Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

A novel triple aqua, phenoxo and carboxylato bridged dinickel(II) complex and its magnetic and comparative biomimetic catalytic studies with analogous dinickel(II) complexes

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Table S1. Selected bond angles (°) for complexes **1–3**.

Bond Angles	**1**	**2**	**3**
Ni1–O1–Ni2	101.77(6)	100.30(4)	104.72(6)
Ni1–O2–Ni2	106.32(7)	101.25(4)	93.30(6)
O2–Ni1–N1	152.58(6)	166.87(4)	164.45(6)
O2–Ni1–O1	76.02(5)	78.19(4)	77.60(6)
N1–Ni1–O1	89.36(6)	88.69(4)	86.93(6)
O2–Ni1–N2	91.31(6)	97.73(4)	99.62(6)
N1–Ni1–N2	96.44(6)	95.37(4)	95.71(7)
O1–Ni1–N2	161.53(6)	172.59(4)	175.29(6)
O2–Ni1–N3	100.94(6)		
N1–Ni1–N3	104.31(6)		
O1–Ni1–N3	99.41(6)		
N2–Ni1–N3	96.14(6)		
N1–Ni1–N7		89.56(5)	
O2–Ni1–N7		91.49(4)	
N7–Ni1–O1		96.62(4)	
N7–Ni1–N2		89.63(5)	
N1–Ni1–N8		87.76(5)	
O2–Ni1–N8		92.22(4)	
N7–Ni1–N8		174.46(5)	
O1–Ni1–N8		88.16(4)	
N2–Ni1–N8		85.81(5)	
O3–Ni1–O1			92.47(6)
O3–Ni1–N1			88.49(6)
O3–Ni1–O5			178.62(6)
O1–Ni1–O5			88.90(6)
N1–Ni1–O5			91.38(6)
O3– Ni1–N2			91.50(7)
O5–Ni1–N2			87.14(7)
O3–Ni1–O2			93.75(6)
O5–Ni1–O2			86.75(6)
O2–Ni2–O1	75.85(5)	80.20(4)	76.01(6)
O2–Ni2–N4	155.36(6)	169.01(4)	94.45(7)
O1–Ni2–N4	88.62(6)	89.52(4)	86.99(6)
O2–Ni2–N5	91.25(6)	97.41(4)	89.45(7)
O1–Ni2–N5	158.47(6)	107.51(4)	165.26(7)
N4– Ni2–N5	97.10(7)	89.37(5)	96.63(7)
O2–Ni2–N6	101.22(6)		169.83(6)
O1–Ni2–N6	102.27(6)		100.01(6)
N4–Ni2–N6	100.71(6)		94.68(7)
N5–Ni2–N6	97.05(7)		93.94(7)
N4–Ni2–N9		94.40(5)	
N9–Ni2–O1		152.74(4)	
N9–Ni2–O2		93.01(4)	
N9–Ni2–N5		99.51(5)	
O1–Ni2–O4			90.10(6)
N4–Ni2–O4			176.60(7)
O4–Ni2–N5			85.75(7)
O4–Ni2–N6			87.56(6)
O4–Ni2–O2			83.12(6)

