

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

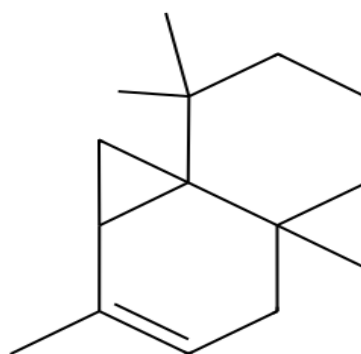
NumAliphaticRings: 3

NumAromaticCarbocycles: 0

NumAromaticHeterocycles: 0

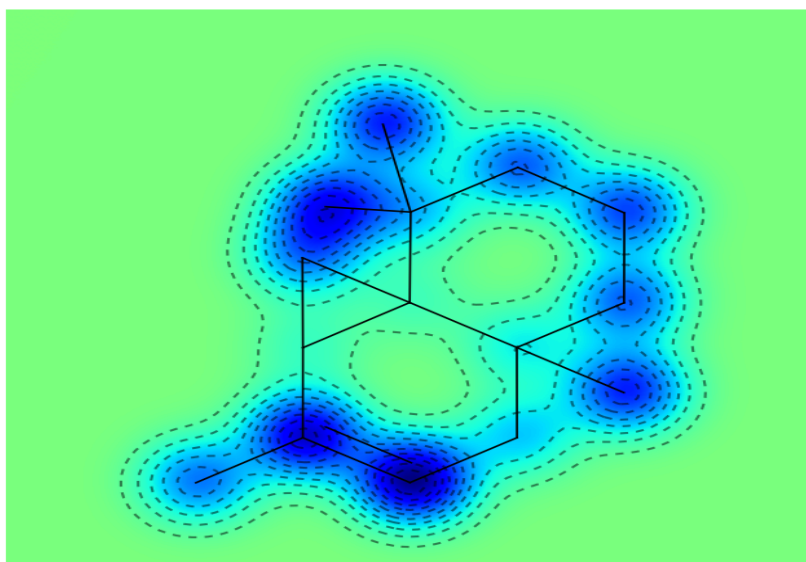
NumAromaticRings: 0

ExactMolWt: 204.188

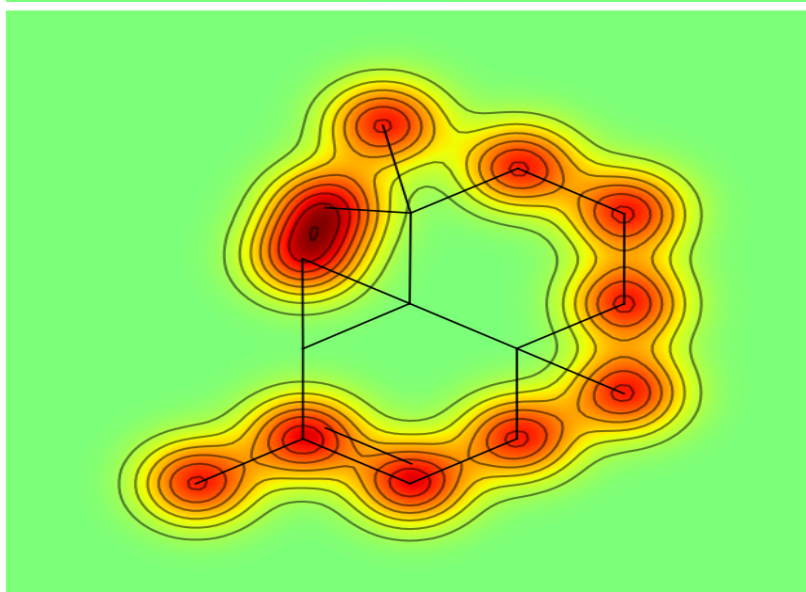


Prediction from Global model: 0.493 -log(mg/l)

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

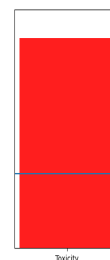
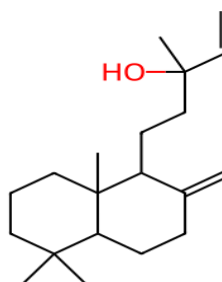
allylic_oxid Stat: Tox

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

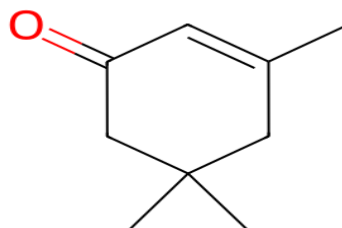
GROUPS:

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

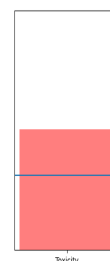
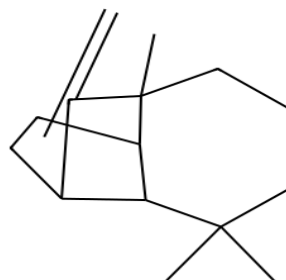
GROUPS:

