











Name	Formula	SMILES	InChI	Structure
AR	AR	[Ar]	InChI=1S/Ar	
N2	N2	N#N	InChI=1S/N2/c1-2	
HE	HE	[He]	InChI=1S/He	
H2	H2	[H][H]	InChI=1S/H2/h1H	
H	H	[H]	InChI=1S/H	
O2	O2	[O][O]	InChI=1S/O2/c1-2	
O	O	[O]	InChI=1S/O	
H2O	H2O	O	InChI=1S/H2O/h1H2	
OH	HO	[OH]	InChI=1S/HO/h1H	
				

OHV	HO	[OH]	InChI=1S/HO/h1H	
H2O2	H2O2	OO	InChI=1S/H2O2/c1-2/h1-2H	
HO2	HO2	[O]O	InChI=1S/HO2/c1-2/h1H	
CO	CO	[C]=O	InChI=1S/CO/c1-2	
CO2	CO2	O=C=O	InChI=1S/CO2/c2-1-3	
HOCO	CHO2	[C](=O)O	InChI=1S/CHO2/c2-1-3/h(H,2,3)	
CH4	CH4	C	InChI=1S/CH4/h1H4	
CH3	CH3	[CH3]	InChI=1S/CH3/h1H3	
CH2	CH2	triplet[CH2]	InChI=1S/CH2/h1H2	
CH2(S)	CH2	singlet[CH2]	InChI=1S/CH2/h1H2	

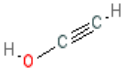
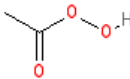
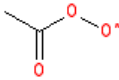



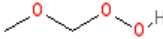


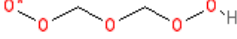
C	C	[C]	InChI=1S/C	
CH	CH	[CH]	InChI=1S/CH/H1h	
CHV	CH	[CH]	InChI=1S/CH/H1h	
CH3O2H	CH4O2	COO	InChI=1S/CH4O2/c1-3-2/h2H,1H3	
CH3O2	CH3O2	CO[O]	InChI=1S/CH3O2/c1-3-2/h1H3	
CH2O2H	CH3O2	[CH2]OO	InChI=1S/CH3O2/c1-3-2/h2H,1H2	
CH3OH	CH4O	CO	InChI=1S/CH4O/c1-2/h2H,1H3	
CH3O	CH3O	C[O]	InChI=1S/CH3O/c1-2/h1H3	
CH2OH	CH3O	[CH2]O	InChI=1S/CH3O/c1-2/h2H,1H2	
CH2O	CH2O	C=O	InChI=1S/CH2O/c1-2/h1H2	

HCO	CHO	[CH]=O	InChI=1S/CHO/c1-2/h1H	
HCOH	CH2O	singlet[CH]O	InChI=1S/CH2O/c1-2/h1-2H	
HO2CHO	CH2O3	O=COO	InChI=1S/CH2O3/c2-1-4-3/h1,3H	
HOCH2O2H	CH4O3	OCOO	InChI=1S/CH4O3/c2-1-4-3/h2-3H,1H2	
HOCH2O2	CH3O3	[O]OCO	InChI=1S/CH3O3/c2-1-4-3/h2H,1H2	
OCH2O2H	CH3O3	[O]COO	InChI=1S/CH3O3/c2-1-4-3/h3H,1H2	
HOCH2O	CH3O2	[O]CO	InChI=1S/CH3O2/c2-1-3/h2H,1H2	
O2CHO	CHO3	[O]OC=O	InChI=1S/CHO3/c2-1-4-3/h1H	
HOCHO	CH2O2	O=CO	InChI=1S/CH2O2/c2-1-3/h1H,(H,2,3)	
OCHO	CHO2	[O]C=O	InChI=1S/CHO2/c2-1-3/h1H	

C2H6	C2H6	CC	InChI=1S/C2H6/c1-2/h1-2H3	
C2H5	C2H5	[CH2]C	InChI=1S/C2H5/c1-2/h1H2,2H3	
C2H5O2H	C2H6O2	CCOO	InChI=1S/C2H6O2/c1-2-4-3/h3H,2H2,1H3	
C2H5O2	C2H5O2	CCO[O]	InChI=1S/C2H5O2/c1-2-4-3/h2H2,1H3	
C2H4	C2H4	C=C	InChI=1S/C2H4/c1-2/h1-2H2	
C2H3	C2H3	[CH]=C	InChI=1S/C2H3/c1-2/h1H,2H2	
CHOCHO	C2H2O2	O=CC=O	InChI=1S/C2H2O2/c3-1-2-4/h1-2H	
C2H3OOH	C2H4O2	C=COO	InChI=1S/C2H4O2/c1-2-4-3/h2-3H,1H2	
C2H3OO	C2H3O2	C=C(O[O])	InChI=1S/C2H3O2/c1-2-4-3/h2H,1H2	
CHCHO	C2H2O	[CH]CO	InChI=1S/C2H2O/c1-2-3/h1-2H	

C2H2	C2H2	C#C	InChI=1S/C2H2/c1-2/h1-2H	
C2H	C2H	[C]#C	InChI=1S/C2H/c1-2/h1H	
H2CC	C2H2	[C]=C	InChI=1S/C2H2/c1-2/H1h2	
C2H5OH	C2H6O	CCO	InChI=1S/C2H6O/c1-2-3/h3H,2H2,1H3	
C2H5O	C2H5O	CC[O]	InChI=1S/C2H5O/c1-2-3/h2H2,1H3	
PC2H4OH	C2H5O	[CH2]CO	InChI=1S/C2H5O/c1-2-3/h3H,1-2H2	
SC2H4OH	C2H5O	C[CH]O	InChI=1S/C2H5O/c1-2-3/h2-3H,1H3	
O2C2H4OH	C2H5O3	[O]OCCO	InChI=1S/C2H5O3/c3-1-2-5-4/h3H,1-2H2	
C2H4O2H	C2H5O2	[CH2]COO	InChI=1S/C2H5O2/c1-2-4-3/h3H,1-2H2	
C2H4O1-2	C2H4O	C1CO1	InChI=1S/C2H4O/c1-2-3-1/h1-2H2	

C2H3O1-2	C2H3O	[CH]1CO1	InChI=1S/C2H3O/c1-2-3-1/h1H,2H2	
CH3CHO	C2H4O	CC=O	InChI=1S/C2H4O/c1-2-3/h2H,1H3	
CH3CO	C2H3O	C[C]=O	InChI=1S/C2H3O/c1-2-3/h1H3	
CH2CHO	C2H3O	[CH2]C=O	InChI=1S/C2H3O/c1-2-3/h2H,1H2	
O2CH2CHO	C2H3O3	[O]OCC=O	InChI=1S/C2H3O3/c3-1-2-5-4/h1H,2H2	
HO2CH2CO	C2H3O3	O=[C]COO	InChI=1S/C2H3O3/c3-1-2-5-4/h4H,2H2	
C2H3OH	C2H4O	C=CO	InChI=1S/C2H4O/c1-2-3/h2-3H,1H2	
C2H2OH	C2H3O	[CH]=CO	InChI=1S/C2H3O/c1-2-3/h1-3H	
CH2CO	C2H2O	C=C=O	InChI=1S/C2H2O/c1-2-3/h1H2	
HCCO	C2HO	[CH]=C=O	InChI=1S/C2HO/c1-2-3/h1H	

HCCOH	C2H2O	C#CO	InChI=1S/C2H2O/c1-2-3/h1,3H	
CH3CO3H	C2H4O3	CC(=O)OO	InChI=1S/C2H4O3/c1-2(3)5-4/h4H,1H3	
CH3CO3	C2H3O3	CC(=O)O[O]	InChI=1S/C2H3O3/c1-2(3)5-4/h1H3	
CH3CO2	C2H3O2	CC([O])=O	InChI=1S/C2H3O2/c1-2(3)4/h1H3	
CH3OCH3	C2H6O	COC	InChI=1S/C2H6O/c1-3-2/h1-2H3	
CH3OCH2	C2H5O	[CH2]OC	InChI=1S/C2H5O/c1-3-2/h1H2,2H3	
CH3OCH2O2H	C2H6O3	COCOO	InChI=1S/C2H6O3/c1-4-2-5-3/h3H,2H2,1H3	
CH3OCH2O2	C2H5O3	COCO[O]	InChI=1S/C2H5O3/c1-4-2-5-3/h2H2,1H3	
CH2OCH2O2H	C2H5O3	[CH2]OCOO	InChI=1S/C2H5O3/c1-4-2-5-3/h3H,1-2H2	
O2CH2OCH2O2H	C2H5O5	[O]OCOCOO	InChI=1S/C2H5O5/c3-6-1-5-2-7-4/h3H,1-2H2	

HO2CH2OCHO	C2H4O4	O=COCOO	InChI=1S/C2H4O4/c3-1-5-2-6-4/h1,4H,2H2	
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OCH2OCHO	C2H3O3	[O]COC=O	InChI=1S/C2H3O3/c3-1-5-2-4/h1H,2H2	
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HOCH2OCO	C2H3O3	O=[C]OCO	InChI=1S/C2H3O3/c3-1-5-2-4/h3H,1H2	
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CH3OCH2OH	C2H6O2	COCO	InChI=1S/C2H6O2/c1-4-2-3/h3H,2H2,1H3	
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CH3OCH2O	C2H5O2	COC[O]	InChI=1S/C2H5O2/c1-4-2-3/h2H2,1H3	
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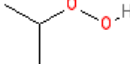
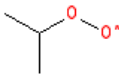
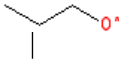



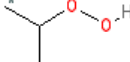
CH3OCHO	C2H4O2	COC=O	InChI=1S/C2H4O2/c1-4-2-3/h2H,1H3	
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CH3OCO	C2H3O2	CO[C]=O	InChI=1S/C2H3O2/c1-4-2-3/h1H3	
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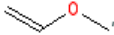
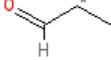

CH2OCHO	C2H3O2	[CH2]OC=O	InChI=1S/C2H3O2/c1-4-2-3/h2H,1H2	
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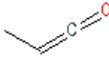


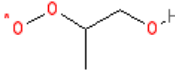




C3H8	C3H8	CCC	InChI=1S/C3H8/c1-3-2/h3H2,1-2H3	
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IC3H7	C3H7	C[CH]C	InChI=1S/C3H7/c1-3-2/h3H,1-2H3	
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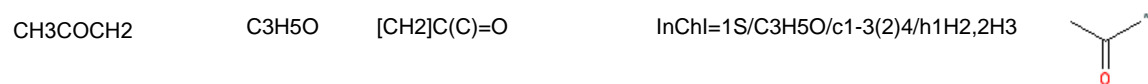
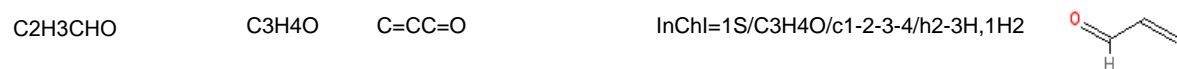
NC3H7	C3H7	[CH2]CC	InChI=1S/C3H7/c1-3-2/h1,3H2,2H3	
NC3H7O2H	C3H8O2	CCCCO	InChI=1S/C3H8O2/c1-2-3-5-4/h4H,2-3H2,1H3	
NC3H7O2	C3H7O2	CCCO[O]	InChI=1S/C3H7O2/c1-2-3-5-4/h2-3H2,1H3	
IC3H7O2H	C3H8O2	CC(C)OO	InChI=1S/C3H8O2/c1-3(2)5-4/h3-4H,1-2H3	
IC3H7O2	C3H7O2	CC(C)O[O]	InChI=1S/C3H7O2/c1-3(2)5-4/h3H,1-2H3	
NC3H7O	C3H7O	CCC[O]	InChI=1S/C3H7O/c1-2-3-4/h2-3H2,1H3	
IC3H7O	C3H7O	CC(C)[O]	InChI=1S/C3H7O/c1-3(2)4/h3H,1-2H3	
C3H6OOH1-2	C3H7O2	C[CH]COO	InChI=1S/C3H7O2/c1-2-3-5-4/h2,4H,3H2,1H3	
C3H6OOH1-3	C3H7O2	[CH2]CCOO	InChI=1S/C3H7O2/c1-2-3-5-4/h4H,1-3H2	
C3H6OOH2-1	C3H7O2	[CH2]C(C)OO	InChI=1S/C3H7O2/c1-3(2)5-4/h3-4H,1H2,2H3	

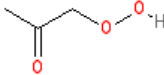


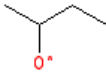

C3H6OOH1-2O2	C3H7O4	CC(COO)O[O]	InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3-4H,2H2,1H3	
C3H6OOH1-3O2	C3H7O4	[O]OCCCCO	InChI=1S/C3H7O4/c4-6-2-1-3-7-5/h4H,1-3H2	
C3H6OOH2-1O2	C3H7O4	CC(CO[O])OO	InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3,5H,2H2,1H3	
C3KET12	C3H6O3	CC(C=O)OO	InChI=1S/C3H6O3/c1-3(2-4)6-5/h2-3,5H,1H3	
C3KET13	C3H6O3	O=CCCCO	InChI=1S/C3H6O3/c4-2-1-3-6-5/h2,5H,1,3H2	
C3H51-2,3OOH	C3H7O4	[CH2]C(COO)OO	InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3-5H,1-2H2	
C3H52-1,3OOH	C3H7O4	OOC[CH]COO	InChI=1S/C3H7O4/c4-6-2-1-3-7-5/h1,4-5H,2-3H2	
C3H5O1-2OOH-3	C3H6O3	C1C(O1)C(OO)	InChI=1S/C3H6O3/c4-6-2-3-1-5-3/h3-4H,1-2H2	
C3H5O1-3OOH-2	C3H6O3	C1C(OO)C(O1)	InChI=1S/C3H6O3/c4-6-3-1-5-2-3/h3-4H,1-2H2	
C3H6O1-2	C3H6O	CC1CO1	InChI=1S/C3H6O/c1-3-2-4-3/h3H,2H2,1H3	

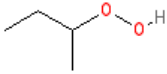



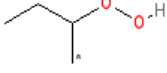
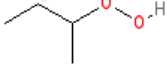
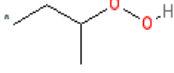
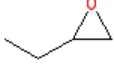


C3H6O1-3	C3H6O	C1COC1	InChI=1S/C3H6O/c1-2-4-3-1/h1-3H2	
C3H6	C3H6	C=CC	InChI=1S/C3H6/c1-3-2/h3H,1H2,2H3	
C3H5-A	C3H5	[CH2]C=C	InChI=1S/C3H5/c1-3-2/h3H,1-2H2	
C3H5-S	C3H5	[CH]=CC	InChI=1S/C3H5/c1-3-2/h1,3H,2H3	
C3H5-T	C3H5	C=[C]C	InChI=1S/C3H5/c1-3-2/h1H2,2H3	
CC3H6	C3H6	C1CC1	InChI=1S/C3H6/c1-2-3-1/h1-3H2	
C3H5O	C3H5O	C=CC[O]	InChI=1S/C3H5O/c1-2-3-4/h2H,1,3H2	
CH2CHOCH2	C3H5O	C=CO[CH2]	InChI=1S/C3H5O/c1-3-4-2/h3H,1-2H2	
CH3CHCHO	C3H5O	C[CH]C=O	InChI=1S/C3H5O/c1-2-3-4/h2-3H,1H3	
AC4H7OOH	C4H8O2	C=CCOOC	InChI=1S/C4H8O2/c1-3-4-6-5-2/h3H,1,4H2,2H3	

C3H6OH1-2	C3H7O	C(O)[CH]C	InChI=1S/C3H7O/c1-2-3-4/h2,4H,3H2,1H3	
CH3CHCO	C3H4O	CC=C=O	InChI=1S/C3H4O/c1-2-3-4/h2H,1H3	
AC3H5OOH	C3H6O2	C=CCOO	InChI=1S/C3H6O2/c1-2-3-5-4/h2,4H,1,3H2	
C3H6OH2-1	C3H7O	[CH2]C(O)C	InChI=1S/C3H7O/c1-3(2)4/h3-4H,1H2,2H3	
HOC3H6O2	C3H7O3	C(O)C(O[O])C	InChI=1S/C3H7O3/c1-3(2-4)6-5/h3-4H,2H2,1H3	
SC3H5OH	C3H6O	CC=CO	InChI=1S/C3H6O/c1-2-3-4/h2-4H,1H3	
IC3H5OH	C3H6O	C=C(C)O	InChI=1S/C3H6O/c1-3(2)4/h4H,1H2,2H3	
C3H5OH	C3H6O	C=CCO	InChI=1S/C3H6O/c1-2-3-4/h2,4H,1,3H2	
CH2CCH2OH	C3H5O	C=[C]CO	InChI=1S/C3H5O/c1-2-3-4/h4H,1,3H2	
C3H4-P	C3H4	C#CC	InChI=1S/C3H4/c1-3-2/h1H,2H3	

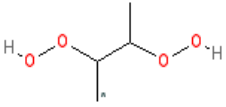
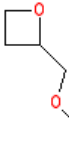
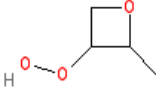
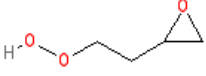
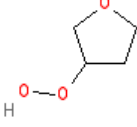
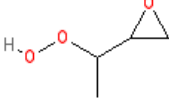
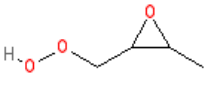

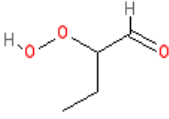
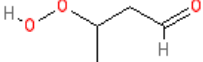
C3H4-A	C3H4	C=C=C	InChI=1S/C3H4/c1-3-2/h1-2H2	
C3H3	C3H3	C#C[CH2]	InChI=1S/C3H3/c1-3-2/h1H,2H2	
CC3H4	C3H4	C1=CC1	InChI=1S/C3H4/c1-2-3-1/h1-2H,3H2	
C3H2	C3H2	C=C=[C]	InChI=1S/C3H2/c1-3-2/H1h2	
H2CCC(S)	C3H2	C=C=[C]	InChI=1S/C3H2/c1-3-2/H1h2	
C3H2(S)	C3H2	C=C=[C]	InChI=1S/C3H2/c1-3-2/H1h2	
C3H2C	C3H2	C1=C[C]1	InChI=1S/C3H2/c1-2-3-1/h1-2H	
PC3H4OH-2	C3H5O	C[C]=CO	InChI=1S/C3H5O/c1-2-3-4/h3-4H,1H3	
SC3H4OH	C3H5O	C=C([CH2])O	InChI=1S/C3H5O/c1-3(2)4/h4H,1-2H2	
C3H3O	C3H3O	C=C=C([O])	InChI=1S/C3H3O/c1-2-3-4/h3H,1H2	



CH3COCH2O	C3H5O2	CC(=O)C[O]	InChI=1S/C3H5O2/c1-3(5)2-4/h2H2,1H3	
C3KET21	C3H6O3	CC(=O)COO	InChI=1S/C3H6O3/c1-3(4)2-6-5/h5H,2H2,1H3	
C4H10	C4H10	CCCC	InChI=1S/C4H10/c1-3-4-2/h3-4H2,1-2H3	
PC4H9	C4H9	[CH2]CCC	InChI=1S/C4H9/c1-3-4-2/h1,3-4H2,2H3	
SC4H9	C4H9	C[CH]CC	InChI=1S/C4H9/c1-3-4-2/h3H,4H2,1-2H3	
PC4H9O	C4H9O	CCCC[O]	InChI=1S/C4H9O/c1-2-3-4-5/h2-4H2,1H3	
SC4H9O	C4H9O	CCC(C)[O]	InChI=1S/C4H9O/c1-3-4(2)5/h4H,3H2,1-2H3	
PC4H9O2	C4H9O2	CCCCO[O]	InChI=1S/C4H9O2/c1-2-3-4-6-5/h2-4H2,1H3	
SC4H9O2	C4H9O2	CCC(C)O[O]	InChI=1S/C4H9O2/c1-3-4(2)6-5/h4H,3H2,1-2H3	
PC4H9O2H	C4H10O2	CCCCOO	InChI=1S/C4H10O2/c1-2-3-4-6-5/h5H,2-4H2,1H3	

SC4H9O2H	C4H10O2	CCC(C)OO	InChI=1S/C4H10O2/c1-3-4(2)6-5/h4-5H,3H2,1-2H3	
C4H8OOH1-2	C4H9O2	CC[CH]COO	InChI=1S/C4H9O2/c1-2-3-4-6-5/h3,5H,2,4H2,1H3	
C4H8OOH1-3	C4H9O2	C[CH]CCOO	InChI=1S/C4H9O2/c1-2-3-4-6-5/h2,5H,3-4H2,1H3	
C4H8OOH1-4	C4H9O2	[CH2]CCCCOO	InChI=1S/C4H9O2/c1-2-3-4-6-5/h5H,1-4H2	
C4H8OOH2-1	C4H9O2	[CH2]C(CC)OO	InChI=1S/C4H9O2/c1-3-4(2)6-5/h4-5H,2-3H2,1H3	
C4H8OOH2-3	C4H9O2	C[CH]C(C)OO	InChI=1S/C4H9O2/c1-3-4(2)6-5/h3-5H,1-2H3	
C4H8OOH2-4	C4H9O2	[CH2]CC(C)OO	InChI=1S/C4H9O2/c1-3-4(2)6-5/h4-5H,1,3H2,2H3	
C4H8O1-2	C4H8O	CCC1CO1	InChI=1S/C4H8O/c1-2-4-3-5-4/h4H,2-3H2,1H3	
C4H8O1-3	C4H8O	CC1CCO1	InChI=1S/C4H8O/c1-4-2-3-5-4/h4H,2-3H2,1H3	
C4H8O1-4	C4H8O	C1CCOC1	InChI=1S/C4H8O/c1-2-4-5-3-1/h1-4H2	

C4H8O2-3	C4H8O	CC1OC1C	InChI=1S/C4H8O/c1-3-4(2)5-3/h3-4H,1-2H3	
C4H8OOH1-2O2	C4H9O4	CCC(COO)O[O]	InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h4-5H,2-3H2,1H3	
C4H8OOH1-3O2	C4H9O4	CC(CCOO)O[O]	InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h4-5H,2-3H2,1H3	
C4H8OOH1-4O2	C4H9O4	[O]OCCCCOO	InChI=1S/C4H9O4/c5-7-3-1-2-4-8-6/h5H,1-4H2	
C4H8OOH2-1O2	C4H9O4	CCC(CO[O])OO	InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h4,6H,2-3H2,1H3	
C4H8OOH2-3O2	C4H9O4	CC(O[O])C(C)OO	InChI=1S/C4H9O4/c1-3(7-5)4(2)8-6/h3-5H,1-2H3	
C4H8OOH2-4O2	C4H9O4	CC(CCO[O])OO	InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h4,6H,2-3H2,1H3	
C4H71-2,4OOH	C4H9O4	[CH2]C(OO)CC(OO)	InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h4-6H,1-3H2	
C4H72-1,3OOH	C4H9O4	CC(OO)[CH]C(OO)	InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h2,4-6H,3H2,1H3	
C4H72-1,4OOH	C4H9O4	C(OO)C[CH]C(OO)	InChI=1S/C4H9O4/c5-7-3-1-2-4-8-6/h1,5-6H,2-4H2	

C4H71-2,3OOH	C4H9O4	[CH2]C(OO)C(OO)C	InChI=1S/C4H9O4/c1-3(7-5)4(2)8-6/h3-6H,1H2,2H3	
C4H7O1-3OOH-4	C4H8O3	C1CC(O1)C(OO)	InChI=1S/C4H8O3/c5-7-3-4-1-2-6-4/h4-5H,1-3H2	
C4H7O1-3OOH-2	C4H8O3	C1C(OO)C(O1)C	InChI=1S/C4H8O3/c1-3-4(7-5)2-6-3/h3-5H,2H2,1H3	
C4H7O1-2OOH-4	C4H8O3	C1C(O1)CC(OO)	InChI=1S/C4H8O3/c5-7-2-1-4-3-6-4/h4-5H,1-3H2	
C4H7O1-4OOH-2	C4H8O3	C1C(OO)CC(O1)	InChI=1S/C4H8O3/c5-7-4-1-2-6-3-4/h4-5H,1-3H2	
C4H7O1-2OOH-3	C4H8O3	C1C(O1)C(OO)C	InChI=1S/C4H8O3/c1-3(7-5)4-2-6-4/h3-5H,2H2,1H3	
C4H7O2-3OOH-1	C4H8O3	C(OO)C1C(O1)C	InChI=1S/C4H8O3/c1-3-4(7-3)2-6-5/h3-5H,2H2,1H3	
C4H72-1OOH	C4H8O2	CC=CCOO	InChI=1S/C4H8O2/c1-2-3-4-6-5/h2-3,5H,4H2,1H3	
NC4KET12	C4H8O3	CCC(C=O)OO	InChI=1S/C4H8O3/c1-2-4(3-5)7-6/h3-4,6H,2H2,1H3	
NC4KET13	C4H8O3	CC(CC=O)OO	InChI=1S/C4H8O3/c1-4(7-6)2-3-5/h3-4,6H,2H2,1H3	

NC4KET14	C4H8O3	O=CCCCOO	InChI=1S/C4H8O3/c5-3-1-2-4-7-6/h3,6H,1-2,4H2	
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NC4KET21	C4H8O3	CCC(=O)COO	InChI=1S/C4H8O3/c1-2-4(5)3-7-6/h6H,2-3H2,1H3	
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NC4KET23	C4H8O3	CC(=O)C(C)OO	InChI=1S/C4H8O3/c1-3(5)4(2)7-6/h4,6H,1-2H3	
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NC4KET24	C4H8O3	CC(=O)CCOO	InChI=1S/C4H8O3/c1-4(5)2-3-7-6/h6H,2-3H2,1H3	
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C4H71-3OOH	C4H8O2	C=CC(C)OO	InChI=1S/C4H8O2/c1-3-4(2)6-5/h3-5H,1H2,2H3	
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C4H71-3,4OOH	C4H9O4	[CH2]CC(OO)C(OO)	InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h4-6H,1-3H2	
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C4H72-3,4OOH	C4H9O4	C[CH]C(OO)C(OO)	InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h2,4-6H,3H2,1H3	
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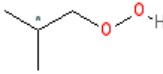
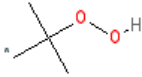

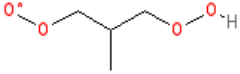
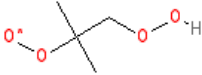

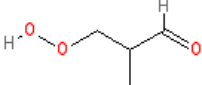
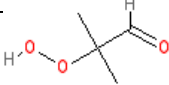


HO2CH2CHO	C2H4O3	C(COO)=O	InChI=1S/C2H4O3/c3-1-2-5-4/h1,4H,2H2	
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IC4H10	C4H10	CC(C)C	InChI=1S/C4H10/c1-4(2)3/h4H,1-3H3	
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IC4H9	C4H9	[CH2]C(C)C	InChI=1S/C4H9/c1-4(2)3/h4H,1H2,2-3H3	
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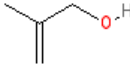
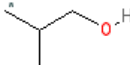
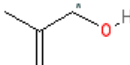
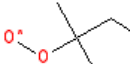

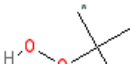
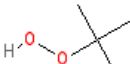
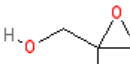


TC4H9	C4H9	CCC	InChI=1S/C4H9/c1-4(2)3/h1-3H3	
TC4H9O	C4H9O	CC(C)(C)[O]	InChI=1S/C4H9O/c1-4(2,3)5/h1-3H3	
IC4H9O	C4H9O	CC(C)C[O]	InChI=1S/C4H9O/c1-4(2)3-5/h4H,3H2,1-2H3	
IC4H8O	C4H8O	CC1(C)CO1	InChI=1S/C4H8O/c1-4(2)3-5-4/h3H2,1-2H3	
IC3H7CHO	C4H8O	CC(C)C=O	InChI=1S/C4H8O/c1-4(2)3-5/h3-4H,1-2H3	
IC3H7CO	C4H7O	CC(C)[C]=O	InChI=1S/C4H7O/c1-4(2)3-5/h4H,1-2H3	
IC3H6CHO	C4H7O	[CH2]C(C)C=O	InChI=1S/C4H7O/c1-4(2)3-5/h3-4H,1H2,2H3	
TC3H6CHO	C4H7O	CCC=O	InChI=1S/C4H7O/c1-4(2)3-5/h3H,1-2H3	
IC3H5CHO	C4H6O	C=C(C)C=O	InChI=1S/C4H6O/c1-4(2)3-5/h3H,1H2,2H3	
TC3H6O2CHO	C4H7O3	CC(C)(C=O)O[O]	InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h3H,1-2H3	

IC3H5O2HCHO	C4H7O3	[CH2]C(C)(C=O)OO	InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h3,6H,1H2,2H3	
TC3H6O2HCO	C4H7O3	CC(C)([C]=O)OO	InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h6H,1-2H3	
TC3H6OCHO	C4H7O2	CC(C)([O])C=O	InChI=1S/C4H7O2/c1-4(2,6)3-5/h3H,1-2H3	
IC3H6CO	C4H6O	CC(C)=C=O	InChI=1S/C4H6O/c1-4(2)3-5/h1-2H3	
IC3H5CO	C4H5O	C=C(C)[C]=O	InChI=1S/C4H5O/c1-4(2)3-5/h1H2,2H3	
IC3H4CHO-A	C4H5O	C=C([CH2])C=O	InChI=1S/C4H5O/c1-4(2)3-5/h3H,1-2H2	
SC4H7OH-I	C4H8O	CC(C)=CO	InChI=1S/C4H8O/c1-4(2)3-5/h3,5H,1-2H3	
IC4H9O2	C4H9O2	CC(C)CO[O]	InChI=1S/C4H9O2/c1-4(2)3-6-5/h4H,3H2,1-2H3	
TC4H9O2	C4H9O2	CC(C)(C)O[O]	InChI=1S/C4H9O2/c1-4(2,3)6-5/h1-3H3	
IC4H8O2H-I	C4H9O2	[CH2]C(C)COO	InChI=1S/C4H9O2/c1-4(2)3-6-5/h4-5H,1,3H2,2H3	

IC4H8O2H-T	C4H9O2	CCCOO	InChI=1S/C4H9O2/c1-4(2)3-6-5/h5H,3H2,1-2H3	
TC4H8O2H-I	C4H9O2	[CH2]C(C)(C)OO	InChI=1S/C4H9O2/c1-4(2,3)6-5/h5H,1H2,2-3H3	
CC4H8O	C4H8O	C1C(C)CO1	InChI=1S/C4H8O/c1-4-2-5-3-4/h4H,2-3H2,1H3	
IC4H8OOH-IO2	C4H9O4	CC(CO[O])COO	InChI=1S/C4H9O4/c1-4(2-7-5)3-8-6/h4-5H,2-3H2,1H3	
IC4H8OOH-TO2	C4H9O4	CC(C)(COO)O[O]	InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h5H,3H2,1-2H3	
TC4H8OOH-IO2	C4H9O4	CC(C)(CO[O])OO	InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h6H,3H2,1-2H3	
IC4KETII	C4H8O3	CC(C=O)COO	InChI=1S/C4H8O3/c1-4(2-5)3-7-6/h2,4,6H,3H2,1H3	
IC4KETIT	C4H8O3	CC(C)(C=O)OO	InChI=1S/C4H8O3/c1-4(2,3-5)7-6/h3,6H,1-2H3	
TIC4H7Q2-I	C4H9O4	[CH2]C(C)(COO)OO	InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h5-6H,1,3H2,2H3	
IIC4H7Q2-I	C4H9O4	[CH2]C(COO)COO	InChI=1S/C4H9O4/c1-4(2-7-5)3-8-6/h4-6H,1-3H2	

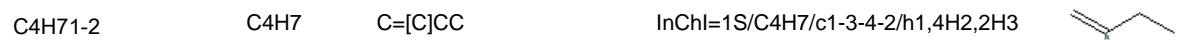
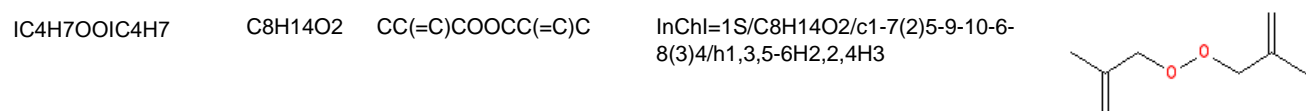
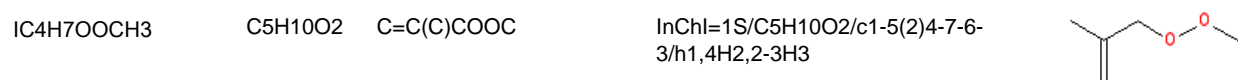
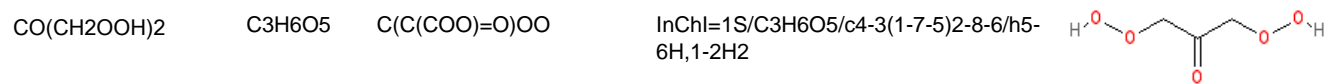
IIC4H7Q2-T	C4H9O4	C[C](COO)COO	InChI=1S/C4H9O4/c1-4(2-7-5)3-8-6/h5-6H,2-3H2,1H3	
IC4H7OOH	C4H8O2	C=C(C)COO	InChI=1S/C4H8O2/c1-4(2)3-6-5/h5H,1,3H2,2H3	
IC4H9O2H	C4H10O2	CC(C)COO	InChI=1S/C4H10O2/c1-4(2)3-6-5/h4-5H,3H2,1-2H3	
TC4H9O2H	C4H10O2	CC(C)(C)OO	InChI=1S/C4H10O2/c1-4(2,3)6-5/h5H,1-3H3	
IC4H8	C4H8	C=C(C)C	InChI=1S/C4H8/c1-4(2)3/h1H2,2-3H3	
IC4H7	C4H7	[CH2]C(=C)C	InChI=1S/C4H7/c1-4(2)3/h1-2H2,3H3	
IC4H7-I1	C4H7	[CH]=C(C)C	InChI=1S/C4H7/c1-4(2)3/h1H,2-3H3	
IC4H7O2	C4H7O2	C=C(C)CO[O]	InChI=1S/C4H7O2/c1-4(2)3-6-5/h1,3H2,2H3	
IC4H6OOH-I	C4H7O2	C=C([CH2])COO	InChI=1S/C4H7O2/c1-4(2)3-6-5/h5H,1-3H2	
CCYCCOOC-T1	C4H7O2	C[C]1COOC1	InChI=1S/C4H7O2/c1-4-2-5-6-3-4/h2-3H2,1H3	



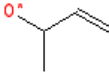

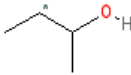
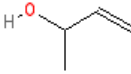



C2CYCOOC-I1	C4H7O2	[CH2]C1(C)COO1	InChI=1S/C4H7O2/c1-4(2)3-5-6-4/h1,3H2,2H3	
IC4H7O	C4H7O	C=C(C)C[O]	InChI=1S/C4H7O/c1-4(2)3-5/h1,3H2,2H3	
CVCYCCOC	C4H6O	C=C1COC1	InChI=1S/C4H6O/c1-4-2-5-3-4/h1-3H2	
CCYC2OCO	C4H7O2	CC1(C[O])CO1	InChI=1S/C4H7O2/c1-4(2-5)3-6-4/h2-3H2,1H3	
CCYCCOOC-I2	C4H7O2	CC1[CH]OOC1	InChI=1S/C4H7O2/c1-4-2-5-6-3-4/h2,4H,3H2,1H3	
CHOIC3H6O	C4H7O2	CC(C=O)C[O]	InChI=1S/C4H7O2/c1-4(2-5)3-6/h2,4H,3H2,1H3	
IC3H5OOCH2	C4H7O2	C=C(C)OO[CH2]	InChI=1S/C4H7O2/c1-4(2)6-5-3/h1,3H2,2H3	
CCYCCO-T1	C3H5O	C[C]1C(O1)	InChI=1S/C3H5O/c1-3-2-4-3/h2H2,1H3	
IC4H8OH-IT	C4H9O	CCCO	InChI=1S/C4H9O/c1-4(2)3-5/h5H,3H2,1-2H3	
IC4H8OH-TI	C4H9O	[CH2]C(C)(C)O	InChI=1S/C4H9O/c1-4(2,3)5/h5H,1H2,2-3H3	

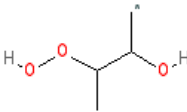
IC4H7OH	C4H8O	C=C(C)CO	InChI=1S/C4H8O/c1-4(2)3-5/h5H,1,3H2,2H3	
IC4H8OH	C4H9O	[CH2]C(C)CO	InChI=1S/C4H9O/c1-4(2)3-5/h4-5H,1,3H2,2H3	
IC4H6OH	C4H7O	C=C(C)[CH]O	InChI=1S/C4H7O/c1-4(2)3-5/h3,5H,1H2,2H3	
TQJC4H8OH	C4H9O3	CC(C)(CO)O[O]	InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h5H,3H2,1-2H3	
TQC4H8OI	C4H9O3	CC(C)(C[O])OO	InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h6H,3H2,1-2H3	
QC4H7OHP	C4H9O3	[CH2]C(C)(CO)OO	InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h5-6H,1,3H2,2H3	
TQC4H7OHI	C4H9O3	CC(C)([CH]O)OO	InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h3,5-6H,1-2H3	
CCY(CCO)COH	C4H8O2	CC1(CO)CO1	InChI=1S/C4H8O2/c1-4(2-5)3-6-4/h5H,2-3H2,1H3	
C2CY(COC)OH	C4H8O2	CC1(C)C(O)O1	InChI=1S/C4H8O2/c1-4(2)3(5)6-4/h3,5H,1-2H3	
IQJC4H8OH	C4H9O3	CC(C)(CO[O])O	InChI=1S/C4H9O3/c1-4(2,5)3-7-6/h5H,3H2,1-2H3	

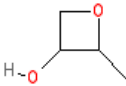
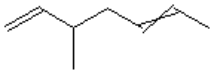

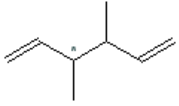
IC3H6OHCHO	C4H8O2	CC(C)(C=O)O	InChI=1S/C4H8O2/c1-4(2,6)3-5/h3,6H,1-2H3	
IQC4H8OT	C4H9O3	CC(C)(COO)[O]	InChI=1S/C4H9O3/c1-4(2,5)3-7-6/h6H,3H2,1-2H3	
IQC4H7OHT	C4H9O3	[CH2]C(C)(COO)O	InChI=1S/C4H9O3/c1-4(2,5)3-7-6/h5-6H,1,3H2,2H3	
CCY(CCOC)OH	C4H8O2	CC1(COC1)O	InChI=1S/C4H8O2/c1-4(5)2-6-3-4/h5H,2-3H2,1H3	
CH2COHCH2OOH	C3H6O3	C=C(COO)O	InChI=1S/C3H6O3/c1-3(4)2-6-5/h4-5H,1-2H2	
TC3H6OH	C3H7O	CCO	InChI=1S/C3H7O/c1-3(2)4/h4H,1-2H3	
TQC4H7OHIO2	C4H9O5	CC(C)(C(O)O[O])OO	InChI=1S/C4H9O5/c1-4(2,9-7)3(5)8-6/h3,5,7H,1-2H3	
TQC4H7OHTO2	C4H9O5	CC(C)(C(O)OO)O[O]	InChI=1S/C4H9O5/c1-4(2,9-7)3(5)8-6/h3,5-6H,1-2H3	
TQC4H7OHIQ-I	C4H9O5	CC(C)(C([O])OO)OO	InChI=1S/C4H9O5/c1-4(2,9-7)3(5)8-6/h3,6-7H,1-2H3	
TQC4H7OHIQ-P	C4H9O5	[CH2]C(C)(C(O)OO)OO	InChI=1S/C4H9O5/c1-4(2,9-7)3(5)8-6/h3,5-7H,1H2,2H3	

IC3H5COHQ	C4H8O3	C=C(C)C(O)OO	InChI=1S/C4H8O3/c1-3(2)4(5)7-6/h4-6H,1H2,2H3	
CH2CQCOHQ	C3H6O5	C=C(OO)C(O)OO	InChI=1S/C3H6O5/c1-2(7-5)3(4)8-6/h3-6H,1H2	
IC3H5Q	C3H6O2	C=C(C)OO	InChI=1S/C3H6O2/c1-3(2)5-4/h4H,1H2,2H3	
COHQCYC(COC)	C4H8O4	CC1(CO1)C(O)OO	InChI=1S/C4H8O4/c1-4(2-7-4)3(5)8-6/h3,5-6H,2H2,1H3	
QCYC(CCOC)OH	C4H8O4	CC1(COC1O)OO	InChI=1S/C4H8O4/c1-4(8-6)2-7-3(4)5/h3,5-6H,2H2,1H3	
HOCOCQ(CH3)2	C4H8O4	CC(C)(C(=O)O)OO	InChI=1S/C4H8O4/c1-4(2,8-7)3(5)6/h7H,1-2H3,(H,5,6)	
IQC4H7OHTO2	C4H9O5	CC(COO)(CO[O])O	InChI=1S/C4H9O5/c1-4(5,2-8-6)3-9-7/h5-6H,2-3H2,1H3	
IQC4H8OTQ-I	C4H9O5	CC(COO)(COO)[O]	InChI=1S/C4H9O5/c1-4(5,2-8-6)3-9-7/h6-7H,2-3H2,1H3	
IQC4H7OHTQ-P	C4H9O5	[CH2]C(COO)(COO)O	InChI=1S/C4H9O5/c1-4(5,2-8-6)3-9-7/h5-7H,1-3H2	
CHOC(CH3)OHCH2Q	C4H8O4	CC(C=O)(COO)O	InChI=1S/C4H8O4/c1-4(6,2-5)3-8-7/h2,6-7H,3H2,1H3	


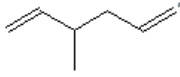



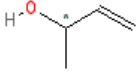
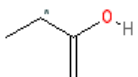

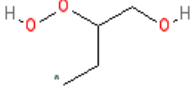
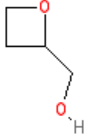


C4H71-4	C4H7	<chem>[CH2]CC=C</chem>	InChI=1S/C4H7/c1-3-4-2/h3H,1-2,4H2	
C4H72-2	C4H7	<chem>C[C]=CC</chem>	InChI=1S/C4H7/c1-3-4-2/h3H,1-2H3	
C4H71-O	C4H7O	<chem>C=CC([O])C</chem>	InChI=1S/C4H7O/c1-3-4(2)/h3-4H,1H2,2H3	
PC4H8OH-2	C4H9O	<chem>C(O)[CH]CC</chem>	InChI=1S/C4H9O/c1-2-3-4-5/h3,5H,2,4H2,1H3	
SC4H8OH-1	C4H9O	<chem>[CH2]C(O)CC</chem>	InChI=1S/C4H9O/c1-3-4(2)/h4-5H,2-3H2,1H3	
SC4H8OH-3	C4H9O	<chem>CC(O)[CH]C</chem>	InChI=1S/C4H9O/c1-3-4(2)/h3-5H,1-2H3	
C4H71-3OH	C4H8O	<chem>C=CC(O)C</chem>	InChI=1S/C4H8O/c1-3-4(2)/h3-5H,1H2,2H3	
C4H71-4OH	C4H8O	<chem>C=CCC(O)</chem>	InChI=1S/C4H8O/c1-2-3-4-5/h2,5H,1,3-4H2	
C4H71-1OH	C4H8O	<chem>C(O)=CCC</chem>	InChI=1S/C4H8O/c1-2-3-4-5/h3-5H,2H2,1H3	
C4H71-2OH	C4H8O	<chem>C=C(O)CC</chem>	InChI=1S/C4H8O/c1-3-4(2)/h5H,2-3H2,1H3	

C4H72-1OH	C4H8O	CC=CC(O)	InChI=1S/C4H8O/c1-2-3-4-5/h2-3,5H,4H2,1H3	
C4H72-2OH	C4H8O	CC=C(O)C	InChI=1S/C4H8O/c1-3-4(2)5/h3,5H,1-2H3	
SQC4H8OP	C4H9O3	CCC(OO)C([O])	InChI=1S/C4H9O3/c1-2-4(3-5)7-6/h4,6H,2-3H2,1H3	
PQC4H8OS	C4H9O3	CCC([O])C(OO)	InChI=1S/C4H9O3/c1-2-4(5)3-7-6/h4,6H,2-3H2,1H3	
PQC4H7OHS-3	C4H9O3	C[CH]C(O)C(OO)	InChI=1S/C4H9O3/c1-2-4(5)3-7-6/h2,4-6H,3H2,1H3	
NC4KET12OH	C4H8O2	C(=O)C(O)CC	InChI=1S/C4H8O2/c1-2-4(6)3-5/h3-4,6H,2H2,1H3	
SQC4H7OHS-4	C4H9O3	CC(OO)C(O)[CH2]	InChI=1S/C4H9O3/c1-3(5)4(2)7-6/h3-6H,1H2,2H3	
SQC4H8OS	C4H9O3	CC(OO)C([O])C	InChI=1S/C4H9O3/c1-3(5)4(2)7-6/h3-4,6H,1-2H3	
NC4KET23OH	C4H8O2	CC(O)C(=O)C	InChI=1S/C4H8O2/c1-3(5)4(2)6/h3,5H,1-2H3	
SC4H8OH-3O2	C4H9O3	CC(O)C(O[O])C	InChI=1S/C4H9O3/c1-3(5)4(2)7-6/h3-5H,1-2H3	

CCY(COCC)OH	C4H8O2	CC(O1)C(O)C1	InChI=1S/C4H8O2/c1-3-4(5)2-6-3/h3-5H,2H2,1H3	
C4H7O2-1	C4H7O	CC=CC[O]	InChI=1S/C4H7O/c1-2-3-4-5/h2-3H,4H2,1H3	
C4H6-1	C4H6	C#CCC	InChI=1S/C4H6/c1-3-4-2/h1H,4H2,2H3	
AC3H5OCH2	C4H7O	C=CCO[CH2]	InChI=1S/C4H7O/c1-3-4-5-2/h3H,1-2,4H2	
SC3H5OCH2-1	C4H7O	[CH2]OC=CC	InChI=1S/C4H7O/c1-3-4-5-2/h3-4H,2H2,1H3	
C8H141-5,3-4	C8H14	C=CC(C)C(C)C=C	InChI=1S/C8H14/c1-5-7(3)8(4)6-2/h5-8H,1-2H2,3-4H3	
C8H141-5,3	C8H14	C=CC(C)CC=CC	InChI=1S/C8H14/c1-4-6-7-8(3)5-2/h4-6,8H,2,7H2,1,3H3	
C8H142-6	C8H14	CC=CCCC=CC	InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h3-6H,7-8H2,1-2H3	
C8H131-5,3-4,TA	C8H13	C=CCC(C)C=C	InChI=1S/C8H13/c1-5-7(3)8(4)6-2/h5-7H,1-2H2,3-4H3	
C8H131-5,3,TA	C8H13	C=CCCC=CC	InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-6H,2,7H2,1,3H3	

C8H131-5,3,SA	C8H13	<chem>C=CC(C)[CH]C=CC</chem>	InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-8H,2H2,1,3H3	
C8H131-5,3,PA	C8H13	<chem>[CH2]C=CCC(C)C=C</chem>	InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-6,8H,1-2,7H2,3H3	
C8H132-6,SA	C8H13	<chem>CC=C[CH]CC=CC</chem>	InChI=1S/C8H13/c1-3-5-7-8-6-4-2/h3-7H,8H2,1-2H3	
C8H132-6,PA	C8H13	<chem>[CH2]C=CCCC=CC</chem>	InChI=1S/C8H13/c1-3-5-7-8-6-4-2/h3-6H,1,7-8H2,2H3	
C6H101-3,3	C6H10	<chem>C=CC(C)=CC</chem>	InChI=1S/C6H10/c1-4-6(3)5-2/h4-5H,1H2,2-3H3	
C8H131-5,3-4,TAO	C8H13O	<chem>C=CC(C)C(C)([O])C=C</chem>	InChI=1S/C8H13O/c1-5-7(3)8(4,9)6-2/h5-7H,1-2H2,3-4H3	
C8H131-5,3,TAO	C8H13O	<chem>C=CC(C)([O])CC=CC</chem>	InChI=1S/C8H13O/c1-4-6-7-8(3,9)5-2/h4-6H,2,7H2,1,3H3	
C8H131-5,3,SAO	C8H13O	<chem>C=CC(C)C([O])C=CC</chem>	InChI=1S/C8H13O/c1-4-6-8(9)7(3)5-2/h4-8H,2H2,1,3H3	
C8H131-5,3,PAO	C8H13O	<chem>C=CC(C)CC=CC[O]</chem>	InChI=1S/C8H13O/c1-3-8(2)6-4-5-7-9/h3-5,8H,1,6-7H2,2H3	
C8H132-6,SAO	C8H13O	<chem>CC=CCC([O])C=CC</chem>	InChI=1S/C8H13O/c1-3-5-7-8(9)6-4-2/h3-6,8H,7H2,1-2H3	

C8H132-6,PAO	C8H13O	<chem>CC=CCCC=CC[O]</chem>	InChI=1S/C8H13O/c1-2-3-4-5-6-7-8-9/h2-3,6-7H,4-5,8H2,1H3	
C7H111-5,3,6P	C7H11	<chem>[CH]=CCC(C)C=C</chem>	InChI=1S/C7H11/c1-4-6-7(3)5-2/h1,4-5,7H,2,6H2,3H3	
C7H111-5,1P	C7H11	<chem>[CH]=CCCC=CC</chem>	InChI=1S/C7H11/c1-3-5-7-6-4-2/h1,3-4,6H,5,7H2,2H3	
C4H64,2-1OH	C4H7O	<chem>C=C[CH]CO</chem>	InChI=1S/C4H7O/c1-2-3-4-5/h2-3,5H,1,4H2	
C4H63,1-1OH	C4H7O	<chem>C[CH]C=CO</chem>	InChI=1S/C4H7O/c1-2-3-4-5/h2-5H,1H3	
C4H63,1-3OH	C4H7O	<chem>C=CCO</chem>	InChI=1S/C4H7O/c1-3-4(2)5/h3,5H,1H2,2H3	
C4H63,1-2OH	C4H7O	<chem>C=C(O)[CH]C</chem>	InChI=1S/C4H7O/c1-3-4(2)5/h3,5H,2H2,1H3	
C4H5OH-13	C4H6O	<chem>C=CC=CO</chem>	InChI=1S/C4H6O/c1-2-3-4-5/h2-5H,1H2	
SQC4H7OHP-4	C4H9O3	<chem>[CH2]CC(CO)OO</chem>	InChI=1S/C4H9O3/c1-2-4(3-5)7-6/h4-6H,1-3H2	
CY(CCCO)COH	C4H8O2	<chem>OCC1CCO1</chem>	InChI=1S/C4H8O2/c5-3-4-1-2-6-4/h4-5H,1-3H2	

NC4KET21OH	C4H8O2	CCC(=O)CO	InChI=1S/C4H8O2/c1-2-4(6)3-5/h5H,2-3H2,1H3	
C2H5CHOHCO	C4H7O2	CCC(O)[C]=O	InChI=1S/C4H7O2/c1-2-4(6)3-5/h4,6H,2H2,1H3	
CH3COCOCH3	C4H7O2	C[C](O)C(C)=O	InChI=1S/C4H7O2/c1-3(5)4(2)6/h5H,1-2H3	
C2H4COCH2OH	C4H7O2	C[CH]C(=O)CO	InChI=1S/C4H7O2/c1-2-4(6)3-5/h2,5H,3H2,1H3	
CH3COHCO	C3H4O2	CC(O)=C=O	InChI=1S/C3H4O2/c1-3(5)2-4/h5H,1H3	
CH2COHCHO	C3H4O2	C=C(O)C=O	InChI=1S/C3H4O2/c1-3(5)2-4/h2,5H,1H2	
SQC4H7OHP-4O2	C4H9O5	[O]OCCC(CO)OO	InChI=1S/C4H9O5/c5-3-4(9-7)1-2-8-6/h4-5,7H,1-3H2	
PQC4H7OHS-3O2	C4H9O5	CC(O[O])C(O)COO	InChI=1S/C4H9O5/c1-3(9-7)4(5)2-8-6/h3-6H,2H2,1H3	
SQC4H7OHS-4O2	C4H9O5	CC(OO)C(O)CO[O]	InChI=1S/C4H9O5/c1-3(9-7)4(5)2-8-6/h3-5,7H,2H2,1H3	
C4H7O2-1,3OOH	C4H9O5	CC(OO)C([O])COO	InChI=1S/C4H9O5/c1-3(9-7)4(5)2-8-6/h3-4,6-7H,2H2,1H3	

NC4KET13OH-2	C4H8O4	CC(OO)C(O)C=O	InChI=1S/C4H8O4/c1-3(8-7)4(6)2-5/h2-4,6-7H,1H3	
NC4KET24OH-1	C4H8O4	O=C(CO)CCOO	InChI=1S/C4H8O4/c5-3-4(6)1-2-8-7/h5,7H,1-3H2	
NC4KET24OH-3	C4H8O4	CC(=O)C(O)COO	InChI=1S/C4H8O4/c1-3(5)4(6)2-8-7/h4,6-7H,2H2,1H3	
C4H6OHOOH1-4-3	C4H8O3	C=CC(CO)OO	InChI=1S/C4H8O3/c1-2-4(3-5)7-6/h2,4-6H,1,3H2	
C4H6OHOOH2-2-1	C4H8O3	CC=C(O)C(OO)	InChI=1S/C4H8O3/c1-2-4(5)3-7-6/h2,5-6H,3H2,1H3	
C4H6OHOOH1-3-4	C4H8O3	C=CC(O)C(OO)	InChI=1S/C4H8O3/c1-2-4(5)3-7-6/h2,4-6H,1,3H2	
C4H6OHOOH1-2-3	C4H8O3	C=C(O)C(C)OO	InChI=1S/C4H8O3/c1-3(5)4(2)7-6/h4-6H,1H2,2H3	
HOCH2CHO	C2H4O2	O=CCO	InChI=1S/C2H4O2/c3-1-2-4/h1,4H,2H2	
C4H71-4OOH	C4H8O2	C=CCCCOO	InChI=1S/C4H8O2/c1-2-3-4-6-5/h2,5H,1,3-4H2	
C4H71-4O2	C4H7O2	C=CCCCO[O]	InChI=1S/C4H7O2/c1-2-3-4-6-5/h2H,1,3-4H2	

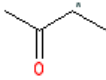
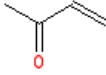
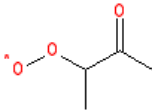
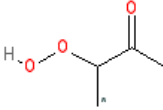
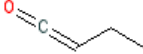





C4H6I-3OOH4	C4H7O2	C=C[CH]COO	InChI=1S/C4H7O2/c1-2-3-4-6-5/h2-3,5H,1,4H2	
C4H6O1-3OOH4	C4H7O3	C=CC([O])COO	InChI=1S/C4H7O3/c1-2-4(5)3-7-6/h2,4,6H,1,3H2	
C4H6O2-1OOH4	C4H7O3	[O]CC=CCOO	InChI=1S/C4H7O3/c5-3-1-2-4-7-6/h1-2,6H,3-4H2	
HOCH2COCH2	C3H5O2	[CH2]C(=O)CO	InChI=1S/C3H5O2/c1-3(5)2-4/h4H,1-2H2	
HOCH2CO	C2H3O2	O=[C]CO	InChI=1S/C2H3O2/c3-1-2-4/h3H,1H2	
HOCHCHO	C2H3O2	O=C[CH]O	InChI=1S/C2H3O2/c3-1-2-4/h1-3H	
PC3H4OH-3	C3H5O	C=C[CH]O	InChI=1S/C3H5O/c1-2-3-4/h2-4H,1H2	
PC3H4OH-1	C3H5O	CC=[C]O	InChI=1S/C3H5O/c1-2-3-4/h2,4H,1H3	
CH3COCHOH	C3H5O2	CC(=O)[CH]O	InChI=1S/C3H5O2/c1-3(5)2-4/h2,4H,1H3	
SC2H2OH	C2H3O	C=[C]O	InChI=1S/C2H3O/c1-2-3/h3H,1H2	

