

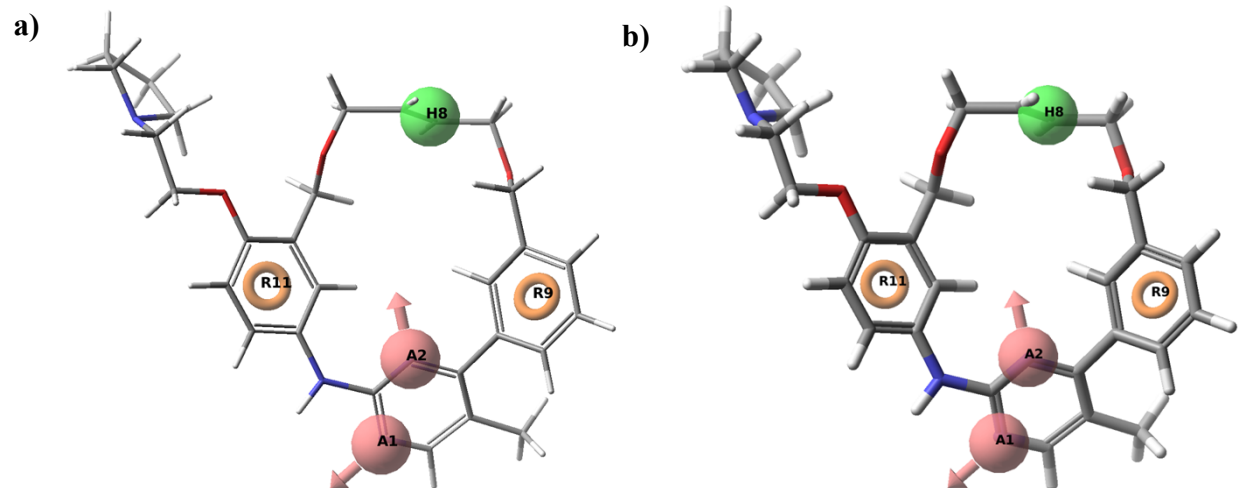
**Supplementary Table 1.** Summary of crystal structure used for the e-pharmacophore generation with their constituent co-crystal ligand with the number of hit molecule after screening against the zinc database.

<b>Proteins</b>	<b>Ligands</b>	<b>Hypothesis</b>	<b>Selected compounds</b>
2B7A	IZA	AADRRR	443
2W1I	L0I	ADDRR	2000
2XA4	AZ5	ADHR	1997
3E63	5B2	ADDRRR	734
3E64	5B3	ADDDRRR	246
3FUP	MI1	AADRR	246
3IOK	1P6	ADRRRR	71
3JY9	JZH	AADDDR	278
3KCK	3KC	AADRRRR	37
3KRR	DQX	AARRRR	919
3Q32	J2I	ADRR	3483
3TJC	0TP	ADDRRR	935
3TJD	6TP	ADDRRR	1567
3E62	5B1	ADDRR	2795
3LPB	NVB	ADRRRR	561

