

Supplementary file 1

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Benchmarking different docking protocols for predicting the binding poses of ligands complexed with cyclooxygenase enzymes and screening chemical libraries

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Table S1. The performance of docking methods on 18 COX1-inhibitor complexes in terms of percent of docking solutions at different RMSD cutoffs.

COX-1	% ≤ 1 Å	% ≤ 2 Å	% > 4 Å	% > 5 Å	% > 6 Å
Gold (ChemPLP)	42.77	77.77	18.88	18.88	17.22
Gold (GoldScore)	37.22	71.66	11.11	11.11	11.11
Gold (ChemScore)	47.22	83.88	16.11	16.11	12.77
Gold (ASP)	37.22	77.22	17.22	17.22	17.22
Autodock (10 Runs)	61.11	88.89	11.11	11.11	11.11
Autodock (50 Runs)	61.11	88.89	5.55	5.55	5.55
LeadIT (FlexX)	22.22	66.67	27.77	27.77	27.77
MVD	61.11	77.78	22.22	16.66	16.66
Glide	94.44	100	0	0	0

Table S2. The performance of docking methods on 32 COX2-inhibitor complexes in terms of percent of docking solutions at different RMSD cutoffs.

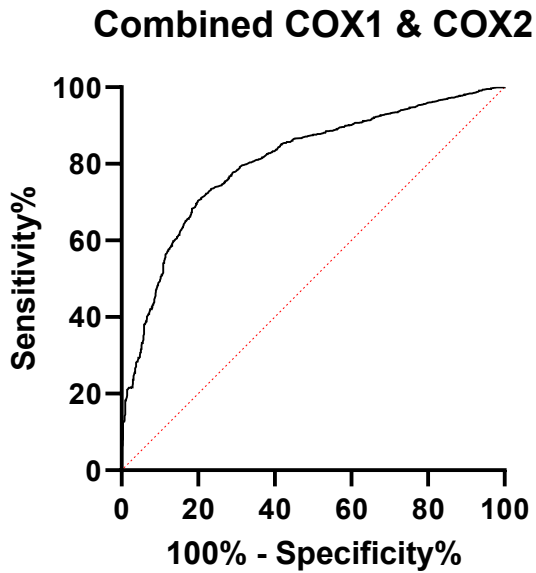
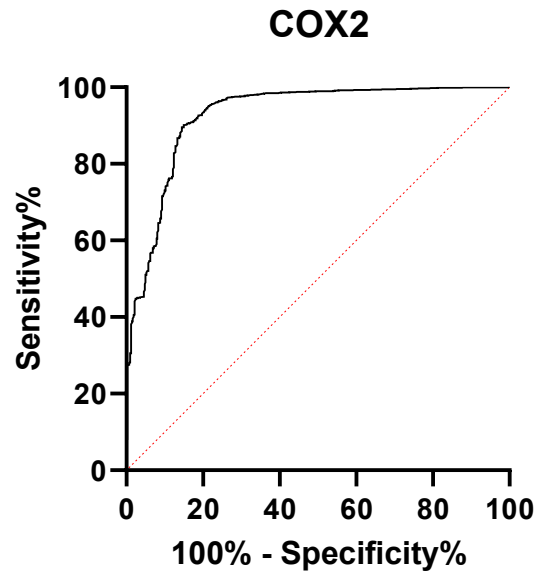
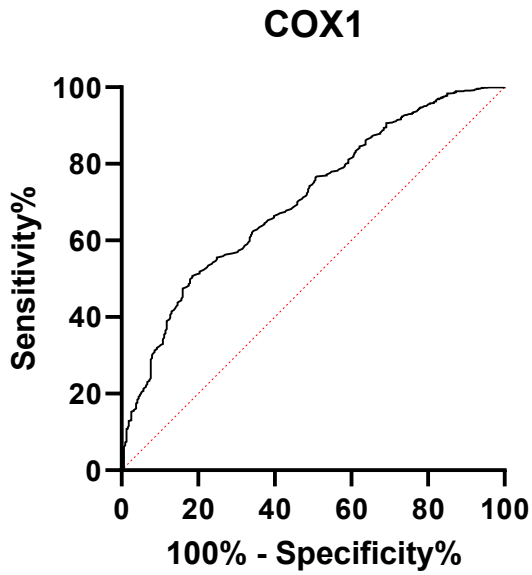
COX-2	% ≤ 1 Å	% ≤ 2 Å	% > 4 Å	% > 5 Å	% > 6 Å
Gold (ChemPLP)	43.32	75.76	17.87	17.57	8.18
Gold (GoldScore)	22.11	52.12	26.66	20.91	9.69
Gold (ChemScore)	39.69	69.7	15.75	14.24	11.21
Gold (ASP)	33.93	75.76	14.84	14.84	13.03
Autodock (10 Runs)	42.42	75.76	15.15	9.09	9.09
Autodock (50 Runs)	42.42	78.79	12.12	9.09	9.09
LeadIT (FlexX)	18.18	57.58	30.3	30.3	21.21

