# Synthesis, characterization and utility of a series of novel copper(II) complexes as an excellent surface disinfectant against nosocomial infections

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Supplementary Material

**Table S1.** Crystallographic data and refinement parameters for complexes **5a-5f**.

| **Complex** | **5a** | **5b** | **5c** | **5d** | **5e** | **5f** |
|---|---|---|---|---|---|---|
| **CCDC** | 2052523 | 2052524 | 2052525 | 2052526 | 2052527 | 2052528 |
| **Empirical formula** | $C_{21}H_{18}CuFN_3O_4$ | $C_{21}H_{18}CuClN_3O_4$ | $C_{21}H_{18}CuBrN_3O_4$ | $C_{23}H_{21}CuIN_4O_4$ | $C_{21}H_{19}CuN_3O_4$ | $C_{28}H_{25}CuN_3O_4$ |
| **$M_r$ [g mol$^{-1}$]** | 458.92 | 475.37 | 519.83 | 607.88 | 440.93 | 531.05 |
| **crystal system** | triclinic | triclinic | triclinic | triclinic | triclinic | monoclinic |
| **space group** | *P*-1 | *P*-1 | *P*-1 | *P*-1 | *P*-1 | $P2_1/n$ |
| ***a* [Å]** | 9.0860(2) | 9.1761(3) | 9.0332(3) | 8.9881(3) | 9.1448(7) | 8.5888(3) |
| **b [Å]** | 9.1382(2) | 9.2338(3) | 9.2739(3) | 9.2451(4) | 9.1465(7) | 10.4392(4) |
| ***c* [Å]** | 13.8154(3) | 14.1378(4) | 14.3155(4) | 16.5516(7) | 13.5672(11) | 27.4486(8) |
| ***α* [deg]** | 100.565(2) | 99.591(2) | 98.566(2) | 74.599(4) | 100.002(7) | 90.0 |
| ***β* [deg]** | 99.858(2) | 98.741(2) | 98.464(2) | 86.394(3) | 100.450(7) | 92.294(3) |
| ***γ* [deg]** | 114.860(2) | 115.625(3) | 115.332(3) | 64.904(4) | 115.079(8) | 90.0 |
| ***V* [Å$^3$]** | 982.71(4) | 1030.62(6) | 1041.57(6) | 1198.86(9) | 969.95(15) | 2459.07(15) |
| ***Z*** | 2 | 2 | 2 | 2 | 2 | 4 |
| **$\rho_{calc}$ [g cm$^{-3}$]** | 1.551 | 1.532 | 1.658 | 1.684 | 1.510 | 1.434 |
| **$\mu$ [mm$^{-1}$]** | 1.155 | 1.222 | 3.000 | 2.235 | 1.159 | 0.928 |
| ***F*(000)** | 470.0 | 486 | 522 | 602 | 454 | 1100 |
| **crystal size [mm]$^3$** | 0.17×0.15×0.13 | 0.25×0.22×0.2 | 0.2×0.18×0.16 | 0.26×0.24×0.2 | 0.22×0.2×0.18 | 0.17×0.16×0.12 |
| **$\theta_{range}$ [deg]** | 3.36-25.87 | 3.27-25.82 | 3.19-27.40 | 3.34-27.434 | 3.18-25.26 | 3.18-27.32 |
| **reflections collected** | 8810 | 8168 | 14511 | 15511 | 6887 | 21387 |
| **Indep reflections** | 3669 | 3863 | 4391 | 5085 | 3354 | 5188 |
| **$R_{int}$** | 0.0328 | 0.0330 | 0.0393 | 0.0634 | 0.0443 | 0.1338 |
| **Parameters refined** | 273 | 273 | 273 | 301 | 264 | 327 |
| **GOF on *F*$^2$** | 1.043 | 1.034 | 1.044 | 1.069 | 1.020 | 1.053 |
| **R1, wR2 [I > 2σ(I)]** | 0.0323, 0.0787 | 0.0359, 0.0927 | 0.0330, 0.0690 | 0.0671, 0.1750 | 0.0489, 0.1361 | 0.0631, 0.1660 |
| **R1, wR2 (all data)** | 0.0399, 0.0821 | 0.0418, 0.0980 | 0.0467, 0.0726 | 0.1091, 0.1963 | 0.0646, 0.1485 | 0.0903, 0.1921 |
| **residuals [e Å$^{-3}$]** | 0.27, -0.25 | 0.315, -0.348 | 0.742, -0.657 | 0.630, -0.867 | 0.362, -0.463 | 0.388, -0.817 |

**Table S2.** Coordination bond lengths (Å) and angles (˚) for complexes **5a**, **5b**, and **5c**.

| | **5a** | **5b** | **5c** |
|---|---|---|---|
| Cu-O(1) | 1.9000(14) | 1.8994(16) | 1.9030(14) |
| Cu-O(2) | 1.8671(15) | 1.8633(17) | 1.8681(15) |
| Cu-N(2) | 1.9244(17) | 1.923(2) | 1.9217(18) |
| Cu-N(3) | 2.0233(17) | 2.0289(19) | 2.0253(17) |
| | | | |
| O(1)-Cu-N(2) | 83.34(6) | 83.31(7) | 83.38(7) |
| O(1)-Cu-N(3) | 92.10(7) | 92.20(7) | 92.24(7) |
| O(2)-Cu-O(1) | 176.86(6) | 175.59(8) | 174.61(7) |
| O(2)-Cu-N(2) | 93.59(7) | 93.50(8) | 93.43(7) |
| O(2)-Cu-N(3) | 90.92(7) | 90.79(8) | 90.90(7) |
| N(2)-Cu-N(3) | 173.99(7) | 175.29(8) | 175.57(7) |

**Table S3.** Coordination bond lengths (Å) and angles (˚) for complexes **5d**, **5e**, and **5f**.

| | **5d** | **5e** | **5f** |
|---|---|---|---|
| Cu-O(1) | 1.896(4) | 1.894(3) | 1.910(2) |
| Cu-O(2) | 1.846(4) | 1.859(3) | 1.912(2) |
| Cu-N(2) | 1.913(4) | 1.916(3) | 1.915(3) |
| Cu-N(3) | 2.022(4) | 2.021(3) | 1.991(3) |
| Cu-O(2)' | - | - | 2.711(3) |
| | | | |
| O(1)-Cu-N(2) | 83.26(16) | 83.23(11) | 82.72(11) |
| O(1)-Cu-N(3) | 91.62(16) | 91.94(12) | 98.96(11) |
| O(2)-Cu-O(1) | 176.24(17) | 177.15(9) | 165.11(11) |
| O(2)-Cu-N(2) | 93.99(16) | 93.97(11) | 91.53(10) |
| O(2)-Cu-N(3) | 91.41(16) | 90.81(11) | 89.82(10) |
| N(2)-Cu-N(3) | 171.66(19) | 173.41(12) | 166.56(11) |

O(2)' at 1-x, 1-y, 1-z.

**Table S4**. Hydrogen bond parameters (Å /°) for complexes **5a-5f**.

| **complex** | D-H | A | d(D-H) | d(H..A) | d(D..A) | <DHA | Symmetry code |
|---|---|---|---|---|---|---|---|
| **5a** | N3-H3a | O1 | 0.89 | 2.24 | 3.013(3) | 145 | 1-x,-y,1-z |
| | N3-H3b | O4 | 0.89 | 2.14 | 3.019(3) | 168 | -1+x,-1+y,z |
| **5b** | N3-H3a | O4 | 0.89 | 2.15 | 3.021(3) | 168 | -1+x,-1+y,z |
| | N3-H3b | O1 | 0.89 | 2.24 | 3.016(3) | 146 | -x,1-y,1-z |
| **5c** | N3-H3a | O1 | 0.89 | 2.20 | 2.969(3) | 145 | 2-x,1-y,1-z |
| | N3-H3b | O4 | 0.89 | 2.14 | 3.014(2) | 169 | 1+x,1+y,z |
| **5d** | N3-H3a | O1 | 0.89 | 2.21 | 2.988(6) | 147 | 2-x,1-y,1-z |
| | N3-H3b | O4 | 0.89 | 2.18 | 3.054(6) | 168 | 1+x,-1+y,z |
| **5e** | N3-H3a | O4 | 0.89 | 2.17 | 3.046(4) | 168 | -1+x,-1+y,z |
| | N3-H3b | O1 | 0.89 | 2.25 | 3.015(4) | 143 | -x,1-y,1-z |
| **5f** | N3-H3a | O4 | 0.89 | 2.20 | 3.020(4) | 153 | 2-x,1-y,1-z |

**Table S5**. Analysis of C-H...π-ring interactions for complexes **5a-5f**.

| X-H | Cg | d(X-H) | d(H..Cg) | d(X..Cg) | <XHCg | Symmetry code |
|---|---|---|---|---|---|---|
| **5a** | | | | | | |
| C15-H15a | Cg1 | 0.96 | 2.90 | 3.625(4) | 133 | 1+x, 1+y, z |
| **5b** | | | | | | |
| C15-H15c | Cg1 | 0.96 | 2.85 | 3.556(4) | 131 | 1+x, 1+y, z |
| **5c** | | | | | | |
| C15-H15a | Cg1 | 0.96 | 2.79 | 3.509(3) | 132 | -1+x, -1+y, z |
| **5d** | | | | | | |
| C15-H15a | Cg1 | 0.96 | 2.98 | 3.739(8) | 136 | -1+x, 1+y, z |
| **5e** | | | | | | |
| C15-H15c | Cg1 | 0.96 | 2.84 | 3.627(6) | 139 | 1+x, 1+y, z |
| **5f** | | | | | | |
| C6-H6 | Cg7 | 0.93 | 2.93 | 3.732(5) | 146 | x, 1+y, z |
| C14-H14b | Cg6 | 0.96 | 2.98 | 3.680(4) | 131 | 1-x, 1-y, 1-z |
| C15-H15a | Cg2 | 0.96 | 2.63 | 3.517(4) | 154 | 2-x, 1-y, 1-z |
| C26-H26 | Cg5 | 0.93 | 2.78 | 3.549(6) | 141 | 3/2-x, -1/2+y, 1/2-z |

Cg1 = aniline ring C16/C21. For **5f** Cg2 = Cu/O2/C8/C12/C13/N2; Cg5 = benzohydrazide ring C2/C7; Cg6 = benzhydrylamine phenyl ring C17/C22; Cg7 = benzhydrylamine phenyl ring C23/C28.

**Table S6**: Electrostatic properties of metal complexes **(5a-5f)** calculated using DFT methods.

| **S.No** | **Compound** | **HOMO** | **LUMO** | **Chemical potentia** | **Chemical hardnes** | **Electrophilicity index (ω)= $\mu^2/2\eta$** | **Chemical softness** |
|---|---|---|---|---|---|---|---|
| **1** | **5a** | -16.06 | -14.79 | -15.43 | 0.64 | 187.13 | 1.57 |
| **2** | **5b** | -15.85 | -14.64 | -15.24 | 0.61 | 191.83 | 1.65 |
| **3** | **5c** | -15.71 | -14.48 | -15.09 | 0.61 | 185.78 | 1.63 |
| **4** | **5d** | -15.45 | -14.28 | -14.86 | 0.585 | 188.73 | 1.70 |
| **5** | **5e** | -16.04 | -14.75 | -15.40 | 0.65 | 183.51 | 1.55 |
| **6** | **5f** | -5.59 | -1.87 | -3.73 | 1.86 | 3.74 | 0.54 |

**Table S7**: Results of cyclic voltammogram of complexes **5a-5f**.

| Sr. No. | Name of the Copper compounds | Epc1(V) | Epc2 (V) | Epa1 (V) |
|---|---|---|---|---|
| 1 | [CuL(4F-An)] (5a) | -0.51 | 0.37 | 0.45 |
| 2 | [CuL(4Cl-An)] (5b) | -0.53 | 0.35 | 0.46 |
| 3 | [CuL(4Br-An)] (5c) | -0.56 | 0.34 | 0.46 |
| 4 | [CuL(4I-An)] (5d) | -0.60 | 0.32 | 0.43 |
| 5 | [CuL(An)] (5e) | -0.51 | 0.36 | 0.46 |
| 6 | [CuL(Benzhydrylamine)] (5f) | -0.53 | 0.34 | 0.44 |

**Table S8.** Details of the HRMS study of copper complexes **5a-5f**.

| Complex | Formula | Ion Peak m/z $[M+H]^+$ | |
|---|---|---|---|
| | | Calculated | Found |
| **5a** | C21H18O4N3CuF | 459.0656 | 459.0438 |
| **5b** | C21H18O4N3CuCl | 475.0360 | 475.0761 |
| **5c** | C21H18O4N3CuBr | 518.9855 | 519.1699 |
| **5d** | C21H18O4N3CuI | 566.9716 | 567.0185 |
| **5e** | C21H19O4N3Cu | 441.0750 | 441.4246 |
| **5f** | C28H25O4N3Cu | 531.1219 | 531.0933 |

**Table S9**: Antimicrobial efficacy of individual ligands and the Minimum Inhibitory Concentration (MIC) of the compounds (µg/mL). No killing indicates that no significant difference in bacterial survival till 512 µg/mL.

| | | S. *aureus* | *K. pneumoniae* | *E. coli* |
|---|---|---|---|---|
| 1. | Copper acetate | No Killing | No Killing | No Killing |
| | Complex 4 | No Killing | No Killing | No Killing |
| | 4-Chloroaniline | No Killing | No Killing | No Killing |
| | **5b** [CuL(4Cl-An)] | 20.62 µg/mL | >64 µg/mL | 44.45 µg/mL |
| 2. | Copper acetate | No Killing | No Killing | No Killing |
| | Complex 4 | No Killing | No Killing | No Killing |
| | Aniline | 10% | No Killing | No Killing |
| | **5e** [CuL(An)] | 11.89 µg/mL | No Killing | >64 µg/mL |
| 3. | Copper acetate | No Killing | No Killing | No Killing |
| | Complex 4 | No Killing | No Killing | No Killing |
| | Benzhydrylamine | 20% | No Killing | No Killing |
| | **5f** [CuL(Benzhydrylamine)] | 2.435 µg/mL | >64 µg/mL | 25.29 µg/mL |

**Table S10: Summary of TGA results**.

| Code | Compound | Temperature Range(°C) | Weight Loss Found/(Calcd.) | Assignment |
|---|---|---|---|---|
| 5a | CuL(4F-An) | 25-240<br><br>240-350 | 30.05(29.09)<br><br>23.77(24.25) | Loss of 4-flouroaniline and CO molecule<br>Loss of NO and $NO_2$ |
| 5b | CuL(4Cl-An) | 25-230<br><br>230-360 | 36.09(36.54)<br><br>25.02(26.75) | Loss of 4-chloroaniline and $CO_2$ molecule<br>Loss of NO and $NO_2$ |
| 5c | CuL(4Br-An) | 25-270<br><br>270-360 | 33.09(33.83)<br><br>25.31(24.62) | Loss of 4-bromoaniline<br>Loss of $CO_2$ and $N_2O$ molecule |
| 5d | CuL(4I-An) | 25-240<br><br>240-390 | 45.57(45.87)<br><br>30.41(29.29) | Loss of 4-iodoaniline, CO and NO<br>Loss of CO, $CO_2$ and $NO_2$ |
| 5e | CuL(An) | 25-240<br><br>240-370 | 24.52(24.00)<br><br>31.26(32.85) | Loss of aniline and one $CH_3$ molecule<br>Loss of CO, NO and $NO_2$ |
| 5f | CuL(Benzhydrylamine) | 25-160<br><br>160-330 | 12.06(11.73)<br><br>52.09(52.12) | Loss of two $CH_3OH$ molecule<br>Loss of benzhydrylamine, and two NO molecule |

