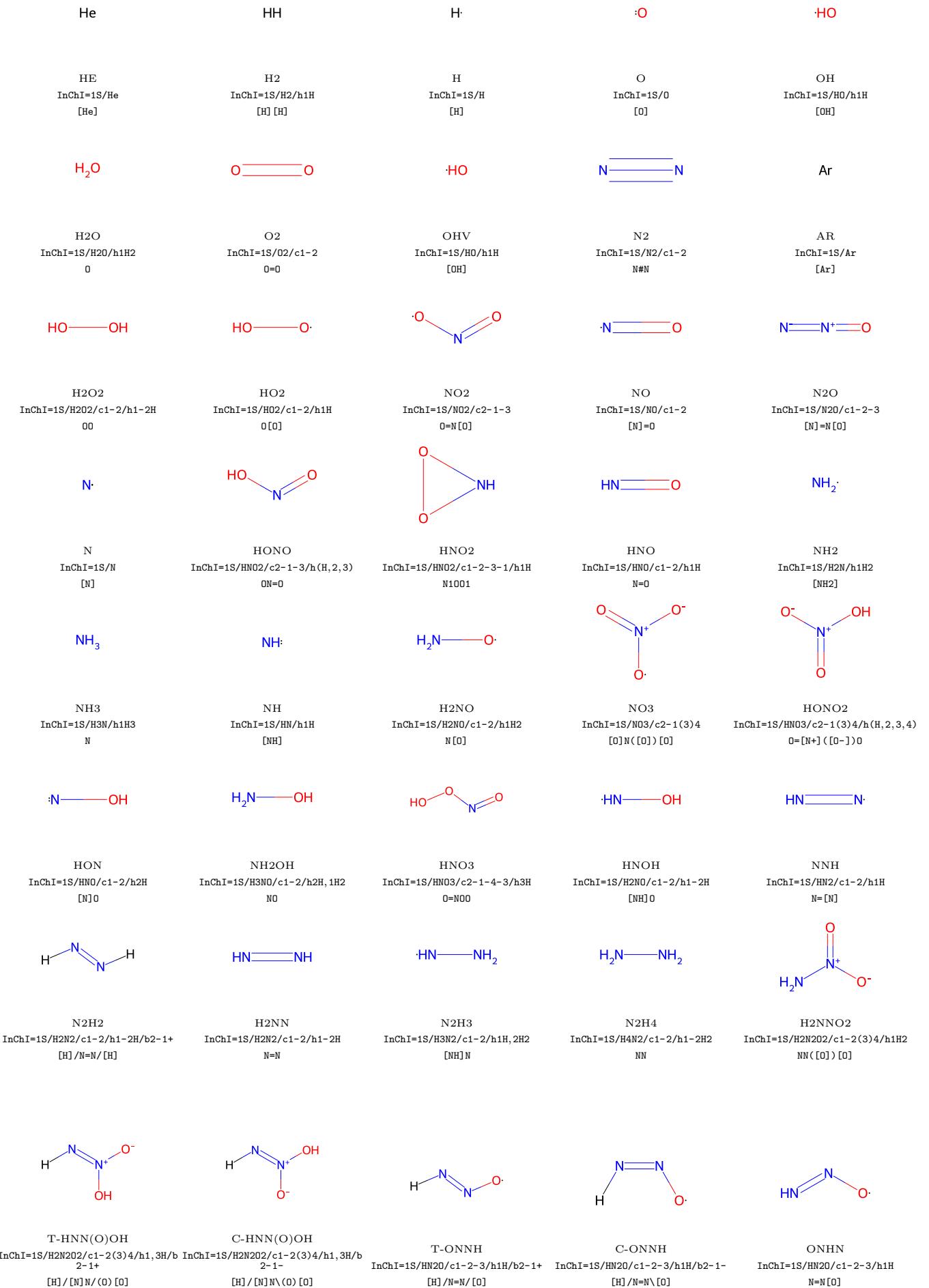


C3MechV4.0 species dictionary

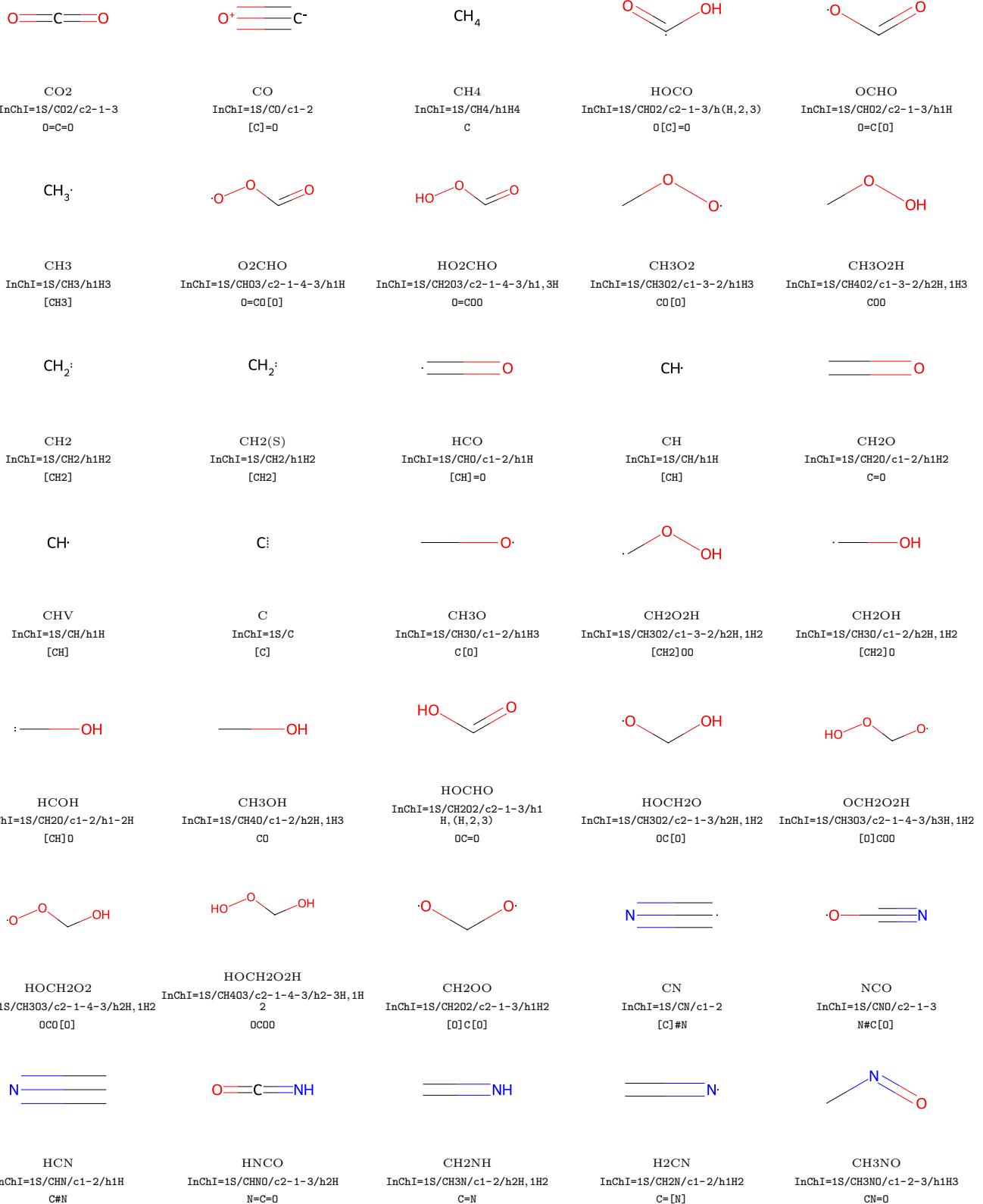
Luna Pratali Maffei, Raymond Langer, Yuki Murakami, Scott W. Wagnon,
Pengzhi Wang, Jiaxin Liu, Mohsin Raza, Yuxiang Zhu, Sanket Girhe,
Christian Schwenzer, Joachim Beeckmann, Stephen J. Klippenstein, Tiziano Faravelli,
Heinz Pitsch, Peter Kelly Senecal, Henry J. Curran

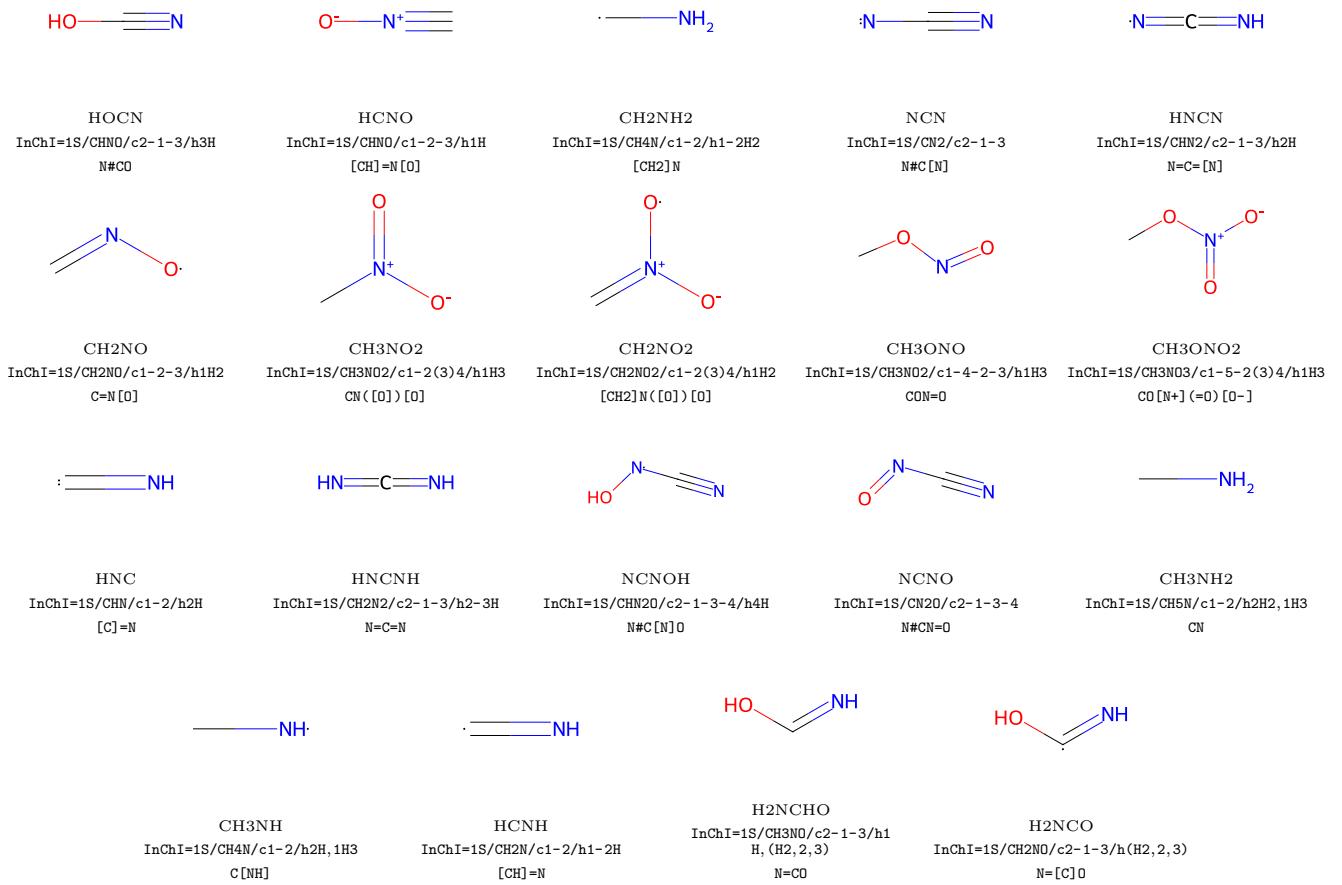
Each figure shows a species with its name in the kinetic model, its International Chemical Identifier (InChI), and its simplified molecular-input line-entry system (SMILES) formula.

1 C₀ species

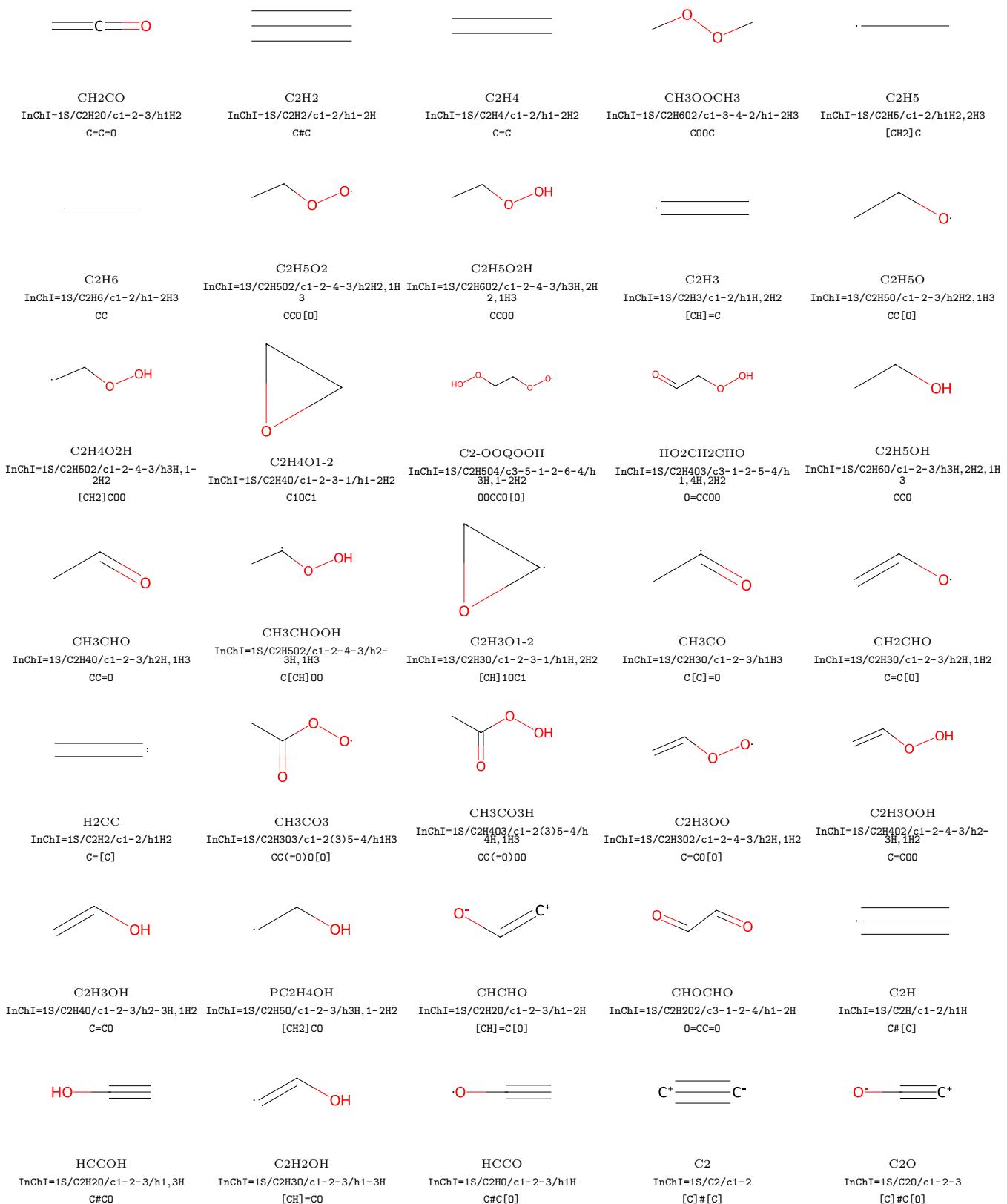


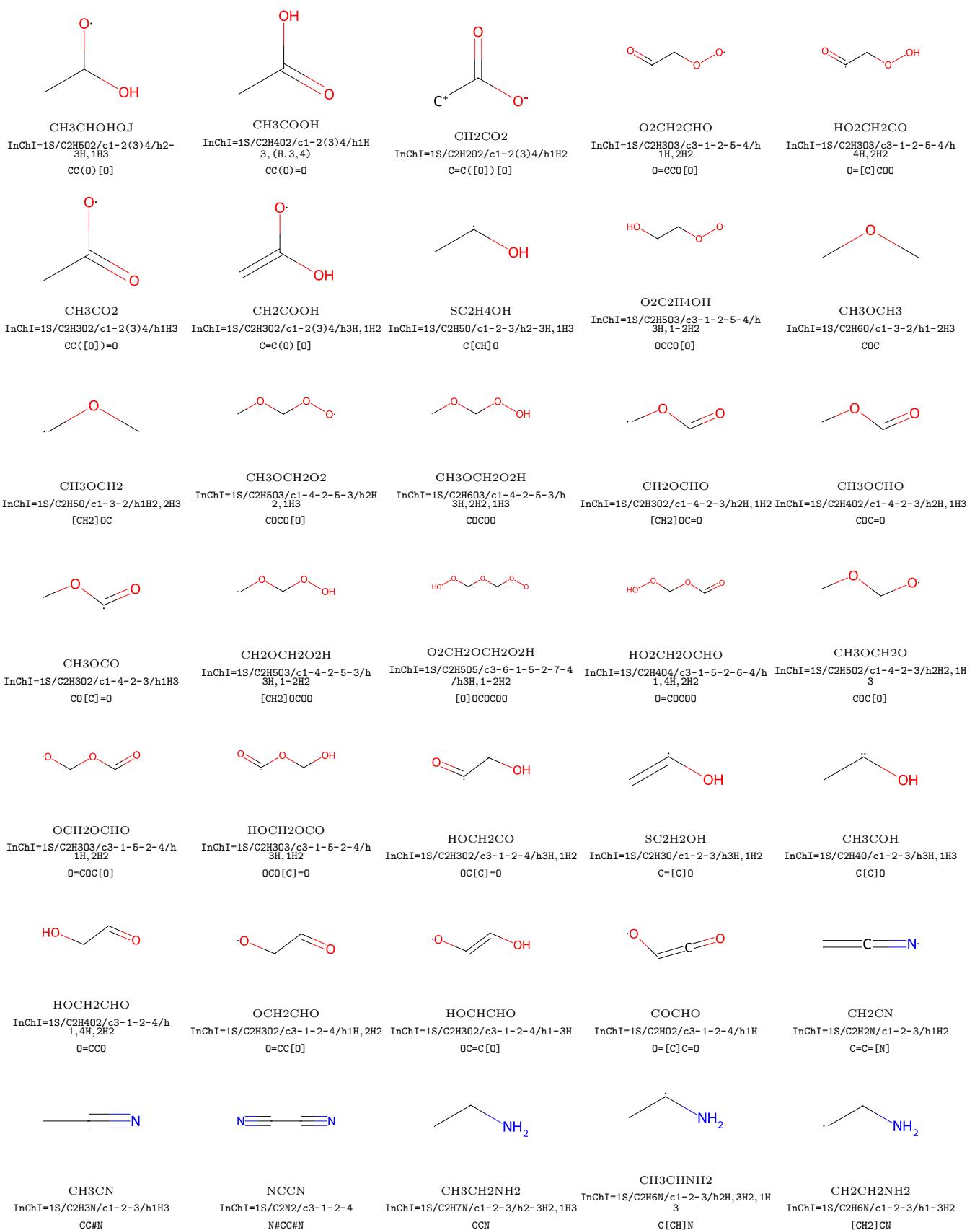
2 C₁ species

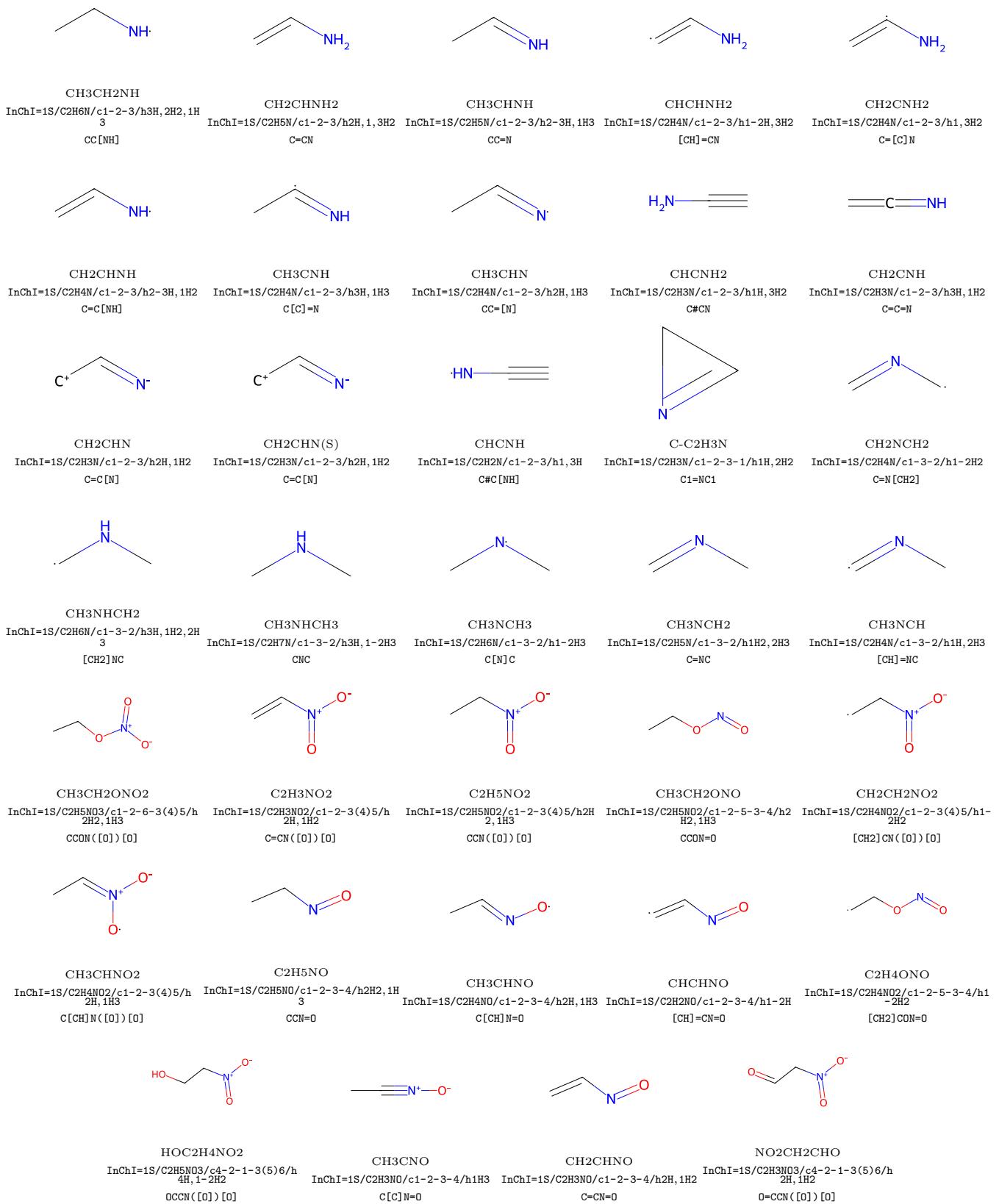




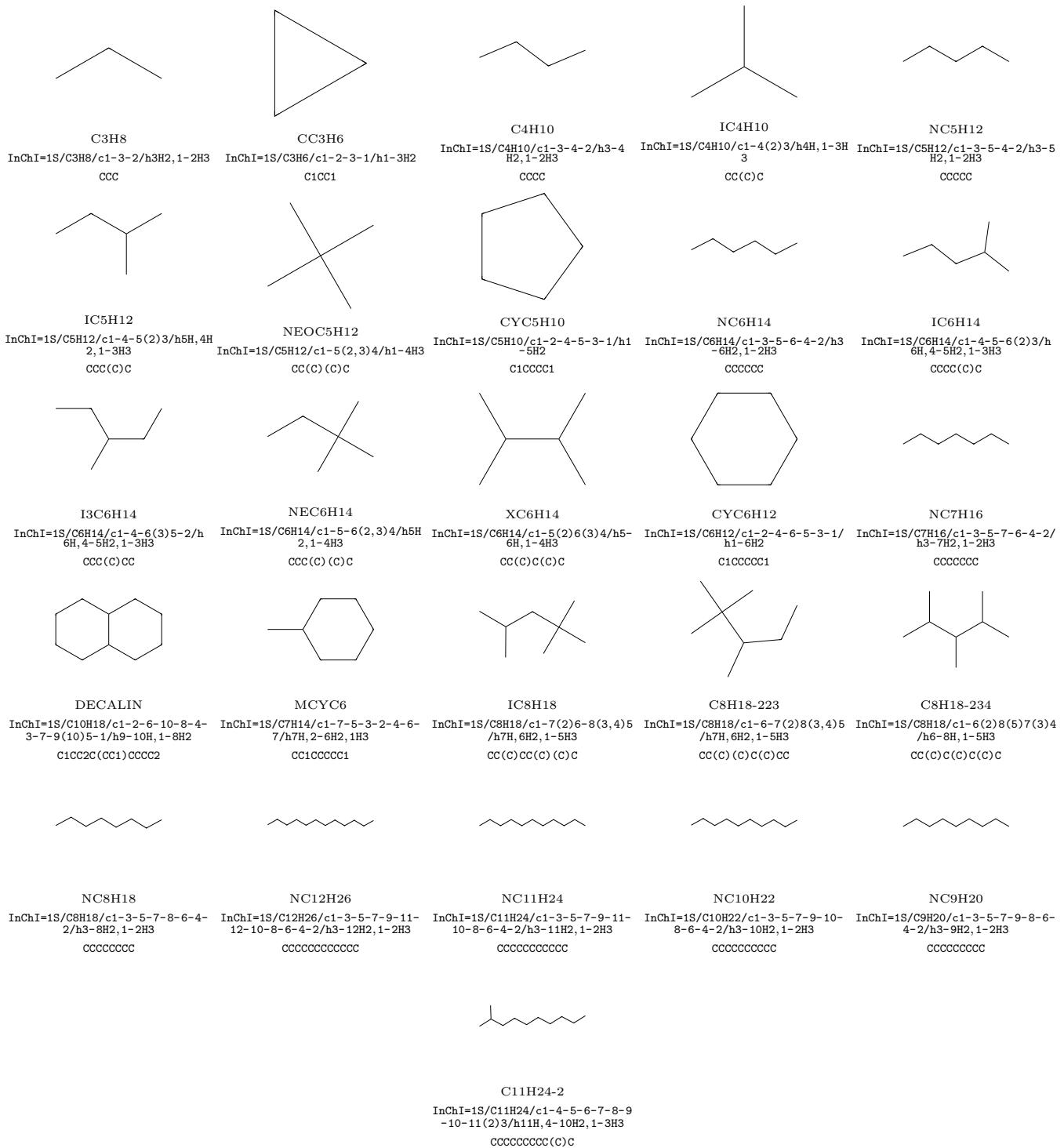
3 C₂ species



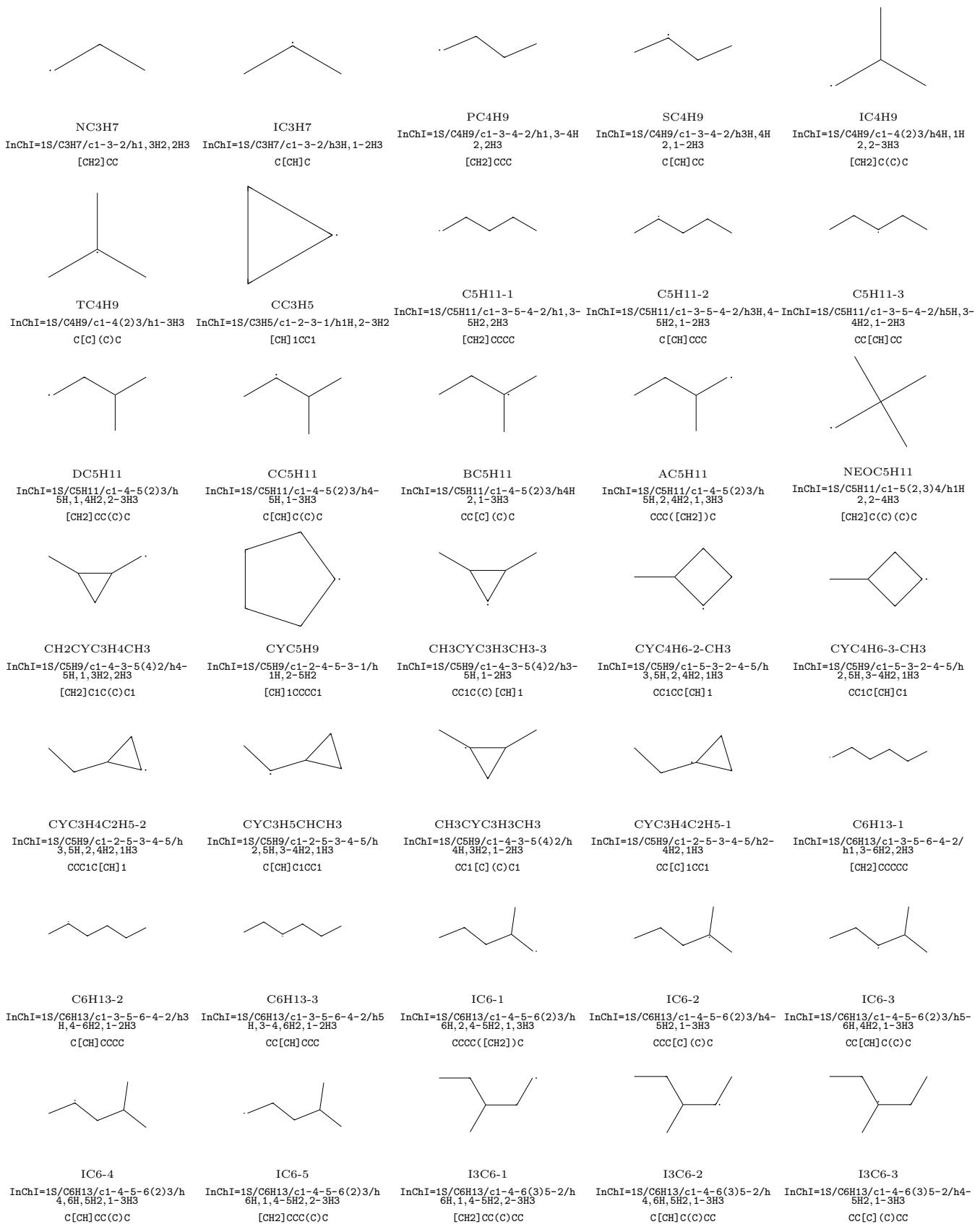


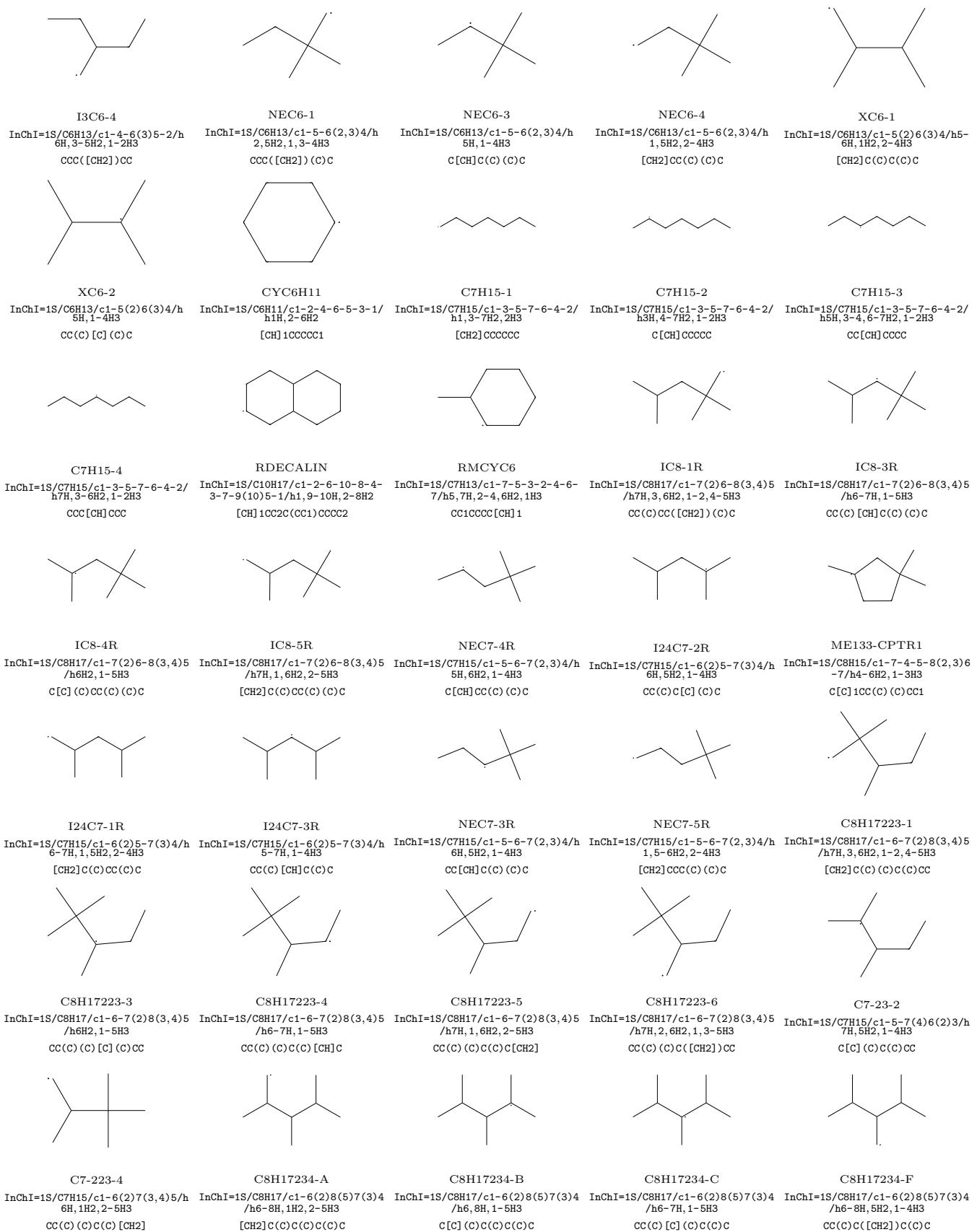


4 Alkanes

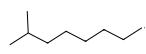
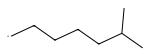
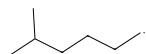
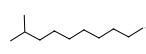
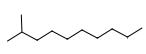


5 Alkyl radicals









C11H23-2I

$\text{InChI}=1\text{S}/\text{C}1\text{H}23/\text{c}1\text{--}4\text{--}5\text{--}6\text{--}7\text{--}8\text{--}9$ $\text{--}10\text{--}11(2)\text{3/h4,11H,5--10H2,1--3H3}$	$\text{InChI}=1\text{S}/\text{C}1\text{H}23/\text{c}1\text{--}4\text{--}5\text{--}6\text{--}7\text{--}8\text{--}9$ $\text{--}10\text{--}11(2)\text{3/h11H,1,4--10H2,2--3H3}$
$\text{C}[\text{CH}] \text{CCCCCCC}(\text{C})\text{C}$	$[\text{CH2}]\text{CCCCCCC}(\text{C})\text{C}$

C11H23-2J

/C11H23/c1-4-5-6-7-8-9
2)3/h11H,1,4-10H2,2-3H3
CH₂]CCCCCCCC(C)C

C7H15-2F

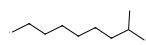
C7H15/c1-4-5-6-
H, 1, 4-6H2, 2-3H3
[CH2]CCCC(C)C

C8H17-2G

C8H17/c1-4-5-6-
8H,1,4-7H2,2-3H3
[CH2]CCCC(C)C

C9H19-2H

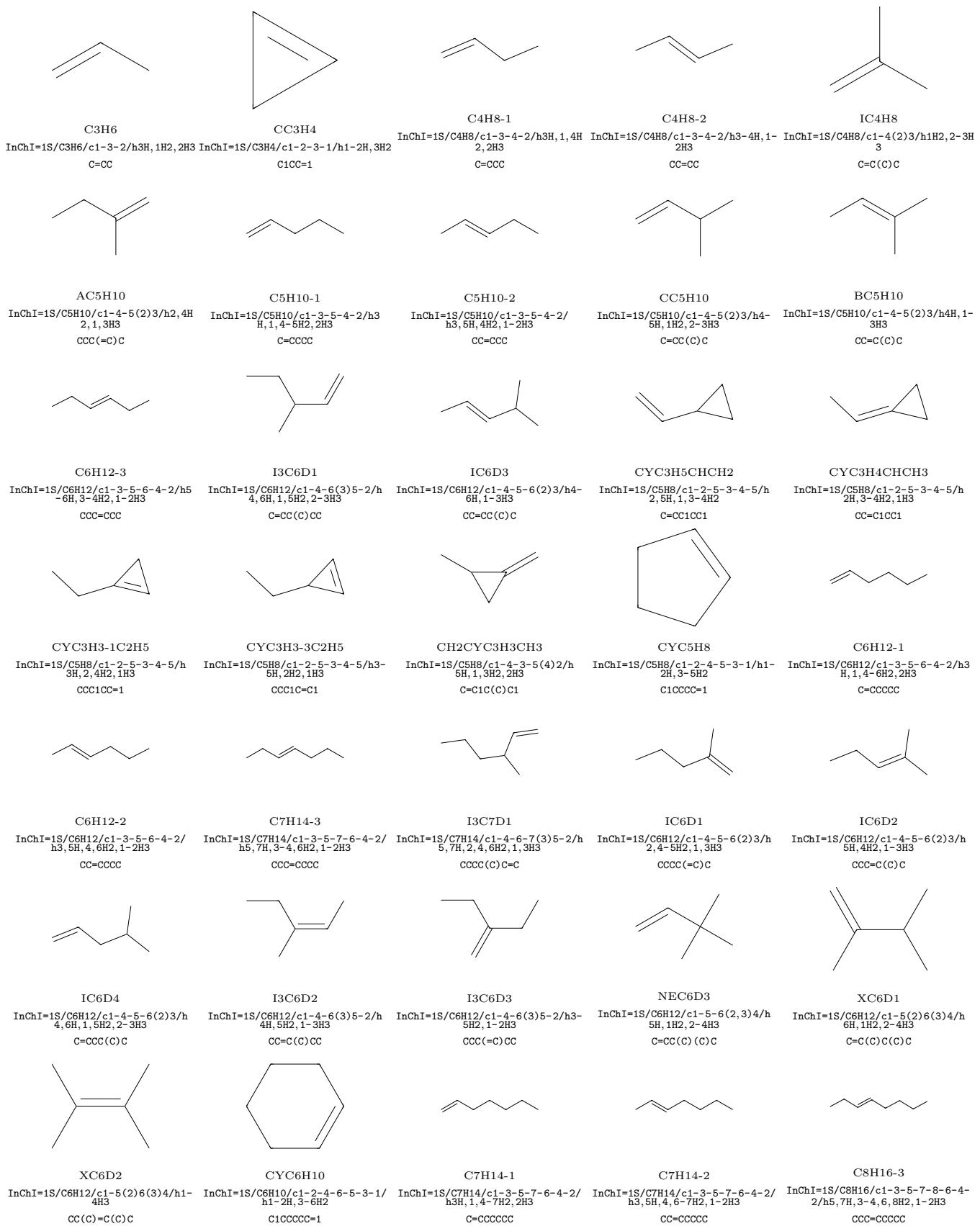
$\text{C}_9\text{H}_{19}/\text{c}1\text{-}4\text{-}5\text{-}6\text{-}7\text{-}8\text{-}$
 $\text{h9H}, 1,4\text{-}8\text{H}2, 2\text{-}3\text{H}3$
 $[\text{CH}_2]\text{CCCCC}(\text{C})\text{C}$

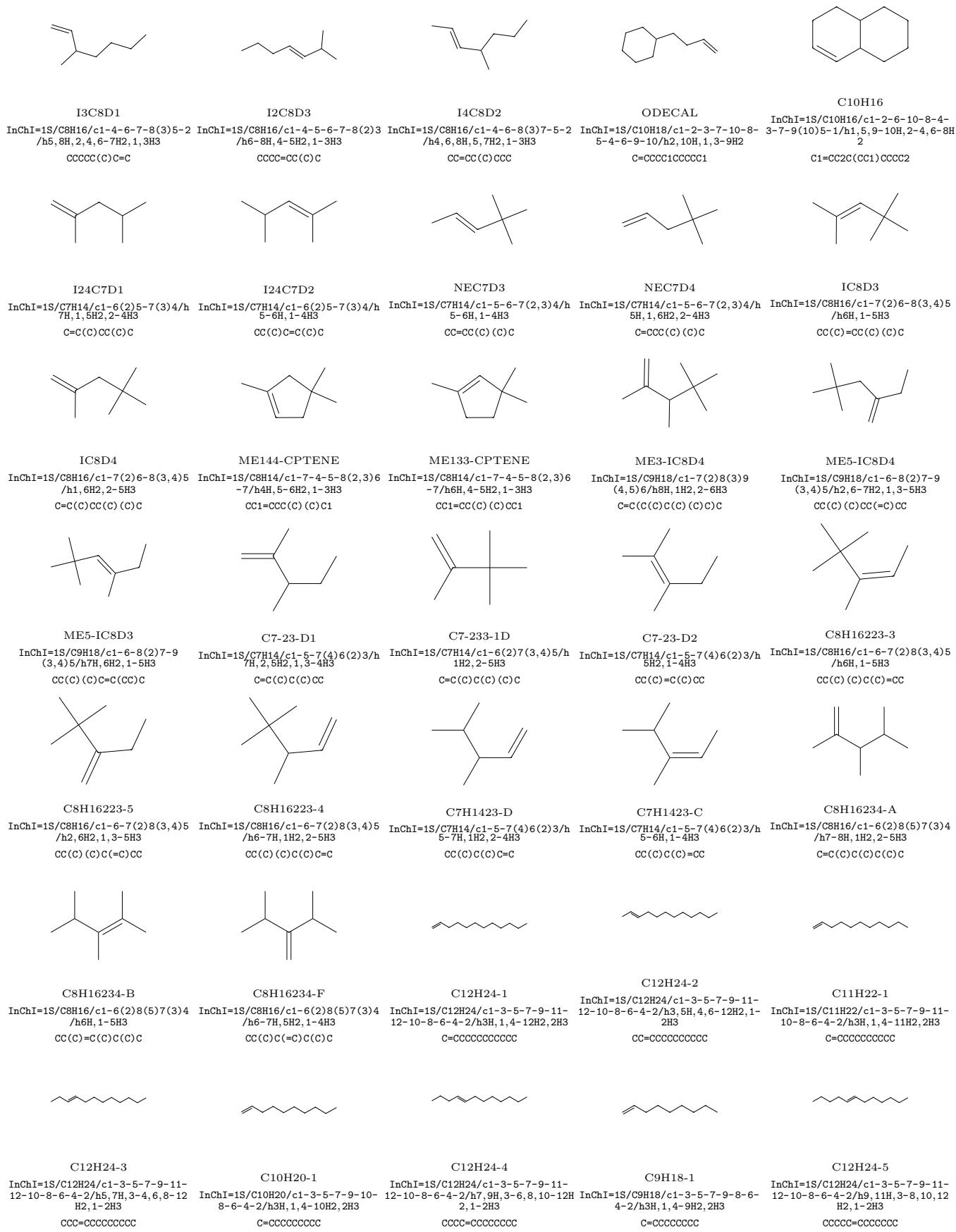


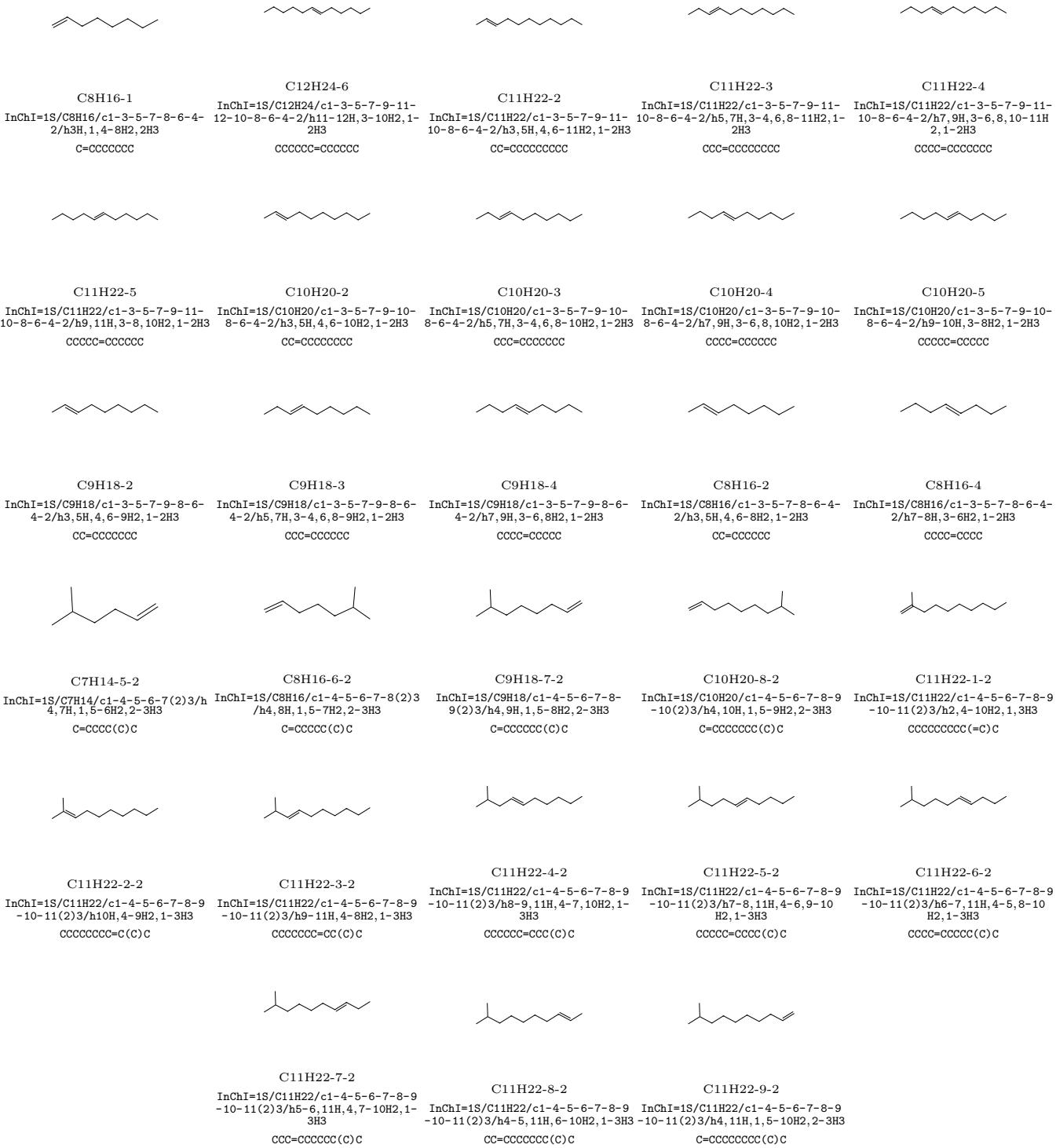
C10H21-2I

InChI=1S/C10H21/c1-4-5-6-7-8-9
 -10(2)3/h10H,1,4-9H2,2-3H3
 [CH₂]CCCCCCC(C)C

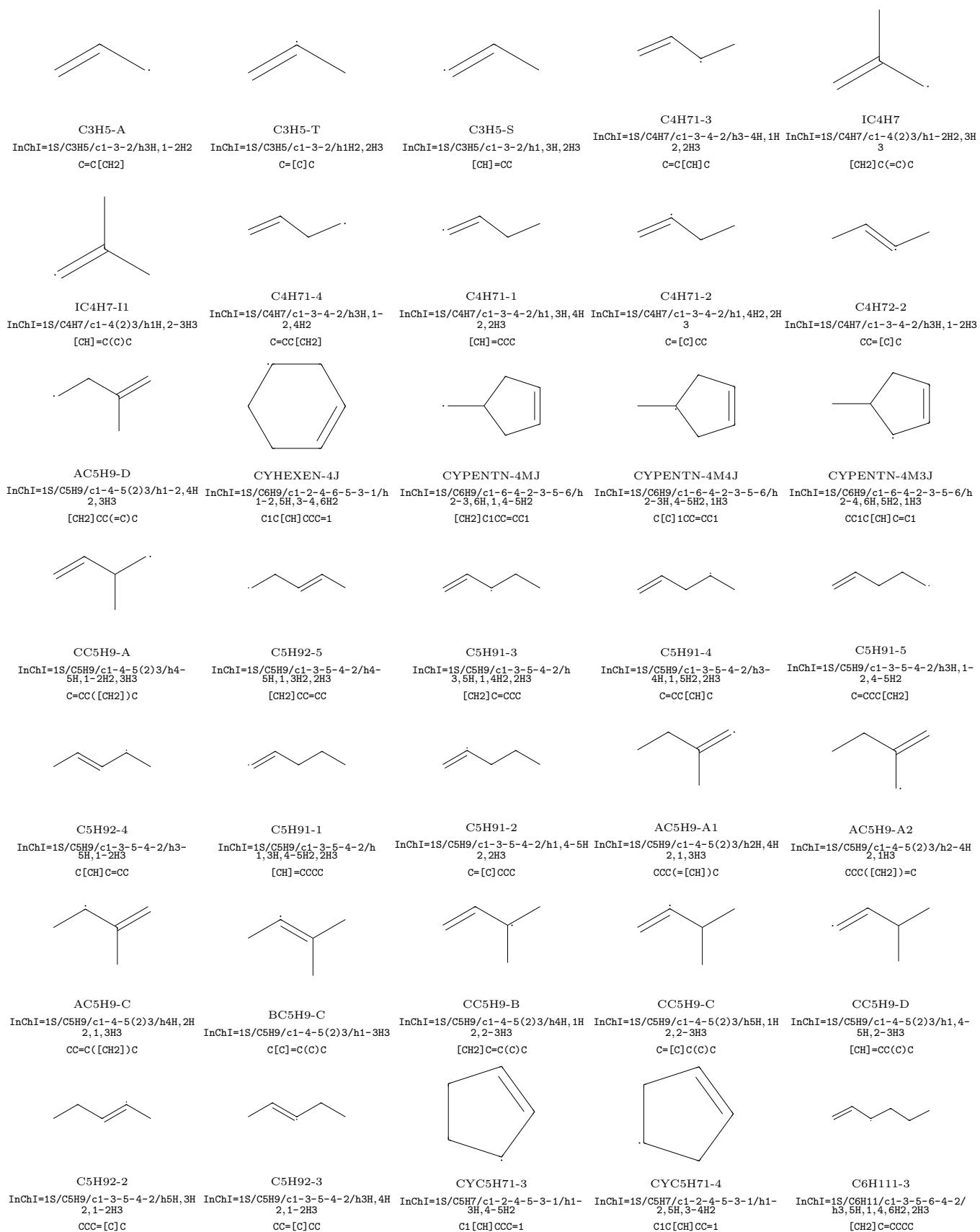
6 Alkenes

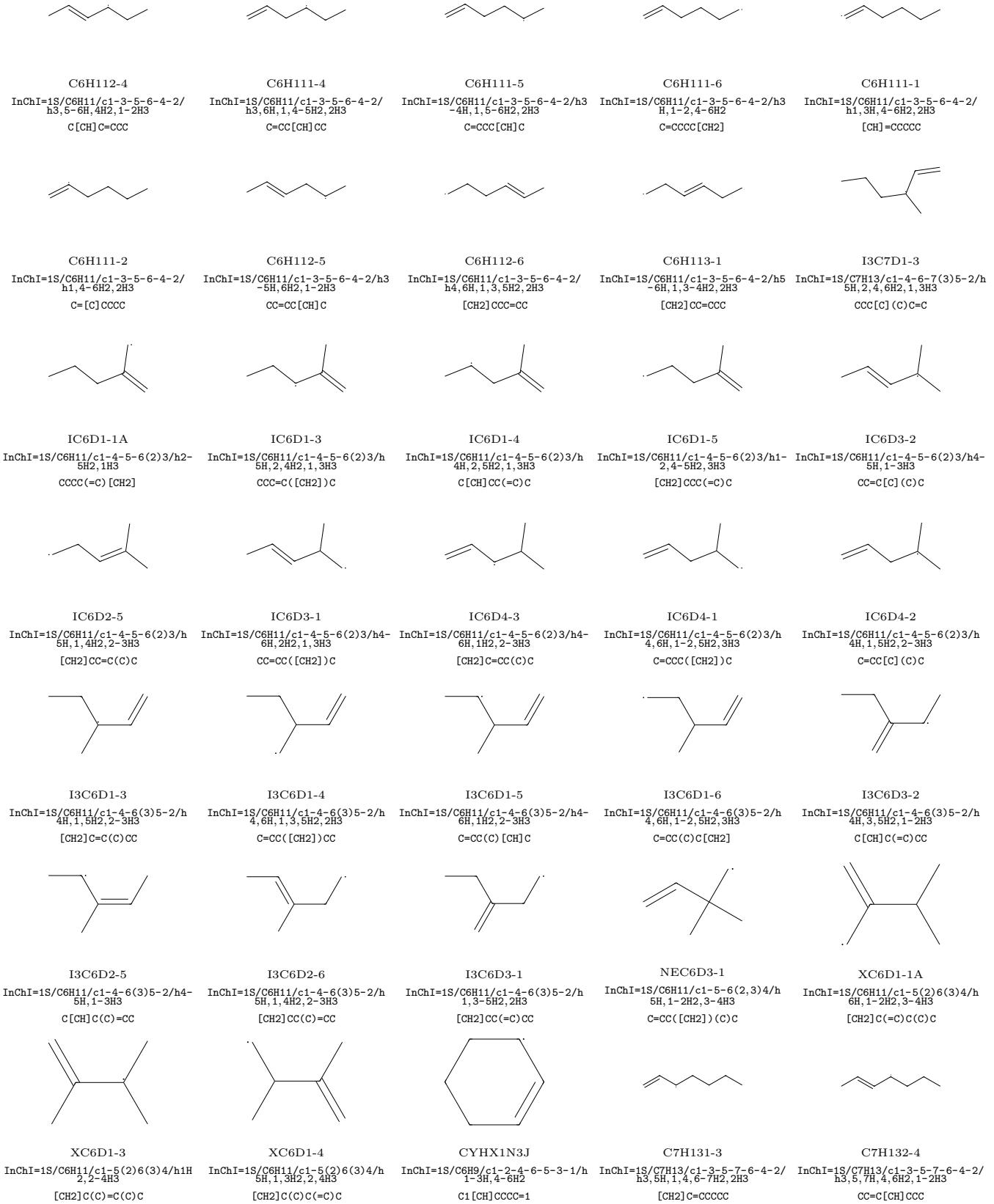


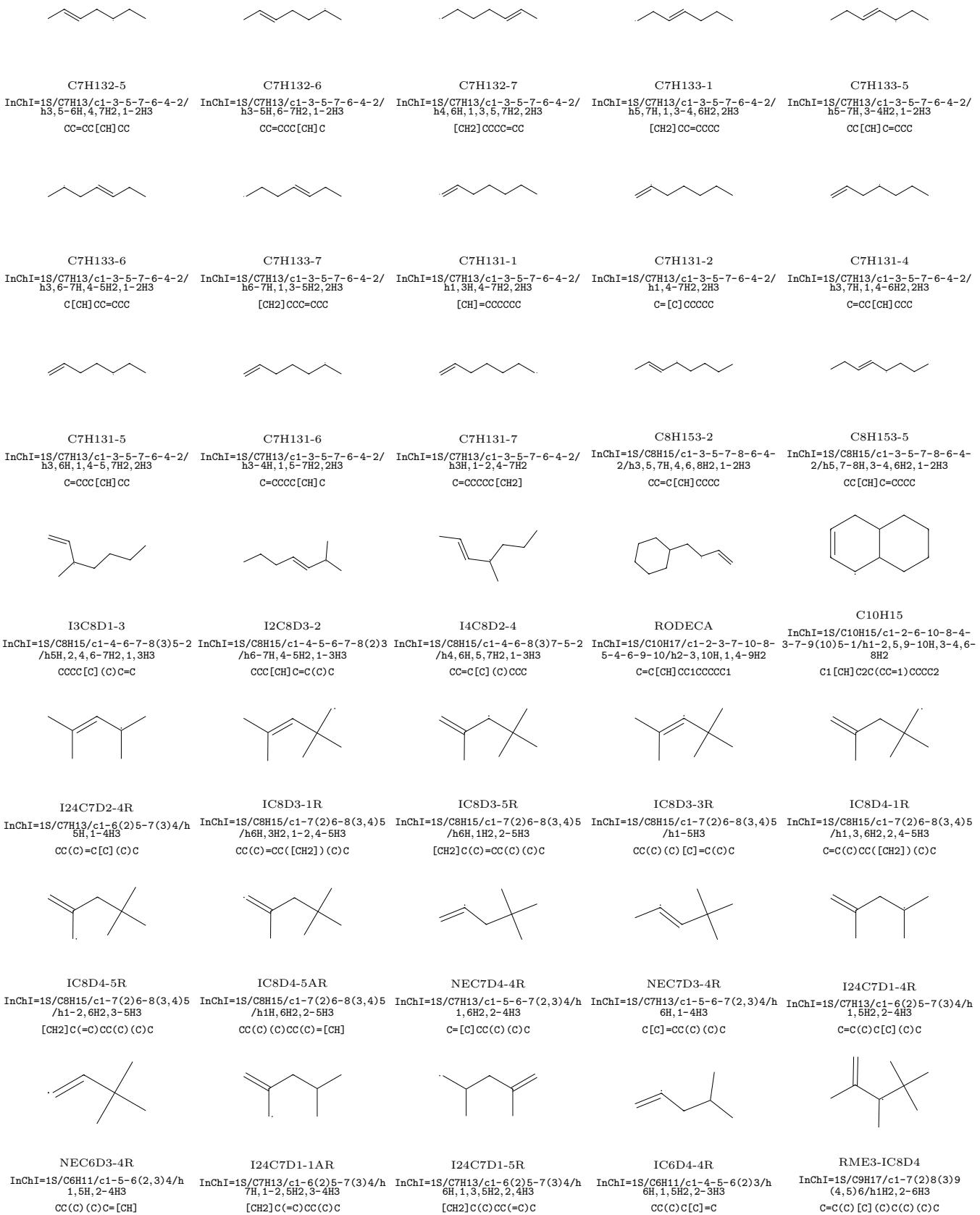


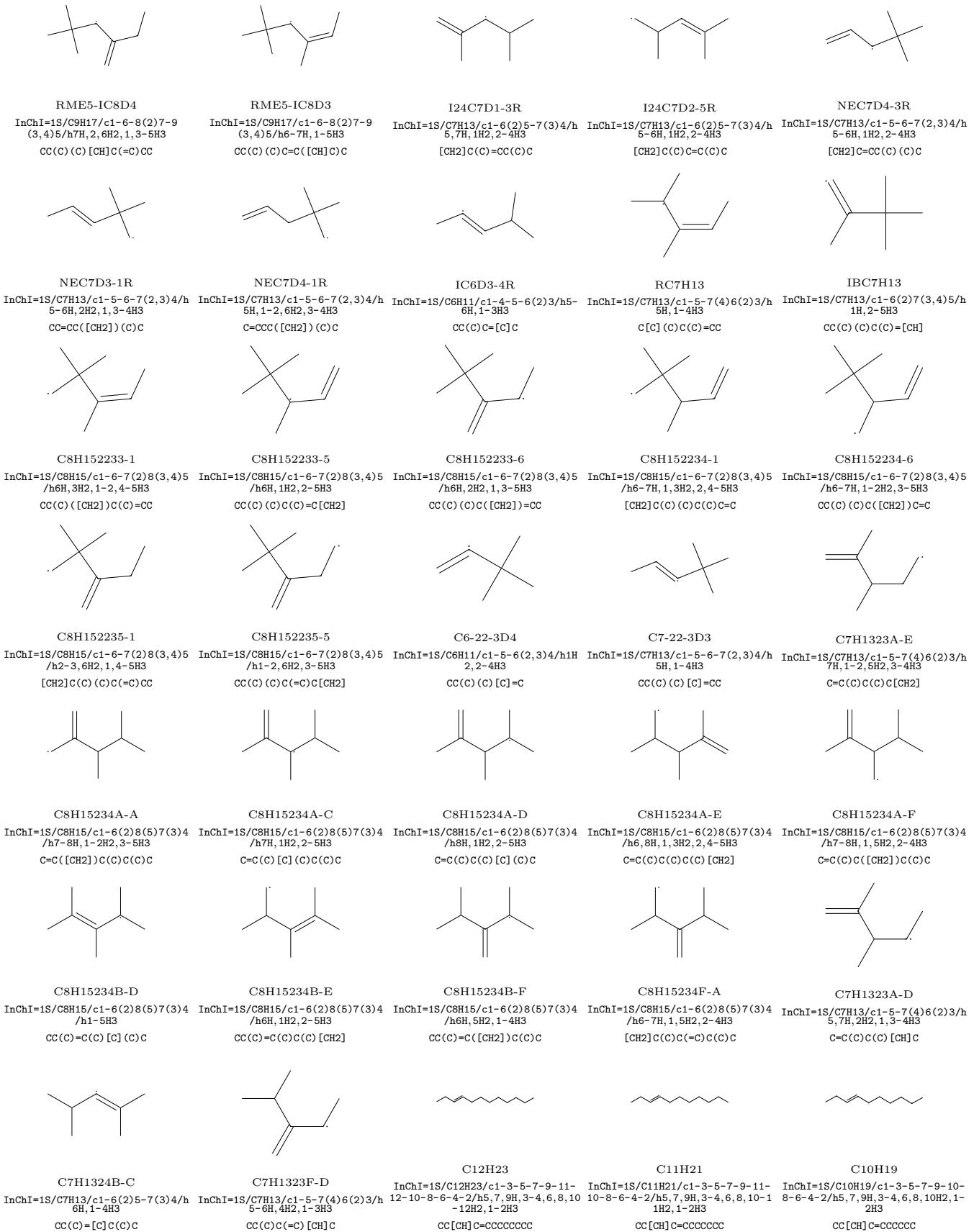


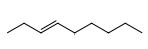
7 Alkenyl radicals



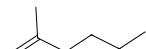




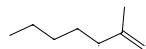




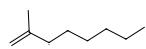
C9H17
InChI=1S/C9H17/c1-3-5-7-9-8-6-4-2/h5,7,9H,3-4,6,8H2,1-2H3
CC[CH]C=CCCCC



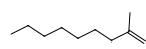
C7H13-1-2
InChI=1S/C7H13/c1-4-5-6-7(2)3/h6H,2,4-5H2,1,3H3
CCC[CH]C(=C)C



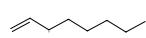
C8H15-1-2
InChI=1S/C8H15/c1-4-5-6-7-8(2)3/h7H,2,4-6H2,1,3H3
CCCC[CH]C(=C)C



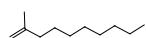
C9H17-1-2
InChI=1S/C9H17/c1-4-5-6-7-8-9(2)3/h8H,2,4-7H2,1,3H3
CCCCC[CH]C(=C)C



C10H19-1-2
InChI=1S/C10H19/c1-4-5-6-7-8-9-10(2)3/h9H,2,4-8H2,1,3H3
CCCCCC[CH]C(=C)C

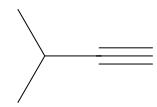
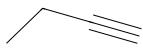
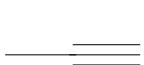


C8H15
InChI=1S/C8H15/c1-3-5-7-8-6-4-2/h3,5H,1,4,6-8H2,2H3
C=C[CH]CCCCC



C11H21-1-2
InChI=1S/C11H21/c1-4-5-6-7-8-9-10-11(2)3/h10H,2,4-9H2,1,3H3
CCCCCCC[CH]C(=C)C

8 Alkynes



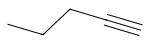
C3H4-P
InChI=1S/C3H4/c1-3-2/h1H,2H3
C#CC

H2CCC(S)
InChI=1S/C3H2/c1-3-2/h1H2
C=C=[C]

C4H6-1
InChI=1S/C4H6/c1-3-4-2/h1H,4H
2,2H3
C#CCC

C4H6-2
InChI=1S/C4H6/c1-3-4-2/h1-2H3
CC#CC

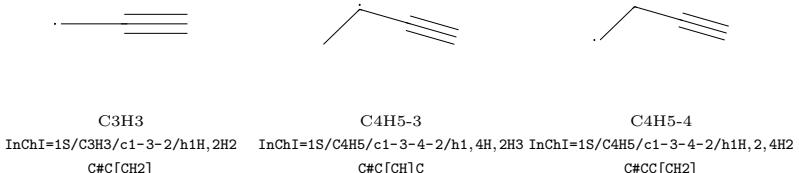
IC5T1
InChI=1S/C5H8/c1-4-5(2)3/h
1,5H,2-3H3
C#CCC(C)C



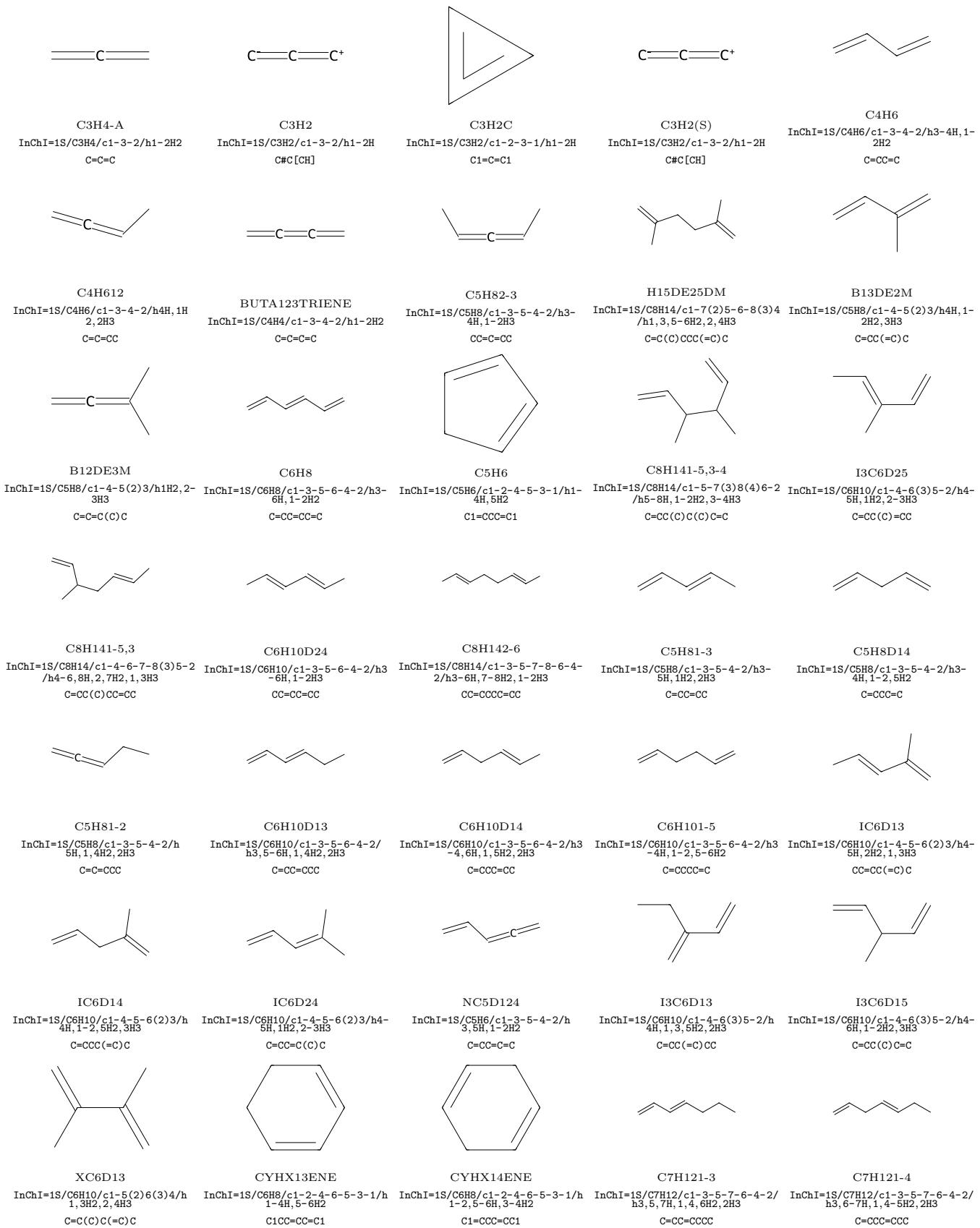
C5H8-2
InChI=1S/C5H8/c1-3-5-4-2/h3H2,1-
2H3
CCC#CC

