


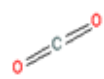
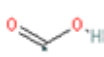










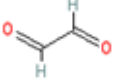
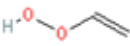
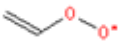






Supporting Information for: An updated experimental and kinetic modeling study of n-heptane oxidation




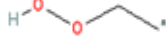





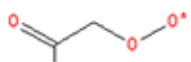
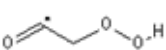
Name	Formula	SMILES	InChI	Structure
AR	AR	[Ar]	InChI=1S/Ar	
N2	N2	N#N	InChI=1S/N2/c1-2	
HE	HE	[He]	InChI=1S/He	
H2	H2	[H][H]	InChI=1S/H2/h1H	
H	H	[H]	InChI=1S/H	
O2	O2	[O][O]	InChI=1S/O2/c1-2	
O	O	[O]	InChI=1S/O	
H2O	H2O	O	InChI=1S/H2O/h1H2	
OH	HO	[OH]	InChI=1S/HO/h1H	
OHV	HO	[OH]	InChI=1S/HO/h1H	




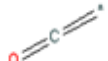
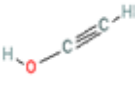
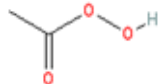
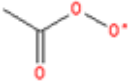




H2O2	H2O2	OO	InChI=1S/H2O2/c1-2/h1-2H	
HO2	HO2	[O]O	InChI=1S/HO2/c1-2/h1H	
CO	CO	[C]=O	InChI=1S/CO/c1-2	
CO2	CO2	O=C=O	InChI=1S/CO2/c2-1-3	
HOCO	CHO2	[C](=O)O	InChI=1S/CHO2/c2-1-3/h(H,2,3)	
CH4	CH4	C	InChI=1S/CH4/h1H4	
CH3	CH3	[CH3]	InChI=1S/CH3/h1H3	
CH2	CH2	triplet[CH2]	InChI=1S/CH2/h1H2	
CH2(S)	CH2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





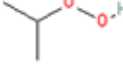
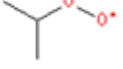




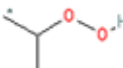
HOCH2O2H	CH4O3	OCOO	InChI=1S/CH4O3/c2-1-4-3/h2-3H,1H2	
HOCH2O2	CH3O3	[O]OCO	InChI=1S/CH3O3/c2-1-4-3/h2H,1H2	
OCH2O2H	CH3O3	[O]COO	InChI=1S/CH3O3/c2-1-4-3/h3H,1H2	
HOCH2O	CH3O2	[O]CO	InChI=1S/CH3O2/c2-1-3/h2H,1H2	
O2CHO	CHO3	[O]OC=O	InChI=1S/CHO3/c2-1-4-3/h1H	
HOCHO	CH2O2	O=CO	InChI=1S/CH2O2/c2-1-3/h1H,(H,2,3)	
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	

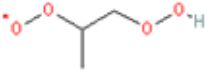

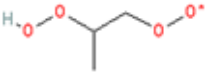
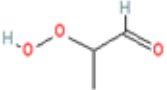



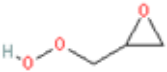
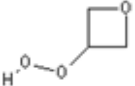

C2H4	C2H4	C=C	InChI=1S/C2H4/c1-2/h1-2H2	
C2H3	C2H3	[CH]=C	InChI=1S/C2H3/c1-2/h1H,2H2	
CHOCHO	C2H2O2	O=CC=O	InChI=1S/C2H2O2/c3-1-2-4/h1-2H	
C2H3OOH	C2H4O2	C=COO	InChI=1S/C2H4O2/c1-2-4-3/h2-3H,1H2	
C2H3OO	C2H3O2	C=C(O[O])	InChI=1S/C2H3O2/c1-2-4-3/h2H,1H2	
CHCHO	C2H2O	[CH]CO	InChI=1S/C2H2O/c1-2-3/h1-2H	
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	




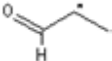

PC2H4OH	C2H5O	[CH2]CO	InChI=1S/C2H5O/c1-2-3/h3H,1-2H2	
SC2H4OH	C2H5O	C[CH]O	InChI=1S/C2H5O/c1-2-3/h2-3H,1H3	
O2C2H4OH	C2H5O3	[O]OCCO	InChI=1S/C2H5O3/c3-1-2-5-4/h3H,1-2H2	
C2H4O2H	C2H5O2	[CH2]COO	InChI=1S/C2H5O2/c1-2-4-3/h3H,1-2H2	
C2H4O1-2	C2H4O	C1CO1	InChI=1S/C2H4O/c1-2-3-1/h1-2H2	
C2H3O1-2	C2H3O	[CH]1CO1	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	
OCH2OCHO	C2H3O3	[O]COC=O	InChI=1S/C2H3O3/c3-1-5-2-4/h1H,2H2	
HOCH2OCO	C2H3O3	O=[C]OCO	InChI=1S/C2H3O3/c3-1-5-2-4/h3H,1H2	
CH3OCH2O	C2H5O2	COC[O]	InChI=1S/C2H5O2/c1-4-2-3/h2H2,1H3	
CH3OCHO	C2H4O2	COC=O	InChI=1S/C2H4O2/c1-4-2-3/h2H,1H3	
CH3OCO	C2H3O2	CO[C]=O	InChI=1S/C2H3O2/c1-4-2-3/h1H3	
CH2OCHO	C2H3O2	[CH2]OC=O	InChI=1S/C2H3O2/c1-4-2-3/h2H,1H2	
C3H8	C3H8	CCC	InChI=1S/C3H8/c1-3-2/h3H2,1-2H3	

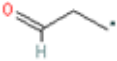
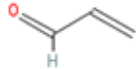


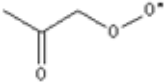
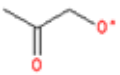
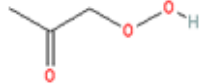



IC3H7	C3H7	C[CH]C	InChI=1S/C3H7/c1-3-2/h3H,1-2H3	
NC3H7	C3H7	[CH2]CC	InChI=1S/C3H7/c1-3-2/h1,3H2,2H3	
NC3H7O2H	C3H8O2	CCCOO	InChI=1S/C3H8O2/c1-2-3-5-4/h4H,2-3H2,1H3	
NC3H7O2	C3H7O2	CCCO[O]	InChI=1S/C3H7O2/c1-2-3-5-4/h2-3H2,1H3	
IC3H7O2H	C3H8O2	CC(C)OO	InChI=1S/C3H8O2/c1-3(2)5-4/h3-4H,1-2H3	
IC3H7O2	C3H7O2	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	

C3H600H1-202	C3H7O4	CC(COO)O[O]	InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3-4H,2H2,1H3	
C3H600H1-302	C3H7O4	[O]OCCCCO	InChI=1S/C3H7O4/c4-6-2-1-3-7-5/h4H,1-3H2	
C3H600H2-102	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	
C3H51-2,300H	C3H7O4	[CH2]C(COO)OO	InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3-5H,1-2H2	
C3H52-1,300H	C3H7O4	OOC[CH]COO	InChI=1S/C3H7O4/c4-6-2-1-3-7-5/h1,4-5H,2-3H2	
C3H501-200H-3	C3H6O3	C1C(O1)C(OO)	InChI=1S/C3H6O3/c4-6-2-3-1-5-3/h3-4H,1-2H2	
C3H501-300H-2	C3H6O3	C1C(OO)C(O1)	InChI=1S/C3H6O3/c4-6-3-1-5-2-3/h3-4H,1-2H2	
C3H601-2	C3H6O	CC1CO1	InChI=1S/C3H6O/c1-3-2-4-3/h3H,2H2,1H3	
C3H601-3	C3H6O	C1COC1	InChI=1S/C3H6O/c1-2-4-3-1/h1-3H2	

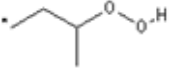
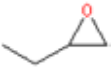



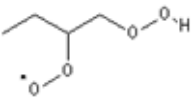
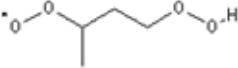

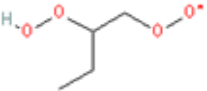
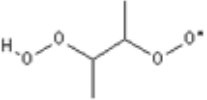
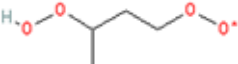
C3H6	C3H6	C=CC	InChI=1S/C3H6/c1-3-2/h3H,1H2,2H3	
C3H5-A	C3H5	[CH2]C=C	InChI=1S/C3H5/c1-3-2/h3H,1-2H2	
C3H5-S	C3H5	[CH]=CC	InChI=1S/C3H5/c1-3-2/h1,3H,2H3	
C3H5-T	C3H5	C=[C]C	InChI=1S/C3H5/c1-3-2/h1H2,2H3	
CC3H6	C3H6	C1CC1	InChI=1S/C3H6/c1-2-3-1/h1-3H2	
C3H5O	C3H5O	C=CC[O]	InChI=1S/C3H5O/c1-2-3-4/h2H,1,3H2	
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	

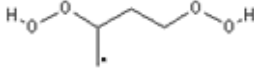
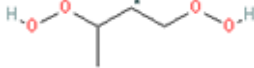

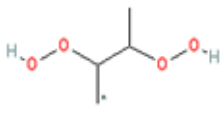
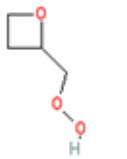
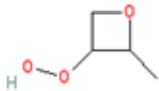
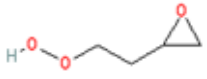
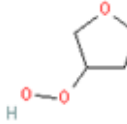
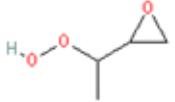

AC3H5OOH	C3H6O2	C=CCOO	InChI=1S/C3H6O2/c1-2-3-5-4/h2,4H,1,3H2	
C3H6OH2-1	C3H7O	[CH2]C(O)C	InChI=1S/C3H7O/c1-3(2)4/h3-4H,1H2,2H3	
HOC3H6O2	C3H7O3	C(O)C(O[O])C	InChI=1S/C3H7O3/c1-3(2-4)6-5/h3-4H,2H2,1H3	
SC3H5OH	C3H6O	CC=CO	InChI=1S/C3H6O/c1-2-3-4/h2-4H,1H3	
IC3H5OH	C3H6O	C=C(C)O	InChI=1S/C3H6O/c1-3(2)4/h4H,1H2,2H3	
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	

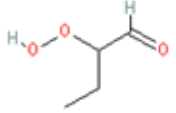
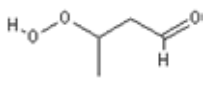
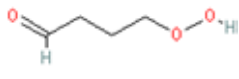
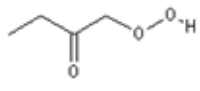
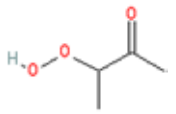
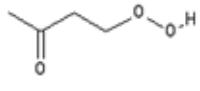
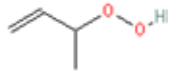
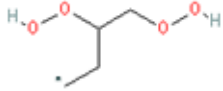
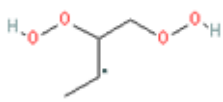
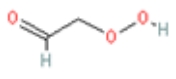

C3H2	C3H2	C=C=[C]	InChI=1S/C3H2/c1-3-2/H1h2	
H2CCC(S)	C3H2	C=C=[C]	InChI=1S/C3H2/c1-3-2/H1h2	
C3H2(S)	C3H2	C=C=[C]	InChI=1S/C3H2/c1-3-2/H1h2	
C3H2C	C3H2	C1=C[C]1	InChI=1S/C3H2/c1-2-3-1/h1-2H	
PC3H4OH-2	C3H5O	C[C]=CO	InChI=1S/C3H5O/c1-2-3-4/h3-4H,1H3	
SC3H4OH	C3H5O	C=C([CH2])O	InChI=1S/C3H5O/c1-3(2)4/h4H,1-2H2	
C3H3O	C3H3O	C=C=C([O])	InChI=1S/C3H3O/c1-2-3-4/h3H,1H2	
C3H3O2H	C3H4O2	C=C=C(OO)	InChI=1S/C3H4O2/c1-2-3-5-4/h3-4H,1H2	
C2HCHO	C3H2O	C#CC=O	InChI=1S/C3H2O/c1-2-3-4/h1,3H	
C2H5CHO	C3H6O	CCC=O	InChI=1S/C3H6O/c1-2-3-4/h3H,2H2,1H3	
C2H5CO	C3H5O	CC[C]=O	InChI=1S/C3H5O/c1-2-3-4/h2H2,1H3	




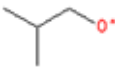

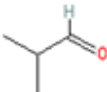
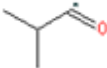
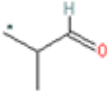
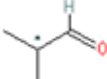
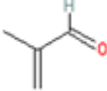
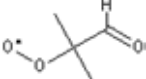
CH2CH2CHO	C3H5O	[CH2]CC=O	InChI=1S/C3H5O/c1-2-3-4/h3H,1-2H2	
C2H3CHO	C3H4O	C=CC=O	InChI=1S/C3H4O/c1-2-3-4/h2-3H,1H2	
C2H3CO	C3H3O	C=C[C]=O	InChI=1S/C3H3O/c1-2-3-4/h2H,1H2	
CH3COCH3	C3H6O	CC(C)=O	InChI=1S/C3H6O/c1-3(2)4/h1-2H3	
CH3COCH2	C3H5O	[CH2]C(C)=O	InChI=1S/C3H5O/c1-3(2)4/h1H2,2H3	
CH3COCH2O2	C3H5O3	CC(=O)CO[O]	InChI=1S/C3H5O3/c1-3(4)2-6-5/h2H2,1H3	
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	

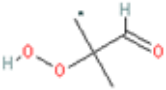
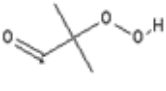
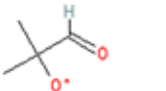
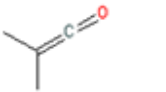
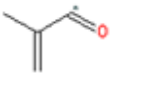
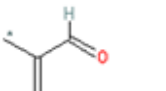
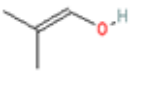
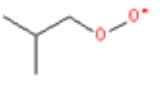
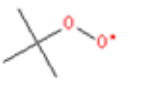
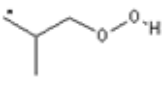
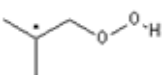
PC4H9O	C4H9O	CCCC[O]	InChI=1S/C4H9O/c1-2-3-4-5/h2-4H2,1H3	
SC4H9O	C4H9O	CCC(C)[O]	InChI=1S/C4H9O/c1-3-4(2)5/h4H,3H2,1-2H3	
PC4H9O2	C4H9O2	CCCCO[O]	InChI=1S/C4H9O2/c1-2-3-4-6-5/h2-4H2,1H3	
SC4H9O2	C4H9O2	CCC(C)O[O]	InChI=1S/C4H9O2/c1-3-4(2)6-5/h4H,3H2,1-2H3	
PC4H9O2H	C4H10O2	CCCCOO	InChI=1S/C4H10O2/c1-2-3-4-6-5/h5H,2-4H2,1H3	
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	

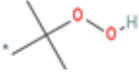

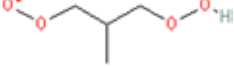
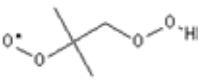
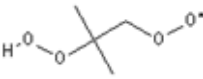
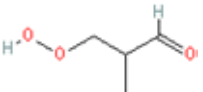
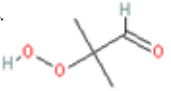
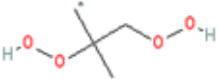
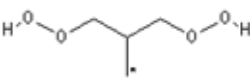
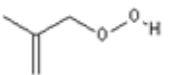
C4H8OOH2-4	C4H9O2	[CH2]CC(C)OO	InChI=1S/C4H9O2/c1-3-4(2)6-5/h4-5H,1,3H2,2H3	
C4H8O1-2	C4H8O	CCC1CO1	InChI=1S/C4H8O/c1-2-4-3-5-4/h4H,2-3H2,1H3	
C4H8O1-3	C4H8O	CC1CCO1	InChI=1S/C4H8O/c1-4-2-3-5-4/h4H,2-3H2,1H3	
C4H8O1-4	C4H8O	C1CCOC1	InChI=1S/C4H8O/c1-2-4-5-3-1/h1-4H2	
C4H8O2-3	C4H8O	CC1OC1C	InChI=1S/C4H8O/c1-3-4(2)5-3/h3-4H,1-2H3	
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	

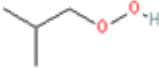
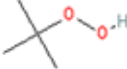



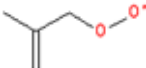
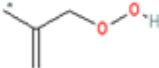




C4H71-2,400H	C4H9O4	[CH2]C(OO)CC(OO)	InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h4-6H,1-3H2	
C4H72-1,300H	C4H9O4	CC(OO)[CH]C(OO)	InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h2,4-6H,3H2,1H3	
C4H72-1,400H	C4H9O4	C(OO)C[CH]C(OO)	InChI=1S/C4H9O4/c5-7-3-1-2-4-8-6/h1,5-6H,2-4H2	
C4H71-2,300H	C4H9O4	[CH2]C(OO)C(OO)C	InChI=1S/C4H9O4/c1-3(7-5)4(2)8-6/h3-6H,1H2,2H3	
C4H701-300H-4	C4H8O3	C1CC(O1)C(OO)	InChI=1S/C4H8O3/c5-7-3-4-1-2-6-4/h4-5H,1-3H2	
C4H701-300H-2	C4H8O3	C1C(OO)C(O1)C	InChI=1S/C4H8O3/c1-3-4(7-5)2-6-3/h3-5H,2H2,1H3	
C4H701-200H-4	C4H8O3	C1C(O1)CC(OO)	InChI=1S/C4H8O3/c5-7-2-1-4-3-6-4/h4-5H,1-3H2	
C4H701-400H-2	C4H8O3	C1C(OO)CC(O1)	InChI=1S/C4H8O3/c5-7-4-1-2-6-3-4/h4-5H,1-3H2	
C4H701-200H-3	C4H8O3	C1C(O1)C(OO)C	InChI=1S/C4H8O3/c1-3(7-5)4-2-6-4/h3-5H,2H2,1H3	
C4H702-300H-1	C4H8O3	C(OO)C1C(O1)C	InChI=1S/C4H8O3/c1-3-4(7-3)2-6-5/h3-5H,2H2,1H3	
C4H72-100H	C4H8O2	CC=CCOO	InChI=1S/C4H8O2/c1-2-3-4-6-5/h2-3,5H,4H2,1H3	

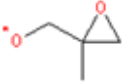
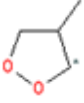
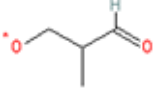
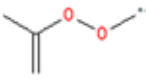

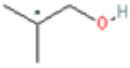
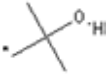

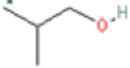
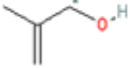

NC4KET12	C4H8O3	CCC(C=O)OO	InChI=1S/C4H8O3/c1-2-4(3-5)7-6/h3-4,6H,2H2,1H3	
NC4KET13	C4H8O3	CC(CC=O)OO	InChI=1S/C4H8O3/c1-4(7-6)2-3-5/h3-4,6H,2H2,1H3	
NC4KET14	C4H8O3	O=CCCCOO	InChI=1S/C4H8O3/c5-3-1-2-4-7-6/h3,6H,1-2,4H2	
NC4KET21	C4H8O3	CCC(=O)COO	InChI=1S/C4H8O3/c1-2-4(5)3-7-6/h6H,2-3H2,1H3	
NC4KET23	C4H8O3	CC(=O)C(C)OO	InChI=1S/C4H8O3/c1-3(5)4(2)7-6/h4,6H,1-2H3	
NC4KET24	C4H8O3	CC(=O)CCOO	InChI=1S/C4H8O3/c1-4(5)2-3-7-6/h6H,2-3H2,1H3	
C4H71-3OOH	C4H8O2	C=CC(C)OO	InChI=1S/C4H8O2/c1-3-4(2)6-5/h3-5H,1H2,2H3	
C4H71-3,4OOH	C4H9O4	[CH2]CC(OO)C(OO)	InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h4-6H,1-3H2	
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	
HO2CH2CHO	C2H4O3	C(COO)=O	InChI=1S/C2H4O3/c3-1-2-5-4/h1,4H,2H2	
IC4H10	C4H10	CC(C)C	InChI=1S/C4H10/c1-4(2)3/h4H,1-3H3	