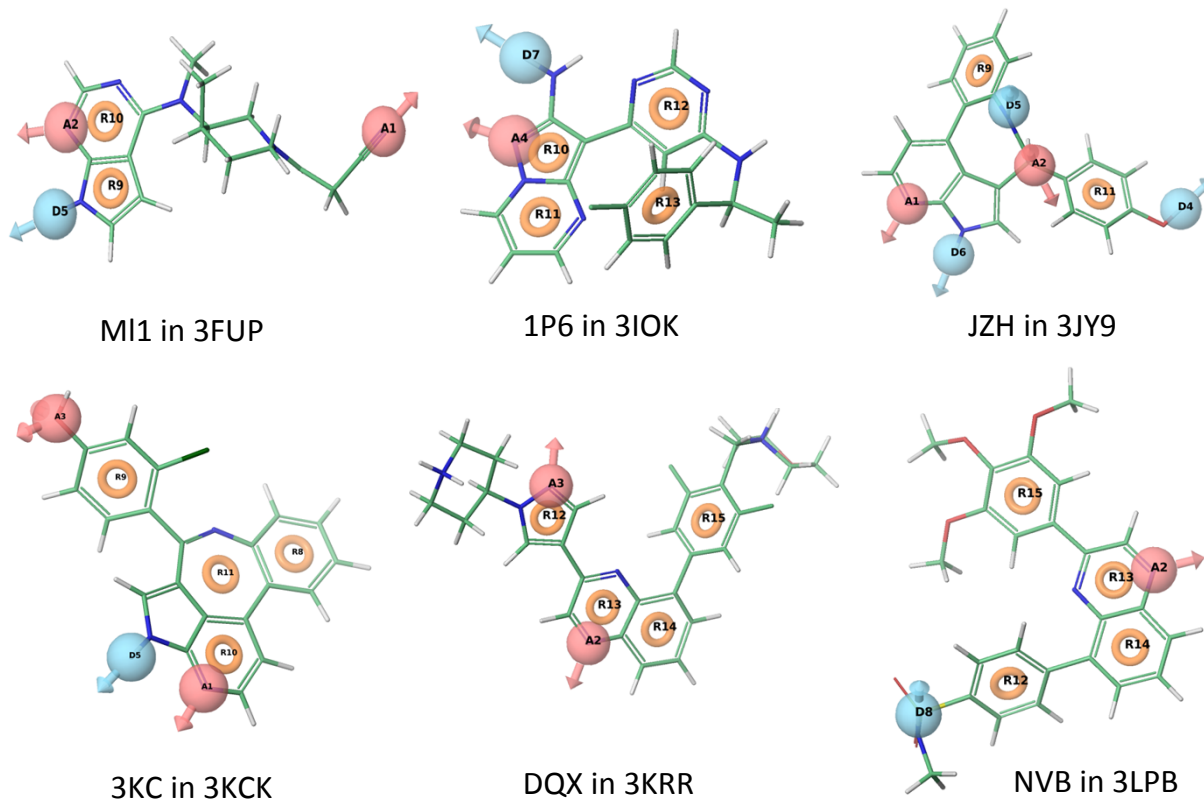
Supplementary Table 2. Summary of docking and MM/GBSA results for 27 lead molecules.

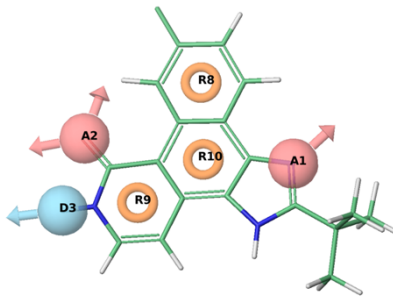
<b>Compound ID</b>	<b>Docking score</b>	<b>MMGBSA <math>\Delta G_{\text{Bind}}</math> (kcal/mol)</b>	<b>MMGBSA <math>\Delta G_{\text{Bind}}</math> Coulomb (kcal/mol)</b>	<b>MMGBSA <math>\Delta G_{\text{Bind}}</math> Hbond (kcal/mol)</b>	<b>MMGBSA <math>\Delta G_{\text{Bind}}</math> Solv GB (kcal/mol)</b>	<b>MMGBSA <math>\Delta G_{\text{Bind}}</math> vdW (kcal/mol)</b>
ZINC08764499	-10.16	-71.52	-3.70	-0.21	28.89	-58.71
ZINC29078467	-9.84	-59.71	83.77	-3.26	-61.08	-42.16
ZINC06624166	-9.3	-64.8	-22.86	-1.59	22.64	-43.27
ZINC79189191	-8.79	-61.86	-4.60	-0.39	20.71	-47.51
ZINC12899088	-8.73	-79.00	-20.93	-0.9	28.06	-50.97
ZINC00138875	-8.68	-62.55	-17.15	-0.68	21.11	-35.11
ZINC02130359	-8.38	-59.95	4.85	-2.02	18.32	-50.26
ZINC36369819	-8.21	-74.30	-13.43	-1.33	25.59	-52.98
ZINC70666323	-8.18	-68.62	-7.34	-0.38	16.98	-49.24