PC4H8OH-1	C4H9O	CCC[CH](O)	InChI=1S/C4H9O/c1-2-3-4-5/h4-5H,2-3H2,1H3	
PC4H8OH-3	C4H9O	C[CH]CC(O)	InChI=1S/C4H9O/c1-2-3-4-5/h2,5H,3-4H2,1H3	
C4H7O1-4	C4H7O	C=CCC[O]	InChI=1S/C4H7O/c1-2-3-4-5/h2H,1,3-4H2	
PC4H8OH-4	C4H9O	[CH2]CCC(O)	InChI=1S/C4H9O/c1-2-3-4-5/h5H,1-4H2	
SC4H8OH-2	C4H9O	C[C](O)CC	InChI=1S/C4H9O/c1-3-4(2)/h5H,3H2,1-2H3	
CH2COHCO	C3H3O2	C=C(O)[C](=O)	InChI=1S/C3H3O2/c1-3(5)2-4/h5H,1H2	
C4H72-2O2	C4H7O2	CC=C(C)O[O]	InChI=1S/C4H7O2/c1-3-4(2)6-5/h3H,1-2H3	
C4H71-1O2	C4H7O2	CCC=CO[O]	InChI=1S/C4H7O2/c1-2-3-4-6-5/h3-4H,2H2,1H3	
C4H71-2O2	C4H7O2	C=C(CC)O[O]	InChI=1S/C4H7O2/c1-3-4(2)6-5/h2-3H2,1H3	
C3H6OH1-1	C3H7O	CC[CH]O	InChI=1S/C3H7O/c1-2-3-4/h3-4H,2H2,1H3	

PC4H8OH-2O2	C4H9O3	CCC(O[O])C(O)	InChI=1S/C4H9O3/c1-2-4(3-5)7-6/h4-5H,2-3H2,1H3	
SC4H8OH-1O2	C4H9O3	CCC(O)C(O[O])	InChI=1S/C4H9O3/c1-2-4(5)3-7-6/h4-5H,2-3H2,1H3	
C4H71-3OOCH3	C5H10O2	C=CC(C)OOC	InChI=1S/C5H10O2/c1-4-5(2)7-6-3/h4-5H,1H2,2-3H3	
C4H72-1OOCH3	C5H10O2	CC=CCOOC	InChI=1S/C5H10O2/c1-3-4-5-7-6-2/h3-4H,5H2,1-2H3	
C4H6	C4H6	C=CC=C	InChI=1S/C4H6/c1-3-4-2/h3-4H,1-2H2	
C4H612	C4H6	C=C=CC	InChI=1S/C4H6/c1-3-4-2/h4H,1H2,2H3	
C4H6-2	C4H6	CC#CC	InChI=1S/C4H6/c1-3-4-2/h1-2H3	
C4H5-I	C4H5	C=[C]C=C	InChI=1S/C4H5/c1-3-4-2/h3H,1-2H2	
C4H5-N	C4H5	[CH]=CC=C	InChI=1S/C4H5/c1-3-4-2/h1,3-4H,2H2	
C4H5-2	C4H5	CC#C[CH2]	InChI=1S/C4H5/c1-3-4-2/h1H2,2H3	

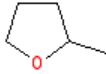

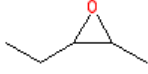

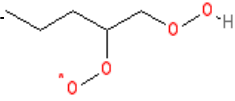
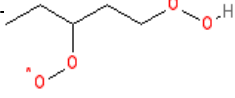
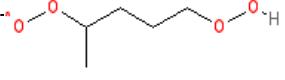
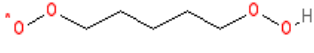
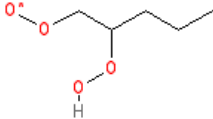
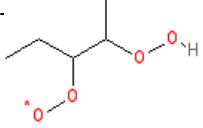
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C4H3-I	C4H3	C#C[C]=C	InChI=1S/C4H3/c1-3-4-2/h1H,2H2	
C4H3-N	C4H3	[CH]=CC#C	InChI=1S/C4H3/c1-3-4-2/h1-3H	
C4H2	C4H2	C#CC#C	InChI=1S/C4H2/c1-3-4-2/h1-2H	
C4H6O25	C4H6O	C1C=CCO1	InChI=1S/C4H6O/c1-2-4-5-3-1/h1-2H,3-4H2	
C2H3CHOCH2	C4H6O	C=CC1CO1	InChI=1S/C4H6O/c1-2-4-3-5-4/h2,4H,1,3H2	
C4H4O	C4H4O	CC#CC=O	InChI=1S/C4H4O/c1-2-3-4-5/h4H,1H3	
C4H6O23	C4H6O	C1OC=CC1	InChI=1S/C4H6O/c1-2-4-5-3-1/h1,3H,2,4H2	
CH2CHCHCHO	C4H5O	[CH2]C=CC=O	InChI=1S/C4H5O/c1-2-3-4-5/h2-4H,1H2	
H2C4O	C4H2O	C#CC1=C(O1)	InChI=1S/C4H2O/c1-2-4-3-5-4/h1,3H	

NC3H7CHO	C4H8O	CCCC=O	InChI=1S/C4H8O/c1-2-3-4-5/h4H,2-3H2,1H3	
NC3H7CO	C4H7O	CCC[C]=O	InChI=1S/C4H7O/c1-2-3-4-5/h2-3H2,1H3	
C3H6CHO-1	C4H7O	[CH2]CCC=O	InChI=1S/C4H7O/c1-2-3-4-5/h4H,1-3H2	
C3H6CHO-2	C4H7O	C[CH]CC=O	InChI=1S/C4H7O/c1-2-3-4-5/h2,4H,3H2,1H3	
C3H6CHO-3	C4H7O	CC[CH]C=O	InChI=1S/C4H7O/c1-2-3-4-5/h3-4H,2H2,1H3	
SC3H5CHO	C4H6O	CC=CC=O	InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3	
SC3H5CO	C4H5O	CC=C[C]=O	InChI=1S/C4H5O/c1-2-3-4-5/h2-3H,1H3	
C2H5COCH3	C4H8O	CCC(C)=O	InChI=1S/C4H8O/c1-3-4(2)5/h3H2,1-2H3	
C2H5COCH2	C4H7O	[CH2]C(=O)CC	InChI=1S/C4H7O/c1-3-4(2)5/h2-3H2,1H3	
CH2CH2COCH3	C4H7O	[CH2]CC(C)=O	InChI=1S/C4H7O/c1-3-4(2)5/h1,3H2,2H3	

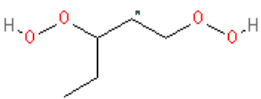
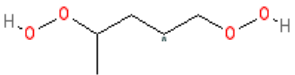

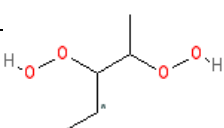
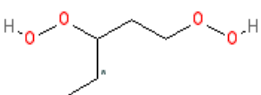
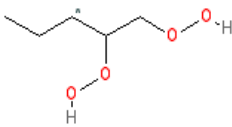
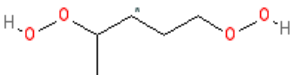


CH ₃ CHCOCH ₃	C ₄ H ₇ O	C[CH]C(C)=O	InChI=1S/C ₄ H ₇ O/c1-3-4(2)5/h3H,1-2H3	
C ₂ H ₃ COCH ₃	C ₄ H ₆ O	C=CC(C)=O	InChI=1S/C ₄ H ₆ O/c1-3-4(2)5/h3H,1H2,2H3	
CH ₃ CHOOCOCH ₃	C ₄ H ₇ O ₃	CC(=O)C(C)O[O]	InChI=1S/C ₄ H ₇ O ₃ /c1-3(5)4(2)7-6/h4H,1-2H3	
CH ₂ CHOOHCOCH ₃	C ₄ H ₇ O ₃	[CH ₂]C(OO)C(C)=O	InChI=1S/C ₄ H ₇ O ₃ /c1-3(5)4(2)7-6/h4,6H,2H2,1H3	
C ₂ H ₅ CHCO	C ₄ H ₆ O	CCC=C=O	InChI=1S/C ₄ H ₆ O/c1-2-3-4-5/h3H,2H2,1H3	
NC ₅ H ₁₂	C ₅ H ₁₂	CCCCC	InChI=1S/C ₅ H ₁₂ /c1-3-5-4-2/h3-5H2,1-2H3	
C ₅ H ₁₁ -1	C ₅ H ₁₁	[CH ₂]CCCC	InChI=1S/C ₅ H ₁₁ /c1-3-5-4-2/h1,3-5H2,2H3	
C ₅ H ₁₁ -2	C ₅ H ₁₁	C[CH]CCC	InChI=1S/C ₅ H ₁₁ /c1-3-5-4-2/h3H,4-5H2,1-2H3	
C ₅ H ₁₁ -3	C ₅ H ₁₁	CC[CH]CC	InChI=1S/C ₅ H ₁₁ /c1-3-5-4-2/h5H,3-4H2,1-2H3	
C ₅ H ₁₁ O ₂ H-1	C ₅ H ₁₂ O ₂	CCCCCOO	InChI=1S/C ₅ H ₁₂ O ₂ /c1-2-3-4-5-7-6/h6H,2-5H2,1H3	

C5H11O2H-2	C5H12O2	CCCC(C)OO	InChI=1S/C5H12O2/c1-3-4-5(2)7-6/h5-6H,3-4H2,1-2H3	
C5H11O2H-3	C5H12O2	CCC(CC)OO	InChI=1S/C5H12O2/c1-3-5(4-2)7-6/h5-6H,3-4H2,1-2H3	
C5H11O2-1	C5H11O2	CCCCCO[O]	InChI=1S/C5H11O2/c1-2-3-4-5-7-6/h2-5H2,1H3	
C5H11O2-2	C5H11O2	CCCC(C)O[O]	InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h5H,3-4H2,1-2H3	
C5H11O2-3	C5H11O2	CCC(CC)O[O]	InChI=1S/C5H11O2/c1-3-5(4-2)7-6/h5H,3-4H2,1-2H3	
C5H11O-1	C5H11O	CCCCC[O]	InChI=1S/C5H11O/c1-2-3-4-5-6/h2-5H2,1H3	
C5H11O-2	C5H11O	CCCC(C)[O]	InChI=1S/C5H11O/c1-3-4-5(2)6/h5H,3-4H2,1-2H3	
C5H11O-3	C5H11O	CCC(CC)[O]	InChI=1S/C5H11O/c1-3-5(6)4-2/h5H,3-4H2,1-2H3	
C5H10OOH1-2	C5H11O2	CCC[CH]COO	InChI=1S/C5H11O2/c1-2-3-4-5-7-6/h4,6H,2-3,5H2,1H3	
C5H10OOH1-3	C5H11O2	CC[CH]CCOO	InChI=1S/C5H11O2/c1-2-3-4-5-7-6/h3,6H,2,4-5H2,1H3	

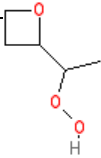
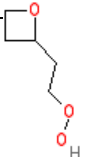
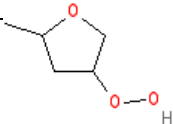
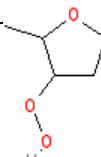
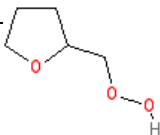
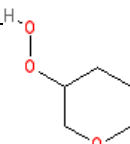
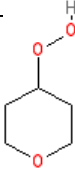
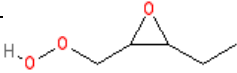
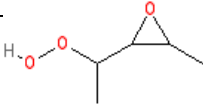
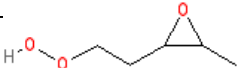
C5H10OOH1-4	C5H11O2	C[CH]CCCCOO	InChI=1S/C5H11O2/c1-2-3-4-5-7-6/h2,6H,3-5H2,1H3	
C5H10OOH1-5	C5H11O2	[CH2]CCCCOO	InChI=1S/C5H11O2/c1-2-3-4-5-7-6/h6H,1-5H2	
C5H10OOH2-1	C5H11O2	CCCC([CH2])OO	InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h5-6H,2-4H2,1H3	
C5H10OOH2-3	C5H11O2	CC[CH]C(C)OO	InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h4-6H,3H2,1-2H3	
C5H10OOH2-4	C5H11O2	C[CH]CC(C)OO	InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h3,5-6H,4H2,1-2H3	
C5H10OOH2-5	C5H11O2	[CH2]CCC(C)OO	InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h5-6H,1,3-4H2,2H3	
C5H10OOH3-1	C5H11O2	[CH2]CC(CC)OO	InChI=1S/C5H11O2/c1-3-5(4-2)7-6/h5-6H,1,3-4H2,2H3	
C5H10OOH3-2	C5H11O2	C[CH]C(CC)OO	InChI=1S/C5H11O2/c1-3-5(4-2)7-6/h3,5-6H,4H2,1-2H3	
C5H10O1-2	C5H10O	CCCC1CO1	InChI=1S/C5H10O/c1-2-3-5-4-6-5/h5H,2-4H2,1H3	
C5H10O1-3	C5H10O	CCC1CCO1	InChI=1S/C5H10O/c1-2-5-3-4-6-5/h5H,2-4H2,1H3	

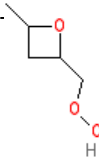
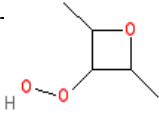

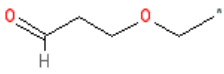
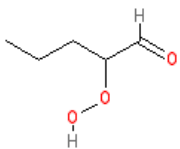
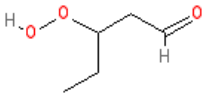
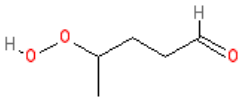
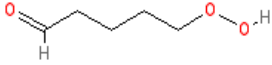
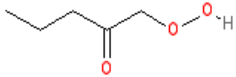
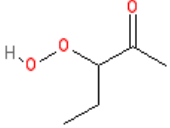
C5H10O1-4	C5H10O	CC1CCCCO1	InChI=1S/C5H10O/c1-5-3-2-4-6-5/h5H,2-4H2,1H3	
C5H10O1-5	C5H10O	C1CCOCC1	InChI=1S/C5H10O/c1-2-4-6-5-3-1/h1-5H2	
C5H10O2-3	C5H10O	CCC1C(C)O1	InChI=1S/C5H10O/c1-3-5-4(2)6-5/h4-5H,3H2,1-2H3	
C5H10O2-4	C5H10O	CC1CC(C)O1	InChI=1S/C5H10O/c1-4-3-5(2)6-4/h4-5H,3H2,1-2H3	
C5H10OOH1-2O2	C5H11O4	CCCC(COO)O[O]	InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h5-6H,2-4H2,1H3	
C5H10OOH1-3O2	C5H11O4	CCC(CCOO)O[O]	InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h5-6H,2-4H2,1H3	
C5H10OOH1-4O2	C5H11O4	CC(CCCOO)O[O]	InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h5-6H,2-4H2,1H3	
C5H10OOH1-5O2	C5H11O4	C(CCOO)CCO[O]	InChI=1S/C5H11O4/c6-8-4-2-1-3-5-9-7/h6H,1-5H2	
C5H10OOH2-1O2	C5H11O4	CCCC(CO[O])OO	InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h5,7H,2-4H2,1H3	
C5H10OOH2-3O2	C5H11O4	CCC(C(C)OO)O[O]	InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h4-6H,3H2,1-2H3	

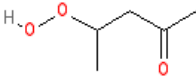
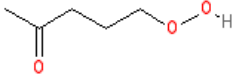
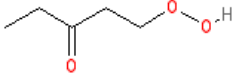
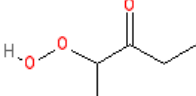
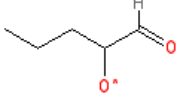
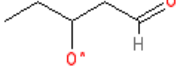
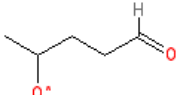

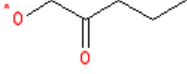
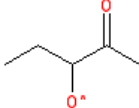
C5H10OOH2-4O2	C5H11O4	CC(CC(C)O[O])OO	InChI=1S/C5H11O4/c1-4(8-6)3-5(2)9-7/h4-6H,3H2,1-2H3	
C5H10OOH2-5O2	C5H11O4	CC(CCCO[O])OO	InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h5,7H,2-4H2,1H3	
C5H10OOH3-1O2	C5H11O4	CCC(CCO[O])OO	InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h5,7H,2-4H2,1H3	
C5H10OOH3-2O2	C5H11O4	CCC(C(C)O[O])OO	InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h4-5,7H,3H2,1-2H3	
C5H91-2,3OOH	C5H11O4	CCC(C([CH2])OO)OO	InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h4-7H,2-3H2,1H3	
C5H91-2,4OOH	C5H11O4	[CH2]C(CC(C)OO)OO	InChI=1S/C5H11O4/c1-4(8-6)3-5(2)9-7/h4-7H,1,3H2,2H3	
C5H91-2,5OOH	C5H11O4	[CH2]C(CCCOO)OO	InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h5-7H,1-4H2	
C5H91-3,4OOH	C5H11O4	[CH2]CC(C(C)OO)OO	InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h4-7H,1,3H2,2H3	
C5H91-3,5OOH	C5H11O4	[CH2]CC(CCOO)OO	InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h5-7H,1-4H2	
C5H91-4,5OOH	C5H11O4	[CH2]CCC(COO)OO	InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h5-7H,1-4H2	

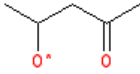
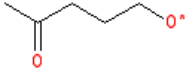
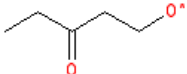
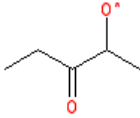
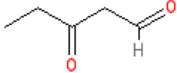
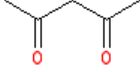
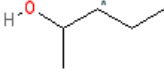
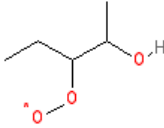
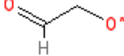
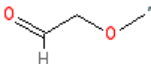
C5H92-1,3OOH	C5H11O4	CCC([CH]COO)OO	InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h3,5-7H,2,4H2,1H3	
C5H92-1,4OOH	C5H11O4	CC(C[CH]COO)OO	InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h2,5-7H,3-4H2,1H3	
C5H92-1,5OOH	C5H11O4	C([CH]COO)CCOO	InChI=1S/C5H11O4/c6-8-4-2-1-3-5-9-7/h2,6-7H,1,3-5H2	
C5H92-3,4OOH	C5H11O4	C[CH]C(C(C)OO)OO	InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h3-7H,1-2H3	
C5H92-3,5OOH	C5H11O4	C[CH]C(CCOO)OO	InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h2,5-7H,3-4H2,1H3	
C5H92-4,5OOH	C5H11O4	C[CH]CC(COO)OO	InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h2,5-7H,3-4H2,1H3	
C5H93-1,2OOH	C5H11O4	CC[CH]C(COO)OO	InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h3,5-7H,2,4H2,1H3	
C5H93-1,4OOH	C5H11O4	CC([CH]CCOO)OO	InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h3,5-7H,2,4H2,1H3	
C5H93-1,5OOH	C5H11O4	[CH](CCOO)CCOO	InChI=1S/C5H11O4/c6-8-4-2-1-3-5-9-7/h1,6-7H,2-5H2	
C5H93-2,4OOH	C5H11O4	CC([CH]C(C)OO)OO	InChI=1S/C5H11O4/c1-4(8-6)3-5(2)9-7/h3-7H,1-2H3	

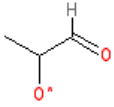
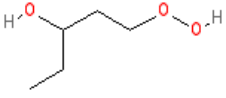
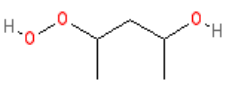
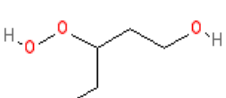
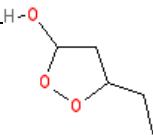
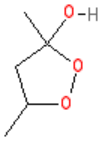
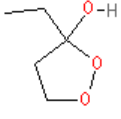
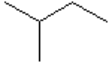
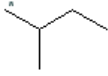

C5H91-3OOH	C5H10O2	C=CC(CC)OO	InChI=1S/C5H10O2/c1-3-5(4-2)7-6/h3,5-6H,1,4H2,2H3	
C5H91-4OOH	C5H10O2	C=CCC(C)OO	InChI=1S/C5H10O2/c1-3-4-5(2)7-6/h3,5-6H,1,4H2,2H3	
C5H91-5OOH	C5H10O2	C=CCCCOO	InChI=1S/C5H10O2/c1-2-3-4-5-7-6/h2,6H,1,3-5H2	
C5H92-1OOH	C5H10O2	CCC=CCOO	InChI=1S/C5H10O2/c1-2-3-4-5-7-6/h3-4,6H,2,5H2,1H3	
C5H92-4OOH	C5H10O2	CC=CC(C)OO	InChI=1S/C5H10O2/c1-3-4-5(2)7-6/h3-6H,1-2H3	
C5H92-5OOH	C5H10O2	CC=CCCCOO	InChI=1S/C5H10O2/c1-2-3-4-5-7-6/h2-3,6H,4-5H2,1H3	
C5H9O1-2OOH-3	C5H10O3	CCC(C1CO1)OO	InChI=1S/C5H10O3/c1-2-4(8-6)5-3-7-5/h4-6H,2-3H2,1H3	
C5H9O1-2OOH-4	C5H10O3	CC(CC1CO1)OO	InChI=1S/C5H10O3/c1-4(8-6)2-5-3-7-5/h4-6H,2-3H2,1H3	
C5H9O1-2OOH-5	C5H10O3	C(CC1CO1)COO	InChI=1S/C5H10O3/c6-8-3-1-2-5-4-7-5/h5-6H,1-4H2	
C5H9O1-3OOH-2	C5H10O3	CCC1C(CO1)OO	InChI=1S/C5H10O3/c1-2-4-5(8-6)3-7-4/h4-6H,2-3H2,1H3	

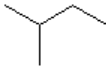
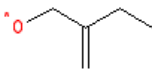
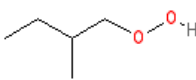
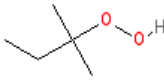
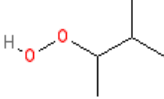
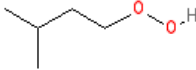
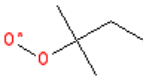
C5H9O1-3OOH-4	C5H10O3	CC(C1CCO1)OO	InChI=1S/C5H10O3/c1-4(8-6)5-2-3-7-5/h4-6H,2-3H2,1H3	
C5H9O1-3OOH-5	C5H10O3	C1COC1CCOO	InChI=1S/C5H10O3/c6-8-4-2-5-1-3-7-5/h5-6H,1-4H2	
C5H9O1-4OOH-2	C5H10O3	CC1CC(CO1)OO	InChI=1S/C5H10O3/c1-4-2-5(8-6)3-7-4/h4-6H,2-3H2,1H3	
C5H9O1-4OOH-3	C5H10O3	CC1C(CCO1)OO	InChI=1S/C5H10O3/c1-4-5(8-6)2-3-7-4/h4-6H,2-3H2,1H3	
C5H9O1-4OOH-5	C5H10O3	C1CC(COO)OC1	InChI=1S/C5H10O3/c6-8-4-5-2-1-3-7-5/h5-6H,1-4H2	
C5H9O1-5OOH-2	C5H10O3	C1CC(COC1)OO	InChI=1S/C5H10O3/c6-8-5-2-1-3-7-4-5/h5-6H,1-4H2	
C5H9O1-5OOH-3	C5H10O3	C1COCCC1OO	InChI=1S/C5H10O3/c6-8-5-1-3-7-4-2-5/h5-6H,1-4H2	
C5H9O2-3OOH-1	C5H10O3	CCC1C(COO)O1	InChI=1S/C5H10O3/c1-2-4-5(8-4)3-7-6/h4-6H,2-3H2,1H3	
C5H9O2-3OOH-4	C5H10O3	CC1C(C(C)OO)O1	InChI=1S/C5H10O3/c1-3-5(7-3)4(2)8-6/h3-6H,1-2H3	
C5H9O2-3OOH-5	C5H10O3	CC1C(CCOO)O1	InChI=1S/C5H10O3/c1-4-5(8-4)2-3-7-6/h4-6H,2-3H2,1H3	

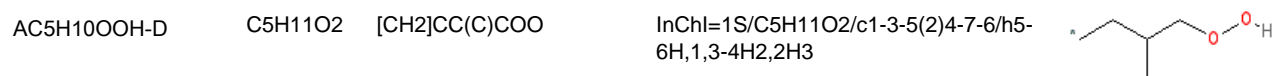
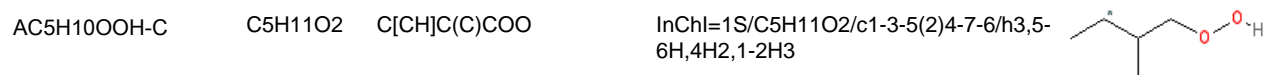
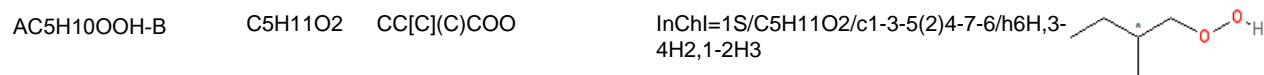
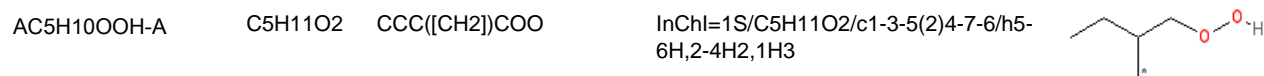
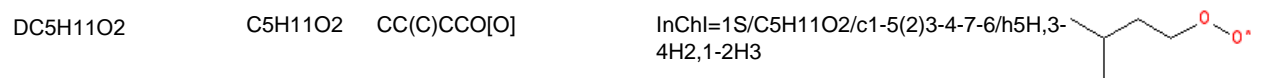
C5H9O2-4OOH-1	C5H10O3	CC1CC(COO)O1	InChI=1S/C5H10O3/c1-4-2-5(8-4)3-7-6/h4-6H,2-3H2,1H3	
C5H9O2-4OOH-3	C5H10O3	CC1C(C(C)O1)OO	InChI=1S/C5H10O3/c1-3-5(8-6)4(2)7-3/h3-6H,1-2H3	
C5H9O1-2O-5	C5H9O2	C(CC1CO1)C[O]	InChI=1S/C5H9O2/c6-3-1-2-5-4-7-5/h5H,1-4H2	
CH2CH2OCH2CH2CH(C5H9O2	[CH2]COCCCC=O		InChI=1S/C5H9O2/c1-2-7-5-3-4-6/h4H,1-3,5H2	
NC5KET12	C5H10O3	CCCC(C=O)OO	InChI=1S/C5H10O3/c1-2-3-5(4-6)8-7/h4-5,7H,2-3H2,1H3	
NC5KET13	C5H10O3	CCC(CC=O)OO	InChI=1S/C5H10O3/c1-2-5(8-7)3-4-6/h4-5,7H,2-3H2,1H3	
NC5KET14	C5H10O3	CC(CCC=O)OO	InChI=1S/C5H10O3/c1-5(8-7)3-2-4-6/h4-5,7H,2-3H2,1H3	
NC5KET15	C5H10O3	C(CC=O)CCOO	InChI=1S/C5H10O3/c6-4-2-1-3-5-8-7/h4,7H,1-3,5H2	
NC5KET21	C5H10O3	CCCC(COO)=O	InChI=1S/C5H10O3/c1-2-3-5(6)4-8-7/h7H,2-4H2,1H3	
NC5KET23	C5H10O3	CCC(C(C)=O)OO	InChI=1S/C5H10O3/c1-3-5(8-7)4(2)6/h5,7H,3H2,1-2H3	

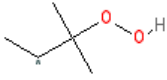
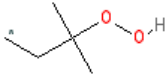
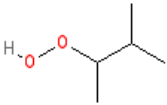
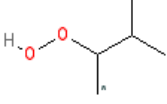
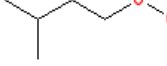
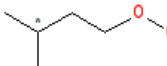
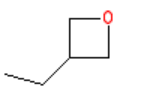
NC5KET24	C5H10O3	CC(CC(C)OO)=O	InChI=1S/C5H10O3/c1-4(6)3-5(2)8-7/h5,7H,3H2,1-2H3	
NC5KET25	C5H10O3	CC(CCCOO)=O	InChI=1S/C5H10O3/c1-5(6)3-2-4-8-7/h7H,2-4H2,1H3	
NC5KET31	C5H10O3	CCC(CCOO)=O	InChI=1S/C5H10O3/c1-2-5(6)3-4-8-7/h7H,2-4H2,1H3	
NC5KET32	C5H10O3	CCC(C(C)OO)=O	InChI=1S/C5H10O3/c1-3-5(6)4(2)8-7/h4,7H,3H2,1-2H3	
NC5KET120	C5H9O2	CCCC(C=O)[O]	InChI=1S/C5H9O2/c1-2-3-5(7)4-6/h4-5H,2-3H2,1H3	
NC5KET130	C5H9O2	CCC(CC=O)[O]	InChI=1S/C5H9O2/c1-2-5(7)3-4-6/h4-5H,2-3H2,1H3	
NC5KET140	C5H9O2	CC(CCC=O)[O]	InChI=1S/C5H9O2/c1-5(7)3-2-4-6/h4-5H,2-3H2,1H3	
NC5KET150	C5H9O2	C(CC=O)CC[O]	InChI=1S/C5H9O2/c6-4-2-1-3-5-7/h4H,1-3,5H2	
NC5KET210	C5H9O2	CCCC(C[O])=O	InChI=1S/C5H9O2/c1-2-3-5(7)4-6/h2-4H2,1H3	
NC5KET230	C5H9O2	CCC(C(C)=O)[O]	InChI=1S/C5H9O2/c1-3-5(7)4(2)6/h5H,3H2,1-2H3	


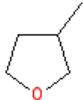


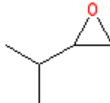
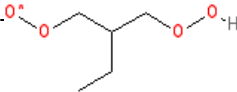
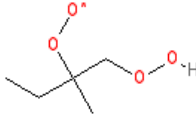
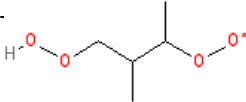
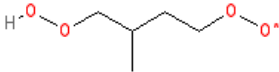
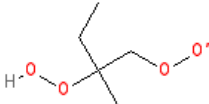
NC5KET24O	C5H9O2	CC(CC(C)=O)[O]	InChI=1S/C5H9O2/c1-4(6)3-5(2)7/h4H,3H2,1-2H3	
NC5KET25O	C5H9O2	CC(CCC[O])=O	InChI=1S/C5H9O2/c1-5(7)3-2-4-6/h2-4H2,1H3	
NC5KET31O	C5H9O2	CCC(CC[O])=O	InChI=1S/C5H9O2/c1-2-5(7)3-4-6/h2-4H2,1H3	
NC5KET32O	C5H9O2	CCC(C(C)[O])=O	InChI=1S/C5H9O2/c1-3-5(7)4(2)6/h4H,3H2,1-2H3	
NC5DIONE13	C5H8O2	C(=O)CC(=O)CC	InChI=1S/C5H8O2/c1-2-5(7)3-4-6/h4H,2-3H2,1H3	
NC5DIONE24	C5H8O2	CC(=O)CC(=O)C	InChI=1S/C5H8O2/c1-4(6)3-5(2)7/h3H2,1-2H3	
C5H10OH23	C5H11O	CC[CH]C(C)O	InChI=1S/C5H11O/c1-3-4-5(2)6/h4-6H,3H2,1-2H3	
O2C5H10OH23	C5H11O3	CCC(C(C)O)O[O]	InChI=1S/C5H11O3/c1-3-5(8-7)4(2)6/h4-6H,3H2,1-2H3	
OCH2CHO	C2H3O2	C(C[O])=O	InChI=1S/C2H3O2/c3-1-2-4/h1H,2H2	
CH2OCH2CHO	C3H5O2	[CH2]OCC=O	InChI=1S/C3H5O2/c1-5-3-2-4/h2H,1,3H2	

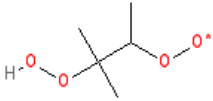
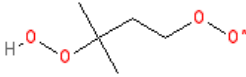
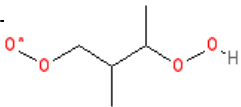
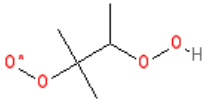
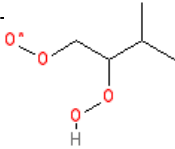
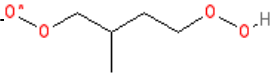
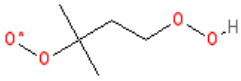
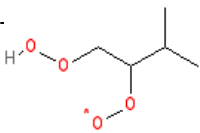
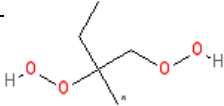
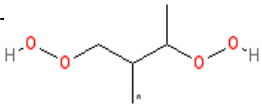
C2H4OCHO	C3H5O2	CC(C=O)[O]	InChI=1S/C3H5O2/c1-3(5)2-4/h2-3H,1H3	
C5H10OOH1-3OH	C5H12O3	C(OO)CC(O)CC	InChI=1S/C5H12O3/c1-2-5(6)3-4-8-7/h5-7H,2-4H2,1H3	
C5H10OOH2-4OH	C5H12O3	CC(OO)CC(O)C	InChI=1S/C5H12O3/c1-4(6)3-5(2)8-7/h4-7H,3H2,1-2H3	
C5H10OOH3-1OH	C5H12O3	C(O)CC(OO)CC	InChI=1S/C5H12O3/c1-2-5(8-7)3-4-6/h5-7H,2-4H2,1H3	
NC5CYCPER13	C5H10O3	C1(O)CC(OO1)CC	InChI=1S/C5H10O3/c1-2-4-3-5(6)8-7-4/h4,6H,2-3H2,1H3	
NC5CYCPER24	C5H10O3	CC1(O)CC(OO1)C	InChI=1S/C5H10O3/c1-4-3-5(2,6)8-7-4/h4,6H,3H2,1-2H3	
NC5CYCPER31	C5H10O3	C(OO1)CC1(O)CC	InChI=1S/C5H10O3/c1-2-5(6)3-4-7-8-5/h6H,2-4H2,1H3	
IC5H12	C5H12	CCC(C)C	InChI=1S/C5H12/c1-4-5(2)3/h5H,4H2,1-3H3	
AC5H11	C5H11	CCC([CH2])C	InChI=1S/C5H11/c1-4-5(2)3/h5H,2,4H2,1,3H3	
BC5H11	C5H11	CCCC	InChI=1S/C5H11/c1-4-5(2)3/h4H2,1-3H3	

CC5H11	C5H11	C[CH]C(C)C	InChI=1S/C5H11/c1-4-5(2)3/h4-5H,1-3H3	
DC5H11	C5H11	[CH2]CC(C)C	InChI=1S/C5H11/c1-4-5(2)3/h5H,1,4H2,2-3H3	
AC5H9O-A2	C5H9O	CCC(=C)C[O]	InChI=1S/C5H9O/c1-3-5(2)4-6/h2-4H2,1H3	
AC5H11O2H	C5H12O2	CCC(C)COO	InChI=1S/C5H12O2/c1-3-5(2)4-7-6/h5-6H,3-4H2,1-2H3	
BC5H11O2H	C5H12O2	CCC(C)(C)OO	InChI=1S/C5H12O2/c1-4-5(2,3)7-6/h6H,4H2,1-3H3	
CC5H11O2H	C5H12O2	CC(C)C(C)OO	InChI=1S/C5H12O2/c1-4(2)5(3)7-6/h4-6H,1-3H3	
DC5H11O2H	C5H12O2	CC(C)CCOO	InChI=1S/C5H12O2/c1-5(2)3-4-7-6/h5-6H,3-4H2,1-2H3	
AC5H11O2	C5H11O2	CCC(C)CO[O]	InChI=1S/C5H11O2/c1-3-5(2)4-7-6/h5H,3-4H2,1-2H3	
BC5H11O2	C5H11O2	CCC(C)(C)O[O]	InChI=1S/C5H11O2/c1-4-5(2,3)7-6/h4H2,1-3H3	
CC5H11O2	C5H11O2	CC(C)C(C)O[O]	InChI=1S/C5H11O2/c1-4(2)5(3)7-6/h4-5H,1-3H3	

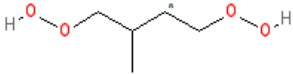
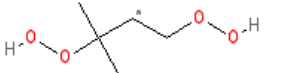
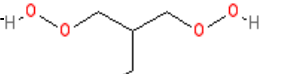
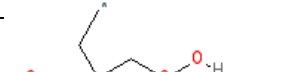
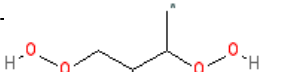
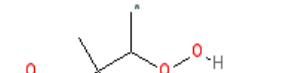
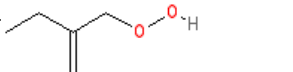
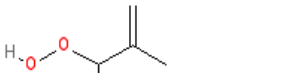
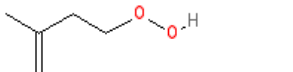
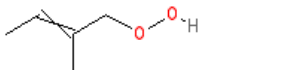


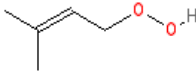
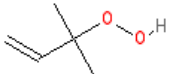
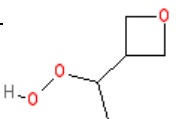
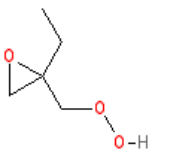
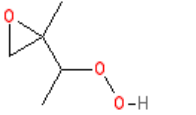
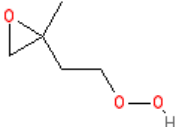
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BC5H10OOH-D	C5H11O2	[CH2]CC(C)(C)OO	InChI=1S/C5H11O2/c1-4-5(2,3)7-6/h6H,1,4H2,2-3H3	
CC5H10OOH-A	C5H11O2	[CH2]C(C)C(C)OO	InChI=1S/C5H11O2/c1-4(2)5(3)7-6/h4-6H,1H2,2-3H3	
CC5H10OOH-B	C5H11O2	CCC(C)OO	InChI=1S/C5H11O2/c1-4(2)5(3)7-6/h5-6H,1-3H3	
CC5H10OOH-D	C5H11O2	CC(C)C([CH2])OO	InChI=1S/C5H11O2/c1-4(2)5(3)7-6/h4-6H,3H2,1-2H3	
DC5H10OOH-A	C5H11O2	[CH2]C(C)CCOO	InChI=1S/C5H11O2/c1-5(2)3-4-7-6/h5-6H,1,3-4H2,2H3	
DC5H10OOH-B	C5H11O2	CCCCOO	InChI=1S/C5H11O2/c1-5(2)3-4-7-6/h6H,3-4H2,1-2H3	
DC5H10OOH-C	C5H11O2	CC(C)[CH]COO	InChI=1S/C5H11O2/c1-5(2)3-4-7-6/h3,5-6H,4H2,1-2H3	
A-AC5H10O	C5H10O	CCC1COC1	InChI=1S/C5H10O/c1-2-5-3-6-4-5/h5H,2-4H2,1H3	
A-BC5H10O	C5H10O	CCC1(C)CO1	InChI=1S/C5H10O/c1-3-5(2)4-6-5/h3-4H2,1-2H3	

A-CC5H10O	C5H10O	CC1COC1C	InChI=1S/C5H10O/c1-4-3-6-5(4)2/h4-5H,3H2,1-2H3	
A-DC5H10O	C5H10O	CC1CCOC1	InChI=1S/C5H10O/c1-5-2-3-6-4-5/h5H,2-4H2,1H3	
B-CC5H10O	C5H10O	CC1C(C)(C)O1	InChI=1S/C5H10O/c1-4-5(2,3)6-4/h4H,1-3H3	
B-DC5H10O	C5H10O	CC1(C)CCO1	InChI=1S/C5H10O/c1-5(2)3-4-6-5/h3-4H2,1-2H3	
C-DC5H10O	C5H10O	CC(C)C1CO1	InChI=1S/C5H10O/c1-4(2)5-3-6-5/h4-5H,3H2,1-2H3	
AC5H10OOH-AO2	C5H11O4	CCC(COO)CO[O]	InChI=1S/C5H11O4/c1-2-5(3-8-6)4-9-7/h5-6H,2-4H2,1H3	
AC5H10OOH-BO2	C5H11O4	CCC(C)(COO)O[O]	InChI=1S/C5H11O4/c1-3-5(2,9-7)4-8-6/h6H,3-4H2,1-2H3	
AC5H10OOH-CO2	C5H11O4	CC(COO)C(C)O[O]	InChI=1S/C5H11O4/c1-4(3-8-6)5(2)9-7/h4-6H,3H2,1-2H3	
AC5H10OOH-DO2	C5H11O4	CC(CCO[O])COO	InChI=1S/C5H11O4/c1-5(4-9-7)2-3-8-6/h5,7H,2-4H2,1H3	
BC5H10OOH-AO2	C5H11O4	CCC(C)(CO[O])OO	InChI=1S/C5H11O4/c1-3-5(2,9-7)4-8-6/h7H,3-4H2,1-2H3	

BC5H10OOH-CO2	C5H11O4	CC(C(C)(C)OO)O[O]	InChI=1S/C5H11O4/c1-4(8-6)5(2,3)9-7/h4,7H,1-3H3	
BC5H10OOH-DO2	C5H11O4	CC(C)(CCO[O])OO	InChI=1S/C5H11O4/c1-5(2,9-7)3-4-8-6/h7H,3-4H2,1-2H3	
CC5H10OOH-AO2	C5H11O4	CC(CO[O])C(C)OO	InChI=1S/C5H11O4/c1-4(3-8-6)5(2)9-7/h4-5,7H,3H2,1-2H3	
CC5H10OOH-BO2	C5H11O4	CC(C(C)(C)O[O])OO	InChI=1S/C5H11O4/c1-4(8-6)5(2,3)9-7/h4,6H,1-3H3	
CC5H10OOH-DO2	C5H11O4	CC(C)C(CO[O])OO	InChI=1S/C5H11O4/c1-4(2)5(9-7)3-8-6/h4-5,7H,3H2,1-2H3	
DC5H10OOH-AO2	C5H11O4	CC(CCOO)CO[O]	InChI=1S/C5H11O4/c1-5(4-9-7)2-3-8-6/h5-6H,2-4H2,1H3	
DC5H10OOH-BO2	C5H11O4	CC(C)(CCOO)O[O]	InChI=1S/C5H11O4/c1-5(2,9-7)3-4-8-6/h6H,3-4H2,1-2H3	
DC5H10OOH-CO2	C5H11O4	CC(C)C(COO)O[O]	InChI=1S/C5H11O4/c1-4(2)5(9-7)3-8-6/h4-6H,3H2,1-2H3	
C5H9A-A,BOOH	C5H11O4	CCC([CH2])(COO)OO	InChI=1S/C5H11O4/c1-3-5(2,9-7)4-8-6/h6-7H,2-4H2,1H3	
C5H9A-A,COOH	C5H11O4	[CH2]C(COO)C(C)OO	InChI=1S/C5H11O4/c1-4(3-8-6)5(2)9-7/h4-7H,1,3H2,2H3	

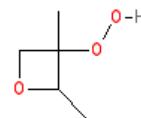
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C5H9A-B,COOH	C5H11O4	CC(C([CH2]))(C)OO)OO	InChI=1S/C5H11O4/c1-4(8-6)5(2,3)9-7/h4,6-7H,2H2,1,3H3	
C5H9A-B,DOOH	C5H11O4	[CH2]C(C)(CCOO)OO	InChI=1S/C5H11O4/c1-5(2,9-7)3-4-8-6/h6-7H,1,3-4H2,2H3	
C5H9A-C,DOOH	C5H11O4	[CH2]C(C)C(COO)OO	InChI=1S/C5H11O4/c1-4(2)5(9-7)3-8-6/h4-7H,1,3H2,2H3	
C5H9B-A,AOOH	C5H11O4	CC[C](COO)COO	InChI=1S/C5H11O4/c1-2-5(3-8-6)4-9-7/h6-7H,2-4H2,1H3	
C5H9B-A,COOH	C5H11O4	C[C](COO)C(C)OO	InChI=1S/C5H11O4/c1-4(3-8-6)5(2)9-7/h5-7H,3H2,1-2H3	
C5H9B-A,DOOH	C5H11O4	C[C](CCOO)COO	InChI=1S/C5H11O4/c1-5(4-9-7)2-3-8-6/h6-7H,2-4H2,1H3	
C5H9B-C,DOOH	C5H11O4	CCC(COO)OO	InChI=1S/C5H11O4/c1-4(2)5(9-7)3-8-6/h5-7H,3H2,1-2H3	
C5H9C-A,AOOH	C5H11O4	C[CH]C(COO)COO	InChI=1S/C5H11O4/c1-2-5(3-8-6)4-9-7/h2,5-7H,3-4H2,1H3	
C5H9C-A,BOOH	C5H11O4	C[CH]C(C)(COO)OO	InChI=1S/C5H11O4/c1-3-5(2,9-7)4-8-6/h3,6-7H,4H2,1-2H3	

C5H9C-A,DOOH	C5H11O4	CC([CH]COO)COO	InChI=1S/C5H11O4/c1-5(4-9-7)2-3-8-6/h2,5-7H,3-4H2,1H3	
C5H9C-B,DOOH	C5H11O4	CC(C)([CH]COO)OO	InChI=1S/C5H11O4/c1-5(2,9-7)3-4-8-6/h3,6-7H,4H2,1-2H3	
C5H9D-A,AOOH	C5H11O4	[CH2]CC(COO)COO	InChI=1S/C5H11O4/c1-2-5(3-8-6)4-9-7/h5-7H,1-4H2	
C5H9D-A,BOOH	C5H11O4	[CH2]CC(C)(COO)OO	InChI=1S/C5H11O4/c1-3-5(2,9-7)4-8-6/h6-7H,1,3-4H2,2H3	
C5H9D-A,COOH	C5H11O4	CC(COO)C([CH2])OO	InChI=1S/C5H11O4/c1-4(3-8-6)5(2)9-7/h4-7H,2-3H2,1H3	
C5H9D-B,COOH	C5H11O4	[CH2]C(C(C)(C)OO)OO	InChI=1S/C5H11O4/c1-4(8-6)5(2,3)9-7/h4,6-7H,1H2,2-3H3	
C5H9A-AOOH	C5H10O2	CCC(=C)COO	InChI=1S/C5H10O2/c1-3-5(2)4-7-6/h6H,2-4H2,1H3	
C5H9A-COOH	C5H10O2	C=C(C)C(C)OO	InChI=1S/C5H10O2/c1-4(2)5(3)7-6/h5-6H,1H2,2-3H3	
C5H9A-DOOH	C5H10O2	C=C(C)CCOO	InChI=1S/C5H10O2/c1-5(2)3-4-7-6/h6H,1,3-4H2,2H3	
C5H9B-AOOH	C5H10O2	CC=C(C)COO	InChI=1S/C5H10O2/c1-3-5(2)4-7-6/h3,6H,4H2,1-2H3	

C5H9B-DOOH	C5H10O2	<chem>CC(C)=CCOO</chem>	InChI=1S/C5H10O2/c1-5(2)3-4-7-6/h3,6H,4H2,1-2H3	
C5H9C-AOOH	C5H10O2	<chem>C=CC(C)COO</chem>	InChI=1S/C5H10O2/c1-3-5(2)4-7-6/h3,5-6H,1,4H2,2H3	
C5H9C-BOOH	C5H10O2	<chem>C=CC(C)(C)OO</chem>	InChI=1S/C5H10O2/c1-4-5(2,3)7-6/h4,6H,1H2,2-3H3	
C5H9OA-AOOH-B	C5H10O3	<chem>CCC1(COC1)OO</chem>	InChI=1S/C5H10O3/c1-2-5(8-6)3-7-4-5/h6H,2-4H2,1H3	
C5H9OA-AOOH-C	C5H10O3	<chem>CC(C1COC1)OO</chem>	InChI=1S/C5H10O3/c1-4(8-6)5-2-7-3-5/h4-6H,2-3H2,1H3	
C5H9OA-AOOH-D	C5H10O3	<chem>C(COO)C1COC1</chem>	InChI=1S/C5H10O3/c6-8-2-1-5-3-7-4-5/h5-6H,1-4H2	
C5H9OA-BOOH-A	C5H10O3	<chem>CCC1(CO1)COO</chem>	InChI=1S/C5H10O3/c1-2-5(3-7-5)4-8-6/h6H,2-4H2,1H3	
C5H9OA-BOOH-C	C5H10O3	<chem>CC(C1(C)CO1)OO</chem>	InChI=1S/C5H10O3/c1-4(8-6)5(2)3-7-5/h4,6H,3H2,1-2H3	
C5H9OA-BOOH-D	C5H10O3	<chem>CC1(CCOO)CO1</chem>	InChI=1S/C5H10O3/c1-5(4-7-5)2-3-8-6/h6H,2-4H2,1H3	
C5H9OA-COOH-A	C5H10O3	<chem>CC1C(CO1)COO</chem>	InChI=1S/C5H10O3/c1-4-5(2-7-4)3-8-6/h4-6H,2-3H2,1H3	

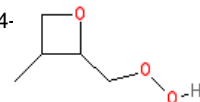
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InChI=1S/C5H10O3/c1-4-5(2,8-6)3-7-4/h4,6H,3H2,1-2H3



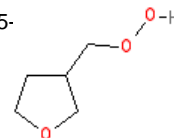
C5H9OA-COOH-D C5H10O3 CC1COC1COO

InChI=1S/C5H10O3/c1-4-2-7-5(4)3-8-6/h4-6H,2-3H2,1H3



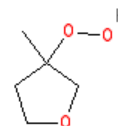
C5H9OA-DOOH-A C5H10O3 C1COCC1COO

InChI=1S/C5H10O3/c6-8-4-5-1-2-7-3-5/h5-6H,1-4H2



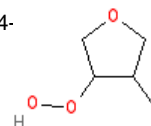
C5H9OA-DOOH-B C5H10O3 CC1(CCOC1)OO

InChI=1S/C5H10O3/c1-5(8-6)2-3-7-4-5/h6H,2-4H2,1H3



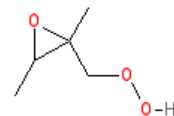
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InChI=1S/C5H10O3/c1-4-2-7-3-5(4)8-6/h4-6H,2-3H2,1H3



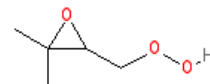
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InChI=1S/C5H10O3/c1-4-5(2,8-4)3-7-6/h4,6H,3H2,1-2H3



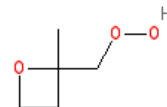
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InChI=1S/C5H10O3/c1-5(2)4(8-5)3-7-6/h4,6H,3H2,1-2H3



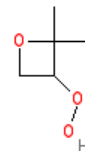
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InChI=1S/C5H10O3/c1-5(4-8-6)2-3-7-5/h6H,2-4H2,1H3



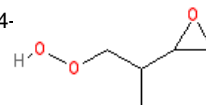
C5H9OB-DOOH-C C5H10O3 CC1(C)C(CO1)OO

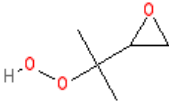
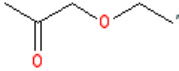
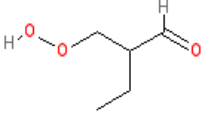
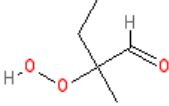
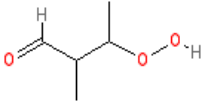
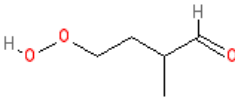
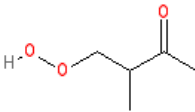
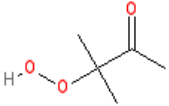
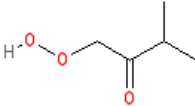
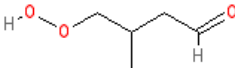
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C5H9OC-DOOH-A C5H10O3 CC(COO)C1CO1


InChI=1S/C5H10O3/c1-4(2-8-6)5-3-7-5/h4-6H,2-3H2,1H3

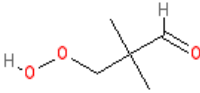
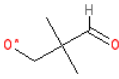


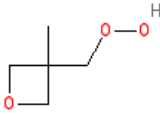










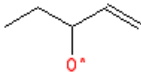
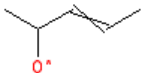
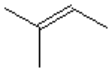
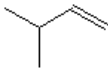
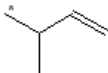
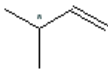
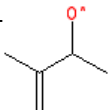
C5H9OC-DOOH-B	C5H10O3	CC(C)(C1CO1)OO	InChI=1S/C5H10O3/c1-5(2,8-6)4-3-7-4/h4,6H,3H2,1-2H3	
CH3COCH2OCH2CH2	C5H9O2	[CH2]COCC(C)=O	InChI=1S/C5H9O2/c1-3-7-4-5(2)6/h1,3-4H2,2H3	
IC5KETAA	C5H10O3	CCC(C=O)COO	InChI=1S/C5H10O3/c1-2-5(3-6)4-8-7/h3,5,7H,2,4H2,1H3	
IC5KETAB	C5H10O3	CCC(C)(C=O)OO	InChI=1S/C5H10O3/c1-3-5(2,4-6)8-7/h4,7H,3H2,1-2H3	
IC5KETAC	C5H10O3	CC(C=O)C(C)OO	InChI=1S/C5H10O3/c1-4(3-6)5(2)8-7/h3-5,7H,1-2H3	
IC5KETAD	C5H10O3	CC(CCOO)C=O	InChI=1S/C5H10O3/c1-5(4-6)2-3-8-7/h4-5,7H,2-3H2,1H3	
IC5KETCA	C5H10O3	CC(COO)C(C)=O	InChI=1S/C5H10O3/c1-4(3-8-7)5(2)6/h4,7H,3H2,1-2H3	
IC5KETCB	C5H10O3	CC(C(C)(C)OO)=O	InChI=1S/C5H10O3/c1-4(6)5(2,3)8-7/h7H,1-3H3	
IC5KETCD	C5H10O3	CC(C)C(COO)=O	InChI=1S/C5H10O3/c1-4(2)5(6)3-8-7/h4,7H,3H2,1-2H3	
IC5KETDA	C5H10O3	CC(CC=O)COO	InChI=1S/C5H10O3/c1-5(2-3-6)4-8-7/h3,5,7H,2,4H2,1H3	

IC5KETDB	C5H10O3	CC(C)(CC=O)OO	InChI=1S/C5H10O3/c1-5(2,8-7)3-4-6/h4,7H,3H2,1-2H3	
IC5KETDC	C5H10O3	CC(C)C(C=O)OO	InChI=1S/C5H10O3/c1-4(2)5(3-6)8-7/h3-5,7H,1-2H3	
IC5KETAAO	C5H9O2	CCC(C=O)C[O]	InChI=1S/C5H9O2/c1-2-5(3-6)4-7/h3,5H,2,4H2,1H3	
IC5KETABO	C5H9O2	CCC(C)(C=O)[O]	InChI=1S/C5H9O2/c1-3-5(2,7)4-6/h4H,3H2,1-2H3	
IC5KETACO	C5H9O2	CC(C=O)C(C)[O]	InChI=1S/C5H9O2/c1-4(3-6)5(2)7/h3-5H,1-2H3	
IC5KETADO	C5H9O2	CC(CC[O])C=O	InChI=1S/C5H9O2/c1-5(4-7)2-3-6/h4-5H,2-3H2,1H3	
IC5KETCAO	C5H9O2	CC(C[O])C(C)=O	InChI=1S/C5H9O2/c1-4(3-6)5(2)7/h4H,3H2,1-2H3	
IC5KETCBO	C5H9O2	CC(C(C)(C)[O])=O	InChI=1S/C5H9O2/c1-4(6)5(2,3)7/h1-3H3	
IC5KETCDO	C5H9O2	CC(C)C(C[O])=O	InChI=1S/C5H9O2/c1-4(2)5(7)3-6/h4H,3H2,1-2H3	
IC5KETDAO	C5H9O2	CC(CC=O)C[O]	InChI=1S/C5H9O2/c1-5(4-7)2-3-6/h3,5H,2,4H2,1H3	

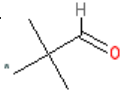
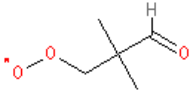
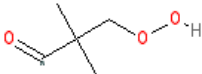
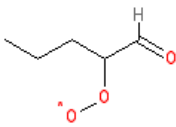
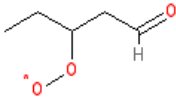
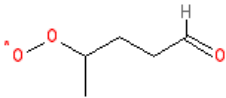
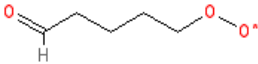