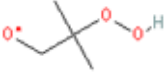
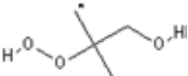
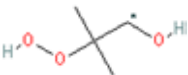
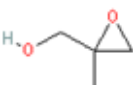
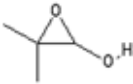
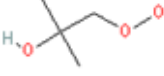
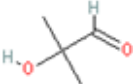
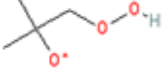
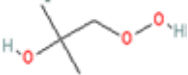

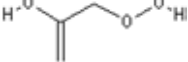
IC4H9	C4H9	[CH2]C(C)C	InChI=1S/C4H9/c1-4(2)3/h4H,1H2,2-3H3	
TC4H9	C4H9	CCC	InChI=1S/C4H9/c1-4(2)3/h1-3H3	
TC4H9O	C4H9O	CC(C)(C)[O]	InChI=1S/C4H9O/c1-4(2,3)5/h1-3H3	
IC4H9O	C4H9O	CC(C)C[O]	InChI=1S/C4H9O/c1-4(2)3-5/h4H,3H2,1-2H3	
IC4H8O	C4H8O	CC1(C)CO1	InChI=1S/C4H8O/c1-4(2)3-5-4/h3H2,1-2H3	
IC3H7CHO	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	


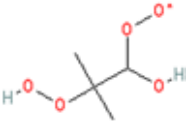
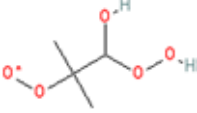
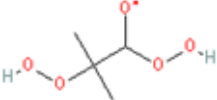
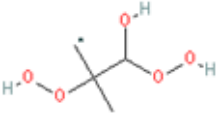
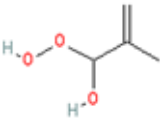
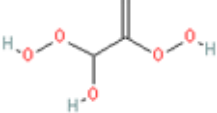
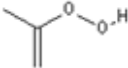
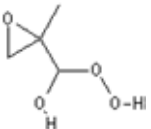
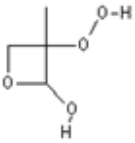
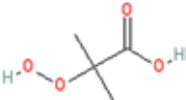
IC3H5O2HCHO	C4H7O3	[CH2]C(C)(C=O)OO	InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h3,6H,1H2,2H3	
TC3H6O2HCO	C4H7O3	CC(C)([C]=O)OO	InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h6H,1-2H3	
TC3H6OCHO	C4H7O2	CC(C)([O])C=O	InChI=1S/C4H7O2/c1-4(2,6)3-5/h3H,1-2H3	
IC3H6CO	C4H6O	CC(C)=C=O	InChI=1S/C4H6O/c1-4(2)3-5/h1-2H3	
IC3H5CO	C4H5O	C=C(C)[C]=O	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	






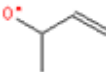

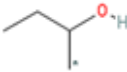
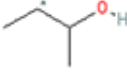
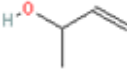

IC4H9O2H	C4H10O2	CC(C)COO	InChI=1S/C4H10O2/c1-4(2)3-6-5/h4-5H,3H2,1-2H3	
TC4H9O2H	C4H10O2	CC(C)(C)OO	InChI=1S/C4H10O2/c1-4(2,3)6-5/h5H,1-3H3	
IC4H8	C4H8	C=C(C)C	InChI=1S/C4H8/c1-4(2)3/h1H2,2-3H3	
IC4H7	C4H7	[CH2]C(=C)C	InChI=1S/C4H7/c1-4(2)3/h1-2H2,3H3	
IC4H7-11	C4H7	[CH]=C(C)C	InChI=1S/C4H7/c1-4(2)3/h1H,2-3H3	
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	

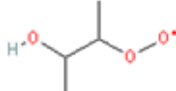
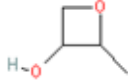

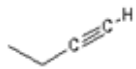


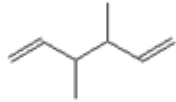
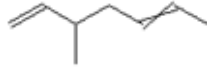

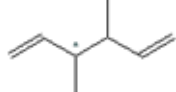
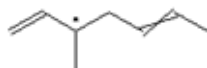
TQC4H8OI	C4H9O3	CC(C)(C[O])OO	InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h6H,3H2,1-2H3	
QC4H7OHP	C4H9O3	[CH2]C(C)(CO)OO	InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h5-6H,1,3H2,2H3	
TQC4H7OHI	C4H9O3	CC(C)([CH]O)OO	InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h3,5-6H,1-2H3	
CCY(CCO)COH	C4H8O2	CC1(CO)CO1	InChI=1S/C4H8O2/c1-4(2-5)3-6-4/h5H,2-3H2,1H3	
C2CY(COC)OH	C4H8O2	CC1(C)C(O)O1	InChI=1S/C4H8O2/c1-4(2)3(5)6-4/h3,5H,1-2H3	
IQC4H8OH	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	
TQC4H7OHIQ2	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	
CO(CH2OOH)2	C3H6O5	C(C(COO)=O)OO	InChI=1S/C3H6O5/c4-3(1-7-5)2-8-6/h5-6H,1-2H2	
CH3COCHO	C3H4O2	CC(C=O)=O	InChI=1S/C3H4O2/c1-3(5)2-4/h2H,1H3	
IC3H5OCH2	C4H7O	C=C(C)O[CH2]	InChI=1S/C4H7O/c1-4(2)5-3/h1,3H2,2H3	
IC4H7OOCH3	C5H10O2	C=C(C)COOC	InChI=1S/C5H10O2/c1-5(2)4-7-6-3/h1,4H2,2-3H3	
IC4H7OOIC4H7	C8H14O2	CC(=C)COOCC(=C)C	InChI=1S/C8H14O2/c1-7(2)5-9-10-6-8(3)4/h1,3,5-6H2,2,4H3	
C4H8-1	C4H8	C=CCC	InChI=1S/C4H8/c1-3-4-2/h3H,1,4H2,2H3	
C4H8-2	C4H8	CC=CC	InChI=1S/C4H8/c1-3-4-2/h3-4H,1-2H3	

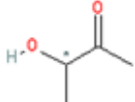
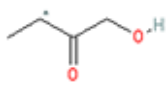
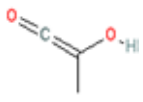
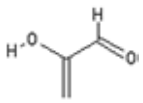
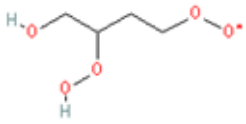
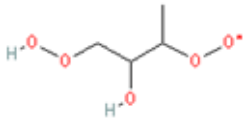
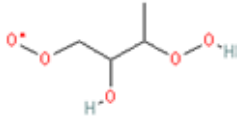
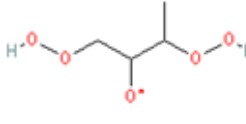
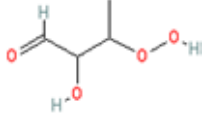
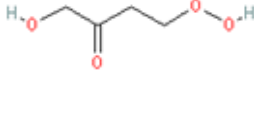
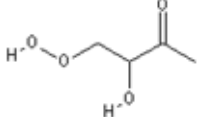
C4H71-1	C4H7	[CH]=CCC	InChI=1S/C4H7/c1-3-4-2/h1,3H,4H2,2H3	
C4H71-2	C4H7	C=[C]CC	InChI=1S/C4H7/c1-3-4-2/h1,4H2,2H3	
C4H71-3	C4H7	C=C[CH]C	InChI=1S/C4H7/c1-3-4-2/h3-4H,1H2,2H3	
C4H71-4	C4H7	[CH2]CC=C	InChI=1S/C4H7/c1-3-4-2/h3H,1-2,4H2	
C4H72-2	C4H7	C[C]=CC	InChI=1S/C4H7/c1-3-4-2/h3H,1-2H3	
C4H71-0	C4H7O	C=CC([O])C	InChI=1S/C4H7O/c1-3-4(2)5/h3-4H,1H2,2H3	
PC4H8OH-2	C4H9O	C(O)[CH]CC	InChI=1S/C4H9O/c1-2-3-4-5/h3,5H,2,4H2,1H3	
SC4H8OH-1	C4H9O	[CH2]C(O)CC	InChI=1S/C4H9O/c1-3-4(2)5/h4-5H,2-3H2,1H3	
SC4H8OH-3	C4H9O	CC(O)[CH]C	InChI=1S/C4H9O/c1-3-4(2)5/h3-5H,1-2H3	
C4H71-3OH	C4H8O	C=CC(O)C	InChI=1S/C4H8O/c1-3-4(2)5/h3-5H,1H2,2H3	
C4H71-4OH	C4H8O	C=CCC(O)	InChI=1S/C4H8O/c1-2-3-4-5/h2,5H,1,3-4H2	

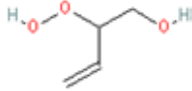
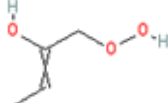
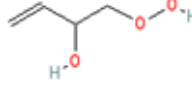
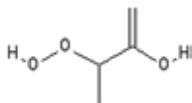
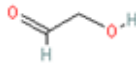

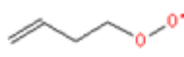

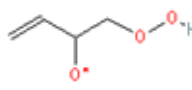

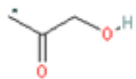
C4H71-10H	C4H8O	C(O)=CCC	InChI=1S/C4H8O/c1-2-3-4-5/h3-5H,2H2,1H3	
C4H71-20H	C4H8O	C=C(O)CC	InChI=1S/C4H8O/c1-3-4(2)5/h5H,2-3H2,1H3	
C4H72-10H	C4H8O	CC=CC(O)	InChI=1S/C4H8O/c1-2-3-4-5/h2-3,5H,4H2,1H3	
C4H72-20H	C4H8O	CC=C(O)C	InChI=1S/C4H8O/c1-3-4(2)5/h3,5H,1-2H3	
SQC4H80P	C4H9O3	CCC(OO)C([O])	InChI=1S/C4H9O3/c1-2-4(3-5)7-6/h4,6H,2-3H2,1H3	
PQC4H80S	C4H9O3	CCC([O])C(OO)	InChI=1S/C4H9O3/c1-2-4(5)3-7-6/h4,6H,2-3H2,1H3	
PQC4H70HS-3	C4H9O3	C[CH]C(O)C(OO)	InChI=1S/C4H9O3/c1-2-4(5)3-7-6/h2,4-6H,3H2,1H3	
NC4KET120H	C4H8O2	C(=O)C(O)CC	InChI=1S/C4H8O2/c1-2-4(6)3-5/h3-4,6H,2H2,1H3	
SQC4H70HS-4	C4H9O3	CC(OO)C(O)[CH2]	InChI=1S/C4H9O3/c1-3(5)4(2)7-6/h3-6H,1H2,2H3	
SQC4H80S	C4H9O3	CC(OO)C([O])C	InChI=1S/C4H9O3/c1-3(5)4(2)7-6/h3-4,6H,1-2H3	
NC4KET230H	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	[CH]=CCC(C)C=C	InChI=1S/C7H11/c1-4-6-7(3)5-2/h1,4-5,7H,2,6H2,3H3	
C7H111-5,1P	C7H11	[CH]=CCCC=CC	InChI=1S/C7H11/c1-3-5-7-6-4-2/h1,3-4,6H,5,7H2,2H3	
C4H64,2-10H	C4H7O	[CH2]C=CCO	InChI=1S/C4H7O/c1-2-3-4-5/h2-3,5H,1,4H2	
C4H63,1-10H	C4H7O	C[CH]C=CO	InChI=1S/C4H7O/c1-2-3-4-5/h2-5H,1H3	
C4H63,1-30H	C4H7O	C=CCO	InChI=1S/C4H7O/c1-3-4(2)5/h3,5H,1H2,2H3	
C4H63,1-20H	C4H7O	C=C(O)[CH]C	InChI=1S/C4H7O/c1-3-4(2)5/h3,5H,2H2,1H3	
C4H50H-13	C4H6O	C=CC=CO	InChI=1S/C4H6O/c1-2-3-4-5/h2-5H,1H2	
SQC4H70HP-4	C4H9O3	[CH2]CC(CO)OO	InChI=1S/C4H9O3/c1-2-4(3-5)7-6/h4-6H,1-3H2	
CY(CCCO)COH	C4H8O2	OCC1CCO1	InChI=1S/C4H8O2/c5-3-4-1-2-6-4/h4-5H,1-3H2	
NC4KET210H	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	


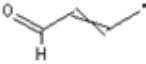
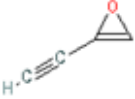
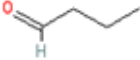

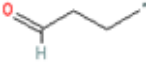
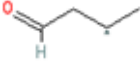
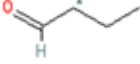
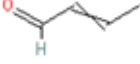

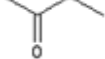
CH3COCOCH3	C4H7O2	C[C](O)C(C)=O	InChI=1S/C4H7O2/c1-3(5)4(2)6/h5H,1-2H3	
C2H4COCH2OH	C4H7O2	C[CH]C(=O)CO	InChI=1S/C4H7O2/c1-2-4(6)3-5/h2,5H,3H2,1H3	
CH3COHCO	C3H4O2	CC(O)=C=O	InChI=1S/C3H4O2/c1-3(5)2-4/h5H,1H3	
CH2COHCHO	C3H4O2	C=C(O)C=O	InChI=1S/C3H4O2/c1-3(5)2-4/h2,5H,1H2	
SQC4H7OHP-4O2	C4H9O5	[O]OCCC(CO)OO	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	

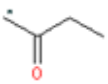
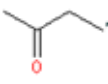
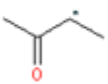
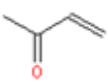
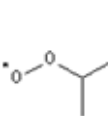
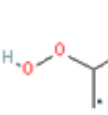
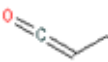




C4H6OHOH1-4-3	C4H8O3	C=CC(CO)OO	InChI=1S/C4H8O3/c1-2-4(3-5)7-6/h2,4-6H,1,3H2	
C4H6OHOH2-2-1	C4H8O3	CC=C(O)C(OO)	InChI=1S/C4H8O3/c1-2-4(5)3-7-6/h2,5-6H,3H2,1H3	
C4H6OHOH1-3-4	C4H8O3	C=CC(O)C(OO)	InChI=1S/C4H8O3/c1-2-4(5)3-7-6/h2,4-6H,1,3H2	
C4H6OHOH1-2-3	C4H8O3	C=C(O)C(C)OO	InChI=1S/C4H8O3/c1-3(5)4(2)7-6/h4-6H,1H2,2H3	
HOCH2CHO	C2H4O2	O=CCO	InChI=1S/C2H4O2/c3-1-2-4/h1,4H,2H2	
C4H71-40OH	C4H8O2	C=CCCCO	InChI=1S/C4H8O2/c1-2-3-4-6-5/h2,5H,1,3H,4H2	
C4H71-4O2	C4H7O2	C=CCCC[O]	InChI=1S/C4H7O2/c1-2-3-4-6-5/h2H,1,3-4H2	
C4H61-30OH4	C4H7O2	C=C[CH]COO	InChI=1S/C4H7O2/c1-2-3-4-6-5/h2-3,5H,1,4H2	
C4H601-30OH4	C4H7O3	C=CC([O])COO	InChI=1S/C4H7O3/c1-2-4(5)3-7-6/h2,4,6H,1,3H2	
C4H602-10OH4	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)5/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	
C4H71-300CH3	C5H10O2	C=CC(C)OOC	InChI=1S/C5H10O2/c1-4-5(2)7-6-3/h4-5H,1H2,2-3H3	
C4H72-100CH3	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	
C4H5-1	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	
C4H4	C4H4	C#CC=C	InChI=1S/C4H4/c1-3-4-2/h1,4H,2H2	
C4H3-1	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)/h3H2,1-2H3	

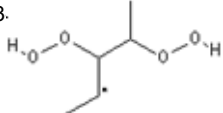
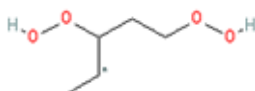
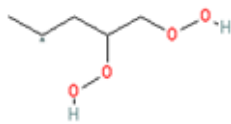
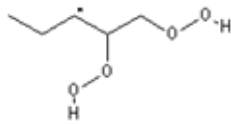

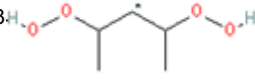
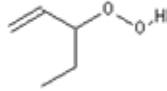
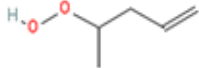


C2H5COCH2	C4H7O	[CH2]C(=O)CC	InChI=1S/C4H7O/c1-3-4(2)5/h2-3H2,1H3	
CH2CH2COCH3	C4H7O	[CH2]CC(C)=O	InChI=1S/C4H7O/c1-3-4(2)5/h1,3H2,2H3	
CH3CHCOCH3	C4H7O	C[CH]C(C)=O	InChI=1S/C4H7O/c1-3-4(2)5/h3H,1-2H3	
C2H3COCH3	C4H6O	C=CC(C)=O	InChI=1S/C4H6O/c1-3-4(2)5/h3H,1H2,2H3	
CH3CHOOCOCH3	C4H7O3	CC(=O)C(C)O[O]	InChI=1S/C4H7O3/c1-3(5)4(2)7-6/h4H,1-2H3	
CH2CHOOHCOCH3	C4H7O3	[CH2]C(OO)C(C)=O	InChI=1S/C4H7O3/c1-3(5)4(2)7-6/h4,6H,2H2,1H3	
C2H5CHCO	C4H6O	CCC=C=O	InChI=1S/C4H6O/c1-2-3-4-5/h3H,2H2,1H3	
NC5H12	C5H12	CCCCC	InChI=1S/C5H12/c1-3-5-4-2/h3-5H2,1-2H3	
C5H11-1	C5H11	[CH2]CCCC	InChI=1S/C5H11/c1-3-5-4-2/h1,3-5H2,2H3	
C5H11-2	C5H11	C[CH]CCC	InChI=1S/C5H11/c1-3-5-4-2/h3H,4-5H2,1-2H3	
C5H11-3	C5H11	CC[CH]CC	InChI=1S/C5H11/c1-3-5-4-2/h5H,3-4H2,1-2H3	

C5H11O2H-1	C5H12O2	CCCCCOO	InChI=1S/C5H12O2/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	

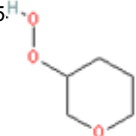
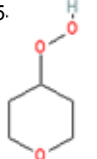
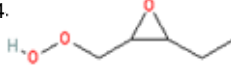
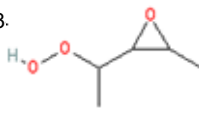
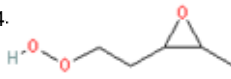
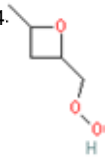
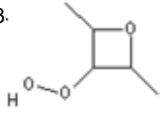
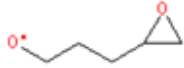
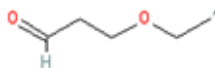
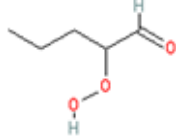
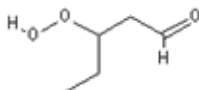
C5H1000H1-4	C5H11O2	C[CH]CCCCOO	InChI=1S/C5H11O2/c1-2-3-4-5-7-6/h2,6H,3-5H2,1H3	
C5H1000H1-5	C5H11O2	[CH2]CCCCOO	InChI=1S/C5H11O2/c1-2-3-4-5-7-6/h6H,1-5H2	
C5H1000H2-1	C5H11O2	CCCC([CH2])OO	InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h5-6H,2-4H2,1H3	
C5H1000H2-3	C5H11O2	CC[CH]C(C)OO	InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h4-6H,3H2,1-2H3	
C5H1000H2-4	C5H11O2	C[CH]CC(C)OO	InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h3,5-6H,4H2,1-2H3	
C5H1000H2-5	C5H11O2	[CH2]CCC(C)OO	InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h5-6H,1,3-4H2,2H3	
C5H1000H3-1	C5H11O2	[CH2]CC(CC)OO	InChI=1S/C5H11O2/c1-3-5(4-2)7-6/h5-6H,1,3-4H2,2H3	
C5H1000H3-2	C5H11O2	C[CH]C(CC)OO	InChI=1S/C5H11O2/c1-3-5(4-2)7-6/h3,5-6H,4H2,1-2H3	
C5H1001-2	C5H10O	CCCC1CO1	InChI=1S/C5H10O/c1-2-3-5-4-6-5/h5H,2-4H2,1H3	
C5H1001-3	C5H10O	CCC1CCO1	InChI=1S/C5H10O/c1-2-5-3-4-6-5/h5H,2-4H2,1H3	
C5H1001-4	C5H10O	CC1CCCO1	InChI=1S/C5H10O/c1-5-3-2-4-6-5/h5H,2-4H2,1H3	

