

ENSEMBLE SUMMARY									
Score <sup>1</sup>	Average				StDev			IC <sub>50</sub> (nM)	Ligand
	Cpd	Bin	Crash	Polar	Score	Crash	Polar		
9.86	23	0	-1.48	3.36	0.97	0.63	0.54	57	35
9.28	38	0	-1.26	3.19	2.25	0.45	1.00	60	S-5
8.88	45	0	-1.52	3.29	0.60	0.54	0.57	60	R-5
10.85	7	1	-1.71	3.24	0.60	0.40	0.47	88	R-36
10.71	9	1	-1.81	3.32	0.64	0.48	0.48	88	S-36
11.67	2	1	-1.12	3.84	0.73	0.36	0.52	180	R-13
10.36	15	1	-1.56	3.53	0.46	0.64	0.73	180	S-13
9.79	25	1	-1.79	2.89	0.76	0.49	0.51	200	R-33
9.79	26	1	-2.05	2.99	0.72	0.44	0.53	200	S-33
11.71	1	1	-1.25	3.12	0.70	0.39	0.25	210	R-12
10.52	13	1	-1.79	3.10	0.51	0.50	0.34	210	S-12
10.39	14	1	-1.69	3.01	0.76	0.34	0.42	290	34
9.59	30	0	-1.73	3.38	0.91	0.61	0.57	300	23
7.91	56	0	-0.57	3.08	1.83	0.19	0.77	360	24
9.96	21	1	-1.13	3.42	0.69	0.36	0.56	400	S-4
9.76	27	1	-1.27	2.94	0.69	0.33	0.28	400	R-4
9.73	29	1	-1.12	3.37	0.93	0.46	0.52	400	29
10.14	18	1	-1.88	3.07	0.91	1.26	0.43	750	S-14
9.73	28	1	-2.44	3.26	2.46	1.25	0.86	750	R-14
9.48	34	1	-1.83	3.68	1.18	0.62	0.85	1160	R-28
8.20	54	0	-2.05	3.15	1.00	0.77	0.71	1160	S-28
10.17	17	1	-1.45	3.10	1.32	1.08	0.50	1180	7
9.43	36	1	-1.08	3.31	1.19	0.52	0.46	1200	S-3
9.08	41	1	-1.21	3.62	2.26	0.39	0.95	1200	R-3
9.96	22	1	-2.21	3.45	0.88	0.67	0.85	1220	R-32
8.68	50	0	-1.97	3.12	2.16	0.78	0.83	1220	S-32
10.98	4	0	-1.80	3.21	1.84	0.78	0.66	1250	R-15
10.53	12	1	-2.06	3.04	0.68	0.78	0.45	1250	S-15
9.14	40	1	-0.95	2.94	3.15	0.43	1.06	1280	6
9.56	31	1	-0.86	3.20	0.79	0.37	0.49	1300	2
10.97	6	0	-1.33	3.21	1.04	0.54	0.29	1360	R-10
10.78	8	0	-1.20	3.41	0.85	0.58	0.23	1360	R-9
10.25	16	0	-2.01	3.12	0.60	0.83	0.19	1360	S-10
10.59	11	0	-1.10	3.41	0.89	0.34	0.32	1380	R-31
10.03	19	1	-1.71	3.26	0.51	0.51	0.57	1380	S-31
9.80	24	1	-1.50	3.09	0.57	0.69	0.26	1380	S-9
11.35	3	0	-0.91	3.24	0.65	0.29	0.18	1410	S-11
10.98	5	0	-1.11	3.23	1.04	0.51	0.22	1410	R-11
9.47	35	1	-1.63	2.67	0.71	0.55	0.34	1420	S-18
8.51	51	1	-1.94	2.43	2.20	0.69	0.71	1420	R-18
9.55	32	1	-1.52	3.58	0.77	0.54	0.45	1460	R-27
9.01	42	1	-1.01	3.43	1.02	0.37	0.48	1460	25
8.78	46	1	-1.85	3.39	0.78	0.48	0.49	1460	S-27
10.70	10	0	-1.56	3.45	1.46	1.32	0.50	1580	8
9.97	20	0	-1.57	3.92	0.76	0.59	0.48	2300	S-17
8.97	43	1	-1.64	3.20	2.74	1.87	0.36	2300	R-17
8.95	44	1	-2.40	2.58	0.79	1.03	0.40	2770	S-19
8.74	47	1	-2.72	2.59	1.50	1.23	0.42	2770	R-19
9.32	37	1	-0.74	3.14	0.80	0.31	0.51	3200	1
8.26	53	1	-3.49	2.91	2.27	2.29	0.66	3370	S-20
8.09	55	1	-3.53	2.71	2.22	1.73	0.62	3370	R-20
9.52	33	1	-0.88	3.28	0.84	0.28	0.36	3500	R-22
9.19	39	1	-0.90	3.18	0.55	0.17	0.47	3500	S-22
4.90	58	1	-7.32	2.71	3.15	4.29	0.91	4200	S-21
4.61	59	1	-7.69	2.61	3.54	3.87	0.79	4200	R-21
8.69	49	1	-1.64	3.40	2.23	0.59	0.98	5710	S-30
8.27	52	1	-1.66	3.43	1.00	0.68	0.66	5710	R-30
4.29	60	1	-8.26	2.58	2.95	2.61	0.58	7200	R-16
3.68	61	1	-8.57	2.56	2.88	2.75	0.45	7200	S-16
8.70	48	1	-1.37	3.63	1.06	0.35	0.56	14300	S-26
7.50	57	1	-1.50	3.21	2.30	0.88	1.03	14300	R-26

  

BINNING ANALYSIS		
	BIN SUM	% CORRECT BINNING
ENSEMBLE SUMMARY	45	74%

<sup>1</sup>Score: Surflex-Dock uses an empirical scoring function that approximates  $-\log(K_d)$ . The scoring function is described in detail in reference 21.