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Supplementary material:

Table 1: Analysis of active site residues of JAK3 from co-crystal structures with inhibitors

PDB ID	L828	F833	V836	A853	M902	E903	G908	R953	L956	A966	D967	L905
1YVJ	N	N	HP	N	HP	HB	HP	HB	HP	N	HP	HB
3LXK	HP	N	HP	HP	N	HB	N	N	HP	HP	N	HB
3LXL	HP	N	HP	HP	N	HB	N	N	HP	N	N	HB
3PJC	HP	HP	HP	N	N	HB	N	N	HP	N	N	HB
4HVD	HP	N	N	HP	N	HB	N	N	HP	N	N	HB
4HVG	HP	N	N	HP	N	HB	N	N	HP	N	N	HB
4HVH	HP	N	N	HP	N	HB	N	N	HP	N	N	HB
4HVI	N	N	HP	HP	N	HB	N	N	HP	N	N	HB
3ZC6	HP	N	HP	HP	N	HB	HP	N	HP	N	N	HB
4I6Q	HP	N	N	HP	N	HB	N	N	HP	N	N	HB

Table 2: Statistical Parameter of the 3D-QSAR AAHR.92

PLS factor	SD	R^2	F	P	RMSE	q^2	P- R
1	0.8153	0.4188	62	$9.622e^{-12}$	0.8514	0.312	0.5656
2	0.6687	0.6135	67.5	$2.83e^{-18}$	0.862	0.2947	0.5702
3	0.5649	0.7274	74.7	$1.234e^{-23}$	0.7327	0.4904	0.7146
4	0.4209	0.8505	118	$2.046e^{-33}$	0.7018	0.5325	0.7545
5	0.3588	0.8926	136.3	$3.226e^{-38}$	0.6529	0.5953	0.8164
6	0.2666	0.9422	162.5	$5.186e^{-43}$	0.6674	0.5772	0.7911
7	0.2342	0.9559	214.2	$8.8e^{-47}$	0.6472	0.6023	0.8178

SD: standard deviation of the regression; F: variance ratio; P: significance level of variance ratio; RMSE: root mean square error; q2: squared value for the predicted activities; P R: Pearson R value for the correlation between predicted and observed activity for the test set; R^2: squared value of the regression

Table 3: Molecular Docking Analysis of the Lead Compounds

Lead	ZINC Database ID	XP Score	Glide Energy	Interacting Residues	MBAE ΔE	RMSD
Lead 1	ZINC72419848	-12.96	-72.20	Glu903, Leu905, Tyr904	-125.12	0.610
Lead 2	ZINC72145366	-12.94	-72.97	Glu903, Leu905, Tyr904	-131.82	0.320
Lead 3	ZINC08991673	-12.81	-71.11	Glu903, Leu905,ASH967	-125.29	053
Lead 4	ZINC72162601	-12.47	-66.80	Glu903, Leu905	-105.36	0.602
Lead 5	ZINC72157582	-12.28	-69.345	Glu903, Leu905	-81.278	0.554
Lead 6	ZINC72418290	-12.13	-71.60	Leu905,ASH967	-80.78	0.610
Lead 7	ZINC40757269	-11.40	-71.81	Leu905,ASH967	-116.22	0.571
Lead 8	ZINC44963631	-11.18	-79.84	Asn954, Lys855	-157.68	0.39
Lead 9	ZINC03280240	-11.19	-79.34	-	-135.23	0.359
Lead 10	ZINC63631329	-11.18	-63.48	Leu905	-137.99	0.63
CP-690550 (Tofacitinib)		-9.86	-92.23	Glu903, Lys855	-150.28	

Table 4: (Available with authors)

Table 5: ADME properties of Lead Compounds

Lead	QPlog Po/w[a]	QP logS[b]	QPlog HERG[c]	QPlog BB[d]	QPP MDCK[e]	% Human Oral Absorption[f]
1	0.94	-2.85	-4.93	-1.79	47.39	69.27
2	1.85	-3.53	-5.17	-1.32	175.39	84.03
3	1.31	-3.71	-5.19	-2.42	30.50	64.50
4	2.37	-4.16	-5.28	-1.22	176.46	87.08
5	2.52	-4.15	-5.03	-1.24	179.57	88.10
6	1.45	-3.39	-3.34	-2.30	3.91	52.57
7	2.49	-3.95	-6.18	-1.04	448.43	94.52
8	4.85	-5.9	-4.44	-0.29	2536.76	100
9	2.28	-4.38	-6.07	-1.57	88.70	81.66
10	2.49	-3.95	-6.18	-1.04	448.43	94.59

a) Predicted octanol/water partition co-efficient log P (acceptable range: -2.0 to 6.5); b), Predicted aqueous solubility; S in mol/L acceptable range: -6.5 to 0.5); c) Predicted IC50 value for blockage of HERG K+ channels (acceptable range: below -6.0).; d) Predicted Blood Brain Barrier permeability (acceptable range: -3 to1.2); e) Predicted apparent MDCK cell permeability in nm/s; f Percentage of human oral absorption (<25% is poor and >80% is high).