

# Photophysical, Cyclic Voltammetry, Electron Paramagnetic Resonance, X-ray Molecular Structure, DFT Calculations and Molecular Docking Study of a new Mn(III) Metalloporphyrin

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## Contents

1. IR spectroscopy.....	2
2. X-ray Molecular structure.....	4
3. Hirshfeld surface analysis.....	7
4. EPR spectroscopy.....	8

## 1. IR spectroscopy

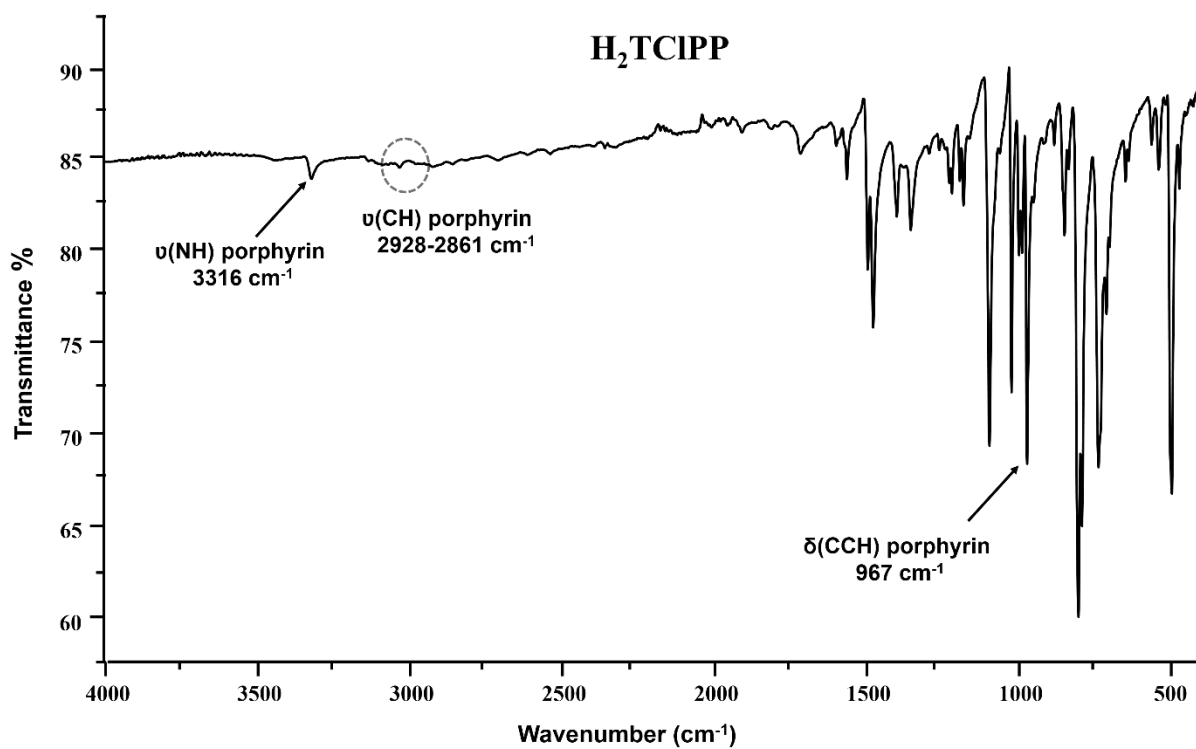


Figure S1. Neat IR spectrum of H<sub>2</sub>TCIPP.

