Supporting Information

One-Pot Three-Component Synthesis of Hydroxyacetylated Imidazo[1,2-a]pyridines via Visible-Light-Mediated Halogen Atom Transfer

Jalaj Kumar Pathak,[a]]Namrata Rastogi[a] [b]*
[a]Medicinal & Process Chemistry Division, CSIR-Central Drug Research Institute, Sector 10, Jankipuram extension, Sitapur Road, P.O. Box 173, Lucknow 226031, India.
[b]Academy of Scientific and Innovative Research, Ghaziabad 201002, India

* Corresponding author's e-mail: namrata.rastogi.cdri@csir.res.in

Table of Contents

1. General Information

Unless mentioned otherwise, all reactions were carried out under nitrogen atmosphere in flame-dried glassware. All reactions were monitored by TLC, visualization was effected with UV and/or by developing in iodine. The NMR Chemical shifts are reported in δ (ppm) relative to TMS as the internal standard for ^{1}H, ^{13}C and TFA as the internal standard for ^{19}F. To describe spin multiplicity, standard abbreviations such as s, d, t, q, m, dd referring to singlet, doublet, triplet, quartet, multiplet and doublet of doublet respectively, are used.

The *α*-bromo ketones and 2-aminopyridines for *in-situ* generation of imidazo[1,2-*a*]pyridines were obtained commercially. The diazo esters were synthesized from corresponding *α*-bromo esters following the reported procedure.[1] All other reagents and catalysts were purchased from commercial suppliers and used without further purification.

Caution! Diazo compounds should be cautiously handled in a fume hood with Personal Safety Equipment (PPE) since they are toxic and potentially explosive.

2. Instrumentation Details

Melting points were recorded on a Precision melting point apparatus and are uncorrected. NMR spectra were recorded on a Bruker Avance spectrometer at 400/500 MHz (^{1}H), 100 MHz/125 MHz (^{13}C) and 376 MHz (^{19}F). The ESI-HRMS spectra were recorded on Agilent 6520-Q-Tof LC/MS system. The visible light irradiation was performed using high power blue LEDs (455 nm) (make: Original Opulant America, power = 3 W, luminous flux/radiant flux = 687 mW at 700 mA) fitted in an aluminium block. The block contains 6 holes to hold vials and is fit with water inlet-outlet nozzles. The vials are placed in holes on the block and irradiated from bottom at a distance of approximately 2 cm. The reaction temperature can be maintained by circulating water through the aluminium block via inlet-outlet nozzles (Figure S1).

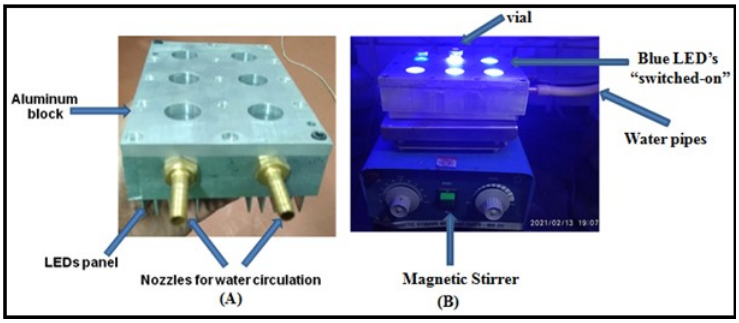


Figure S1. (A) Picture of the visible light photoreactor; (B) Experimental set-up

3. General Procedures

3.1. General procedure for the synthesis of hydroxyacetylated imidazo[1,2-*a*]pyridines 5

To a 5 mL snap vial equipped with a magnetic stir bar were added 2-aminopyridine **1** (0.2 mmol), *α*-bromo ketone **2** (0.2 mmol), diazo ester **4** (0.4 mmol), and iodine (5 mg, 0.02 mmol)

in DCE (2.0 mL). The resulting reaction mixture was stirred at room temperature (≈25 °C) in open air under irradiation with 3 W blue LEDs (455 nm). After completion of the reaction (10-12 h; TLC monitoring), the reaction mixture was concentrated under reduced pressure. The crude residue was purified by column chromatography on silica gel (100–200 mesh) using hexane/ethyl acetate as eluent to afford the pure product **5**.

3.2. Procedure for the synthesis of methyl 2-oxo-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)acetate 7[2]

In an oven-dried 10 mL round-bottom flask, equipped with a magnetic stir bar, were added methyl 2-hydroxy-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)acetate **5a** (56 mg, 0.2 mmol) and Dess-Martin periodinane (339 mg, 0.8 mmol) in DCM (2.0 mL). The resulting mixture was stirred at room temperature and was concentrated under reduced pressure after completion of the reaction (4 h; TLC monitoring). The crude residue was purified by column chromatography on silica gel (100–200 mesh) using hexane/ethyl acetate as eluent to afford the pure product **7**.

3.3. Procedure for the synthesis of 1-(2-phenylimidazo[1,2-a]pyridin-3-yl)ethane-1,2-diol 8

In an oven-dried 10 mL round-bottom flask, equipped with a magnetic stir bar, methyl 2-hydroxy-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)acetate **5a** (56 mg, 0.2 mmol) was dissolved in anhydrous THF (2.0 mL) followed by portionwise addition of $LiAlH_4$ (8 mg, 0.2 mmol) at 0 °C. The resulting mixture was brought to room temperature and stirred until completion of the reaction (1 h; TLC monitoring). Subsequently, the reaction was carefully quenched by the sequential addition of ice-cold water (2 mL), 15% aqueous NaOH solution (2 mL), and DCM (5 mL). Anhydrous $MgSO_4$ was then added, and the mixture was stirred for an additional 15 min at room temperature, followed by filtration. The filter cake was washed with a 10:1 mixture of DCM/MeOH (10 mL × 4), and the combined filtrates were concentrated under reduced pressure. The crude residue was purified by column chromatography on silica gel (100–200 mesh) using hexane/ethyl acetate as the eluent to afford the pure product **8**.

3.4. Procedure for the radical trapping reaction

To a 5 mL snap vial, equipped with a magnetic stirring bar, 2-aminopyridine **1a** (18 mg, 0.2 mmol), phenacyl bromide **2a** (39 mg, 0.2 mmol), methyl diazoacetate (40 mg, 0.4 mmol) and I_2 (5 mg, 0.02 mmol) were dissolved in DCE (2.0 mL). Further, TEMPO (93 mg, 0.6 mmol) was added and the resulting reaction mixture was stirred in open air at room temperature (≈ 25 ^oC) under the irradiation of 3 W blue LEDs (455 nm). After 2h, the reaction mixture was concentrated under reduced pressure and the crude reaction mixture was analysed by High Resolution Mass Spectrometry (HRMS).

3.5. Procedure for the Light On-Off experiment

To a 5 mL snap vial, equipped with a magnetic stir bar, were added 2-aminopyridine **1a** (18 mg, 0.2 mmol), phenacyl bromide **2a** (39 mg, 0.2 mmol), **4a** methyl diazoacetate (40 mg, 0.4 mmol), and I_2 (5 mg, 0.02 mmol) in DCE (2.0 mL). The resulting reaction mixture was stirred at room temperature (≈25 °C) in open air and was subjected to alternating light and dark conditions for fixed time intervals (2 h). Irradiation was carried out using 3 W blue LEDs (455 nm) during the first (0-2 h), third (4-6 h), fifth (8-10 h), and seventh (12-14 h) phases, whereas the reaction mixture was stirred in the absence of light during the second (2-4 h), fourth (6-8 h), and sixth (10-12 h) phases. Product formation was observed exclusively during the irradiated periods, while no reaction progress occurred under dark conditions.

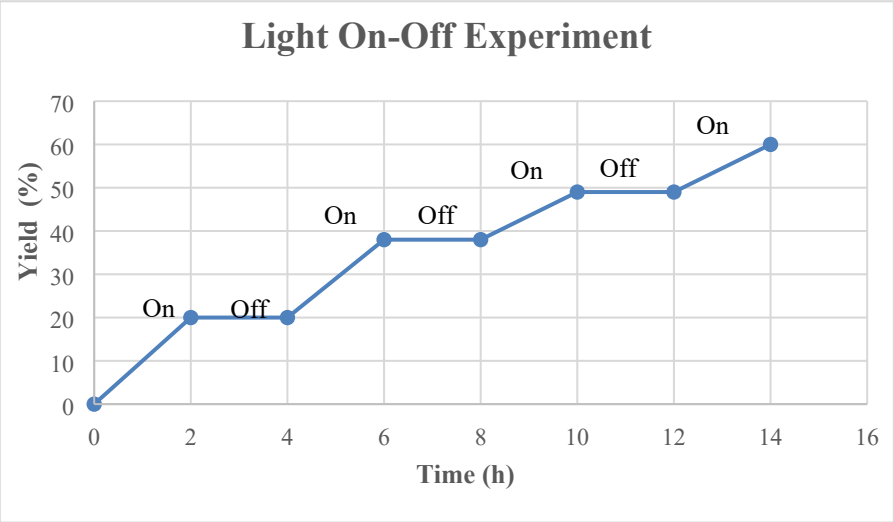
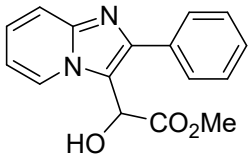


Figure S2. Light on-off experiment

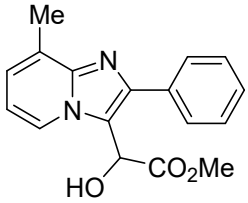
4. Spectroscopic Data

Methyl 2-hydroxy-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)acetate (5a)



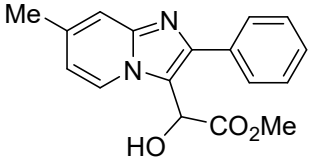
White solid; yield 88% (50 mg); R_f 0.50 (30% EtOAc/hexane); Mp 191-193 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.21 (d, J = 6.7 Hz, 1H), 7.74 (d, J = 7.2 Hz, 2H), 7.66 (d, J = 9.0 Hz, 1H), 7.46 (t, J = 7.2 Hz, 2H), 7.40 (t, J = 7.1 Hz, 1H), 7.23-7.26 (d, J = 8.3 Hz, 1H merged with solvent peak), 6.84 (t, J = 6.5 Hz, 1H), 5.85 (s, 1H), 3.74 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.46, 145.33, 145.00, 133.07, 128.95, 128.55, 128.33, 125.77, 125.57, 117.23, 116.33, 112.88, 65.05, 53.30; **HRMS** for $C_{16}H_{15}N_2O_3^+$: calcd. $[M+H]^+$: 283.1077, found: 283.1085

Methyl 2-hydroxy-2-(8-methyl-2-phenylimidazo[1,2-a]pyridin-3-yl)acetate (5b)



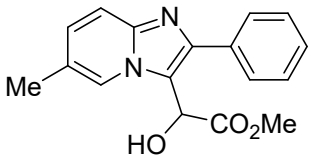
White solid; yield 66% (39 mg); R_f 0.50 (30% EtOAc/hexane); Mp 170-172 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 (d, *J* = 6.7 Hz, 1H), 7.69 (d, *J* = 7.3 Hz, 2H), 7.40 (t, *J* = 7.3 Hz, 2H), 7.35 (t, *J* = 7.2 Hz, 1H), 7.02 (d, *J* = 6.7 Hz, 1H), 6.73 (t, *J* = 6.8 Hz, 1H), 5.77 (s, 1H), 3.70 (s, 3H), 2.62 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 172.74, 145.58, 145.46, 133.53, 129.16, 128.49, 128.17, 127.50, 124.40, 123.00, 116.42, 112.87, 65.12, 53.37, 17.16; **HRMS** for $C_{17}H_{17}N_2O_3^+$: calcd. $[M+H]^+$: 297.1234, found 297.1245

Methyl 2-hydroxy-2-(7-methyl-2-phenylimidazo[1,2-a]pyridin-3-yl)acetate (5c)



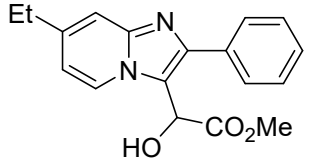
White solid; yield 55% (33 mg); R_f 0.50 (30% EtOAc/hexane); Mp 166-168 °C; **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.35 (d, *J* = 6.9 Hz, 1H), 7.80 (d, *J* = 7.6 Hz, 2H), 7.52 (t, *J* = 7.5 Hz, 2H), 7.43 (t, *J* = 7.3 Hz, 1H), 7.15 (d, *J* = 6.8 Hz, 1H), 6.91 (t, *J* = 6.9 Hz, 1H), 6.47 (br s, 1H), 5.81 (s, 1H), 3.62 (s, 3H), 2.54 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 171.76, 145.20, 143.69, 134.56, 129.07, 129.00, 128.38, 126.93, 124.36, 124.31, 118.54, 112.80, 64.96, 52.84, 17.07; **HRMS** for $C_{17}H_{17}N_2O_3^+$: calcd. $[M+H]^+$: 297.1234, found: 297.1237

Methyl 2-hydroxy-2-(6-methyl-2-phenylimidazo[1,2-a]pyridin-3-yl)acetate (5d)



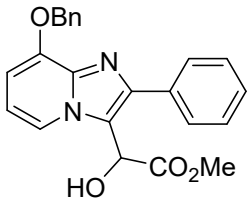
White solid; yield 75% (44 mg); R_f 0.50 (30% EtOAc/hexane); Mp 186-188 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.74 (d, *J* = 7.4 Hz, 2H), 7.57 (d, *J* = 9.1 Hz, 1H), 7.46 (t, *J* = 7.3 Hz, 2H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 9.0 Hz, 1H), 5.83 (s, 1H), 3.75 (s, 3H), 2.35 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 171.72, 144.10, 143.91, 134.57, 129.00, 128.94, 128.74, 128.34, 123.96, 121.89, 117.83, 116.87, 64.88, 52.85, 18.39; **HRMS** for $C_{17}H_{17}N_2O_3^+$: calcd. $[M+H]^+$: 297.1234, found: 297.1237

Methyl 2-(7-ethyl-2-phenylimidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5e)



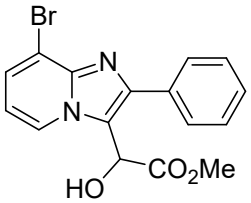
White solid; yield 72% (43 mg); R_f 0.50 (30% EtOAc/hexane); Mp 165-167 °C; **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.41 (d, J = 7.1 Hz, 1H), 7.79 (d, J = 7.3 Hz, 2H), 7.51 (t, J = 7.5 Hz, 2H), 7.42 (t, J = 7.2 Hz, 2H), 6.91 (d, J = 7.0 Hz, 1H), 6.47 (d, J = 4.0 Hz, 1H), 5.80 (d, J = 3.8 Hz, 1H), 3.64 (s, 3H), 2.68 (q, J = 7.5 Hz, 2H), 1.24 (t, J = 7.5 Hz, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 171.77, 145.32, 144.05, 142.42, 134.57, 129.01, 128.91, 128.34, 126.13, 117.51, 114.29, 114.23, 64.97, 52.85, 28.13, 14.98; **HRMS** for $C_{17}H_{17}N_2O_3^+$: calcd. $[M+H]^+$: 297.1234, found: 297.1243

Methyl 2-(8-(benzyloxy)-2-phenylimidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5f)



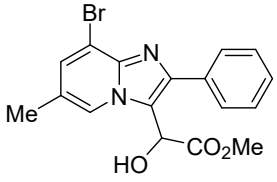
White solid; yield 68% (53 mg); R_f 0.50 (30% EtOAc/hexane); Mp 151-153 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.08 (d, J = 6.4 Hz, 1H), 7.77 (d, J = 7.6 Hz, 2H), 7.48-7.53 (m, 4H), 7.36-7.44 (m, 4H), 6.83-6.90 (m, 2H), 6.46 (d, J = 4.0 Hz, 1H), 5.79 (d, J = 3.9 Hz, 1H), 5.33 (s, 2H), 3.61 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 171.68, 147.78, 143.34, 139.36, 136.89, 134.38, 129.03, 128.98, 128.59, 128.52, 128.38, 119.38, 119.11, 112.76, 104.30, 70.48, 64.86, 52.85; **HRMS** for $C_{23}H_{21}N_2O_4^+$: calcd. $[M+H]^+$: 389.1496, found: 389.1489

Methyl 2-(8-bromo-2-phenylimidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5g)



White solid; yield 68% (49 mg); R_f 0.50 (30% EtOAc/hexane); Mp 164-165 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.53 (d, J = 6.7 Hz, 1H), 7.80 (d, J = 7.2 Hz, 2H), 7.72 (d, J = 7.2 Hz, 1H), 7.54 (t, J = 7.2 Hz, 2H), 7.46 (t, J = 7.2 Hz, 1H), 6.96 (t, J = 7.1 Hz, 1H), 6.59 (d, J = 4.1 Hz, 1H), 5.82 (d, J = 4.0 Hz, 1H), 3.63 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 170.44, 143.57, 141.61, 132.86, 128.15, 127.82, 127.53, 125.37, 119.20, 112.30, 109.80, 64.02, 52.00; **HRMS** for $C_{16}H_{14}BrN_2O_3^+$: calcd. $[M+H]^+$: 361.0182, found: 361.0193

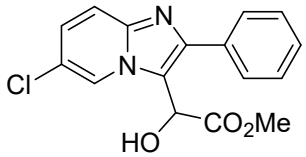
Methyl 2-(8-bromo-6-methyl-2-phenylimidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5h)



White solid; yield 53% (40 mg); R_f 0.50 (30% EtOAc/hexane); Mp 165-166 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.31 (s, 1H), 7.78 (d, J = 7.3 Hz, 2H), 7.62 (s, 1H), 7.52 (t, J = 7.4 Hz, 2H),

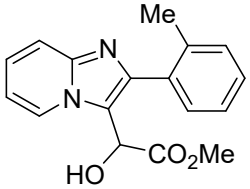
7.44 (t, J = 7.3 Hz, 1H), 6.55 (d, J = 4.2 Hz, 1H), 5.79 (d, J = 4.2 Hz, 1H), 3.61 (s, 3H), 2.32 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 171.42, 144.41, 141.63, 133.98, 131.07, 129.06, 128.66, 123.64, 122.63, 119.91, 110.29, 64.92, 52.93, 18.03; **HRMS** for $C_{17}H_{16}BrN_2O_3^+$: calcd. $[M+H]^+$: 375.0339, found: 375.0350

Methyl 2-(6-chloro-2-phenylimidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5i)



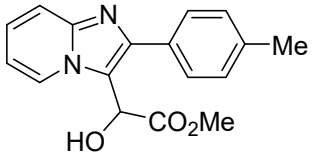
White solid; yield 55% (35 mg); R_f 0.50 (30% EtOAc/hexane); Mp 182-184 °C; **^{1}H NMR** (500 MHz, DMSO-d_6) 8.67 (d, J = 1.3 Hz, 1H), 7.80 (d, J = 7.2 Hz, 2H), 7.73 (d, J = 9.5 Hz, 1H), 7.53 (t, J = 7.5 Hz, 2H), 7.42-7.47 (m, 2H), 6.62 (d, J = 3.8 Hz, 1H), 5.85 (d, J = 3.4 Hz, 1H), 3.64 (s, 1H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 171.37, 145.11, 143.32, 133.85, 129.12, 128.98, 128.77, 126.72, 124.43, 119.61, 118.83, 118.40, 64.81, 53.03; **HRMS** for $C_{16}H_{14}ClN_2O_3^+$: calcd. $[M+H]^+$: 317.0687, found: 317.0694

Methyl 2-hydroxy-2-(2-(o-tolyl)imidazo[1,2-a]pyridin-3-yl)acetate (5j)



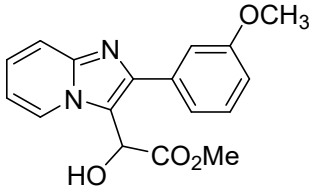
White solid; yield 89% (53 mg); R_f 0.50 (30% EtOAc/hexane); Mp 191-193 °C; **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.48 (d, J = 6.3 Hz, 1H), 7.63 (d, J = 9.1 Hz, 1H), 7.32-7.36 (m, 4H), 7.26-7.29 (m, 1H), 7.01 (t, J = 6.7 Hz, 1H), 6.40 (d, J = 3.6 Hz, 1H), 5.43 (s, 1H), 3.53 (s, 3H), 2.27 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d6) δ 171.60, 144.92, 144.48, 137.91, 133.67, 130.93, 130.66, 128.71, 126.37, 125.82, 125.63, 118.87, 117.38, 112.74, 64.84, 52.65, 20.40; **HRMS** for $C_{17}H_{17}N_2O_3^+$: calcd. $[M+H]^+$: 297.1234, found: 297.1239

Methyl 2-hydroxy-2-(2-(*p*-tolyl)imidazo[1,2-a]pyridin-3-yl)acetate (5k)



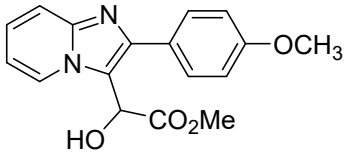
White solid; yield 89% (53 mg); R_f 0.50 (30% EtOAc/hexane); Mp 171-172 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.23 (d, J = 6.9 Hz, 1H), 7.61 (d, J = 9.1 Hz, 1H), 7.58 (d, J = 7.7 Hz, 2H), 7.21-7.24 (m, 3H), 6.82 (t, J = 6.8 Hz, 1H), 5.84 (s, 1H), 3.72 (s, 3H), 2.39 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 172.71, 145.98, 145.18, 138.15, 130.44, 129.30, 128.85, 125.43, 125.33, 117.41, 115.78, 112.69, 65.15, 53.41, 21.34; **HRMS** for $C_{17}H_{17}N_2O_3^+$: calcd. $[M+H]^+$: 297.1234, found: 297.1242

Methyl 2-hydroxy-2-(2-(3-methoxyphenyl)imidazo[1,2-a]pyridin-3-yl)acetate (5l)



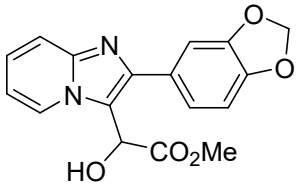
White solid; yield 88% (55 mg); R_f 0.50 (30% EtOAc/hexane); Mp 161-162 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.28 (d, *J* = 6.7 Hz, 1H), 7.54 (d, *J* = 9.0 Hz, 1H), 7.24-7.27 (m, 1H merged with solvent peak), 7.17-7.22 (m, 3H), 6.88 (d, *J* = 7.7 Hz, 1H), 6.79 (t, *J* = 6.7 Hz, 1H), 5.85 (s, 1H), 3.82 (s, 3H), 3.71 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 172.50, 159.60, 145.65, 145.21, 134.75, 129.51, 125.54, 125.45, 121.33, 117.35, 116.29, 114.46, 113.95, 112.67, 65.08, 55.27, 53.27; **HRMS** for $C_{17}H_{17}N_2O_4^+$: calcd. $[M+H]^+$: 313.1183, found: 313.1196

Ethyl 2-hydroxy-2-(2-(4-methoxyphenyl)imidazo[1,2-a]pyridin-3-yl)acetate (5m)



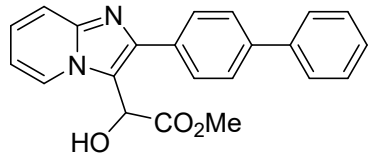
White solid; yield 85% (53 mg); R_f 0.50 (30% EtOAc/hexane); Mp 158-160 °C; **^{1}H NMR** (500 MHz, DMSO-*d6*) δ 8.50 (d, *J* = 6.9 Hz, 1H), 7.74 (d, *J* = 8.7 Hz, 2H), 7.62 (d, *J* = 9.0 Hz, 1H), 7.30-7.34 (m, 1H), 7.08 (d, *J* = 8.7 Hz, 2H), 6.97-7.00 (m, 1H), 6.48 (d, *J* = 4.1 Hz, 1H), 5.81 (d, *J* = 4.0 Hz, 1H), 3.83 (s, 3H), 3.64 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 171.76, 159.69, 144.76, 144.21, 130.24, 126.82, 126.61, 125.67, 117.37, 117.23, 114.53, 112.62, 65.02, 55.67, 52.86; **HRMS** for $C_{17}H_{17}N_2O_4$+: calcd. $[M+H]^+$: 313.1183, found: 313.1194

Methyl 2-(2-(benzo[d][1,3]dioxol-5-yl)imidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5n)



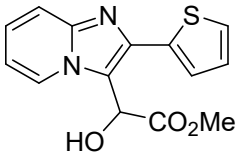
White solid; yield 78% (51 mg); R_f 0.50 (30% EtOAc/hexane); Mp 156-158 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.20 (d, *J* = 6.8 Hz, 1H), 7.60 (d, *J* = 9.0 Hz, 1H), 7.17-7.26 (m, 3H), 6.86 (d, *J* = 7.9 Hz, 1H), 6.81 (t, *J* = 6.6 Hz, 1H), 6.01 (s, 2H), 5.83 (s, 1H), 3.77 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 171.70, 148.01, 147.70, 144.64, 144.07, 128.37, 126.58, 125.81, 122.77, 117.58, 117.27, 112.74, 109.16, 108.94, 101.68, 64.89, 52.88; **HRMS** for $C_{17}H_{15}N_2O_5^+$: calcd. $[M+H]^+$: 327.0975, found: 327.0986

Methyl 2-(2-([1,1'-biphenyl]-4-yl)imidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5o)



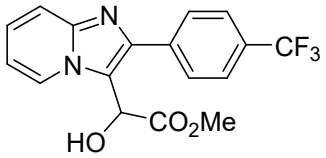
White solid; yield 88% (63 mg); R_f 0.50 (30% EtOAc/hexane); Mp 175-176 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.29 (d, *J* = 6.8 Hz, 1H), 7.70 (d, *J* = 8.1 Hz, 2H), 7.56-7.60 (m, 5H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.36 (t, *J* = 7.3 Hz, 1H), 7.16 (t, *J* = 7.7 Hz, 1H), 6.77 (t, *J* = 6.6 Hz, 1H), 5.89 (s, 1H), 3.72 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 171.48, 144.11, 142.17, 140.55, 139.95, 132.14, 129.62, 129.50, 128.21, 127.42, 127.17, 127.04, 118.58, 116.68, 113.75, 64.84, 52.99; **HRMS** for $C_{22}H_{19}N_2O_3^+$: calcd. $[M+H]^+$: 359.1390, found: 359.1399

Methyl 2-hydroxy-2-(2-(thiophen-2-yl)imidazo[1,2-a]pyridin-3-yl)acetate (5p)



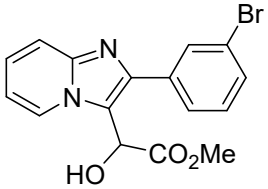
White solid; yield 65% (37 mg); R_f 0.50 (30% EtOAc/hexane); Mp 182-183 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.24 (d, *J* = 6.8 Hz, 1H), 7.63 (d, *J* = 9.0 Hz, 1H), 7.42 (d, *J* = 3.4 Hz, 2H), 7.22-7.26 (d, *J* = 8.4 Hz, 1H), 7.13 (t, *J* = 3.8 Hz, 1H), 6.82 (t, *J* = 6.7 Hz, 1H), 6.03 (s, 1H), 3.77 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 171.45, 144.80, 138.31, 137.25, 128.49, 127.51, 126.78, 126.23, 126.18, 117.20, 117.13, 113.00, 64.85, 52.90; **HRMS** for $C_{14}H_{13}N_2O_3S^+$: calcd. $[M+H]^+$: 289.0641, found: 289.0652

Methyl 2-hydroxy-2-(2-(4-(trifluoromethyl)phenyl)imidazo[1,2-a]pyridin-3-yl)acetate (5q)



White solid; yield 76% (53 mg); R_f 0.50 (30% EtOAc/hexane); Mp 166-168 °C; **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.53 (d, *J* = 6.2 Hz, 1H), 8.04 (d, *J* = 7.3 Hz, 2H), 7.88 (d, *J* = 7.3 Hz, 2H), 7.69 (d, *J* = 8.7 Hz, 1H), 7.38 (t, *J* = 7.3 Hz, 1H), 7.04 (t, *J* = 5.8 Hz, 1H), 6.59 (s, 1H), 5.90 (s, 1H), 3.62 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 170.56, 144.07, 141.53, 137.53, 128.64, 123.87 (q, $^1J_{C\text{-}F}$ = 270.4 Hz), 127.69 (q, $^2J_{C\text{-}F}$ = 31.6 Hz), 125.77, 125.43, 125.01 (q appearing as d, $^3J_{C\text{-}F}$ = 3.2 Hz), 118.23, 116.68, 112.29, 63.80, 51.99; **^{19}F NMR** (376 MHz, $CDCl_3$) δ -64.30; **HRMS** for $C_{17}H_{14}F_3N_2O_3^+$: calcd. $[M+H]^+$: 351.0951, found: 351.0959

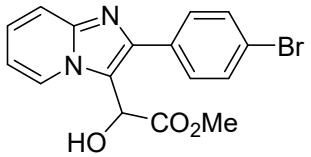
Methyl 2-(2-(3-bromophenyl)imidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5r)



White solid; yield 79% (57 mg); R_f 0.50 (30% EtOAc/hexane); Mp 185-186 °C; **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.52 (d, *J* = 7.0 Hz, 1H), 7.99 (s, 1H), 7.81 (d, *J* = 7.7 Hz, 1H), 7.63-7.67 (m, 2H), 7.48 (t, *J* = 7.9 Hz, 1H), 7.36-7.39 (m, 1H), 7.03 (t, *J* = 6.8 Hz, 1H), 6.56 (d, *J* = 2.7

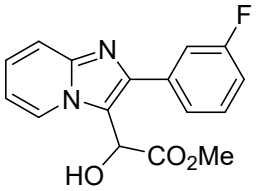
Hz, 1H), 5.85 (s, 1H), 3.62 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 171.50, 144.89, 142.44, 136.74, 131.43, 131.25, 131.21, 127.84, 126.67, 126.26, 122.36, 118.69, 117.54, 113.14, 64.75, 52.92; **HRMS** for $C_{16}H_{14}BrN_2O_3^+$: calcd. $[M+H]^+$: 361.0182, found: 361.0190

Methyl 2-(2-(4-bromophenyl)imidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5s)



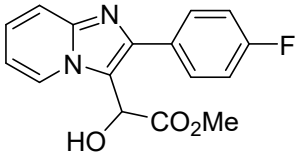
White solid; yield 82% (59 mg); R_f 0.50 (30% EtOAc/hexane); Mp 171-172 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.23 (d, J = 6.7 Hz, 1H), 7.55 (d, J = 9.1 Hz, 1H), 7.47 (s, 4H), 7.24 (t, J = 7.9 Hz, 1H), 6.83 (t, J = 6.7 Hz, 1H), 5.75 (s, 1H), 3.73 (s, 3H); **^{13}C NMR** (125 MHz, CD_3OD) δ 172.80, 146.62, 144.57, 135.75, 133.33, 131.65, 129.93, 127.94, 127.64, 119.25, 117.50, 114.24, 66.08, 53.32; **HRMS** for $C_{16}H_{14}BrN_2O_3^+$: calcd. $[M+H]^+$: 361.0182, found: 361.0194

Methyl 2-(2-(3-fluorophenyl)imidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5t)



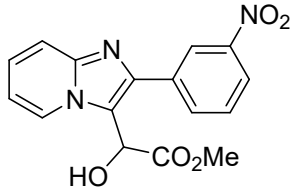
White solid; yield 70% (42 mg); R_f 0.50 (30% EtOAc/hexane); Mp 194-196 °C; **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.52 (d, J = 6.9 Hz, 1H), 7.65-7.67 (m, 2H), 7.54-7.61 (m, 2H), 7.35-7.38 (m, 1H), 7.26-7.30 (m, 1H), 7.02-7.04 (m, 1H), 6.56 (d, J = 4.0 Hz, 1H), 5.88 (d, J = 3.6 Hz, 1H), 3.63 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 171.55, 162.71 (d, $^1J_{C\text{-}F}$ = 241.7 Hz), 144.84, 142.74, 136.79 (d, $^3J_{C\text{-}F}$ = 8.1 Hz), 131.10 (d, $^3J_{C\text{-}F}$ = 8.3 Hz), 126.67, 126.21, 125.00, 118.63, 117.53, 115.48 (d, $^2J_{C\text{-}F}$ = 22.4 Hz), 115.26 (d, $^2J_{C\text{-}F}$ = 20.9 Hz), 113.10, 64.73, 52.91; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.46; **HRMS** for $C_{16}H_{14}FN_2O_3^+$: calcd. $[M+H]^+$: 301.0983, found: 301.0990

Methyl 2-(2-(4-fluorophenyl)imidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5u)



