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


# Electronic Supplementary Information

## Mononuclear copper(II) Schiff base complexes as effective models for phenoxazinone synthase

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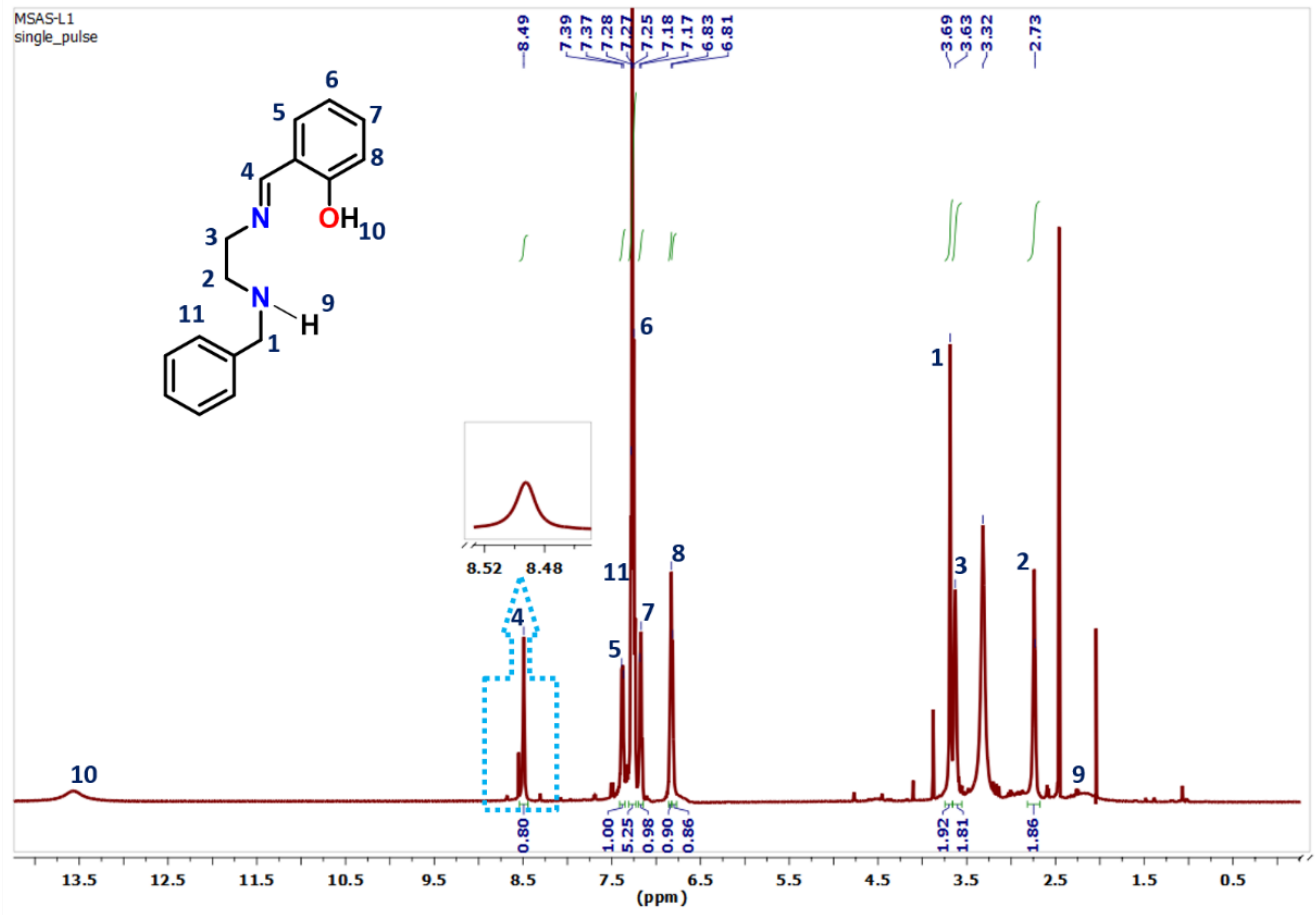


