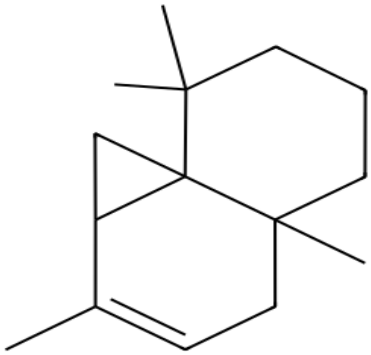
VERA: Similarity and Grouping:

PREMIER
PRIORITISATION AND RISK EVALUATION
OF MEDICINES IN THE ENVIRONMENT



Molecule Input:

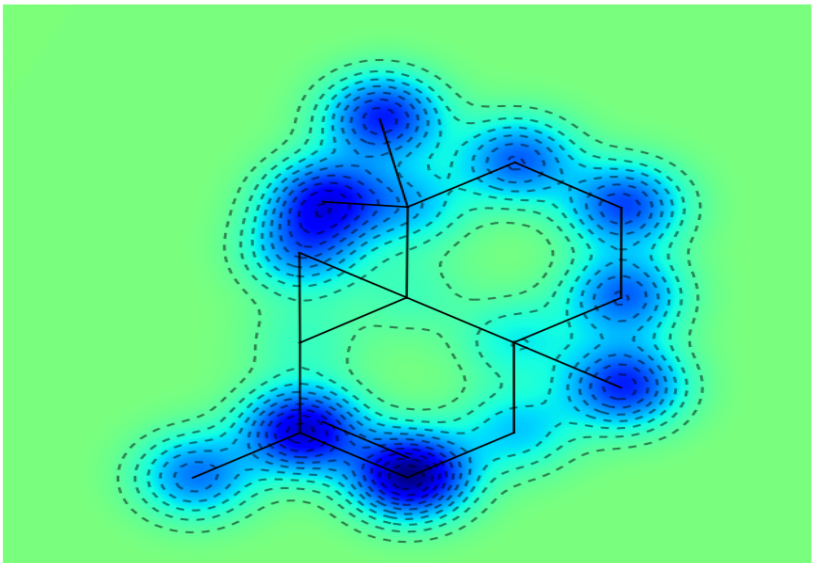
TotGroups: 2

['allylic_oxid', 'CC4']

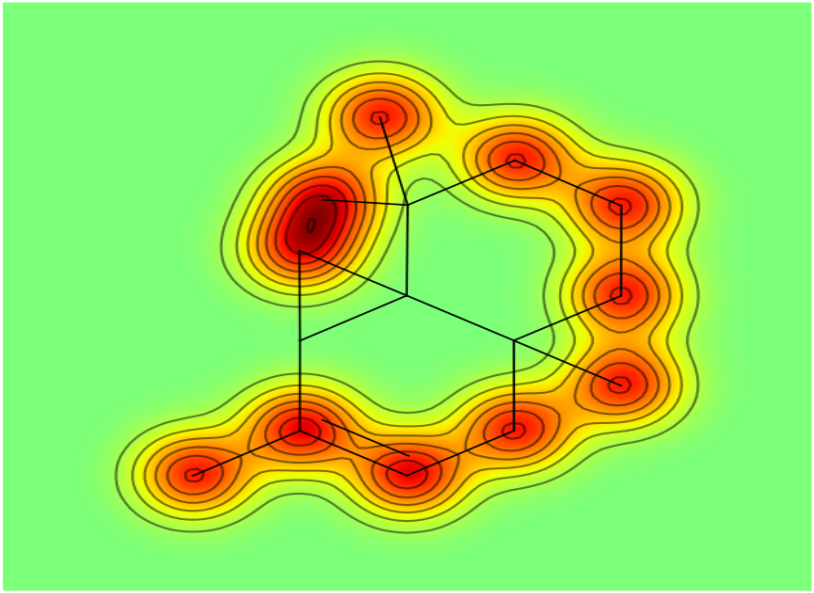
LogP: 4.559
MaxPartialCharge: -0.012
MinPartialCharge: -0.085
NumHAcceptors: 0
NumHDonors: 0
NumRotatableBonds: 0
NumAliphaticRings: 3
NumAromaticCarbocycles: 0
NumAromaticHeterocycles: 0
NumAromaticRings: 0
ExactMolWt: 204.188

Prediction from Global model: 0.459 -log(mg/l)

GasteigerCharges:



CrippenContribs:



Molecules with the highest group similarity

1) SMILES: C=CC(C)(O)CCC1C(=C)CCC2C(C)(C)CCCC12C

ExpValue: 0.92 -log(mg/l)