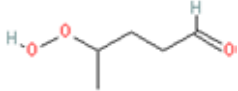
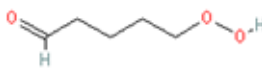
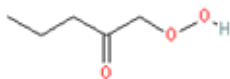
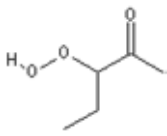
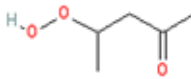
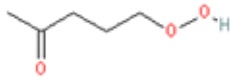
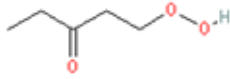
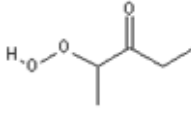
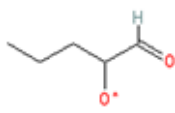
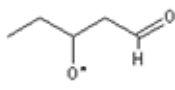
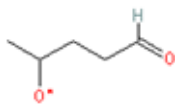
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C5H1002-3	C5H100	CCC1C(C)O1	InChI=1S/C5H10O/c1-3-5-4(2)6-5/h4-5H,3H2,1-2H3	
C5H1002-4	C5H100	CC1CC(C)O1	InChI=1S/C5H10O/c1-4-3-5(2)6-4/h4-5H,3H2,1-2H3	
C5H1000H1-202	C5H11O4	CCCC(COO)O[O]	InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h5-6H,2-4H2,1H3	
C5H1000H1-302	C5H11O4	CCC(CCOO)O[O]	InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h5-6H,2-4H2,1H3	
C5H1000H1-402	C5H11O4	CC(CCCOO)O[O]	InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h5-6H,2-4H2,1H3	
C5H1000H1-502	C5H11O4	C(CCOO)CCO[O]	InChI=1S/C5H11O4/c6-8-4-2-1-3-5-9-7/h6H,1-5H2	
C5H1000H2-102	C5H11O4	CCCC(CO[O])OO	InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h5,7H,2-4H2,1H3	
C5H1000H2-302	C5H11O4	CCC(C(C)OO)O[O]	InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h4-6H,3H2,1-2H3	
C5H1000H2-402	C5H11O4	CC(CC(C)O[O])OO	InChI=1S/C5H11O4/c1-4(8-6)3-5(2)9-7/h4-6H,3H2,1-2H3	
C5H1000H2-502	C5H11O4	CC(CCCO[O])OO	InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h5,7H,2-4H2,1H3	

C5H1000H3-102	C5H11O4	CCC(CCO[O])OO	InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h5,7H,2-4H2,1H3	
C5H1000H3-202	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	
C5H91-2,300H	C5H11O4	CCC(C([CH2])OO)OO	InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h4,7H,2-3H2,1H3	
C5H91-2,400H	C5H11O4	[CH2]C(CC(C)OO)OO	InChI=1S/C5H11O4/c1-4(8-6)3-5(2)9-7/h4,7H,1,3H2,2H3	
C5H91-2,500H	C5H11O4	[CH2]C(CCCOO)OO	InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h5,7H,1-4H2	
C5H91-3,400H	C5H11O4	[CH2]CC(C(C)OO)OO	InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h4,7H,1,3H2,2H3	
C5H91-3,500H	C5H11O4	[CH2]CC(CCOO)OO	InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h5,7H,1-4H2	
C5H91-4,500H	C5H11O4	[CH2]CCC(COO)OO	InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h5,7H,1-4H2	
C5H92-1,300H	C5H11O4	CCC([CH]COO)OO	InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h3,5-7H,2,4H2,1H3	
C5H92-1,400H	C5H11O4	CC(C[CH]COO)OO	InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h2,5-7H,3-4H2,1H3	
C5H92-1,500H	C5H11O4	C([CH]COO)CCOO	InChI=1S/C5H11O4/c6-8-4-2-1-3-5-9-7/h2,6-7H,1,3-5H2	

C5H92-3,400H	C5H11O4	C[CH]C(C(C)OO)OO	InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h3-7H,1-2H3	
C5H92-3,500H	C5H11O4	C[CH]C(CCOO)OO	InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h2,5-7H,3-4H2,1H3	
C5H92-4,500H	C5H11O4	C[CH]CC(COO)OO	InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h2,5-7H,3-4H2,1H3	
C5H93-1,200H	C5H11O4	CC[CH]C(COO)OO	InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h3,5-7H,2,4H2,1H3	
C5H93-1,400H	C5H11O4	CC([CH]CCOO)OO	InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h3,5-7H,2,4H2,1H3	
C5H93-1,500H	C5H11O4	[CH](CCOO)CCOO	InChI=1S/C5H11O4/c6-8-4-2-1-3-5-9-7/h1,6-7H,2-5H2	
C5H93-2,400H	C5H11O4	CC([CH]C(C)OO)OO	InChI=1S/C5H11O4/c1-4(8-6)3-5(2)9-7/h3-7H,1-2H3	
C5H91-300H	C5H10O2	C=CC(CC)OO	InChI=1S/C5H10O2/c1-3-5(4-2)7-6/h3,5-6H,1,4H2,2H3	
C5H91-400H	C5H10O2	C=CCC(C)OO	InChI=1S/C5H10O2/c1-3-4-5(2)7-6/h3,5-6H,1,4H2,2H3	
C5H91-500H	C5H10O2	C=CCCCOO	InChI=1S/C5H10O2/c1-2-3-4-5-7-6/h2,6H,1,3-5H2	
C5H92-100H	C5H10O2	CCC=CCOO	InChI=1S/C5H10O2/c1-2-3-4-5-7-6/h3-4,6H,2,5H2,1H3	



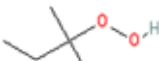

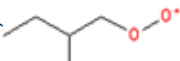

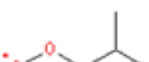
C5H92-400H	C5H10O2	CC=CC(C)OO	InChI=1S/C5H10O2/c1-3-4-5(2)7-6/h3-6H,1-2H3	
C5H92-500H	C5H10O2	CC=CCCCO	InChI=1S/C5H10O2/c1-2-3-4-5-7-6/h2-3,6H,4-5H2,1H3	
C5H901-200H-3	C5H10O3	CCC(C1CO1)OO	InChI=1S/C5H10O3/c1-2-4(8-6)5-3-7-5/h4-6H,2-3H2,1H3	
C5H901-200H-4	C5H10O3	CC(CC1CO1)OO	InChI=1S/C5H10O3/c1-4(8-6)2-5-3-7-5/h4-6H,2-3H2,1H3	
C5H901-200H-5	C5H10O3	C(CC1CO1)COO	InChI=1S/C5H10O3/c6-8-3-1-2-5-4-7-5/h5-6H,1-4H2	
C5H901-300H-2	C5H10O3	CCC1C(CO1)OO	InChI=1S/C5H10O3/c1-2-4-5(8-6)3-7-4/h4-6H,2-3H2,1H3	
C5H901-300H-4	C5H10O3	CC(C1CCO1)OO	InChI=1S/C5H10O3/c1-4(8-6)5-2-3-7-5/h4-6H,2-3H2,1H3	
C5H901-300H-5	C5H10O3	C1COC1CCOO	InChI=1S/C5H10O3/c6-8-4-2-5-1-3-7-5/h5-6H,1-4H2	
C5H901-400H-2	C5H10O3	CC1CC(CO1)OO	InChI=1S/C5H10O3/c1-4-2-5(8-6)3-7-4/h4-6H,2-3H2,1H3	
C5H901-400H-3	C5H10O3	CC1C(CCO1)OO	InChI=1S/C5H10O3/c1-4-5(8-6)2-3-7-4/h4-6H,2-3H2,1H3	
C5H901-400H-5	C5H10O3	C1CC(COO)OC1	InChI=1S/C5H10O3/c6-8-4-5-2-1-3-7-5/h5-6H,1-4H2	

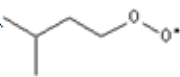

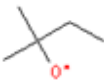
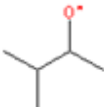
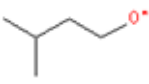
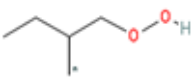
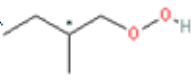
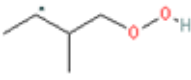
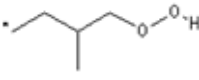
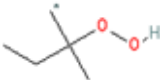
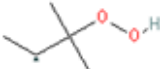
C5H901-500H-2	C5H1003	C1CC(COC1)OO	InChI=1S/C5H10O3/c6-8-5-2-1-3-7-4-5/h5-6H,1-4H2	
C5H901-500H-3	C5H1003	C1COCCC1OO	InChI=1S/C5H10O3/c6-8-5-1-3-7-4-2-5/h5-6H,1-4H2	
C5H902-300H-1	C5H1003	CCC1C(COO)O1	InChI=1S/C5H10O3/c1-2-4-5(8-4)3-7-6/h4-6H,2-3H2,1H3	
C5H902-300H-4	C5H1003	CC1C(C(C)OO)O1	InChI=1S/C5H10O3/c1-3-5(7-3)4(2)8-6/h3-6H,1-2H3	
C5H902-300H-5	C5H1003	CC1C(CCOO)O1	InChI=1S/C5H10O3/c1-4-5(8-4)2-3-7-6/h4-6H,2-3H2,1H3	
C5H902-400H-1	C5H1003	CC1CC(COO)O1	InChI=1S/C5H10O3/c1-4-2-5(8-4)3-7-6/h4-6H,2-3H2,1H3	
C5H902-400H-3	C5H1003	CC1C(C(C)O1)OO	InChI=1S/C5H10O3/c1-3-5(8-6)4(2)7-3/h3-6H,1-2H3	
C5H901-20-5	C5H9O2	C(CC1CO1)C[O]	InChI=1S/C5H9O2/c6-3-1-2-5-4-7-5/h5H,1-4H2	
CH2CH2OCH2CH2CHO	C5H9O2	[CH2]COCCC=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	

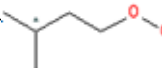
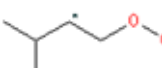
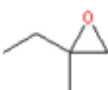
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NC5KET15	C5H10O3	C(CC=O)CCOO	InChI=1S/C5H10O3/c6-4-2-1-3-5-8-7/h4,7H,1-3,5H2	
NC5KET21	C5H10O3	CCCC(COO)=O	InChI=1S/C5H10O3/c1-2-3-5(6)4-8-7/h7H,2-4H2,1H3	
NC5KET23	C5H10O3	CCC(C(C)=O)OO	InChI=1S/C5H10O3/c1-3-5(8-7)4(2)6/h5,7H,3H2,1-2H3	
NC5KET24	C5H10O3	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	
NC5KET240	C5H9O2	CC(CC(C)=O)[O]	InChI=1S/C5H9O2/c1-4(6)3-5(2)7/h4H,3H2,1-2H3	
NC5KET250	C5H9O2	CC(CCC[O])=O	InChI=1S/C5H9O2/c1-5(7)3-2-4-6/h2-4H2,1H3	
NC5KET310	C5H9O2	CCC(CC[O])=O	InChI=1S/C5H9O2/c1-2-5(7)3-4-6/h2-4H2,1H3	
NC5KET320	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	

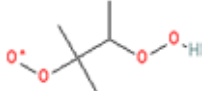
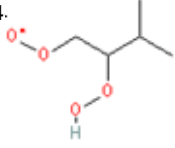
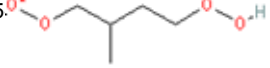
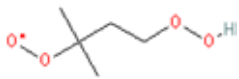
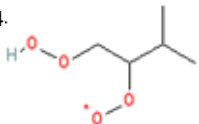
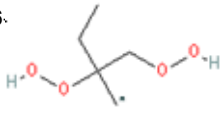
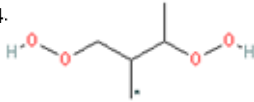

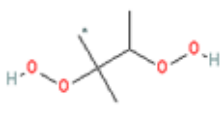
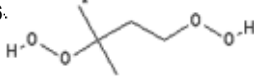
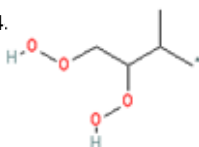
OCH2CHO	C2H3O2	C(C[O])=O	InChI=1S/C2H3O2/c3-1-2-4/h1H,2H2	
CH2OCH2CHO	C3H5O2	[CH2]OCC=O	InChI=1S/C3H5O2/c1-5-3-2-4/h2H,1,3H2	
C2H4OCHO	C3H5O2	CC(C=O)[O]	InChI=1S/C3H5O2/c1-3(5)2-4/h2-3H,1H3	
C5H10OOH1-3OH	C5H12O3	C(OOH)CC(OH)CC	InChI=1S/C5H12O3/c1-2-5(6)3-4-8-7/h5-7H,2-4H2,1H3	
C5H10OOH2-4OH	C5H12O3	CC(OOH)CC(OH)C	InChI=1S/C5H12O3/c1-4(6)3-5(2)8-7/h4-7H,3H2,1-2H3	
C5H10OOH3-1OH	C5H12O3	C(OH)CC(OOH)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	

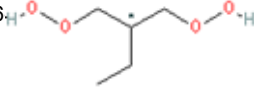
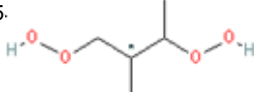

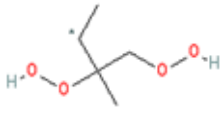
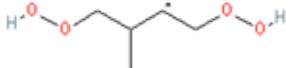
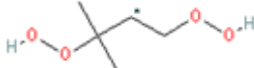
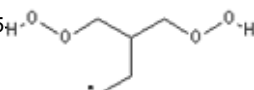
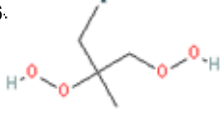
BC5H11	C5H11	CCCC	InChI=1S/C5H11/c1-4-5(2)3/h4H2,1-3H3	
CC5H11	C5H11	C[CH]C(C)C	InChI=1S/C5H11/c1-4-5(2)3/h4-5H,1-3H3	
DC5H11	C5H11	[CH2]CC(C)C	InChI=1S/C5H11/c1-4-5(2)3/h5H,1,4H2,2-3H3	
AC5H9O-A2	C5H9O	CCC(=C)C[O]	InChI=1S/C5H9O/c1-3-5(2)4-6/h2-4H2,1H3	
AC5H11O2H	C5H12O2	CCC(C)COO	InChI=1S/C5H12O2/c1-3-5(2)4-7-6/h5-6H,3-4H2,1-2H3	
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	

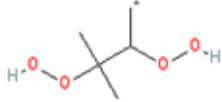
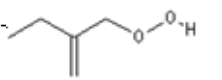
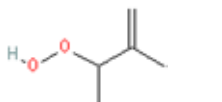
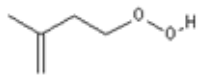
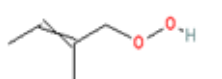
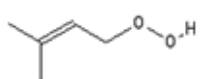
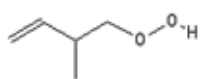
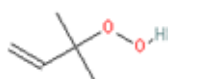
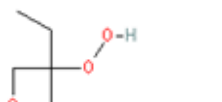
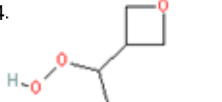
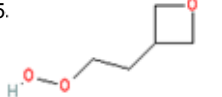
DC5H11O2	C5H11O2	CC(C)CCO[O]	InChI=1S/C5H11O2/c1-5(2)3-4-7-6/h5H,3-4H2,1-2H3	
AC5H11O	C5H11O	CCC(C)C[O]	InChI=1S/C5H11O/c1-3-5(2)4-6/h5H,3-4H2,1-2H3	
BC5H11O	C5H11O	CCC(C)(C)[O]	InChI=1S/C5H11O/c1-4-5(2,3)6/h4H2,1-3H3	
CC5H11O	C5H11O	CC(C)C(C)[O]	InChI=1S/C5H11O/c1-4(2)5(3)6/h4-5H,1-3H3	
DC5H11O	C5H11O	CC(C)CC[O]	InChI=1S/C5H11O/c1-5(2)3-4-6/h5H,3-4H2,1-2H3	
AC5H10OOH-A	C5H11O2	CCC([CH2])COO	InChI=1S/C5H11O2/c1-3-5(2)4-7-6/h5-6H,2-4H2,1H3	
AC5H10OOH-B	C5H11O2	CCCCOO	InChI=1S/C5H11O2/c1-3-5(2)4-7-6/h6H,3-4H2,1-2H3	
AC5H10OOH-C	C5H11O2	C[CH]C(C)COO	InChI=1S/C5H11O2/c1-3-5(2)4-7-6/h3,5-6H,4H2,1-2H3	
AC5H10OOH-D	C5H11O2	[CH2]CC(C)COO	InChI=1S/C5H11O2/c1-3-5(2)4-7-6/h5-6H,1,3-4H2,2H3	
BC5H10OOH-A	C5H11O2	CCC([CH2])(C)OO	InChI=1S/C5H11O2/c1-4-5(2,3)7-6/h6H,2,4H2,1,3H3	
BC5H10OOH-C	C5H11O2	C[CH]C(C)(C)OO	InChI=1S/C5H11O2/c1-4-5(2,3)7-6/h4,6H,1-3H3	

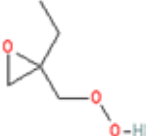
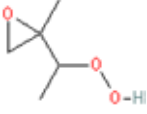
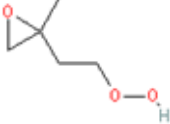
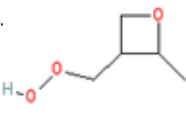
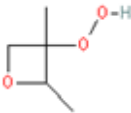
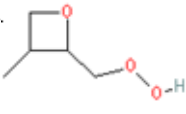
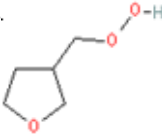
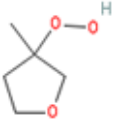
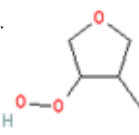
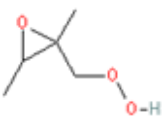
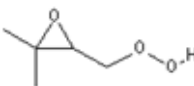
BC5H10OOH-D	C5H11O2	[CH2]CC(C)(C)OO	InChI=1S/C5H11O2/c1-4-5(2,3)7-6/h6H,1,4H2,2-3H3	
CC5H10OOH-A	C5H11O2	[CH2]C(C)C(C)OO	InChI=1S/C5H11O2/c1-4(2)5(3)7-6/h4-6H,1H2,2-3H3	
CC5H10OOH-B	C5H11O2	CCC(C)OO	InChI=1S/C5H11O2/c1-4(2)5(3)7-6/h5-6H,1-3H3	
CC5H10OOH-D	C5H11O2	CC(C)C([CH2])OO	InChI=1S/C5H11O2/c1-4(2)5(3)7-6/h4-6H,3H2,1-2H3	
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-AC5H100	C5H10O	CCC1COC1	InChI=1S/C5H10O/c1-2-5-3-6-4-5/h5H,2-4H2,1H3	
A-BC5H100	C5H10O	CCC1(C)CO1	InChI=1S/C5H10O/c1-3-5(2)4-6-5/h3-4H2,1-2H3	
A-CC5H100	C5H10O	CC1COC1C	InChI=1S/C5H10O/c1-4-3-6-5(4)2/h4-5H,3H2,1-2H3	
A-DC5H100	C5H10O	CC1CCOC1	InChI=1S/C5H10O/c1-5-2-3-6-4-5/h5H,2-4H2,1H3	

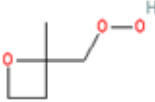

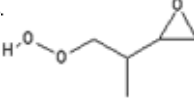
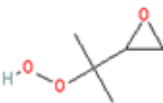
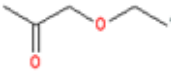
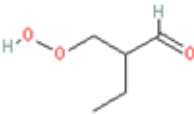
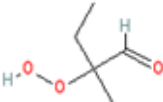
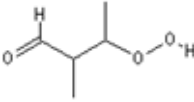
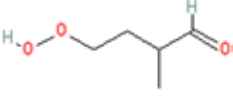
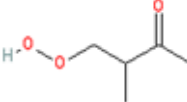
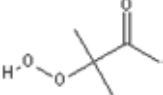
B-CC5H10O	C5H10O	CC1C(C)(C)O1	InChI=1S/C5H10O/c1-4-5(2,3)6-4/h4H,1-3H3	
B-DC5H10O	C5H10O	CC1(C)CCO1	InChI=1S/C5H10O/c1-5(2)3-4-6-5/h3-4H2,1-2H3	
C-DC5H10O	C5H10O	CC(C)C1CO1	InChI=1S/C5H10O/c1-4(2)5-3-6-5/h4-5H,3H2,1-2H3	
AC5H10OOH-AO2	C5H11O4	CCC(COO)CO[O]	InChI=1S/C5H11O4/c1-2-5(3-8-6)4-9-7/h5-6H,2-4H2,1H3	
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	