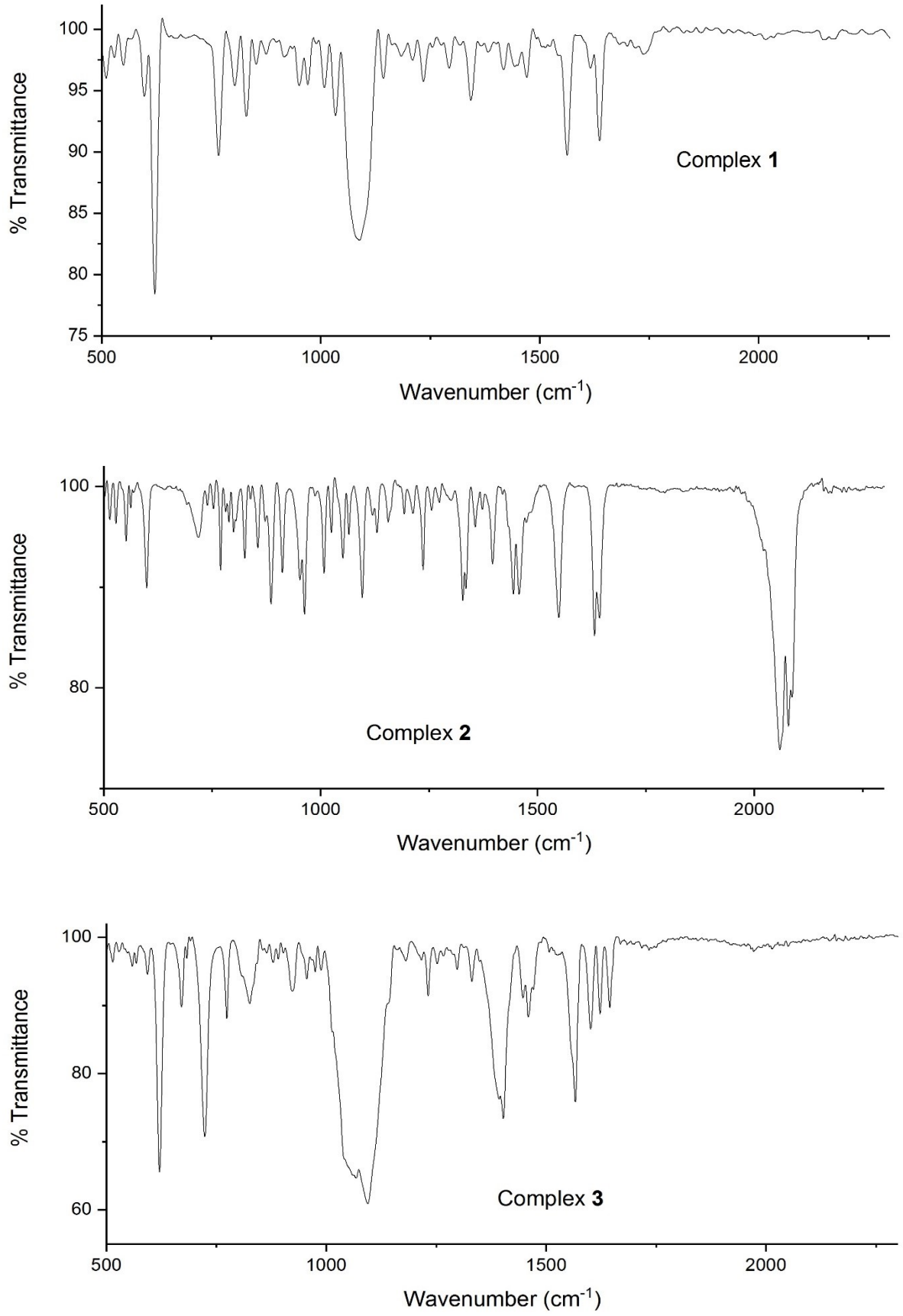

Fig.S1. IR spectra of complexes **1**–**3**.

