Electronic Supplementary Information

Ligand influence in electrocatalytic properties of Cu(II) triazole complexes for hydrogen peroxide detection in aqueous media

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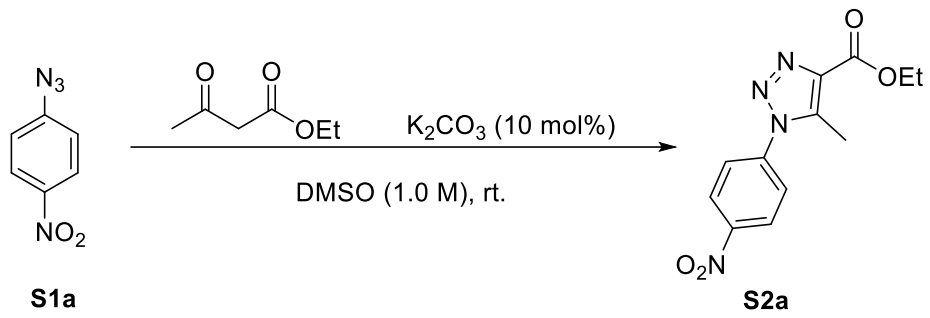
1. Synthesis of **copper (II) complexes $Cu(L^{NO2})_2$, $Cu(L^{Br})_2$ and $Cu(L^{OMe})_2$**

1.1.*Synthesis Synthesis of Ethyl 1-Aryl-5-methyl-1H-1,2,3-triazole-4-carboxylate* ***S2a-c***.

Exemplified for ***S2a***.

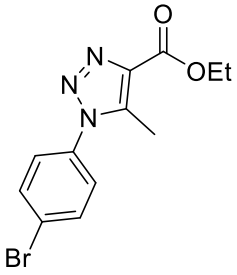


S1a **S2a**

Catalytic K_2CO_3 (252 mg, 1.82 mmol, 10 mol%) were added to a solution of phenylazide **S1a** (3.01 g, 18.32 mmol, 1.0 equiv.) and ethyl acetoacetate (2.54 mL, 20.11 mmol, 1.1 equiv) in DMSO (18.3 mL, 1.0 M). The resulting reaction mixture was stirred at room temperature for 3 h. The progress of the reaction was monitored by TLC. Then, cold water (30 mL) was added, obtaining a precipitate that was filtered and washed successively with cold water and vacuum drying. Triazole **S2a** was purified by crystallization with EtOH and then with AcOEt, obtaining 4.63 g as yellow crystals (92% yield). **m.p**.: 178–180°C; **IR** (cm^{-1}) *ν*: 3120, 3099, 3080 (C_{ar}-H), 2977, 2937, 2870 (C_{sp}^3-H), 1721 (C=O), 1597 (C_{ar}- C_{ar}), 1566 (N=N), 1533, 1346 (Ar-NO_2), 1249 (CO-O), 980 (N-N=N); **^{1}H NMR** (500 MHz, $CDCl_3$) δ (ppm): 8.44 (d, *J* = 8.9 Hz, 1H), 7.73 (d, *J* = 9.0 Hz, 1H), 4.45 (q, *J* = 7.1 Hz, 1H), 2.67 (s, 1H), 1.43 (t, *J* = 7.1 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ (ppm): 161.4 (C=O), 148.3 (C), 140.3 (C), 138.9 (C), 137.5 (C), 126.0 (CH), 125.3 (CH), 61.5 (CH_2), 14.4 (CH_3), 10.3 (CH_3). **HRESIMS**: Calculated to $C_{12}H_{13}N_4O_4$ $[M+H]^+$: *m/z* 277.0937, found: 277.0909. (Figure S16-18).

For the synthesis of triazoles **S2b** and **S2c**, the same procedure described for **S2a** was used, obtaining:

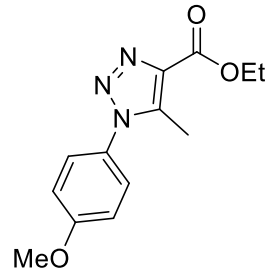
Ethyl 1-(4-bromophenyl)-5-methyl-1H-1,2,3-triazole-4-carboxylate (**S2b**):



S2b

White crystals in THF (92% yield from 4-bromophenylazide **S1b**); **m.p**.: 176–178°C; **IR** (cm^{-1}) *ν*: 3099, 3067 (C_{Ar}-H), 1717 (C=O), 1562 (N=N), 1248 (CO-O), 981 (N-N=N), 840 (Ar-Br); **^{1}H NMR** (500 MHz, $CDCl_3$) *δ* (ppm): 7.67 (d, *J* = 7.5 Hz, 2H), 7.32 (d, *J* = 7.8 Hz, 2H), 4.41 (q, *J* = 6.7 Hz, 2H), 2.55 (s, 3H), 1.39 (t, *J* = 6.8 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) *δ* (ppm): 161.5 (C=O), 138.8 (C), 136.9 (C), 134.4 (C), 133.0 (CH), 126.9 (CH), 124.2 (C), 61.2 (CH_2), 14.4 (CH_3), 10.1 (CH_3); **HRESIMS**: Calculated to $C_{12}H_{13}BrN_3O_2$ $[M+H]^+$: *m/z* 310.0191, found: 310.0159. (Figure S19-21)

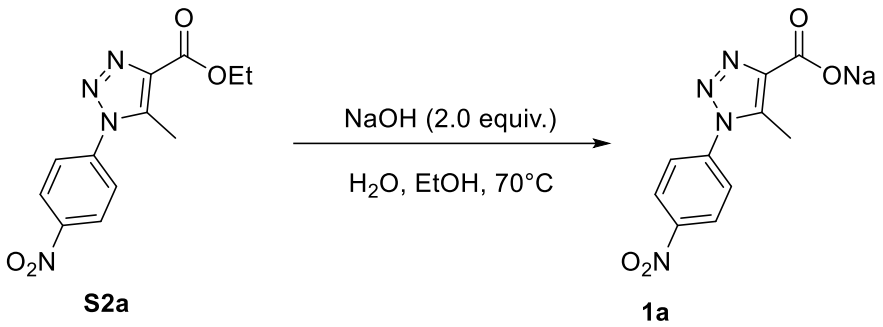
Ethyl 1-(4-methoxyphenyl)-5-methyl-1H-1,2,3-triazole-4-carboxylate (**S2c**):



S2c

White crystals in THF (82% yield from 4-methoxyphenylazide **S1c**); **m.p.:** 140–142°C; **IR** (cm^{-1}) *ν*: 3086, 3004 (C_{Ar}-H), 1709 (C=O), 1564 (N=N), 1247 (CO-O), 982 (N-N=N); **^{1}H-NMR** (500 MHz. $CDCl_3$) *δ* (ppm): 7.32 (d, *J* = 5.4 Hz, 2H), 7.02 (d, *J* = 5.1 Hz, 2H), 4.43 (q, *J* = 6.2 Hz, 2H), 3.85 (s, 3H), 2.52 (s, 3H), 1.41 (t, *J* = 6.1 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) *δ* (ppm): 161.8 (C=O), 160.7 (C), 139.1 (C), 136.5 (C), 128.2 (C), 126.9 (CH), 114.8 (CH), 61.1 (CH_2), 55.8 (CH_3), 14.5 (CH_3), 10.1 (CH_3); **HRESIMS**: Calculated to $C_{13}H_{16}N_3O_3$ $[M+H]^+$: *m/z* 262.1192, found: 262.1152. (Figure S22-24)

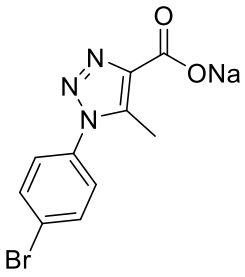
1.2.*Synthesis of bidentate triazole ligands **1a-b.*** Exemplified for **1a**.



NaOH (579 mg, 14.48 mmol, 2.0 equiv.) and H_2O (7.0 mL) was added to a solution of ethyl 5-methyl-1-(4-nitrophenyl)-1*H*-1,2,3-triazole-4-carboxylate (**S2a**) (2.0 g, 7.24 mmol) in EtOH (50 mL) at rt. The resulting mixture was warmed to 70 °C for 3 h and then cooled to room temperature. The resulting precipitate was filtered (washed with cold EtOH) and dried in vacuo to give sodium 5-methyl-1-(4-nitrophenyl)-1*H*-1,2,3-triazole-4-carboxylate **1a** as a white solid (1.92 g, 98% yield). **m.p.:** >300 °C; **IR** (KBr, cm^{-1}) 3506 (O-H, residual moisture), 3114 and 3080 (C_{Ar}-H), 1623 (C=O), 1601 (N=N), 1444 and 1346 (Ar-NO_2), 1095 (CO-O). **^{1}H-NMR** (400 MHz, DMSO-*d*6 + CDCl3) δ (ppm): 8.41 (d, *J* = 8.9 Hz, 2H), 7.85 (d, *J* = 8.9 Hz, 2H), 2.55 (s, 3H).; **HRESIMS**: Calculated to $C_{10}H_7N_4O4_3$ $[M-H]^-$: *m/z* 247.0473, found: 247.0465. (Figure S25-26)

For the synthesis of **1b**, the same procedure described for **1a** was used, obtaining:

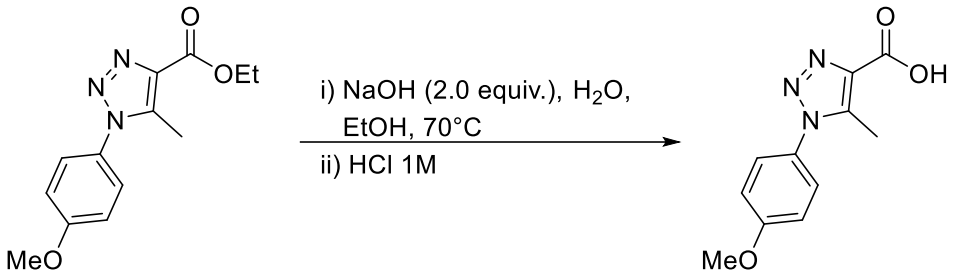
Sodium 5-methyl-1-(4-nitrophenyl)-1H-1,2,3-triazole-4-carboxylate (**1b**):



1b

White solid (77% yield from **S2b**). **m.p.:** 176-178 °C; **IR** (KBr, cm^{-1}) 3510 (O-H, residual moisture), 3095 (C_{Ar}-H), 1615 (C=O), 1496 (N=N), 1066 (CO-O), 840 (Ar-Br). **^{1}H-NMR** (400 MHz, DMSO-d_6) δ (ppm): 7.69 (d, J = 8.6 Hz, 2H), 7.36 (d, J = 8.7 Hz, 2H), 2.36 (s, 3H); **^{13}C NMR** (101 MHz, DMSO-d_6) δ (ppm): 168.24 (CO), 143.72 (C), 137.95 (C), 135.88 (C), 134.28 (CH), 128.59 (CH), 124.85 (C), 10.80 (CH_3); **HRESIMS**: Calculated to $C_{10}H_7BrN_3O_2$ $[M-H]^-$: *m/z* 279.9727, found: 279.9734. (Figure S27-29)

1.3.*Synthesis of bidentate triazole ligands **1c.***

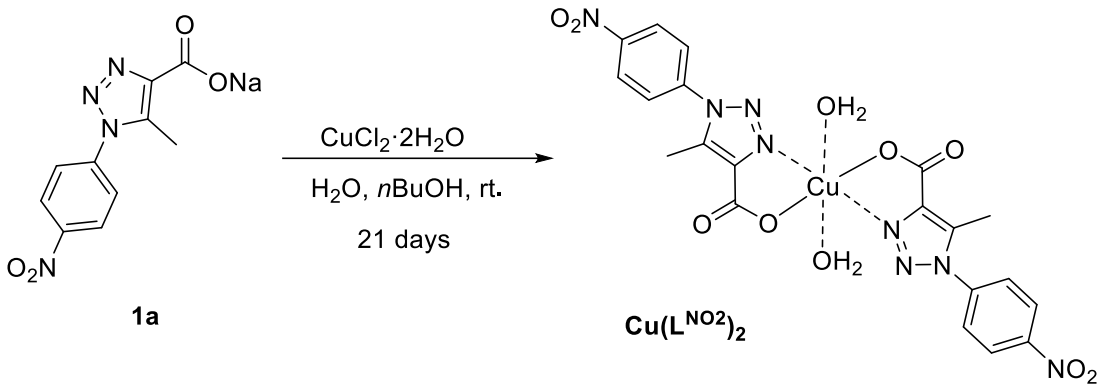


S2c **1c**

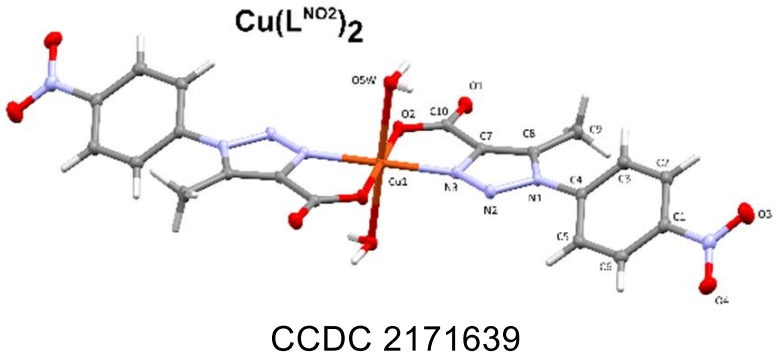
NaOH (612.32 mg, 15.31 mmol, 2.0 equiv.) and H_2O (7.6 mL) was added to a solution of ethyl *1-(4-methoxyphenyl)-5-methyl-1H-1,2,3-triazole-4-carboxylate* (**S2c**) (2.0 g, 7.65 mmol) in EtOH (50 mL) at rt. The resulting mixture was warmed to 70 °C for 3 h and then cooled to room temperature. Then, the volatile fraction (EtOH) was evaporated in vacuo and water (50 mL) was added. The resulting mixture was acidified with 1M HCl to pH 3 and extracted with $CHCl_3$ (3 x 20 mL). The combined organic layers were dried over Na_2SO_4, filtered and concentrated in vacuo to give 1-(4-methoxyphenyl)-5-methyl-1H-1,2,3-triazole-4-carboxylic acid **1c** (1.67 g, 93%) as a white solid which was used without purification in the next step. **m.p.:** 193 - 194 °C; **IR** (KBr, cm^{-1}) ν: 3077 (COO-H), 3050 (C_{Ar}-H), 1687

(C=O), 1518 (N=N), 1272 (CO-O). **^{1}H-NMR** (400 MHz, DMSO-d_6) δ (ppm): 13.11 (s, 1H), 7.53 (d, J = 8.9 Hz, 2H), 7.15 (d, J = 8.9 Hz, 2H), 3.84 (s, 3H), 2.45 (s, 3H).; (101 MHz, DMSO-d_6) δ (ppm): 162.70 (CO), 160.21 (C), 139.09 (C), 136.32 (C), 128.14 (C), 127.01 (CH), 114.77 (CH), 55.64 (CH_3), 9.69 (CH_3).; **HRESIMS**: Calculated to $C_{11}H_{10}N_3O_3$ $[M-H]^-$: m/z 232.0728, found: 232.0733. (Figure S30-32)

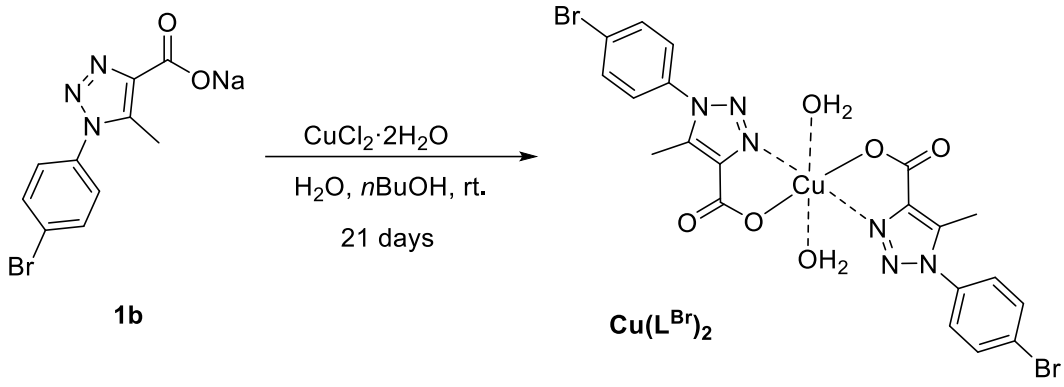
1.4. *Synthesis of copper (II) complex* ***Cu(L^{NO2})$_2$***



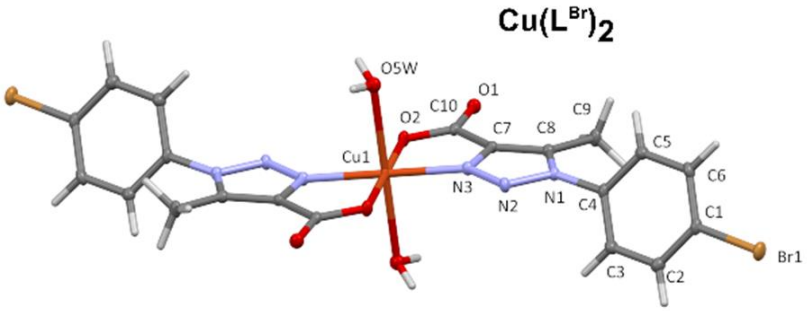
A solution of $CuCl_2 \cdot 2H_2O$ (6.31 mg, 37.01 µmol) in *n*BuOH (4 mL) was carefully added to a solution of sodium 1-(4-nitrophenyl)-5-methyl-*1H*-1,2,3-triazole-4-carboxylate (**1a**) (20.0 mg, 74.02 µmol) in water (4 mL) contained in a vial. The vial was sealed, and a light blue precipitate was obtained after 21 days. The precipitate was crystallized from DMF obtaining light blue single crystals of $Cu(L^{NO_2})_2$ after 4 days (9.30 mg, 42%). **m.p.:** 235-237 °C (dec.). **IR** (KBr, cm^{-1}) *ν*: 3409 (O-H), 3118 and 3069 (C_{Ar-H}), 1653 (C=O), 1530 (N=N), 1525 and1350 (Ar-NO_2), 1317 (CO-O) (Figure S33). UV/Vis (DMF): λ_{max} = 276 nm (Figure S4). $Cu(L^{NO_2})_2$ structure was confirmed by X-ray crystallography (CCDC 2171639).



