Supporting Information

for

Reaction of a Nitrosyl Complex of Mn(II)-porphyrinate with Superoxide: NOD Activity is More Favorable Over SOD Activity

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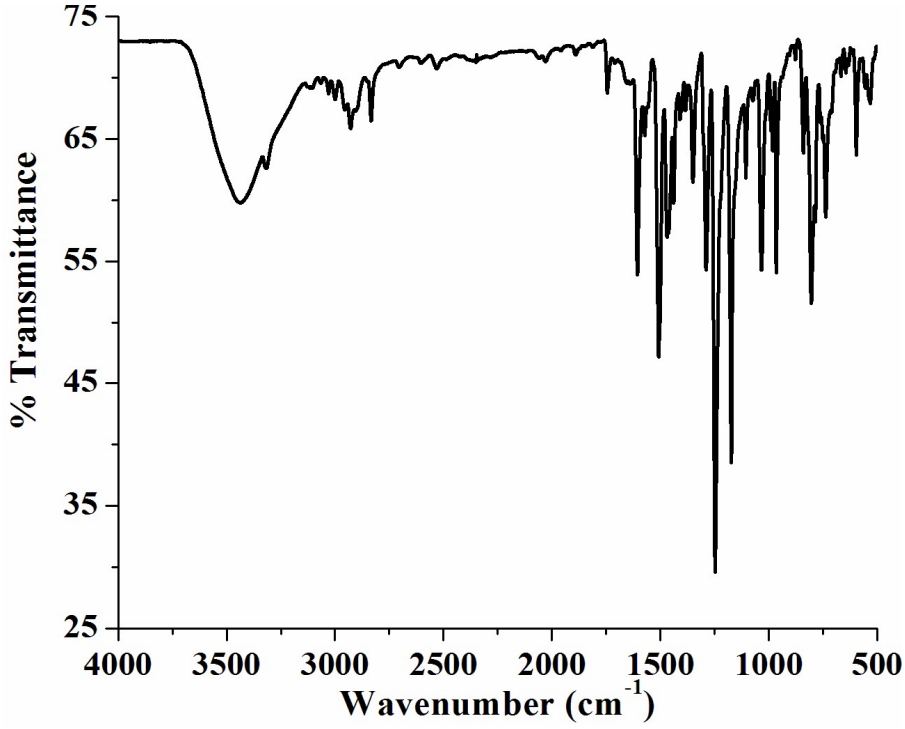

Figure S1. FT-IR spectrum of ligand **$TMPPH_2$** in KBr.

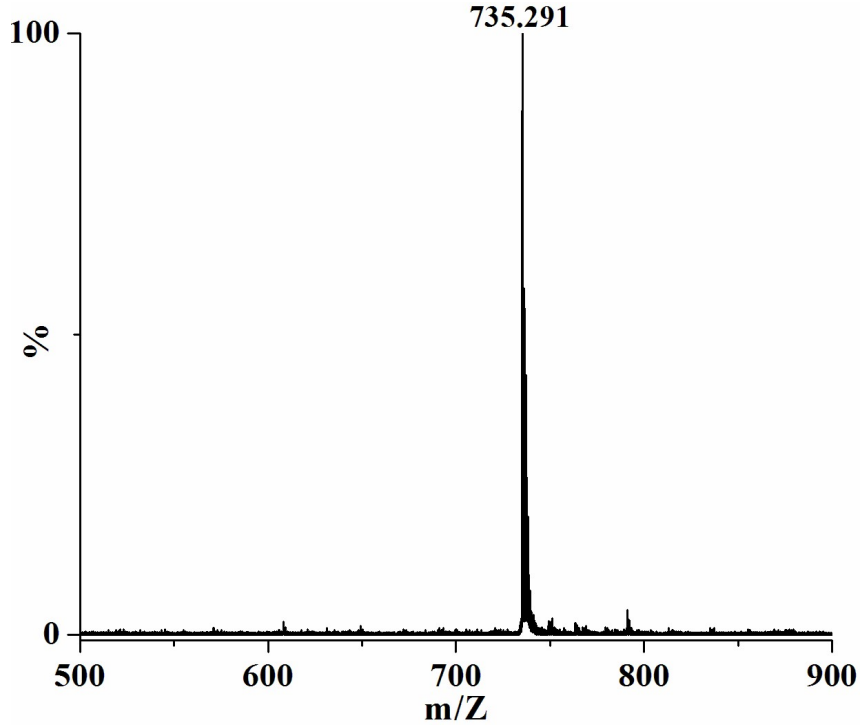

Figure S2. ESI-mass spectrum of ligand **$TMPPH_2$** in acetonitrile.

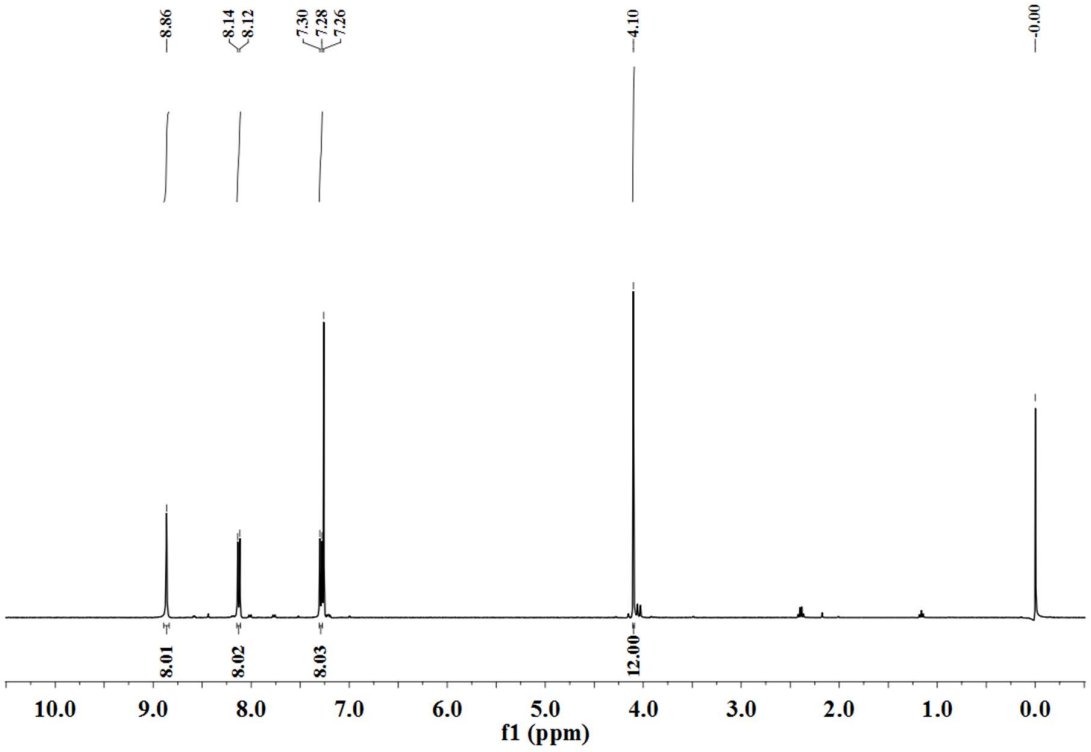

Figure S3. ^{1}H NMR spectrum of ligand **TMPPH$_2$** in $CDCl_3$.

