Electronic Supporting Information

Manganese Matere Bonds in biological systems: PDB inspection and DFT calculations

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Table S1. List of PDB codes (PDBID), coordinated ligands (L_1 to L_4), interacting partner (LB), intermolecular Mn···LB distance (d, in Å) and L–Mn···LB angle (α, in degrees).

PDBID	L_1	L_2	L_3	L_4	LB	d	α
6EZJ	HIS	GLU	HIS	HIS	5LD	2.803	158.3
1WBL	GLU	ASP	ASP	HOH	HIS	2.804	164.2
6ILB	HIS	SER	ASP	HIS	GLU	2.836	170.8
4XSM	GLU	ASP	HIS	TLZ	GLU	2.892	161.1
4M0V	ASP	HIS	ASP	HOH	HIS	2.906	166.8
6B8W	GLU	HIS	TYR	HOH	HIS	2.961	163.8
2BAN	ASP	GLU	ASP	HOH	GLY	2.970	166.7
2P7P	HIS	HIS	GLU	SO4	TYR	3.041	170.0
5NMP	HIS	HIS	ASP	SIN	GLN	3.122	169.7
4O4K	ASP	HIS	ASP	HIS	HIS	3.164	167.9
1YNY	HIS	HIS	ASP	HOH	LYS	3.229	168.7
7Y1T	SER	SER	ASP	GLN	GLU	3.317	174.4
3BG5	ASP	LYS	HIS	HIS	PYR	3.391	166.5
1OG0	CYS	HIS	GLU	ASP	ARG	3.395	168.3
3F2C	HIS	HIS	GLU	ASN	CYS	3.499	169.3
5OEY	GLU	ASP	GLU	PO4	ASP	3.549	172.0
1LU2	GLU	ASP	ASP	HIS	SER	3.591	176.6
8ICT	DG	ASP	ASP	DCP	ASP	3.643	168.1
1KFL	CYS	HIS	GLU	ASP	ARG	3.646	162.6

1RIT	GLU	ASP	ASP	HIS	VAL	3.684	158.5
5ZT0	ASP	HIS	ASP	PO4	HIS	3.697	160.7
7MPQ	ASP	GLU	ASP	5GP	TYR	3.733	172.3
5D09	CYS	HIS	GLU	ASP	ARG	3.753	162.7
2DVF	GLU	ASP	ASP	HIS	VAL	3.834	169.2
6TVV	ASP	ASP	HIS	ASP	ASP	3.840	170.4
5CZ0	CYS	HIS	GLU	ASP	ARG	3.841	160.1
4D69	GLU	ASP	ASP	HIS	ILE	3.860	175.0
5DCD	CYS	HIS	GLU	ASP	ARG	3.872	174.1
3DKY	HIS	ASP	HIS	HIS	HIS	3.912	171.9
1V6O	GLU	ASP	ASP	HIS	VAL	3.928	162.0
6S2U	HIS	HIS	ASP	ASP	TYR	3.957	161.5
7ZR1	ASP	HIS	ASP	HIS	HIS	3.982	167.2
5FPL	LEU	LEU	THR	GLU	VAL	4.024	167.0
3NQW	HIS	HIS	ASP	ASP	ASN	4.055	158.8
1MSD	HIS	HIS	ASP	HIS	GLN	4.057	174.6
5FY9	ASN	LEU	THR	GLU	VAL	4.058	169.0
5O5L	ASP	ILE	ASP	ONM	PHE	4.137	167.2
4GBW	ASP	ASP	GLU	PO4	GLU	4.141	175.7
4YTQ	GLU	ASP	HIS	GLU	HIS	4.148	176.4
1LUL	GLU	ASP	ASP	HIS	ILE	4.206	169.7
2A8R	GLU	GLU	GLU	POP	ASP	4.328	178.6
4K20	GLU	ASP	ASP	HIS	VAL	4.387	167.9
8AMU	HIS	ASP	HIS	HIS	TYR	4.571	163.7

