

# Supplementary Materials

**Table S1.** P-values of the statistical test on the difference between CATHER and other methods' TM-scores in Table 1. "HHP", "EIG", "SPX", "MUS" and "MAP" represent the methods HHpred, EigenTHREADER, SPARKS-X, MUSTER and map\_align, respectively.

Targets	HHP	SPX	EIG	MUS	MAP
Easy	2.20E-15	1.51E-07	9.81E-15	2.55E-08	6.9E-10
Medium	6.34E-15	1.56E-04	1.45E-10	2.07E-03	1.87E-06
Hard	4.35E-17	1.48E-07	3.04E-10	5.92E-10	7.77E-11
Overall	3.07E-15	3.04E-06	8.82E-13	6.00E-09	1.14E-08

**Table S2.** P-values of the statistical test between the difference of CATHER and other methods' TM-scores in Table 2.

Targets	HHP	SPX	EIG	MUS	MAP
TBM	0.41	0.0039	1.61E-07	0.47	5.34E-06
TBM/FM	1.21E-05	0.002	0.0008	7.22E-08	0.002
FM	1.40E-08	9.56E-08	0.002	1.78E-09	3.97E-06
Overall	8.63E-07	1.18E-04	5.06E-06	2.91E-05	0.002

**Table S3.** Comparison between CATHER and the top servers in CASP12.

Targets	CATHER	QUARK	RaptorX	Zhang-Server	BAKER-ROSETTASERVER
TBM	0.7163	0.791	0.7797	0.7949	0.7858
TBM/FM	0.5442	0.5258	0.5023	0.5467	0.4955
FM	0.3426	0.3355	0.3159	0.3438	0.3261
Overall	0.5183	0.5409	0.5239	0.5495	0.5299

**Table S4.** The average TM-scores of the top models of different methods on the benchmark datasets.

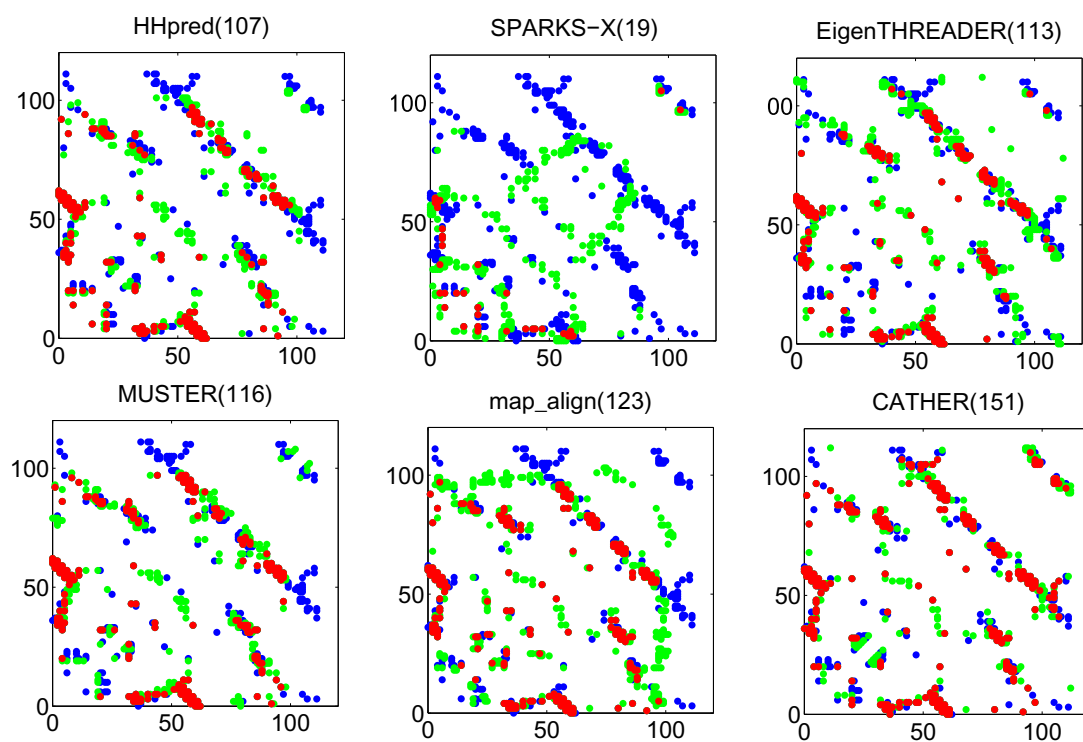
Target	Test480			CASP12		
	CATHER	PRF-align	PRF_cr	CATHER	PRF-align	PRF_cr
Easy (TBM)	0.7471	0.7295	0.7228	0.7163	0.6578	0.6984
Medium (TBM/FM)	0.5426	0.4561	0.5342	0.5442	0.3522	0.4927
Hard (FM)	0.4561	0.3128	0.4317	0.3426	0.2488	0.2966
Overall	0.6485	0.5901	0.6256	0.5183	0.4226	0.4822

