

Supporting Information

High Phenoxazinone Synthase Activity of Two Mononuclear *cis*-Dichloro Cobalt(II) Complexes with Rigid Pyridyl Scaffold

Arabinda Muley,[†] Kalai Selvan Karumban,[†] Sadananda Kumbhakar, Bishnubasu Giri and Somnath Maji*

Department of Chemistry, Indian Institute of Technology, Hyderabad, Kandi, Sangareddy 502284, Telangana, India

[†] These authors contributed equally to this work.

Email address: smaji@chy.iith.ac.in (Somnath Maji)

Figure captions

Fig. S1. ^1H NMR spectra of L^1 in CDCl_3 in room temperature.

Fig. S2. FT-IR spectra of (a) [1] and (b) [2].

Fig. S3. Increase in phenoxazinone absorbance during the catalytic oxidation of (a) 0.10×10^{-2} M, (b) 0.25×10^{-2} M, (c) 0.50×10^{-2} M and (d) 0.75×10^{-2} M *o*-aminophenol with 1×10^{-4} M complex [1] at room temperature (25 °C) (left) and respective rate constant determination (right).

Fig. S4. Increase in phenoxazinone absorbance during the catalytic oxidation of (a) 0.10×10^{-2} M, (b) 0.25×10^{-2} M, (c) 0.50×10^{-2} M and (d) 0.75×10^{-2} M *o*-aminophenol with 1×10^{-4} M complex [2] at room temperature (25 °C) (left) and respective rate constant determination (right).

Fig. S5. Initial rate versus substrate concentration plot for the oxidation of *o*-aminophenol catalyzed by [2] at room temperature (25 °C).

Fig. S6. Lineweaver-Burk plots for the oxidation of *o*-aminophenol catalyzed by [2] at room temperature (25 °C).

Fig. S7. *o*-aminophenol oxidation of 10^{-2} M substrate by 10^{-4} M of $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ in methanol at room temperature (25 °C) (a) and zoomed version (b).

Fig. S8. *o*-aminophenol oxidation of 10^{-2} M substrate in methanol only (blank test) at room temperature (25 °C) (a) and zoomed version (b).

Fig. S9. ESI-MS spectra for the formation of phenoxazinone upon addition of complex to *o*-aminophenol.

Fig. S10. Evidence of adduct formation along with peroxide found via mass spectrometry (a), (c) and (e) (zoomed of (b)) for [1] and [2] with their simulated mass spectra (b), (d) and (f).

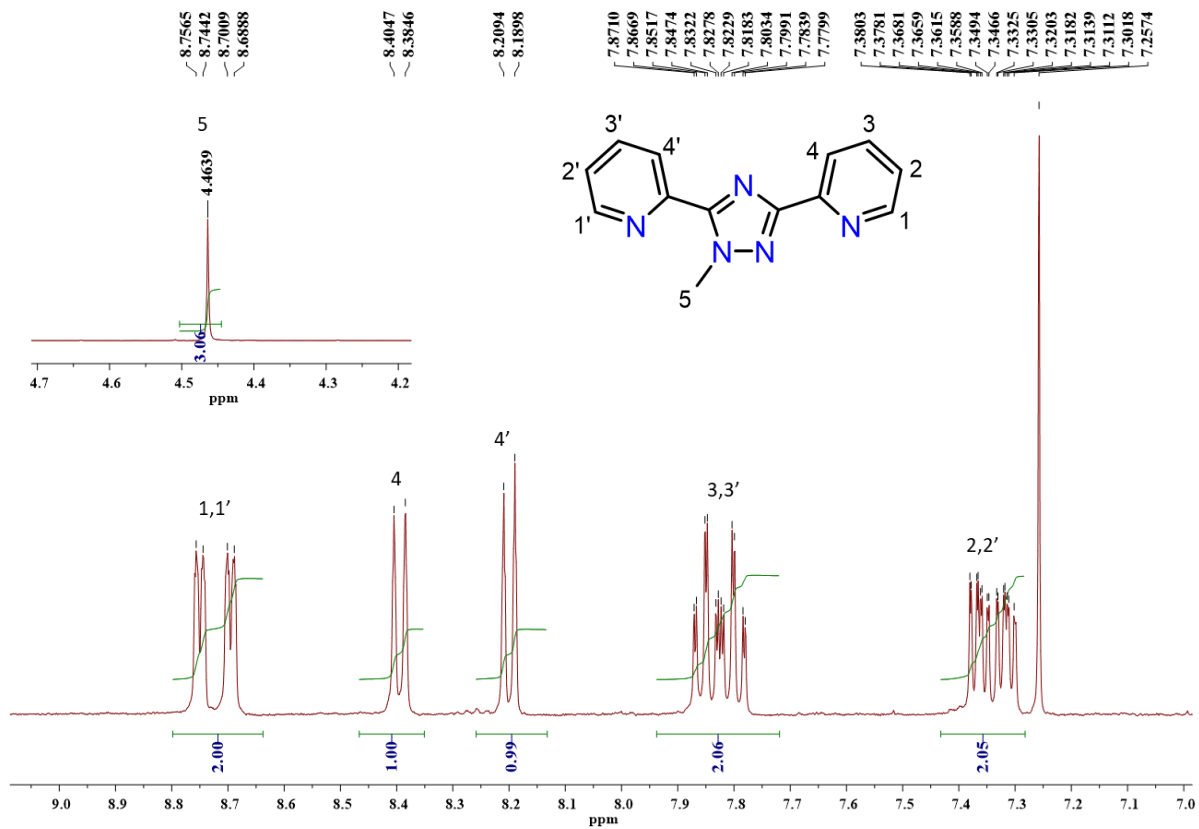


Fig. S1 ¹H NMR spectra of **L¹** in CDCl₃ in room temperature.