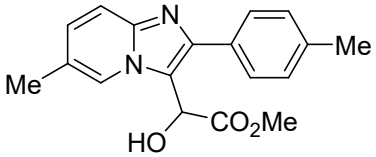
White solid; yield 70% (42 mg); R_f 0.50 (30% EtOAc/hexane); Mp 174-176 °C; **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.50 (d, J = 6.9 Hz, 1H), 7.82-7.85 (m, 2H), 7.65 (d, J = 9.0 Hz, 1H), 7.35 (t, J = 8.8 Hz, 3H), 7.00-7.03 (m, 1H), 6.51 (s, 1H), 5.81 (s, 1H), 3.63 (s, 3H); **^{13}C NMR** (100 MHz, CD_3OD) δ 172.80, 164.55 (d, $^1J_{C\text{-}F}$ = 245.5 Hz), 146.33, 144.50, 132.20 (d, $^3J_{C\text{-}F}$ = 8.2 Hz), 130.62 (d, $^4J_{C\text{-}F}$ = 3.2 Hz), 128.12, 127.67, 119.07, 117.27, 116.62 (d, $^2J_{C\text{-}F}$ = 21.8 Hz), 114.33, 66.08, 53.30; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.47; **HRMS** for $C_{16}H_{14}FN_2O_3^+$: calcd. $[M+H]^+$: 301.0983, found: 301.0994

Methyl 2-hydroxy-2-(2-(3-nitrophenyl)imidazo[1,2-a]pyridin-3-yl)acetate (5v)



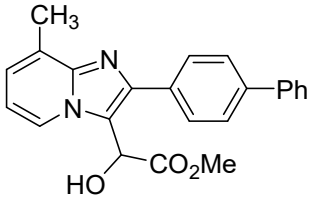
White solid; yield 58% (38 mg); R_f 0.50 (30% EtOAc/hexane); Mp 165-166 °C; **^{1}H NMR** (500 MHz, DMSO-d_6) δ 8.68 (t, J = 1.8 Hz, 1H), 8.57 (d, J = 6.9 Hz, 1H), 8.26-8.29 (m, 2H), 7.81 (t, J = 8.0 Hz, 1H), 7.70 (d, J = 9.0 Hz, 1H), 7.40 (t, J = 7.5 Hz, 1H), 7.06 (t, J = 6.5 Hz, 1H), 6.64 (d, J = 3.4 Hz, 1H), 5.94 (d, J = 3.0 Hz, 1H), 3.64 (s, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 171.44, 148.56, 145.01, 141.65, 135.97, 135.07, 130.71, 126.76, 126.53, 123.36, 123.12, 119.19, 117.63, 113.35, 64.68, 52.96; **HRMS** for $C_{16}H_{14}N_3O_5^+$: calcd. $[M+H]^+$: 328.0928, found: 328.0935

Methyl 2-hydroxy-2-(6-methyl-2-(p-tolyl)imidazo[1,2-a]pyridin-3-yl)acetate (5w)



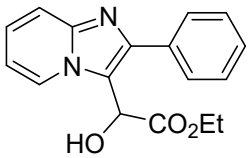
White solid; yield 79% (49 mg); R_f 0.50 (30% EtOAc/hexane); Mp 182-184 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.52 (d, J = 6.8 Hz, 2H), 7.46 (d, J = 8.9 Hz, 1H), 7.17 (d, J = 6.7 Hz, 2H), 7.03 (d, J = 8.6 Hz, 1H), 5.80 (s, 1H), 3.71 (s, 3H), 2.37 (s, 3H), 2.31 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 171.72, 144.03, 143.77, 137.74, 131.58, 129.59, 128.83, 128.75, 123.95, 121.87, 117.55, 116.68, 64.91, 52.83, 21.29, 18.37; **HRMS** for $C_{18}H_{19}N_2O_3^+$: calcd. $[M+H]^+$: 311.1390, found: 311.1401

Methyl 2-(2-([1,1'-biphenyl]-4-yl)-8-methylimidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5x)



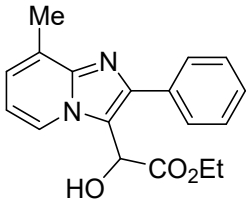
White solid; yield 76% (57 mg); R_f 0.50 (30% EtOAc/hexane); Mp 141-143 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.35 (d, J = 6.6 Hz, 1H), 7.90 (d, J = 7.8 Hz, 2H), 7.82 (d, J = 7.8 Hz, 2H), 7.76 (d, J = 7.3 Hz, 2H), 7.51 (t, J = 7.2 Hz, 2H), 7.40 (t, J = 6.9 Hz, 1H), 7.16 (d, J = 6.0 Hz, 1H), 6.91 (t, J = 6.7 Hz, 1H), 6.49 (d, J = 3.7 Hz, 1H), 5.87 (d, J = 3.6 Hz, 1H), 3.64 (s, 3H), 2.55 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 171.75, 145.29, 143.26, 140.15, 140.03, 133.67, 129.55, 129.49, 128.08, 127.28, 127.13, 126.95, 124.36, 118.68, 112.83, 65.01, 52.88, 17.07; **HRMS** for $C_{23}H_{21}N_2O_3^+$: calcd. $[M+H]^+$: 373.1547, found: 373.1551

Ethyl 2-hydroxy-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)acetate (5y)[3]



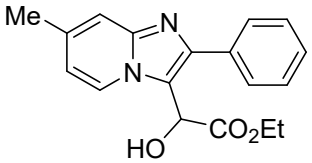
White solid; yield 85% (50 mg); R_f 0.50 (30% EtOAc/hexane); Mp 171-173 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.25 (d, *J* = 6.4 Hz, 1H), 7.72 (d, *J* = 6.8 Hz, 2H), 7.62 (d, *J* = 8.8 Hz, 1H), 7.37-7.42 (m, 3H), 7.23 (t, *J* = 7.5 Hz, 1H), 6.82 (t, *J* = 6.2 Hz, 1H), 5.81 (s, 1H), 4.08-4.28 (m, 2H), 1.15 (t, *J* = 6.8 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 172.03, 145.43, 144.99, 133.16, 128.98, 128.51, 128.30, 125.66, 125.47, 117.27, 116.35, 112.76, 65.07, 62.73, 13.94; **HRMS** for $C_{17}H_{17}N_2O_3^+$: calcd. $[M+H]^+$: 297.1234, found: 297.1247

Ethyl 2-hydroxy-2-(8-methyl-2-phenylimidazo[1,2-a]pyridin-3-yl)acetate (5z)[3]



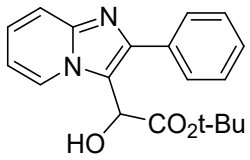
White solid; yield 73% (45 mg); R_f 0.50 (30% EtOAc/hexane); Mp 165-167 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 6.8 Hz, 1H), 7.73 (d, *J* = 7.0 Hz, 2H), 7.41 (t, *J* = 7.3 Hz, 2H), 7.34 (t, *J* = 7.3 Hz, 1H), 7.04 (d, *J* = 6.8 Hz, 1H), 6.75 (t, *J* = 6.9 Hz, 1H), 5.75 (s, 1H), 4.07-4.26 (m, 2H), 2.64 (s, 3H), 1.15 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 172.18, 145.54, 145.34, 133.65, 129.15, 128.38, 128.06, 127.40, 124.27, 123.14, 116.71, 112.65, 65.15, 62.63, 17.15, 13.97; **HRMS** for $C_{19}H_{19}N_2O_3^+$: calcd. $[M+H]^+$: 311.1390, found: 311.1405

Ethyl 2-hydroxy-2-(7-methyl-2-phenylimidazo[1,2-a]pyridin-3-yl)acetate (5aa)



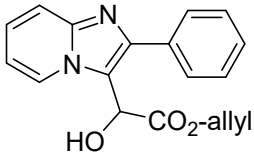
White solid; yield 68% (42 mg); R_f 0.50 (30% EtOAc/hexane); Mp 161-163 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 (d, *J* = 6.8 Hz, 1H), 7.69 (d, *J* = 7.1 Hz, 2H), 7.34-7.42 (m, 4H), 6.63 (d, *J* = 6.6 Hz, 1H), 5.77 (s, 1H), 4.09-4.27 (m, 2H), 2.38 (s, 3H), 1.16 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 171.23, 145.25, 143.97, 136.35, 134.62, 128.96, 128.92, 128.32, 125.94, 117.59, 115.62, 115.14, 65.05, 61.61, 21.23, 14.37; **HRMS** for $C_{18}H_{19}N_2O_3^+$: calcd. $[M+H]^+$: 311.1390, found: 311.1400

***tert*-Butyl 2-hydroxy-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)acetate (5ab) NRJP**



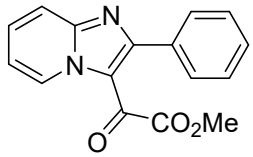
White solid; yield 80% (52 mg); R_f 0.50 (30% EtOAc/hexane); Mp 154-155 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.58 (d, J = 6.8 Hz, 1H), 7.83 (d, J = 7.6 Hz, 2H), 7.64 (d, J = 9.0 Hz, 1H), 7.51 (t, J = 7.5 Hz, 2H), 7.42 (t, J = 7.3 Hz, 1H), 7.33 (t, J = 7.3 Hz, 1H), 7.00 (t, J = 6.8 Hz, 1H), 6.35 (br s, 1H), 5.66 (s, 1H), 1.30 (s, 9H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 170.96, 144.11, 144.08, 131.97, 129.17, 128.87, 128.79, 127.12, 125.70, 117.12, 116.64, 113.67, 84.57, 65.26, 27.82; **HRMS** for $C_{19}H_{21}N_2O_3^+$: calcd. $[M+H]^+$: 325.1547, found: 325.1560

Allyl 2-hydroxy-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)acetate (5ac)



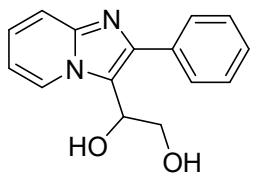
White solid; yield 84% (52 mg); R_f 0.50 (30% EtOAc/hexane); Mp 113-115 °C; **^{1}H NMR** (500 MHz, DMSO-*d6*) δ 8.54 (d, J = 6.9 Hz, 1H), 7.82 (d, J = 7.3 Hz, 2H), 7.65 (d, J = 9.0 Hz, 1H), 7.51 (t, J = 7.5 Hz, 2H), 7.43 (t, J = 7.3 Hz, 1H), 7.34 (t, J = 7.7 Hz, 1H), 7.00 (t, J = 6.7 Hz, 1H), 6.57 (d, J = 4.1 Hz, 1H), 5.87 (d, J = 4.0 Hz, 1H), 5.76-5.83 (m, 1H), 5.04-5.10 (m, 2H), 4.59 (d, J = 5.0 Hz, 2H); **^{13}C NMR** (125 MHz, DMSO-d_6) δ 170.85, 144.87, 144.25, 134.44, 132.58, 129.03, 129.00, 128.48, 126.77, 125.89, 118.10, 118.07, 117.41, 112.76, 65.73, 65.04; **HRMS** for $C_{18}H_{17}N_2O_3^+$: calcd. $[M+H]^+$: 309.1234, found: 309.1242

Methyl 2-oxo-2-(2-phenylimidazo[1,2-a]pyridin-3-yl)acetate (7)



White solid; yield 80% (45 mg); R_f 0.50 (20% EtOAc/hexane); Mp 133-135 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.68 (d, J = 6.7 Hz, 1H), 7.84 (d, J = 8.8 Hz, 1H), 7.60-7.67 (m, 3H), 7.49-7.50 (m, 3H), 7.21 (t, J = 6.6 Hz, 1H), 3.29 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 176.45, 163.83, 158.66, 148.27, 133.54, 131.13, 129.65, 129.58, 129.13, 128.46, 118.06, 117.68, 115.88, 52.22; **HRMS** for $C_{16}H_{13}N_2O_3^+$: calcd. $[M+H]^+$: 281.0921, found: 281.0923

1-(2-Phenylimidazo[1,2-a]pyridin-3-yl)ethane-1,2-diol (8)



White solid; yield 88% (45 mg); R_f 0.50 (50% EtOAc/hexane); Mp 111-113 °C; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.70 (d, J = 6.9 Hz, 1H), 7.80 (d, J = 7.7 Hz, 2H), 7.58 (d, J = 9.0 Hz, 1H), 7.47 (t, J = 7.5 Hz, 2H), 7.38 (t, J = 7.1 Hz, 1H), 7.25 (t, J = 7.8 Hz, 1H), 6.88 (t, J = 6.8 Hz, 1H), 5.71 (d, J = 3.1 Hz, 1H), 5.20-5.24 (m, 1H), 5.08 (t, J = 5.2 Hz, 1H), 3.86-3.96 (m, 2H);

^{13}C NMR (100 MHz, DMSO-d_6) δ 144.69, 143.34, 135.26, 129.22, 128.73, 127.92, 127.87, 124.87, 121.47, 117.24, 111.78, 66.94, 63.73; **HRMS** for $C_{15}H_{15}N_2O_2^+$: calcd. $[M+H]^+$: 255.1128, found: 255.1140

5. References

1) P. Zhao, Y. Liu, Y. Zhang, L. Wang, and Y. Ma, *Org. Lett.*, 2024, **26**, 2511–2516.

2) Z. Liu, X. Guo, Z. Chen, L. Wu and K. Yang, *Synthesis*, 2024, **56**, 1756–1764.

3) N. Meena, Bhawani, Sonam, K. Rangan and A. Kumar, *J. Org. Chem.*, 2023, **88**, 3022–3034.