**Fig. S1** [1]HNMR (500 MHz) spectrum of ligand **L1**(H) was recorded in DMSO-$d_6$.

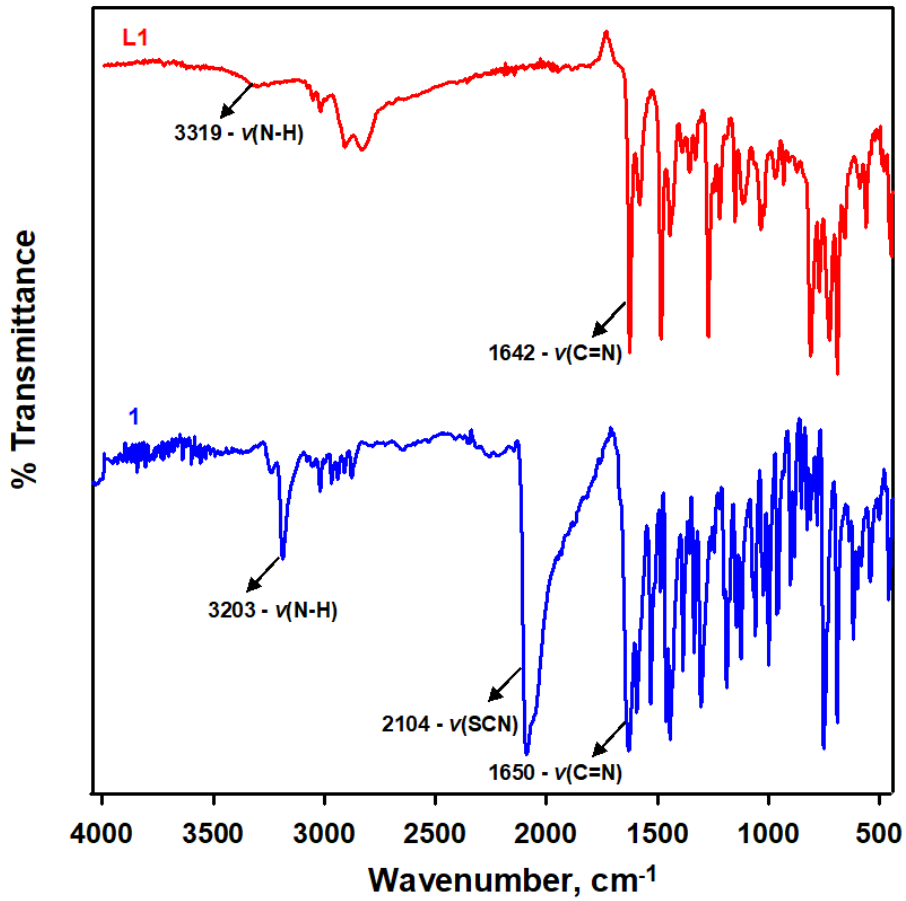


**Fig. S2** ATR spectra of ligand **L1**(H) and IR spectra of complex **1.**

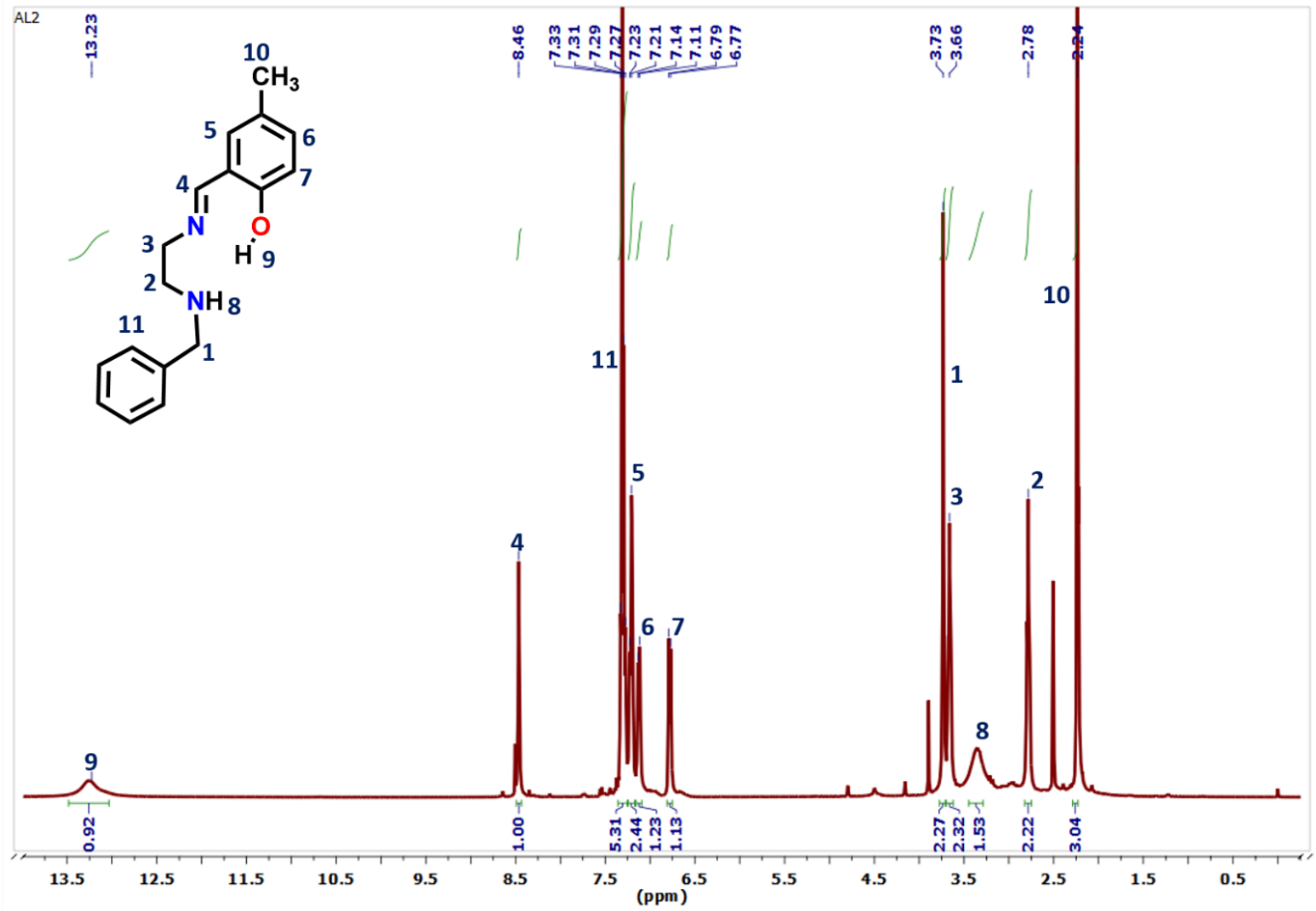


**Fig. S3** $^{1}$H NMR spectrum (500 MHz) of ligand **L2**(H) was recorded in DMSO-$d_6$.

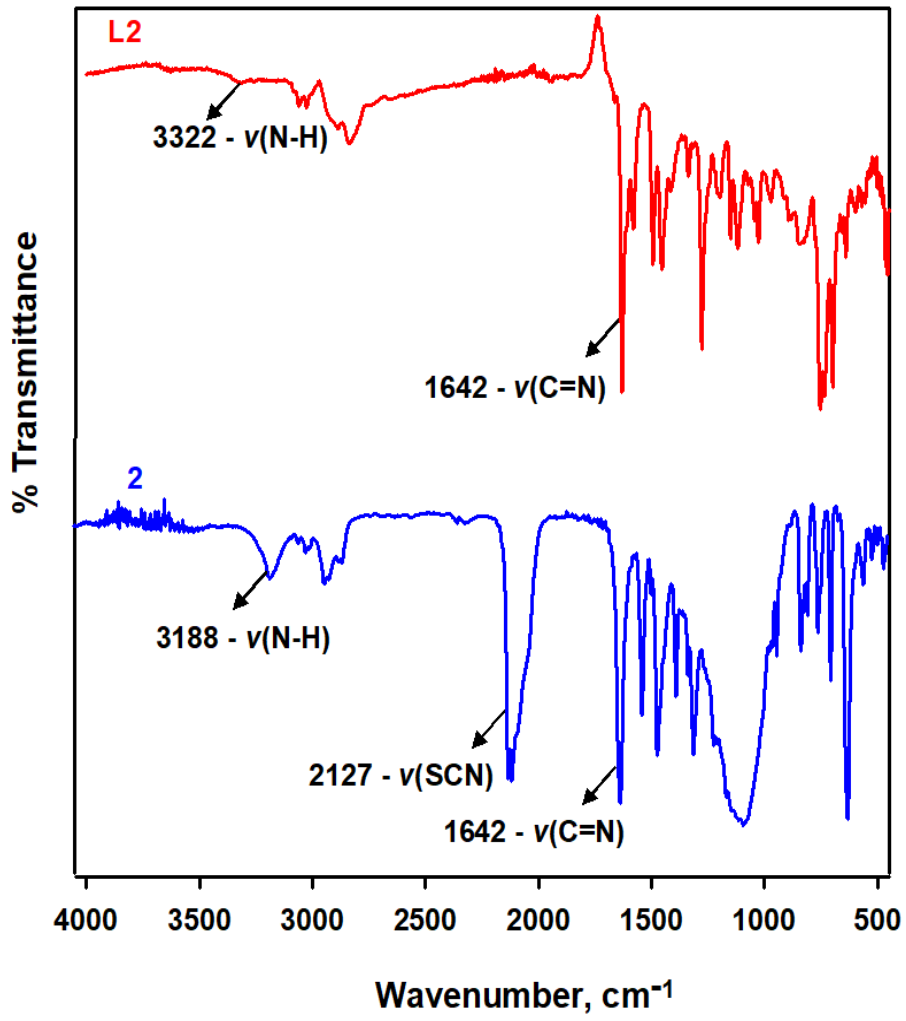


**Fig. S4** ATR spectra of ligand **L2**(H) and IR spectra of complex **2.**

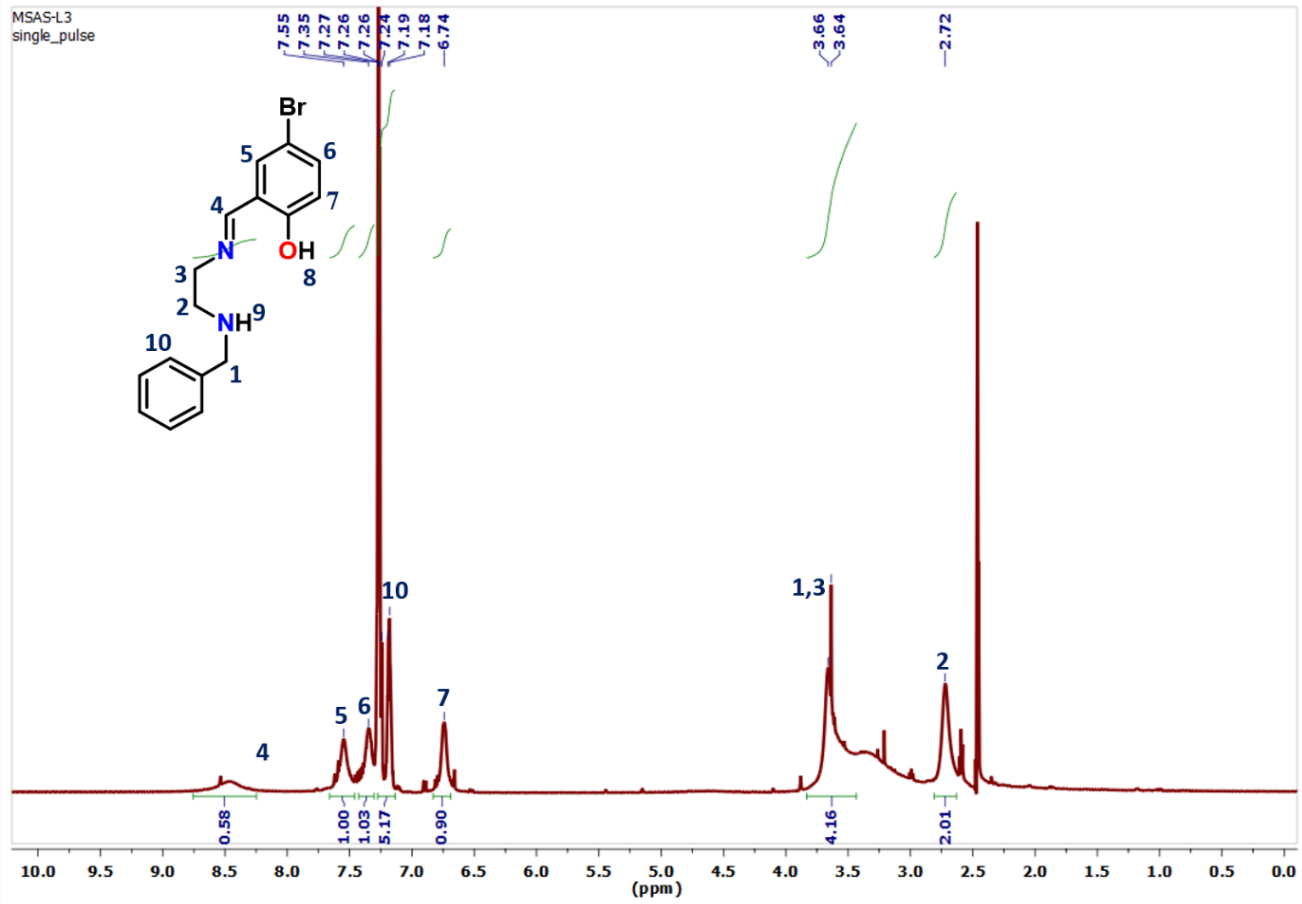


**Fig. S5** $^{1}$H NMR (500 MHz) spectrum of ligand **L3**(H) was recorded in DMSO-$d_6$.

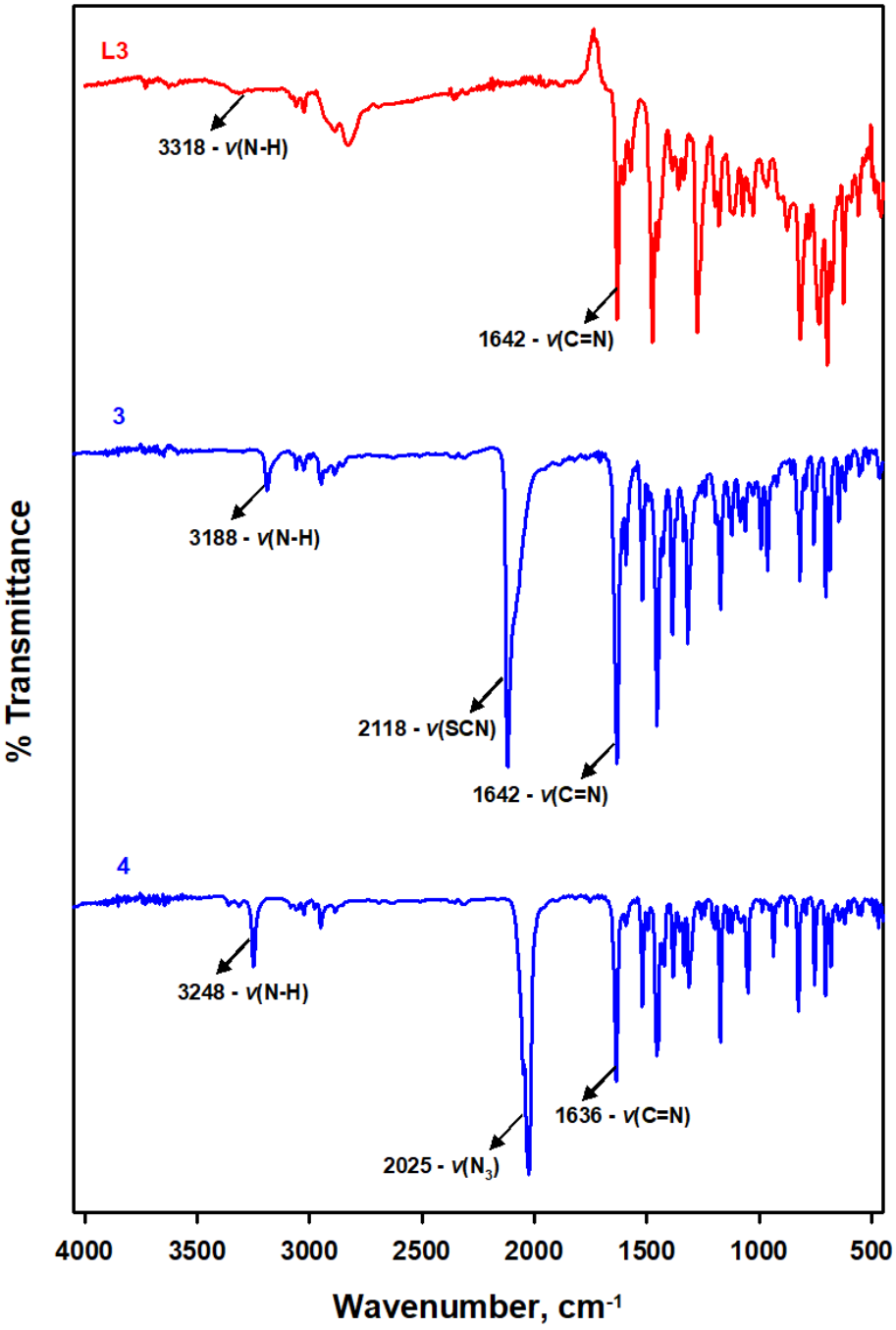


**Fig. S6** ATR spectra of ligand **L3**(H) and IR spectra of complex **3** and **4.**

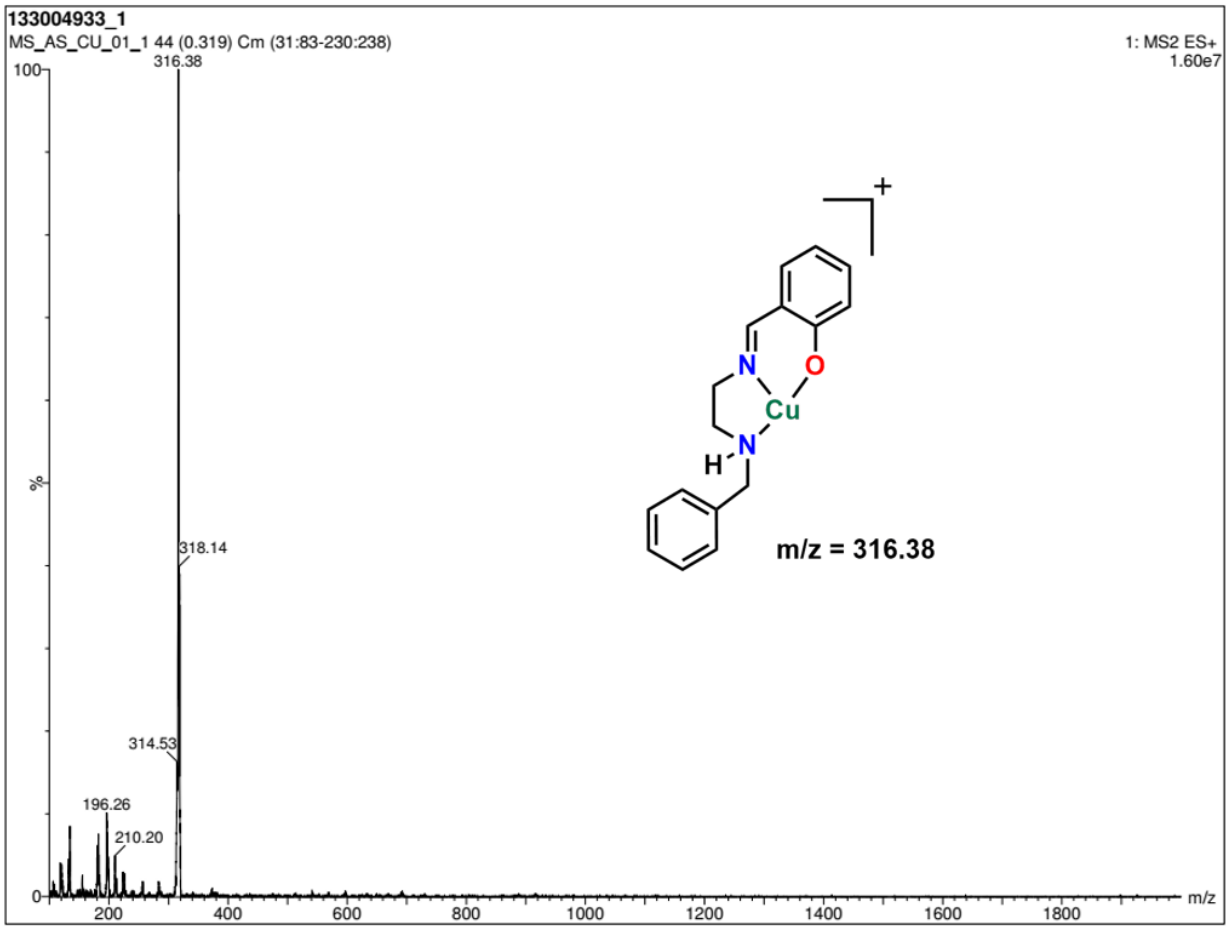