SimilarityVega: 0.753

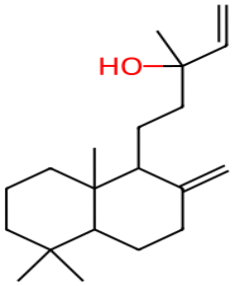
SimilarityGrouping: 0.817

Grp_Similarity_Mean: 0.785

Groups in common: 4

TotGroups 9

GROUPS:
Al_OH Stat: Neutro
allylic_oxid Stat: Tox
CH2_Terminal Stat: Tox
CC4 Stat: Tox
Al_bicycle Stat: Tox
Alerts: []



2) SMILES: CC1=CC(=O)CC(C)(C)C1

ExpValue: -2.4 -log(mg/l)

SimilarityVega: 0.6940000000000001

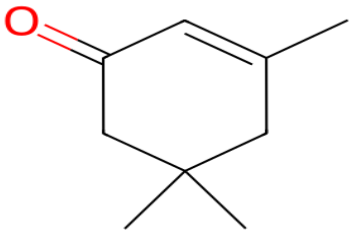
SimilarityGrouping: 0.706

Grp_Similarity_Mean: 0.7

Groups in common: 3

TotGroups 4

GROUPS:
allylic_oxid Stat: Tox
CC4 Stat: Tox
ketone_aliphatic Stat: Neutro
Alerts: []



3) SMILES: C=C1C2CCC3C2C(C)(C)CCCC13C

ExpValue: -1.01 -log(mg/l)

SimilarityVega: 0.93

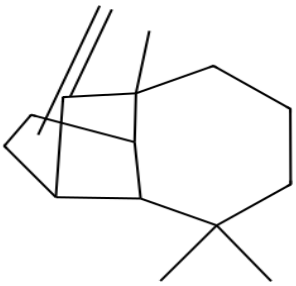
SimilarityGrouping: 0.7

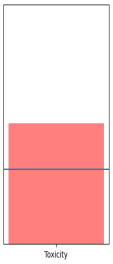
Grp_Similarity_Mean: 0.815

Groups in common: 3

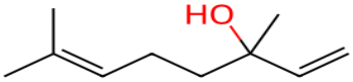
TotGroups 5

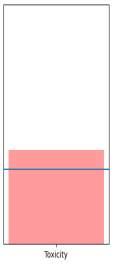
GROUPS:
allylic_oxid Stat: Tox
CH2_Terminal Stat: Tox
CC4 Stat: Tox
Alerts: []



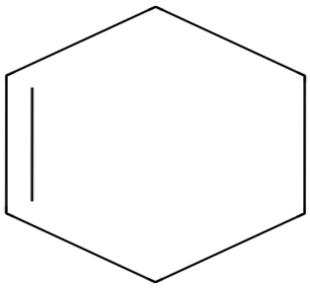


4) SMILES: C=CC(C)(O)CCC=C(C)C
ExpValue: -1.589 -log(mg/l)
SimilarityVega: 0.661
SimilarityGrouping: 0.7
Grp_Similarity_Mean: 0.68
Groups in common: 3
TotGroups 5
GROUPS:
Al_OH Stat: Neutro
allylic_oxid Stat: Tox
CH2_Terminal Stat: Tox
CC4 Stat: Tox
Alerts: []

