

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]}*

^aMedicinal & Process Chemistry Division, CSIR-Central Drug Research Institute, Sector 10, Jankipuram extension, Sitapur Road, P.O. Box 173, Lucknow 226031, India.

^bAcademy 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.....	1
2. Instrumentation Details.....	1
3. General Procedures.....	1-3
4. Spectroscopic Data.....	3-13
5. References.....	13
6. Copies of ¹ H, ¹³ C, ¹⁹ F and HRMS Spectra.....	13-46

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 ^1H , ^{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 (^1H), 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).

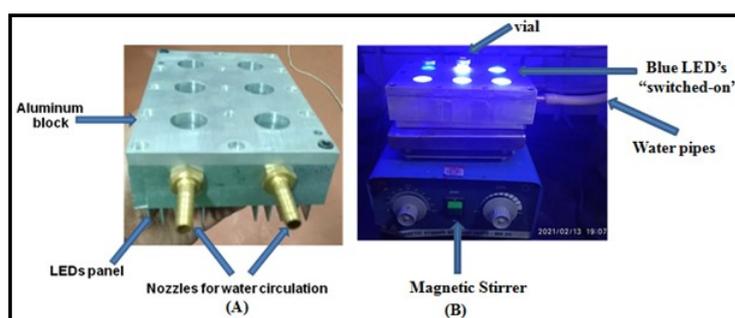


Figure S1. (A) Picture of the visible light photoreactor; (B) Experimental set-up

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 **7²**

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 LiAlH₄ (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 MgSO₄ 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 \times 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 I₂ (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 °C) 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 I₂ (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.

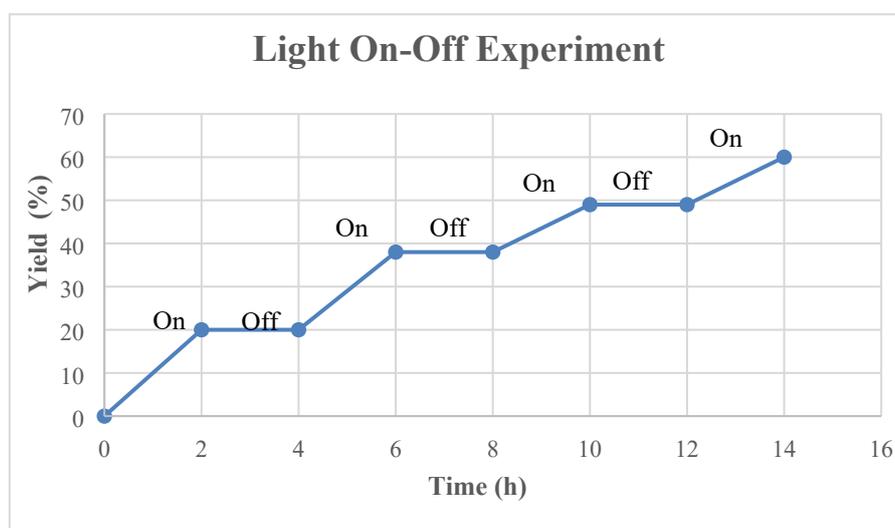
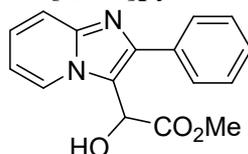


Figure S2. Light on-off experiment

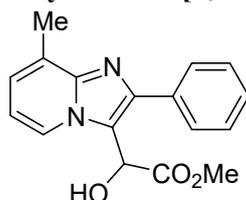
4. Spectroscopic Data

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



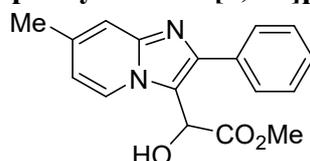
White solid; yield 88% (50 mg); R_f 0.50 (30% EtOAc/hexane); Mp 191-193 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.21 (d, J = 6.7 Hz, 1H), 7.74 (d, J = 7.2 Hz, 2H), 7.66 (d, J = 9.0 Hz, 1H), 7.46 (t, J = 7.2 Hz, 2H), 7.40 (t, J = 7.1 Hz, 1H), 7.23-7.26 (d, J = 8.3 Hz, 1H merged with solvent peak), 6.84 (t, J = 6.5 Hz, 1H), 5.85 (s, 1H), 3.74 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) 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 C₁₆H₁₅N₂O₃⁺: calcd. [M+H]⁺: 283.1077, found: 283.1085

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



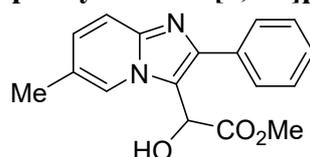
White solid; yield 66% (39 mg); R_f 0.50 (30% EtOAc/hexane); Mp 170-172 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.06 (d, $J = 6.7$ Hz, 1H), 7.69 (d, $J = 7.3$ Hz, 2H), 7.40 (t, $J = 7.3$ Hz, 2H), 7.35 (t, $J = 7.2$ Hz, 1H), 7.02 (d, $J = 6.7$ Hz, 1H), 6.73 (t, $J = 6.8$ Hz, 1H), 5.77 (s, 1H), 3.70 (s, 3H), 2.62 (s, 3H); $^{13}\text{C NMR}$ (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 $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 297.1234, found 297.1245

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



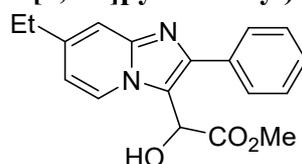
White solid; yield 55% (33 mg); R_f 0.50 (30% EtOAc/hexane); Mp 166-168 °C; $^1\text{H NMR}$ (500 MHz, $\text{DMSO}-d_6$) δ 8.35 (d, $J = 6.9$ Hz, 1H), 7.80 (d, $J = 7.6$ Hz, 2H), 7.52 (t, $J = 7.5$ Hz, 2H), 7.43 (t, $J = 7.3$ Hz, 1H), 7.15 (d, $J = 6.8$ Hz, 1H), 6.91 (t, $J = 6.9$ Hz, 1H), 6.47 (br s, 1H), 5.81 (s, 1H), 3.62 (s, 3H), 2.54 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO}-d_6$) 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 $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 297.1234, found: 297.1237

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



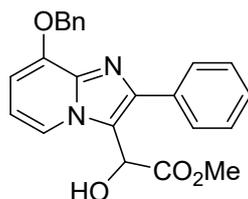
White solid; yield 75% (44 mg); R_f 0.50 (30% EtOAc/hexane); Mp 186-188 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.96 (s, 1H), 7.74 (d, $J = 7.4$ Hz, 2H), 7.57 (d, $J = 9.1$ Hz, 1H), 7.46 (t, $J = 7.3$ Hz, 2H), 7.40 (t, $J = 7.3$ Hz, 1H), 7.11 (d, $J = 9.0$ Hz, 1H), 5.83 (s, 1H), 3.75 (s, 3H), 2.35 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO}-d_6$) 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 $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 297.1234, found: 297.1237

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



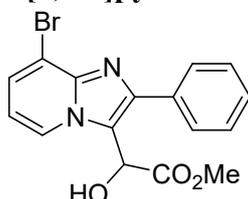
White solid; yield 72% (43 mg); R_f 0.50 (30% EtOAc/hexane); Mp 165-167 °C; $^1\text{H NMR}$ (500 MHz, DMSO- d_6) δ 8.41 (d, $J = 7.1$ Hz, 1H), 7.79 (d, $J = 7.3$ Hz, 2H), 7.51 (t, $J = 7.5$ Hz, 2H), 7.42 (t, $J = 7.2$ Hz, 2H), 6.91 (d, $J = 7.0$ Hz, 1H), 6.47 (d, $J = 4.0$ Hz, 1H), 5.80 (d, $J = 3.8$ Hz, 1H), 3.64 (s, 3H), 2.68 (q, $J = 7.5$ Hz, 2H), 1.24 (t, $J = 7.5$ Hz, 3H); $^{13}\text{C NMR}$ (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 $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 297.1234, found: 297.1243

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



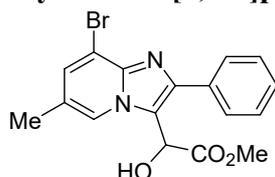
White solid; yield 68% (53 mg); R_f 0.50 (30% EtOAc/hexane); Mp 151-153 °C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 8.08 (d, $J = 6.4$ Hz, 1H), 7.77 (d, $J = 7.6$ Hz, 2H), 7.48-7.53 (m, 4H), 7.36-7.44 (m, 4H), 6.83-6.90 (m, 2H), 6.46 (d, $J = 4.0$ Hz, 1H), 5.79 (d, $J = 3.9$ Hz, 1H), 5.33 (s, 2H), 3.61 (s, 3H); $^{13}\text{C NMR}$ (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 $\text{C}_{23}\text{H}_{21}\text{N}_2\text{O}_4^+$: calcd. $[\text{M}+\text{H}]^+$: 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; $^1\text{H NMR}$ (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); $^{13}\text{C NMR}$ (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 $\text{C}_{16}\text{H}_{14}\text{BrN}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 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; $^1\text{H NMR}$ (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),

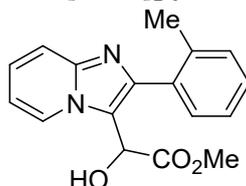
7.44 (t, $J = 7.3$ Hz, 1H), 6.55 (d, $J = 4.2$ Hz, 1H), 5.79 (d, $J = 4.2$ Hz, 1H), 3.61 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 171.42, 144.41, 141.63, 133.98, 131.07, 129.06, 128.66, 123.64, 122.63, 119.91, 110.29, 64.92, 52.93, 18.03; HRMS for $\text{C}_{17}\text{H}_{16}\text{BrN}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 375.0339, found: 375.0350

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



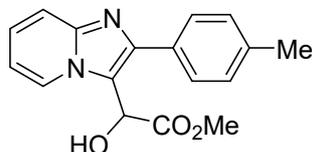
White solid; yield 55% (35 mg); R_f 0.50 (30% EtOAc/hexane); Mp 182-184 °C; ^1H NMR (500 MHz, DMSO- d_6) 8.67 (d, $J = 1.3$ Hz, 1H), 7.80 (d, $J = 7.2$ Hz, 2H), 7.73 (d, $J = 9.5$ Hz, 1H), 7.53 (t, $J = 7.5$ Hz, 2H), 7.42-7.47 (m, 2H), 6.62 (d, $J = 3.8$ Hz, 1H), 5.85 (d, $J = 3.4$ Hz, 1H), 3.64 (s, 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 $\text{C}_{16}\text{H}_{14}\text{ClN}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 317.0687, found: 317.0694

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



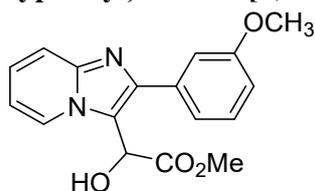
White solid; yield 89% (53 mg); R_f 0.50 (30% EtOAc/hexane); Mp 191-193 °C; ^1H NMR (500 MHz, DMSO- d_6) δ 8.48 (d, $J = 6.3$ Hz, 1H), 7.63 (d, $J = 9.1$ Hz, 1H), 7.32-7.36 (m, 4H), 7.26-7.29 (m, 1H), 7.01 (t, $J = 6.7$ Hz, 1H), 6.40 (d, $J = 3.6$ Hz, 1H), 5.43 (s, 1H), 3.53 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (125 MHz, DMSO- d_6) 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 $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 297.1234, found: 297.1239

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



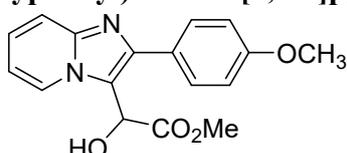
White solid; yield 89% (53 mg); R_f 0.50 (30% EtOAc/hexane); Mp 171-172 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.23 (d, $J = 6.9$ Hz, 1H), 7.61 (d, $J = 9.1$ Hz, 1H), 7.58 (d, $J = 7.7$ Hz, 2H), 7.21-7.24 (m, 3H), 6.82 (t, $J = 6.8$ Hz, 1H), 5.84 (s, 1H), 3.72 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) 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 $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 297.1234, found: 297.1242

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



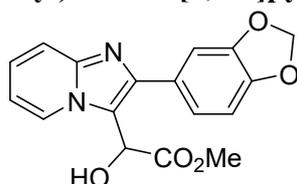
White solid; yield 88% (55 mg); R_f 0.50 (30% EtOAc/hexane); Mp 161-162 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.28 (d, $J = 6.7$ Hz, 1H), 7.54 (d, $J = 9.0$ Hz, 1H), 7.24-7.27 (m, 1H merged with solvent peak), 7.17-7.22 (m, 3H), 6.88 (d, $J = 7.7$ Hz, 1H), 6.79 (t, $J = 6.7$ Hz, 1H), 5.85 (s, 1H), 3.82 (s, 3H), 3.71 (s, 3H); $^{13}\text{C NMR}$ (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 $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_4^+$: calcd. $[\text{M}+\text{H}]^+$: 313.1183, found: 313.1196

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



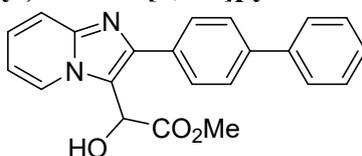
White solid; yield 85% (53 mg); R_f 0.50 (30% EtOAc/hexane); Mp 158-160 °C; $^1\text{H NMR}$ (500 MHz, $\text{DMSO-}d_6$) δ 8.50 (d, $J = 6.9$ Hz, 1H), 7.74 (d, $J = 8.7$ Hz, 2H), 7.62 (d, $J = 9.0$ Hz, 1H), 7.30-7.34 (m, 1H), 7.08 (d, $J = 8.7$ Hz, 2H), 6.97-7.00 (m, 1H), 6.48 (d, $J = 4.1$ Hz, 1H), 5.81 (d, $J = 4.0$ Hz, 1H), 3.83 (s, 3H), 3.64 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO-}d_6$) 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 $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_4^+$: calcd. $[\text{M}+\text{H}]^+$: 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)



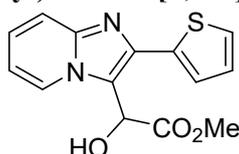
White solid; yield 78% (51 mg); R_f 0.50 (30% EtOAc/hexane); Mp 156-158 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.20 (d, $J = 6.8$ Hz, 1H), 7.60 (d, $J = 9.0$ Hz, 1H), 7.17-7.26 (m, 3H), 6.86 (d, $J = 7.9$ Hz, 1H), 6.81 (t, $J = 6.6$ Hz, 1H), 6.01 (s, 2H), 5.83 (s, 1H), 3.77 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO-}d_6$) 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 $\text{C}_{17}\text{H}_{15}\text{N}_2\text{O}_5^+$: calcd. $[\text{M}+\text{H}]^+$: 327.0975, found: 327.0986

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



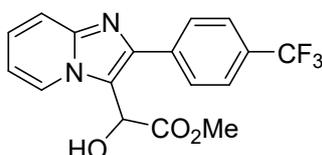
White solid; yield 88% (63 mg); R_f 0.50 (30% EtOAc/hexane); Mp 175-176 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.29 (d, $J = 6.8$ Hz, 1H), 7.70 (d, $J = 8.1$ Hz, 2H), 7.56-7.60 (m, 5H), 7.45 (t, $J = 7.5$ Hz, 2H), 7.36 (t, $J = 7.3$ Hz, 1H), 7.16 (t, $J = 7.7$ Hz, 1H), 6.77 (t, $J = 6.6$ Hz, 1H), 5.89 (s, 1H), 3.72 (s, 3H); $^{13}\text{C NMR}$ (100 MHz, $\text{DMSO}-d_6$) 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 $\text{C}_{22}\text{H}_{19}\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 359.1390, found: 359.1399