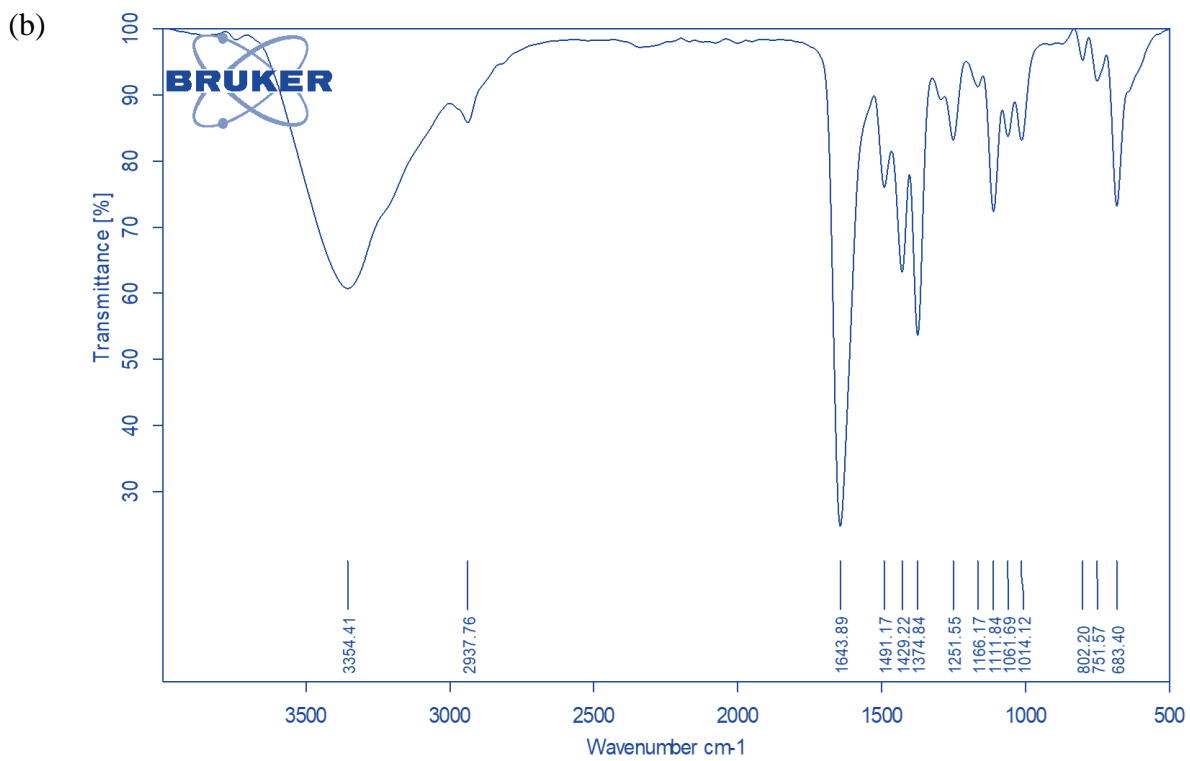
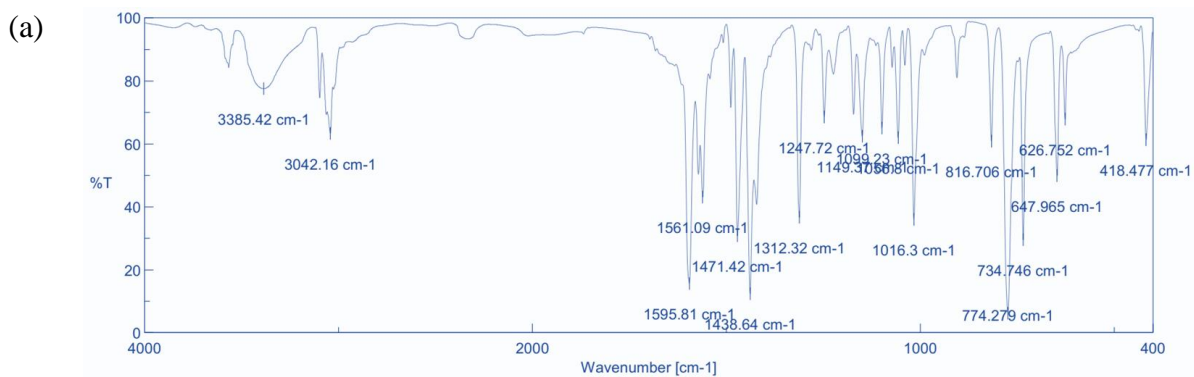


Fig. S2. FT-IR spectra of (a) [1] and (b) [2].

