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Supplementary Information

Manganese(II) complexes of tridentate 3N ligands as functional models of phenoxazinone synthase: Impact of ligand steric hindrance on reactivity

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Figure S1

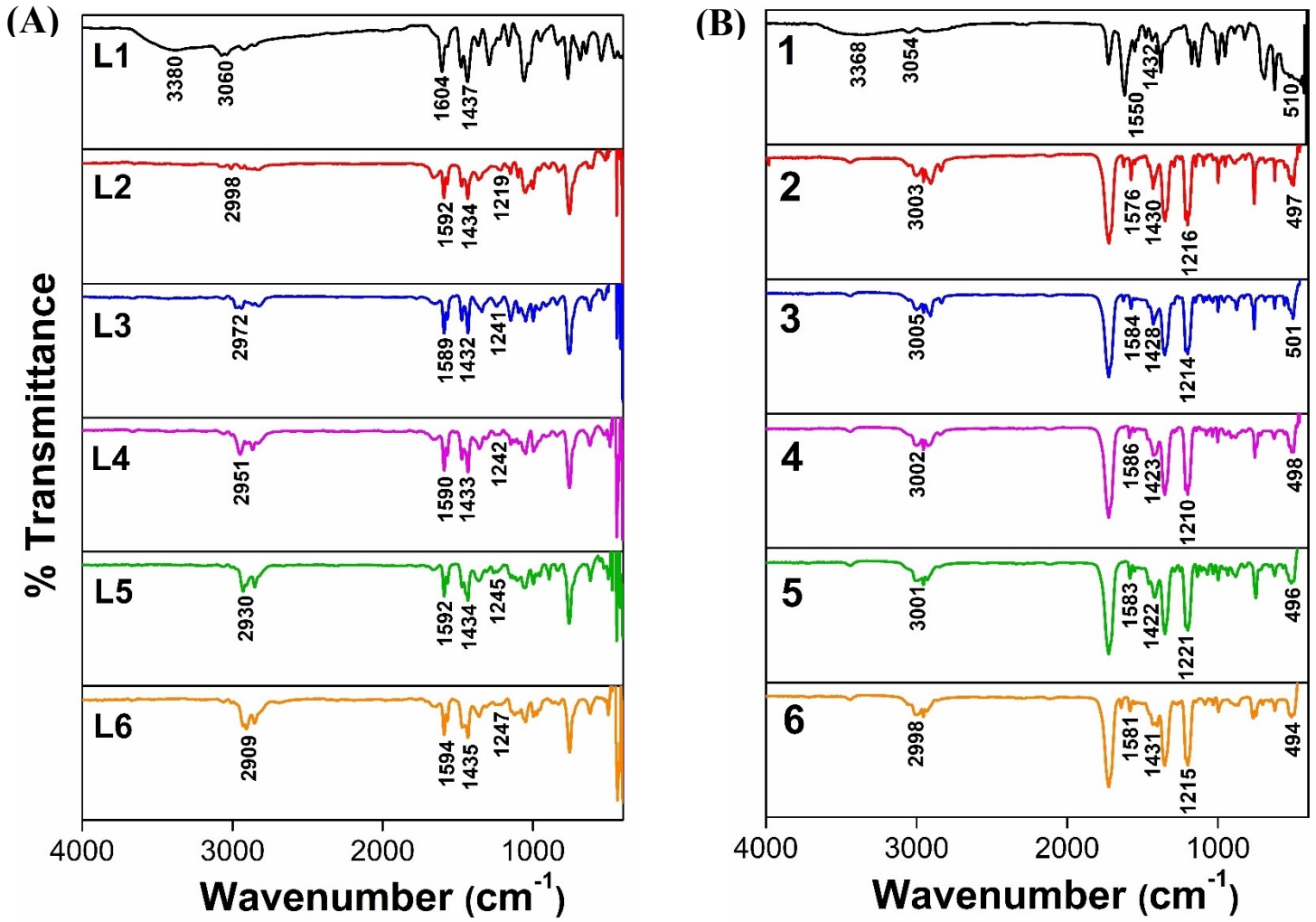


Fig. S1 ATR-FTIR spectra of ligands **L1**–**L6** and their corresponding manganese(II) complexes **1**–**6**, respectively.

Table S1

Table S1. ATR-FTIR spectral data for ligands and their respective manganese(II) complexes.

	Group of stretching frequency (cm^{-1})				
Compound	**υ(C–H)**	**υ(C=N_{py})**	**υ(C–N_{py})**	**υ(C–$N_{3°\ amine}$)**	**υ(Mn–N)**
L1	3060	1604	1437	–	–
L2	2998	1592	1434	1219	–
L3	2972	1589	1432	1241	–
L4	2951	1590	1433	1242	–
L5	2930	1592	1434	1245	–
L6	2909	1594	1436	1247	–
1	3054	1550	1432	–	510
2	3003	1576	1430	1216	497
3	3005	1584	1428	1214	501
4	3002	1586	1423	1210	498
5	3001	1583	1422	1221	496
6	2998	1581	1431	1215	494

Figure S2

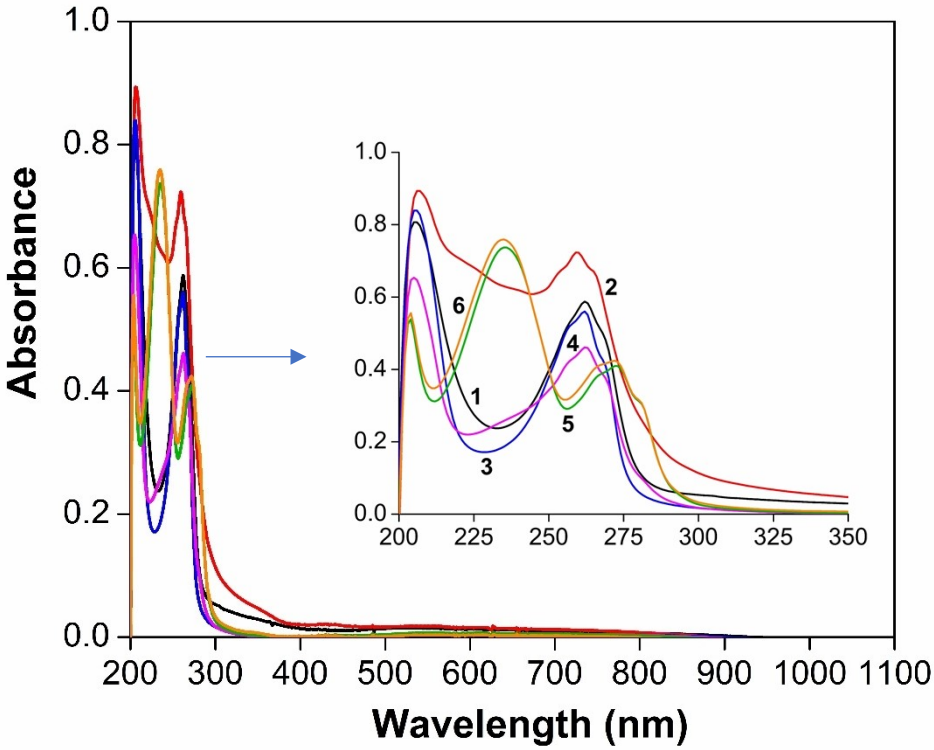


Fig. S2 Electronic absorption spectra of complexes **1**–**6** in methanol at RT.

Table S2

Table S2. UV-vis spectral data[a] of manganese(II) complexes **1**–**6** in methanol.

Complexes	λ_{max} (nm), ε (M^{-1} cm^{-1})
$[Mn(L1)Cl_2]$ **1**	205 (31,428) 260 (22,878) 268 (20,688)
$[Mn(L2)Cl_2]$ **2**	206 (32,251) 223 (24,955) 260 (26,078) 266 (23,698)
$[Mn(L3)Cl_2]$ **3**	206 (15,117) 257 (9,361) 262 (10,094) 270 (7,384)
$[Mn(L4)Cl_2]$ **4**	205 (11,775) 256 (7,465) 263 (7,373) 269 (6,769)
$[Mn(L5)Cl_2]$ **5**	204 (11,682) 235 (15,920) 266 (8,192) 273 (8,839) 281 (6,591)
$[Mn(L6)Cl_2]$ **6**	204 (15,002) 235 (20,493) 266 (10,988) 272 (11,447) 281 (8,293)

[a]Concentration of manganese(II) complexes: 3×10^{-3} M in methanol solution at 25 °C.

Figure S3 and S4

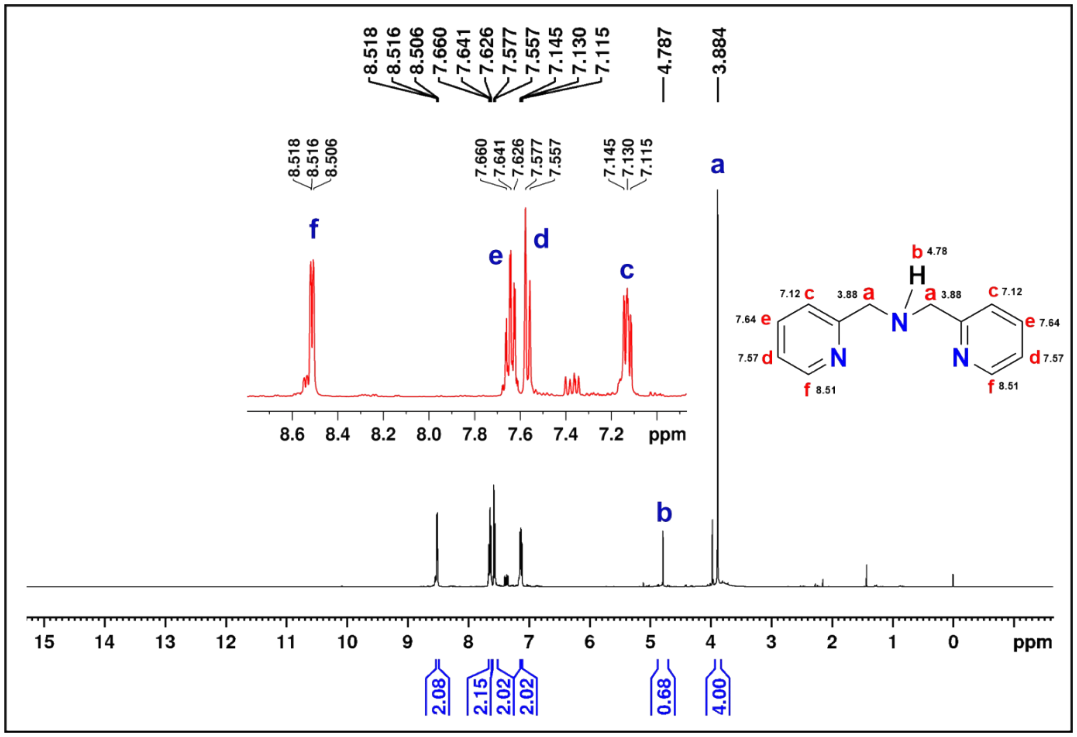


Fig. S3. ^{1}H NMR spectrum of **L1** in $CDCl_3$ at 298 K.

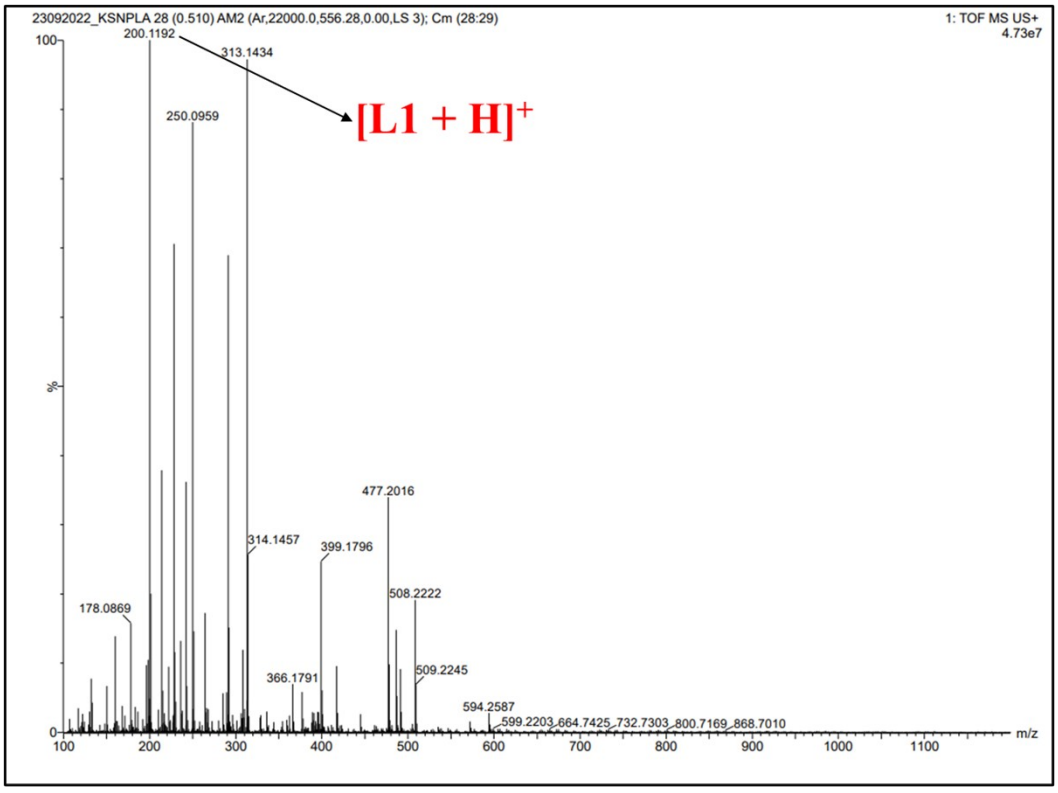


Fig. S4 High Resolution Mass Spectrum of **L1** in methanol solution.

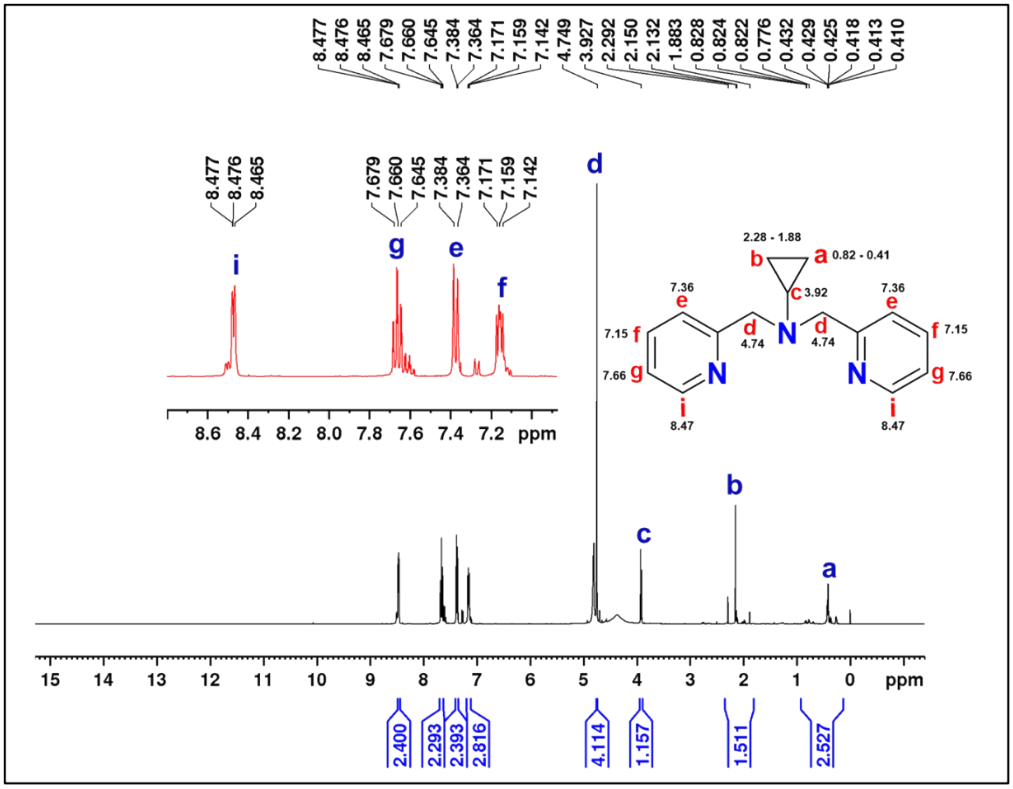


Figure S5 and S6

Fig. S5 ^{1}H NMR spectrum of **L2** in $CDCl_3$ at 298 K.

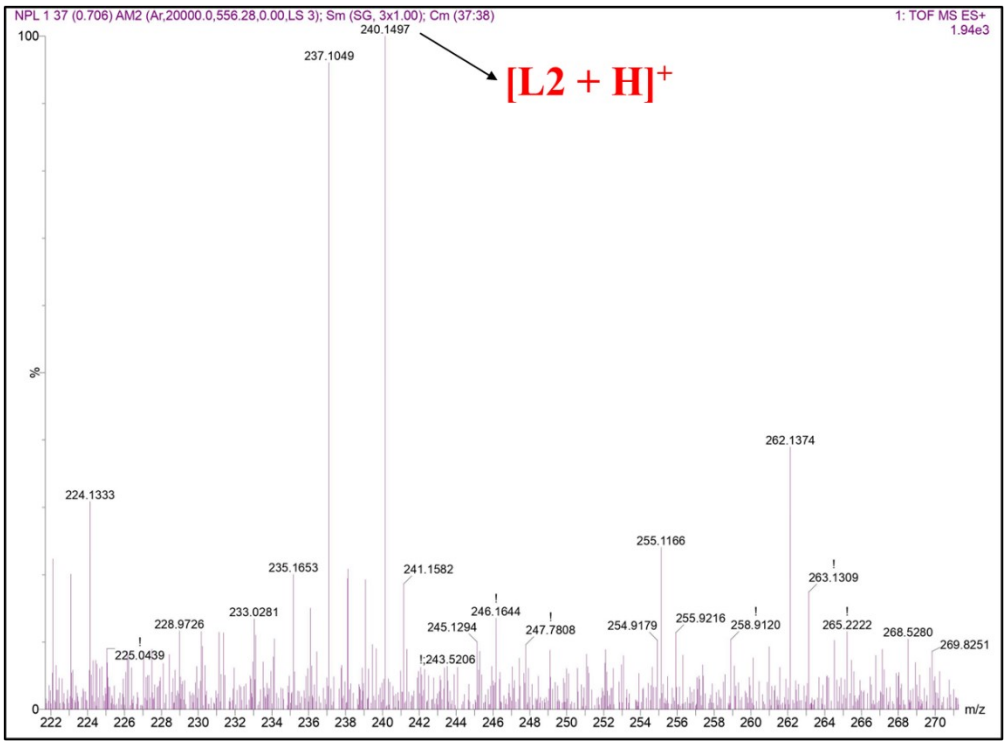


Fig. S6 High Resolution Mass Spectrum of **L2** in methanol solution.

Figure S7 and S8

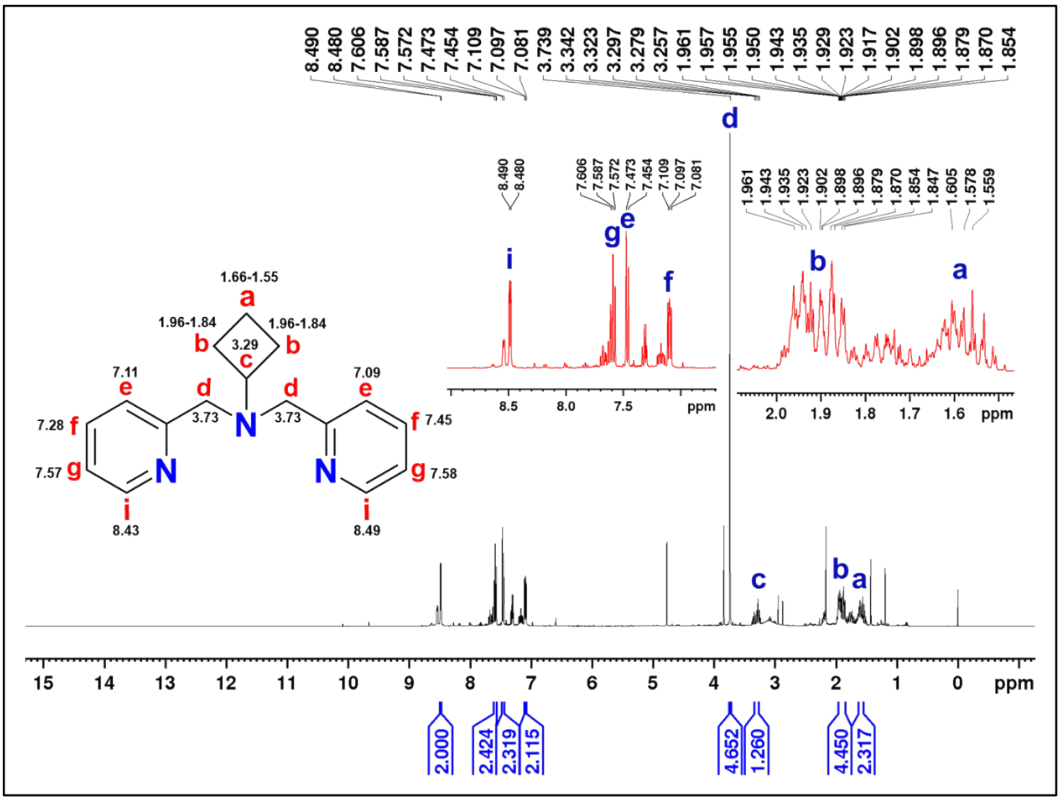


Fig. S7 ^{1}H NMR spectrum of **L3** in $CDCl_3$ at 298 K.

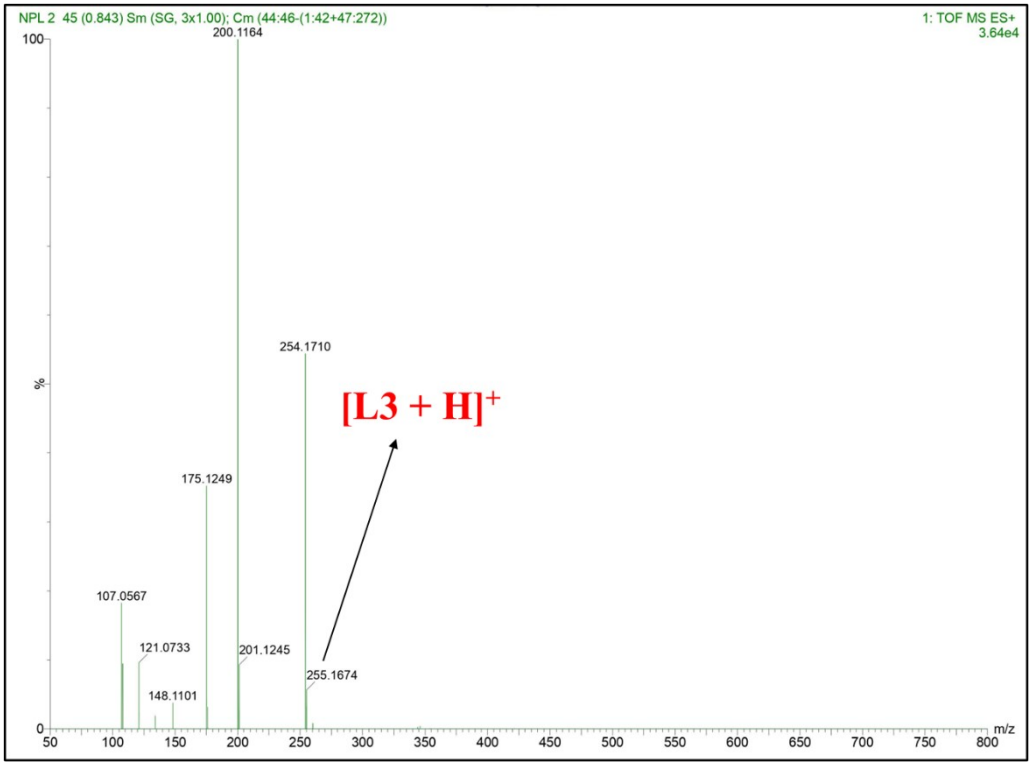


Fig. S8 High Resolution Mass Spectrum of **L3** in methanol solution.

