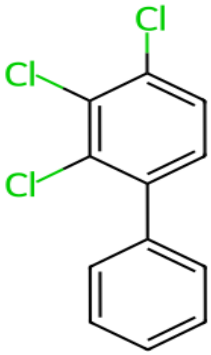
VERA: Similarity and Grouping:

PREMIER
PRIORITISATION AND RISK EVALUATION
OF MEDICINES IN THE ENVIRONMENT



Molecule Input:

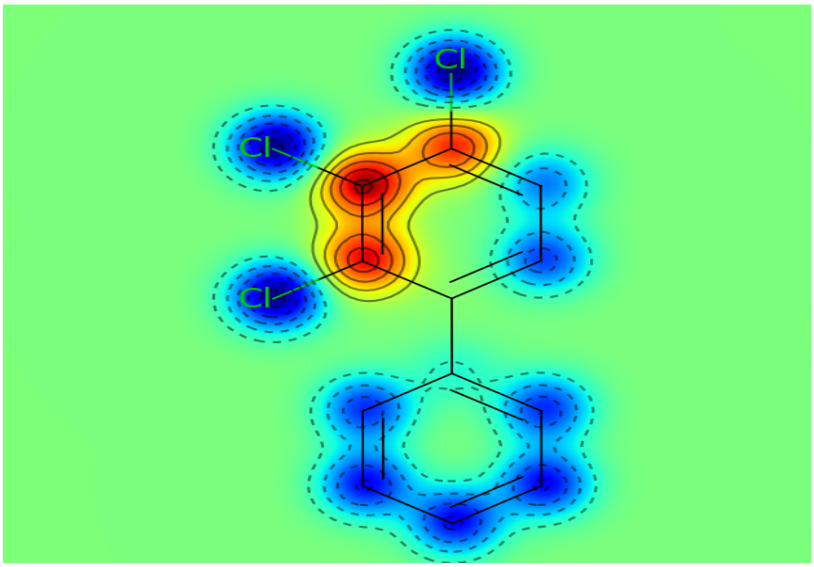
TotGroups: 2

['benzene', 'Ar_Cl_Br']

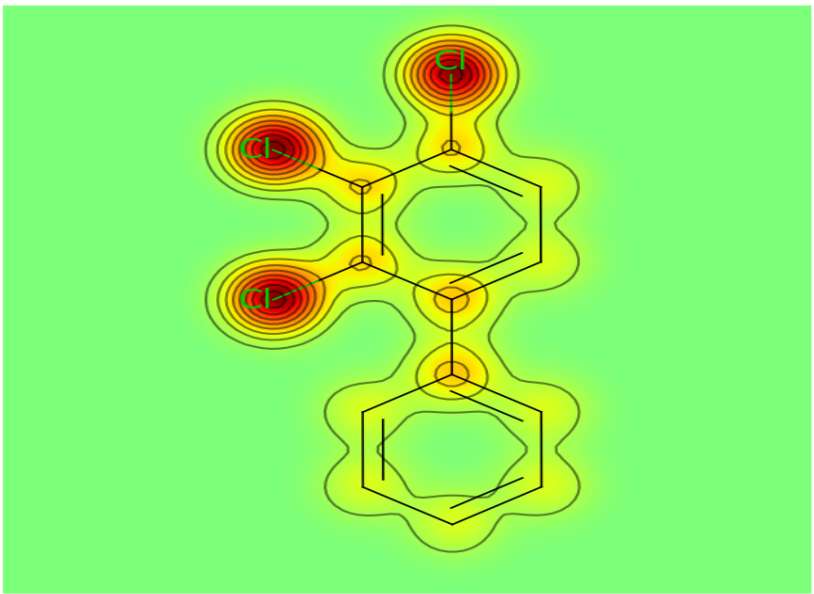
LogP: 5.314
MaxPartialCharge: 0.078
MinPartialCharge: -0.083
NumHAcceptors: 0
NumHDonors: 0
NumRotatableBonds: 1
NumAliphaticRings: 0
NumAromaticCarbocycles: 2
NumAromaticHeterocycles: 0
NumAromaticRings: 2
ExactMolWt: 255.961