**Fig. S7** Mass spectral data of complex **1** recorded in acetonitrile**.**

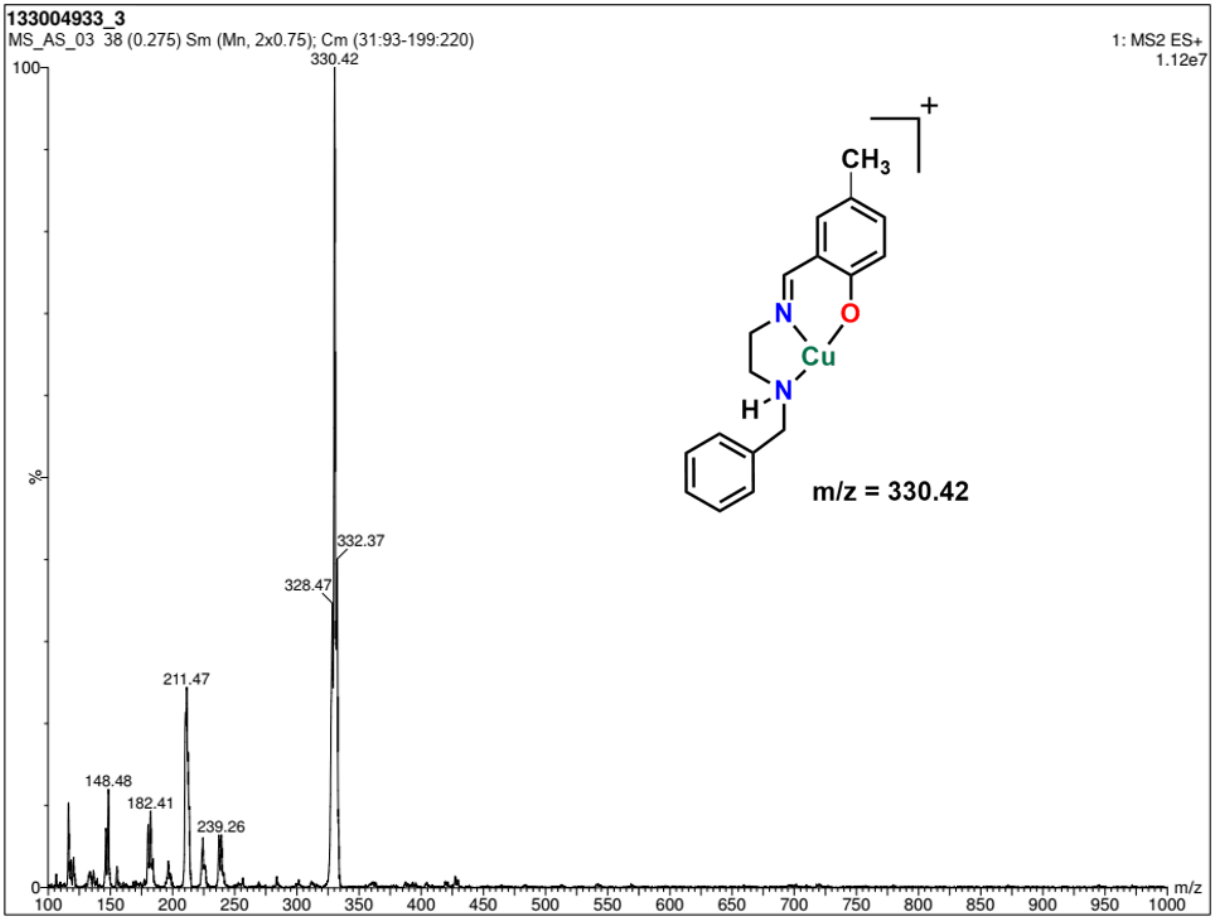


**Fig. S8** Mass spectral data of complex **2** recorded in acetonitrile**.**

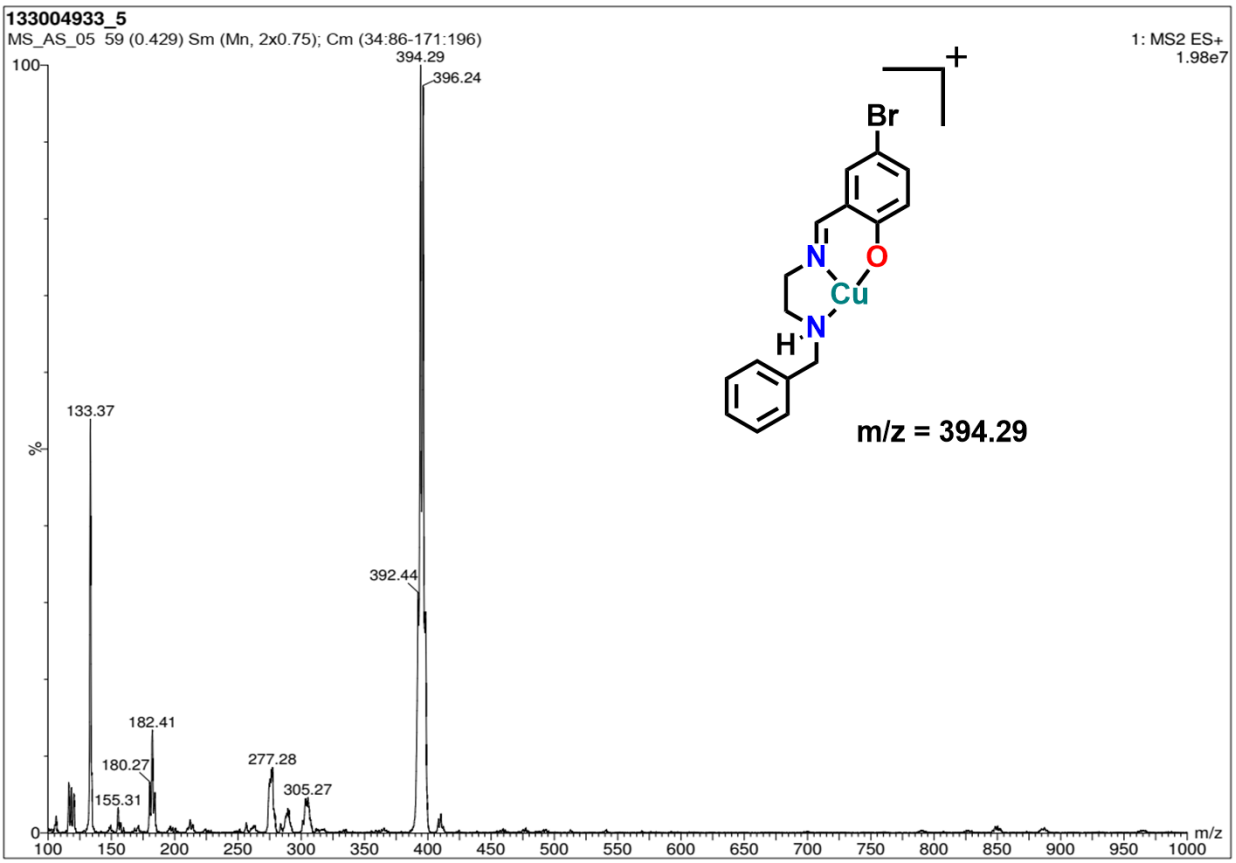


**Fig. S9** Mass spectral data of complex **3** recorded in acetonitrile**.**

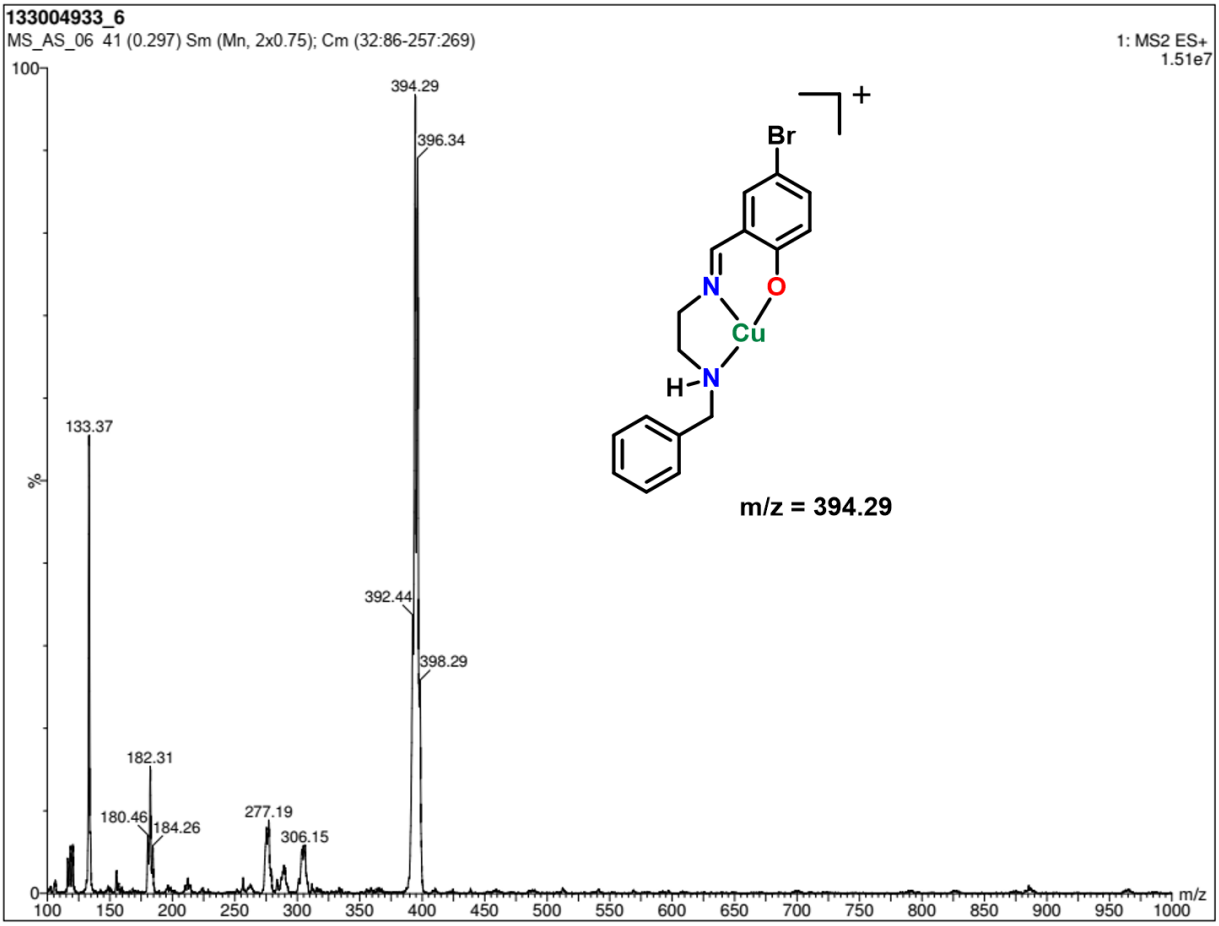


**Fig. S10** Mass spectral data of complex **4** recorded in acetonitrile**.**

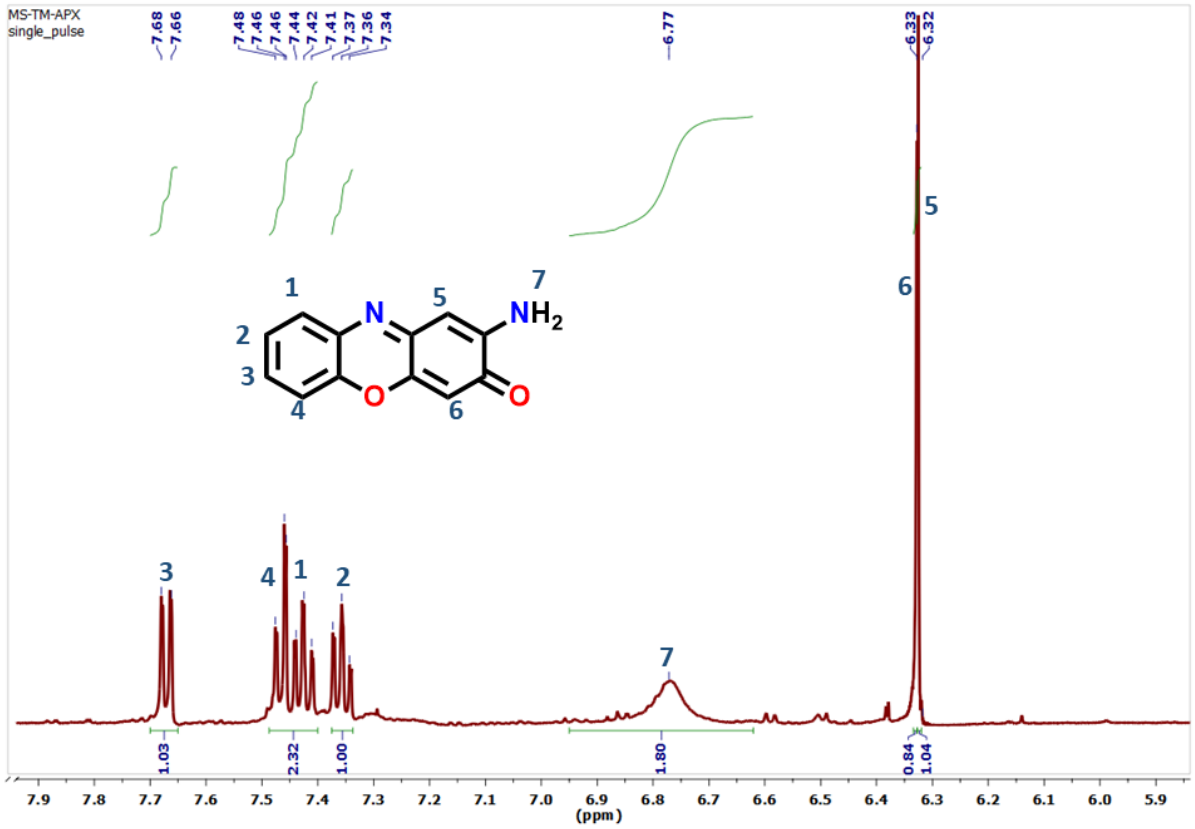


**Fig. S11** $^{1}$H NMR (500 MHz, 300 K) spectrum was recorded in DMSO-$d_6$ for the reaction mixture of *o*-aminophenol (25 mM) and a complex **3** (5 mM) in oxygen saturated methanol