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

Supporting Information

The first report of a tetra-azide bound mononuclear cobalt(III) complex and its comparative biomimetic catalytic activity with tri-azide bound cobalt(III) compounds

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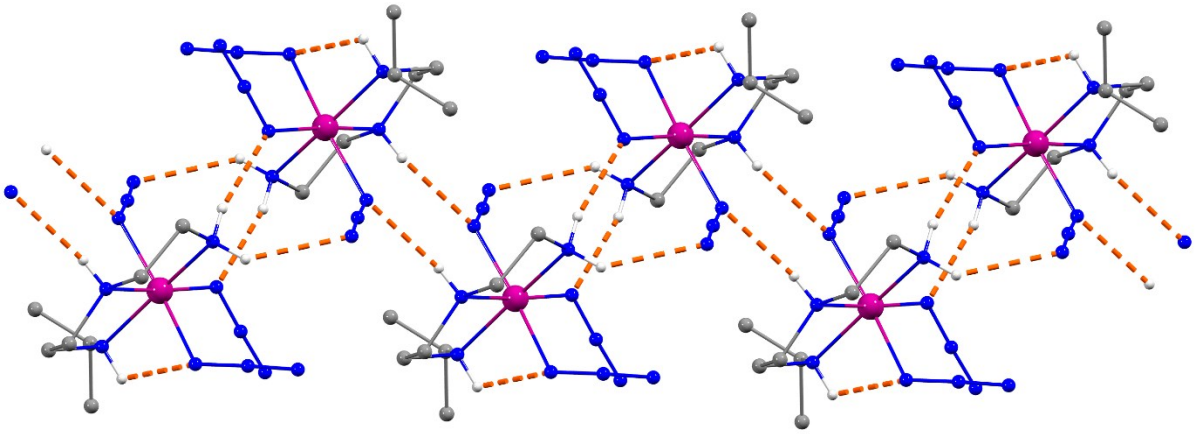

Fig. S1. Hydrogen bonded supramolecular chain structure of **2** propagating along the *a* axis.

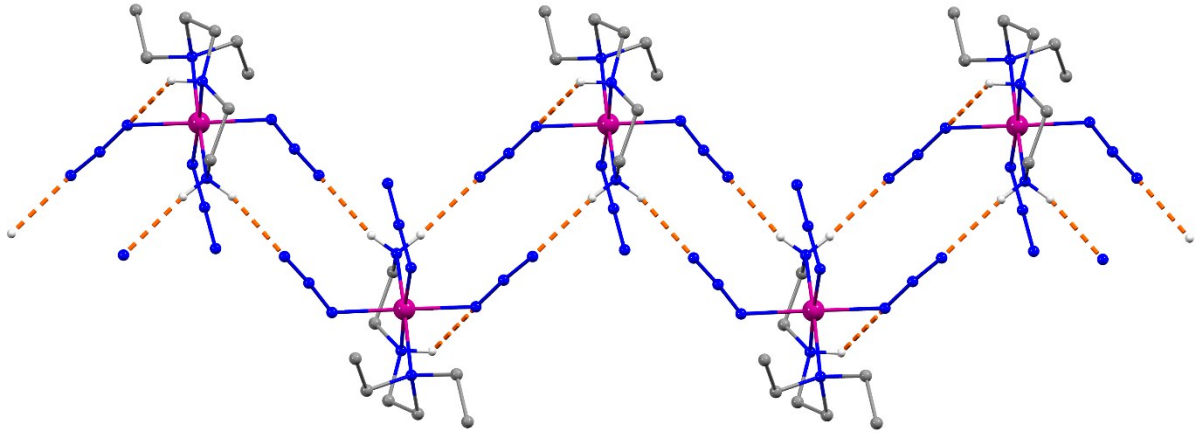

Fig. S2. Hydrogen bonded zig-zag supramolecular chain structure of **3** propagating along the *c* axis.