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



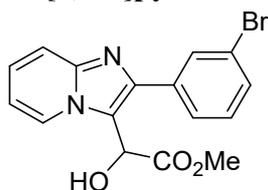
White solid; yield 65% (37 mg); R_f 0.50 (30% EtOAc/hexane); Mp 182-183 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.24 (d, $J = 6.8$ Hz, 1H), 7.63 (d, $J = 9.0$ Hz, 1H), 7.42 (d, $J = 3.4$ Hz, 2H), 7.22-7.26 (d, $J = 8.4$ Hz, 1H), 7.13 (t, $J = 3.8$ Hz, 1H), 6.82 (t, $J = 6.7$ Hz, 1H), 6.03 (s, 1H), 3.77 (s, 3H); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO}-d_6$) 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 $\text{C}_{14}\text{H}_{13}\text{N}_2\text{O}_3\text{S}^+$: calcd. $[\text{M}+\text{H}]^+$: 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; $^1\text{H NMR}$ (500 MHz, $\text{DMSO}-d_6$) 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); $^{13}\text{C NMR}$ (125 MHz, $\text{DMSO}-d_6$) δ 170.56, 144.07, 141.53, 137.53, 128.64, 123.87 (q, $^1J_{\text{C-F}} = 270.4$ Hz), 127.69 (q, $^2J_{\text{C-F}} = 31.6$ Hz), 125.77, 125.43, 125.01 (q appearing as d, $^3J_{\text{C-F}} = 3.2$ Hz), 118.23, 116.68, 112.29, 63.80, 51.99; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -64.30; **HRMS** for $\text{C}_{17}\text{H}_{14}\text{F}_3\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 351.0951, found: 351.0959

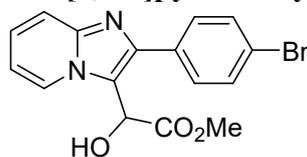
Methyl 2-(2-(3-bromophenyl)imidazo[1,2-a]pyridin-3-yl)-2-hydroxyacetate (5r)



White solid; yield 79% (57 mg); R_f 0.50 (30% EtOAc/hexane); Mp 185-186 °C; $^1\text{H NMR}$ (500 MHz, $\text{DMSO}-d_6$) 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, $J = 2.7$

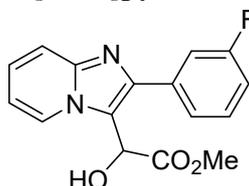
Hz, 1H), 5.85 (s, 1H), 3.62 (s, 3H); ^{13}C NMR (125 MHz, DMSO- d_6) δ 171.50, 144.89, 142.44, 136.74, 131.43, 131.25, 131.21, 127.84, 126.67, 126.26, 122.36, 118.69, 117.54, 113.14, 64.75, 52.92; HRMS for $\text{C}_{16}\text{H}_{14}\text{BrN}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 361.0182, found: 361.0190

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



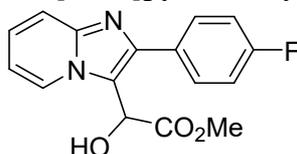
White solid; yield 82% (59 mg); R_f 0.50 (30% EtOAc/hexane); Mp 171-172 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.23 (d, $J = 6.7$ Hz, 1H), 7.55 (d, $J = 9.1$ Hz, 1H), 7.47 (s, 4H), 7.24 (t, $J = 7.9$ Hz, 1H), 6.83 (t, $J = 6.7$ Hz, 1H), 5.75 (s, 1H), 3.73 (s, 3H); ^{13}C NMR (125 MHz, CD_3OD) δ 172.80, 146.62, 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 $\text{C}_{16}\text{H}_{14}\text{BrN}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 361.0182, found: 361.0194

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



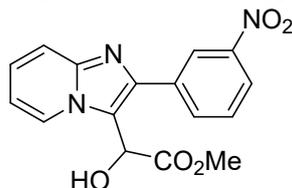
White solid; yield 70% (42 mg); R_f 0.50 (30% EtOAc/hexane); Mp 194-196 °C; ^1H NMR (500 MHz, DMSO- d_6) δ 8.52 (d, $J = 6.9$ Hz, 1H), 7.65-7.67 (m, 2H), 7.54-7.61 (m, 2H), 7.35-7.38 (m, 1H), 7.26-7.30 (m, 1H), 7.02-7.04 (m, 1H), 6.56 (d, $J = 4.0$ Hz, 1H), 5.88 (d, $J = 3.6$ Hz, 1H), 3.63 (s, 3H); ^{13}C NMR (125 MHz, DMSO- d_6) δ 171.55, 162.71 (d, $^1J_{\text{C-F}} = 241.7$ Hz), 144.84, 142.74, 136.79 (d, $^3J_{\text{C-F}} = 8.1$ Hz), 131.10 (d, $^3J_{\text{C-F}} = 8.3$ Hz), 126.67, 126.21, 125.00, 118.63, 117.53, 115.48 (d, $^2J_{\text{C-F}} = 22.4$ Hz), 115.26 (d, $^2J_{\text{C-F}} = 20.9$ Hz), 113.10, 64.73, 52.91; ^{19}F NMR (376 MHz, CDCl_3) δ -113.46; HRMS for $\text{C}_{16}\text{H}_{14}\text{FN}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 301.0983, found: 301.0990

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



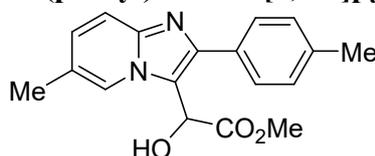
White solid; yield 70% (42 mg); R_f 0.50 (30% EtOAc/hexane); Mp 174-176 °C; ^1H NMR (500 MHz, DMSO- d_6) δ 8.50 (d, $J = 6.9$ Hz, 1H), 7.82-7.85 (m, 2H), 7.65 (d, $J = 9.0$ Hz, 1H), 7.35 (t, $J = 8.8$ Hz, 3H), 7.00-7.03 (m, 1H), 6.51 (s, 1H), 5.81 (s, 1H), 3.63 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD) δ 172.80, 164.55 (d, $^1J_{\text{C-F}} = 245.5$ Hz), 146.33, 144.50, 132.20 (d, $^3J_{\text{C-F}} = 8.2$ Hz), 130.62 (d, $^4J_{\text{C-F}} = 3.2$ Hz), 128.12, 127.67, 119.07, 117.27, 116.62 (d, $^2J_{\text{C-F}} = 21.8$ Hz), 114.33, 66.08, 53.30; ^{19}F NMR (376 MHz, CDCl_3) δ -113.47; HRMS for $\text{C}_{16}\text{H}_{14}\text{FN}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 301.0983, found: 301.0994

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



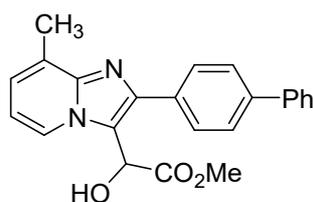
White solid; yield 58% (38 mg); R_f 0.50 (30% EtOAc/hexane); Mp 165-166 °C; $^1\text{H NMR}$ (500 MHz, DMSO- d_6) δ 8.68 (t, J = 1.8 Hz, 1H), 8.57 (d, J = 6.9 Hz, 1H), 8.26-8.29 (m, 2H), 7.81 (t, J = 8.0 Hz, 1H), 7.70 (d, J = 9.0 Hz, 1H), 7.40 (t, J = 7.5 Hz, 1H), 7.06 (t, J = 6.5 Hz, 1H), 6.64 (d, J = 3.4 Hz, 1H), 5.94 (d, J = 3.0 Hz, 1H), 3.64 (s, 3H); $^{13}\text{C NMR}$ (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 $\text{C}_{16}\text{H}_{14}\text{N}_3\text{O}_5^+$: calcd. $[\text{M}+\text{H}]^+$: 328.0928, found: 328.0935

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



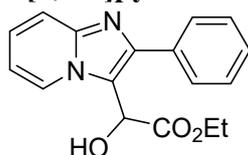
White solid; yield 79% (49 mg); R_f 0.50 (30% EtOAc/hexane); Mp 182-184 °C; $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.00 (s, 1H), 7.52 (d, J = 6.8 Hz, 2H), 7.46 (d, J = 8.9 Hz, 1H), 7.17 (d, J = 6.7 Hz, 2H), 7.03 (d, J = 8.6 Hz, 1H), 5.80 (s, 1H), 3.71 (s, 3H), 2.37 (s, 3H), 2.31 (s, 3H); $^{13}\text{C NMR}$ (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 $\text{C}_{18}\text{H}_{19}\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 311.1390, found: 311.1401

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



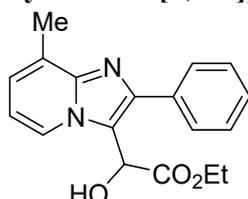
White solid; yield 76% (57 mg); R_f 0.50 (30% EtOAc/hexane); Mp 141-143 °C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 8.35 (d, J = 6.6 Hz, 1H), 7.90 (d, J = 7.8 Hz, 2H), 7.82 (d, J = 7.8 Hz, 2H), 7.76 (d, J = 7.3 Hz, 2H), 7.51 (t, J = 7.2 Hz, 2H), 7.40 (t, J = 6.9 Hz, 1H), 7.16 (d, J = 6.0 Hz, 1H), 6.91 (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); $^{13}\text{C NMR}$ (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 $\text{C}_{23}\text{H}_{21}\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 373.1547, found: 373.1551

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



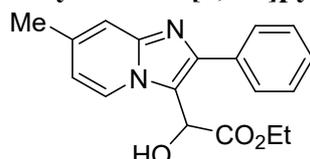
White solid; yield 85% (50 mg); R_f 0.50 (30% EtOAc/hexane); Mp 171-173 °C; **¹H NMR** (500 MHz, CDCl₃) δ 8.25 (d, J = 6.4 Hz, 1H), 7.72 (d, J = 6.8 Hz, 2H), 7.62 (d, J = 8.8 Hz, 1H), 7.37-7.42 (m, 3H), 7.23 (t, J = 7.5 Hz, 1H), 6.82 (t, J = 6.2 Hz, 1H), 5.81 (s, 1H), 4.08-4.28 (m, 2H), 1.15 (t, J = 6.8 Hz, 3H); **¹³C NMR** (125 MHz, CDCl₃) 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 C₁₇H₁₇N₂O₃⁺: 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



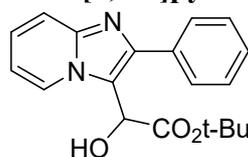
White solid; yield 73% (45 mg); R_f 0.50 (30% EtOAc/hexane); Mp 165-167 °C; **¹H NMR** (400 MHz, CDCl₃) δ 8.09 (d, J = 6.8 Hz, 1H), 7.73 (d, J = 7.0 Hz, 2H), 7.41 (t, J = 7.3 Hz, 2H), 7.34 (t, J = 7.3 Hz, 1H), 7.04 (d, J = 6.8 Hz, 1H), 6.75 (t, J = 6.9 Hz, 1H), 5.75 (s, 1H), 4.07-4.26 (m, 2H), 2.64 (s, 3H), 1.15 (t, J = 7.1 Hz, 3H); **¹³C NMR** (125 MHz, CDCl₃) 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 C₁₉H₁₉N₂O₃⁺: calcd. [M+H]⁺: 311.1390, found: 311.1405

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



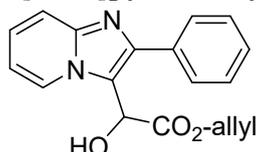
White solid; yield 68% (42 mg); R_f 0.50 (30% EtOAc/hexane); Mp 161-163 °C; **¹H NMR** (500 MHz, CDCl₃) δ 8.13 (d, J = 6.8 Hz, 1H), 7.69 (d, J = 7.1 Hz, 2H), 7.34-7.42 (m, 4H), 6.63 (d, J = 6.6 Hz, 1H), 5.77 (s, 1H), 4.09-4.27 (m, 2H), 2.38 (s, 3H), 1.16 (t, J = 7.0 Hz, 3H); **¹³C NMR** (125 MHz, DMSO-*d*₆) 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 C₁₈H₁₉N₂O₃⁺: calcd. [M+H]⁺: 311.1390, found: 311.1400

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



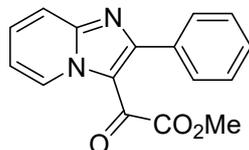
White solid; yield 80% (52 mg); R_f 0.50 (30% EtOAc/hexane); Mp 154-155 °C; $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 8.58 (d, J = 6.8 Hz, 1H), 7.83 (d, J = 7.6 Hz, 2H), 7.64 (d, J = 9.0 Hz, 1H), 7.51 (t, J = 7.5 Hz, 2H), 7.42 (t, J = 7.3 Hz, 1H), 7.33 (t, J = 7.3 Hz, 1H), 7.00 (t, J = 6.8 Hz, 1H), 6.35 (br s, 1H), 5.66 (s, 1H), 1.30 (s, 9H); $^{13}\text{C NMR}$ (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 $\text{C}_{19}\text{H}_{21}\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 325.1547, found: 325.1560

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



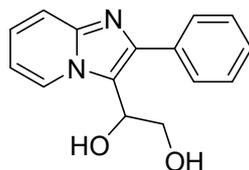
White solid; yield 84% (52 mg); R_f 0.50 (30% EtOAc/hexane); Mp 113-115 °C; $^1\text{H NMR}$ (500 MHz, DMSO- d_6) δ 8.54 (d, J = 6.9 Hz, 1H), 7.82 (d, J = 7.3 Hz, 2H), 7.65 (d, J = 9.0 Hz, 1H), 7.51 (t, J = 7.5 Hz, 2H), 7.43 (t, J = 7.3 Hz, 1H), 7.34 (t, J = 7.7 Hz, 1H), 7.00 (t, J = 6.7 Hz, 1H), 6.57 (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); $^{13}\text{C NMR}$ (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 $\text{C}_{18}\text{H}_{17}\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 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; $^1\text{H NMR}$ (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); $^{13}\text{C NMR}$ (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 $\text{C}_{16}\text{H}_{13}\text{N}_2\text{O}_3^+$: calcd. $[\text{M}+\text{H}]^+$: 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; $^1\text{H NMR}$ (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, $\text{DMSO-}d_6$) 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 $\text{C}_{15}\text{H}_{15}\text{N}_2\text{O}_2^+$: calcd. $[\text{M}+\text{H}]^+$: 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 ^1H , ^{13}C , ^{19}F and HRMS Spectra