MVD	27.27	66.67	24.24	21.21	15.15
Glide	93.94	100	0	0	0

Table S3. Enrichment factors calculated based on the docking scores for active ligands/decoys at 0.1% top ranking structures.

	COX1	COX2
	EF 0.1%	EF 0.1%
AD4	40	31
GLIDE	19	20
GOLD	8	23
FlexX	29	12

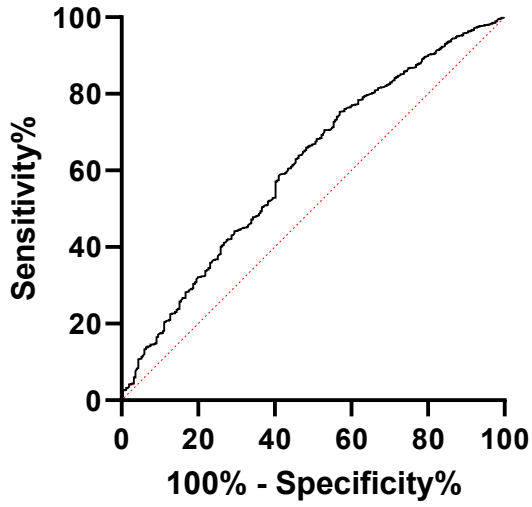
Glide data



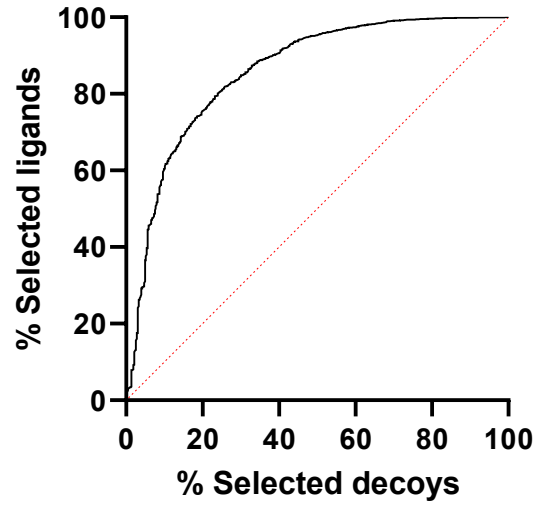
	COX1	COX2	Combined
AUC	0.7041	0.9275	0.8055
Std. Error	0.01426	0.007629	0.007556
95% CI	0.6762 to 0.7321	0.9126 to 0.9425	0.7907 to 0.8203
P value	<0.0001	<0.0001	<0.0001