at 60 $^{o}$C for 6 hrs after the work-up. The $^{1}$H NMR spectrum confirms the formation of 2-amino-phenoxazine-3-one (APX) in the reaction mixture as the product.

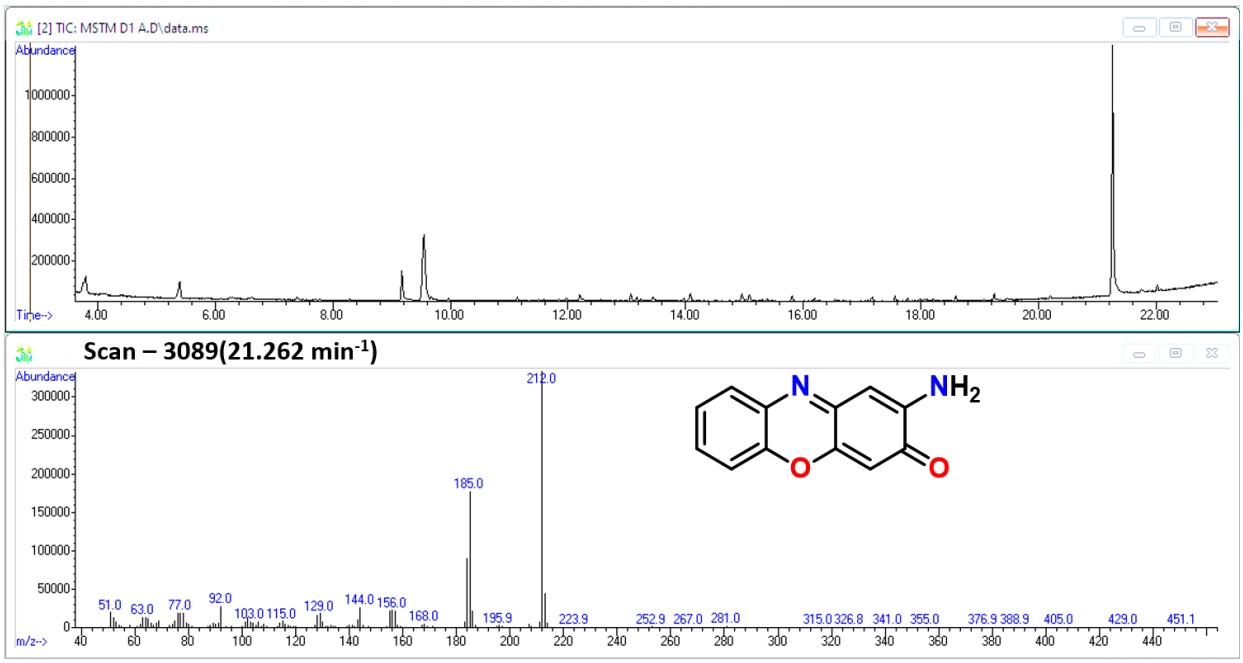


**Fig. S12** GC-MS data was recorded in methanol for the reaction mixture of *o*-aminophenol (25 mM) and a complex **3** (5 mM) in oxygen-saturated methanol at 60 °C for 6 hrs after the work-up. Among the given spectra (top) total ion chromatogram and (bottom) mass spectrum of the product, 2-amino-phenoxazine-3-one (APX) with m/z = 212.0 at 21.262 min. The peaks observed in the chromatogram with the retention time of 9.543 min and 9.17 min are (3-bromophenyl)methanamine and *o*-aminophenol, respectively.