Cartesian coordinates of the PDB models regarding 2P7P, 3BG5 and 3DKY structures

2P7P

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C      5.8160000   -7.2650000   24.8380000
C      6.1870000   -7.9340000   26.1230000
N      6.4580000   -7.2310000   27.2760000
C      6.3350000   -9.2440000   26.4360000
C      6.7590000   -8.0780000   28.2440000
N      6.6920000   -9.3050000   27.7610000
C     14.0500000  -13.6220000   23.0810000
C     13.1560000  -12.4040000   22.8770000
O     11.9390000  -12.5440000   22.7840000
N     13.7460000  -11.2150000   22.8260000
C     12.9660000   -9.9940000   22.6410000
C     13.3280000   -9.2940000   21.3540000
O     14.4950000   -9.0670000   21.0690000
C     13.1540000   -9.0380000   23.8190000
C     12.5760000   -9.5590000   25.1140000
C     13.3190000  -10.3960000   25.9470000
C     11.2770000   -9.2390000   25.4930000
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C	12.7750000	-10.9000000	27.1310000
C	10.7220000	-9.7370000	26.6640000
C	11.4770000	-10.5670000	27.4800000
O	10.9240000	-11.0610000	28.6430000
N	12.3100000	-8.9460000	20.5790000
C	12.5230000	-8.3070000	19.2880000
C	9.2620000	-12.9240000	25.2700000
C	8.8380000	-12.8210000	26.7340000
O	7.9730000	-11.9710000	27.0570000
O	9.3710000	-13.5950000	27.5660000
C	2.1600000	-14.2820000	29.3640000
C	3.5820000	-13.8330000	29.2420000
N	4.5910000	-14.6660000	28.8140000
C	4.1590000	-12.6310000	29.4690000
C	5.7310000	-13.9980000	28.7840000
N	5.4960000	-12.7600000	29.1770000
Mn	7.3710000	-11.1630000	28.8930000
S	7.0340000	-10.6650000	32.1730000
O	8.4990000	-10.8200000	32.2390000
O	6.6360000	-9.4440000	32.9000000
O	6.6320000	-10.5760000	30.7490000
O	6.3650000	-11.8200000	32.7970000
H	15.1263779	-13.3991425	23.0545906
H	14.2295585	-8.8200820	23.9202719
H	12.6699983	-8.0814202	23.5612822
H	10.6739559	-8.5884475	24.8513603
H	14.3444582	-10.6567106	25.6722660
H	9.6901623	-9.5180514	26.9460222
H	13.3542135	-11.5497024	27.7901319
H	10.7285814	-12.0067007	28.5104798
H	11.9212645	-10.3392226	22.6196211
H	13.5243505	-7.8595150	19.2992801
H	6.6302049	-6.6257891	24.4601360
H	5.6052206	-8.0261492	24.0762669
H	6.4187580	-6.2228303	27.3611787
H	6.2601720	-10.1402494	25.8259546
H	6.9962610	-7.8155637	29.2740011
H	10.2142552	-12.3894036	25.1300239
H	9.4400313	-13.9759318	25.0150794
H	1.5335493	-13.4358647	29.6744375
H	2.0416807	-15.0780522	30.1170848
H	4.4686294	-15.6433306	28.5805556
H	3.7340077	-11.6997942	29.8337143
H	6.7006894	-14.3928652	28.4766577
H	4.9158335	-6.6390940	24.9468305
H	1.7665130	-14.6597229	28.4064800
H	8.5198683	-12.4794411	24.5934599
H	13.7959246	-14.0639614	24.0553039
H	13.8041027	-14.3622385	22.3081881
H	12.4770111	-9.0364200	18.4626616
H	11.7684646	-7.5258381	19.1171745
H	11.3828817	-9.2753796	20.8130630
H	14.7528938	-11.1255468	22.7626296