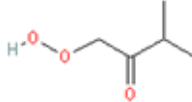
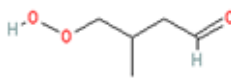
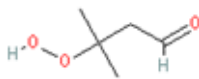
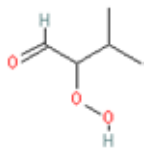
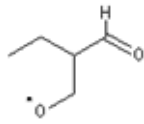
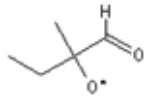
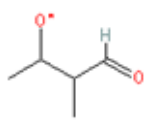
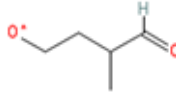
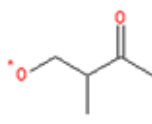
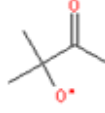
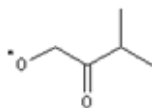
CC5H10OOH-BO2	C5H11O4	CC(C(C)(C)O[O])OO	InChI=1S/C5H11O4/c1-4(8-6)5(2,3)9-7/h4,6H,1-3H3	
CC5H10OOH-DO2	C5H11O4	CC(C)C(CO[O])OO	InChI=1S/C5H11O4/c1-4(2)5(9-7)3-8-6/h4,5,7H,3H2,1-2H3	
DC5H10OOH-AO2	C5H11O4	CC(CCOO)CO[O]	InChI=1S/C5H11O4/c1-5(4-9-7)2-3-8-6/h5,6H,2-4H2,1H3	
DC5H10OOH-BO2	C5H11O4	CC(C)(CCOO)O[O]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

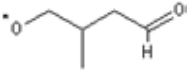
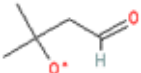
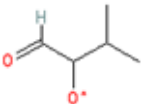
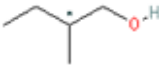
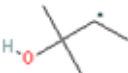
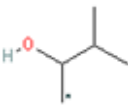
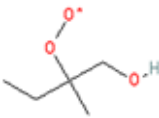
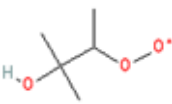
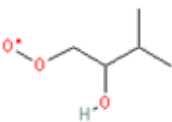
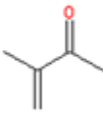
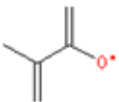
C5H9B-A,AOOH	C5H11O4	CC[C](COO)COO	InChI=1S/C5H11O4/c1-2-5(3-8-6)4-9-7/h6-7H,2-4H2,1H3	
C5H9B-A,COOH	C5H11O4	C[C](COO)C(C)OO	InChI=1S/C5H11O4/c1-4(3-8-6)5(2)9-7/h5-7H,3H2,1-2H3	
C5H9B-A,DOOH	C5H11O4	C[C](CCOO)COO	InChI=1S/C5H11O4/c1-5(4-9-7)2-3-8-6/h6-7H,2-4H2,1H3	
C5H9B-C,DOOH	C5H11O4	CCC(COO)OO	InChI=1S/C5H11O4/c1-4(2)5(9-7)3-8-6/h5-7H,3H2,1-2H3	
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	CC(C)=CCOO	InChI=1S/C5H10O2/c1-5(2)3-4-7-6/h3,6H,4H2,1-2H3	
C5H9C-AOOH	C5H10O2	C=CC(C)COO	InChI=1S/C5H10O2/c1-3-5(2)4-7-6/h3,5-6H,1,4H2,2H3	
C5H9C-BOOH	C5H10O2	C=CC(C)(C)OO	InChI=1S/C5H10O2/c1-4-5(2,3)7-6/h4,6H,1H2,2-3H3	
C5H90A-AOOH-B	C5H10O3	CCC1(COC1)OO	InChI=1S/C5H10O3/c1-2-5(8-6)3-7-4-5/h6H,2-4H2,1H3	
C5H90A-AOOH-C	C5H10O3	CC(C1COC1)OO	InChI=1S/C5H10O3/c1-4(8-6)5-2-7-3-5/h4.6H,2-3H2,1H3	
C5H90A-AOOH-D	C5H10O3	C(COO)C1COC1	InChI=1S/C5H10O3/c6-8-2-1-5-3-7-4-5/h5.6H,1-4H2	





C5H90A-BOOH-A	C5H10O3	CCC1(CO1)COO	InChI=1S/C5H10O3/c1-2-5(3-7-5)4-8-6/h6H,2-4H2,1H3	
C5H90A-BOOH-C	C5H10O3	CC(C1(C)CO1)OO	InChI=1S/C5H10O3/c1-4(8-6)5(2)3-7-5/h4,6H,3H2,1-2H3	
C5H90A-BOOH-D	C5H10O3	CC1(CCOO)CO1	InChI=1S/C5H10O3/c1-5(4-7-5)2-3-8-6/h6H,2-4H2,1H3	
C5H90A-COOH-A	C5H10O3	CC1C(CO1)COO	InChI=1S/C5H10O3/c1-4-5(2-7-4)3-8-6/h4,6H,2-3H2,1H3	
C5H90A-COOH-B	C5H10O3	CC1C(C)(CO1)OO	InChI=1S/C5H10O3/c1-4-5(2,8-6)3-7-4/h4,6H,3H2,1-2H3	
C5H90A-COOH-D	C5H10O3	CC1COC1COO	InChI=1S/C5H10O3/c1-4-2-7-5(4)3-8-6/h4,6H,2-3H2,1H3	
C5H90A-DOOH-A	C5H10O3	C1COCC1COO	InChI=1S/C5H10O3/c6-8-4-5-1-2-7-3-5/h5,6H,1-4H2	
C5H90A-DOOH-B	C5H10O3	CC1(CCO1)OO	InChI=1S/C5H10O3/c1-5(8-6)2-3-7-4-5/h6H,2-4H2,1H3	
C5H90A-DOOH-C	C5H10O3	CC1COCC1OO	InChI=1S/C5H10O3/c1-4-2-7-3-5(4)8-6/h4,6H,2-3H2,1H3	
C5H90B-COOH-A	C5H10O3	CC1C(C)(COO)O1	InChI=1S/C5H10O3/c1-4-5(2,8-4)3-7-6/h4,6H,3H2,1-2H3	
C5H90B-COOH-D	C5H10O3	CC1(C)C(COO)O1	InChI=1S/C5H10O3/c1-5(2)4(8-5)3-7-6/h4,6H,3H2,1-2H3	


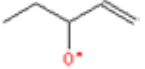
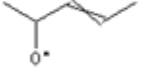

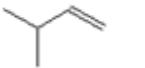

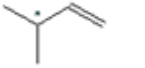
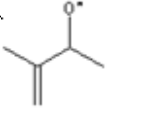
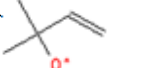
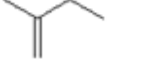

C5H9OB-DOOH-A	C5H10O3	CC1(CCO1)COO	InChI=1S/C5H10O3/c1-5(4-8-6)2-3-7-5/h6H,2-4H2,1H3	
C5H9OB-DOOH-C	C5H10O3	CC1(C)C(CO1)OO	InChI=1S/C5H10O3/c1-5(2)4(8-6)3-7-5/h4,6H,3H2,1-2H3	
C5H9OC-DOOH-A	C5H10O3	CC(COO)C1CO1	InChI=1S/C5H10O3/c1-4(2-8-6)5-3-7-5/h4-6H,2-3H2,1H3	
C5H9OC-DOOH-B	C5H10O3	CC(C)(C1CO1)OO	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	

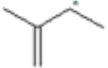
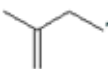

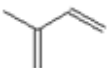
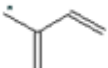
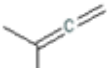
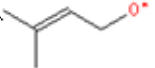
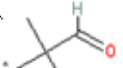

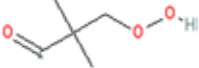
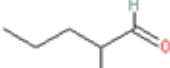
IC5KETCD	C5H10O3	CC(C)C(COO)=O	InChI=1S/C5H10O3/c1-4(2)5(6)3-8-7/h4,7H,3H2,1-2H3	
IC5KETDA	C5H10O3	CC(CC=O)COO	InChI=1S/C5H10O3/c1-5(2-3-6)4-8-7/h3,5,7H,2,4H2,1H3	
IC5KETDB	C5H10O3	CC(C)(CC=O)OO	InChI=1S/C5H10O3/c1-5(2,8-7)3-4-6/h4,7H,3H2,1-2H3	
IC5KETDC	C5H10O3	CC(C)C(C=O)OO	InChI=1S/C5H10O3/c1-4(2)5(3-6)8-7/h3-5,7H,1-2H3	
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	

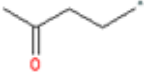
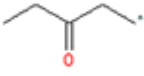
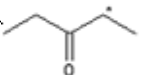
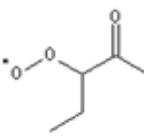
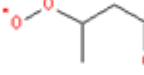
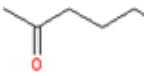
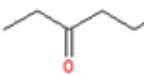
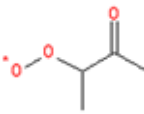
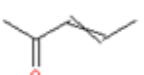
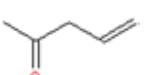
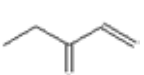
AC3H4COCH3	C5H7O	C=C([CH2])C(C)=O	InChI=1S/C5H7O/c1-4(2)5(3)6/h1-2H2,3H3	
NEOC5H12	C5H12	CC(C)(C)C	InChI=1S/C5H12/c1-5(2,3)4/h1-4H3	
NEOC5H11	C5H11	[CH2]C(C)(C)C	InChI=1S/C5H11/c1-5(2,3)4/h1H2,2-4H3	
NEOC5H11O2H	C5H12O2	CC(C)(C)COO	InChI=1S/C5H12O2/c1-5(2,3)4-7-6/h6H,4H2,1-3H3	
NEOC5H11O2	C5H11O2	CC(C)(C)CO[O]	InChI=1S/C5H11O2/c1-5(2,3)4-7-6/h4H2,1-3H3	
NEOC5H11O	C5H11O	CC(C)(C)C[O]	InChI=1S/C5H11O/c1-5(2,3)4-6/h4H2,1-3H3	
NEOC5H10OOH	C5H11O2	[CH2]C(C)(C)COO	InChI=1S/C5H11O2/c1-5(2,3)4-7-6/h6H,1,4H2,2-3H3	
NEO-C5H10O	C5H10O	CC1(C)COC1	InChI=1S/C5H10O/c1-5(2)3-6-4-5/h3-4H2,1-2H3	
NEOC5H10OOH-O2	C5H11O4	CC(C)(COO)CO[O]	InChI=1S/C5H11O4/c1-5(2,3-8-6)4-9-7/h6H,3-4H2,1-2H3	
NEOC5H9Q2	C5H11O4	[CH2]C(C)(COO)COO	InChI=1S/C5H11O4/c1-5(2,3-8-6)4-9-7/h6-7H,1,3-4H2,2H3	
NEOC5KET	C5H10O3	CC(C)(C=O)COO	InChI=1S/C5H10O3/c1-5(2,3-6)4-8-7/h3,7H,4H2,1-2H3	




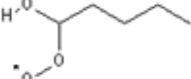
NEOC5KETOX	C5H9O2	CC(C)(C=O)C[O]	InChI=1S/C5H9O2/c1-5(2,3-6)4-7/h3H,4H2,1-2H3	
NEOC5KEJOL	C5H9O2	CC(C)(CO)[C]=O	InChI=1S/C5H9O2/c1-5(2,3-6)4-7/h6H,3H2,1-2H3	
IC4H6Q2-II	C4H8O4	C=C(COO)COO	InChI=1S/C4H8O4/c1-4(2-7-5)3-8-6/h5-6H,1-3H2	
NEOC5H9O-OOH	C5H10O3	CC1(COC1)COO	InChI=1S/C5H10O3/c1-5(4-8-6)2-7-3-5/h6H,2-4H2,1H3	
C5H10-1	C5H10	C=CCCC	InChI=1S/C5H10/c1-3-5-4-2/h3H,1,4-5H2,2H3	
C5H10-2	C5H10	CC=CCC	InChI=1S/C5H10/c1-3-5-4-2/h3,5H,4H2,1-2H3	
C5H81-3	C5H8	C=CC=CC	InChI=1S/C5H8/c1-3-5-4-2/h3-5H,1H2,2H3	
C5H91-3	C5H9	C=C[CH]CC	InChI=1S/C5H9/c1-3-5-4-2/h3,5H,1,4H2,2H3	
C5H91-4	C5H9	C=CC[CH]C	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	
C5H901-3	C5H9O	C=CC(CC)[O]	InChI=1S/C5H9O/c1-3-5(6)4-2/h3,5H,1,4H2,2H3	
C5H902-4	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	
AC5H90-C	C5H9O	C=C(C)C(C)[O]	InChI=1S/C5H9O/c1-4(2)5(3)6/h5H,1H2,2-3H3	
CC5H90-B	C5H9O	C=CC(C)(C)[O]	InChI=1S/C5H9O/c1-4-5(2,3)6/h4H,1H2,2-3H3	
AC5H10	C5H10	CCC(=C)C	InChI=1S/C5H10/c1-4-5(2)3/h2,4H2,1,3H3	
AC5H9-A2	C5H9	CCC(=C)[CH2]	InChI=1S/C5H9/c1-4-5(2)3/h2-4H2,1H3	

AC5H9-C	C5H9	C[CH]C(=C)C	InChI=1S/C5H9/c1-4-5(2)/h4H,2H2,1,3H3	
AC5H9-D	C5H9	[CH2]CC(=C)C	InChI=1S/C5H9/c1-4-5(2)/h1-2,4H2,3H3	
B2E2M10J	C5H9O	CC=C(C)C[O]	InChI=1S/C5H9O/c1-3-5(2)4-6/h3H,4H2,1-2H3	
B13DE2M	C5H8	C=CC(=C)C	InChI=1S/C5H8/c1-4-5(2)3/h4H,1-2H2,3H3	
B13DE2MJ	C5H7	C=CC(=C)[CH2]	InChI=1S/C5H7/c1-4-5(2)3/h4H,1-3H2	
B12DE3M	C5H8	[CH2]=[C]=CC	InChI=1S/C5H8/c1-4-5(2)3/h1H2,2-3H3	
B2E3M10J	C5H9O	CC(C)=CC[O]	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-102	C5H9O3	CCCC(O[O])C(=O)	InChI=1S/C5H9O3/c1-2-3-5(4-6)8-7/h4-5H,2-3H2,1H3	

PC4H8CHO-202	C5H9O3	CCC(O[O])CC(=O)	InChI=1S/C5H9O3/c1-2-5(8-7)3-4-6/h4-5H,2-3H2,1H3	
PC4H8CHO-302	C5H9O3	CC(O[O])CCC(=O)	InChI=1S/C5H9O3/c1-5(8-7)3-2-4-6/h4-5H,2-3H2,1H3	
PC4H8CHO-402	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	
NC3H7COCH3	C5H10O	CC(=O)CCC	InChI=1S/C5H10O/c1-3-4-5(2)6/h3-4H2,1-2H3	
C2H5COC2H5	C5H10O	CCC(=O)CC	InChI=1S/C5H10O/c1-3-5(6)4-2/h3-4H2,1-2H3	
NC3H7COCH2	C5H9O	[CH2]C(=O)CCC	InChI=1S/C5H9O/c1-3-4-5(2)6/h2-4H2,1H3	
CH3CH2CHCOCH3	C5H9O	CC(=O)[CH]CC	InChI=1S/C5H9O/c1-3-4-5(2)6/h4H,3H2,1-2H3	
CH3CHCH2COCH3	C5H9O	CC(=O)C[CH]C	InChI=1S/C5H9O/c1-3-4-5(2)6/h3H,4H2,1-2H3	

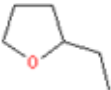
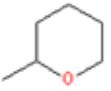
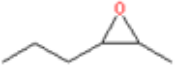

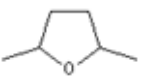

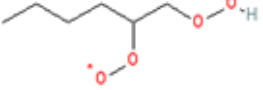
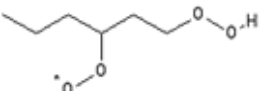
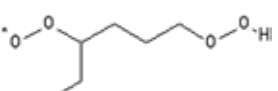

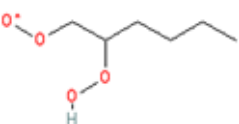
CH ₂ CH ₂ CH ₂ COCH ₃	C ₅ H ₉ O	CC(=O)CC[CH ₂]	InChI=1S/C ₅ H ₉ O/c1-3-4-5(2)/h1,3-4H ₂ ,2H ₃	
CH ₂ CH ₂ COC ₂ H ₅	C ₅ H ₉ O	[CH ₂]CC(=O)CC	InChI=1S/C ₅ H ₉ O/c1-3-5(6)4-2/h1,3-4H ₂ ,2H ₃	
CH ₃ CHCOC ₂ H ₅	C ₅ H ₉ O	C[CH]C(=O)CC	InChI=1S/C ₅ H ₉ O/c1-3-5(6)4-2/h3H,4H ₂ ,1-2H ₃	
NC52ONEO2-3	C ₅ H ₉ O ₃	CC(=O)C(O[O])CC	InChI=1S/C ₅ H ₉ O ₃ /c1-3-5(8-7)4(2)6/h5H,3H ₂ ,1-2H ₃	
NC52ONEO2-4	C ₅ H ₉ O ₃	CC(=O)CC(O[O])C	InChI=1S/C ₅ H ₉ O ₃ /c1-4(6)3-5(2)8-7/h5H,3H ₂ ,1-2H ₃	
NC52ONEO2-5	C ₅ H ₉ O ₃	CC(=O)CCC(O[O])	InChI=1S/C ₅ H ₉ O ₃ /c1-5(6)3-2-4-8-7/h2-4H ₂ ,1H ₃	
NC53ONEO2-1	C ₅ H ₉ O ₃	C(O[O])CC(=O)CC	InChI=1S/C ₅ H ₉ O ₃ /c1-2-5(6)3-4-8-7/h2-4H ₂ ,1H ₃	
NC53ONEO2-2	C ₅ H ₉ O ₃	CC(O[O])C(=O)CC	InChI=1S/C ₅ H ₉ O ₃ /c1-3-5(6)4(2)8-7/h4H,3H ₂ ,1-2H ₃	
NC52ONE-3	C ₅ H ₈ O	CC(=O)C=CC	InChI=1S/C ₅ H ₈ O/c1-3-4-5(2)/h3-4H,1-2H ₃	
NC52ONE-4	C ₅ H ₈ O	CC(=O)CC=C	InChI=1S/C ₅ H ₈ O/c1-3-4-5(2)6/h3H,1,4H ₂ ,2H ₃	
NC53ONE-1	C ₅ H ₈ O	C=CC(=O)CC	InChI=1S/C ₅ H ₈ O/c1-3-5(6)4-2/h3H,1,4H ₂ ,2H ₃	