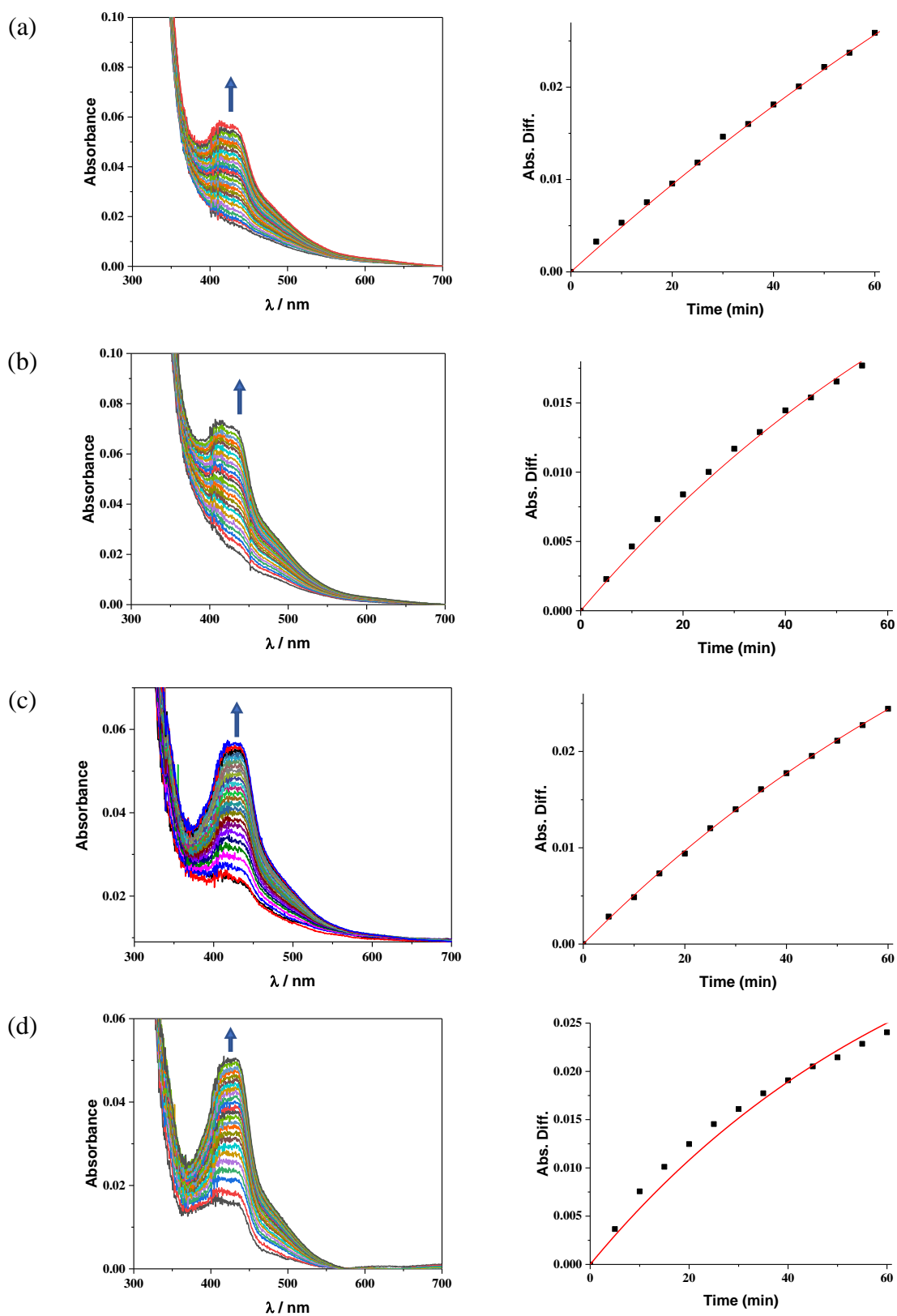


Fig. S3. Increase in phenoxazinone absorbance during the catalytic oxidation of (a) 0.10×10^{-2} M, (b) 0.25×10^{-2} M, (c) 0.50×10^{-2} M and (d) 0.75×10^{-2} M *o*-aminophenol with 1×10^{-4} M complex [1] at room temperature (25 °C) (left) and respective rate constant determination (right).

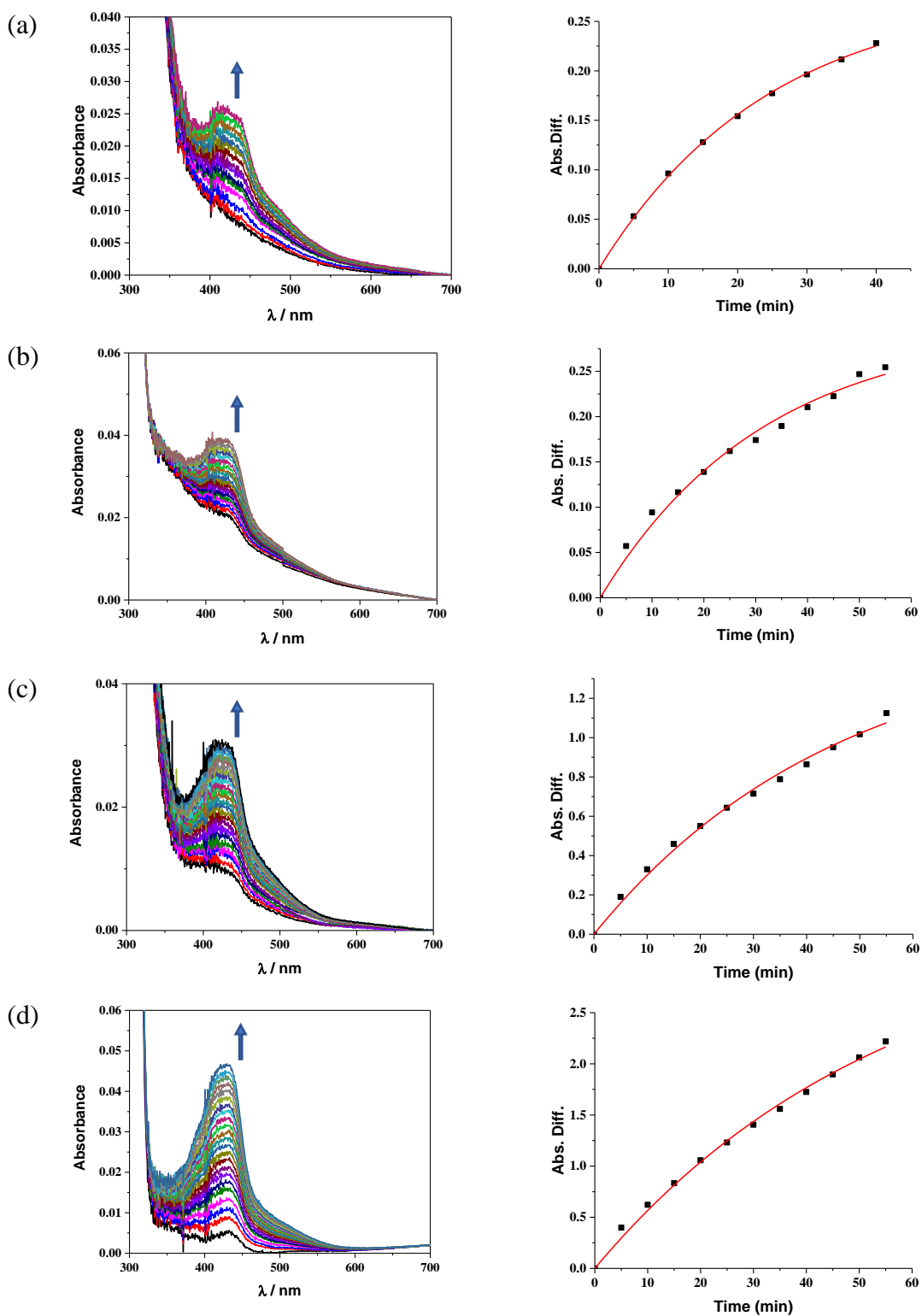


Fig. S4. Increase in phenoxazinone absorbance during the catalytic oxidation of (a) 0.10×10^{-2} M, (b) 0.25×10^{-2} M, (c) 0.50×10^{-2} M and (d) 0.75×10^{-2} M *o*-aminophenol with 1×10^{-4} M complex [2] at room temperature (25 °C) (left) and respective rate constant determination (right).

