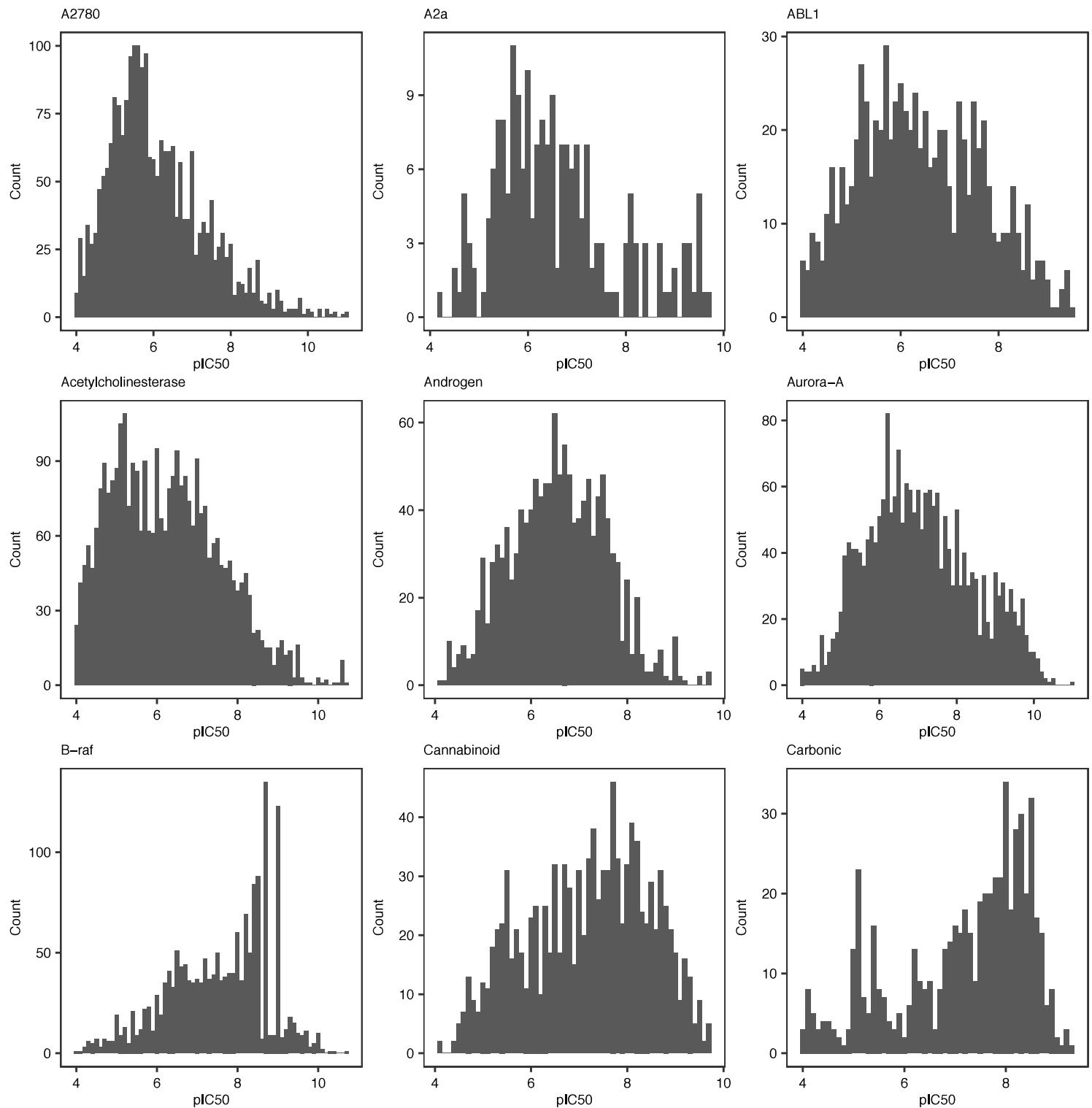
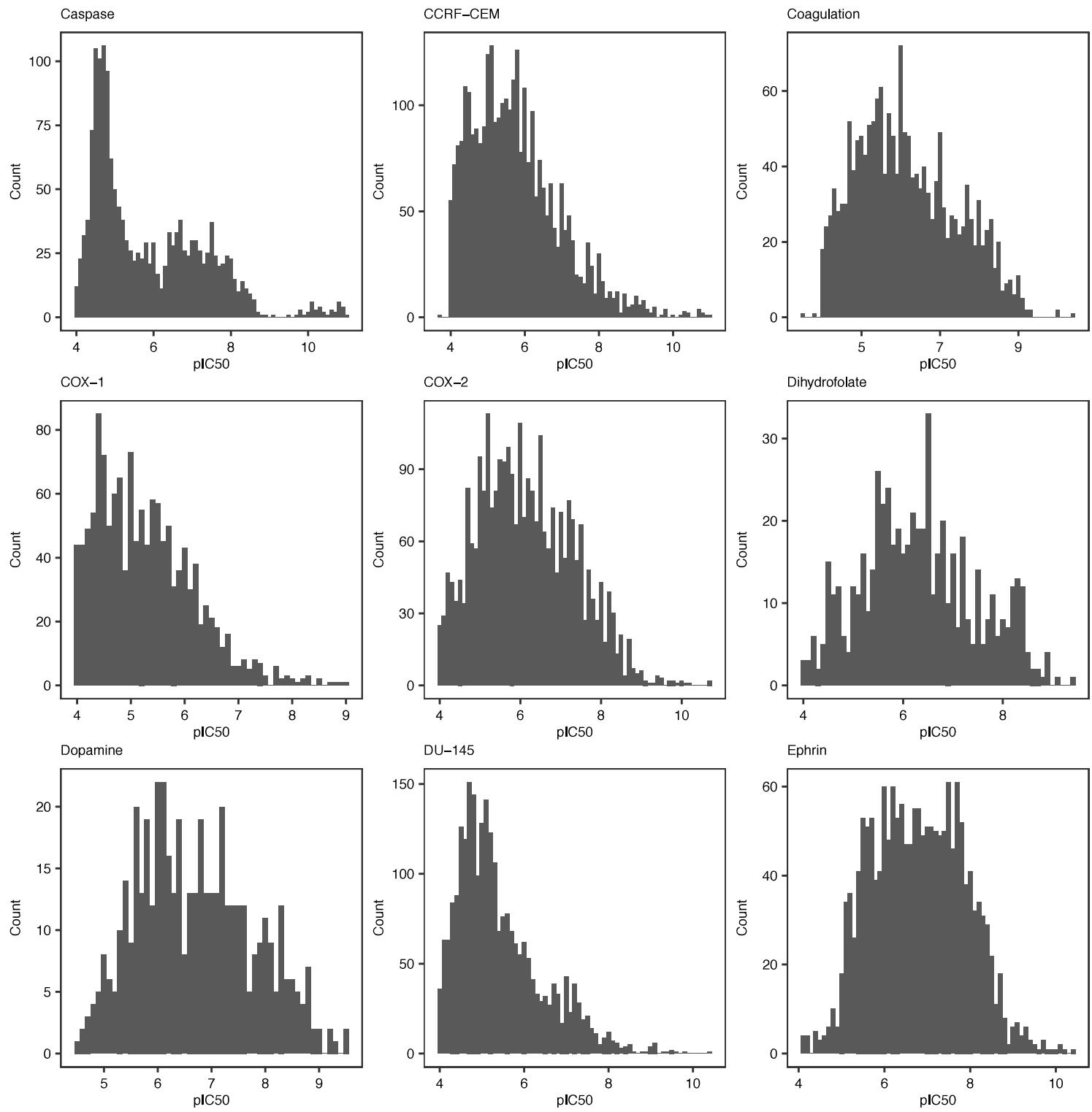
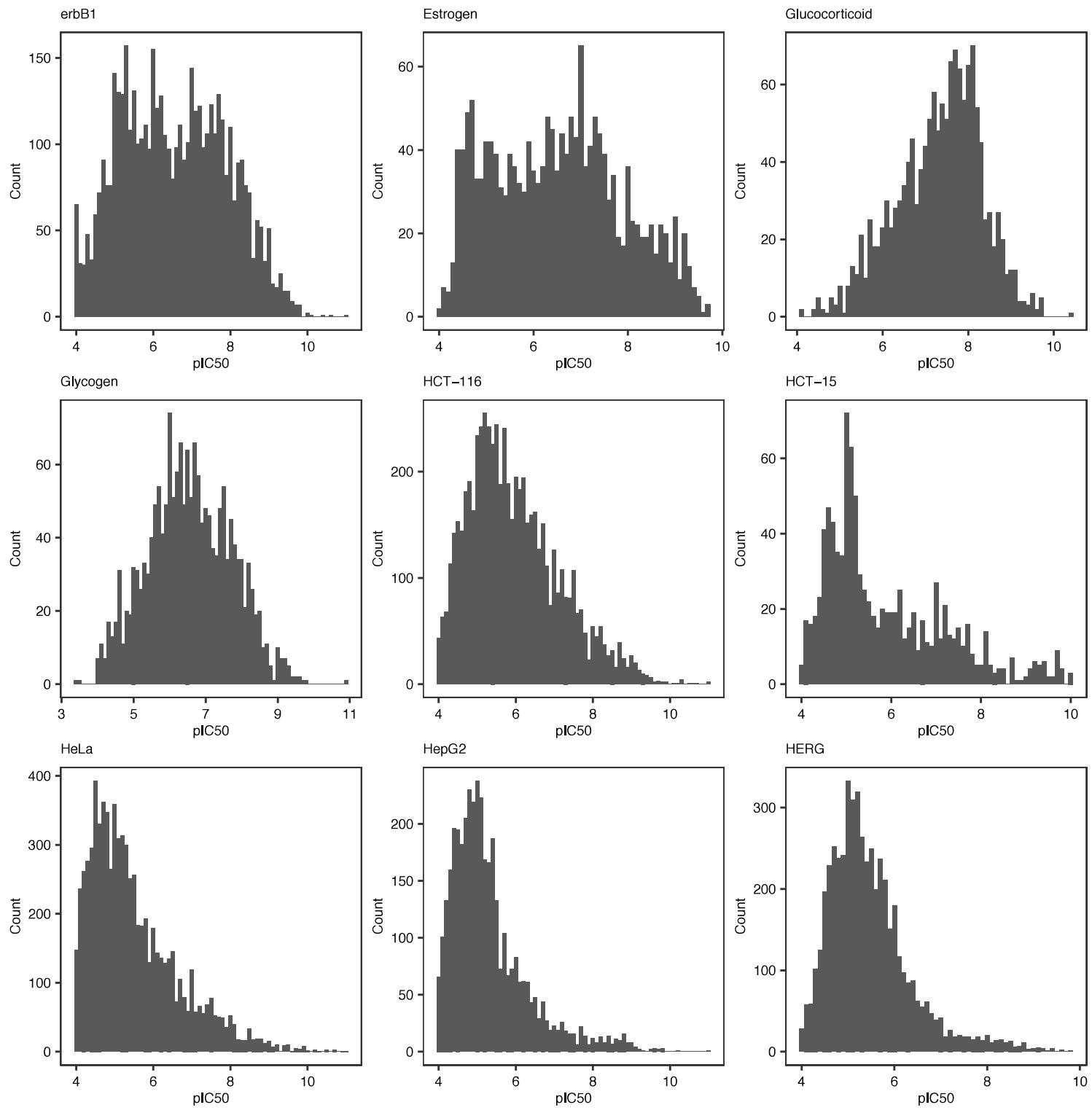
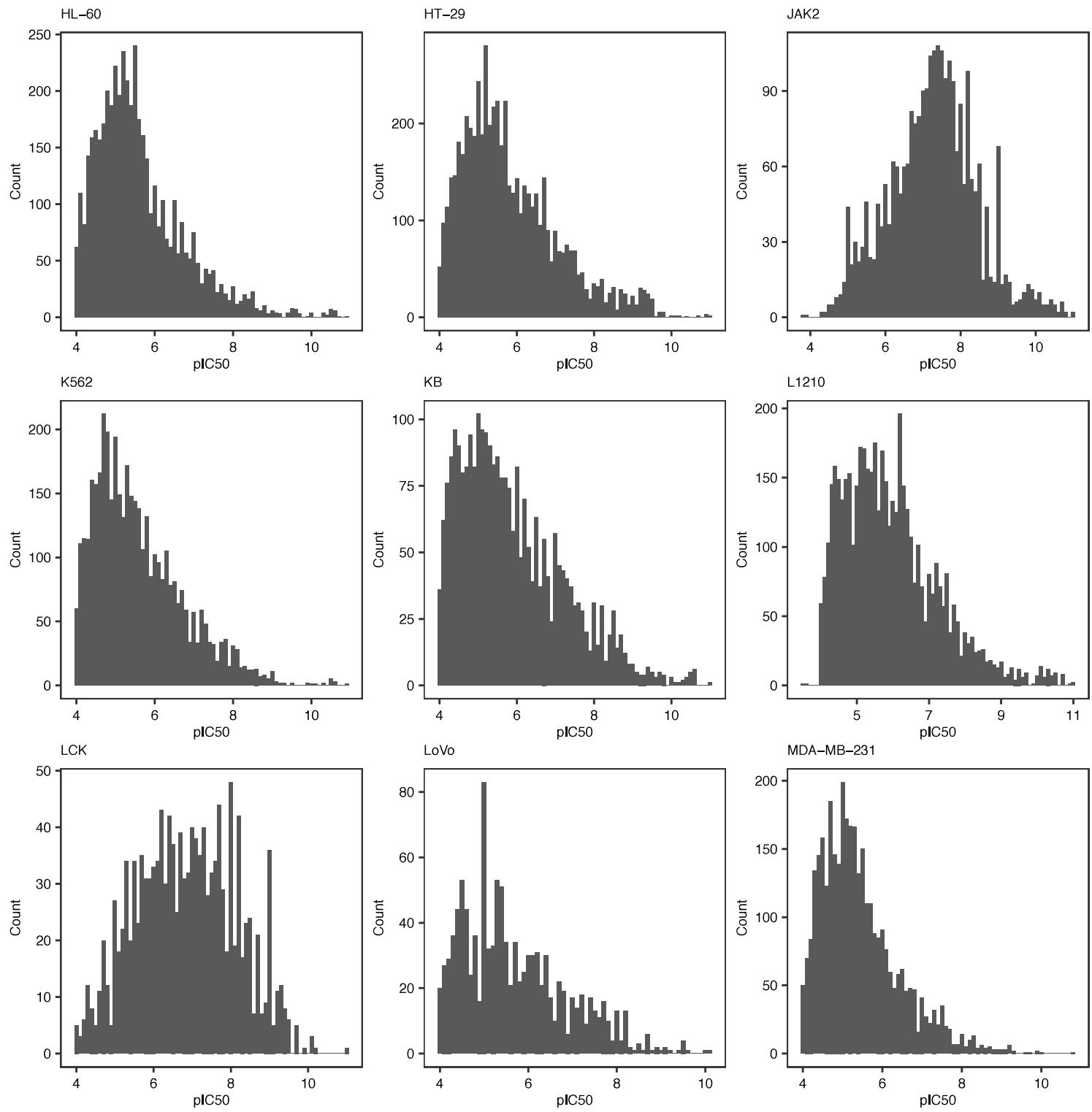


Supplementary Figure 1

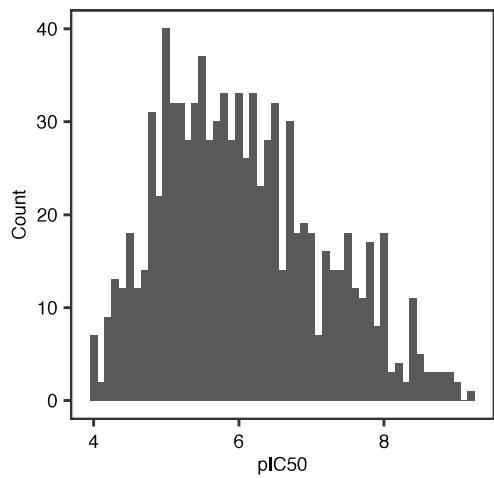




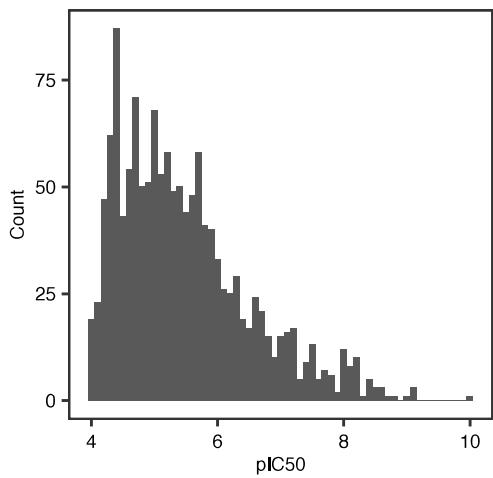




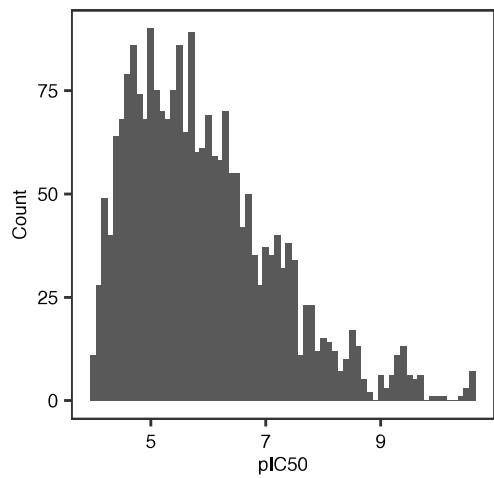
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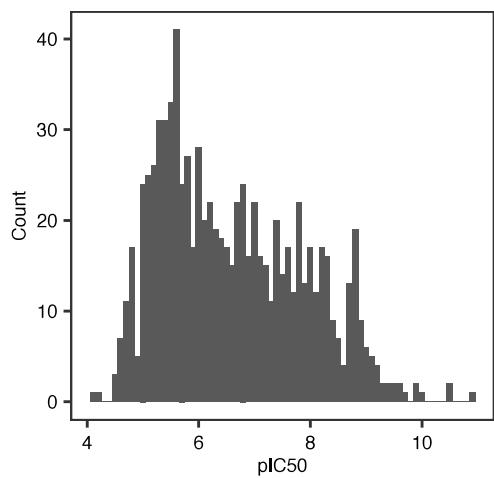
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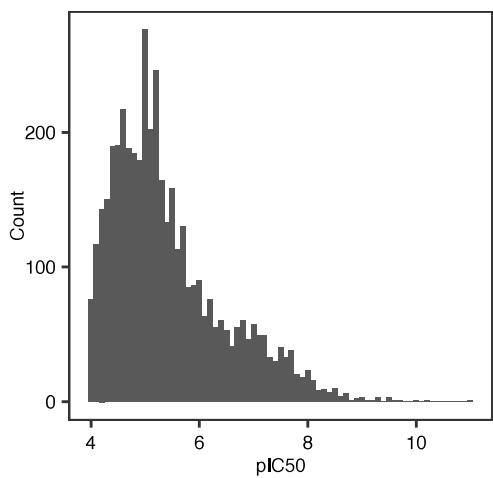
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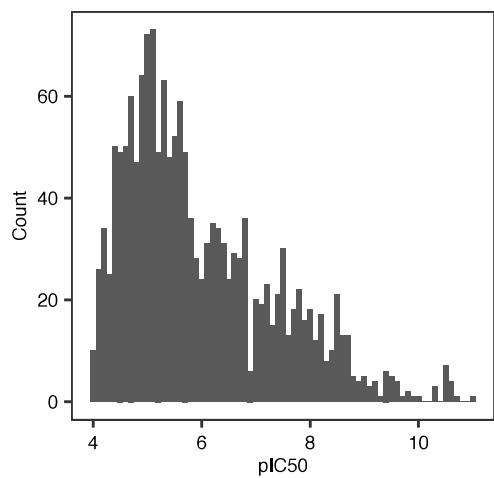
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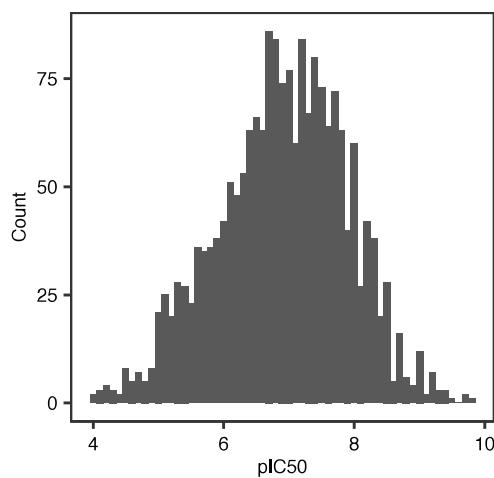
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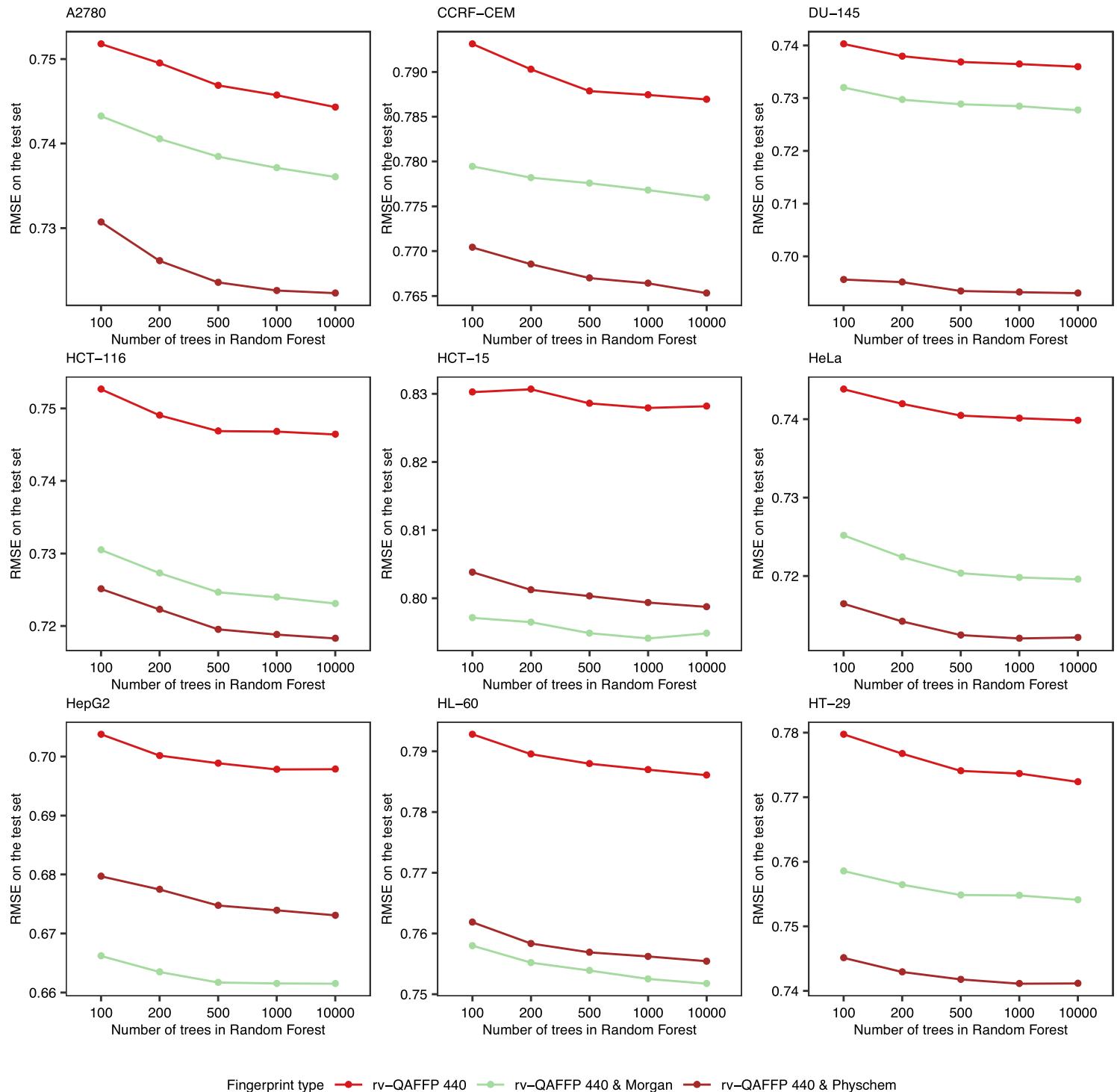
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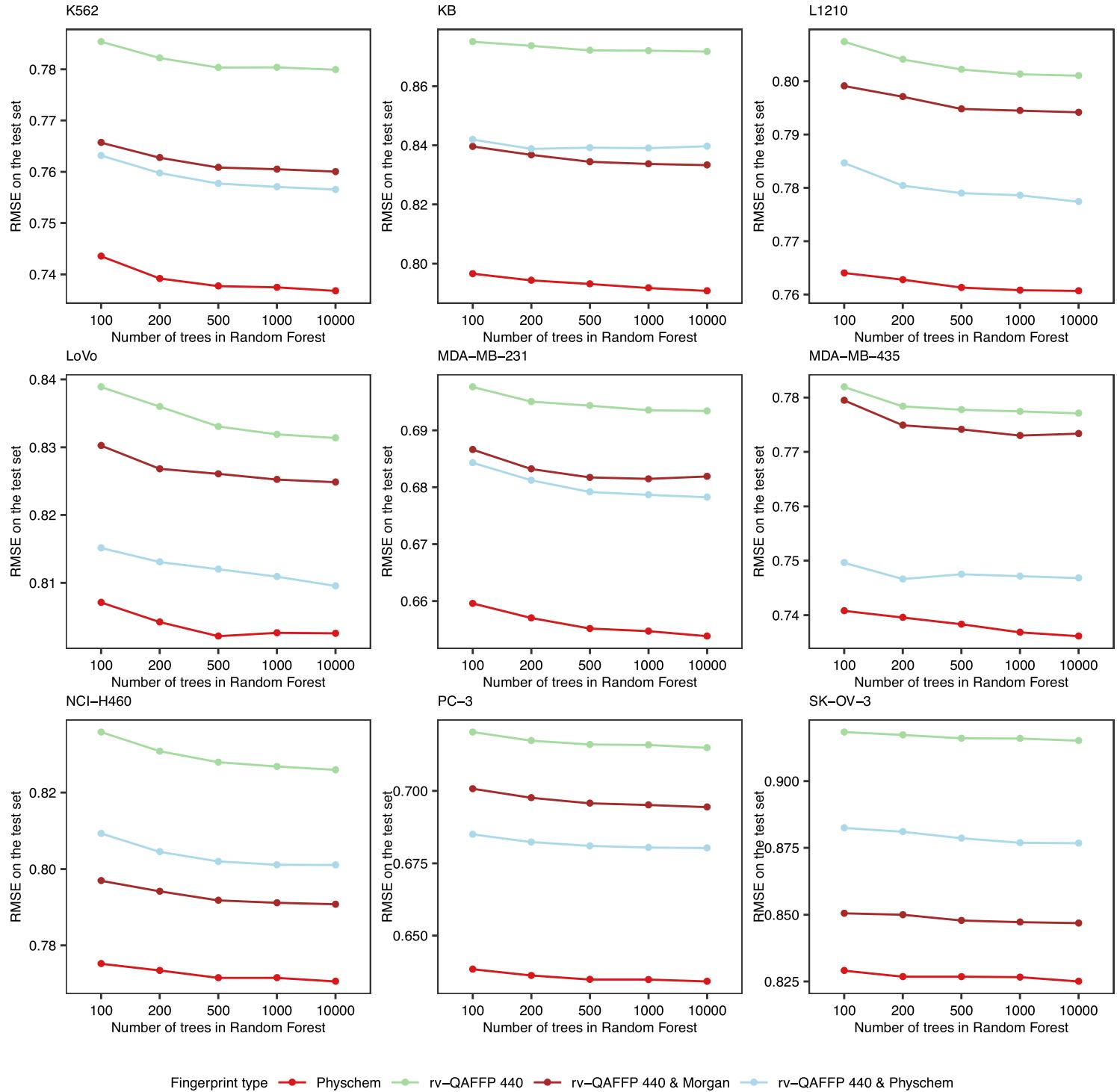


