

Supporting Information

For

Selective C₃ Nitrosation of Imidazopyridines using AgNO₃ as the NO source

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(1) General Information

^1H , ^{13}C , and DEPT NMR spectra were recorded on a 400 MHz Varian Unity Plus or Varian Mercury plus spectrometer. The chemical shift (δ) values are reported in parts per million (ppm), and the coupling constants (J) are given in Hz. The spectra were recorded using CDCl_3 as a solvent. ^1H NMR chemical shifts are referenced to tetramethylsilane (TMS) (0 ppm). ^{13}C NMR was referenced to CDCl_3 (77.0 ppm) or DMSO-d_6 (39.51 ppm). The abbreviations used are as follows: s, singlet; d, doublet; t, triplet; q, quartet; dd, doublet of doublet; ddd, doublet of doublet; dt, doublet of triplets; td, triplet of doublet; m, multiplet. Mass spectra and high-resolution mass spectra (HRMS) were measured using the ESI (FT-MS solariX) at National Sun Yat-Sen University, Kaohsiung, Taiwan. Melting points were determined on an EZ-Melt (Automated melting point apparatus). All products reported showed ^1H NMR spectra in agreement with the assigned structures. Reaction progress and product mixtures were routinely monitored by TLC using Merck TLC aluminum sheets (silica gel 60 F254). Column chromatography was carried out with 230–400 mesh silica gel 60 (Merck) and a mixture of hexane/ethyl acetate or hexane as eluent. Preparative TLC was run on Merck TLC aluminum sheets (silica gel 60 F254).

(2) Mechanistic studies:

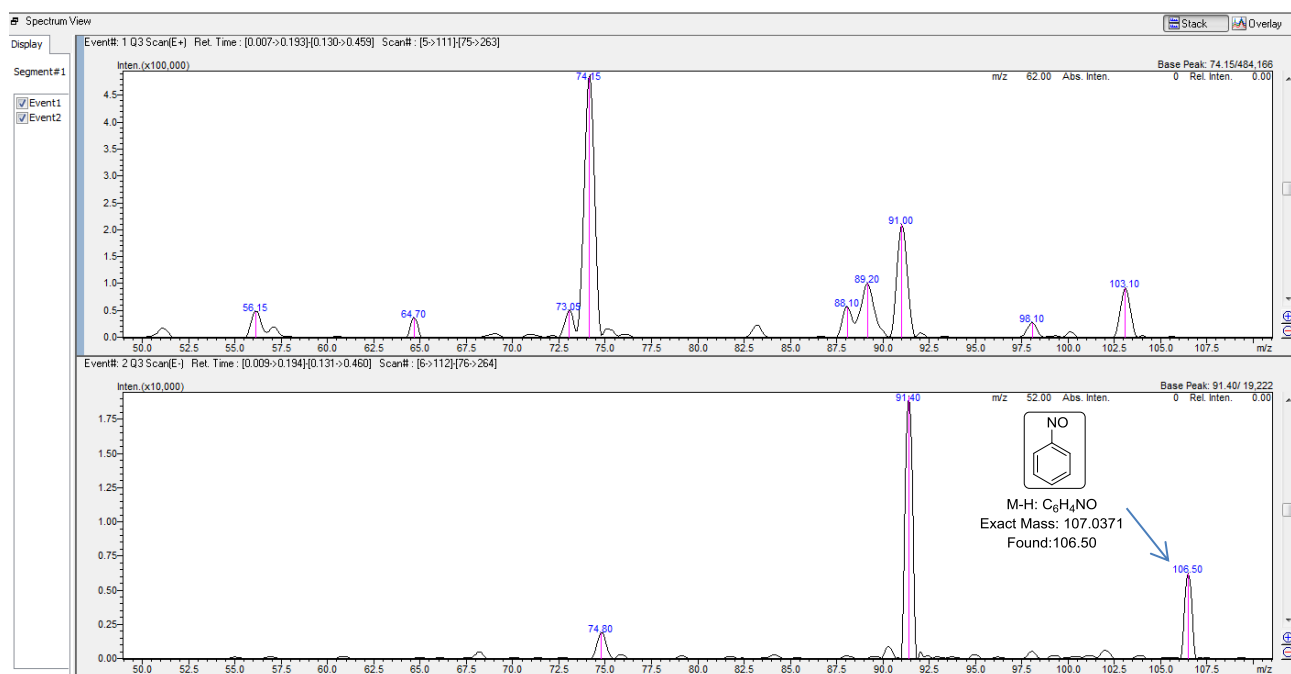
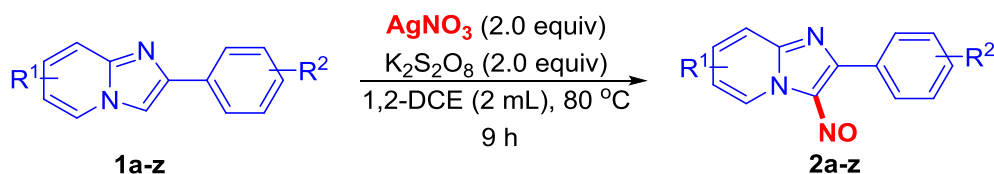


Fig S1: LC-MS observed trapping intermediate of 1, 4-Cyclohexadiene (1, 4-CHD) in the presence of starting material (1a).

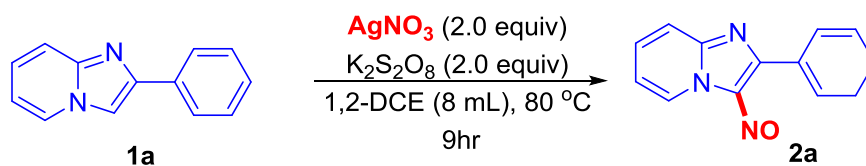
(3) Experimental Procedures

(i) The General Experimental Procedure for the Synthesis of 3-nitroso-2-phenylimidazo [1, 2-*a*] pyridine derivatives using AgNO₃ as the "NO" Source.



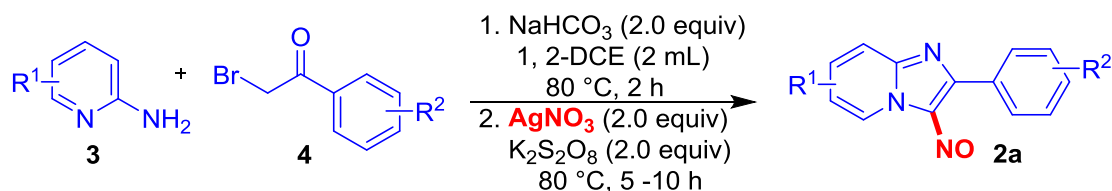
To an oven-dried sealed tube was charged with 2-phenylimidazo[1, 2-*a*]pyridine derivatives **1a-1z**¹ (0.2 mmol), AgNO₃ (2.0 equiv), K₂S₂O₈ (2.0 equiv) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of the reaction (7 ~ 9 h) by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 20 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate, and the combined ethyl acetate layer was given brine wash (1X20 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford pure heteroaryl nitrosation **2a-2z** in 65-90% yields.

(ii) The General Experimental Procedure for the Gram Scale Synthesis of 3-nitroso-2-phenylimidazo[1, 2-*a*] pyridine derivatives using AgNO₃ as the "NO" Source.



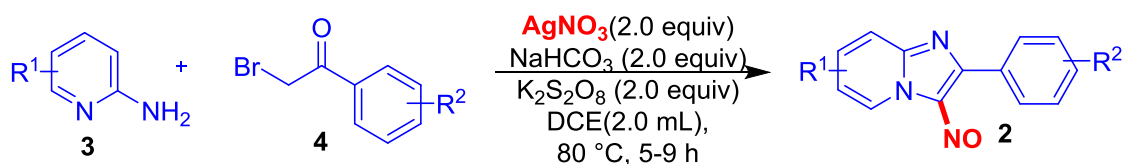
To an oven-dried sealed tube was charged with 2-phenylimidazo[1, 2-*a*]pyridine derivatives **1a** (5.15 mmol), AgNO₃ (2.0 equiv), K₂S₂O₈ (2.0 equiv) and 1, 2-Dichloroethane (8.0 mL) allowed to stir at 80 °C until the completion of the reaction (9 h) by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 30 mL of water. The water layer was extracted with (3X20 mL) of ethyl acetate, and the combined ethyl acetate layer was given brine wash (1X30 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford pure heteroaryl nitrosation **2a** in 56% yields.

(iii) The General Experimental Procedure Sequential one-spot strategy for the synthesis of 3-nitroso-2-phenylimidazo[1, 2-*a*] pyridine derivatives using AgNO₃ as the "NO" Source.



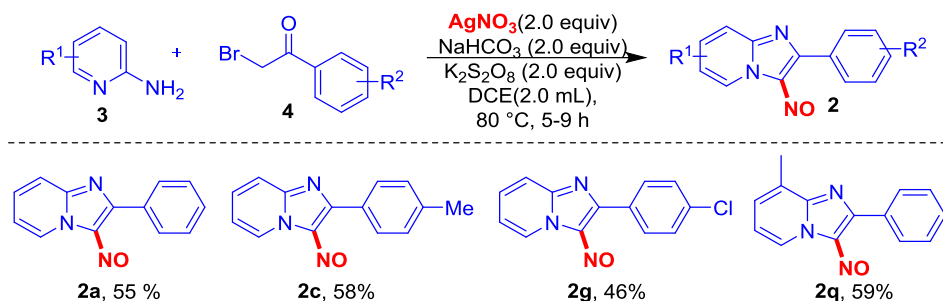
To an oven-dried sealed tube was charged with 2-aminopyridine derivatives **3** (0.2 mmol), 2-bromoacetophenone derivatives **4** (0.2 mmol), NaHCO₃ (2.0 equiv), and 1, 2-Dichloroethane (8.0 mL) allowed to stir at 80 °C for 2 h. Followed by the addition of AgNO₃ (2.0 equiv), K₂S₂O₈ (2.0 equiv), and allowed to stir at 80 °C until the completion of the reaction (5-10 h) by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 20 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate, and the combined ethyl acetate layer was given brine wash (1X20 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford pure heteroaryl nitrosation **2a**, **2c**, **2g**, **2l**, **2n**, **2q**, **2r** in 64-84% yields.

(iv) The General Experimental Procedure for the One-pot strategy for the synthesis of 3-nitroso-2-phenylimidazo [1, 2-*a*] pyridine derivatives using AgNO₃ as the "NO" Source.



To an oven-dried sealed tube was charged with 2-aminopyridine derivatives **3** (0.2 mmol), 2-bromoacetophenone derivatives **4** (0.2 mmol), AgNO₃ (2.0 equiv), NaHCO₃ (2.0 equiv), K₂S₂O₈ (2.0 equiv) and 1, 2-Dichloroethane (8.0 mL) allowed to stir at 80 °C until the completion of the reaction (5-9 h) by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 20 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate, and the combined ethyl acetate layer was given brine wash (1X20 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford pure heteroaryl nitrosation **2a**, **2c**, **2g**, **2q** 46-59% yields.

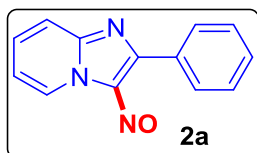
Scheme S1. One-pot strategy for the synthesis of 3-nitroso-2-phenylimidazo [1, 2-*a*] pyridine derivatives.^{a, b}



^a Reaction conditions: **3** (0.2 mmol), **4** (0.2 mmol), AgNO_3 (2.0 equiv), NaHCO_3 (2.0 equiv), $\text{K}_2\text{S}_2\text{O}_8$ (2.0 equiv), 1,2-Dichloroethane (1.0 mL), 80 °C, 5-9 h. ^b Isolated yield.

(4) Spectral Characterization

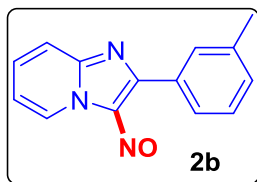
3-nitroso-2-phenylimidazo[1, 2-*a*]pyridine (2a**)**²: Following the general procedure, a 15 mL reaction tube



was charged with 2-phenylimidazo[1, 2-*a*]pyridine (**1a**) (38 mg, 0.2 mmol), AgNO_3 (0.4 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was

cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 3-nitroso-2-phenylimidazo[1, 2-*a*]pyridine (**2a**) as a green solid (40 mg, yield = 90%); Mp. 162.2-162.8 °C; ¹H NMR (400 MHz, CDCl_3) δ 9.95 (dt, J = 6.7, 1.2 Hz, 1H), 8.70 – 8.66 (m, 2H), 7.89 – 7.82 (m, 2H), 7.61 – 7.54 (m, 3H), 7.29 – 7.25 (m, 1H); ¹³C NMR (101 MHz, CDCl_3) δ 153.37, 136.09, 131.58, 131.54, 130.83, 128.84, 126.50, 119.53, 117.50.

3-nitroso-2-(*m*-tolyl)imidazo[1, 2-*a*]pyridine (2b**)**³: Following the general procedure, a 15 mL reaction tube

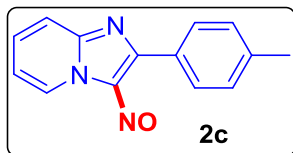


was charged with 2-(*m*-tolyl)imidazo[1, 2-*a*]pyridine (**1b**) (42 mg, 0.2 mmol), AgNO_3 (0.4 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was

cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 3-nitroso-2-(*m*-tolyl)imidazo[1, 2-*a*]pyridine (**2b**) as a green solid (39 mg, yield = 83%); Mp. 144.4-145.1 °C; ¹H NMR (400 MHz, CDCl_3) δ 9.95 (dt, J = 6.7, 1.2 Hz, 1H), 8.49

(dt, $J = 3.6, 1.8, 0.7$ Hz, 2H), 7.89 – 7.82 (m, 2H), 7.48 – 7.39 (m, 2H), 7.29 – 7.24 (m, 1H), 2.49 (d, $J = 0.7$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 160.11, 153.25, 145.61, 138.61, 136.19, 132.54, 131.29, 131.22, 128.78, 128.19, 126.56, 119.52, 117.39, 21.44.

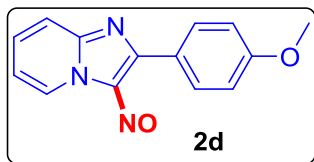
3-nitroso-2-(*p*-tolyl)imidazo[1, 2-*a*]pyridine (2c)⁴ : Following the general procedure, a 15 mL reaction tube



was charged with 2-(*p*-tolyl)imidazo[1, 2-*a*]pyridine (**1c**) (42 mg, 0.2 mmol), AgNO_3 (0.4 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the

reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 3-nitroso-2-(*p*-tolyl)imidazo[1, 2-*a*]pyridine (**2c**) as a green solid (41 mg, yield = 86%); Mp. 208.0-209.0 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.95 (dt, $J = 6.8, 1.2$ Hz, 1H), 8.61 – 8.57 (m, 2H), 7.88 – 7.81 (m, 2H), 7.39 – 7.35 (m, 2H), 7.25 (td, $J = 6.5, 2.0$ Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 160.03, 153.19, 145.78, 142.37, 136.19, 130.78, 129.67, 128.66, 126.60, 119.33, 117.32, 21.63.

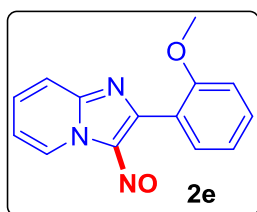
2-(4-methoxyphenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (2d)² : Following the general procedure, a 15 mL



reaction tube was charged with 2-(4-methoxyphenyl)imidazo[1, 2-*a*]pyridine (**1d**) (45 mg, 0.2 mmol), AgNO_3 (0.4 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (0.4 mmol) and 1,2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction

by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 2-(4-methoxyphenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (**2d**) as a green solid (40 mg, yield = 80%); Mp. 220.4-221.5 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.97 (dt, $J = 6.7, 1.2$ Hz, 1H), 8.71 – 8.65 (m, 2H), 7.84 – 7.80 (m, 2H), 7.22 (ddd, $J = 6.7, 4.8, 3.5$ Hz, 1H), 7.09 – 7.04 (m, 2H), 3.92 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 162.94, 159.79, 153.02, 146.10, 136.36, 132.65, 126.77, 124.08, 119.07, 117.18, 114.46, 55.48.

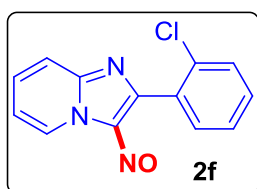
2-(2-methoxyphenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (2e)² : Following the general procedure, a 15 mL



reaction tube was charged with 2-(2-methoxyphenyl)imidazo[1, 2-*a*]pyridine (**1e**) (45 mg, 0.2 mmol), AgNO_3 (0.4 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion,

the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 2-(2-methoxyphenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (**2e**) as a green solid (38 mg, yield = 76%); Mp. 110.8-111.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.89 (dt, *J* = 6.7, 1.2 Hz, 1H), 7.95 – 7.90 (m, 2H), 7.83 (ddd, *J* = 8.7, 7.1, 1.4 Hz, 1H), 7.54 (ddd, *J* = 8.3, 7.5, 1.8 Hz, 1H), 7.29 (dd, *J* = 6.9, 1.3 Hz, 1H), 7.17 – 7.11 (m, 2H), 3.89 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 153.61, 135.45, 133.84, 132.17, 126.14, 120.75, 120.69, 119.39, 117.73, 111.82, 56.05.

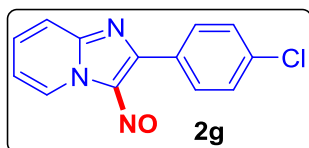
2-(2-chlorophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (2f**)²** : Following the general procedure, a 15 mL



reaction tube was charged with 2-(2-chlorophenyl)imidazo[1, 2-*a*]pyridine (**1f**) (46 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The

water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 2-(2-chlorophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (**2f**) as a green solid (37 mg, yield = 72%); Mp. 146.2-146.7 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.86 (dt, *J* = 6.6, 1.2 Hz, 1H), 7.98 – 7.85 (m, 3H), 7.62 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.49 (dtd, *J* = 19.4, 7.5, 1.6 Hz, 2H), 7.35 (td, *J* = 6.9, 1.3 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 160.94, 153.34, 145.07, 135.64, 134.25, 133.78, 131.40, 130.76, 130.58, 126.66, 126.13, 119.95, 117.92.

2-(4-chlorophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (2g**)²** : Following the general procedure, a 15 mL

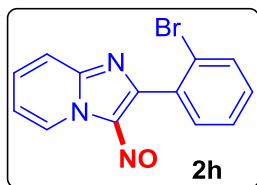


reaction tube was charged with 2-(4-chlorophenyl)imidazo[1, 2-*a*]pyridine (**1g**) (46 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After

completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 2-(4-chlorophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (**2g**) as a green solid (35 mg, yield = 68%); Mp. 219.8-220.5 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.92 (dt, *J* = 6.6, 1.2 Hz, 1H), 8.69 – 8.63 (m, 2H), 7.86 (dd, *J* = 3.7, 1.0 Hz, 2H), 7.58 – 7.48 (m, 2H), 7.31 – 7.26 (m, 1H);

^{13}C NMR (101 MHz, CDCl_3) δ 158.56, 153.17, 145.59, 138.30, 136.26, 131.96, 129.97, 129.17, 126.52, 119.75, 117.50.

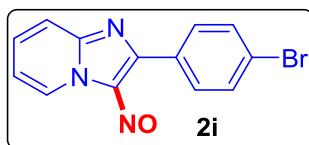
2-(2-bromophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (2h**)²** : Following the general procedure, a 15 mL



reaction tube was charged with 2-(2-bromophenyl)imidazo[1, 2-*a*]pyridine (**1h**) (55 mg, 0.2 mmol), AgNO_3 (0.4 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The

water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 2-(2-bromophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (**2h**) as a green solid (38 mg, yield = 63%); Mp. 118.6-119.2 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.84 (dt, J = 6.8, 1.2 Hz, 1H), 8.01 – 7.77 (m, 4H), 7.53 – 7.33 (m, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 162.18, 153.17, 144.94, 135.63, 133.72, 133.66, 132.79, 131.45, 127.16, 126.11, 123.35, 119.96, 117.91.

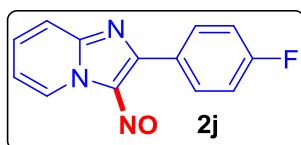
2-(4-bromophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (2i**)³** : Following the general procedure, a 15 mL



reaction tube was charged with 2-(4-bromophenyl)imidazo[1, 2-*a*]pyridine (**1i**) (55 mg, 0.2 mmol), AgNO_3 (0.4 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (0.4 mmol) and 1,2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After

completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate, and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 2-(4-bromophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (**2i**) as a green solid (50 mg, yield = 83%); Mp. 199.3-199.7 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.92 (d, J = 6.3 Hz, 1H), 8.61 – 8.56 (m, 2H), 7.86 (d, J = 2.9 Hz, 2H), 7.72 – 7.68 (m, 2H), 7.28 (d, J = 7.1 Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 145.61, 136.23, 132.14, 130.46, 126.96, 126.55, 119.78, 117.54.

2-(4-fluorophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (2j**)²** : Following the general procedure, a 15 mL

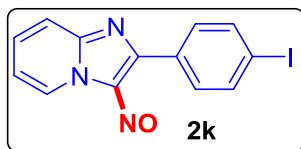


reaction tube was charged with 2-(4-fluorophenyl)imidazo[1, 2-*a*]pyridine (**1j**) (42 mg, 0.2 mmol), AgNO_3 (0.4 mmol), $\text{K}_2\text{S}_2\text{O}_8$ (0.4 mmol) and 1,2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After

completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced

pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 2-(4-fluorophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (**2j**) as a green solid (31 mg, yield = 65%); Mp. 120-121 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.93 (dt, *J* = 6.7, 1.2 Hz, 1H), 8.80 – 8.66 (m, 2H), 7.90 – 7.84 (m, 2H), 7.32 – 7.22 (m, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 166.65, 164.40 (*J_F* = 252 Hz), 158.76, 153.05, 145.64, 136.37, 133.06, 132.97 (*J_F* = 8.7 Hz), 127.66 (*J_F* = 3.1 Hz), 126.61, 119.66, 117.42, 116.22 (d, *J_F* = 21.4 Hz), 116.01.

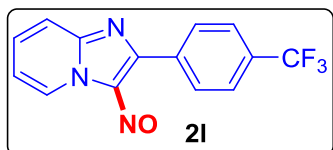
2-(4-iodophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (2k**)** : Following the general procedure, a 15 mL



reaction tube was charged with 2-(4-iodophenyl)imidazo[1, 2-*a*]pyridine (**1k**) (64 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After

completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 2-(4-iodophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (**2k**) as a green solid (57 mg, yield = 82%); Mp. 194.8-195.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.90 (dt, *J* = 6.7, 1.2 Hz, 1H), 8.47 – 8.35 (m, 2H), 7.92 – 7.82 (m, 4H), 7.31 – 7.25 (m, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 158.68, 153.07, 145.51, 138.11, 136.28, 132.12, 130.89, 126.52, 119.80, 117.50, 99.52. HRMS (ESI) calcd for C₁₃H₉N₃O₁ [M + H]⁺: 349.9790; found: 349.9792.

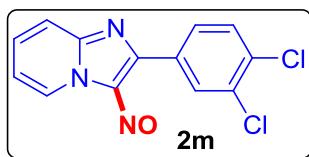
3-nitroso-2-(4-(trifluoromethyl)phenyl)imidazo[1, 2-*a*]pyridine (2l**)³** : Following the general procedure, a



15 mL reaction tube was charged with 2-(4-(trifluoromethyl)phenyl)imidazo[1, 2-*a*]pyridine (**1l**) (52 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of

reaction by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 3-nitroso-2-(4-(trifluoromethyl)phenyl)imidazo[1, 2-*a*]pyridine (**2l**) as a green solid (39 mg, yield = 68%); Mp. 163.7-164.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.91 (dt, *J* = 6.7, 1.2 Hz, 1H), 8.82 (dt, *J* = 7.9, 0.9 Hz, 2H), 7.92 – 7.79 (m, 4H), 7.32 (td, *J* = 6.6, 2.0 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 158.01, 153.36, 145.41, 136.23, 134.82, 131.00 (*q*, *J_{CF3}* = 32.4 Hz), 126.43, 125.72 (*q*, *J_{CF3}* = 3.7 Hz), 125.69, 125.65, 125.61, 120.15 (*q*, *J_{CF3}* = 242.2 Hz), 117.73.

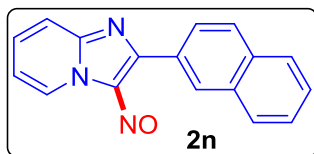
2-(3,4-dichlorophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (2m)³ : Following the general procedure, a 15 mL



reaction tube was charged with 2-(3,4-dichlorophenyl)imidazo[1, 2-*a*]pyridine (**1m**) (53 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction

by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 2-(3,4-dichlorophenyl)-3-nitrosoimidazo[1, 2-*a*]pyridine (**2m**) as a green solid (44 mg, yield = 75%); Mp. 194.7-195.4 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.89 (dt, *J* = 6.8, 1.2 Hz, 1H), 8.82 (d, *J* = 2.0 Hz, 1H), 8.58 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.88 – 7.85 (m, 2H), 7.63 (d, *J* = 8.5 Hz, 1H), 7.30 (dt, *J* = 6.7, 4.2 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 153.11, 145.41, 136.30, 136.23, 133.36, 132.10, 131.43, 130.87, 129.73, 126.45, 120.05, 117.62.

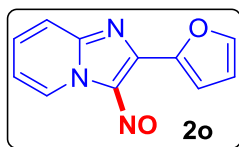
2-(naphthalen-2-yl)-3-nitrosoimidazo[1, 2-*a*]pyridine (2n)⁴ : Following the general procedure, a 15 mL



reaction tube was charged with 2-(naphthalen-2-yl)imidazo[1, 2-*a*]pyridine (**1n**) (38 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction

by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 2-(naphthalen-2-yl)-3-nitrosoimidazo[1, 2-*a*]pyridine (**2n**) as a green solid (41 mg, yield = 76%); Mp. 206.2-206.7 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.97 (d, *J* = 5.9 Hz, 1H), 9.33 – 9.29 (m, 1H), 8.76 (dd, *J* = 8.7, 1.6 Hz, 1H), 8.06 – 7.99 (m, 2H), 7.94 – 7.85 (m, 3H), 7.57 (dddd, *J* = 16.6, 8.1, 6.8, 1.3 Hz, 2H), 7.26 (s, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 159.82, 145.83, 136.18, 134.86, 133.27, 132.16, 129.55, 128.92, 128.47, 127.91, 127.74, 126.60, 126.59, 126.57, 119.52, 117.47.