1.5.*Synthesis of copper (II) complex* ***Cu(L^{Br})$_2$***

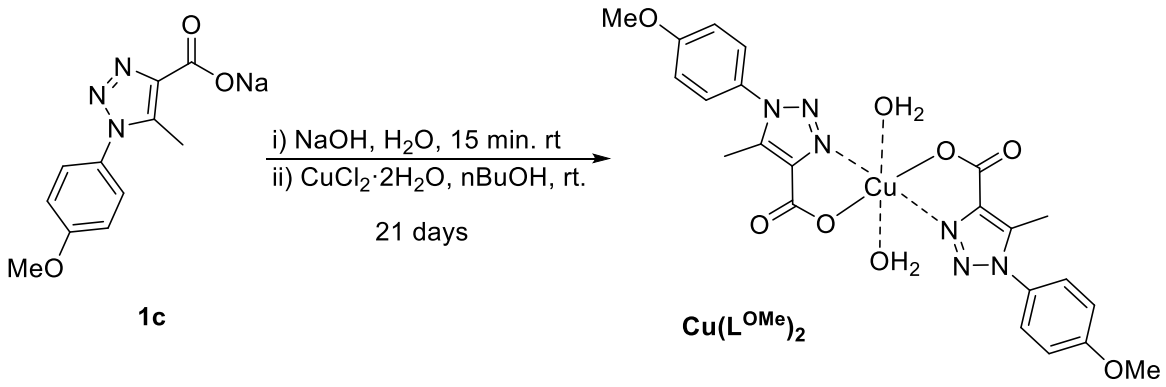


A solution of $CuCl_2 \cdot 2H_2O$ (5.61 mg, 32.89 µmol) in *n*BuOH (4 mL) was carefully added to a solution of sodium 1-(4-bromophenyl)-5-methyl-*1H*-1,2,3-triazole-4-carboxylate (**1b**) (20.0 mg, 65.77 µmol) in water (4 mL) contained in a vial. The vial was sealed, and light blue single crystals of $Cu(L^{Br})_2$ were obtained after 21 days (12.37 mg, 57%). **m.p.:** 222-225 °C (dec.). **IR** (KBr, cm^{-1}) ν: 3226 (O-H), 3106 and 3054 (C_{Ar-H}), 1657 (C=O), 1582 (N=N), 1313 (CO-O), 1010 (N-N=N), 850 (Ar-Br) (Figure S34). UV/Vis (DMF): λ_{max} = 267 nm (Figure S5). $Cu(L^{Br})_2$ structure was confirmed by X-ray crystallography (CCDC 2171641).

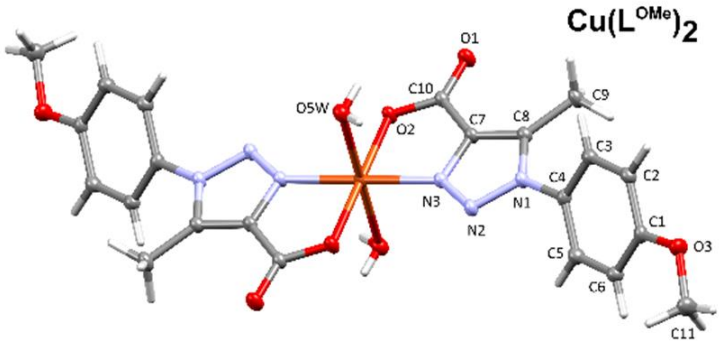


CCDC 2171641

1.6.*Synthesis of copper (II) complex* ***Cu(L^{OMe})$_2$***



A solution of $CuCl_2 \cdot 2H_2O$ (7.31 mg, 42.88 µmol) in *n*BuOH (8 mL) was carefully added to a solution of 1-(4-methoxyphenyl)-5-methyl-*1H*-1,2,3-triazole-4-carboxylic acid (**1c**) (20.0 mg, 85.75 µmol) in water (8 mL) contained in a vial, previously treated with NaOH (43.0 µL, 2.0 M, 85.75 µmol) for 30 min. The vial was sealed, and blue single crystals of $Cu(L^{MeO})_2$ were obtained 21 days (21.8 mg, 90%). **m.p.:** 225-230 °C (dec.). **IR** (KBr, cm^{-1}) ν: 3540 and 3428 (O-H), 3054 (C_{Ar}-H), 1634 (C=O), 1522 (N=N), 1246 (CO-O), 1021 (C_{Ar}-OMe) (Figure S35). UV/Vis (DMF): λ_{max} = 265 nm (Figure S6). $Cu(L^{OMe})_2$ structure was confirmed by X-ray crystallography (CCDC 2171640).



CCDC 2171640

2. Crystallography data of $Cu(L^{NO_2})_2$, $Cu(L^{Br})_2$ and $Cu(L^{OMe})_2$ complexes

Table S1. Data and experimental details for $Cu(L^{NO2})_2$, $Cu(L^{Br})_2$ and $Cu(L^{OMe})_2$

Crystal data	**$Cu(L^{NO_2})_2$**	**$Cu(L^{Br})_2$**	**$Cu(L^{OMe})_2$**
Ideal formula	$C_{20}H_{18}CuN_8O_{10}$, 2(C_3H_7NO), 2(H_2O)	$C_{20}H_{18}Br_2CuN_6O_6$, 3(H_2O)	$C_{22}H_{24}CuN_6O_8$, 2(H_2O)
Crystal system, Space group	P-1	P-1	P 21/c
Crystal size (mm)	0.10 × 0.09 × 0.04	0.08 × 0.07 × 0.03	0.10 × 0.09 × 0.04
Temperature (K)	100	100	100
a,*b*,*c* (Å)	7.3942(4), 8.0737(4), 15.2816(8)	7.2584(4), 11.4225(6), 16.6484(8)	11.7258(5), 10.2545(4), 10.9905(4)
α, β, γ (°)	102.804(2), 92.714(2), 109.580(2),	105.3322(18), 98.0427(18), 100.6246(18)	90, 107.7260(10), 90
V (Å^3)	830.79(8)	1282.18(12)	1258.78(9)
Z	1	2	2
Calculated density (g cm^{-3})	1.551	1.854	1.583
μ (mm^{-1})	0.741	4.03	0.936
Data Collection			
Θ range (˚)	2.76 to 28.27	1.95 to 28.28	2.70 to 30.03
Absorption correction	multi-scan Bruker Sadabs-2016/2		
T_{min}, T_{max}	0.9171, 0.9705	0.7771, 0.8496	0.942, 0.877
Nº. of measured, independent and observed [I>2σ] reflections	30694, 4111, 3732	50780, 6375, 5178	24114, 3673, 3150
[R_{int}]	0.0387	0.042	
Data completeness to 28.27ºθ (%)	99.9	99.9	99.8
Refinenment			
Refinemment	Full-matrix least squaes on F^2		
Number of reflections, parameters, restraints	4111, 251, 0	6375, 387,9	3673, 192,0
R_1(all), wR_2 (all)	0.0328, 0.0673	0.0378, 0.0681	0.0447, 0.0921
R_1 [$I > 2\sigma(I)$], wR_2	0.0275, 0.0645	0.0263, 0.062	0.034, 0.0831
GoF	1.047	1.037	1.05
$\Delta\rho_{max}$ (eÅ^{-3})/$\Delta\rho_{min}$ (eÅ^{-3})	0.37/-0.39	0.91/-0.37	1.38/-0.63

Table S2. Hydrogen Bonds distances (Å) and angles (°) for $Cu(L^{NO2})_2$, $Cu(L^{Br})_2$ and $Cu(L^{OMe})_2$

Donor-H..Acceptor	**D - H**	**H...A**	**D...A**	**D-H...A**
$Cu(L^{NO2})_2$				
O5W-H51..O1^{i}	0.83(2)	1.97(2)	2.7841(14)	166(2)
O5W-H52..O7	0.84(2)	1.93(2)	2.7698(15)	176(2)
O6W-H61..O7	0.84(2)	2.13(2)	2.9459(16)	167(2)
O6W-H62..O1^{i}	0.85(2)	2.01(2)	2.8558(15)	170(2)
Symmetry code: i (1-x,2-y,1-z) ii()				
$Cu(L^{Br})_2$				
(O6W-H62A)_3..O2_2	0.862(17)	1.992(18)	2.840(2)	167(3)
(O6W-H61A)_3^a..O8W	3 0.90(2)	1.92(3)	2.787(3)	161(6)
(O6W-H61B)_3^b..O7W_3	0.90(2)	2.17(5)	2.816(3)	128(5)
(O7W-H71A)_3^a..O6W_3	0.86(2)	1.97(2)	2.816(3)	169(6)
(O8W-H81B)_3^b..O6W_3	0.907(19)	2.05(4)	2.787(3)	138(5)
(O8W-H82A)_3..O1_1	0.865(17)	1.907(18)	2.763(2)	170(3)
(O5W-H5A)_2..O7W_3^{i}	0.79(3)	2.05(3)	2.826(2)	172(3)
(O7W-H72A)_3..N2_1^{ii}	0.828(17)	2.38(2)	3.147(3)	155(3)
(O5W- H5B)_2..O1_2^{iii}	0.78(3)	2.00(3)	2.772(2)	172(3)
(C9-H9B)_1..Br1_2^{iv}	0.98	2.88	3.826(2)	163.7
(O5W- H51A)_1..O1_1^{v}	0.80(3)	1.96(3)	2.762(2)	175(3)
(O5W-H51B)_1..O6W_3^{v}	0.78(3)	2.26(3)	3.005(2)	161(3)
(O8W-H81A)_3^a..O7W_3^{v}	0.89(2)	1.97(2)	2.860(3)	171(6)
(O7W-H71B)_3^b..O8W_3^{vi}	0.85(2)	2.13(4)	2.860(3)	143(6)
Symmetry codes: (i) −x+2, −y+1, −z+1; (ii) −x+1, −y+1, −z+2; (iii) −x+1, −y+1, −z+1; (iv) x, y−1, z+1; (v) x−1, y, z; (vi) x+1, y, z.				
$Cu(L^{OMe})_2$				
O5W-H51W..O1^{i}	0.80(2)	2.06(2)	2.8553(18)	174(2)
O5W-H52W..O6W^{ii}	0.73(3)	2.14(3)	2.818(2)	155(2)
O6W-H61W..O2^{iii}	0.82(3)	2.00(3)	2.8205(19)	175(3)
O6W-H62W..O1^{iv}	0.79(3)	2.15(3)	2.8962(19)	159(3)
C3-H3..O5W^{iv}	0.95	2.48	3.400(2)	163

C9-H9B..O3^{v}	0.98	2.50	3.165(2)	125
Symmetry codes: (i) -x,-1/2+y,1/2-z, (ii) x,1/2-y,-1/2+z, (iii) -x,1-y,1-z, (iv) x,3/2-y,1/2+z, (v) 1-x,2-y,2-z				

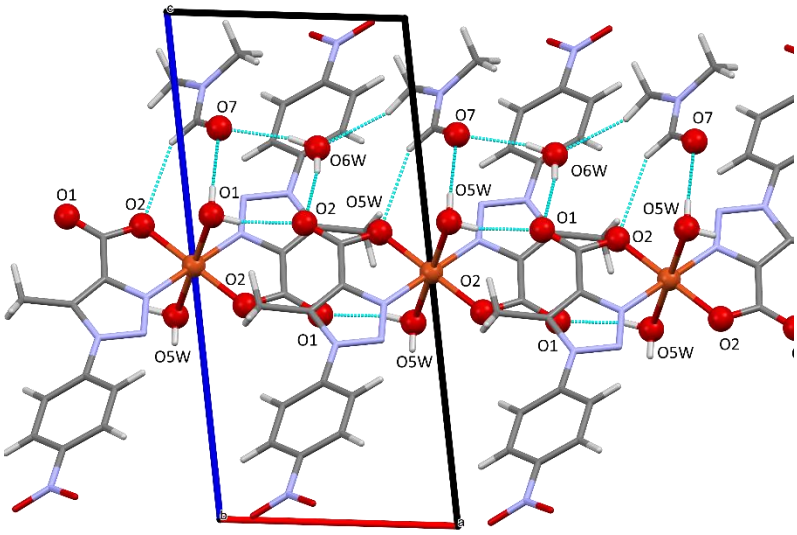


Figure S1. Infinite chain along [1 0 0] direction for Cu(L^{NO2})$_2$. Symmetry codes omitted for clarify

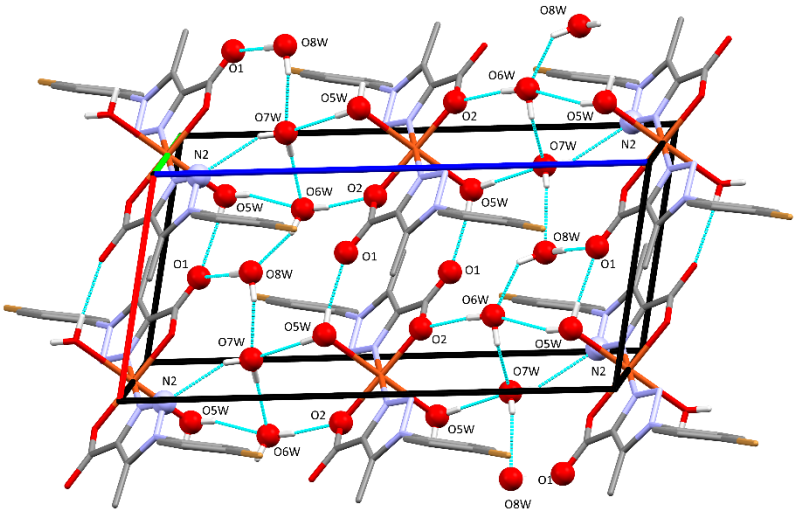


Figure S2. Projection along b-axis with 2D-Networks along ac plane for $Cu(L^{Br})_2$. Symmetry codes omitted for clarify