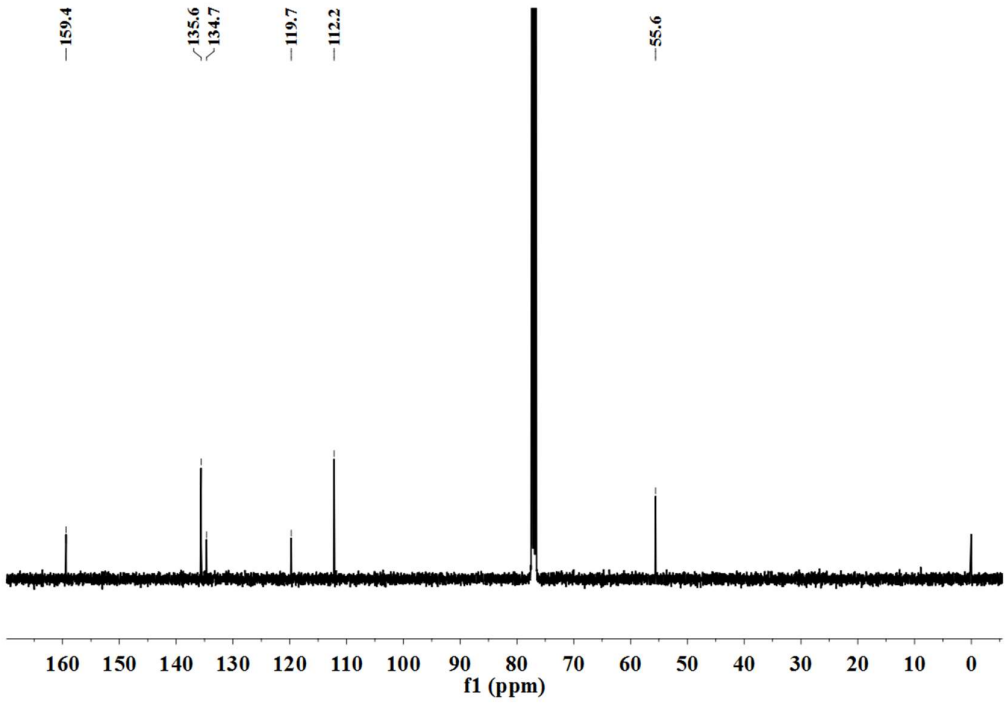

Figure S4. ^{13}C NMR spectrum of ligand **TMPPH$_2$** in $CDCl_3$.

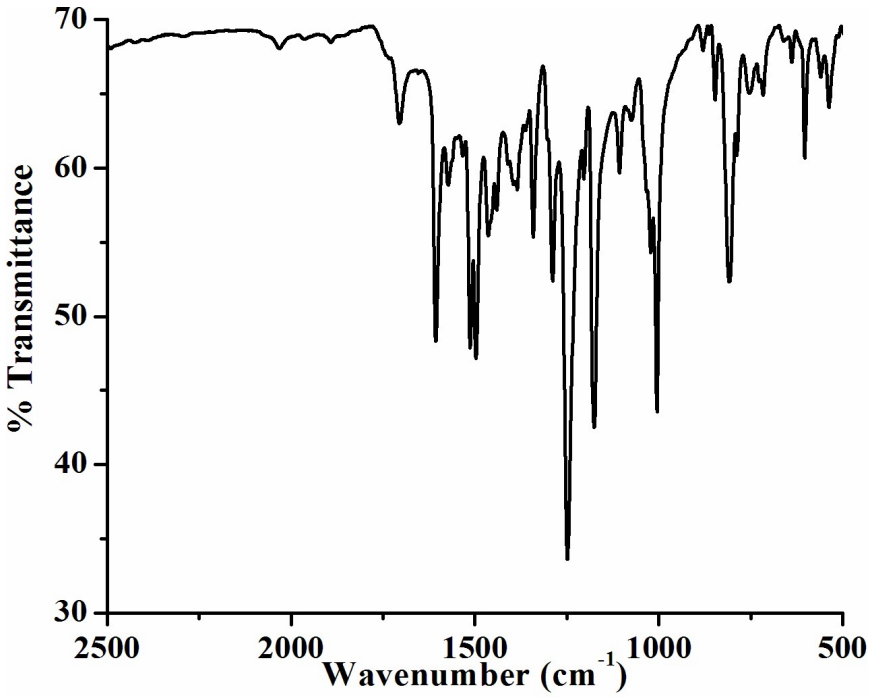

Figure S5. FT-IR spectrum of complex **1a** in KBr.

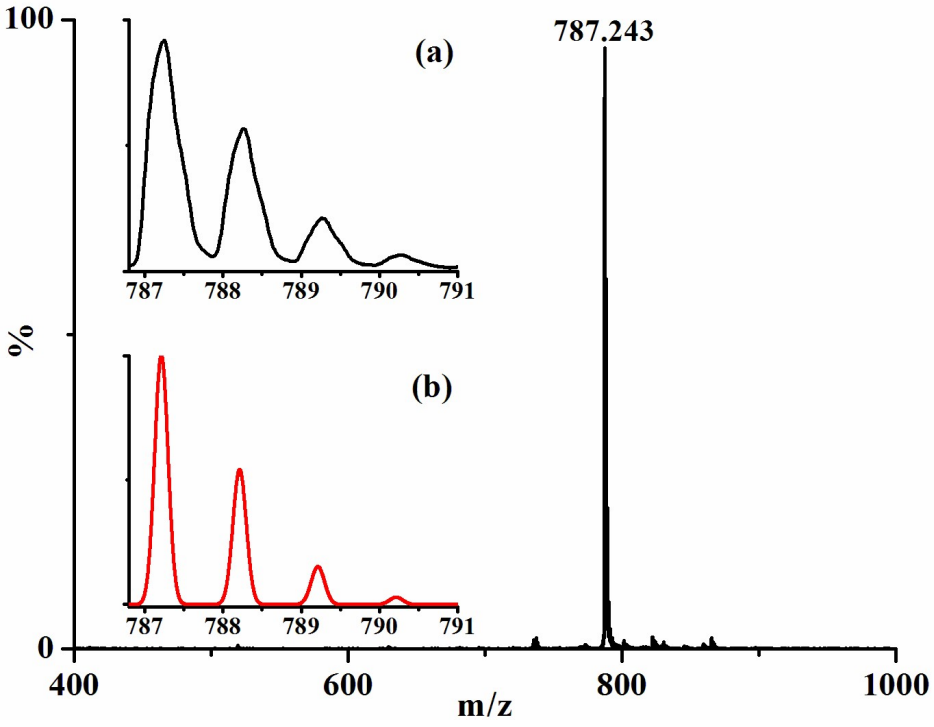

Figure S6. ESI-mass spectrum of complex **1a** in acetonitrile. [Inset: (a) experimental and (b) simulated isotopic distribution pattern].

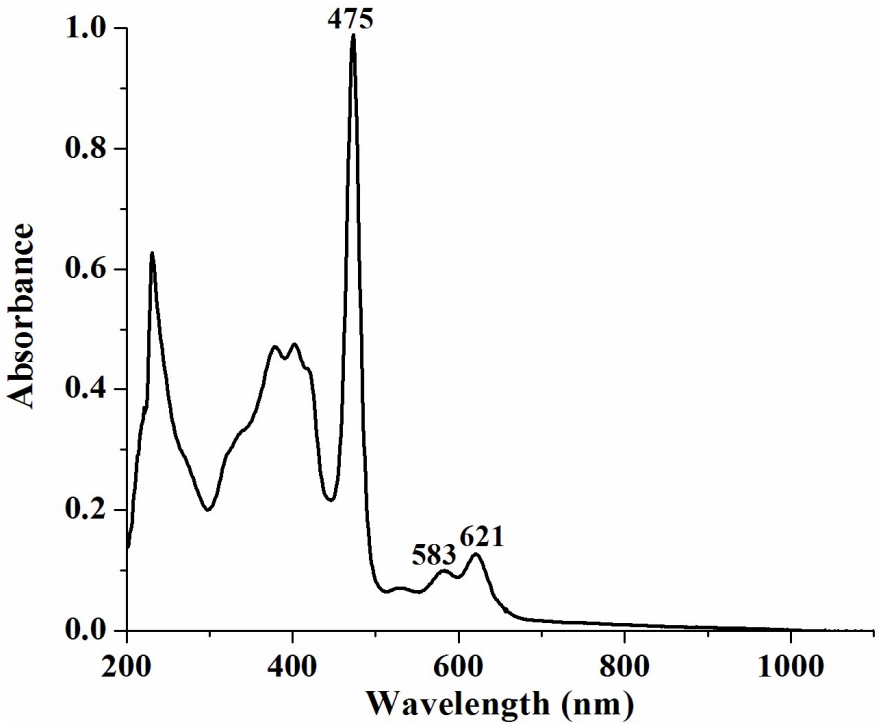

Figure S7. UV-visible spectrum of complex **1a** in dichloromethane at RT.