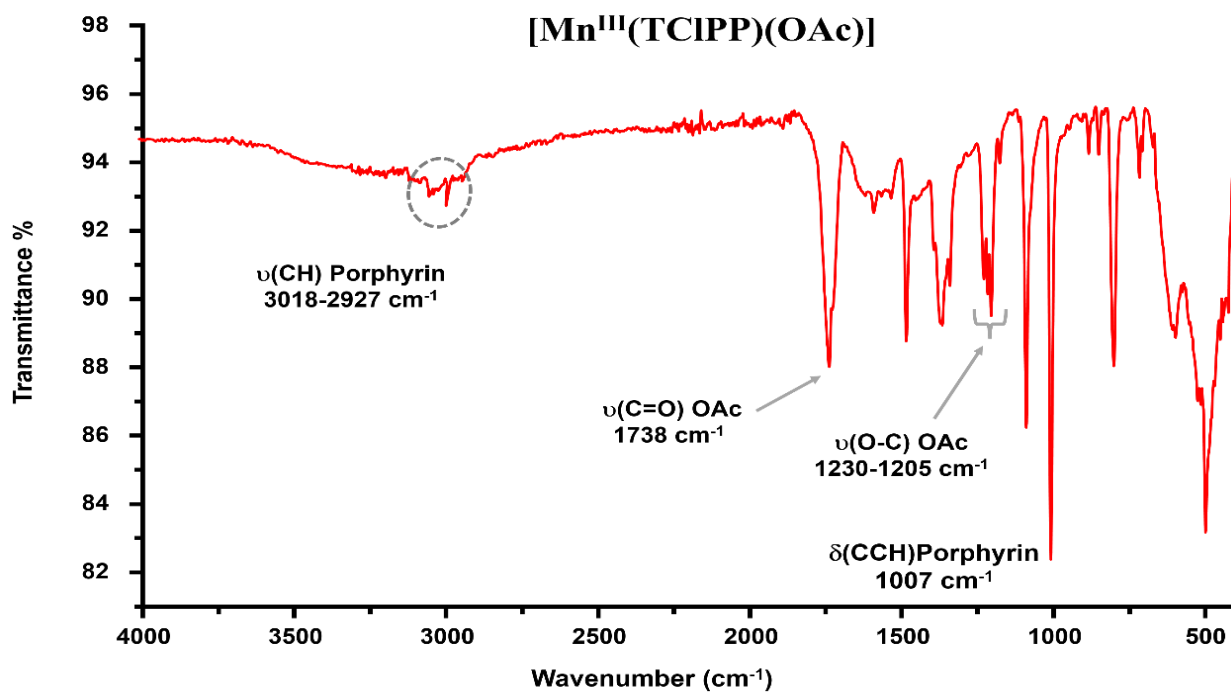


Figure S2. Neat IR spectrum of [Mn<sup>III</sup>(TCIPP)(OAc)].

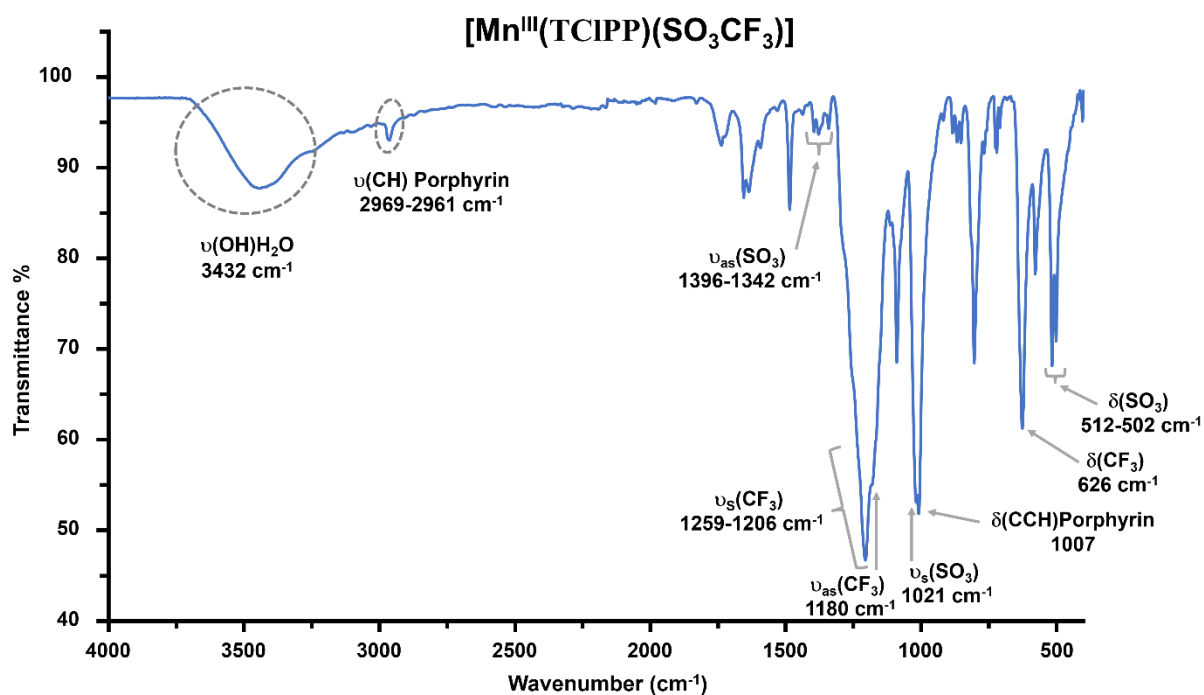


Figure S3. Neat IR spectrum of [Mn<sup>III</sup>(TCIPP)SO<sub>3</sub>CF<sub>3</sub>].