**Table S5.** List of 83 CASP12 domains.

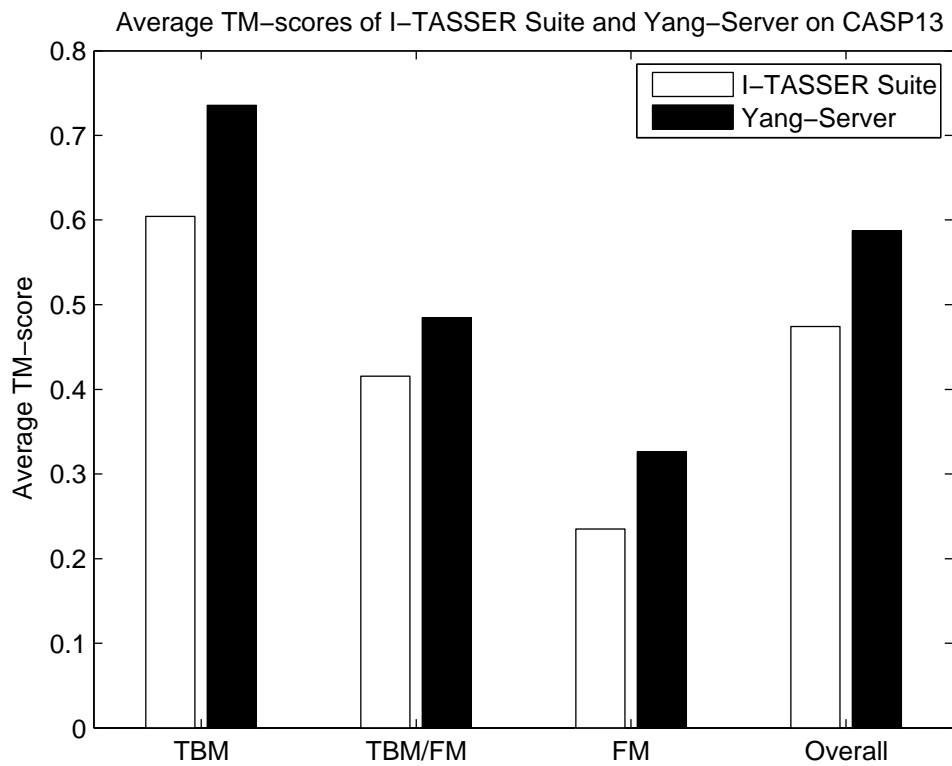
Domain ID	Classification	Target	Residues in domain
T0858-D1	FM	T0858	129
T0860-D1	TBM	T0860	136
T0861-D1	TBM	T0861	132
T0862-D1	FM	T0862	101
T0863-D1	FM	T0863	133
T0863-D2	FM	T0863	358
T0864-D1	FM	T0864	246
T0865-D1	TBM	T0865	62
T0866-D1	FM	T0866	104
T0867-D1	TBM	T0867	104
T0868-D1	FM/TBM	T0868	116
T0869-D1	FM	T0869	104
T0870-D1	FM	T0870	123
T0872-D1	TBM	T0872	88
T0877-D1	TBM	T0877	142
T0878-D1	FM	T0878	347
T0879-D1	TBM	T0879	220
T0880-D1	FM	T0880	26
T0880-D2	FM	T0880	157
T0881-D1	TBM	T0881	202
T0882-D1	TBM	T0882	24
T0884-D1	FM/TBM	T0884	71
T0885-D1	TBM	T0885	114
T0886-D1	FM	T0886	69
T0886-D2	FM	T0886	127
T0888-D1	FM	T0888	171
T0889-D1	TBM	T0889	239
T0890-D1	FM/TBM	T0890	82
T0890-D2	FM	T0890	106
T0891-D1	TBM	T0891	12
T0892-D1	FM/TBM	T0892	69
T0892-D2	FM	T0892	110
T0893-D1	TBM	T0893	73
T0893-D2	TBM	T0893	169
T0894-D1	FM	T0894	89
T0894-D2	FM/TBM	T0894	84
T0895-D1	TBM	T0895	120
T0896-D1	FM/TBM	T0896	86
T0896-D2	FM/TBM	T0896	201