Figure S9 and S10

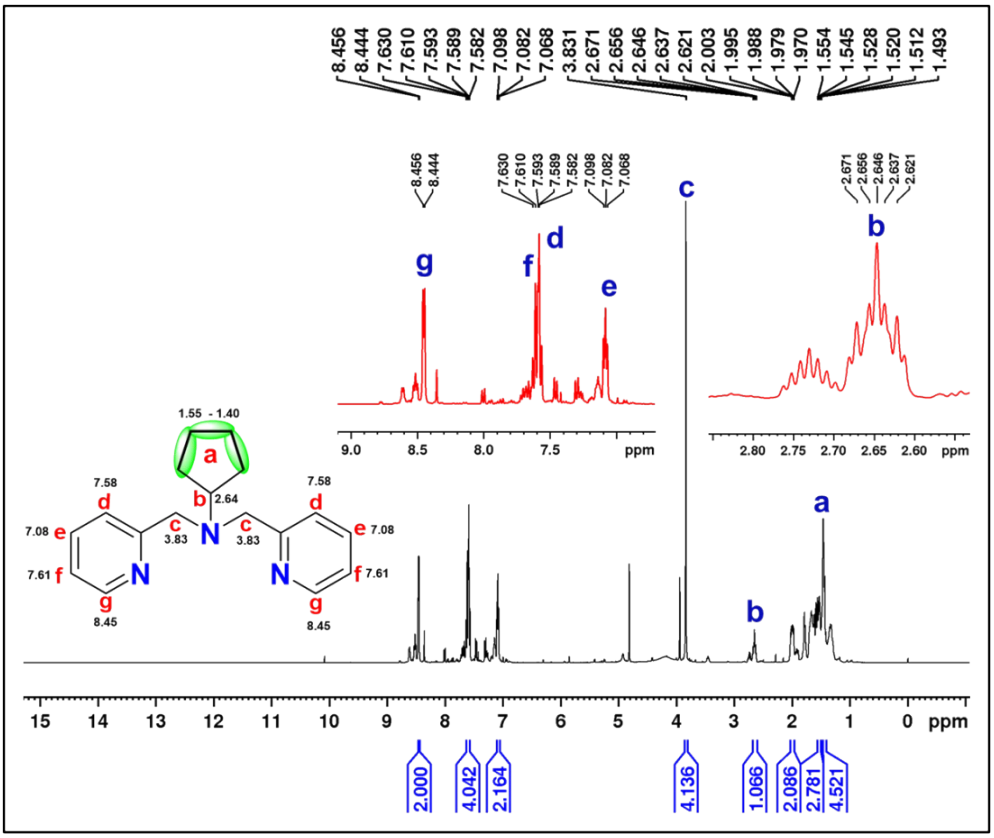
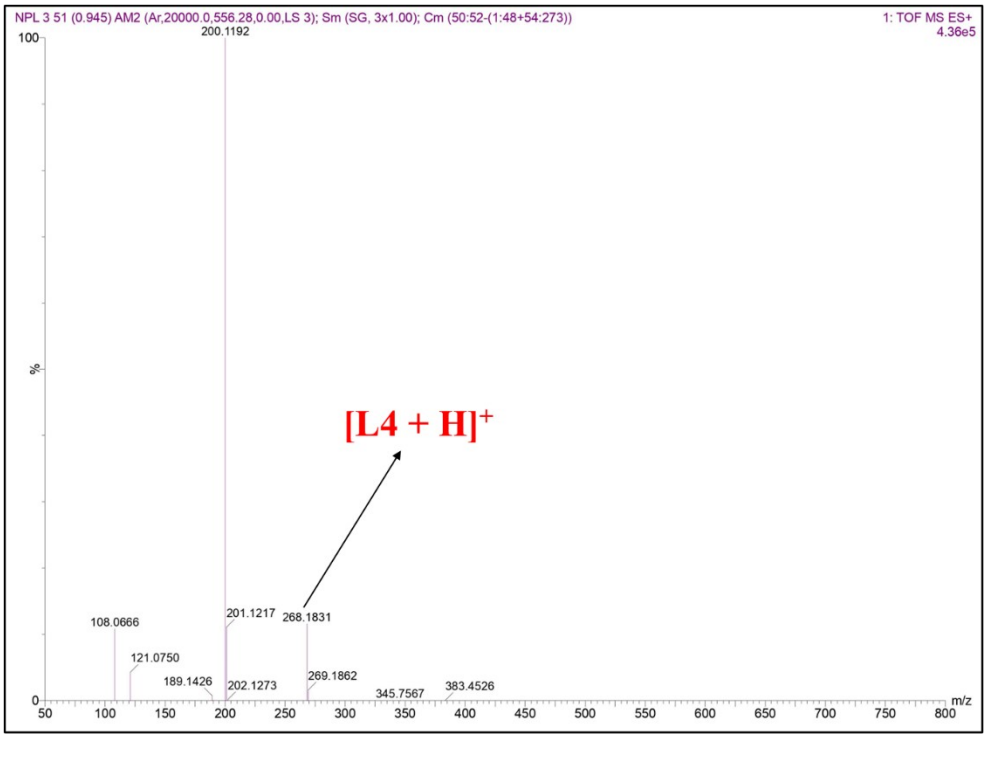


Fig. S9 ^{1}H



NMR spectrum of **L4** in $CDCl_3$ at 298 K.

Fig. S10 High Resolution Mass Spectrum of **L4** in methanol solution.

Figure S11 and S12

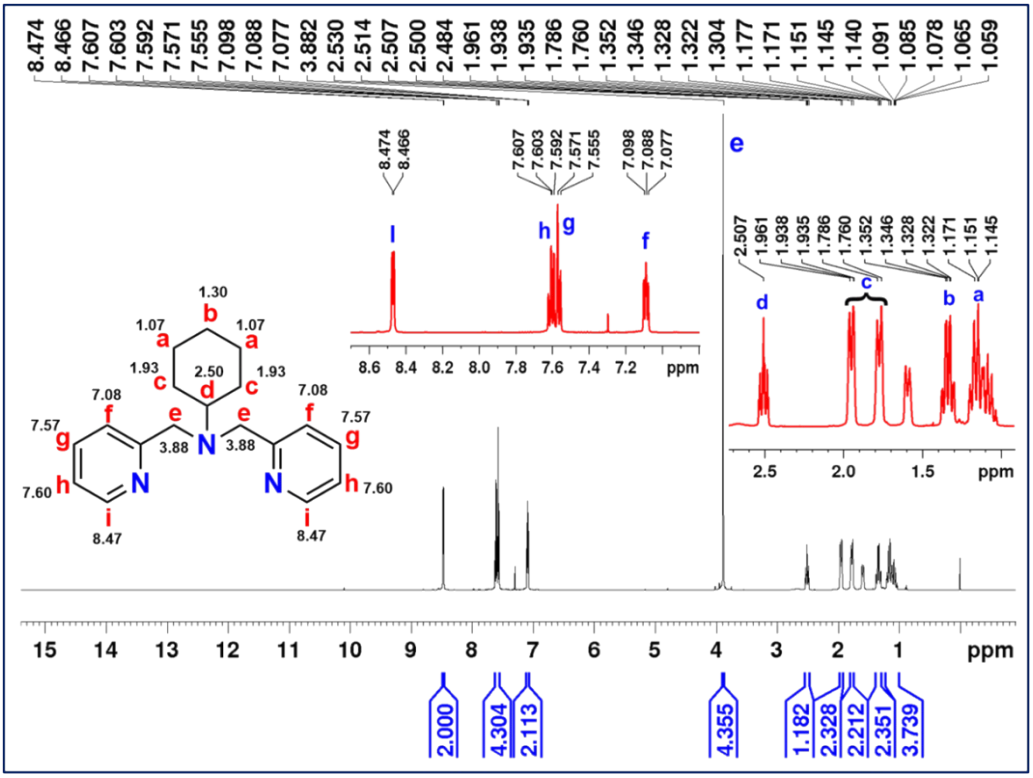


Fig. S11 ^{1}H NMR spectrum of **L5** in $CDCl_3$ at 298 K.

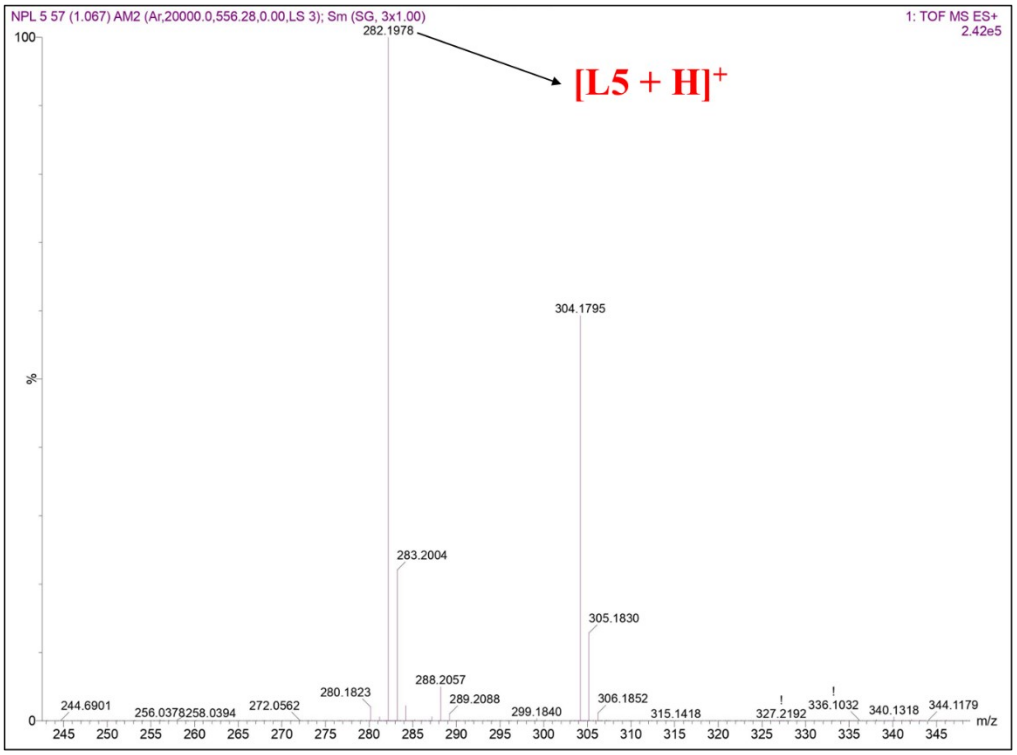


Fig. S12 High Resolution Mass Spectrum of **L5** in methanol solution.

Figure S13 and S14

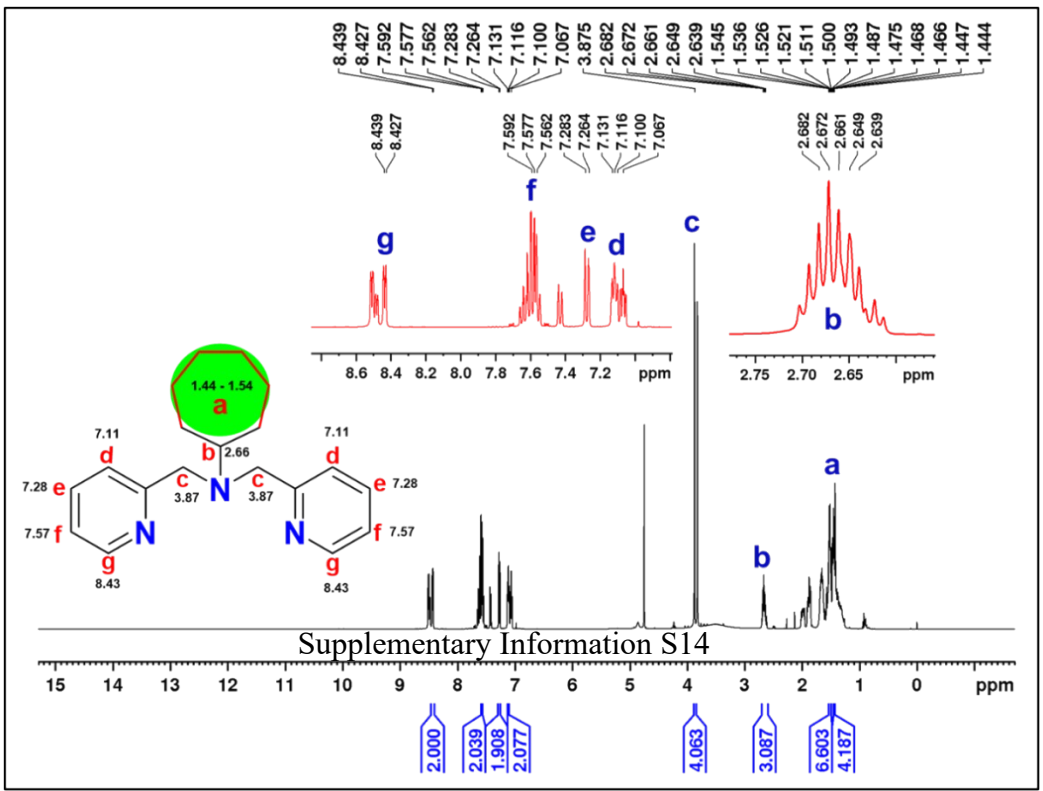


Fig. S13 ^{1}H NMR spectrum of **L6** in $CDCl_3$ at 298 K.

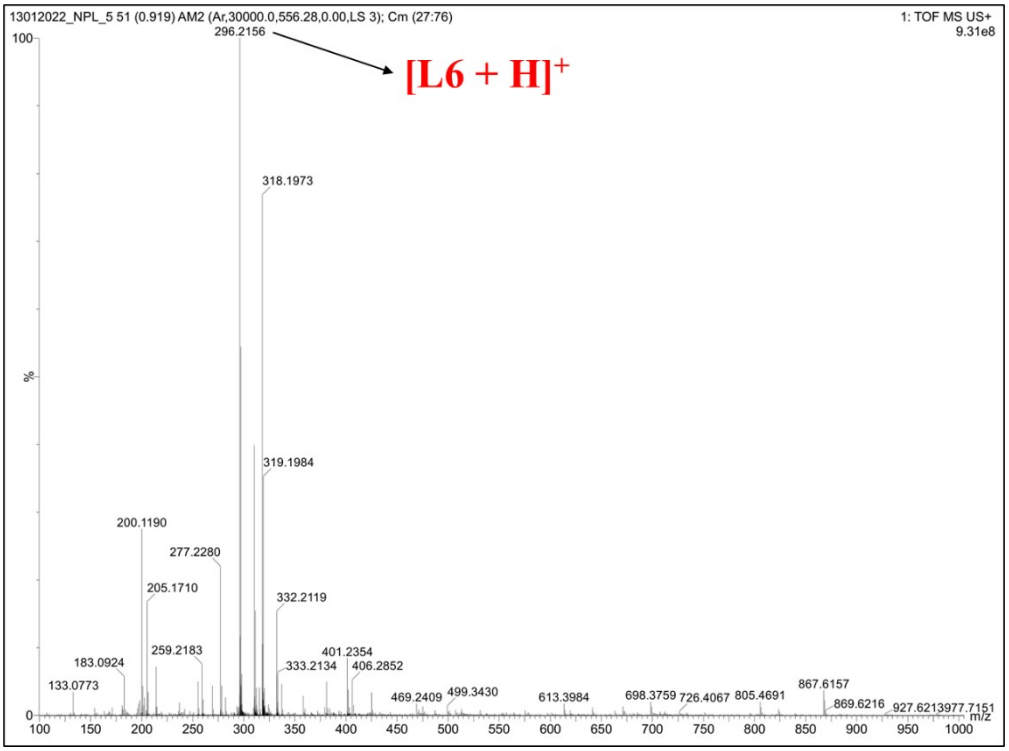


Fig. S14 High Resolution Mass Spectrum of **L6** in methanol solution.

Table S3

Table S3. Selected crystallographic data for ligand **L5**.

Compound	**L5**
CCDC	2430690
Formula	$C_{18}H_{23}N_3$
Formula weight	281.39
Temperature, K	110.0
Wavelength, Å	1.54178
Crystal system	Monoclinic
Space group	C1*c*1
a/Å	6.2324(4)
b/Å	18.1633(11)
c/Å	c = 14.3366(9)
α /°	90
B /°	102.317(2)
γ /°	90
Volume Å^3	1585.56(17)
Z	4
Density, Mg/m^3	1.179
Absorption coefficient, mm^{-1}	0.543
F(000)	608
Crystal size, mm^3	0.349 x 0.217 x 0.25
Theta range for data collection	4.869 to 62.387°
Index ranges	-6<=h<=6, -20<=k<=20, -16<=l<=16
Reflections collected	18558
Independent reflections	2445 [R(int) = 0.0365]
Completeness to theta = 25.242°	98.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4628 and 0.3837
Data / restraints / parameters	2445 / 2 / 190
Goodness[c]-of-fit on F^2	1.092
[a]R_1, [b]wR_2	0.0271, 0.0624
R indices (all data)	R_1 = 0.0286, wR_2 = 0.0635
Extinction coefficient	n/a
e.Å^{-3}	0.112, -0.151

[a]$R_1 = \sum||F_o| - |F_c||/\sum|F_o|$.[b] $wR_2(F_o^2) = [\sum[w(F_o^2 - F_c^2)^2 / \sum wF_o^4]^{1/2}$.[c] GOF = $\sum[w(F_o^2 - F_c^2)^2 /(N_{obs} - N_{params})]^{1/2}$.

Table S4

Table S4. The selected bond length [Å] and bond angle [˚] for ligand **L5**. Highlighted data are indicating lowest to highest of bond length [Å] and bond angle [˚]

Ligand L5	
Bond length [Å]	
N(1)–C(1)	1.466(3)
N(1)–C(7)	1.461(3)
N(1)–C(13)	1.481(3)
N(2)–C(2)	1.338(3)
N(2)–C(6)	1.342(3)
N(3)–C(8)	1.343(3)
N(3)–C(12)	1.344(3)
Bond Angle [˚]	
C(1)–N(1)–C(13)	114.13(15)
C(7)–N(1)–C(1)	110.26(15)
C(7)–N(1)–C(13)	112.09(15)
C(2)–N(2)–C(6)	117.05(19)
C(8)–N(3)–C(12)	117.37(18)

Figure S15

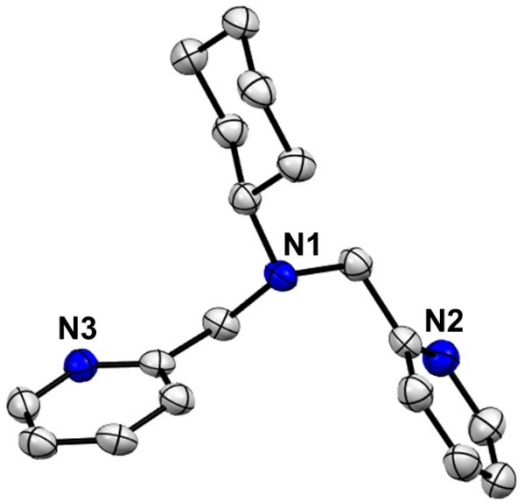


Fig. S15 ORTEP diagram of ligand **L5** showing 50% probability thermal ellipsoids and labeling scheme for selected atoms. All the hydrogen atoms are omitted for better clarity. Only one component of the asymmetric unit is shown.

Crystal description of ligand L5: The molecular structure of the **L5** ligand is displayed in Figure S15. The ligand **L5** keeps one chiral centre, however, the single-center face

Cc space group clearly suggest that the compound crystalize as a racemate. X-ray crystallography indicates that **L5** crystallizes in a trigonal planar monoclinic crystal arrangement with the space group *Cc* and cell parameters: a = 6.2324(4) Å, b = 18.1633(11) Å, c = 14.3366(9) Å, α = 90˚, β = 102.317(2)˚, γ = 90˚ (Table S3), and the crystal structure of **L5** is oblique, with selected bond distances and angle are provided in Table S4. The pyridine nitrogen bond lengths (N(2)–C(2), 1.338(3) Å; N(3)–C(8), 1.343(3) Å) are shorter than the tertiary amine nitrogen bond lengths (N(1)–C(1), 1.466(3) Å, N(1)–C(7), 1.461(3) Å, N(1)–C(13), 1.481(3) Å) due to the π-electron delocalization in the pyridine ring system. The bond angle around tertiary amine nitrogen are C(1)–N(1)–C(13): 114.13(15) Å, C(7)–N(1)–C(1): 110.26(15) Å, and C(7)–N(1)–C(13): 112.09(15) Å. Overall, all the C–N bond distances and C–N–C bond angle are different, clearly demonstrating the influence of bond pair-lone pair repulsion in pyridine nitrogen and tertiary amine in **L5**.

Figure S16

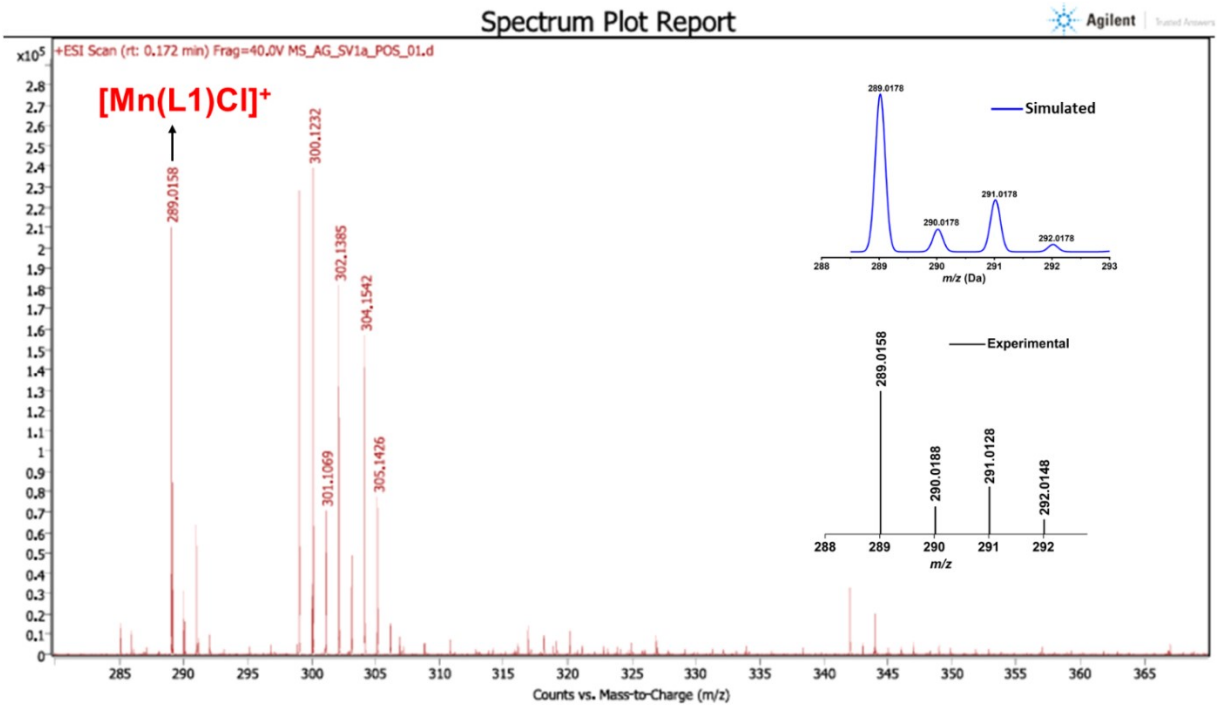


Fig. S16 High Resolution Mass Spectrum of the $[Mn^{II}(L1)Cl]^+$ ion for complex **1** recorded in methanol solution (1×10^{-3} M). The blue trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak at *m/z* 289.0158.

Figure S17

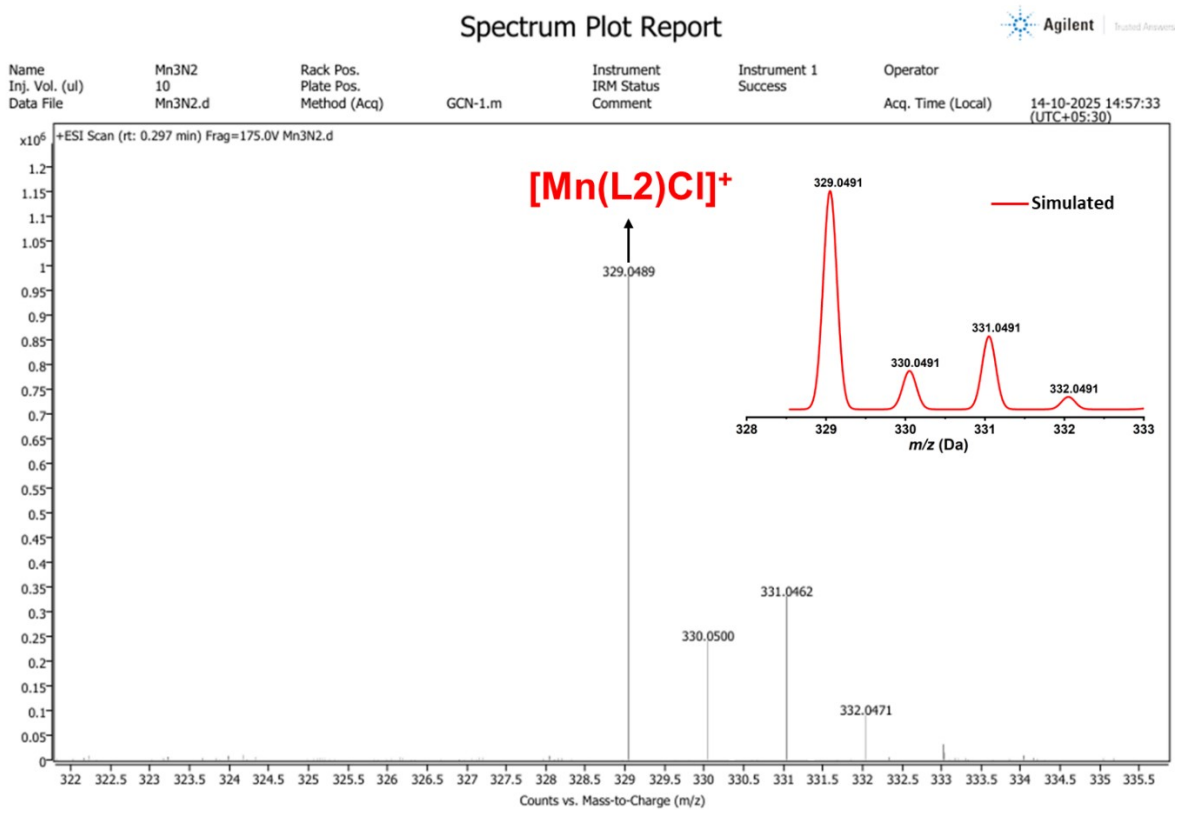


Fig. S17 High Resolution Mass Spectrum of the $[Mn^{II}(L2)Cl]^+$ ion for complex **2** recorded in methanol solution (1×10^{-3} M). The red trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak at *m/z* 329.0489.