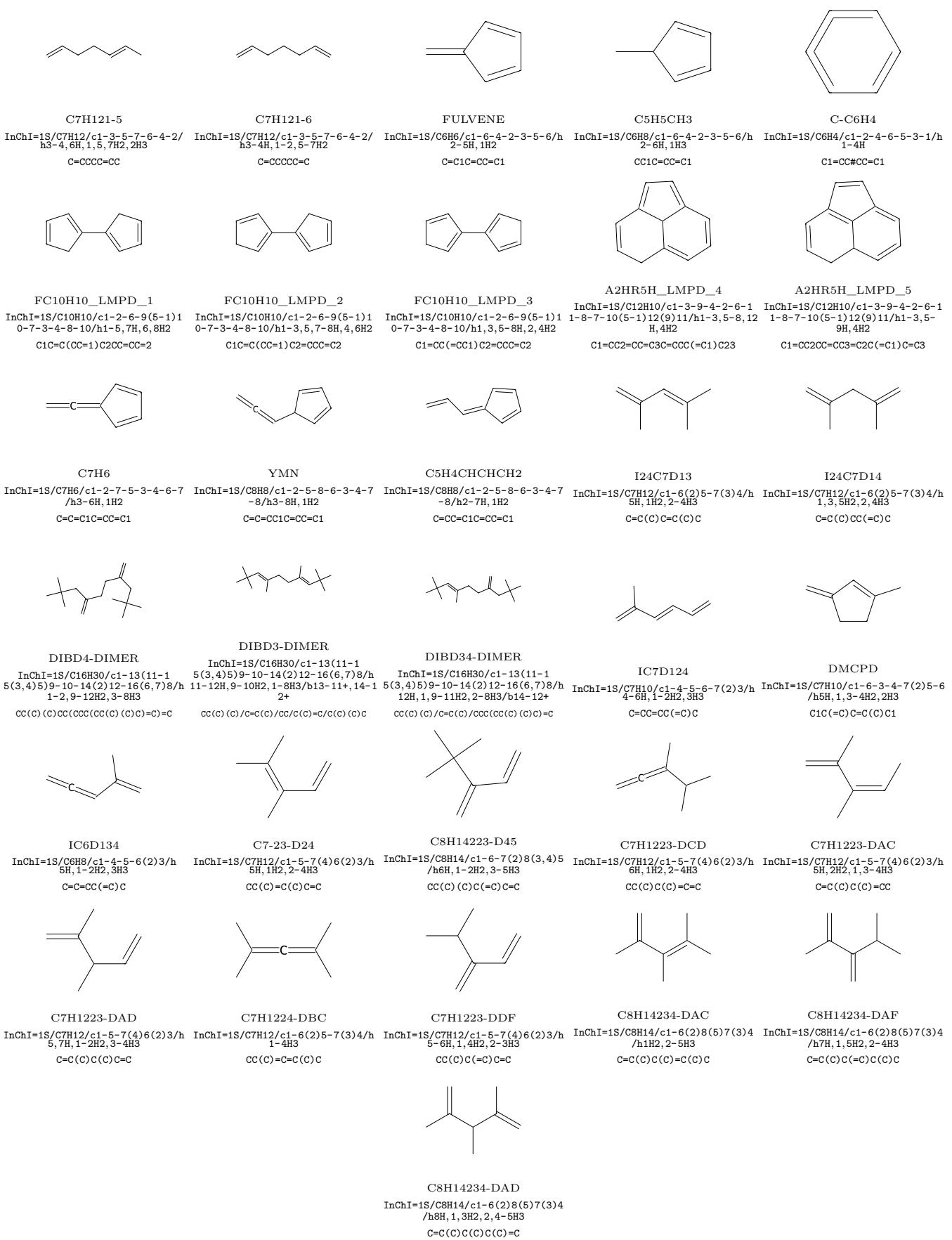
C5H8-1
InChI=1S/C5H8/c1-3-5-4-2/h1H,4-
5H2,2H3
C#CCCC

9 Alkynyl radicals

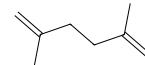
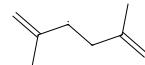
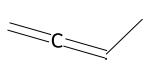
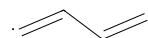
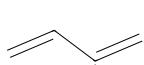


10 Polyenes





11 Polyenyl radicals



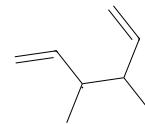
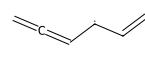
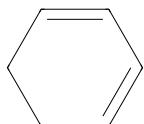
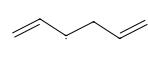
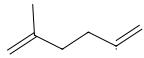
C4H5-I
InChI=1S/C4H5/c1-3-4-2/h3H,1-2H2
C=C[C]=C

C4H5-N
InChI=1S/C4H5/c1-3-4-2/h1,3-4H,2H2
[CH]=CC=C

C4H5-2
InChI=1S/C4H5/c1-3-4-2/h1H2,2H3
C=CC=C

H15DE25DM-S
InChI=1S/C8H13/c1-7(2)5-6-8(3)4/h5H,1,3,6H2,2,4H3
[CH2]C(C)=CCC(=C)C

H15DE25DM-A
InChI=1S/C8H13/c1-7(2)5-6-8(3)4/h1-3,5-6H2,4H3
[CH2]C(=C)CCC(=C)C



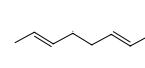
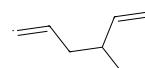
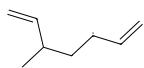
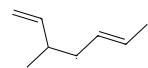
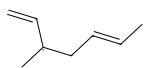
H15DE2M-T
InChI=1S/C7H11/c1-4-5-6-7(2)3/h1-2,5-6H2,3H3
C=[C]CCC(=C)C

C6H9-A
InChI=1S/C6H9/c1-3-5-6-4-2/h3-5H,1-2,6H2
[CH2]C=CCCC=C

CYC6H7
InChI=1S/C6H7/c1-4-6-5-3-1/h1-5H,6H2
C1C=CC[CH]C=1

C6H7-2
InChI=1S/C6H7/c1-3-5-6-4-2/h3-5H,1-2H2
C=CC=C

C8H131-5,3-TA
InChI=1S/C8H13/c1-5-7(3)8(4)6-2/h5-7H,1-2H2,3-4H3
C=CCC(C)C=C



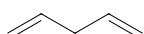
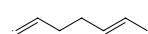
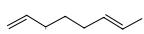
C8H131-5,3,TA
InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-6H,2,7H2,1,3H3
C=CCCC=CC

C8H131-5,3,SA
InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-8H,2H2,1,3H3
C=CC(C)[CH]C=CC

C8H131-5,3,PA
InChI=1S/C8H13/c1-4-6-7-8(3)5-2/h4-6,8H,1-2,7H2,3H3
[CH2]C=CCC(C)C=C

C7H111-5,3,6P
InChI=1S/C7H11/c1-4-6-7(3)5-2/h1,3-4H,5H2
[CH]=CCC(C)=C

C8H132-6,SA
InChI=1S/C8H13/c1-3-5-7-8-6-4-2/h3-7H,8H2,1-2H3
CC=C[CH]CC=CC



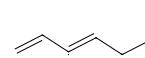
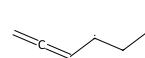
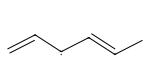
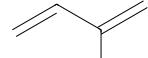
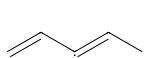
C8H132-6,PA
InChI=1S/C8H13/c1-3-5-7-8-6-4-2/h2H3-6H,1-7H2,2H3
[CH2]C=CCCC=CC

C7H111-5,1P
InChI=1S/C7H11/c1-3-5-7-6-4-2/h1,3-4,6H,5,7H2,2H3
[CH]=CCCC=CC

CVCCJCVC
InChI=1S/C5H7/c1-3-5-4-2/h3-5H,1-2H2
C=CC=C

C5H7-14-1
InChI=1S/C5H7/c1-3-5-4-2/h1,3-4H,2,5H2
[CH]=CCC=C

C5H7-13-2
InChI=1S/C5H7/c1-3-5-4-2/h4-5H,1H2,2H3
C=[C]C=CC



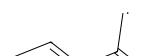
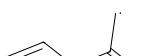
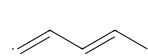
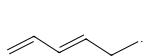
C5H7-13-3
InChI=1S/C5H7/c1-3-5-4-2/h3-4H,1H2,2H3
[CH2]C=C=CC

B13DE2MJ
InChI=1S/C5H7/c1-4-5(2)3/h4H,1-3H2
C=CC([CH2])=C

CVCCJCVC
InChI=1S/C6H9/c1-3-5-6-4-2/h3-6H,1H2,2H3
C=CC=C

C6H9-13-2
InChI=1S/C6H9/c1-3-5-6-4-2/h5-6H,1,4H2,2H3
C=[C]C=CC

C6H9-13-3
InChI=1S/C6H9/c1-3-5-6-4-2/h3-6H,1,4H2,2H3
[CH2]C=C=CC



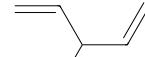
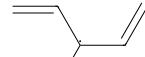
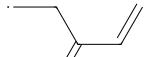
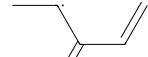
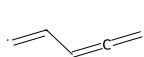
C6H9-13-6
InChI=1S/C6H9/c1-3-5-6-4-2/h3-5H,1-2,4H2
C=CC=CC[CH2]

P13DE1J
InChI=1S/C5H7/c1-3-5-4-2/h1,3-5H,2H3
[CH]=CC=CC

IC6D14-1
InChI=1S/C6H9/c1-4-5-6(2)3/h4H,1-3,5H2
C=CCC(=C)[CH2]

IC6D13-5R
InChI=1S/C6H9/c1-4-5-6(2)3/h4-5H,1-2H2,3H3
[CH2]C=CC(=C)C

IC6D13-1AR
InChI=1S/C6H9/c1-4-5-6(2)3/h4-5H,2-3H2,1H3
CC=CC(=C)[CH2]



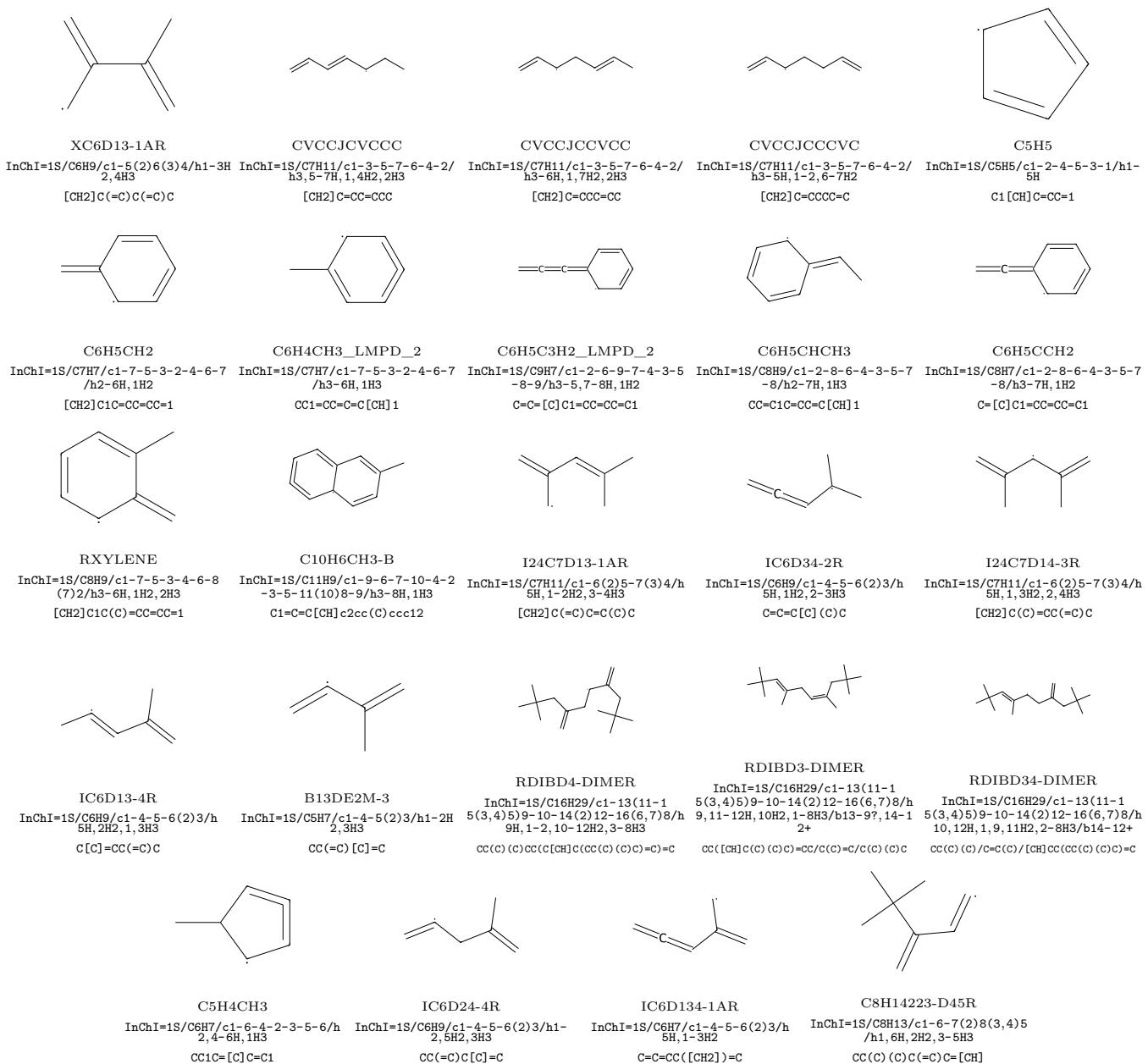
NC5D124-5R
InChI=1S/C5H5/c1-3-5-4-2/h1-3,5H,2H2
[OH]=CC=C

I3C6D13-5
InChI=1S/C6H9/c1-4-6(3)5-2/h4-5H,1-3H2,2H3
C=CC([CH2])=CC

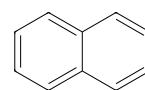
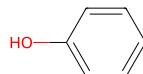
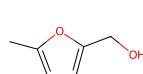
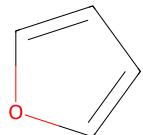
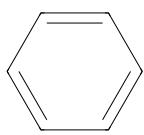
I3C6D13-6
InChI=1S/C6H9/c1-4-6(3)5-2/h4-5H,1-3,5H2
C=CC(C)=C

I3C6D15-3
InChI=1S/C6H9/c1-4-6(3)5-2/h4-5H,1-2H2,3H3
C=CC(C)=C

I3C6D15-4
InChI=1S/C6H9/c1-4-6(3)5-2/h4-6H,1-3H2
C=CC([CH2])=C



12 Aromatics (molecules)



C6H6

InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H
C1=CC=CC=C1

FURAN

InChI=1S/C4H4O/c1-2-4-5-3-1/h1-4H
C1=COC=C1

DMTHFOH1D2-4

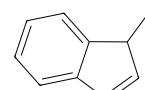
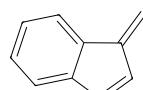
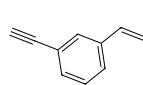
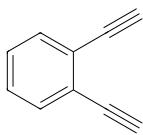
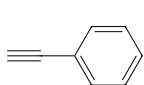
InChI=1S/C6H8O2/c1-5-2-3-6(4-7)8-5/h2-3,7H,4H2,1H3
CC1OC(CC=1)CO

C6H5OH

InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H
OC1=CC=CC=C1

NAPH

InChI=1S/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H
C1=CC2C(C=C1)=CC=CC=2



C6H5C2H

InChI=1S/C8H6/c1-2-8-6-4-3-5-7
-8/h1,3-7H
C#CC1C=CC=CC=1

C6H4(C2H)2

InChI=1S/C10H6/c1-3-9-7-5-6-8-10(9)4-2/h1-5,8H
C#Cc1cccc1C#C

C2HC6H4C2H3

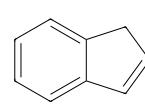
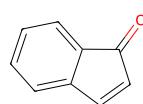
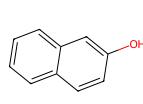
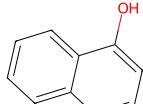
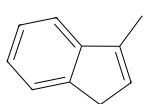
InChI=1S/C10H8/c1-3-9-6-5-7-10
(4-2)8-9/h1,4-8H,2H2
C#Cc1cccc(C=C)c1

C9H6CH2

InChI=1S/C10H8/c1-8-6-7-9-4-2-3-5-10(8)9/h2-7H,1H2
C=C1C2C(CC=CC=2)=C1

MEINDENE_LMPD_1

InChI=1S/C10H10/c1-8-6-7-9-4-2-3-5-10(8)9/h2-6H,7H2,1H3
CC1C2C(CC=CC=2)=C1



MEINDENE_LMPD_2

InChI=1S/C10H10/c1-8-6-7-9-4-2-3-5-10(8)9/h2-6H,7H2,1H3
CC1C2C(CC=CC=2)=C1

NAPHOH-A

InChI=1S/C10H8O/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7,11H
OC1C2C(CC=CC=2)=C1

NAPHOH-B

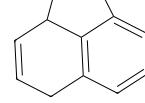
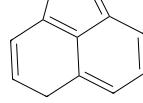
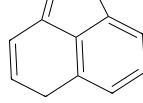
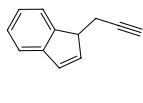
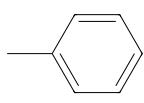
InChI=1S/C10H8O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7,11H
C1C2C(CC=CC=2)=C1

C9H6O

InChI=1S/C9H6O/c10-9-6-5-7-3-1-2-4-8(7)9/h1-6H
O=C1C2C(CC=CC=2)=C1

IND

InChI=1S/C9H8/c1-2-5-9-7-3-6-8-4-10(9)4-1/h1-6H,7H2
C1=CC2=C(C=C1)CC=C2



C6H5CH3

InChI=1S/C7H8/c1-7-5-3-2-4-6-7
-11-6-3-4-7-12(10)11/h1,3-4,6-10
/h2-6H,1H3
CC1=CC=CC=C1

C9H7C3H3

InChI=1S/C12H10/c1-2-5-10-8-9-11-6-3-4-7-12(10)11/h1,3-4,6-10
H,5H2
C#CCC1=CC=CC=C1

A2HR5H_LMPD_1

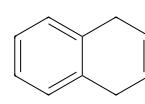
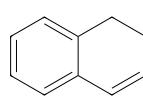
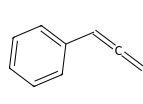
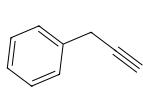
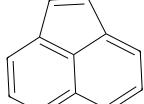
InChI=1S/C12H10/c1-3-9-4-2-6-1-1-8-7-10(5-1)12(9)11/h1-3,5-6,8H,4,7H2
C1=CC2=C3C(CC2)=CCCC=C1

A2HR5H_LMPD_2

InChI=1S/C12H10/c1-3-9-4-2-6-1-1-8-7-10(5-1)12(9)11/h1-3,5-6,8H,4,7H2
C1=CC2=CCC=C2C(CC2)=C3

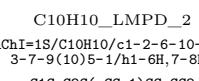
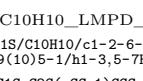
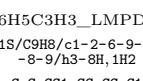
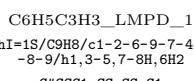
A2HR5H_LMPD_3

InChI=1S/C12H10/c1-3-9-4-2-6-1-1-8-7-10(5-1)12(9)11/h1-3,5-8,11
H,4H2
C1=CC2=C3C(CC2)=C3C(CC2)=C2

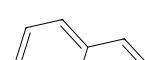
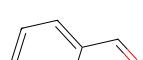
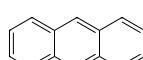
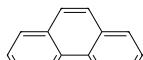
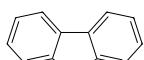


C12H8

InChI=1S/C12H8/c1-3-9-4-2-6-11
-8-7-10(5-1)12(9)11/h1-8H
C1=CC2=C3C(CC2)=C1



InChI=1S/C10H10/c1-2-6-10-8-4-3-7-9(10)5-1/h1-6H,7-8H2
C1=CC2=C(CC2)=CCC=C2



FLUORENE

InChI=1S/C13H10/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)12/h1-8
H,9H2
C1=CC2=C(C=C1)C3C(CC2)=C1

PHNTHRNLMPD_1

InChI=1S/C14H10/c1-3-7-13(5-1)9-10-12-6-2-4-8-14(12)13/h1-14-8-4-3-7-13(14)9-11(12)5-1/h1-10H
C1=C=CC2=C(C=C1)C3C(CC2)=C1

PHNTHRNLMPD_2

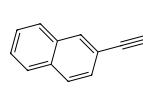
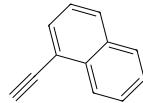
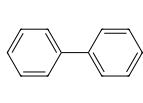
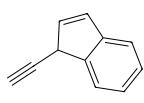
InChI=1S/C14H10/c1-2-6-12-10-1-1-6-9-8-10H
C1=CC2=C(C=C1)C3C(CC2)=C1

C6H5CHO

InChI=1S/C7H6O/c8-6-7-4-2-1-3-5-7-1/h1-6H
O=CC1=CC=CC=C1

C10H10_LMPD_2

InChI=1S/C10H10/c1-2-6-10-8-4-3-7-9(10)5-1/h1-6H,7-8H2
C1=CC2=C(CC2)=CCC=C2



C9H7C2H

InChI=1S/C11H8/c1-2-9-7-8-10-5-3-4-6-11(9)10/h1,3-9H
C#CC1C=CC2=C1C=CC2

BIPHENYL

InChI=1S/C12H10/c1-3-7-11(8-1)12-9-5-2-6-10-12/h1-10H
C1=CC=CC2=C(C=C1)C2C=CC=C2

A2C2HA

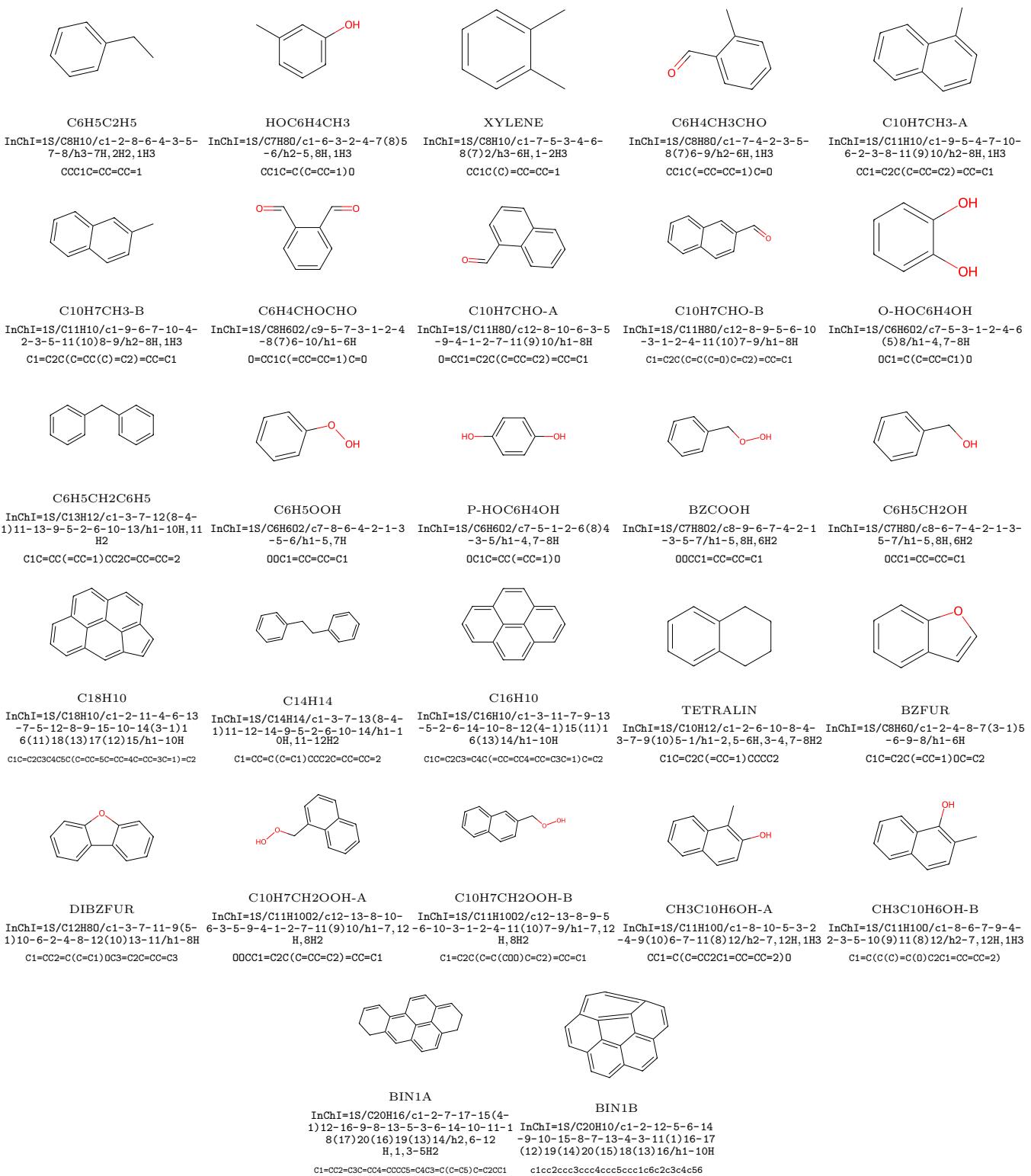
InChI=1S/C12H8/c1-2-10-7-5-8-1-1-6-3-4-9-12(10)11/h1,3-9H
C#CC1=CC=CC2=C(C=C1)C2C=CC=C2

A2C2HB

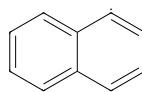
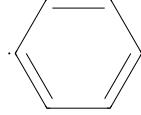
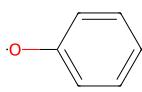
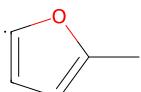
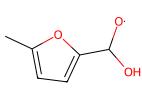
InChI=1S/C12H8/c1-2-10-7-8-11-5-3-4-6-12(11)9-10/h1,3-9H
C#CC1=CC=CC2=C(C=C1)C2C=CC=C2

C18H14

InChI=1S/C18H14/c1-2-12-6-7-15-9-8-13-4-3-5-14-10-11-16(12)8(15)17(13)14/h3-11H,2H2,1H3
CCC1C2C3=C4C(C=CC=C4C3=CC=C1)=CC=



13 Aromatics (radicals)



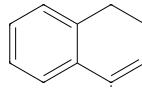
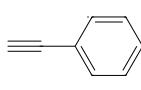
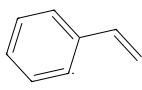
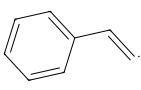
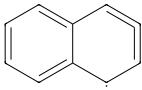
DMTHFOH1D2-4-1OJ
InChI=1S/C6H7O3/c1-4-2-3-5(9-4)6(7)8/h2-3,6-7H,1H3
CC1OC(=CC=1)C(O)[0]

MF25J
InChI=1S/C5H5O/c1-5-3-2-4-6-5/h2-3H,1H3
CC10[C]C=CC=1

C6H5O
InChI=1S/C6H5O/c7-6-4-2-1-3-5-6/h1-5H
[0]C1=CC=CC=C1

C6H5
InChI=1S/C6H5/c1-2-4-6-5-3-1/h1-5H
C1[CH]C=CC=C1

NAPH-A
InChI=1S/C10H7/c1-2-6-10-8-4-3-7-9(10)5-1/h1-3,5-8H
[C]1=CC2=C(C=C1)C=CC=C2



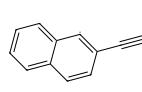
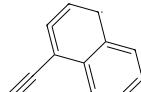
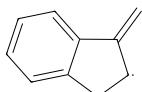
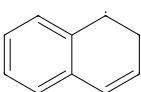
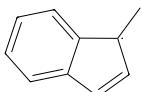
NAPH-B
InChI=1S/C10H7/c1-2-6-10-8-4-3-7-9(10)5-1/h1-3,5-8H
[C]1=CC2=C(C=C1)C=CC=C2

C6H5CHCH
InChI=1S/C8H7/c1-2-8-6-4-3-5-7/h8-1H7
[CH]=CC1C=CC=CC1

C6H4C2H3
InChI=1S/C8H5/c1-2-8-6-4-3-5-7/h8-2H,1H2
C=CC1=C=CC=C[CH]1

C6H4C2H
InChI=1S/C8H5/c1-2-8-6-4-3-5-7/h8-1H3,3-6H
C#CC1=C=CC=C[CH]1

MEINDR
InChI=1S/C10H9/c1-2-6-10-8-4-3-7-9(10)5-1/h1-3,5-6H,4,8H2
C1C=C2C(=CC=C1)CCC=[C]2



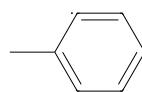
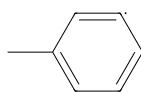
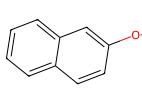
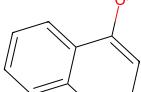
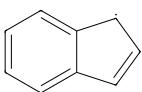
MEINDENYL
InChI=1S/C10H9/c1-8-6-7-9-4-2-3-5-10(8)9/h2-7H,1H3
CC1=C2C(=CC=C1)C=CC=C2

C10H9
InChI=1S/C10H9/c1-2-6-10-8-4-3-7-9(10)5-1/h1-3,5-8H,4H2
C1C=C2C([CH]C=1)=CCC=C2

MEINDRSR
InChI=1S/C10H9/c1-8-6-7-9-4-2-3-5-10(8)9/h2-6H,1,7H2
C=C1C2C(=CC=C2)C[CH]1

A2C2HA-
InChI=1S/C12H7/c1-2-10-7-5-8-1-6-3-4-9-12(10)11/h1,3-6,8-9H
C#CC1=C=CC=C[CH]1

A2C2HB-
InChI=1S/C12H7/c1-2-10-7-8-11-5-3-4-6-12(11)9-10/h1,3-8H
C#CC1=[C]C2=CC=CC=C12



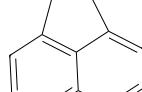
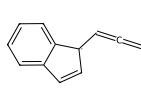
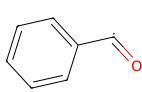
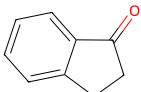
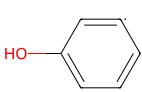
C9H7
InChI=1S/C9H7/c1-2-5-9-7-3-6-8/h9-4-1/h1-7H
[CH]1C=C2C(=C=C1)=CC=C2

NAPH-O-A
InChI=1S/C10H70/c11-10-7-3-5-8/h4-1-2-6-9(8)10/h1-7H
[0]C1C2C(=CC=C1)=CC=C2

NAPH-O-B
InChI=1S/C10H70/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H
C1C2C(=CC=C1)=CC=C2

C6H4CH3_LMPD_1
InChI=1S/C7H7/c1-7-5-3-2-4-6-7/h2-3,5-6H,1H3
CC1=C[CH]C=CC=1

C6H4CH3_LMPD_3
InChI=1S/C7H7/c1-7-5-3-2-4-6-7/h2-5H,1H3
CC1=CC=CC=[C]1



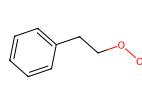
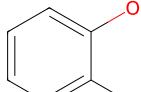
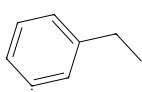
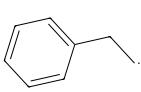
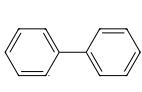
C6H4OH
InChI=1S/C6H5O/c7-6-4-2-1-3-5-6/h1-2,4-5,7H
OC1=C[C]C=CC=C1

C9H7O
InChI=1S/C9H70/c10-9-6-5-7-3-1/h2-4-8(7)9/h1-5H,6H2
O=C1C[CH]c2cccccc21

C6H5CO
InChI=1S/C7H5O/c8-6-7-4-2-1-3-5-7/h1-5H
O=[C]C1=CC=CC=C1

C9H6C3H3
InChI=1S/C12H9/c1-2-5-10-8-9-1-6-3-4-7-12(10)11/h3-9H,1H2
C=C=C[C]1C=CC2=CC=CC=C12

A2R5H
InChI=1S/C12H9/c1-3-9-4-2-6-11-8-7-10(5-1)12(9)11/h1-7H,8H2
[CH]1CC2=CC=CC=C2C1=CC=C3



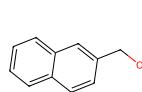
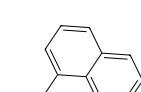
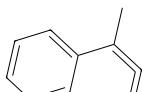
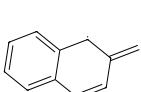
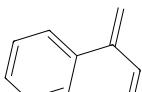
C12H9
InChI=1S/C12H9/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-9H
C1C=CC(=CC=C1)C2[C]C=CC=C2

C6H5CH2CH2
InChI=1S/C8H9/c1-2-8-6-4-3-5-7/h8-3-7H,1-2H2
[CH2]CC1C=CC=CC=C1

C6H4C2H5
InChI=1S/C8H9/c1-2-8-6-4-3-5-7/h8-3-4-6-7H,2H2,1H3
CCC1=CC=C[C]1C

OC6H4CH3
InChI=1S/C7H7/c1-6-4-2-3-5-7(6)8/h2-5H,1H3
CC1C(=CC=C1)[0]

C6H5CH2CH2OO
InChI=1S/C8H9O2/c9-10-7-6-8-4-2-1-3-5-8/h1-5H,6-7H2
[0]OCCC1C=CC=CC=C1



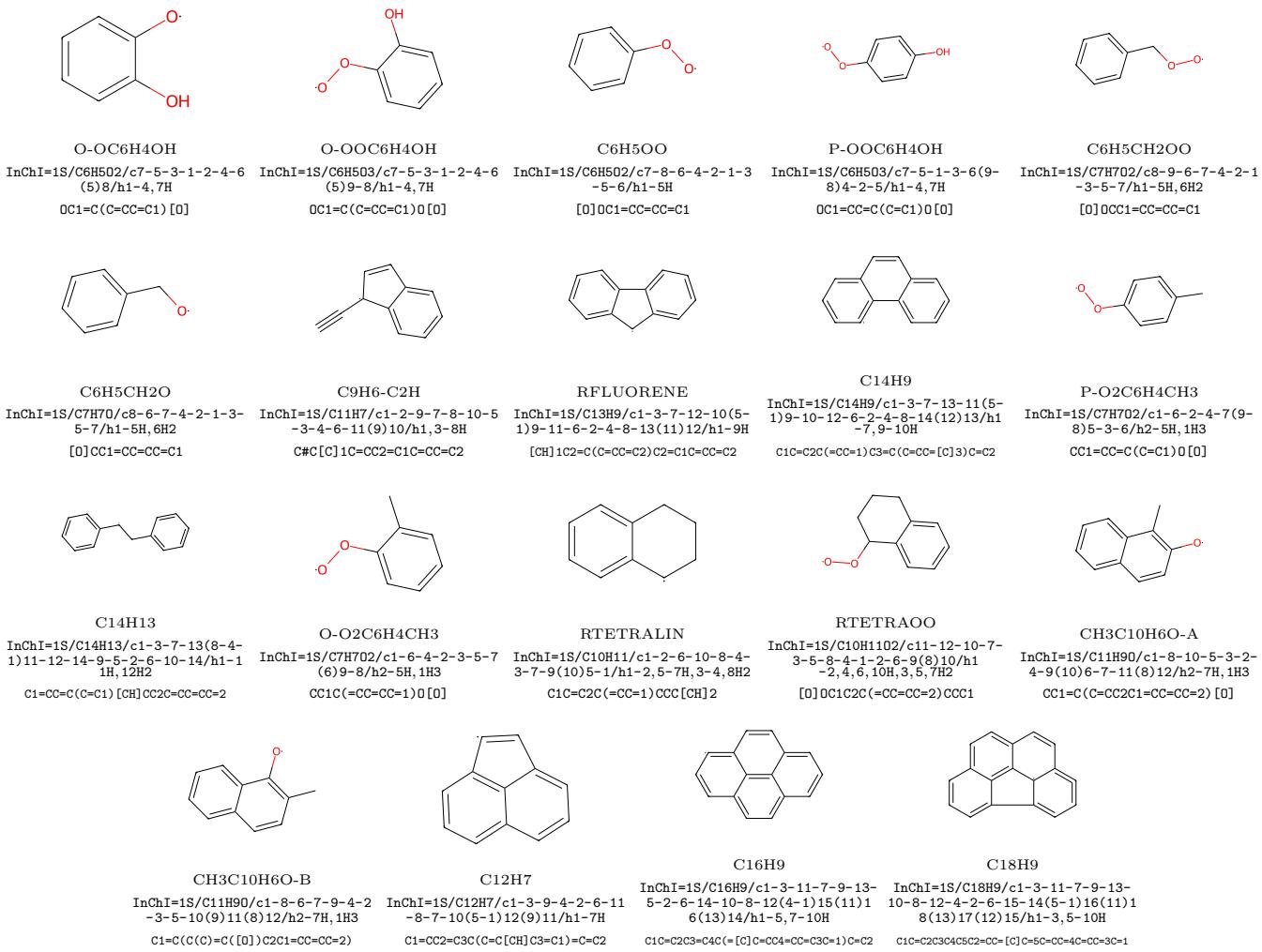
C10H7CH2-A
InChI=1S/C11H9/c1-9-5-4-7-10-6/h2-8H,1H2
[CH2]C1=C2C=CC=CC=C1

C10H7CH2-B
InChI=1S/C11H9/c1-9-6-7-10-4-2/h3-5-11(10)8-9/h2-8H,1H2
C1=C2C=C([CH2])C=CC2=CC=C1

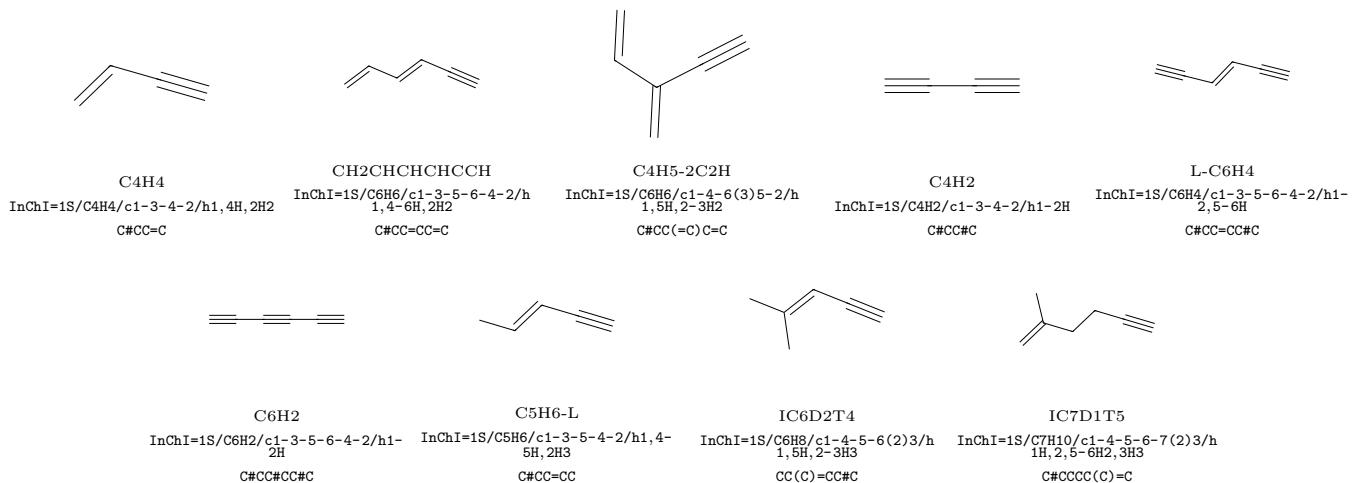
C10H6CH3-A
InChI=1S/C11H9/c1-9-5-4-7-10-6/h2-4,6-8H,1H3
CC1=C=CC[CH]c2cccccc21

C10H7CH2O-A
InChI=1S/C11H9O/c12-8-10-6-3-5/h4-1-2-7-11(9)10/h1-7H,8H2
[0]CC1=C2C(=C=C1)C=CC=C1

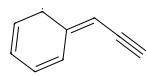
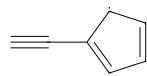
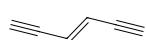
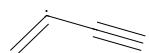
C10H7CH2O-B
InChI=1S/C11H9O/c12-8-9-5-6-10/h3-1-2-4-11(10)7-9/h1-7H,8H2
C1=C2C(C=C(C[0])C=C2)=CC=C1



14 Other hydro-carbon molecules



15 Other hydro-carbon radicals



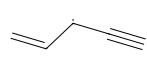
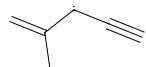
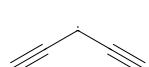
C4H3-N
InChI=1S/C4H3/c1-3-4-2
[CH]=CC#C

C4H3-I
InChI=1S/C4H3/c1-3-4-2/h1H,2H2
C#C[C]=C

C6H3
InChI=1S/C6H3/c1-3-5-6
2,5H
C#CC=C=C=[CH]

ChI=1S/C7H5/c1-2-7-5-3
/h1,3-6H

C6H5C3H2_LMPD_1
 hI=1S/C9H7/c1-2-6-9-7-4-3-5
 -8-9/h1,3-8H
 [CH]=C=CC1=CC=CC=C1

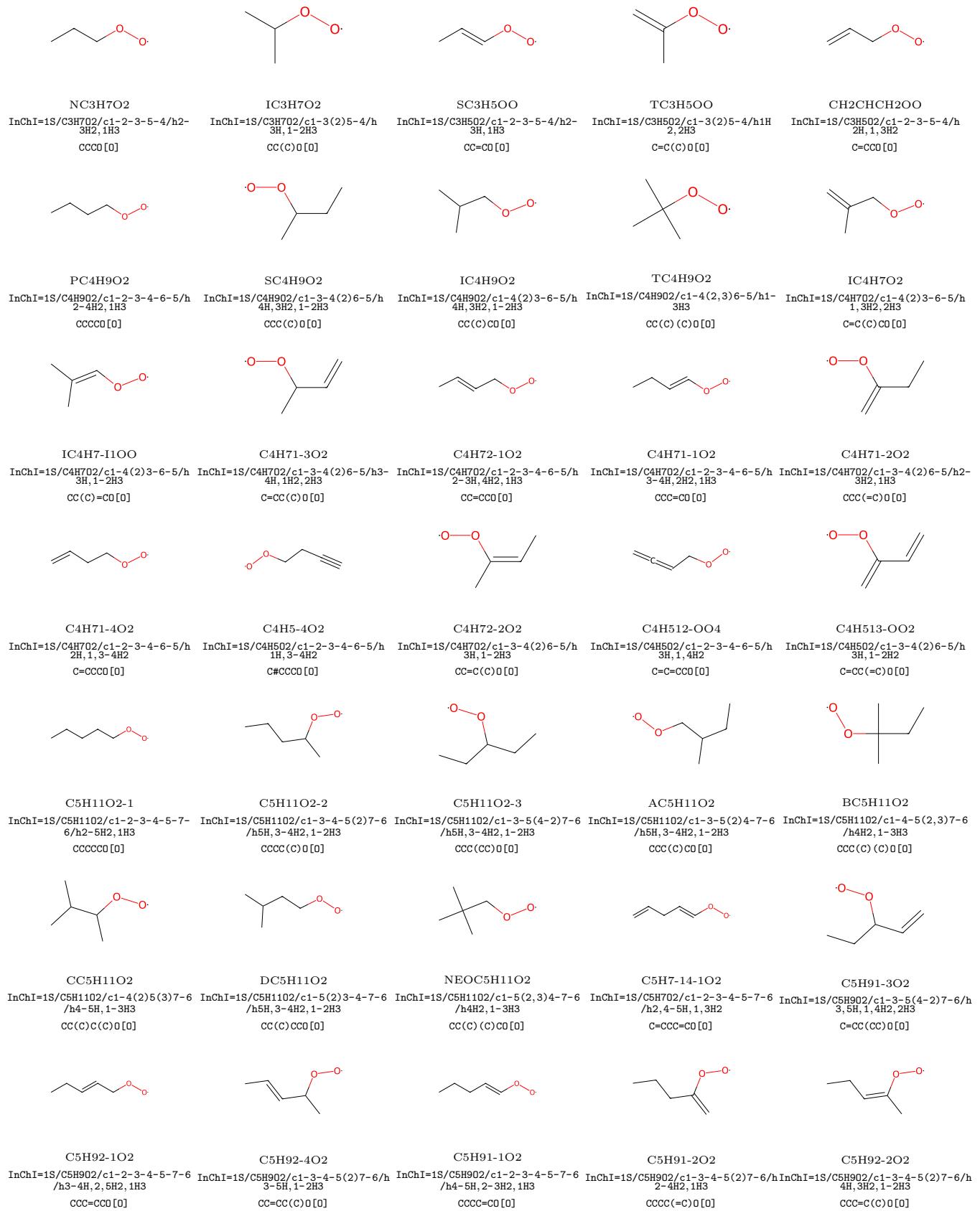


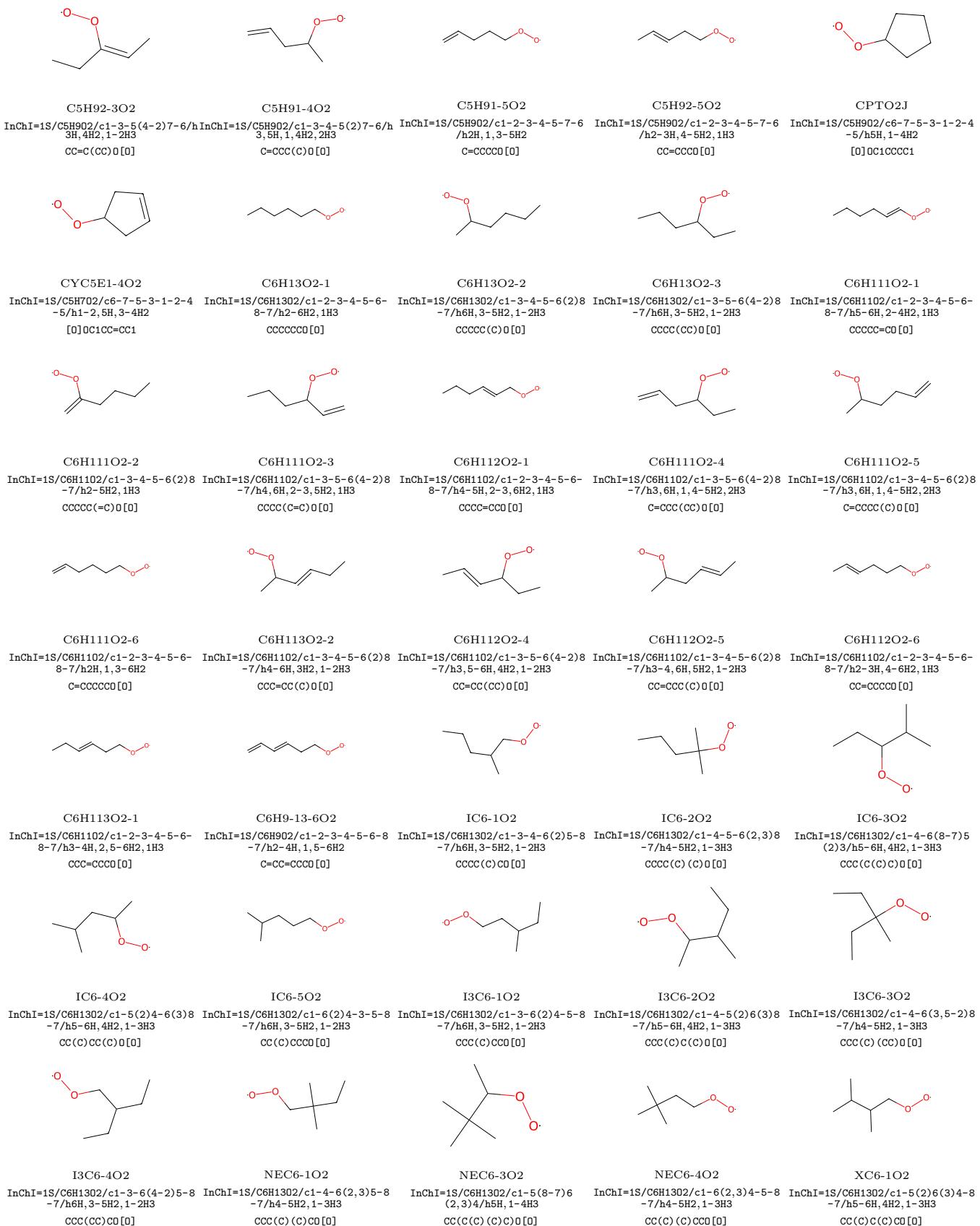
C5H3
InChI=1S/C5H3/c1-3-5-4-2/h1-2,5H
C#CC=C=[CH]

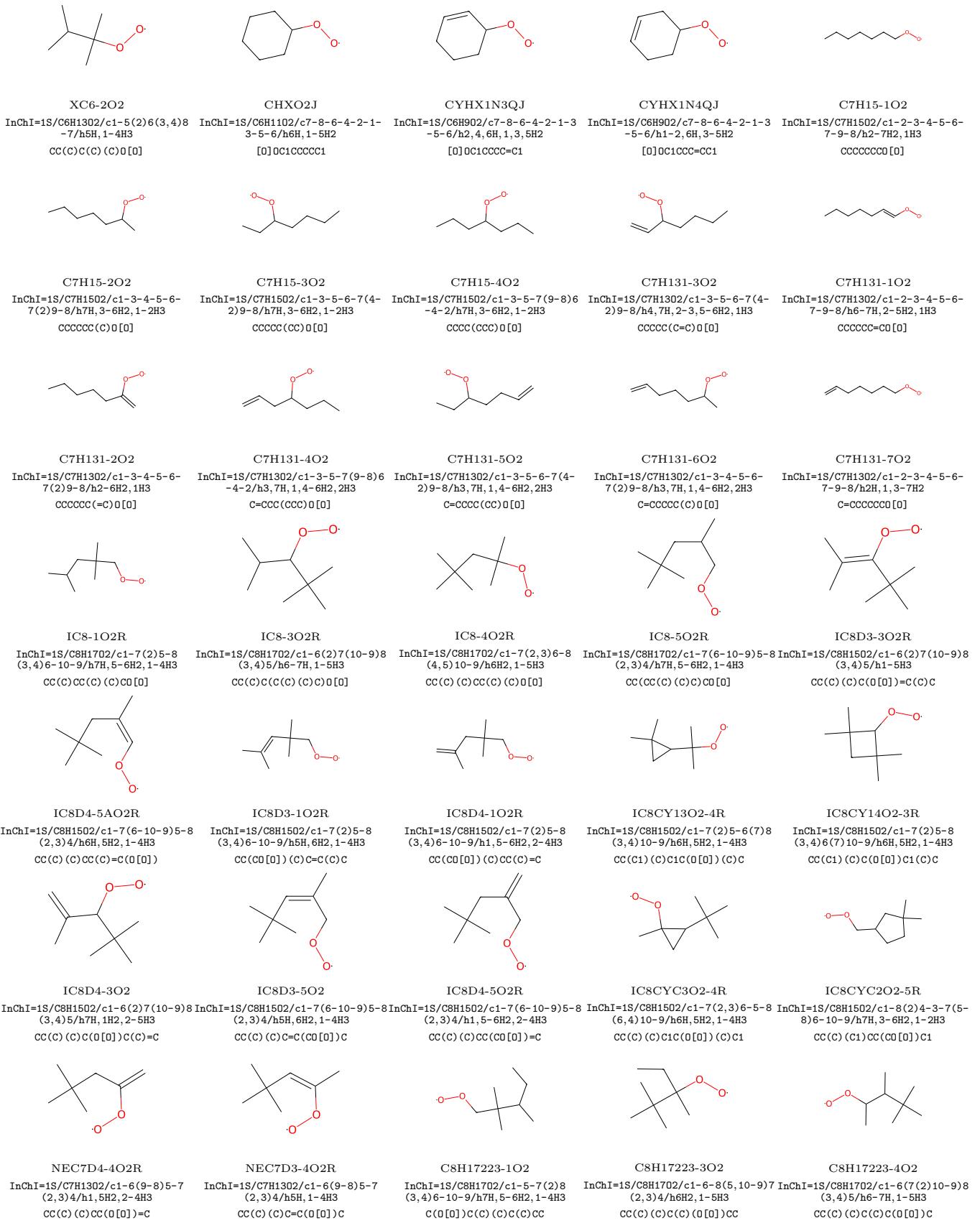
IC6D2T4-1R
 InChI=1S/C6H7/c1-4-5-6(2)3/h1,5H,2H2,3H3
 CC([CH2])=CC#C

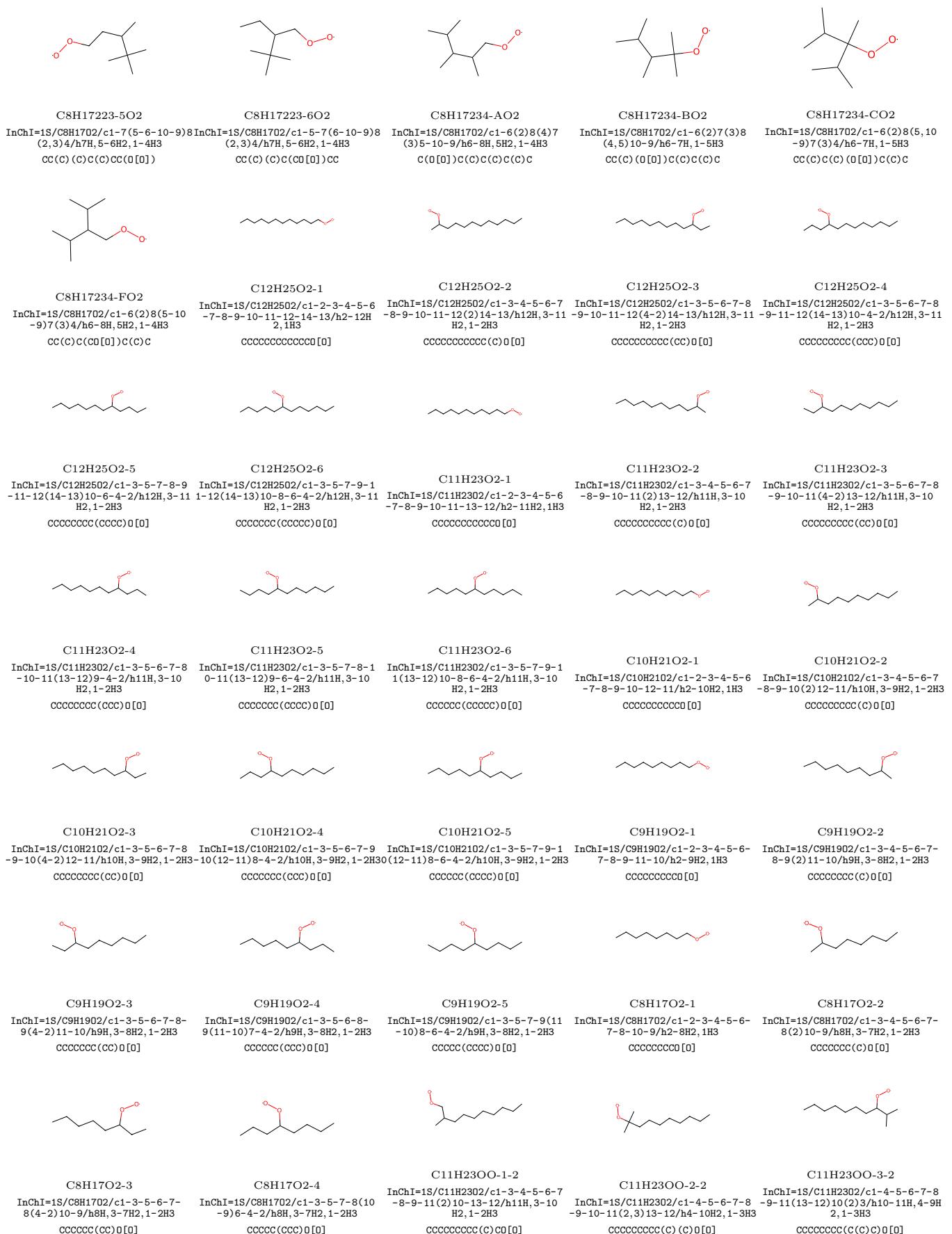
C#CCVCCJ
 InChI=1S/C5H5/c1-3-5-4-2/h1,4-5H,2H2
 [CH2]C=CC#C

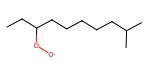
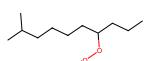
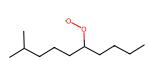
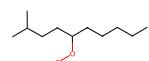
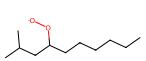
16 Peroxy radicals











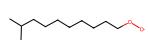
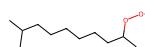
C11H23OO-4-2
InChI=1S/C11H23O2/c1-4-5-6-7-8
-11(13-12)9-10(2)3/h10-11H,4-9H
2,1-3H3
CCCCCCC(CC(C)C)O[0]

C11H23OO-5-2
InChI=1S/C11H23O2/c1-4-5-6-7-1
1(13-12)9-8-10(2)3/h10-11H,4-9H
-12)9-6-7-10(2)3/h10-11H,4-9H
2,1-3H3
CCCCCC(CCC(C)C)O[0]

C11H23OO-6-2
InChI=1S/C11H23O2/c1-4-5-8-11(13
InChI=1S/C11H23O2/c1-4-7-11(13-1
2)9-6-5-8-10(2)3/h10-11H,4-9H
2,1-3H3
CCCC(CCCC(C)C)O[0]

C11H23OO-7-2
InChI=1S/C11H23O2/c1-4-11(13-1
2)9-7-5-6-8-10(2)3/h10-11H,4-9H
2,1-3H3
CCCC(CCCC(C)C)O[0]

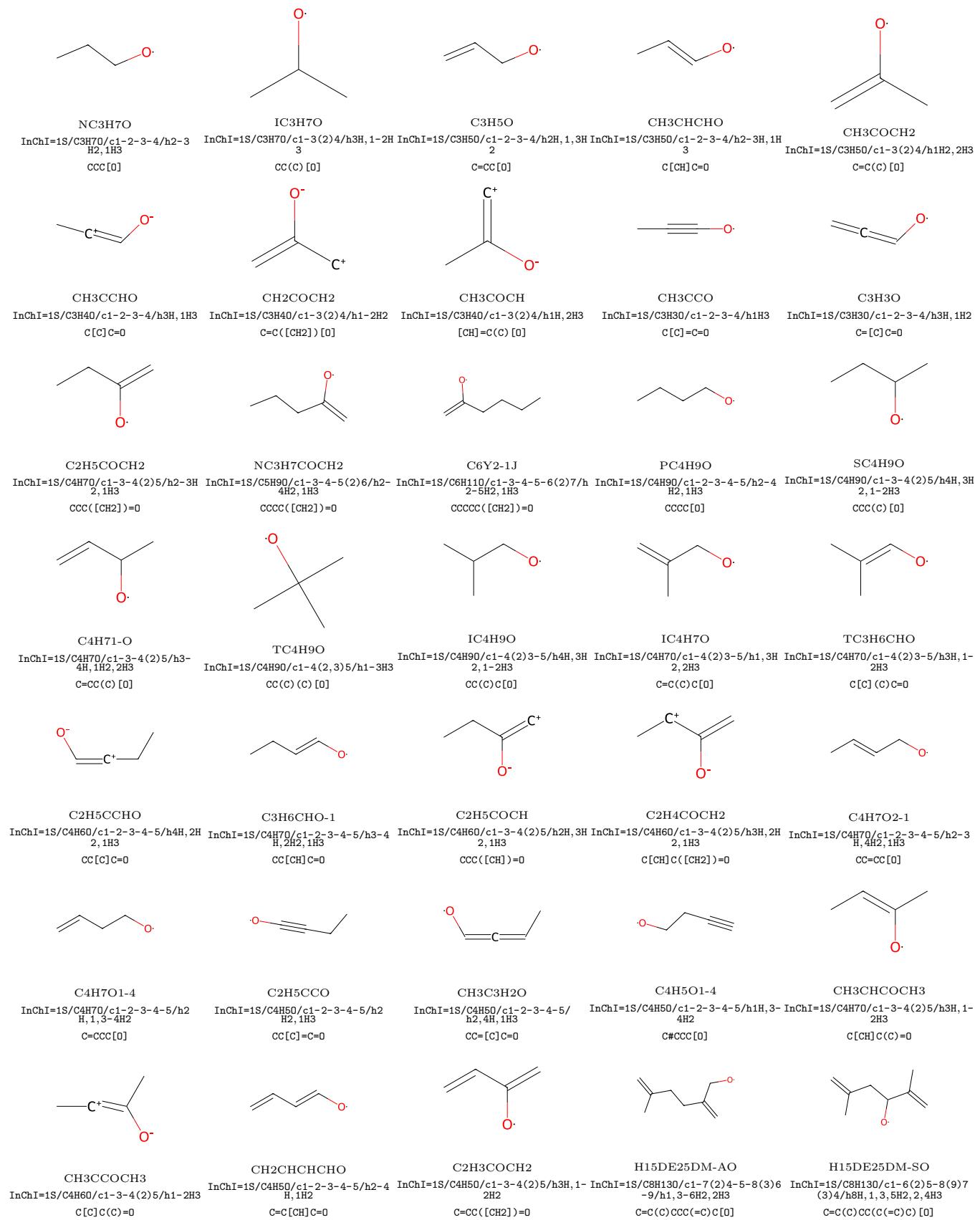
C11H23OO-8-2
InChI=1S/C11H23O2/c1-4-11(13-1
2)9-7-5-6-8-10(2)3/h10-11H,4-9H
2,1-3H3
CCC(CCCCC(C)C)O[0]

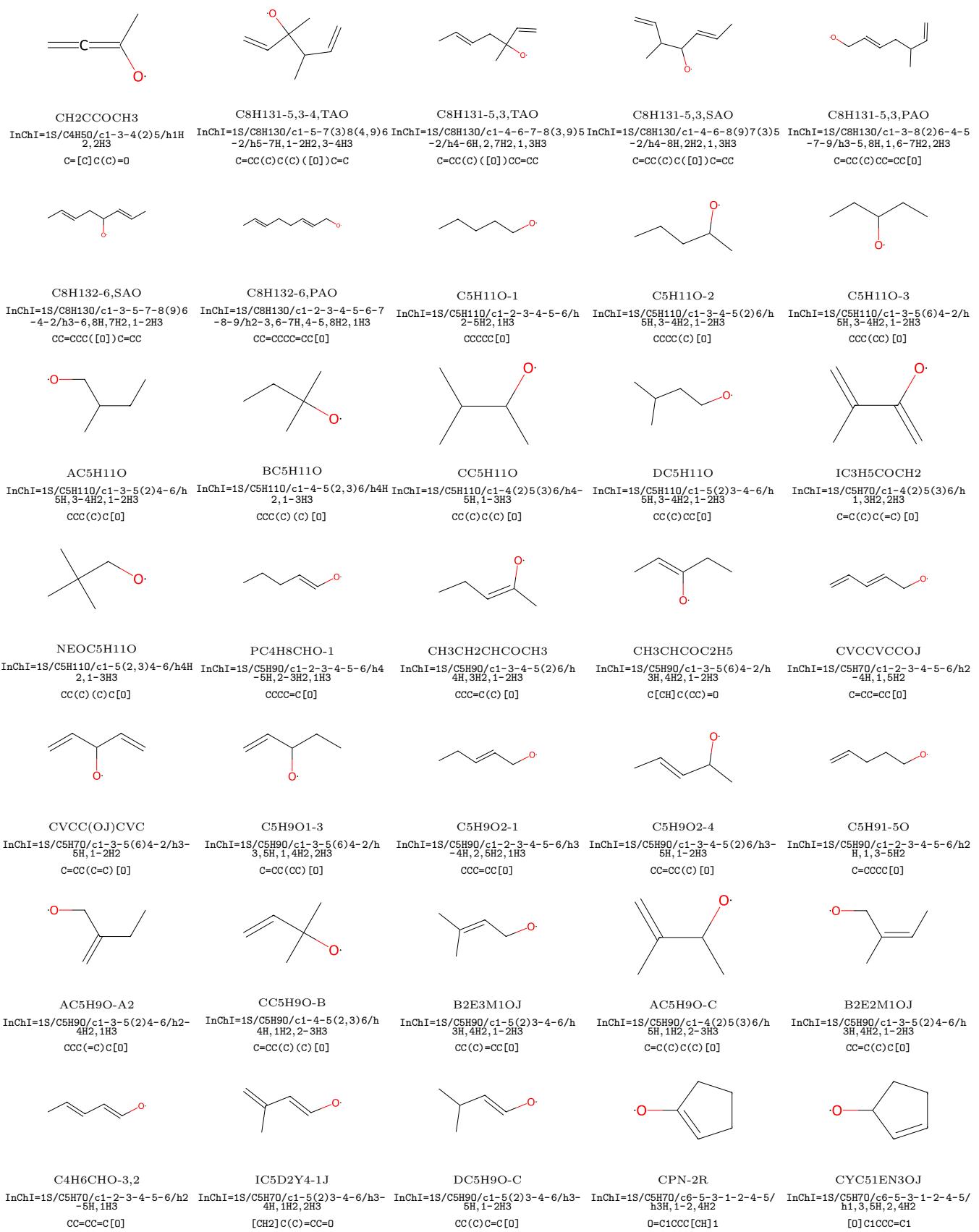


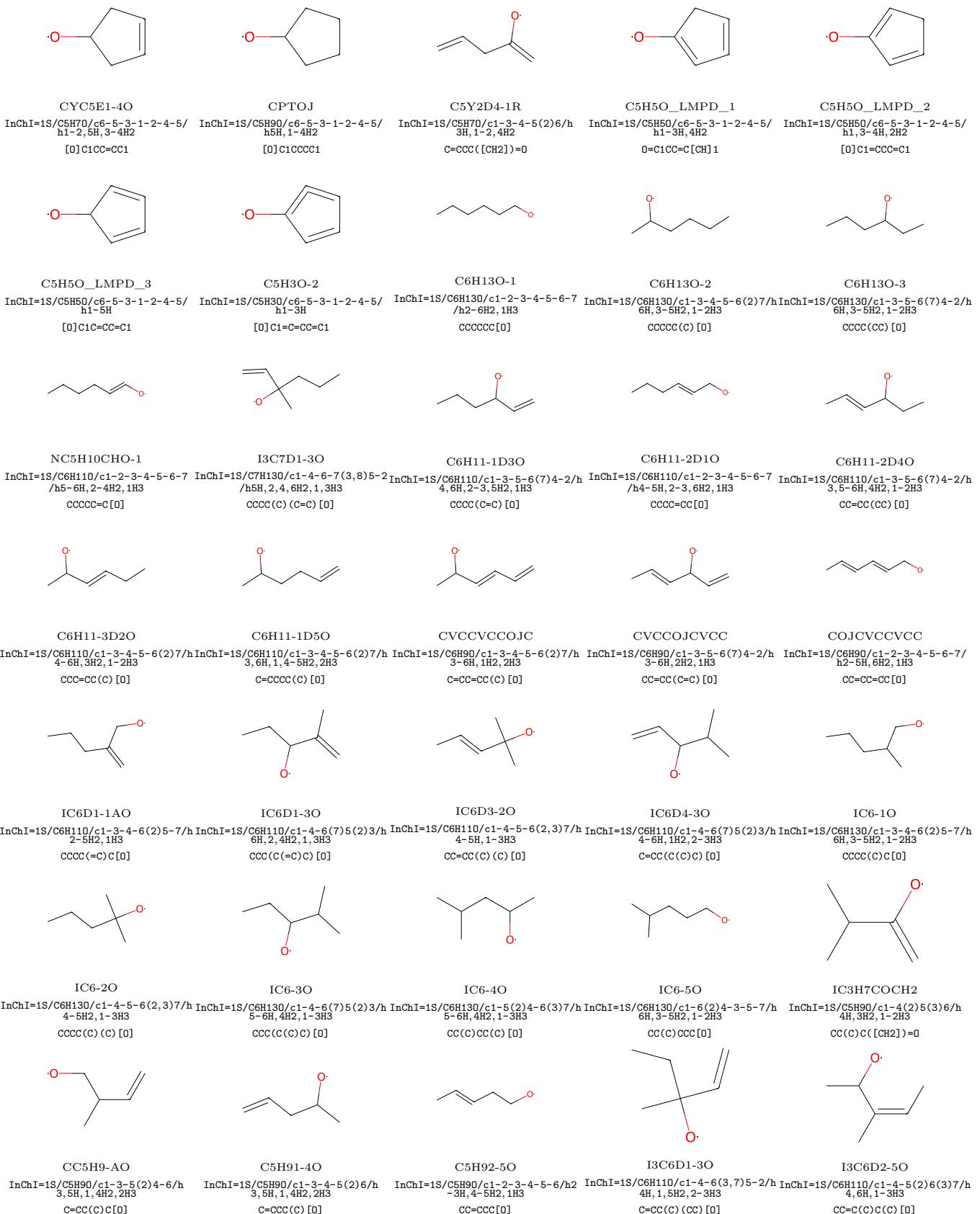
C11H23OO-9-2
InChI=1S/C11H23O2/c1-10(2)8-6-4
-5-7-9-11(3)13-12/h10-11H,4-9H
2,1-3H3
CC(C)CCCCCCC(C)O[0]

