Supporting Information

CoDockPP: a Multistage Approach for Global and Site-specific Protein-protein Docking

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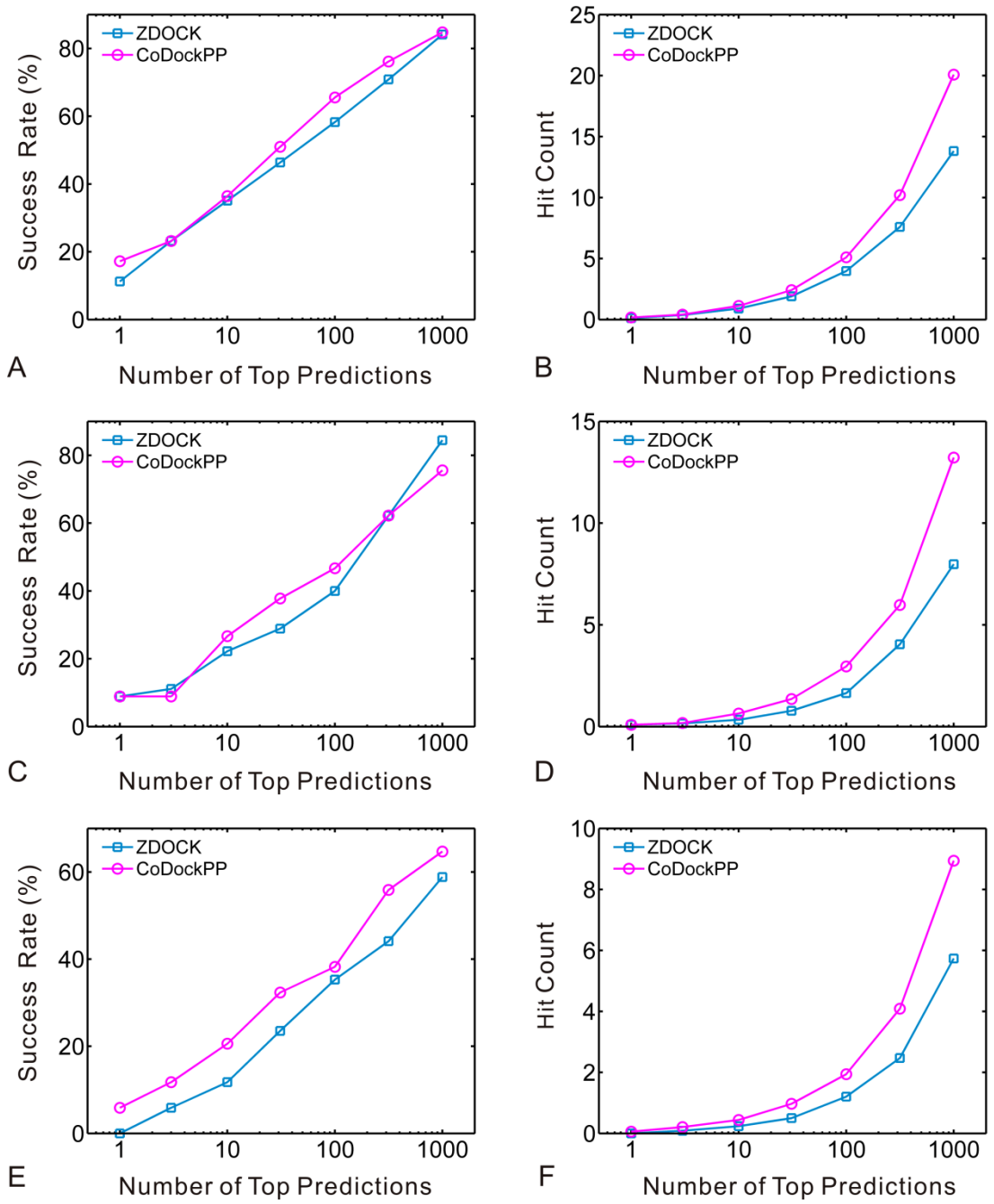

Figure S1. Success rate and hit count comparisons for global unbound docking test of three categories in benchmark 5.0. (A), (C) and (E) show the docking success rates of ZDOCK and CoDockPP for rigid-body, medium difficulty and difficult cases, respectively. (B), (D) and (F) show the hit counts of ZDOCK and CoDockPP for rigid-body, medium difficulty and difficult cases, respectively.