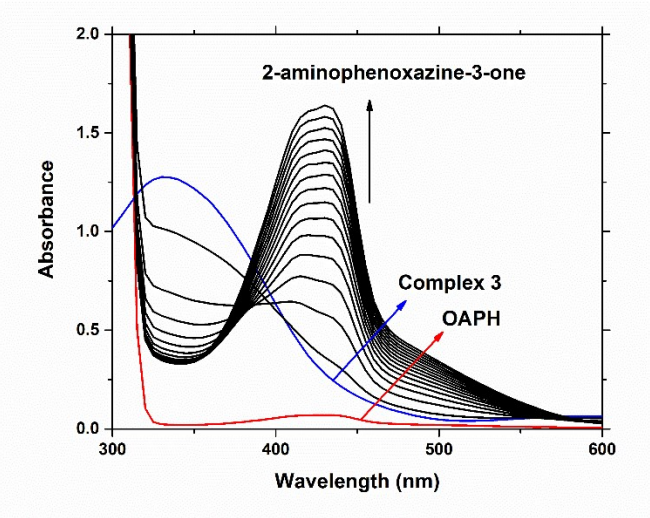

Fig. S3. The time resolved spectral profile showing oxidation of *o*-aminophenol (1.0×10^{-2} M) catalysed by **3** (1×10^{-5} M) in dioxygen-saturated methanol. The spectra were recorded at 5 min intervals under aerobic conditions at room temperature.

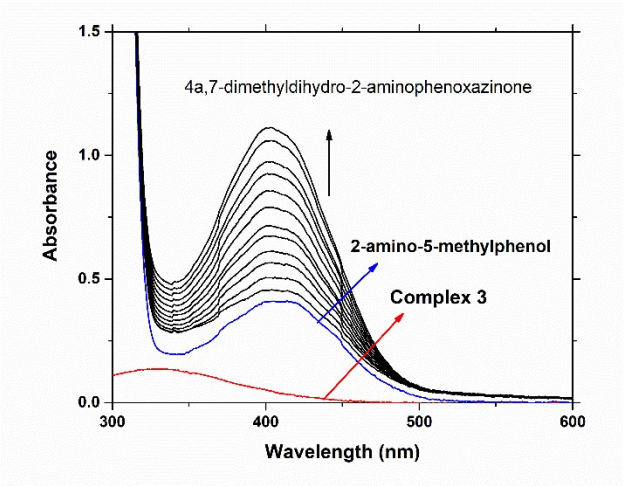

Fig. S4. The time resolved spectral profile showing oxidation of 2-amino-5-methylphenol (5×10^{-3} M) catalysed by **3** (2×10^{-5} M) in dioxygen-saturated methanol. The spectra were recorded at 5 min intervals under aerobic conditions at room temperature.

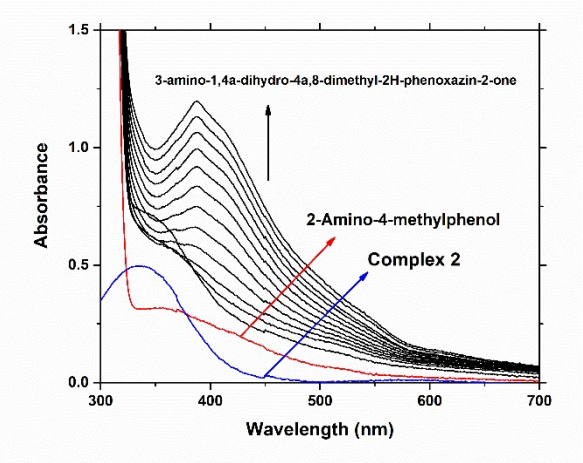

Fig S5. Increase of the phenoxazinone band at 388 nm after the addition of 2-amino-4-methylphenol to a methanol solution with complexes **1** and **2**. The spectra were recorded at 5 min intervals.