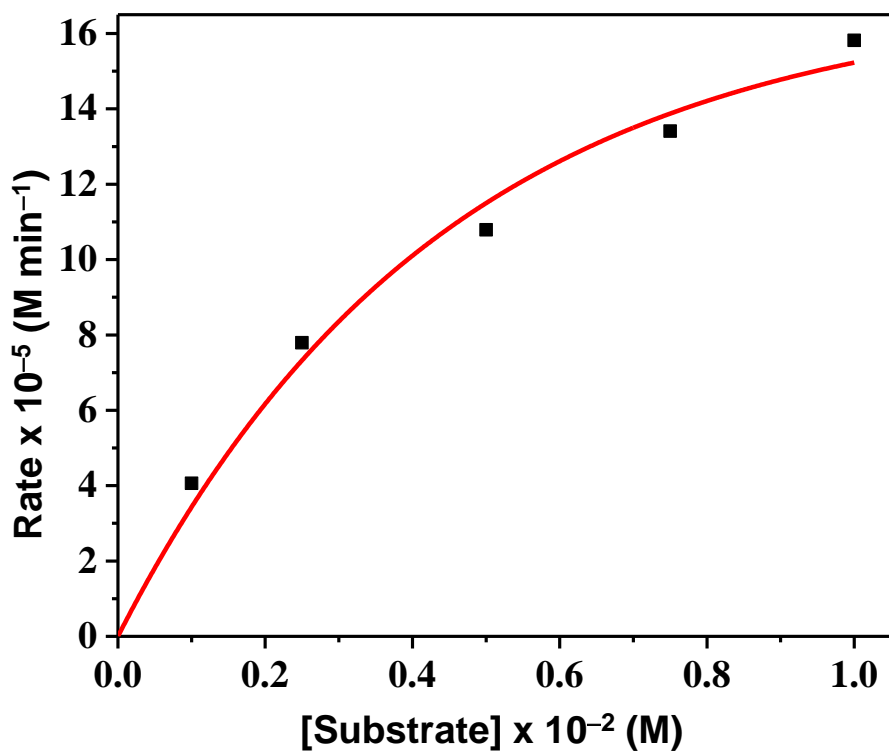


Fig. S5 Initial rate versus substrate concentration plot for the oxidation of *o*-aminophenol catalyzed by [2] at room temperature (25 °C).

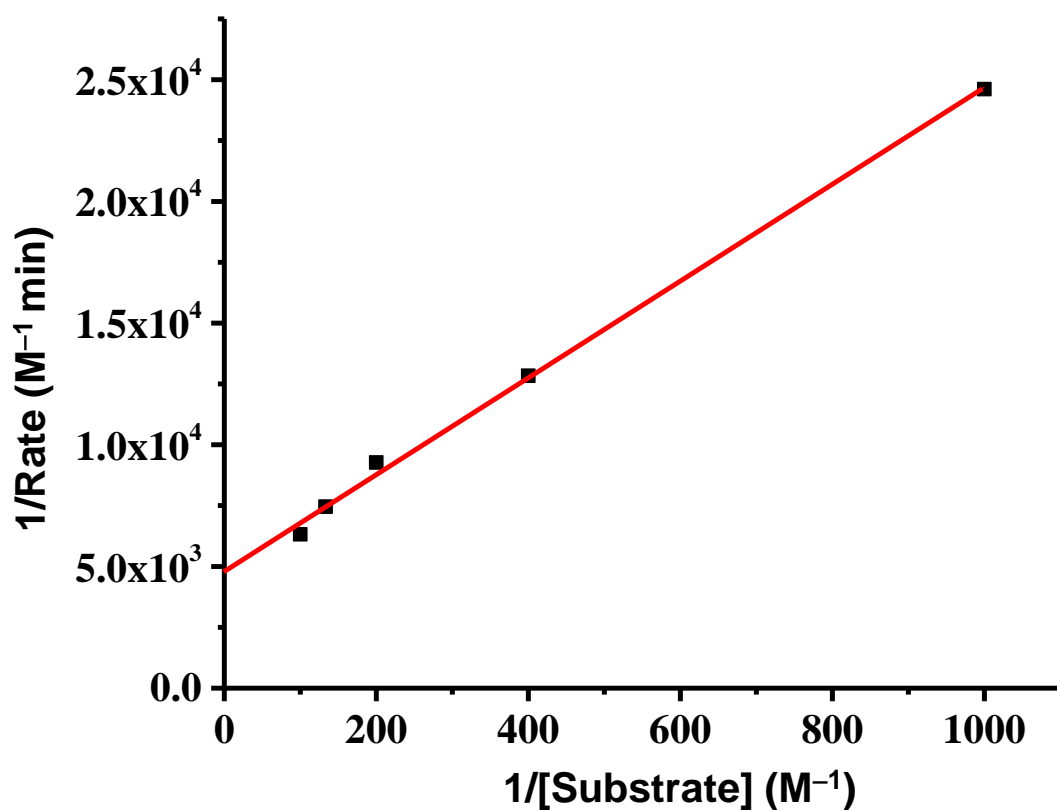


Fig. S6 Lineweaver-Burk plots for the oxidation of *o*-aminophenol catalyzed by [2] at room temperature (25 °C).