6. Copies of ^{1}H, ^{13}C, ^{19}F and HRMS Spectra

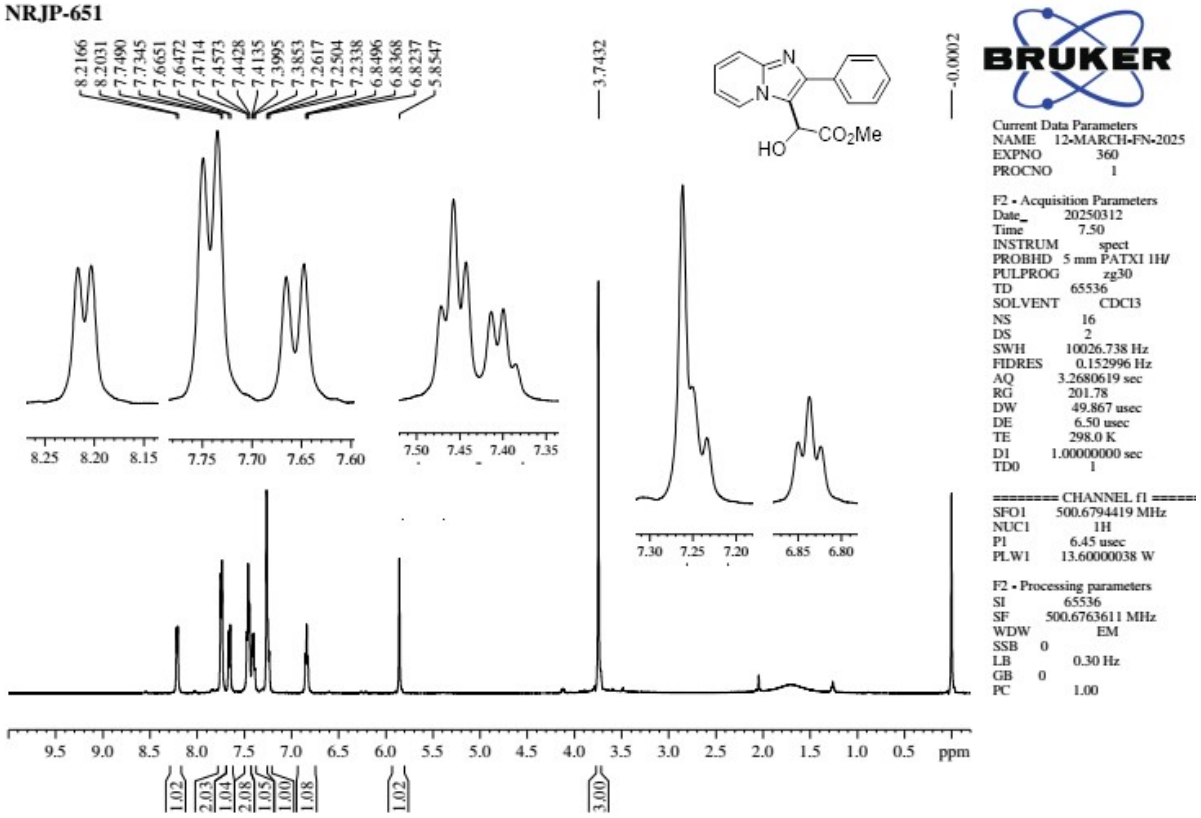


Figure S3. ^{1}H NMR Spectrum of 5a

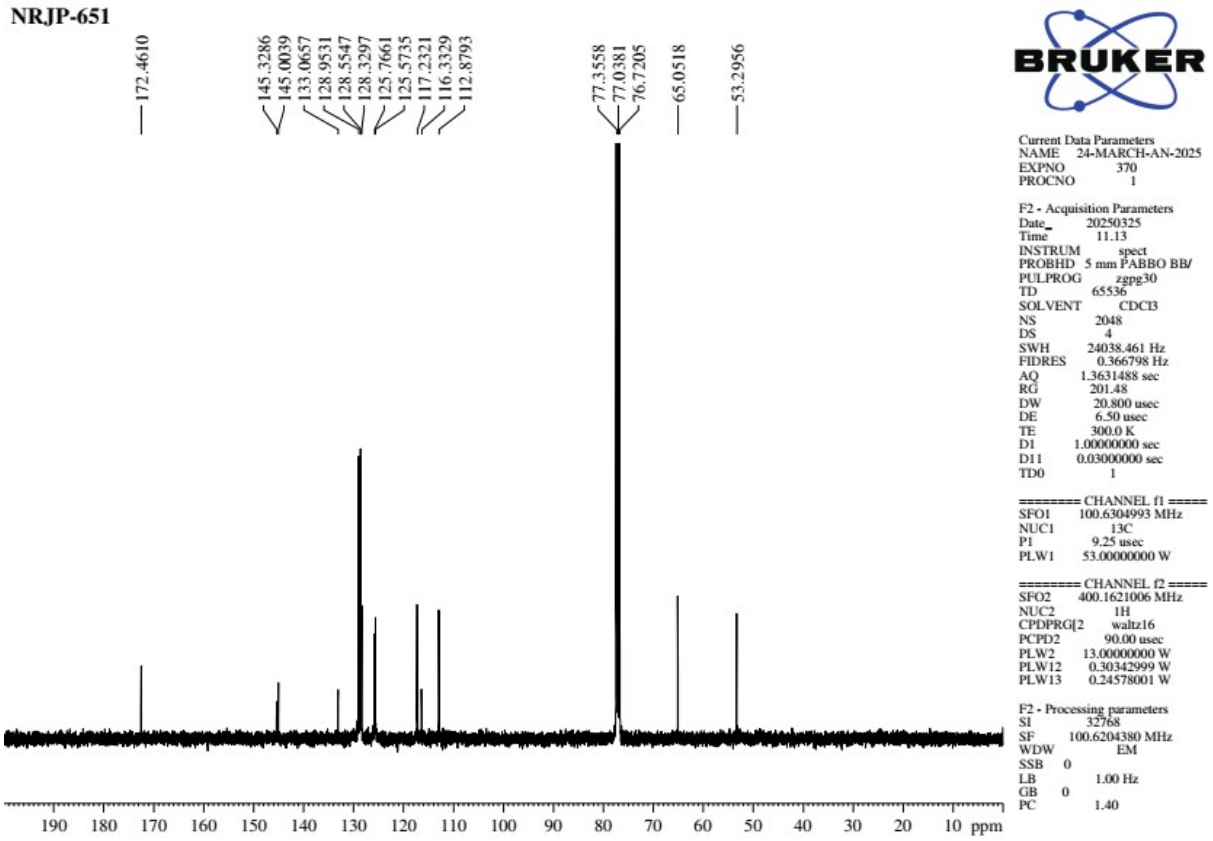


Figure S4. ^{13}C NMR Spectrum of 5a

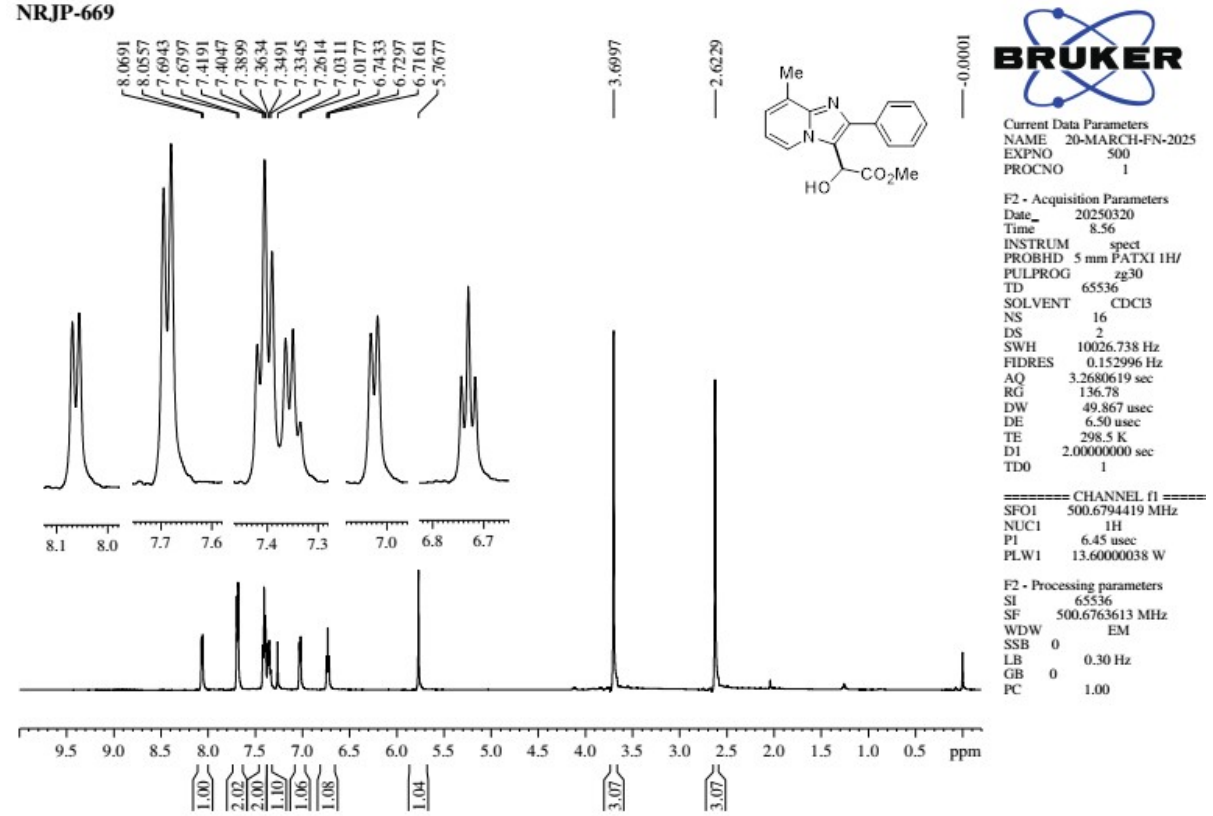


Figure S5. ^{1}H NMR Spectrum of 5b

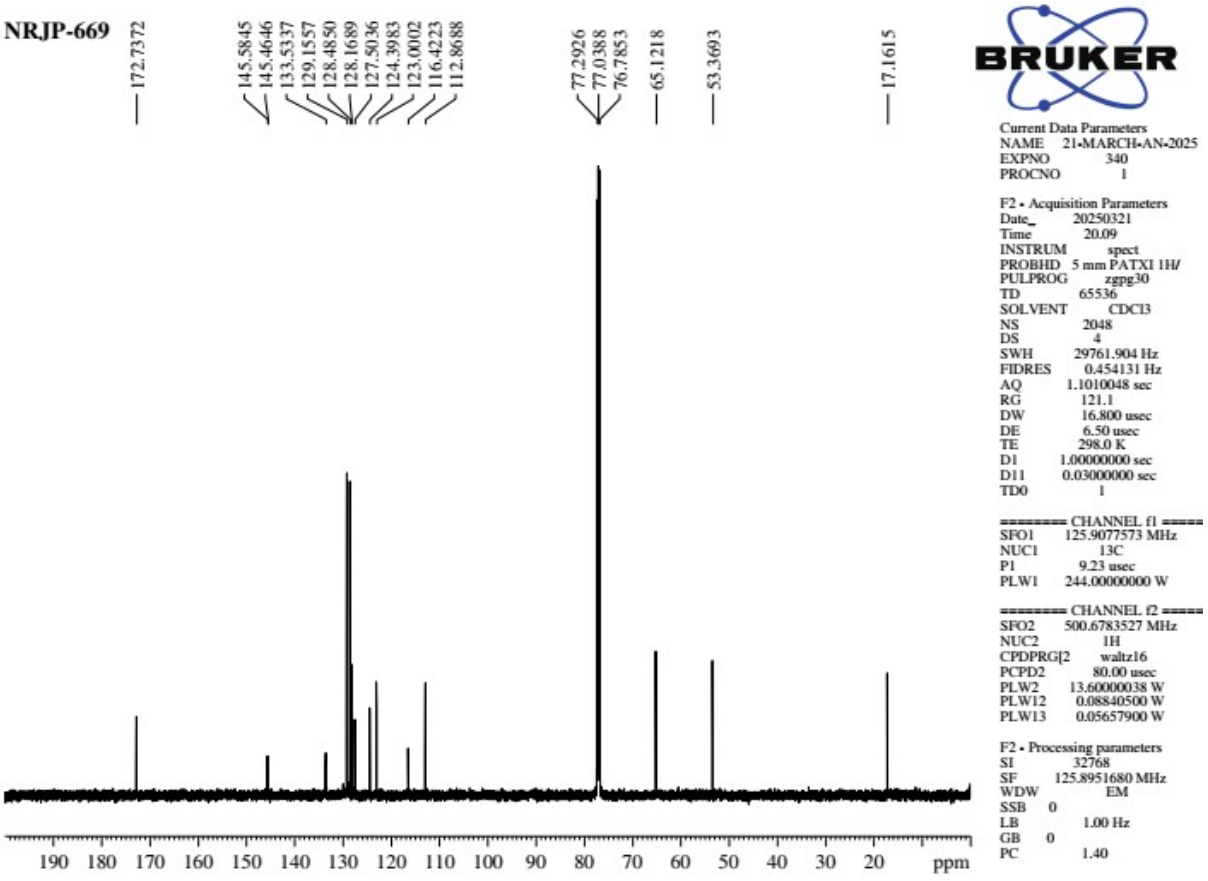


Figure S6. ^{13}C NMR Spectrum of 5b

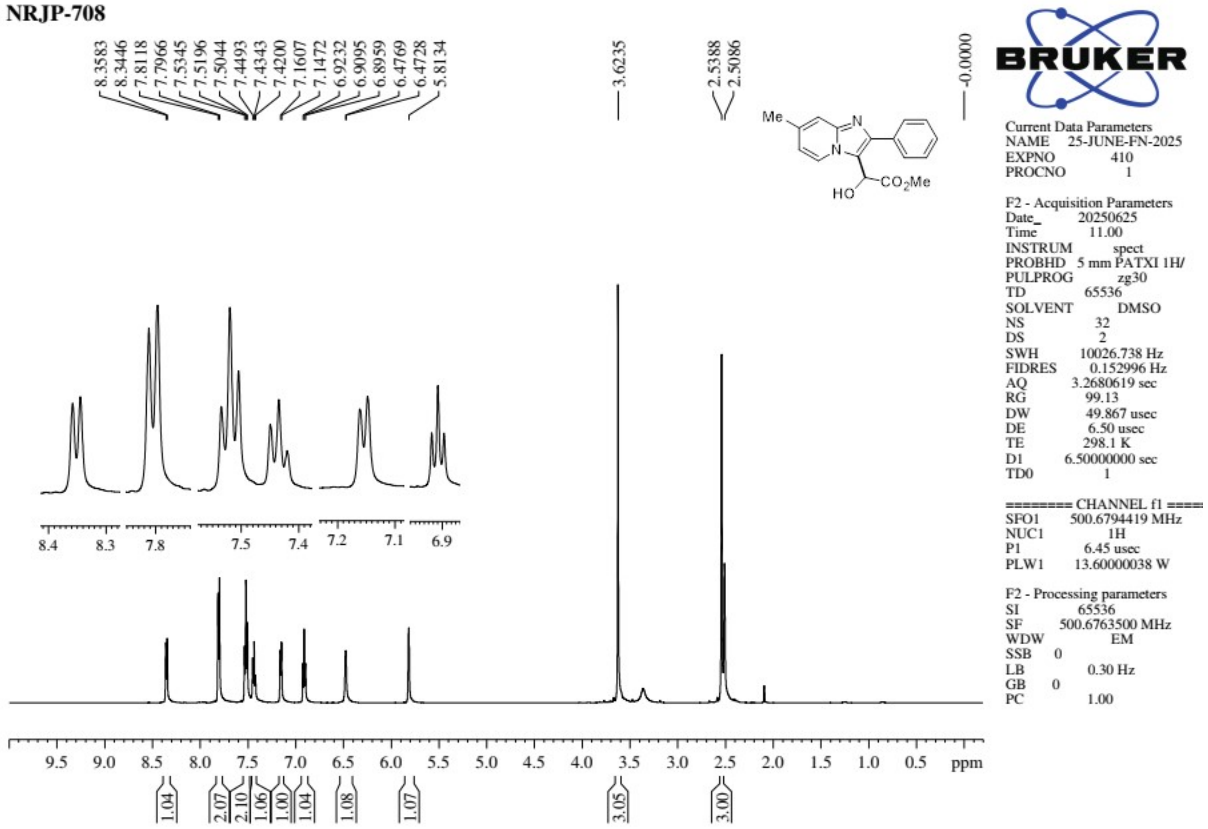


Figure S7. ^{1}H NMR Spectrum of 5c

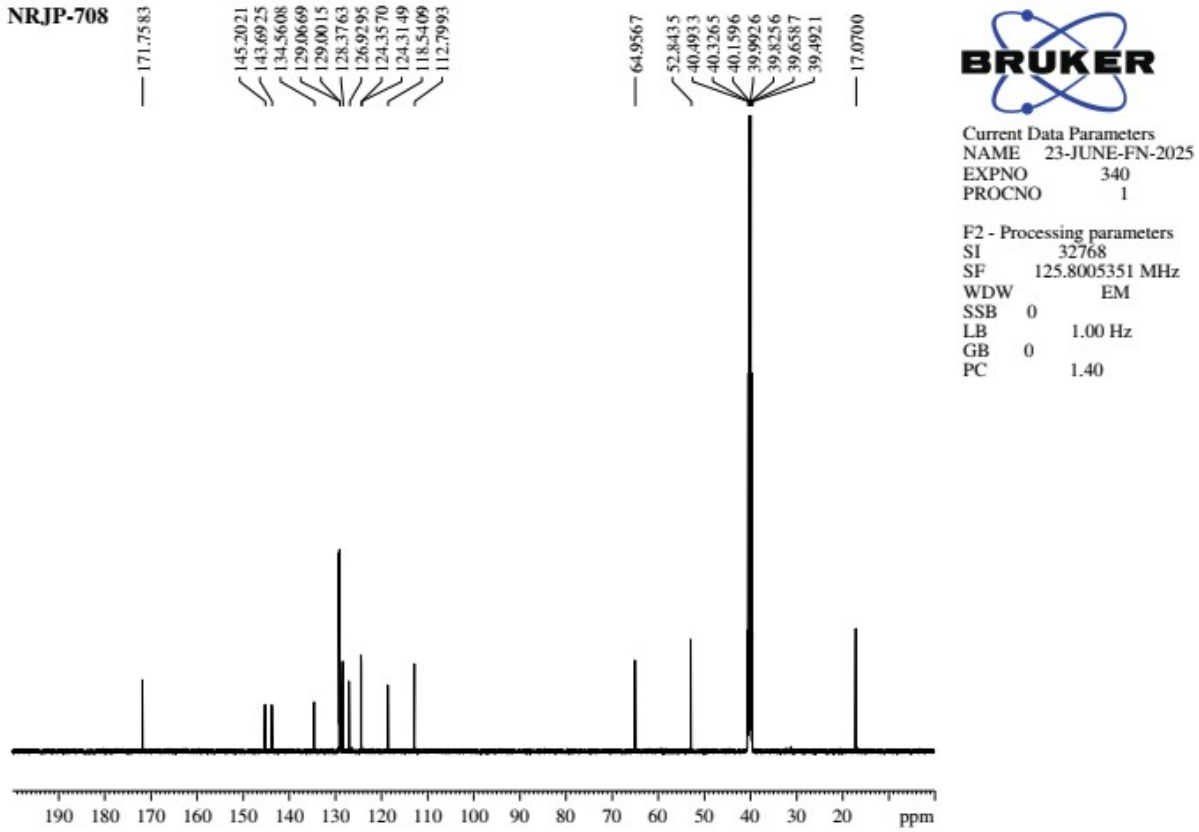


Figure S8. ^{13}C NMR Spectrum of 5c

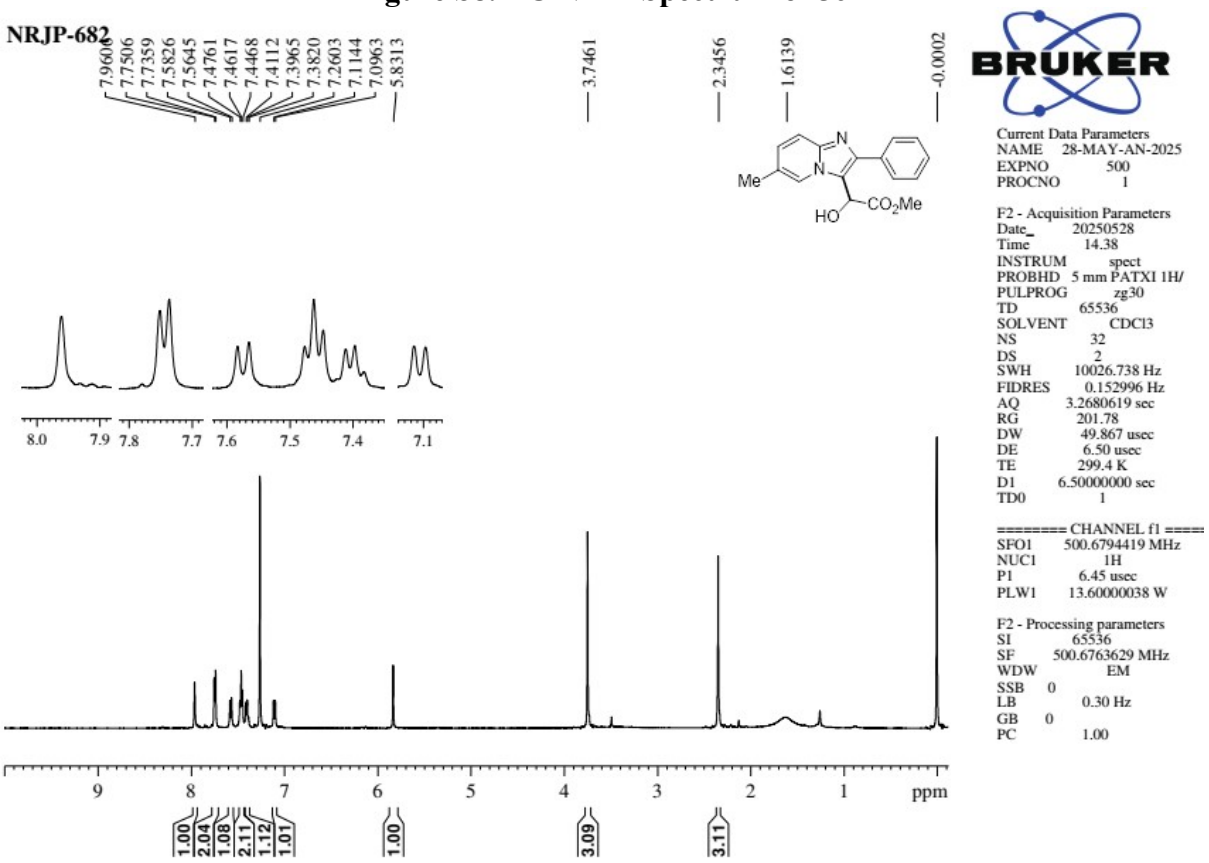


Figure S9. ^{1}H NMR Spectrum of 5d

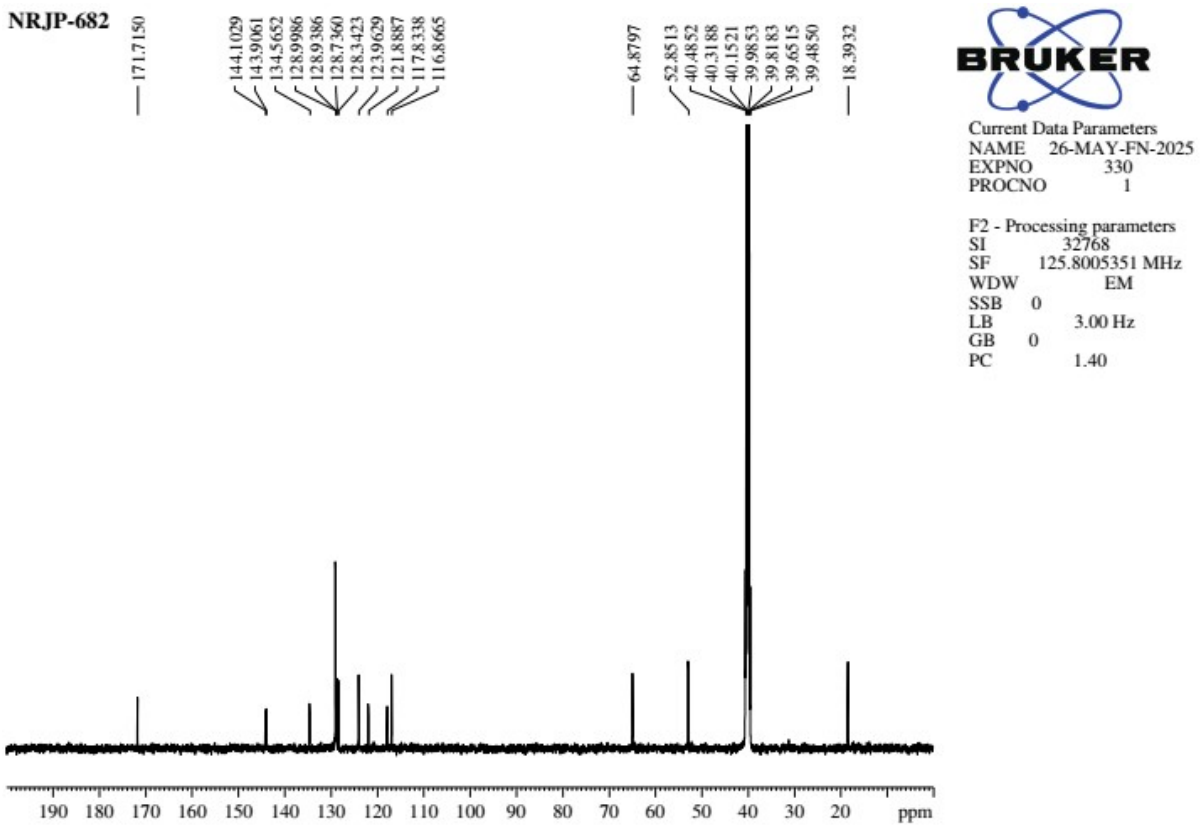


Figure S10. ^{13}C NMR Spectrum of 5d

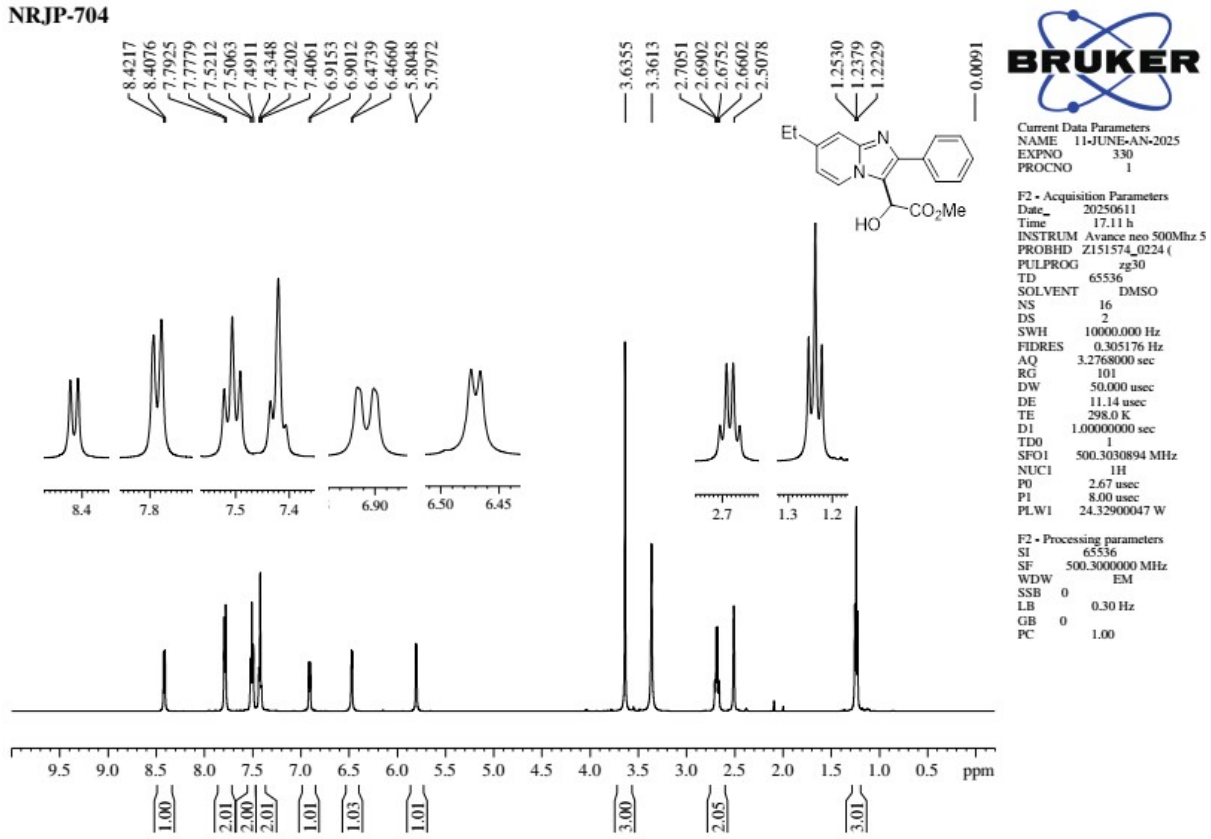


Figure S11. ^{1}H NMR Spectrum of 5e

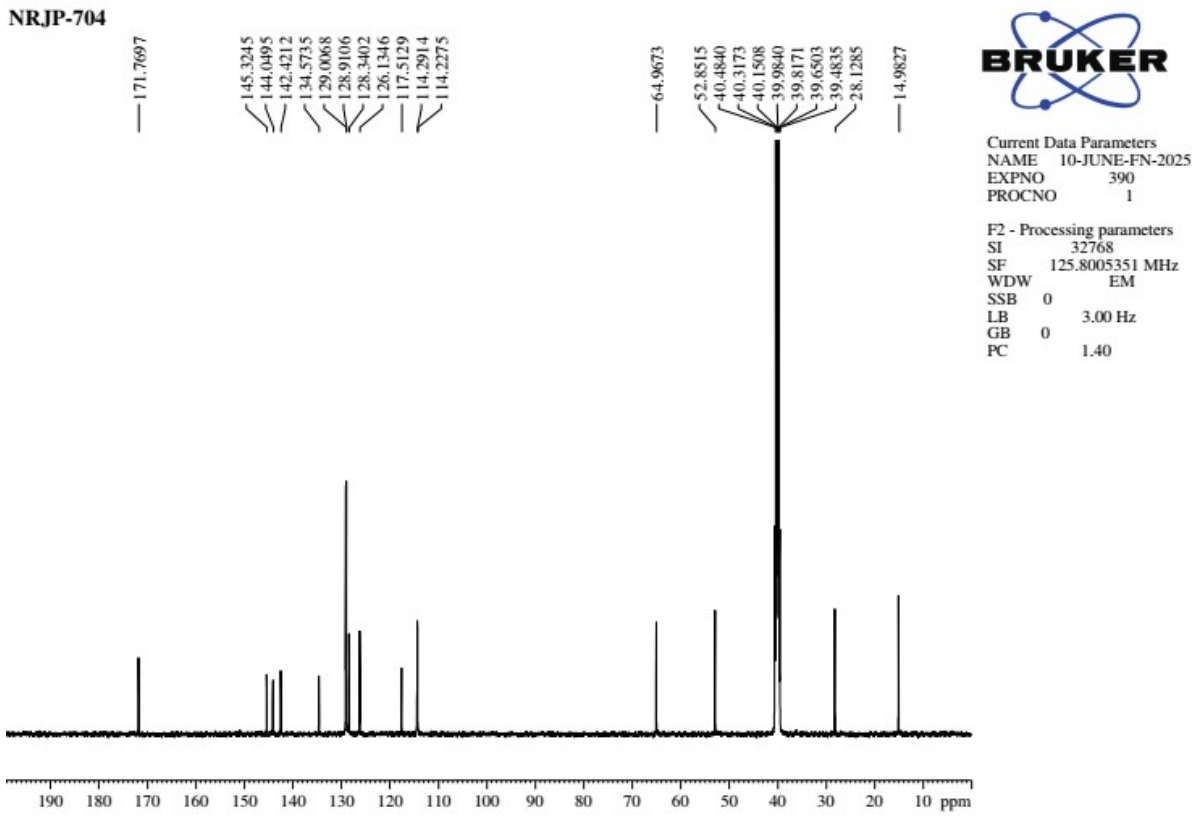


Figure S12. ^{13}C NMR Spectrum of 5e

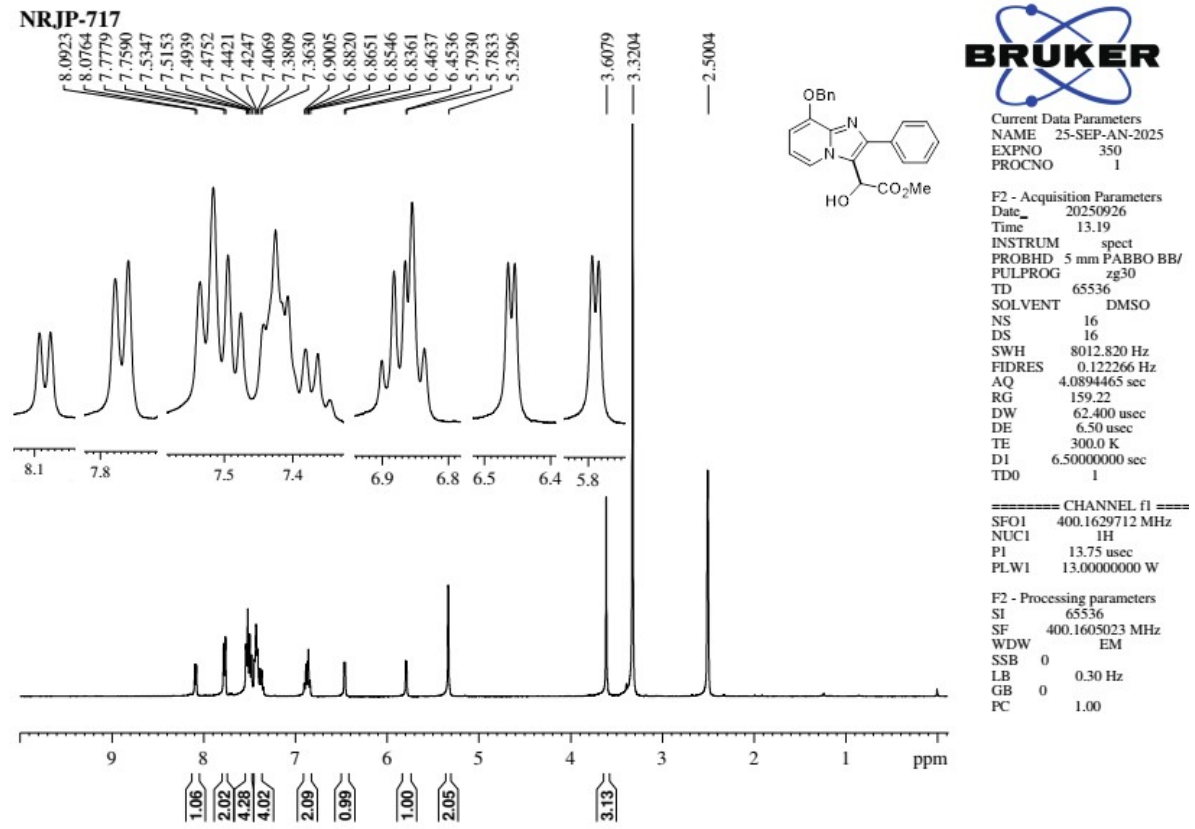


Figure S13. ^{1}H NMR Spectrum of 5f

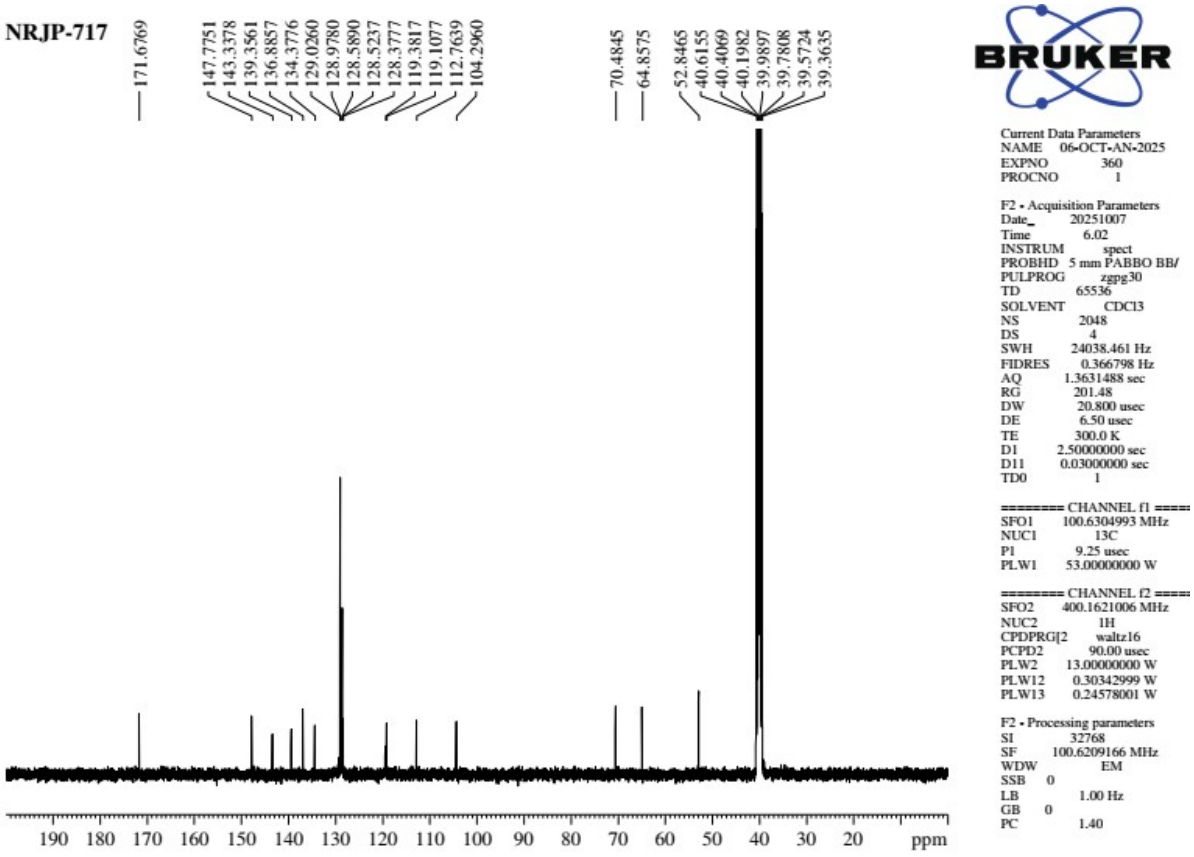


Figure S14. ^{13}C NMR Spectrum of 5f

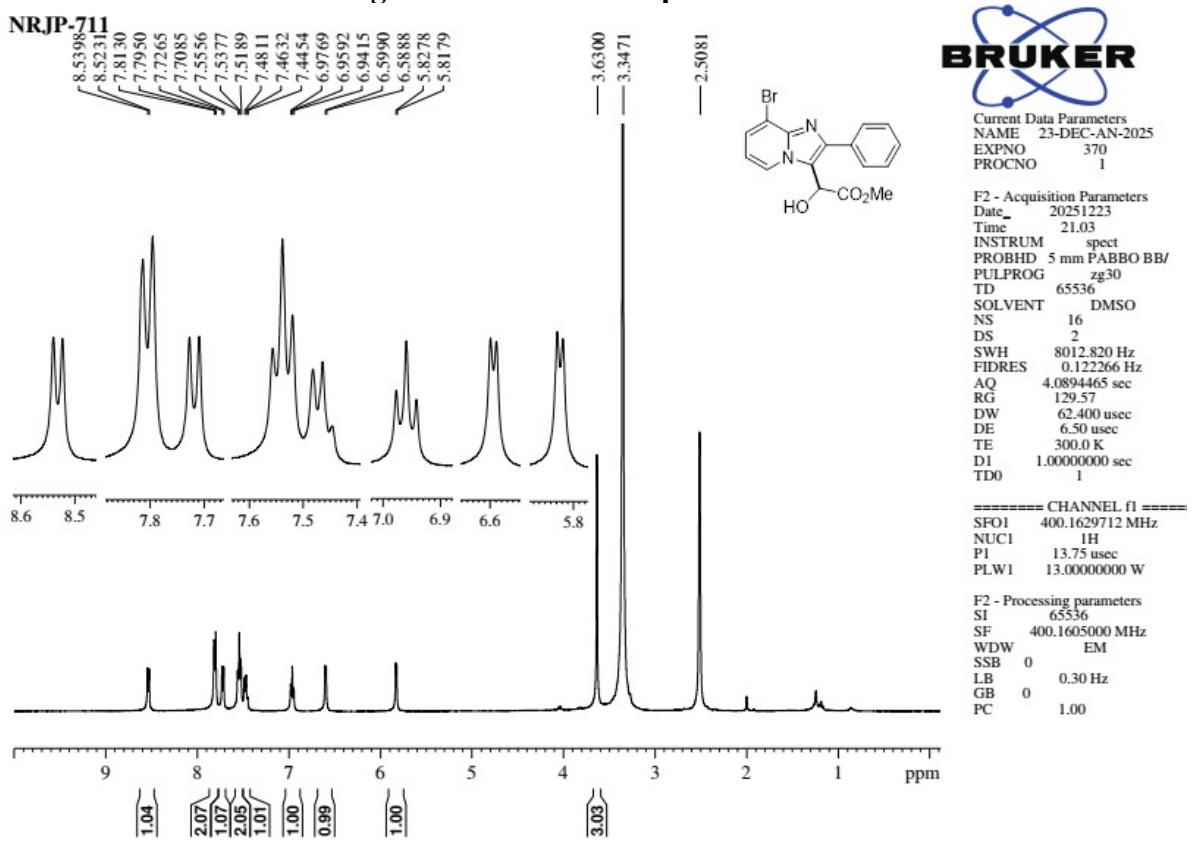