ZINC02160787	-8.12	-60.65	-4.29	-4.39	16.76	-42.21
ZINC09215995	-8.06	-83.29	-20.49	-1.31	22.30	-48.76
ZINC12901690	-9.72	-66.97	-3.68	-0.47	24.02	-49.08
ZINC70666306	-8.69	-68.30	-25.52	-0.67	32.25	-45.74
ZINC12296487	-8.63	-70.35	-16.55	-0.76	29.50	-58.19
ZINC32124076	-8.57	-76.50	-18.68	-1.43	31.56	-50.32
ZINC00391857	-8.11	-57.52	-11.73	-0.71	25.31	-40.76
ZINC09130685	-8.02	-83.73	-16.32	-1.4	26.56	-61.06
ZINC00517863	-8.74	-38.28	-18.64	-0.66	22.88	-23.07
ZINC12892087	-8.12	-57.95	-20.84	-0.68	29.28	-43.7
ZINC00138886	-9.08	-66.16	-19.23	-0.70	25.41	-41.36
ZINC04000352	-8.8	-72.23	-12.32	-0.60	24.03	-55.86
ZINC00241869	-8.74	-68.76	-15.96	-0.70	21.9	-41.34
ZINC12898945	-8.5	-67.46	-21.83	-2.66	24.42	-37.39
ZINC12901845	-8.41	-71.26	-17.24	-0.97	19.92	-46.77
ZINC70666656	-8.29	-78.94	-12.11	-0.91	26.1	-54.54
ZINC01293793	-8.27	-59.6	6.72	-0.96	22.72	-49.95
ZINC08765154	-8.2	-66.7	-5.83	-0.39	16.48	-46.69
ZINC36369819	-8.21	-74.3	-13.43	-1.33	25.59	-52.98