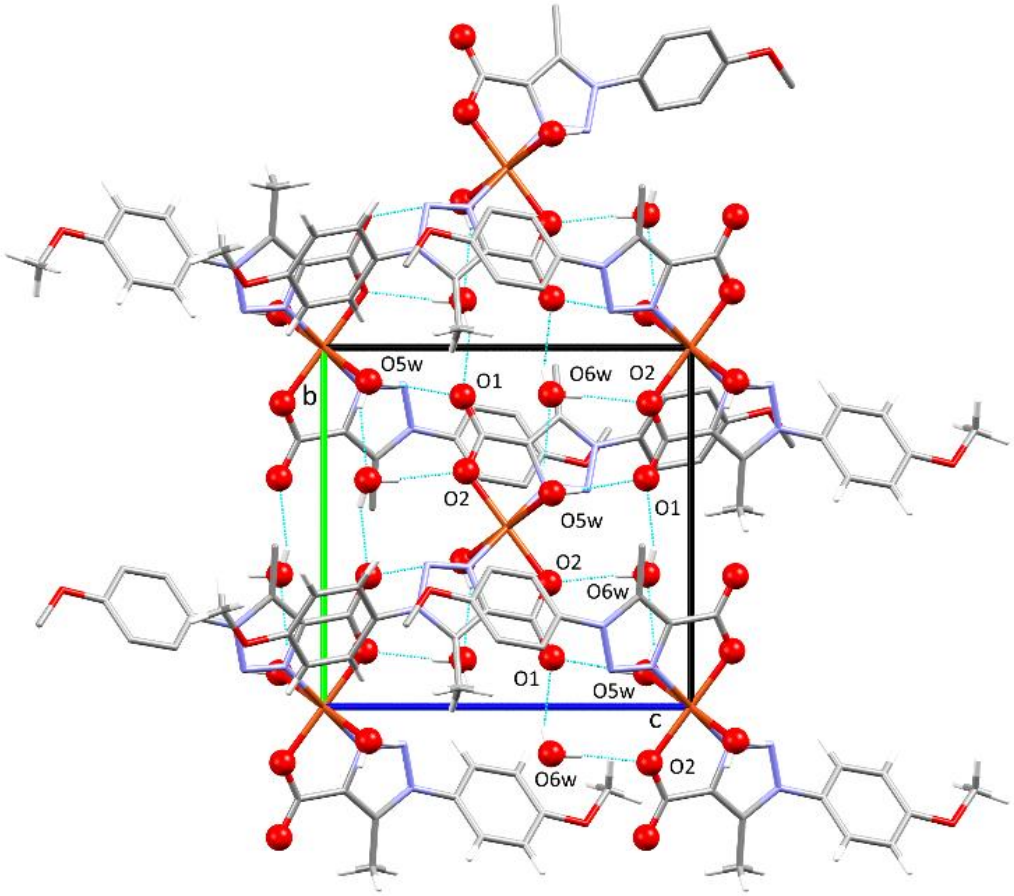


Figure S3. Projection along a-axis with 2D-Networks along bc plane for $Cu(L^{OMe})_2$. Symmetry codes omitted for clarify

Table S3. Selected geometric parameters bonds (Å) and angles (°) for $Cu(L^{NO2})_2$, $Cu(L^{Br})_2$ and $Cu(L^{MeO})_2$

	$Cu(L^{NO2})_2$	**$Cu(L^{Br})_2$_A**	**$Cu(L^{Br})_2$_B**	**$Cu(L^{OMe})_2$**
Cu1-O2	1.9701(9)	1.9519(14)	1.9761(14)	1.9816(12)
Cu1-O2i	1.9701(9)	1.9520(14)	1.9761(14)	1.9816(12)
Cu1-N3	1.9959(11)	2.0212(17)	2.0012(17)	1.9837(14)
Cu1-N3i	1.9959(11)	2.0213(17)	2.0012(17)	1.9837(14)
Cu1- O5W	2.3940(11)	2.3704(16)	2.3545(16)	2.4323(13)
Cu1-O5Wi	2.3940(11)	2.3704(16)	2.3545(16)	2.4323(13)
N1-N2	1.3611(15)	1.356(2)	1.357(2)	1.3581(19)
N2-N3	1.3002(16)	1.308(2)	1.305(2)	1.3077(19)
O2-Cu1-$O2^i$	180	180	180	180
O5-Cu1-$O5w^i$	180	180	180	180
N3-Cu1-$N3^i$	180	180	180	180
O2-Cu1-N3	82.72(4)	82.82(6)	82.37(6)	82.39(5)
O2-Cu1-$N3^i$	97.28(4)	97.18(6)	97.63(6)	97.61(5)
O2-Cu1 O5W	90.77(4)	88.91(6)	90.88(6)	90.49(5)
O2-Cu1 $O5W^i$	89.23(4)	91.09(6)	89.12(6)	89.51(5)
N3 Cu1 O5W	88.81(4)	90.34(6)	90.27(6)	94.28(5)
N3 Cu1 $O5W^i$	91.19(4)	89.66(6)	89.73(6)	85.72(5)
Symmetry codes: (i)	2-x, 2-y, 1-z	-x, 1-y, 2-z	2-x, 1-y, 1-z	-x, 1-y, 1-z

Table S4. coordination polyhedral parameters

	$Cu(L^{NO2})_2$	**$Cu(L^{Br})_2$**	**$Cu(L^{Br})_2$**	**$Cu(L^{OMe})_2$**
Vp	12.6013	12.3694	12.3021	12.4458
Qe	1.0274	1.0203	1.0193	1.0223
BAV	27.8032	19.2271	21.472	20.0309

3. Electronic absorption spectra (UV-Vis)

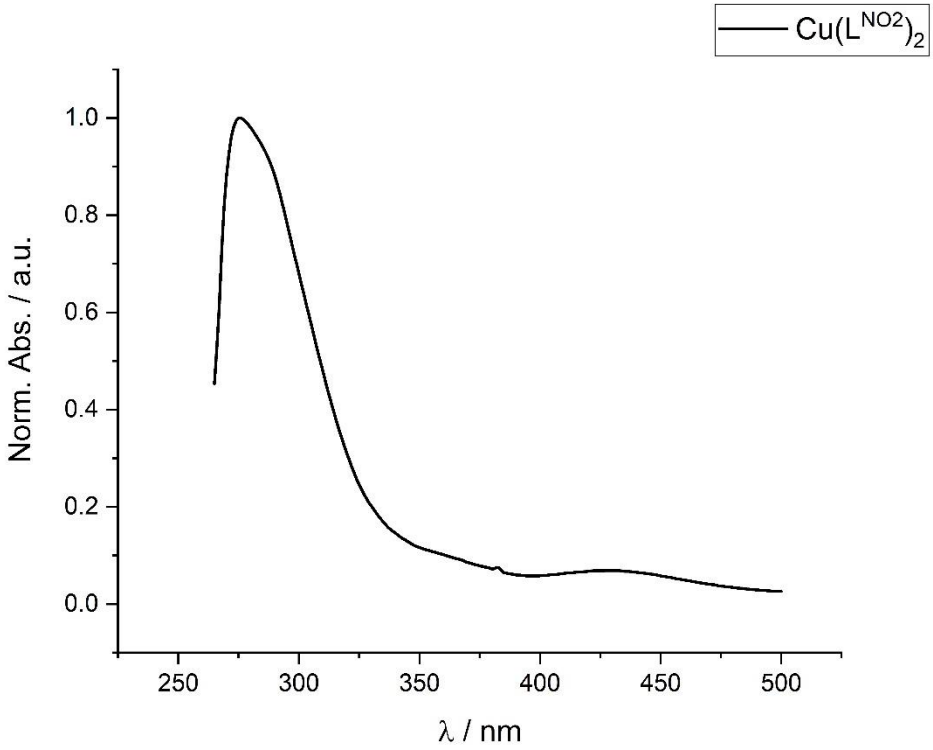


Figure S4 Electronic spectra of $Cu(L^{NO_2})_2$ recorded in DMF 10 μM.

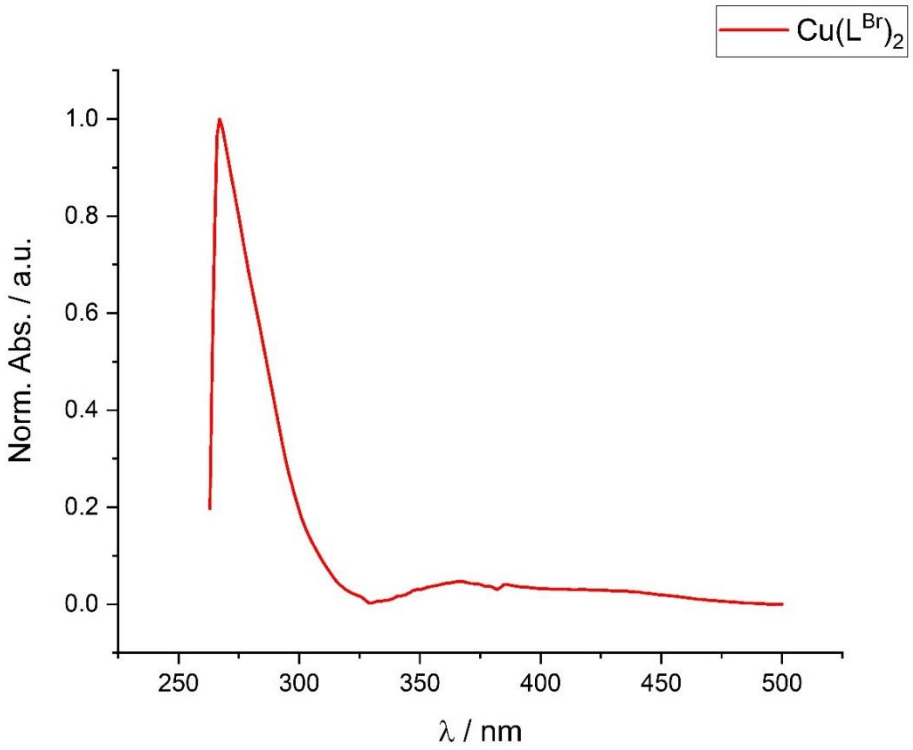


Figure S5 Electronic spectra of $Cu(L^{Br})_2$ recorded in DMF 10 μM.

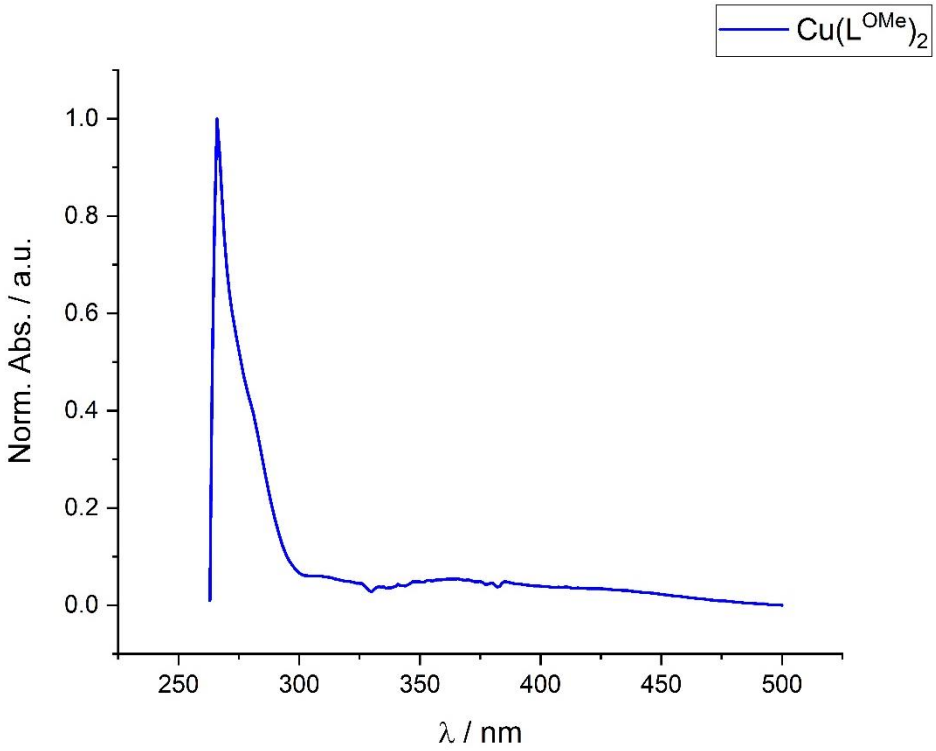


Figure S6 Electronic spectra of $Cu(L^{OMe})_2$ recorded in DMF 10 μM.

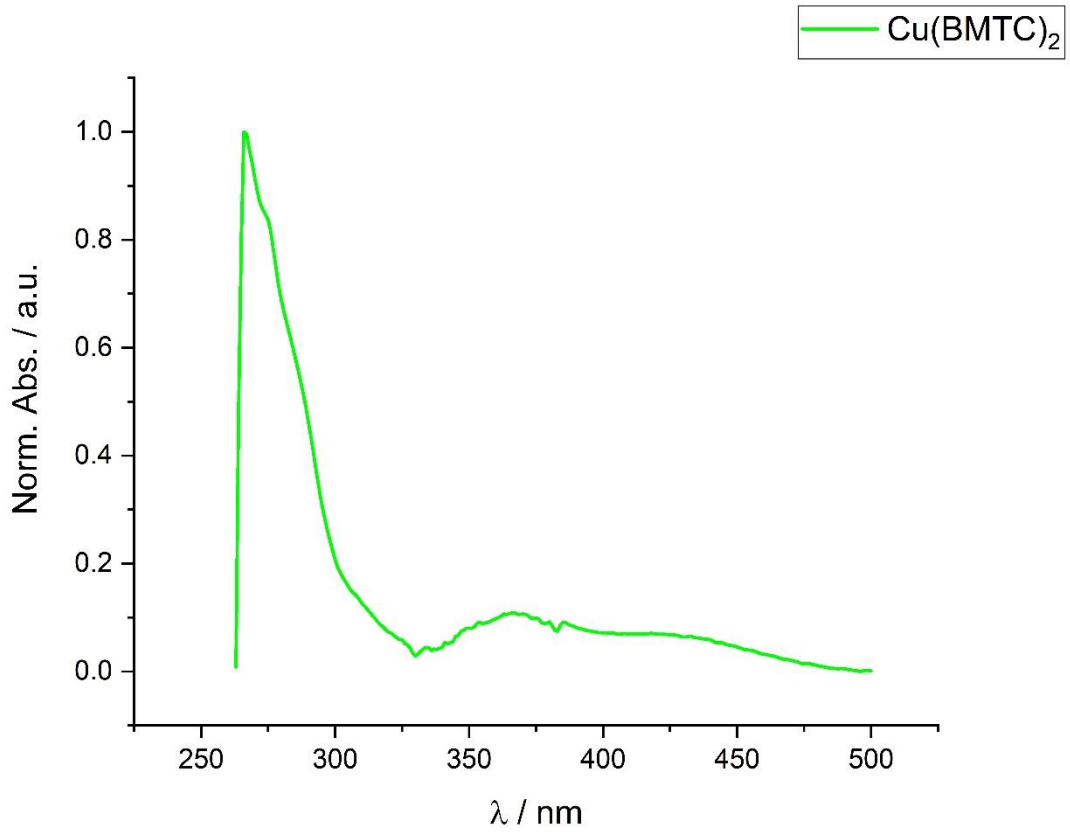


Figure S7 Electronic spectra of $Cu(BMTC)_2$ recorded in DMF 10 μM.

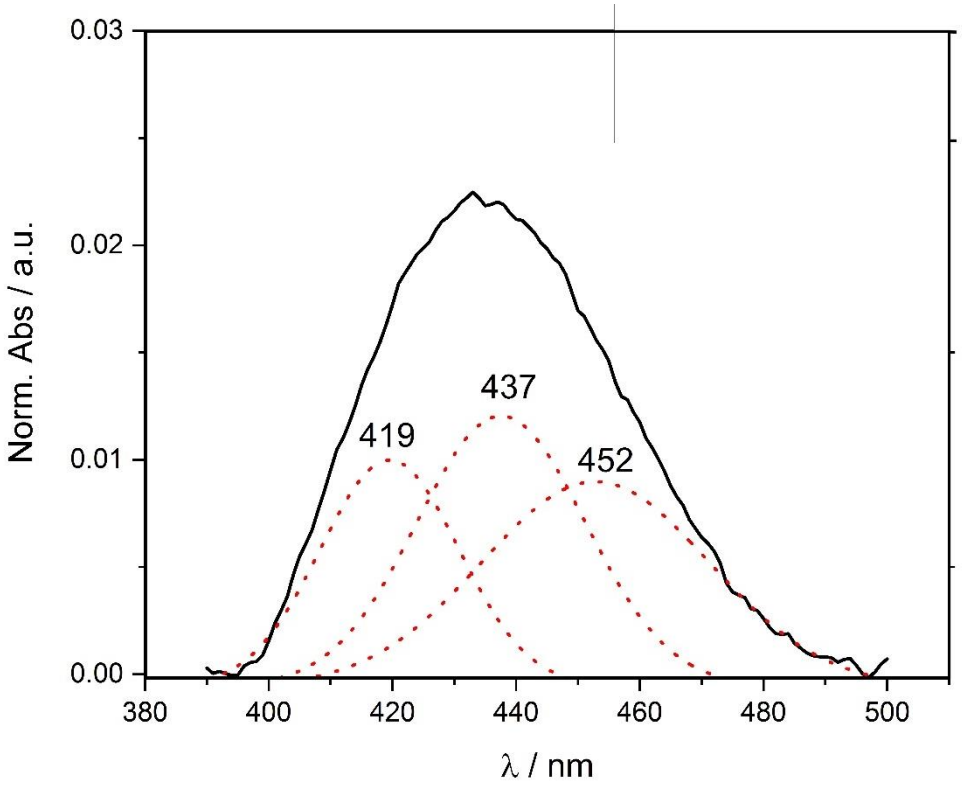


Figure S8 *d-d* transition of $Cu(L^{NO_2})_2$.

