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Article

DNA and BSA Interaction Studies and Antileukemic Evaluation of Polyaromatic Thiosemicarbazones and Their Copper Complexes

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Supplementary Informations

L_1 (CCDC 2164725)

Crystal data: $C_{14}H_{15}N_3S_1$, Mr = 257.35, orthorhombic, space group Pcab, a = 7.5832(3), b = 12.3944(5), c = 28.4373(11) Å, V = 2672.8(2) Å^3, Z = 8, ρ_{calc} = 1.279 Mg·m^{-3}, T = 293.15 K, F(000) = 1088, crystal dimensions = 0.20 × 0.20 × 0.20 mm, indexes range= −9 < h < 9, −15 < k < 15, −35 < l < 35, collected reflections = 30191, unique reflections = 2736, refined parameters = 223, goodness-of-fit = 1.058, R factor = 0.0350, wR2 = 0.0941, residual electron density = 0.21 and −0.16 eÅ^{-3}.

L_3 (CCDC 2164721)

Crystal data: $C_{18}H_{16}Cl_1N_3S_1$, Mr = 341.85, orthorhombic, space group $Pca2_1$, a = 7.9863(8), b = 9.7195(9), c = 21.2622(19) Å, V = 1650.4(3)Å^3, Z = 4, ρ_{calc} = 1.376 Mg·m^{-3}, T = 296.15 K, F(000) = 712, crystal dimensions = 0.10 × 0.10 × 0.10 mm, index range = −9 < h <10, −12 < k < 12, −26 < l < 26, collected reflections = 19173, unique reflections = 1924, refined parameters = 210, goodness-of-fit = 1.012, R factor = 0.0497, wR2 = 0.1054, residual electron density = 0.23 and −0.26 eÅ^{-3}.

L_4 (CCDC 2164724)

Crystal data: $C_{17}H_{14}Cl_1N_3S_1$, Mr = 327.82, monoclinic, space group $P2_1/c$, a = 10.9230(7), b = 8.8750(4), c = 15.8800(16) Å, β = 94.226(9)°, V = 1535.2(7) Å^3, Z = 4, ρ_{calc} = 1.418 Mg·m^{-3}, T = 293.15 K, F(000) = 680, crystal dimensions = 0.20 × 0.20 × 0.20 mm, index range = −13 < h < 13, −3 < k < 10, −4 < l < 19, collected reflections = 3007, unique reflections = 2905, refined parameters = 207, goodness-of-fit = 0.887, R factor = 0.0520, wR2 = 0.0975, residual electron density = 0.22 and −0.22 eÅ^{-3}.

$[Cu^I(L_1)_2](HSO_4)$ (**1**) (CCDC 2164723)

Crystal data: $C_{28}H_{31}Cu_1N_6O_4S_3$, Mr = 675.31, triclinic, space group P-1, a = 11.6646(5), b = 14.9211(7), c = 9.0074(8) Å, α = 90.609(7), β = 95.373(4), γ = 74.663(5)°, V = 1505.1(2) Å^3, Z = 2, ρ_{calc} = 1.490 Mg·m^{-3}, T = 293.15 K, F(000) = 700, crystal dimensions = 0.10 × 0.10 × 0.10 mm, index range −14 < h < 14, −18 < k < 18, −1< l < 10, collected reflections = 5669, unique reflections = 5667, refined parameters = 381, goodness-of-fit = 1.048, R factor = 0.0551, wR2 = 0.1486, residual electron density = 1.10 and −0.68 eÅ^{-3}.

L_5 (CCDC 2164722)

Crystal data: $C_{13}H_{13}N_3S_1$, Mr = 243.32, triclinic, space group P-1, a = 5.8381(7), b = 8.7678(11), c = 12.8504(16) Å, α= 72.4065(19), β = 86.5610(19), γ = 81.701(2)°, V = 620.35(13) Å^3, Z = 2, ρ_{calc} = 1.303 Mg·m^{-3}, T = 293.15 K, F(000) = 256, crystal dimensions = 0.10 × 0.10 × 0.10 mm, index range = −8 < h < 8, −12 < k < 12, −18 < l < 18, collected reflections = 10130, unique reflections = 3906, refined parameters = 206, goodness-of-fit = 1.075, R factor = 0.0418, wR2 = 0.1251, residual electron density = 0.26 and −0.14 eÅ^{-3}.

$[Cu^I_2(SO_4)(L_2)_5]$ (**2**). (CCDC 2164726)

Crystal data: $C_{65}H_{71}Cu_2N_{15}O_7S_6$, Mr = 1493.80, triclinic, space group *P*-1, a = 10.4703(11), b = 14.6148(15), c = 25.4741(26) Å, α = 96.778(2), β = 94.401(2), γ = 109.416(1)°, V = 3622.6(6) Å^3, Z = 2, ρ_{calc} = 1.369 Mg·m^{-3}, T = 293.15 K, F(000) = 1552, crystal dimensions = 0.20 × 0.10 × 0.210 mm, index range −13 < h < 13, −18 < k < 18, −31 < l < 31, collected reflections = 43186, unique reflections = 14866, refined parameters = 829, goodness-of-fit = 1.065, R factor = 0.0603, wR2 = 0.1769, residual electron density = 0.58 and −0.35 eÅ^{-3}.

In this structure, a solvent mask was calculated and 61 electrons were found in a volume of 410 Å^3 in 1 void per unit cell. This is consistent with the presence of 3[H_2O] per Formula Unit which account for 60 electrons per unit cell.