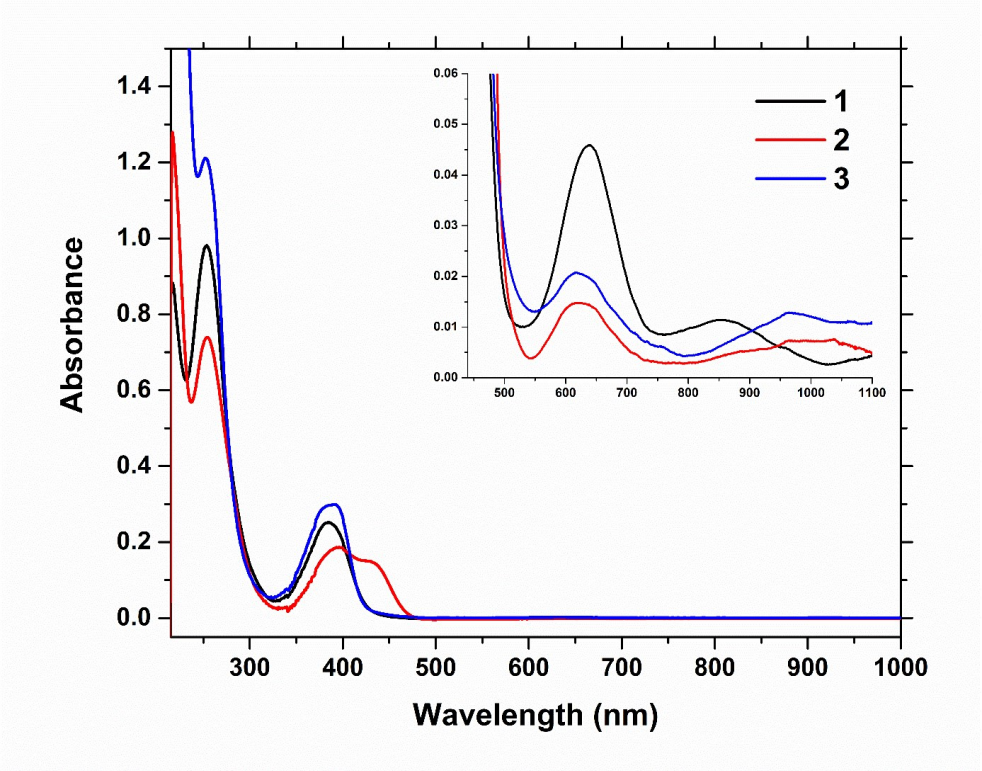

Fig. S2. UV-Vis Spectra of the complexes **1–3** at [Complex] = $5x10^{-5}$ (M) whereas the inset spectra were recorded at [Complex] = $1x10^{-3}$ (M).

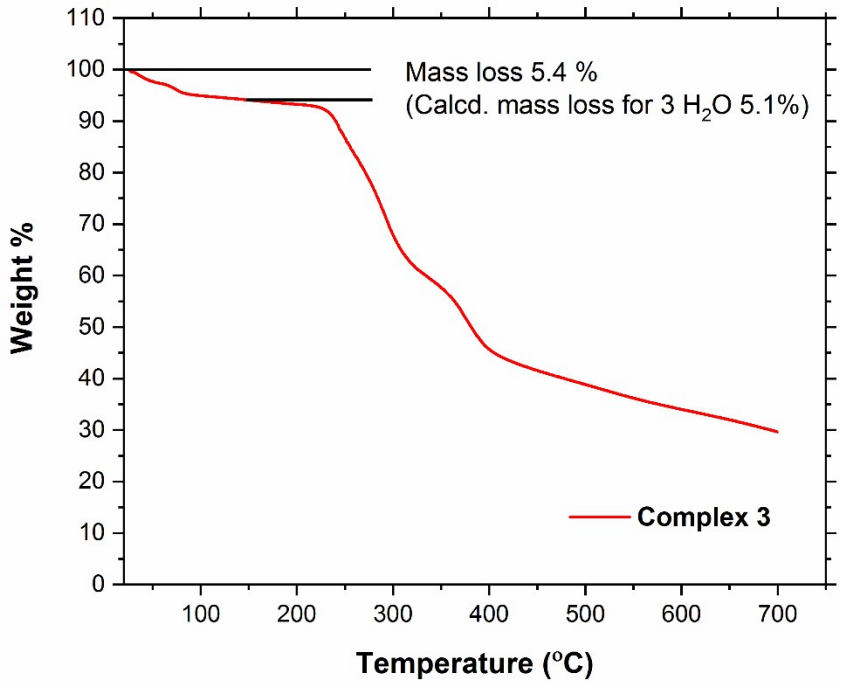

Fig. S3. TGA plot for complex **3**.

