

Supplementary data

Table S1. Summary of the dataset.

Peptide length	PDB code	Free protein	Classification
5	1jq8	1zwp	easy
5	1mf4	3nju	easy
5	1nvq	4hyi	easy
5	1v1t	1n99	easy
5	2aij	2afy	easy
5	2hpl	2ccq	easy
5	2m0v	2kjd	easy
5	3fp2	3fp3	easy
5	3hds	3hf5	easy
5	4hdq	4hdo	easy
5	4ny3	2ixm	easy
5	4x3o	5yqo	easy
5	5e33	5egy	easy
5	5ggp	5ggp	easy
5	5kds	5kdn	easy
5	5onp	5jvi	easy
5	6f4s	4gjz	easy
6	1ddv	1ddw	easy
6	1f8h	1eh2	easy
6	1jw6	2uu8	easy
6	1ywi	1ywj	easy
6	2ds8	2ds5	easy
6	2ymt	4bcx	easy
6	3emh	6e1z	easy
6	4fii	2j0i	easy
6	4j8b	4j87	easy
6	4m91	4m90	easy
6	4r5i	4r5k	easy
6	4x2h	4wp5	easy
6	5bs2	5bs1	easy
6	5gu4	3px8	easy
6	5njc	5njb	easy
6	5oj5	2xbg	easy
6	6cwp	6cwq	easy
7	1czy	1f3v	easy
7	1p7v	2pwa	easy
7	3agy	3agx	easy
7	3emw	3ek9	easy
7	3s9c	3s9b	easy

7	3shb	3sox	easy
7	3wgx	3wge	easy
7	4ep2	3kt2	easy
7	4leb	4le8	easy
7	4ouc	4qtc	easy
7	4qbr	3a1a	easy
7	5fpx	5fpz	easy
7	5i7z	2lc7	easy
7	5lyn	5lyp	easy
7	6n3e	6n3d	easy
8	1jd5	1jd4	easy
8	1t74	5v8q	easy
8	1w80	1b9k	easy
8	1yy6	2flw	easy
8	2c3i	1xws	easy
8	2e4h	2e3h	easy
8	2fgr	2fgq	easy
8	2jkg	2j kf	easy
8	2xcb	2xcc	easy
8	3av9	4ah9	medium
8	3r42	3r3q	easy
8	4c5a	4c5c	easy
8	4nrx	3kzd	easy
8	4odk	4odo	easy
8	4oz1	4oz0	easy
8	5fv6	5fv5	easy
8	5m5r	2xzg	easy
8	5o9u	5o6h	easy
8	5wyi	3rls	easy
9	1lb6	1lb4	easy
9	2ka9	3gsl	easy
9	2khh	2jp7	easy
9	3i5r	1pht	easy
9	3obq	3obs	easy
9	4bt9	4bt8	easy
9	4pge	6GB6	easy
9	4u0c	5jpa	easy
9	5dai	3lx1	easy
9	5n22	5n1u	easy
9	5t0k	5vsc	easy
9	5wfv	5wfl	medium
10	1ywo	1y0m	easy
10	2fka	3oo0	easy
10	2ke1	1xwh	easy

10	2o9v	2o2w	easy
10	2r7g	3pom	easy
10	4m5s	2y1y	easy
10	4pd1	6fgc	medium
10	4yje	3nmw	easy
10	5huw	4u5u	easy
10	5nqv	5nqs	medium
10	5ow5	5nbt	easy
10	5xxq	3gfc	easy
10	6b27	6b26	easy
10	6ej7	6foa	easy
11	1d8d	3e33	medium
11	1l2z	1gyf	medium
11	1r17	2ral	easy
11	1rxz	1rwz	easy
11	2jnw	2a1i	difficult
11	2qos	1lf7	difficult
11	3bej	1osh	easy
11	3g2s	1jwf	easy
11	3p72	1p9a	difficult
11	3v2o	3so8	easy
11	4hom	4fke	medium
11	4xc2	1gnu	medium
11	4z2o	4z27	easy
11	5crw	3wt1	difficult
11	5xhz	1wi7	easy
12	2aq9	2jf2	difficult
12	2cch	4eoj	easy
12	2ht9	2cq9	easy
12	2rol	2k2m	medium
12	2xrw	4qtd	medium
12	4cc2	4cc4	medium
12	4gq6	4gq4	difficult
12	4j2c	1lvf	easy
12	4lzf	4ld1	medium
12	4nuu	3rrc	easy
12	4qh7	3dvh	easy
12	4zoz	4zoy	easy
12	5d94	3vtu	medium
12	5n85	4ipc	easy
12	6h7b	6h7a	medium
13	1cqg	1trs	medium
13	1eg4	1eg3	easy
13	1o0p	3v4m	medium

13	2las	2mw5	easy
13	2p1o	2p1m	difficult
13	2v8c	2vk3	medium
13	3bqo	3l82	medium
13	4lk9	4ljn	easy
13	4mvi	4iax	difficult
13	4oyk	4p09	difficult
13	4uqy	4uqx	medium
13	5di8	5hyf	difficult
13	5v3r	2oew	easy
13	6e5x	5dvw	easy
14	1a0n	3ua6	medium
14	1mv0	1muz	medium
14	2jqk	2jqh	easy
14	3pe4	3pe3	medium
14	3zrj	3zri	easy
14	4a2a	4a2b	easy
14	5ei3	1ipc	easy
14	5j3q	2qkm	easy
14	6co4	5irs	medium
15	1nrl	4x1f	easy
15	2fym	6bfy	difficult
15	2ivz	1crz	difficult
15	2vzg	2vzc	easy
15	3h1z	1e42	medium
15	4txr	2lxm	easy
15	5yay	5yaz	difficult
15	6f0y	1roc	medium
16	1pmx	1imx	difficult
16	2i94	4yi8	easy
16	2koh	2k1z	difficult
16	3et3	5y2t	easy
16	4iga	4qyw	easy
16	4xek	2lk4	easy
16	5ajn	5fv9	medium
16	5efi	3gmo	easy
17	1f47	1f46	easy
17	2lsi	2lsy	difficult
17	6dei	3n4s	easy
17	6f6d	4ask	medium
17	6fbk	6elm	difficult
18	1j2x	1i27	easy
18	1yfn	1ox8	difficult
18	2kbr	2kbq	easy

18	3plu	1m94	difficult
18	3tiw	3qq7	easy
18	6f0w	6ey1	difficult
18	6g5g	1epw	easy
19	2cny	2co3	medium
19	2hwn	1l6e	easy
19	3aa0	3aa7	difficult
19	4dg3	5n3j	difficult
19	5fml	6fs8	easy
19	5v2p	1t3s	easy
20	1vpp	1mkk	difficult
20	2nnu	1dto	difficult
20	2xpn	2xpl	easy
20	5tgi	3hpc	difficult

Table S2. The ranks given by the global docking programs and GalaxyPepDock for the entire dataset.

Peptide length	PDB code	ZDOCK ^a	HawkDock ^a	FRODOCK ^a	MDockPeP _SA ^a	MDockPeP _HA ^a	CABS- dock_SA ^a	CABS- dock_HA ^a	HPEPDOCK ^a	pepATTRACT ^a	GalaxyPepDock ^a
5	1jq8								19:3.960 (0.583)	2:3.679 (0.458)	3:3.927 (0.667)
5	1mf4			7:2.803 (0.700)							4:2.464 (0.700)
5	1nvq		47:3.014 (0.500)	79:2.987 (0.333)	4:3.880 (0.667)	4:3.880 (0.667)			6:2.989 (0.500)		4:2.987 (0.667)
5	1vlt								15:3.613 (0.333)		1:0.906 (0.833)
5	2aij	99:3.404 (0.435)							11:1.132 (0.739)		1:1.244 (0.609)
5	2hpl	69:3.664 (0.632)	8:3.952 (0.842)	2:3.058 (0.421)	16:3.591 (0.632)	16:3.591 (0.632)			1:2.663 (0.579)		1:3.257 (0.737)
5	2m0v		5:3.073 (0.353)		56:3.893 (0.235)	56:3.893 (0.235)			43:2.098 (0.529)	11:2.922 (0.412)	5:2.634 (0.706)
5	3fp2		21:2.594 (0.500)						2:2.328 (0.875)		1:2.152 (0.750)
5	3hds								83:3.551 (0.571)		3:2.538 (0.619)
5	4hdq	36:3.598 (0.273)			16:3.837 (0.364)	16:3.837 (0.364)	7:3.916 (0.227)	7:3.916 (0.227)	21:3.215 (0.682)	1:2.795 (0.455)	
5	4ny3				18:3.660 (0.533)	18:3.660 (0.533)			8:3.831 (0.400)	14:3.851 (0.333)	

