Electronic Supplementary Material (ESI) for New Journal of Chemistry.

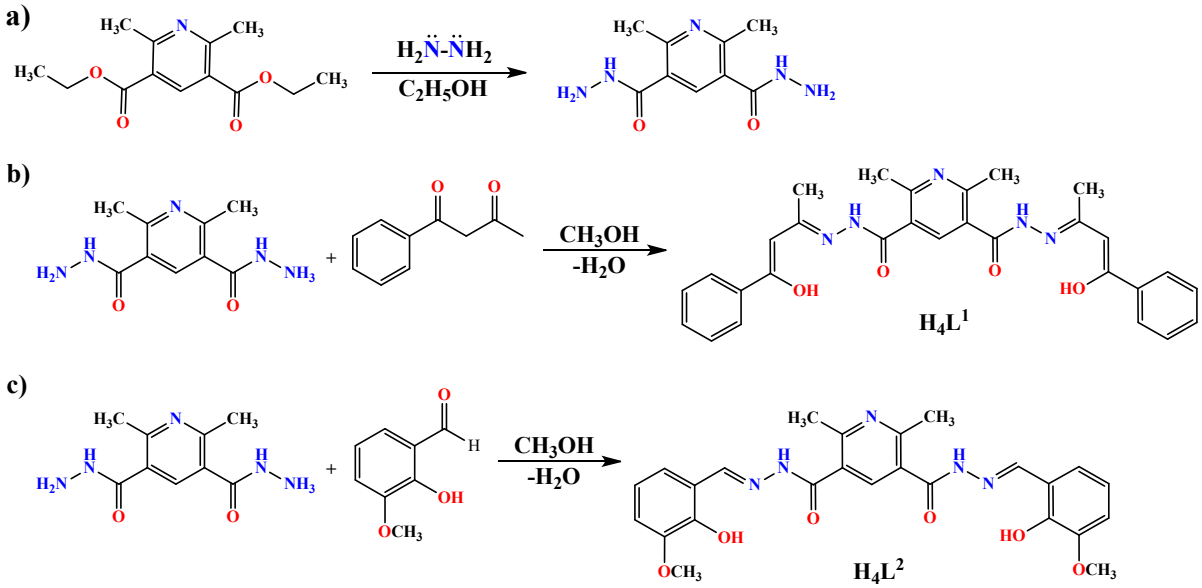
Dinuclear oxidovandium complexes with dihydrazone ligands derived from diethyl 2,6-dimethylpyridine-3,5-dicarboxylate obtained from Hantzsch reaction; crystal structure and catalytic activity

Fatemeh Soltani,[a] Rahman Bikas,[a,*] Neda Heydari,[b] Anna Kozakiewicz-Piekarz [c]

[a] *Department of Chemistry, Faculty of Science, Imam Khomeini International University, 34148-96818, Qazvin, Iran*

[b] *Department of Chemistry, Faculty of Science, University of Zanjan, 45371-38791, Zanjan, Iran*

[c] *Department of Biomedical and Polymer Chemistry, Faculty of Chemistry, Nicolaus Copernicus University in Torun, 87-100, Torun, Poland*



Scheme S1. Synthesis pathway of a) dihydrazide compound, b) H_4L^1 and c) H_4L^2

Table S1. Hydrogen bonding interactions for **1** and **2** (Å, °)

D–H···A	D–H	H···A	D···A	D–H···A
Complex **1**				
C15–H15C···N11^{ii}	0.98	2.62	3.488(6)	148
O24A–H24A···O21^{iii}	0.84	2.02	2.840(14)	167
O24A–H24A···N25^{iii}	0.84	2.49	2.964(12)	117
N25–H25A···O21^{iv}	0.87	2.29	3.088(6)	152
N25–H25A···O22^{iv}	0.87	2.36	3.080(5)	141
N25–H25B···O1W	0.89	2.06	2.948(7)	175
N25–H25C···O21	0.88	1.91	2.781(5)	173
N25–H25D···O22^{v}	0.87	1.98	2.833(5)	166
N25–H25D···O24B^{v}	0.87	2.36	2.824(15)	114
O1W–H1WA···N19^{vi}	0.94	1.78	2.720(15)	180
Complex **2**				
C6A–H6A···O21A^{i}	0.98	2.65	3.133(6)	110
C6A–H6C···O22B^{ii}	0.98	2.61	3.573(6)	168
C6B–H6F···O21B^{iii}	0.98	2.65	3.288(6)	123
O1W–H1WA···O14B^{iv}	0.86	2.28	3.091(5)	158
O1W–H1WB···N18A	0.86	2.02	2.841(5)	161
N24–H24A···O21A	0.99	1.86	2.827(5)	163
N24–H24B···O1W^{v}	0.99	1.95	2.909(5)	161
N24–H24C···O22A^{vi}	0.99	1.83	2.829(5)	175
N24–H24D···O5B^{i}	0.99	2.34	2.966(5)	120
N24–H24D···O8B^{i}	0.99	1.99	2.967(5)	166
N23–H23A···O22B^{vii}	0.99	1.88	2.867(5)	166
N23–H23B···O1W^{iv}	0.99	2.16	3.100(5)	156
N23–H23C···O22A^{iii}	0.99	2.34	2.990(5)	122
N23–H23C···O21B	0.99	2.04	2.765(5)	128
N23–H23D···O5A^{iii}	0.99	2.08	2.890(5)	137
N23–H23D···O8A^{iii}	0.99	2.07	2.931(5)	144

Symmetry codes: for **1** (ii) x, −y+1, z−1/2; (iii) x, y, z−1; (iv) x, −y+2, z+1/2; (v) x, y, z+1; (vi) −x+1, −y+1, −z+2; for **2** (i) −x+1, y−1/2, −z+3/2; (ii) x, y−1, z; (iii) −x+2, y+1/2, −z+3/2; (iv) −x+2, −y+1, −z+1; (v) −x+1, −y+1, −z+1; (vi) x−1, y, z; (vii) x+1, y, z.