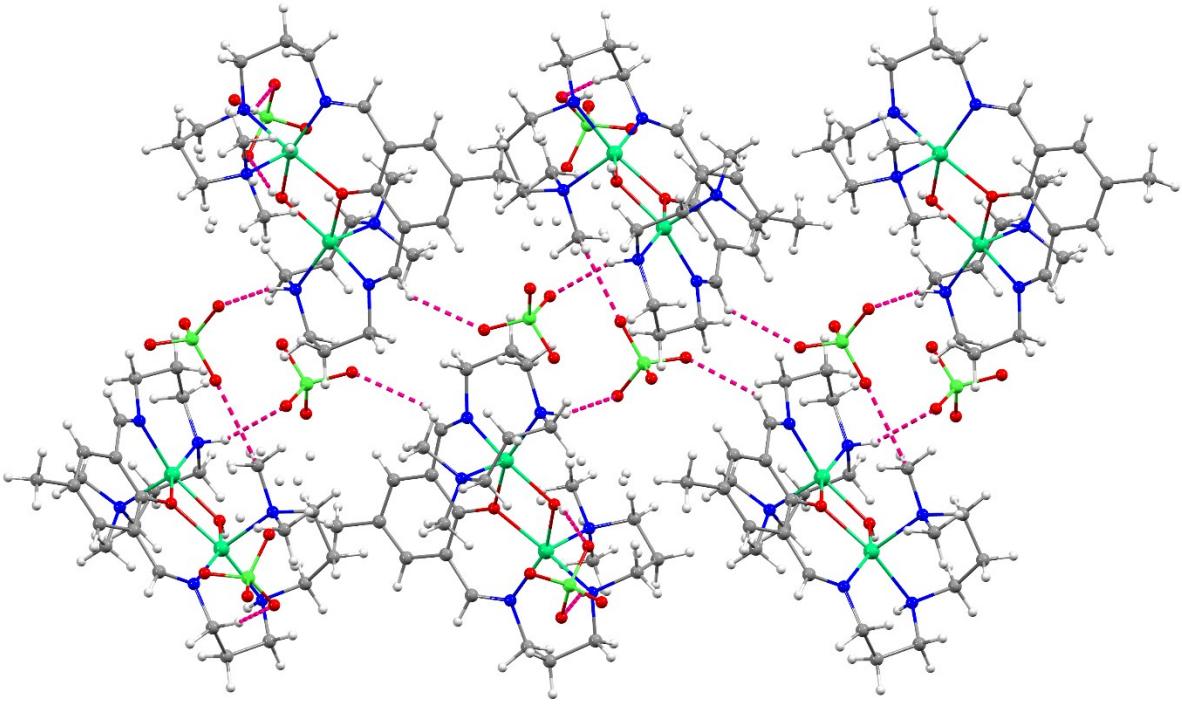

Fig. S4. The crystal packing of complex **1** displaying different hydrogen bonding interactions.