Prediction from Linear model: 0.048 -log(mg/l)

GasteigerCharges:



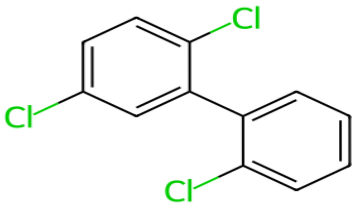
CrippenContribs:

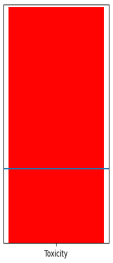


Molecules with the highest group similarity

1) SMILES: Clc1ccc(Cl)c(-c2ccccc2Cl)c1
ExpValue: 1.472 -log(mg/l)
SimilarityVega: 0.975
SimilarityGrouping: 0.875
Grp_Similarity_Mean: 0.925
Groups in common: 3
TotGroups 3

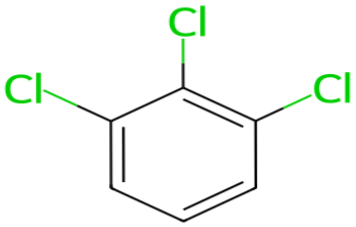
GROUPS:
Ar_Cl_Br Stat: Tox
Alerts: []

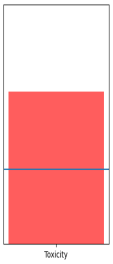




2) SMILES: Clc1cccc(Cl)c1Cl
ExpValue: -0.338 -log(mg/l)
SimilarityVega: 0.781
SimilarityGrouping: 0.875
Grp_Similarity_Mean: 0.828
Groups in common: 3
TotGroups 3

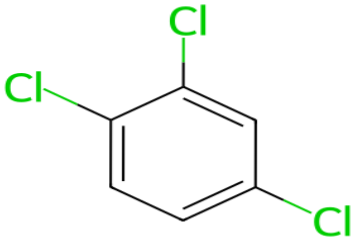
GROUPS:
Ar_Cl_Br Stat: Tox
Alerts: []



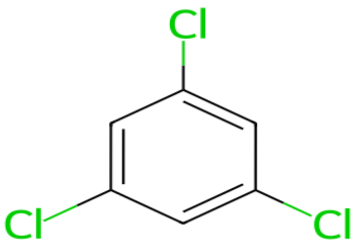


3) SMILES: Clc1ccc(Cl)c(Cl)c1
ExpValue: -0.412 -log(mg/l)
SimilarityVega: 0.78
SimilarityGrouping: 0.875
Grp_Similarity_Mean: 0.828
Groups in common: 3
TotGroups 3

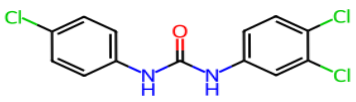
GROUPS:
Ar_Cl_Br Stat: Tox
Alerts: []

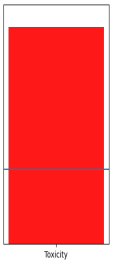


4) SMILES: Clc1cc(Cl)cc(Cl)c1
ExpValue: -0.512 -log(mg/l)
SimilarityVega: 0.773
SimilarityGrouping: 0.875
Grp_Similarity_Mean: 0.824
Groups in common: 3
TotGroups 3
GROUPS:
Ar_Cl_Br Stat: Tox
Alerts: []