Vanilloid



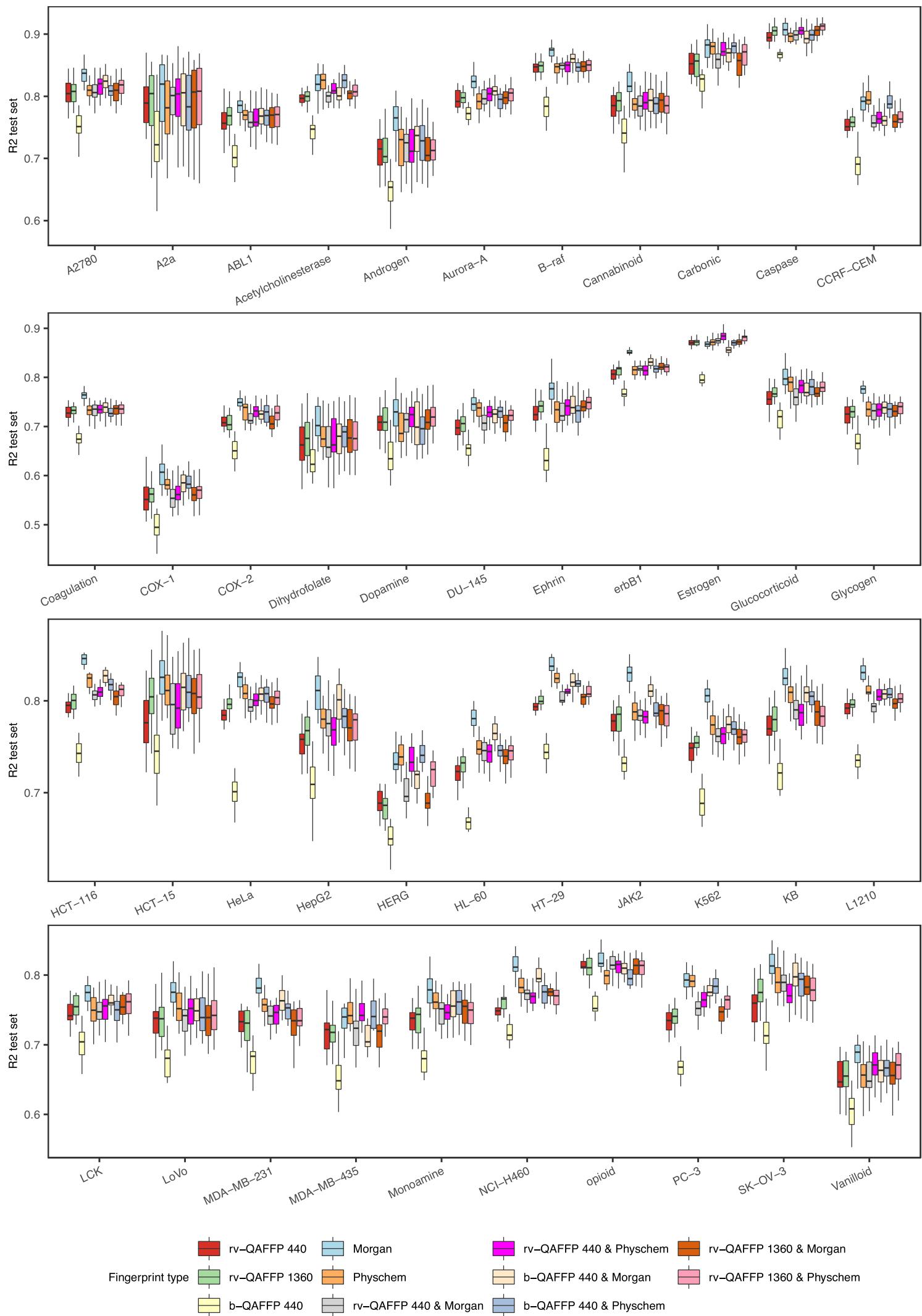
Supplementary Figure 2



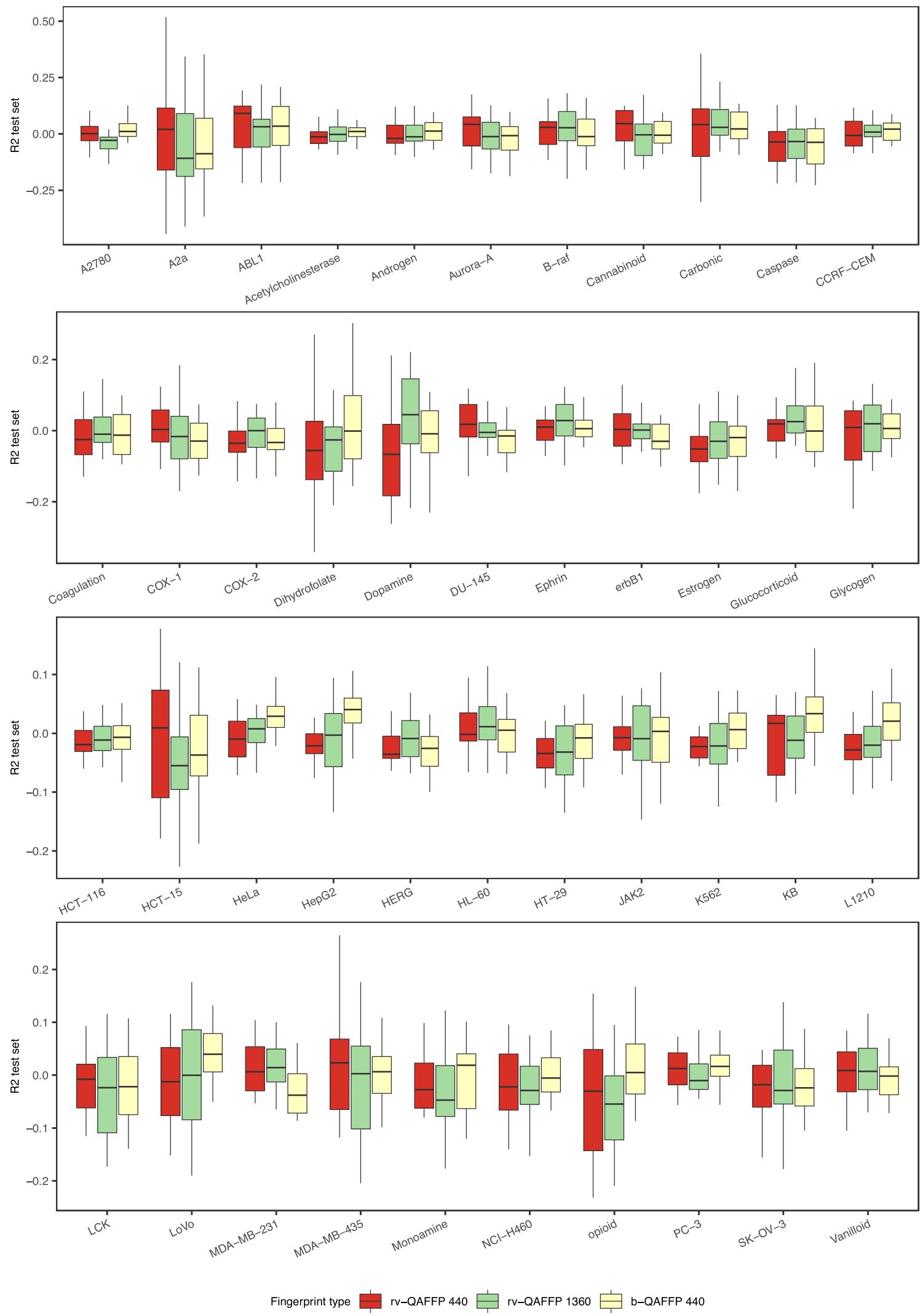


Fingerprint type — ● Physchem ● rv-QAFFP 440 ● rv-QAFFP 440 & Morgan ● rv-QAFFP 440 & Physchem

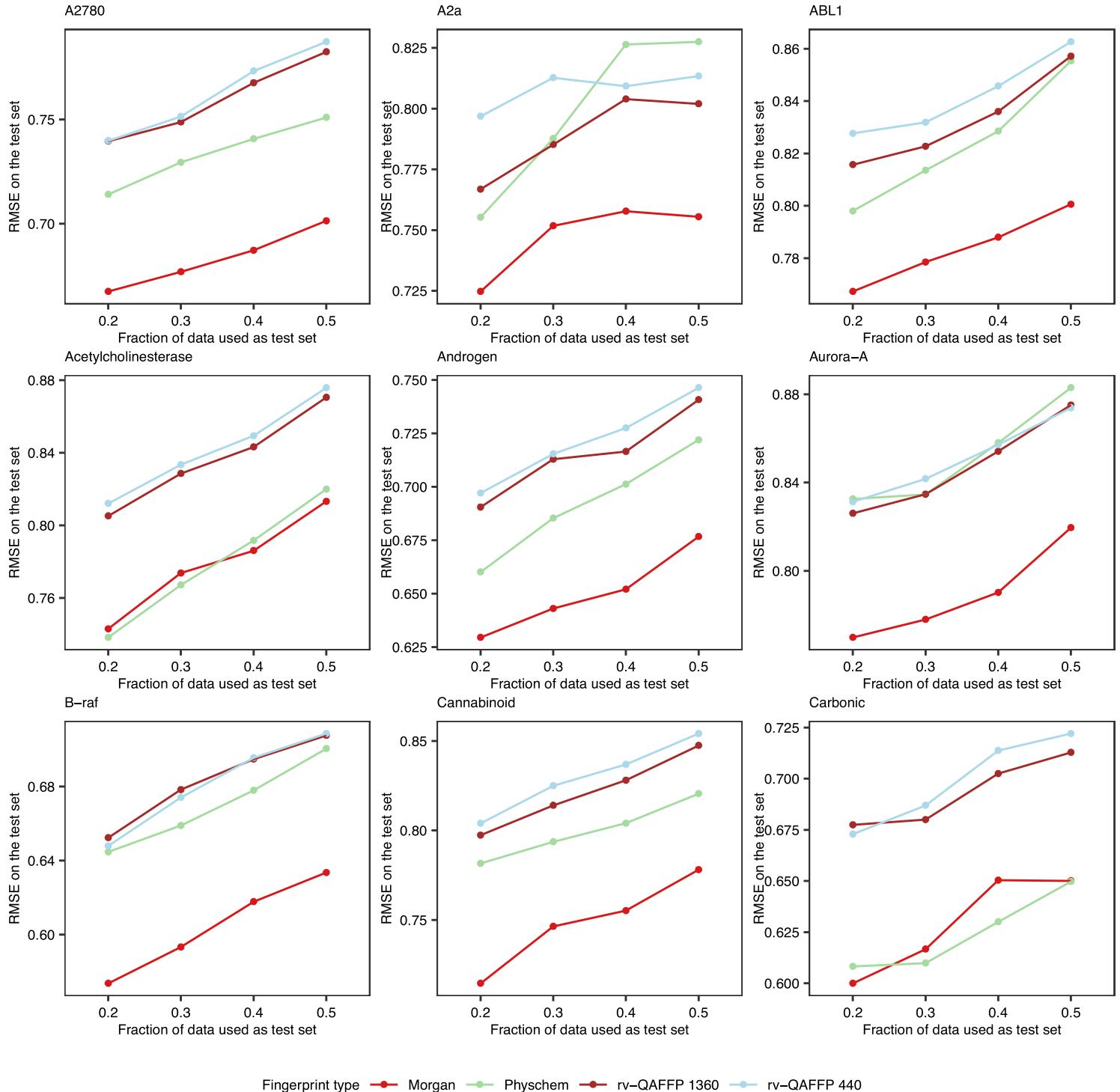
Supplementary Figure 3



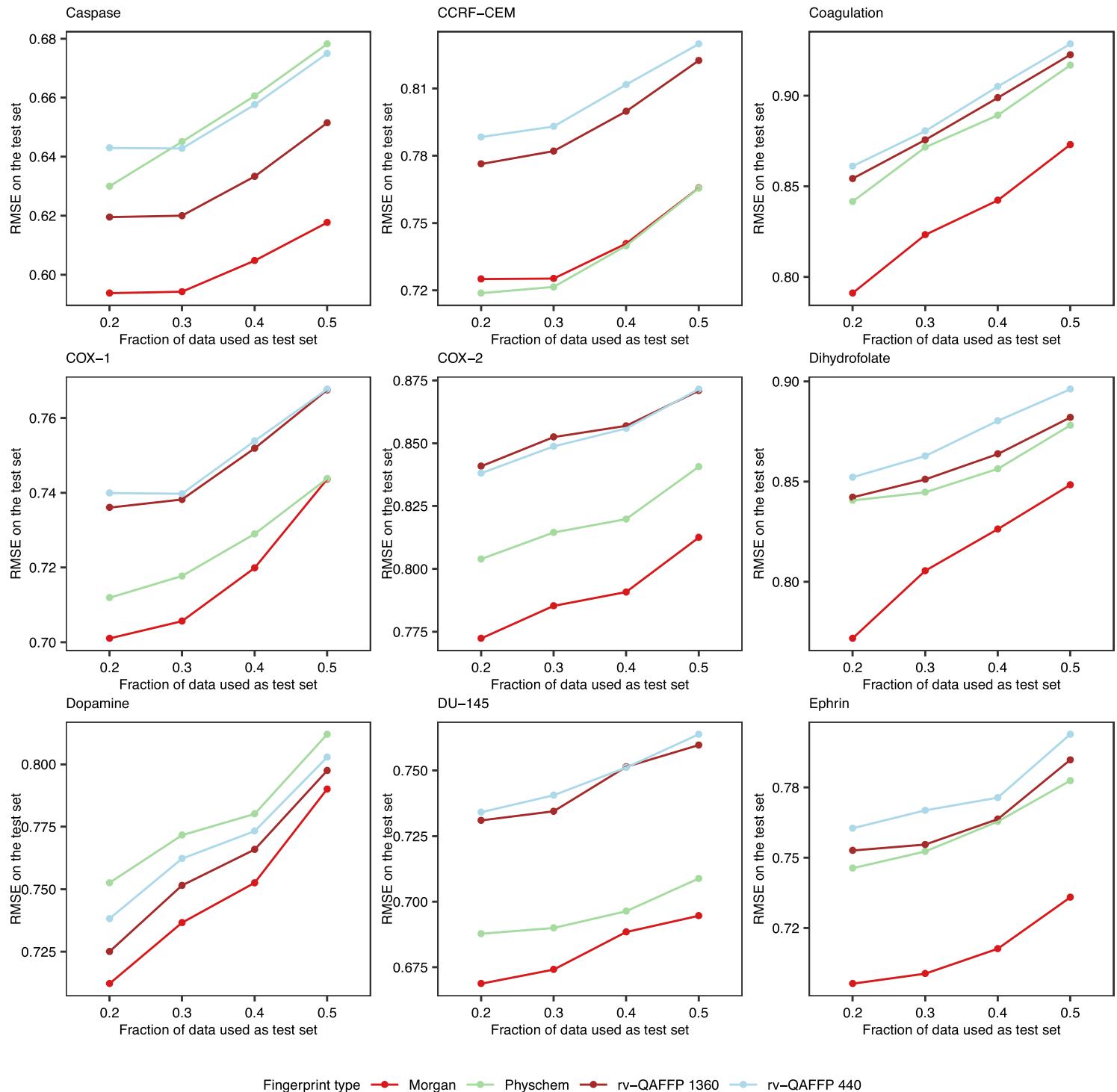
Supplementary Figure 4



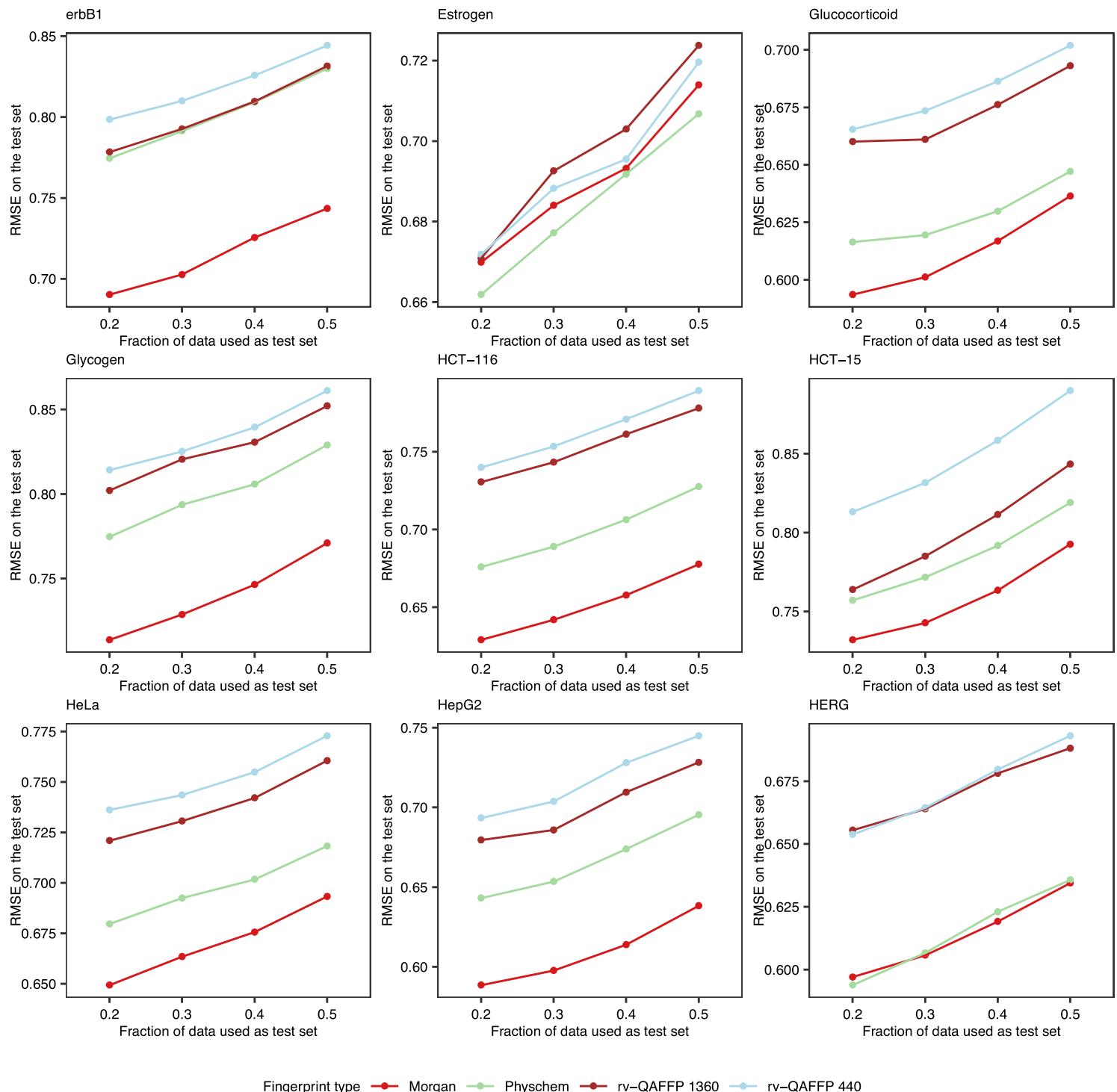
Supplementary Figure 5



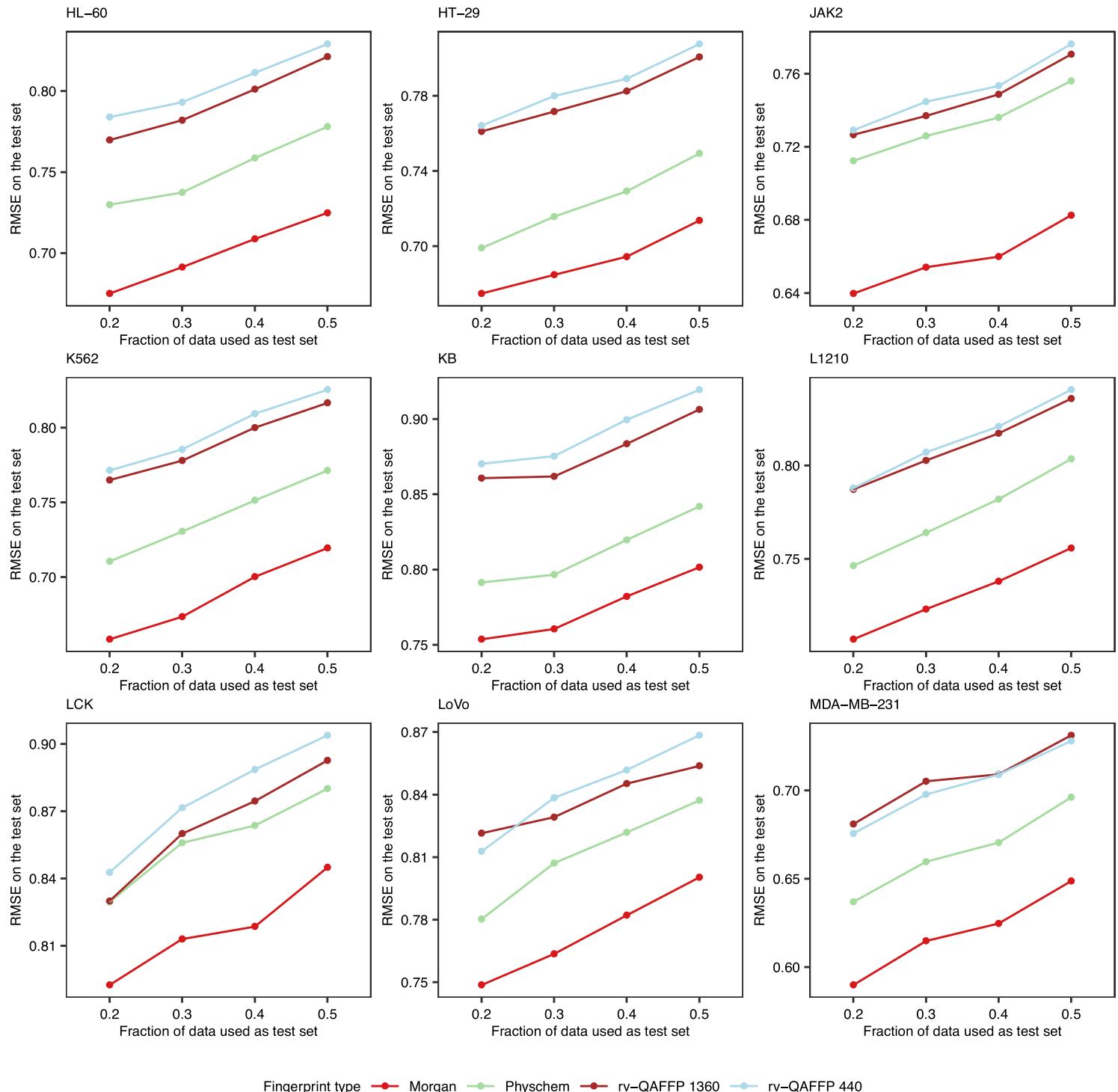
Fingerprint type — Morgan — Physchem — rv-QAFFP 1360 — rv-QAFFP 440



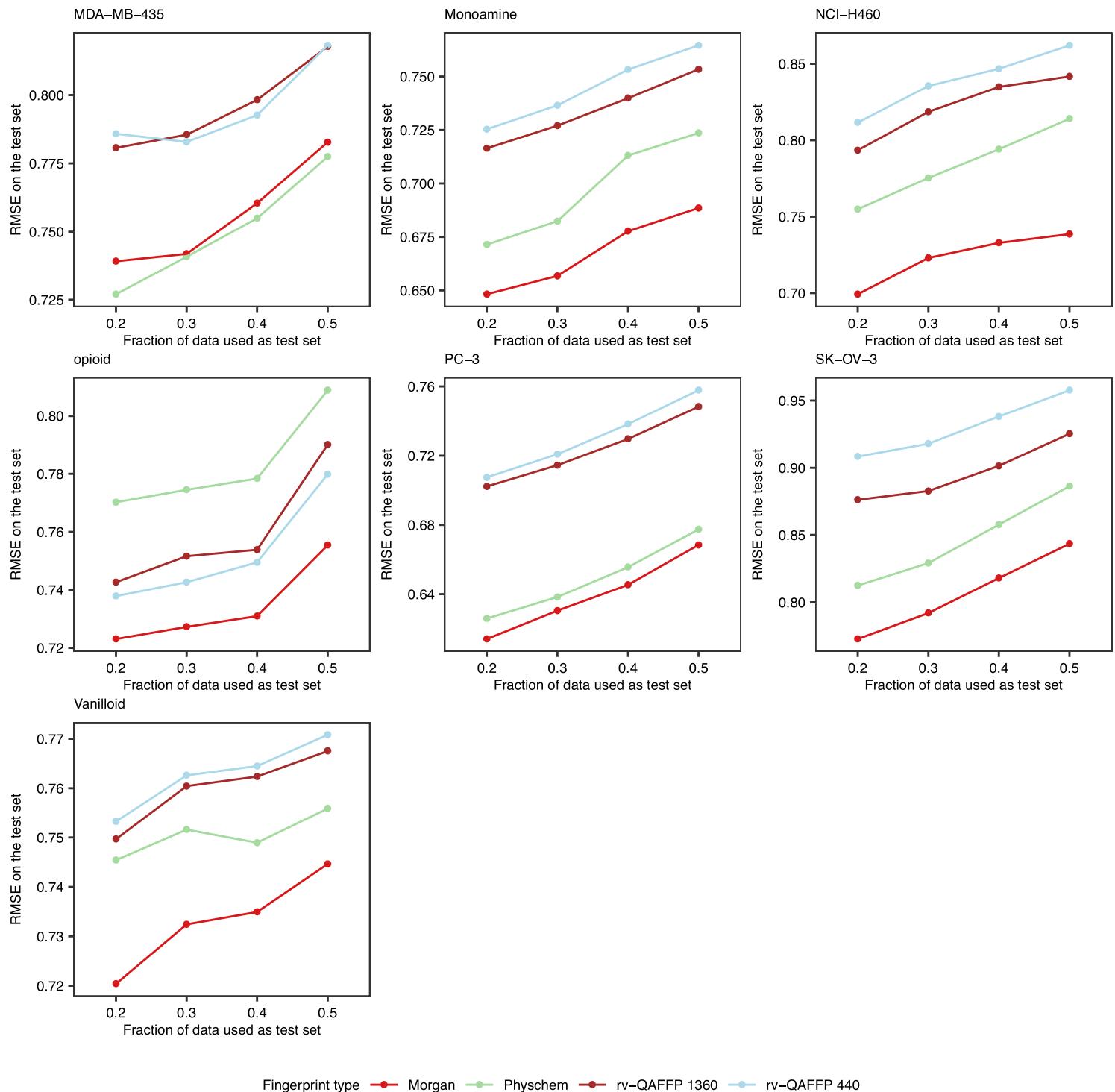
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Fingerprint type — Morgan — Physchem — rv-QAFFP 1360 — rv-QAFFP 440

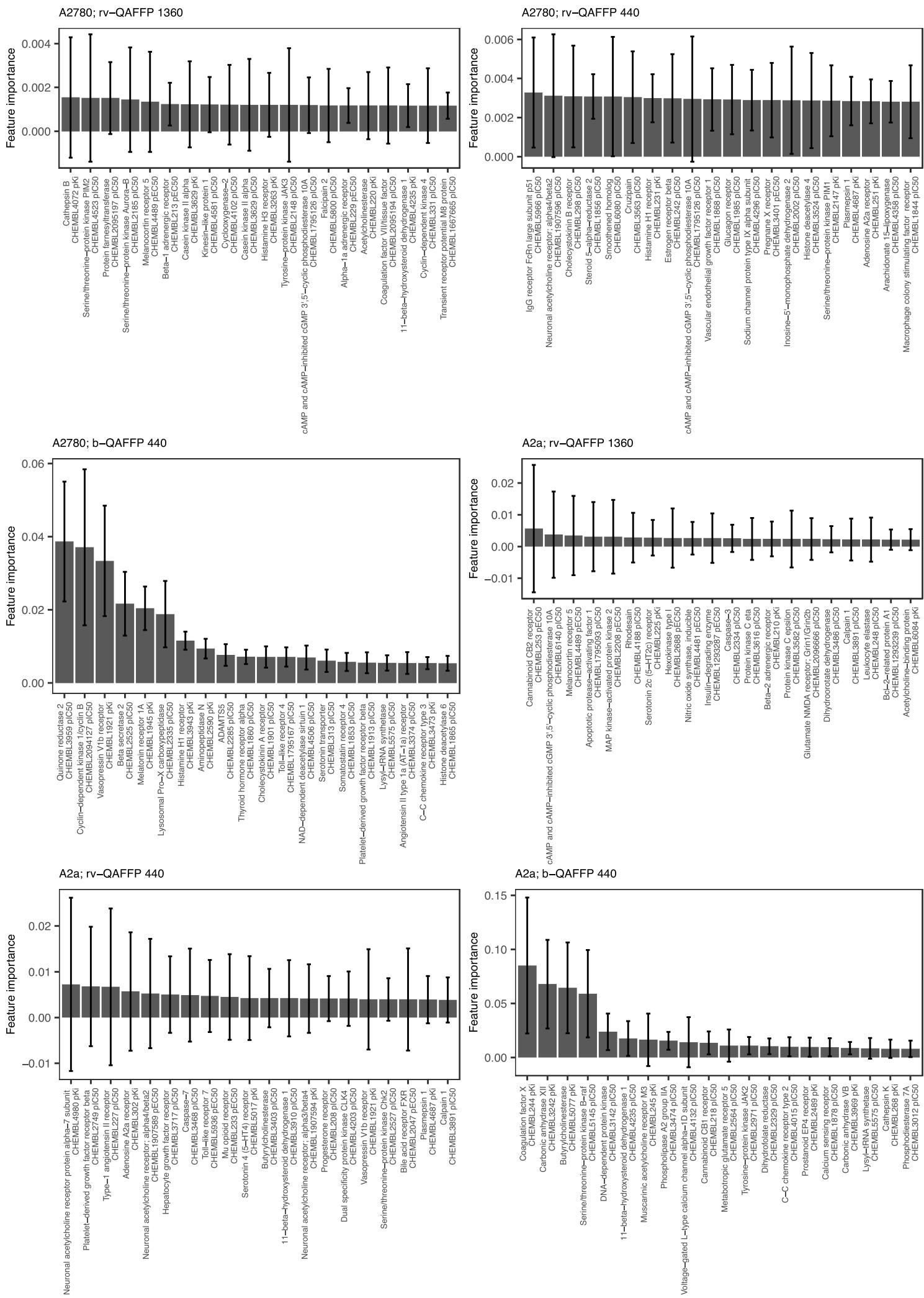


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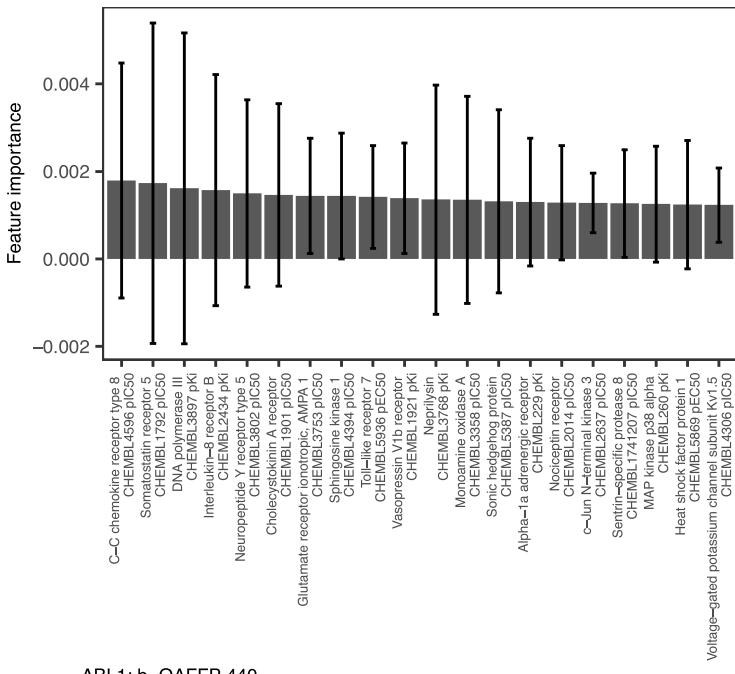