5	4x3o				41:2.863 (0.571)	41:2.863 (0.571)			21:3.159 (0.667)		4:3.665 (0.476)
5	5e33								1:2.119 (0.808)		
5	5ggp			5:2.717 (0.875)	21:3.495 (0.500)	21:3.495 (0.500)			57:3.079 (0.750)	13:3.578 (1.000)	
5	5kds										
5	5onp						2:3.466 (0.407)	2:3.466 (0.407)	16:3.731 (0.630)		
5	6f4s								94:3.875 (0.615)		
6	1ddv				3:3.780 (0.214)	3:3.780 (0.214)			60:3.531 (0.357)		1:1.384 (0.714)
6	1f8h				14:2.768 (0.667)	14:2.768 (0.667)					1:2.652 (0.733)
6	1jw6										3:3.318 (0.500)
6	1ywi	50:3.956 (0.471)	12:2.100 (0.471)	4:3.068 (0.471)			2:3.473 (0.294)	2:3.473 (0.294)	3:3.763 (0.647)	4:1.791 (0.882)	
6	2ds8			5:3.943 (0.294)			4:2.075 (0.471)	4:2.075 (0.471)	1:2.541 (0.647)		1:1.238 (0.824)
6	2ymt		91:2.798 (0.579)	5:2.917 (0.632)	4:3.419 (0.684)	4:3.419 (0.684)			5:3.701 (0.684)	2:2.207 (0.789)	1:1.222 (0.684)
6	3emh				60:3.480 (0.438)	60:3.480 (0.438)			33:3.930 (0.375)	4:3.971 (0.562)	1:1.919 (0.875)
6	4fii	2:2.550 (0.643)	3:2.109 (0.643)	6:3.091 (0.393)			3:2.905 (0.321)	3:2.905 (0.321)	5:1.539 (0.607)	27:2.414 (0.750)	1:2.574 (0.464)

6	4j8b							73:3.311 (0.524)		
6	4m9l		48:3.310 (0.375)					15:1.972 (0.812)		1:2.539 (0.812)
6	4r5i			21:3.102 (0.577)	1:1.819 (0.731)	1:1.819 (0.731)		5:3.013 (0.615)	13:3.109 (0.615)	1:1.162 (0.885)
6	4x2h	3:3.053 (0.679)		71:2.511 (0.286)	1:2.848 (0.429)	1:2.848 (0.429)				
6	5bs2									
6	5gu4	3:2.491 (0.700)	11:3.900 (0.400)	1:2.012 (0.750)	23:3.251 (0.700)	23:3.251 (0.700)		3:1.571 (0.750)		1:2.513 (0.950)
6	5njc							53:3.819 (0.393)	27:3.710 (0.536)	
6	5oj5									
6	6cwp									
7	1czy	64:3.126 (0.538)	9:2.547 (0.615)	19:3.389 (0.385)	3:2.605 (0.769)	3:2.605 (0.769)				1:2.598 (0.654)
7	1p7v	72:3.841 (0.538)						33:3.906 (0.385)		1:2.483 (0.538)
7	3agy				8:2.770 (0.647)	8:2.770 (0.647)		34:2.993 (0.765)	20:3.439 (0.353)	1:3.134 (0.529)
7	3emw	74:3.843 (0.286)			44:3.964 (0.524)	44:3.964 (0.524)				4:2.800 (0.333)
7	3s9c	92:3.370 (0.393)			29:3.089 (0.536)	29:3.089 (0.536)				1:2.414 (0.571)

7	3shb							4:2.760 (0.842)		1:1.852 (0.895)	
7	3wgx	7:3.383 (0.600)	39:3.200 (0.350)	1:2.960 (0.400)	7:3.949 (0.300)	7:3.949 (0.300)		21:3.165 (0.600)	9:2.700 (0.500)	1:1.905 (0.550)	
7	4ep2							3:1.590 (0.722)		2:1.272 (0.750)	
7	4leb		67:3.914 (0.333)								
7	4ouc										
7	4qbr		62:3.051 (0.370)							1:2.973 (0.370)	
7	5fpx				8:3.879 (0.423)	8:3.879 (0.423)					
7	5i7z				85:3.571 (0.667)	85:3.571 (0.667)		67:3.596 (0.533)		7:1.709 (1.000)	
7	5lyn		83:3.066 (0.476)	67:3.468 (0.476)	9:2.545 (0.524)	9:2.545 (0.524)	8:3.707 (0.333)	8:3.707 (0.333)	1:2.722 (0.381)	9:3.406 (0.238)	1:1.978 (0.857)
7	6n3e	44:3.390 (0.381)								9:3.741 (0.619)	
8	1jd5							31:3.929 (0.346)		1:1.479 (0.846)	
8	1t74						1:2.384 (0.667)	1:2.384 (0.667)		1:2.036 (0.611)	
8	1w80									10:3.173 (0.450)	
8	1yy6		21:3.849 (0.435)		18:3.735 (0.435)	18:3.735 (0.435)		16:2.925 (0.478)		1:2.653 (0.609)	

8	2c3i						29:3.910 (0.370)	44:3.816 (0.296)	1:2.693 (0.556)
8	2e4h		33:3.968 (0.353)				1:3.276 (0.471)		
8	2fgr								1:3.915 (0.700)
8	2jkg	68:3.834 (0.500)	23:3.967 (0.571)	42:3.283 (0.357)			44:3.968 (0.429)	38:3.710 (0.500)	3:3.719 (0.571)
8	2xcb						13:3.643 (0.609)		1:2.168 (0.435)
8	3av9								
8	3r42				43:3.938 (0.609)	43:3.938 (0.609)	6:2.751 (0.826)		1:2.155 (0.783)
8	4c5a								
8	4nxr		7:3.919 (0.423)				19:3.209 (0.577)		1:2.373 (0.769)
8	4odk								
8	4oz1				6:4.000 (0.591)	6:4.000 (0.591)			
8	5fv6	23:3.658 (0.273)							
8	5m5r						8:3.330 (0.429)		1:3.168 (0.762)
8	5o9u	39:2.685 (0.476)					5:3.960 (0.500)		1:3.312 (0.452)
8	5wyi								

9	1lb6	81:3.491 (0.556)	8:2.742 (0.333)	16:3.494 (0.556)	16:3.494 (0.556)			3:2.793 (0.519)	1:2.853 (0.593)
9	2ka9								
9	2khh					6:3.899 (0.250)	6:3.899 (0.250)		1:3.889 (0.350)
9	3i5r		1:3.329 (0.350)	1:3.897 (0.750)	1:3.897 (0.750)		1:3.068 (0.600)	7:3.042 (0.600)	1:2.092 (0.750)
9	3obq	57:3.827 (0.619)	8:3.392 (0.238)	12:3.739 (0.381)	12:3.739 (0.381)		7:2.460 (0.619)		1:2.597 (0.714)
9	4bt9	52:2.682 (0.737)	7:2.977 (0.421)	39:2.844 (0.579)	39:2.844 (0.579)		7:1.579 (0.789)		1:2.656 (0.632)
9	4pge	63:3.248 (0.419)		84:3.916 (0.558)	84:3.916 (0.558)		23:2.214 (0.535)		1:2.411 (0.581)
9	4u0c								
9	5dai								1:1.222 (0.812)
9	5n22								
9	5t0k								2:2.918 (0.692)
9	5wfv			90:3.904 (0.393)	90:3.904 (0.393)				1:2.043 (0.786)
10	1ywo	33:3.638 (0.429)	16:2.559 (0.429)	13:3.983 (0.571)	13:3.983 (0.571)		3:3.289 (0.571)		1:3.597 (0.643)
10	2fka						13:3.955 (0.615)		1:3.210 (0.538)
10	2ke1			98:3.146 (0.706)	98:3.146 (0.706)				3:2.860 (0.676)

10	2o9v			18:3.417 (0.438)	4:1.646 (0.812)	4:1.646 (0.812)			10:3.819 (0.625)	41:2.796 (0.625)	1:1.551 (0.625)
10	2r7g				11:3.657 (0.379)	11:3.657 (0.379)			9:3.417 (0.586)		6:1.868 (0.793)
10	4m5s								27:2.468 (0.346)		
10	4pd1				12:3.489 (0.567)	12:3.489 (0.567)			9:2.971 (0.500)		1:1.909 (0.633)
10	4yje	34:3.680 (0.558)									
10	5huw										2:2.307 (0.667)
10	5nqv				40:3.434 (0.500)	40:3.434 (0.500)	1:3.914 (0.346)	1:3.914 (0.346)	12:3.450 (0.423)		
10	5ow5	26:2.087 (0.706)	36:2.631 (0.529)	23:2.507 (0.471)	100:1.376 (0.824)	100:1.376 (0.824)			22:3.886 (0.412)	7:3.977 (0.294)	
10	5xxq								4:3.941 (0.310)		
10	6b27				2:2.072 (0.652)	2:2.072 (0.652)			20:2.521 (0.435)		2:2.073 (0.783)
10	6ej7								61:3.339 (0.406)		
11	1d8d				75:4.371 (0.303)	32:4.346 (0.394)			50:4.545 (0.242)		3:4.229 (0.242)
11	1l2z				51:4.268 (0.471)				5:3.802 (0.471)		3:3.970 (0.471)
11	1r17										1:1.605 (0.811)

11	1rxz								63:4.277 (0.206)		1:2.810 (0.618)
11	2jnw										1:4.087 (0.591)
11	2qos				1:4.119 (0.300)	7:3.288 (0.300)					
11	3bej		19:4.764 (0.450)		71:4.928 (0.350)	94:3.667 (0.550)	8:2.983 (0.350)		2:4.271 (0.550)		1:2.401 (0.550)
11	3g2s	63:4.060 (0.577)							86:4.409 (0.231)		1:3.394 (0.615)
11	3p72										
11	3v2o	96:3.624 (0.520)	19:3.964 (0.320)	5:3.154 (0.280)	17:3.877 (0.440)	48:3.125 (0.560)	4:4.714 (0.280)		3:2.663 (0.680)	3:4.020 (0.360)	1:3.743 (0.720)
11	4hom										
11	4xc2							5:4.176 (0.500)			7:4.944 (0.471)
11	4z2o					47:1.615 (0.844)					
11	5crw										
11	5xhz					30:4.202 (0.500)	3:3.280 (0.333)	7:4.397 (0.417)			1:4.121 (0.625)
12	2aq9										1:3.920 (0.500)
12	2cch	80:4.212 (0.382)	32:3.809 (0.324)		1:4.406 (0.618)				4:3.185 (0.382)		1:3.878 (0.618)
12	2ht9										8:4.685 (0.571)
12	2rol				66:4.407 (0.550)	60:4.737 (0.400)	2:4.947 (0.300)		4:3.298 (0.250)		

