

REDAN: Relative Entropy-Based Dynamical Allosteric Network Model

Supplementary Information

Hongyu Zhou, Peng Tao*

Department of Chemistry, Center for Scientific Computation, Center for Drug Discovery,
Design, and Delivery (CD4), Southern Methodist University, Dallas, Texas 75275, United States

* Corresponding author

Email: ptao@smu.edu

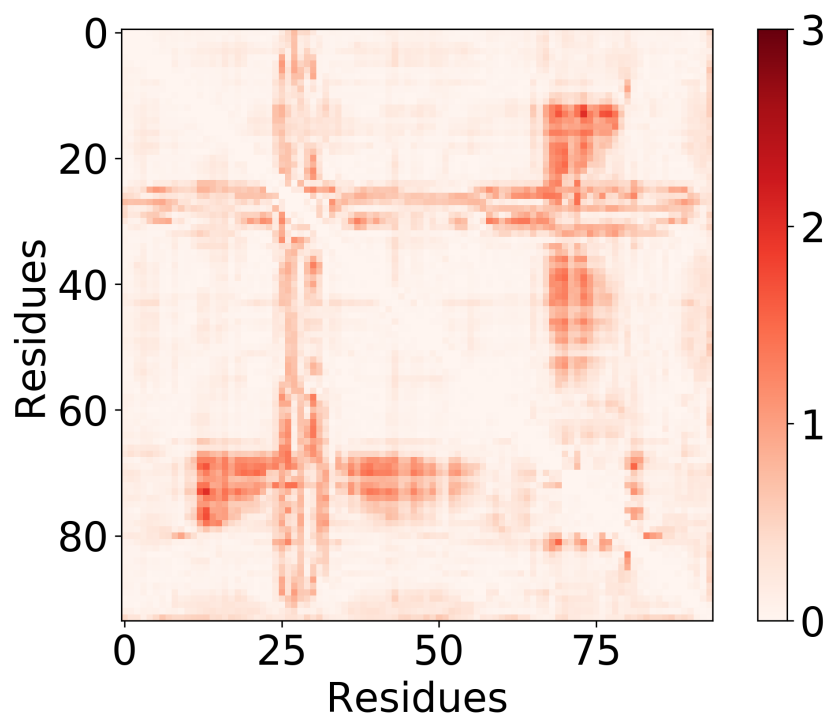


Figure S1: Perturbation relative entropy (*PRE*) matrix for all residue pairs for PDZ2

