

Appendix A: Detailed information about compounds with best score

(In silico search of tubulin polymerization inhibitors, by *H. K. Sahakyan, G. G. Arakelov, K.*

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Pubchem CID	Score	molWeight	mfScore	Natom	molArea	molLogP	HBA	HBD	drugLikeness
692750	-43.45	329	-35.72	43	361	2.61	7	1	-0.213
647614	-41.74	482	-84.06	69	554	2.7	8	3	0.319
5056984	-41.42	468	-45.45	62	512	2.67	10	1	0.49
5346822	-41.04	479	-58.99	64	507	4.68	10	2	0.211
2933439	-39.86	492	-85.29	68	556	4.42	8	2	0.406
6568705	-39.73	508	-131.41	65	543	4.96	7	2	1.268
5321825	-39.71	440	-8.811	60	491	3.87	8	4	0.189
2535591	-39.62	442	-25.39	54	459	2.04	12	1	0.135
336635	-39.58	498	-81.00	70	562	2.83	10	1	0.291
4419227	-39.52	482	-45.57	65	531	2.92	10	1	0.637
17585330	-38.95	452	-31.71	61	480	2.94	9	2	1.216
Colchicine	-38.49	399	-111.14	54	438	2.72	8	1	0.956

Pubchem CID – PubChem Compound Identifier

Score – ICM binding score

molWeight – Molecular weight

mfScore – Potential of mean force score

Natom – Number of atoms in ligand

molArea – Molecular Area

molLogP – Lipophilicity

HBA and **HBD** – H-bond acceptors and donors respectively

drugLikeness – Predicted drug likeness property