T0896-D3	FM	T0896	161
T0897-D1	FM	T0897	138
T0897-D2	FM	T0897	124
T0898-D1	FM	T0898	106
T0898-D2	FM/TBM	T0898	55
T0899-D1	FM	T0899	269
T0899-D2	FM	T0899	88
T0900-D1	FM	T0900	102
T0901-D1	FM/TBM	T0901	223
T0901-D2	FM	T0901	70
T0902-D1	TBM	T0902	231
T0903-D1	TBM	T0903	524
T0904-D1	FM	T0904	251
T0905-D1	FM	T0905	242
T0905-D2	FM	T0905	66
T0909-D1	FM/TBM	T0909	333
T0912-D1	TBM	T0912	414
T0912-D2	FM/TBM	T0912	83
T0912-D3	FM	T0912	103
T0913-D1	TBM	T0913	338
T0914-D1	FM	T0914	158
T0914-D2	FM	T0914	162
T0915-D1	FM	T0915	154
T0917-D1	TBM	T0917	391
T0918-D1	FM	T0918	108
T0918-D2	FM	T0918	123
T0918-D3	FM	T0918	159
T0920-D1	TBM	T0920	321
T0920-D2	TBM	T0920	241
T0921-D1	TBM	T0921	138
T0922-D1	TBM	T0922	74
T0923-D1	FM	T0923	286
T0928-D1	TBM	T0928	343
T0941-D1	FM	T0941	341
T0942-D1	TBM	T0942	223
T0942-D2	TBM	T0942	214
T0943-D1	FM/TBM	T0943	73
T0943-D2	TBM	T0943	451
T0944-D1	TBM	T0944	253
T0945-D1	FM/TBM	T0945	396
T0946-D1	FM	T0946	80
T0946-D2	TBM	T0946	212
T0947-D1	TBM	T0947	175
T0948-D1	TBM	T0948	149

