**Supplementary figures**

Figure S1

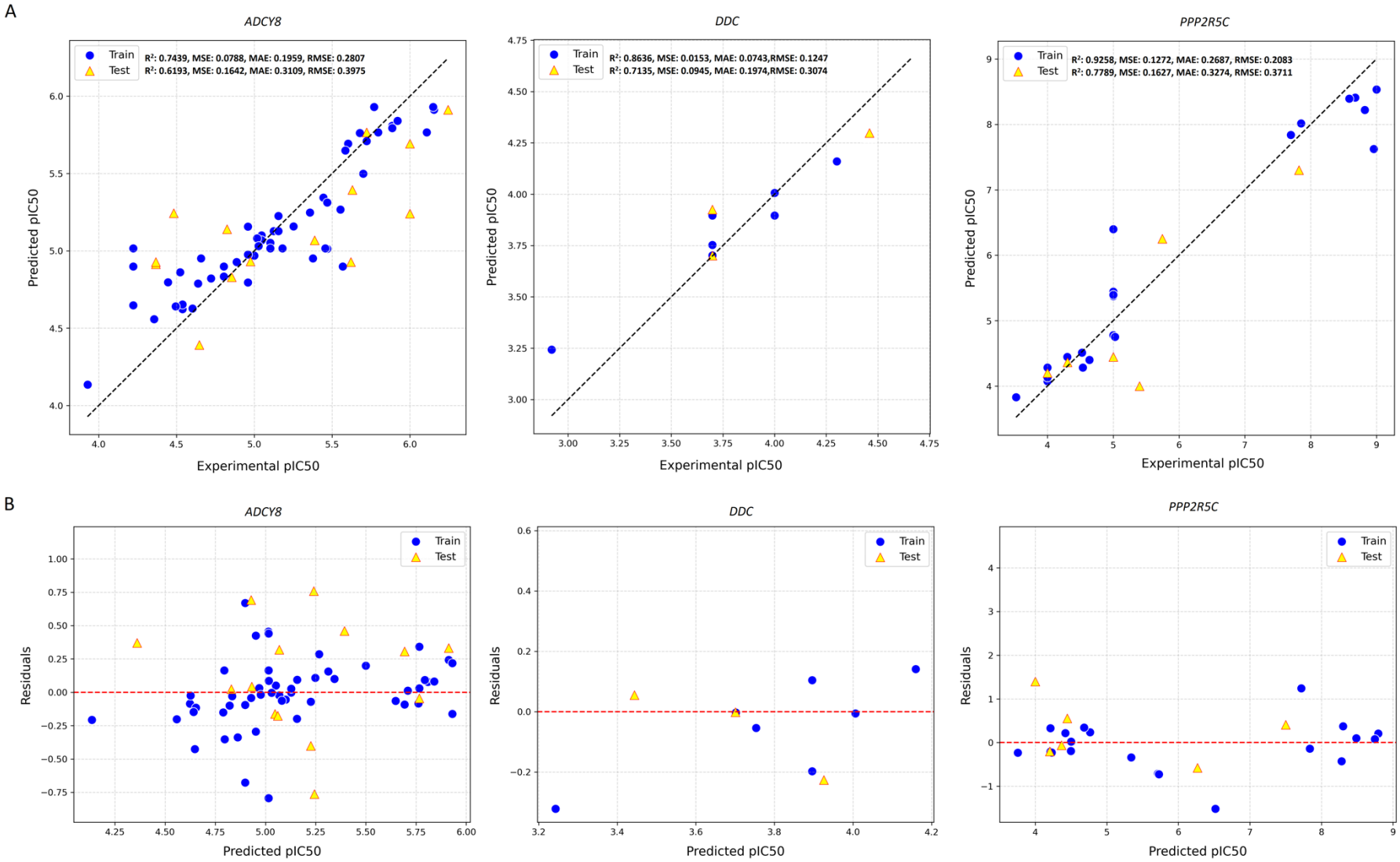

A
ADCY8
Train
Test
R²: 0.7439, MSE: 0.0788, MAE: 0.1959, RMSE: 0.2807
R²: 0.6193, MSE: 0.1642, MAE: 0.3109, RMSE: 0.3975
Predicted pIC50
Experimental pIC50
DDC
R²: 0.8636, MSE: 0.0153, MAE: 0.0743,RMSE: 0.1247
R²: 0.7135, MSE: 0.0945, MAE: 0.1974,RMSE: 0.3074
PPP2R5C
R²: 0.9258, MSE: 0.1272, MAE: 0.2687, RMSE: 0.2083
R²: 0.7789, MSE: 0.1627, MAE: 0.3274, RMSE: 0.3711
B
Residuals
Predicted pIC50

Figure S2