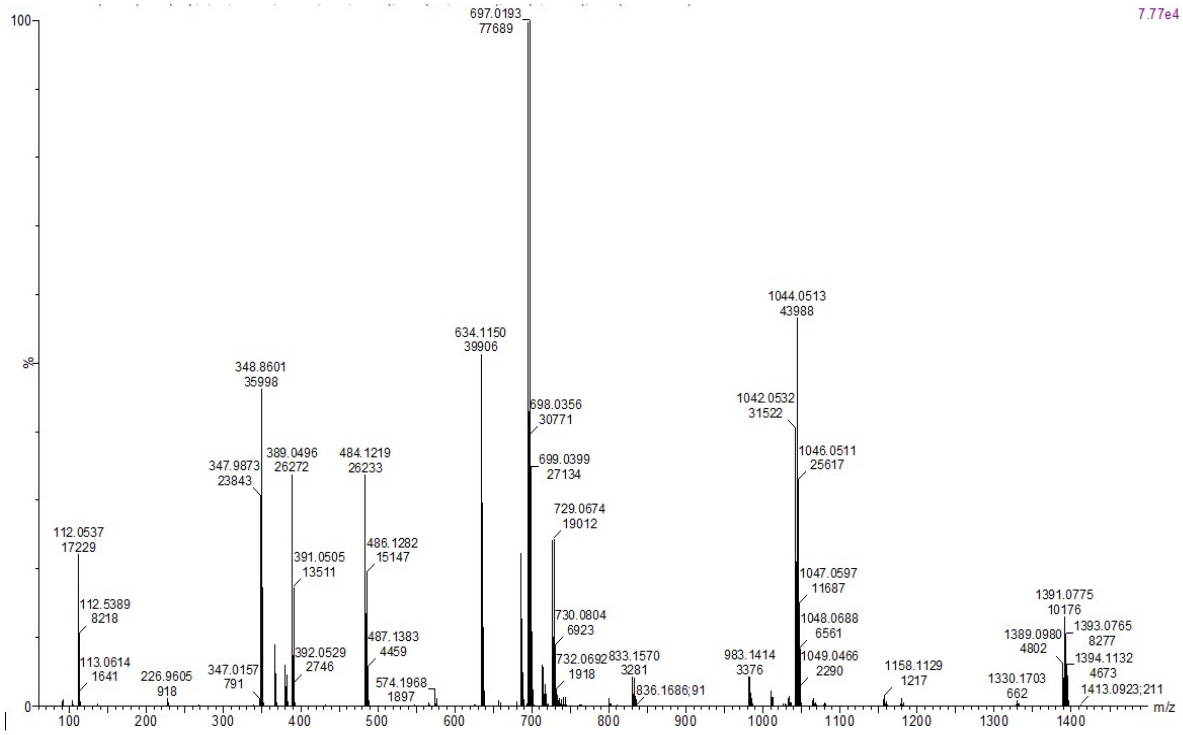



**Figure S1(a):** Whole HRMS spectrum of copper complex **5a**.

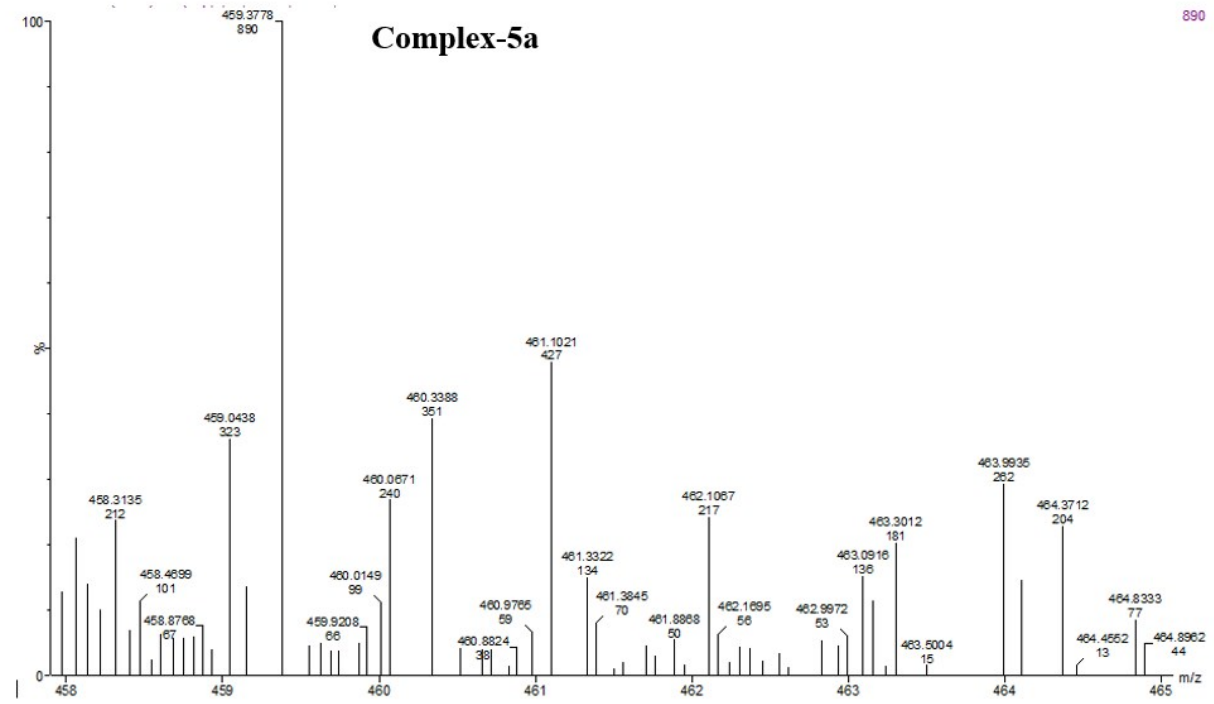



**Figure S1(b):** Partial HRMS spectrum of copper complex **5a**.

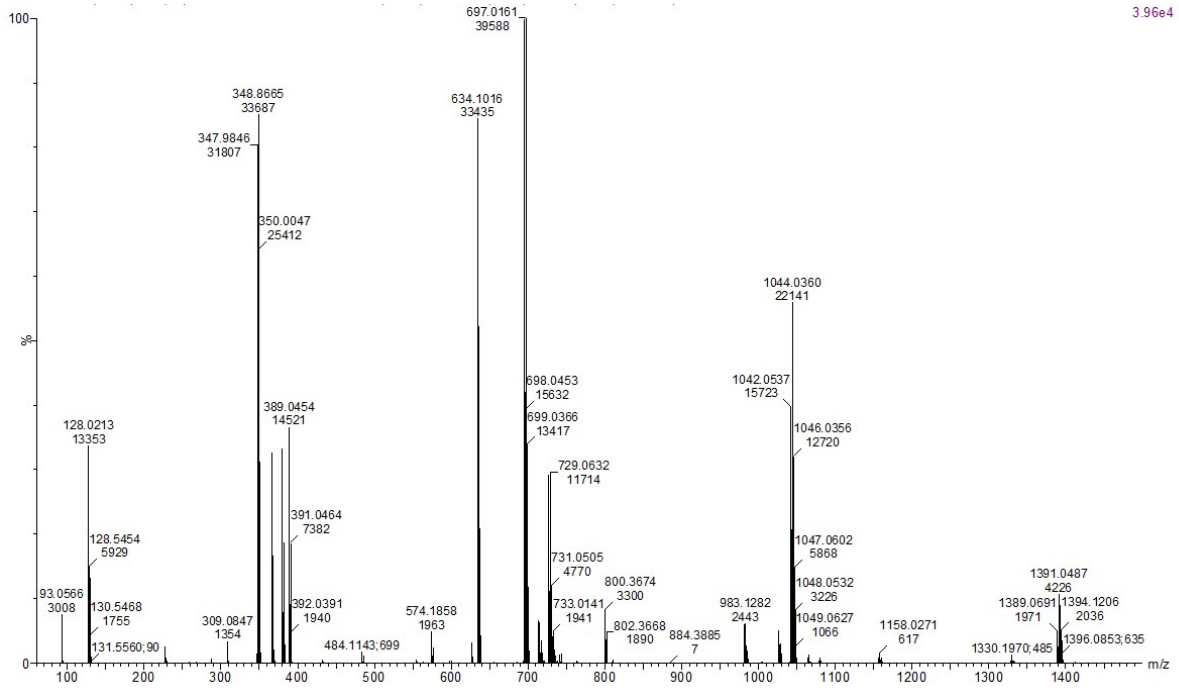



**Figure S2(a):** Whole HRMS spectrum of copper complex **5b**.

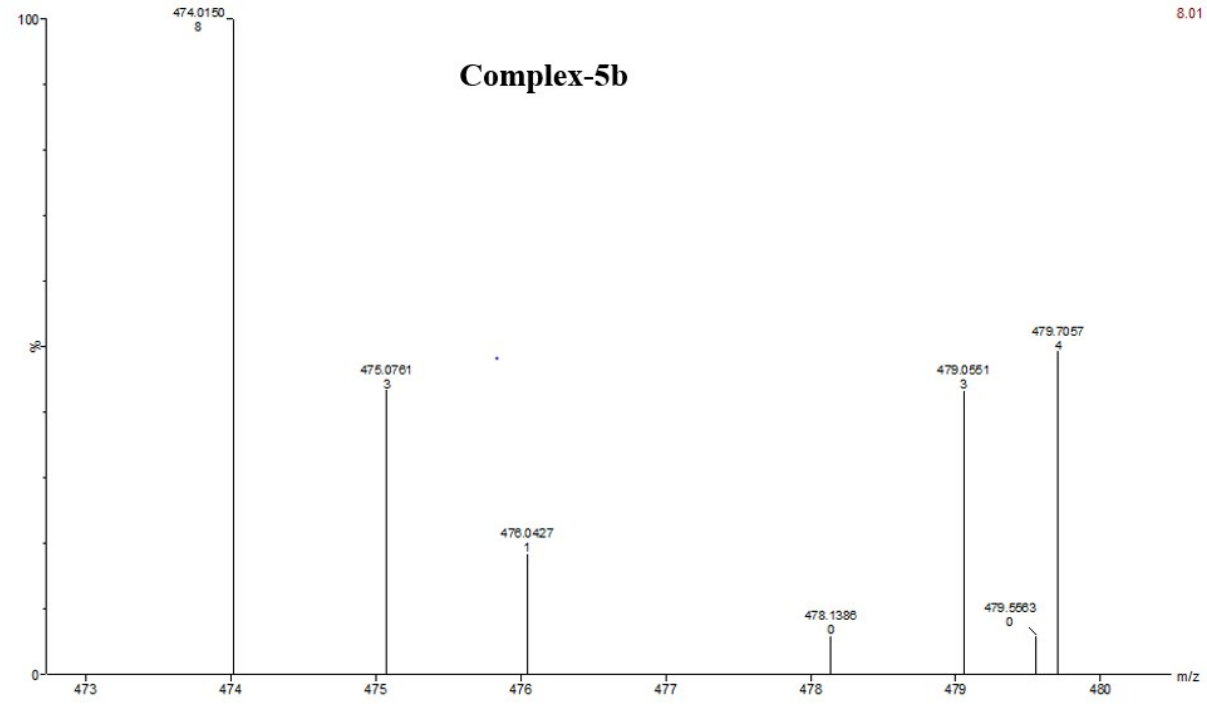



**Figure S2(b):** Partial HRMS spectrum of copper complex **5b**.

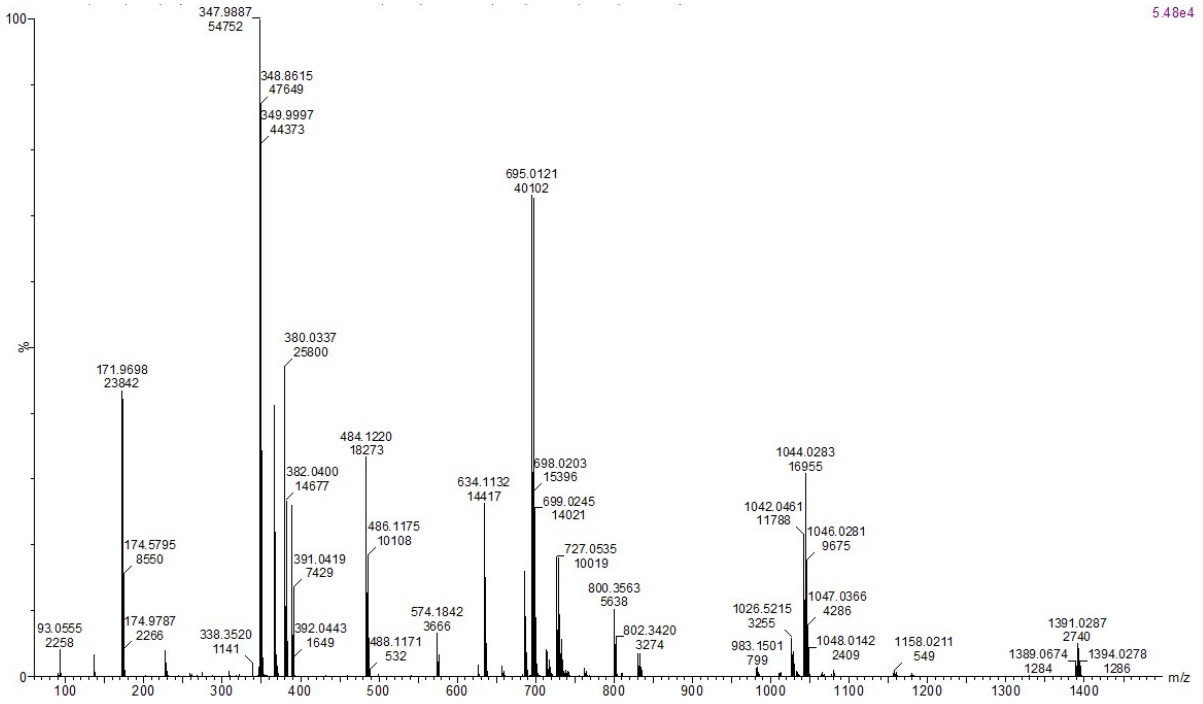



**Figure S3(a):** Whole HRMS spectrum of copper complex **5c**.

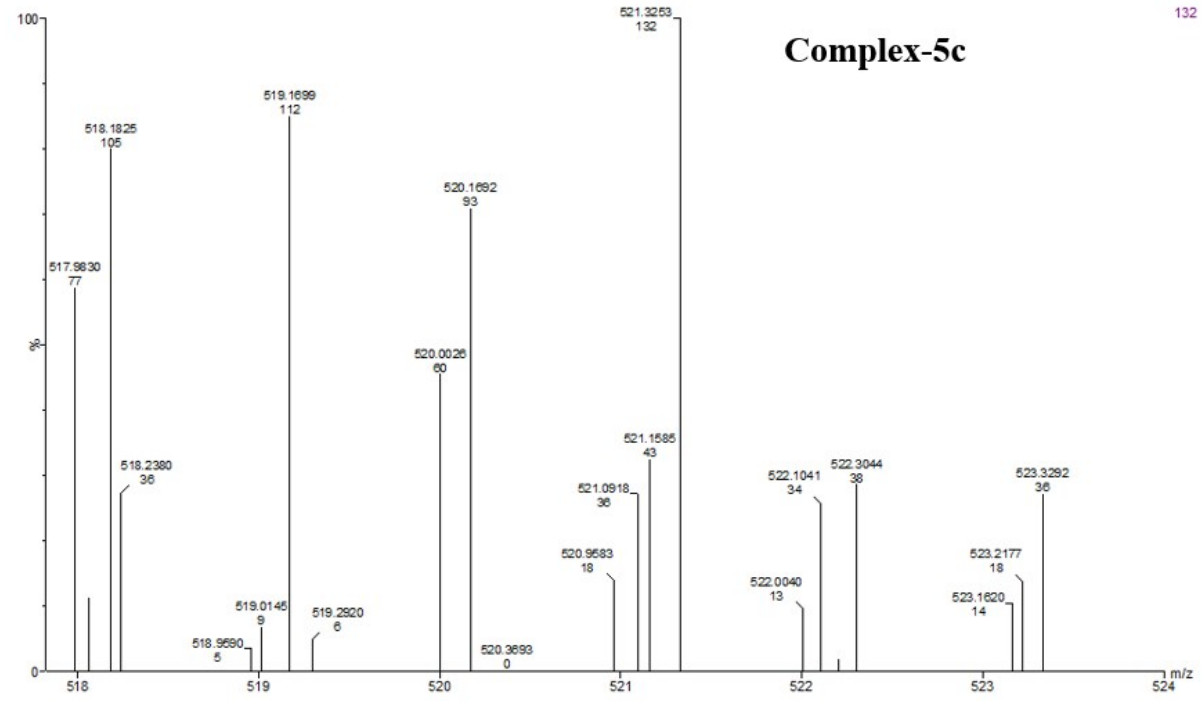



**Figure S3(b):** Partial HRMS spectrum of copper complex **5c**.

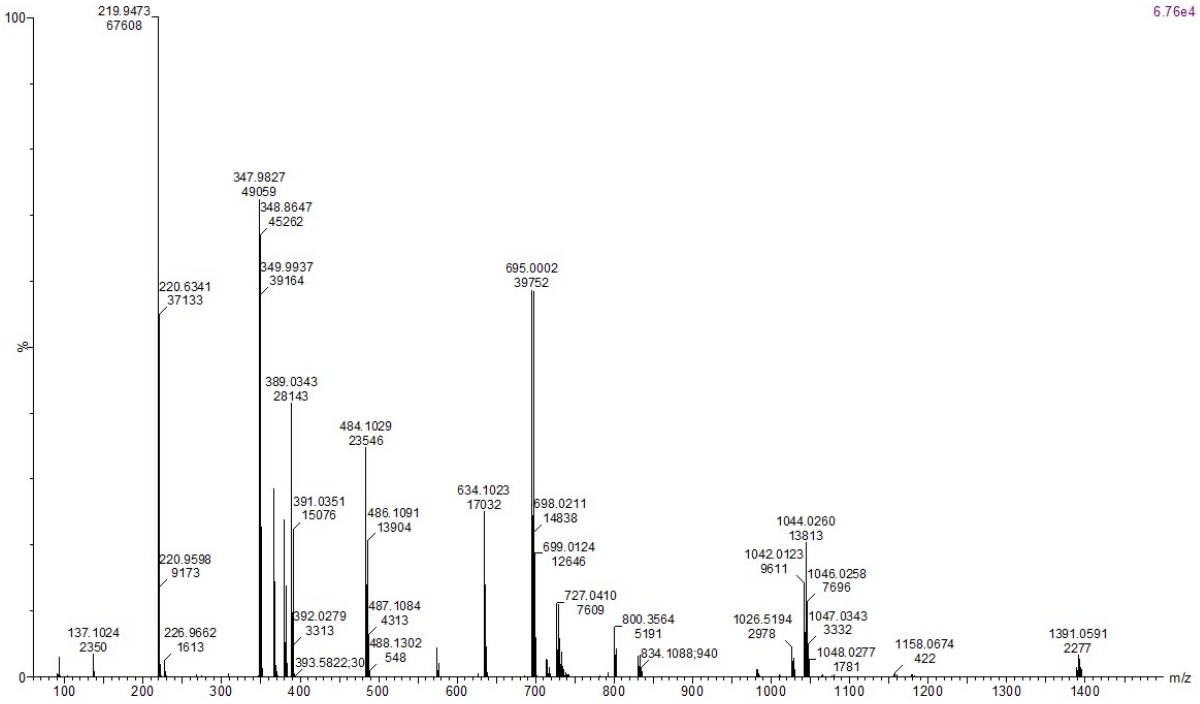



**Figure S4(a):** Whole HRMS spectrum of copper complex **5d**.

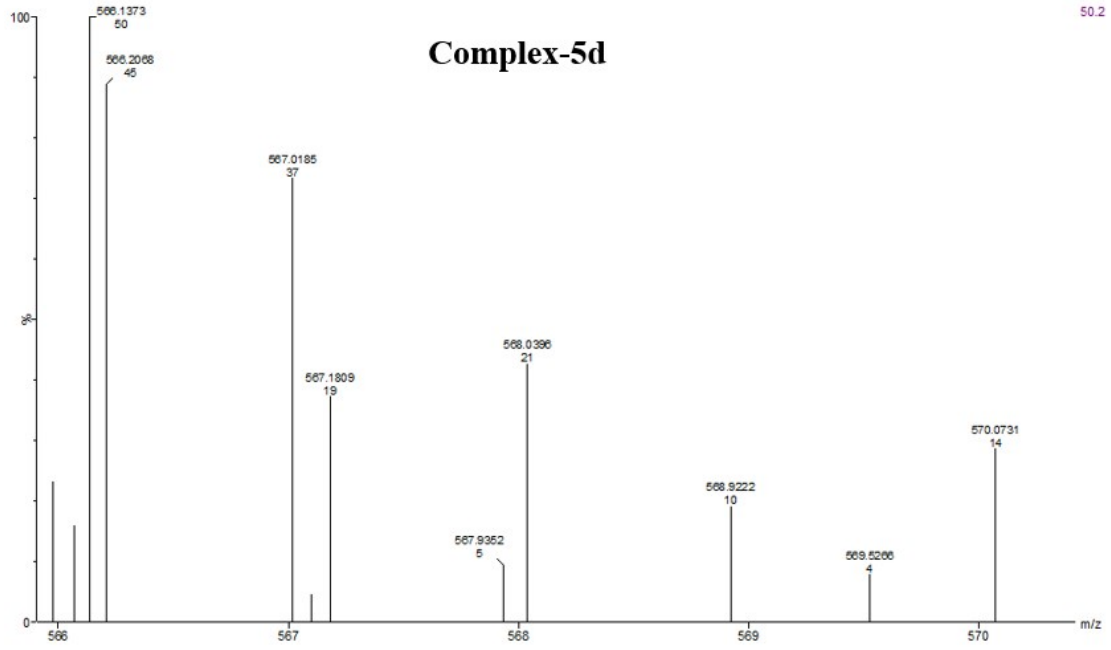



**Figure S4(b):** Partial HRMS spectrum of copper complex **5d**.

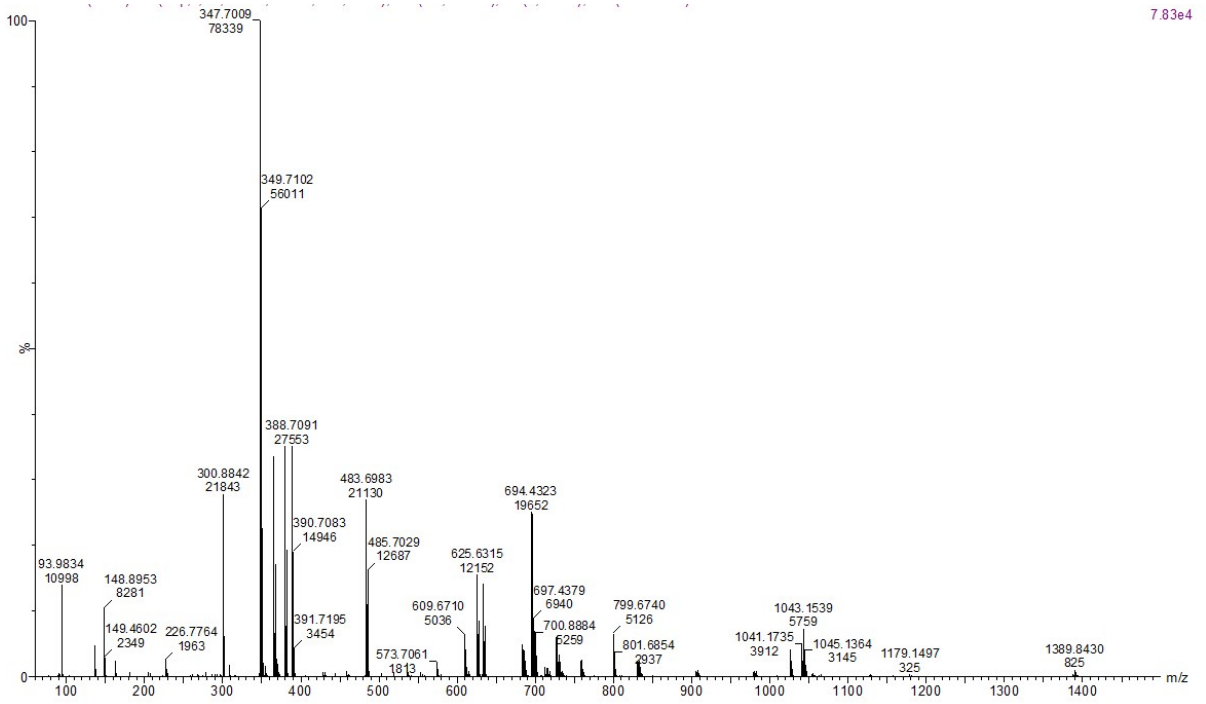