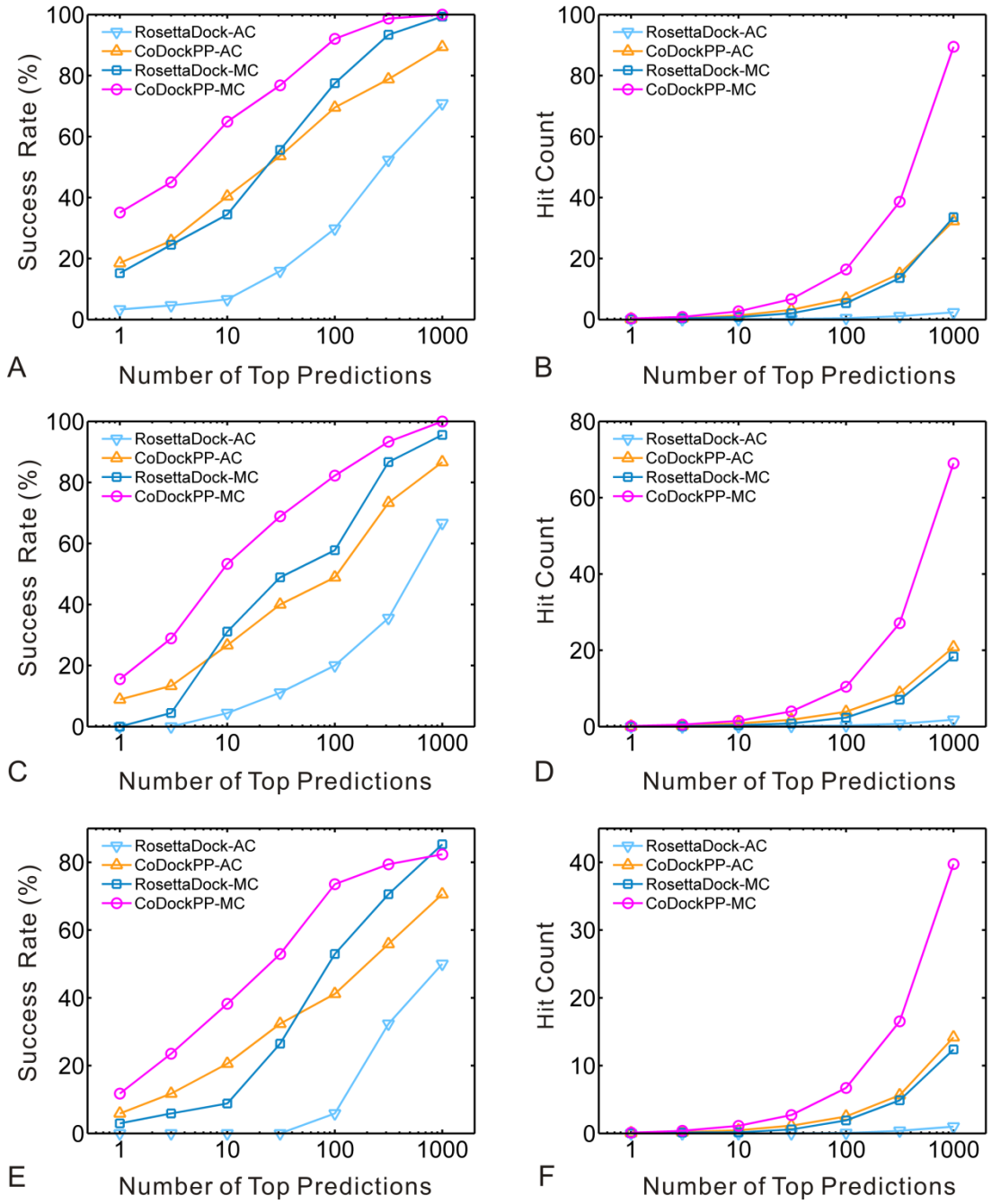

Figure S2. Success rate and hit count comparisons for site-specific unbound docking test of three categories in benchmark 5.0. (A), (C) and (E) show the docking success rates of RosettaDock and CoDockPP for rigid-body, medium difficulty and difficult cases, respectively. (B), (D) and (F) show the hit counts of RosettaDock and CoDockPP for rigid-body, medium difficulty and difficult cases, respectively. The docking tests of ambiguous constraints and multiple constraints are shown in the figures with different markers.