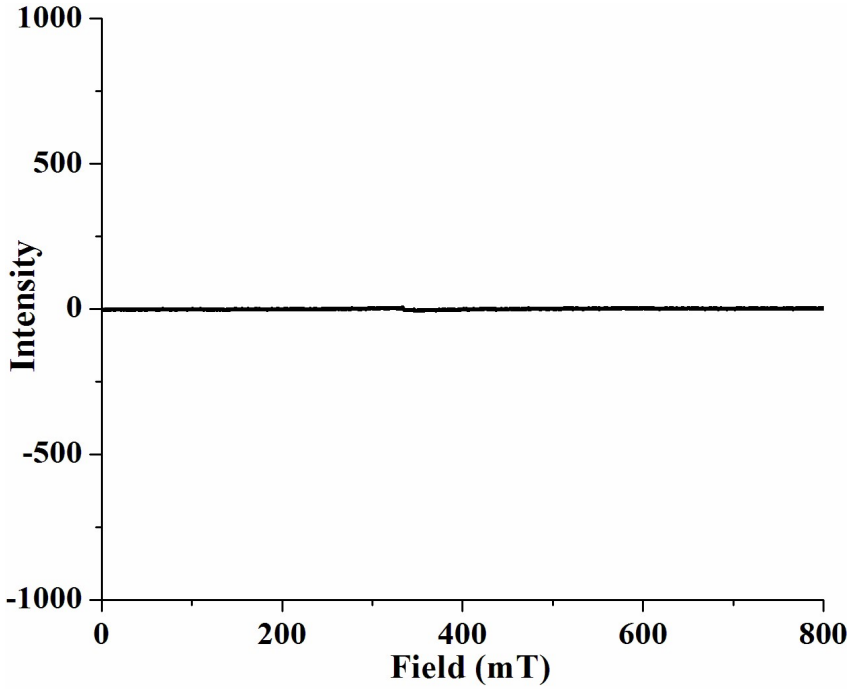

Figure S8. X-band EPR spectrum of complex **1a** in dichloromethane at 77K.

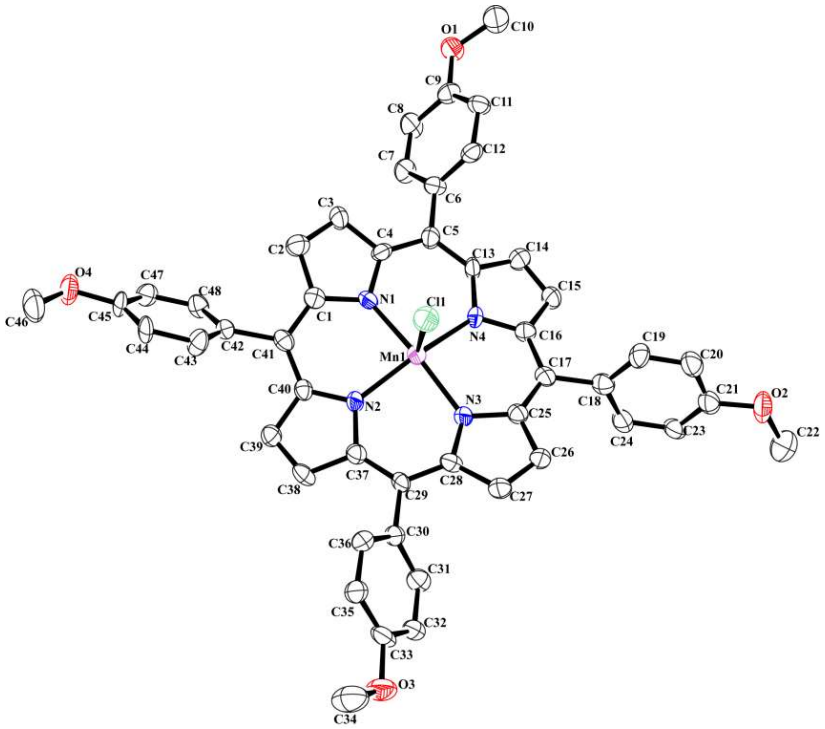

Figure S9. ORTEP diagram of complex **1a** (30% thermal ellipsoid plot, H-atoms are omitted for clarity).

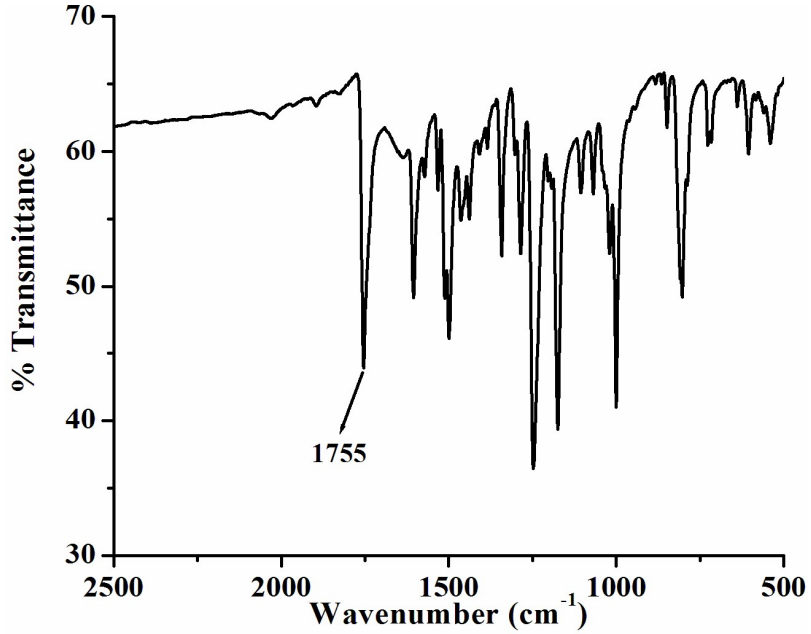

Figure S10. FT-IR spectrum of complex **1** in KBr.

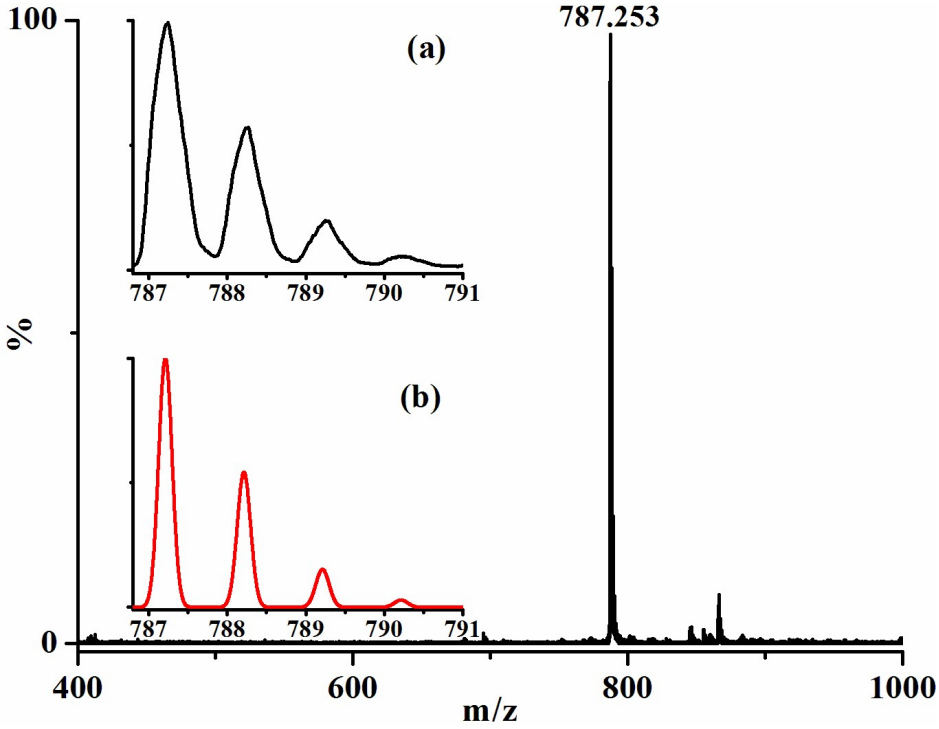

Figure S11. ESI-mass spectrum of complex **1** in acetonitrile. [Inset: (a) experimental and (b) simulated isotopic distribution pattern].