Figure S18

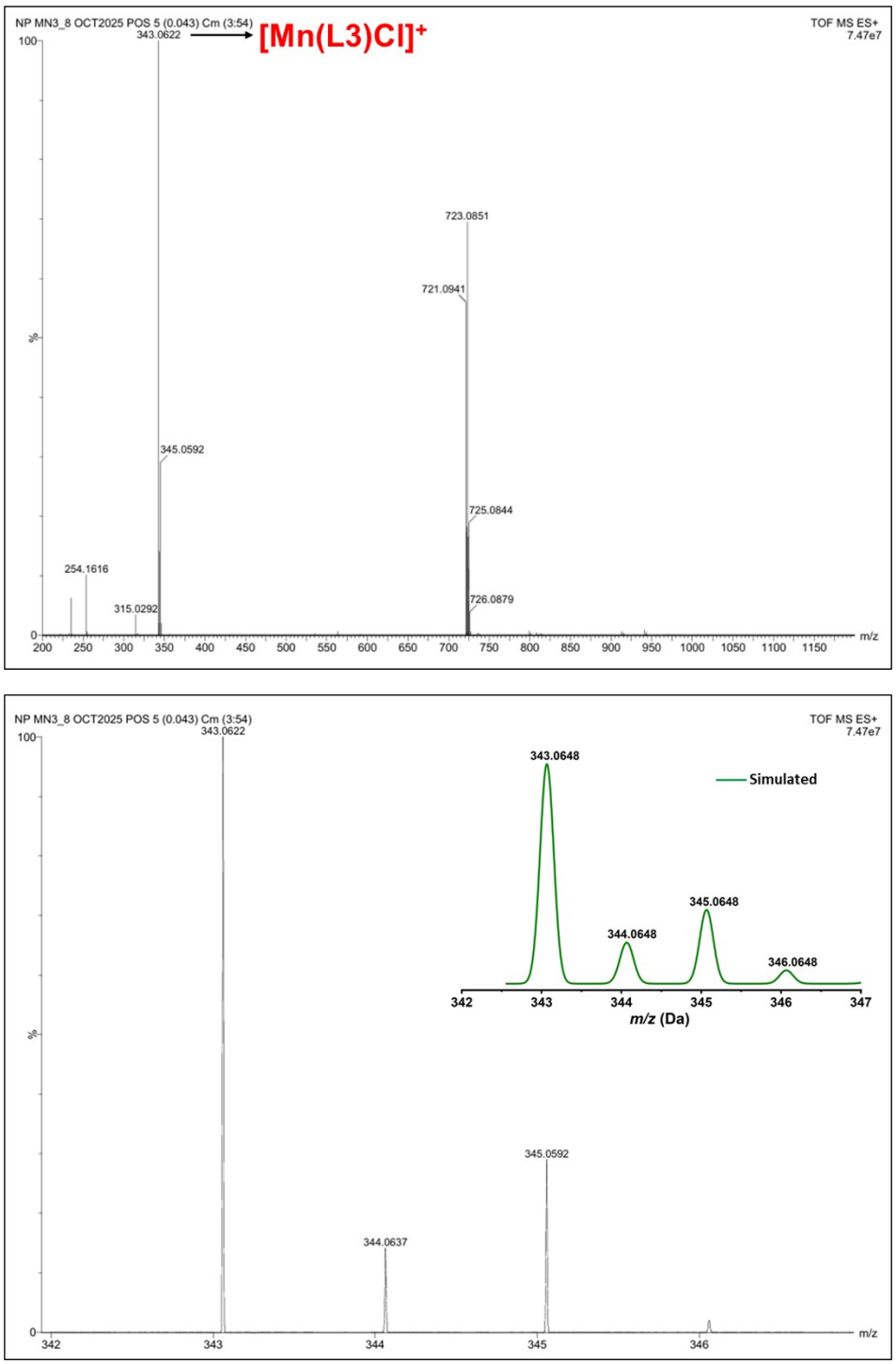


Fig. S18 High Resolution Mass Spectrum of the $[Mn^{II}(L3)Cl]^+$ ion for complex **3** recorded in methanol solution (1×10^{-3} M). The green trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak at *m/z* 343.0622.

Figure S19

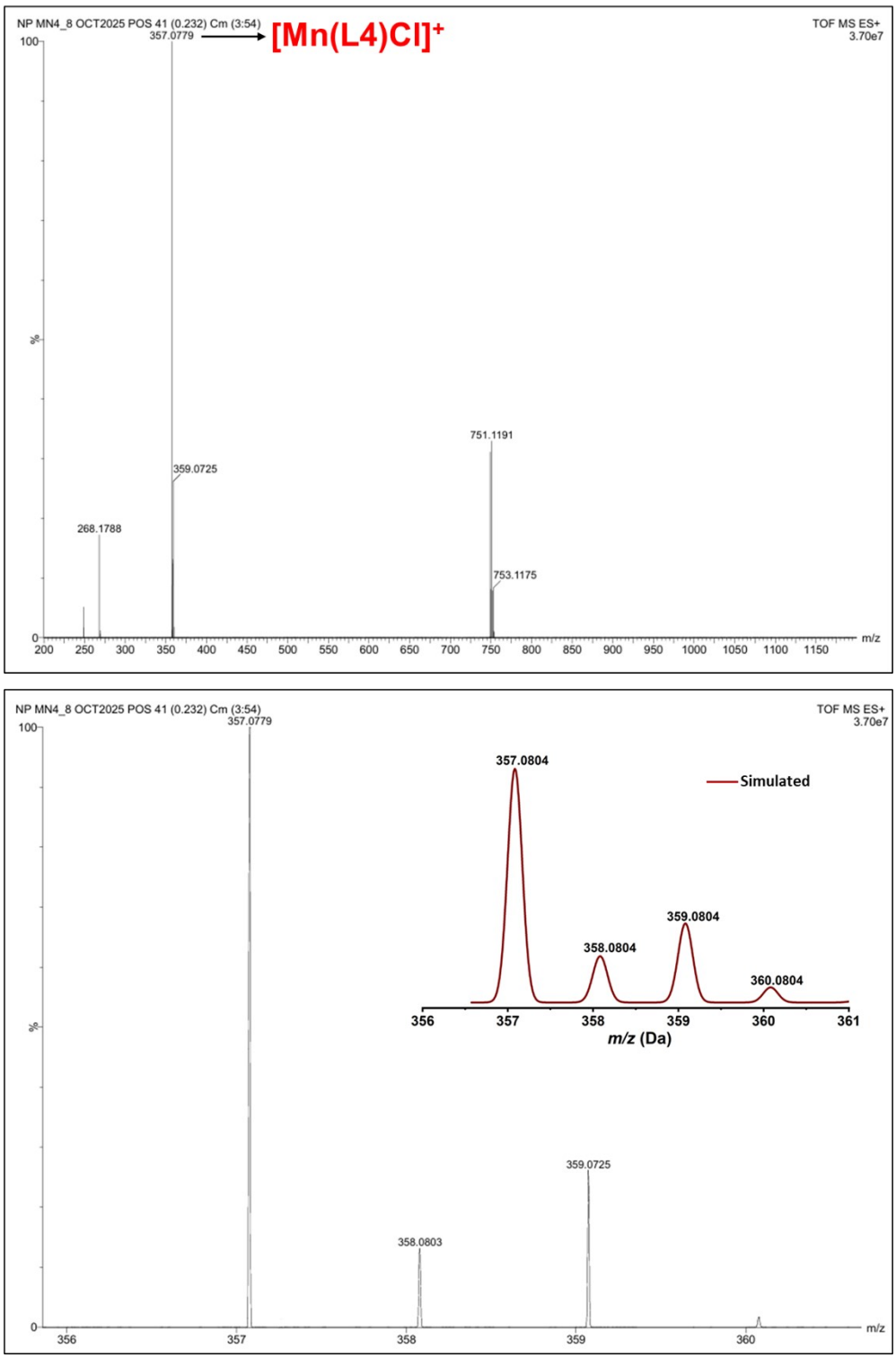


Fig. S19 High Resolution Mass Spectrum of the $[Mn^{II}(L4)Cl]^+$ ion for complex **4** recorded in methanol solution (1×10^{-3} M). The brown trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak at *m/z* 357.0779.

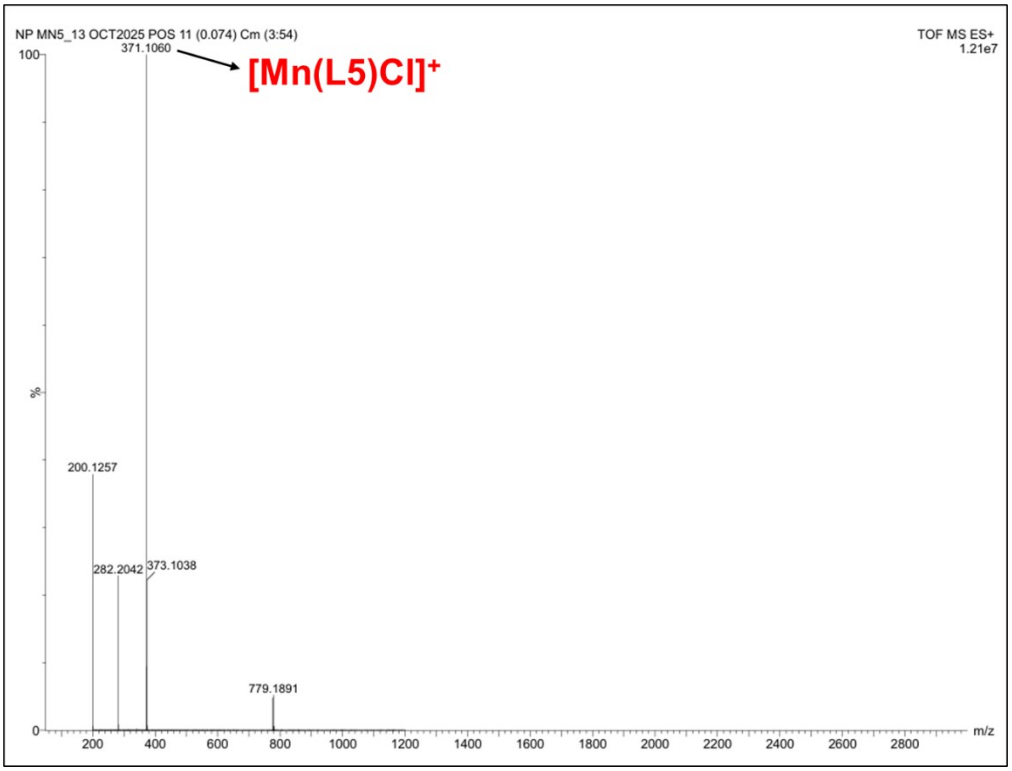

NP MN5_13 OCT2025 POS 11 (0.074) Cm (3:54)
TOF MS ES+
1.21e7
371.1060
[Mn(L5)Cl]+
200.1257
282.2042
373.1038
779.1891
m/z

Figure S20

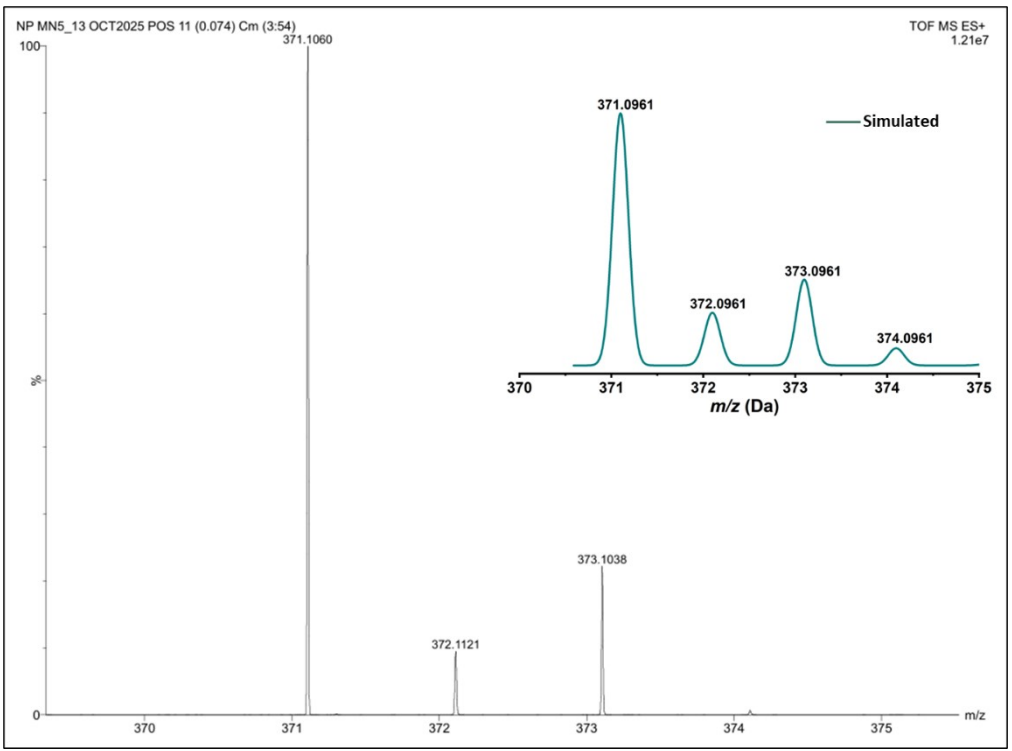

NP MN5_13 OCT2025 POS 11 (0.074) Cm (3:54)
TOF MS ES+
1.21e7
371.1060
371.0961
Simulated
372.0961
373.0961
374.0961
m/z (Da)
373.1038
372.1121
m/z

Fig. S20 High Resolution Mass Spectrum of the $[Mn^{II}(L5)Cl]^+$ ion for complex **5** recorded in methanol solution (1×10^{-3} M). The teal trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak observed at *m/z* 371.1060.

Figure S21

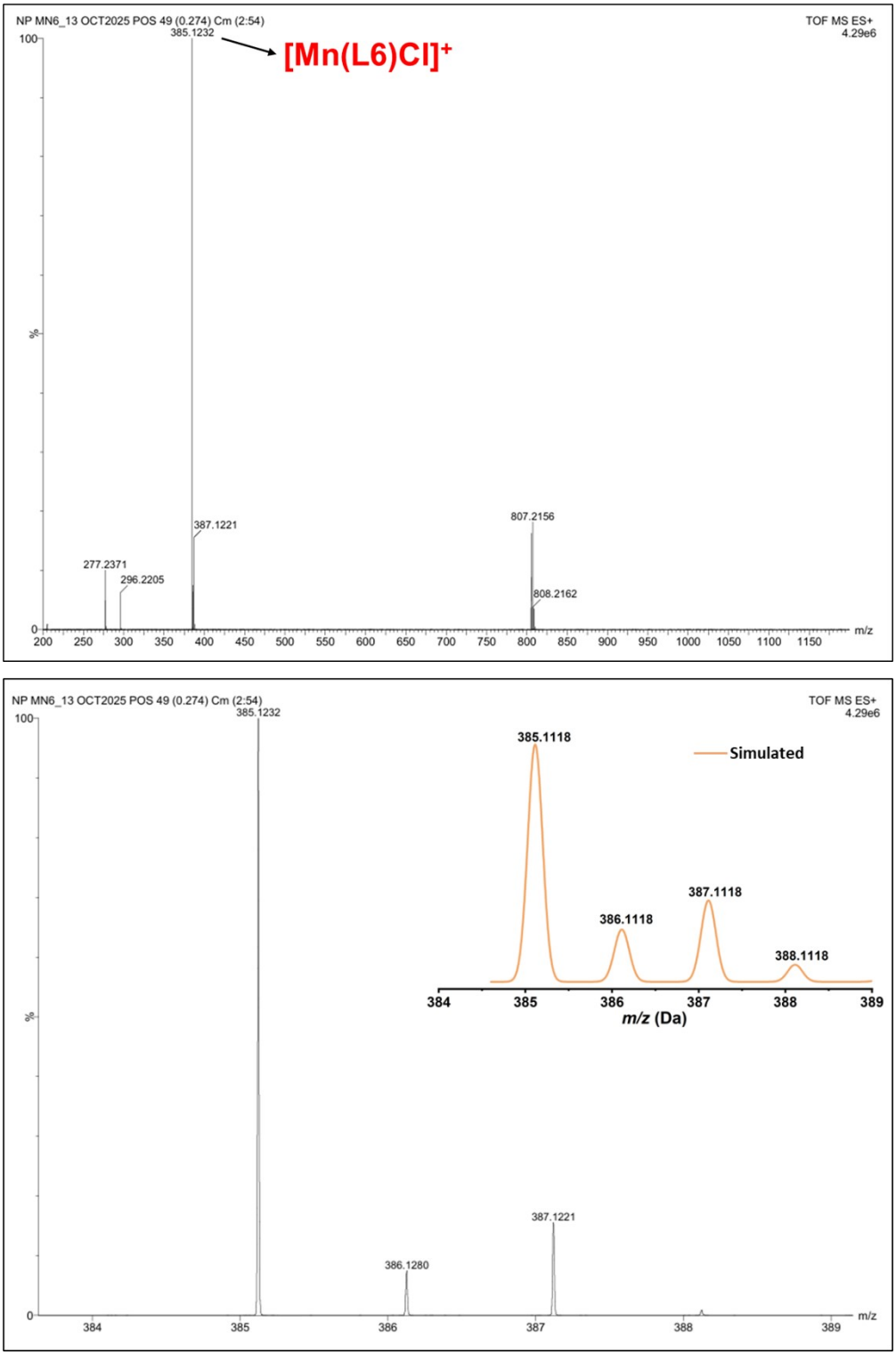


Fig. S21 High Resolution Mass Spectrum of the $[Mn^{II}(L6)Cl]^+$ ion for complex **6** recorded in methanol solution (1×10^{-3} M). The orange trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak observed at *m/z* 385.1232.

Figure S22

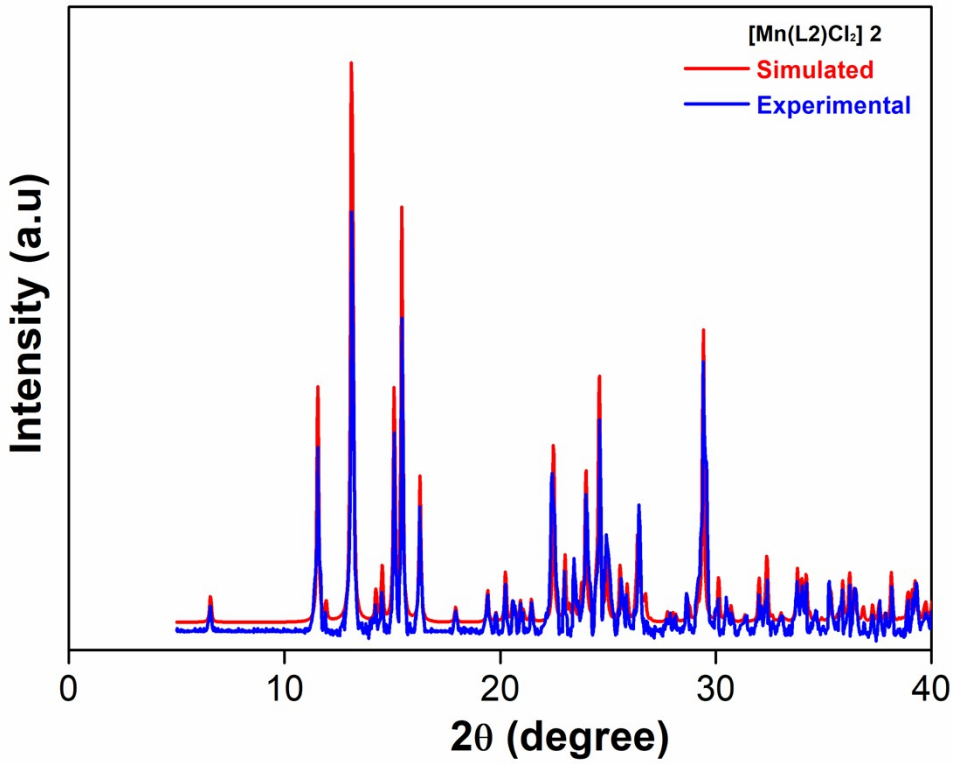


Fig S22. Experimental X-ray powder diffraction pattern (blue line) of manganese(II) complex **2** compared with the simulated XRPD pattern (red line).

Figure S23

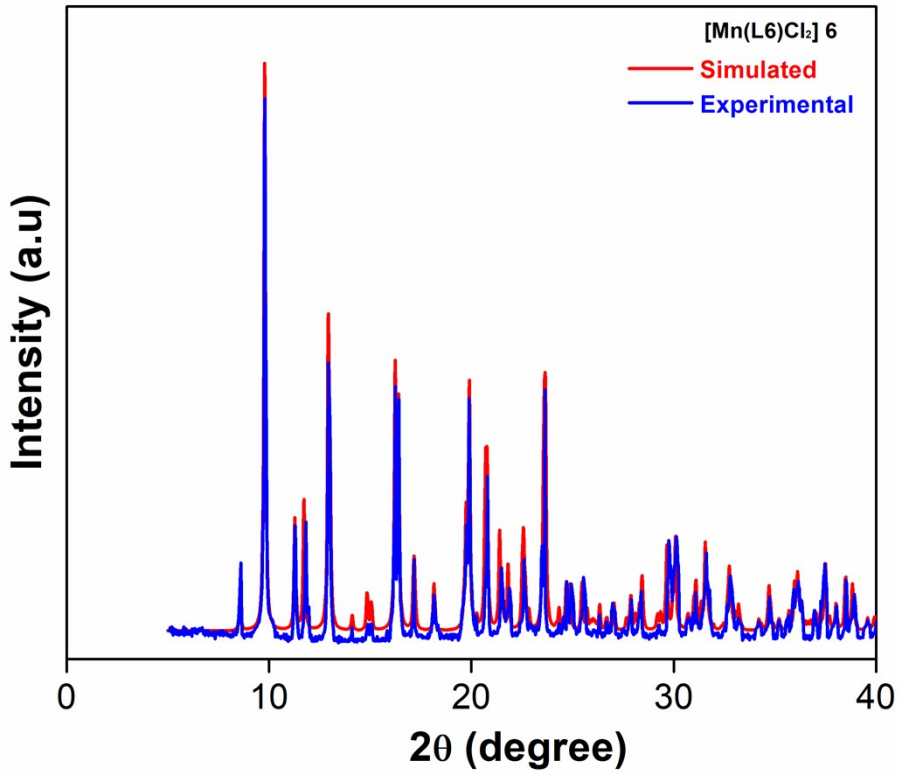


Fig S23. Experimental X-ray powder diffraction pattern (blue line) of manganese(II) complex **6** compared with the simulated XRPD pattern (red line).

Figure S24

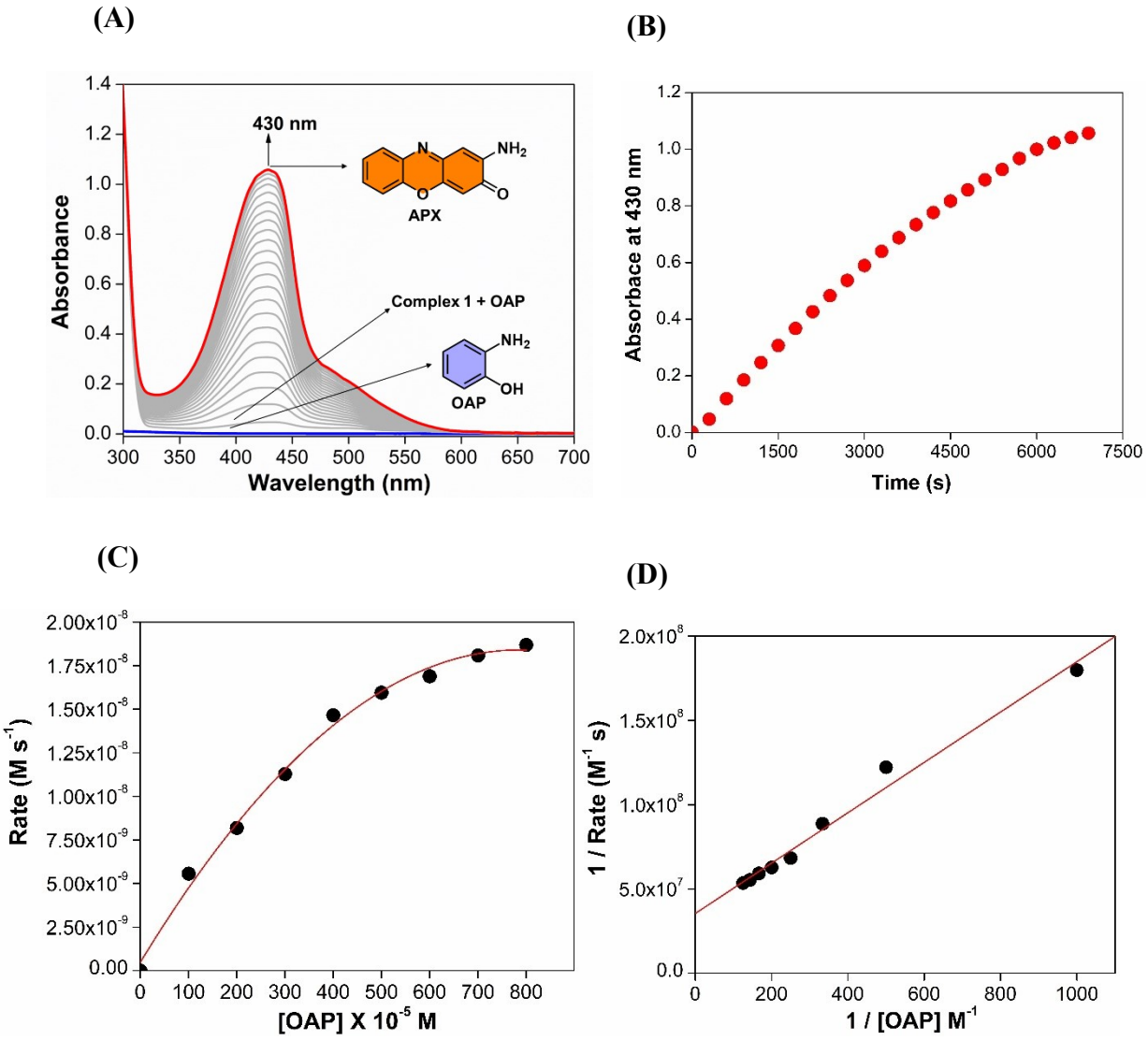


Fig. S24 (A) UV-vis spectral scans for biomimetic oxidation of OAP (1.0×10^{-3} M to 8.0×10^{-3} M in O_2 saturated methanol at 25 ˚C, increase the 2-aminophenoxazine-3-one product at 430 nm for the fixed concentration (1.0×10^{-5} M) of complex **1**. (B) Time trace. (C) Michaelis-Menten plot. (D) Lineweaver-Burk plot.