**Figure S5(a):** Whole HRMS spectrum of copper complex **5e**.

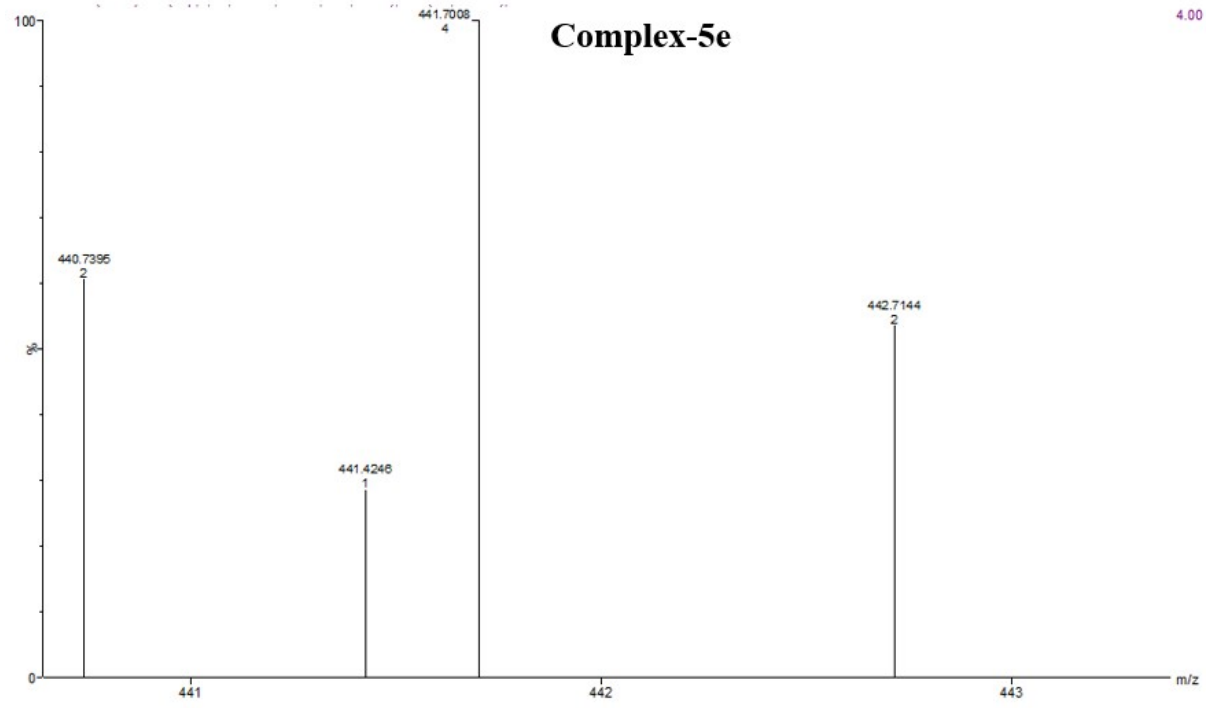



**Figure S5(b):** Partial HRMS spectrum of copper complex **5e**.

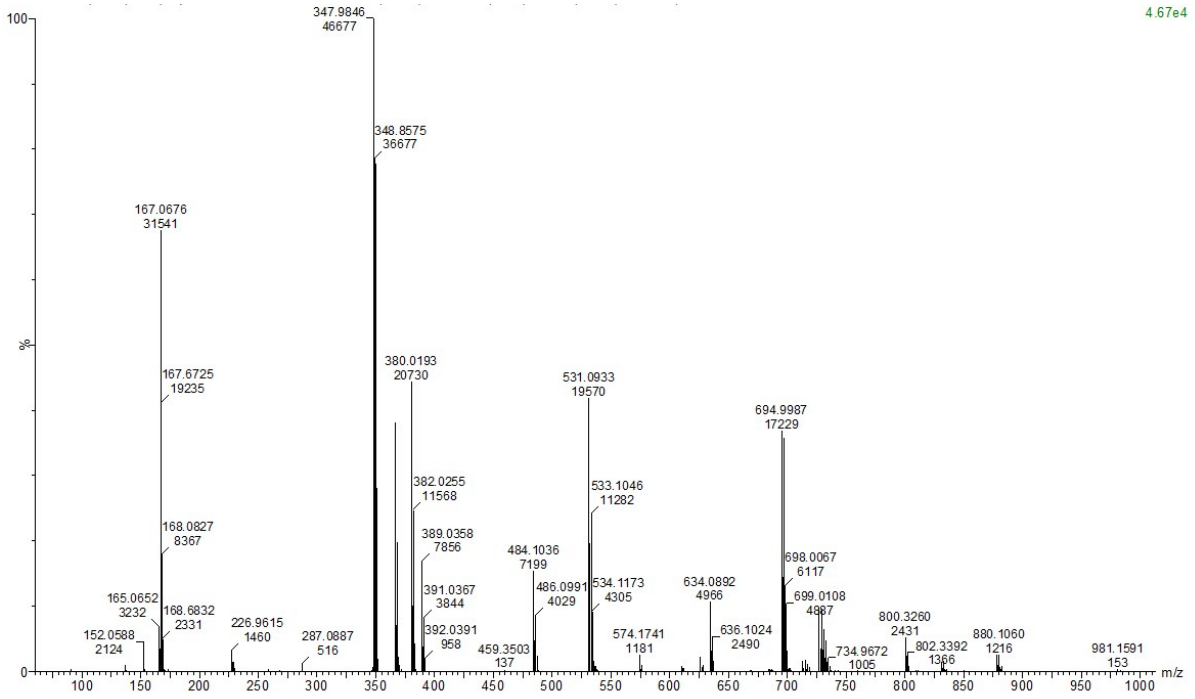



**Figure S6(a):** Whole HRMS spectrum of copper complex **5f**.

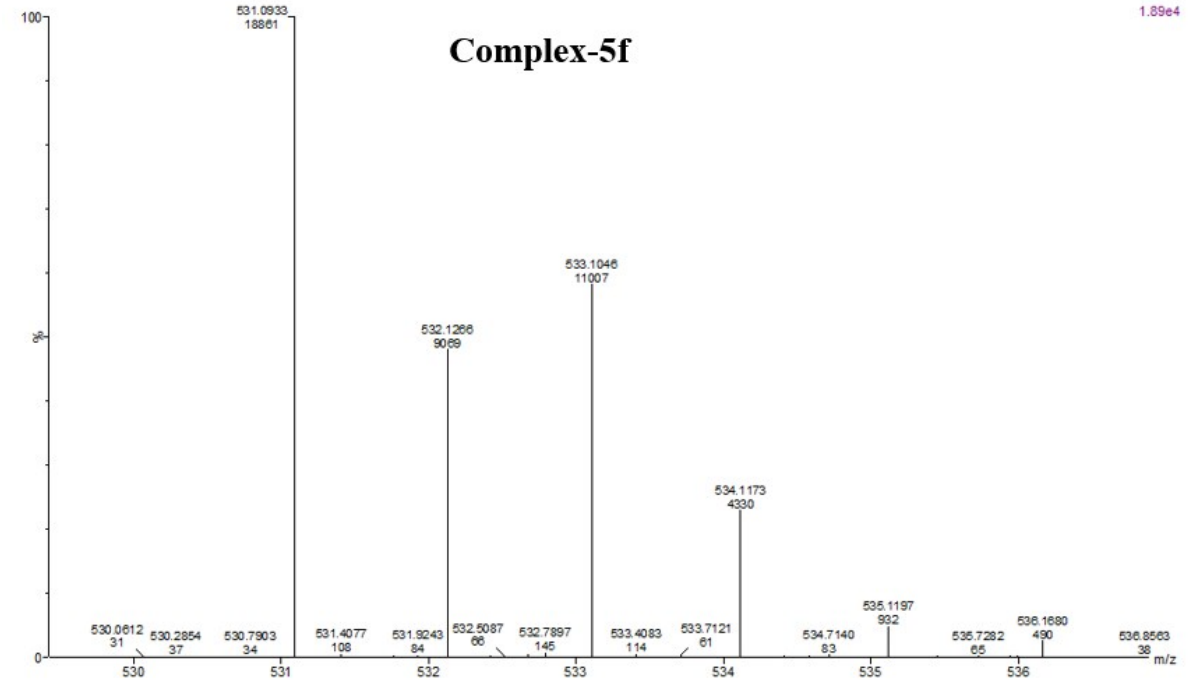
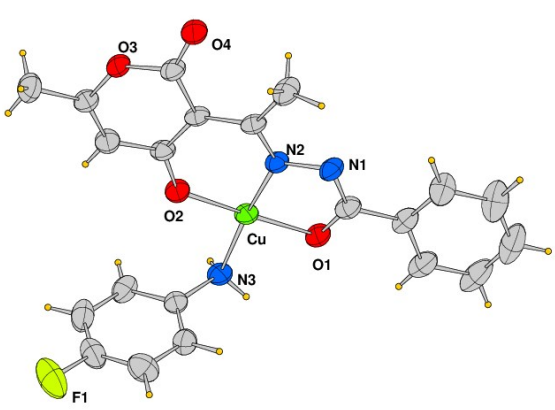
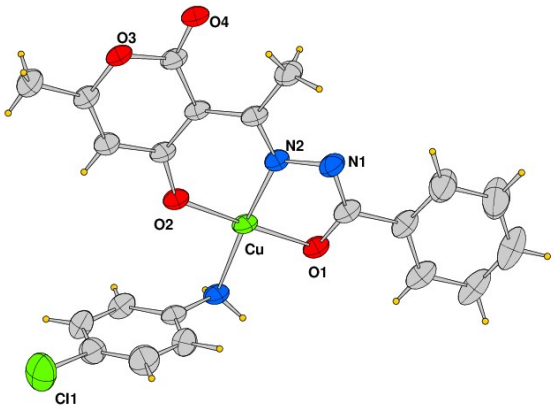


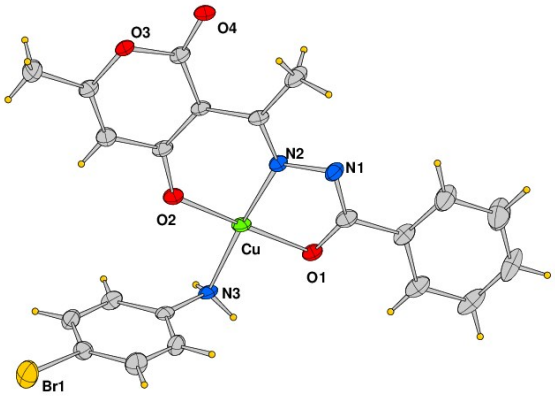

**Figure S6(b):** Partial HRMS spectrum of copper complex **5f**.



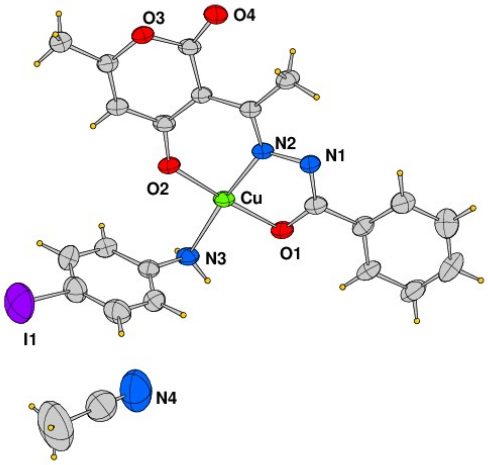

**5a**



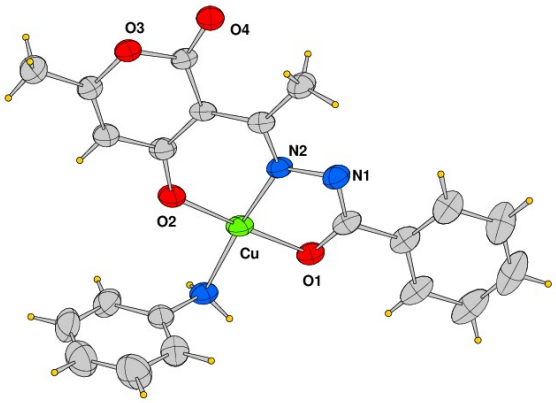

**5b**




**5c**




**5d**




**5e**

**Figure S7:** Molecular structure of complexes **5a–5e** (ORTEP diagrams with ellipsoid probability at 50%).

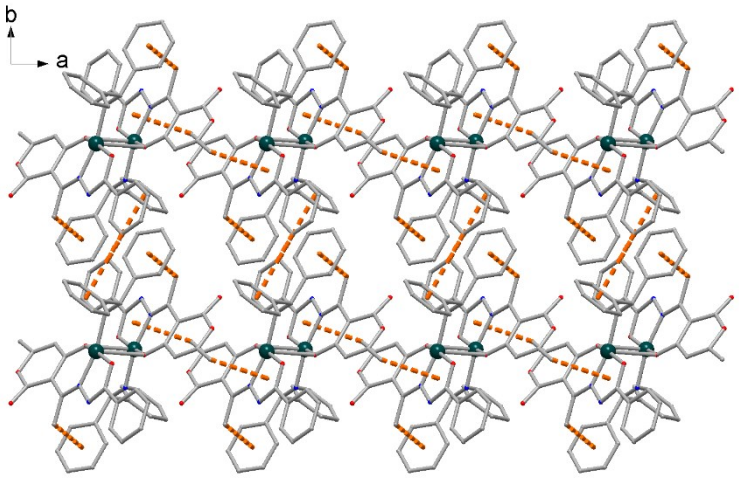



**Figure S8:** 3D architecture viewed down axis *c* in the crystal packing of **5f** built by C-H…π-ring interactions (parameters reported in Table 5S).