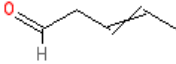
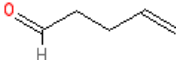
IC5KETDBO	C5H9O2	CC(C)(CC=O)[O]	InChI=1S/C5H9O2/c1-5(2,7)3-4-6/h4H,3H2,1-2H3	
IC5KETDCO	C5H9O2	CC(C)C(C=O)[O]	InChI=1S/C5H9O2/c1-4(2)5(7)3-6/h3-5H,1-2H3	
AC5H10OH	C5H11O	CCCCO	InChI=1S/C5H11O/c1-3-5(2)4-6/h6H,3-4H2,1-2H3	
BC5H10OH	C5H11O	C[CH]C(C)(C)O	InChI=1S/C5H11O/c1-4-5(2,3)6/h4,6H,1-3H3	
CC5H10OH	C5H11O	CC(C)C([CH2])O	InChI=1S/C5H11O/c1-4(2)5(3)6/h4-6H,3H2,1-2H3	
AO2C5H10OH	C5H11O3	CCC(C)(CO)O[O]	InChI=1S/C5H11O3/c1-3-5(2,4-6)8-7/h6H,3-4H2,1-2H3	
BO2C5H10OH	C5H11O3	CC(C(C)(C)O)O[O]	InChI=1S/C5H11O3/c1-4(8-7)5(2,3)6/h4,6H,1-3H3	
CO2C5H10OH	C5H11O3	CC(C)C(CO[O])O	InChI=1S/C5H11O3/c1-4(2)5(6)3-8-7/h4-6H,3H2,1-2H3	
IC3H5COCH3	C5H8O	C=C(C)C(C)=O	InChI=1S/C5H8O/c1-4(2)5(3)6/h1H2,2-3H3	
IC3H5COCH2	C5H7O	C=C(C)C(=C)[O]	InChI=1S/C5H7O/c1-4(2)5(3)6/h1,3H2,2H3	

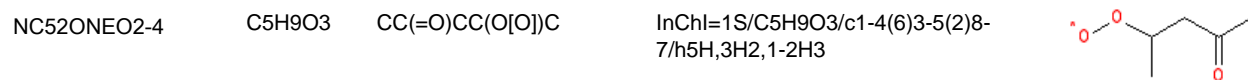
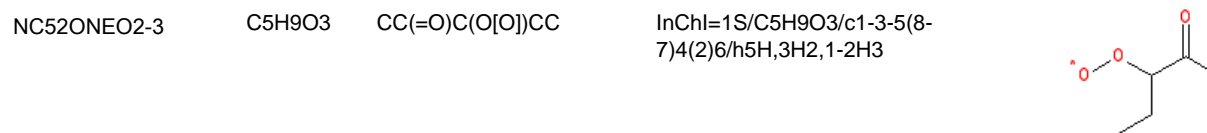
AC3H4COCH3	C5H7O	<chem>C=C([CH2])C(C)=O</chem>	InChI=1S/C5H7O/c1-4(2)5(3)6/h1-2H2,3H3	
NEOC5H12	C5H12	<chem>CC(C)(C)C</chem>	InChI=1S/C5H12/c1-5(2,3)4/h1-4H3	
NEOC5H11	C5H11	<chem>[CH2]C(C)(C)C</chem>	InChI=1S/C5H11/c1-5(2,3)4/h1H2,2-4H3	
NEOC5H11O2H	C5H12O2	<chem>CC(C)(C)COO</chem>	InChI=1S/C5H12O2/c1-5(2,3)4-7-6/h6H,4H2,1-3H3	
NEOC5H11O2	C5H11O2	<chem>CC(C)(C)CO[O]</chem>	InChI=1S/C5H11O2/c1-5(2,3)4-7-6/h4H2,1-3H3	
NEOC5H11O	C5H11O	<chem>CC(C)(C)C[O]</chem>	InChI=1S/C5H11O/c1-5(2,3)4-6/h4H2,1-3H3	
NEOC5H10OOH	C5H11O2	<chem>[CH2]C(C)(C)COO</chem>	InChI=1S/C5H11O2/c1-5(2,3)4-7-6/h6H,1,4H2,2-3H3	
NEO-C5H10O	C5H10O	<chem>CC1(C)COC1</chem>	InChI=1S/C5H10O/c1-5(2)3-6-4-5/h3-4H2,1-2H3	
NEOC5H10OOH-O2	C5H11O4	<chem>CC(C)(COO)CO[O]</chem>	InChI=1S/C5H11O4/c1-5(2,3-8-6)4-9-7/h6H,3-4H2,1-2H3	
NEOC5H9Q2	C5H11O4	<chem>[CH2]C(C)(COO)COO</chem>	InChI=1S/C5H11O4/c1-5(2,3-8-6)4-9-7/h6-7H,1,3-4H2,2H3	

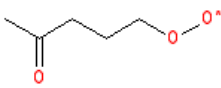
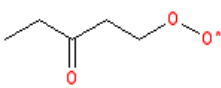
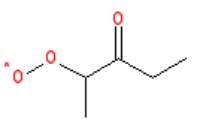
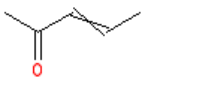
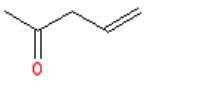
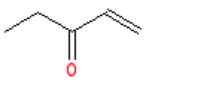




NEOC5KET	C5H10O3	<chem>CC(C)(C=O)COO</chem>	InChI=1S/C5H10O3/c1-5(2,3-6)4-7/h3,7H,4H2,1-2H3	
NEOC5KETOX	C5H9O2	<chem>CC(C)(C=O)C[O]</chem>	InChI=1S/C5H9O2/c1-5(2,3-6)4-7/h3H,4H2,1-2H3	
NEOC5KEJOL	C5H9O2	<chem>CC(C)(CO)[C]=O</chem>	InChI=1S/C5H9O2/c1-5(2,3-6)4-7/h6H,3H2,1-2H3	
IC4H6Q2-II	C4H8O4	<chem>C=C(COO)COO</chem>	InChI=1S/C4H8O4/c1-4(2-7-5)3-8-6/h5-6H,1-3H2	
NEOC5H9O-OOH	C5H10O3	<chem>CC1(COC1)COO</chem>	InChI=1S/C5H10O3/c1-5(4-8-6)2-7-3-5/h6H,2-4H2,1H3	
C5H10-1	C5H10	<chem>C=CCCC</chem>	InChI=1S/C5H10/c1-3-5-4-2/h3H,1,4-5H2,2H3	
C5H10-2	C5H10	<chem>CC=CCC</chem>	InChI=1S/C5H10/c1-3-5-4-2/h3,5H,4H2,1-2H3	
C5H81-3	C5H8	<chem>C=CC=CC</chem>	InChI=1S/C5H8/c1-3-5-4-2/h3-5H,1H2,2H3	
C5H91-3	C5H9	<chem>C=C[CH]CC</chem>	InChI=1S/C5H9/c1-3-5-4-2/h3,5H,1,4H2,2H3	
C5H91-4	C5H9	<chem>C=CC[CH]C</chem>	InChI=1S/C5H9/c1-3-5-4-2/h3-4H,1,5H2,2H3	

C5H91-5	C5H9	C=CCC[CH2]	InChI=1S/C5H9/c1-3-5-4-2/h3H,1-2,4-5H2	
C5H92-4	C5H9	CC=C[CH]C	InChI=1S/C5H9/c1-3-5-4-2/h3-5H,1-2H3	
C5H92-5	C5H9	[CH2]CC=CC	InChI=1S/C5H9/c1-3-5-4-2/h4-5H,1,3H2,2H3	
C5H9O1-3	C5H9O	C=CC(CC)[O]	InChI=1S/C5H9O/c1-3-5(6)4-2/h3,5H,1,4H2,2H3	
C5H9O2-4	C5H9O	CC=CC(C)[O]	InChI=1S/C5H9O/c1-3-4-5(2)6/h3-5H,1-2H3	
BC5H10	C5H10	CC=C(C)C	InChI=1S/C5H10/c1-4-5(2)3/h4H,1-3H3	
CC5H10	C5H10	C=CC(C)C	InChI=1S/C5H10/c1-4-5(2)3/h4-5H,1H2,2-3H3	
CC5H9-A	C5H9	C=CC([CH2])C	InChI=1S/C5H9/c1-4-5(2)3/h4-5H,1-2H2,3H3	
CC5H9-B	C5H9	C=CCC	InChI=1S/C5H9/c1-4-5(2)3/h4H,1H2,2-3H3	
AC5H9O-C	C5H9O	C=C(C)C(C)[O]	InChI=1S/C5H9O/c1-4(2)5(3)6/h5H,1H2,2-3H3	

CC5H9O-B	C5H9O	<chem>C=CC(C)(C)[O]</chem>	InChI=1S/C5H9O/c1-4-5(2,3)6/h4H,1H2,2-3H3	
AC5H10	C5H10	<chem>CCC(=C)C</chem>	InChI=1S/C5H10/c1-4-5(2)3/h2,4H2,1,3H3	
AC5H9-A2	C5H9	<chem>CCC(=C)[CH2]</chem>	InChI=1S/C5H9/c1-4-5(2)3/h2-4H2,1H3	
AC5H9-C	C5H9	<chem>C[CH]C(=C)C</chem>	InChI=1S/C5H9/c1-4-5(2)3/h4H,2H2,1,3H3	
AC5H9-D	C5H9	<chem>[CH2]CC(=C)C</chem>	InChI=1S/C5H9/c1-4-5(2)3/h1-2,4H2,3H3	
B2E2M1OJ	C5H9O	<chem>CC=C(C)C[O]</chem>	InChI=1S/C5H9O/c1-3-5(2)4-6/h3H,4H2,1-2H3	
B13DE2M	C5H8	<chem>C=CC(=C)C</chem>	InChI=1S/C5H8/c1-4-5(2)3/h4H,1-2H2,3H3	
B13DE2MJ	C5H7	<chem>C=CC(=C)[CH2]</chem>	InChI=1S/C5H7/c1-4-5(2)3/h4H,1-3H2	
B12DE3M	C5H8	<chem>[CH2]=[C]=CC</chem>	InChI=1S/C5H8/c1-4-5(2)3/h1H2,2-3H3	
B2E3M1OJ	C5H9O	<chem>CC(C)=CC[O]</chem>	InChI=1S/C5H9O/c1-5(2)3-4-6/h3H,4H2,1-2H3	

TC4H8CHO	C5H9O	[CH2]C(C)(C)C=O	InChI=1S/C5H9O/c1-5(2,3)4-6/h4H,1H2,2-3H3	
O2C4H8CHO	C5H9O3	CC(C)(C=O)CO[O]	InChI=1S/C5H9O3/c1-5(2,3-6)4-8-7/h3H,4H2,1-2H3	
O2HC4H8CO	C5H9O3	CC(C)([C]=O)COO	InChI=1S/C5H9O3/c1-5(2,3-6)4-8-7/h7H,4H2,1-2H3	
PC4H8CHO-1O2	C5H9O3	CCCC(O[O])C(=O)	InChI=1S/C5H9O3/c1-2-3-5(4-6)8-7/h4-5H,2-3H2,1H3	
PC4H8CHO-2O2	C5H9O3	CCC(O[O])CC(=O)	InChI=1S/C5H9O3/c1-2-5(8-7)3-4-6/h4-5H,2-3H2,1H3	
PC4H8CHO-3O2	C5H9O3	CC(O[O])CCC(=O)	InChI=1S/C5H9O3/c1-5(8-7)3-2-4-6/h4-5H,2-3H2,1H3	
PC4H8CHO-4O2	C5H9O3	C(O[O])CCCC(=O)	InChI=1S/C5H9O3/c6-4-2-1-3-5-8-7/h4H,1-3,5H2	
C4H7CHO-2	C5H8O	CCC=CC(=O)	InChI=1S/C5H8O/c1-2-3-4-5-6/h3-5H,2H2,1H3	
C4H7CHO-3	C5H8O	CC=CCC(=O)	InChI=1S/C5H8O/c1-2-3-4-5-6/h2-3,5H,4H2,1H3	
C4H7CHO-4	C5H8O	C=CCCC(=O)	InChI=1S/C5H8O/c1-2-3-4-5-6/h2,5H,1,3-4H2	



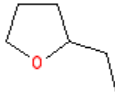
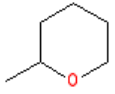
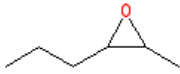
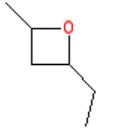
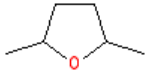
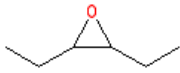
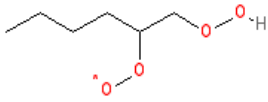
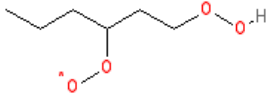
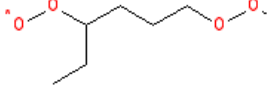
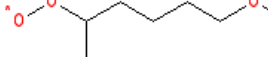
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NC53ONEO2-1	C5H9O3	C(O[O])CC(=O)CC	InChI=1S/C5H9O3/c1-2-5(6)3-4-8-7/h2-4H2,1H3	
NC53ONEO2-2	C5H9O3	CC(O[O])C(=O)CC	InChI=1S/C5H9O3/c1-3-5(6)4(2)8-7/h4H,3H2,1-2H3	
NC52ONE-3	C5H8O	CC(=O)C=CC	InChI=1S/C5H8O/c1-3-4-5(2)6/h3-4H,1-2H3	
NC52ONE-4	C5H8O	CC(=O)CC=C	InChI=1S/C5H8O/c1-3-4-5(2)6/h3H,1,4H2,2H3	
NC53ONE-1	C5H8O	C=CC(=O)CC	InChI=1S/C5H8O/c1-3-5(6)4-2/h3H,1,4H2,2H3	
NC5H11OH	C5H12O	CCCCC(O)	InChI=1S/C5H12O/c1-2-3-4-5-6/h6H,2-5H2,1H3	
C5H10OH11	C5H11O	CCCC[CH](O)	InChI=1S/C5H11O/c1-2-3-4-5-6/h5-6H,2-4H2,1H3	
C5H10OH12	C5H11O	CCC[CH]CO	InChI=1S/C5H11O/c1-2-3-4-5-6/h4,6H,2-3,5H2,1H3	
C5H10OH13	C5H11O	CC[CH]CC(O)	InChI=1S/C5H11O/c1-2-3-4-5-6/h3,6H,2,4H2,1H3	

C5H10OH14	C5H11O	C[CH]CCC(O)	InChI=1S/C5H11O/c1-2-3-4-5-6/h2,6H,3-5H2,1H3	
C5H10OH15	C5H11O	[CH2]CCCC(O)	InChI=1S/C5H11O/c1-2-3-4-5-6/h6H,1-5H2	
C5H10OH-1O2	C5H11O3	CCCCC(O)(O[O])	InChI=1S/C5H11O3/c1-2-3-4-5(6)8-7/h5-6H,2-4H2,1H3	
C5H10OH-2O2	C5H11O3	CCCC(O[O])C(O)	InChI=1S/C5H11O3/c1-2-3-5(4-6)8-7/h5-6H,2-4H2,1H3	
C5H10OH-3O2	C5H11O3	CCC(O[O])CC(O)	InChI=1S/C5H11O3/c1-2-5(8-7)3-4-6/h5-6H,2-4H2,1H3	
C5H10OH-4O2	C5H11O3	CC(O[O])CCC(O)	InChI=1S/C5H11O3/c1-5(8-7)3-2-4-6/h5-6H,2-4H2,1H3	
C5H10OH-5O2	C5H11O3	C(O[O])CCCC(O)	InChI=1S/C5H11O3/c6-4-2-1-3-5-8-7/h6H,1-5H2	
C5H9OH1-1	C5H10O	CCCC=C(O)	InChI=1S/C5H10O/c1-2-3-4-5-6/h4-6H,2-3H2,1H3	
C5H9OH1-2	C5H10O	CCC=CC(O)	InChI=1S/C5H10O/c1-2-3-4-5-6/h3-4,6H,2,5H2,1H3	
C5H9OH1-3	C5H10O	CC=CCC(O)	InChI=1S/C5H10O/c1-2-3-4-5-6/h2-3,6H,4-5H2,1H3	

C5H9OH1-4	C5H10O	C=CCCC(O)	InChI=1S/C5H10O/c1-2-3-4-5/h2,6H,1,3-5H2	
NC6H14	C6H14	CCCCCC	InChI=1S/C6H14/c1-3-5-6-4-2/h3-6H2,1-2H3	
C6H13-1	C6H13	[CH2]CCCCC	InChI=1S/C6H13/c1-3-5-6-4-2/h1,3-6H2,2H3	
C6H13-2	C6H13	C[CH]CCCC	InChI=1S/C6H13/c1-3-5-6-4-2/h3H,4-6H2,1-2H3	
C6H13-3	C6H13	CC[CH]CCC	InChI=1S/C6H13/c1-3-5-6-4-2/h5H,3-4,6H2,1-2H3	
C6H13OOH-1	C6H14O2	C(OO)CCCCC	InChI=1S/C6H14O2/c1-2-3-4-5-6-7/h7H,2-6H2,1H3	
C6H13OOH-2	C6H14O2	CC(OO)CCCC	InChI=1S/C6H14O2/c1-3-4-5-6(2)8-7/h6-7H,3-5H2,1-2H3	
C6H13OOH-3	C6H14O2	CCC(OO)CCC	InChI=1S/C6H14O2/c1-3-5-6(4-2)8-7/h6-7H,3-5H2,1-2H3	
C6H13O2-1	C6H13O2	C(O[O])CCCCC	InChI=1S/C6H13O2/c1-2-3-4-5-6-8-7/h2-6H2,1H3	
C6H13O2-2	C6H13O2	CC(O[O])CCCC	InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h6H,3-5H2,1-2H3	

C6H13O2-3	C6H13O2	CCC(O[O])CCC	InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h6H,3-5H2,1-2H3	
C6H13O-1	C6H13O	C([O])CCCCC	InChI=1S/C6H13O/c1-2-3-4-5-6-7/h2-6H2,1H3	
C6H13O-2	C6H13O	CC([O])CCCC	InChI=1S/C6H13O/c1-3-4-5-6(2)7/h6H,3-5H2,1-2H3	
C6H13O-3	C6H13O	CCC([O])CCC	InChI=1S/C6H13O/c1-3-5-6(7)4-2/h6H,3-5H2,1-2H3	
C6H12OOH1-2	C6H13O2	C(OO)[CH]CCCC	InChI=1S/C6H13O2/c1-2-3-4-5-6-8-7/h5,7H,2-4,6H2,1H3	
C6H12OOH1-3	C6H13O2	C(OO)C[CH]CCC	InChI=1S/C6H13O2/c1-2-3-4-5-6-8-7/h4,7H,2-3,5-6H2,1H3	
C6H12OOH1-4	C6H13O2	C(OO)CC[CH]CC	InChI=1S/C6H13O2/c1-2-3-4-5-6-8-7/h3,7H,2,4-6H2,1H3	
C6H12OOH1-5	C6H13O2	C(OO)CCC[CH]C	InChI=1S/C6H13O2/c1-2-3-4-5-6-8-7/h2,7H,3-6H2,1H3	
C6H12OOH2-1	C6H13O2	[CH2]C(OO)CCCC	InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h6-7H,2-5H2,1H3	
C6H12OOH2-3	C6H13O2	CC(OO)[CH]CCC	InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h5-7H,3-4H2,1-2H3	

C6H12OOH2-4	C6H13O2	CC(OO)C[CH]CC	InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h4,6-7H,3,5H2,1-2H3	
C6H12OOH2-5	C6H13O2	CC(OO)CC[CH]C	InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h3,6-7H,4-5H2,1-2H3	
C6H12OOH2-6	C6H13O2	CC(OO)CCC[CH2]	InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h6-7H,1,3-5H2,2H3	
C6H12OOH3-1	C6H13O2	[CH2]CC(OO)CCC	InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h6-7H,2-5H2,1H3	
C6H12OOH3-2	C6H13O2	C[CH]C(OO)CCC	InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h4,6-7H,3,5H2,1-2H3	
C6H12OOH3-4	C6H13O2	CCC(OO)[CH]CC	InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h5-7H,3-4H2,1-2H3	
C6H12OOH3-5	C6H13O2	CCC(OO)C[CH]C	InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h3,6-7H,4-5H2,1-2H3	
C6H12OOH3-6	C6H13O2	CCC(OO)CC[CH2]	InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h6-7H,1,3-5H2,2H3	
C6H12O1-2	C6H12O	C1C(O1)CCCC	InChI=1S/C6H12O/c1-2-3-4-6-5-7-6/h6H,2-5H2,1H3	
C6H12O1-3	C6H12O	C1CC(O1)CCC	InChI=1S/C6H12O/c1-2-3-6-4-5-7-6/h6H,2-5H2,1H3	

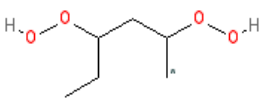
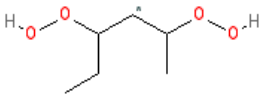
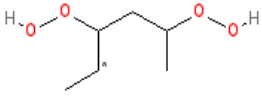
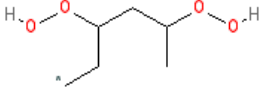
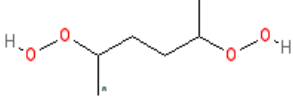
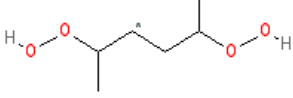
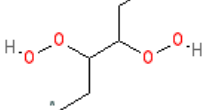
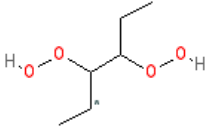
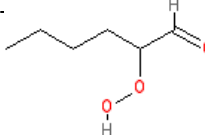
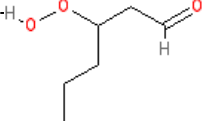
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C6H12O1-5	C6H12O	C1CCCC(O1)C	InChI=1S/C6H12O/c1-6-4-2-3-5-7-6/h6H,2-5H2,1H3	
C6H12O2-3	C6H12O	CC1C(O1)CCC	InChI=1S/C6H12O/c1-3-4-6-5(2)7-6/h5-6H,3-4H2,1-2H3	
C6H12O2-4	C6H12O	CC1CC(O1)CC	InChI=1S/C6H12O/c1-3-6-4-5(2)7-6/h5-6H,3-4H2,1-2H3	
C6H12O2-5	C6H12O	CC1CCC(O1)C	InChI=1S/C6H12O/c1-5-3-4-6(2)7-5/h5-6H,3-4H2,1-2H3	
C6H12O3-4	C6H12O	CCC1C(O1)CC	InChI=1S/C6H12O/c1-3-5-6(4-2)7-5/h5-6H,3-4H2,1-2H3	
C6H12OOH1-2O2	C6H13O4	C(OO)C(O[O])CCCC	InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h6-7H,2-5H2,1H3	
C6H12OOH1-3O2	C6H13O4	C(OO)CC(O[O])CCC	InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h6-7H,2-5H2,1H3	
C6H12OOH1-4O2	C6H13O4	C(OO)CCC(O[O])CC	InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h6-7H,2-5H2,1H3	
C6H12OOH1-5O2	C6H13O4	C(OO)CCCC(O[O])C	InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h6-7H,2-5H2,1H3	

C6H12OOH2-1O2	C6H13O4	C(O[O])C(OO)CCCC	InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h6,8H,2-5H2,1H3	
C6H12OOH2-3O2	C6H13O4	CC(OO)C(O[O])CCC	InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h5-7H,3-4H2,1-2H3	
C6H12OOH2-4O2	C6H13O4	CC(OO)CC(O[O])CC	InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h5-7H,3-4H2,1-2H3	
C6H12OOH2-5O2	C6H13O4	CC(OO)CCC(O[O])C	InChI=1S/C6H13O4/c1-5(9-7)3-4-6(2)10-8/h5-7H,3-4H2,1-2H3	
C6H12OOH2-6O2	C6H13O4	CC(OO)CCCC(O[O])	InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h6,8H,2-5H2,1H3	
C6H12OOH3-1O2	C6H13O4	C(O[O])CC(OO)CCC	InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h6,8H,2-5H2,1H3	
C6H12OOH3-2O2	C6H13O4	CC(O[O])C(OO)CCC	InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h5-6,8H,3-4H2,1-2H3	
C6H12OOH3-4O2	C6H13O4	CCC(OO)C(O[O])CC	InChI=1S/C6H13O4/c1-3-5(9-7)6(4-2)10-8/h5-7H,3-4H2,1-2H3	
C6H12OOH3-5O2	C6H13O4	CCC(OO)CC(O[O])C	InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h5-6,8H,3-4H2,1-2H3	
C6H12OOH3-6O2	C6H13O4	CCC(OO)CCC(O[O])	InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h6,8H,2-5H2,1H3	

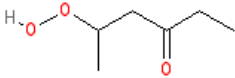
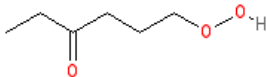

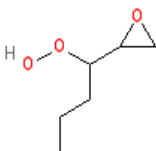
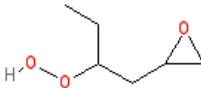
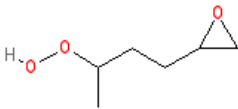

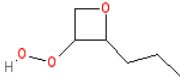
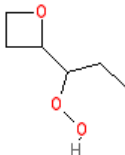
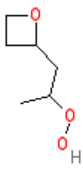
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C6H11-1D4OOH	C6H12O2	<chem>C=CCC(OO)CC</chem>	InChI=1S/C6H12O2/c1-3-5-6(4-2)8-7/h3,6-7H,1,4-5H2,2H3	
C6H11-1D5OOH	C6H12O2	<chem>C=CCCC(OO)C</chem>	InChI=1S/C6H12O2/c1-3-4-5-6(2)8-7/h3,6-7H,1,4-5H2,2H3	
C6H11-1D6OOH	C6H12O2	<chem>C=CCCCC(OO)</chem>	InChI=1S/C6H12O2/c1-2-3-4-5-6-8-7/h2,7H,1,3-6H2	
C6H11-2D1OOH	C6H12O2	<chem>C(OO)C=CCCC</chem>	InChI=1S/C6H12O2/c1-2-3-4-5-6-8-7/h4-5,7H,2-3,6H2,1H3	
C6H11-2D4OOH	C6H12O2	<chem>CC=CC(OO)CC</chem>	InChI=1S/C6H12O2/c1-3-5-6(4-2)8-7/h3,5-7H,4H2,1-2H3	
C6H11-2D5OOH	C6H12O2	<chem>CC=CCC(OO)C</chem>	InChI=1S/C6H12O2/c1-3-4-5-6(2)8-7/h3-4,6-7H,5H2,1-2H3	
C6H11-2D6OOH	C6H12O2	<chem>CC=CCCC(OO)</chem>	InChI=1S/C6H12O2/c1-2-3-4-5-6-8-7/h2-3,7H,4-6H2,1H3	
C6H11-3D1OOH	C6H12O2	<chem>C(OO)CC=CCC</chem>	InChI=1S/C6H12O2/c1-2-3-4-5-6-8-7/h3-4,7H,2,5-6H2,1H3	
C6H11-3D2OOH	C6H12O2	<chem>CC(OO)C=CCC</chem>	InChI=1S/C6H12O2/c1-3-4-5-6(2)8-7/h4-7H,3H2,1-2H3	

C6H11Q12-3	C6H13O4	<chem>C(OO)C(OO)[CH]CCC</chem>	InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h4,6-8H,2-3,5H2,1H3	
C6H11Q12-4	C6H13O4	<chem>C(OO)C(OO)C[CH]CC</chem>	InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h3,6-8H,2,4-5H2,1H3	
C6H11Q12-5	C6H13O4	<chem>C(OO)C(OO)CC[CH]C</chem>	InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h2,6-8H,3-5H2,1H3	
C6H11Q12-6	C6H13O4	<chem>C(OO)C(OO)CCC[CH2]</chem>	InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h6-8H,1-5H2	
C6H11Q13-2	C6H13O4	<chem>C(OO)[CH]C(OO)CCC</chem>	InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h4,6-8H,2-3,5H2,1H3	
C6H11Q13-4	C6H13O4	<chem>C(OO)CC(OO)[CH]CC</chem>	InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h3,6-8H,2,4-5H2,1H3	
C6H11Q13-5	C6H13O4	<chem>C(OO)CC(OO)C[CH]C</chem>	InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h2,6-8H,3-5H2,1H3	
C6H11Q13-6	C6H13O4	<chem>C(OO)CC(OO)CC[CH2]</chem>	InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h6-8H,1-5H2	
C6H11Q14-2	C6H13O4	<chem>C(OO)[CH]CC(OO)CC</chem>	InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h3,6-8H,2,4-5H2,1H3	
C6H11Q14-3	C6H13O4	<chem>C(OO)C[CH]C(OO)CC</chem>	InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h4,6-8H,2-3,5H2,1H3	

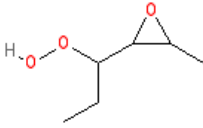
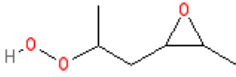
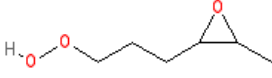
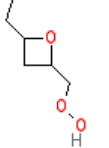
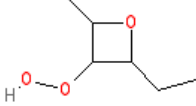
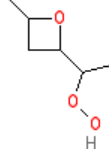

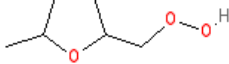
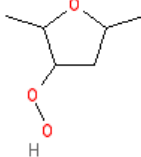

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C6H11Q14-6	C6H13O4	<chem>C(OO)CCC(OO)C[CH2]</chem>	InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h6-8H,1-5H2	
C6H11Q15-2	C6H13O4	<chem>C(OO)[CH]CCC(OO)C</chem>	InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h3,6-8H,2,4-5H2,1H3	
C6H11Q15-3	C6H13O4	<chem>C(OO)C[CH]CC(OO)C</chem>	InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h2,6-8H,3-5H2,1H3	
C6H11Q15-4	C6H13O4	<chem>C(OO)CC[CH]C(OO)C</chem>	InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h4,6-8H,2-3,5H2,1H3	
C6H11Q15-6	C6H13O4	<chem>C(OO)CCCC(OO)[CH2]</chem>	InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h6-8H,1-5H2	
C6H11Q23-1	C6H13O4	<chem>[CH2]C(OO)C(OO)CCC</chem>	InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h5-8H,2-4H2,1H3	
C6H11Q23-4	C6H13O4	<chem>CC(OO)C(OO)[CH]CC</chem>	InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h4-8H,3H2,1-2H3	
C6H11Q23-5	C6H13O4	<chem>CC(OO)C(OO)C[CH]C</chem>	InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h3,5-8H,4H2,1-2H3	
C6H11Q23-6	C6H13O4	<chem>CC(OO)C(OO)CC[CH2]</chem>	InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h5-8H,1,3-4H2,2H3	

C6H11Q24-1	C6H13O4	[CH2]C(OO)CC(OO)CC	InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h5-8H,2-4H2,1H3	
C6H11Q24-3	C6H13O4	CC(OO)[CH]C(OO)CC	InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h4-8H,3H2,1-2H3	
C6H11Q24-5	C6H13O4	CC(OO)CC(OO)[CH]C	InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h3,5-8H,4H2,1-2H3	
C6H11Q24-6	C6H13O4	CC(OO)CC(OO)C[CH2]	InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h5-8H,1,3-4H2,2H3	
C6H11Q25-1	C6H13O4	[CH2]C(OO)CCC(OO)C	InChI=1S/C6H13O4/c1-5(9-7)3-4-6(2)10-8/h5-8H,1,3-4H2,2H3	
C6H11Q25-3	C6H13O4	CC(OO)[CH]CC(OO)C	InChI=1S/C6H13O4/c1-5(9-7)3-4-6(2)10-8/h3,5-8H,4H2,1-2H3	
C6H11Q34-1	C6H13O4	[CH2]CC(OO)C(OO)CC	InChI=1S/C6H13O4/c1-3-5(9-7)6(4-2)10-8/h5-8H,1,3-4H2,2H3	
C6H11Q34-2	C6H13O4	C[CH]C(OO)C(OO)CC	InChI=1S/C6H13O4/c1-3-5(9-7)6(4-2)10-8/h3,5-8H,4H2,1-2H3	
C6KET12	C6H12O3	C(=O)C(OO)CCCC	InChI=1S/C6H12O3/c1-2-3-4-6(5-7)9-8/h5-6,8H,2-4H2,1H3	
C6KET13	C6H12O3	C(=O)CC(OO)CCC	InChI=1S/C6H12O3/c1-2-3-6(9-8)4-5-7/h5-6,8H,2-4H2,1H3	

C6KET14	C6H12O3	<chem>C(=O)CCC(OO)CC</chem>	InChI=1S/C6H12O3/c1-2-6(9-8)4-3-5-7/h5-6,8H,2-4H2,1H3	
C6KET15	C6H12O3	<chem>C(=O)CCCC(OO)C</chem>	InChI=1S/C6H12O3/c1-6(9-8)4-2-3-5-7/h5-6,8H,2-4H2,1H3	
C6KET21	C6H12O3	<chem>C(OO)C(=O)CCCC</chem>	InChI=1S/C6H12O3/c1-2-3-4-6(7)5-9-8/h8H,2-5H2,1H3	
C6KET23	C6H12O3	<chem>CC(=O)C(OO)CCC</chem>	InChI=1S/C6H12O3/c1-3-4-6(9-8)5(2)7/h6,8H,3-4H2,1-2H3	
C6KET24	C6H12O3	<chem>CC(=O)CC(OO)CC</chem>	InChI=1S/C6H12O3/c1-3-6(9-8)4-5(2)7/h6,8H,3-4H2,1-2H3	
C6KET25	C6H12O3	<chem>CC(=O)CCC(OO)C</chem>	InChI=1S/C6H12O3/c1-5(7)3-4-6(2)9-8/h6,8H,3-4H2,1-2H3	
C6KET26	C6H12O3	<chem>CC(=O)CCCC(OO)</chem>	InChI=1S/C6H12O3/c1-6(7)4-2-3-5-9-8/h8H,2-5H2,1H3	
C6KET31	C6H12O3	<chem>C(OO)CC(=O)CCC</chem>	InChI=1S/C6H12O3/c1-2-3-6(7)4-5-9-8/h8H,2-5H2,1H3	
C6KET32	C6H12O3	<chem>CC(OO)C(=O)CCC</chem>	InChI=1S/C6H12O3/c1-3-4-6(7)5(2)9-8/h5,8H,3-4H2,1-2H3	
C6KET34	C6H12O3	<chem>CCC(=O)C(OO)CC</chem>	InChI=1S/C6H12O3/c1-3-5(7)6(4-2)9-8/h6,8H,3-4H2,1-2H3	

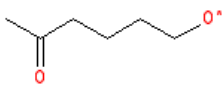
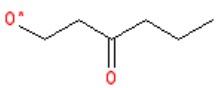
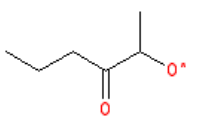
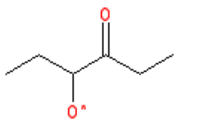
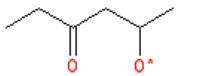
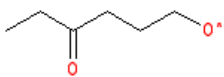
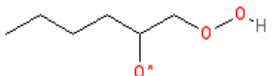
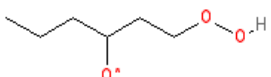
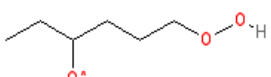
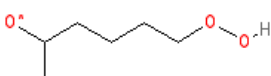
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C6KET36	C6H12O3	CCC(=O)CCC(OO)	InChI=1S/C6H12O3/c1-2-6(7)4-3-5-9-8/h8H,2-5H2,1H3	
C5H91-1	C5H9	CCCC=[CH]	InChI=1S/C5H9/c1-3-5-4-2/h1,3H,4-5H2,2H3	
C6H11O12-3OOH	C6H12O3	C1C(O1)C(OO)CCC	InChI=1S/C6H12O3/c1-2-3-5(9-7)6-4-8-6/h5-7H,2-4H2,1H3	
C6H11O12-4OOH	C6H12O3	C1C(O1)CC(OO)CC	InChI=1S/C6H12O3/c1-2-5(9-7)3-6-4-8-6/h5-7H,2-4H2,1H3	
C6H11O12-5OOH	C6H12O3	C1C(O1)CCC(OO)C	InChI=1S/C6H12O3/c1-5(9-7)2-3-6-4-8-6/h5-7H,2-4H2,1H3	
C6H11O12-6OOH	C6H12O3	C1C(O1)CCCC(OO)	InChI=1S/C6H12O3/c7-9-4-2-1-3-6-5-8-6/h6-7H,1-5H2	
C6H11O13-2OOH	C6H12O3	C1C(OO)C(O1)CCC	InChI=1S/C6H12O3/c1-2-3-5-6(9-7)4-8-5/h5-7H,2-4H2,1H3	
C6H11O13-4OOH	C6H12O3	C1CC(O1)C(OO)CC	InChI=1S/C6H12O3/c1-2-5(9-7)6-3-4-8-6/h5-7H,2-4H2,1H3	
C6H11O13-5OOH	C6H12O3	C1CC(O1)CC(OO)C	InChI=1S/C6H12O3/c1-5(9-7)4-6-2-3-8-6/h5-7H,2-4H2,1H3	

C6H11O13-6OOH	C6H12O3	C1CC(O1)CCC(OO)	InChI=1S/C6H12O3/c7-9-4-1-2-6-3-5-8-6/h6-7H,1-5H2	
C6H11O14-2OOH	C6H12O3	C1C(OO)CC(O1)CC	InChI=1S/C6H12O3/c1-2-5-3-6(9-7)4-8-5/h5-7H,2-4H2,1H3	
C6H11O14-3OOH	C6H12O3	C1CC(OO)C(O1)CC	InChI=1S/C6H12O3/c1-2-5-6(9-7)3-4-8-5/h5-7H,2-4H2,1H3	
C6H11O14-5OOH	C6H12O3	C1CCC(O1)C(OO)C	InChI=1S/C6H12O3/c1-5(9-7)6-3-2-4-8-6/h5-7H,2-4H2,1H3	
C6H11O14-6OOH	C6H12O3	C1CCC(O1)CC(OO)	InChI=1S/C6H12O3/c7-9-5-3-6-2-1-4-8-6/h6-7H,1-5H2	
C6H11O15-2OOH	C6H12O3	C1C(OO)CCC(O1)C	InChI=1S/C6H12O3/c1-5-2-3-6(9-7)4-8-5/h5-7H,2-4H2,1H3	
C6H11O15-3OOH	C6H12O3	C1CC(OO)CC(O1)C	InChI=1S/C6H12O3/c1-5-4-6(9-7)2-3-8-5/h5-7H,2-4H2,1H3	
C6H11O15-4OOH	C6H12O3	C1CCC(OO)C(O1)C	InChI=1S/C6H12O3/c1-5-6(9-7)3-2-4-8-5/h5-7H,2-4H2,1H3	
C6H11O15-6OOH	C6H12O3	C1CCCC(O1)C(OO)	InChI=1S/C6H12O3/c7-9-5-6-3-1-2-4-8-6/h6-7H,1-5H2	
C6H11O23-1OOH	C6H12O3	C(OO)C1C(O1)CCC	InChI=1S/C6H12O3/c1-2-3-5-6(9-5)4-8-7/h5-7H,2-4H2,1H3	


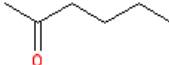

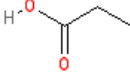






C6H11O23-4OOH	C6H12O3	CC1C(O1)C(OO)CC	InChI=1S/C6H12O3/c1-3-5(9-7)6-4(2)8-6/h4-7H,3H2,1-2H3	
C6H11O23-5OOH	C6H12O3	CC1C(O1)CC(OO)C	InChI=1S/C6H12O3/c1-4(9-7)3-6-5(2)8-6/h4-7H,3H2,1-2H3	
C6H11O23-6OOH	C6H12O3	CC1C(O1)CCC(OO)	InChI=1S/C6H12O3/c1-5-6(9-5)3-2-4-8-7/h5-7H,2-4H2,1H3	
C6H11O24-1OOH	C6H12O3	C(OO)C1CC(O1)CC	InChI=1S/C6H12O3/c1-2-5-3-6(9-5)4-8-7/h5-7H,2-4H2,1H3	
C6H11O24-3OOH	C6H12O3	CC1C(OO)C(O1)CC	InChI=1S/C6H12O3/c1-3-5-6(9-7)4(2)8-5/h4-7H,3H2,1-2H3	
C6H11O24-5OOH	C6H12O3	CC1CC(O1)C(OO)C	InChI=1S/C6H12O3/c1-4-3-6(8-4)5(2)9-7/h4-7H,3H2,1-2H3	
C6H11O24-6OOH	C6H12O3	CC1CC(O1)CC(OO)	InChI=1S/C6H12O3/c1-5-4-6(9-5)2-3-8-7/h5-7H,2-4H2,1H3	
C6H11O25-1OOH	C6H12O3	C(OO)C1CCC(O1)C	InChI=1S/C6H12O3/c1-5-2-3-6(9-5)4-8-7/h5-7H,2-4H2,1H3	
C6H11O25-3OOH	C6H12O3	CC1C(OO)CC(O1)C	InChI=1S/C6H12O3/c1-4-3-6(9-7)5(2)8-4/h4-7H,3H2,1-2H3	
C6H11O34-1OOH	C6H12O3	C(OO)CC1C(O1)CC	InChI=1S/C6H12O3/c1-2-5-6(9-5)3-4-8-7/h5-7H,2-4H2,1H3	

C6H11O34-2OOH	C6H12O3	CC(OO)C1C(O1)CC	InChI=1S/C6H12O3/c1-3-5-6(8-5)4(2)9-7/h4-7H,3H2,1-2H3	
C4H7O12-4	C4H7O	C1C(O1)C[CH2]	InChI=1S/C4H7O/c1-2-4-3-5-4/h4H,1-3H2	
C4H7O13-4	C4H7O	C1CC(O1)[CH2]	InChI=1S/C4H7O/c1-4-2-3-5-4/h4H,1-3H2	
C4H7O23-1	C4H7O	CC1C(O1)[CH2]	InChI=1S/C4H7O/c1-3-4(2)5-3/h3-4H,1H2,2H3	
C5H9O12-5	C5H9O	C1C(O1)CC[CH2]	InChI=1S/C5H9O/c1-2-3-5-4-6-5/h5H,1-4H2	
C5H9O13-5	C5H9O	C1CC(O1)C[CH2]	InChI=1S/C5H9O/c1-2-5-3-4-6-5/h5H,1-4H2	
C5H9O14-5	C5H9O	C1CCC(O1)[CH2]	InChI=1S/C5H9O/c1-5-3-2-4-6-5/h5H,1-4H2	
C5H9O23-1	C5H9O	CCC1C(O1)[CH2]	InChI=1S/C5H9O/c1-3-5-4(2)6-5/h4-5H,2-3H2,1H3	
C5H9O23-5	C5H9O	[CH2]CC1C(O1)C	InChI=1S/C5H9O/c1-3-5-4(2)6-5/h4-5H,1,3H2,2H3	
C5H9O24-1	C5H9O	[CH2]C1CC(O1)C	InChI=1S/C5H9O/c1-4-3-5(2)6-4/h4-5H,1,3H2,2H3	

AC3H5CHO	C4H6O	C=CCC=O	InChI=1S/C4H6O/c1-2-3-4-5/h2,4H,1,3H2	
PC4H9CO	C5H9O	CCCC[C]=O	InChI=1S/C5H9O/c1-2-3-4-5-6/h2-4H2,1H3	
C6KET12O	C6H11O2	C(=O)C([O])CCCC	InChI=1S/C6H11O2/c1-2-3-4-6(8)5-7/h5-6H,2-4H2,1H3	
C6KET13O	C6H11O2	C(=O)CC([O])CCC	InChI=1S/C6H11O2/c1-2-3-6(8)4-5-7/h5-6H,2-4H2,1H3	
C6KET14O	C6H11O2	C(=O)CCC([O])CC	InChI=1S/C6H11O2/c1-2-6(8)4-3-5-7/h5-6H,2-4H2,1H3	
C6KET15O	C6H11O2	C(=O)CCCC([O])C	InChI=1S/C6H11O2/c1-6(8)4-2-3-5-7/h5-6H,2-4H2,1H3	
C6KET21O	C6H11O2	C([O])C(=O)CCCC	InChI=1S/C6H11O2/c1-2-3-4-6(8)5-7/h2-5H2,1H3	
C6KET23O	C6H11O2	CC(=O)C([O])CCC	InChI=1S/C6H11O2/c1-3-4-6(8)5(2)7/h6H,3-4H2,1-2H3	
C6KET24O	C6H11O2	CC(=O)CC([O])CC	InChI=1S/C6H11O2/c1-3-6(8)4-5(2)7/h6H,3-4H2,1-2H3	
C6KET25O	C6H11O2	CC(=O)CCC([O])C	InChI=1S/C6H11O2/c1-5(7)3-4-6(2)8/h5H,3-4H2,1-2H3	

C6KET26O	C6H11O2	CC(=O)CCCC([O])	InChI=1S/C6H11O2/c1-6(8)4-2-3-5-7/h2-5H2,1H3	
C6KET31O	C6H11O2	CCCC(=O)CC([O])	InChI=1S/C6H11O2/c1-2-3-6(8)4-5-7/h2-5H2,1H3	
C6KET32O	C6H11O2	CCCC(=O)C([O])C	InChI=1S/C6H11O2/c1-3-4-6(8)5(2)7/h5H,3-4H2,1-2H3	
C6KET34O	C6H11O2	CCC([O])C(=O)CC	InChI=1S/C6H11O2/c1-3-5(7)6(8)4-2/h5H,3-4H2,1-2H3	
C6KET35O	C6H11O2	CC([O])CC(=O)CC	InChI=1S/C6H11O2/c1-3-6(8)4-5(2)7/h5H,3-4H2,1-2H3	
C6KET36O	C6H11O2	C([O])CCC(=O)CC	InChI=1S/C6H11O2/c1-2-6(8)4-3-5-7/h2-5H2,1H3	
C6H12OOH1-2O	C6H13O3	C(OO)C([O])CCCC	InChI=1S/C6H13O3/c1-2-3-4-6(7)5-9-8/h6,8H,2-5H2,1H3	
C6H12OOH1-3O	C6H13O3	C(OO)CC([O])CCC	InChI=1S/C6H13O3/c1-2-3-6(7)4-5-9-8/h6,8H,2-5H2,1H3	
C6H12OOH1-4O	C6H13O3	C(OO)CCC([O])CC	InChI=1S/C6H13O3/c1-2-6(7)4-3-5-9-8/h6,8H,2-5H2,1H3	
C6H12OOH1-5O	C6H13O3	C(OO)CCCC([O])C	InChI=1S/C6H13O3/c1-6(7)4-2-3-5-9-8/h6,8H,2-5H2,1H3	

C6H12OOH2-1O	C6H13O3	C([O])C(OO)CCCC	InChI=1S/C6H13O3/c1-2-3-4-6(5-7)9-8/h6,8H,2-5H2,1H3	
C6H12OOH2-3O	C6H13O3	CC(OO)C([O])CCC	InChI=1S/C6H13O3/c1-3-4-6(7)5(2)9-8/h5-6,8H,3-4H2,1-2H3	
C6H12OOH2-4O	C6H13O3	CC(OO)CC([O])CC	InChI=1S/C6H13O3/c1-3-6(7)4-5(2)9-8/h5-6,8H,3-4H2,1-2H3	
C6H12OOH2-5O	C6H13O3	CC(OO)CCC([O])C	InChI=1S/C6H13O3/c1-5(7)3-4-6(2)9-8/h5-6,8H,3-4H2,1-2H3	
C6H12OOH2-6O	C6H13O3	CC(OO)CCCC([O])	InChI=1S/C6H13O3/c1-6(9-8)4-2-3-5-7/h6,8H,2-5H2,1H3	
C6H12OOH3-1O	C6H13O3	C([O])CC(OO)CCC	InChI=1S/C6H13O3/c1-2-3-6(9-8)4-5-7/h6,8H,2-5H2,1H3	
C6H12OOH3-2O	C6H13O3	CC([O])C(OO)CCC	InChI=1S/C6H13O3/c1-3-4-6(9-8)5(2)7/h5-6,8H,3-4H2,1-2H3	
C6H12OOH3-4O	C6H13O3	CCC(OO)C([O])CC	InChI=1S/C6H13O3/c1-3-5(7)6(4-2)9-8/h5-6,8H,3-4H2,1-2H3	
C6H12OOH3-5O	C6H13O3	CCC(OO)CC([O])C	InChI=1S/C6H13O3/c1-3-6(9-8)4-5(2)7/h5-6,8H,3-4H2,1-2H3	
C6H12OOH3-6O	C6H13O3	CCC(OO)CCC([O])	InChI=1S/C6H13O3/c1-2-6(9-8)4-3-5-7/h6,8H,2-5H2,1H3	

NC5H11CHO	C6H12O	CCCCC=O	InChI=1S/C6H12O/c1-2-3-4-5-6-7/h6H,2-5H2,1H3	
C6Y2	C6H12O	CC(=O)CCCC	InChI=1S/C6H12O/c1-3-4-5-6(2)7/h3-5H2,1-2H3	
CH3COOH	C2H4O2	CC(=O)O	InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)	
C2H5COOH	C3H6O2	CCC(=O)O	InChI=1S/C3H6O2/c1-2-3(4)5/h2H2,1H3,(H,4,5)	
C6H12-1	C6H12	C=CCCCC	InChI=1S/C6H12/c1-3-5-6-4-2/h3H,1,4-6H2,2H3	
C6H12-2	C6H12	CC=CCCC	InChI=1S/C6H12/c1-3-5-6-4-2/h3,5H,4,6H2,1-2H3	
C6H12-3	C6H12	CCC=CCC	InChI=1S/C6H12/c1-3-5-6-4-2/h5-6H,3-4H2,1-2H3	
C6H111-3	C6H11	C=C[CH]CCC	InChI=1S/C6H11/c1-3-5-6-4-2/h3,5H,1,4,6H2,2H3	
C6H111-4	C6H11	C=CC[CH]CC	InChI=1S/C6H11/c1-3-5-6-4-2/h3,6H,1,4-5H2,2H3	
C6H111-5	C6H11	C=CCC[CH]C	InChI=1S/C6H11/c1-3-5-6-4-2/h3-4H,1,5-6H2,2H3	

C6H111-6	C6H11	C=CCCC[CH2]	InChI=1S/C6H11/c1-3-5-6-4-2/h3H,1-2,4-6H2	
C6H112-4	C6H11	CC=C[CH]CC	InChI=1S/C6H11/c1-3-5-6-4-2/h3,5-6H,4H2,1-2H3	
C6H112-5	C6H11	CC=CC[CH]C	InChI=1S/C6H11/c1-3-5-6-4-2/h3-5H,6H2,1-2H3	
C6H112-6	C6H11	CC=CCC[CH2]	InChI=1S/C6H11/c1-3-5-6-4-2/h4,6H,1,3,5H2,2H3	
C6H113-1	C6H11	CCC=CC[CH2]	InChI=1S/C6H11/c1-3-5-6-4-2/h5-6H,1,3-4H2,2H3	
C6H12OH-1J2	C6H13O	C(O)[CH]CCCC	InChI=1S/C6H13O/c1-2-3-4-5-6-7/h5,7H,2-4,6H2,1H3	
C6H12OH-2J1	C6H13O	[CH2]C(O)CCCC	InChI=1S/C6H13O/c1-3-4-5-6(2)7/h6-7H,2-5H2,1H3	
C6H12OH-2J3	C6H13O	CC(O)[CH]CCC	InChI=1S/C6H13O/c1-3-4-5-6(2)7/h5-7H,3-4H2,1-2H3	
C6H12OH-3J2	C6H13O	C[CH]C(O)CCC	InChI=1S/C6H13O/c1-3-5-6(7)4-2/h4,6-7H,3,5H2,1-2H3	
C6H12OH-3J4	C6H13O	CCC(O)[CH]CC	InChI=1S/C6H13O/c1-3-5-6(7)4-2/h5-7H,3-4H2,1-2H3	

C6H12OH-1O2-2	C6H13O3	C(O)C(O[O])CCCC	InChI=1S/C6H13O3/c1-2-3-4-6(5-7)9-8/h6-7H,2-5H2,1H3	
C6H12OH-2O2-1	C6H13O3	C(O[O])C(O)CCCC	InChI=1S/C6H13O3/c1-2-3-4-6(7)5-9-8/h6-7H,2-5H2,1H3	
C6H12OH-2O2-3	C6H13O3	CC(O)C(O[O])CCC	InChI=1S/C6H13O3/c1-3-4-6(9-8)5(2)7/h5-7H,3-4H2,1-2H3	
C6H12OH-3O2-2	C6H13O3	CC(O[O])C(O)CCC	InChI=1S/C6H13O3/c1-3-4-6(7)5(2)9-8/h5-7H,3-4H2,1-2H3	
C6H12OH-3O2-4	C6H13O3	CCC(O)C(O[O])CC	InChI=1S/C6H13O3/c1-3-5(7)6(4-2)9-8/h5-7H,3-4H2,1-2H3	
PC4H9CHO	C5H10O	CCCCC=O	InChI=1S/C5H10O/c1-2-3-4-5-6/h5H,2-4H2,1H3	
PC4H8CHO-1	C5H9O	CCC[CH]C=O	InChI=1S/C5H9O/c1-2-3-4-5-6/h4-5H,2-3H2,1H3	
PC4H8CHO-2	C5H9O	CC[CH]CC=O	InChI=1S/C5H9O/c1-2-3-4-5-6/h3,5H,2,4H2,1H3	
PC4H8CHO-3	C5H9O	C[CH]CCC=O	InChI=1S/C5H9O/c1-2-3-4-5-6/h2,5H,3-4H2,1H3	
PC4H8CHO-4	C5H9O	[CH2]CCCC=O	InChI=1S/C5H9O/c1-2-3-4-5-6/h5H,1-4H2	

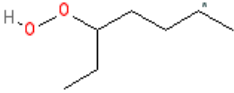
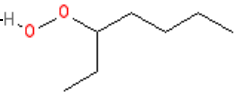
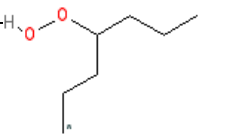
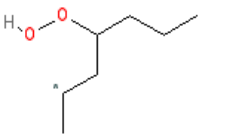
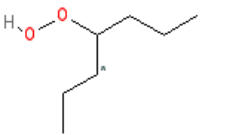



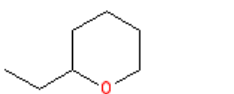
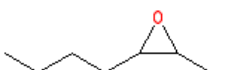
C6H11-1D3O	C6H11O	<chem>C=CC([O])CCC</chem>	InChI=1S/C6H11O/c1-3-5-6(7)4-2/h4,6H,2-3,5H2,1H3	
C6H11-1D4O	C6H11O	<chem>C=CCC([O])CC</chem>	InChI=1S/C6H11O/c1-3-5-6(7)4-2/h3,6H,1,4-5H2,2H3	
C6H11-1D5O	C6H11O	<chem>C=CCCC([O])C</chem>	InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3,6H,1,4-5H2,2H3	
C6H11-1D6O	C6H11O	<chem>C=CCCCC([O])</chem>	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2H,1,3-6H2	
C6H11-2D1O	C6H11O	<chem>C([O])C=CCCC</chem>	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h4-5H,2-3,6H2,1H3	
C6H11-2D4O	C6H11O	<chem>CC=CC([O])CC</chem>	InChI=1S/C6H11O/c1-3-5-6(7)4-2/h3,5-6H,4H2,1-2H3	
C6H11-2D5O	C6H11O	<chem>CC=CCC([O])C</chem>	InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3-4,6H,5H2,1-2H3	
C6H11-2D6O	C6H11O	<chem>CC=CCCC([O])</chem>	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2-3H,4-6H2,1H3	
C6H11-3D1O	C6H11O	<chem>CCC=CCC([O])</chem>	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h3-4H,2,5-6H2,1H3	
C6H11-3D2O	C6H11O	<chem>CCC=CC([O])C</chem>	InChI=1S/C6H11O/c1-3-4-5-6(2)7/h4-6H,3H2,1-2H3	

NC5H11CO	C6H11O	CCCCC[C]=O	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2-5H2,1H3	
NC5H10CHO-1	C6H11O	CCCC[CH]C=O	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h5-6H,2-4H2,1H3	
NC5H10CHO-2	C6H11O	CCC[CH]CC=O	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h4,6H,2-3,5H2,1H3	
NC5H10CHO-3	C6H11O	CC[CH]CCC=O	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h3,6H,2,4-5H2,1H3	
NC5H10CHO-4	C6H11O	C[CH]CCCC=O	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2,6H,3-5H2,1H3	
NC5H10CHO-5	C6H11O	[CH2]CCCCC=O	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h6H,1-5H2	
C6H10D13	C6H10	C=CC=CCC	InChI=1S/C6H10/c1-3-5-6-4-2/h3,5-6H,1,4H2,2H3	
C6H10D24	C6H10	CC=CC=CC	InChI=1S/C6H10/c1-3-5-6-4-2/h3-6H,1-2H3	
C6H10I-5	C6H10	C=CCCC=C	InChI=1S/C6H10/c1-3-5-6-4-2/h3-4H,1-2,5-6H2	
C6H9-A	C6H9	C=CC[CH]C=C	InChI=1S/C6H9/c1-3-5-6-4-2/h3-5H,1-2,6H2	

