Supporting information

Guanine-Copper coordination polymers: Crystal analysis and application as thin film precursors

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Table S1: Selected hydrogen bonding distances (Å) and bond angles (°) in **1–3**.

D—H…A[#]	D…A	H…A	D—H…A
1			
N(1)—H(1)...Cl(2)	3.145(3)	2.31	163
N(2A)—H(2A1)...Cl(2)^{i}	3.435(3)	2.66	150
N(1A)—H(1A)...O(6A)^{ii}	2.891(3)	2.05	166
N(1B)—H(1B)...Cl(2)^{iii}	3.408(3)	2.56	168
N(2A)—H(2A2)...O(6B)^{ii}	2.824(4)	2.04	151
N(2)—H(2A)...Cl(3)^{iv}	3.360(3)	2.52	165
N(2)—H(2B)...O(1M)^{v}	2.983(4)	2.20	151
N(2)—H(2B1)...O(2M)^{iii}	2.930(4)	2.11	160
O(2M)—H2O2...O(6A)^{ii}	2.859(4)	2.54	104
O(1M)—H2O1...Cl(1)^{vi}	3.160(3)	2.33	166
C(8)—H(8)...Cl(1)^{vii}	3.552(3)	2.63	174
C(8A)—H(8A)...O(6)	2.950(5)	2.42	116
C(8A)—H(8A)...Cl(3)^{vii}	3.573(4)	2.75	149
C(8B)—H(8B)...Cl(3)	3.656(4)	2.78	157
C(8B)—H(8B)...O(6)	2.972(4)	2.48	113
C(11A)—H(11D)...Cl(3)^{i}	3.627(8)	2.79	150
C(11C)—H(11E)...O(1M)^{viii}	3.182(10)	2.35	149
C(11C)—H(11E)...N(9B)	2.685(11)	2.30	104
2			
N(1)—H(1)…Cl(2)^{ix}	3.201(5)	2.38	160
N(2)—H(2A)...Cl(1)	3.403(6)	2.58	160
N(2)—H(2B)...Cl(2)^{ix}	3.423(6)	2.67	147
C(8)—H(8)...Cl(1)^{x}	3.494(6)	2.69	146
C(9)—H(9B)...Cl(1)^{x}	3.616(6)	2.71	156
C(11)—H(11)...O(6)^{xi}	3.172(7)	2.24	177
3			
N(1)—H(1)…Br(2)^{xii}	3.313(8)	2.50	159
N(2)—H(2A)...Br(1)	3.470(8)	2.64	161
N(2)—H(2B)...Br(2)^{xii}	3.473(8)	2.70	150
C(8)—H(8)...Br(1)^{xiii}	3.601(9)	2.79	146
C(9)—H(9A)...Br(1)^{xiii}	3.687(9)	2.77	158
C(11)—H(11)...O(6)^{xiv}	3.212(11)	2.28	175

[#]Symmetry of A: (*i*) -1+x,y,z (*ii*) 1-x,1-y,1-z (*iii*) 2-x,1-y,1-z (*iv*) x,-1+y,z (*v*) 1+x,y,z (*vi*) -1+x,-1+y,z (*vii*) 2-x,2-y,-z (*viii*) 1+x,1+y,z (*ix*) 1–x,-y,1-z (*x*) -1+x,1/2-y,-1/2+z (x*i*) 1-x,1/2+y,3/2-z (*xii*) 1+x,y,z (*xiii*) -1+x,1/2-y,-1/2+z (*xiv*) 1-x,1/2+y,1/2-z; where A= acceptor and D= donor

Table S2: Observed bond lengths (Å) between constituent atoms.

Bond	N9-propargyl Guanine[4i]	**2**	**3**
C2-N1	1.369	1.361	1.364
C2-N2	1.335	1.337	1.332
C2-N3	1.319	1.332	1.326
C4-C5	1.387	1.366	1.366
C4-N9	1.362	1.371	1.363
C4-N3	1.351	1.356	1.367
C5-N7	1.390	1.384	1.391
C5-C6	1.408	1.417	1.421
C6-O6	1.241	1.226	1.228
C6-N1	1.393	1.403	1.401
C8-N7	1.304	1.321	1.308
C8-N9	1.380	1.375	1.376
C9-N9	1.467	1.473	1.482
C9-C10	1.456	1.484	1.470
C10-C11	1.183	1.213	1.214
Cu1-C10	------	2.053	2.066
Cu1-C11	------	2.077	2.072
Cu1-N3	------	2.052	2.051
Cu2-N7	------	1.952	1.954

Figure S1: (a) Crystal lattice of **3** when viewed along *a*-axis. (b) Corresponding bond lengths and distances (Å) in **3**.

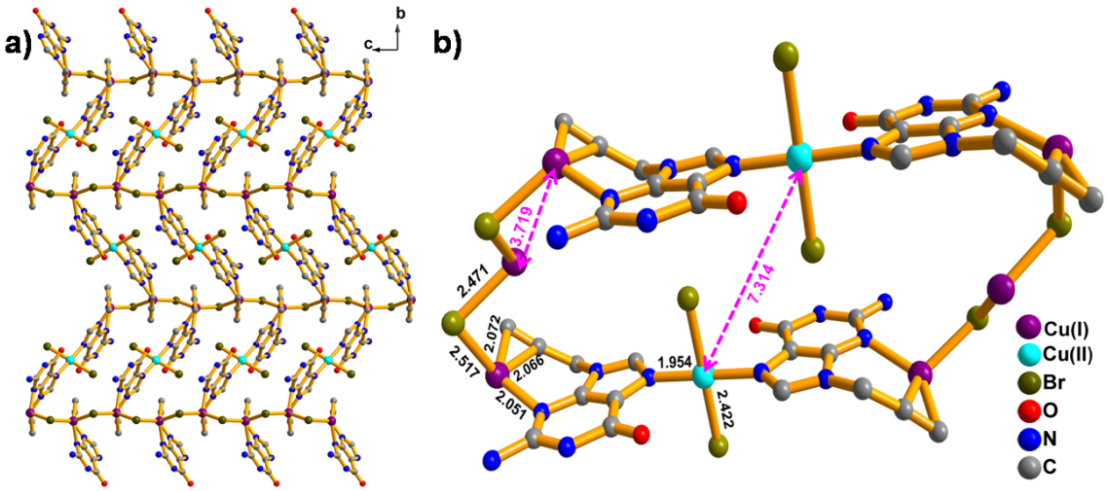


Figure S2: SEM images of thin films from **1–3** (T_1 = 450 °C; a, c, e), (T_2 = 600 °C; b, d, f). Scale: 1 μm.