Figure S25

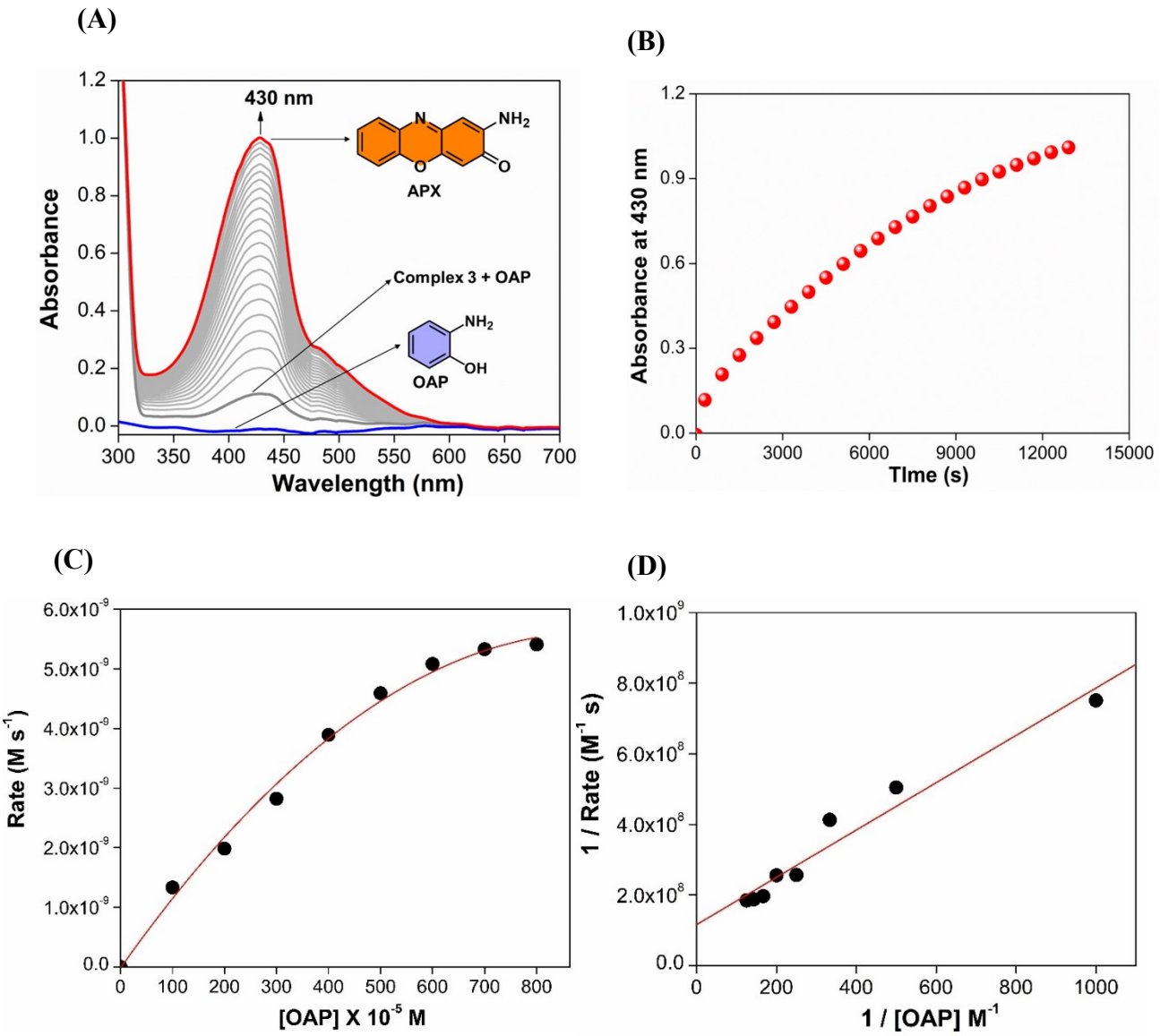


Fig. S25 (A) UV-vis spectral scans for biomimetic oxidation of OAP (1.0×10^{-3} M to 8.0×10^{-3} M in O_2 saturated methanol at 25 ˚C, increase the 2-aminophenoxazine-3-one product at 430 nm for the fixed concentration (1.0×10^{-5} M) of complex **3**. (B) Time trace. (C) Michaelis-Menten plot. (D) Lineweaver-Burk plot.

Figure S26

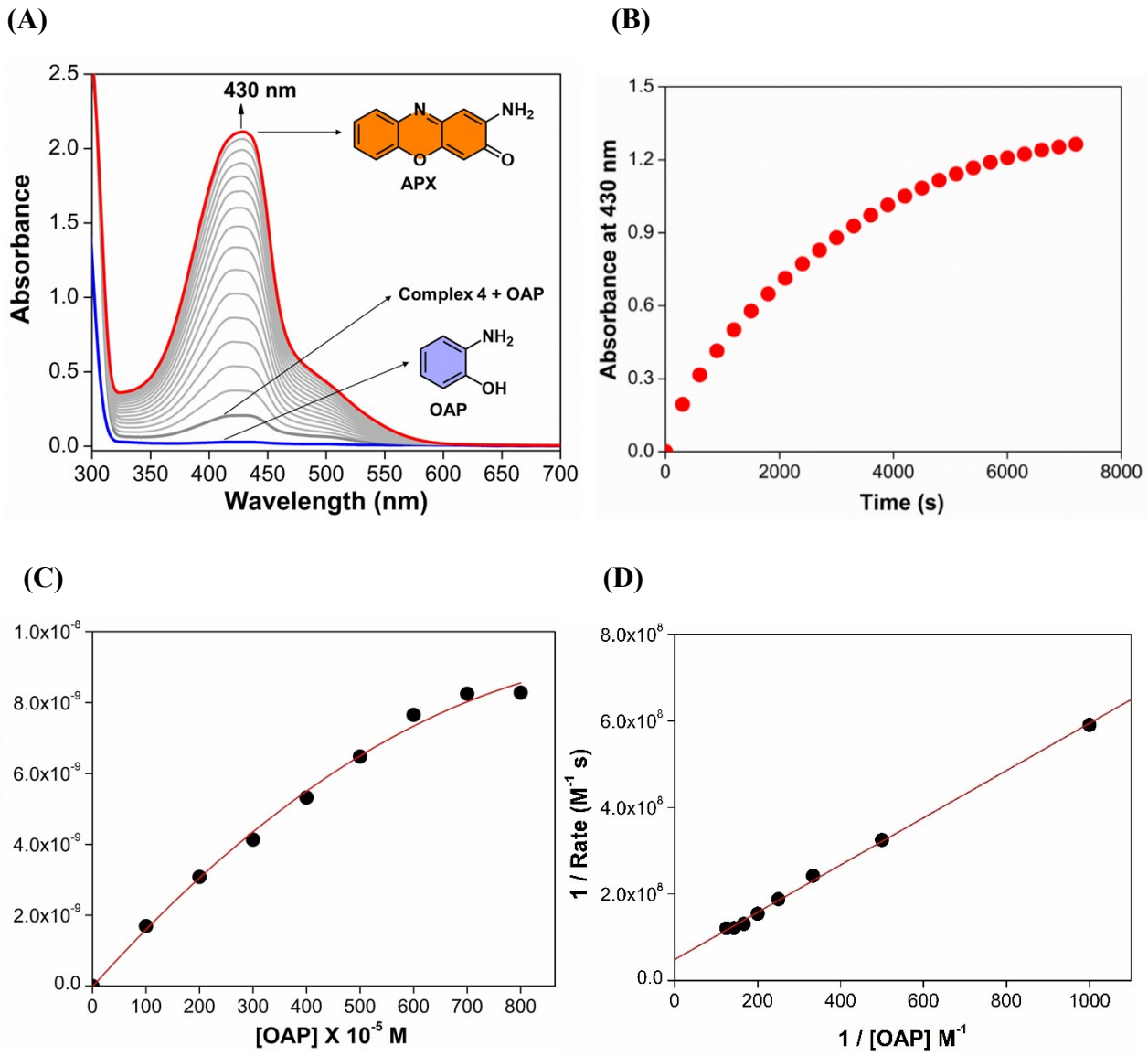


Fig. S26 (A) UV-vis spectral scans for biomimetic oxidation of OAP (1.0×10^{-3} M to 8.0×10^{-3} M in O_2 saturated methanol at 25 ˚C, increase the 2-aminophenoxazine-3-one product at 430 nm for the fixed concentration (1.0×10^{-5} M) of complex **4**. (B) Time trace. (C) Michaelis-Menten plot. (D) Lineweaver-Burk plot.

Figure S27

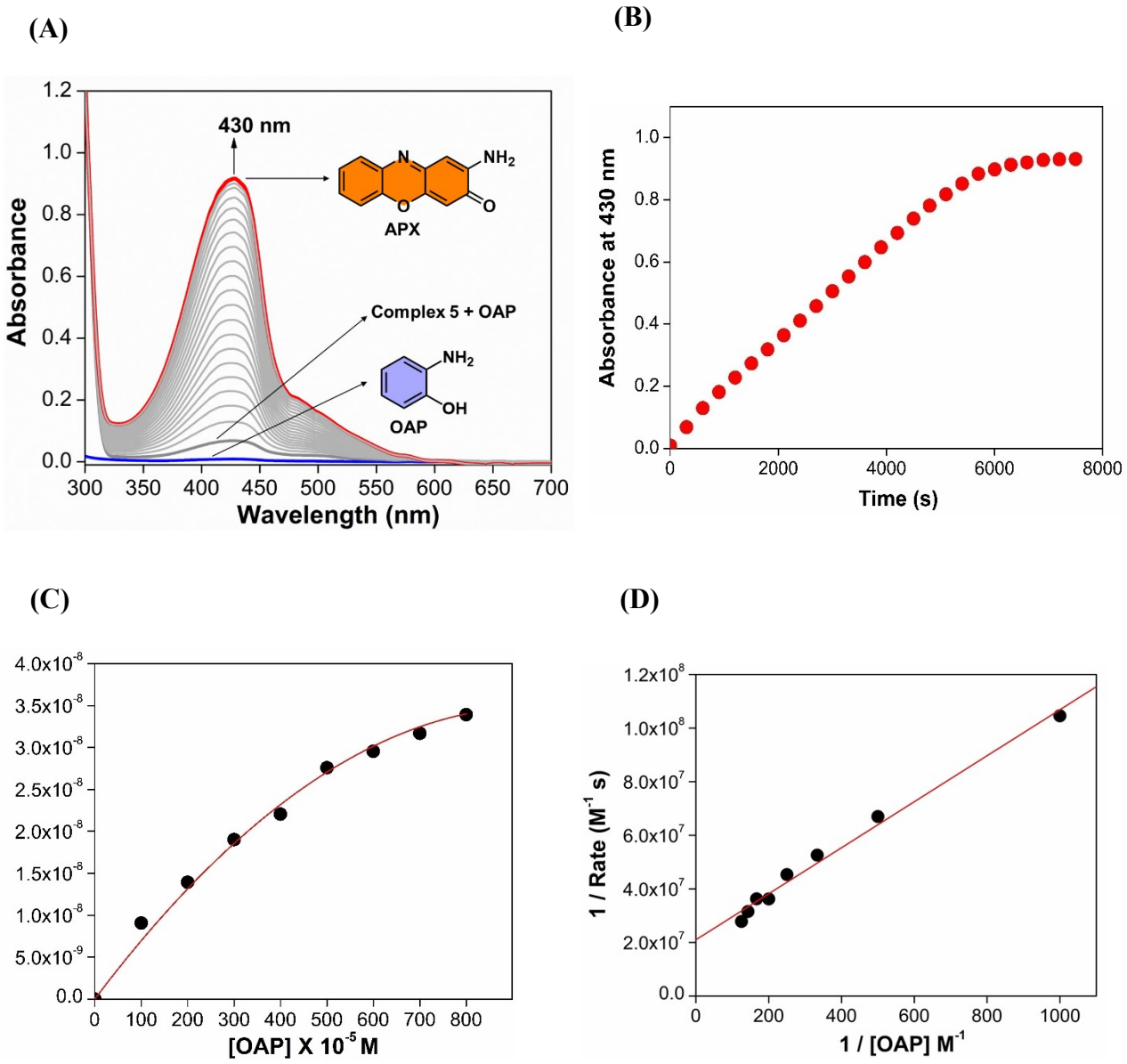


Fig. S27 (A) UV-vis spectral scans for biomimetic oxidation of OAP (1.0×10^{-3} M to 8.0×10^{-3} M in O_2 saturated methanol at 25 ˚C, increase the 2-aminophenoxazine-3-one product at 430 nm for the fixed concentration (1.0×10^{-5} M) of complex **5**. (B) Time trace. (C) Michaelis-Menten plot. (D) Lineweaver-Burk plot.

Figure S28

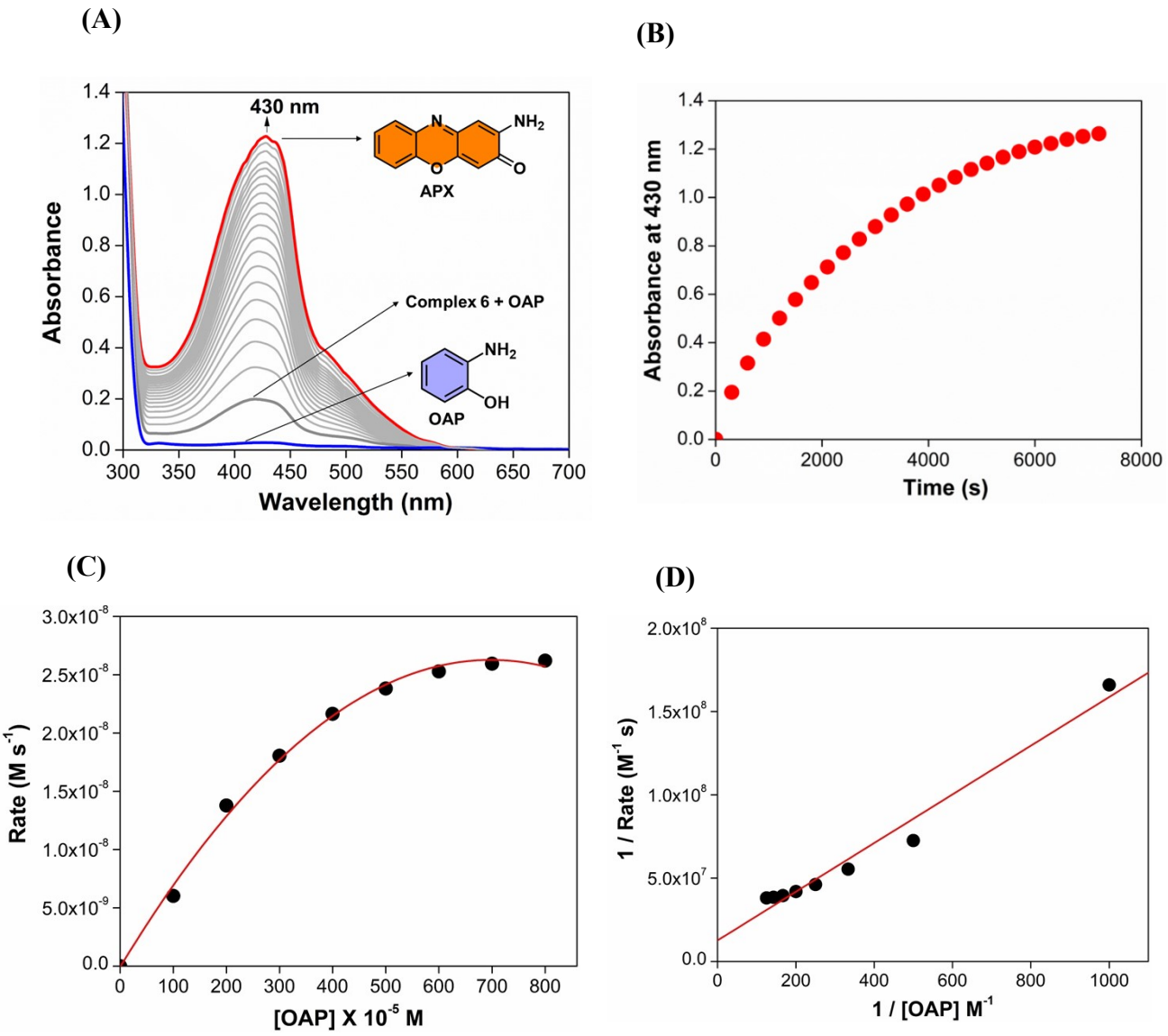


Fig. S28 (A) UV-vis spectral scans for biomimetic oxidation of OAP (1.0×10^{-3} M to 8.0×10^{-3} M in O_2 saturated methanol at 25 ˚C, increase the 2-aminophenoxazine-3-one product at 430 nm for the fixed concentration (1.0×10^{-5} M) of complex **6**. (B) Time trace. (C) Michaelis-Menten plot. (D) Lineweaver-Burk plot.

Figure S29

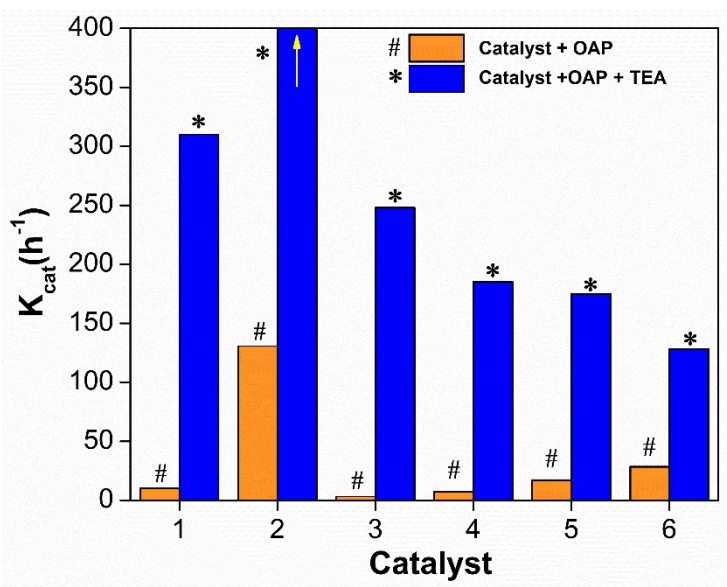


Fig. S29 Comparison of turnover numbers (TON) of oxidative coupling of OAP to APX by manganese(II) complexes **1**–**6** in the presence and absence of base of triethylamine.

Figure S30

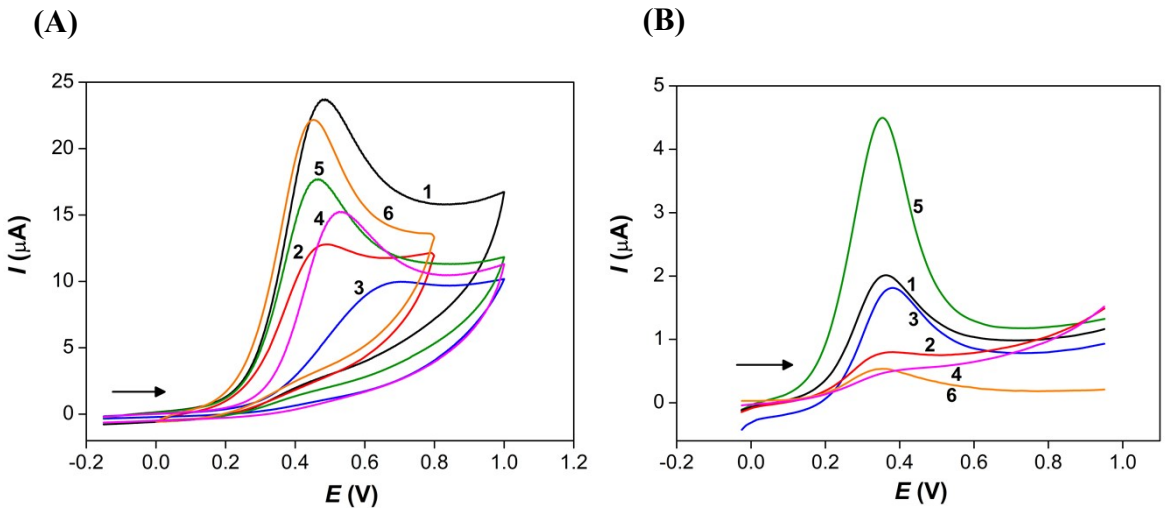


Fig. S30 (A) Cyclic voltammograms of 1 mM manganese(II) complexes **1**–**6** in methanol solution at 25 °C. Supporting electrolyte: 0.1M $TBAPF_6$. Scan Rate 50 mV s^{-1}. (B) Differential pulse voltammograms of $[Mn(L)Cl_2]$ **1**–**6**. Scan Rate: 5 mV s^{-1}.

Figure S31

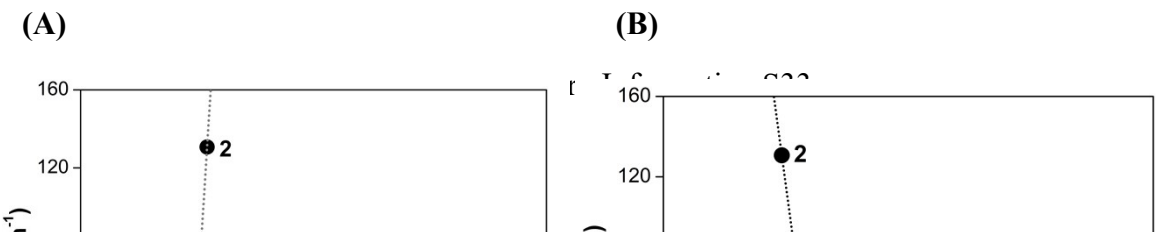


Fig. S31 (A) Correlation plots of $E_{1/2}$ (V) values for [Mn(L)Cl_2] **1**–**6** *vs*. the turnover numbers (k_{cat}, h^{-1}) and (B) $E_{1/2}$ (V) values of [Mn(L)(OAP)] adducts *vs*. the turnover numbers (k_{cat}, h^{-1}).

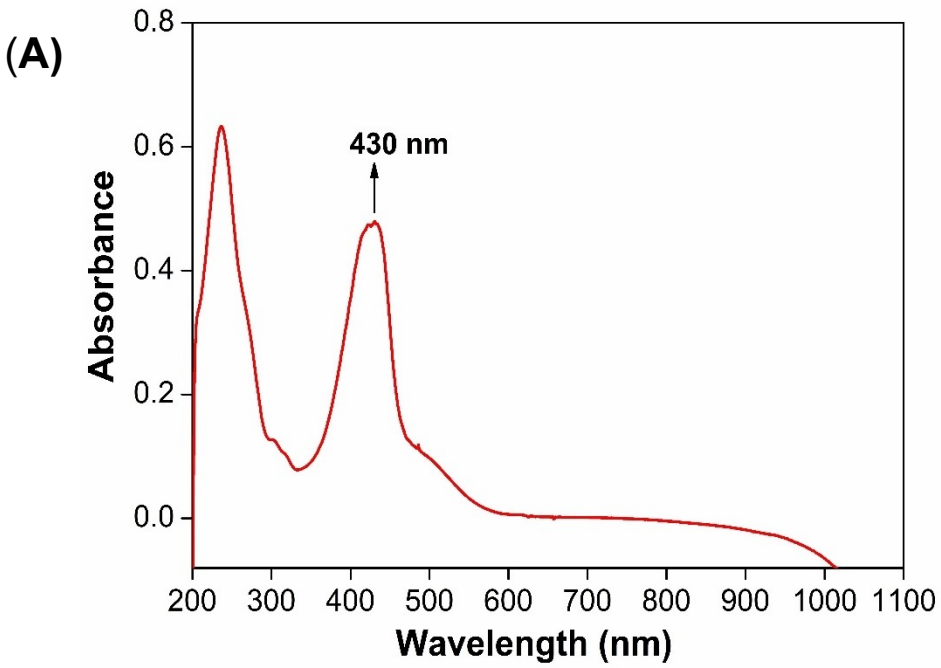


Figure S32

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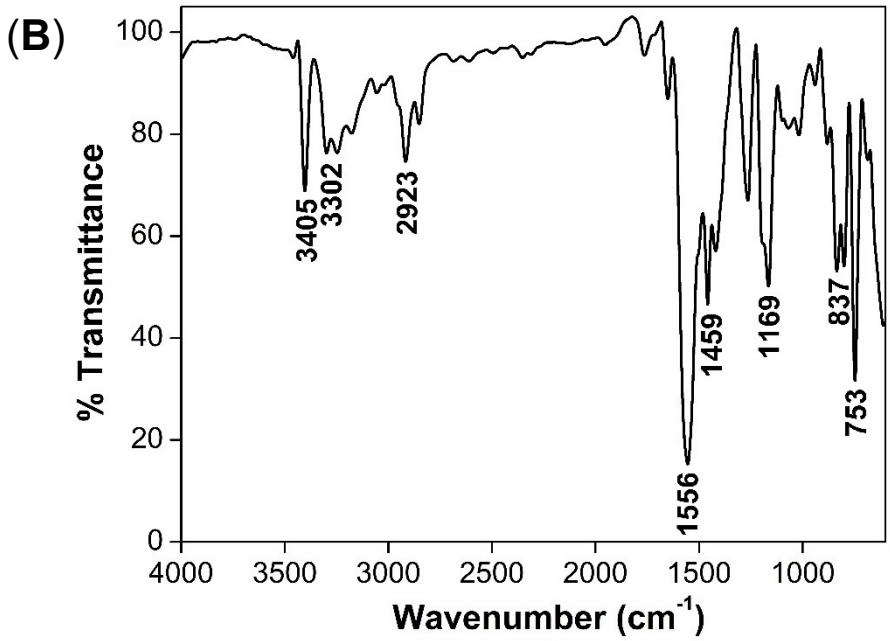


Fig. S32 (A) UV-vis spectrum of isolated product of 2-aminophenoxazine-3-one in methanol at 25 ˚C. (B) ATR-FTIR spectrum of isolated product of the 2-aminophenoxazine-3-one product.

Figure S33 and S34

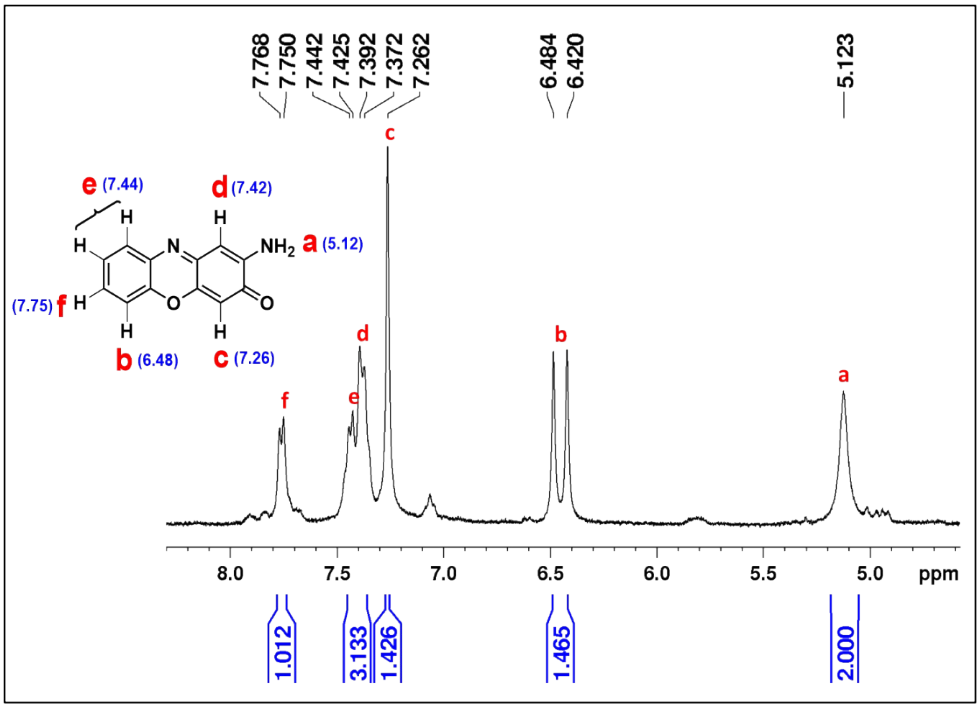


Fig. S33 ^{1}H NMR spectrum of 2-aminophenoxazine-3-one in $CDCl_3$ at 298 K.