12	2xrw					1:4.466 (0.217)		1:2.665 (0.652)
12	4cc2		4:2.359 (0.679)	2:4.329 (0.357)		24:4.940 (0.286)		1:4.524 (0.607)
12	4gq6		89:3.503 (0.294)					1:4.966 (0.441)
12	4j2c							
12	4lzf							2:4.327 (0.478)
12	4nuu					67:4.734 (0.250)		
12	4qh7	64:4.567 (0.382)	6:4.677 (0.353)		8:4.898 (0.294)	66:1.795 (0.559)	9:4.300 (0.353)	2:3.027 (0.735)
12	4zoz		22:4.146 (0.241)	19:3.684 (0.310)	5:4.995 (0.207)	6:4.354 (0.241)		5:4.579 (0.414)
12	5d94	98:4.820 (0.219)	91:4.391 (0.469)			25:4.095 (0.219)		1:4.908 (0.500)
12	5n85		33:3.812 (0.409)	11:3.642 (0.500)		15:4.710 (0.227)		
12	6h7b		2:3.276 (0.429)	2:3.283 (0.464)		84:3.490 (0.393)		
13	1cqq							2:3.899 (0.556)
13	1eg4					37:2.939 (0.667)		4:4.953 (0.619)
13	1o0p							1:3.494 (0.615)
13	2las				3:4.139 (0.294)			

13	2p1o								3:3.715 (0.379)
13	2v8c								1:3.468 (0.577)
13	3bqo								1:2.629 (0.660)
13	4lk9						22:4.001 (0.290)		1:1.473 (0.677)
13	4mvi								
13	4oyk						26:4.625 (0.333)		
13	4uqy			6:4.026 (0.406)	35:4.748 (0.469)		1:4.447 (0.250)		
13	5di8								1:4.760 (0.455)
13	5v3r		33:2.364 (0.647)				98:4.782 (0.294)		1:1.575 (0.588)
13	6e5x	4:4.309 (0.346)	25:3.779 (0.692)		58:3.564 (0.462)	1:4.602 (0.269)	5:3.347 (0.615)	13:4.987 (0.462)	
14	1a0n				47:4.634 (0.316)				
14	1mv0			17:4.157 (0.458)	19:4.569 (0.542)		6:4.046 (0.333)	52:4.273 (0.417)	1:3.416 (0.667)
14	2jqk		37:3.536 (0.438)	77:4.886 (0.250)		5:3.687 (0.625)	2:3.634 (0.750)	21:4.804 (0.312)	1:4.260 (0.375)
14	3pe4								1:3.202 (0.758)
14	3zrj		13:4.278 (0.318)	49:4.069 (0.455)	11:4.940 (0.318)			5:2.794 (0.682)	1:1.750 (0.864)
14	4a2a								1:3.006 (0.560)

14	5ei3						25:3.987 (0.292)		1:2.961 (0.750)
14	5j3q	85:4.778 (0.276)		9:4.710 (0.241)	3:4.706 (0.241)	1:4.939 (0.345)	3:4.901 (0.241)	13:4.563 (0.310)	
14	6co4					5:3.706 (0.273)	2:3.541 (0.364)		
15	1nrl				2:4.770 (0.211)	4:3.019 (0.316)	4:4.904 (0.211)		1:1.496 (0.789)
15	2fym								1:2.536 (0.862)
15	2ivz					3:4.374 (0.361)			1:3.519 (0.472)
15	2vzg		5:4.440 (0.308)			7:4.340 (0.385)	21:4.811 (0.385)		2:3.225 (0.615)
15	3h1z								1:3.690 (0.667)
15	4txr					5:3.359 (0.227)			
15	5yay						98:4.866 (0.250)		
15	6f0y								
16	1pmx				93:4.680 (0.400)		54:4.512 (0.467)		1:2.973 (0.667)
16	2i94			8:4.961 (0.333)					
16	2koh						96:4.991 (0.269)		2:4.687 (0.538)
16	3et3								1:3.340 (0.667)

16	4iga			33:4.773 (0.368)			5:4.628 (0.368)	5:4.748 (0.526)
16	4xek	4:2.768 (0.304)			2:4.913 (0.348)	7:4.217 (0.261)	37:4.484 (0.304)	3:2.162 (0.739)
16	5ajn		20:4.450 (0.250)				5:4.271 (0.438)	
16	5efi			13:4.535 (0.290)				
17	1f47	37:4.667 (0.421)					5:4.833 (0.211)	1:4.811 (0.421)
17	2lsi							2:2.273 (0.517)
17	6dei							
17	6f6d							1:2.408 (0.518)
17	6fbk				5:4.561 (0.545)	2:3.275 (0.591)		
18	1j2x						53:4.578 (0.476)	2:3.913 (0.571)
18	1yfn			8:3.687 (0.371)		4:4.621 (0.229)		
18	2kbr			63:4.941 (0.500)	1:4.578 (0.350)	3:4.592 (0.250)	7:4.497 (0.250)	70:4.657 (0.350)
18	3plu						7:3.561 (0.400)	
18	3tiw		4:4.643 (0.259)	2:3.986 (0.704)	2:3.822 (0.630)		5:4.379 (0.407)	1:2.605 (0.593)
18	6f0w							1:3.591 (0.477)

18	6g5g	55:4.529 (0.414)		63:2.549 (0.414)					
19	2cny						90:4.316 (0.286)		
19	2hwn	2:3.938 (0.452)	16:3.044 (0.258)	7:1.995 (0.419)	1:1.026 (0.258)	6:1.895 (0.387)	2:3.248 (0.387)		7:1.164 (0.741)
19	3aa0								1:2.401 (0.482)
19	4dg3						5:4.423 (0.240)		1:4.268 (0.580)
19	5fml								
19	5v2p						47:4.861 (0.250)		1:1.918 (0.531)
20	1vpp								
20	2nnu						83:4.952 (0.522)		2:3.444 (0.565)
20	2xpn	15:4.257 (0.344)							
20	5tgi								

^a Blank space represents prediction failure. The number before the “:” indicates the best rank of the near-native prediction, followed by IL_RMSD and f_{nat} .

Table S3. The ranks given by the local docking programs for the entire dataset.

Peptide length	PDB code	DINC ^a	ADCP ^a	Vina_SA ^a	Vina_HA ^a	MDockPeP _SA ^a	MDockPeP _HA ^a	GOLD_SA ^a	GOLD_HA ^a	Surflex ^a	HADDOCK ^a	HPEPDOCK ^a
5	1jq8		11:3.836 (0.667)					2:3.606 (0.583)	6:3.835 (0.625)	76:3.276 (0.458)	2:2.563 (0.875)	89:3.344 (0.583)
5	1mf4			25:3.999 (0.350)		2:3.723 (0.450)	2:3.723 (0.450)	3:2.128 (0.650)	2:2.444 (0.700)	11:2.605 (0.700)	21:2.701 (0.600)	
5	1nvq	15:3.452 (0.500)	10:3.447 (0.667)	5:3.908 (0.500)	8:3.954 (0.417)	23:3.111 (0.500)	23:3.111 (0.500)	52:3.722 (0.417)	50:3.701 (0.583)	8:3.747 (0.500)	43:3.726 (0.500)	3:3.592 (0.750)
5	1v1t		12:3.877 (0.556)			55:3.937 (0.667)	55:3.937 (0.667)	2:2.557 (0.944)	43:3.053 (0.389)	7:2.524 (0.778)	4:2.725 (0.667)	1:3.146 (0.333)
5	2aij	2:1.157 (0.783)	1:1.288 (0.826)	7:1.922 (0.652)	12:1.909 (0.652)	2:3.624 (0.391)	2:3.624 (0.391)	1:1.220 (0.826)	1:1.217 (0.696)	1:1.668 (0.826)	1:1.661 (0.913)	4:1.849 (0.609)
5	2hpl	4:2.540 (0.632)	1:3.674 (0.737)	1:2.887 (0.579)	1:2.894 (0.579)	16:3.421 (0.474)	16:3.421 (0.474)	12:2.717 (0.632)	3:0.976 (0.842)	1:3.716 (0.842)	2:3.591 (0.632)	1:2.613 (0.684)
5	2m0v	23:3.887 (0.412)	5:3.674 (0.765)	37:2.849 (0.529)	15:2.900 (0.529)	6:3.941 (0.353)	6:3.941 (0.353)	12:3.231 (0.706)	16:3.082 (0.647)	1:2.173 (0.471)	18:3.231 (0.588)	5:2.556 (0.588)
5	3fp2	92:3.700 (0.500)	84:3.929 (0.562)	21:2.875 (0.750)		19:2.834 (0.812)	19:2.834 (0.812)	23:3.286 (0.625)	15:3.023 (0.625)	8:2.585 (0.812)	9:2.354 (0.812)	35:3.100 (0.562)
5	3hds	95:3.410 (0.571)	18:3.485 (0.476)	32:3.674 (0.429)		39:3.991 (0.667)	39:3.991 (0.667)	21:3.546 (0.333)		11:2.402 (0.619)		23:2.820 (0.524)
5	4hdq	1:3.437 (0.818)	1:3.883 (0.500)	1:3.084 (0.818)	1:3.301 (0.727)	1:2.805 (0.773)	1:2.805 (0.773)	1:2.587 (0.455)	1:3.201 (0.591)	1:3.708 (0.727)	2:3.722 (0.682)	76:2.805 (0.364)
5	4ny3	1:3.738 (0.800)	24:3.604 (0.467)	1:3.743 (0.800)	1:3.625 (0.800)	6:3.769 (0.467)	6:3.769 (0.467)	4:3.990 (0.200)	4:3.439 (0.667)	18:3.904 (0.533)	8:3.421 (0.867)	14:3.655 (0.533)