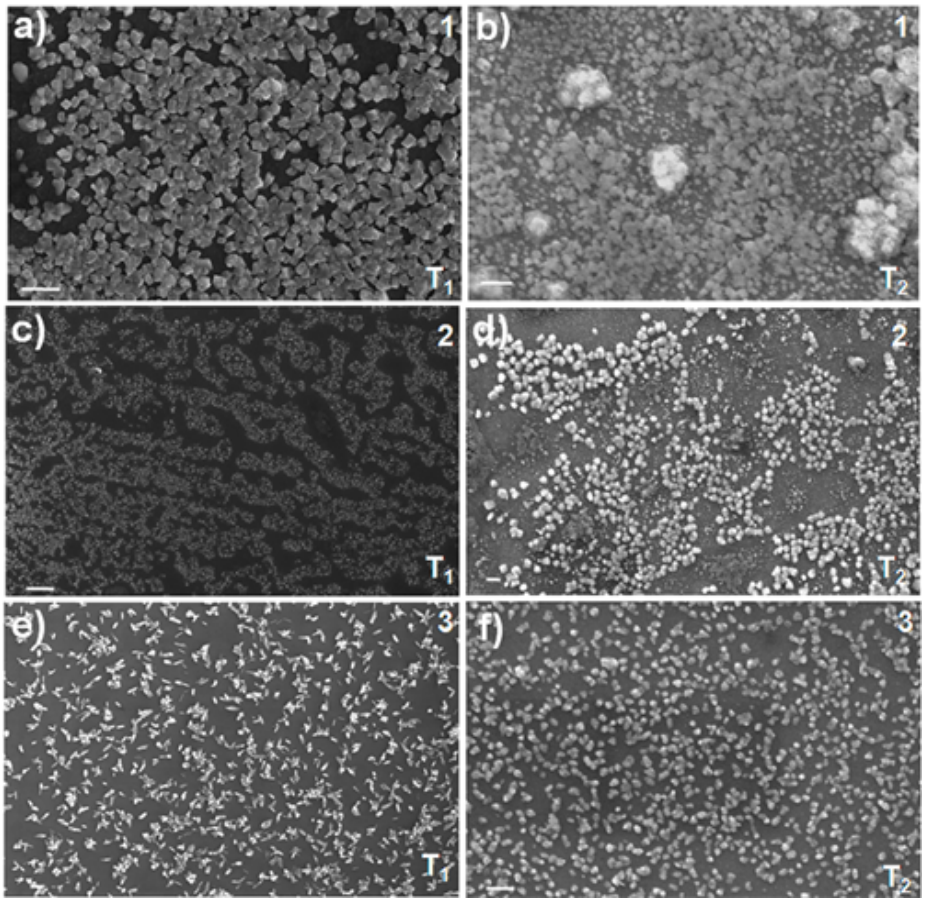


Figure S3: SEM images of thin films from $CuCl_2$, $CuBr_2$ on Si(100) (T_1 = 450 °C; a, c), (T_2 = 600 °C; b, d). scale: 2 µm.

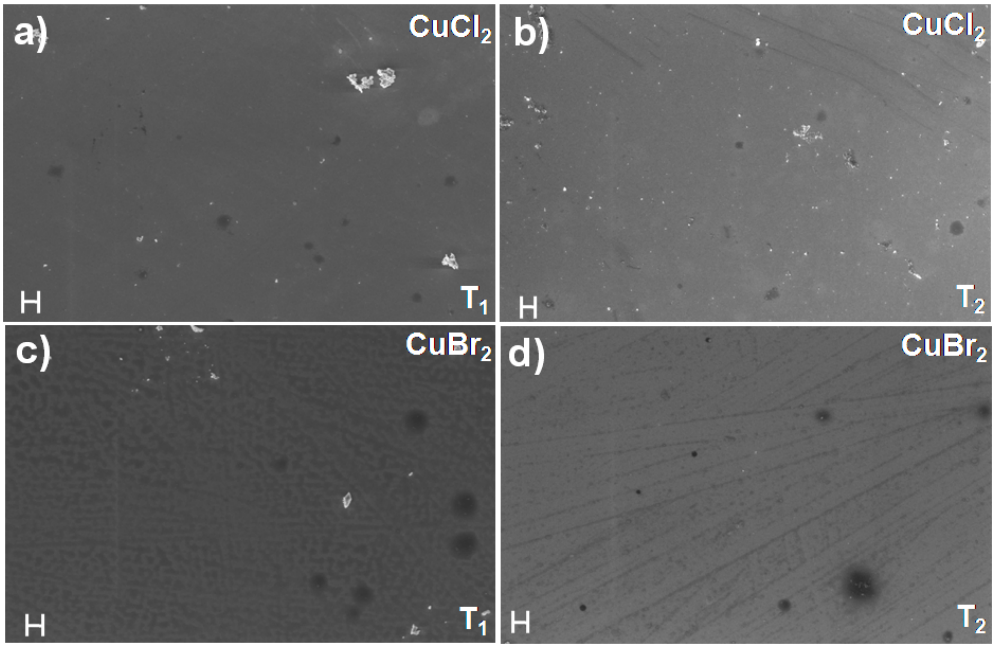


Figure S4: AFM images of thin film from **1**. (a) AFM image at T_1 [1.9×1.9 µm]. (b) AFM image at T_2 [5×5 µm]. (c & e) 3D image and diameter-height profile of panel [a] respectively. (d & f) 3D image and diameter-height profile of panel [b] respectively.