2P7P-H substitution of the OH phenolic group

C	5.81600000	-7.26500000	24.83800000
C	6.18700000	-7.93400000	26.12300000
N	6.45800000	-7.23100000	27.27600000
C	6.33500000	-9.24400000	26.43600000
C	6.75900000	-8.07800000	28.24400000
N	6.69200000	-9.30500000	27.76100000
C	14.05000000	-13.62200000	23.08100000
C	13.15600000	-12.40400000	22.87700000
O	11.93900000	-12.54400000	22.78400000
N	13.74600000	-11.21500000	22.82600000
C	12.96600000	-9.99400000	22.64100000
C	13.32800000	-9.29400000	21.35400000
O	14.49500000	-9.06700000	21.06900000
C	13.15400000	-9.03800000	23.81900000
C	12.57600000	-9.55900000	25.11400000
C	13.31900000	-10.39600000	25.94700000
C	11.27700000	-9.23900000	25.49300000
C	12.77500000	-10.90000000	27.13100000
C	10.72200000	-9.73700000	26.66400000
C	11.47700000	-10.56700000	27.48000000
N	12.31000000	-8.94600000	20.57900000
C	12.52300000	-8.30700000	19.28800000
C	9.26200000	-12.92400000	25.27000000
C	8.83800000	-12.82100000	26.73400000
O	7.97300000	-11.97100000	27.05700000
O	9.37100000	-13.59500000	27.56600000
C	2.16000000	-14.28200000	29.36400000
C	3.58200000	-13.83300000	29.24200000
N	4.59100000	-14.66600000	28.81400000
C	4.15900000	-12.63100000	29.46900000
C	5.73100000	-13.99800000	28.78400000
N	5.49600000	-12.76000000	29.17700000
Mn	7.37100000	-11.16300000	28.89300000
S	7.03400000	-10.66500000	32.17300000
O	8.49900000	-10.82000000	32.23900000
O	6.63600000	-9.44400000	32.90000000
O	6.63200000	-10.57600000	30.74900000
O	6.36500000	-11.82000000	32.79700000
H	15.12637790	-13.39914250	23.05459060
H	14.22955850	-8.82008200	23.92027190
H	12.66999830	-8.08142020	23.56128220
H	10.67395590	-8.58844750	24.85136030
H	14.34445820	-10.65671060	25.67226600
H	9.69016230	-9.51805140	26.94602220
H	13.35421350	-11.54970240	27.79013190
H	11.92126450	-10.33922260	22.61962110
H	13.52435050	-7.85951500	19.29928010
H	6.63020490	-6.62578910	24.46013600
H	5.60522060	-8.02614920	24.07626690
H	6.41875800	-6.22283030	27.36117870
H	6.26017200	-10.14024940	25.82595460
H	6.99626100	-7.81556370	29.27400110
H	10.21425520	-12.38940360	25.13002390
H	9.44003130	-13.97593180	25.01507940
H	1.53354930	-13.43586470	29.67443750
H	2.04168070	-15.07805220	30.11708480
H	4.46862940	-15.64333060	28.58055560
H	3.73400770	-11.69979420	29.83371430
H	6.70068940	-14.39286520	28.47665770
H	4.91583350	-6.63909400	24.94683050
H	1.76651300	-14.65972290	28.40648000

H	8.51986830	-12.47944110	24.59345990
H	13.79592460	-14.06396140	24.05530390
H	13.80410270	-14.36223850	22.30818810
H	12.47701110	-9.03642000	18.46266160
H	11.76846460	-7.52583810	19.11717450
H	11.38288170	-9.27537960	20.81306300
H	14.75289380	-11.12554680	22.76262960
H	11.04800089	-10.95022886	28.38221694

3BG5

C	50.3860000	75.6220000	51.7850000
C	49.7000000	76.7390000	52.5620000
O	49.8900000	76.8100000	53.7990000
O	48.9600000	77.5860000	52.0220000
C	43.8670000	76.6810000	56.3140000
N	45.1900000	76.3570000	55.7000000
C	48.5880000	73.3340000	59.3590000
C	48.8250000	74.3040000	58.2460000
N	49.4880000	73.9580000	57.0890000
C	48.5070000	75.6150000	58.1230000
C	49.5590000	75.0120000	56.2950000
N	48.9780000	76.0330000	56.9030000
C	51.7700000	80.8190000	58.3910000
C	50.8740000	80.1710000	57.3790000
N	50.9650000	80.4300000	56.0290000
C	49.8910000	79.2470000	57.5170000
C	50.0690000	79.7070000	55.3800000
N	49.4040000	78.9800000	56.2600000
Mn	47.7610000	77.2670000	55.1760000
C	43.4500000	78.4730000	51.9620000
O	42.3670000	78.1360000	52.6130000
O	43.4350000	78.5020000	50.6490000
C	44.6080000	78.7860000	52.6710000
O	45.6340000	77.9690000	52.6300000
C	44.6840000	80.0520000	53.4810000
H	51.4611797	75.6103394	52.0148474
H	49.9698608	74.6532006	52.1023949
H	44.0000913	76.9184722	57.3781520
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H	47.9271824	73.7831540	60.1114108
H	48.1114417	72.4093998	58.9977375
H	49.8893313	73.0449315	56.9059175
H	47.9797010	76.2683867	58.8139606
H	50.0209169	75.0775579	55.3052683
H	51.4494433	80.5391388	59.4015450
H	51.7380071	81.9180042	58.3196112
H	51.6315422	81.0674199	55.6094795
H	49.5131720	78.7657696	58.4147436
H	49.9406092	79.6722483	54.2981578
H	45.6414570	80.0826413	54.0137261
H	43.8335756	80.1207116	54.1785573
H	44.6121287	80.9215237	52.8058429
H	45.0223208	76.1510172	54.7110977
H	45.5024857	75.4683271	56.0966497
H	50.2284108	75.7554757	50.7086389
H	49.5271158	73.0541523	59.8627467
H	43.1550515	75.8469225	56.2184595
H	52.8174528	80.5008095	58.2683199
H	41.6885261	77.9591107	51.9361226