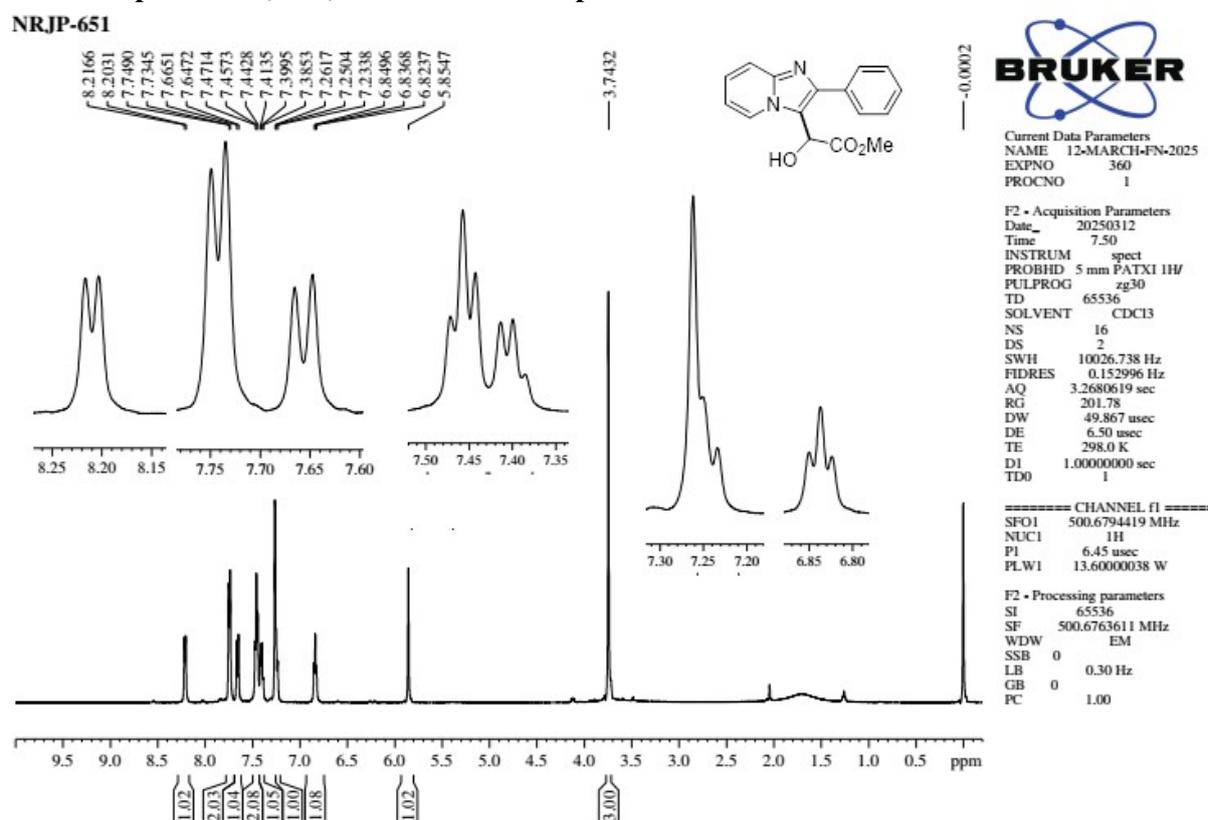
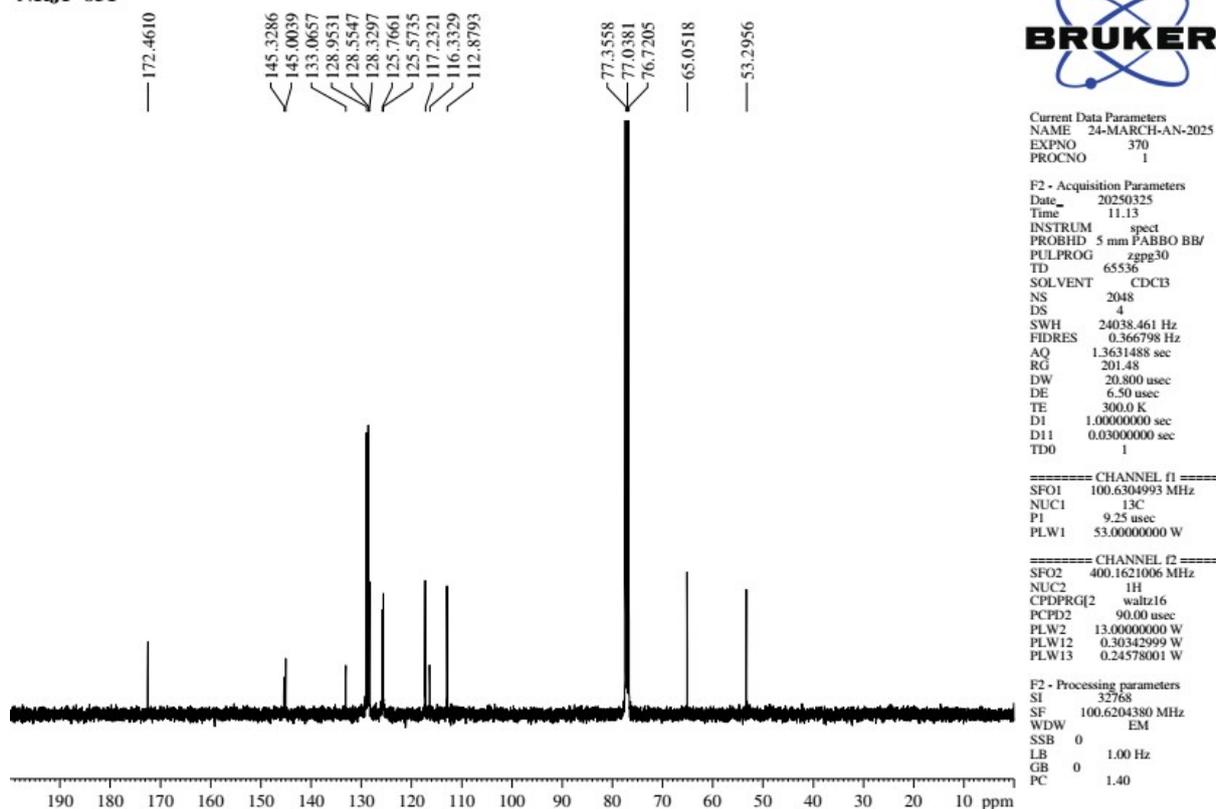
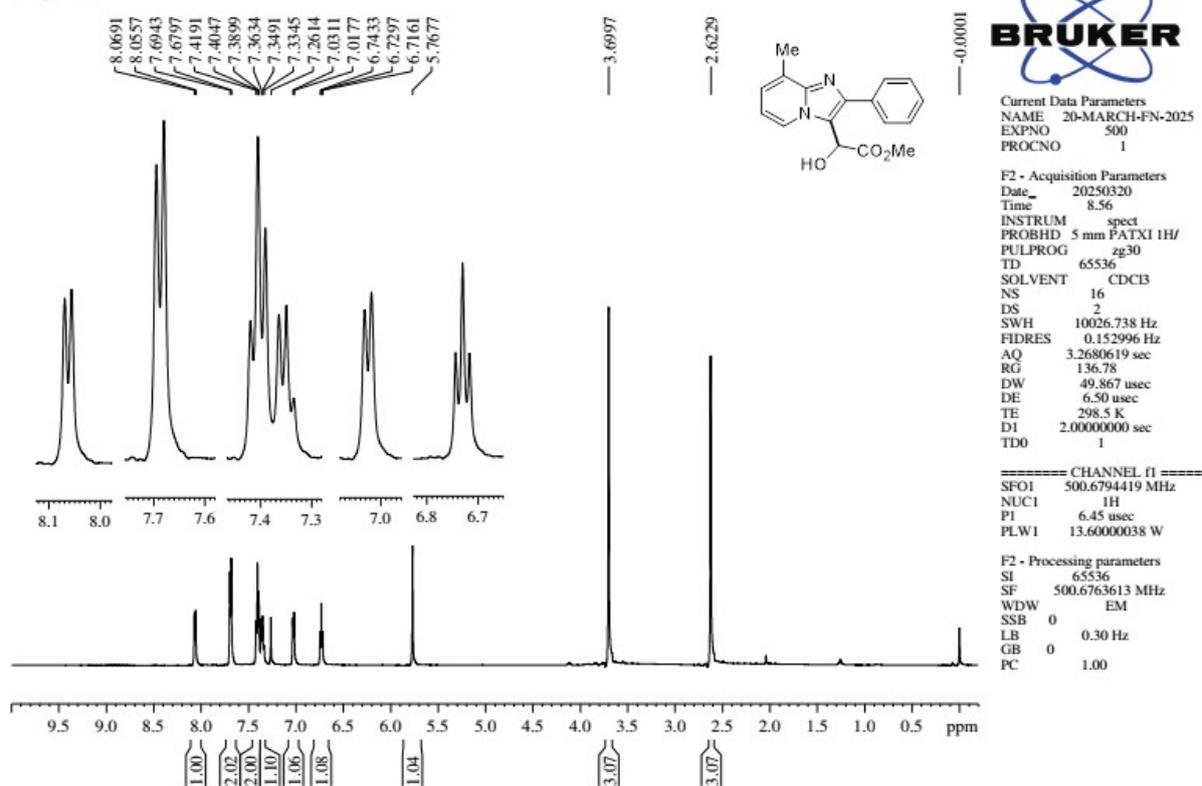