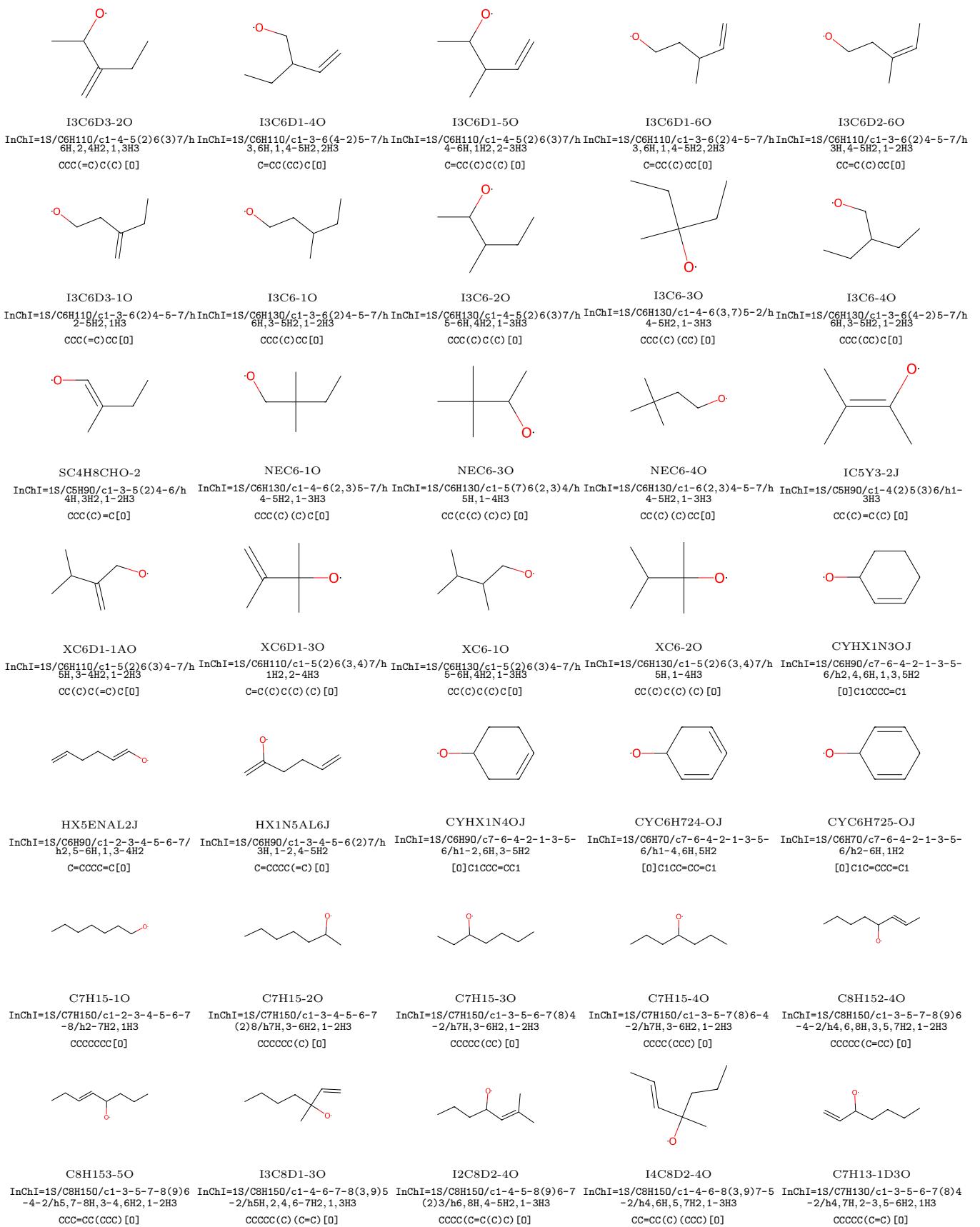
C11H23OO-10-2
InChI=1S/C11H23O2/c1-11(2)9-7-5
-3-4-6-8-10-13-12/h11H,3-10
H2,1-2H3
CC(O)CCCCCCCCO[0]

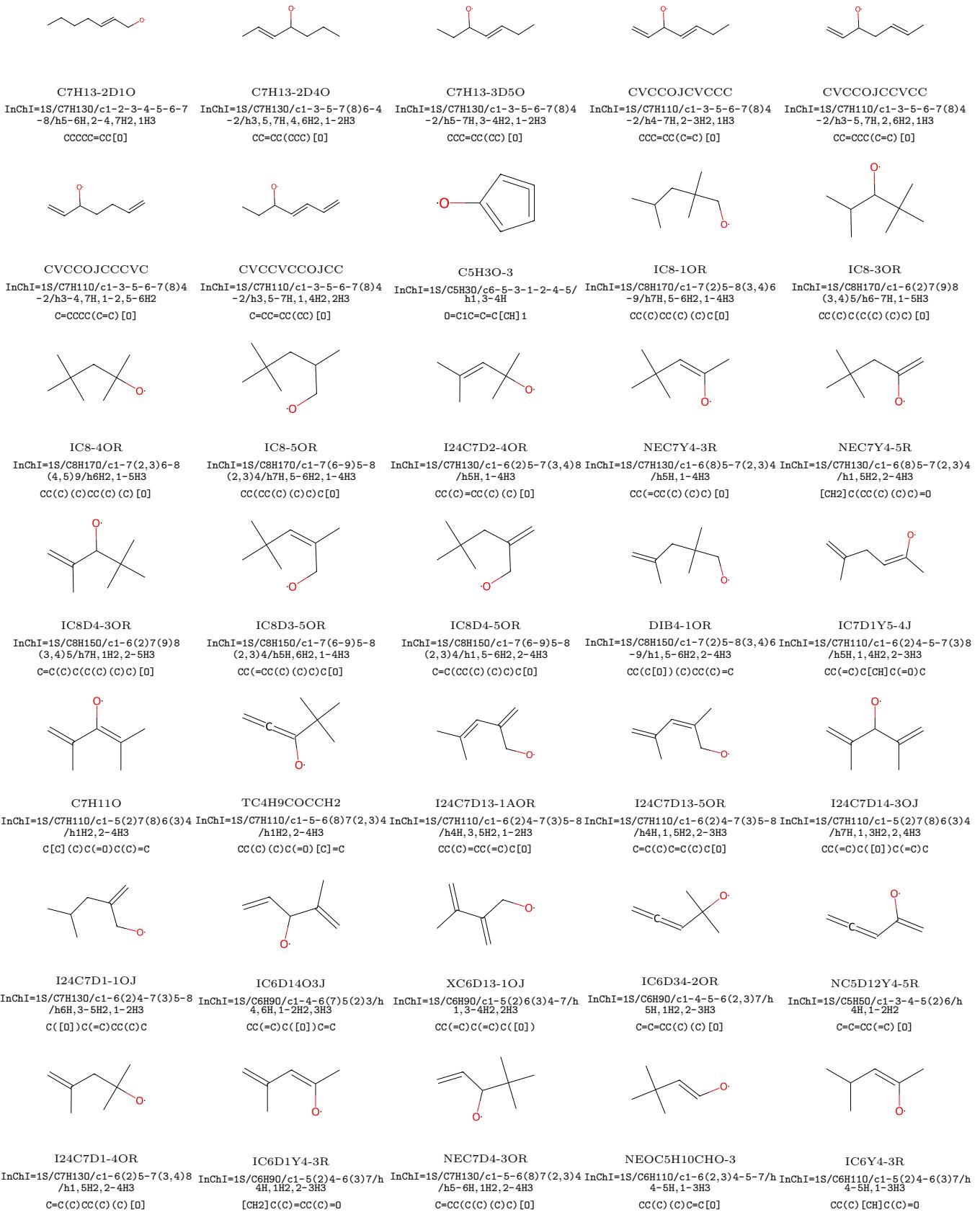
17 Oxy radicals

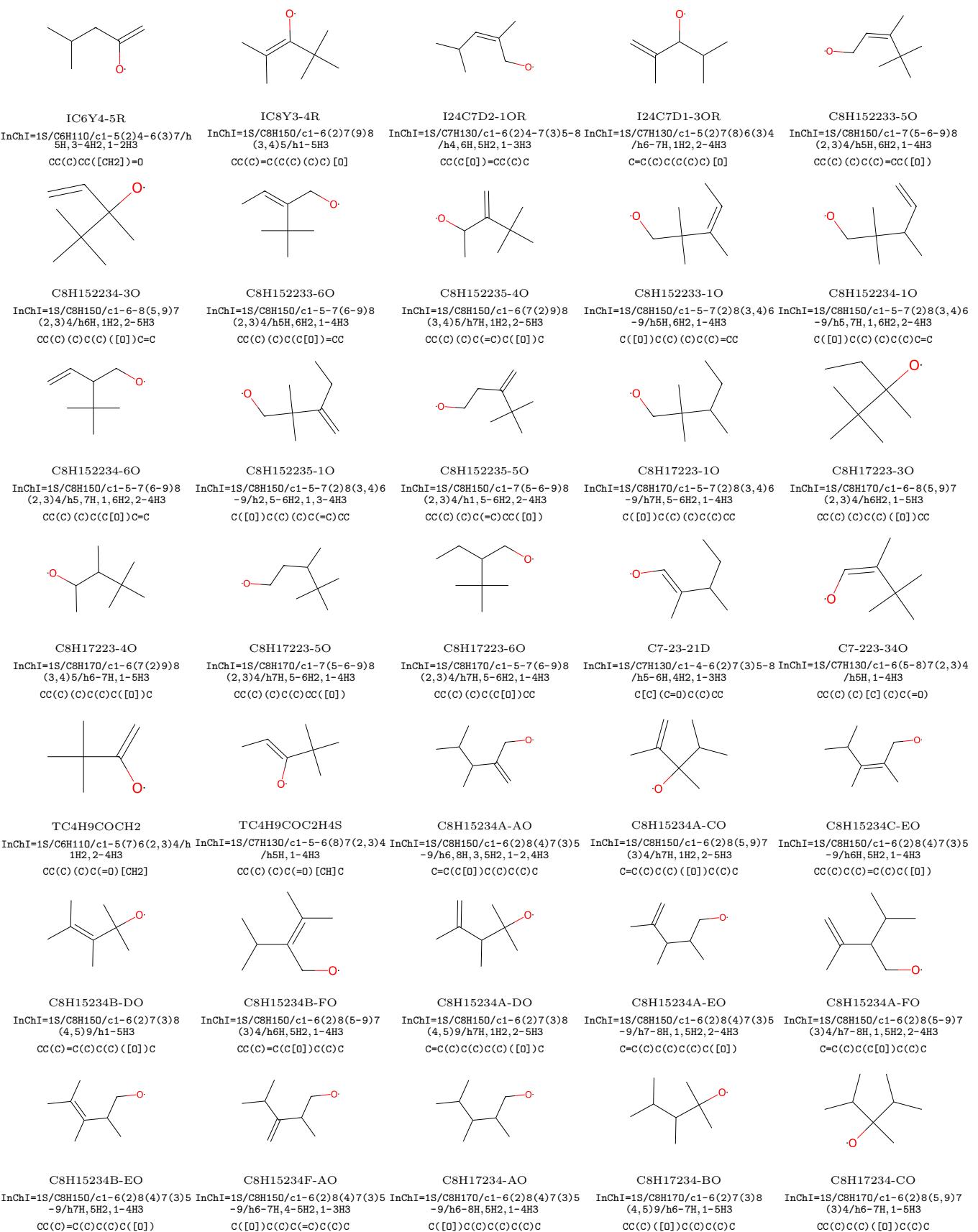


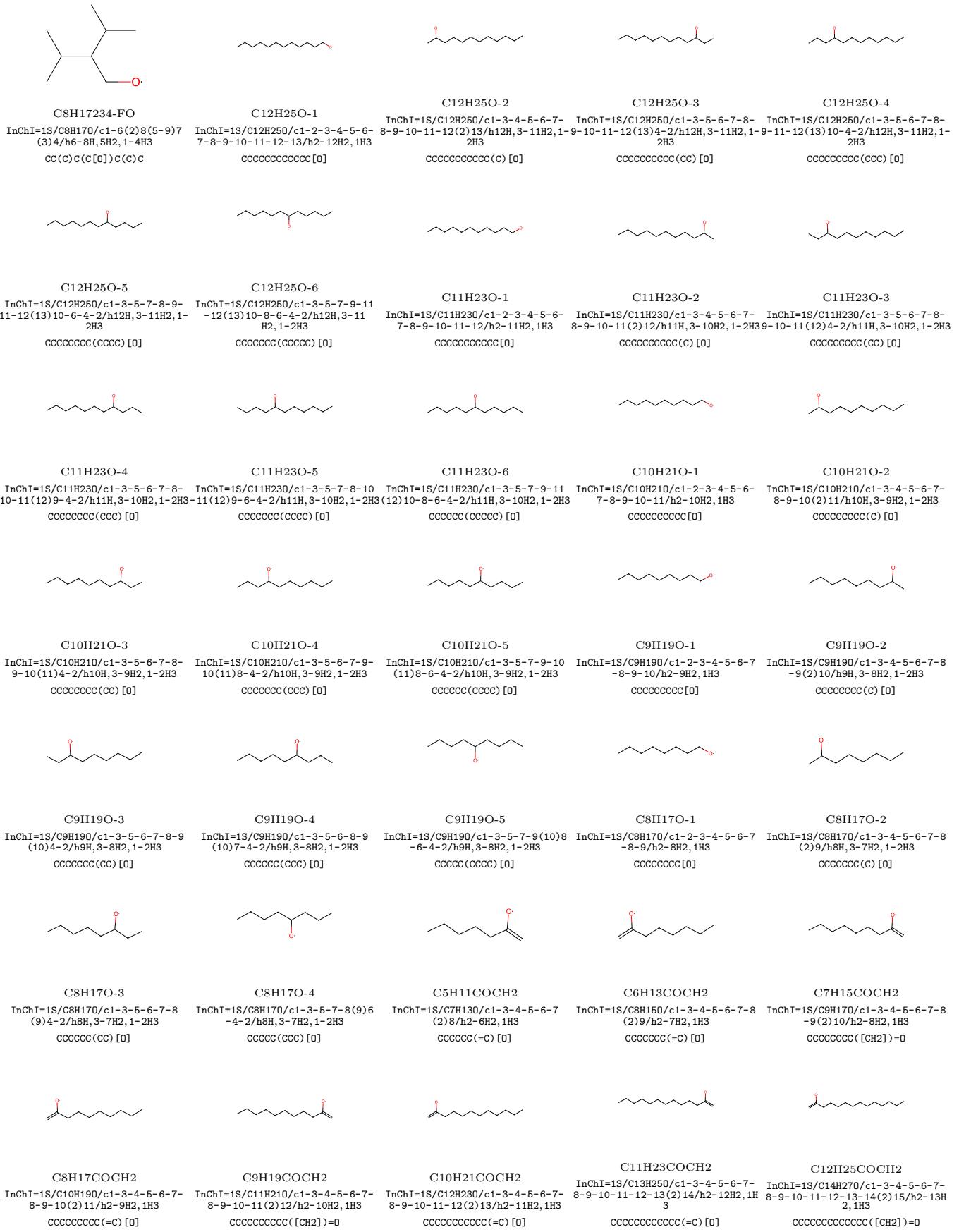














IC5H11COCH₂

InChI=1S/C7H13O/c1-6(2)4-5-7(3)8 InChI=1S/C8H15O/c1-7(2)5-4-6-8
/h6H,3-5H2,1-2H3 (3)9/h7H,3-6H2,1-2H3 InChI=1S/C9H17O/c1-8(2)6-4-5-7
-9(3)10/h8H,3-7H2,1-2H3 InChI=1S/C10H19O/c1-9(2)7-5-4-6
-8-10(3)11/h9H,3-8H2,1-2H3
CC(C)CCC(=C) [0] CC(C)CCCC(=C) [0] CC(C)CCCCC(=C) [0] CC(C)CCCCC(=C) [0]

IC6H13COCH₂

InChI=1S/C8H15O/c1-7(2)5-4-6-8
(3)9/h7H,3-6H2,1-2H3
CC(C)CCCC(=C) [0]

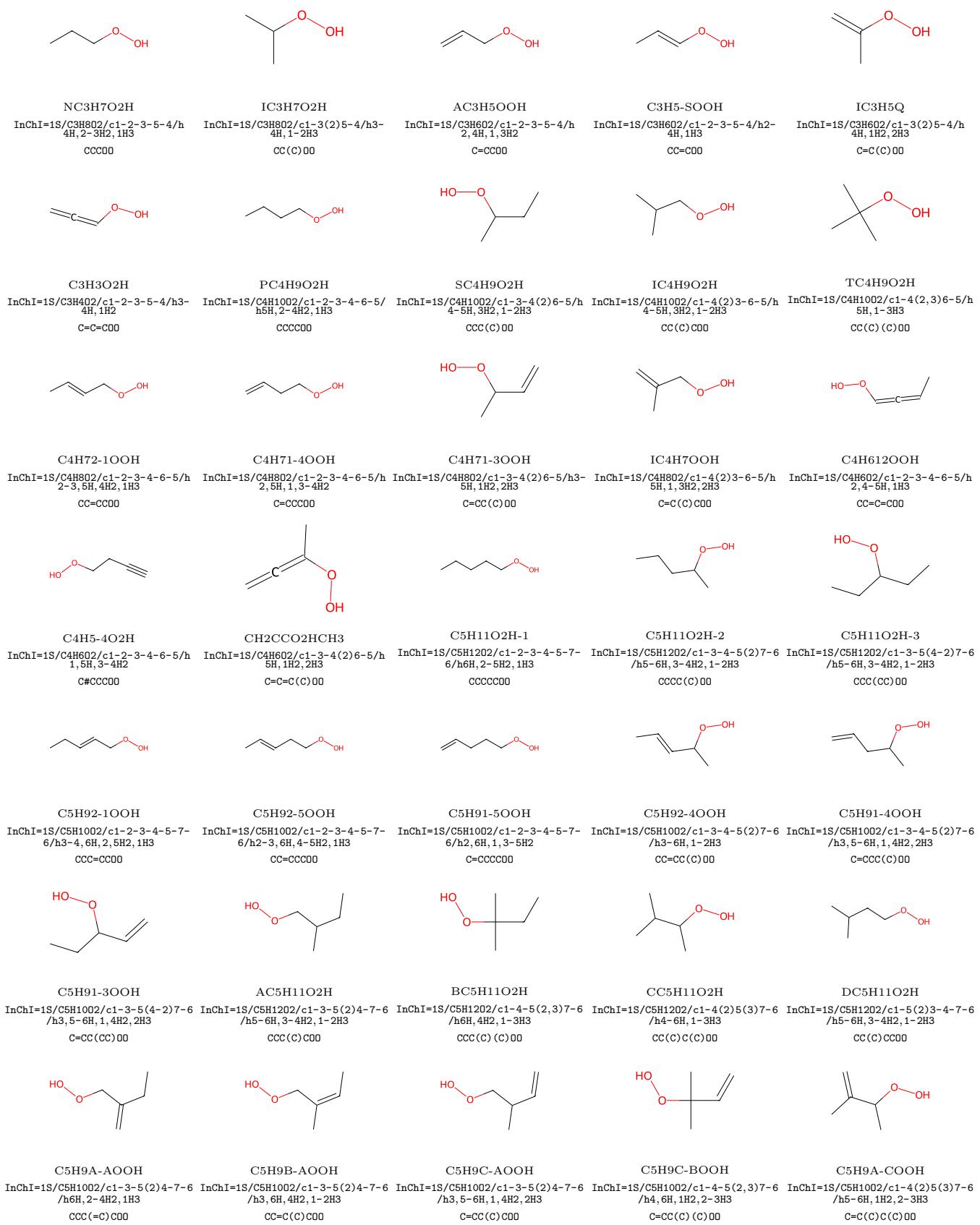
IC7H15COCH₂

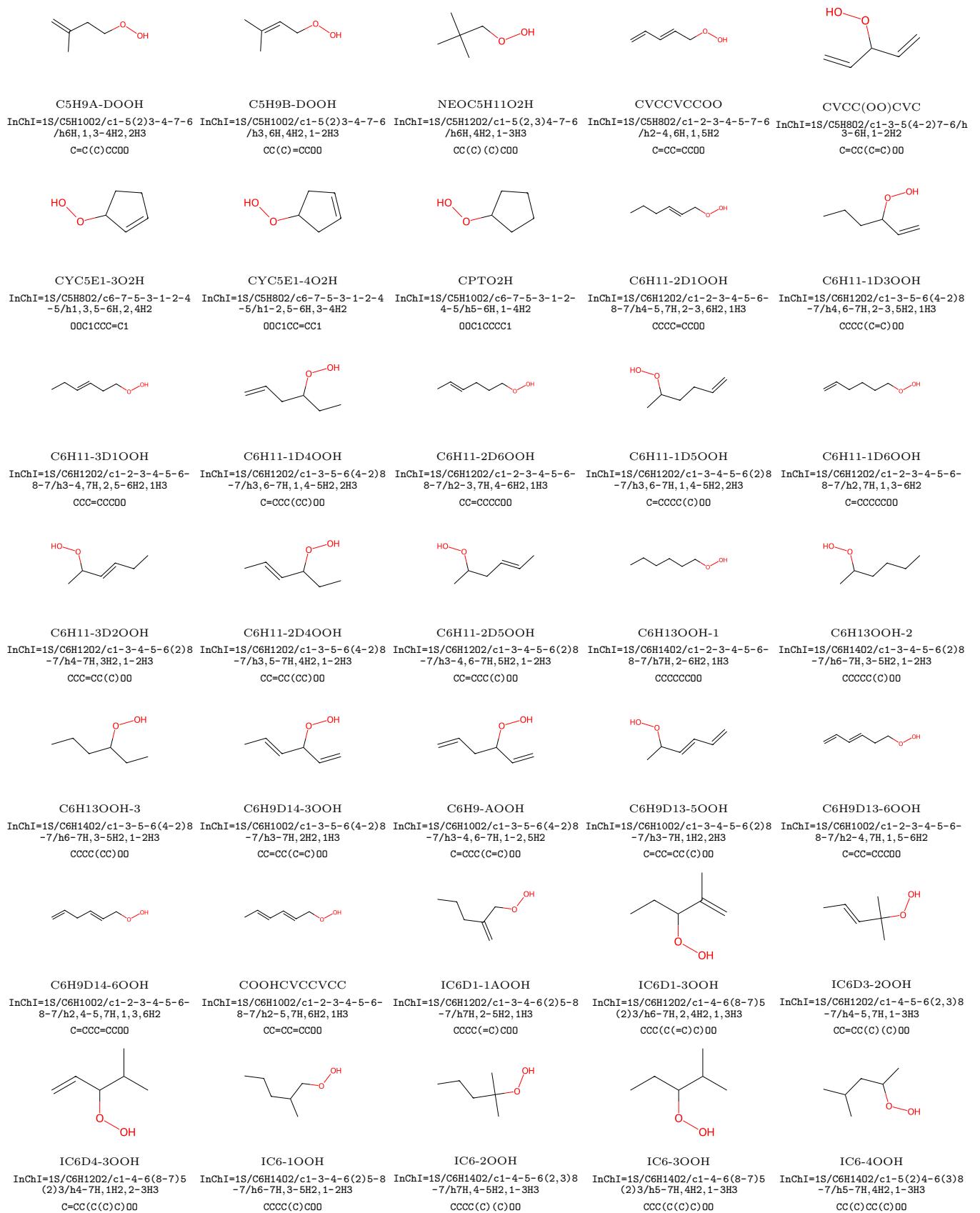
InChI=1S/C9H17O/c1-8(2)6-4-5-7
-9(3)10/h8H,3-7H2,1-2H3
CC(C)CCCC(=C) [0]

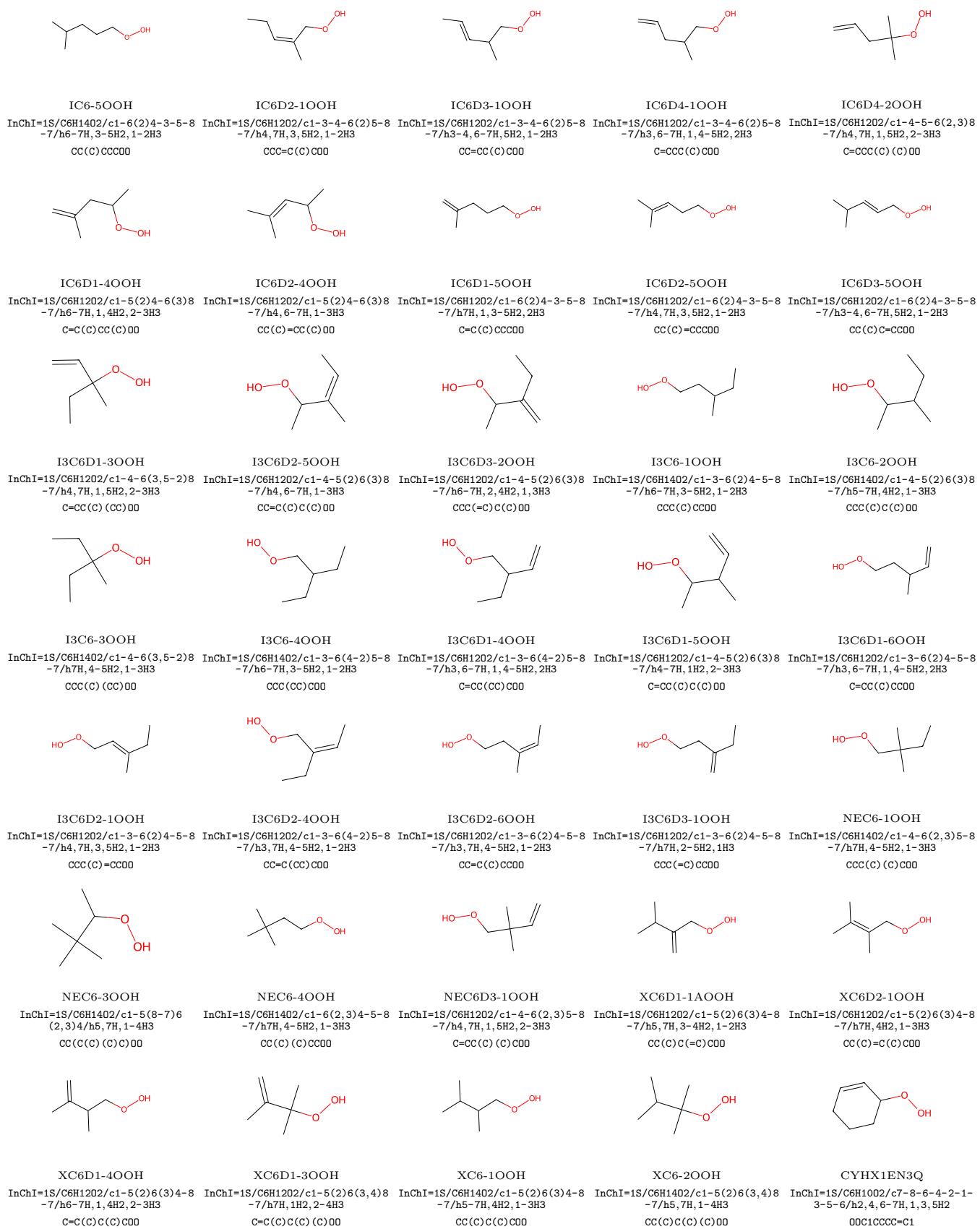
IC8H17COCH₂

InChI=1S/C10H19O/c1-9(2)7-5-4-6
-8-10(3)11/h9H,3-8H2,1-2H3
CC(C)CCCCC(=C) [0]

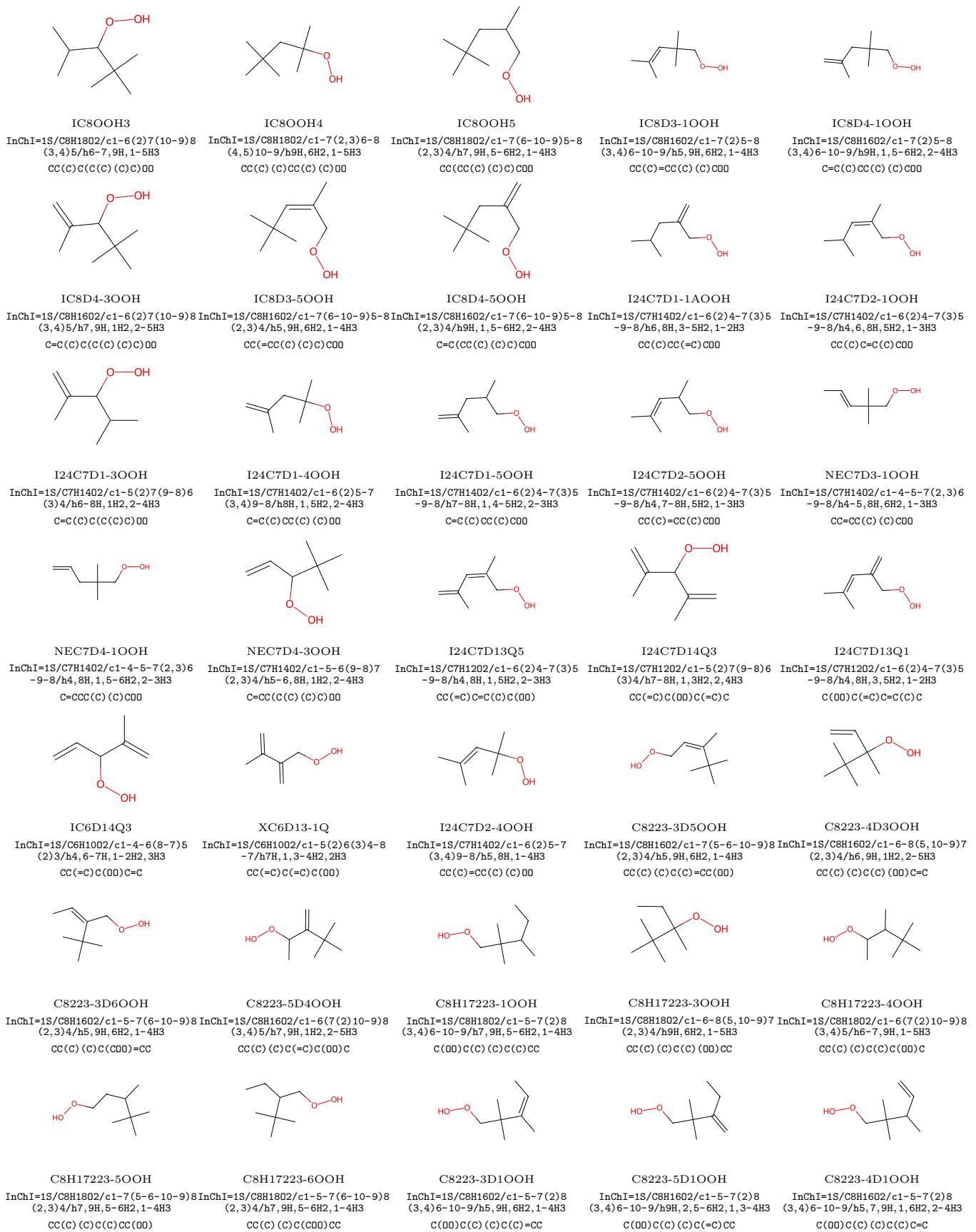
18 Hydroperoxides (molecules)

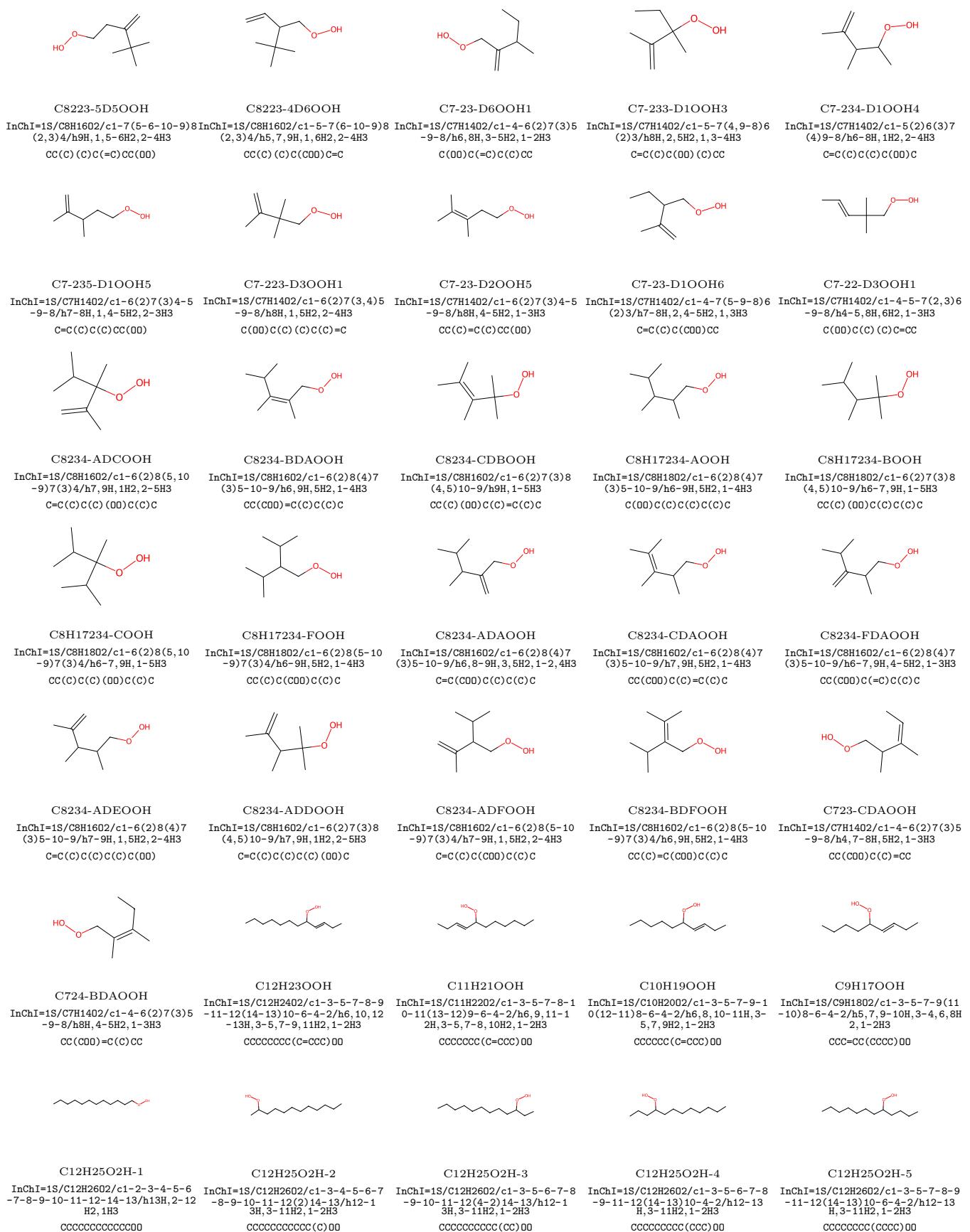


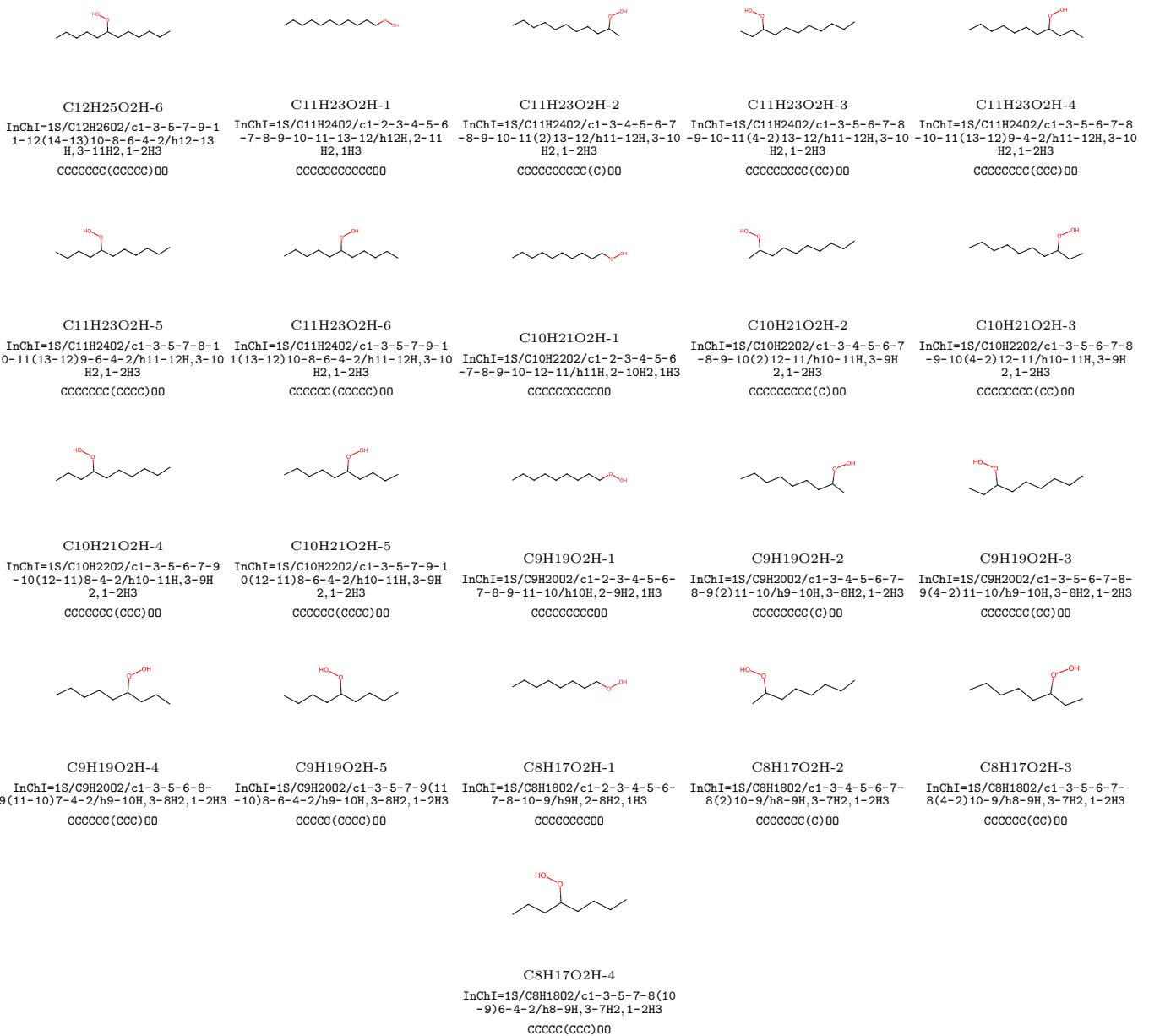




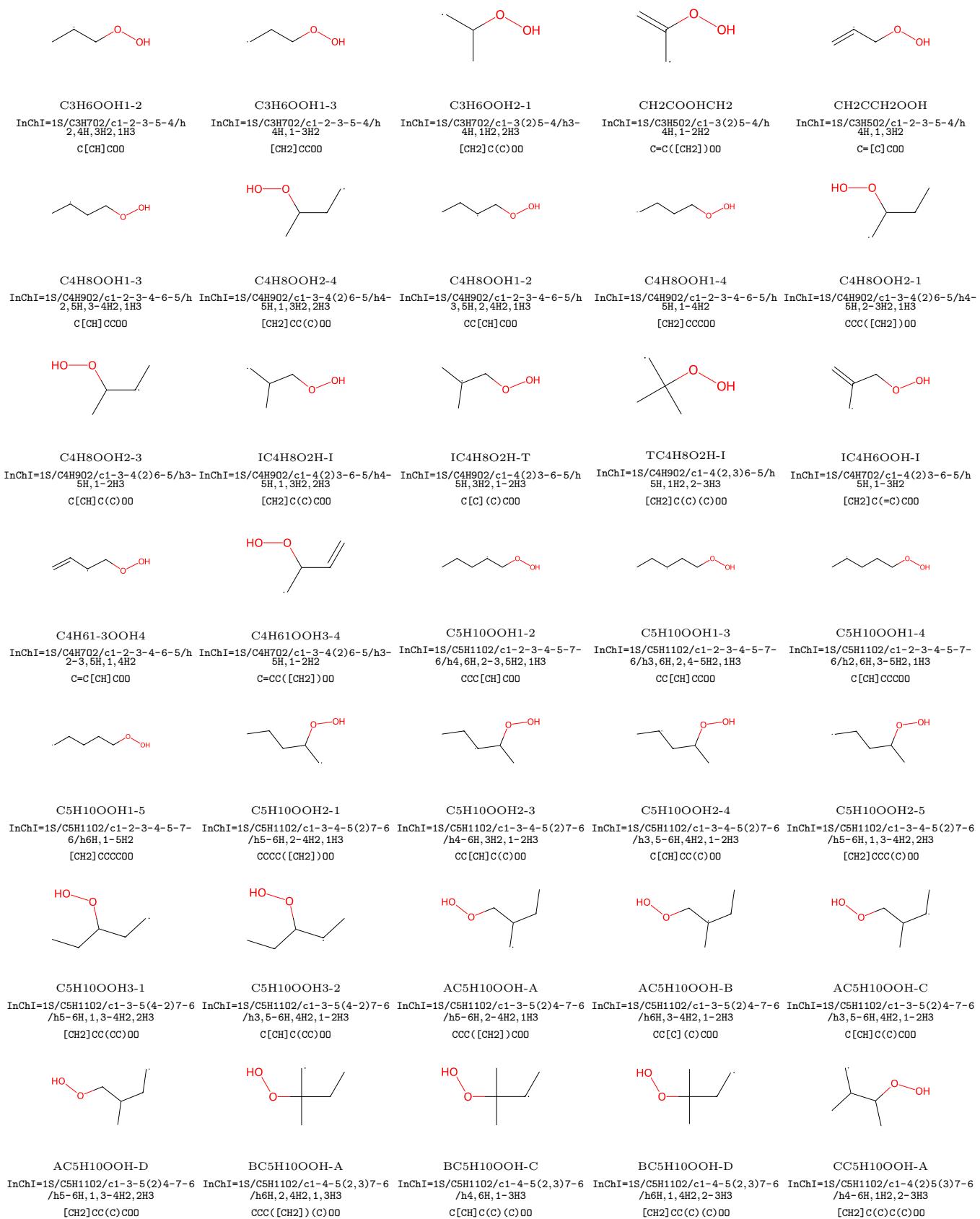


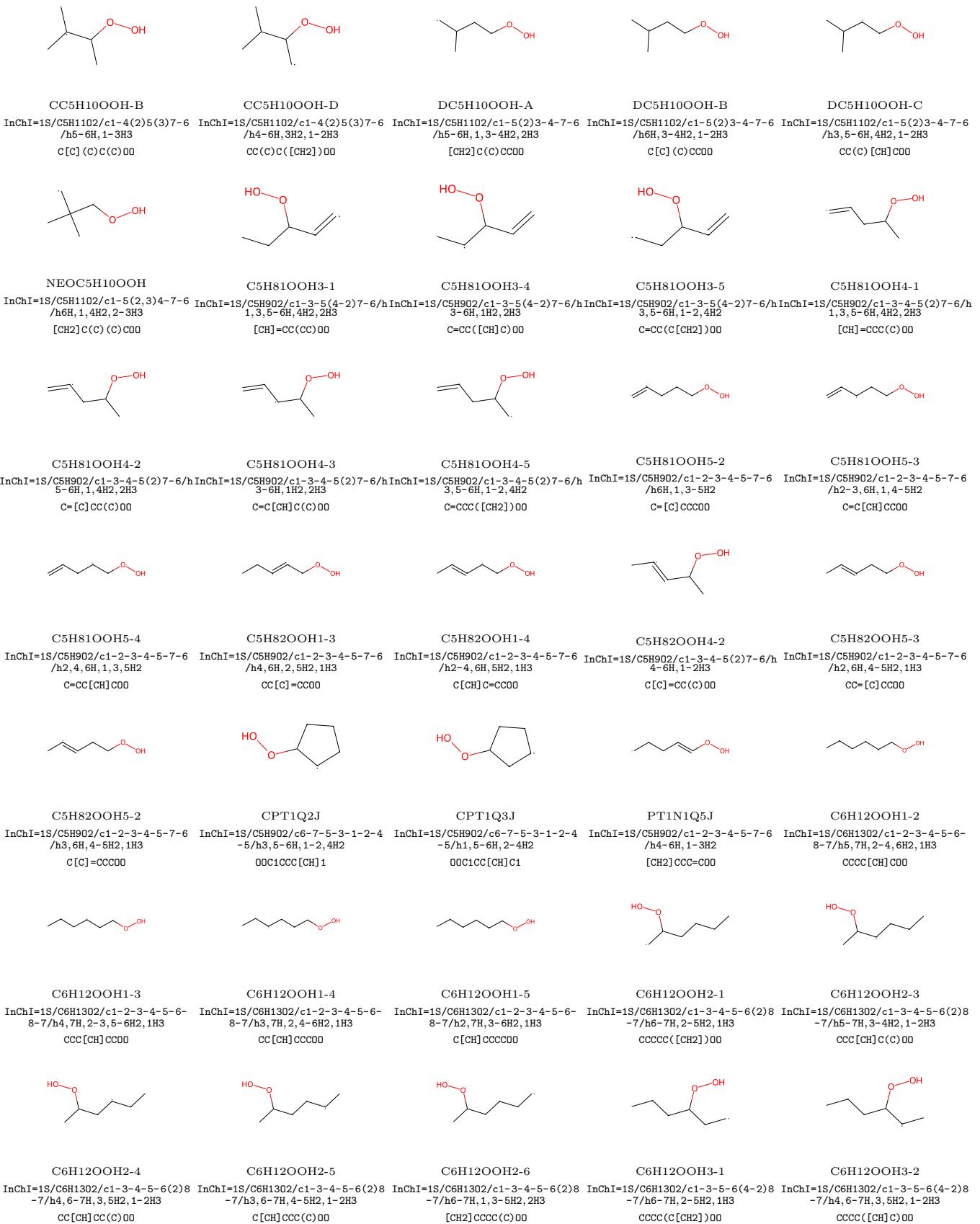


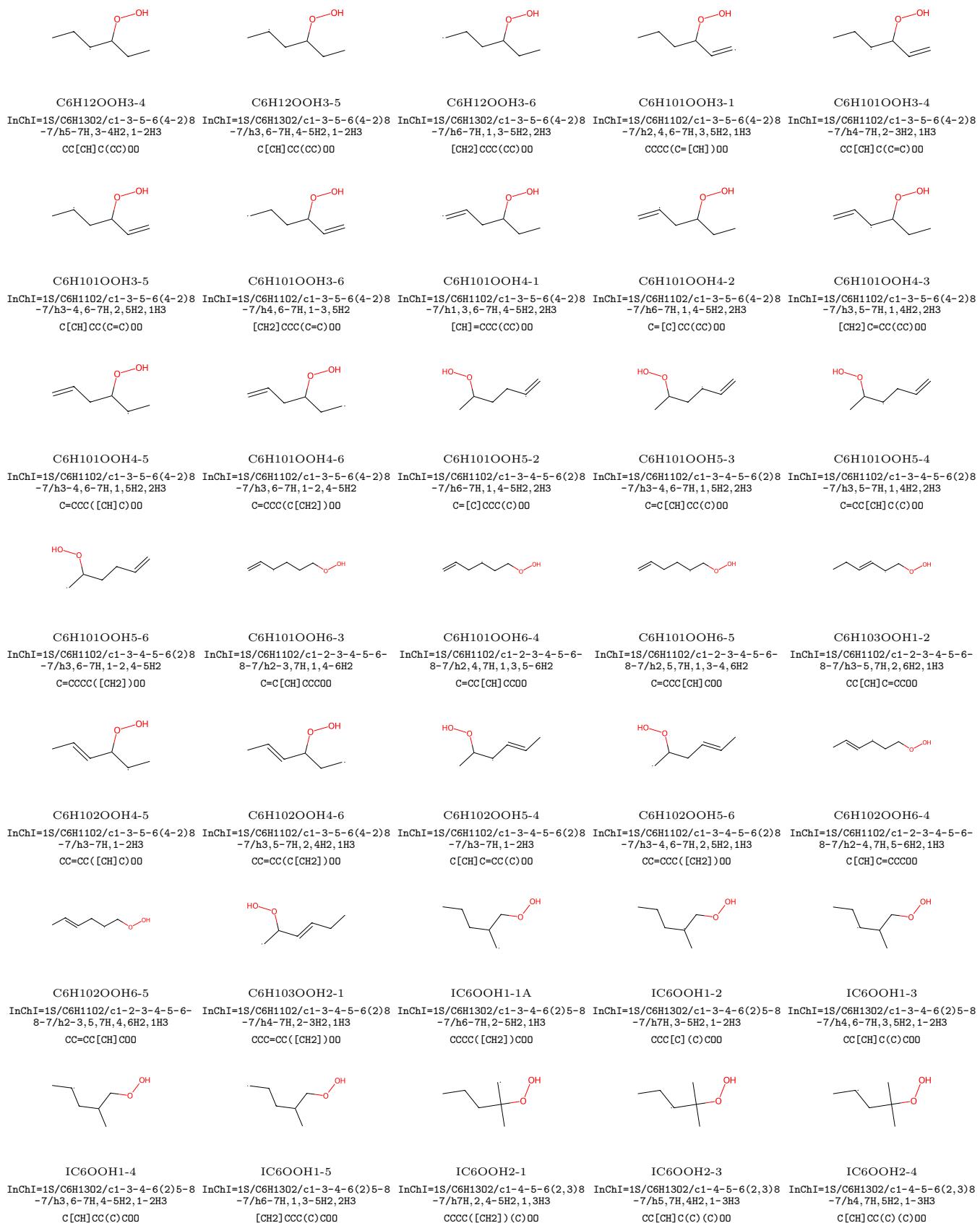


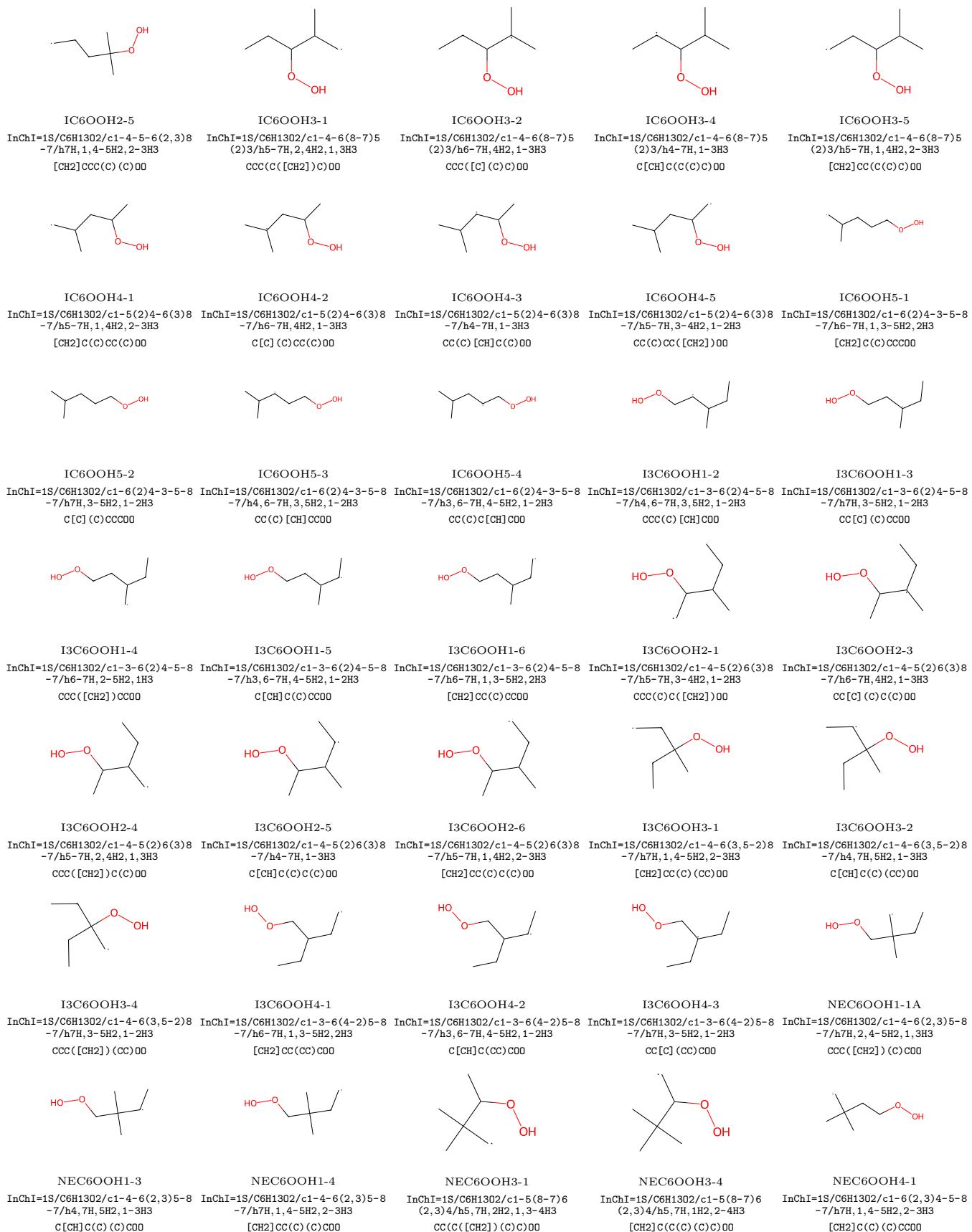


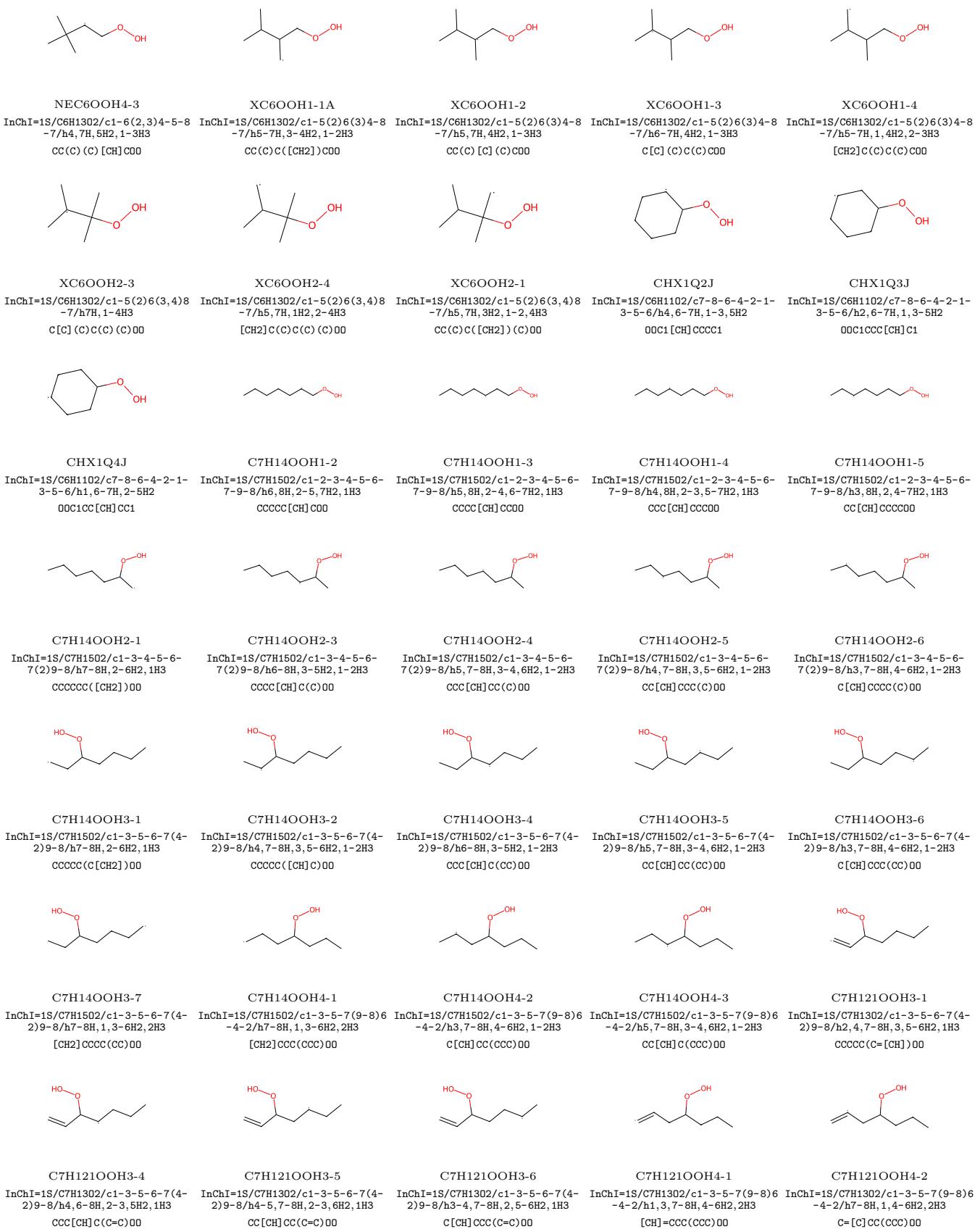
19 Hydroperoxides (radicals)