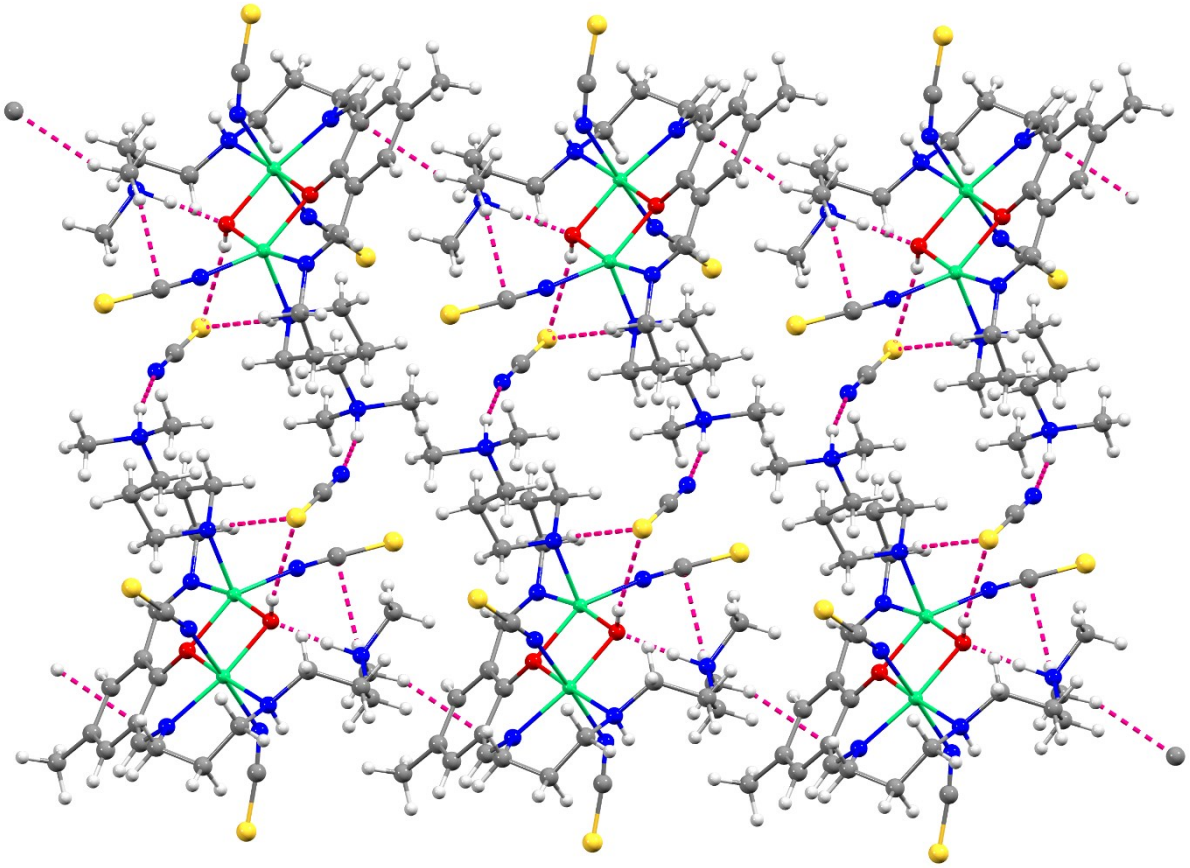

Fig. S5. The crystal packing of complex **2** displaying different weak non-covalent interactions.