Figure S3. ^1H NMR Spectrum of 5a

NRJP-651

Figure S4. ¹³C NMR Spectrum of 5a

NRJP-669

Figure S5. ¹H NMR Spectrum of 5b

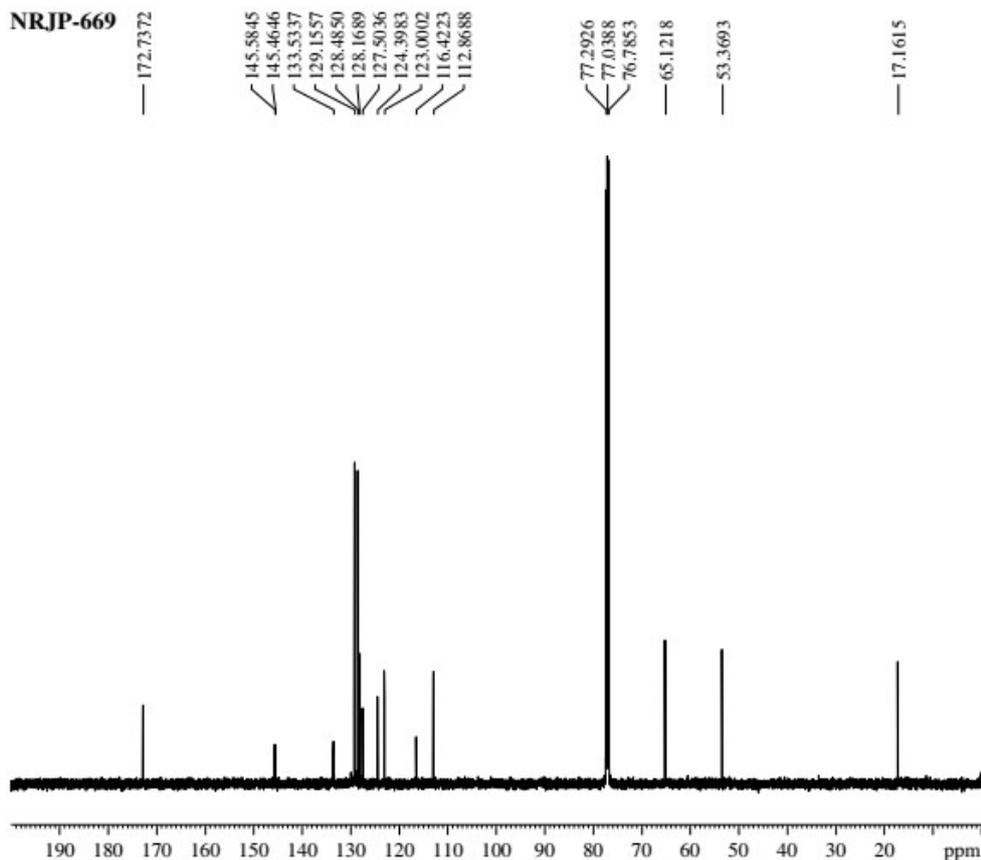


Figure S6. ¹³C NMR Spectrum of 5b

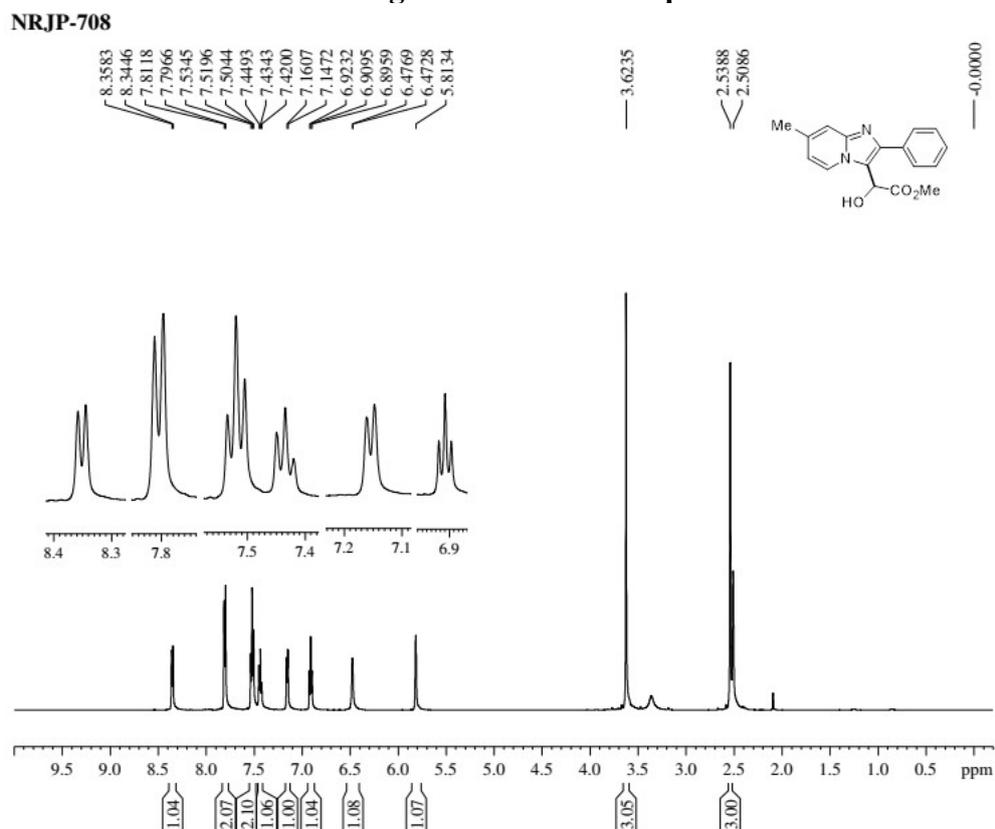


Figure S7. ¹H NMR Spectrum of 5c

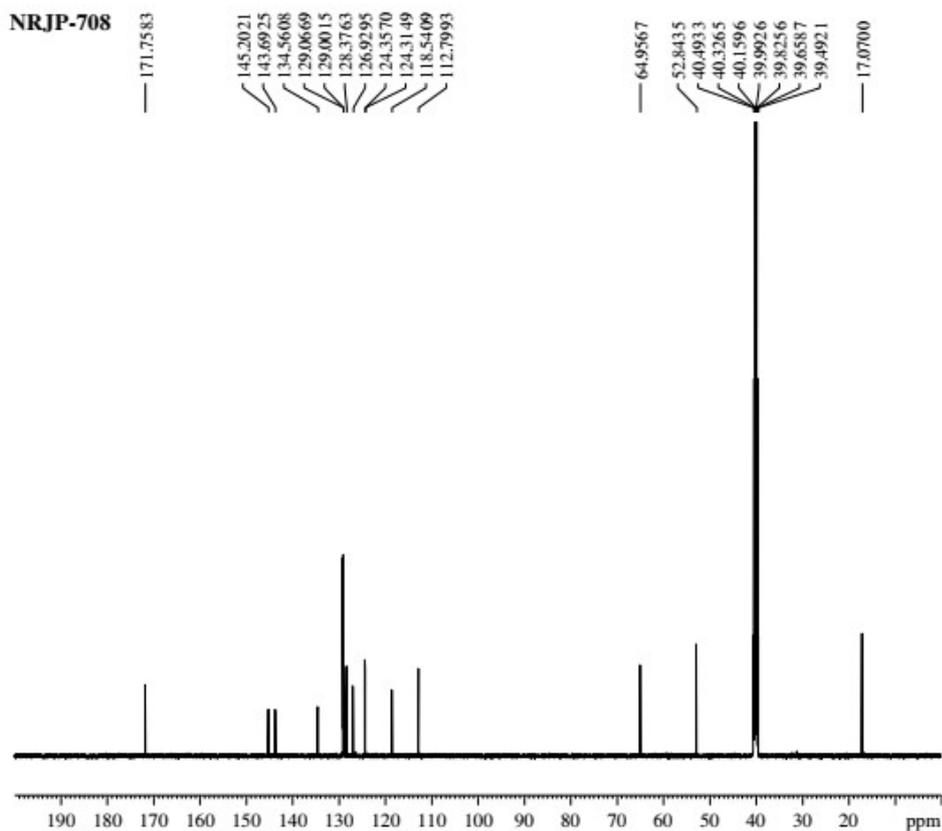


Figure S8. ¹³C NMR Spectrum of 5c

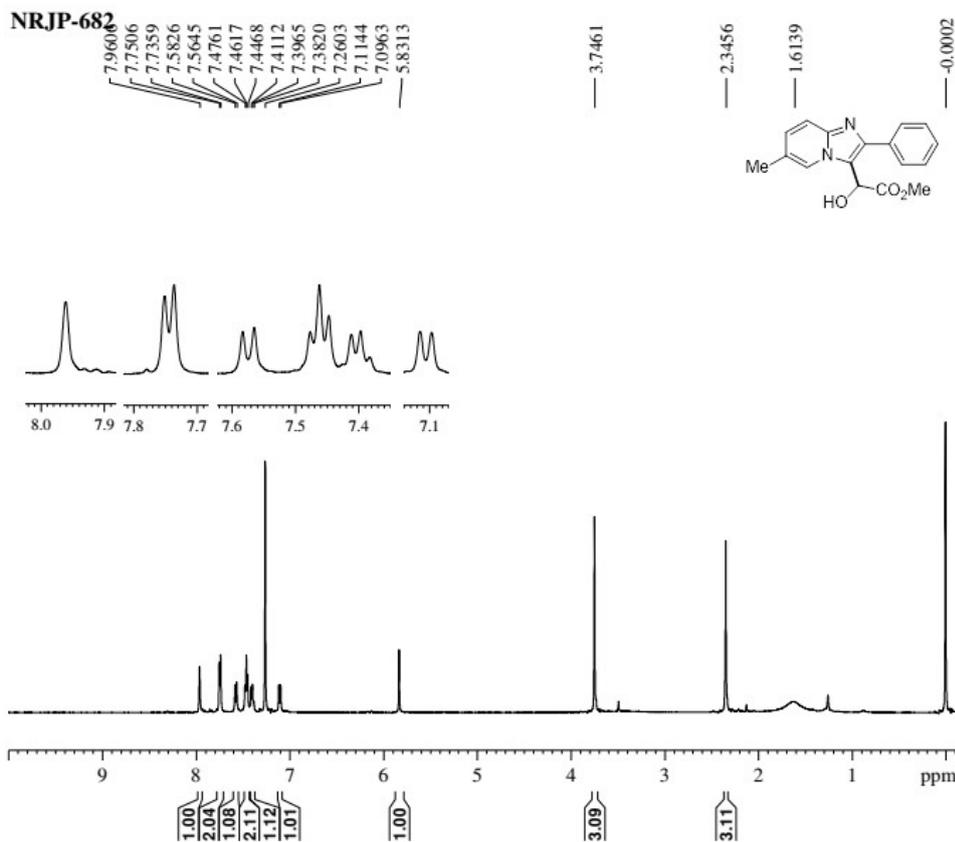


Figure S9. ¹H NMR Spectrum of 5d



Current Data Parameters
NAME 23-JUNE-FN-2025
EXPNO 340
PROCNO 1

F2 - Processing parameters
SI 32768
SF 125.8005351 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



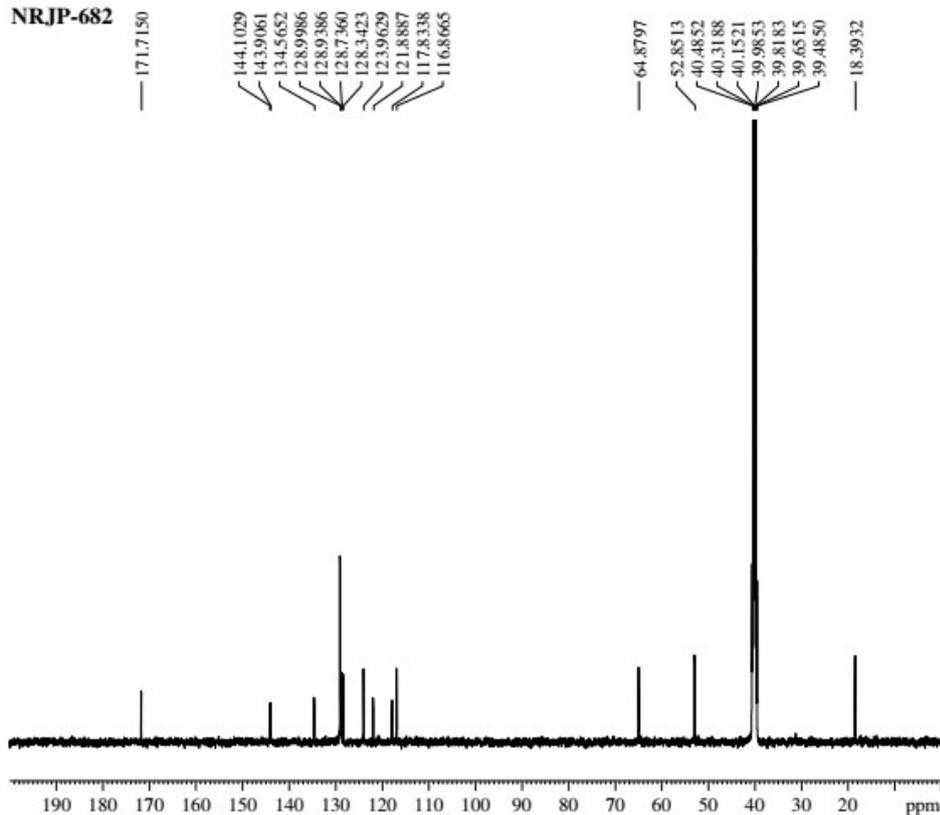
Current Data Parameters
NAME 28-MAY-AN-2025
EXPNO 500
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250528
Time 14.38
INSTRUM spect
PROBHD 5 mm PATX1 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 32
DS 2
SWH 10026.738 Hz
FIDRES 0.152996 Hz
AQ 3.2680619 sec
RG 201.78
DW 49.867 usec
DE 6.50 usec
TE 299.4 K
D1 6.50000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.6794419 MHz
NUC1 1H
P1 6.45 usec
PLW1 13.60000038 W

F2 - Processing parameters
SI 65536
SF 500.6763629 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRJP-682

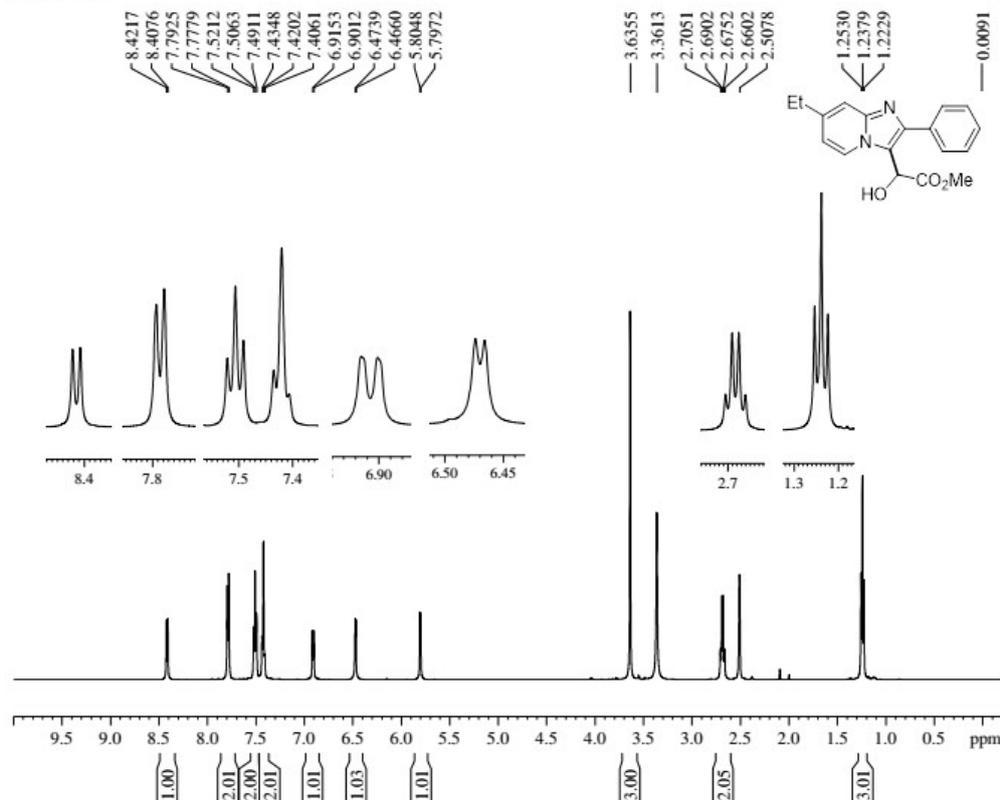


Current Data Parameters
 NAME 26-MAY-FN-2025
 EXPNO 330
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 125.8005351 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Figure S10. ¹³C NMR Spectrum of 5d

NRJP-704



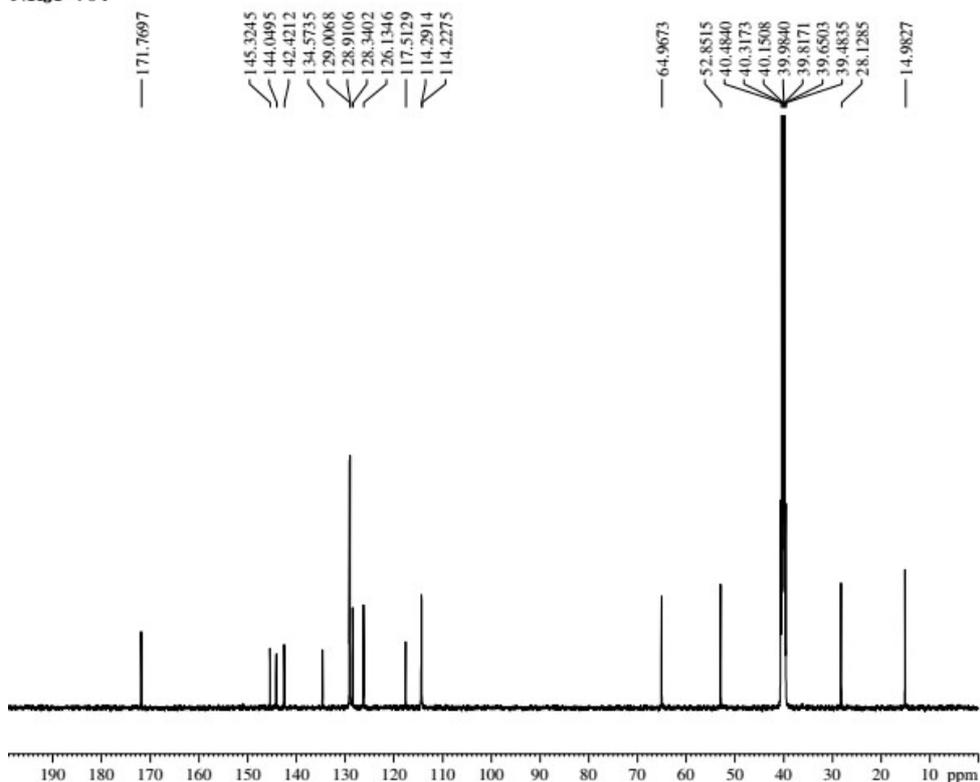
Current Data Parameters
 NAME 11-JUNE-AN-2025
 EXPNO 330
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250611
 Time 17.11 h
 INSTRUM Avance neo 500Mhz 5
 PROBHD Z151574_0224 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2768000 sec
 RG 101
 DW 50.000 usec
 DE 11.14 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1
 SFO1 500.300894 MHz
 NUC1 1H
 PO 2.67 usec
 P1 8.00 usec
 PLW1 24.32900047 W

F2 - Processing parameters
 SI 65536
 SF 500.300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

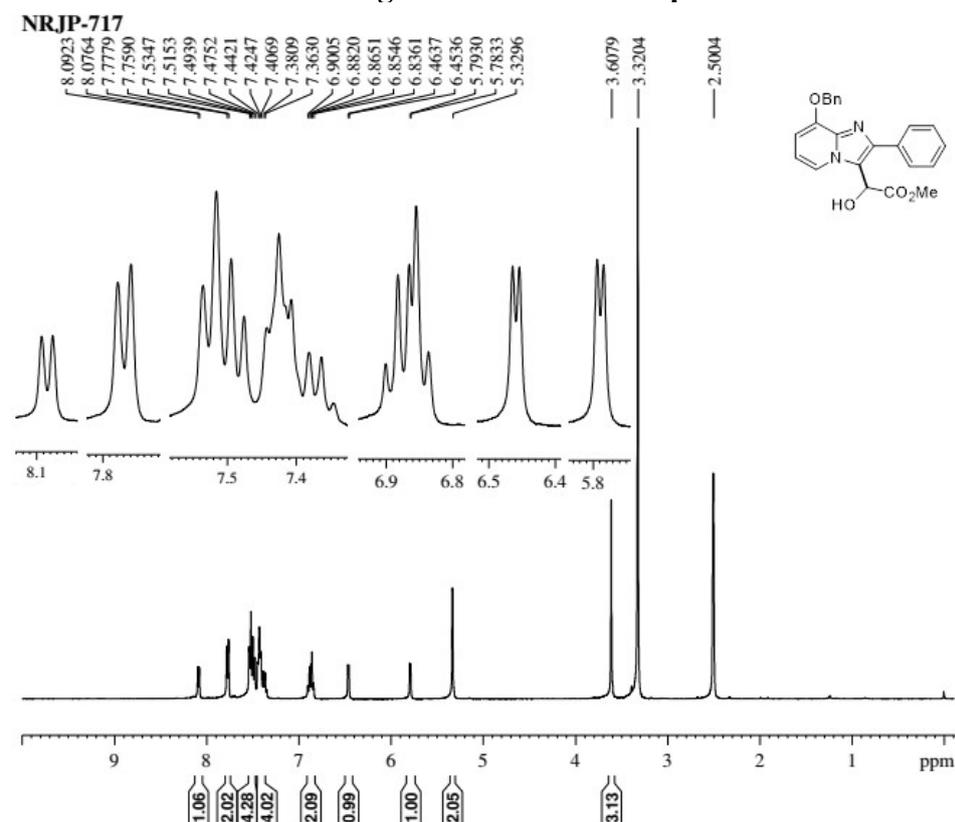
Figure S11. ¹H NMR Spectrum of 5e

NRJP-704



Current Data Parameters
 NAME 10-JUNE-FN-2025
 EXPNO 390
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 125.8005351 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Figure S12. ¹³C NMR Spectrum of 5e

Current Data Parameters
 NAME 25-SEP-AN-2025
 EXPNO 350
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250926
 Time 13.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 16
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 159.22
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 6.50000000 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 400.1605023 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S13. ¹H NMR Spectrum of 5f