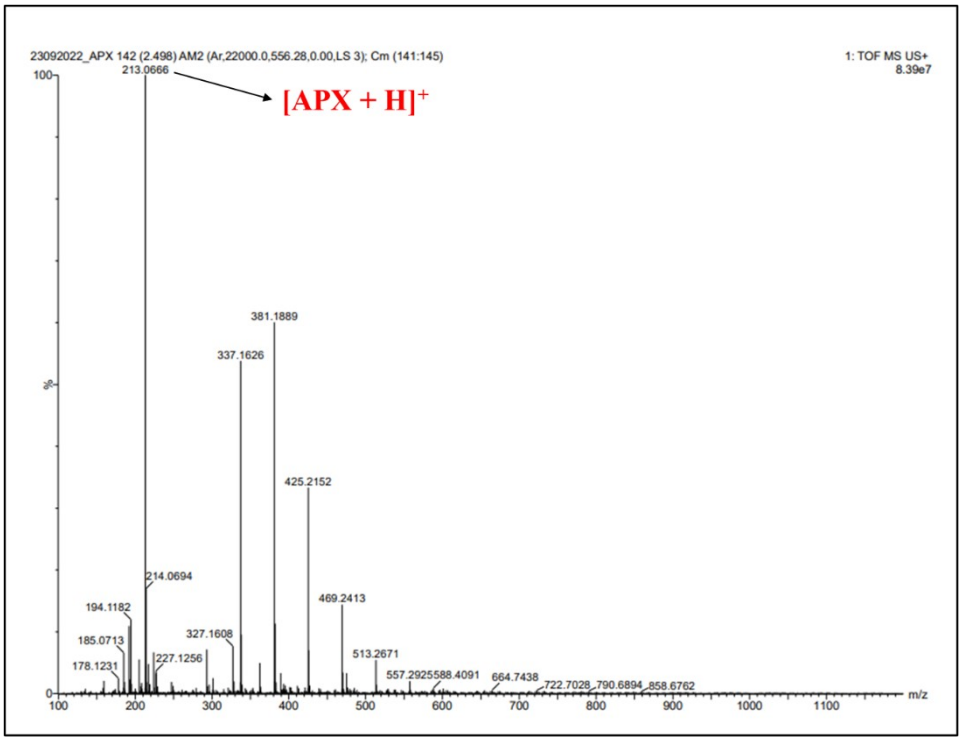


Fig. S34 High Resolution Mass Spectrum of 2-aminophenoxazine-3-one in methanol solution.

Figure S35 **and S36**

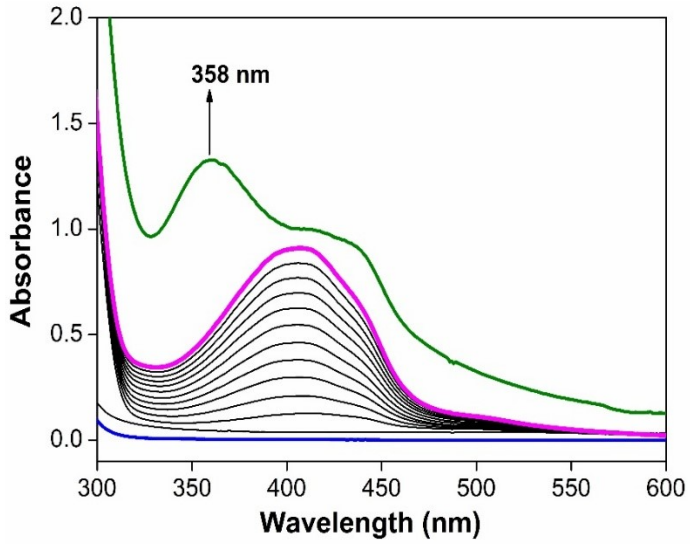
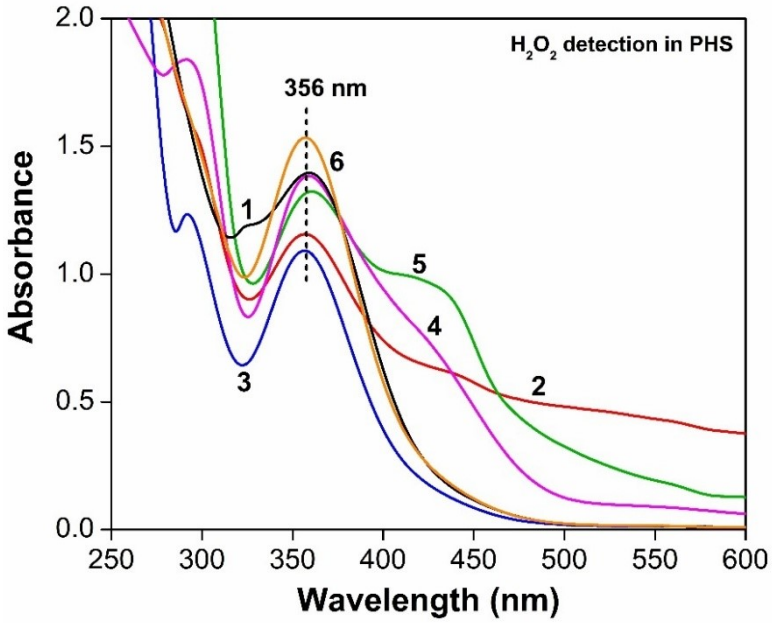


Fig. S35 Detection of H_2O_2 by UV-vis spectroscopy during oxidation of *o*-aminophenol catalysed by complex **5** in O_2 saturated methanol solution.



$$H_2O_2 + 2KI + H_2SO_4 \rightarrow I_2 + K_2SO_4 + 2H_2O$$

$$KI + I_2\,(aq) \rightarrow K^+ + I_3^-$$

Fig. S36 Detection of H_2O_2 by UV-vis spectroscopy during oxidation of *o*-aminophenol catalysed by complexes **1**–**6** in O_2 saturated methanol solution.

Figure S37

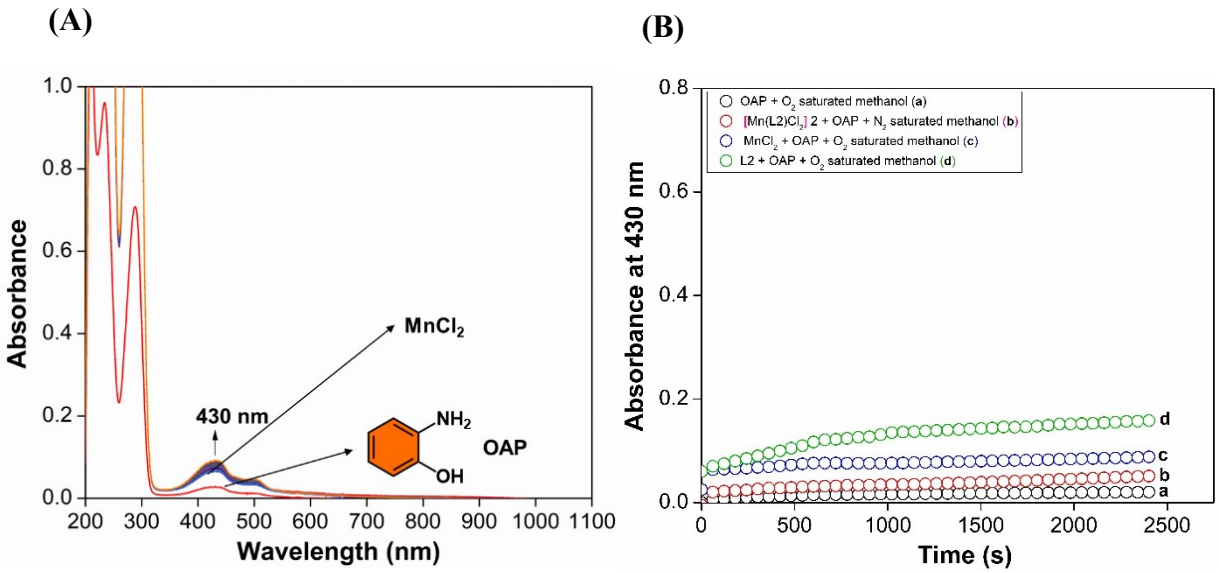


Fig. S37 Control experiment for PHS activity; (A) Oxidation of OAP by $MnCl_2.4H_2O$ salt in dioxygen saturated methanol at room temperature. (B) Time-dependent traces for the reactions: (a) OAP with O_2 saturated methanol, (b) Complex **2** with OAP in N_2-saturated methanol, (c) $MnCl_2.4H_2O$ with OAP in the O_2 saturated methanol and (d) ligand **L2** with OAP in O_2 saturated methanol solution.

Figure S38 and S39

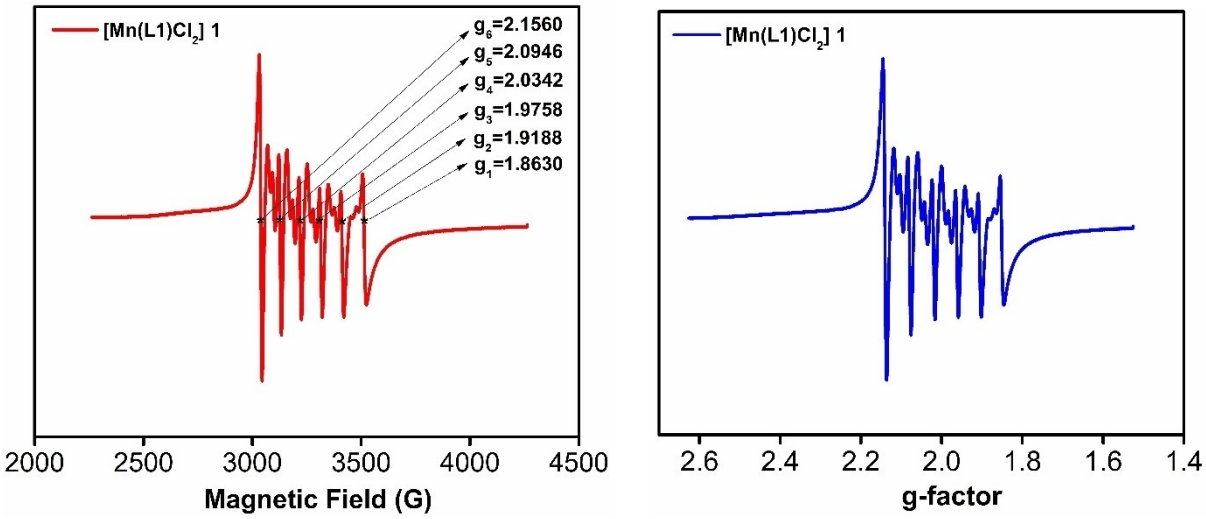


Fig. S38 EPR spectrum complex **1**: Conc.: (3 × 10^{-3} M in methanol at 77 K. Center field: 3250.00 G; Sweep width: 750.00 G; Microwave Frequency: 9.104062 GHz; Power: 0.99800 (mW).

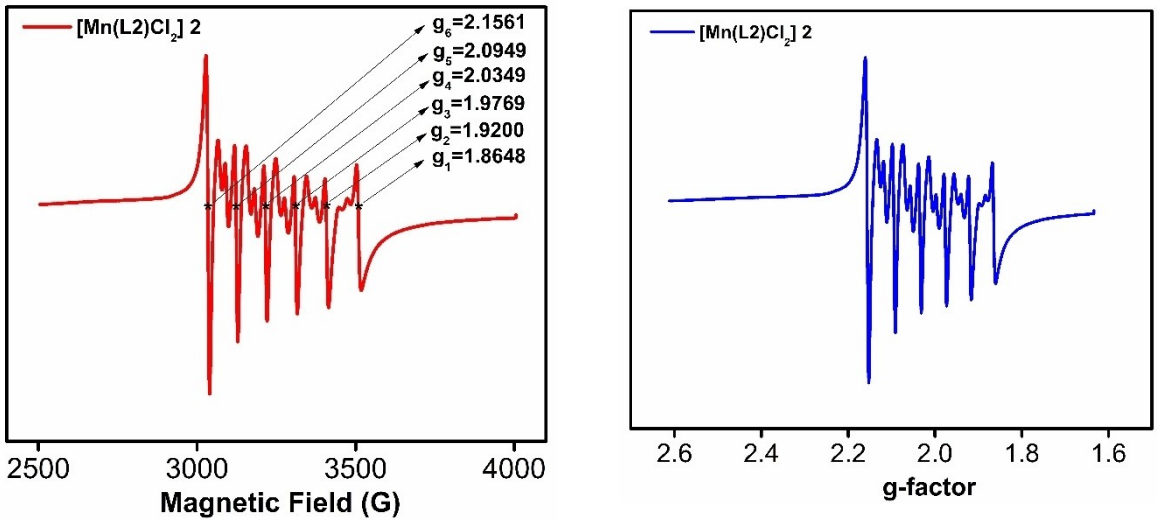


Fig. S39 EPR spectrum complex **2**: Conc.: (3 × 10^{-3} M in methanol at 77 K. Center field: 3250.513 G; Sweep Width: 750.00 G; Microwave Frequency: 9.157336 GHz; Power: 0.99800 (mW).

Figure S40 and S41

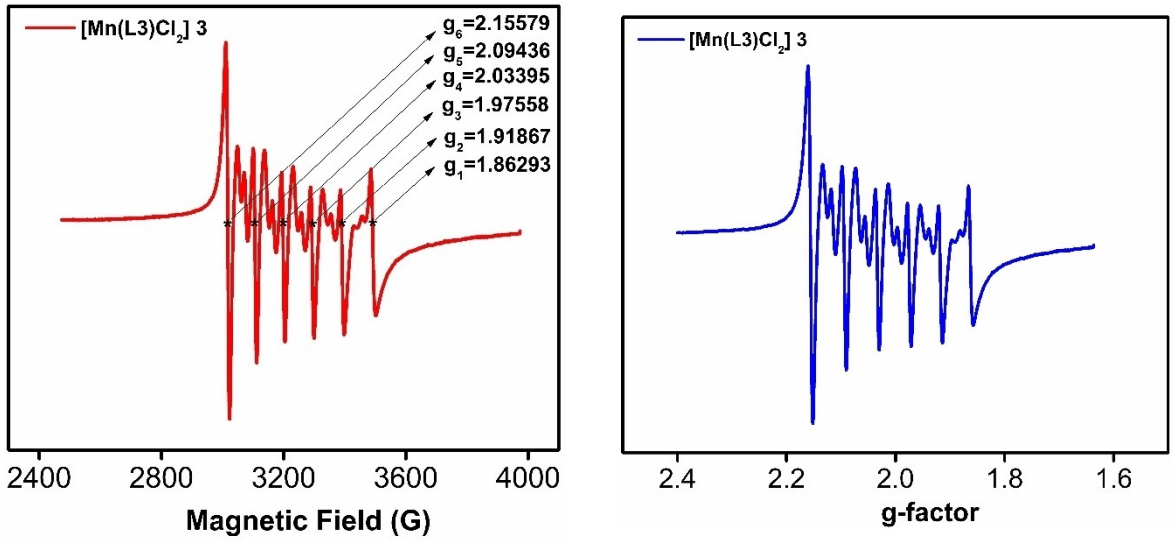


Fig. S40 EPR spectrum complex **3**. Conc.: (3×10^{-3} M in methanol at 77 K. Center field: 3220.365 G; Sweep Width: 750.00 G; Microwave Frequency: 9.103461 GHz; Power: 0.99800 (mW).

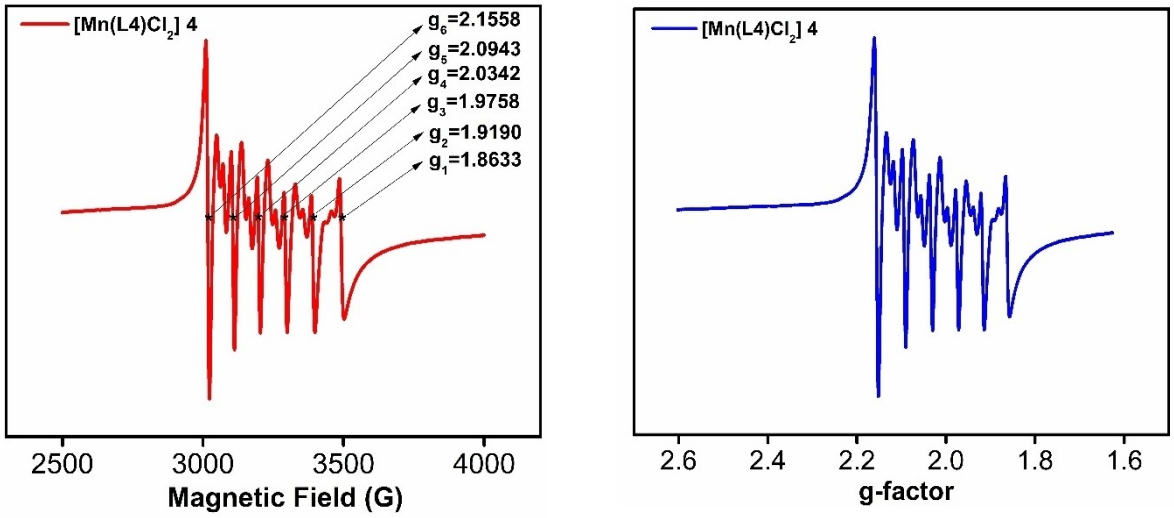


Fig. S41 EPR spectrum complex **4**. Conc.: (3×10^{-3} M in methanol at 77 K. Center field: 3220.000 G; Sweep Width: 750.00 G; Microwave Frequency: 9.104018 GHz; Power: 0.99800 (mW).

Figure S42 and S43

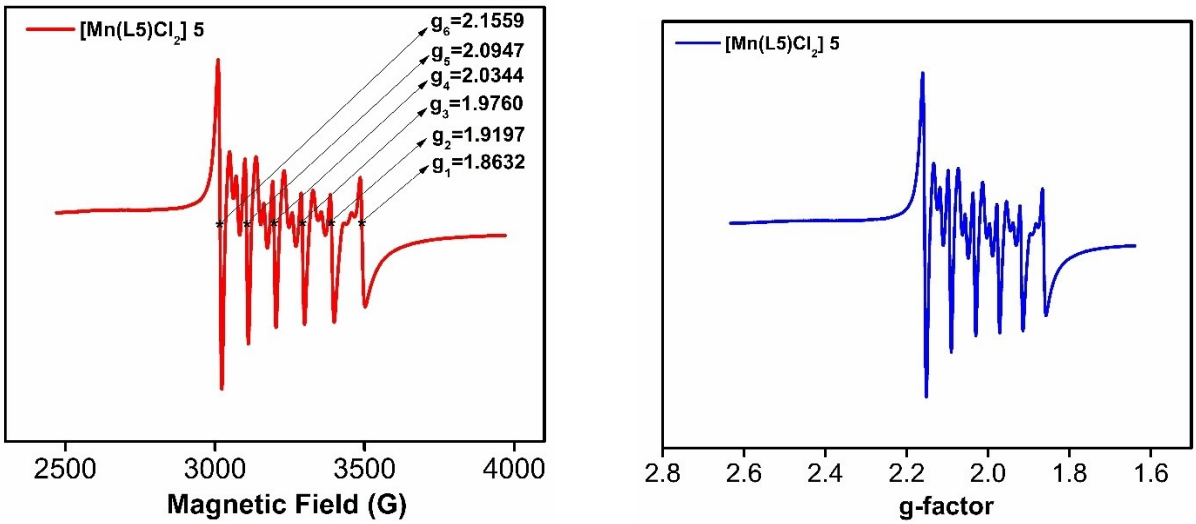


Fig. S42 EPR spectrum complex **5**. Conc.: (3×10^{-3} M in methanol at 77 K. Center field: 3220.000 G; Sweep Width: 750.00 G; Microwave Frequency: 9.104263 GHz; Power: 0.99800 (mW).

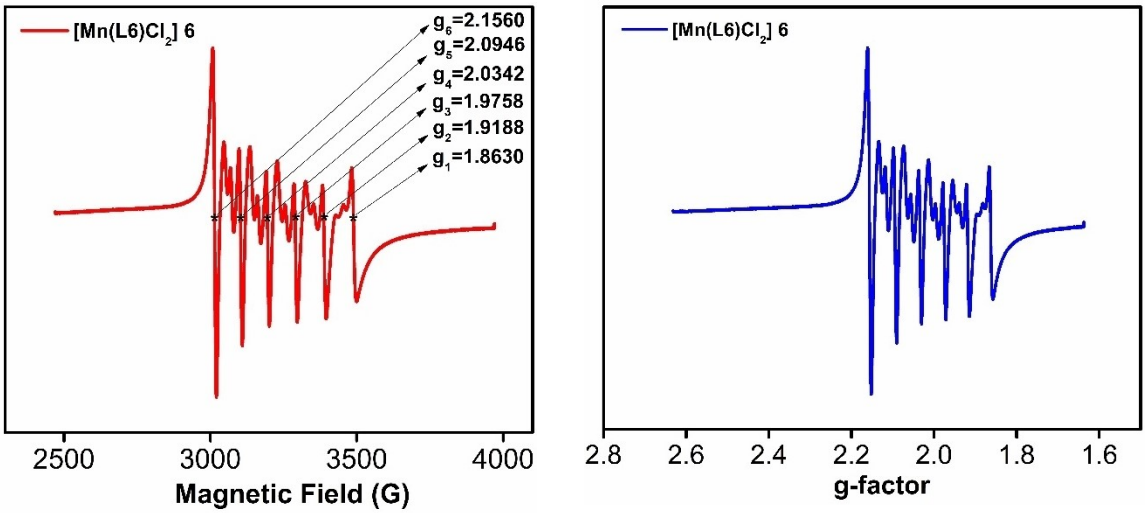


Fig. S43 EPR spectrum complex **6**. Conc.: (3×10^{-3} M in methanol at 77 K. Center field: 3220.000 G; Sweep Width: 750.00 G; Microwave Frequency: 9.097549 GHz; Power: 0.99500 (mW).

Figure S44

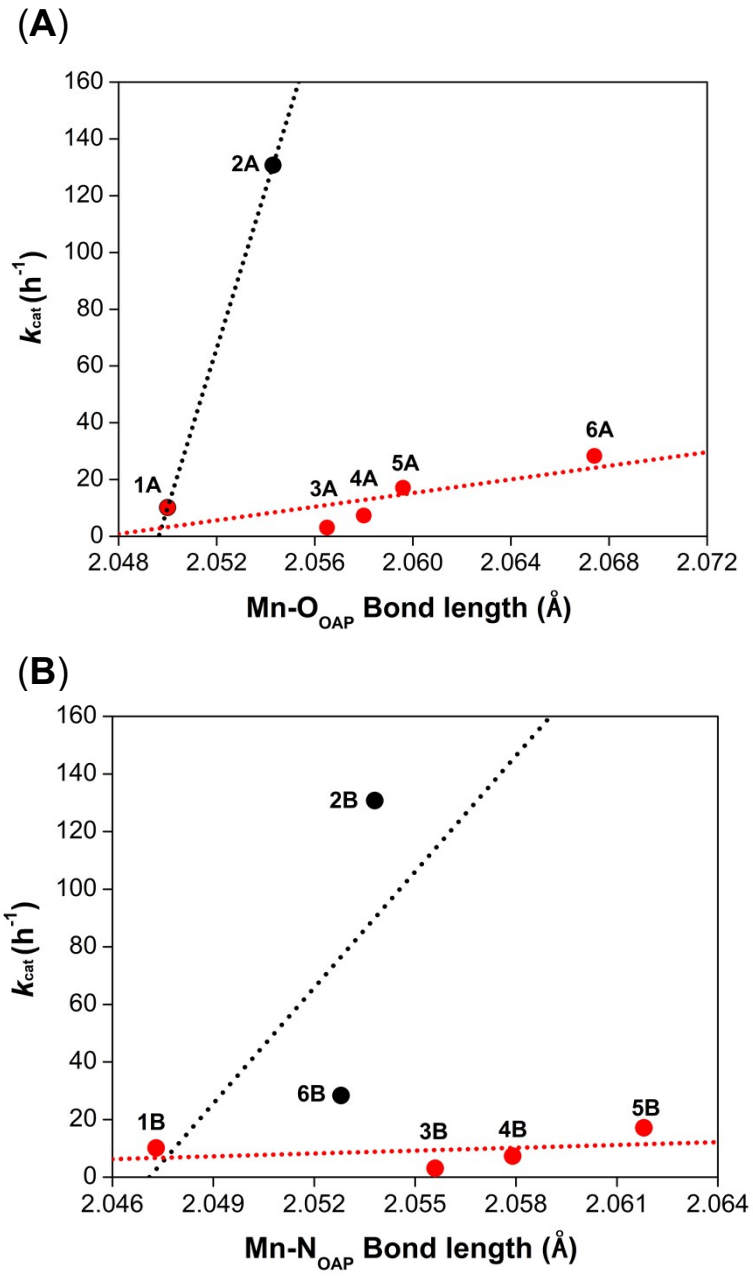


Fig. S44 (A) Correlation plot of turnover number (TON) versus Mn–O_{OAP} bond length (Å) for the [Mn(L)(OAP)] **1A**–**6A** adducts and (B) Mn–N_{OAP} bond length (Å) for the [Mn(L)(OAP)] **1B**–**6B** adducts.