Table S1. The training set of 975 protein–protein complexes used for deriving knowledge-based scoring function.

PDB entry									
137L	1A3A	1A4U	1ADE	1AUO	1B2P	1B34	1B43	1BD9	1BDY
1BG8	1BKP	1BPL	1C02	1C77	1C94	1CIQ	1CPJ	1CQ3	1D0N
1D2C	1D2O	1D9C	1DC5	1DEV	1DJT	1DLE	1DQZ	1DYS	1E15
1E5L	1E7N	1EGP	1EM8	1EV7	1EZG	1F2T	1F3U	1F46	1F60
1FA8	1FGU	1FS0	1FVK	1FWL	1FZR	1G0S	1G2Q	1G8E	1GMJ
1GO3	1GXJ	1GY7	1GYJ	1H6K	1H7E	1HA4	1HF2	1HJR	1HSS
1HUC	1HUL	1I07	1I2O	1I4J	1I4S	1I7N	1ID1	1IED	1IGQ
1IJY	1IPI	1IRQ	1IU8	1JK6	1JNP	1K3R	1K9X	1KCX	1KPT
1KTJ	1KTN	1KZQ	1L0W	1L2U	1L7J	1LBQ	1LBV	1LGQ	1LHP
1LJ9	1LM5	1M45	1M4J	1MBY	1MK4	1MKB	1MKF	1MKK	1MMI
1MNA	1MTP	1MY7	1MYL	1N1J	1N5B	1NA6	1NO4	1NOZ	1NXM
1NYE	1O0W	1OCK	1OR7	1OTK	1OTV	1OV9	1P27	1P5H	1PCF
1PUG	1PVU	1Q2H	1Q67	1QO7	1QQG	1QSD	1QSJ	1QUQ	1QYA
1QYC	1R0M	1R0V	1R12	1R1T	1R1U	1R4C	1R5P	1R8J	1R8O
1R8W	1REG	1RK4	1RVE	1RW0	1RZN	1S3O	1S7H	1S7O	1SFL
1SFN	1SGM	1SH8	1SMN	1SMX	1SND	1SQE	1SQU	1SV0	1SW6
1T06	1T11	1T33	1T4D	1T5O	1T6F	1T70	1TE5	1TFO	1TKL
1TKS	1TLU	1TVN	1TW9	1U07	1UFB	1UFI	1UGQ	1UI6	1UII
1UIR	1UIU	1UJN	1ULH	1ULK	1UT4	1UZ3	1V5X	1V8H	1VB5
1VC1	1VDE	1VE2	1VF6	1VH4	1VH5	1VHI	1VQ3	1VS3	1VSC
1W5R	1W9C	1WLT	1WMH	1WMI	1WMW	1WTJ	1WU9	1WY5	1WZ3
1X2I	1X6I	1X94	1XAO	1XEW	1XG2	1XLY	1XXO	1XYF	1Y14
1Y6Z	1Y7Y	1Y96	1Y9W	1YE5	1YJG	1YOZ	1YPT	1Z4E	1Z9M
1ZGR	1ZHG	1ZOQ	1ZRS	1ZTD	1ZV1	1ZVP	1ZX2	1ZYM	1ZZG
2A61	2A8F	2AEJ	2AN1	2AVT	2AZJ	2BAY	2BLS	2BPD	2C2X
2C3T	2C5J	2CAR	2CMG	2CO5	2CUY	2D0J	2D13	2D4U	2D68
2D7E	2DBB	2DFU	2DM9	2DPL	2DQW	2DSB	2DST	2DVW	2DYO
2E0K	2E10	2E31	2E5B	2E9Y	2EBE	2ECR	2EEN	2EFR	2EIU
2EJ8	2EMQ	2EOA	2EQ5	2ETX	2F5J	2F6L	2FBN	2FHZ	2FIP
2FJR	2FQM	2FSD	2FSF	2FXO	2GEC	2GIY	2GOM	2GOP	2GT2
2GTD	2GWF	2GZ4	2H0Q	2H1E	2HIQ	2HKN	2HOW	2HQL	2HYX
2I00	2I3S	2I4L	2I5Q	2IB0	2IOB	2IPB	2IPR	2J67	2J8N
2JJ7	2NPT	2NRC	2NVW	2NWI	2NX4	2NXN	2NXO	2NZ7	2O27
2O70	2O7M	2OAM	2OHC	2OPT	2OQQ	2OR2	2OVI	2OWY	2P04
2P19	2P1J	2P62	2PA6	2PEO	2PEQ	2PFB	2PJU	2PL2	2PVP
2Q8O	2Q8R	2Q8T	2QCW	2QDO	2QDQ	2QSF	2QSU	2QXV	2QYA
2QYP	2R6U	2RBH	2RCZ	2RG7	2RSP	2SPC	2VOK	2VT1	2VVW
2W01	2W1V	2W4S	2W6A	2W8M	2WFV	2WUA	2WUJ	2X3V	2X4I
2X5Q	2X5S	2X6G	2X78	2XCC	2XHF	2XPP	2XT4	2XTY	2XWX
2Y0Q	2Y3W	2YLE	2YML	2YQ1	2YSW	2YVS	2YVU	2YWB	2YY0
2YYV	2Z3Q	2Z5E	2ZB9	2ZCG	2ZCI	2ZCN	2ZD7	2ZF3	2ZGL
2ZIG	2ZNJ	2ZVR	2ZVY	2ZZ8	3A5P	3A7O	3ABD	3AG5	3AGD
3AGX	3AKJ	3AMI	3ASY	3AU4	3AY3	3AZD	3B3G	3BAT	3BIL
3BT3	3C0T	3C57	3C90	3CAI	3CG6	3COO	3CPT	3CS5	3CT6
3CUO	3CYP	3D1B	3D3K	3D7A	3DAL	3DLQ	3DO8	3DP7	3DQG
3DRE	3DS2	3DXE	3E3M	3E57	3E6D	3E7D	3E96	3EAB	3EAR
3EBN	3ECY	3EES	3EFY	3EGC	3EGO	3EP1	3EPU	3ER6	3ERJ