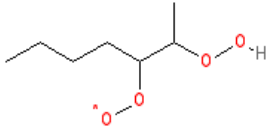
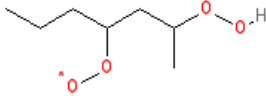
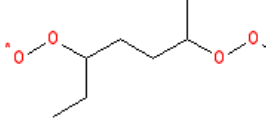

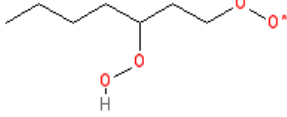
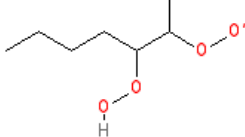
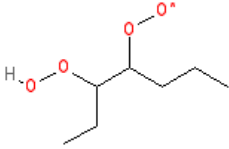
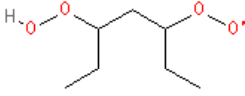
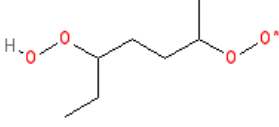
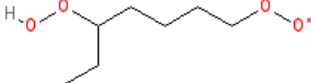
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C7H15-1	C7H15	[CH2]CCCCC	InChI=1S/C7H15/c1-3-5-7-6-4-2/h1,3-7H2,2H3	
C7H15-2	C7H15	C[CH]CCCC	InChI=1S/C7H15/c1-3-5-7-6-4-2/h3H,4-7H2,1-2H3	
C7H15-3	C7H15	CC[CH]CCCC	InChI=1S/C7H15/c1-3-5-7-6-4-2/h5H,3-4,6-7H2,1-2H3	
C7H15-4	C7H15	CCC[CH]CCC	InChI=1S/C7H15/c1-3-5-7-6-4-2/h7H,3-6H2,1-2H3	
C7H15OOH-1	C7H16O2	C(OO)CCCCC	InChI=1S/C7H16O2/c1-2-3-4-5-6-7-9-8/h8H,2-7H2,1H3	
C7H15OOH-2	C7H16O2	CC(OO)CCCC	InChI=1S/C7H16O2/c1-3-4-5-6-7(2)9-8/h7H,8H,3-6H2,1-2H3	
C7H15OOH-3	C7H16O2	CCC(OO)CCCC	InChI=1S/C7H16O2/c1-3-5-6-7(4-2)9-8/h7H,8H,3-6H2,1-2H3	
C7H15OOH-4	C7H16O2	CCCC(OO)CCC	InChI=1S/C7H16O2/c1-3-5-7(9-8)6-4-2/h7H,8H,3-6H2,1-2H3	
C7H15-1O2	C7H15O2	C(O[O])CCCCC	InChI=1S/C7H15O2/c1-2-3-4-5-6-7-9-8/h2-7H2,1H3	

C7H15-2O2	C7H15O2	CC(O[O])CCCCC	InChI=1S/C7H15O2/c1-3-4-5-6-7(2)9-8/h7H,3-6H2,1-2H3	
C7H15-3O2	C7H15O2	CCC(O[O])CCCC	InChI=1S/C7H15O2/c1-3-5-6-7(4-2)9-8/h7H,3-6H2,1-2H3	
C7H15-4O2	C7H15O2	CCCC(O[O])CCC	InChI=1S/C7H15O2/c1-3-5-7(9-8)6-4-2/h7H,3-6H2,1-2H3	
C7H15-1O	C7H15O	C([O])CCCCCC	InChI=1S/C7H15O/c1-2-3-4-5-6-7-8/h2-7H2,1H3	
C7H15-2O	C7H15O	CC([O])CCCCC	InChI=1S/C7H15O/c1-3-4-5-6-7(2)8/h7H,3-6H2,1-2H3	
C7H15-3O	C7H15O	CCC([O])CCCC	InChI=1S/C7H15O/c1-3-5-6-7(8)4-2/h7H,3-6H2,1-2H3	
C7H15-4O	C7H15O	CCCC([O])CCC	InChI=1S/C7H15O/c1-3-5-7(8)6-4-2/h7H,3-6H2,1-2H3	
C7H14OOH1-2	C7H15O2	C(OO)[CH]CCCCC	InChI=1S/C7H15O2/c1-2-3-4-5-6-7-9-8/h6,8H,2-5,7H2,1H3	
C7H14OOH1-3	C7H15O2	C(OO)C[CH]CCCC	InChI=1S/C7H15O2/c1-2-3-4-5-6-7-9-8/h5,8H,2-4,6-7H2,1H3	
C7H14OOH1-4	C7H15O2	C(OO)CC[CH]CCC	InChI=1S/C7H15O2/c1-2-3-4-5-6-7-9-8/h4,8H,2-3,5-7H2,1H3	

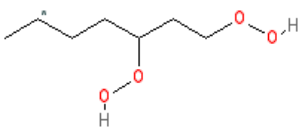
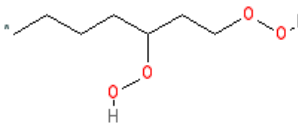
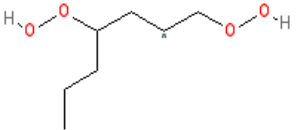
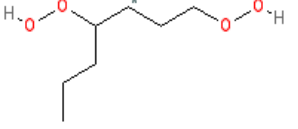
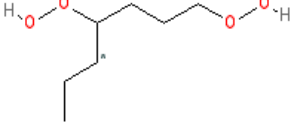
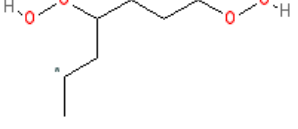
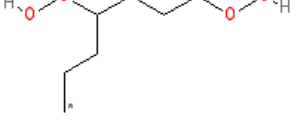
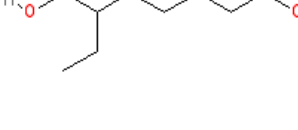
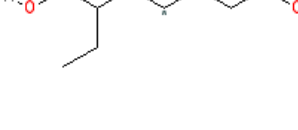
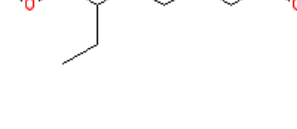
C7H14OOH1-5	C7H15O2	C(OO)CCC[CH]CC	InChI=1S/C7H15O2/c1-2-3-4-5-6-7-9-8/h3,8H,2,4-7H2,1H3	
C7H14OOH2-1	C7H15O2	[CH2]C(OO)CCCC	InChI=1S/C7H15O2/c1-3-4-5-6-7(2)9-8/h7-8H,2-6H2,1H3	
C7H14OOH2-3	C7H15O2	CC(OO)[CH]CCCC	InChI=1S/C7H15O2/c1-3-4-5-6-7(2)9-8/h6-8H,3-5H2,1-2H3	
C7H14OOH2-4	C7H15O2	CC(OO)C[CH]CCC	InChI=1S/C7H15O2/c1-3-4-5-6-7(2)9-8/h5,7-8H,3-4,6H2,1-2H3	
C7H14OOH2-5	C7H15O2	CC(OO)CC[CH]CC	InChI=1S/C7H15O2/c1-3-4-5-6-7(2)9-8/h4,7-8H,3,5-6H2,1-2H3	
C7H14OOH2-6	C7H15O2	CC(OO)CCC[CH]C	InChI=1S/C7H15O2/c1-3-4-5-6-7(2)9-8/h3,7-8H,4-6H2,1-2H3	
C7H14OOH3-1	C7H15O2	[CH2]CC(OO)CCCC	InChI=1S/C7H15O2/c1-3-5-6-7(4-2)9-8/h7-8H,2-6H2,1H3	
C7H14OOH3-2	C7H15O2	C[CH]C(OO)CCCC	InChI=1S/C7H15O2/c1-3-5-6-7(4-2)9-8/h4,7-8H,3,5-6H2,1-2H3	
C7H14OOH3-4	C7H15O2	CCC(OO)[CH]CCC	InChI=1S/C7H15O2/c1-3-5-6-7(4-2)9-8/h6-8H,3-5H2,1-2H3	
C7H14OOH3-5	C7H15O2	CCC(OO)C[CH]CC	InChI=1S/C7H15O2/c1-3-5-6-7(4-2)9-8/h5,7-8H,3-4,6H2,1-2H3	

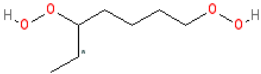
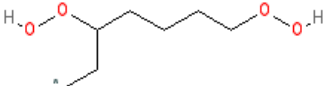
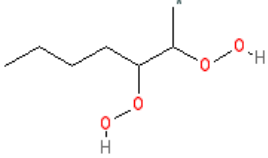
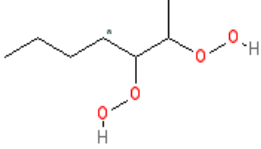
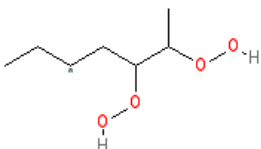
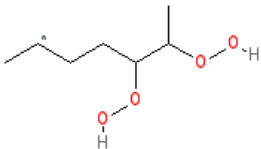
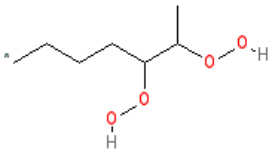
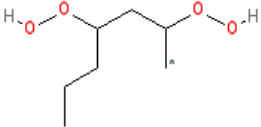
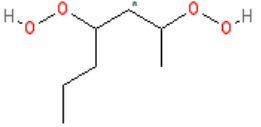
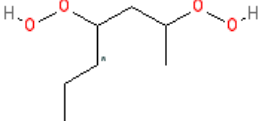
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C7H14OOH3-7	C7H15O2	CCC(OO)CCC[CH2]	InChI=1S/C7H15O2/c1-3-5-6-7(4-2)9-8/h7-8H,1,3-6H2,2H3	
C7H14OOH4-1	C7H15O2	CCCC(OO)CC[CH2]	InChI=1S/C7H15O2/c1-3-5-7(9-8)6-4-2/h7-8H,1,3-6H2,2H3	
C7H14OOH4-2	C7H15O2	CCCC(OO)C[CH]C	InChI=1S/C7H15O2/c1-3-5-7(9-8)6-4-2/h3,7-8H,4-6H2,1-2H3	
C7H14OOH4-3	C7H15O2	CCCC(OO)[CH]CC	InChI=1S/C7H15O2/c1-3-5-7(9-8)6-4-2/h5,7-8H,3-4,6H2,1-2H3	
C7H14O1-2	C7H14O	C1C(O1)CCCCC	InChI=1S/C7H14O/c1-2-3-4-5-7-6-8-7/h7H,2-6H2,1H3	
C7H14O1-3	C7H14O	C1CC(O1)CCCC	InChI=1S/C7H14O/c1-2-3-4-7-5-6-8-7/h7H,2-6H2,1H3	
C7H14O1-4	C7H14O	C1CCC(O1)CCC	InChI=1S/C7H14O/c1-2-4-7-5-3-6-8-7/h7H,2-6H2,1H3	
C7H14O1-5	C7H14O	C1CCCC(O1)CC	InChI=1S/C7H14O/c1-2-7-5-3-4-6-8-7/h7H,2-6H2,1H3	
C7H14O2-3	C7H14O	CC1C(O1)CCCC	InChI=1S/C7H14O/c1-3-4-5-7-6(2)8-7/h6-7H,3-5H2,1-2H3	

C7H14O2-4	C7H14O	CC1CC(O1)CCC	InChI=1S/C7H14O/c1-3-4-7-5-6(2)8-7/h6-7H,3-5H2,1-2H3	
C7H14O2-5	C7H14O	CC1CCC(O1)CC	InChI=1S/C7H14O/c1-3-7-5-4-6(2)8-7/h6-7H,3-5H2,1-2H3	
C7H14O2-6	C7H14O	CC1CCCC(O1)C	InChI=1S/C7H14O/c1-6-4-3-5-7(2)8-6/h6-7H,3-5H2,1-2H3	
C7H14O3-4	C7H14O	CCC1C(O1)CCC	InChI=1S/C7H14O/c1-3-5-7-6(4-2)8-7/h6-7H,3-5H2,1-2H3	
C7H14O3-5	C7H14O	CCC1CC(O1)CC	InChI=1S/C7H14O/c1-3-6-5-7(4-2)8-6/h6-7H,3-5H2,1-2H3	
C7H14OOH1-2O2	C7H15O4	C(OO)C(O[O])CCCCC	InChI=1S/C7H15O4/c1-2-3-4-5-7(11-9)6-10-8/h7-8H,2-6H2,1H3	
C7H14OOH1-3O2	C7H15O4	C(OO)CC(O[O])CCCC	InChI=1S/C7H15O4/c1-2-3-4-7(11-9)5-6-10-8/h7-8H,2-6H2,1H3	
C7H14OOH1-4O2	C7H15O4	C(OO)CCC(O[O])CCC	InChI=1S/C7H15O4/c1-2-4-7(11-9)5-3-6-10-8/h7-8H,2-6H2,1H3	
C7H14OOH1-5O2	C7H15O4	C(OO)CCCC(O[O])CC	InChI=1S/C7H15O4/c1-2-7(11-9)5-3-4-6-10-8/h7-8H,2-6H2,1H3	
C7H14OOH2-1O2	C7H15O4	C(O[O])C(OO)CCCCC	InChI=1S/C7H15O4/c1-2-3-4-5-7(11-9)6-10-8/h7,9H,2-6H2,1H3	

C7H14OOH2-3O2	C7H15O4	CC(OO)C(O[O])CCCC	InChI=1S/C7H15O4/c1-3-4-5-7(11-9)6(2)10-8/h6-8H,3-5H2,1-2H3	
C7H14OOH2-4O2	C7H15O4	CC(OO)CC(O[O])CCC	InChI=1S/C7H15O4/c1-3-4-7(11-9)5-6(2)10-8/h6-8H,3-5H2,1-2H3	
C7H14OOH2-5O2	C7H15O4	CC(OO)CCC(O[O])CC	InChI=1S/C7H15O4/c1-3-7(11-9)5-4-6(2)10-8/h6-8H,3-5H2,1-2H3	
C7H14OOH2-6O2	C7H15O4	CC(OO)CCCC(O[O])C	InChI=1S/C7H15O4/c1-6(10-8)4-3-5-7(2)11-9/h6-8H,3-5H2,1-2H3	
C7H14OOH3-1O2	C7H15O4	C(O[O])CC(OO)CCCC	InChI=1S/C7H15O4/c1-2-3-4-7(11-9)5-6-10-8/h7,9H,2-6H2,1H3	
C7H14OOH3-2O2	C7H15O4	CC(O[O])C(OO)CCCC	InChI=1S/C7H15O4/c1-3-4-5-7(11-9)6(2)10-8/h6-7,9H,3-5H2,1-2H3	
C7H14OOH3-4O2	C7H15O4	CCC(OO)C(O[O])CCC	InChI=1S/C7H15O4/c1-3-5-7(11-9)6(4-2)10-8/h6-8H,3-5H2,1-2H3	
C7H14OOH3-5O2	C7H15O4	CCC(OO)CC(O[O])CC	InChI=1S/C7H15O4/c1-3-6(10-8)5-7(4-2)11-9/h6-8H,3-5H2,1-2H3	
C7H14OOH3-6O2	C7H15O4	CCC(OO)CCC(O[O])C	InChI=1S/C7H15O4/c1-3-7(11-9)5-4-6(2)10-8/h6-7,9H,3-5H2,1-2H3	
C7H14OOH3-7O2	C7H15O4	CCC(OO)CCCC(O[O])	InChI=1S/C7H15O4/c1-2-7(11-9)5-3-4-6-10-8/h7,9H,2-6H2,1H3	

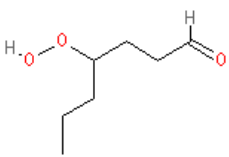
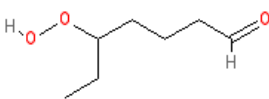
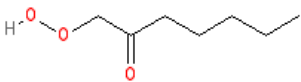
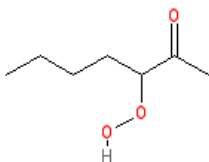
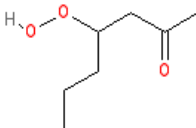
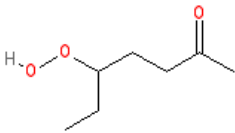
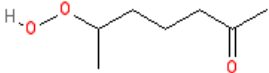
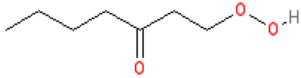
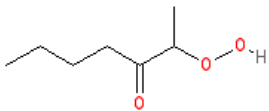
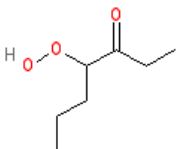
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C7H14OOH4-2O2	C7H15O4	CCCC(OO)CC(O[O])C	InChI=1S/C7H15O4/c1-3-4-7(11-9)5-6(2)10-8/h6-7,9H,3-5H2,1-2H3	
C7H14OOH4-3O2	C7H15O4	CCCC(OO)C(O[O])CC	InChI=1S/C7H15O4/c1-3-5-7(11-9)6(4-2)10-8/h6-7,9H,3-5H2,1-2H3	
C7H13Q12-3	C7H15O4	C(OO)C(OO)[CH]CCCC	InChI=1S/C7H15O4/c1-2-3-4-5-7(11-9)6-10-8/h5,7-9H,2-4,6H2,1H3	
C7H13Q12-4	C7H15O4	C(OO)C(OO)C[CH]CCC	InChI=1S/C7H15O4/c1-2-3-4-5-7(11-9)6-10-8/h4,7-9H,2-3,5-6H2,1H3	
C7H13Q12-5	C7H15O4	C(OO)C(OO)CC[CH]CC	InChI=1S/C7H15O4/c1-2-3-4-5-7(11-9)6-10-8/h3,7-9H,2,4-6H2,1H3	
C7H13Q12-6	C7H15O4	C(OO)C(OO)CCC[CH]C	InChI=1S/C7H15O4/c1-2-3-4-5-7(11-9)6-10-8/h2,7-9H,3-6H2,1H3	
C7H13Q13-2	C7H15O4	C(OO)[CH]C(OO)CCCC	InChI=1S/C7H15O4/c1-2-3-4-7(11-9)5-6-10-8/h5,7-9H,2-4,6H2,1H3	
C7H13Q13-4	C7H15O4	C(OO)CC(OO)[CH]CCC	InChI=1S/C7H15O4/c1-2-3-4-7(11-9)5-6-10-8/h4,7-9H,2-3,5-6H2,1H3	
C7H13Q13-5	C7H15O4	C(OO)CC(OO)C[CH]CC	InChI=1S/C7H15O4/c1-2-3-4-7(11-9)5-6-10-8/h3,7-9H,2,4-6H2,1H3	

C7H13Q13-6	C7H15O4	C(OO)CC(OO)CC[CH]C	InChI=1S/C7H15O4/c1-2-3-4-7(11-9)5-6-10-8/h2,7-9H,3-6H2,1H3	
C7H13Q13-7	C7H15O4	C(OO)CC(OO)CCC[CH2]	InChI=1S/C7H15O4/c1-2-3-4-7(11-9)5-6-10-8/h7-9H,1-6H2	
C7H13Q14-2	C7H15O4	C(OO)[CH]CC(OO)CCC	InChI=1S/C7H15O4/c1-2-4-7(11-9)5-3-6-10-8/h3,7-9H,2,4-6H2,1H3	
C7H13Q14-3	C7H15O4	C(OO)C[CH]C(OO)CCC	InChI=1S/C7H15O4/c1-2-4-7(11-9)5-3-6-10-8/h5,7-9H,2-4,6H2,1H3	
C7H13Q14-5	C7H15O4	C(OO)CCC(OO)[CH]CC	InChI=1S/C7H15O4/c1-2-4-7(11-9)5-3-6-10-8/h4,7-9H,2-3,5-6H2,1H3	
C7H13Q14-6	C7H15O4	C(OO)CCC(OO)C[CH]C	InChI=1S/C7H15O4/c1-2-4-7(11-9)5-3-6-10-8/h2,7-9H,3-6H2,1H3	
C7H13Q14-7	C7H15O4	C(OO)CCC(OO)CC[CH2]	InChI=1S/C7H15O4/c1-2-4-7(11-9)5-3-6-10-8/h7-9H,1-6H2	
C7H13Q15-2	C7H15O4	C(OO)[CH]CCC(OO)CC	InChI=1S/C7H15O4/c1-2-7(11-9)5-3-4-6-10-8/h4,7-9H,2-3,5-6H2,1H3	
C7H13Q15-3	C7H15O4	C(OO)C[CH]CC(OO)CC	InChI=1S/C7H15O4/c1-2-7(11-9)5-3-4-6-10-8/h3,7-9H,2,4-6H2,1H3	
C7H13Q15-4	C7H15O4	C(OO)CC[CH]C(OO)CC	InChI=1S/C7H15O4/c1-2-7(11-9)5-3-4-6-10-8/h5,7-9H,2-4,6H2,1H3	

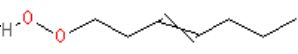
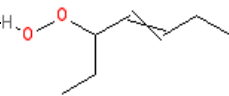
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C7H13Q15-7	C7H15O4	C(OO)CCCC(OO)C[CH2]	InChI=1S/C7H15O4/c1-2-7(11-9)5-3-4-6-10-8/h7-9H,1-6H2	
C7H13Q23-1	C7H15O4	[CH2]C(OO)C(OO)CCCC	InChI=1S/C7H15O4/c1-3-4-5-7(11-9)6(2)10-8/h6-9H,2-5H2,1H3	
C7H13Q23-4	C7H15O4	CC(OO)C(OO)[CH]CCC	InChI=1S/C7H15O4/c1-3-4-5-7(11-9)6(2)10-8/h5-9H,3-4H2,1-2H3	
C7H13Q23-5	C7H15O4	CC(OO)C(OO)C[CH]CC	InChI=1S/C7H15O4/c1-3-4-5-7(11-9)6(2)10-8/h4,6-9H,3,5H2,1-2H3	
C7H13Q23-6	C7H15O4	CC(OO)C(OO)CC[CH]C	InChI=1S/C7H15O4/c1-3-4-5-7(11-9)6(2)10-8/h3,6-9H,4-5H2,1-2H3	
C7H13Q23-7	C7H15O4	CC(OO)C(OO)CCC[CH2]	InChI=1S/C7H15O4/c1-3-4-5-7(11-9)6(2)10-8/h6-9H,1,3-5H2,2H3	
C7H13Q24-1	C7H15O4	[CH2]C(OO)CC(OO)CCC	InChI=1S/C7H15O4/c1-3-4-7(11-9)5-6(2)10-8/h6-9H,2-5H2,1H3	
C7H13Q24-3	C7H15O4	CC(OO)[CH]C(OO)CCC	InChI=1S/C7H15O4/c1-3-4-7(11-9)5-6(2)10-8/h5-9H,3-4H2,1-2H3	
C7H13Q24-5	C7H15O4	CC(OO)CC(OO)[CH]CC	InChI=1S/C7H15O4/c1-3-4-7(11-9)5-6(2)10-8/h4,6-9H,3,5H2,1-2H3	

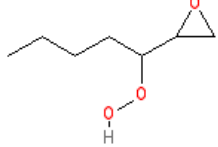
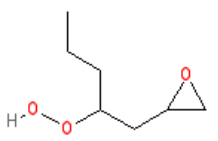
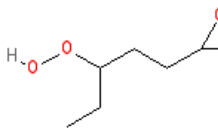
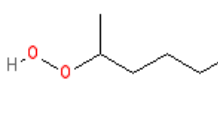
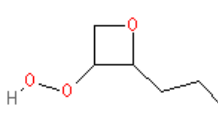
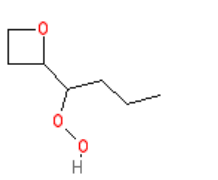
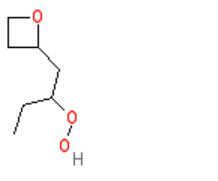
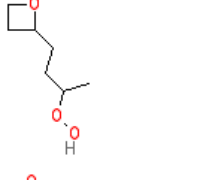
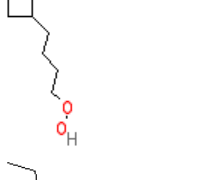
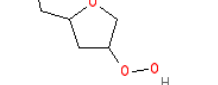
C7H13Q24-6	C7H15O4	CC(OO)CC(OO)C[CH]C	InChI=1S/C7H15O4/c1-3-4-7(11-9)5-6(2)10-8/h3,6-9H,4-5H2,1-2H3	
C7H13Q24-7	C7H15O4	CC(OO)CC(OO)CC[CH2]	InChI=1S/C7H15O4/c1-3-4-7(11-9)5-6(2)10-8/h6-9H,1,3-5H2,2H3	
C7H13Q25-1	C7H15O4	[CH2]C(OO)CCC(OO)CC	InChI=1S/C7H15O4/c1-3-7(11-9)5-4-6(2)10-8/h6-9H,2-5H2,1H3	
C7H13Q25-3	C7H15O4	CC(OO)[CH]CC(OO)CC	InChI=1S/C7H15O4/c1-3-7(11-9)5-4-6(2)10-8/h4,6-9H,3,5H2,1-2H3	
C7H13Q25-4	C7H15O4	CC(OO)C[CH]C(OO)CC	InChI=1S/C7H15O4/c1-3-7(11-9)5-4-6(2)10-8/h5-9H,3-4H2,1-2H3	
C7H13Q25-6	C7H15O4	CC(OO)CCC(OO)[CH]C	InChI=1S/C7H15O4/c1-3-7(11-9)5-4-6(2)10-8/h3,6-9H,4-5H2,1-2H3	
C7H13Q25-7	C7H15O4	CC(OO)CCC(OO)C[CH2]	InChI=1S/C7H15O4/c1-3-7(11-9)5-4-6(2)10-8/h6-9H,1,3-5H2,2H3	
C7H13Q26-1	C7H15O4	CC(OO)CCCC(OO)[CH2]	InChI=1S/C7H15O4/c1-6(10-8)4-3-5-7(2)11-9/h6-9H,1,3-5H2,2H3	
C7H13Q26-3	C7H15O4	CC(OO)CC[CH]C(OO)C	InChI=1S/C7H15O4/c1-6(10-8)4-3-5-7(2)11-9/h4,6-9H,3,5H2,1-2H3	
C7H13Q26-4	C7H15O4	CC(OO)C[CH]CC(OO)C	InChI=1S/C7H15O4/c1-6(10-8)4-3-5-7(2)11-9/h3,6-9H,4-5H2,1-2H3	

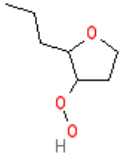
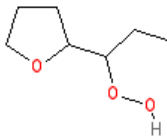
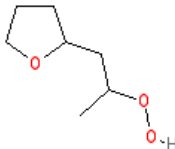
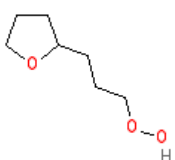
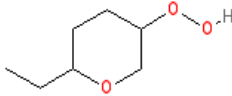
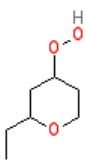
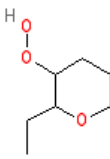
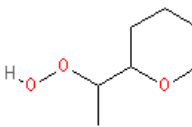
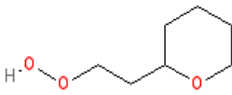
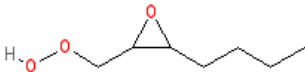
C7H13Q34-1	C7H15O4	[CH2]CC(OO)C(OO)CCC	InChI=1S/C7H15O4/c1-3-5-7(11-9)6(4-2)10-8/h6-9H,2-5H2,1H3	
C7H13Q34-2	C7H15O4	C[CH]C(OO)C(OO)CCC	InChI=1S/C7H15O4/c1-3-5-7(11-9)6(4-2)10-8/h4,6-9H,3,5H2,1-2H3	
C7H13Q34-5	C7H15O4	CCC(OO)C(OO)[CH]CC	InChI=1S/C7H15O4/c1-3-5-7(11-9)6(4-2)10-8/h5-9H,3-4H2,1-2H3	
C7H13Q34-6	C7H15O4	CCC(OO)C(OO)C[CH]C	InChI=1S/C7H15O4/c1-3-5-7(11-9)6(4-2)10-8/h3,6-9H,4-5H2,1-2H3	
C7H13Q34-7	C7H15O4	CCC(OO)C(OO)CC[CH2]	InChI=1S/C7H15O4/c1-3-5-7(11-9)6(4-2)10-8/h6-9H,1,3-5H2,2H3	
C7H13Q35-1	C7H15O4	CCC(OO)CC(OO)C[CH2]	InChI=1S/C7H15O4/c1-3-6(10-8)5-7(4-2)11-9/h6-9H,1,3-5H2,2H3	
C7H13Q35-2	C7H15O4	CCC(OO)CC(OO)[CH]C	InChI=1S/C7H15O4/c1-3-6(10-8)5-7(4-2)11-9/h3,6-9H,4-5H2,1-2H3	
C7H13Q35-4	C7H15O4	CCC(OO)[CH]C(OO)CC	InChI=1S/C7H15O4/c1-3-6(10-8)5-7(4-2)11-9/h5-9H,3-4H2,1-2H3	
C7KET12	C7H14O3	C(=O)C(OO)CCCCC	InChI=1S/C7H14O3/c1-2-3-4-5-7(6-8)10-9/h6-7,9H,2-5H2,1H3	
C7KET13	C7H14O3	C(=O)CC(OO)CCCC	InChI=1S/C7H14O3/c1-2-3-4-7(10-9)5-6-8/h6-7,9H,2-5H2,1H3	

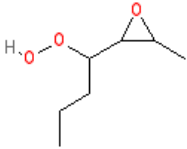
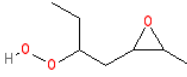
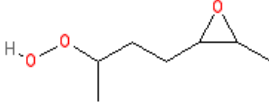
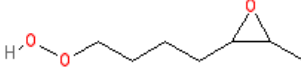
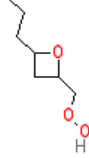
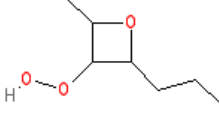
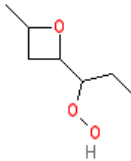
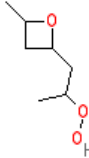

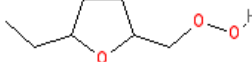
C7KET14	C7H14O3	<chem>C(=O)CCC(OO)CCC</chem>	InChI=1S/C7H14O3/c1-2-4-7(10-9)5-3-6-8/h6-7,9H,2-5H2,1H3	
C7KET15	C7H14O3	<chem>C(=O)CCCC(OO)CC</chem>	InChI=1S/C7H14O3/c1-2-7(10-9)5-3-4-6-8/h6-7,9H,2-5H2,1H3	
C7KET21	C7H14O3	<chem>C(OO)C(=O)CCCCC</chem>	InChI=1S/C7H14O3/c1-2-3-4-5-7(8)6-10-9/h9H,2-6H2,1H3	
C7KET23	C7H14O3	<chem>CC(=O)C(OO)CCCC</chem>	InChI=1S/C7H14O3/c1-3-4-5-7(10-9)6(2)8/h7,9H,3-5H2,1-2H3	
C7KET24	C7H14O3	<chem>CC(=O)CC(OO)CCC</chem>	InChI=1S/C7H14O3/c1-3-4-7(10-9)5-6(2)8/h7,9H,3-5H2,1-2H3	
C7KET25	C7H14O3	<chem>CC(=O)CCC(OO)CC</chem>	InChI=1S/C7H14O3/c1-3-7(10-9)5-4-6(2)8/h7,9H,3-5H2,1-2H3	
C7KET26	C7H14O3	<chem>CC(=O)CCCC(OO)C</chem>	InChI=1S/C7H14O3/c1-6(8)4-3-5-7(2)10-9/h7,9H,3-5H2,1-2H3	
C7KET31	C7H14O3	<chem>C(OO)CC(=O)CCCC</chem>	InChI=1S/C7H14O3/c1-2-3-4-7(8)5-6-10-9/h9H,2-6H2,1H3	
C7KET32	C7H14O3	<chem>CC(OO)C(=O)CCCC</chem>	InChI=1S/C7H14O3/c1-3-4-5-7(8)6(2)10-9/h6,9H,3-5H2,1-2H3	
C7KET34	C7H14O3	<chem>CCC(=O)C(OO)CCC</chem>	InChI=1S/C7H14O3/c1-3-5-7(10-9)6(8)4-2/h7,9H,3-5H2,1-2H3	

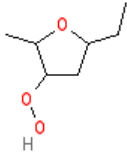
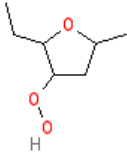
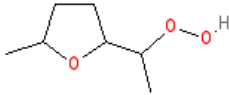
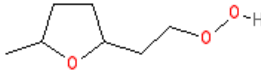
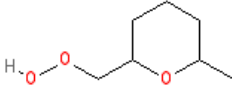
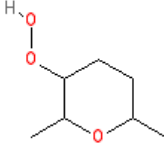
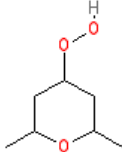
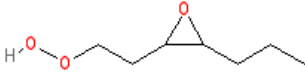
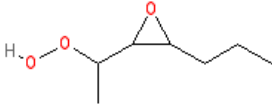
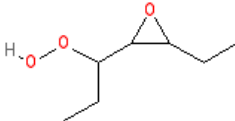
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C7KET36	C7H14O3	CCC(=O)CCC(OO)C	InChI=1S/C7H14O3/c1-3-7(8)5-4-6(2)10-9/h6,9H,3-5H2,1-2H3	
C7KET37	C7H14O3	CCC(=O)CCCC(OO)	InChI=1S/C7H14O3/c1-2-7(8)5-3-4-6-10-9/h9H,2-6H2,1H3	
C7KET41	C7H14O3	C(OO)CCC(=O)CCC	InChI=1S/C7H14O3/c1-2-4-7(8)5-3-6-10-9/h9H,2-6H2,1H3	
C7KET42	C7H14O3	CC(OO)CC(=O)CCC	InChI=1S/C7H14O3/c1-3-4-7(8)5-6(2)10-9/h6,9H,3-5H2,1-2H3	
C7KET43	C7H14O3	CCC(OO)C(=O)CCC	InChI=1S/C7H14O3/c1-3-5-6(8)7(4-2)10-9/h7,9H,3-5H2,1-2H3	
C7H13-1D3OOH	C7H14O2	C=CC(OO)CCCC	InChI=1S/C7H14O2/c1-3-5-6-7(4-2)9-8/h4,7-8H,2-3,5-6H2,1H3	
C7H13-1D4OOH	C7H14O2	C=CCC(OO)CCC	InChI=1S/C7H14O2/c1-3-5-7(9-8)6-4-2/h3,7-8H,1,4-6H2,2H3	
C7H13-1D5OOH	C7H14O2	C=CCCC(OO)CC	InChI=1S/C7H14O2/c1-3-5-6-7(4-2)9-8/h3,7-8H,1,4-6H2,2H3	
C7H13-1D6OOH	C7H14O2	C=CCCCC(OO)C	InChI=1S/C7H14O2/c1-3-4-5-6-7(2)9-8/h3,7-8H,1,4-6H2,2H3	

C7H13-2D1OOH	C7H14O2	C(OO)C=CCCC	InChI=1S/C7H14O2/c1-2-3-4-5-6-7-9-8/h5-6,8H,2-4,7H2,1H3	
C7H13-2D4OOH	C7H14O2	CC=CC(OO)CCC	InChI=1S/C7H14O2/c1-3-5-7(9-8)6-4-2/h3,5,7-8H,4,6H2,1-2H3	
C7H13-2D5OOH	C7H14O2	CC=CCC(OO)CC	InChI=1S/C7H14O2/c1-3-5-6-7(4-2)9-8/h3,5,7-8H,4,6H2,1-2H3	
C7H13-2D6OOH	C7H14O2	CC=CCCC(OO)C	InChI=1S/C7H14O2/c1-3-4-5-6-7(2)9-8/h3-4,7-8H,5-6H2,1-2H3	
C7H13-2D7OOH	C7H14O2	CC=CCCCC(OO)	InChI=1S/C7H14O2/c1-2-3-4-5-6-7-9-8/h2-3,8H,4-7H2,1H3	
C7H13-3D1OOH	C7H14O2	C(OO)CC=CCCC	InChI=1S/C7H14O2/c1-2-3-4-5-6-7-9-8/h4-5,8H,2-3,6-7H2,1H3	
C7H13-3D2OOH	C7H14O2	CC(OO)C=CCCC	InChI=1S/C7H14O2/c1-3-4-5-6-7(2)9-8/h5-8H,3-4H2,1-2H3	
C7H13-3D5OOH	C7H14O2	CCC=CC(OO)CC	InChI=1S/C7H14O2/c1-3-5-6-7(4-2)9-8/h5-8H,3-4H2,1-2H3	
C7H13-3D6OOH	C7H14O2	CCC=CCC(OO)C	InChI=1S/C7H14O2/c1-3-4-5-6-7(2)9-8/h4-5,7-8H,3,6H2,1-2H3	
C7H13-3D7OOH	C7H14O2	CCC=CCCC(OO)	InChI=1S/C7H14O2/c1-2-3-4-5-6-7-9-8/h3-4,8H,2,5-7H2,1H3	

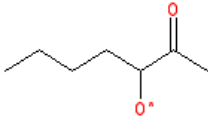
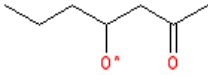
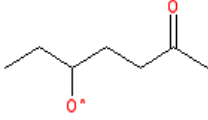
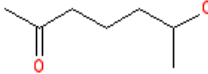
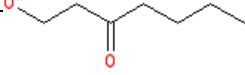
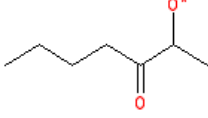
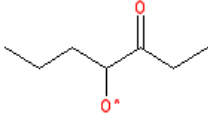
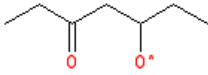
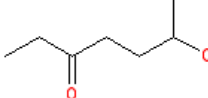
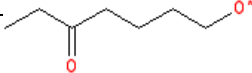
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C7H13O12-4OOH	C7H14O3	C1C(O1)CC(OO)CCC	InChI=1S/C7H14O3/c1-2-3-6(10-8)4-7-5-9-7/h6-8H,2-5H2,1H3	
C7H13O12-5OOH	C7H14O3	C1C(O1)CCC(OO)CC	InChI=1S/C7H14O3/c1-2-6(10-8)3-4-7-5-9-7/h6-8H,2-5H2,1H3	
C7H13O12-6OOH	C7H14O3	C1C(O1)CCCC(OO)C	InChI=1S/C7H14O3/c1-6(10-8)3-2-4-7-5-9-7/h6-8H,2-5H2,1H3	
C7H13O13-2OOH	C7H14O3	C1C(OO)C(O1)CCCC	InChI=1S/C7H14O3/c1-2-3-4-6-7(10-8)5-9-6/h6-8H,2-5H2,1H3	
C7H13O13-4OOH	C7H14O3	C1CC(O1)C(OO)CCC	InChI=1S/C7H14O3/c1-2-3-7(10-8)6-4-5-9-6/h6-8H,2-5H2,1H3	
C7H13O13-5OOH	C7H14O3	C1CC(O1)CC(OO)CC	InChI=1S/C7H14O3/c1-2-6(10-8)5-7-3-4-9-7/h6-8H,2-5H2,1H3	
C7H13O13-6OOH	C7H14O3	C1CC(O1)CCC(OO)C	InChI=1S/C7H14O3/c1-6(10-8)2-3-7-4-5-9-7/h6-8H,2-5H2,1H3	
C7H13O13-7OOH	C7H14O3	C1CC(O1)CCCC(OO)	InChI=1S/C7H14O3/c8-10-5-2-1-3-7-4-6-9-7/h7-8H,1-6H2	
C7H13O14-2OOH	C7H14O3	C1C(OO)CC(O1)CCC	InChI=1S/C7H14O3/c1-2-3-6-4-7(10-8)5-9-6/h6-8H,2-5H2,1H3	

C7H13O14-3OOH	C7H14O3	C1CC(OO)C(O1)CCC	InChI=1S/C7H14O3/c1-2-3-6-7(10-8)4-5-9-6/h6-8H,2-5H2,1H3	
C7H13O14-5OOH	C7H14O3	C1CCC(O1)C(OO)CC	InChI=1S/C7H14O3/c1-2-6(10-8)7-4-3-5-9-7/h6-8H,2-5H2,1H3	
C7H13O14-6OOH	C7H14O3	C1CCC(O1)CC(OO)C	InChI=1S/C7H14O3/c1-6(10-8)5-7-3-2-4-9-7/h6-8H,2-5H2,1H3	
C7H13O14-7OOH	C7H14O3	C1CCC(O1)CCC(OO)	InChI=1S/C7H14O3/c8-10-6-2-4-7-3-1-5-9-7/h7-8H,1-6H2	
C7H13O15-2OOH	C7H14O3	C1C(OO)CCC(O1)CC	InChI=1S/C7H14O3/c1-2-6-3-4-7(10-8)5-9-6/h6-8H,2-5H2,1H3	
C7H13O15-3OOH	C7H14O3	C1CC(OO)CC(O1)CC	InChI=1S/C7H14O3/c1-2-6-5-7(10-8)3-4-9-6/h6-8H,2-5H2,1H3	
C7H13O15-4OOH	C7H14O3	C1CCC(OO)C(O1)CC	InChI=1S/C7H14O3/c1-2-6-7(10-8)4-3-5-9-6/h6-8H,2-5H2,1H3	
C7H13O15-6OOH	C7H14O3	C1CCCC(O1)C(OO)C	InChI=1S/C7H14O3/c1-6(10-8)7-4-2-3-5-9-7/h6-8H,2-5H2,1H3	
C7H13O15-7OOH	C7H14O3	C1CCCC(O1)CC(OO)	InChI=1S/C7H14O3/c8-10-6-4-7-3-1-2-5-9-7/h7-8H,1-6H2	
C7H13O23-1OOH	C7H14O3	C(OO)C1C(O1)CCCC	InChI=1S/C7H14O3/c1-2-3-4-6-7(10-6)5-9-8/h6-8H,2-5H2,1H3	

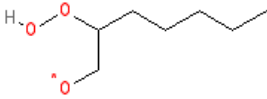
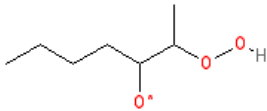
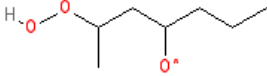
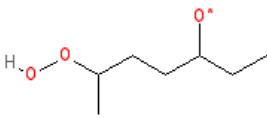
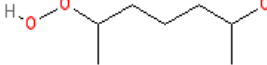
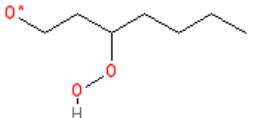
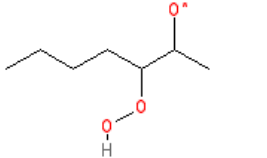
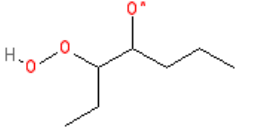
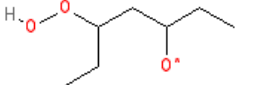
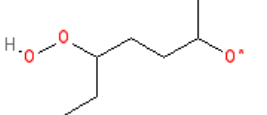
C7H13O23-4OOH	C7H14O3	CC1C(O1)C(OO)CCC	InChI=1S/C7H14O3/c1-3-4-6(10-8)7-5(2)9-7/h5-8H,3-4H2,1-2H3	
C7H13O23-5OOH	C7H14O3	CC1C(O1)CC(OO)CC	InChI=1S/C7H14O3/c1-3-6(10-8)4-7-5(2)9-7/h5-8H,3-4H2,1-2H3	
C7H13O23-6OOH	C7H14O3	CC1C(O1)CCC(OO)C	InChI=1S/C7H14O3/c1-5(10-8)3-4-7-6(2)9-7/h5-8H,3-4H2,1-2H3	
C7H13O23-7OOH	C7H14O3	CC1C(O1)CCCC(OO)	InChI=1S/C7H14O3/c1-6-7(10-6)4-2-3-5-9-8/h6-8H,2-5H2,1H3	
C7H13O24-1OOH	C7H14O3	C(OO)C1CC(O1)CCC	InChI=1S/C7H14O3/c1-2-3-6-4-7(10-6)5-9-8/h6-8H,2-5H2,1H3	
C7H13O24-3OOH	C7H14O3	CC1C(OO)C(O1)CCC	InChI=1S/C7H14O3/c1-3-4-6-7(10-8)5(2)9-6/h5-8H,3-4H2,1-2H3	
C7H13O24-5OOH	C7H14O3	CC1CC(O1)C(OO)CC	InChI=1S/C7H14O3/c1-3-6(10-8)7-4-5(2)9-7/h5-8H,3-4H2,1-2H3	
C7H13O24-6OOH	C7H14O3	CC1CC(O1)CC(OO)C	InChI=1S/C7H14O3/c1-5-3-7(9-5)4-6(2)10-8/h5-8H,3-4H2,1-2H3	
C7H13O24-7OOH	C7H14O3	CC1CC(O1)CCC(OO)	InChI=1S/C7H14O3/c1-6-5-7(10-6)3-2-4-9-8/h6-8H,2-5H2,1H3	
C7H13O25-1OOH	C7H14O3	C(OO)C1CCC(O1)CC	InChI=1S/C7H14O3/c1-2-6-3-4-7(10-6)5-9-8/h6-8H,2-5H2,1H3	

C7H13O25-3OOH	C7H14O3	CC1C(OO)CC(O1)CC	InChI=1S/C7H14O3/c1-3-6-4-7(10-8)5(2)9-6/h5-8H,3-4H2,1-2H3	
C7H13O25-4OOH	C7H14O3	CC1CC(OO)C(O1)CC	InChI=1S/C7H14O3/c1-3-6-7(10-8)4-5(2)9-6/h5-8H,3-4H2,1-2H3	
C7H13O25-6OOH	C7H14O3	CC1CCC(O1)C(OO)C	InChI=1S/C7H14O3/c1-5-3-4-7(9-5)6(2)10-8/h5-8H,3-4H2,1-2H3	
C7H13O25-7OOH	C7H14O3	CC1CCC(O1)CC(OO)	InChI=1S/C7H14O3/c1-6-2-3-7(10-6)4-5-9-8/h6-8H,2-5H2,1H3	
C7H13O26-1OOH	C7H14O3	C(OO)C1CCCC(O1)C	InChI=1S/C7H14O3/c1-6-3-2-4-7(10-6)5-9-8/h6-8H,2-5H2,1H3	
C7H13O26-3OOH	C7H14O3	CC1C(OO)CCC(O1)C	InChI=1S/C7H14O3/c1-5-3-4-7(10-8)6(2)9-5/h5-8H,3-4H2,1-2H3	
C7H13O26-4OOH	C7H14O3	CC1CC(OO)CC(O1)C	InChI=1S/C7H14O3/c1-5-3-7(10-8)4-6(2)9-5/h5-8H,3-4H2,1-2H3	
C7H13O34-1OOH	C7H14O3	C(OO)CC1C(O1)CCC	InChI=1S/C7H14O3/c1-2-3-6-7(10-6)4-5-9-8/h6-8H,2-5H2,1H3	
C7H13O34-2OOH	C7H14O3	CC(OO)C1C(O1)CCC	InChI=1S/C7H14O3/c1-3-4-6-7(9-6)5(2)10-8/h5-8H,3-4H2,1-2H3	
C7H13O34-5OOH	C7H14O3	CCC1C(O1)C(OO)CC	InChI=1S/C7H14O3/c1-3-5-7(9-5)6(4-2)10-8/h5-8H,3-4H2,1-2H3	

C7H13O34-6OOH	C7H14O3	CCC1C(O1)CC(OO)C	InChI=1S/C7H14O3/c1-3-6-7(9-6)4-5(2)10-8/h5-8H,3-4H2,1-2H3	
C7H13O34-7OOH	C7H14O3	CCC1C(O1)CCC(OO)	InChI=1S/C7H14O3/c1-2-6-7(10-6)4-3-5-9-8/h6-8H,2-5H2,1H3	
C7H13O35-1OOH	C7H14O3	CCC1CC(O1)CC(OO)	InChI=1S/C7H14O3/c1-2-6-5-7(10-6)3-4-9-8/h6-8H,2-5H2,1H3	
C7H13O35-2OOH	C7H14O3	CCC1CC(O1)C(OO)C	InChI=1S/C7H14O3/c1-3-6-4-7(9-6)5(2)10-8/h5-8H,3-4H2,1-2H3	
C7H13O35-4OOH	C7H14O3	CCC1C(OO)C(O1)CC	InChI=1S/C7H14O3/c1-3-5-7(10-8)6(4-2)9-5/h5-8H,3-4H2,1-2H3	
C7KET120	C7H13O2	C(=O)C([O])CCCCC	InChI=1S/C7H13O2/c1-2-3-4-5-7(9)6-8/h6-7H,2-5H2,1H3	
C7KET130	C7H13O2	C(=O)CC([O])CCCC	InChI=1S/C7H13O2/c1-2-3-4-7(9)5-6-8/h6-7H,2-5H2,1H3	
C7KET140	C7H13O2	C(=O)CCC([O])CCC	InChI=1S/C7H13O2/c1-2-4-7(9)5-3-6-8/h6-7H,2-5H2,1H3	
C7KET150	C7H13O2	C(=O)CCCC([O])CC	InChI=1S/C7H13O2/c1-2-7(9)5-3-4-6-8/h6-7H,2-5H2,1H3	
C7KET210	C7H13O2	C([O])C(=O)CCCCC	InChI=1S/C7H13O2/c1-2-3-4-5-7(9)6-8/h2-6H2,1H3	

C7KET23O	C7H13O2	<chem>CC(=O)C([O])CCCC</chem>	InChI=1S/C7H13O2/c1-3-4-5-7(9)6(2)8/h7H,3-5H2,1-2H3	
C7KET24O	C7H13O2	<chem>CC(=O)CC([O])CCC</chem>	InChI=1S/C7H13O2/c1-3-4-7(9)5-6(2)8/h7H,3-5H2,1-2H3	
C7KET25O	C7H13O2	<chem>CC(=O)CCC([O])CC</chem>	InChI=1S/C7H13O2/c1-3-7(9)5-4-6(2)8/h7H,3-5H2,1-2H3	
C7KET26O	C7H13O2	<chem>CC(=O)CCCC([O])C</chem>	InChI=1S/C7H13O2/c1-6(8)4-3-5-7(2)9/h6H,3-5H2,1-2H3	
C7KET31O	C7H13O2	<chem>C([O])CC(=O)CCCC</chem>	InChI=1S/C7H13O2/c1-2-3-4-7(9)5-6-8/h2-6H2,1H3	
C7KET32O	C7H13O2	<chem>CC([O])C(=O)CCCC</chem>	InChI=1S/C7H13O2/c1-3-4-5-7(9)6(2)8/h6H,3-5H2,1-2H3	
C7KET34O	C7H13O2	<chem>CCC(=O)C([O])CCC</chem>	InChI=1S/C7H13O2/c1-3-5-7(9)6(8)4-2/h7H,3-5H2,1-2H3	
C7KET35O	C7H13O2	<chem>CCC(=O)CC([O])CC</chem>	InChI=1S/C7H13O2/c1-3-6(8)5-7(9)4-2/h6H,3-5H2,1-2H3	
C7KET36O	C7H13O2	<chem>CCC(=O)CCC([O])C</chem>	InChI=1S/C7H13O2/c1-3-7(9)5-4-6(2)8/h6H,3-5H2,1-2H3	
C7KET37O	C7H13O2	<chem>CCC(=O)CCCC([O])</chem>	InChI=1S/C7H13O2/c1-2-7(9)5-3-4-6-8/h2-6H2,1H3	

C7KET41O	C7H13O2	CCCC(=O)CCC([O])	InChI=1S/C7H13O2/c1-2-4-7(9)5-3-6-8/h2-6H2,1H3	
C7KET42O	C7H13O2	CCCC(=O)CC([O])C	InChI=1S/C7H13O2/c1-3-4-7(9)5-6(2)8/h6H,3-5H2,1-2H3	
C7KET43O	C7H13O2	CCCC(=O)C([O])CC	InChI=1S/C7H13O2/c1-3-5-7(9)6(8)4-2/h6H,3-5H2,1-2H3	
C7Y24	C7H12O2	CC(=O)CC(=O)CCC	InChI=1S/C7H12O2/c1-3-4-7(9)5-6(2)8/h3-5H2,1-2H3	
C7Y13	C7H12O2	C(=O)CC(=O)CCCC	InChI=1S/C7H12O2/c1-2-3-4-7(9)5-6-8/h6H,2-5H2,1H3	
C7Y35	C7H12O2	CCC(=O)CC(=O)CC	InChI=1S/C7H12O2/c1-3-6(8)5-7(9)4-2/h3-5H2,1-2H3	
C7H14OOH1-2O	C7H15O3	C(OO)C([O])CCCCC	InChI=1S/C7H15O3/c1-2-3-4-5-7(8)6-10-9/h7,9H,2-6H2,1H3	
C7H14OOH1-3O	C7H15O3	C(OO)CC([O])CCCC	InChI=1S/C7H15O3/c1-2-3-4-7(8)5-6-10-9/h7,9H,2-6H2,1H3	
C7H14OOH1-4O	C7H15O3	C(OO)CCC([O])CCC	InChI=1S/C7H15O3/c1-2-4-7(8)5-3-6-10-9/h7,9H,2-6H2,1H3	
C7H14OOH1-5O	C7H15O3	C(OO)CCCC([O])CC	InChI=1S/C7H15O3/c1-2-7(8)5-3-4-6-10-9/h7,9H,2-6H2,1H3	

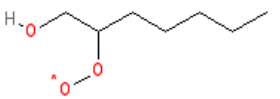
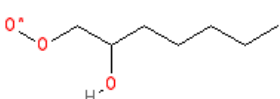
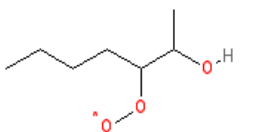
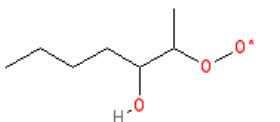
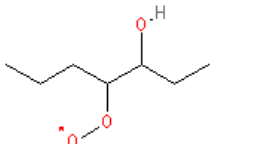
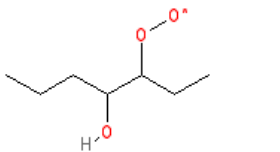
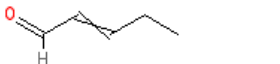
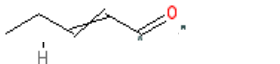
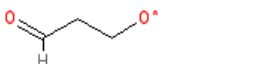
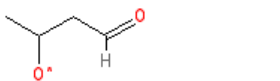
C7H14OOH2-1O	C7H15O3	C([O])C(OO)CCCC	InChI=1S/C7H15O3/c1-2-3-4-5-7(6-8)10-9/h7,9H,2-6H2,1H3	
C7H14OOH2-3O	C7H15O3	CC(OO)C([O])CCCC	InChI=1S/C7H15O3/c1-3-4-5-7(8)6(2)10-9/h6-7,9H,3-5H2,1-2H3	
C7H14OOH2-4O	C7H15O3	CC(OO)CC([O])CCC	InChI=1S/C7H15O3/c1-3-4-7(8)5-6(2)10-9/h6-7,9H,3-5H2,1-2H3	
C7H14OOH2-5O	C7H15O3	CC(OO)CCC([O])CC	InChI=1S/C7H15O3/c1-3-7(8)5-4-6(2)10-9/h6-7,9H,3-5H2,1-2H3	
C7H14OOH2-6O	C7H15O3	CC(OO)CCCC([O])C	InChI=1S/C7H15O3/c1-6(8)4-3-5-7(2)10-9/h6-7,9H,3-5H2,1-2H3	
C7H14OOH3-1O	C7H15O3	C([O])CC(OO)CCCC	InChI=1S/C7H15O3/c1-2-3-4-7(10-9)5-6-8/h7,9H,2-6H2,1H3	
C7H14OOH3-2O	C7H15O3	CC([O])C(OO)CCCC	InChI=1S/C7H15O3/c1-3-4-5-7(10-9)6(2)8/h6-7,9H,3-5H2,1-2H3	
C7H14OOH3-4O	C7H15O3	CCC(OO)C([O])CCC	InChI=1S/C7H15O3/c1-3-5-6(8)7(4-2)10-9/h6-7,9H,3-5H2,1-2H3	
C7H14OOH3-5O	C7H15O3	CCC(OO)CC([O])CC	InChI=1S/C7H15O3/c1-3-6(8)5-7(4-2)10-9/h6-7,9H,3-5H2,1-2H3	
C7H14OOH3-6O	C7H15O3	CCC(OO)CCC([O])C	InChI=1S/C7H15O3/c1-3-7(10-9)5-4-6(2)8/h6-7,9H,3-5H2,1-2H3	