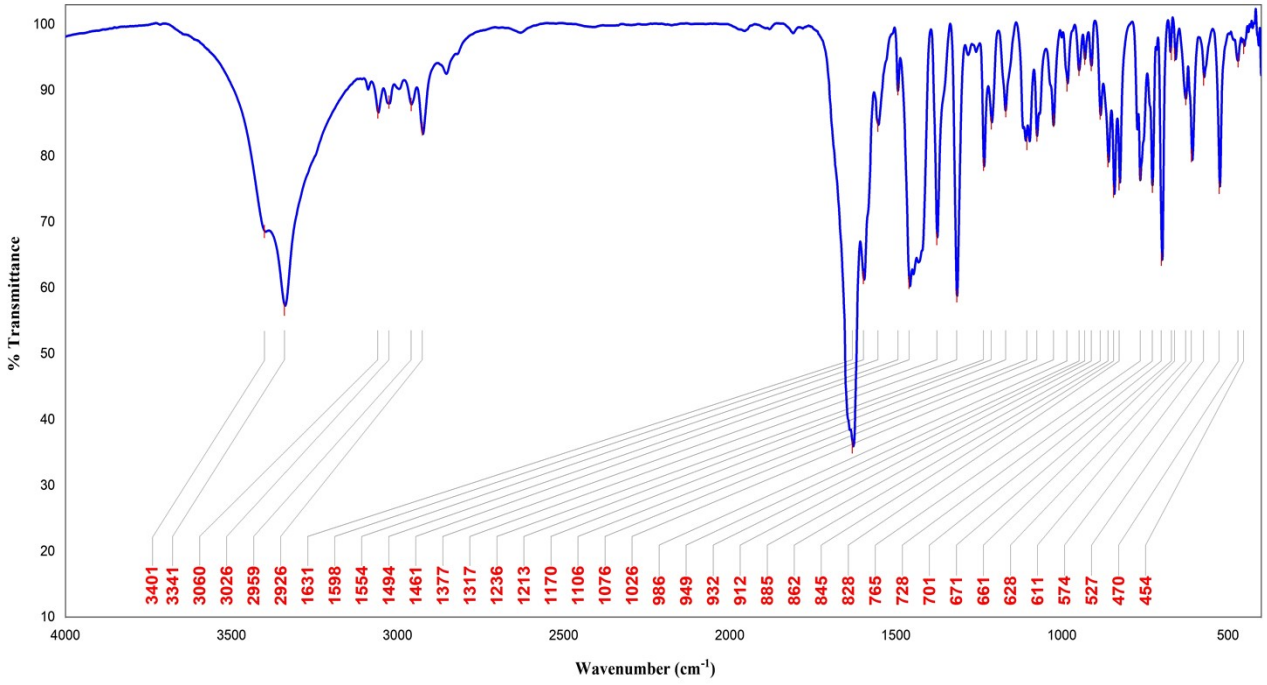


Fig. S1. FT-IR spectrum of H_4L^1

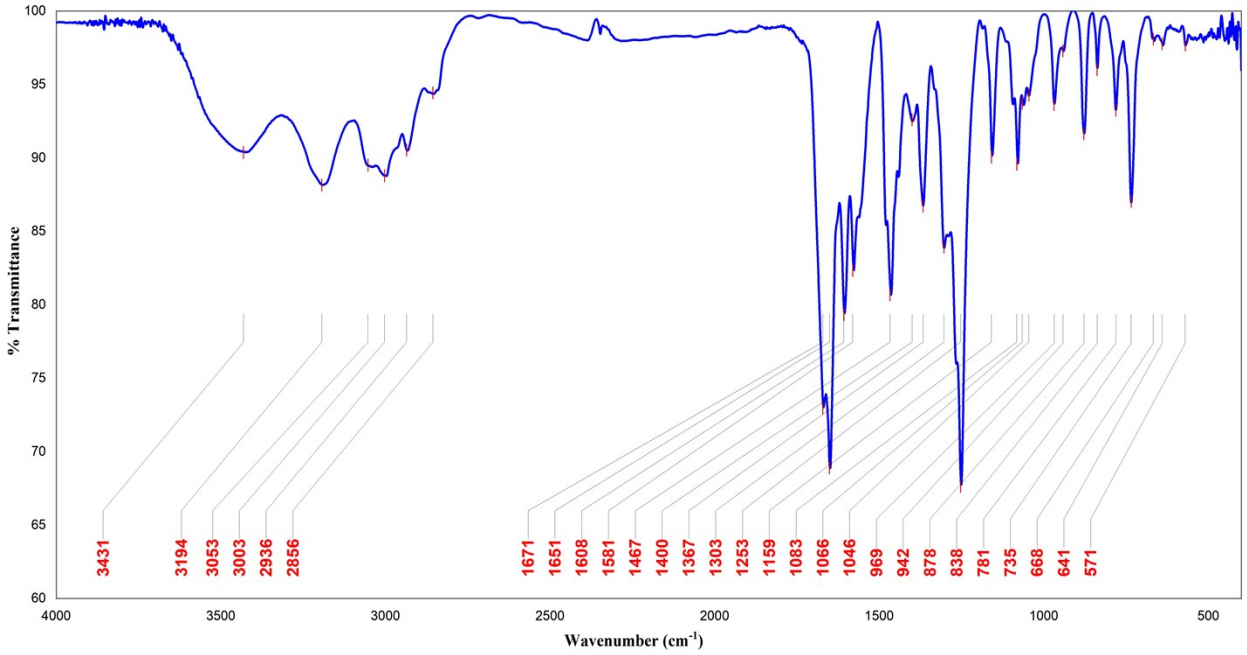


Fig. S2. FT-IR spectrum of H_4L^2

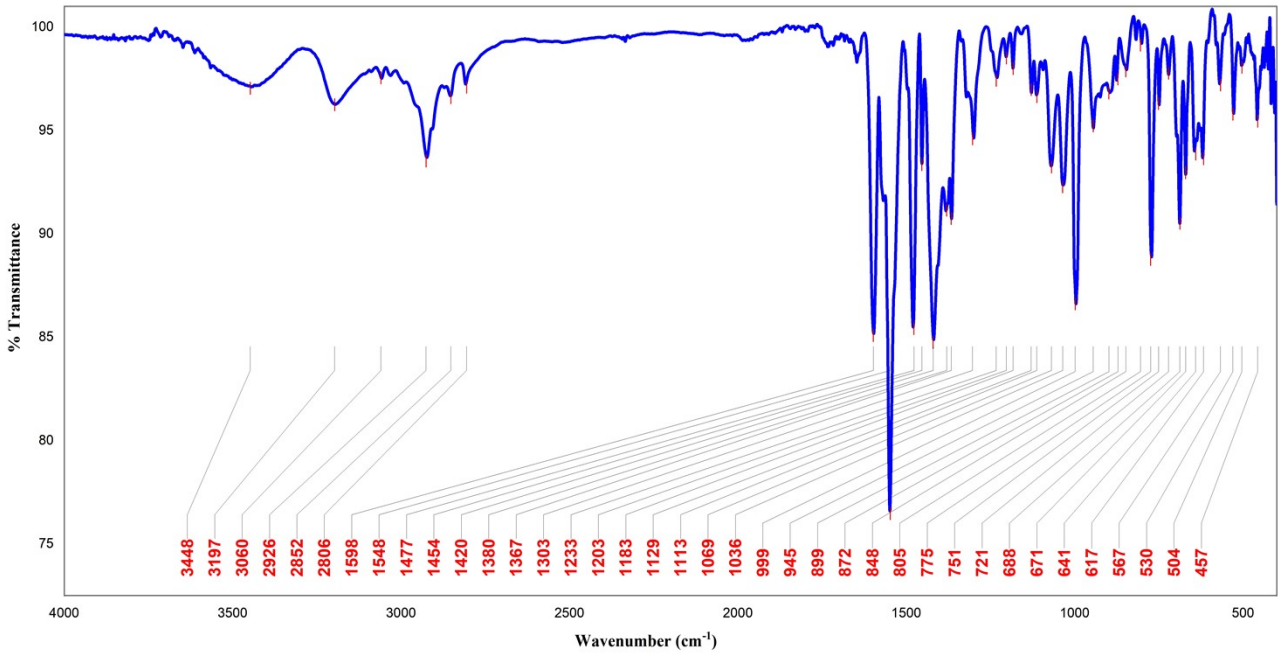


Fig. S3. FT-IR spectrum of compound **1**

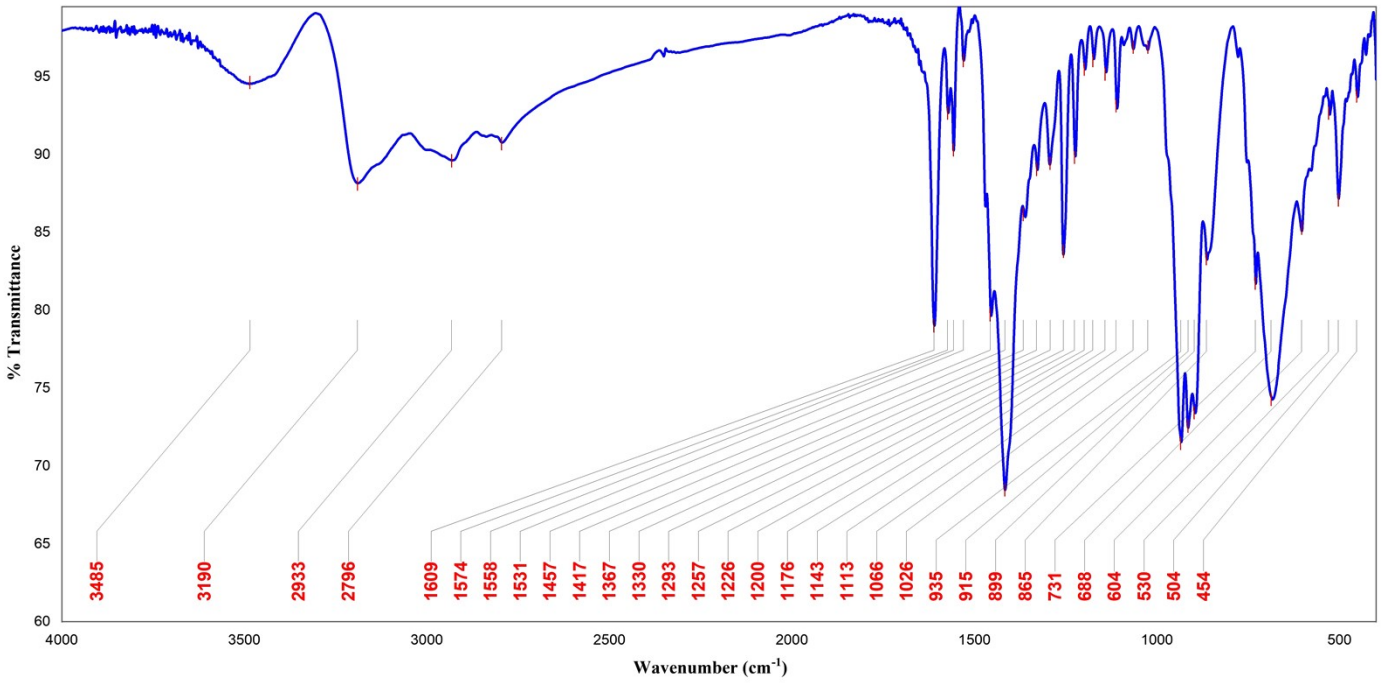


Fig. S4. FT-IR spectrum of compound **2**

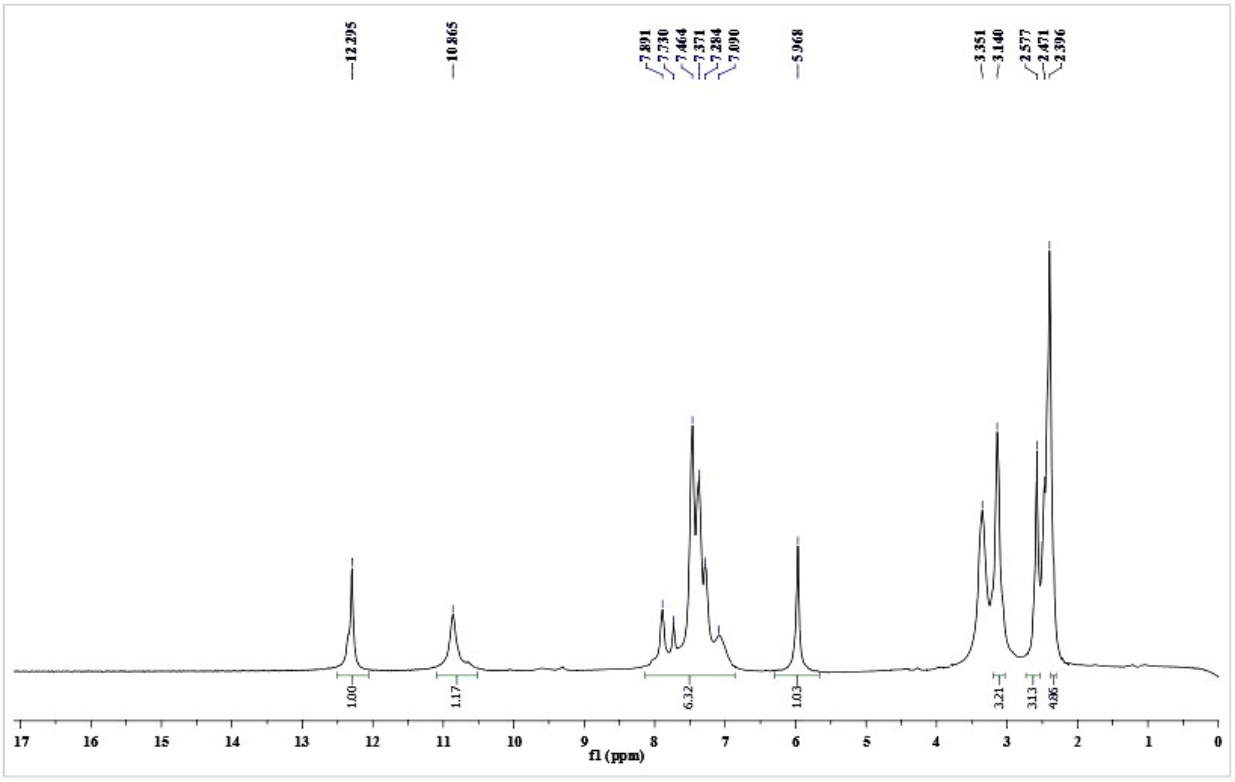


