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Electronic Supplementary Information

Using theoretical calculations to predict the redox potential of mononuclear manganese complexes

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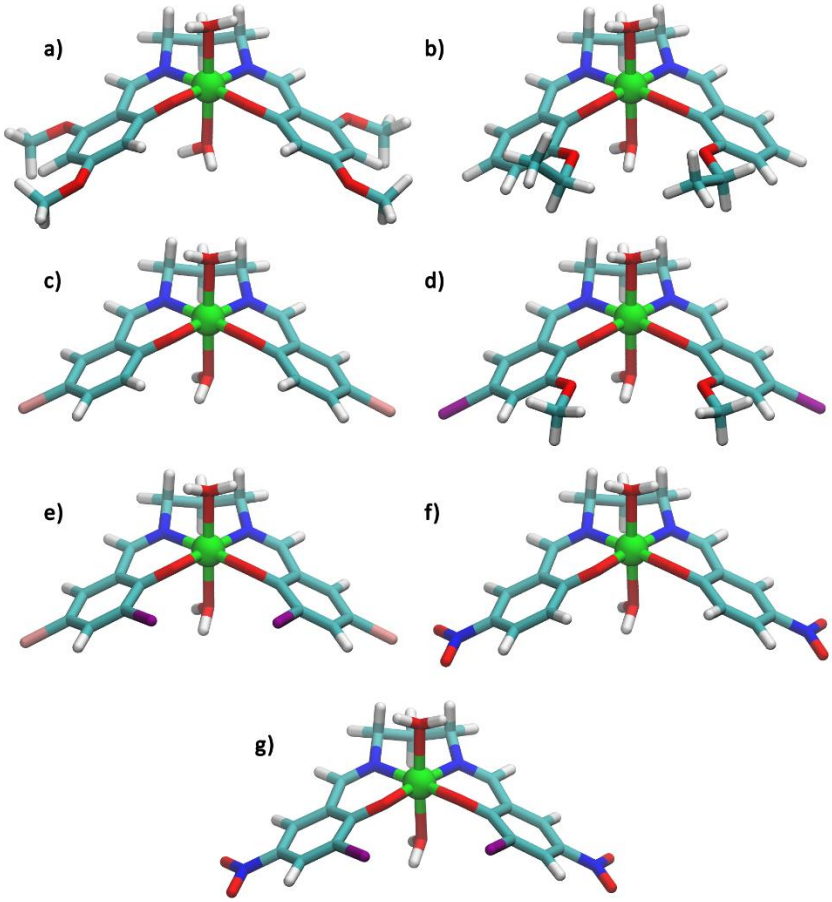

Fig. S1 Optimized structure of the all complexes. A) Complex-1 B) Complex-2. Atoms are represented with the following colours: H: white, C: cyan, N: blue, O: red, Mn: green, Br: purple.

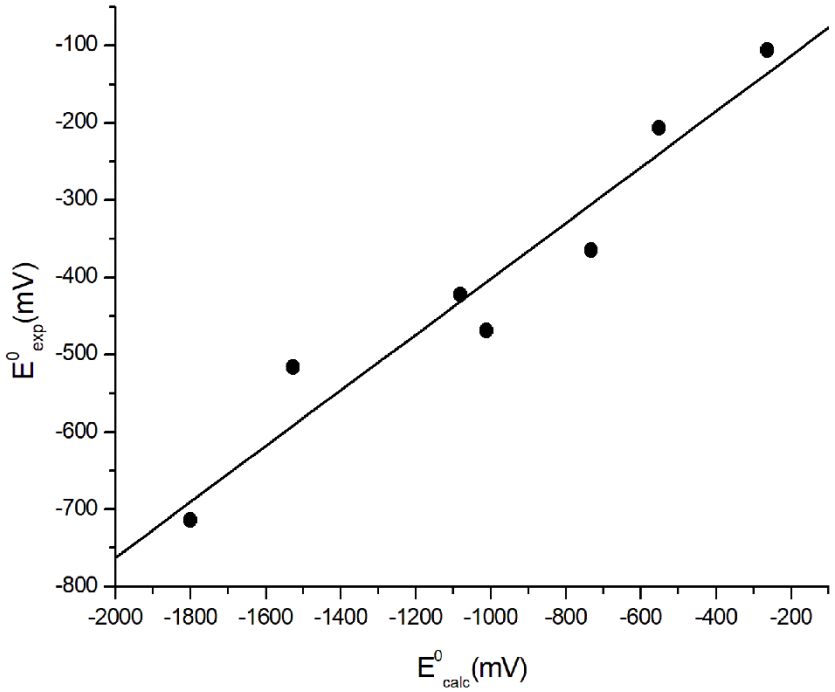

Fig. S2 Plot of calculated and experimental redox potentials for the manganese complexes. Calculations were performed at B3LYP/6-31G**/LANL2DZ in vacuum. Solid line represents the linear regression of the data. Regression coefficient (R) is 0.96.