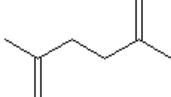
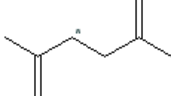
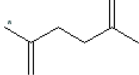
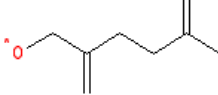
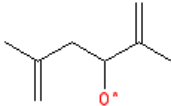
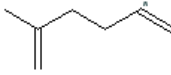
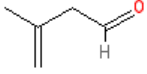
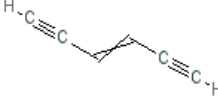
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C7H14OOH4-1O	C7H15O3	CCCC(OO)CCC([O])	InChI=1S/C7H15O3/c1-2-4-7(10-9)5-3-6-8/h7,9H,2-6H2,1H3	
C7H14OOH4-2O	C7H15O3	CCCC(OO)CC([O])C	InChI=1S/C7H15O3/c1-3-4-7(10-9)5-6(2)8/h6-7,9H,3-5H2,1-2H3	
C7H14OOH4-3O	C7H15O3	CCCC(OO)C([O])CC	InChI=1S/C7H15O3/c1-3-5-7(10-9)6(8)4-2/h6-7,9H,3-5H2,1-2H3	
C6H11O13-6	C6H11O	C1CC(O1)CC[CH2]	InChI=1S/C6H11O/c1-2-3-6-4-5-7-6/h6H,1-5H2	
C6H11O14-6	C6H11O	C1CCC(O1)C[CH2]	InChI=1S/C6H11O/c1-2-6-4-3-5-7-6/h6H,1-5H2	
C6H11O15-6	C6H11O	C1CCCC(O1)[CH2]	InChI=1S/C6H11O/c1-6-4-2-3-5-7-6/h6H,1-5H2	
C6H11O23-1	C6H11O	[CH2]C1C(O1)CCC	InChI=1S/C6H11O/c1-3-4-6-5(2)7-6/h5-6H,2-4H2,1H3	
C6H11O23-6	C6H11O	CC1C(O1)CC[CH2]	InChI=1S/C6H11O/c1-3-4-6-5(2)7-6/h5-6H,1,3-4H2,2H3	
C6H11O24-1	C6H11O	[CH2]C1CC(O1)CC	InChI=1S/C6H11O/c1-3-6-4-5(2)7-6/h5-6H,2-4H2,1H3	

C6H11O24-6	C6H11O	CC1CC(O1)C[CH2]	InChI=1S/C6H11O/c1-3-6-4-5(2)7-6/h5-6H,1,3-4H2,2H3	
C6H11O34-1	C6H11O	CCC1C(O1)C[CH2]	InChI=1S/C6H11O/c1-3-5-6(4-2)7-5/h5-6H,1,3-4H2,2H3	
C6Y2-1J	C6H11O	[CH2]C(=O)CCCC	InChI=1S/C6H11O/c1-3-4-5-6(2)7/h2-5H2,1H3	
C6Y3-6J	C6H11O	[CH2]CCC(=O)CC	InChI=1S/C6H11O/c1-3-5-6(7)4-2/h1,3-5H2,2H3	
C6Y3-1J	C6H11O	[CH2]CC(=O)CCC	InChI=1S/C6H11O/c1-3-5-6(7)4-2/h2-5H2,1H3	
C7H14-1	C7H14	C=CCCCC	InChI=1S/C7H14/c1-3-5-7-6-4-2/h3H,1,4-7H2,2H3	
C7H14-2	C7H14	CC=CCCC	InChI=1S/C7H14/c1-3-5-7-6-4-2/h3,5H,4,6-7H2,1-2H3	
C7H14-3	C7H14	CCC=CCCC	InChI=1S/C7H14/c1-3-5-7-6-4-2/h5,7H,3-4,6H2,1-2H3	
C7H131-3	C7H13	C=C[CH]CCCC	InChI=1S/C7H13/c1-3-5-7-6-4-2/h3,5H,1,4,6-7H2,2H3	
C7H131-4	C7H13	C=CC[CH]CCC	InChI=1S/C7H13/c1-3-5-7-6-4-2/h3,7H,1,4-6H2,2H3	

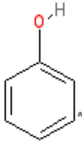
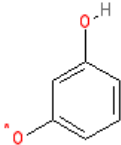
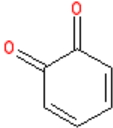
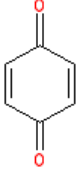
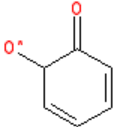
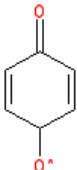
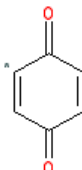


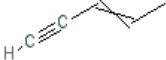
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C7H131-6	C7H13	<chem>C=CCCC[CH]C</chem>	InChI=1S/C7H13/c1-3-5-7-6-4-2/h3-4H,1,5-7H2,2H3	
C7H131-7	C7H13	<chem>C=CCCCC[CH2]</chem>	InChI=1S/C7H13/c1-3-5-7-6-4-2/h3H,1-2,4-7H2	
C7H132-4	C7H13	<chem>CC=C[CH]CCC</chem>	InChI=1S/C7H13/c1-3-5-7-6-4-2/h3,5,7H,4,6H2,1-2H3	
C7H132-5	C7H13	<chem>CC=CC[CH]CC</chem>	InChI=1S/C7H13/c1-3-5-7-6-4-2/h3,5-6H,4,7H2,1-2H3	
C7H132-6	C7H13	<chem>CC=CCC[CH]C</chem>	InChI=1S/C7H13/c1-3-5-7-6-4-2/h3-5H,6-7H2,1-2H3	
C7H132-7	C7H13	<chem>CC=CCCC[CH2]</chem>	InChI=1S/C7H13/c1-3-5-7-6-4-2/h4,6H,1,3,5,7H2,2H3	
C7H133-1	C7H13	<chem>[CH2]CC=CCCC</chem>	InChI=1S/C7H13/c1-3-5-7-6-4-2/h5,7H,1,3-4,6H2,2H3	
C7H133-5	C7H13	<chem>CCC=C[CH]CC</chem>	InChI=1S/C7H13/c1-3-5-7-6-4-2/h5-7H,3-4H2,1-2H3	
C7H133-6	C7H13	<chem>CCC=CC[CH]C</chem>	InChI=1S/C7H13/c1-3-5-7-6-4-2/h3,6-7H,4-5H2,1-2H3	

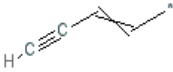




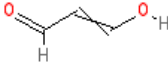


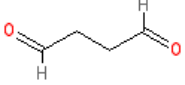
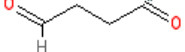
C7H133-7	C7H13	CCC=CCC[CH2]	InChI=1S/C7H13/c1-3-5-7-6-4-2/h6-7H,1,3-5H2,2H3	
C7H13-1D3O	C7H13O	C=CC([O])CCCC	InChI=1S/C7H13O/c1-3-5-6-7(8)4-2/h4,7H,2-3,5-6H2,1H3	
C7H13-2D4O	C7H13O	CC=CC([O])CCC	InChI=1S/C7H13O/c1-3-5-7(8)6-4-2/h3,5,7H,4,6H2,1-2H3	
C7H13-3D5O	C7H13O	CCC=CC([O])CC	InChI=1S/C7H13O/c1-3-5-6-7(8)4-2/h5-7H,3-4H2,1-2H3	
C7H14OH-1J2	C7H15O	C(O)[CH]CCCCC	InChI=1S/C7H15O/c1-2-3-4-5-6-7-8/h6,8H,2-5,7H2,1H3	
C7H14OH-2J1	C7H15O	[CH2]C(O)CCCCC	InChI=1S/C7H15O/c1-3-4-5-6-7(2)8/h7-8H,2-6H2,1H3	
C7H14OH-2J3	C7H15O	CC(O)[CH]CCCC	InChI=1S/C7H15O/c1-3-4-5-6-7(2)8/h6-8H,3-5H2,1-2H3	
C7H14OH-3J2	C7H15O	C[CH]C(O)CCCC	InChI=1S/C7H15O/c1-3-5-6-7(8)4-2/h4,7-8H,3,5-6H2,1-2H3	
C7H14OH-3J4	C7H15O	CCC(O)[CH]CCC	InChI=1S/C7H15O/c1-3-5-6-7(8)4-2/h6-8H,3-5H2,1-2H3	
C7H14OH-4J3	C7H15O	CC[CH]C(O)CCC	InChI=1S/C7H15O/c1-3-5-7(8)6-4-2/h5,7-8H,3-4,6H2,1-2H3	

C7H14OH-1O2-2	C7H15O3	C(O)C(O[O])CCCCC	InChI=1S/C7H15O3/c1-2-3-4-5-7(6-8)10-9/h7-8H,2-6H2,1H3	
C7H14OH-2O2-1	C7H15O3	C(O[O])C(O)CCCCC	InChI=1S/C7H15O3/c1-2-3-4-5-7(8)6-10-9/h7-8H,2-6H2,1H3	
C7H14OH-2O2-3	C7H15O3	CC(O)C(O[O])CCCC	InChI=1S/C7H15O3/c1-3-4-5-7(10-9)6(2)8/h6-8H,3-5H2,1-2H3	
C7H14OH-3O2-2	C7H15O3	CC(O[O])C(O)CCCC	InChI=1S/C7H15O3/c1-3-4-5-7(8)6(2)10-9/h6-8H,3-5H2,1-2H3	
C7H14OH-3O2-4	C7H15O3	CCC(O)C(O[O])CCC	InChI=1S/C7H15O3/c1-3-5-7(10-9)6(8)4-2/h6-8H,3-5H2,1-2H3	
C7H14OH-4O2-3	C7H15O3	CCC(O[O])C(O)CCC	InChI=1S/C7H15O3/c1-3-5-6(8)7(4-2)10-9/h6-8H,3-5H2,1-2H3	
C5D2Y1	C5H8O	C(=O)C=CCC	InChI=1S/C5H8O/c1-2-3-4-5-6/h3-5H,2H2,1H3	
C5D2Y1-1R	C5H7O	CCC=C[C]=O	InChI=1S/C5H7O/c1-2-3-4-5-6/h3-4H,2H2,1H3	
C3Y1-3OR	C3H5O2	C([O])CC=O	InChI=1S/C3H5O2/c4-2-1-3-5/h2H,1,3H2	
C4Y1-3OR	C4H7O2	CC([O])CC=O	InChI=1S/C4H7O2/c1-4(6)2-3-5/h3-4H,2H2,1H3	

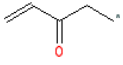
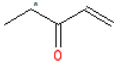
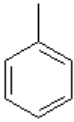
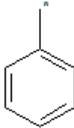
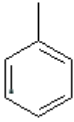
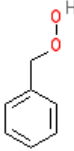
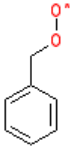
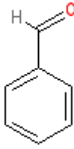
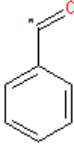
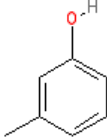
C6D2Y1	C6H10O	CCCC=CC(=O)	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h4-6H,2-3H2,1H3	
C6D2Y1-1R	C6H9O	CCCC=C[C](=O)	InChI=1S/C6H9O/c1-2-3-4-5-6-7/h4-5H,2-3H2,1H3	
H15DE25DM	C8H14	C=C(C)CCC(=C)C	InChI=1S/C8H14/c1-7(2)5-6-8(3)4/h1,3,5-6H2,2,4H3	
H15DE25DM-S	C8H13	C=C(C)[CH]CC(=C)C	InChI=1S/C8H13/c1-7(2)5-6-8(3)4/h5H,1,3,6H2,2,4H3	
H15DE25DM-A	C8H13	C=C([CH2])CCC(=C)C	InChI=1S/C8H13/c1-7(2)5-6-8(3)4/h1-3,5-6H2,4H3	
H15DE25DM-AO	C8H13O	C=C(C)CCC(=C)C[O]	InChI=1S/C8H13O/c1-7(2)4-5-8(3)6-9/h1,3-6H2,2H3	
H15DE25DM-SO	C8H13O	C=C(C)CC(C(=C)C)[O]	InChI=1S/C8H13O/c1-6(2)5-8(9)7(3)4/h8H,1,3,5H2,2,4H3	
H15DE2M-T	C7H11	C=[C]CCC(=C)C	InChI=1S/C7H11/c1-4-5-6-7(2)3/h1-2,5-6H2,3H3	
IC4H7CHO	C5H8O	C=C(C)CC=O	InChI=1S/C5H8O/c1-5(2)3-4-6/h4H,1,3H2,2H3	
L-C6H4	C6H4	C#CC=CC#C	InChI=1S/C6H4/c1-3-5-6-4-2/h1-2,5-6H	

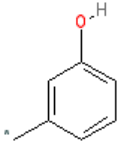
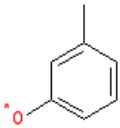
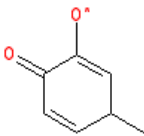
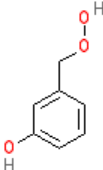
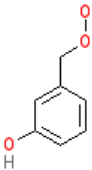
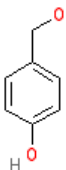
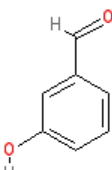
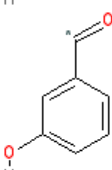
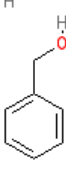
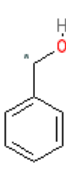
C-C6H4	C6H4	<chem>C#CC#CC=C</chem>	InChI=1S/C6H4/c1-3-5-6-4-2/h1,4H,2H2	
C6H3	C6H3	<chem>C#C[C]=CC#C</chem>	InChI=1S/C6H3/c1-3-5-6-4-2/h1-2,5H	
C6H2	C6H2	<chem>C#CC#CC#C</chem>	InChI=1S/C6H2/c1-3-5-6-4-2/h1-2H	
C6H6	C6H6	<chem>C1=CC=CC=C1</chem>	InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H	
FULVENE	C6H6	<chem>C=C1C=CC=C1</chem>	InChI=1S/C6H6/c1-6-4-2-3-5-6/h2-5H,1H2	
C6H5	C6H5	<chem>C1=[C]C=CC=C1</chem>	InChI=1S/C6H5/c1-2-4-6-5-3-1/h1-5H	
C6H5OO	C6H5O2	<chem>C1=C(O[O])C=CC=C1</chem>	InChI=1S/C6H5O2/c7-8-6-4-2-1-3-5-6/h1-5H	
C6H5OOH	C6H6O2	<chem>C1=C(OO)C=CC=C1</chem>	InChI=1S/C6H6O2/c7-8-6-4-2-1-3-5-6/h1-5,7H	
C6H5OH	C6H6O	<chem>C1(O)=CC=CC=C1</chem>	InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H	
C6H5O	C6H5O	<chem>C1([O])=CC=CC=C1</chem>	InChI=1S/C6H5O/c7-6-4-2-1-3-5-6/h1-5H	

C6H4OH	C6H5O	C1=[C]C=C(O)C=C1	InChI=1S/C6H5O/c7-6-4-2-1-3-5-6/h1-2,4-5,7H	
OC6H4OH	C6H5O2	C1=C([O])C=C(O)C=C1	InChI=1S/C6H5O2/c7-5-2-1-3-6(8)4-5/h1-4,7H	
O-C6H4O2	C6H4O2	C1(=O)C(=O)C=CC=C1	InChI=1S/C6H4O2/c7-5-3-1-2-4-6(5)8/h1-4H	
P-C6H4O2	C6H4O2	C1(=O)C=CC(=O)C=C1	InChI=1S/C6H4O2/c7-5-1-2-6(8)4-3-5/h1-4H	
O-OC6H5OJ	C6H5O2	C1(=O)C([O])C=CC=C1	InChI=1S/C6H5O2/c7-5-3-1-2-4-6(5)8/h1-5H	
P-OC6H5OJ	C6H5O2	C1(=O)C=CC([O])C=C1	InChI=1S/C6H5O2/c7-5-1-2-6(8)4-3-5/h1-5H	
P-C6H3O2	C6H3O2	C1(=O)[C]=CC(=O)C=C1	InChI=1S/C6H3O2/c7-5-1-2-6(8)4-3-5/h1-3H	
C5H6	C5H6	C1C=CC=C1	InChI=1S/C5H6/c1-2-4-5-3-1/h1-4H,5H2	
C5H5	C5H5	[CH]1C=CC=C1	InChI=1S/C5H5/c1-2-4-5-3-1/h1-5H	
C5H6-L	C5H6	C#CC=CC	InChI=1S/C5H6/c1-3-5-4-2/h1,4-5H,2H3	

C#CCVCCJ	C5H5	C#CC=C[CH2]	InChI=1S/C5H5/c1-3-5-4-2/h1,4-5H,2H2	
C5H7	C5H7	C1C[CH]C=C1	InChI=1S/C5H7/c1-2-4-5-3-1/h1-3H,4-5H2	
CVCCJCVC	C5H7	C=C[CH]C=C	InChI=1S/C5H7/c1-3-5-4-2/h3-5H,1-2H2	
CVCCVCCJ	C5H7	C=CC=C[CH2]	InChI=1S/C5H7/c1-3-5-4-2/h3-5H,1-2H2	
CVCCJCVCOH	C5H7O	C=C[CH]C=C(O)	InChI=1S/C5H7O/c1-2-3-4-5-6/h2-6H,1H2	
HOCVCCVO	C3H4O2	C(O)=CC=O	InChI=1S/C3H4O2/c4-2-1-3-5/h1-4H	
CVCCVCCOH	C5H8O	C=CC=CC(O)	InChI=1S/C5H8O/c1-2-3-4-5-6/h2-4,6H,1,5H2	
OC5H7O	C5H7O2	C(=O)[CH]CCC(=O)	InChI=1S/C5H7O2/c6-4-2-1-3-5-7/h2,4-5H,1,3H2	
OC4H6O	C4H6O2	C(=O)CCC(=O)	InChI=1S/C4H6O2/c5-3-1-2-4-6/h3-4H,1-2H2	
OC4H5O	C4H5O2	C(=O)CC[C](=O)	InChI=1S/C4H5O2/c5-3-1-2-4-6/h3H,1-2H2	

O2CCHOOJ	C2HO4	C(=O)(O)C(=O)[O]	InChI=1S/C2HO4/c3-1(4)2(5)6/h(H,3,4)	
HOVCCCJVO	C3H3O2	C(O)=C[C]=O	InChI=1S/C3H3O2/c4-2-1-3-5/h1-2,4H	
C5H5OH	C5H6O	C1(O)C=CC=C1	InChI=1S/C5H6O/c6-5-3-1-2-4-5/h1-6H	
C5H5O	C5H5O	C1([O])C=CC=C1	InChI=1S/C5H5O/c6-5-3-1-2-4-5/h1-5H	
C5H4OH	C5H5O	[C](O)1C=CC=C1	InChI=1S/C5H5O/c6-5-3-1-2-4-5/h1-4,6H	
C5H4O	C5H4O	C1(=O)C=CC=C1	InChI=1S/C5H4O/c6-5-3-1-2-4-5/h1-4H	
C5H3O	C5H3O	C1(=O)[C]=CC=C1	InChI=1S/C5H3O/c6-5-3-1-2-4-5/h1-3H	
CJVCCVCCVO	C5H5O	[CH]=CC=CC=O	InChI=1S/C5H5O/c1-2-3-4-5-6/h1-5H	
CVCCVCCJVO	C5H5O	C=CC=C[C]=O	InChI=1S/C5H5O/c1-2-3-4-5-6/h2-4H,1H2	
CJVCCVO	C3H3O	[CH]=CC=O	InChI=1S/C3H3O/c1-2-3-4/h1-3H	

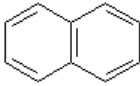
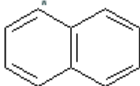
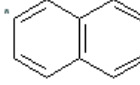
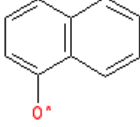
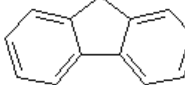
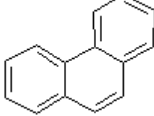
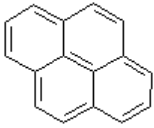



PC2H4COC2H3	C5H7O	<chem>[CH2]CC(=O)C=C</chem>	InChI=1S/C5H7O/c1-3-5(6)4-2/h3H,1-2,4H2	
SC2H4COC2H3	C5H7O	<chem>C=CC(=O)[CH]C</chem>	InChI=1S/C5H7O/c1-3-5(6)4-2/h3-4H,1H2,2H3	
C6H5CH3	C7H8	<chem>c1cc(C)ccc1</chem>	InChI=1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3	
C6H5CH2	C7H7	<chem>c1cc([CH2])ccc1</chem>	InChI=1S/C7H7/c1-7-5-3-2-4-6-7/h2-6H,1H2	
C6H4CH3	C7H7	<chem>Cc1c[c]ccc1</chem>	InChI=1S/C7H7/c1-7-5-3-2-4-6-7/h2-3,5-6H,1H3	
BZCOOH	C7H8O2	<chem>c1c(COO)cccc1</chem>	InChI=1S/C7H8O2/c8-9-6-7-4-2-1-3-5-7/h1-5,8H,6H2	
C6H5CH2OO	C7H7O2	<chem>c1c(CO[O])cccc1</chem>	InChI=1S/C7H7O2/c8-9-6-7-4-2-1-3-5-7/h1-5H,6H2	
C6H5CHO	C7H6O	<chem>c1c(C=O)cccc1</chem>	InChI=1S/C7H6O/c8-6-7-4-2-1-3-5-7/h1-6H	
C6H5CO	C7H5O	<chem>C1=CC([C]=O)=CC=C1</chem>	InChI=1S/C7H5O/c8-6-7-4-2-1-3-5-7/h1-5H	
HOC6H4CH3	C7H8O	<chem>C1=CC(C)=CC(O)=C1</chem>	InChI=1S/C7H8O/c1-6-3-2-4-7(8)5-6/h2-5,8H,1H3	

HOC6H4CH2	C7H7O	C1=CC([CH2])=CC(O)=C1	InChI=1S/C7H7O/c1-6-3-2-4-7(8)5-6/h2-5,8H,1H2	
OC6H4CH3	C7H7O	C1=CC(C)=CC([O])=C1	InChI=1S/C7H7O/c1-6-3-2-4-7(8)5-6/h2-5H,1H3	
OCH3C6H4O	C7H7O2	CC1C=CC(=O)C([O])=C1	InChI=1S/C7H7O2/c1-5-2-3-6(8)7(9)4-5/h2-5H,1H3	
HOC6H4CH2OOH	C7H8O3	C1=CC(COO)=CC(O)=C1	InChI=1S/C7H8O3/c8-7-3-1-2-6(4-7)5-10-9/h1-4,8-9H,5H2	
HOC6H4CH2OO	C7H7O3	C1=CC(CO[O])=CC(O)=C1	InChI=1S/C7H7O3/c8-7-3-1-2-6(4-7)5-10-9/h1-4,8H,5H2	
HOC6H4CH2O	C7H7O2	[O]Cc1ccc(O)cc1	InChI=1S/C7H7O2/c8-5-6-1-3-7(9)4-2-6/h1-4,9H,5H2	
HOC6H4CHO	C7H6O2	C1=CC(C=O)=CC(O)=C1	InChI=1S/C7H6O2/c8-5-6-2-1-3-7(9)4-6/h1-5,9H	
HOC6H4CO	C7H5O2	C1=CC([C]=O)=CC(O)=C1	InChI=1S/C7H5O2/c8-5-6-2-1-3-7(9)4-6/h1-4,9H	
C6H5CH2OH	C7H8O	C1=CC(CO)=CC=C1	InChI=1S/C7H8O/c8-6-7-4-2-1-3-5-7/h1-5,8H,6H2	
C6H5CHOH	C7H7O	C1=CC([CH]O)=CC=C1	InChI=1S/C7H7O/c8-6-7-4-2-1-3-5-7/h1-6,8H	

C ₆ H ₅ CH ₂ O	C ₇ H ₇ O	C1=CC(C[O])=CC=C1	InChI=1S/C ₇ H ₇ O/c8-6-7-4-2-1-3-5-7/h1-5H,6H2	
C ₆ H ₅ C ₂ H ₅	C ₈ H ₁₀	C1=CC(CC)=CC=C1	InChI=1S/C ₈ H ₁₀ /c1-2-8-6-4-3-5-7-8/h3-7H,2H2,1H3	
C ₆ H ₅ CHCH ₃	C ₈ H ₉	C1=CC([CH]C)=CC=C1	InChI=1S/C ₈ H ₉ /c1-2-8-6-4-3-5-7-8/h2-7H,1H3	
C ₆ H ₅ CH ₂ CH ₂	C ₈ H ₉	C1=CC(C[CH ₂])=CC=C1	InChI=1S/C ₈ H ₉ /c1-2-8-6-4-3-5-7-8/h3-7H,1-2H2	
C ₆ H ₅ C ₂ H ₃	C ₈ H ₈	C1=CC(C=C)=CC=C1	InChI=1S/C ₈ H ₈ /c1-2-8-6-4-3-5-7-8/h2-7H,1H2	
C ₆ H ₅ CCH ₂	C ₈ H ₇	C1=CC([C]=C)=CC=C1	InChI=1S/C ₈ H ₇ /c1-2-8-6-4-3-5-7-8/h3-7H,1H2	
C ₆ H ₅ CHCH	C ₈ H ₇	C1=CC(C=[CH])=CC=C1	InChI=1S/C ₈ H ₇ /c1-2-8-6-4-3-5-7-8/h1-7H	
C ₁₄ H ₁₄	C ₁₄ H ₁₄	c(cc1)ccc1CCc2ccc(cc2)	InChI=1S/C ₁₄ H ₁₄ /c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-14/h1-10H,11-12H2	
C ₁₄ H ₁₃	C ₁₄ H ₁₃	c(cc1)ccc1[CH]Cc2ccc(cc2)	InChI=1S/C ₁₄ H ₁₃ /c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-14/h1-11H,12H2	
C ₁₄ H ₁₂	C ₁₄ H ₁₂	c(cc1)ccc1C=Cc2ccc(cc2)	InChI=1S/C ₁₄ H ₁₂ /c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-14/h1-12H	

C14H11	C14H11	<chem>c(cc1)ccc1[C]=Cc2ccc(cc2)</chem>	InChI=1S/C14H11/c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-14/h1-11H	
C14H13OOH	C14H14O2	<chem>c(cc1)ccc1C(OO)Cc2ccc(cc2)</chem>	InChI=1S/C14H14O2/c15-16-14(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-10,14-15H,11H2	
C14H13OO	C14H13O2	<chem>c(cc1)ccc1C(O[O])Cc2ccc(cc2)</chem>	InChI=1S/C14H13O2/c15-16-14(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-10,14H,11H2	
C14H12OOH	C14H13O2	<chem>C(=C1)C=C(C=C1)C(OO)[CH]C(C=C2)=CC(=C2)</chem>	InChI=1S/C14H13O2/c15-16-14(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-11,14-15H	
C14H12O2H-1O2	C14H13O4	<chem>C(=C1)C=C(C=C1)C(OO)C(O[O])C(C=C2)=CC(=C2)</chem>	InChI=1S/C14H13O4/c15-17-13(11-7-3-1-4-8-11)14(18-16)12-9-5-2-6-10-12/h1-10,13-15H	
C14H11O-1O2H	C14H12O3	<chem>C(=C1)C=C(C=C1)C(=O)C(OO)C(C=C2)=CC(=C2)</chem>	InChI=1S/C14H12O3/c15-13(11-7-3-1-4-8-11)14(17-16)12-9-5-2-6-10-12/h1-10,14,16H	
C14H13O	C14H13O	<chem>c(cc1)ccc1C([O])Cc2ccc(cc2)</chem>	InChI=1S/C14H13O/c15-14(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-10,14H,11H2	
C14H12O	C14H12O	<chem>O=C(CC1C=CC=CC=1)C1C=CC=CC=1</chem>	InChI=1S/C14H12O/c15-14(13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-10H,11H2	
O-O2C6H4CH3	C7H7O2	<chem>C1(C)=C(O[O])C=CC=C1</chem>	InChI=1S/C7H7O2/c1-6-4-2-3-5-7(6)9-8/h2-5H,1H3	
OC6H4CH2	C7H6O	<chem>C=C1C=CC=CC1=O</chem>	InChI=1S/C7H6O/c1-6-4-2-3-5-7(6)8/h2-5H,1H2	

C6H5CHOOCH3	C8H9O2	CC(O[O])C1C=CC=CC=1	InChI=1S/C8H9O2/c1-7(10-9)8-5-3-2-4-6-8/h2-7H,1H3	
C6H5CH2CH2OO	C8H9O2	[O]OCCC1C=CC=CC=1	InChI=1S/C8H9O2/c9-10-7-6-8-4-2-1-3-5-8/h1-5H,6-7H2	
C7H6	C7H6	C=C=C1C=CC=C1	InChI=1S/C7H6/c1-2-7-5-3-4-6-7/h3-6H,1H2	
C7H5	C7H5	[CH]=C=C1C=CC=C1	InChI=1S/C7H5/c1-2-7-5-3-4-6-7/h1,3-6H	
IND	C9H8	C1=CC=C2CC=CC2=C1	InChI=1S/C9H8/c1-2-5-9-7-3-6-8(9)4-1/h1-6H,7H2	
C10H9	C10H9	[CH]1CC=CC2C=CC=CC=21	InChI=1S/C10H9/c1-2-6-10-8-4-3-7-9(10)5-1/h1-3,5-8H,4H2	
C10H10	C10H10	C1C=CC2CCC=CC=2C=1	InChI=1S/C10H10/c1-2-6-10-8-4-3-7-9(10)5-1/h1-3,5-7H,4,8H2	
C5H5CH3	C6H8	CC1C=CC=C1	InChI=1S/C6H8/c1-6-4-2-3-5-6/h2-6H,1H3	
C9H7	C9H7	[CH]1C=CC2=CC=CC=C12	InChI=1S/C9H7/c1-2-5-9-7-3-6-8(9)4-1/h1-7H	
C9H6O	C9H6O	C1=CC=CC2=C1C(=O)C(=	InChI=1S/C9H6O/c10-9-6-5-7-3-1-2-4-8(7)9/h1-6H	

NAPH	C10H8	<chem>C1C=CC2C=CC=CC=2C=1</chem>	InChI=1S/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H	
NAPH-	C10H7	<chem>[C]1=CC=CC2=C1C=C(C=C2)</chem>	InChI=1S/C10H7/c1-2-6-10-8-4-3-7-9(10)5-1/h1-7H	
NAPHV	C10H7	<chem>C1=[C]C=CC2=C1C=C(C=C2)</chem>	InChI=1S/C10H7/c1-2-6-10-8-4-3-7-9(10)5-1/h1-3,5-8H	
NAPHO	C10H7O	<chem>[O]C1=CC=CC2C=CC=CC=21</chem>	InChI=1S/C10H7O/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H	
FLUORENE	C13H10	<chem>C1=CC=C2C(=C1)CC1=CC=CC=C12</chem>	InChI=1S/C13H10/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)12/h1-8H,9H2	
C14H10	C14H10	<chem>C1=CC=C2C(C=CC3=CC=CC=C32)=C1</chem>	InChI=1S/C14H10/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1-10H	
C16H10	C16H10	<chem>C1=CC2=CC=C3C=CC=C4C=CC(=C1)C2=C43</chem>	InChI=1S/C16H10/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h1-10H	
C*CC*C*O	C4H4O	<chem>C=CC=C=O</chem>	InChI=1S/C4H4O/c1-2-3-4-5/h2-3H,1H2	
X135C6H8	C6H8	<chem>C=CC=CC=C</chem>	InChI=1S/C6H8/c1-3-5-6-4-2/h3-6H,1-2H2	
X16C7H113	C7H11	<chem>[CH2]C=CCCC=C</chem>	InChI=1S/C7H11/c1-3-5-7-6-4-2/h3-5H,1-2,6-7H2	

X16C7H114	C7H11	<chem>C=CC[CH]CC=C</chem>	InChI=1S/C7H11/c1-3-5-7-6-4-2/h3-4,7H,1-2,5-6H2	
X15C7H113	C7H11	<chem>[CH2]C=CCC=CC</chem>	InChI=1S/C7H11/c1-3-5-7-6-4-2/h3-6H,1,7H2,2H3	
X15C7H114	C7H11	<chem>C=CC[CH]C=CC</chem>	InChI=1S/C7H11/c1-3-5-7-6-4-2/h3-4,6-7H,1,5H2,2H3	
AEC7H11A	C7H11	<chem>[CH2]C(=C)CCC=C</chem>	InChI=1S/C7H11/c1-4-5-6-7(2)3/h4H,1-3,5-6H2	
AEC7H11C	C7H11	<chem>[CH2]C(C)=CCC=C</chem>	InChI=1S/C7H11/c1-4-5-6-7(2)3/h4,6H,1-2,5H2,3H3	
AEC7H11D	C7H11	<chem>[CH2]C=CCC(=C)C</chem>	InChI=1S/C7H11/c1-4-5-6-7(2)3/h4-5H,1-2,6H2,3H3	
GKC7H11M	C7H11	<chem>[CH2]C(C=C)CC=C</chem>	InChI=1S/C7H11/c1-4-6-7(3)5-2/h4-5,7H,1-3,6H2	
GKC7H11I	C7H11	<chem>C=CCCC=C</chem>	InChI=1S/C7H11/c1-4-6-7(3)5-2/h4-5H,1-2,6H2,3H3	
GKC7H11J	C7H11	<chem>[CH2]C=CC(C)C=C</chem>	InChI=1S/C7H11/c1-4-6-7(3)5-2/h4-7H,1-2H2,3H3	
X16C7H12	C7H12	<chem>C=CCCCC=C</chem>	InChI=1S/C7H12/c1-3-5-7-6-4-2/h3-4H,1-2,5-7H2	

X15C7H12	C7H12	C=CCCC=CC	InChI=1S/C7H12/c1-3-5-7-6-4-2/h3-4,6H,1,5,7H2,2H3	
AEC7H12	C7H12	C=CCCC(=C)C	InChI=1S/C7H12/c1-4-5-6-7(2)3/h4H,1-2,5-6H2,3H3	
GKC7H12	C7H12	C=CCC(C)C=C	InChI=1S/C7H12/c1-4-6-7(3)5-2/h4-5,7H,1-2,6H2,3H3	
MCH1ENE	C7H12	CC1=CCCCC1	InChI=1S/C7H12/c1-7-5-3-2-4-6-7/h5H,2-4,6H2,1H3	
MCH2ENE	C7H12	CC1C=CCCC1	InChI=1S/C7H12/c1-7-5-3-2-4-6-7/h3,5,7H,2,4,6H2,1H3	
MCH3ENE	C7H12	CC1CC=CCC1	InChI=1S/C7H12/c1-7-5-3-2-4-6-7/h2-3,7H,4-6H2,1H3	
CHXDCH2	C7H12	C=C1CCCCC1	InChI=1S/C7H12/c1-7-5-3-2-4-6-7/h1-6H2	
MCH1N3J	C7H11	CC1=C[CH]CCC1	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h3,5H,2,4,6H2,1H3	
MCH1N4J	C7H11	CC1=CC[CH]CC1	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2,5H,3-4,6H2,1H3	
MCH1N5J	C7H11	CC1=CCC[CH]C1	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h3,6H,2,4-5H2,1H3	

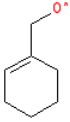

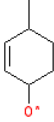

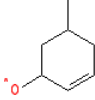


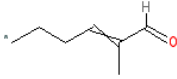
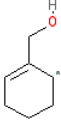
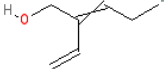
MCH1N6J	C7H11	<chem>CC1=CCCC[CH]1</chem>	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h5-6H,2-4H2,1H3	
MCH2N4J	C7H11	<chem>CC1C=C[CH]CC1</chem>	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2-3,5,7H,4,6H2,1H3	
MCH2N5J	C7H11	<chem>CC1C=CC[CH]C1</chem>	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h3-5,7H,2,6H2,1H3	
MCH2N6J	C7H11	<chem>CC1[CH]CCC=C1</chem>	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h3,5-7H,2,4H2,1H3	
MCH2NCH2J	C7H11	<chem>[CH2]C1C=CCCC1</chem>	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h3,5,7H,1-2,4,6H2	
MCH3N1J	C7H11	<chem>C[C]1CC=CCC1</chem>	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2-3H,4-6H2,1H3	
MCH3N5J	C7H11	<chem>CC1C[CH]C=CC1</chem>	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2-4,7H,5-6H2,1H3	
MCH3N6J	C7H11	<chem>CC1[CH]CC=CC1</chem>	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2-3,6-7H,4-5H2,1H3	
MCH3NCH2J	C7H11	<chem>[CH2]C1CC=CCC1</chem>	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2-3,7H,1,4-6H2	
CHXDCH22J	C7H11	<chem>[CH2]C1=CCCCC1</chem>	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h5H,1-4,6H2	

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









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CHXDCH24J	C7H11	<chem>C=C1CC[CH]CC1</chem>	InChI=1S/C7H11/c1-7-5-3-2-4-6-7/h2H,1,3-6H2	
IKC7H12	C7H12	<chem>CCC(C)=CC=C</chem>	InChI=1S/C7H12/c1-4-6-7(3)5-2/h4,6H,1,5H2,2-3H3	
IKC7H11G	C7H11	<chem>[CH2]CC(C)=CC=C</chem>	InChI=1S/C7H11/c1-4-6-7(3)5-2/h4,6H,1-2,5H2,3H3	
X15C7H116	C7H11	<chem>C=CCCC=[C]C</chem>	InChI=1S/C7H11/c1-3-5-7-6-4-2/h3,6H,1,5,7H2,2H3	
GIC7H11L	C7H11	<chem>[CH2]CC=C(C)C=C</chem>	InChI=1S/C7H11/c1-4-6-7(3)5-2/h5-6H,1-2,4H2,3H3	
C5H7-1	C5H7	<chem>[CH]=C(C)C=C</chem>	InChI=1S/C5H7/c1-4-5(2)3/h2,4H,1H2,3H3	
X12C7H117	C7H11	<chem>[CH2]CCCC=C=C</chem>	InChI=1S/C7H11/c1-3-5-7-6-4-2/h6H,1-3,5,7H2	
CJCC*C*C	C5H7	<chem>[CH2]CC=C=C</chem>	InChI=1S/C5H7/c1-3-5-4-2/h5H,1-3H2	
ACC7H12	C7H12	<chem>CC(=C)C=CCC</chem>	InChI=1S/C7H12/c1-4-5-6-7(2)3/h5-6H,2,4H2,1,3H3	

ACC7H11F	C7H11	<chem>[CH2]CC=CC(=C)C</chem>	InChI=1S/C7H11/c1-4-5-6-7(2)3/h5-6H,1-2,4H2,3H3	
C5H7-4	C5H7	<chem>[CH]=CC(=C)C</chem>	InChI=1S/C5H7/c1-4-5(2)3/h1,4H,2H2,3H3	
CEC7H12	C7H12	<chem>CC(C)C=CC=C</chem>	InChI=1S/C7H12/c1-4-5-6-7(2)3/h4-7H,1H2,2-3H3	
CEC7H11A	C7H11	<chem>[CH2]C(C)C=CC=C</chem>	InChI=1S/C7H11/c1-4-5-6-7(2)3/h4-7H,1-2H2,3H3	
GKC7H11G	C7H11	<chem>[CH]=CC(C)CC=C</chem>	InChI=1S/C7H11/c1-4-6-7(3)5-2/h2,4-5,7H,1,6H2,3H3	
X13C7H117	C7H11	<chem>[CH2]CCC=CC=C</chem>	InChI=1S/C7H11/c1-3-5-7-6-4-2/h3,5,7H,1-2,4,6H2	
X13C7H116	C7H11	<chem>C=CC=CC[CH]C</chem>	InChI=1S/C7H11/c1-3-5-7-6-4-2/h3-5,7H,1,6H2,2H3	
X24C7H12	C7H12	<chem>CC=CC=CCC</chem>	InChI=1S/C7H12/c1-3-5-7-6-4-2/h3,5-7H,4H2,1-2H3	
X24C7H117	C7H11	<chem>[CH2]CC=CC=CC</chem>	InChI=1S/C7H11/c1-3-5-7-6-4-2/h4-7H,1,3H2,2H3	
C5H713-1	C5H7	<chem>[CH]=CC=CC</chem>	InChI=1S/C5H7/c1-3-5-4-2/h1,3-5H,2H3	

X14C7H117	C7H11	<chem>[CH2]CC=CCC=C</chem>	InChI=1S/C7H11/c1-3-5-7-6-4-2/h3,6-7H,1-2,4-5H2	
C5H81-4	C5H8	<chem>C=CCC=C</chem>	InChI=1S/C5H8/c1-3-5-4-2/h3-4H,1-2,5H2	
C5H714-1	C5H7	<chem>[CH]=CCC=C</chem>	InChI=1S/C5H7/c1-3-5-4-2/h1,3-4H,2,5H2	
C5H714-4	C5H7	<chem>C=[C]CC=C</chem>	InChI=1S/C5H7/c1-3-5-4-2/h3H,1-2,5H2	
GMC7H12	C7H12	<chem>C=CC(=C)CCC</chem>	InChI=1S/C7H12/c1-4-6-7(3)5-2/h5H,2-4,6H2,1H3	
GMC7H11L	C7H11	<chem>[CH2]CCC(=C)C=C</chem>	InChI=1S/C7H11/c1-4-6-7(3)5-2/h5H,1-4,6H2	
KMC7H11G	C7H11	<chem>[CH2]CC(=C)CC=C</chem>	InChI=1S/C7H11/c1-4-6-7(3)5-2/h4H,1-3,5-6H2	
X16C7H112	C7H11	<chem>C=[C]CCCC=C</chem>	InChI=1S/C7H11/c1-3-5-7-6-4-2/h3H,1-2,5-7H2	
MCH1N3OJ	C7H11O	<chem>CC1=CC([O])CCC1</chem>	InChI=1S/C7H11O/c1-6-3-2-4-7(8)5-6/h5,7H,2-4H2,1H3	
MCH1N6OJ	C7H11O	<chem>CC1=CCCCC1[O]</chem>	InChI=1S/C7H11O/c1-6-4-2-3-5-7(6)8/h4,7H,2-3,5H2,1H3	

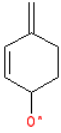

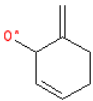
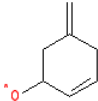
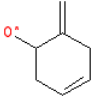


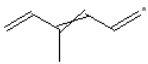
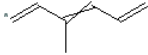

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MCH2N1OJ	C7H11O	CC1([O])C=CCCC1	InChI=1S/C7H11O/c1-7(8)5-3-2-4-6-7/h3,5H,2,4,6H2,1H3	
MCH2N4OJ	C7H11O	CC1C=CC([O])CC1	InChI=1S/C7H11O/c1-6-2-4-7(8)5-3-6/h2,4,6-7H,3,5H2,1H3	
MCH3N2OJ	C7H11O	CC1CCC=CC1[O]	InChI=1S/C7H11O/c1-6-4-2-3-5-7(6)8/h3,5-7H,2,4H2,1H3	
MCH3N5OJ	C7H11O	CC1CC=CC([O])C1	InChI=1S/C7H11O/c1-6-3-2-4-7(8)5-6/h2,4,6-7H,3,5H2,1H3	
CHXDCH22OJ	C7H11O	C=C1CCCCC1[O]	InChI=1S/C7H11O/c1-6-4-2-3-5-7(6)8/h7H,1-5H2	
HC6H10CHO-GL	C7H11O	[CH2]CCC(C)=CC=O	InChI=1S/C7H11O/c1-3-4-7(2)5-6-8/h5-6H,1,3-4H2,2H3	
BC6H10CHO-AF	C7H11O	[CH2]CCC=C(C)C=O	InChI=1S/C7H11O/c1-3-4-5-7(2)6-8/h5-6H,1,3-4H2,2H3	
MCH1CH2OH6J	C7H11O	OCC1=CCCC[CH]1	InChI=1S/C7H11O/c8-6-7-4-2-1-3-5-7/h4-5,8H,1-3,6H2	
HX13N3CH2OH6J	C7H11O	[CH2]CC=C(C=C)CO	InChI=1S/C7H11O/c1-3-5-7(4-2)6-8/h4-5,8H,1-3,6H2	

BT13N2CH2OH1J	C5H7O	[CH]=C(C=C)CO	InChI=1S/C5H7O/c1-3-5(2)4-6/h2-3,6H,1,4H2	
CYHX1N3*O	C6H8O	O=C1C=CCCC1	InChI=1S/C6H8O/c7-6-4-2-1-3-5-6/h2,4H,1,3,5H2	
CYHX1N3*O4J	C6H7O	[O]C1=CCCC=C1	InChI=1S/C6H7O/c7-6-4-2-1-3-5-6/h2,4-5H,1,3H2	
X135C6H73OJ	C6H7O	[CH2]C=CC(=O)C=C	InChI=1S/C6H7O/c1-3-5-6(7)4-2/h3-5H,1-2H2	
X2C6H10CHO-16	C7H11O	[CH2]CCC=CCC=O	InChI=1S/C7H11O/c1-2-3-4-5-6-7-8/h4-5,7H,1-3,6H2	
X3C6H11CHO-27	C7H11O	[CH2]CCC=CC(C)=O	InChI=1S/C7H11O/c1-3-4-5-6-7(2)8/h5-6H,1,3-4H2,2H3	
JC6H10CHO-LG	C7H11O	[CH2]CC(C)C=CC=O	InChI=1S/C7H11O/c1-3-7(2)5-4-6-8/h4-7H,1,3H2,2H3	
DC6H10CHO-FA	C7H11O	[CH2]C(C)CC=CC=O	InChI=1S/C7H11O/c1-7(2)5-3-4-6-8/h3-4,6-7H,1,5H2,2H3	
HX2*CH21*O6J	C7H11O	[CH2]CCCC(=C)C=O	InChI=1S/C7H11O/c1-3-4-5-7(2)6-8/h6H,1-5H2	
MCH13DIEN	C7H10	CC1=CC=CCC1	InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h2-3,5H,4,6H2,1H3	

MCH14DIEN	C7H10	CC1=CCC=CC1	InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h2-3,6H,4-5H2,1H3	
MCH15DIEN	C7H10	CC1=CCCC=CC1	InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h3,5-6H,2,4H2,1H3	
MCH24DIEN	C7H10	CC1C=CC=CC1	InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h2-5,7H,6H2,1H3	
MCH25DIEN	C7H10	CC1C=CCC=CC1	InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h3-7H,2H2,1H3	
CHXDCH22N	C7H10	C=C1C=CCCC1	InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h3,5H,1-2,4,6H2	
CHXDCH23N	C7H10	C=C1CC=CCC1	InChI=1S/C7H10/c1-7-5-3-2-4-6-7/h2-3H,1,4-6H2	
MCH13N5J	C7H9	CC1=C[CH]C=CC1	InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-5H,6H2,1H3	
MCH13N6J	C7H9	CC1=CCC=C[CH]1	InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-3,5-6H,4H2,1H3	
MCH13NCH2J	C7H9	C=C1[CH]C=CCC1	InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-3,5H,1,4,6H2	
MCH14NCH2J	C7H9	[CH2]C1=CCC=CC1	InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-3,6H,1,4-5H2	

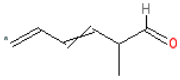
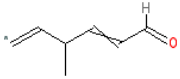
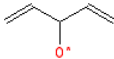
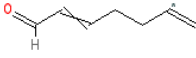
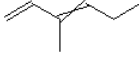

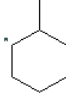

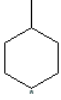
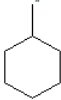
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MCH15NCH2J	C7H9	<chem>C=C1[CH]CCC=C1</chem>	InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h3,5-6H,1-2,4H2	
MCH25N4J	C7H9	<chem>CC1C=C[CH]C=C1</chem>	InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-7H,1H3	
MCH24NCH2J	C7H9	<chem>[CH2]C1C=CC=CC1</chem>	InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-5,7H,1,6H2	
MCH25NCH2J	C7H9	<chem>[CH2]C1C=CCC=C1</chem>	InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h3-7H,1-2H2	
CHXDCH22N5J	C7H9	<chem>C=C1C=CC[CH]C1</chem>	InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h3-5H,1-2,6H2	
CHXDCH23N5J	C7H9	<chem>C=C1C[CH]C=CC1</chem>	InChI=1S/C7H9/c1-7-5-3-2-4-6-7/h2-4H,1,5-6H2	
MCH13N5OJ	C7H9O	<chem>CC1=CC=CC([O])C1</chem>	InChI=1S/C7H9O/c1-6-3-2-4-7(8)5-6/h2-4,7H,5H2,1H3	
MCH13N6OJ	C7H9O	<chem>CC1=CC=CCC1[O]</chem>	InChI=1S/C7H9O/c1-6-4-2-3-5-7(6)8/h2-4,7H,5H2,1H3	
MCH13NCH2OJ	C7H9O	<chem>[O]CC1=CC=CCC1</chem>	InChI=1S/C7H9O/c8-6-7-4-2-1-3-5-7/h1-2,4H,3,5-6H2	

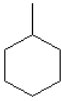
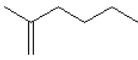
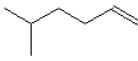
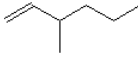
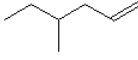
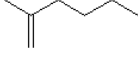
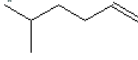
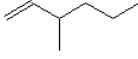
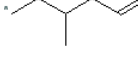
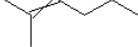
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MCH14N6OJ	C7H9O	<chem>CC1=CCC=CC1[O]</chem>	InChI=1S/C7H9O/c1-6-4-2-3-5-7(6)8/h3-5,7H,2H2,1H3	
MCH14NCH2OJ	C7H9O	<chem>[O]CC1=CCC=CC1</chem>	InChI=1S/C7H9O/c8-6-7-4-2-1-3-5-7/h1-2,5H,3-4,6H2	
MCH15N3OJ	C7H9O	<chem>CC1=CC([O])CC=C1</chem>	InChI=1S/C7H9O/c1-6-3-2-4-7(8)5-6/h2-3,5,7H,4H2,1H3	
MCH15NCH2OJ	C7H9O	<chem>[O]CC1=CCCC=C1</chem>	InChI=1S/C7H9O/c8-6-7-4-2-1-3-5-7/h2,4-5H,1,3,6H2	
MCH24N1OJ	C7H9O	<chem>C1(C)([O])C=CC=CC1</chem>	InChI=1S/C7H9O/c1-7(8)5-3-2-4-6-7/h2-5H,6H2,1H3	
MCH24N6OJ	C7H9O	<chem>CC1C=CC=CC1[O]</chem>	InChI=1S/C7H9O/c1-6-4-2-3-5-7(6)8/h2-7H,1H3	
X135C7H97OJ	C7H9O	<chem>C=CC=CC=CC[O]</chem>	InChI=1S/C7H9O/c1-2-3-4-5-6-7-8/h2-6H,1,7H2	
MCH25N1OJ	C7H9O	<chem>CC1([O])C=CCC=C1</chem>	InChI=1S/C7H9O/c1-7(8)5-3-2-4-6-7/h3-6H,2H2,1H3	
MCH25N4OJ	C7H9O	<chem>CC1C=CC([O])C=C1</chem>	InChI=1S/C7H9O/c1-6-2-4-7(8)5-3-6/h2-7H,1H3	

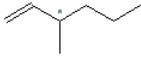
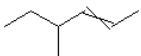
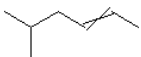
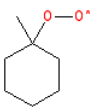
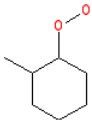
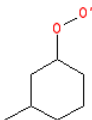
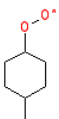
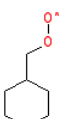
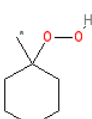
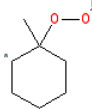
CHXDCH22N4OJ	C7H9O	<chem>C=C1C=CC([O])CC1</chem>	InChI=1S/C7H9O/c1-6-2-4-7(8)5-3-6/h2,4,7H,1,3,5H2	
CHXDCH22N6OJ	C7H9O	<chem>C=C1C=CCCC1[O]</chem>	InChI=1S/C7H9O/c1-6-4-2-3-5-7(6)8/h2,4,7H,1,3,5H2	
CHXDCH23N2OJ	C7H9O	<chem>C=C1CCC=CC1[O]</chem>	InChI=1S/C7H9O/c1-6-4-2-3-5-7(6)8/h3,5,7H,1-2,4H2	
CHXDCH23N5OJ	C7H9O	<chem>C=C1CC=CC([O])C1</chem>	InChI=1S/C7H9O/c1-6-3-2-4-7(8)5-6/h2,4,7H,1,3,5H2	
CHXDCH23N6OJ	C7H9O	<chem>C=C1CC=CCC1[O]</chem>	InChI=1S/C7H9O/c1-6-4-2-3-5-7(6)8/h2-3,7H,1,4-5H2	
X135C7H96J	C7H9	<chem>C=CC=CC=[C]C</chem>	InChI=1S/C7H9/c1-3-5-7-6-4-2/h3,5-7H,1H2,2H3	
X135C7H97J	C7H9	<chem>[CH2]C=CC=CC=C</chem>	InChI=1S/C7H9/c1-3-5-7-6-4-2/h3-7H,1-2H2	
GIKC7H9-L	C7H9	<chem>[CH]=CC=C(C)C=C</chem>	InChI=1S/C7H9/c1-4-6-7(3)5-2/h1,4-6H,2H2,3H3	
GIKC7H9-G	C7H9	<chem>[CH]=CC(C)=CC=C</chem>	InChI=1S/C7H9/c1-4-6-7(3)5-2/h2,4-6H,1H2,3H3	
X124C7H97J	C7H9	<chem>[CH2]CC=CC=C=C</chem>	InChI=1S/C7H9/c1-3-5-7-6-4-2/h5-7H,1-3H2	

C*C*CC*C	C5H6	C=C=CC=C	InChI=1S/C5H6/c1-3-5-4-2/h3,5H,1-2H2	
C*C*CC*CJ	C5H5	[CH]=CC=C=C	InChI=1S/C5H5/c1-3-5-4-2/h1,3,5H,2H2	
ACEC7H9-F	C7H9	[CH]=CC=CC(=C)C	InChI=1S/C7H9/c1-4-5-6-7(2)3/h1,4-6H,2H2,3H3	
ACEC7H9-A	C7H9	[CH]=C(C)C=CC=C	InChI=1S/C7H9/c1-4-5-6-7(2)3/h2,4-6H,1H2,3H3	
ACEC7H9-A2	C7H9	[CH2]C(=C)C=CC=C	InChI=1S/C7H9/c1-4-5-6-7(2)3/h4-6H,1-3H2	
GKMC7H9-L	C7H9	[CH]=CCC(=C)C=C	InChI=1S/C7H9/c1-4-6-7(3)5-2/h1,4-5H,2-3,6H2	
GKMC7H9-G	C7H9	[CH]=CC(=C)CC=C	InChI=1S/C7H9/c1-4-6-7(3)5-2/h2,4-5H,1,3,6H2	
X126C7H95J	C7H9	[CH2]C=CCC=C=C	InChI=1S/C7H9/c1-3-5-7-6-4-2/h3,5-6H,1-2,7H2	
C5H713-4	C5H7	C=CC=[C]C	InChI=1S/C5H7/c1-3-5-4-2/h3,5H,1H2,2H3	
GIKC7H9-M	C7H9	[CH2]C=CC([CH2])=C[CH2]	InChI=1S/C7H9/c1-4-6-7(3)5-2/h4-6H,1-3H2	

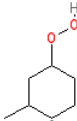
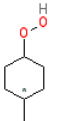
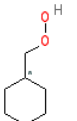
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X136C7H97J	C7H9	<chem>[CH]=CCC=CC=C</chem>	InChI=1S/C7H9/c1-3-5-7-6-4-2/h1,3-4,6-7H,2,5H2	
IKC6H8CHO-GL	C7H9O	<chem>[CH]=CC=C(C)CC=O</chem>	InChI=1S/C7H9O/c1-3-4-7(2)5-6-8/h1,3-4,6H,5H2,2H3	
AC4H6CHO-DA	C5H7O	<chem>[CH]=C(C)CC=O</chem>	InChI=1S/C5H7O/c1-5(2)3-4-6/h1,4H,3H2,2H3	
X24C6H8CHO-72	C7H9O	<chem>C[C]=CC=CCC=O</chem>	InChI=1S/C7H9O/c1-2-3-4-5-6-7-8/h3-5,7H,6H2,1H3	
CYHX13N1J	C6H7	<chem>[C]1=CC=CCC1</chem>	InChI=1S/C6H7/c1-2-4-6-5-3-1/h1-3H,4,6H2	
X135C6H72	C6H7	<chem>C=[C]C=CC=C</chem>	InChI=1S/C6H7/c1-3-5-6-4-2/h3,5-6H,1-2H2	
ADC6H8CHO-FA	C7H9O	<chem>[CH]=C(C)CC=CC=O</chem>	InChI=1S/C7H9O/c1-7(2)5-3-4-6-8/h1,3-4,6H,5H2,2H3	
X25C6H8CHO-72	C7H9O	<chem>C[C]=CCC=CC=O</chem>	InChI=1S/C7H9O/c1-2-3-4-5-6-7-8/h3,5-7H,4H2,1H3	
CYHX24N1*O	C6H6O	<chem>O=C1C=CC=CC1</chem>	InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-4H,5H2	