Fingerprint type — Morgan — Physchem — rv-QAFFP 1360 — rv-QAFFP 440

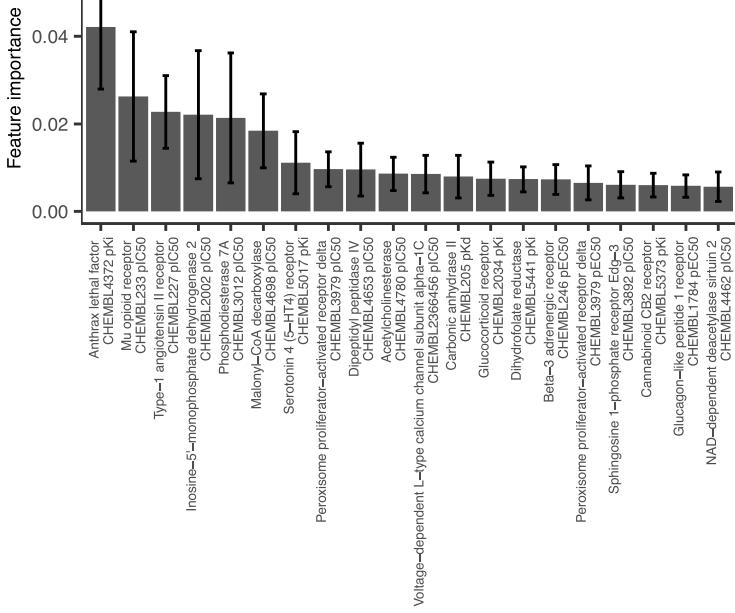
Supplementary Figure 6



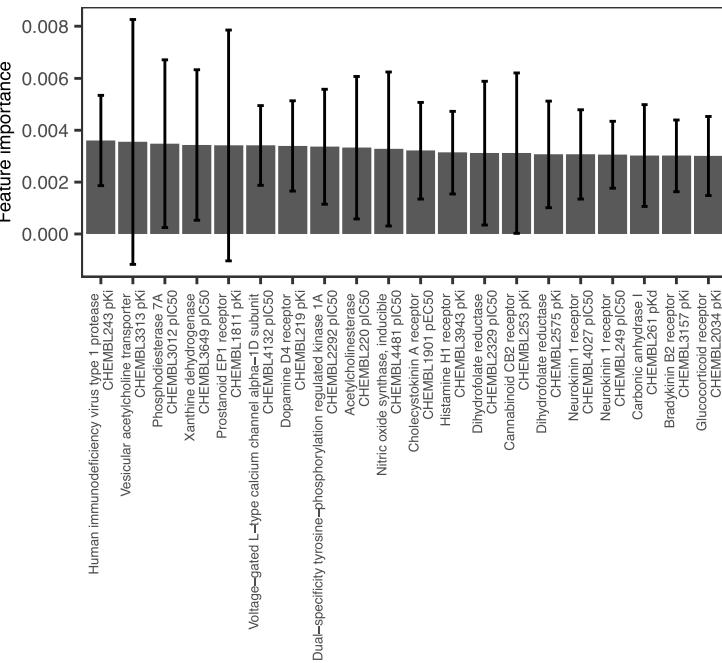
ABL1; rv-QAFFP 1360



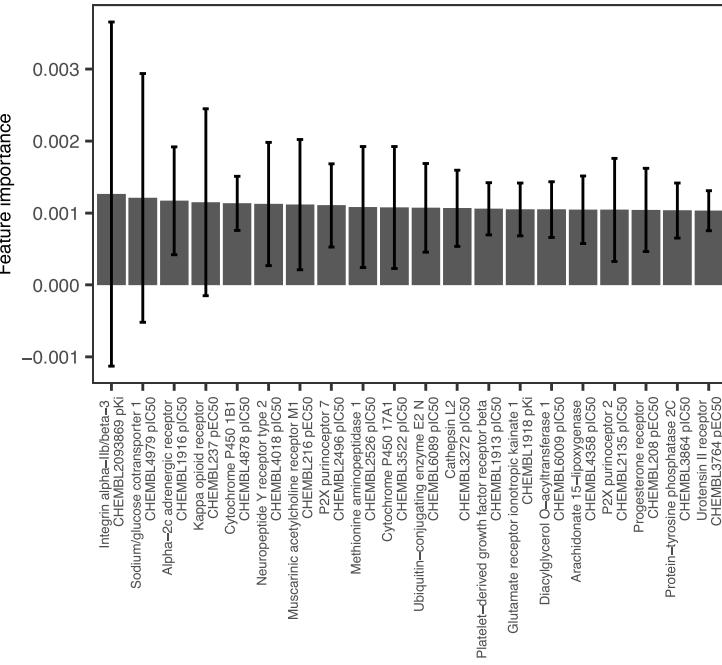
ABL1; b-QAFFP 440



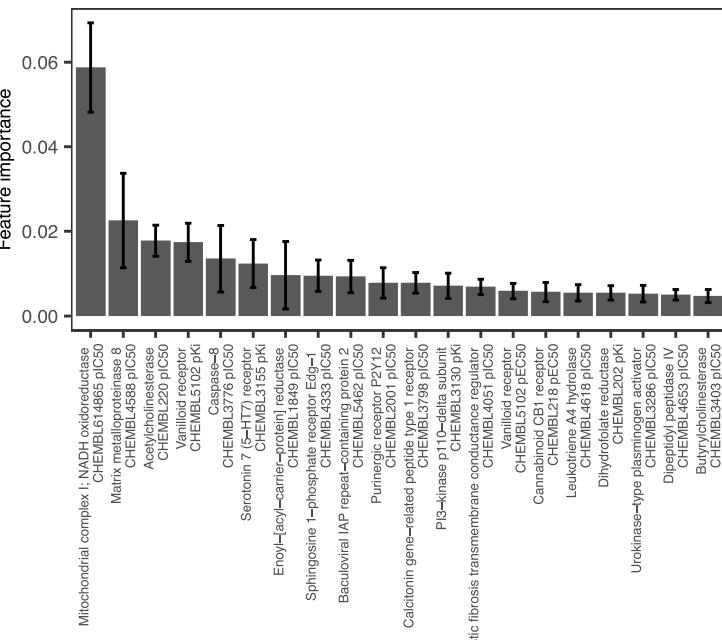
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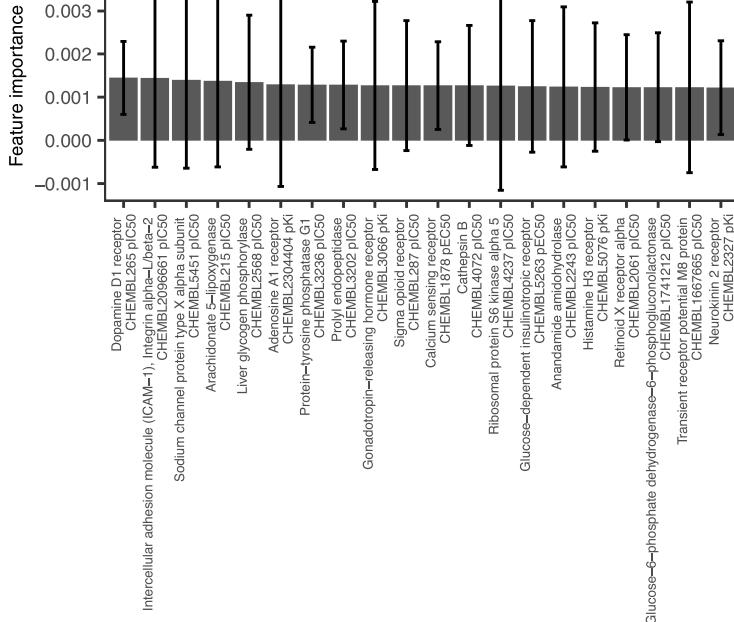
Acetylcholinesterase; rv-QAFFP 1360



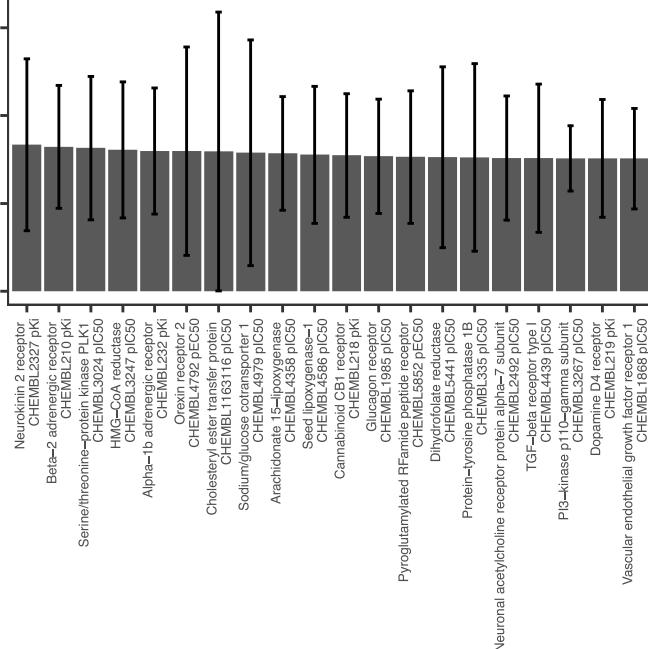
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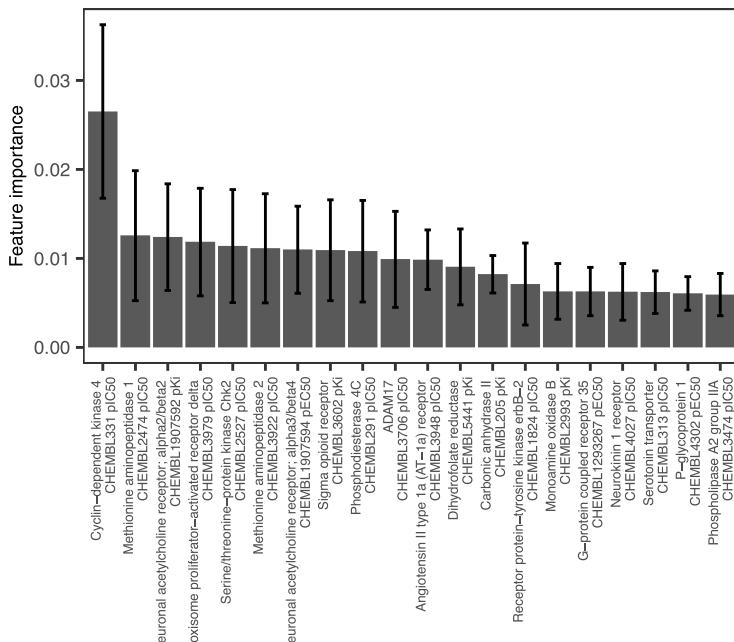
Androgen; rv-QAFFP 1360



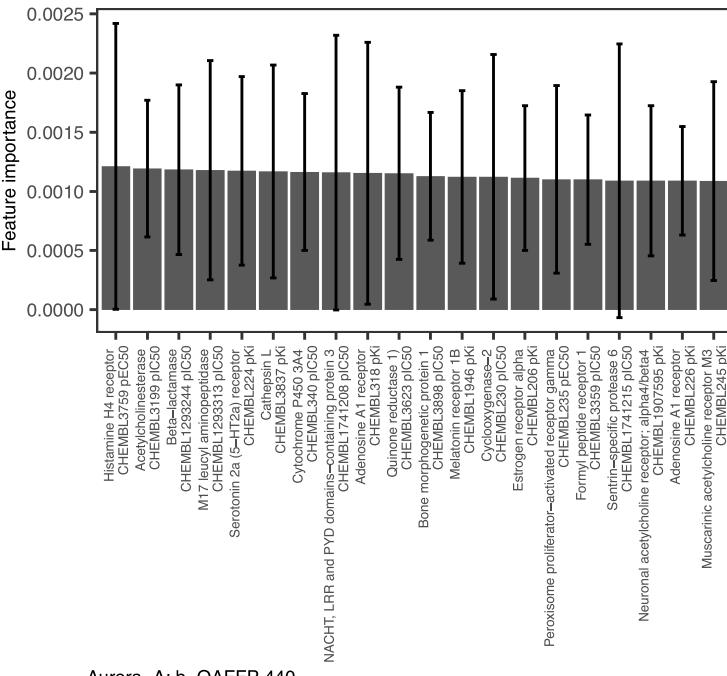
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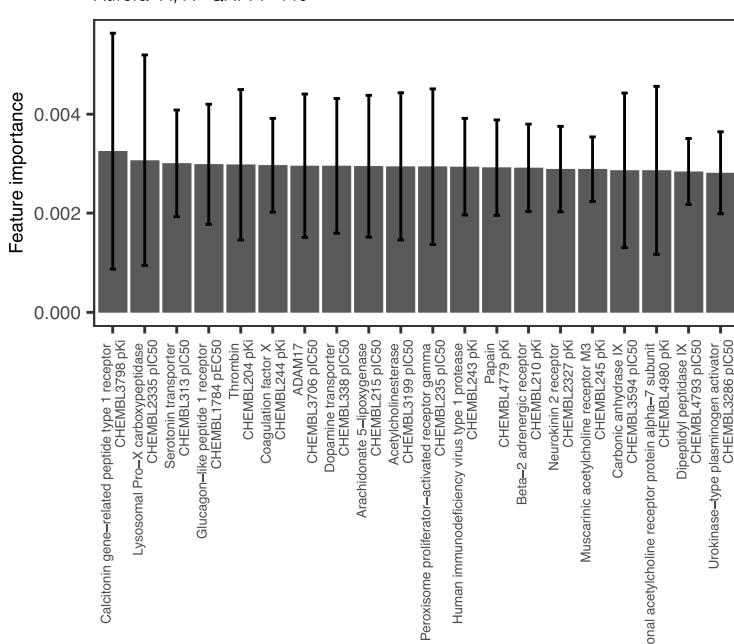
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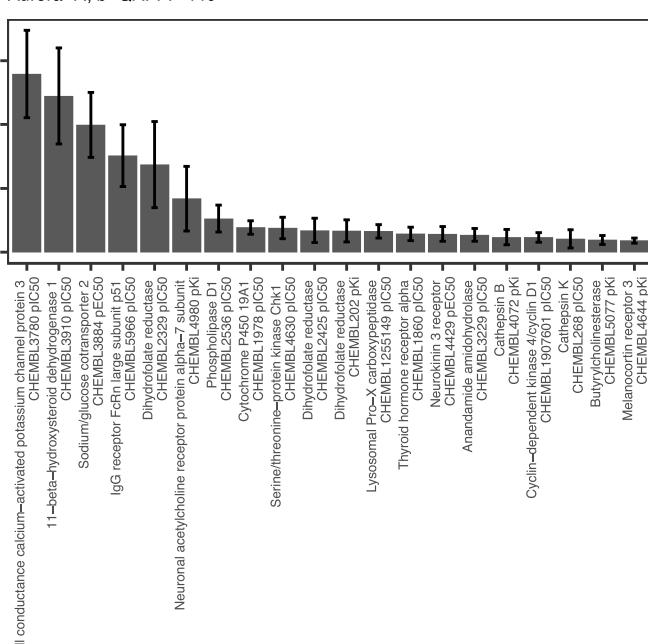
Aurora-A; rv-QAFFP 1360



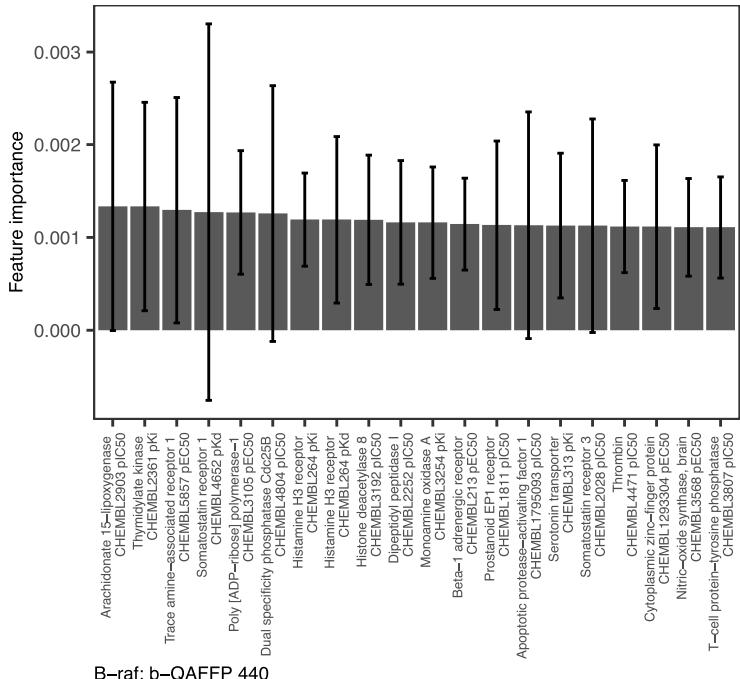
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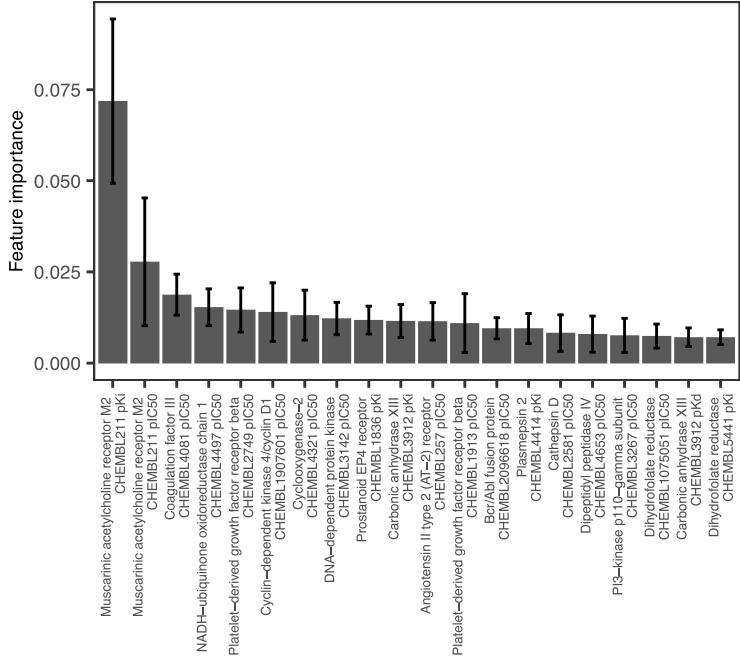
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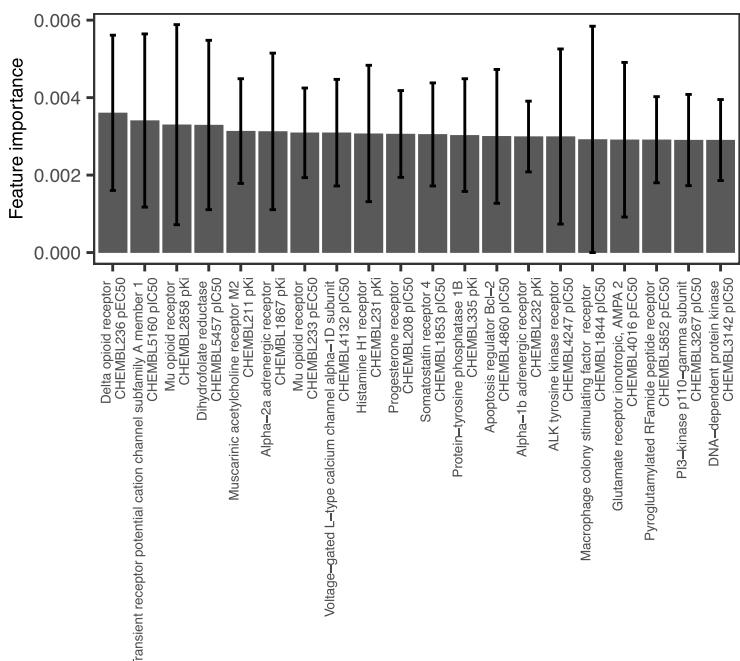
B-raf; rv-QAFFP 1360



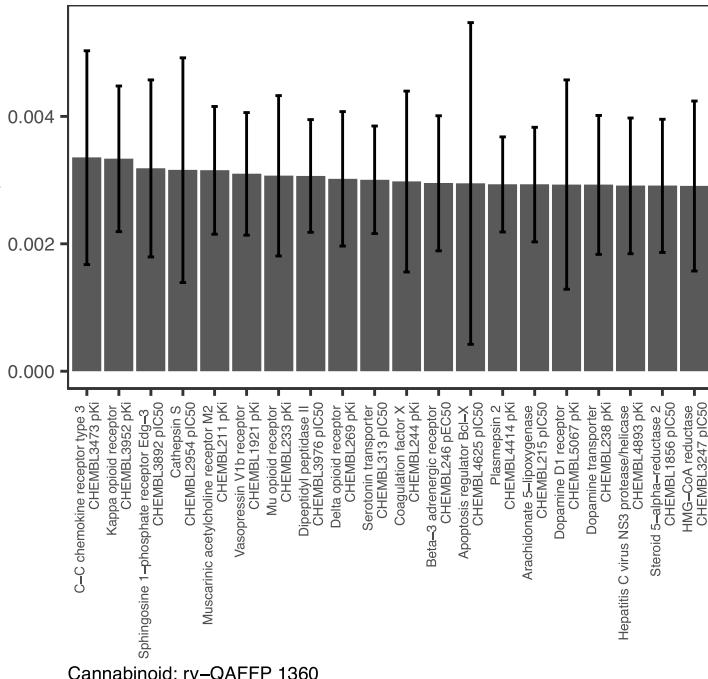
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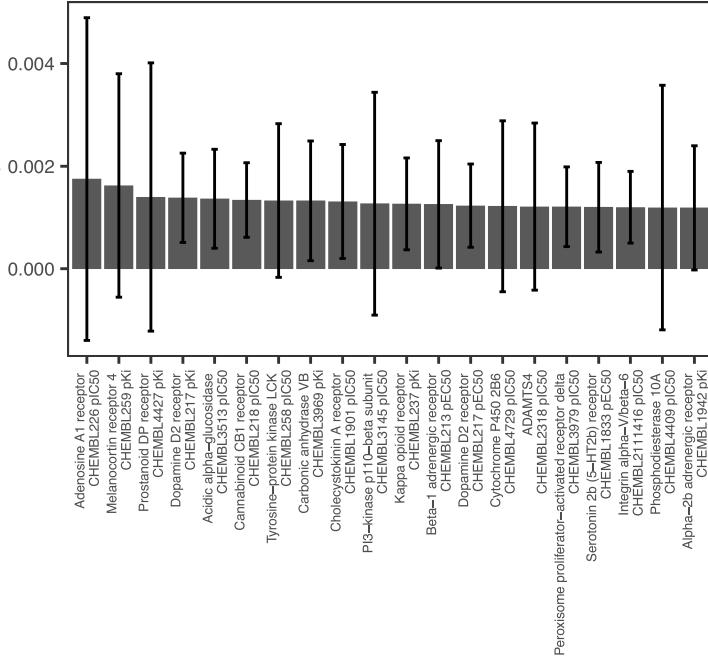
Cannabinoid; rv-QAFFP 440



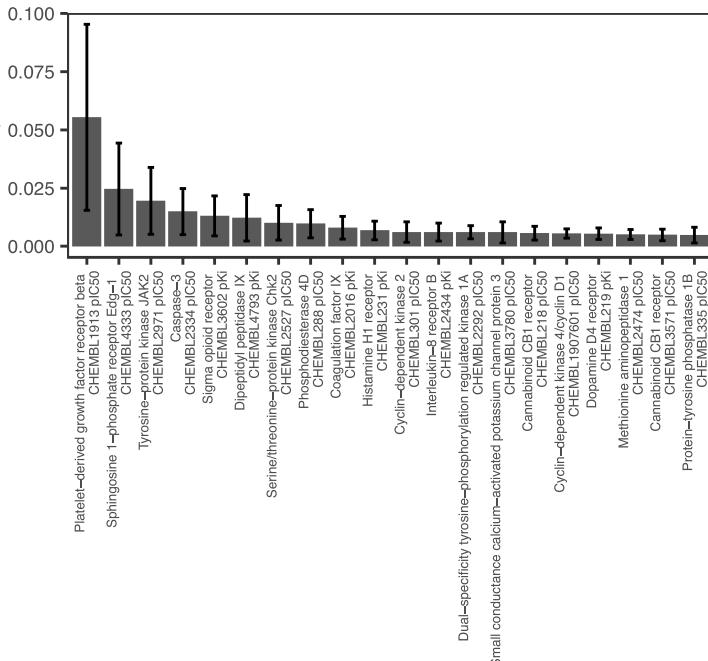
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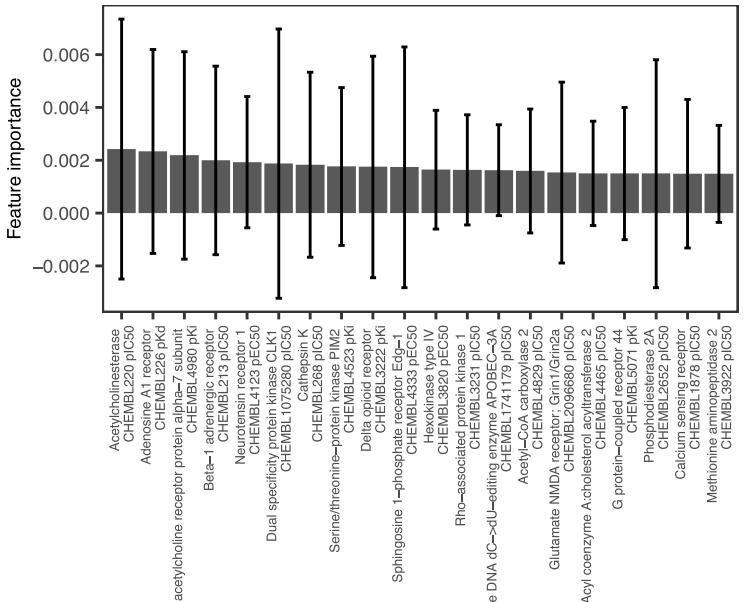
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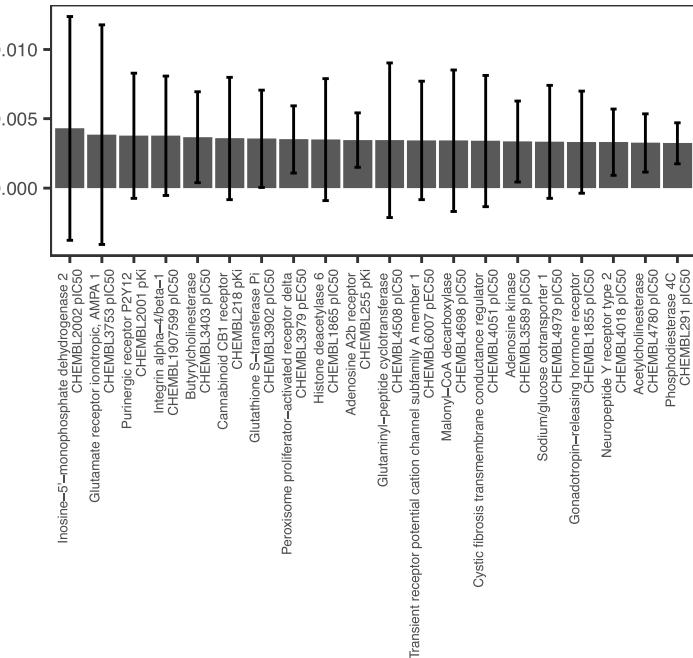
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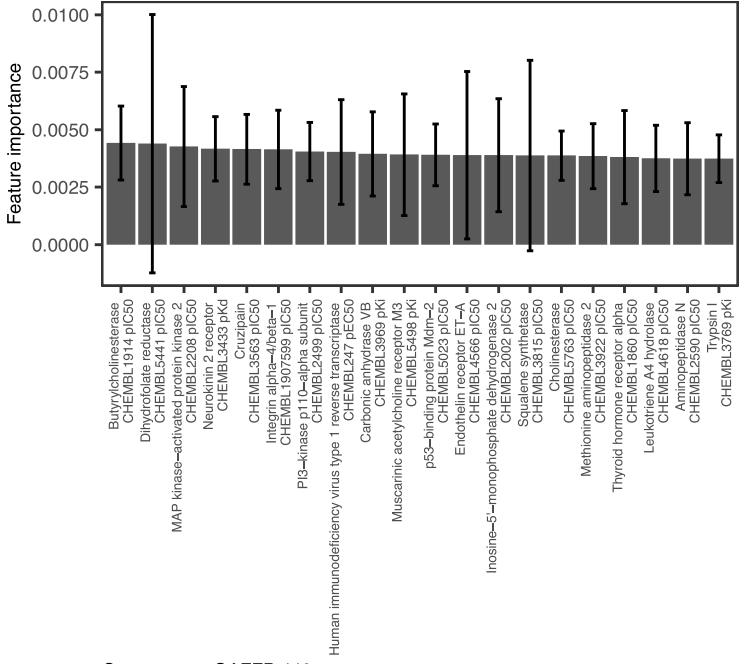
Carbonic; rv-QAFFP 1360