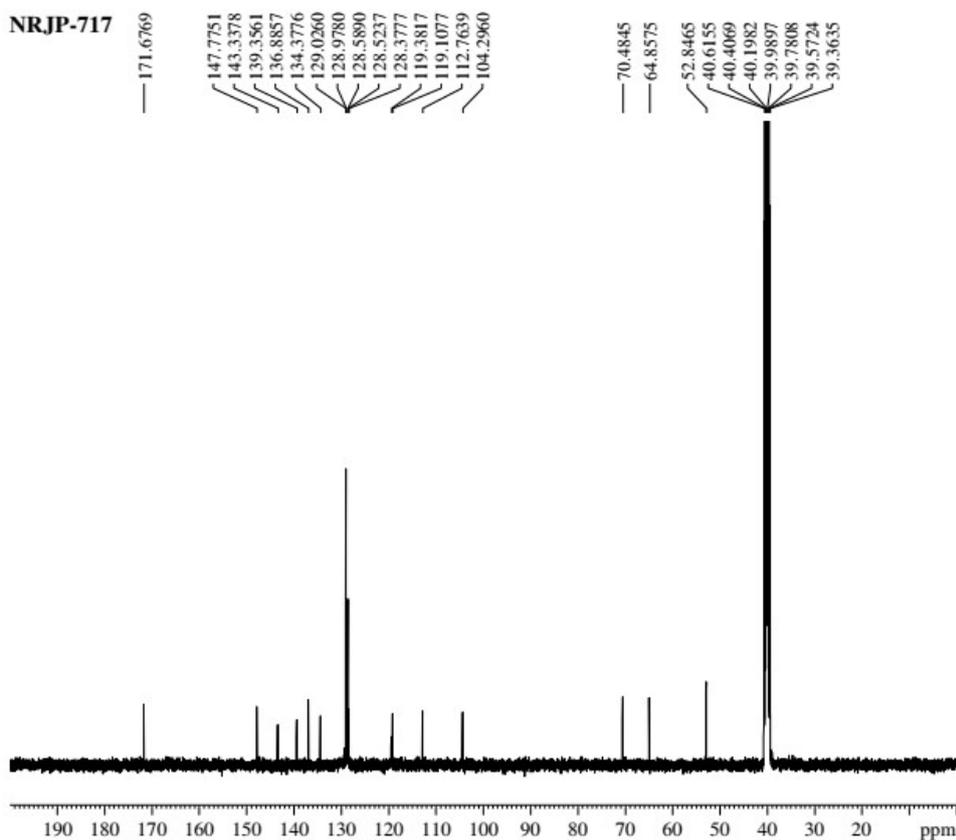


Figure S14. ¹³C NMR Spectrum of 5f

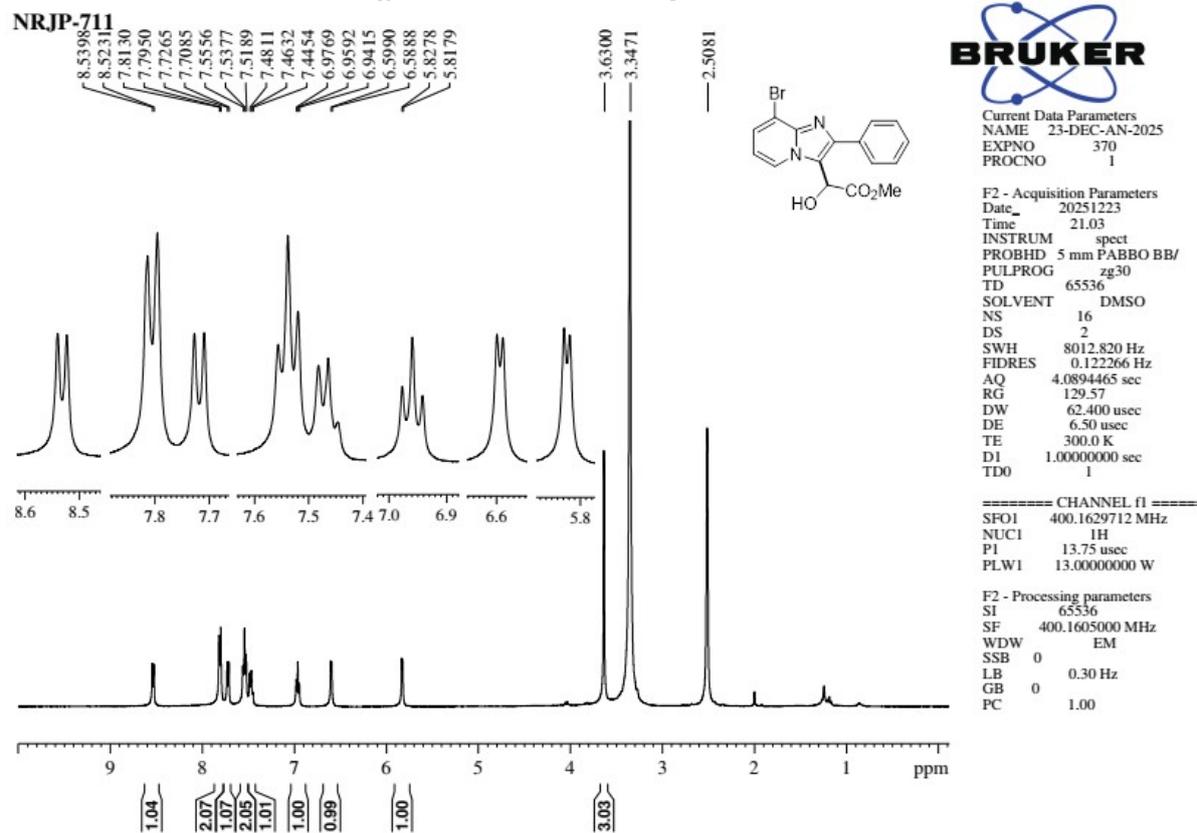
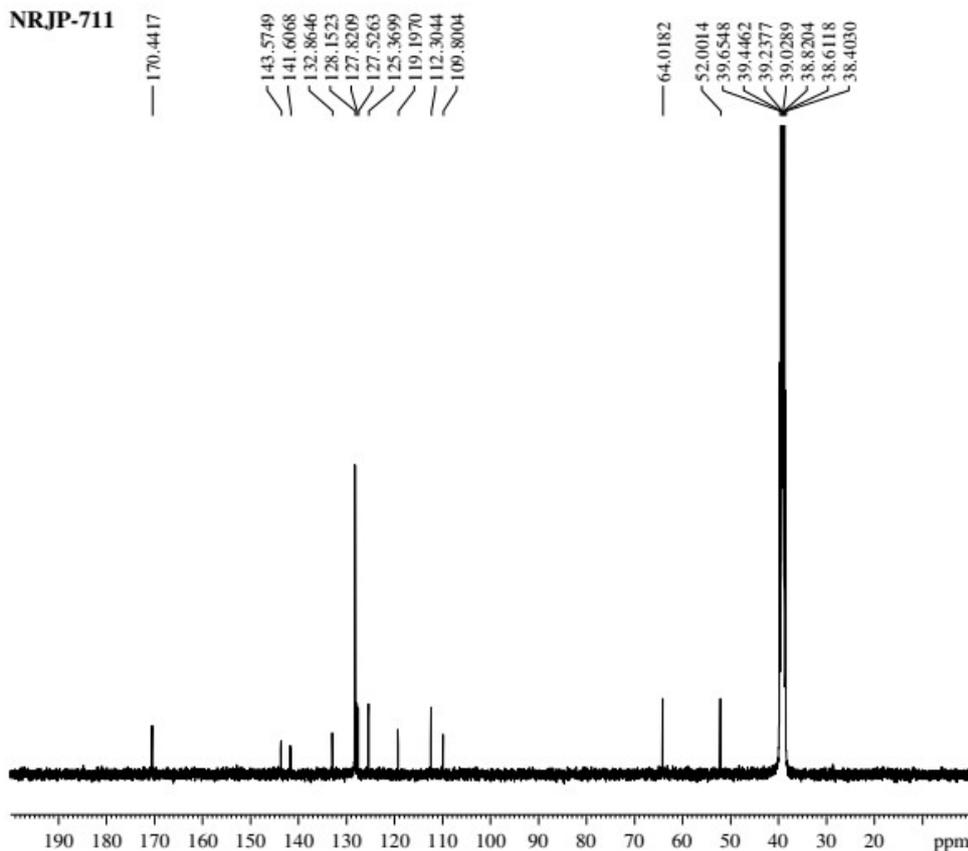


Figure S15. ¹H NMR Spectrum of 5g

NRJP-711



Current Data Parameters
 NAME 19-DEC-AN-2025
 EXPNO 340
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251220
 Time 4.02
 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

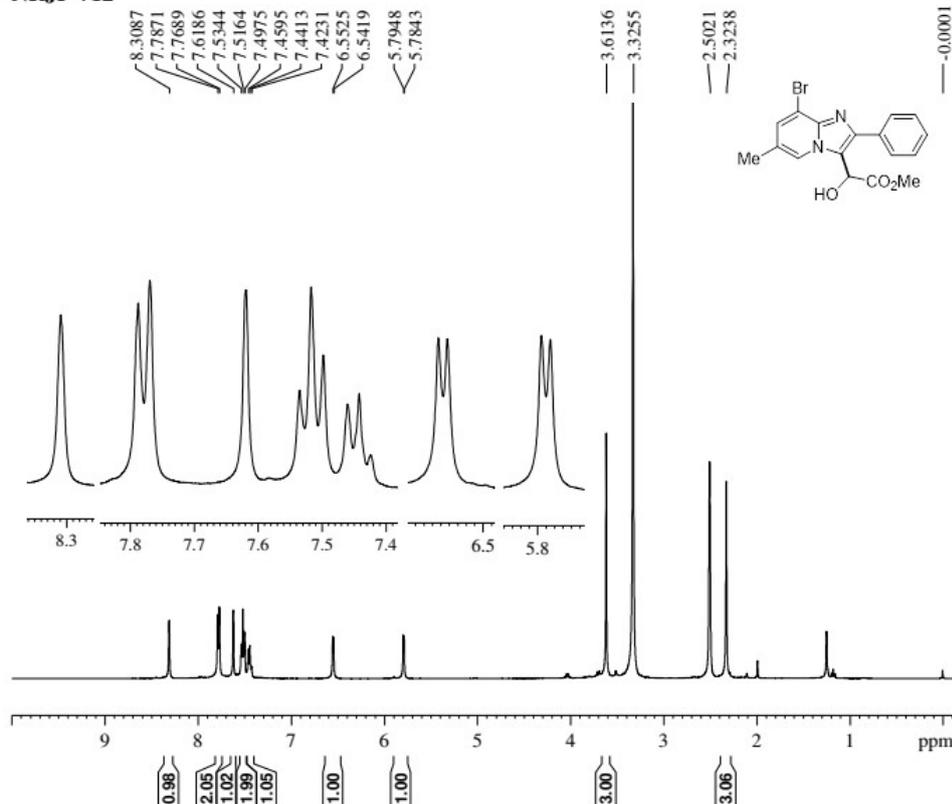
===== CHANNEL f1 =====
 SFO1 100.6304993 MHz
 NUC1 13C
 P1 9.25 usec
 PLW1 53.00000000 W

===== CHANNEL f2 =====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.00000000 W
 PLW12 0.30342999 W
 PLW13 0.24578001 W

F2 - Processing parameters
 SI 32768
 SF 100.6205353 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure S16. ¹³C NMR Spectrum of 5g

NRJP-712



Current Data Parameters
 NAME 19-SEP-FN-2025
 EXPNO 350
 PROCNO 1

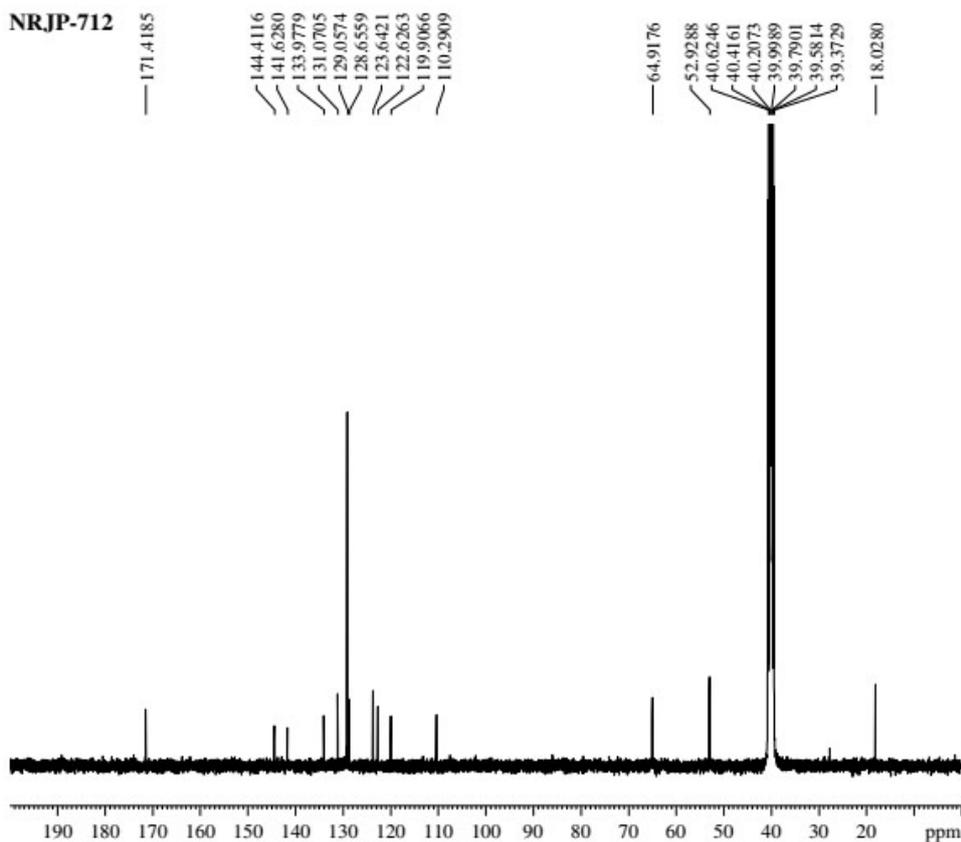
F2 - Acquisition Parameters
 Date_ 20250919
 Time 17.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 8
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 145.29
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 4.00000000 sec
 TD0 1

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

F2 - Processing parameters
 SI 65536
 SF 400.1605012 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S17. ¹H NMR Spectrum of 5h

NRJP-712



Current Data Parameters
 NAME 11-SEP-AN-2025
 EXPNO 320
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250912
 Time 3.09
 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 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

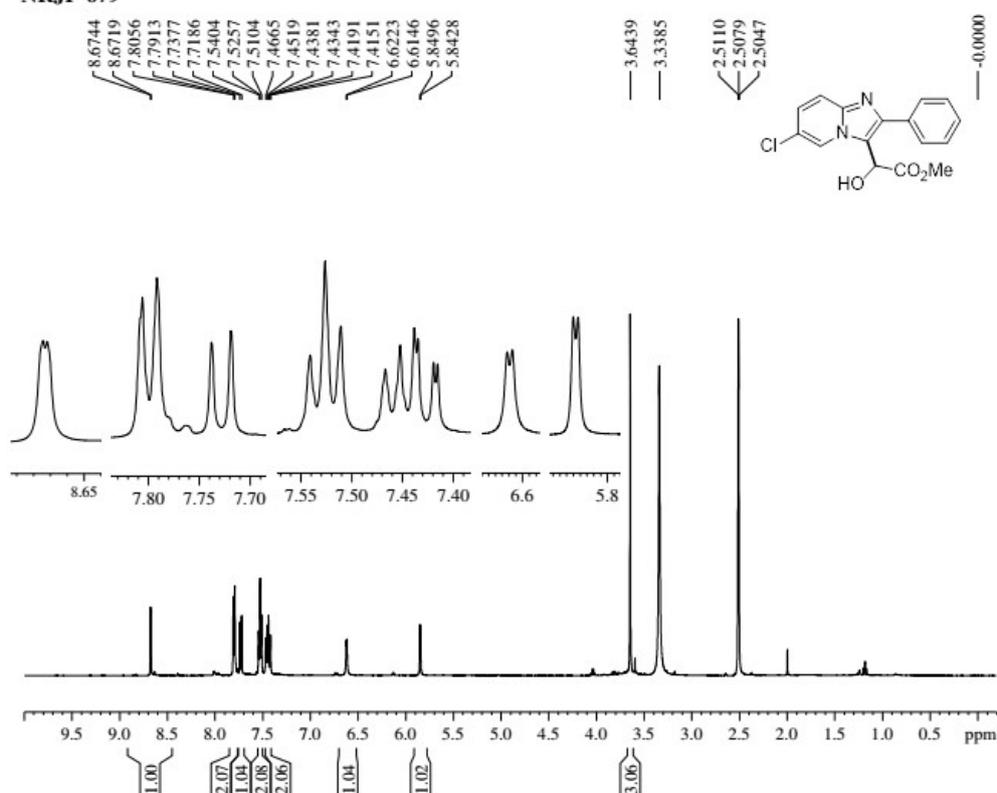
==== CHANNEL f1 =====
 SFO1 100.6304993 MHz
 NUC1 13C
 P1 9.25 usec
 PLW1 53.00000000 W