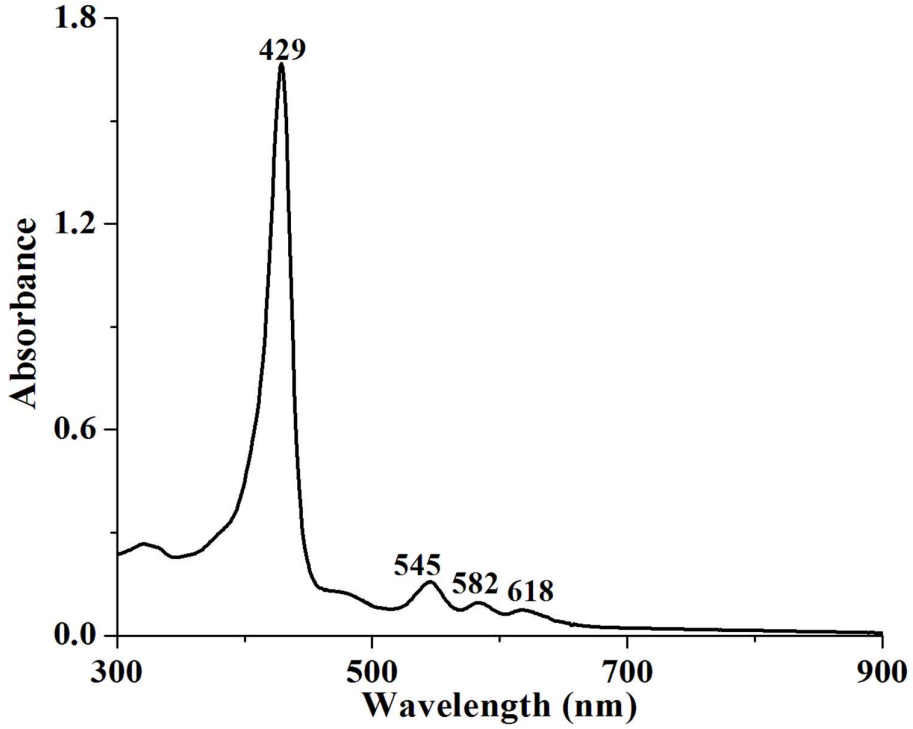

Figure S12. UV-visible spectrum of complex **1** in dichloromethane at RT.

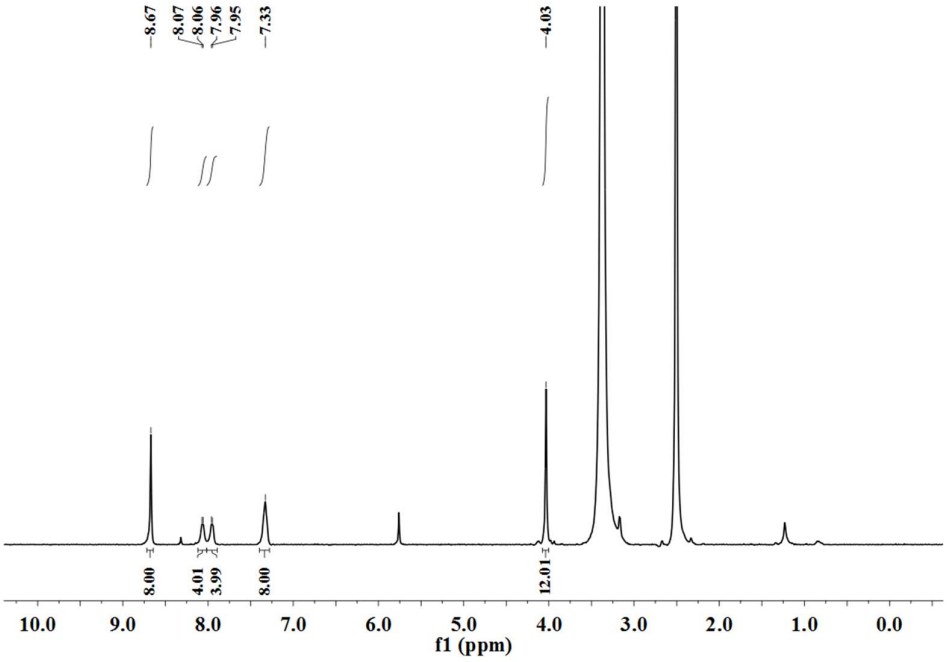

Figure S13. ^{1}H NMR spectrum of complex **1** in DMSO-d_6.

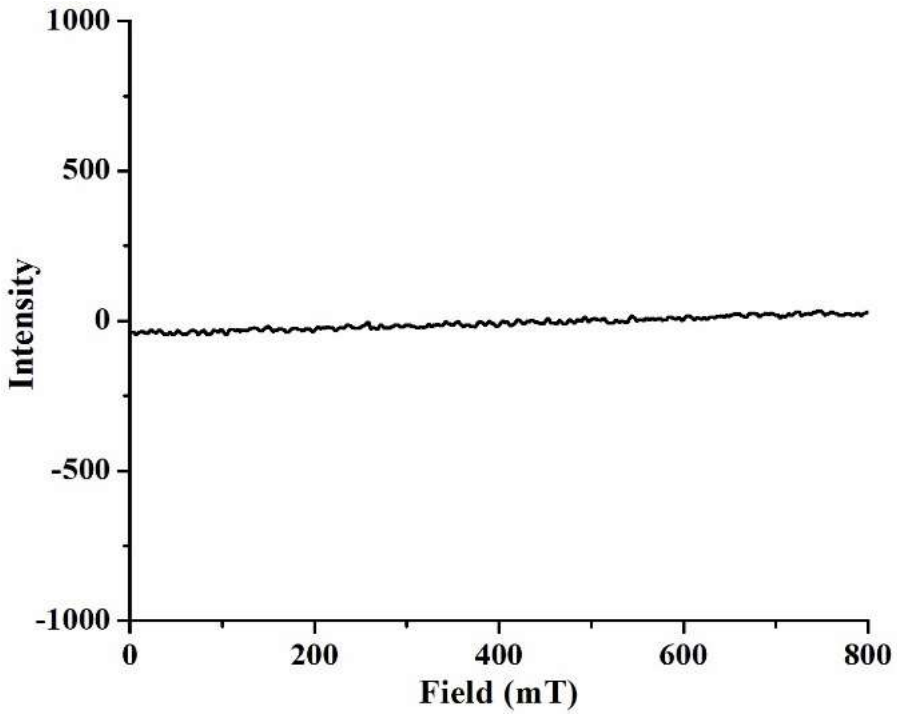

Figure S14. X-band EPR spectrum of complex **1** in THF at 77K.

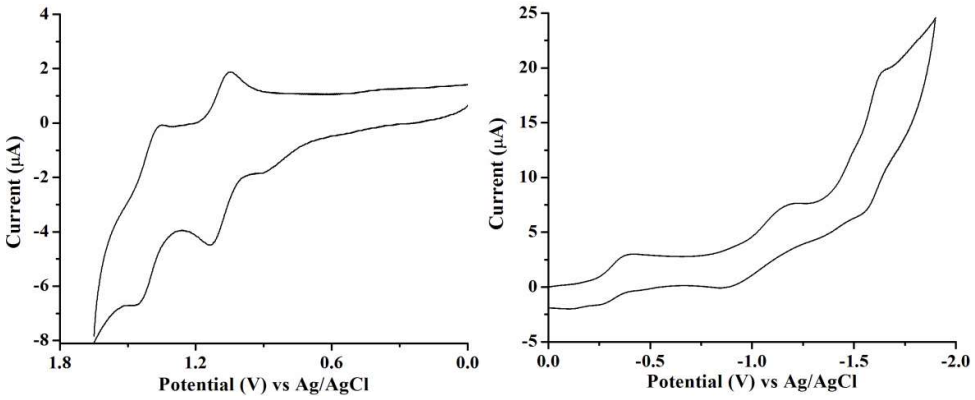

Figure S15. Cyclic voltammograms of complex **1** in dichloromethane *vs.* Ag/AgCl, supporting electrolyte 0.1 M TBAP, Scan rate 0.1 v/s.