2-(furan-2-yl)-3-nitrosoimidazo[1, 2-*a*]pyridine (2o)² : Following the general procedure, a 15 mL reaction

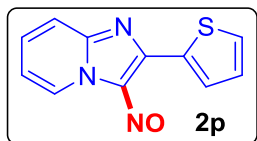


tube was charged with 2-(furan-2-yl)imidazo[1, 2-*a*]pyridine (**1o**) (37 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture

was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude

compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 2-(furan-2-yl)-3-nitrosoimidazo[1, 2-*a*]pyridine (**2o**) as a green solid (36 mg, yield = 85%); Mp. 193.8-194.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.87 (dt, *J* = 6.7, 1.2 Hz, 1H), 7.88 – 7.81 (m, 4H), 7.29 – 7.23 (m, 1H), 6.70 (dd, *J* = 3.5, 1.7 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 151.11, 147.16, 146.55, 146.46, 136.43, 126.46, 119.45, 118.87, 117.52, 113.34.

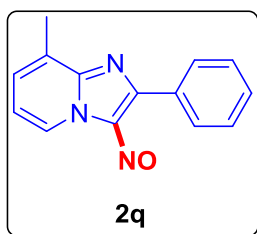
3-nitroso-2-(thiophen-2-yl)imidazo[1, 2-*a*]pyridine (2p**)²** : Following the general procedure, a 15 mL



reaction tube was charged with 2-(thiophen-2-yl)imidazo[1, 2-*a*]pyridine (**1p**) (40 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the

reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 3-nitroso-2-(thiophen-2-yl)imidazo[1, 2-*a*]pyridine (**2p**) as a green solid (37 mg, yield = 81%); Mp. 190.8-191.4 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.88 (dt, *J* = 6.7, 1.2 Hz, 1H), 8.49 (dd, *J* = 3.8, 1.2 Hz, 1H), 7.85 – 7.78 (m, 2H), 7.74 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.29 – 7.21 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 155.71, 146.34, 136.51, 134.15, 133.35, 133.03, 129.10, 126.61, 119.20, 117.16.

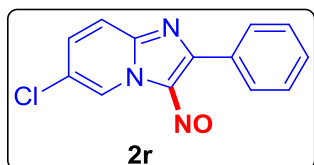
8-methyl-3-nitroso-2-phenylimidazo[1, 2-*a*]pyridine (2q**)⁴** : Following the general procedure, a 15 mL



reaction tube was charged with 8-methyl-2-phenylimidazo[1, 2-*a*]pyridine (**1q**) (42 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1,2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl

acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 8-methyl-3-nitroso-2-phenylimidazo[1, 2-*a*]pyridine (**2q**) as a green solid (37 mg, yield = 78%); Mp. 131.4-131.9 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.81 (d, *J* = 6.8 Hz, 1H), 8.73 – 8.65 (m, 2H), 7.63 (dt, *J* = 7.2, 1.2 Hz, 1H), 7.58 – 7.52 (m, 3H), 7.15 (t, *J* = 7.0 Hz, 1H), 2.76 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 159.37, 153.76, 145.58, 135.42, 131.84, 131.33, 130.83, 128.74, 127.92, 124.24, 119.42, 16.51.

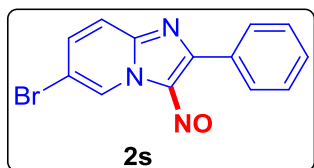
6-chloro-3-nitroso-2-phenylimidazo[1, 2-*a*]pyridine (2r)² : Following the general procedure, a 15 mL



reaction tube was charged with 6-chloro-2-phenylimidazo[1, 2-*a*]pyridine (**1r**) (46 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with

10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 6-chloro-3-nitroso-2-phenylimidazo[1, 2-*a*]pyridine (**2r**) as a green solid (41 mg, yield = 80%); Mp. 213.2-214.0 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.02 (t, *J* = 1.4 Hz, 1H), 8.69 – 8.64 (m, 2H), 7.80 (d, *J* = 1.4 Hz, 2H), 7.63 – 7.54 (m, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 159.81, 153.13, 143.78, 136.64, 131.82, 131.25, 130.81, 128.94, 127.45, 124.42, 117.76.

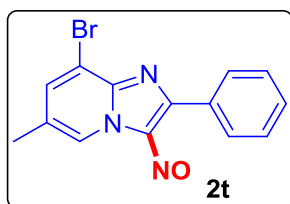
6-bromo-3-nitroso-2-phenylimidazo[1, 2-*a*]pyridine (2s)³ : Following the general procedure, a 15 mL



reaction tube was charged with 6-bromo-2-phenylimidazo[1, 2-*a*]pyridine (**1s**) (55 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with

10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 6-bromo-3-nitroso-2-phenylimidazo[1, 2-*a*]pyridine (**2s**) as a green solid (47 mg, yield = 78%); Mp. 217.3-218.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.10 (dd, *J* = 1.9, 0.8 Hz, 1H), 8.68 – 8.65 (m, 2H), 7.90 (dd, *J* = 9.2, 2.0 Hz, 1H), 7.74 (dd, *J* = 9.3, 0.8 Hz, 1H), 7.63 – 7.54 (m, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 159.62, 152.95, 143.93, 138.96, 131.82, 131.22, 130.82, 128.94, 126.42, 118.05, 113.88, 77.32, 77.00, 76.68.

8-bromo-6-methyl-3-nitroso-2-phenylimidazo[1, 2-*a*]pyridine (2t)² : Following the general procedure, a 15

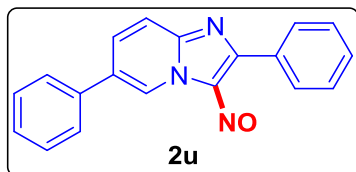


mL reaction tube was charged with 8-bromo-6-methyl-2-phenylimidazo[1, 2-*a*]pyridine (**1t**) (57 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1,2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was cooled to room temperature and

diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was

purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 8-bromo-6-methyl-3-nitroso-2-phenylimidazo[1, 2-*a*]pyridine (**2t**) as a green solid (48 mg, yield = 76%); Mp. 168.2-169.6 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.13 (s, 1H), 9.06 – 9.04 (m, 2H), 8.29 (s, 1H), 7.94 (dd, *J* = 8.0, 6.8 Hz, 3H), 2.80 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 159.98, 140.71, 131.75, 131.33, 131.01, 130.74, 128.83, 111.71, 18.16.

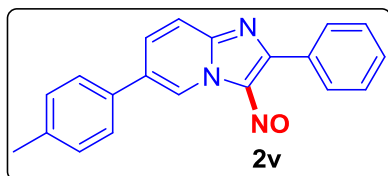
3-nitroso-2,6-diphenylimidazo[1, 2-*a*]pyridine (2u**)** : Following the general procedure, a 15 mL reaction



tube was charged with 2,6-diphenylimidazo[1, 2-*a*]pyridine (**1u**) (54 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was cooled to room temperature and diluted

with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 3-nitroso-2, 6-diphenylimidazo[1, 2-*a*]pyridine (**2u**) as a green solid (48 mg, yield = 81%); Mp. 171.6-172.3 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.21 (dd, *J* = 1.9, 0.9 Hz, 1H), 8.71 – 8.68 (m, 2H), 8.09 (dd, *J* = 9.1, 1.9 Hz, 1H), 7.93 (dd, *J* = 9.1, 0.9 Hz, 1H), 7.63 – 7.45 (m, 8H); ¹³C NMR (101 MHz, CDCl₃) δ 135.99, 134.48, 131.68, 131.43, 130.84, 129.43, 129.03, 128.89, 127.15, 123.91, 117.19. HRMS (ESI) calcd for C₁₉ H₁₄N₃O [M + H]⁺: 300.1137; found: 300.1138.

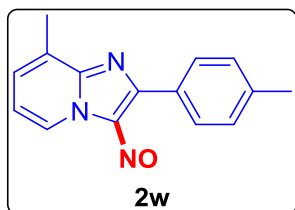
3-nitroso-2-phenyl-6-(*p*-tolyl)imidazo[1, 2-*a*]pyridine (2v**)** : Following the general procedure, a 15 mL



reaction tube was charged 2-phenyl-6-(*p*-tolyl)imidazo[1, 2-*a*]pyridine (**1v**) (57 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was cooled to room

temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 3-nitroso-2-phenyl-6-(*p*-tolyl)imidazo[1, 2-*a*]pyridine (**2v**) as a green solid (49 mg, yield = 79%); Mp. 221.5-222.4 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.21 (s, 1H), 8.71 (d, *J* = 7.3 Hz, 2H), 8.12 – 8.08 (m, 1H), 7.95 (d, *J* = 9.0 Hz, 1H), 7.64 – 7.48 (m, 6H), 7.37 – 7.33 (m, 2H), 2.45 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 139.27, 136.09, 134.65, 132.38, 131.76, 130.85, 130.16, 128.93, 126.98, 123.77, 117.05, 21.21. HRMS (ESI) calcd for C₂₀H₁₆N₃O [M + H]⁺: 314.1293; found: 314.1296

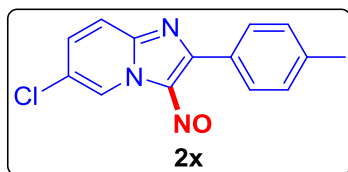
8-methyl-3-nitroso-2-(*p*-tolyl)imidazo[1, 2-*a*]pyridine (2w)³ : Following the general procedure, a 15 mL



reaction tube was charged with 8-methyl-2-(*p*-tolyl)imidazo[1, 2-*a*]pyridine (**1w**) (44 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was cooled to room temperature and diluted with

10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 8-methyl-3-nitroso-2-(*p*-tolyl)imidazo[1, 2-*a*]pyridine (**2w**) as a green solid (35 mg, yield = 69%); Mp. 169.2-170.1 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.83 (d, *J* = 6.4 Hz, 1H), 8.63 – 8.57 (m, 2H), 7.65 (d, *J* = 7.1 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.15 (t, *J* = 6.9 Hz, 1H), 2.76 (s, 3H), 2.46 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 159.71, 145.99, 142.15, 135.79, 130.82, 129.61, 128.99, 127.87, 124.67, 119.30, 21.65, 16.55.

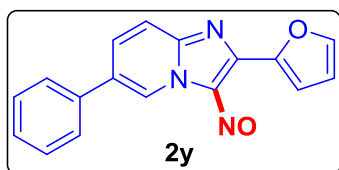
6-chloro-3-nitroso-2-(*p*-tolyl)imidazo[1, 2-*a*]pyridine (2x)² : Following the general procedure, a 15 mL



reaction tube was charged with 6-chloro-2-(*p*-tolyl)imidazo[1, 2-*a*]pyridine (**1x**) (49 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was cooled to room

temperature and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 6-chloro-3-nitroso-2-(*p*-tolyl)imidazo[1,2-*a*]pyridine (**2x**) as a green solid (43 mg, yield = 79%); Mp. 228.0-229.0 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.99 (t, *J* = 1.5 Hz, 1H), 8.57 – 8.53 (m, 2H), 7.76 (d, *J* = 1.5 Hz, 2H), 7.37 – 7.33 (m, 2H), 2.45 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 159.69, 152.91, 143.80, 142.65, 136.68, 130.72, 129.75, 128.33, 127.18, 124.44, 117.55, 21.64.

2-(furan-2-yl)-3-nitroso-6-phenylimidazo[1, 2-*a*]pyridine (2y) : Following the general procedure, a 15 mL

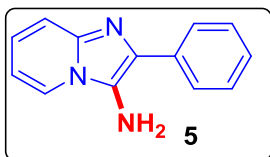


reaction tube was charged with 2-(furan-2-yl)-6-phenylimidazo[1, 2-*a*]pyridine (**1y**) (52 mg, 0.2 mmol), AgNO₃ (0.4 mmol), K₂S₂O₈ (0.4 mmol) and 1, 2-Dichloroethane (1.0 mL) allowed to stir at 80 °C until the completion of reaction by TLC. After completion, the reaction mixture was cooled to room temperature

and diluted with 10 mL of water. The water layer was extracted with (3X10 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1X10 mL). The final ethyl acetate layer was dried over sodium sulfate and concentrated under reduced pressure to get the crude compound. The obtained crude was

purified using column chromatography by eluting from (Hex/EA = 8/2) to afford the corresponding 2-(furan-2-yl)-3-nitroso-6-phenylimidazo[1, 2-*a*]pyridine (**2y**) as a green solid (47 mg, yield = 81%); Mp. 198.5-199.2 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.14 (dd, *J* = 1.9, 0.9 Hz, 1H), 8.06 (dd, *J* = 9.0, 1.9 Hz, 1H), 7.90 – 7.86 (m, 2H), 7.83 (dd, *J* = 3.5, 0.7 Hz, 1H), 7.61 – 7.58 (m, 2H), 7.55 – 7.45 (m, 3H), 6.70 (dd, *J* = 3.5, 1.7 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 151.22, 147.17, 146.66, 136.16, 135.30, 134.32, 129.43, 129.04, 127.11, 123.76, 118.84, 117.28, 113.38. HRMS (ESI) calcd for C₁₇H₁₂N₃O₂ [M + H]⁺: 290.0930; found: 290.0933.

2-phenylimidazo[1, 2-*a*]pyridin-3-amine (5**)²**: To a stirred solution of **2a** (0.1 g, 0.45 mmol) in glacial acetic



acid (2 mL) was added iron powder (0.075 g, 1.35 mmol). The resulting suspension was stirred at 100 °C for 3 h. After completion of the reaction (as determined by TLC), the reaction mixture was filtered through a bed of celite to remove the iron residue,

which was washed with ethyl acetate (30 mL). The filtrate was partitioned with 2 M KOH, and the basic layer was further extracted with ethyl acetate (3 × 25 mL). The combined organic extracts were washed with brine (35 mL), dried with anhydrous Na₂SO₄, and concentrated under reduced pressure. The obtained crude was purified using column chromatography by eluting from (Hex/EA = 6/4) to afford the corresponding 2-phenylimidazo[1, 2-*a*]pyridin-3-amine (**3**) as a yellow solid (88 mg, yield = 86%); Mp. 119-121 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.99 (d, *J* = 6.8 Hz, 1H), 7.94 (d, *J* = 7.6 Hz, 2H), 7.53 (d, *J* = 9.2 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.29 (dd, *J* = 14.8, 7.2 Hz, 1H), 7.09 (d, *J* = 7.6 Hz, 1H), 6.78 (d, *J* = 6.8 Hz, 1H), 3.51 (s, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 140.69, 134.05, 132.49, 128.67, 128.29, 127.17, 127.05, 126.90, 123.43, 122.76, 121.88, 117.04, 111.79.