Fig. S5. ^{1}H NMR spectrum of H_4L^1 in DMSO-d_6

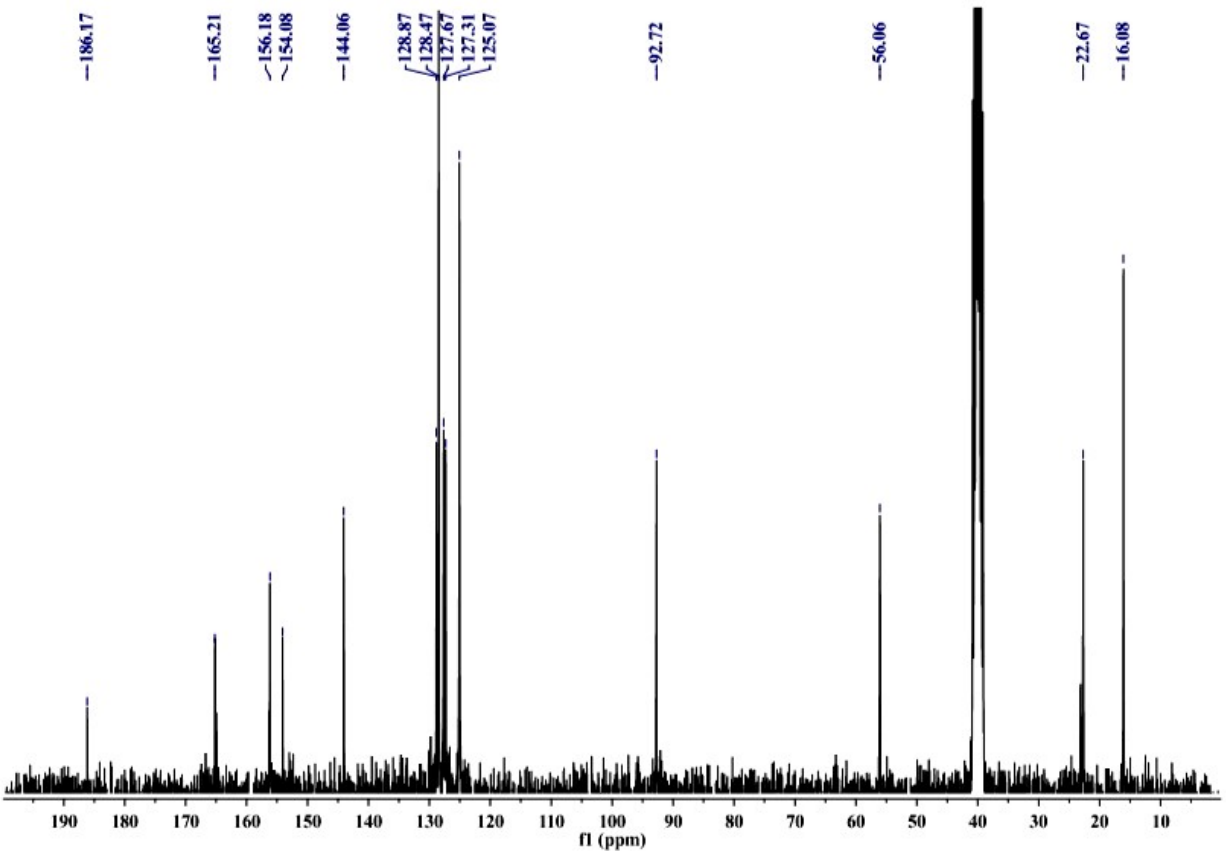


Fig. S6. ^{13}C NMR spectrum of H_4L^1 in DMSO-d_6

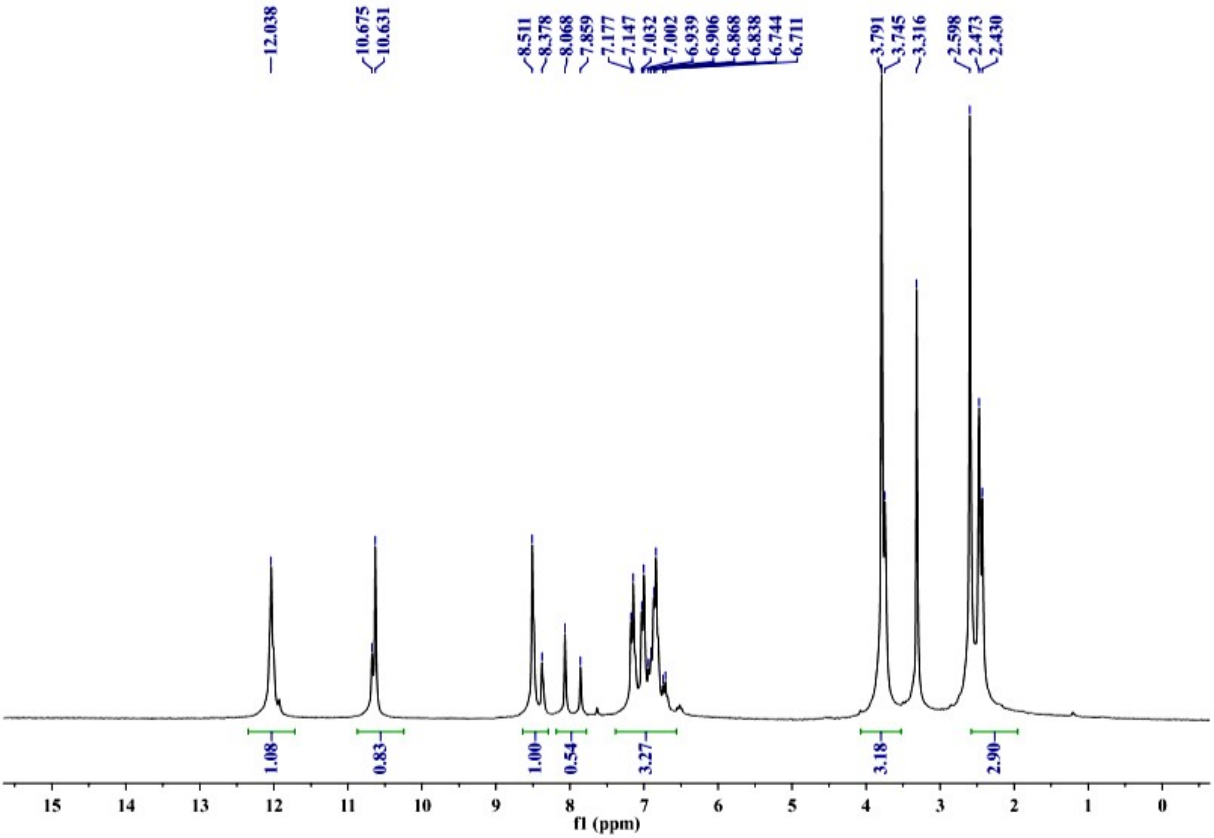


Fig. S7. ^{1}H NMR spectrum of H_4L^2 in DMSO-d_6

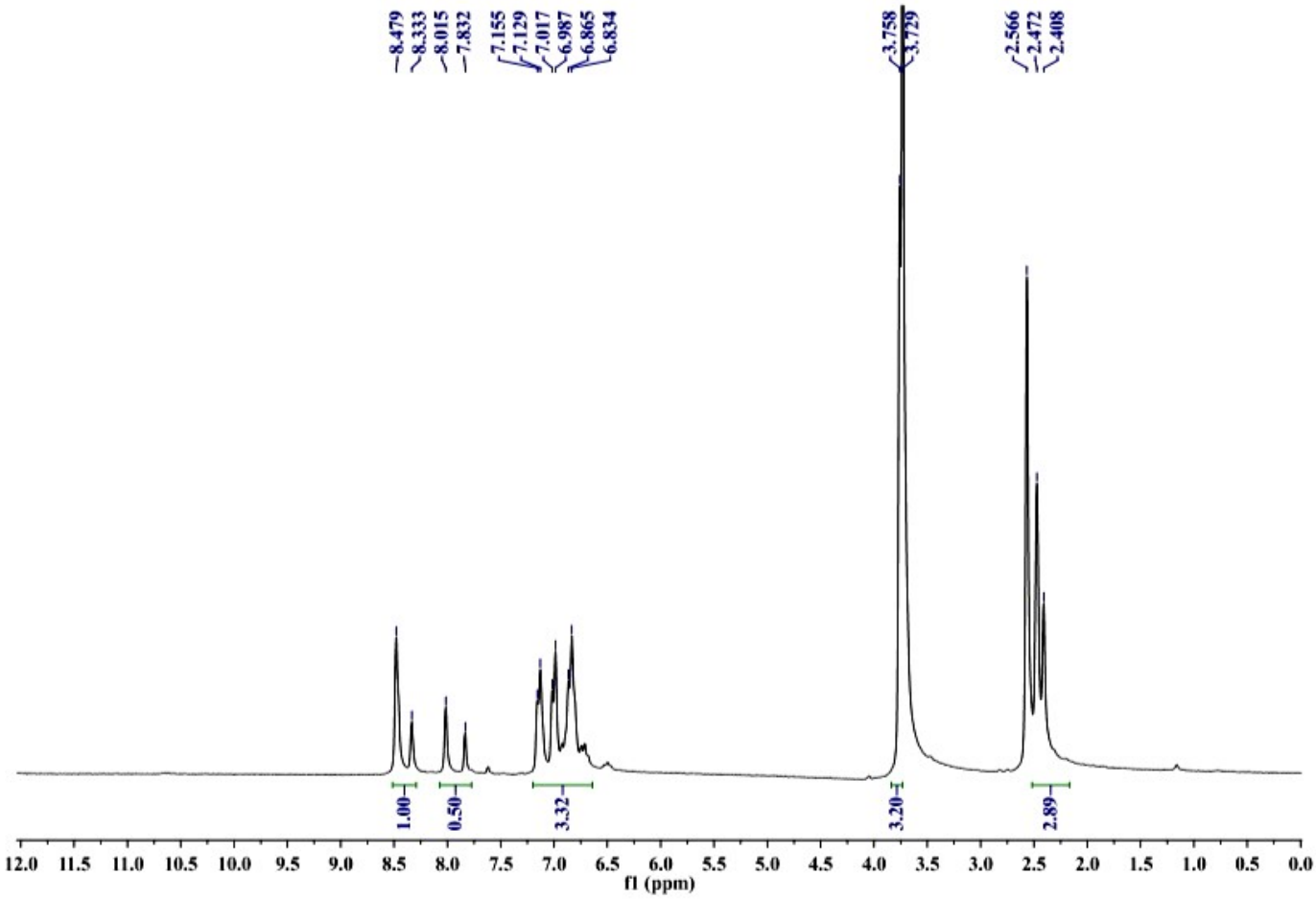


Fig. S8. ^{1}H NMR spectrum of H_4L^2 in DMSO-d_6 + D_2O

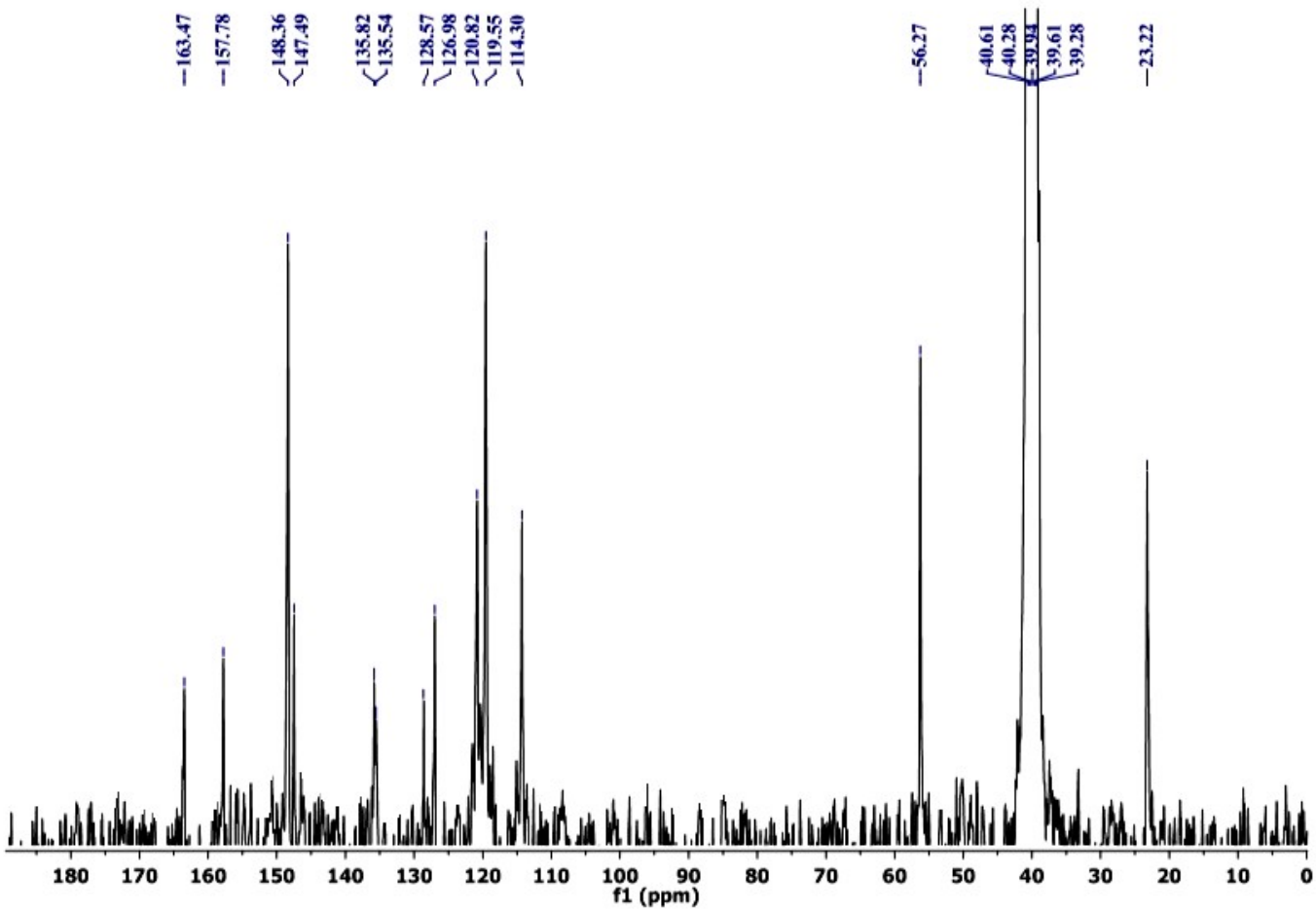