3EUS	3EWO	3F13	3F1L	3F31	3F3H	3FCH	3FD4	3FFE	3FFL
3FGN	3FHU	3FK6	3FK9	3FPN	3FV6	3FX7	3FXD	3FYF	3G17
3G1G	3G1S	3G4O	3G67	3G79	3G8L	3GDM	3GDO	3GFK	3GGN
3GQ2	3GT6	3GWA	3GWY	3H00	3HDE	3HE4	3HE5	3HGT	3HGU
3HJ2	3HMT	3HO7	3HR0	3HS3	3HTU	3HUH	3I00	3I17	3I2Z
3I3G	3I6X	3ID3	3IHM	3IJT	3IKK	3INO	3IWZ	3IX0	3K1R
3K2Y	3K6T	3K86	3KAJ	3KDG	3KF6	3KGK	3KH8	3KP7	3KXS
3KZ3	3L18	3L32	3L7H	3L7O	3L8U	3LJB	3LQ7	3LRU	3LW3
3LYX	3M3I	3M5R	3M8E	3M8J	3MAB	3MEX	3MGK	3MGM	3MJK
3MKQ	3MP4	3MQ0	3MYO	3N3E	3NDD	3NFY	3NGH	3NJ2	3NJD
3NK6	3NKD	3NRP	3NUI	3NVA	3O9O	3OAK	3OL4	3ONM	3OT7
3OY2	3P3A	3P8T	3PIM	3PNO	3PNY	3PRA	3PRB	3QAS	3QIT
3QMQ	3QQ6	3QR2	3QT5	3R3P	3R4Y	3R7S	3RKC	3RNQ	3RRS
3RV1	3S02	3SK1	3SR3	3SRI	3SSW	3SWK	3SXO	3SXY	3SXZ
3SZH	3T43	3T5X	3T7J	3TCV	3TE8	3TG9	3TOE	3TOJ	3TQT
3TU3	3TV0	3TYY	3U80	3UEB	3UEP	3ULB	3UMZ	3UT4	3UV0
3V67	3V69	3V6G	3VBA	3VJZ	3VN0	3VOQ	3VPJ	3VSK	3VUQ
3VZ9	3W0E	3W35	3W6Q	3W8G	3WFI	3WHR	3WJE	3WMD	3WSC
3WTD	3WVB	3WVZ	3WXZ	3WYD	3YGS	3ZCD	3ZIB	3ZIH	3ZIT
3ZPN	3ZSS	3ZVQ	3ZWL	3ZYL	4A3T	4A5B	4A5U	4ABM	4ABX
4AIH	4AK9	4AN6	4B6I	4B8A	4B93	4BI8	4BI9	4BK6	4BL7
4BRO	4C1B	4C5G	4C86	4CIJ	4CT6	4CU5	4D48	4D6K	4D7K
4D9O	4D9S	4DEX	4DJG	4DM7	4DQZ	4E1P	4E1R	4E2A	4EGT
4EJQ	4EQA	4FBD	4FGW	4FOL	4FQN	4FW1	4FZ2	4FZO	4G1O
4G2B	4G6T	4G7X	4G94	4G9M	4GDO	4GEH	4GF3	4GFK	4GVB
