

Evolutionary analyses of sequence and structure space unravel the structural facets of SOD1

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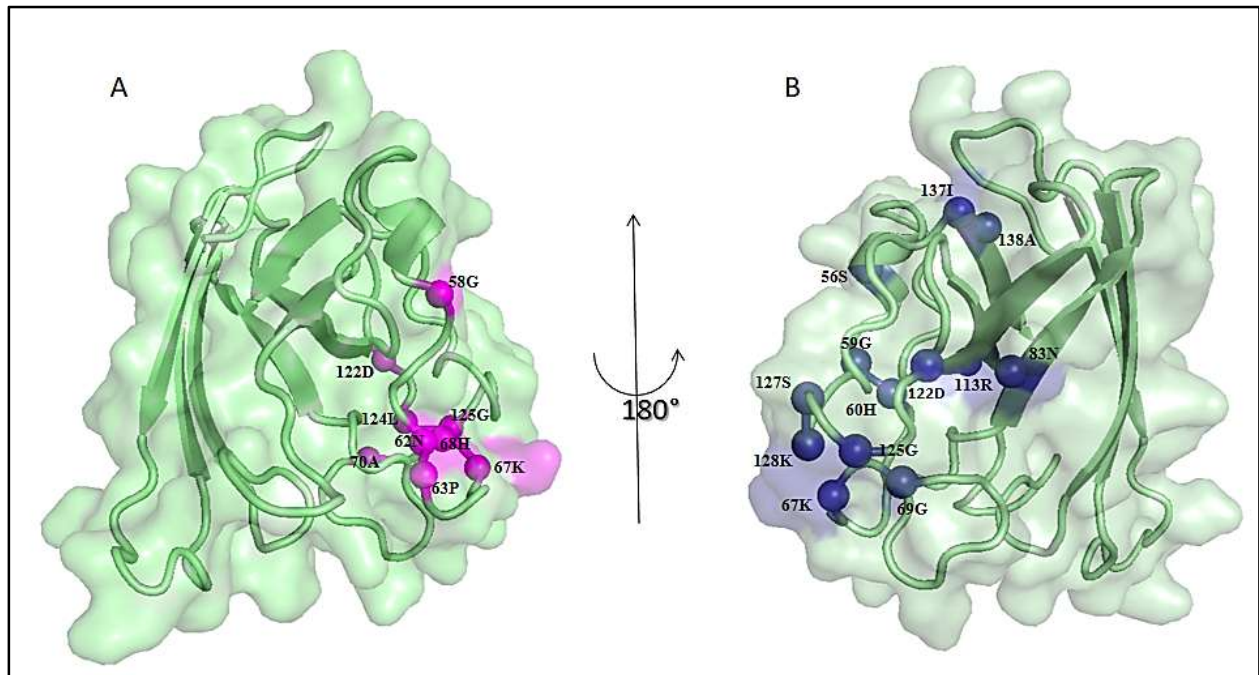
