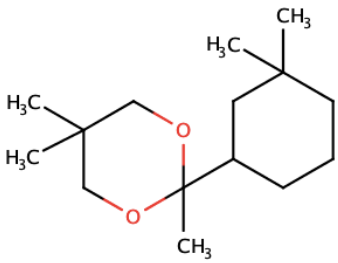
1.

Commercial name: Fructaplex©

IUPAC Name: 2-(3,3-dimethylcyclohexyl)-2,5,5-trimethyl-1,3-dioxane
SMILES: CC1(C)CCCC(C1)C2(C)OCC(C)(C)CO2

Molecular weight:	240.39 g/mol
Volume (cubic Angstroems):	258.88
Atoms number (non-hydrogen):	17
miLogP:	4.43

Structure:



Biological Properties:

Predicted Druglikeness[i]:

GPCR ligand	-0.23
Ion channel modulator	-0.03
Kinase inhibitor	-0.6
Nuclear receptor ligand	0.15
Protease inhibitor	-0.28
Enzyme inhibitor	0.15

Commercial name: Fructaplex©

IUPAC Name: 2-(3,3-dimethylcyclohexyl)-2,5,5-trimethyl-1,3-dioxane
SMILES: CC1(C)CCCC(C1)C2(C)OCC(C)(C)CO2

Predicted Olfactory Receptor Activity[ii]:

OR2L13	83.715%
OR1G1	82.761%
OR10J5	80.569%
OR2W1	78.180%
OR7A2	77.696%

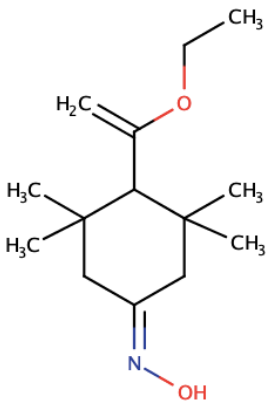
2.

Commercial name: Sylvoxime©

IUPAC Name: N-[4-(1-ethoxyethenyl)-3,3,5,5tetramethylcyclohexylidene]hydroxylamine
SMILES: CCOC(=C)C1C(C)(C)CC(CC1(C)C)=NO

Molecular weight:	239.36
Volume (cubic Angstroems):	252.83
Atoms number (non-hydrogen):	17
miLogP:	4.33

Structure:



Biological Properties:

Predicted Druglikeness:

GPCR ligand	-0.6
Ion channel modulator	-0.41
Kinase inhibitor	-0.93
Nuclear receptor ligand	-0.17
Protease inhibitor	-0.39
Enzyme inhibitor	0.01

Commercial name: Sylvoxime©

IUPAC Name: N-[4-(1-ethoxyethenyl)-3,3,5,5tetramethylcyclohexylidene]hydroxylamine
SMILES: CCOC(=C)C1C(C)(C)CC(CC1(C)C)=NO

Predicted Olfactory Receptor Activity:

OR52D1	71.900%
OR1G1	70.394%
0R52I2	70.392%
OR52I1	70.390%
OR2Y1	70.378%

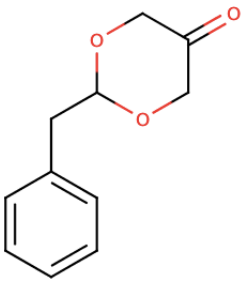
3.

Commercial name: Hyperflor©

IUPAC Name: 2-benzyl-1,3-dioxan-5-one
SMILES: O=C1COC(CC2=CC=CC=C2)OC1

Molecular weight:	192.21 g/mol
Volume (cubic Angstroems):	177.39
Atoms number (non-hydrogen):	14
miLogP:	1.09

Structure:



Biological Properties:

Predicted Druglikeness:

GPCR ligand	-0.27
Ion channel modulator	-0.39
Kinase inhibitor	-1.02
Nuclear receptor ligand	-0.81
Protease inhibitor	-0.51
Enzyme inhibitor	0.07

Commercial name: Hyperflor©

IUPAC Name: 2-benzyl-1,3-dioxan-5-one
SMILES: O=C1COC(CC2=CC=CC=C2)OC1

Predicted Olfactory Receptor Activity:

OR1D2	86.325%
OR1A1	80.362%
OR2G2	73.955%
OR2W1	73.590%
OR10G9	72.690%
OR10D4	72.329%
OR4C6	71.154%
OR10G7	70.886%
OR5F1	70.743%
OR2L2	70.680%
OR7A10	70.344%
OR5AU1	70.259%
OR10G8	69.059%
OR2L13	68.728%
OR10G6	68.210%
OR10G4	68.189%
OR4D5	67.655%
OR10D3	66.975%
OR2AK2	66.533%
OR8H3	66.529%
OR8H1	66.274%
OR2T10	66.212%
OR2D3	66.110%
OR12D2	65.730%
OR1M1	65.712%
OR4D6	65.692%
OR4D9	64.976%
OR4K3	64.712%
OR11H6	64.639%
OR1F2	64.240%
OR10A7	64.109%
OR8U8	63.919%
OR51L1	63.820%
OR3A1	63.457%
OR4C46	63.137%
OR4C3	62.763%
OR1N1	62.353%

Commercial name: Hyperflor©

IUPAC Name: 2-benzyl-1,3-dioxan-5-one
SMILES: O=C1COC(CC2=CC=CC=C2)OC1

Predicted Olfactory Receptor Activity (continued):

OR7D2	61.584%
OR5T1	61.259%
OR8B4	61.181%
OR1I1	60.284%
OR5D14	60.222%
OR2L5	59.252%
OR8D1	59.186%
OR7C2	59.091%
OR2T2	58.897%
OR5AC2	58.697%
OR2A25	58.670%
OR4A15	58.637%
OR4D10	58.521%
OR4N5	57.579%
OR8U1	57.562%
OR2T5	57.550%
OR7A5	57.486%
OR2AE1	57.100%
OR51H1	57.022%
OR10H1	56.678%
OR2A7	56.514%
OR6V1	56.478%
OR2T29	56.274%
OR8B12	56.060%
OR1J2	56.029%
OR2D2	55.979%
OR4F3/4F16 /4F2	55.752%
OR10A2	55.276%
OR8B8	55.060%
OR8D4	54.561%
OR8B3	54.334%
OR2A2	53.894%
OR7C1	53.423%
OR9A2	53.282%
OR8B2	53.127%
OR4F5	53.079%
OR7A17	52.601%

Commercial name: Hyperflor©

IUPAC Name: 2-benzyl-1,3-dioxan-5-one
SMILES: O=C1COC(CC2=CC=CC=C2)OC1

Predicted Olfactory Receptor Activity (continued):

OR9K2	52.595%
OR4S1	52.444%
OR10V1	52.040%
OR2T35	52.028%
OR10K1	51.964%
OR2A4	51.907%
OR10H5	51.151%
OR4F4	51.020%
OR4F21	50.973%
OR1L6	50.968%
OR2M4	50.912%
OR10H2	50.851%
Y1035_ HUMAN	50.799%
OR10A3	50.571%

[i] Molinspiration Cheminformatics

[ii] **ODORactor: a web server for deciphering olfactory coding.**
Liu X, Su X, Wang F, Huang Z, Wang Q, Li Z, Zhang R, Wu L, Pan Y, Chen Y, Zhuang H, Chen G, Shi T, Zhang J*. Bioinformatics, 2011, 27: 2302-2303.