4H0P	4HA7	4HBE	4HEH	4HL6	4HPL	4HR9	4HWI	4HX8	4HYE
4HZA	4I4N	4IHN	4ILF	4ILH	4J0E	4J11	4J4L	4J6U	4J7A
4J7P	4J7R	4JAK	4JAR	4JBA	4JDX	4JE3	4JEH	4JHP	4JOI
4JTM	4JVU	4JVW	4K5A	4KBM	4KK2	4KKQ	4KN8	4KP2	4KT6
4KTI	4KV2	4KY9	4KYX	4L0K	4L0N	4L0R	4L1C	4L2W	4L4Y
4L6W	4LE5	4LJL	4LLD	4LN9	4LO8	4LQC	4LUB	4M23	4M6B
4MAC	4MDU	4ML1	4MQV	4MT8	4MUO	4MYZ	4NK0	4NSW	4O0Q
4O4B	4O7H	4OGD	4OM7	4OUH	4P0U	4P61	4P93	4P96	4PAS
4PBZ	4PEO	4PGG	4PRS	4PU7	4PVC	4PZ9	4Q20	4Q25	4Q9B
4QFQ	4QGK	4QLP	4QXZ	4R3Q	4R77	4RDJ	4RIE	4RJV	4RS8
4S1V	4TQ1	4TQJ	4TRH	4TRT	4U1F	4U4P	4U9C	4UED	4UU3
4UUL	4UVJ	4V17	4W4K	4W4R	4WMJ	4WVR	4WWR	4WXM	4X1E
4X9Z	4XBX	4XD9	4XFQ	4XHT	4XO2	4XZ7	4XZA	4YAE	4YIF
4YJY	4YMR	4YNH	4YXC	4YZE	4Z1A	4Z27	4Z9J	4ZBW	4ZDS
4ZEQ	4ZGB	4ZMU	4ZOQ	4ZQ8	4ZQS	4ZVD	4ZXZ	5A49	5AB4
5AYQ	5B02	5B08	5B4N	5B52	5BTO	5BXX	5C21	5C6H	5C6K
5CES	5CFO	5CJ0	5CJ1	5CS1	5CV0	5CWT	5D5P	5DDT	5DMB
5DOI	5E5N	5ECW	5ELL	5EN8	5EPW	5ESC	5F22	5F3K	5F5S
5FCN	5FHK	5FVK	5FYA	5G1E	5G23	5GI4	5GK2	5GKC	5GKK
5GN2	5GPI	5GPL	5GQ0	5GTU	5GZ1	5H2Y	5H69	5H6T	5H6W
5H78	5HEC	5HO3	5HPG	5HST	5HU7	5I5I	5I8J	5IF3	5IFZ
5IOJ	5IWB	5IY3	5J0K	5J4A	5J4I	5J8Y	5J9I	5JFZ	5JHM
5JKJ	5JNH	5K3D	5K3H	5K7M	5KN4	5L04	5LOY	5LSL	5LUS
5M7R	5M97	5MLK	5N76	5NBT	5NCK	5OWU	5RUB	5TS9	5TT4
5TZ5	5U96	5V2I	5V6B	5V6G	5V8Z	5VKY	5WOF	5WSX	5WUY
5WWO	5WXL	5WYG	5XBH	5XGS					