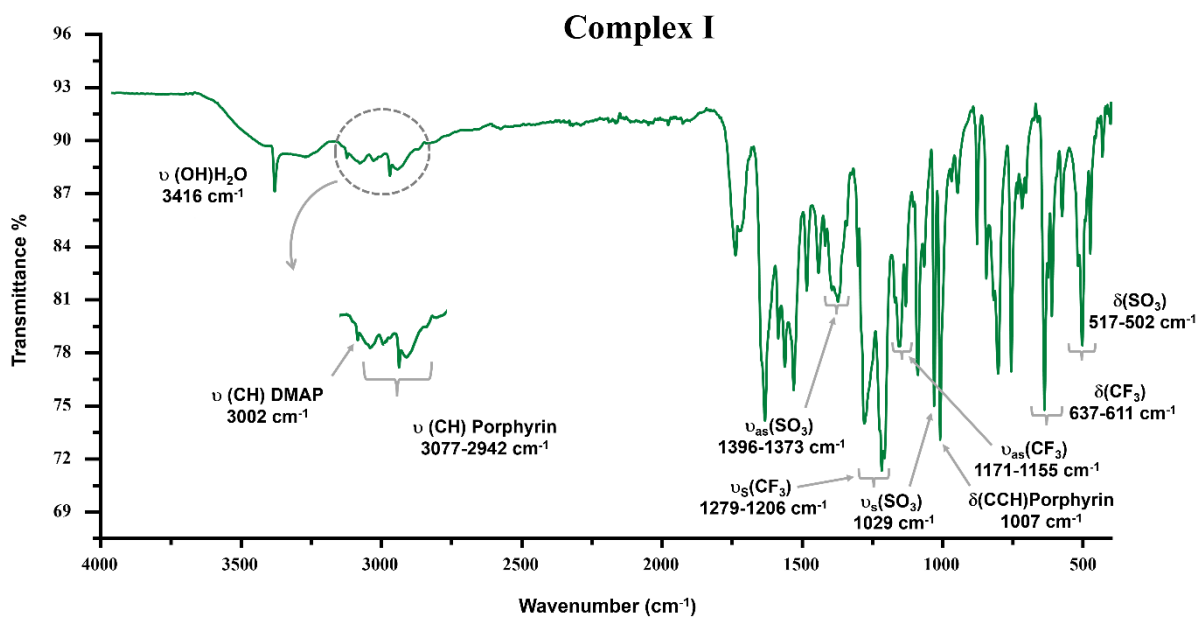


Figure S4. Neat IR spectrum of Complex I.

## 2. . X-ray Molecular structure

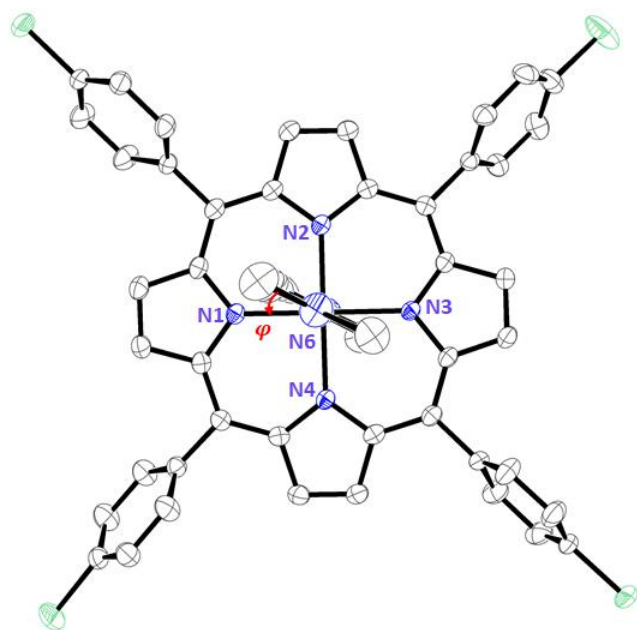


Figure S5. Top view of the  $[\text{Mn}^{\text{III}}(\text{TCIPP})(\text{DMAP})_2]^+$  ion complex showing the dihedral angle  $\varphi$  between the DMAP plane axial ligands and the closest N(pyrrole)-Mn-N(DMAP).