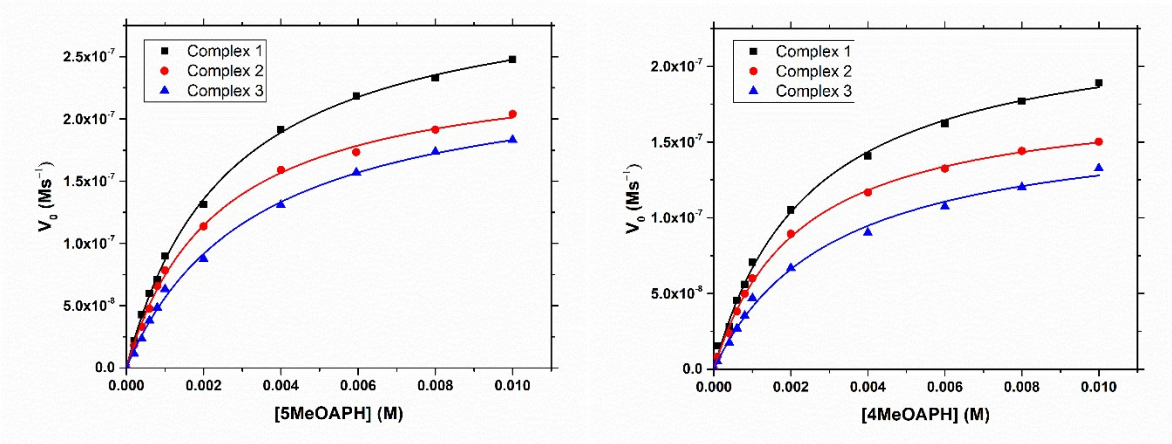

Fig. S6. Initial rate versus substrate concentration plot for the oxidation of substituted aminophenols (left side for 2-amino-5-methylphenol and right side for 2-amino-4-methylphenol) in dioxygen-saturated methanol catalysed by complexes **1**–**3** at room temperature. Symbols and solid lines represent the experimental and simulated profiles, respectively.

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

	1	**2**	**3**
N1–Co1–N2	90.2(2)	86.15(6)	85.07(7)
N1–Co1–N3		170.76(6)	171.38(7)
N1–Co1–N4	87.1(2)	90.05(6)	87.87(8)
N1–Co1–N7	173.9(3)	90.41(6)	94.82(7)
N1–Co1–N10	85.6(3)	91.49(6)	87.64(7)
N1–Co1–N13	93.3(3)		
N2–Co1–N3		86.09(6)	86.33(7)
N2–Co1–N4	87.4(2)	86.54(6)	84.91(8)
N2–Co1–N7	94.3(2)	176.10(6)	177.25(8)
N2–Co1–N10	175.8(3)	89.57(6)	88.25(8)
N2–Co1–N13	89.5(3)		
N4–Co1–N3		94.49(6)	91.97(7)
N4–Co1–N7	89.1(3)	91.65(6)	92.35(7)
N4–Co1–N10	91.6(3)	175.71(6)	172.11(7)
N4–Co1–N13	176.9(3)		
N7–Co1–N3		97.49(6)	93.79(7)
N7–Co1–N10	89.7(3)	92.35(6)	94.49(7)
N7–Co1–N13	90.7(3)		
N10–Co1–N3		83.43(6)	91.50(6)
N10–Co1–N13	91.5(3)		
N–N–N(azide)	176.0(9) 176.1(7) 176.1(8) 178.1(9)	176.88(17) 176.89(16) 177.86(18)	175.7(2) 176.2(2) 176.2(2)
N–N–Co	117.1(5) 125.4(5) 120.2(5) 120.6(5)	119.33(11) 120.73(11) 119.73(11)	122.32(13) 121.13(14) 120.77(13)