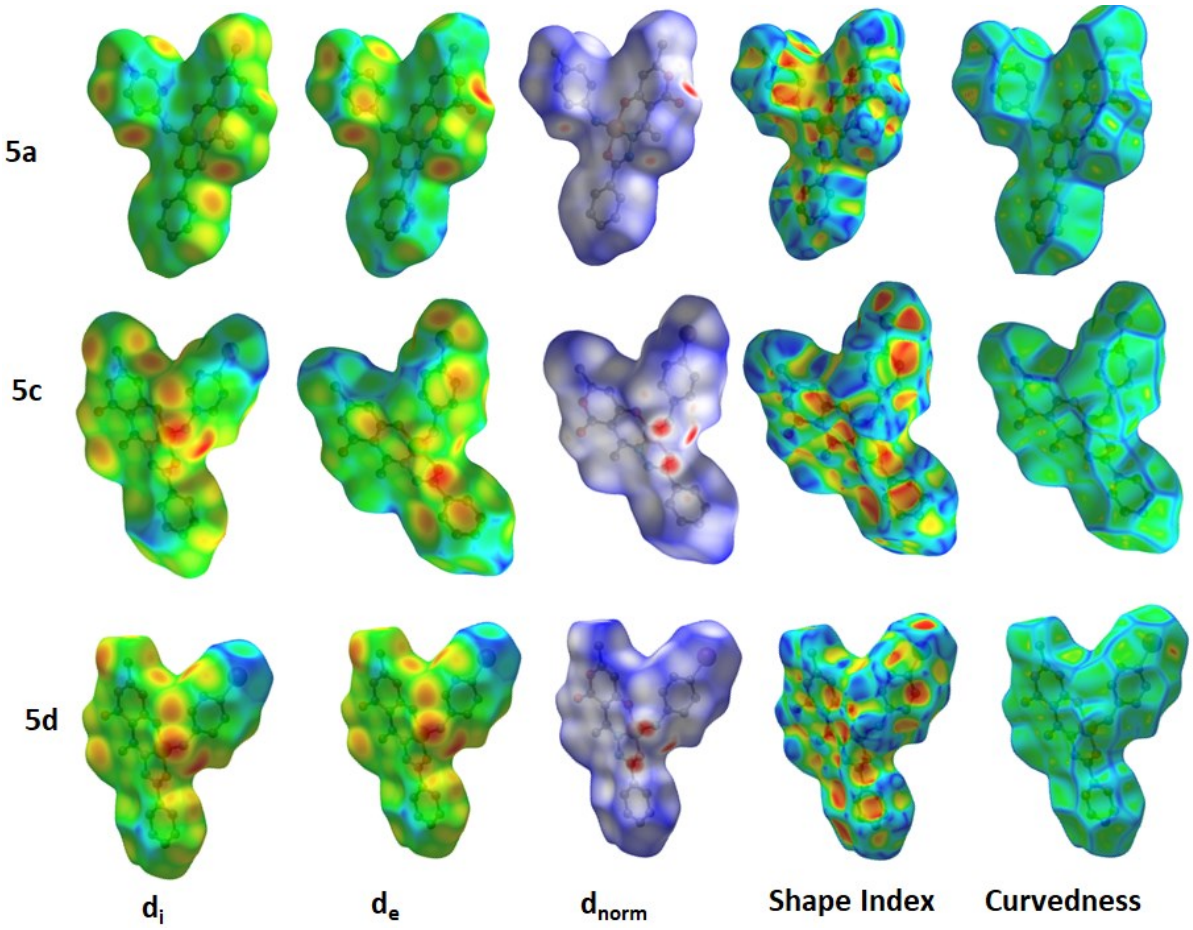



**Figure S9:** Hirshfeld surface analysis of complexes **5a**, **5c** and **5d**.

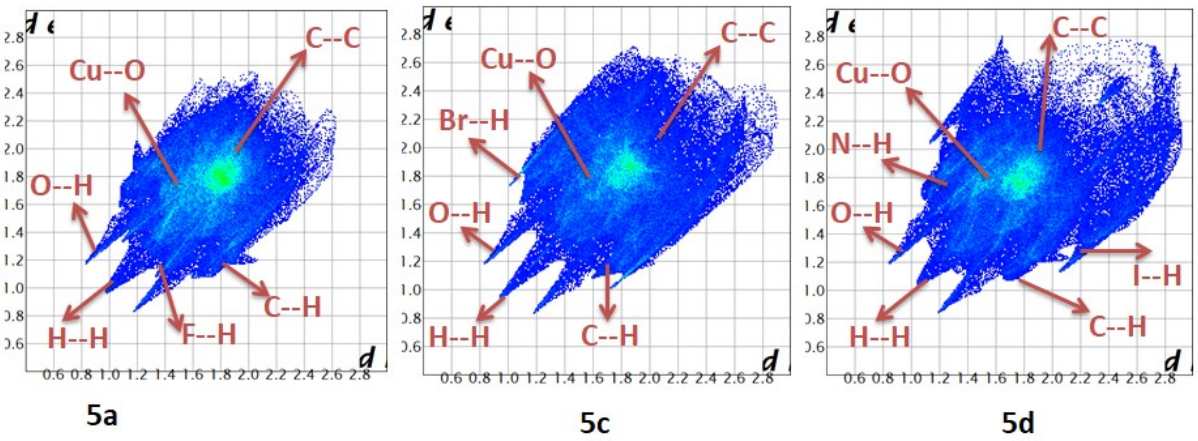



**Figure S10:** 2D fingerprint plots for complexes **5a**, **5c** and **5d**.

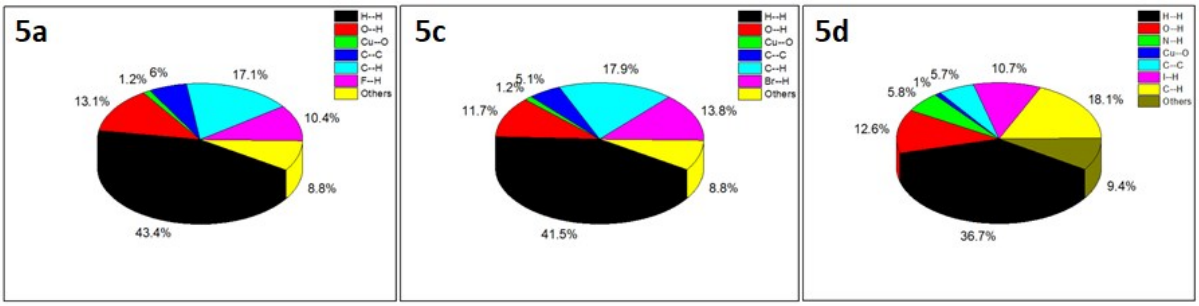



**Figure S11:** Relative percentage contributions of several intermolecular interactions on the Hirshfeld surface area of these complexes.