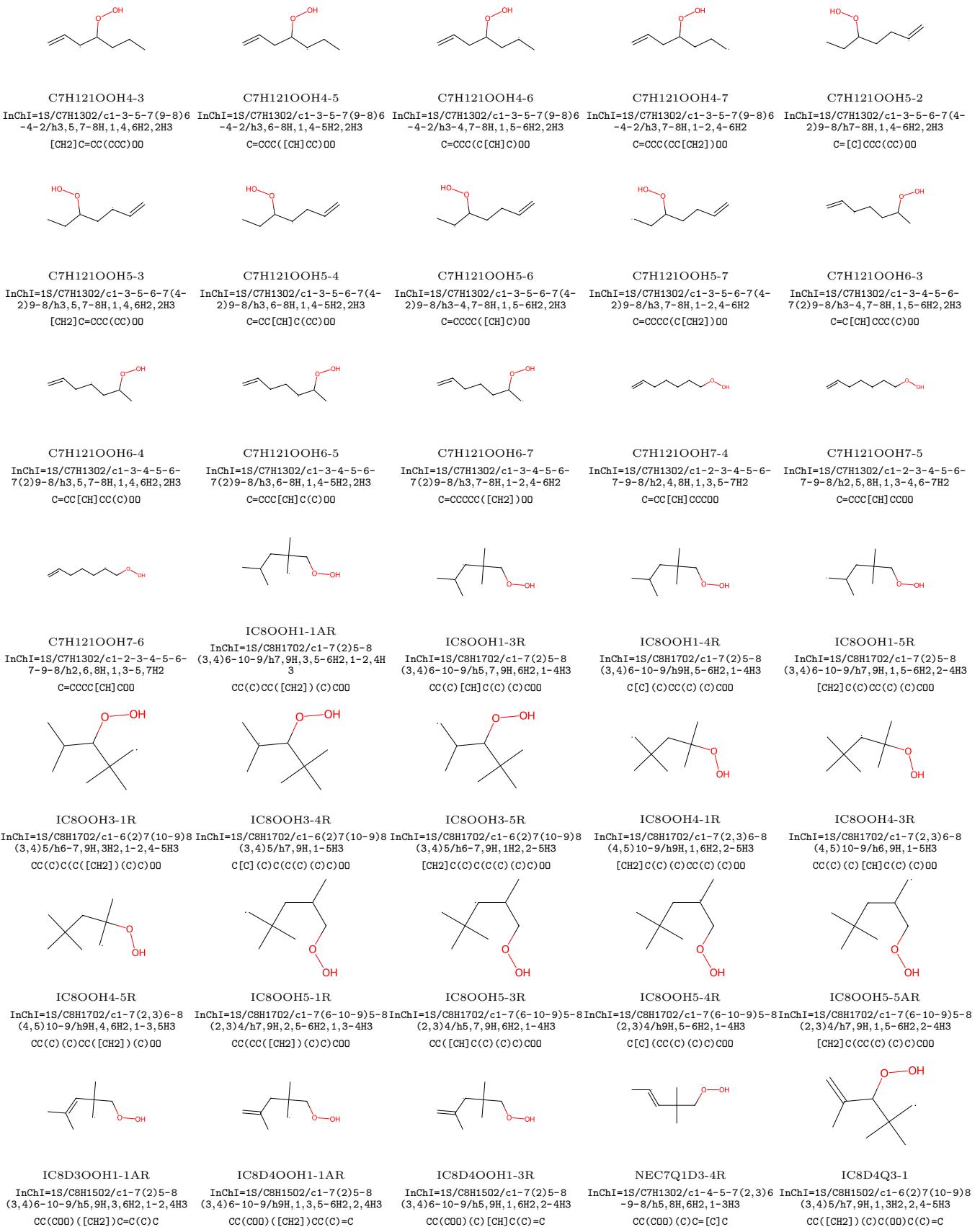


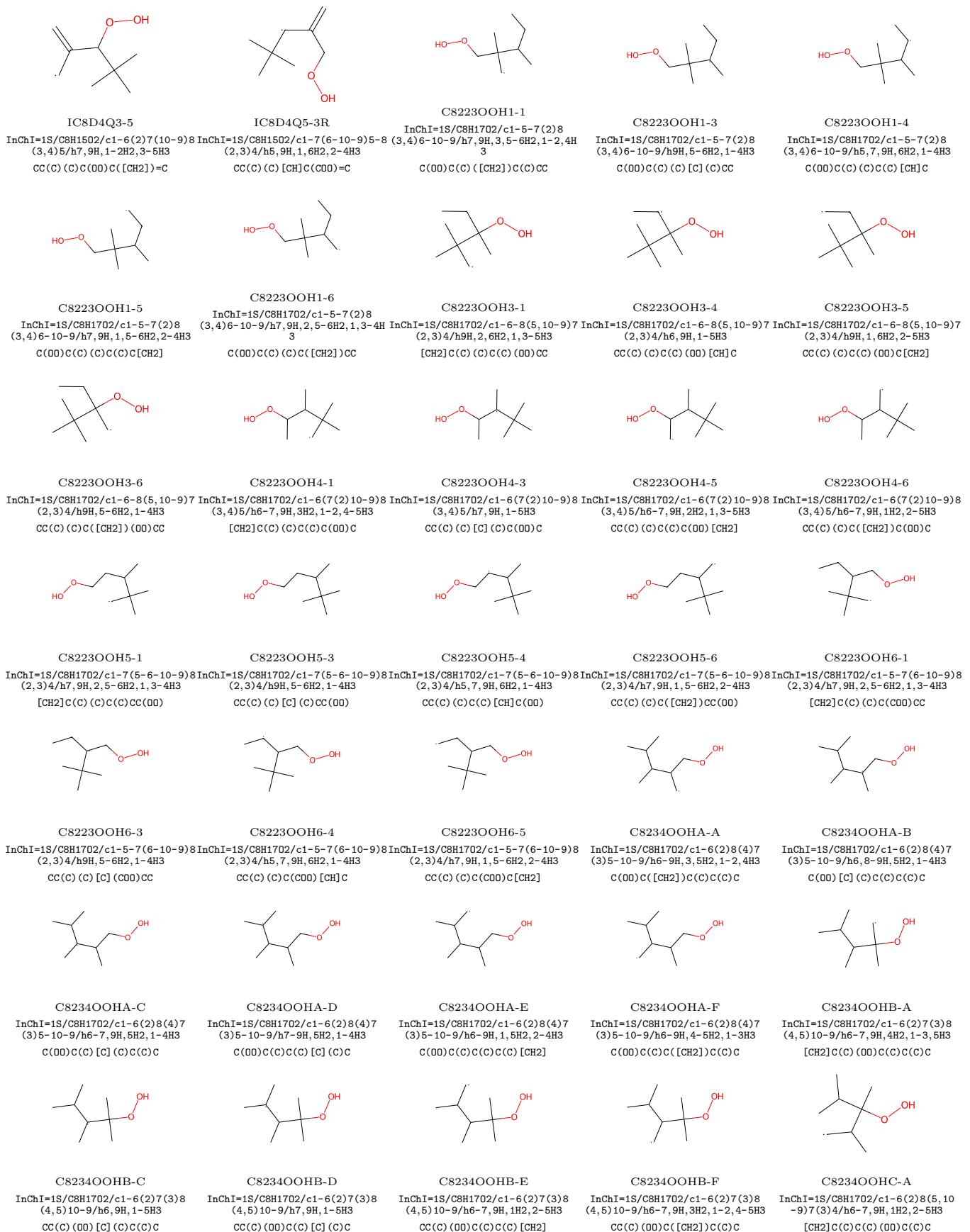




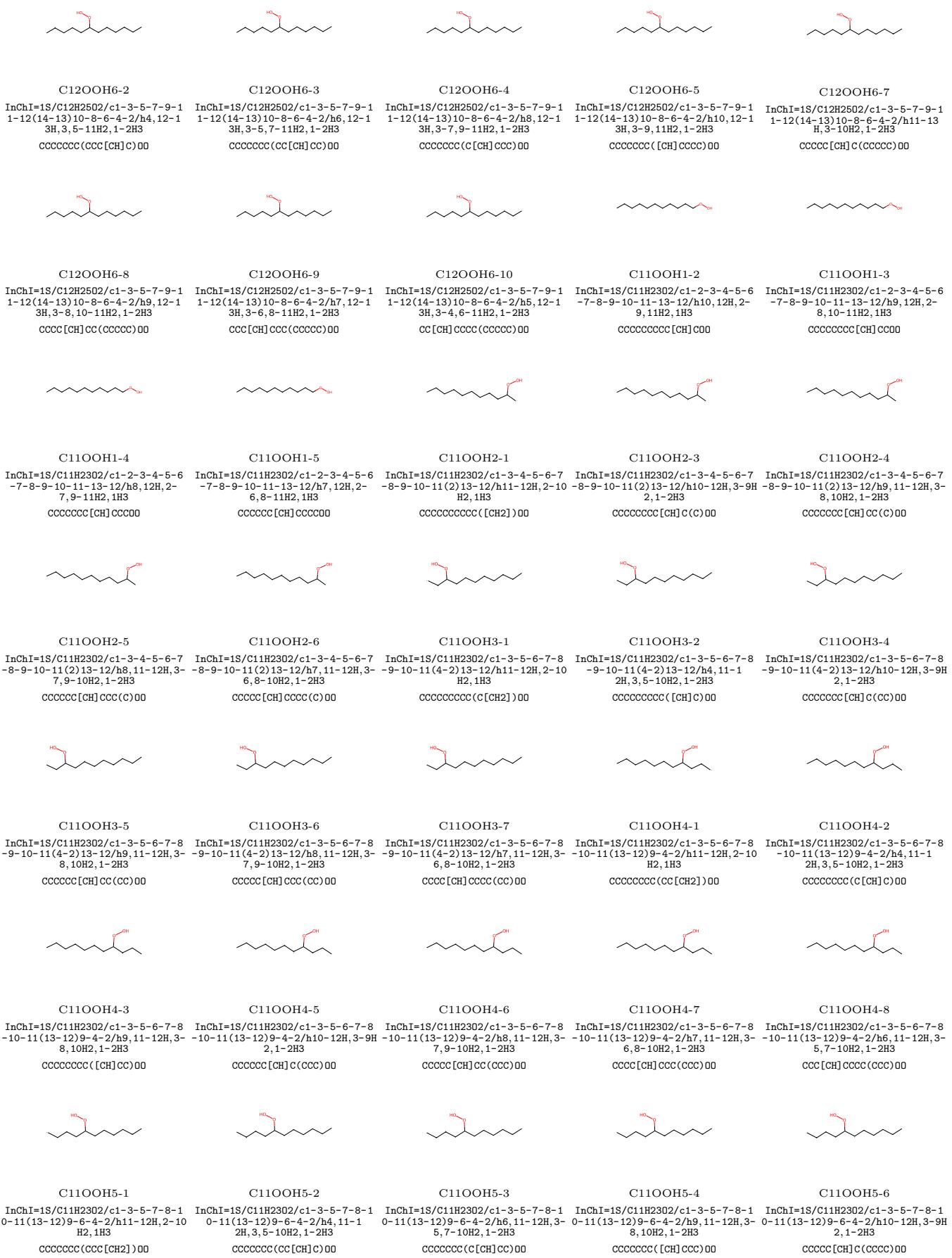


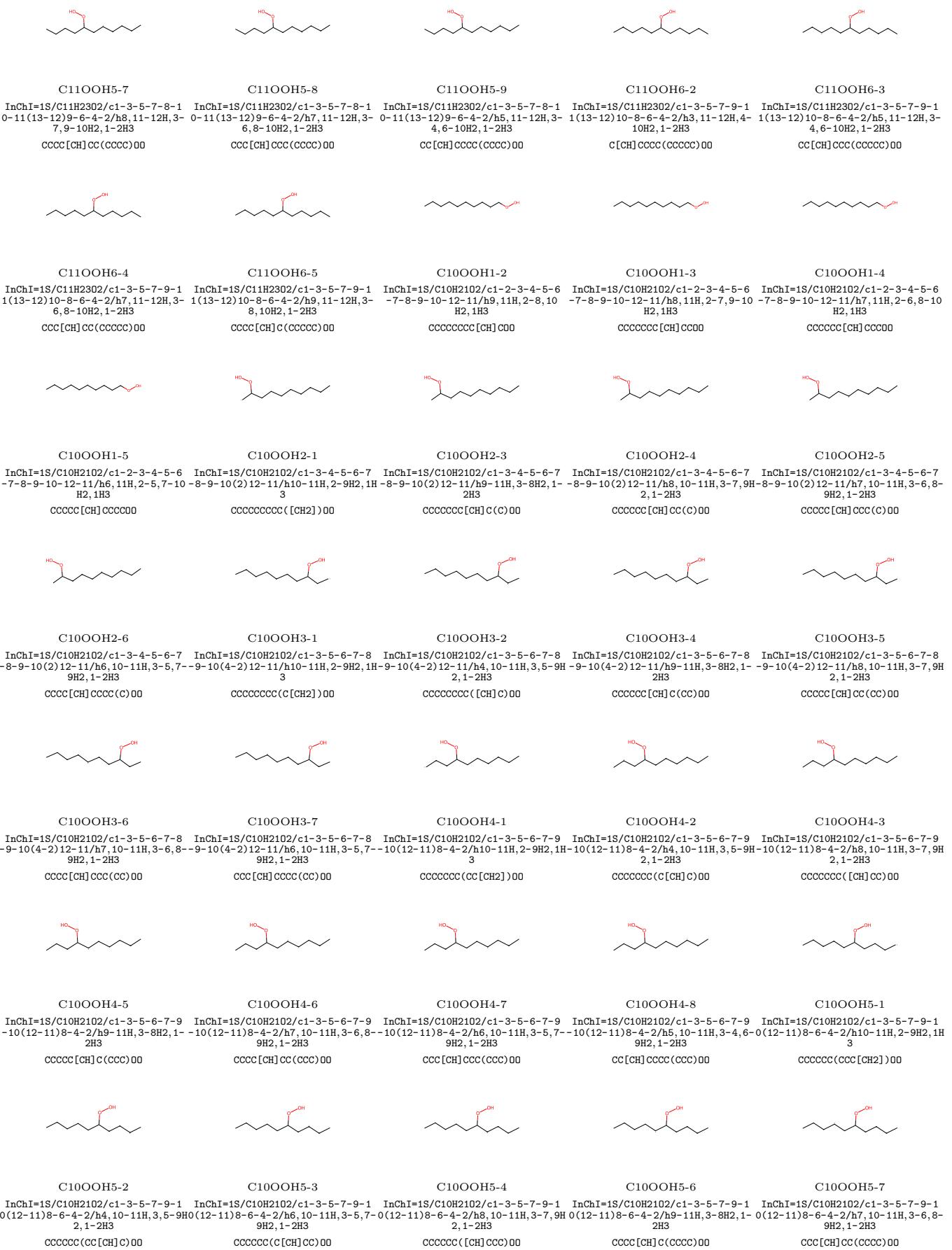


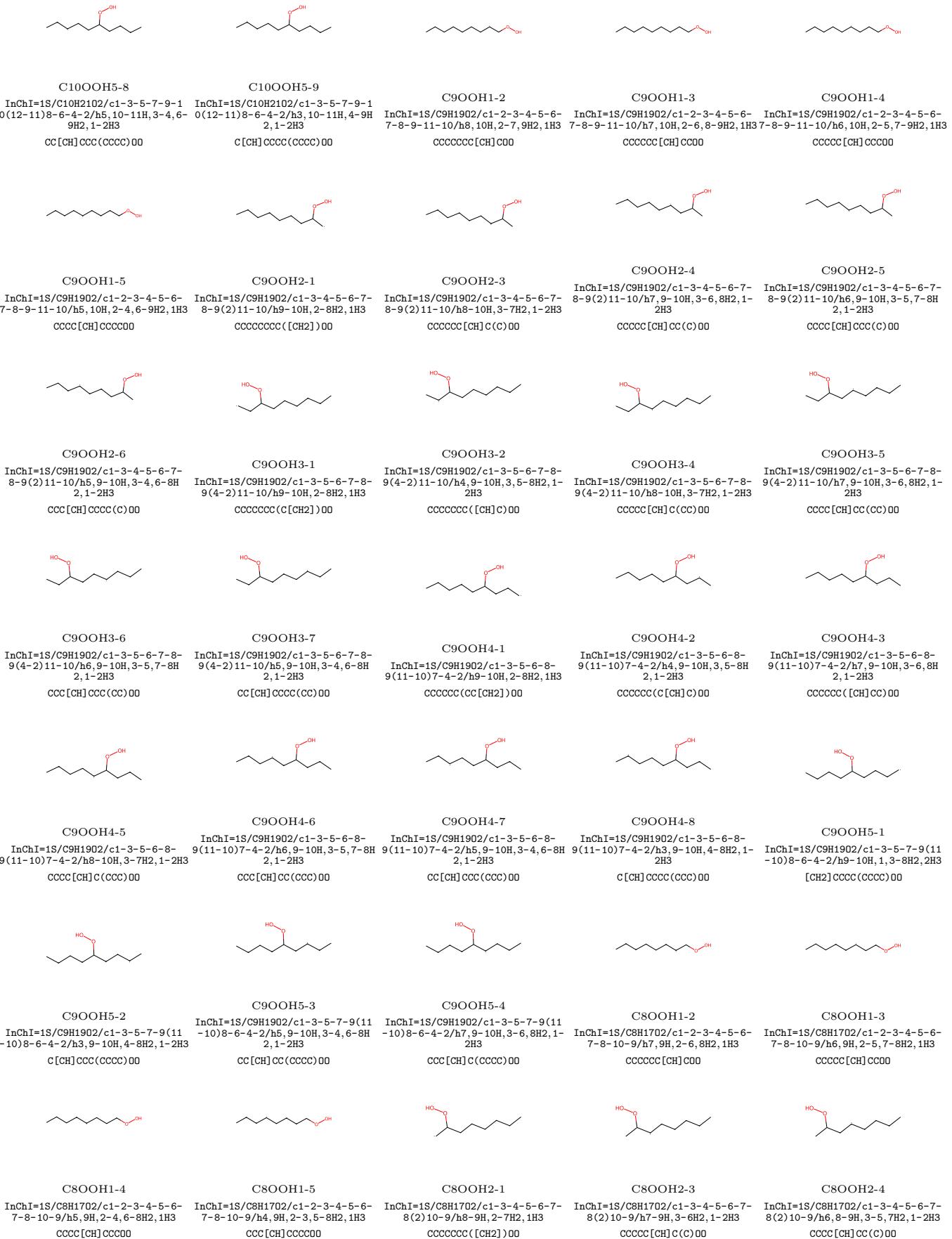


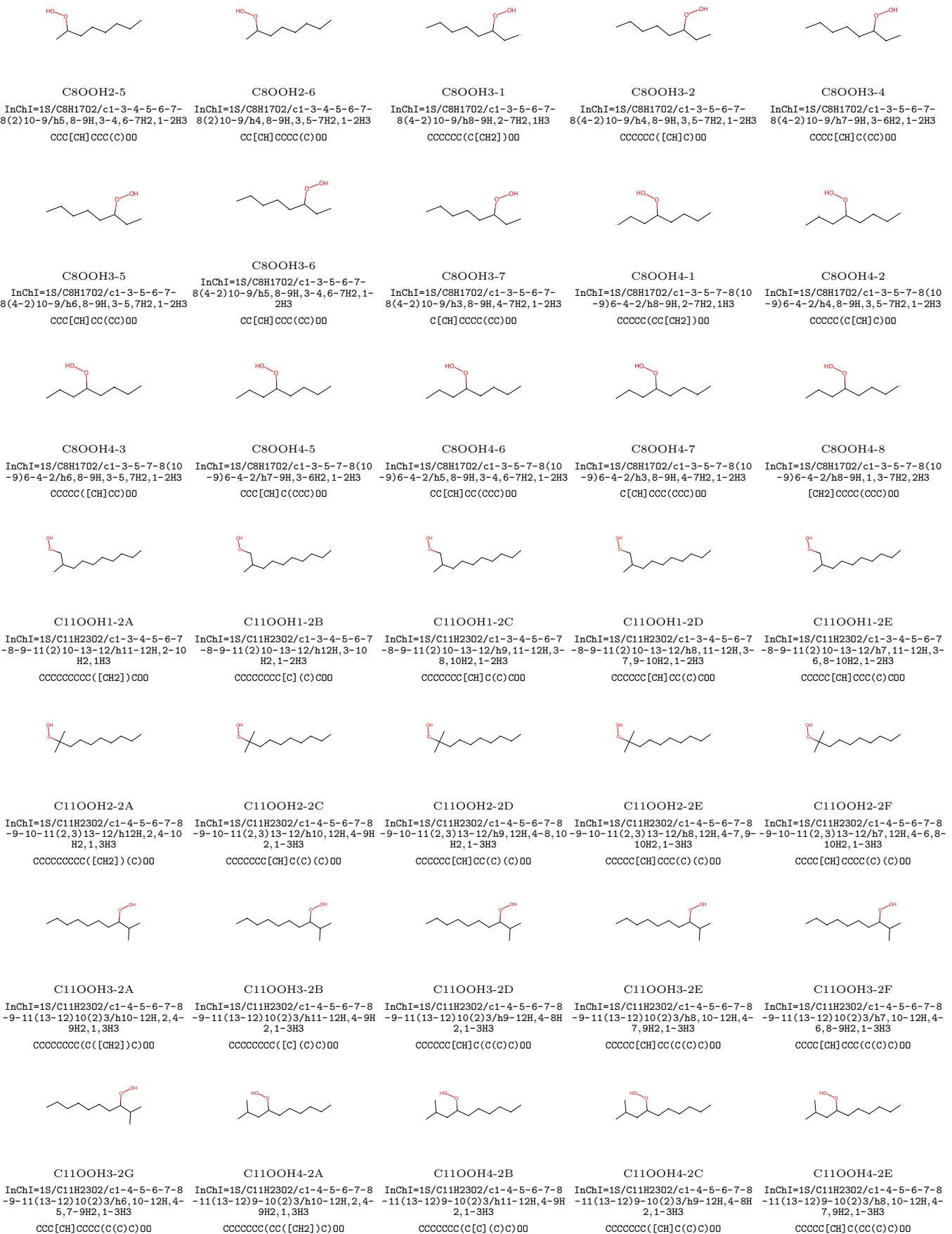


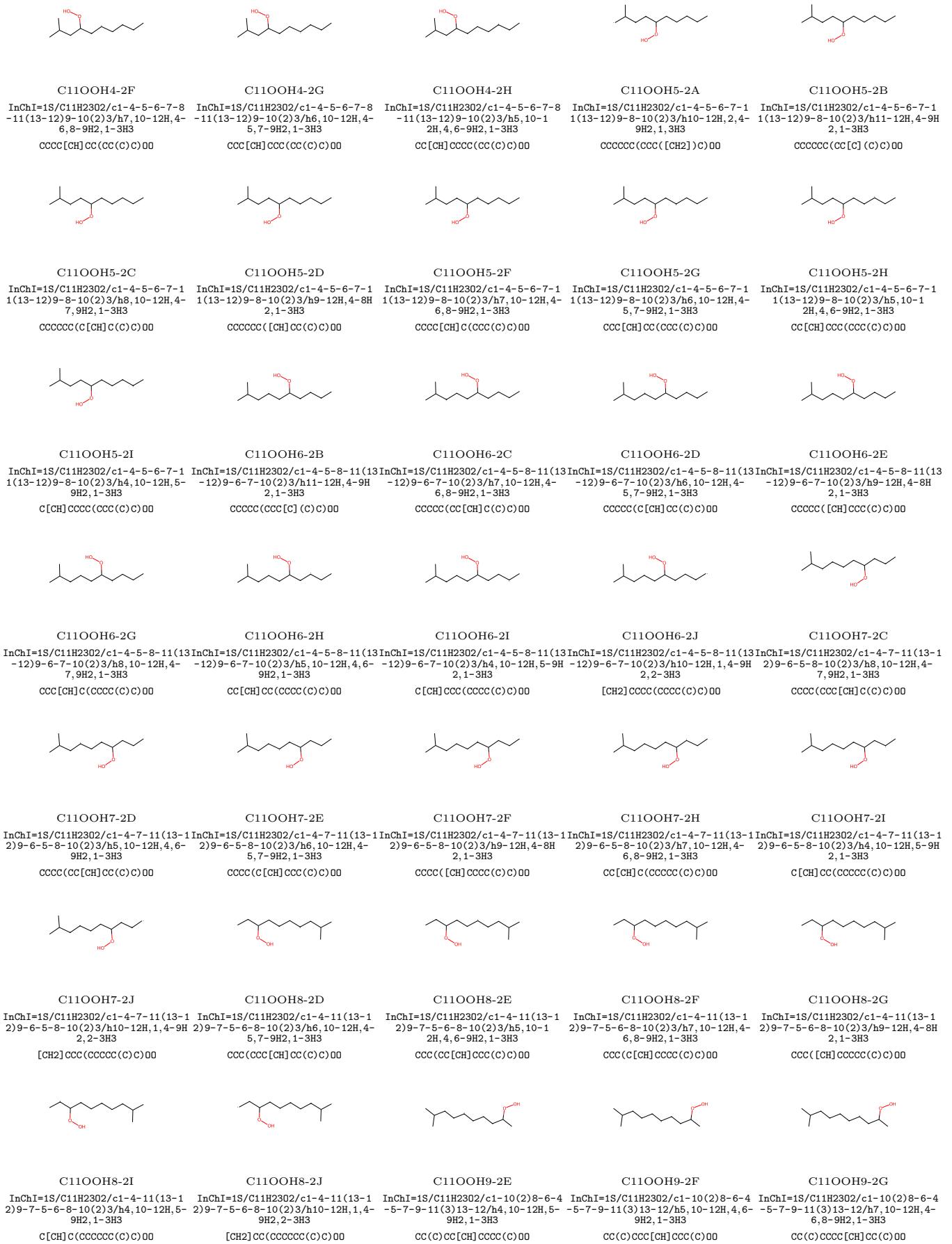


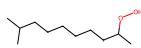




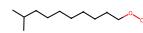
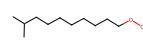
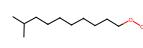
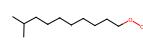
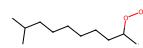






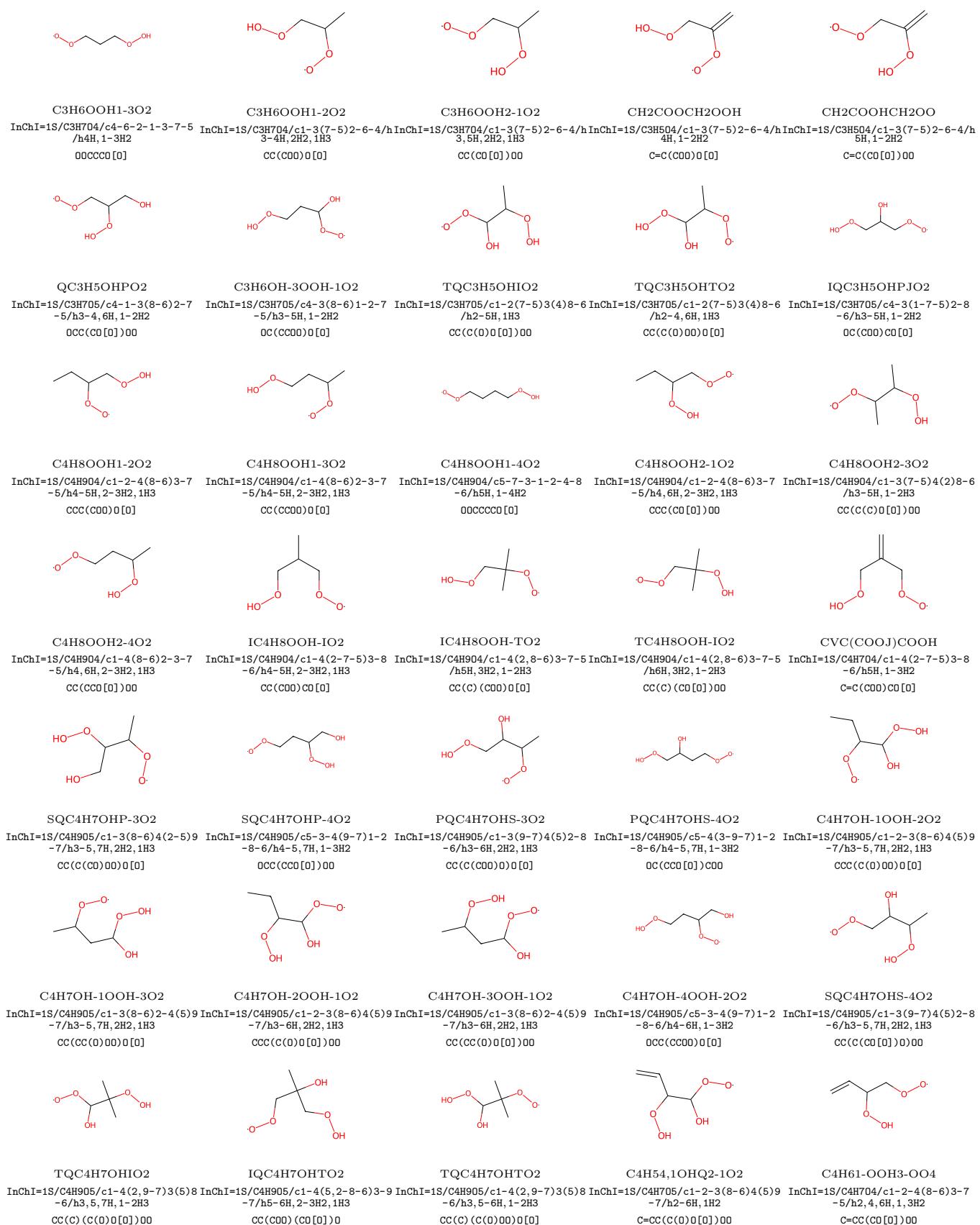


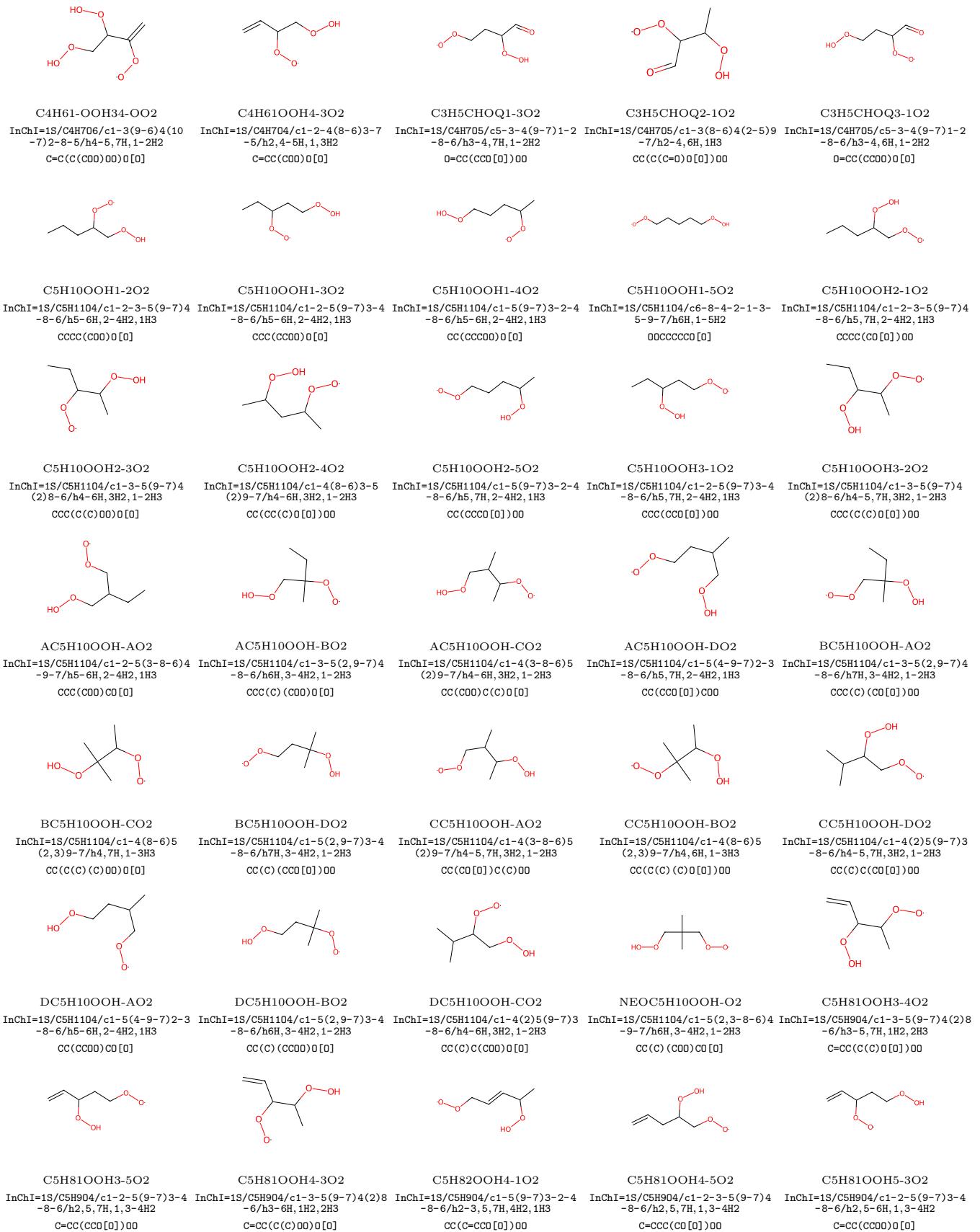
C11OOH9-2H
InChI=1S/C11H23O2/c1-10(2)8-6-4 InChI=1S/C11H23O2/c1-10(2)8-6-4 InChI=1S/C11H23O2/c1-11(2)9-7-5 InChI=1S/C11H23O2/c1-11(2)9-7-5 InChI=1S/C11H23O2/c1-11(2)9-7-5
-5-7-9-11(3)13-12/h9-12H,4-8H -5-7-9-11(3)13-12/h10-12H,3-9H -3-4-6-8-10-13-12/h3,11-12H,4- 3-4-6-8-10-13-12/h4,11-1 3-4-6-8-10-13-12/h6,11-12H,3-
2,1-3H3 2,1-2H3 10H2,1-2H3 2H,3,5-10H2,1-2H3 5,7-10H2,1-2H3
CC(C)CCCC[CH]C(C)OO CC(C)CCCCC([CH2])OO CC(C)CCC[CH]CCCCOO CC(C)CCCC[CH]CCCO CC(C)CCCC[CH]CCOO

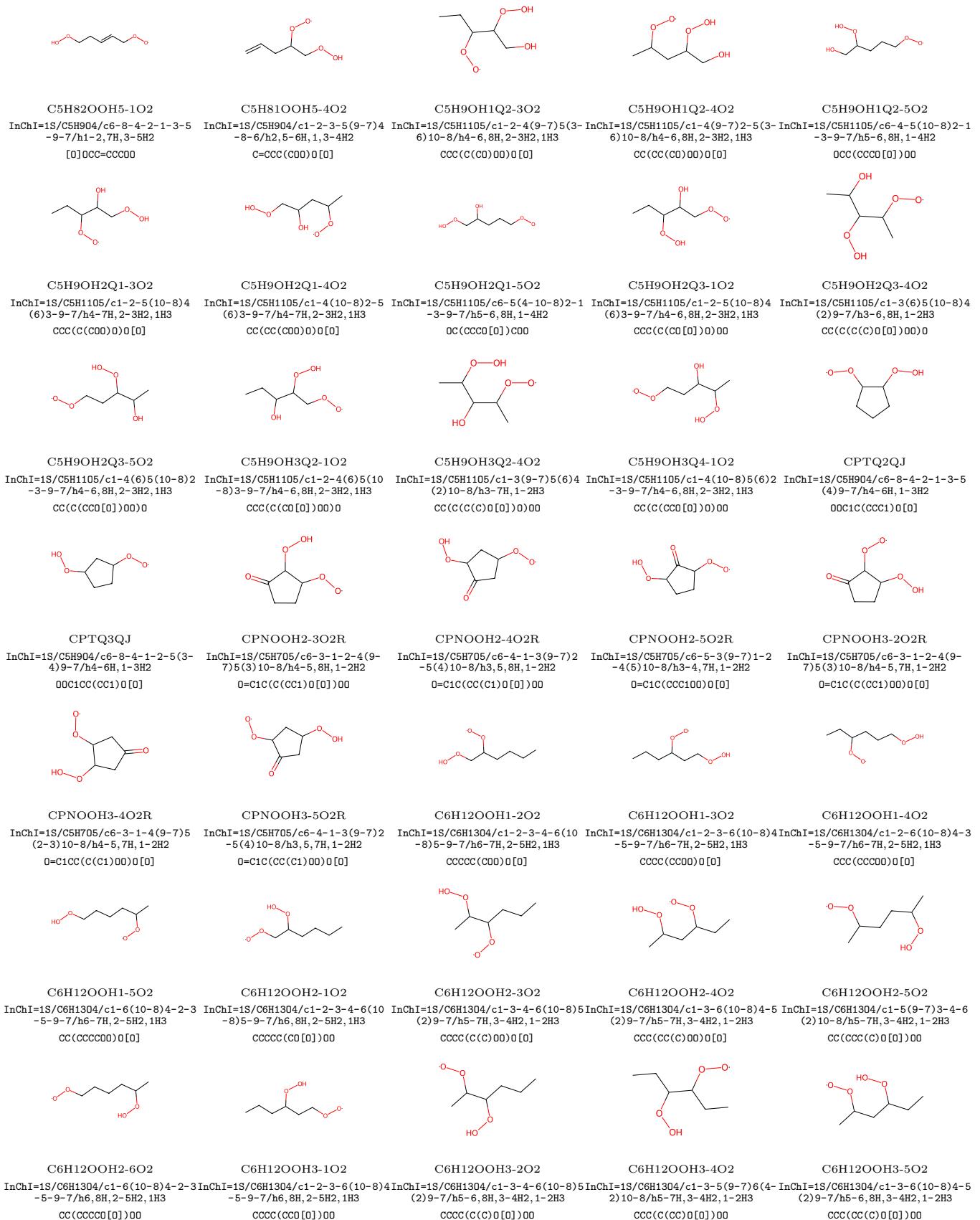


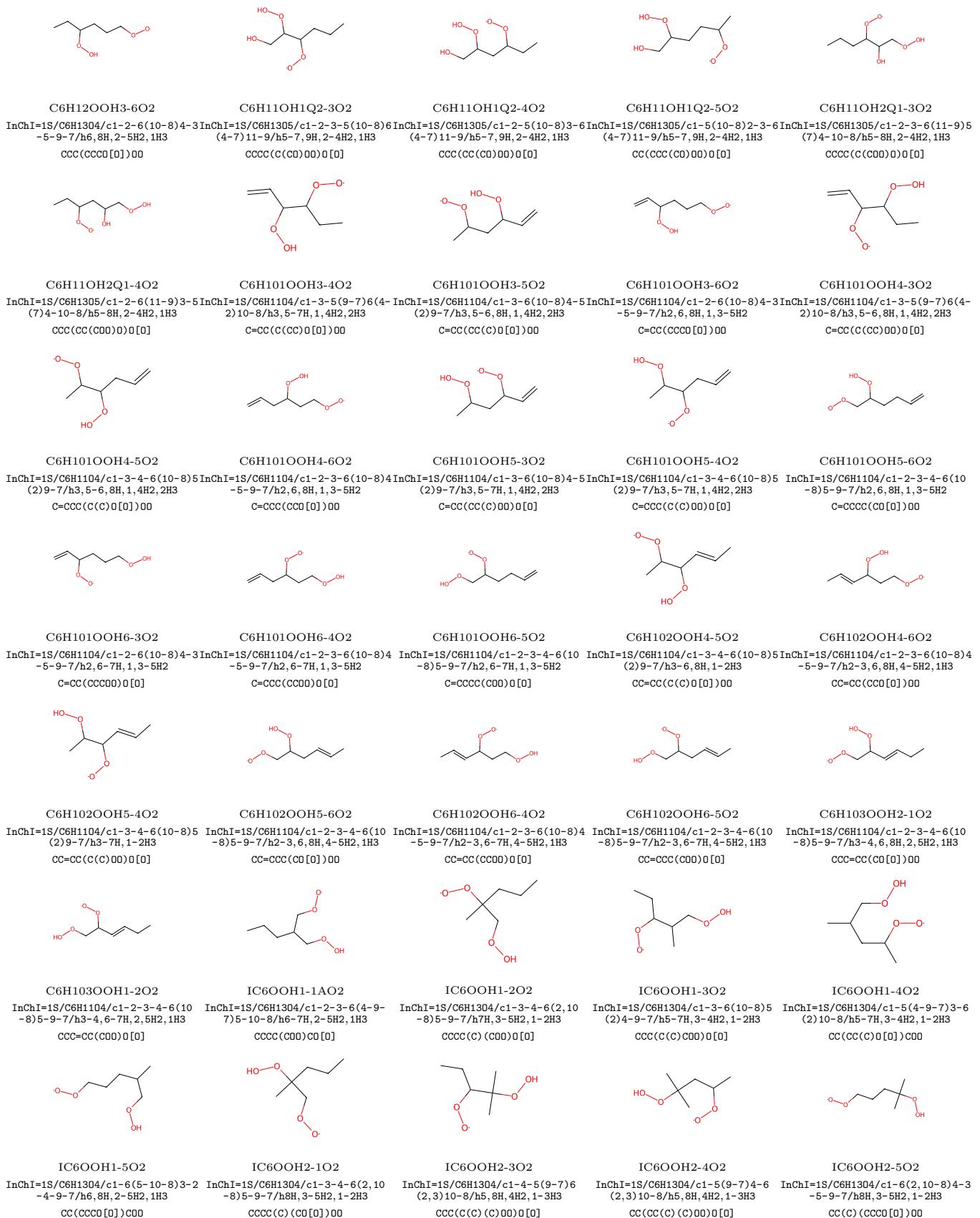
C11OOH10-2I
InChI=1S/C11H23O2/c1-11(2)9-7-5
-3-4-6-8-10-13-12/h8,11-12H,3-
7,9-10H2,1-2H3
CC(C)CCCCC[CH]COO

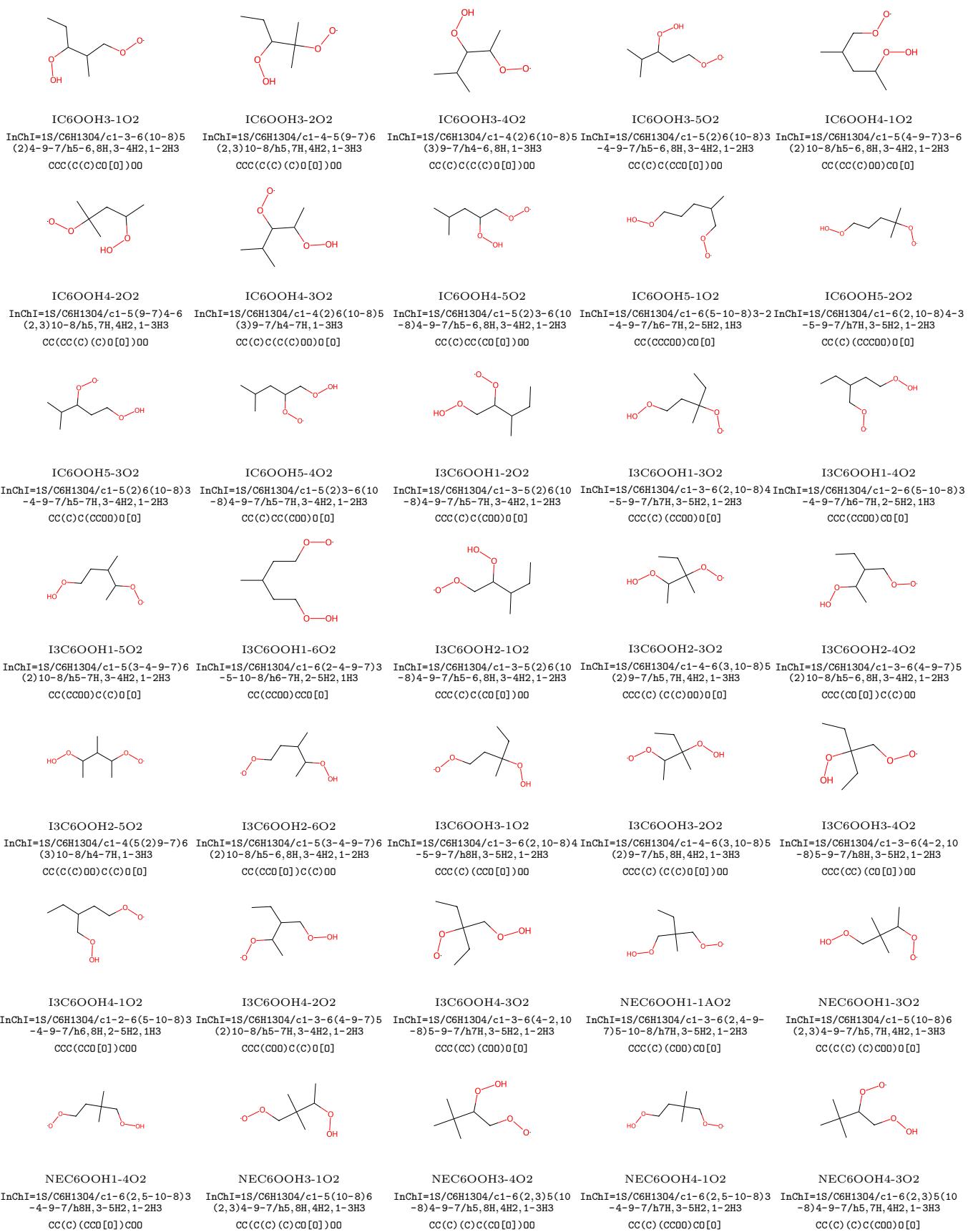
20 Peroxy hydroperoxides

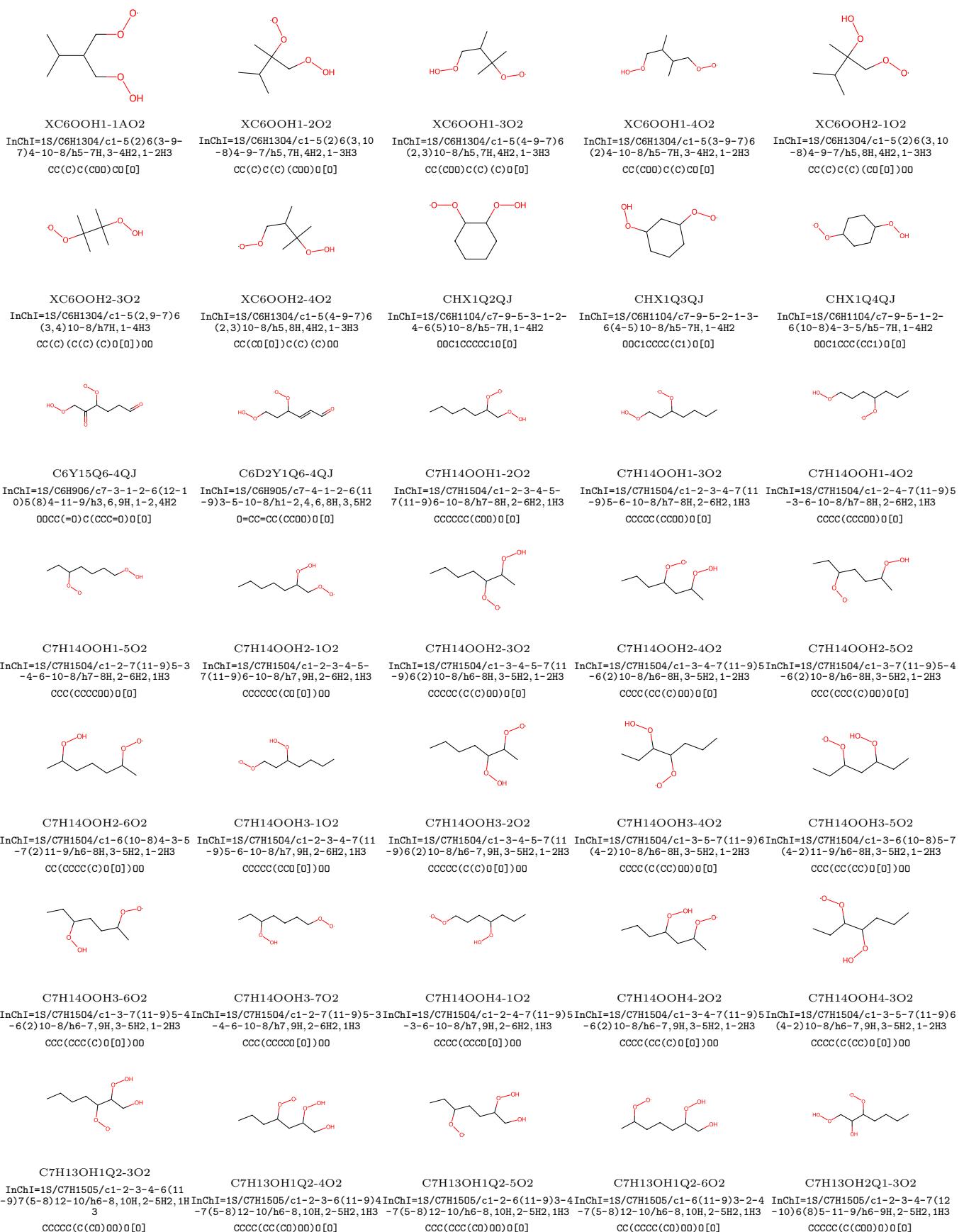


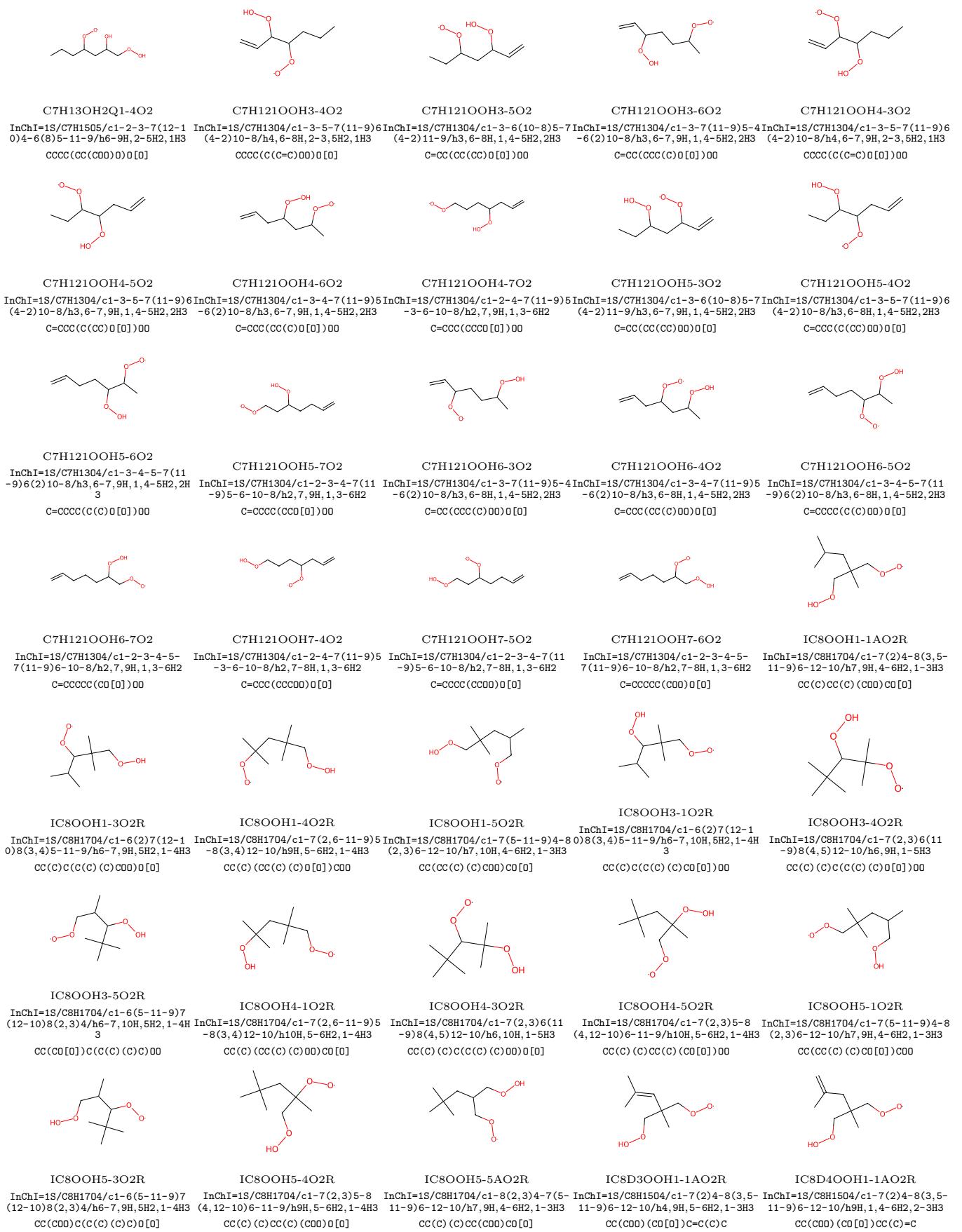


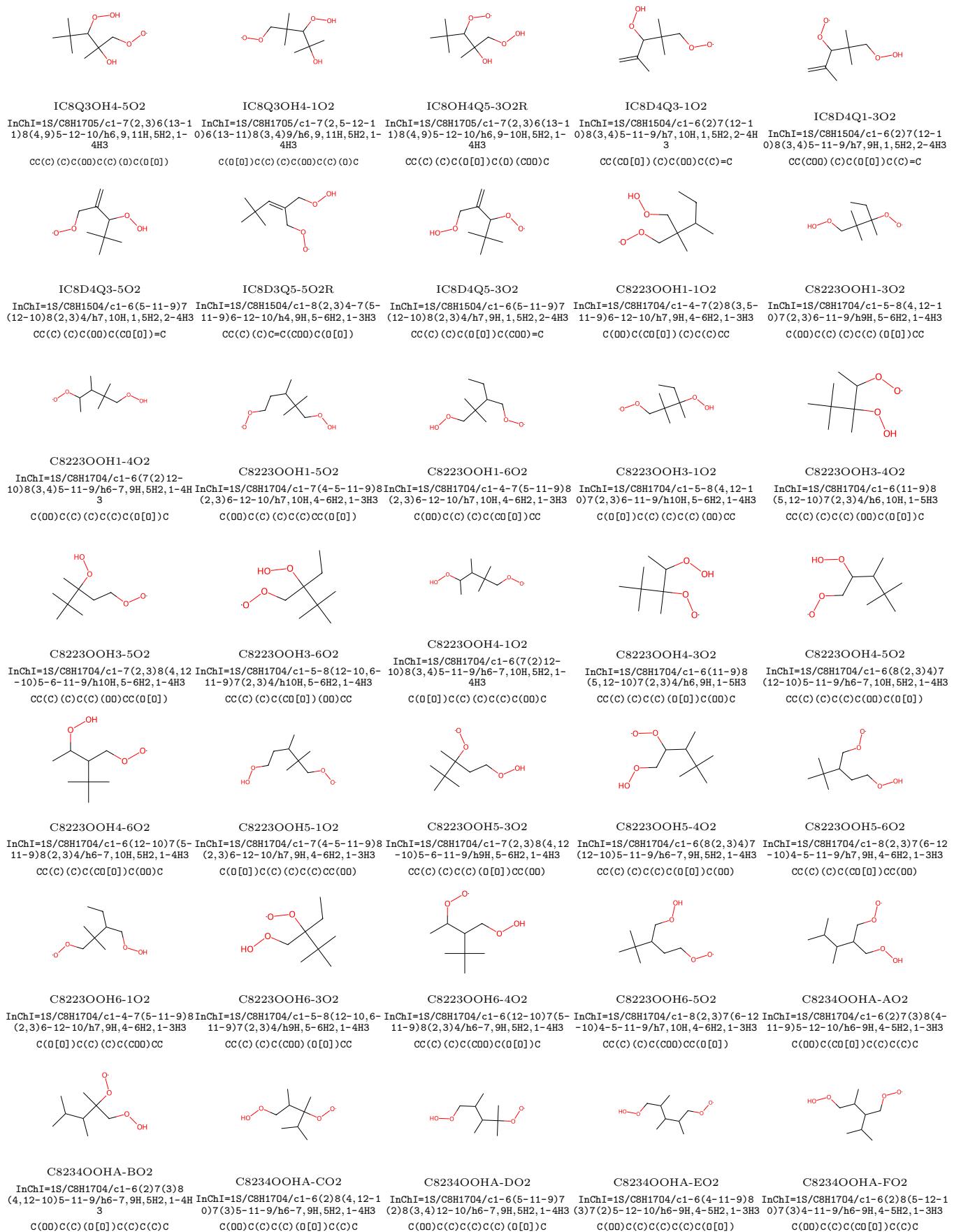


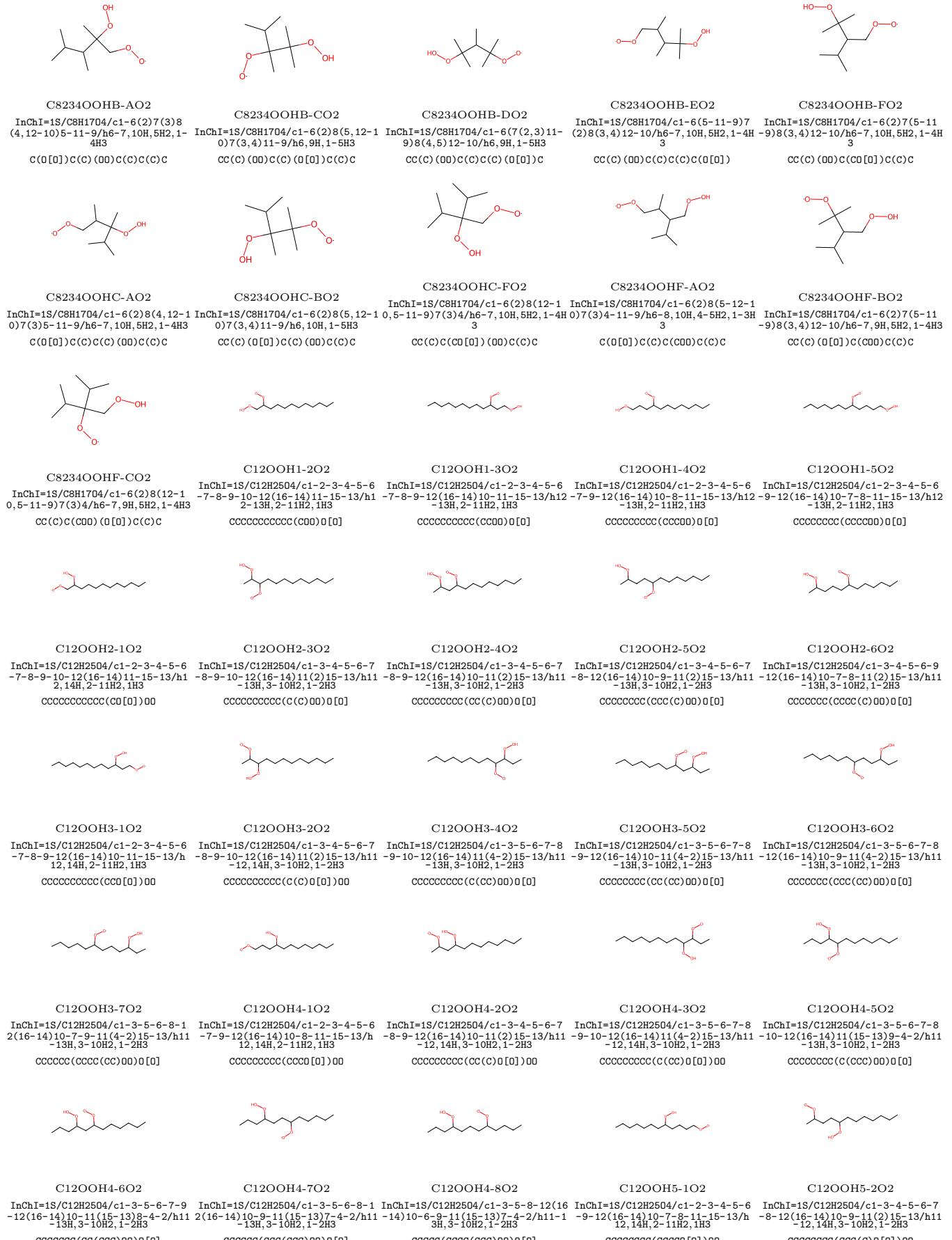


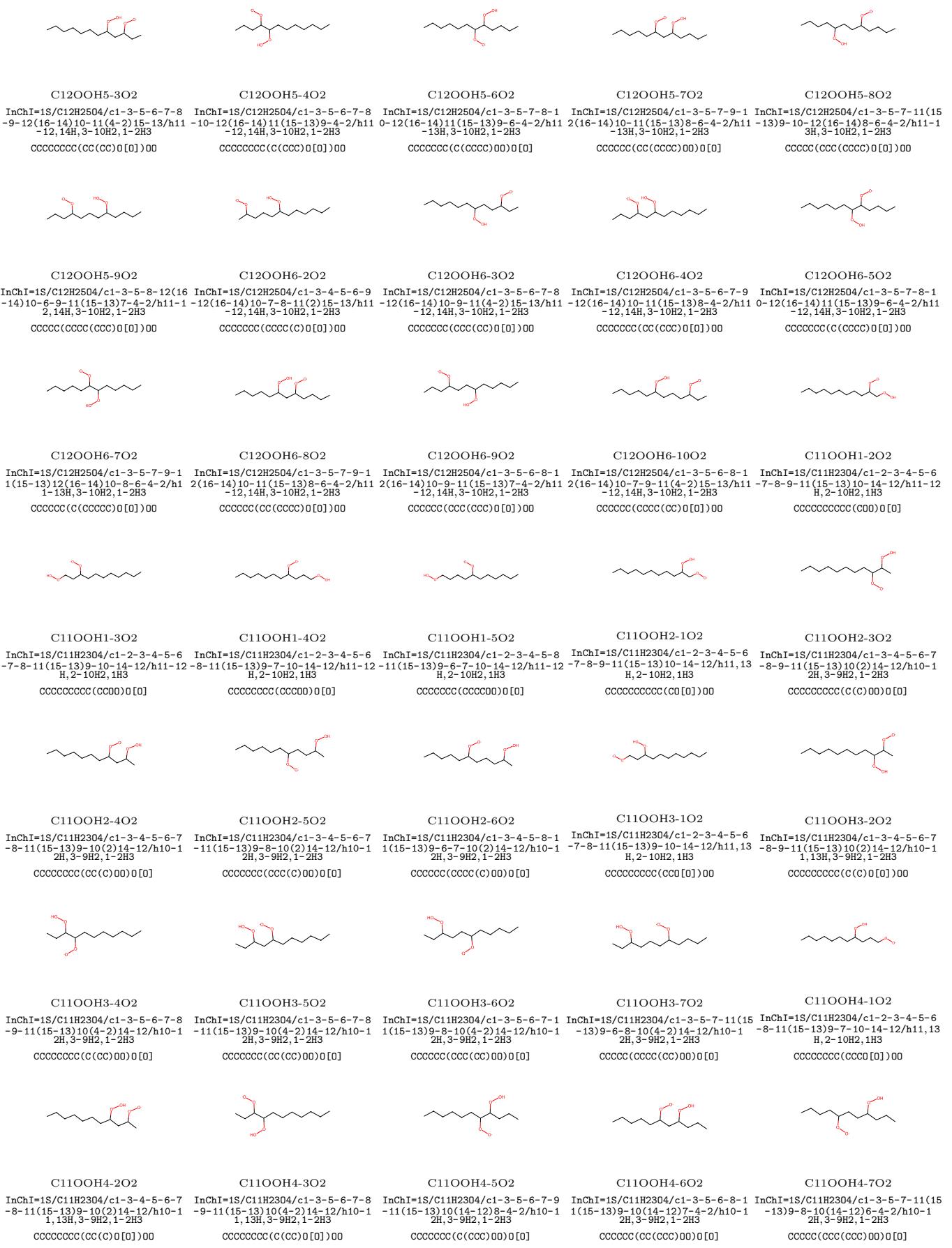


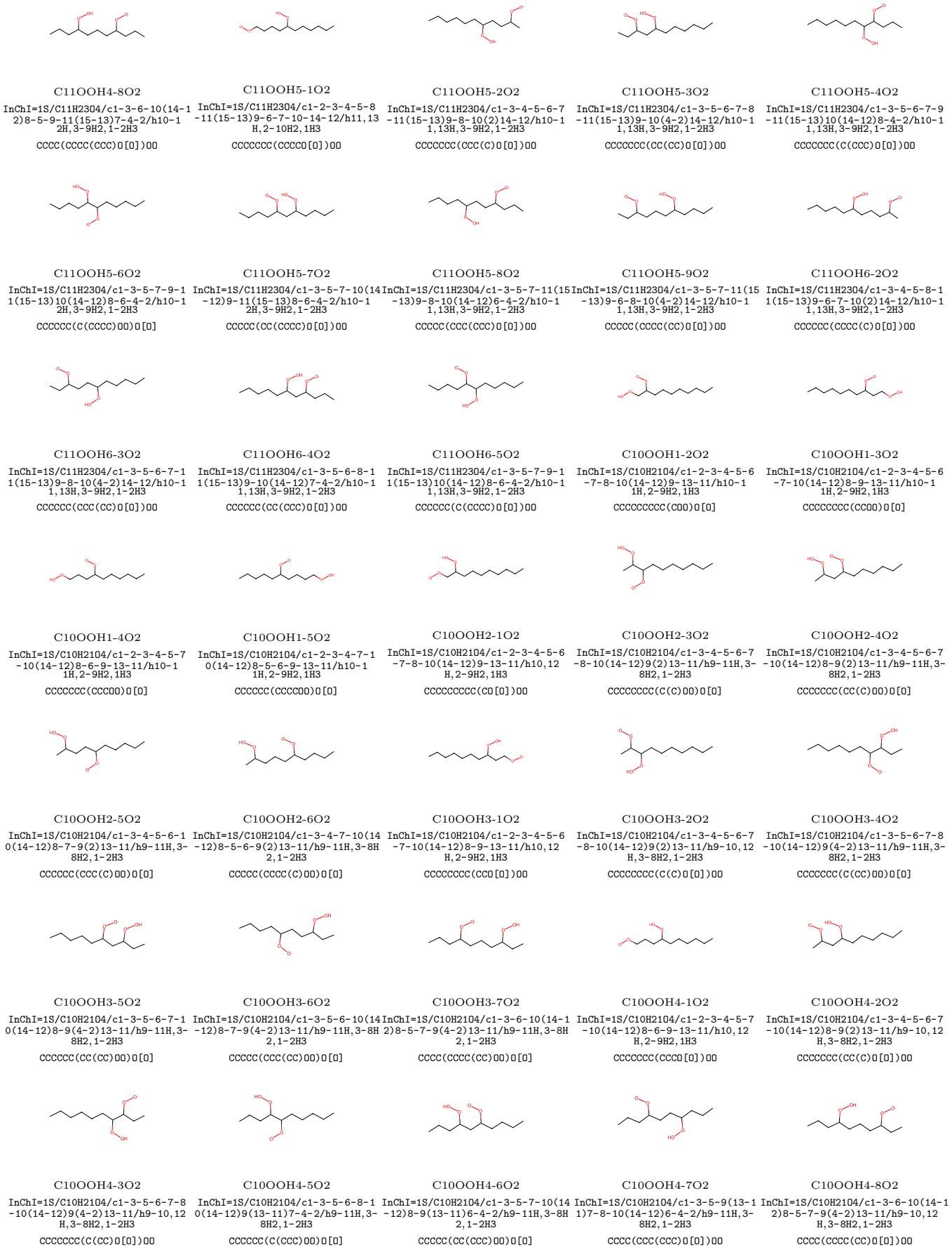


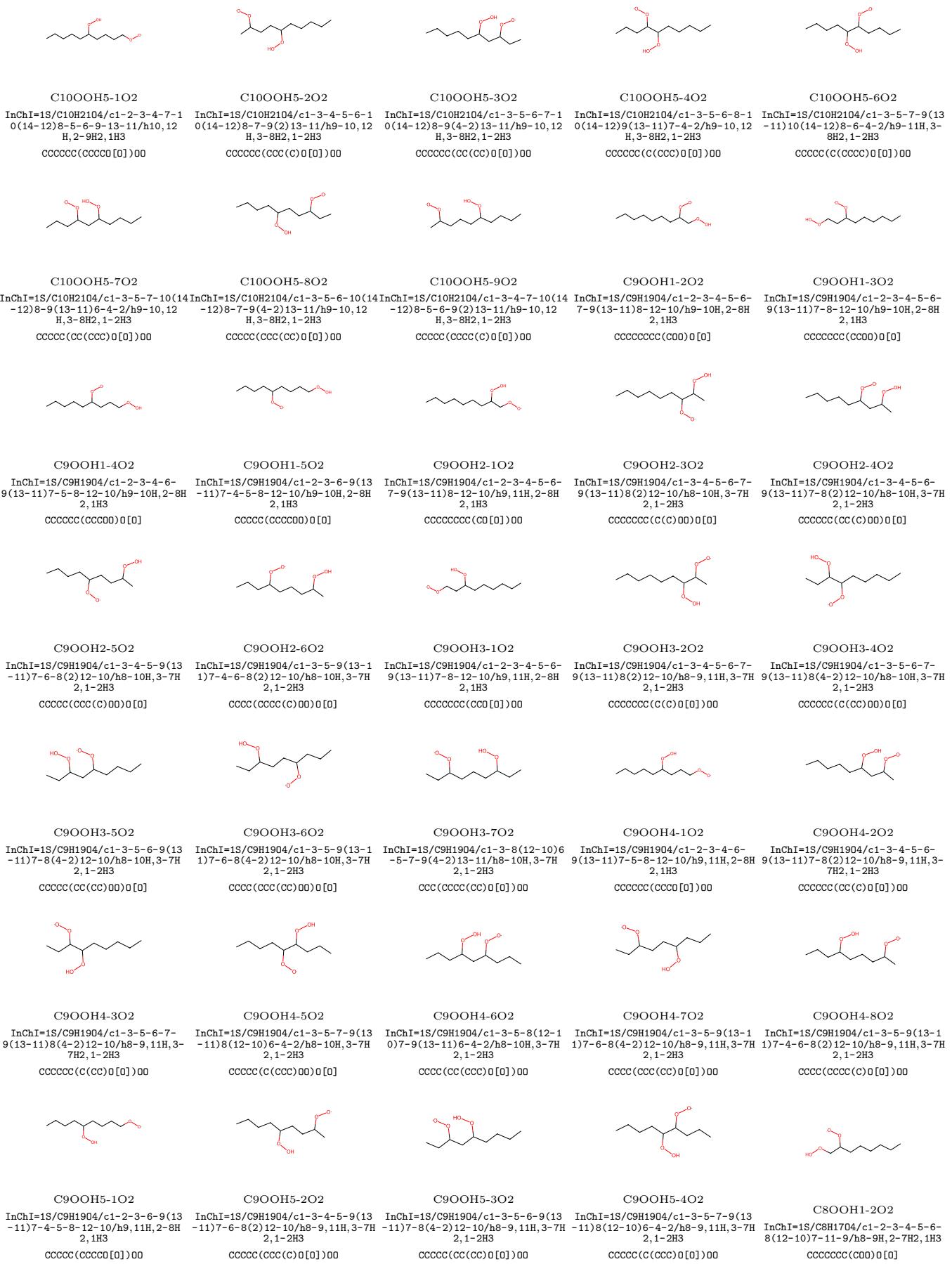


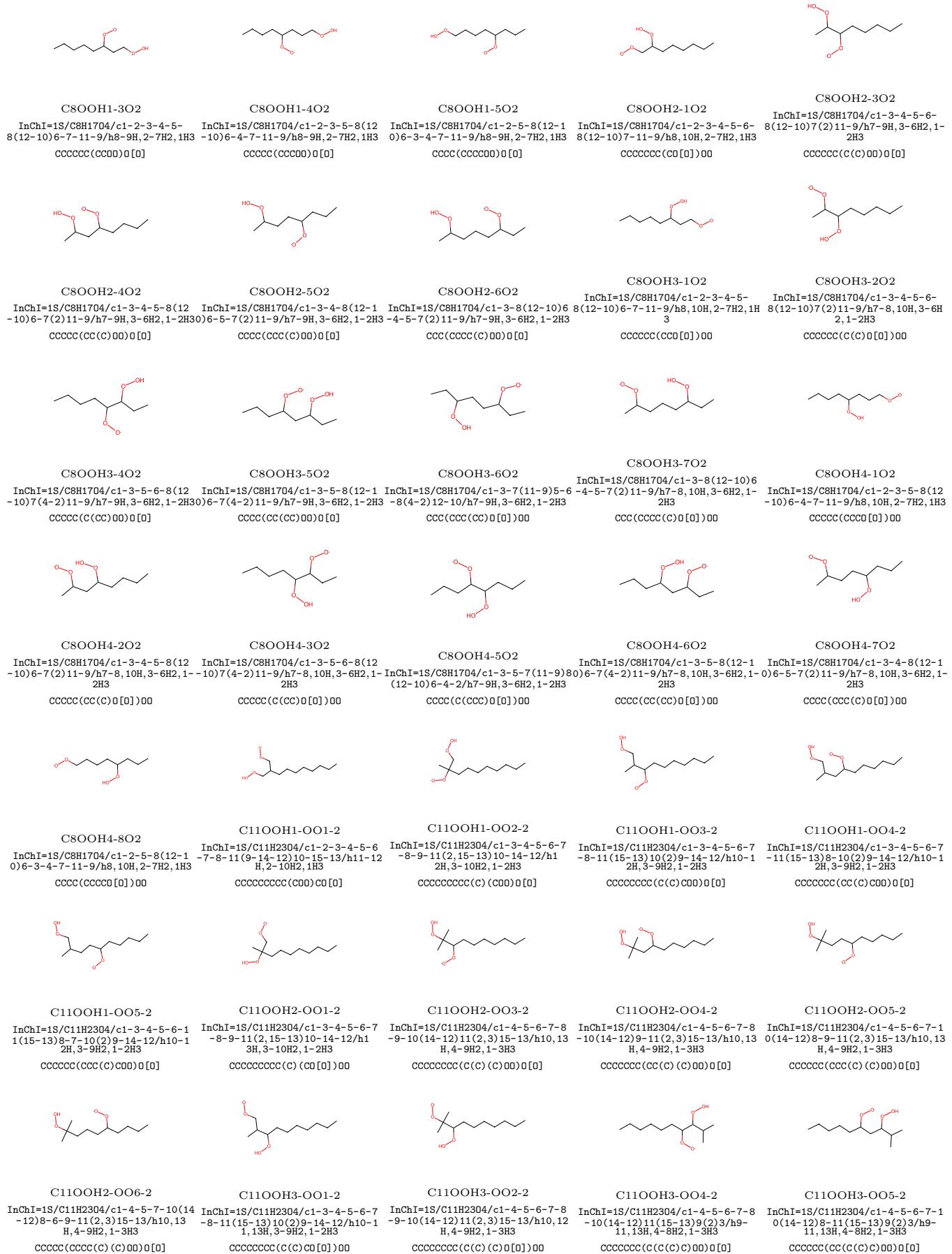


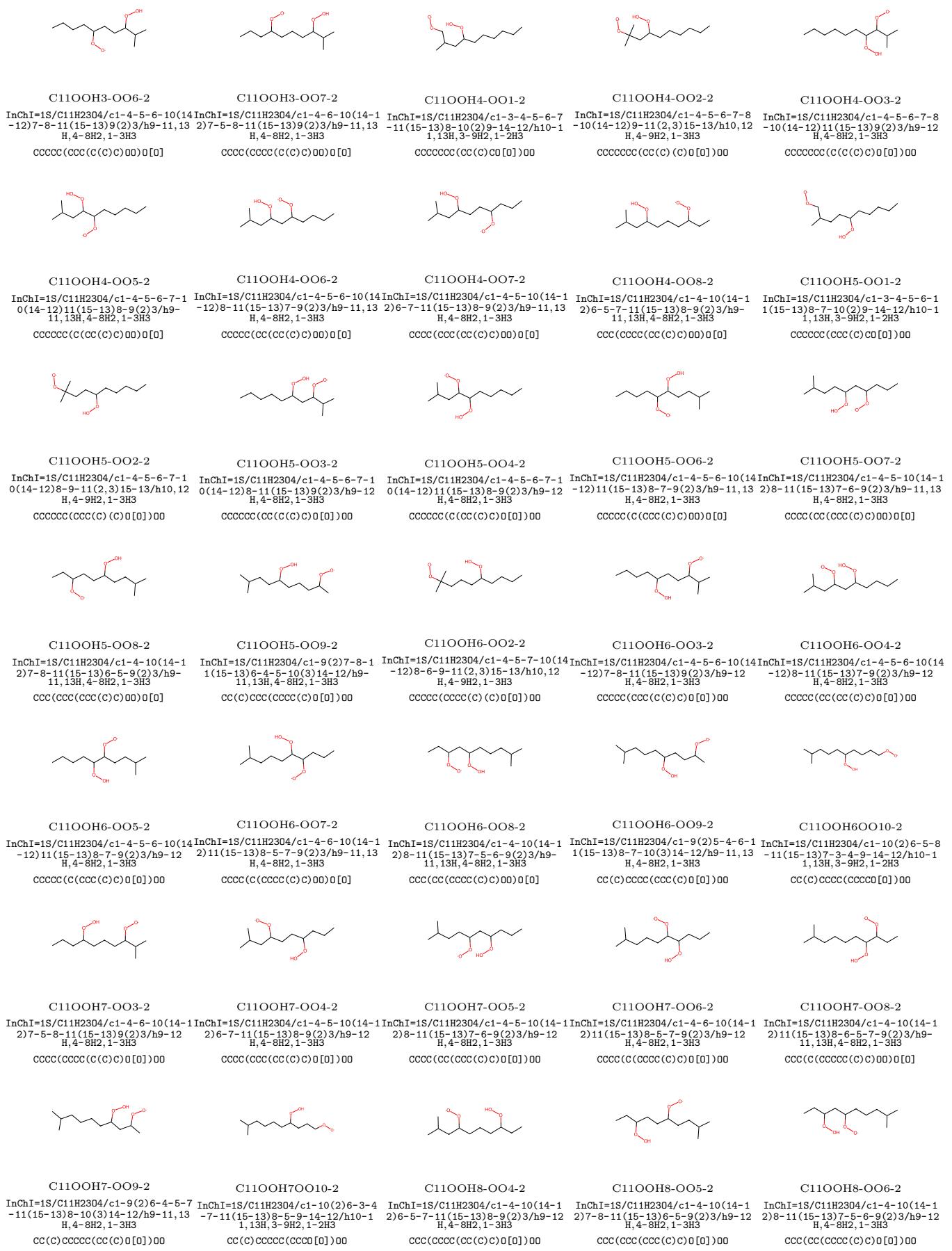




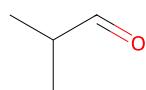
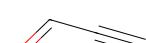
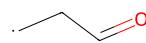
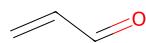
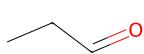