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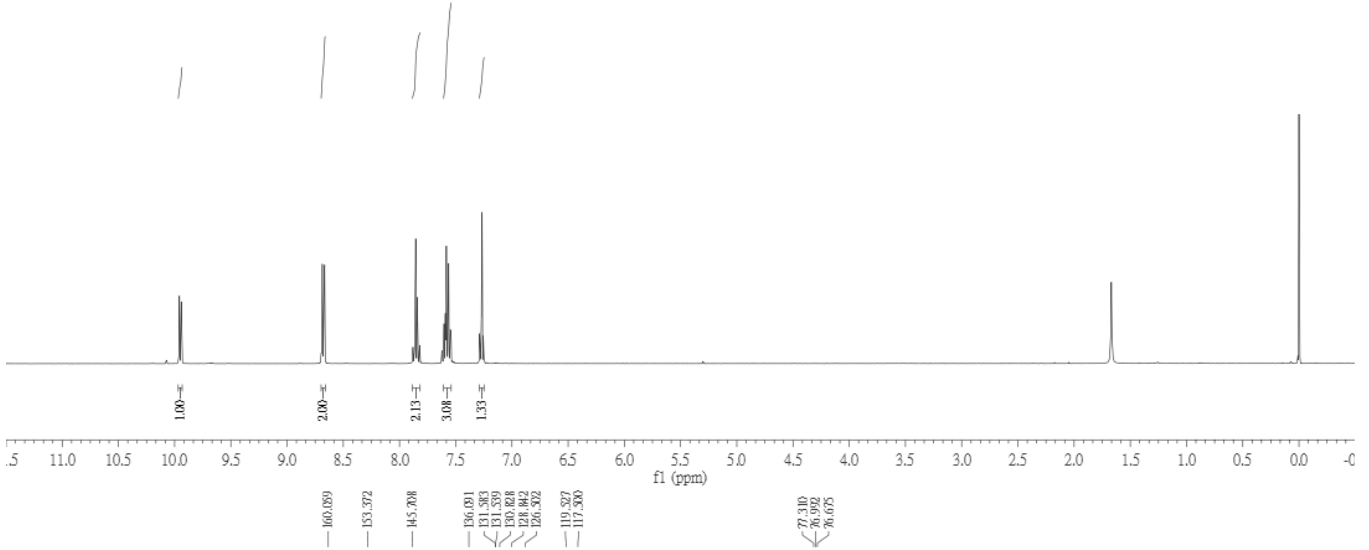
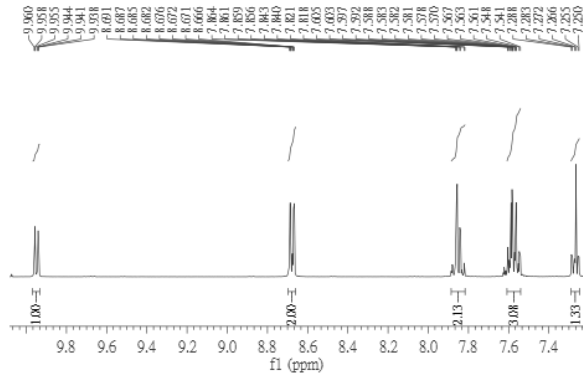
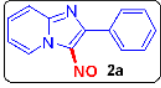
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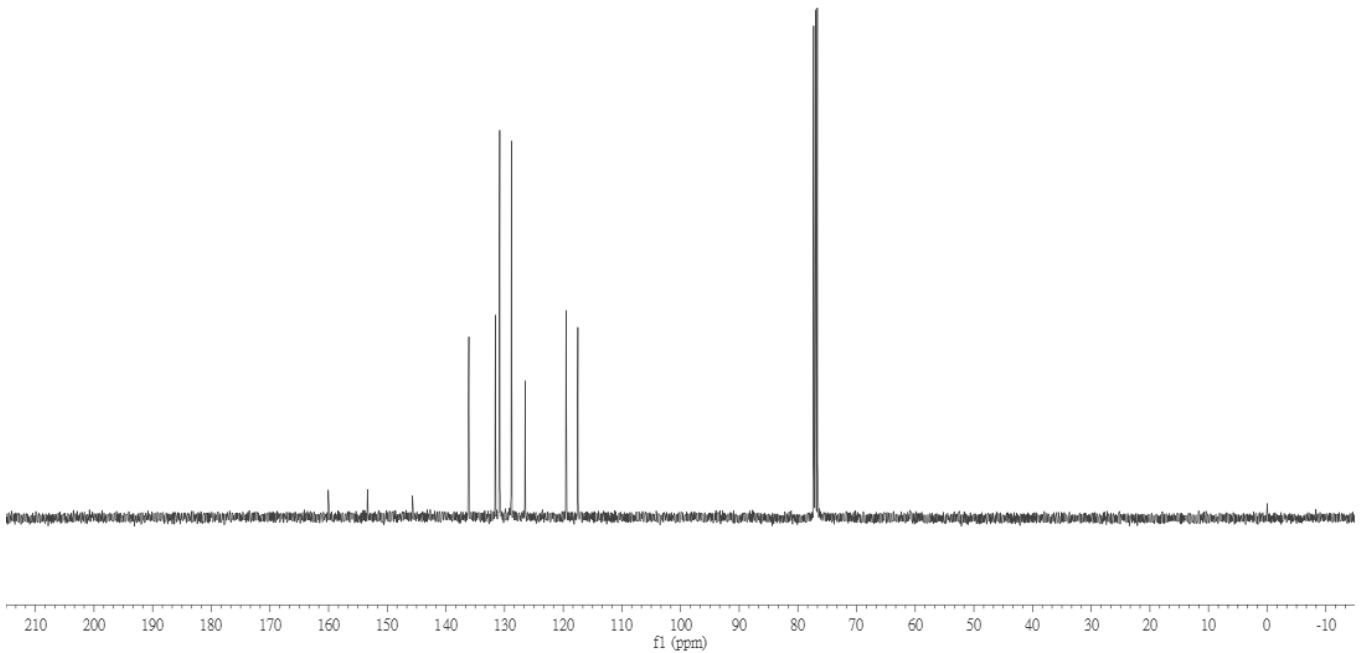
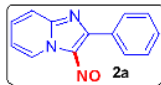
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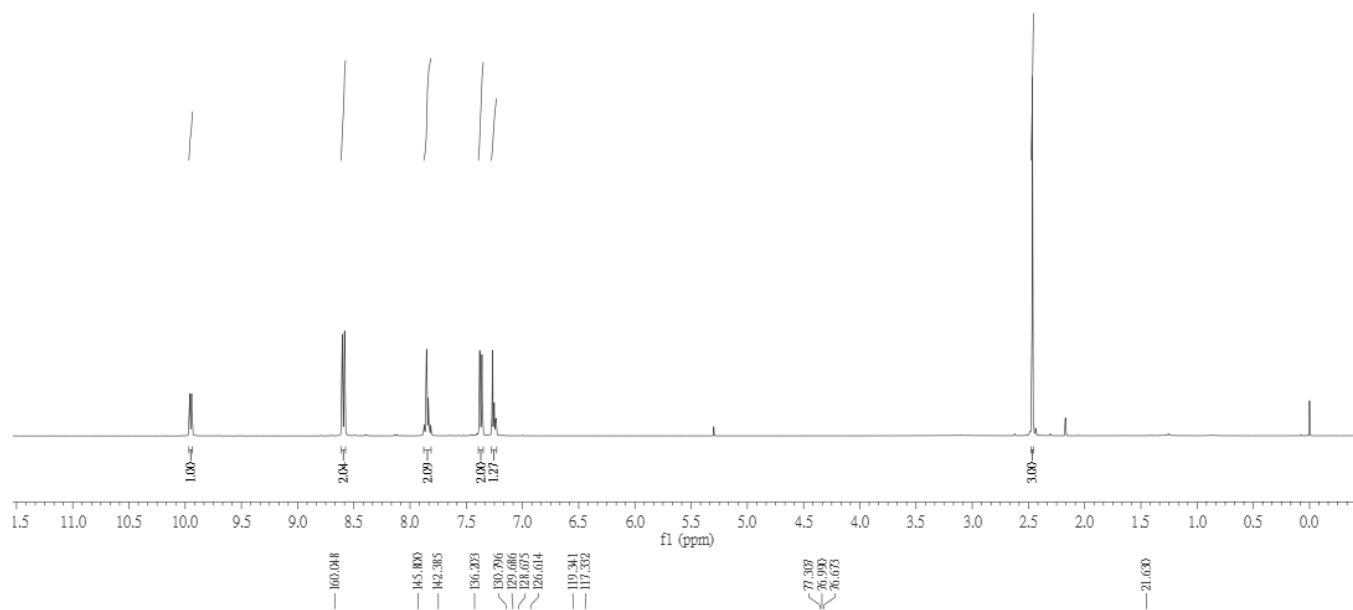
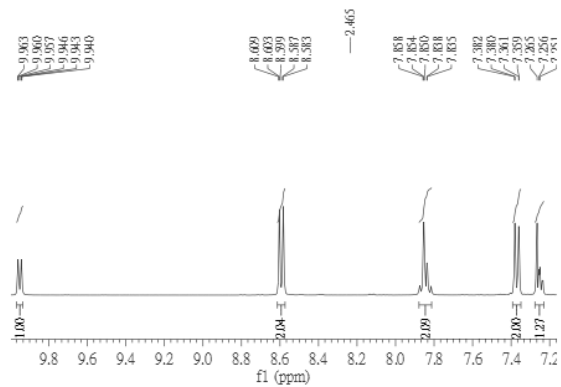
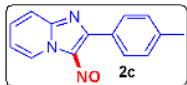
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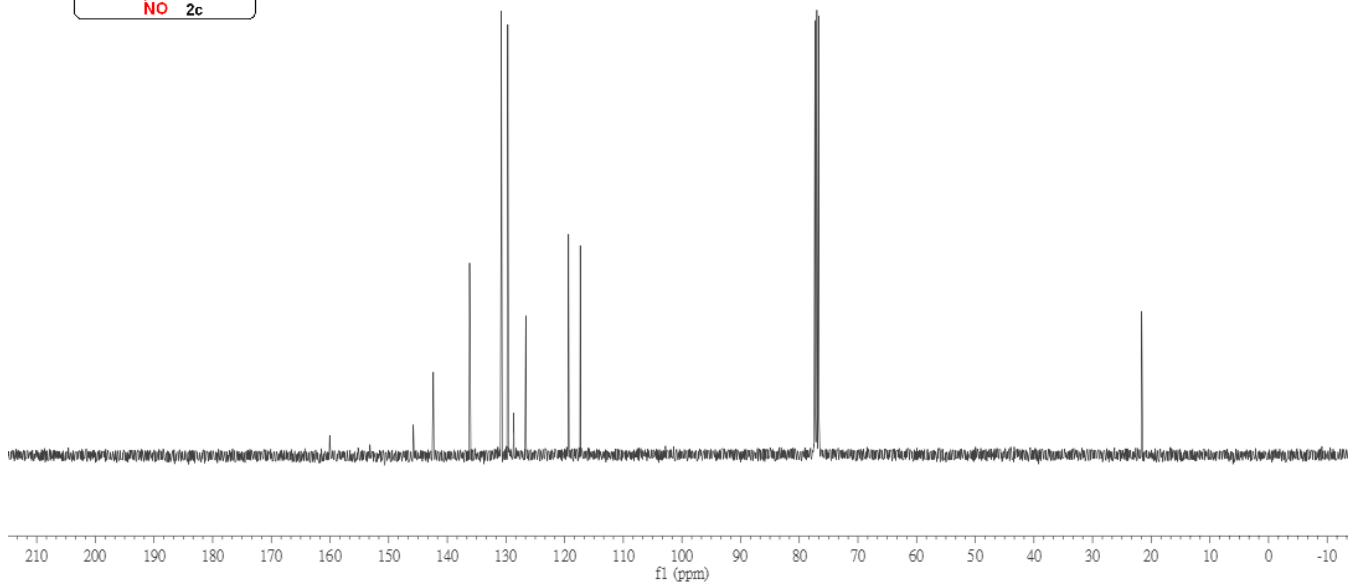
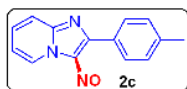
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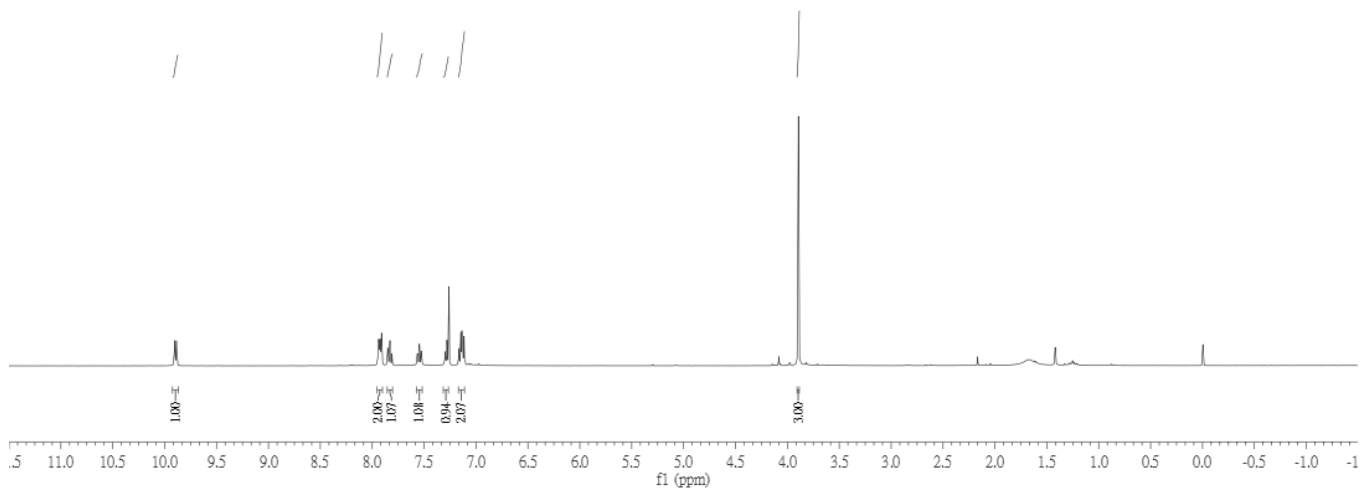
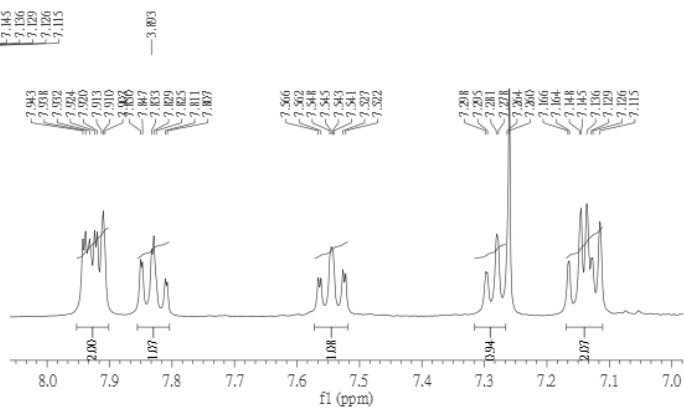
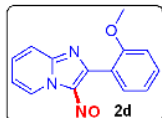
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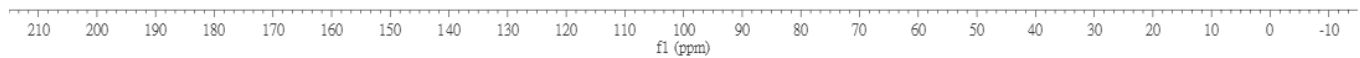
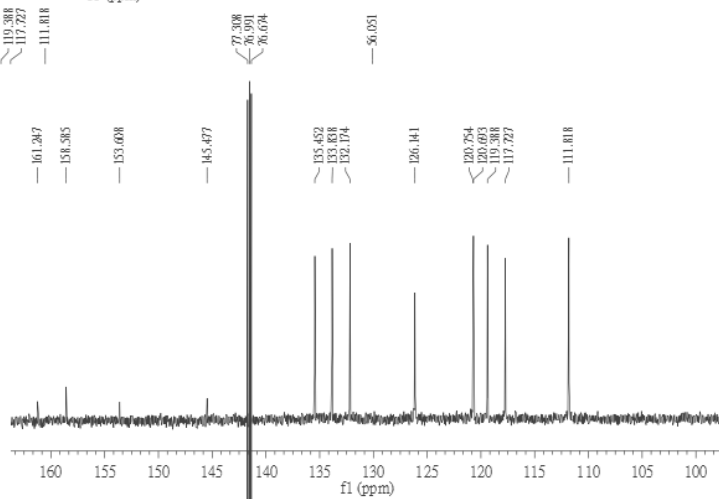
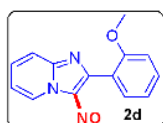
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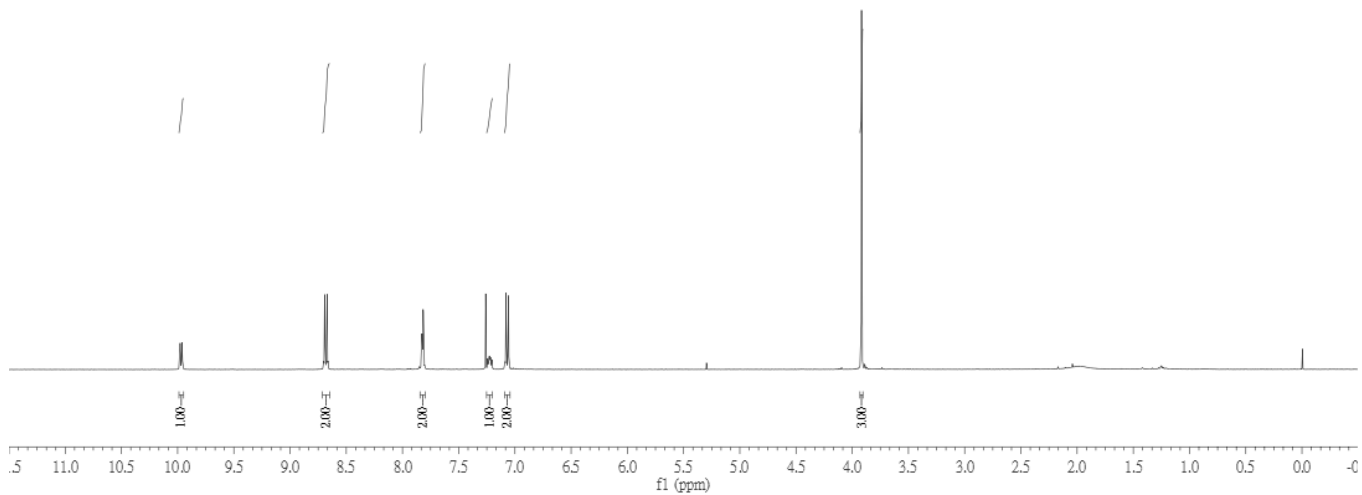
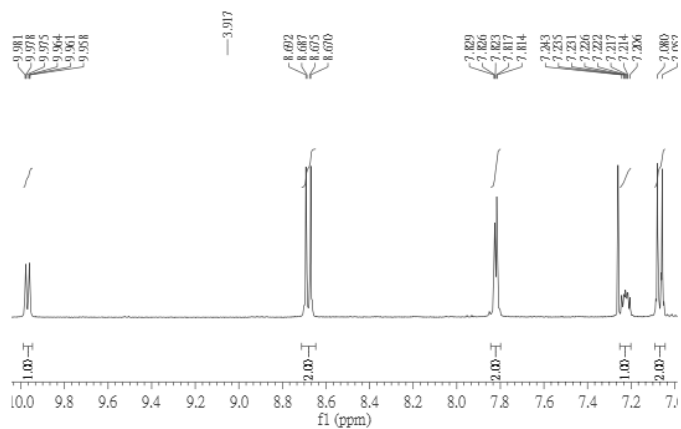
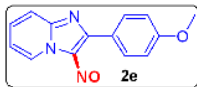
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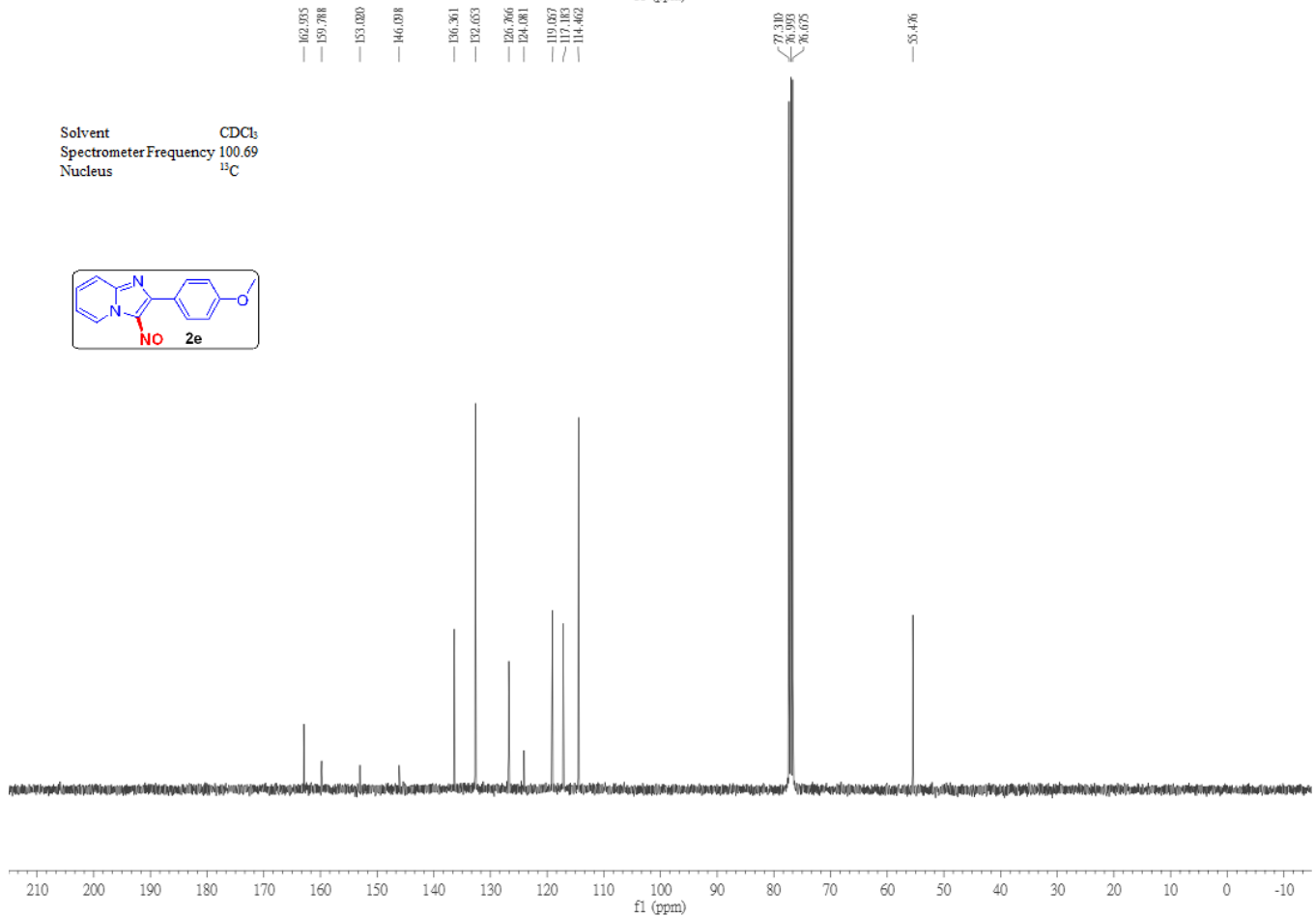
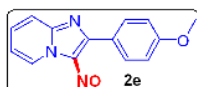
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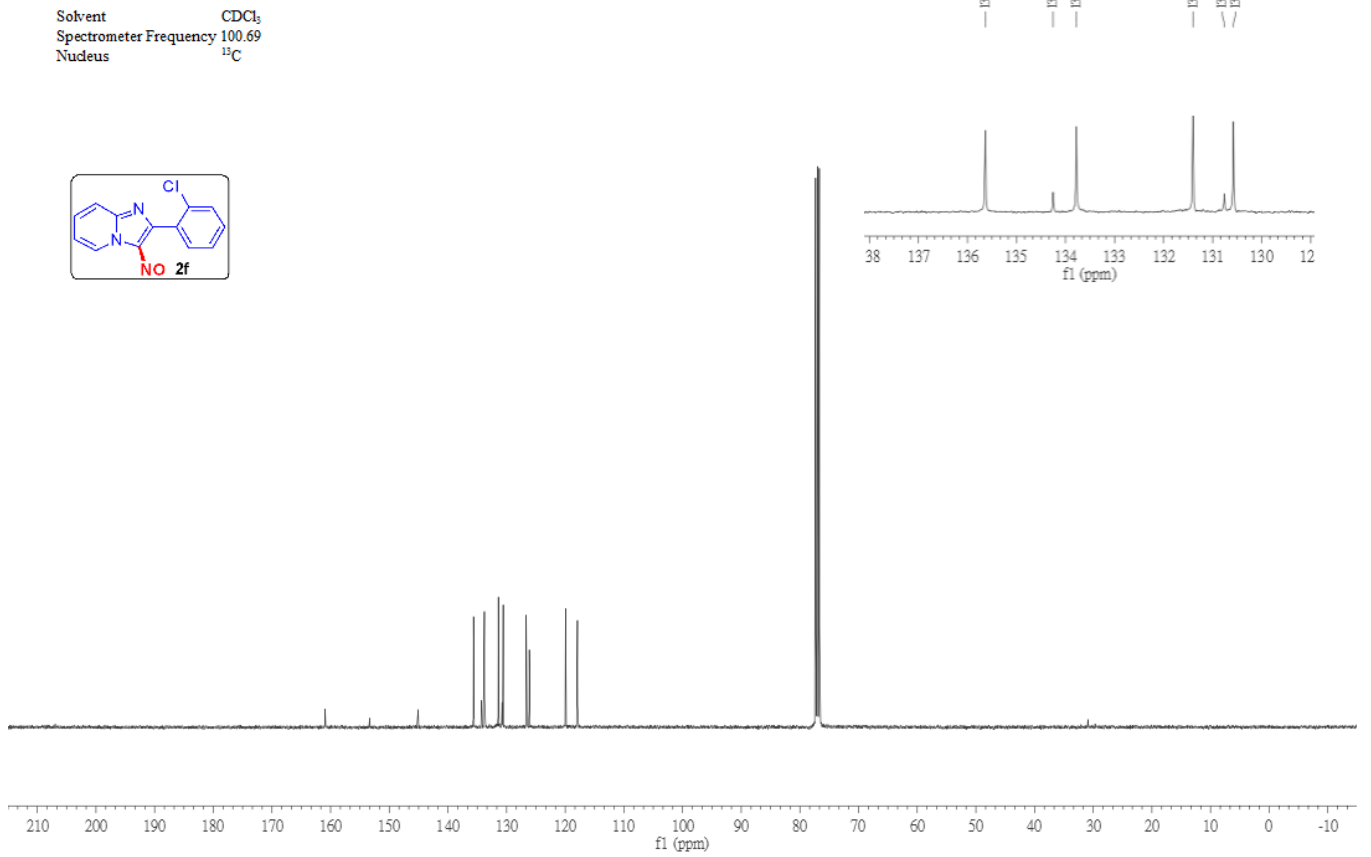
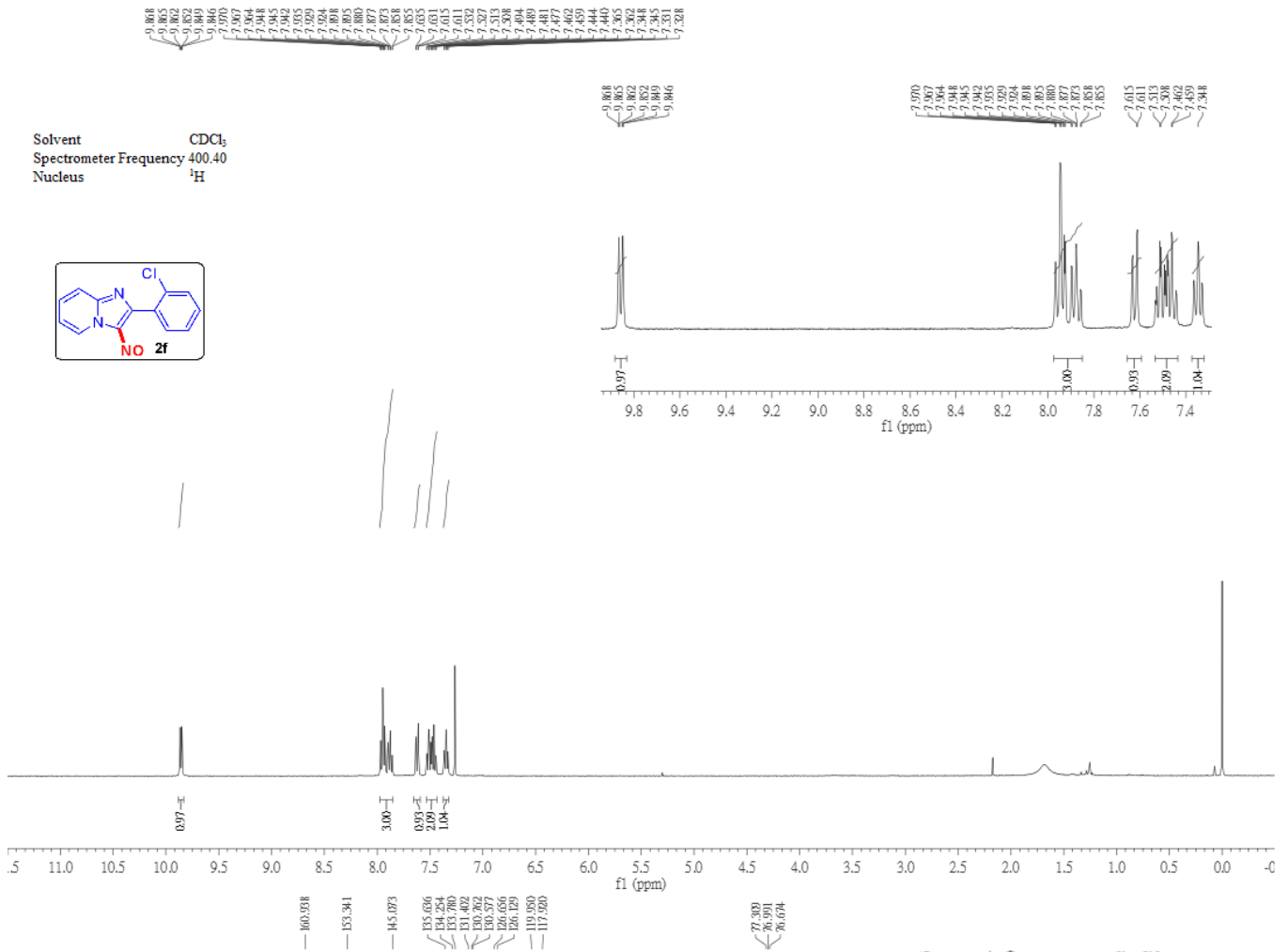


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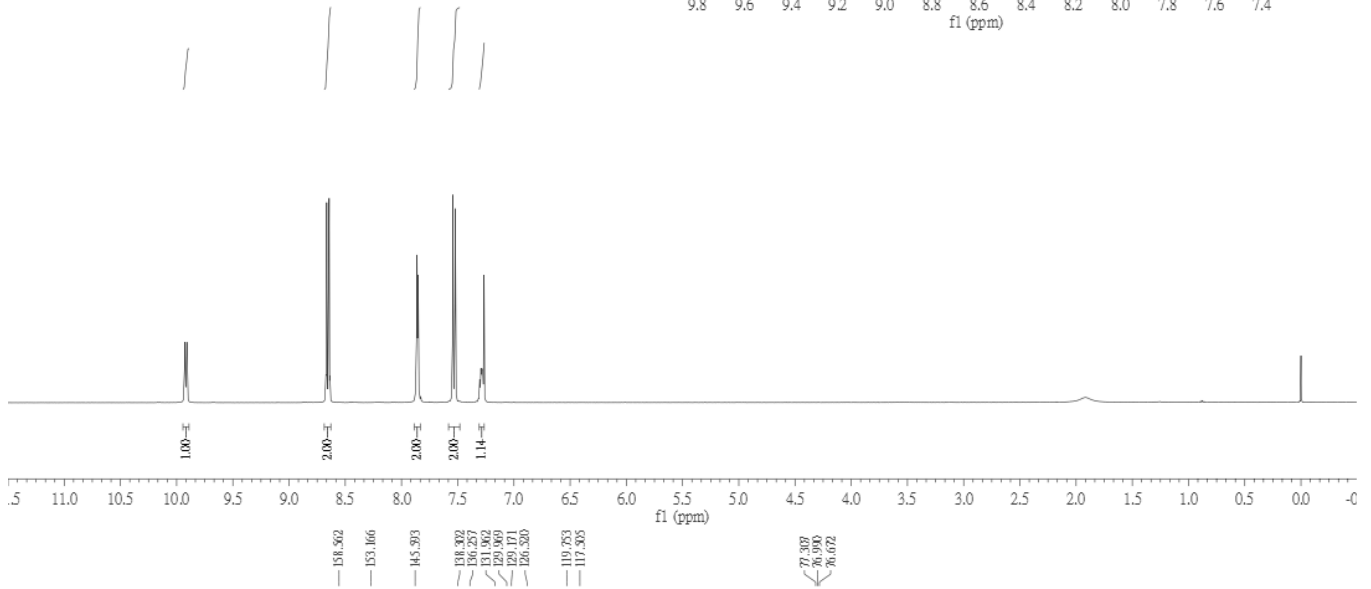
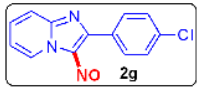