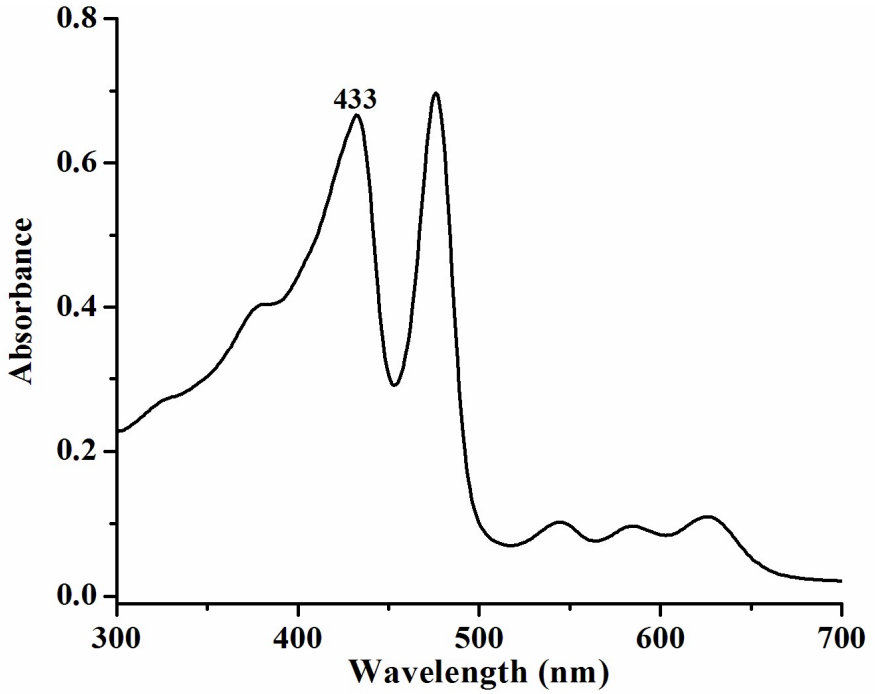

Figure S16: UV-visible spectrum of the reaction mixture of complex **1a** and *t*BuOOH at −40 °C in THF.

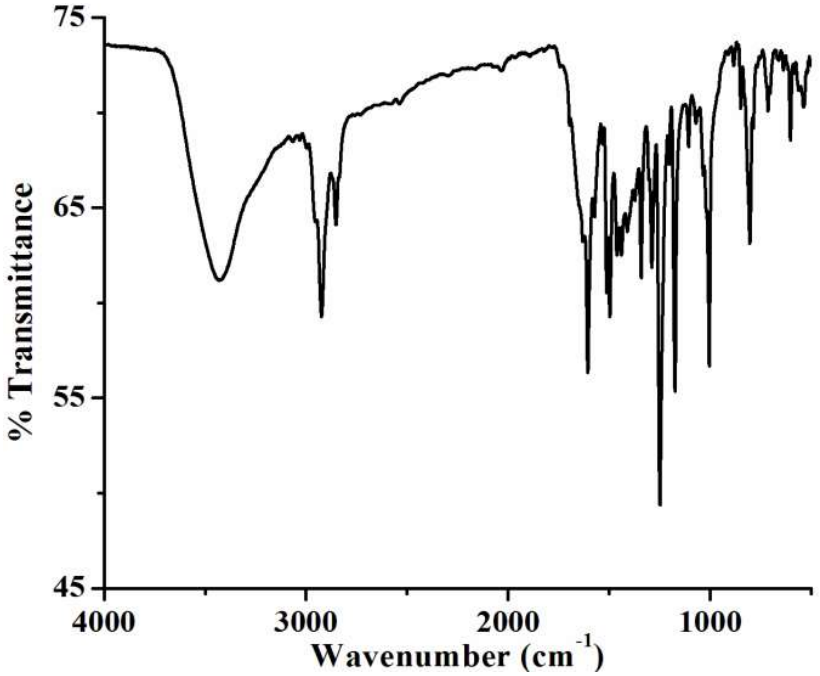

Figure S17. FT-IR spectrum of complex **2** in KBr.

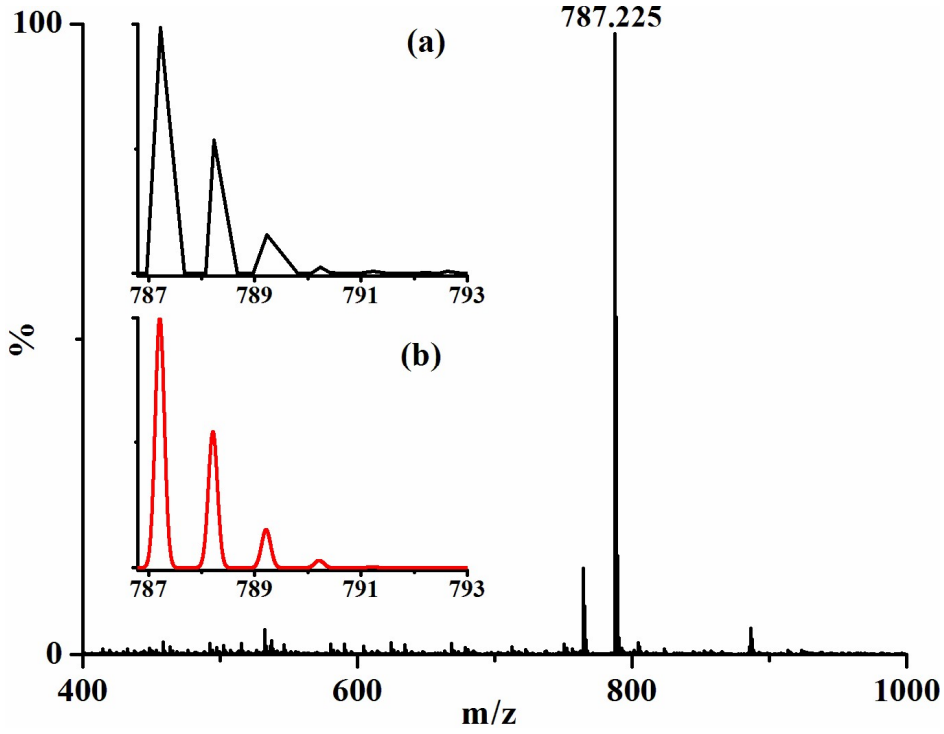

Figure S18. ESI-mass spectrum of complex **2** in acetonitrile. [Inset: (a) experimental and (b) simulated isotopic distribution pattern].

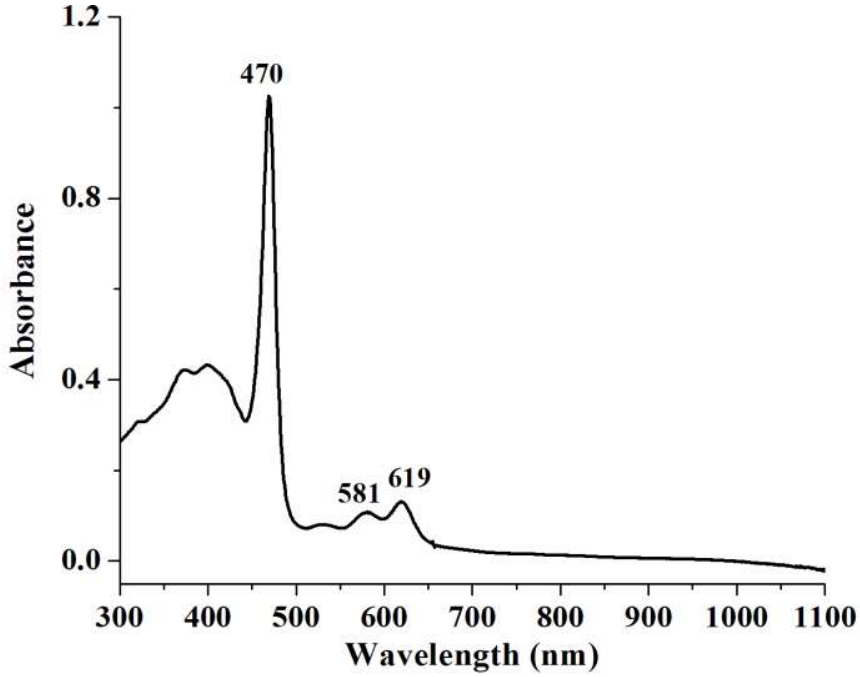

Figure S19. UV-visible spectrum of complex **2** in THF.