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:

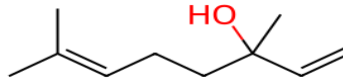
Al_OH Stat: Neutro

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

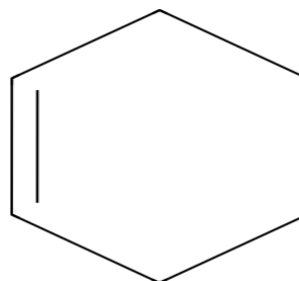
Groups in common: 2

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:

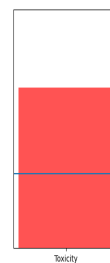
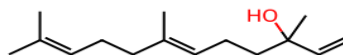
Al_OH Stat: Neutro

allylic_oxid Stat: Tox

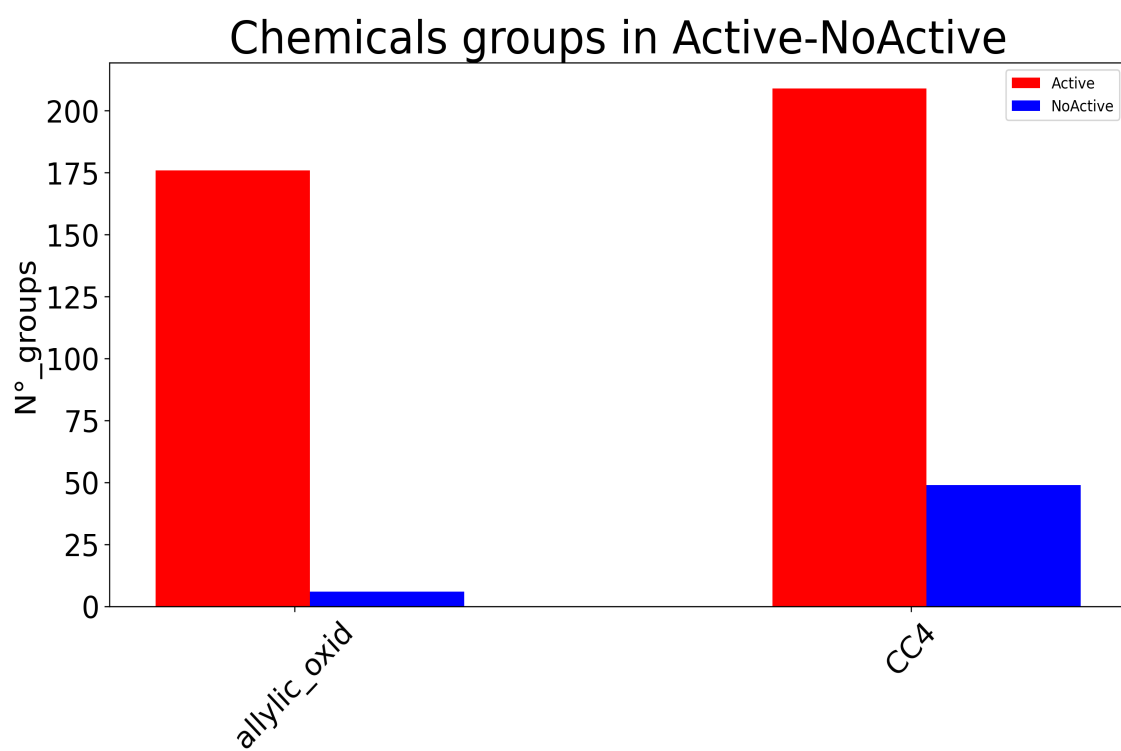
CH2_Terminal Stat: Tox

CC4 Stat: Tox

Alerts: []



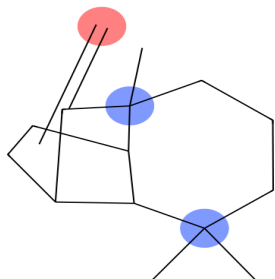
Molecule Input: Bar Chart for groups in Dataset find in target



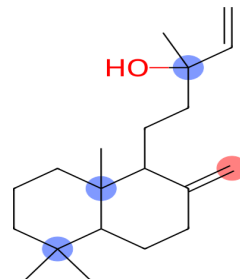
Reasoning

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

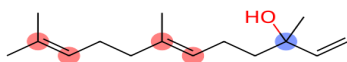
Smile: C=C1C2CCC3C2C(C)(C)CCCC13C
 ExpValue: -1.01 -log(mg/l)
 Similarity: 0.93



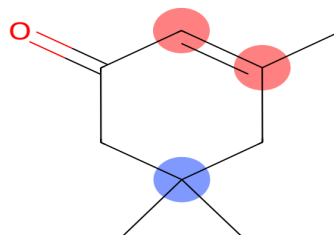
Smile: C=CC(C)(O)CCC1C(=C)CCC2C(C)(C)CCCC12C
 ExpValue: 0.92 -log(mg/l)
 Similarity: 0.753