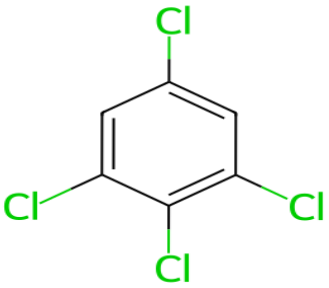


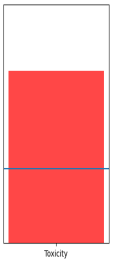
5) SMILES: O=C(Nc1ccc(Cl)cc1)Nc1ccc(Cl)c(Cl)c1
ExpValue: 1.043 -log(mg/l)
SimilarityVega: 0.76
SimilarityGrouping: 0.844
Grp_Similarity_Mean: 0.802
Groups in common: 3
TotGroups 4
GROUPS:
urea Stat: Tox
Ar_Cl_Br Stat: Tox
Alerts: []



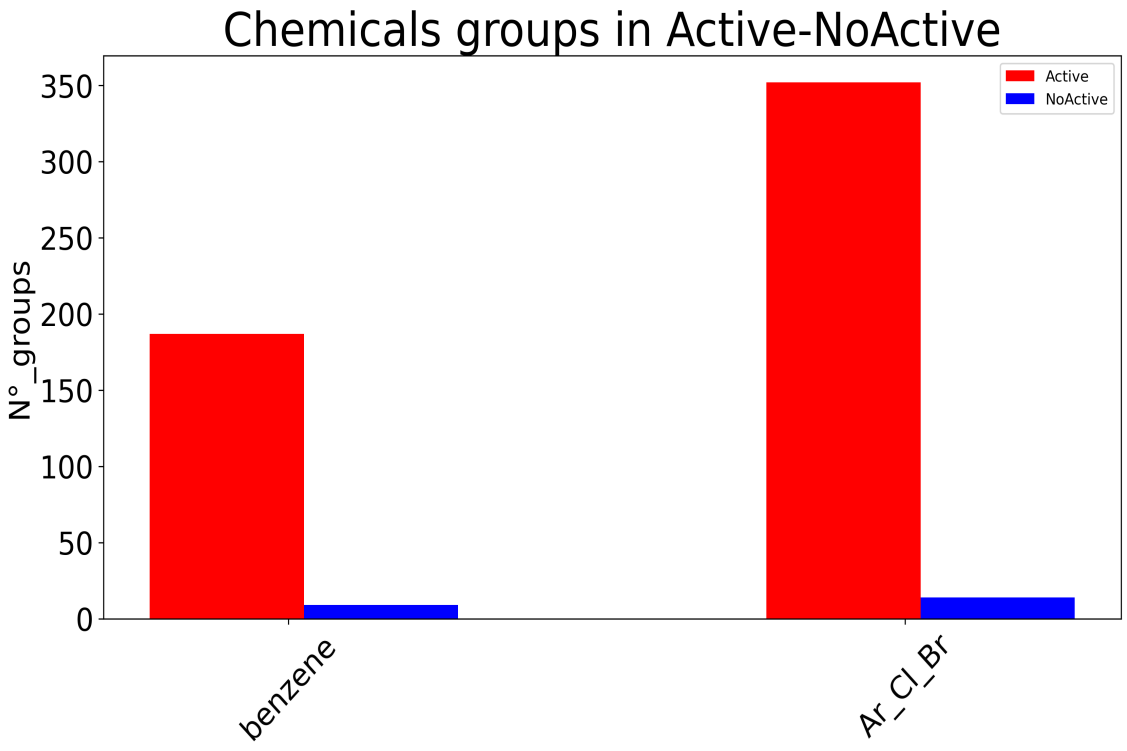


6) SMILES: Clc1cc(Cl)c(Cl)c(Cl)c1
ExpValue: 0.098 -log(mg/l)
SimilarityVega: 0.758
SimilarityGrouping: 0.844
Grp_Similarity_Mean: 0.801
Groups in common: 3
TotGroups 4
GROUPS:
Ar_Cl_Br Stat: Tox
Alerts: []





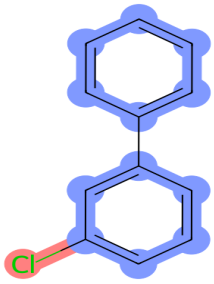
Molecule Input: Bar Chart for groups in Dataset find in target