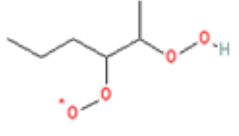
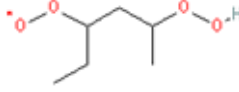
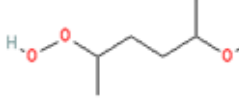
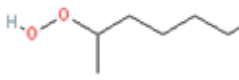
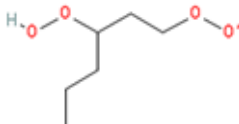
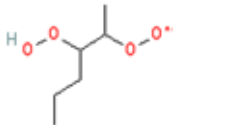
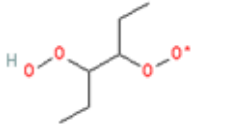
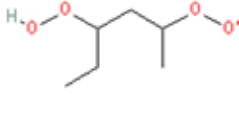
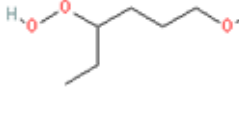
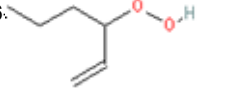
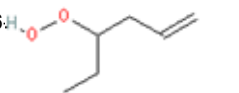
NC5H11OH	C5H12O	CCCCC(OH)	InChI=1S/C5H12O/c1-2-3-4-5-6/h6H,2-5H2,1H3	
C5H10OH11	C5H11O	CCCC[CH](OH)	InChI=1S/C5H11O/c1-2-3-4-5-6/h5-6H,2-4H2,1H3	
C5H10OH12	C5H11O	CCC[CH]CO	InChI=1S/C5H11O/c1-2-3-4-5-6/h4,6H,2-3,5H2,1H3	
C5H10OH13	C5H11O	CC[CH]CC(OH)	InChI=1S/C5H11O/c1-2-3-4-5-6/h3,6H,2,4-5H2,1H3	
C5H10OH14	C5H11O	C[CH]CCC(OH)	InChI=1S/C5H11O/c1-2-3-4-5-6/h2,6H,3-5H2,1H3	
C5H10OH15	C5H11O	[CH2]CCCC(OH)	InChI=1S/C5H11O/c1-2-3-4-5-6/h6H,1-5H2	
C5H10OH-102	C5H11O3	CCCC(OH)(O[O])	InChI=1S/C5H11O3/c1-2-3-4-5(6)8-7/h5-6H,2-4H2,1H3	
C5H10OH-202	C5H11O3	CCCC(O[O])C(OH)	InChI=1S/C5H11O3/c1-2-3-5(4-6)8-7/h5-6H,2-4H2,1H3	
C5H10OH-302	C5H11O3	CCC(O[O])CC(OH)	InChI=1S/C5H11O3/c1-2-5(8-7)3-4-6/h5-6H,2-4H2,1H3	
C5H10OH-402	C5H11O3	CC(O[O])CCC(OH)	InChI=1S/C5H11O3/c1-5(8-7)3-2-4-6/h5-6H,2-4H2,1H3	
C5H10OH-502	C5H11O3	C(O[O])CCCC(OH)	InChI=1S/C5H11O3/c6-4-2-1-3-5-8-7/h6H,1-5H2	

C5H9OH1-1	C5H10O	CCCC=C(OH)	InChI=1S/C5H10O/c1-2-3-4-5-6/h4-6H,2-3H2,1H3	
C5H9OH1-2	C5H10O	CCC=CC(OH)	InChI=1S/C5H10O/c1-2-3-4-5-6/h3-4,6H,2,5H2,1H3	
C5H9OH1-3	C5H10O	CC=CCC(OH)	InChI=1S/C5H10O/c1-2-3-4-5-6/h2-3,6H,4-5H2,1H3	
C5H9OH1-4	C5H10O	C=CCCC(OH)	InChI=1S/C5H10O/c1-2-3-4-5-6/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/c1-2-3-4-5-6-8-7/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	

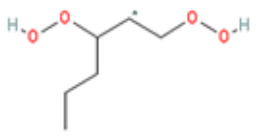
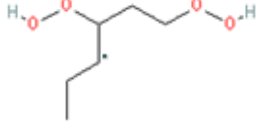
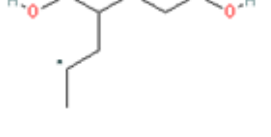
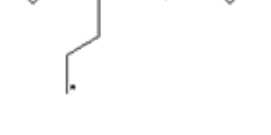
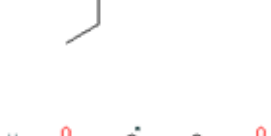
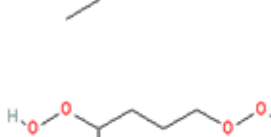
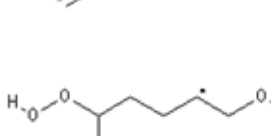
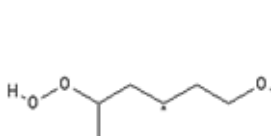

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C6H13O2-2	C6H13O2	CC(O[O])CCCC	InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h6H,3-5H2,1-2H3	
C6H13O2-3	C6H13O2	CCC(O[O])CCC	InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h6H,3-5H2,1-2H3	
C6H13O-1	C6H13O	C([O])CCCC	InChI=1S/C6H13O/c1-2-3-4-5-6-7/h2-6H2,1H3	
C6H13O-2	C6H13O	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	

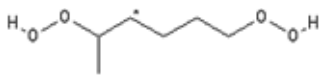
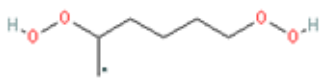
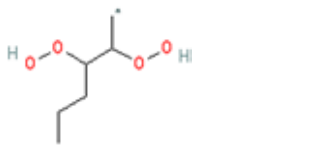
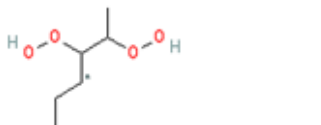
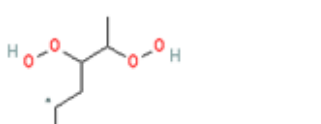
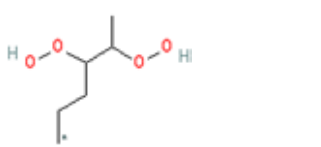
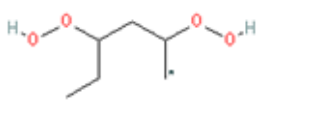
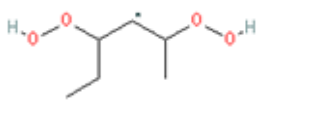
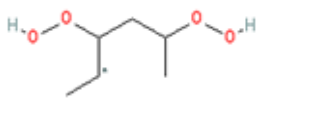
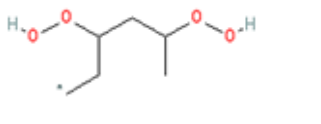
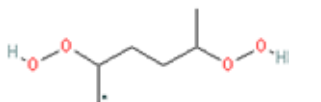
C6H1200H2-3	C6H13O2	CC(OO)[CH]CCC	InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h5-7H,3-4H2,1-2H3	
C6H1200H2-4	C6H13O2	CC(OO)C[CH]CC	InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h4,6H,3,5H2,1-2H3	
C6H1200H2-5	C6H13O2	CC(OO)CC[CH]C	InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h3,6H,4-5H2,1-2H3	
C6H1200H2-6	C6H13O2	CC(OO)CCC[CH2]	InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h6-7H,1,3-5H2,2H3	
C6H1200H3-1	C6H13O2	[CH2]CC(OO)CCC	InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h6-7H,2-5H2,1H3	
C6H1200H3-2	C6H13O2	C[CH]C(OO)CCC	InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h4,6-7H,3,5H2,1-2H3	
C6H1200H3-4	C6H13O2	CCC(OO)[CH]CC	InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h5-7H,3-4H2,1-2H3	
C6H1200H3-5	C6H13O2	CCC(OO)C[CH]C	InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h3,6-7H,4-5H2,1-2H3	
C6H1200H3-6	C6H13O2	CCC(OO)CC[CH2]	InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h6-7H,1,3-5H2,2H3	
C6H1201-2	C6H12O	C1C(O1)CCCC	InChI=1S/C6H12O/c1-2-3-4-6-5-7-6/h6H,2-5H2,1H3	
C6H1201-3	C6H12O	C1CC(O1)CCC	InChI=1S/C6H12O/c1-2-3-6-4-5-7-6/h6H,2-5H2,1H3	

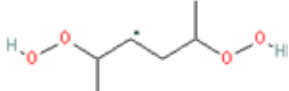
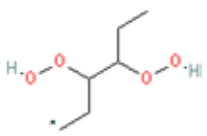
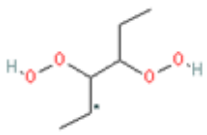
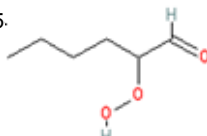
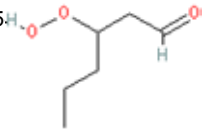
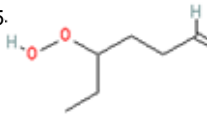
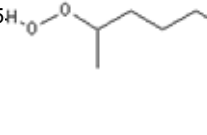
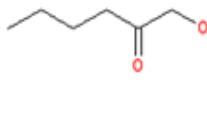
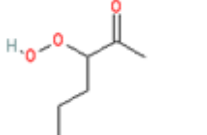
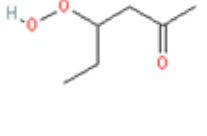
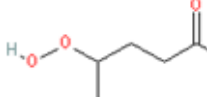
C6H12O1-4	C6H12O	C1CCC(O1)CC	InChI=1S/C6H12O/c1-2-6-4-3-5-7-6/h6H,2-5H2,1H3	
C6H12O1-5	C6H12O	C1CCCC(O1)C	InChI=1S/C6H12O/c1-6-4-2-3-5-7-6/h6H,2-5H2,1H3	
C6H12O2-3	C6H12O	CC1C(O1)CCC	InChI=1S/C6H12O/c1-3-4-6-5(2)7-6/h5-6H,3-4H2,1-2H3	
C6H12O2-4	C6H12O	CC1CC(O1)CC	InChI=1S/C6H12O/c1-3-6-4-5(2)7-6/h5-6H,3-4H2,1-2H3	
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	<chem>CC(OO)C(O[O])CCC</chem>	InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h5-7H,3-4H2,1-2H3	
C6H12OOH2-4O2	C6H13O4	<chem>CC(OO)CC(O[O])CC</chem>	InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h5-7H,3-4H2,1-2H3	
C6H12OOH2-5O2	C6H13O4	<chem>CC(OO)CCC(O[O])C</chem>	InChI=1S/C6H13O4/c1-5(9-7)3-4-6(2)10-8/h5-7H,3-4H2,1-2H3	
C6H12OOH2-6O2	C6H13O4	<chem>CC(OO)CCCC(O[O])</chem>	InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h6,8H,2-5H2,1H3	
C6H12OOH3-1O2	C6H13O4	<chem>C(O[O])CC(OO)CCC</chem>	InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h6,8H,2-5H2,1H3	
C6H12OOH3-2O2	C6H13O4	<chem>CC(O[O])C(OO)CCC</chem>	InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h5-6,8H,3-4H2,1-2H3	
C6H12OOH3-4O2	C6H13O4	<chem>CCC(OO)C(O[O])CC</chem>	InChI=1S/C6H13O4/c1-3-5(9-7)6(4-2)10-8/h5-7H,3-4H2,1-2H3	
C6H12OOH3-5O2	C6H13O4	<chem>CCC(OO)CC(O[O])C</chem>	InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h5-6,8H,3-4H2,1-2H3	
C6H12OOH3-6O2	C6H13O4	<chem>CCC(OO)CCC(O[O])</chem>	InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h6,8H,2-5H2,1H3	
C6H11-1D3OOH	C6H12O2	<chem>C=CC(OO)CCC</chem>	InChI=1S/C6H12O2/c1-3-5-6(4-2)8-7/h4,6,7H,2-3,5H2,1H3	
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	

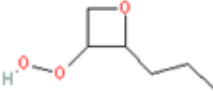
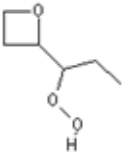
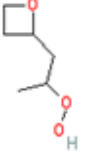

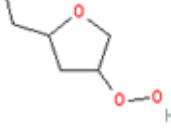
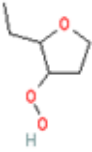
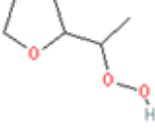
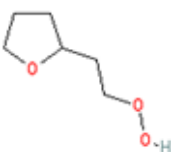
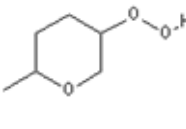
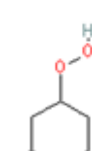
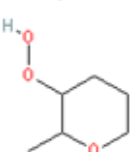
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C6H11-1D600H	C6H12O2	C=CCCCC(OO)	InChI=1S/C6H12O2/c1-2-3-4-5-6-8-7/h2,7H,1,3-6H2	
C6H11-2D100H	C6H12O2	C(OO)C=CCCC	InChI=1S/C6H12O2/c1-2-3-4-5-6-8-7/h4-5,7H,2-3,6H2,1H3	
C6H11-2D400H	C6H12O2	CC=CC(OO)CC	InChI=1S/C6H12O2/c1-3-5-6(4-2)8-7/h3,5H,7H,4H2,1-2H3	
C6H11-2D500H	C6H12O2	CC=CCC(OO)C	InChI=1S/C6H12O2/c1-3-4-5-6(2)8-7/h3-4,6-7H,5H2,1-2H3	
C6H11-2D600H	C6H12O2	CC=CCCC(OO)	InChI=1S/C6H12O2/c1-2-3-4-5-6-8-7/h2-3,7H,4-6H2,1H3	
C6H11-3D100H	C6H12O2	C(OO)CC=CCC	InChI=1S/C6H12O2/c1-2-3-4-5-6-8-7/h3-4,7H,2,5-6H2,1H3	
C6H11-3D200H	C6H12O2	CC(OO)C=CCC	InChI=1S/C6H12O2/c1-3-4-5-6(2)8-7/h4-7H,3H2,1-2H3	
C6H11Q12-3	C6H13O4	C(OO)C(OO)[CH]CCC	InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h4,6-8H,2-3,5H2,1H3	
C6H11Q12-4	C6H13O4	C(OO)C(OO)C[CH]CC	InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h3,6-8H,2,4-5H2,1H3	
C6H11Q12-5	C6H13O4	C(OO)C(OO)CC[CH]C	InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h2,6-8H,3-5H2,1H3	

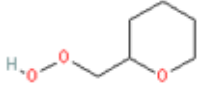
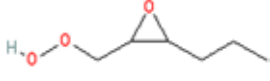
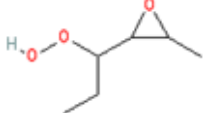
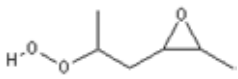
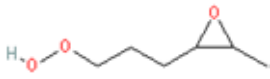
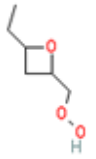
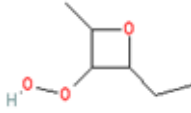
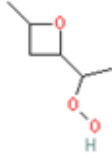
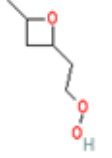
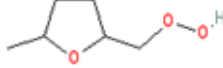
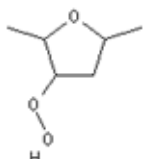
C6H11Q12-6	C6H13O4	C(OO)C(OO)CCC[CH2]	InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h6-8H,1-5H2	
C6H11Q13-2	C6H13O4	C(OO)[CH]C(OO)CCC	InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h4,6-8H,2-3,5H2,1H3	
C6H11Q13-4	C6H13O4	C(OO)CC(OO)[CH]CC	InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h3,6-8H,2,4-5H2,1H3	
C6H11Q13-5	C6H13O4	C(OO)CC(OO)C[CH]C	InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h2,6-8H,3-5H2,1H3	
C6H11Q13-6	C6H13O4	C(OO)CC(OO)CC[CH2]	InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h6-8H,1-5H2	
C6H11Q14-2	C6H13O4	C(OO)[CH]CC(OO)CC	InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h3,6-8H,2,4-5H2,1H3	
C6H11Q14-3	C6H13O4	C(OO)C[CH]C(OO)CC	InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h4,6-8H,2-3,5H2,1H3	
C6H11Q14-5	C6H13O4	C(OO)CCC(OO)[CH]C	InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h2,6-8H,3-5H2,1H3	
C6H11Q14-6	C6H13O4	C(OO)CCC(OO)C[CH2]	InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h6-8H,1-5H2	
C6H11Q15-2	C6H13O4	C(OO)[CH]CCC(OO)C	InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h3,6-8H,2,4-5H2,1H3	
C6H11Q15-3	C6H13O4	C(OO)C[CH]CC(OO)C	InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h2,6-8H,3-5H2,1H3	

C6H11Q15-4	C6H13O4	C(OO)CC[CH]C(OO)C	InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h4,6-8H,2-3,5H2,1H3	
C6H11Q15-6	C6H13O4	C(OO)CCCC(OO)[CH2]	InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h6-8H,1-5H2	
C6H11Q23-1	C6H13O4	[CH2]C(OO)C(OO)CCC	InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h5-8H,2-4H2,1H3	
C6H11Q23-4	C6H13O4	CC(OO)C(OO)[CH]CC	InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h4-8H,3H2,1-2H3	
C6H11Q23-5	C6H13O4	CC(OO)C(OO)C[CH]C	InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h3,5-8H,4H2,1-2H3	
C6H11Q23-6	C6H13O4	CC(OO)C(OO)CC[CH2]	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	C(=O)CCC(OO)CC	InChI=1S/C6H12O3/c1-2-6(9-8)4-3-5-7/h5,6,8H,2-4H2,1H3	
C6KET15	C6H12O3	C(=O)CCCC(OO)C	InChI=1S/C6H12O3/c1-6(9-8)4-2-3-5-7/h5,6,8H,2-4H2,1H3	
C6KET21	C6H12O3	C(OO)C(=O)CCCC	InChI=1S/C6H12O3/c1-2-3-4-6(7)5-9-8/h8H,2-5H2,1H3	
C6KET23	C6H12O3	CC(=O)C(OO)CCC	InChI=1S/C6H12O3/c1-3-4-6(9-8)5(2)7/h6,8H,3-4H2,1-2H3	
C6KET24	C6H12O3	CC(=O)CC(OO)CC	InChI=1S/C6H12O3/c1-3-6(9-8)4-5(2)7/h6,8H,3-4H2,1-2H3	
C6KET25	C6H12O3	CC(=O)CCC(OO)C	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	
C6KET35	C6H12O3	<chem>CCC(=O)CC(OO)C</chem>	InChI=1S/C6H12O3/c1-3-6(7)4-5(2)9-8/h5,8H,3-4H2,1-2H3	
C6KET36	C6H12O3	<chem>CCC(=O)CCC(OO)</chem>	InChI=1S/C6H12O3/c1-2-6(7)4-3-5-9-8/h8H,2-5H2,1H3	
C5H91-1	C5H9	<chem>CCCC=[CH]</chem>	InChI=1S/C5H9/c1-3-5-4-2/h1,3H,4-5H2,2H3	
C6H11O12-300H	C6H12O3	<chem>C1C(O1)C(OO)CCC</chem>	InChI=1S/C6H12O3/c1-2-3-5(9-7)6-4-8-6/h5-7H,2-4H2,1H3	
C6H11O12-400H	C6H12O3	<chem>C1C(O1)CC(OO)CC</chem>	InChI=1S/C6H12O3/c1-2-5(9-7)3-6-4-8-6/h5-7H,2-4H2,1H3	
C6H11O12-500H	C6H12O3	<chem>C1C(O1)CCC(OO)C</chem>	InChI=1S/C6H12O3/c1-5(9-7)2-3-6-4-8-6/h5-7H,2-4H2,1H3	
C6H11O12-600H	C6H12O3	<chem>C1C(O1)CCCC(OO)</chem>	InChI=1S/C6H12O3/c7-9-4-2-1-3-6-5-8-6/h6-7H,1-5H2	

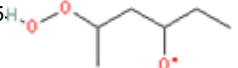
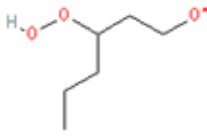
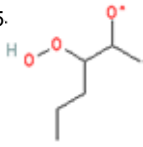
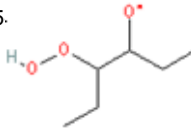
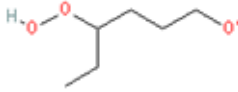

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C6H11O13-400H	C6H12O3	C1CC(O1)C(OO)CC	InChI=1S/C6H12O3/c1-2-5(9-7)6-3-4-8-6/h5-7H,2-4H2,1H3	
C6H11O13-500H	C6H12O3	C1CC(O1)CC(OO)C	InChI=1S/C6H12O3/c1-5(9-7)4-6-2-3-8-6/h5-7H,2-4H2,1H3	
C6H11O13-600H	C6H12O3	C1CC(O1)CCC(OO)	InChI=1S/C6H12O3/c7-9-4-1-2-6-3-5-8-6/h6-7H,1-5H2	
C6H11O14-200H	C6H12O3	C1C(OO)CC(O1)CC	InChI=1S/C6H12O3/c1-2-5-3-6(9-7)4-8-5/h5-7H,2-4H2,1H3	
C6H11O14-300H	C6H12O3	C1CC(OO)C(O1)CC	InChI=1S/C6H12O3/c1-2-5-6(9-7)3-4-8-5/h5-7H,2-4H2,1H3	
C6H11O14-500H	C6H12O3	C1CCC(O1)C(OO)C	InChI=1S/C6H12O3/c1-5(9-7)6-3-2-4-8-6/h5-7H,2-4H2,1H3	
C6H11O14-600H	C6H12O3	C1CCC(O1)CC(OO)	InChI=1S/C6H12O3/c7-9-5-3-6-2-1-4-8-6/h6-7H,1-5H2	
C6H11O15-200H	C6H12O3	C1C(OO)CCC(O1)C	InChI=1S/C6H12O3/c1-5-2-3-6(9-7)4-8-5/h5-7H,2-4H2,1H3	
C6H11O15-300H	C6H12O3	C1CC(OO)CC(O1)C	InChI=1S/C6H12O3/c1-5-4-6(9-7)2-3-8-5/h5-7H,2-4H2,1H3	
C6H11O15-400H	C6H12O3	C1CCC(OO)C(O1)C	InChI=1S/C6H12O3/c1-5-6(9-7)3-2-4-8-5/h5-7H,2-4H2,1H3	

