**Table S1**. Hydrogen bonds for $[Cu^{II}_2(Ale)_4(H_2O)_2]\cdot 2H_2O$ (Å and °)

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(5)-H(5A)...O(57)#2 | 0.91 | 2.19 | 2.942(3) | 139.4 |
| N(5)-H(5A)...O(84)#2 | 0.91 | 2.51 | 3.200(3) | 132.5 |
| N(5)-H(5B)...O(1)#2 | 0.91 | 1.95 | 2.843(4) | 168.4 |
| N(5)-H(5C)...O(4)#3 | 0.91 | 2.11 | 2.963(3) | 156.0 |
| N(66)-H(66A)...O(55)#4 | 0.91 | 2.22 | 3.103(4) | 164.0 |
| N(66)-H(66A)...O(56)#4 | 0.91 | 2.35 | 3.024(4) | 130.4 |
| N(66)-H(66B)...O(5)#5 | 0.91 | 2.19 | 2.936(4) | 138.3 |
| N(66)-H(66B)...O(2)#6 | 0.91 | 2.64 | 3.288(4) | 128.5 |
| N(66)-H(66C)...O(9)#1 | 0.91 | 2.32 | 3.069(4) | 139.2 |
| N(66)-H(66C)...O(21) | 0.91 | 2.30 | 3.058(4) | 140.7 |
| O(57)-H(57)...O(55)#4 | 0.84 | 1.77 | 2.541(3) | 152.4 |
| O(2)-H(2)...O(1)#3 | 0.84 | 1.85 | 2.510(3) | 135.0 |
| O(5)-H(5)...O(6)#7 | 0.84 | 1.87 | 2.539(3) | 135.1 |
| O(56)-H(56)...O(58)#1 | 0.84 | 1.77 | 2.535(3) | 150.0 |
| O(99)-H(1W)...O(84)#8 | 0.825(18) | 2.36(2) | 3.174(4) | 168(4) |
| O(99)-H(2W)...O(6)#7 | 0.809(18) | 2.00(2) | 2.798(3) | 170(4) |
| O(3)-H(3)...O(58) | 0.84 | 1.98 | 2.813(3) | 170.5 |

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z #2 -x+1,-y+2,-z+1 #3 -x+1, y+1/2, -z+1/2

#4 x,-y+3/2,z+1/2 #5 x-1,y,z #6 -x,y-1/2,-z+1/2

#7 -x+1,-y+2,-z #8 x,-y+3/2,z-1/2

**Table S2**. Hydrogen bonds for $[Co^{II}(Pam)_2(H_2O)_2]$ (Å and °)

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(1)-H(1C)...O(1)#2 | 0.89 | 2.35 | 3.038(7) | 134.0 |
| N(1)-H(1C)...O(4)#3 | 0.89 | 2.32 | 3.107(7) | 147.0 |
| N(1)-H(1A)...O(2)#4 | 0.89 | 2.14 | 2.977(7) | 155.4 |
| N(1)-H(1A)...O(7)#5 | 0.89 | 2.60 | 3.125(7) | 118.9 |
| N(1)-H(1B)...O(6)#6 | 0.89 | 2.30 | 3.085(6) | 147.1 |
| N(1)-H(1B)...O(3)#7 | 0.89 | 2.61 | 3.239(7) | 128.2 |
| O(7)-H(71)...O(6)#3 | 0.91(8) | 1.89(8) | 2.743(6) | 156(7) |
| O(7)-H(72)...O(8)#4 | 0.84(9) | 2.13(9) | 2.889(6) | 150(8) |
| O(7)-H(72)...O(5)#1 | 0.84(9) | 2.51(8) | 2.911(7) | 111(7) |
| O(8)-H(8)...O(1)#8 | 0.82 | 2.14 | 2.850(6) | 145.3 |
| O(8)-H(8)...O(5) | 0.82 | 2.68 | 3.124(6) | 115.9 |
| O(2)-H(2)...O(6)#9 | 0.82 | 2.11 | 2.509(6) | 109.8 |
| O(5)-H(5)...O(3)#8 | 0.82 | 1.86 | 2.473(6) | 130.3 |

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 x+1,y,z #3 -x+1,-y+1,-z+1

#4 -x+1/2,y-1/2,-z+3/2 #5 x+1/2,-y+1/2,z+1/2

#6 -x+3/2,y-1/2,-z+3/2 #7 -x+1,-y+1,-z+2 #8 -x+1/2,y+1/2,-z+3/2

#9 x-1/2,-y+3/2,z+1/2

**Table S3**. Hydrogen bonds for $[Ni(Pam)_2(H_2O)_2]$ (Å and °).

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| O(9)-H(14)...O(7)#2 | 0.98(7) | 1.55(7) | 2.522(3) | 173(6) |
| O(6)-H(13)...O(8) | 0.86(6) | 2.75(6) | 3.105(3) | 106(4) |
| O(6)-H(13)...O(2)#3 | 0.86(6) | 2.04(6) | 2.840(3) | 155(5) |
| O(3)-H(12)...O(7)#4 | 0.97(5) | 1.81(5) | 2.741(3) | 160(4) |
| N(1)-H(1C)...O(1)#4 | 0.89 | 2.36 | 3.122(4) | 143.4 |
| N(1)-H(1C)...O(2)#5 | 0.89 | 2.30 | 3.032(4) | 138.8 |
| N(1)-H(1A)...O(7)#6 | 0.89 | 2.30 | 3.081(4) | 147.2 |
| N(1)-H(1B)...O(3)#7 | 0.89 | 2.65 | 3.148(4) | 116.5 |
| N(1)-H(1B)...O(9)#8 | 0.89 | 2.12 | 2.971(4) | 159.4 |
| O(3)-H(3)...O(8)#1 | 0.73(5) | 2.51(5) | 2.921(3) | 117(5) |
| O(3)-H(3)...O(6)#8 | 0.73(5) | 2.25(5) | 2.887(3) | 145(5) |
| O(8)-H15…O(5)#2 | 1.20(4) | 1.27(4) | 2.464(3) | 171(5) |