Table S2. Success rate and hit count comparisons for global unbound docking test

Method	Top 1	Top 10	Top 100	Top 1000
Rigid-body (151)				
ZDOCK	11.3%/0.11 [a]	35.1%/0.90	58.3%/3.97	84.1%/13.80
CoDockPP	17.2%/0.17	36.4%/1.12	65.6%/5.10	84.8%/20.07
Medium difficulty (45)				
ZDOCK	8.9%/0.09	22.2%/0.33	40.0%/1.64	84.4%/7.98
CoDockPP	8.9%/0.09	26.7%/0.64	46.7%/2.96	75.6%/13.22
Difficult (34)				
ZDOCK	0.0%/0.00	11.8%/0.24	35.3%/1.21	58.8%/5.74
CoDockPP	5.9%/0.06	20.6%/0.44	38.2%/1.94	64.7%/8.94
All (230)				
ZDOCK	9.1%/0.09	29.1%/0.69	51.3%/3.11	80.4%/11.47
CoDockPP	13.9%/0.14	32.2%/0.93	57.8%/4.21	80.0%/17.09

[a] The first number is the success rate and the second number is the hit count.

Table S3. Success rate and hit count comparisons for site-specific unbound docking test

Method	Ambiguous constraints test				Multiple constraints test			
	Top 1	Top 10	Top 100	Top 1000	Top 1	Top 10	Top 100	Top 1000
Rigid-body (151)								
RosettaDock	3.3%/0.03 [a]	6.6%/0.09	29.8%/0.46	70.9%/2.36	15.2%/0.15	34.4%/0.82	77.5%/5.37	99.3%/33.56
CoDockPP	18.5%/0.19	40.4%/1.35	69.5%/6.93	89.4%/32.29	35.1%/0.35	64.9%/2.71	92.1%/16.44	100.0%/89.43
Medium difficulty (45)								
RosettaDock	0.0%/0.00	4.4%/0.04	20.0%/0.29	66.7%/1.80	0.0%/0.00	31.1%/0.36	57.8%/2.33	95.6%/18.36
CoDockPP	8.9%/0.09	26.7%/0.82	48.9%/3.89	86.7%/20.84	15.6%/0.16	53.3%/1.51	82.2%/10.44	100.0%/69.00
Difficult (34)								
RosettaDock	0.0%/0.00	0.0%/0.00	5.9%/0.06	50%/1.00	2.9%/0.03	8.8%/0.15	52.9%/1.91	85.3%/12.38
CoDockPP	5.9%/0.06	20.6%/0.47	41.2%/2.50	70.6%/14.18	11.8%/0.12	38.2%/1.12	73.5%/6.71	82.4%/39.74
All (230)								
RosettaDock	2.2%/0.02	5.2%/0.07	24.3%/0.37	67.4%/2.05	10.4%/0.10	30.0%/0.63	70.0%/4.27	96.5%/27.45
CoDockPP	14.8%/0.15	34.8%/1.12	61.3%/5.68	86.1%/27.37	27.8%/0.28	58.7%/2.24	87.4%/13.80	97.4%/78.09

[a] The first number is the success rate and the second number is the hit count.