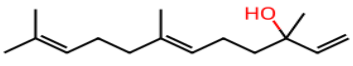




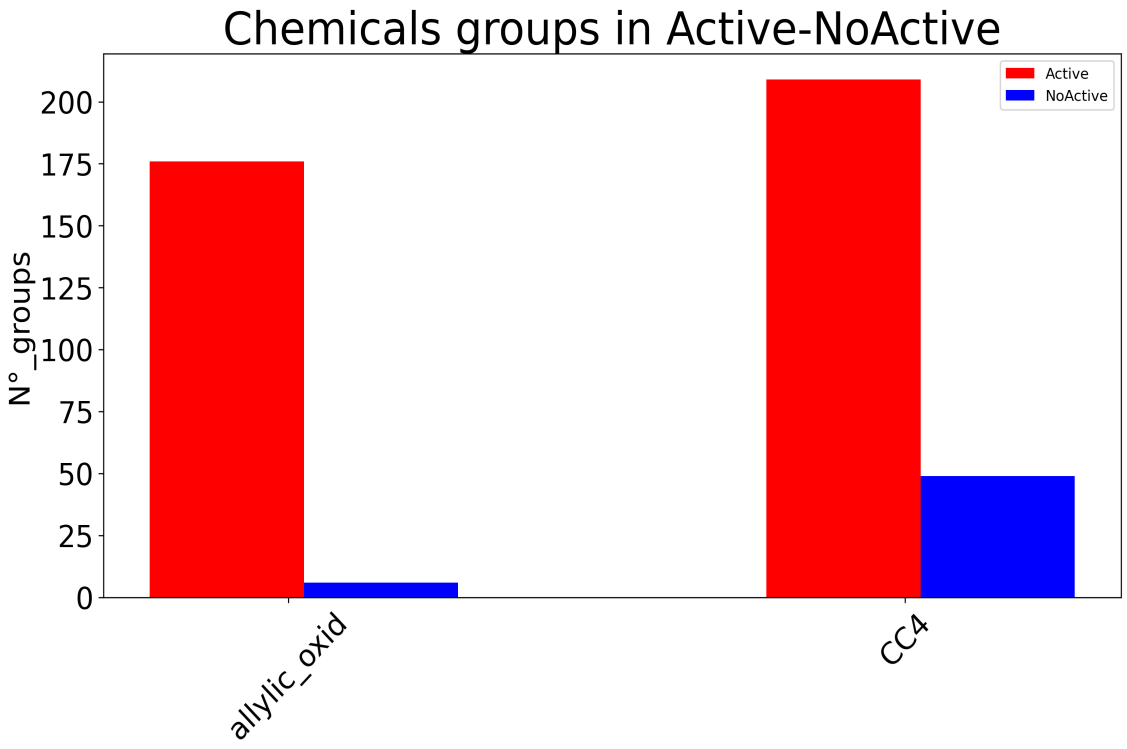
5) SMILES: C1=CCCCC1
ExpValue: -0.762 -log(mg/l)
SimilarityVega: 0.752
SimilarityGrouping: 0.7
Grp_Similarity_Mean: 0.726
Groups in common: 2
TotGroups 2
GROUPS:
allylic_oxid Stat: Tox
Alerts: []



6) SMILES: C=CC(C)(O)CCC=C(C)CCC=C(C)C
ExpValue: -0.155 -log(mg/l)
SimilarityVega: 0.712
SimilarityGrouping: 0.693
Grp_Similarity_Mean: 0.702
Groups in common: 3
TotGroups 7
GROUPS:
Al_OH Stat: Neutro
allylic_oxid Stat: Tox
CH2_Terminal Stat: Tox
CC4 Stat: Tox
Alerts: []



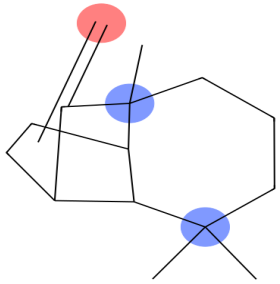
Molecule Input: Bar Chart for groups in Dataset find in target



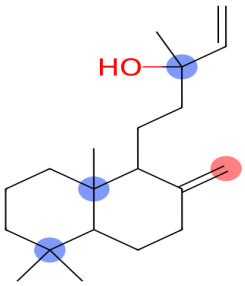
Reasoning

Ortogonal Research based on copresence of group with high prevalence allylic_oxid and GRP CC4

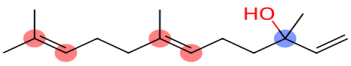
Smile: C=C1C2CCC3C2C(C)(C)CCCC13C
ExpValue: -1.01 -log(mg/l)
Similarity: 0.93



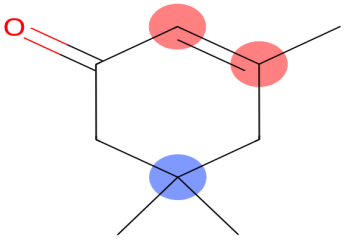
Smile: C=CC(C)(O)CCC1C(=C)CCC2C(C)(C)CCCC12C
ExpValue: 0.92 -log(mg/l)
Similarity: 0.753



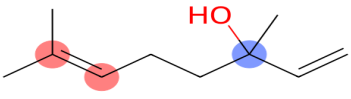
Smile: C=CC(C)(O)CCC=C(C)CCC=C(C)C
ExpValue: -0.155 -log(mg/l)
Similarity: 0.712



Smile: CC1=CC(=O)CC(C)(C)C1
ExpValue: -2.4 -log(mg/l)
Similarity: 0.6940000000000001