Fig. S9. ^{13}C NMR spectrum of H_4L^2 in DMSO-d_6

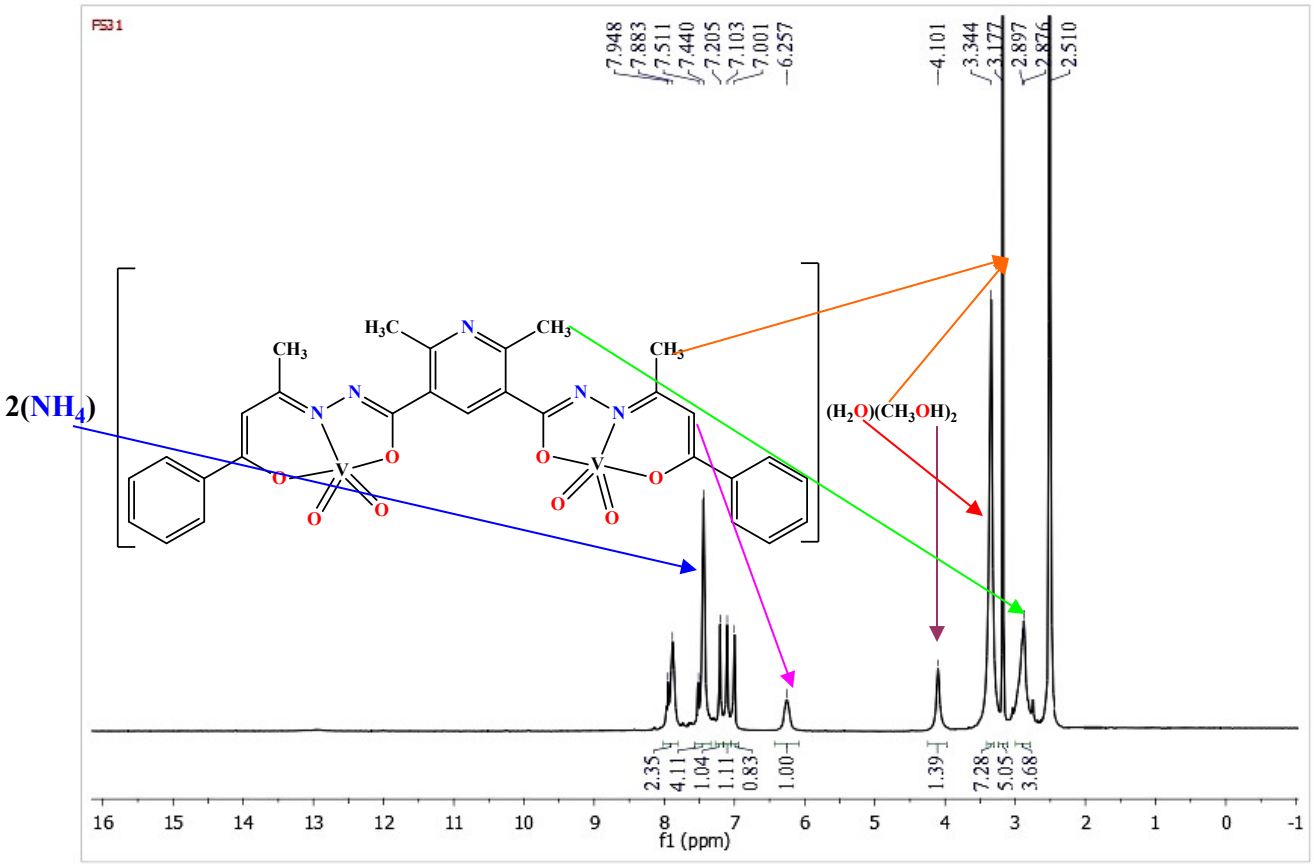


Fig. S10. ^{1}H NMR spectrum of complex **1** in DMSO-d_6

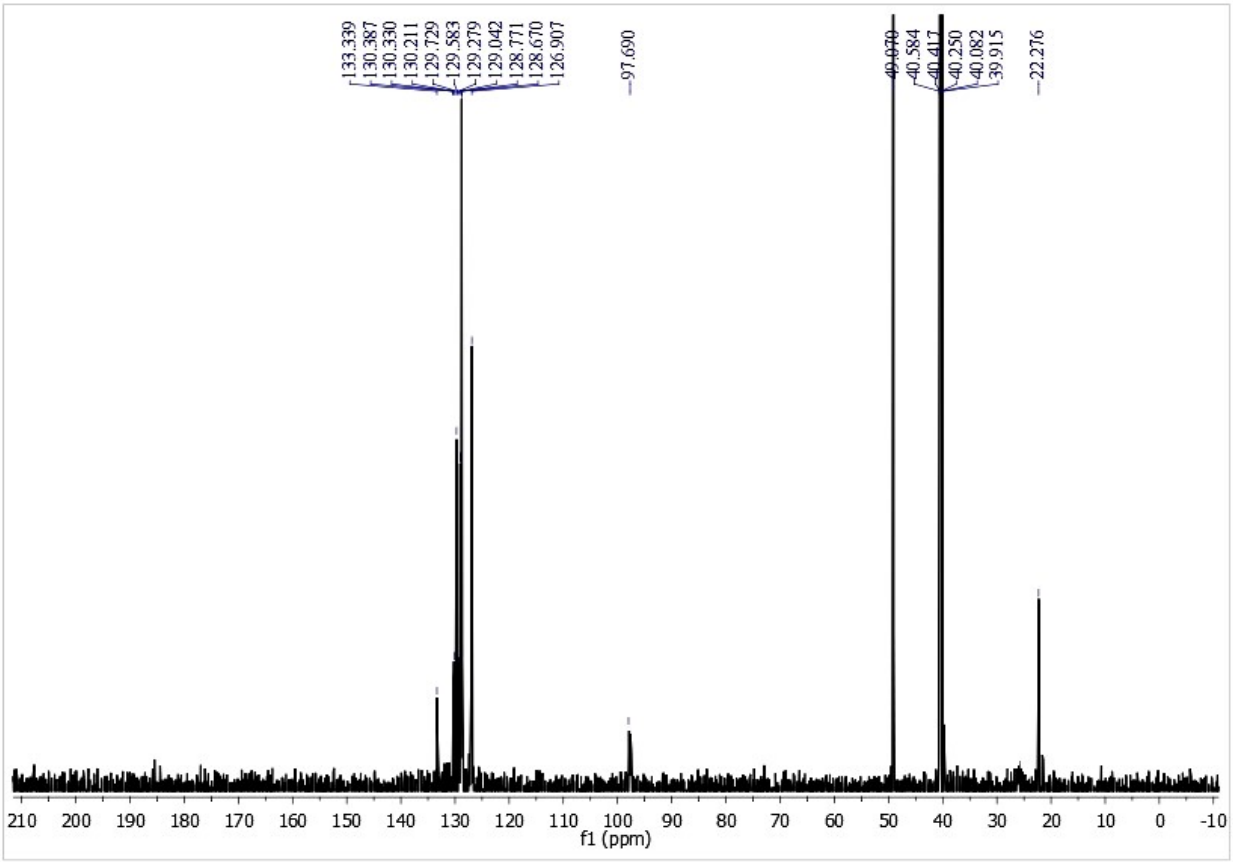


Fig. S11. ^{13}C NMR spectrum of complex **1** in DMSO-d_6

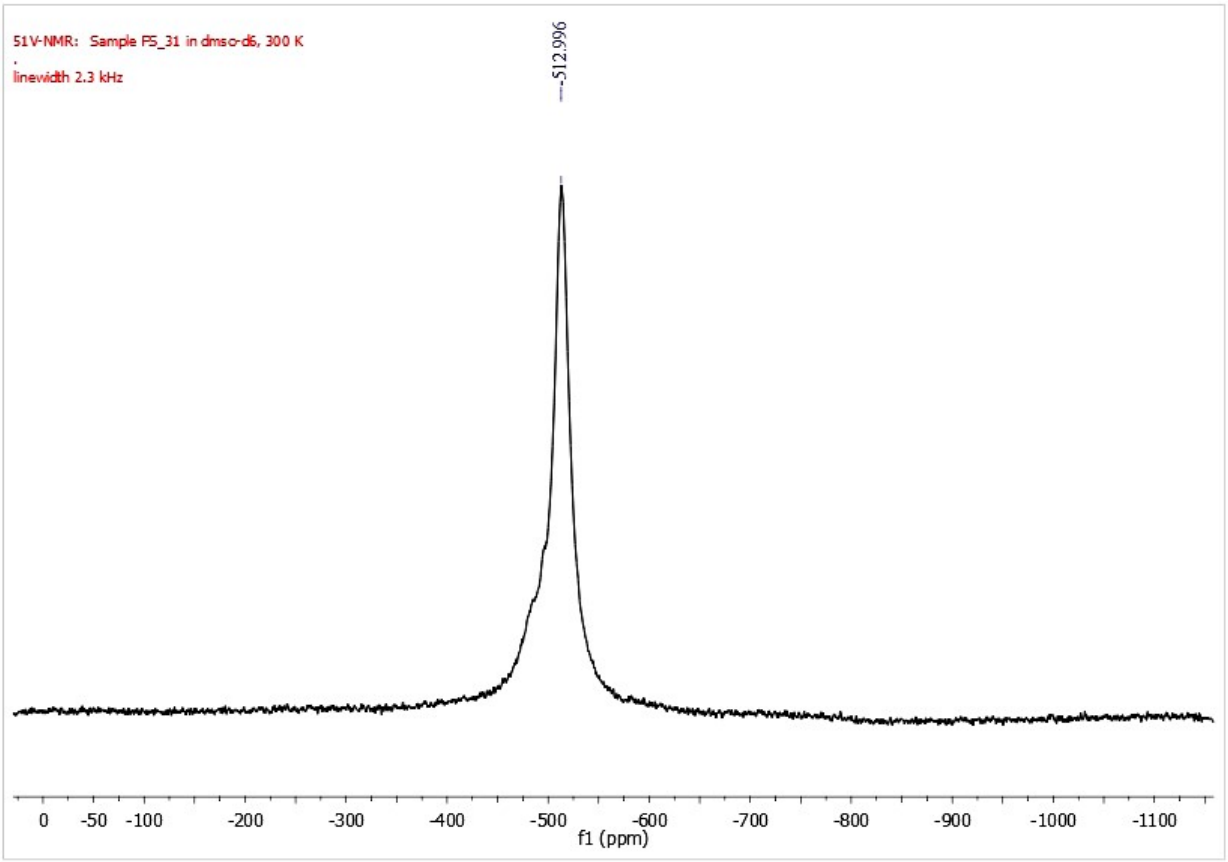


Fig. S12. ^{51}V NMR spectrum of complex **1** in DMSO-d_6

