Table S4 - CPORT sensitivity and specificity versus rank of the first one-star structure.

Complex	CPORT predictions				Rank of the first one-star structure	# of one-star structures
	Receptor		Ligand			
	Sensitivity	Specificity	Sensitivity	Specificity		
1ACB	0.769	0.541	1.000	0.357	29	16
1AK4	0.800	0.327	1.000	0.175	205	5
1AKJ	0.346	0.136	0.485	0.239	47	6
1AVX	0.576	0.345	0.933	0.241	113	5
1AY7	0.750	0.218	0.882	0.500	5	15
1B6C	0.571	0.179	0.591	0.325	1	8
1BUH	0.500	0.145	0.722	0.342	226	3
1BVN	0.606	0.339	0.905	0.452	1	48
1CGI	0.543	0.487	0.905	0.594	20	53
1DFJ	0.615	0.511	0.576	0.373	1	50
1E6E	0.483	0.292	0.724	0.600	1	49
1E96	0.625	0.208	0.588	0.286	50	24
1EAW	0.600	0.429	0.938	0.441	8	10
1EWY	0.381	0.190	0.778	0.452	10	18
1EZU	0.645	0.328	0.535	0.500	365	1
1F51	0.469	0.238	0.704	0.432	119	9
1FC2	0.529	0.127	0.733	0.314	349	1
1GP2	0.600	0.467	0.452	0.215	107	9
1HE1	0.818	0.500	0.656	0.375	2	10
1HIA	0.379	0.212	1.000	0.417	83	31
1I4D	0.385	0.139	0.526	0.294	109	3
1MAH	0.633	0.339	0.636	0.341	59	3
1ML0	0.207	0.125	0.680	0.472	62	4
1PPE	0.441	0.357	1.000	0.517	1	86
1TMQ	0.600	0.356	0.767	0.535	1	70

1UDI	0.630	0.354	0.759	0.550	37	3
1WQ1	0.459	0.362	0.724	0.512	47	6
2BTF	0.500	0.182	0.621	0.333	234	1
2MTA	0.565	0.220	0.938	0.385	72	18
2PCC	0.400	0.140	0.438	0.212	244	1
2SIC	0.645	0.400	1.000	0.271	4	45
2SNI	0.581	0.360	1.000	0.593	78	12
7CEI	0.500	0.173	0.750	0.319	31	5