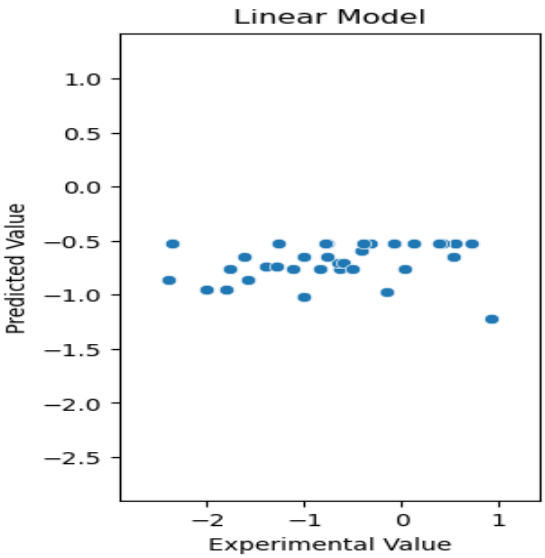


Smile: C=CC(C)(O)CCC=C(C)C
ExpValue: -1.589 -log(mg/l)
Similarity: 0.661



Local Linear Model

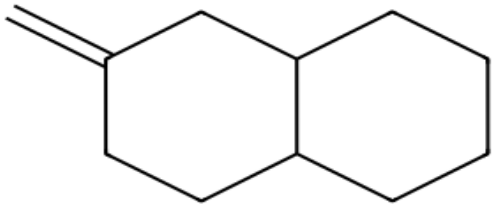
The target assessment was made by using Global model model not by this Local model



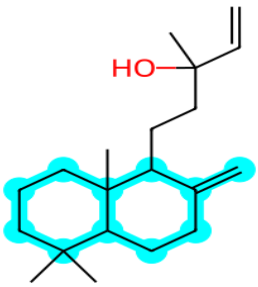
Mean square error: 0.72

Scaffold

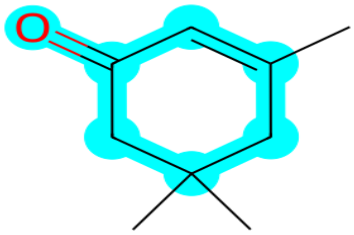
Scaffold analysis



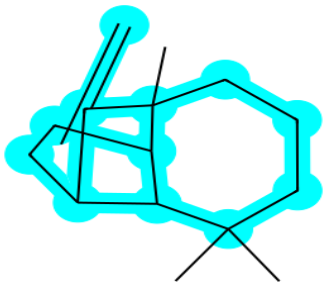
Smile: C=CC(C)(O)CCC1C(=C)CCC2C(C)(C)CCCC12C
ExpValue: 0.92 -log(mg/l)
Similarity: 0.753



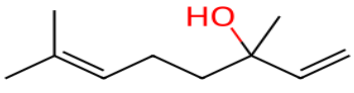
Smile: CC1=CC(=O)CC(C)(C)C1
ExpValue: -2.4 -log(mg/l)
Similarity: 0.6940000000000001



Smile: C=C1C2CCC3C2C(C)(C)CCCC13C
ExpValue: -1.01 -log(mg/l)
Similarity: 0.93



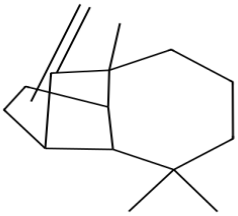
Smile: C=CC(C)(O)CCC=C(C)C
ExpValue: -1.589 -log(mg/l)
Similarity: 0.661



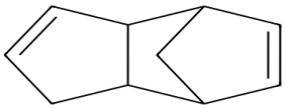
Descriptors

Calculator Similarity descriptor

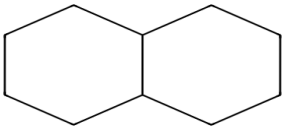
Smile: C=C1C2CCC3C2C(C)(C)CCCC13C
ExpValue: -1.01 -log(mg/l)
DistanceCityBlock: 0.324
LogP:4.415000000000004
MW: 204.187800768



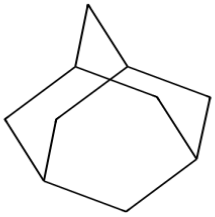
Smile: C1=CC2C3C=CC(C3)C2C1
ExpValue: -1.771 -log(mg/l)
DistanceCityBlock: 4.126
LogP:2.3846000000000007
MW: 132.093900384



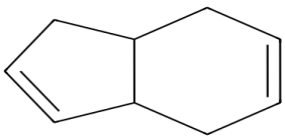
Smile: C1CCC2CCCCC2C1
ExpValue: 0.433 -log(mg/l)
DistanceCityBlock: 4.426
LogP:3.3668000000000022
MW: 138.140850576



Smile: C1C2CC3CC1CC(C2)C3
ExpValue: 0.553 -log(mg/l)
DistanceCityBlock: 5.146
LogP:2.832600000000001
MW: 136.125200512



Smile: C1=CCC2CC=CC2C1
ExpValue: -0.642 -log(mg/l)
DistanceCityBlock: 5.156
LogP:2.5287000000000006
MW: 120.093900384



Smile: CC=C1CC2C=CC1C2
ExpValue: -0.844 -log(mg/l)
DistanceCityBlock: 5.255
LogP:2.5287000000000006
MW: 120.093900384