CEC6H8CHO-AF	C7H9O	<chem>[CH]=CC=CC(C)C=O</chem>	InChI=1S/C7H9O/c1-3-4-5-7(2)6-8/h1,3-7H,2H3	
GJC6H8CHO-LG	C7H9O	<chem>[CH]=CC(C)C=CC=O</chem>	InChI=1S/C7H9O/c1-3-7(2)5-4-6-8/h1,3-7H,2H3	
C5H714-3OJ	C5H7O	<chem>C=CC([O])C=C</chem>	InChI=1S/C5H7O/c1-3-5(6)4-2/h3-5H,1-2H2	
X14C6H8CHO-72	C7H9O	<chem>C(=O)C=CCC[C]=C</chem>	InChI=1S/C7H9O/c1-2-3-4-5-6-7-8/h5-7H,1,3-4H2	
GIC7H12	C7H12	<chem>C=CC(C)=CCC</chem>	InChI=1S/C7H12/c1-4-6-7(3)5-2/h5-6H,2,4H2,1,3H3	
MCHR1	C7H13	<chem>C[C]1CCCCC1</chem>	InChI=1S/C7H13/c1-7-5-3-2-4-6/h2-6H2,1H3	
MCHR2	C7H13	<chem>CC1[CH]CCCC1</chem>	InChI=1S/C7H13/c1-7-5-3-2-4-6/h5,7H,2-4,6H2,1H3	
MCHR3	C7H13	<chem>CC1C[CH]CCC1</chem>	InChI=1S/C7H13/c1-7-5-3-2-4-6/h3,7H,2,4-6H2,1H3	
MCHR4	C7H13	<chem>CC1CC[CH]CC1</chem>	InChI=1S/C7H13/c1-7-5-3-2-4-6/h2,7H,3-6H2,1H3	
CYCHEXCH2	C7H13	<chem>[CH2]C1CCCCC1</chem>	InChI=1S/C7H13/c1-7-5-3-2-4-6-7/h7H,1-6H2	

MCH	C7H14	CC1CCCCC1	InChI=1S/C7H14/c1-7-5-3-2-4-6-7/h7H,2-6H2,1H3	
AC7H14	C7H14	C=C(C)CCCC	InChI=1S/C7H14/c1-4-5-6-7(2)3/h2,4-6H2,1,3H3	
EC7H14	C7H14	C=CCCC(C)C	InChI=1S/C7H14/c1-4-5-6-7(2)3/h4,7H,1,5-6H2,2-3H3	
GC7H14	C7H14	C=CC(C)CCC	InChI=1S/C7H14/c1-4-6-7(3)5-2/h5,7H,2,4,6H2,1,3H3	
KC7H14	C7H14	C=CCC(C)CC	InChI=1S/C7H14/c1-4-6-7(3)5-2/h4,7H,1,5-6H2,2-3H3	
AC7H13F	C7H13	[CH2]CCCC(=C)C	InChI=1S/C7H13/c1-4-5-6-7(2)3/h1-2,4-6H2,3H3	
EC7H13A	C7H13	[CH2]C(C)CCC=C	InChI=1S/C7H13/c1-4-5-6-7(2)3/h4,7H,1-2,5-6H2,3H3	
GC7H13L	C7H13	[CH2]CCC(C)C=C	InChI=1S/C7H13/c1-4-6-7(3)5-2/h5,7H,1-2,4,6H2,3H3	
KC7H13G	C7H13	[CH2]CC(C)CC=C	InChI=1S/C7H13/c1-4-6-7(3)5-2/h4,7H,1-2,5-6H2,3H3	
AC7H13C	C7H13	[CH2]C(C)=CCCC	InChI=1S/C7H13/c1-4-5-6-7(2)3/h6H,2,4-5H2,1,3H3	

GC7H13I	C7H13	<chem>C=CCCCC</chem>	InChI=1S/C7H13/c1-4-6-7(3)5-2/h5H,2,4,6H2,1,3H3	
KC7H13J	C7H13	<chem>[CH2]C=CC(C)CC</chem>	InChI=1S/C7H13/c1-4-6-7(3)5-2/h4,6-7H,1,5H2,2-3H3	
EC7H13D	C7H13	<chem>[CH2]C=CCC(C)C</chem>	InChI=1S/C7H13/c1-4-5-6-7(2)3/h4-5,7H,1,6H2,2-3H3	
MCH10O	C7H13O2	<chem>CC1(O[O])CCCCC1</chem>	InChI=1S/C7H13O2/c1-7(9-8)5-3-2-4-6-7/h2-6H2,1H3	
MCH20O	C7H13O2	<chem>CC1CCCCC1O[O]</chem>	InChI=1S/C7H13O2/c1-6-4-2-3-5-7(6)9-8/h6-7H,2-5H2,1H3	
MCH30O	C7H13O2	<chem>CC1CCCC(O[O])C1</chem>	InChI=1S/C7H13O2/c1-6-3-2-4-7(5-6)9-8/h6-7H,2-5H2,1H3	
MCH40O	C7H13O2	<chem>CC1CCC(O[O])CC1</chem>	InChI=1S/C7H13O2/c1-6-2-4-7(9-8)5-3-6/h6-7H,2-5H2,1H3	
CHXCH2OO	C7H13O2	<chem>[O]OCC1CCCCC1</chem>	InChI=1S/C7H13O2/c8-9-6-7-4-2-1-3-5-7/h7H,1-6H2	
MCH1QX	C7H13O2	<chem>[CH2]C1(OO)CCCCC1</chem>	InChI=1S/C7H13O2/c1-7(9-8)5-3-2-4-6-7/h8H,1-6H2	
MCH1QJ2	C7H13O2	<chem>CC1(OO)[CH]CCCC1</chem>	InChI=1S/C7H13O2/c1-7(9-8)5-3-2-4-6-7/h5,8H,2-4,6H2,1H3	

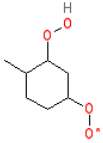
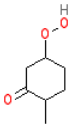
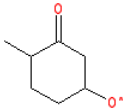
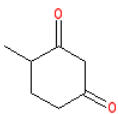
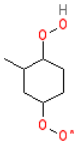
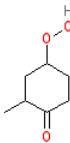
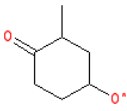
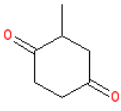
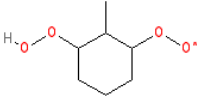
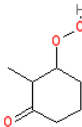
MCH1QJ3	C7H13O2	CC1(OO)C[CH]CCC1	InChI=1S/C7H13O2/c1-7(9-8)5-3-2-4-6-7/h3,8H,2,4-6H2,1H3	
MCH1QJ4	C7H13O2	CC1(OO)CC[CH]CC1	InChI=1S/C7H13O2/c1-7(9-8)5-3-2-4-6-7/h2,8H,3-6H2,1H3	
MCH2QX	C7H13O2	[CH2]C1CCCCC1OO	InChI=1S/C7H13O2/c1-6-4-2-3-5-7(6)9-8/h6-8H,1-5H2	
MCH2QJ3	C7H13O2	CC1CCC[CH]C1OO	InChI=1S/C7H13O2/c1-6-4-2-3-5-7(6)9-8/h5-8H,2-4H2,1H3	
MCH2QJ1	C7H13O2	C[C]1CCCCC1OO	InChI=1S/C7H13O2/c1-6-4-2-3-5-7(6)9-8/h7-8H,2-5H2,1H3	
MCH2QJ4	C7H13O2	CC1CC[CH]CC1OO	InChI=1S/C7H13O2/c1-6-4-2-3-5-7(6)9-8/h3,6-8H,2,4-5H2,1H3	
MCH2QJ5	C7H13O2	CC1C[CH]CCC1OO	InChI=1S/C7H13O2/c1-6-4-2-3-5-7(6)9-8/h2,6-8H,3-5H2,1H3	
MCH2QJ6	C7H13O2	CC1[CH]CCCC1OO	InChI=1S/C7H13O2/c1-6-4-2-3-5-7(6)9-8/h4,6-8H,2-3,5H2,1H3	
MCH3QJ2	C7H13O2	CC1[CH]C(OO)CCC1	InChI=1S/C7H13O2/c1-6-3-2-4-7(5-6)9-8/h5-8H,2-4H2,1H3	
MCH3QJ5	C7H13O2	CC1C[CH]CC(OO)C1	InChI=1S/C7H13O2/c1-6-3-2-4-7(5-6)9-8/h2,6-8H,3-5H2,1H3	

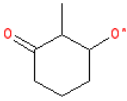
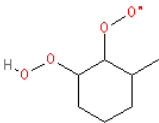
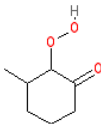
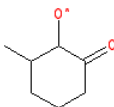
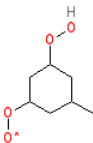
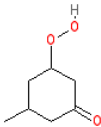
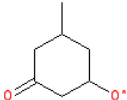
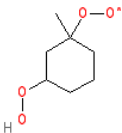
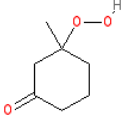
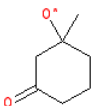
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MCH3QJ6	C7H13O2	CC1[CH]CCC(OO)C1	InChI=1S/C7H13O2/c1-6-3-2-4-7(5-6)9-8/h3,6-8H,2,4-5H2,1H3	
MCH4QJ3	C7H13O2	CC1C[CH]C(OO)CC1	InChI=1S/C7H13O2/c1-6-2-4-7(9-8)5-3-6/h4,6-8H,2-3,5H2,1H3	
MCH4QJ2	C7H13O2	CC1[CH]CC(OO)CC1	InChI=1S/C7H13O2/c1-6-2-4-7(9-8)5-3-6/h2,6-8H,3-5H2,1H3	
MCH4QJ1	C7H13O2	C[C]1CCC(OO)CC1	InChI=1S/C7H13O2/c1-6-2-4-7(9-8)5-3-6/h7-8H,2-5H2,1H3	
CHXJ1CH2Q	C7H13O2	OOC[C]1CCCCC1	InChI=1S/C7H13O2/c8-9-6-7-4-2-1-3-5-7/h8H,1-6H2	
CHXJ2CH2Q	C7H13O2	O OCC1[CH]CCCC1	InChI=1S/C7H13O2/c8-9-6-7-4-2-1-3-5-7/h4,7-8H,1-3,5-6H2	
C7ENE-ONE	C7H12O	C=CCCC(C)C=O	InChI=1S/C7H12O/c1-3-4-5-7(2)6-8/h3,6-7H,1,4-5H2,2H3	
C7ENE-ONEJ	C7H11O	C=CCCC(C)[C]=O	InChI=1S/C7H11O/c1-3-4-5-7(2)6-8/h3,7H,1,4-5H2,2H3	
C7ENEJ-ONE	C7H11O	[CH2]C=CCC(C)C=O	InChI=1S/C7H11O/c1-3-4-5-7(2)6-8/h3-4,6-7H,1,5H2,2H3	

MCHYO23	C7H12O	CC1CCCC2OC21	InChI=1S/C7H12O/c1-5-3-2-4-6-7(5)8-6/h5-7H,2-4H2,1H3	
MCHO	C7H12O	C1CC(C=O)CCC1	InChI=1S/C7H12O/c8-6-7-4-2-1-3-5-7/h6-7H,1-5H2	
MCHYO25	C7H12O	CC1CC2CCCC1O2	InChI=1S/C7H12O/c1-5-4-6-2-3-7(5)8-6/h5-7H,2-4H2,1H3	
MCH1OOH	C7H14O2	CC1(OO)CCCCC1	InChI=1S/C7H14O2/c1-7(9-8)5-3-2-4-6-7/h8H,2-6H2,1H3	
MCH2OOH	C7H14O2	CC1CCCCC1OO	InChI=1S/C7H14O2/c1-6-4-2-3-5-7(6)9-8/h6-8H,2-5H2,1H3	
MCH3OOH	C7H14O2	CC1CCCC(OO)C1	InChI=1S/C7H14O2/c1-6-3-2-4-7(5-6)9-8/h6-8H,2-5H2,1H3	
MCH4OOH	C7H14O2	CC1CCC(OO)CC1	InChI=1S/C7H14O2/c1-6-2-4-7(9-8)5-3-6/h6-8H,2-5H2,1H3	
CHXCH2OOH	C7H14O2	O OCC1CCCCC1	InChI=1S/C7H14O2/c8-9-6-7-4-2-1-3-5-7/h7-8H,1-6H2	
MCH1OJ	C7H13O	CC1([O])CCCCC1	InChI=1S/C7H13O/c1-7(8)5-3-2-4-6-7/h2-6H2,1H3	
MCH2OJ	C7H13O	CC1CCCCC1[O]	InChI=1S/C7H13O/c1-6-4-2-3-5-7(6)8/h6-7H,2-5H2,1H3	

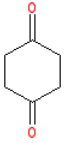
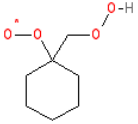
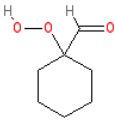
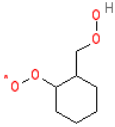
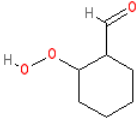
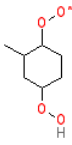
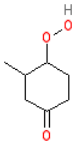
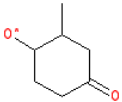
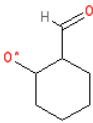
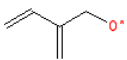
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MCH4OJ	C7H13O	CC1CCC([O])CC1	InChI=1S/C7H13O/c1-6-2-4-7(8)5-3-6/h6-7H,2-5H2,1H3	
CHXCH2OJ	C7H13O	[O]CC1CCCCC1	InChI=1S/C7H13O/c8-6-7-4-2-1-3-5-7/h7H,1-6H2	
CHXYCO-2	C7H12O	C1OC2CCCCC12	InChI=1S/C7H12O/c1-2-4-7-6(3-1)5-8-7/h6-7H,1-5H2	
CCOCCCCC.	C7H13O	[CH2]CCCCC(C)=O	InChI=1S/C7H13O/c1-3-4-5-6-7(2)8/h1,3-6H2,2H3	
CC.CCCCCO	C7H13O	C[CH]CCCCC=O	InChI=1S/C7H13O/c1-2-3-4-5-6-7-8/h2,7H,3-6H2,1H3	
IC6H12CHO5	C7H13O	C(=O)C(C)CCC[CH2]	InChI=1S/C7H13O/c1-3-4-5-7(2)6-8/h6-7H,1,3-5H2,2H3	
IC6H12CHO2	C7H13O	[CH2]C(C)CCCC=O	InChI=1S/C7H13O/c1-7(2)5-3-4-6-8/h6-7H,1,3-5H2,2H3	
IC6H12CHO3	C7H13O	C(=O)CCC(C)C[CH2]	InChI=1S/C7H13O/c1-3-7(2)5-4-6-8/h6-7H,1,3-5H2,2H3	
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MCH2Q3QJ	C7H13O4	CC1CCCC(O[O])C1OO	InChI=1S/C7H13O4/c1-5-3-2-4-6(10-8)7(5)11-9/h5-7,9H,2-4H2,1H3	
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MCH2O3OJ	C7H11O2	CC1CCCC([O])C1=O	InChI=1S/C7H11O2/c1-5-3-2-4-6(8)7(5)9/h5-6H,2-4H2,1H3	
MCH2Q1QJ	C7H13O4	CC1(O[O])CCCCC1OO	InChI=1S/C7H13O4/c1-7(11-9)5-3-2-4-6(7)10-8/h6,8H,2-5H2,1H3	
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CHX1O2O	C6H8O2	C1(=O)C(=O)CCCC1	InChI=1S/C6H8O2/c7-5-3-1-2-4-6(5)8/h1-4H2	
MCH2QXQJ	C7H13O4	[O]OCC1CCCCC1OO	InChI=1S/C7H13O4/c8-10-5-6-3-1-2-4-7(6)11-9/h6-7,9H,1-5H2	
MCH2OXQ	C7H12O3	O=C1CCCCC1COO	InChI=1S/C7H12O3/c8-7-4-2-1-3-6(7)5-10-9/h6,9H,1-5H2	
MCH2OXOJ	C7H11O2	[O]CC1CCCCC1=O	InChI=1S/C7H11O2/c8-5-6-3-1-2-4-7(6)9/h6H,1-5H2	

MCH2Q4QJ	C7H13O4	CC1CCC(O[O])CC1OO	InChI=1S/C7H13O4/c1-5-2-3-6(10-8)-7(5)11-9/h5-7,9H,2-4H2,1H3	
MCH2O4Q	C7H12O3	CC1CCC(OO)CC1=O	InChI=1S/C7H12O3/c1-5-2-3-6(10-9)-7(5)8/h5-6,9H,2-4H2,1H3	
MCH2O4OJ	C7H11O2	CC1CCC([O])CC1=O	InChI=1S/C7H11O2/c1-5-2-3-6(8)-7(5)9/h5-6H,2-4H2,1H3	
MCH2O4O	C7H10O2	CC1CCC(=O)CC1=O	InChI=1S/C7H10O2/c1-5-2-3-6(8)-7(5)9/h5H,2-4H2,1H3	
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MCH2O5Q	C7H12O3	CC1CC(OO)CCC1=O	InChI=1S/C7H12O3/c1-5-4-6(10-9)2-3-7(5)8/h5-6,9H,2-4H2,1H3	
MCH2O5OJ	C7H11O2	CC1CC([O])CCC1=O	InChI=1S/C7H11O2/c1-5-4-6(8)2-3-7(5)9/h5-6H,2-4H2,1H3	
MCH2O5O	C7H10O2	C1(C)C(=O)CCC(=O)C1	InChI=1S/C7H10O2/c1-5-4-6(8)2-3-7(5)9/h5H,2-4H2,1H3	
MCH2Q6QJ	C7H13O4	CC1C(O[O])CCCC1OO	InChI=1S/C7H13O4/c1-5-6(10-8)3-2-4-7(5)11-9/h5-8H,2-4H2,1H3	
MCH2O6Q	C7H12O3	CC1C(=O)CCCC1OO	InChI=1S/C7H12O3/c1-5-6(8)3-2-4-7(5)10-9/h5,7,9H,2-4H2,1H3	

MCH2O6OJ	C7H11O2	CC1C(=O)CCCC1[O]	InChI=1S/C7H11O2/c1-5-6(8)3-2-4-7(5)9/h5-6H,2-4H2,1H3	
MCH3Q2QJ	C7H13O4	CC1CCCC(OO)C1O[O]	InChI=1S/C7H13O4/c1-5-3-2-4-6(10-8)7(5)11-9/h5-8H,2-4H2,1H3	
MCH3O2Q	C7H12O3	CC1CCCC(=O)C1OO	InChI=1S/C7H12O3/c1-5-3-2-4-6(8)7(5)10-9/h5,7,9H,2-4H2,1H3	
MCH3O2OJ	C7H11O2	CC1CCCC(=O)C1[O]	InChI=1S/C7H11O2/c1-5-3-2-4-6(8)7(5)9/h5,7H,2-4H2,1H3	
MCH3Q5QJ	C7H13O4	CC1CC(O[O])CC(OO)C1	InChI=1S/C7H13O4/c1-5-2-6(10-8)4-7(3-5)11-9/h5-8H,2-4H2,1H3	
MCH3O5Q	C7H12O3	CC1CC(=O)CC(OO)C1	InChI=1S/C7H12O3/c1-5-2-6(8)4-7(3-5)10-9/h5,7,9H,2-4H2,1H3	
MCH3O5OJ	C7H11O2	CC1CC(=O)CC([O])C1	InChI=1S/C7H11O2/c1-5-2-6(8)4-7(9)3-5/h5-6H,2-4H2,1H3	
MCH3Q1QJ	C7H13O4	CC1(O[O])CCCC(OO)C1	InChI=1S/C7H13O4/c1-7(11-9)4-2-3-6(5-7)10-8/h6,8H,2-5H2,1H3	
MCH3O1Q	C7H12O3	CC1(OO)CCCC(=O)C1	InChI=1S/C7H12O3/c1-7(10-9)4-2-3-6(8)5-7/h9H,2-5H2,1H3	
MCH3O1OJ	C7H11O2	CC1([O])CCCC(=O)C1	InChI=1S/C7H11O2/c1-7(9)4-2-3-6(8)5-7/h2-5H2,1H3	

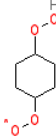
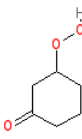
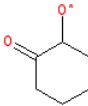
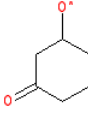
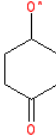
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MCH4O3Q	C7H12O3	CC1CCC(=O)C(OO)C1	InChI=1S/C7H12O3/c1-5-2-3-6(8)7(4-5)10-9/h5,7,9H,2-4H2,1H3	
MCH4O3OJ	C7H11O2	CC1CCC(=O)C([O])C1	InChI=1S/C7H11O2/c1-5-2-3-6(8)7(9)4-5/h5,7H,2-4H2,1H3	
MCH3O4O	C7H10O2	C1(C)CC(=O)C(=O)CC1	InChI=1S/C7H10O2/c1-5-2-3-6(8)7(9)4-5/h5H,2-4H2,1H3	
MCH4Q2QJ	C7H13O4	CC1CCC(OO)CC1O[O]	InChI=1S/C7H13O4/c1-5-2-3-6(10-8)4-7(5)11-9/h5-8H,2-4H2,1H3	
MCH4O2Q	C7H12O3	CC1CCC(=O)CC1OO	InChI=1S/C7H12O3/c1-5-2-3-6(8)4-7(5)10-9/h5,7,9H,2-4H2,1H3	
MCH4O2OJ	C7H11O2	CC1CCC(=O)CC1[O]	InChI=1S/C7H11O2/c1-5-2-3-6(8)4-7(5)9/h5,7H,2-4H2,1H3	
MCH4Q1QJ	C7H13O4	CC1(O[O])CCC(OO)CC1	InChI=1S/C7H13O4/c1-7(11-9)4-2-6(10-8)3-5-7/h6,8H,2-5H2,1H3	
MCH4O1Q	C7H12O3	CC1(OO)CCC(=O)CC1	InChI=1S/C7H12O3/c1-7(10-9)4-2-6(8)3-5-7/h9H,2-5H2,1H3	
MCH4O1OJ	C7H11O2	CC1([O])CCC(=O)CC1	InChI=1S/C7H11O2/c1-7(9)4-2-6(8)3-5-7/h2-5H2,1H3	

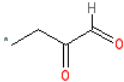
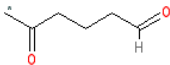
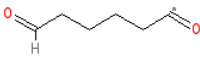
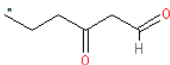
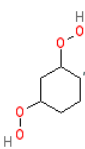
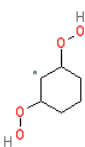
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MCHXQ1QJ	C7H13O4	<chem>[O]OC1(COO)CCCCC1</chem>	InChI=1S/C7H13O4/c8-10-6-7(11-9)4-2-1-3-5-7/h8H,1-6H2	
CHXCHO1Q	C7H12O3	<chem>O=CC1(OO)CCCCC1</chem>	InChI=1S/C7H12O3/c8-6-7(10-9)4-2-1-3-5-7/h6,9H,1-5H2	
MCHXQ2QJ	C7H13O4	<chem>[O]OC1CCCCC1COO</chem>	InChI=1S/C7H13O4/c8-10-5-6-3-1-2-4-7(6)11-9/h6-8H,1-5H2	
CHXCHO2Q	C7H12O3	<chem>O=CC1CCCCC1OO</chem>	InChI=1S/C7H12O3/c8-5-6-3-1-2-4-7(6)10-9/h5-7,9H,1-4H2	
MCH3Q6QJ	C7H13O4	<chem>CC1CC(OO)CCC1O[O]</chem>	InChI=1S/C7H13O4/c1-5-4-6(10-8)2-3-7(5)11-9/h5-8H,2-4H2,1H3	
MCH3O6Q	C7H12O3	<chem>CC1CC(=O)CCC1OO</chem>	InChI=1S/C7H12O3/c1-5-4-6(8)2-3-7(5)10-9/h5,7,9H,2-4H2,1H3	
MCH3O6OJ	C7H11O2	<chem>CC1CC(=O)CCC1[O]</chem>	InChI=1S/C7H11O2/c1-5-4-6(8)2-3-7(5)9/h5,7H,2-4H2,1H3	
CHXCHO2OJ	C7H11O2	<chem>[O]C1CCCCC1C=O</chem>	InChI=1S/C7H11O2/c8-5-6-3-1-2-4-7(6)9/h5-7H,1-4H2	
IC5H7OJ	C5H7O	<chem>C=C(C[O])C=C</chem>	InChI=1S/C5H7O/c1-3-5(2)4-6/h3H,1-2,4H2	

CHX	C6H12	C1CCCCC1	InChI=1S/C6H12/c1-2-4-6-5-3-1/h1-6H2	
CHXRAD	C6H11	[CH]1CCCCC1	InChI=1S/C6H11/c1-2-4-6-5-3-1/h1H,2-6H2	
CHXO2H	C6H12O2	OOC1CCCCC1	InChI=1S/C6H12O2/c7-8-6-4-2-1-3-5-6/h6-7H,1-5H2	
CHXO2J	C6H11O2	[O]OC1CCCCC1	InChI=1S/C6H11O2/c7-8-6-4-2-1-3-5-6/h6H,1-5H2	
CHX1Q2J	C6H11O2	OOC1[CH]CCCC1	InChI=1S/C6H11O2/c7-8-6-4-2-1-3-5-6/h4,6-7H,1-3,5H2	
CHX1Q3J	C6H11O2	OOC1C[CH]CCC1	InChI=1S/C6H11O2/c7-8-6-4-2-1-3-5-6/h2,6-7H,1,3-5H2	
CHX1Q4J	C6H11O2	OOC1CC[CH]CC1	InChI=1S/C6H11O2/c7-8-6-4-2-1-3-5-6/h1,6-7H,2-5H2	
CYCHEXENE	C6H10	C1=CCCCC1	InChI=1S/C6H10/c1-2-4-6-5-3-1/h1-2H,3-6H2	
HX1EN3Q6J	C6H11O2	[CH2]CCC(C=C)OO	InChI=1S/C6H11O2/c1-3-5-6(4-2)8-7/h4,6-H,1-3,5H2	
C2H2OOH	C2H3O2	[CH]=COO	InChI=1S/C2H3O2/c1-2-4-3/h1-3H	

HX1EN1Q6J	C6H11O2	[CH2]CCCC=COO	InChI=1S/C6H11O2/c1-2-3-4-5-6-8-7/h5-7H,1-4H2	
BT1EN1Q4J	C4H7O2	[CH2]CC=COO	InChI=1S/C4H7O2/c1-2-3-4-6-5/h3-5H,1-2H2	
CHXYO12	C6H10O	C1CCC2OC2C1	InChI=1S/C6H10O/c1-2-4-6-5(3-1)7-6/h5-6H,1-4H2	
CHX1*O	C6H10O	O=C1CCCCC1	InChI=1S/C6H10O/c7-6-4-2-1-3-5-6/h1-5H2	
CHX1*O2J	C6H9O	O=C1[CH]CCCC1	InChI=1S/C6H9O/c7-6-4-2-1-3-5-6/h4H,1-3,5H2	
HX1N3*O6J	C6H9O	[CH2]CCC(=O)C=C	InChI=1S/C6H9O/c1-3-5-6(7)4-2/h4H,1-3,5H2	
BT1N3*O4J	C4H5O	[CH2]C(=O)C=C	InChI=1S/C4H5O/c1-3-4(2)5/h3H,1-2H2	
HEX5ENAL	C6H10O	C=CCCCC=O	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h2,6H,1,3-5H2	
HX5ENAL1J	C6H9O	C=CCCC[C]=O	InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2H,1,3-5H2	
HX5ENAL4J	C6H9O	[CH2]C=CCCC=O	InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2-3,6H,1,4-5H2	

HX1EN6Q6J	C6H11O2	<chem>C=CCCC[CH]OO</chem>	InChI=1S/C6H11O2/c1-2-3-4-5-6-8-7/h2,6-7H,1,3-5H2	
HX1EN4Q6J	C6H11O2	<chem>[CH2]CC(CC=C)OO</chem>	InChI=1S/C6H11O2/c1-3-5-6(4-2)8-7/h3,6-7H,1-2,4-5H2	
BT1EN4Q4J	C4H7O2	<chem>C=CC[CH]OO</chem>	InChI=1S/C4H7O2/c1-2-3-4-6-5/h2,4-5H,1,3H2	
CHXYO13	C6H10O	<chem>C1C2CCCC1O2</chem>	InChI=1S/C6H10O/c1-2-5-4-6(3-1)7-5/h5-6H,1-4H2	
CHX1*O3J	C6H9O	<chem>O=C1C[CH]CCC1</chem>	InChI=1S/C6H9O/c7-6-4-2-1-3-5-6/h2H,1,3-5H2	
HXEN4AL6J	C6H9O	<chem>[CH2]CC(=O)CC=C</chem>	InChI=1S/C6H9O/c1-3-5-6(7)4-2/h3H,1-2,4-5H2	
HX1EN5Q6J	C6H11O2	<chem>[CH2]C(CCC=C)OO</chem>	InChI=1S/C6H11O2/c1-3-4-5-6(2)8-7/h3,6-7H,1-2,4-5H2	
CHXYO14	C6H10O	<chem>C1CC2CCC1O2</chem>	InChI=1S/C6H10O/c1-2-6-4-3-5(1)7-6/h5-6H,1-4H2	
CHX1*O4J	C6H9O	<chem>O=C1CC[CH]CC1</chem>	InChI=1S/C6H9O/c7-6-4-2-1-3-5-6/h1H,2-5H2	
HX1N5AL6J	C6H9O	<chem>[CH2]C(=O)CCC=C</chem>	InChI=1S/C6H9O/c1-3-4-5-6(2)7/h3H,1-2,4-5H2	

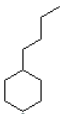
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CHX1Q3QJ	C6H11O4	[O]OC1CCCC(OO)C1	InChI=1S/C6H11O4/c7-9-5-2-1-3-6(4-5)10-8/h5-7H,1-4H2	
CHX1Q4QJ	C6H11O4	[O]OC1CCC(OO)CC1	InChI=1S/C6H11O4/c7-9-5-1-2-6(10-8)4-3-5/h5-7H,1-4H2	
CHX1*O2Q	C6H10O3	O=C1CCCCC1OO	InChI=1S/C6H10O3/c7-5-3-1-2-4-6(5)9-8/h6,8H,1-4H2	
CHX1*O3Q	C6H10O3	O=C1CCCC(OO)C1	InChI=1S/C6H10O3/c7-5-2-1-3-6(4-5)9-8/h6,8H,1-4H2	
CHX1*O4Q	C6H10O3	O=C1CCC(OO)CC1	InChI=1S/C6H10O3/c7-5-1-3-6(9-8)4-2-5/h6,8H,1-4H2	
CHX1*O2OJ	C6H9O2	[O]C1CCCCC1=O	InChI=1S/C6H9O2/c7-5-3-1-2-4-6(5)8/h5H,1-4H2	
CHX1*O3OJ	C6H9O2	[O]C1CCCC(=O)C1	InChI=1S/C6H9O2/c7-5-2-1-3-6(8)4-5/h5H,1-4H2	
CHX1*O4OJ	C6H9O2	[O]C1CCC(=O)CC1	InChI=1S/C6H9O2/c7-5-1-2-6(8)4-3-5/h5H,1-4H2	
HX12AL6J	C6H9O2	[CH2]CCCC(=O)C=O	InChI=1S/C6H9O2/c1-2-3-4-6(8)5-7/h5H,1-4H2	

BUT12AL4J	C4H5O2	[CH2]CC(=O)C=O	InChI=1S/C4H5O2/c1-2-4(6)3-5/h3H,1-2H2	
HX15AL6J	C6H9O2	[CH2]C(=O)CCCC=O	InChI=1S/C6H9O2/c1-6(8)4-2-3-5-7/h5H,1-4H2	
HX16AL1J	C6H9O2	O=[C]CCCCC=O	InChI=1S/C6H9O2/c7-5-3-1-2-4-6-8/h5H,1-4H2	
HX13AL6J	C6H9O2	[CH2]CCC(=O)CC=O	InChI=1S/C6H9O2/c1-2-3-6(8)4-5-7/h5H,1-4H2	
BUT13AL4J	C4H5O2	[CH2]C(=O)CC=O	InChI=1S/C4H5O2/c1-4(6)2-3-5/h3H,1-2H2	
HX14AL6J	C6H9O2	[CH2]CC(=O)CCC=O	InChI=1S/C6H9O2/c1-2-6(8)4-3-5-7/h5H,1-4H2	
CHX1Q2Q3J	C6H11O4	OOC1[CH]CCCC1OO	InChI=1S/C6H11O4/c7-9-5-3-1-2-4-6(5)10-8/h3,5-8H,1-2,4H2	
CHX1Q2Q4J	C6H11O4	OOC1C[CH]CCC1OO	InChI=1S/C6H11O4/c7-9-5-3-1-2-4-6(5)10-8/h1,5-8H,2-4H2	
CHX1Q3Q4J	C6H11O4	OOC1[CH]CCC(OO)C1	InChI=1S/C6H11O4/c7-9-5-2-1-3-6(4-5)10-8/h2,5-8H,1,3-4H2	
CHX1Q3Q2J	C6H11O4	OOC1[CH]C(OO)CCC1	InChI=1S/C6H11O4/c7-9-5-2-1-3-6(4-5)10-8/h4-8H,1-3H2	

CHX1Q3Q5J	C6H11O4	OOC1C[CH]CC(OO)C1	InChI=1S/C6H11O4/c7-9-5-2-1-3-6(4-5)10-8/h1,5-8H,2-4H2	
CHX1Q4Q2J	C6H11O4	OOC1[CH]CC(OO)CC1	InChI=1S/C6H11O4/c7-9-5-1-2-6(10-8)4-3-5/h1,5-8H,2-4H2	
CYHX1EN3Q	C6H10O2	OOC1C=CCCC1	InChI=1S/C6H10O2/c7-8-6-4-2-1-3-5-6/h2,4,6-7H,1,3,5H2	
CYHX1N3OJ	C6H9O	[O]C1C=CCCC1	InChI=1S/C6H9O/c7-6-4-2-1-3-5-6/h2,4,6H,1,3,5H2	
HX2N1AL6J	C6H9O	[CH2]CCC=CC=O	InChI=1S/C6H9O/c1-2-3-4-5-6-7/h4-6H,1-3H2	
HXEN6AL1J	C6H9O	[CH]=CCCCC=O	InChI=1S/C6H9O/c1-2-3-4-5-6-7/h1-2,6H,3-5H2	
HX1N1Q6AL	C6H10O3	O=CCCCC=COO	InChI=1S/C6H10O3/c7-5-3-1-2-4-6-9-8/h4-6,8H,1-3H2	
HX1NOJ6AL	C6H9O2	O=C[CH]CCCC=O	InChI=1S/C6H9O2/c7-5-3-1-2-4-6-8/h3,5-6H,1-2,4H2	
HEX15EN3Q	C6H10O2	C=CCC(C=C)OO	InChI=1S/C6H10O2/c1-3-5-6(4-2)8-7/h3-4,6-7H,1-2,5H2	
HX15EN3OJ	C6H9O	C=CCC([O])C=C	InChI=1S/C6H9O/c1-3-5-6(7)4-2/h3-4,6H,1-2,5H2	

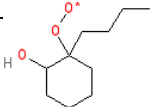
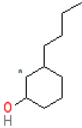
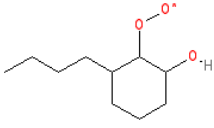
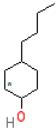
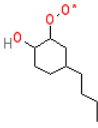
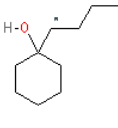
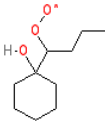
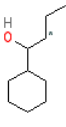
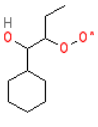
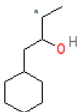
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H1N5OJ6AL	C6H9O2	C=CCCC([O])C=O	InChI=1S/C6H9O2/c1-2-3-4-6(8)5-7/h2,5-6H,1,3-4H2	
HCOCJ*O	C2HO2	O=[C]C=O	InChI=1S/C2HO2/c3-1-2-4/h1H	
CYHX1EN4Q	C6H10O2	OOC1CC=CCC1	InChI=1S/C6H10O2/c7-8-6-4-2-1-3-5-6/h1-2,6-7H,3-5H2	
CYHX1N4OJ	C6H9O	[O]C1CC=CCC1	InChI=1S/C6H9O/c7-6-4-2-1-3-5-6/h1-2,6H,3-5H2	
AC3H4CHO1	C4H5O	[CH]=CCC=O	InChI=1S/C4H5O/c1-2-3-4-5/h1-2,4H,3H2	
HEX15EN1Q	C6H10O2	C=CCCC=COO	InChI=1S/C6H10O2/c1-2-3-4-5-6-8-7/h2,5-7H,1,3-4H2	
HX15EN1OJ	C6H9O	C=CCC[CH]C=O	InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2,5-6H,1,3-4H2	
HX1N4Q6AL	C6H10O3	C=CCC(CC=O)OO	InChI=1S/C6H10O3/c1-2-3-6(9-8)4-5-7/h2,5-6,8H,1,3-4H2	
H1N4OJ6AL	C6H9O2	C=CCC([O])CC=O	InChI=1S/C6H9O2/c1-2-3-6(8)4-5-7/h2,5-6H,1,3-4H2	

PRO13DIAL	C3H4O2	O=CCC=O	InChI=1S/C3H4O2/c4-2-1-3-5/h2-3H,1H2	
PRO13AL1J	C3H3O2	O=[C]CC=O	InChI=1S/C3H3O2/c4-2-1-3-5/h2H,1H2	
HX1N3Q6AL	C6H10O3	C=CC(CCC=O)OO	InChI=1S/C6H10O3/c1-2-6(9-8)4-3-5-7/h2,5-6,8H,1,3-4H2	
H1N3OJ6AL	C6H9O2	C=CC([O])CCC=O	InChI=1S/C6H9O2/c1-2-6(8)4-3-5-7/h2,5-6H,1,3-4H2	
C6H12-16	C6H12	[CH2]CCCC[CH2]	InChI=1S/C6H12/c1-3-5-6-4-2/h1-6H2	
CHXOJ	C6H11O	[O]C1CCCCC1	InChI=1S/C6H11O/c7-6-4-2-1-3-5-6/h6H,1-5H2	
CYHX1N3J	C6H9	[CH]1C=CCCC1	InChI=1S/C6H9/c1-2-4-6-5-3-1/h1-3H,4-6H2	
CYHX1N4J	C6H9	[CH]1CC=CCC1	InChI=1S/C6H9/c1-2-4-6-5-3-1/h1-2,5H,3-4,6H2	
HX13EN6J	C6H9	[CH2]CC=CC=C	InChI=1S/C6H9/c1-3-5-6-4-2/h3,5-6H,1-2,4H2	
CYHX13ENE	C6H8	C1=CCCC=C1	InChI=1S/C6H8/c1-2-4-6-5-3-1/h1-4H,5-6H2	

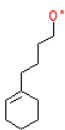
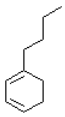
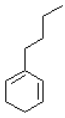
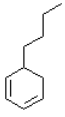
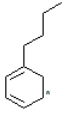
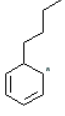
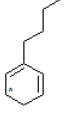
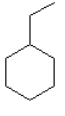
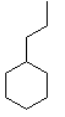

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CYHX14ENE	C6H8	C1=CCC=CC1	InChI=1S/C6H8/c1-2-4-6-5-3-1/h1-2,5-6H,3-4H2	
NBCH	C10H20	CCCCC1CCCCC1	InChI=1S/C10H20/c1-2-3-7-10-8-5-4-6-9-10/h10H,2-9H2,1H3	
C10H20-4	C10H20	CCCC=CCCCC	InChI=1S/C10H20/c1-3-5-7-9-10-8-6-4-2/h7,9H,3-6,8,10H2,1-2H3	
C10H20-5	C10H20	CCCCC=CCCC	InChI=1S/C10H20/c1-3-5-7-9-10-8-6-4-2/h9-10H,3-8H2,1-2H3	
C10H19	C10H19	CCCC=C[CH]CCCC	InChI=1S/C10H19/c1-3-5-7-9-10-8-6-4-2/h7,9-10H,3-6,8H2,1-2H3	
NBCH-1J	C10H19	CCCC[C]1CCCCC1	InChI=1S/C10H19/c1-2-3-7-10-8-5-4-6-9-10/h2-9H2,1H3	
NBCH-2J	C10H19	CCCCC1[CH]CCCC1	InChI=1S/C10H19/c1-2-3-7-10-8-5-4-6-9-10/h8,10H,2-7,9H2,1H3	
NBCH-3J	C10H19	CCCCC1C[CH]CCC1	InChI=1S/C10H19/c1-2-3-7-10-8-5-4-6-9-10/h5,10H,2-4,6-9H2,1H3	
NBCH-4J	C10H19	CCCCC1CC[CH]CC1	InChI=1S/C10H19/c1-2-3-7-10-8-5-4-6-9-10/h4,10H,2-3,5-9H2,1H3	

NBCH-AJ	C10H19	CCC[CH]C1CCCCC1	InChI=1S/C10H19/c1-2-3-7-10-8-5-4-6-9-10/h7,10H,2-6,8-9H2,1H3	
NBCH-BJ	C10H19	CC[CH]CC1CCCCC1	InChI=1S/C10H19/c1-2-3-7-10-8-5-4-6-9-10/h3,10H,2,4-9H2,1H3	
NBCH-CJ	C10H19	C[CH]CCCC1CCCCC1	InChI=1S/C10H19/c1-2-3-7-10-8-5-4-6-9-10/h2,10H,3-9H2,1H3	
NBCH-DJ	C10H19	[CH2]CCCC1CCCCC1	InChI=1S/C10H19/c1-2-3-7-10-8-5-4-6-9-10/h10H,1-9H2	
NBCH-1ENE	C10H18	CCCCC1=CCCCC1	InChI=1S/C10H18/c1-2-3-7-10-8-5-4-6-9-10/h8H,2-7,9H2,1H3	
NBCH-2ENE	C10H18	CCCCC1C=CCCC1	InChI=1S/C10H18/c1-2-3-7-10-8-5-4-6-9-10/h5,8,10H,2-4,6-7,9H2,1H3	
NBCH-3ENE	C10H18	CCCCC1CC=CCC1	InChI=1S/C10H18/c1-2-3-7-10-8-5-4-6-9-10/h4-5,10H,2-3,6-9H2,1H3	
NBCH-A-ENE	C10H18	CCCC=C1CCCCC1	InChI=1S/C10H18/c1-2-3-7-10-8-5-4-6-9-10/h7H,2-6,8-9H2,1H3	
NBCH-B-ENE	C10H18	CCC=CC1CCCCC1	InChI=1S/C10H18/c1-2-3-7-10-8-5-4-6-9-10/h3,7,10H,2,4-6,8-9H2,1H3	
NBCH-C-ENE	C10H18	CC=CCC1CCCCC1	InChI=1S/C10H18/c1-2-3-7-10-8-5-4-6-9-10/h2-3,10H,4-9H2,1H3	

NBCH-D-ENE	C10H18	<chem>C=CCCC1CCCCC1</chem>	InChI=1S/C10H18/c1-2-3-7-10-8-5-4-6-9-10/h2,10H,1,3-9H2	
NBCH-1N-AJ	C10H17	<chem>CCC[CH]C1=CCCCC1</chem>	InChI=1S/C10H17/c1-2-3-7-10-8-5-4-6-9-10/h7-8H,2-6,9H2,1H3	
NBCH-1N3J	C10H17	<chem>CCCCC1=C[CH]CCC1</chem>	InChI=1S/C10H17/c1-2-3-7-10-8-5-4-6-9-10/h5,8H,2-4,6-7,9H2,1H3	
NBCH-1N6J	C10H17	<chem>CCCCC1=CCCC[CH]1</chem>	InChI=1S/C10H17/c1-2-3-7-10-8-5-4-6-9-10/h8-9H,2-7H2,1H3	
NBCH-2N4J	C10H17	<chem>CCCCC1C=C[CH]CC1</chem>	InChI=1S/C10H17/c1-2-3-7-10-8-5-4-6-9-10/h4-5,8,10H,2-3,6-7,9H2,1H3	
NBCH-3N5J	C10H17	<chem>CCCCC1CC=C[CH]C1</chem>	InChI=1S/C10H17/c1-2-3-7-10-8-5-4-6-9-10/h4-6,10H,2-3,7-9H2,1H3	
NBCH-AN-BJ	C10H17	<chem>CC[CH]C=C1CCCCC1</chem>	InChI=1S/C10H17/c1-2-3-7-10-8-5-4-6-9-10/h3,7H,2,4-6,8-9H2,1H3	
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NBCH-CN-DJ	C10H17	<chem>[CH2]C=CCC1CCCCC1</chem>	InChI=1S/C10H17/c1-2-3-7-10-8-5-4-6-9-10/h2-3,10H,1,4-9H2	
NBCH-1J-2OH	C10H19O	<chem>CCCC[C]1C(O)CCCC1</chem>	InChI=1S/C10H19O/c1-2-3-6-9-7-4-5-8-10(9)11/h10-11H,2-8H2,1H3	

NBCH-1OO-2OH	C10H19O3	CCCCC1(O[O])C(O)CCCC1	InChI=1S/C10H19O3/c1-2-3-7-10(13-12)8-5-4-6-9(10)11/h9,11H,2-8H2,1H3	
NBCH-2J-3OH	C10H19O	CCCCC1[CH]C(O)CCC1	InChI=1S/C10H19O/c1-2-3-5-9-6-4-7-10(11)8-9/h8-11H,2-7H2,1H3	
NBCH-2OO-3OH	C10H19O3	CCCCC1C(O[O])C(O)CCC1	InChI=1S/C10H19O3/c1-2-3-5-8-6-4-7-9(11)10(8)13-12/h8-11H,2-7H2,1H3	
NBCH-3J-4OH	C10H19O	CCCCC1C[CH]C(O)CC1	InChI=1S/C10H19O/c1-2-3-4-9-5-7-10(11)8-6-9/h7,9-11H,2-6,8H2,1H3	
NBCH-3OO-4OH	C10H19O3	CCCCC1CC(O[O])C(O)CC1	InChI=1S/C10H19O3/c1-2-3-4-8-5-6-9(11)10(7-8)13-12/h8-11H,2-7H2,1H3	
NBCH-1OH-AJ	C10H19O	CCC[CH]C1(O)CCCCC1	InChI=1S/C10H19O/c1-2-3-7-10(11)8-5-4-6-9-10/h7,11H,2-6,8-9H2,1H3	
NBCH-1OH-AOO	C10H19O3	CCCC(O[O])C1(O)CCCCC1	InChI=1S/C10H19O3/c1-2-6-9(13-12)10(11)7-4-3-5-8-10/h9,11H,2-8H2,1H3	
NBCH-AOH-BJ	C10H19O	CC[CH]C(O)C1CCCCC1	InChI=1S/C10H19O/c1-2-6-10(11)9-7-4-3-5-8-9/h6,9-11H,2-5,7-8H2,1H3	
NBCH-AOH-BOO	C10H19O3	CCC(O[O])C(O)C1CCCCC1	InChI=1S/C10H19O3/c1-2-9(13-12)10(11)8-6-4-3-5-7-8/h8-11H,2-7H2,1H3	
NBCH-BOH-CJ	C10H19O	C[CH]C(O)CC1CCCCC1	InChI=1S/C10H19O/c1-2-10(11)8-9-6-4-3-5-7-9/h2,9-11H,3-8H2,1H3	

NBCH-BOH-COO	C10H19O3	<chem>CC(O[O])C(O)CC1CCCCC1</chem>	InChI=1S/C10H19O3/c1-8(13-12)10(11)7-9-5-3-2-4-6-9/h8-11H,2-7H2,1H3	
NBCH-COH-DJ	C10H19O	<chem>[CH2]C(O)CCC1CCCCC1</chem>	InChI=1S/C10H19O/c1-9(11)7-8-10-5-3-2-4-6-10/h9-11H,1-8H2	
NBCH-COH-DOO	C10H19O3	<chem>C(O[O])C(O)CCC1CCCCC1</chem>	InChI=1S/C10H19O3/c11-10(8-13-12)7-6-9-4-2-1-3-5-9/h9-11H,1-8H2	
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NBCH1N6OJ	C10H17O	<chem>CCCCC1=CCCCC1([O])</chem>	InChI=1S/C10H17O/c1-2-3-6-9-7-4-5-8-10(9)11/h7,10H,2-6,8H2,1H3	
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NBCH-AN-BOJ	C10H17O	<chem>CCC([O])CC1=CCCCC1</chem>	InChI=1S/C10H17O/c1-2-10(11)8-9-6-4-3-5-7-9/h6,10H,2-5,7-8H2,1H3	
NBCH-BN-COJ	C10H17O	<chem>CC([O])CCC1=CCCCC1</chem>	InChI=1S/C10H17O/c1-9(11)7-8-10-5-3-2-4-6-10/h5,9H,2-4,6-8H2,1H3	

NBCH-CN-DOJ	C10H17O	C([O])CCCC1=CCCCC1	InChI=1S/C10H17O/c11-9-5-4-8-10-6-2-1-3-7-10/h6H,1-5,7-9H2	
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NBCH-2N4N	C10H16	CCCCC1C=CC=CC1	InChI=1S/C10H16/c1-2-3-7-10-8-5-4-6-9-10/h4-6,8,10H,2-3,7,9H2,1H3	
NBCH1N3N5J	C10H15	CCCCC1=CC=C[CH]C1	InChI=1S/C10H15/c1-2-3-7-10-8-5-4-6-9-10/h4-6,8H,2-3,7,9H2,1H3	
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ECH-BJ	C8H15	[CH2]CC1CCCCC1	InChI=1S/C8H15/c1-2-8-6-4-3-5-7-8/h8H,1-7H2	
NPCH-CJ	C9H17	[CH2]CCC1CCCCC1	InChI=1S/C9H17/c1-2-6-9-7-4-3-5-8-9/h9H,1-8H2	
C6H5C4H9	C10H14	CCCCc1ccccc1	InChI=1S/C10H14/c1-2-3-7-10-8-5-4-6-9-10/h4-6,8-9H,2-3,7H2,1H3	

NBCH-1O2	C10H19O2	CCCCC1(O[O])CCCCC1	InChI=1S/C10H19O2/c1-2-3-7-10(12-11)8-5-4-6-9-10/h2-9H2,1H3	
NBCH-2O2	C10H19O2	CCCCC1C(O[O])CCCC1	InChI=1S/C10H19O2/c1-2-3-6-9-7-4-5-8-10(9)12-11/h9-10H,2-8H2,1H3	
NBCH-3O2	C10H19O2	CCCCC1CC(O[O])CCC1	InChI=1S/C10H19O2/c1-2-3-5-9-6-4-7-10(8-9)12-11/h9-10H,2-8H2,1H3	
NBCH-4O2	C10H19O2	CCCCC1CCC(O[O])CC1	InChI=1S/C10H19O2/c1-2-3-4-9-5-7-10(12-11)8-6-9/h9-10H,2-8H2,1H3	
NBCH-AO2	C10H19O2	CCCC(O[O])C1CCCCC1	InChI=1S/C10H19O2/c1-2-6-10(12-11)9-7-4-3-5-8-9/h9-10H,2-8H2,1H3	
NBCH-BO2	C10H19O2	CCC(O[O])CC1CCCCC1	InChI=1S/C10H19O2/c1-2-10(12-11)8-9-6-4-3-5-7-9/h9-10H,2-8H2,1H3	
NBCH-CO2	C10H19O2	CC(O[O])CCC1CCCCC1	InChI=1S/C10H19O2/c1-9(12-11)7-8-10-5-3-2-4-6-10/h9-10H,2-8H2,1H3	
NBCH-DO2	C10H19O2	C(O[O])CCCC1CCCCC1	InChI=1S/C10H19O2/c11-12-9-5-4-8-10-6-2-1-3-7-10/h10H,1-9H2	
NBCH-1OJ	C10H19O	CCCCC1([O])CCCCC1	InChI=1S/C10H19O/c1-2-3-7-10(11)8-5-4-6-9-10/h2-9H2,1H3	
NBCH-2OJ	C10H19O	CCCCC1C([O])CCCC1	InChI=1S/C10H19O/c1-2-3-6-9-7-4-5-8-10(9)11/h9-10H,2-8H2,1H3	

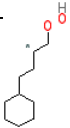
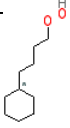
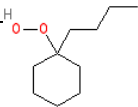
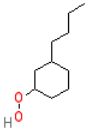
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NBCH-4OJ	C10H19O	CCCCC1CCC([O])CC1	InChI=1S/C10H19O/c1-2-3-4-9-5-7-10(11)8-6-9/h9-10H,2-8H2,1H3	
NBCH-AOJ	C10H19O	CCCC([O])C1CCCCC1	InChI=1S/C10H19O/c1-2-6-10(11)9-7-4-3-5-8-9/h9-10H,2-8H2,1H3	
NBCH-BOJ	C10H19O	CCC([O])CC1CCCCC1	InChI=1S/C10H19O/c1-2-10(11)8-9-6-4-3-5-7-9/h9-10H,2-8H2,1H3	
NBCH-COJ	C10H19O	CC([O])CCC1CCCCC1	InChI=1S/C10H19O/c1-9(11)7-8-10-5-3-2-4-6-10/h9-10H,2-8H2,1H3	
NBCH-DOJ	C10H19O	C([O])CCCC1CCCCC1	InChI=1S/C10H19O/c11-9-5-4-8-10-6-2-1-3-7-10/h10H,1-9H2	
NBCH-1Q-2J	C10H19O2	CCCCC1(OO)[CH]CCCC1	InChI=1S/C10H19O2/c1-2-3-7-10(12-11)8-5-4-6-9-10/h8,11H,2-7,9H2,1H3	
NBCH-1Q-3J	C10H19O2	CCCCC1(OO)C[CH]CCC1	InChI=1S/C10H19O2/c1-2-3-7-10(12-11)8-5-4-6-9-10/h5,11H,2-4,6-9H2,1H3	
NBCH-1Q-4J	C10H19O2	CCCCC1(OO)CC[CH]CC1	InChI=1S/C10H19O2/c1-2-3-7-10(12-11)8-5-4-6-9-10/h4,11H,2-3,5-9H2,1H3	
NBCH-1Q-AJ	C10H19O2	CCC[CH]C1(OO)CCCCC1	InChI=1S/C10H19O2/c1-2-3-7-10(12-11)8-5-4-6-9-10/h7,11H,2-6,8-9H2,1H3	

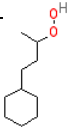
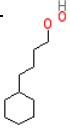
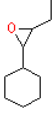
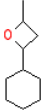
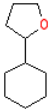
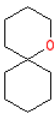
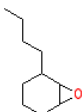
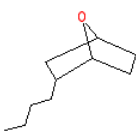
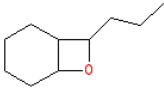
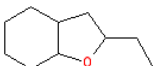
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NBCH-1Q-CJ	C10H19O2	C[CH]CCC1(OO)CCCCC1	InChI=1S/C10H19O2/c1-2-3-7-10(12-11)8- 5-4-6-9-10/h2,11H,3-9H2,1H3	
NBCH-1Q-DJ	C10H19O2	[CH2]CCCC1(OO)CCCCC1	InChI=1S/C10H19O2/c1-2-3-7-10(12-11)8- 5-4-6-9-10/h11H,1-9H2	
NBCH-2Q-1J	C10H19O2	CCCC[C]1C(OO)CCCC1	InChI=1S/C10H19O2/c1-2-3-6-9-7-4-5-8- 10(9)12-11/h10-11H,2-8H2,1H3	
NBCH-2Q-3J	C10H19O2	CCCCC1C(OO)[CH]CCC1	InChI=1S/C10H19O2/c1-2-3-6-9-7-4-5-8- 10(9)12-11/h8-11H,2-7H2,1H3	
NBCH-2Q-AJ	C10H19O2	CCC[CH]C1C(OO)CCCC1	InChI=1S/C10H19O2/c1-2-3-6-9-7-4-5-8- 10(9)12-11/h6,9-11H,2-5,7-8H2,1H3	
NBCH-2Q-4J	C10H19O2	CCCCC1C(OO)C[CH]CC1	InChI=1S/C10H19O2/c1-2-3-6-9-7-4-5-8- 10(9)12-11/h5,9-11H,2-4,6-8H2,1H3	
NBCH-2Q-6J	C10H19O2	CCCCC1C(OO)CCC[CH]1	InChI=1S/C10H19O2/c1-2-3-6-9-7-4-5-8- 10(9)12-11/h7,9-11H,2-6,8H2,1H3	
NBCH-2Q-5J	C10H19O2	CCCCC1C(OO)CC[CH]C1	InChI=1S/C10H19O2/c1-2-3-6-9-7-4-5-8- 10(9)12-11/h4,9-11H,2-3,5-8H2,1H3	
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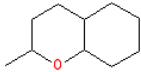