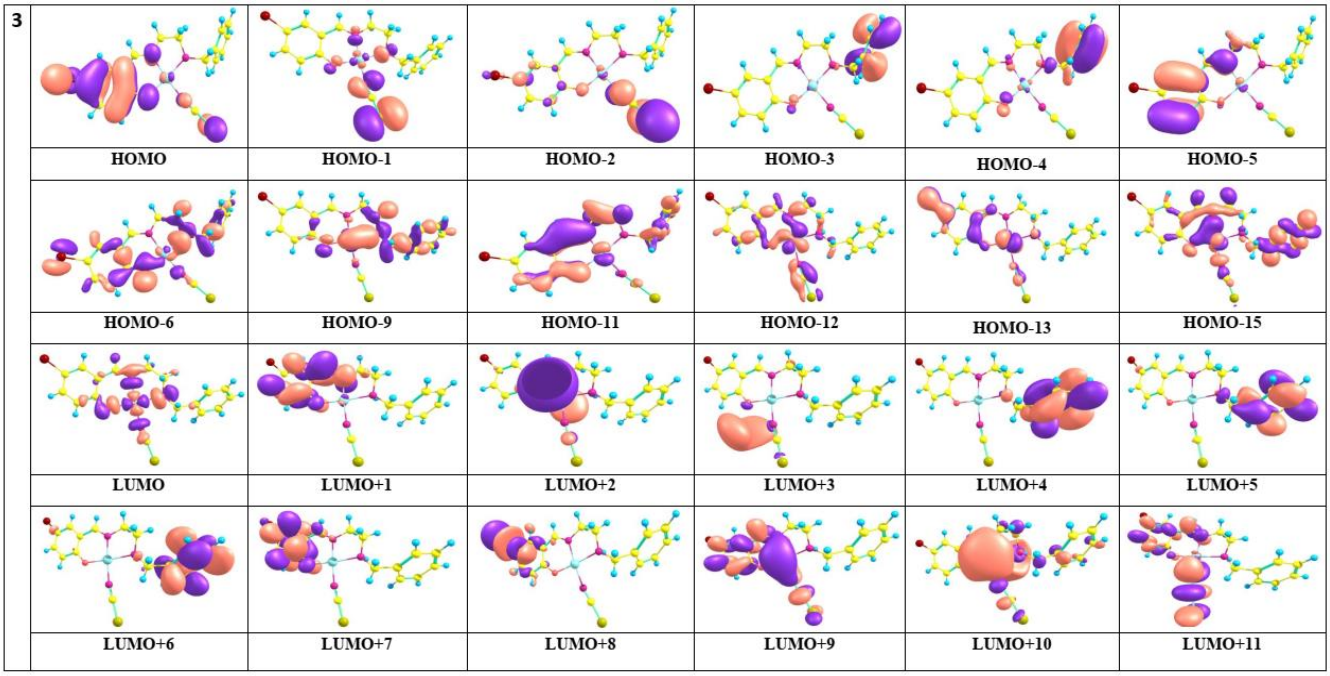


**Fig. S13** Frontier molecular orbitals (FMO) of complex **3.**

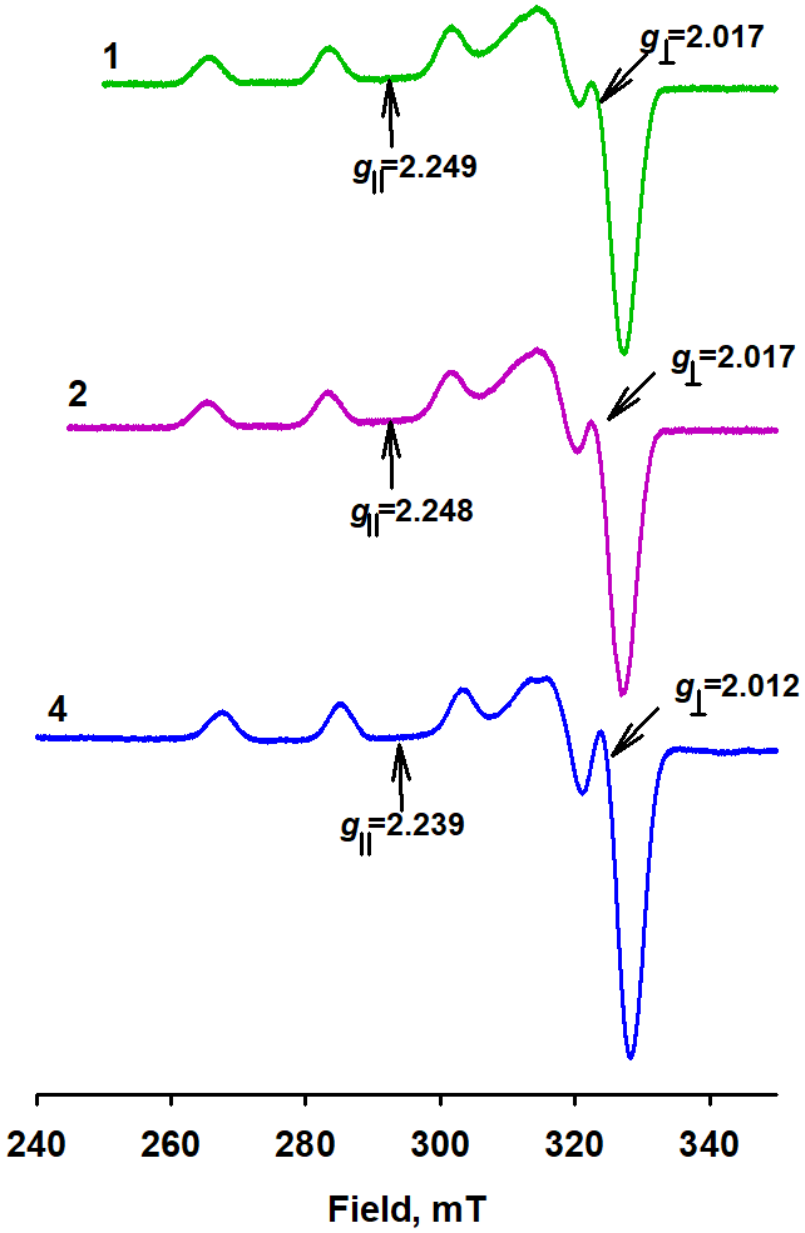


**Fig. S14** EPR spectra of **1**, **2** and **4** were measured at 77 K in methanol/DMF (4:1) solution.

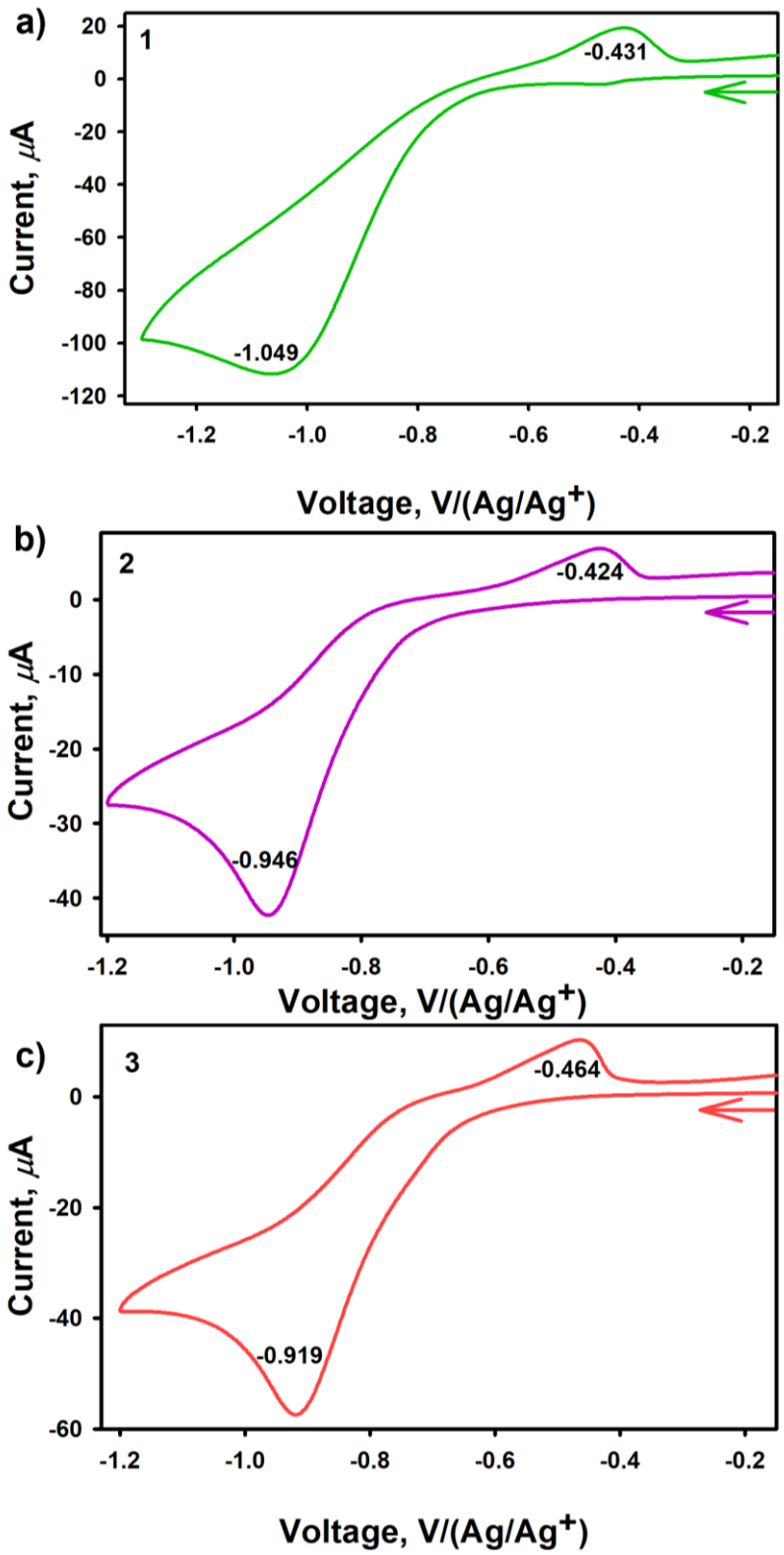


**Fig. S15** Cyclic voltammogram of the complexes **1-3 (a-c)** in methanol:DMF (9:1); tetrabutylammonium hexafluorophosphate (TBAHFP) (0.1 M) as the supporting electrolyte; scan rate - 0.1 V/ s. Working electrode – glassy carbon, Auxillary electrode - platinum wire.

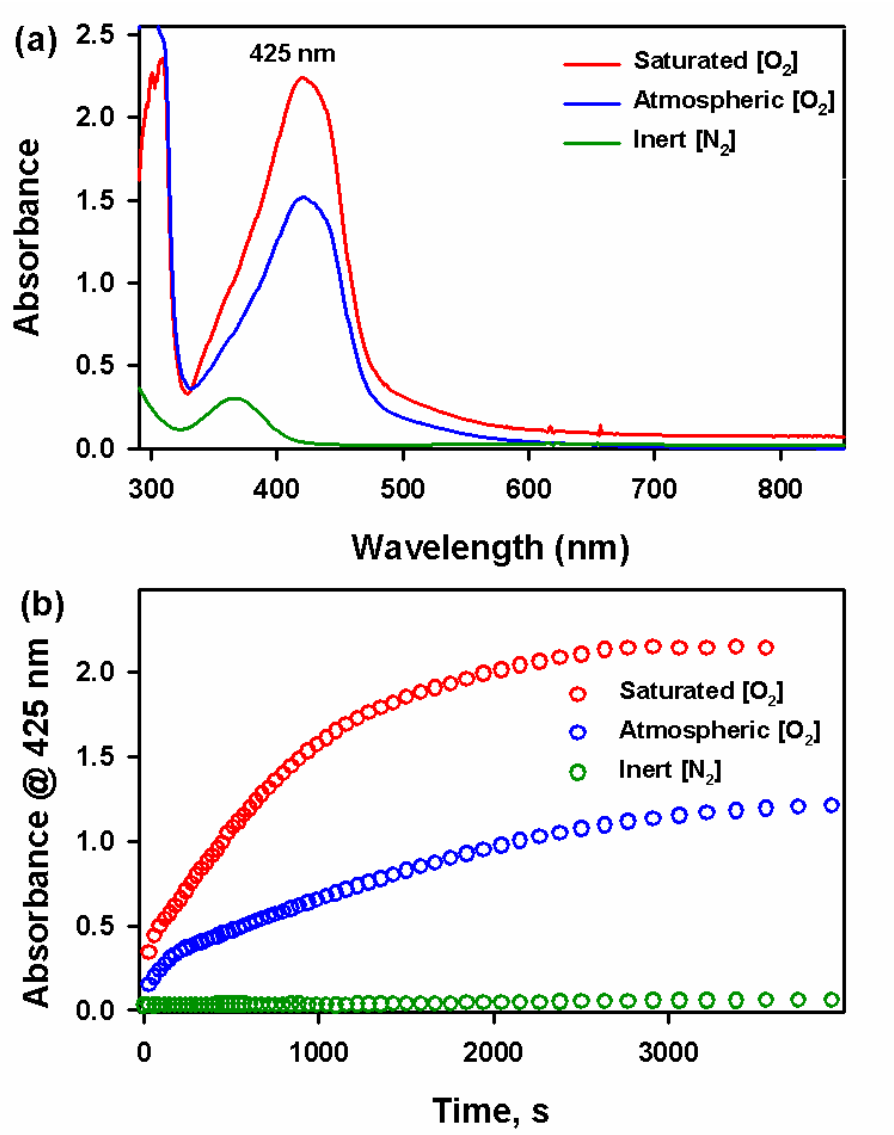


**Fig. S16 (a)** UV-vis spectra for the reaction of complex **1** (0.1 mM) OAP (20 mM) in methanol with different oxygen environment. **(b)** Time profiles for the formation of the 2-amino-phenoxazine-3-one with an absorption at 425 nm.

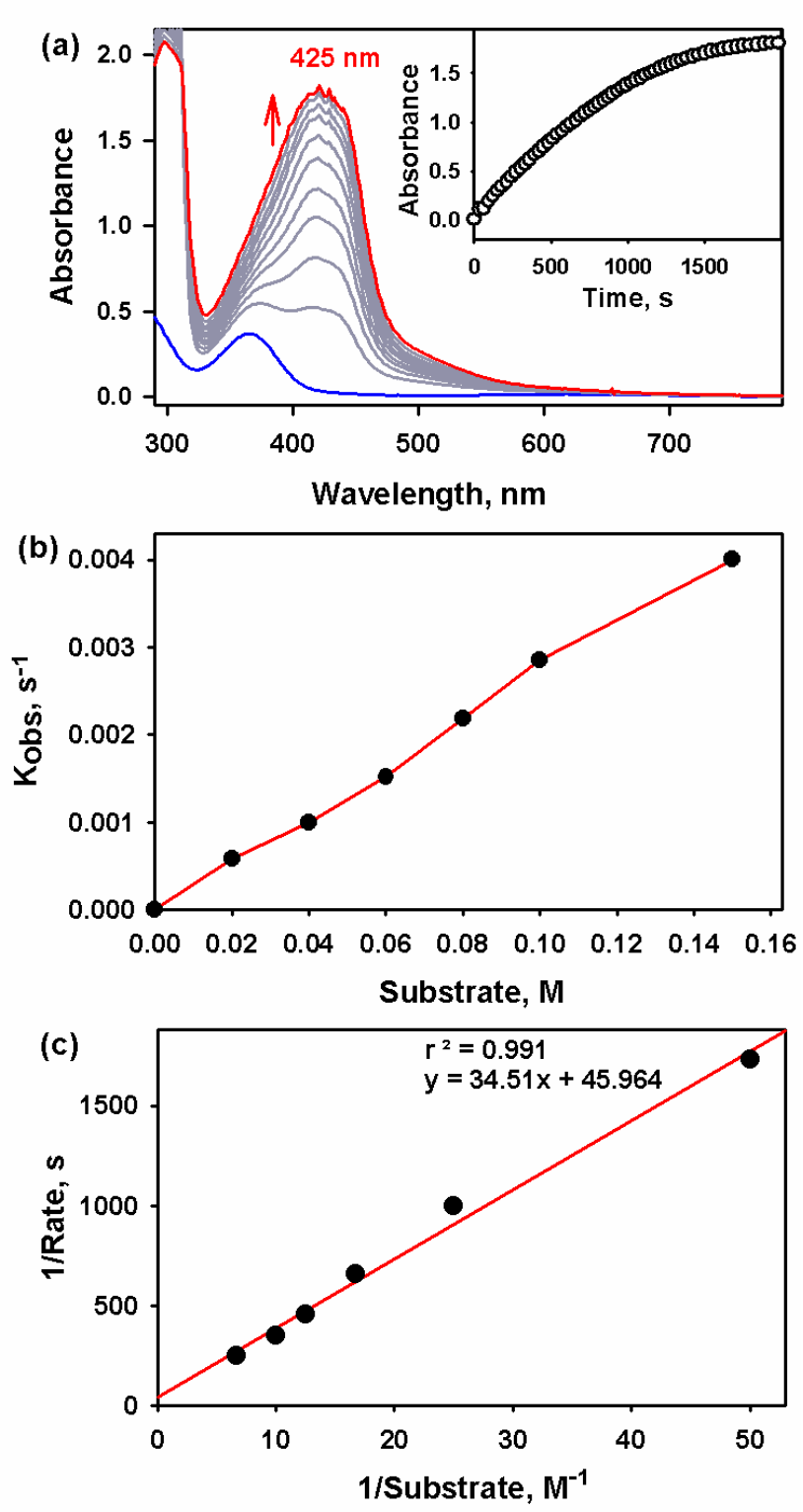


**Fig. S17 (a)** UV-vis spectral profile for the formation of phenoxazinone chromophore peak at 425 nm in the reaction of complex **1** (0.1 mM) with OAP (60 mM). **(b)** The plot of rate *vs* substrate concentration. **(c)** Lineweaver-Burk plot for the complex **1**.