GOLD data

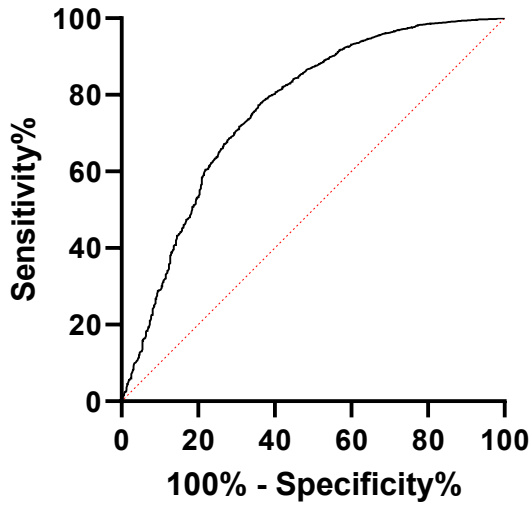
COX1



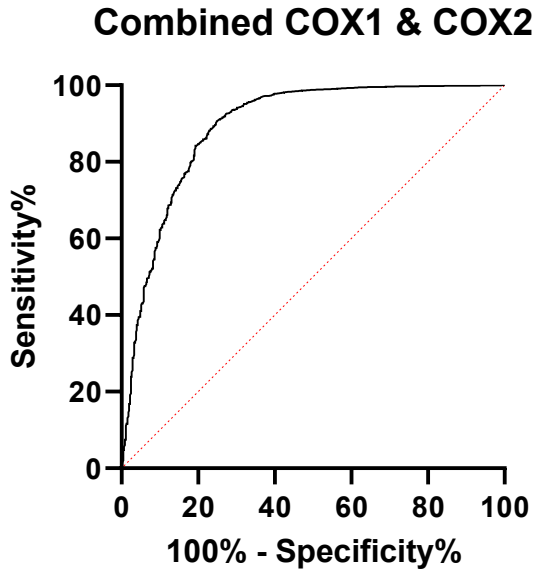
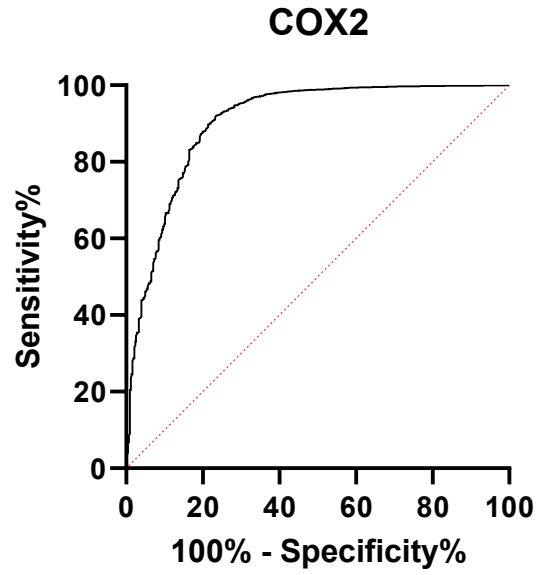
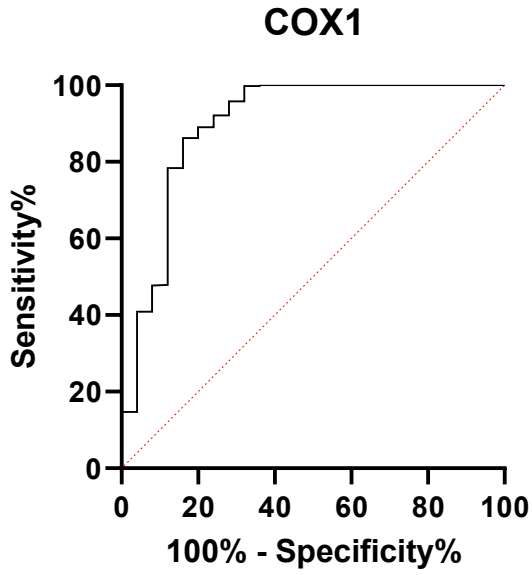
COX2



Combined COX1 & COX2



AutoDock Vina (adt4.2 force field)



FlexX results (LeadIT)