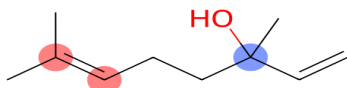
Smile: C=CC(C)(O)CCC=C(C)CCC=C(C)C
 ExpValue: -0.155 -log(mg/l)
 Similarity: 0.712



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

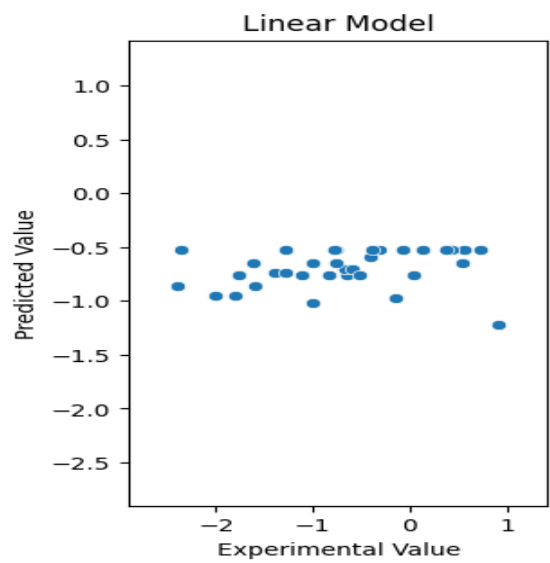


Smile: C=CC(C)(O)CCC=C(C)C
 ExpValue: -1.589 -log(mg/l)
 Similarity: 0.661



Local Linear Model

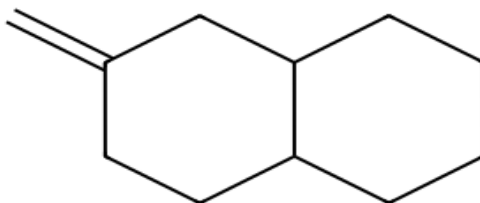
The target assessment was made by using Global model model not by this Local model



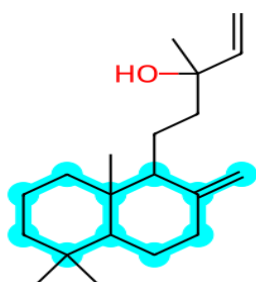
Mean square error: 0.72

Scaffold

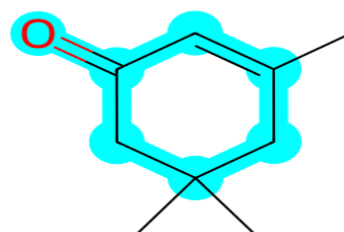
Scaffold analysis



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



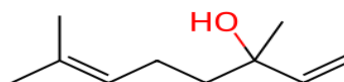
Smile: CC1=CC(=O)CC(C)(C)C1
 ExpValue: -2.4 -log(mg/l)
 Similarity: 0.6940000000000001



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



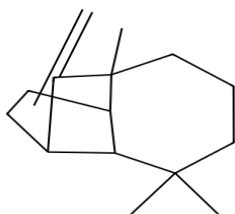
Smile: C=CC(C)(O)CCC=C(C)C
 ExpValue: -1.589 -log(mg/l)
 Similarity: 0.661



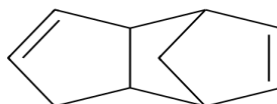
Descriptors

Calculator Similarity descriptor

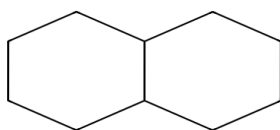
Smile: C=C1C2CCC3C2C(C)(C)CCCC13C
 ExpValue: -1.01 -log(mg/l)
 DistanceCityBlock: 0.324
 LogP: 4.415000000000004
 MW: 204.187800768



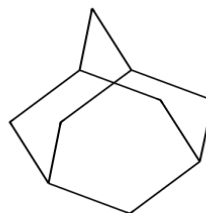
Smile: C1=CC2C3C=CC(C3)C2C1
 ExpValue: -1.771 -log(mg/l)
 DistanceCityBlock: 4.126
 LogP: 2.3846000000000007
 MW: 132.093900384



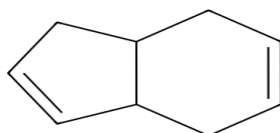
Smile: C1CCC2CCCCC2C1
 ExpValue: 0.433 -log(mg/l)
 DistanceCityBlock: 4.426
 LogP: 3.3668000000000022
 MW: 138.140850576



Smile: C1C2CC3CC1CC(C2)C3
 ExpValue: 0.553 -log(mg/l)
 DistanceCityBlock: 5.146
 LogP: 2.8326000000000001
 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