C6H11015-600H	C6H12O3	C1CCCC(O1)C(OO)	InChI=1S/C6H12O3/c7-9-5-6-3-1-2-4-8-6/h6-7H,1-5H2	
C6H11023-100H	C6H12O3	C(OO)C1C(O1)CCC	InChI=1S/C6H12O3/c1-2-3-5-6(9-5)4-8-7/h5-7H,2-4H2,1H3	
C6H11023-400H	C6H12O3	CC1C(O1)C(OO)CC	InChI=1S/C6H12O3/c1-3-5(9-7)6-4(2)8-6/h4-7H,3H2,1-2H3	
C6H11023-500H	C6H12O3	CC1C(O1)CC(OO)C	InChI=1S/C6H12O3/c1-4(9-7)3-6-5(2)8-6/h4-7H,3H2,1-2H3	
C6H11023-600H	C6H12O3	CC1C(O1)CCC(OO)	InChI=1S/C6H12O3/c1-5-6(9-5)3-2-4-8-7/h5-7H,2-4H2,1H3	
C6H11024-100H	C6H12O3	C(OO)C1CC(O1)CC	InChI=1S/C6H12O3/c1-2-5-3-6(9-5)4-8-7/h5-7H,2-4H2,1H3	
C6H11024-300H	C6H12O3	CC1C(OO)C(O1)CC	InChI=1S/C6H12O3/c1-3-5-6(9-7)4(2)8-5/h4-7H,3H2,1-2H3	
C6H11024-500H	C6H12O3	CC1CC(O1)C(OO)C	InChI=1S/C6H12O3/c1-4-3-6(8-4)5(2)9-7/h4-7H,3H2,1-2H3	
C6H11024-600H	C6H12O3	CC1CC(O1)CC(OO)	InChI=1S/C6H12O3/c1-5-4-6(9-5)2-3-8-7/h5-7H,2-4H2,1H3	
C6H11025-100H	C6H12O3	C(OO)C1CCC(O1)C	InChI=1S/C6H12O3/c1-5-2-3-6(9-5)4-8-7/h5-7H,2-4H2,1H3	
C6H11025-300H	C6H12O3	CC1C(OO)CC(O1)C	InChI=1S/C6H12O3/c1-4-3-6(9-7)5(2)8-4/h4-7H,3H2,1-2H3	

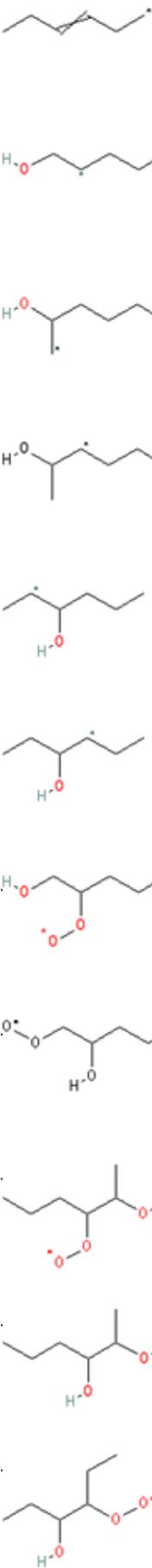

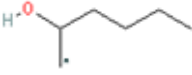
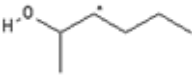
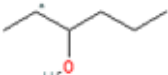
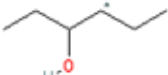
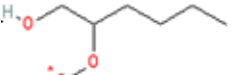
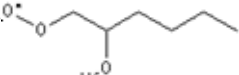
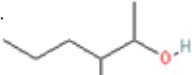
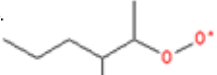
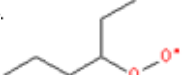
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C6H11034-200H	C6H12O3	CC(OO)C1C(O1)CC	InChI=1S/C6H12O3/c1-3-5-6(8-5)4(2)9-7/h4-7H,3H2,1-2H3	
C4H7012-4	C4H7O	C1C(O1)C[CH2]	InChI=1S/C4H7O/c1-2-4-3-5-4/h4H,1-3H2	
C4H7013-4	C4H7O	C1CC(O1)[CH2]	InChI=1S/C4H7O/c1-4-2-3-5-4/h4H,1-3H2	
C4H7023-1	C4H7O	CC1C(O1)[CH2]	InChI=1S/C4H7O/c1-3-4(2)5-3/h3-4H,1H2,2H3	
C5H9012-5	C5H9O	C1C(O1)CC[CH2]	InChI=1S/C5H9O/c1-2-3-5-4-6-5/h5H,1-4H2	
C5H9013-5	C5H9O	C1CC(O1)C[CH2]	InChI=1S/C5H9O/c1-2-5-3-4-6-5/h5H,1-4H2	
C5H9014-5	C5H9O	C1CCC(O1)[CH2]	InChI=1S/C5H9O/c1-5-3-2-4-6-5/h5H,1-4H2	
C5H9023-1	C5H9O	CCC1C(O1)[CH2]	InChI=1S/C5H9O/c1-3-5-4(2)6-5/h4-5H,2-3H2,1H3	
C5H9023-5	C5H9O	[CH2]CC1C(O1)C	InChI=1S/C5H9O/c1-3-5-4(2)6-5/h4-5H,1,3H2,2H3	
C5H9024-1	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	
C6KET120	C6H11O2	C(=O)C([O])CCCC	InChI=1S/C6H11O2/c1-2-3-4-6(8)5-7/h5-6H,2-4H2,1H3	
C6KET130	C6H11O2	C(=O)CC([O])CCC	InChI=1S/C6H11O2/c1-2-3-6(8)4-5-7/h5-6H,2-4H2,1H3	
C6KET140	C6H11O2	C(=O)CCC([O])CC	InChI=1S/C6H11O2/c1-2-6(8)4-3-5-7/h5-6H,2-4H2,1H3	
C6KET150	C6H11O2	C(=O)CCCC([O])C	InChI=1S/C6H11O2/c1-6(8)4-2-3-5-7/h5-6H,2-4H2,1H3	
C6KET210	C6H11O2	C([O])C(=O)CCCC	InChI=1S/C6H11O2/c1-2-3-4-6(8)5-7/h2-5H2,1H3	
C6KET230	C6H11O2	CC(=O)C([O])CCC	InChI=1S/C6H11O2/c1-3-4-6(8)5(2)7/h6H,3-4H2,1-2H3	
C6KET240	C6H11O2	CC(=O)CC([O])CC	InChI=1S/C6H11O2/c1-3-6(8)4-5(2)7/h6H,3-4H2,1-2H3	
C6KET250	C6H11O2	CC(=O)CCC([O])C	InChI=1S/C6H11O2/c1-5(7)3-4-6(2)8/h5H,3-4H2,1-2H3	
C6KET260	C6H11O2	CC(=O)CCCC([O])	InChI=1S/C6H11O2/c1-6(8)4-2-3-5-7/h2-5H2,1H3	

C6KET310	C6H11O2	CCCC(=O)CC([O])	InChI=1S/C6H11O2/c1-2-3-6(8)4-5-7/h2-5H2,1H3	
C6KET320	C6H11O2	CCCC(=O)C([O])C	InChI=1S/C6H11O2/c1-3-4-6(8)5(2)7/h5H,3-4H2,1-2H3	
C6KET340	C6H11O2	CCC([O])C(=O)CC	InChI=1S/C6H11O2/c1-3-5(7)6(8)4-2/h5H,3-4H2,1-2H3	
C6KET350	C6H11O2	CC([O])CC(=O)CC	InChI=1S/C6H11O2/c1-3-6(8)4-5(2)7/h5H,3-4H2,1-2H3	
C6KET360	C6H11O2	C([O])CCC(=O)CC	InChI=1S/C6H11O2/c1-2-6(8)4-3-5-7/h2-5H2,1H3	
C6H12OOH1-20	C6H13O3	C(OO)C([O])CCCC	InChI=1S/C6H13O3/c1-2-3-4-6(7)5-9-8/h6,8H,2-5H2,1H3	
C6H12OOH1-30	C6H13O3	C(OO)CC([O])CCC	InChI=1S/C6H13O3/c1-2-3-6(7)4-5-9-8/h6,8H,2-5H2,1H3	
C6H12OOH1-40	C6H13O3	C(OO)CCC([O])CC	InChI=1S/C6H13O3/c1-2-6(7)4-3-5-9-8/h6,8H,2-5H2,1H3	
C6H12OOH1-50	C6H13O3	C(OO)CCCC([O])C	InChI=1S/C6H13O3/c1-6(7)4-2-3-5-9-8/h6,8H,2-5H2,1H3	
C6H12OOH2-10	C6H13O3	C([O])C(OO)CCCC	InChI=1S/C6H13O3/c1-2-3-4-6(5-7)9-8/h6,8H,2-5H2,1H3	
C6H12OOH2-30	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	

C6H12OOH2-40	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	
C6H12OOH2-50	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	
C6H12OOH2-60	C6H13O3	CC(OO)CCCC([O])	InChI=1S/C6H13O3/c1-6(9-8)4-2-3-5-7/h6,8H,2-5H2,1H3	
C6H12OOH3-10	C6H13O3	C([O])CC(OO)CCC	InChI=1S/C6H13O3/c1-2-3-6(9-8)4-5-7/h6,8H,2-5H2,1H3	
C6H12OOH3-20	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	
C6H12OOH3-40	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	
C6H12OOH3-50	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	
C6H12OOH3-60	C6H13O3	CCC(OO)CCC([O])	InChI=1S/C6H13O3/c1-2-6(9-8)4-3-5-7/h6,8H,2-5H2,1H3	
NC5H11CHO	C6H12O	CCCCCC=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)	

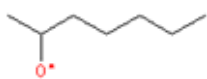
C2H5COOH	C3H6O2	CCC(=O)O	InChI=1S/C3H6O2/c1-2-3(4)5/h2H2,1H3,(H,4,5)	
C6H12-1	C6H12	C=CCCC	InChI=1S/C6H12/c1-3-5-6-4-2/h3H,1,4-6H2,2H3	
C6H12-2	C6H12	CC=CCCC	InChI=1S/C6H12/c1-3-5-6-4-2/h3,5H,4,6H2,1-2H3	
C6H12-3	C6H12	CCC=CCC	InChI=1S/C6H12/c1-3-5-6-4-2/h5-6H,3-4H2,1-2H3	
C6H111-3	C6H11	C=C[CH]CCC	InChI=1S/C6H11/c1-3-5-6-4-2/h3,5H,1,4,6H2,2H3	
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	
C6H120H-1J2	C6H13O	C(O)[CH]CCCC	InChI=1S/C6H13O/c1-2-3-4-5-6-7/h5,7H,2-4,6H2,1H3	
C6H120H-2J1	C6H13O	[CH2]C(O)CCCC	InChI=1S/C6H13O/c1-3-4-5-6(2)/h6-7H,2-5H2,1H3	
C6H120H-2J3	C6H13O	CC(O)[CH]CCC	InChI=1S/C6H13O/c1-3-4-5-6(2)/h5-7H,3-4H2,1-2H3	
C6H120H-3J2	C6H13O	C[CH]C(O)CCC	InChI=1S/C6H13O/c1-3-5-6(7)4-2/h4,6-7H,3,5H2,1-2H3	
C6H120H-3J4	C6H13O	CCC(O)[CH]CC	InChI=1S/C6H13O/c1-3-5-6(7)4-2/h5-7H,3-4H2,1-2H3	
C6H120H-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	
C6H120H-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	
C6H120H-2O2-3	C6H13O3	CC(O)C(O[O])CCC	InChI=1S/C6H13O3/c1-3-4-6(9-8)5(2)/h5-7H,3-4H2,1-2H3	
C6H120H-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	
C6H120H-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	

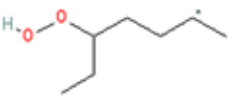
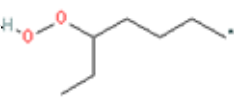
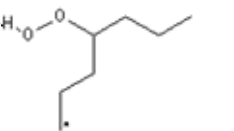
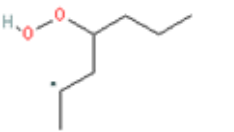
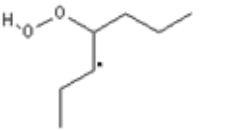
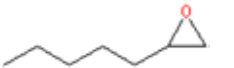

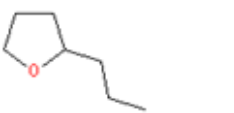
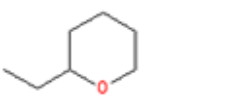
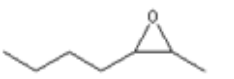
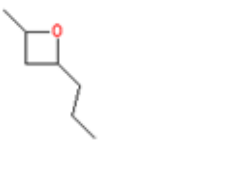
PC4H9CHO	C5H10O	CCCCC=O	InChI=1S/C5H10O/c1-2-3-4-5-6/h5H,2-4H2,1H3	
PC4H8CHO-1	C5H9O	CCC[CH]C=O	InChI=1S/C5H9O/c1-2-3-4-5-6/h4-5H,2-3H2,1H3	
PC4H8CHO-2	C5H9O	CC[CH]CC=O	InChI=1S/C5H9O/c1-2-3-4-5-6/h3,5H,2,4H2,1H3	
PC4H8CHO-3	C5H9O	C[CH]CCC=O	InChI=1S/C5H9O/c1-2-3-4-5-6/h2,5H,3-4H2,1H3	
PC4H8CHO-4	C5H9O	[CH2]CCCC=O	InChI=1S/C5H9O/c1-2-3-4-5-6/h5H,1-4H2	
C6H11-1D3O	C6H11O	C=CC([O])CCC	InChI=1S/C6H11O/c1-3-5-6(7)4-2/h4,6H,2-3,5H2,1H3	
C6H11-1D4O	C6H11O	C=CCC([O])CC	InChI=1S/C6H11O/c1-3-5-6(7)4-2/h3,6H,1,4-5H2,2H3	
C6H11-1D5O	C6H11O	C=CCCC([O])C	InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3,6H,1,4-5H2,2H3	
C6H11-1D6O	C6H11O	C=CCCCC([O])	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2H,1,3-6H2	
C6H11-2D1O	C6H11O	C([O])C=CCCC	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h4-5H,2-3,6H2,1H3	
C6H11-2D4O	C6H11O	CC=CC([O])CC	InChI=1S/C6H11O/c1-3-5-6(7)4-2/h3,5-6H,4H2,1-2H3	

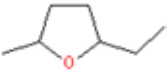
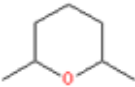


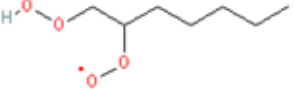
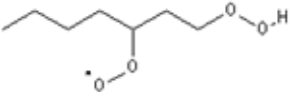
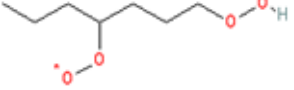
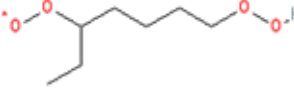
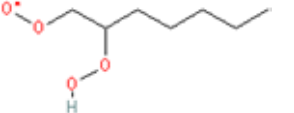
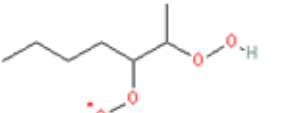
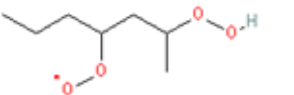
C6H11-2D5O	C6H11O	<chem>CC=CCC([O])C</chem>	InChI=1S/C6H11O/c1-3-4-5-6(2)/h3-4,6H,5H2,1-2H3	
C6H11-2D6O	C6H11O	<chem>CC=CCCC([O])</chem>	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2-3H,4-6H2,1H3	
C6H11-3D1O	C6H11O	<chem>CCC=CCC([O])</chem>	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h3-4H,2,5-6H2,1H3	
C6H11-3D2O	C6H11O	<chem>CCC=CC([O])C</chem>	InChI=1S/C6H11O/c1-3-4-5-6(2)/h4-6H,3H2,1-2H3	
NC5H11CO	C6H11O	<chem>CCCCC[C]=O</chem>	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2-5H2,1H3	
NC5H10CHO-1	C6H11O	<chem>CCCC[CH]C=O</chem>	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h5-6H,2-4H2,1H3	
NC5H10CHO-2	C6H11O	<chem>CCC[CH]CC=O</chem>	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h4,6H,2-3,5H2,1H3	
NC5H10CHO-3	C6H11O	<chem>CC[CH]CCC=O</chem>	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h3,6H,2,4-5H2,1H3	
NC5H10CHO-4	C6H11O	<chem>C[CH]CCCC=O</chem>	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2,6H,3-5H2,1H3	
NC5H10CHO-5	C6H11O	<chem>[CH2]CCCCC=O</chem>	InChI=1S/C6H11O/c1-2-3-4-5-6-7/h6H,1-5H2	
C6H10D13	C6H10	<chem>C=CC=CCC</chem>	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	
C6H101-5	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	
NC7H16	C7H16	CCCCCCC	InChI=1S/C7H16/c1-3-5-7-6-4-2/h3-7H2,1-2H3	
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	
C7H1500H-1	C7H16O2	C(OO)CCCCC	InChI=1S/C7H16O2/c1-2-3-4-5-6-7-9-8/h8H,2-7H2,1H3	
C7H1500H-2	C7H16O2	CC(OO)CCCC	InChI=1S/C7H16O2/c1-3-4-5-6-7(2)9-8/h7H,8H,3-6H2,1-2H3	
C7H1500H-3	C7H16O2	CCC(OO)CCCC	InChI=1S/C7H16O2/c1-3-5-6-7(4-2)9-8/h7H,8H,3-6H2,1-2H3	

C7H1500H-4	C7H16O2	CCCC(OO)CCC	InChI=1S/C7H16O2/c1-3-5-7(9-8)6-4-2/h7H,8H,3-6H2,1-2H3	
C7H15-102	C7H15O2	C(O[O])CCCCCC	InChI=1S/C7H15O2/c1-2-3-4-5-6-7-9-8/h2-7H2,1H3	
C7H15-202	C7H15O2	CC(O[O])CCCCC	InChI=1S/C7H15O2/c1-3-4-5-6-7(2)9-8/h7H,3-6H2,1-2H3	
C7H15-302	C7H15O2	CCC(O[O])CCCC	InChI=1S/C7H15O2/c1-3-5-6-7(4-2)9-8/h7H,3-6H2,1-2H3	
C7H15-402	C7H15O2	CCCC(O[O])CCC	InChI=1S/C7H15O2/c1-3-5-7(9-8)6-4-2/h7H,3-6H2,1-2H3	
C7H15-10	C7H15O	C([O])CCCCCC	InChI=1S/C7H15O/c1-2-3-4-5-6-7-8/h2-7H2,1H3	
C7H15-20	C7H15O	CC([O])CCCCCC	InChI=1S/C7H15O/c1-3-4-5-6-7(2)8/h7H,3-6H2,1-2H3	
C7H15-30	C7H15O	CCC([O])CCCC	InChI=1S/C7H15O/c1-3-5-6-7(8)4-2/h7H,3-6H2,1-2H3	
C7H15-40	C7H15O	CCCC([O])CCC	InChI=1S/C7H15O/c1-3-5-7(8)6-4-2/h7H,3-6H2,1-2H3	
C7H1400H1-2	C7H15O2	C(OO)[CH]CCCCC	InChI=1S/C7H15O2/c1-2-3-4-5-6-7-9-8/h6,8H,2-5,7H2,1H3	
C7H1400H1-3	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	