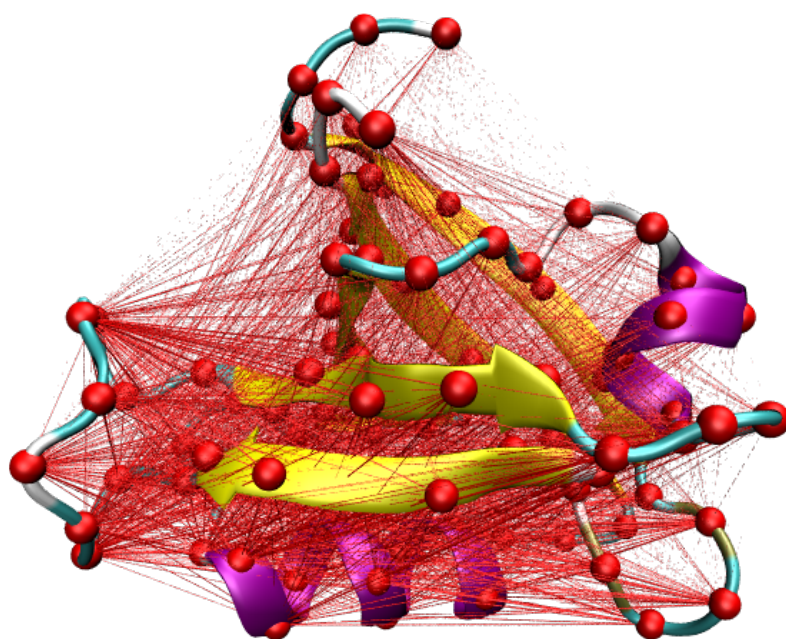


Figure S2: Allosteric network connecting residue pairs with significant *PRE*

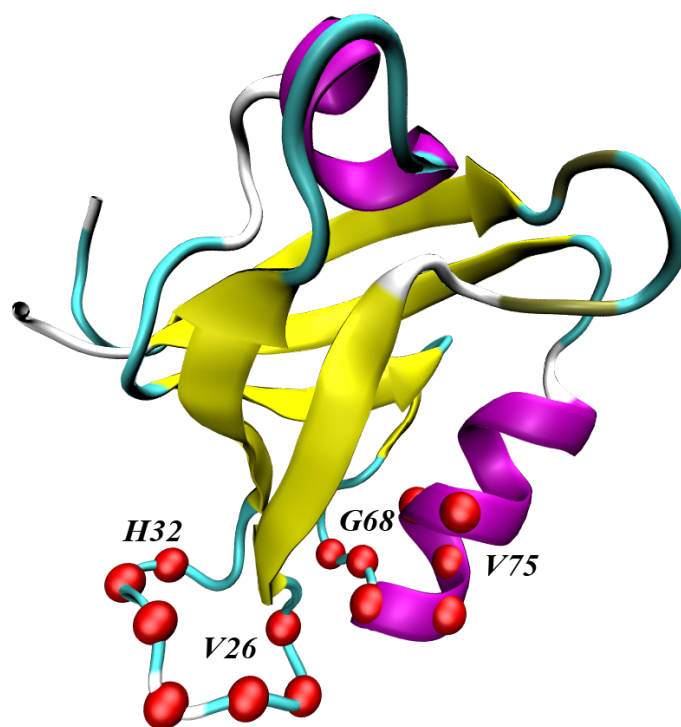


Figure S3: Top 15 Residues with highest total *PRE*

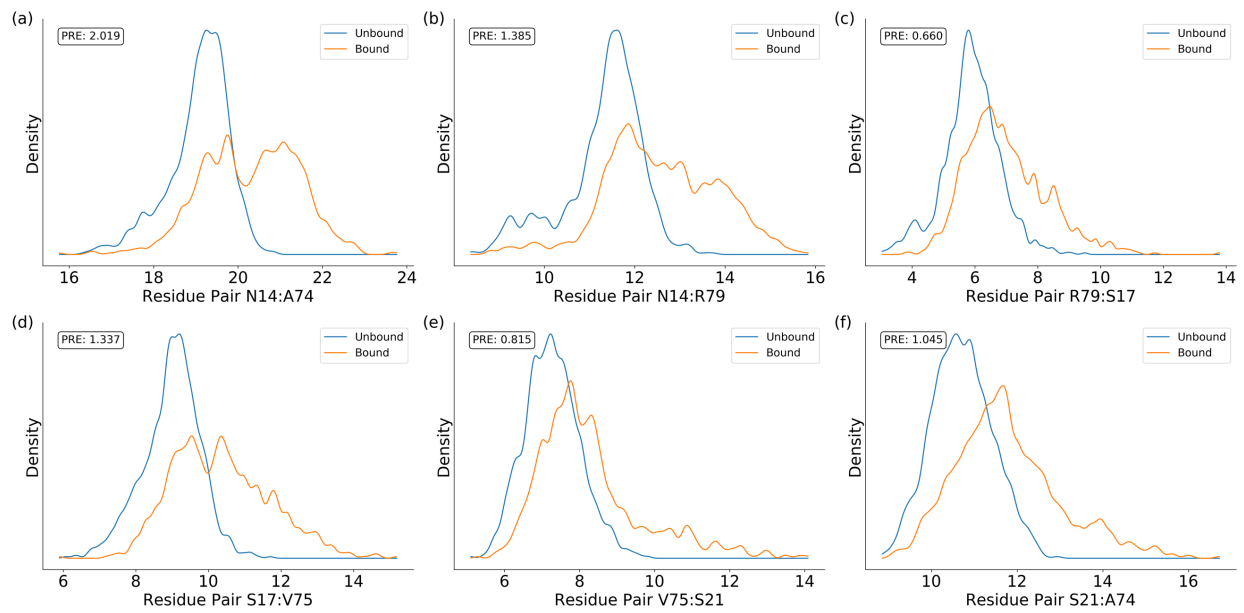


Figure S4: Decomposition of the distribution difference between N14:A74 into allosteric pathway with residue pairs N14:R79; R79:S17; S17:V75; V75:S21; and S21:A74. Distance distribution in unbound and bound states for: (a) N14:A74; (b) N14:R79; (c) R79:S17; (d) S17:V75; (e) V75:S21; and (f) S21:A74.

