

Supplementary Materials

A study on allosteric communication in U1A-snRNA binding interactions: network analysis combined with molecular dynamics data

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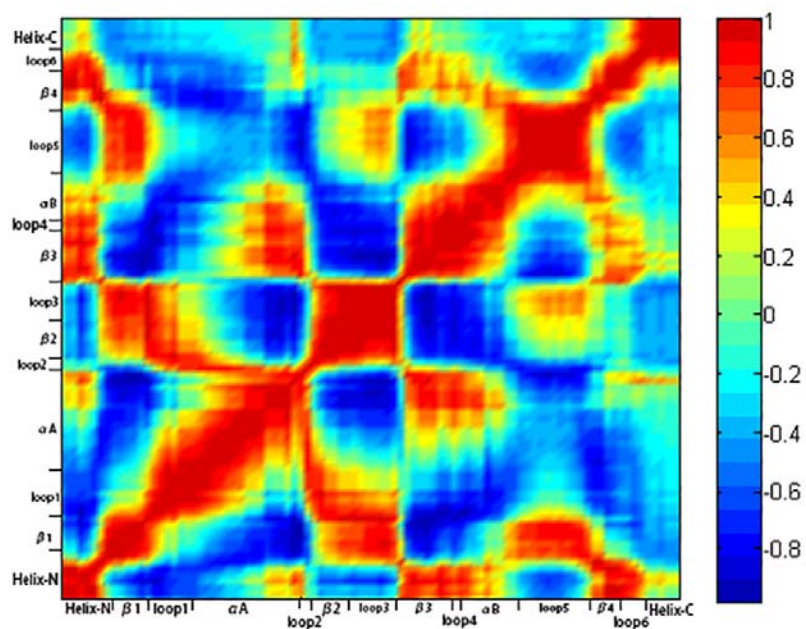


Figure S1. Fluctuation cross-correlations calculated using the dominant ten lowest motional modes for U1A protein. As shown in the color bar, the blue regions indicate negative correlations and the green-yellow-red regions present positive correlations.

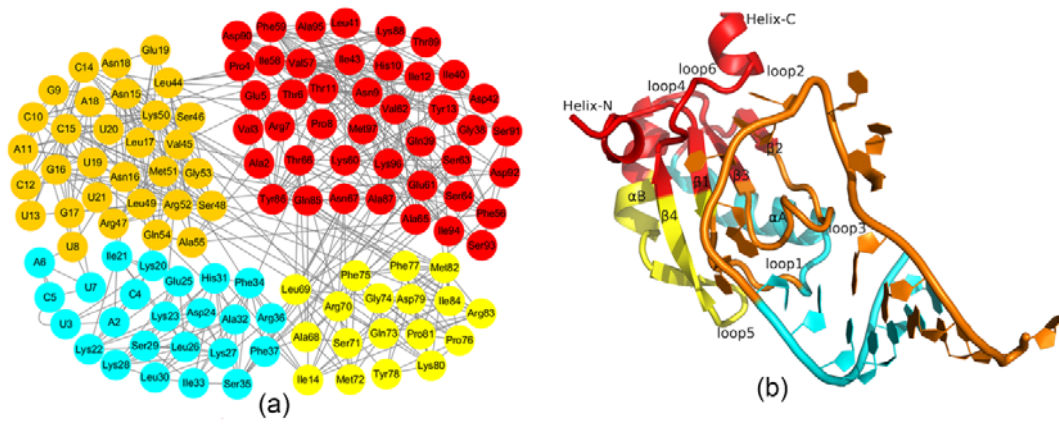


Figure S2. Four community structures of U1A-snRNA system obtained with Girvan-Newman algorithm, in which residue indexes (a) and their positions in the structure (b) are coded in red, cyan, orange and yellow, respectively.

Table S1. Residue list in decreasing order of its degree value in U1A-snRNA complex network

Rank	Residue Num	Degree values	Rank	Residue Num	Degree values
1	12	14	25	10	9
2	51	14	26	26	9
3	11	13	27	27	9
4	59	13	28	35	9
5	65	13	29	46	9
6	82	13	30	48	9
7	15	12	31	55	9
8	13	11	32	66	9
9	52	11	33	67	9
10	58	11	34	73	9
11	86	11	35	80	9
12	87	11	36	81	9
13	9	10	37	83	9
14	14	10	38	84	9
15	16	10	39	85	9
16	45	10	40	90	9
17	50	10	41	5	8
18	54	10	42	17	8
19	56	10	43	18	8
20	57	10	44	21	8
21	62	10	45	25	8
22	64	10	46	28	8
23	68	10	47	29	8
24	69	10	48	30	8

Table S1 (Continued)

Rank	Residue Num	Degree values	Rank	Residue Num	Degree values
49	31	8	73	91	7
50	34	8	74	92	7
51	40	8	75	94	7
52	43	8	76	95	7
53	44	8	77	4	6
54	47	8	78	7	6
55	49	8	79	8	6
56	53	8	80	19	6
57	60	8	81	20	6
58	76	8	82	24	6
59	88	8	83	39	6
60	6	7	84	41	6
61	22	7	85	42	6
62	23	7	86	63	6
63	32	7	87	71	6
64	33	7	88	36	5
65	37	7	89	78	5
66	38	7	90	79	5
67	61	7	91	89	5
68	70	7	92	93	5
69	72	7	93	96	5
70	74	7	94	3	4
71	75	7	95	97	3
72	77	7	96	2	2

Table S2. Residue list in decreasing order of its betweenness value in U1A-snRNA complex network

Rank	Residue Num	Betweenness	Rank	Residue Num	Betweenness
1	73	0.314	25	38	0.183
2	74	0.313	26	47	0.175
3	68	0.311	27	3	0.174
4	69	0.308	28	36	0.17
5	70	0.3	29	48	0.168
6	53	0.299	30	35	0.166
7	71	0.298	31	34	0.162
8	72	0.297	32	33	0.158
9	77	0.294	33	32	0.154
10	80	0.293	34	30	0.146
11	75	0.291	35	29	0.143
12	52	0.284	36	28	0.139
13	76	0.27	37	27	0.135
14	63	0.257	38	26	0.133
15	62	0.249	39	25	0.132
16	79	0.248	40	87	0.12
17	18	0.245	41	21	0.11
18	78	0.242	42	64	0.104
19	10	0.231	43	89	0.1
20	37	0.231	44	51	0.099
21	9	0.219	45	90	0.096
22	67	0.217	46	8	0.088
23	65	0.216	47	50	0.083
24	66	0.204	48	91	0.083

Table S2 (Continued)

Rank	Residue Num	Betweenness	Rank	Residue Num	Betweenness
49	19	0.078	73	96	0.017
50	7	0.076	74	45	0.016
51	39	0.072	75	16	0.014
52	40	0.064	76	42	0.014
53	6	0.063	77	46	0.014
54	59	0.06	78	54	0.014
55	23	0.057	79	61	0.014
56	24	0.057	80	82	0.014
57	5	0.054	81	49	0.012
58	93	0.054	82	85	0.012
59	22	0.051	83	14	0.011
60	12	0.04	84	88	0.009
61	4	0.034	85	43	0.008
62	95	0.034	86	44	0.008
63	58	0.027	87	55	0.004
64	86	0.022	88	60	0.004
65	17	0.021	89	15	0.003
66	81	0.021	90	13	0.001
67	11	0.02	91	56	0.001
68	41	0.02	92	2	0
69	83	0.019	93	20	0
70	84	0.019	94	31	0
71	92	0.018	95	94	0
72	57	0.017	96	97	0