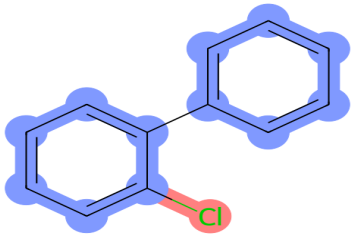
Reasoning

Ortogonal Research based on copresence of group with high prevalence Ar_Cl_Br and GRP benzene

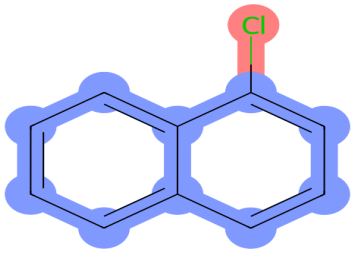
Smile: Clc1cccc(-c2ccccc2)c1
ExpValue: -0.894 -log(mg/l)
Similarity: 0.864



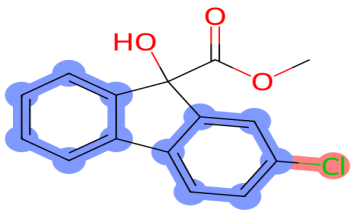
Smile: Clc1ccccc1-c1ccccc1
ExpValue: -0.604 -log(mg/l)
Similarity: 0.864



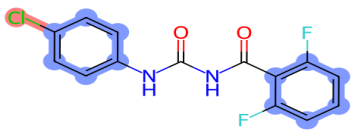
Smile: Clc1cccc2ccccc12
ExpValue: -0.23 -log(mg/l)
Similarity: 0.761



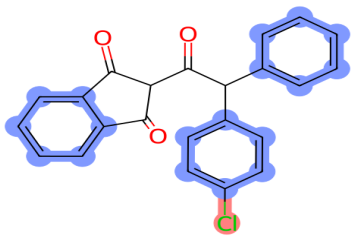
Smile: COC(=O)C1(O)c2ccccc2-c2ccc(Cl)cc21
ExpValue: -0.158 -log(mg/l)
Similarity: 0.749



Smile: O=C(NC(=O)c1c(F)cccc1F)Nc1ccc(Cl)cc1
ExpValue: -2.631 -log(mg/l)
Similarity: 0.722

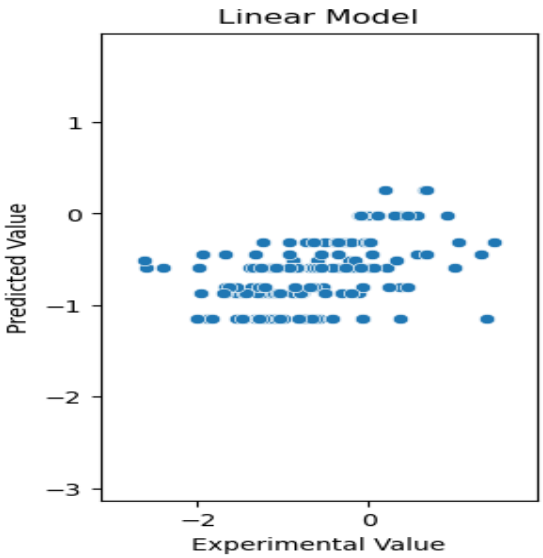


Smile:
O=C1c2ccccc2C(=O)C1C(=O)C(c1ccccc1)c1ccc(Cl)cc1
ExpValue: 0.328 -log(mg/l)
Similarity: 0.678



Local Linear Model

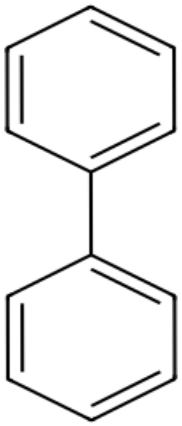
The target assessment was made by using Linear model model not by this Local model