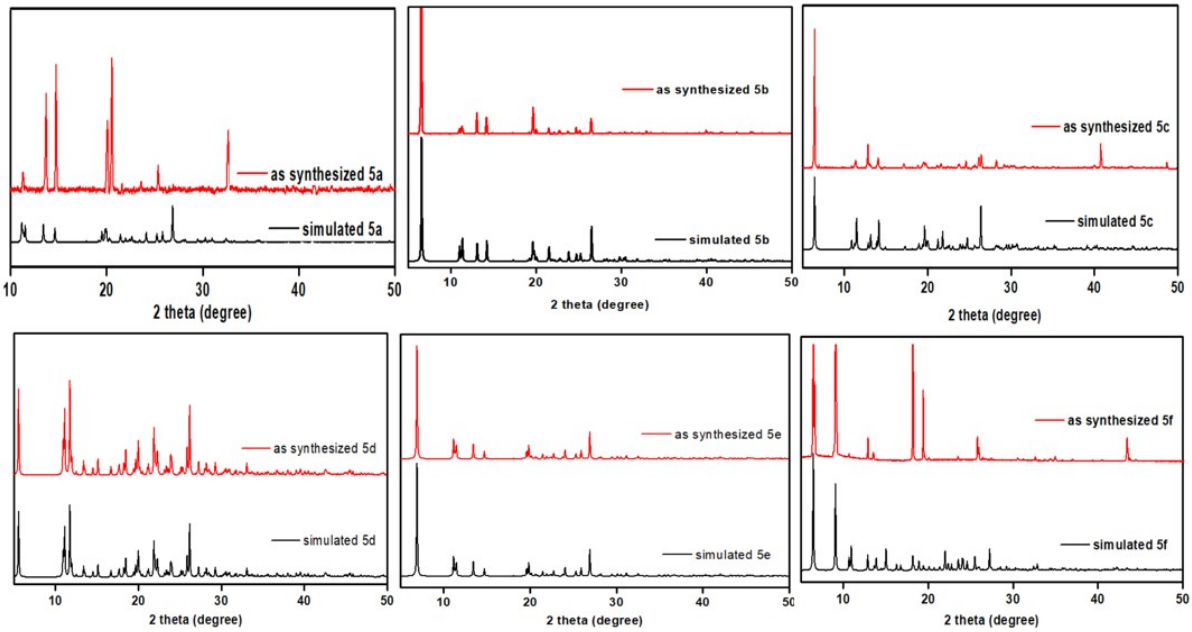



**Figure S12:** Powder XRD spectra of **5a-5f** complexes.

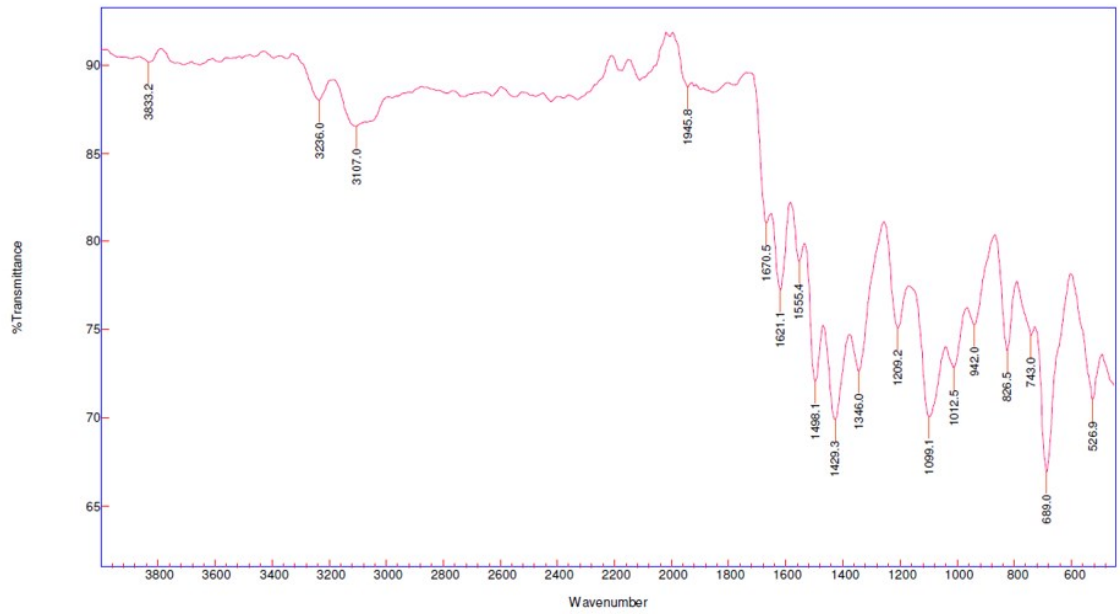



**Figure S13 (a):** FT-IR spectrum of complexe [CuL(4F-An)] **(5a)**.

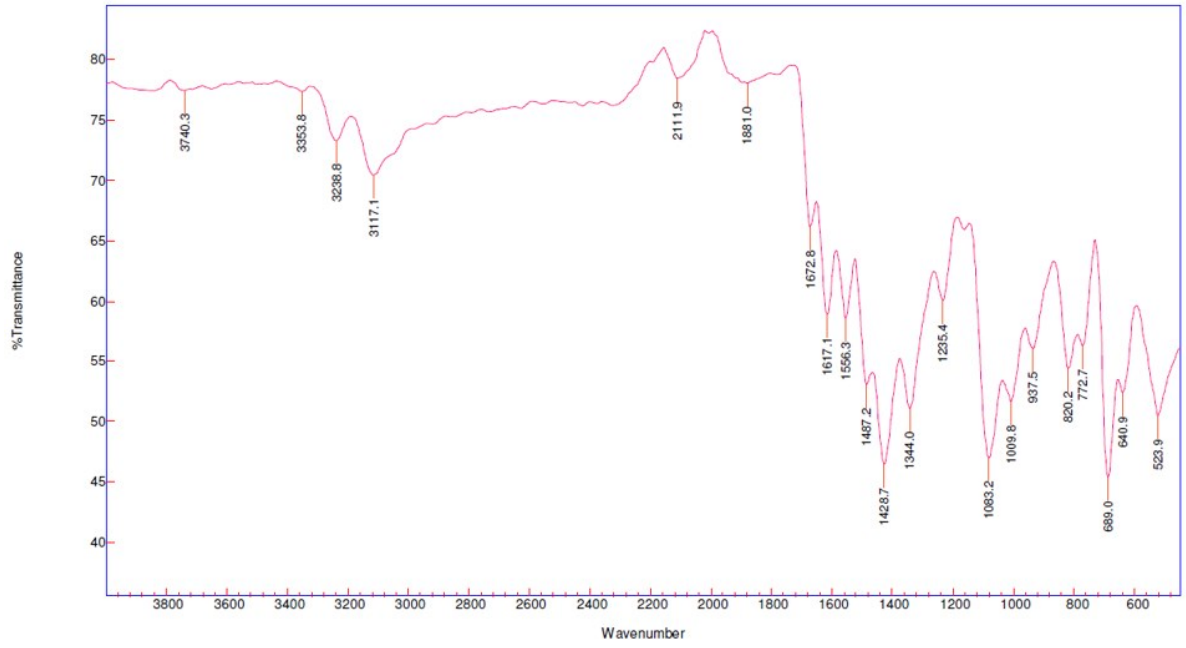



**Figure S13 (b):** FT-IR spectrum of complex [CuL(4Cl-An)] **(5b)**.

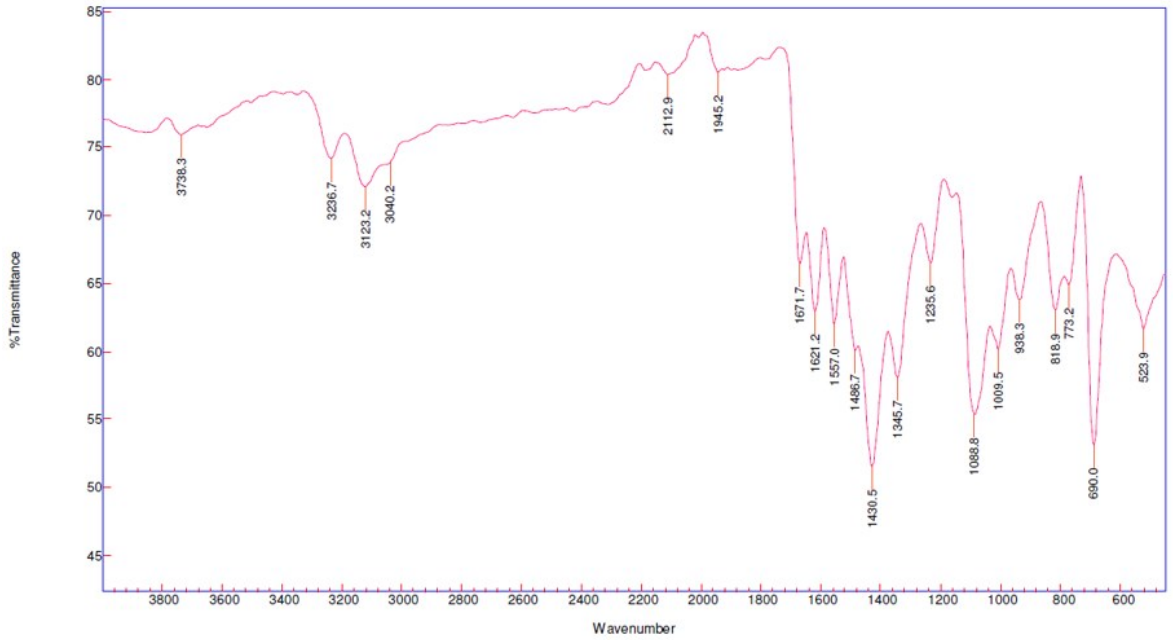



**Figure S13 (c):** FT-IR spectrum of complex [CuL(4Br-An)] **(5c)**.

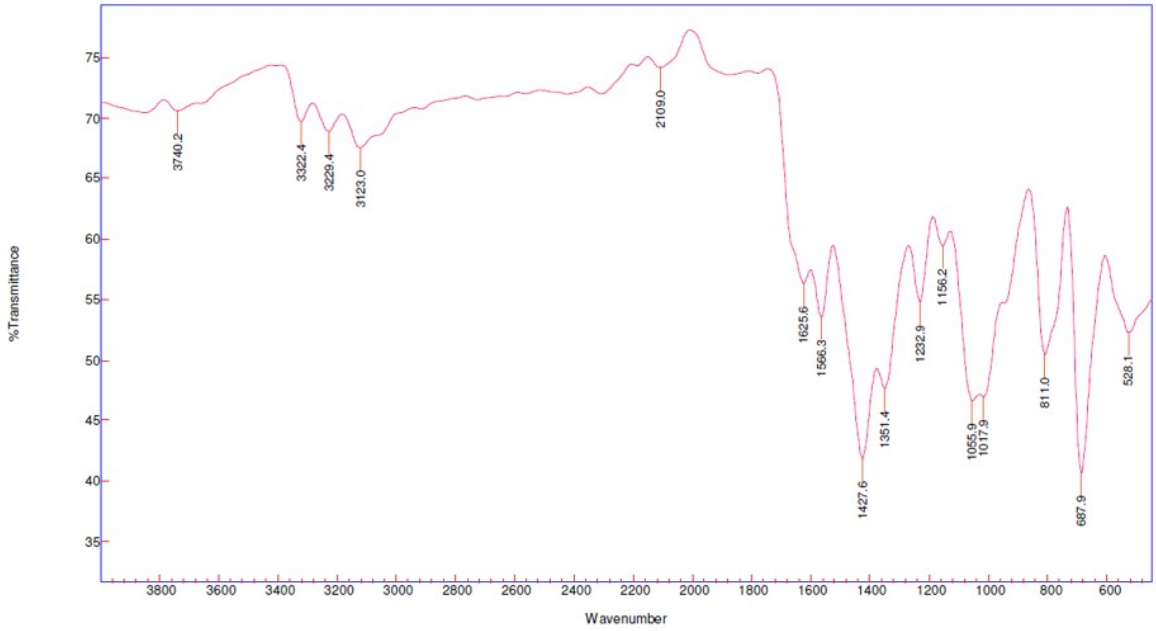



**Figure S13 (d):** FT-IR spectrum of complex [CuL(4I-An)] **(5d)**.

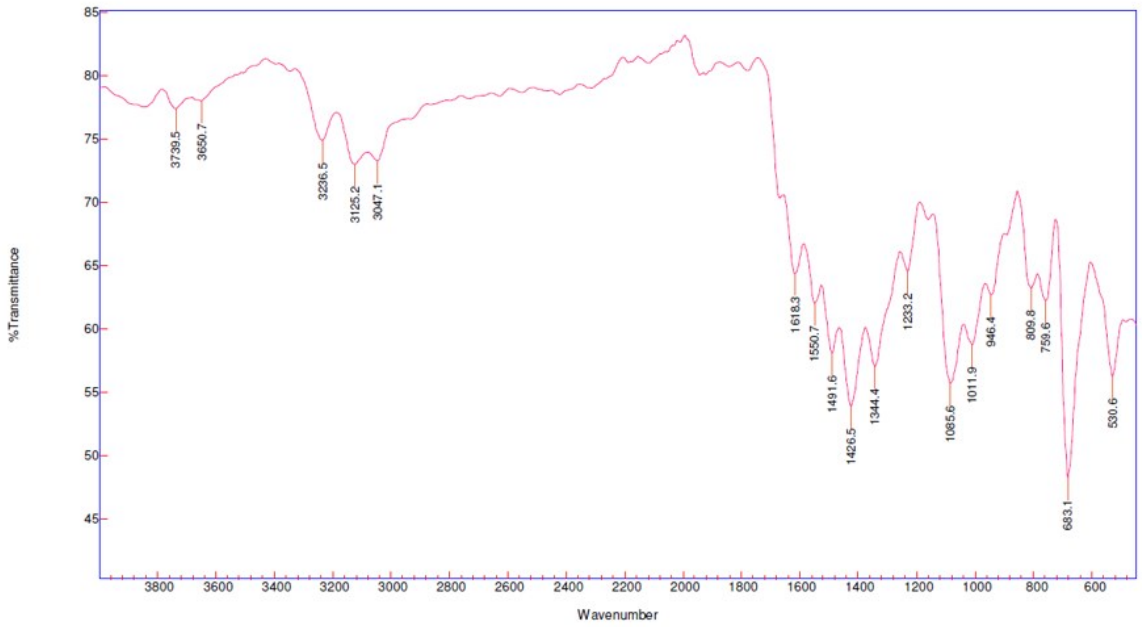



**Figure S13 (e):** FT-IR spectrum of complex [CuL(An)] **(5e)**.

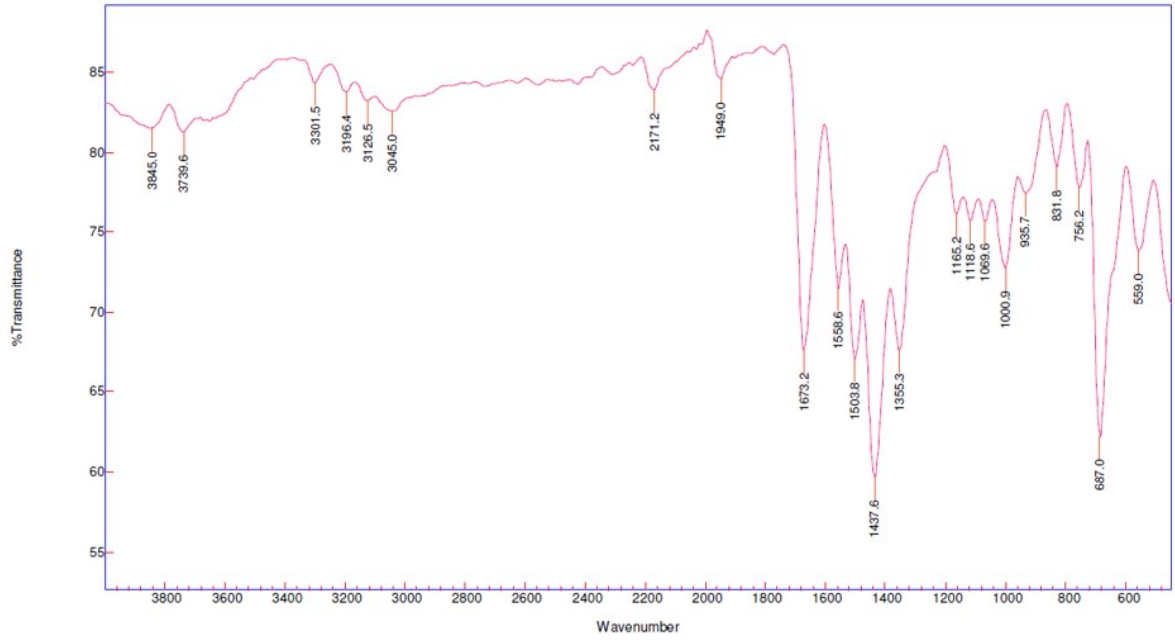



**Figure S13 (f):** FT-IR spectrum of complex [CuL(Benzhydrylamine)] **(5f)**.

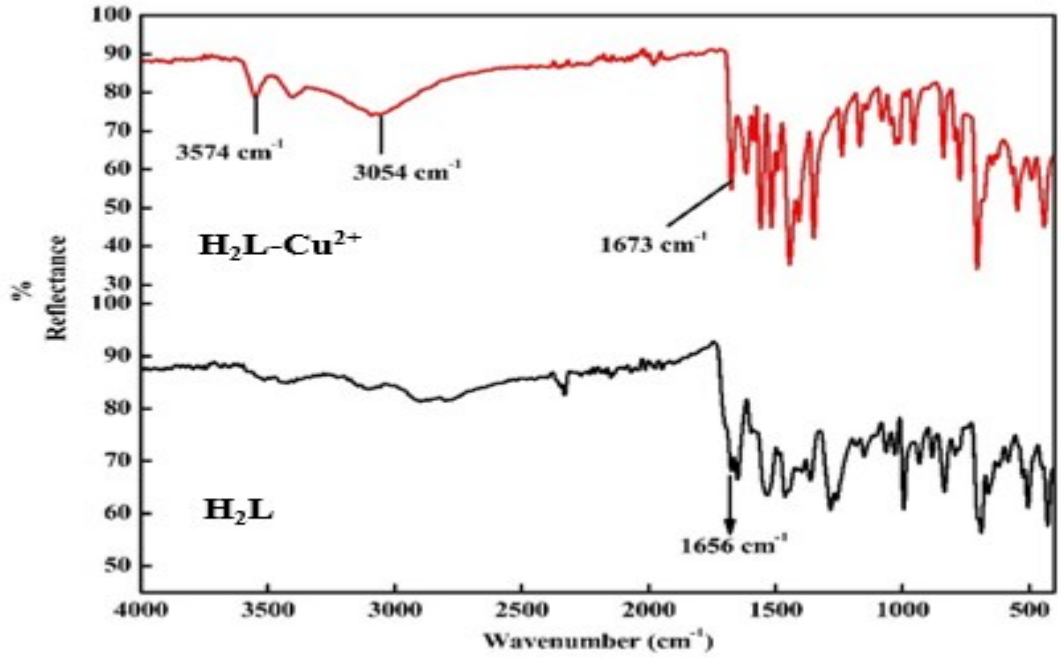



**Figure S13 (g):** FT-IR spectra of synthesized ligand **$H_2L$** and complex **$H_2L$-$Cu^{2+}$**.

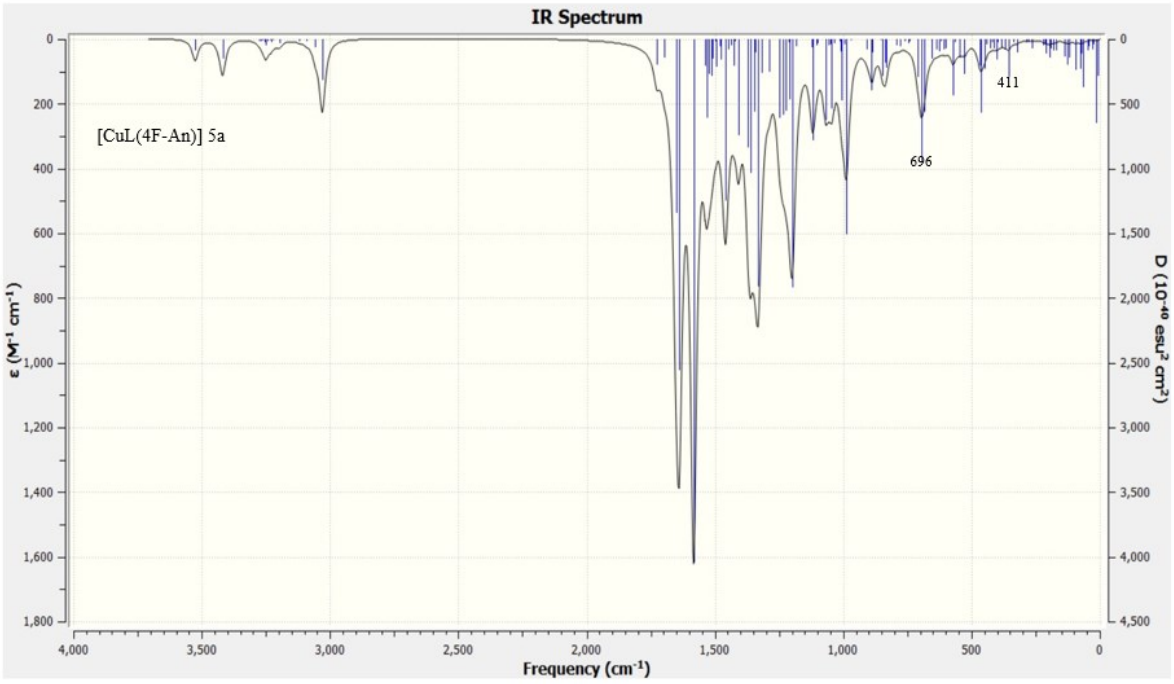



**Figure S13 (h):** Computed FT-IR spectrum of complex [CuL(4F-An)] **(5a)**.

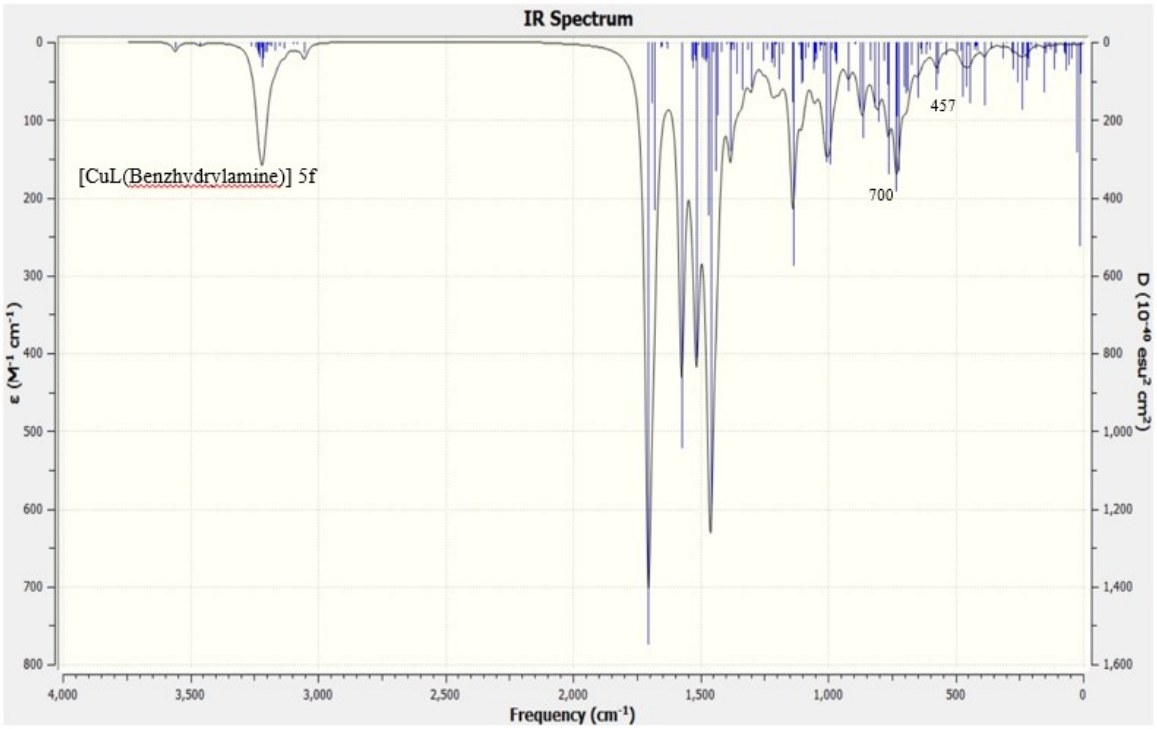



**Figure S13 (i):** Computed FT-IR spectrum of complex [CuL(Benzhydrylamine)] **(5f)**.

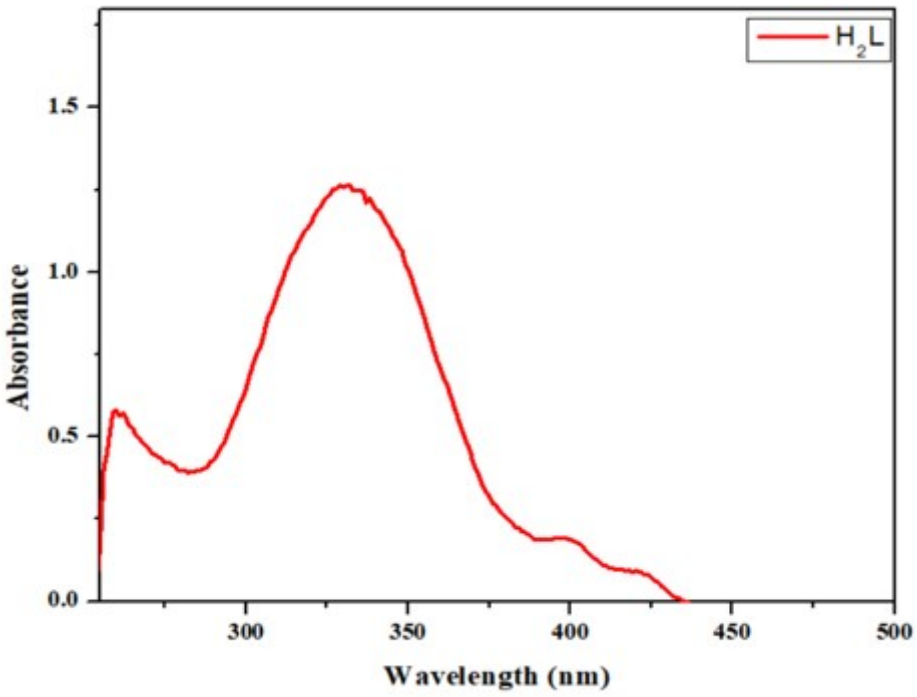



**Figure S14 (a):** UV- vis spectrum of ligand **$H_2L$**.

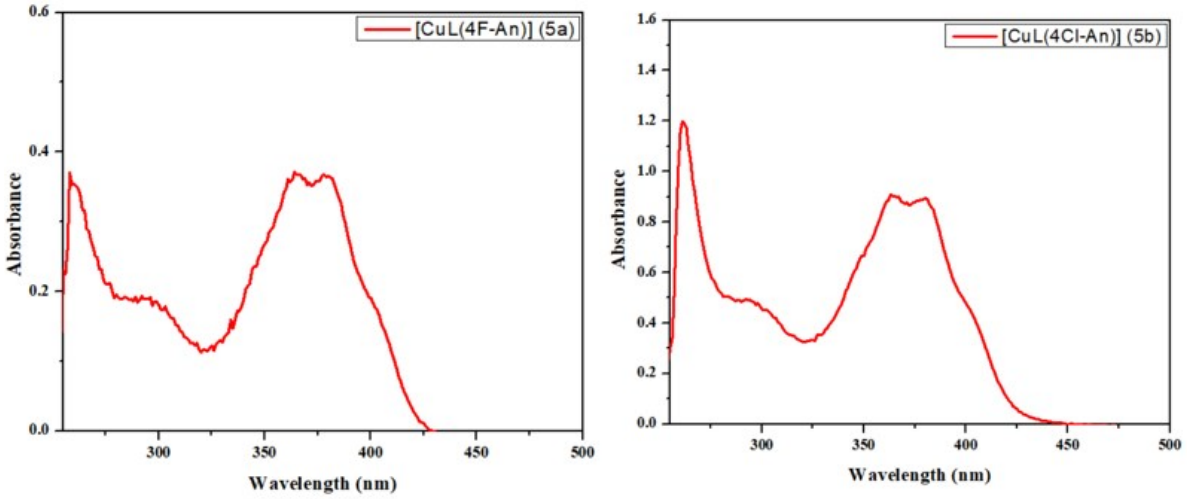