21 Aldehydes (molecules and radicals)



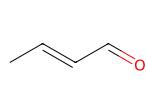
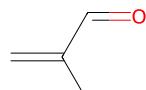
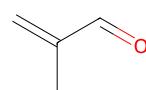
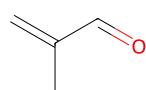
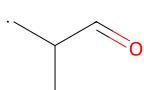
C2H5CHO
InChI=1S/C3H6O/c1-2-3-4/h3H,2H
CCC=O

C2H3CHO
InChI=1S/C3H4O/c1-2-3-4/h2-3H,1H
C=CC=O

CH2CH2CHO
InChI=1S/C3H5O/c1-2-3-4/h3H,1-2H
[CH2]CC=O

C2HCHO
InChI=1S/C3H2O/c1-2-3-4/h1,3H
C#CC=O

IC3H7CHO
InChI=1S/C4H8O/c1-4(2)3-5/h3-4H,1H2,2H3
CC(C)C=O



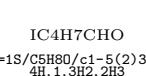
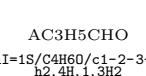
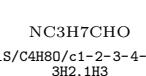
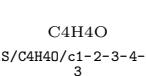
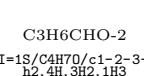
IC3H6CHO
InChI=1S/C4H7O/c1-4(2)3-5/h3-4H,1H2,2H3
[CH2]C(C)C=O

IC3H5CHO
InChI=1S/C4H6O/c1-4(2)3-5/h3H,1H
C=C(C)C=O

IC3H4CHO-A
InChI=1S/C4H5O/c1-4(2)3-5/h3H,1-2H
[CH2]C(=C)C=O

IC4YAA
InChI=1S/C4H4O/c1-4(2-5)3-6/h2-3H,1H2
C=C(C=O)C=O

SC3H5CHO
InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3
CC=CC=O



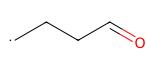
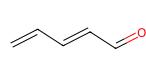
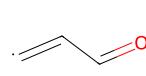
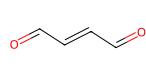
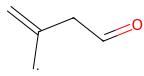
C3H6CHO-2
InChI=1S/C4H7O/c1-2-3-4-5/h2-4H,3H2,1H3
C[CH]CC=O

C4H4O
InChI=1S/C4H4O/c1-2-3-4-5/h4H,1H
CC#CC=O

NC3H7CHO
InChI=1S/C4H8O/c1-2-3-4-5/h4H,2-3H2,1H3
CCCC=O

AC3H5CHO
InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1-3H2
C=CCC=O

IC4H7CHO
InChI=1S/C5H8O/c1-5(2)3-4-6/h4H,1-3H2
C=C(C)CC=O



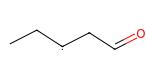
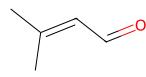
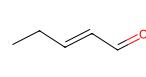
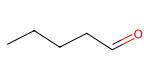
IC4H7CHO-A
InChI=1S/C5H7O/c1-5(2)3-4-6/h4H,1-3H2
[CH2]C(=C)CC=O

OVCCVCCVO
InChI=1S/C4H4O2/c5-3-1-2-4-6/h1-4H
O=CC=CC=O

CJVCCVO
InChI=1S/C3H3O/c1-2-3-4/h1-3H
[CH]=CC=O

CVCCVCCVO
InChI=1S/C5H6O/c1-2-3-4-5-6/h2
C=CC=CC=O

C3H6CHO-3
InChI=1S/C4H7O/c1-2-3-4-5/h4H,1-3H2
[CH2]CCC=O



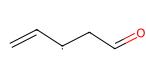
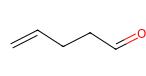
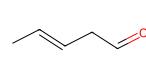
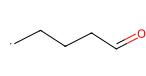
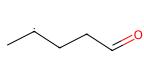
PC4H9CHO
InChI=1S/C5H10O/c1-2-3-4-5-6/h5H,2-4H2,1H3
CCCCC=O

TC4H8CHO
InChI=1S/C5H9O/c1-5(2,3)4-6/h4H,1H2,2-3H3
[CH2]C(C)(C)C=O

C4H7CHO-2
InChI=1S/C5H8O/c1-2-3-4-5-6/h3
-5H,2H2,1H3
CCC=CC=O

IC5D2Y4
InChI=1S/C5H8O/c1-5(2)3-4-6/h3-4H,1-2H3
CC(C)=CC=O

PC4H8CHO-2
InChI=1S/C5H9O/c1-2-3-4-5-6/h3,5H,2,4H2,1H3
CC[CH]CC=O



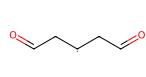
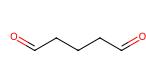
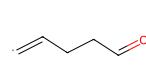
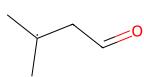
PC4H8CHO-3
InChI=1S/C5H9O/c1-2-3-4-5-6/h2,5H,3-4H2,1H3
C[CH]CCC=O

PC4H8CHO-4
InChI=1S/C5H9O/c1-2-3-4-5-6/h5
H,1-4H2
[CH2]CCCC=O

C4H7CHO-3
InChI=1S/C5H8O/c1-2-3-4-5-6/h2
-3,5H,4H2,1H3
CC=CCC=O

C4H7CHO-4
InChI=1S/C5H8O/c1-2-3-4-5-6/h2,5H,1-3H2
C=CCCC=O

C4H6CHO-4,3
InChI=1S/C5H7O/c1-2-3-4-5-6/h2-3H,1,4H2
C=C[CH]CC=O



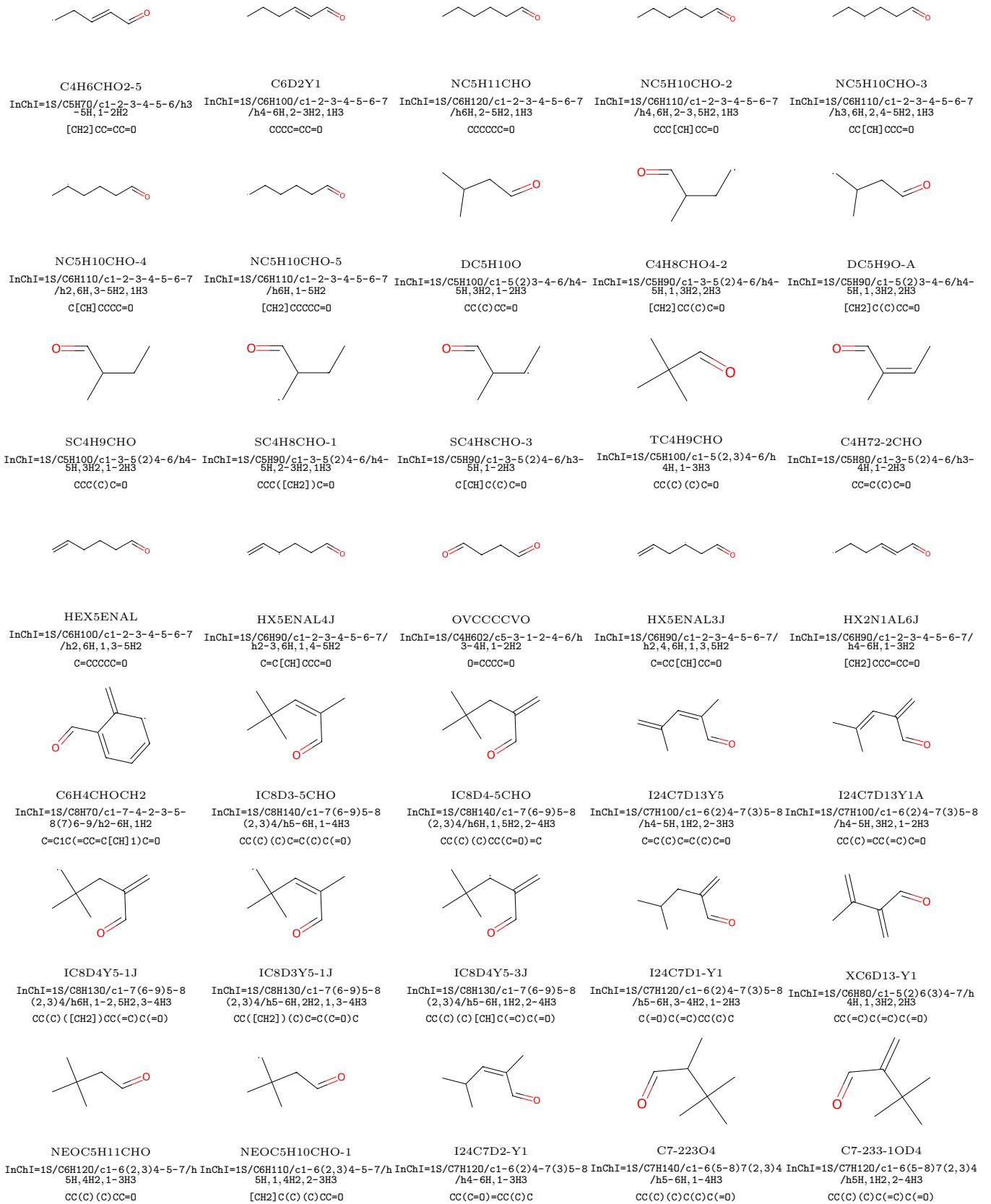
DC5H9O-B
InChI=1S/C5H9O/c1-5(2)3-4-6/h4H,3H2,1-2H3
CCCC=O

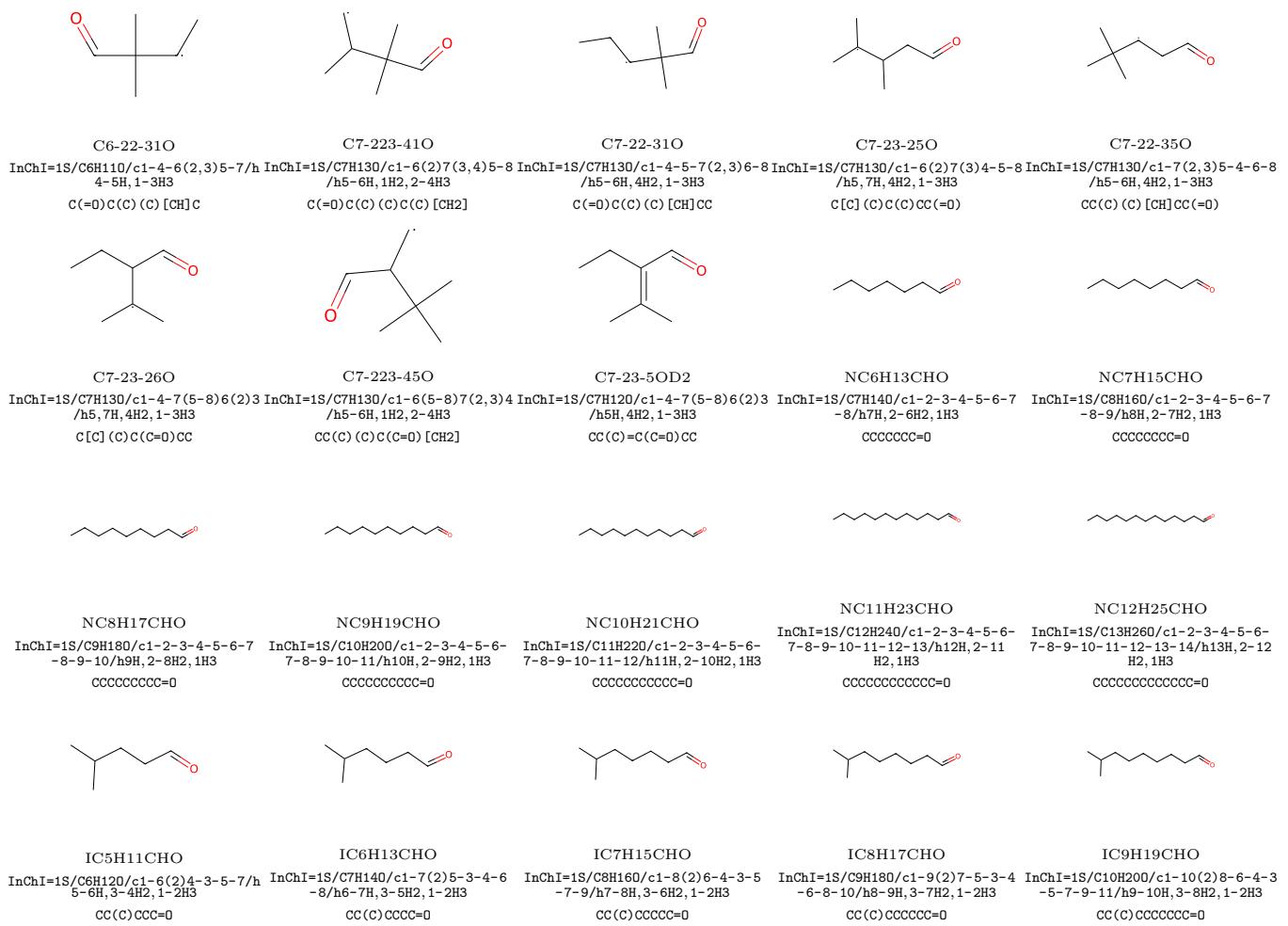
IC5D2Y14
InChI=1S/C5H6O2/c1-5(4-7)2-3-6/h2-4H,1H3
CC(=CC=O)C=O

C4H6CHO4-5
InChI=1S/C5H7O/c1-2-3-4-5-6/h1
-2,5H,3-4H2
[CH]=CCCC=O

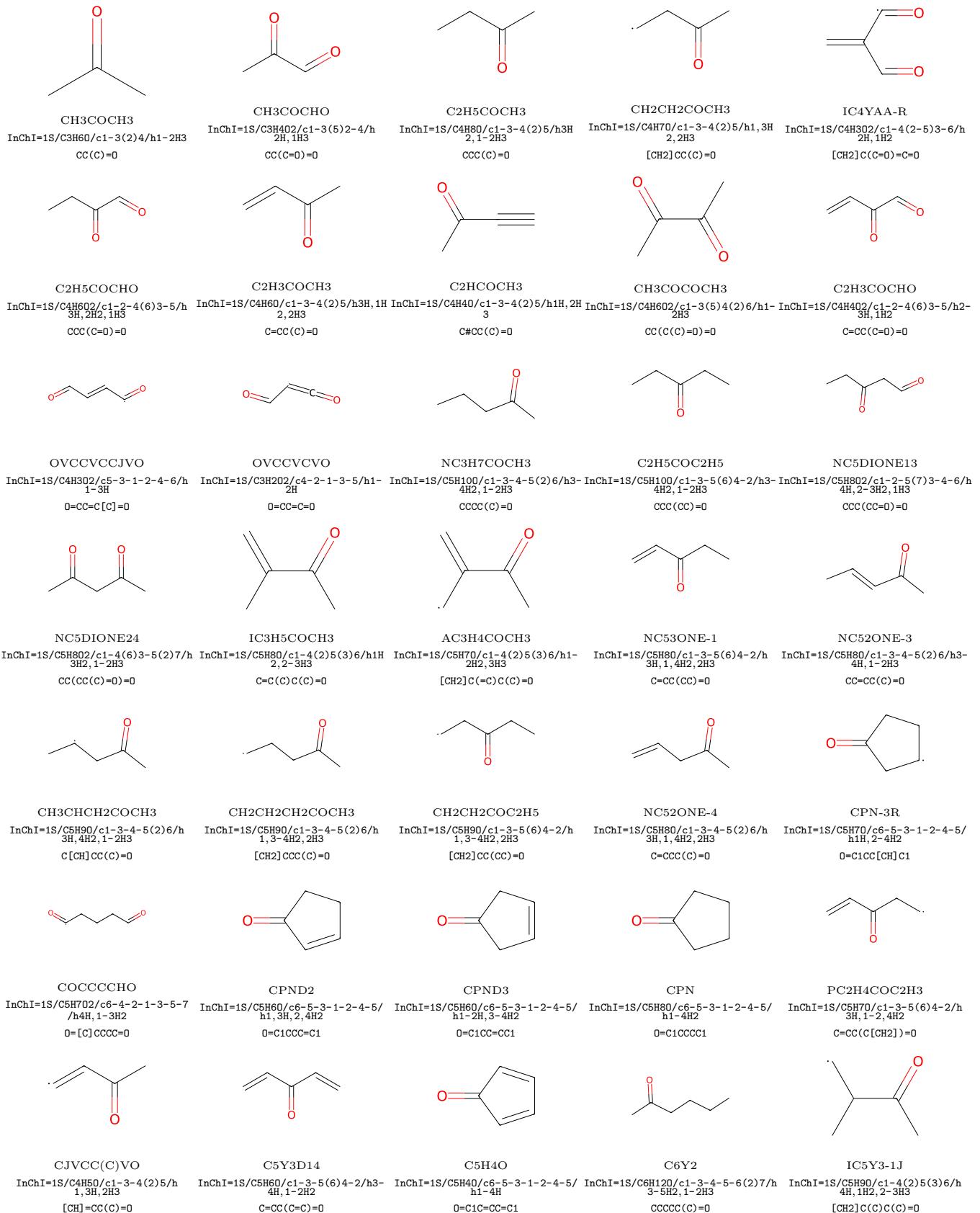
CHOCCCCHO
InChI=1S/C5H8O2/c6-4-2-1-3-5-7
/h4-5H,1-3H2
O=CCCCCC=O

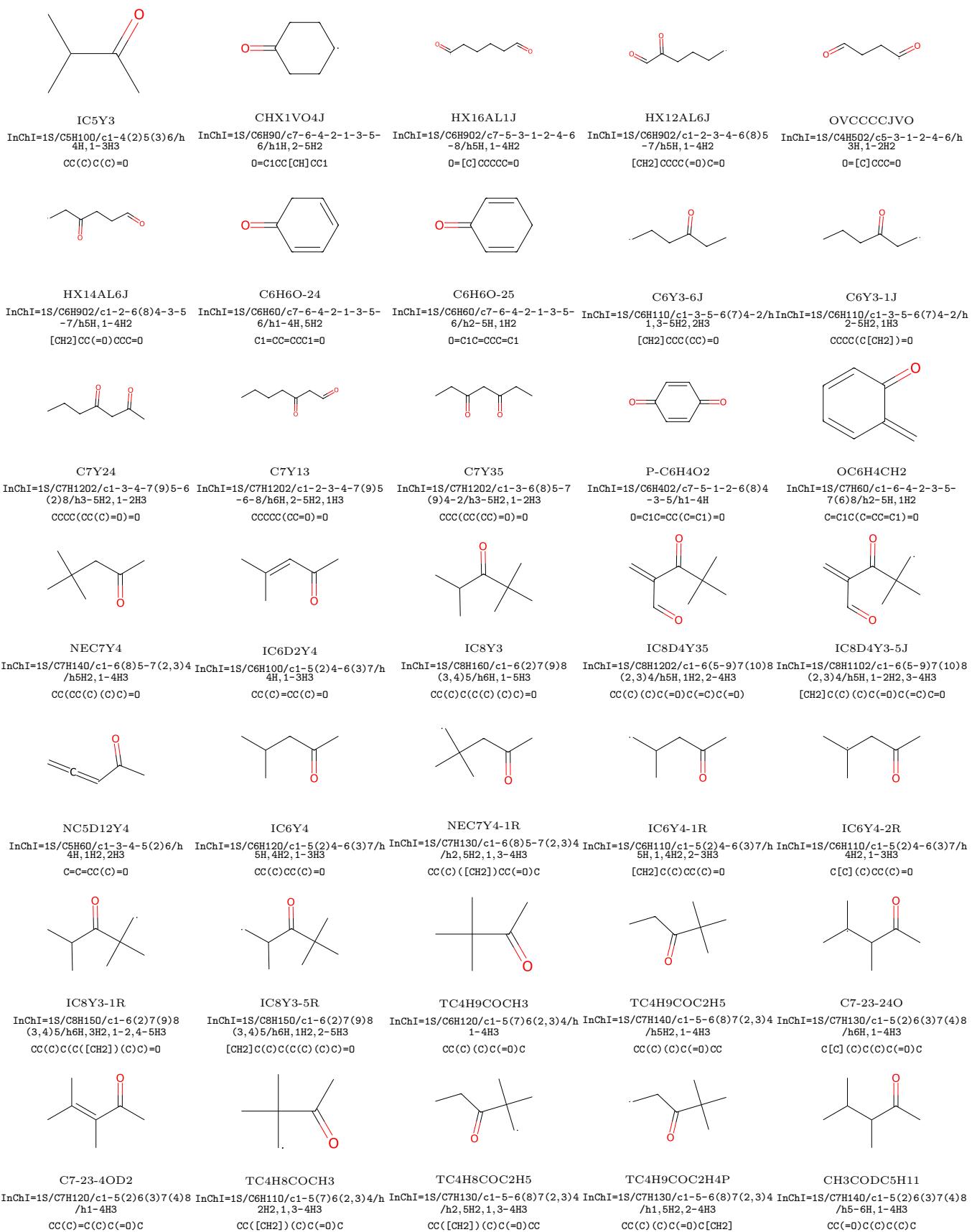
CHOCHHCCHCHO
InChI=1S/C5H7O2/c6-4-2-1-3-5-7
/h1,4-5H,2-3H2
O=CC[CH]CC=O

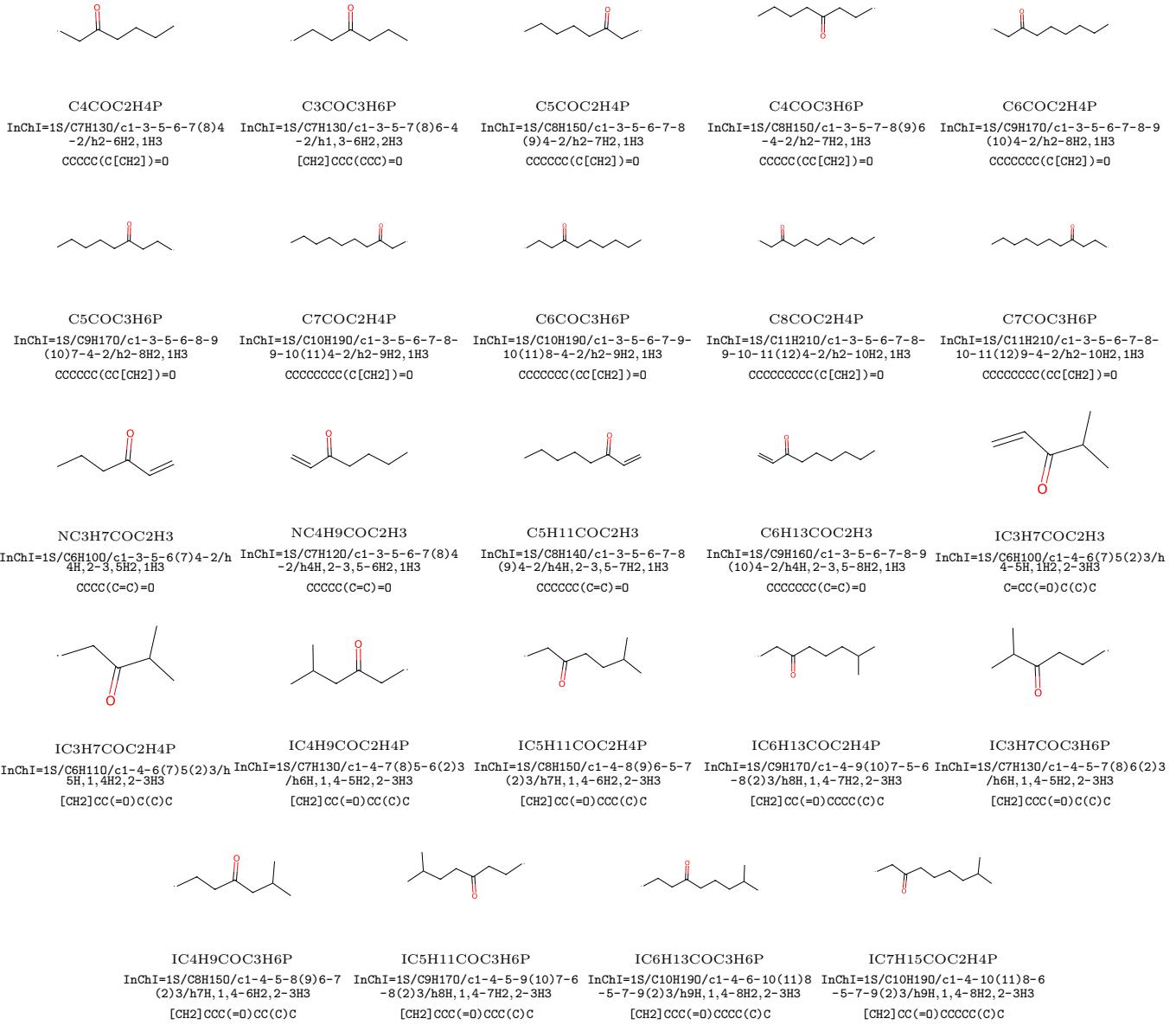




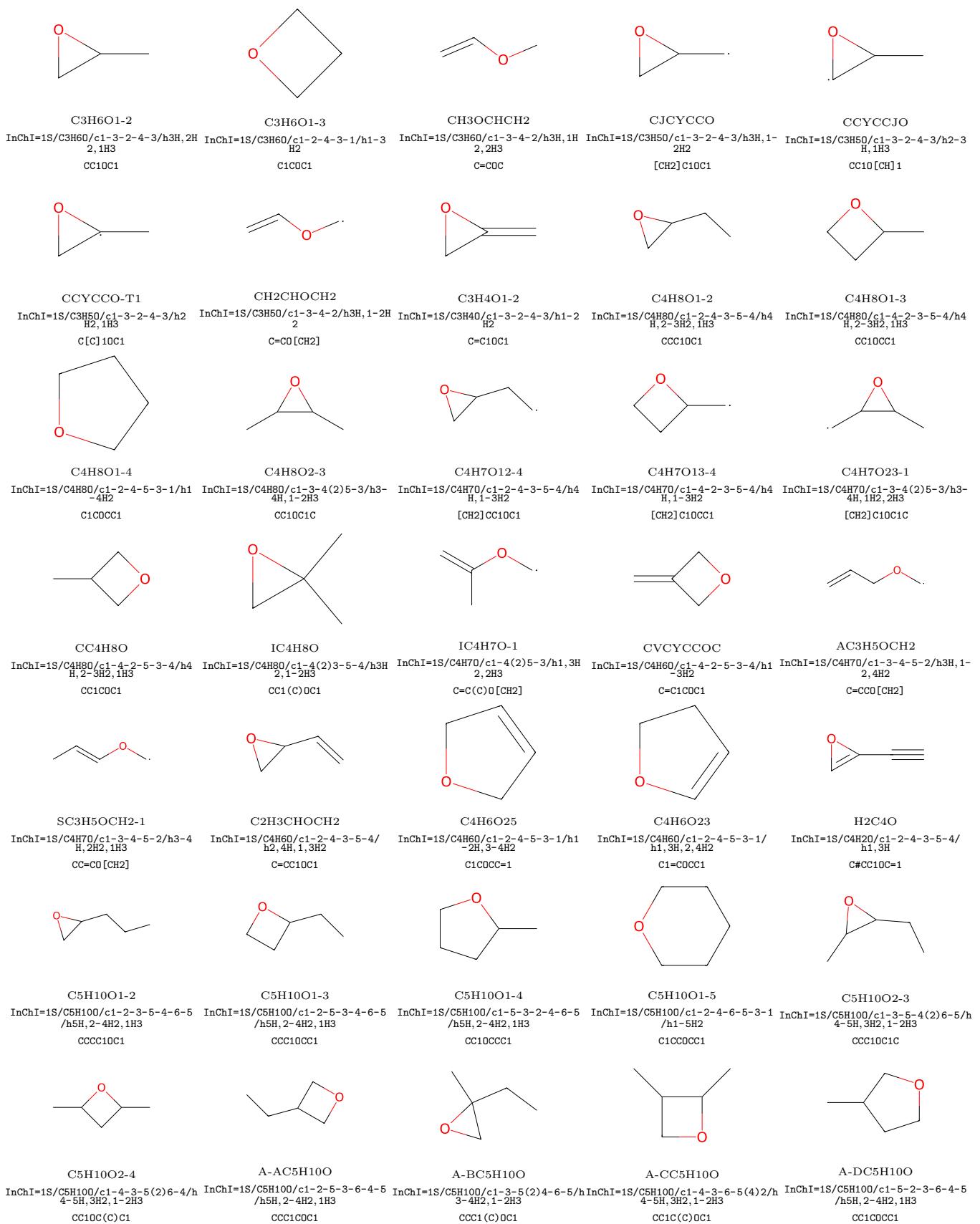
22 Ketones (molecules and radicals)

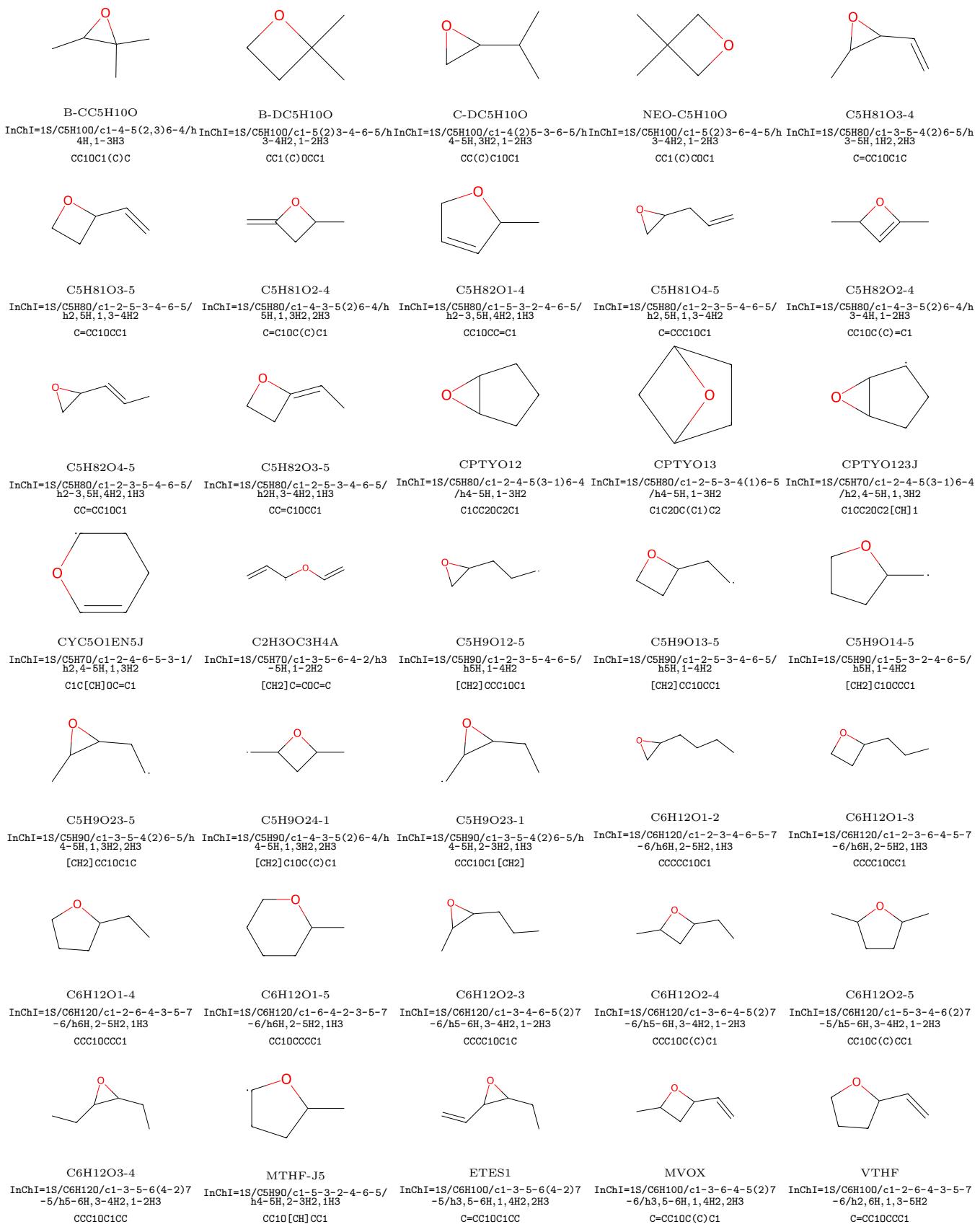


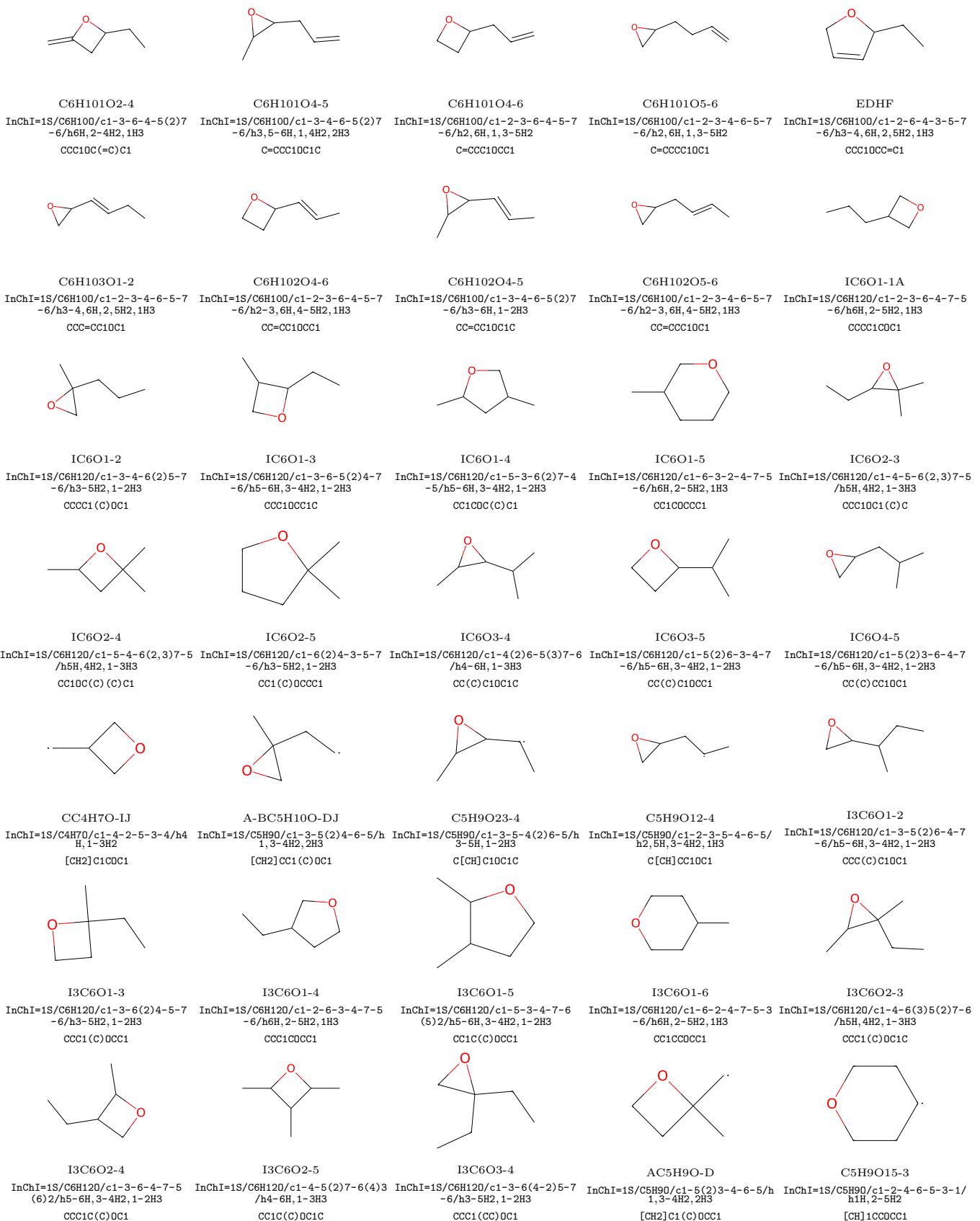


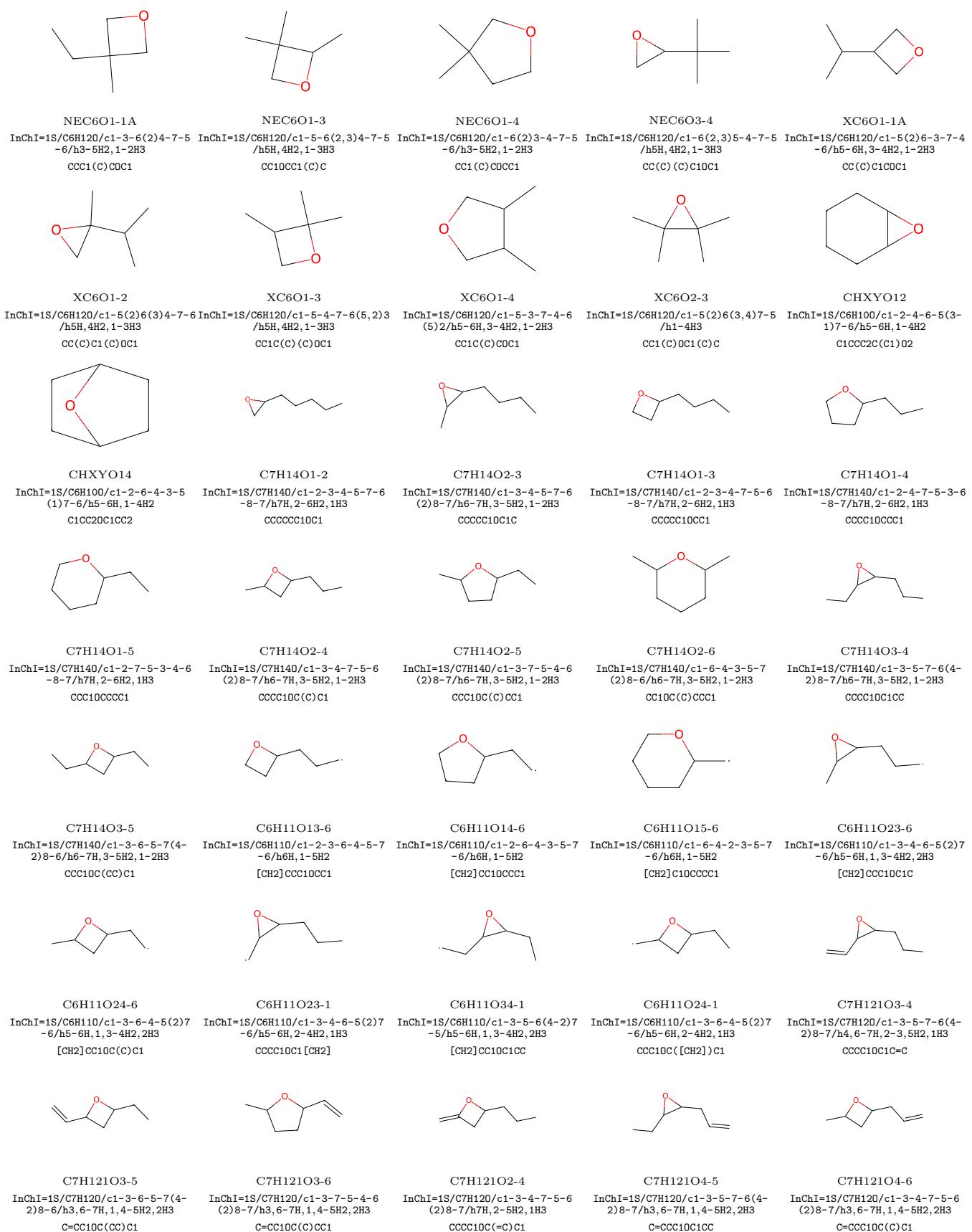


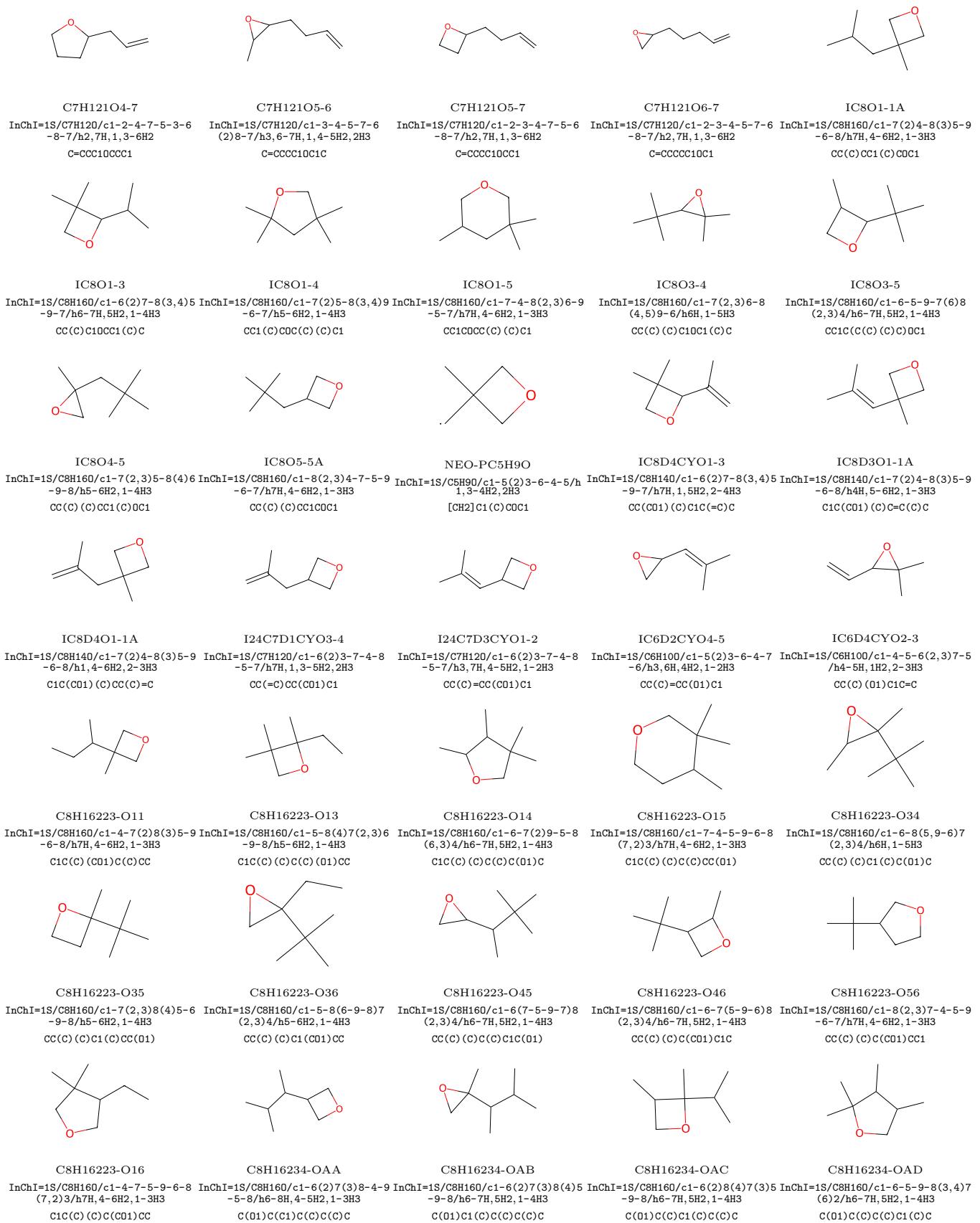
23 Ethers (molecules and radicals)

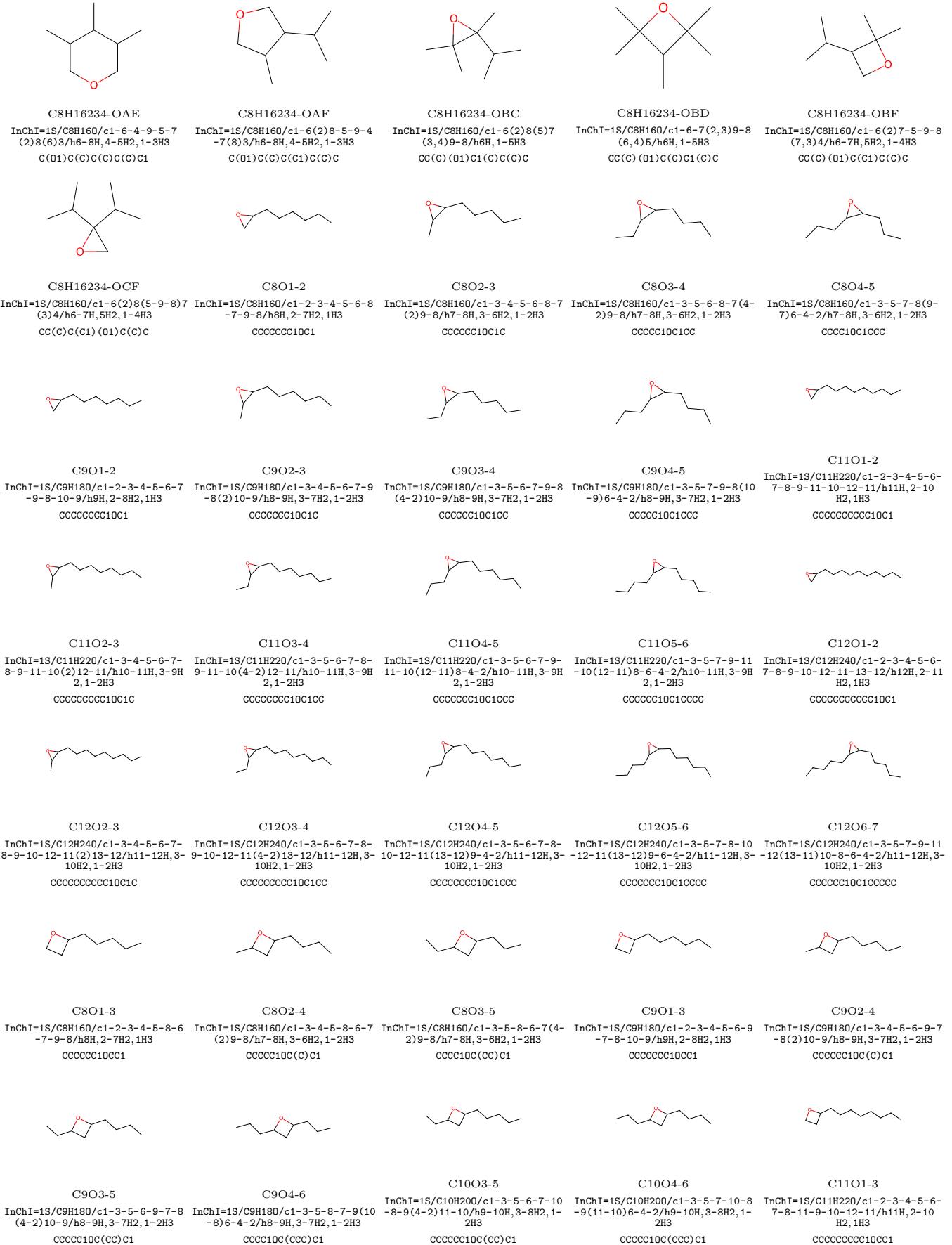




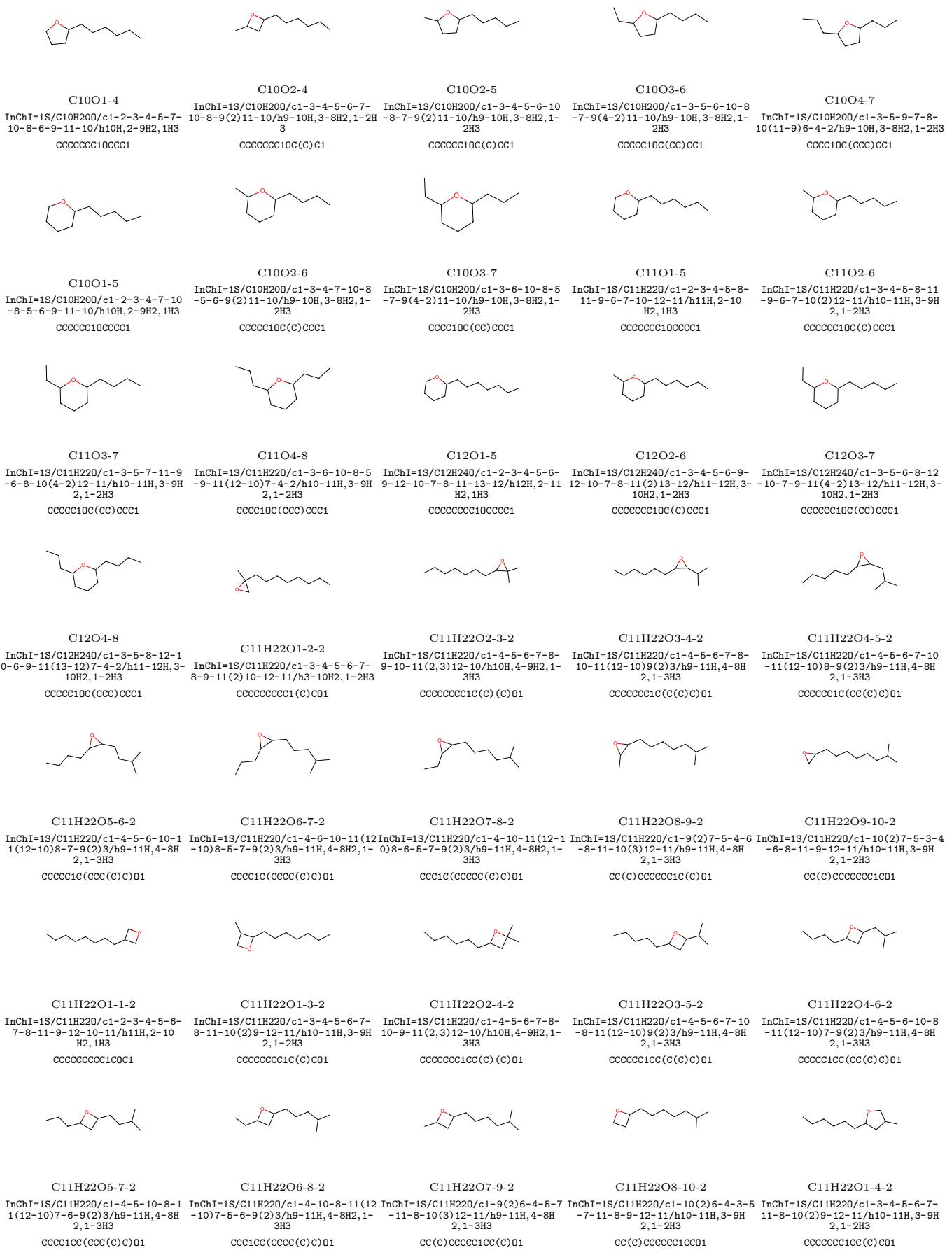


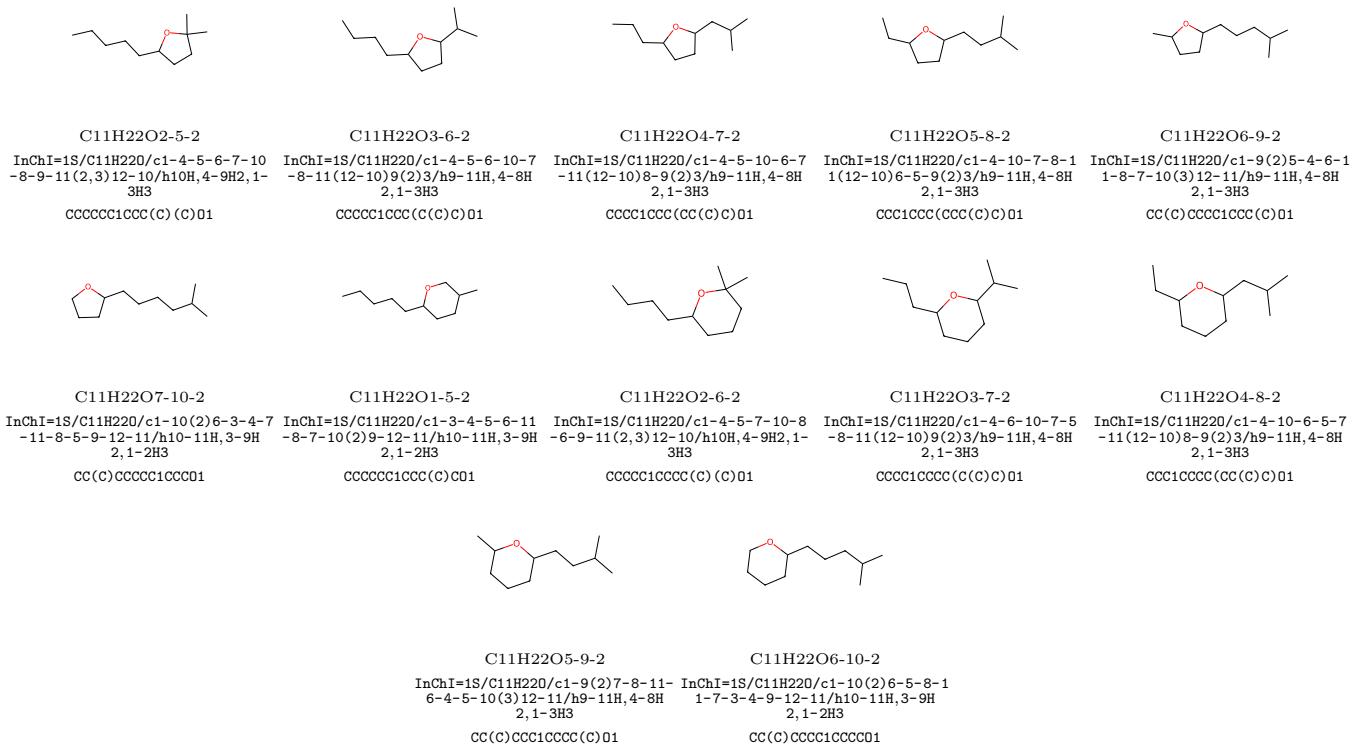




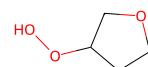
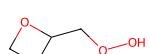
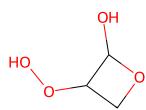
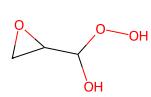
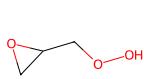








24 Ether-hydroperoxides



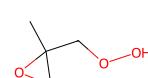
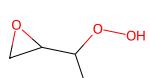
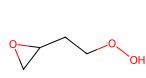
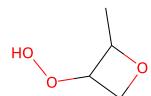
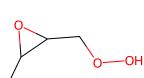
C3H5O1-2OOH-3
InChI=1S/C3H6O3/c4-6-2-3-1-5-3
/h3-4H, 1-2H2
00CC1OC1

COHOOCY(COC)
InChI=1S/C3H6O4/c4-3(7-5)2-1-6
-2/h2-5H, 1H2
OC(C1OC1)OO

OHCY(COCC)OOH
InChI=1S/C3H6O4/c4-3-2(7-5)1-6
-3/h2-5H, 1H2
OC1OC100

C4H7O1-3OOH-4
InChI=1S/C4H8O3/c5-7-3-4-1-2-6
-4/h4-5H, 1-3H2
00CC1OCC1

C4H7O1-4OOH-2
InChI=1S/C4H8O3/c5-7-4-1-2-6-3
-4/h4-5H, 1-3H2
00C1OCOC1



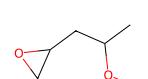
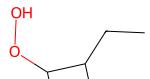
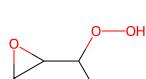
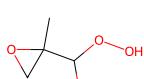
C4H7O2-3OOH-1
InChI=1S/C4H8O3/c1-3-4(7-3)2-6
-5/h3-5H, 2H2, 1H3
CC1OC1COO

C4H7O1-3OOH-2
InChI=1S/C4H8O3/c1-3-4(7-5)2-6
-3/h3-5H, 2H2, 1H3
CC1OCC100

C4H7O1-2OOH-4
InChI=1S/C4H8O3/c5-7-2-1-4-3-6
-4/h4-5H, 1-3H2
00CCC10C1

C4H7O1-2OOH-3
InChI=1S/C4H8O3/c1-3(7-5)4-2-6
-4/h3-5H, 2H2, 1H3
CC(C1OC1)OO

ET12IC4-1OOH
InChI=1S/C4H8O3/c1-4(8-6)2-5-3
-5/h5H, 2-3H2, 1H3
CC1(COO)OC1



COHQCYC(COC)

InChI=1S/C4H8O4/c1-4(2-7-4)3(5)8
-6/h3, 5-6H, 2H2, 1H3
CC1(C(O)OO)OC1

QCYC(CCOC)OH

InChI=1S/C4H8O4/c1-4(8-6)2-7-3
(4)5/h3, 5-6H, 2H2, 1H3
CC1(C(O)OC1)OO

C5H9O1-2OOH-3

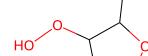
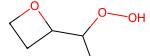
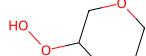
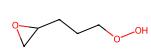
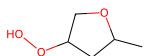
InChI=1S/C5H10O3/c1-2-4(8-6)5-3
-7-5/h4-6H, 2-3H2, 1H3
CCC(C1OC1)OO

C5H9O1-3OOH-2

InChI=1S/C5H10O3/c1-2-4-5(8-6)3
-7-4/h4-6H, 2-3H2, 1H3
CCC1OCC100

C5H9O1-2OOH-4

InChI=1S/C5H10O3/c1-4(8-6)2-5-3
-7-5/h4-6H, 2-3H2, 1H3
CC(CC1OC1)OO



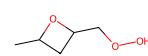
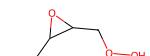
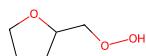
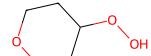
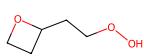
C5H9O1-4OOH-2
InChI=1S/C5H10O3/c1-4-2-5(8-6)3
-7-4/h4-6H, 2-3H2, 1H3
CC1OCC(C1)OO

C5H9O1-2OOH-5
InChI=1S/C5H10O3/c6-8-3-1-2-5-
4-7-5/h5-6H, 1-4H2
00CCCC1OC1

C5H9O1-5OOH-2
InChI=1S/C5H10O3/c6-8-5-2-1-3-
7-4-5/h5-6H, 1-4H2
00C1COCCC1

C5H9O1-3OOH-4
InChI=1S/C5H10O3/c1-4(8-6)5-2-3
-7-5/h4-6H, 2-3H2, 1H3
CC(C1OC1)OO

C5H9O1-4OOH-3
InChI=1S/C5H10O3/c1-4-5(8-6)2-3
-7-4/h4-6H, 2-3H2, 1H3
CC1OCCC100



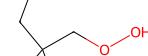
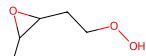
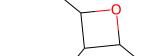
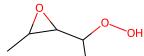
C5H9O1-3OOH-5
InChI=1S/C5H10O3/c6-8-4-2-5-1-
3-7-5/h5-6H, 1-4H2
00CCC1OCC1

C5H9O1-5OOH-3
InChI=1S/C5H10O3/c6-8-5-1-3-7-
4-2-5/h5-6H, 1-4H2
00C1CCOCC1

C5H9O1-4OOH-5
InChI=1S/C5H10O3/c6-8-4-5-2-1-
3-7-5/h5-6H, 1-4H2
00CC1OCC1

C5H9O2-3OOH-1
InChI=1S/C5H10O3/c1-2-4-5(8-4)3
-7-6/h4-6H, 2-3H2, 1H3
CCC1OCC100

C5H9O2-4OOH-1
InChI=1S/C5H10O3/c1-4-2-5(8-4)3
-7-6/h4-6H, 2-3H2, 1H3
CC1OC(C1)COO



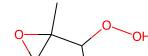
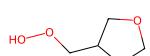
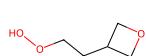
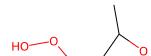
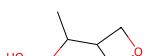
C5H9O2-3OOH-4
InChI=1S/C5H10O3/c1-3-5(7-3)4
(2)8-6/h3-6H, 1-2H3
CC1OC1C(C)OO

C5H9O2-4OOH-3
InChI=1S/C5H10O3/c1-3-5(8-6)4
(2)7-3/h3-6H, 1-2H3
CC1OC(C)C100

C5H9O2-3OOH-5
InChI=1S/C5H10O3/c1-4-5(8-4)2-3
-7-6/h4-6H, 2-3H2, 1H3
CC1OC1CCOO

C5H9OA-AAOOH-B
InChI=1S/C5H10O3/c1-2-5(8-6)3-7
-4-5/h6H, 2-4H2, 1H3
CCC1(COC1)OO

C5H9OA-BOOH-A
InChI=1S/C5H10O3/c1-2-5(3-7-5)4
-8-6/h6H, 2-4H2, 1H3
CCC1(COO)OC1



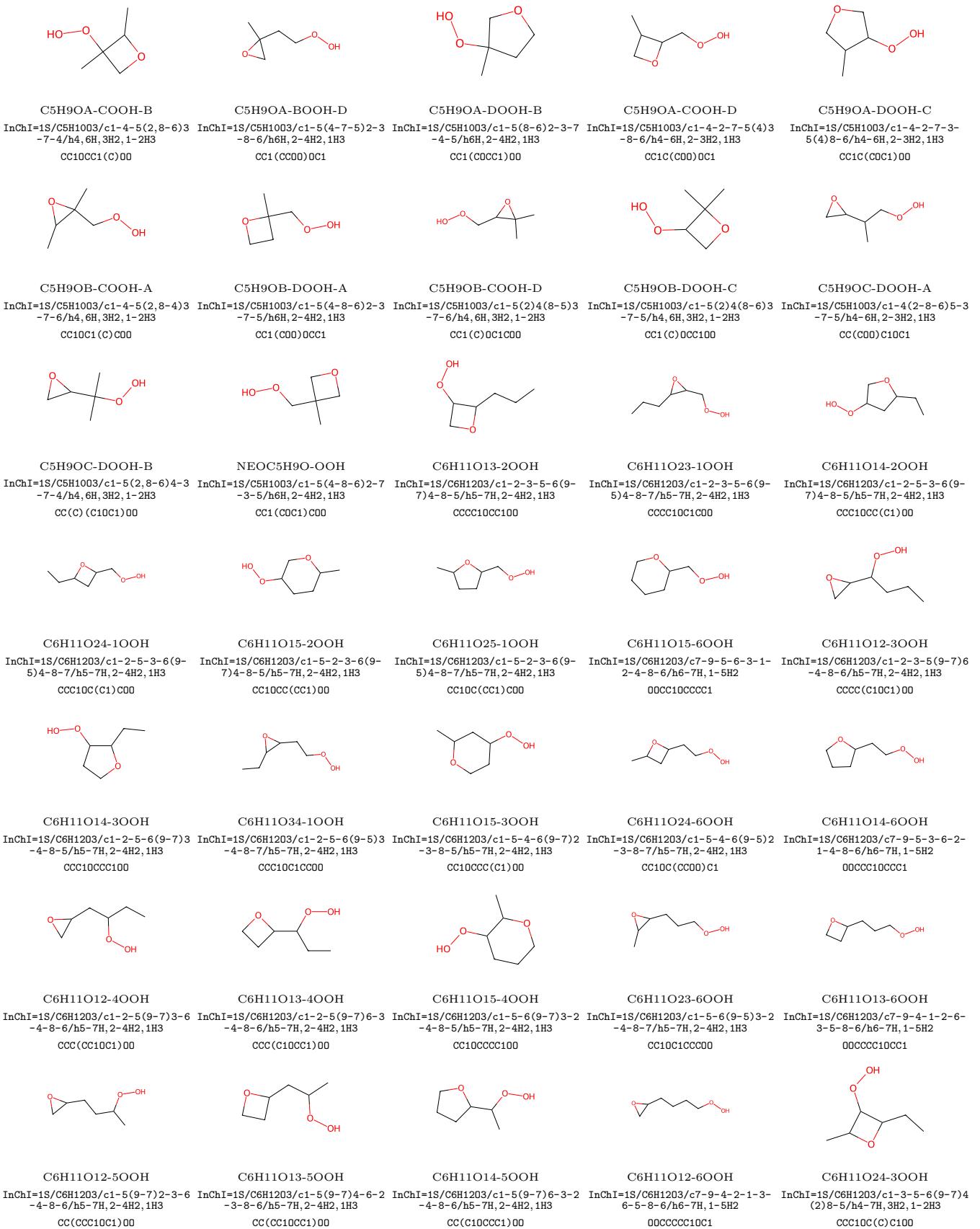
C5H9OA-AAOOH-C
InChI=1S/C5H10O3/c1-4(8-6)5-2-7
-3-5/h4-6H, 2-3H2, 1H3
CC(C1OC1)OO

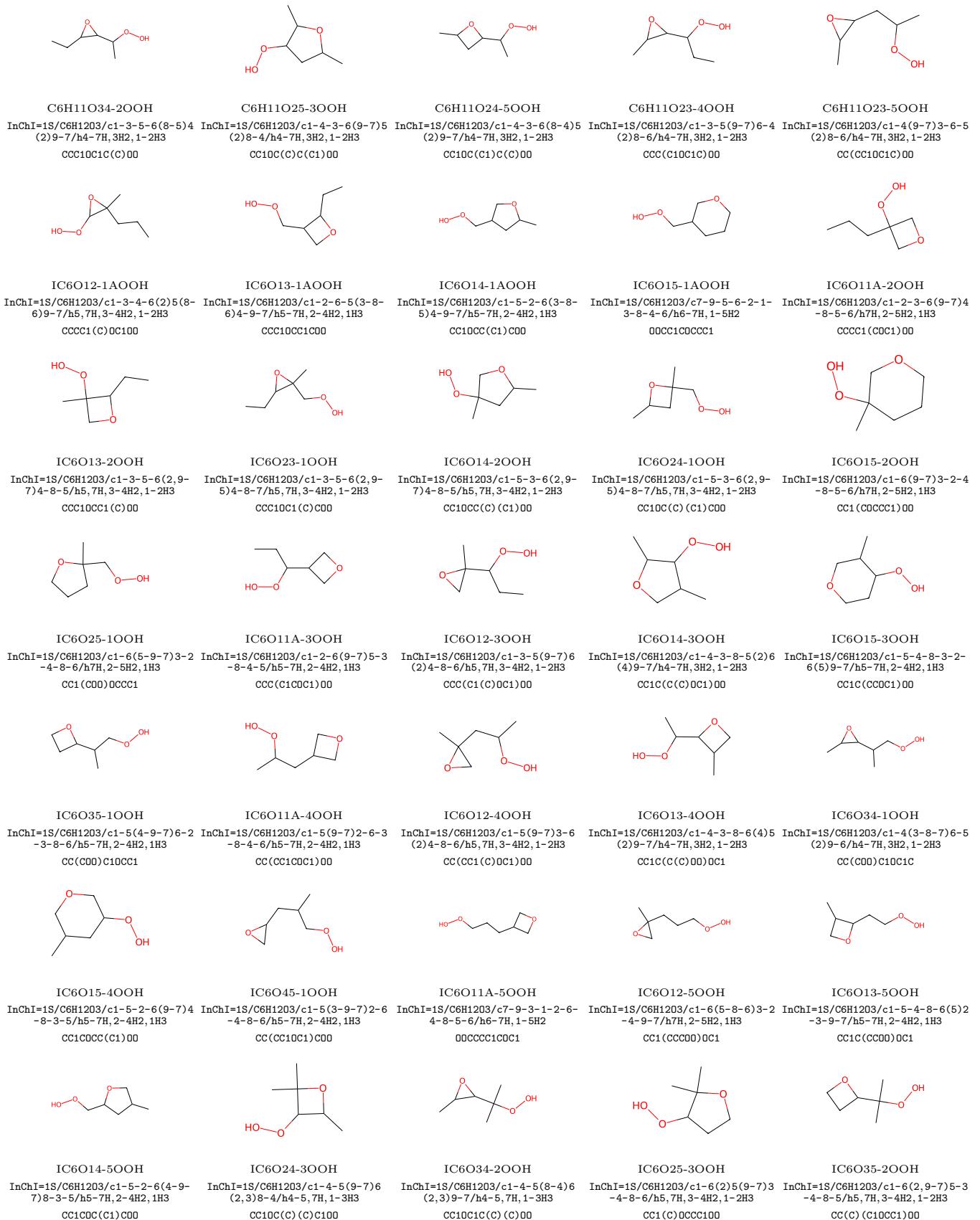
C5H9OA-COOH-A
InChI=1S/C5H10O3/c1-4-5(2-7-4)3
-8-6/h4-6H, 2-3H2, 1H3
CC1OCC1C00