Figure S45

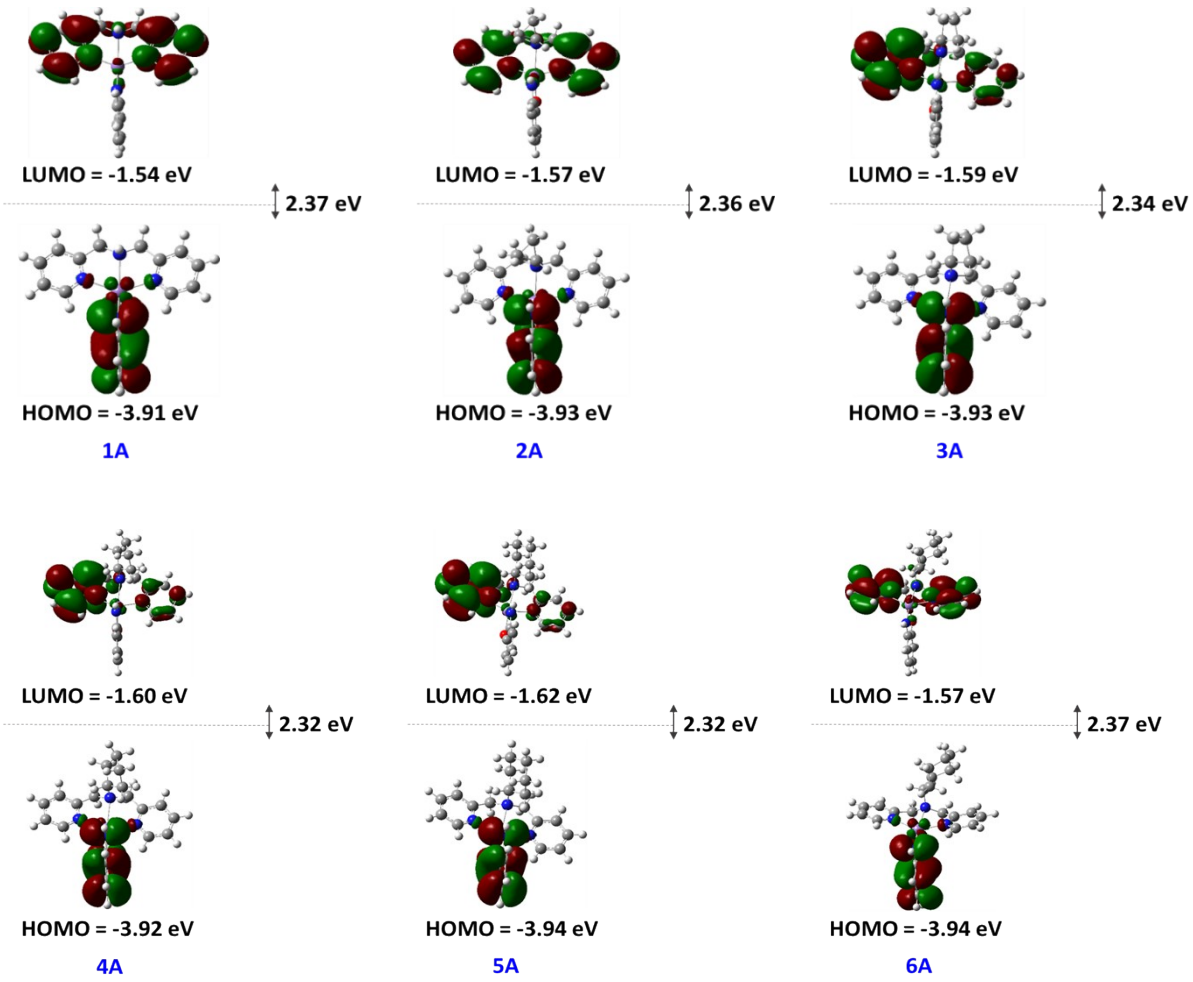


Fig. S45 HOMO and LUMO band gap energy profile diagram for OAP adducts **1A**–**6A** were performed with unrestricted B3LYP-D3 with the Grimme's dispersion corrections, employing the def2-TZVP (TZVP = valence triple-ζ polarized) basis set and methanol as a solvent CPCM method.

Figure S46

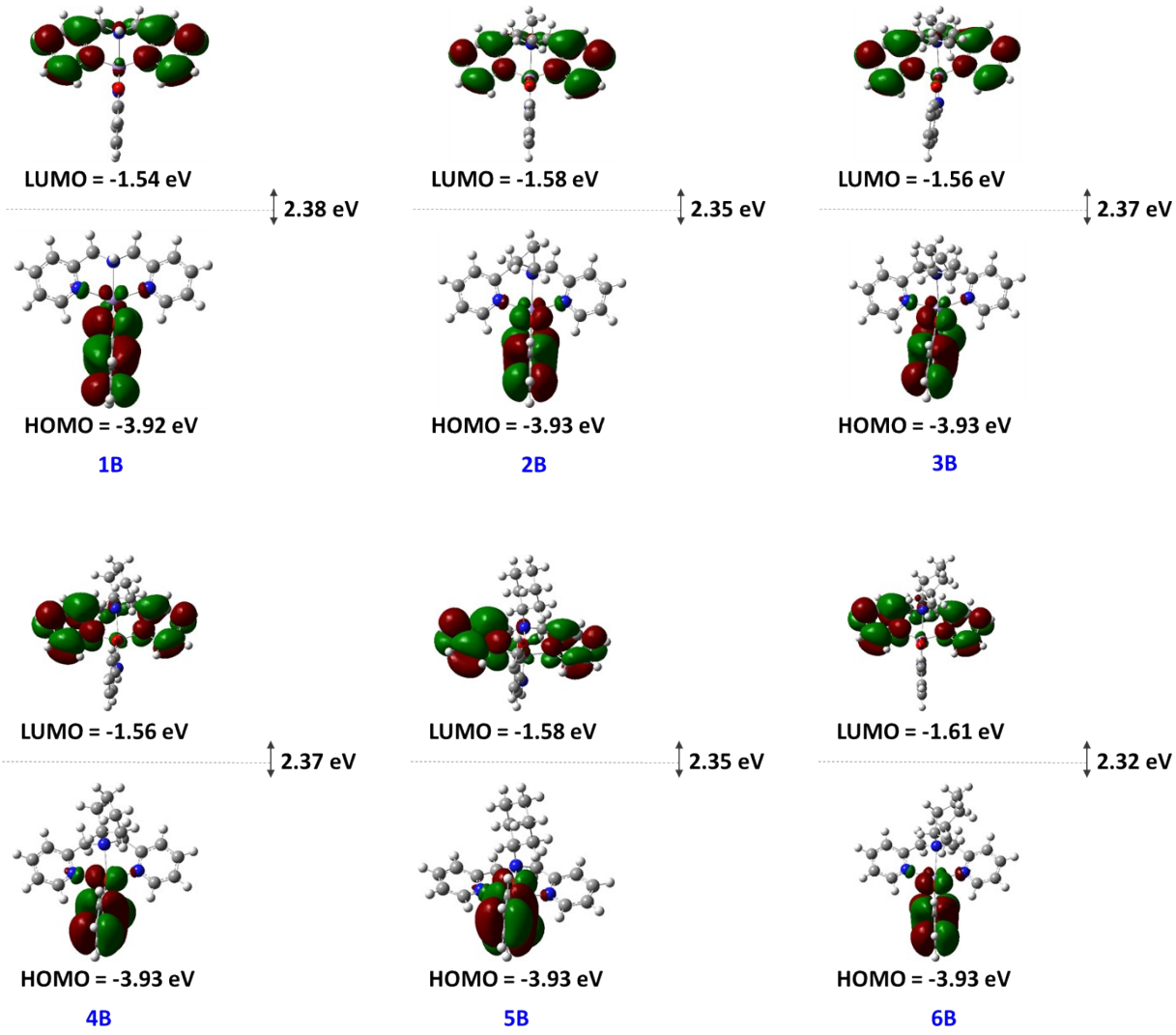


Fig. S46 HOMO and LUMO band gap energy profile diagram for OAP adducts **1B**–**6B** were performed with unrestricted B3LYP-D3 with the Grimme's dispersion corrections, employing the def2-TZVP (TZVP = valence triple-ζ polarized) basis set and methanol as a solvent CPCM method.

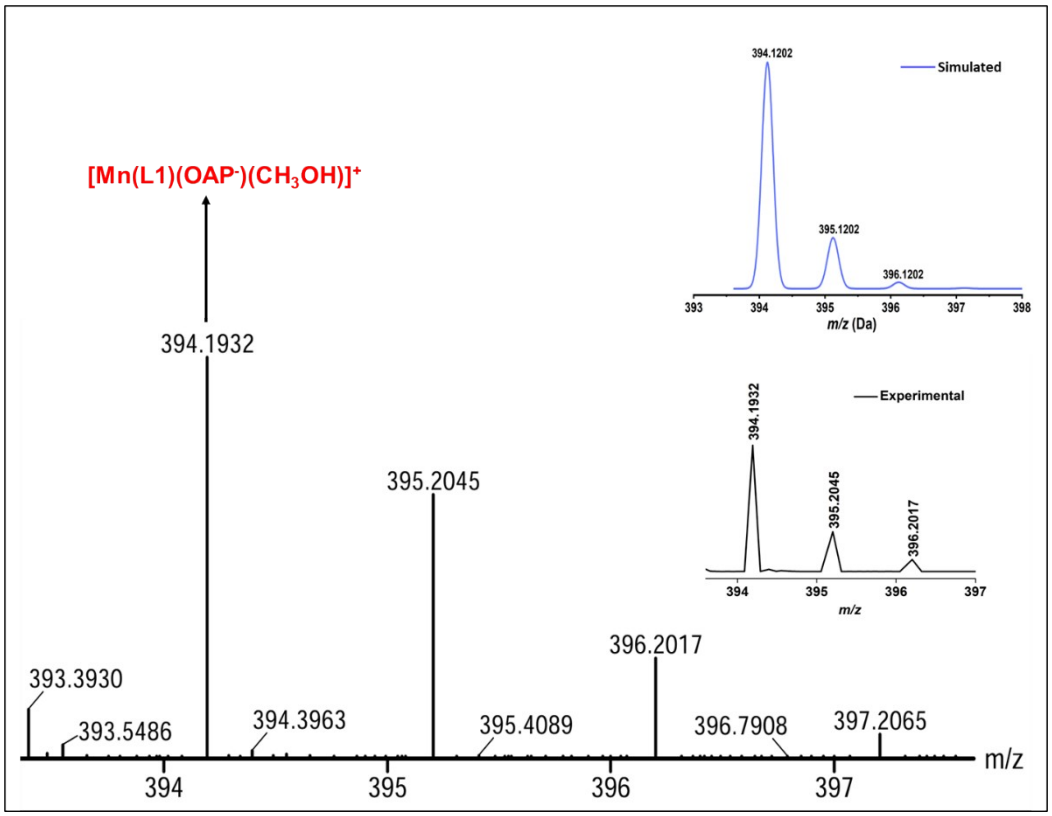


Figure S47

Fig. S47 High Resolution Mass Spectrum of the $[Mn^{II}(L1)(OAP^{-})(CH_3OH)]^{+}$ ion for OAP-adduct **1**, obtained from a 1:50 mixture of $[Mn(L1)Cl_2]$ **1** and *o*-aminophenol, recorded

in O_2 saturated methanol solution. The blue trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak observed at *m/z* 394.1932.

Figure S48

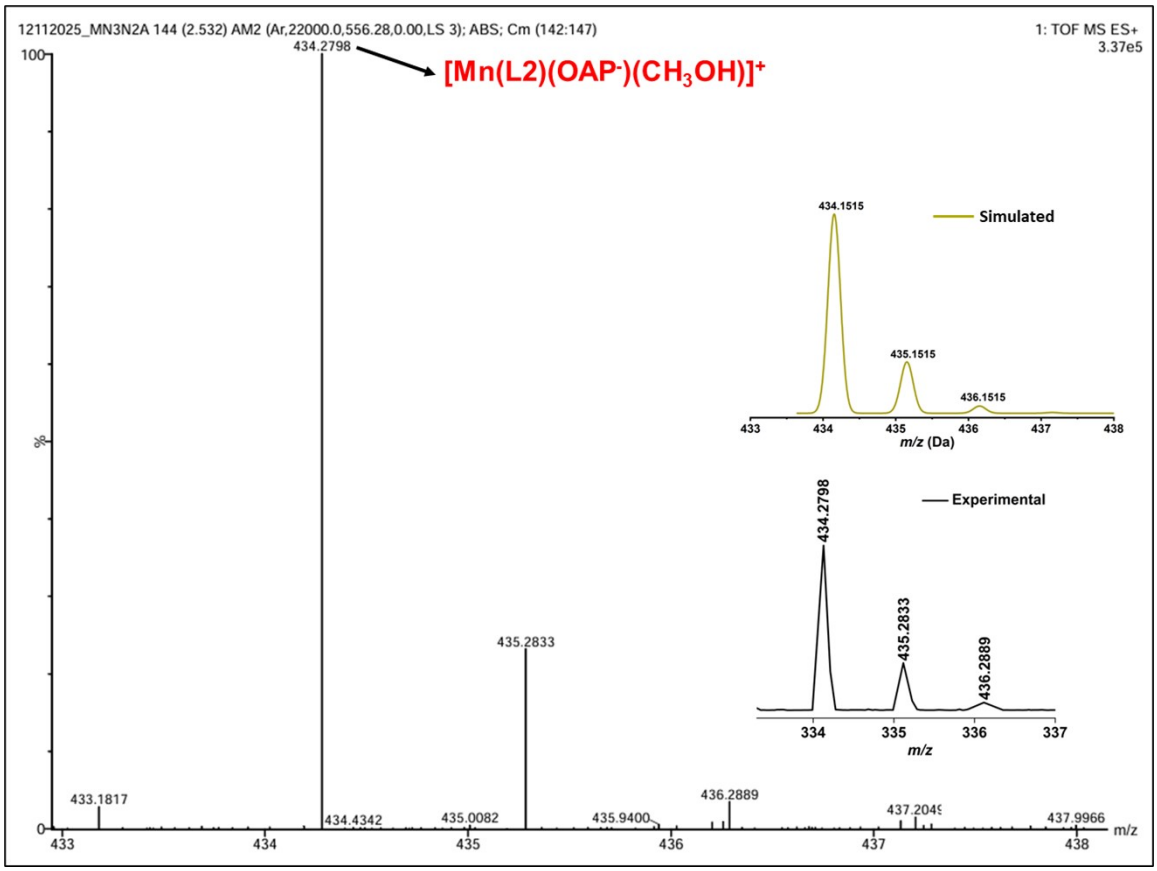


Fig. S48 High Resolution Mass Spectrum of the $[Mn^{II}(L2)(OAP^{-})(CH_3OH)]^{+}$ ion for OAP-adduct **2**, obtained from a 1:50 mixture of $[Mn(L2)Cl_2]$ **2** and *o*-aminophenol, recorded in O_2 saturated methanol solution. The yellow trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak observed at *m/z* 434.2798.

Figure S49

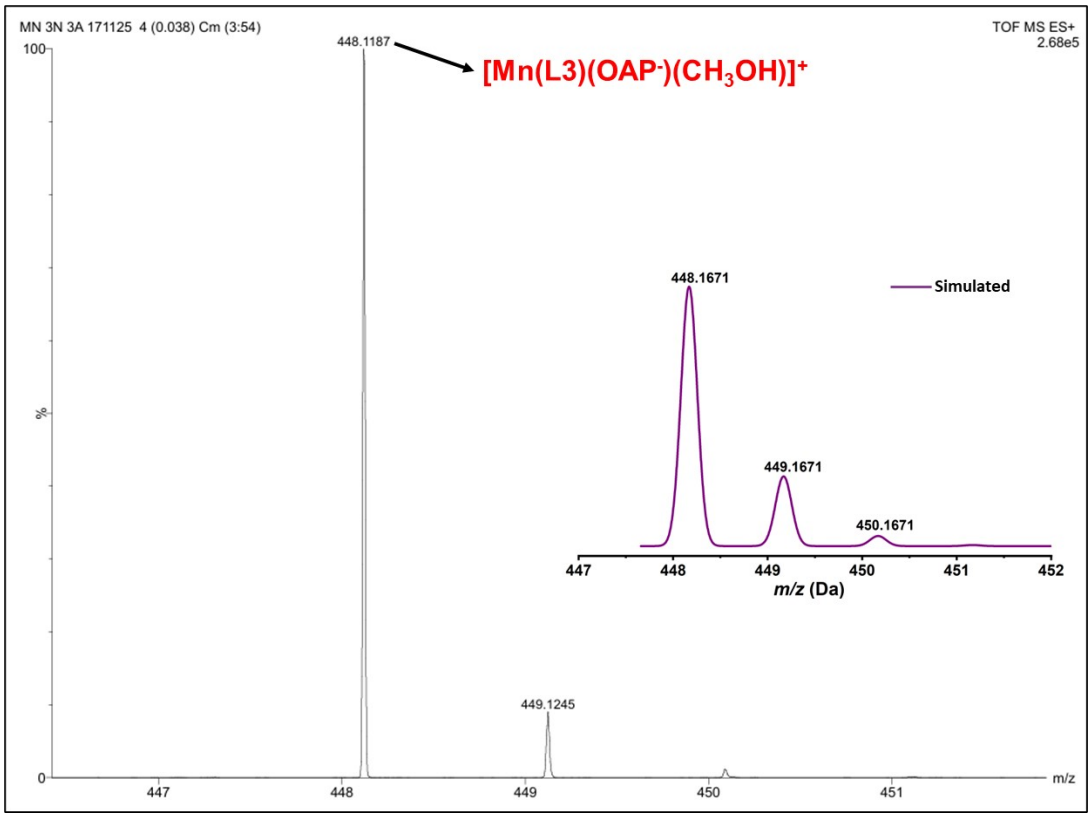


Fig. S49 High Resolution Mass Spectrum of the $[Mn^{II}(L3)(OAP^{-})(CH_3OH)]^{+}$ ion for OAP-adduct **3**, obtained from a 1:50 mixture of $[Mn(L3)Cl_2]$ **3** and *o*-aminophenol, recorded in O_2 saturated methanol solution. The violet trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak observed at *m/z* 448.1187.

Figure S50

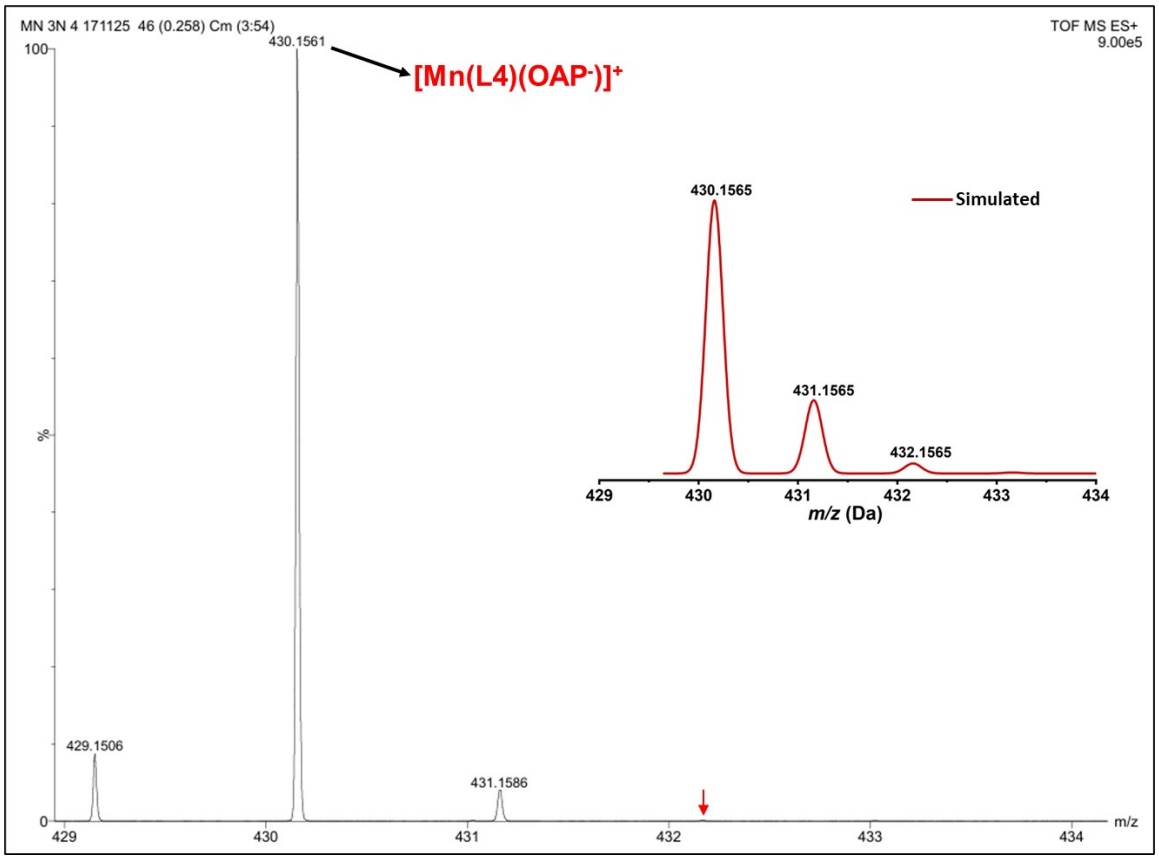


Fig. S50 High Resolution Mass Spectrum of the $[Mn^{II}(L4)(OAP^{-})]^{+}$ ion for OAP-adduct **4**, obtained from a 1:50 mixture of $[Mn(L4)Cl_2]$ **4** and *o*-aminophenol, recorded in O_2 saturated methanol solution. The brown trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak observed at *m/z* 430.1561.

Figure S51

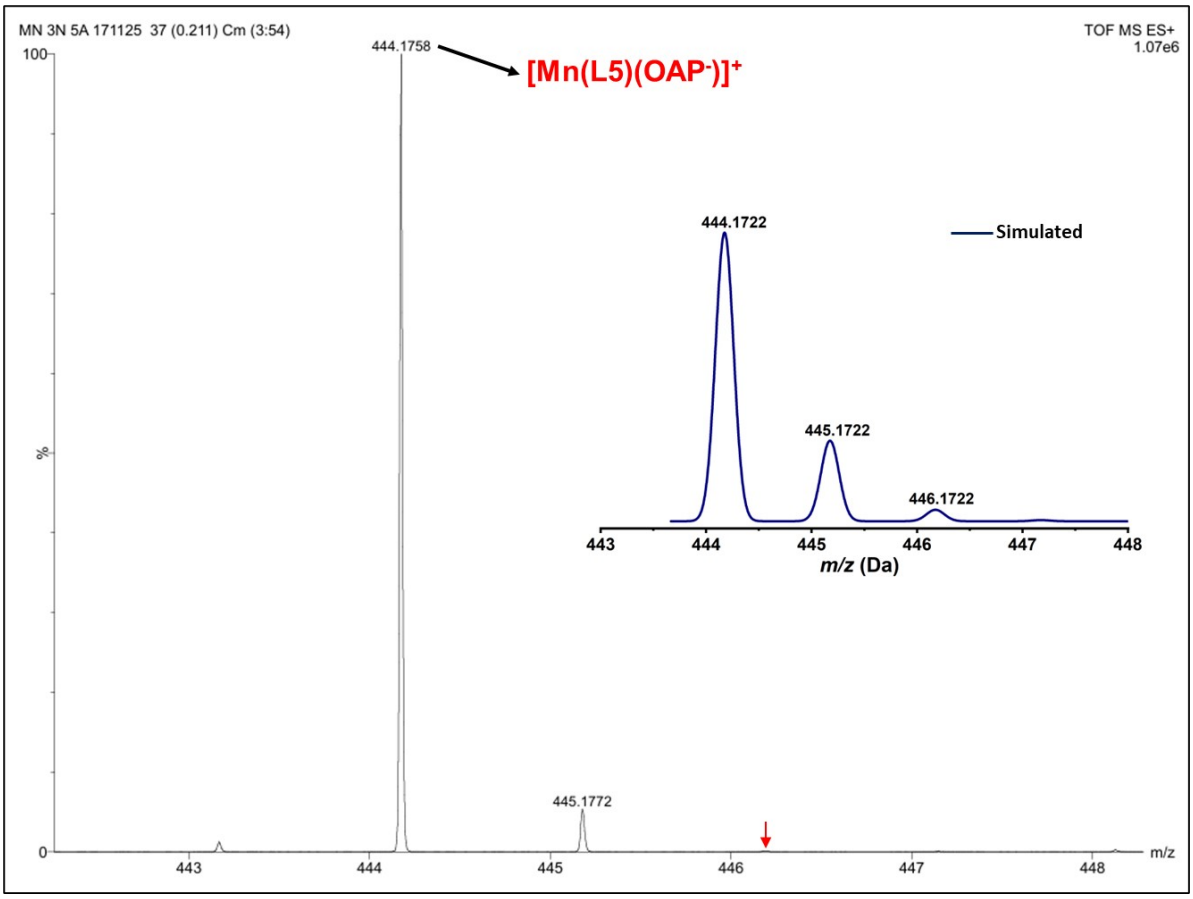


Fig. S51 High Resolution Mass Spectrum of the $[Mn^{II}(L5)(OAP^{-})]^{+}$ ion for OAP-adduct **5**, obtained from a 1:50 mixture of $[Mn(L5)Cl_2]$ **5** and *o*-aminophenol, recorded in O_2 saturated methanol solution. The dark-blue trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak observed at *m/z* 444.1758.

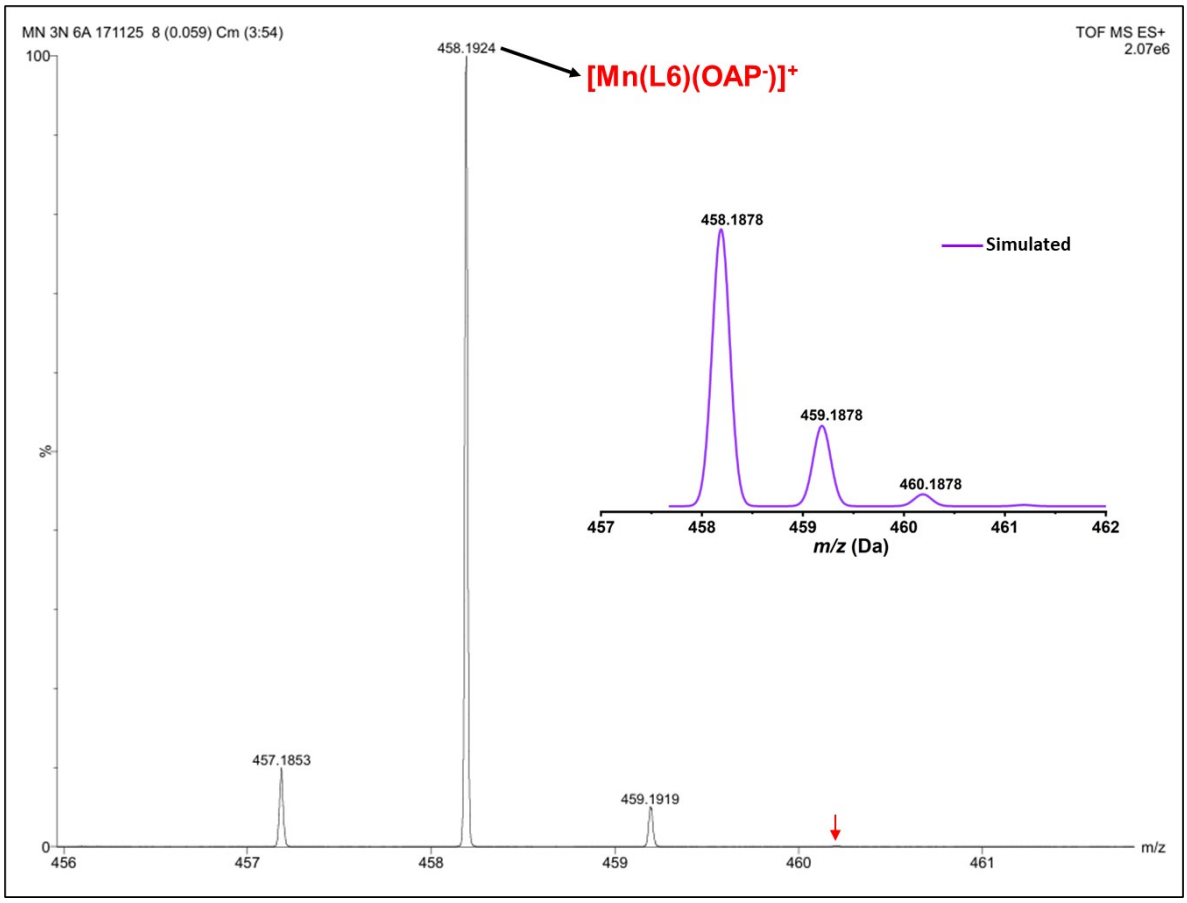


Figure S52

Fig. S52 High Resolution Mass Spectrum of the $[Mn^{II}(L6)(OAP^{-})]^{+}$ ion for OAP-adduct **6**, obtained from a 1:50 mixture of $[Mn(L6)Cl_2]$ **6** and *o*-aminophenol, recorded in O_2 saturated methanol solution. The bluish-purple trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak observed at *m/z* 458.1924.