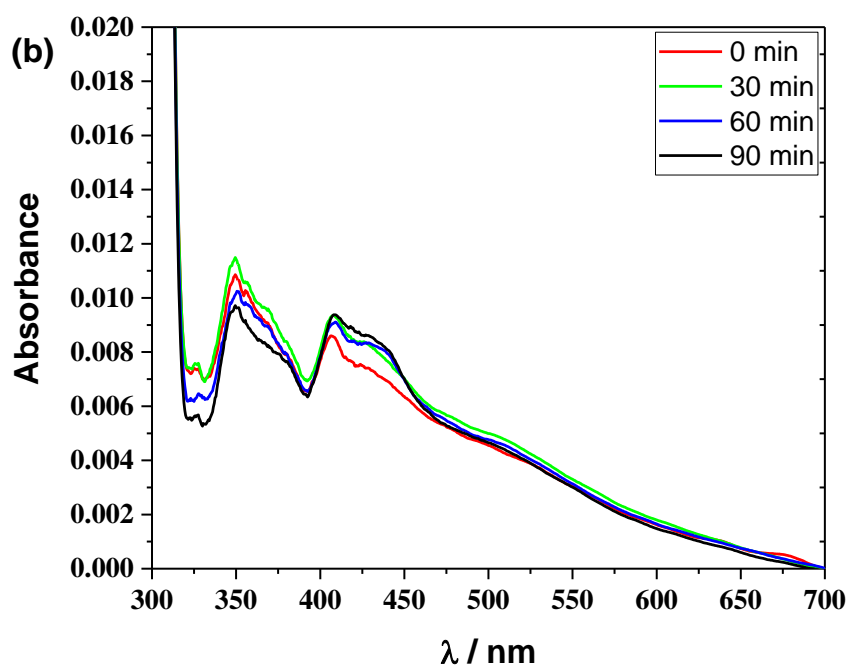
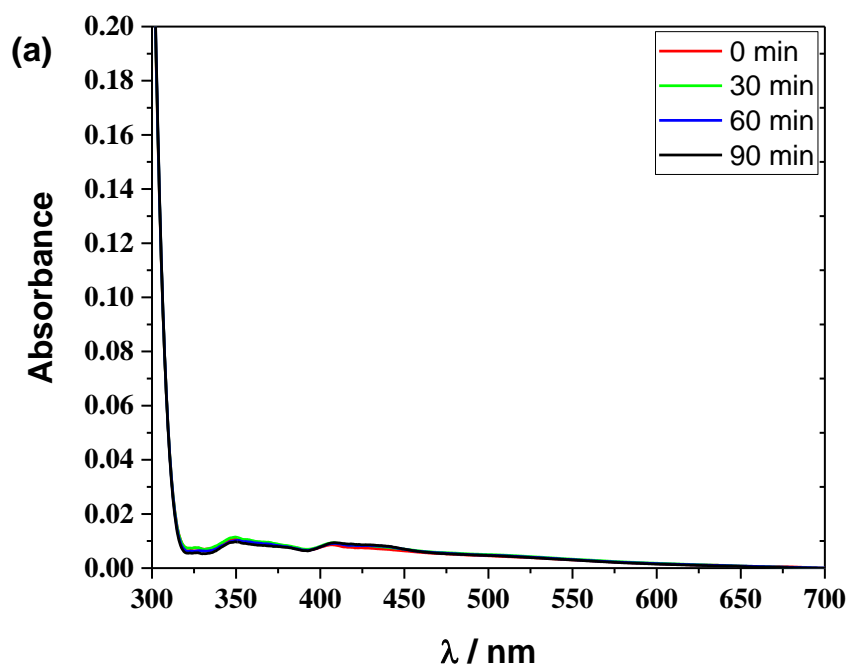


Fig. S7 o -aminophenol oxidation of 10^{-2} M substrate by 10^{-4} M of $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ in methanol at room temperature (25°C) (a) and zoomed version (b).

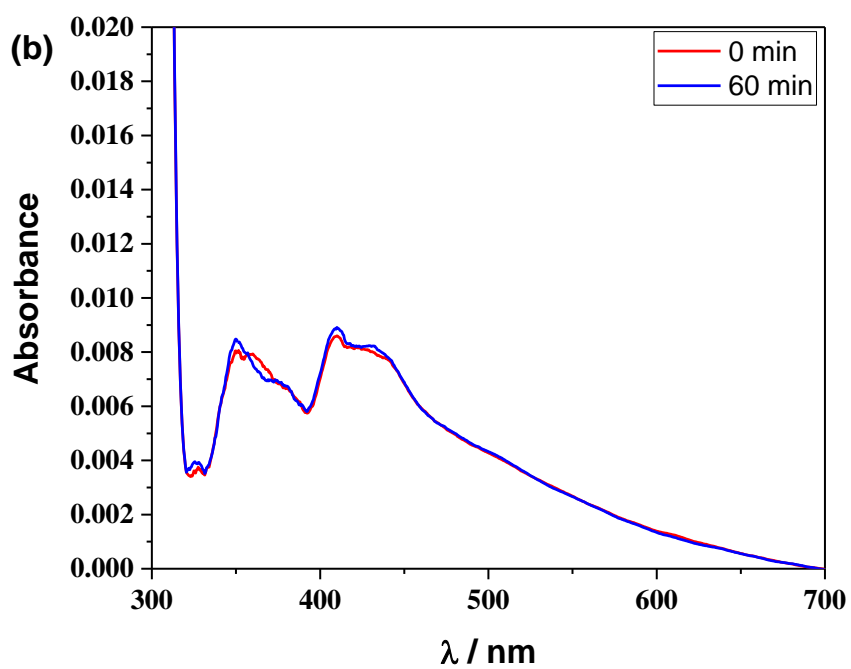
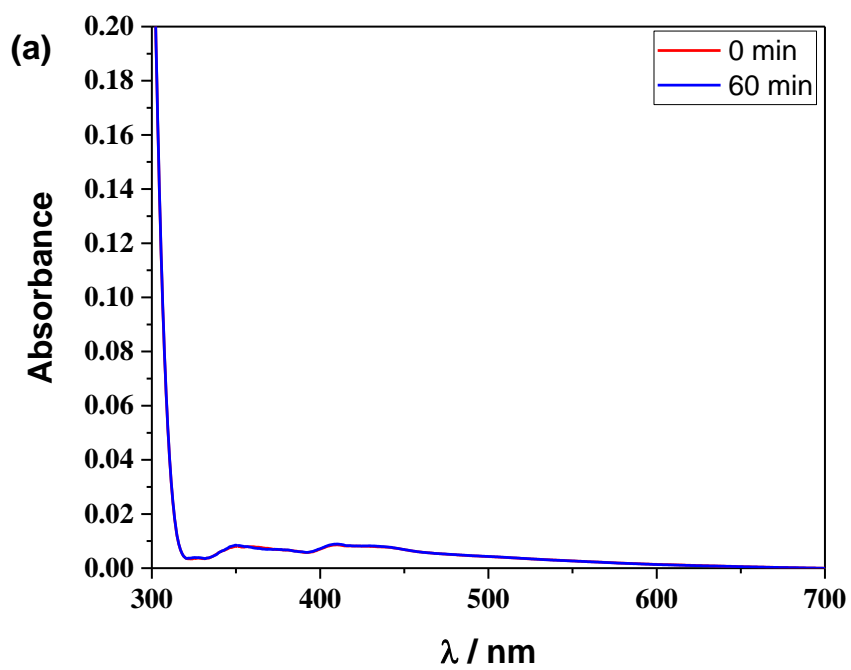


Fig. S8. *o*-aminophenol oxidation of 10⁻² M substrate in methanol only (blank test) at room temperature (25 °C) (a) and zoomed version (b).