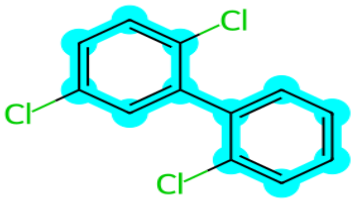
Mean square error: 0.46

Scaffold

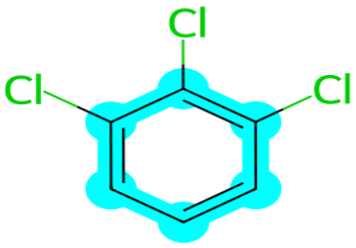
Scaffold analysis



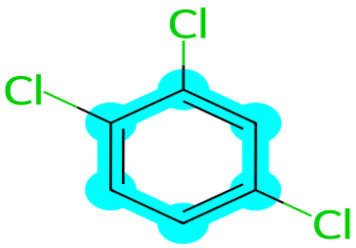
Smile: Clc1ccc(Cl)c(-c2ccccc2Cl)c1
ExpValue: 1.472 -log(mg/l)
Similarity: 0.975



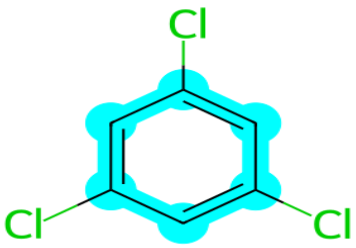
Smile: Clc1cccc(Cl)c1Cl
ExpValue: -0.338 -log(mg/l)
Similarity: 0.781



Smile: Clc1ccc(Cl)c(Cl)c1
ExpValue: -0.412 -log(mg/l)
Similarity: 0.78



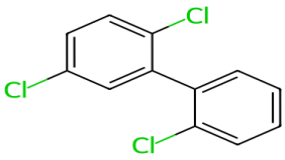
Smile: Clc1cc(Cl)cc(Cl)c1
ExpValue: -0.512 -log(mg/l)
Similarity: 0.773



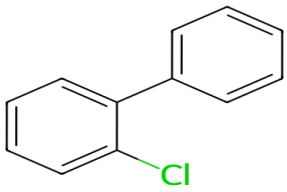
Descriptors

Calculator Similarity descriptor

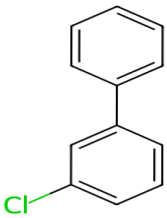
Smile: Clc1ccc(Cl)c(-c2ccccc2Cl)c1
ExpValue: 1.472 -log(mg/l)
DistanceCityBlock: 0.285
LogP:5.313800000000002
MW: 255.961333264



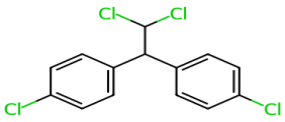
Smile: Clc1ccccc1-c1ccccc1
ExpValue: -0.604 -log(mg/l)
DistanceCityBlock: 2.931
LogP:4.007000000000002
MW: 188.039277968



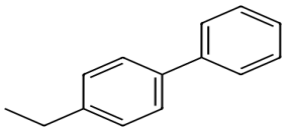
Smile: Clc1cccc(-c2ccccc2)c1
ExpValue: -0.894 -log(mg/l)
DistanceCityBlock: 3.002
LogP:4.007000000000002
MW: 188.039277968



Smile: Clc1ccc(C(c2ccc(Cl)cc2)C(Cl)Cl)cc1
ExpValue: -0.642 -log(mg/l)
DistanceCityBlock: 3.631
LogP:5.929000000000002
MW: 317.95366104



Smile: CCc1ccc(-c2ccccc2)cc1
ExpValue: 0.223 -log(mg/l)
DistanceCityBlock: 4.554
LogP:3.916000000000002
MW: 182.109550448



Smile: Clc1cccc2ccccc12
ExpValue: -0.23 -log(mg/l)
DistanceCityBlock: 4.638
LogP:3.4932000000000016
MW: 162.023627904