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z  #2 x-1/2,-y+3/2,z+1/2  #3 -x+1/2,y-1/2,-z+1/2

#4 -x+1,-y+2,-z  #5 x+1,y,z  #6 -x+3/2,y+1/2,-z+1/2

#7 x+1/2,-y+5/2,z+1/2  #8 -x+1/2,y+1/2,-z+1/2

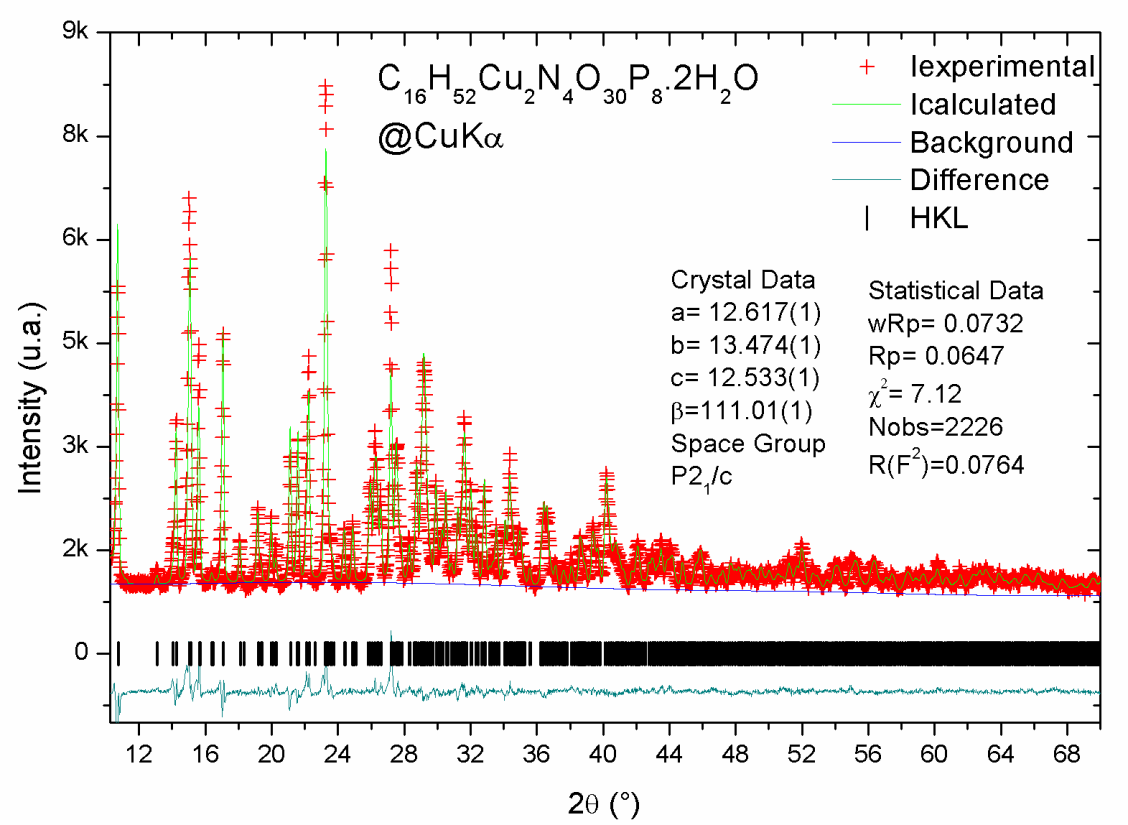


**Figure S1**- Rietveld refinement for the $C_{16}H_{52}Cu_2N_4O_{30}P_8 \cdot 2H_2O$ compound, indicating the experimental data, the calculated intensities, the background function, the difference curve and the Bragg positions.

**Table S4**. Level of BSA binding of the complexes after 48 h incubation

| Compound | Interaction with BSA(%) | Compound | Interaction with BSA(%) |
|---|---|---|---|
| $([Cu^{II}(Pam)]\cdot H_2O)_n$ | 98 | $[Cu^{II}_2(Ale)_4(H_2O)_2]$ | 94 |
| $[Co^{II}(Pam)_2(H_2O)_2]$ | 76 | $[Co^{II}_2(Ale)_4(H_2O)_2]$ | 54 |
| $[Ni^{II}(Pam)_2(H_2O)_2]$ | 91 | $[Ni^{II}_2(Ale)_4(H_2O)_2]$ | 88 |
| $[Mn^{II}(Pam)_2(H_2O)_2]$ | 0 | $[Mn^{II}_2(Ale)_4(H_2O)_2]$ | 52 |