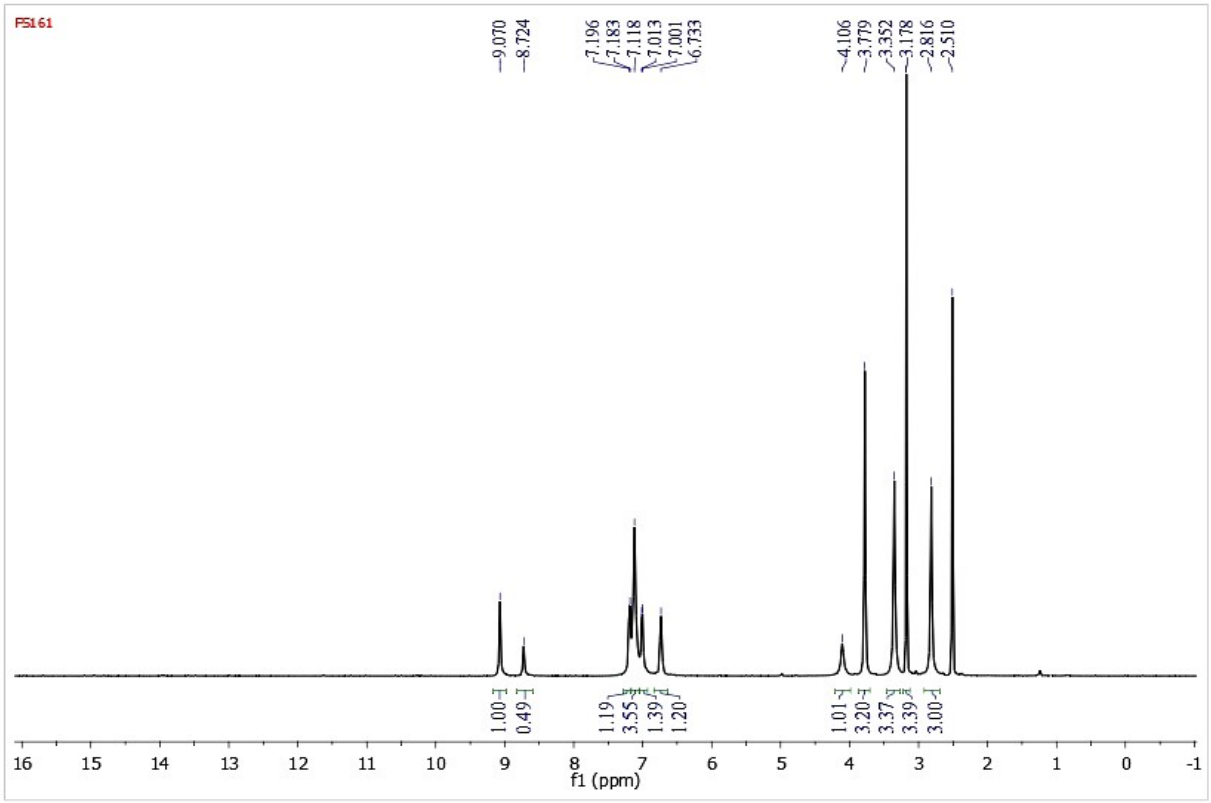


Fig. S13. ^{1}H NMR spectrum of complex **2** in DMSO-d_6 (300 MHz)

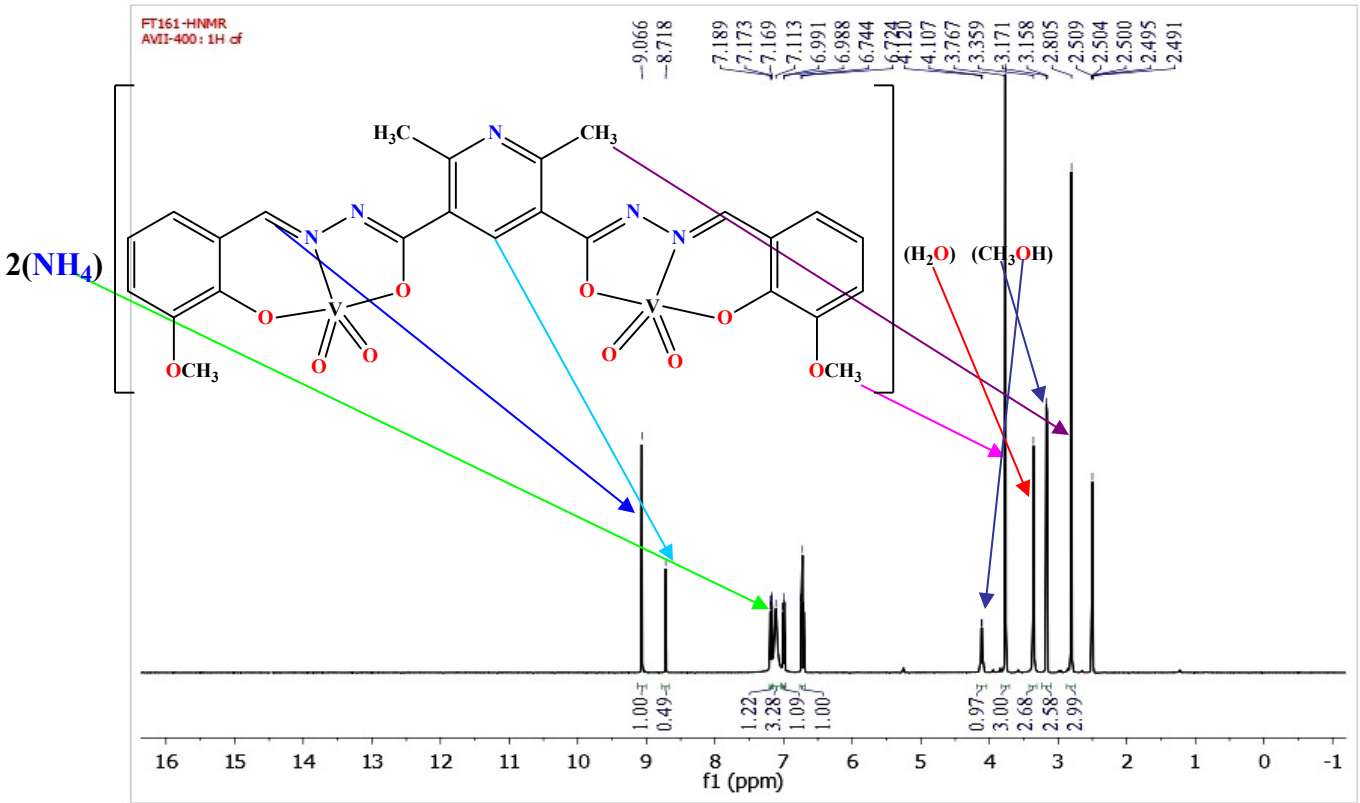


Fig. S14. ^{1}H NMR spectrum of complex **2** in DMSO-d_6 (400 MHz)

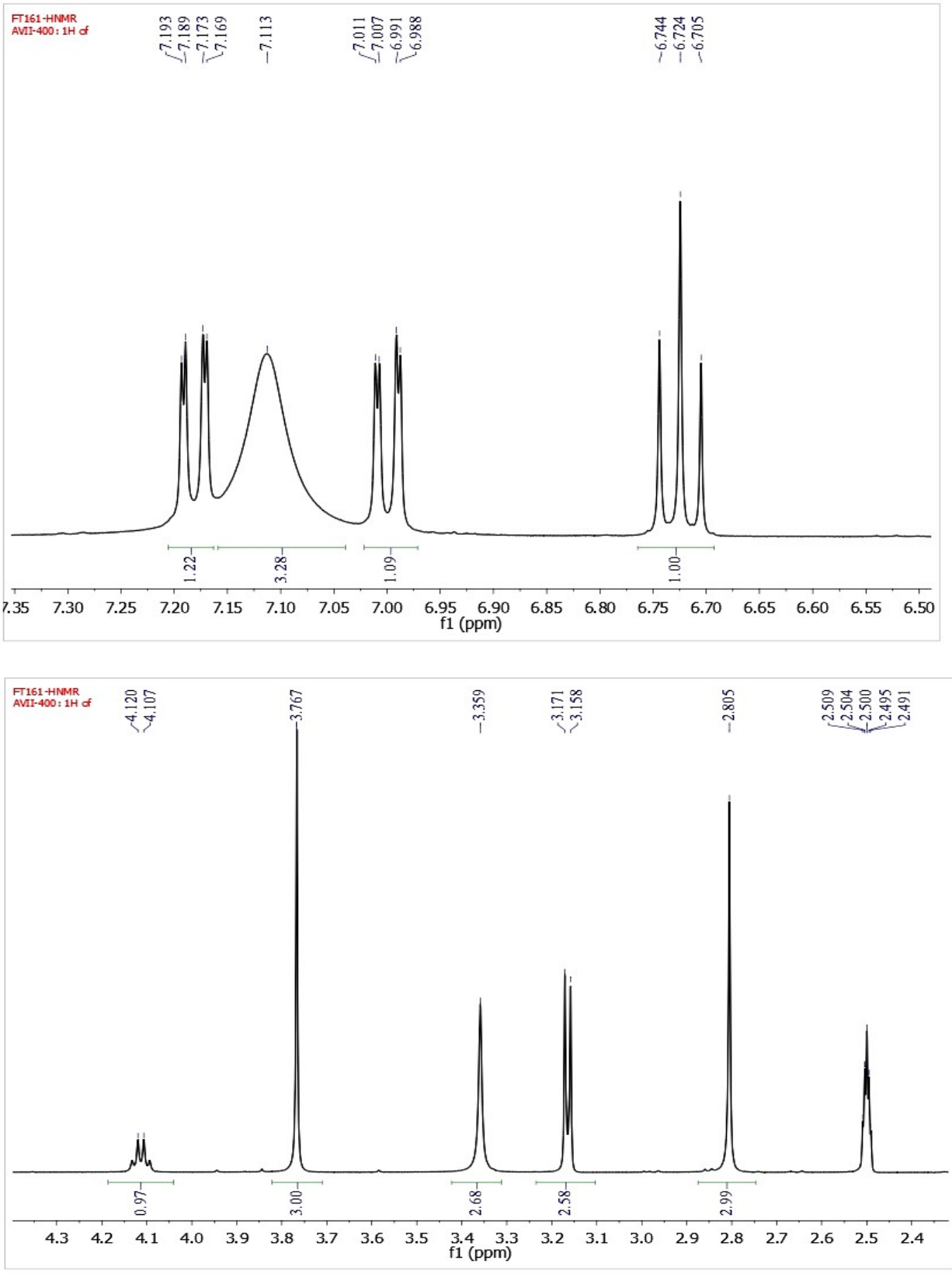


Fig. S15. Expanded ^{1}H NMR spectrum of complex **2** in DMSO-d_6 (top 6.5-7.5 ppm; bottom 2.3-4.3 ppm)