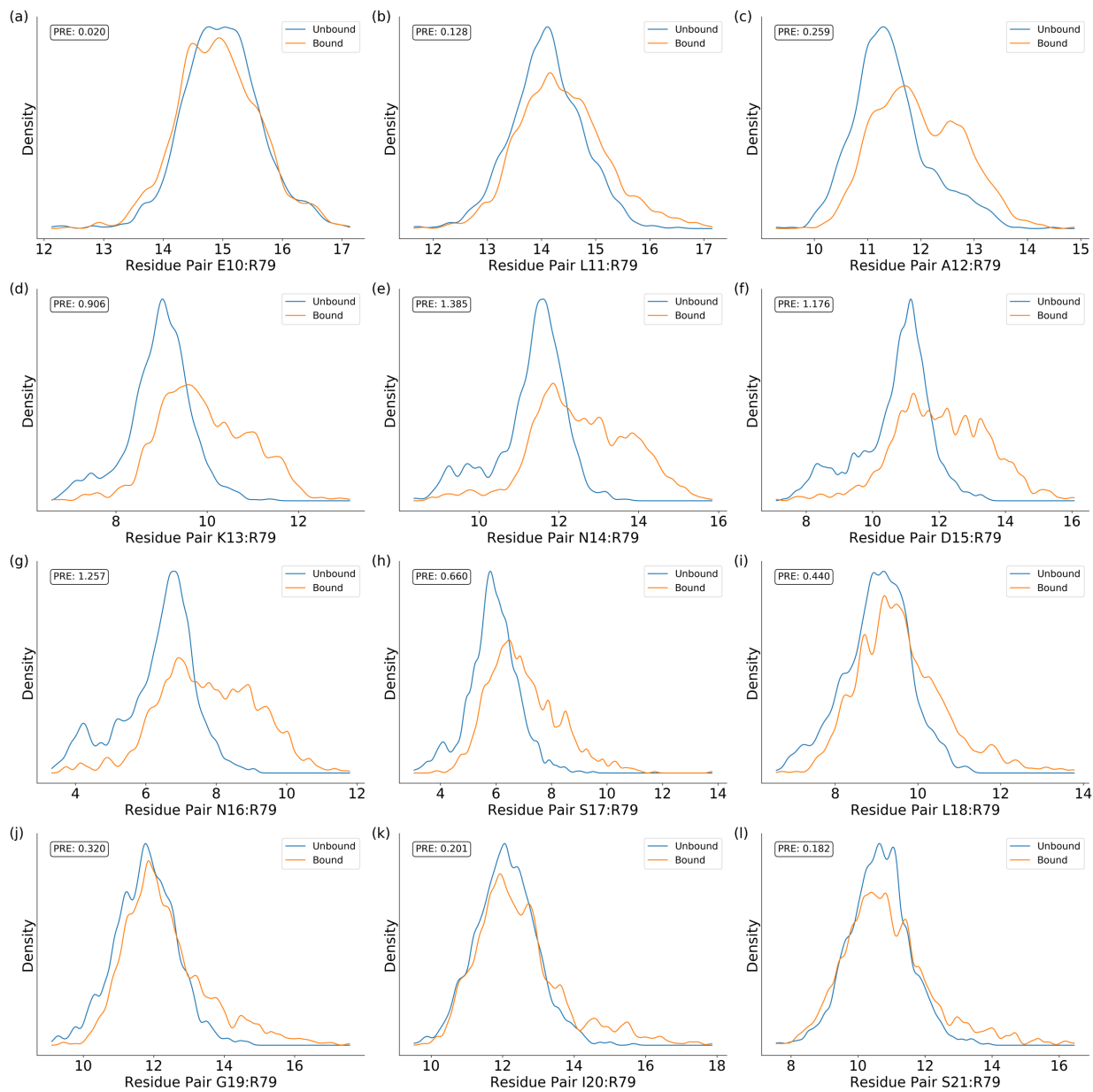


Figure S5: Distributions between residue R79 with residues E10 through S21: (a) E10:R19; (b) L11:R79; (c) A12:R79; (d) K13:R79; (e) N14:R79; (f) D15:R79; (g) N16:R79; (h) S17:R79; (i) L18:R79; (j) G19:R79; (k) I20:R79; (l) S21:R79.

