Supporting Information

Predictive Power of Molecular Dynamics Receptor Structures in Virtual Screening

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SUPPORTING TABLES

Table SI Structures Used in Study

System	*Structure*
RT X-rays:	1BQM, 1DLO, 1EP4, 1FK9, 1HMV, 1HVN, 1KLM, 1RT1,1RT4, 1RTD, 1VRT, 1VRU, 2HMI, 2ZD1, 3DLK
RT Binders:	Rilpivirine/TMC-278, Etravirine/TMC-125, DPC-083, Efavirenz, MKC-442, RDEA-806, S-1153, 8-Cl TBO, HEPT, UC-781, GW678248, MIV-150, Trovirdine/PETT, UK-453061, MK-4965, S-DABO-3W, Loviride/Alpha-APA, Nevirapine, HBY-097, Delavirdine
RT Decoys:	National Cancer Institute Diversity Set II (http://dtp.cancer.gov)
W191G X-rays:	1AA4, 1AC4, 1AC8, 1AEB, 1AED, 1AEE, 1AEF, 1AEG, 1AEH, 1AEJ, 1AEK, 1AEM, 1AEN, 1AEO, 1AEQ, 1AES, 1AET, 1AEU, 1AEV, 1BEJ, 1CMP, 1CMQ, 1CMT, 1RYC, 2ANZ, 2AQD, 2AS1, 2AS2, 2AS3, 2AS4, 2AS6, 2EUN, 2EUO, 2EUP, 2EUQ, 2EUR, 2EUS, 2EUT, 2EUU, 2RBT, 2RBU, 2RBV, 2RBW, 2RBX, 2RBY, 2RBZ, 2RC0, 2RC1, 2RC2
W191G Binders and Decoys:	Shoichet Lab at UCSF provided the list of binders/non-binders. (http://shoichetlab.compbio.ucsf.edu/take-away.php)

Table SII Predictive Power of MD Structures Compared to X-ray models and Random Ranking

Receptor	**System**	**Nr. MD Structures with Higher Predictive Power than Mean X-ray model**	**%**	**Nr. MD Structures with Higher Predictive Power than Random Ranking**	**%**
RT	α-APA bound	788	31.5	2496	99.8
	UC-781 bound	566	22.6	2497	99.9
	unbound open	1239	49.6	632	25.3
	unbound closed	1288	51.5	523	20.9
W191G	2a5mt bound	298	12.0	2350	94.0

	unbound open	20	0.8	1790	71.6
	unbound closed	4	0.2	2206	88.2

Table SIII Mean Fluctuations of the Binding Site With Respect to Mean AUC Values

Receptor	System	<AUC>	All-atom <RMSF> [Å]	C^{α}-atom <RMSF> [Å]
RT	α-APA bound	0.77	0.91	0.73
	UC-781 bound	0.75	0.84	0.65
	unbound open	0.44	1.22	1.05
	unbound closed	0.44	1.34	1.19
W191G	2a5mt bound	0.66	0.93	0.54
	unbound open	0.58	1.38	0.91
	unbound closed	0.59	1.22	0.81

SUPPORTING FIGURES

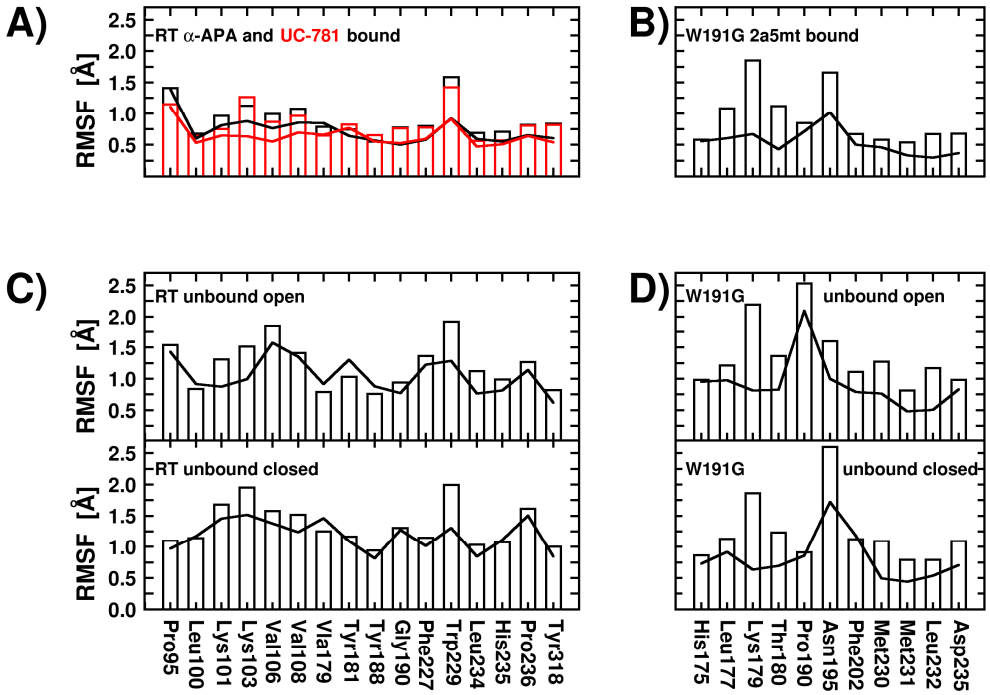

Figure S1. Root-mean-square fluctuations (RMSF) of binding site residues from molecular dynamics simulations of RT (left), and W191G (right). A) and B) show ligand-bound simulation fluctuations, C) and D) show unbound simulation fluctuations. Bars indicate the backbone C^{α}-atom positions RMSF values. Lines indicate all atom RMSF values. In all cases, RMSF values were calculated using sampling of 50 ns.