5	4x3o	1:3.332 (0.571)	4:2.620 (0.762)	1:3.442 (0.524)	2:3.186 (0.571)	3:2.453 (0.619)	3:2.453 (0.619)	1:2.747 (0.762)	1:3.117 (0.667)	6:1.682 (0.667)	21:3.120 (0.571)	8:2.943 (0.714)
5	5e33	1:1.523 (0.808)	4:1.623 (0.692)	1:3.659 (0.577)	1:2.427 (0.731)			1:2.180 (0.808)	1:2.172 (0.808)	1:2.220 (0.769)	17:2.129 (0.846)	2:1.722 (0.808)
5	5ggp	46:3.016 (0.875)	70:2.117 (0.875)	25:2.581 (0.750)		2:3.649 (0.875)	2:3.649 (0.875)	1:2.966 (0.750)	1:2.678 (0.750)	18:1.665 (1.000)	2:3.557 (0.500)	
5	5kds		71:3.937 (0.778)							12:3.905 (0.778)		
5	5onp	1:1.278 (0.889)	1:1.012 (0.889)	1:2.838 (0.815)	1:2.954 (0.815)	43:3.265 (0.556)	43:3.265 (0.556)	1:2.748 (0.852)	1:2.915 (0.741)	1:2.731 (0.778)		5:3.142 (0.444)
5	6f4s		81:3.477 (0.615)		23:3.660 (0.538)				41:3.917 (0.692)		23:3.008 (0.769)	
6	1ddv	24:3.664 (0.643)	6:3.309 (0.571)	11:3.687 (0.571)	19:3.605 (0.714)	2:3.186 (0.214)	2:3.186 (0.214)	4:3.738 (0.643)	12:3.858 (0.643)	32:3.433 (0.429)	1:3.752 (0.786)	50:3.115 (0.357)
6	1f8h	6:3.236 (0.667)	3:3.617 (0.733)	4:3.335 (0.600)	9:3.692 (0.800)	7:3.492 (0.533)	7:3.492 (0.533)	2:3.551 (0.733)	1:3.600 (0.667)	39:3.177 (0.467)	23:3.414 (0.333)	97:3.362 (0.533)
6	1jw6									63:3.513 (0.400)	46:3.797 (0.600)	
6	1ywi	23:3.044 (0.471)	1:3.674 (0.471)	7:3.872 (0.529)	12:3.903 (0.529)			3:3.764 (0.412)	1:2.432 (0.471)	1:2.639 (0.353)	1:3.935 (0.412)	12:1.243 (0.647)
6	2ds8	35:3.944 (0.471)	1:2.927 (0.529)	1:1.562 (0.765)	9:2.606 (0.882)	5:2.136 (0.824)	5:2.136 (0.824)	22:3.940 (0.353)	72:3.121 (0.529)	2:3.459 (0.353)	1:2.925 (0.941)	6:2.840 (0.647)
6	2ymt	8:2.877 (0.579)	3:2.317 (0.632)	12:1.945 (0.789)	40:2.738 (0.368)	10:3.232 (0.632)	10:3.232 (0.632)	1:2.682 (0.579)		1:1.535 (0.684)	1:2.758 (0.842)	26:1.853 (0.684)
6	3emh	53:3.717 (0.250)	3:3.411 (0.750)	30:3.722 (0.438)		15:3.614 (0.375)	15:3.614 (0.375)	2:3.730 (0.688)	1:2.214 (0.938)	1:3.982 (0.688)	1:3.456 (0.688)	

6	4fii	49:3.493 (0.500)	13:3.631 (0.429)	8:3.437 (0.464)	19:2.704 (0.607)	9:3.122 (0.357)	9:3.122 (0.357)	21:3.314 (0.321)	16:3.647 (0.500)	3:2.765 (0.500)	1:1.779 (0.857)	4:3.937 (0.321)
6	4j8b		41:3.272 (0.667)						21:3.903 (0.476)		7:3.662 (0.762)	61:3.917 (0.524)
6	4m9l	6:3.456 (0.562)	2:3.894 (0.625)	9:3.571 (0.562)	40:3.568 (0.625)	87:3.692 (0.312)	87:3.692 (0.312)	6:3.350 (0.688)	5:2.516 (0.688)	71:3.838 (0.500)	15:3.001 (0.562)	13:3.218 (0.438)
6	4r5i	2:3.088 (0.731)	6:2.723 (0.731)	1:2.684 (0.654)	7:3.390 (0.654)	6:1.349 (0.769)	6:1.349 (0.769)	1:3.114 (0.615)	1:2.791 (0.615)	1:3.588 (0.385)		4:1.437 (0.769)
6	4x2h	25:2.198 (0.536)	3:3.534 (0.429)	7:2.188 (0.571)	6:3.837 (0.536)	1:2.280 (0.500)	1:2.280 (0.500)	6:2.757 (0.429)	10:2.773 (0.500)	16:2.698 (0.464)	1:2.904 (0.821)	
6	5bs2										86:3.222 (0.545)	43:2.761 (0.727)
6	5gu4	19:3.417 (0.650)	1:1.955 (0.900)	11:3.290 (0.750)		2:2.727 (0.650)	2:2.727 (0.650)	3:3.778 (0.800)	3:3.993 (0.700)	1:3.470 (0.700)	3:2.711 (0.750)	12:3.511 (0.650)
6	5njc	1:3.812 (0.357)	2:1.237 (0.857)	4:3.839 (0.357)	2:3.862 (0.357)	2:1.123 (0.750)	2:1.123 (0.750)	2:3.863 (0.464)	1:3.987 (0.429)	1:3.803 (0.321)	14:3.591 (0.571)	
6	5oj5	23:3.850 (0.333)	1:2.951 (0.800)	21:3.320 (0.400)	14:2.884 (0.467)	29:3.611 (0.667)	29:3.611 (0.667)	20:3.267 (0.733)	20:3.716 (0.667)	5:3.453 (0.667)		
6	6cwp		2:3.378 (0.700)			56:2.857 (0.550)	56:2.857 (0.550)	33:3.941 (0.600)	35:3.630 (0.300)	49:3.471 (0.250)	1:2.233 (0.700)	
7	1czy	11:3.319 (0.538)	1:1.104 (0.885)	4:3.117 (0.692)	8:3.412 (0.654)	2:2.558 (0.615)	2:2.558 (0.615)	1:1.964 (0.577)	2:3.656 (0.346)	1:2.322 (0.615)	9:3.771 (0.538)	1:2.944 (0.577)
7	1p7v	64:3.510 (0.462)	8:3.479 (0.462)	8:2.728 (0.615)	22:2.907 (0.577)	20:3.368 (0.462)	20:3.368 (0.462)	10:3.600 (0.500)	7:2.425 (0.654)	9:3.322 (0.423)	13:3.018 (0.654)	9:2.568 (0.538)
7	3agy	80:3.511 (0.529)	4:2.977 (0.647)			1:2.172 (0.588)	1:2.172 (0.588)				4:3.790 (0.588)	1:1.839 (0.706)