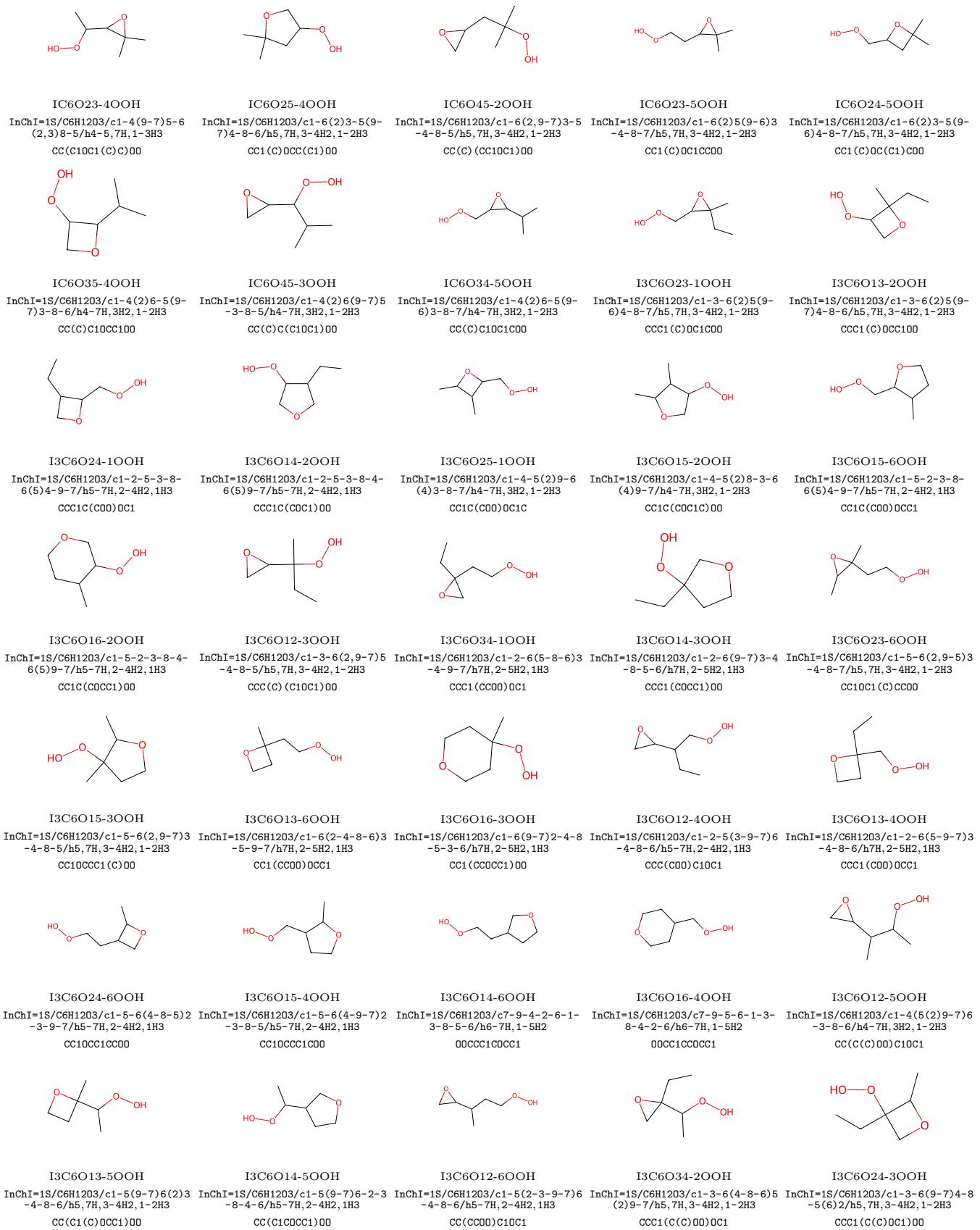
C5H9OA-AAOOH-D
InChI=1S/C5H10O3/c6-8-2-1-5-3-
7-4-5/h5-6H, 1-4H2
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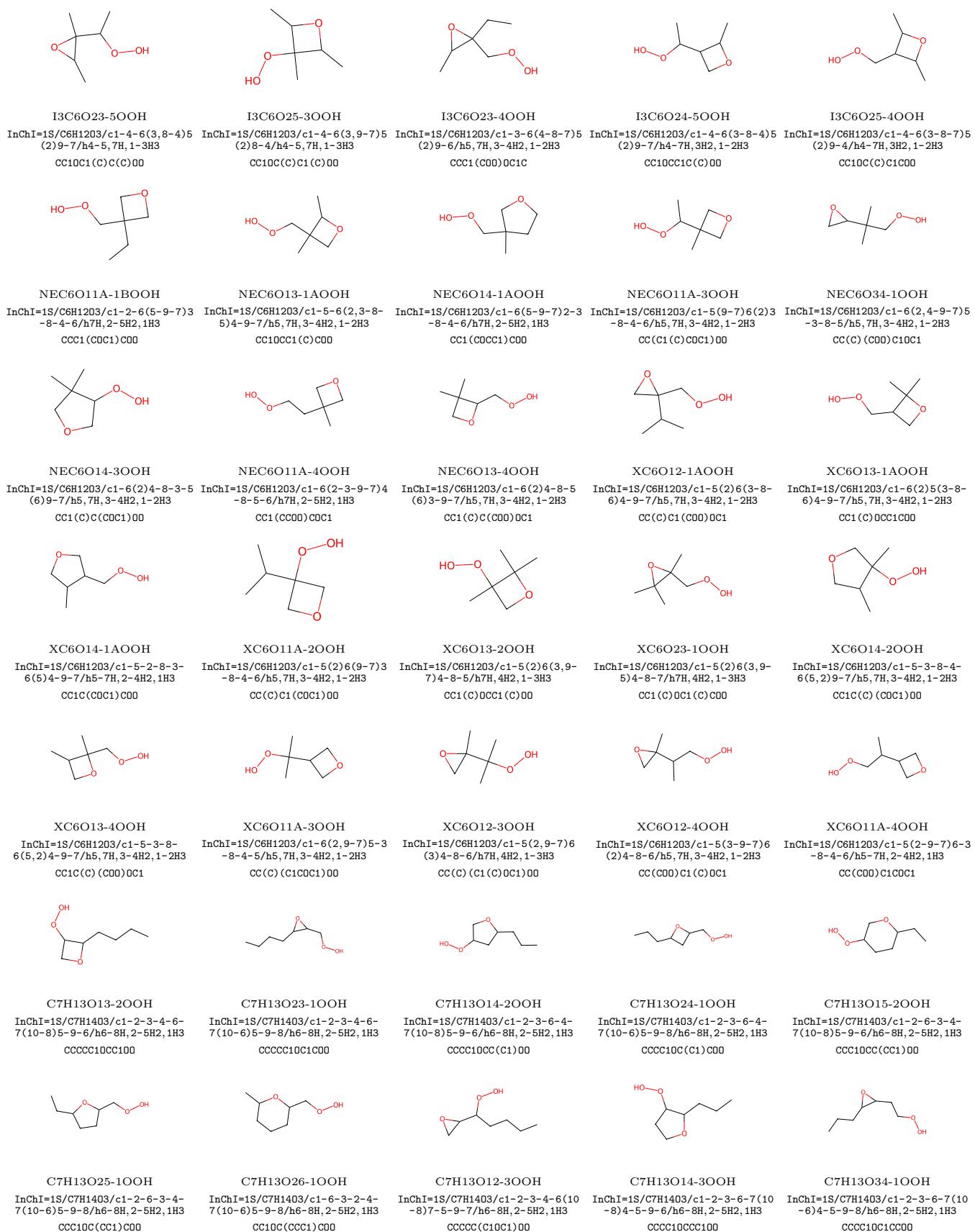
C5H9OA-DOOH-A
InChI=1S/C5H10O3/c6-8-4-5-1-2-
7-3-5/h5-6H, 1-4H2
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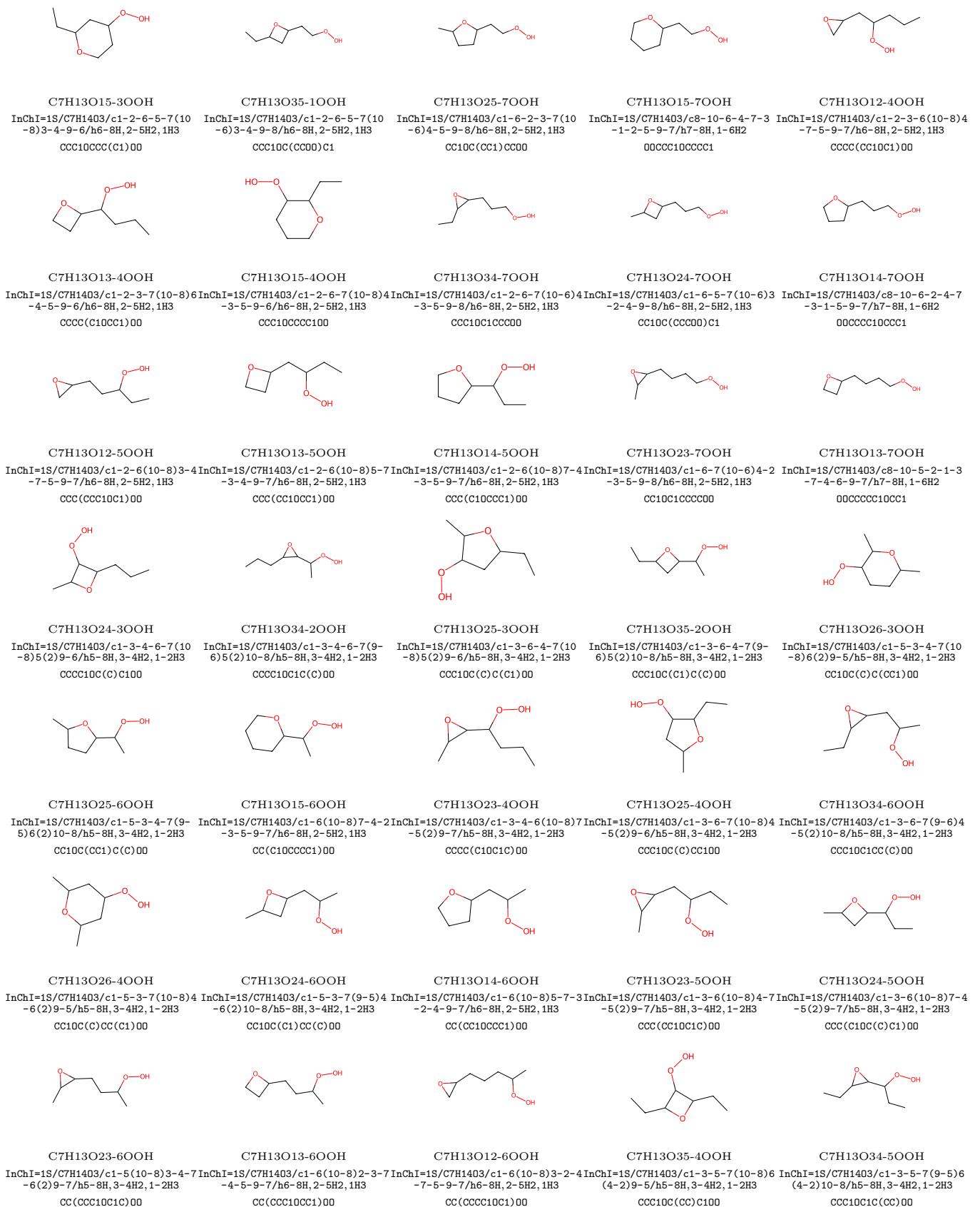
C5H9OA-BOOH-C
InChI=1S/C5H10O3/c1-4(8-6)5(2)3
-7-5/h4-6H, 3H2, 1-2H3
CC(C1OC1)OO

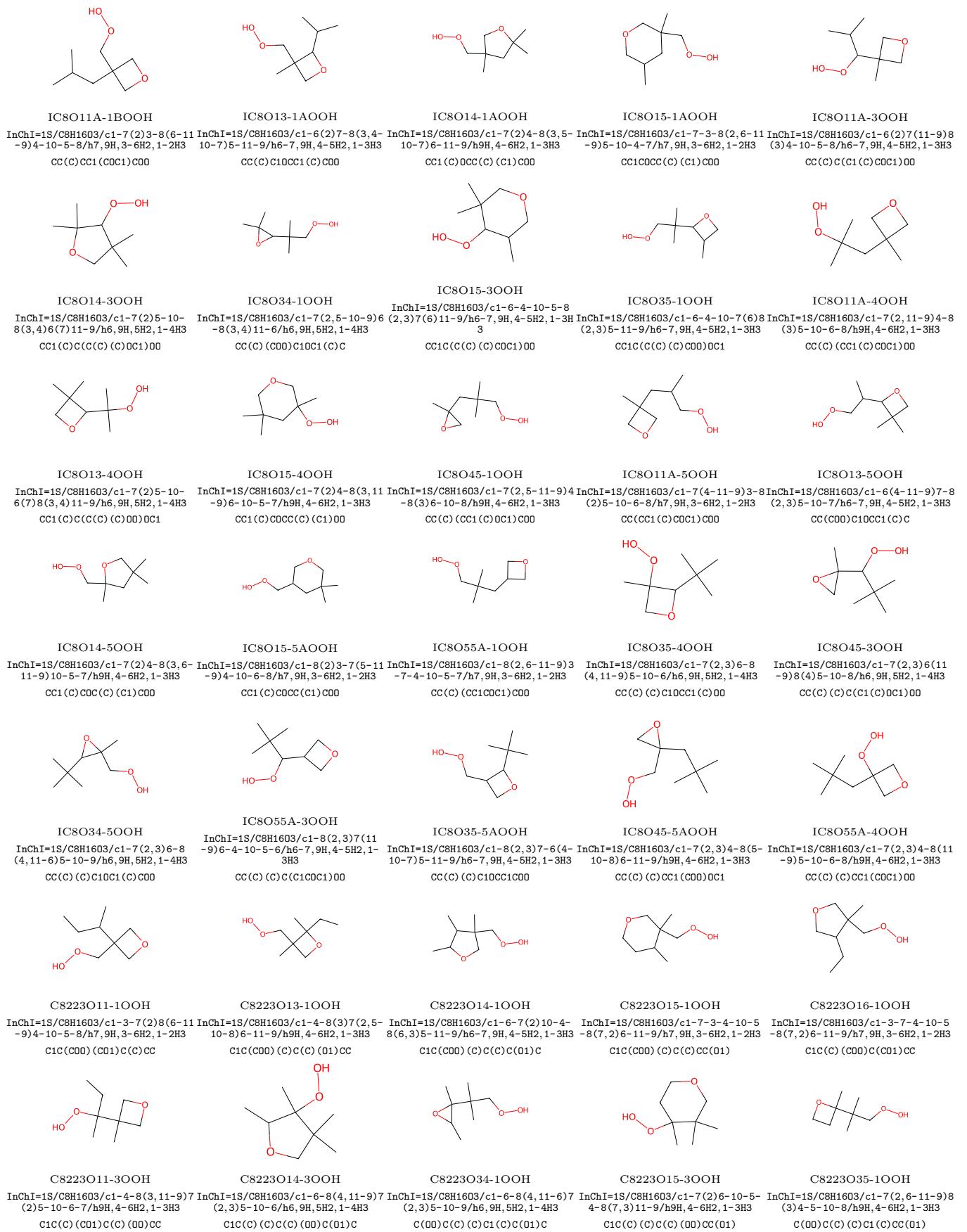


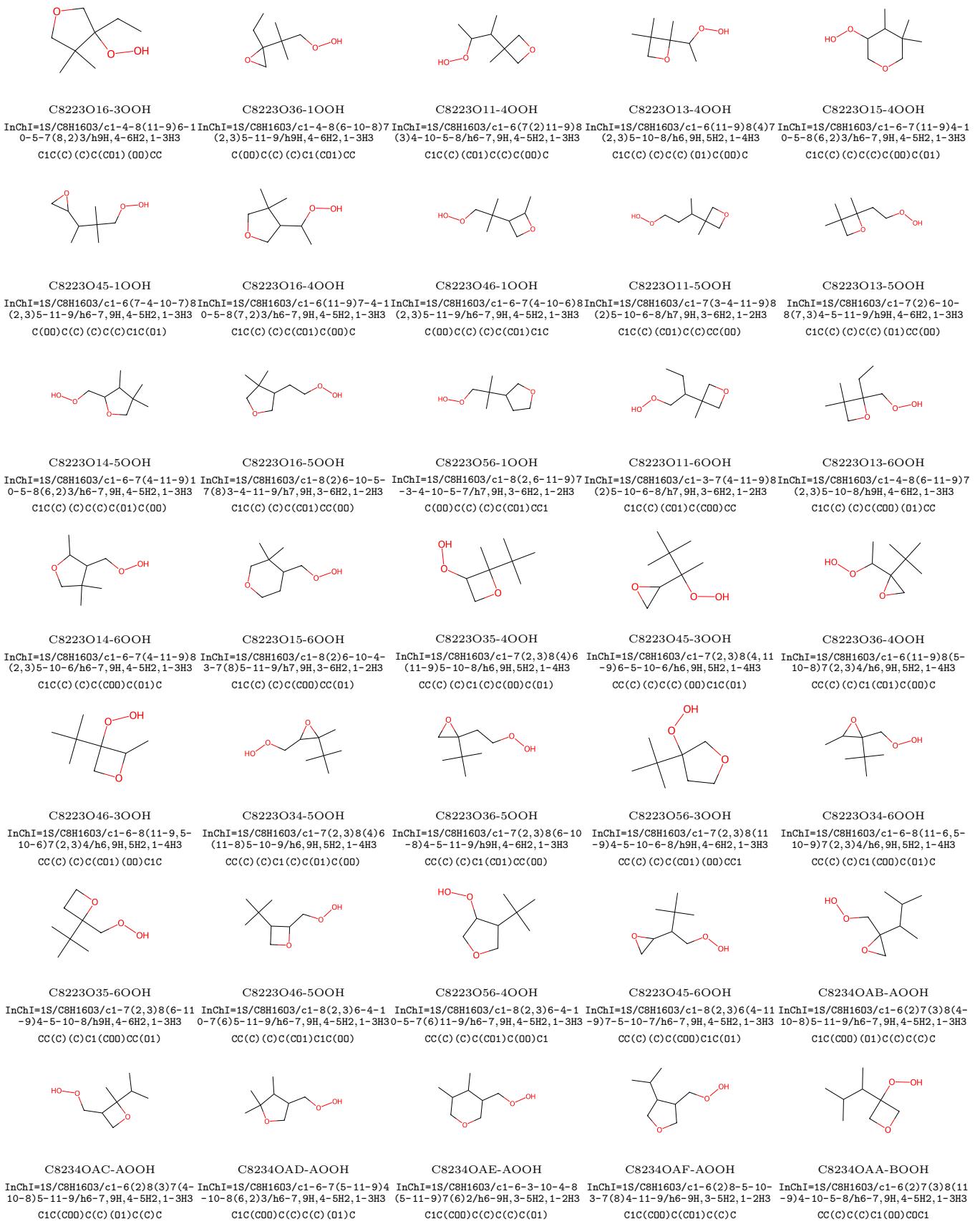


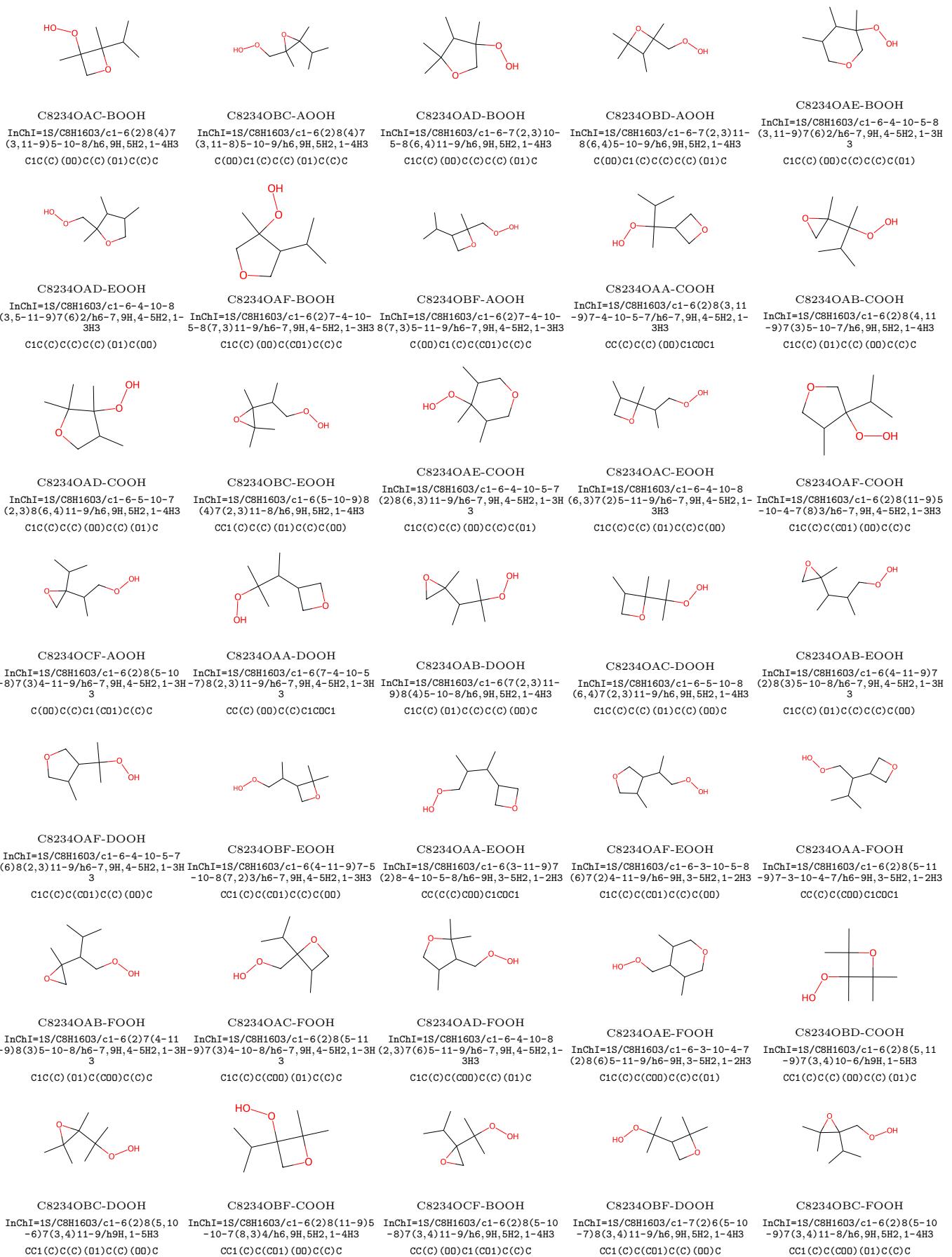


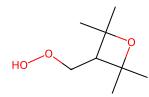








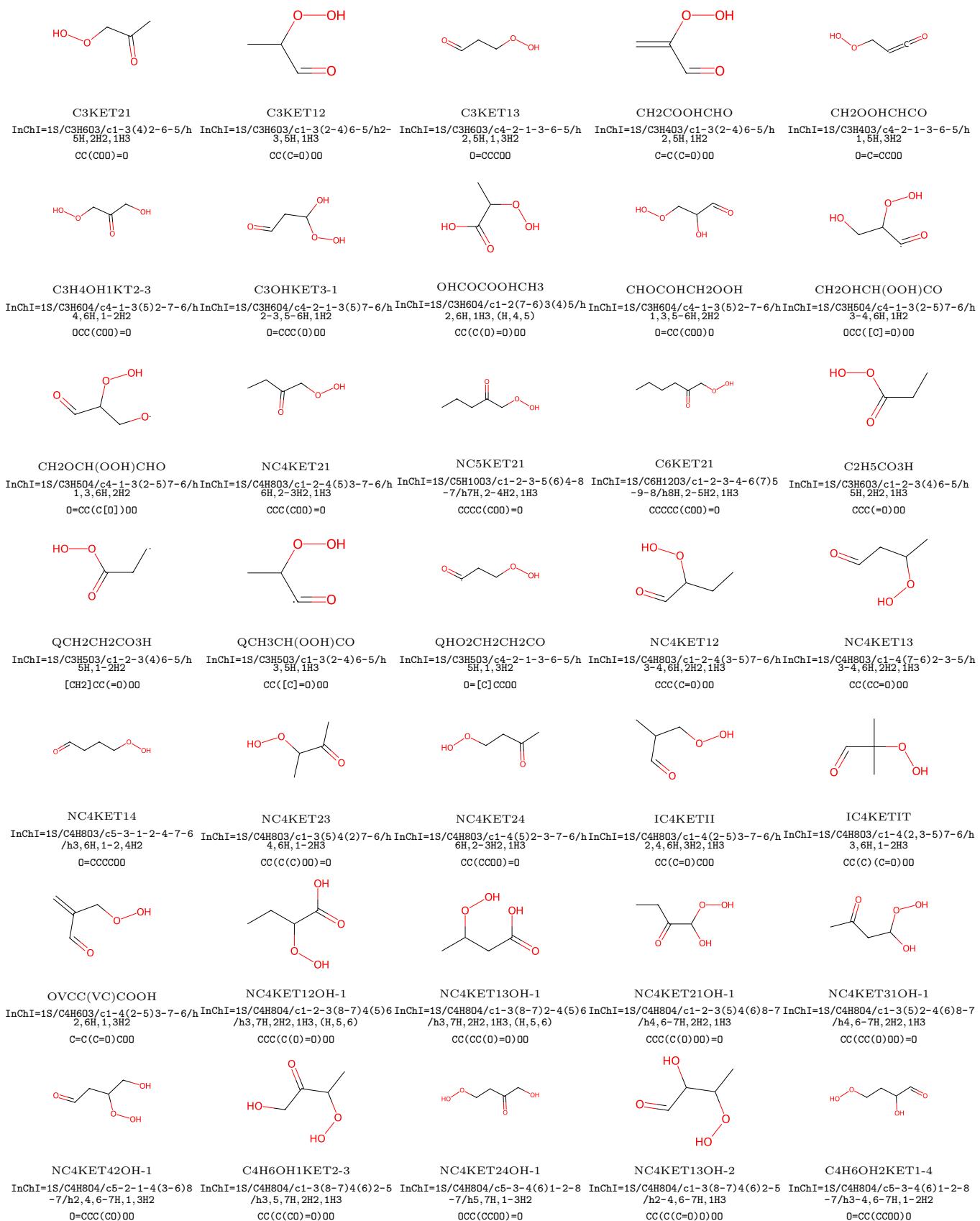


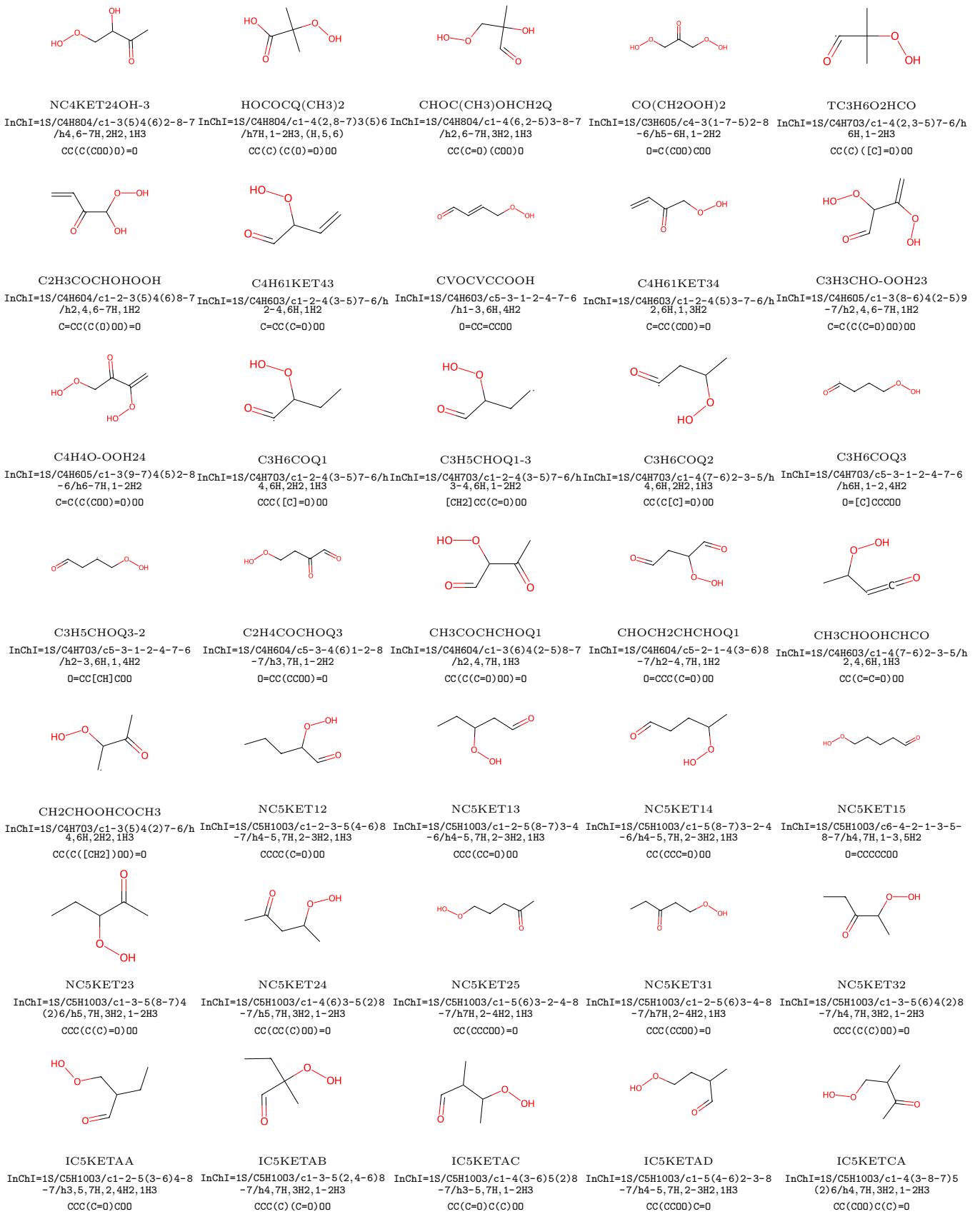


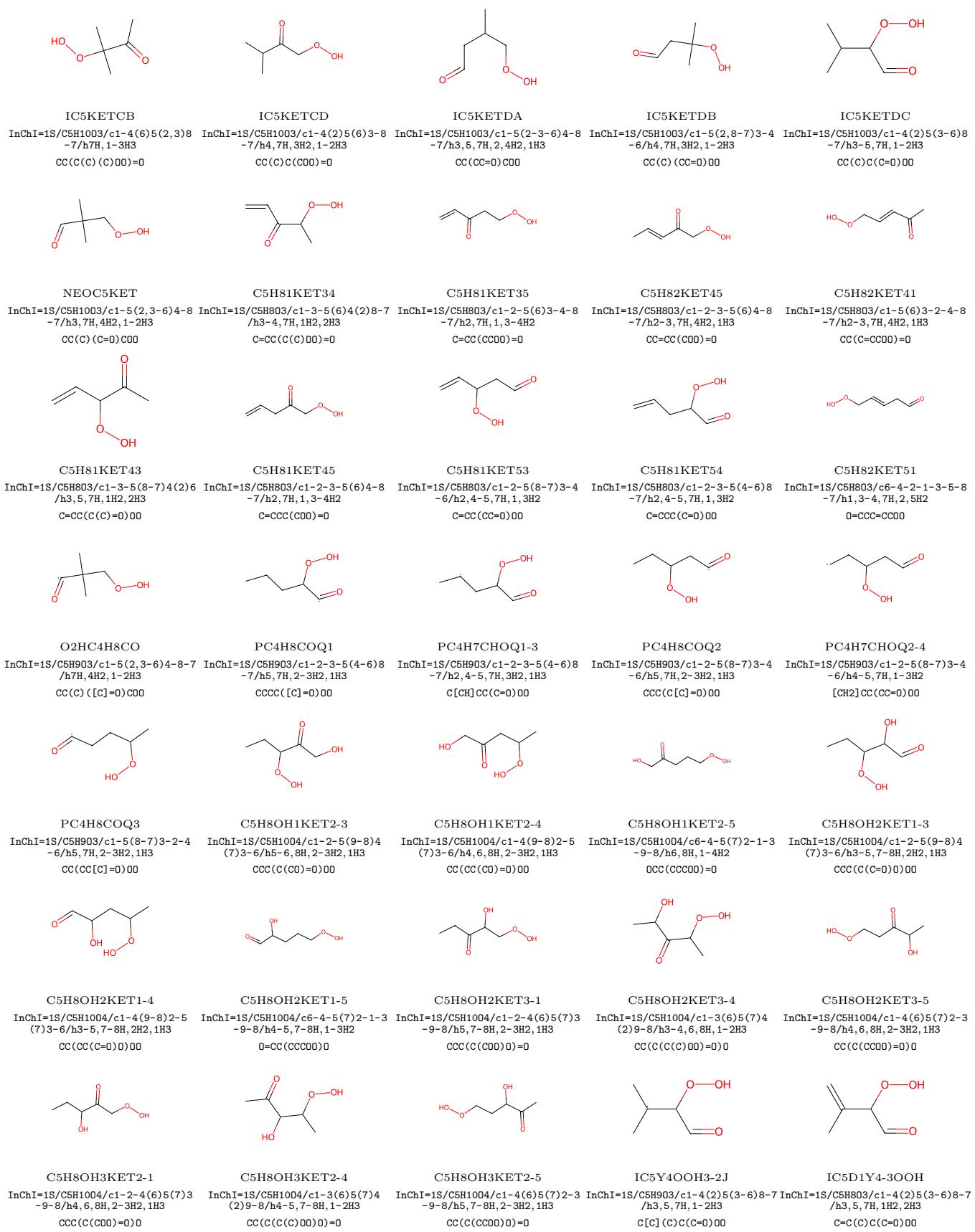
C8234OBD-FOOH

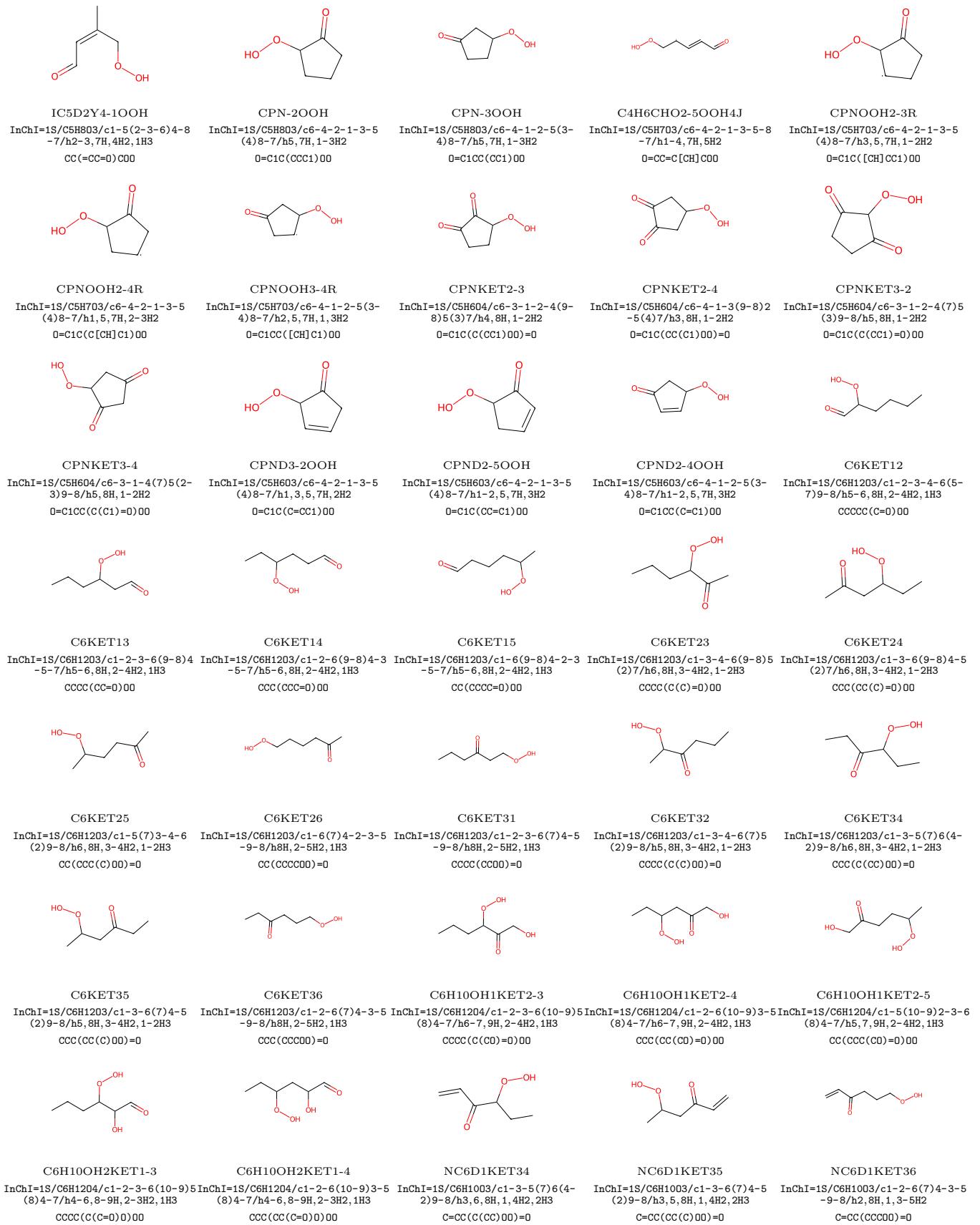
InChI=1S/C8H16O3/c1-7(2)6(5-10
-9)8(3,4)11-7/h6,9H,5H2,1-4H3
cc1(c)c(c(=O)O)c(c(=O)O)c1C

