

Supplementary Table I: comparison of the ensemble-docking results to the individual ones (a ligand against its own PDB-related structure). In red the ones for which the preferred ensemble target is better than the PDB-related one (this correspond to a better score obtained)

N°	Ligand PDB ID	Original PDB target	Docking score in the original PDB target	Preferred PDB target in the Ensemble docking	Docking score in the ensemble docking
1	KSA	MD_1R0P	82	MD_1R0P	81
2	AM7	MD_2RFN	101	MD_2RFN	102
3	AM8	MD_2RFS	88	MD_2RFS	86
4	CKK	MD_3C1X	105	MD_3C1X	105
5	LKG	MD_3CCN	80	MD_3CCN	76
6	L5G	MD_3CD8	85	MD_3CD8	82
7	1FN	MD_3CE3	95	MD_3CE3	95
8	319	MD_3CTH	92	MD_3CTH	90
9	320	MD_3CTJ	89	MD_3CTH	92
10	IHX	MD_3F66	82	MD_3F66	81
11	3F82	MD_3F82	99	MD_3F82	98
12	3EFJ	MD_3EFJ	101	MD_3EFJ	102
13	MT4	MD_3EFK	96	MD_2RFN	99
14	ZZY	MD_2WD1	80	MD_2WD1	78
15	ATP	MD_3DKC	106	MD_3DKC	102
16	SX8	MD_3DKF	82	MD_3CCN	84
17	VGH	MD_2WGJ	82	MD_2WGJ	82
18	DFQ	MD_3A4P	81	MD_3A4P	79
19	L8V	MD_3L8V	82	MD_2RFN	85
20	B2D	MD_3I5N	83	MD_3I5N	86
21	88Z	MD_3LQ8	100	MD_3LQ8	99
99	PFY	MD_2WKM	88	MD_2WKM	88
23	Q6W	MD_3Q6W	90	MD_3Q6W	93
24	3QT	MD_3QTI	85	MD_3QTI	84
25	M97	MD_3RHK	83	MD_3RHK	83
26	KRW	MD_3ZXZ	82	MD_3CCN	87
27	OJL	MD_4DEI	94	MD_4DEI	93
28	OJ3	MD_4GG5	79	MD_4GG5	77
29	L1X	MD_4EEV	106	MD_3F86	111
30	DF6	MD_3VW8	98	MD_3VW8	98
31	1JC	MD_4IWD	98	MD_4IWD	97
32	5TF	MD_3ZCL	75	MD_3CCN	76
33	W97	MD_3ZC5	79	MD_2RFN	81
34	6XE	MD_3ZBX	78	MD_3CCN	82
35	1RU	MD_4KNB	84	MD_4KNB	83
36	DWF	MD_4MXC	102	MD_4MXC	100
37	44X	MD_4XYF	93	MD_4XYF	93
38	3E8	MD_4R1V	95	MD_4R1V	94
39	46G	MD_4XMO	76	MD_2WKM	79
40	5B4	MD_5DG5	95	MD_5DG5	94
41	5T1	MD_5EYD	86	MD_5EYD	83
42	5QQ	MD_5EOB	80	MD_3CCN	84
43	5SZ	MD_5EYC	80	MD_5EYC	80
44	84P	MD_5UAF		MD_5UAF	
45	66L	5HTI	94	MD_3F66	93

Supplementary table II: most used c-Met inhibitors as pointed by SelleckChem (www.selleckchem.com/c-Met.html) and AdooQ Biosciences (www.adooq.com/met.html)

compound names	PubChem IDs	Tanimoto
Crizotinib	11626560	0.31
Cabozantinib	25102847	0.24
Foretinib	42642645	0.29
PHA-665752	10461815	0.39
SU11274	9549297	0.38
JNJ-38877618	57654476	0.27
Glumetinib	117797905	0.30
Altiratinib	54576299	0.27
BMS-777607	24794418	0.31
Tivantinib	11494412	0.31
JNJ-38877605	46911863	0.28
PF-04217903	17754438	0.30
Capmatinib	25145656	0.31
BMS-754807	24785538	0.33
BMS-794833	44155856	0.32
AMG-208	24864821	0.29
MK-2461	44137946	0.29
Golvatinib	16118392	0.29
AMG-458	24764449	0.34
NVP-BVU972	44206063	0.26
Tepotinib	25171648	0.29
AMG	44181686	0.34
Merestinib	44603533	0.33
S49076	49809909	0.36
NPS-1034	46194178	0.35
Savolitinib	68289010	0.29
SAR-125844	25182860	0.35
SGX-523	24779724	0.26
Glesatinib	24901704	0.36
BMS-817378	44137813	0.34
MK-8033	45142457	0.28
norcantharidin	93004	0.12