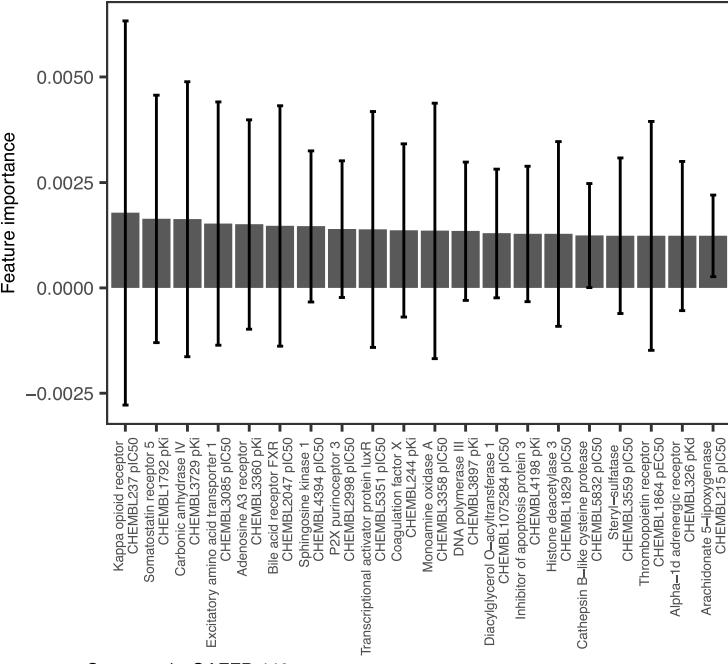
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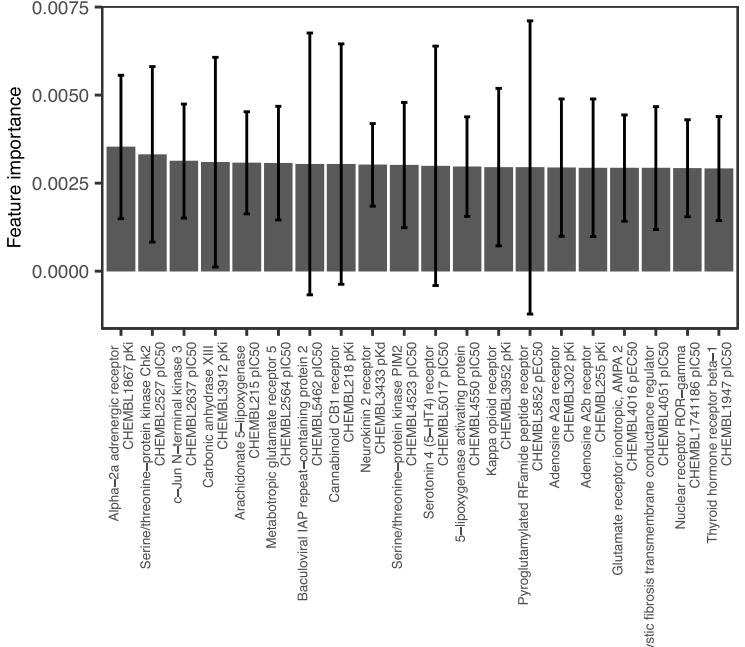
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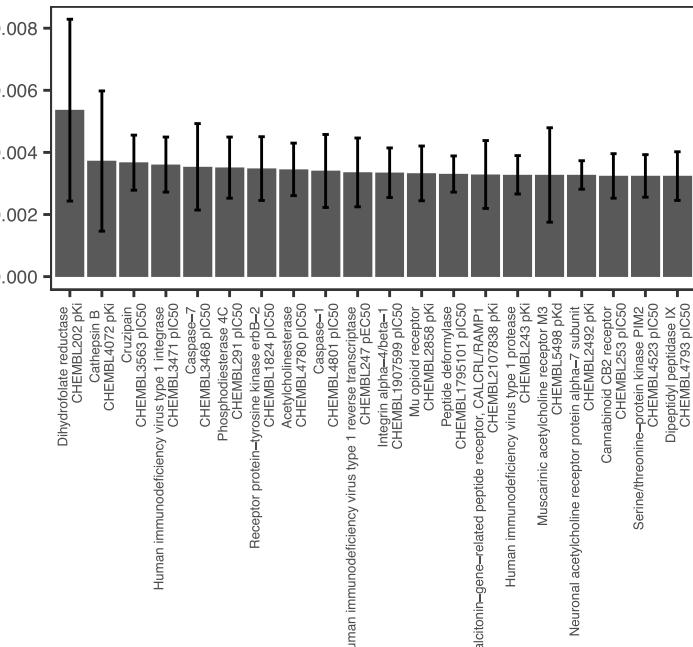
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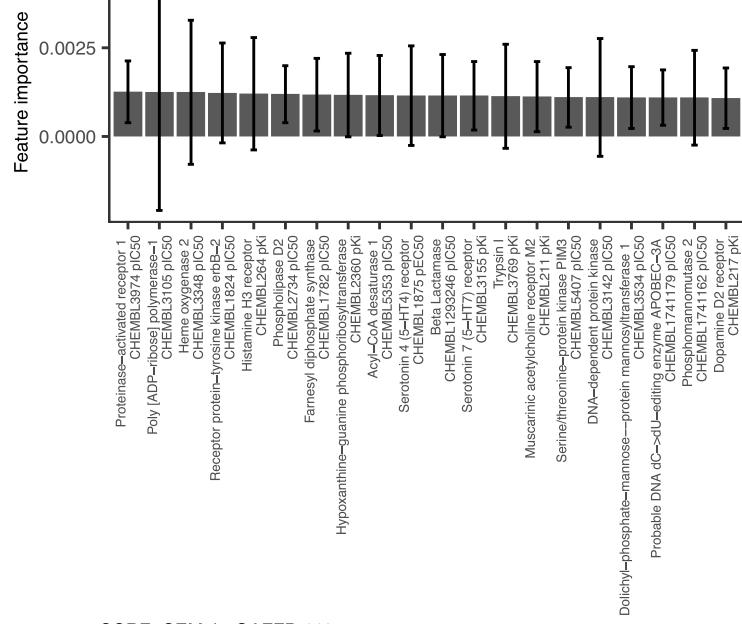
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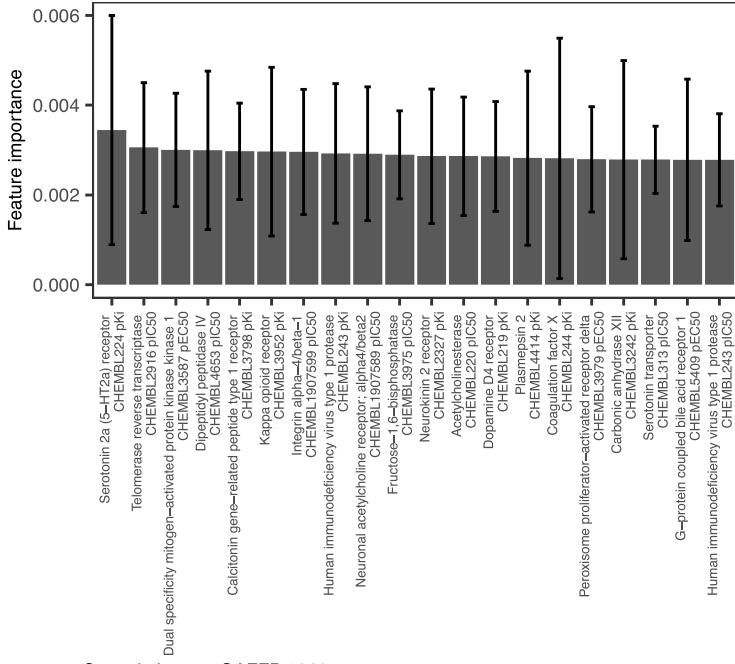
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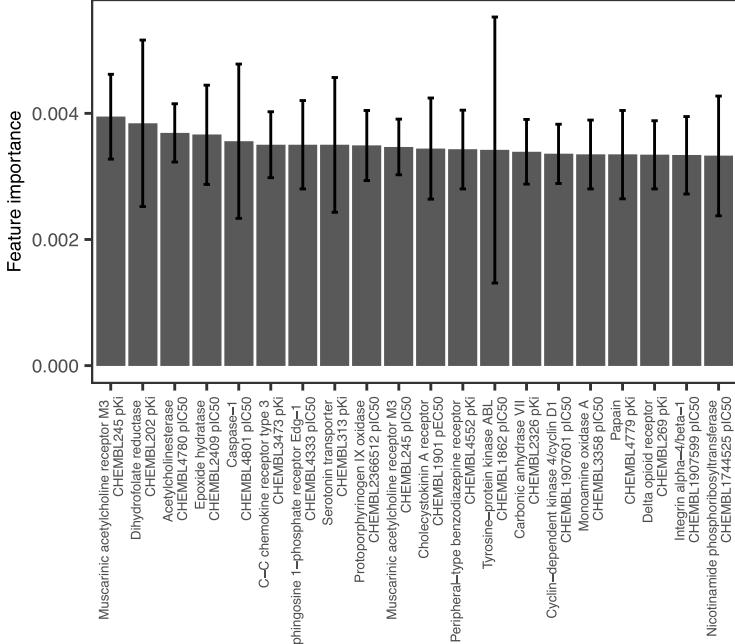
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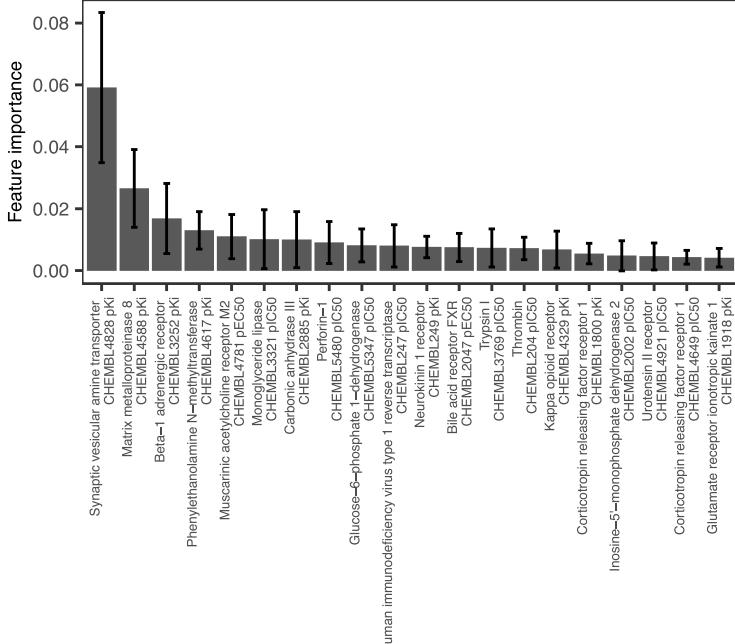
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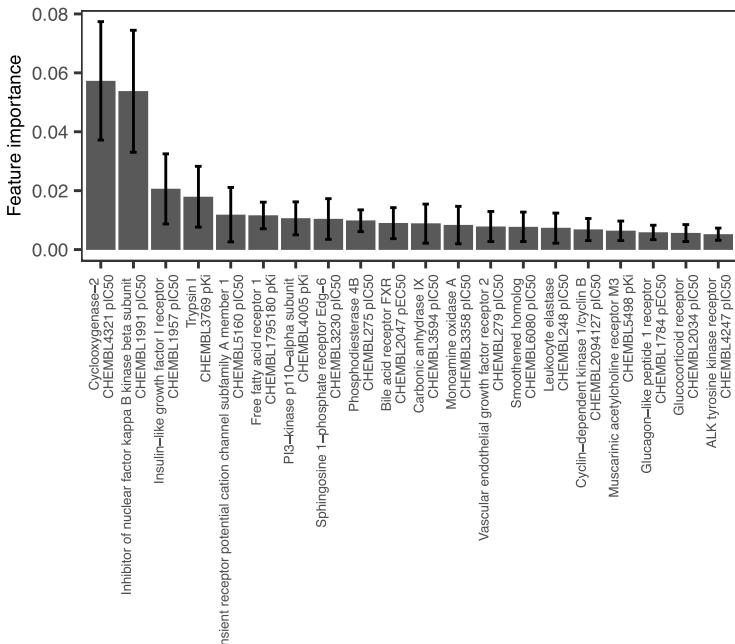
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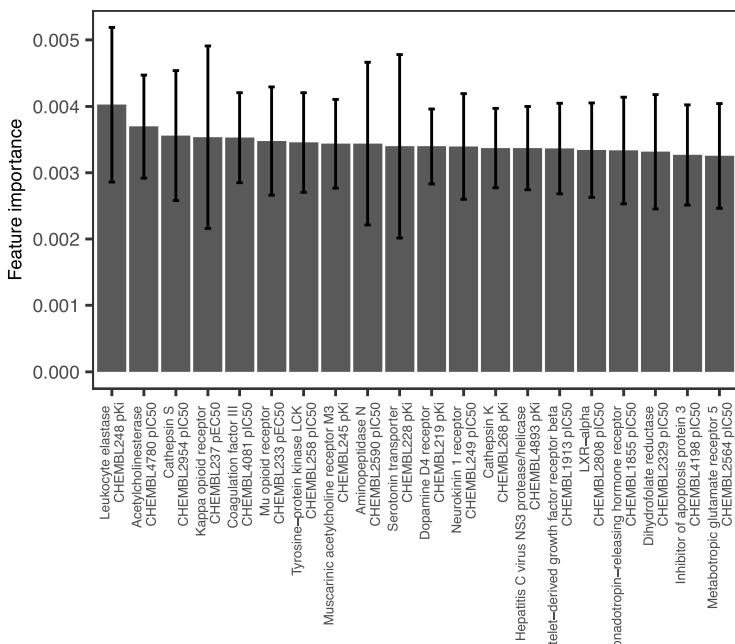
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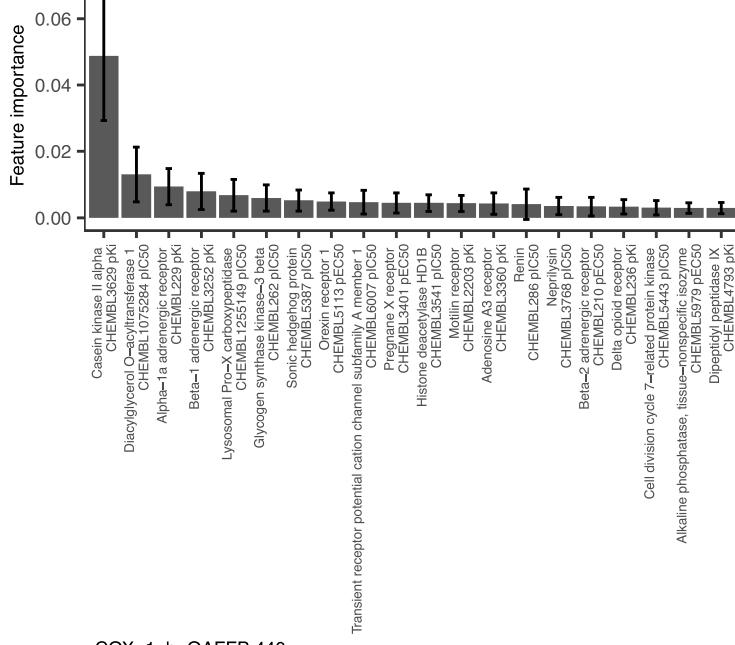
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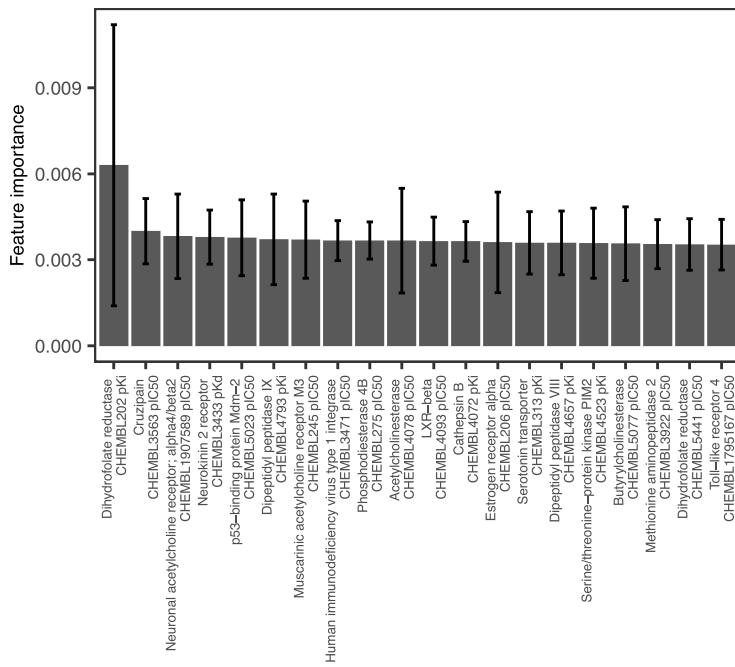
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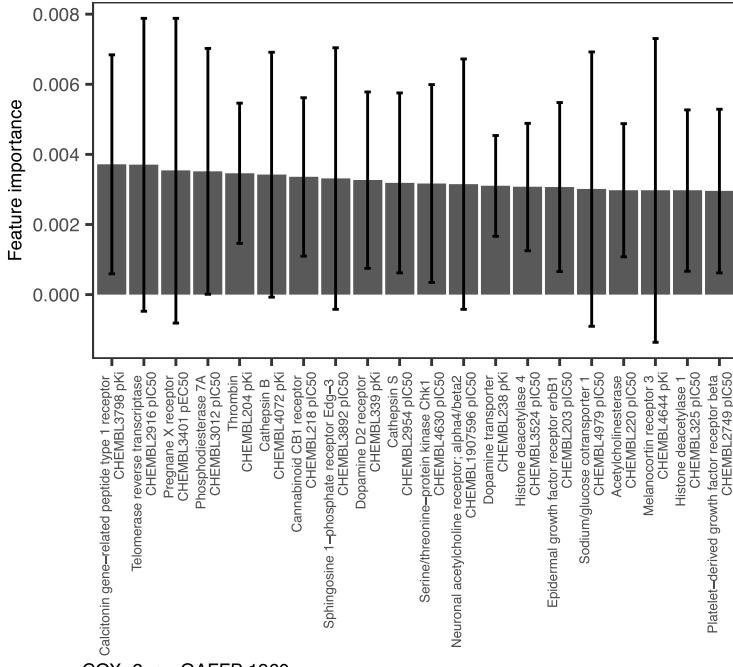
COX-1; rv-QAFFP 1360



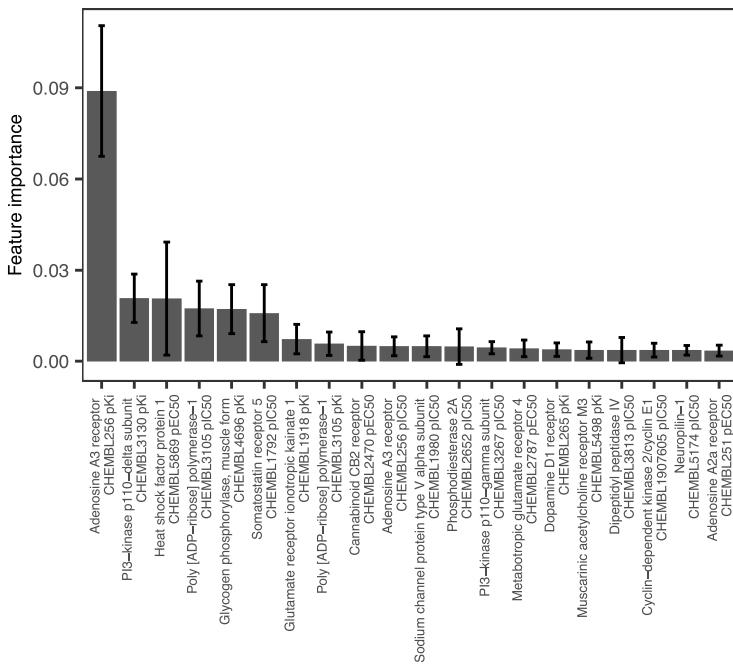
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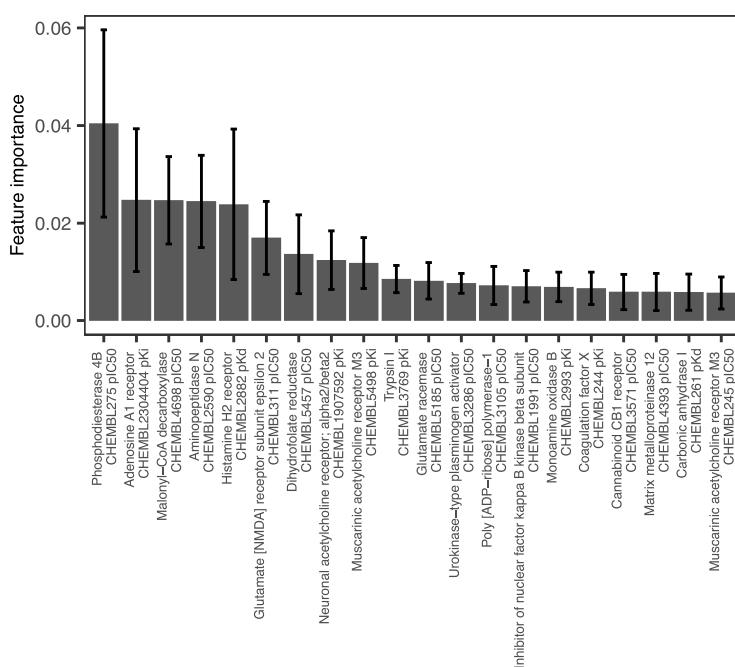
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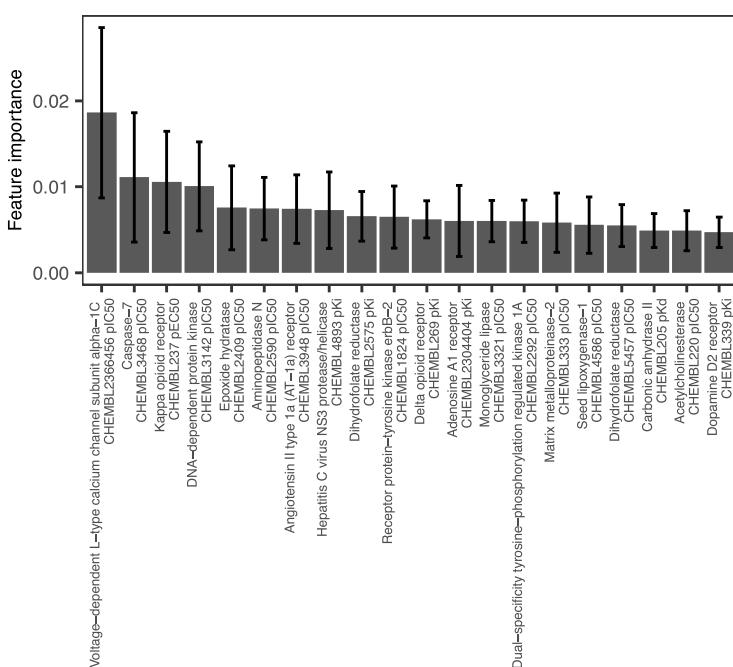
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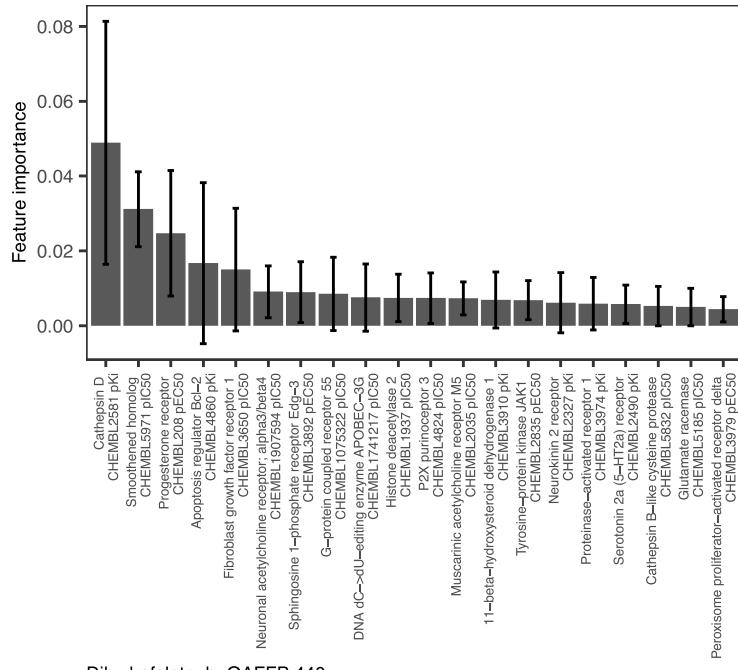
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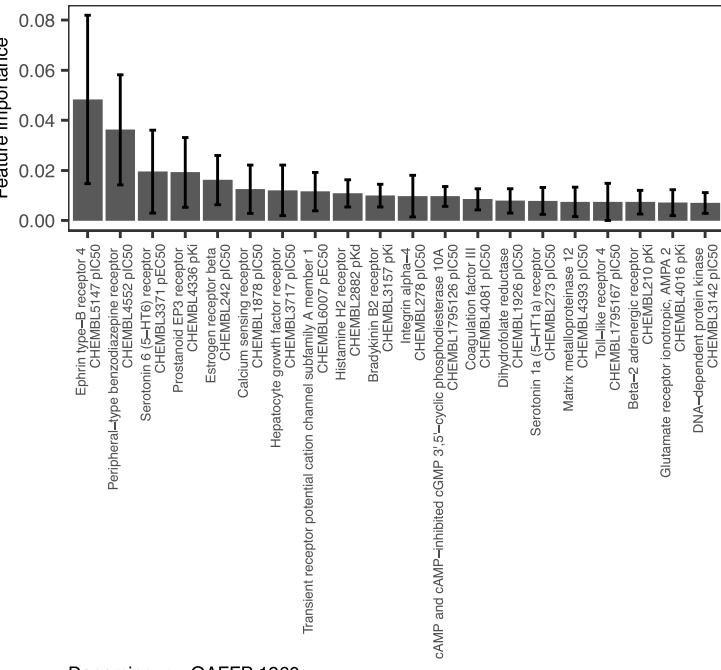
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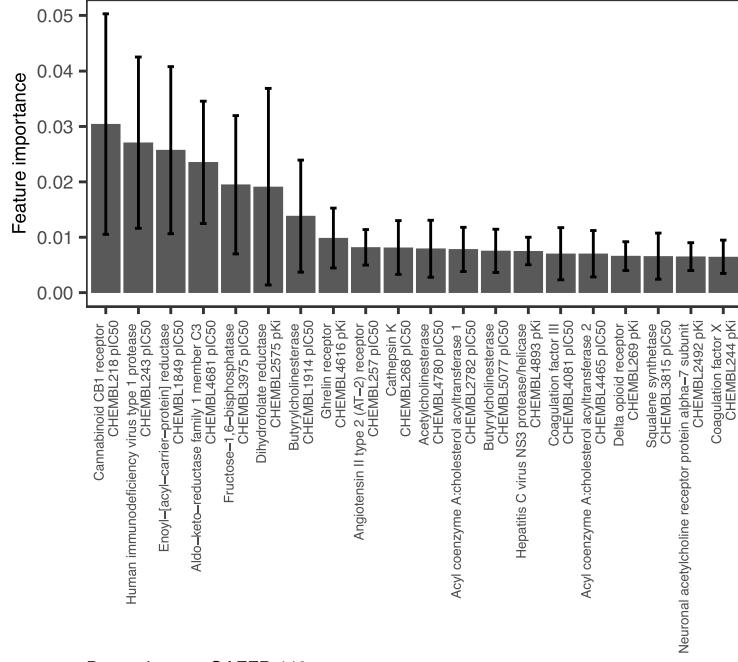
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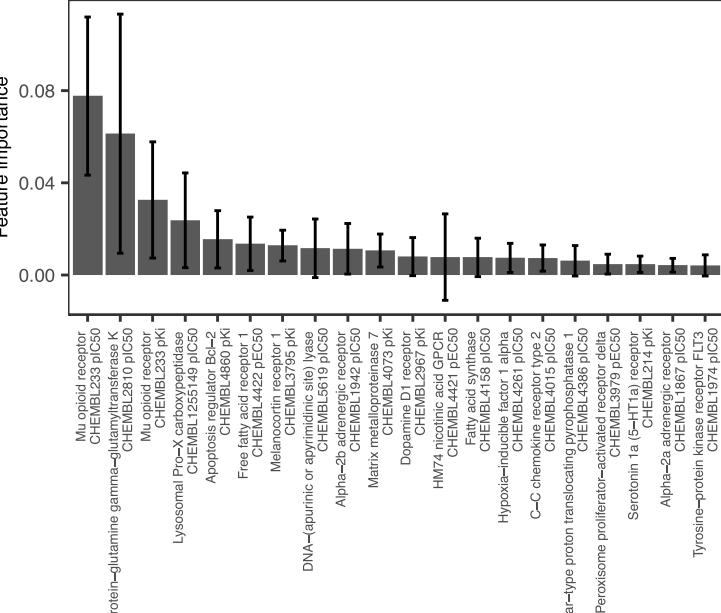
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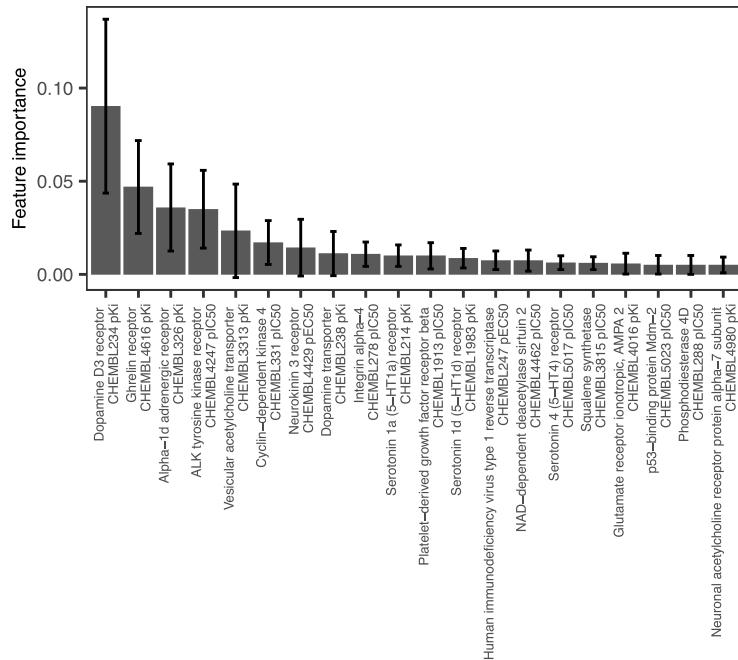
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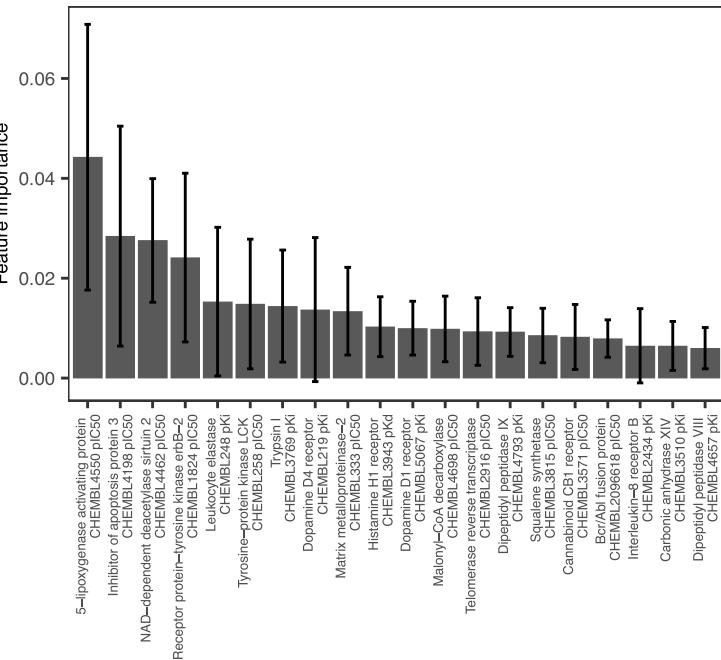
Dopamine; rv-QAFFP 1360