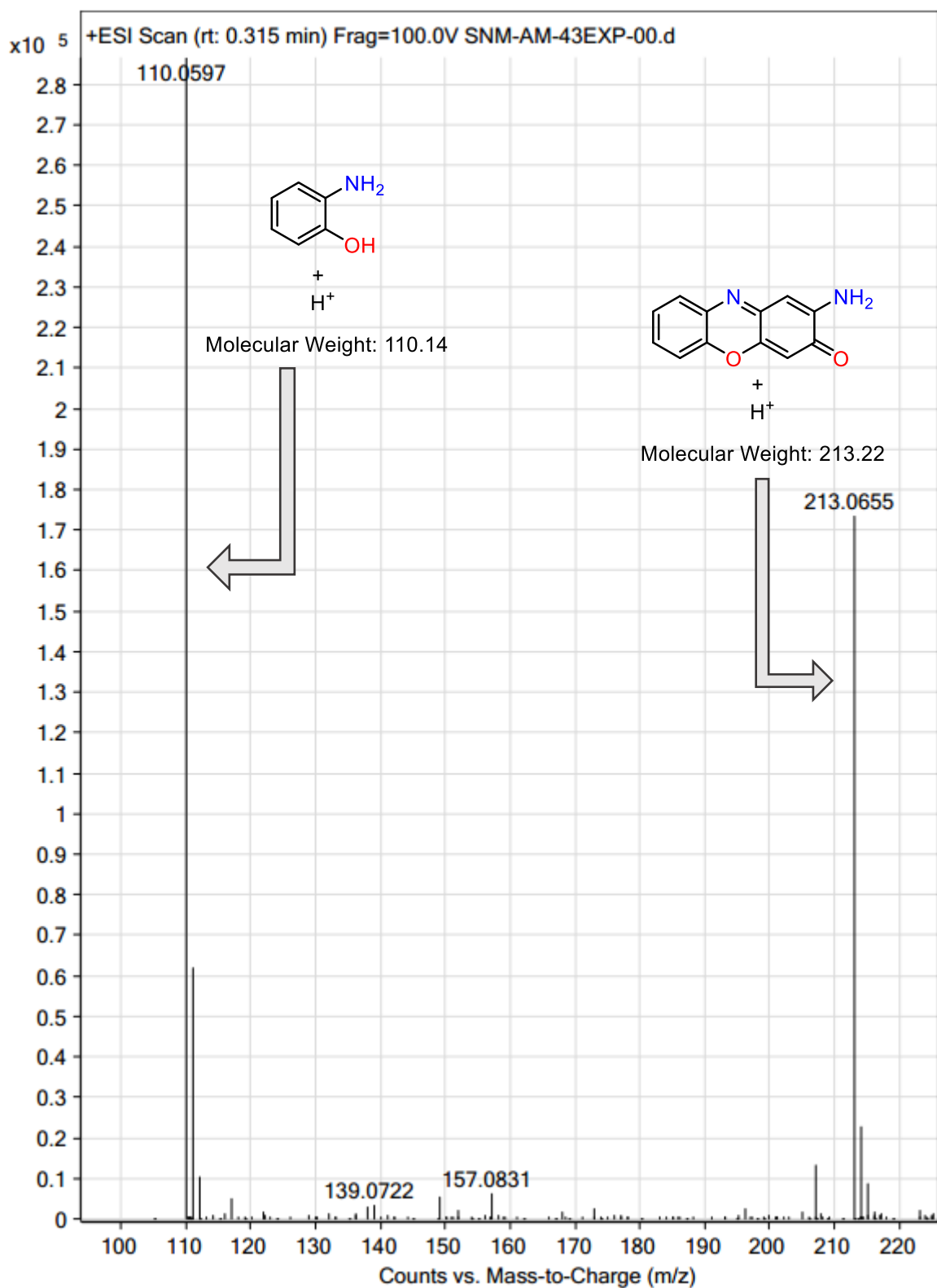
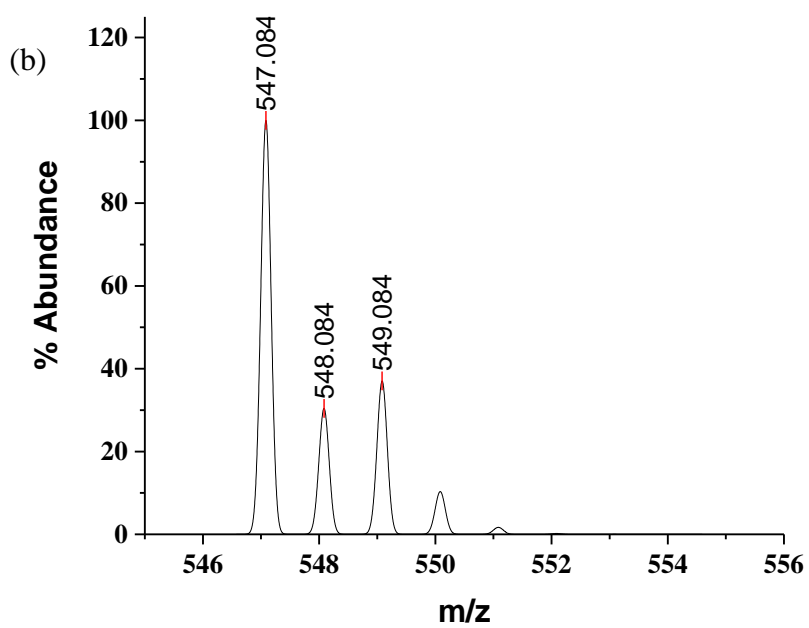
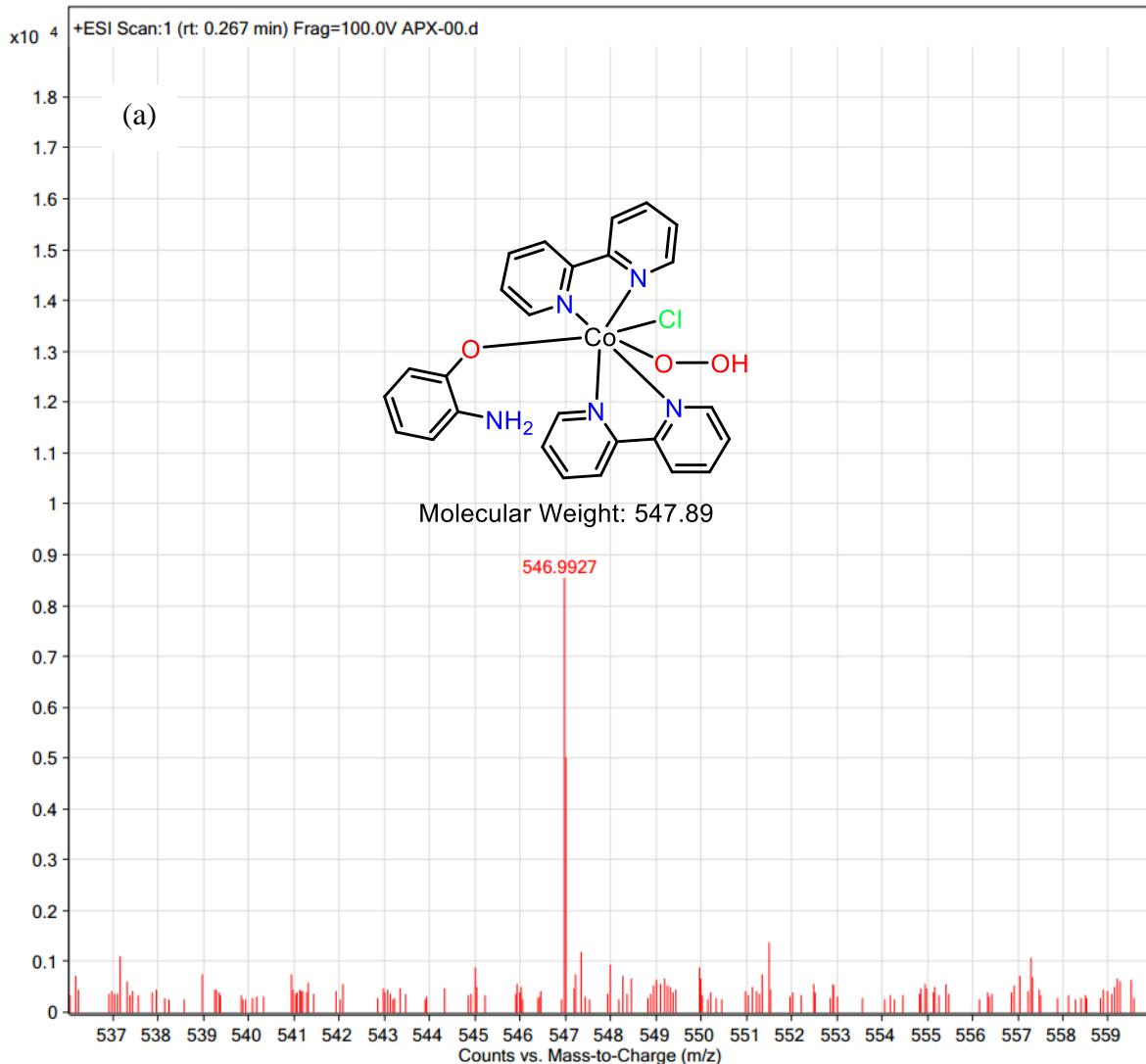