7	3emw	67:2.954 (0.476)	4:3.637 (0.762)	14:3.432 (0.619)		22:3.781 (0.476)	22:3.781 (0.476)		84:3.965 (0.524)			80:3.589 (0.619)
7	3s9c	1:2.509 (0.714)	15:3.507 (0.429)	1:2.119 (0.714)	1:2.092 (0.750)	3:3.232 (0.536)	3:3.232 (0.536)	17:3.740 (0.500)	9:3.020 (0.536)	31:3.734 (0.536)		
7	3shb	30:3.996 (0.579)	36:1.694 (0.789)	10:3.516 (0.526)	18:2.877 (0.526)	9:2.354 (0.737)	9:2.354 (0.737)	22:3.689 (0.421)	21:3.707 (0.632)		40:3.003 (0.579)	8:3.701 (0.632)
7	3wgx		8:3.628 (0.750)			21:2.998 (0.600)	21:2.998 (0.600)	29:3.379 (0.550)	64:2.218 (0.600)	10:3.674 (0.450)	20:1.856 (0.750)	21:3.128 (0.650)
7	4ep2	1:2.467 (0.778)	1:1.075 (0.722)	4:2.366 (0.750)	1:2.370 (0.806)			1:1.485 (0.722)	1:1.329 (0.778)	5:3.938 (0.417)	9:3.274 (0.361)	
7	4leb										50:3.997 (0.714)	
7	4ouc											
7	4qbr	24:3.854 (0.481)	24:3.451 (0.593)	14:3.490 (0.407)	23:2.975 (0.407)	82:2.488 (0.407)	82:2.488 (0.407)	4:3.149 (0.630)	2:1.617 (0.778)	44:2.604 (0.519)	17:3.270 (0.704)	58:1.549 (0.741)
7	5fpx	23:3.846 (0.462)	76:2.858 (0.462)	20:3.652 (0.500)	28:3.940 (0.423)	1:3.886 (0.385)	1:3.886 (0.385)	52:3.157 (0.462)	8:3.928 (0.385)		24:3.985 (0.500)	
7	5i7z		34:2.610 (0.733)	31:2.646 (0.733)		7:3.474 (0.467)	7:3.474 (0.467)				3:2.938 (0.667)	71:3.337 (0.267)
7	5lyn	14:3.920 (0.381)	7:1.579 (0.810)			10:2.416 (0.571)	10:2.416 (0.571)	4:3.362 (0.667)	3:2.330 (0.476)	42:2.658 (0.619)	3:2.128 (0.857)	1:2.906 (0.429)
7	6n3e		86:3.506 (0.476)			15:3.900 (0.524)	15:3.900 (0.524)			1:3.071 (0.476)	44:3.900 (0.476)	
8	1jd5	49:3.829 (0.308)	5:2.504 (0.885)	7:3.661 (0.462)	42:3.736 (0.538)	66:3.102 (0.500)	66:3.102 (0.500)	1:3.122 (0.654)	1:2.652 (0.808)			

8	1t74		1:3.383 (0.444)				8:3.462 (0.556)	8:3.462 (0.556)		15:3.092 (0.333)	17:3.895 (0.444)	
8	1w80		26:2.797 (0.700)	15:3.581 (0.300)	54:3.653 (0.350)	2:3.344 (0.700)	2:3.344 (0.700)	4:3.900 (0.500)	21:3.205 (0.450)	5:3.541 (0.750)	9:3.397 (0.850)	81:3.082 (0.400)
8	1yy6	11:3.303 (0.522)	50:3.985 (0.522)	3:3.047 (0.609)	2:3.862 (0.565)	4:3.582 (0.565)	4:3.582 (0.565)	8:3.594 (0.261)	10:3.624 (0.435)	25:3.895 (0.348)	35:3.520 (0.565)	10:3.524 (0.391)
8	2c3i		32:3.970 (0.519)						65:3.195 (0.370)	25:3.984 (0.370)	41:3.210 (0.852)	68:2.689 (0.593)
8	2e4h		3:3.071 (0.471)					1:2.214 (0.529)	2:3.016 (0.471)	8:3.802 (0.353)	25:3.859 (0.647)	23:2.328 (0.294)
8	2fgr		25:3.338 (0.900)									
8	2jkg							29:4.000 (0.214)			13:3.815 (0.571)	
8	2xcb		1:3.103 (0.609)	50:2.646 (0.652)		89:3.741 (0.304)	89:3.741 (0.304)		39:3.710 (0.261)	62:3.396 (0.391)	1:2.549 (0.696)	14:3.230 (0.478)
8	3av9	3:3.426 (0.368)	47:3.992 (0.316)	4:3.661 (0.368)	5:3.943 (0.579)	29:3.395 (0.421)	29:3.395 (0.421)					
8	3r42	2:3.058 (0.652)	16:3.405 (0.696)	2:3.313 (0.783)	11:3.212 (0.652)	22:3.964 (0.609)	22:3.964 (0.609)	4:3.794 (0.391)	1:3.267 (0.391)	3:3.886 (0.478)	25:3.838 (0.652)	
8	4c5a										36:3.962 (0.571)	
8	4nrx	31:3.224 (0.615)	12:2.392 (0.538)			2:3.773 (0.462)	2:3.773 (0.462)	21:2.895 (0.385)	24:3.110 (0.462)	2:3.044 (0.577)	3:2.511 (0.577)	88:2.431 (0.423)
8	4odk	30:3.325 (0.444)	13:3.734 (0.667)	6:3.575 (0.500)	19:3.517 (0.333)	2:3.574 (0.500)	2:3.574 (0.500)		50:2.763 (0.556)		5:3.416 (0.500)	23:3.340 (0.444)

8	4oz1		5:3.971 (0.545)				3:3.730 (0.545)	3:3.730 (0.545)	12:3.547 (0.364)	2:3.903 (0.364)		1:3.070 (0.773)	
8	5fv6						84:3.964 (0.455)	84:3.964 (0.455)	55:3.539 (0.364)	8:3.875 (0.455)		2:3.535 (0.727)	
8	5m5r								23:3.710 (0.476)	4:3.577 (0.476)			8:3.840 (0.476)
8	5o9u		2:1.563 (0.643)				6:2.346 (0.667)	6:2.346 (0.667)	45:2.416 (0.429)			1:1.558 (0.714)	
8	5wyi	40:3.628 (0.500)	55:3.333 (0.600)	12:2.653 (0.600)	10:3.924 (0.600)				2:3.054 (0.450)	3:3.074 (0.400)	11:3.862 (0.500)		
9	1lb6		6:3.897 (0.630)	12:3.842 (0.556)			66:3.911 (0.481)	66:3.911 (0.481)	24:2.904 (0.630)	42:3.033 (0.481)		5:3.146 (0.704)	
9	2ka9											50:3.482 (0.571)	
9	2khh						4:3.510 (0.300)	4:3.510 (0.300)	15:3.264 (0.350)	22:3.879 (0.500)	21:3.900 (0.400)	49:3.474 (0.500)	
9	3i5r	66:3.983 (0.400)	14:3.821 (0.600)		52:3.428 (0.250)		1:2.631 (0.850)	1:2.631 (0.850)			17:2.826 (0.600)	18:2.698 (0.600)	19:2.872 (0.600)
9	3obq	32:3.453 (0.571)	3:3.898 (0.476)	3:3.928 (0.619)	1:3.372 (0.571)		24:3.900 (0.333)	24:3.900 (0.333)	10:3.351 (0.524)	8:3.659 (0.524)	28:3.979 (0.619)		8:3.985 (0.476)
9	4bt9	1:3.633 (0.789)	7:2.545 (0.789)	6:3.126 (0.737)	4:3.469 (0.632)		10:3.904 (0.789)	10:3.904 (0.789)	7:3.341 (0.737)	9:3.695 (0.789)	6:2.130 (0.842)	25:1.795 (1.000)	18:1.133 (0.895)
9	4pge		5:2.512 (0.651)				26:3.233 (0.442)	26:3.233 (0.442)	2:3.800 (0.395)	8:2.253 (0.674)	1:2.452 (0.581)	6:3.235 (0.512)	65:3.745 (0.349)
9	4u0c											23:3.936 (0.714)	72:3.856 (0.500)

9	5dai	61:2.517 (0.750)	4:3.432 (0.469)	17:3.245 (0.594)			51:3.661 (0.406)	13:3.668 (0.406)	83:3.405 (0.375)			
9	5n22									7:3.244 (0.714)		
9	5t0k	1:3.362 (0.487)	4:3.323 (0.667)	1:3.828 (0.410)	20:3.685 (0.462)		4:3.681 (0.436)	9:2.852 (0.436)	46:3.925 (0.385)			
9	5wfv	23:3.513 (0.750)	1:3.922 (0.786)	54:3.388 (0.607)		2:3.730 (0.679)	2:3.730 (0.679)	10:3.236 (0.643)	40:2.896 (0.679)			
10	1ywo		90:3.759 (0.571)			7:3.815 (0.500)	7:3.815 (0.500)		1:3.178 (0.786)	1:2.912 (0.571)	6:3.974 (0.643)	
10	2fka		88:3.855 (0.692)			22:2.555 (0.692)	22:2.555 (0.692)				22:2.459 (0.615)	
10	2kel		41:2.817 (0.647)			14:2.931 (0.735)	14:2.931 (0.735)					
10	2o9v			46:3.576 (0.500)		10:3.454 (0.750)	10:3.454 (0.750)	1:3.404 (0.500)	24:3.678 (0.500)	20:2.363 (0.688)	13:3.712 (0.625)	98:2.759 (0.688)
10	2r7g		7:3.736 (0.517)			3:3.886 (0.345)	3:3.886 (0.345)		90:3.996 (0.207)			16:3.988 (0.379)
10	4m5s		2:3.651 (0.692)	18:3.863 (0.731)		1:2.437 (0.731)	1:2.437 (0.731)		100:3.949 (0.385)	2:2.290 (0.731)		2:3.833 (0.462)
10	4pd1	8:3.881 (0.433)	30:3.903 (0.500)			68:2.987 (0.600)	68:2.987 (0.600)	18:3.711 (0.567)	24:3.597 (0.500)	18:3.320 (0.567)		14:3.949 (0.367)
10	4yje							25:3.310 (0.488)	4:2.343 (0.581)	24:3.627 (0.349)	1:2.651 (0.651)	
10	5huw							2:3.841 (0.472)			1:3.165 (0.500)	52:2.910 (0.389)