Dopamine; rv-QAFFP 440

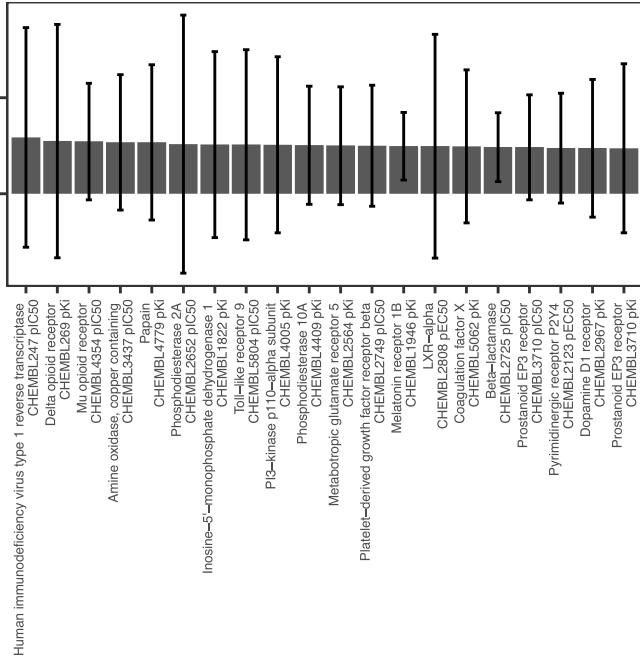


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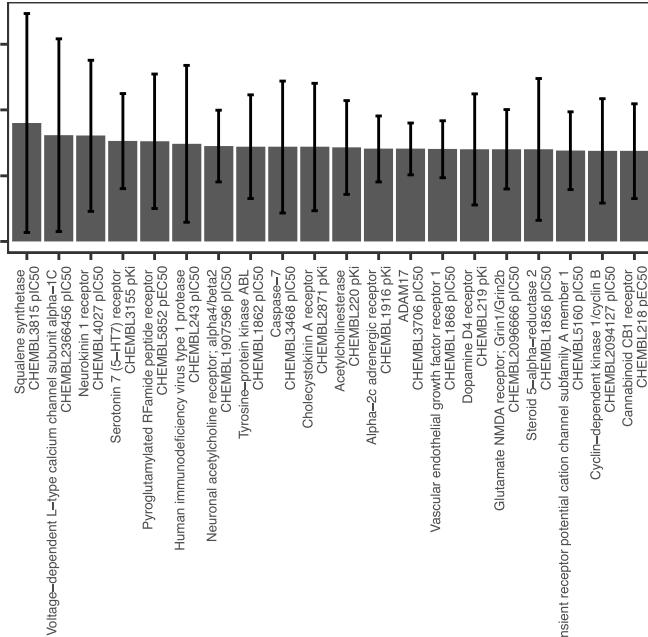
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Feature importance



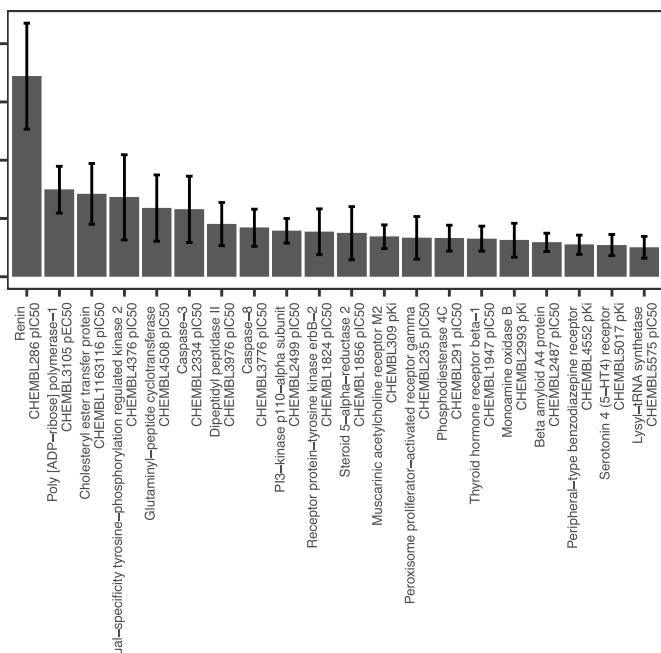
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Feature importance



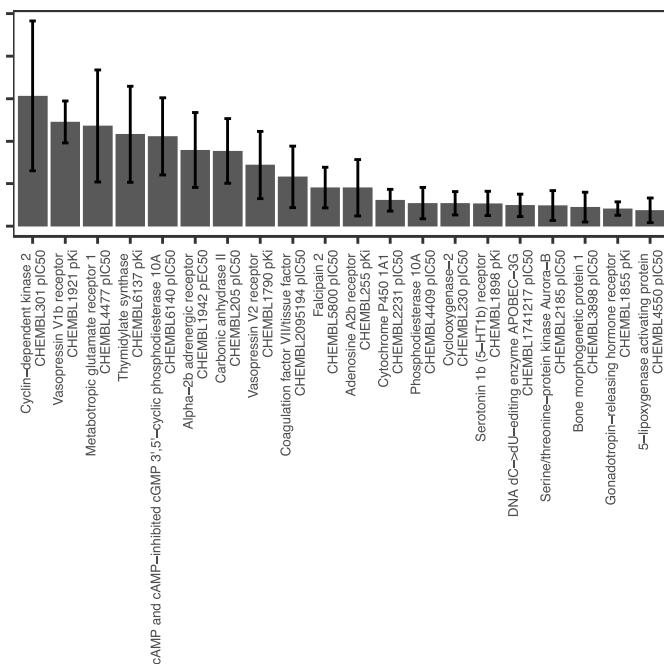
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Feature importance



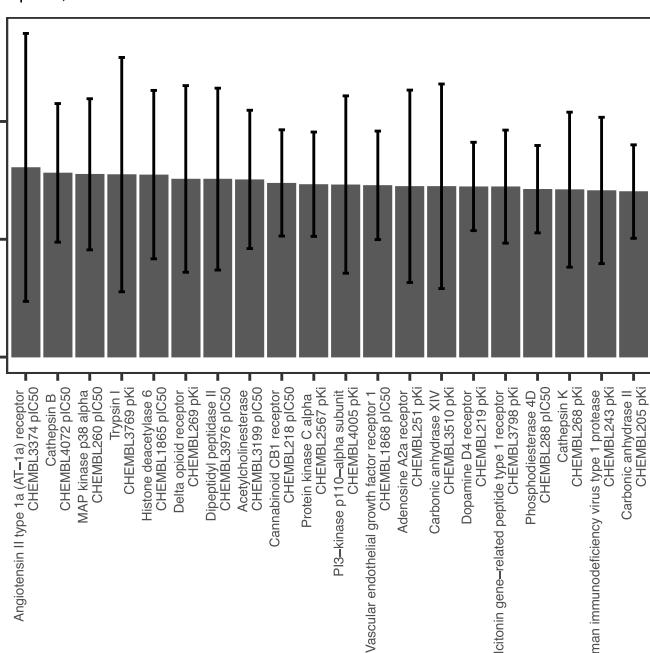
Ephrin; rv-QAFFP 1360

Feature importance



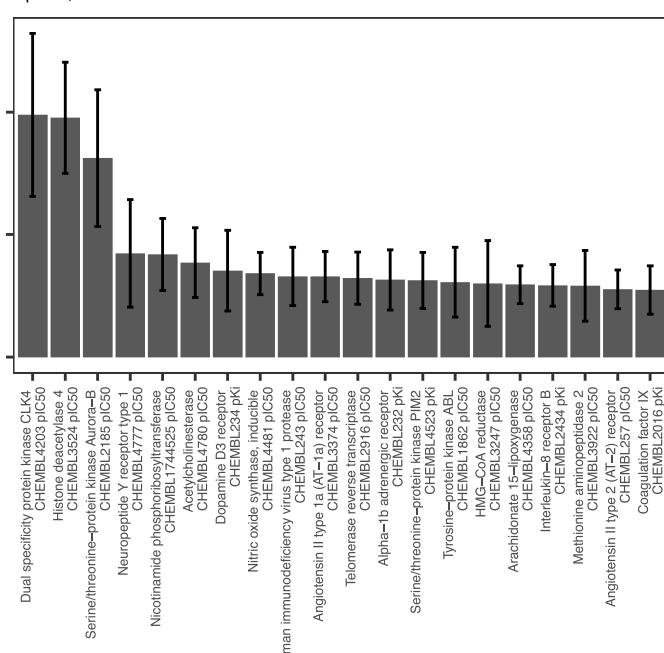
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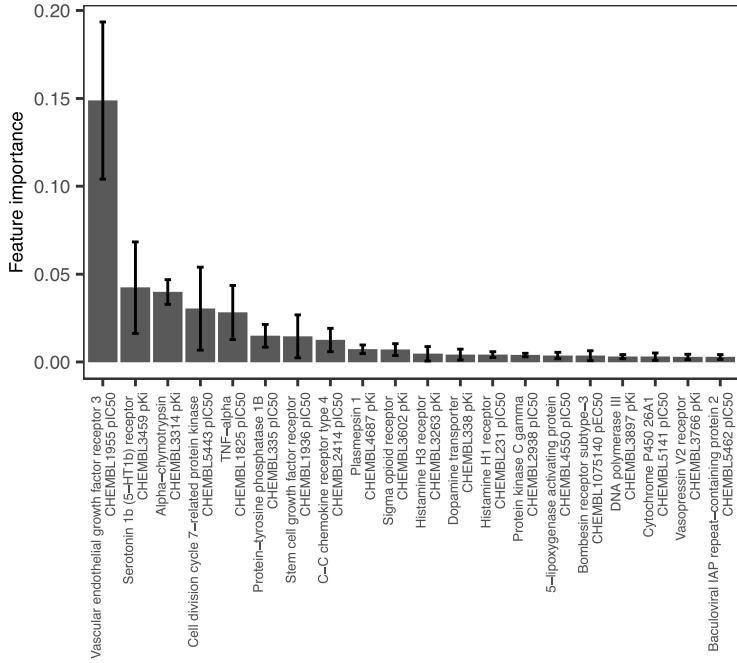


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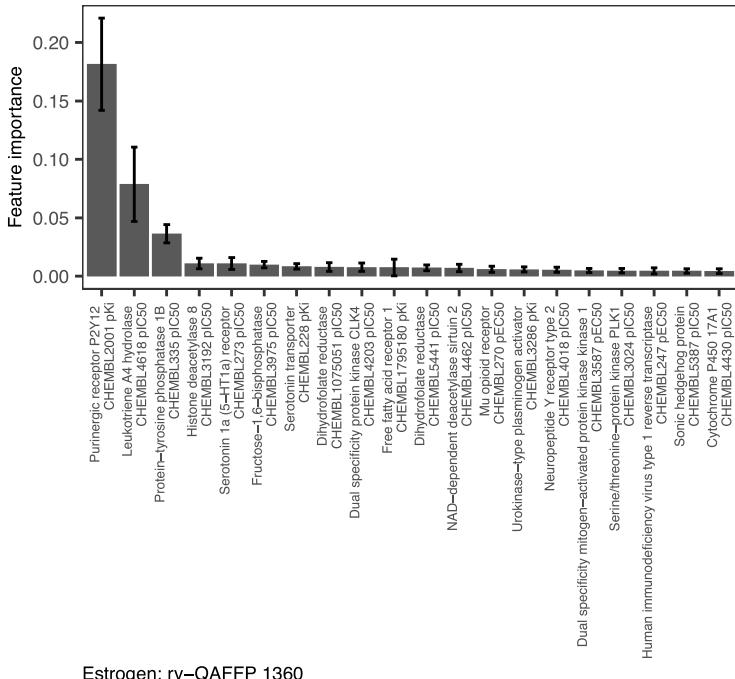
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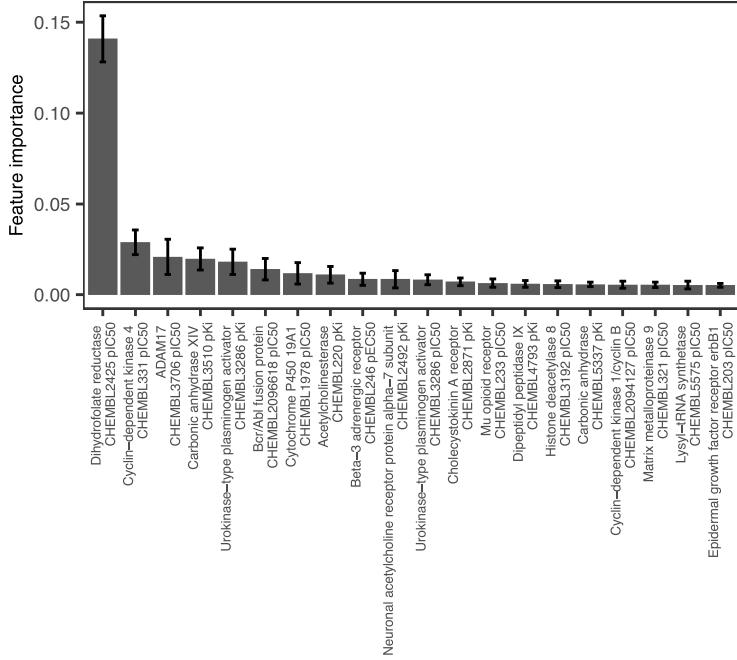
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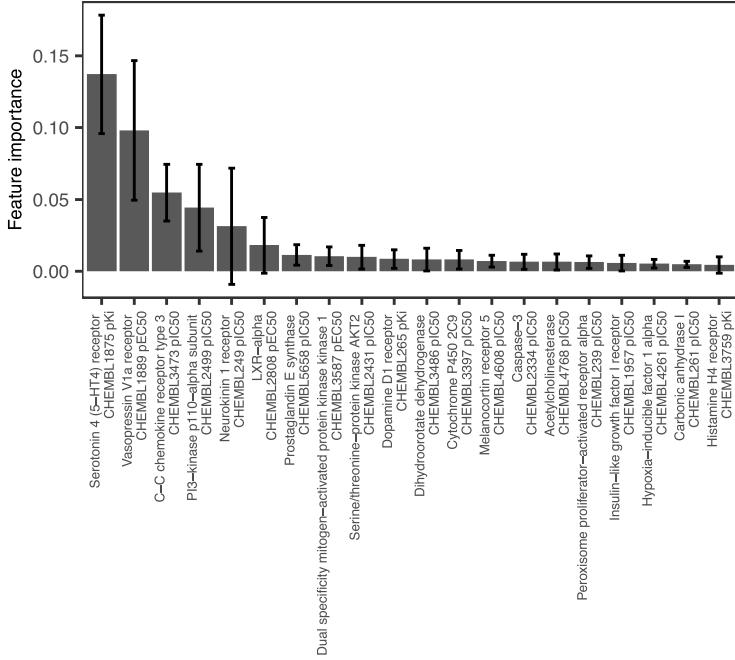
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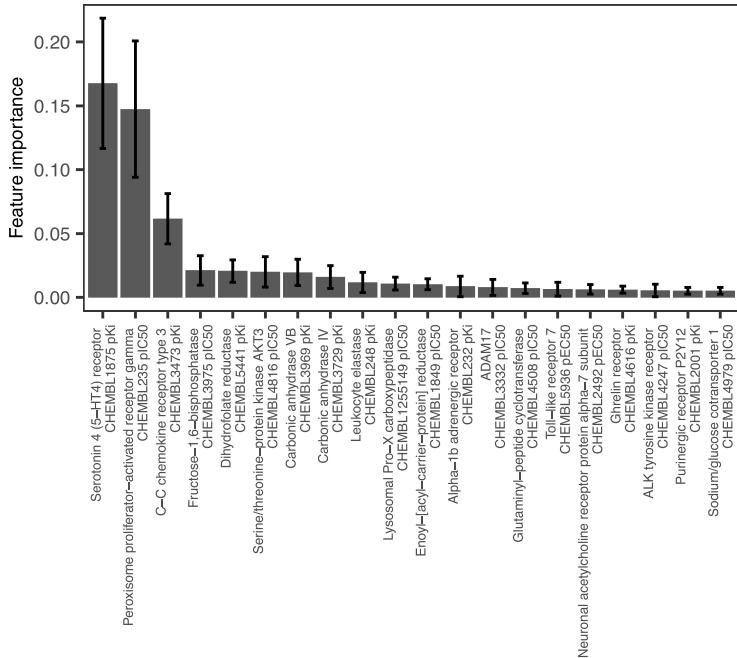
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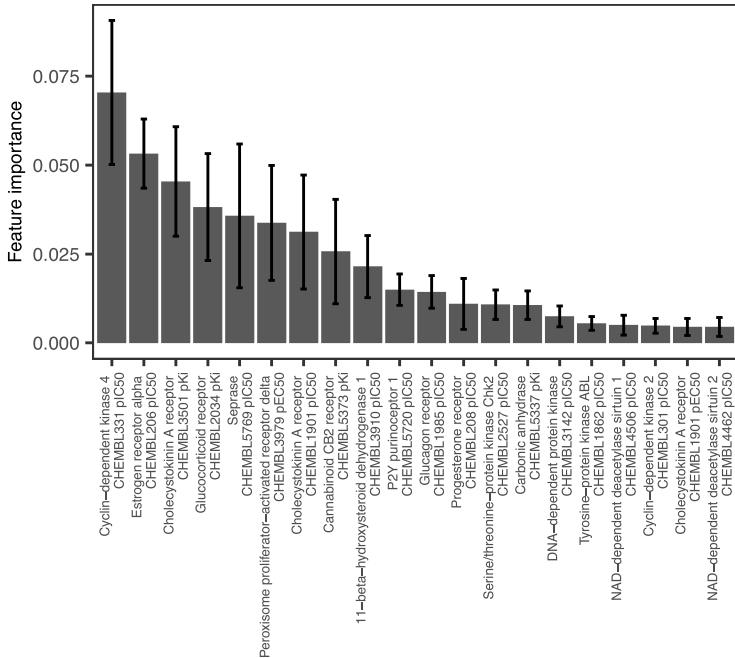
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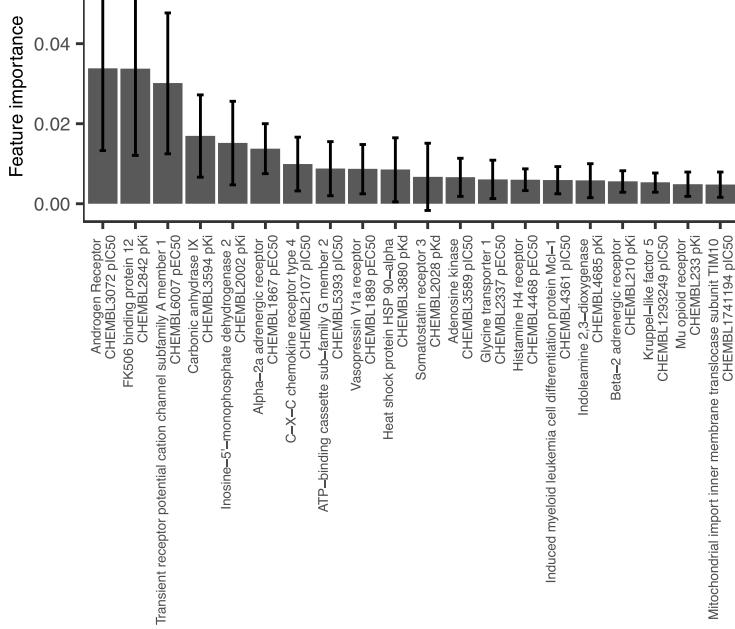
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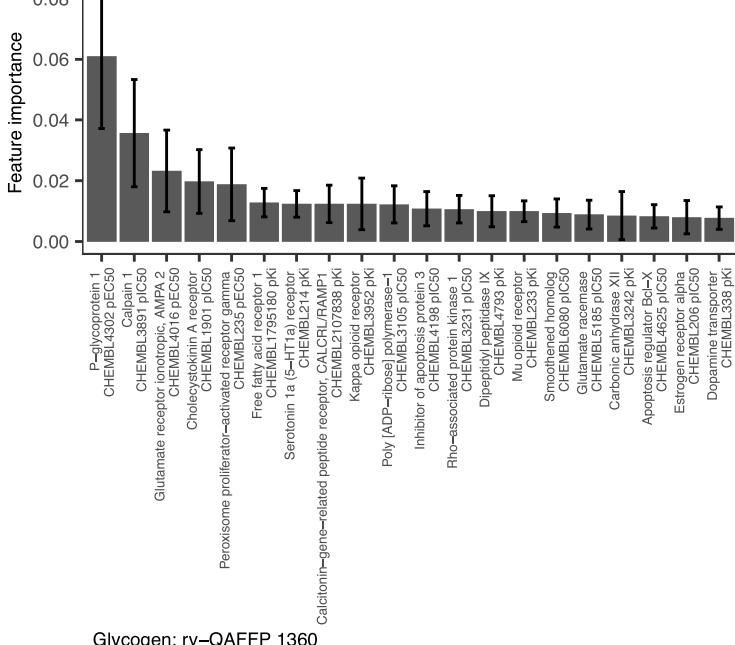
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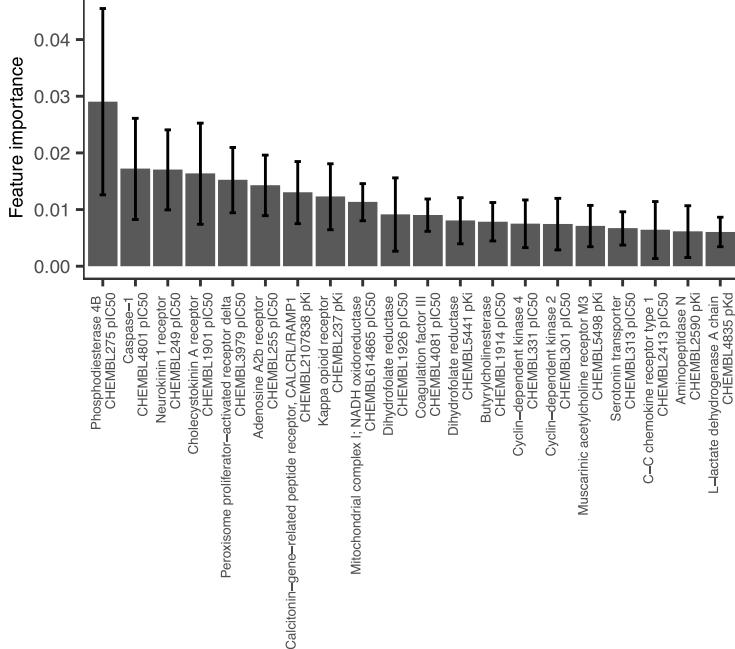
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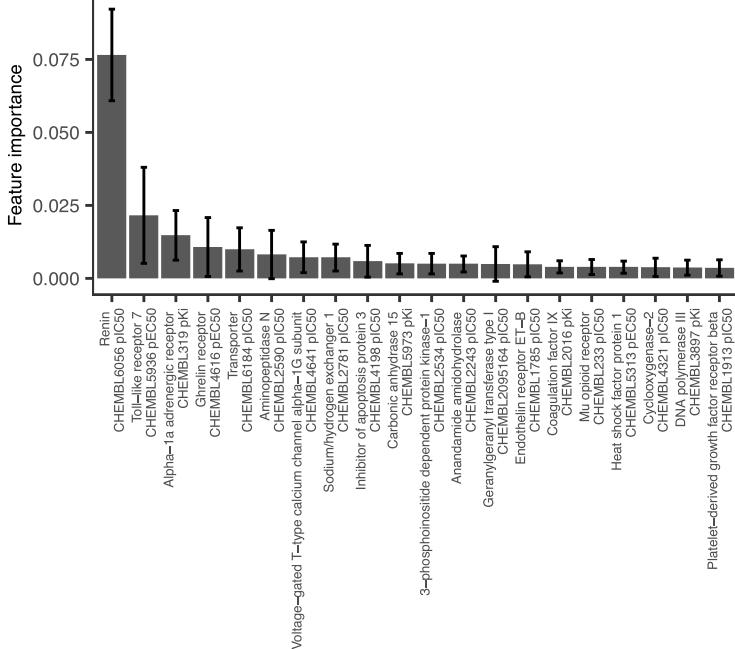
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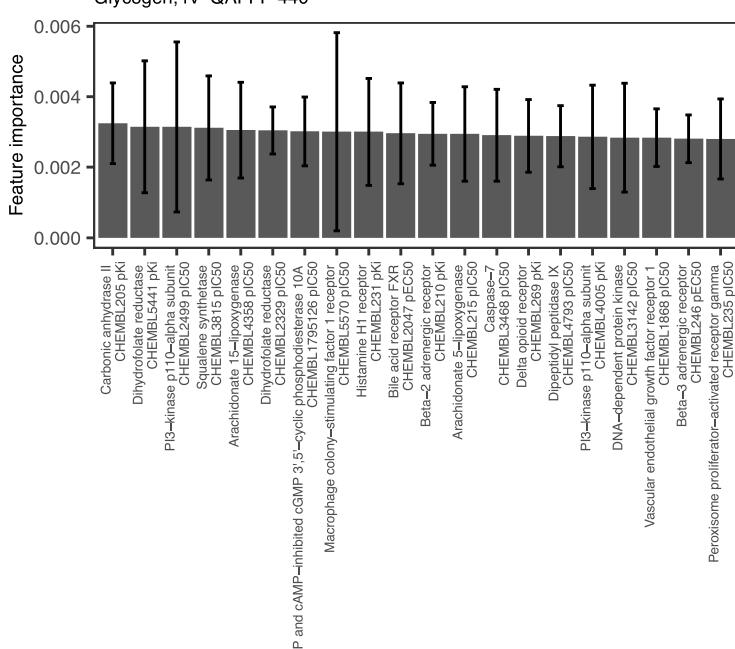
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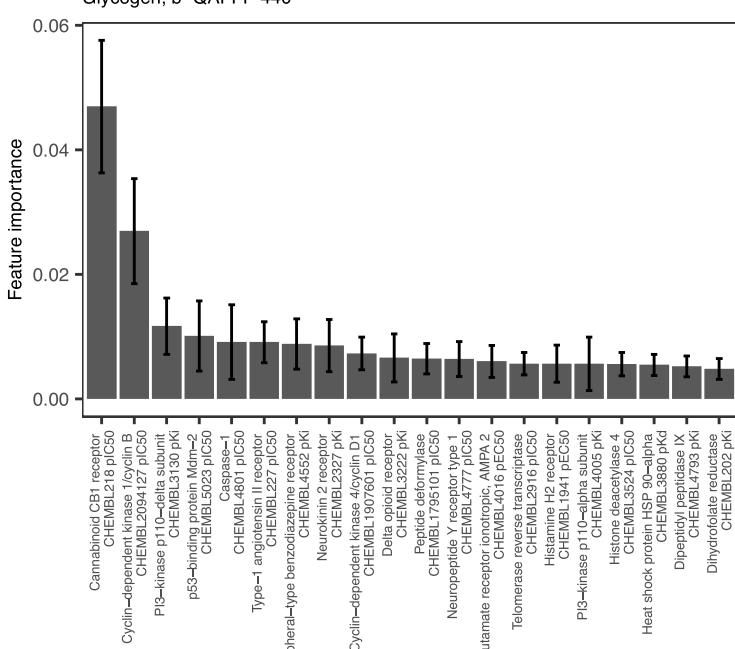
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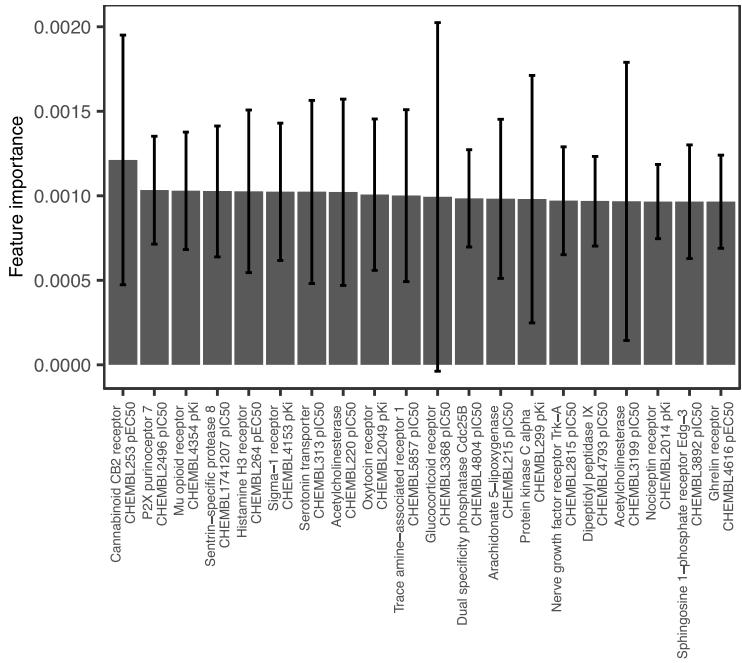
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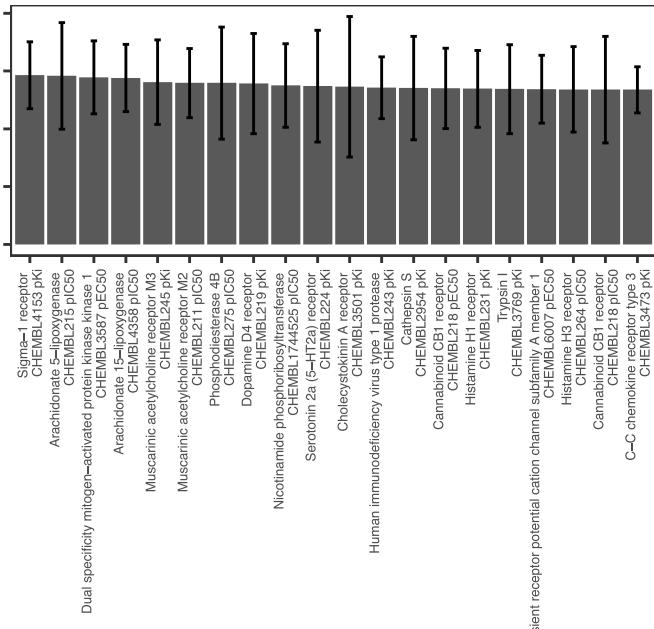
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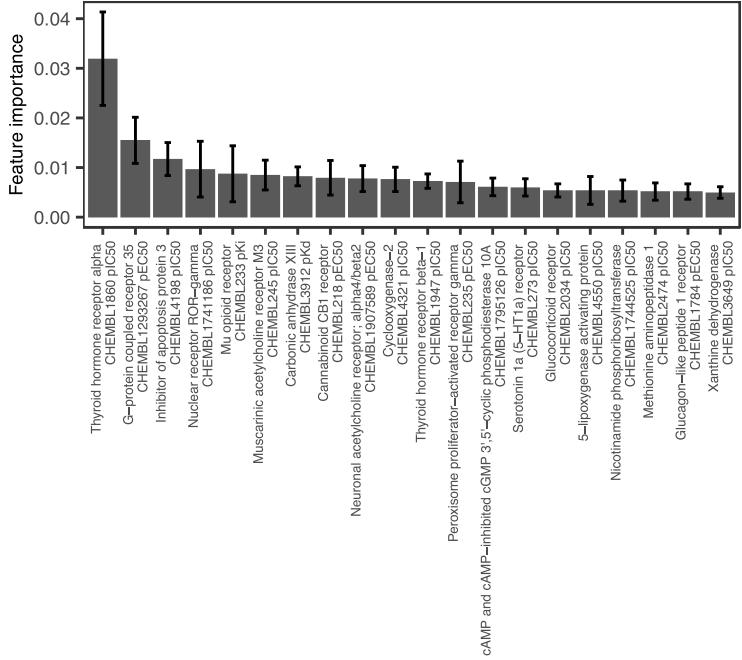
HCT-116; rv-QAFFP 1360