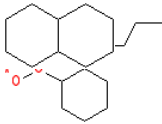
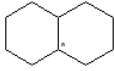
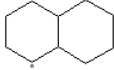
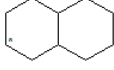
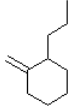
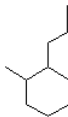
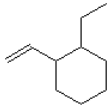
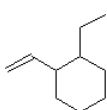
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NBCH-3Q-2J	C10H19O2	CCCCC1[CH]C(OO)CCC1	InChI=1S/C10H19O2/c1-2-3-5-9-6-4-7-10(8-9)12-11/h8-11H,2-7H2,1H3	
NBCH-3Q-4J	C10H19O2	CCCCC1CC(OO)[CH]CC1	InChI=1S/C10H19O2/c1-2-3-5-9-6-4-7-10(8-9)12-11/h7,9-11H,2-6,8H2,1H3	
NBCH-3Q-1J	C10H19O2	CCCC[C]1CC(OO)CCC1	InChI=1S/C10H19O2/c1-2-3-5-9-6-4-7-10(8-9)12-11/h10-11H,2-8H2,1H3	
NBCH-3Q-5J	C10H19O2	CCCCC1CC(OO)C[CH]C1	InChI=1S/C10H19O2/c1-2-3-5-9-6-4-7-10(8-9)12-11/h4,9-11H,2-3,5-8H2,1H3	
NBCH-3Q-6J	C10H19O2	CCCCC1CC(OO)CC[CH]1	InChI=1S/C10H19O2/c1-2-3-5-9-6-4-7-10(8-9)12-11/h6,9-11H,2-5,7-8H2,1H3	
NBCH-3Q-AJ	C10H19O2	CCC[CH]C1CC(OO)CCC1	InChI=1S/C10H19O2/c1-2-3-5-9-6-4-7-10(8-9)12-11/h5,9-11H,2-4,6-8H2,1H3	
NBCH-3Q-BJ	C10H19O2	CC[CH]CC1CC(OO)CCC1	InChI=1S/C10H19O2/c1-2-3-5-9-6-4-7-10(8-9)12-11/h3,9-11H,2,4-8H2,1H3	
NBCH-4Q-3J	C10H19O2	CCCCC1C[CH]C(OO)CC1	InChI=1S/C10H19O2/c1-2-3-4-9-5-7-10(12-11)8-6-9/h7,9-11H,2-6,8H2,1H3	
NBCH-4Q-2J	C10H19O2	CCCCC1[CH]CC(OO)CC1	InChI=1S/C10H19O2/c1-2-3-4-9-5-7-10(12-11)8-6-9/h5,9-11H,2-4,6-8H2,1H3	

NBCH-4Q-1J	C10H19O2	CCCC[C]1CCC(OO)CC1	InChI=1S/C10H19O2/c1-2-3-4-9-5-7-10(12-11)8-6-9/h10-11H,2-8H2,1H3	
NBCH-4Q-AJ	C10H19O2	CCC[CH]C1CCC(OO)CC1	InChI=1S/C10H19O2/c1-2-3-4-9-5-7-10(12-11)8-6-9/h4,9-11H,2-3,5-8H2,1H3	
NBCH-AQ-1J	C10H19O2	CCCC(OO)[C]1CCCCC1	InChI=1S/C10H19O2/c1-2-6-10(12-11)9-7-4-3-5-8-9/h10-11H,2-8H2,1H3	
NBCH-AQ-BJ	C10H19O2	CC[CH]C(OO)C1CCCCC1	InChI=1S/C10H19O2/c1-2-6-10(12-11)9-7-4-3-5-8-9/h6,9-11H,2-5,7-8H2,1H3	
NBCH-AQ-CJ	C10H19O2	C[CH]CC(OO)C1CCCCC1	InChI=1S/C10H19O2/c1-2-6-10(12-11)9-7-4-3-5-8-9/h2,9-11H,3-8H2,1H3	
NBCH-AQ-2J	C10H19O2	CCCC(OO)C1[CH]CCCCC1	InChI=1S/C10H19O2/c1-2-6-10(12-11)9-7-4-3-5-8-9/h7,9-11H,2-6,8H2,1H3	
NBCH-AQ-DJ	C10H19O2	[CH2]CCC(OO)C1CCCCC1	InChI=1S/C10H19O2/c1-2-6-10(12-11)9-7-4-3-5-8-9/h9-11H,1-8H2	
NBCH-AQ-3J	C10H19O2	CCCC(OO)C1C[CH]CCCC1	InChI=1S/C10H19O2/c1-2-6-10(12-11)9-7-4-3-5-8-9/h4,9-11H,2-3,5-8H2,1H3	
NBCH-AQ-4J	C10H19O2	CCCC(OO)C1CC[CH]CC1	InChI=1S/C10H19O2/c1-2-6-10(12-11)9-7-4-3-5-8-9/h3,9-11H,2,4-8H2,1H3	
NBCH-BQ-AJ	C10H19O2	CCC(OO)[CH]C1CCCCC1	InChI=1S/C10H19O2/c1-2-10(12-11)8-9-6-4-3-5-7-9/h8-11H,2-7H2,1H3	

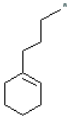
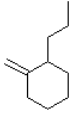


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NBCH-BQ-1J	C10H19O2	CCC(OO)C[C]1CCCCC1	InChI=1S/C10H19O2/c1-2-10(12-11)8-9-6-4-3-5-7-9/h10-11H,2-8H2,1H3	
NBCH-BQ-DJ	C10H19O2	[CH2]CC(OO)CC1CCCCC1	InChI=1S/C10H19O2/c1-2-10(12-11)8-9-6-4-3-5-7-9/h9-11H,1-8H2	
NBCH-BQ-2J	C10H19O2	CCC(OO)CC1[CH]CCCCC1	InChI=1S/C10H19O2/c1-2-10(12-11)8-9-6-4-3-5-7-9/h6,9-11H,2-5,7-8H2,1H3	
NBCH-BQ-3J	C10H19O2	CCC(OO)CC1C[CH]CCCC1	InChI=1S/C10H19O2/c1-2-10(12-11)8-9-6-4-3-5-7-9/h4,9-11H,2-3,5-8H2,1H3	
NBCH-CQ-BJ	C10H19O2	CC(OO)[CH]CC1CCCCC1	InChI=1S/C10H19O2/c1-9(12-11)7-8-10-5-3-2-4-6-10/h7,9-11H,2-6,8H2,1H3	
NBCH-CQ-DJ	C10H19O2	[CH2]C(OO)CCC1CCCCC1	InChI=1S/C10H19O2/c1-9(12-11)7-8-10-5-3-2-4-6-10/h9-11H,1-8H2	
NBCH-CQ-AJ	C10H19O2	CC(OO)C[CH]C1CCCCC1	InChI=1S/C10H19O2/c1-9(12-11)7-8-10-5-3-2-4-6-10/h8-11H,2-7H2,1H3	
NBCH-CQ-1J	C10H19O2	CC(OO)CC[C]1CCCCC1	InChI=1S/C10H19O2/c1-9(12-11)7-8-10-5-3-2-4-6-10/h9,11H,2-8H2,1H3	
NBCH-CQ-2J	C10H19O2	CC(OO)CCC1[CH]CCCCC1	InChI=1S/C10H19O2/c1-9(12-11)7-8-10-5-3-2-4-6-10/h5,9-11H,2-4,6-8H2,1H3	

NBCH-DQ-CJ	C10H19O2	C(OO)[CH]CCC1CCCCC1	InChI=1S/C10H19O2/c11-12-9-5-4-8-10-6-2-1-3-7-10/h5,10-11H,1-4,6-9H2	
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NBCH-DQ-AJ	C10H19O2	C(OO)CC[CH]C1CCCCC1	InChI=1S/C10H19O2/c11-12-9-5-4-8-10-6-2-1-3-7-10/h8,10-11H,1-7,9H2	
NBCH-DQ-1J	C10H19O2	C(OO)CCC[C]1CCCCC1	InChI=1S/C10H19O2/c11-12-9-5-4-8-10-6-2-1-3-7-10/h11H,1-9H2	
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NBCH-2OOH	C10H20O2	CCCCC1C(OO)CCCC1	InChI=1S/C10H20O2/c1-2-3-6-9-7-4-5-8-10(9)12-11/h9-11H,2-8H2,1H3	
NBCH-3OOH	C10H20O2	CCCCC1CC(OO)CCC1	InChI=1S/C10H20O2/c1-2-3-5-9-6-4-7-10(8-9)12-11/h9-11H,2-8H2,1H3	
NBCH-4OOH	C10H20O2	CCCCC1CCC(OO)CC1	InChI=1S/C10H20O2/c1-2-3-4-9-5-7-10(12-11)8-6-9/h9-11H,2-8H2,1H3	
NBCH-AOOH	C10H20O2	CCCC(OO)C1CCCCC1	InChI=1S/C10H20O2/c1-2-6-10(12-11)9-7-4-3-5-8-9/h9-11H,2-8H2,1H3	
NBCH-BOOH	C10H20O2	CCC(OO)CC1CCCCC1	InChI=1S/C10H20O2/c1-2-10(12-11)8-9-6-4-3-5-7-9/h9-11H,2-8H2,1H3	

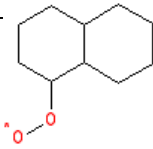
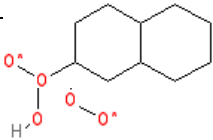
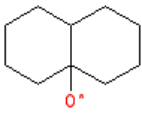
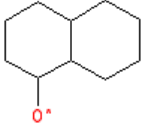
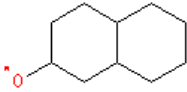
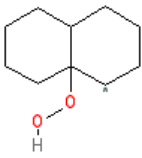
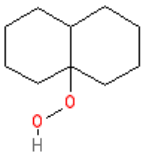
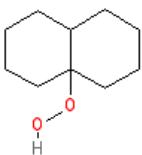
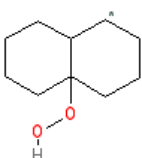
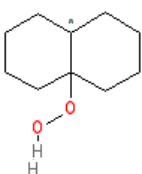
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NBCH-DOOH	C10H20O2	C(OO)CCCC1CCCCC1	InChI=1S/C10H20O2/c11-12-9-5-4-8-10-6-2-1-3-7-10/h10-11H,1-9H2	
NBCHYOAB	C10H18O	CCC(O2)C2C1CCCCC1	InChI=1S/C10H18O/c1-2-9-10(11-9)8-6-4-3-5-7-8/h8-10H,2-7H2,1H3	
NBCHYOAC	C10H18O	CC(O2)CC2C1CCCCC1	InChI=1S/C10H18O/c1-8-7-10(11-8)9-5-3-2-4-6-9/h8-10H,2-7H2,1H3	
NBCHYOAD	C10H18O	C(O2)CCC2C1CCCCC1	InChI=1S/C10H18O/c1-2-5-9(6-3-1)10-7-4-8-11-10/h9-10H,1-8H2	
NBCHYO1D	C10H18O	C(O2)CCCC12CCCCC1	InChI=1S/C10H18O/c1-2-6-10(7-3-1)8-4-5-9-11-10/h1-9H2	
NBCHYO23	C10H18O	CCCCC1C2C(O2)CCC1	InChI=1S/C10H18O/c1-2-3-5-8-6-4-7-9-10(8)11-9/h8-10H,2-7H2,1H3	
NBCHYO25	C10H18O	CCCCC1C2CCC(O2)C1	InChI=1S/C10H18O/c1-2-3-4-8-7-9-5-6-10(8)11-9/h8-10H,2-7H2,1H3	
NBCHYO2A	C10H18O	CCCC(O2)C1C2CCCC1	InChI=1S/C10H18O/c1-2-5-9-8-6-3-4-7-10(8)11-9/h8-10H,2-7H2,1H3	
NBCHYO2B	C10H18O	CCC(O2)CC1C2CCCC1	InChI=1S/C10H18O/c1-2-9-7-8-5-3-4-6-10(8)11-9/h8-10H,2-7H2,1H3	

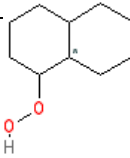
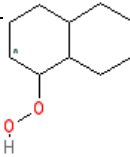
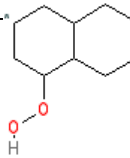
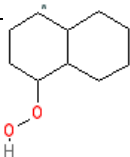
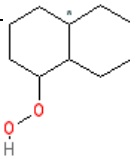
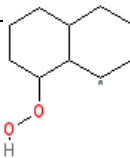
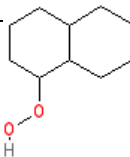
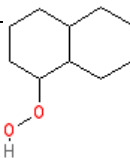
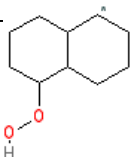
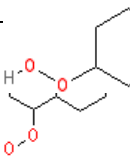
NBCHYO2C	C10H18O	CC(O2)CCC1C2CCCC1	InChI=1S/C10H18O/c1-8-6-7-9-4-2-3-5-10(9)11-8/h8-10H,2-7H2,1H3	
C10ENE-AL	C10H18O	C(=O)CCCC=CCCC	InChI=1S/C10H18O/c1-2-3-4-5-6-7-8-9-10-11/h5-6,10H,2-4,7-9H2,1H3	
DECALIN	C10H18	C1CCCC(C12)CCCC2	InChI=1S/C10H18/c1-2-6-10-8-4-3-7-9(10)5-1/h9-10H,1-8H2	
DCL-1R	C10H17	C2CC[C](C1)C(C2)CCC1	InChI=1S/C10H17/c1-2-6-10-8-4-3-7-9(10)5-1/h9H,1-8H2	
DCL-2R	C10H17	C2C[CH]C(C1)C(C2)CCC1	InChI=1S/C10H17/c1-2-6-10-8-4-3-7-9(10)5-1/h5,9-10H,1-4,6-8H2	
DCL-3R	C10H17	C2[CH]CC(C1)C(C2)CCC1	InChI=1S/C10H17/c1-2-6-10-8-4-3-7-9(10)5-1/h1,9-10H,2-8H2	
NPCH-2CH2	C10H18	C1CCCC(=C)C1CCC	InChI=1S/C10H18/c1-3-6-10-8-5-4-7-9(10)2/h10H,2-8H2,1H3	
NPCHD1A-2M	C10H18	C1CCCC(C)C1CC=C	InChI=1S/C10H18/c1-3-6-10-8-5-4-7-9(10)2/h3,9-10H,1,4-8H2,2H3	
ECH-2V	C10H18	C1CCCC(CC)C1C=C	InChI=1S/C10H18/c1-3-9-7-5-6-8-10(9)4-2/h3,9-10H,1,4-8H2,2H3	
ECH-2V-1AR	C10H17	C1CCCC(C[CH2])C1C=C	InChI=1S/C10H17/c1-3-9-7-5-6-8-10(9)4-2/h3,9-10H,1-2,4-8H2	

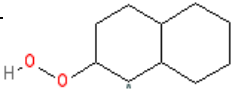
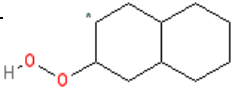
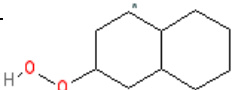
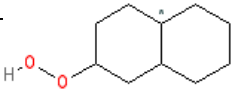
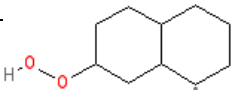
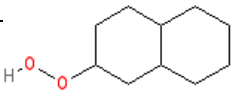
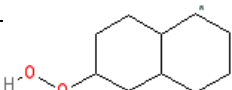
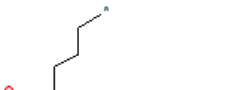
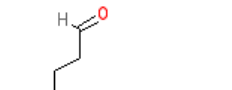
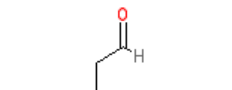
ECH2V-6R	C10H17	<chem>C1CC[CH]C(CC)C1C=C</chem>	InChI=1S/C10H17/c1-3-9-7-5-6-8-10(9)4-2/h3,8-10H,1,4-7H2,2H3	
ECH2V-3R	C10H17	<chem>[CH]1CCCC(CC)C1C=C</chem>	InChI=1S/C10H17/c1-3-9-7-5-6-8-10(9)4-2/h3,7,9-10H,1,4-6,8H2,2H3	
ECHD2	C8H14	<chem>C1CCC=CC1CC</chem>	InChI=1S/C8H14/c1-2-8-6-4-3-5-7-8/h4,6,8H,2-3,5,7H2,1H3	
ECHD3	C8H14	<chem>C1CC=CCC1CC</chem>	InChI=1S/C8H14/c1-2-8-6-4-3-5-7-8/h3-4,8H,2,5-7H2,1H3	
ECHD1A1	C8H12	<chem>C1CCCC=C1C=C</chem>	InChI=1S/C8H12/c1-2-8-6-4-3-5-7-8/h2,6H,1,3-5,7H2	
ECHD1-1AR	C8H13	<chem>C1CCCC=C1C[CH2]</chem>	InChI=1S/C8H13/c1-2-8-6-4-3-5-7-8/h6H,1-5,7H2	
ECHD2A-2R	C8H13	<chem>C1CC(=CC)[CH]CC1</chem>	InChI=1S/C8H13/c1-2-8-6-4-3-5-7-8/h2,6H,3-5,7H2,1H3	
ECHD2-4R	C8H13	<chem>C1C[CH]C=CC1CC</chem>	InChI=1S/C8H13/c1-2-8-6-4-3-5-7-8/h3-4,6,8H,2,5,7H2,1H3	
ECHD24	C8H12	<chem>C1C=CC=CC1CC</chem>	InChI=1S/C8H12/c1-2-8-6-4-3-5-7-8/h3-6,8H,2,7H2,1H3	
CYDED1-6R	C10H17	<chem>C1CC=CCCC[CH]CC1</chem>	InChI=1S/C10H17/c1-2-4-6-8-10-9-7-5-3-1/h1-2,9H,3-8,10H2	

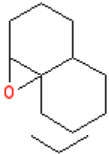
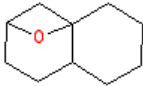
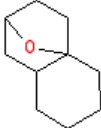
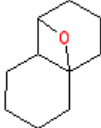
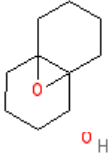
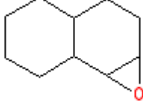
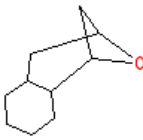
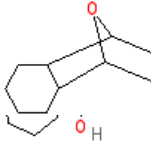
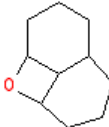
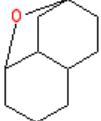
PBCHD1-1AR	C10H17	C1CCCC=C1CCC[CH2]	InChI=1S/C10H17/c1-2-3-7-10-8-5-4-6-9-10/h8H,1-7,9H2	
PBCHD1A-2R	C10H17	C1CCC[CH]C1CCC=C	InChI=1S/C10H17/c1-2-3-7-10-8-5-4-6-9-10/h2,8,10H,1,3-7,9H2	
NPCHD1A-2MR	C10H17	C1CCCC([CH2])C1CC=C	InChI=1S/C10H17/c1-3-6-10-8-5-4-7-9(10)2/h3,9-10H,1-2,4-8H2	
CYHD1-2R	C6H9	C1CCC[C]=C1	InChI=1S/C6H9/c1-2-4-6-5-3-1/h1H,2,4-6H2	
NPCH-2CH2-1AR	C10H17	C1CCCC(CC[CH2])C1=C	InChI=1S/C10H17/c1-3-6-10-8-5-4-7-9(10)2/h10H,1-8H2	
NPCH-2CH2-6R	C10H17	C1CC[CH]C(CCC)C1=C	InChI=1S/C10H17/c1-3-6-10-8-5-4-7-9(10)2/h8,10H,2-7H2,1H3	
NC10D17-10R	C10H17	C=CCCCC=CC[CH2]	InChI=1S/C10H17/c1-3-5-7-9-10-8-6-4-2/h3,6,8H,1-2,4-5,7,9-10H2	
NC10D17-6R	C10H17	C=CCCC[CH]C=CCC	InChI=1S/C10H17/c1-3-5-7-9-10-8-6-4-2/h3,6,8,10H,1,4-5,7,9H2,2H3	
NC10D19-4R	C10H17	C=CC[CH]CCCCC=C	InChI=1S/C10H17/c1-3-5-7-9-10-8-6-4-2/h3-4,7H,1-2,5-6,8-10H2	
NC10D19-3R	C10H17	C=C[CH]CCCCC=C	InChI=1S/C10H17/c1-3-5-7-9-10-8-6-4-2/h3-5H,1-2,6-10H2	

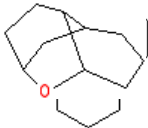
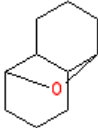
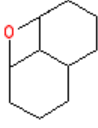
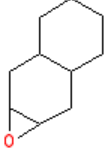
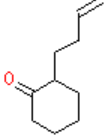
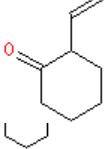
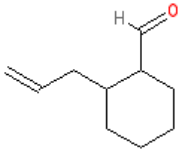
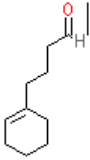
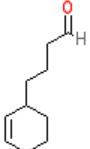
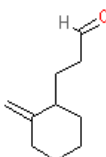
NC10D16-10R	C10H17	<chem>C=CCCCC=CCC[CH2]</chem>	InChI=1S/C10H17/c1-3-5-7-9-10-8-6-4-2/h3,8,10H,1-2,4-7,9H2	
NC8D16-8R	C8H13	<chem>C=CCCCC=C[CH2]</chem>	InChI=1S/C8H13/c1-3-5-7-8-6-4-2/h3-5H,1-2,6-8H2	
DCLD1	C10H16	<chem>C1CCCCC2C1=CCCC2</chem>	InChI=1S/C10H16/c1-2-6-10-8-4-3-7-9(10)5-1/h5,10H,1-4,6-8H2	
DCLD2	C10H16	<chem>C1CCCCC2C1C=CCC2</chem>	InChI=1S/C10H16/c1-2-6-10-8-4-3-7-9(10)5-1/h1,5,9-10H,2-4,6-8H2	
DCLD3	C10H16	<chem>C1CCCCC2C1CC=CC2</chem>	InChI=1S/C10H16/c1-2-6-10-8-4-3-7-9(10)5-1/h1-2,9-10H,3-8H2	
DCLD6	C10H16	<chem>C1CCCCC2=C1CCCC2</chem>	InChI=1S/C10H16/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H2	
DCLOOH1	C10H18O2	<chem>C1CCCCC2C1(OO)CCCC2</chem>	InChI=1S/C10H18O2/c11-12-10-7-3-1-5-9(10)6-2-4-8-10/h9,11H,1-8H2	
DCLOOH2	C10H18O2	<chem>C1CCCCC2C1C(OO)CCC2</chem>	InChI=1S/C10H18O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h8-11H,1-7H2	
DCLOOH3	C10H18O2	<chem>C1CCCCC2C1CC(OO)CC2</chem>	InChI=1S/C10H18O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h8-11H,1-7H2	
DCL-1O2R	C10H17O2	<chem>C1CCCCC2C1(O[O])CCCC2</chem>	InChI=1S/C10H17O2/c11-12-10-7-3-1-5-9(10)6-2-4-8-10/h9H,1-8H2	

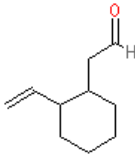
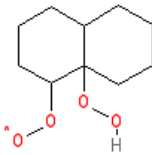
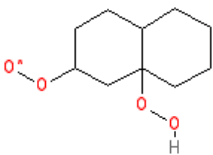
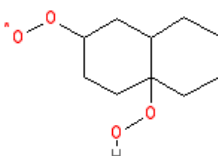
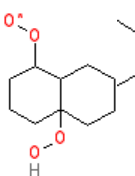
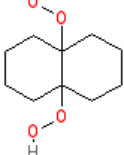
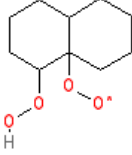
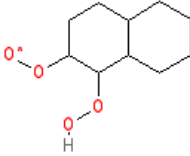
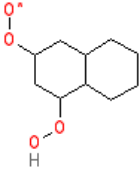
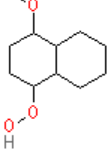
DCL-202R	C10H17O2	C1CCCC2C1C(O[O])CCC2	InChI=1S/C10H17O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h8-10H,1-7H2	
DCL-302R	C10H17O2	C1CCCC2C1CC(O[O])CC2	InChI=1S/C10H17O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h8-10H,1-7H2	
DCL-10R	C10H17O	C1CCCC2C1([O])CCCC2	InChI=1S/C10H17O/c11-10-7-3-1-5-9(10)6-2-4-8-10/h9H,1-8H2	
DCL-20R	C10H17O	C1CCCC2C1C([O])CCC2	InChI=1S/C10H17O/c11-10-7-3-5-8-4-1-2-6-9(8)10/h8-10H,1-7H2	
DCL-30R	C10H17O	C1CCCC2C1CC([O])CC2	InChI=1S/C10H17O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h8-10H,1-7H2	
DCLOOH1-2R	C10H17O2	C1CCCC2C1(OO)[CH]CCC2	InChI=1S/C10H17O2/c11-12-10-7-3-1-5-9(10)6-2-4-8-10/h7,9,11H,1-6,8H2	
DCLOOH1-3R	C10H17O2	C1CCCC2C1(OO)C[CH]CC2	InChI=1S/C10H17O2/c11-12-10-7-3-1-5-9(10)6-2-4-8-10/h3,9,11H,1-2,4-8H2	
DCLOOH1-4R	C10H17O2	C1CCCC2C1(OO)CC[CH]C2	InChI=1S/C10H17O2/c11-12-10-7-3-1-5-9(10)6-2-4-8-10/h1,9,11H,2-8H2	
DCLOOH1-5R	C10H17O2	C1CCCC2C1(OO)CCC[CH]2	InChI=1S/C10H17O2/c11-12-10-7-3-1-5-9(10)6-2-4-8-10/h5,9,11H,1-4,6-8H2	
DCLOOH1-6R	C10H17O2	C1CCC[C]2C1(OO)CCCC2	InChI=1S/C10H17O2/c11-12-10-7-3-1-5-9(10)6-2-4-8-10/h11H,1-8H2	

DCLOOH2-1R	C10H17O2	C1CCCC2[C]1C(OO)CCC2	InChI=1S/C10H17O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h8,10-11H,1-7H2	
DCLOOH2-3R	C10H17O2	C1CCCC2C1C(OO)[CH]CC2	InChI=1S/C10H17O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h7-11H,1-6H2	
DCLOOH2-4R	C10H17O2	C1CCCC2C1C(OO)C[CH]C2	InChI=1S/C10H17O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h3,8-11H,1-2,4-7H2	
DCLOOH2-5R	C10H17O2	C1CCCC2C1C(OO)CC[CH]C2	InChI=1S/C10H17O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h5,8-11H,1-4,6-7H2	
DCLOOH2-6R	C10H17O2	C1CCC[C]2C1C(OO)CCC2	InChI=1S/C10H17O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h9-11H,1-7H2	
DCLOOH2-2AR	C10H17O2	[CH]1CCCC2C1C(OO)CCC2	InChI=1S/C10H17O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h6,8-11H,1-5,7H2	
DCLOOH2-3AR	C10H17O2	C1[CH]CCC2C1C(OO)CCC2	InChI=1S/C10H17O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h2,8-11H,1,3-7H2	
DCLOOH2-4AR	C10H17O2	C1C[CH]CC2C1C(OO)CCC2	InChI=1S/C10H17O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h1,8-11H,2-7H2	
DCLOOH2-5AR	C10H17O2	C1CC[CH]C2C1C(OO)CCC2	InChI=1S/C10H17O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h4,8-11H,1-3,5-7H2	
DCLOOH3-1R	C10H17O2	C1CCCC2[C]1CC(OO)CC2	InChI=1S/C10H17O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h8,10-11H,1-7H2	

DCLOOH3-2R	C10H17O2	C1CCCC2C1[CH]C(OO)CC	InChI=1S/C10H17O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h7-11H,1-6H2	
DCLOOH3-4R	C10H17O2	C1CCCC2C1CC(OO)[CH]C	InChI=1S/C10H17O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h6,8-11H,1-5,7H2	
DCLOOH3-5R	C10H17O2	C1CCCC2C1CC(OO)C[CH]	InChI=1S/C10H17O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h5,8-11H,1-4,6-7H2	
DCLOOH3-6R	C10H17O2	C1CCC[C]2C1CC(OO)CC2	InChI=1S/C10H17O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h9-11H,1-7H2	
DCLOOH3-2AR	C10H17O2	[CH]1CCCC2C1CC(OO)CC	InChI=1S/C10H17O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h4,8-11H,1-3,5-7H2	
DCLOOH3-3AR	C10H17O2	C1[CH]CCC2C1CC(OO)CC	InChI=1S/C10H17O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h2,8-11H,1,3-7H2	
DCLOOH3-5AR	C10H17O2	C1CC[CH]C2C1CC(OO)CC	InChI=1S/C10H17O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h3,8-11H,1-2,4-7H2	
PBCHY2-1AR	C10H17O	C(C[CH2])CC1C(=O)CCCC	InChI=1S/C10H17O/c1-2-3-6-9-7-4-5-8-10(9)11/h9H,1-8H2	
NPCHY1A-2MR	C10H17O	C(CC=O)C1C([CH2])CCCC	InChI=1S/C10H17O/c1-9-5-2-3-6-10(9)7-4-8-11/h8-10H,1-7H2	
ECHY1A-2ER	C10H17O	C1C(CC=O)C(C[CH2])CCC	InChI=1S/C10H17O/c1-2-9-5-3-4-6-10(9)7-8-11/h8-10H,1-7H2	

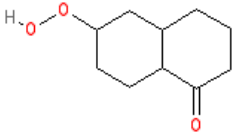
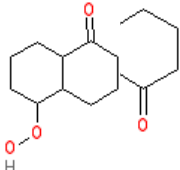
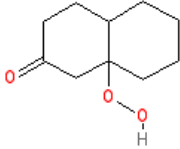
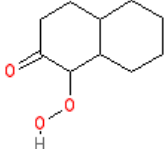
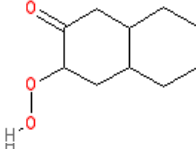
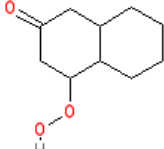
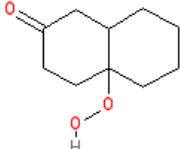
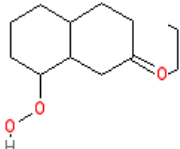
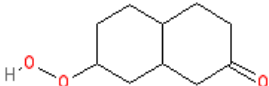
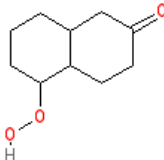
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DCLO1-3	C10H16O	C1CCCC2C13CC(O3)CC2	InChI=1S/C10H16O/c1-2-6-10-7-9(11-10)5-4-8(10)3-1/h8-9H,1-7H2	
DCLO1-4	C10H16O	C1CCCC2C13CCC(O3)C2	InChI=1S/C10H16O/c1-2-5-10-6-4-9(11-10)7-8(10)3-1/h8-9H,1-7H2	
DCLO1-5	C10H16O	C1CCCC2C13CCCC2(O3)	InChI=1S/C10H16O/c1-2-6-10-7-3-5-9(11-10)8(10)4-1/h8-9H,1-7H2	
DCLO1-6	C10H16O	C1CCCC2(O3)C13CCCC2	InChI=1S/C10H16O/c1-2-6-10-8-4-3-7-9(10,5-1)11-10/h1-8H2	
DCLO2-3	C10H16O	C1CCCC2C1C3C(O3)CC2	InChI=1S/C10H16O/c1-2-4-8-7(3-1)5-6-9-10(8)11-9/h7-10H,1-6H2	
DCLO2-4	C10H16O	C1CCCC2C1C3CC(O3)C2	InChI=1S/C10H16O/c1-2-4-9-7(3-1)5-8-6-10(9)11-8/h7-10H,1-6H2	
DCLO2-5	C10H16O	C1CCCC2C1C3CCC2(O3)	InChI=1S/C10H16O/c1-2-4-8-7(3-1)9-5-6-10(8)11-9/h7-10H,1-6H2	
DCLO2-2A	C10H16O	C1(O3)CCCC2C1C3CCC2	InChI=1S/C10H16O/c1-3-7-4-2-6-9-10(7)8(5-1)11-9/h7-10H,1-6H2	
DCLO2-3A	C10H16O	C1C(O3)CCC2C1C3CCC2	InChI=1S/C10H16O/c1-2-7-4-5-8-6-9(7)10(3-1)11-8/h7-10H,1-6H2	

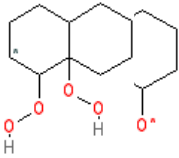
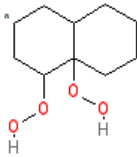
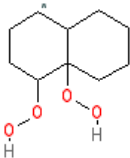
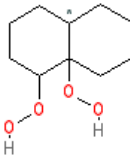
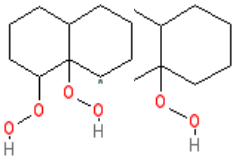
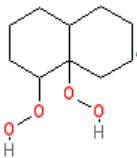
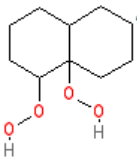
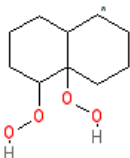
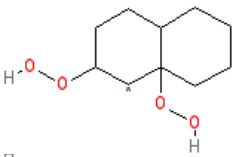
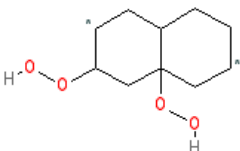
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DCLO2-5A	C10H16O	C1CCC(O3)C2C1C3CCC2	InChI=1S/C10H16O/c1-3-7-8-4-2-6-10(7)11-9(8)5-1/h7-10H,1-6H2	
DCLO3-3A	C10H16O	C1C(O3)CCC2C1CC3CC2	InChI=1S/C10H16O/c1-3-9-5-8-6-10(11-9)4-2-7(1)8/h7-10H,1-6H2	
DCLO3-4	C10H16O	C1CCCC2C1CC3C(O3)C2	InChI=1S/C10H16O/c1-2-4-8-6-10-9(11-10)5-7(8)3-1/h7-10H,1-6H2	
PBCHD1AY2	C10H16O	C(C=C)CC1C(=O)CCCC1	InChI=1S/C10H16O/c1-2-3-6-9-7-4-5-8-10(9)11/h2,9H,1,3-8H2	
ECHD1AY2	C8H12O	C1C(C=C)C(=O)CCC1	InChI=1S/C8H12O/c1-2-7-5-3-4-6-8(7)9/h2,7H,1,3-6H2	
NPCHD1A-2CHO	C10H16O	C(C=C)C1C(C=O)CCCC1	InChI=1S/C10H16O/c1-2-5-9-6-3-4-7-10(9)8-11/h2,8-10H,1,3-7H2	
PBCHD1Y1A	C10H16O	C(CC=O)CC1=CCCCC1	InChI=1S/C10H16O/c11-9-5-4-8-10-6-2-1-3-7-10/h6,9H,1-5,7-8H2	
PBCHD2Y1A	C10H16O	C(CC=O)CC1C=CCCC1	InChI=1S/C10H16O/c11-9-5-4-8-10-6-2-1-3-7-10/h2,6,9-10H,1,3-5,7-8H2	
NPCHY1A-2CH2	C10H16O	C(CC=O)C1C(=C)CCCC1	InChI=1S/C10H16O/c1-9-5-2-3-6-10(9)7-4-8-11/h8,10H,1-7H2	

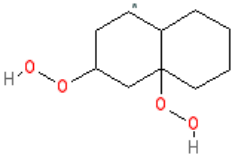
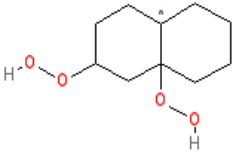
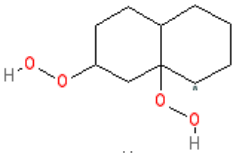
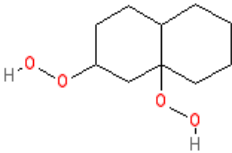
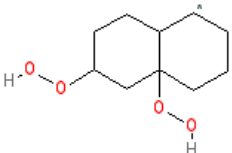
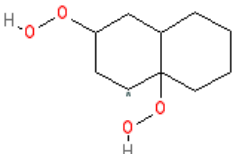
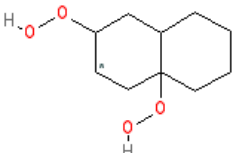
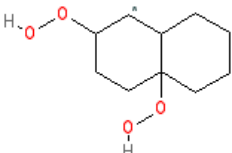
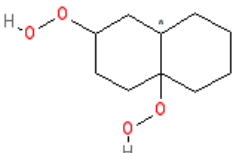
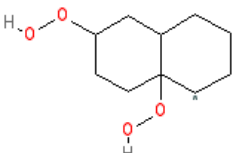
ECHY1A-2V	C10H16O	C1C(CC=O)C(C=C)CCC1	InChI=1S/C10H16O/c1-2-9-5-3-4-6-10(9)7-8-11/h2,8-10H,1,3-7H2	
DCLOOH1-2O2R	C10H17O4	C1CCCC2C1(OO)C(O[O])C	InChI=1S/C10H17O4/c11-13-9-6-3-5-8-4-1-2-7-10(8,9)14-12/h8-9,12H,1-7H2	
DCLOOH1-3O2R	C10H17O4	C1CCCC2C1(OO)CC(O[O])	InChI=1S/C10H17O4/c11-13-9-5-4-8-3-1-2-6-10(8,7-9)14-12/h8-9,12H,1-7H2	
DCLOOH1-4O2R	C10H17O4	C1CCCC2C1(OO)CCC(O[O])C2	InChI=1S/C10H17O4/c11-13-9-4-6-10(14-12)5-2-1-3-8(10)7-9/h8-9,12H,1-7H2	
DCLOOH1-5O2R	C10H17O4	C1CCCC2C1(OO)CCCC2(O[O])	InChI=1S/C10H17O4/c11-13-9-5-3-7-10(14-12)6-2-1-4-8(9)10/h8-9,12H,1-7H2	
DCLOOH1-6O2R	C10H17O4	C1CCCC2(O[O])C1(OO)CC	InChI=1S/C10H17O4/c11-13-9-5-1-2-6-10(9,14-12)8-4-3-7-9/h11H,1-8H2	
DCLOOH2-1O2R	C10H17O4	C1CCCC2C1(O[O])C(OO)C	InChI=1S/C10H17O4/c11-13-9-6-3-5-8-4-1-2-7-10(8,9)14-12/h8-9,11H,1-7H2	
DCLOOH2-3O2R	C10H17O4	C1CCCC2C1C(OO)C(O[O])	InChI=1S/C10H17O4/c11-13-9-6-5-7-3-1-2-4-8(7)10(9)14-12/h7-10,12H,1-6H2	
DCLOOH2-4O2R	C10H17O4	C1CCCC2C1C(OO)CC(O[O])C2	InChI=1S/C10H17O4/c11-13-8-5-7-3-1-2-4-9(7)10(6-8)14-12/h7-10,12H,1-6H2	
DCLOOH2-5O2R	C10H17O4	C1CCCC2C1C(OO)CCC2(O[O])	InChI=1S/C10H17O4/c11-13-9-5-6-10(14-12)8-4-2-1-3-7(8)9/h7-11H,1-6H2	

DCLOOH2-6O2R	C10H17O4	C1CCCC2(O[O])C1C(OO)C CC2	InChI=1S/C10H17O4/c11-13-9-5-3-7-10(14-12)6-2-1-4-8(9)10/h8-9,11H,1-7H2	
DCLOOH2-2AO2R	C10H17O4	C1(O[O])CCCC2C1C(OO)C CC2	InChI=1S/C10H17O4/c11-13-8-5-1-3-7-4-2-6-9(14-12)10(7)8/h7-11H,1-6H2	
DCLOOH2-3AO2R	C10H17O4	C1C(O[O])CCC2C1C(OO)C CC2	InChI=1S/C10H17O4/c11-13-8-5-4-7-2-1-3-10(14-12)9(7)6-8/h7-10,12H,1-6H2	
DCLOOH2-4AO2R	C10H17O4	C1CC(O[O])CC2C1C(OO)C CC2	InChI=1S/C10H17O4/c11-13-8-4-5-9-7(6-8)2-1-3-10(9)14-12/h7-10,12H,1-6H2	
DCLOOH2-5AO2R	C10H17O4	C1CCC(O[O])C2C1C(OO)C CC2	InChI=1S/C10H17O4/c11-13-9-5-1-3-7-8(9)4-2-6-10(7)14-12/h7-11H,1-6H2	
DCLOOH3-1O2R	C10H17O4	C1CCCC2C1(O[O])CC(OO) CC2	InChI=1S/C10H17O4/c11-13-9-5-4-8-3-1-2-6-10(8,7-9)14-12/h8-9,11H,1-7H2	
DCLOOH3-2O2R	C10H17O4	C1CCCC2C1C(O[O])C(OO) CC2	InChI=1S/C10H17O4/c11-13-9-6-5-7-3-1-2-4-8(7)10(9)14-12/h7-11H,1-6H2	
DCLOOH3-4O2R	C10H17O4	C1CCCC2C1CC(OO)C(O[O]) C2	InChI=1S/C10H17O4/c11-13-9-5-7-3-1-2-4-8(7)6-10(9)14-12/h7-11H,1-6H2	
DCLOOH3-5O2R	C10H17O4	C1CCCC2C1CC(OO)CC2(O[O])	InChI=1S/C10H17O4/c11-13-8-5-7-3-1-2-4-9(7)10(6-8)14-12/h7-11H,1-6H2	
DCLOOH3-6O2R	C10H17O4	C1CCCC2(O[O])C1CC(OO) CC2	InChI=1S/C10H17O4/c11-13-9-4-6-10(14-12)5-2-1-3-8(10)7-9/h8-9,11H,1-7H2	

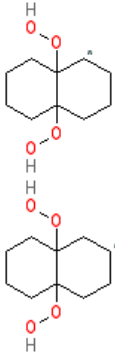
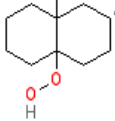
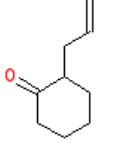
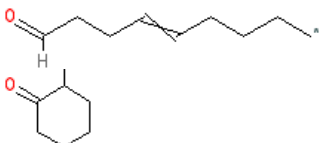
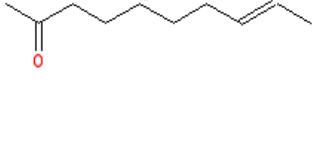

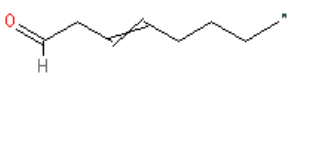
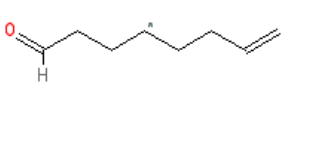
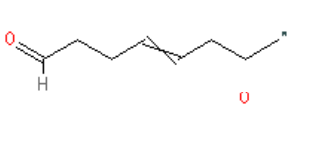
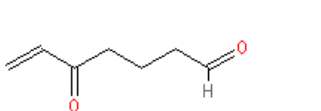
DCLOOH3-2AO2R	C10H17O4	C1(O[O])CCCC2C1CC(OO)CC2	InChI=1S/C10H17O4/c11-13-8-5-4-7-2-1-3-10(14-12)9(7)6-8/h7-11H,1-6H2	
DCLOOH3-3AO2R	C10H17O4	C1C(O[O])CCC2C1CC(OO)CC2	InChI=1S/C10H17O4/c11-13-9-3-1-7-2-4-10(14-12)6-8(7)5-9/h7-11H,1-6H2	
DCLOOH3-5AO2R	C10H17O4	C1CCC(O[O])C2C1CC(OO)CC2	InChI=1S/C10H17O4/c11-13-8-4-5-9-7(6-8)2-1-3-10(9)14-12/h7-11H,1-6H2	
DCLKET2-1	C10H16O3	C1CCCC2C1(OO)C(=O)CC2	InChI=1S/C10H16O3/c11-9-6-3-5-8-4-1-2-7-10(8,9)13-12/h8,12H,1-7H2	
DCLKET2-3	C10H16O3	C1CCCC2C1C(=O)C(OO)CC2	InChI=1S/C10H16O3/c11-10-8-4-2-1-3-7(8)5-6-9(10)13-12/h7-9,12H,1-6H2	
DCLKET2-4	C10H16O3	C1CCCC2C1C(=O)CC(OO)C2	InChI=1S/C10H16O3/c11-10-6-8(13-12)5-7-3-1-2-4-9(7)10/h7-9,12H,1-6H2	
DCLKET2-5	C10H16O3	C1CCCC2C1C(=O)CCC2(OO)	InChI=1S/C10H16O3/c11-9-5-6-10(13-12)8-4-2-1-3-7(8)9/h7-8,10,12H,1-6H2	
DCLKET2-6	C10H16O3	C1CCCC2(OO)C1C(=O)CC2	InChI=1S/C10H16O3/c11-9-5-3-7-10(13-12)6-2-1-4-8(9)10/h8,12H,1-7H2	
DCLKET2-2A	C10H16O3	C1(OO)CCCC2C1C(=O)CC2	InChI=1S/C10H16O3/c11-8-5-1-3-7-4-2-6-9(13-12)10(7)8/h7,9-10,12H,1-6H2	
DCLKET2-3A	C10H16O3	C1C(OO)CCC2C1C(=O)CC2	InChI=1S/C10H16O3/c11-10-3-1-2-7-4-5-8(13-12)6-9(7)10/h7-9,12H,1-6H2	

DCLKET2-4A	C10H16O3	<chem>C1CC(OO)CC2C1C(=O)CC2</chem>	InChI=1S/C10H16O3/c11-10-3-1-2-7-6-8(13-12)4-5-9(7)10/h7-9,12H,1-6H2	
DCLKET2-5A	C10H16O3	<chem>C1CCC(OO)C2C1C(=O)CC2</chem>	InChI=1S/C10H16O3/c11-9-5-1-4-8-7(9)3-2-6-10(8)13-12/h7-8,10,12H,1-6H2	
DCLKET3-1	C10H16O3	<chem>C1CCCC2C1(OO)CC(=O)C2</chem>	InChI=1S/C10H16O3/c11-9-5-4-8-3-1-2-6-10(8,7-9)13-12/h8,12H,1-7H2	
DCLKET3-2	C10H16O3	<chem>C1CCCC2C1C(OO)C(=O)C2</chem>	InChI=1S/C10H16O3/c11-9-6-5-7-3-1-2-4-8(7)10(9)13-12/h7-8,10,12H,1-6H2	
DCLKET3-4	C10H16O3	<chem>C1CCCC2C1CC(=O)C(OO)C2</chem>	InChI=1S/C10H16O3/c11-9-5-7-3-1-2-4-8(7)6-10(9)13-12/h7-8,10,12H,1-6H2	
DCLKET3-5	C10H16O3	<chem>C1CCCC2C1CC(=O)CC2(OO)</chem>	InChI=1S/C10H16O3/c11-8-5-7-3-1-2-4-9(7)10(6-8)13-12/h7,9-10,12H,1-6H2	
DCLKET3-6	C10H16O3	<chem>C1CCCC2(OO)C1CC(=O)C2</chem>	InChI=1S/C10H16O3/c11-9-4-6-10(13-12)5-2-1-3-8(10)7-9/h8,12H,1-7H2	
DCLKET3-2A	C10H16O3	<chem>C1(OO)CCCC2C1CC(=O)C2</chem>	InChI=1S/C10H16O3/c11-8-5-4-7-2-1-3-10(13-12)9(7)6-8/h7,9-10,12H,1-6H2	
DCLKET3-3A	C10H16O3	<chem>C1C(OO)CCC2C1CC(=O)C2</chem>	InChI=1S/C10H16O3/c11-9-3-1-7-2-4-10(13-12)6-8(7)5-9/h7-8,10,12H,1-6H2	
DCLKET3-5A	C10H16O3	<chem>C1CCC(OO)C2C1CC(=O)C2</chem>	InChI=1S/C10H16O3/c11-8-4-5-9-7(6-8)2-1-3-10(9)13-12/h7,9-10,12H,1-6H2	

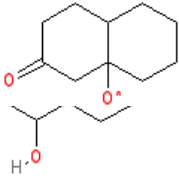
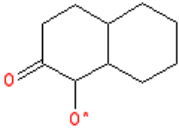
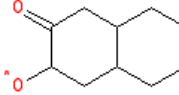
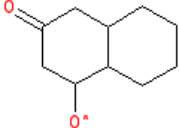
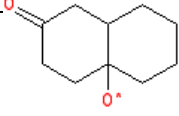
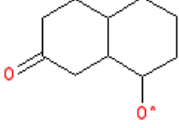
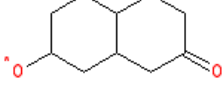
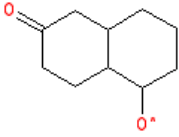
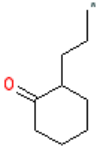
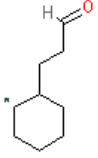
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DCLQ12-4R	C10H17O4	C1CCCC2C1(OO)C(OO)C[CH]C2	InChI=1S/C10H17O4/c11-13-9-6-3-5-8-4- 1-2-7-10(8,9)14-12/h3,8-9,11-12H,1-2,4- 7H2	
DCLQ12-5R	C10H17O4	C1CCCC2C1(OO)C(OO)C C[CH]2	InChI=1S/C10H17O4/c11-13-9-6-3-5-8-4- 1-2-7-10(8,9)14-12/h5,8-9,11-12H,1-4,6- 7H2	
DCLQ12-6R	C10H17O4	C1CCC[C]2C1(OO)C(OO)C CC2	InChI=1S/C10H17O4/c11-13-9-6-3-5-8-4- 1-2-7-10(8,9)14-12/h9,11-12H,1-7H2	
DCLQ12-2AR	C10H17O4	[CH]1CCCC2C1(OO)C(OO) CCC2	InChI=1S/C10H17O4/c11-13-9-6-3-5-8-4- 1-2-7-10(8,9)14-12/h7-9,11-12H,1-6H2	
DCLQ12-3AR	C10H17O4	C1[CH]CCC2C1(OO)C(OO) CCC2	InChI=1S/C10H17O4/c11-13-9-6-3-5-8-4- 1-2-7-10(8,9)14-12/h2,8-9,11-12H,1,3- 7H2	
DCLQ12-4AR	C10H17O4	C1C[CH]CC2C1(OO)C(OO) CCC2	InChI=1S/C10H17O4/c11-13-9-6-3-5-8-4- 1-2-7-10(8,9)14-12/h1,8-9,11-12H,2-7H2	
DCLQ12-5AR	C10H17O4	C1CC[CH]C2C1(OO)C(OO) CCC2	InChI=1S/C10H17O4/c11-13-9-6-3-5-8-4- 1-2-7-10(8,9)14-12/h4,8-9,11-12H,1-3,5- 7H2	
DCLQ13-2R	C10H17O4	C1CCCC2C1(OO)[CH]C(O O)CC2	InChI=1S/C10H17O4/c11-13-9-5-4-8-3-1- 2-6-10(8,7-9)14-12/h7-9,11-12H,1-6H2	
DCLQ13-4R	C10H17O4	C1CCCC2C1(OO)CC(OO)[CH]C2	InChI=1S/C10H17O4/c11-13-9-5-4-8-3-1- 2-6-10(8,7-9)14-12/h5,8-9,11-12H,1-4,6- 7H2	

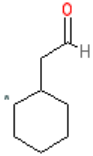
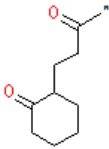
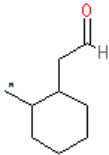
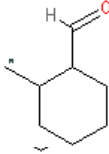
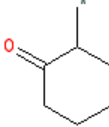
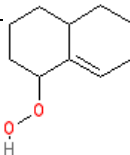
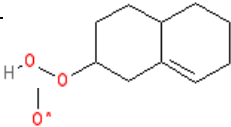
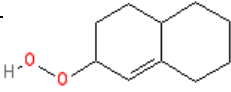
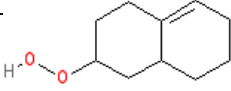
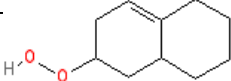
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DCLQ13-6R	C10H17O4	C1CCC[C]2C1(OO)CC(OO)CC2	InChI=1S/C10H17O4/c11-13-9-5-4-8-3-1-2-6-10(8,7-9)14-12/h9,11-12H,1-7H2	
DCLQ13-2AR	C10H17O4	[CH]1CCCC2C1(OO)CC(O)CC2	InChI=1S/C10H17O4/c11-13-9-5-4-8-3-1-2-6-10(8,7-9)14-12/h6,8-9,11-12H,1-5,7H2	
DCLQ13-3AR	C10H17O4	C1[CH]CCC2C1(OO)CC(O)CC2	InChI=1S/C10H17O4/c11-13-9-5-4-8-3-1-2-6-10(8,7-9)14-12/h2,8-9,11-12H,1,3-7H2	
DCLQ13-5AR	C10H17O4	C1CC[CH]C2C1(OO)CC(O)CC2	InChI=1S/C10H17O4/c11-13-9-5-4-8-3-1-2-6-10(8,7-9)14-12/h3,8-9,11-12H,1-2,4-7H2	
DCLQ14-2R	C10H17O4	C1CCCC2C1(OO)[CH]CC(OO)C2	InChI=1S/C10H17O4/c11-13-9-4-6-10(14-12)5-2-1-3-8(10)7-9/h6,8-9,11-12H,1-5,7H2	
DCLQ14-3R	C10H17O4	C1CCCC2C1(OO)C[CH]C(OO)C2	InChI=1S/C10H17O4/c11-13-9-4-6-10(14-12)5-2-1-3-8(10)7-9/h4,8-9,11-12H,1-3,5-7H2	
DCLQ14-5R	C10H17O4	C1CCCC2C1(OO)CCC(OO)[CH]2	InChI=1S/C10H17O4/c11-13-9-4-6-10(14-12)5-2-1-3-8(10)7-9/h7-9,11-12H,1-6H2	
DCLQ14-6R	C10H17O4	C1CCC[C]2C1(OO)CCC(O)C2	InChI=1S/C10H17O4/c11-13-9-4-6-10(14-12)5-2-1-3-8(10)7-9/h9,11-12H,1-7H2	
DCLQ14-2AR	C10H17O4	[CH]1CCCC2C1(OO)CCC(OO)C2	InChI=1S/C10H17O4/c11-13-9-4-6-10(14-12)5-2-1-3-8(10)7-9/h5,8-9,11-12H,1-4,6-7H2	