10	5nqv	57:3.892 (0.500)	12:2.987 (0.731)		35:3.574 (0.500)	12:3.728 (0.538)	12:3.728 (0.538)	16:3.918 (0.346)		38:3.998 (0.462)	1:3.476 (0.462)	
10	5ow5	31:3.832 (0.471)	2:3.738 (0.765)			1:3.991 (0.412)	1:3.991 (0.412)	36:3.165 (0.471)	1:3.423 (0.412)	6:3.956 (0.294)	3:3.232 (0.412)	21:1.861 (0.588)
10	5xxq							3:3.978 (0.379)	5:3.625 (0.241)	5:3.994 (0.276)	11:3.980 (0.448)	20:3.737 (0.345)
10	6b27	15:3.094 (0.435)	20:2.858 (0.478)	35:3.794 (0.522)		1:1.975 (0.652)	1:1.975 (0.652)	1:3.469 (0.478)	1:2.450 (0.565)			
10	6ej7		3:3.934 (0.438)					4:3.747 (0.562)	1:3.422 (0.500)	1:3.564 (0.375)	5:3.908 (0.594)	5:3.562 (0.375)
11	1d8d		2:4.666 (0.455)			50:4.892 (0.273)		3:4.072 (0.394)	3:4.153 (0.424)	45:4.253 (0.212)	6:4.451 (0.545)	2:4.563 (0.212)
11	1l2z					49:4.086 (0.588)	92:4.636 (0.471)	5:4.930 (0.412)	18:4.456 (0.353)	38:4.985 (0.353)		
11	1r17							38:3.969 (0.453)	60:4.354 (0.585)		12:4.977 (0.377)	
11	1rxz		5:2.542 (0.735)			39:4.423 (0.294)		4:3.374 (0.382)	1:4.938 (0.382)	67:4.756 (0.265)	3:4.898 (0.382)	
11	2jnw		24:4.226 (0.682)			17:4.685 (0.364)	27:4.975 (0.500)					
11	2qos	42:4.936 (0.250)	33:4.861 (0.300)			1:4.241 (0.250)	4:2.373 (0.550)	7:4.932 (0.250)	6:4.732 (0.350)	58:4.926 (0.200)	5:4.767 (0.650)	
11	3bej	6:4.623 (0.450)	6:3.716 (0.450)	17:4.600 (0.350)		2:4.814 (0.650)	1:4.767 (0.250)	9:3.980 (0.550)	3:4.801 (0.300)	8:4.907 (0.250)	5:4.871 (0.300)	6:4.062 (0.350)
11	3g2s						47:4.671 (0.500)					34:4.997 (0.385)

11	3p72		21:4.858 (0.500)			95:4.250 (0.750)	85:4.541 (0.292)		1:4.761 (0.292)	15:4.777 (0.625)	
11	3v2o	28:4.953 (0.440)	1:4.241 (0.720)	18:4.911 (0.560)		42:4.525 (0.440)	51:4.039 (0.520)	5:3.704 (0.400)	20:4.222 (0.240)		9:1.897 (0.840) 3:4.071 (0.520)
11	4hom	5:4.923 (0.304)	10:4.146 (0.522)	12:3.662 (0.543)	5:3.877 (0.435)			9:4.327 (0.413)	8:4.678 (0.348)		13:3.316 (0.565)
11	4xc2	28:4.201 (0.382)	97:4.122 (0.294)	17:4.974 (0.294)	54:4.716 (0.353)			4:4.671 (0.353)	1:4.022 (0.353)		93:4.363 (0.618)
11	4z2o		3:3.461 (0.594)			57:4.856 (0.438)		4:4.218 (0.562)	72:4.579 (0.500)		21:4.693 (0.312)
11	5crw	42:4.769 (0.364)							79:4.626 (0.500)		
11	5xhz		72:4.955 (0.375)			83:4.783 (0.333)		19:4.905 (0.375)	44:4.567 (0.542)		1:3.427 (0.458) 83:3.667 (0.292)
12	2aq9	48:4.357 (0.300)		51:4.810 (0.300)	29:4.524 (0.500)			25:4.562 (0.400)	1:4.195 (0.400)		
12	2cch		1:4.939 (0.382)			18:4.104 (0.471)	2:3.121 (0.618)	1:3.288 (0.500)	1:3.534 (0.529)		13:4.402 (0.412) 3:4.737 (0.206)
12	2ht9		98:4.715 (0.857)			5:4.523 (0.857)	13:4.527 (0.714)		8:4.827 (0.429)		64:3.719 (0.286)
12	2rol		25:4.526 (0.500)	2:3.759 (0.350)		7:4.455 (0.300)	6:4.958 (0.350)	1:4.837 (0.400)	4:3.110 (0.350)		29:4.739 (0.550) 7:4.689 (0.350)
12	2xrw		9:3.949 (0.783)				29:4.463 (0.391)		43:4.913 (0.348)		19:4.420 (0.609)
12	4cc2		42:3.274 (0.679)	47:3.893 (0.536)		4:4.277 (0.536)	4:3.057 (0.714)	35:4.751 (0.214)	4:4.859 (0.464)	1:4.218 (0.393)	18:4.973 (0.393)

12	4gq6	37:4.865 (0.441)			59:4.263 (0.294)	44:4.792 (0.294)	12:4.444 (0.265)	1:4.531 (0.382)			
12	4j2c	32:4.900 (0.333)	12:4.327 (0.571)			75:4.573 (0.286)	27:4.354 (0.381)	16:4.793 (0.333)	83:4.531 (0.476)	43:4.548 (0.429)	59:4.460 (0.238)
12	4lzf						37:4.549 (0.435)				
12	4nuu	43:4.915 (0.250)	2:4.985 (0.350)	25:4.786 (0.350)	4:4.705 (0.350)	10:2.828 (0.750)	27:4.104 (0.200)	3:4.850 (0.550)	98:3.087 (0.350)		
12	4qh7		73:4.595 (0.471)		30:2.643 (0.647)	17:4.136 (0.441)	1:3.942 (0.441)	3:4.826 (0.412)	41:4.446 (0.294)	4:4.643 (0.353)	
12	4zoz	17:4.798 (0.345)	18:4.895 (0.241)		41:3.762 (0.310)	7:4.107 (0.552)				74:3.785 (0.448)	1:3.262 (0.448)
12	5d94	37:4.828 (0.344)	93:3.909 (0.469)		17:4.325 (0.406)	2:3.801 (0.500)		9:4.394 (0.219)	46:4.777 (0.312)	14:4.474 (0.500)	79:4.287 (0.281)
12	5n85	5:3.698 (0.500)	3:4.050 (0.591)	10:3.956 (0.682)	1:3.224 (0.591)	5:3.334 (0.364)	5:4.954 (0.364)	3:4.918 (0.227)	11:4.298 (0.227)	1:3.628 (0.273)	
12	6h7b	13:4.835 (0.464)	4:4.447 (0.429)	7:4.095 (0.357)	16:3.457 (0.429)	2:3.297 (0.464)	2:3.146 (0.464)	3:4.671 (0.321)	14:4.508 (0.286)	56:4.821 (0.321)	96:3.741 (0.286)
13	1cqg										
13	1eg4								69:4.314 (0.476)		
13	1o0p		15:4.646 (0.731)		31:4.665 (0.423)			1:4.896 (0.500)			
13	2las										
13	2p1o							76:4.334 (0.379)			

13	2v8c											
13	3bqo		8:4.138 (0.540)						12:4.407 (0.280)		1:4.367 (0.340)	
13	4lk9						22:4.827 (0.226)			4:4.491 (0.226)	2:4.808 (0.419)	
13	4mvi											
13	4oyk					24:4.632 (0.333)						
13	4uqy	2:3.974 (0.531)	1:3.542 (0.438)	6:3.587 (0.500)	6:2.732 (0.719)	18:2.914 (0.688)	21:3.634 (0.531)	2:3.779 (0.375)	4:3.574 (0.344)		1:4.565 (0.469)	1:4.778 (0.281)
13	5di8	27:4.819 (0.455)	38:4.680 (0.667)									
13	5v3r		40:4.713 (0.235)						57:4.782 (0.235)		1:4.146 (0.529)	
13	6e5x	12:3.998 (0.731)	1:3.913 (0.846)	6:4.004 (0.692)		23:3.893 (0.731)		54:4.798 (0.500)	90:4.649 (0.385)	1:3.921 (0.731)		5:3.258 (0.577)
14	1a0n					24:4.832 (0.263)	34:4.579 (0.474)					
14	1mv0	1:4.407 (0.375)		4:4.087 (0.500)	15:4.640 (0.500)		32:4.625 (0.458)	7:4.435 (0.458)	54:4.155 (0.250)		1:4.994 (0.417)	5:3.426 (0.292)
14	2jqk		4:3.980 (0.312)			35:4.284 (0.562)	6:4.439 (0.250)		95:4.769 (0.312)			
14	3pe4								83:4.634 (0.273)		13:3.627 (0.485)	53:4.285 (0.212)
14	3zrj	14:4.524 (0.545)	1:4.515 (0.727)	16:4.499 (0.682)		3:4.172 (0.591)	17:4.594 (0.545)			58:4.870 (0.500)		4:4.385 (0.409)