**Figure S14 (b):** UV- vis spectra of synthesized complexes **5a** and **5b**.

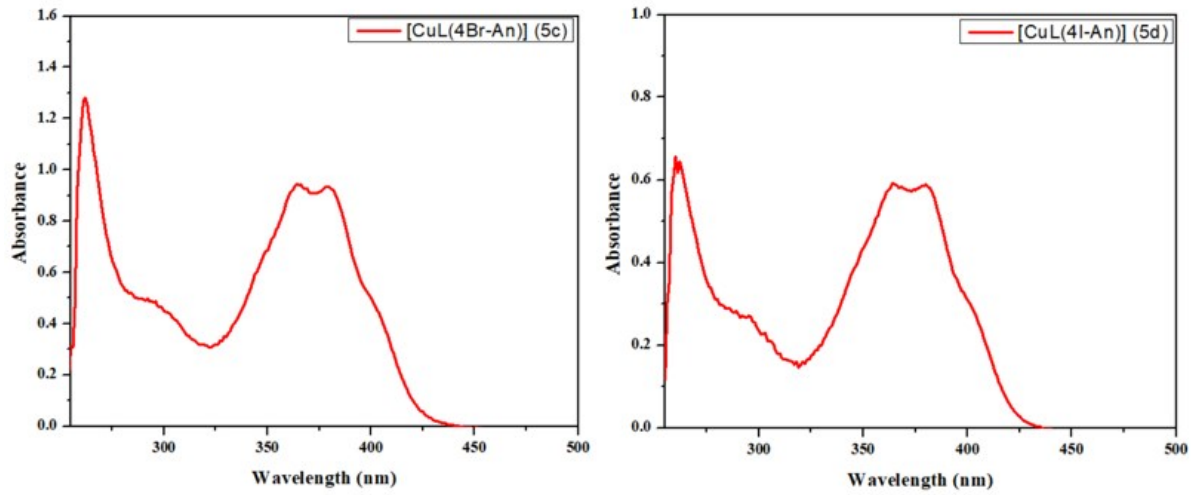



**Figure S14 (c):** UV- vis spectra of synthesized complexes **5c** and **5d**.

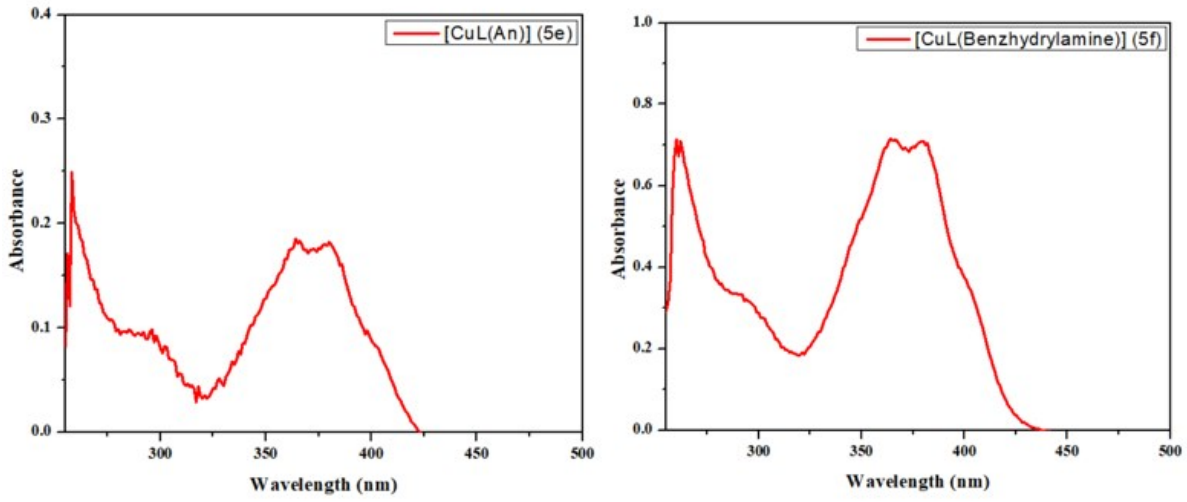



**Figure S14 (d):** UV- vis spectra of synthesized complexes **5e** and **5f**.

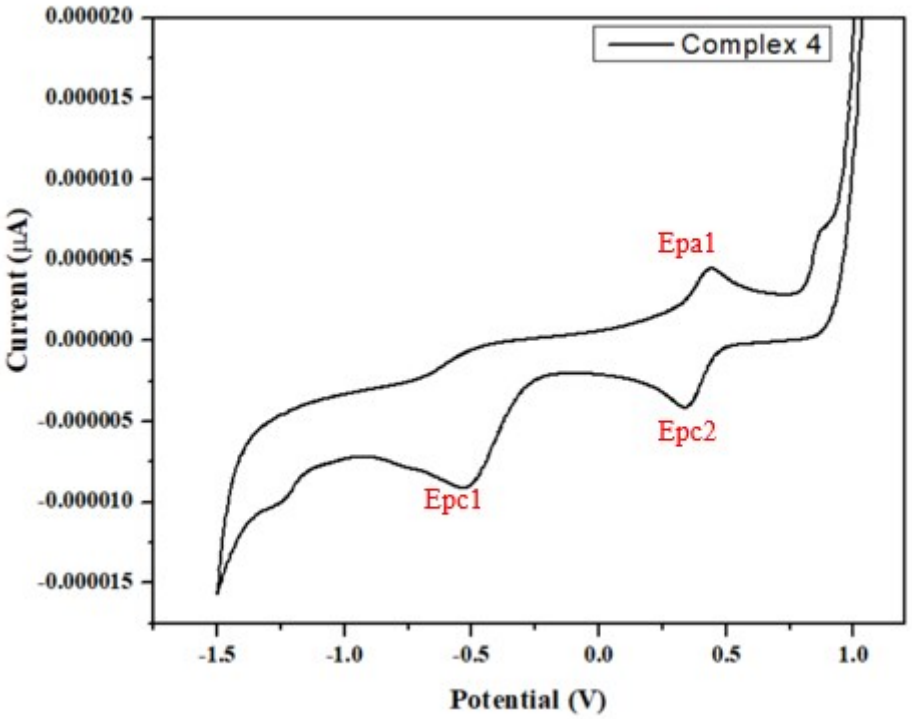



**Figure S15 (a):** Cyclicvoltammetric response of complex **4** using 0.05 M KCl solution at scan rate of 25 mV/sec.

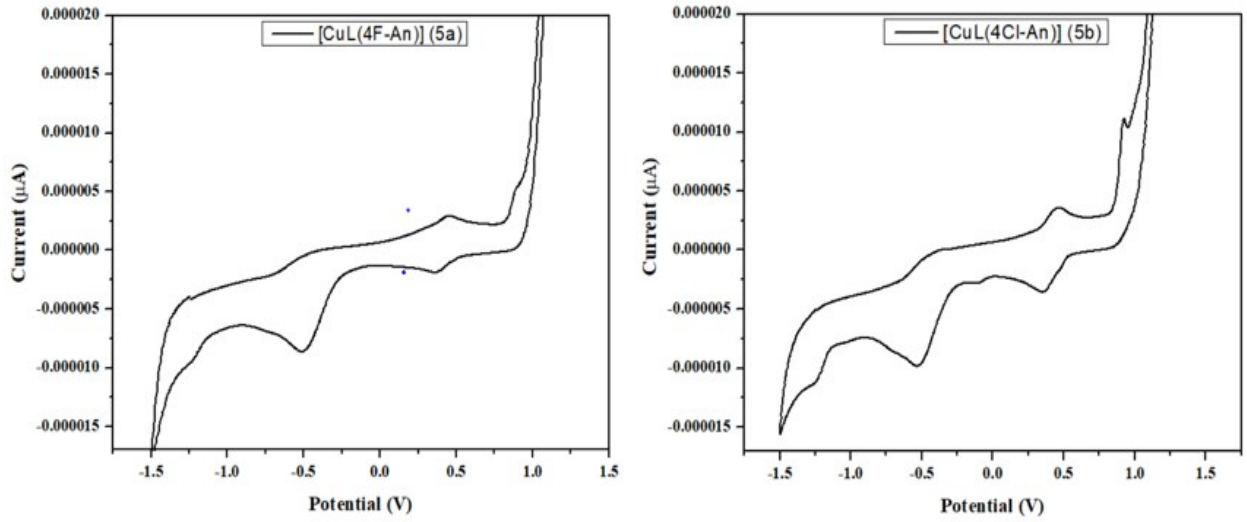



**Figure S15 (b):** Cyclicvoltammetric response complexes **5a** and **5b** using 0.05 M KCl solution at scan rate of 25 mV/sec.

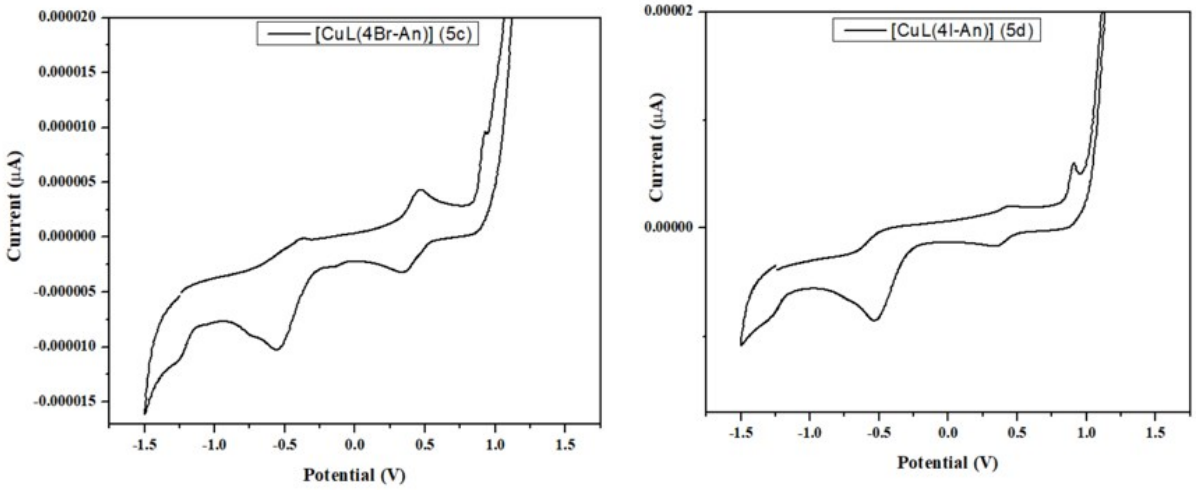



**Figure S15 (c):** Cyclicvoltammetric response complexes **5c** and **5d** using 0.05 M KCl solution at scan rate of 25 mV/sec.

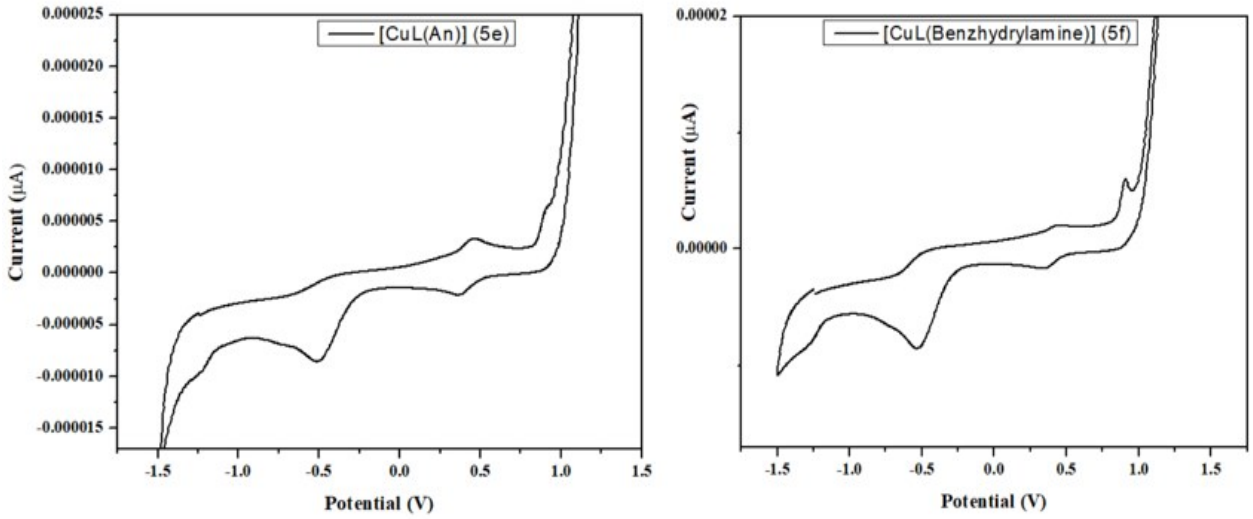



**Figure S15 (d):** Cyclicvoltammetric response complexes **5e** and **5f** using 0.05 M KCl solution at scan rate of 25 mV/sec.

‡ All the potentials are referenced to Ag/AgCl electrode.

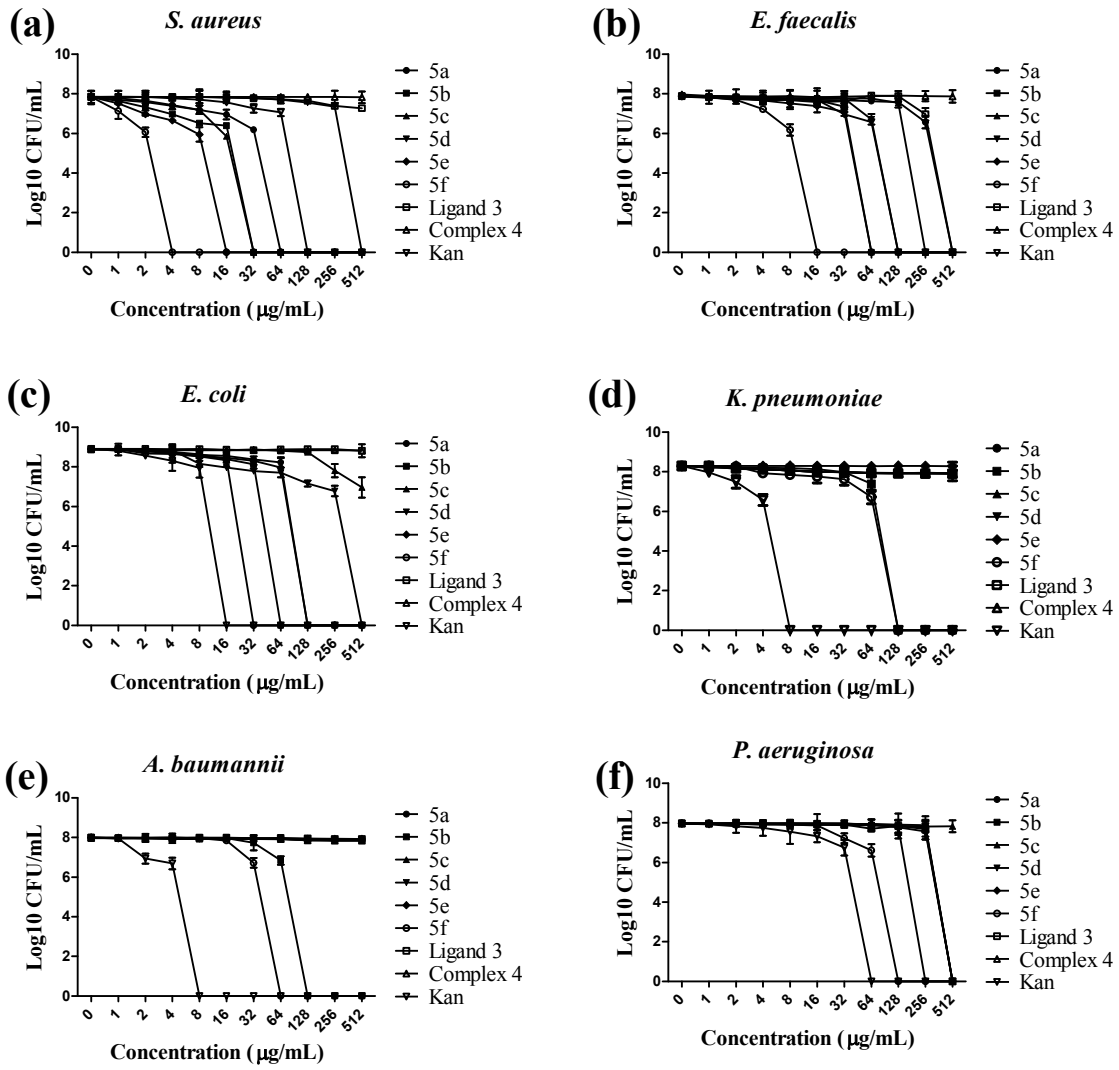



**Figure S16:** Log CFU/mL of all bacteria used in the study in the presence of various concentration of complexes **4**, **5a-5f**, ligand (**3**) and Kanamycin as comparison after 24h of treatment. Data represent mean±SD for all data point. Each experiment was performed at least twice in duplicate.