3DKY

C	10.9280000	17.9500000	-47.7960000
C	9.8980000	18.4670000	-46.8760000
N	9.1790000	19.6100000	-47.1450000
C	9.4670000	18.0270000	-45.6730000
C	8.3600000	19.8560000	-46.1410000
N	8.5070000	18.9060000	-45.2440000
C	9.8400000	21.5780000	-51.7550000
C	9.5730000	21.2630000	-50.3220000
O	9.4730000	22.2310000	-49.5300000
O	9.4390000	20.0580000	-50.0060000
C	15.8530000	19.0140000	-47.7260000
C	14.5730000	19.7620000	-47.7220000
N	13.7360000	19.7870000	-48.8120000
C	13.9770000	20.5090000	-46.7800000
C	12.6890000	20.5280000	-48.5400000
N	12.8110000	20.9770000	-47.3050000
C	11.8230000	19.5840000	-41.9030000
C	11.8180000	20.6910000	-42.9190000
N	12.5650000	21.8410000	-42.7580000
C	11.1360000	20.8410000	-44.0720000
C	12.3330000	22.6570000	-43.7690000
N	11.4660000	22.0800000	-44.5790000
C	3.9570000	17.7070000	-43.2210000
C	3.2410000	18.7420000	-44.0570000
O	2.2870000	18.4250000	-44.7400000
N	3.7270000	19.9760000	-43.9940000
C	3.0860000	21.1390000	-44.6220000
C	1.6160000	21.3080000	-44.2440000
O	0.8570000	21.9270000	-45.0100000
C	3.2840000	21.1670000	-46.1560000
C	4.6660000	21.5720000	-46.5800000
N	5.4270000	20.8270000	-47.4530000
C	5.4340000	22.6240000	-46.2270000
C	6.5960000	21.4170000	-47.6270000
N	6.6320000	22.5050000	-46.8900000
N	1.2430000	20.7870000	-43.0630000
C	-0.1390000	20.8230000	-42.5530000
Mn	10.5050000	22.0400000	-47.1880000
H	4.3274023	16.9144245	-43.8868680
H	3.0121768	20.1751825	-46.5471849
H	2.5352582	21.8707733	-46.5504291
H	5.2154215	23.4560755	-45.5607005
H	7.3747905	21.0648304	-48.3073433
H	3.5907712	22.0226691	-44.1978951
H	-0.7321900	21.4103881	-43.2649853
H	11.9381995	18.2305145	-47.4601942
H	10.7388701	18.3705570	-48.7937968
H	9.7131655	17.1338079	-45.1022164
H	7.7190471	20.7250839	-46.0133289
H	7.9674373	18.8010623	-44.3931612
H	9.9672059	22.6511590	-51.9465280
H	10.7384589	21.0317865	-52.0777729
H	16.3425863	19.0999951	-46.7476383
H	16.5511812	19.4048983	-48.4831943
H	13.9116314	19.3017175	-49.6845796
H	14.3015437	20.7439604	-45.7696845
H	11.8416670	20.6579727	-49.2176273
H	11.3910188	19.9124945	-40.9444643
H	11.2248078	18.7418453	-42.2738868
H	13.1689564	22.0279145	-41.9658436
H	10.4589816	20.1530448	-44.5679385

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H    12.7840805   23.6390513  -43.8978383
H     4.7892557   18.0945025  -42.6140664
H     3.2206656   17.2360900  -42.5540966
H    -0.1753616   21.3001323  -41.5627039
H    -0.5515082   19.8051302  -42.4898890
H     9.0074606   21.1937381  -52.3618667
H    15.6998488   17.9427105  -47.9311710
H    12.8403723   19.2114348  -41.7065419
H     5.0946917   19.9941722  -47.9251069
H    10.8945684   16.8529149  -47.8577616
H     4.5275565   20.1536620  -43.4047660
H     1.9288616   20.2668219  -42.5354481
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