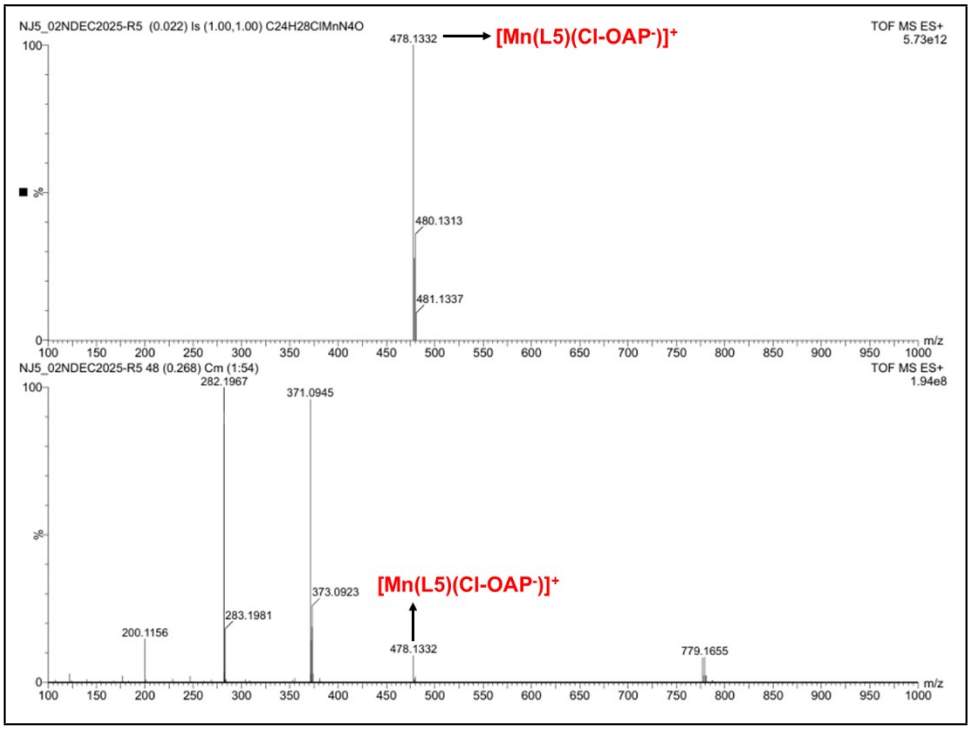


Figure S53

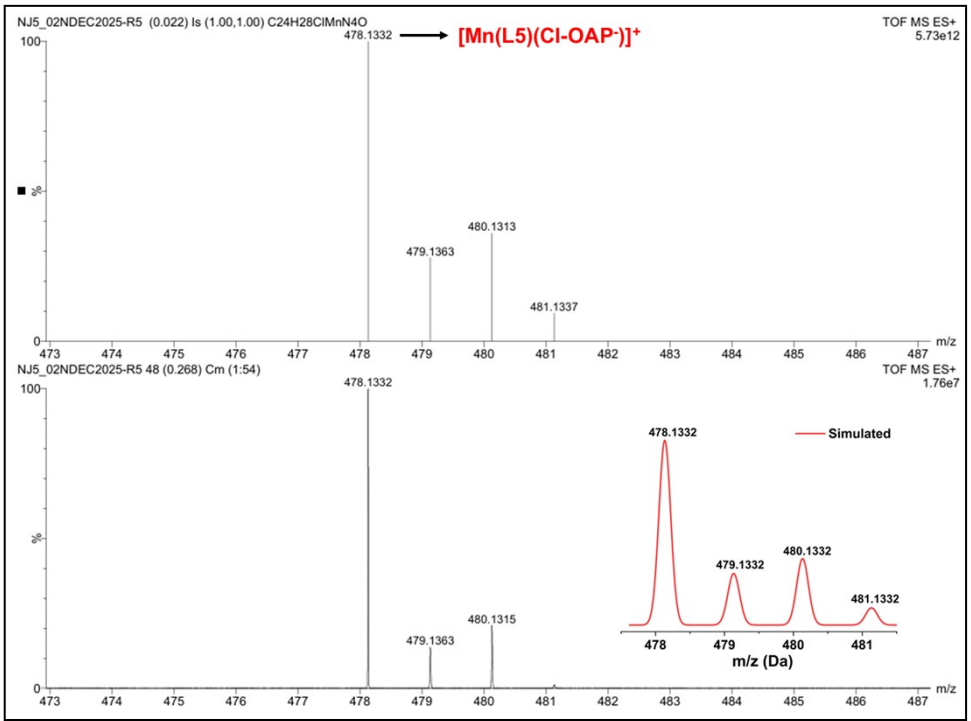


Fig. S53 High Resolution Mass Spectrum of the $[Mn^{II}(L5)(Cl\text{-}OAP^{-})]^{+}$ ion for Cl-OAP-adduct **5**, obtained from a 1:50 mixture of $[Mn(L5)Cl_2]$ **5** and 5-chloroaminophenol, recorded in O_2 saturated methanol solution. The red trace represents the simulated isotopic distribution, while the black trace corresponds to the experimental isotopic pattern of the peak observed at *m/z* 478.1332.

Cartesian Coordinates

Complex 1

6	-4.742908000	0.917716000	-0.405401000
1	-5.751289000	1.285441000	-0.542521000
6	-4.475290000	-0.445662000	-0.452301000
1	-5.259612000	-1.169243000	-0.623842000
1	-2.894059000	-1.911670000	-0.326246000
25	0.000008000	-0.686287000	0.163337000
17	0.000006000	-2.358590000	-1.580559000
17	-0.000042000	-1.634113000	2.364509000
7	2.160113000	-0.011261000	-0.065431000
7	0.000006000	1.618893000	-0.242347000
7	-2.160102000	-0.011252000	-0.065470000
6	3.166510000	-0.865066000	-0.282480000
1	2.894074000	-1.911680000	-0.326186000

6	4.475298000	-0.445669000	-0.452285000
1	5.259620000	-1.169251000	-0.623825000
6	3.697533000	1.804539000	-0.189597000
6	2.413004000	1.303141000	-0.015789000
6	1.237414000	2.204357000	0.281214000
1	1.132819000	2.282810000	1.366768000
6	-1.237406000	2.204366000	0.281192000
1	-1.132823000	2.282841000	1.366745000
6	-2.412996000	1.303147000	-0.015808000
6	-3.697529000	1.804545000	-0.189590000
1	-3.869127000	2.872030000	-0.158067000
6	-3.166499000	-0.865057000	-0.282519000
1	1.425186000	3.211645000	-0.100331000
1	-1.425173000	3.211647000	-0.100375000
1	3.869128000	2.872025000	-0.158091000
6	4.742912000	0.917711000	-0.405409000
1	5.751290000	1.285437000	-0.542548000
1	0.000016000	1.688034000	-1.256696000

Complex 2

6	-4.720931000	0.659207000	-0.001583000
1	-5.727607000	1.055137000	-0.028548000
6	-4.448055000	-0.610737000	-0.494200000
1	-5.226215000	-1.233494000	-0.912227000
1	-2.860080000	-2.040506000	-0.830359000
25	-0.000060000	-1.018994000	0.148075000
17	-0.000076000	-2.520627000	-1.724583000
17	-0.000054000	-1.505046000	2.518778000
7	2.143798000	-0.335654000	0.058876000
7	0.000016000	1.404131000	0.339747000

7	-2.143905000	-0.335590000	0.058885000
6	3.140205000	-1.067676000	-0.447379000
1	2.859915000	-2.040524000	-0.830506000
6	4.447943000	-0.610847000	-0.494197000
1	5.226085000	-1.233600000	-0.912265000
6	3.682410000	1.421595000	0.517635000
6	2.400087000	0.890806000	0.535546000
6	1.225475000	1.628450000	1.129521000
1	1.054815000	1.222195000	2.128318000
6	-1.225526000	1.628609000	1.129359000
1	-1.054969000	1.222449000	2.128210000
6	-2.400145000	0.890939000	0.535416000
6	-3.682447000	1.421775000	0.517433000
1	-3.859137000	2.419178000	0.896466000
6	-3.140337000	-1.067616000	-0.447312000
1	1.239848000	0.858429000	-2.077406000
1	-1.239334000	0.858725000	-2.077870000
1	1.454279000	2.693679000	1.233088000
1	-1.454279000	2.693862000	1.232807000
6	0.000205000	2.235211000	-0.858040000
1	0.000293000	3.300418000	-0.633017000
6	0.753580000	1.822444000	-2.087667000
1	1.281596000	2.594029000	-2.630654000
6	-0.752847000	1.822625000	-2.087934000
1	-1.280483000	2.594330000	-2.631120000
1	3.859135000	2.418953000	0.896771000
6	4.720868000	0.659035000	-0.001443000
1	5.727562000	1.054922000	-0.028348000

Complex 3

6	4.784145000	0.504970000	-0.230287000
1	5.786122000	0.899422000	-0.336893000
6	4.541966000	-0.598233000	0.579191000
1	5.340339000	-1.088397000	1.118183000
1	2.983018000	-1.901999000	1.321250000
25	0.074548000	-1.204189000	0.130631000
17	0.086203000	-2.244691000	2.293378000
17	0.087813000	-2.267522000	-2.043149000
7	-2.087821000	-0.571978000	0.020002000
7	0.034523000	1.050741000	-0.628694000
7	2.219770000	-0.486612000	0.046428000
6	-3.086262000	-1.243987000	0.604188000
1	-2.786642000	-2.064896000	1.243399000
6	-4.416602000	-0.912111000	0.412964000
1	-5.194733000	-1.479002000	0.904173000
6	-3.677873000	0.864852000	-1.013818000
6	-2.367459000	0.468233000	-0.771957000
6	-1.195780000	1.166394000	-1.422925000
1	-1.014364000	0.668706000	-2.377465000
6	1.246495000	1.132291000	-1.463739000
1	1.081232000	0.512717000	-2.347212000
6	2.446917000	0.576532000	-0.737075000
6	3.721418000	1.104439000	-0.893647000
1	3.872726000	1.972947000	-1.520208000
6	3.239483000	-1.058234000	0.693256000
1	-1.457248000	2.204134000	-1.647297000
1	1.446688000	2.153965000	-1.800507000
1	-3.874524000	1.716816000	-1.650735000
6	-4.714977000	0.163260000	-0.417205000
1	-5.742310000	0.456268000	-0.589458000

6	0.137689000	1.991292000	0.504364000
6	0.210068000	3.527282000	0.296644000
6	-1.025199000	2.206971000	1.495151000
1	1.011940000	1.678187000	1.076016000
6	-0.520779000	3.663669000	1.657834000
1	-0.423083000	3.862288000	-0.525989000
1	1.197772000	3.973648000	0.191160000
1	-1.997969000	2.196960000	1.007481000
1	-1.060534000	1.556370000	2.367702000
1	-1.277490000	4.441649000	1.739721000
1	0.182278000	3.761778000	2.485193000

Complex 4

6	4.782031000	0.348223000	-0.296214000
1	5.783035000	0.731606000	-0.444168000
6	4.533149000	-0.623380000	0.665116000
1	5.325022000	-1.019884000	1.284648000
1	2.971465000	-1.820119000	1.564835000
25	0.090076000	-1.327154000	0.218362000
17	0.031975000	-2.065546000	2.507510000
17	0.161284000	-2.746495000	-1.727606000
7	-2.066529000	-0.751168000	-0.013236000
7	0.050320000	0.837720000	-0.813909000
7	2.220468000	-0.614778000	0.083267000
6	-3.061769000	-1.375428000	0.626773000
1	-2.757552000	-2.128836000	1.342057000
6	-4.393832000	-1.074651000	0.400722000
1	-5.169247000	-1.600726000	0.939337000
6	-3.663965000	0.569831000	-1.180724000
6	-2.350979000	0.209423000	-0.898589000

6	-1.184436000	0.857738000	-1.610153000
1	-0.999397000	0.279573000	-2.517446000
6	1.257723000	0.756876000	-1.657724000
1	1.078256000	-0.010657000	-2.413526000
6	2.453762000	0.323090000	-0.846224000
6	3.727150000	0.832081000	-1.059737000
1	3.884070000	1.598434000	-1.806467000
6	3.232110000	-1.074754000	0.824201000
1	-1.462737000	1.865552000	-1.929848000
1	1.472107000	1.694326000	-2.177641000
1	-3.865377000	1.357775000	-1.894016000
6	-4.697739000	-0.083038000	-0.525997000
1	-5.726726000	0.183973000	-0.728202000
6	0.175383000	1.936341000	0.183760000
6	0.352251000	3.370245000	-0.385270000
6	-0.965623000	2.057089000	1.199292000
1	1.070350000	1.688692000	0.756890000
6	-0.309489000	4.309158000	0.655234000
1	-0.128484000	3.469002000	-1.359553000
1	1.407716000	3.599722000	-0.530558000
6	-0.671567000	3.408293000	1.851123000
1	-0.989879000	1.217616000	1.893878000
1	-1.934356000	2.105780000	0.698066000
1	0.339870000	5.136973000	0.940269000
1	-1.219643000	4.743802000	0.237185000
1	0.181130000	3.314209000	2.529652000
1	-1.511699000	3.791487000	2.430799000

Complex 5

6	4.771472000	0.322603000	-0.293727000

1	5.759074000	0.733092000	-0.458093000
6	4.534864000	-0.545773000	0.764691000
1	5.323415000	-0.833152000	1.445682000
1	2.998593000	-1.705036000	1.753333000
25	0.145141000	-1.495294000	0.289137000
17	0.122738000	-1.898451000	2.649008000
17	0.239290000	-3.047665000	-1.558217000
7	-2.038257000	-0.999919000	0.003820000
7	0.045930000	0.564279000	-0.976362000
7	2.243080000	-0.710363000	0.125661000
6	-3.024080000	-1.524056000	0.738256000
1	-2.714097000	-2.196333000	1.528050000
6	-4.357528000	-1.220890000	0.516338000
1	-5.125894000	-1.664503000	1.133567000
6	-3.644640000	0.215705000	-1.263246000
6	-2.332052000	-0.140106000	-0.978817000
6	-1.167996000	0.379317000	-1.788483000
1	-0.940013000	-0.383711000	-2.535518000
6	1.274869000	0.415236000	-1.779869000
1	1.135040000	-0.448804000	-2.432298000
6	2.463891000	0.128747000	-0.896340000
6	3.720373000	0.668717000	-1.133384000
1	3.865972000	1.353989000	-1.957275000
6	3.250486000	-1.037021000	0.939769000
1	-1.459606000	1.280804000	-2.331254000
1	1.478444000	1.279613000	-2.416277000
1	-3.852703000	0.920856000	-2.056610000
6	-4.670735000	-0.334964000	-0.508127000
1	-5.700117000	-0.068833000	-0.709487000
6	0.085046000	1.820501000	-0.156598000

6	-0.033630000	3.118845000	-0.970294000
6	-0.925373000	1.829475000	0.994970000
1	1.077206000	1.809311000	0.302097000
6	0.195184000	4.340426000	-0.071970000
1	-1.032771000	3.187806000	-1.410312000
1	0.680823000	3.129518000	-1.795071000
6	-0.701812000	3.047520000	1.897567000
1	-1.943539000	1.864803000	0.599156000
1	-0.842428000	0.912855000	1.580329000
6	-0.778151000	4.355171000	1.107357000
1	0.094573000	5.254352000	-0.662121000
1	1.223539000	4.320795000	0.305566000
1	-1.439632000	3.043824000	2.703220000
1	0.282716000	2.966715000	2.371597000
1	-0.569910000	5.206341000	1.760368000
1	-1.798081000	4.487339000	0.729080000

Complex 6

6	3.787871000	-2.419774000	-0.550697000
1	4.832622000	-2.625461000	-0.742977000
6	3.106599000	-3.100018000	0.451268000
1	3.596251000	-3.847088000	1.059731000
1	1.190241000	-3.279988000	1.437661000
25	-1.031980000	-1.310075000	0.254058000
17	-1.197414000	-1.755527000	2.604277000
17	-1.870429000	-2.608902000	-1.596161000
7	-2.541600000	0.358756000	0.145794000
7	-0.004205000	0.508126000	-0.956651000
7	1.123306000	-1.876798000	-0.057848000
6	-3.580315000	0.505251000	0.972428000

1	-3.662904000	-0.235128000	1.757733000
6	-4.489229000	1.543780000	0.843569000
1	-5.317806000	1.628845000	1.532301000
6	-3.210735000	2.317354000	-1.030102000
6	-2.348693000	1.245770000	-0.840299000
6	-1.164003000	0.982505000	-1.737829000
1	-1.444246000	0.184632000	-2.428454000
6	0.964101000	-0.210096000	-1.803486000
1	0.386900000	-0.777386000	-2.536795000
6	1.776165000	-1.212012000	-1.020165000
6	3.114006000	-1.460829000	-1.295451000
1	3.618093000	-0.901869000	-2.072088000
6	1.771303000	-2.794886000	0.663804000
1	-0.940115000	1.871031000	-2.334353000
1	1.621723000	0.459682000	-2.361408000
1	-3.024179000	3.025515000	-1.825923000
6	-4.298837000	2.464799000	-0.179036000
1	-4.982582000	3.293721000	-0.306550000
6	0.573682000	1.628462000	-0.127701000
6	1.362761000	2.667802000	-0.963102000
1	-0.308773000	2.137360000	0.262248000
6	1.326604000	1.101488000	1.098628000
6	2.898554000	2.595111000	-0.931578000
1	1.068573000	3.663877000	-0.624565000
1	1.023122000	2.612988000	-1.998864000
1	2.136199000	0.437578000	0.798441000
1	0.638486000	0.487608000	1.682980000
6	1.918238000	2.204709000	1.990914000
6	3.526442000	3.299506000	0.277931000
1	3.245111000	1.558969000	-0.978238000

1	3.272548000	3.077941000	-1.838060000
6	3.355965000	2.586281000	1.621025000
1	1.274895000	3.091286000	1.978391000
1	1.917436000	1.845451000	3.022649000
1	4.596400000	3.435015000	0.094406000
1	3.098284000	4.306063000	0.347181000
1	3.959548000	1.671491000	1.617807000
1	3.771604000	3.223217000	2.407543000

Manganese(II)-aminophenolate adducts

Mn^{II}-OAP adduct 1A

6	-1.587601000	4.821597000	-0.260772000
1	-1.927495000	5.847825000	-0.309657000
6	-2.438260000	3.778768000	-0.606357000
1	-3.453438000	3.962335000	-0.929108000
1	-2.555619000	1.627104000	-0.808877000
25	0.107125000	0.060150000	-0.138163000
7	2.066340000	-1.143139000	-0.162473000
7	1.930905000	1.571053000	0.024179000
7	-0.704661000	2.205894000	-0.146560000
6	2.108298000	-2.421875000	-0.545283000
1	1.156426000	-2.854832000	-0.826752000
6	3.287663000	-3.147339000	-0.589472000
1	3.280033000	-4.181600000	-0.903303000
6	4.424618000	-1.177281000	0.158012000
6	3.198435000	-0.524048000	0.187370000
6	3.069500000	0.905319000	0.663499000
1	2.877824000	0.886256000	1.739921000
6	1.489225000	2.804873000	0.680202000
1	1.424797000	2.603628000	1.753204000

6	0.115699000	3.204525000	0.193714000
6	-0.291606000	4.532061000	0.141321000
1	0.398935000	5.320362000	0.409009000
6	-1.950930000	2.483617000	-0.538319000
1	4.014160000	1.436793000	0.514331000
1	2.191004000	3.634035000	0.549399000
1	5.326303000	-0.647085000	0.434059000
6	4.468007000	-2.508061000	-0.231070000
1	5.411258000	-3.037578000	-0.260165000
1	2.164615000	1.773387000	-0.943956000
6	-2.104660000	-1.694574000	-0.608322000
6	-1.983622000	-1.590180000	0.827687000
6	-2.886167000	-2.286117000	1.631745000
6	-3.908808000	-3.079934000	1.085318000
6	-4.028869000	-3.181104000	-0.293660000
6	-3.135092000	-2.494617000	-1.126711000
1	-4.593756000	-3.606294000	1.740166000
1	-3.233260000	-2.577874000	-2.205931000
8	-1.010473000	-0.832682000	1.330218000
1	-2.778288000	-2.197717000	2.708517000
7	-1.185648000	-0.988018000	-1.342299000
1	-1.310164000	-1.115740000	-2.337900000
1	-4.811203000	-3.789611000	-0.733959000

Mn^{II}-OAP adduct 2A

6	0.301385000	4.889398000	-0.448607000
1	0.337291000	5.966440000	-0.350338000
6	1.471104000	4.155372000	-0.609242000
1	2.438667000	4.635992000	-0.643340000
1	2.246481000	2.145917000	-0.821677000

25	0.167867000	-0.090298000	-0.420206000
7	-1.212554000	-1.826124000	-0.696329000
7	-2.095120000	0.727023000	0.030500000
7	0.199303000	2.137471000	-0.681351000
6	-0.711508000	-3.063410000	-0.804230000
1	0.362819000	-3.124612000	-0.924487000
6	-1.506061000	-4.195835000	-0.760538000
1	-1.061140000	-5.176329000	-0.854429000
6	-3.393087000	-2.751433000	-0.463983000
6	-2.530107000	-1.662806000	-0.532236000
6	-3.058397000	-0.244389000	-0.497758000
1	-3.272091000	0.036655000	-1.530298000
6	-2.223102000	2.055202000	-0.589940000
1	-2.470686000	1.913662000	-1.643759000
6	-0.931554000	2.839277000	-0.537325000
6	-0.915899000	4.222755000	-0.407405000
1	-1.843469000	4.763382000	-0.275721000
6	1.373407000	2.777537000	-0.713577000
1	-4.019606000	-0.220917000	0.024410000
1	-3.033155000	2.636584000	-0.137670000
1	-4.452903000	-2.591018000	-0.317161000
6	-2.875780000	-4.032951000	-0.583596000
1	-3.530427000	-4.893046000	-0.533558000
6	2.597559000	-0.774435000	0.924601000
6	2.895514000	-0.859534000	-0.487072000
6	4.186947000	-1.204393000	-0.884148000
6	5.203598000	-1.471311000	0.048256000
6	4.921246000	-1.391620000	1.404586000
6	3.632702000	-1.046106000	1.833131000
1	6.196835000	-1.737192000	-0.294954000

1	3.417599000	-0.985849000	2.896712000
8	1.920702000	-0.605328000	-1.359497000
1	4.390294000	-1.262884000	-1.948900000
7	1.308913000	-0.431760000	1.248945000
1	1.158077000	-0.389023000	2.248242000
1	5.692980000	-1.594924000	2.138952000
6	-2.037403000	0.851274000	1.486999000
6	-3.246398000	1.108317000	2.346374000
6	-2.507874000	-0.209634000	2.426083000
1	-1.132686000	1.365549000	1.786704000
1	-4.220088000	1.095056000	1.874001000
1	-3.150004000	1.817487000	3.157098000
1	-1.889040000	-0.414803000	3.288821000
1	-3.009607000	-1.079972000	2.027879000

Mn^{II}-OAP adduct 3A

6	-0.145324000	4.753432000	-0.869202000
1	-0.233326000	5.832006000	-0.866930000
6	1.105611000	4.146106000	-0.914524000
1	2.014937000	4.729289000	-0.951735000
1	2.103552000	2.225161000	-0.928193000
25	0.299672000	-0.194717000	-0.469385000
7	-0.828830000	-2.121453000	-0.728761000
7	-2.088382000	0.338163000	-0.263450000
7	0.066178000	1.997817000	-0.857247000
6	-0.203354000	-3.299183000	-0.623628000
1	0.878162000	-3.257593000	-0.595020000
6	-0.886134000	-4.502198000	-0.548423000
1	-0.340919000	-5.431961000	-0.467940000
6	-2.924919000	-3.251279000	-0.668983000

6	-2.168045000	-2.089635000	-0.759461000
6	-2.808810000	-0.736695000	-0.963411000
1	-2.775604000	-0.523049000	-2.033511000
6	-2.345459000	1.661399000	-0.846089000
1	-2.611534000	1.521198000	-1.895356000
6	-1.138716000	2.574589000	-0.819824000
6	-1.280902000	3.958625000	-0.819253000
1	-2.267895000	4.399665000	-0.775278000
6	1.164257000	2.763380000	-0.902657000
1	-3.864459000	-0.779115000	-0.675035000
1	-3.197660000	2.164755000	-0.381479000
1	-4.004939000	-3.192928000	-0.678062000
6	-2.275524000	-4.474116000	-0.566781000
1	-2.845670000	-5.391061000	-0.495935000
6	2.742425000	-0.519008000	0.990490000
6	3.117903000	-0.528034000	-0.404887000
6	4.466842000	-0.645041000	-0.739310000
6	5.467185000	-0.759468000	0.240736000
6	5.109886000	-0.756516000	1.581709000
6	3.762446000	-0.637925000	1.947505000
1	6.506352000	-0.848624000	-0.054537000
1	3.489201000	-0.633489000	2.999359000
8	2.157757000	-0.419944000	-1.321478000
1	4.728768000	-0.647092000	-1.792848000
7	1.401143000	-0.392059000	1.252347000
1	1.197582000	-0.396946000	2.243078000
1	5.868018000	-0.844713000	2.352145000
6	-2.315190000	0.250002000	1.190273000
6	-1.741905000	1.319838000	2.142812000
6	-3.715187000	0.471482000	1.826874000