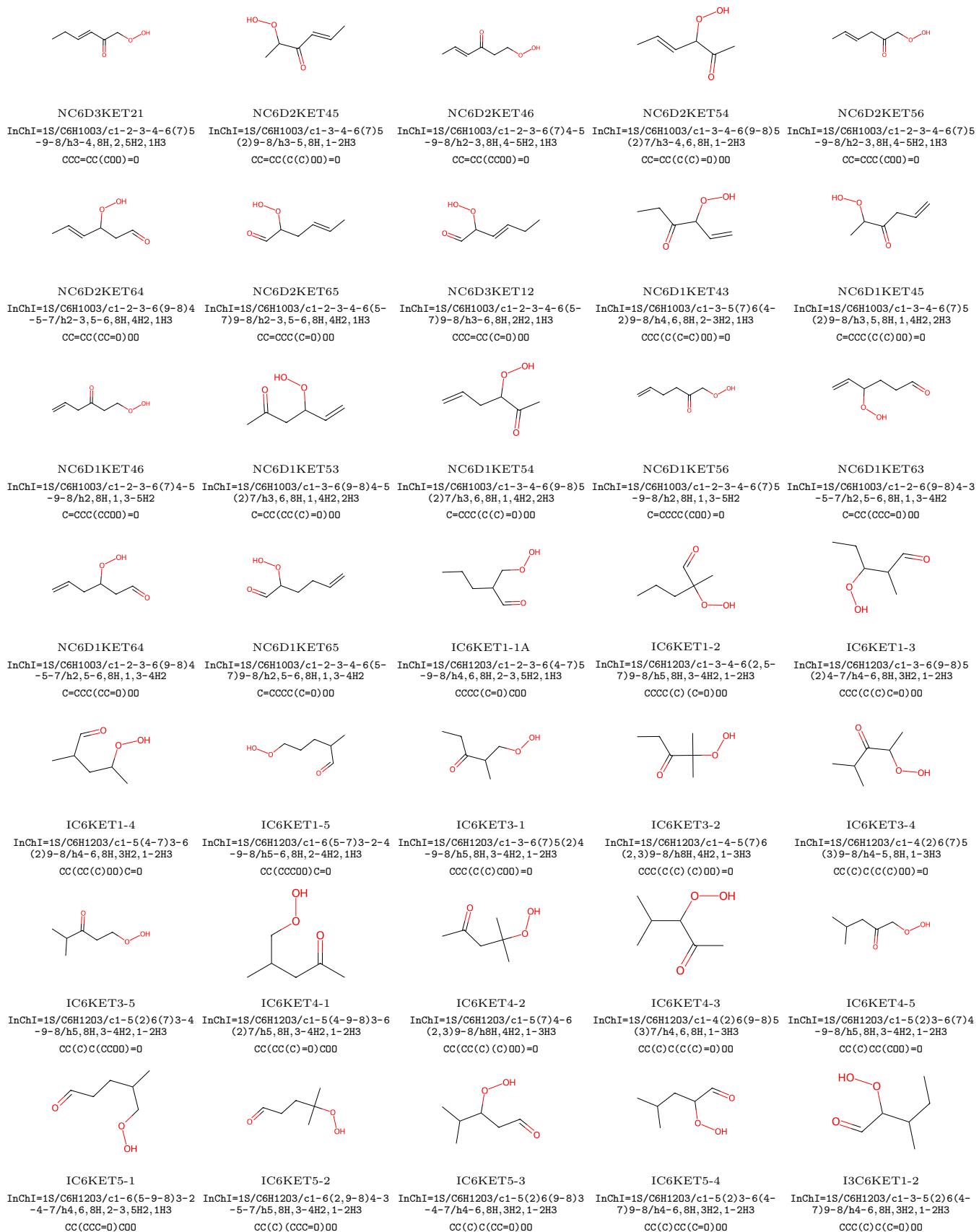
25 Carbonyl-hydroperoxides

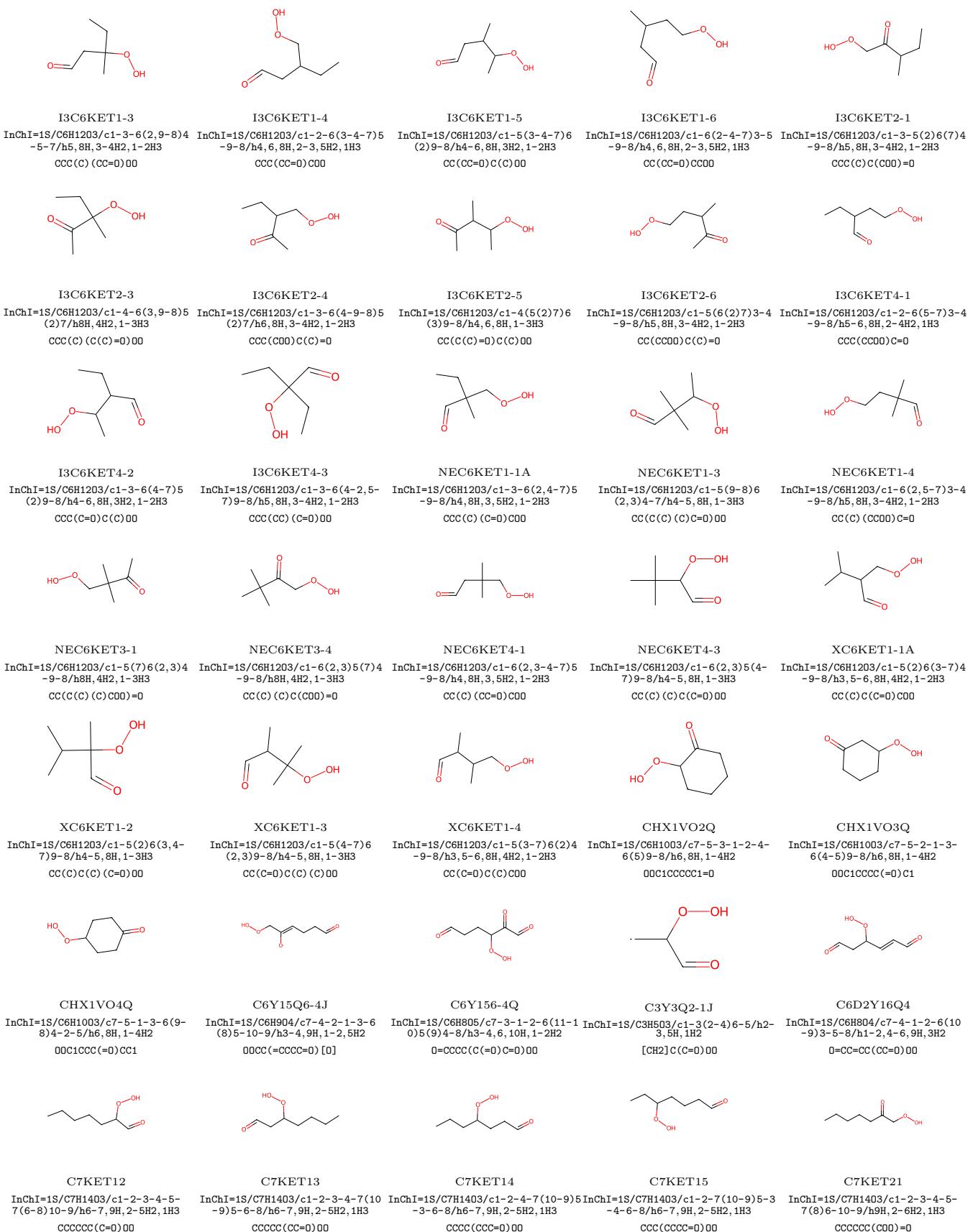


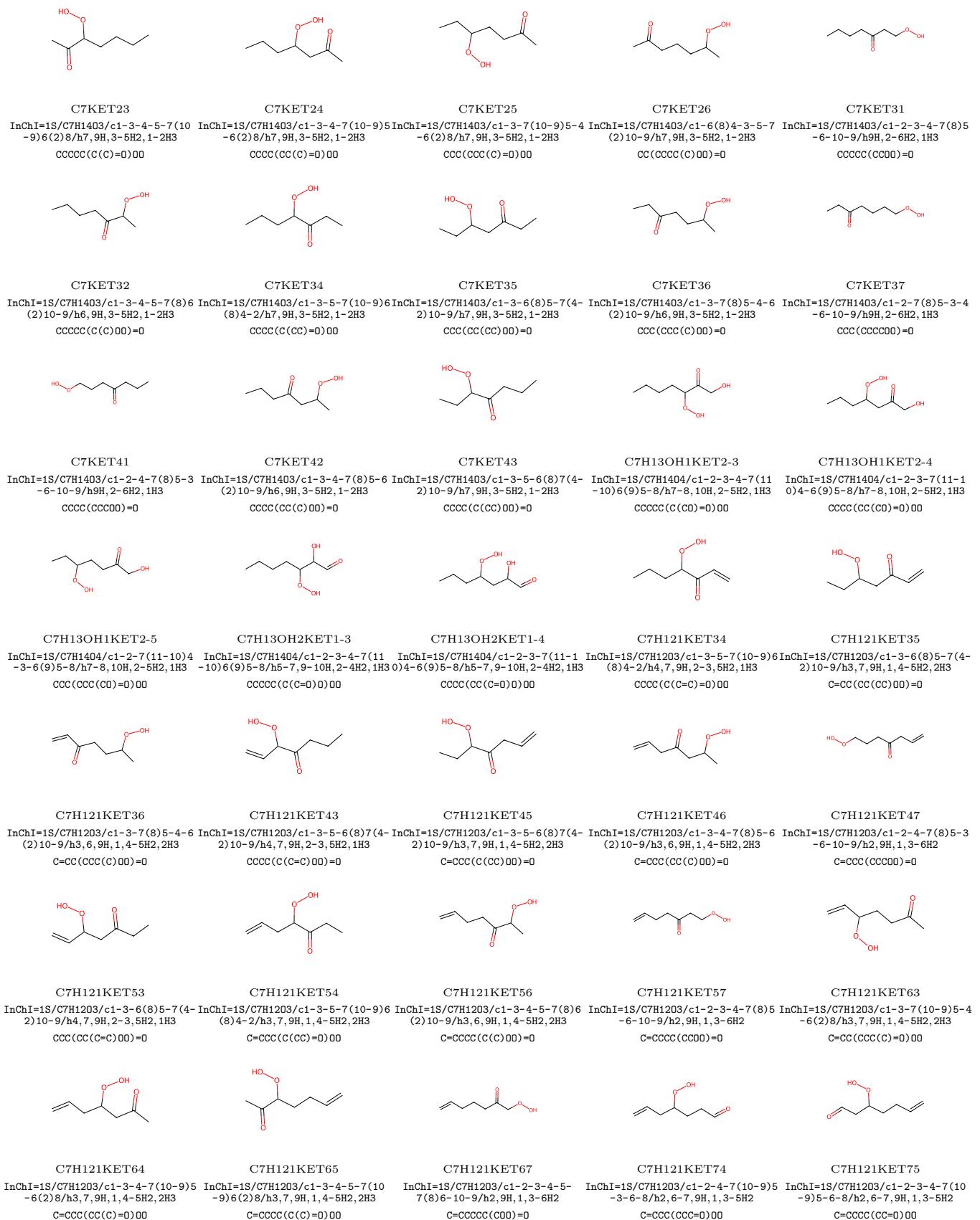


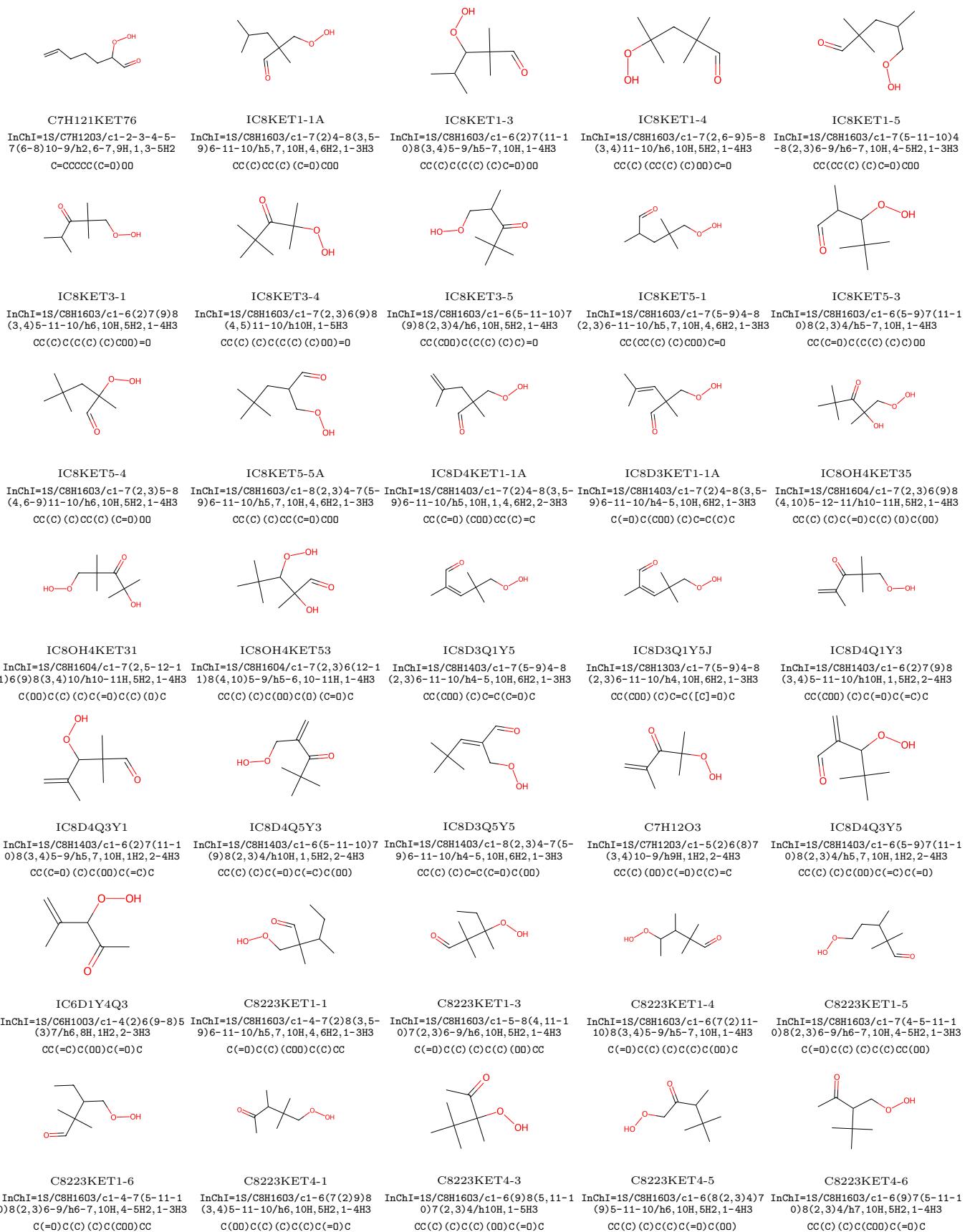


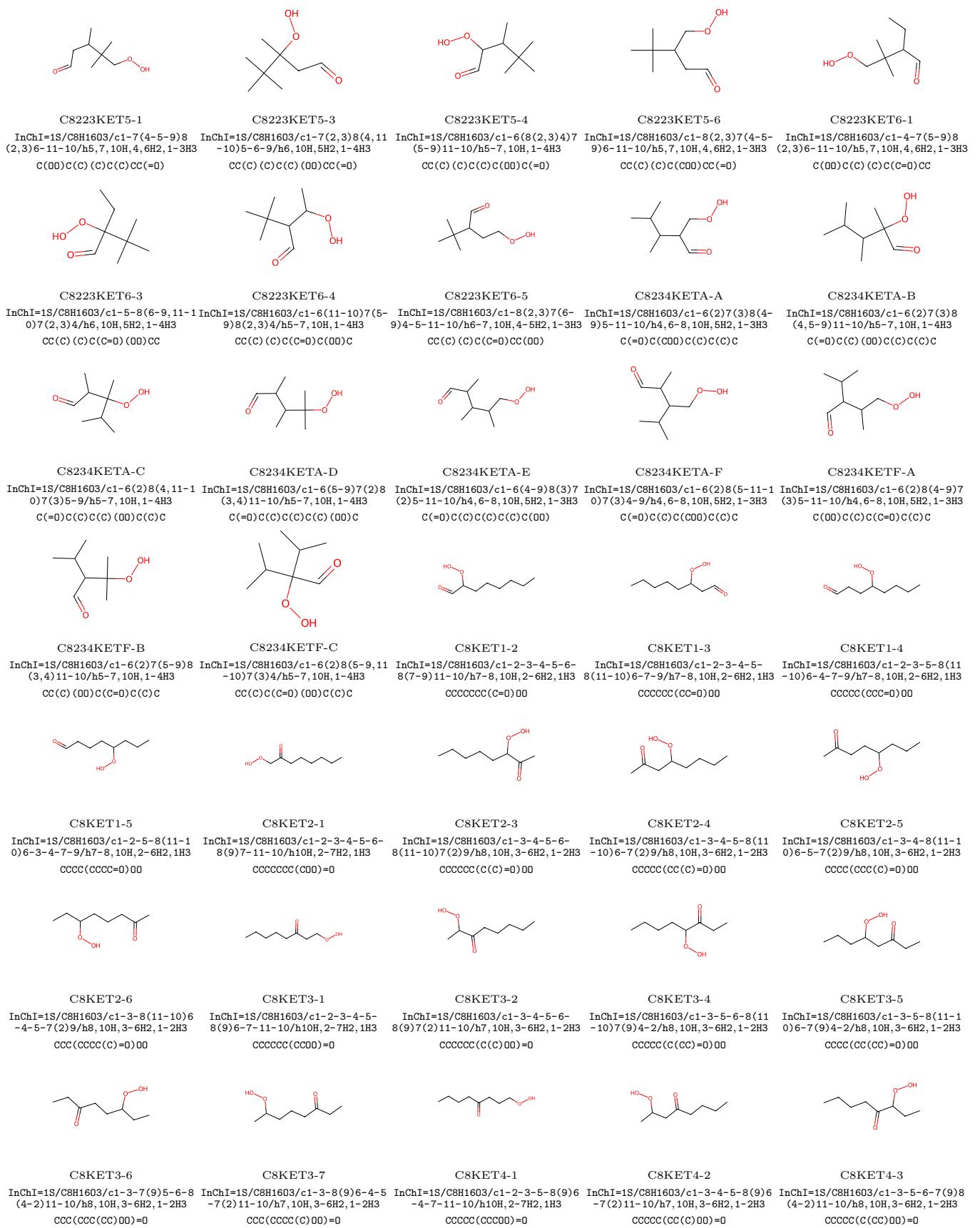


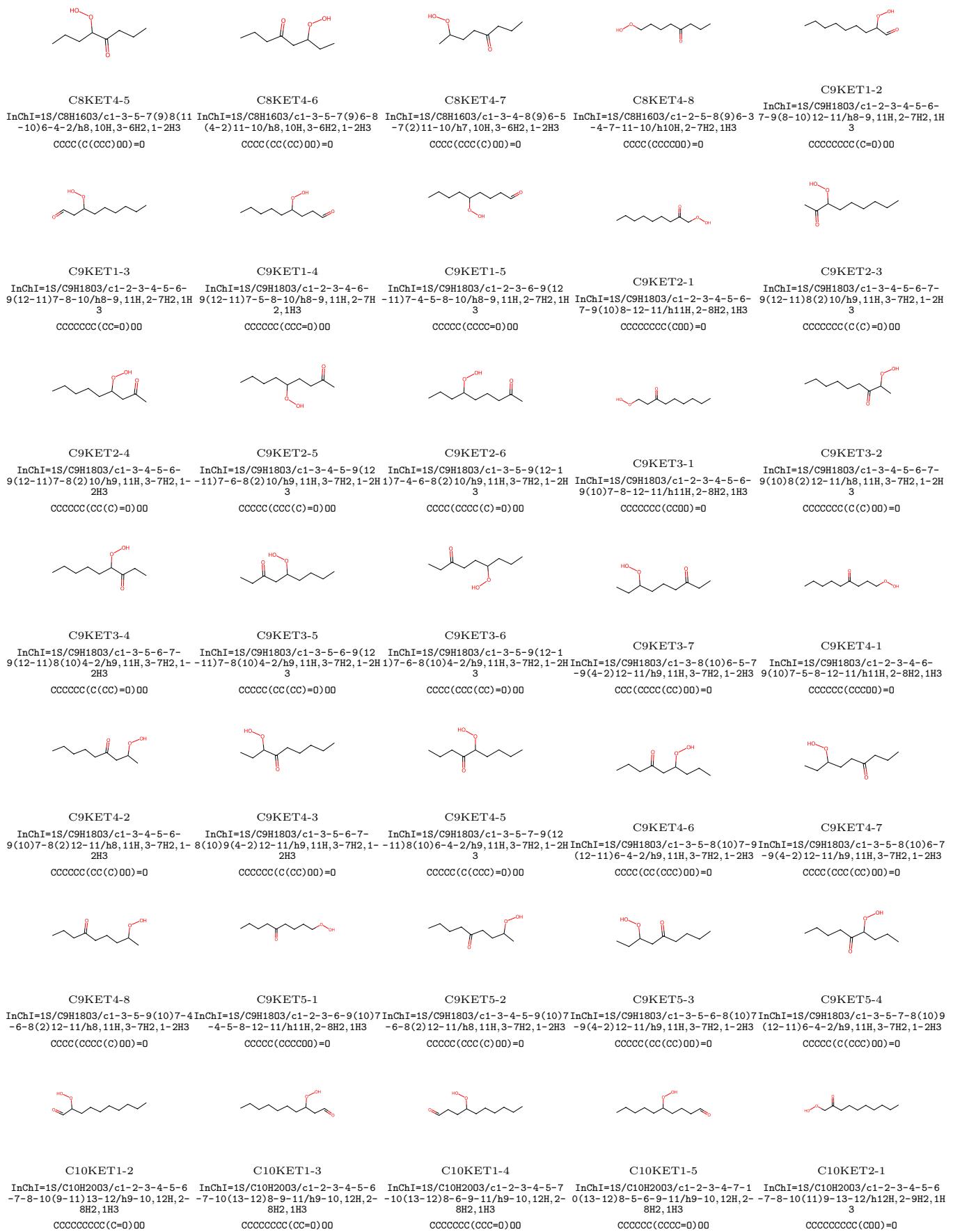


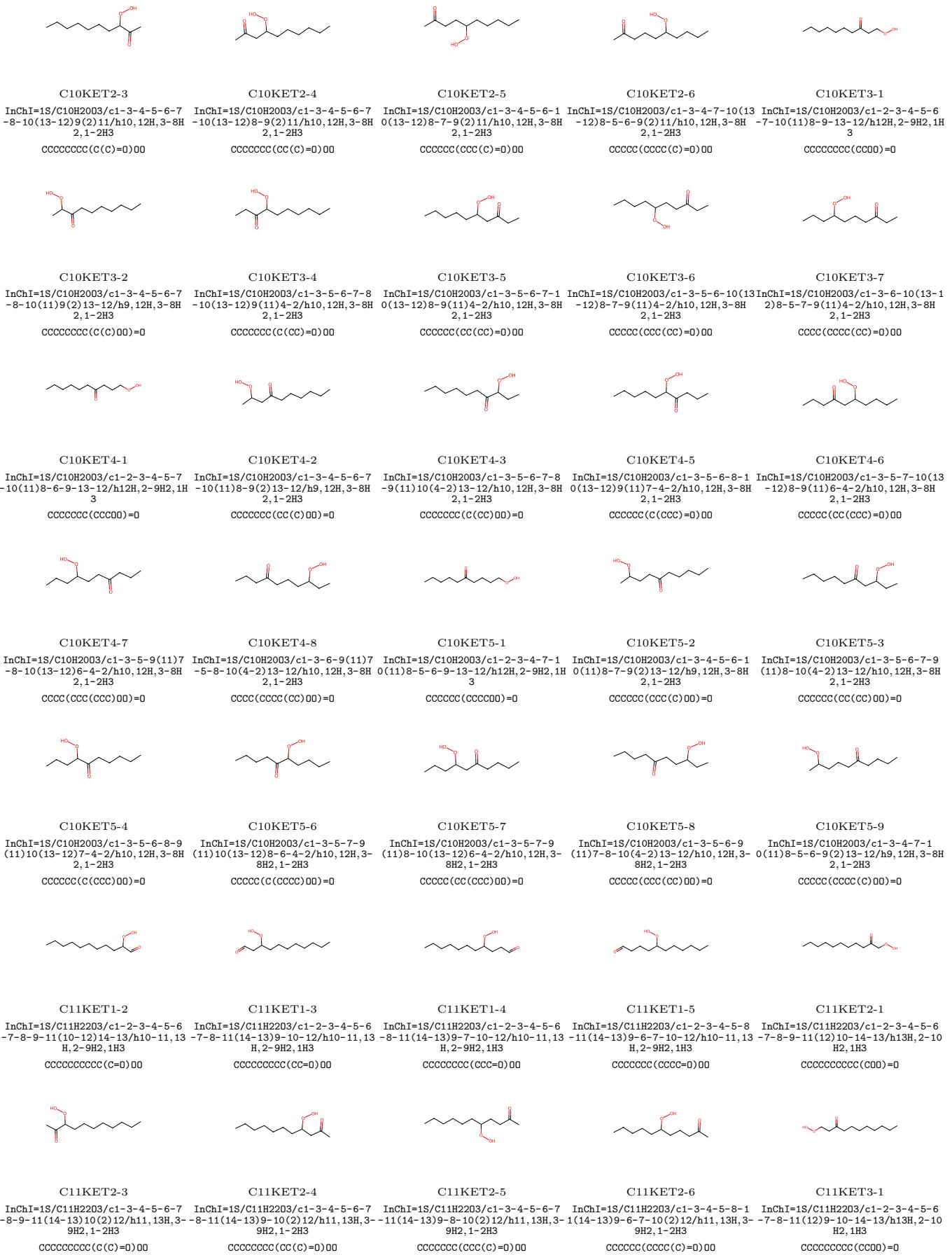


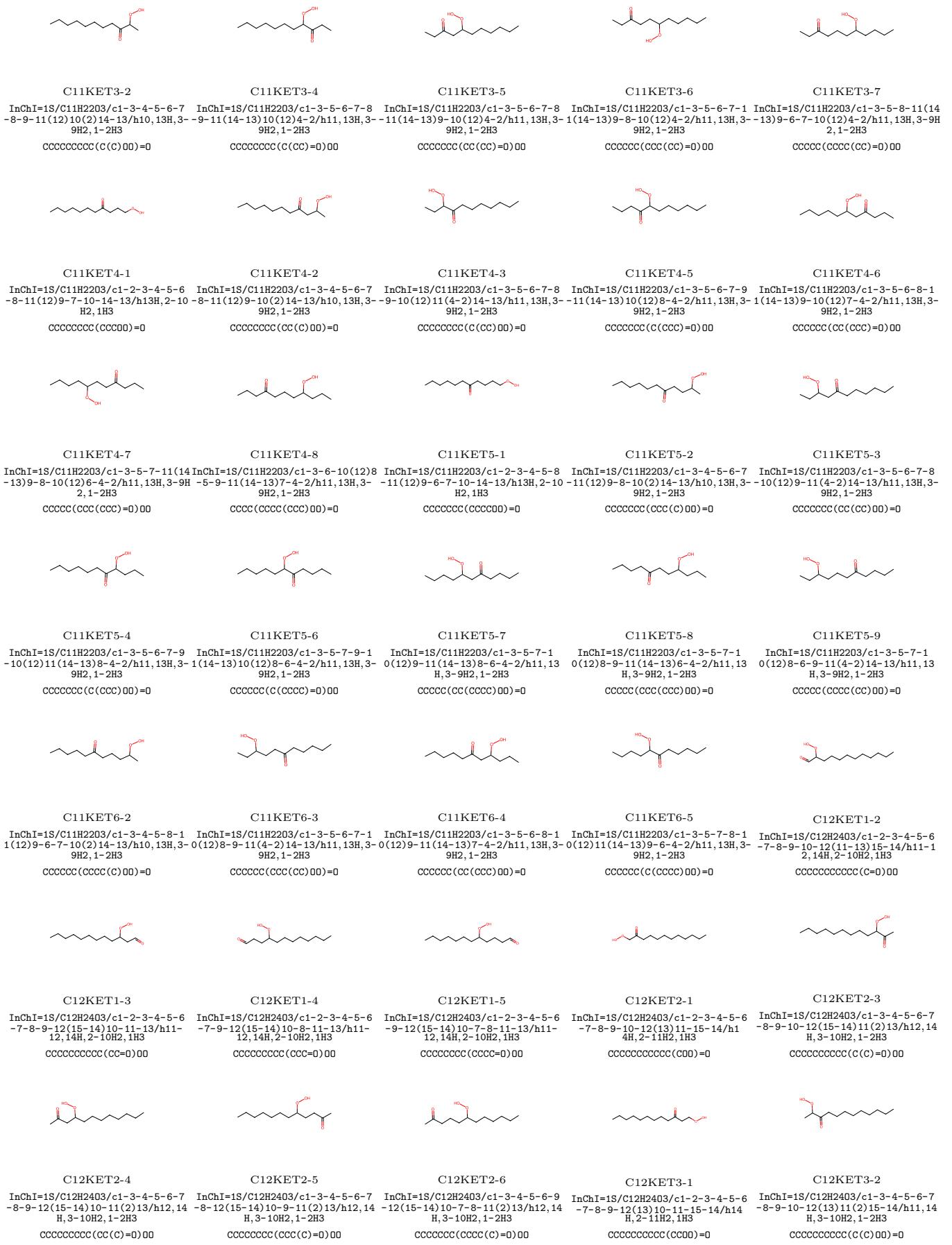


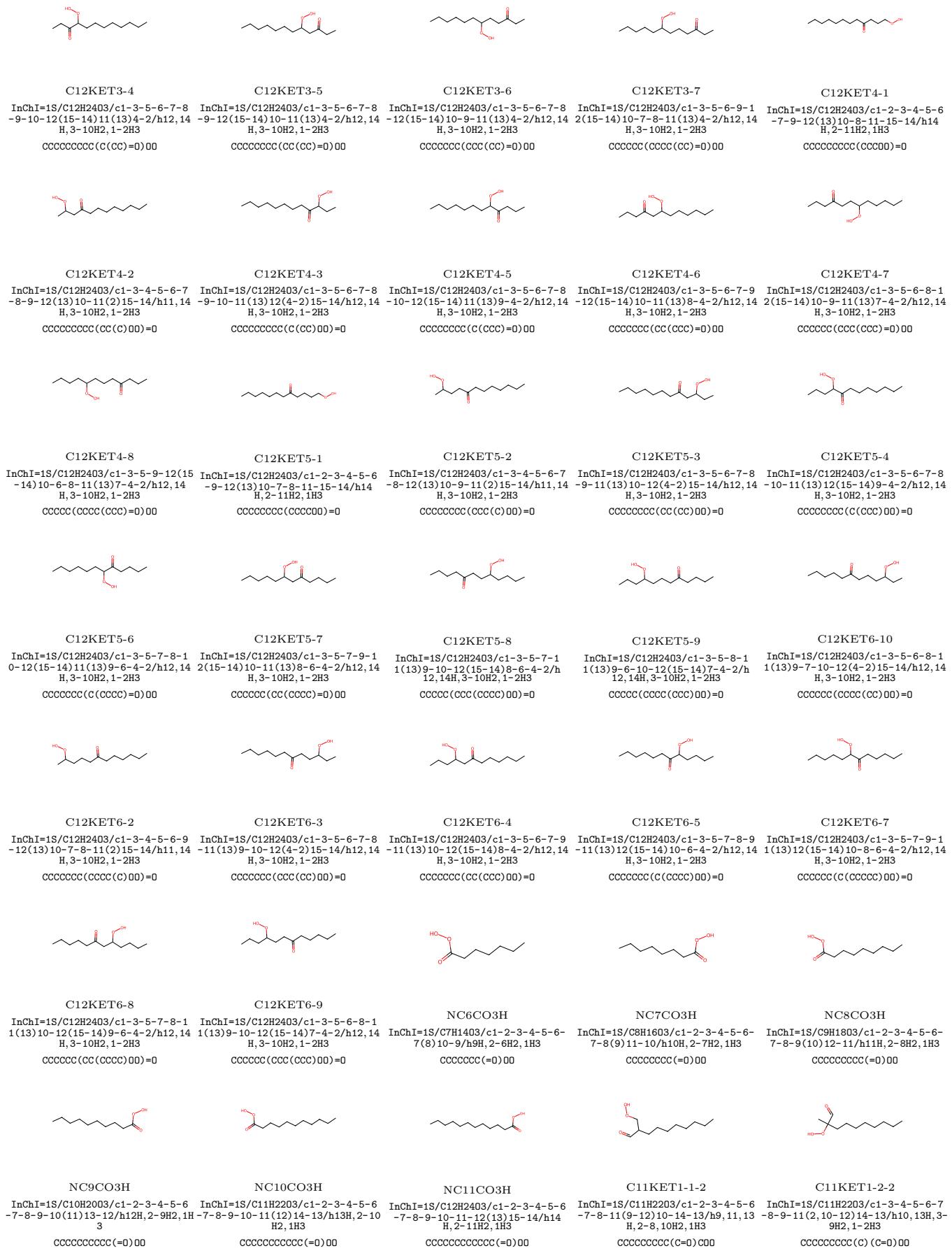


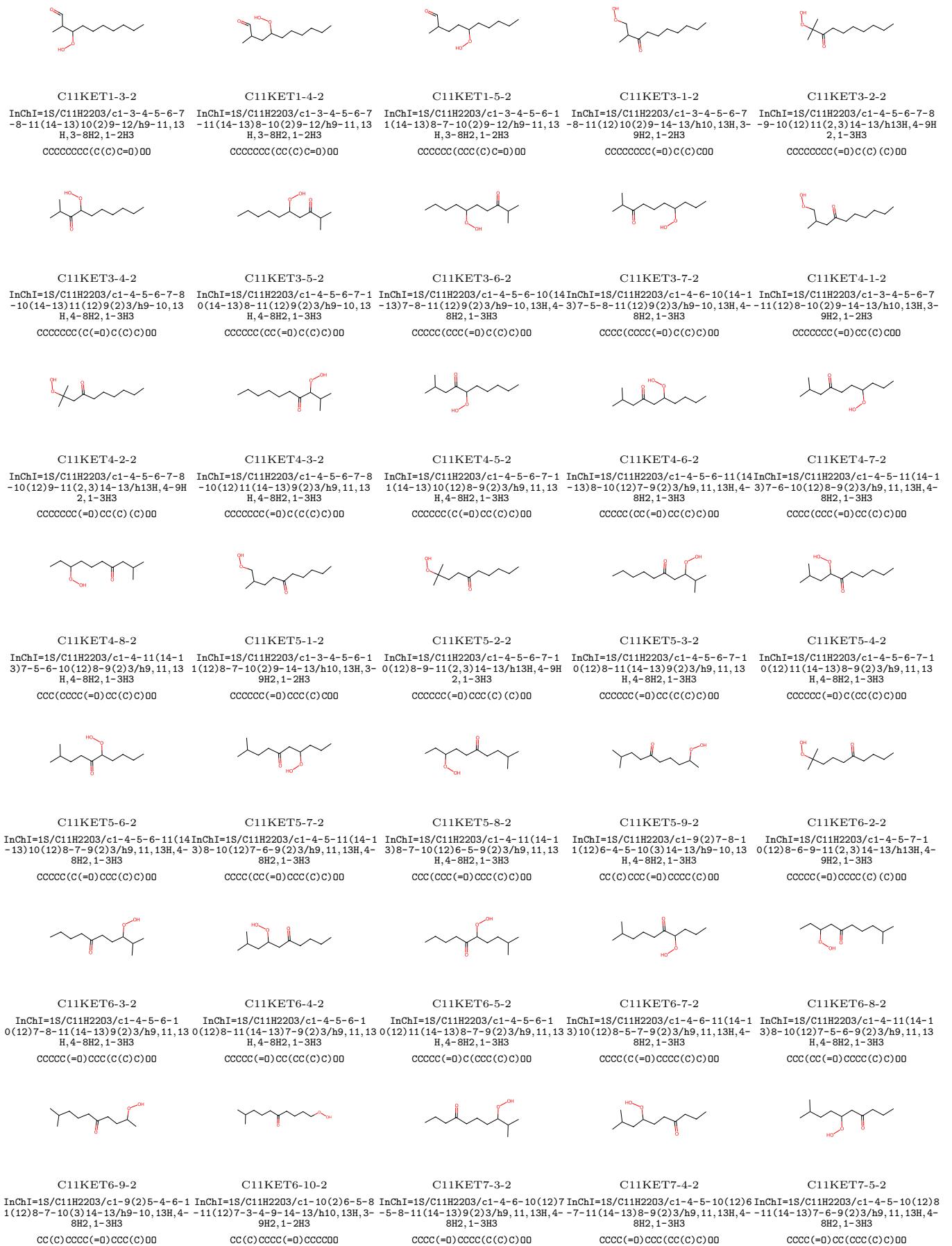


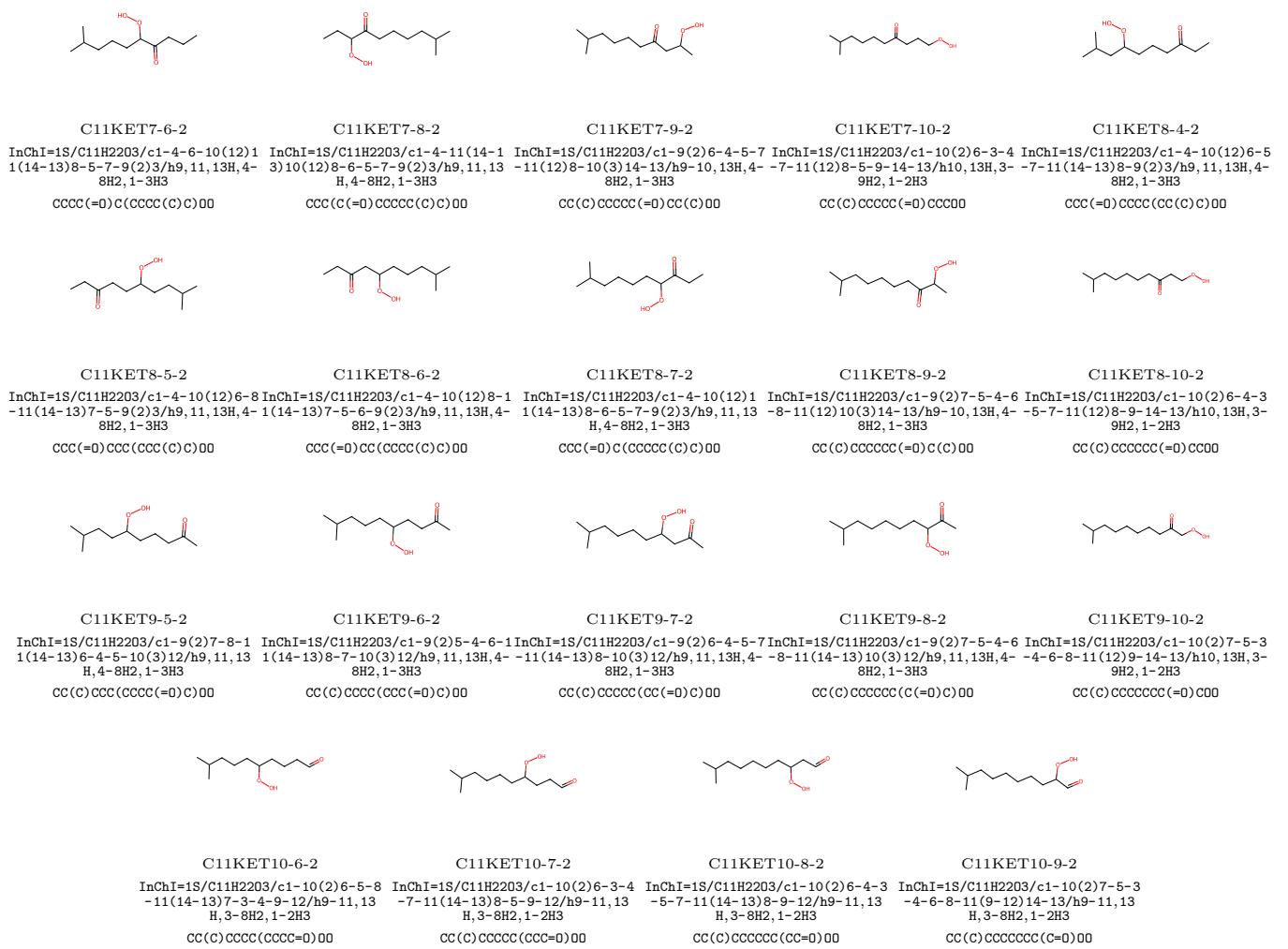




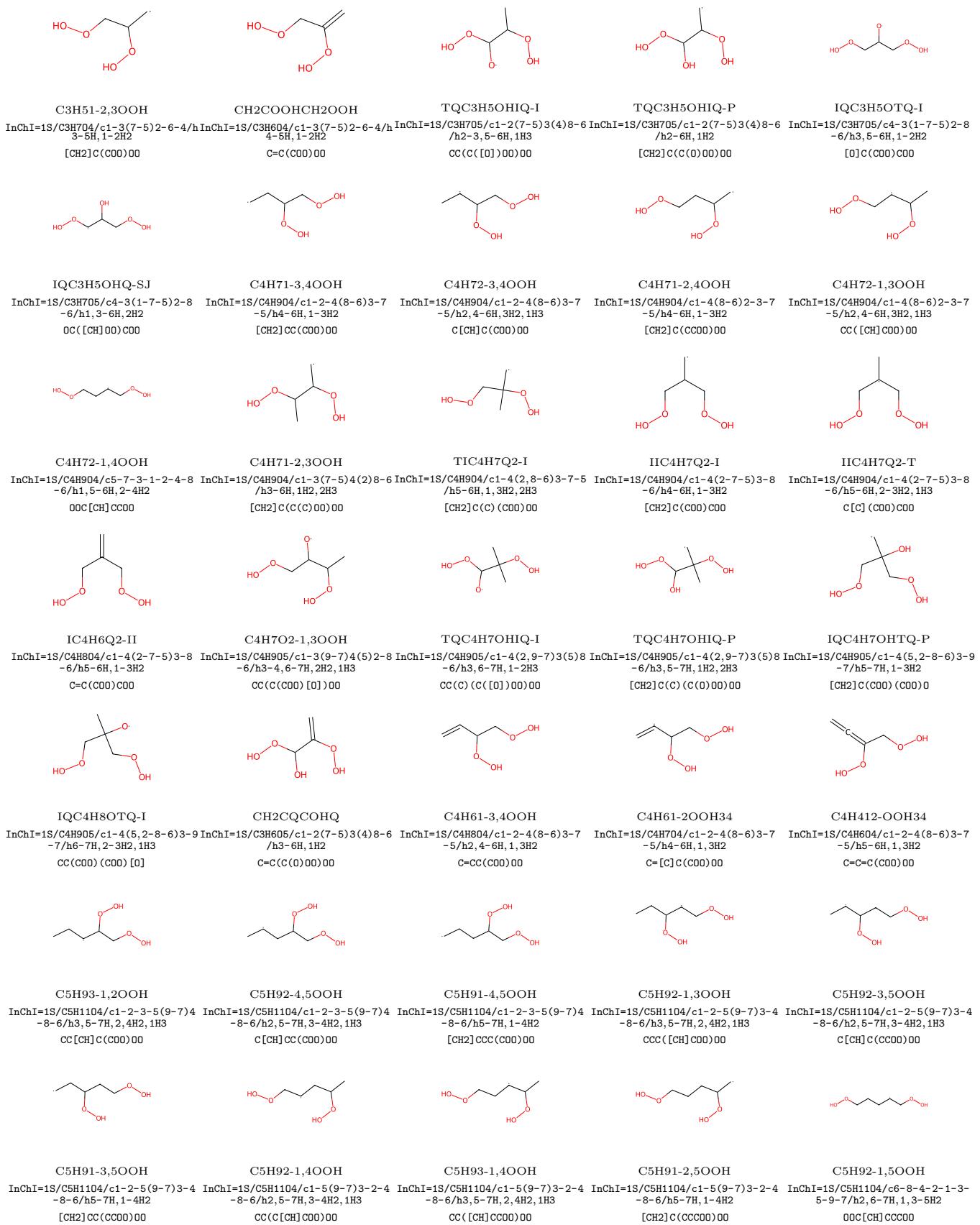


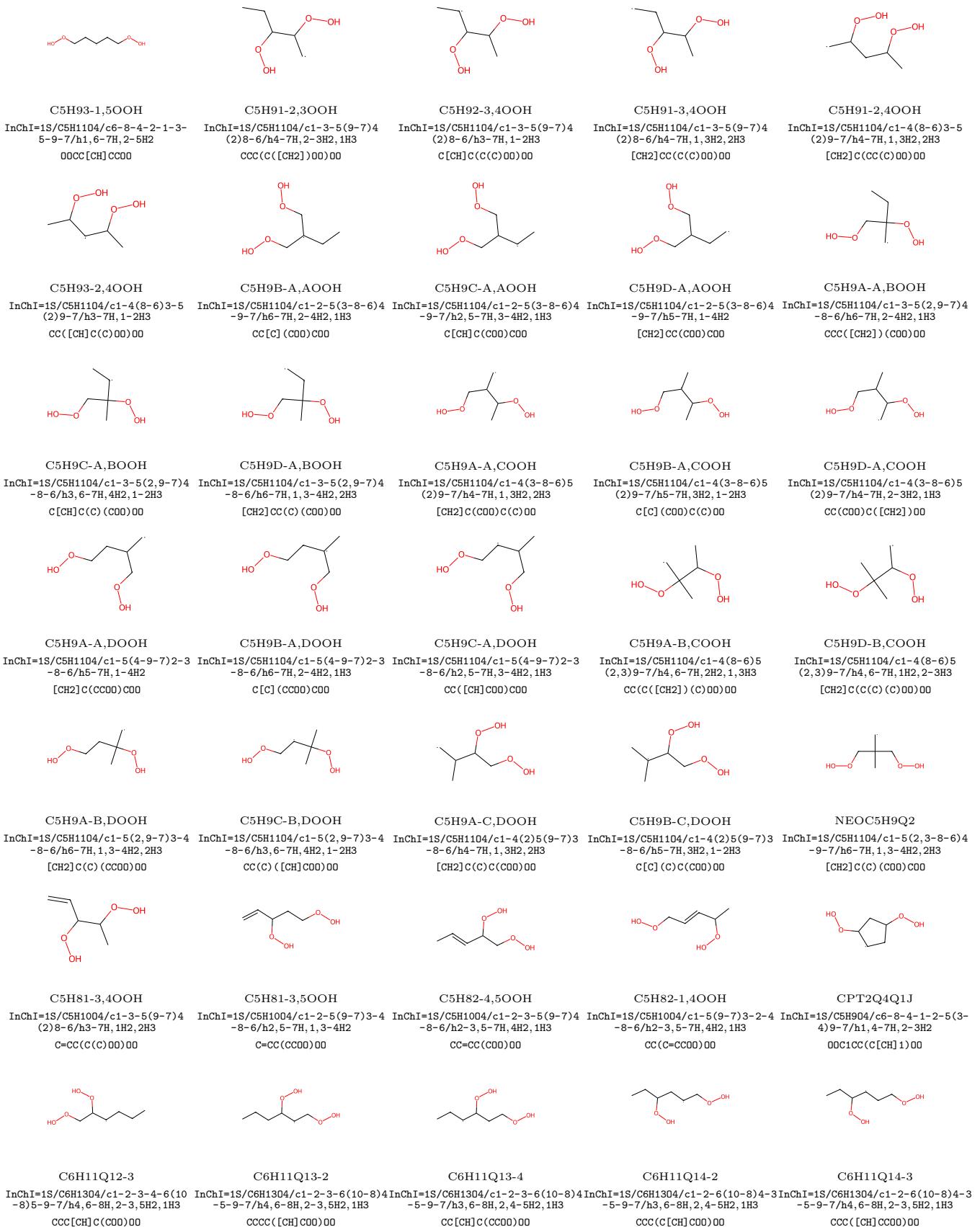


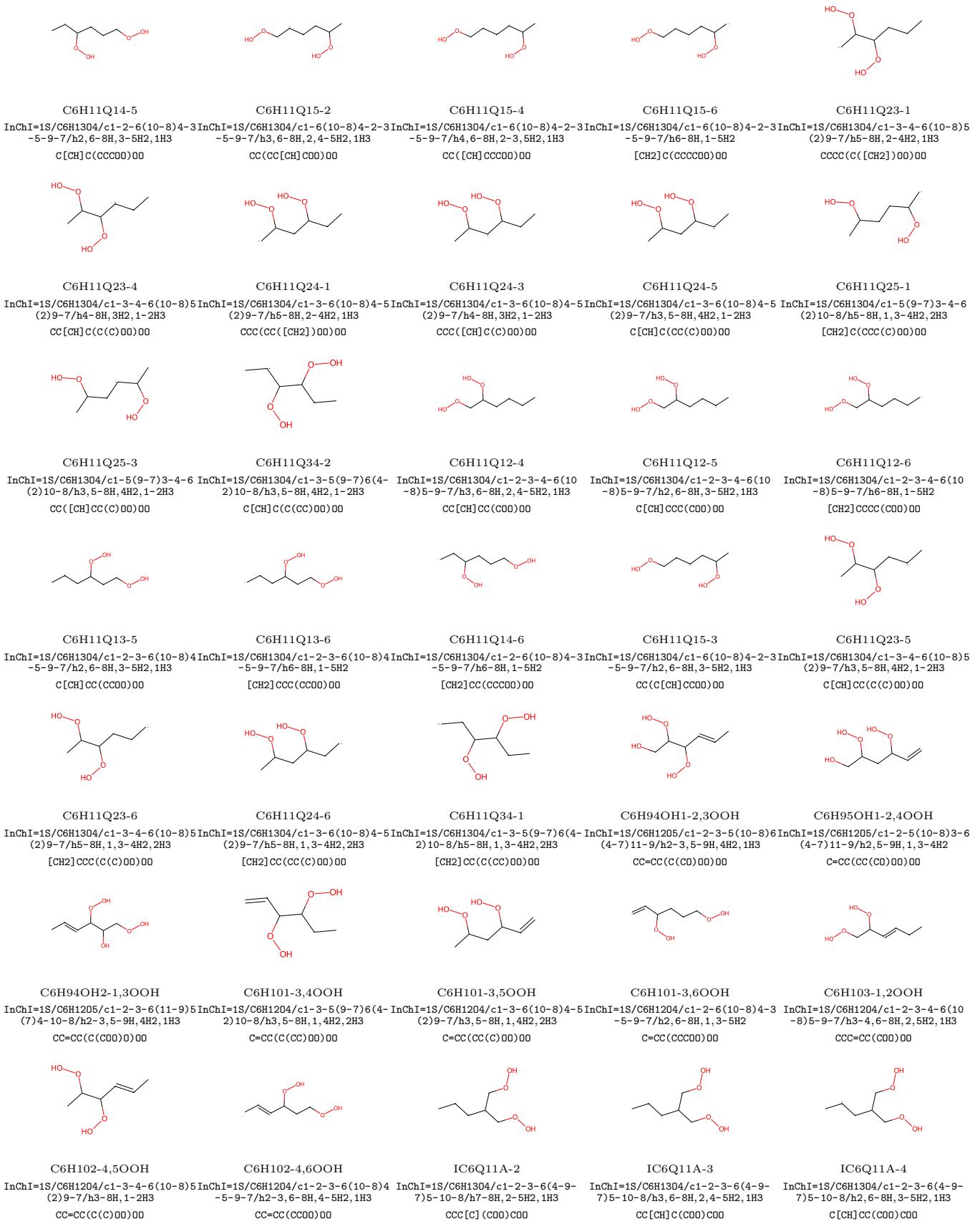


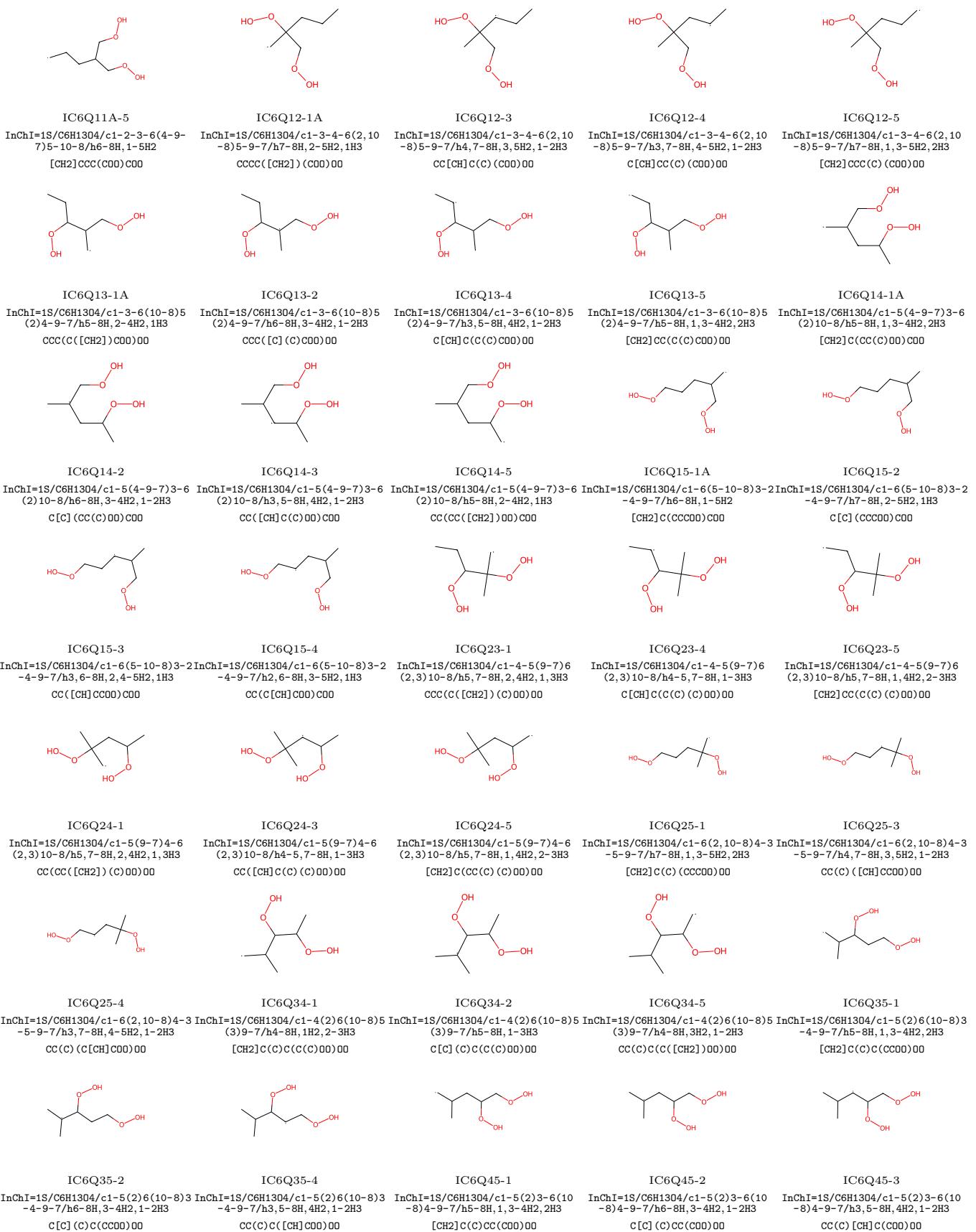


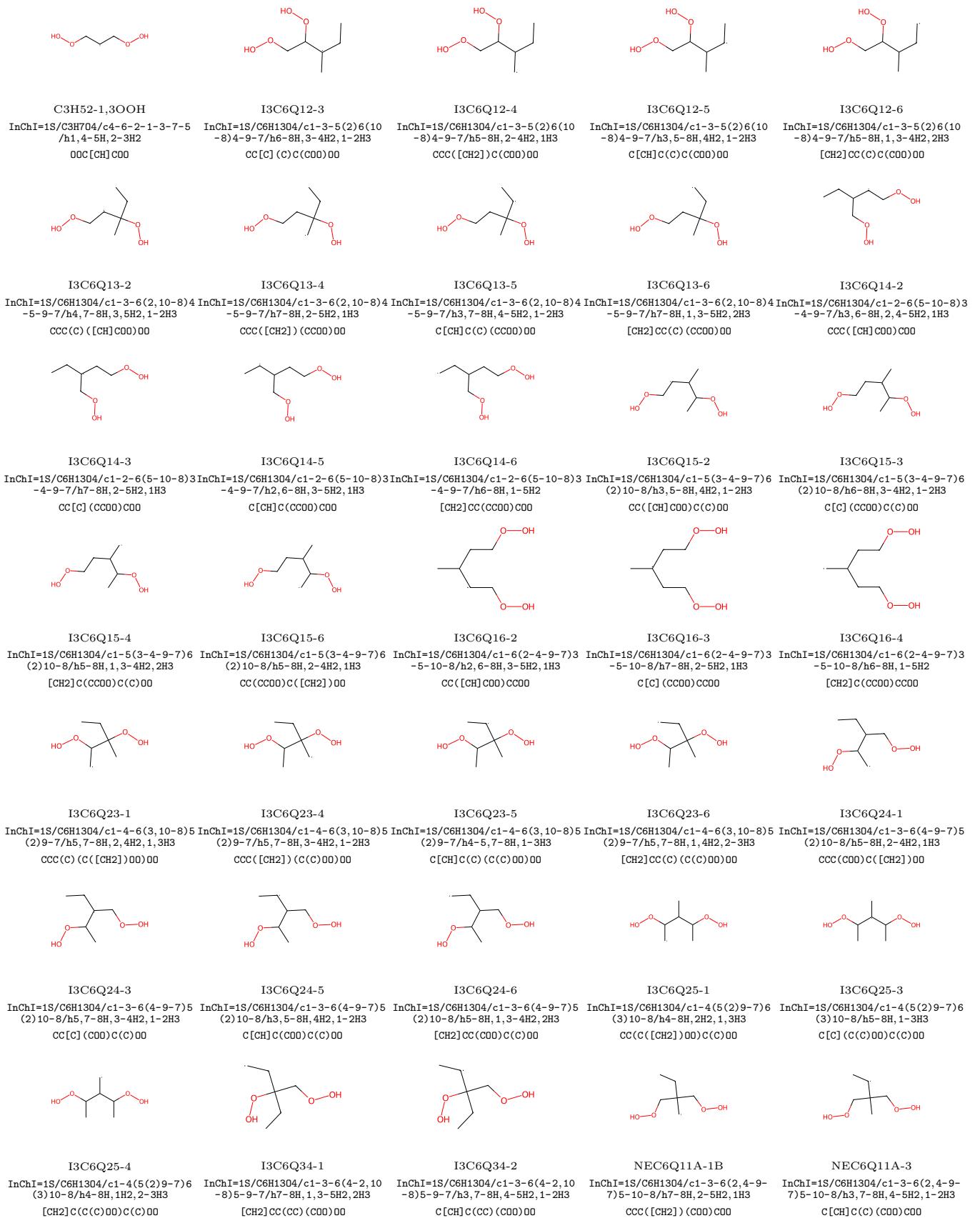
26 Di-hydroperoxy radicals

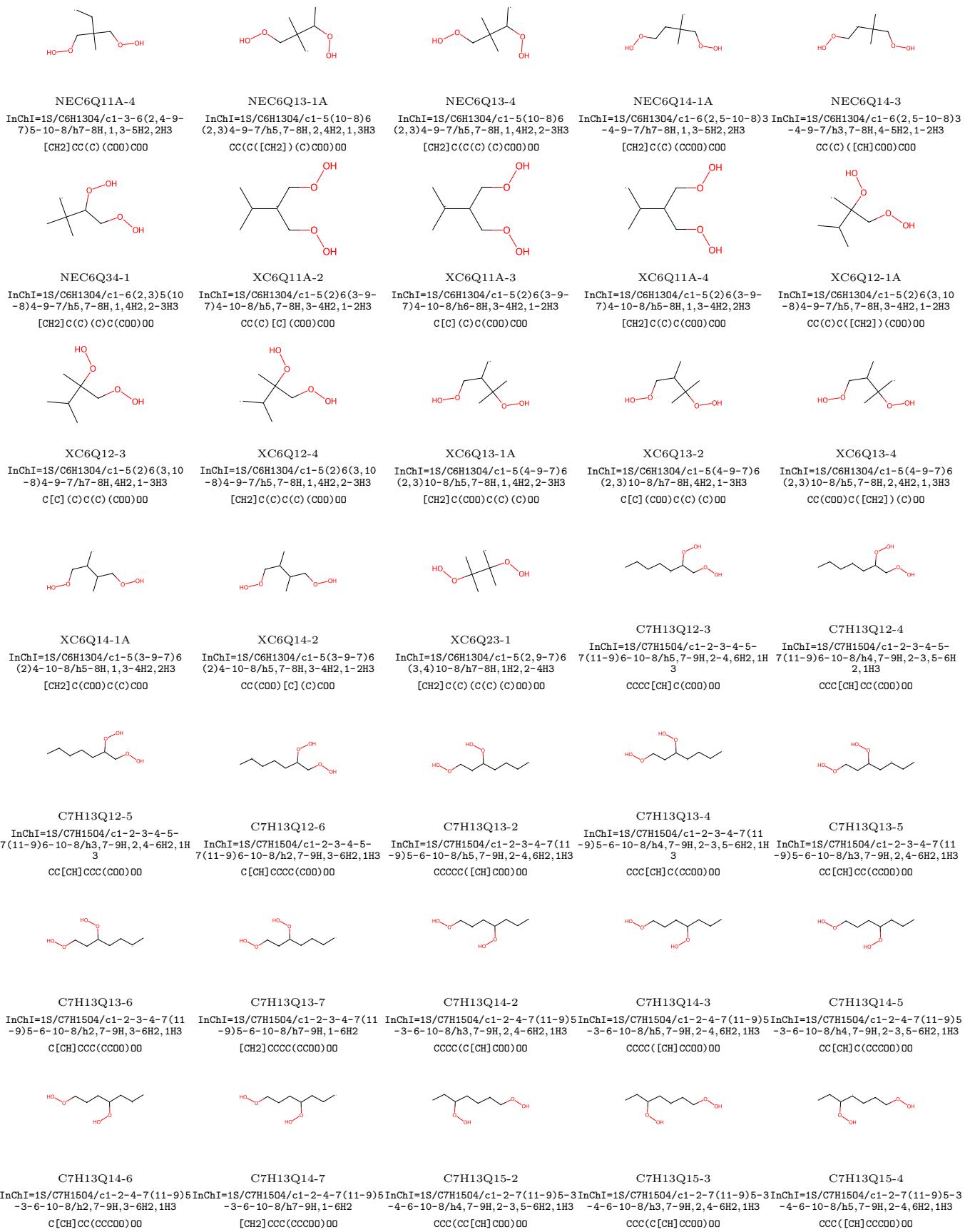


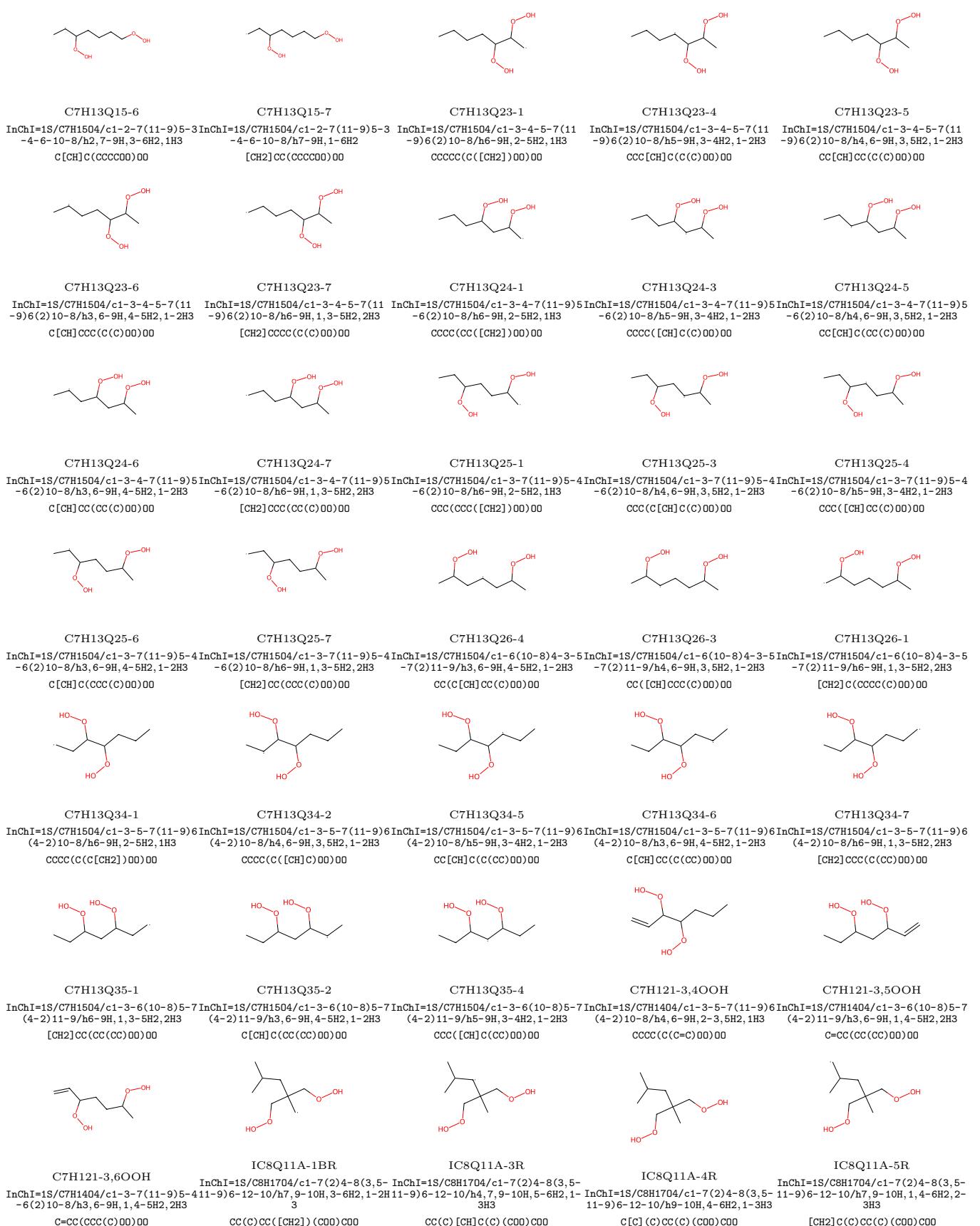


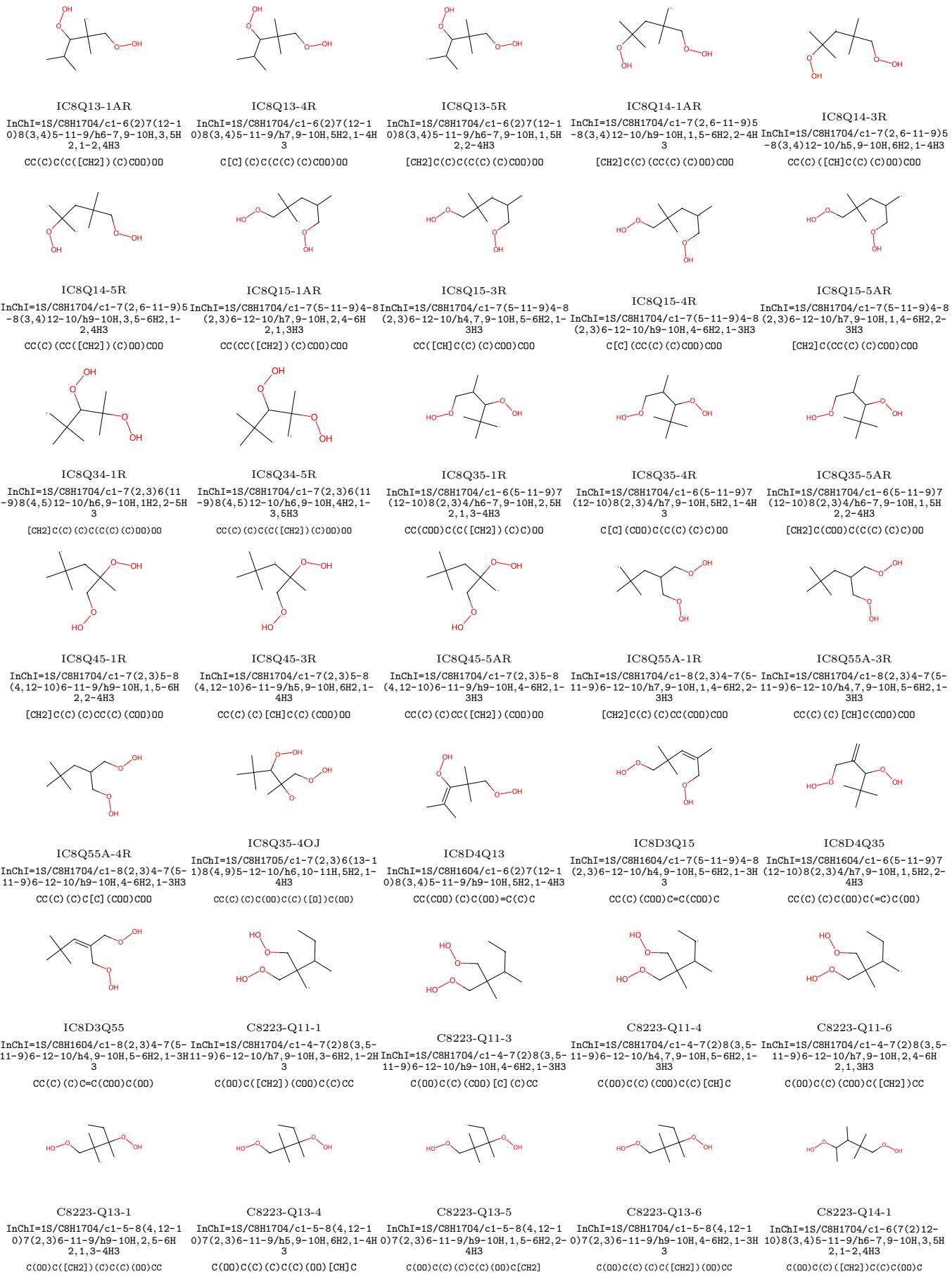


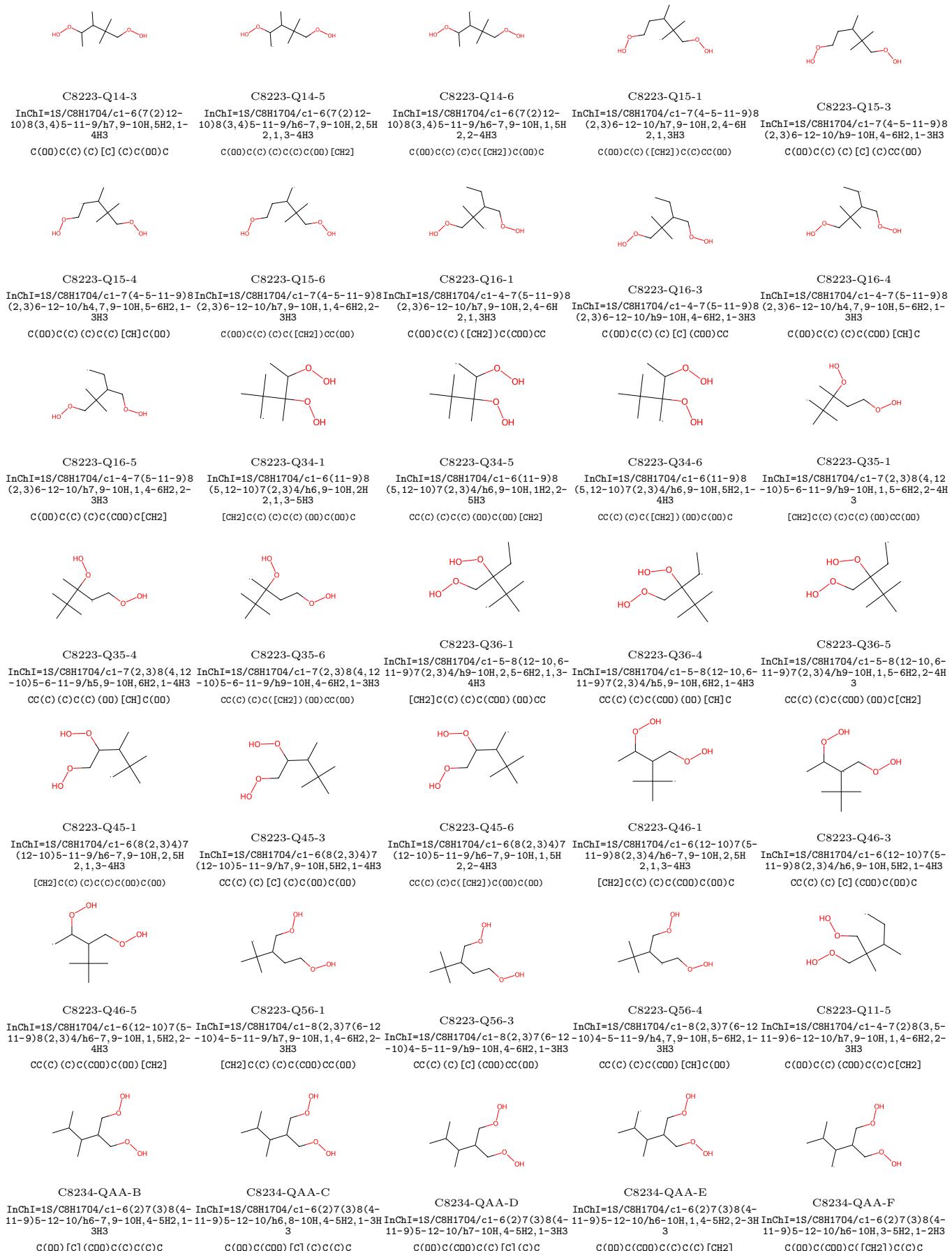


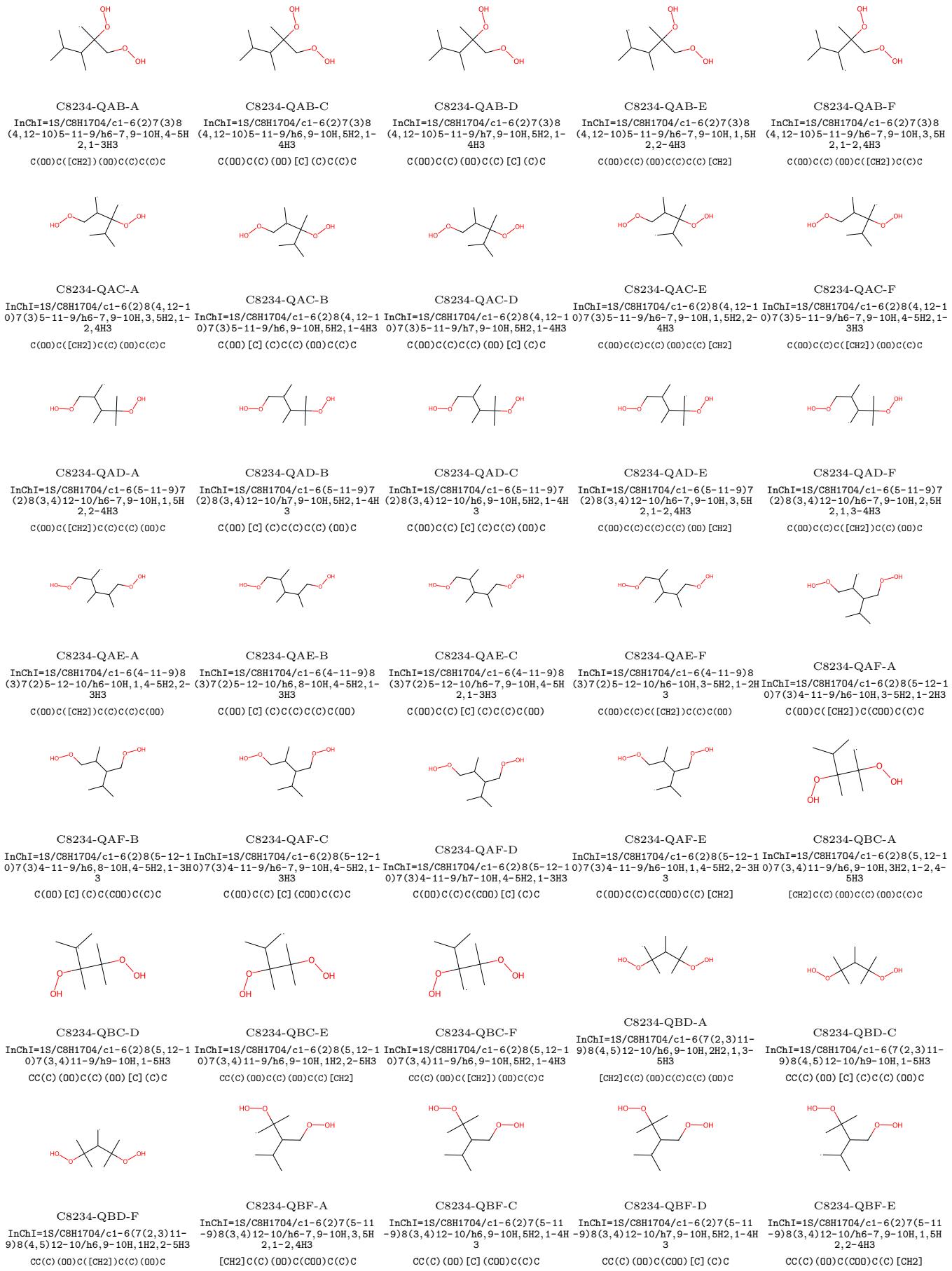


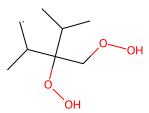




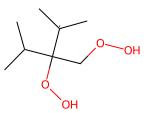






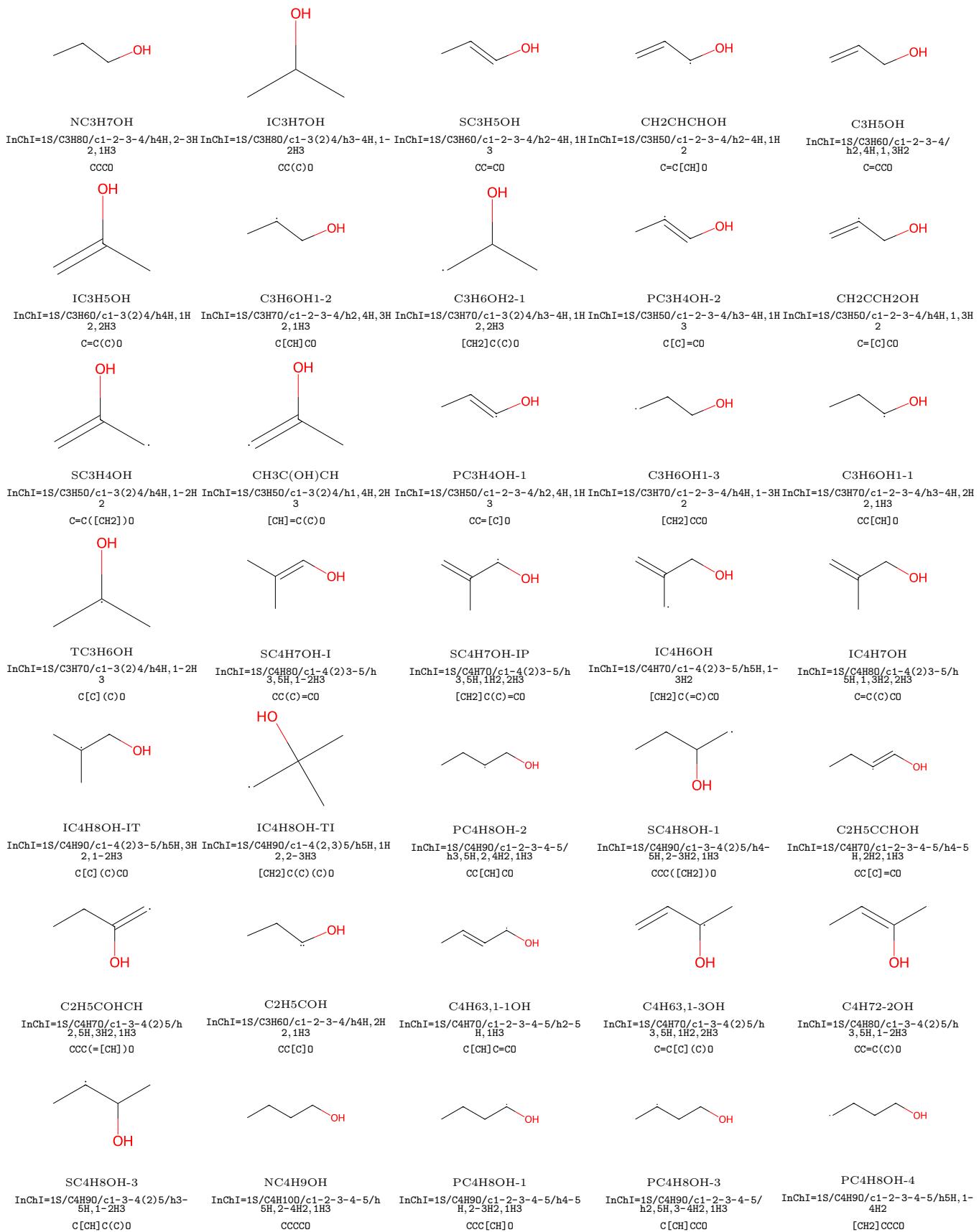


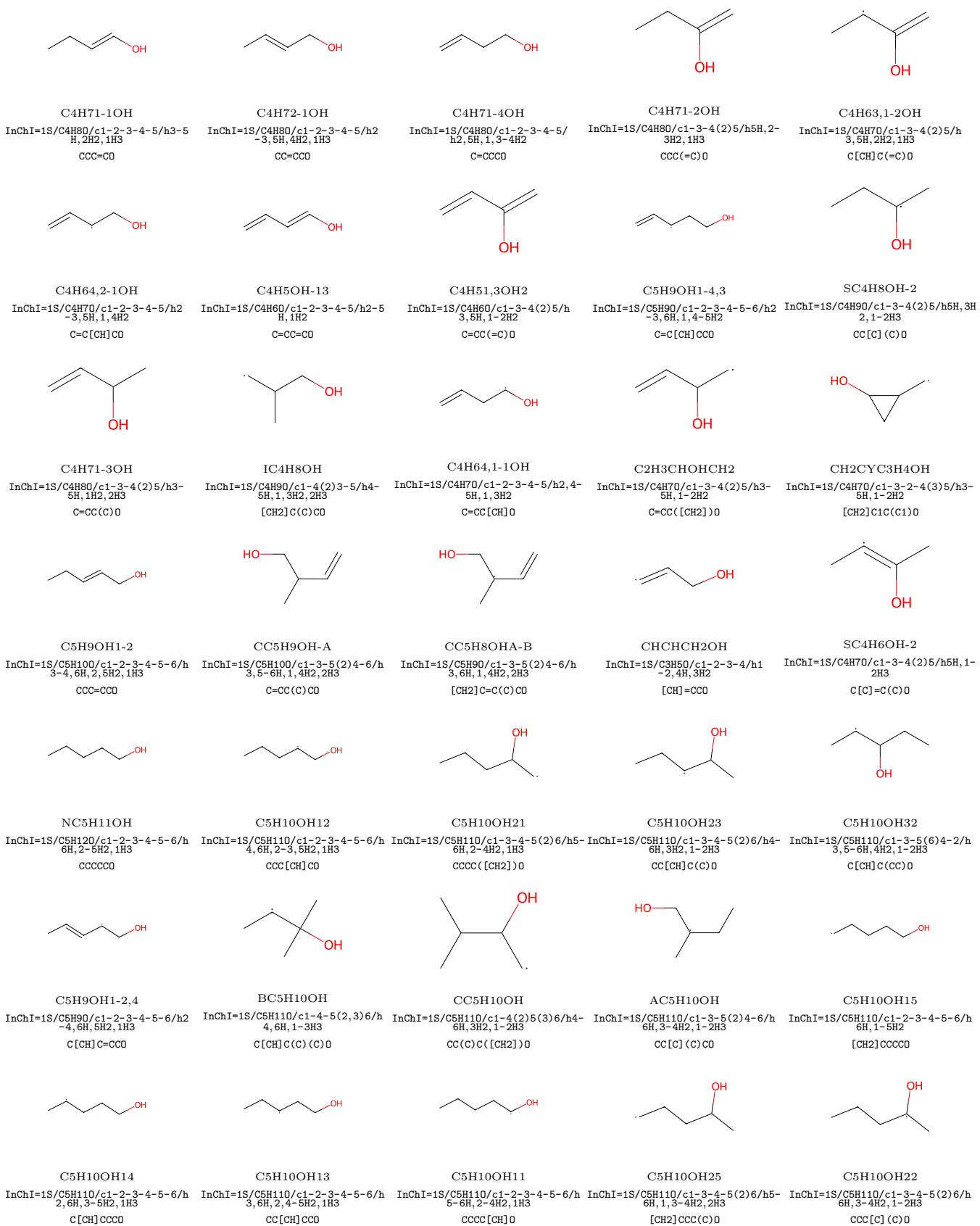
C8234-QCF-A

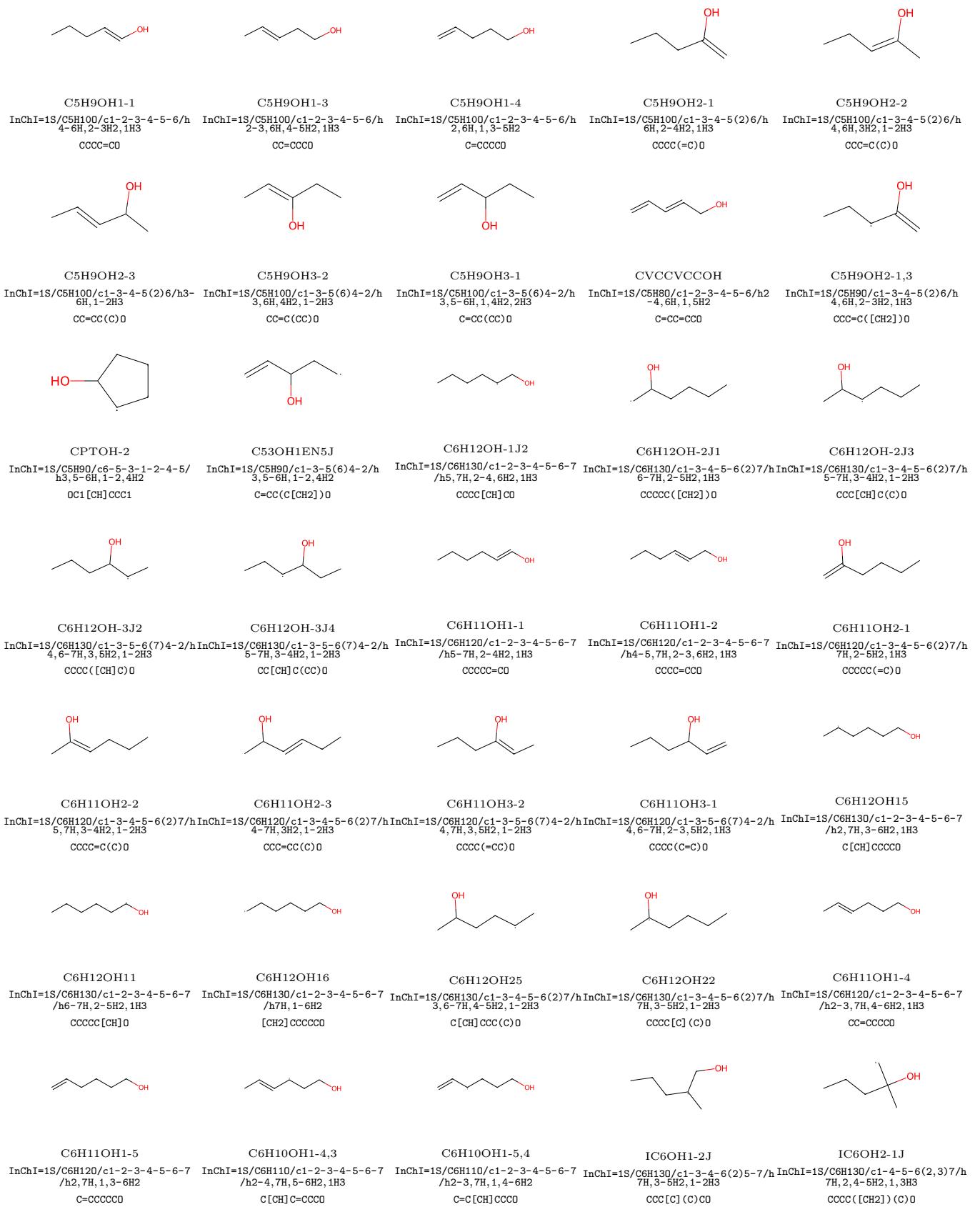


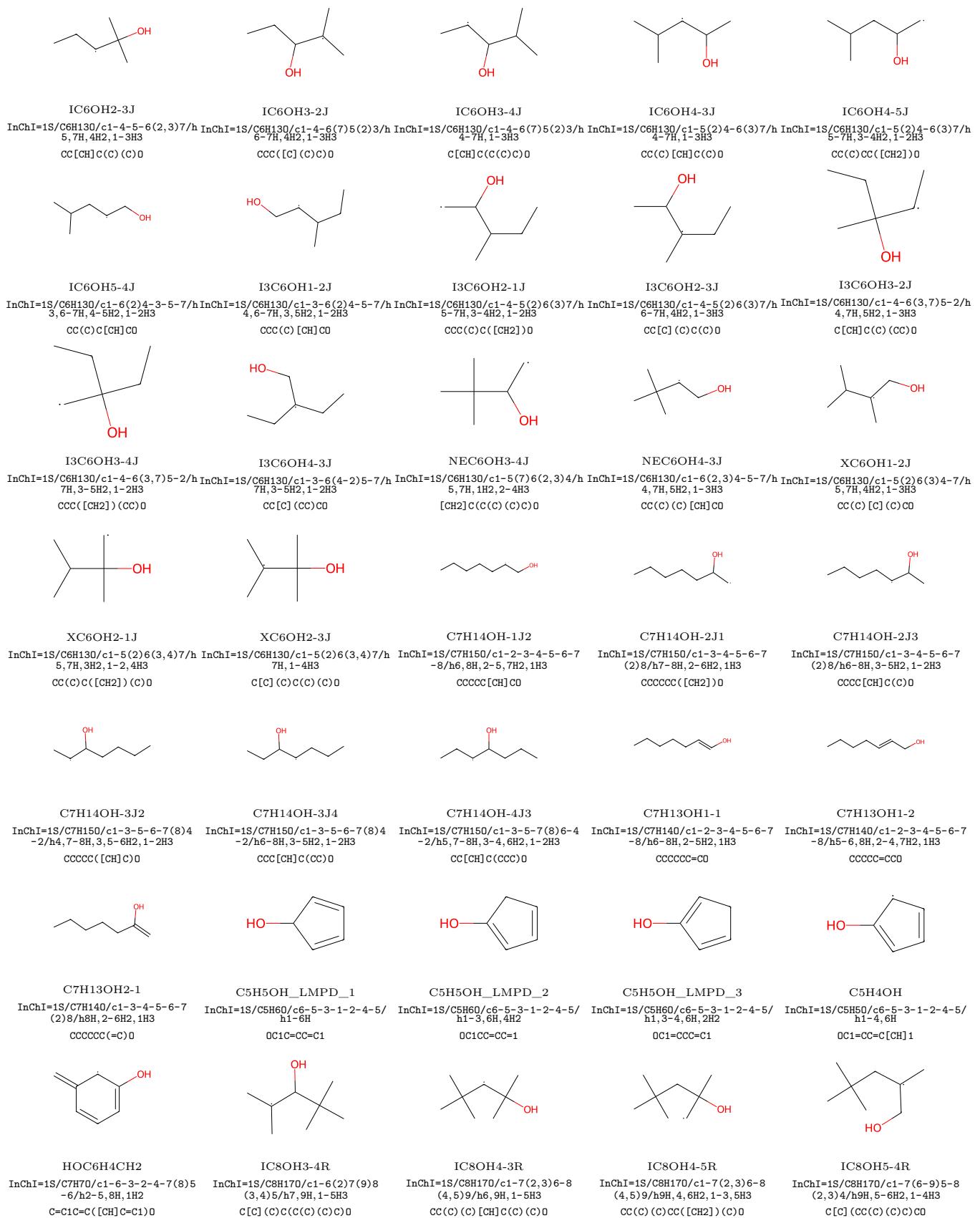
C8234-QCF-B

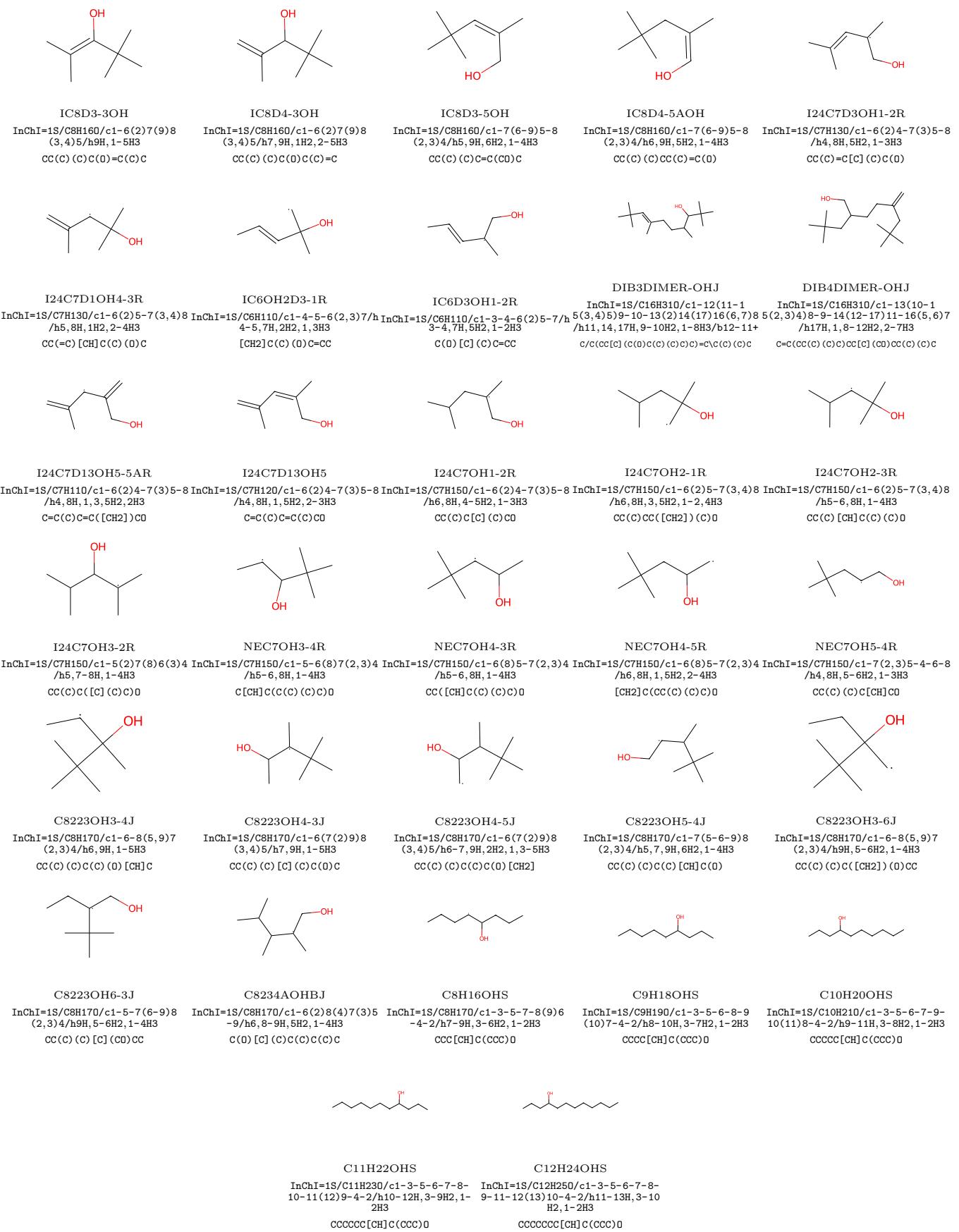
27 Alcohols (molecules and radicals)