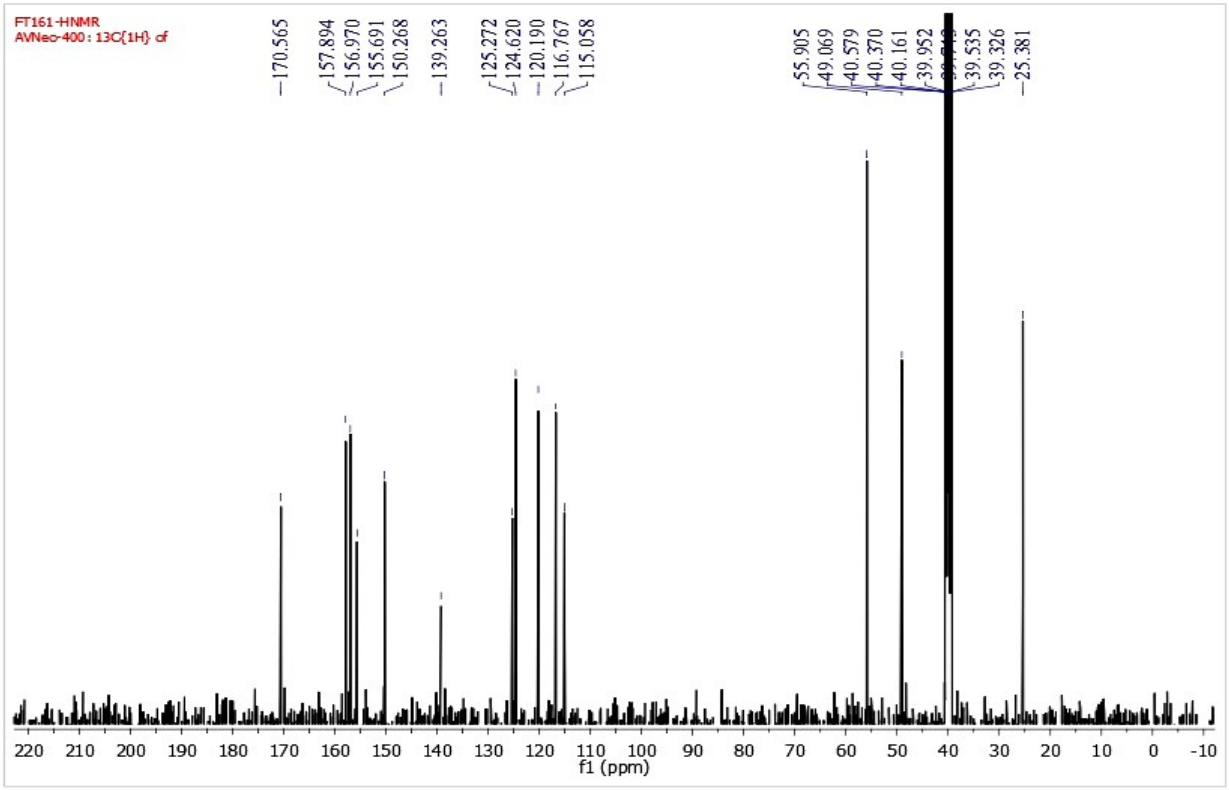


Fig. S16. ^{13}C NMR spectrum of complex **2** in DMSO-d_6

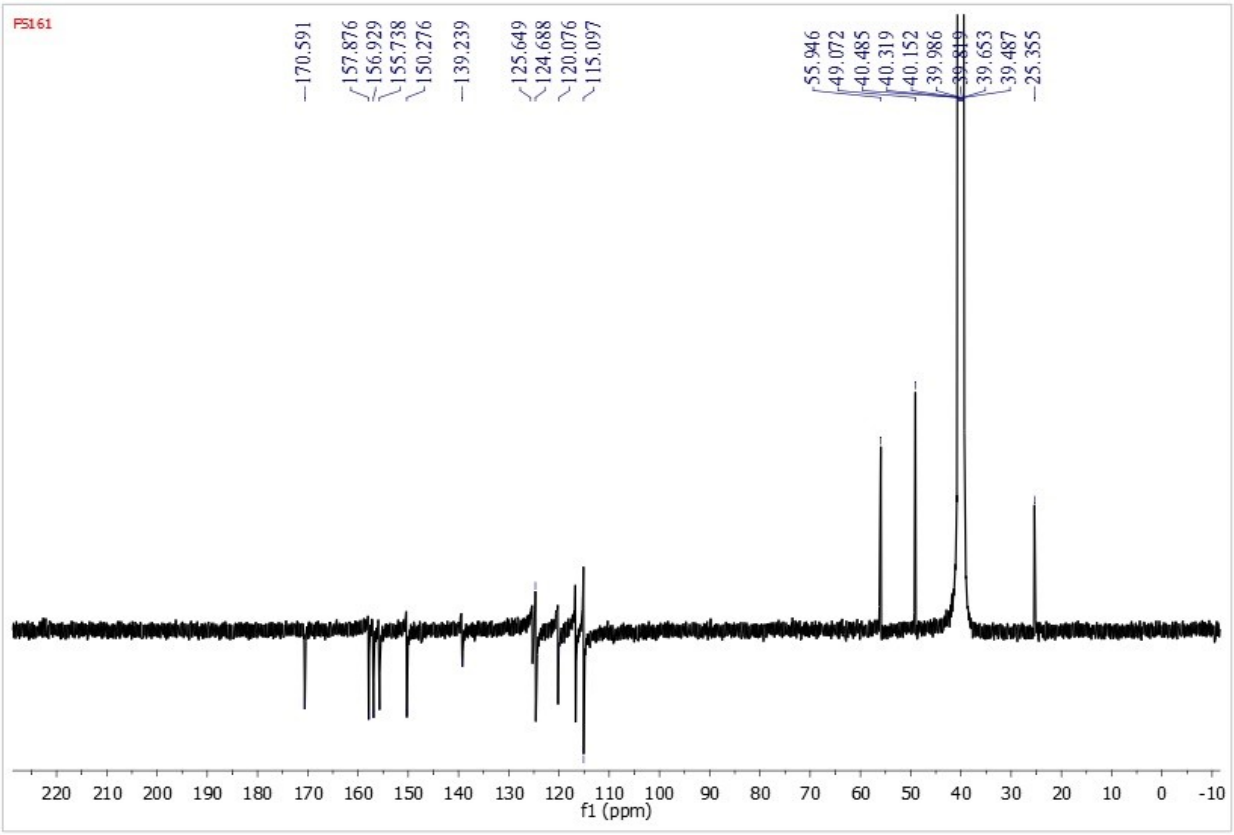


Fig. S17. DEPT ^{13}C NMR spectrum of complex **2** in DMSO-d_6

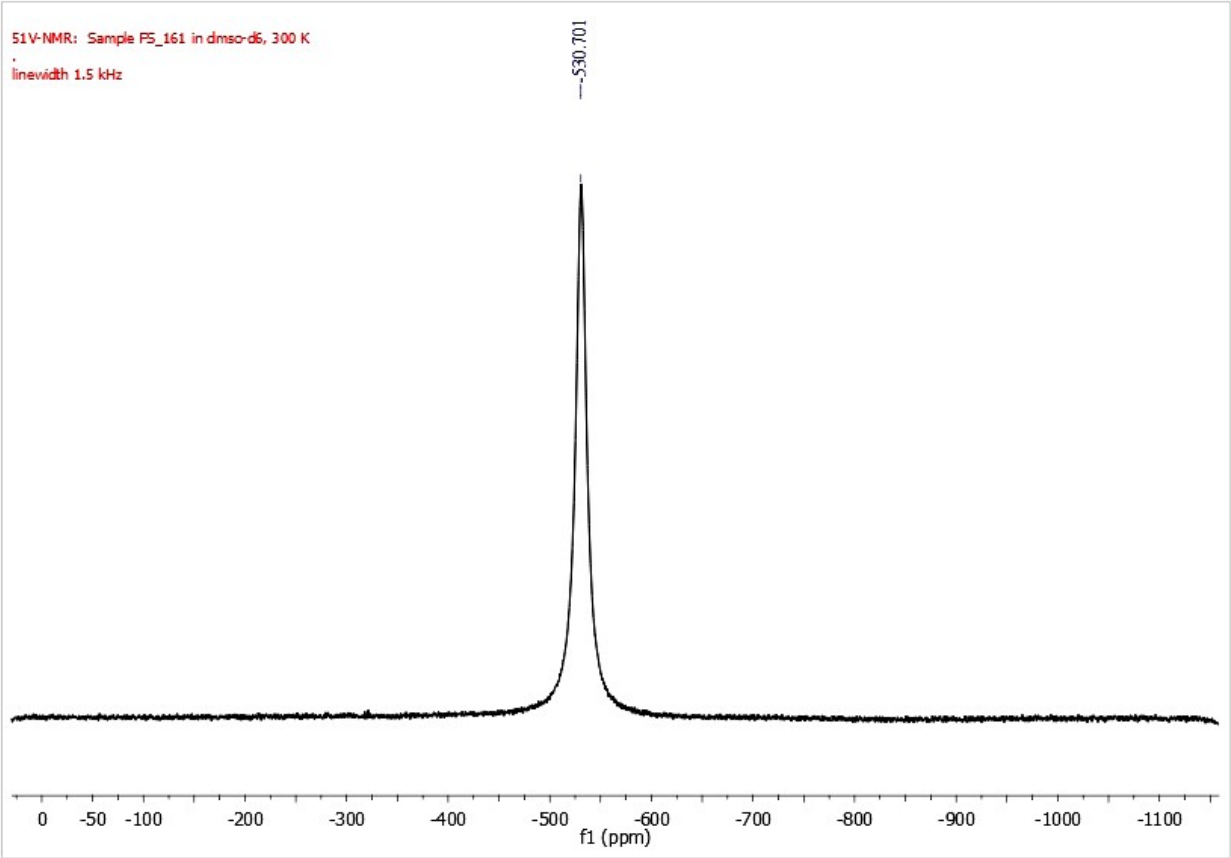


Fig. S18. ^{51}V NMR spectrum of complex **2** in DMSO-d_6

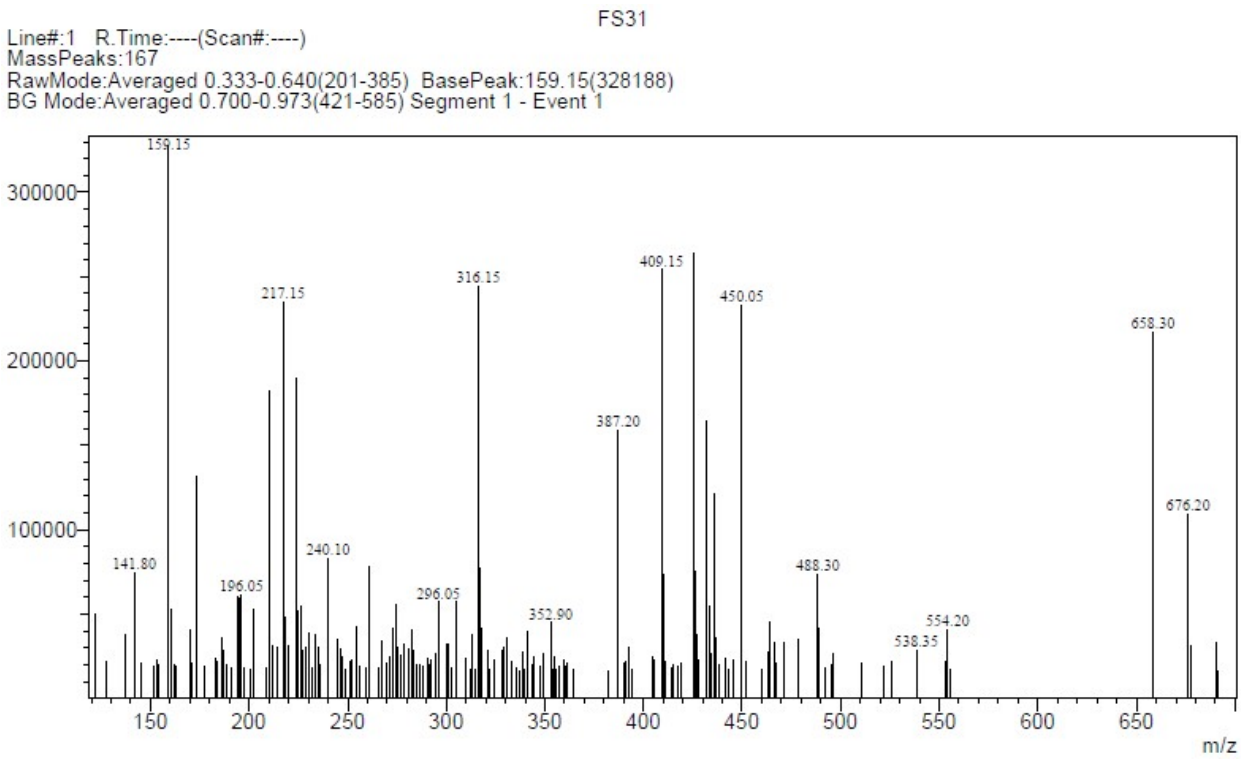


Fig. S19. Mass spectrum of complex **1**