1	-1.942255000	-0.728174000	1.499654000
6	-2.978362000	1.083287000	3.047010000
1	-1.770261000	2.317515000	1.706509000
1	-0.746175000	1.141107000	2.544083000
1	-4.295210000	1.226545000	1.294860000
1	-4.337893000	-0.407641000	1.986139000
1	-3.427422000	1.960360000	3.509489000
1	-2.782319000	0.336733000	3.816895000

Mn^{II}-OAP adduct 4A

6	0.302166000	-4.702772000	-0.965675000
1	0.477960000	-5.770095000	-0.997696000
6	-0.988548000	-4.202285000	-0.825810000
1	-1.843570000	-4.859143000	-0.749544000
1	-2.133973000	-2.374566000	-0.665125000
25	-0.519554000	0.191057000	-0.438963000
7	0.414326000	2.207017000	-0.710015000
7	1.959226000	-0.139747000	-0.563052000
7	-0.130853000	-1.974122000	-0.867922000
6	-0.249415000	3.321789000	-0.388640000
1	-1.296365000	3.193238000	-0.145254000
6	0.358273000	4.567129000	-0.355890000
1	-0.215676000	5.444506000	-0.093131000
6	2.403449000	3.488375000	-0.982037000
6	1.719380000	2.280276000	-1.007276000
6	2.380378000	0.986091000	-1.414656000
1	2.059036000	0.766467000	-2.435059000
6	2.228245000	-1.441850000	-1.187984000
1	2.347230000	-1.290095000	-2.262567000
6	1.110401000	-2.447766000	-1.009979000

6	1.363803000	-3.815548000	-1.057327000
1	2.380104000	-4.172352000	-1.160003000
6	-1.157824000	-2.829689000	-0.777861000
1	3.466884000	1.114283000	-1.437445000
1	3.167484000	-1.880723000	-0.841242000
1	3.460204000	3.514136000	-1.210714000
6	1.712178000	4.648521000	-0.656416000
1	2.225293000	5.600850000	-0.630319000
6	-2.947484000	0.311075000	1.078693000
6	-3.355186000	0.294147000	-0.307668000
6	-4.717102000	0.304755000	-0.609280000
6	-5.699339000	0.334614000	0.395024000
6	-5.311243000	0.351285000	1.727258000
6	-3.950173000	0.340414000	2.060449000
1	-6.749190000	0.342100000	0.125151000
1	-3.651988000	0.353227000	3.105509000
8	-2.411021000	0.268244000	-1.246238000
1	-5.004099000	0.292057000	-1.656166000
7	-1.594456000	0.301327000	1.306949000
1	-1.366847000	0.317191000	2.292408000
1	-6.055357000	0.373674000	2.515907000
6	2.495419000	-0.001540000	0.815222000
6	2.020465000	-1.071182000	1.808499000
6	4.046293000	0.020846000	0.956104000
1	2.108180000	0.954745000	1.173292000
6	3.000098000	-0.904984000	2.970068000
1	2.131710000	-2.072302000	1.385697000
1	0.973758000	-0.942832000	2.085347000
6	4.357301000	-0.744331000	2.264769000
1	4.408178000	1.048465000	0.991501000

1	4.529634000	-0.451319000	0.099693000
1	2.755372000	-0.000614000	3.535027000
1	2.979930000	-1.743576000	3.666805000
1	5.095474000	-0.233384000	2.883280000
1	4.760743000	-1.731871000	2.029374000

Mn^{II}-OAP adduct 5A

6	0.467951000	4.622892000	-1.190337000
1	0.429011000	5.703714000	-1.228531000
6	1.679166000	3.964974000	-1.001610000
1	2.606428000	4.509603000	-0.892233000
1	2.577631000	2.007767000	-0.792210000
25	0.643354000	-0.322187000	-0.578940000
7	-0.524118000	-2.222942000	-0.862602000
7	-1.776677000	0.315447000	-0.824242000
7	0.550357000	1.862461000	-1.076171000
6	-0.039013000	-3.405036000	-0.471399000
1	1.006194000	-3.417508000	-0.190018000
6	-0.819447000	-4.549643000	-0.416422000
1	-0.386569000	-5.486626000	-0.095620000
6	-2.664258000	-3.221901000	-1.172229000
6	-1.814723000	-2.124772000	-1.214019000
6	-2.265422000	-0.767977000	-1.694855000
1	-1.823681000	-0.613534000	-2.681511000
6	-1.841327000	1.626552000	-1.485994000
1	-1.919163000	1.463161000	-2.562676000
6	-0.615382000	2.487427000	-1.265225000
6	-0.692910000	3.875596000	-1.321859000
1	-1.651595000	4.356921000	-1.463231000
6	1.672684000	2.581997000	-0.946644000

1	-3.350772000	-0.759425000	-1.826053000
1	-2.733560000	2.190235000	-1.205407000
1	-3.704328000	-3.109519000	-1.446371000
6	-2.158873000	-4.452343000	-0.770751000
1	-2.803710000	-5.320254000	-0.728932000
6	2.892442000	-0.525035000	1.184186000
6	3.433646000	-0.640986000	-0.150289000
6	4.814751000	-0.752121000	-0.310301000
6	5.690434000	-0.754961000	0.788411000
6	5.173777000	-0.644594000	2.071814000
6	3.790407000	-0.530736000	2.262836000
1	6.759006000	-0.841816000	0.628415000
1	3.391535000	-0.443927000	3.269975000
8	2.588705000	-0.632993000	-1.179667000
1	5.202237000	-0.836772000	-1.320790000
7	1.527194000	-0.417163000	1.271469000
1	1.205341000	-0.337381000	2.227152000
1	5.834945000	-0.644413000	2.931432000
6	-2.389272000	0.279570000	0.538871000
6	-1.724189000	1.285579000	1.483546000
6	-3.916415000	0.446917000	0.571766000
1	-2.158623000	-0.719424000	0.921927000
6	-2.253894000	1.128530000	2.912297000
1	-1.928398000	2.304499000	1.140860000
1	-0.641080000	1.152363000	1.467722000
6	-4.448226000	0.289745000	2.001523000
1	-4.188937000	1.437539000	0.195926000
1	-4.401144000	-0.284839000	-0.076011000
6	-3.775876000	1.269865000	2.964092000
1	-1.777882000	1.867094000	3.561534000

1	-1.967286000	0.142342000	3.294004000
1	-5.531886000	0.428973000	2.007895000
1	-4.260823000	-0.735159000	2.340769000
1	-4.138168000	1.109647000	3.982659000
1	-4.051689000	2.293512000	2.686534000

Mn^{II}-OAP adduct 6A

6	-1.329963000	-4.312468000	0.203693000
1	-1.832284000	-5.249648000	0.404764000
6	-0.466396000	-4.191660000	-0.877884000
1	-0.272638000	-5.022690000	-1.541413000
1	0.844857000	-2.813959000	-1.909602000
25	0.934939000	0.104716000	-0.597132000
7	0.535977000	2.332992000	-0.451970000
7	-1.079266000	0.453434000	0.822729000
7	-0.062003000	-1.910319000	-0.307453000
6	0.984642000	3.263255000	-1.299172000
1	1.519935000	2.896170000	-2.165963000
6	0.790915000	4.620176000	-1.089876000
1	1.168747000	5.339288000	-1.802931000
6	-0.364980000	4.052416000	0.929209000
6	-0.128416000	2.712735000	0.649744000
6	-0.560116000	1.603401000	1.580035000
1	0.327268000	1.268956000	2.120908000
6	-1.030490000	-0.790688000	1.604410000
1	-0.125019000	-0.744431000	2.213182000
6	-0.895130000	-2.018863000	0.735593000
6	-1.545532000	-3.211923000	1.023650000
1	-2.214127000	-3.272532000	1.871698000
6	0.151111000	-2.968549000	-1.092293000

1	-1.273912000	1.989805000	2.315017000
1	-1.873260000	-0.903133000	2.290678000
1	-0.912853000	4.327924000	1.820217000
6	0.102219000	5.019544000	0.048567000
1	-0.073626000	6.068926000	0.245811000
6	-2.405099000	0.779962000	0.197971000
6	-3.590076000	0.737244000	1.194375000
1	-2.297349000	1.821078000	-0.109682000
6	-2.624061000	-0.011755000	-1.095551000
6	-4.477310000	-0.517851000	1.198324000
1	-4.231195000	1.598128000	0.990084000
1	-3.200276000	0.908943000	2.199897000
1	-2.528955000	-1.081867000	-0.914179000
1	-1.813486000	0.252500000	-1.777661000
6	-3.977125000	0.243467000	-1.777716000
6	-5.573351000	-0.502567000	0.125215000
1	-3.876830000	-1.425729000	1.095754000
1	-4.959303000	-0.584864000	2.177190000
6	-5.090217000	-0.702515000	-1.312857000
1	-4.282771000	1.286278000	-1.638879000
1	-3.846377000	0.108103000	-2.854091000
1	-6.305635000	-1.282787000	0.353302000
1	-6.109776000	0.450655000	0.196169000
1	-4.731636000	-1.731779000	-1.428359000
1	-5.948569000	-0.601283000	-1.983798000
8	2.186085000	-0.022526000	1.043814000
7	2.672620000	-0.338449000	-1.589178000
6	3.708643000	-0.566629000	-0.715344000
6	5.008359000	-0.959808000	-1.071308000
6	6.009065000	-1.166782000	-0.112632000

6	5.726991000	-0.986244000	1.234121000
6	4.434188000	-0.596201000	1.620649000
6	3.416618000	-0.385765000	0.689453000
1	5.235941000	-1.101147000	-2.124545000
1	7.000811000	-1.469209000	-0.430527000
1	6.492782000	-1.142453000	1.985274000
1	4.195891000	-0.453030000	2.670061000
1	2.943258000	-0.489104000	-2.551750000

Mn^{II}-OAP adduct 1B

6	4.074224000	-3.085399000	0.366762000
1	4.930138000	-3.732114000	0.508702000
6	2.782686000	-3.587188000	0.480118000
1	2.599757000	-4.627467000	0.709978000
1	0.692596000	-3.044474000	0.383873000
25	0.123046000	0.038120000	-0.208282000
7	-0.401970000	2.265206000	0.032118000
7	2.122114000	1.283218000	0.085423000
7	1.893758000	-1.421166000	0.013495000
6	-1.641019000	2.674225000	0.320927000
1	-2.382760000	1.891015000	0.417148000
6	-1.962499000	4.011147000	0.493513000
1	-2.977326000	4.301560000	0.726562000
6	0.339792000	4.528381000	0.075222000
6	0.577786000	3.168871000	-0.091112000
6	1.943604000	2.631599000	-0.456971000
1	2.004361000	2.561249000	-1.546686000
6	3.252039000	0.530240000	-0.462490000
1	3.211391000	0.617063000	-1.551948000
6	3.135446000	-0.932975000	-0.098411000

6	4.253882000	-1.739487000	0.077760000
1	5.245442000	-1.315317000	-0.007074000
6	1.720804000	-2.715528000	0.298349000
1	2.722886000	3.328708000	-0.134421000
1	4.222281000	0.922347000	-0.143008000
1	1.152749000	5.235895000	-0.019276000
6	-0.948988000	4.954508000	0.366626000
1	-1.158356000	6.007784000	0.500165000
1	2.218695000	1.340728000	1.095740000
6	-2.290457000	-1.356250000	-0.833219000
6	-2.217110000	-1.331110000	0.609703000
6	-3.245925000	-1.916569000	1.347184000
6	-4.348861000	-2.527757000	0.726948000
6	-4.422793000	-2.553360000	-0.658489000
6	-3.403515000	-1.972949000	-1.425518000
1	-5.131367000	-2.972884000	1.330788000
1	-3.467509000	-1.995917000	-2.510163000
8	-1.165750000	-0.747467000	1.180841000
1	-3.172266000	-1.887362000	2.429991000
7	-1.246674000	-0.764174000	-1.501240000
1	-1.359172000	-0.808356000	-2.505333000
1	-5.266852000	-3.019714000	-1.154688000

Mn^{II}-OAP adduct 2B

6	-0.673924000	4.915207000	-0.305504000
1	-0.857189000	5.971187000	-0.156192000
6	0.618402000	4.443394000	-0.503276000
1	1.467671000	5.111892000	-0.515781000
1	1.782682000	2.647055000	-0.823275000
25	0.197074000	-0.005088000	-0.643366000

7	-0.845336000	-1.994451000	-0.715786000
7	-2.150589000	0.346028000	0.017338000
7	-0.216803000	2.214030000	-0.672696000
6	-0.116336000	-3.114008000	-0.798007000
1	0.943063000	-2.966125000	-0.968489000
6	-0.673252000	-4.375649000	-0.673722000
1	-0.049593000	-5.255472000	-0.745935000
6	-2.795241000	-3.310611000	-0.356059000
6	-2.161926000	-2.080970000	-0.498974000
6	-2.941338000	-0.784264000	-0.475926000
1	-3.222452000	-0.559994000	-1.506441000
6	-2.566560000	1.631500000	-0.561151000
1	-2.794028000	1.469854000	-1.617038000
6	-1.464622000	2.663153000	-0.488567000
6	-1.729369000	4.012799000	-0.292947000
1	-2.745815000	4.345810000	-0.132076000
6	0.801101000	3.080851000	-0.676877000
1	-3.879402000	-0.924265000	0.070558000
1	-3.472907000	2.018958000	-0.083929000
1	-3.860273000	-3.350718000	-0.169815000
6	-2.041919000	-4.472275000	-0.447404000
1	-2.514576000	-5.439415000	-0.336593000
6	3.026590000	-0.410837000	-0.526095000
6	2.584194000	-0.333569000	0.847314000
6	3.528171000	-0.452256000	1.867176000
6	4.893855000	-0.642083000	1.596115000
6	5.322698000	-0.713592000	0.278192000
6	4.396461000	-0.599476000	-0.767179000
1	5.600902000	-0.729752000	2.413062000
1	4.738085000	-0.656798000	-1.797314000

8	1.287015000	-0.151168000	1.086919000
1	3.175795000	-0.393581000	2.892414000
7	2.049406000	-0.291738000	-1.482987000
1	2.422614000	-0.354751000	-2.420888000
1	6.372805000	-0.858651000	0.049327000
6	-2.025737000	0.458911000	1.471458000
6	-3.212986000	0.561355000	2.392266000
6	-2.316326000	-0.655540000	2.422121000
1	-1.173794000	1.072846000	1.733465000
1	-4.199042000	0.429797000	1.965433000
1	-3.165923000	1.274186000	3.204218000
1	-1.631871000	-0.784090000	3.249511000
1	-2.728092000	-1.580752000	2.045775000

Mn^{II}-OAP adduct 3B

6	3.463190000	-3.614374000	-0.619065000
1	4.261688000	-4.341457000	-0.549946000
6	2.137820000	-4.026058000	-0.712020000
1	1.870655000	-5.073356000	-0.719010000
1	0.104053000	-3.308754000	-0.861438000
25	-0.245433000	-0.259076000	-0.709252000
7	-0.667115000	1.951013000	-0.879877000
7	1.846552000	0.949607000	-0.249285000
7	1.431842000	-1.745036000	-0.784430000
6	-1.927225000	2.390835000	-0.814880000
1	-2.691108000	1.624443000	-0.864320000
6	-2.237888000	3.735593000	-0.685426000
1	-3.269991000	4.053249000	-0.637004000
6	0.115717000	4.188931000	-0.668136000
6	0.343297000	2.825961000	-0.809624000

6	1.732103000	2.245422000	-0.937551000
1	1.924359000	2.081659000	-1.999774000
6	2.970302000	0.146151000	-0.740321000
1	3.137807000	0.407319000	-1.787109000
6	2.703891000	-1.343146000	-0.693245000
6	3.749034000	-2.257465000	-0.606801000
1	4.768187000	-1.904066000	-0.523286000
6	1.154642000	-3.055449000	-0.790706000
1	2.474148000	2.967942000	-0.581072000
1	3.905432000	0.366380000	-0.217009000
1	0.951011000	4.872828000	-0.600222000
6	-1.193595000	4.649576000	-0.610146000
1	-1.395312000	5.706940000	-0.499073000
6	-2.882046000	-1.326688000	-0.435080000
6	-2.436013000	-1.031277000	0.907529000
6	-3.320828000	-1.222667000	1.968728000
6	-4.630321000	-1.690856000	1.768490000
6	-5.062328000	-1.974594000	0.480596000
6	-4.195030000	-1.793689000	-0.604910000
1	-5.292123000	-1.826888000	2.616170000
1	-4.539389000	-2.016422000	-1.611328000
8	-1.193784000	-0.584063000	1.081111000
1	-2.967611000	-0.994784000	2.969676000
7	-1.967021000	-1.114885000	-1.436740000
1	-2.345240000	-1.326103000	-2.350683000
1	-6.069929000	-2.335940000	0.306452000
6	1.812554000	1.141731000	1.211384000
6	2.017183000	-0.044231000	2.175402000
6	2.922836000	1.918894000	1.969730000
1	0.847692000	1.599095000	1.435131000

6	2.671375000	0.958133000	3.161065000
1	2.756512000	-0.754957000	1.808833000
1	1.120678000	-0.582673000	2.475206000
1	3.909774000	1.758936000	1.533071000
1	2.771827000	2.986444000	2.124383000
1	3.544165000	0.611854000	3.711852000
1	1.947004000	1.368416000	3.865153000

Mn^{II}-OAP adduct 4B

6	3.021851000	-3.982288000	-0.732342000
1	3.763823000	-4.767652000	-0.671204000
6	1.665033000	-4.289910000	-0.740478000
1	1.317250000	-5.311961000	-0.688431000
1	-0.312284000	-3.417140000	-0.818121000
25	-0.405097000	-0.347504000	-0.763929000
7	-0.693909000	1.873977000	-1.070429000
7	1.793424000	0.721390000	-0.516726000
7	1.136500000	-1.964447000	-0.876904000
6	-1.900143000	2.427002000	-0.921017000
1	-2.729040000	1.732028000	-0.863497000
6	-2.080593000	3.799393000	-0.835648000
1	-3.072893000	4.211138000	-0.716242000
6	0.295784000	4.038849000	-1.042270000
6	0.390699000	2.656548000	-1.131842000
6	1.701684000	1.938831000	-1.343123000
1	1.739522000	1.630635000	-2.389981000
6	2.823392000	-0.203753000	-1.003694000
1	2.977393000	-0.011636000	-2.067306000
6	2.438950000	-1.662472000	-0.870038000
6	3.412584000	-2.653624000	-0.795486000

1	4.459276000	-2.379875000	-0.780777000
6	0.757559000	-3.247786000	-0.811759000
1	2.537702000	2.624649000	-1.176989000
1	3.792439000	-0.040765000	-0.523288000
1	1.189740000	4.646448000	-1.080636000
6	-0.959287000	4.617747000	-0.896930000
1	-1.058749000	5.692832000	-0.823964000
6	-3.102738000	-1.155650000	-0.280287000
6	-2.564910000	-0.786122000	1.009017000
6	-3.409526000	-0.788607000	2.118788000
6	-4.766545000	-1.137858000	2.017631000
6	-5.287390000	-1.492355000	0.781105000
6	-4.462233000	-1.499168000	-0.351313000
1	-5.395493000	-1.128063000	2.900415000
1	-4.876702000	-1.776339000	-1.316929000
8	-1.277059000	-0.454935000	1.088592000
1	-2.985714000	-0.506127000	3.077470000
7	-2.220858000	-1.131438000	-1.332495000
1	-2.662681000	-1.385316000	-2.206289000
1	-6.332631000	-1.764484000	0.683254000
6	1.898398000	1.056740000	0.928103000
6	1.946931000	-0.143487000	1.879236000
6	3.102265000	1.943014000	1.349255000
1	0.978632000	1.598869000	1.159147000
6	2.344050000	0.511939000	3.201782000
1	2.728336000	-0.845565000	1.578971000
1	0.997057000	-0.675134000	1.911251000
6	3.448783000	1.506692000	2.795680000
1	2.844949000	3.000525000	1.290926000
1	3.952333000	1.788117000	0.682784000

1	1.485446000	1.045951000	3.619248000
1	2.676969000	-0.207928000	3.950131000
1	3.518174000	2.352696000	3.479775000
1	4.417361000	1.002768000	2.809432000

Mn^{II}-OAP adduct 5B

6	1.652440000	-4.668159000	-0.801310000
1	2.150950000	-5.624599000	-0.712680000
6	0.264124000	-4.588530000	-0.770445000
1	-0.350183000	-5.471088000	-0.661000000
1	-1.397154000	-3.203618000	-0.852815000
25	-0.654502000	-0.248855000	-0.841382000
7	-0.362436000	1.941576000	-1.215814000
7	1.798481000	0.198401000	-0.779236000
7	0.393327000	-2.215396000	-1.010938000
6	-1.350639000	2.810901000	-0.991171000
1	-2.324823000	2.374522000	-0.807642000
6	-1.144283000	4.182272000	-0.985711000
1	-1.969645000	4.855382000	-0.801157000
6	1.169964000	3.749587000	-1.437783000
6	0.879535000	2.392250000	-1.435990000
6	1.912775000	1.330283000	-1.716725000
1	1.712351000	0.941606000	-2.717354000
6	2.492994000	-0.997975000	-1.273003000
1	2.621035000	-0.896977000	-2.352669000
6	1.728479000	-2.285503000	-1.045877000
6	2.392309000	-3.503363000	-0.939593000
1	3.473752000	-3.530496000	-0.959284000
6	-0.322682000	-3.339586000	-0.876001000
1	2.912291000	1.772114000	-1.739517000

1	3.499953000	-1.096667000	-0.860394000
1	2.183831000	4.085945000	-1.606948000
6	0.141376000	4.657217000	-1.213618000
1	0.343441000	5.720285000	-1.209078000
6	-3.419075000	-0.443263000	-0.116861000
6	-2.706314000	-0.179563000	1.112235000
6	-3.432070000	-0.009149000	2.290638000
6	-4.834733000	-0.088062000	2.316107000
6	-5.523176000	-0.343332000	1.138352000
6	-4.820110000	-0.518212000	-0.061024000
1	-5.368223000	0.050130000	3.249542000
1	-5.365255000	-0.715832000	-0.980149000
8	-1.376800000	-0.109040000	1.072364000
1	-2.877405000	0.189856000	3.202410000
7	-2.646893000	-0.597238000	-1.241318000
1	-3.204705000	-0.769988000	-2.067248000
1	-6.605833000	-0.406842000	1.138305000
6	2.135680000	0.578849000	0.628815000
6	1.883060000	-0.573927000	1.605662000
6	3.551156000	1.144033000	0.826025000
1	1.422569000	1.369936000	0.880282000
6	2.084204000	-0.115494000	3.052789000
1	2.576519000	-1.394434000	1.397642000
1	0.870257000	-0.953502000	1.476856000
6	3.759185000	1.597618000	2.275975000
1	4.292900000	0.378761000	0.577128000
1	3.728581000	1.988529000	0.158949000
6	3.481313000	0.467456000	3.268222000
1	1.912188000	-0.956505000	3.728768000
1	1.331076000	0.642102000	3.295866000

1	4.776742000	1.975928000	2.400069000
1	3.084769000	2.435281000	2.486307000
1	3.590125000	0.828765000	4.294021000
1	4.226424000	-0.324376000	3.130312000

Mn^{II}-OAP adduct 6B

6	1.390932000	-4.173080000	-1.430096000
1	1.914496000	-5.117021000	-1.507009000
6	0.043917000	-4.138043000	-1.088840000
1	-0.512809000	-5.043859000	-0.894193000
1	-1.625383000	-2.806989000	-0.734725000
25	-0.964407000	0.181656000	-0.743322000
7	-0.609624000	2.390218000	-0.584613000
7	1.542844000	0.621253000	-0.934074000
7	0.067209000	-1.755697000	-1.224046000
6	-1.519249000	3.182007000	-0.009600000
1	-2.460893000	2.710413000	0.242199000
6	-1.278590000	4.521500000	0.255123000
1	-2.040985000	5.128454000	0.722731000
6	0.906685000	4.222943000	-0.680902000
6	0.586792000	2.892819000	-0.918604000
6	1.537275000	1.935961000	-1.596771000
1	1.182193000	1.792018000	-2.619411000
6	2.013656000	-0.446252000	-1.828165000
1	1.730979000	-0.170759000	-2.846395000
6	1.365605000	-1.781842000	-1.546775000
6	2.061207000	-2.979256000	-1.662047000
1	3.111820000	-2.970846000	-1.919429000
6	-0.579193000	-2.903494000	-0.998154000
1	2.531965000	2.387473000	-1.665091000

1	3.101076000	-0.552683000	-1.832660000
1	1.884373000	4.599113000	-0.950092000
6	-0.040406000	5.049294000	-0.088701000
1	0.188722000	6.088309000	0.108630000
6	2.240204000	0.690510000	0.395359000
6	3.780503000	0.842266000	0.281851000
1	1.862777000	1.615186000	0.835985000
6	1.774345000	-0.434896000	1.324136000
6	4.651755000	-0.397011000	0.545892000
1	4.094709000	1.623189000	0.978829000
1	4.018785000	1.236950000	-0.707666000
1	1.958662000	-1.409185000	0.868933000
1	0.692529000	-0.351772000	1.431363000
6	2.425445000	-0.419104000	2.716216000
6	4.907925000	-0.676873000	2.032010000
1	4.227635000	-1.286737000	0.071791000
1	5.617064000	-0.230162000	0.060441000
6	3.717038000	-1.237721000	2.810191000
1	2.609349000	0.612842000	3.035647000
1	1.708997000	-0.832511000	3.430333000
1	5.740805000	-1.380665000	2.121971000
1	5.242072000	0.254167000	2.504331000
1	3.504603000	-2.252480000	2.454060000
1	4.003532000	-1.336637000	3.861601000
8	-1.717744000	-0.232561000	1.118572000
7	-2.919956000	-0.145126000	-1.275321000
6	-3.690310000	-0.497634000	-0.195456000
6	-5.056204000	-0.820806000	-0.226060000
6	-5.760251000	-1.165850000	0.935505000
6	-5.108211000	-1.195230000	2.160177000

6	-3.740397000	-0.878688000	2.220316000
6	-3.014804000	-0.533208000	1.080873000
1	-5.572990000	-0.798688000	-1.181791000
1	-6.815099000	-1.409007000	0.869484000
1	-5.642864000	-1.460444000	3.065048000
1	-3.214133000	-0.897519000	3.169628000
1	-3.447198000	-0.145460000	-2.138549000