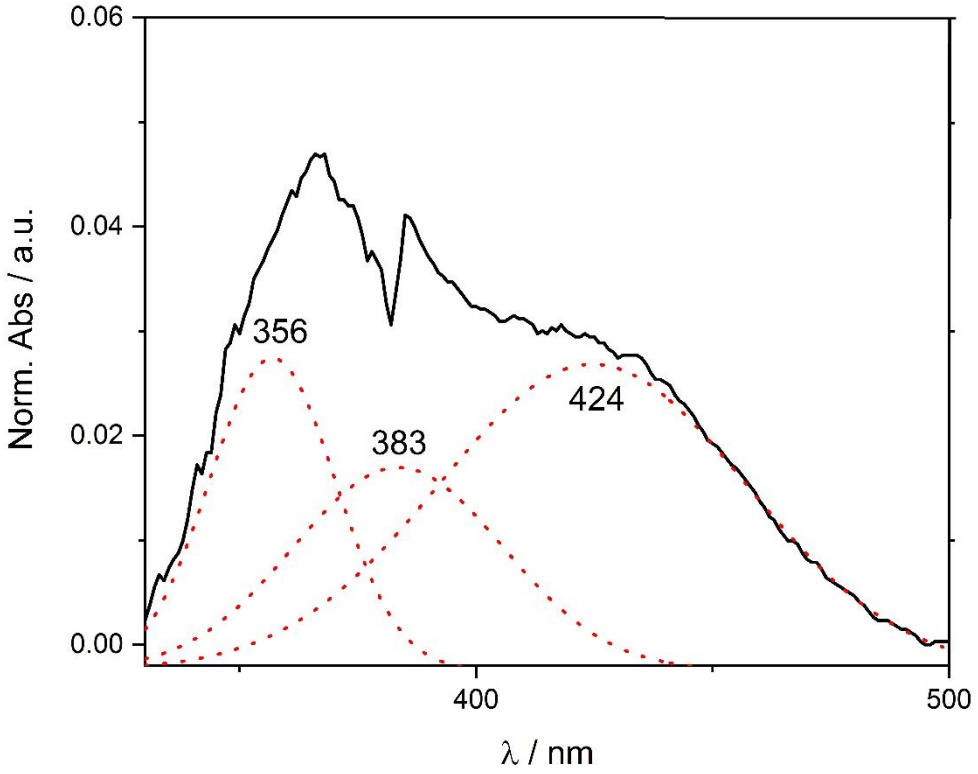


Figure S9 *d-d* transition of $Cu(L^{Br})_2$.

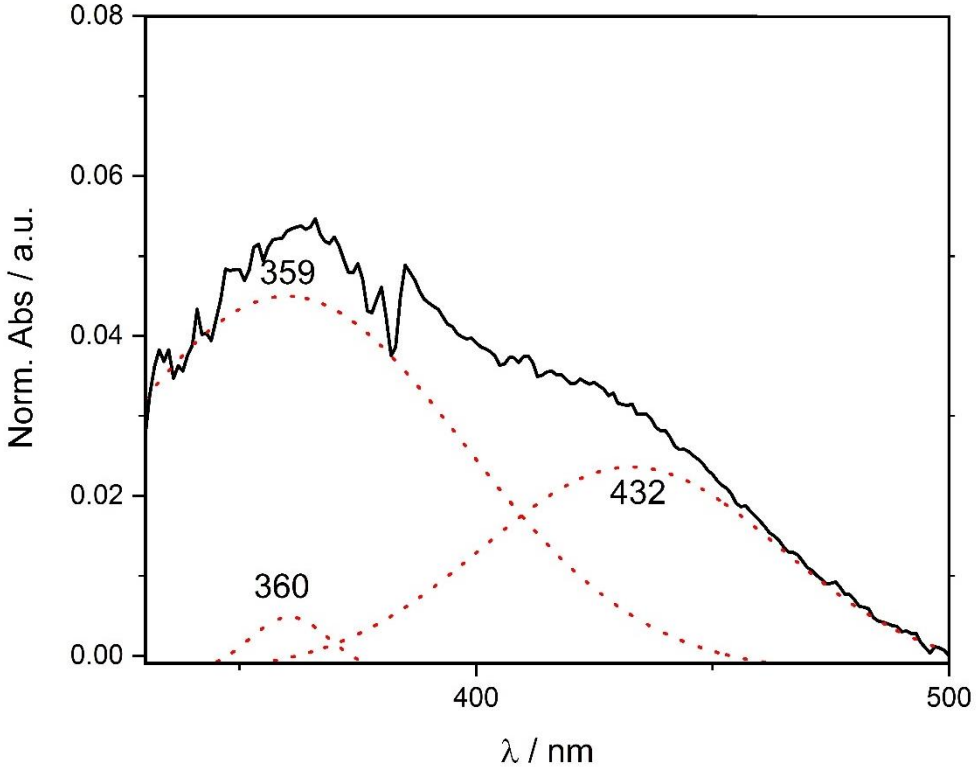


Figure S10 *d-d* transition of $Cu(L^{OMe})_2$.

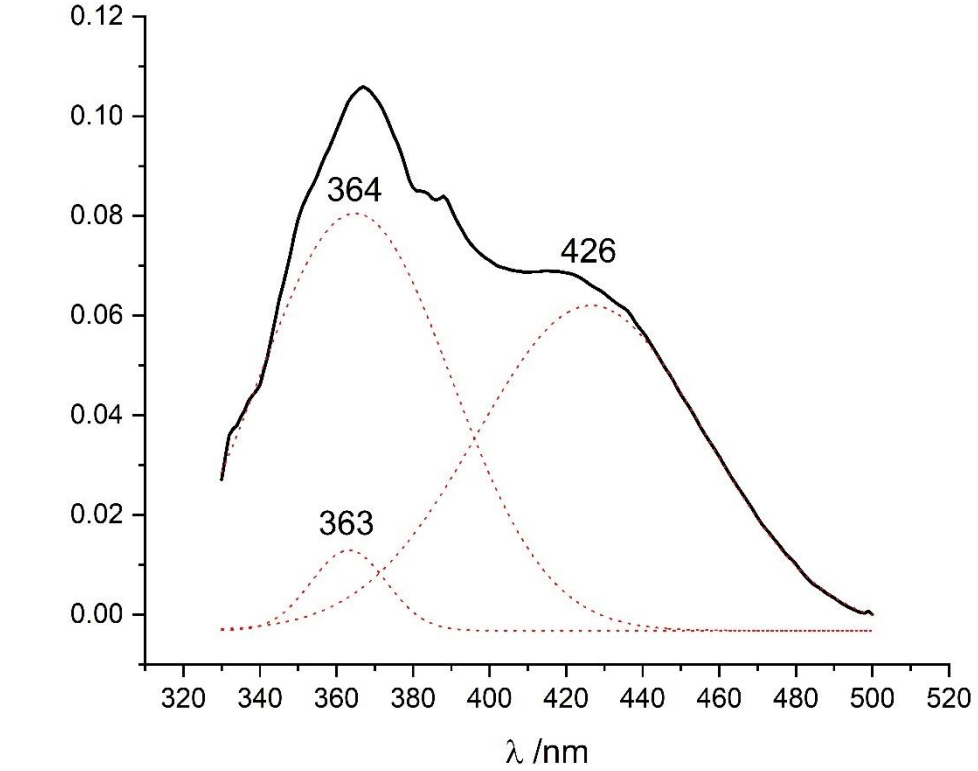


Figure S11 *d-d* transition of $Cu(BMTC)_2$.

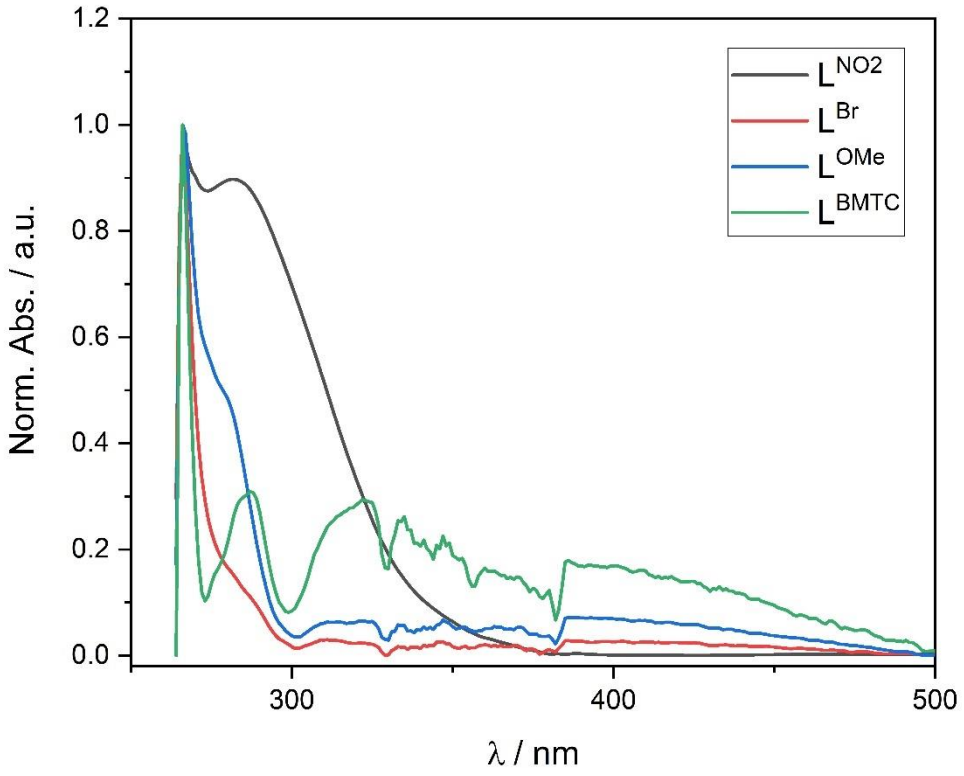


Figure S12 Electronic spectra of Ligands recorded in DMF 10 μM.

4. Cyclic voltammogram characterization

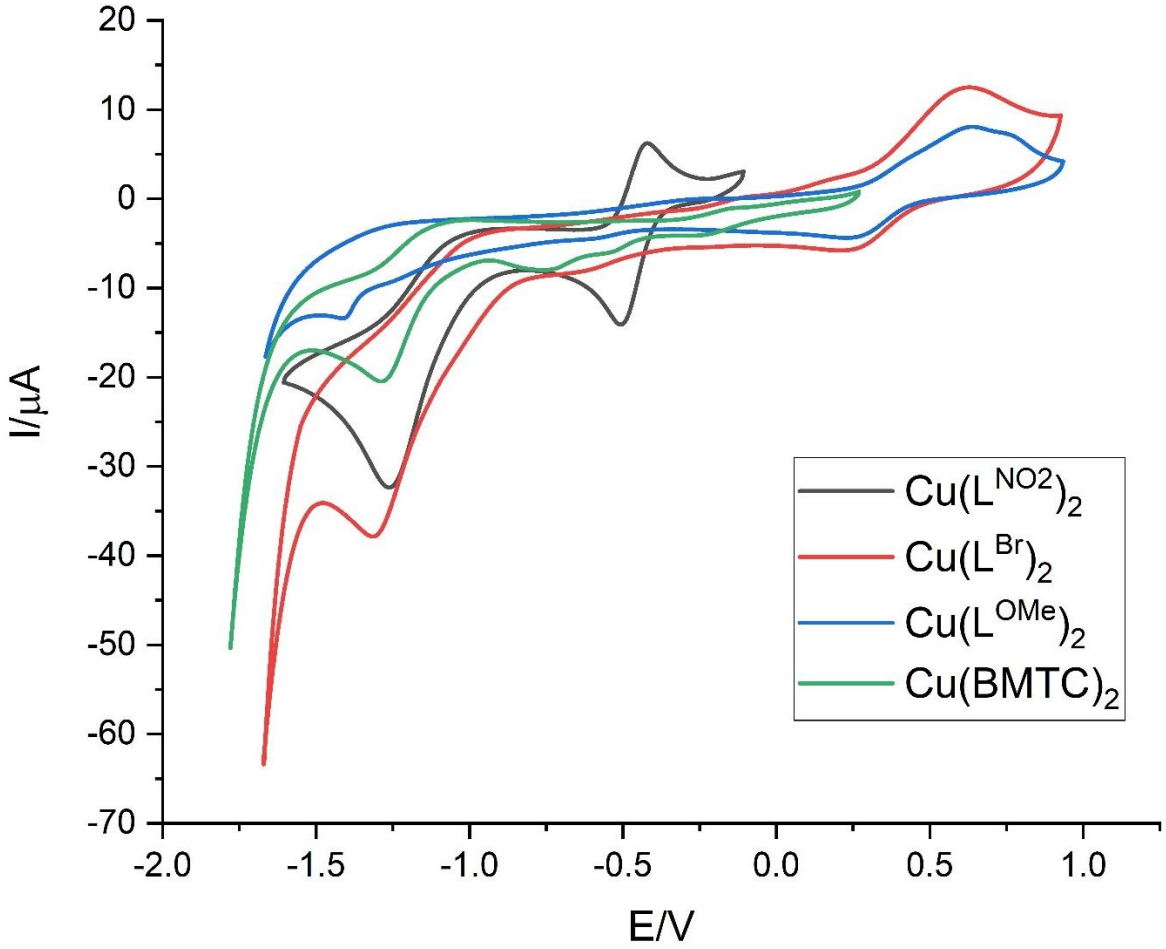


Figure S13 Cyclic voltammograms of complexes $Cu(L^{NO2})_2$, $Cu(L^{Br})_2$, and $Cu(L^{OMe})_2$, and $Cu(BMTC)_2$, recorded in DMF containing 0.1 M *n*-$Bu_4N^+PF_6^-$ at a glassy carbon working electrode at 298 K, v = 100 mVs^{-1}, reference electrode Ag/Ag^+, internal reference $Cp_2Fe^{0/+}$.

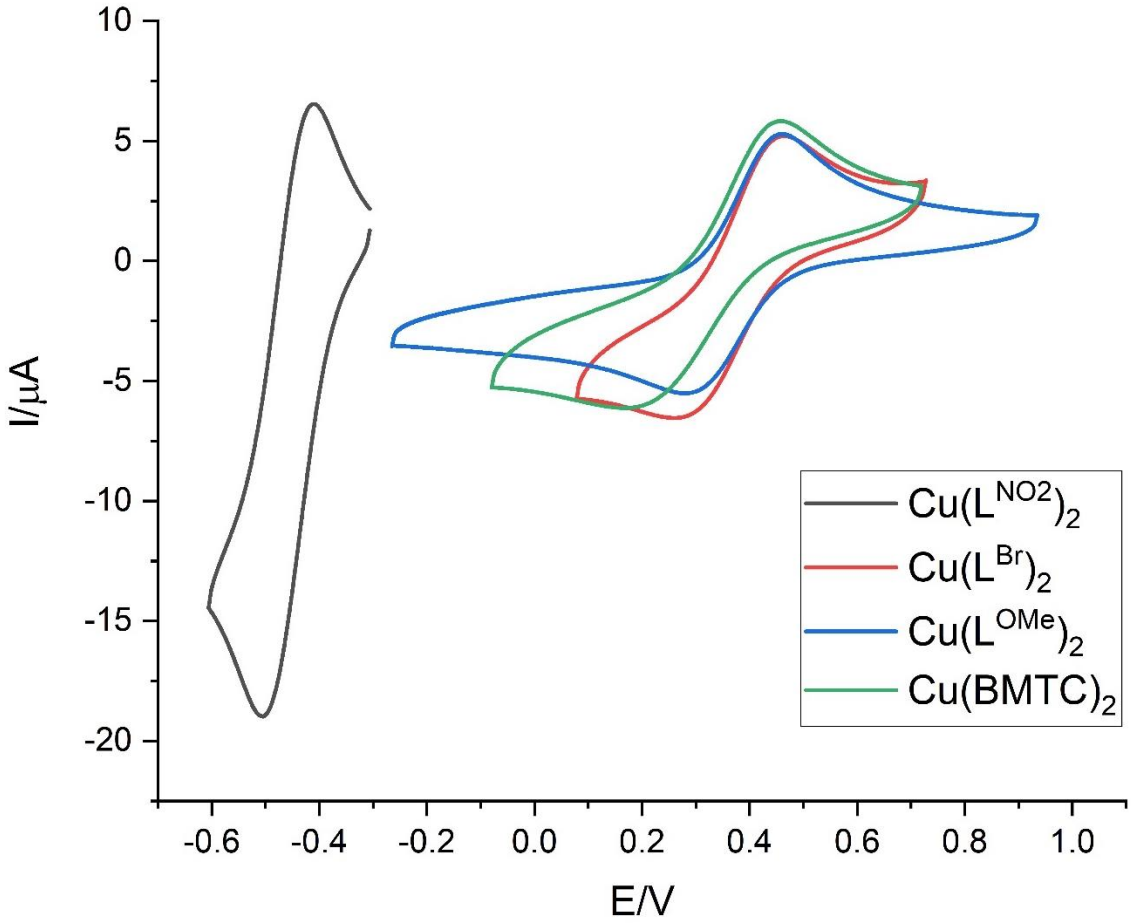


Figure S14 $Cu^{1+/2+}$ couple of complexes $Cu(L^{NO2})_2$, $Cu(L^{Br})_2$, and $Cu(L^{OMe})_2$, and $Cu(BMTC)_2$ in cyclic voltammograms recorded in DMF containing 0.1 M *n*-$Bu_4N^+PF_6^-$ at a glassy carbon working electrode at 298 K, v = 100 mVs^{-1}, reference electrode Ag/Ag^+, internal reference $Cp_2Fe^{0/+}$.