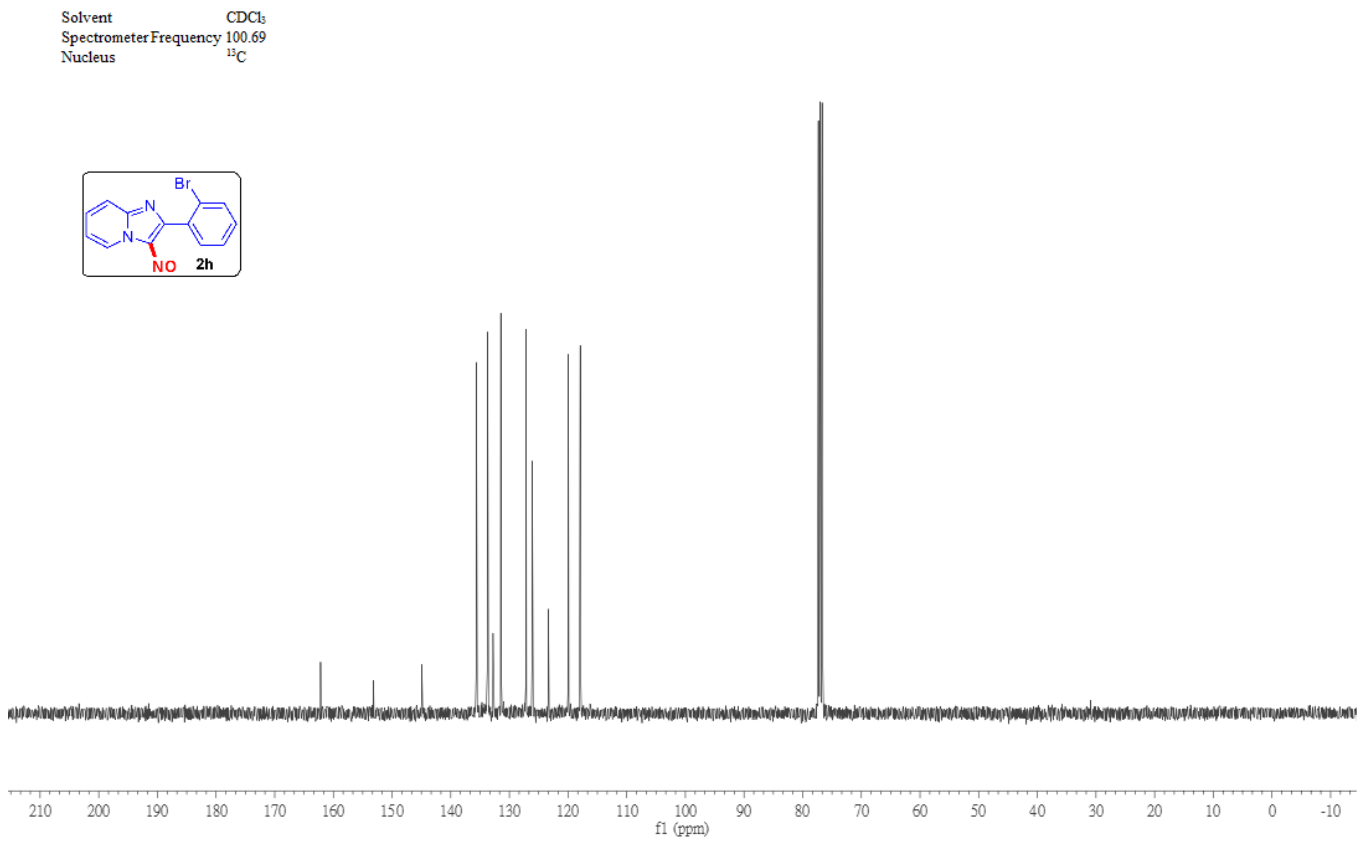
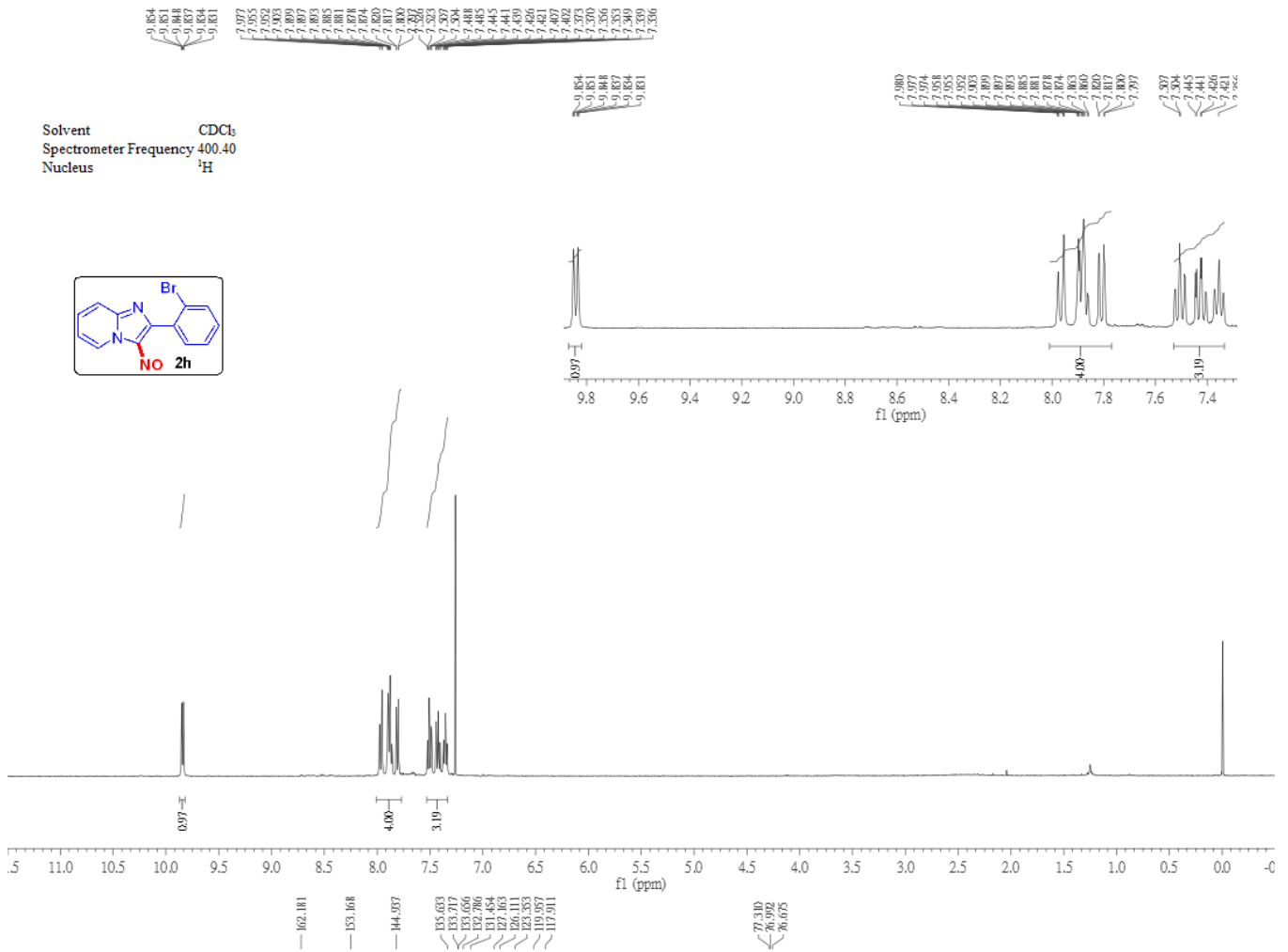
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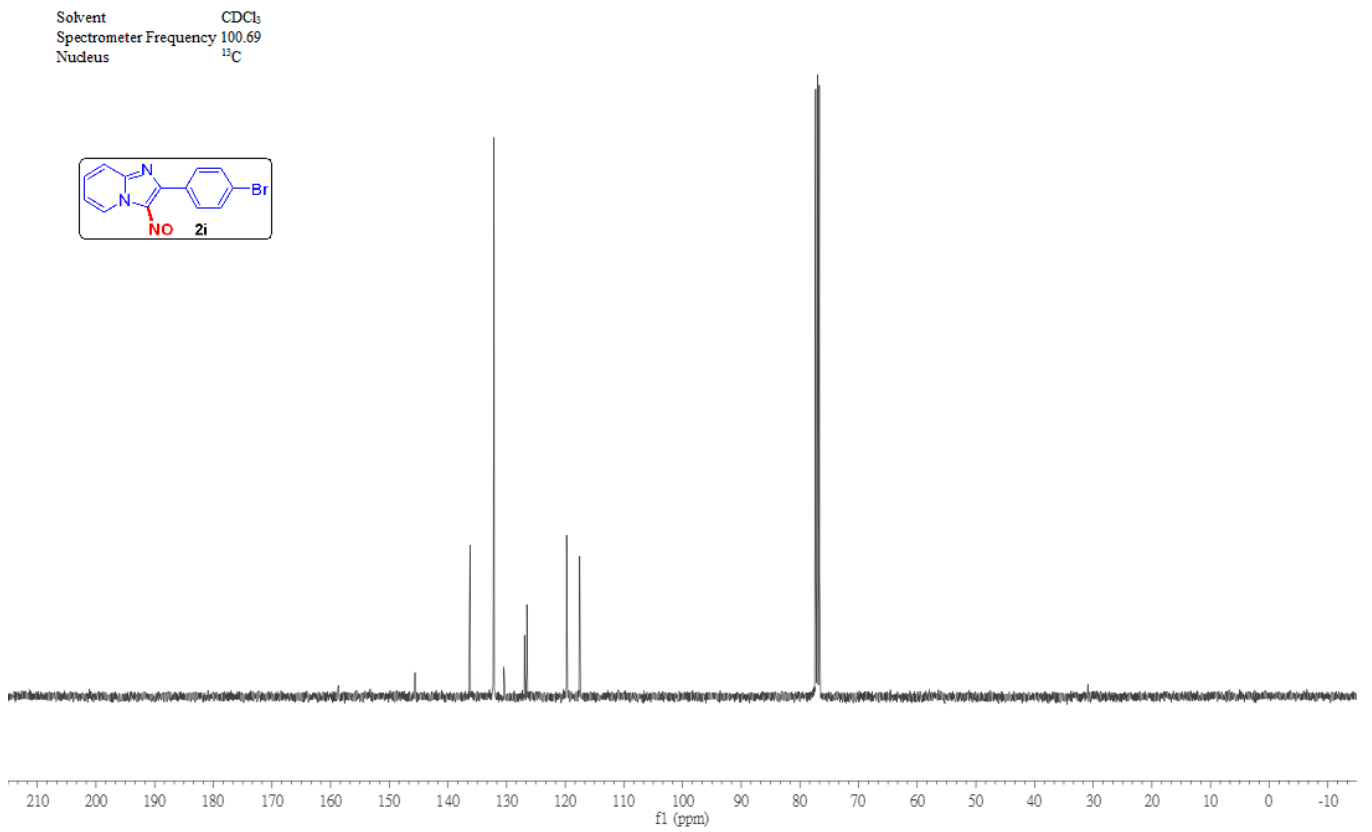
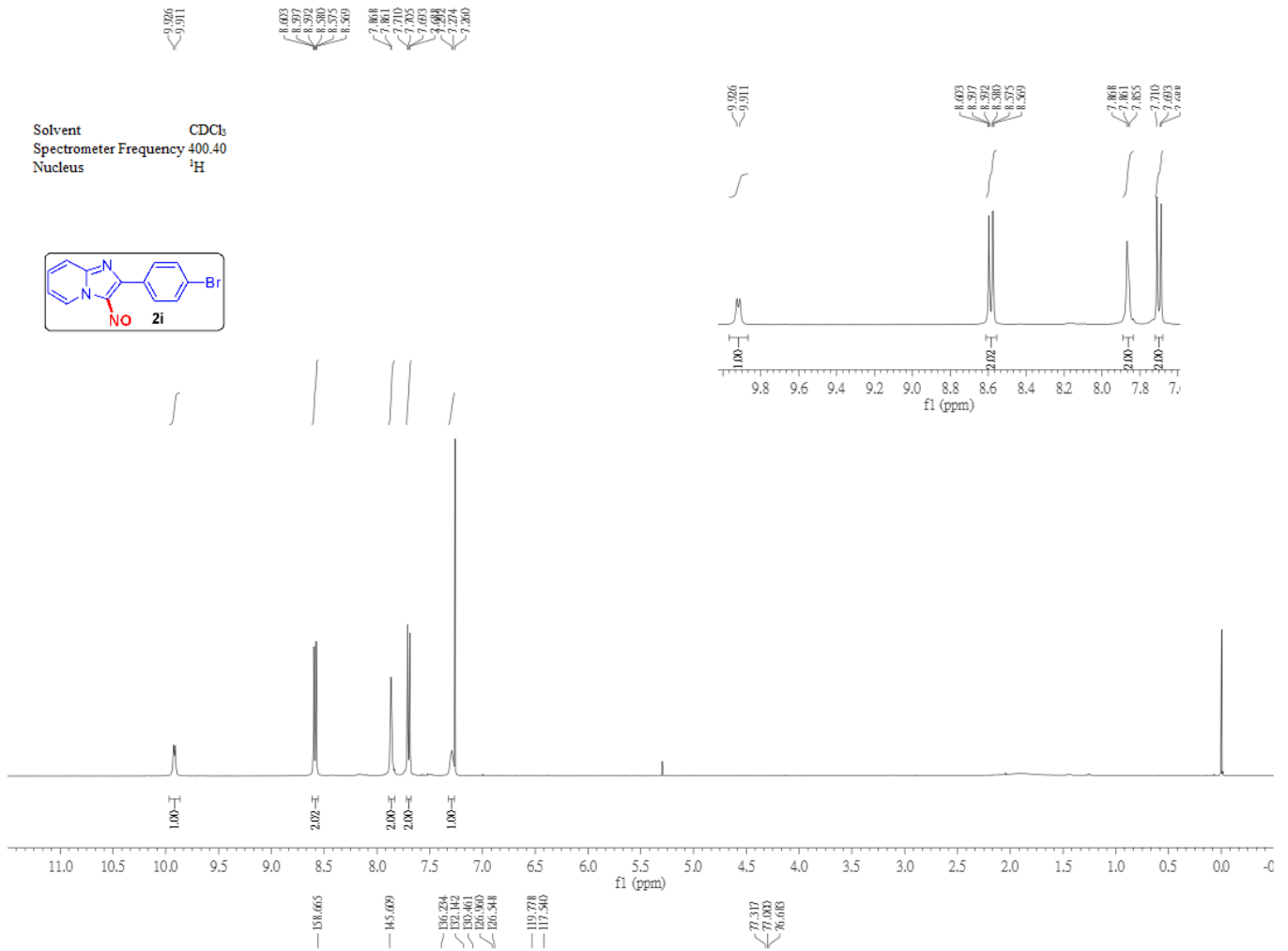




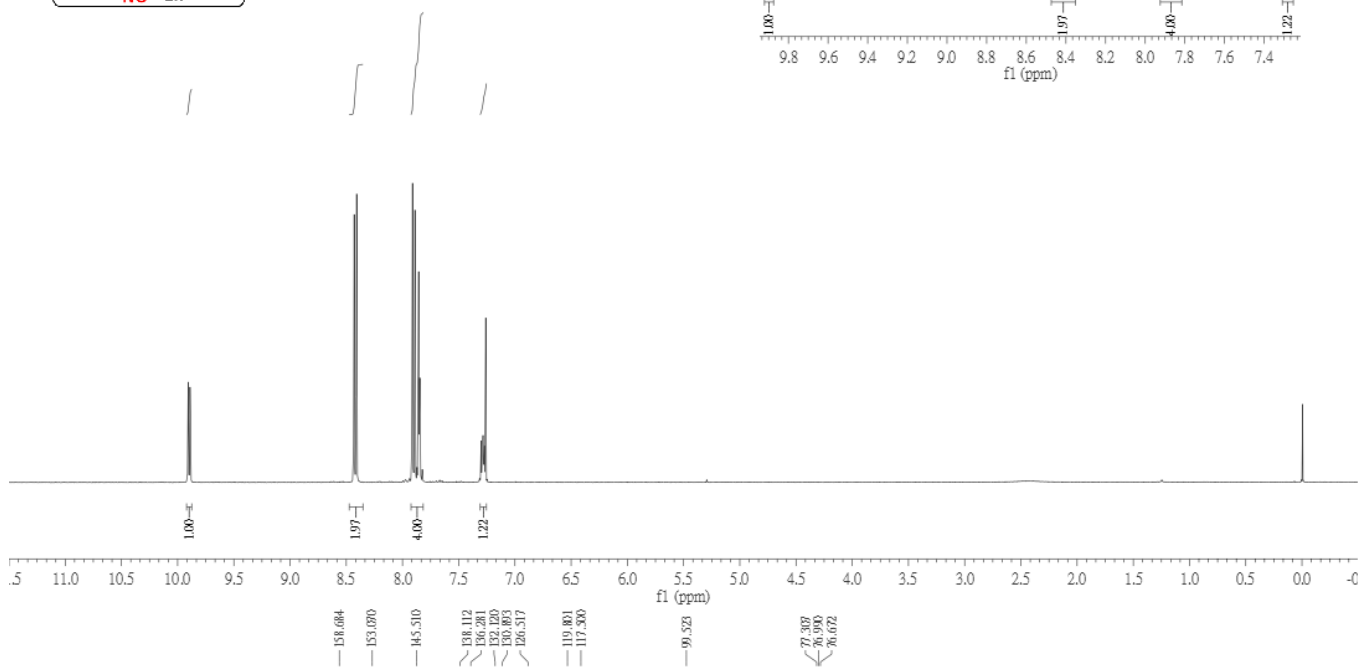
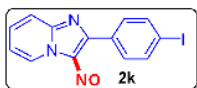
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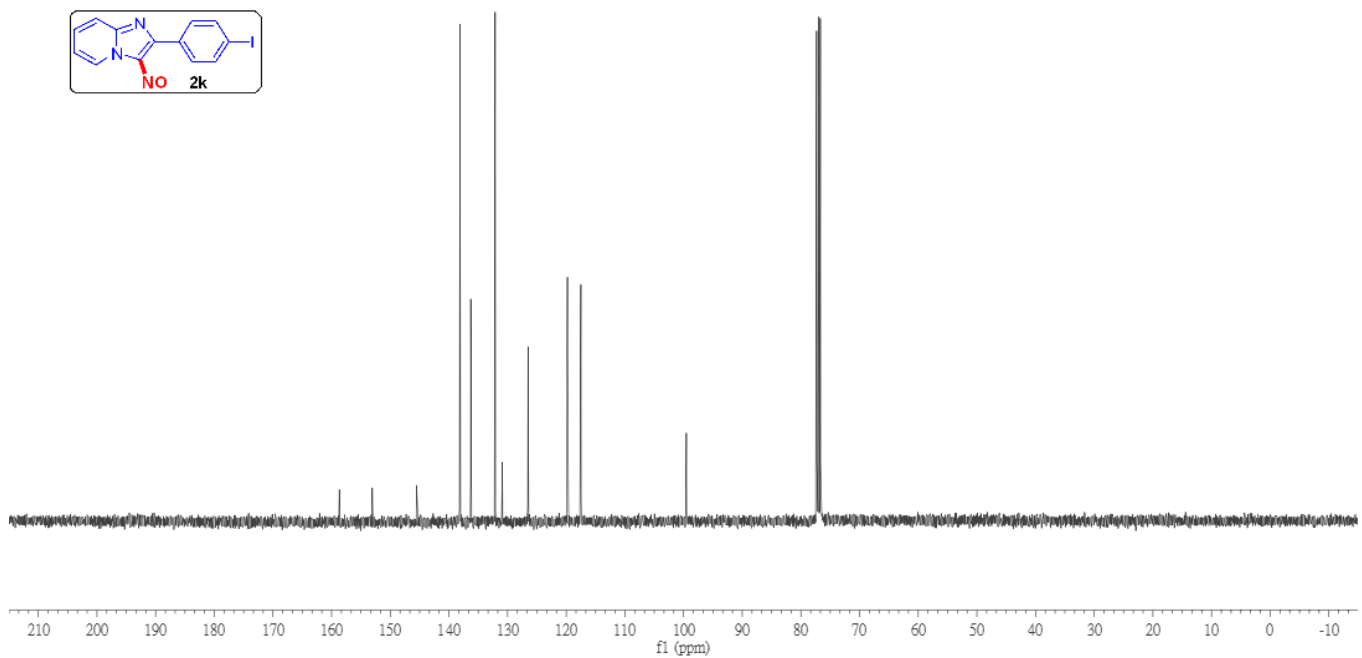
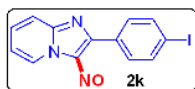




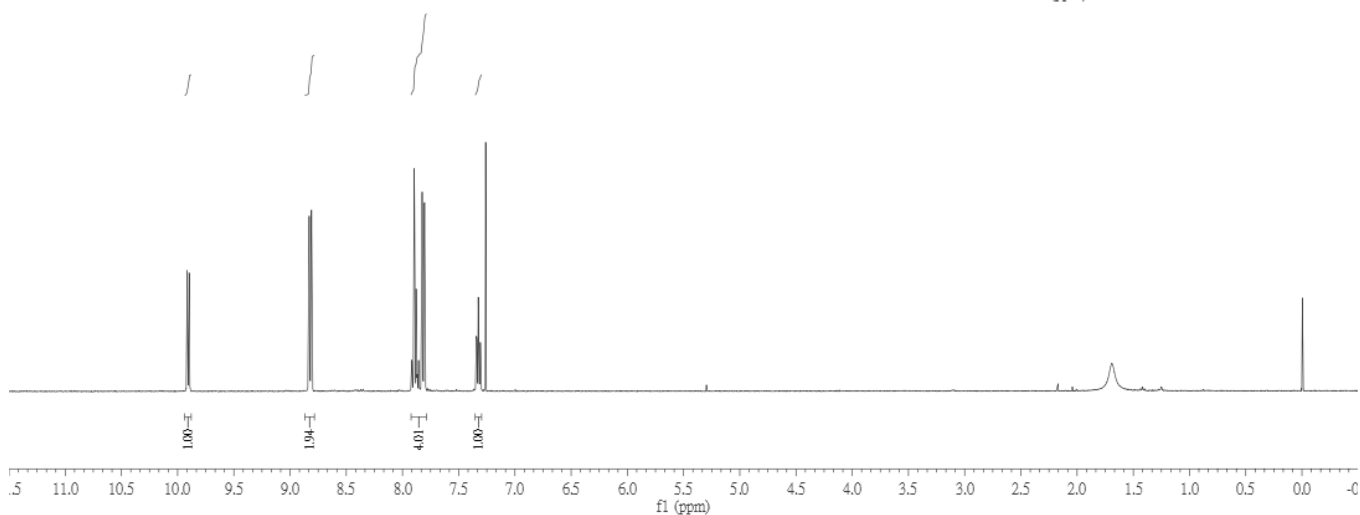
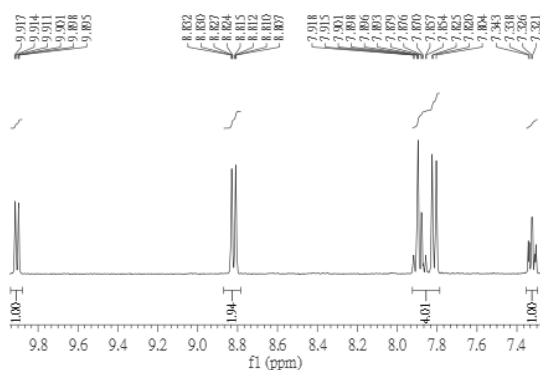
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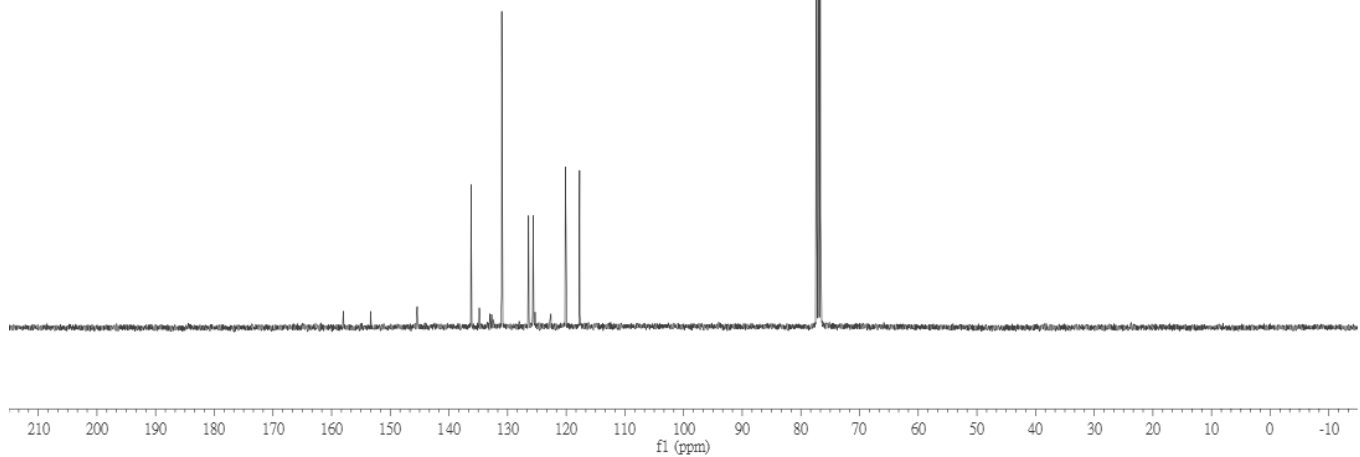
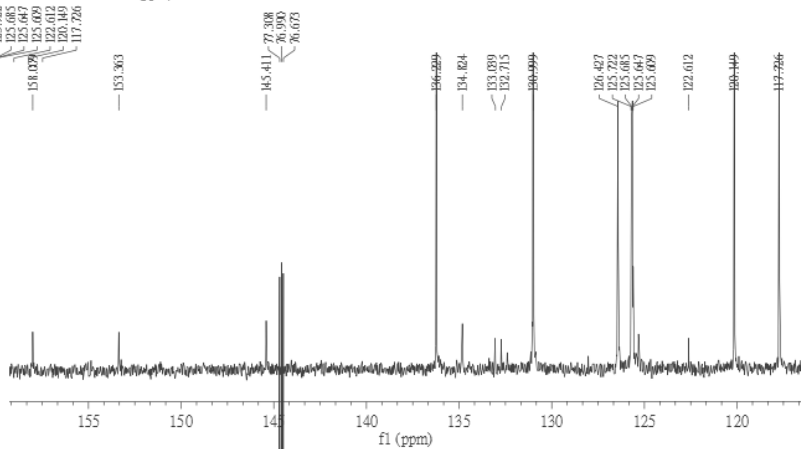
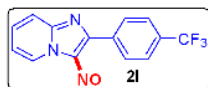
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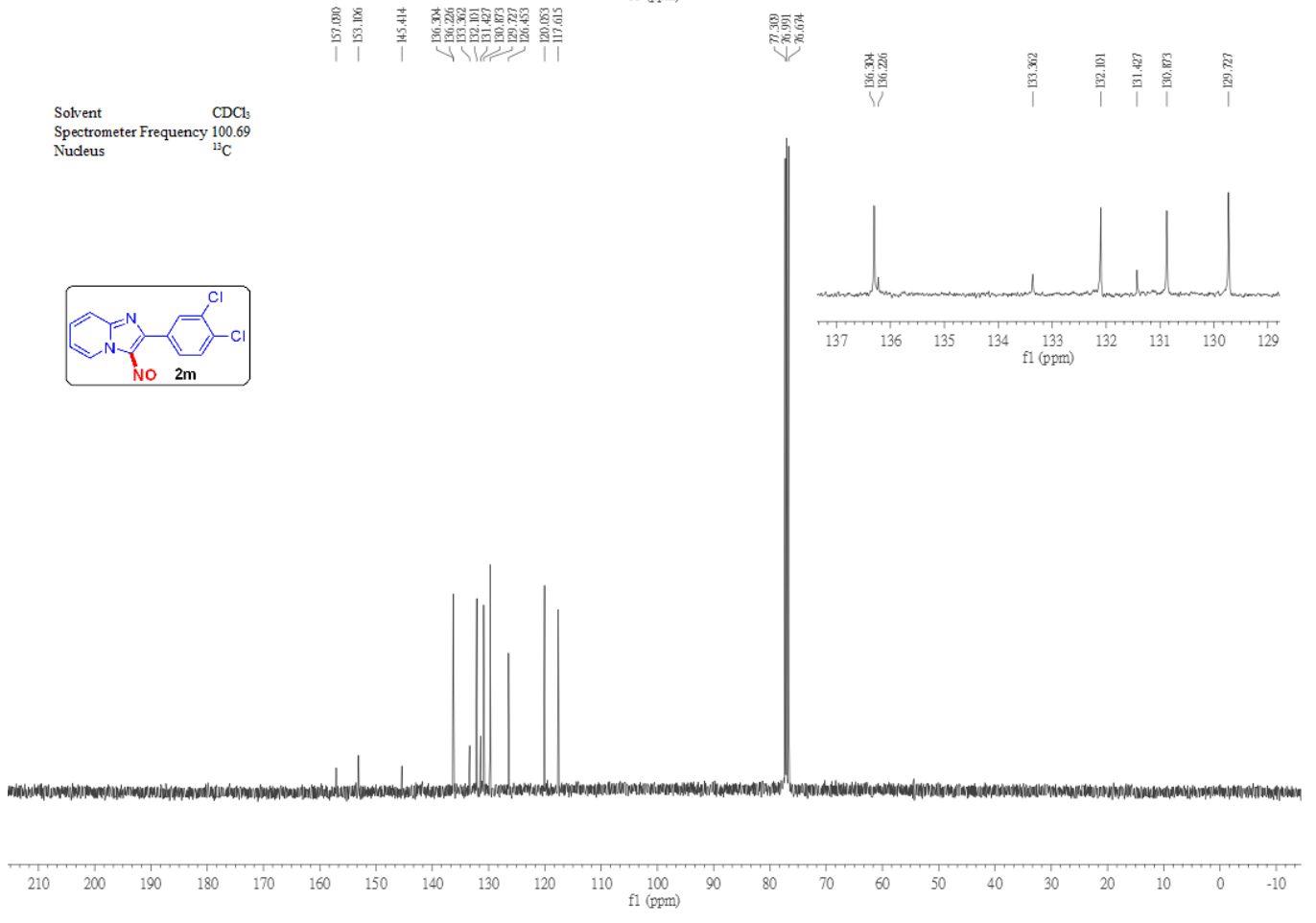
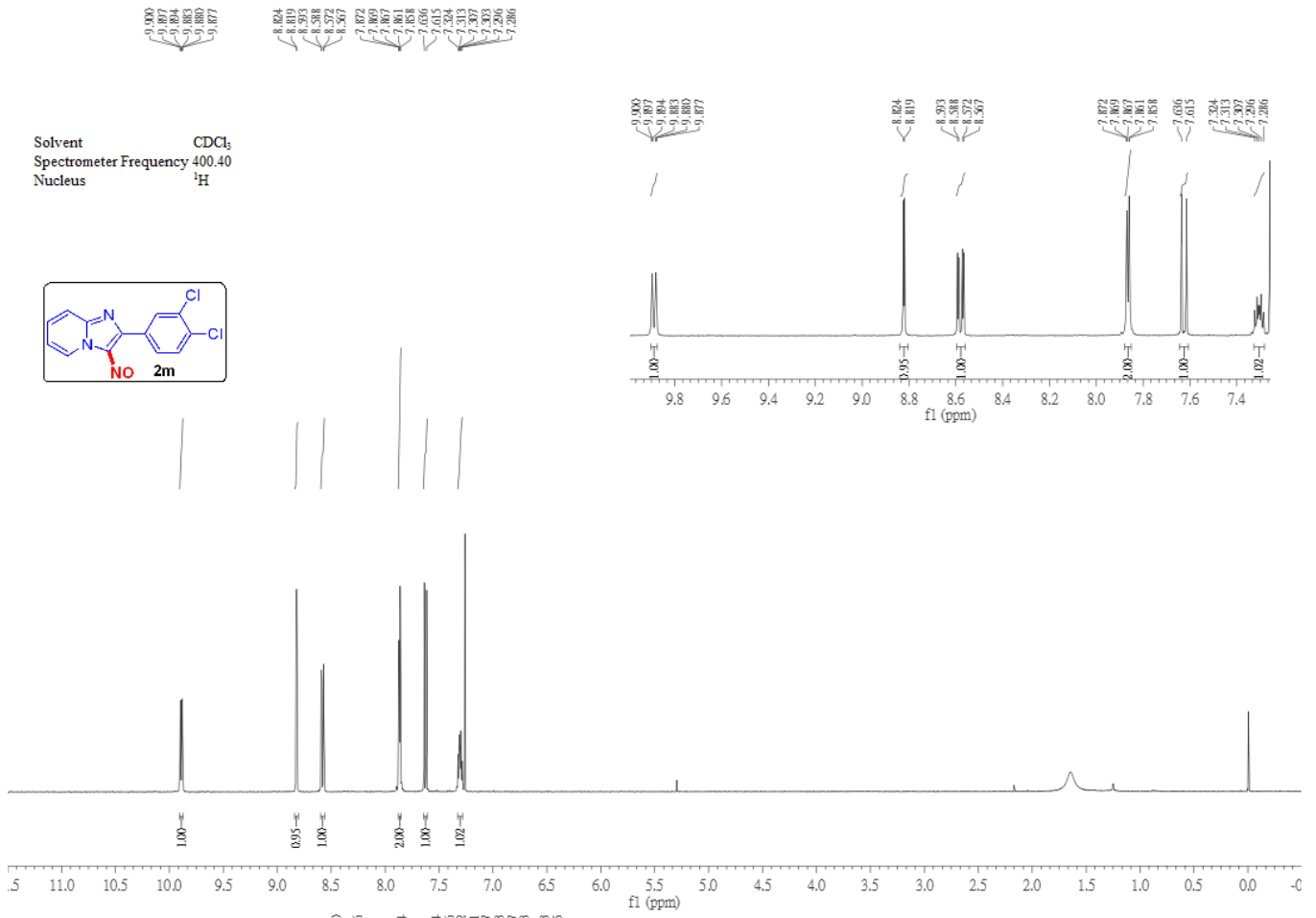


