

S1 Table. The hit frequencies for all proteins of standard protein dataset before and after score normalization in the reverse docking by DOCK, Glide and AutoDock Vina.

Protein	Hit frequency ^a	Hit frequency ^b	Hit frequency ^c	Hit frequency ^d	Hit frequency ^e	Hit frequency ^f
1b9v	3	3	0	21	0	47
1bcd	1	116	0	39	5	74
1c8k	59	140	0	25	0	0
1d3g	66	14	326	31	1267	1
1e66	26	254	209	37	1102	32
1h00	10	29	0	34	3	10
1j4h	0	27	0	71	0	0
1kvo	22	24	0	26	3	14
1l2s	1	62	1	71	0	52
1li4	27	124	6	65	37	22
1lru	46	92	8	110	0	48
1mv9	1	15	261	34	26	6
1njs	5	45	84	41	0	116
1q4x	4	9	342	18	110	4
1qw6	438	58	0	53	460	31
1r9o	13	2	0	77	0	36
1s3b	67	3	395	77	402	2
1sj0	0	6	11	19	4	80
1sqt	4	4	1	6	0	33
1syn	18	33	11	12	11	7
1udt	937	94	55	53	79	11
1uyg	0	0	113	15	8	43
1vso	3	27	0	29	0	19
1xl2	26	35	0	17	1	15
1ype	3	31	1	30	0	20
1zw5	1607	52	1	94	6	75
2aa2	1	279	16	19	1	399
2am9	2	83	16	14	3	162
2ayw	1	7	5	29	0	48
2azr	0	60	0	92	3	157
2b8t	2	35	18	55	0	86
2cnk	0	41	0	70	0	32
2e1w	39	50	0	35	0	0
2etr	8	38	1	15	0	7
2fsz	1	51	6	28	1	89
2gtk	1	11	138	48	0	44
2h7l	39	26	56	36	5	13
2hv5	6	3	316	14	291	50
2hzi	13	165	266	33	112	50
2i0e	2	18	0	31	1	28
2i78	1	22	0	31	5	21
2ica	0	2	6	54	0	109
2nnq	12	181	1	25	10	23

2of2	1	32	1	26	0	8
2oi0	121	39	9	85	0	0
2oj9	1	28	2	18	0	50
2ojg	10	36	8	29	0	12
2owb	8	27	8	32	1	4
2p2i	7	28	226	89	6	25
2p54	2	3	33	12	0	12
2qd9	0	43	8	91	0	20
2rgp	26	64	7	43	2	11
2v3f	4	54	0	52	3	30
2vt4	36	29	11	31	64	5
2zdt	7	37	74	25	0	16
2zec	1	46	0	7	0	44
2znp	1	5	78	50	0	0
3bgs	1	31	24	152	0	35
3biz	2	34	5	18	7	49
3bkl	36	25	2	40	7	17
3bqd	5	334	103	47	0	2
3bwm	1	223	4	47	4	518
3bz3	1	47	13	47	0	29
3c4f	2	98	22	15	9	134
3ccw	6	68	0	45	0	47
3chp	52	1	211	74	607	132
3cjo	4	25	0	57	0	0
3cqw	30	14	0	44	4	14
3d0e	5	1	0	48	0	8
3d4q	4	42	58	13	19	8
3e37	2	22	13	70	0	22
3el8	2	78	0	26	0	8
3eml	2	47	26	28	11	28
3eqh	391	38	27	56	0	7
3f07	0	190	46	602	1	133
3f9m	2	27	1	73	3	354
3frj	94	4	7	27	7	11
3g0e	2	80	28	20	0	79
3g6z	0	18	4	16	0	6
3hl5	0	48	0	40	0	71
3hmm	198	63	5	64	42	7
3kba	0	108	74	18	3	3
3kgc	1	60	31	22	0	63
3kl6	5	0	8	64	2	80
3krj	2	4	35	40	11	45
3l3m	130	55	38	32	31	11
3l5d	2	29	0	21	0	0
3lan	3	14	113	52	97	106
3ln1	3	52	82	31	23	36
3lpb	7	6	4	19	0	0

3lq8	4	0	19	17	1	79
3m2w	2	20	2	37	0	19
3max	5	43	823	396	14	354
3nf7	0	48	0	19	0	33
3nxo	38	29	2	23	27	6
3nxu	22	0	15	55	6	14
3ny8	3	0	0	10	18	3
3odu	22	33	0	10	0	14
3pbl	4	3	1	64	6	21
830c	142	73	0	58	8	41

^aThe hit frequency for DOCK before score normalization

^bThe hit frequency for DOCK after score normalization

^cThe hit frequency for Glide before score normalization

^dThe hit frequency for Glide after score normalization

^eThe hit frequency for AutoDock Vina before score normalization

^fThe hit frequency for AutoDock Vina after score normalization