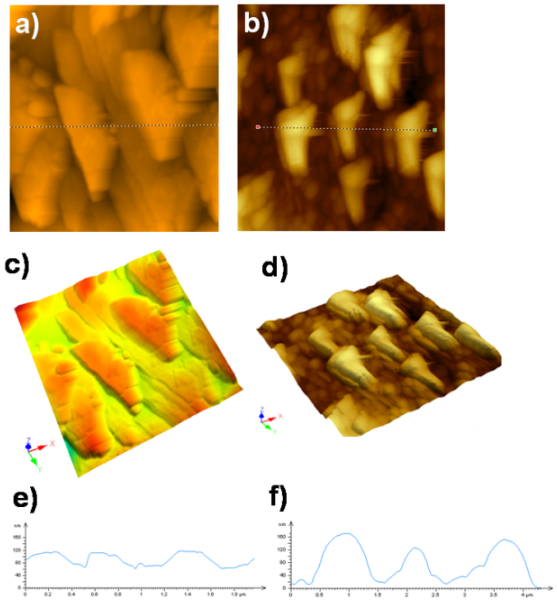


Figure S5: AFM images of thin film from **2**. (a) AFM image at T_1 [1.9×1.9 µm]. (b) AFM image at T_2 [1.3×1.3 µm]. (c & e) 3D image and diameter-height profile of panel [a] respectively. (d & f) 3D image and diameter-height profile of panel [b] respectively.

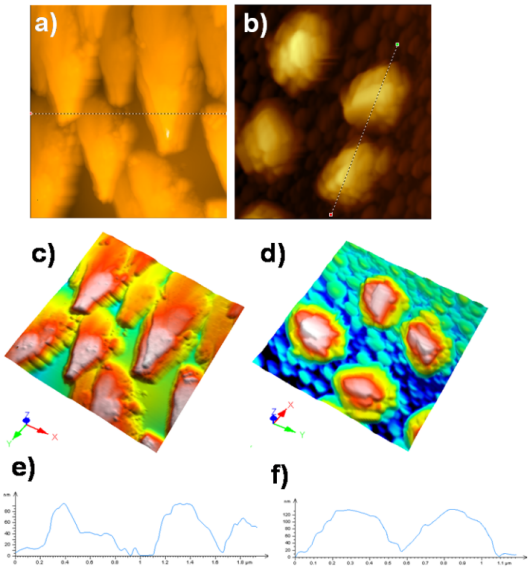


Figure S6: AFM images of thin film from **3**. (a) AFM image at T_1 [2.1×2.1 µm]. (b) AFM image at T_2 [0.9×1.3 µm]. (c & e) 3D image and diameter-height profile of panel [a] respectively. (d & f) 3D image and diameter-height profile of panel [b] respectively.

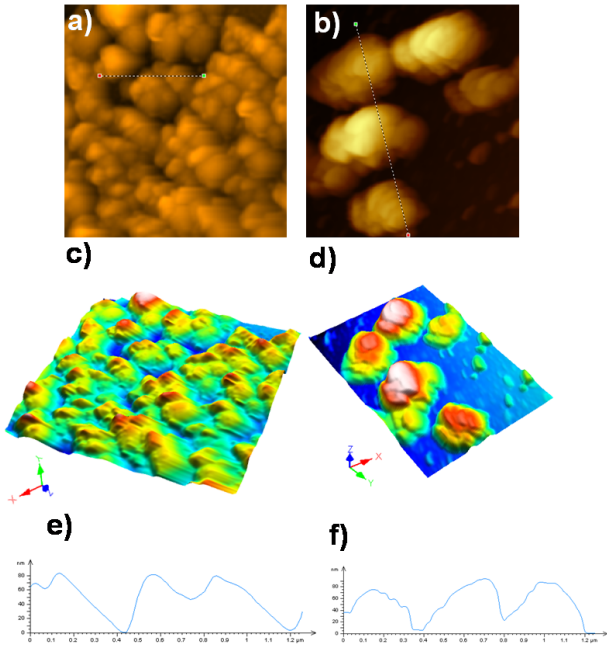


Figure S7: IR spectrum of N9-propargylguanine.