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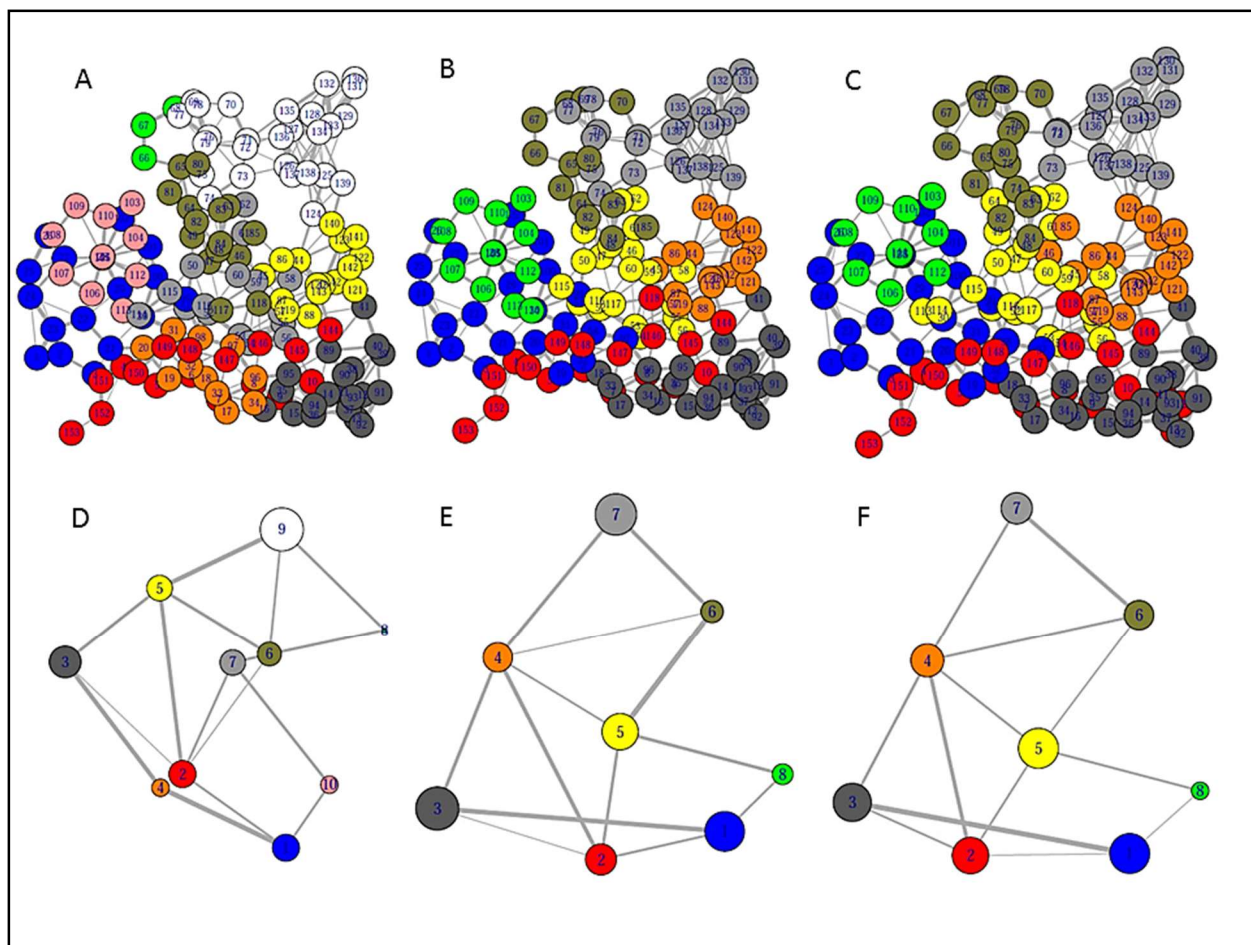
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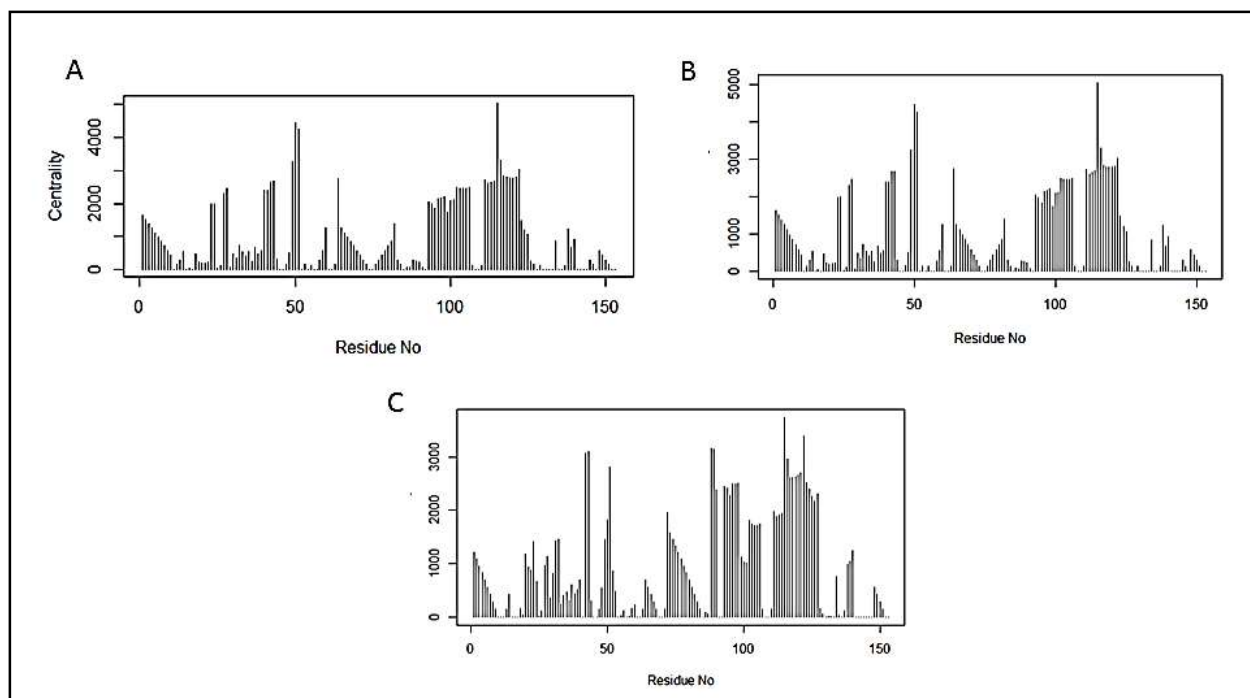
Supplementary Figures



