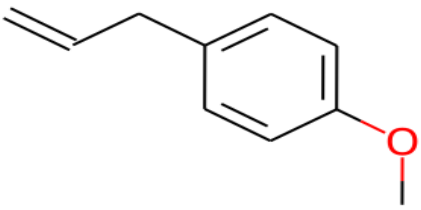
VERA: Similarity and Grouping:

CONCERTREACH
CONCERTING EXPERIMENTAL DATA AND IN SILICO MODELS FOR REACH



Molecule Input:

TotGroups: 5

['allylic_oxid', 'methoxy', 'benzCH2', 'Ar_OR', 'CH2_Terminal']

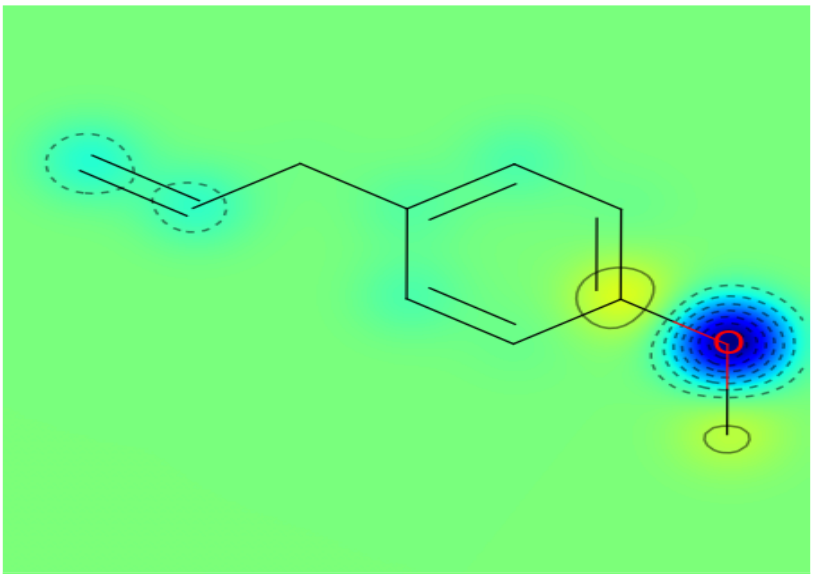
Structural Alers: f_SA38

LogP: 2.424
MaxPartialCharge: 0.118
MinPartialCharge: -0.497
NumHAcceptors: 1
NumHDonors: 0
NumRotatableBonds: 3
NumAliphaticRings: 0
NumAromaticCarbocycles: 1
NumAromaticHeterocycles: 0
NumAromaticRings: 1
ExactMolWt: 148.089

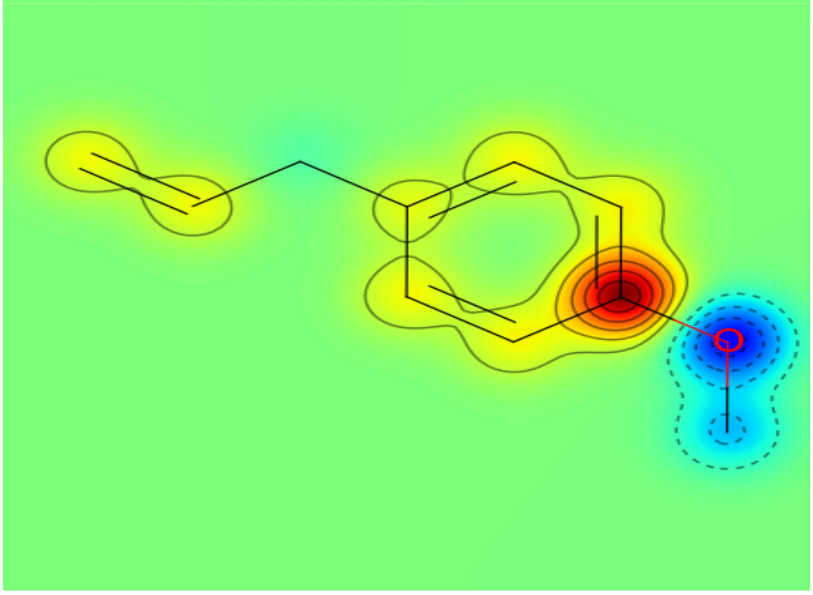
Experimental Value is known: Active

Prediction: Active***(5)