14	4a2a	11:3.672 (0.680)		46:4.931 (0.280)		44:4.571 (0.280)		36:4.259 (0.400)	29:4.622 (0.400)		33:4.515 (0.320)
14	5ei3	13:4.348 (0.458)	1:4.816 (0.333)			73:4.832 (0.458)	56:4.972 (0.500)		41:3.973 (0.333)		9:4.081 (0.417)
14	5j3q	11:4.904 (0.379)	87:4.999 (0.310)	9:4.885 (0.241)	19:4.244 (0.448)	4:4.338 (0.379)	5:4.064 (0.310)	1:4.403 (0.379)	6:4.662 (0.207)		19:4.464 (0.207)
14	6co4		16:4.958 (0.409)	5:4.249 (0.500)	26:4.147 (0.545)				9:4.921 (0.273)	5:4.861 (0.727)	6:2.872 (0.364)
15	1nrl	1:4.811 (0.579)		34:4.553 (0.526)	1:4.946 (0.211)	32:4.812 (0.368)	25:4.983 (0.737)	5:4.685 (0.421)	90:4.862 (0.421)		49:3.951 (0.211)
15	2fym							7:4.997 (0.241)	87:4.562 (0.448)		
15	2ivz			26:4.938 (0.278)		13:4.179 (0.472)	24:4.524 (0.528)		77:4.636 (0.361)		
15	2vzg		69:4.473 (0.692)								55:4.671 (0.308)
15	3h1z	38:4.495 (0.556)	1:3.394 (0.694)		58:3.536 (0.611)	88:4.640 (0.472)			9:4.626 (0.333)	47:4.757 (0.417)	
15	4txr		68:4.628 (0.227)			65:4.610 (0.364)	2:4.881 (0.318)	19:4.523 (0.318)	22:4.708 (0.318)	29:4.910 (0.545)	2:4.309 (0.409)
15	5yay	64:4.052 (0.417)		18:4.437 (0.583)		5:4.493 (0.333)	8:4.960 (0.306)	26:3.665 (0.250)	1:4.935 (0.306)		85:3.958 (0.222)
15	6f0y							2:4.240 (0.577)			
16	1pmx		17:4.931 (0.600)			4:4.725 (0.600)	35:4.509 (0.733)				53:4.555 (0.400)

16	2i94	100:4.315 (0.458)						28:4.844 (0.250)		17:3.735 (0.458)	9:4.724 (0.250)	
16	2koh		26:4.020 (0.577)									50:4.580 (0.538)
16	3et3			3:4.524 (0.286)	1:4.823 (0.429)	3:4.672 (0.238)	6:3.663 (0.571)		4:4.814 (0.333)		67:4.473 (0.476)	33:4.756 (0.238)
16	4iga		11:4.353 (0.684)			6:4.326 (0.579)	22:4.431 (0.263)					53:4.489 (0.263)
16	4xek	93:4.973 (0.391)	8:4.946 (0.304)			3:4.438 (0.304)	2:4.638 (0.348)			2:4.455 (0.435)		42:4.851 (0.391)
16	5ajn		97:4.733 (0.375)					21:4.332 (0.250)	27:4.417 (0.375)	1:5.000 (0.438)	9:4.403 (0.406)	
16	5efi	60:4.521 (0.387)	4:3.668 (0.452)	25:4.269 (0.581)		12:4.410 (0.290)	1:4.605 (0.258)		2:4.805 (0.323)	1:4.573 (0.355)		46:4.960 (0.258)
17	1f47								4:4.342 (0.211)		17:4.810 (0.474)	61:4.695 (0.421)
17	2lsi		77:4.295 (0.345)									
17	6dei			11:4.306 (0.237)		8:4.646 (0.342)	4:4.355 (0.395)		1:4.396 (0.368)		1:4.931 (0.316)	4:3.669 (0.237)
17	6f6d											
17	6fbk					85:4.719 (0.500)	42:4.402 (0.500)					
18	1j2x	49:4.715 (0.286)				1:4.912 (0.333)	68:4.859 (0.333)					

18	1yfn	99:4.892 (0.200)	27:4.981 (0.343)	20:4.756 (0.400)	29:3.337 (0.400)	9:3.730 (0.486)	12:4.803 (0.343)	12:4.564 (0.200)	14:4.538 (0.200)	5:3.747 (0.343)	
18	2kbr		5:4.465 (0.350)	36:4.933 (0.450)		1:4.811 (0.300)	11:4.254 (0.500)				36:4.710 (0.300)
18	3plu					1:3.679 (0.667)	1:4.432 (0.600)				
18	3tiw					5:4.435 (0.481)	2:4.932 (0.259)		17:4.605 (0.259)		5:2.853 (0.556)
18	6f0w			52:4.172 (0.386)	42:4.982 (0.500)		34:4.769 (0.295)		32:4.333 (0.205)		1:4.638 (0.295)
18	6g5g		1:3.458 (0.621)								
19	2cny							5:4.641 (0.206)		13:4.674 (0.508)	
19	2hwn		8:3.833 (0.419)				11:4.400 (0.258)			13:3.726 (0.548)	1:3.273 (0.355)
19	3aa0		1:4.762 (0.411)				29:3.546 (0.393)				
19	4dg3										
19	5fml		55:4.751 (0.296)			51:4.283 (0.259)	61:4.708 (0.333)			25:3.762 (0.407)	
19	5v2p	19:4.941 (0.250)	5:2.733 (0.562)	29:4.599 (0.500)		5:4.088 (0.438)	1:3.472 (0.375)		28:4.070 (0.344)	33:4.111 (0.562)	46:4.729 (0.250)
20	1vpp										
20	2nnu		78:4.433 (0.391)			2:4.631 (0.304)	13:4.636 (0.348)		84:4.517 (0.304)		27:4.950 (0.304)

20	2xpn	15:4.901 (0.312)	1:4.964 (0.344)
20	5tgi		

^a Blank space represents prediction failure. The number before the “:” indicates the best rank of the near-native prediction, followed by IL_RMSD and f_{nat} .

Table S4. The ranks given by AutoDock or Vina-based docking programs with the binding sites defined by the peptide length.

Peptide length	PDB code	DINC_site ^a	ADCP_site ^a	Vina_SA_site ^a	Vina_HA_site ^a	MDockPeP_SA_site ^a
5	1jq8		12:3.793 (0.667)			
5	1mf4		21:3.965 (0.650)			2:2.894 (0.550)
5	1nvq	19:3.142 (0.500)	13:3.541 (0.667)	5:3.825 (0.500)	7:3.257 (0.500)	6:3.937 (0.667)
5	1v1t		18:3.829 (0.556)			46:3.712 (0.778)
5	2aij	2:1.324 (0.783)	1:1.395 (0.783)	5:1.235 (0.696)	9:1.668 (0.696)	1:1.468 (0.652)
5	2hpl	1:3.929 (0.526)	1:3.681 (0.684)	1:2.688 (0.632)	1:2.893 (0.579)	11:3.835 (0.421)
5	2m0v		1:3.489 (0.706)	6:2.950 (0.529)	39:2.249 (0.647)	2:3.801 (0.412)
5	3fp2	69:3.364 (0.375)	39:3.991 (0.625)	13:3.742 (0.438)		4:2.993 (0.688)
5	3hds	94:3.499 (0.429)	15:2.543 (0.714)	41:3.568 (0.381)		91:3.069 (0.714)
5	4hdq	1:3.345 (0.818)	1:3.971 (0.727)	1:3.391 (0.773)	1:3.315 (0.727)	1:2.678 (0.818)
5	4ny3	1:3.707 (0.800)	18:3.512 (0.400)	1:3.721 (0.800)	1:3.636 (0.800)	7:3.807 (0.467)
5	4x3o	2:3.116 (0.524)	1:2.518 (0.810)	1:3.554 (0.571)	3:3.441 (0.571)	5:2.227 (0.714)
5	5e33	8:3.902 (0.423)	4:1.600 (0.731)	15:2.720 (0.615)	33:2.435 (0.577)	5:3.613 (0.615)
5	5ggp	51:3.510 (0.750)	91:3.749 (0.750)	23:2.988 (0.750)		5:3.589 (0.750)
5	5kds					
5	5onp	1:2.630 (0.815)	1:2.844 (0.815)	1:2.945 (0.815)	1:2.957 (0.815)	
5	6f4s				19:3.713 (0.538)	53:3.870 (0.615)
6	1ddv	90:3.390 (0.643)	1:3.781 (0.429)	8:3.607 (0.714)	37:3.668 (0.714)	1:3.896 (0.714)
6	1f8h	4:3.281 (0.800)	21:3.611 (0.733)	18:3.748 (0.600)	3:3.550 (0.733)	3:3.617 (0.533)
6	1jw6					
6	1ywi	13:3.062 (0.412)	1:3.617 (0.471)	5:3.992 (0.529)	7:3.955 (0.471)	
6	2ds8	4:2.669 (0.765)	1:2.966 (0.588)	1:1.081 (0.765)	7:2.453 (0.882)	8:2.420 (0.412)
6	2ymt	15:2.335 (0.632)	4:2.053 (0.789)	10:2.176 (0.526)	2:2.828 (0.368)	2:2.018 (0.684)
6	3emh		3:1.410 (0.625)	44:3.465 (0.500)	22:3.647 (0.500)	12:3.986 (0.438)