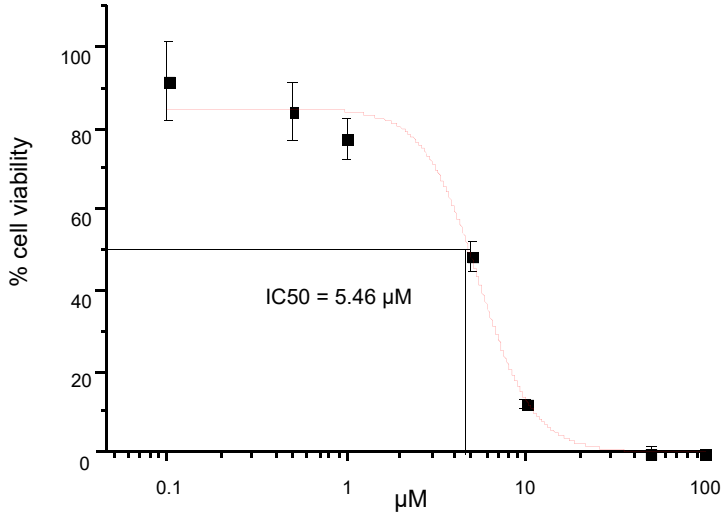

Figure S1. U937 cell viability curve after treatment with $[Cu^I(L_1)_2](HSO_4)$ (**1**) at different concentrations.

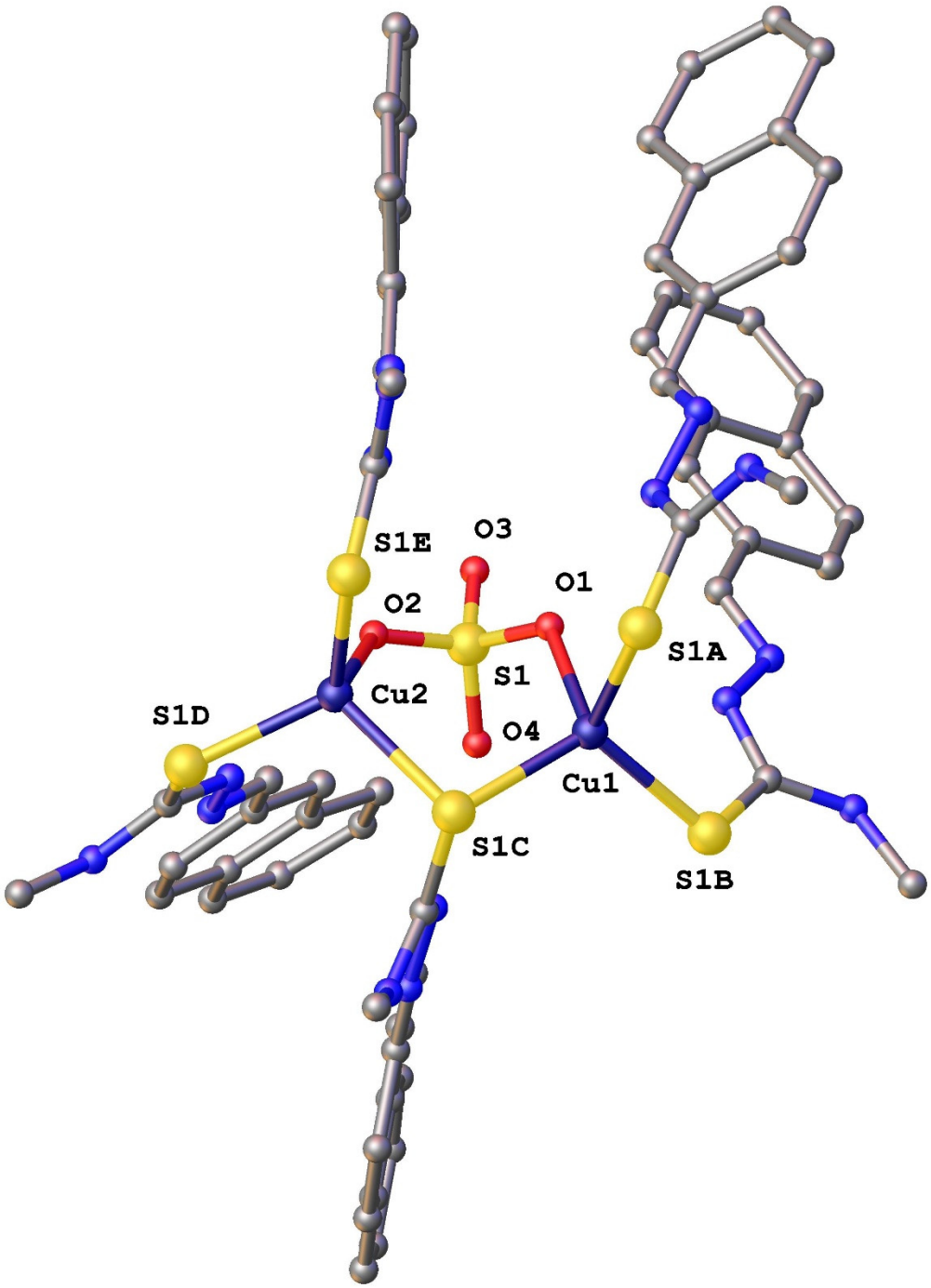

Figure S2. Representation of complex [$Cu^{I}_2(SO_4)(L_2)_5$] (**2**).