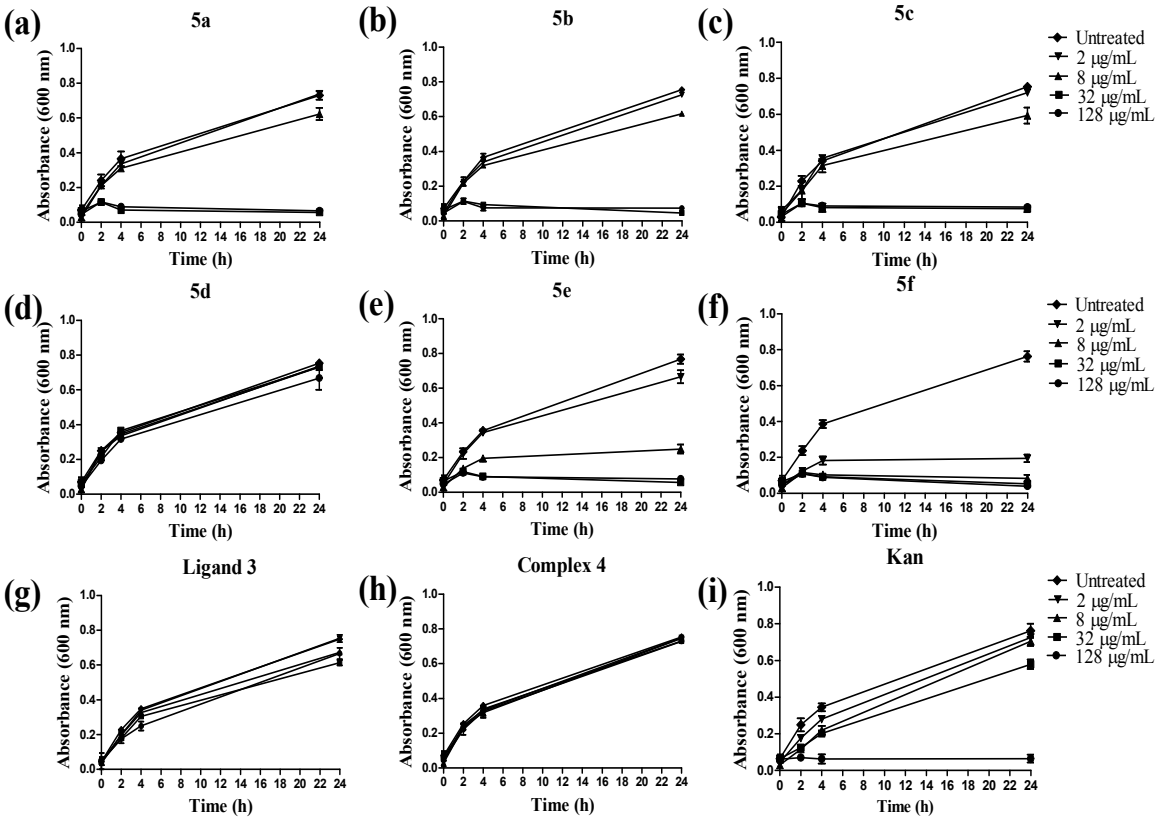



**Figure S17:** Impact on growth of *S. aureus* in the presence of various concentrations of compounds used in this study. Data represent mean±SD for all data point. Each experiment was performed at least twice in duplicate.

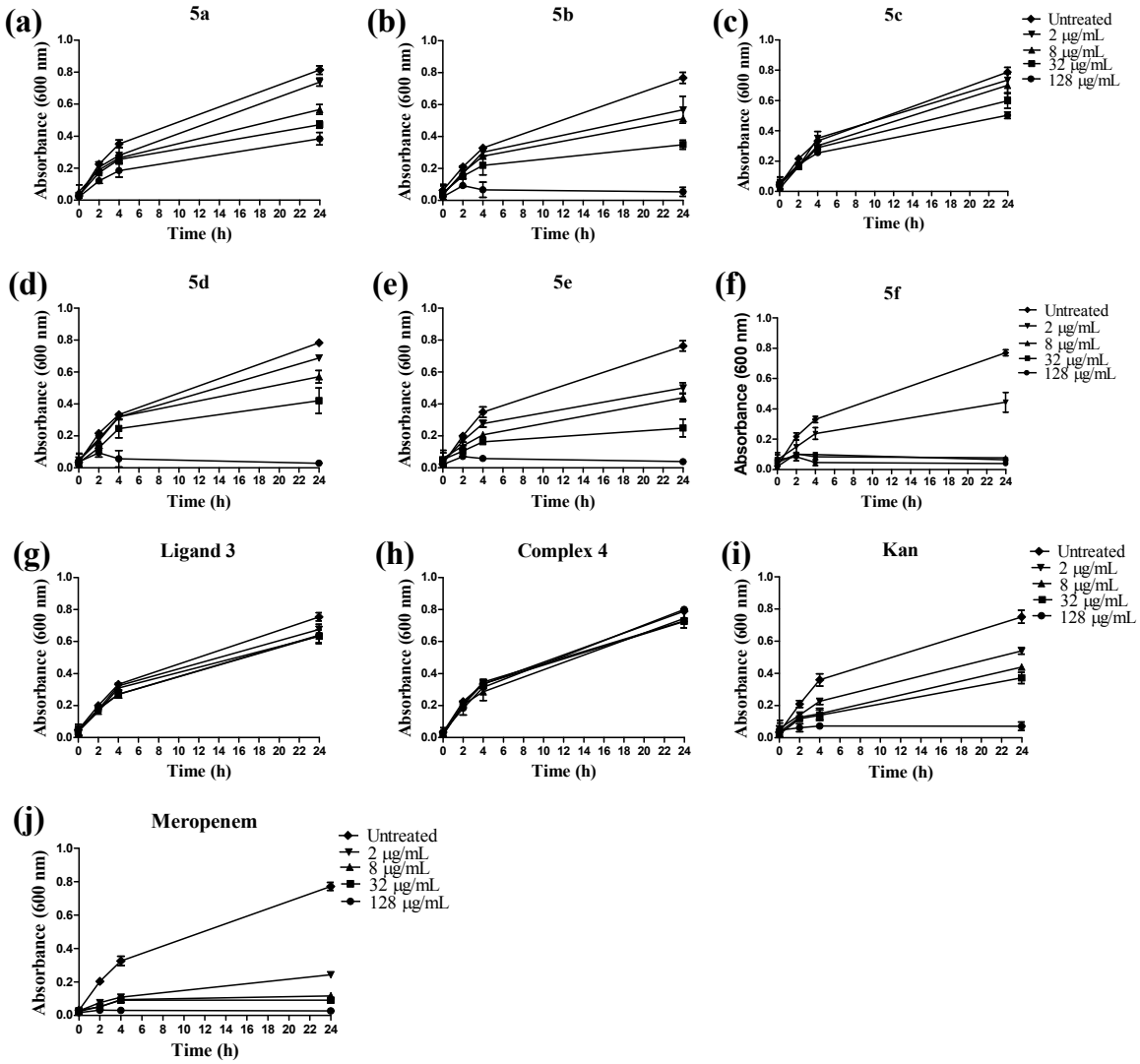



**Figure S18:** Impact on growth of *E. faecalis* in the presence of various concentrations of compounds used in this study. Data represent mean±SD for all data point. Each experiment was performed at least twice in duplicate. Meropenem, a third generation antibiotic was also used as control to show that MIC of compound 5f is comparable to this drug.

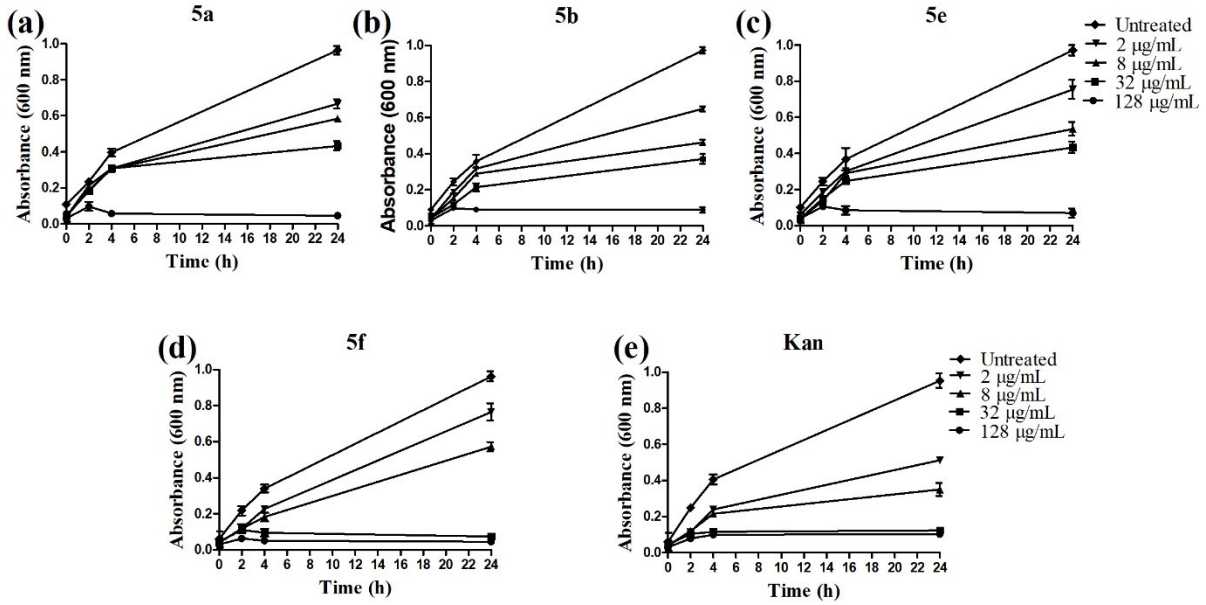



**Figure S19:** Impact on growth of *E. coli* in the presence of various concentrations of compounds used in this study. Data represent mean±SD for all data point. Each experiment was performed at least twice in duplicate. Note: No effect on growth in presence of complexes **4**, **5c**, **5d**, and ligand **3**.

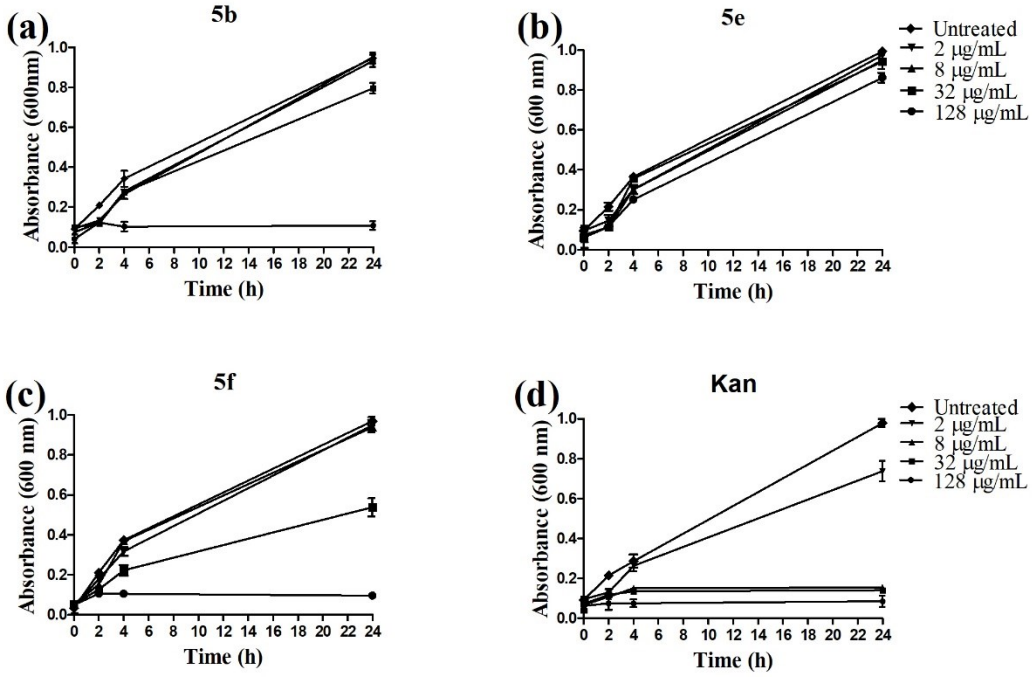



**Figure S20:** Impact on growth of *A. baumannii* in the presence of various concentrations of compounds used in this study. Data represent mean±SD for all data point. Each experiment was performed at least twice in duplicate. Note: No effect on growth in presence of complexes **4**, **5a**, **5c**, **5d**, and ligand **3**.

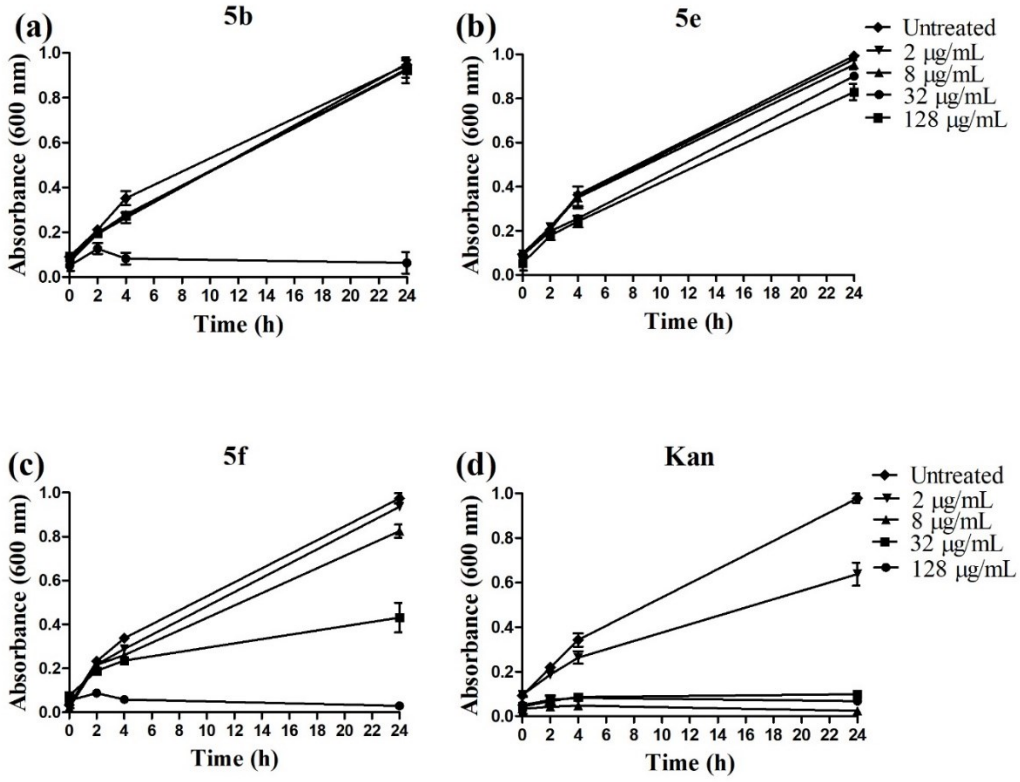



**Figure S21:** Impact on growth of *K. pneumoniae* in the presence of various concentrations of compounds used in this study. Data represent mean±SD for all data point. Each experiment was performed at least twice in duplicate. Note: No effect on growth in presence of complexes **4**, **5a**, **5c**, **5d**, and ligand **3**.

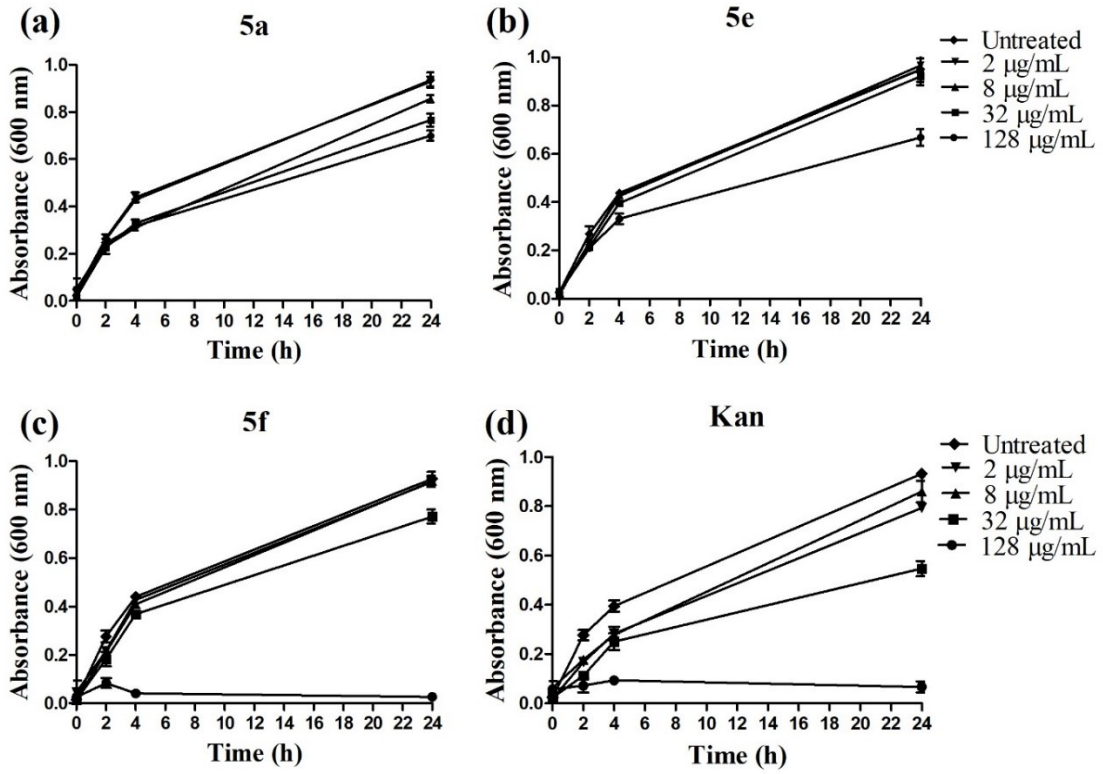



**Figure S22:** Impact on growth of P. aeruginosa in the presence of various concentrations of compounds used in this study. Data represent mean±SD for all data point. Each experiment was performed at least twice in duplicate. Note: No effect on growth in presence of complexes **4**, **5b**, **5c**, **5d**, and ligand **3**.