Table S6. List of 104 CASP13 domains.

Domain ID	Classification	Target	Residues in domain
T0950-D1	FM	T0950	342
T0951-D1	TBM	T0951	256
T0953s1-D1	FM	T0953s1	67
T0953s2-D1	FM/TBM	T0953s2	44
T0953s2-D2	FM	T0953s2	111
T0953s2-D3	FM	T0953s2	93
T0954-D1	TBM	T0954	336
T0955-D1	FM/TBM	T0955	41
T0957s1-D1	FM	T0957s1	108
T0957s1-D2	TBM	T0957s1	54
T0957s2-D1	FM	T0957s2	135
T0958-D1	FM/TBM	T0958	77
T0958-D1	TBM	T0958	180
T0960-D2	FM	T0960	84
T0960-D3	TBM	T0960	89
T0960-D5	TBM	T0960	105
T0961-D1	TBM	T0961	503
T0962-D1	TBM	T0962	177
T0964-D1	TBM	T0964	95
T0965-D1	TBM	T0965	313
T0966-D1	TBM	T0966	492
T0967-D1	TBM	T0967	79
T0968s1-D1	FM	T0968s1	119
T0968s2-D1	FM	T0968s2	116
T0969-D1	FM	T0969	354
T0974-D1	TBM	T0974	128
T0974s1-D1	TBM	T0974s1	69
T0975-D1	FM	T0975	293
T0976-D1	TBM	T0976	120
T0976-D2	TBM	T0976	124
T0977-D1	TBM	T0977	301
T0977-D2	TBM	T0977	204
T0978-D1	FM/TBM	T0978	413
T0979-D1	TBM	T0979	92
T0980s1-D1	FM	T0980s1	105
T0981-D1	TBM	T0981	86
T0981-D2	FM	T0981	80
T0981-D3	FM/TBM	T0981	203
T0981-D4	TBM	T0981	111
T0981-D5	TBM	T0981	127
T0982-D1	TBM	T0982	135
T0982-D2	TBM	T0982	132
T0983-D1	TBM	T0983	236
T0985-D1	TBM	T0985	842
T0986s1-D1	FM/TBM	T0986s1	92
T0986s2-D1	FM	T0986s2	155
T0987-D1	FM	T0987	185
T0987-D2	FM	T0987	207
T0989-D1	FM	T0989	134
T0989-D2	FM	T0989	112
T0990-D1	FM	T0990	76
T0990-D2	FM	T0990	231
T0990-D3	FM	T0990	213
T0991-D1	FM	T0991	111
T0992-D1	FM/TBM	T0992	107
T0993s1-D1	TBM	T0993s1	263
T0993s2-D1	TBM	T0993s2	98
T0995-D1	TBM	T0995	294
T0996-D1	TBM	T0996	107
T0996-D2	TBM	T0996	127
T0996-D3	TBM	T0996	100
T0996-D4	TBM	T0996	133
T0996-D5	TBM	T0996	121
T0996-D6	TBM	T0996	104
T0996-D7	TBM	T0996	140
T0997-D1	FM/TBM	T0997	185
T0998-D1	FM	T0998	166
T0999-D2	TBM	T0999	453
T0999-D3	TBM	T0999	180
T0999-D4	TBM	T0999	244
T0999-D6	TBM	T0999	288
T1000-D2	FM	T1000	431
T1001-D1	FM	T1001	139
T1002-D1	TBM	T1002	59
T1002-D2	TBM	T1002	59
T1002-D3	TBM	T1002	144
T1003-D1	TBM	T1003	437
T1004-D1	TBM	T1004	86
T1004-D2	TBM	T1004	77
T1005-D1	FM/TBM	T1005	326
T1006-D1	TBM	T1006	77
T1008-D1	FM/TBM	T1008	77
T1009-D1	TBM	T1009	718
T1010-D1	FM	T1010	210
T1011-D1	TBM	T1011	302
T1013-D1	TBM	T1013	288
T1014-D1	TBM	T1014	159
T1014-D2	TBM	T1014	117
T1015s1-D1	FM	T1015s1	88
T1015s2-D1	TBM	T1015s2	129
T1016-D1	TBM	T1016	202
T1017s1-D1	TBM	T1017s1	110
T1017s2-D1	FM	T1017s2	128
T1018-D1	TBM	T1018	334
T1018s1-D1	FM/TBM	T1018s1	58
T1018s2-D1	TBM	T1018s2	88
T1020-D1	TBM	T1020	322
T1021s1-D1	TBM	T1021s1	145
T1021s2-D1	TBM	T1021s2	349
T1021s3-D1	FM	T1021s3	178
T1021s3-D2	FM	T1021s3	101
T1022s1-D1	FM	T1022s1	156
T1022s1-D2	TBM	T1022s1	57
T1022s2-D1	TBM	T1022s2	525



**Fig. S1.** The match of the native contact map and the contact maps of the predicted structure models. Blue points: the contacts of native structure; Green points: the contacts of the models; Red points: the match of two maps. The number in each title means the number of matched contacts.



**Fig. S2.** The average TM-scores of I-TASSER Suite (white bars) and Yang-Server (black bars) for CASP13 domains.