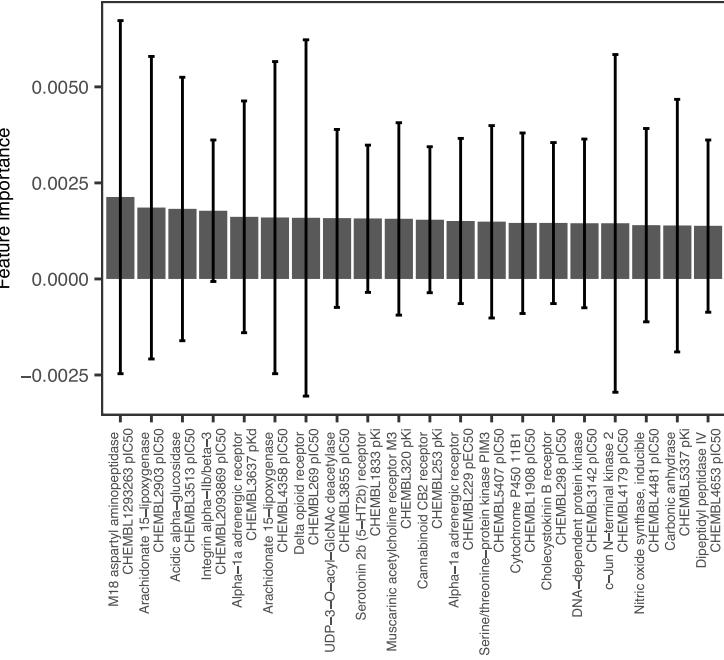
HCT-116; rv-QAFFP 440



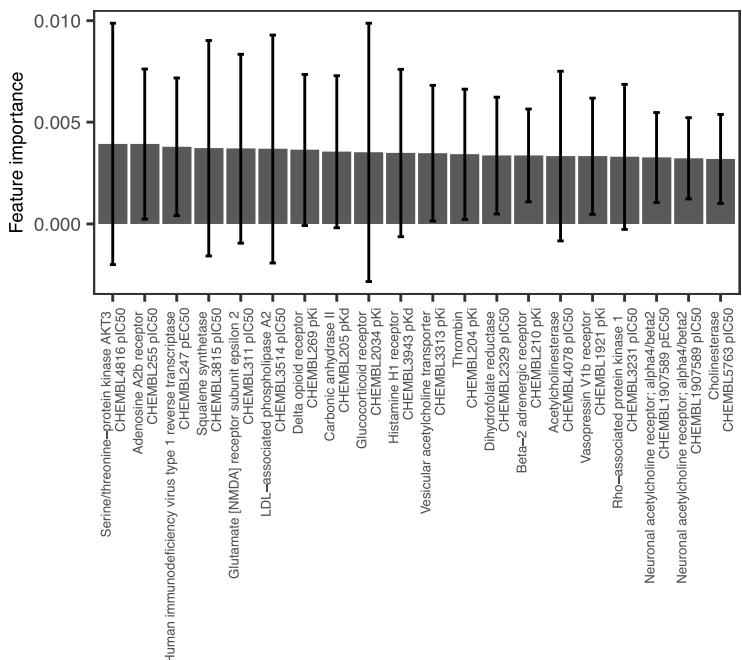
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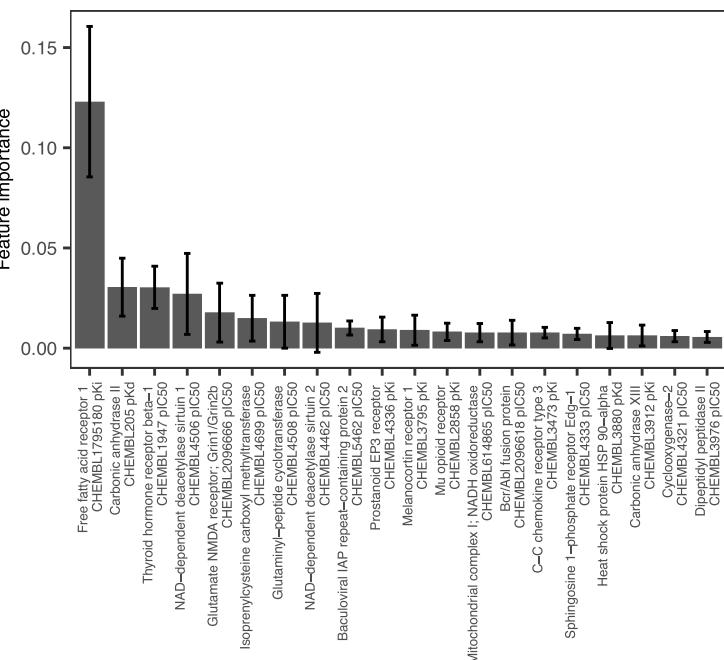
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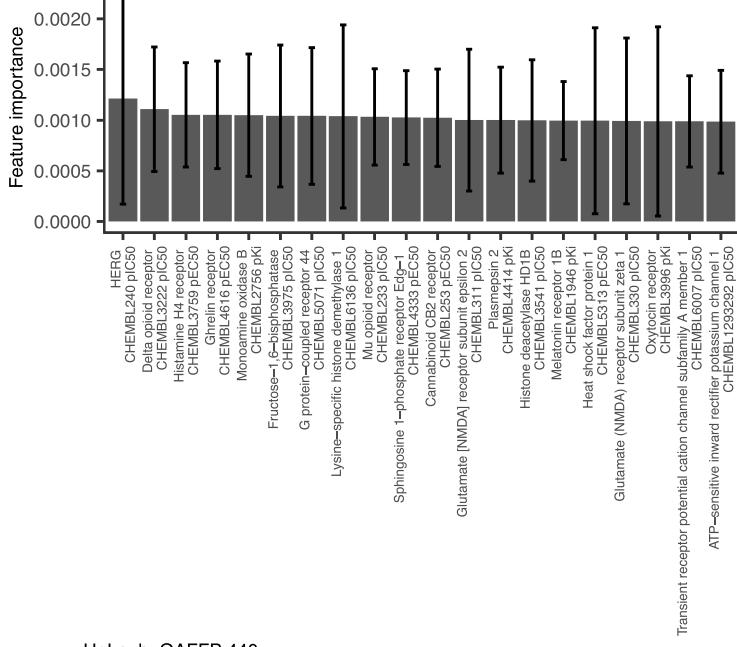
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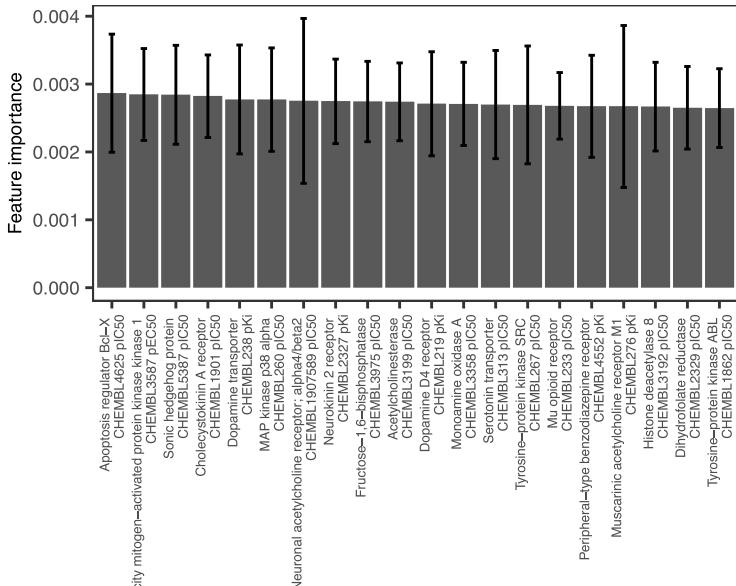
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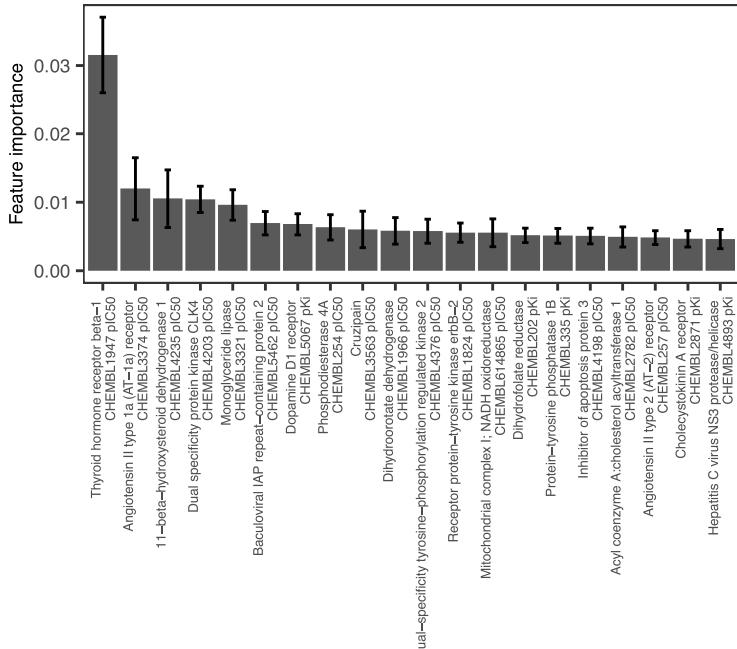
HeLa; rv-QAFFP 1360



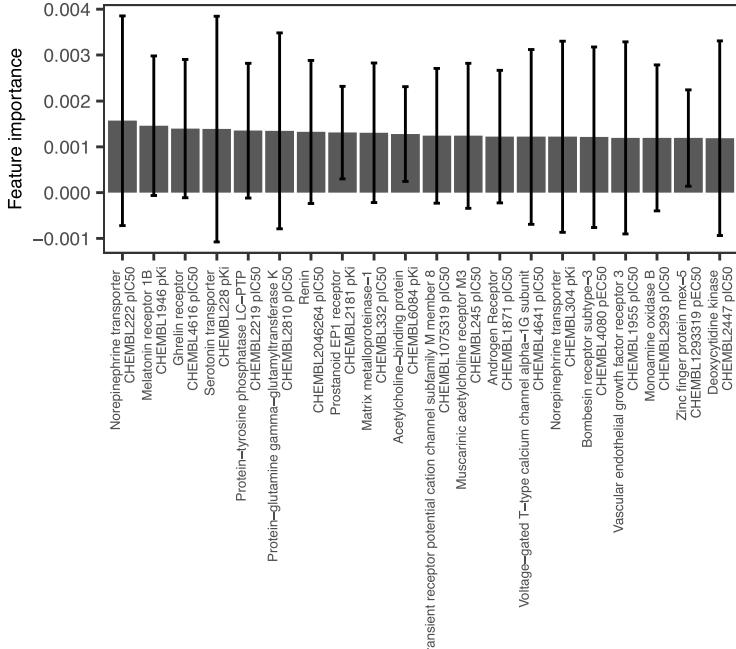
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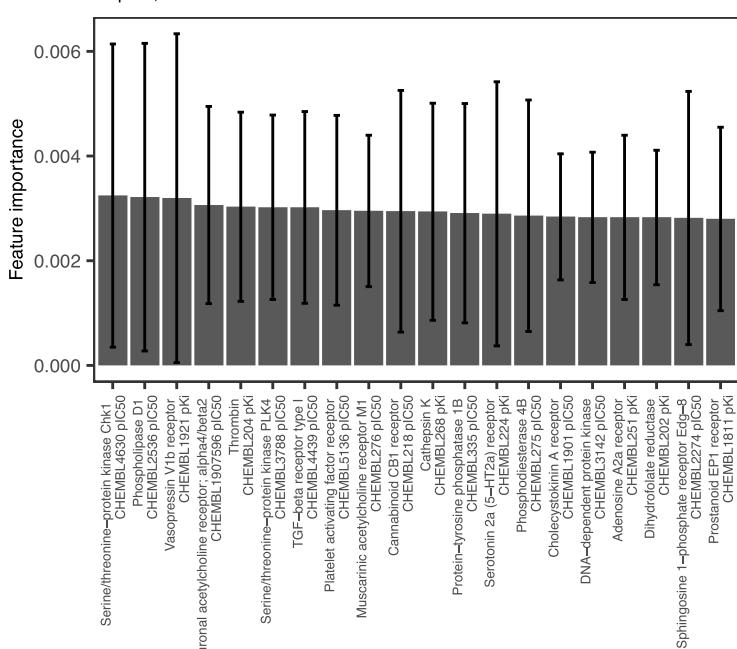
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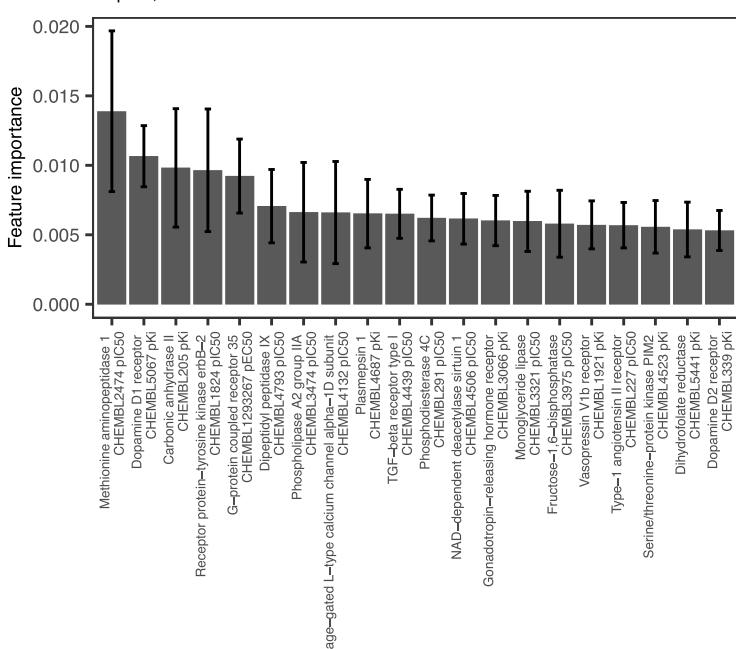
HepG2; rv-QAFFP 1360

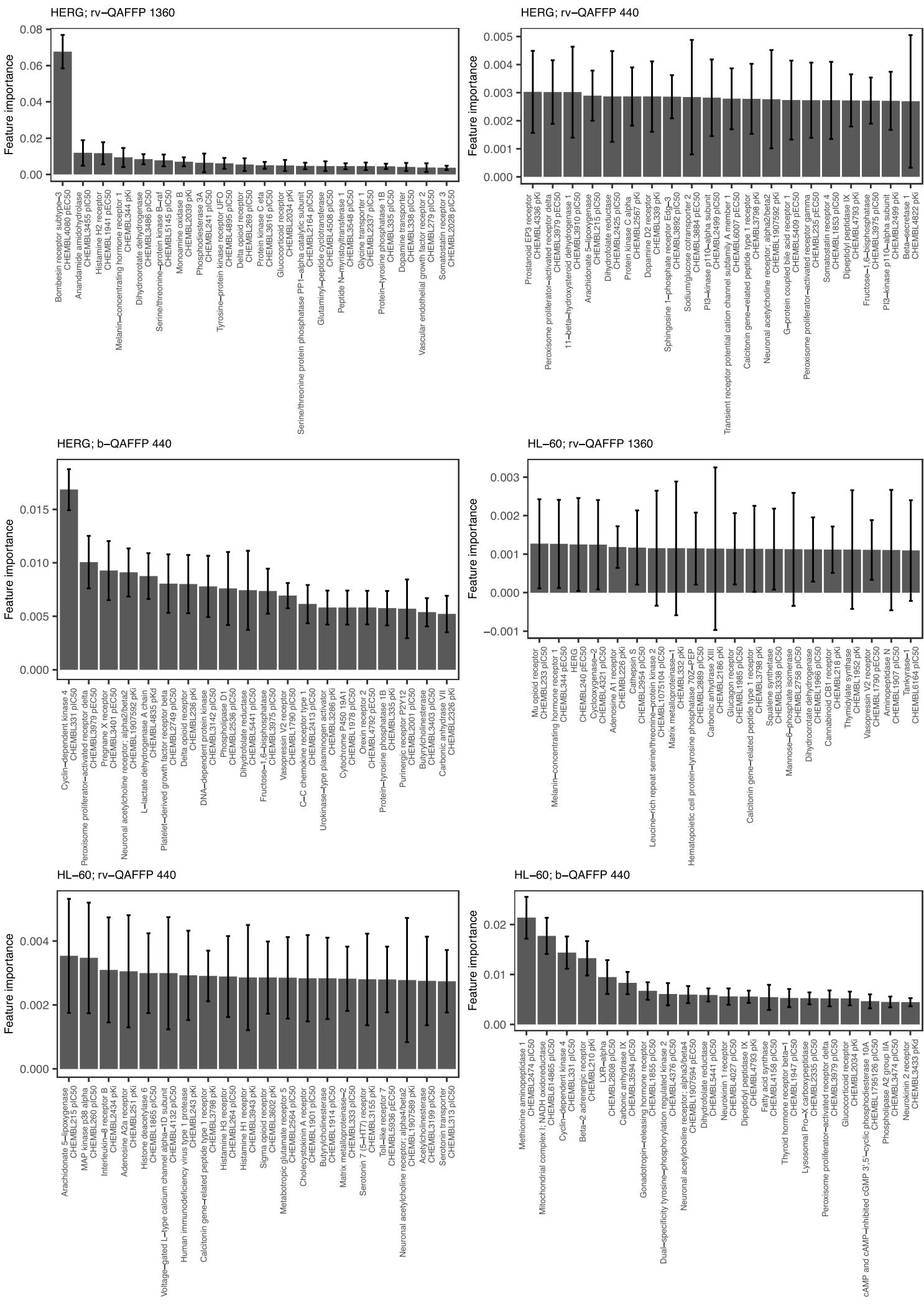


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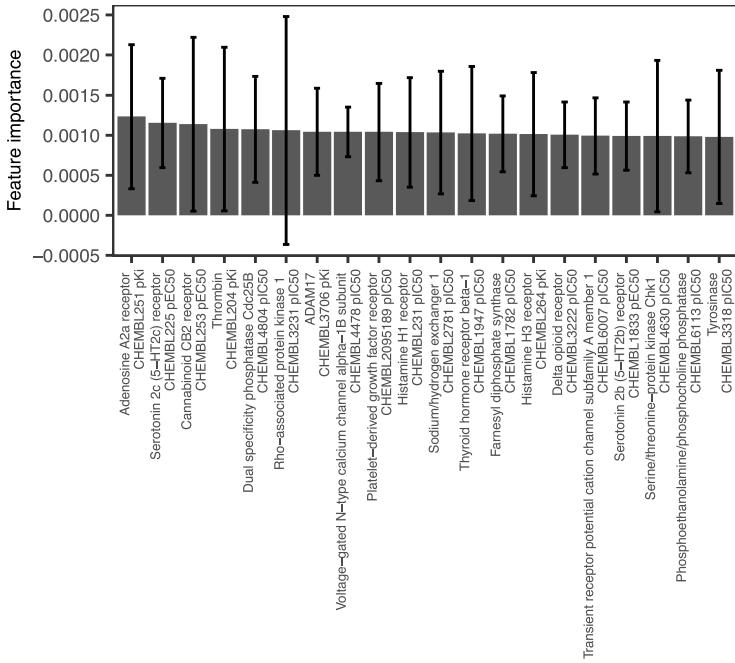


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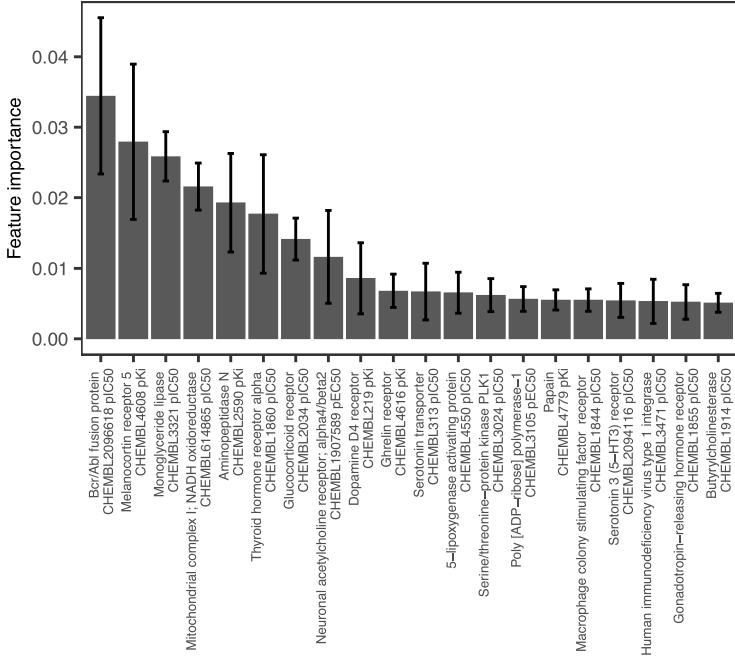