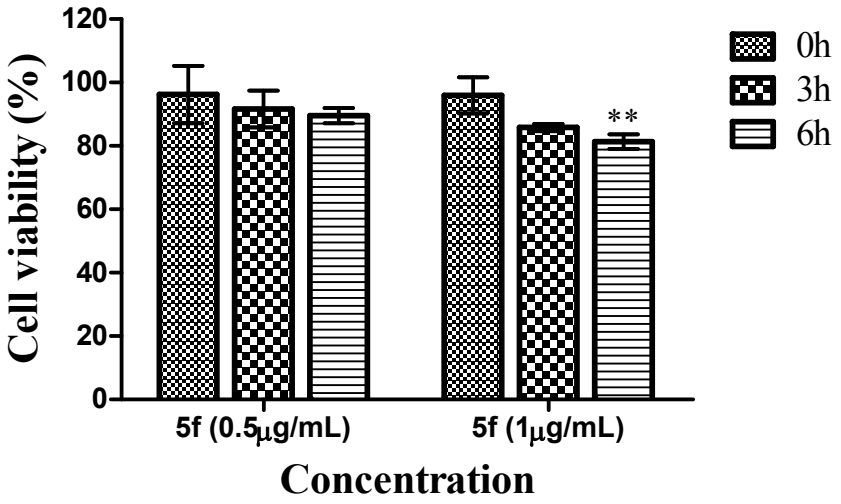



**Figure S23**: MTT assay indicate negligible cell toxicity of the residual compound **[CuL(Benzhydrylamine)] 5f**. Data indicate precent cell viability of HEK-293 kidney cell line at 3 hours and 6 hours of direct exposure of the residual compound to the cell . Data represent mean ± SD (**P<0.01). Each experiment was performed at least twice in triplicate.

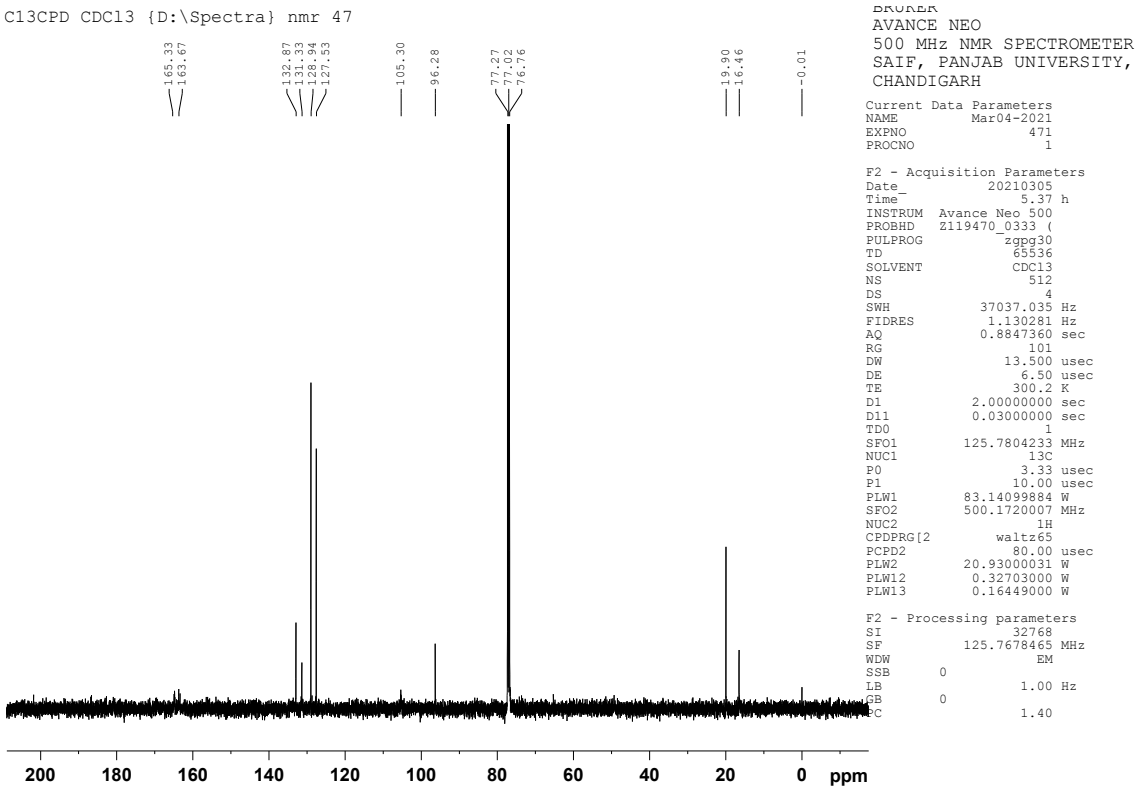



**Figure S24:** $^{13}$C-NMR Spectrum of $\mathbf{H_2L}$ in $CDCl_3$.

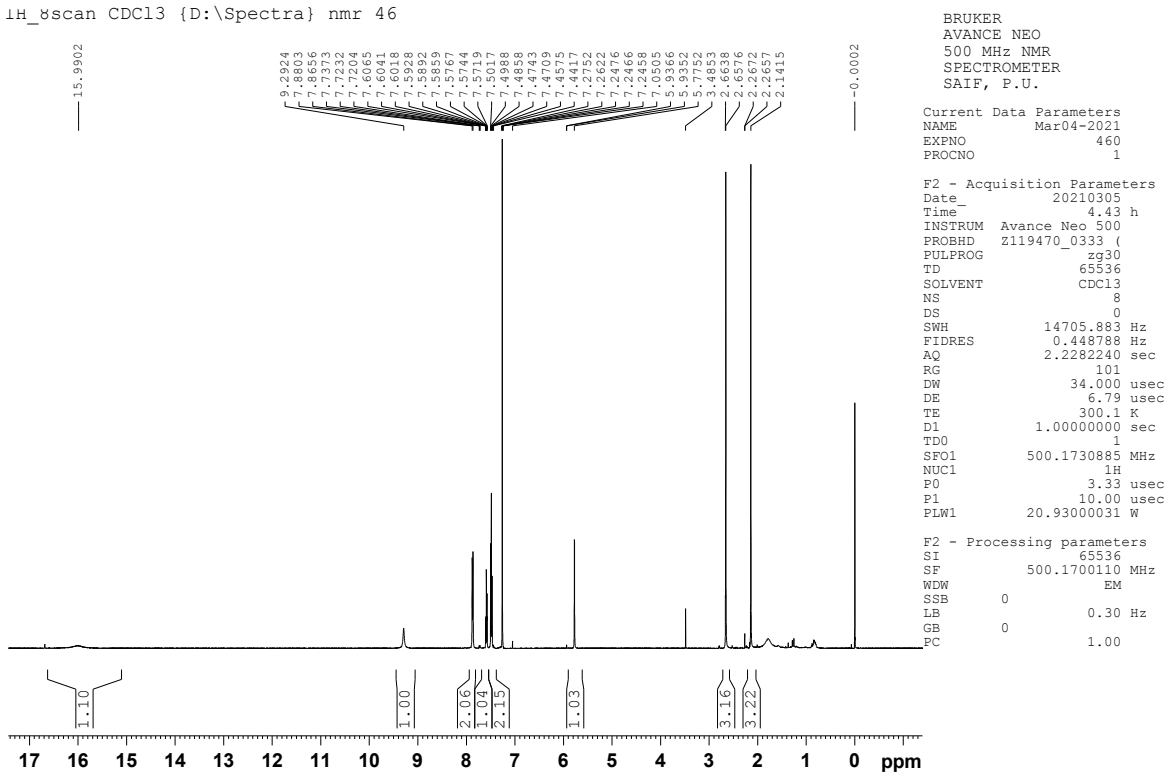



**Figure S25 (a):** $^{1}$H-NMR Spectrum of ligand $\mathbf{H_2L}$ in $CDCl_3$ (Whole Spectrum).

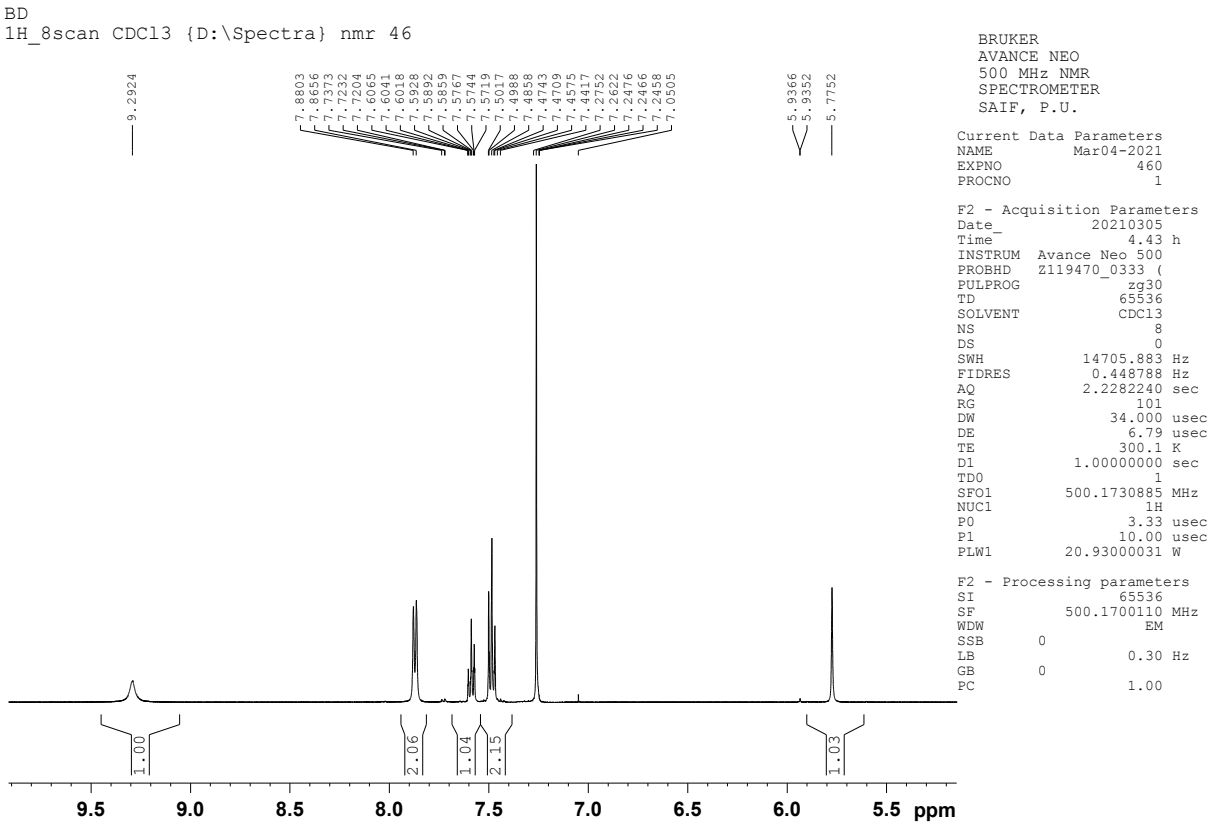



**Figure S25 (b):** $^{1}$H-NMR Spectrum of ligand **$H_2$L** in $CDCl_3$ (Partial Spectrum).

## TGA and DSC analysis of complexes 5a-5f

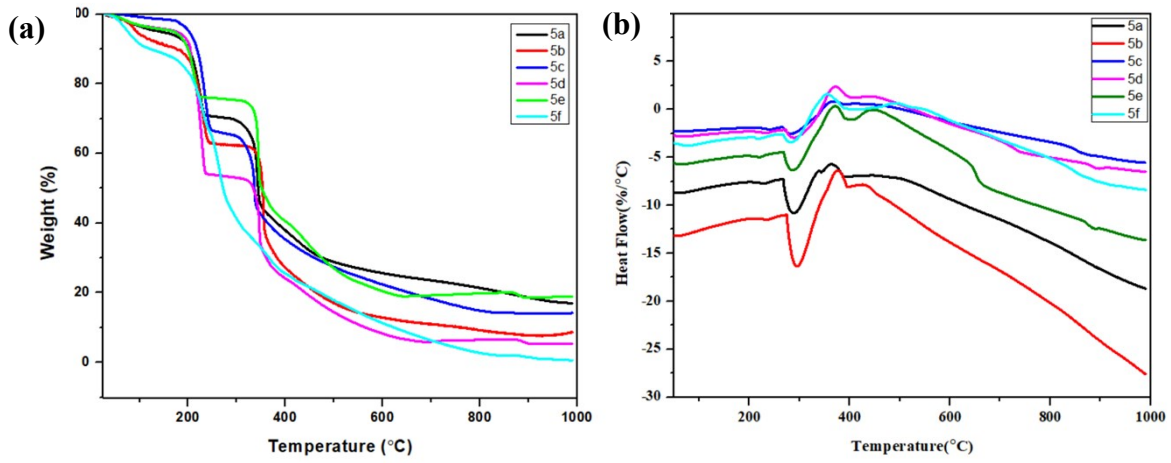



**Figure S26: (a)**Thermo gravimetric curves of all solvated metal complexes and **(b)** DSC plot of all solvated metal complexes.

Thermal gravimetric analysis was performed to check the thermal stability of all the synthesized copper complexes over the temperature range 25-1000 °C under nitrogen

atmosphere. The weight loss pattern is explained in **Table-S10**. In all the copper complexes described and evaluated in this manuscript, the residue is CuO. In case of DSC analysis, the sharp endothermic peak in the range of 285-295 °C for complexes 5a-5f was in good agreement with TGA data.

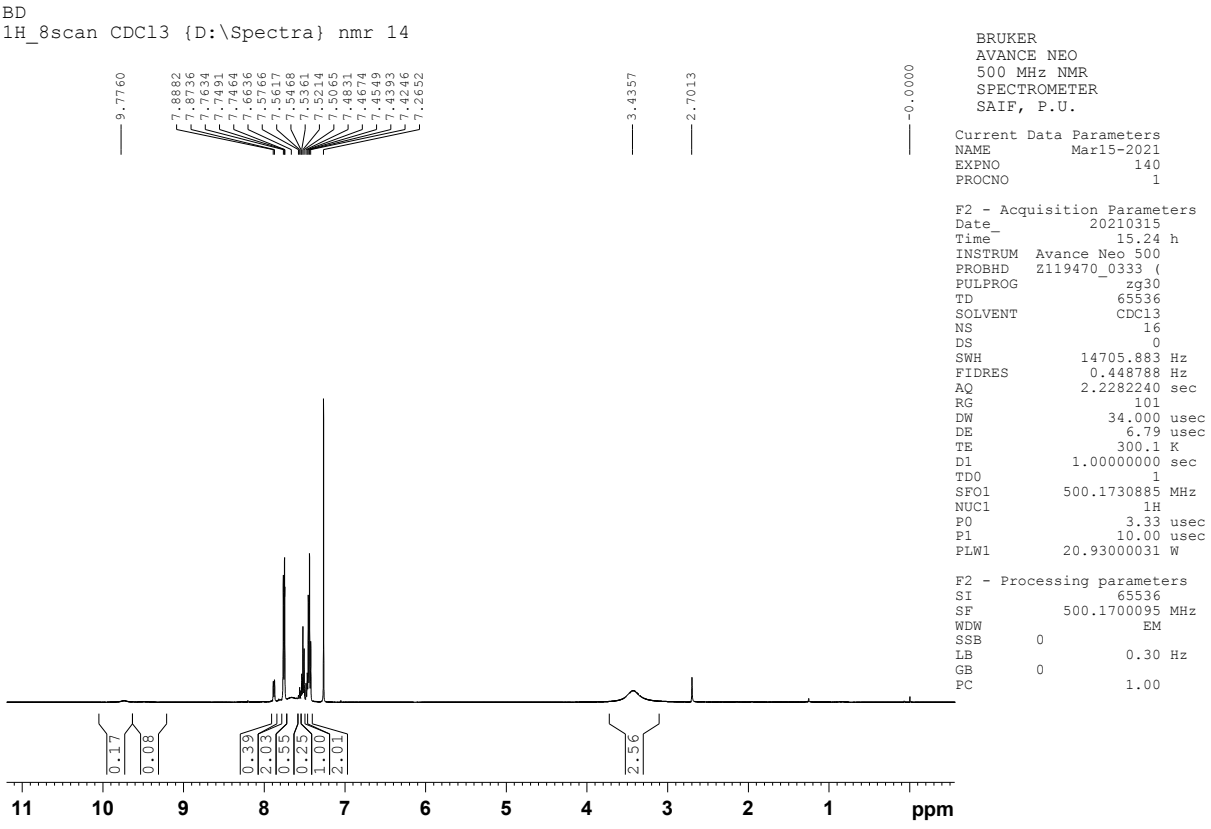



**Figure S27:** $^{1}$H-NMR Spectra of benzohydrazide in $CDCl_3$.