==== CHANNEL f2 =====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 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 S18. ¹³C NMR Spectrum of 5h

NRJP-679



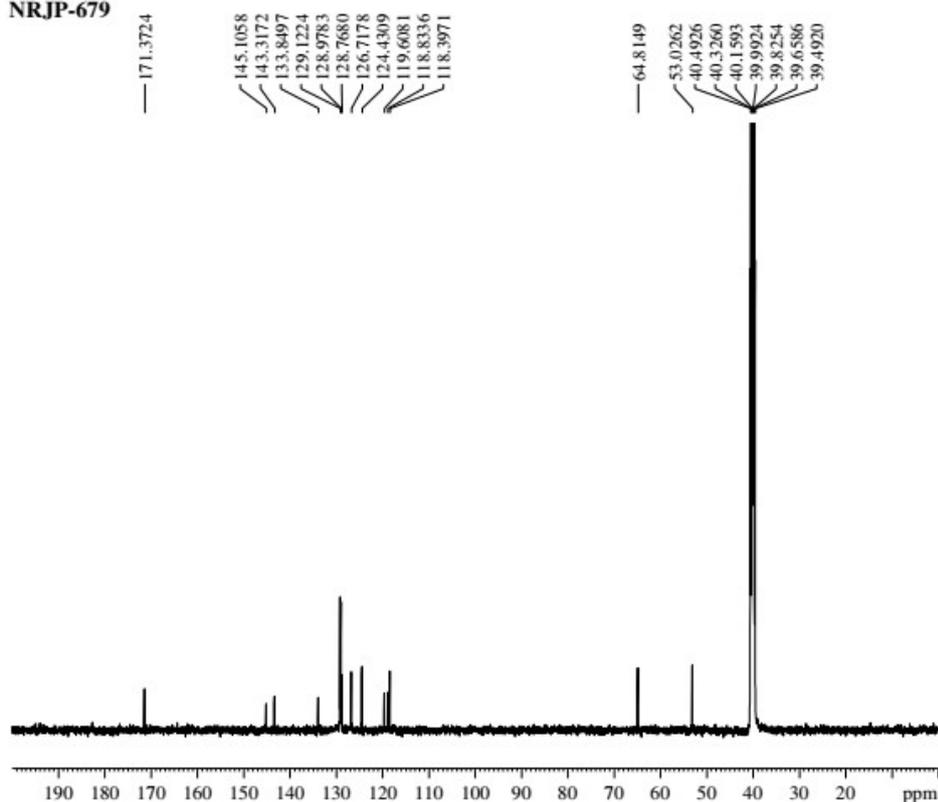
Current Data Parameters
 NAME 10-JUNE-AN-2025
 EXPNO 380
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250610
 Time 16.32 h
 INSTRUM Avance neo 500Mhz
 PROBHD Z151574_0224 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2768000 sec
 RG 101
 DW 50.000 usec
 DE 11.14 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.3030894 MHz
 NUC1 1H
 P0 8.00 usec
 P1 2.67 usec
 PLW1 24.32900047 W

F2 - Processing parameters
 SI 65536
 SF 500.3000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S19. ¹H NMR Spectrum of 5i

NRJP-679

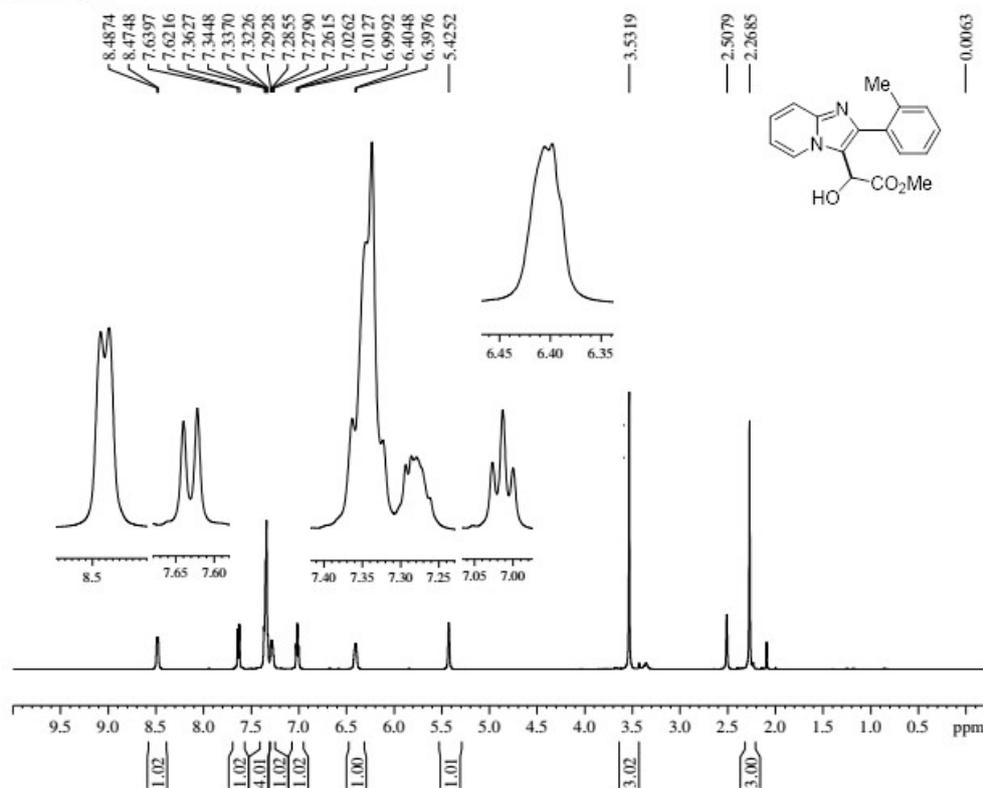


Current Data Parameters
 NAME 09-JUNE-AN-2025
 EXPNO 350
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 125.8005351 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Figure S20. ¹³C NMR Spectrum of 5i

NRJP-691



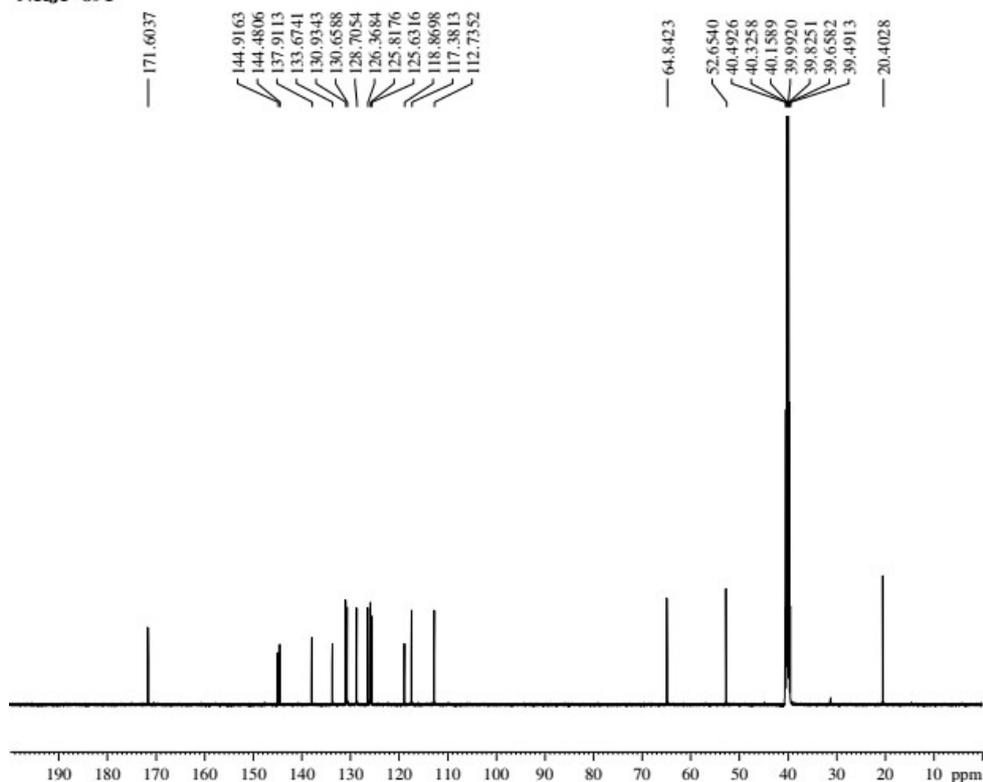
Current Data Parameters
 NAME 20-JUNE-AN-2025
 EXPNO 510
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250620
 Time 15:43 h
 INSTRUM Avance neo 500MHz 5i
 PROBHID Z151574_0224 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2768000 sec
 RG 80.6
 DW 50.000 usec
 DE 11.14 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.3030894 MHz
 NUC1 1H
 P0 2.67 usec
 P1 8.00 usec
 PLW1 24.32900047 W

F2 - Processing parameters
 SI 65536
 SF 500.3000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S21. ¹H NMR Spectrum of 5j

NRJP-691

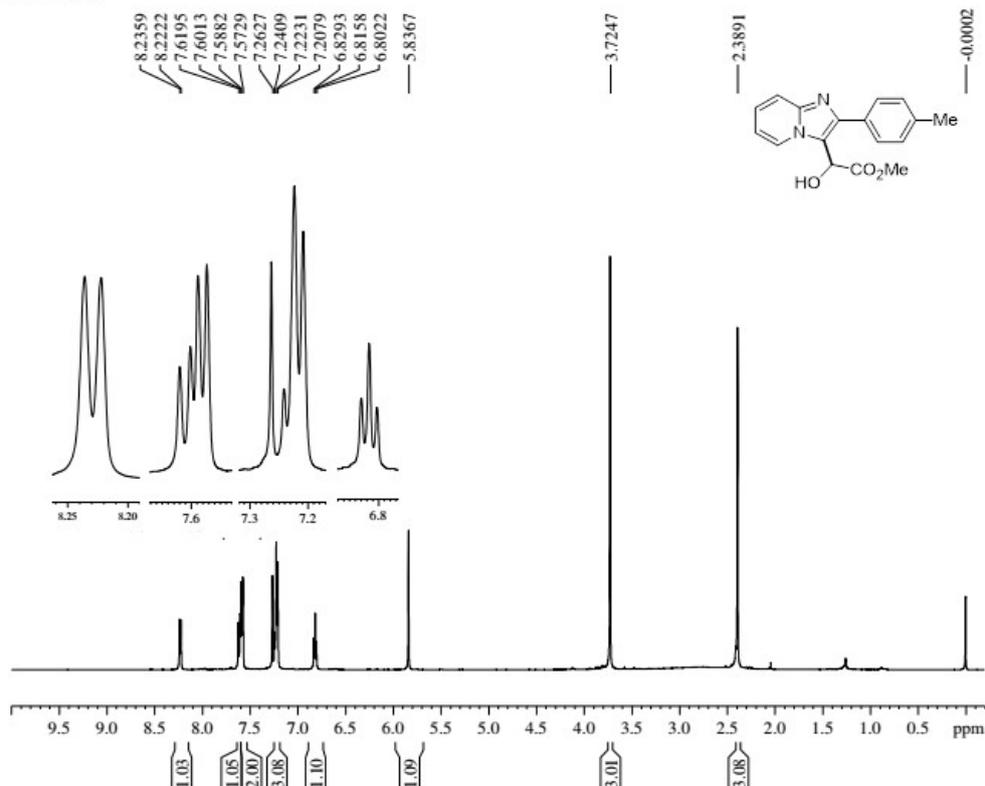


Current Data Parameters
 NAME 19-JUNE-AN-2025
 EXPNO 310
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 125.8005351 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure S22. ¹³C NMR Spectrum of 5j

NRJP-662

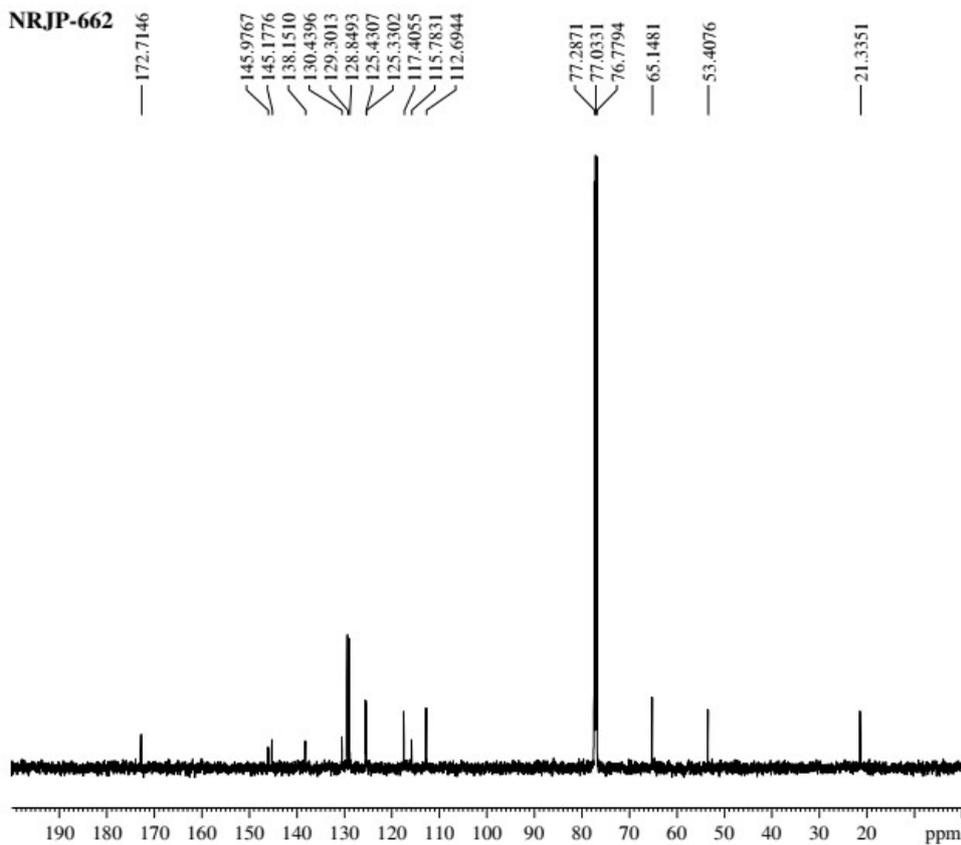


Current Data Parameters
 NAME 18-FEB-AN-2025
 EXPNO 340
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250218
 Time 15.56 h
 INSTRUM Avance neo 500Mhz
 PROBHD Z151574_0224 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2768000 sec
 RG 101
 DW 50.000 usec
 DE 11.14 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.3050894 MHz
 NUC1 1H
 PO 2.67 usec
 P1 8.00 usec
 PLW1 24.32900047 W

F2 - Processing parameters
 SI 65536
 SF 500.300108 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S23. ¹H NMR Spectrum of 5k