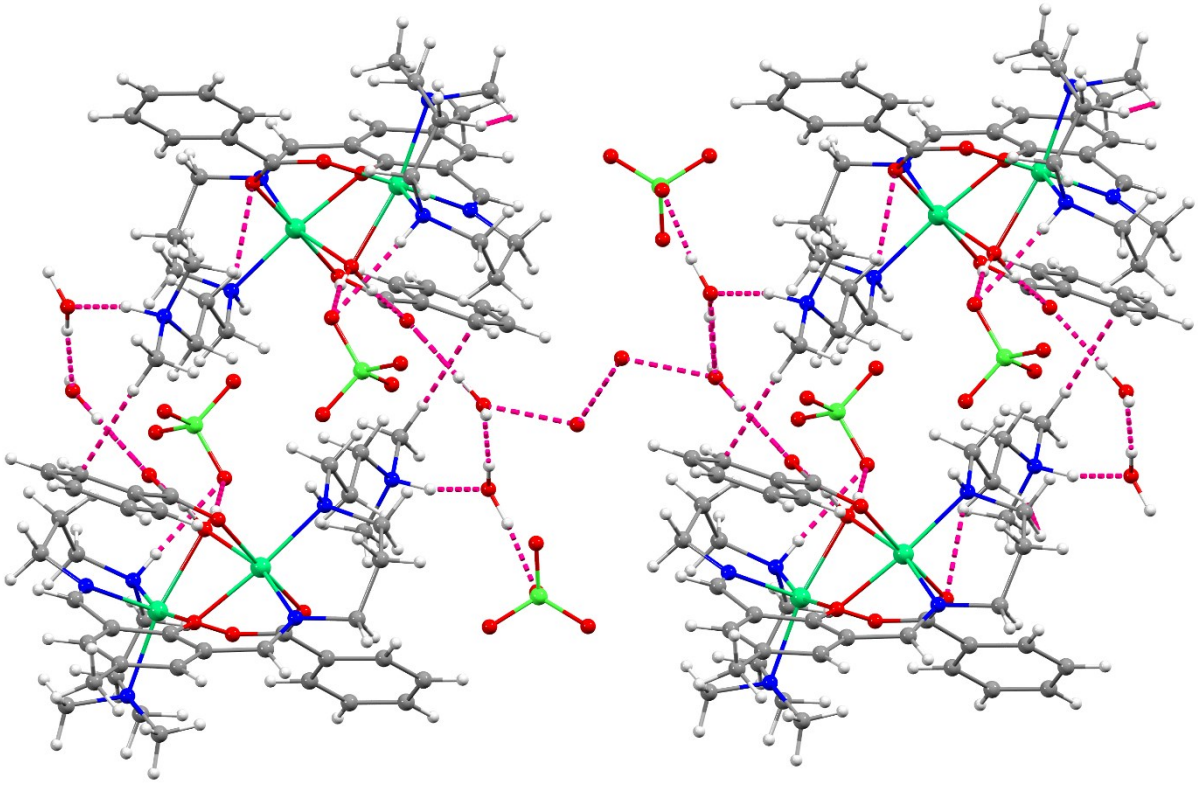

Fig. S6. The crystal packing of complex **3** displaying different hydrogen bonding interactions.

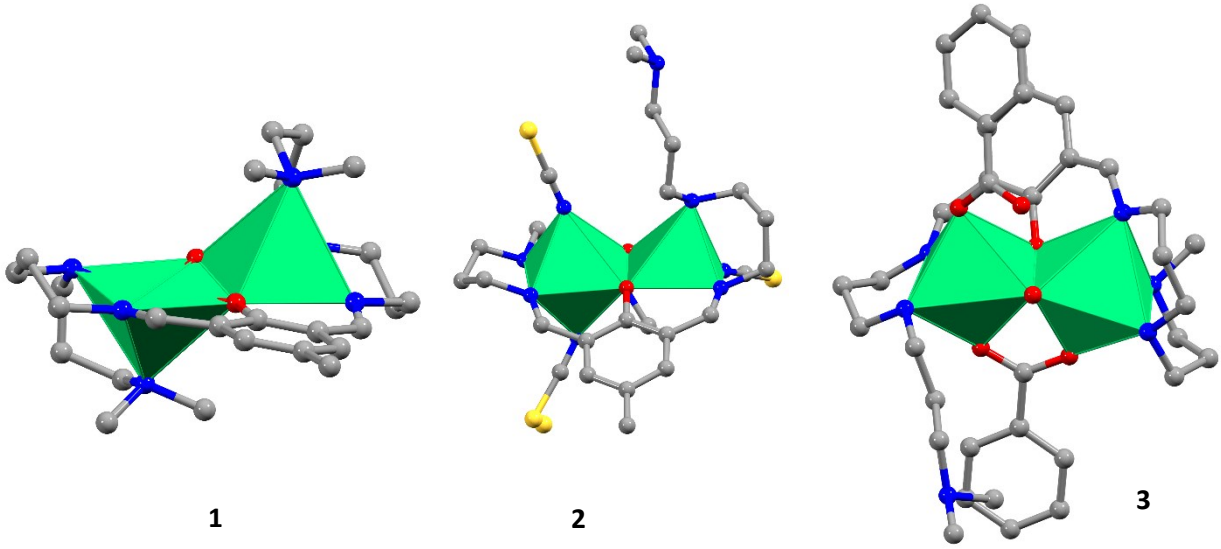

Fig. S7. Crystal structures of **1–3** showing edge sharing bi-polyhedral structures and hydrogen atoms have been omitted for clarity.

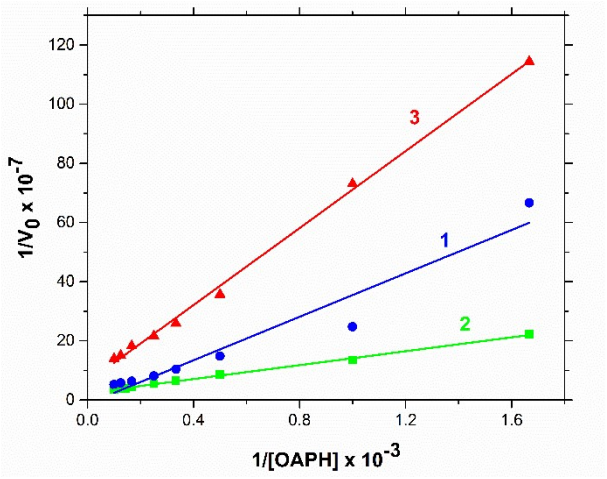

Fig. S8. Linear Lineweaver–Burk plots for the oxidation of *o*-aminophenol catalysed by **1-3**. Symbols and solid lines represent experimental and simulated profiles, respectively.