**Supplementary Figure 1.** Alignment of two top score pharmacophore sites with the most active compound.

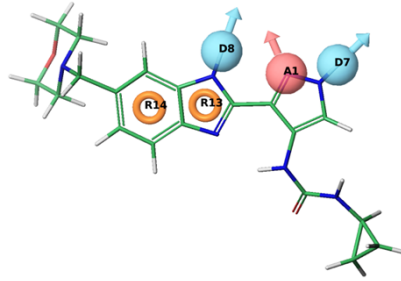


**Supplementary Figure 2.** E-Pharmacophore sites predicted from the 15 co-crystallized compounds of Jak2.

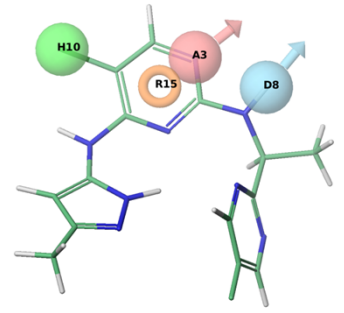




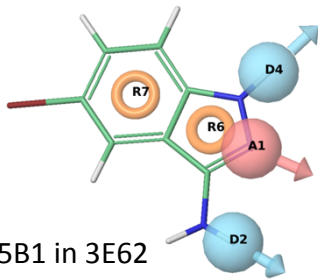
IZA in 2B7A



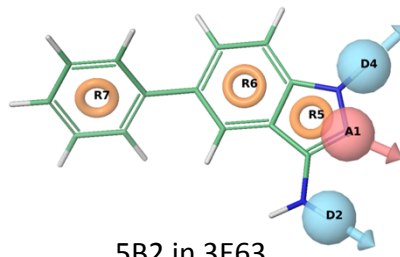
LOI in 2W1I



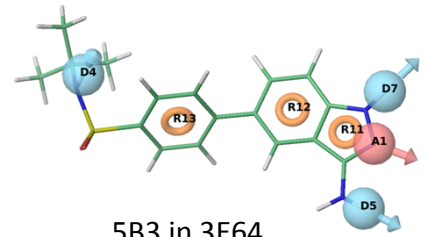
AZ5 in 2XA4



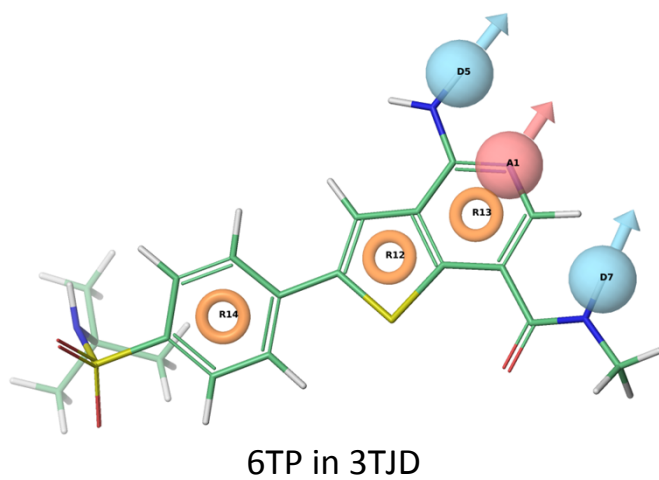
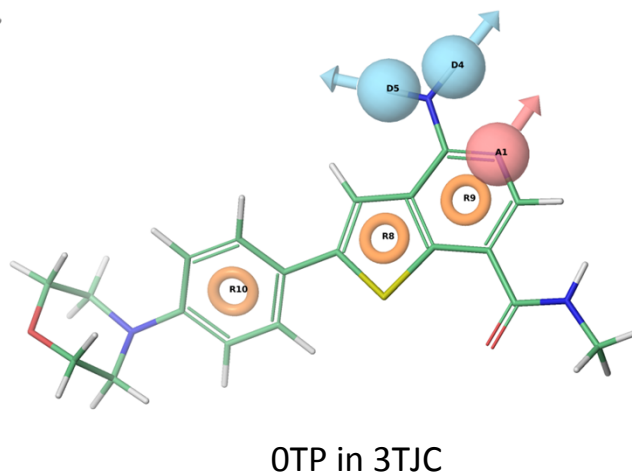
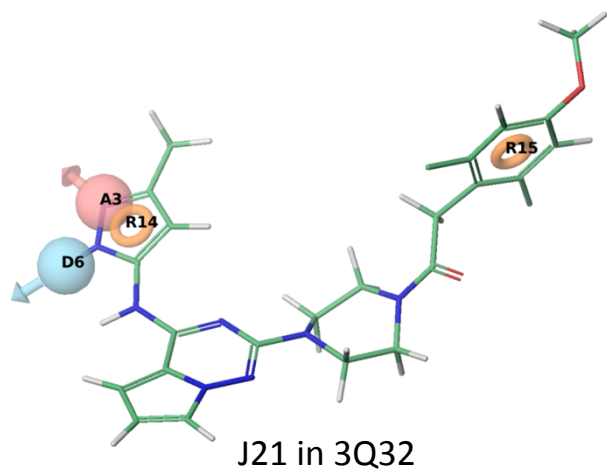
5B1 in 3E62