5. SEM

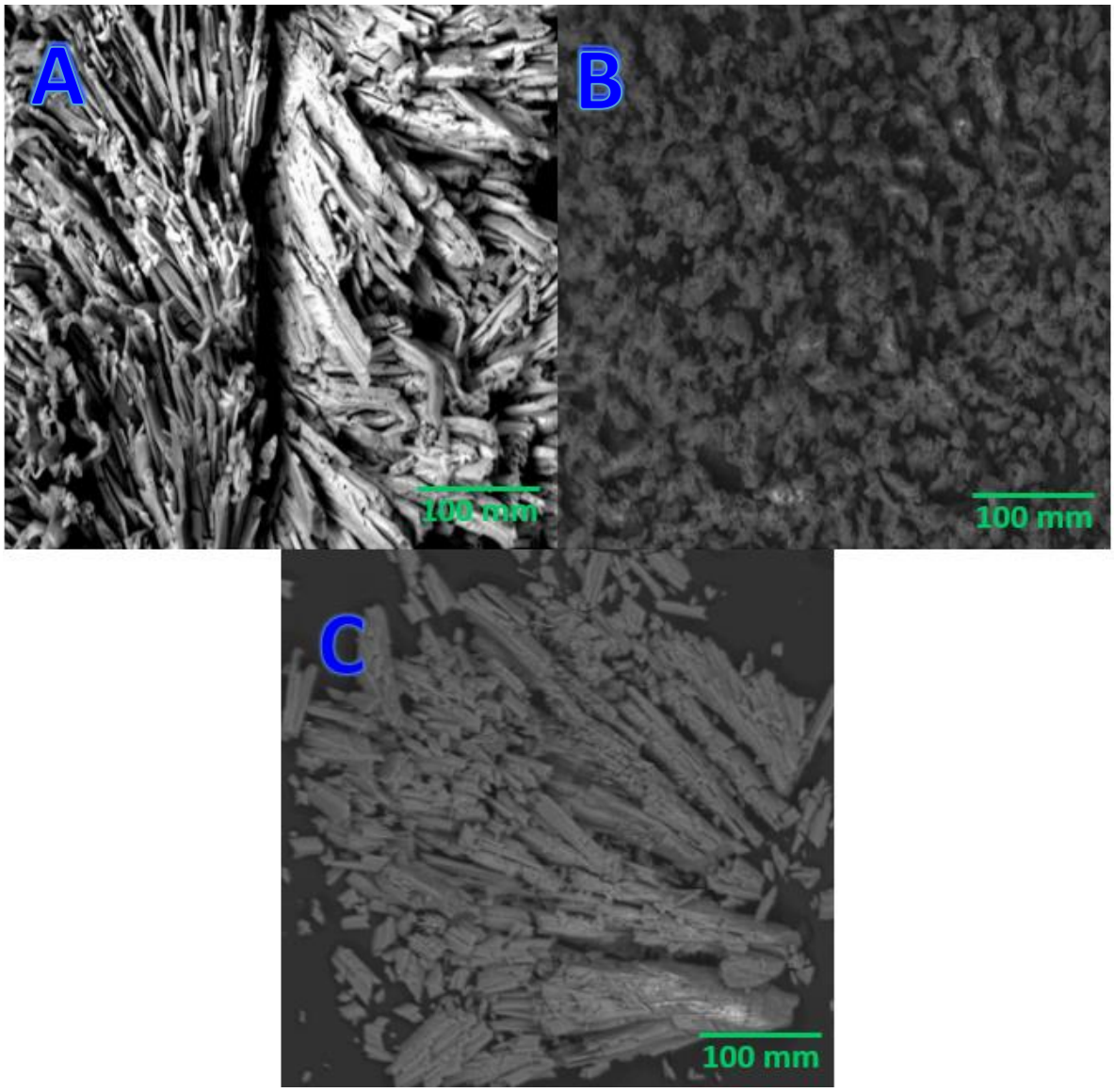


Figure S15 FE-SEM image for $Cu(L^{OMe})_2$ (A), $Cu(L^{Br})_2$ (B) and $Cu(L^{NO_2})_2$ (C).

6. IR and NMR Spectra

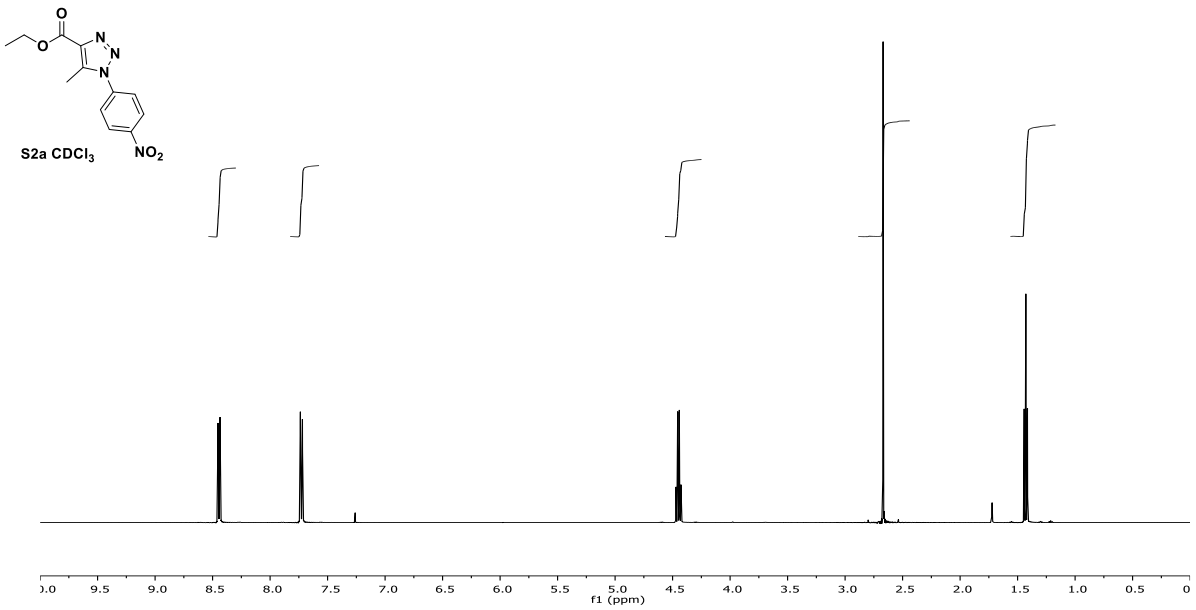


Figure S16. ^{1}H-NMR of triazole **S2a**.

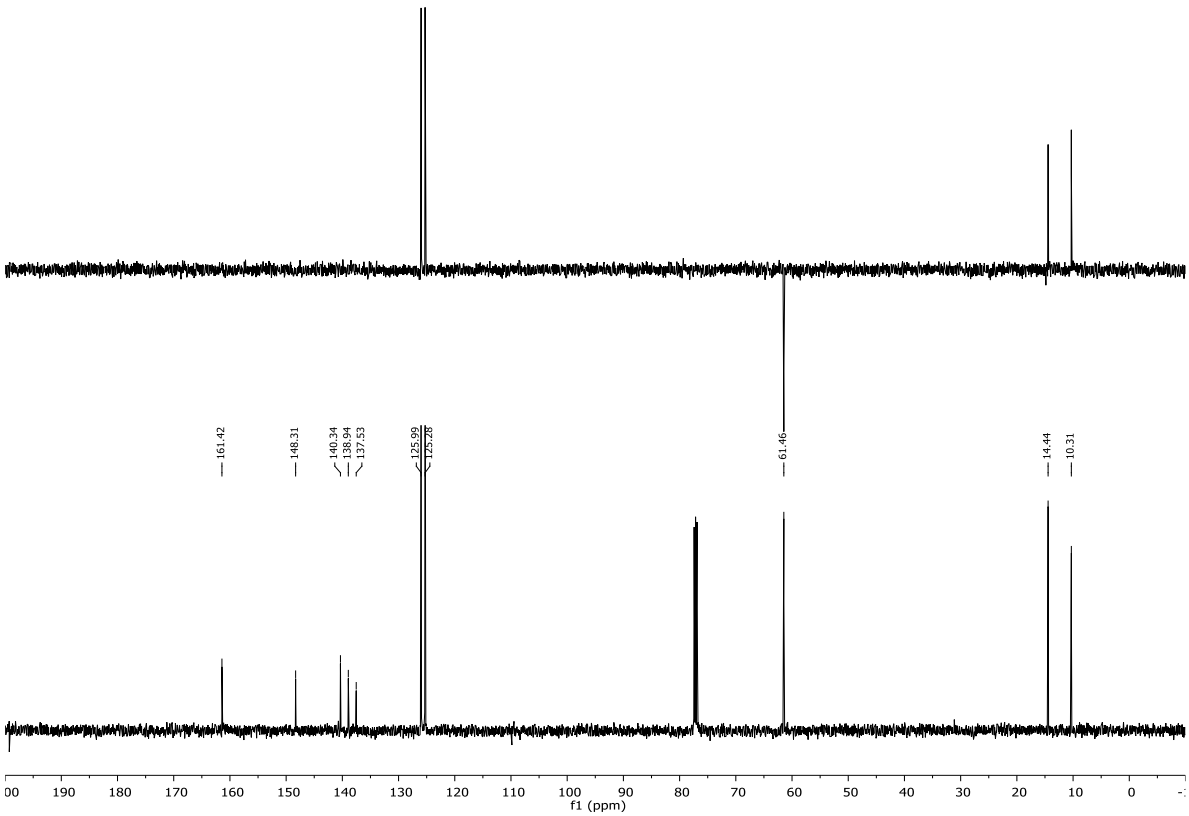


Figure S17. ^{13}C-NMR and DEPT-135 of triazole **S2a**.

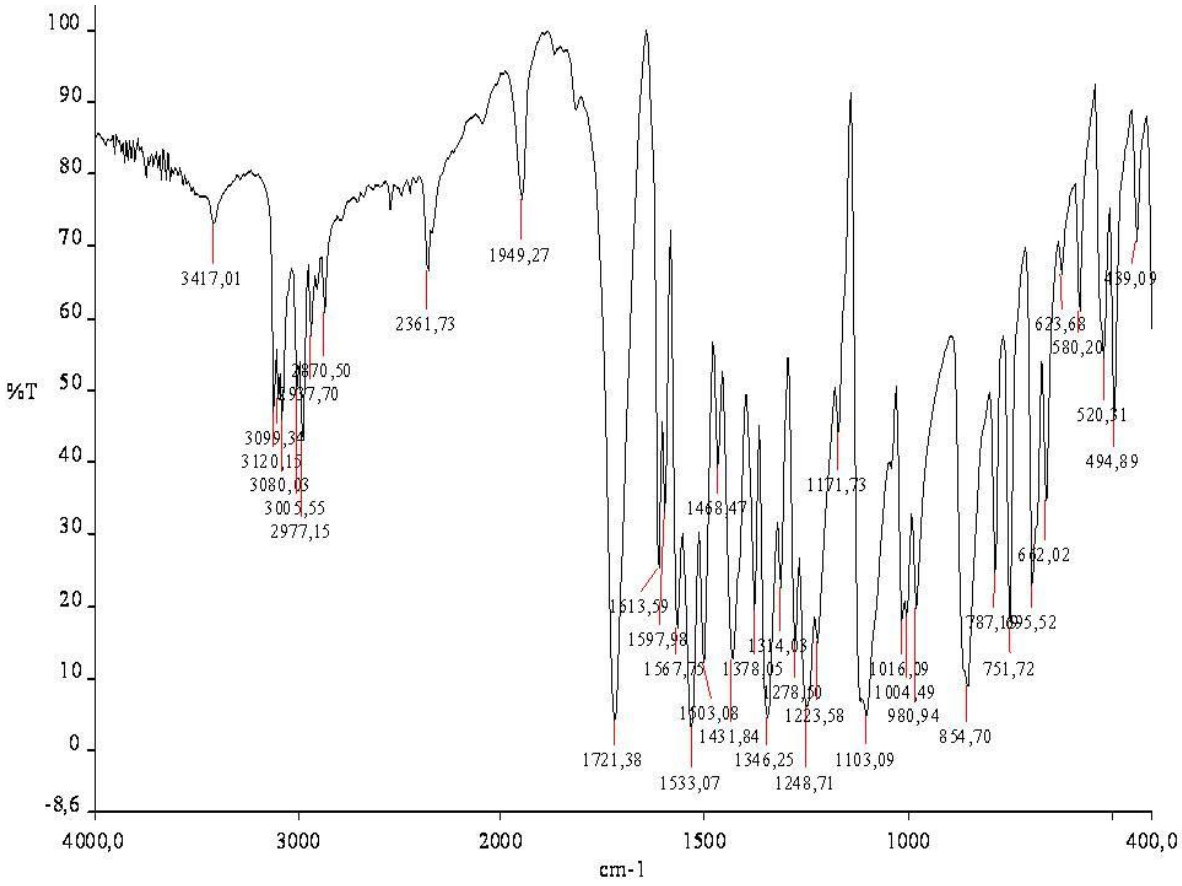


Figure S18. FT-IR of triazole **S2a**.

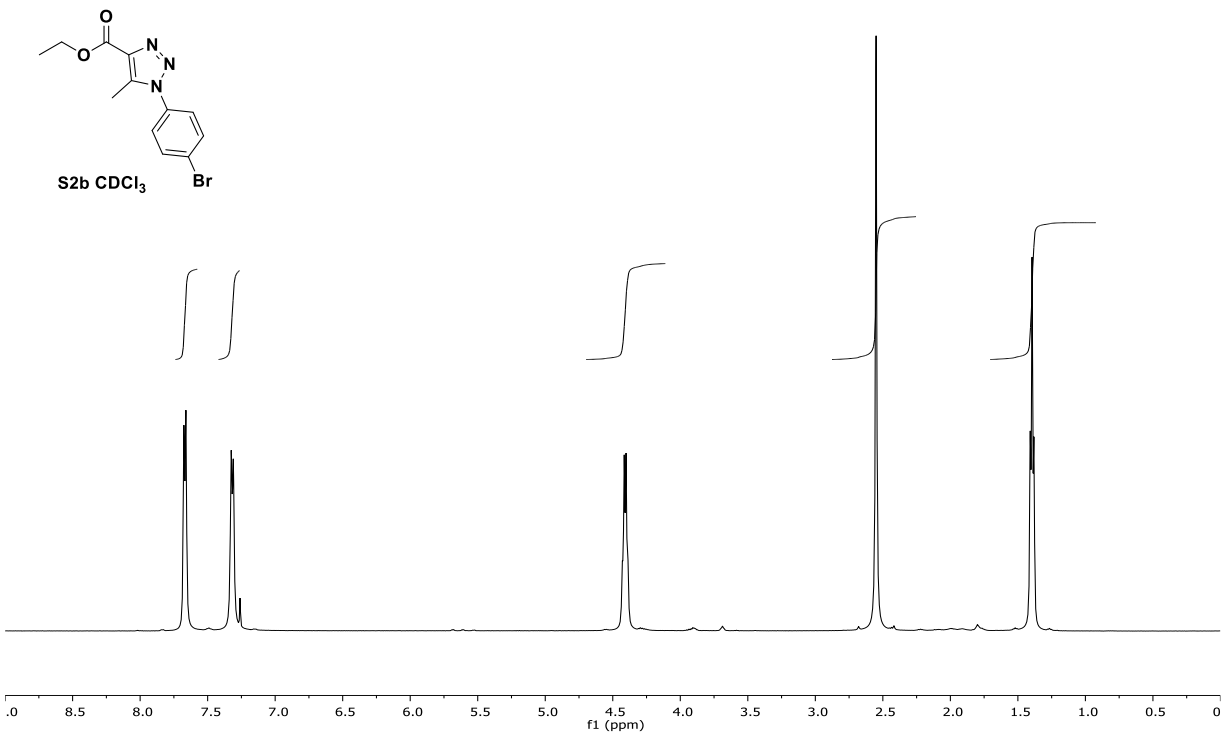


Figure S19. ^{1}H-NMR of triazole **S2b**.