GasteigerCharges:



CrippenContribs:



Molecules with the highest group similarity

1) SMILES: C=CCc1ccc(OC)cc1

Class: Active

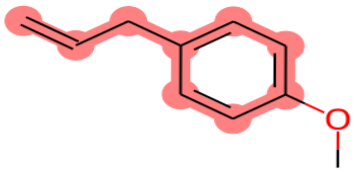
SimilarityVega: 1.0

SimilarityGrouping: 1.0

Grp_Similarity_Mean: 1.0

Groups in common: 5

TotGroups 5



GROUPS:
allylic_oxid Stat: Neutro
methoxy Stat: Neutro
benzCH2 Stat: Neutro
Ar_OR Stat: Neutro
CH2_Terminal Stat: Neutro
Alerts: ['f_SA38']

2) SMILES: C=CCc1ccc(O)c(OC)c1

Class: NON-Active

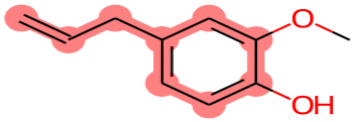
SimilarityVega: 0.896

SimilarityGrouping: 0.953

Grp_Similarity_Mean: 0.924

Groups in common: 5

TotGroups 8



GROUPS:
allylic_oxid Stat: Neutro
methoxy Stat: Neutro
phenol Stat: Neutro
phenol_noOrthoHbond Stat: Neutro
benzCH2 Stat: Neutro
Ar_OR Stat: Neutro
op_diphenolo_OR Stat: Neutro
CH2_Terminal Stat: Neutro
Alerts: ['f_SA38']

3) SMILES: C=CCc1ccc(OC)c(OC)c1

Class: Active

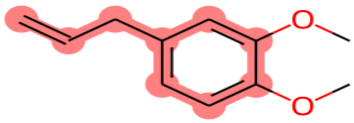
SimilarityVega: 0.896

SimilarityGrouping: 0.953

Grp_Similarity_Mean: 0.924

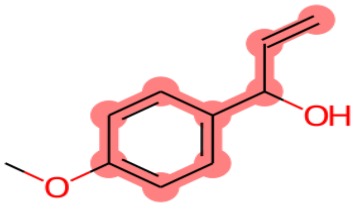
Groups in common: 5

TotGroups 8

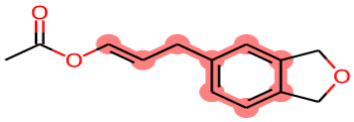


GROUPS:
allylic_oxid Stat: Neutro
methoxy Stat: Neutro
benzCH2 Stat: Neutro
Ar_OR Stat: Neutro
op_diphenolo_OR Stat: Neutro
CH2_Terminal Stat: Neutro
Alerts: ['f_SA38']