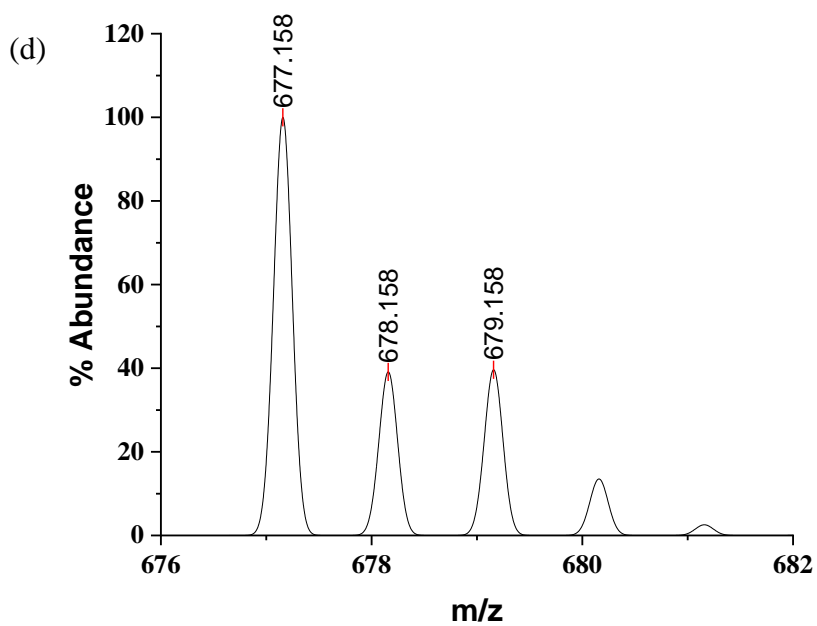
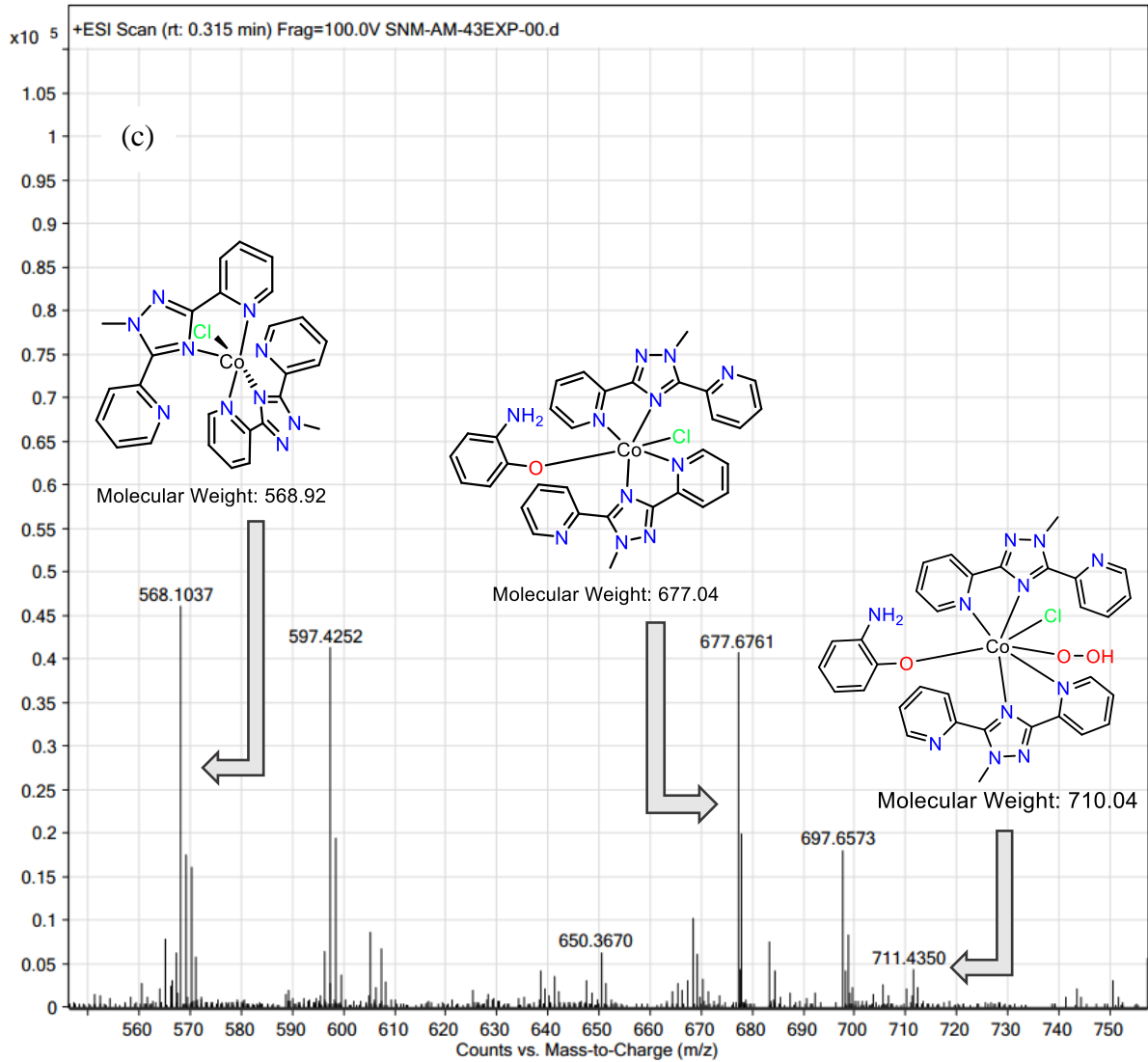