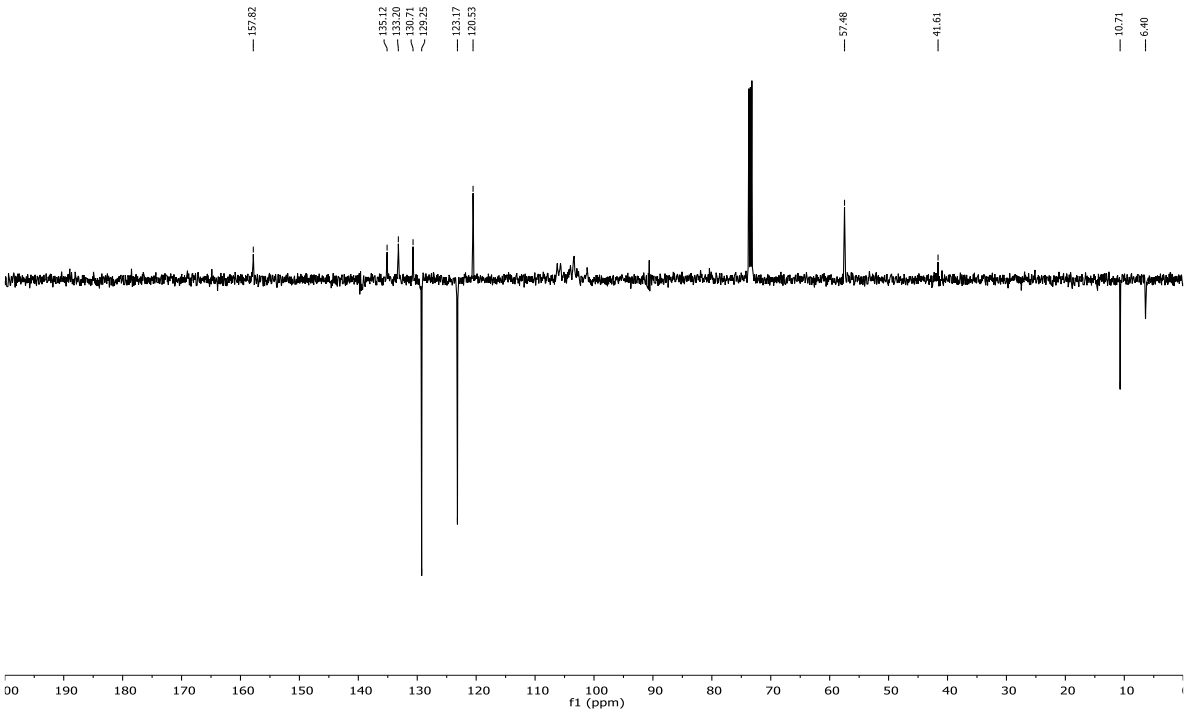


Figure S20. ^{13}C-NMR-APT of triazole **S2b**.

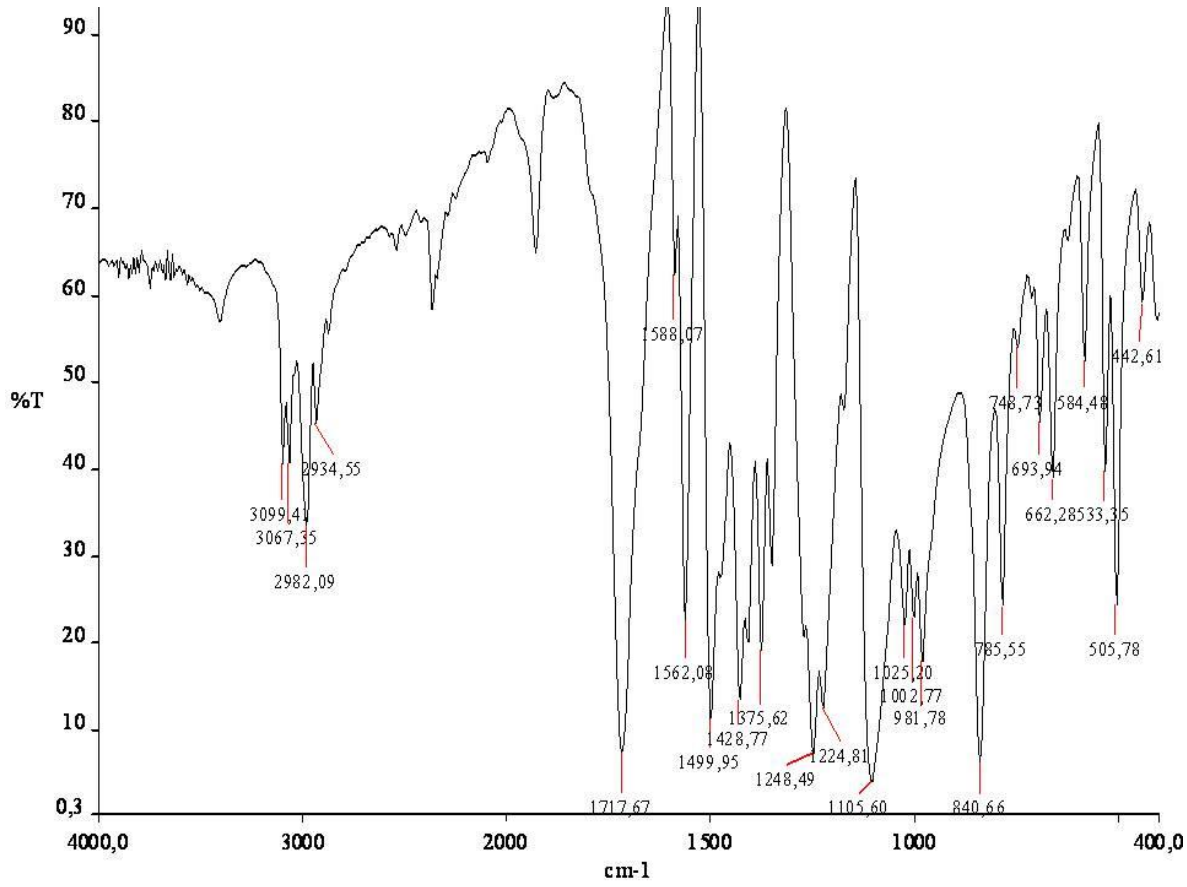


Figure S21. FT-IR of triazole **S2b**.

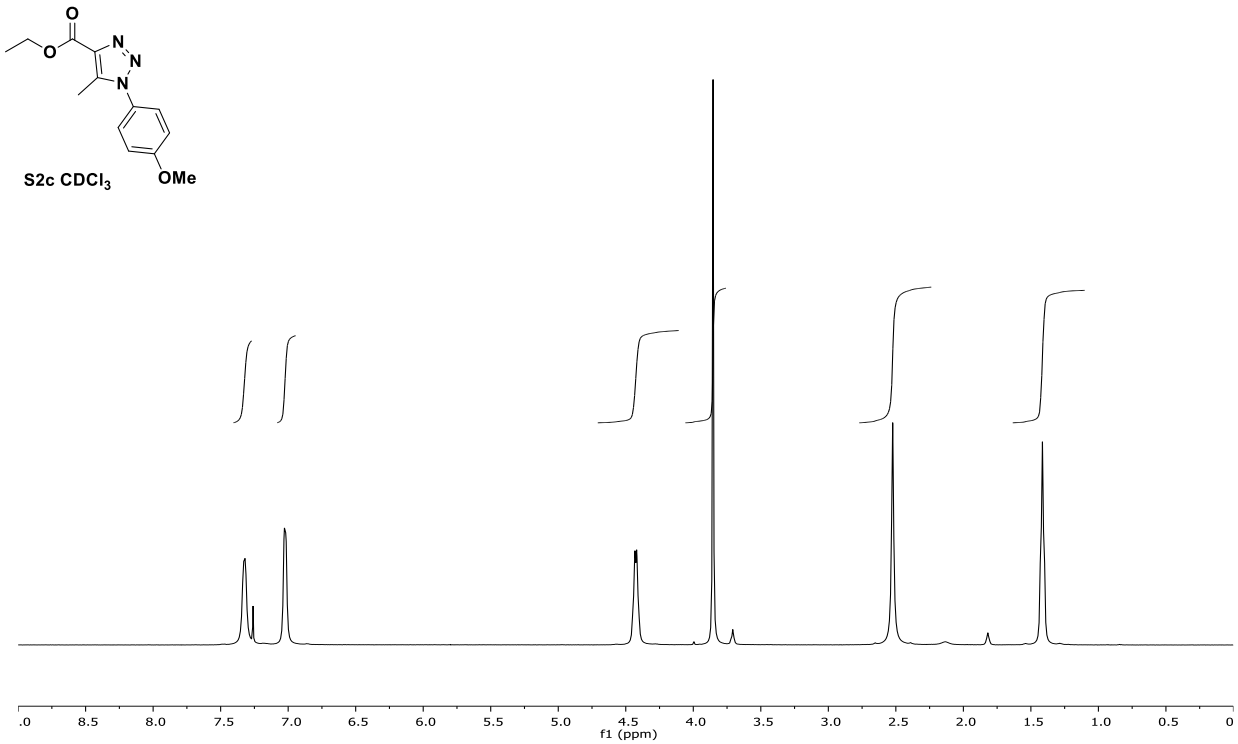


Figure S22. ^{1}H-NMR of triazole **S2c**.

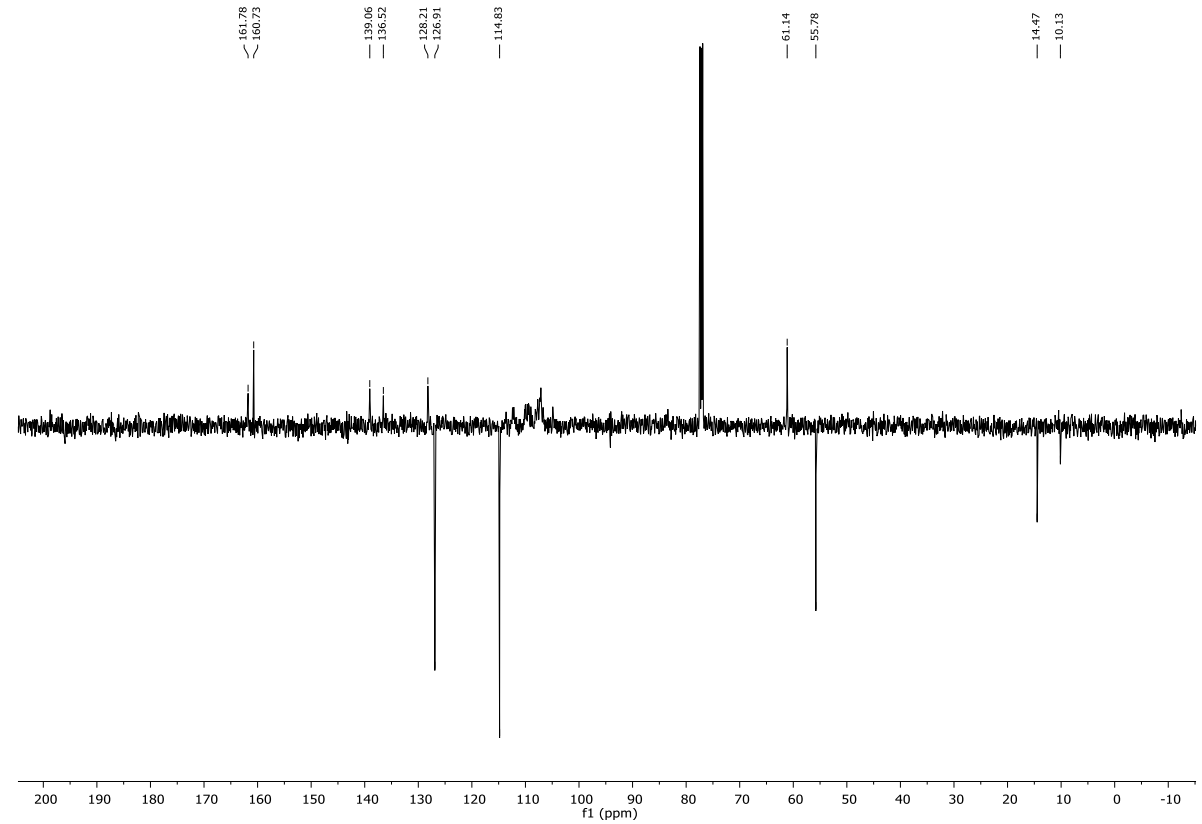


Figure S23. ^{13}C-NMR-APT of triazole **S2c**.

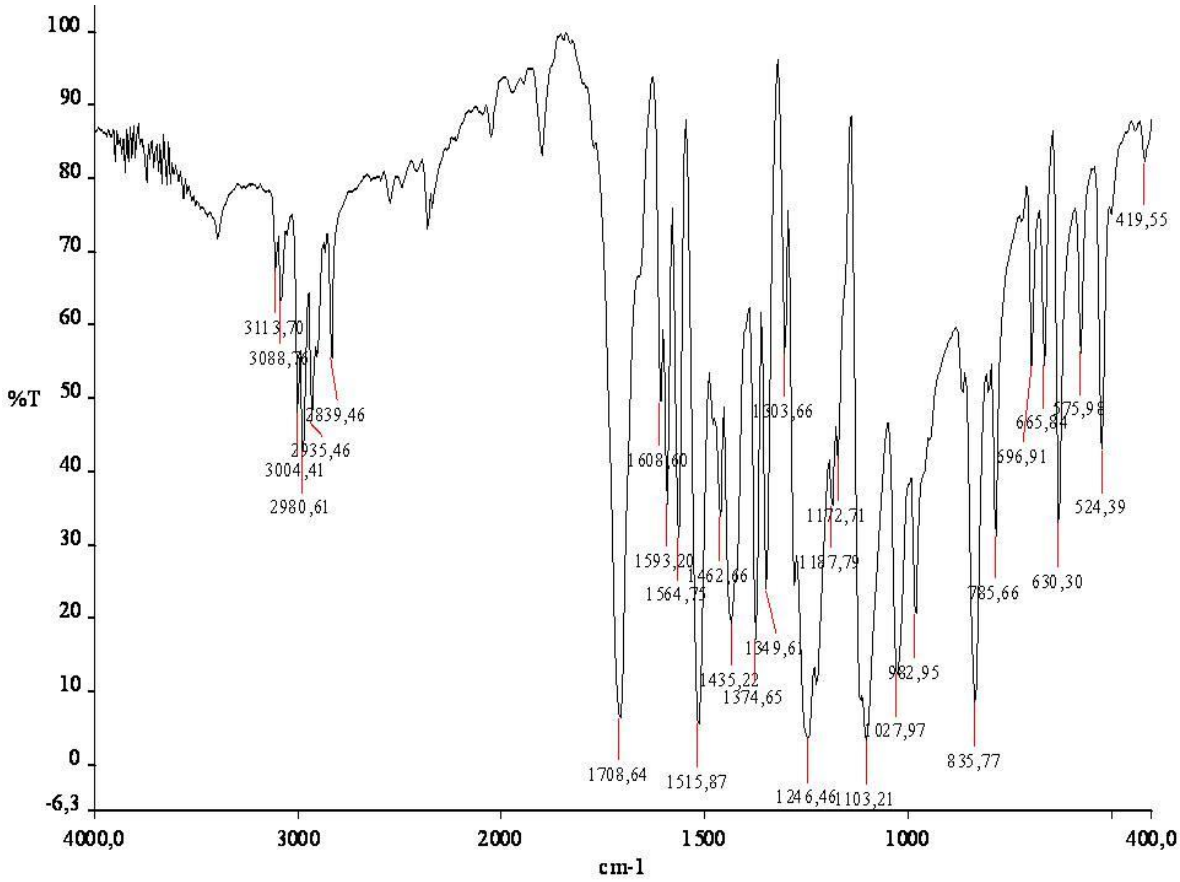


Figure S24. FT-IR of triazole **S2c**.