6	4fii	5:3.729 (0.429)	50:3.609 (0.357)	5:3.400 (0.429)	4:3.507 (0.321)	7:2.141 (0.500)
6	4j8b		38:3.862 (0.619)			88:3.791 (0.571)
6	4m9l	33:3.575 (0.562)	26:3.926 (0.500)	13:3.513 (0.562)	4:3.857 (0.562)	43:3.742 (0.625)
6	4r5i	10:2.585 (0.769)	6:3.841 (0.500)	15:2.727 (0.731)	1:2.560 (0.808)	7:1.897 (0.808)
6	4x2h	10:2.108 (0.536)	4:3.816 (0.393)	4:2.014 (0.571)	4:3.828 (0.536)	2:3.574 (0.250)
6	5bs2		98:3.867 (0.818)			21:3.826 (0.636)
6	5gu4	78:2.159 (0.700)	1:1.788 (1.000)	16:3.175 (0.600)	6:3.842 (0.850)	1:3.796 (0.700)
6	5njc	8:3.940 (0.357)	1:1.180 (0.857)	11:1.089 (0.714)	6:2.416 (0.607)	5:1.133 (0.750)
6	5oj5	10:3.602 (0.533)	1:2.846 (0.800)	16:3.433 (0.400)	12:3.057 (0.467)	19:3.535 (0.733)
6	6cwp					39:3.476 (0.600)
7	1czy	18:2.688 (0.615)	2:1.392 (0.923)	28:2.912 (0.654)	2:3.498 (0.654)	4:3.815 (0.385)
7	1p7v	70:3.505 (0.423)	6:3.175 (0.538)		35:2.827 (0.731)	38:2.481 (0.462)
7	3agy		2:2.645 (0.647)	38:3.753 (0.471)	14:3.744 (0.647)	2:2.872 (0.588)
7	3emw			29:3.822 (0.476)		58:3.326 (0.524)
7	3s9c	1:2.309 (0.786)	20:3.523 (0.321)	1:2.540 (0.643)	1:2.342 (0.750)	13:2.812 (0.464)
7	3shb	34:2.928 (0.632)	32:1.740 (0.895)			6:2.163 (0.684)
7	3wgx		8:1.803 (0.800)	55:3.070 (0.650)		2:3.741 (0.450)
7	4ep2	2:2.453 (0.778)	1:1.142 (0.667)	2:2.286 (0.750)	1:2.300 (0.750)	3:3.459 (0.250)
7	4leb					
7	4ouc					
7	4qbr	17:3.059 (0.481)	68:3.727 (0.519)	8:3.122 (0.333)		22:3.723 (0.370)
7	5fpx	20:3.984 (0.269)		32:3.837 (0.462)	1:3.902 (0.385)	13:3.808 (0.462)
7	5i7z		43:3.402 (0.667)			22:3.441 (0.467)
7	5lyn	21:3.501 (0.429)	9:1.537 (0.810)			10:2.244 (0.667)
7	6n3e					
8	ljd5	4:3.669 (0.538)	5:2.901 (0.885)	21:3.714 (0.462)	48:3.728 (0.538)	61:2.549 (0.615)

8	1t74		1:3.386 (0.333)			9:2.633 (0.667)
8	1w80	70:3.812 (0.500)				18:2.747 (0.750)
8	1yy6	8:3.196 (0.609)		7:2.477 (0.652)	8:2.977 (0.522)	17:3.194 (0.652)
8	2c3i					29:3.671 (0.778)
8	2e4h		9:3.551 (0.471)			
8	2fgr		54:3.890 (0.650)			
8	2jkg					
8	2xcb		1:2.296 (0.913)			
8	3av9	31:3.935 (0.632)		41:3.962 (0.421)		32:3.393 (0.579)
8	3r42	6:2.589 (0.739)	24:3.180 (0.739)	17:2.122 (0.739)	14:2.428 (0.696)	46:3.384 (0.696)
8	4c5a					
8	4nxr		47:3.917 (0.538)			27:3.515 (0.538)
8	4odk	5:3.224 (0.444)	58:3.520 (0.500)	53:2.522 (0.500)	18:3.127 (0.556)	8:3.923 (0.389)
8	4oz1		8:2.930 (0.727)			14:3.593 (0.545)
8	5fv6			17:3.762 (0.727)		
8	5m5r		56:3.939 (0.524)			
8	5o9u		19:1.523 (0.667)			1:2.386 (0.714)
8	5wyi		79:3.379 (0.500)			
9	1lb6		9:3.785 (0.556)		2:3.870 (0.556)	10:3.286 (0.593)
9	2ka9					
9	2khh					
9	3i5r					5:1.638 (0.700)
9	3obq	35:3.180 (0.476)	1:3.637 (0.619)	3:3.420 (0.619)	17:3.757 (0.619)	35:2.666 (0.571)
9	4bt9	3:3.630 (0.789)	16:1.986 (0.842)		20:3.172 (0.632)	23:1.729 (0.737)
9	4pge	38:3.888 (0.279)	33:3.895 (0.442)			36:3.406 (0.465)
9	4u0c	9:3.302 (0.643)				

9	5dai	31:2.888 (0.656)		5:3.548 (0.469)	34:3.393 (0.500)	
9	5n22					
9	5t0k		84:3.925 (0.436)	2:3.635 (0.462)		
9	5wfv		16:3.538 (0.643)	30:3.163 (0.821)		
10	1ywo					59:3.693 (0.786)
10	2fka					
10	2ke1					
10	2o9v					7:3.623 (0.312)
10	2r7g		6:3.994 (0.414)			4:3.914 (0.345)
10	4m5s		40:3.783 (0.654)			1:2.372 (0.769)
10	4pd1	39:3.851 (0.400)				63:3.044 (0.600)
10	4yje	21:3.728 (0.349)				16:2.484 (0.605)
10	5huw					
10	5nqv	22:3.375 (0.577)	19:3.307 (0.808)	10:3.406 (0.577)	55:3.345 (0.769)	27:2.894 (0.654)
10	5ow5		8:3.030 (0.765)			19:1.298 (0.765)
10	5xxq					
10	6b27					6:3.949 (0.478)
10	6ej7					
11	1d8d					
11	1l2z					
11	1r17					
11	1rxz		2:3.185 (0.735)			
11	2jnw	37:4.719 (0.318)				
11	2qos	9:4.963 (0.200)	26:4.847 (0.250)	11:4.878 (0.300)	5:4.642 (0.250)	7:4.592 (0.300)
11	3bej		54:4.138 (0.250)			1:4.943 (0.650)
11	3g2s					

11	3p72		3:4.524 (0.417)		
11	3v2o	5:3.974 (0.400)	3:3.036 (0.760)		29:4.551 (0.360)
11	4hom	64:4.652 (0.348)	28:4.622 (0.326)		35:4.980 (0.283)
11	4xc2			30:4.541 (0.235)	2:4.759 (0.265)
11	4z2o		3:2.843 (0.812)		
11	5crw				38:4.805 (0.227)
11	5xhz				
12	2aq9				
12	2cch				58:4.680 (0.500)
12	2ht9				
12	2rol				46:4.919 (0.300)
12	2xrw				
12	4cc2	10:3.999 (0.464)		8:4.172 (0.536)	5:4.852 (0.393)
12	4gq6	1:4.607 (0.471)			16:4.515 (0.235)
12	4j2c		15:4.705 (0.429)		
12	4lzf				
12	4nuu		26:4.874 (0.450)		85:3.502 (0.550)
12	4qh7				13:4.142 (0.471)
12	4zoz		55:4.980 (0.379)		43:4.958 (0.241)
12	5d94		1:4.004 (0.562)		16:4.861 (0.312)
12	5n85	61:4.730 (0.591)	3:3.767 (0.409)	29:4.935 (0.409)	22:2.885 (0.545)
12	6h7b			32:4.251 (0.464)	38:4.855 (0.393)
13	1cqq				
13	1eg4				
13	1o0p		6:4.585 (0.577)		50:4.605 (0.538)
13	2las				

13	2p1o				
13	2v8c				
13	3bqo				
13	4lk9				
13	4mvi				
13	4oyk				
13	4uqy		27:4.779 (0.344)	45:3.864 (0.562)	41:3.230 (0.594) 2:4.573 (0.469)
13	5di8				
13	5v3r				
13	6e5x				1:4.789 (0.615)
14	1a0n				
14	1mv0	31:4.545 (0.500)			
14	2jqk				31:4.789 (0.375)
14	3pe4				
14	3zrj		2:4.175 (0.636)		
14	4a2a				
14	5ei3		4:4.575 (0.250)		33:4.010 (0.292) 26:4.991 (0.333)
14	5j3q			9:4.412 (0.345)	46:4.069 (0.345) 1:4.633 (0.448)
14	6co4	40:4.106 (0.455)	15:3.885 (0.591)		18:4.249 (0.500)
15	1nrl				
15	2fym				
15	2ivz				
15	2vzg				
15	3h1z				
15	4txr				
15	5yay				

15	6f0y		
16	1pmx		12:4.287 (0.400)
16	2i94		
16	2koh		
16	3et3	61:4.723 (0.286)	
16	4iga		
16	4xek		
16	5ajn		
16	5efi	50:4.784 (0.290)	26:4.938 (0.452)
17	1f47		
17	2lsi		
17	6dei		
17	6f6d		
17	6fbk		
18	1j2x		94:4.729 (0.476)
18	1yfn		
18	2kbr	10:4.321 (0.350)	33:4.934 (0.250)
18	3plu		
18	3tiw		11:4.056 (0.630)
18	6f0w		27:4.782 (0.295) 59:4.977 (0.386)
18	6g5g		
19	2cny		
19	2hwn		
19	3aa0		
19	4dg3		
19	5fml		

19	5v2p	
20	1vpp	
20	2nnu	
20	2xpn	1:3.949 (0.406)
20	5tgi	

^a Blank space represents prediction failure. The number before the “:” indicates the best rank of the near-native prediction, followed by IL_RMSD and f_{nat} .