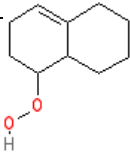
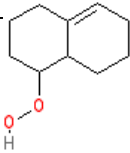
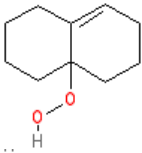
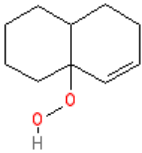
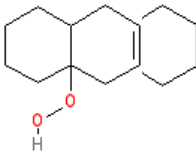
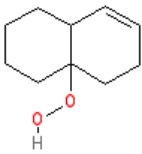
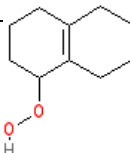
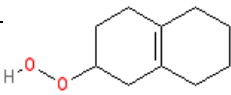
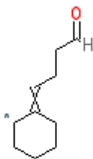
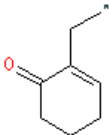
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DCLQ14-5AR	C10H17O4	<chem>C1CC[CH]C2C1(OO)CCC(OO)C2</chem>	InChI=1S/C10H17O4/c11-13-9-4-6-10(14-12)5-2-1-3-8(10)7-9/h3,8-9,11-12H,1-2,4-7H2	
DCLQ15-2R	C10H17O4	<chem>C1CCCC2C1(OO)[CH]CCC2(OO)</chem>	InChI=1S/C10H17O4/c11-13-9-5-3-7-10(14-12)6-2-1-4-8(9)10/h7-9,11-12H,1-6H2	
DCLQ15-3R	C10H17O4	<chem>C1CCCC2C1(OO)C[CH]CC2(OO)</chem>	InChI=1S/C10H17O4/c11-13-9-5-3-7-10(14-12)6-2-1-4-8(9)10/h3,8-9,11-12H,1-2,4-7H2	
DCLQ15-4R	C10H17O4	<chem>C1CCCC2C1(OO)CC[CH]C2(OO)</chem>	InChI=1S/C10H17O4/c11-13-9-5-3-7-10(14-12)6-2-1-4-8(9)10/h5,8-9,11-12H,1-4,6-7H2	
DCLQ15-6R	C10H17O4	<chem>C1CCC[C]2C1(OO)CCCC2(OO)</chem>	InChI=1S/C10H17O4/c11-13-9-5-3-7-10(14-12)6-2-1-4-8(9)10/h9,11-12H,1-7H2	
DCLQ15-2AR	C10H17O4	<chem>[CH]1CCCC2C1(OO)CCCC2(OO)</chem>	InChI=1S/C10H17O4/c11-13-9-5-3-7-10(14-12)6-2-1-4-8(9)10/h6,8-9,11-12H,1-5,7H2	
DCLQ15-3AR	C10H17O4	<chem>C1[CH]CCC2C1(OO)CCCC2(OO)</chem>	InChI=1S/C10H17O4/c11-13-9-5-3-7-10(14-12)6-2-1-4-8(9)10/h2,8-9,11-12H,1,3-7H2	
DCLQ15-4AR	C10H17O4	<chem>C1C[CH]CC2C1(OO)CCCC2(OO)</chem>	InChI=1S/C10H17O4/c11-13-9-5-3-7-10(14-12)6-2-1-4-8(9)10/h1,8-9,11-12H,2-7H2	
DCLQ15-5AR	C10H17O4	<chem>C1CC[CH]C2C1(OO)CCCC2(OO)</chem>	InChI=1S/C10H17O4/c11-13-9-5-3-7-10(14-12)6-2-1-4-8(9)10/h4,8-9,11-12H,1-3,5-7H2	


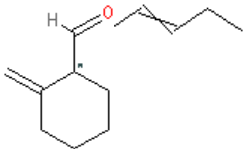
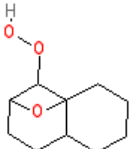
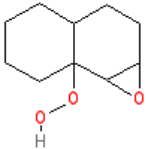
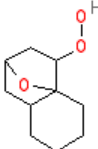
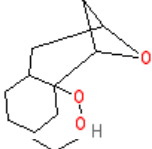
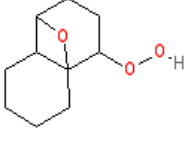
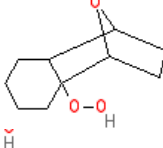
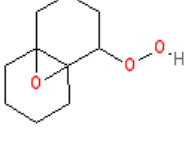
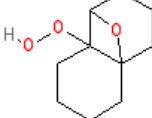
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DCLQ16-3R	C10H17O4	<chem>C1CCCC2(OO)C1(OO)C[C]HCC2</chem>	InChI=1S/C10H17O4/c11-13-9-5-1-2-6-10(9,14-12)8-4-3-7-9/h1,11-12H,2-8H2	
NPCHD1AY2	C9H14O	<chem>C(C=C)C1C(=O)CCCC1</chem>	InChI=1S/C9H14O/c1-2-5-8-6-3-4-7-9(8)10/h2,8H,1,3-7H2	
NC9D4Y1-9R	C9H15O	<chem>C(=O)CCC=CCCC[CH2]</chem>	InChI=1S/C9H15O/c1-2-3-4-5-6-7-8-9-10/h5-6,9H,1-4,7-8H2	
NC9D1Y8-5R	C9H15O	<chem>C=CCC[CH]CCC(=O)C</chem>	InChI=1S/C9H15O/c1-3-4-5-6-7-8-9(2)10/h3,6H,1,4-5,7-8H2,2H3	
NC9D4Y9-1R	C9H15O	<chem>[CH2]CCC=CCCCC(=O)</chem>	InChI=1S/C9H15O/c1-2-3-4-5-6-7-8-9-10/h4-5,9H,1-3,6-8H2	
NC8D3Y1-8R	C8H13O	<chem>C(=O)CC=CCCC[CH2]</chem>	InChI=1S/C8H13O/c1-2-3-4-5-6-7-8-9/h5-6,8H,1-4,7H2	
NC8D1Y8-5R	C8H13O	<chem>C=CCC[CH]CCC(=O)</chem>	InChI=1S/C8H13O/c1-2-3-4-5-6-7-8-9/h2,5,8H,1,3-4,6-7H2	
NC8D4Y8-1R	C8H13O	<chem>[CH2]CCC=CCCC(=O)</chem>	InChI=1S/C8H13O/c1-2-3-4-5-6-7-8-9/h4-5,8H,1-3,6-7H2	
NC7D1Y37	C7H10O2	<chem>C=CC(=O)CCCC(=O)</chem>	InChI=1S/C7H10O2/c1-2-7(9)5-3-4-6-8/h2,6H,1,3-5H2	

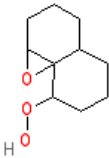
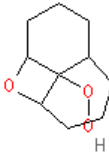
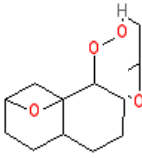
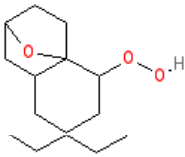
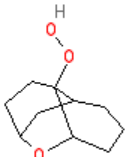
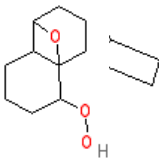
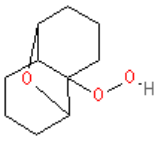
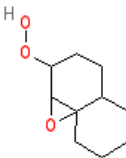
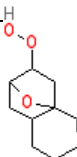
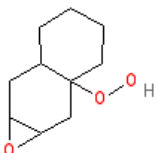
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DCLKET2-1O	C10H15O2	<chem>C1CCCC2C1([O])C(=O)CC</chem>	InChI=1S/C10H15O2/c11-9-6-3-5-8-4-1-2-7-10(8,9)12/h8H,1-7H2	
DCLKET2-3O	C10H15O2	<chem>C1CCCC2C1C(=O)C([O])C</chem>	InChI=1S/C10H15O2/c11-9-6-5-7-3-1-2-4-8(7)10(9)12/h7-9H,1-6H2	
DCLKET2-4O	C10H15O2	<chem>C1CCCC2C1C(=O)CC([O])</chem>	InChI=1S/C10H15O2/c11-8-5-7-3-1-2-4-9(7)10(12)6-8/h7-9H,1-6H2	
DCLKET2-5O	C10H15O2	<chem>C1CCCC2C1C(=O)CCC2([O])</chem>	InChI=1S/C10H15O2/c11-9-5-6-10(12)8-4-2-1-3-7(8)9/h7-9H,1-6H2	
DCLKET2-6O	C10H15O2	<chem>C1CCCC2([O])C1C(=O)CC</chem>	InChI=1S/C10H15O2/c11-9-5-3-7-10(12)6-2-1-4-8(9)10/h8H,1-7H2	
DCLKET2-2AO	C10H15O2	<chem>C1([O])CCCC2C1C(=O)CC</chem>	InChI=1S/C10H15O2/c11-8-5-1-3-7-4-2-6-9(12)10(7)8/h7-8,10H,1-6H2	
DCLKET2-3AO	C10H15O2	<chem>C1C([O])CCC2C1C(=O)CC</chem>	InChI=1S/C10H15O2/c11-8-5-4-7-2-1-3-10(12)9(7)6-8/h7-9H,1-6H2	
DCLKET2-4AO	C10H15O2	<chem>C1CC([O])CC2C1C(=O)CC</chem>	InChI=1S/C10H15O2/c11-8-4-5-9-7(6-8)2-1-3-10(9)12/h7-9H,1-6H2	
DCLKET2-5AO	C10H15O2	<chem>C1CCC([O])C2C1C(=O)CC</chem>	InChI=1S/C10H15O2/c11-9-5-1-3-7-8(9)4-2-6-10(7)12/h7-9H,1-6H2	

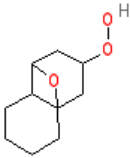
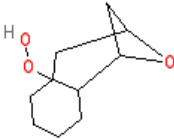
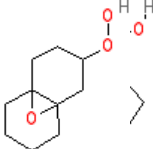
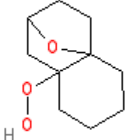
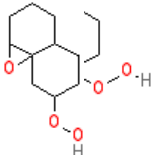
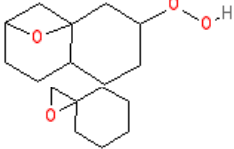
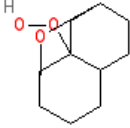
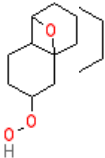
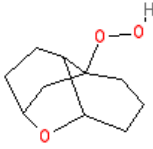
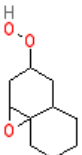
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DCLKET3-2O	C10H15O2	C1CCCC2C1C([O])C(=O)C2	InChI=1S/C10H15O2/c11-9-6-5-7-3-1-2-4-8(7)10(9)12/h7-8,10H,1-6H2	
DCLKET3-4O	C10H15O2	C1CCCC2C1CC(=O)C([O])C2	InChI=1S/C10H15O2/c11-9-5-7-3-1-2-4-8(7)6-10(9)12/h7-9H,1-6H2	
DCLKET3-5O	C10H15O2	C1CCCC2C1CC(=O)CC2([O])	InChI=1S/C10H15O2/c11-8-5-7-3-1-2-4-9(7)10(12)6-8/h7,9-10H,1-6H2	
DCLKET3-6O	C10H15O2	C1CCCC2([O])C1CC(=O)C2	InChI=1S/C10H15O2/c11-9-4-6-10(12)5-2-1-3-8(10)7-9/h8H,1-7H2	
DCLKET3-2AO	C10H15O2	C1([O])CCCC2C1CC(=O)C2	InChI=1S/C10H15O2/c11-8-5-4-7-2-1-3-10(12)9(7)6-8/h7,9-10H,1-6H2	
DCLKET3-3AO	C10H15O2	C1C([O])CCC2C1CC(=O)C2	InChI=1S/C10H15O2/c11-9-3-1-7-2-4-10(12)6-8(7)5-9/h7-9H,1-6H2	
DCLKET3-5AO	C10H15O2	C1CCC([O])C2C1CC(=O)C2	InChI=1S/C10H15O2/c11-8-4-5-9-7(6-8)2-1-3-10(9)12/h7,9-10H,1-6H2	
NPCHY2-1AR	C9H15O	C(C[CH2])C1C(=O)CCCC1	InChI=1S/C9H15O/c1-2-5-8-6-3-4-7-9(8)10/h8H,1-7H2	
NPCHY1A-2R	C9H15O	C(CC=O)C1[CH]CCCC1	InChI=1S/C9H15O/c10-8-4-7-9-5-2-1-3-6-9/h5,8-9H,1-4,6-7H2	

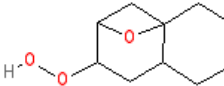
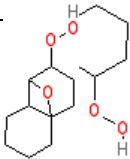
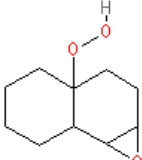
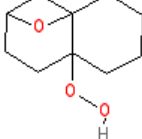
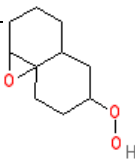
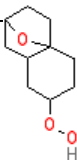
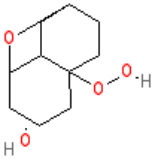
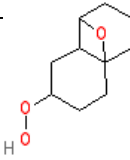
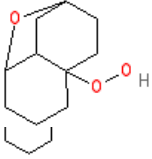
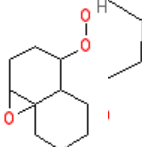
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PBCHY2A2-1AR	C10H15O2	C([CH2])(=O)CCC1C(=O)CCC1	InChI=1S/C10H15O2/c1-8(11)6-7-9-4-2-3-5-10(9)12/h9H,1-7H2	
ECHY1A-2MR	C9H15O	C1C(CC=O)C([CH2])CCC1	InChI=1S/C9H15O/c1-8-4-2-3-5-9(8)6-7-10/h7-9H,1-6H2	
MCHY1A-2MR	C8H13O	C1C(C=O)C([CH2])CCC1	InChI=1S/C8H13O/c1-7-4-2-3-5-8(7)6-9/h6-8H,1-5H2	
MCHY2-1AR	C7H11O	C1C([CH2])C(=O)CCC1	InChI=1S/C7H11O/c1-6-4-2-3-5-7(6)8/h6H,1-5H2	
DCLD1-2AOOH	C10H16O2	C1(OO)CCCC2C1=CCCC2	InChI=1S/C10H16O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h6,8,10-11H,1-5,7H2	
DCLD1-3AOOH	C10H16O2	C1C(OO)CCC2C1=CCCC2	InChI=1S/C10H16O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h4,8,10-11H,1-3,5-7H2	
DCLD1-3OOH	C10H16O2	C1CCCC2C1=CC(OO)CC2	InChI=1S/C10H16O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h7-8,10-11H,1-6H2	
DCLD1-4AOOH	C10H16O2	C1CC(OO)CC2C1=CCCC2	InChI=1S/C10H16O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h3,9-11H,1-2,4-7H2	
DCLD1-4OOH	C10H16O2	C1CCCC2C1=CCC(OO)C2	InChI=1S/C10H16O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h5,9-11H,1-4,6-7H2	

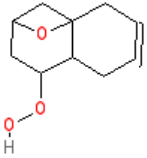
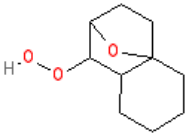
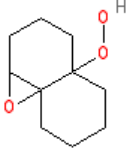
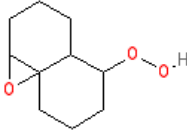
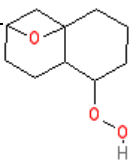
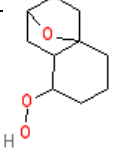
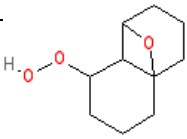
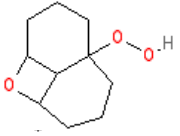
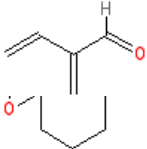
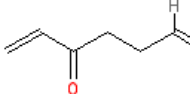
DCLD1-5OOH	C10H16O2	C1CCCC2C1=CCCC2(OO)	InChI=1S/C10H16O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h5,9-11H,1-4,6-7H2	
DCLD1-5AOOH	C10H16O2	C1CCC(OO)C2C1=CCCC2	InChI=1S/C10H16O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h4,9-11H,1-3,5-7H2	
DCLD1-6OOH	C10H16O2	C1CCCC2(OO)C1=CCCC2	InChI=1S/C10H16O2/c11-12-10-7-3-1-5-9(10)6-2-4-8-10/h5,11H,1-4,6-8H2	
DCLD2-1OOH	C10H16O2	C1CCCC2C1(OO)C=CCC2	InChI=1S/C10H16O2/c11-12-10-7-3-1-5-9(10)6-2-4-8-10/h3,7,9,11H,1-2,4-6,8H2	
DCLD3-1OOH	C10H16O2	C1CCCC2C1(OO)CC=CC2	InChI=1S/C10H16O2/c11-12-10-7-3-1-5-9(10)6-2-4-8-10/h1,3,9,11H,2,4-8H2	
DCLD4-1OOH	C10H16O2	C1CCCC2C1(OO)CCC=C2	InChI=1S/C10H16O2/c11-12-10-7-3-1-5-9(10)6-2-4-8-10/h1,5,9,11H,2-4,6-8H2	
DCLD6-2OOH	C10H16O2	C1CCCC2=C1C(OO)CCC2	InChI=1S/C10H16O2/c11-12-10-7-3-5-8-4-1-2-6-9(8)10/h10-11H,1-7H2	
DCLD6-3OOH	C10H16O2	C1CCCC2=C1CC(OO)CC2	InChI=1S/C10H16O2/c11-12-10-6-5-8-3-1-2-4-9(8)7-10/h10-11H,1-7H2	
PBCHD4AY1A-2R	C10H15O	C(CC=O)C=C1[CH]CCCC1	InChI=1S/C10H15O/c11-9-5-4-8-10-6-2-1-3-7-10/h6,8-9H,1-5,7H2	
ECHD1Y6-1AR	C8H11O	C1(=O)C(C[CH2])=CCCC1	InChI=1S/C8H11O/c1-2-7-5-3-4-6-8(7)9/h5H,1-4,6H2	

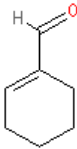
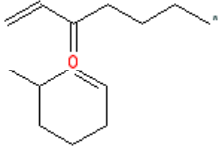
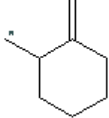
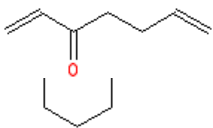
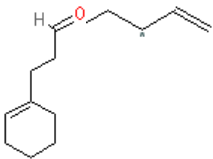


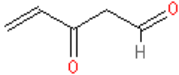
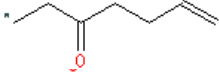
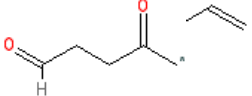
NC8D13-8R	C ₈ H ₁₃	<chem>C=CC=CCCC[CH2]</chem>	InChI=1S/C ₈ H ₁₃ /c1-3-5-7-8-6-4-2/h3,5,7H,1-2,4,6,8H2	
MCHY1A-2CH2-1R	C ₈ H ₁₁ O	<chem>C1[C](C=O)C(=C)CCC1</chem>	InChI=1S/C ₈ H ₁₁ O/c1-7-4-2-3-5-8(7)6-9/h6H,1-5H2	
DCLO13-2OOH	C ₁₀ H ₁₆ O ₃	<chem>C1CCCC2C13C(OO)C(O3)CC2</chem>	InChI=1S/C ₁₀ H ₁₆ O ₃ /c11-13-9-8-5-4-7-3-1-2-6-10(7,9)12-8/h7-9,11H,1-6H2	
DCLO23-1OOH	C ₁₀ H ₁₆ O ₃	<chem>C1CCCC2C1(OO)C3C(O3)CC2</chem>	InChI=1S/C ₁₀ H ₁₆ O ₃ /c11-13-10-6-2-1-3-7(10)4-5-8-9(10)12-8/h7-9,11H,1-6H2	
DCLO14-2OOH	C ₁₀ H ₁₆ O ₃	<chem>C1CCCC2C13C(OO)CC(O3)C2</chem>	InChI=1S/C ₁₀ H ₁₆ O ₃ /c11-13-9-6-8-5-7-3-1-2-4-10(7,9)12-8/h7-9,11H,1-6H2	
DCLO24-1OOH	C ₁₀ H ₁₆ O ₃	<chem>C1CCCC2C1(OO)C3CC(O3)C2</chem>	InChI=1S/C ₁₀ H ₁₆ O ₃ /c11-13-10-4-2-1-3-7(10)5-8-6-9(10)12-8/h7-9,11H,1-6H2	
DCLO15-2OOH	C ₁₀ H ₁₆ O ₃	<chem>C1CCCC2C13C(OO)CCC2(O3)</chem>	InChI=1S/C ₁₀ H ₁₆ O ₃ /c11-13-9-5-4-8-7-3-1-2-6-10(7,9)12-8/h7-9,11H,1-6H2	
DCLO25-1OOH	C ₁₀ H ₁₆ O ₃	<chem>C1CCCC2C1(OO)C3CCC2(O3)</chem>	InChI=1S/C ₁₀ H ₁₆ O ₃ /c11-13-10-6-2-1-3-7(10)8-4-5-9(10)12-8/h7-9,11H,1-6H2	
DCLO16-2OOH	C ₁₀ H ₁₆ O ₃	<chem>C1CCCC2(O3)C13C(OO)C(C3)C2</chem>	InChI=1S/C ₁₀ H ₁₆ O ₃ /c11-12-8-4-3-6-9-5-1-2-7-10(8,9)13-9/h8,11H,1-7H2	
DCLO26-1OOH	C ₁₀ H ₁₆ O ₃	<chem>C1CCCC2(O3)C1(OO)C3C(C3)C2</chem>	InChI=1S/C ₁₀ H ₁₆ O ₃ /c11-13-10-7-2-1-5-9(10)6-3-4-8(10)12-9/h8,11H,1-7H2	

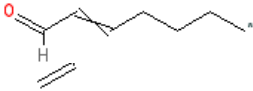
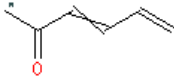
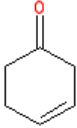
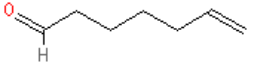
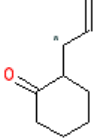
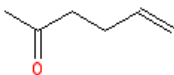
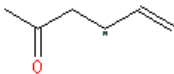

DCLO12-2AOOH	C10H16O3	C1(OO)CCCC2C13C(O3)C CC2	InChI=1S/C10H16O3/c11-13-9-6-2-4-7-3- 1-5-8-10(7,9)12-8/h7-9,11H,1-6H2	
DCLO22A-1OOH	C10H16O3	C1(O3)CCCC2C1(OO)C3C CC2	InChI=1S/C10H16O3/c11-13-10-7-3-1-5- 8(10)12-9(10)6-2-4-7/h7-9,11H,1-6H2	
DCLO13-2AOOH	C10H16O3	C1(OO)CCCC2C13CC(O3) CC2	InChI=1S/C10H16O3/c11-13-9-3-1-2-7-4- 5-8-6-10(7,9)12-8/h7-9,11H,1-6H2	
DCLO14-2AOOH	C10H16O3	C1(OO)CCCC2C13CCC(O 3)C2	InChI=1S/C10H16O3/c11-13-9-3-1-2-7-6- 8-4-5-10(7,9)12-8/h7-9,11H,1-6H2	
DCLO24A-1OOH	C10H16O3	C1CC(O3)CC2C1(OO)C3C CC2	InChI=1S/C10H16O3/c11-13-10-5-4-8-6- 7(10)2-1-3-9(10)12-8/h7-9,11H,1-6H2	
DCLO15-2AOOH	C10H16O3	C1(OO)CCCC2C13CCCC2 (O3)	InChI=1S/C10H16O3/c11-13-9-5-1-3-7-8- 4-2-6-10(7,9)12-8/h7-9,11H,1-6H2	
DCLO25A-1OOH	C10H16O3	C1CCC(O3)C2C1(OO)C3C CC2	InChI=1S/C10H16O3/c11-13-10-6-2-4-8- 7(10)3-1-5-9(10)12-8/h7-9,11H,1-6H2	
DCLO12-3OOH	C10H16O3	C1CCCC2C13C(O3)C(OO) CC2	InChI=1S/C10H16O3/c11-13-8-5-4-7-3-1- 2-6-10(7)9(8)12-10/h7-9,11H,1-6H2	
DCLO14-3OOH	C10H16O3	C1CCCC2C13CC(OO)C(O 3)C2	InChI=1S/C10H16O3/c11-13-9-6-10-4-2-1- 3-7(10)5-8(9)12-10/h7-9,11H,1-6H2	
DCLO34-1OOH	C10H16O3	C1CCCC2C1(OO)CC3C(O 3)C2	InChI=1S/C10H16O3/c11-13-10-4-2-1-3- 7(10)5-8-9(6-10)12-8/h7-9,11H,1-6H2	

DCLO15-3OOH	C10H16O3	C1CCCC2C13CC(OO)CC2	InChI=1S/C10H16O3/c11-13-7-5-9-8-3-1-2-4-10(8,6-7)12-9/h7-9,11H,1-6H2	
DCLO35-1OOH	C10H16O3	C1CCCC2C1(OO)CC3CC2	InChI=1S/C10H16O3/c11-13-10-4-2-1-3-8(10)9-5-7(6-10)12-9/h7-9,11H,1-6H2	
DCLO16-3OOH	C10H16O3	C1CCCC2(O3)C13CC(OO)CC2	InChI=1S/C10H16O3/c11-12-8-3-6-9-4-1-2-5-10(9,7-8)13-9/h8,11H,1-7H2	
DCLO36-1OOH	C10H16O3	C1CCCC2(O3)C1(OO)CC3	InChI=1S/C10H16O3/c11-13-10-5-2-1-4-9(10)6-3-8(7-10)12-9/h8,11H,1-7H2	
DCLO12-3AOOH	C10H16O3	C1C(OO)CCC2C13C(O3)C	InChI=1S/C10H16O3/c11-13-8-5-4-7-2-1-3-9-10(7,6-8)12-9/h7-9,11H,1-6H2	
DCLO13-3AOOH	C10H16O3	C1C(OO)CCC2C13CC(O3)CC2	InChI=1S/C10H16O3/c11-13-9-4-2-7-1-3-8-5-10(7,6-9)12-8/h7-9,11H,1-6H2	
DCLO33A-1OOH	C10H16O3	C1C(O3)CCC2C1(OO)CC3	InChI=1S/C10H16O3/c11-13-10-5-8-3-1-7(10)2-4-9(6-10)12-8/h7-9,11H,1-6H2	
DCLO15-3AOOH	C10H16O3	C1C(OO)CCC2C13CCCC2	InChI=1S/C10H16O3/c11-13-7-3-4-8-9-2-1-5-10(8,6-7)12-9/h7-9,11H,1-6H2	
DCLO35A-1OOH	C10H16O3	C1CCC(O3)C2C1(OO)CC3	InChI=1S/C10H16O3/c11-13-10-5-1-2-9-8(10)4-3-7(6-10)12-9/h7-9,11H,1-6H2	
DCLO12-4OOH	C10H16O3	C1CCCC2C13C(O3)CC(O)C2	InChI=1S/C10H16O3/c11-13-8-5-7-3-1-2-4-10(7)9(6-8)12-10/h7-9,11H,1-6H2	

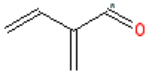
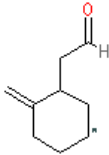
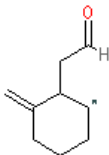
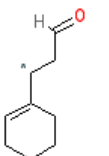
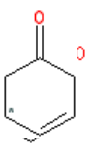
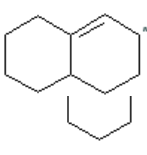
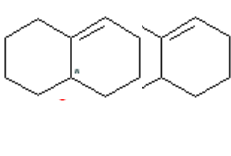
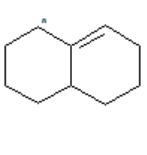
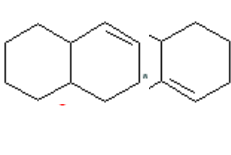
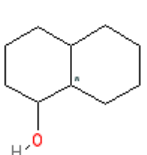
DCLO13-4OOH	C10H16O3	C1CCCC2C13CC(O3)C(O)C2	InChI=1S/C10H16O3/c11-13-8-5-7-3-1-2-4-10(7)6-9(8)12-10/h7-9,11H,1-6H2	
DCLO15-4OOH	C10H16O3	C1CCCC2C13CCC(OO)C2(O3)	InChI=1S/C10H16O3/c11-13-8-4-6-10-5-2-1-3-7(10)9(8)12-10/h7-9,11H,1-6H2	
DCLO45-1OOH	C10H16O3	C1CCCC2C1(OO)CCC3C2(O3)	InChI=1S/C10H16O3/c11-13-10-5-2-1-3-7(10)9-8(12-9)4-6-10/h7-9,11H,1-6H2	
DCLO46-1OOH	C10H16O3	C1CCCC2(O3)C1(OO)CCC3C2	InChI=1S/C10H16O3/c11-13-9-4-1-2-5-10(9)7-8(12-10)3-6-9/h8,11H,1-7H2	
DCLO12-4AOOH	C10H16O3	C1CC(OO)CC2C13C(O3)CC2	InChI=1S/C10H16O3/c11-13-8-4-5-10-7(6)8)2-1-3-9(10)12-10/h7-9,11H,1-6H2	
DCLO14-4AOOH	C10H16O3	C1CC(OO)CC2C13CCC(O3)C2	InChI=1S/C10H16O3/c11-13-9-2-4-10-3-18(12-10)5-7(10)6-9/h7-9,11H,1-6H2	
DCLO44A-1OOH	C10H16O3	C1CC(O3)CC2C1(OO)CCC3C2	InChI=1S/C10H16O3/c11-13-10-3-1-8-5-7(10)6-9(12-8)2-4-10/h7-9,11H,1-6H2	
DCLO15-4AOOH	C10H16O3	C1CC(OO)CC2C13CCCC2(O3)	InChI=1S/C10H16O3/c11-13-7-3-5-10-4-1-2-9(12-10)8(10)6-7/h7-9,11H,1-6H2	
DCLO45A-1OOH	C10H16O3	C1CCC(O3)C2C1(OO)CCC3C2	InChI=1S/C10H16O3/c11-13-10-4-1-2-9-8(10)6-7(12-9)3-5-10/h7-9,11H,1-6H2	
DCLO12-5OOH	C10H16O3	C1CCCC2C13C(O3)CCC2(OO)	InChI=1S/C10H16O3/c11-13-8-4-5-9-10(12-9)6-2-1-3-7(8)10/h7-9,11H,1-6H2	

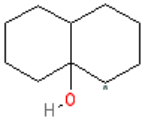
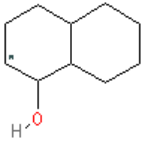
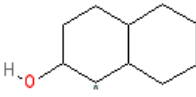
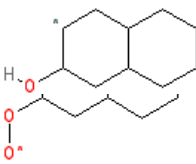
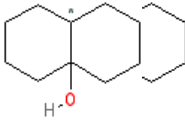
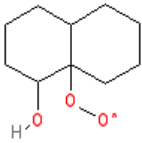
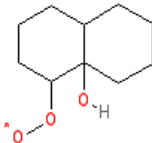
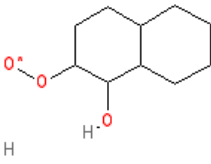
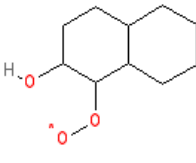
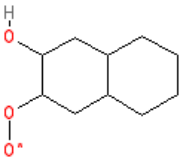
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DCLO14-5OOH	C10H16O3	C1CCCC2C13CCC(O3)C2(InChI=1S/C10H16O3/c11-13-9-7-3-1-2-5-10(7)6-4-8(9)12-10/h7-9,11H,1-6H2	
DCLO56-1OOH	C10H16O3	C1CCCC23C1(OO)CCCC2	InChI=1S/C10H16O3/c11-13-9-5-1-2-7-10(9)8(12-10)4-3-6-9/h8,11H,1-7H2	
DCLO12-5AOOH	C10H16O3	C1CCC(OO)C2C13C(O3)C	InChI=1S/C10H16O3/c11-13-8-4-2-6-10-7(8)3-1-5-9(10)12-10/h7-9,11H,1-6H2	
DCLO13-5AOOH	C10H16O3	C1CCC(OO)C2C13CC(O3)	InChI=1S/C10H16O3/c11-13-9-2-1-5-10-6-7(12-10)3-4-8(9)10/h7-9,11H,1-6H2	
DCLO14-5AOOH	C10H16O3	C1CCC(OO)C2C13CCC(O	InChI=1S/C10H16O3/c11-13-9-2-1-4-10-5-3-7(12-10)6-8(9)10/h7-9,11H,1-6H2	
DCLO15-5AOOH	C10H16O3	C1CCC(OO)C2C13CCCC2	InChI=1S/C10H16O3/c11-13-8-4-2-6-10-5-1-3-7(12-10)9(8)10/h7-9,11H,1-6H2	
DCLO55A-1OOH	C10H16O3	C1CCC3C2C1(OO)CCCC2	InChI=1S/C10H16O3/c11-13-10-5-1-3-7-9(10)8(12-7)4-2-6-10/h7-9,11H,1-6H2	
IC5D13Y1A	C5H6O	C(=O)C(=C)C=C	InChI=1S/C5H6O/c1-3-5(2)4-6/h3-4H,1-2H2	
NC6D1Y36	C6H8O2	C=CC(=O)CCC(=O)	InChI=1S/C6H8O2/c1-2-6(8)4-3-5-7/h2,5H,1,3-4H2	

MCHD1Y1A	C7H10O	<chem>C1C(C=O)=CCCC1</chem>	InChI=1S/C7H10O/c8-6-7-4-2-1-3-5-7/h4,6H,1-3,5H2	
NC7D1Y3-7R	C7H11O	<chem>C=CC(=O)CCC[CH2]</chem>	InChI=1S/C7H11O/c1-3-5-6-7(8)4-2/h4H,1-3,5-6H2	
MCHD1A-2MR	C8H13	<chem>C1C(=C)C([CH2])CCC1</chem>	InChI=1S/C8H13/c1-7-5-3-4-6-8(7)2/h7H,1-6H2	
NC7D16Y3	C7H10O	<chem>C=CC(=O)CCC=C</chem>	InChI=1S/C7H10O/c1-3-5-6-7(8)4-2/h3-4H,1-2,5-6H2	
NPCHD1Y1A	C9H14O	<chem>C(CC=O)C1=CCCCC1</chem>	InChI=1S/C9H14O/c10-8-4-7-9-5-2-1-3-6-9/h5,8H,1-4,6-7H2	
NC7D4Y1-7R	C7H11O	<chem>C(=O)CCC=CC[CH2]</chem>	InChI=1S/C7H11O/c1-2-3-4-5-6-7-8/h3-4,7H,1-2,5-6H2	
NC6D3Y16-1R	C6H7O2	<chem>[C](=O)CC=CCC(=O)</chem>	InChI=1S/C6H7O2/c7-5-3-1-2-4-6-8/h1-2,5H,3-4H2	
NC5D1Y35	C5H6O2	<chem>C=CC(=O)CC(=O)</chem>	InChI=1S/C5H6O2/c1-2-5(7)3-4-6/h2,4H,1,3H2	
NC7D1Y5-7R	C7H11O	<chem>C=CCCC(=O)C[CH2]</chem>	InChI=1S/C7H11O/c1-3-5-6-7(8)4-2/h3H,1-2,4-6H2	
NC5Y14-5R	C5H7O2	<chem>C(=O)CCC(=O)[CH2]</chem>	InChI=1S/C5H7O2/c1-5(7)3-2-4-6/h4H,1-3H2	

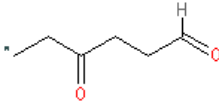
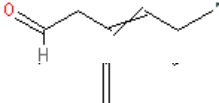
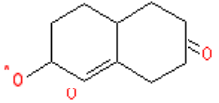
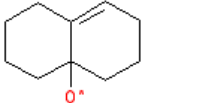
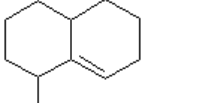
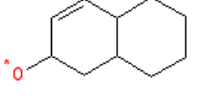

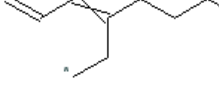


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NC6D13Y5-6R	C6H7O	<chem>C=CC=CC(=O)[CH2]</chem>	InChI=1S/C6H7O/c1-3-4-5-6(2)7/h3-5H,1-2H2	
CYHxD1Y4	C6H8O	<chem>C1C=CCC(=O)C1</chem>	InChI=1S/C6H8O/c7-6-4-2-1-3-5-6/h1-2H,3-5H2	
NC7D1Y7	C7H12O	<chem>C=CCCCC(=O)</chem>	InChI=1S/C7H12O/c1-2-3-4-5-6-7-8/h2,7H,1,3-6H2	
NC7D1Y7-3R	C7H11O	<chem>C=C[CH]CCCC(=O)</chem>	InChI=1S/C7H11O/c1-2-3-4-5-6-7-8/h2-3,7H,1,4-6H2	
ECHY1A-2CH2	C9H14O	<chem>C1C(CC=O)C(=C)CCC1</chem>	InChI=1S/C9H14O/c1-8-4-2-3-5-9(8)6-7-10/h7,9H,1-6H2	
NPCHD1AY2-3AR	C9H13O	<chem>[CH](C=C)C1C(=O)CCCC1</chem>	InChI=1S/C9H13O/c1-2-5-8-6-3-4-7-9(8)10/h2,5,8H,1,3-4,6-7H2	
NC6D1Y5	C6H10O	<chem>C=CCCC(=O)C</chem>	InChI=1S/C6H10O/c1-3-4-5-6(2)7/h3H,1,4-5H2,2H3	
NC6D1Y5-3R	C6H9O	<chem>C=C[CH]CC(=O)C</chem>	InChI=1S/C6H9O/c1-3-4-5-6(2)7/h3-4H,1,5H2,2H3	
NC7D1Y37-5R	C7H9O2	<chem>C=CC(=O)C[CH]CC(=O)</chem>	InChI=1S/C7H9O2/c1-2-7(9)5-3-4-6-8/h2-3,6H,1,4-5H2	

NC7D1Y37-7R	C7H9O2	<chem>C=CC(=O)CCC[C](=O)</chem>	InChI=1S/C7H9O2/c1-2-7(9)5-3-4-6-8/h2H,1,3-5H2	
NC7D16Y3-5R	C7H9O	<chem>C=CC(=O)C[CH]C=C</chem>	InChI=1S/C7H9O/c1-3-5-6-7(8)4-2/h3-5H,1-2,6H2	
NC4D1Y34	C4H4O2	<chem>C=CC(=O)C(=O)</chem>	InChI=1S/C4H4O2/c1-2-4(6)3-5/h2-3H,1H2	
NC4D1Y34-4R	C4H3O2	<chem>C=CC(=O)[C](=O)</chem>	InChI=1S/C4H3O2/c1-2-4(6)3-5/h2H,1H2	
NC6D1Y36-5R	C6H7O2	<chem>C=CC(=O)C[CH]C(=O)</chem>	InChI=1S/C6H7O2/c1-2-6(8)4-3-5-7/h2-3,5H,1,4H2	
NC6D1Y36-6R	C6H7O2	<chem>C=CC(=O)CC[C](=O)</chem>	InChI=1S/C6H7O2/c1-2-6(8)4-3-5-7/h2H,1,3-4H2	
NC5D1Y35-5R	C5H5O2	<chem>C=CC(=O)C[C](=O)</chem>	InChI=1S/C5H5O2/c1-2-5(7)3-4-6/h2H,1,3H2	
NC5D2Y1-5R	C5H7O	<chem>C(=O)C=CC[CH2]</chem>	InChI=1S/C5H7O/c1-2-3-4-5-6/h3-5H,1-2H2	
ECHD1A1-3R	C8H11	<chem>C1C(C=C)=C[CH]CC1</chem>	InChI=1S/C8H11/c1-2-8-6-4-3-5-7-8/h2,4,6H,1,3,5,7H2	
ECHD1A1-6R	C8H11	<chem>[CH]1C(C=C)=CCCC1</chem>	InChI=1S/C8H11/c1-2-8-6-4-3-5-7-8/h2,6-7H,1,3-5H2	

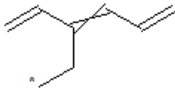
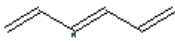
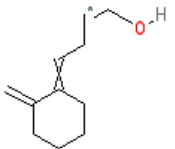
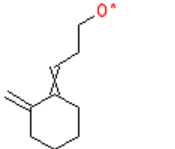
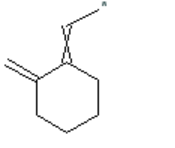
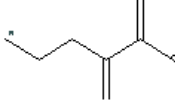
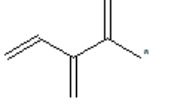
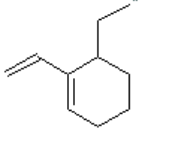
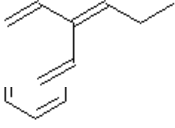
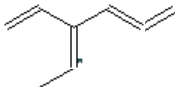
IC5D13Y1A-1AR	C5H5O	<chem>[C](=O)C(=C)C=C</chem>	InChI=1S/C5H5O/c1-3-5(2)4-6/h3H,1-2H2	
ECHY1A-2CH2-5R	C9H13O	<chem>C1C(CC=O)C(=C)CC[CH]1</chem>	InChI=1S/C9H13O/c1-8-4-2-3-5-9(8)6-7-10/h3,7,9H,1-2,4-6H2	
ECHY1A-2CH2-6R	C9H13O	<chem>[CH]1C(CC=O)C(=C)CCC1</chem>	InChI=1S/C9H13O/c1-8-4-2-3-5-9(8)6-7-10/h5,7,9H,1-4,6H2	
NPCHD1Y1A-3AR	C9H13O	<chem>[CH](CC=O)C1=CCCCC1</chem>	InChI=1S/C9H13O/c10-8-4-7-9-5-2-1-3-6-9/h5,7-8H,1-4,6H2	
CYHXD1Y4-6R	C6H7O	<chem>[CH]1C=CCC(=O)C1</chem>	InChI=1S/C6H7O/c7-6-4-2-1-3-5-6/h1-3H,4-5H2	
DCLD1-3R	C10H15	<chem>C1CCCC2C1=C[CH]CC2</chem>	InChI=1S/C10H15/c1-2-6-10-8-4-3-7-9(10)5-1/h1,5,10H,2-4,6-8H2	
DCLD1-6R	C10H15	<chem>C1CCC[C]2C1=CCCC2</chem>	InChI=1S/C10H15/c1-2-6-10-8-4-3-7-9(10)5-1/h5H,1-4,6-8H2	
DCLD1-2AR	C10H15	<chem>[CH]1CCCC2C1=CCCC2</chem>	InChI=1S/C10H15/c1-2-6-10-8-4-3-7-9(10)5-1/h5,7,10H,1-4,6,8H2	
DCLD2-4R	C10H15	<chem>C1CCCC2C1C=C[CH]C2</chem>	InChI=1S/C10H15/c1-2-6-10-8-4-3-7-9(10)5-1/h1-2,5,9-10H,3-4,6-8H2	
DCL-2OH-1R	C10H17O	<chem>C1CCCC2[C]1C(O)CCC2</chem>	InChI=1S/C10H17O/c11-10-7-3-5-8-4-1-2-6-9(8)10/h8,10-11H,1-7H2	

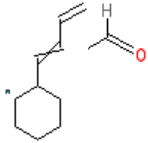
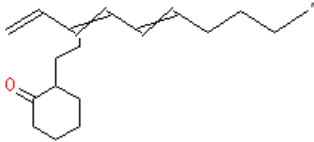


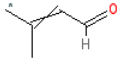

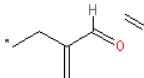

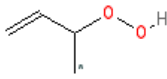

DCL-1OH-2R	C10H17O	C1CCCC2C1(O)[CH]CCC2	InChI=1S/C10H17O/c11-10-7-3-1-5-9(10)6-2-4-8-10/h7,9,11H,1-6,8H2	
DCL-2OH-3R	C10H17O	C1CCCC2C1C(O)[CH]CC2	InChI=1S/C10H17O/c11-10-7-3-5-8-4-1-2-6-9(8)10/h7-11H,1-6H2	
DCL-3OH-2R	C10H17O	C1CCCC2C1[CH]C(O)CC2	InChI=1S/C10H17O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h7-11H,1-6H2	
DCL-3OH-4R	C10H17O	C1CCCC2C1CC(O)[CH]C2	InChI=1S/C10H17O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h6,8-11H,1-5,7H2	
DCL-1OH-6R	C10H17O	C1CCC[C]2C1(O)CCCC2	InChI=1S/C10H17O/c11-10-7-3-1-5-9(10)6-2-4-8-10/h11H,1-8H2	
DCL-2OH-1O2R	C10H17O3	C1CCCC2C1(O[O])C(O)CC2	InChI=1S/C10H17O3/c11-9-6-3-5-8-4-1-2-7-10(8,9)13-12/h8-9,11H,1-7H2	
DCL-1OH-2O2R	C10H17O3	C1CCCC2C1(O)C(O[O])CC2	InChI=1S/C10H17O3/c11-10-7-2-1-4-8(10)5-3-6-9(10)13-12/h8-9,11H,1-7H2	
DCL-2OH-3O2R	C10H17O3	C1CCCC2C1C(O)C(O[O])C2	InChI=1S/C10H17O3/c11-10-8-4-2-1-3-7(8)5-6-9(10)13-12/h7-11H,1-6H2	
DCL-3OH-2O2R	C10H17O3	C1CCCC2C1C(O[O])C(O)C2	InChI=1S/C10H17O3/c11-9-6-5-7-3-1-2-4-8(7)10(9)13-12/h7-11H,1-6H2	
DCL-3OH-4O2R	C10H17O3	C1CCCC2C1CC(O)C(O[O])C2	InChI=1S/C10H17O3/c11-9-5-7-3-1-2-4-8(7)6-10(9)13-12/h7-11H,1-6H2	

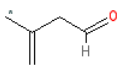

DCL-1OH-6O2R	C10H17O3	<chem>C1CCCC2(O[O])C1(O)CCC2</chem>	InChI=1S/C10H17O3/c11-9-5-1-3-7-10(9,13-12)8-4-2-6-9/h11H,1-8H2	
ECHY2A2-1AR	C8H11O2	<chem>C(=O)C([CH2])C(C1)C(=O)CC1</chem>	InChI=1S/C8H11O2/c1-6(9)7-4-2-3-5-8(7)10/h7H,1-5H2	
NPCH2CHO-1AR	C10H17O	<chem>C(C[CH2])C1C(C=O)CCCC1</chem>	InChI=1S/C10H17O/c1-2-5-9-6-3-4-7-10(9)8-11/h8-10H,1-7H2	
ECHD1Y1A	C8H12O	<chem>C1C(CC=O)=CCCC1</chem>	InChI=1S/C8H12O/c9-7-6-8-4-2-1-3-5-8/h4,7H,1-3,5-6H2	
ECHD1Y1A-1AR	C8H11O	<chem>C1C(C[C]=O)=CCCC1</chem>	InChI=1S/C8H11O/c9-7-6-8-4-2-1-3-5-8/h4H,1-3,5-6H2	
MCHD1AY2	C7H10O	<chem>C1C(=C)C(=O)CCC1</chem>	InChI=1S/C7H10O/c1-6-4-2-3-5-7(6)8/h1-5H2	
MCHD1AY2-6R	C7H9O	<chem>[CH]1C(=C)C(=O)CCC1</chem>	InChI=1S/C7H9O/c1-6-4-2-3-5-7(6)8/h4H,1-3,5H2	
NC6D1Y6	C6H10O	<chem>C=CCCC(=O)</chem>	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h2,6H,1,3-5H2	
NC6D1Y6-3R	C6H9O	<chem>C=C[CH]CCC(=O)</chem>	InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2-3,6H,1,4-5H2	
NC6D1Y6-6R	C6H9O	<chem>C=CCCC[C](=O)</chem>	InChI=1S/C6H9O/c1-2-3-4-5-6-7/h2H,1,3-5H2	

NC6Y14-6R	C6H9O2	<chem>C(=O)CCC(=O)C[CH2]</chem>	InChI=1S/C6H9O2/c1-2-6(8)4-3-5-7/h5H,1-4H2	
NC6D3Y1-6R	C6H9O	<chem>C(=O)CC=CC[CH2]</chem>	InChI=1S/C6H9O/c1-2-3-4-5-6-7/h3-4,6H,1-2,5H2	
DCLD1-3OR	C10H15O	<chem>C1CCCC2C1=CC([O])CC2</chem>	InChI=1S/C10H15O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h7-8,10H,1-6H2	
DCLD1-6OR	C10H15O	<chem>C1CCCC2([O])C1=CCCC2</chem>	InChI=1S/C10H15O/c11-10-7-3-1-5-9(10)6-2-4-8-10/h5H,1-4,6-8H2	
DCLD1-2AOR	C10H15O	<chem>C1([O])CCCC2C1=CCCC2</chem>	InChI=1S/C10H15O/c11-10-7-3-5-8-4-1-2-6-9(8)10/h6,8,10H,1-5,7H2	
DCLD2-4OR	C10H15O	<chem>C1CCCC2C1C=CC([O])C2</chem>	InChI=1S/C10H15O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h5-6,8-10H,1-4,7H2	
PBCHD2-1R	C10H17	<chem>C(CC)C[C]1C=CCCC1</chem>	InChI=1S/C10H17/c1-2-3-7-10-8-5-4-6-9-10/h5,8H,2-4,6-7,9H2,1H3	
NC8D13-4ER	C10H17	<chem>C=CC=C(C[CH2])CCCC</chem>	InChI=1S/C10H17/c1-4-7-9-10(6-3)8-5-2/h5,8H,2-4,6-7,9H2,1H3	
PBCHD21A	C10H16	<chem>C(C=C)CC1C=CCCC1</chem>	InChI=1S/C10H16/c1-2-3-7-10-8-5-4-6-9-10/h2,5,8,10H,1,3-4,6-7,9H2	
PBCHD11A	C10H16	<chem>C(C=C)CC1=CCCCC1</chem>	InChI=1S/C10H16/c1-2-3-7-10-8-5-4-6-9-10/h2,8H,1,3-7,9H2	

NC10D15-10R	C10H17	<chem>C=CCCC=CCCC[CH2]</chem>	InChI=1S/C10H17/c1-3-5-7-9-10-8-6-4-2/h3,9-10H,1-2,4-8H2	
NC10D15-7R	C10H17	<chem>C=CCCC=C[CH]CCC</chem>	InChI=1S/C10H17/c1-3-5-7-9-10-8-6-4-2/h3,8-10H,1,4-7H2,2H3	
NC8D15-8R	C8H13	<chem>C=CCCC=CC[CH2]</chem>	InChI=1S/C8H13/c1-3-5-7-8-6-4-2/h3,6,8H,1-2,4-5,7H2	
NC8D137	C8H12	<chem>C=CC=CCCC=C</chem>	InChI=1S/C8H12/c1-3-5-7-8-6-4-2/h3-5,7H,1-2,6,8H2	
NC8D1V5-8R	C10H17	<chem>C=CCCC(C=C)CC[CH2]</chem>	InChI=1S/C10H17/c1-4-7-9-10(6-3)8-5-2/h4,6,10H,1-3,5,7-9H2	
NC7D16-5MR	C8H13	<chem>C=CCCC([CH2])C=C</chem>	InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-5,8H,1-3,6-7H2	
PBCHD2-1AR	C10H17	<chem>C(C[CH2])CC1C=CCCC1</chem>	InChI=1S/C10H17/c1-2-3-7-10-8-5-4-6-9-10/h5,8,10H,1-4,6-7,9H2	
ECHD2-1AR	C8H13	<chem>C1C(C[CH2])C=CCC1</chem>	InChI=1S/C8H13/c1-2-8-6-4-3-5-7-8/h4,6,8H,1-3,5,7H2	
NPCHD1A3A-2MR	C10H15	<chem>C(C=C)=C1C([CH2])CCCC1</chem>	InChI=1S/C10H15/c1-3-6-10-8-5-4-7-9(10)2/h3,6,9H,1-2,4-5,7-8H2	
NC8D13-4V-8R	C10H15	<chem>C=CC=C(C=C)CCC[CH2]</chem>	InChI=1S/C10H15/c1-4-7-9-10(6-3)8-5-2/h5-6,8H,1-4,7,9H2	

NC6D13-4V-6R	C8H11	<chem>C=CC=C(C=C)C[CH2]</chem>	InChI=1S/C8H11/c1-4-7-8(5-2)6-3/h4-5,7H,1-3,6H2	
X135C6H7-3R	C6H7	<chem>C=C[C]=CC=C</chem>	InChI=1S/C6H7/c1-3-5-6-4-2/h3-5H,1-2H2	
NPCHD3A-2CH2-1AR	C10H15	<chem>C(C[CH2])=C1C(=C)CCCC1</chem>	InChI=1S/C10H15/c1-3-6-10-8-5-4-7-9(10)2/h6H,1-5,7-8H2	
NPCHD3A-2W-1AOR	C10H15O	<chem>C(CC[O])=C1C(=C)CCCC1</chem>	InChI=1S/C10H15O/c1-9-5-2-3-6-10(9)7-4-8-11/h7H,1-6,8H2	
ECHD2A-2CH2-1AR	C9H13	<chem>C1C(=C[CH2])C(=C)CCC1</chem>	InChI=1S/C9H13/c1-3-9-7-5-4-6-8(9)2/h3H,1-2,4-7H2	
NC7D1-34CH2-7R	C9H13	<chem>C=CC(=C)C(=C)CC[CH2]</chem>	InChI=1S/C9H13/c1-5-7-9(4)8(3)6-2/h6H,1-5,7H2	
NC5D14-3CH2-2MR	C7H9	<chem>C=C([CH2])C(=C)C=C</chem>	InChI=1S/C7H9/c1-5-7(4)6(2)3/h5H,1-4H2	
ECHD2-2V-1AR	C10H15	<chem>C1C(C[CH2])C(C=C)CCC1</chem>	InChI=1S/C10H15/c1-3-9-7-5-6-8-10(9)4-2/h3,7,10H,1-2,4-6,8H2	
NC6D13-3V-6R	C8H11	<chem>C=CC(C=C)=CC[CH2]</chem>	InChI=1S/C8H11/c1-4-7-8(5-2)6-3/h5-7H,1-4H2	
NC4D13-2V-1R	C6H7	<chem>[CH]=C(C=C)C=C</chem>	InChI=1S/C6H7/c1-4-6(3)5-2/h3-5H,1-2H2	

PBCHD1A3A-2R	C10H15	<chem>C(C=C)=CC1[CH]CCCC1</chem>	InChI=1S/C10H15/c1-2-3-7-10-8-5-4-6-9-10/h2-3,7-8,10H,1,4-6,9H2	
NC10D135-10R	C10H15	<chem>C=CC=CC=CCCC([CH2])</chem>	InChI=1S/C10H15/c1-3-5-7-9-10-8-6-4-2/h3,5,7,9-10H,1-2,4,6,8H2	
NC8D135-8R	C8H11	<chem>C=CC=CC=CC[CH2]</chem>	InChI=1S/C8H11/c1-3-5-7-8-6-4-2/h3,5-8H,1-2,4H2	
NC6D135-1R	C6H7	<chem>[CH]=CC=CC=C</chem>	InChI=1S/C6H7/c1-3-5-6-4-2/h1,3-6H,2H2	
IC3H5CHCHO	C5H7O	<chem>[CH2]C(C)=CC=O</chem>	InChI=1S/C5H7O/c1-5(2)3-4-6/h3-4H,1H2,2H3	
C4H6CHO1-43	C5H7O	<chem>C=C[CH]CC=O</chem>	InChI=1S/C5H7O/c1-2-3-4-5-6/h2-3,5H,1,4H2	
C4H6CHO1-24	C5H7O	<chem>[CH2]CC(=C)C=O</chem>	InChI=1S/C5H7O/c1-3-5(2)4-6/h4H,1-3H2	
C4H6CHO1-13	C5H7O	<chem>C[CH]C=CC=O</chem>	InChI=1S/C5H7O/c1-2-3-4-5-6/h2-5H,1H3	
C4H61-4OOH3	C4H7O2	<chem>C=CC(OO)[CH2]</chem>	InChI=1S/C4H7O2/c1-3-4(2)6-5/h3-5H,1-2H2	
AC3H5CO	C4H5O	<chem>C=CC[C]=O</chem>	InChI=1S/C4H5O/c1-2-3-4-5/h2H,1,3H2	

AC3H4CH2CHO	C5H7O	[CH2]C(=C)CC=O	InChI=1S/C5H7O/c1-5(2)3-4-6/h4H,1-3H2	
CYDED	C10H18	C1C=CCCCCCCC1	InChI=1S/C10H18/c1-2-4-6-8-10-9-7-5-3-1/h1-2H,3-10H2	
CYDED1-3R	C10H17	C1C=C[CH]CCCCC1	InChI=1S/C10H17/c1-2-4-6-8-10-9-7-5-3-1/h1-3H,4-10H2	
C10H17-13-10	C10H17	C=CC=CCCCC[CH2]	InChI=1S/C10H17/c1-3-5-7-9-10-8-6-4-2/h3,5,7H,1-2,4,6,8-10H2	
C8H13-13-8	C8H13	C=CC=CCCC[CH2]	InChI=1S/C8H13/c1-3-5-7-8-6-4-2/h3,5,7H,1-2,4,6,8H2	
C6H9-13-6	C6H9	C=CC=CC[CH2]	InChI=1S/C6H9/c1-3-5-6-4-2/h3,5-6H,1-2,4H2	
C3H4CHO-2	C4H5O	C=[C]CC=O	InChI=1S/C4H5O/c1-2-3-4-5/h4H,1,3H2	
C3H4CHO-3	C4H5O	[CH]=CCC=O	InChI=1S/C4H5O/c1-2-3-4-5/h1-2,4H,3H2	
CH2CHCHCO	C4H4O	C=CC=C=O	InChI=1S/C4H4O/c1-2-3-4-5/h2-3H,1H2	