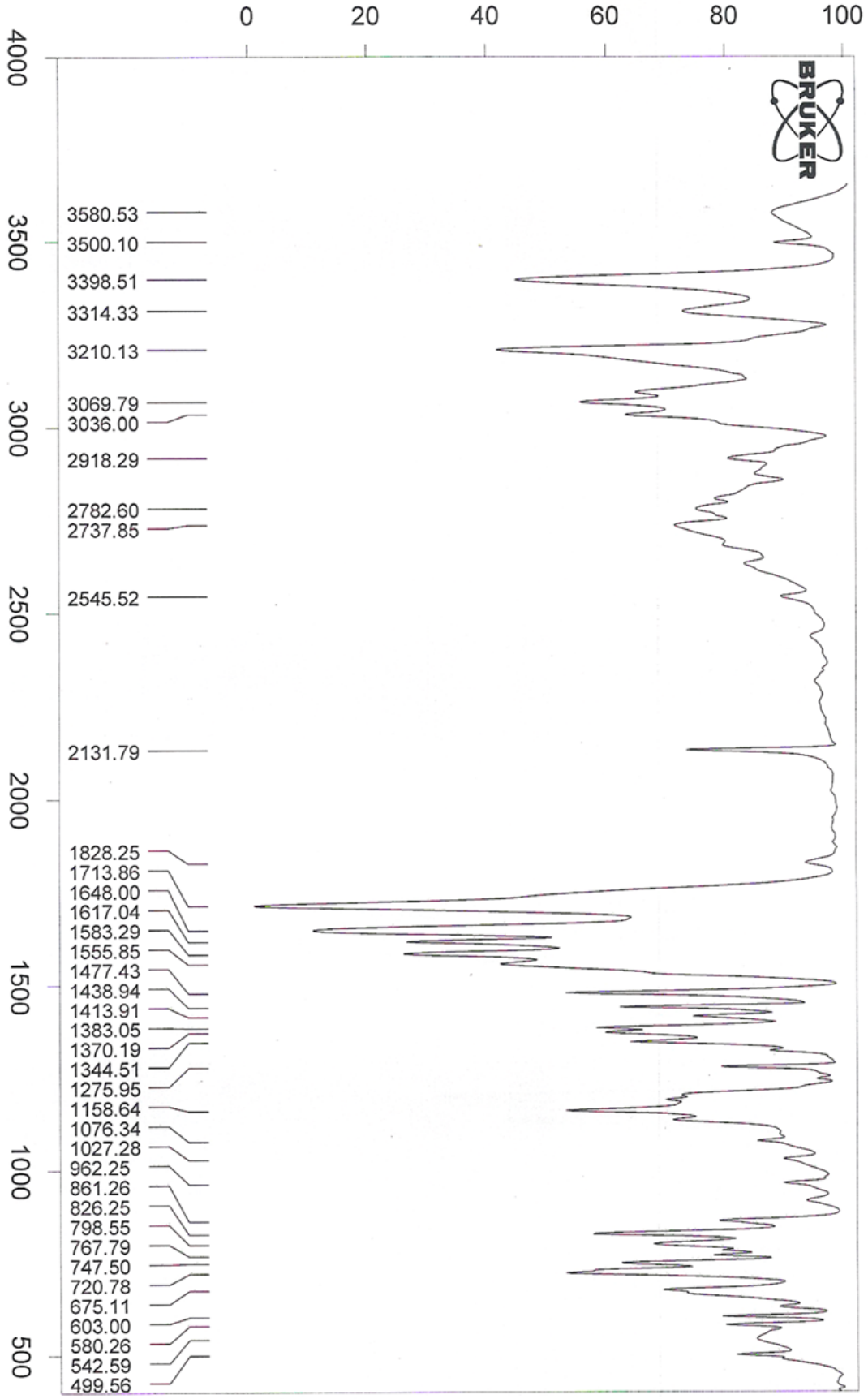


Figure S8: IR spectrum of **2**.

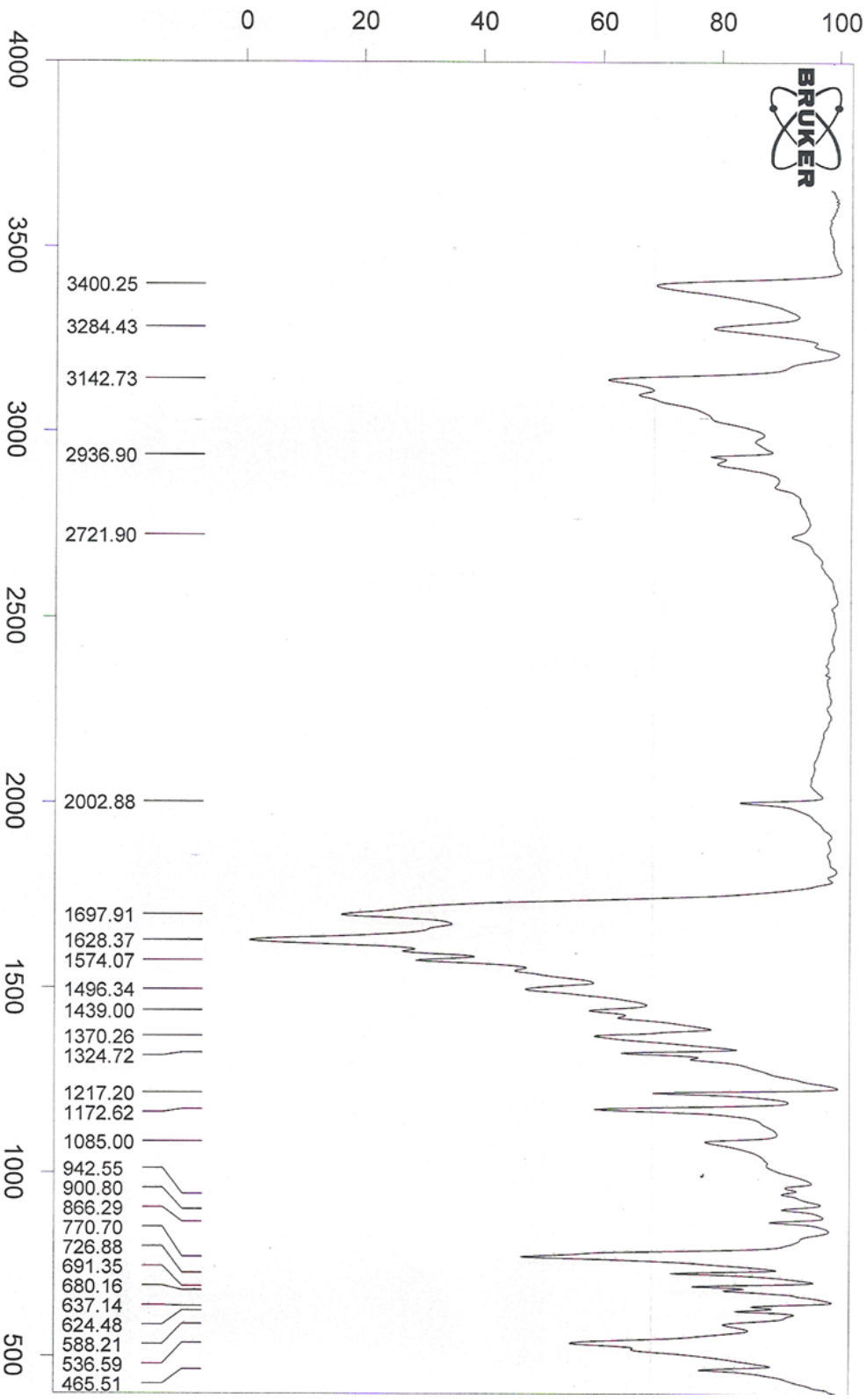


Figure S9: IR spectrum of **3**.