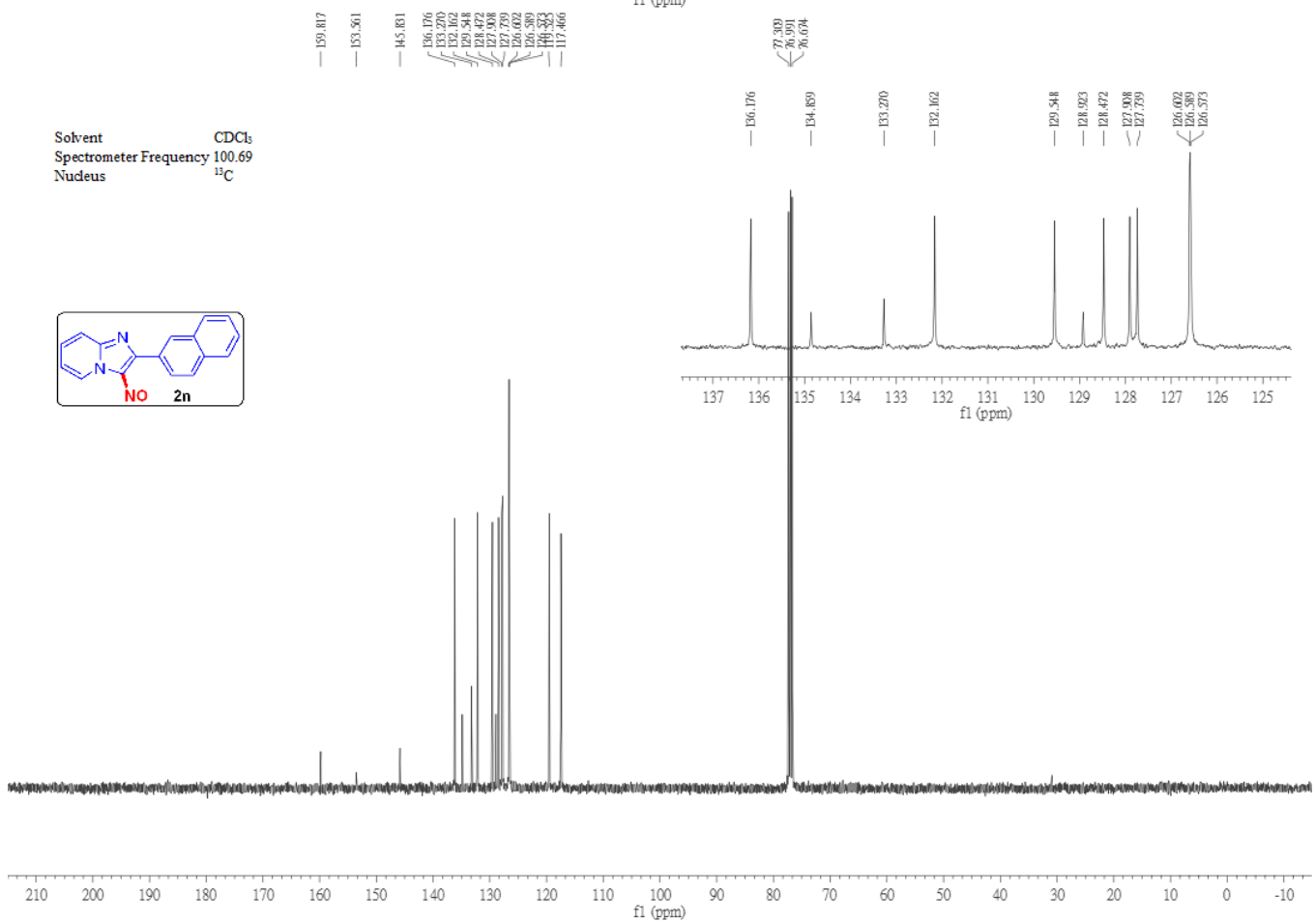
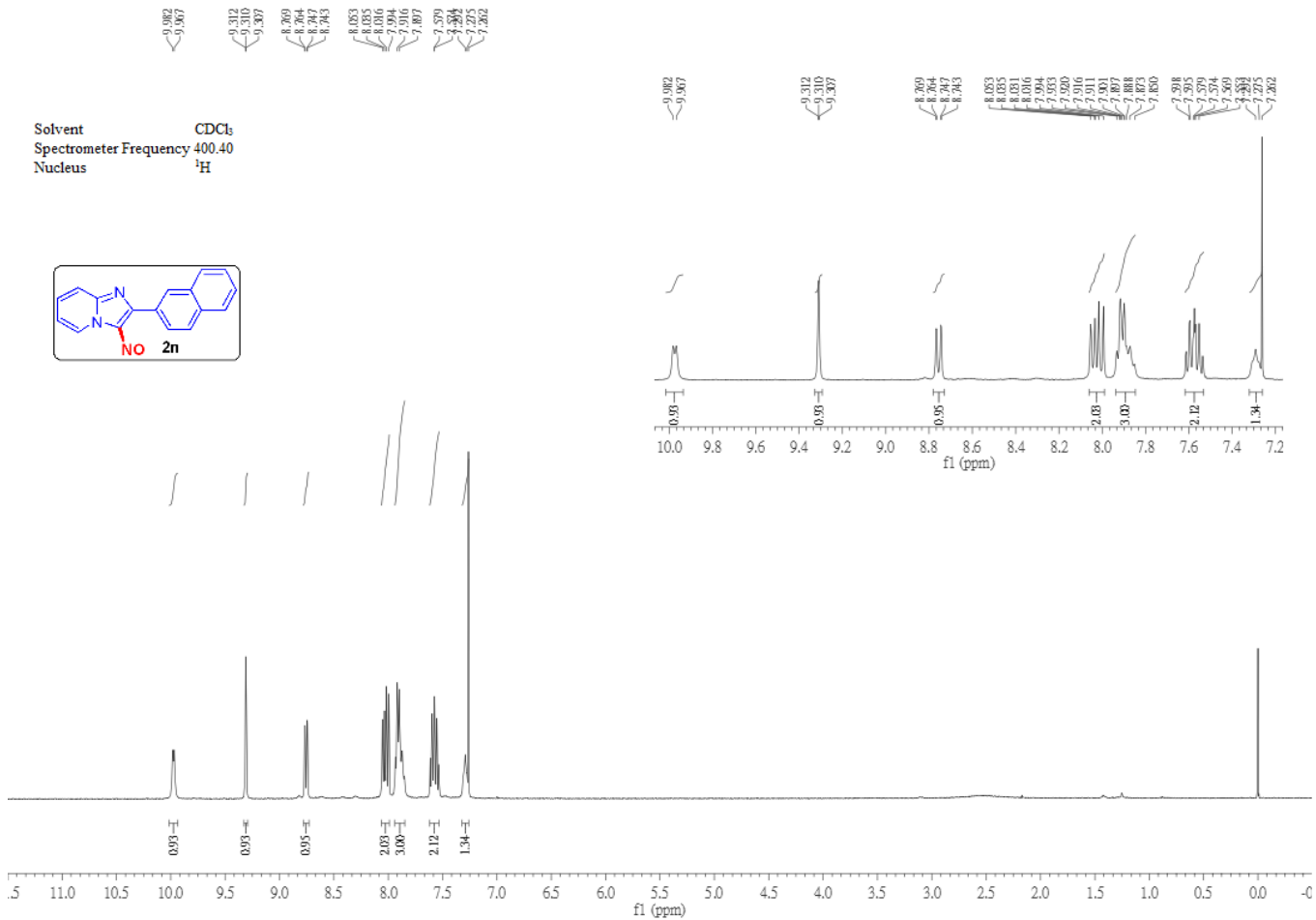
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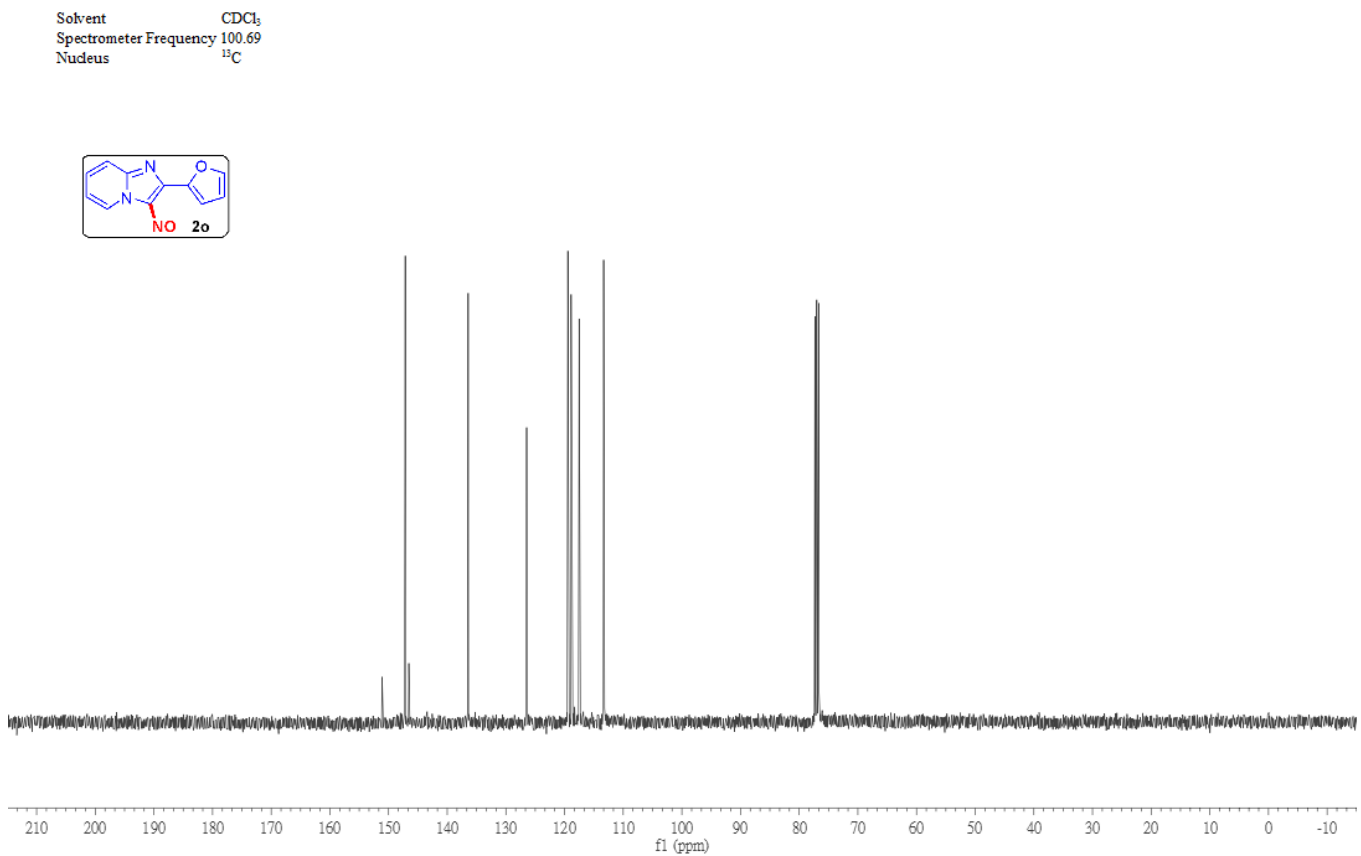
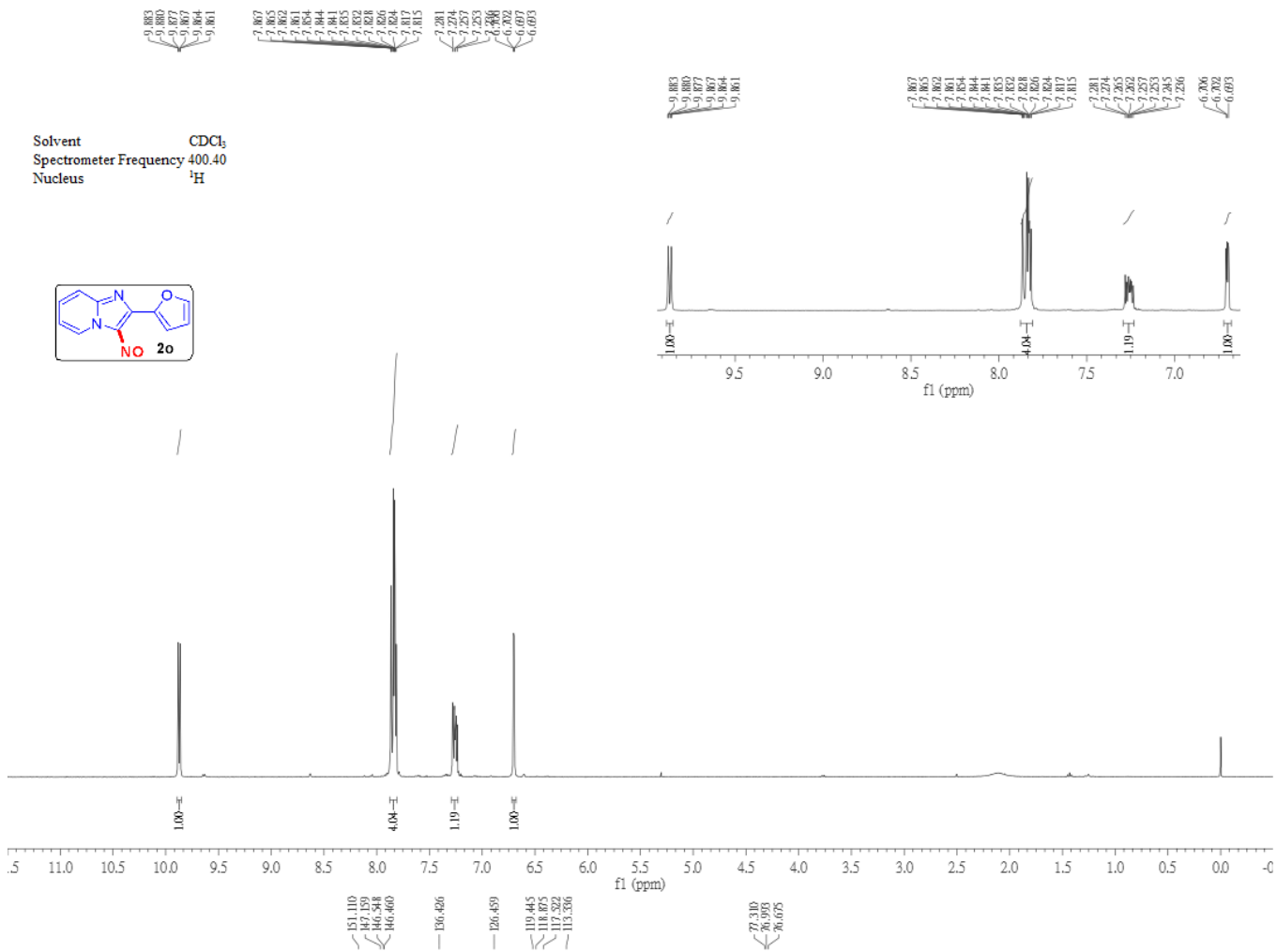


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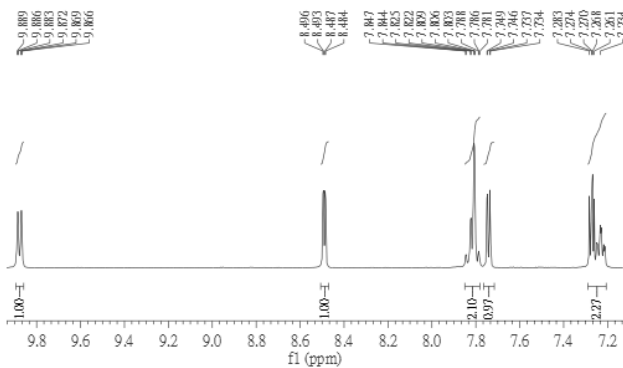
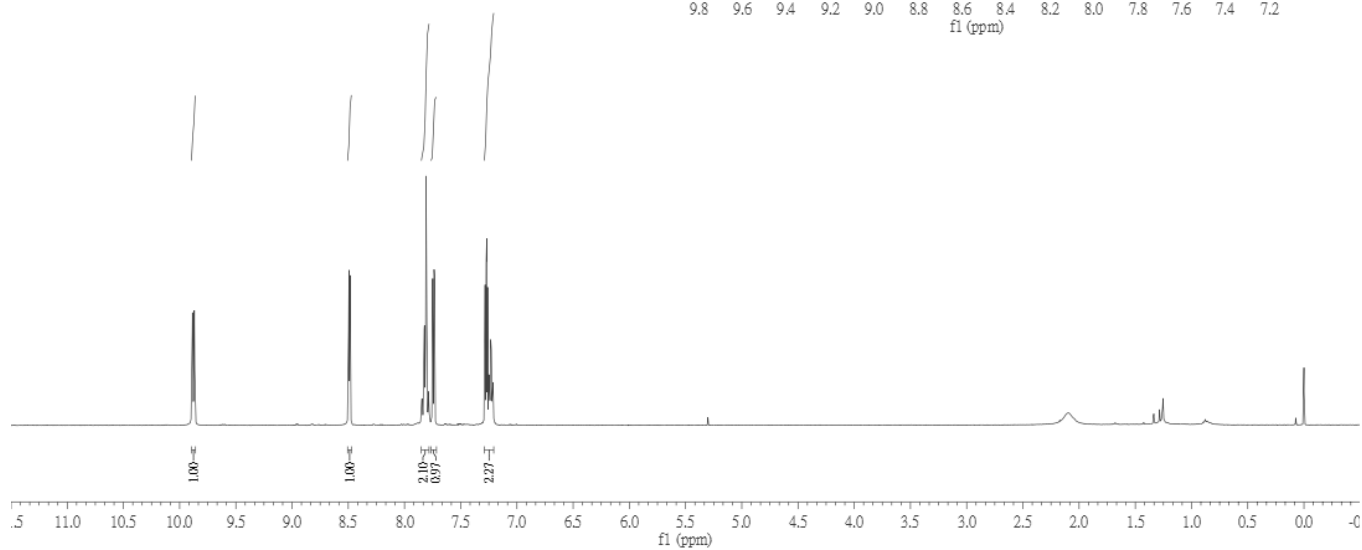




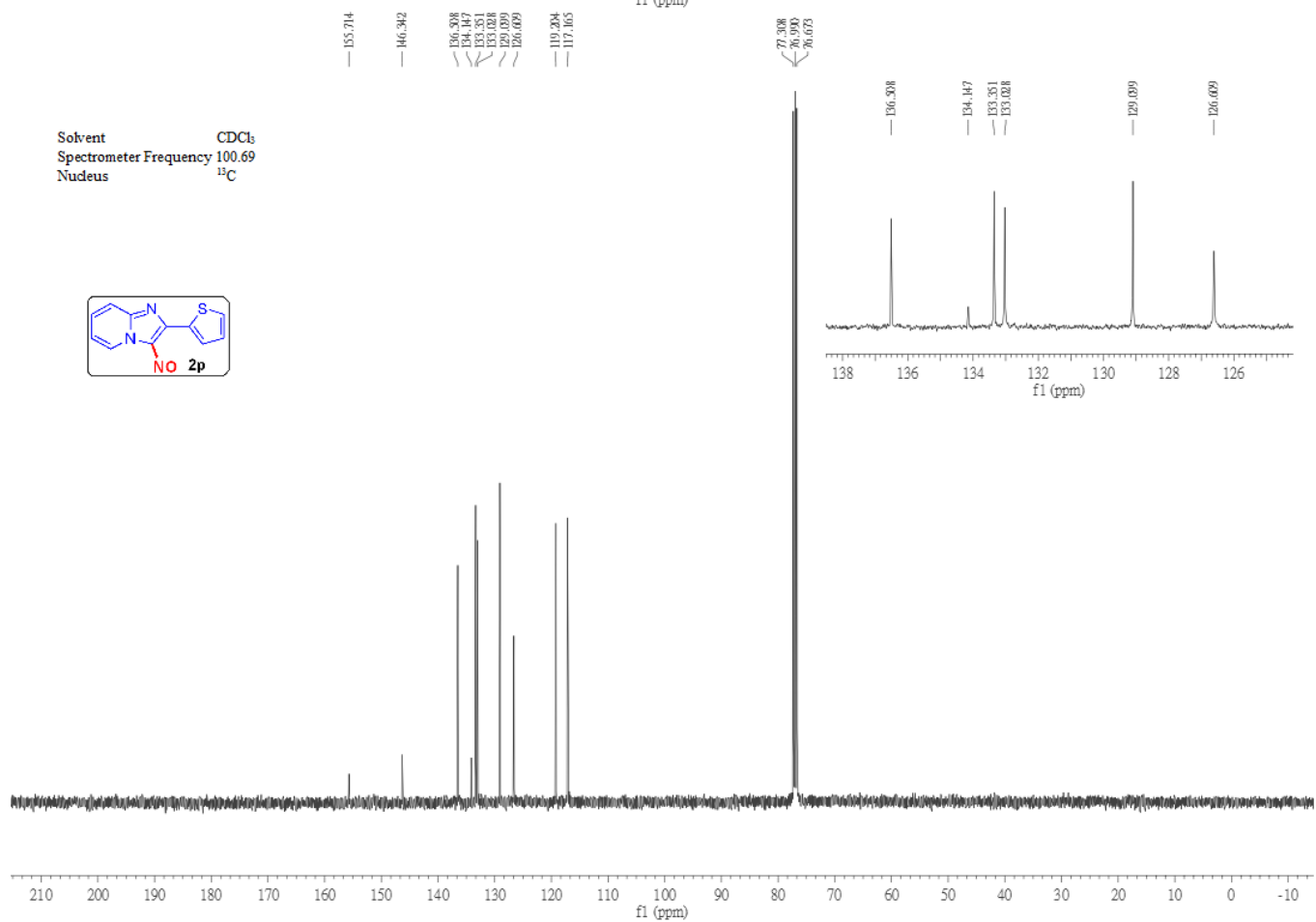
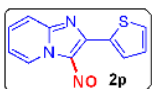