Table S1. Inter- and intra-molecular interactions for I.

<i>Hydrogen bond</i>				
D <sup>a</sup> -H...A <sup>b</sup>	Symmetry	D...A [Å]	D-H...A [°]	
C7-H7...O3	1-x, 1-y, 1-z	3.150(4)	126	
C29-H29...O1	x, -1+y, z	3.334(4)	143	
C48-H48...O2	x, -1+y, z	3.335(5)	162	
C53-H53...O3	-1+x, -1+y, z	3.416(4)	160	
C64-H64...O1	1-x, 1-y, 1-z	2.959(9)	148	
<i>Interactions C-H...Cg</i>				
C-H...Cg ( $\pi$ )	Symmetry code	C...Cg ( $\pi$ )	C-H...Cg	
C23-H23...Cg1	-x, 1-y, 1-z	3.884(4)	164	
C51-H51C...Cg10	1+x, y, z	3.528(4)	132	
C58-H58B...Cg9	-1+x, y, z	3.405(4)	133	
C61-H61A...Cg14	1+x, y, z	3.749(12)	161	
<i>Inter- and Intra-molecular interactions C-X...Cg</i>				
C-X...Cg ( $\pi$ )	Symmetry code	C...Cg	X...Cg	C-H...Cg
C30-Cl2...Cg11	x,-1+y,z	4.949(3)	3.4337(15)	143.39(12)
C42-Cl4...Cg13	x, 1+y, z	4.855(3)	3.4195(15)	137.59(12)
C64-Cl6...Cg14	1-x, 1-y, 1-z	4.710(9)	3.598(3)	118.10(3)
C59-F1...Cg3	1+x, 1+y, z	4.356(5)	3.300(4)	136.30(3)
C59-F2...Cg11	1-x, 1-y, 1-z	4.442(4)	3.297(4)	144.10(3)
C65-Cl9...Cg14	1-x, 1-y, 1-z	4.920(2)	3.811(16)	119.90(9)

<sup>a</sup>: D = donor, <sup>b</sup>: A = acceptor, X =heteroatom, Cg =centroid.

Cg1: is the centroid of the N1/C1-C4 pyrrole five-membered ring.

Cg3: is the centroid of the N3/C11-C14 pyrrole five-membered ring.

Cg9: is the centroid of the N5/C45-C49 phenyl six-membered ring.

Cg10: N7/C52-C56 phenyl six-membered ring.

Cg11: C21-C26 a phenyl ix-membered ring.

Cg13: C33-C38 a phenyl six-membered ring.

Cg14: C39-C44 a phenyl six-membered ring.

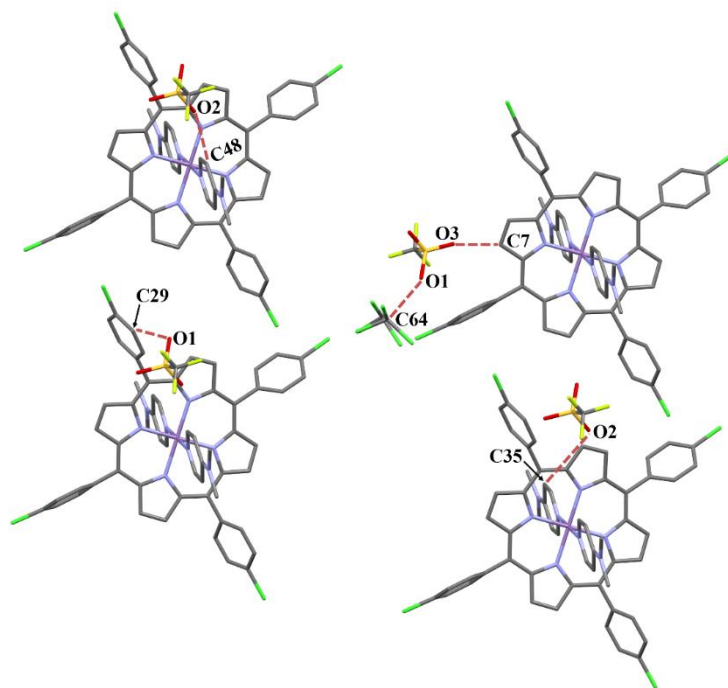


Figure S6. Hydrogen bonds interactions in complex I according to the direction [100].