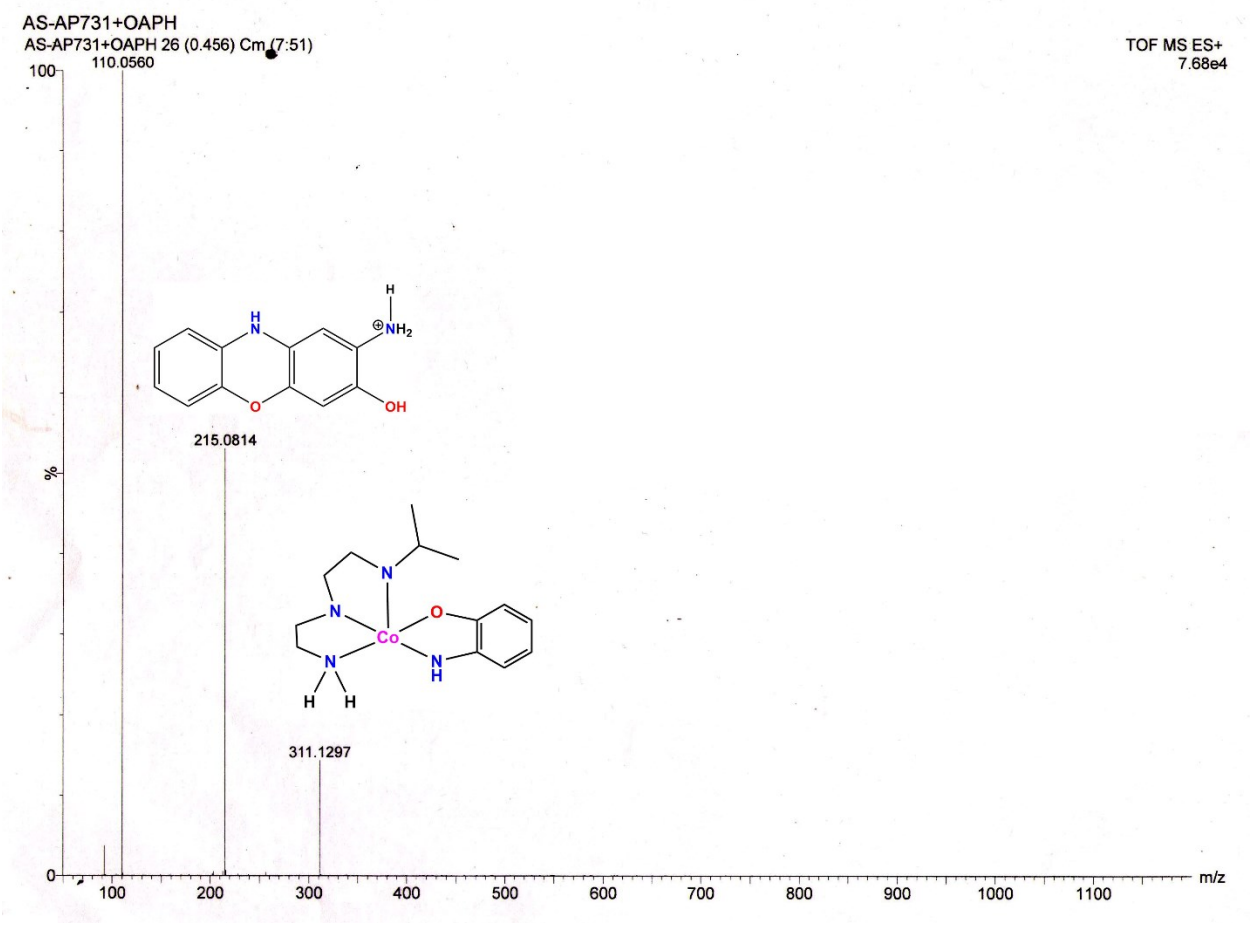

Fig. S7. Electrospray ionization mass spectrum (ESI-MS positive) of a 1:20 mixture of complex **2** and *o*-aminophenol in methanol recorded after 5 min of mixing.