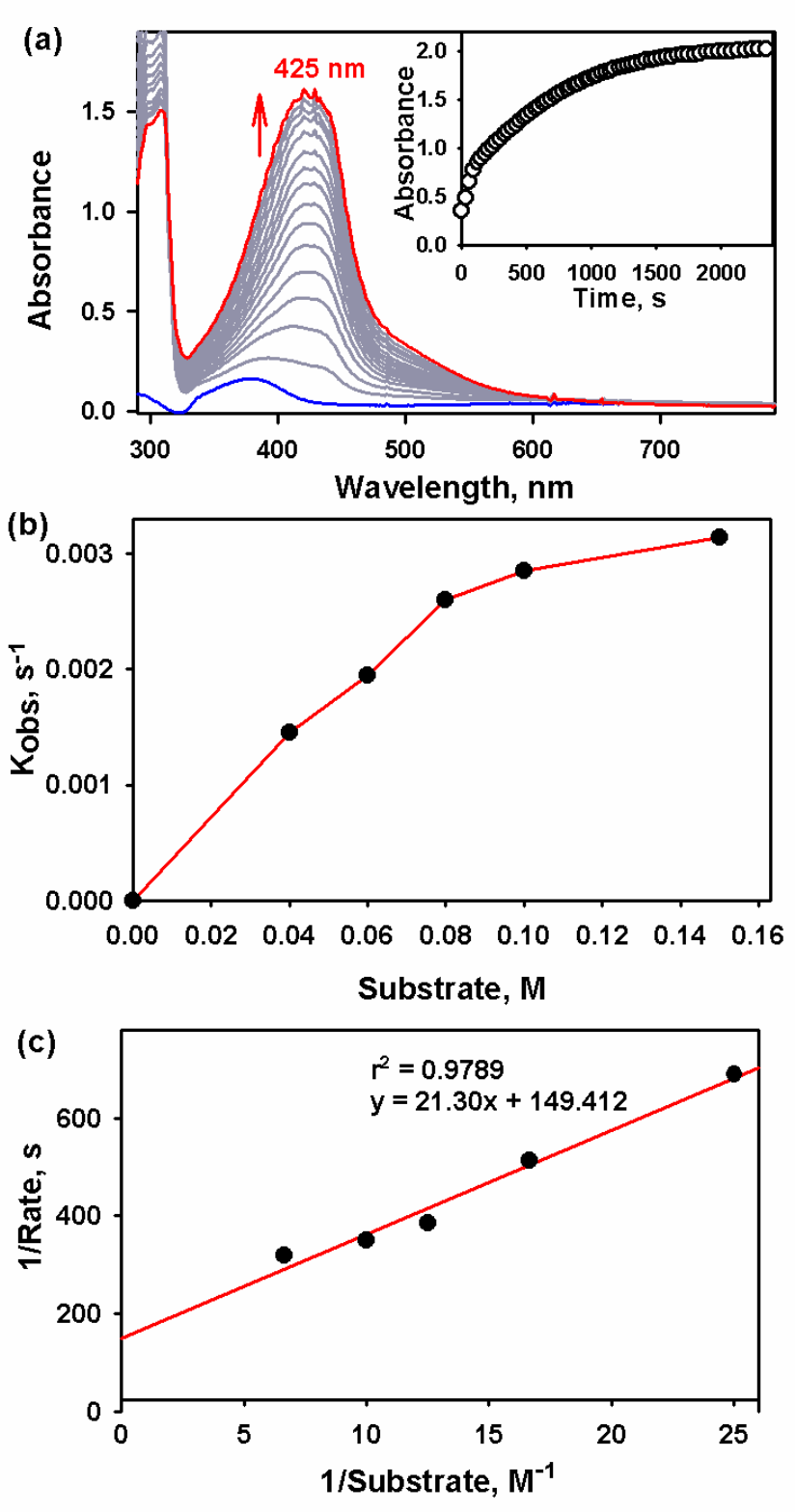


**Fig. S18 (a)** UV-vis spectral profile for the formation of phenoxazinone chromophore peak at 425 nm in the reaction of complex **2** (0.1 mM) with OAP (60 mM). **(b)** The plot of rate *vs* substrate concentration. **(c)** Lineweaver-Burk plot for the complex **2**.

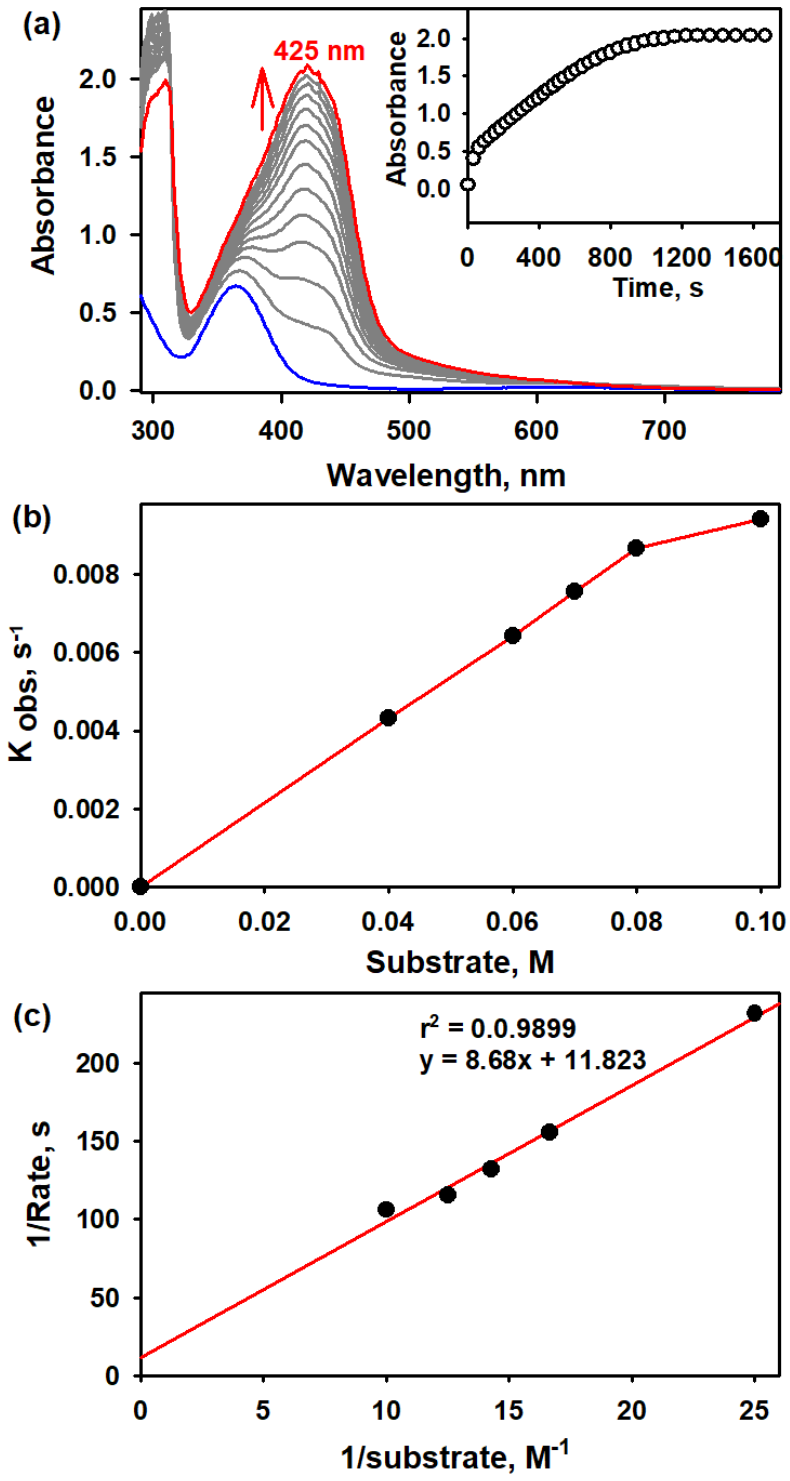


**Fig. S19 (a)** UV-vis spectral profile for the formation of phenoxazinone chromophore peak at 425 nm in the reaction of complex **4** (0.1 mM) with OAP (60 mM). **(b)** The plot of rate *vs* substrate concentration. **(c)** Lineweaver-Burk plot for the complex **4**.

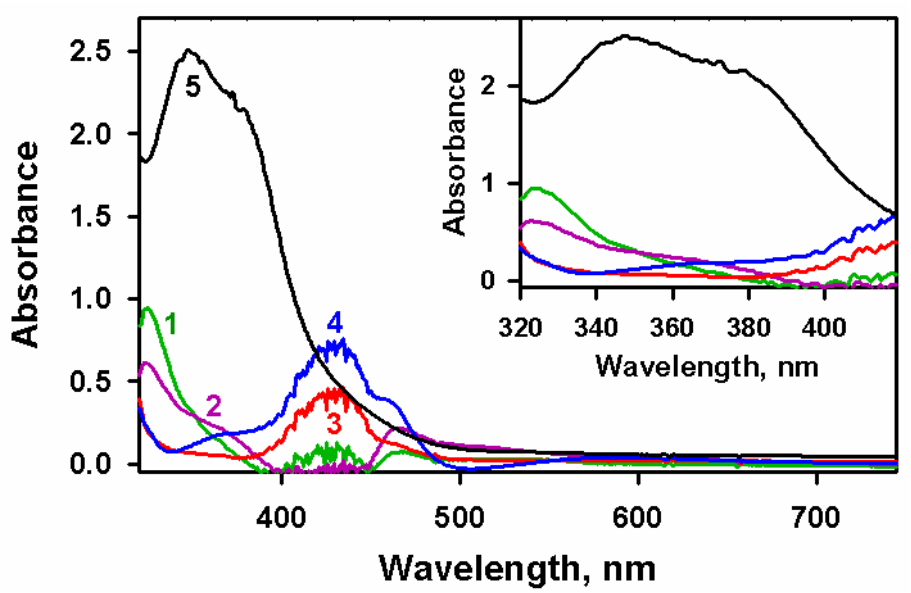


**Fig. S20** UV-vis absorption spectra for the detection of $H_2O_2$ formation in the oxidation of OAP against **1**-**4**, as oxygen reduced product**.** The reaction was monitored by treating the reaction mixture with the excess amount of NaI**.** The inset shows no formation of triiodide ($I_3^-$) ion formation. The black line (**5**) represents the reaction of $H_2O_2$ (0.1 mM) with excess NaI (100 mM) in methnol.

**Table S1.** HOMO - LUMO energy surfaces for the computed absorption spectrum of complex **3** using **m06** functional, with basis sets **6-31G** for C,H,O,S,N and **LANL2DZ** for Cu for 20 excited states.

