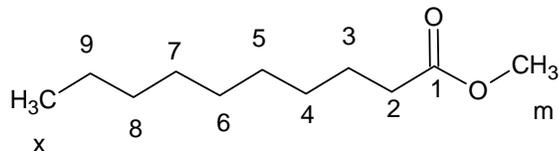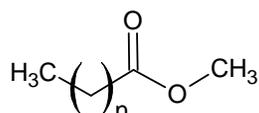# Nomenclature of species

1) Methyl esters :

Numbering of the carbon atoms in ester species:

a. Saturated methyl esters:

n	Name	Name in the models
0	methyl ethanoate	me
1	methyl propanaote	mp
2	methyl butanoate	mb
3	methyl pentanoate	mf
4	methyl hexanoate	mh
5	methyl heptanoate	ms
6	methyl octanoate	mo
7	methyl nonanoate	mn
8	methyl decanoate	md

b. Unsaturated methyl esters:

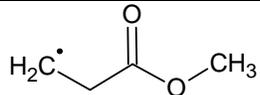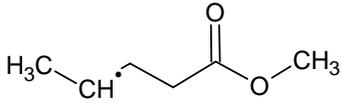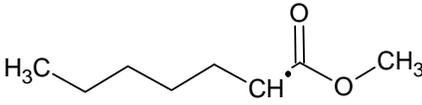Name = "name of the saturated ester " + "position of the double bond" + "d"
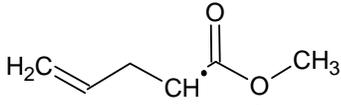
Formula	Name	Name in the model
	2-propenoic acid methyl ester	mp2d
	3-pentenoic acid methyl ester	mf3d
	5-heptanoic acid methyl ester	ms5d

c. methyl esters with two double bonds:

Name = "name of the saturated ester " + "position of the first double bond" + "position of the second double bond" + "d"
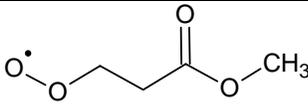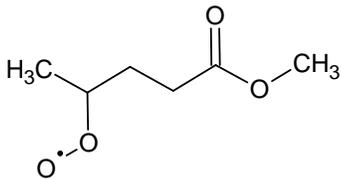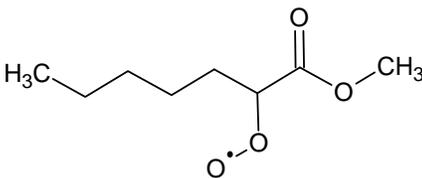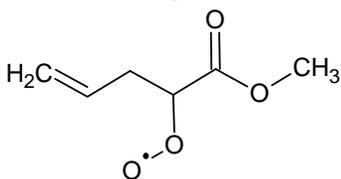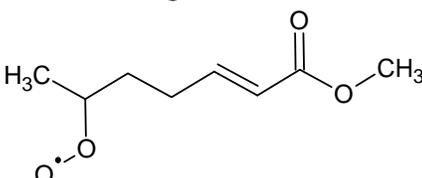
d. Alkyl ester radicals

Name = "name of corresponding ester" + "position of the radical dot" + "j"

Formula	Name in the model
	mp3j
	mf4j
	ms2j
	mf4d2j
	ms2d6j
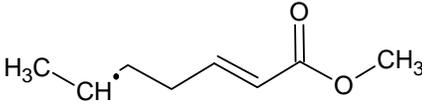
e. Peroxy ester radicals

Name = "name of corresponding ester" + "position of the O-O group" + "oo"
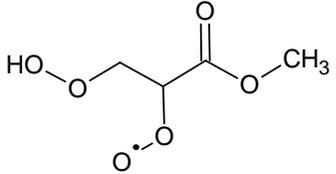
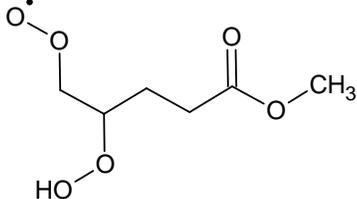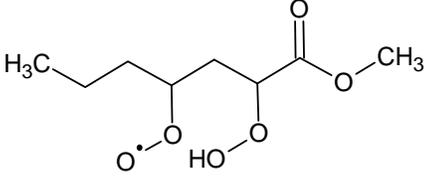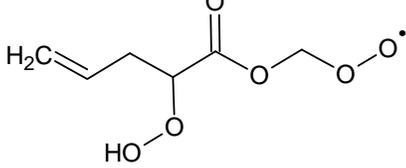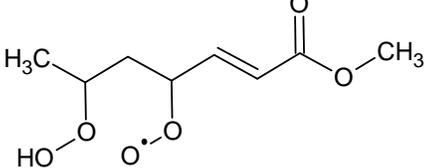| Formula	Name in the model
	mp3oo
	mf4oo
	ms2oo
	mf4d2oo
	ms2d6oo

f. Hydroperoxy alkyl ester radicals:

Name = "name of corresponding ester" + "position of the O-O group" + "oo" + "position of the radical dot" + "j"

Formula	Name in the model
	mp3ooh2j
	mf4ooh5j
	ms2ooh4j
	mf4d2oohmj
	ms2d6ooh4j

g. OOQOOH ester radicals:

Name = "name of corresponding ester" + "position of the O-OH group" + "ooh" + "position of the O-O group" + "o2"
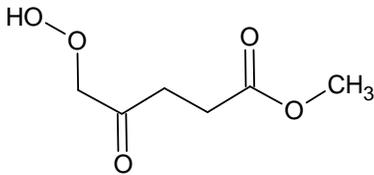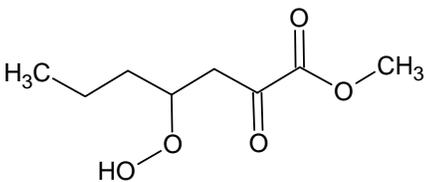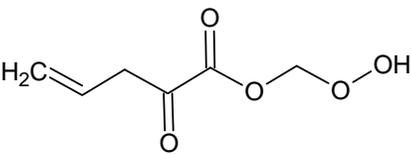
Formula	Name in the model
	mp3ooh2o2
	mf4ooh5o2
	ms2ooh4o2
	mf4d2oohmo2
	ms2d6ooh4o2

h. Ketohydroperoxide ester molecules:

Name = "name of corresponding ester" + "ket" + "position of the carbonyl group" + "position of the O-OH group"
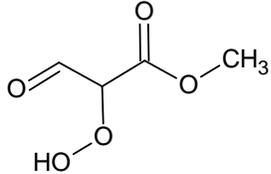
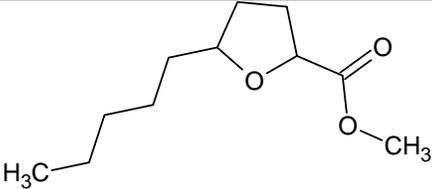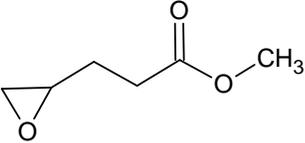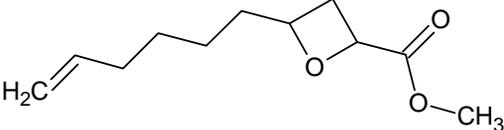| Formula	Name in the model
	mp3ket32
	mf4ket45
	ms2ket24
	mf4d2ket2m
	ms2d6ket64
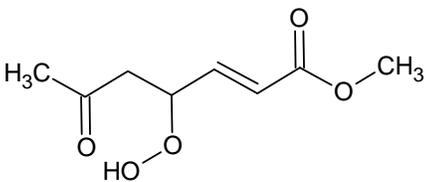
i. Cyclic ethers:

For saturated esters:
Name = "name of corresponding ester" + "o" + "position of the first C-atom embedded in the ring and adjacent to the O-atom" + "position of the second C-atom embedded in the ring and adjacent to the O-atom".
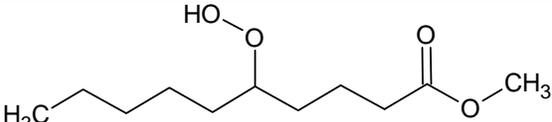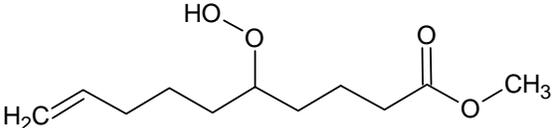
For unsaturated esters (e.g. md9d)
Name = "name of corresponding ester" + "cy" + "position of the first C-atom embedded in the ring and adjacent to the O-atom" + "position of the second C-atom embedded in the ring and adjacent to the O-atom".

Formula	Name in the model
	mdo2-5
	mfo4-5
	md9dcy24

j. Hydroperoxydes:

Name = "name of corresponding ester" + "position of the O-OH group" + "ooh".