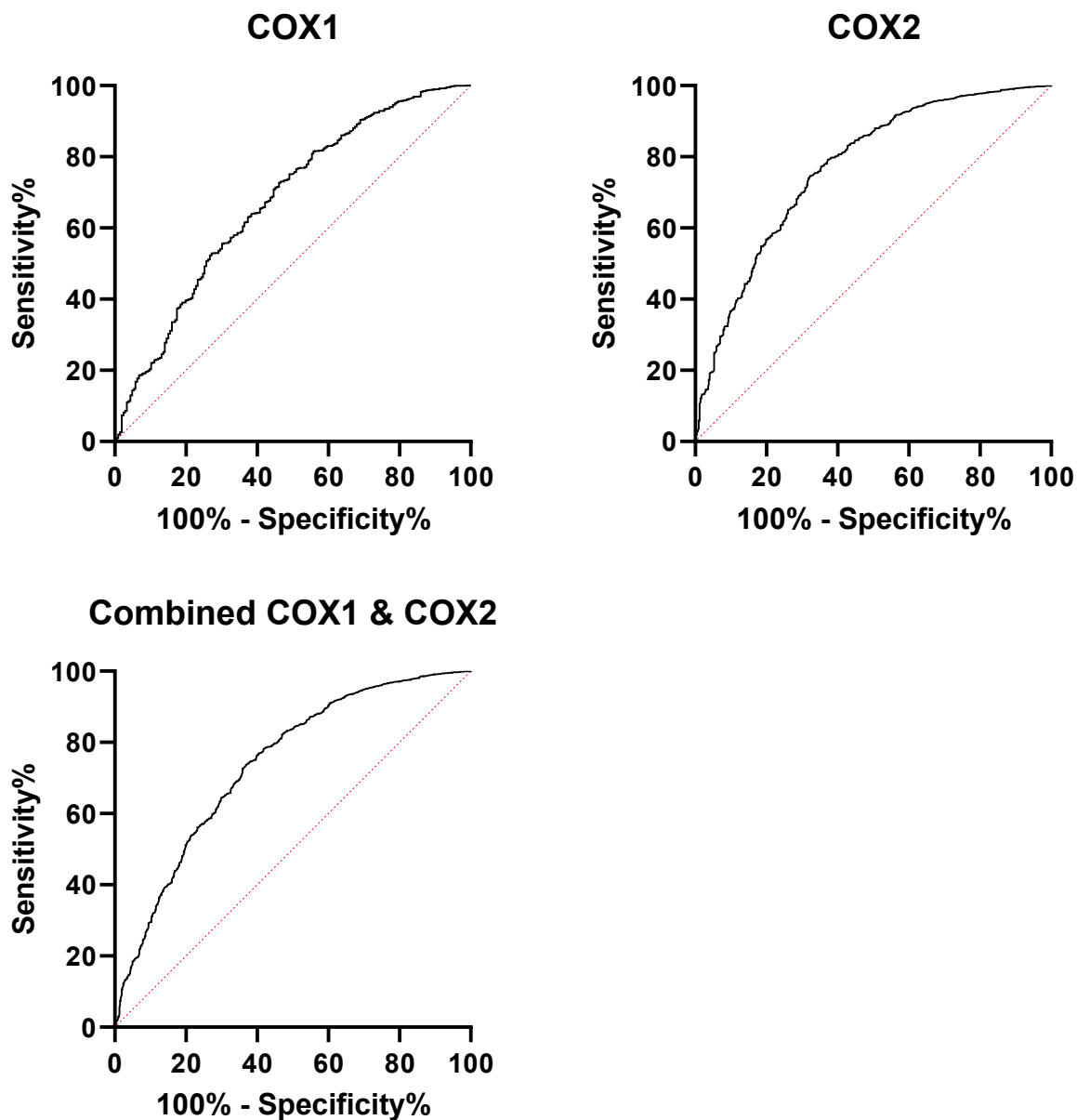


Figure S1. AUC plots of ROC analyses on docking scores for COX1, COX2 and combined COX1 and COX2 active ligands and decoys obtained by the studied docking methods.