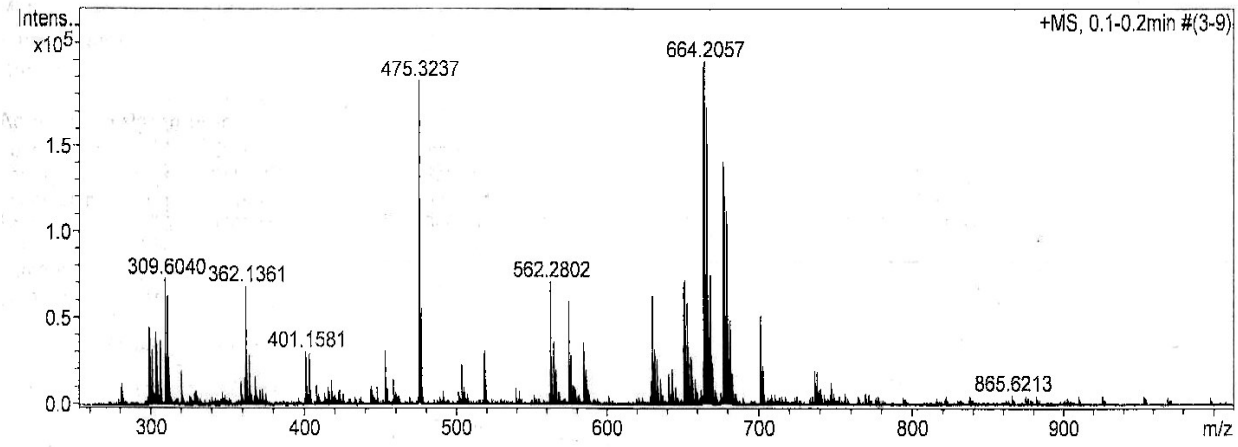

Fig. S9. Electrospray ionization mass spectrum (ESI-MS positive) of **2.**

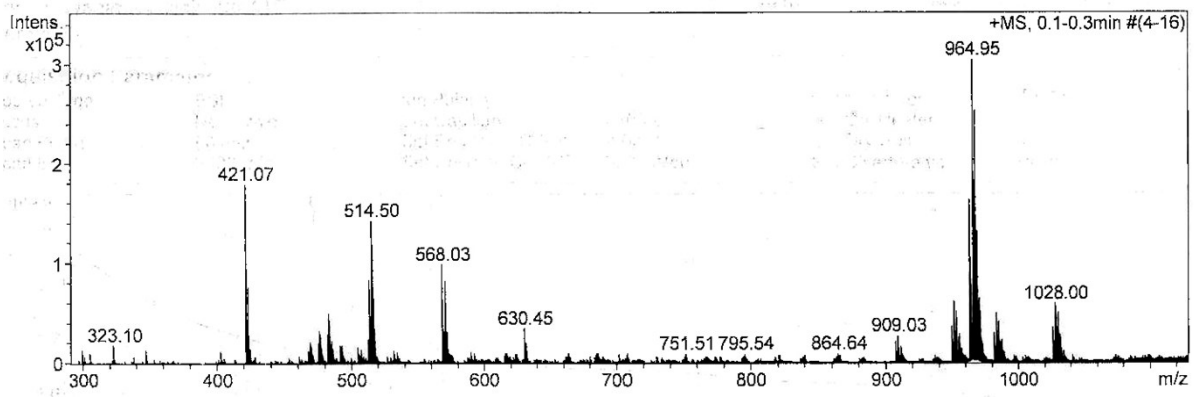

Fig. S10. Electrospray ionization mass spectrum (ESI-MS positive) of a 1:50 mixture of **2** and OAPH in methanol recorded after 10 min of mixing.