Fig. S9 ESI-MS spectra for the formation of phenoxazinone upon addition of complex to *o*-aminophenol.





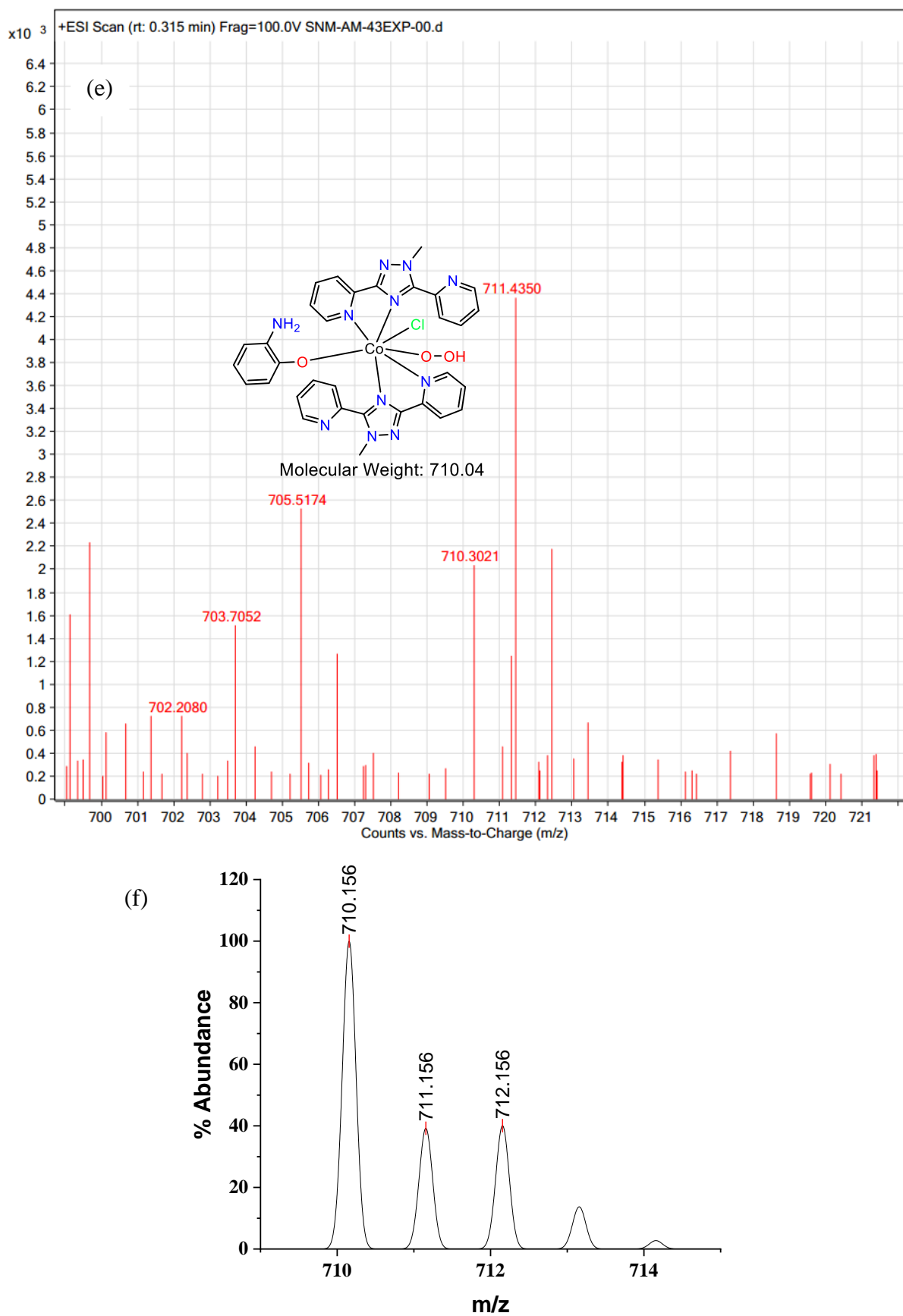


Fig. S10 Evidence of adduct formation along with peroxide found via mass spectrometry (a), (c) and (e) (zoomed of (b)) for [1] and [2] with their simulated mass spectra (b), (d) and (f).