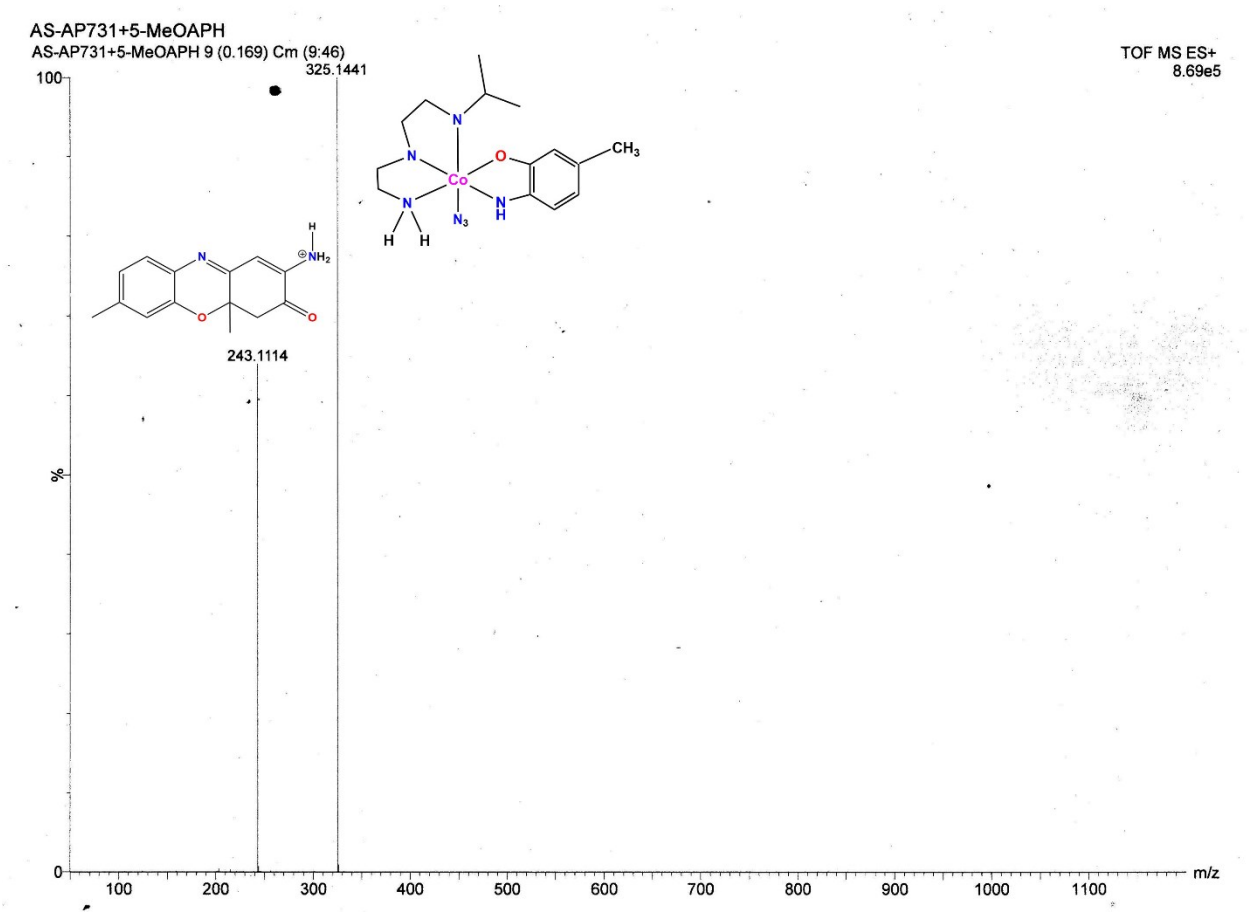

Fig. S8. Electrospray ionization mass spectrum (ESI-MS positive) of a 1:20 mixture of complex **2** and 2-amino-5-methylphenol in methanol recorded after 10 min of mixing.

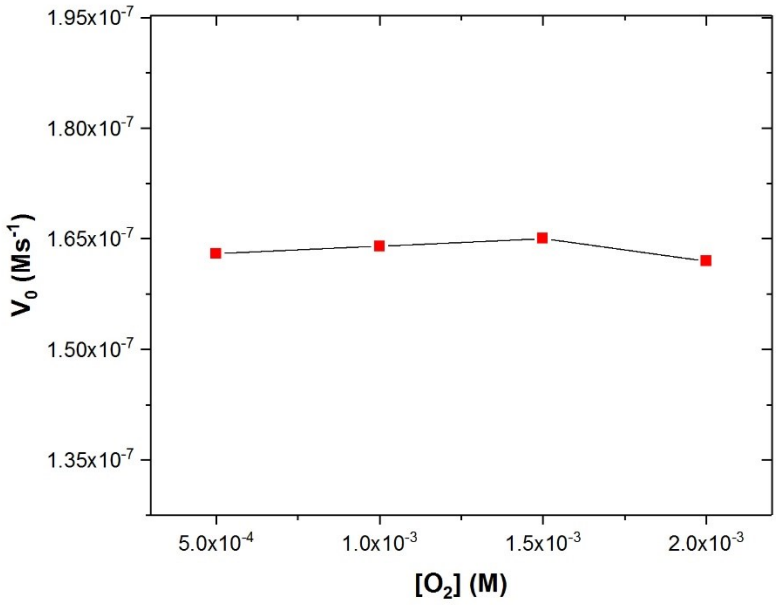

Fig. S9. Rate dependency on the dioxygen concentration for the complex **1** catalysed oxidation of *o*-aminophenol using the concentration of O_2 in air-saturated methanol solution was taken as 2.0 × 10–3 M. [S1]

References

S1 M. Quaranta, M. Murkovicb and I. Klimant, *Analyst,* 2013, **138**, 6243–6245.