| Compound | Excited state | Oscillator Strength (f) | Excitation energy (eV) | Wavelength (nm) | Transition | Coefficient of Transition | Percentage contribution |
|---|---|---|---|---|---|---|---|
| **3** | 1 | 0.0019 | 1.7338 | 715.09 | HOMO – LUMO (β) | 0.67667 | 45.79 |
| | | | | | HOMO-15– LUMO (β) | 0.12256 | 1.50 |
| | | | | | HOMO-13 – LUMO (β) | 0.37657 | 14.18 |
| | | | | | HOMO-12 – LUMO (β) | -0.40907 | 16.73 |
| | | | | | HOMO-9 – LUMO (β) | 0.13152 | 1.73 |
| | | | | | HOMO-7 – LUMO (β) | 0.21819 | 4.76 |
| | | | | | HOMO-6 – LUMO (β) | -0.18707 | 3.49 |
| | | | | | HOMO-5 – LUMO (β) | -0.11776 | 1.39 |
| | | | | | HOMO-1 – LUMO (β) | -0.23333 | 5.45 |
| | | | | | | | |
| | 2 | 0.0050 | 1.7733 | 699.17 | HOMO-12 – LUMO (β) | 0.54921 | 30.16 |
| | | | | | HOMO-22 – LUMO (β) | 0.10836 | 1.17 |
| | | | | | HOMO-15 – LUMO (β) | -0.18284 | 3.34 |
| | | | | | HOMO-13 – LUMO (β) | 0.34553 | 11.94 |
| | | | | | HOMO-9 – LUMO (β) | -0.17334 | 3.00 |
| | | | | | HOMO-7 – LUMO (β | 0.12571 | 1.58 |
| | | | | | HOMO-6 – LUMO (β) | 0.34442 | 11.86 |
| | | | | | HOMO-1 – LUMO (β) | 0.40697 | 16.56 |
| | | | | | HOMO– LUMO (β) | 0.40012 | 16.01 |
| | | | | | | | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | 3 | 0.0006 | 1.9540 | 634.52 | HOMO-9 – LUMO (β) | 0.61536 | 37.87 |
| | | | | | HOMO-18 – LUMO (β) | 0.10095 | 1.02 |
| | | | | | HOMO-17 – LUMO (β) | 0.17686 | 3.13 |
| | | | | | HOMO-15 – LUMO (β) | 0.28562 | 8.16 |
| | | | | | HOMO-14 – LUMO (β) | -0.21780 | 4.74 |
| | | | | | HOMO-12 – LUMO (β) | 0.26325 | 6.93 |
| | | | | | HOMO-11 – LUMO (β) | -0.14962 | 2.24 |
| | | | | | HOMO-10 – LUMO (β) | 0.56722 | 32.17 |
| | | | | | | | |
| | 4 | 0.0002 | 2.1502 | 576.61 | HOMO-11 – LUMO (β) | 0.65348 | 42.70 |
| | | | | | HOMO-26 – LUMO (β) | 0.10350 | 1.07 |
| | | | | | HOMO-23 – LUMO (β) | 0.12550 | 1.58 |
| | | | | | HOMO-16 – LUMO (β) | 0.36384 | 13.24 |
| | | | | | HOMO-15 – LUMO (β) | 0.10681 | 1.14 |
| | | | | | HOMO-12 – LUMO (β) | 0.10721 | 1.15 |
| | | | | | HOMO-5 – LUMO (β) | -0.23133 | 5.35 |
| | | | | | HOMO-2 – LUMO (β) | 0.53856 | 8.41 |
| | | | | | | | |
| | 5 | 0.0003 | 2.7447 | 451.72 | HOMO-13 – LUMO (β) | 0.57371 | 32.91 |
| | | | | | HOMO-20 – LUMO (β) | -0.12812 | 1.64 |
| | | | | | HOMO-19 – LUMO (β) | 0.25189 | 6.34 |
| | | | | | HOMO-12 – LUMO (β) | -0.10750 | 1.16 |
| | | | | | HOMO-11 – LUMO (β) | -0.24962 | 6.23 |
| | | | | | HOMO-7 – LUMO (β) | 0.13269 | 1.76 |
| | | | | | HOMO-2 – LUMO (β) | 0.45304 | 20.52 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | | | HOMO – LUMO (β) | -0.49732 | 24.73 |
| | | | | | | | |
| | 6 | 0.0002 | 2.8500 | 435.03 | HOMO – LUMO+1 (β) | 0.67208 | 45.17 |
| | | | | | HOMO-6 – LUMO (α) | -0.11547 | 1.33 |
| | | | | | HOMO-2 – LUMO (α) | 0.15955 | 2.55 |
| | | | | | HOMO – LUMO (α) | -0.66322 | 43.98 |
| | | | | | HOMO-5 – LUMO+1 (β) | -0.11115 | 1.24 |
| | | | | | HOMO-2 – LUMO+1 (β) | -0.14968 | 2.24 |
| | | | | | | | |
| | 7 | 0.0006 | 2.9071 | 426.49 | HOMO-1 – LUMO (β) | 0.86415 | 74.68 |
| | | | | | HOMO-12 – LUMO (β) | -0.33927 | 11.51 |
| | | | | | HOMO-6 – LUMO (β) | -0.28477 | 8.11 |
| | | | | | | | |
| | 8 | 0.0005 | 3.0435 | 407.37 | HOMO-2 – LUMO (β) | 0.69058 | 47.69 |
| | | | | | HOMO-23 – LUMO (β) | -0.18310 | 3.35 |
| | | | | | HOMO-16 – LUMO (β) | -0.21083 | 4.44 |
| | | | | | HOMO-13 – LUMO (β) | -0.36376 | 13.23 |
| | | | | | HOMO-11 – LUMO (β) | -0.30271 | 9.16 |
| | | | | | HOMO-5 – LUMO (β) | 0.27777 | 7.72 |
| | | | | | HOMO– LUMO (β) | 0.33178 | 11.01 |
| | | | | | | | |
| | 9 | 0.0003 | 3.4428 | 360.12 | HOMO-5 – LUMO+1 (β) | 0.55732 | 31.06 |
| | | | | | HOMO-6 – LUMO (α) | 0.54933 | 30.18 |
| | | | | | HOMO-6 – LUMO+6 (α) | -0.14853 | 2.21 |
| | | | | | HOMO-3 – LUMO (α) | -0.21011 | 4.41 |
| | | | | | HOMO-1 – LUMO+1 (α) | -0.10214 | 1.04 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | | | HOMO – LUMO(α) | -0.11519 | 1.33 |
| | | | | | HOMO – LUMO+6 (α) | 0.29444 | 8.67 |
| | | | | | HOMO-5– LUMO+7 (β) | -0.14941 | 2.23 |
| | | | | | HOMO– LUMO+7 (β) | -0.29747 | 8.85 |
| | | | | | | | |
| | 10 | 0.0018 | 3.5686 | 347.43 | HOMO-3 – LUMO (α) | 0.80703 | 65.12 |
| | | | | | HOMO-6 – LUMO (α) | 0.14397 | 2.07 |
| | | | | | HOMO-5 – LUMO (α) | -0.11612 | 1.35 |
| | | | | | HOMO-1 – LUMO (α) | 0.43375 | 18.81 |
| | | | | | HOMO– LUMO (α) | 0.10638 | 1.13 |
| | | | | | HOMO-5– LUMO+1 (β) | 0.12310 | 1.52 |
| | | | | | HOMO– LUMO+1 (β) | 0.10661 | 1.14 |
| | | | | | | | |
| | 11 | 0.0411 | 3.5889 | 345.47 | HOMO – LUMO+1(β) | 0.57360 | 32.90 |
| | | | | | HOMO-3 – LUMO (α) | -0.13255 | 1.76 |
| | | | | | HOMO-3 – LUMO (α) | -0.10958 | 1.20 |
| | | | | | HOMO-3 – LUMO (α) | 0.56078 | 31.45 |
| | | | | | HOMO – LUMO+1(β) | 0.15100 | 2.28 |
| | | | | | HOMO – LUMO+1(β) | -0.20231 | 4.09 |
| | | | | | HOMO – LUMO+1(β) | 0.33690 | 11.35 |
| | | | | | HOMO – LUMO+1(β) | 0.15640 | 2.47 |
| | | | | | HOMO – LUMO+1(β) | 0.24239 | 5.88 |
| | | | | | | | |
| | 12 | 0.0825 | 3.7744 | 328.49 | HOMO-3 - LUMO(β) | 0.61635 | 37.99 |
| | | | | | HOMO-5 – LUMO+4 (α) | -0.19747 | 3.89 |
| | | | | | HOMO-5 – LUMO+5 (α) | 0.15847 | 2.51 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | | | HOMO-4 – LUMO+3 (α) | -0.25637 | 6.57 |
| | | | | | HOMO-4 – LUMO+5 (α) | 0.14760 | 2.18 |
| | | | | | HOMO– LUMO (α) | 0.22716 | 5.16 |
| | | | | | HOMO-4 - LUMO(β) | -0.38597 | 14.89 |
| | | | | | HOMO-4 – LUMO+5(β) | 0.12763 | 1.63 |
| | | | | | HOMO-4 – LUMO+6(β) | -0.22830 | 5.21 |
| | | | | | HOMO-3 – LUMO+4(β) | 0.25073 | 6.28 |
| | | | | | HOMO-3 – LUMO+5(β) | -0.18360 | 3.37 |
| | | | | | HOMO– LUMO+1(β) | 0.22293 | 4.97 |
| | | | | | | | |
| | 13 | 0.0086 | 3.8945 | 318.36 | HOMO-5 - LUMO(β) | 0.86901 | 75.52 |
| | | | | | HOMO-16 - LUMO(β) | 0.23517 | 5.53 |
| | | | | | HOMO-11 - LUMO(β) | 0.22438 | 5.03 |
| | | | | | HOMO-3 - LUMO(β) | -0.12815 | 1.64 |
| | | | | | HOMO-2 - LUMO(β) | -0.11421 | 1.30 |
| | | | | | | | |
| | 14 | 0.0827 | 3.9261 | 315.80 | HOMO-3 - LUMO(β) | 0.59160 | 34.99 |
| | | | | | HOMO-5– LUMO+4 (α) | 0.21578 | 4.65 |
| | | | | | HOMO-5– LUMO+5 (α) | -0.19006 | 3.61 |
| | | | | | HOMO-4– LUMO+3 (α) | 0.26241 | 6.88 |
| | | | | | HOMO-4– LUMO+5 (α) | -0.17354 | 3.01 |
| | | | | | HOMO– LUMO (α) | 0.15428 | 2.38 |
| | | | | | HOMO-11– LUMO (β) | 0.15142 | 2.29 |
| | | | | | HOMO-6– LUMO (β) | -0.23504 | 5.52 |
| | | | | | HOMO-5– LUMO (β) | 0.25648 | 6.58 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | | | HOMO-4–LUMO (β) | 0.21697 | 4.71 |
| | | | | | HOMO-4–LUMO-5 (β) | -0.13487 | 1.82 |
| | | | | | HOMO-4–LUMO-6 (β) | 0.25454 | 6.48 |
| | | | | | HOMO-3–LUMO-4 (β) | -0.25689 | 6.59 |
| | | | | | HOMO-3–LUMO-5 (β) | 0.15224 | 15.29 |
| | | | | | HOMO–LUMO+1 (β) | 0.14850 | 2.21 |
| | | | | | | | |
| | 15 | 0.0759 | 3.9724 | 312.11 | HOMO-4 - LUMO(β) | 0.80898 | 65.44 |
| | | | | | HOMO-4–LUMO+3 (α) | -0.18667 | 3.48 |
| | | | | | HOMO–LUMO (α) | -0.13513 | 1.83 |
| | | | | | HOMO-12 - LUMO(β) | -0.15873 | 2.52 |
| | | | | | HOMO-6 - LUMO(β) | 0.22653 | 5.13 |
| | | | | | HOMO-4 – LUMO+6(β) | -0.11294 | 1.27 |
| | | | | | HOMO-3 - LUMO(β) | 0.29925 | 8.95 |
| | | | | | HOMO-3 – LUMO+4(β) | 0.16608 | 2.76 |
| | | | | | HOMO-3 – LUMO+5(β) | -0.11830 | 1.39 |
| | | | | | HOMO-LUMO+1(β) | 0.12875 | 1.66 |
| | | | | | | | |
| | 16 | 0.1169 | 4.0813 | 303.78 | HOMO-6 - LUMO(β) | 0.70524 | 49.74 |
| | | | | | HOMO-4–LUMO+3 (α) | 0.15207 | 2.31 |
| | | | | | HOMO-4–LUMO+5 (α) | -0.10763 | 1.16 |
| | | | | | HOMO–LUMO (α) | -0.20093 | 4.04 |
| | | | | | HOMO–LUMO+6 (α) | 0.11883 | 1.41 |
| | | | | | HOMO-12 - LUMO(β) | -0.27982 | 7.83 |
| | | | | | HOMO-4 - LUMO(β) | -0.31565 | 9.96 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | | | HOMO-4-LUMO+6(β) | 0.12280 | 1.51 |
| | | | | | HOMO-3 -LUMO(β) | 0.28345 | 8.03 |
| | | | | | HOMO-3 –LUMO-4(β) | -0.14006 | 1.96 |
| | | | | | HOMO-LUMO+1(β) | -0.18662 | 3.48 |
| | | | | | | | |
| | 17 | 0.0047 | 4.1957 | 295.50 | HOMO–LUMO+7(β) | 0.47109 | 22.19 |
| | | | | | HOMO-6–LUMO (α) | 0.28601 | 8.18 |
| | | | | | HOMO-2–LUMO (α) | 0.23574 | 5.56 |
| | | | | | HOMO-2–LUMO+6 (α) | 0.13309 | 1.77 |
| | | | | | HOMO–LUMO+1 (α) | -0.14076 | 1.98 |
| | | | | | HOMO–LUMO+6 (α) | -0.43846 | 19.22 |
| | | | | | HOMO-6–LUMO (β) | 0.10131 | 1.03 |
| | | | | | HOMO-5–LUMO+1(β) | 0.27365 | 7.49 |
| | | | | | HOMO-2–LUMO+1(β) | -0.25325 | 6.41 |
| | | | | | HOMO-2–LUMO+7(β) | -0.13767 | 1.89 |
| | | | | | HOMO-1–LUMO+1(β) | 0.36071 | 13.01 |
| | | | | | HOMO–LUMO+2(β) | 0.15677 | 2.46 |
| | 18 | 0.0001 | 4.2050 | 294.85 | HOMO-1 –LUMO+1(β) | 0.92232 | 85.07 |
| | | | | | HOMO-6–LUMO (α) | -0.11727 | 1.37 |
| | | | | | HOMO–LUMO+6 (α) | 0.16692 | 2.79 |
| | | | | | HOMO-5–LUMO+1(β) | -0.10376 | 1.07 |
| | | | | | HOMO-2–LUMO+1(β) | 0.13039 | 1.70 |
| | | | | | HOMO–LUMO+7(β) | -0.17716 | 3.14 |
| | | | | | | | |
| | 19 | 0.0003 | 4.2351 eV | 292.75 | HOMO-1 –LUMO (α) | 0.87187 | 76.02 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | | | HOMO-1 – LUMO (α) | -0.42991 | 18.48 |
| | | | | | HOMO-1 – LUMO (α) | -0.20258 | 4.10 |
| | | | | | | | |
| | 20 | 0.0019 | 4.2715 | 290.26 | HOMO-2 – LUMO (α) | 0.90646 | 82.17 |
| | | | | | HOMO-6 – LUMO (α) | -0.12282 | 1.51 |
| | | | | | HOMO-3 – LUMO (α) | -0.17189 | 2.95 |
| | | | | | HOMO-1– LUMO (α) | 0.14212 | 2.02 |
| | | | | | HOMO– LUMO (α) | 0.13860 | 1.92 |
| | | | | | HOMO-5– LUMO+1(β) | -0.14008 | 1.96 |
| | | | | | HOMO– LUMO+7(β) | -0.12489 | 1.56 |
| | | | | | | | |