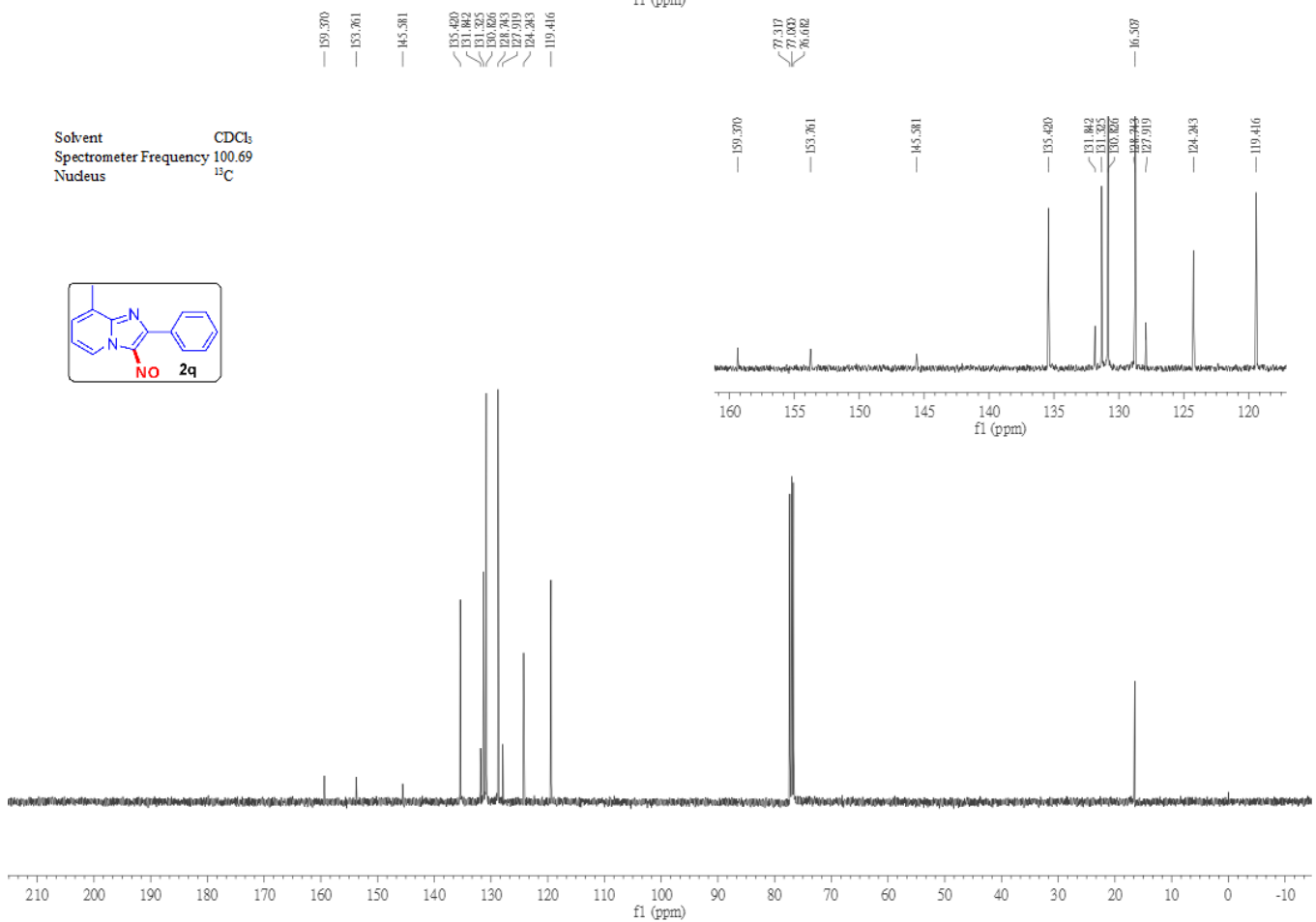
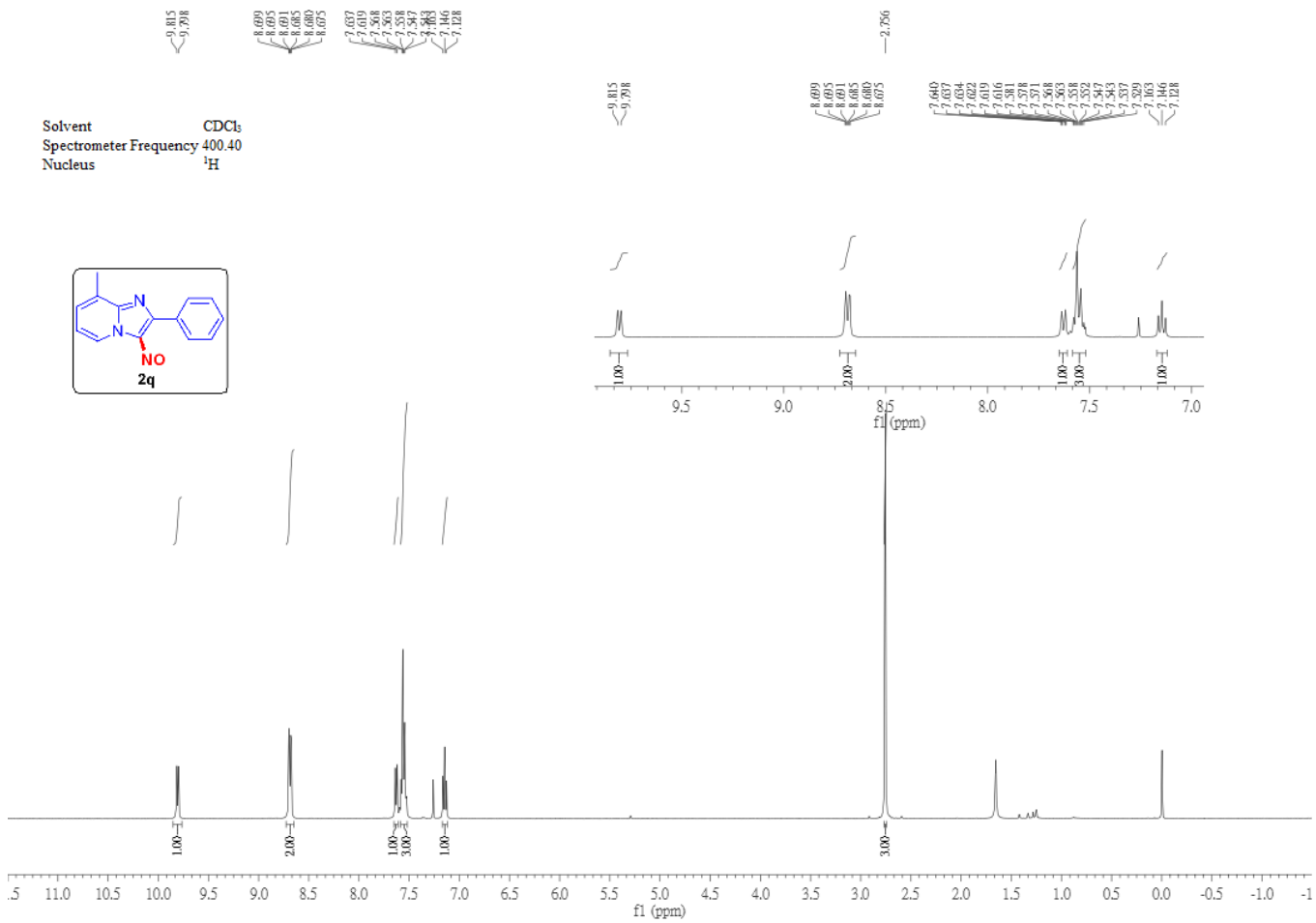


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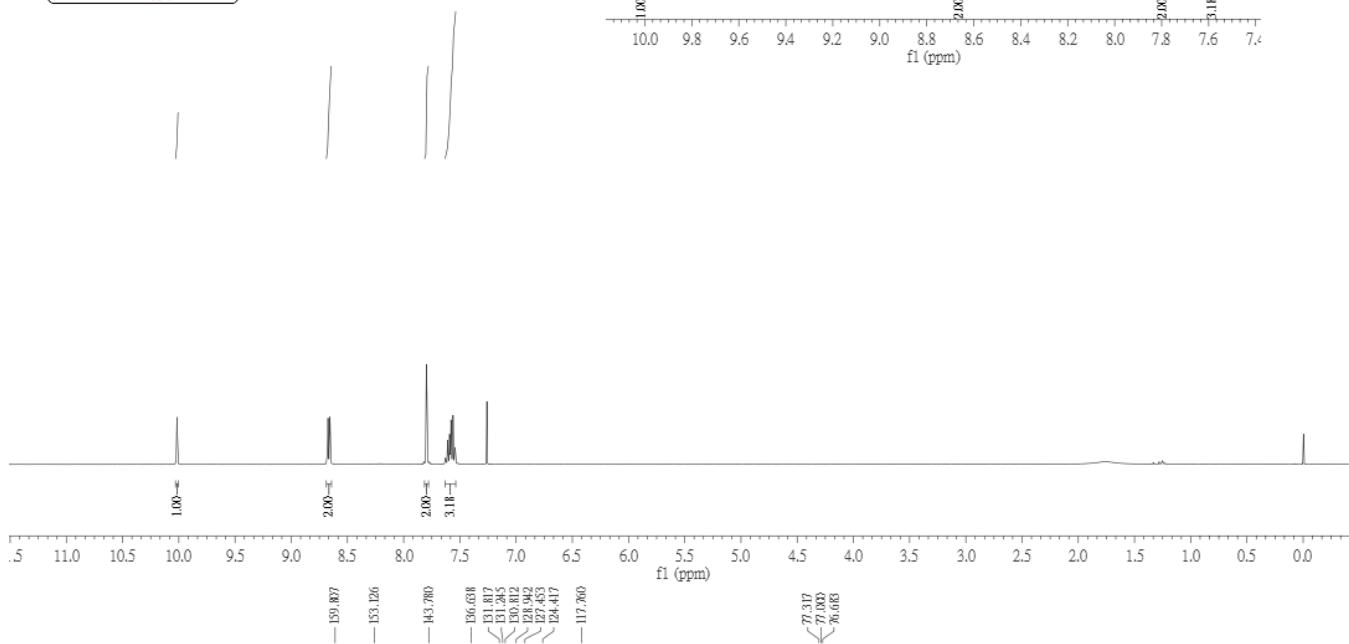
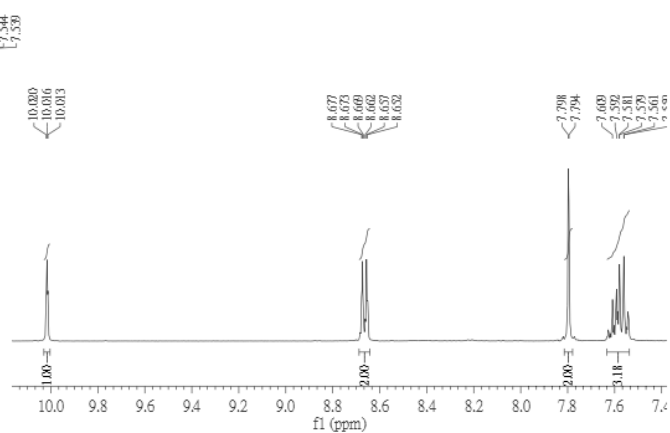


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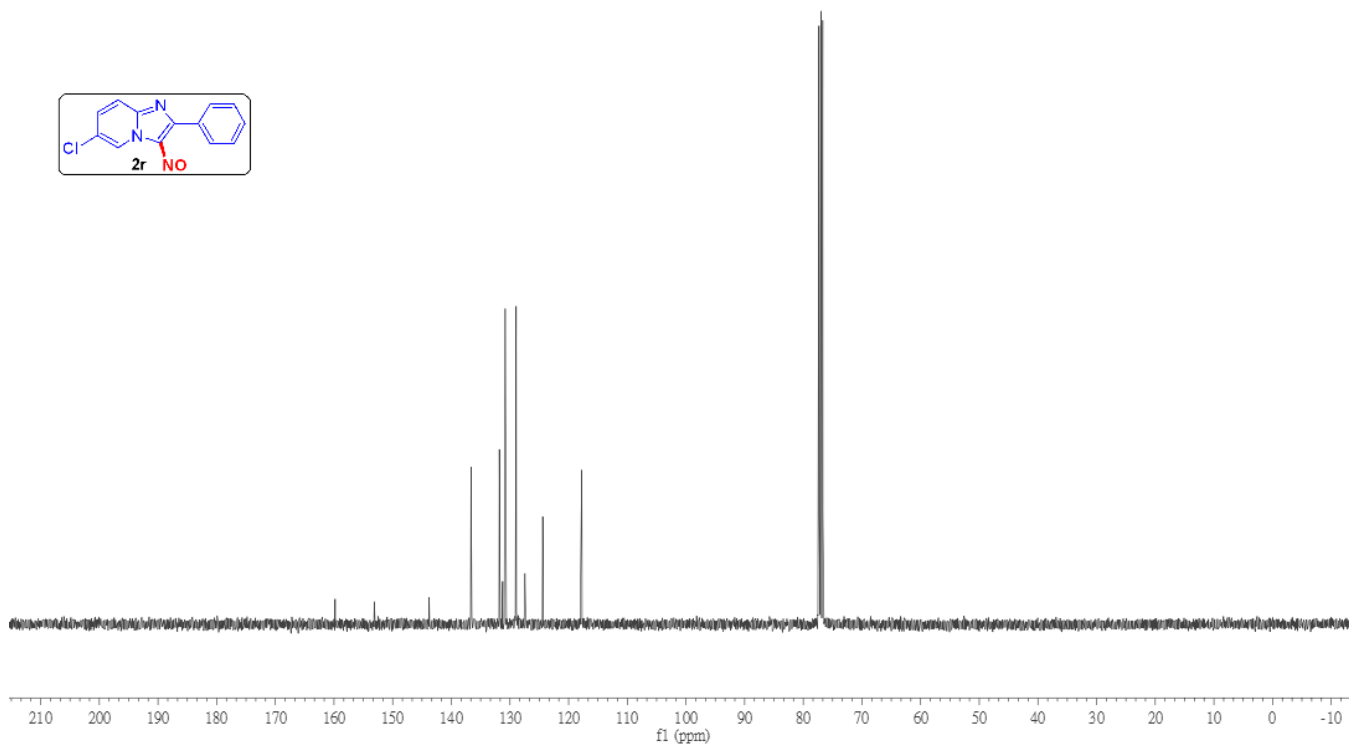




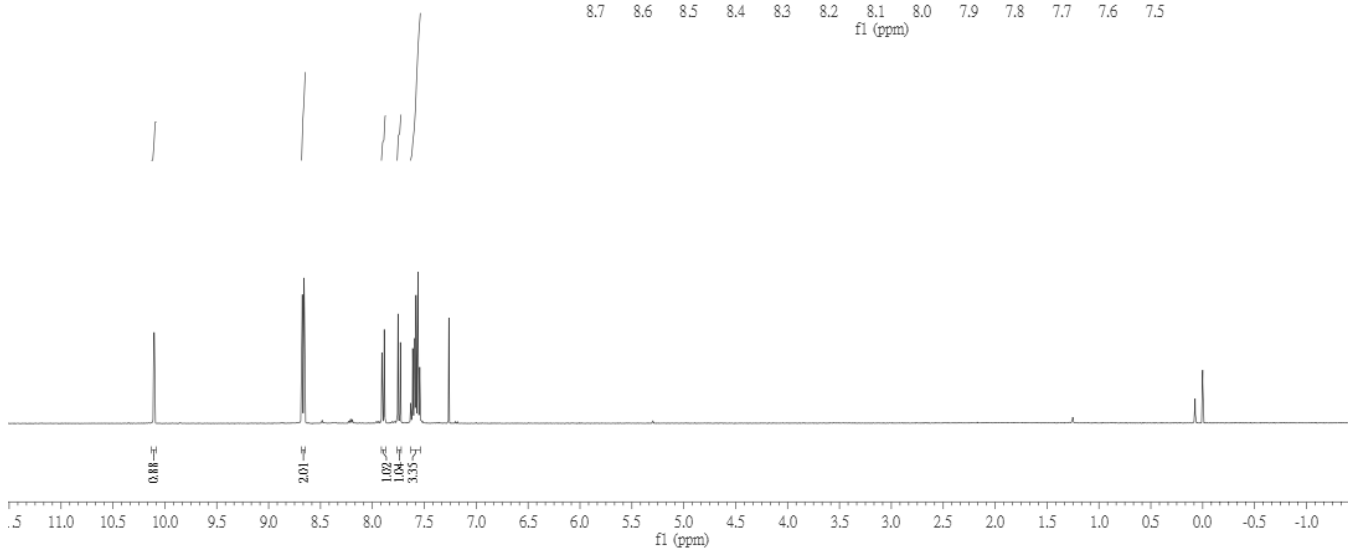
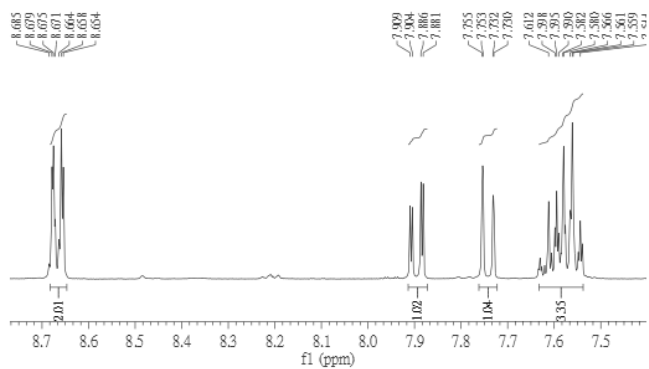
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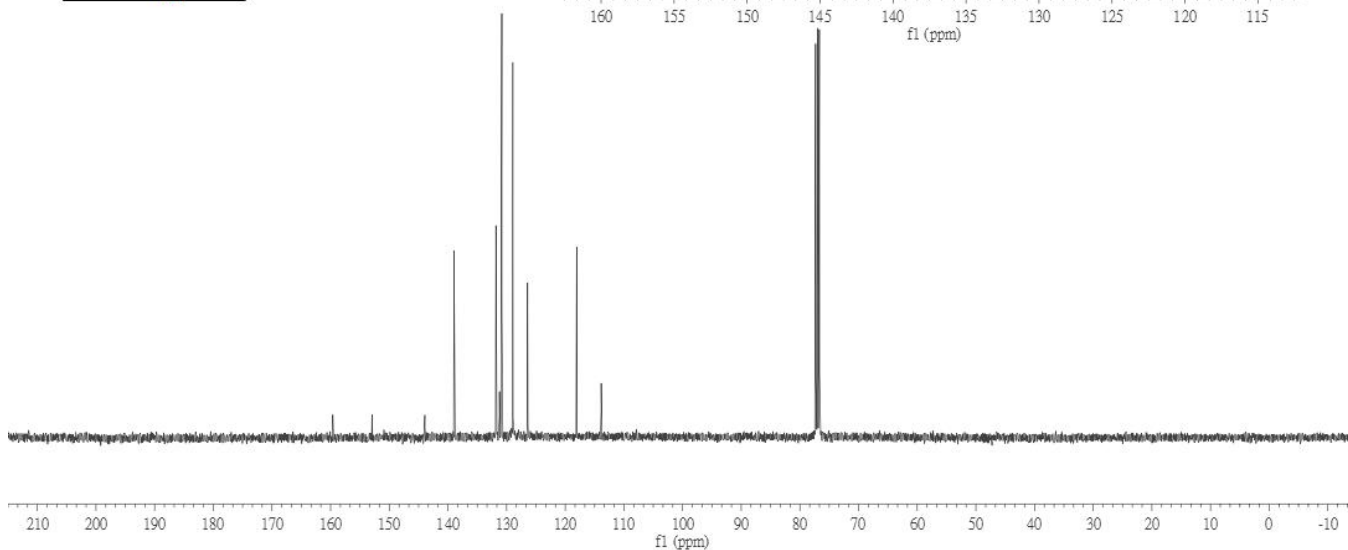
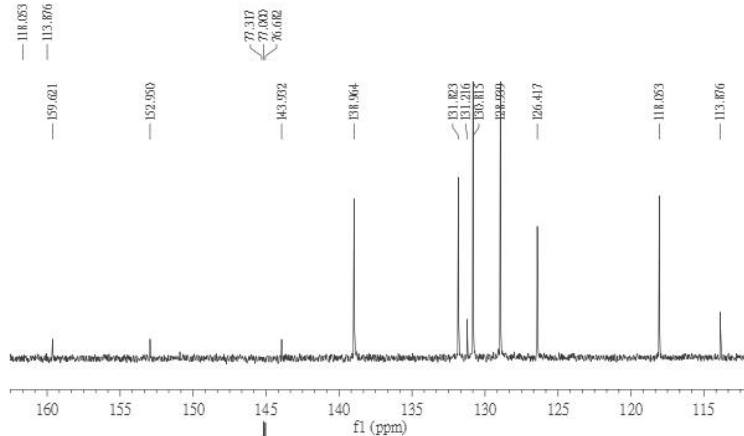
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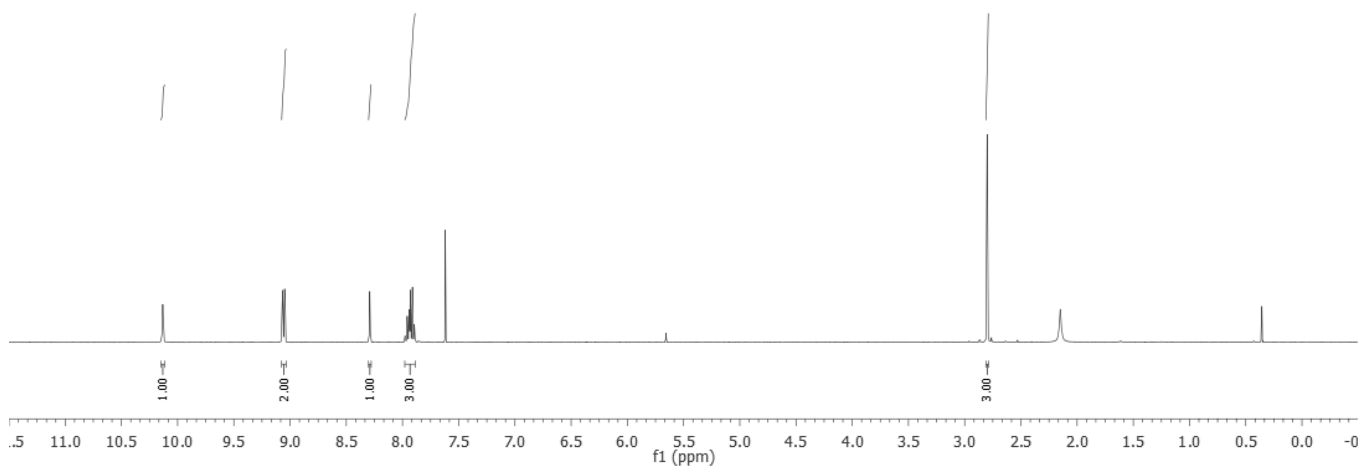
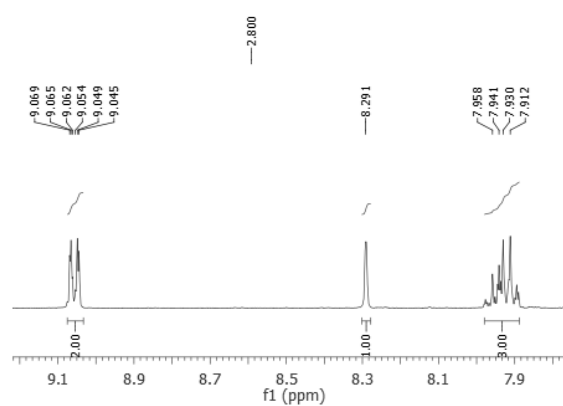
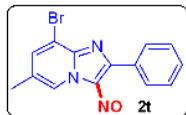
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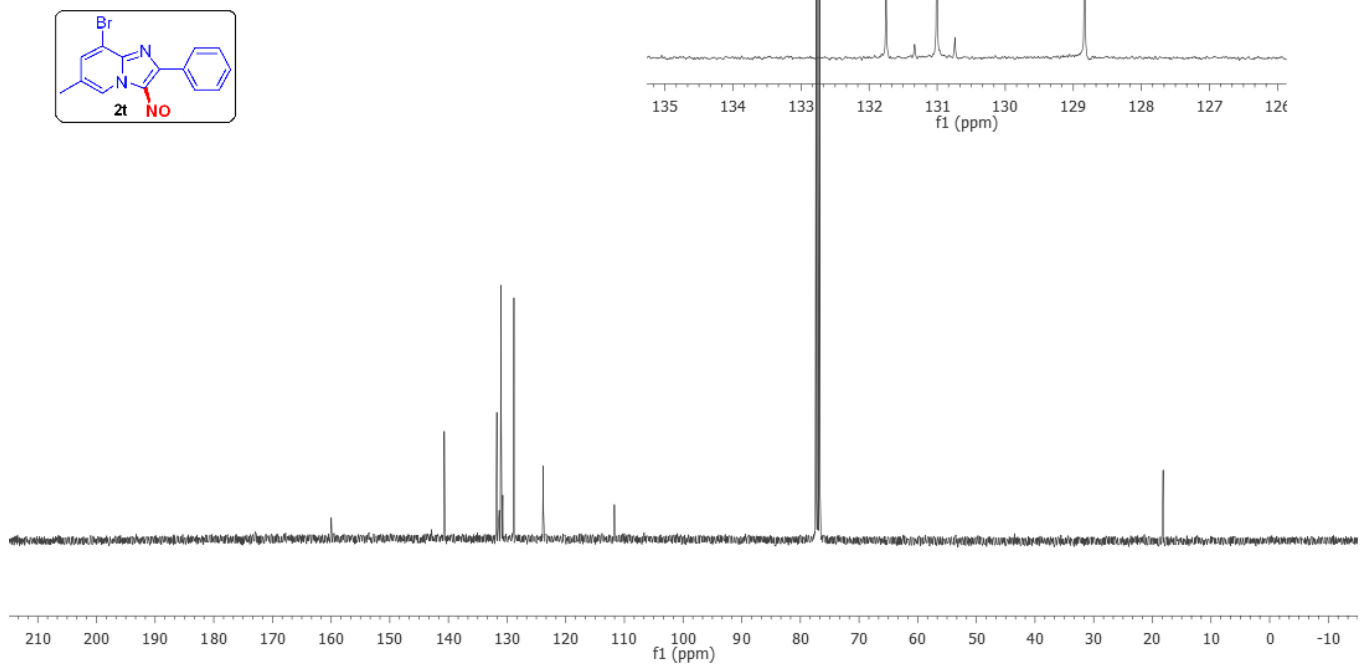
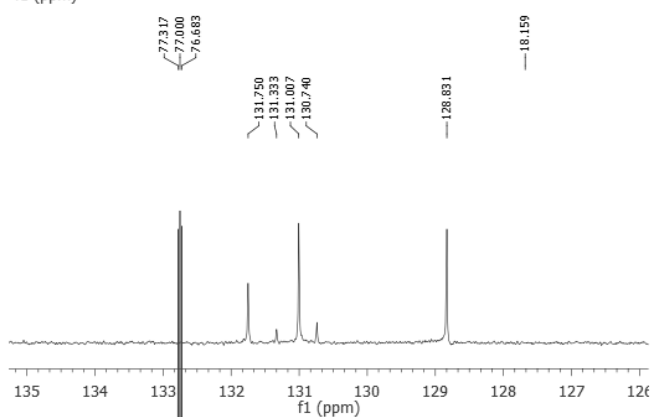
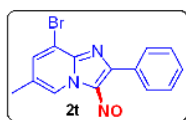
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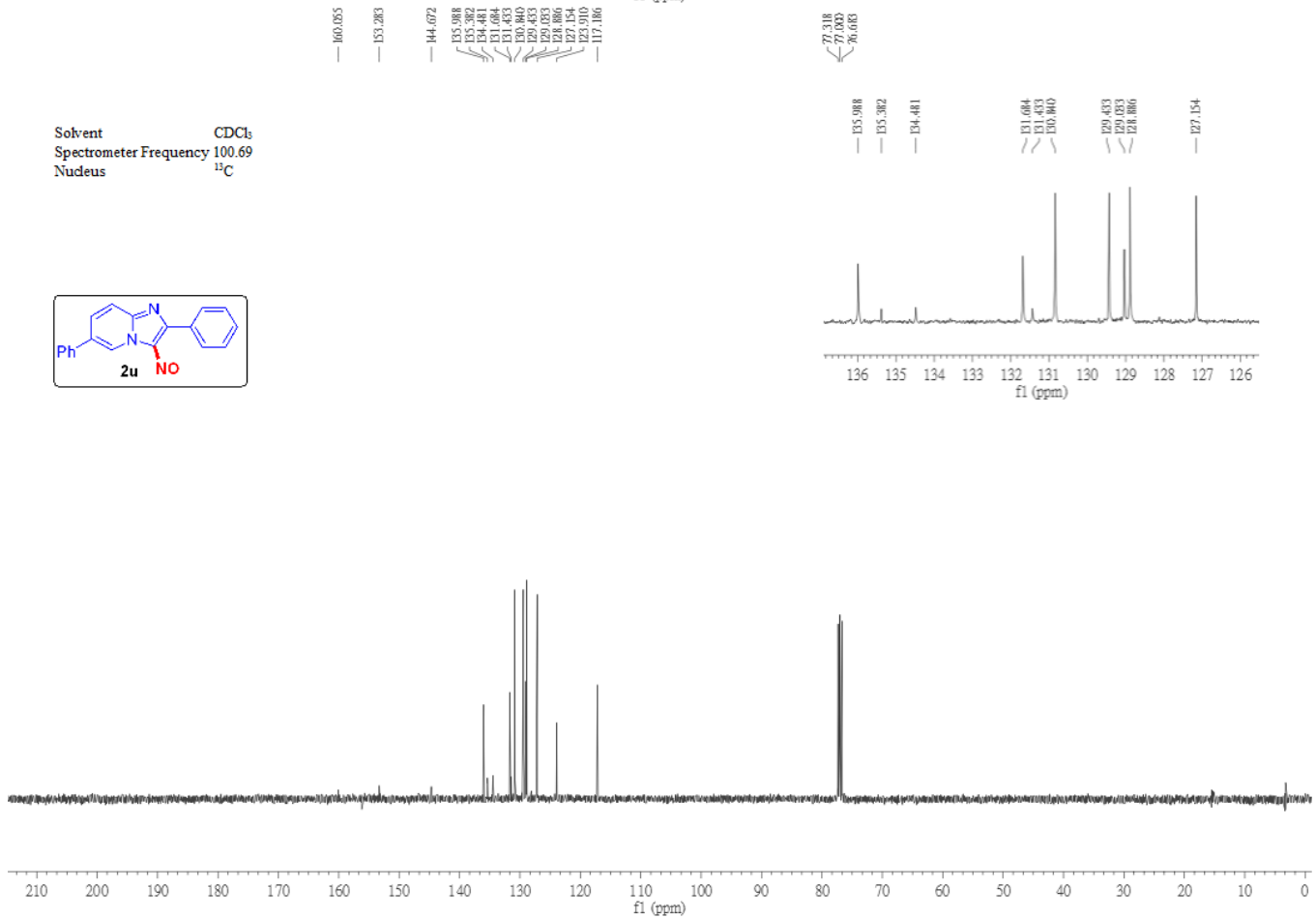
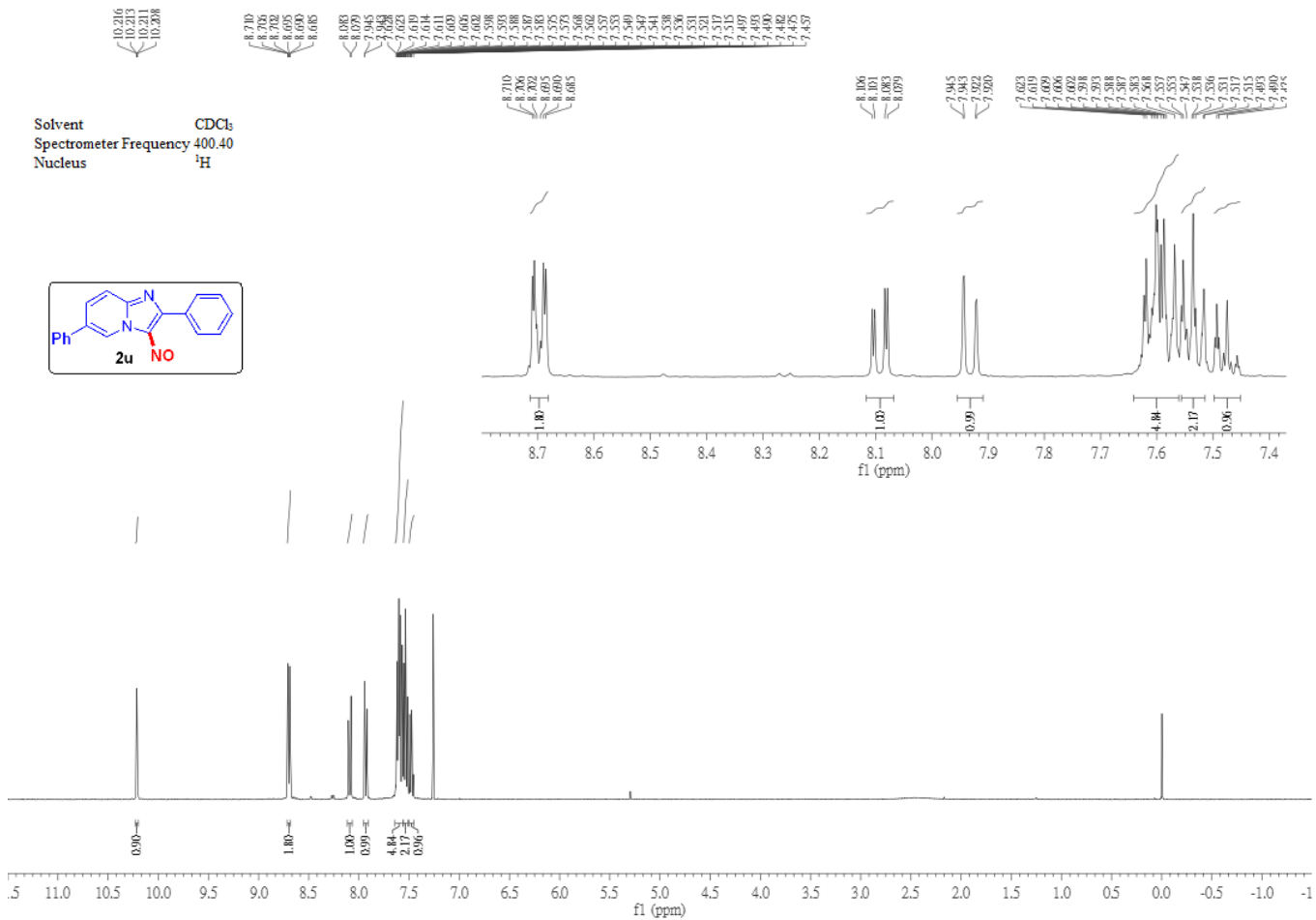