Figure S15. ^{1}H NMR Spectrum of 5g

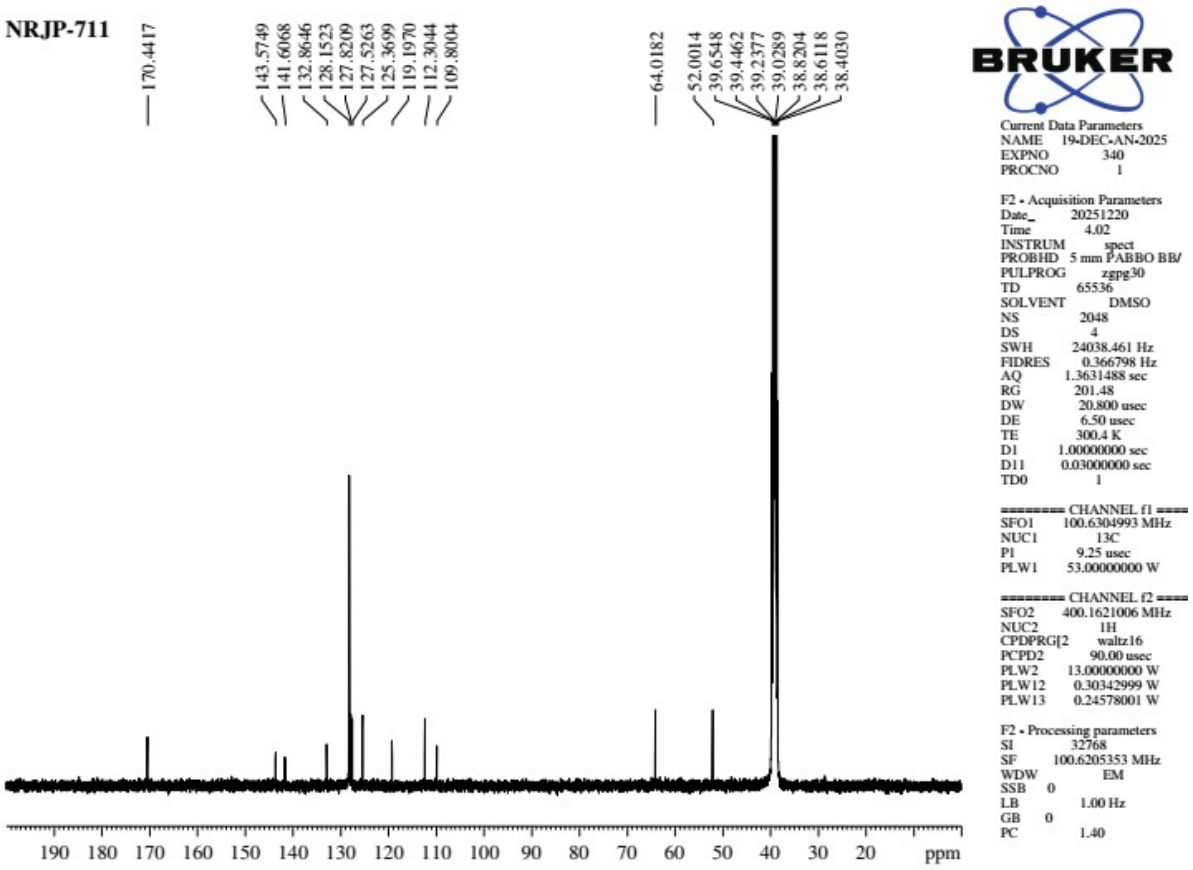


Figure S16. ^{13}C NMR Spectrum of 5g

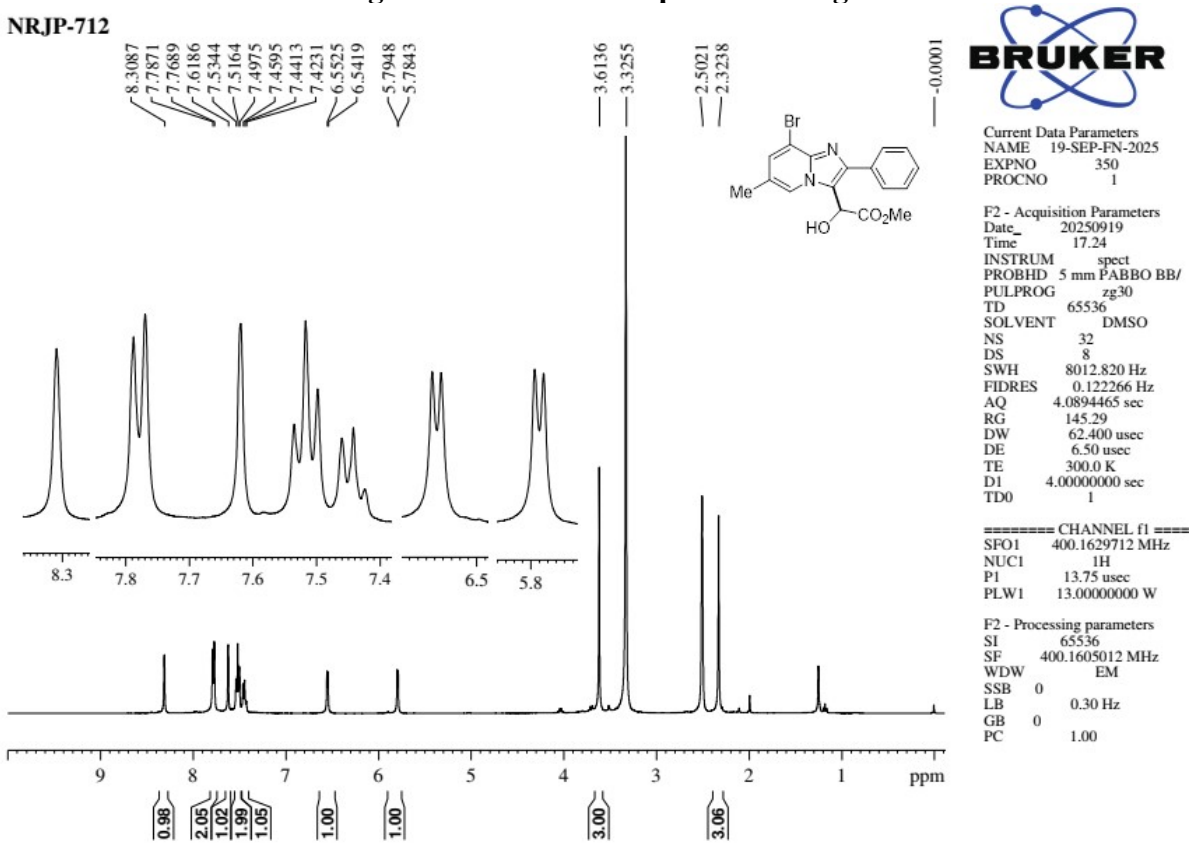


Figure S17. ^{1}H NMR Spectrum of 5h

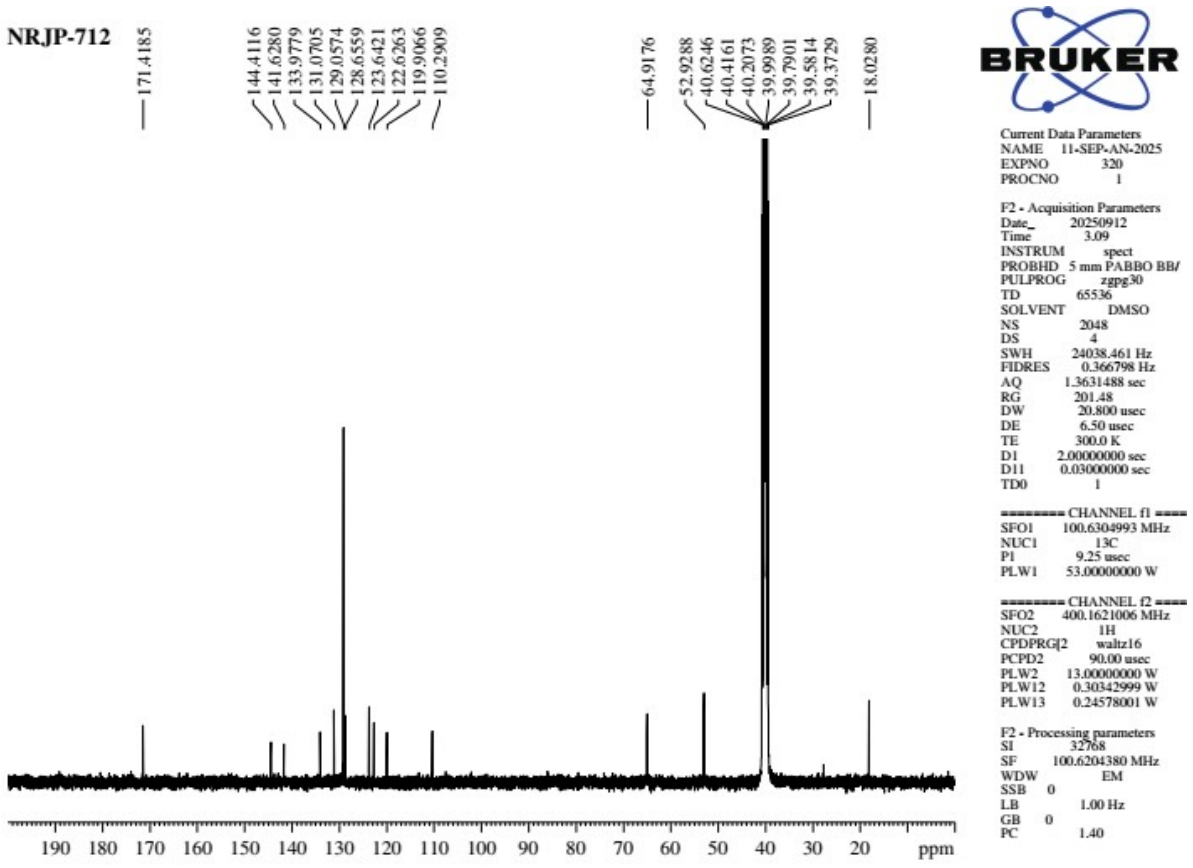


Figure S18. ^{13}C NMR Spectrum of 5h

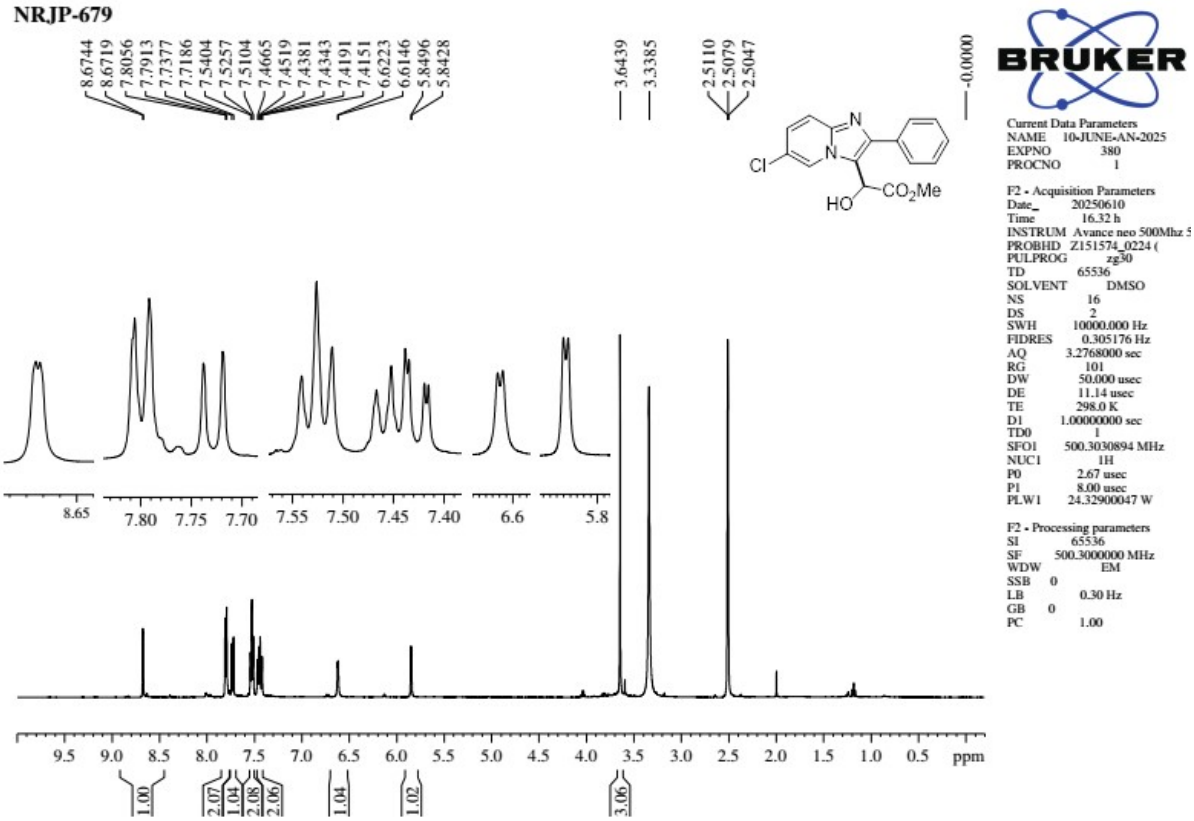


Figure S19. ^{1}H NMR Spectrum of 5i

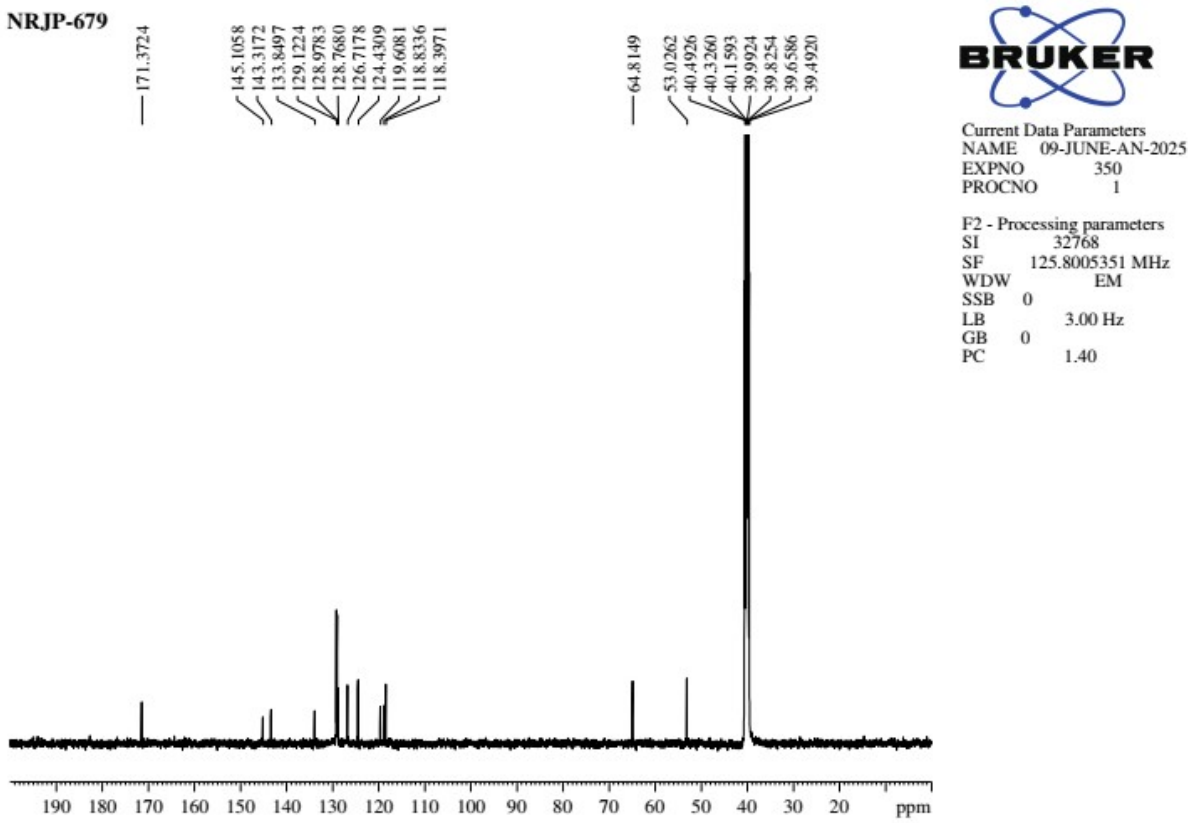


Figure S20. ^{13}C NMR Spectrum of 5i

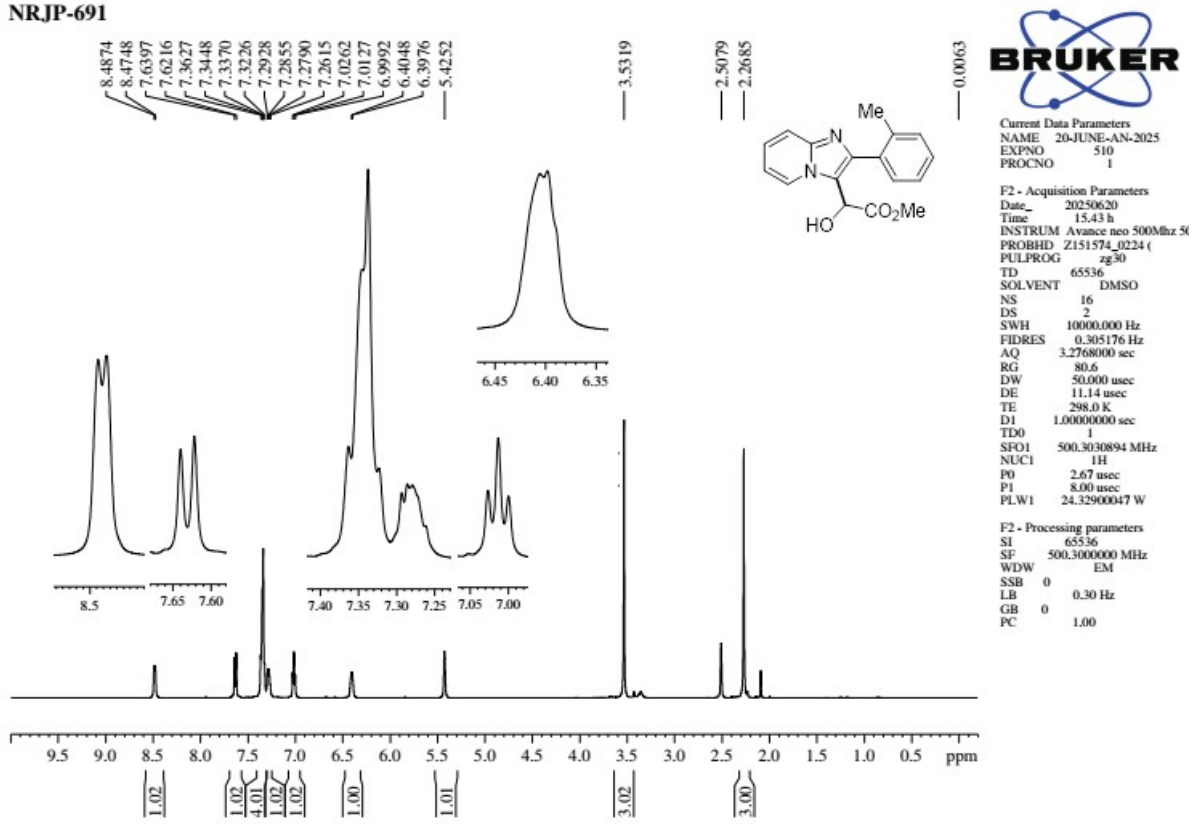


Figure S21. ^{1}H NMR Spectrum of 5j

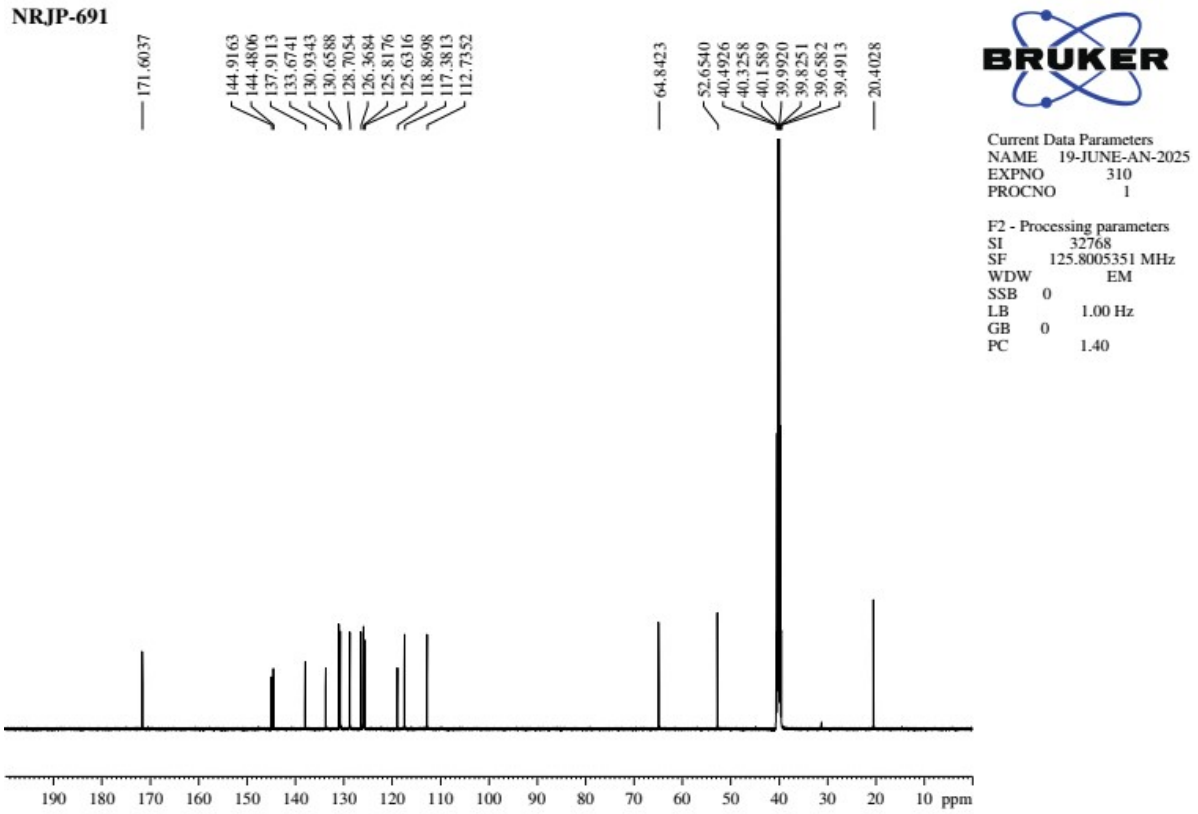


Figure S22. ^{13}C NMR Spectrum of 5j

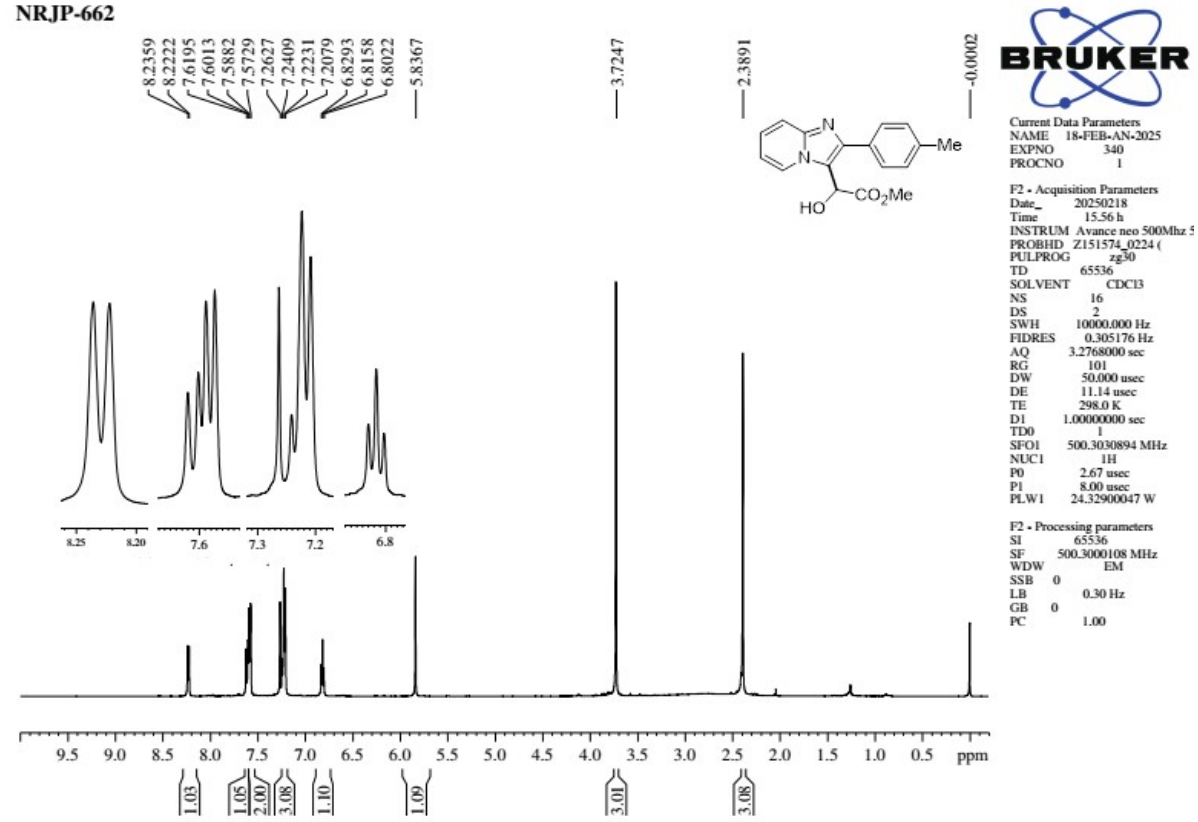


Figure S23. ^{1}H NMR Spectrum of 5k

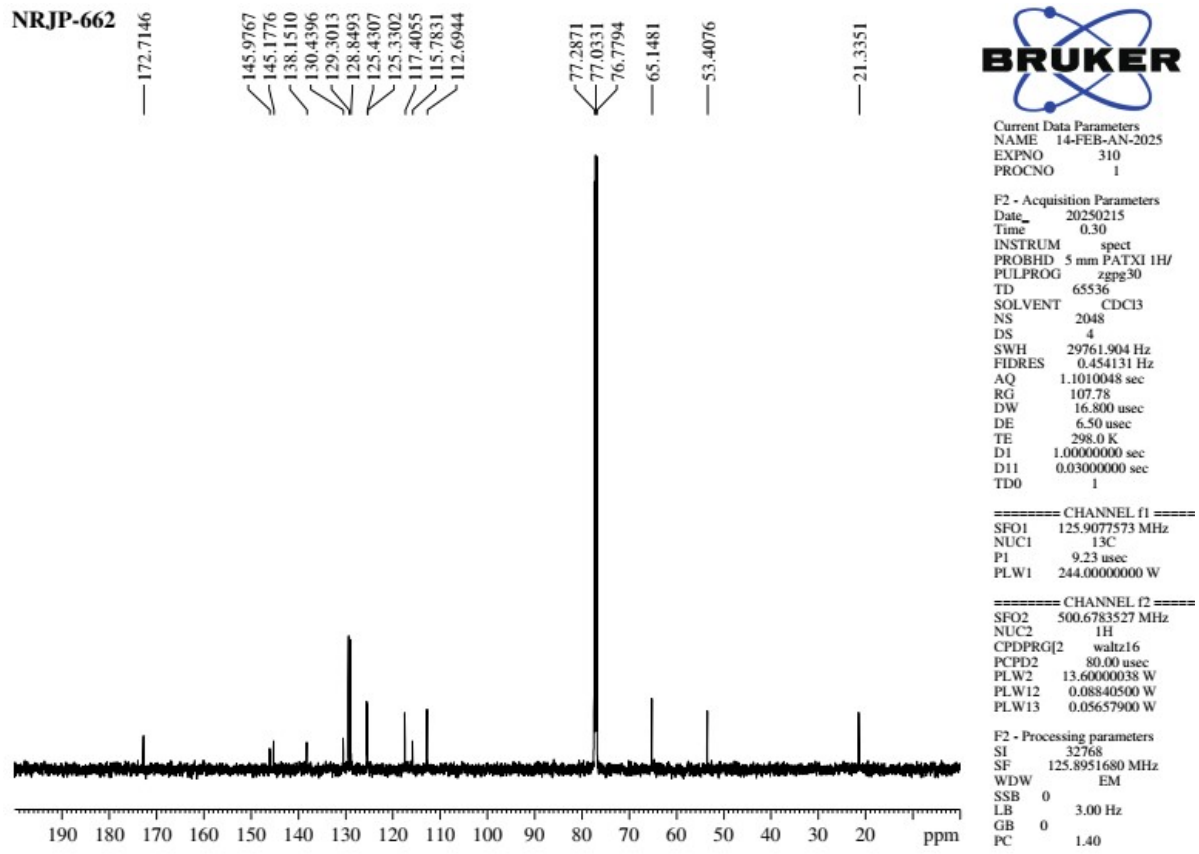


Figure S24. ^{13}C NMR Spectrum of 5k

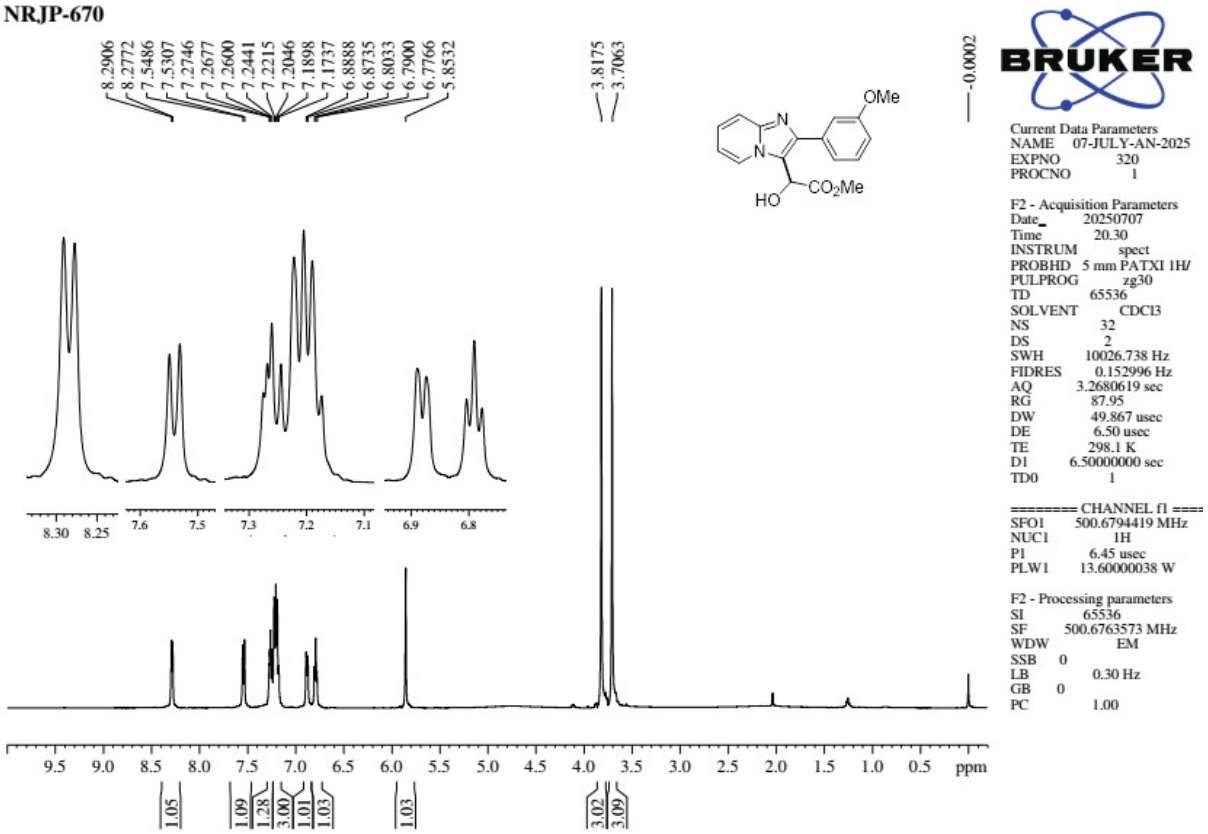


Figure S25. ^{1}H NMR Spectrum of 5l

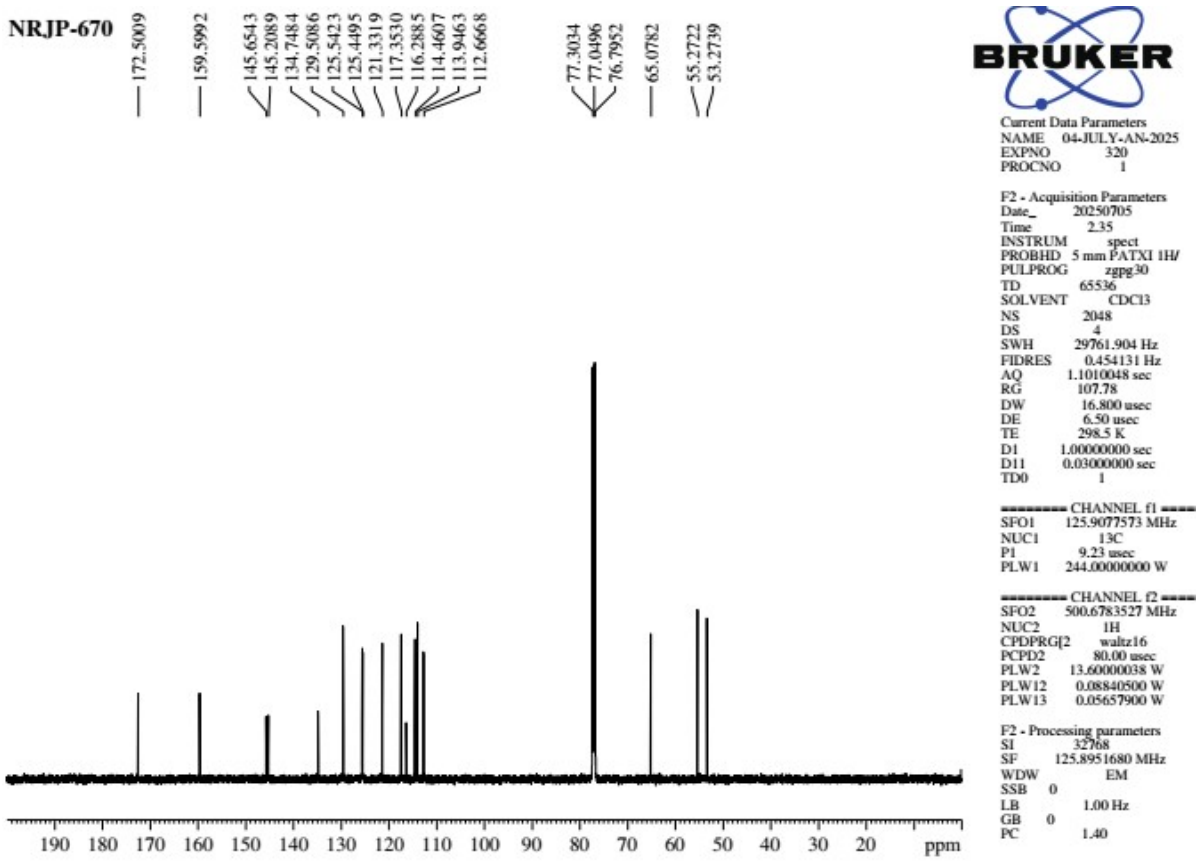


Figure S26. ^{13}C NMR Spectrum of 5l

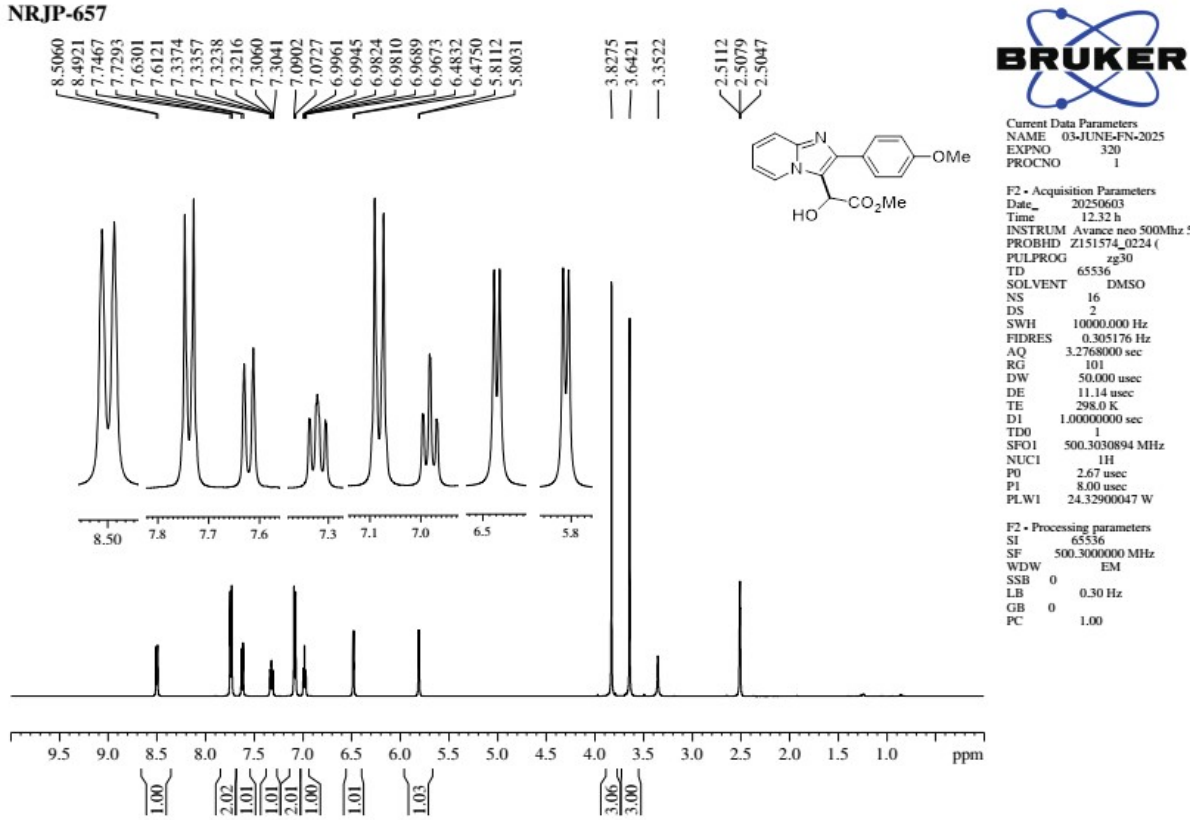


Figure S27. ^{1}H NMR Spectrum of 5m

