BIOINFORMATION

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Supplementary material:

Table 1: Inhibitors selected for the study

S.N	SMO Inhibitors	PubChem CID
1	Cyclopamine	CID 442972
2	Saridegib	CID 25027363
3	Itraconazole	CID 55283
4	LDE-225	CID 24775005
5	TAK-441	CID 44187367
6	BMS-833923 (XL139)	CID 57662985
7	PF-04449913	CID 25166913

Table 2: Docking scores of inhibitors arranged in descending order

S.No	Inhibitor	MolDock Score	Rerank Score	HBond Score
1	BMS 833923 (XL 139)	-189.99	-153.04	-1.9203
2	LDE-225	-175.82	-145.9	-0.2275
3	PF-04449913	-161.97	-130.7	-8.3375
4	Vismodegib	-141.46	-114.6	-3.7154
5	TAK-441	-189.6	-92.568	-3.1279
6	Itraconazole	-189.65	-71.049	-2.0268
7	Cyclopamine	-154.45	-49.784	-0.4258
8	Saridegib	-133.32	15.7613	-2.0484

Table 3: Hydrogen bonding profile of BMS 833923 (XL 139) in SMO receptor

Interacting Residue	Energy Kcal/mol	Length Å
Arg (400)	-1.078	3.38441
Tyr (294)	-0.4696	2.74877
Asn (219)	-1.3049	3.33902

Table 4: *Energy overview of BMS 833923 (XL 139) and its interactions with SMO receptor*

Energy overview: Descriptors	MolDock Score	Rerank Weight	Rerank Score
Total Energy	-204.46		-175.04
External Ligand interactions	-231.09		-199.31
Protein - Ligand interactions	-231.09		-199.31
Steric (by PLP)	-228.24	0.686	-156.57
Steric (by LJ12-6)		0.533	-40.484
Hydrogen bonds	-2.852	0.792	-2.259
Hydrogen bonds (no directionality)			0
Electrostatic (short range)	0	0.892	0
Electrostatic (long range)	0	0.156	0
Cofactor - Ligand	0	0.602	0
Water - Ligand interactions	0	0.988	0
Internal Ligand interactions	26.627		24.272
Torsional strain	0.345	0.938	0.324

Torsional strain (sp2-sp2)		0.636	0
Hydrogen bonds			0
Steric (by PLP)	26.282	0.172	4.52
Steric (by LJ12-6)		0.139	19.428
Electrostatic	0	0.437	0