Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Computational investigation of novel pyrimidine derivatives as potent FAK inhibitors via 3D-QSAR, molecular docking, molecular dynamics simulation and retrosynthesis

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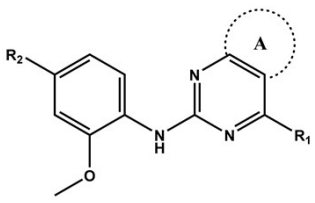
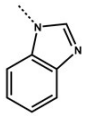
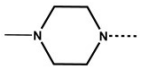
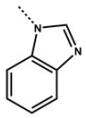
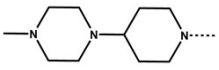
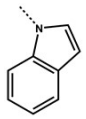
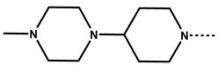
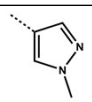
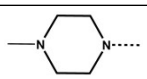
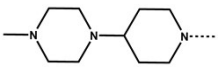
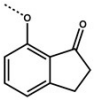
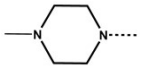
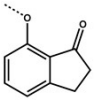
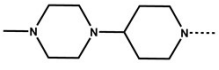
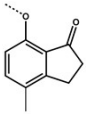
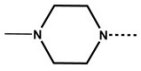
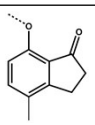
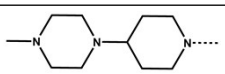
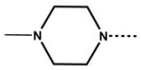
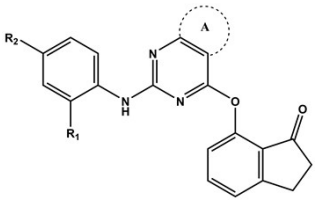
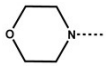
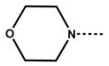
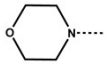
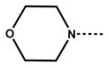
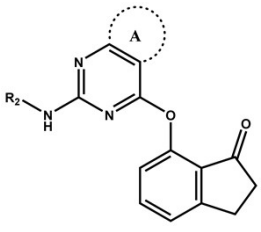
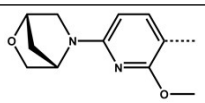
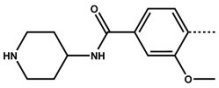
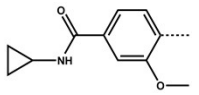
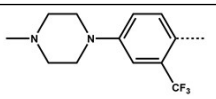
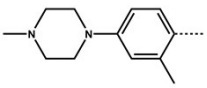
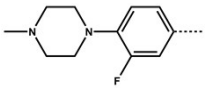
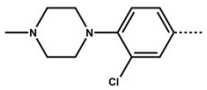
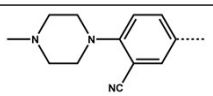
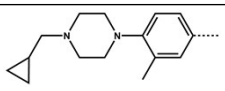
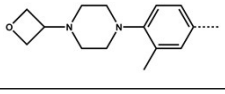
Supplementary Table

Table S1 Chemical structures of the investigated molecules and their pIC_{50} values

No.		Basic structure	A	R_1	R_2	pIC_{50} (exp)	CoMSIA/ HD	
							pIC_{50} (pred)	Residual
1	Training					7.435	7.783	-0.348
2	Training					7.559	7.509	0.05
4	Training					6.843	6.692	0.151
5	Training					6.481	7.032	-0.551
6	Training					6.761	6.862	-0.101
7	Training					8.413	8.127	0.286
8	Test					8.536	7.656	0.880
9	Training					8.690	8.459	0.231
10	Training					8.607	8.355	0.252
11	Training			H		7.978	8.21	-0.232

12	Training			H		7.913	8.193	-0.280
13	Test			OCH_3		7.943	7.838	0.105
18	Training			OCH_3		6.025	5.877	0.148
24	Training			H		6.960	6.835	0.125
25	Training			H		6.611	6.56	0.051
28	Training			OCH_3		7.562	7.316	0.246
31	Training			OCH_3		6.636	6.425	0.211
32	Training			OCH_3		6.184	6.493	-0.309
33	Training			OCH_3		6.609	6.603	0.006
35	Training			-		8.018	8.043	-0.025
36	Training			-		8.724	8.66	0.064
37	Training			-		7.964	8.079	-0.115
38	Test			-		7.001	8.261	-1.26
39	Test			-		8.147	7.864	0.283
40	Training			-		8.249	8.162	0.087
41	Training			-		8.319	8.244	0.075
42	Test			-		7.687	7.782	-0.095
43	Training			-		8.377	8.557	-0.180
44	Training			-		8.199	8.342	-0.143

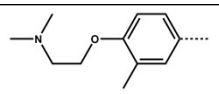
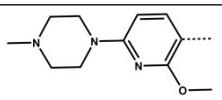
45	Training			-		8.406	8.104	0.302
46	Test			-		8.043	7.798	0.245

Table S2 Statistical parameters of numerous Y-Randomization tests for the CoMSIA/HD model

Model	Q^2	R^2	Model	Q^2	R^2
Random 1	-0.200	0.061	Random 6	-0.225	0.032
Random 2	-0.110	0.127	Random 7	-0.222	0.043
Random 3	-0.402	0.0098	Random 8	-0.164	0.078
Random 4	-0.276	0.105	Random 9	-0.319	0.001
Random 5	-0.178	0.096	Random 10	-0.202	0.126
Original	**0.699**	**0.931**			

Supplementary Figure

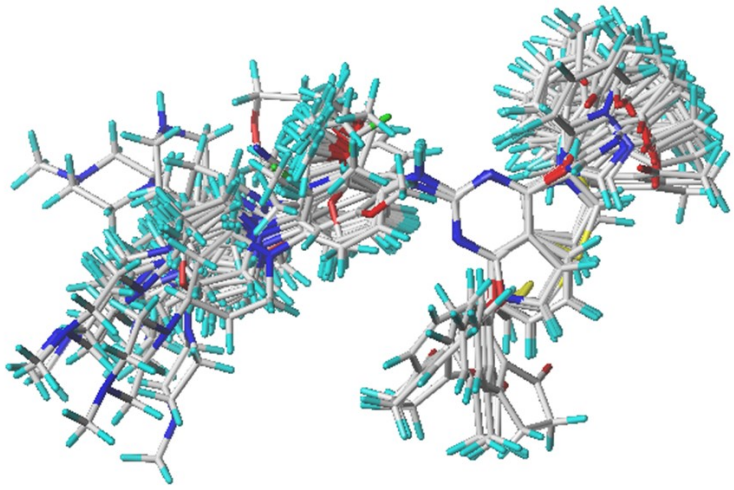


Fig. S1 Alignment of 31 compounds under investigation.