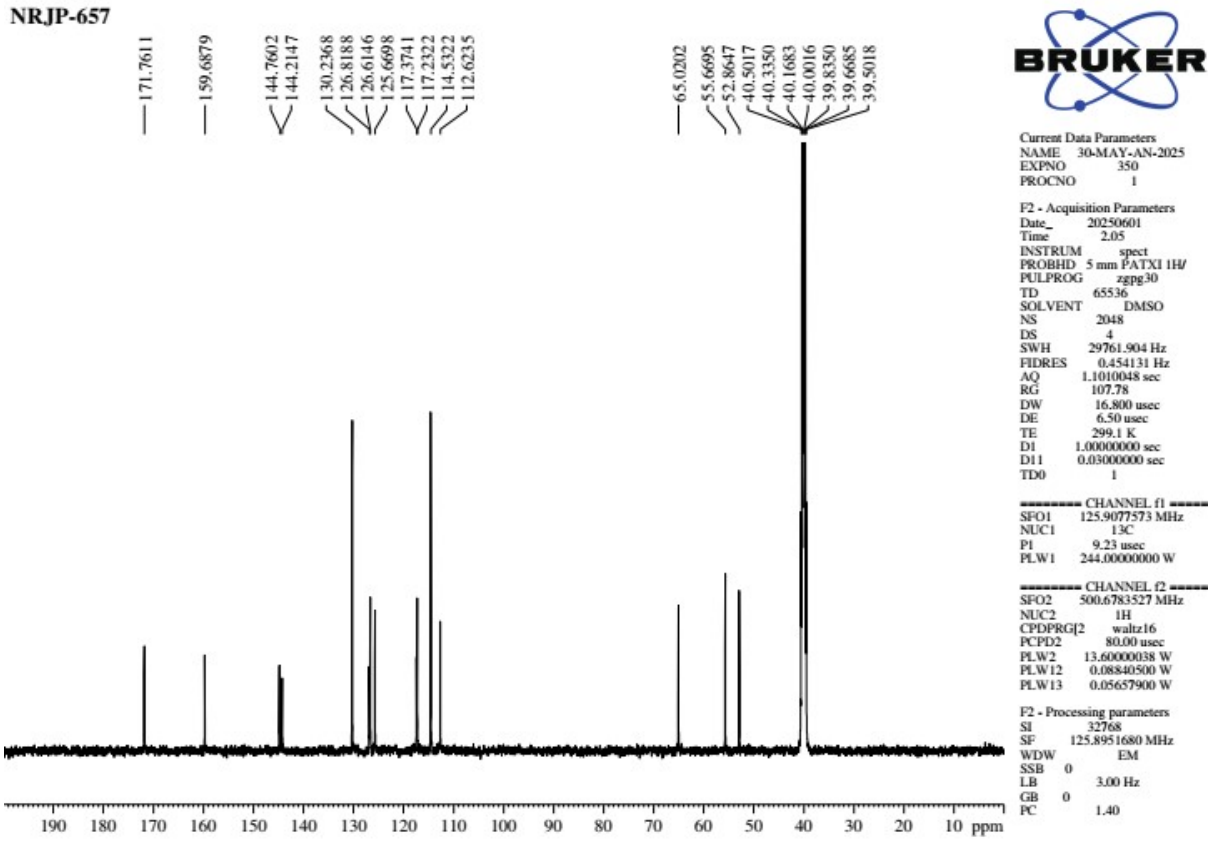


Figure S28. ^{13}C NMR Spectrum of 5m

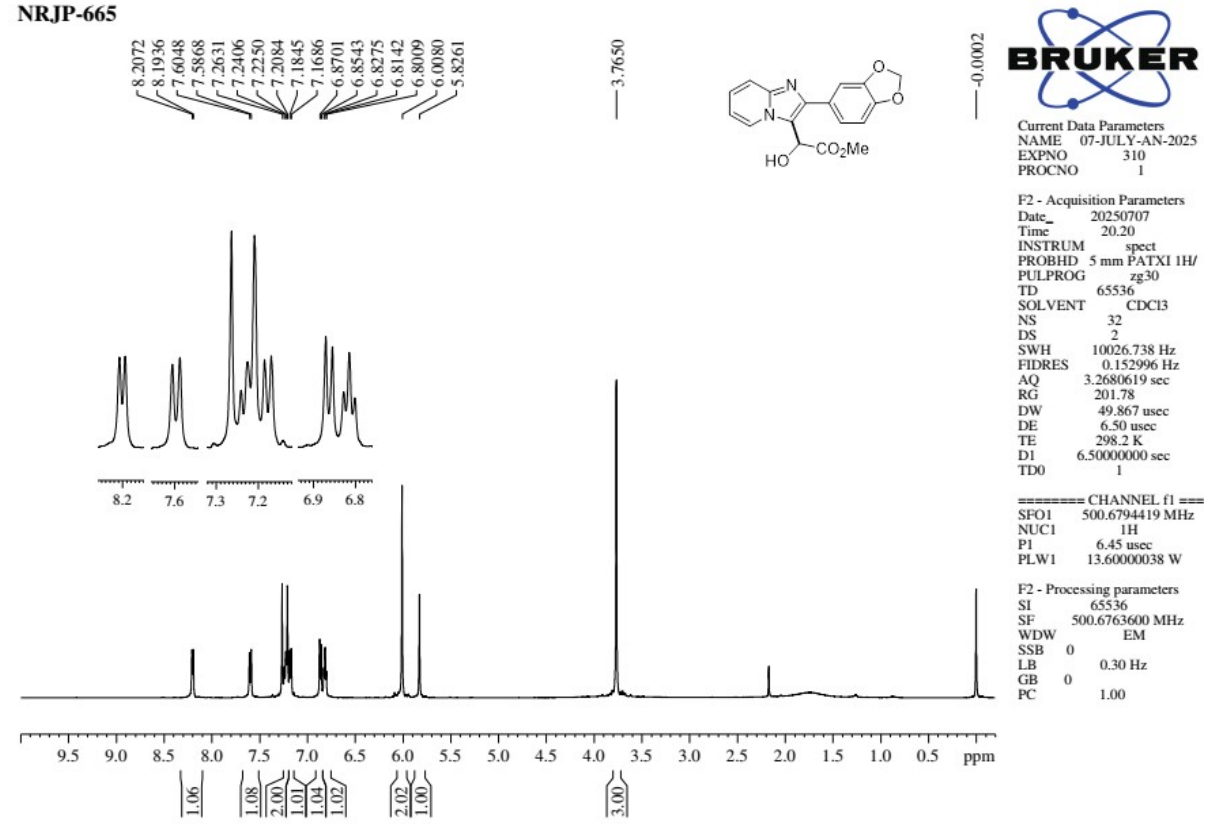


Figure S29. ^{1}H NMR Spectrum of 5n

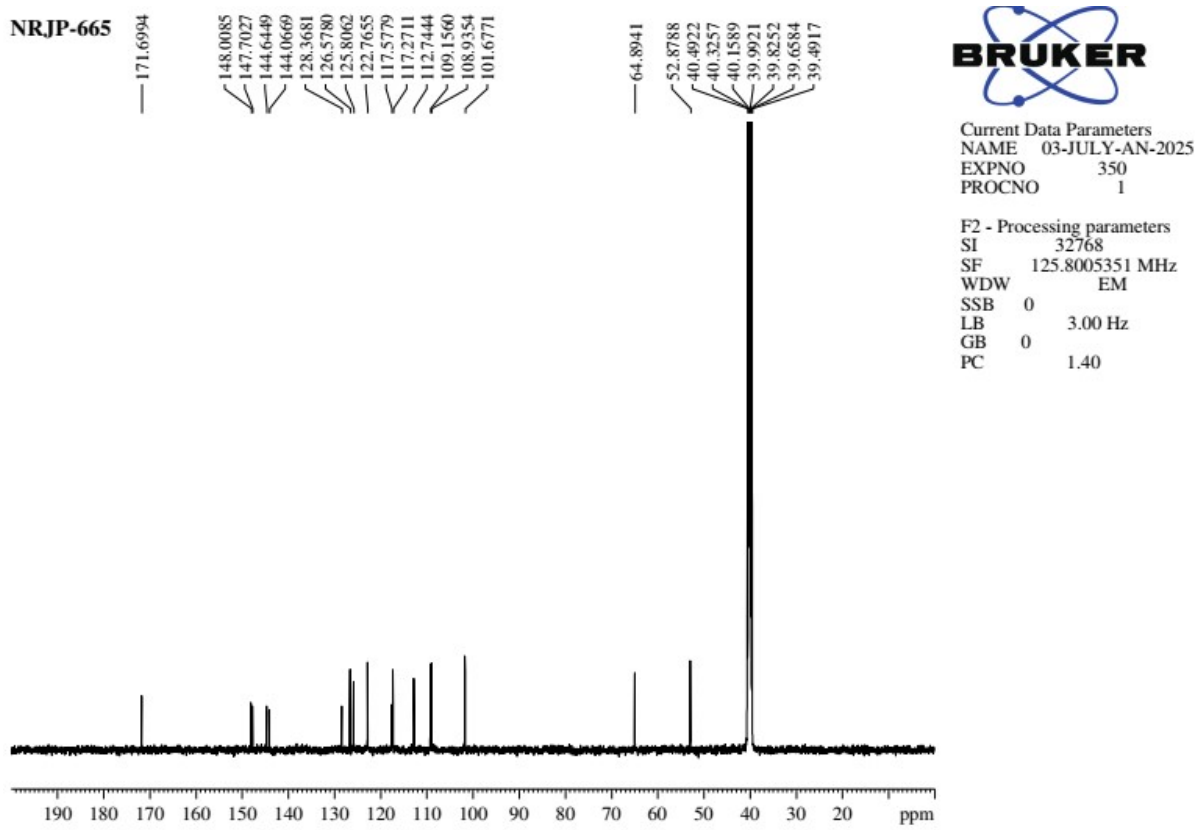


Figure S30. ^{13}C NMR Spectrum of 5n

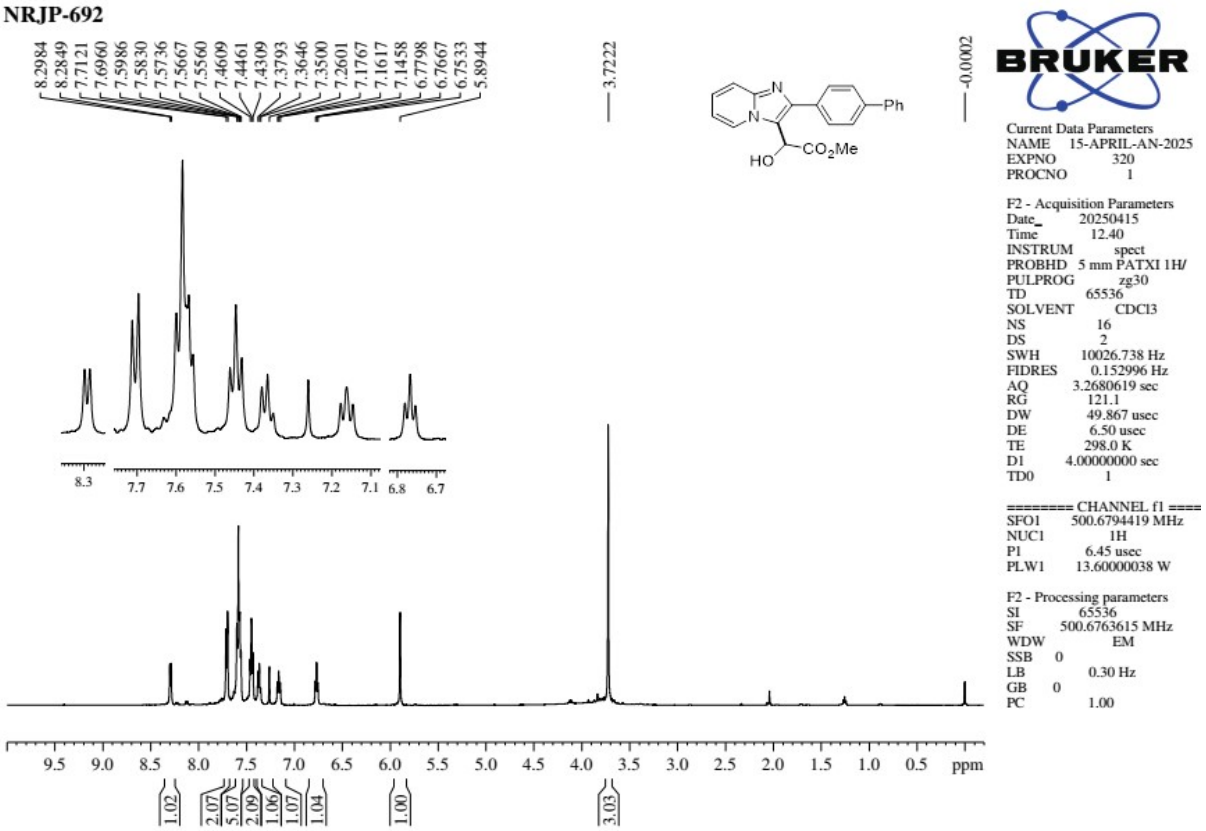


Figure S31. ^{1}H NMR Spectrum of 5o

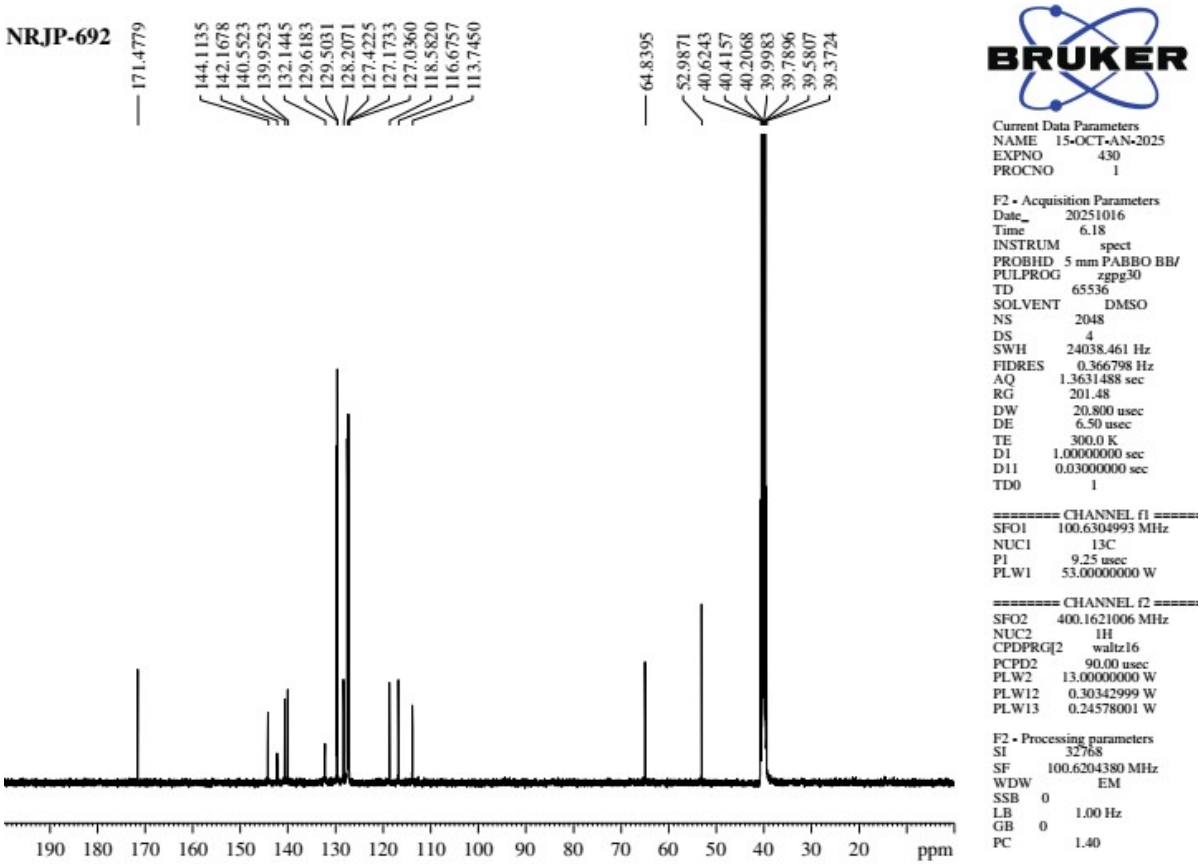


Figure S32. ^{13}C NMR Spectrum of 5o

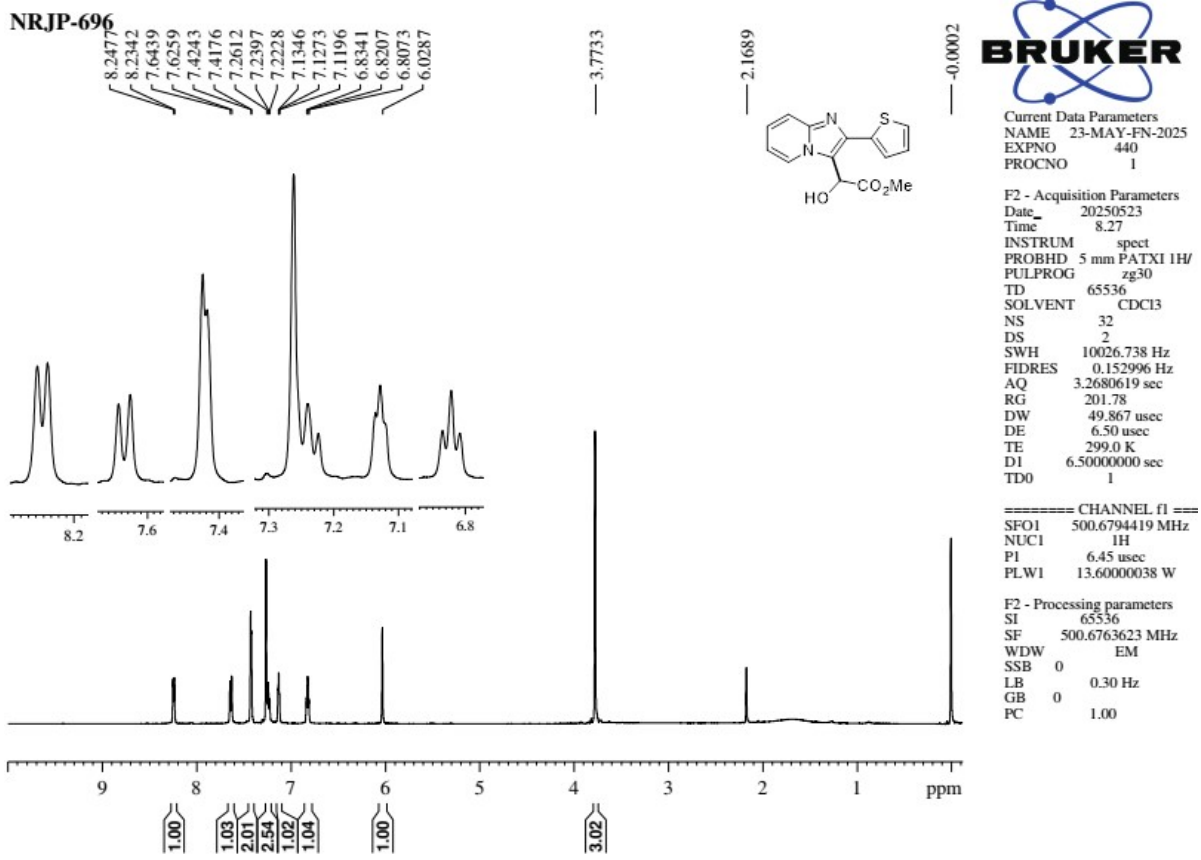


Figure S33. ^{1}H NMR Spectrum of 5p

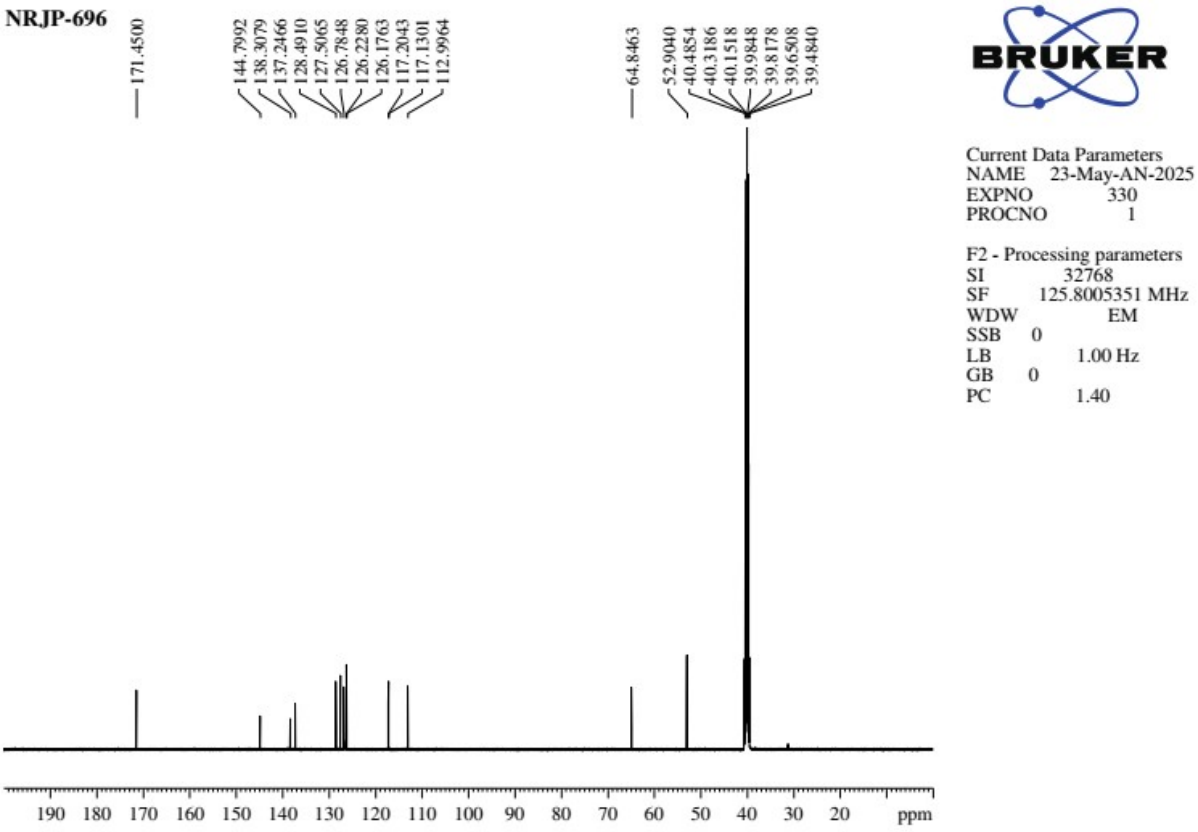


Figure S34. ^{13}C NMR Spectrum of 5p

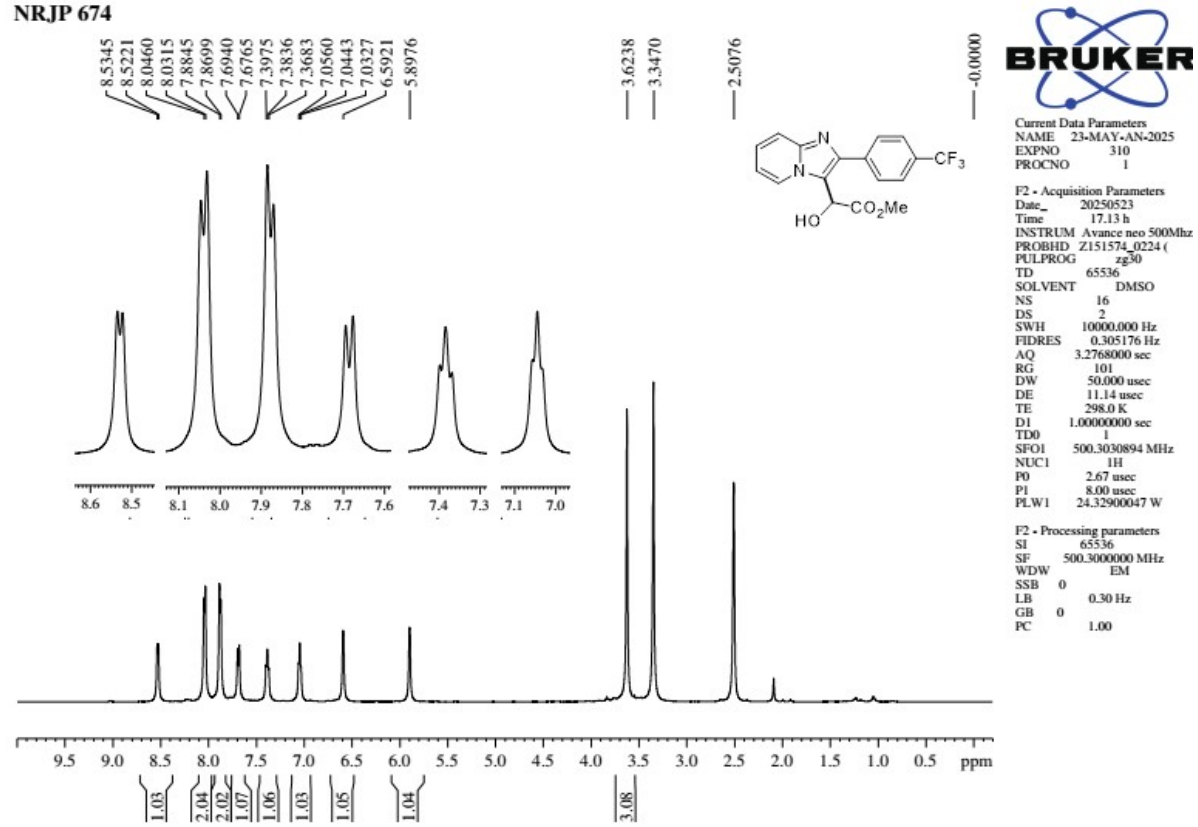


Figure S35. ^{1}H NMR Spectrum of 5q

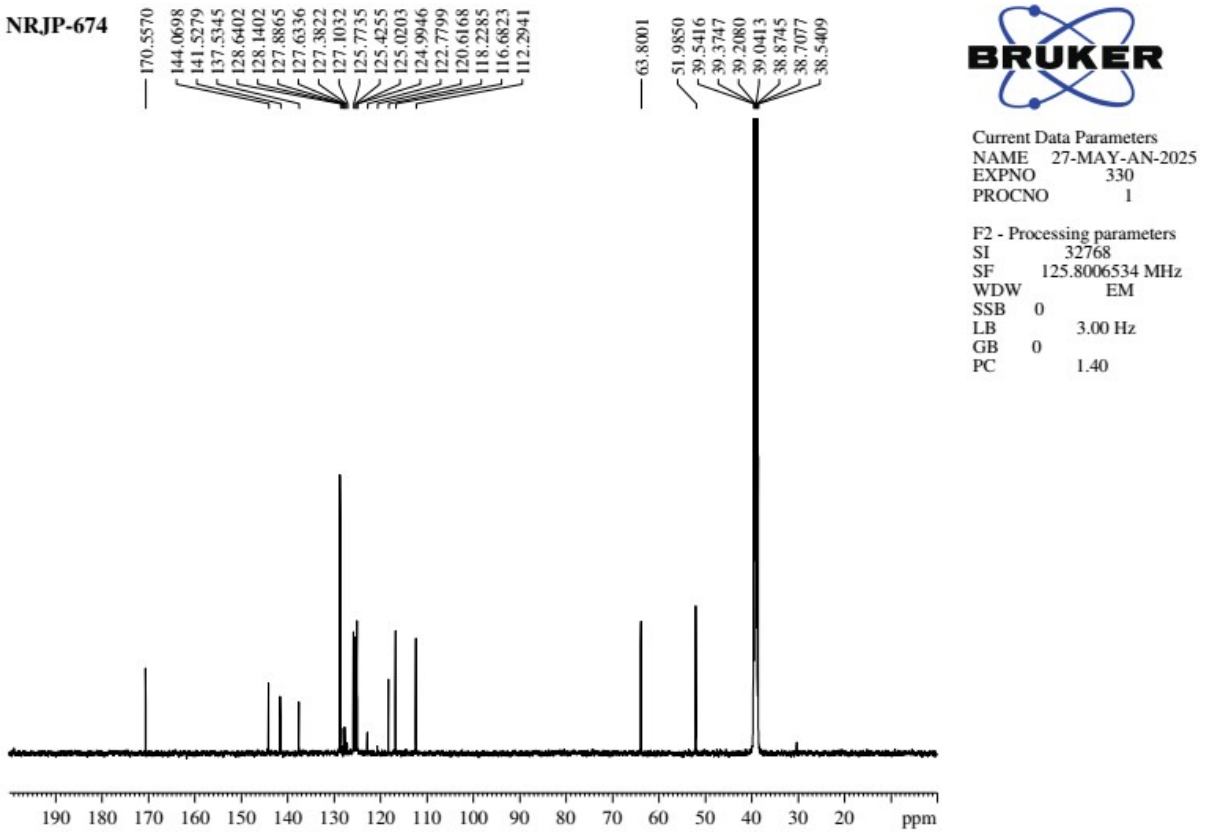


Figure S36. ^{13}C NMR Spectrum of 5q

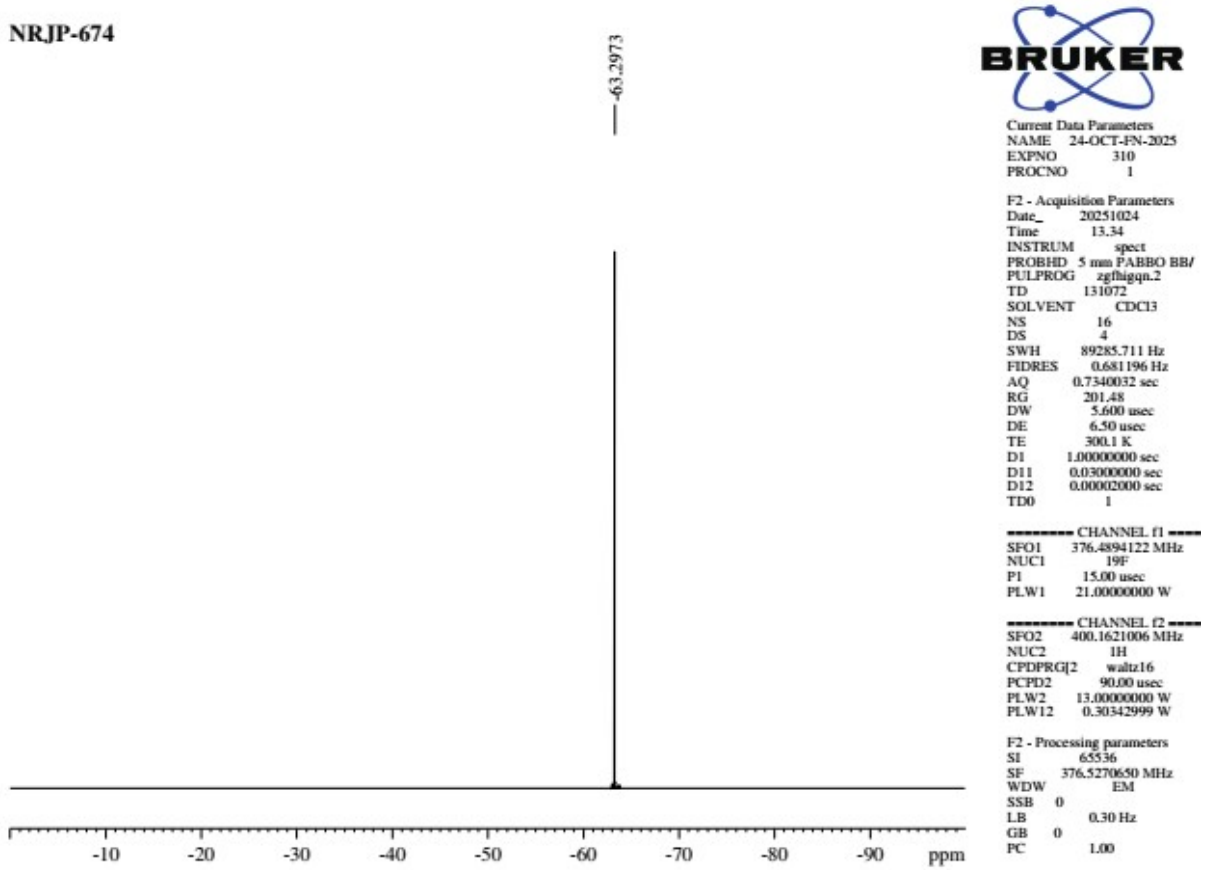


Figure S37. ^{19}F NMR Spectrum of 5q

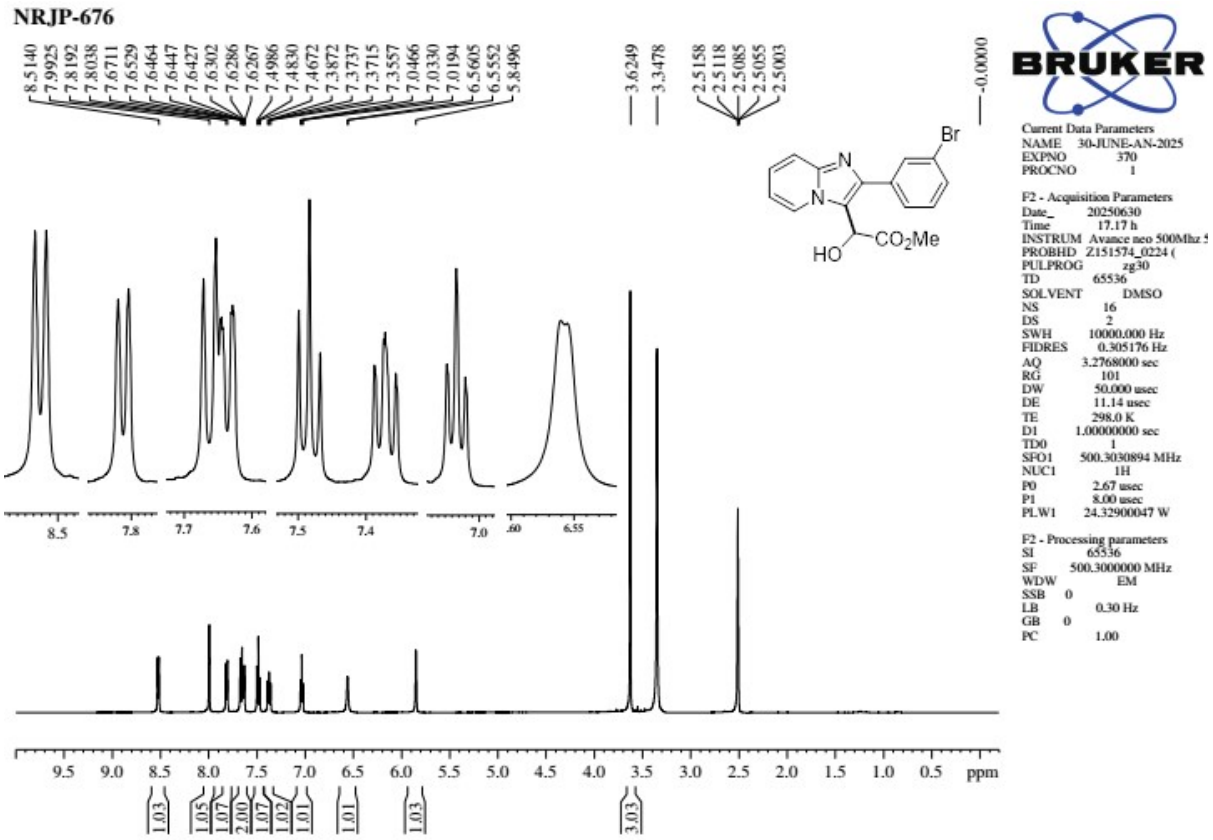


Figure S38. ^{1}H NMR Spectrum of 5r

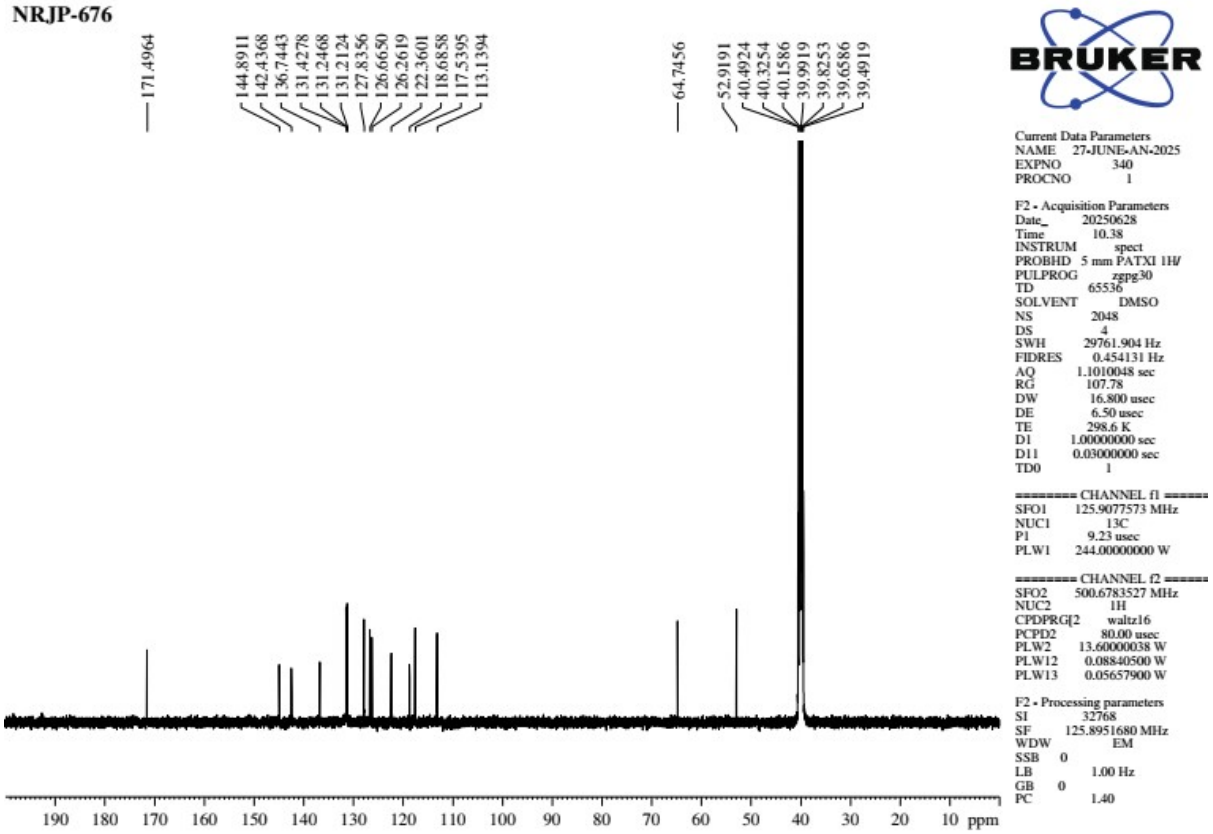


Figure S39. ^{13}C NMR Spectrum of 5r

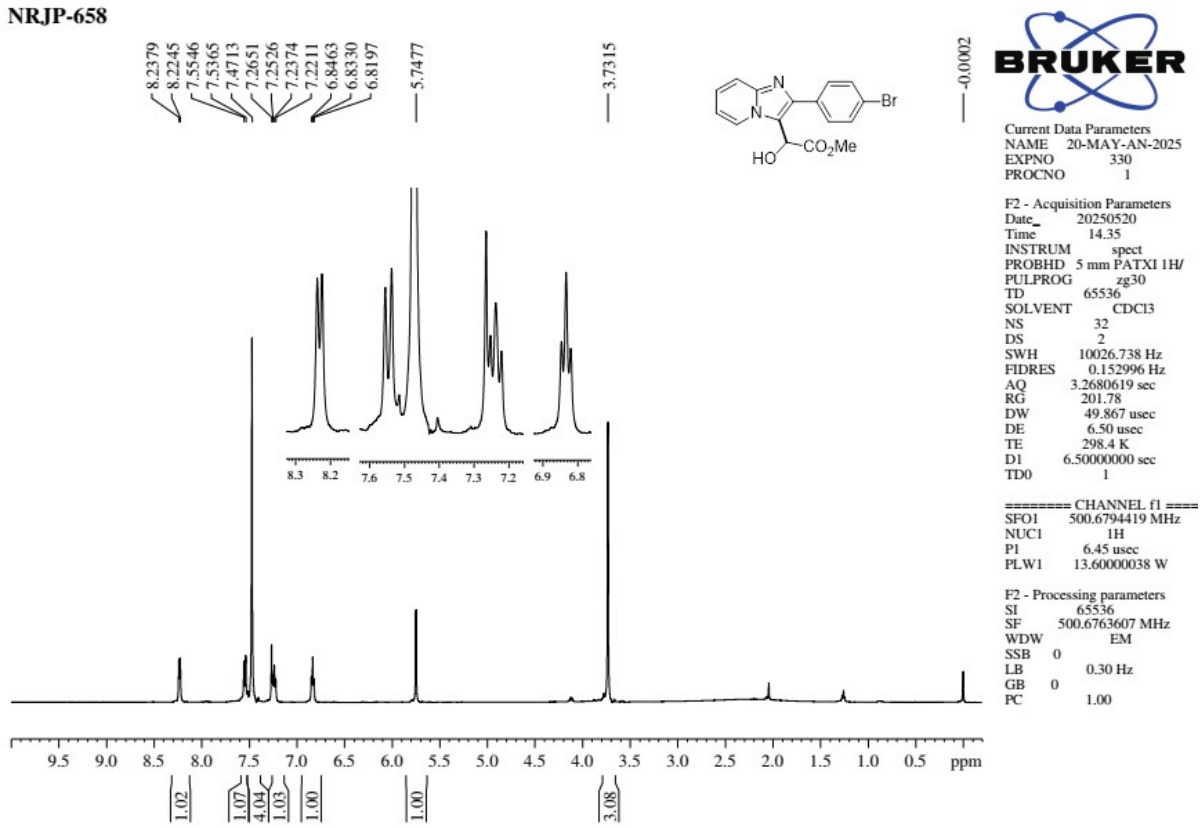


Figure S40. ^{1}H NMR Spectrum of 5s