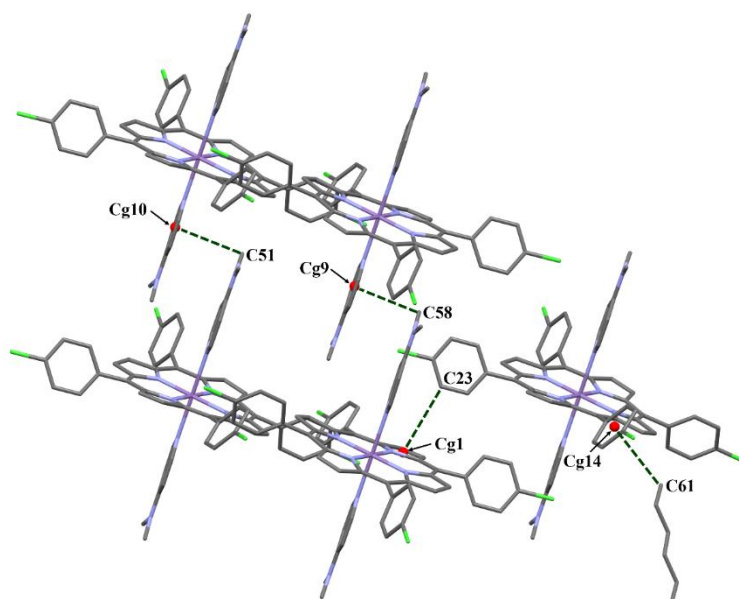


Figure S7. Inter- and intra-molecular interactions C–H...Cg in the crystal lattice of I view along the [010] direction.

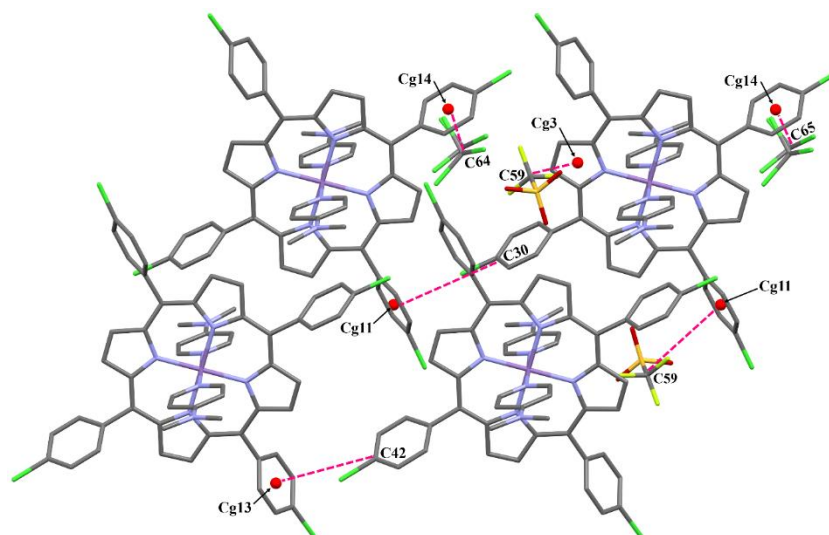


Figure S8. Inter- and intramolecular interactions C–X...Cg in the crystal structure of **I** view along the [100] direction.