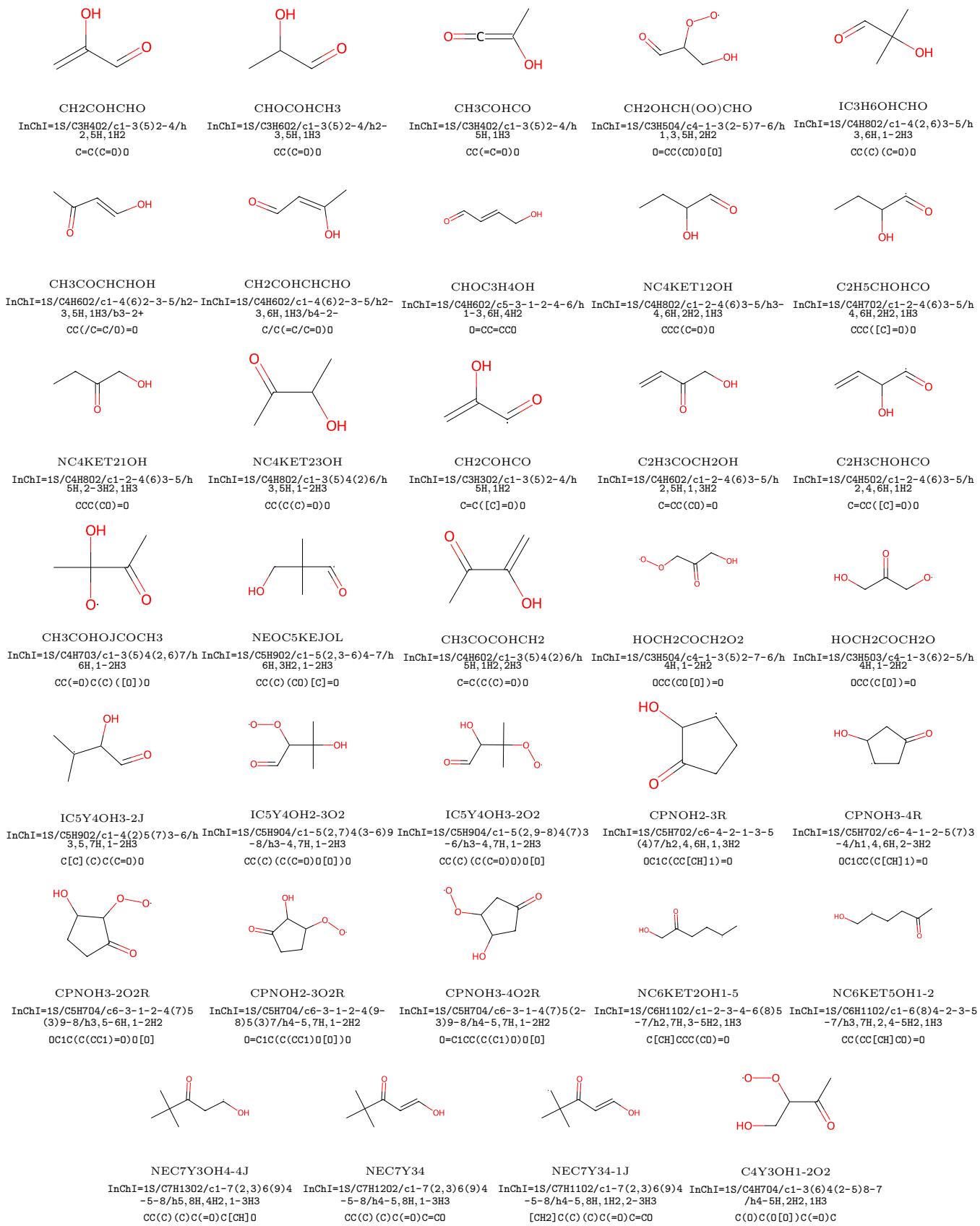


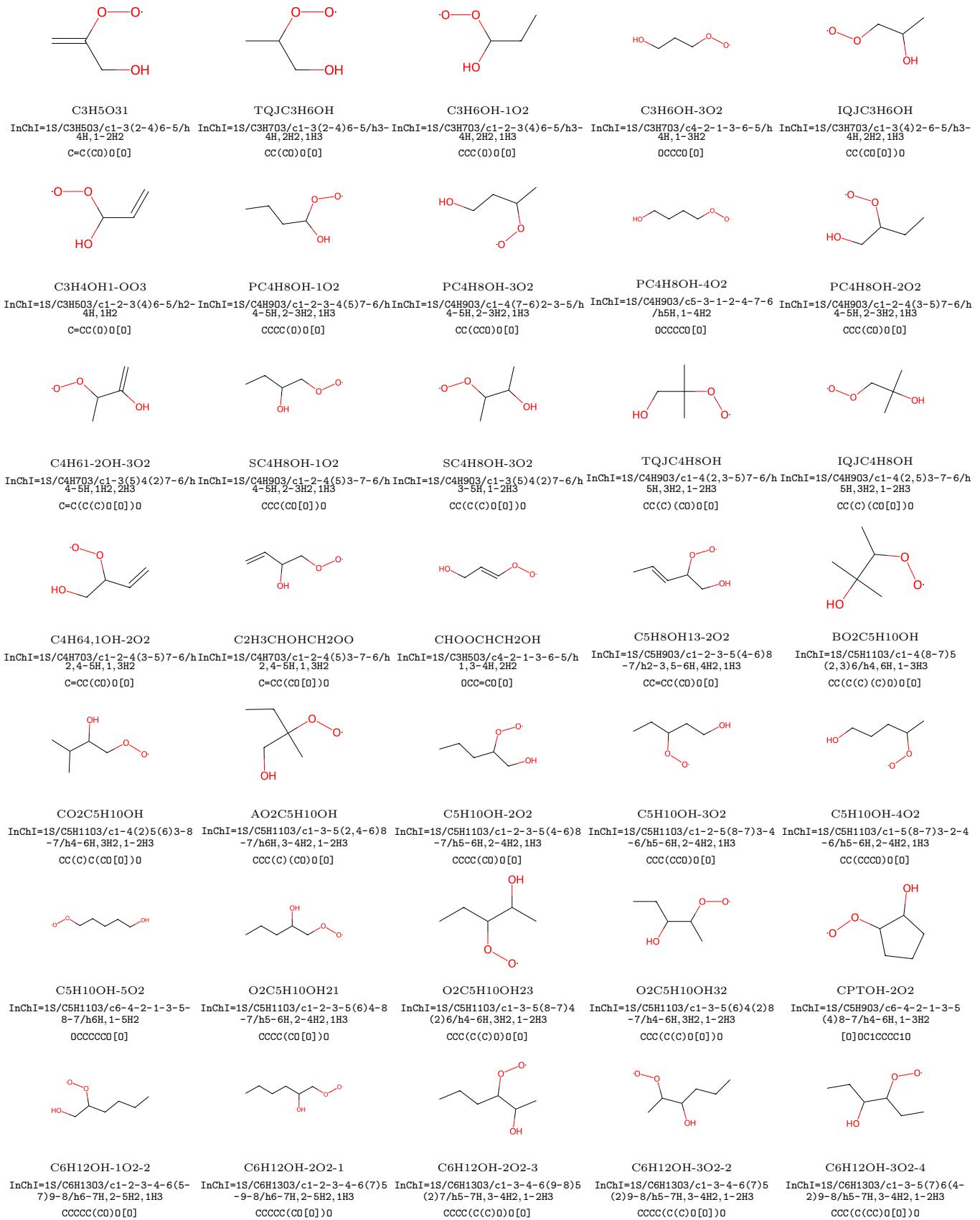


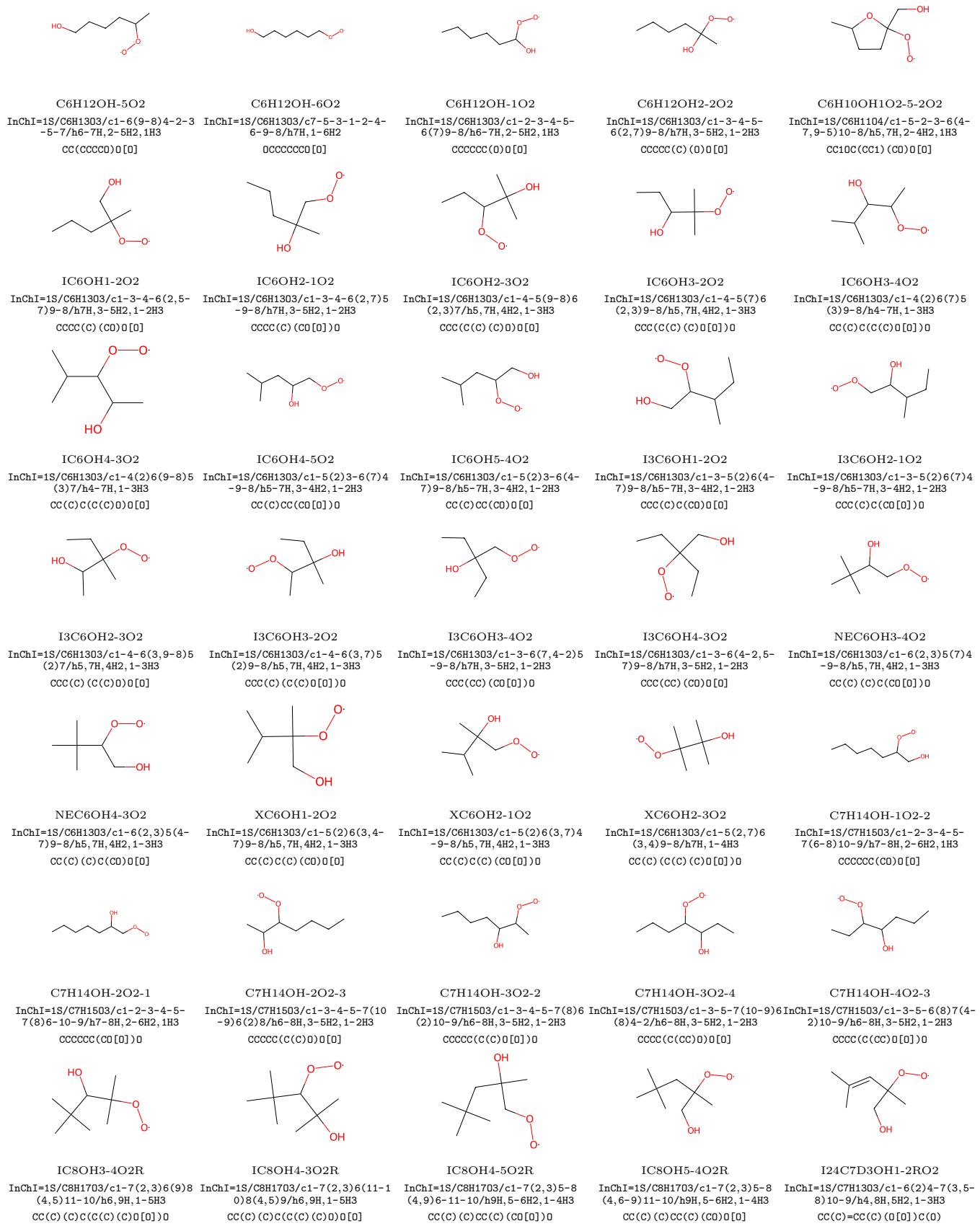


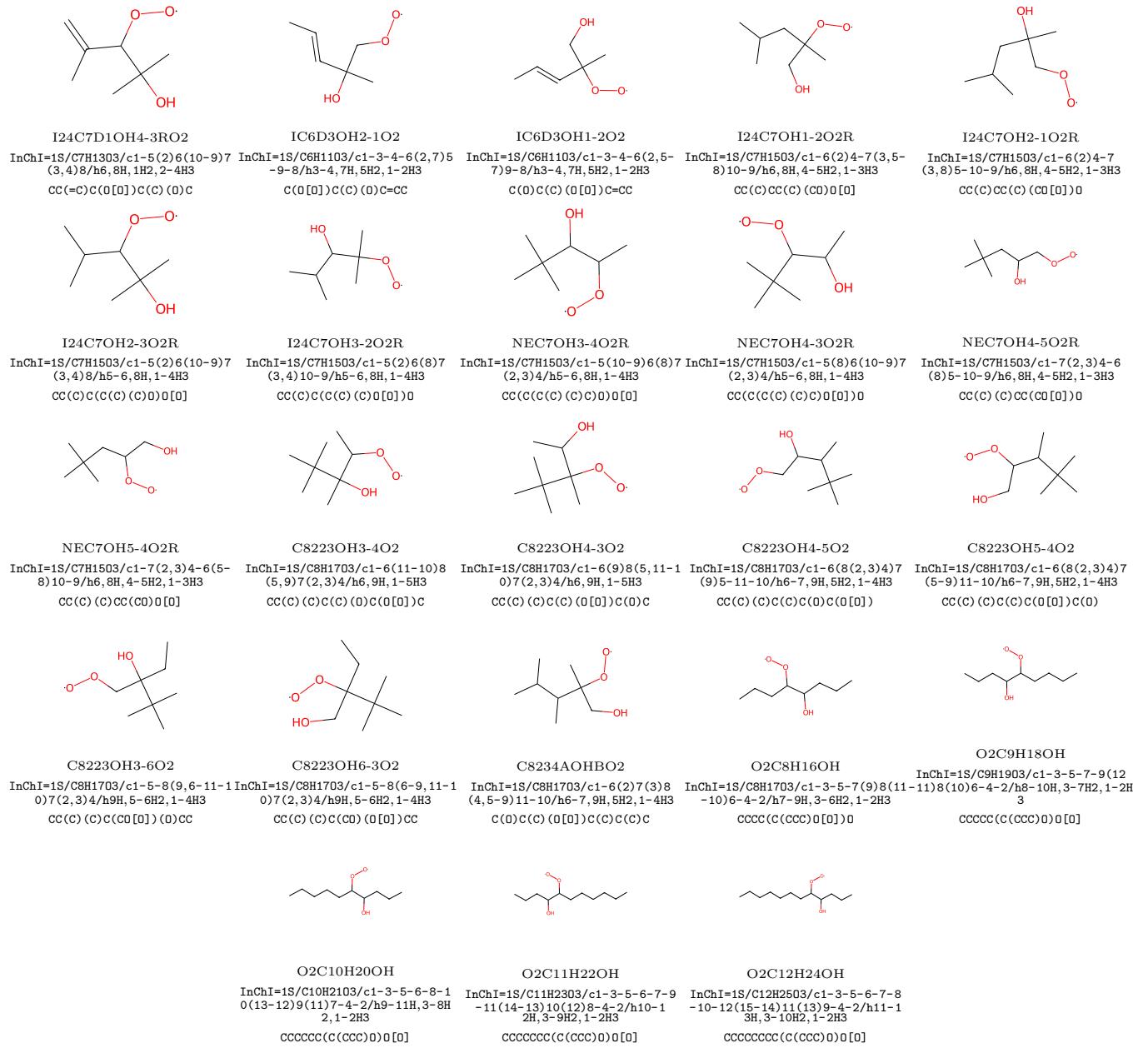


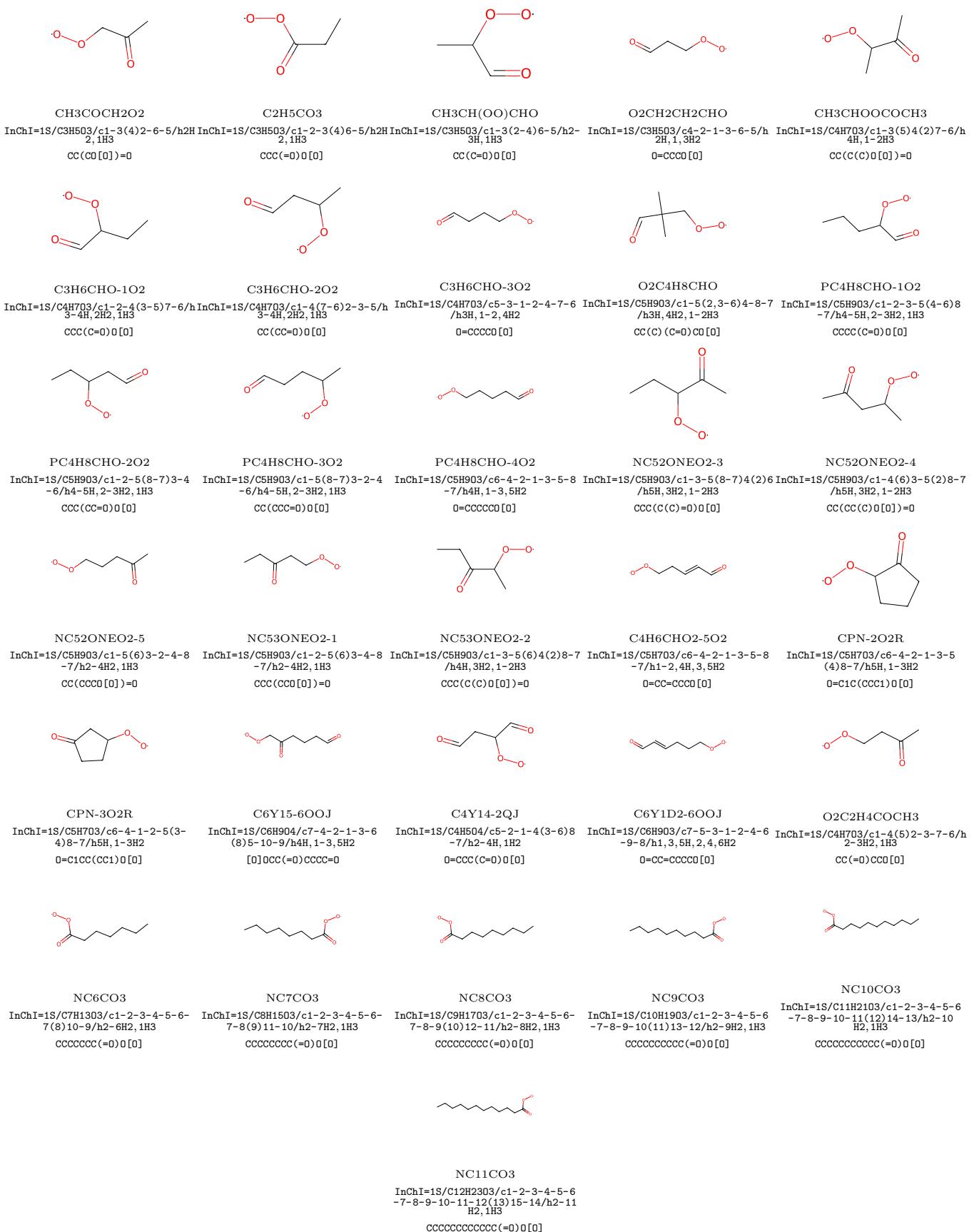
28 Miscellaneous

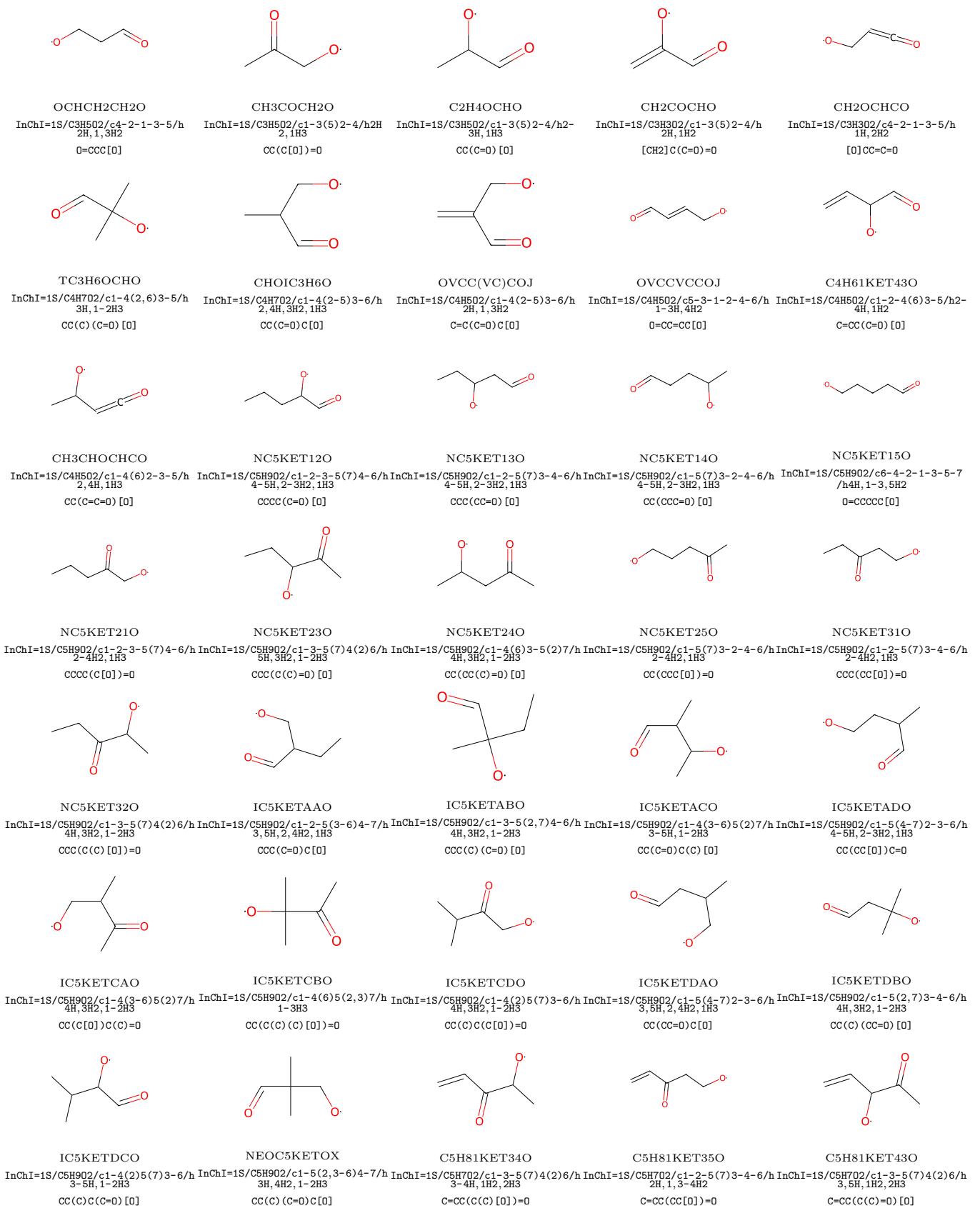


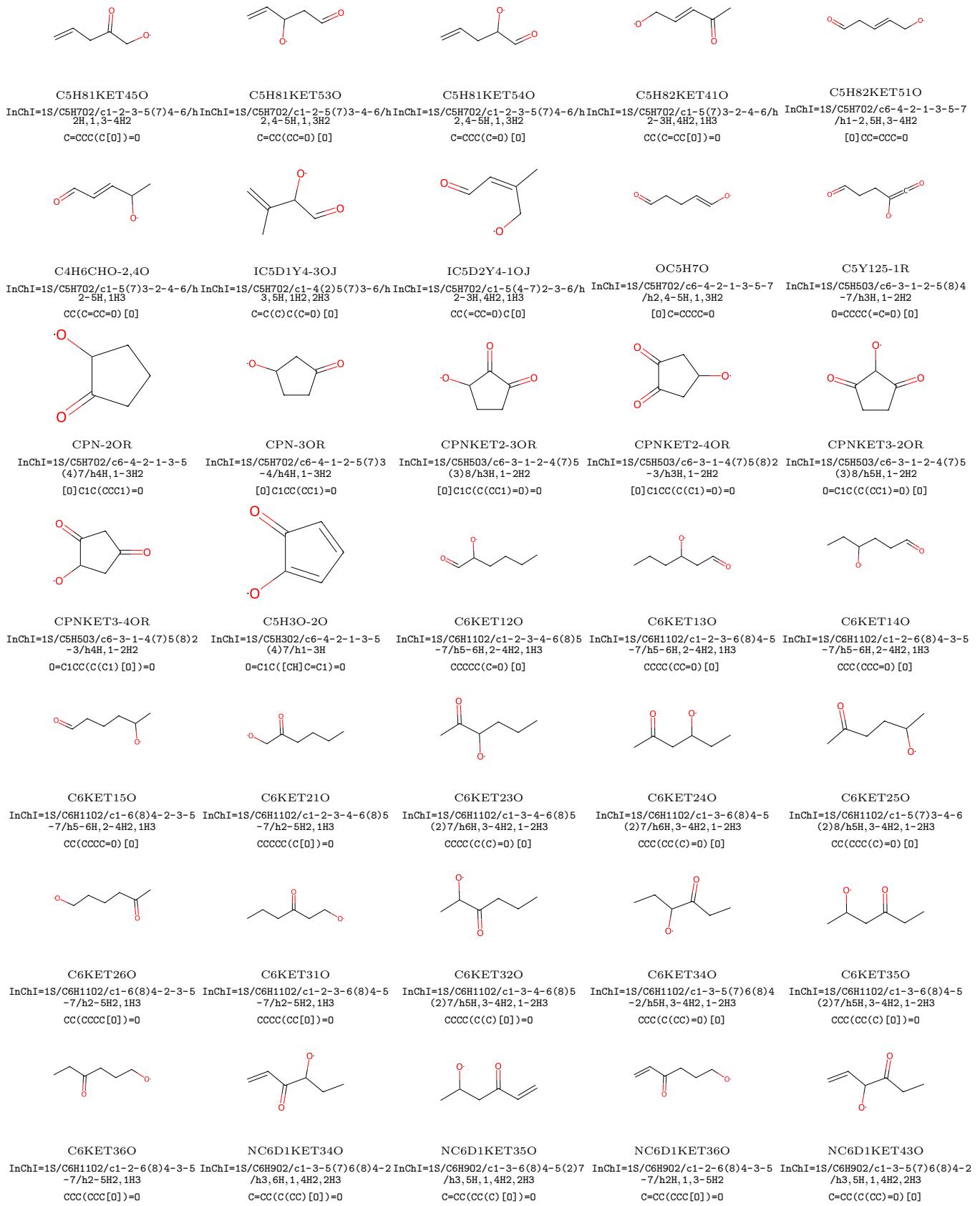


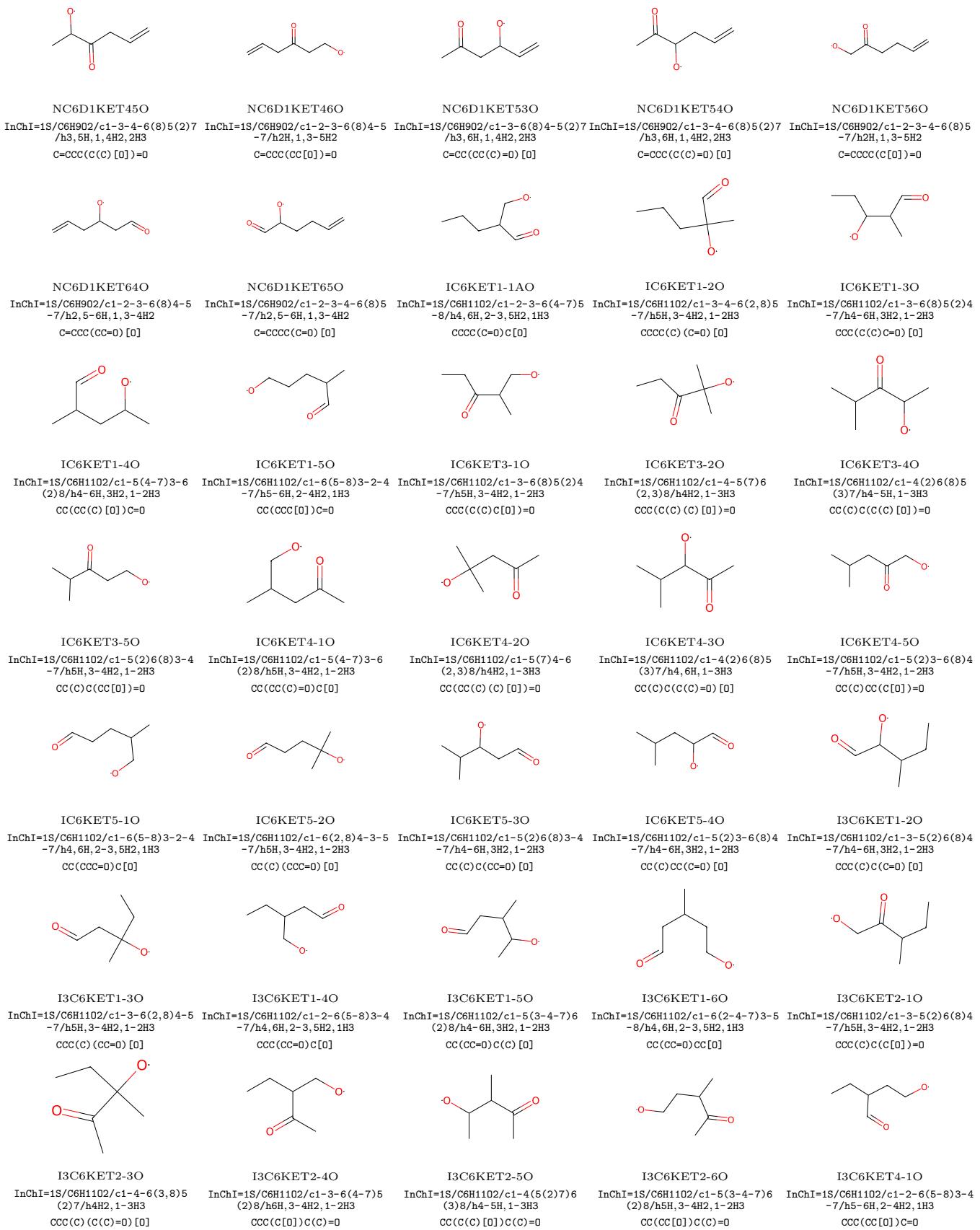


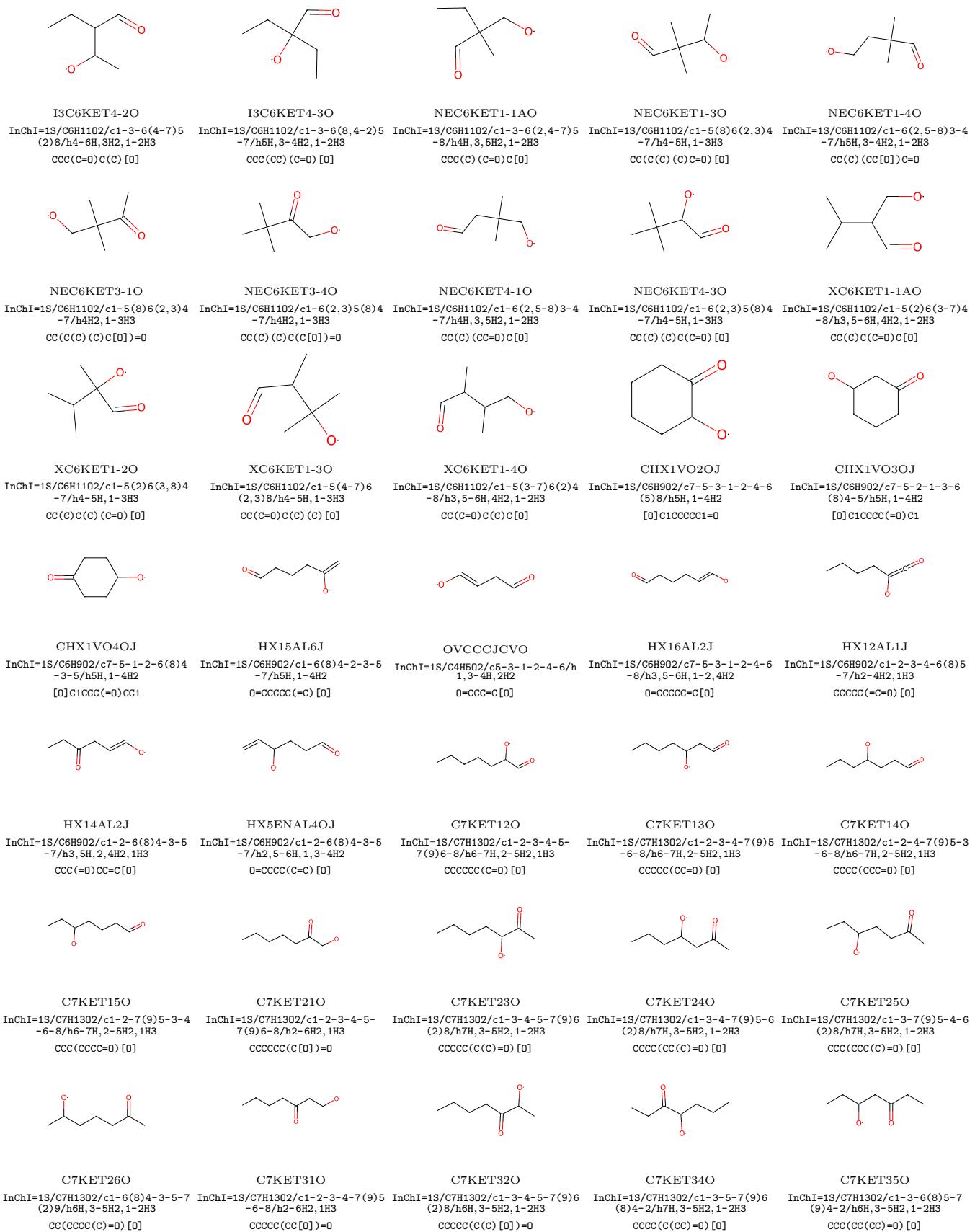


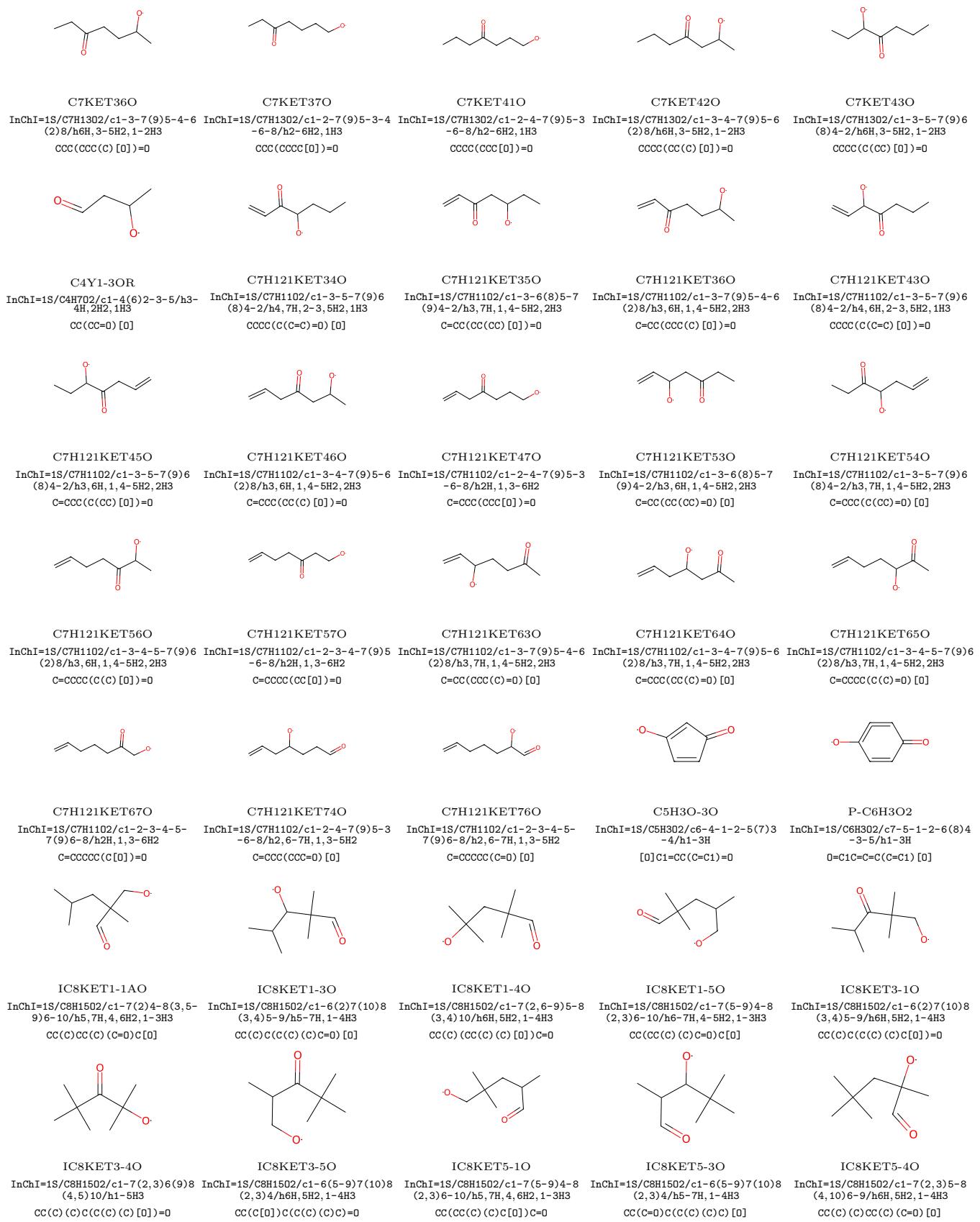


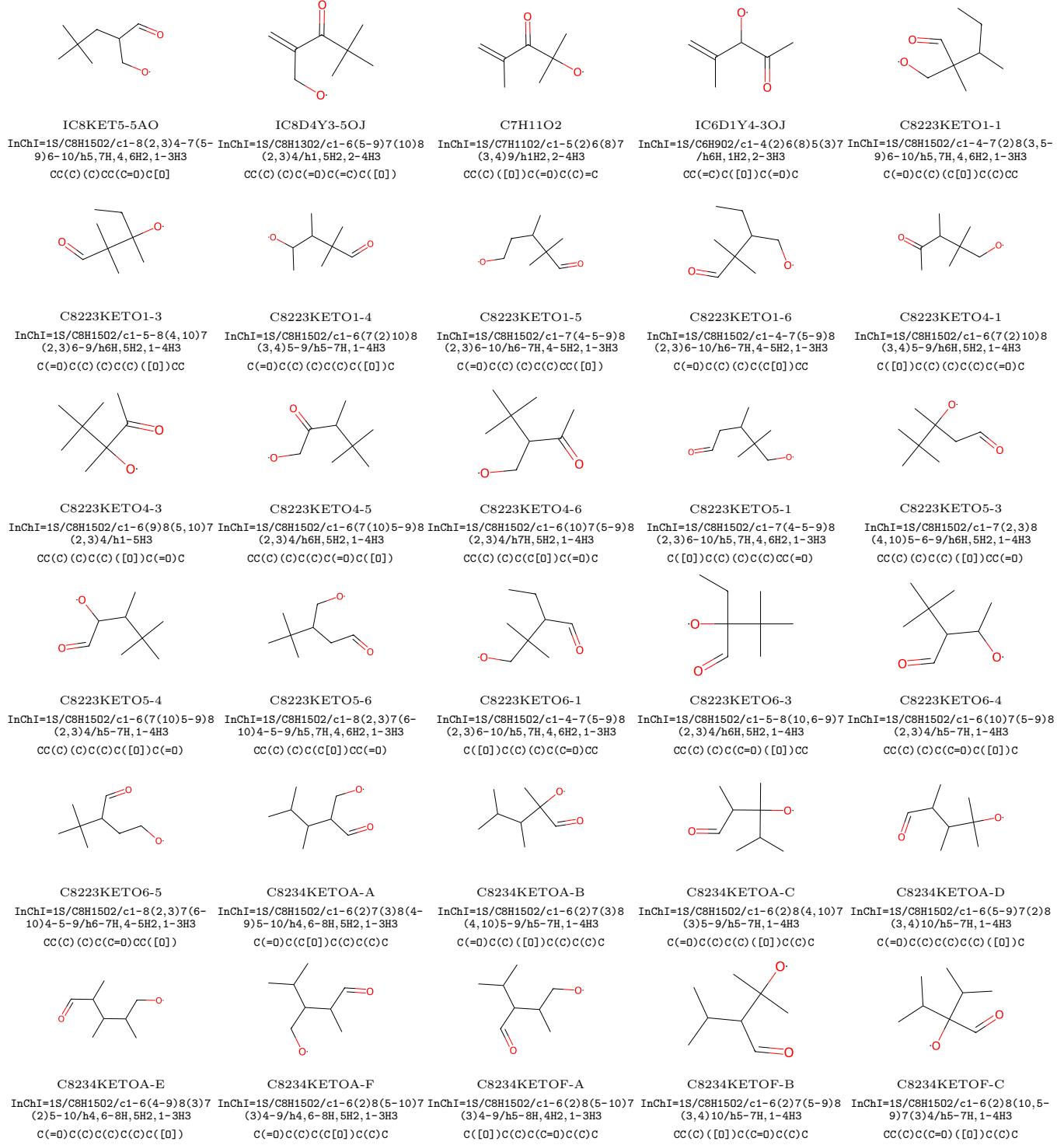


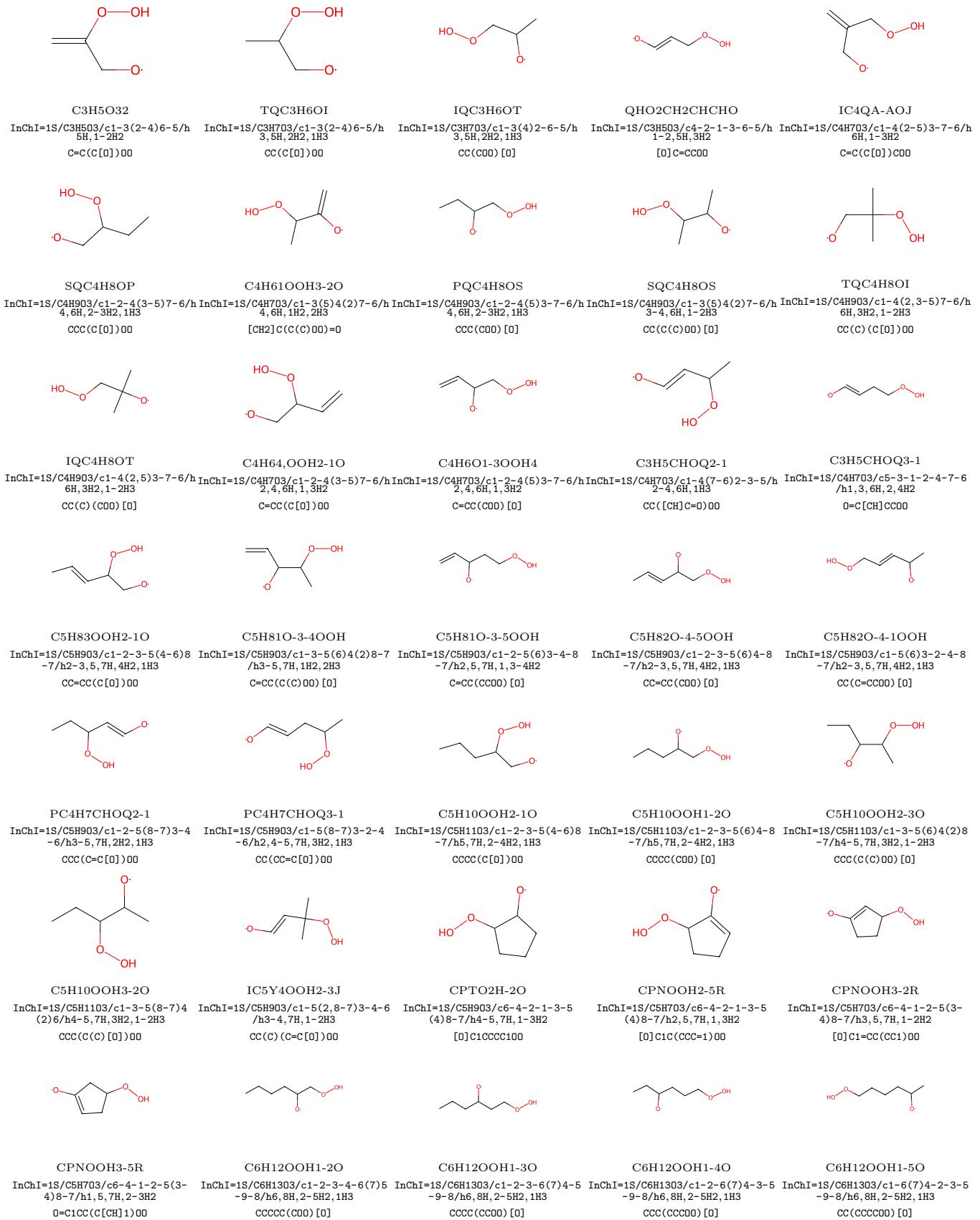


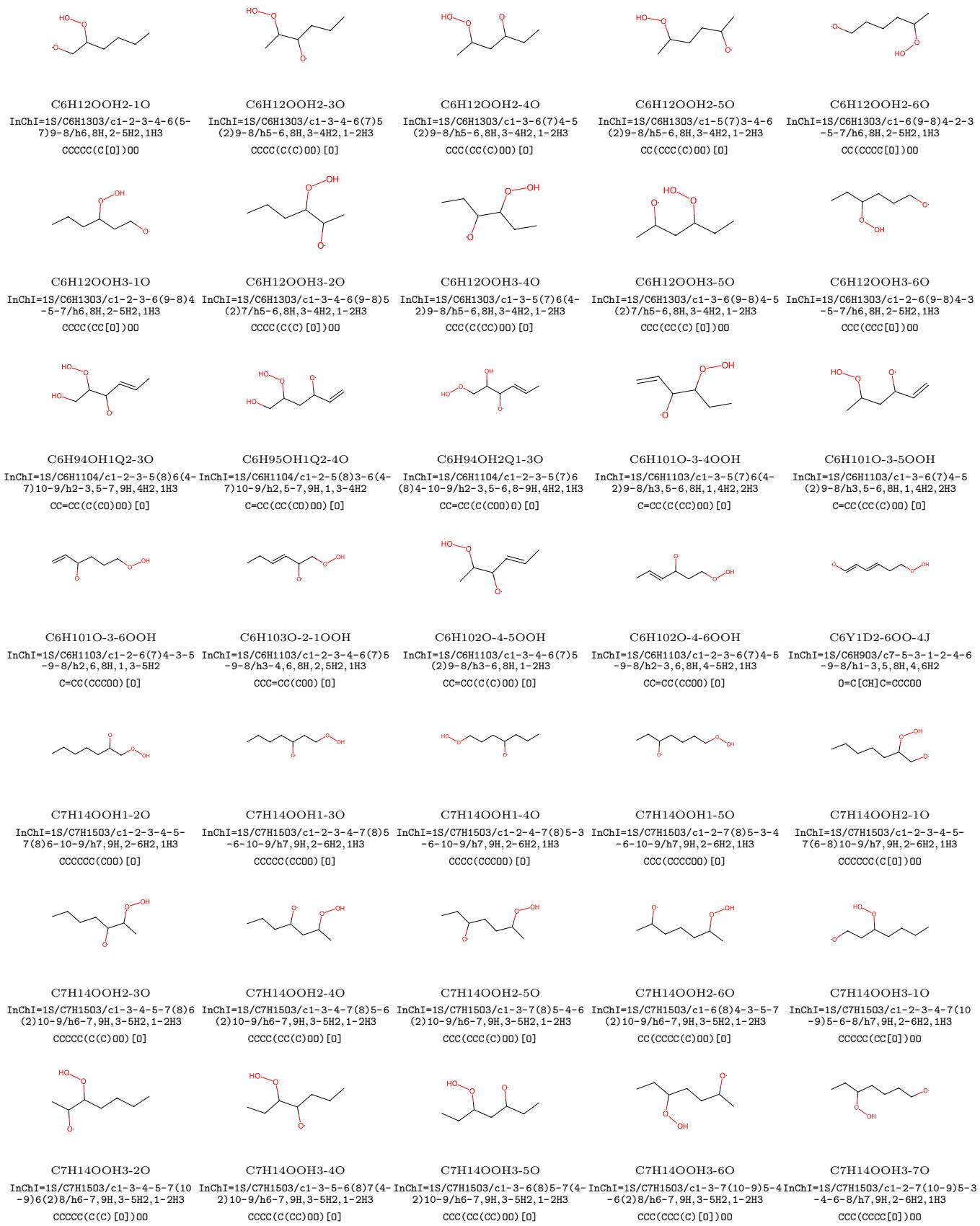


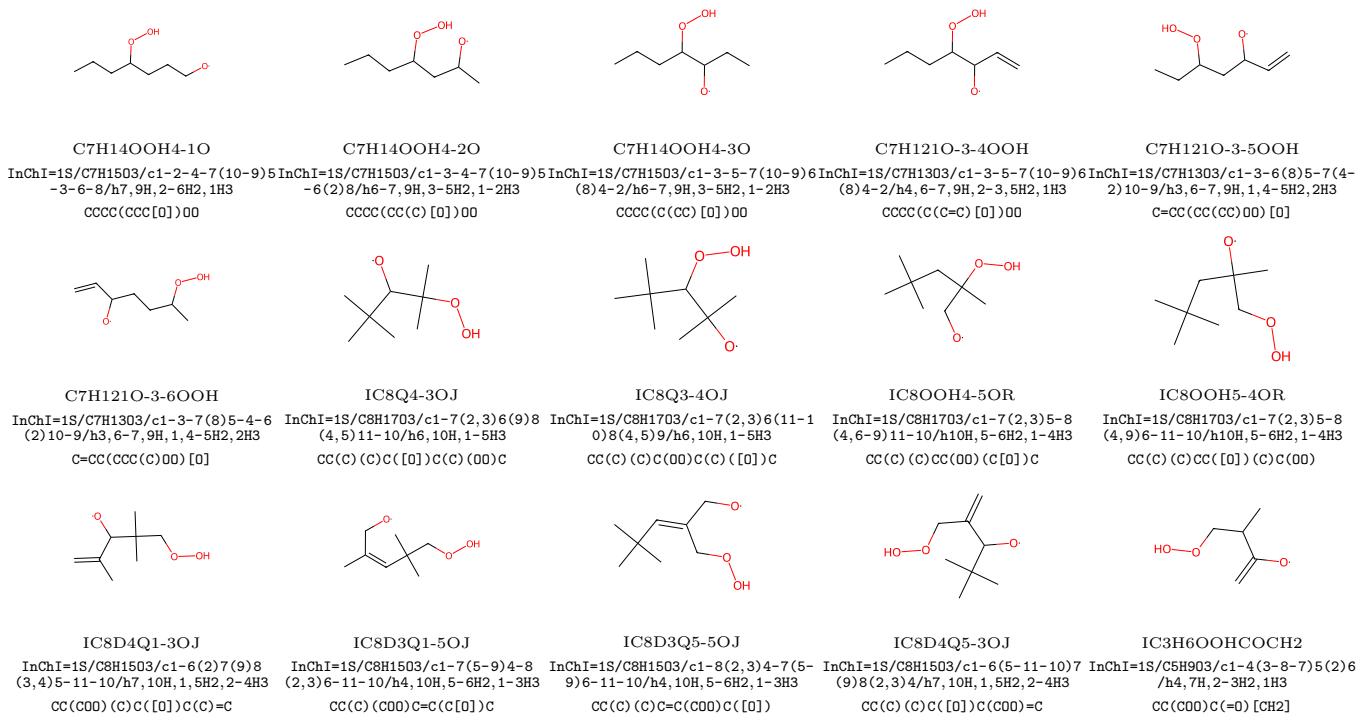


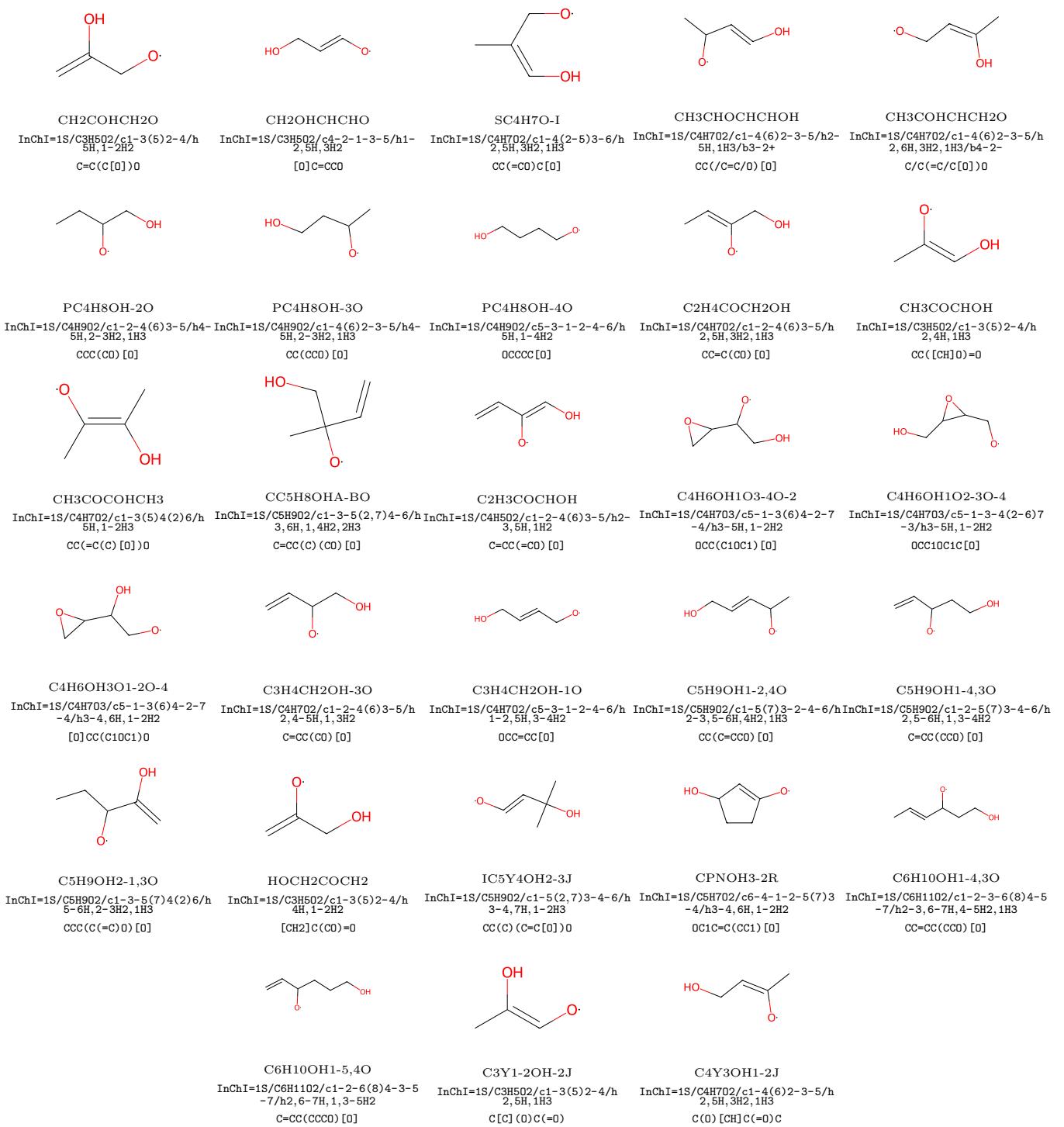


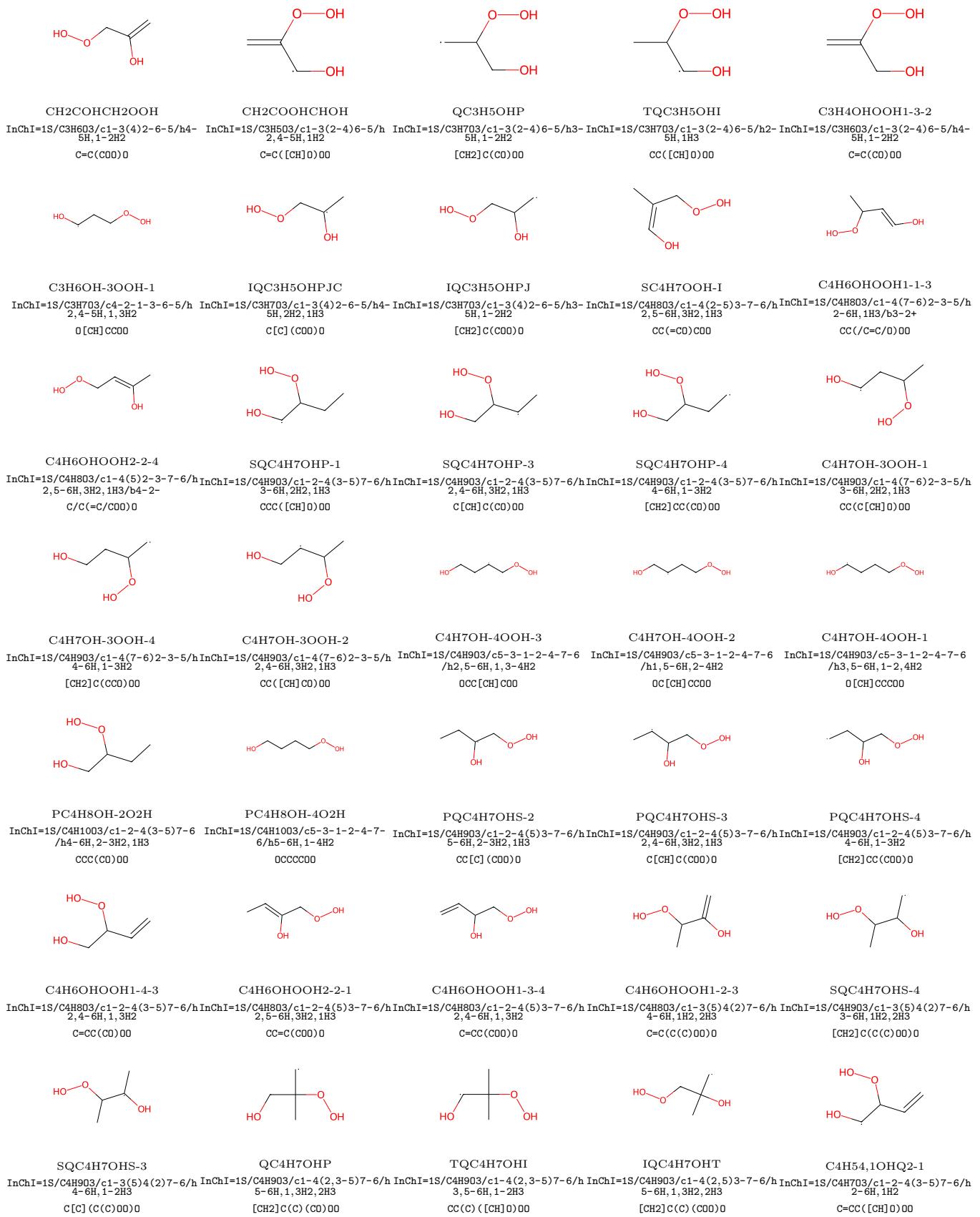


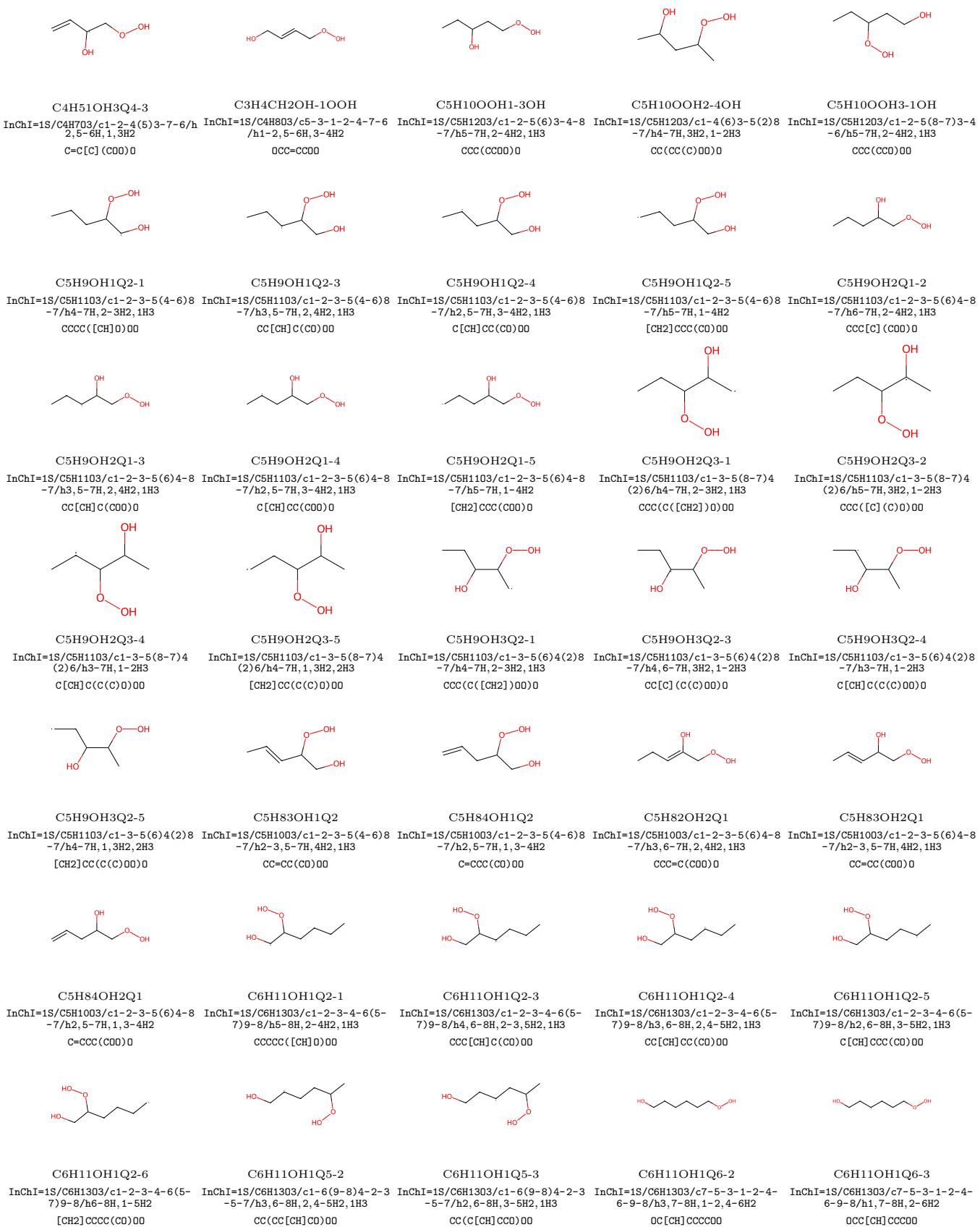


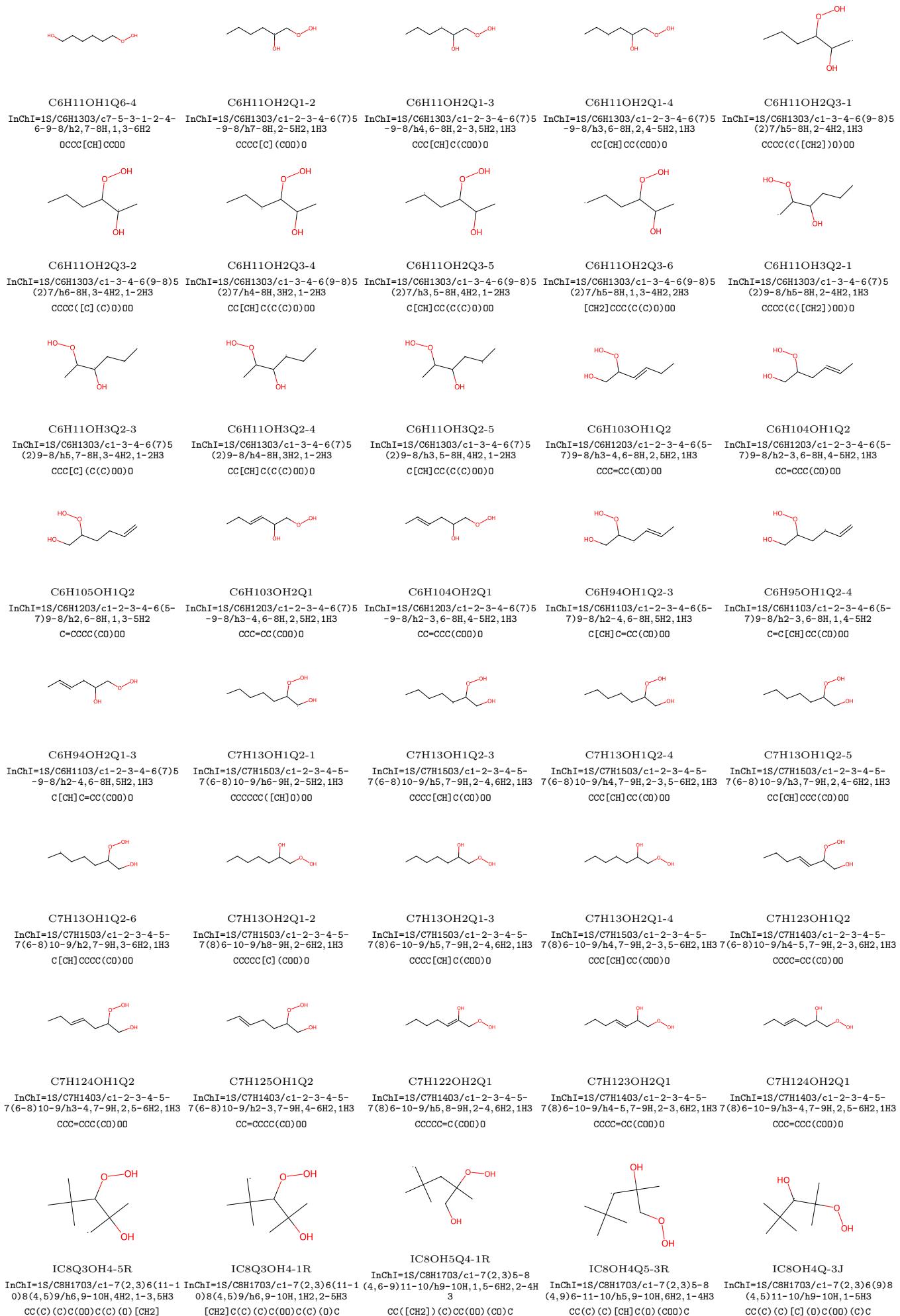


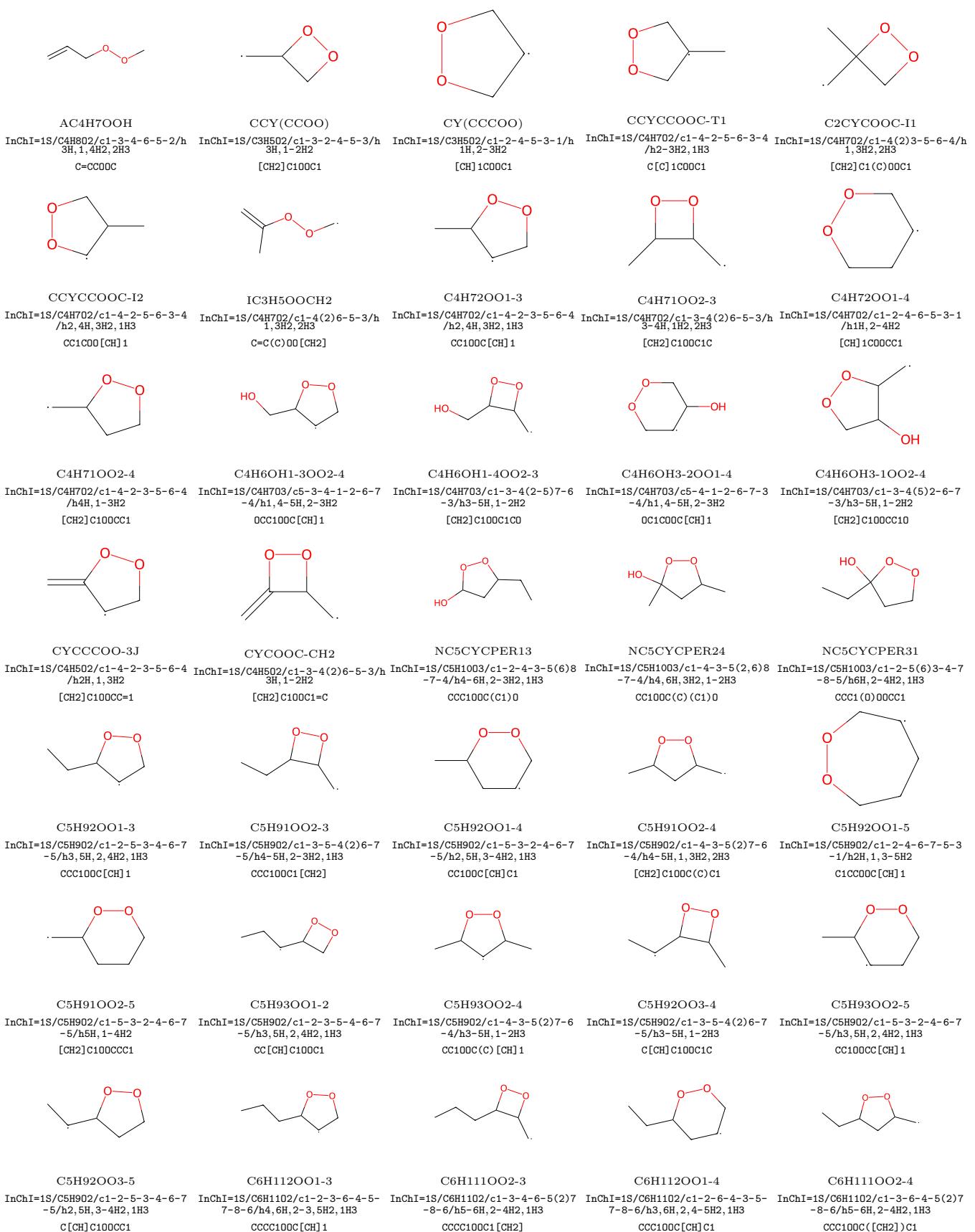


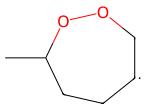




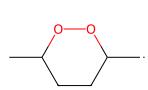




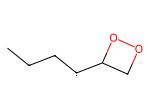




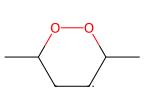
C6H112OO1-5
InChI=1S/C6H11O2/c1-6-4-2-3-5-7-8-6/h3,6H,2,4-5H2,1H3
CC1OOC[CH]CC1



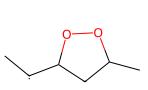
C6H111OO2-5
InChI=1S/C6H11O2/c1-5-3-4-6(2)8-7-5/h5-6H,1,3-4H2,2H3
[CH2]C1OOC(C)CC1



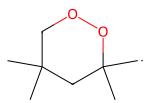
C6H113OO1-2
InChI=1S/C6H11O2/c1-2-3-4-6-5-7-8-6/h4,6H,2-3,5H2,1H3
CCC[CH]C1OOC1



C6H113OO2-5
InChI=1S/C6H11O2/c1-5-3-4-6(2)8-7-5/h3,5-6H,4H2,1-2H3
CC1OOC(C)C[CH]1



C6H112OO3-5
InChI=1S/C6H11O2/c1-3-6-4-5(2)7-8-6/h3,5-6H,4H2,1-2H3
C[CH]C1OOC(C)C1



IC8CYOO14-5R
InChI=1S/C8H15O2/c1-7(2)5-8(3,4)10-9-6-7/h3,5-6H2,1-2,4H3
CC(C1)(C)CC(OO1)(C)[CH2]