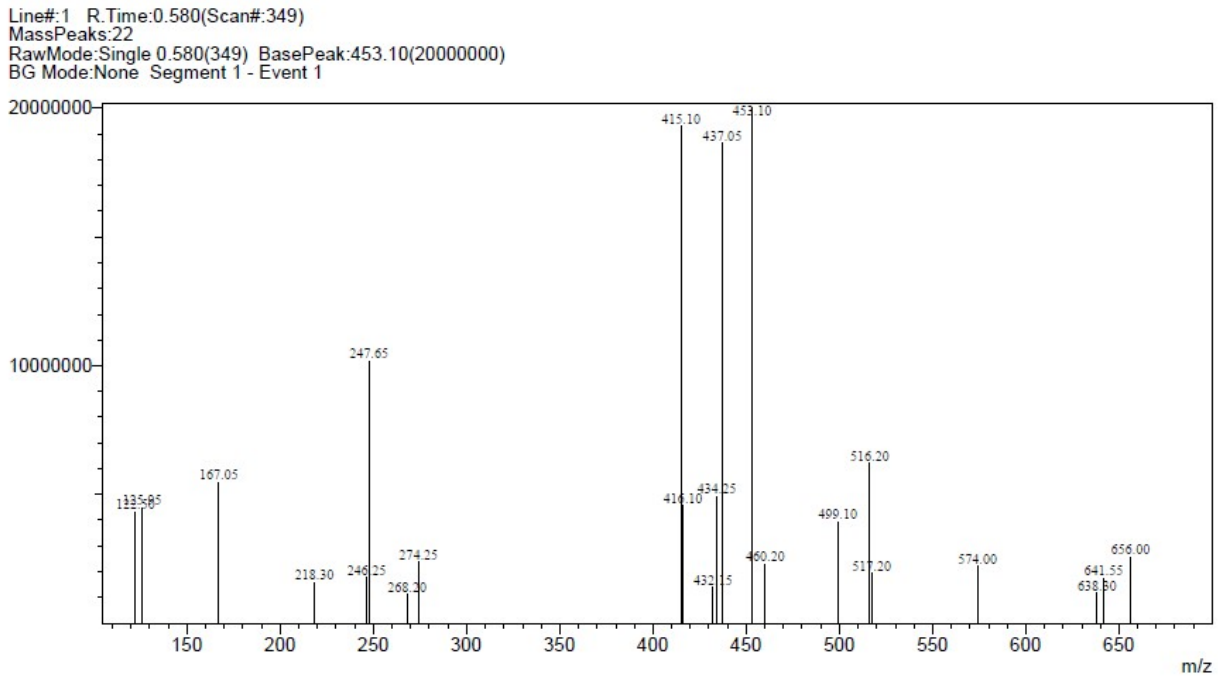


Fig. S20. Mass spectrum of complex **2**

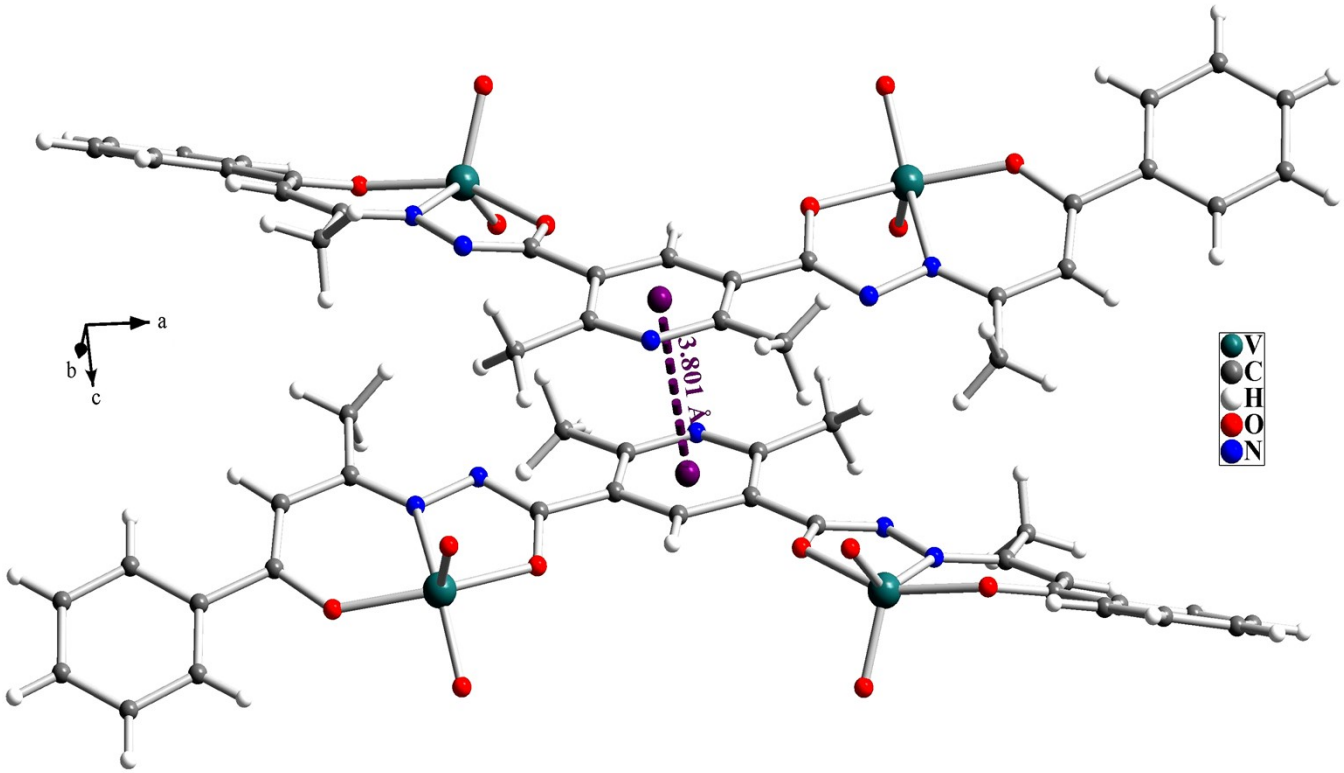


Fig. S21. Intermolecular π···π stacking interaction in the crystal structure of complex **1**

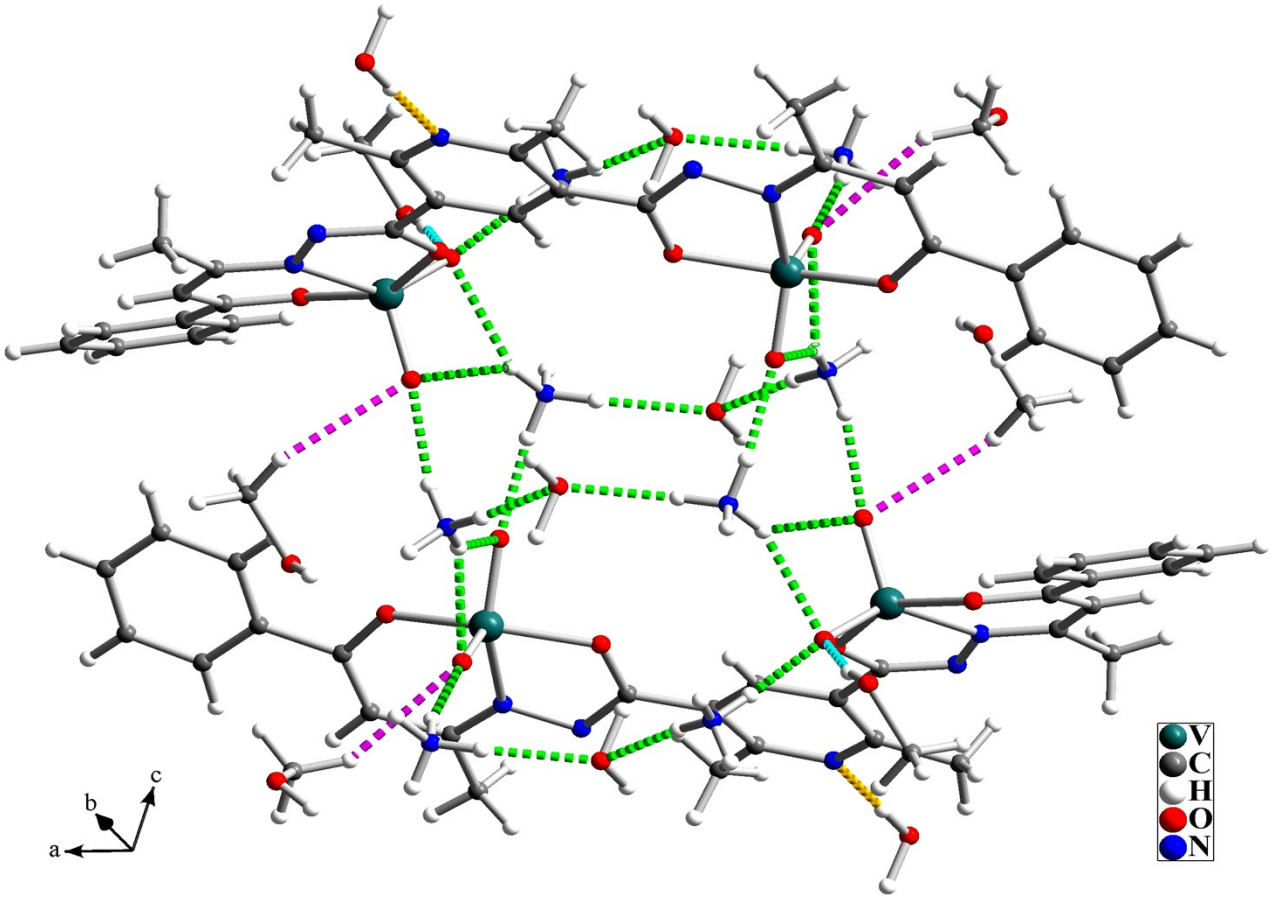


Fig. S22. Hydrogen bond interactions in the crystal structure of complex **1**; O–H···N (orange), O–H···O (blue), N–H···O (green) and C–H···O (pink)