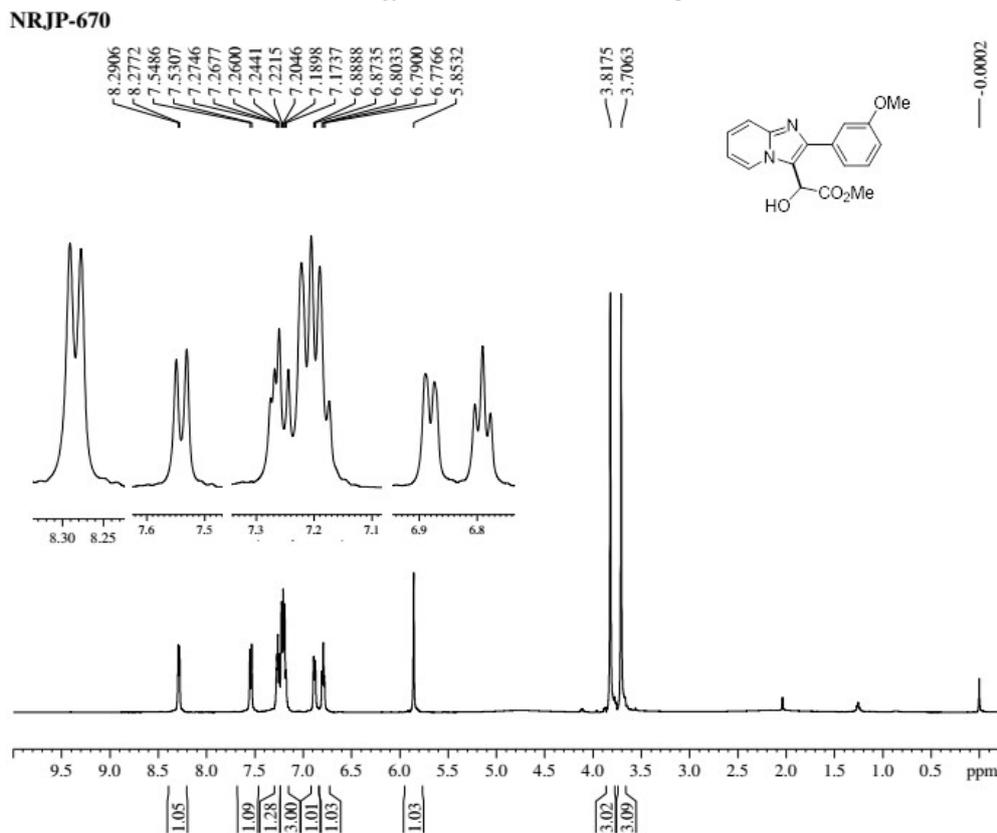
Current Data Parameters
NAME 14-FEB-AN-2025
EXPNO 310
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250215
Time 0.30
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.78
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.9077573 MHz
NUC1 13C
P1 9.23 usec
PLW1 244.0000000 W

==== CHANNEL f2 =====
SFO2 500.6783527 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 13.60000038 W
PLW12 0.08840500 W
PLW13 0.05657900 W

F2 - Processing parameters
SI 32768
SF 125.8951680 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

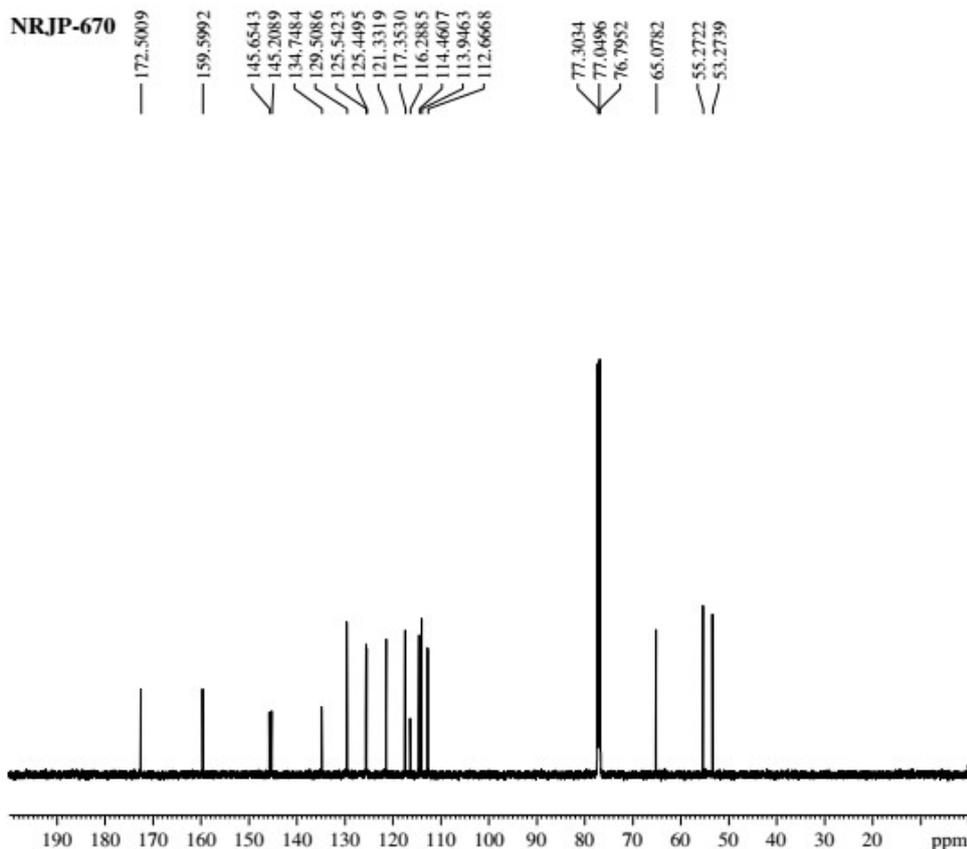


Current Data Parameters
NAME 07-JULY-AN-2025
EXPNO 320
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250707
Time 20.30
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 10026.738 Hz
FIDRES 0.152996 Hz
AQ 3.2680619 sec
RG 87.95
DW 49.867 usec
DE 6.50 usec
TE 298.1 K
D1 6.50000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.6794419 MHz
NUC1 1H
P1 6.45 usec
PLW1 13.60000038 W

F2 - Processing parameters
SI 65536
SF 500.6763573 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 04-JULY-AN-2025
EXPNO 320
PROCNO 1

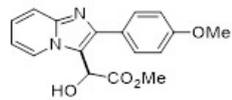
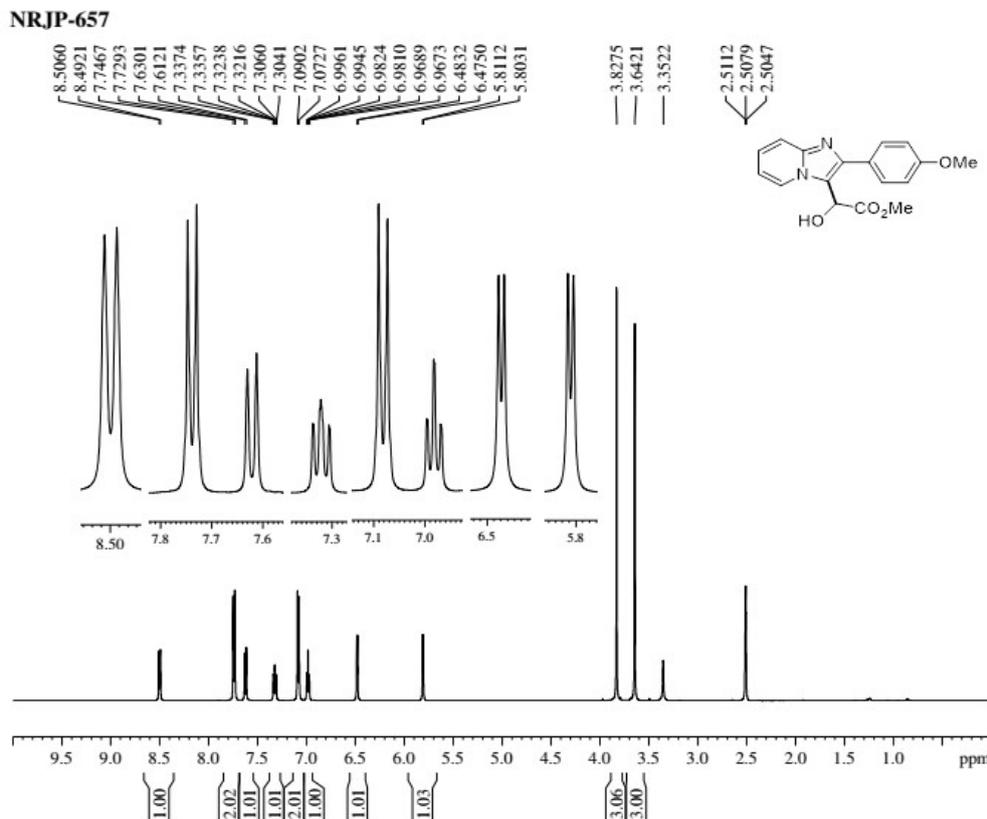
F2 - Acquisition Parameters
Date_ 20250705
Time 2.35
INSTRUM spect
PROBHD 5 mm PAXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 107.78
DW 16.800 usec
DE 6.50 usec
TE 298.5 K
D1 1.0000000 sec
D11 0.03000000 sec
TD0 1

CHANNEL f1
SFO1 125.9077573 MHz
NUC1 13C
P1 9.23 usec
PLW1 244.00000000 W

CHANNEL f2
SFO2 500.6783527 MHz
NUC2 1H
CDDPRG2 waltz16
PCPD2 80.00 usec
PLW2 13.60000038 W
PLW12 0.08840500 W
PLW13 0.05657900 W

F2 - Processing parameters
SI 32768
SF 125.8951680 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S26. ¹³C NMR Spectrum of 5l



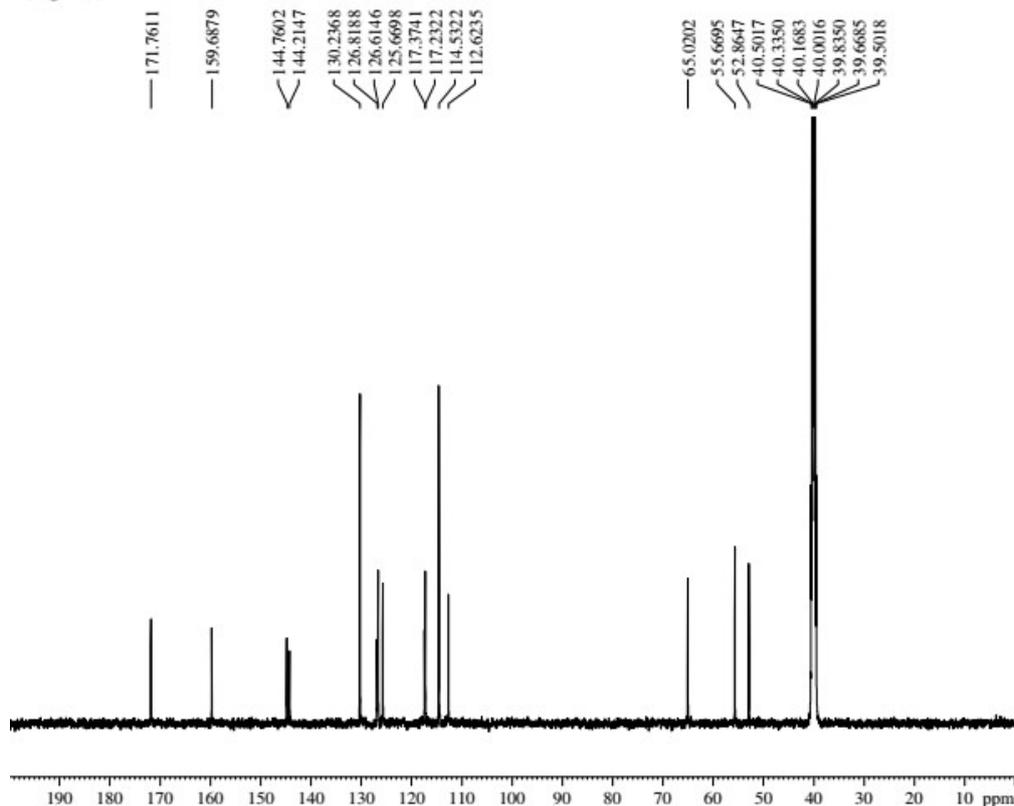
Current Data Parameters
NAME 03-JUNE-FN-2025
EXPNO 320
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250603
Time 12.32 h
INSTRUM Avance neo 500Mhz
PROBHD Z151574-0224 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2768000 sec
RG 101
DW 50.000 usec
DE 11.14 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1
SFO1 500.3030894 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.32900047 W

F2 - Processing parameters
SI 65536
SF 500.3000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S27. ¹H NMR Spectrum of 5m

NRJP-657



Current Data Parameters
 NAME 30-MAY-AN-2025
 EXPNO 350
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250601
 Time 2.05
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 107.78
 DW 16.800 usec
 DE 6.50 usec
 TE 299.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

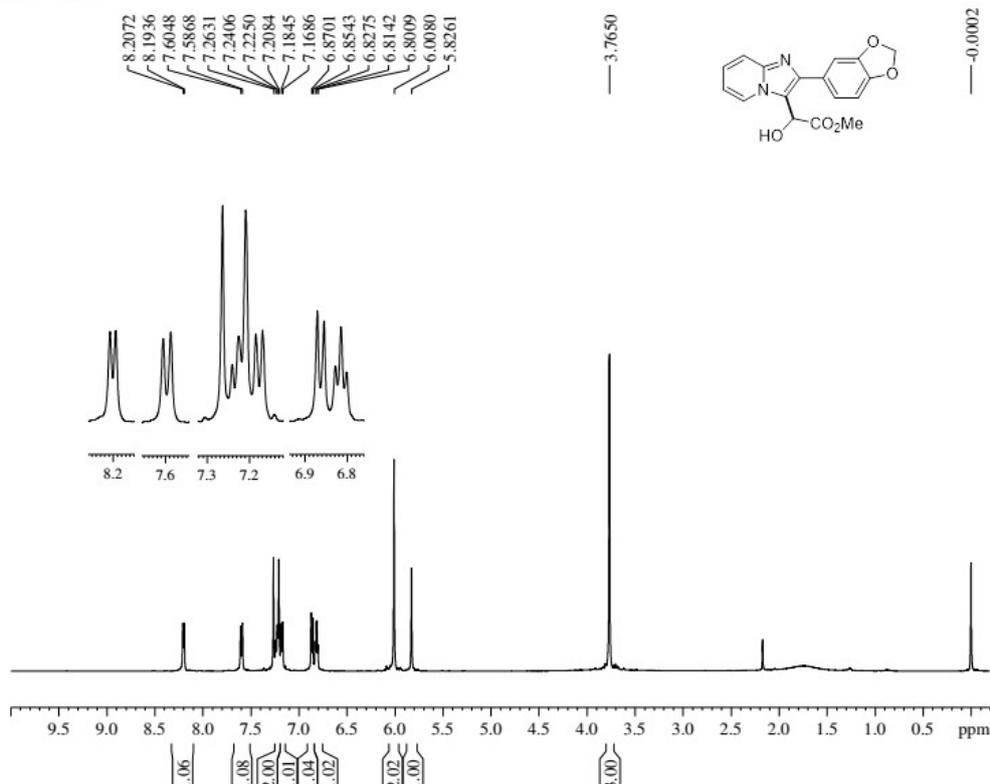
==== CHANNEL f1 ====
 SFO1 125.9077573 MHz
 NUC1 13C
 P1 9.23 usec
 PLW1 244.00000000 W