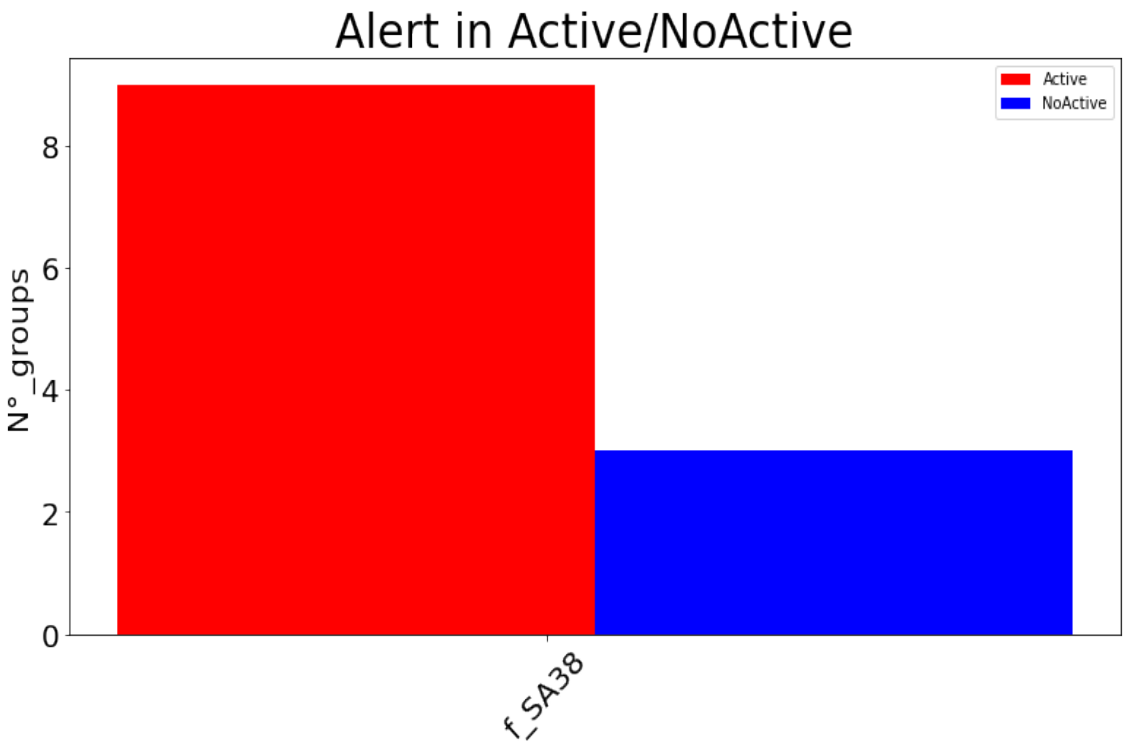
4) SMILES: C=CC(O)c1ccc(OC)cc1
Class: Active
SimilarityVega: 0.92
SimilarityGrouping: 0.769
Grp_Similarity_Mean: 0.844
Groups in common: 3
TotGroups 4
GROUPS:
Al_OH Stat: Neutro
methoxy Stat: Neutro
Ar_OR Stat: Neutro
CH2_Terminal Stat: Neutro
Alerts: ['f_SA38']

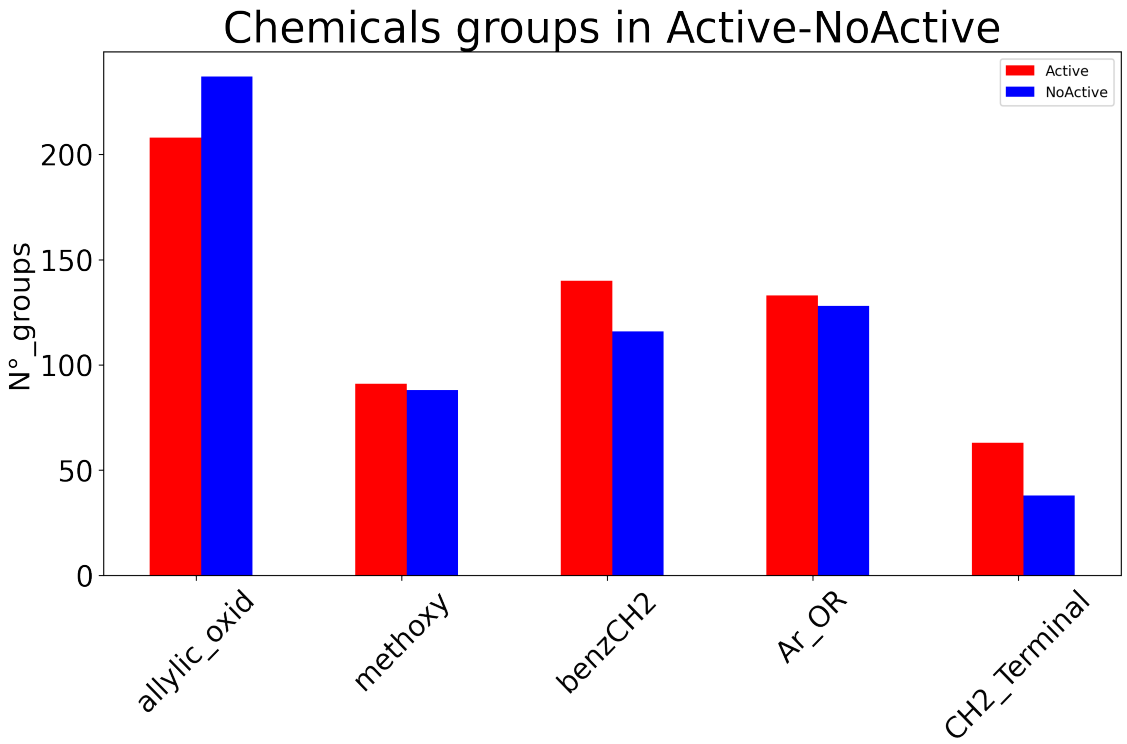


5) SMILES: CC(=O)OC=CCc1ccc2c(c1)COC2
Class: Active
SimilarityVega: 0.732
SimilarityGrouping: 0.617
Grp_Similarity_Mean: 0.674
Groups in common: 2
TotGroups 6
GROUPS:
allylic_oxid Stat: Neutro
bicyclic Stat: Neutro
ester Stat: Neutro
benzCH2 Stat: Neutro
Alerts: ['f_SA38']