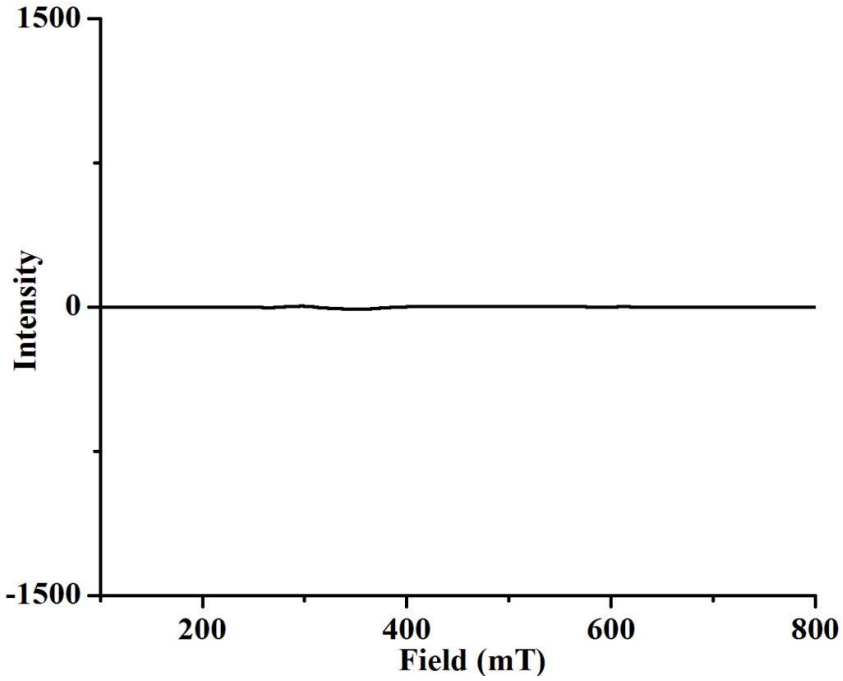

Figure S20. X-band EPR spectrum of complex **2** in THF at 77K.

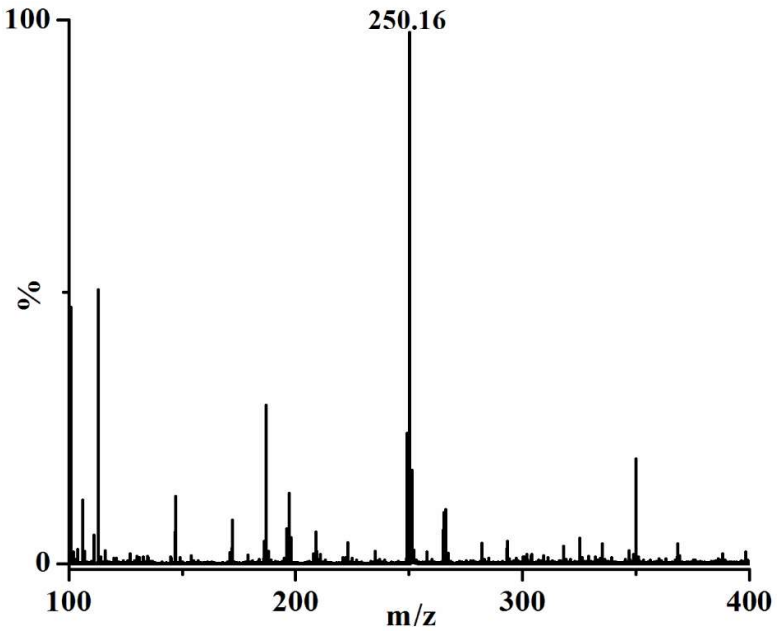

Figure S21. ESI-mass spectrum of 2,4-di-*tert*-butyl-6-nitrophenol in acetonitrile.

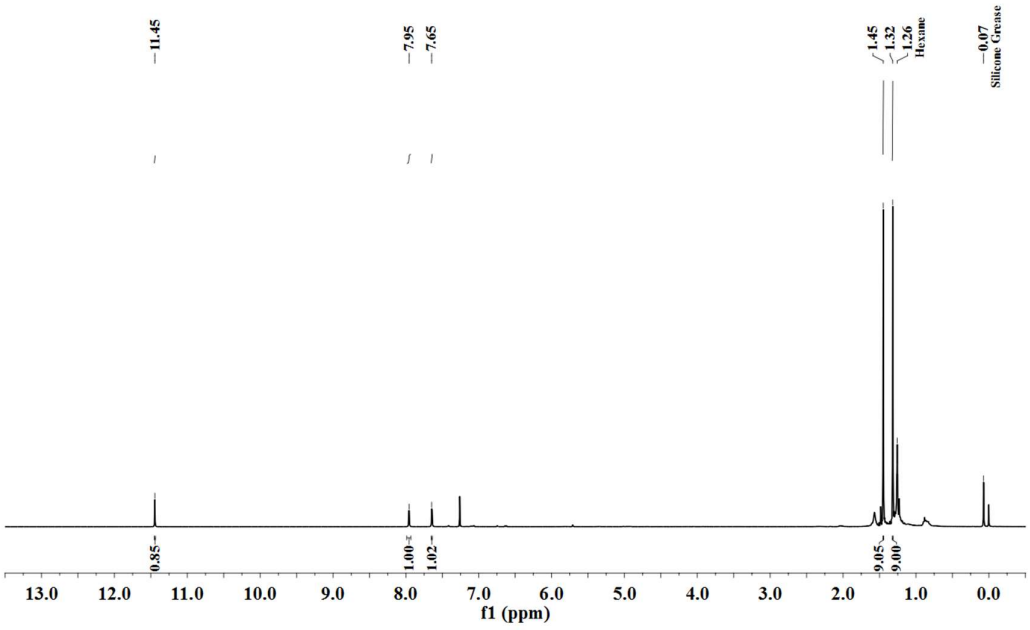

Figure S22. ^{1}H NMR spectrum of 2,4-di-*tert*-butyl-6-nitrophenol in $CDCl_3$.

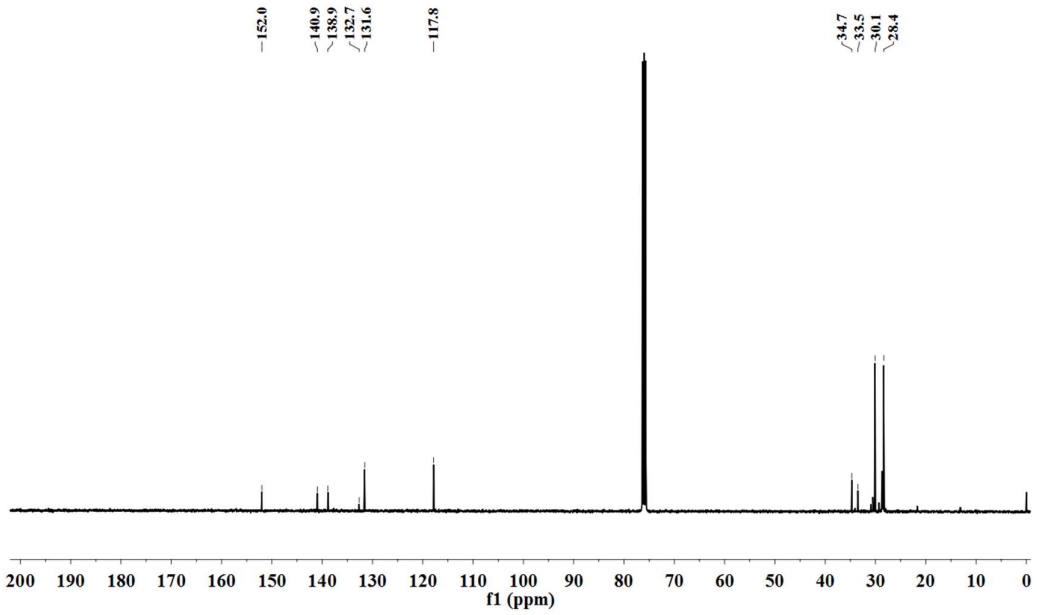

Figure S23. ^{13}C NMR spectrum of 2,4-di-*tert*-butyl-6-nitrophenol in $CDCl_3$.