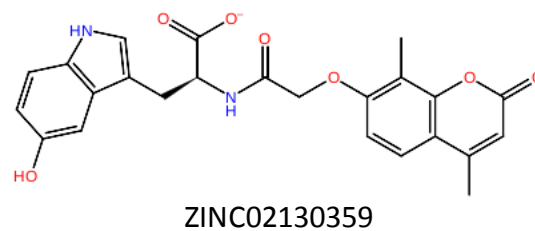
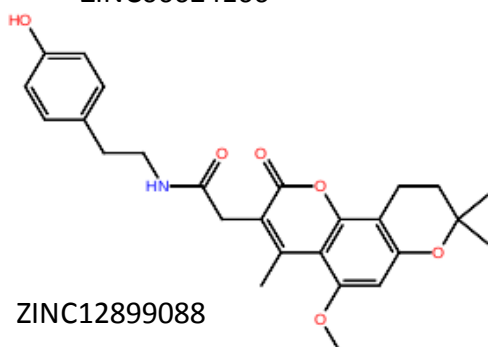
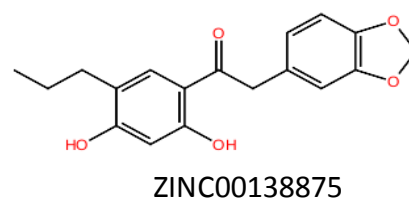
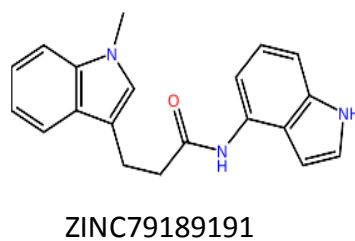
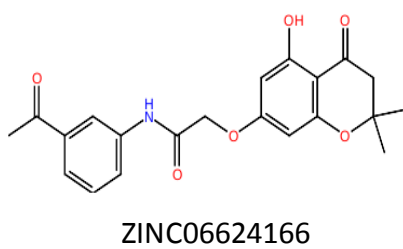
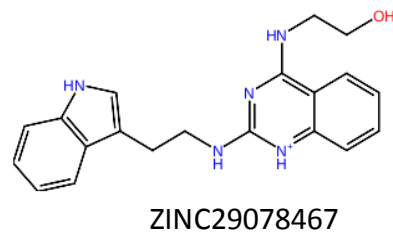
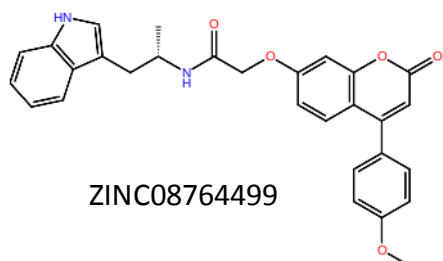
5B2 in 3E63

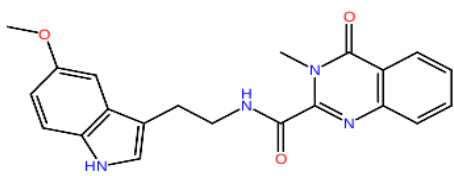


5B3 in 3E64

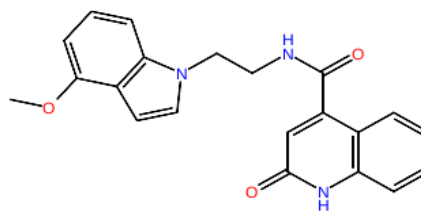


**Supplementary Figure 3.** Chemical structure of 27 hit compounds from Zinc database with their corresponding IDs.

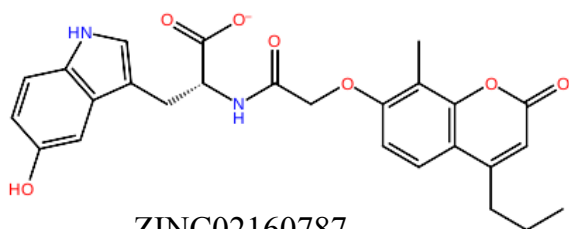




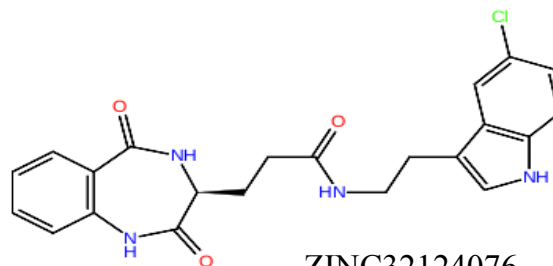
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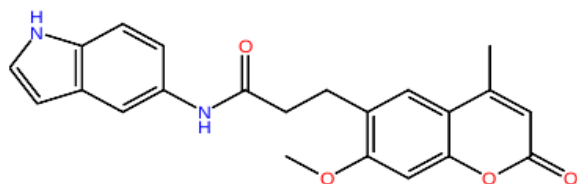
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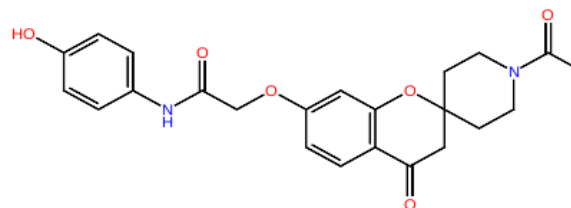
ZINC02160787



ZINC32124076



ZINC70666306



ZINC12296487