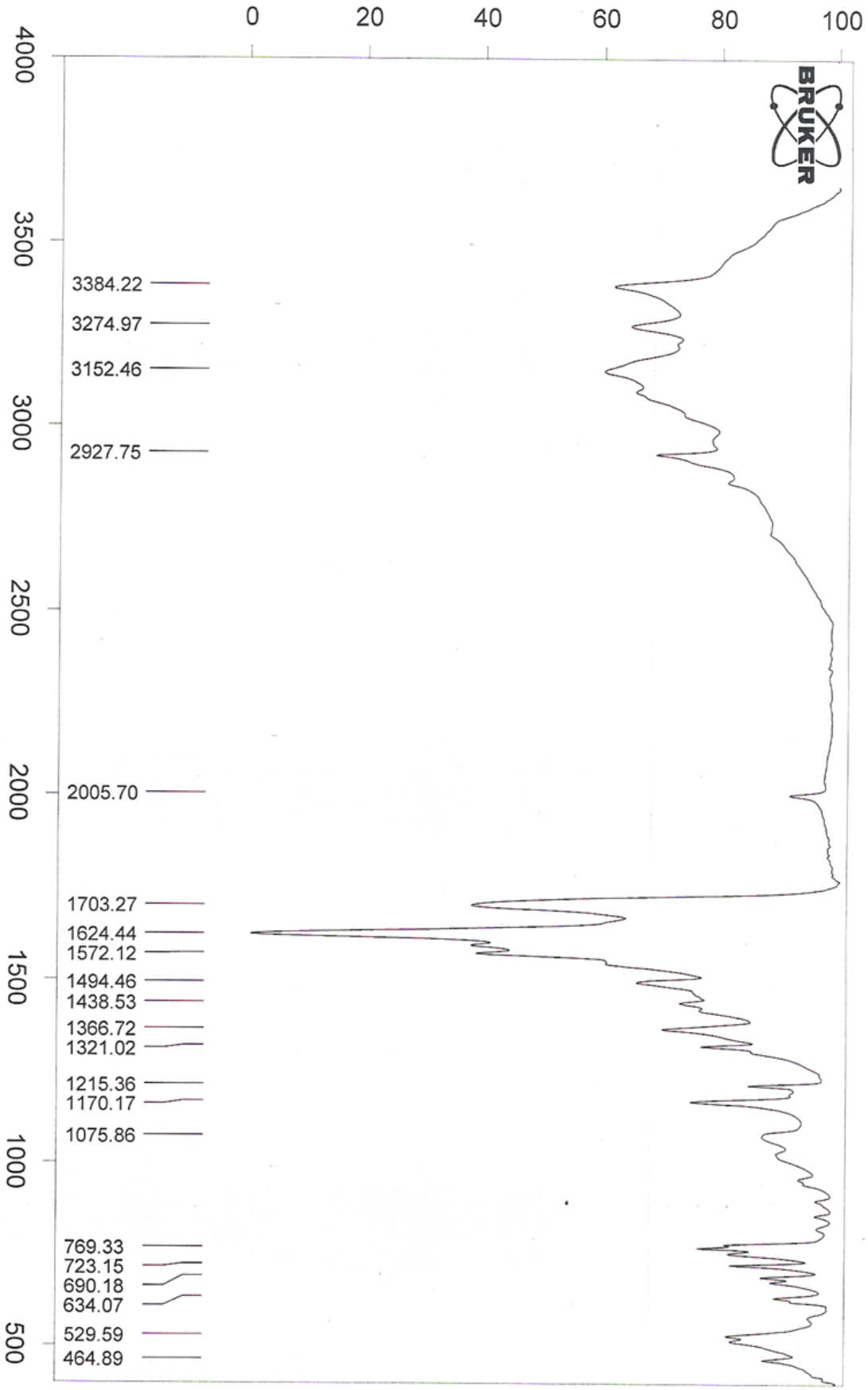


Figure S10: ESI-HRMS of **1**.