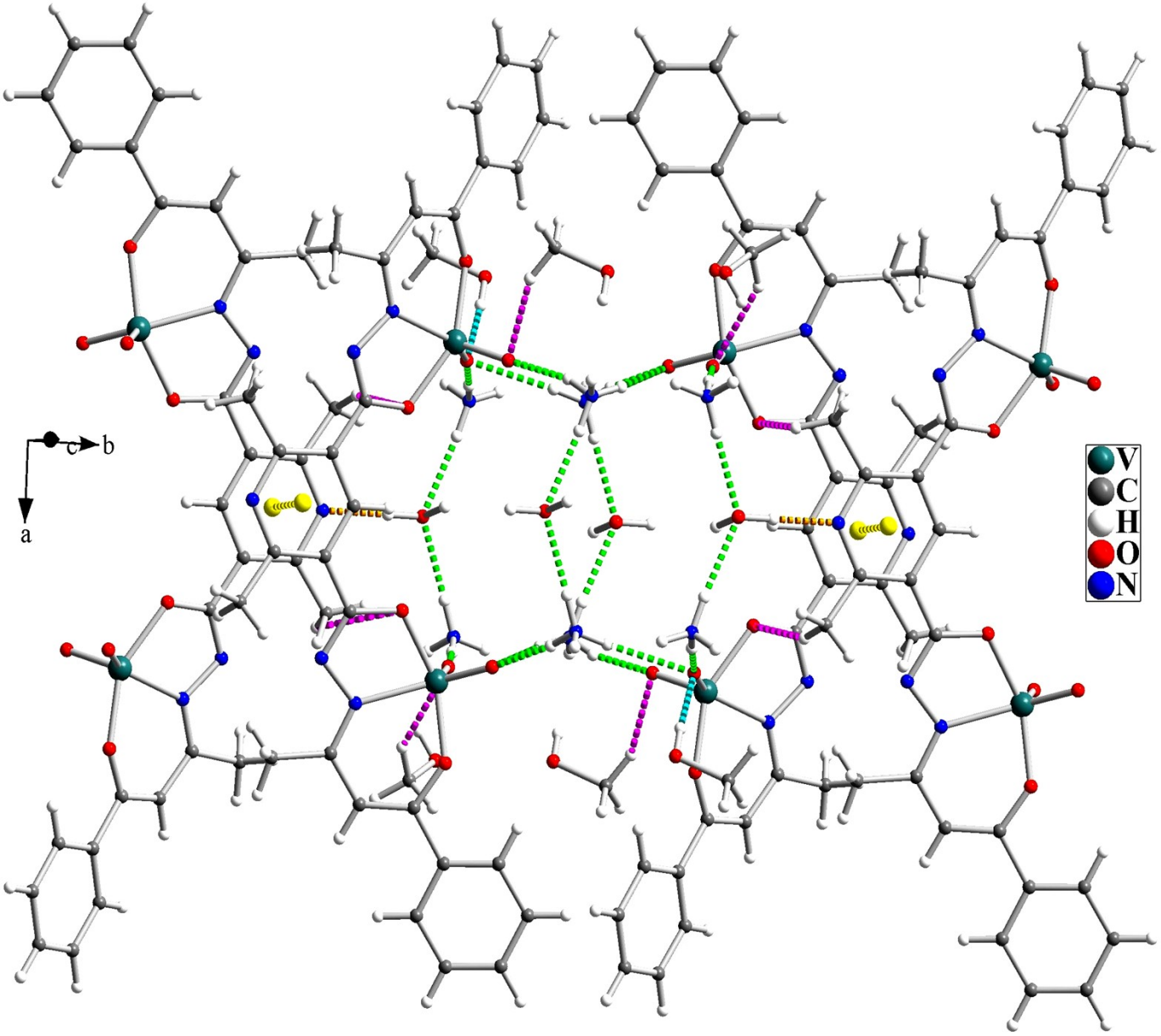


Fig. S23. Intermolecular π···π stacking (yellow dashed line) and O–H···N (orange), O–H···O (blue), N–H···O (green) and C–H···O (pink) hydrogen bond interactions in the crystal structure of complex **1**

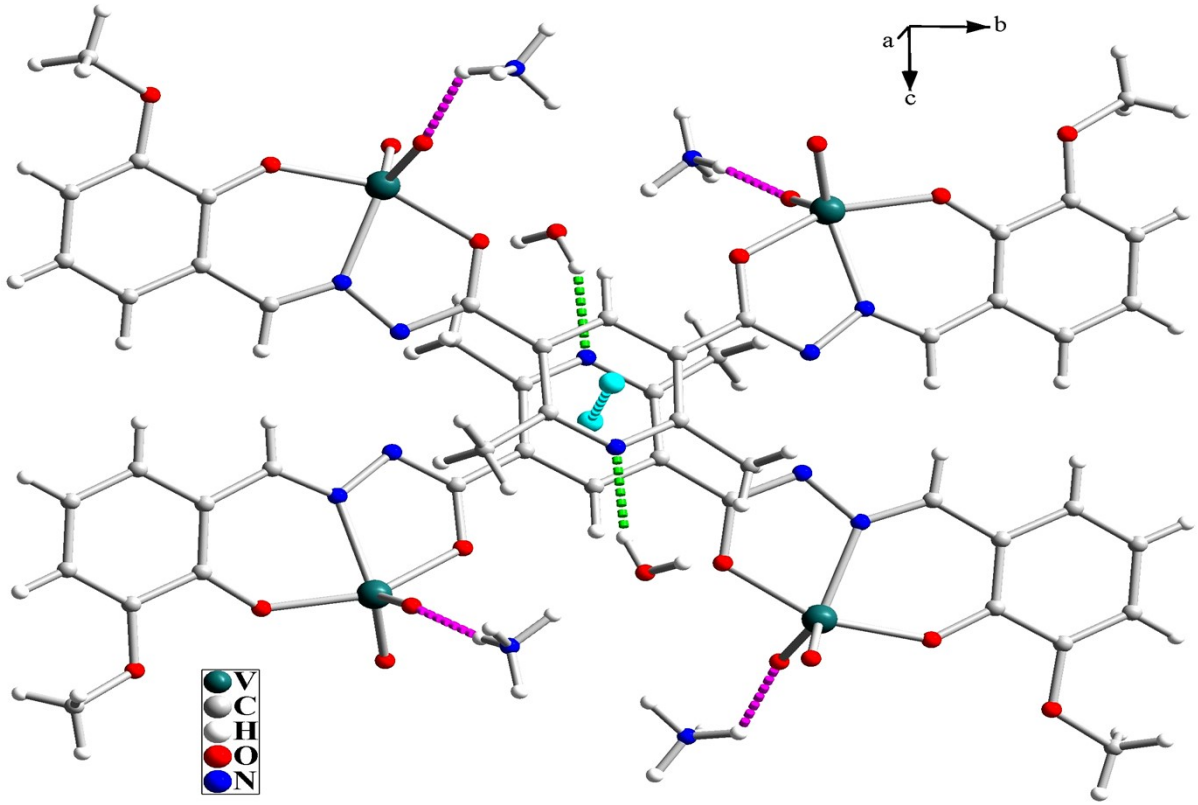


Fig. S24. Intermolecular π···π stacking (blue dashed line) and hydrogen bond interactions O–H···N (green) and N–H···O (pink) in the crystal structure of complex **2**

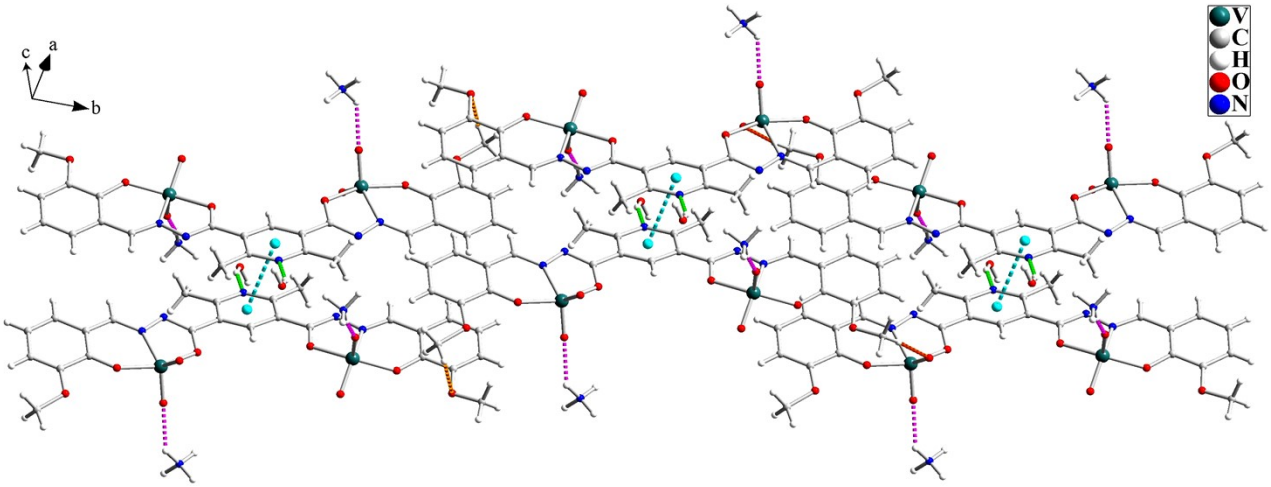


Fig. S25. Intermolecular π···π stacking (blue dashed line) and O–H···N (green), N–H···O (pink) and C–H···O (orange) hydrogen bond interactions in the crystal structure of complex **2**

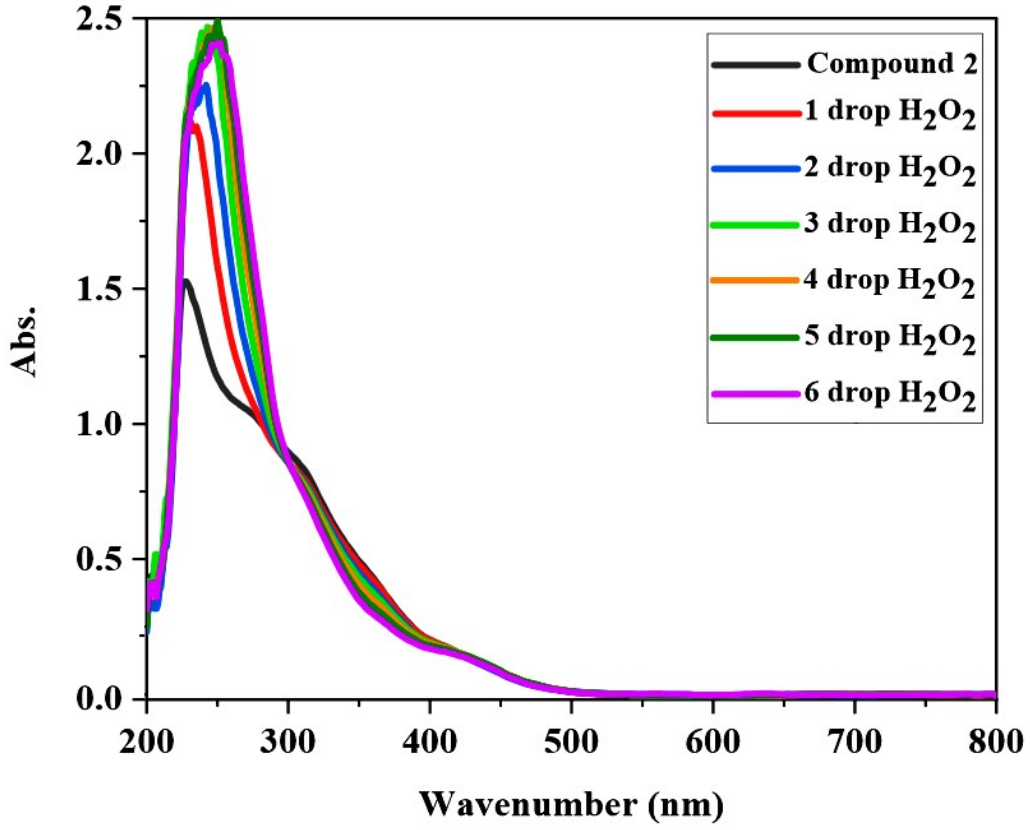


Fig. S26. UV-Vis spectra of complex **2** after addition of diluted H_2O_2 in CH_3OH