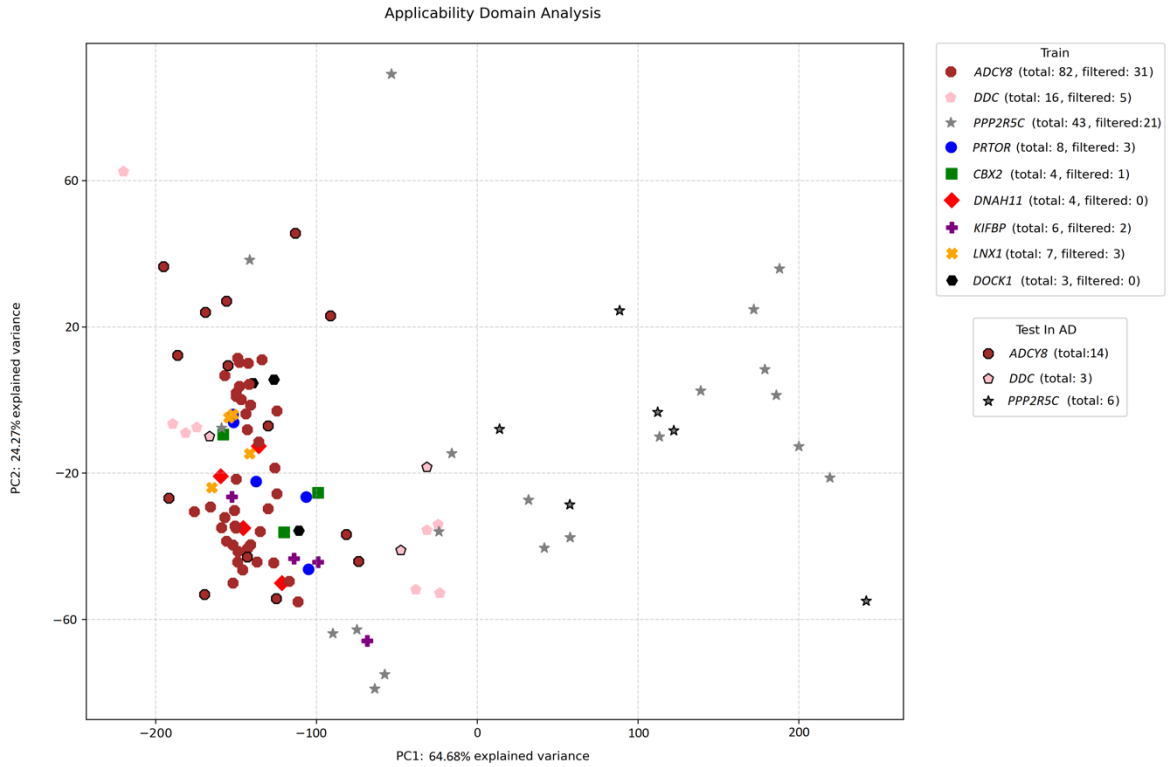

Applicability Domain Analysis
PC2: 24.27% explained variance
PC1: 64.68% explained variance
60
20
−20
−60
−200
−100
0
100
200
Train
ADCY8 (total: 82, filtered: 31)
DDC (total: 16, filtered: 5)
PPP2R5C (total: 43, filtered:21)
PRTOR (total: 8, filtered: 3)
CBX2 (total: 4, filtered: 1)
DNAH11 (total: 4, filtered: 0)
KIFBP (total: 6, filtered: 2)
LNX1 (total: 7, filtered: 3)
DOCK1 (total: 3, filtered: 0)
Test In AD
ADCY8 (total:14)
DDC (total: 3)
PPP2R5C (total: 6)