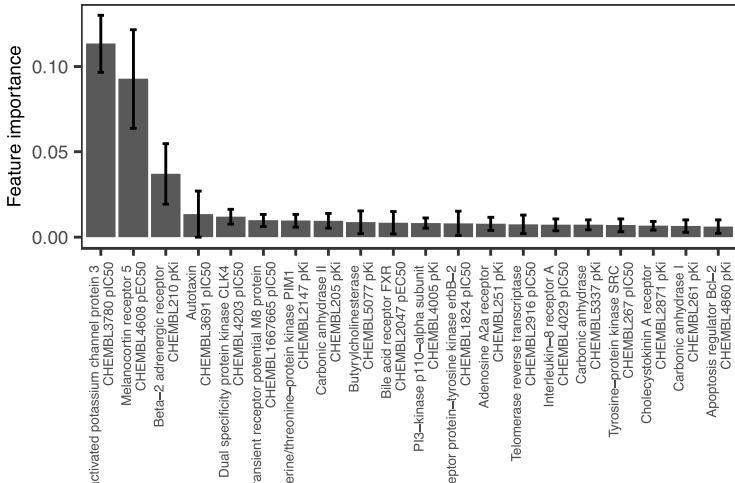
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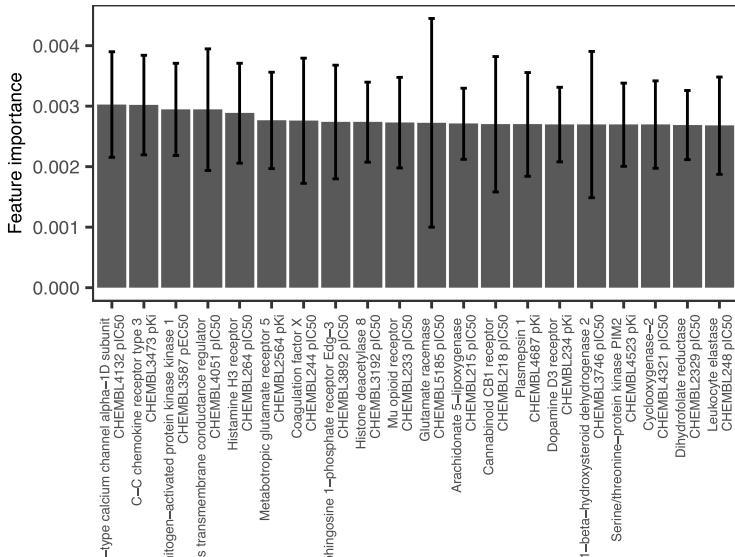
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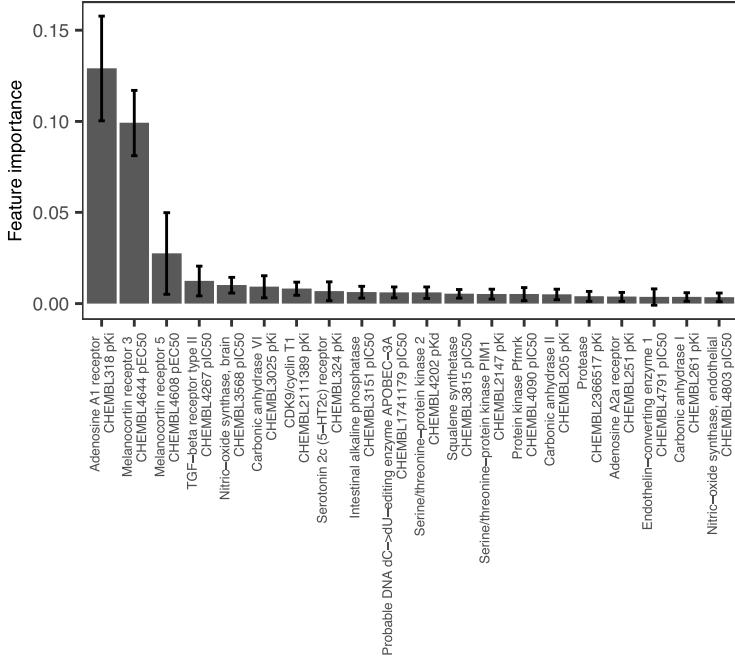
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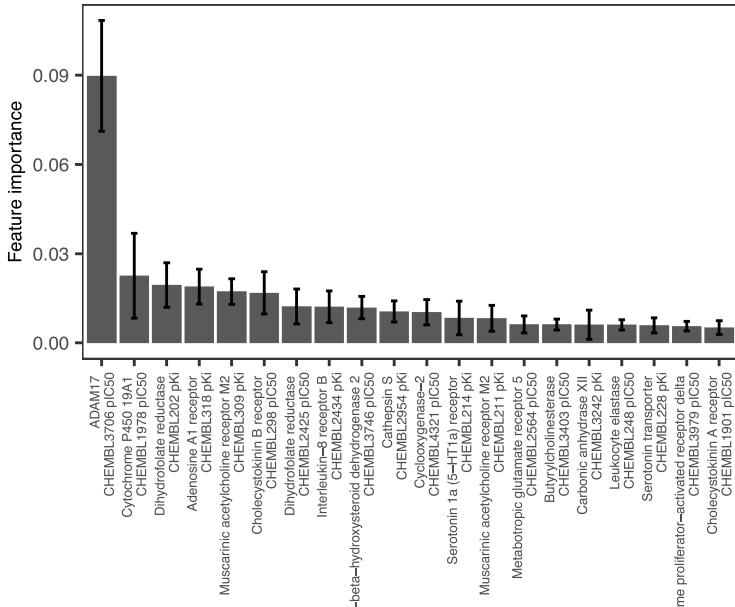
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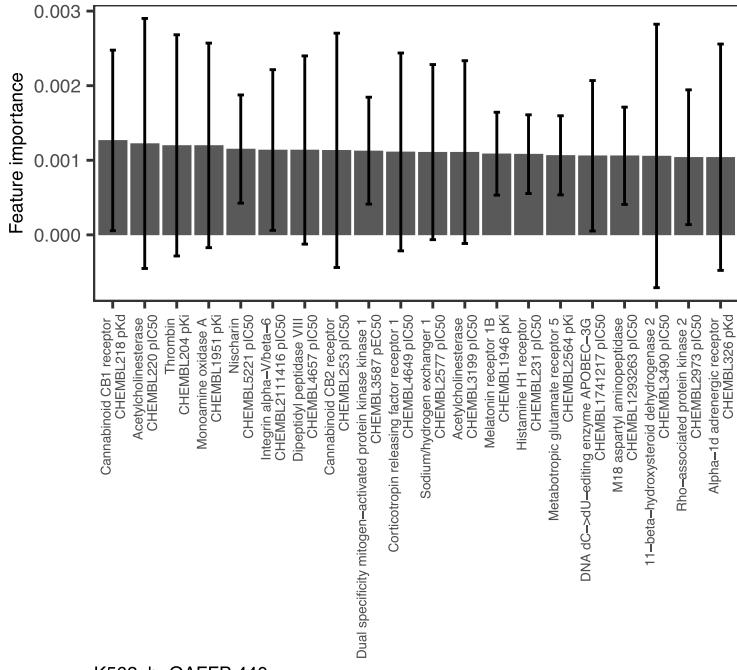
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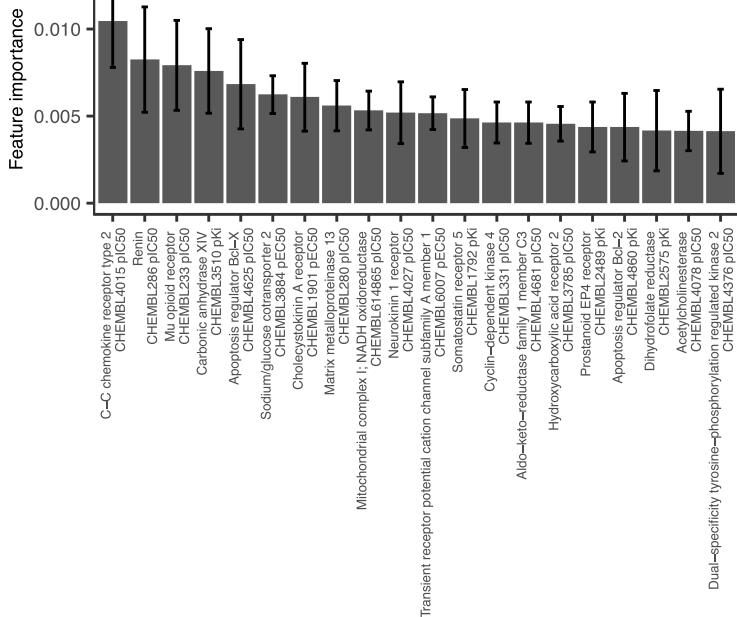
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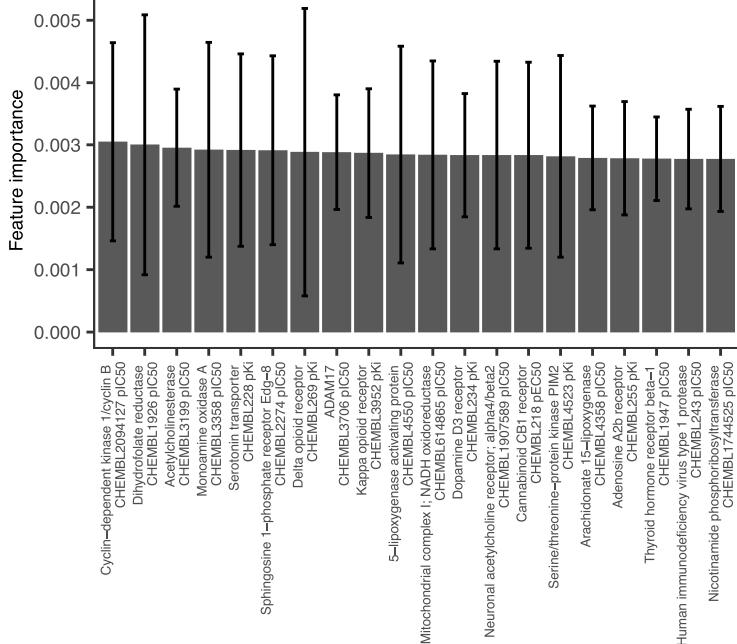
K562; rv-QAFFP 1360



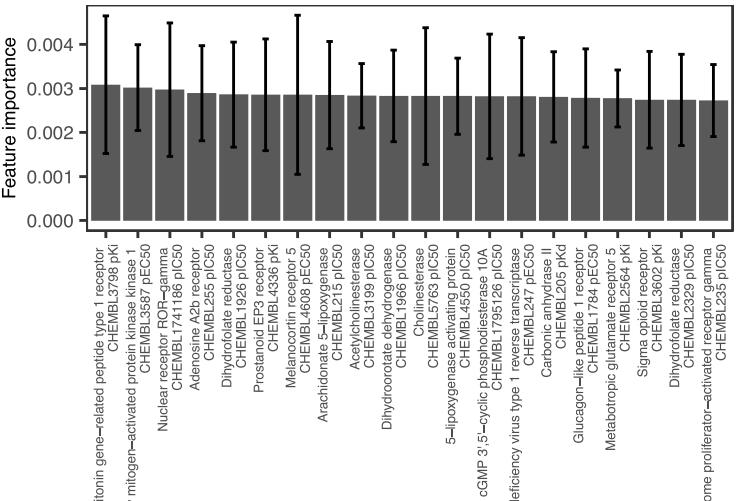
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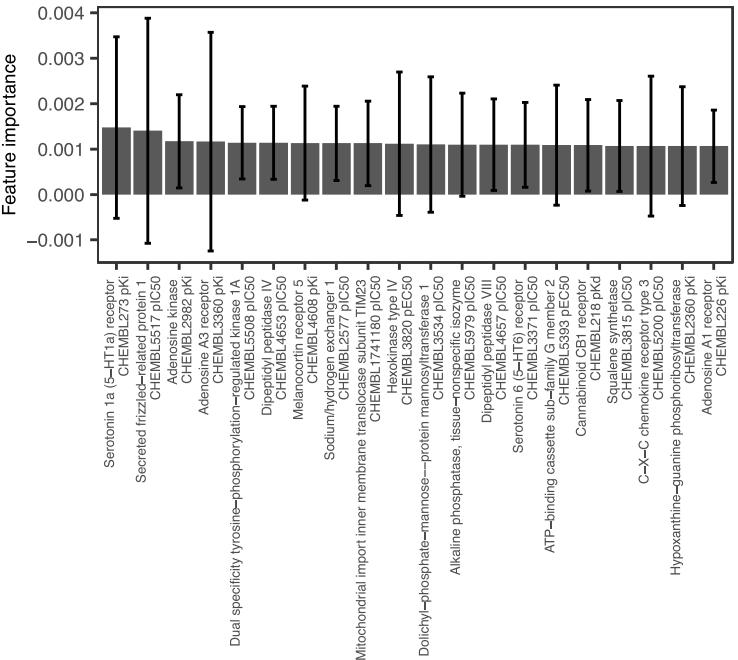
KB; rv-QAFFP 440



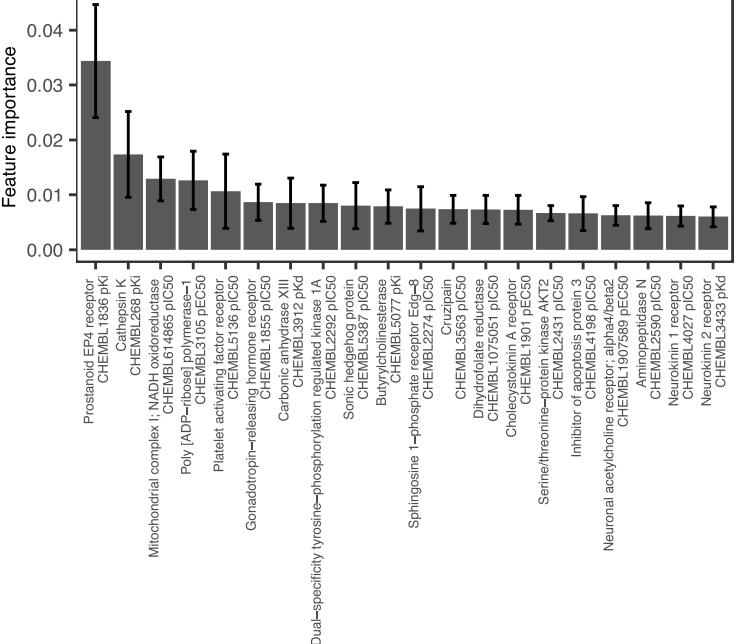
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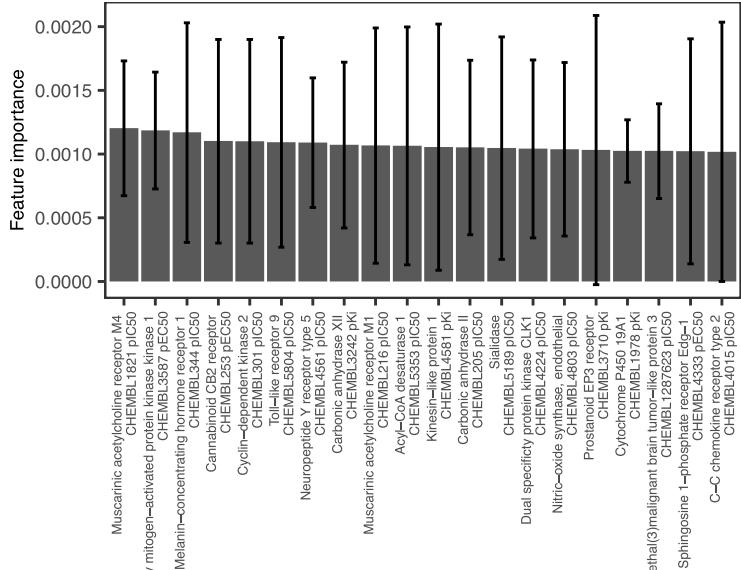
KB; rv-QAFFP 1360



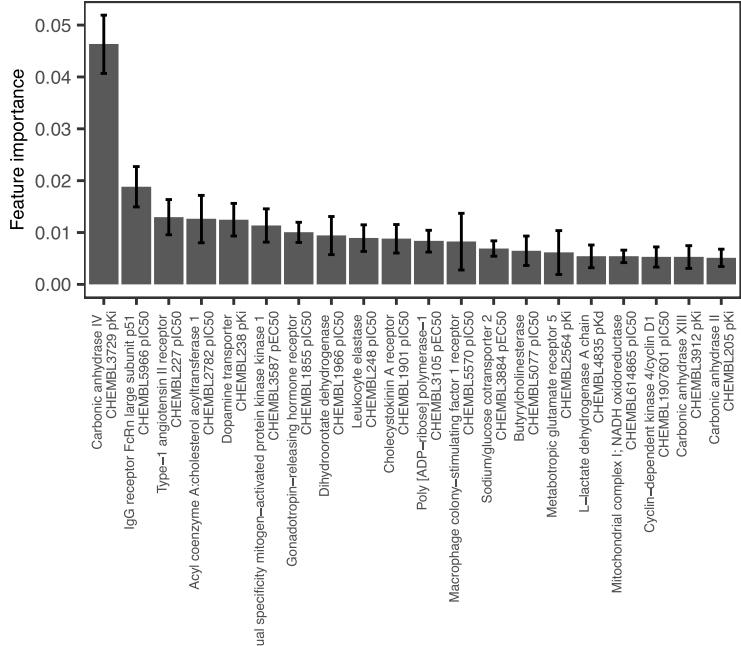
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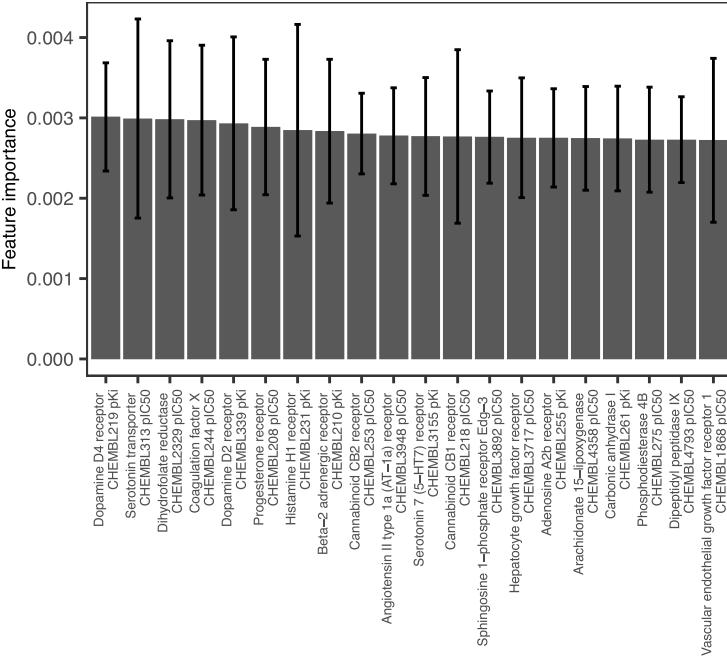
L1210; rv-QAFFP 1360



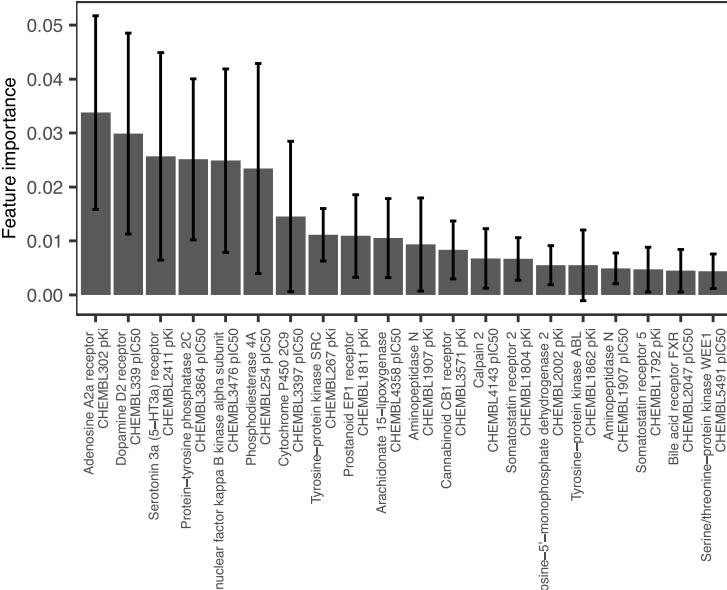
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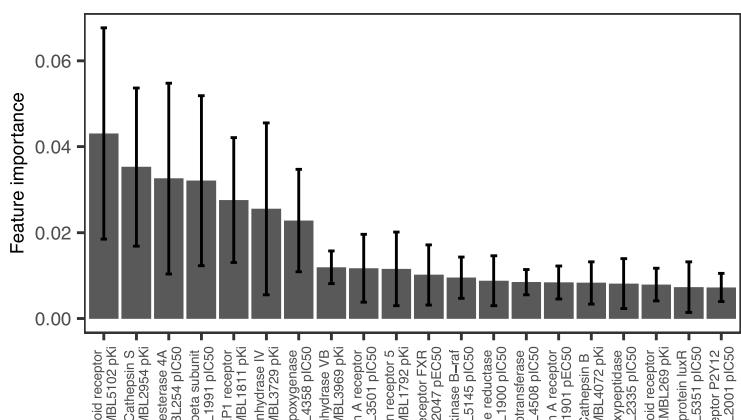
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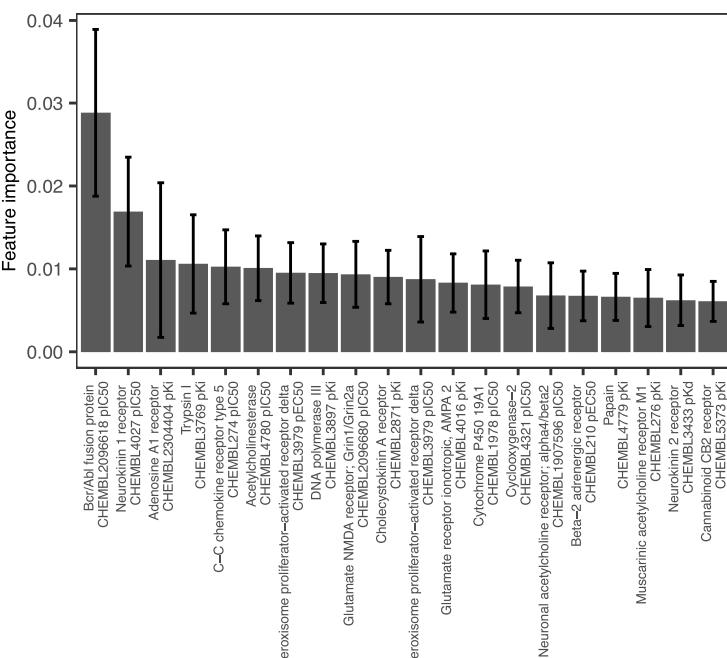
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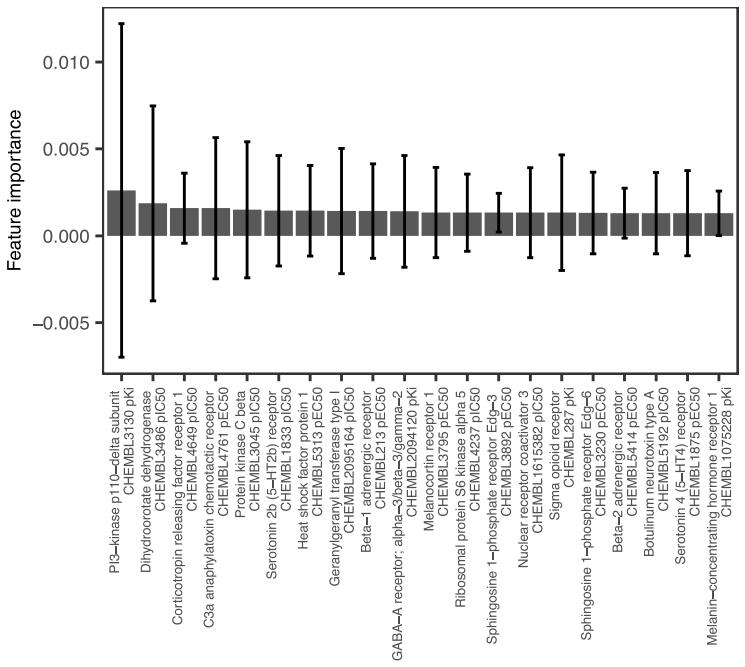
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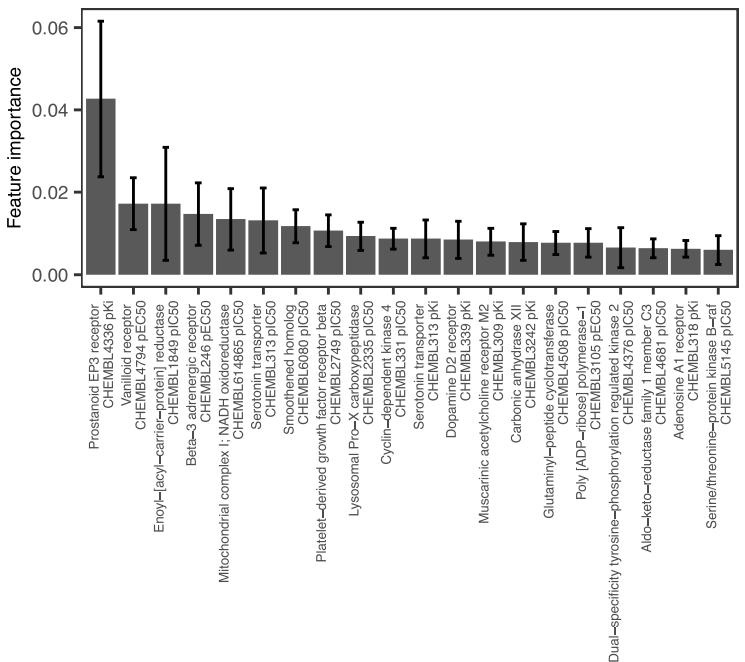
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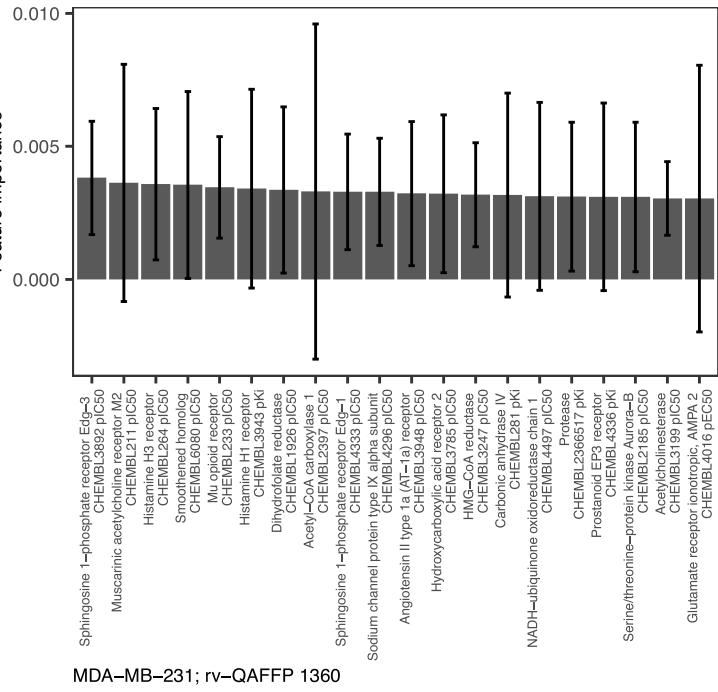
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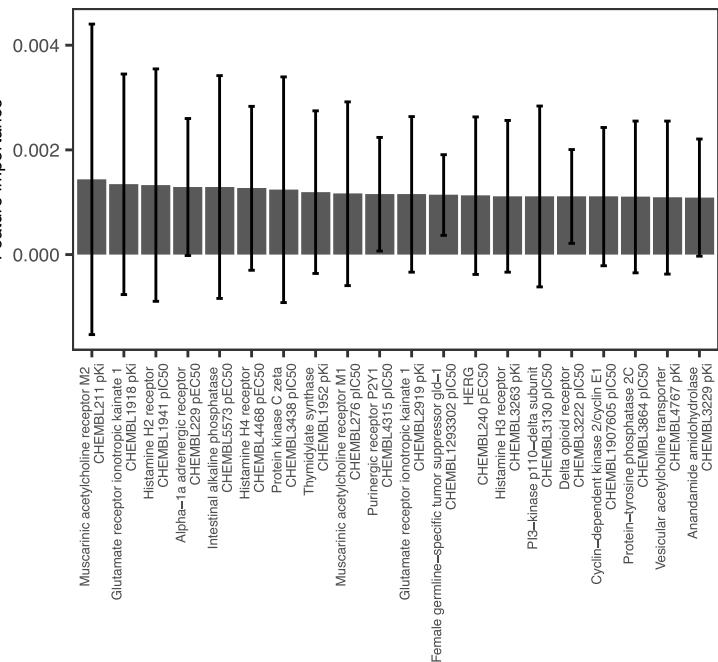
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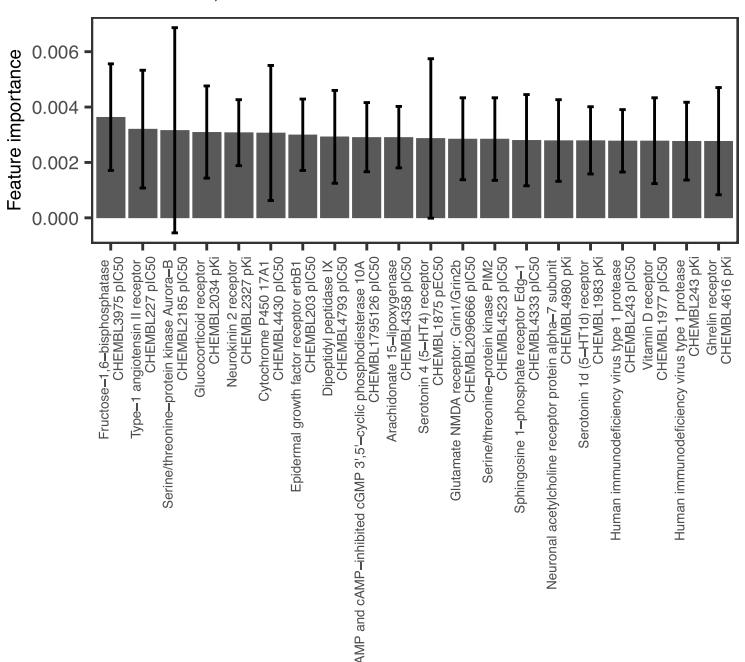
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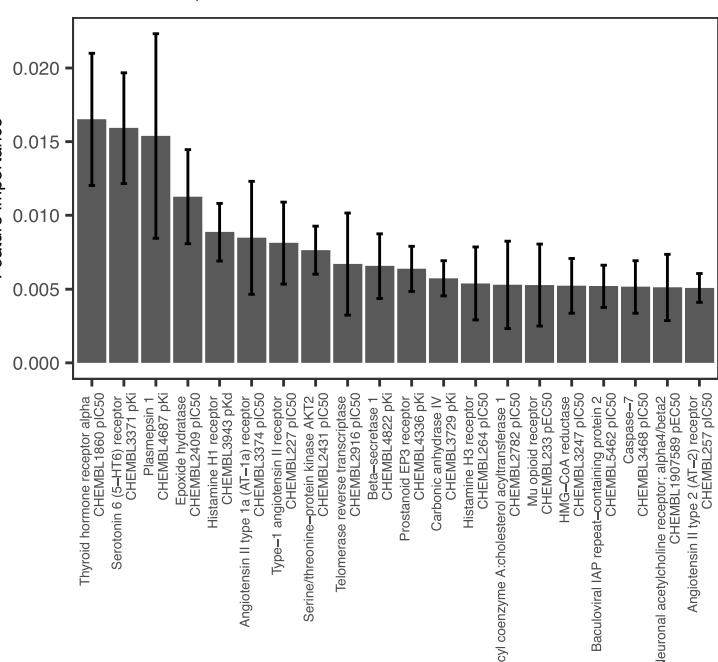
MDA-MB-231; rv-QAFFP 1360