Supplementary Figure 1. This figure designates the consensus structure. (A) Spheres highlighted by magenta color indicates the residues from top MI pairs positioned in loop region. (B) Spheres emphasized by deep blue color designates the residues from top DI pair that were housed in the loop region.



Supplementary Figure 2. (A and D) All residue network and community cluster network of Cu-SOD1. (B and E) All residue network and community cluster network of L4_SOD1. (C and F) Full residue network and simplified community network of L4S_SOD1.



Supplementary Figure 3. Betweenness centrality profile of (A) Cu-SOD1, (B) L4_SOD1 and (C) L4S_SOD1.

Supplementary Table 1: WT SOD1 cluster members

Cluster id	Size	Residue members
1	16	c(1:3, 21:30, 100:102)
2	15	c(4:7, 16:19, 33:35, 149:152)
3	13	c(8:15, 144:148)
4	7	c(20, 31:32, 96:99)
5	13	c(36:41, 89:95)
6	17	c(42:45, 86:88, 119:124, 140:143)
7	16	c(46:49, 62:65, 80:85, 117:118)
8	12	50:61
9	14	66:79
10	14	103:116
11	15	125:139
12	1	153

Important clusters are highlighted in bold face

Supplementary Table 2: apo-SOD1 cluster members

Cluster id	Size	Members
1	23	c(1:3, 19:32, 97:102)
2	17	c(4:10, 144:153)
3	25	c(11:18, 33:41, 89:96)
4	17	c(42:45, 86:88, 119:124, 140:143)
5	15	c(46:49, 63:65, 80:85, 117:118)

6	16	c(50:62, 114:116)
7	29	c(66:79, 125:139)
8	11	103:113

Supplementary Table 3: Zn SOD1 cluster members

Cluster id	Size	Members
1	23	c(1:3, 19:32, 97:102)
2	16	c(4:10, 144:152)
3	25	c(11:18, 33:41, 89:96)
4	17	c(42:44, 84:88, 120:124, 140:143)
5	18	c(45:49, 63:68, 80:83, 117:119)
6	16	c(50:62, 114:116)
7	26	c(69:79, 125:139)
8	11	103:113
9	1	153

Supplementary Table 4: Cu SOD1 cluster members

Cluster id	Size	Members
1	17	c(1:3, 21:30, 99:102)
2	17	c(4:10, 144:153)
3	20	c(11:16, 35:41, 89:95)
4	11	c(17:20, 31:34, 96:98)
5	16	c(42:45, 86:88, 119:123, 140:143)
6	15	c(46:49, 63:65, 80:85, 117:118)
7	16	c(50:62, 114:116)
8	3	66:68
9	27	c(69:79, 124:139)
10	11	103:113

Supplementary Table 5: L4 SOD1 cluster members

Cluster id	Size	Members
1	23	c(1:3, 19:32, 97:102)
2	18	c(4:10, 118, 144:153)
3	25	c(11:18, 33:41, 89:96)
4	17	c(42:45, 86:88, 119:124, 140:143)
5	21	c(46:63, 115:117)
6	13	c(64:70, 80:85)
7	24	c(71:79, 125:139)
8	12	103:114

Supplementary Table 6: L7 SOD1 cluster members

Cluster id	Size	Members
1	26	c(1:3, 17:33, 97:102)
2	9	c(4:6, 148:153)
3	9	c(7:10, 118, 144:147)
4	22	c(11:16, 34:41, 89:96)
5	18	c(42:45, 86:88, 119:124, 139:143)
6	9	c(46:48, 64:65, 80:82, 117)
7	17	c(49:63, 115:116)
8	23	c(66:73, 79, 125:138)
9	8	c(74:78, 83:85)
10	12	103:114

Supplementary Table 7: L4S SOD1 cluster members

Cluster id	Size	Members
1	23	c(1:3, 19:32, 97:102)
2	21	c(4:13, 118, 144:153)
3	22	c(14:18, 33:41, 89:96)
4	19	c(42:46, 85:88, 119:124, 140:143)
5	23	c(47:64, 113:117)
6	17	c(65:70, 74:84)
7	18	c(71:73, 125:139)
8	10	103:112

Supplementary Table 8: DI network members

Color	Size	Members
Yellow	27	c(14,17,18,42,46,54,49,61,93:97,100,103,107,117:125,120,135)
Blue	22	c(15,27:32,62:68,74,78,84,88,90,112,115,133)
Green	9	c(8,10,22,40,86,101,106,137,138)
Grey	7	c(24,33,34,73,76,126,129)
Violet	11	c(23,39,56,58,70,79,81,83,91,92,98)
Brown	3	c(20,53,104)
Turquoise	13	c(5,7,9,11,13,16,19,21,38,51,77,87,89)
Apricot	8	c(4,26,41,43,44,47,48,50)
Tangerine	14	c(36,37,49,52,60,69,72,79,105,109,113,114,121,132)

Supplementary Table 9: MI network members

Color	Number of Members	Members
Violet	1	86
Blue	2	79,81
Grey	1	77
Turquoise	2	13,102
Green	3	c(95,41,43)
Yellow	5	c(42,44,46,118,120)
Brown	6	c(116,117,119,121,124,125)
Tangerine	24	c(5,19,22,29,31,56,58,59,63:70,89,92:94,99,97,122)