Table SI Relevant geometrical parameters of the optimized structures of the Mn^{III} complexes calculated at B3LYP / 6-31G** / LANL2DZ / PCM

	Complex-1	Complex-2	Complex-3	Complex-4	Complex-5	Complex-6	Complex-7
Mn-O1	1.89	1.88	1.88	1.88	1.879	1.88	1.89
Mn-O2	1.88	1.87	1.87	1.87	1.875	1.87	1.89
Mn-O3	2.31	2.30	2.29	2.29	2.292	2.30	2.26
Mn-O4	2.036	2.34	2.33	2.33	2.332	2.36	2.30
Mn-N1	2.02	2.04	2.05	2.05	2.049	2.04	2.04
Mn-N2	2.03	2.05	2.05	2.05	2.054	2.05	2.04
O1-Mn-O2	89.2	89.6	89.1	89.4	89.4	89.3	88.8
O1-Mn-O3	89.1	91.7	94.0	92.4	92.4	88.0	95.0
O1-Mn-O4	91.1	91.6	91.3	92.0	92.0	90.7	90.4
O1-Mn-N1	177.4	178.2	177.1	178.0	178.0	177.8	175.7
O1-Mn-N2	88.3	88.3	88.6	88.3	88.3	88.3	88.7
O2-Mn-O3	94.4	94.2	93.6	94.1	94.1	92.2	92.2
O2-Mn-O4	87.2	88.2	89.0	88.6	88.6	85.7	89.0
O2-Mn-N1	89.03	88.7	88.7	88.7	88.7	89.0	88.4
O2-Mn-N2	175.0	176.7	177.4	176.6	176.7	175.4	177.6
N1-Mn-O3	89.1	88.0	88.0	88.1	88.2	90.6	88.4
N1-Mn-O4	90.6	88.8	86.8	87.5	87.5	90.6	86.3
N1-Mn-N2	93.6	93.4	93.5	93.6	93.6	93.4	94.0
N2-Mn-O3	89.9	88.5	87.7	88.2	88.2	91.7	88.1
N2-Mn-O4	88.4	89.2	89.9	89.2	89.2	90.3	90.9
O3-Mn-O4	178.3	175.9	174.1	174.7	174.7	90.3	174.5

Table SII Relevant geometrical parameters of the optimized structures of the Mn^{III} complexes calculated at B3LYP / 6-31G** / LANL2DZ / SMD

	Complex-1	Complex-2	Complex-3	Complex-4	Complex-5	Complex-6	Complex-7
Mn-O1	1.89	1.88	1.88	1.88	1.89	1.89	1.90
Mn-O2	1.88	1.87	1.88	1.88	1.88	1.89	1.89
Mn-O3	2.32	2.31	2.31	2.30	2.30	2.29	2.27
Mn-O4	2.37	2.35	2.35	2.34	2.33	2.33	2.32
Mn-N1	2.02	2.04	2.05	2.04	2.04	2.04	2.04
Mn-N2	2.03	2.05	2.05	2.05	2.05	2.05	2.04
O1-Mn-O2	89.3	89.7	89.1	89.6	90.0	88.4	89.1
O1-Mn-O3	88.1	88.3	91.9	89.2	90.1	91.8	92.9
O1-Mn-O4	90.7	91.9	91.0	92.0	91.8	90.9	96.4
O1-Mn-N1	177.4	177.3	177.5	177.9	178.5	177.0	176.0
O1-Mn-N2	88.2	88.1	88.5	88.1	88.2	88.6	88.5
O2-Mn-O3	93.2	93.9	92.4	93.3	92.9	93.0	90.5
O2-Mn-O4	87.3	87.3	89.3	88.0	88.1	88.3	89.0
O2-Mn-N1	88.9	88.7	88.8	88.8	88.5	88.9	88.5
O2-Mn-N2	174.8	175.0	177.0	175.3	176.2	176.0	177.6
N1-Mn-O3	90.0	89.5	89.4	89.6	89.7	89.6	90.3
N1-Mn-O4	91.1	90.2	87.7	89.1	88.4	87.7	86.9
N1-Mn-N2	93.7	93.6	93.6	93.7	93.3	93.9	93.8
N2-Mn-O3	91.2	90.5	89.5	90.1	90.4	89.7	89.9
N2-Mn-O4	88.1	88.2	88.9	88.0	88.6	89.1	90.1
O3-Mn-O4	178.7	178.7	176.6	177.7	177.8	89.1	177.2