Figure S3

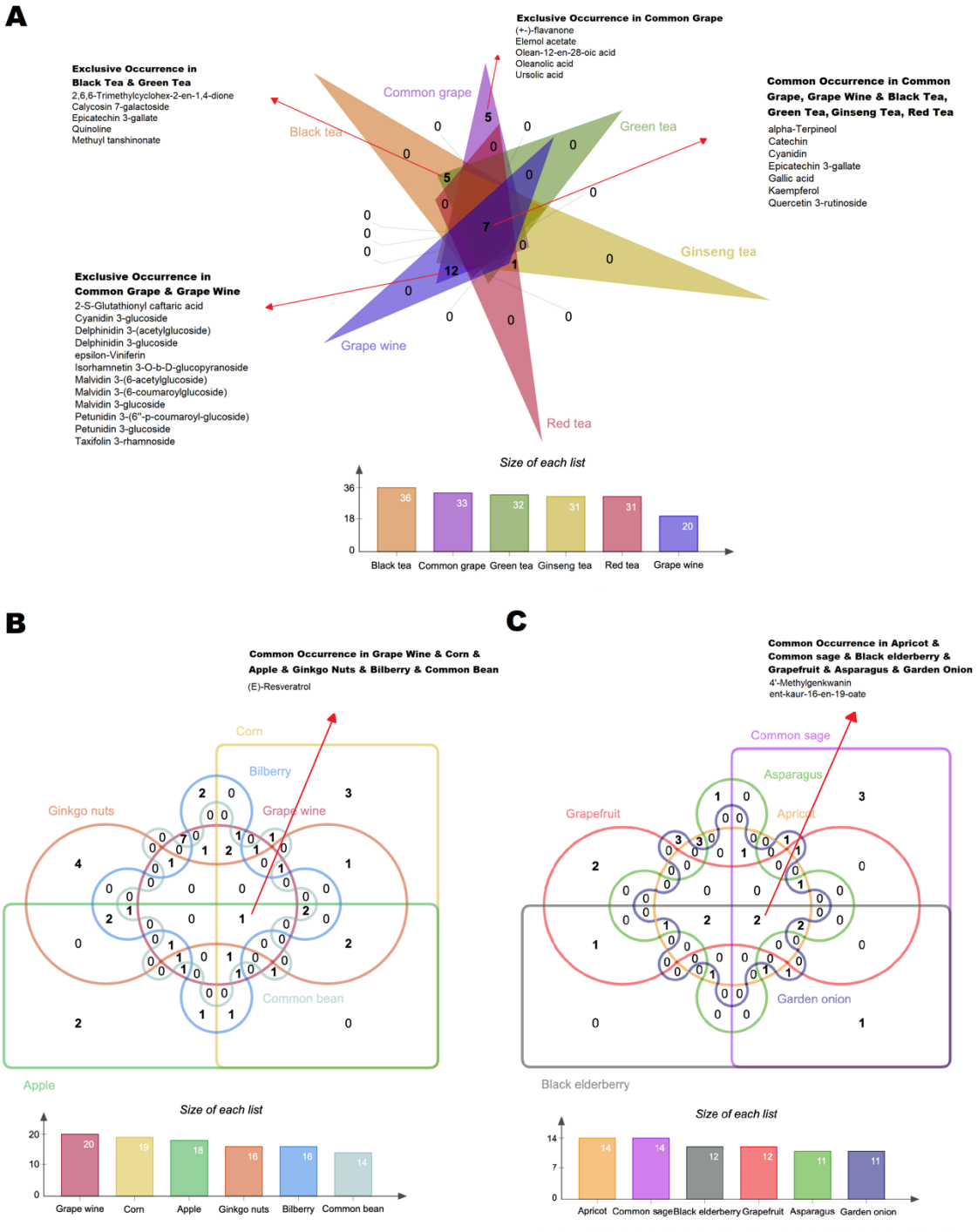

A
Exclusive Occurrence in Common Grape
(+-)-flavanone
Elemol acetate
Olean-12-en-28-oic acid
Oleanolic acid
Ursolic acid
Exclusive Occurrence in Black Tea & Green Tea
2,6,6-Trimethylcyclohex-2-en-1,4-dione
Calycosin 7-galactoside
Epicatechin 3-gallate
Quinoline
Methuyl tanshinonate
Common Occurrence in Common Grape, Grape Wine & Black Tea, Green Tea, Ginseng Tea, Red Tea
alpha-Terpineol
Catechin
Cyanidin
Epicatechin 3-gallate
Gallic acid
Kaempferol
Quercetin 3-rutinoside
Exclusive Occurrence in Common Grape & Grape Wine
2-S-Glutathionyl caftaric acid
Cyanidin 3-glucoside
Delphinidin 3-(acetylglucoside)
Delphinidin 3-glucoside
epsilon-Viniferin
Isorhamnetin 3-O-b-D-glucopyranoside
Malvidin 3-(6-acetylglucoside)
Malvidin 3-(6-coumaroylglucoside)
Malvidin 3-glucoside
Petunidin 3-(6''-p-coumaroyl-glucoside)
Petunidin 3-glucoside
Taxifolin 3-rhamnoside
Common grape
Black tea
Green tea
Ginseng tea
Grape wine
Red tea
Size of each list
Black tea
Common grape
Green tea
Ginseng tea
Red tea
Grape wine
B
Common Occurrence in Grape Wine & Corn & Apple & Ginkgo Nuts & Bilberry & Common Bean
(E)-Resveratrol
Corn
Bilberry
Ginkgo nuts
Grape wine
Common bean
Apple
Size of each list
Grape wine
Corn
Apple
Ginkgo nuts
Bilberry
Common bean
C
Common Occurrence in Apricot & Common sage & Black elderberry & Grapefruit & Asparagus & Garden Onion
4'-Methylgenkwanin
ent-kaur-16-en-19-oate
Common sage
Asparagus
Grapefruit
Apricot
Garden onion
Black elderberry
Size of each list
Apricot
Common sage
Black elderberry
Grapefruit
Asparagus
Garden onion