Table S1: Top 5 residue pairs with the highest *PRE* upon peptide binding

Rank	Residue 1	Residue 2	PRE	Positions
1	N14	A74	2.019	β 1/ β 2 loop - α 3 helix
2	N14	L78	1.733	β 1/ β 2 loop - α 3 helix
3	K13	A74	1.720	β 1/ β 2 loop - α 3 helix
4	N14	T70	1.675	β 1/ β 2 loop - β 5/ α 3 loop
5	N14	T77	1.667	β 1/ β 2 loop - α 3 helix

Table S2: The accumulative allosteric effects for all residues

Rank	Residue	Total PRE	Rank	Residue	Total PRE	Rank	Residue	Total PRE
1	T70	54.9913	33	L66	20.1973	65	D49	13.0417
2	V26	54.8601	34	E47	19.6053	66	V64	13.0148
3	N27	52.6212	35	N80	19.4159	67	A12	12.7549
4	H71	50.4975	36	I20	19.2648	68	G4	12.6076
5	A74	46.7677	37	V40	18.4983	69	G55	12.2800
6	Q73	46.7028	38	I41	18.1236	70	D56	11.9449
7	A69	46.6795	39	A39	18.0600	71	R51	11.9448
8	R31	45.3269	40	V22	17.9820	72	A60	11.9024
9	T28	43.2867	41	S48	17.5738	73	Y36	11.3871
10	S29	38.1434	42	S21	17.1323	74	V9	11.1163
11	V75	37.0717	43	T23	17.1136	75	D5	11.0351
12	K72	35.8782	44	P42	16.8081	76	L59	11.0080
13	H32	34.7514	45	G92	16.6443	77	V84	10.8489
14	V30	32.0371	46	L18	16.5901	78	I52	10.7910
15	G68	30.7605	47	K91	16.3775	79	N62	10.5792
16	S94	29.4638	48	Q83	16.1430	80	V85	10.2575
17	G25	29.4041	49	V37	16.0991	81	L87	10.2471
18	E76	29.1336	50	E67	15.9713	82	L11	9.9817
19	T77	29.0960	51	G50	15.8363	83	L89	9.9431
20	N14	29.0179	52	K38	15.5068	84	F7	9.6712
21	L78	28.9938	53	I35	15.4423	85	V61	9.5903
22	R79	26.6650	54	A45	15.3900	86	R57	9.5262
23	G44	26.5424	55	Q93	15.2973	87	P3	9.3712
24	S17	26.4758	56	E90	15.0831	88	L88	9.1361
25	K13	26.4013	57	A46	14.9597	89	V58	8.9116
26	G33	24.6582	58	S65	14.7508	90	H86	8.7422
27	G82	24.5079	59	H53	14.3638	91	P1	8.4365
28	T81	24.0366	60	K54	14.1894	92	E8	8.3291
29	D15	23.9787	61	G24	13.7044	93	K2	7.4152
30	N16	23.1473	62	G34	13.5056	94	E10	7.0688
31	G19	22.0650	63	G63	13.2646			
32	Q43	21.3449	64	I6	13.0652			

Table S3: Total *PRE* between each community calculated from Kernighan-Lin algorithm (the value inside bracket is the percentage of total allosteric effects for all pair-wised residues)

Total PRE	Commu 1	Commu 2	Commu 3	Commu 4	Commu 5
Commu 1	8.17 (0.8%)	57.39 (5.9%)	65.38 (6.8%)	71.66 (7.4%)	55.47 (5.7%)
Commu 2		11.26 (1.2%)	65.46 (6.8%)	182.93 (19.0%)	51.52 (5.3%)
Commu 3			8.61 (0.9%)	72.45 (7.5%)	119.94(12.4%)
Commu 4				9.25 (1.0%)	173.29 (18.0%)
Commu 5					12.30 (1.3%)

Table S4: the residues in each community for PDZ2

	Residues
Commu 1	1-8, 23, 32-35, 56, 84, 89, 90-92
Commu 2	12-20, 43-44, 46-47, 51-52, 81-82, 83, 87
Commu 3	25-31, 93, 94
Commu 4	66-80
Commu 5	9-11, 21-22, 24, 36-42, 45, 48-50, 53-55, 57-65, 85-86, 88

Table S5: Characteristics of three algorithms

	Girvan-Newman	Kernighan-Lin	Hybrid
Computational Cost	Low	High	Medium
Minimum Search	No	Minimum	Local Minimum
Number of Communities	Auto determined	Need be specified	Auto determined
Cutoff Value Dependent	Yes	No	Yes
Deterministic	Yes	No	Yes
Secondary Structure Conservation	Partially	Most secondary structures	Partially