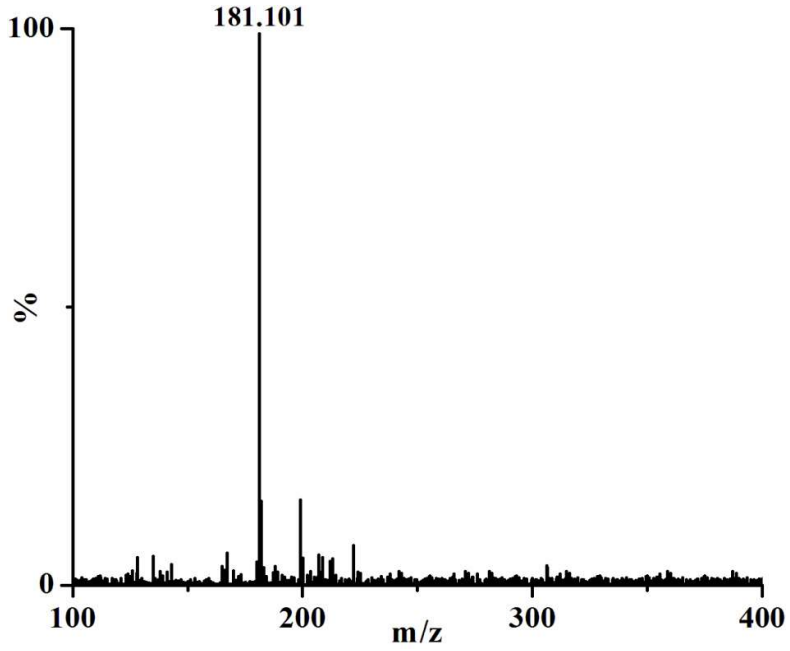

Figure S24. ESI-mass spectrum of 9-fluorenone in acetonitrile.

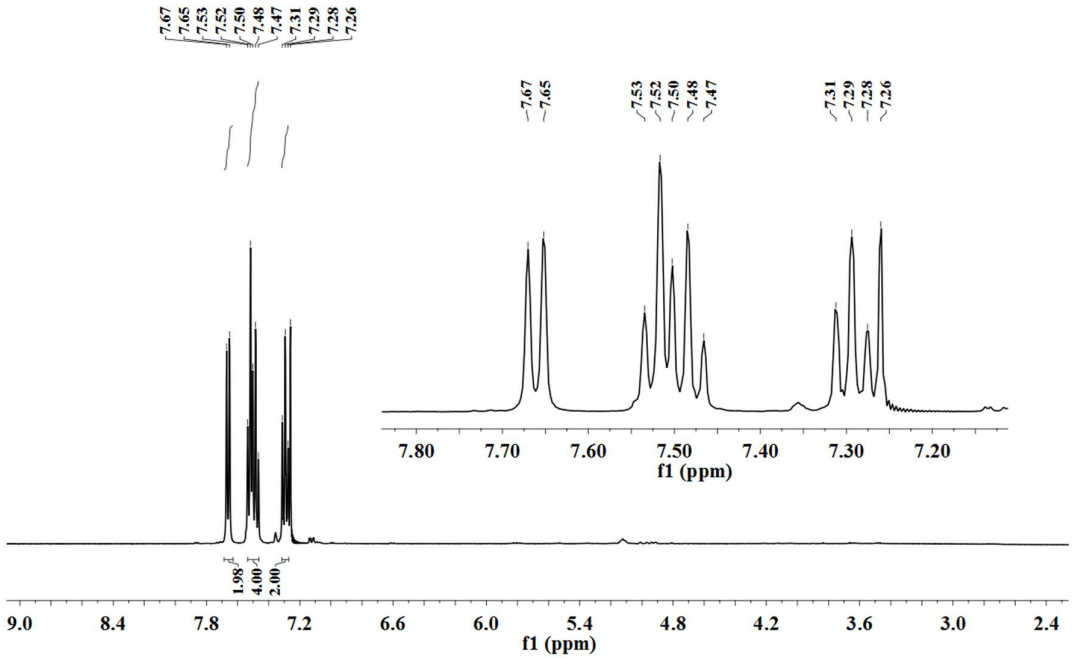

Figure S25. ^{1}H NMR spectrum of 9-fluorenone in $CDCl_3$.

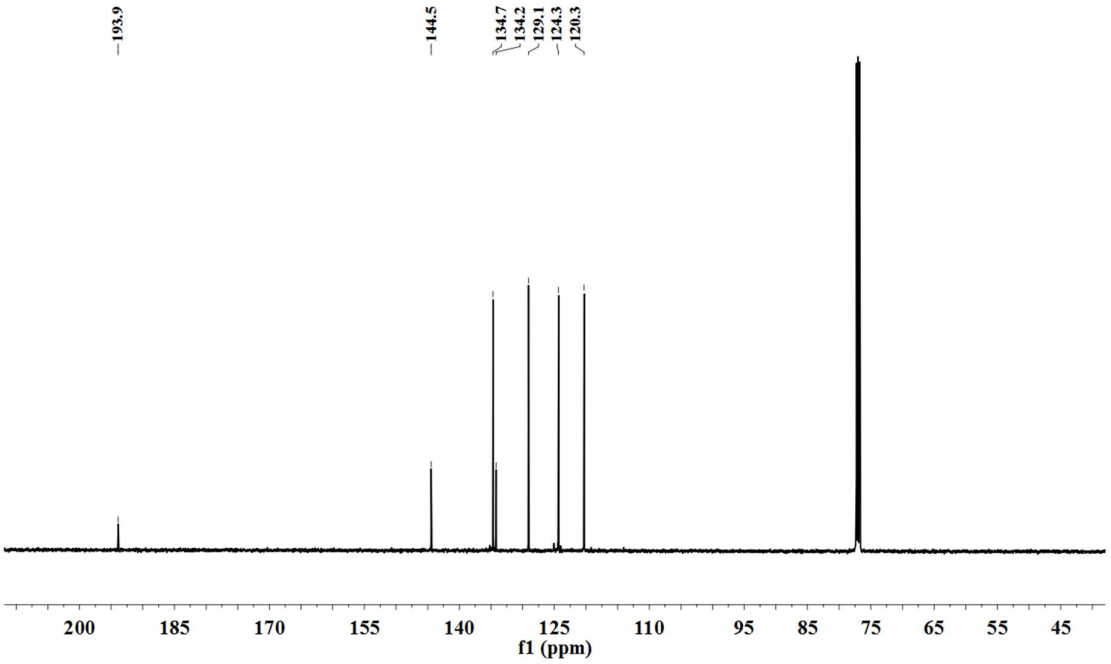

Figure S26. ^{13}C NMR spectrum of 9-fluorenone in $CDCl_3$.

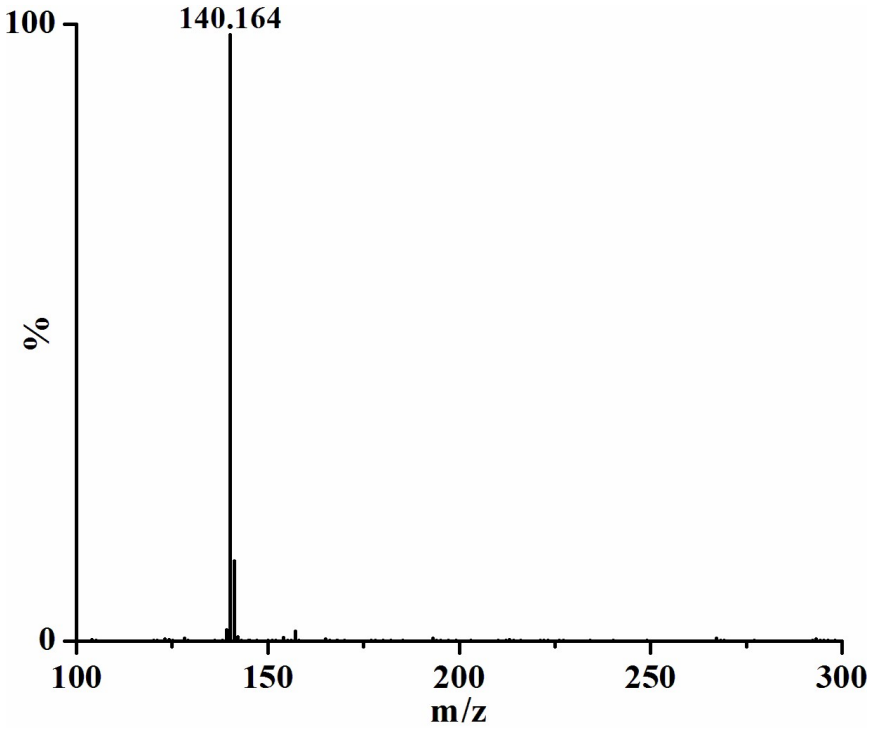

Figure S27. ESI-mass spectrum of $tmpNO_3$ in acetonitrile.