Figure S4

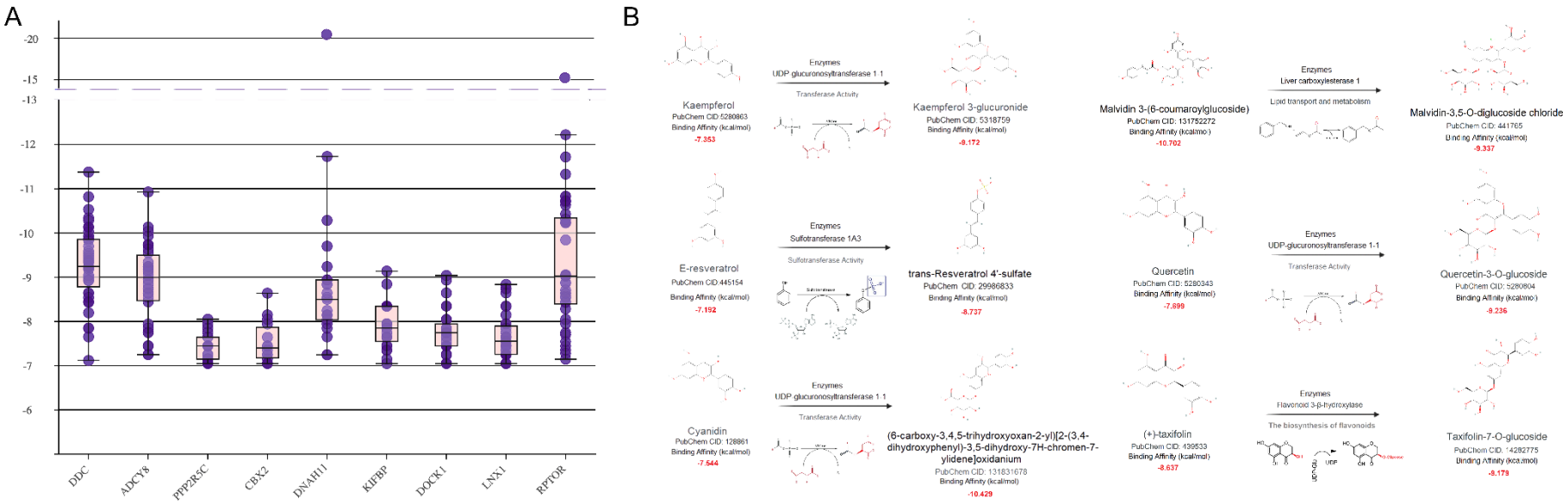

A
-20
-15
-13
-12
-11
-10
-9
-8
-7
-6
DDC
ADCY8
PPP2R5C
CBX2
DNAH11
KIFBP
DOCK1
LNX1
RPTOR
B
Kaempferol
PubChem CID:5280863
Binding Affinity (kcal/mol)
-7.353
Enzymes
UDP glucuronosyltransferase 1 1
Transferase Activity
Kaempferol 3-glucuronide
PubChem CID: 5318759
Binding Affinity (kcal/mol)
-9.172
Malvidin 3-(6-coumaroyl)glucoside)
PubChem CID: 131752272
Binding Affinity (kcal/mol)
-10.702
Enzymes
Liver carboxylesterase 1
Lipid transport and metabolism
Malvidin-3,5-O-diglucoside chloride
PubChem CID: 441765
Binding Affinity (kcal/mol)
-9.337
E-resveratrol
PubChem CID:445154
Binding Affinity (kcal/mol)
-7.192
Enzymes
Sulfotransferase 1A3
Sulfotransferase Activity
trans-Resveratrol 4'-sulfate
PubChem CID: 29986833
Binding Affinity (kcal/mol)
-8.737
Quercetin
PubChem CID: 5280343
Binding Affinity (kcal/mol)
-7.699
Enzymes
UDP-glucuronosyltransferase 1-1
Transferase Activity
Quercetin-3-O-glucoside
PubChem CID: 5280804
Binding Affinity (kcal/mol)
-9.236
Cyanidin
PubChem CID: 128861
Binding Affinity (kcal/mol)
-7.544
Enzymes
UDP glucuronosyltransferase 1 1
Transferase Activity
(6-carboxy-3,4,5-trihydroxyoxan-2-yl)[2-(3,4-dihydroxyphenyl)-3,5-dihydroxy-7H-chromen-7-ylidene]oxidanium
PubChem CID: 131831678
Binding Affinity (kcal/mol)
-10.429
(+)-taxifolin
PubChem CID: 439533
Binding Affinity (kcal/mol)
-8.637
Enzymes
Flavonoid 3-β-hydroxylase
The biosynthesis of flavonoids
Taxifolin-7-O-glucoside
PubChem CID: 14282775
Binding Affinity (kcal/mol)
-8.178