C7H1400H1-4	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	
C7H1400H1-5	C7H15O2	C(OO)CCC[CH]CC	InChI=1S/C7H15O2/c1-2-3-4-5-6-7-9-8/h3,8H,2,4-7H2,1H3	
C7H1400H2-1	C7H15O2	[CH2]C(OO)CCCC	InChI=1S/C7H15O2/c1-3-4-5-6-7(2)9-8/h7H,8H,2-6H2,1H3	
C7H1400H2-3	C7H15O2	CC(OO)[CH]CCCC	InChI=1S/C7H15O2/c1-3-4-5-6-7(2)9-8/h6H,8H,3-5H2,1-2H3	
C7H1400H2-4	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	
C7H1400H2-5	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	
C7H1400H2-6	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	
C7H1400H3-1	C7H15O2	[CH2]CC(OO)CCCC	InChI=1S/C7H15O2/c1-3-5-6-7(4-2)9-8/h7H,8H,2-6H2,1H3	
C7H1400H3-2	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	
C7H1400H3-4	C7H15O2	CCC(OO)[CH]CCC	InChI=1S/C7H15O2/c1-3-5-6-7(4-2)9-8/h6H,8H,3-5H2,1-2H3	
C7H1400H3-5	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	

C7H1400H3-6	C7H15O2	CCC(OO)CC[CH]C	InChI=1S/C7H15O2/c1-3-5-6-7(4-2)9-8/h3,7-8H,4-6H2,1-2H3	
C7H1400H3-7	C7H15O2	CCC(OO)CCC[CH2]	InChI=1S/C7H15O2/c1-3-5-6-7(4-2)9-8/h7H,8H,1,3-6H2,2H3	
C7H1400H4-1	C7H15O2	CCCC(OO)CC[CH2]	InChI=1S/C7H15O2/c1-3-5-7(9-8)6-4-2/h7H,8H,1,3-6H2,2H3	
C7H1400H4-2	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	
C7H1400H4-3	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	
C7H1401-2	C7H14O	C1C(O1)CCCCC	InChI=1S/C7H14O/c1-2-3-4-5-7-6-8-7/h7H,2-6H2,1H3	
C7H1401-3	C7H14O	C1CC(O1)CCCC	InChI=1S/C7H14O/c1-2-3-4-7-5-6-8-7/h7H,2-6H2,1H3	
C7H1401-4	C7H14O	C1CCC(O1)CCC	InChI=1S/C7H14O/c1-2-4-7-5-3-6-8-7/h7H,2-6H2,1H3	
C7H1401-5	C7H14O	C1CCCC(O1)CC	InChI=1S/C7H14O/c1-2-7-5-3-4-6-8-7/h7H,2-6H2,1H3	
C7H1402-3	C7H14O	CC1C(O1)CCCC	InChI=1S/C7H14O/c1-3-4-5-7-6(2)8-7/h6-7H,3-5H2,1-2H3	
C7H1402-4	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	
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C7H14O3-5	C7H14O	CCC1CC(O1)CC	InChI=1S/C7H14O/c1-3-6-5-7(4-2)8-6/h6-7H,3-5H2,1-2H3	
C7H14OOH1-202	C7H15O4	C(OO)C(O[O])CCCC	InChI=1S/C7H15O4/c1-2-3-4-5-7(11-9)6-10-8/h7-8H,2-6H2,1H3	
C7H14OOH1-302	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	
C7H14OOH1-402	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	
C7H14OOH1-502	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	
C7H14OOH2-102	C7H15O4	C(O[O])C(OO)CCCC	InChI=1S/C7H15O4/c1-2-3-4-5-7(11-9)6-10-8/h7,9H,2-6H2,1H3	
C7H14OOH2-302	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	
C7H14OOH2-402	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	

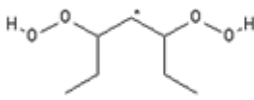
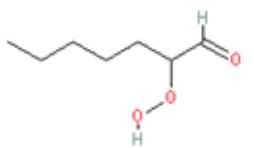
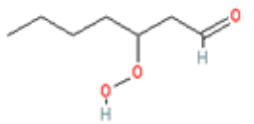
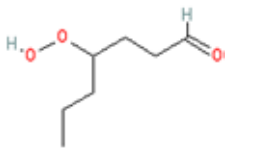
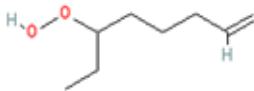
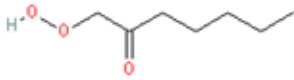
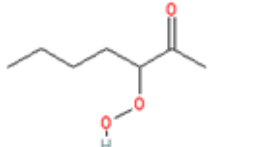
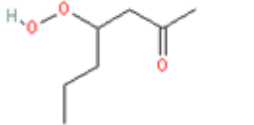
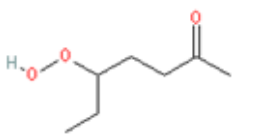
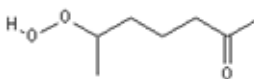
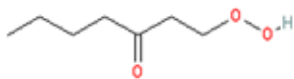
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C7H1400H2-602	C7H15O4	CC(OO)CCCC(O[O])C	InChI=1S/C7H15O4/c1-6(10-8)4-3-5-7(2)11-9/h6-8H,3-5H2,1-2H3	
C7H1400H3-102	C7H15O4	C(O[O])CC(OO)CCCC	InChI=1S/C7H15O4/c1-2-3-4-7(11-9)5-6-10-8/h7,9H,2-6H2,1H3	
C7H1400H3-202	C7H15O4	CC(O[O])C(OO)CCCC	InChI=1S/C7H15O4/c1-3-4-5-7(11-9)6(2)10-8/h6-7,9H,3-5H2,1-2H3	
C7H1400H3-402	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	
C7H1400H3-502	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	
C7H1400H3-602	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	
C7H1400H3-702	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	
C7H1400H4-102	C7H15O4	CCCC(OO)CCC(O[O])	InChI=1S/C7H15O4/c1-2-4-7(11-9)5-3-6-10-8/h7,9H,2-6H2,1H3	
C7H1400H4-202	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	
C7H1400H4-302	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	

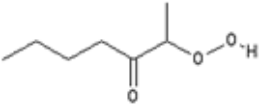
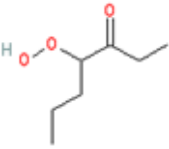
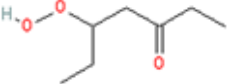
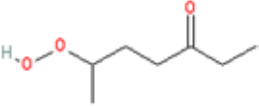
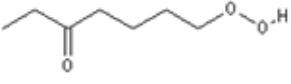
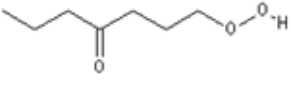
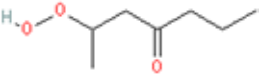
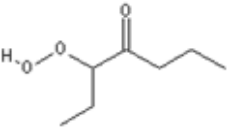
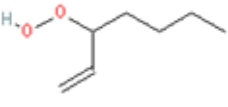
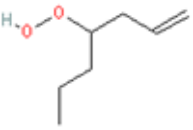
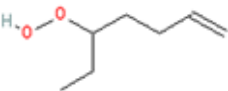
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C7H13Q12-4	C7H15O4	C(OO)C(OO)C[CH]CCC	InChI=1S/C7H15O4/c1-2-3-4-5-7(11-9)6-10-8/h4,7-9H,2-3,5-6H2,1H3	
C7H13Q12-5	C7H15O4	C(OO)C(OO)CC[CH]CC	InChI=1S/C7H15O4/c1-2-3-4-5-7(11-9)6-10-8/h3,7-9H,2,4-6H2,1H3	
C7H13Q12-6	C7H15O4	C(OO)C(OO)CCC[CH]C	InChI=1S/C7H15O4/c1-2-3-4-5-7(11-9)6-10-8/h2,7-9H,3-6H2,1H3	
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	
C7H13Q15-6	C7H15O4	C(OO)CCCC(OO)[CH]C	InChI=1S/C7H15O4/c1-2-7(11-9)5-3-4-6-10-8/h2,7-9H,3-6H2,1H3	
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	
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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	

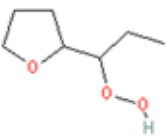
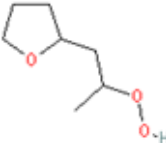
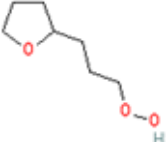
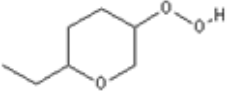
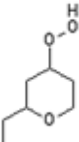
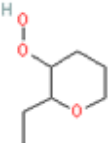
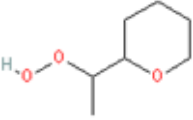
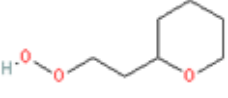

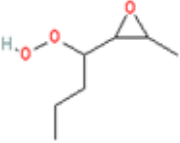
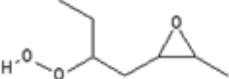
C7H13Q25-7	C7H15O4	<chem>CC(OO)CCC(OO)C[CH2]</chem>	InChI=1S/C7H15O4/c1-3-7(11-9)5-4-6(2)10-8/h6-9H,1,3-5H2,2H3	
C7H13Q26-1	C7H15O4	<chem>CC(OO)CCCC(OO)[CH2]</chem>	InChI=1S/C7H15O4/c1-6(10-8)4-3-5-7(2)11-9/h6-9H,1,3-5H2,2H3	
C7H13Q26-3	C7H15O4	<chem>CC(OO)CC[CH]C(OO)C</chem>	InChI=1S/C7H15O4/c1-6(10-8)4-3-5-7(2)11-9/h4,6-9H,3,5H2,1-2H3	
C7H13Q26-4	C7H15O4	<chem>CC(OO)C[CH]CC(OO)C</chem>	InChI=1S/C7H15O4/c1-6(10-8)4-3-5-7(2)11-9/h3,6-9H,4-5H2,1-2H3	
C7H13Q34-1	C7H15O4	<chem>[CH2]CC(OO)C(OO)CCC</chem>	InChI=1S/C7H15O4/c1-3-5-7(11-9)6(4-2)10-8/h6-9H,2-5H2,1H3	
C7H13Q34-2	C7H15O4	<chem>C[CH]C(OO)C(OO)CCC</chem>	InChI=1S/C7H15O4/c1-3-5-7(11-9)6(4-2)10-8/h4,6-9H,3,5H2,1-2H3	
C7H13Q34-5	C7H15O4	<chem>CCC(OO)C(OO)[CH]CC</chem>	InChI=1S/C7H15O4/c1-3-5-7(11-9)6(4-2)10-8/h5-9H,3-4H2,1-2H3	
C7H13Q34-6	C7H15O4	<chem>CCC(OO)C(OO)C[CH]C</chem>	InChI=1S/C7H15O4/c1-3-5-7(11-9)6(4-2)10-8/h3,6-9H,4-5H2,1-2H3	
C7H13Q34-7	C7H15O4	<chem>CCC(OO)C(OO)CC[CH2]</chem>	InChI=1S/C7H15O4/c1-3-5-7(11-9)6(4-2)10-8/h6-9H,1,3-5H2,2H3	
C7H13Q35-1	C7H15O4	<chem>CCC(OO)CC(OO)C[CH2]</chem>	InChI=1S/C7H15O4/c1-3-6(10-8)5-7(4-2)11-9/h6-9H,1,3-5H2,2H3	
C7H13Q35-2	C7H15O4	<chem>CCC(OO)CC(OO)[CH]C</chem>	InChI=1S/C7H15O4/c1-3-6(10-8)5-7(4-2)11-9/h3,6-9H,4-5H2,1-2H3	

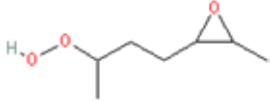
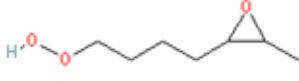
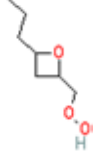
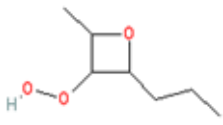
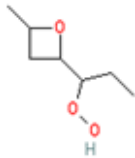
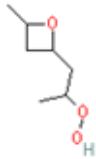

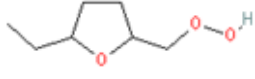
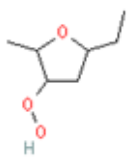
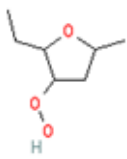
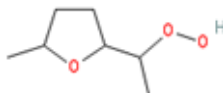
C7H13Q35-4	C7H15O4	CCC(OO)[CH]C(OO)CC	InChI=1S/C7H15O4/c1-3-6(10-8)5-7(4-2)11-9/h5-9H,3-4H2,1-2H3	
C7KET12	C7H14O3	C(=O)C(OO)CCCC	InChI=1S/C7H14O3/c1-2-3-4-5-7(6-8)10-9/h6-7,9H,2-5H2,1H3	
C7KET13	C7H14O3	C(=O)CC(OO)CCCC	InChI=1S/C7H14O3/c1-2-3-4-7(10-9)5-6-8/h6-7,9H,2-5H2,1H3	
C7KET14	C7H14O3	C(=O)CCC(OO)CCC	InChI=1S/C7H14O3/c1-2-4-7(10-9)5-3-6-8/h6-7,9H,2-5H2,1H3	
C7KET15	C7H14O3	C(=O)CCCC(OO)CC	InChI=1S/C7H14O3/c1-2-7(10-9)5-3-4-6-8/h6-7,9H,2-5H2,1H3	
C7KET21	C7H14O3	C(OO)C(=O)CCCCC	InChI=1S/C7H14O3/c1-2-3-4-5-7(8)6-10-9/h9H,2-6H2,1H3	
C7KET23	C7H14O3	CC(=O)C(OO)CCCC	InChI=1S/C7H14O3/c1-3-4-5-7(10-9)6(2)8/h7,9H,3-5H2,1-2H3	
C7KET24	C7H14O3	CC(=O)CC(OO)CCC	InChI=1S/C7H14O3/c1-3-4-7(10-9)5-6(2)8/h7,9H,3-5H2,1-2H3	
C7KET25	C7H14O3	CC(=O)CCC(OO)CC	InChI=1S/C7H14O3/c1-3-7(10-9)5-4-6(2)8/h7,9H,3-5H2,1-2H3	
C7KET26	C7H14O3	CC(=O)CCCC(OO)C	InChI=1S/C7H14O3/c1-6(8)4-3-5-7(2)10-9/h7,9H,3-5H2,1-2H3	
C7KET31	C7H14O3	C(OO)CC(=O)CCCC	InChI=1S/C7H14O3/c1-2-3-4-7(8)5-6-10-9/h9H,2-6H2,1H3	

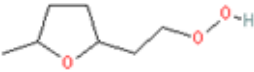
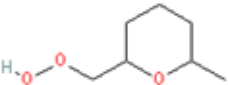
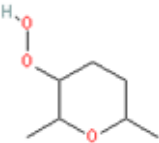
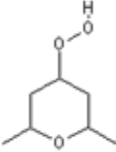
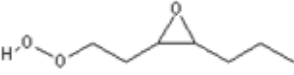
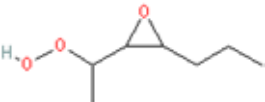
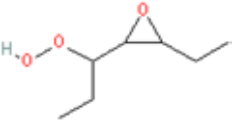
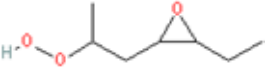
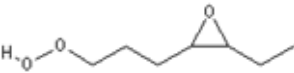
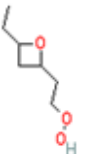
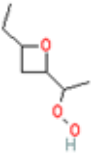
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C7KET34	C7H14O3	<chem>CCC(=O)C(OO)CCC</chem>	InChI=1S/C7H14O3/c1-3-5-7(10-9)6(8)4-2/h7,9H,3-5H2,1-2H3	
C7KET35	C7H14O3	<chem>CCC(=O)CC(OO)CC</chem>	InChI=1S/C7H14O3/c1-3-6(8)5-7(4-2)10-9/h7,9H,3-5H2,1-2H3	
C7KET36	C7H14O3	<chem>CCC(=O)CCC(OO)C</chem>	InChI=1S/C7H14O3/c1-3-7(8)5-4-6(2)10-9/h6,9H,3-5H2,1-2H3	
C7KET37	C7H14O3	<chem>CCC(=O)CCCC(OO)</chem>	InChI=1S/C7H14O3/c1-2-7(8)5-3-4-6-10-9/h9H,2-6H2,1H3	
C7KET41	C7H14O3	<chem>C(OO)CCC(=O)CCC</chem>	InChI=1S/C7H14O3/c1-2-4-7(8)5-3-6-10-9/h9H,2-6H2,1H3	
C7KET42	C7H14O3	<chem>CC(OO)CC(=O)CCC</chem>	InChI=1S/C7H14O3/c1-3-4-7(8)5-6(2)10-9/h6,9H,3-5H2,1-2H3	
C7KET43	C7H14O3	<chem>CCC(OO)C(=O)CCC</chem>	InChI=1S/C7H14O3/c1-3-5-6(8)7(4-2)10-9/h7,9H,3-5H2,1-2H3	
C7H13-1D300H	C7H14O2	<chem>C=CC(OO)CCCC</chem>	InChI=1S/C7H14O2/c1-3-5-6-7(4-2)9-8/h4,7-8H,2-3,5-6H2,1H3	
C7H13-1D400H	C7H14O2	<chem>C=CCC(OO)CCC</chem>	InChI=1S/C7H14O2/c1-3-5-7(9-8)6-4-2/h3,7-8H,1,4-6H2,2H3	
C7H13-1D500H	C7H14O2	<chem>C=CCCC(OO)CC</chem>	InChI=1S/C7H14O2/c1-3-5-6-7(4-2)9-8/h3,7-8H,1,4-6H2,2H3	

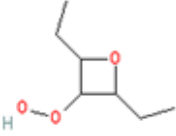
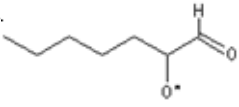
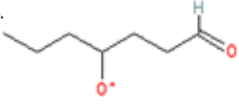
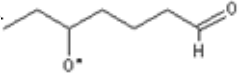
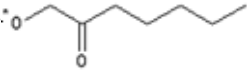
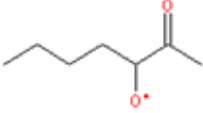
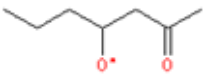
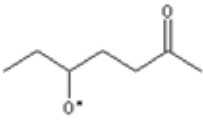
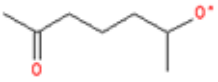
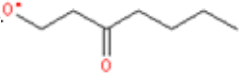
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C7H13-2D100H	C7H14O2	C(OO)C=CCCC	InChI=1S/C7H14O2/c1-2-3-4-5-6-7-9-8/h5-6,8H,2-4,7H2,1H3	
C7H13-2D400H	C7H14O2	CC=CC(OO)CCC	InChI=1S/C7H14O2/c1-3-5-7(9-8)6-4-2/h3,5,7-8H,4,6H2,1-2H3	
C7H13-2D500H	C7H14O2	CC=CCC(OO)CC	InChI=1S/C7H14O2/c1-3-5-6-7(4-2)9-8/h3,5,7-8H,4,6H2,1-2H3	
C7H13-2D600H	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	
C7H13-2D700H	C7H14O2	CC=CCCCC(OO)	InChI=1S/C7H14O2/c1-2-3-4-5-6-7-9-8/h2-3,8H,4-7H2,1H3	
C7H13-3D100H	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	
C7H13-3D200H	C7H14O2	CC(OO)C=CCCC	InChI=1S/C7H14O2/c1-3-4-5-6-7(2)9-8/h5-8H,3-4H2,1-2H3	
C7H13-3D500H	C7H14O2	CCC=CC(OO)CC	InChI=1S/C7H14O2/c1-3-5-6-7(4-2)9-8/h5-8H,3-4H2,1-2H3	
C7H13-3D600H	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	
C7H13-3D700H	C7H14O2	CCC=CCCC(OO)	InChI=1S/C7H14O2/c1-2-3-4-5-6-7-9-8/h3-4,8H,2,5-7H2,1H3	

C7H13O12-300H	C7H14O3	C1C(O1)C(OO)CCCC	InChI=1S/C7H14O3/c1-2-3-4-6(10-8)7-5-9-7/h6-8H,2-5H2,1H3	
C7H13O12-400H	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	
C7H13O12-500H	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	
C7H13O12-600H	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	
C7H13O13-200H	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	
C7H13O13-400H	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	
C7H13O13-500H	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	
C7H13O13-600H	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	
C7H13O13-700H	C7H14O3	C1CC(O1)CCCC(OO)	InChI=1S/C7H14O3/c8-10-5-2-1-3-7-4-6-9-7/h7-8H,1-6H2	
C7H13O14-200H	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	
C7H13O14-300H	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	