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

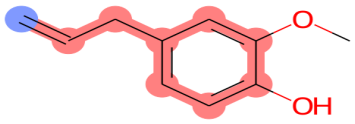




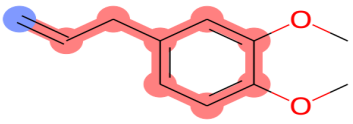
Reasoning

Ortogonal Research based on copresence of alerts ['f_SA38'] and GRP allylic_oxid

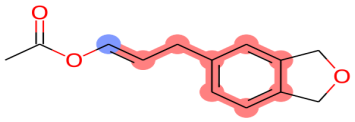
Smile: C=CCc1ccc(O)c(OC)c1
Class: NON-Active
Similarity: 0.896



Smile: C=CCc1ccc(OC)c(OC)c1
Class: Active
Similarity: 0.896



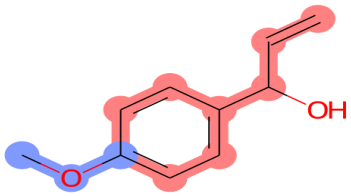
Smile: CC(=O)OC=CCc1ccc2c(c1)COC2
Class: Active
Similarity: 0.732



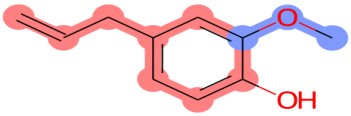
Reasoning

Ortogonal Research based on copresence of alerts ['f_SA38'] and GRP methoxy

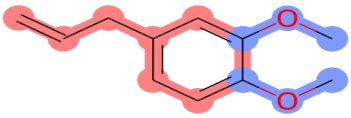
Smile: C=CC(O)c1ccc(OC)cc1
Class: Active
Similarity: 0.92



Smile: C=CCc1ccc(O)c(OC)c1
Class: NON-Active
Similarity: 0.896



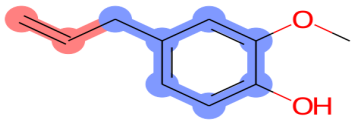
Smile: C=CCc1ccc(OC)c(OC)c1
Class: Active
Similarity: 0.896



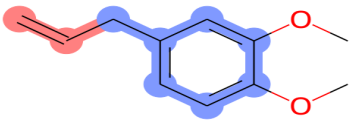
Reasoning

Ortogonal Research based on copresence of alerts ['f_SA38'] and GRP benzCH2

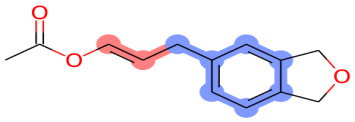
Smile: C=CCc1ccc(O)c(OC)c1
Class: NON-Active
Similarity: 0.896



Smile: C=CCc1ccc(OC)c(OC)c1
Class: Active
Similarity: 0.896



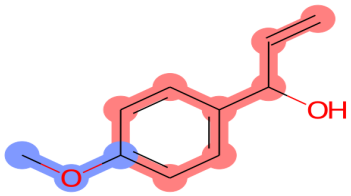
Smile: CC(=O)OC=CCc1ccc2c(c1)COC2
Class: Active
Similarity: 0.732



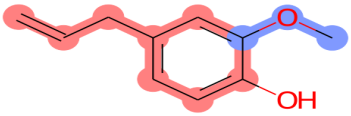
Reasoning

Ortogonal Research based on copresence of alerts ['f_SA38'] and GRP Ar_OR

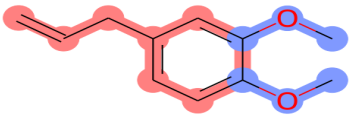
Smile: C=CC(O)c1ccc(OC)cc1
Class: Active
Similarity: 0.92