Figure S5

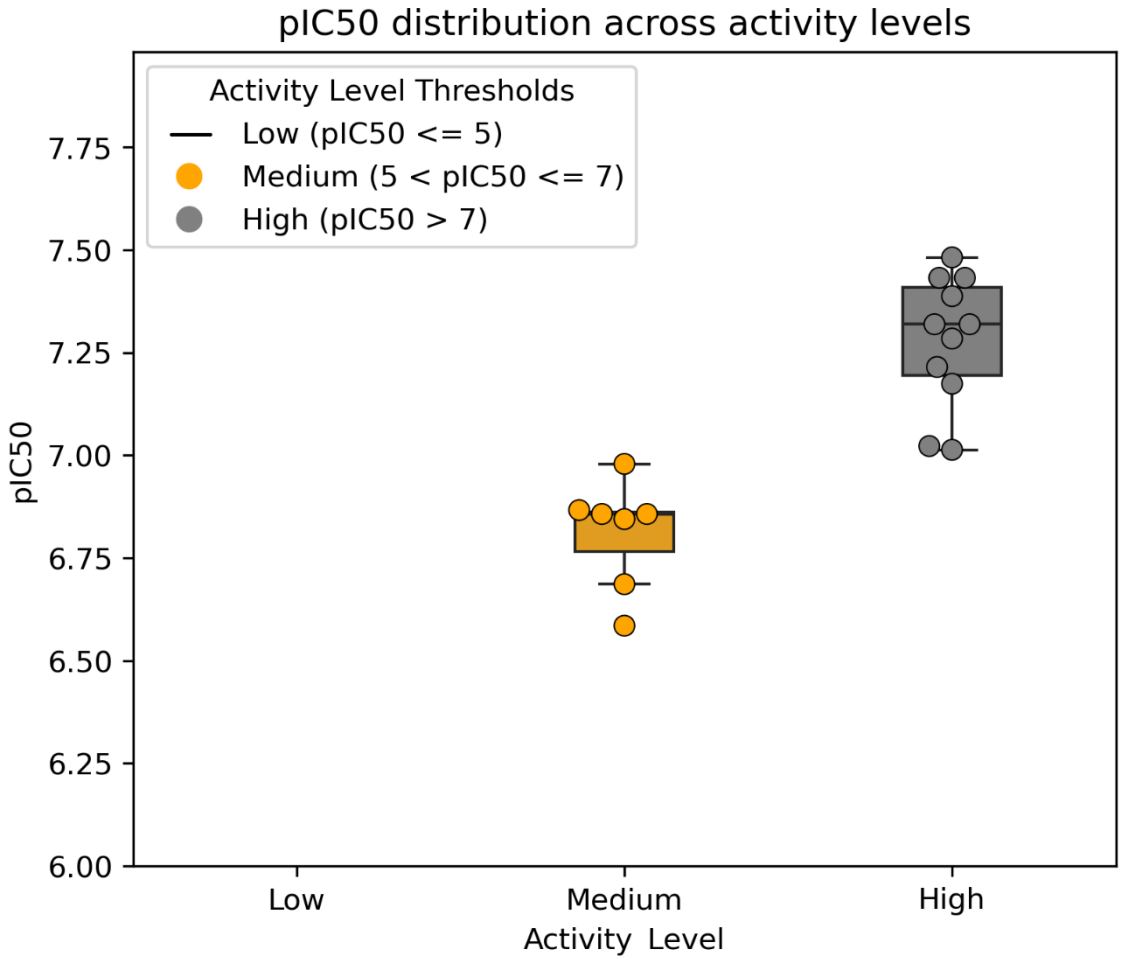
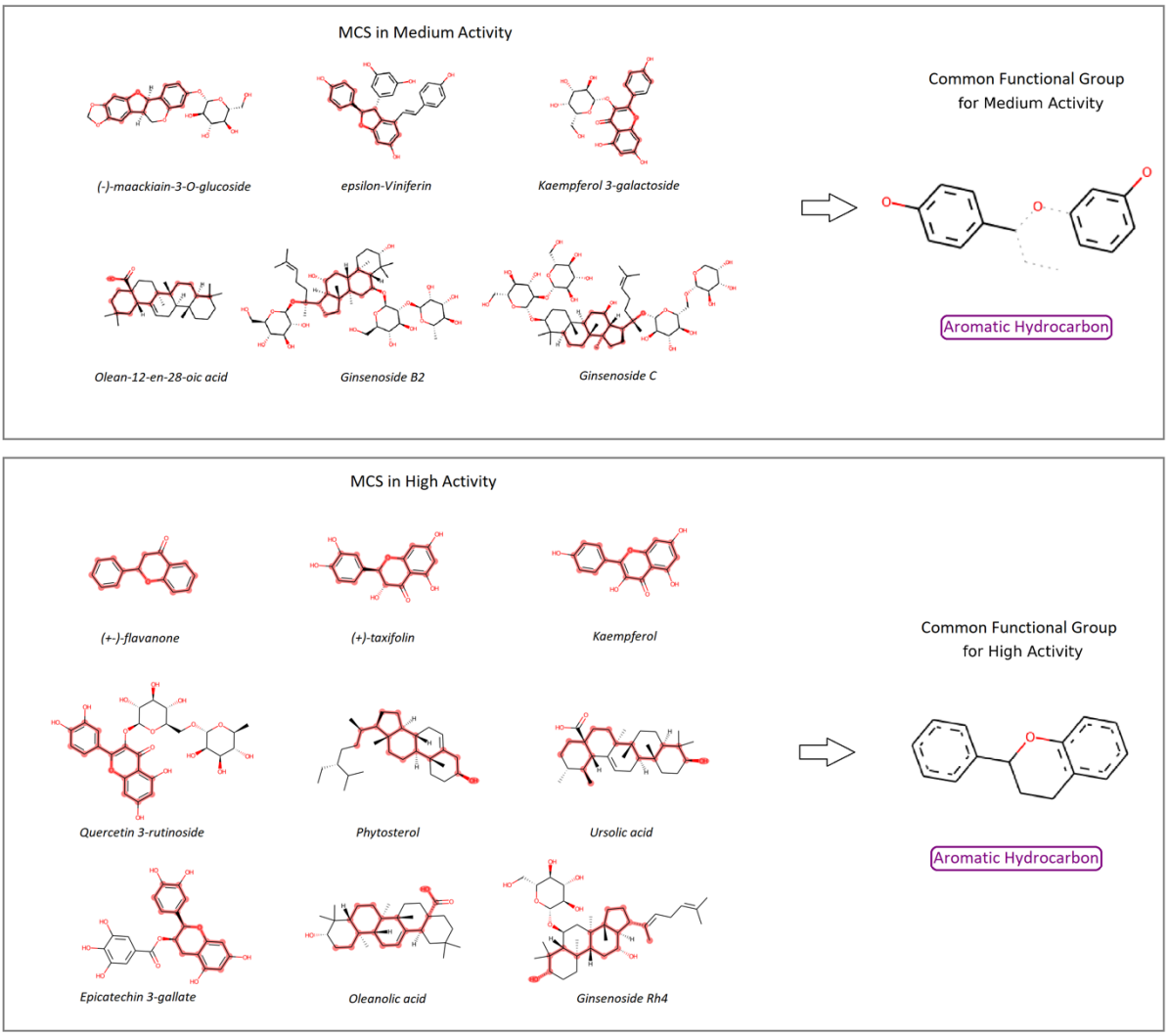

pIC50 distribution across activity levels
Activity Level Thresholds
Low (pIC50 <= 5)
Medium (5 < pIC50 <= 7)
High (pIC50 > 7)
pIC50
7.75
7.50
7.25
7.00
6.75
6.50
6.25
6.00
Low
Medium
High
Activity Level

Figure S6


MCS in Medium Activity
(-)-maackiain-3-O-glucoside
epsilon-Viniferin
Kaempferol 3-galactoside
Olean-12-en-28-oic acid
Ginsenoside B2
Ginsenoside C
Common Functional Group
for Medium Activity
Aromatic Hydrocarbon
MCS in High Activity
(+-)-flavanone
(+)-taxifolin
Kaempferol
Quercetin 3-rutinoside
Phytosterol
Ursolic acid
Epicatechin 3-gallate
Oleanolic acid
Ginsenoside Rh4
Common Functional Group
for High Activity
Aromatic Hydrocarbon