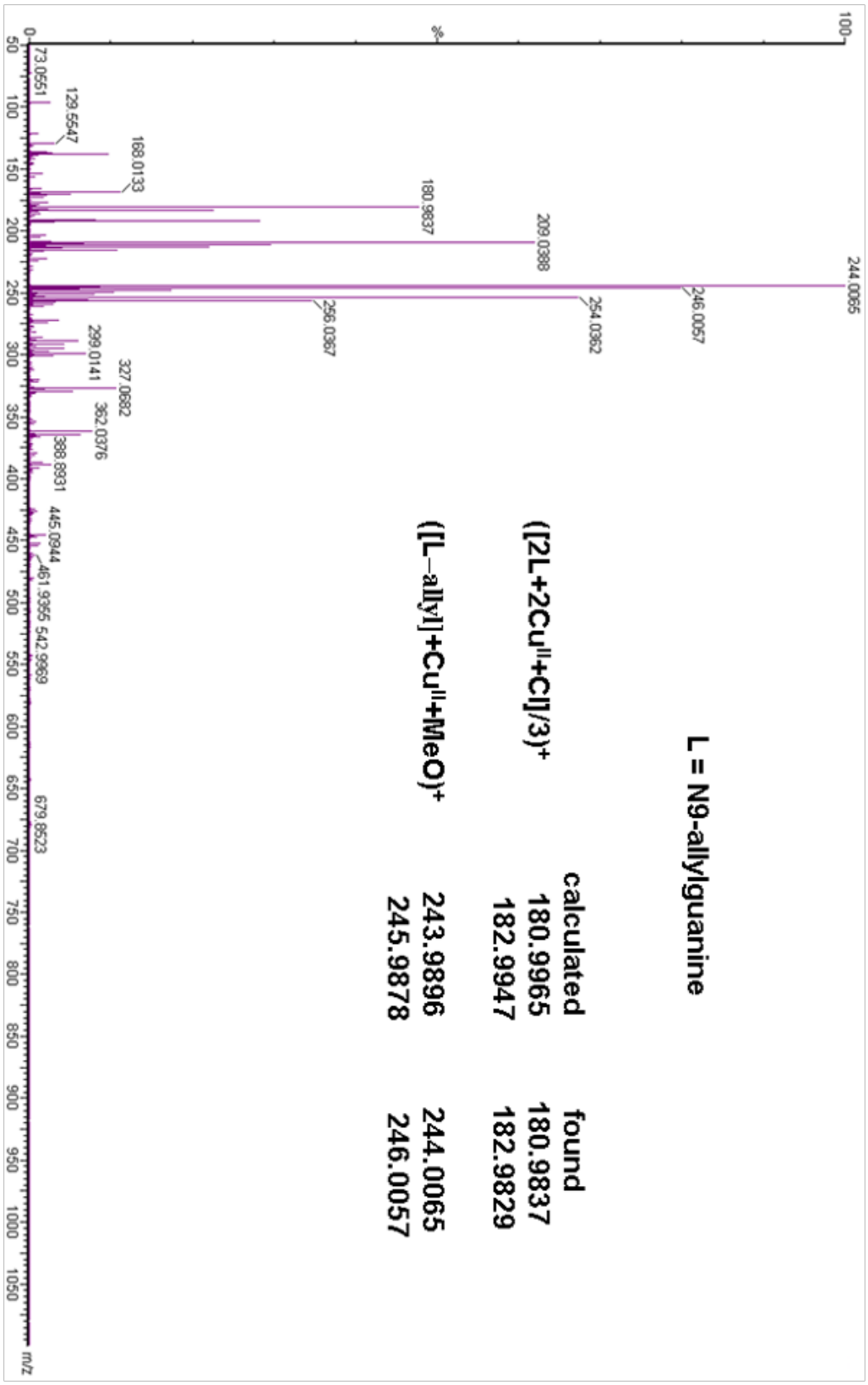


Figure S11: ESI-HRMS of **2**.

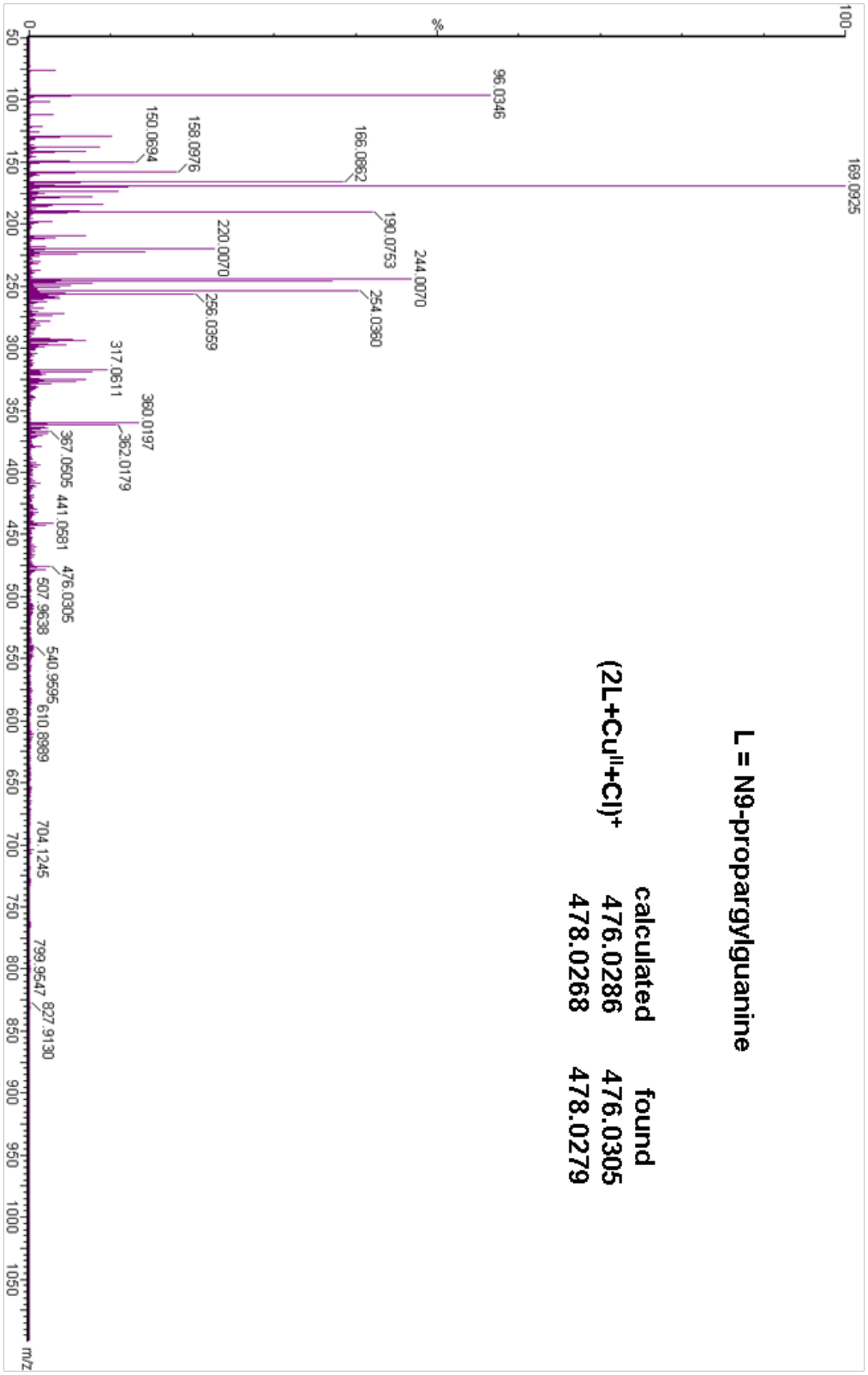


Figure S12: ESI-HRMS of **3**.