### 3. Hirshfeld surface analysis

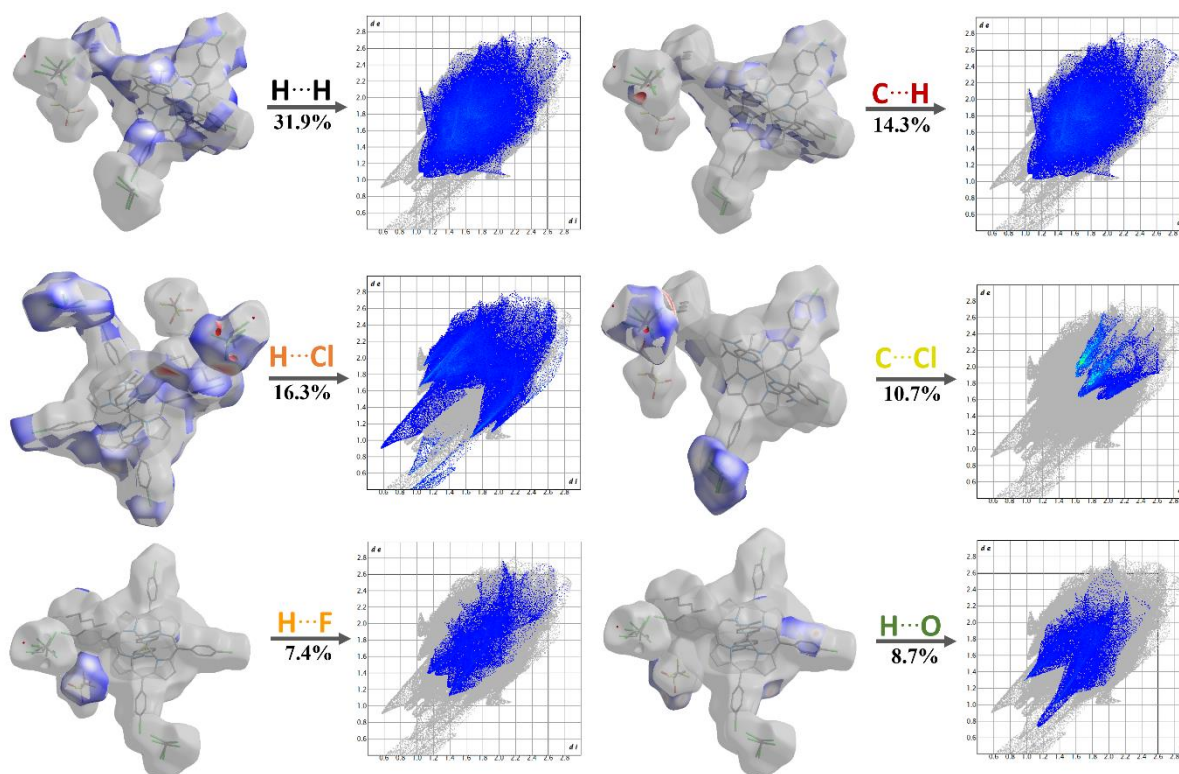


Figure S9. Hirshfeld surface mapped over  $d_{\text{norm}}$  and decomposed fingerprint plots for the dominant interactions for **I**

#### 4. EPR spectroscopy

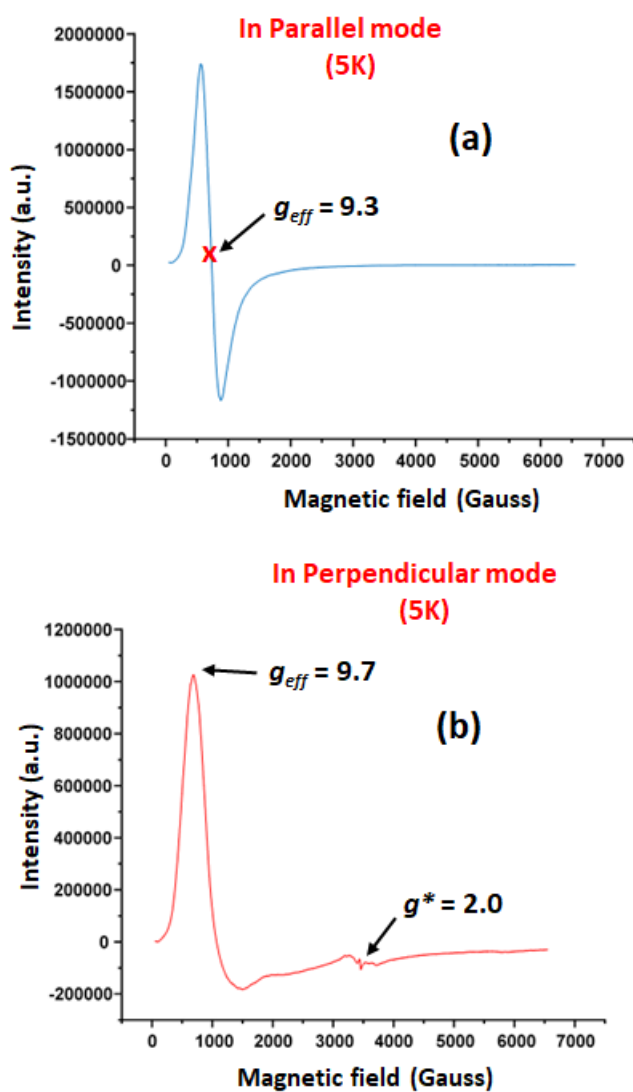


Figure S10. Experimental EPR spectra for complex I in parallel (a) and perpendicular (b) modes at 5 K.