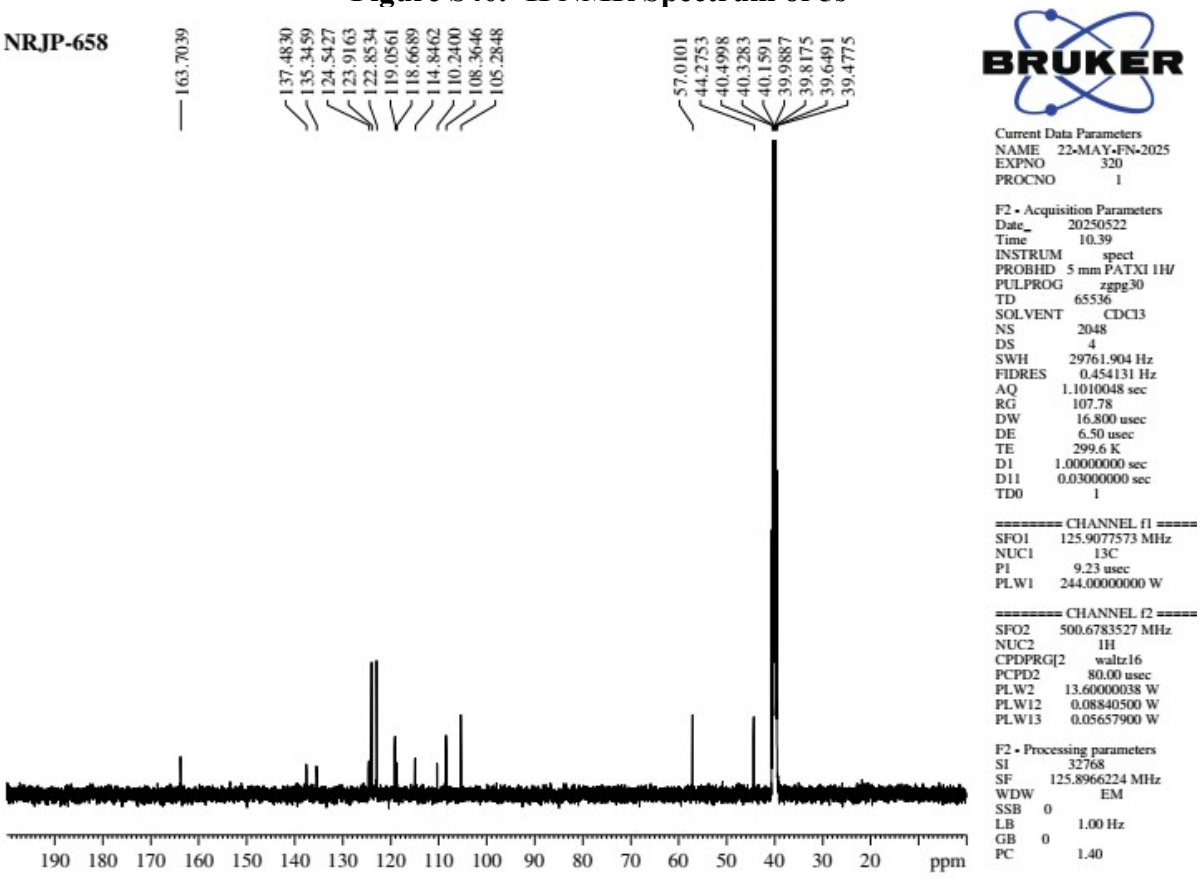


Figure S41. ^{13}C NMR Spectrum of 5s

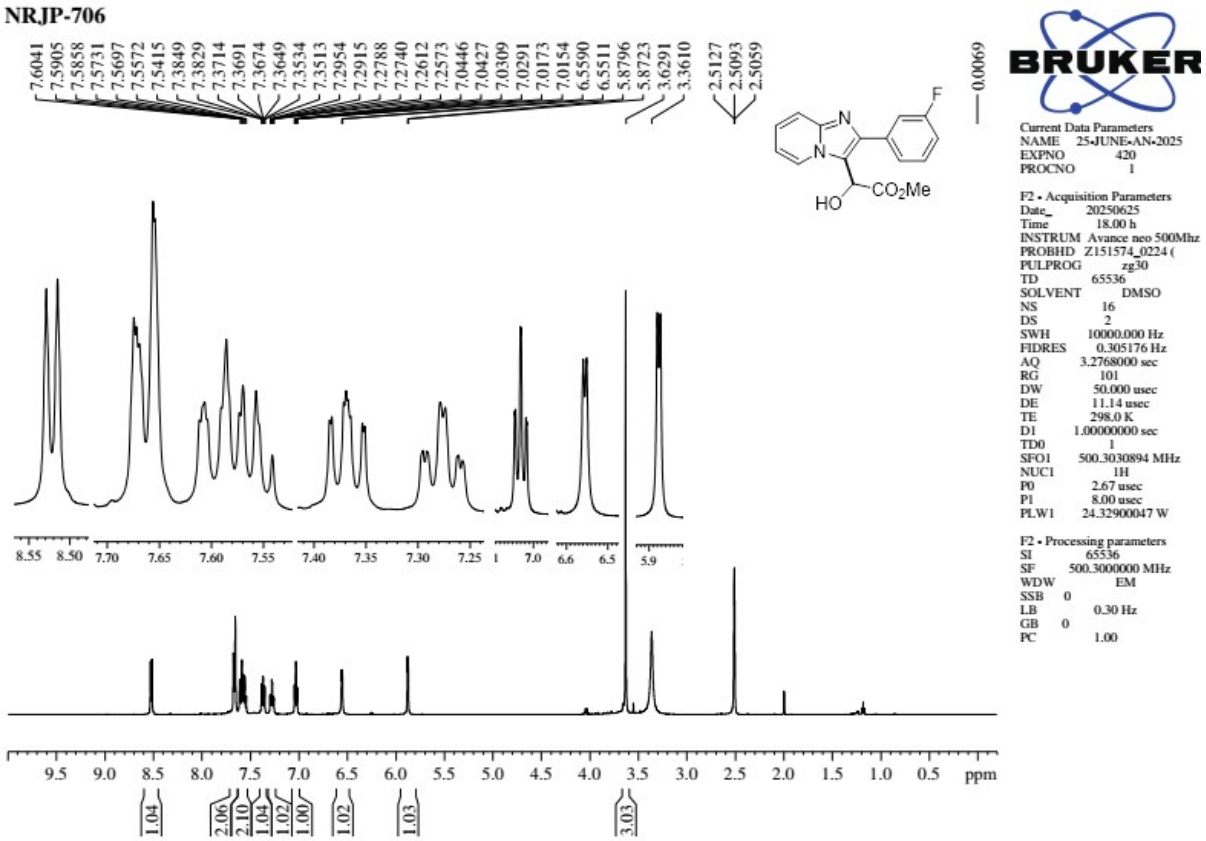


Figure S42. ^{1}H NMR Spectrum of 5t

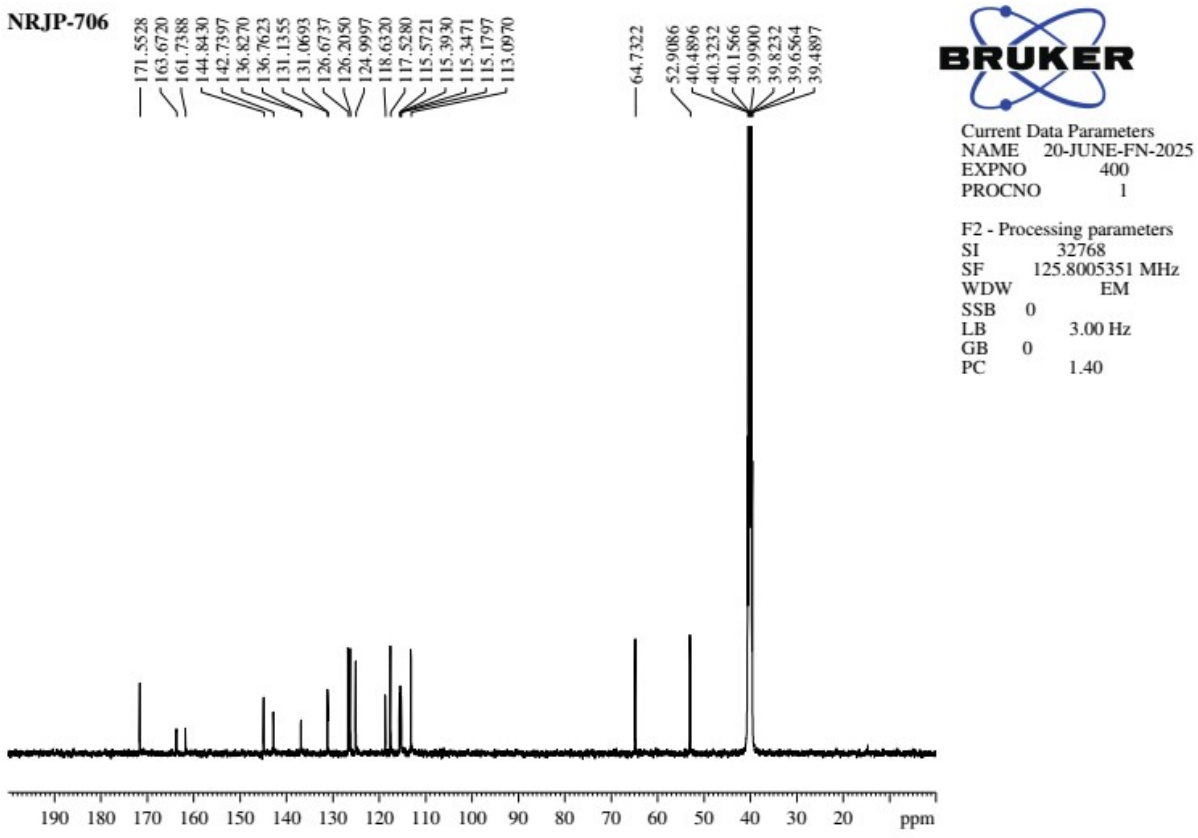


Figure S43. ^{13}C NMR Spectrum of 5t

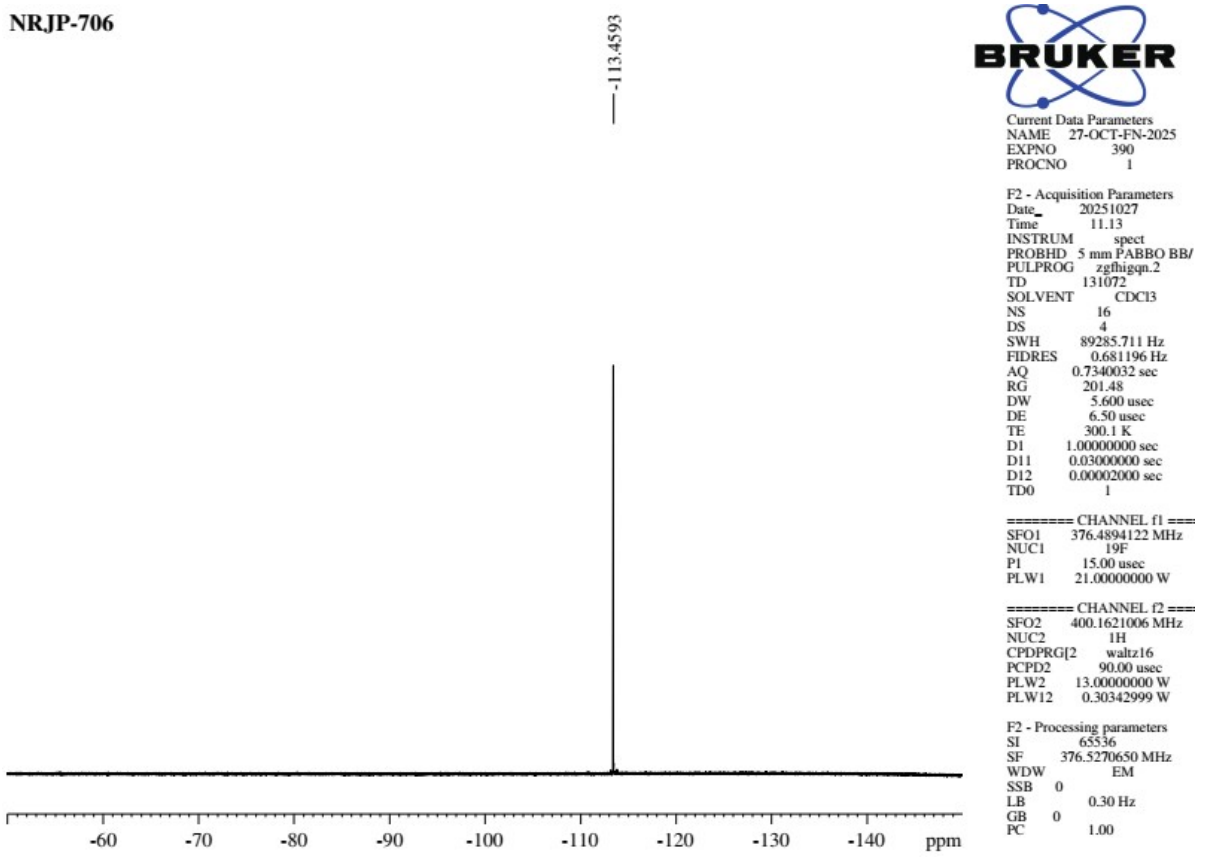


Figure S44. ^{19}F NMR Spectrum of 5t

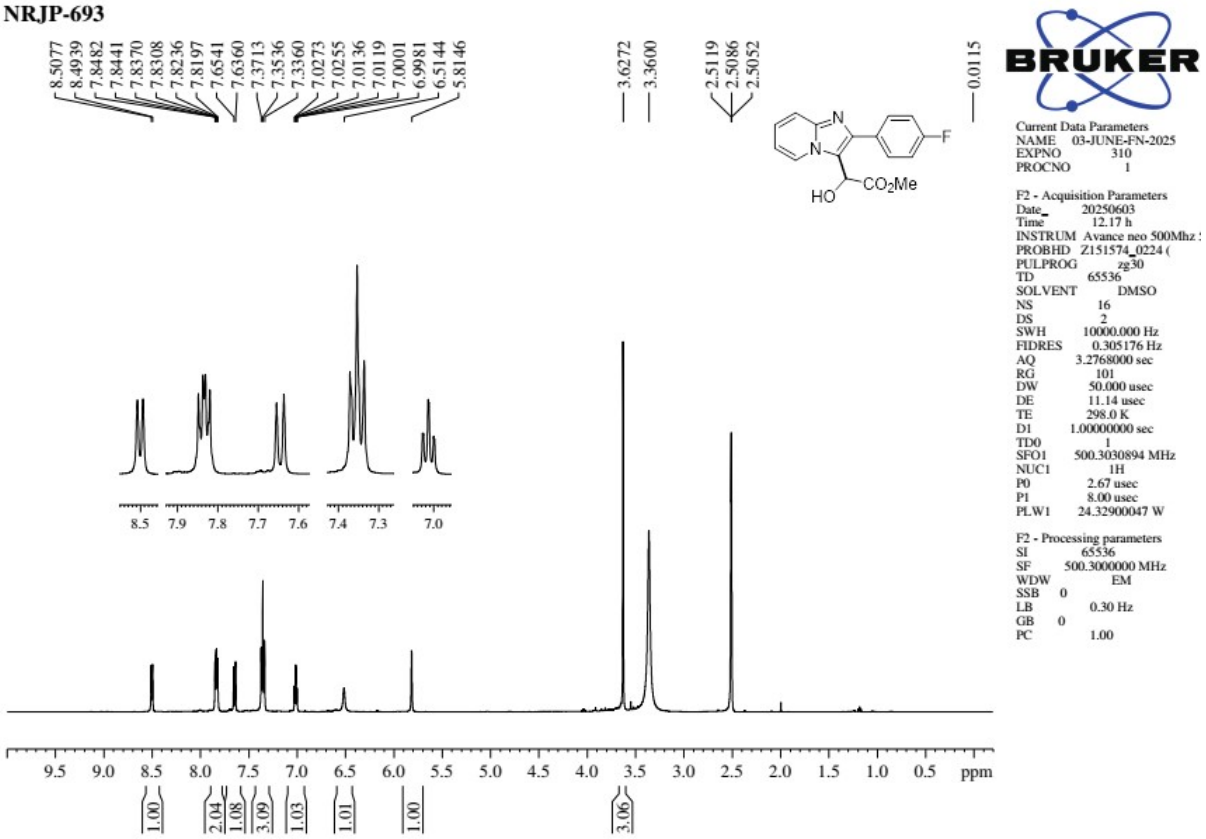


Figure S45. ^{1}H NMR Spectrum of 5u

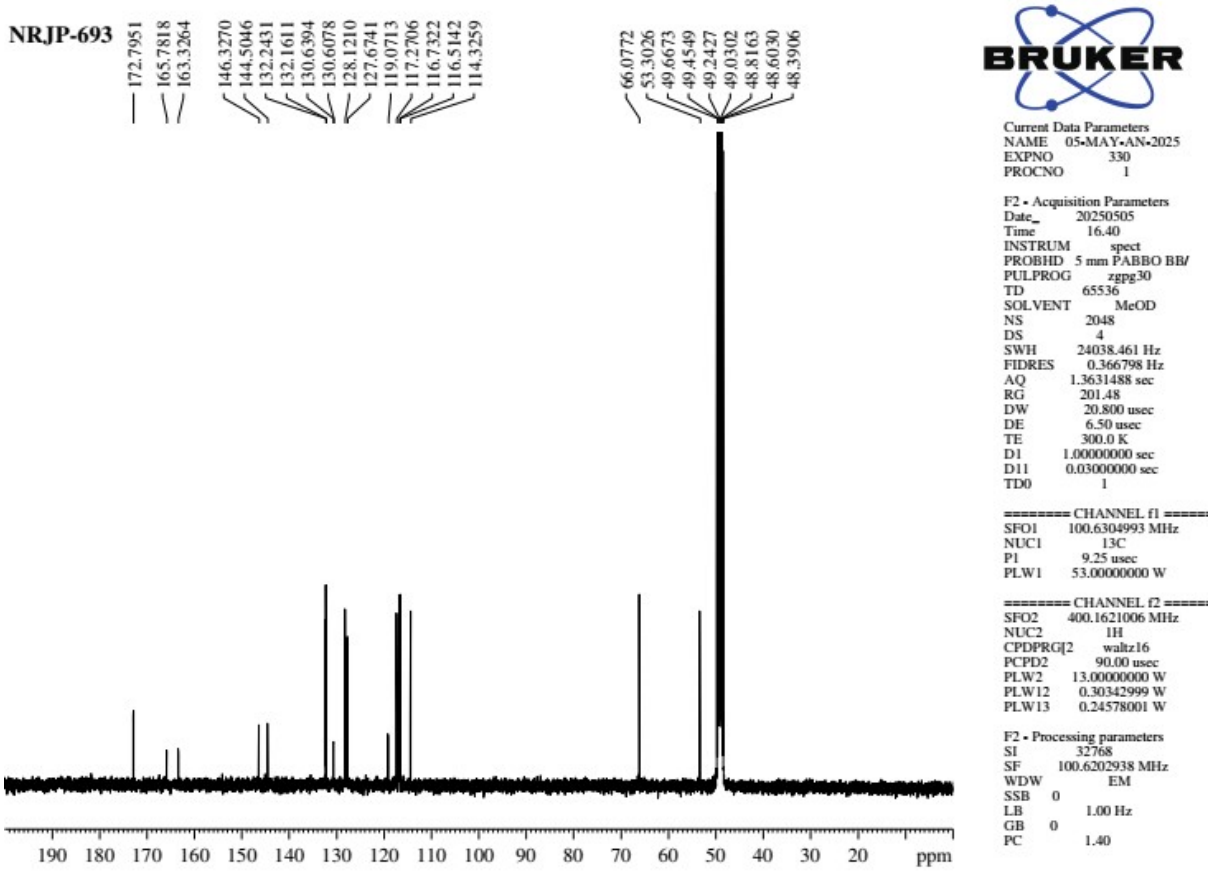


Figure S46. ^{13}C NMR Spectrum of 5u

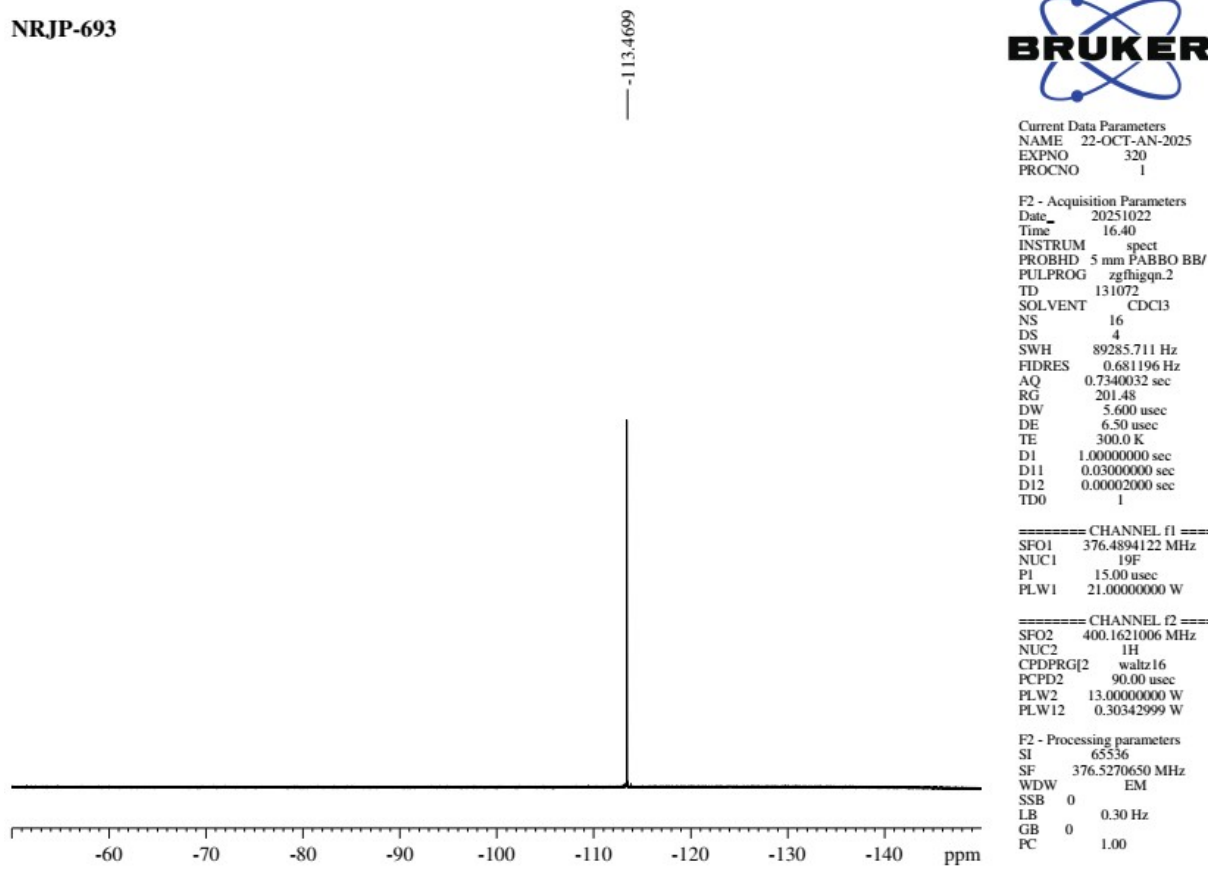


Figure S47. ^{19}F NMR Spectrum of 5u

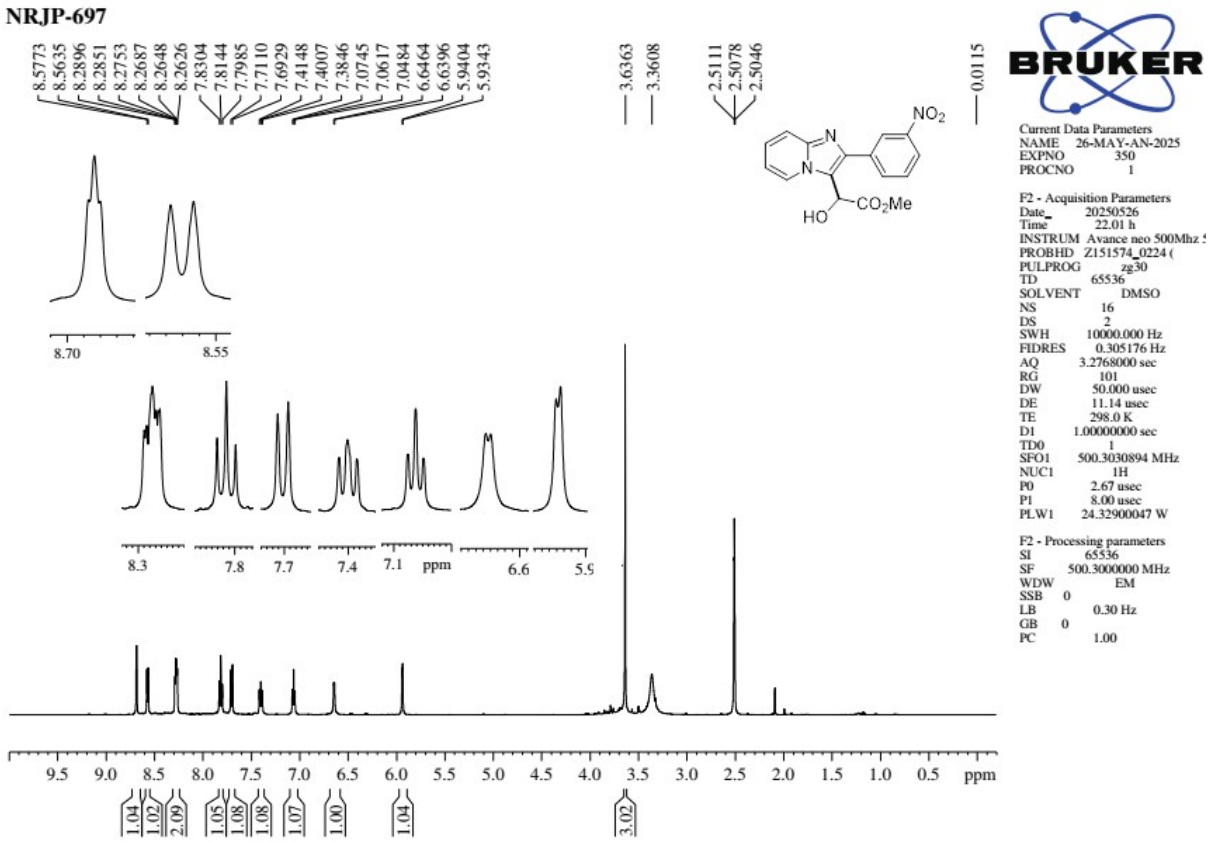


Figure S48. ^{1}H NMR Spectrum of 5v

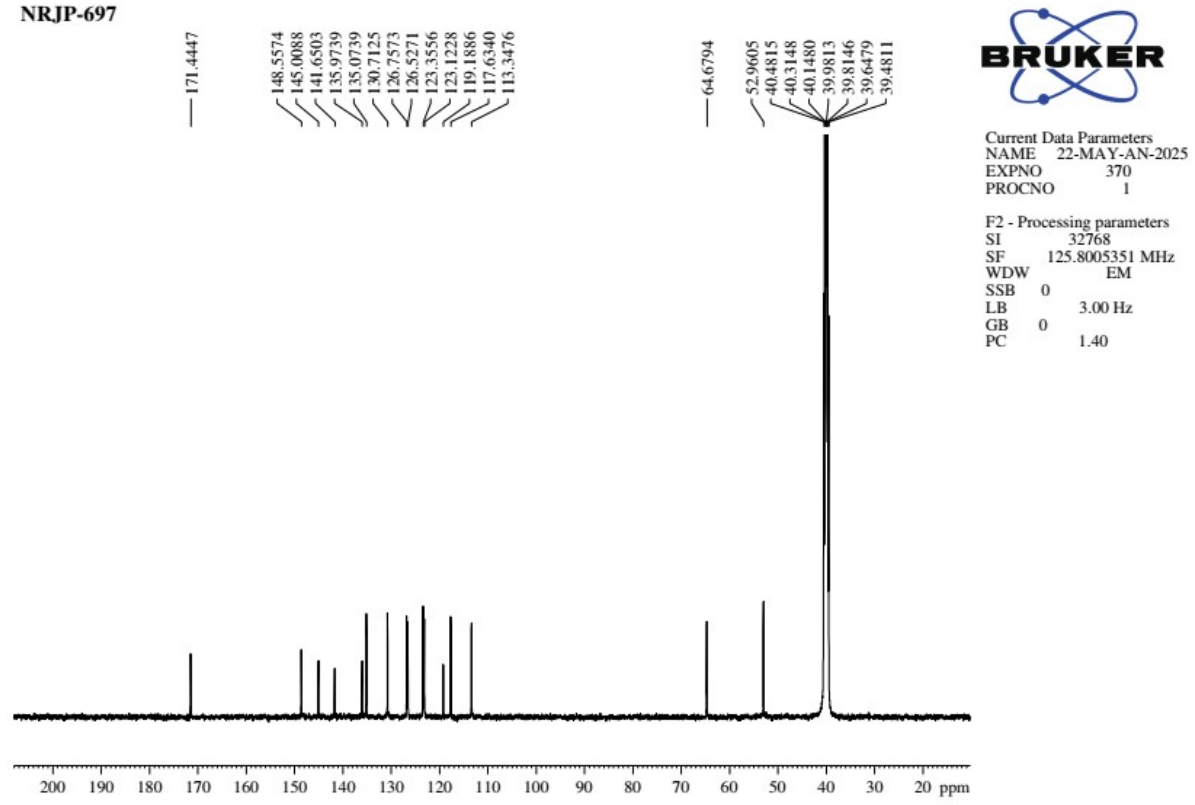


Figure S49. ^{13}C NMR Spectrum of 5v

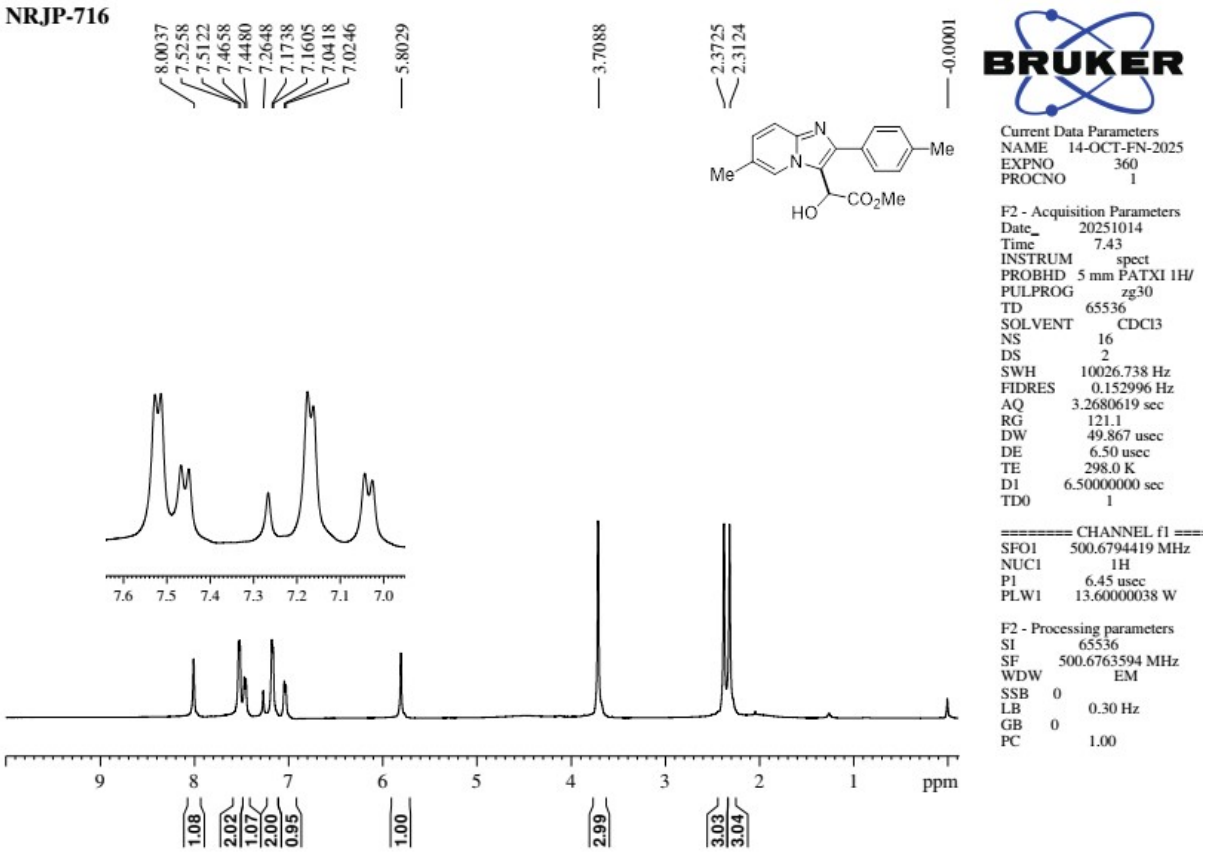


Figure S50. ^{1}H NMR Spectrum of 5w

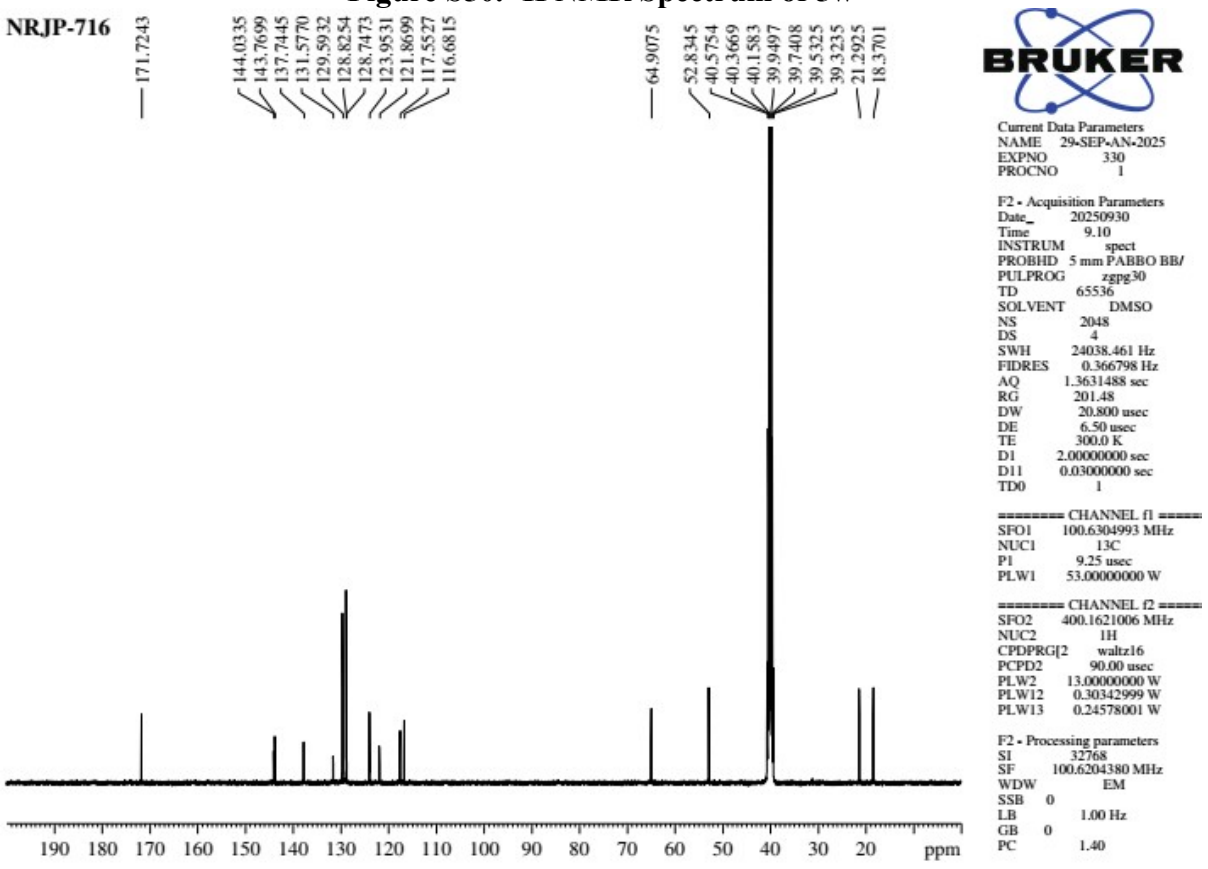
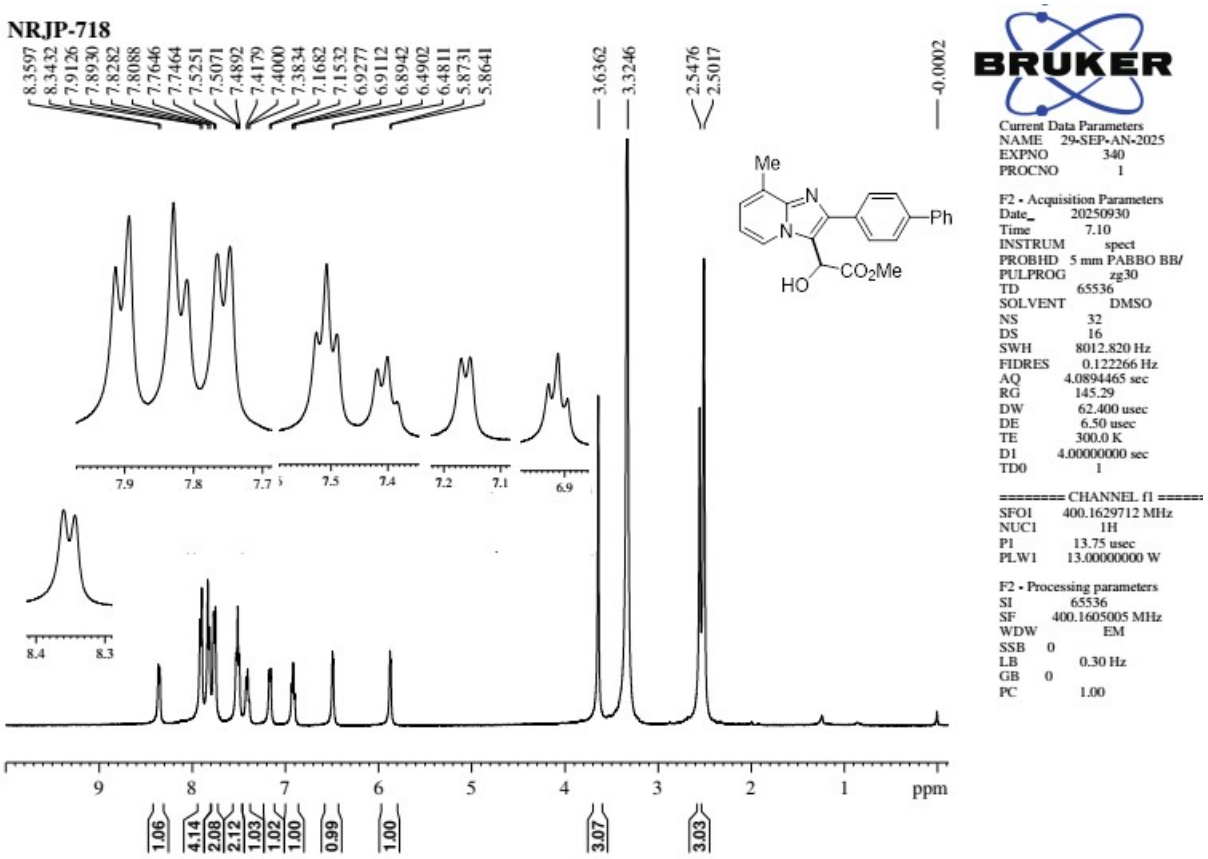


Figure S51. ^{13}C NMR Spectrum of 5w



BRUKER

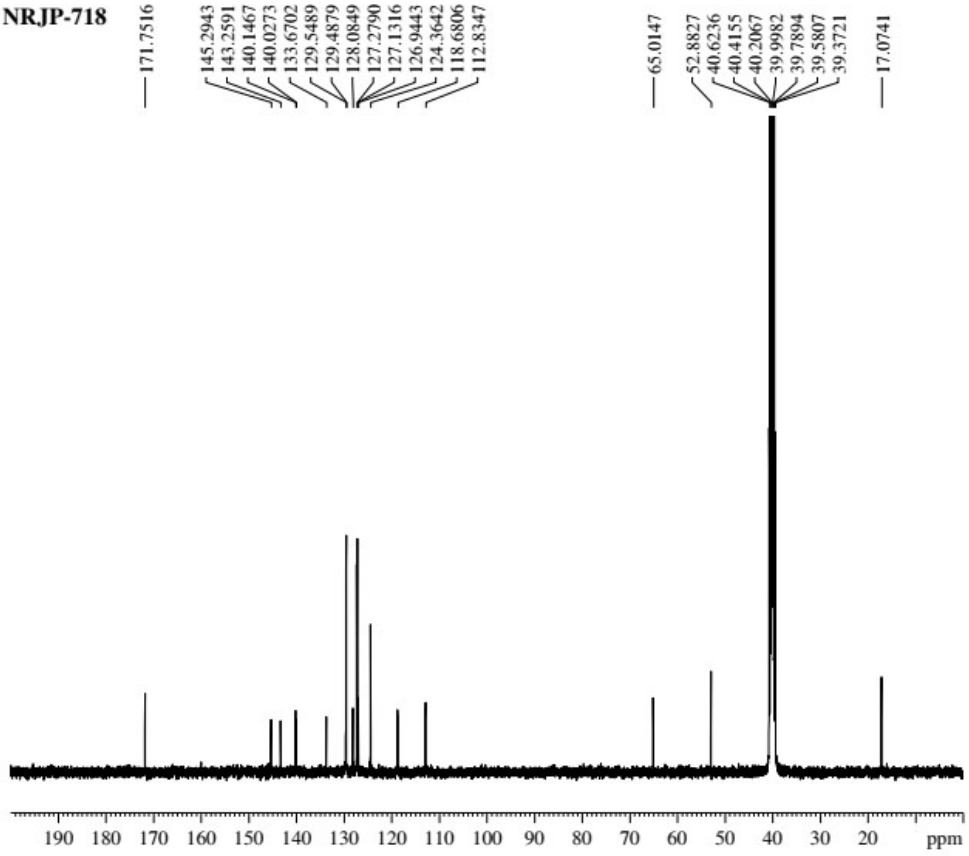
Current Data Parameters
NAME 29-SEP-AN-2025
EXPNO 340
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250930
Time 7.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 16
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 145.29
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 4.00000000 sec
TD0 1

======== CHANNEL f1 ======
SFO1 400.1629712 MHz
NUC1 1H
P1 13.75 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1605005 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S52. ^{1}H NMR Spectrum of 5x



BRUKER

Current Data Parameters
NAME 19-DEC-AN-2025
EXPNO 350
PROCNO 1

F2 - Acquisition Parameters
Date_ 20251220
Time 2.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 201.48
DW 20.800 usec
DE 6.50 usec
TE 300.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ====
SFO1 100.6304993 MHz
NUC1 13C
P1 9.25 usec
PLW1 53.00000000 W

======== CHANNEL f2 ====
SFO2 400.1621006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.30342999 W
PLW13 0.24578001 W

F2 - Processing parameters
SI 32768
SF 100.6204380 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S53. ^{13}C NMR Spectrum of 5x