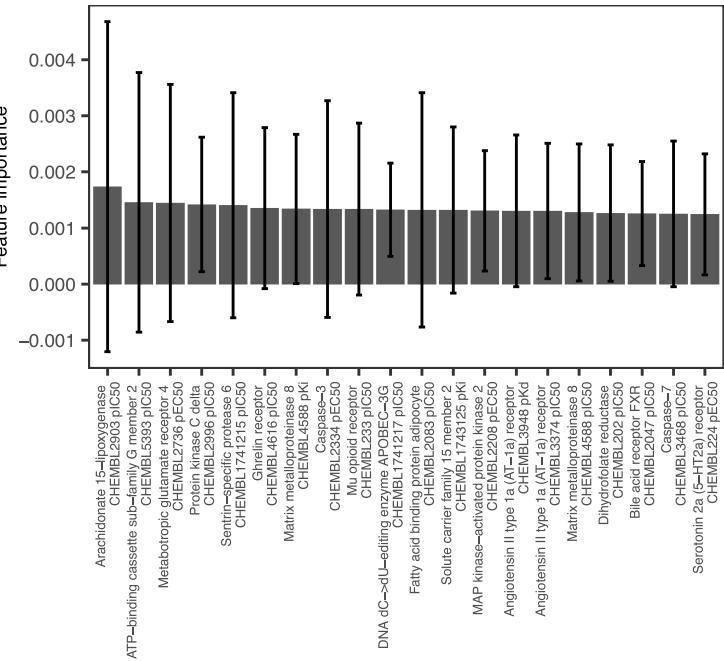
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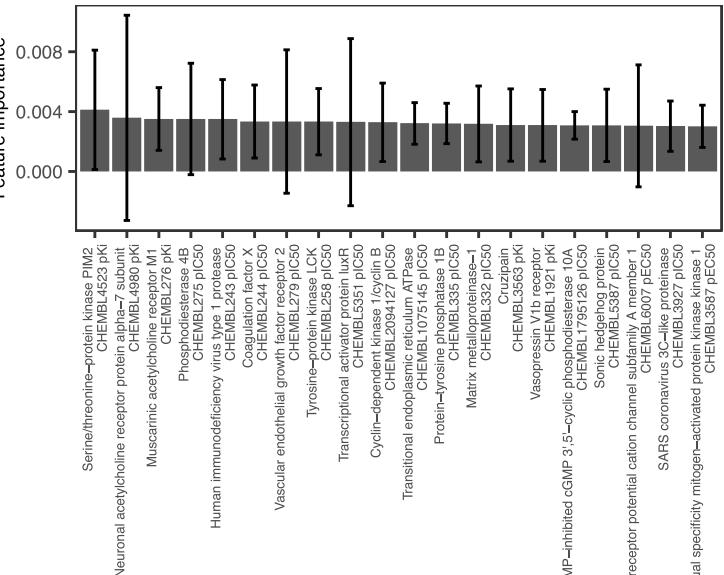
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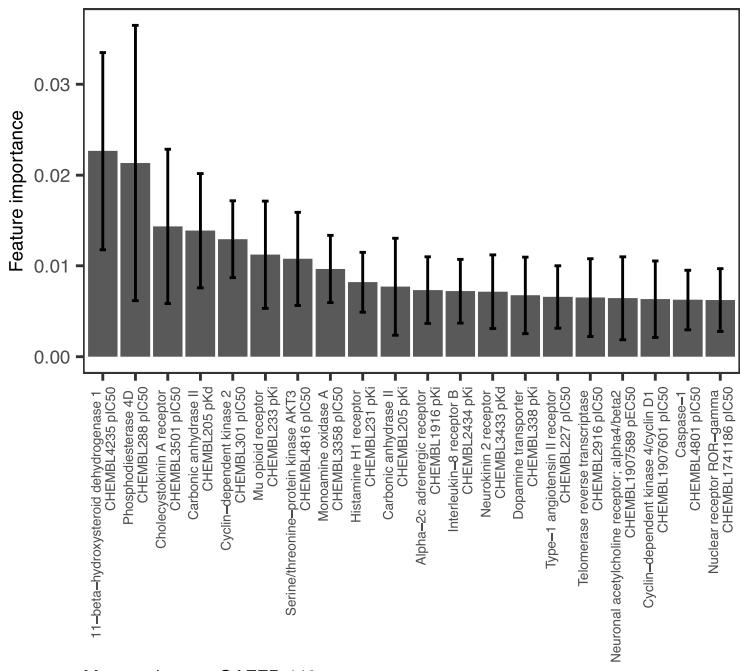
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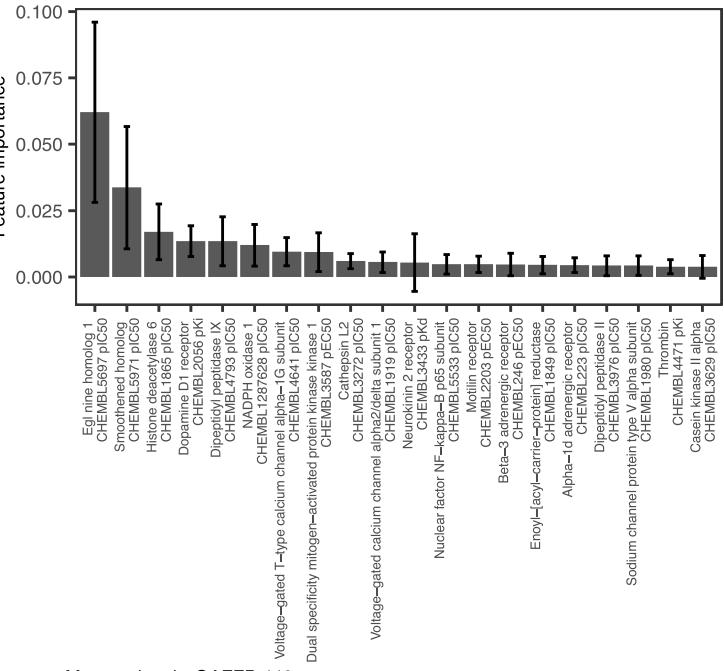
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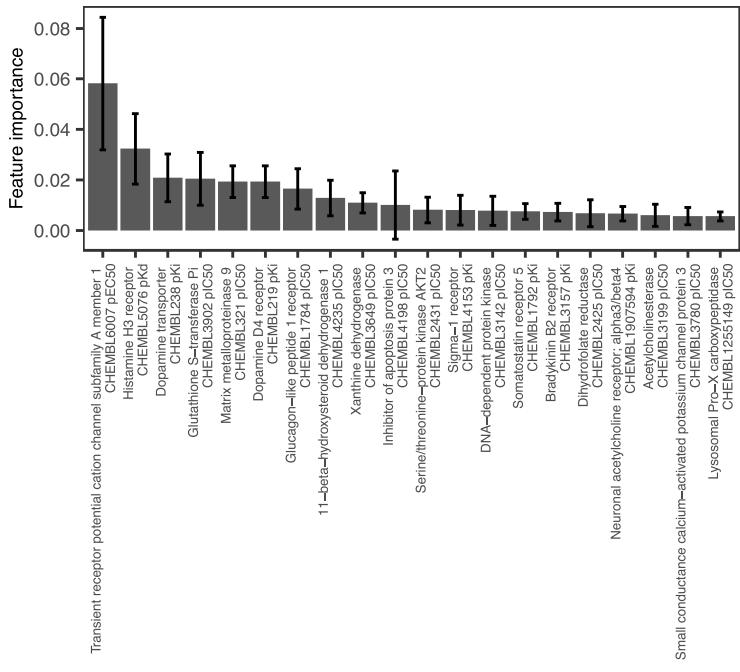
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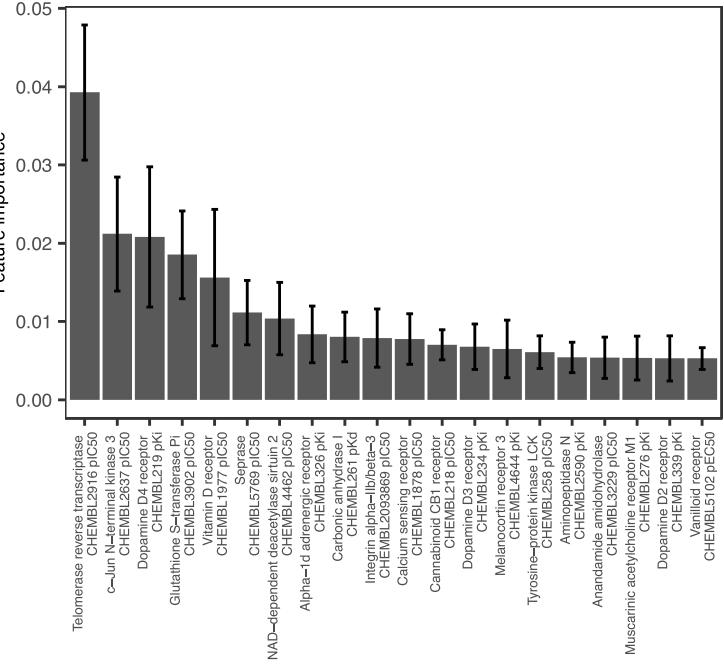
Monoamine; rv-QAFFP 1360



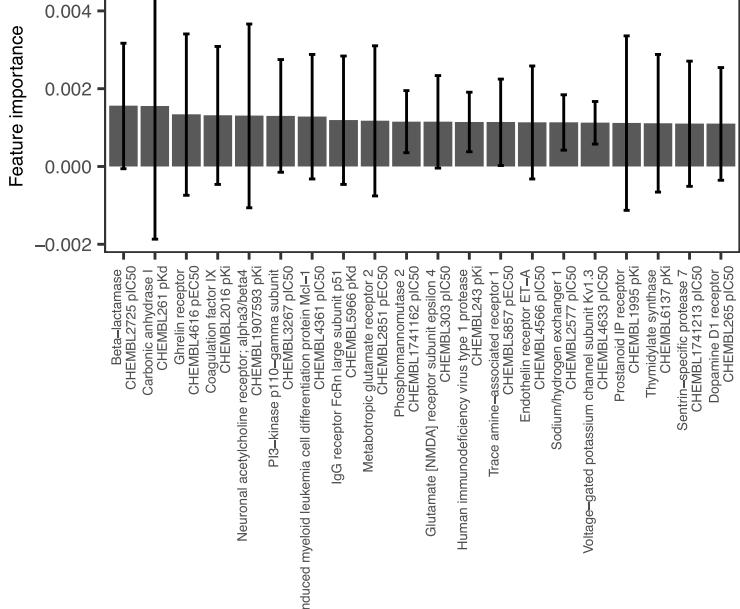
Monoamine; rv-QAFFP 440



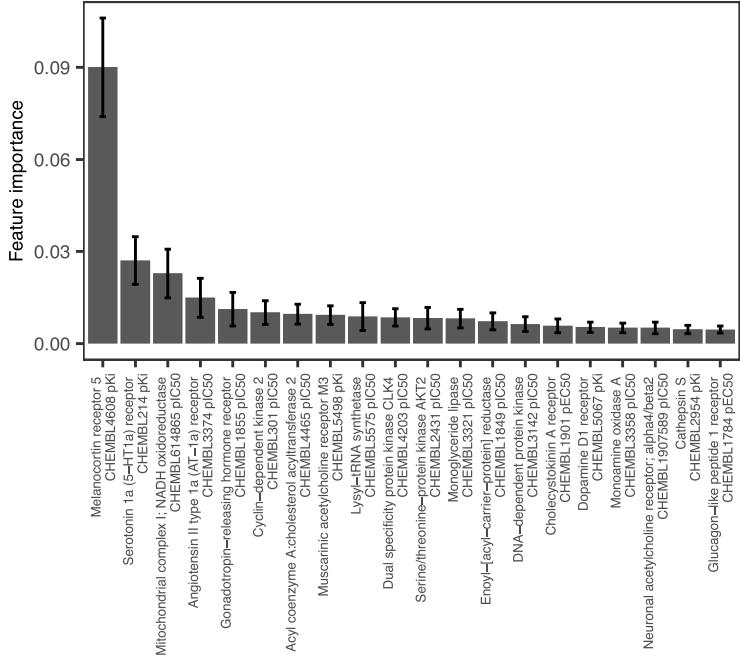
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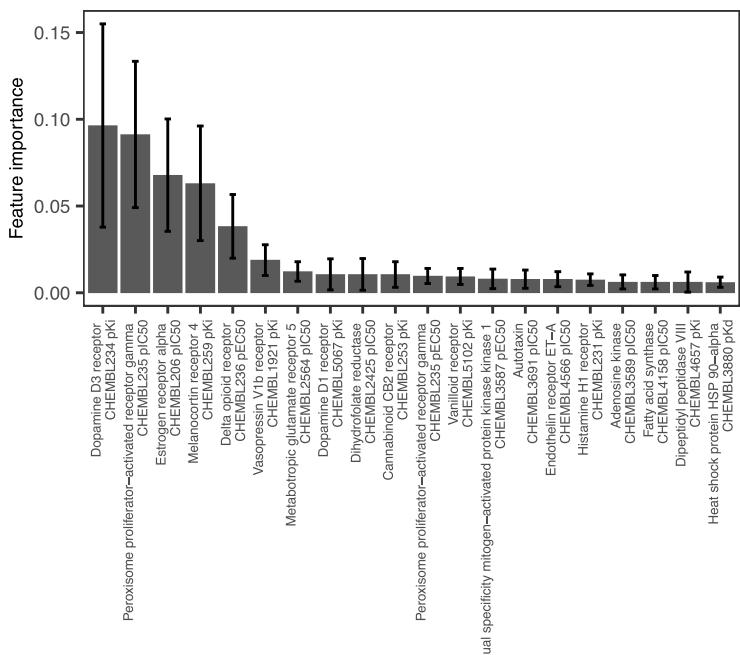
NCI-H460; rv-QAFFP 1360



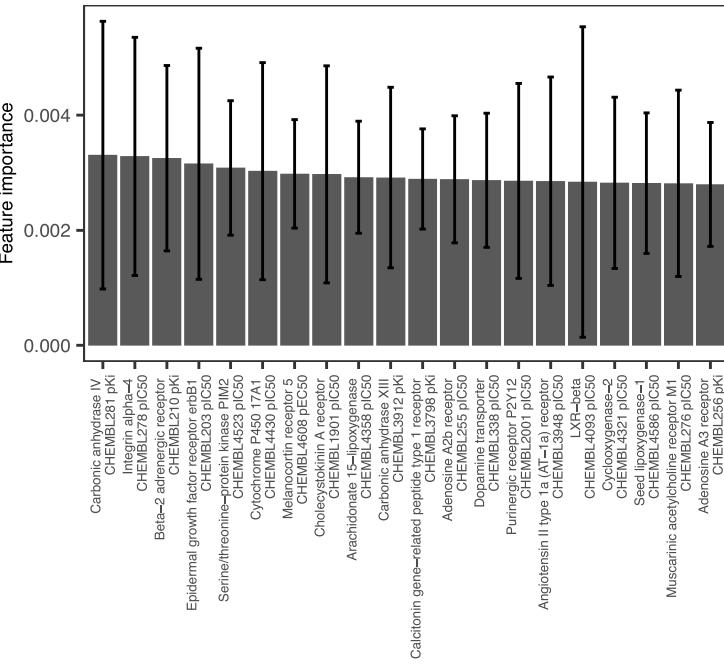
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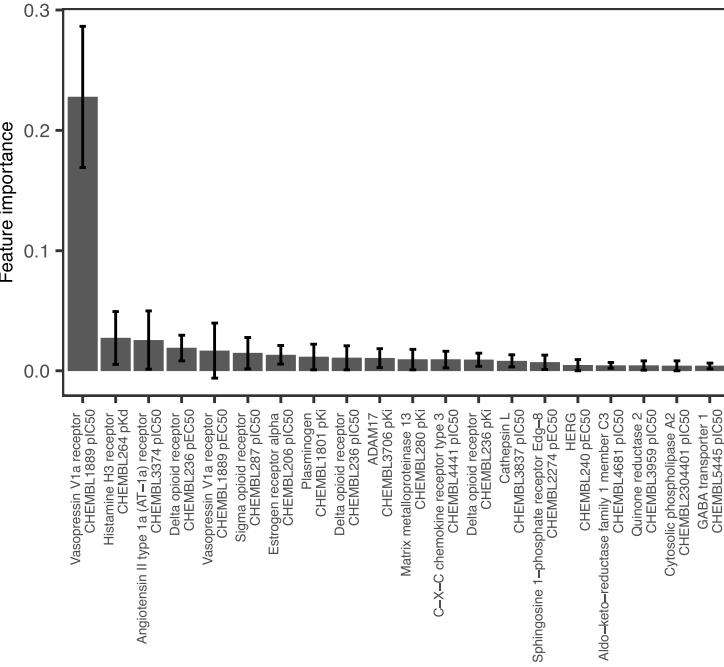
opioid; rv-QAFFP 440



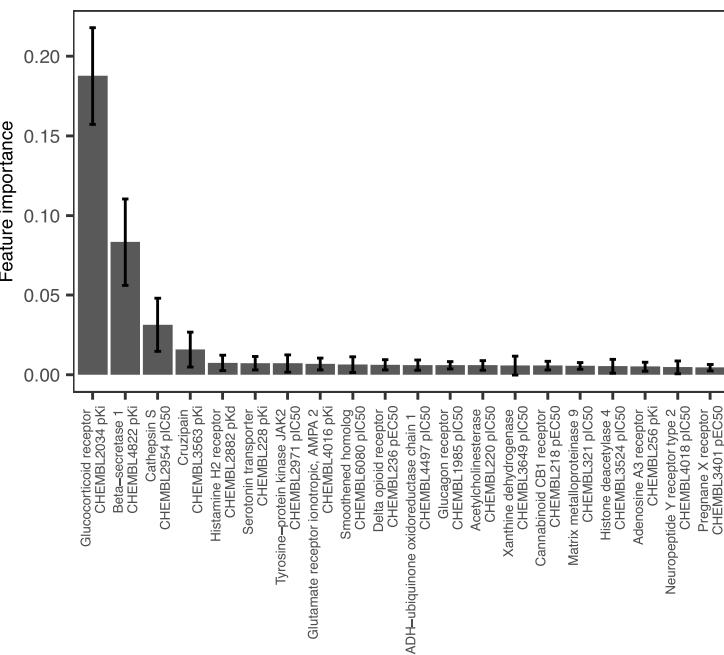
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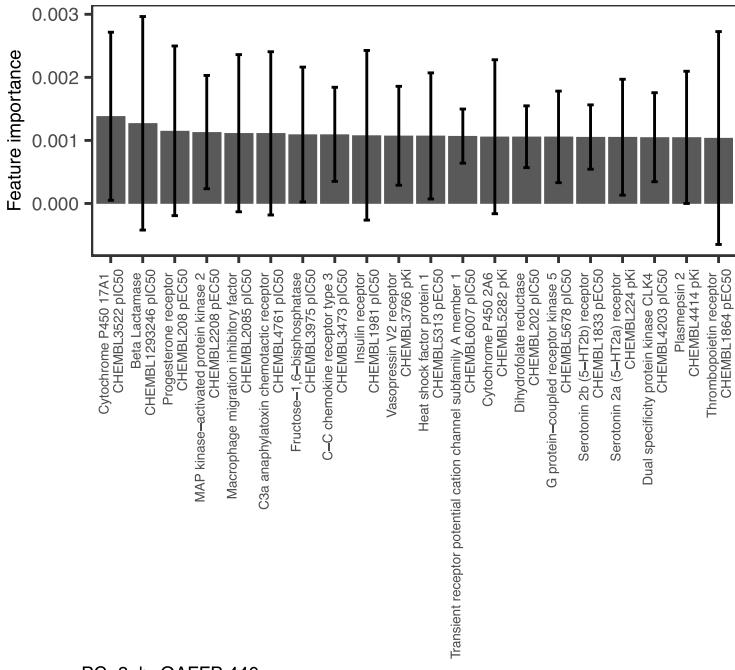
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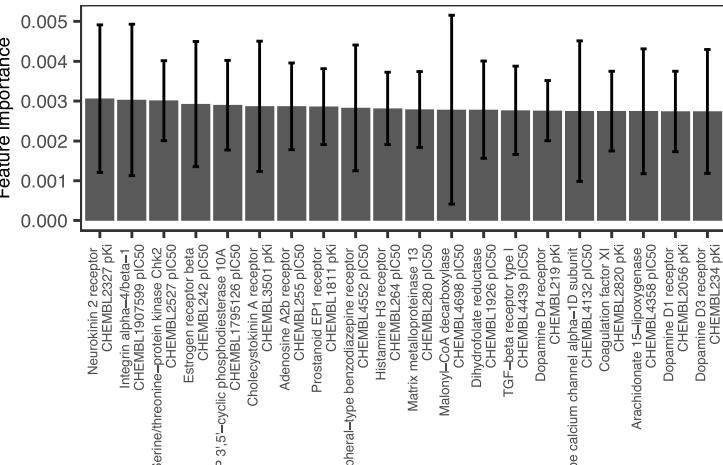
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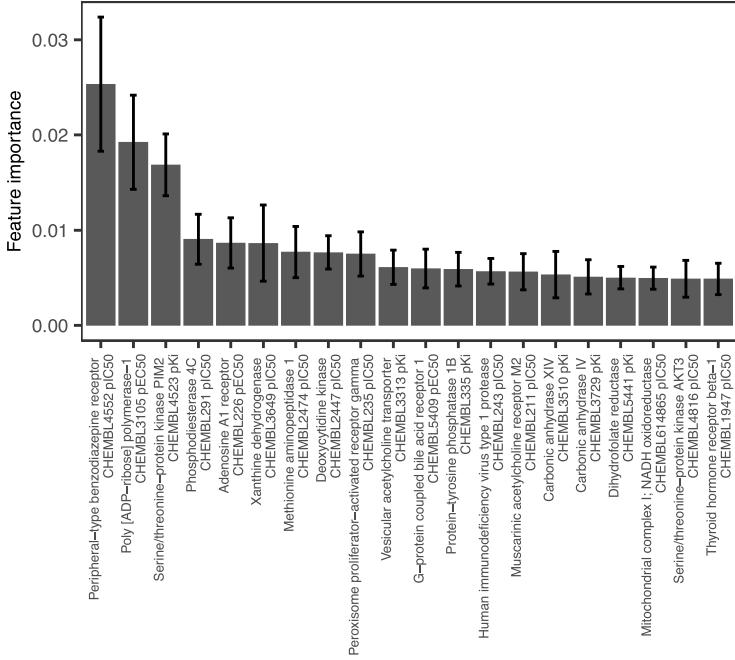
PC-3; rv-QAFFP 1360



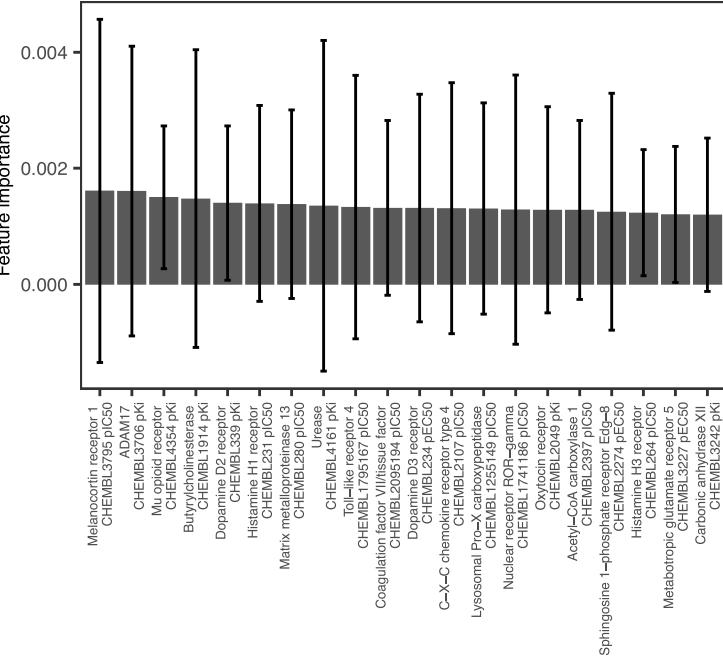
PC-3; rv-QAFFP 440



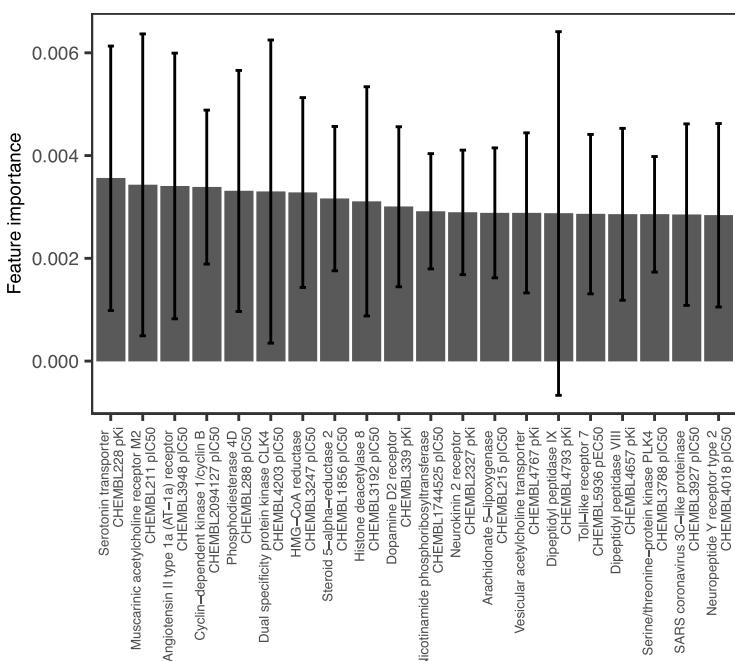
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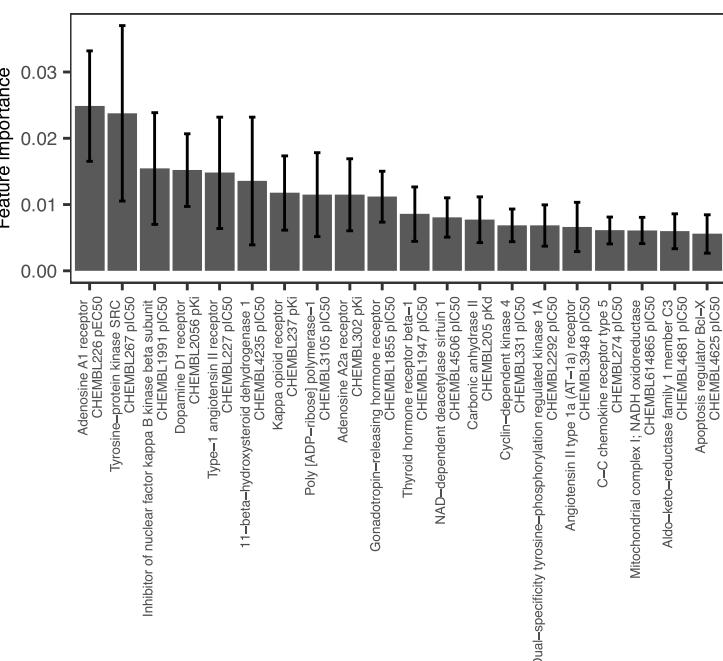
SK-OV-3; rv-QAFFP 1360



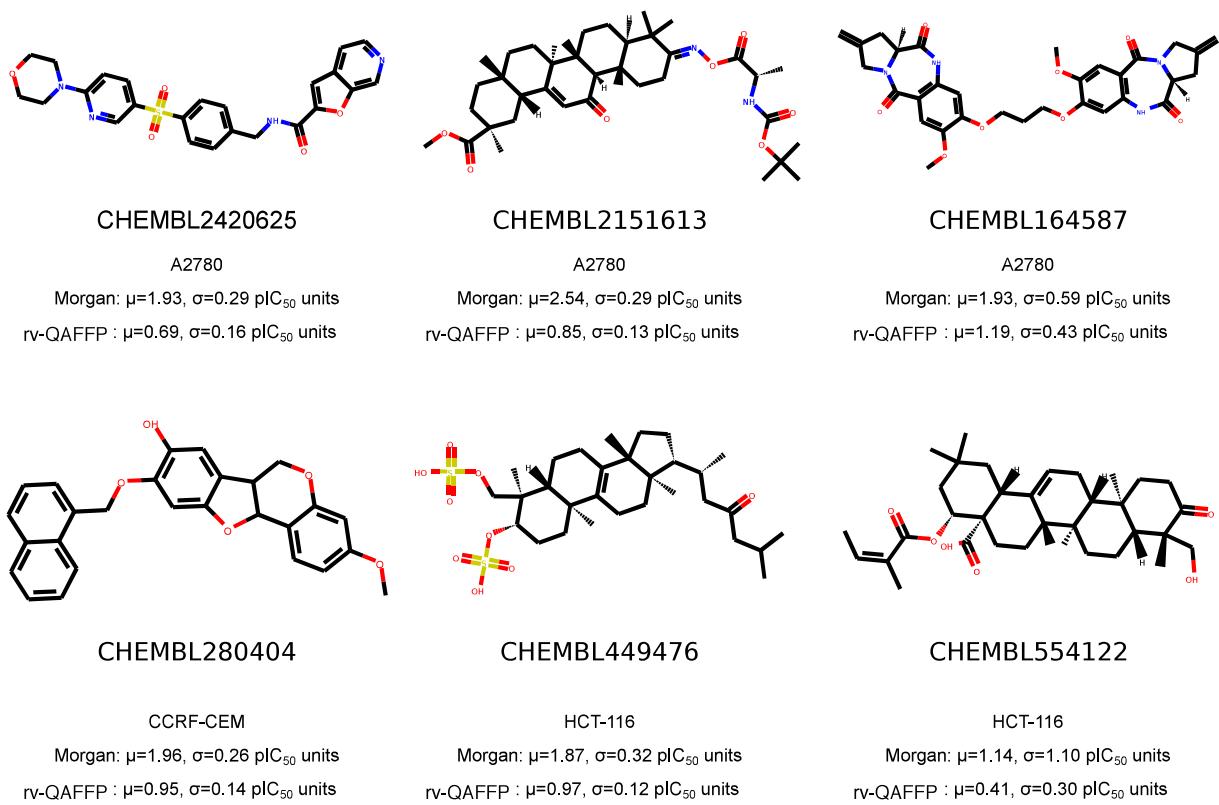
SK-OV-3; rv-QAFFP 440



SK-OV-3; b-QAFFP 440



Supplementary Figure 7



Supplementary Figure 8