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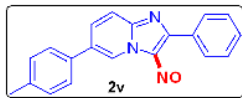


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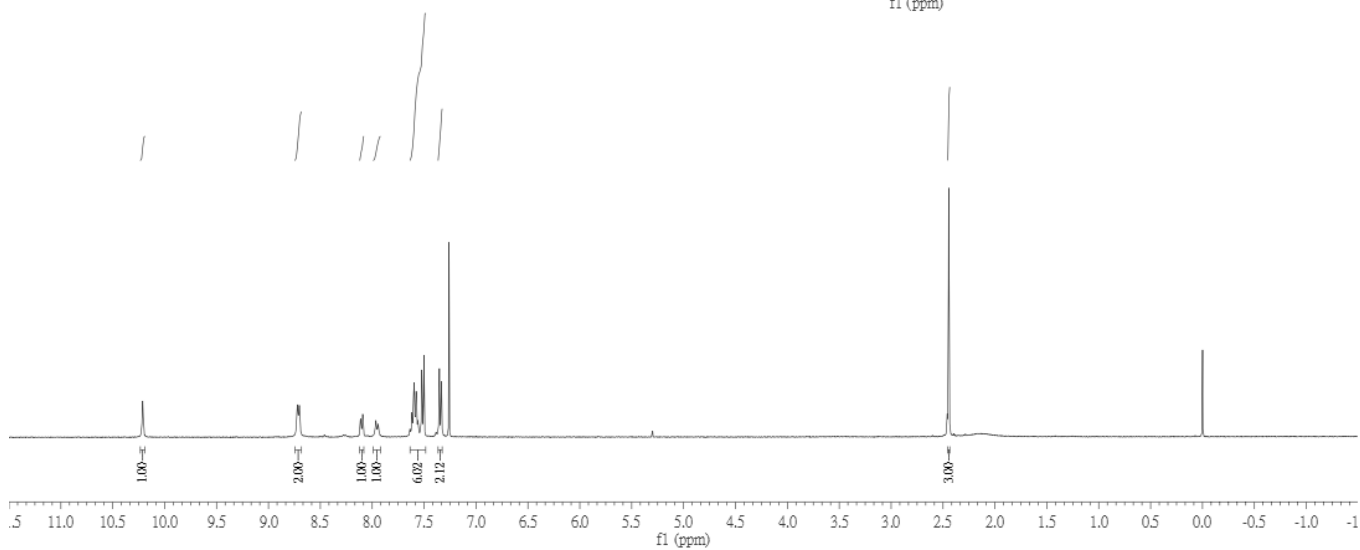
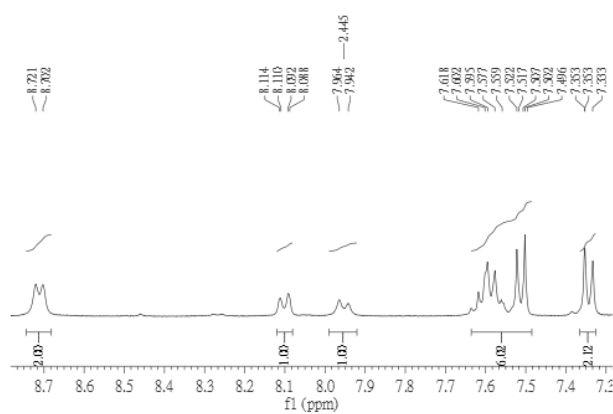




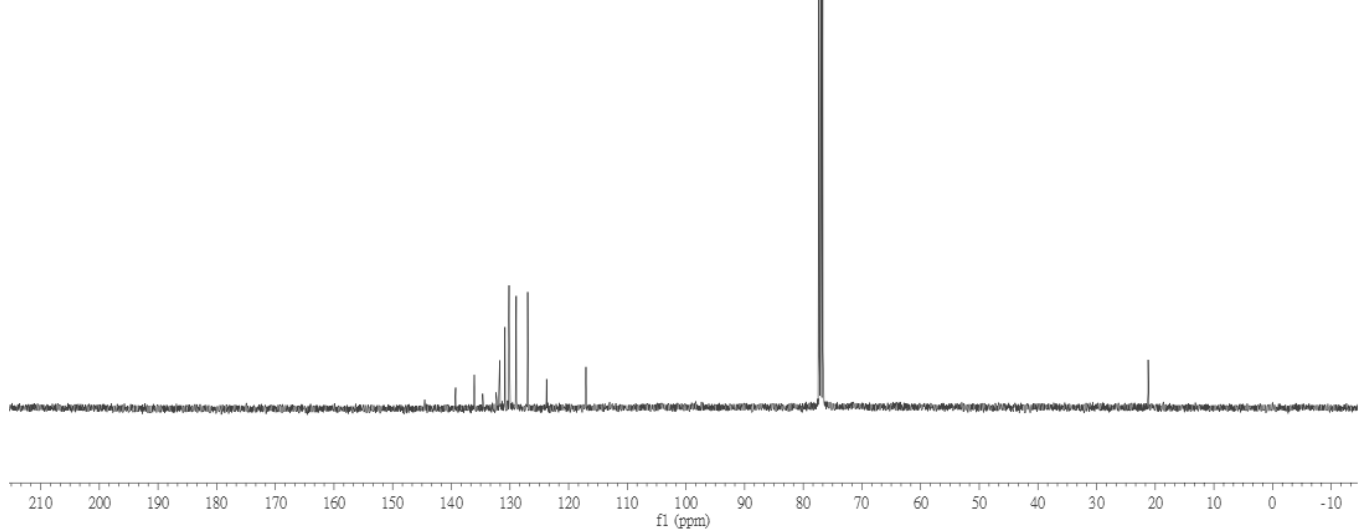
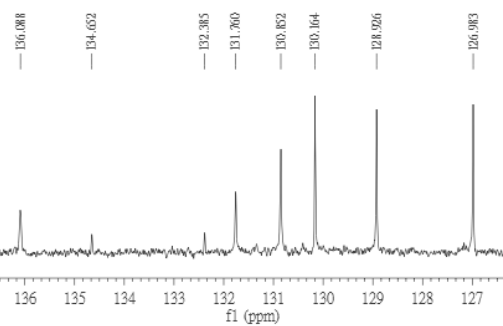
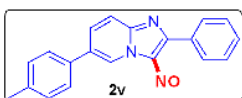
Solvent CDCl_3
 Spectrometer Frequency 400.40
 Nucleus ^1H



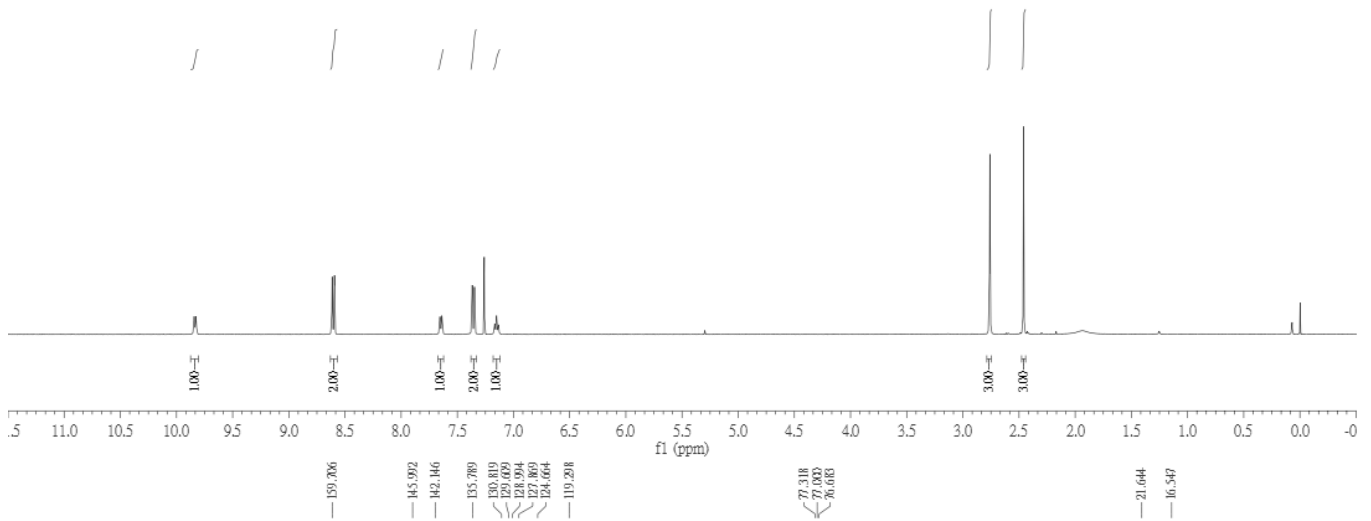
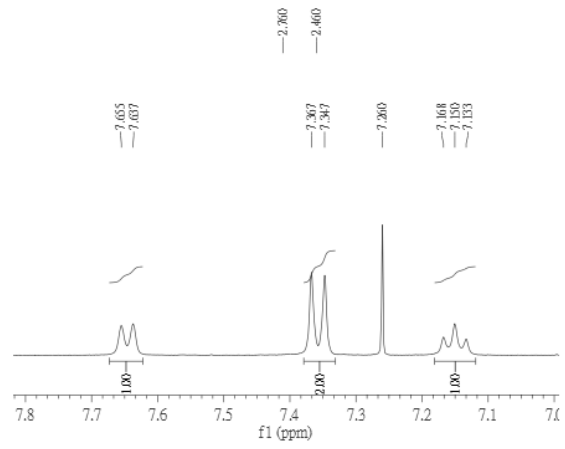
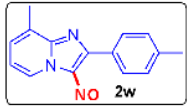
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10.210
8.721
8.702
8.114
8.110
8.092
8.064
7.942
7.618
7.602
7.595
7.579
7.572
7.517
7.509
7.482
7.468
7.333
7.333
7.260



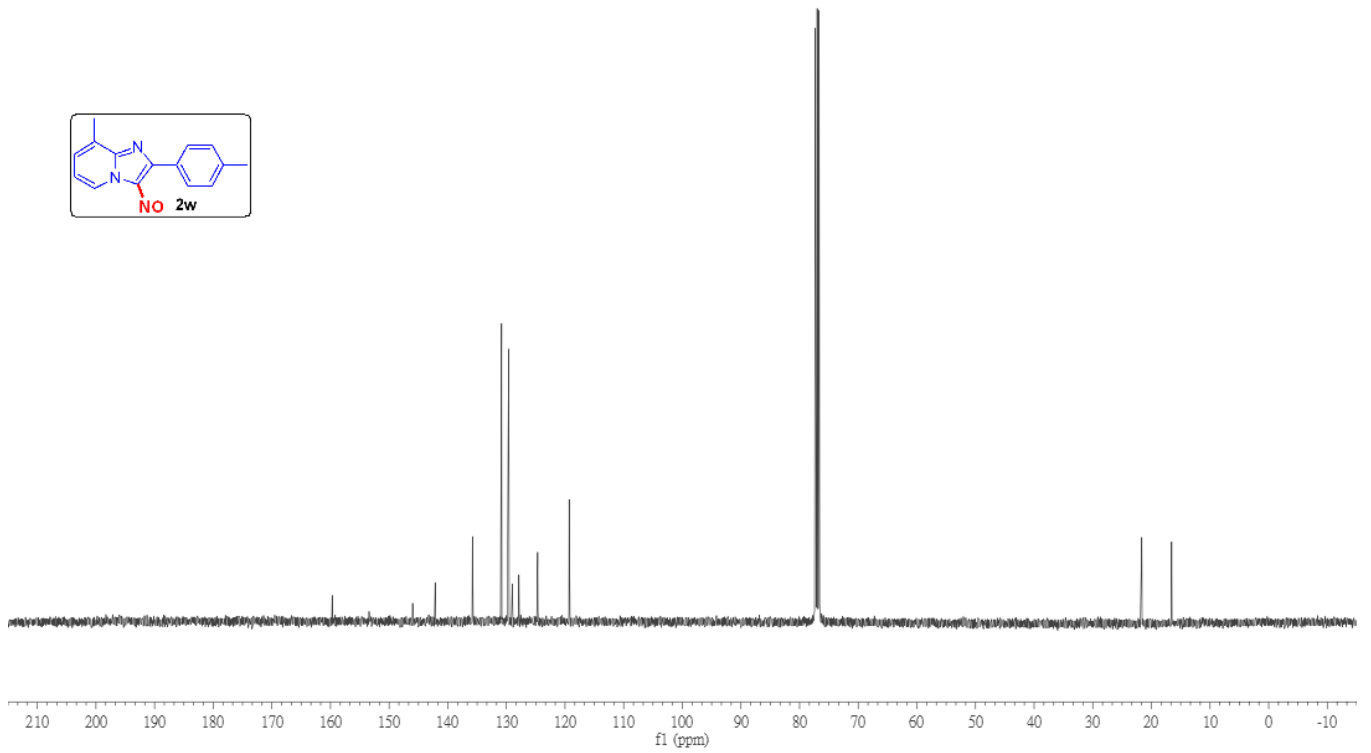
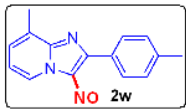
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 Spectrometer Frequency 100.69
 Nucleus ^{13}C

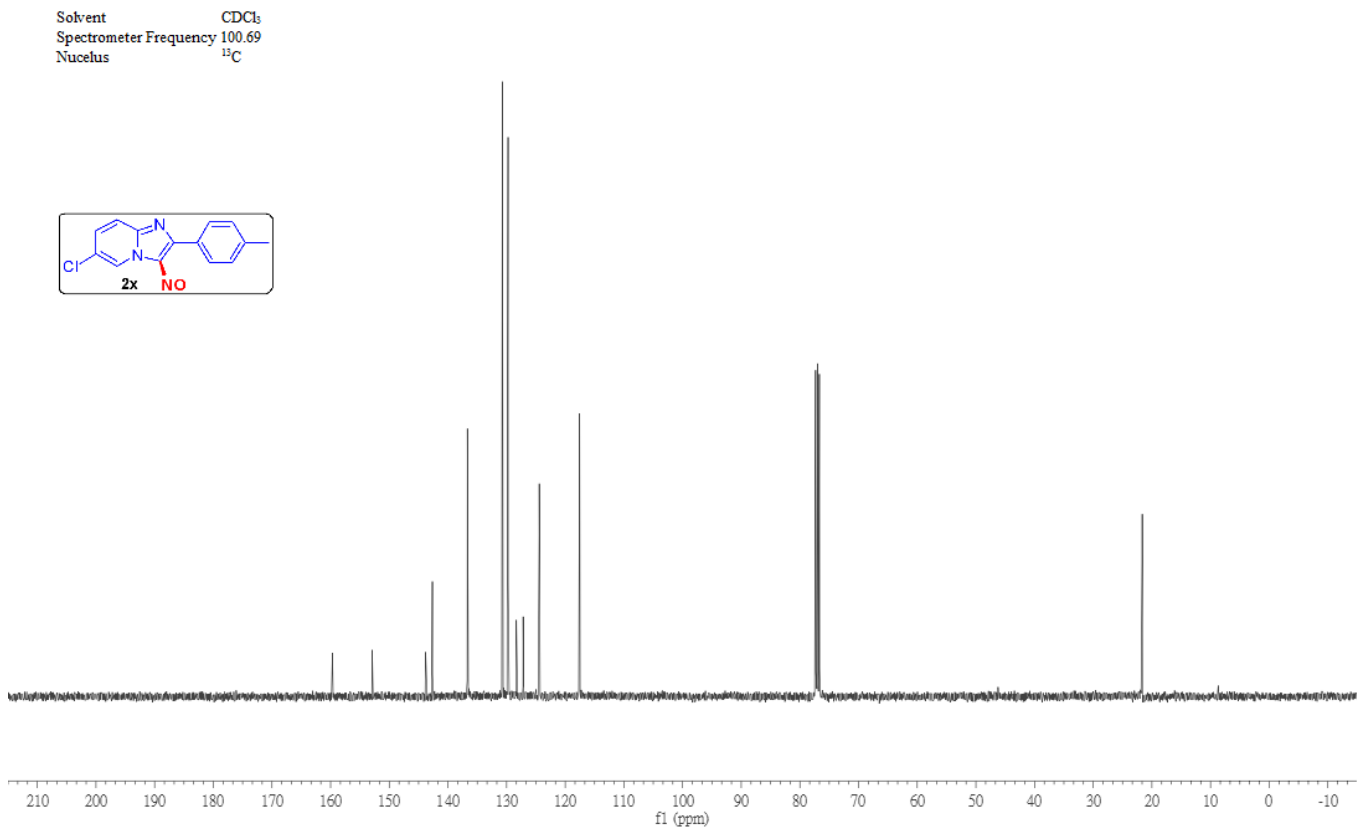
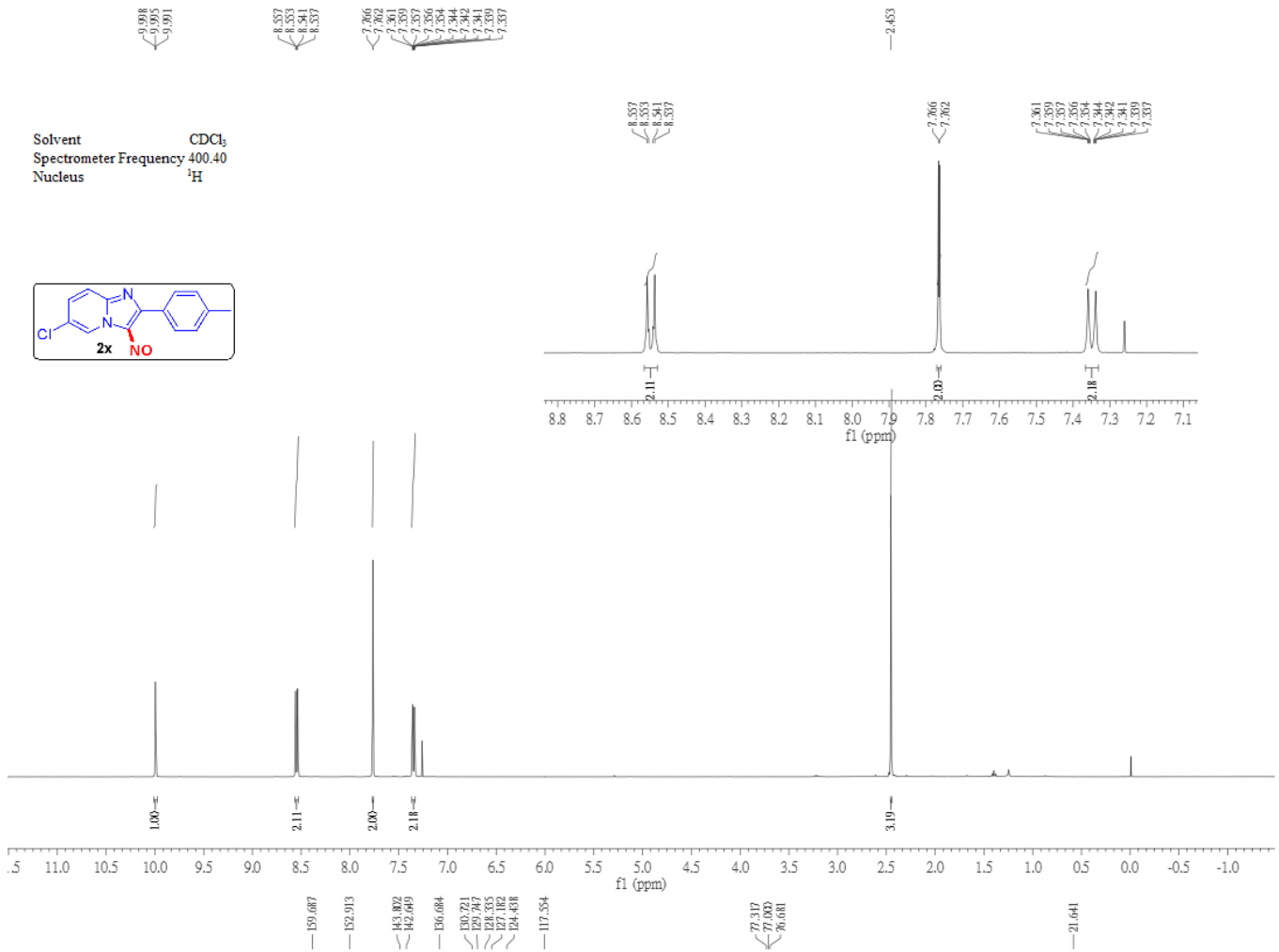