Smile: C=CCc1ccc(O)c(OC)c1
Class: NON-Active
Similarity: 0.896



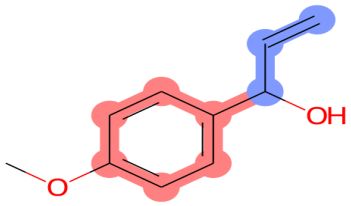
Smile: C=CCc1ccc(OC)c(OC)c1
Class: Active
Similarity: 0.896



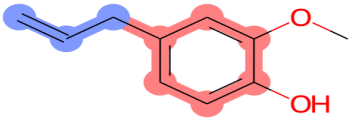
Reasoning

Ortogonal Research based on copresence of alerts ['f_SA38'] and GRP CH2_Terminal

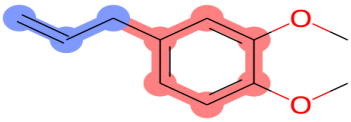
Smile: C=CC(O)c1ccc(OC)cc1
Class: Active
Similarity: 0.92



Smile: C=CCc1ccc(O)c(OC)c1
Class: NON-Active
Similarity: 0.896

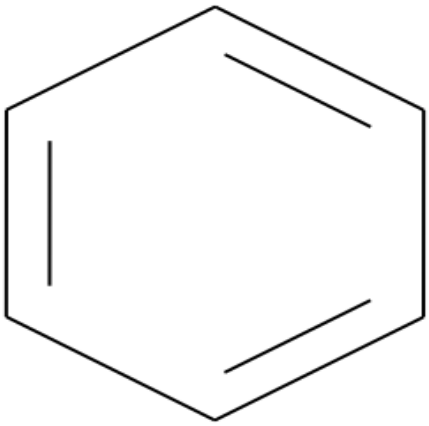


Smile: C=CCc1ccc(OC)c(OC)c1
Class: Active
Similarity: 0.896

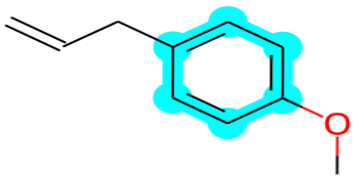


Scaffold

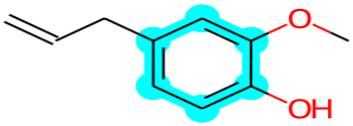
Scaffold analysis



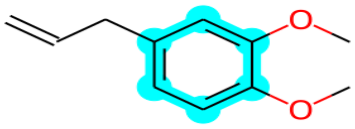
Smile: C=CCc1ccc(OC)cc1
Class: Active
Similarity: 1.0



Smile: C=CCc1ccc(O)c(OC)c1
Class: NON-Active
Similarity: 0.896



Smile: C=CCc1ccc(OC)c(OC)c1
Class: Active
Similarity: 0.896



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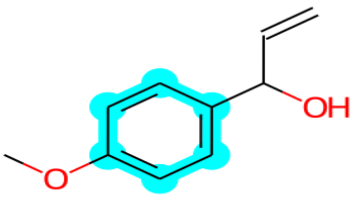
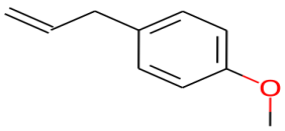


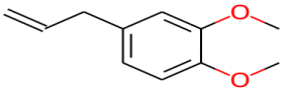
Descriptors

Calculator Similarity descriptor

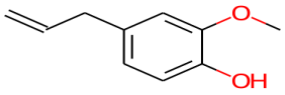
Smile: C=CCc1ccc(OC)cc1
Class: Active
DistanceCityBlock: 0.0
LogP:2.4237
MW: 148.088815004



Smile: C=CCc1ccc(OC)c(OC)c1
Class: Active
DistanceCityBlock: 6.239
LogP:2.4323000000000006
MW: 178.099379688



Smile: C=CCc1ccc(O)c(OC)c1
Class: NON-Active
DistanceCityBlock: 6.718
LogP:2.1292999999999997
MW: 164.083729624



Smile: C=CC(O)c1ccc(OC)cc1
Class: Active
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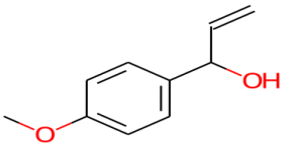
LogP:1.9145999999999999
MW: 164.083729624



Smile: CC(=O)OC=CCc1ccc2c(c1)COC2
Class: Active
DistanceCityBlock: 14.436
LogP:2.3361
MW: 218.094294308