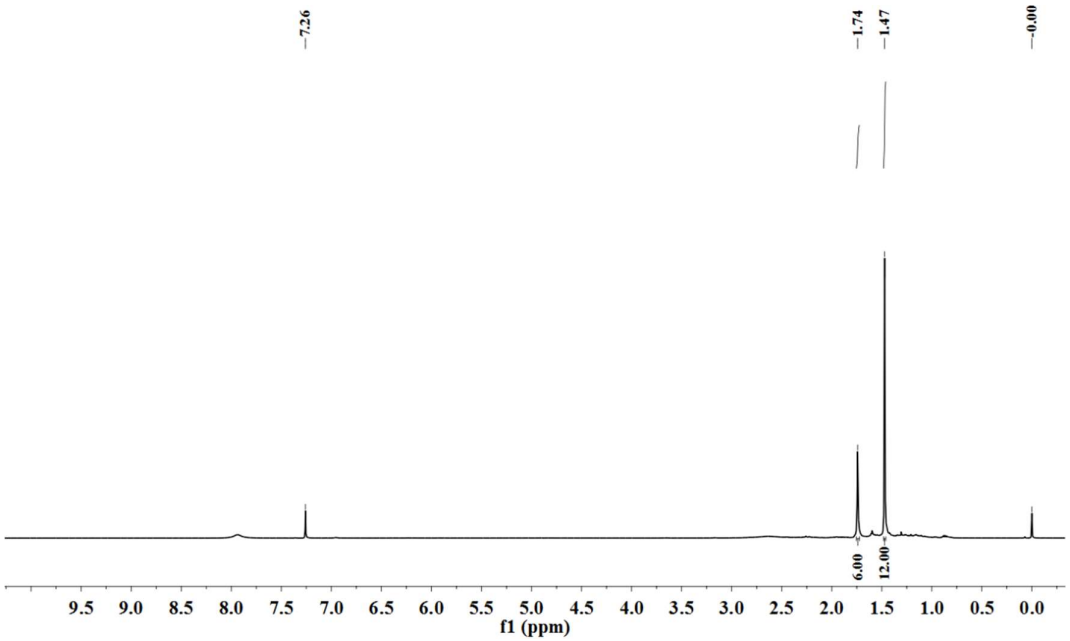

Figure S28. ^1H NMR spectrum of $tmpNO_3$ in $CDCl_3$.

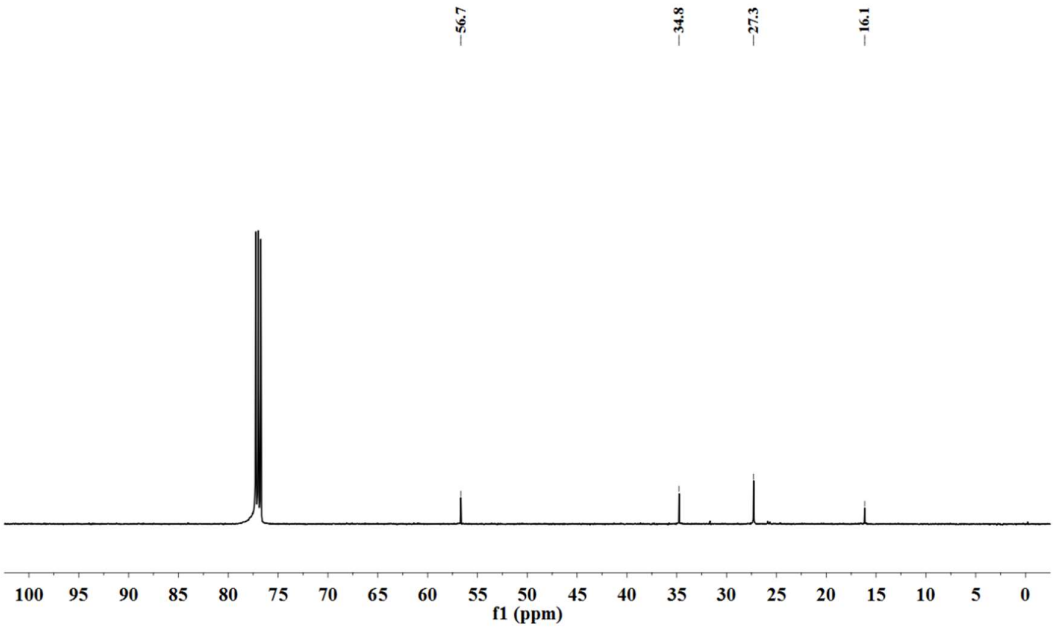

Figure S29. ^{13}C NMR spectrum of $tmpNO_3$ in $CDCl_3$.

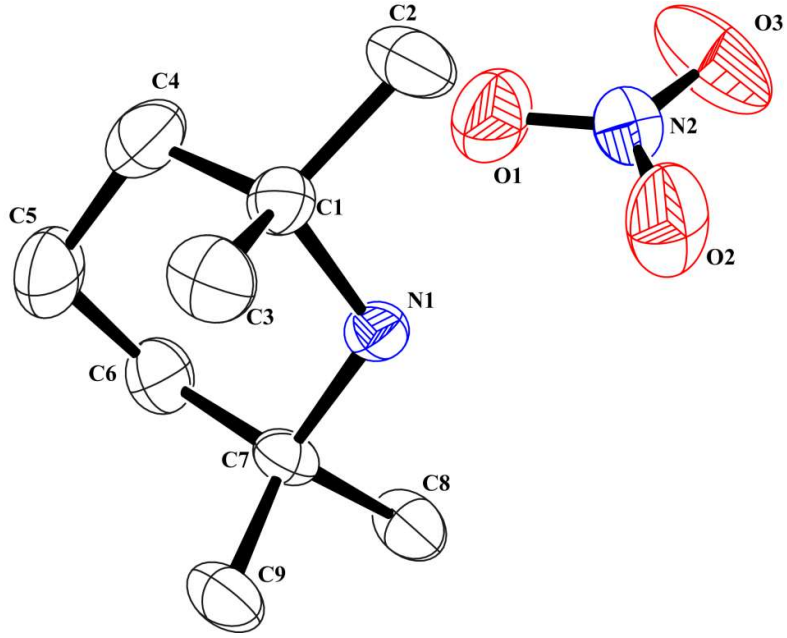

Figure S30. ORTEP diagram of $tmpNO_3$ (30% thermal ellipsoid plot, H-atoms are omitted for clarity).

Table S1. Crystallographic data for complex **2**.

	2
Formulae	$C_{48}H_{38}N_4O_6Mn$
Mol. wt.	821.76
Crystal system	Monoclinic
Space group	P 21/c
Temperature /K	100(2)
Wavelength /Å	0.71073
a /Å	9.8(2)
b /Å	10.4(2)
c /Å	21.2(4)
α/°	90
β/°	111.6(7)
γ/°	90
V/ $Å^3$	2009(68)
Z	2
Density/Mgm^{-3}	1.358
Abs. Coeff. /mm^{-1}	0.385
Abs. correction	none
F(000)	854
Total no. of reflections	3524
Reflections, $I > 2\sigma(I)$	1310
Max. 2θ/°	24.995
Ranges (h, k, l)	$-11 \le h \le 11$ $-12 \le k \le 12$ $-11 \le l \le 25$
Complete to 2θ (%)	0.998
Refinement method	Full-matrix least-squares on F^2
Goof (F^2)	0.841
R indices [$I > 2\sigma(I)$]	0.0904
R indices (all data)	0.1702

Table S2. Selected bond lengths (Å) of complex **2**.

Atoms	**2**
Mn1-N1	1.91(3)
Mn1-N2	1.95(3)
Mn1-O1	2.13(3)
C1-C2	1.28(2)
C2-C3	1.37(3)
C4-C5	1.49(2)
C5-C6	1.32(2)
C6-C7	1.37(2)

Table S3. Selected bond angles (˚) of complex **2**.

Atoms	**2**
N1-Mn1-N2	86.8(12)
N1-Mn1-O1	90.5(14)
C1-C2-C3	105.2(11)
C5-C6-C7	119.3(14)
C8-O2-C9	119.8(7)