**Table S2.** Electrochemical data of the complexes **1-3** in in methanol:DMF (9:1). TBAHFP (0.1 M) as the supporting electrolyte; scan rate - 0.1 V/ s.

| C**omplex** | $E_{pc}$**(V)** | $E_{pa}$**(V)** | $E_{1/2}$**(V)** |
|---|---|---|---|
| 1 | -1.032 | -0.411 | -0.740 |
| 2 | -0.951 | -0.426 | -0.688 |
| 3 | - 0.919 | -0.464 | -0.691 |

**Table S3.** $k_{cat}$ values of previously reported phenoxazinone synthase-like activities of different Cu(II) complexes having salicylaldehyde derivative ligand.

| Sl no. | Catalyst | Solvent | $k_{cat}(h^{-1})$ | Ref. |
|---|---|---|---|---|
| **1** | $[Cu_4(L^4)_4]$ | MeOH | $1.21 \times 10^5$ | **S1** |
| **2** | $[CuL^5{}_2]$ | MeOH | 74.22 | **S2** |
| **3** | $[Cu_2(L^6)_3]ClO_4$ | MeOH | 78.14 | **S3** |
| **4** | $[Cu_2L^7{}_2Cl_2]$ | MeOH | $1.06\times10^3$ | **S4** |
| **5** | $[Cu_2L^7{}_2Cl_2]$ | MeCN | $2.13 \times10^2$ | **S4** |
| **6** | $[Cu_2L^7{}_2Cl_2]$ | DCM | $2.84 \times10^3$ | **S4** |
| **7** | $[CuL^8Na(NCS)]0.5H_2O$ | MeCN | 3.72 | **S5** |
| **8** | $[CuL^8Na(OClO_3)]0.25H_2O$ | MeCN | 5.17 | **S5** |
| **9** | $[CuL^8HgCl_2]$ | MeCN | 8.29 | **S5** |
| **10** | $[Cu_2(L^9)_3]ClO_4$ | MeCN | 78.14 | **S6** |
| **11** | $[Cu(L^{10})(NCS)]_n$ | DMF | 33.76 | **S7** |
| **12** | $[Cu(L^{10})(N3)]_n$ | DMF | 0.96 | **S7** |

Where the abbreviations of, $H_2L^4$ = *N*-(2-hydroxyethyl)-3-methoxysalicylaldimine; $HL^5$ = (*Z*)-2-methoxy-6-(((2-methoxyphenyl)imino) methyl)phenol; $HL^6$ = (*E*)-1-((3-(dimethylamino)-propylimino)methyl)naphthalen-2-ol); $HL^7$ = 2-((*E*)-(2-(benzylthio)ethylimino)methyl)-phenol; $H_2L^8$ = *N,N'*-bis(3-ethoxysalicylidene)-2,2-dimethylpropane-1,3-diamine; $H_2L^9$ = *N,N'*-bis(3-methoxysalicylidene)-2,2-dimethylpropane-1,3-diamine; $HL^{10}$ = (*E*)-4-chloro-2-[(2-propylaminoethylimino)methyl]phenol

Coordinates of the complex **3** using B3LYP level of theory with the basis sets 6-31G for C, H, O, S, N & Br and LANL2DZ for Cu centre.

E=-4064.8780711

| | | | |
|---|---|---|---|
| 29 | 0.637252000 | 0.551766000 | 0.250443000 |
| 35 | -6.740711000 | -0.895557000 | -0.161016000 |
| 16 | 2.446809000 | 4.919297000 | 0.069904000 |
| 8 | -1.045726000 | 1.316497000 | -0.299988000 |
| 7 | -0.227484000 | -1.138207000 | 0.786125000 |
| 7 | 1.687817000 | 2.171110000 | 0.316653000 |
| 7 | 2.407932000 | -0.620090000 | 0.311293000 |
| 1 | 2.817427000 | -0.287191000 | 1.188886000 |
| 6 | 1.973938000 | 3.327871000 | 0.201946000 |
| 6 | -1.506566000 | -1.411031000 | 0.715109000 |
| 1 | -1.836030000 | -2.404249000 | 1.039306000 |
| 6 | -2.531700000 | -0.534826000 | 0.246390000 |
| 6 | -2.256158000 | 0.791136000 | -0.238377000 |
| 6 | -4.902383000 | -0.221405000 | -0.184386000 |
| 6 | -3.872137000 | -1.015817000 | 0.259086000 |
| 1 | -4.070696000 | -2.017727000 | 0.624980000 |
| 6 | 4.742057000 | -0.905670000 | -0.608799000 |
| 6 | -4.651341000 | 1.084056000 | -0.659758000 |
| 1 | -5.475965000 | 1.697620000 | -1.003042000 |
| 6 | 0.738864000 | -2.132846000 | 1.288989000 |
| 1 | 0.321813000 | -3.148643000 | 1.269993000 |
| 1 | 0.984964000 | -1.893038000 | 2.333198000 |
| 6 | -3.360219000 | 1.576122000 | -0.684202000 |
| 1 | -3.146300000 | 2.575340000 | -1.043524000 |
| 6 | 1.997988000 | -2.050276000 | 0.421407000 |
| 1 | 2.800685000 | -2.679702000 | 0.824526000 |
| 1 | 1.768242000 | -2.398423000 | -0.590666000 |

| | | | |
|---|---|---|---|
| 6 | 5.106909000 | -2.117044000 | -1.219954000 |
| 1 | 4.404686000 | -2.617972000 | -1.881307000 |
| 6 | 3.365336000 | -0.306004000 | -0.809816000 |
| 1 | 3.411274000 | 0.784242000 | -0.861645000 |
| 1 | 2.905986000 | -0.671154000 | -1.733804000 |
| 6 | 5.674548000 | -0.255480000 | 0.219999000 |
| 1 | 5.415296000 | 0.697158000 | 0.675386000 |
| 6 | 6.372678000 | -2.673168000 | -1.001656000 |
| 1 | 6.644128000 | -3.605903000 | -1.485732000 |
| 6 | 6.938351000 | -0.811269000 | 0.441728000 |
| 1 | 7.650933000 | -0.295368000 | 1.077089000 |
| 6 | 7.289017000 | -2.022864000 | -0.167318000 |
| 1 | 8.272058000 | -2.451044000 | -0.000346000 |

Cartesian coordinates of complex **6**

| | | | |
|---|---|---|---|
| 29 | 0.416325000 | 0.546353000 | 0.325048000 |
| 8 | -1.472091000 | 1.031005000 | 1.017308000 |
| 7 | -0.487968000 | 0.645919000 | -1.689487000 |
| 7 | 2.113386000 | 0.035745000 | -0.863902000 |
| 1 | 2.543197000 | 0.981730000 | -0.963072000 |
| 6 | -1.709200000 | 0.322149000 | -1.904022000 |
| 1 | -2.000613000 | -0.098753000 | -2.886013000 |
| 6 | -2.792753000 | 0.444241000 | -0.944263000 |
| 6 | -2.591196000 | 0.777101000 | 0.462213000 |
| 6 | 4.287537000 | -1.196264000 | -0.792853000 |
| 6 | -5.053430000 | 0.579742000 | 0.755237000 |
| 6 | 0.527740000 | 0.391863000 | -2.691658000 |
| 1 | 0.114626000 | -0.052715000 | -3.616392000 |
| 1 | 0.992545000 | 1.354316000 | -2.949924000 |
| 6 | -3.791597000 | 0.812190000 | 1.261747000 |
| 1 | -3.653837000 | 1.046584000 | 2.313552000 |
| 6 | 1.613439000 | -0.532746000 | -2.110730000 |
| 1 | 2.405772000 | -0.677270000 | -2.867707000 |
| 1 | 1.173823000 | -1.506591000 | -1.871947000 |
| 6 | 4.546404000 | -2.526435000 | -1.150512000 |
| 6 | 2.999242000 | -0.829817000 | -0.080234000 |
| 1 | 3.212672000 | -0.263945000 | 0.832645000 |
| 1 | 2.447338000 | -1.734236000 | 0.182956000 |
| 6 | 5.223037000 | -0.205465000 | -1.132275000 |
| 1 | 4.996421000 | 0.827604000 | -0.869760000 |
| 6 | 5.724759000 | -2.864053000 | -1.823834000 |
| 6 | 6.398259000 | -0.543756000 | -1.803850000 |
| 1 | 7.118634000 | 0.231882000 | -2.058962000 |
| 6 | 6.655931000 | -1.875436000 | -2.150876000 |

| | | | |
|---|---|---|---|
| 1 | 7.573148000 | -2.137286000 | -2.675947000 |
| 1 | 5.914118000 | -3.900859000 | -2.097403000 |
| 1 | 3.803558000 | -3.280730000 | -0.895580000 |
| 6 | -4.090721000 | 0.192428000 | -1.431673000 |
| 6 | -5.198473000 | 0.269014000 | -0.607956000 |
| 1 | -4.214033000 | -0.061742000 | -2.481914000 |
| 1 | -5.927213000 | 0.628675000 | 1.399040000 |
| 35 | -6.980740000 | -0.061994000 | -1.334631000 |
| 8 | 1.725909000 | 1.581214000 | 1.489416000 |
| 6 | 1.916731000 | 2.859145000 | 1.393550000 |
| 6 | 1.373980000 | 3.744943000 | 2.364607000 |
| 6 | 2.725225000 | 3.442337000 | 0.298385000 |
| 6 | 1.625503000 | 5.112372000 | 2.367504000 |
| 6 | 2.962326000 | 4.856864000 | 0.362834000 |
| 6 | 2.434428000 | 5.667873000 | 1.355625000 |
| 1 | 0.756524000 | 3.282837000 | 3.131329000 |
| 1 | 1.202205000 | 5.748539000 | 3.143781000 |
| 1 | 3.577701000 | 5.296971000 | -0.424928000 |
| 1 | 2.643010000 | 6.738189000 | 1.348045000 |
| 7 | 3.183499000 | 2.652883000 | -0.682098000 |
| 1 | 3.699057000 | 3.229892000 | -1.352313000 |
| 8 | 0.121282000 | -1.741538000 | 0.279082000 |
| 6 | -0.012913000 | -2.532228000 | 1.262683000 |
| 6 | 0.671206000 | -3.858847000 | 1.280418000 |
| 6 | -0.820342000 | -2.183572000 | 2.398528000 |
| 6 | 0.399082000 | -4.715144000 | 2.406635000 |
| 6 | -1.021994000 | -3.052465000 | 3.452830000 |
| 6 | -0.415142000 | -4.335327000 | 3.454780000 |
| 1 | -1.263597000 | -1.191044000 | 2.371423000 |
| 1 | 0.879114000 | -5.696265000 | 2.417100000 |

| | | | |
|---|---|---|---|
| 1 | -1.650023000 | -2.753369000 | 4.291202000 |
| 1 | -0.585007000 | -5.015541000 | 4.288910000 |
| 7 | 1.490971000 | -4.170958000 | 0.278298000 |
| 1 | 1.870908000 | -5.106126000 | 0.474423000 |

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