C7H13O14-500H	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	
C7H13O14-600H	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	
C7H13O14-700H	C7H14O3	C1CCC(O1)CCC(OO)	InChI=1S/C7H14O3/c8-10-6-2-4-7-3-1-5-9-7/h7-8H,1-6H2	
C7H13O15-200H	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	
C7H13O15-300H	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	
C7H13O15-400H	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	
C7H13O15-600H	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	
C7H13O15-700H	C7H14O3	C1CCCC(O1)CC(OO)	InChI=1S/C7H14O3/c8-10-6-4-7-3-1-2-5-9-7/h7-8H,1-6H2	
C7H13O23-100H	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	
C7H13O23-400H	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	
C7H13O23-500H	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	

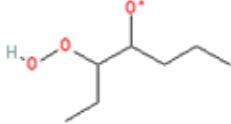
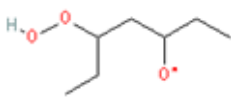
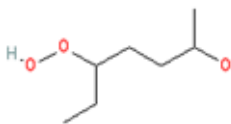
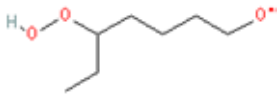
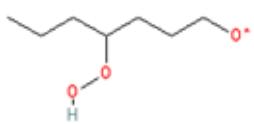
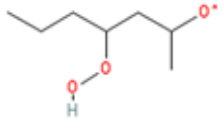
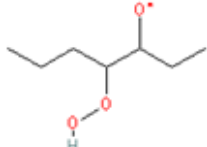

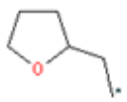
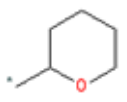
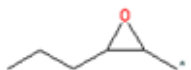
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C7H13023-700H	C7H14O3	CC1C(O1)CCCC(OO)	InChI=1S/C7H14O3/c1-6-7(10-6)4-2-3-5-9-8/h6-8H,2-5H2,1H3	
C7H13024-100H	C7H14O3	C(OO)C1CC(O1)CCC	InChI=1S/C7H14O3/c1-2-3-6-4-7(10-6)5-9-8/h6-8H,2-5H2,1H3	
C7H13024-300H	C7H14O3	CC1C(OO)C(O1)CCC	InChI=1S/C7H14O3/c1-3-4-6-7(10-8)5(2)9-6/h5-8H,3-4H2,1-2H3	
C7H13024-500H	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	
C7H13024-600H	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	
C7H13024-700H	C7H14O3	CC1CC(O1)CCC(OO)	InChI=1S/C7H14O3/c1-6-5-7(10-6)3-2-4-9-8/h6-8H,2-5H2,1H3	
C7H13025-100H	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	
C7H13025-300H	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	
C7H13025-400H	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	
C7H13025-600H	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	


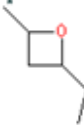
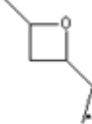

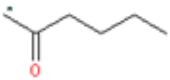
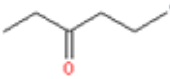
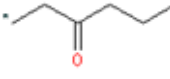




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C7H13026-100H	C7H14O3	C(OO)C1CCCC(O1)C	InChI=1S/C7H14O3/c1-6-3-2-4-7(10-6)5-9-8/h6-8H,2-5H2,1H3	
C7H13026-300H	C7H14O3	CC1C(OO)CCC(O1)C	InChI=1S/C7H14O3/c1-5-3-4-7(10-8)6(2)9-5/h5-8H,3-4H2,1-2H3	
C7H13026-400H	C7H14O3	CC1CC(OO)CC(O1)C	InChI=1S/C7H14O3/c1-5-3-7(10-8)4-6(2)9-5/h5-8H,3-4H2,1-2H3	
C7H13034-100H	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	
C7H13034-200H	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	
C7H13034-500H	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	
C7H13034-600H	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	
C7H13034-700H	C7H14O3	CCC1C(O1)CCC(OO)	InChI=1S/C7H14O3/c1-2-6-7(10-6)4-3-5-9-8/h6-8H,2-5H2,1H3	
C7H13035-100H	C7H14O3	CCC1CC(O1)CC(OO)	InChI=1S/C7H14O3/c1-2-6-5-7(10-6)3-4-9-8/h6-8H,2-5H2,1H3	
C7H13035-200H	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	

C7H13O35-400H	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	
C7KET230	C7H13O2	CC(=O)C([O])CCCC	InChI=1S/C7H13O2/c1-3-4-5-7(9)6(2)8/h7H,3-5H2,1-2H3	
C7KET240	C7H13O2	CC(=O)CC([O])CCC	InChI=1S/C7H13O2/c1-3-4-7(9)5-6(2)8/h7H,3-5H2,1-2H3	
C7KET250	C7H13O2	CC(=O)CCC([O])CC	InChI=1S/C7H13O2/c1-3-7(9)5-4-6(2)8/h7H,3-5H2,1-2H3	
C7KET260	C7H13O2	CC(=O)CCCC([O])C	InChI=1S/C7H13O2/c1-6(8)4-3-5-7(2)9/h6H,3-5H2,1-2H3	
C7KET310	C7H13O2	C([O])CC(=O)CCCC	InChI=1S/C7H13O2/c1-2-3-4-7(9)5-6-8/h2,6H2,1H3	

C7KET320	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	
C7KET340	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	
C7KET350	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	
C7KET360	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	
C7KET370	C7H13O2	<chem>CCC(=O)CCCC([O])</chem>	InChI=1S/C7H13O2/c1-2-7(9)5-3-4-6-8/h2-6H2,1H3	
C7KET410	C7H13O2	<chem>CCCC(=O)CCC([O])</chem>	InChI=1S/C7H13O2/c1-2-4-7(9)5-3-6-8/h2-6H2,1H3	
C7KET420	C7H13O2	<chem>CCCC(=O)CC([O])C</chem>	InChI=1S/C7H13O2/c1-3-4-7(9)5-6(2)8/h6H,3-5H2,1-2H3	
C7KET430	C7H13O2	<chem>CCCC(=O)C([O])CC</chem>	InChI=1S/C7H13O2/c1-3-5-7(9)6(8)4-2/h6H,3-5H2,1-2H3	
C7Y24	C7H12O2	<chem>CC(=O)CC(=O)CCC</chem>	InChI=1S/C7H12O2/c1-3-4-7(9)5-6(2)8/h3-5H2,1-2H3	
C7Y13	C7H12O2	<chem>C(=O)CC(=O)CCCC</chem>	InChI=1S/C7H12O2/c1-2-3-4-7(9)5-6-8/h6H,2-5H2,1H3	
C7Y35	C7H12O2	<chem>CCC(=O)CC(=O)CC</chem>	InChI=1S/C7H12O2/c1-3-6(8)5-7(9)4-2/h3-5H2,1-2H3	

C7H1400H1-20	C7H15O3	C(OO)C([O])CCCC	InChI=1S/C7H15O3/c1-2-3-4-5-7(8)6-10-9/h7,9H,2-6H2,1H3	
C7H1400H1-30	C7H15O3	C(OO)CC([O])CCCC	InChI=1S/C7H15O3/c1-2-3-4-7(8)5-6-10-9/h7,9H,2-6H2,1H3	
C7H1400H1-40	C7H15O3	C(OO)CCC([O])CCC	InChI=1S/C7H15O3/c1-2-4-7(8)5-3-6-10-9/h7,9H,2-6H2,1H3	
C7H1400H1-50	C7H15O3	C(OO)CCCC([O])CC	InChI=1S/C7H15O3/c1-2-7(8)5-3-4-6-10-9/h7,9H,2-6H2,1H3	
C7H1400H2-10	C7H15O3	C([O])C(OO)CCCC	InChI=1S/C7H15O3/c1-2-3-4-5-7(6-8)10-9/h7,9H,2-6H2,1H3	
C7H1400H2-30	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	
C7H1400H2-40	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	
C7H1400H2-50	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	
C7H1400H2-60	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	
C7H1400H3-10	C7H15O3	C([O])CC(OO)CCCC	InChI=1S/C7H15O3/c1-2-3-4-7(10-9)5-6-8/h7,9H,2-6H2,1H3	
C7H1400H3-20	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	

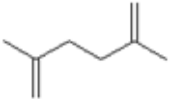
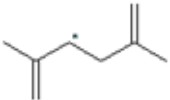
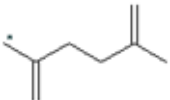
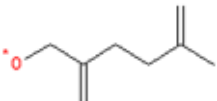
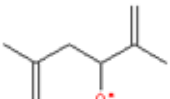
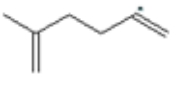
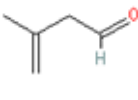
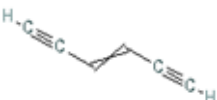
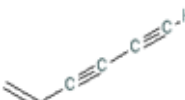
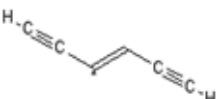
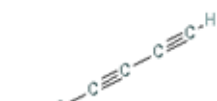
C7H1400H3-40	C7H15O3	CCC(OO)C([O])CCC	InChI=1S/C7H15O3/c1-3-5-6(8)7(4-2)10-9/h6-7,9H,3-5H2,1-2H3	
C7H1400H3-50	C7H15O3	CCC(OO)CC([O])CC	InChI=1S/C7H15O3/c1-3-6(8)5-7(4-2)10-9/h6-7,9H,3-5H2,1-2H3	
C7H1400H3-60	C7H15O3	CCC(OO)CCC([O])C	InChI=1S/C7H15O3/c1-3-7(10-9)5-4-6(2)8/h6-7,9H,3-5H2,1-2H3	
C7H1400H3-70	C7H15O3	CCC(OO)CCCC([O])	InChI=1S/C7H15O3/c1-2-7(10-9)5-3-4-6-8/h7,9H,2-6H2,1H3	
C7H1400H4-10	C7H15O3	CCCC(OO)CCC([O])	InChI=1S/C7H15O3/c1-2-4-7(10-9)5-3-6-8/h7,9H,2-6H2,1H3	
C7H1400H4-20	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	
C7H1400H4-30	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	
C6H11013-6	C6H11O	C1CC(O1)CC[CH2]	InChI=1S/C6H11O/c1-2-3-6-4-5-7-6/h6H,1-5H2	
C6H11014-6	C6H11O	C1CCC(O1)C[CH2]	InChI=1S/C6H11O/c1-2-6-4-3-5-7-6/h6H,1-5H2	
C6H11015-6	C6H11O	C1CCCC(O1)[CH2]	InChI=1S/C6H11O/c1-6-4-2-3-5-7-6/h6H,1-5H2	
C6H11023-1	C6H11O	[CH2]C1C(O1)CCC	InChI=1S/C6H11O/c1-3-4-6-5(2)7-6/h5-6H,2-4H2,1H3	


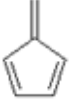

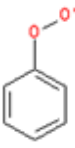
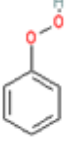
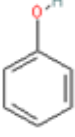
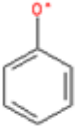
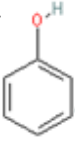
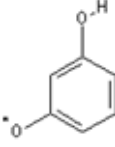
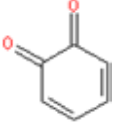
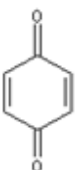
C6H11023-6	C6H11O	CC1C(O1)CC[CH2]	InChI=1S/C6H11O/c1-3-4-6-5(2)7-6/h5-6H,1,3-4H2,2H3	
C6H11024-1	C6H11O	[CH2]C1CC(O1)CC	InChI=1S/C6H11O/c1-3-6-4-5(2)7-6/h5-6H,2-4H2,1H3	
C6H11024-6	C6H11O	CC1CC(O1)C[CH2]	InChI=1S/C6H11O/c1-3-6-4-5(2)7-6/h5-6H,1,3-4H2,2H3	
C6H11034-1	C6H11O	CCC1C(O1)C[CH2]	InChI=1S/C6H11O/c1-3-5-6(4-2)7-5/h5-6H,1,3-4H2,2H3	
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=CCCCCC	InChI=1S/C7H14/c1-3-5-7-6-4-2/h3H,1,4-7H2,2H3	
C7H14-2	C7H14	CC=CCCCC	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	

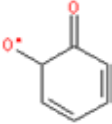
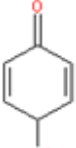
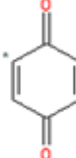



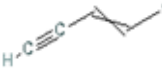




C7H131-4	C7H13	<chem>C=CC[CH]CCC</chem>	InChI=1S/C7H13/c1-3-5-7-6-4-2/h3,7H,1,4-6H2,2H3	
C7H131-5	C7H13	<chem>C=CCC[CH]CC</chem>	InChI=1S/C7H13/c1-3-5-7-6-4-2/h3,6H,1,4-5,7H2,2H3	
C7H131-6	C7H13	<chem>C=CCCC[CH]C</chem>	InChI=1S/C7H13/c1-3-5-7-6-4-2/h3-4H,1,5-7H2,2H3	
C7H131-7	C7H13	<chem>C=CCCCC[CH2]</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-2I1	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-3I4	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	

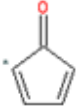


C7H14OH-2O2-1	C7H15O3	<chem>C(O[O])C(O)CCCC</chem>	InChI=1S/C7H15O3/c1-2-3-4-5-7(8)6-10-9/h7-8H,2-6H2,1H3	
C7H14OH-2O2-3	C7H15O3	<chem>CC(O)C(O[O])CCCC</chem>	InChI=1S/C7H15O3/c1-3-4-5-7(10-9)6(2)8/h6-8H,3-5H2,1-2H3	
C7H14OH-3O2-2	C7H15O3	<chem>CC(O[O])C(O)CCCC</chem>	InChI=1S/C7H15O3/c1-3-4-5-7(8)6(2)10-9/h6-8H,3-5H2,1-2H3	
C7H14OH-3O2-4	C7H15O3	<chem>CCC(O)C(O[O])CCC</chem>	InChI=1S/C7H15O3/c1-3-5-7(10-9)6(8)4-2/h6-8H,3-5H2,1-2H3	
C7H14OH-4O2-3	C7H15O3	<chem>CCC(O[O])C(O)CCC</chem>	InChI=1S/C7H15O3/c1-3-5-6(8)7(4-2)10-9/h6-8H,3-5H2,1-2H3	
C5D2Y1	C5H8O	<chem>CCC=CC=O</chem>	InChI=1S/C5H8O/c1-2-3-4-5-6/h3-5H,2H2,1H3	
C5D2Y1-1R	C5H7O	<chem>CCC=C[C]=O</chem>	InChI=1S/C5H7O/c1-2-3-4-5-6/h3-4H,2H2,1H3	
C3Y1-3OR	C3H5O2	<chem>C([O])CC=O</chem>	InChI=1S/C3H5O2/c4-2-1-3-5/h2H,1,3H2	
C4Y1-3OR	C4H7O2	<chem>CC([O])CC=O</chem>	InChI=1S/C4H7O2/c1-4(6)2-3-5/h3-4H,2H2,1H3	
C6D2Y1	C6H10O	<chem>CCCC=CC(=O)</chem>	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h4-6H,2-3H2,1H3	
C6D2Y1-1R	C6H9O	<chem>CCCC=C[C](=O)</chem>	InChI=1S/C6H9O/c1-2-3-4-5-6-7/h4-5H,2-3H2,1H3	

H15DE25DM	C8H14	<chem>C=C(C)CCC(=C)C</chem>	InChI=1S/C8H14/c1-7(2)5-6-8(3)4/h1,3,5-6H2,2,4H3	
H15DE25DM-S	C8H13	<chem>C=C(C)[CH]CC(=C)C</chem>	InChI=1S/C8H13/c1-7(2)5-6-8(3)4/h5H,1,3,6H2,2,4H3	
H15DE25DM-A	C8H13	<chem>C=C([CH2])CCC(=C)C</chem>	InChI=1S/C8H13/c1-7(2)5-6-8(3)4/h1-3,5-6H2,4H3	
H15DE25DM-AO	C8H13O	<chem>C=C(C)CCC(=C)C[O]</chem>	InChI=1S/C8H13O/c1-7(2)4-5-8(3)6-9/h1,3-6H2,2H3	
H15DE25DM-SO	C8H13O	<chem>C=C(C)CC(C(=C)C)[O]</chem>	InChI=1S/C8H13O/c1-6(2)5-8(9)7(3)4/h8H,1,3,5H2,2,4H3	
H15DE2M-T	C7H11	<chem>C=[C]CCC(=C)C</chem>	InChI=1S/C7H11/c1-4-5-6-7(2)3/h1-2,5-6H2,3H3	
IC4H7CHO	C5H8O	<chem>C=C(C)CC=O</chem>	InChI=1S/C5H8O/c1-5(2)3-4-6/h4H,1,3H2,2H3	
L-C6H4	C6H4	<chem>C#CC=CC#C</chem>	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	C1=CC=CC=C1	InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H	
FULVENE	C6H6	C=C1C=CC=C1	InChI=1S/C6H6/c1-6-4-2-3-5-6/h2-5H,1H2	
C6H5	C6H5	C1=[C]C=CC=C1	InChI=1S/C6H5/c1-2-4-6-5-3-1/h1-5H	
C6H5OO	C6H5O2	C1=C(O[O])C=CC=C1	InChI=1S/C6H5O2/c7-8-6-4-2-1-3-5-6/h1-5H	
C6H5OOH	C6H6O2	C1=C(OO)C=CC=C1	InChI=1S/C6H6O2/c7-8-6-4-2-1-3-5-6/h1-5,7H	
C6H5OH	C6H6O	C1(O)=CC=CC=C1	InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H	
C6H5O	C6H5O	C1([O])=CC=CC=C1	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	<chem>C1(=O)C([O])C=CC=C1</chem>	InChI=1S/C6H5O2/c7-5-3-1-2-4-6(5)8/h1-5H	
P-OC6H5OJ	C6H5O2	<chem>C1(=O)C=CC([O])C=C1</chem>	InChI=1S/C6H5O2/c7-5-1-2-6(8)4-3-5/h1-5H	
P-C6H3O2	C6H3O2	<chem>C1(=O)[C]=CC(=O)C=C1</chem>	InChI=1S/C6H3O2/c7-5-1-2-6(8)4-3-5/h1-3H	
C5H6	C5H6	<chem>C1C=CC=C1</chem>	InChI=1S/C5H6/c1-2-4-5-3-1/h1-4H,5H2	
C5H5	C5H5	<chem>[CH]1C=CC=C1</chem>	InChI=1S/C5H5/c1-2-4-5-3-1/h1-5H	
C5H6-L	C5H6	<chem>C#CC=CC</chem>	InChI=1S/C5H6/c1-3-5-4-2/h1,4-5H,2H3	
C#CCVCCJ	C5H5	<chem>C#CC=C[CH2]</chem>	InChI=1S/C5H5/c1-3-5-4-2/h1,4-5H,2H2	
C5H7	C5H7	<chem>C1C[CH]C=C1</chem>	InChI=1S/C5H7/c1-2-4-5-3-1/h1-3H,4-5H2	
CVCCJCVC	C5H7	<chem>C=C[CH]C=C</chem>	InChI=1S/C5H7/c1-3-5-4-2/h3-5H,1-2H2	
CVCCVCCJ	C5H7	<chem>C=CC=C[CH2]</chem>	InChI=1S/C5H7/c1-3-5-4-2/h3-5H,1-2H2	
CVCCJCVCOH	C5H7O	<chem>C=C[CH]C=C(O)</chem>	InChI=1S/C5H7O/c1-2-3-4-5-6/h2-6H,1H2H	

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)	
HOCVCCJVO	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	<chem>C1(=O)[C]=CC=C1</chem>	InChI=1S/C5H3O/c6-5-3-1-2-4-5/h1-3H	
C1VCCVCCVO	C5H5O	<chem>[CH]=CC=CC=O</chem>	InChI=1S/C5H5O/c1-2-3-4-5-6/h1-5H	
CVCCVCCJVO	C5H5O	<chem>C=CC=C[C]=O</chem>	InChI=1S/C5H5O/c1-2-3-4-5-6/h2-4H,1H2	
C1VCCVO	C3H3O	<chem>[CH]=CC=O</chem>	InChI=1S/C3H3O/c1-2-3-4/h1-3H	