Formula	Name in the model
	md5ooh
	md9d5ooh

2) Alkanes
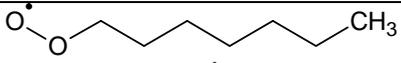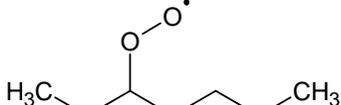
Normal alkanes are named nc_xh_{2x+2}. For example n-heptane is named nc7h16 in the models.

a. Alkyl radicals:

1-heptyl radical is named c7h15-1, 2-heptyl radical is named c7h15-2...
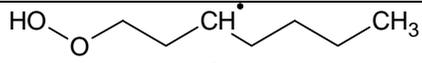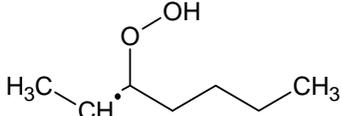
b. Peroxy radicals:

Name = "name of corresponding radical" + "o2-" + "position of the O-O group"

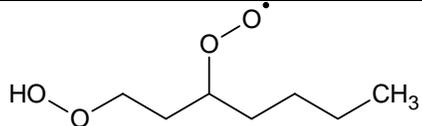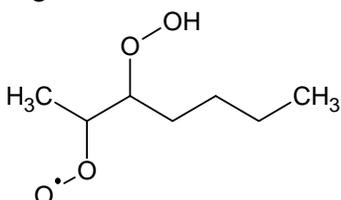| Formula	Name in the model
	c7h15o2-1
	c7h15o2-3

c. Hydroperoxy alkyl radicals:

Name = "name of corresponding radical" + "ooh-" + "position of the O-OH group"

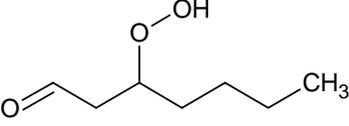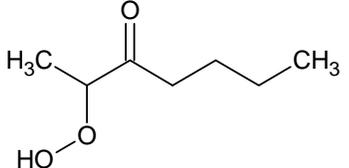| Formula	Name in the model
	c7h14ooh1-3
	c7h15ooh3-2

d. OOQOOH radicals:

Name = "name of corresponding radical minus one H-atom" + "ooh" + "position of the O-OH group" + "-" + "position of the O-O group" + "o2".

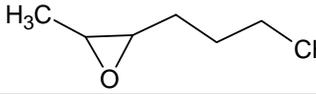| Formula	Name in the model
	c7h14ooh1-3o2
	c7h14ooh3-2o2

e. Ketohydroperoxides:

Name = "nc" + "number of C-atoms in the original alkane" + "ket" + "position of the carbonyl group" + "position of the O-OH group".

Formula	Name in the model
	nc7ket13
	nc7ket32

f. Cyclic ethers:

Name = "formula of the corresponding n-alkane minus two H-atoms" + "o" + "ket" + "position of the first C-atom embedded in the cycle and adjacent to the O-atom" + "-" + "position of the second C-atom embedded in the cycle and adjacent to the O-atom".
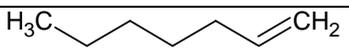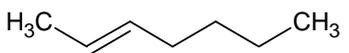Note that the first figure is always less than the second one. For example c7h14o3-1 does not exist and must be written c7h14o1-3.

Formula	Name in the model
	c7h14o1-3
	c7h14o2-3

3) Unsaturated hydrocarbons:

a. Alkenes:

1-heptene is named c7h14-1, 2-heptene is named c7h14-2…

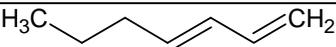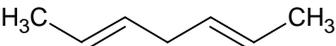| Formula	Name in the model
	c7h14-1
	c7h14-2

b. Alkenyl radicals:

Name = "formula of the corresponding alkene minus one H-atom" + "-" + "position of the double bond" + "position of the radical dot".
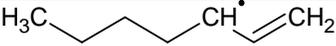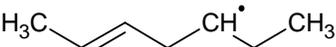
Formula	Name in the model
H₃C⌁⌁CH•⌁CH₂	c7h13-13
H₃C⌁⌁CH•⌁CH₃	c7h13-25

c. Dienes:

Name = "formula of the diene" + "-" + "position of the first double bond" + "position of the second double bond".
Note that the first figure must be less than the second one. For example c7h12-52 does not exist and is written c7h12-25.

Formula	Name in the model
H₃C⌁⌁⌁CH₂	c7h12-13
H₃C⌁⌁⌁CH₃	c7h12-25