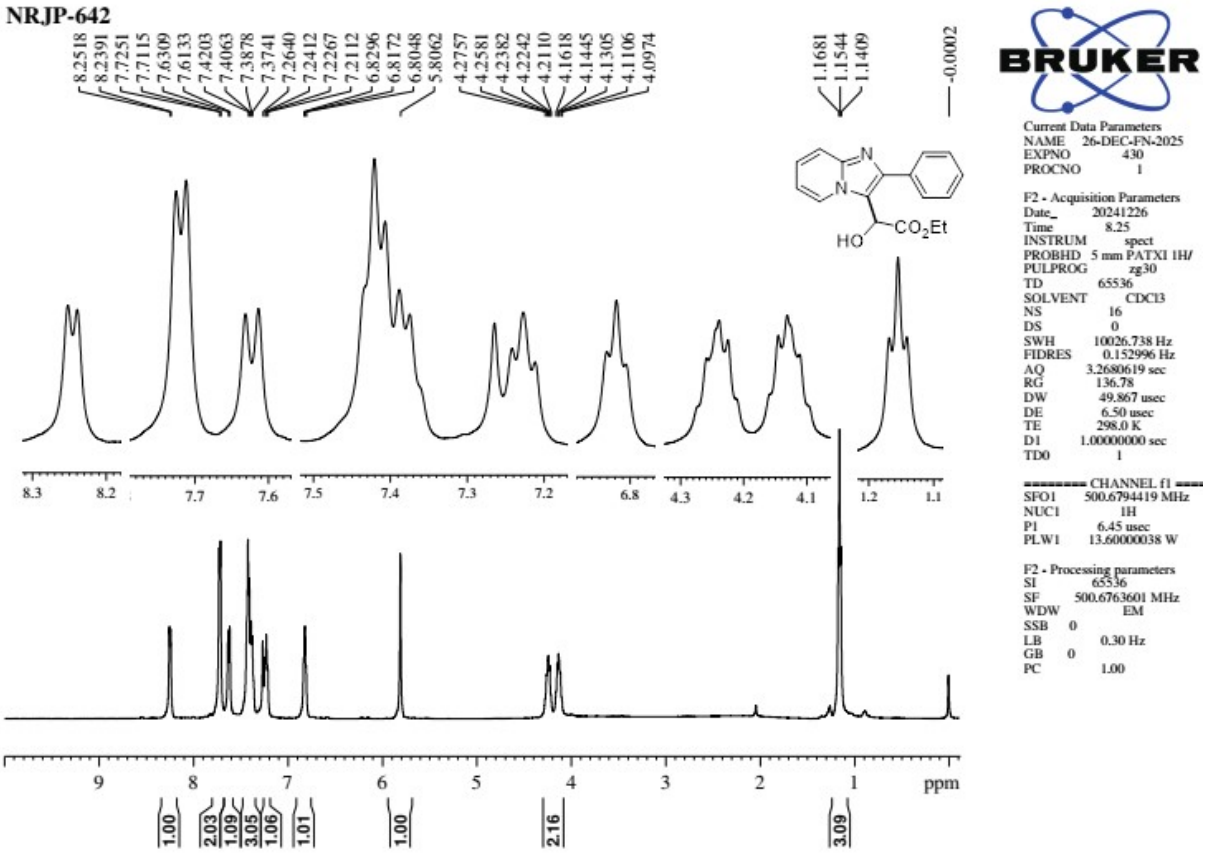


Figure S54. ^{1}H NMR Spectrum of 5y

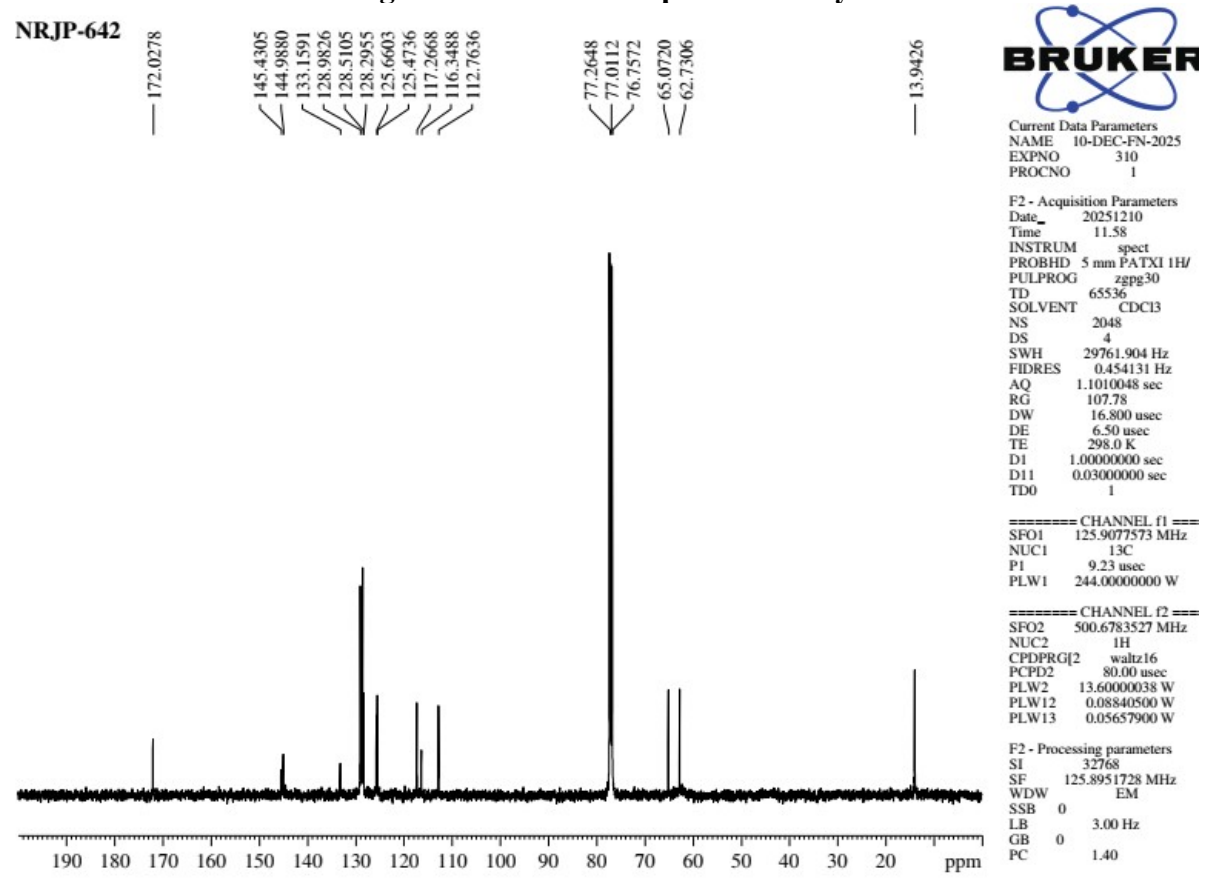


Figure S55. ^{13}C NMR Spectrum of 5y

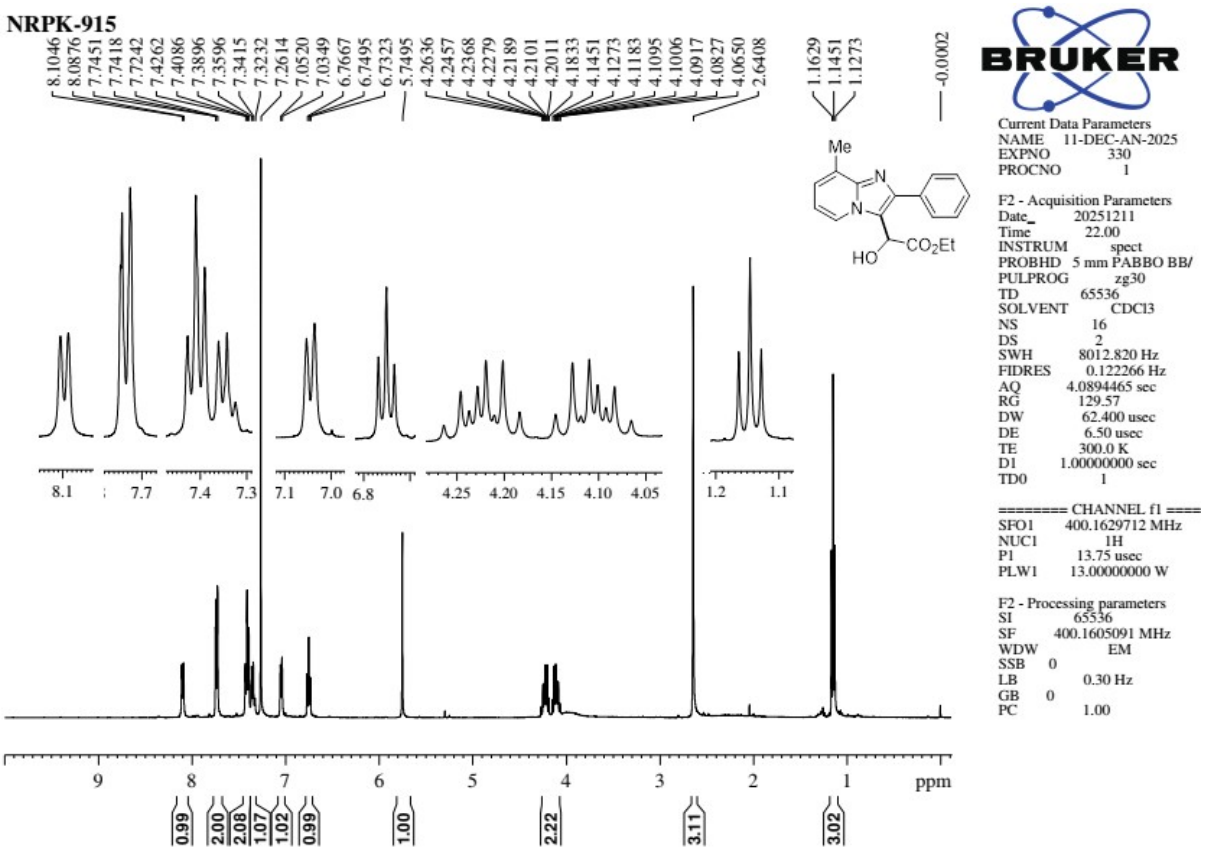


Figure S56. ^{1}H NMR Spectrum of 5z

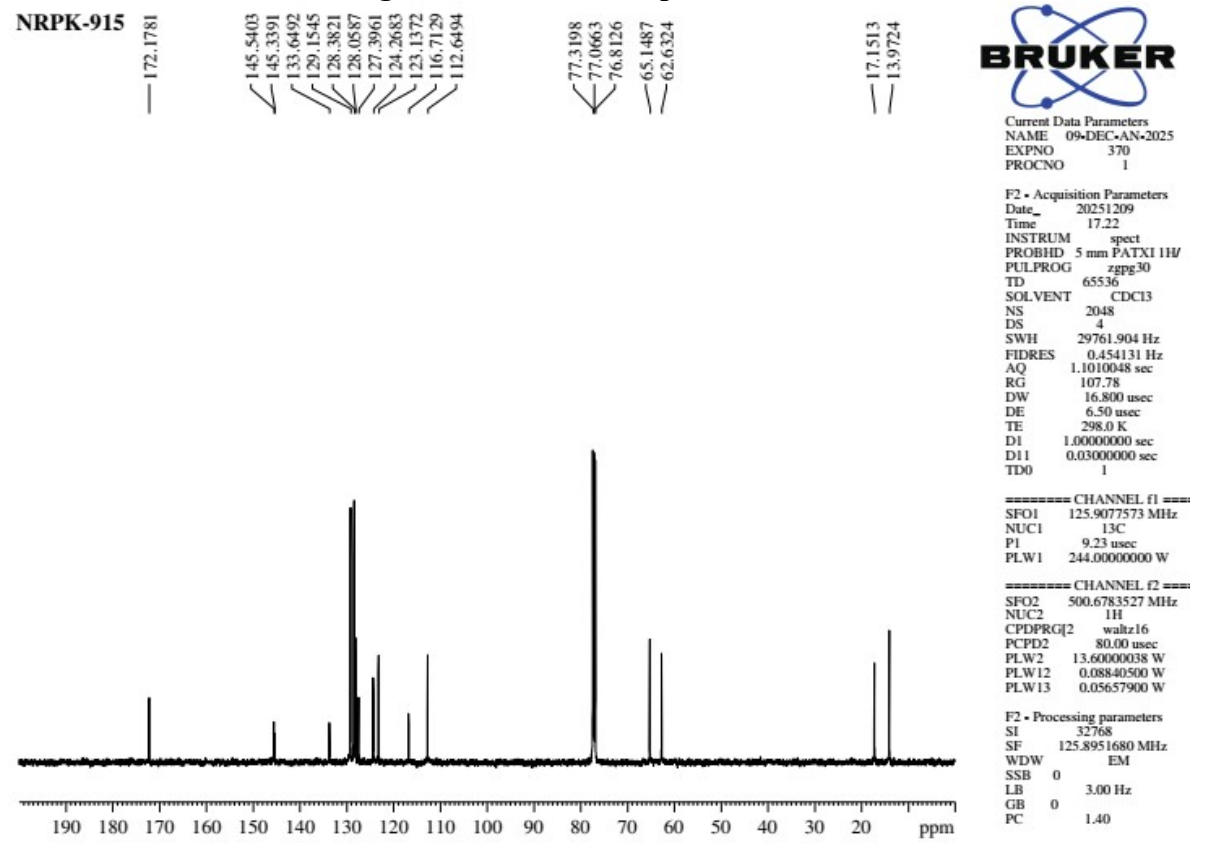


Figure S57. ^{13}C NMR Spectrum of 5z

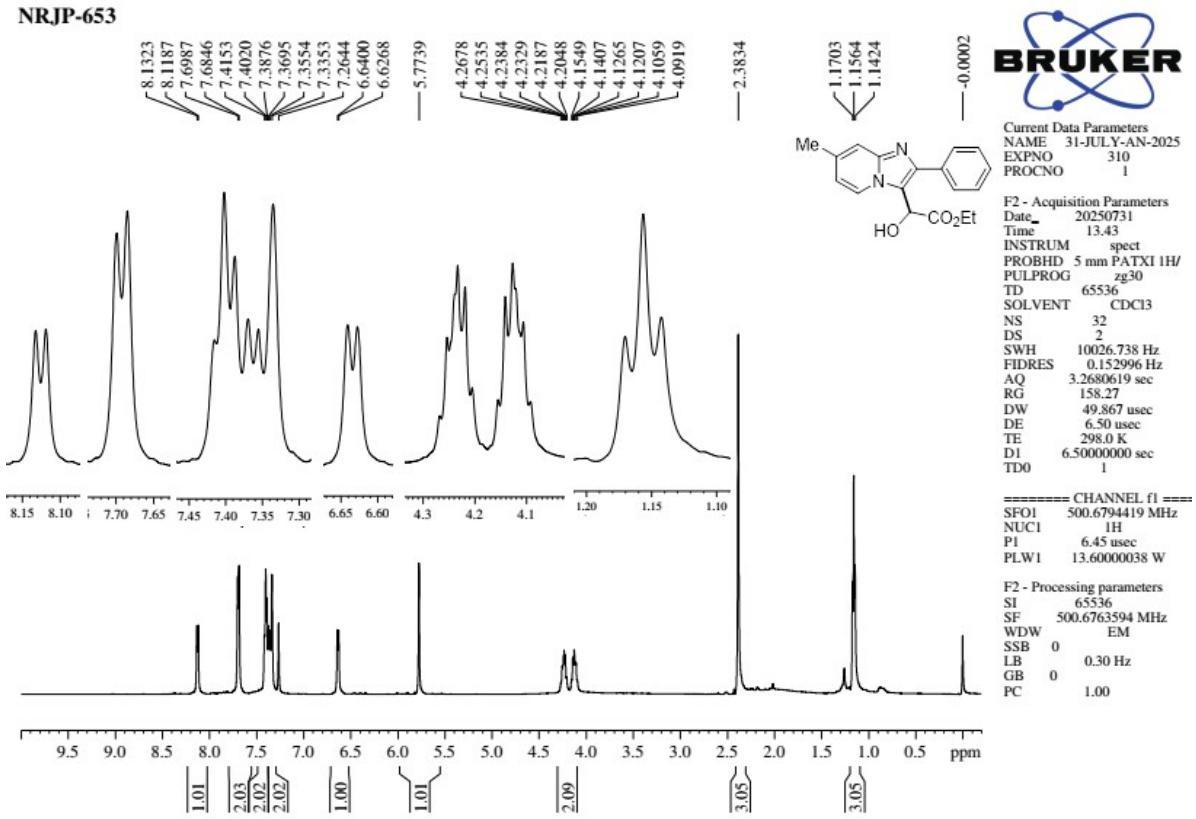


Figure S58. ^{1}H NMR Spectrum of 5aa

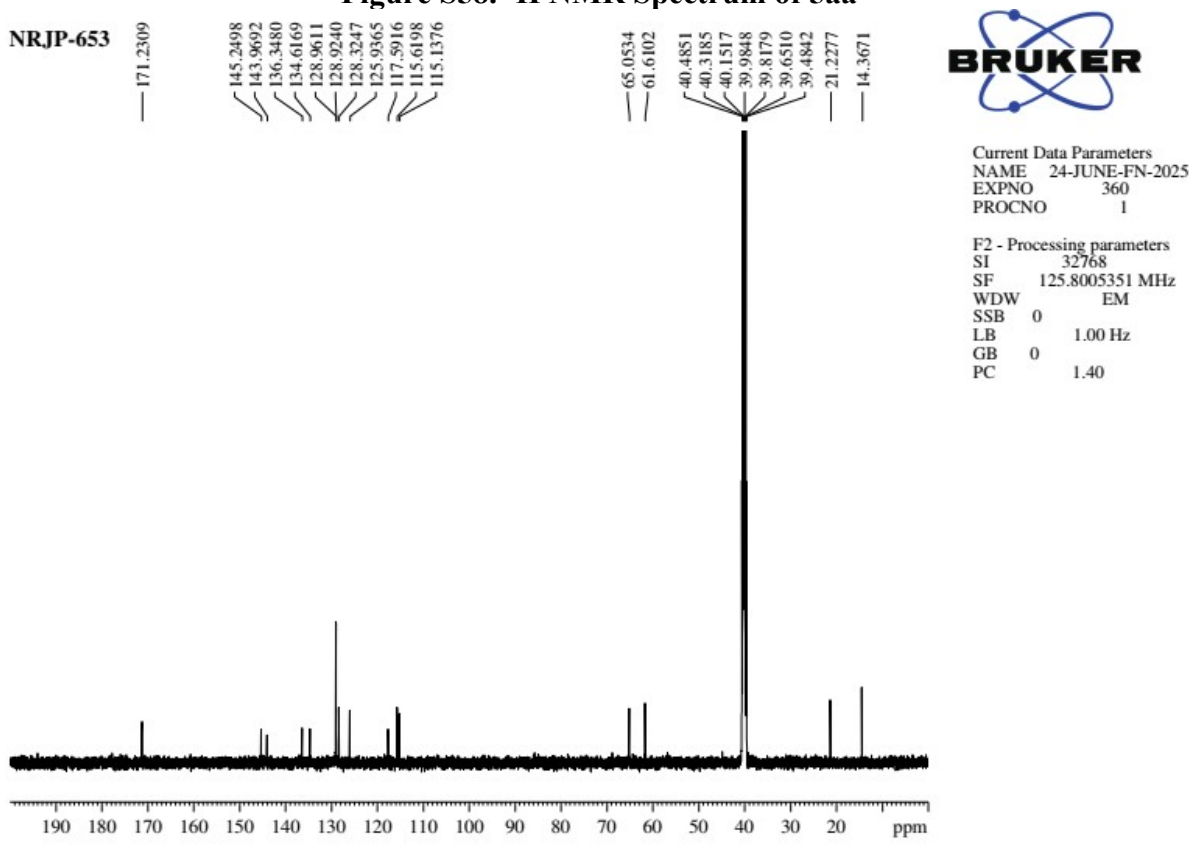


Figure S59. ^{13}C NMR Spectrum of 5aa

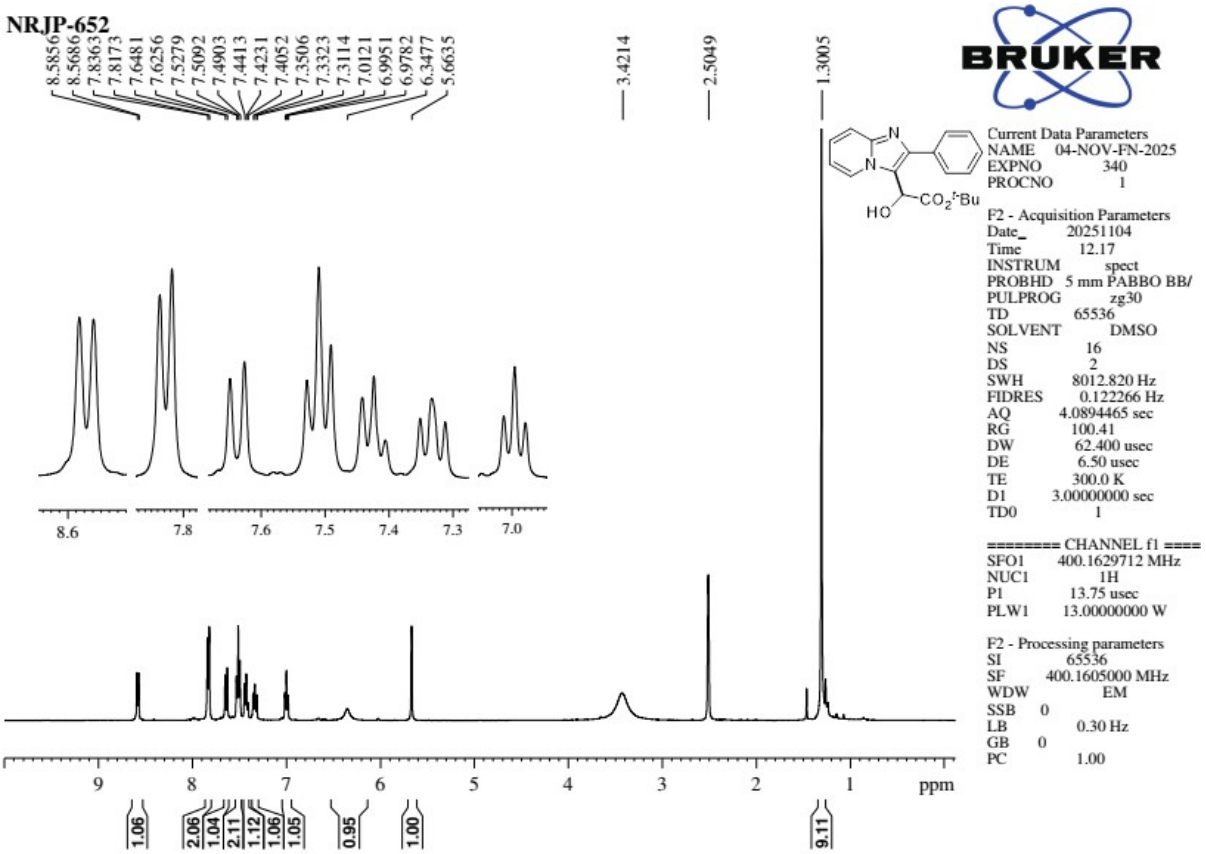


Figure S60. ^{1}H NMR Spectrum of 5ab

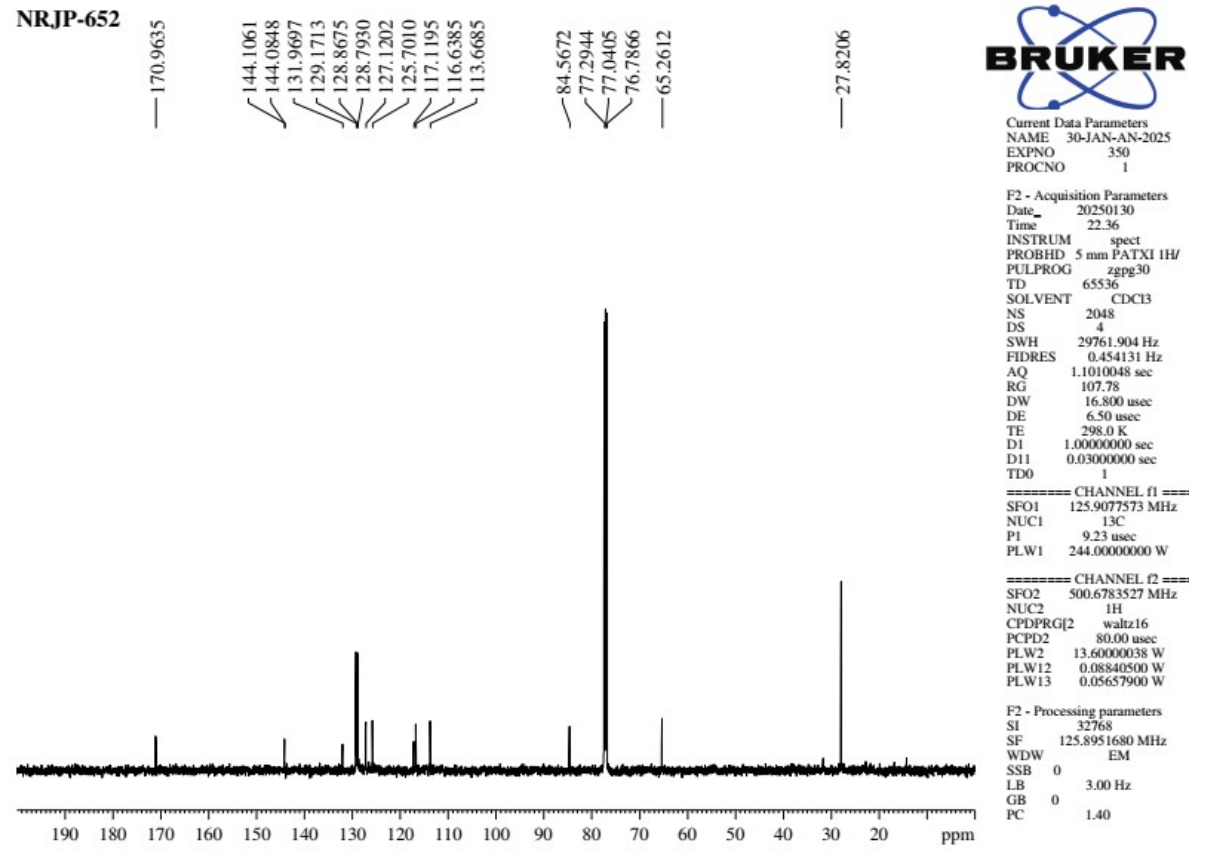


Figure S61. ^{13}C NMR Spectrum of 5ab

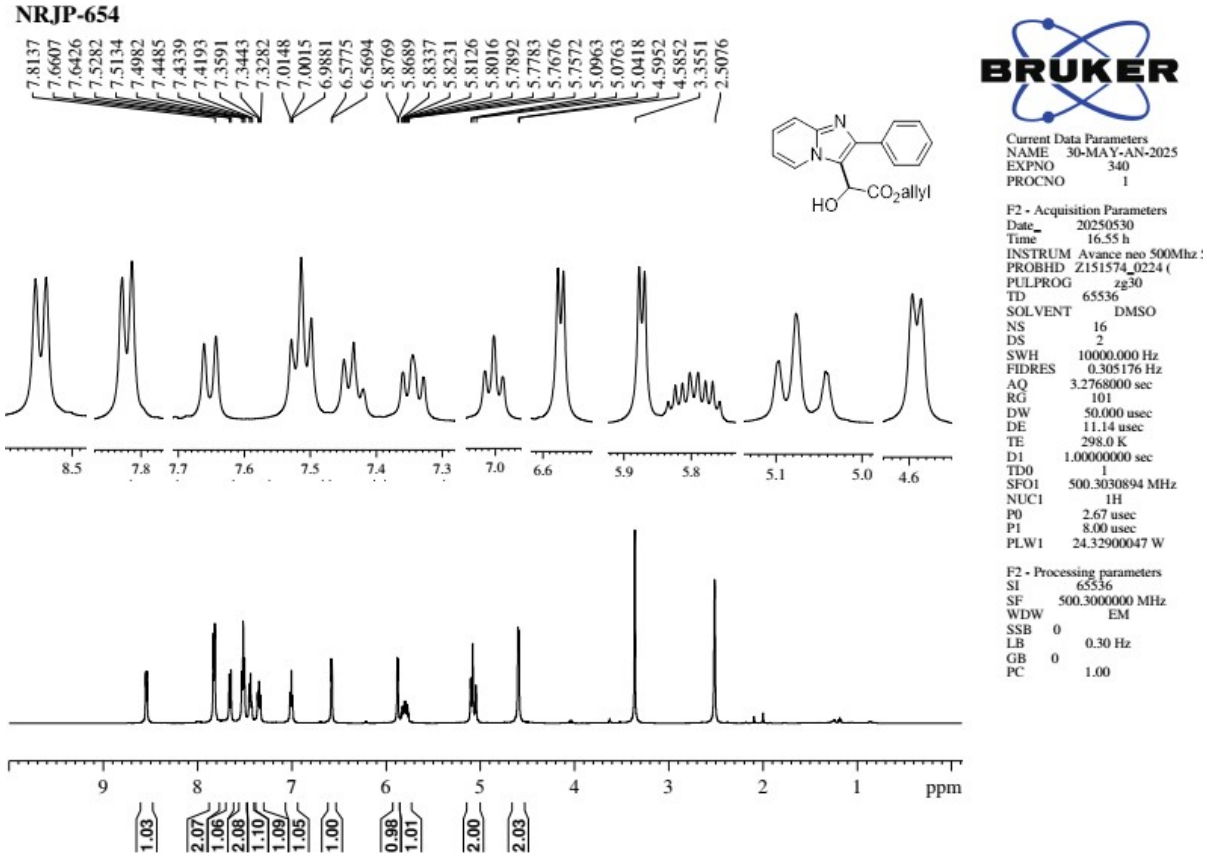


Figure S62. ^{1}H NMR Spectrum of 5ac

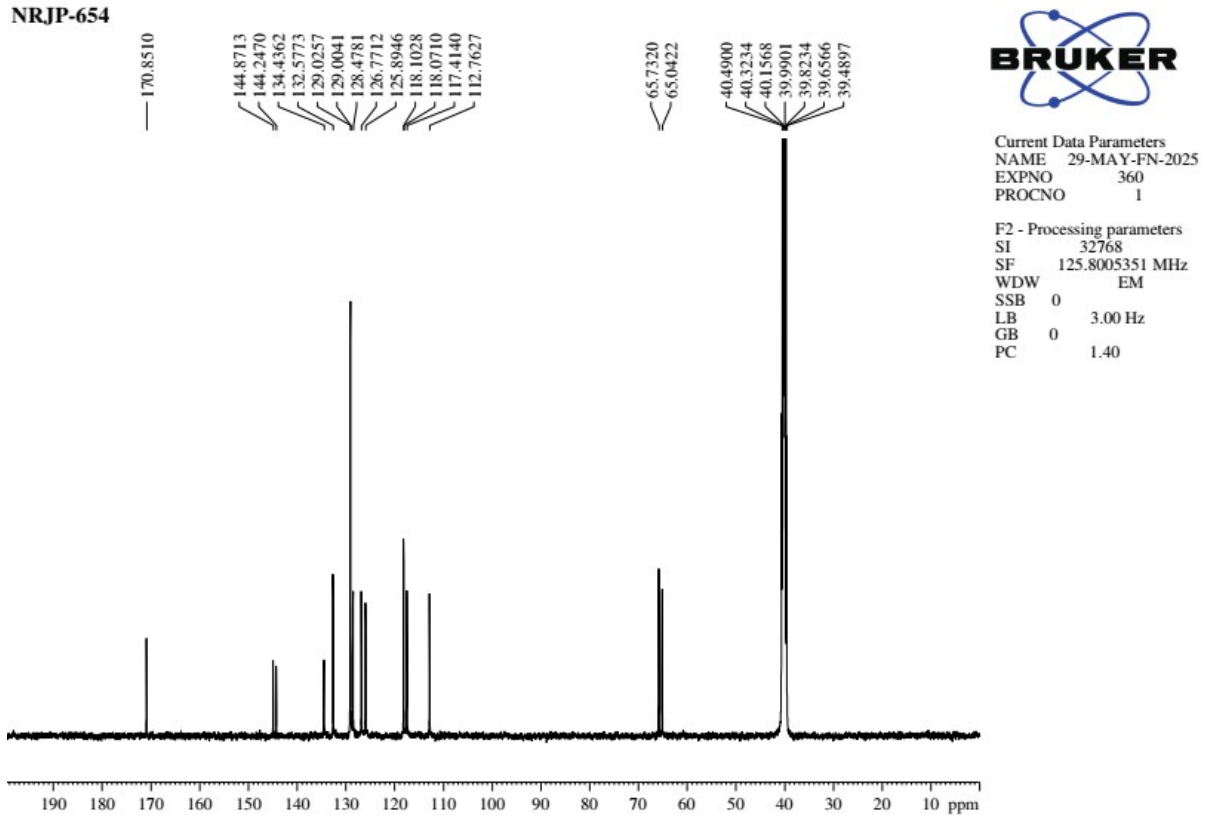


Figure S63. ^{13}C NMR Spectrum of 5ac

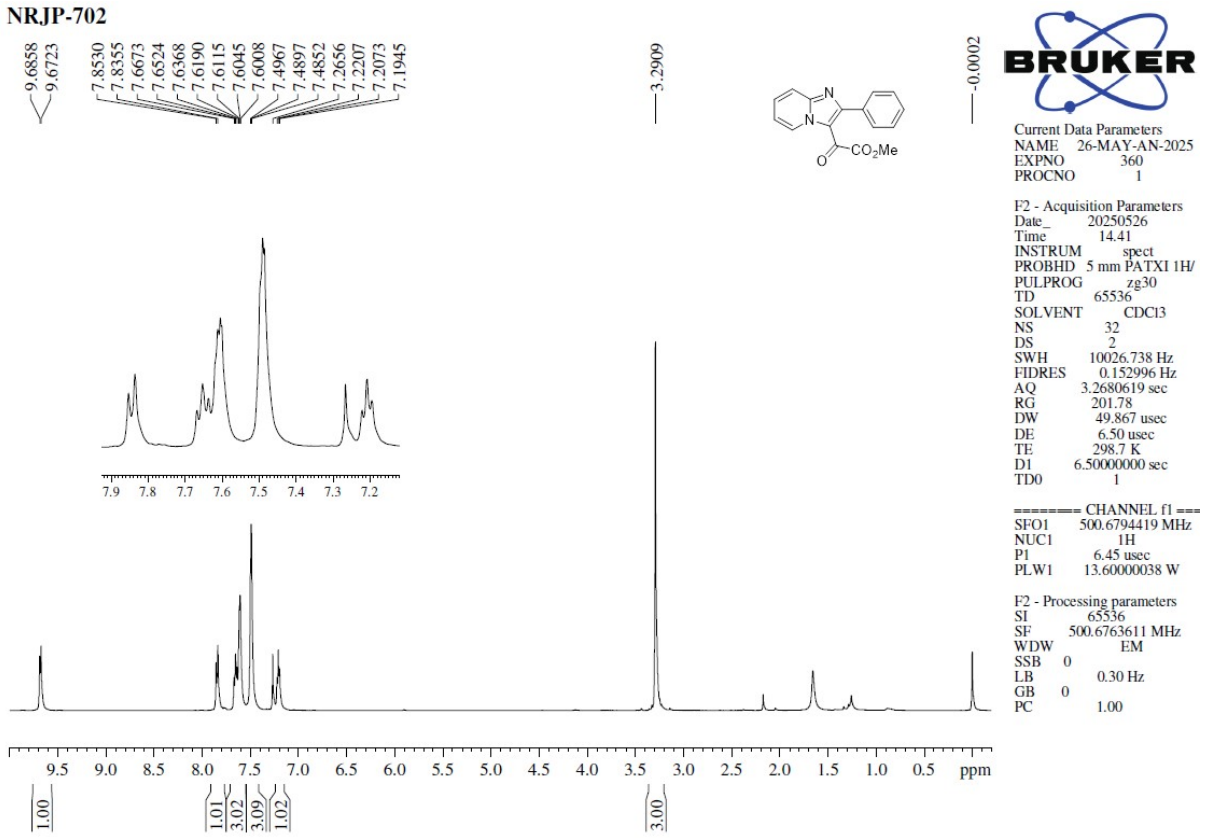


Figure S64. ^{1}H NMR Spectrum of 7

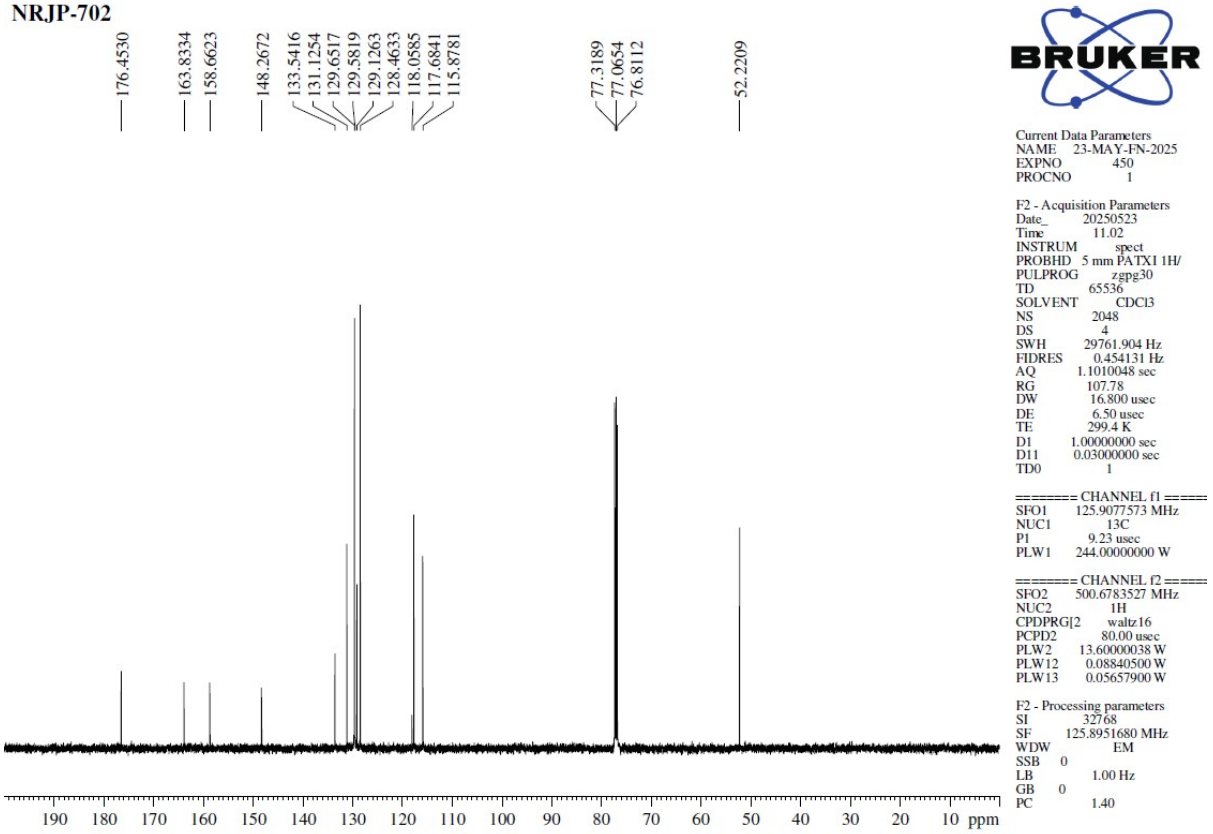
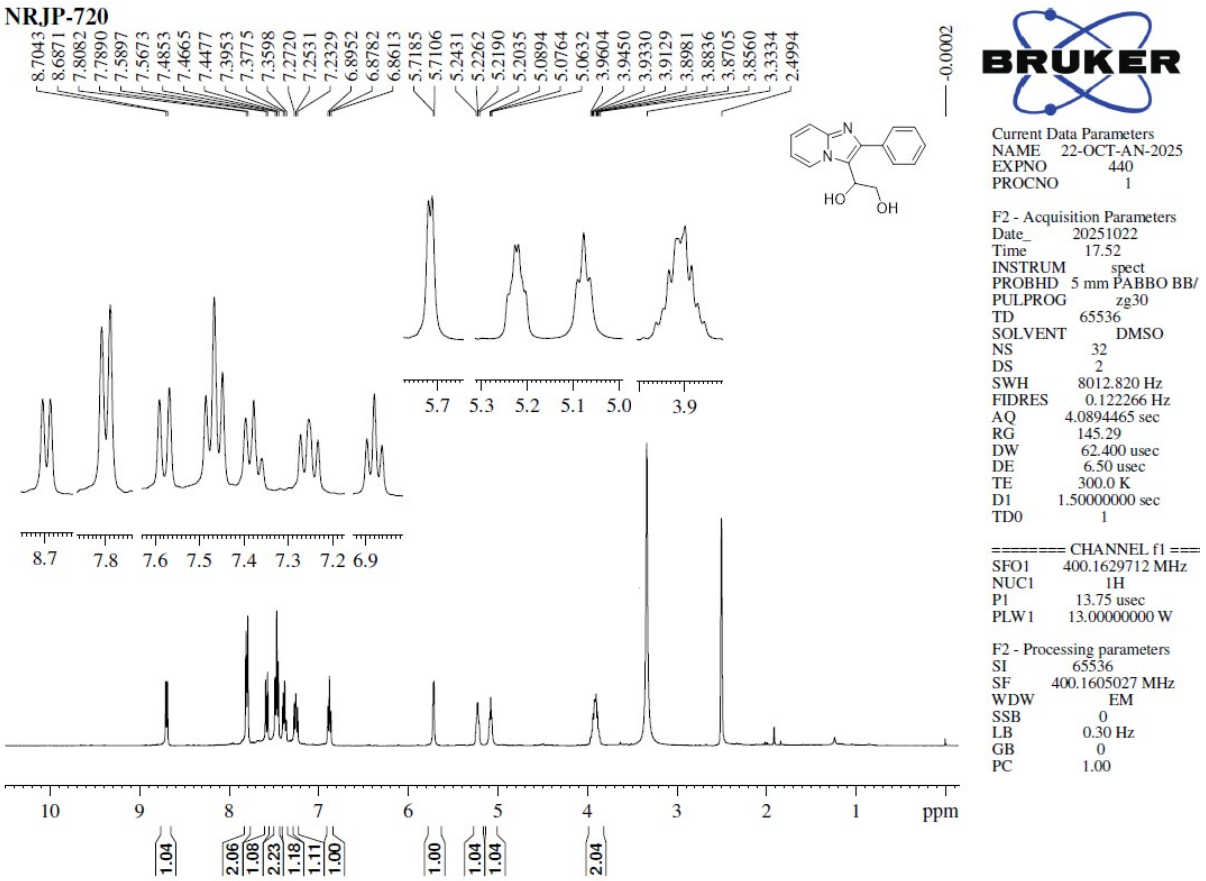


Figure S65. ^{13}C NMR Spectrum of 7



\Figure S66. ^{1}H NMR Spectrum of 8

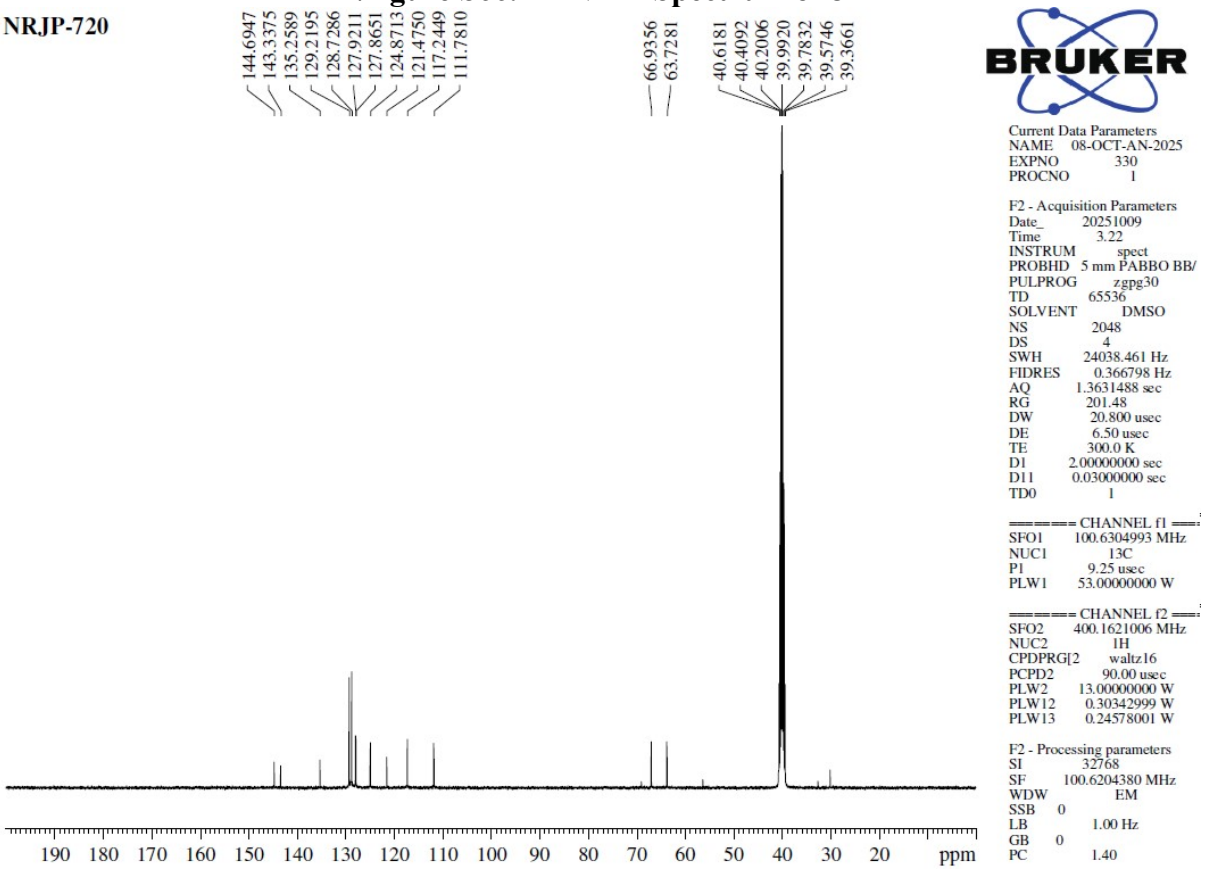


Figure S67. ^{13}C NMR Spectrum of 8

Openlynx Report SAIF, CSIR-CDRI, LUCKNOW
Sample: 447
File:HRMS25I30OCT25_COD
Description:NRJP651 T

Vial:1:D,1
Date:30-Oct-2025
Mass:

ID:HRMS25I30OCT25
Time:11:53:10
Formula:

Printed: Thu Oct 30 14:36:01 2025

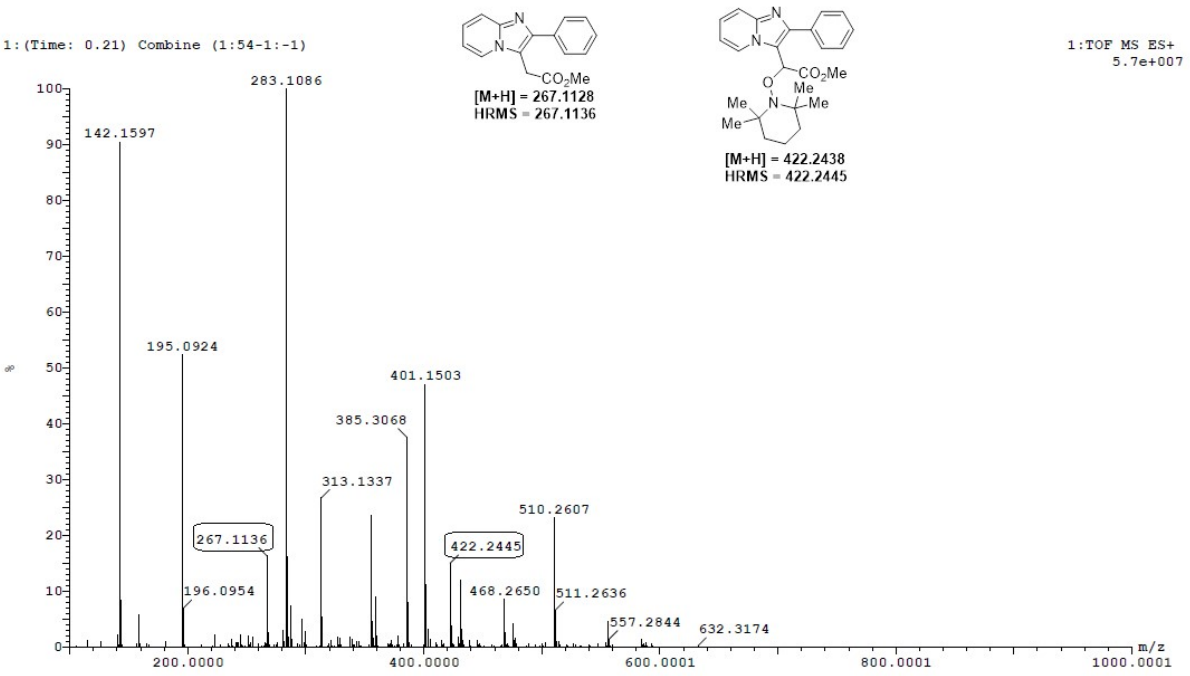


Figure S68. HRMS spectra of 6