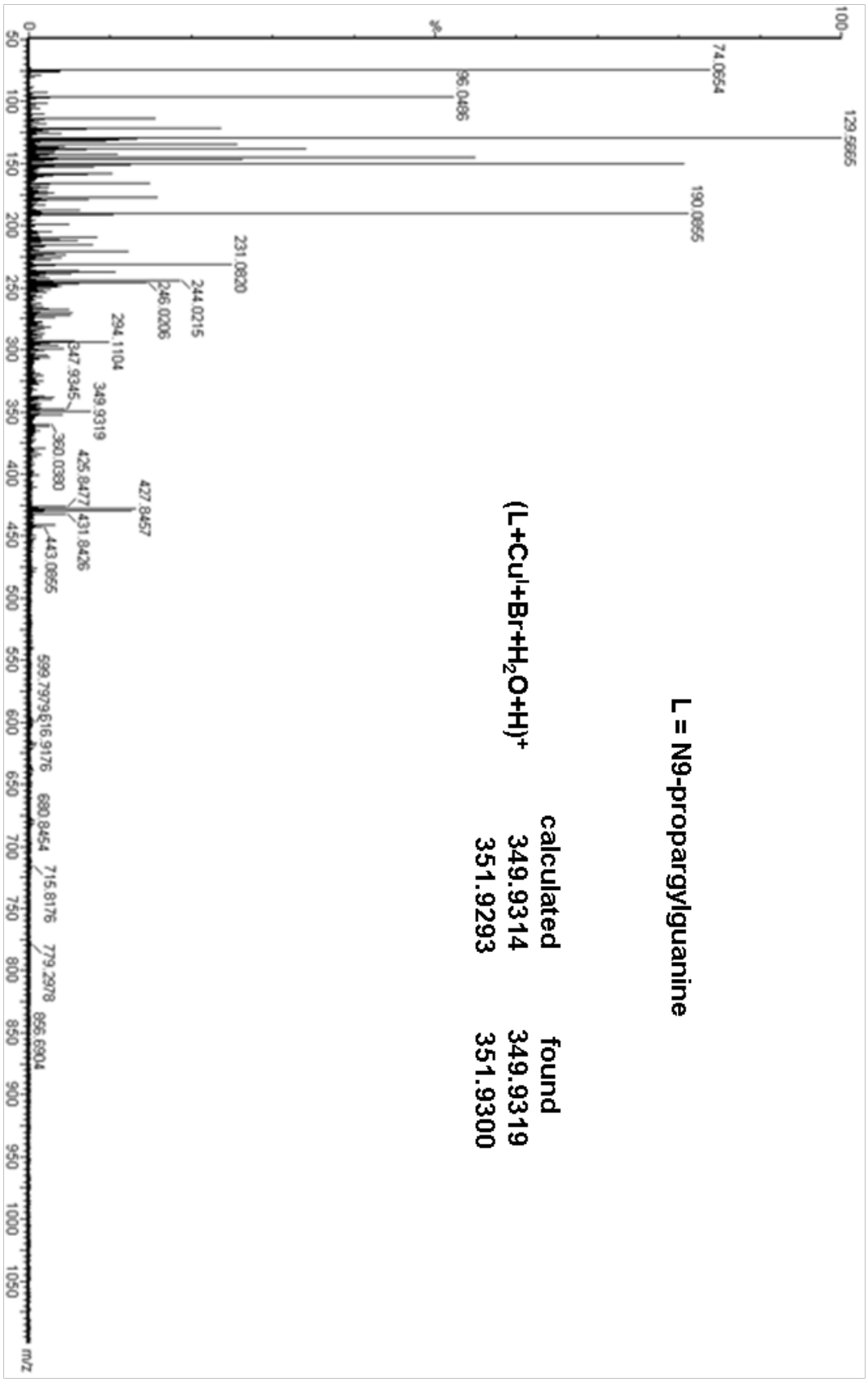
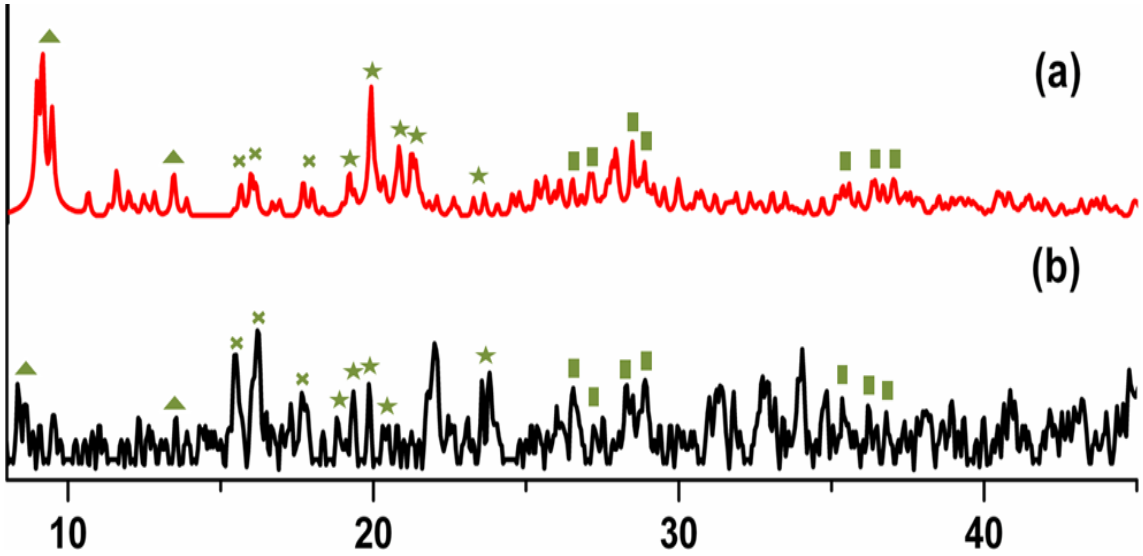
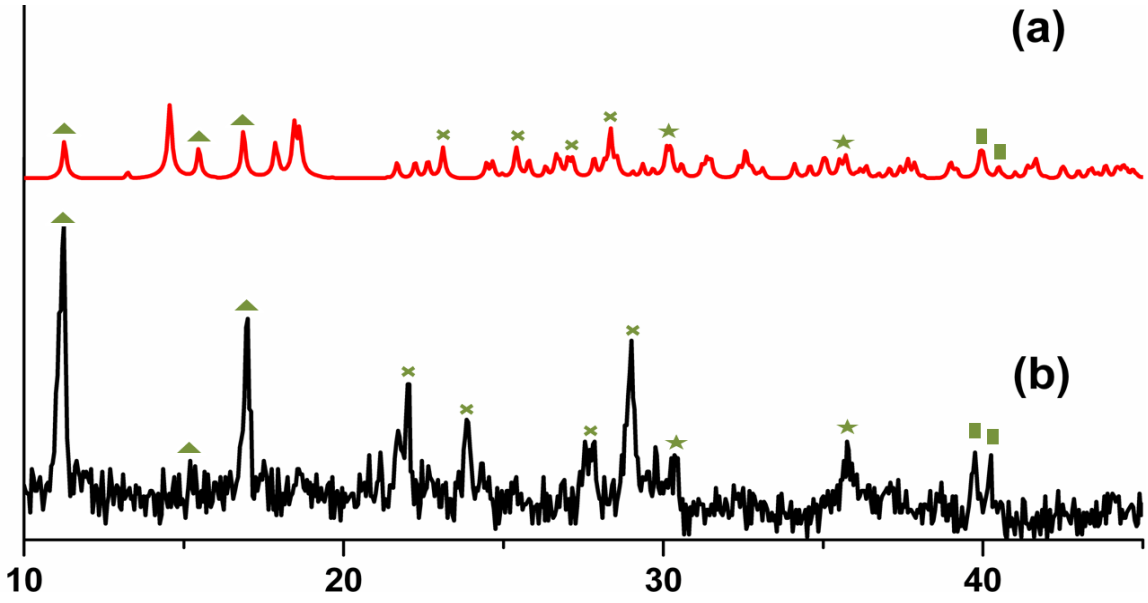