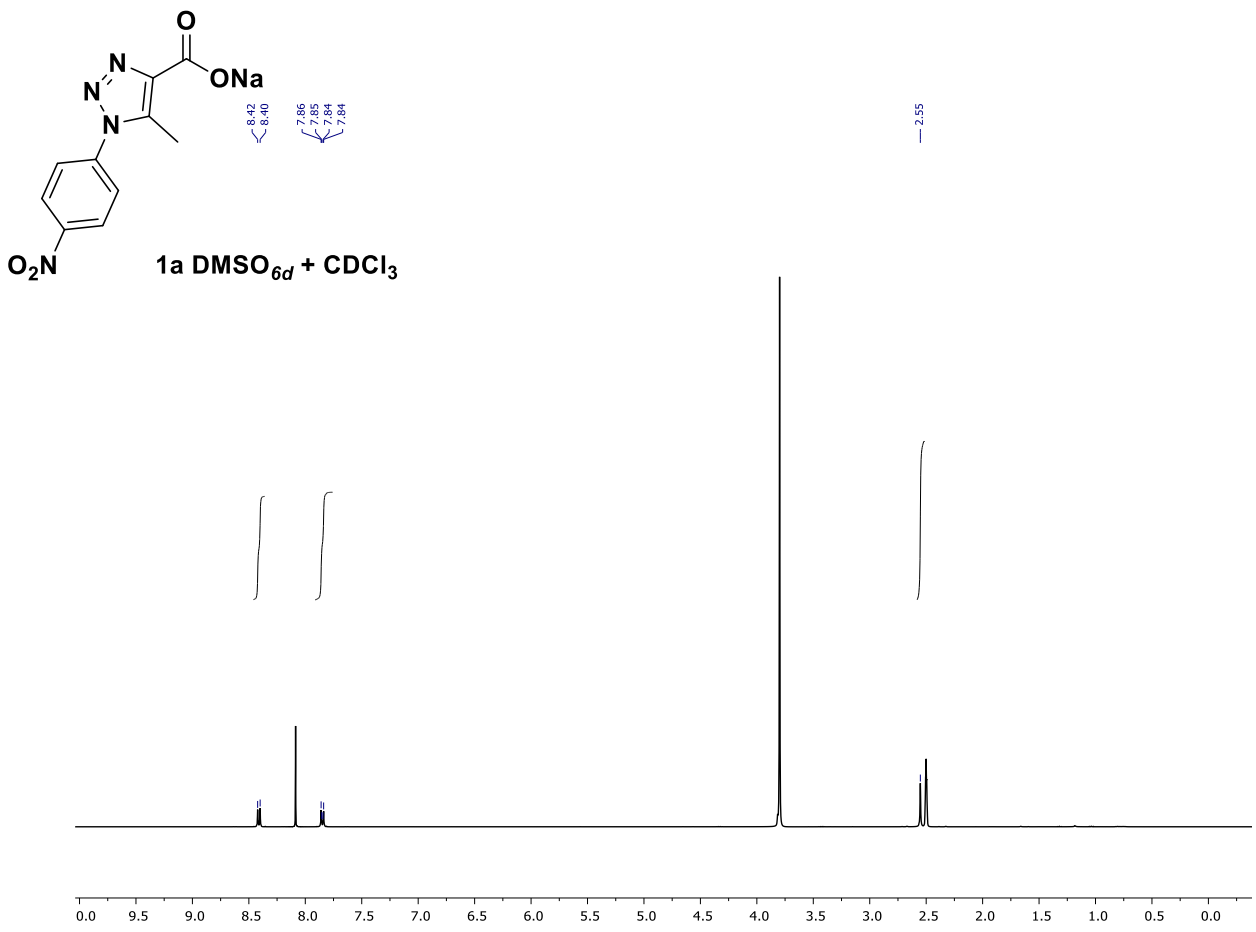


Figure S25. ^{1}H-NMR of triazole **1a**.

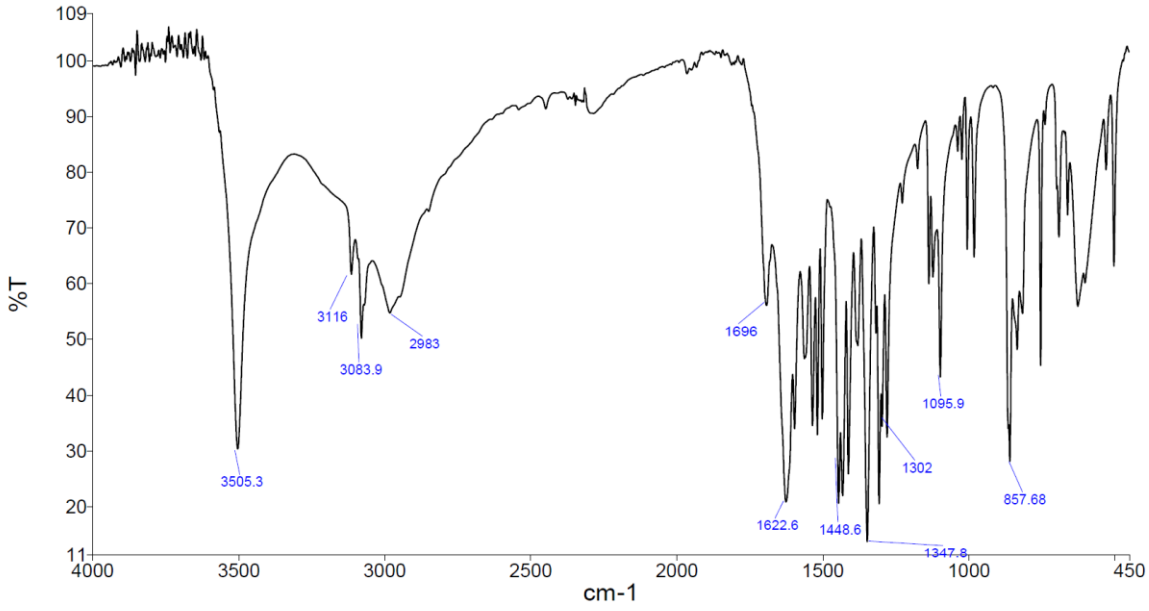


Figure S26. FT-IR of triazole **1a**.

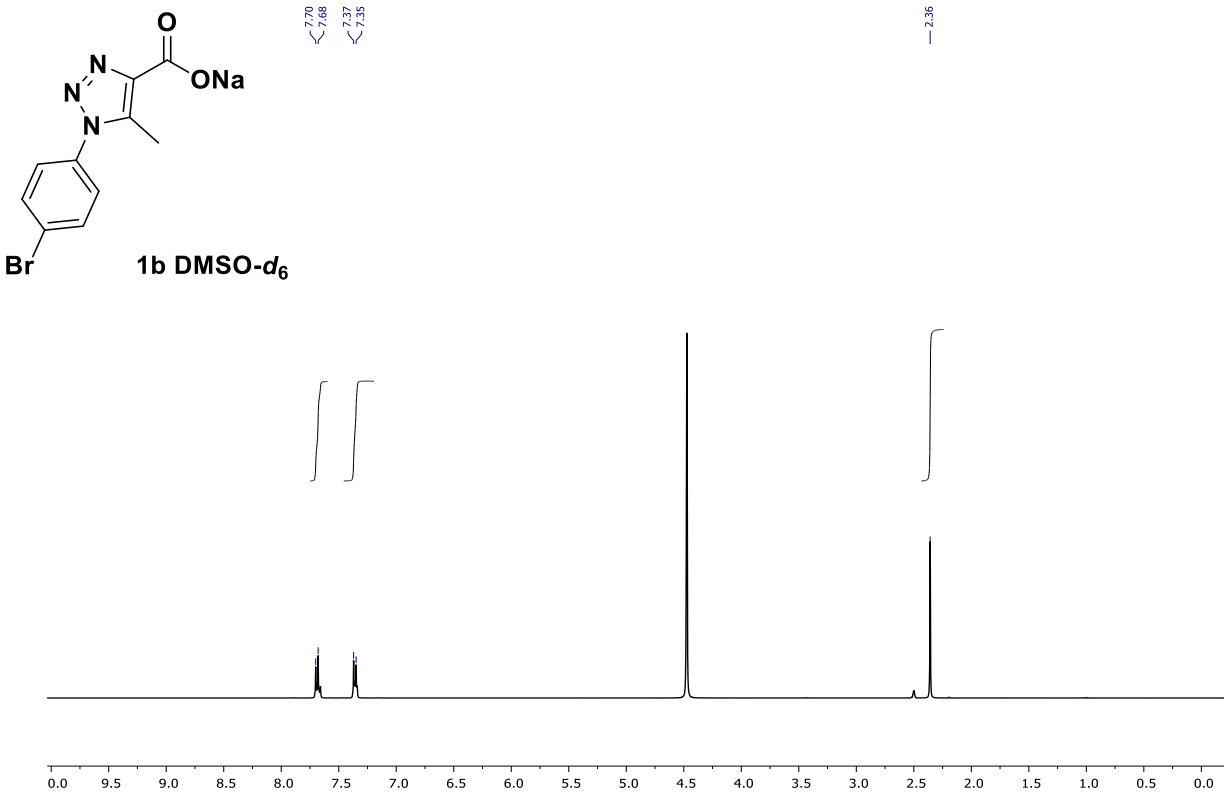


Figure S27. ^{1}H-NMR of triazole **1b**.

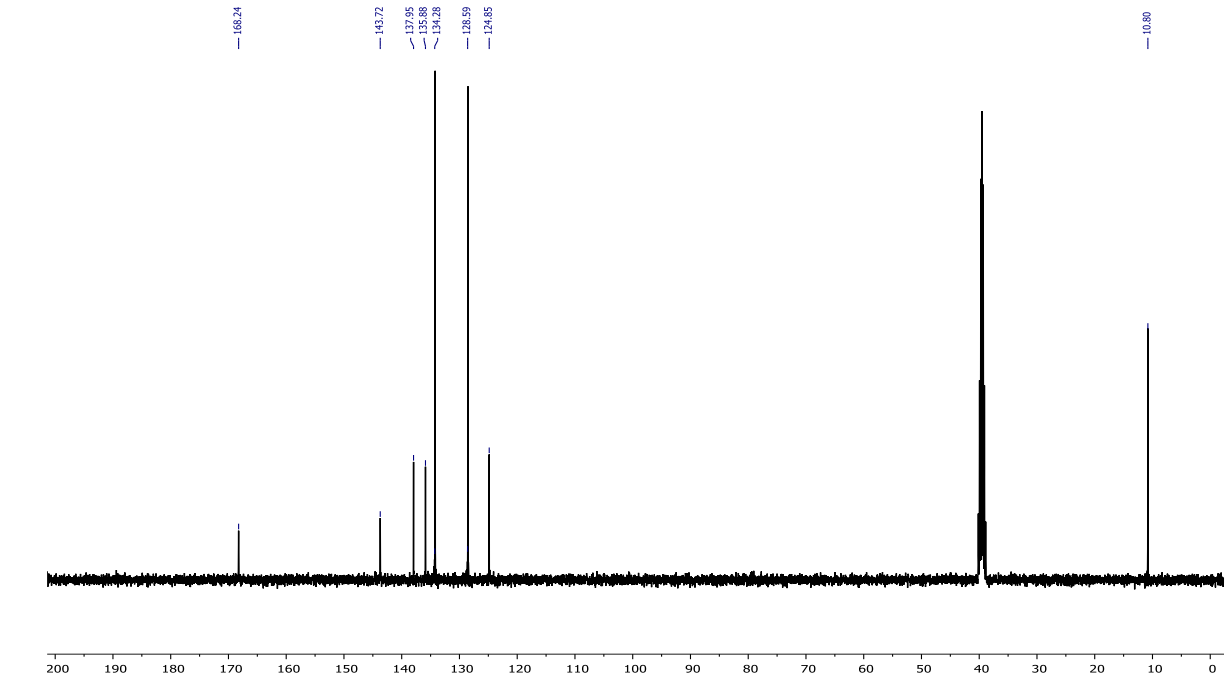


Figure S28. ^{13}C-NMR of triazole **1b**.

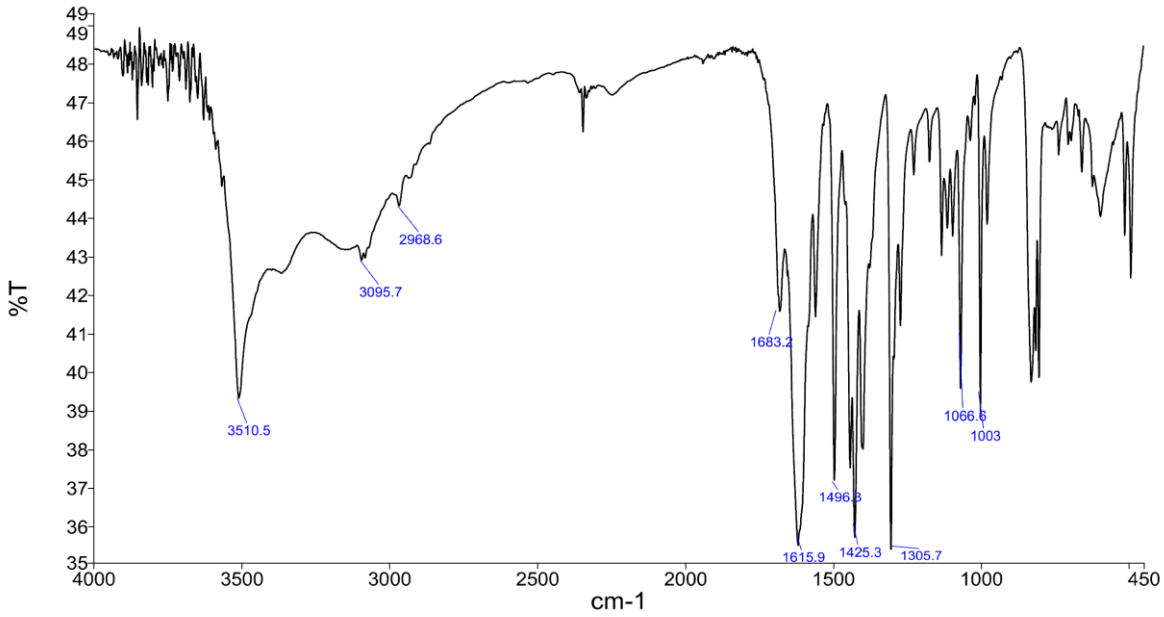


Figure S29. FT-IR of triazole **1b**.

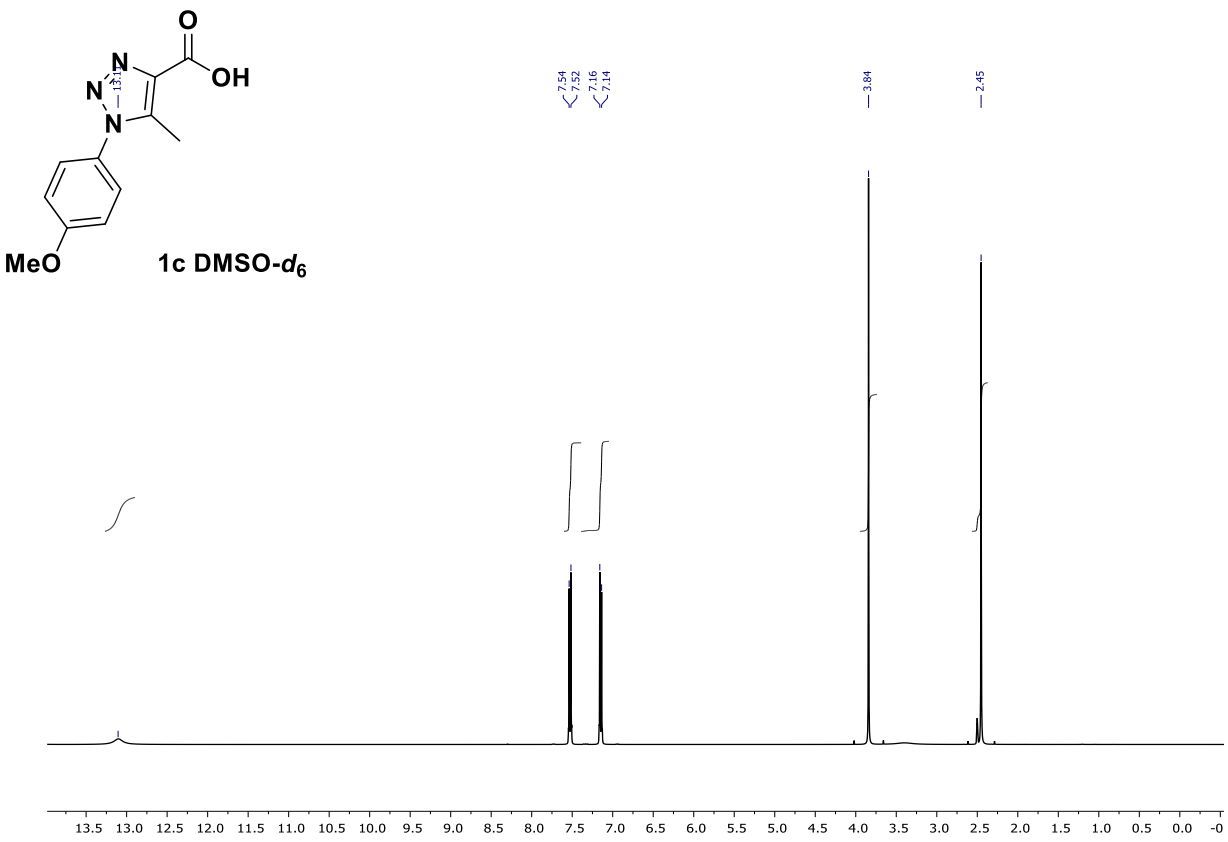


Figure S30. ^{1}H-NMR of triazole **1c**.