Solvent CDCl_3
 Spectrometer Frequency 400.40
 Nucleus ^1H

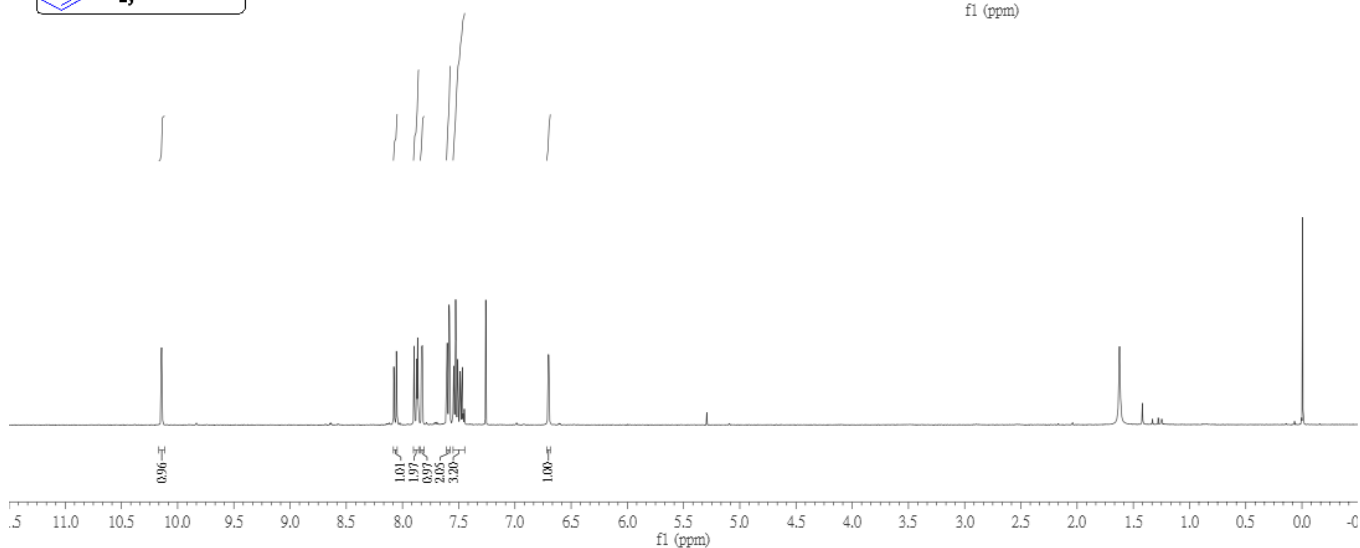
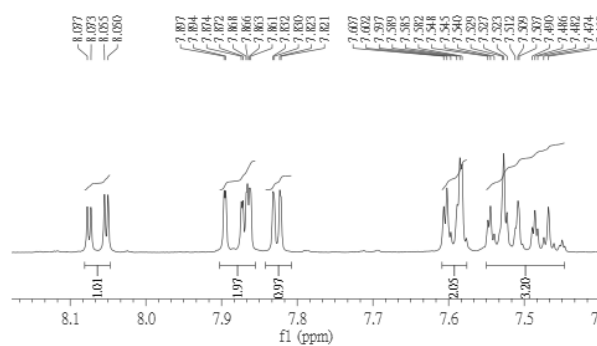
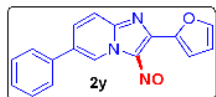


Solvent CDCl_3
 Spectrometer Frequency 100.69
 Nucleus ^{13}C

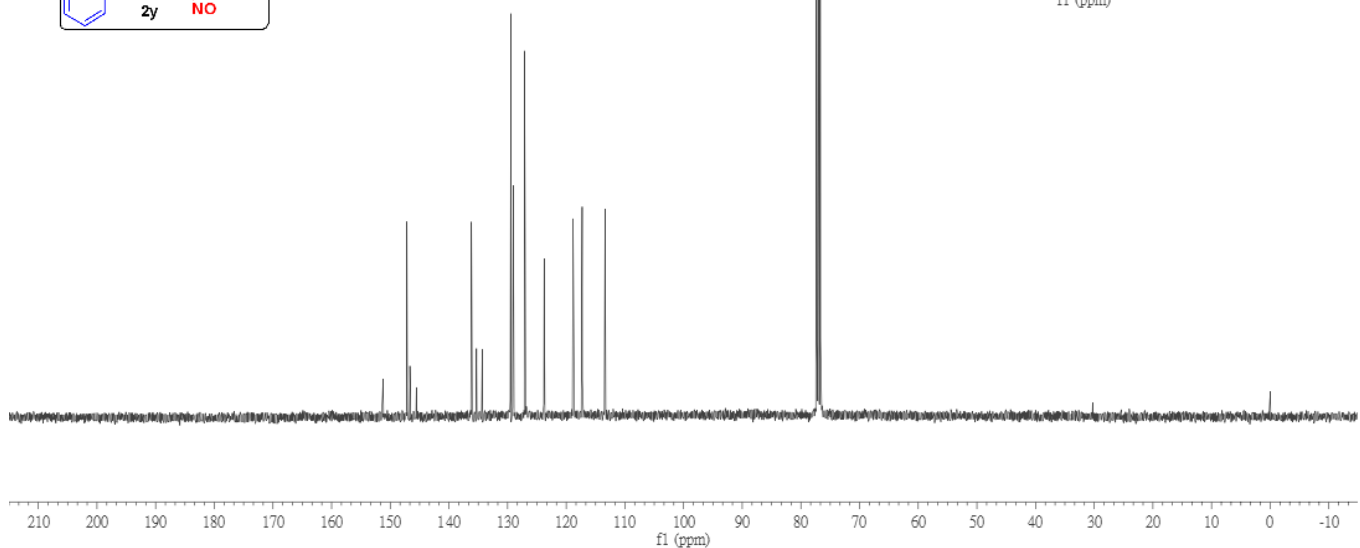
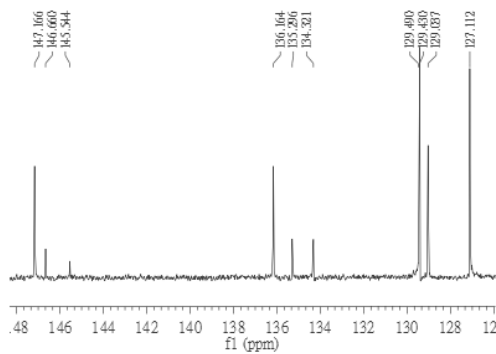
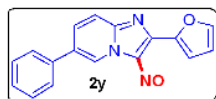




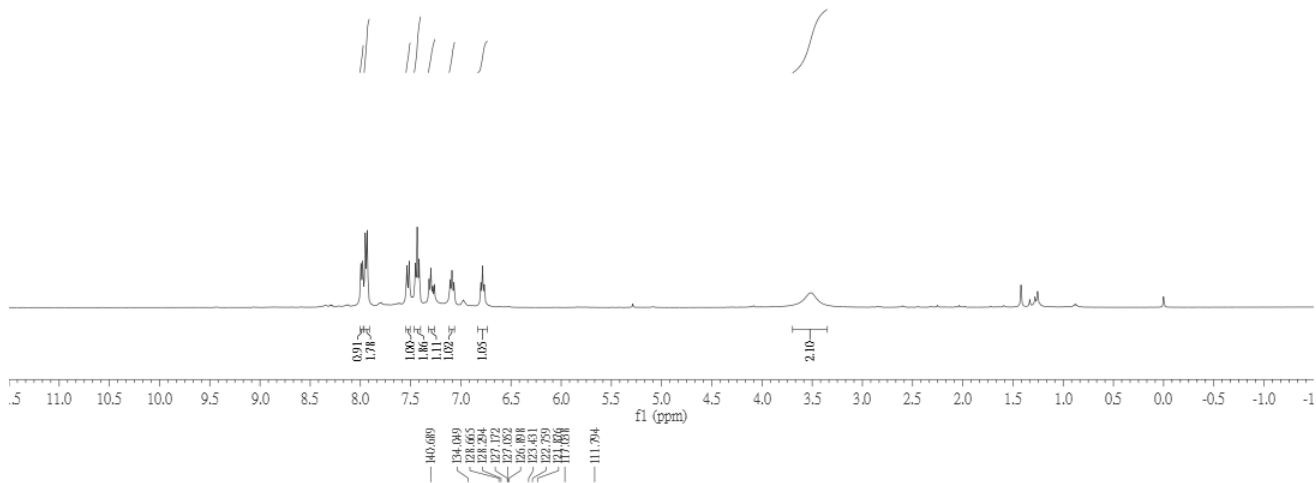
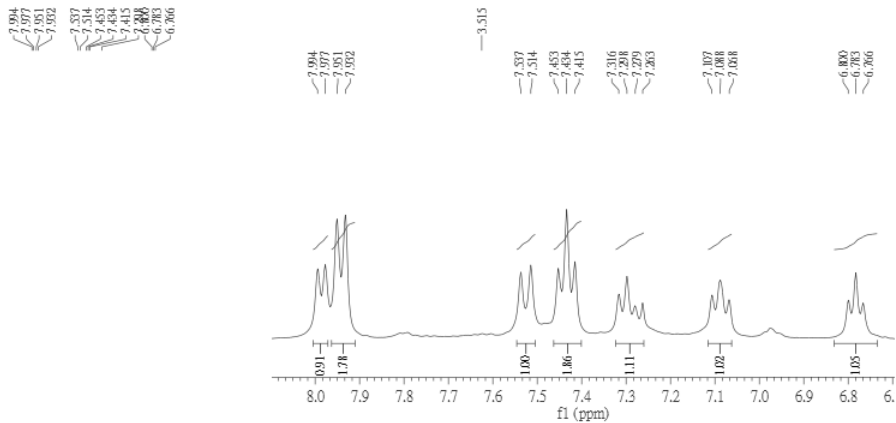
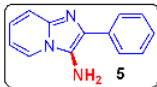
Solvent CDCl_3
 Spectrometer Frequency 400.40
 Nucleus ^1H



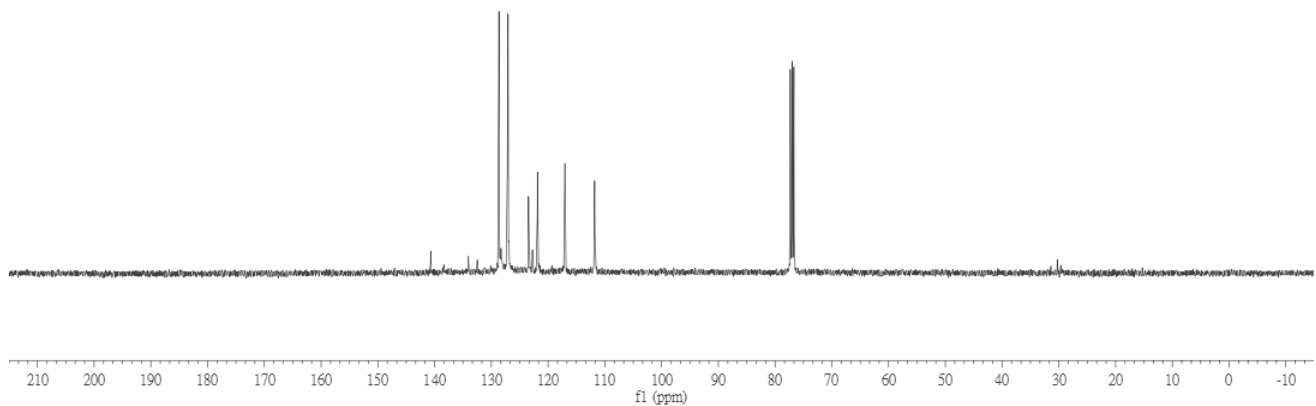
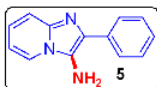
Solvent CDCl_3
 Spectrometer Frequency 100.69
 Nucleus ^{13}C



Solvent CDCl₃
 Spectrometer Frequency 400.40
 Nucleus ¹H



Solvent CDCl₃
 Spectrometer Frequency 100.69
 Nucleus ¹³C



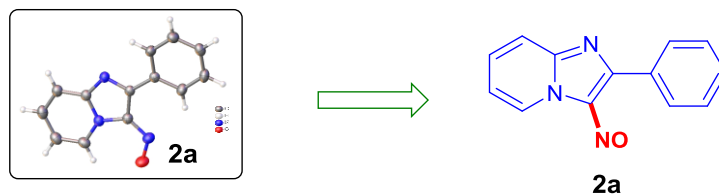


Table 1. Crystal data and structure refinement for **2a**.

Identification code	2a	
Empirical formula	C ₁₃ H ₉ N ₃ O	
Formula weight	223.23	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 10.8002(6) Å	α = 90°.
	b = 8.8240(5) Å	β = 100.264(3)°.
	c = 22.0252(13) Å	γ = 90°.
Volume	2065.4(2) Å ³	
Z	8	
Density (calculated)	1.436 Mg/m ³	
Absorption coefficient	0.095 mm ⁻¹	
F(000)	928	
Crystal size	0.530 x 0.290 x 0.200 mm ³	
Theta range for data collection	3.041 to 26.394°.	
Index ranges	-13 ≤ h ≤ 13, -11 ≤ k ≤ 11, -27 ≤ l ≤ 27	
Reflections collected	34885	
Independent reflections	4196 [R(int) = 0.0429]	
Completeness to theta = 25.242°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9281 and 0.8181	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4196 / 0 / 307	
Goodness-of-fit on F ²	1.067	
Final R indices [I > 2σ(I)]	R1 = 0.0398, wR2 = 0.1084	
R indices (all data)	R1 = 0.0533, wR2 = 0.1221	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.219 and -0.188 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for vsk7. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
O(1)	7648(1)	4062(1)	684(1)	39(1)
N(1)	4269(1)	1023(1)	531(1)	27(1)
N(2)	5388(1)	2750(1)	90(1)	26(1)
N(3)	7117(1)	3124(2)	989(1)	32(1)
C(1)	4319(1)	1858(2)	19(1)	26(1)
C(2)	3459(2)	1900(2)	-535(1)	31(1)
C(3)	3714(2)	2825(2)	-1000(1)	35(1)
C(4)	4813(2)	3714(2)	-913(1)	34(1)
C(5)	5646(2)	3681(2)	-370(1)	31(1)
C(6)	6046(1)	2470(2)	692(1)	27(1)
C(7)	5301(1)	1382(2)	940(1)	25(1)
C(8)	5545(2)	663(2)	1553(1)	27(1)
C(9)	6746(2)	608(2)	1918(1)	32(1)
C(10)	6923(2)	-125(2)	2486(1)	39(1)
C(11)	5924(2)	-802(2)	2696(1)	41(1)
C(12)	4732(2)	-744(2)	2335(1)	40(1)
C(13)	4540(2)	-20(2)	1768(1)	33(1)
O(2)	2435(1)	3848(1)	720(1)	39(1)
N(4)	-880(1)	731(1)	627(1)	26(1)
N(5)	173(1)	2494(1)	168(1)	26(1)
N(6)	1945(1)	2901(2)	1037(1)	32(1)
C(14)	-866(1)	1560(2)	108(1)	25(1)
C(15)	-1746(2)	1562(2)	-439(1)	30(1)
C(16)	-1538(2)	2499(2)	-908(1)	34(1)
C(17)	-458(2)	3420(2)	-838(1)	35(1)
C(18)	398(2)	3417(2)	-304(1)	30(1)
C(19)	854(1)	2254(2)	767(1)	27(1)
C(20)	149(1)	1140(2)	1029(1)	24(1)
C(21)	436(1)	429(2)	1642(1)	25(1)
C(22)	1456(2)	859(2)	2093(1)	31(1)
C(23)	1680(2)	117(2)	2660(1)	35(1)
C(24)	915(2)	-1056(2)	2783(1)	32(1)
C(25)	-93(2)	-1502(2)	2336(1)	34(1)
C(26)	-331(2)	-759(2)	1773(1)	30(1)

Table 3. Bond lengths [Å] and angles [°] for vsk7.

O(1)-N(3)	1.2665(17)
N(1)-C(7)	1.3388(19)
N(1)-C(1)	1.3572(19)
N(2)-C(5)	1.3725(19)
N(2)-C(1)	1.3830(19)
N(2)-C(6)	1.4093(19)
N(3)-C(6)	1.353(2)
C(1)-C(2)	1.395(2)
C(2)-C(3)	1.376(2)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.407(2)
C(3)-H(3B)	0.9500
C(4)-C(5)	1.363(2)
C(4)-H(4A)	0.9500
C(5)-H(5A)	0.9500
C(6)-C(7)	1.422(2)
C(7)-C(8)	1.474(2)
C(8)-C(13)	1.395(2)
C(8)-C(9)	1.398(2)
C(9)-C(10)	1.391(2)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.383(3)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.389(3)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.386(2)
C(12)-H(12A)	0.9500
C(13)-H(13A)	0.9500
O(2)-N(6)	1.2643(17)
N(4)-C(20)	1.3404(19)
N(4)-C(14)	1.3602(19)
N(5)-C(14)	1.3795(19)
N(5)-C(18)	1.3745(19)
N(5)-C(19)	1.4086(19)
N(6)-C(19)	1.348(2)
C(14)-C(15)	1.394(2)
C(15)-C(16)	1.373(2)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.407(2)
C(16)-H(16A)	0.9500
C(17)-C(18)	1.362(2)
C(17)-H(17A)	0.9500
C(18)-H(18A)	0.9500
C(19)-C(20)	1.427(2)
C(20)-C(21)	1.470(2)
C(21)-C(22)	1.398(2)
C(21)-C(26)	1.398(2)
C(22)-C(23)	1.393(2)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.381(2)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.389(2)
C(24)-H(24A)	0.9500

C(25)-C(26)	1.386(2)
C(25)-H(25A)	0.9500
C(26)-H(26A)	0.9500
C(7)-N(1)-C(1)	106.18(13)
C(5)-N(2)-C(1)	122.13(13)
C(5)-N(2)-C(6)	131.72(14)
C(1)-N(2)-C(6)	106.15(12)
O(1)-N(3)-C(6)	116.86(14)
N(1)-C(1)-N(2)	111.72(13)
N(1)-C(1)-C(2)	128.48(14)
N(2)-C(1)-C(2)	119.80(14)
C(3)-C(2)-C(1)	118.42(15)
C(3)-C(2)-H(2A)	120.8
C(1)-C(2)-H(2A)	120.8
C(2)-C(3)-C(4)	120.36(15)
C(2)-C(3)-H(3B)	119.8
C(4)-C(3)-H(3B)	119.8
C(5)-C(4)-C(3)	121.13(15)
C(5)-C(4)-H(4A)	119.4
C(3)-C(4)-H(4A)	119.4
C(4)-C(5)-N(2)	118.16(15)
C(4)-C(5)-H(5A)	120.9
N(2)-C(5)-H(5A)	120.9
N(3)-C(6)-N(2)	128.64(14)
N(3)-C(6)-C(7)	126.59(14)
N(2)-C(6)-C(7)	104.71(13)
N(1)-C(7)-C(6)	111.24(13)
N(1)-C(7)-C(8)	120.37(14)
C(6)-C(7)-C(8)	128.39(14)
C(13)-C(8)-C(9)	119.23(15)
C(13)-C(8)-C(7)	118.25(14)
C(9)-C(8)-C(7)	122.50(14)
C(8)-C(9)-C(10)	119.83(16)
C(8)-C(9)-H(9A)	120.1
C(10)-C(9)-H(9A)	120.1
C(11)-C(10)-C(9)	120.72(16)
C(11)-C(10)-H(10A)	119.6
C(9)-C(10)-H(10A)	119.6
C(10)-C(11)-C(12)	119.47(16)
C(10)-C(11)-H(11A)	120.3
C(12)-C(11)-H(11A)	120.3
C(11)-C(12)-C(13)	120.45(17)
C(11)-C(12)-H(12A)	119.8
C(13)-C(12)-H(12A)	119.8
C(8)-C(13)-C(12)	120.29(16)
C(8)-C(13)-H(13A)	119.9
C(12)-C(13)-H(13A)	119.9
C(20)-N(4)-C(14)	106.17(12)
C(14)-N(5)-C(18)	122.16(13)
C(14)-N(5)-C(19)	106.26(12)
C(18)-N(5)-C(19)	131.58(14)
O(2)-N(6)-C(19)	117.05(14)
N(4)-C(14)-N(5)	111.81(13)
N(4)-C(14)-C(15)	128.23(14)
N(5)-C(14)-C(15)	119.97(14)

C(16)-C(15)-C(14)	118.23(15)
C(16)-C(15)-H(15A)	120.9
C(14)-C(15)-H(15A)	120.9
C(15)-C(16)-C(17)	120.58(15)
C(15)-C(16)-H(16A)	119.7
C(17)-C(16)-H(16A)	119.7
C(18)-C(17)-C(16)	121.03(15)
C(18)-C(17)-H(17A)	119.5
C(16)-C(17)-H(17A)	119.5
C(17)-C(18)-N(5)	118.01(15)
C(17)-C(18)-H(18A)	121.0
N(5)-C(18)-H(18A)	121.0
N(6)-C(19)-N(5)	128.29(14)
N(6)-C(19)-C(20)	126.93(14)
N(5)-C(19)-C(20)	104.77(13)
N(4)-C(20)-C(19)	110.99(13)
N(4)-C(20)-C(21)	120.36(13)
C(19)-C(20)-C(21)	128.63(14)
C(22)-C(21)-C(26)	118.51(14)
C(22)-C(21)-C(20)	123.18(14)
C(26)-C(21)-C(20)	118.30(14)
C(21)-C(22)-C(23)	119.94(15)
C(21)-C(22)-H(22A)	120.0
C(23)-C(22)-H(22A)	120.0
C(24)-C(23)-C(22)	120.92(15)
C(24)-C(23)-H(23A)	119.5
C(22)-C(23)-H(23A)	119.5
C(23)-C(24)-C(25)	119.59(15)
C(23)-C(24)-H(24A)	120.2
C(25)-C(24)-H(24A)	120.2
C(26)-C(25)-C(24)	119.84(16)
C(26)-C(25)-H(25A)	120.1
C(24)-C(25)-H(25A)	120.1
C(25)-C(26)-C(21)	121.19(15)
C(25)-C(26)-H(26A)	119.4
C(21)-C(26)-H(26A)	119.4

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for vsk7. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
O(1)	38(1)	32(1)	48(1)	-2(1)	10(1)	-10(1)
N(1)	29(1)	25(1)	26(1)	-1(1)	3(1)	1(1)
N(2)	30(1)	22(1)	28(1)	-2(1)	6(1)	2(1)
N(3)	31(1)	26(1)	39(1)	-5(1)	6(1)	-4(1)
C(1)	28(1)	21(1)	29(1)	-3(1)	6(1)	2(1)
C(2)	33(1)	27(1)	31(1)	-2(1)	3(1)	2(1)
C(3)	42(1)	31(1)	30(1)	-1(1)	2(1)	6(1)
C(4)	46(1)	28(1)	30(1)	3(1)	12(1)	4(1)
C(5)	38(1)	24(1)	33(1)	1(1)	13(1)	1(1)
C(6)	28(1)	24(1)	27(1)	-4(1)	4(1)	2(1)
C(7)	28(1)	21(1)	27(1)	-4(1)	5(1)	3(1)
C(8)	32(1)	23(1)	26(1)	-3(1)	4(1)	3(1)
C(9)	31(1)	32(1)	33(1)	-3(1)	4(1)	3(1)
C(10)	38(1)	41(1)	34(1)	-1(1)	-2(1)	10(1)
C(11)	50(1)	39(1)	33(1)	7(1)	5(1)	10(1)
C(12)	45(1)	38(1)	39(1)	8(1)	10(1)	0(1)
C(13)	34(1)	31(1)	32(1)	1(1)	2(1)	-1(1)
O(2)	38(1)	34(1)	46(1)	6(1)	7(1)	-10(1)
N(4)	27(1)	25(1)	26(1)	-1(1)	3(1)	1(1)
N(5)	29(1)	23(1)	27(1)	-1(1)	5(1)	2(1)
N(6)	31(1)	28(1)	38(1)	0(1)	5(1)	-5(1)
C(14)	27(1)	22(1)	28(1)	-3(1)	5(1)	2(1)
C(15)	31(1)	28(1)	29(1)	-1(1)	4(1)	4(1)
C(16)	39(1)	33(1)	29(1)	0(1)	1(1)	8(1)
C(17)	45(1)	30(1)	31(1)	4(1)	9(1)	4(1)
C(18)	37(1)	24(1)	33(1)	2(1)	12(1)	1(1)
C(19)	28(1)	24(1)	28(1)	-1(1)	4(1)	2(1)
C(20)	25(1)	22(1)	26(1)	-3(1)	6(1)	3(1)
C(21)	26(1)	23(1)	26(1)	-1(1)	6(1)	4(1)
C(22)	33(1)	27(1)	32(1)	-4(1)	1(1)	-3(1)
C(23)	37(1)	36(1)	29(1)	-5(1)	-3(1)	1(1)
C(24)	38(1)	33(1)	26(1)	3(1)	5(1)	8(1)
C(25)	34(1)	36(1)	33(1)	6(1)	6(1)	0(1)
C(26)	27(1)	33(1)	30(1)	1(1)	2(1)	-2(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for vsk7.

	x	y	z	U(eq)
H(2A)	2715	1304	-589	37
H(3B)	3145	2864	-1382	42
H(4A)	4976	4349	-1238	41
H(5A)	6386	4286	-312	37
H(9A)	7438	1069	1777	39
H(10A)	7740	-160	2732	47
H(11A)	6053	-1304	3084	49
H(12A)	4042	-1204	2478	48
H(13A)	3721	13	1524	39
H(15A)	-2469	931	-485	36
H(16A)	-2130	2527	-1283	41
H(17A)	-325	4053	-1169	42
H(18A)	1130	4034	-258	37
H(22A)	1995	1657	2013	37
H(23A)	2370	421	2966	42
H(24A)	1077	-1554	3172	39
H(25A)	-619	-2315	2416	41
H(26A)	-1027	-1063	1471	36