Figure S13: PXRD spectra of complexes.

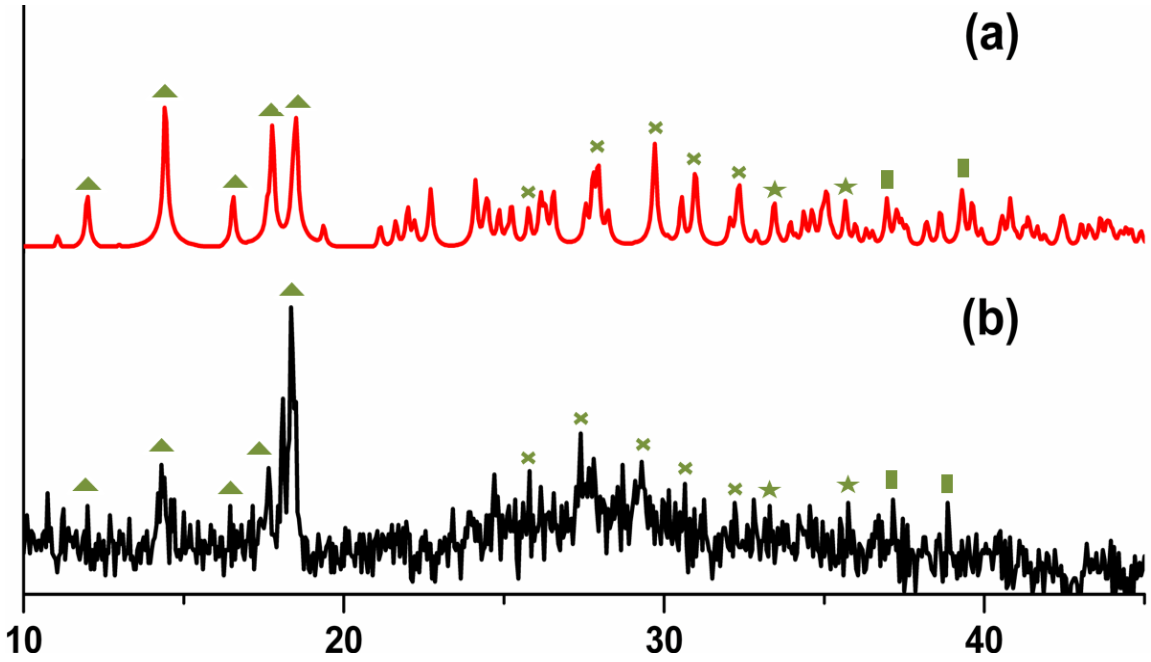
(i) PXRD pattern of **1**. (a) simulated pattern at 100 K (b) observed pattern at 298 K



(ii) PXRD pattern of **2**. (a) simulated pattern at 100 K (b) observed pattern at 298 K



(iii) PXRD pattern of **3**. (a) simulated pattern at 100 K (b) observed pattern at 298 K



The peak correspondence is marked with symbols. The reason for some of peaks are shifted may be attributed to difference in temperature for simulated and observed PXRD data, which causes a difference in the inter-planar distances, thus changing the θ values.