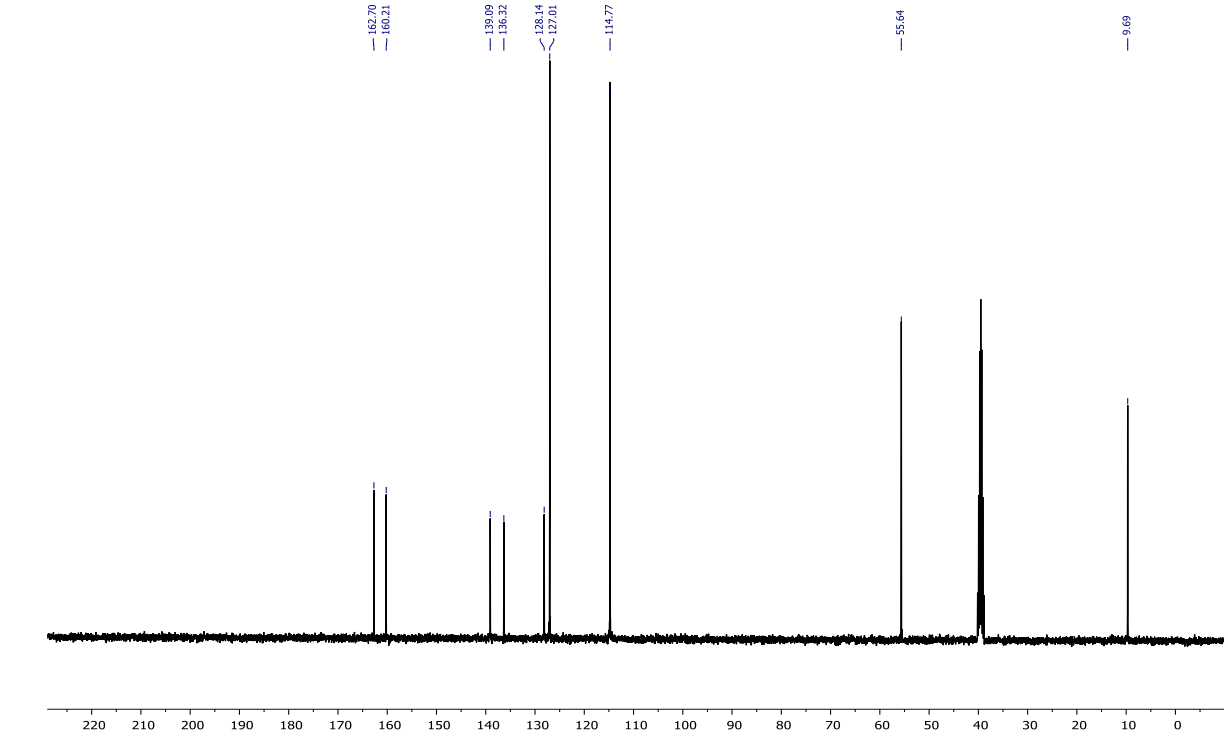


Figure S31. ^{13}C-NMR of triazole **1c**.

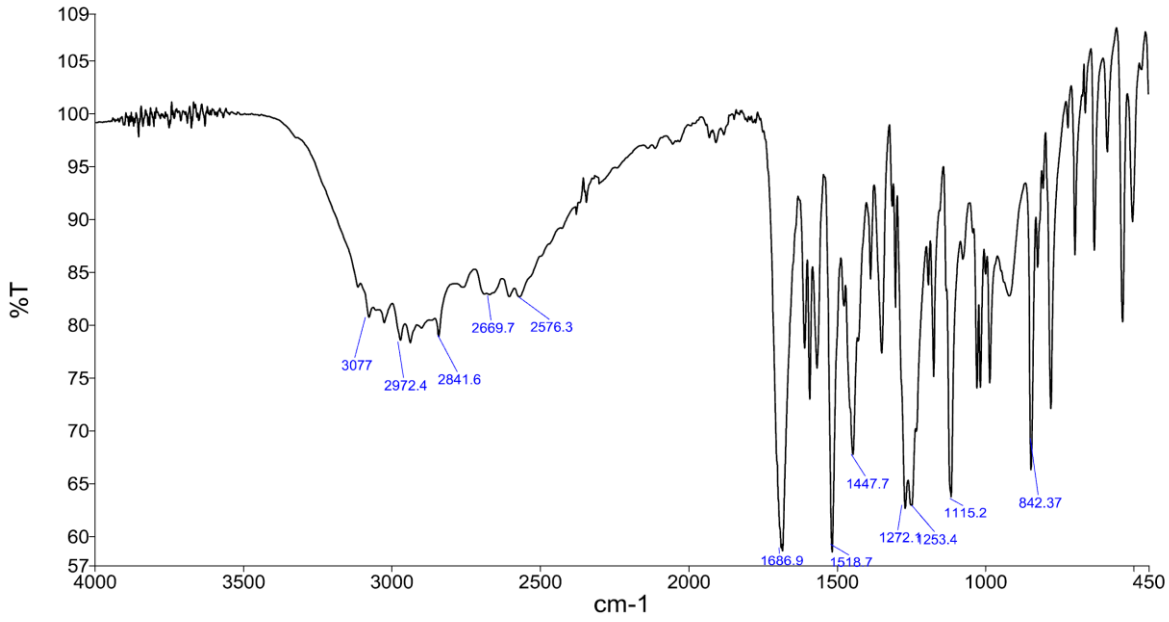


Figure S32. FT-IR of triazole **1c**.

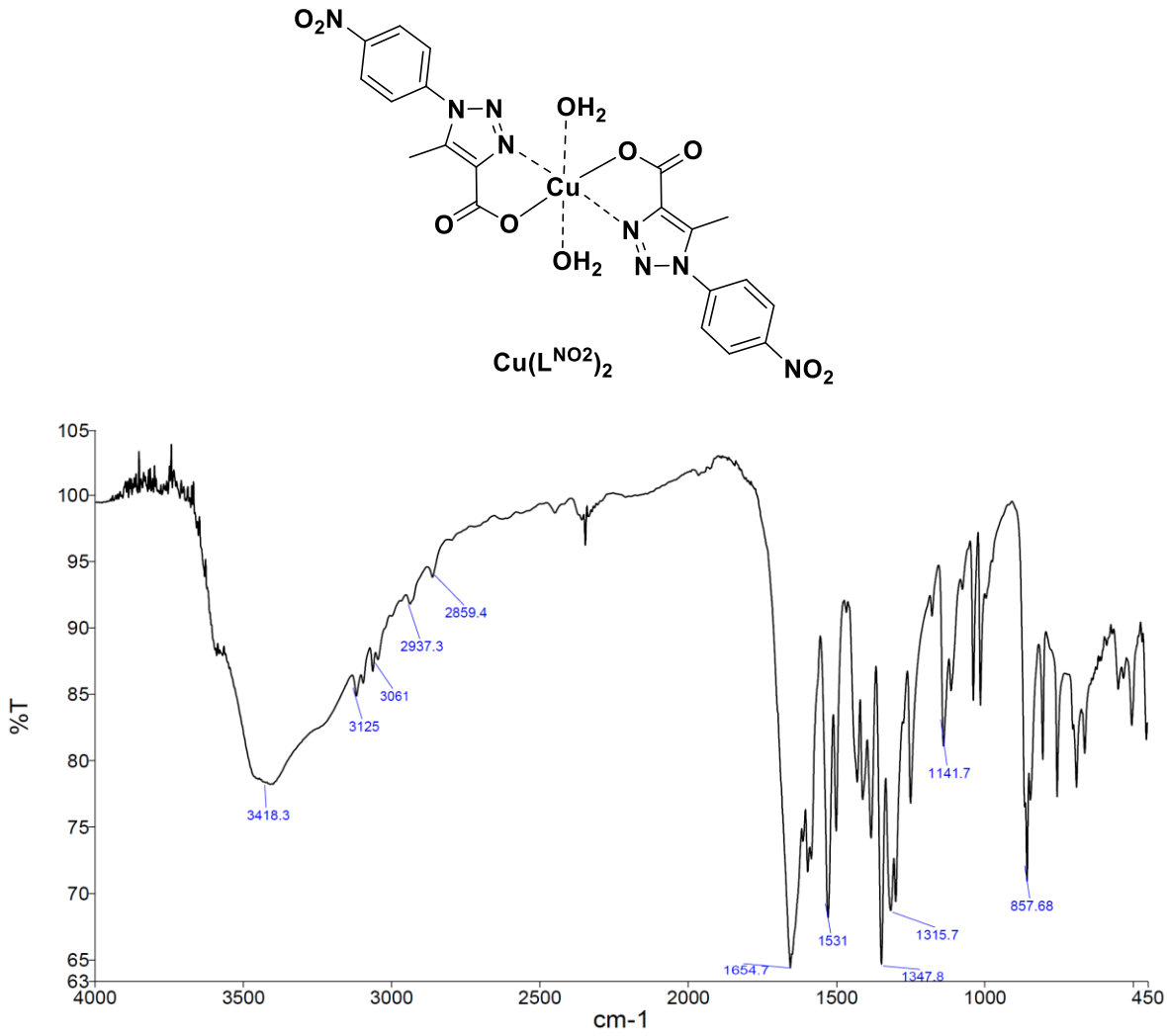


Figure S33. FT-IR of triazole **Cu(L^{NO2})$_2$**

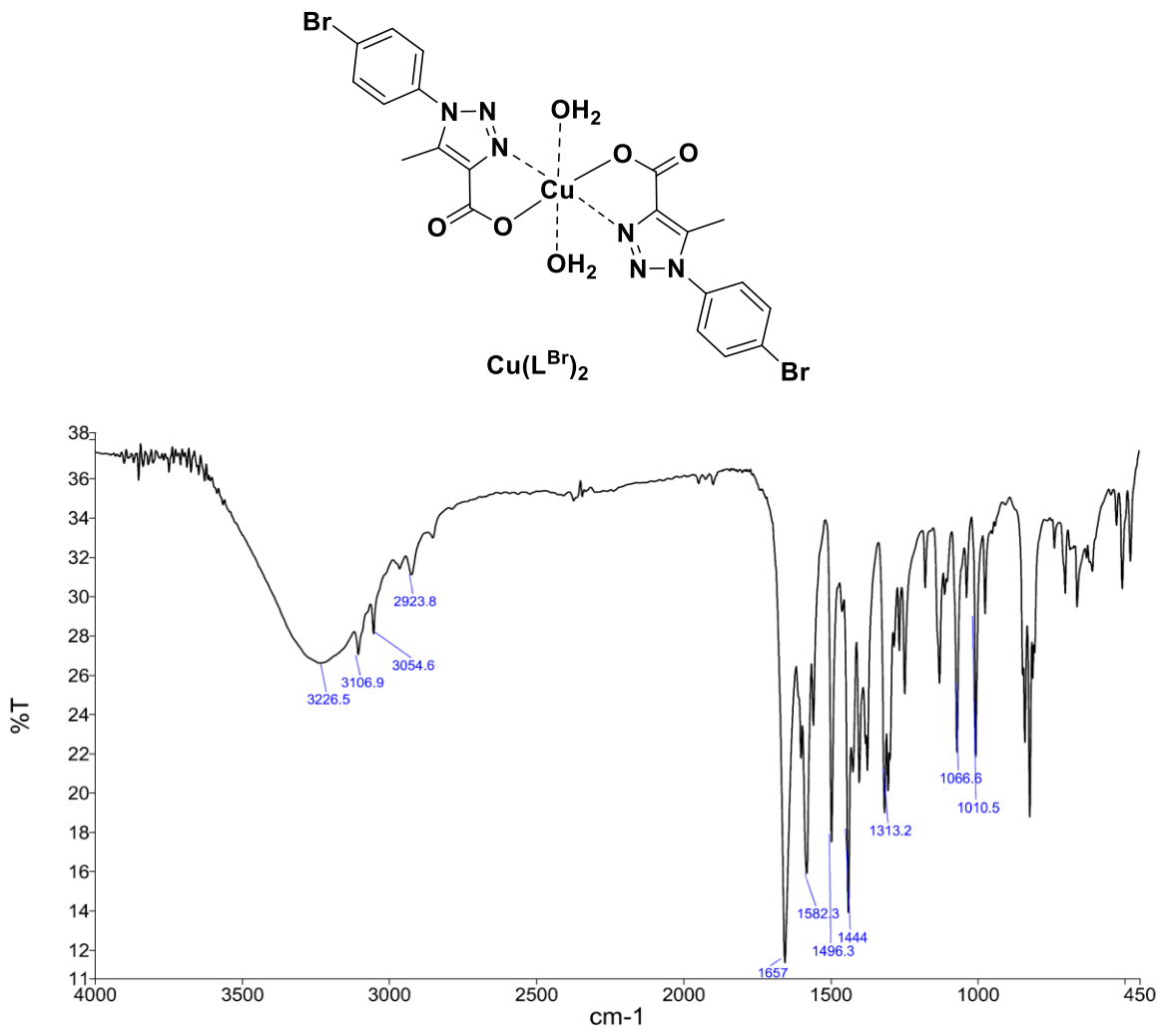


Figure S34. FT-IR of triazole **Cu(L^{Br})$_2$**

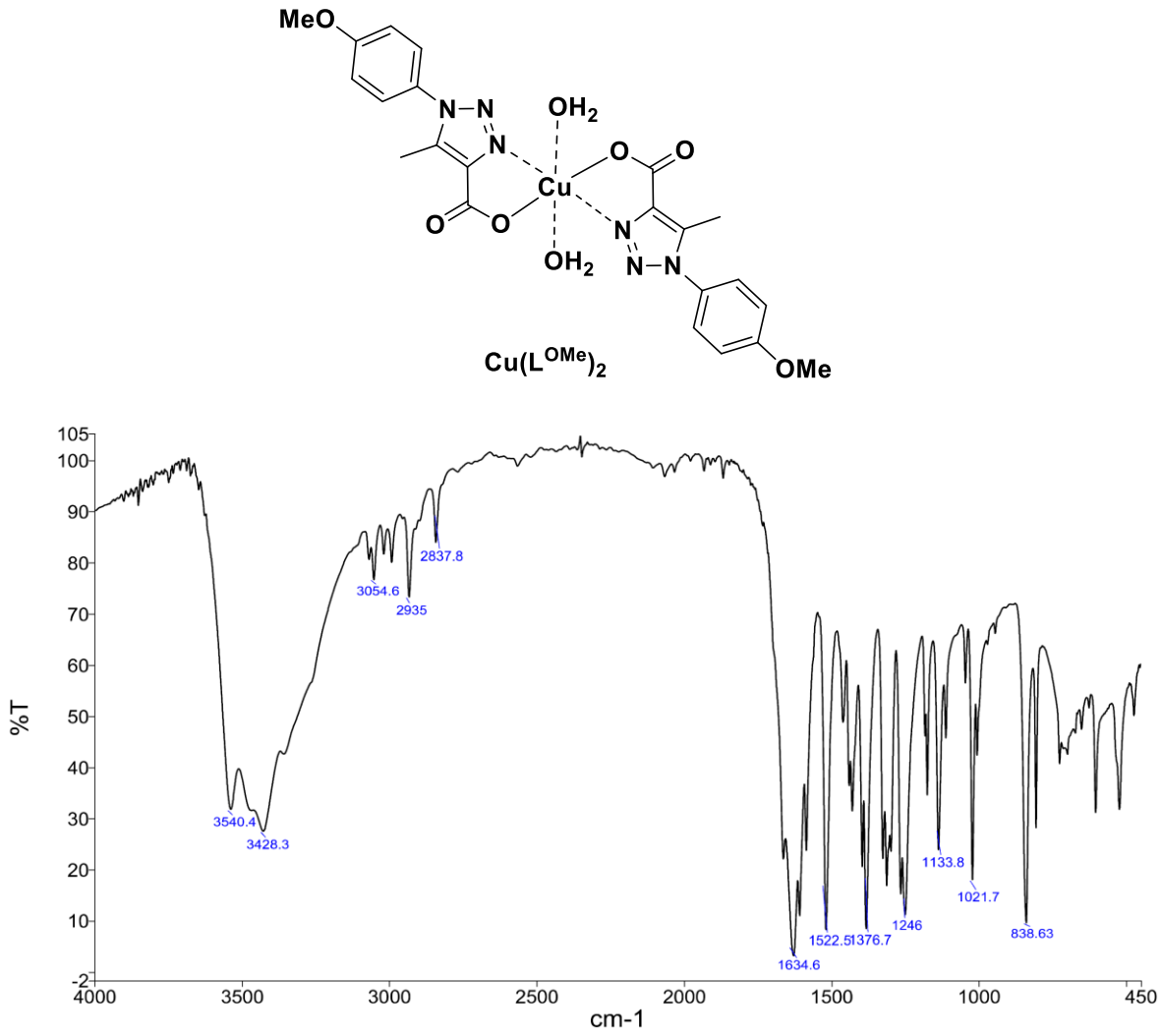


Figure S35. FT-IR of triazole **Cu(L^{OMe})$_2$**