==== CHANNEL f2 ====
 SFO2 500.6783527 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 13.60000038 W
 PLW12 0.08840500 W
 PLW13 0.05657900 W

F2 - Processing parameters
 SI 32768
 SF 125.8951680 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Figure S28. ¹³C NMR Spectrum of 5m

NRJP-665



Current Data Parameters
 NAME 07-JULY-AN-2025
 EXPNO 310
 PROCNO 1

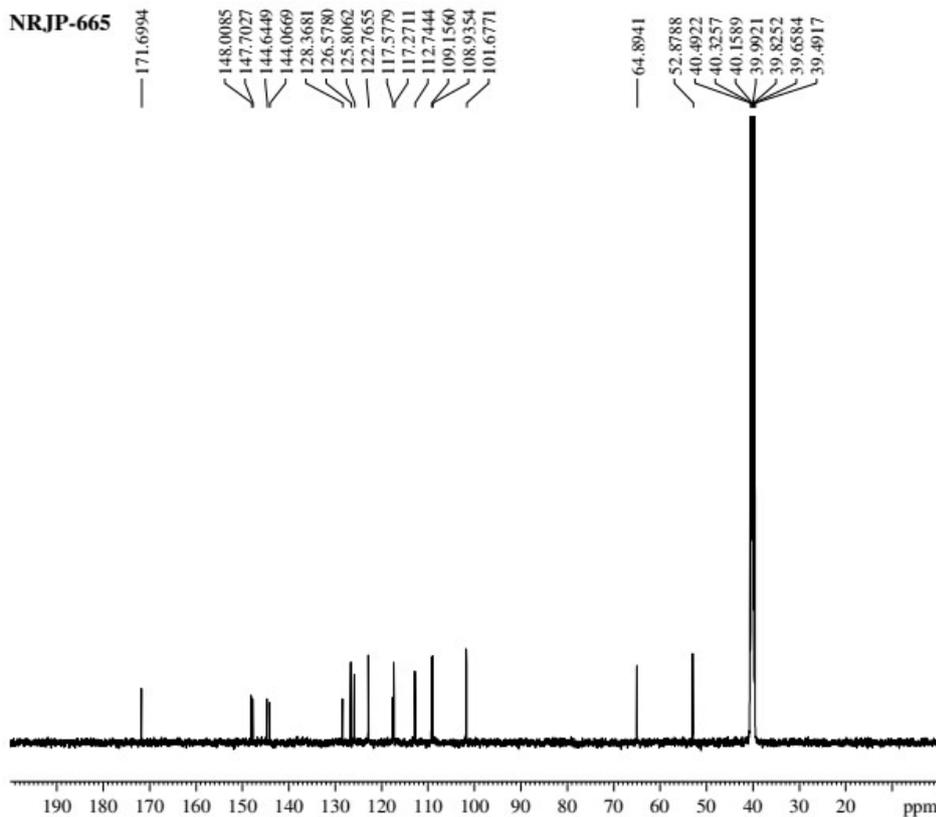
F2 - Acquisition Parameters
 Date_ 20250707
 Time 20.20
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 10026.738 Hz
 FIDRES 0.152996 Hz
 AQ 3.2680619 sec
 RG 201.78
 DW 49.867 usec
 DE 6.50 usec
 TE 298.2 K
 D1 6.50000000 sec
 TDO 1

==== CHANNEL f1 ====
 SFO1 500.6794419 MHz
 NUC1 1H
 P1 6.45 usec
 PLW1 13.60000038 W

F2 - Processing parameters
 SI 65536
 SF 500.6763600 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S29. ¹H NMR Spectrum of 5n

NRJP-665

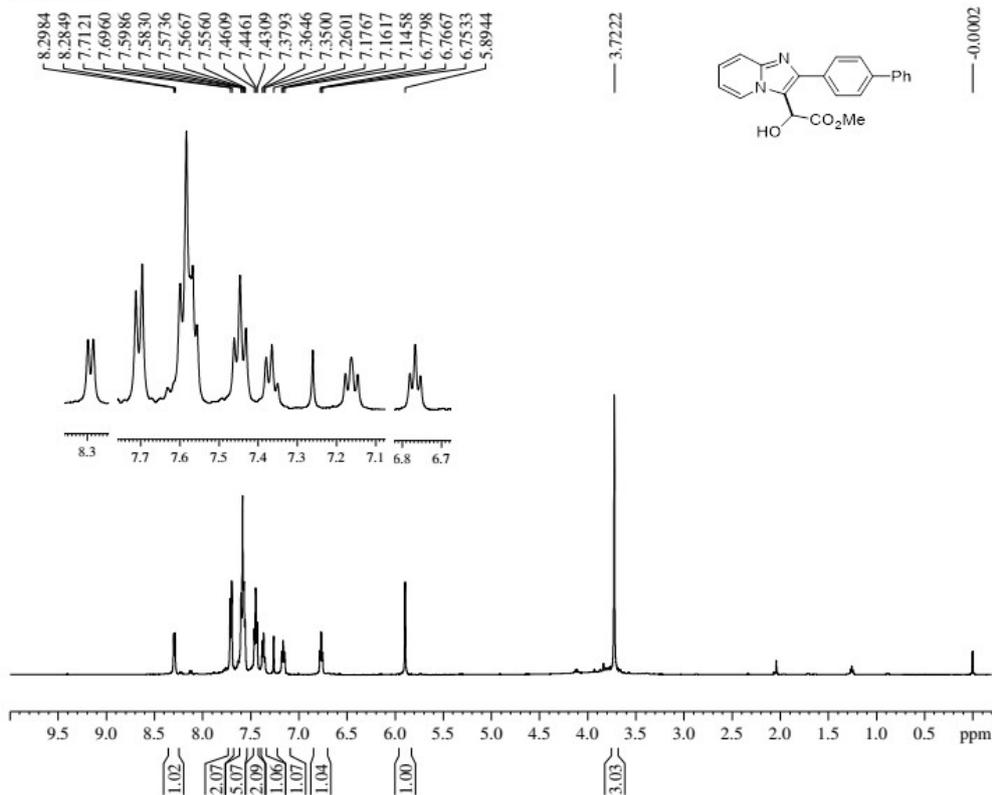


Current Data Parameters
NAME 03-JULY-AN-2025
EXPNO 350
PROCNO 1

F2 - Processing parameters
SI 32768
SF 125.8005351 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Figure S30. ¹³C NMR Spectrum of 5n

NRJP-692



Current Data Parameters
NAME 15-APRIL-AN-2025
EXPNO 320
PROCNO 1

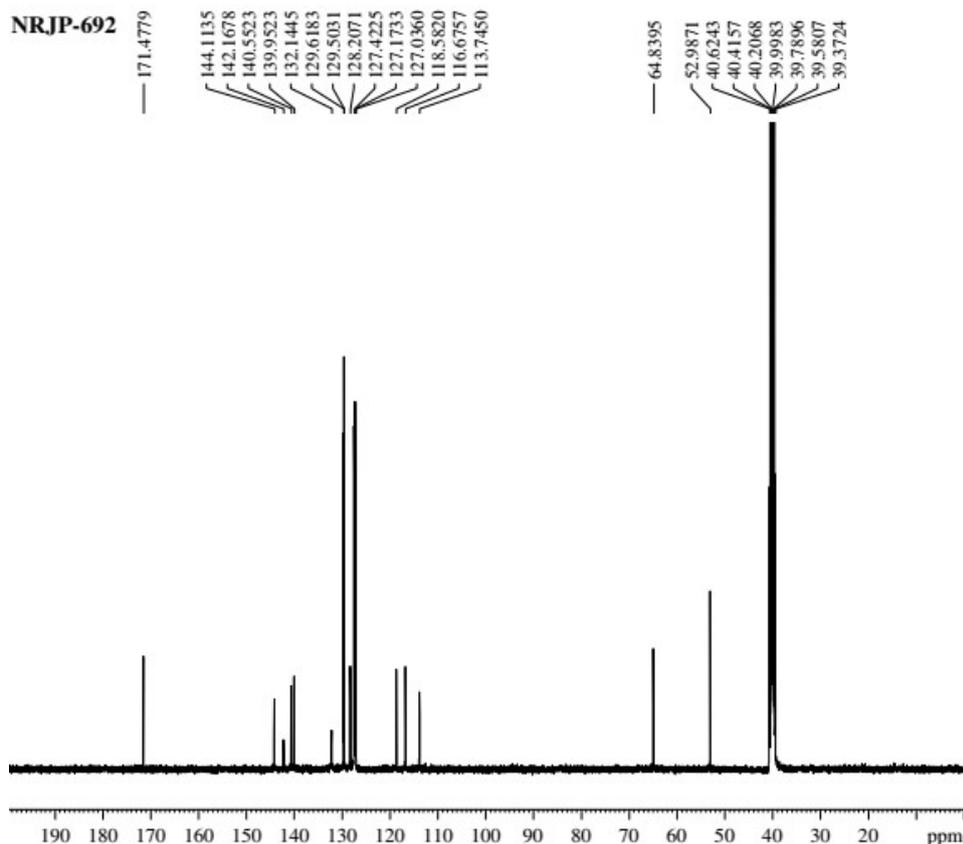
F2 - Acquisition Parameters
Date_ 20250415
Time 12.40
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10026.738 Hz
FIDRES 0.152996 Hz
AQ 3.2680619 sec
RG 121.1
DW 49.867 usec
DE 6.50 usec
TE 298.0 K
D1 4.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.6794419 MHz
NUC1 1H
P1 6.45 usec
PLW1 13.60000038 W

F2 - Processing parameters
SI 65536
SF 500.6763615 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S31. ¹H NMR Spectrum of 5o

NRJP-692



Current Data Parameters
 NAME 15-OCT-A3-2025
 EXPNO 430
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251016
 Time 6.18
 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 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

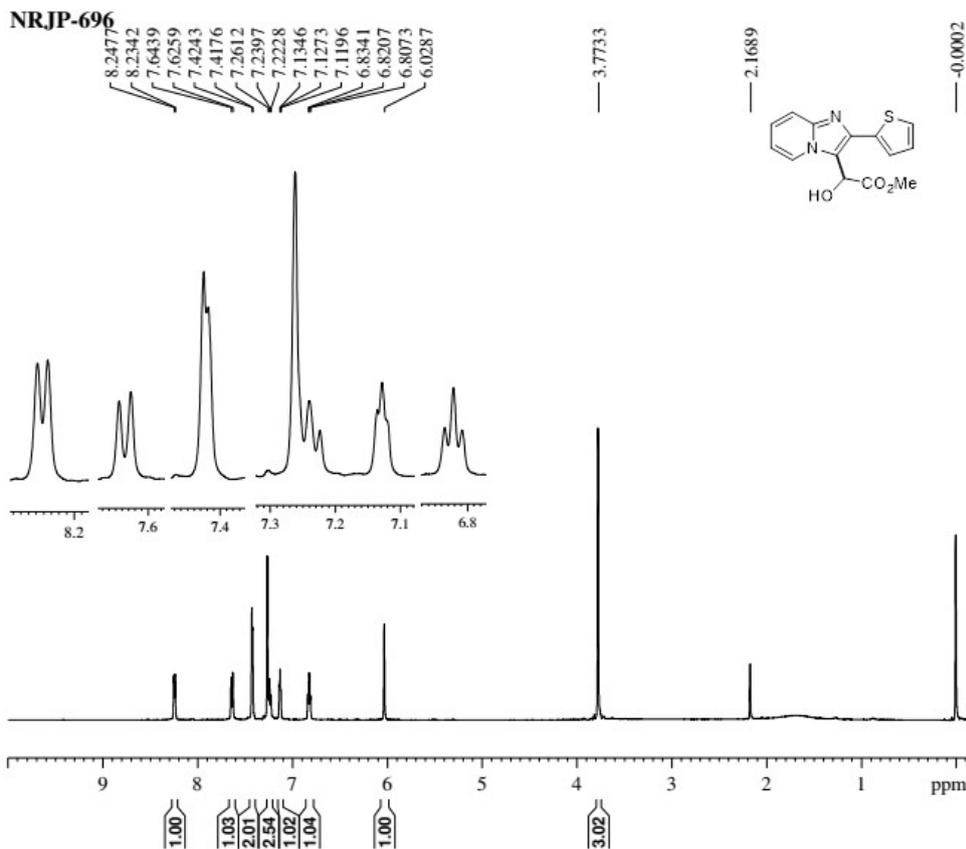
==== CHANNEL f1 =====
 SFO1 100.6304993 MHz
 NUC1 13C
 P1 9.25 usec
 PLW1 53.00000000 W

==== CHANNEL f2 =====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 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 S32. ¹³C NMR Spectrum of 50

NRJP-696



Current Data Parameters
 NAME 23-MAY-FN-2025
 EXPNO 440
 PROCNO 1

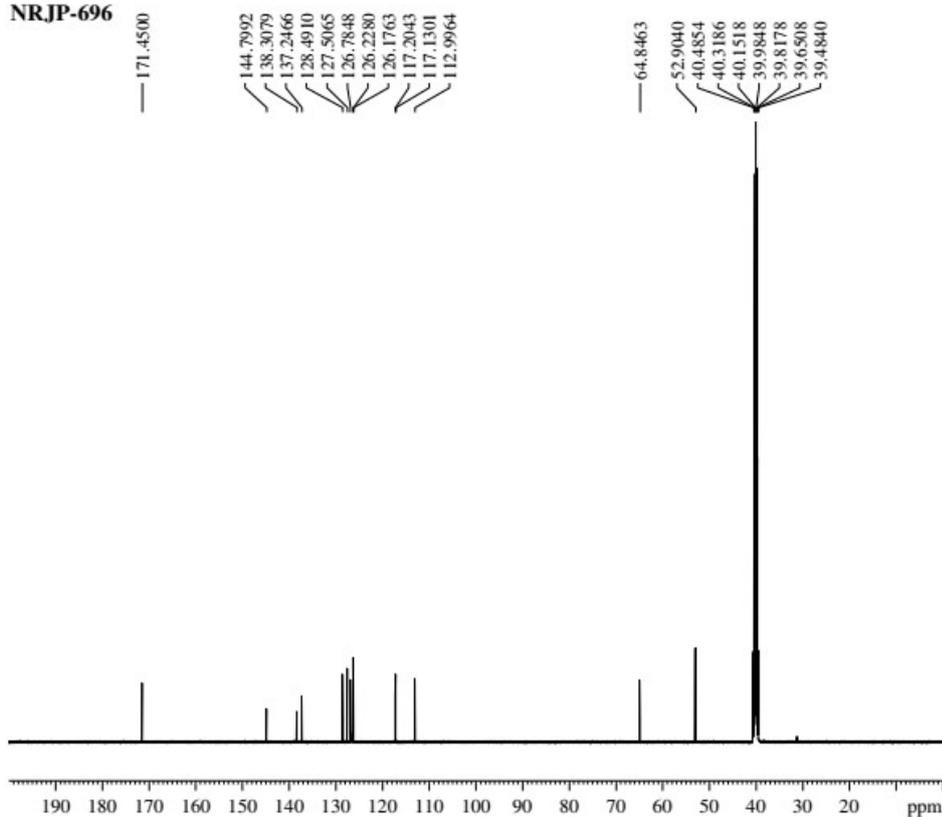
F2 - Acquisition Parameters
 Date_ 20250523
 Time 8.27
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 10026.738 Hz
 FIDRES 0.152996 Hz
 AQ 3.2680619 sec
 RG 201.78
 DW 49.867 usec
 DE 6.50 usec
 TE 299.0 K
 D1 6.50000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.6794419 MHz
 NUC1 1H
 P1 6.45 usec
 PLW1 13.60000038 W

F2 - Processing parameters
 SI 65536
 SF 500.6763623 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S33. ¹H NMR Spectrum of 5p

NRJP-696

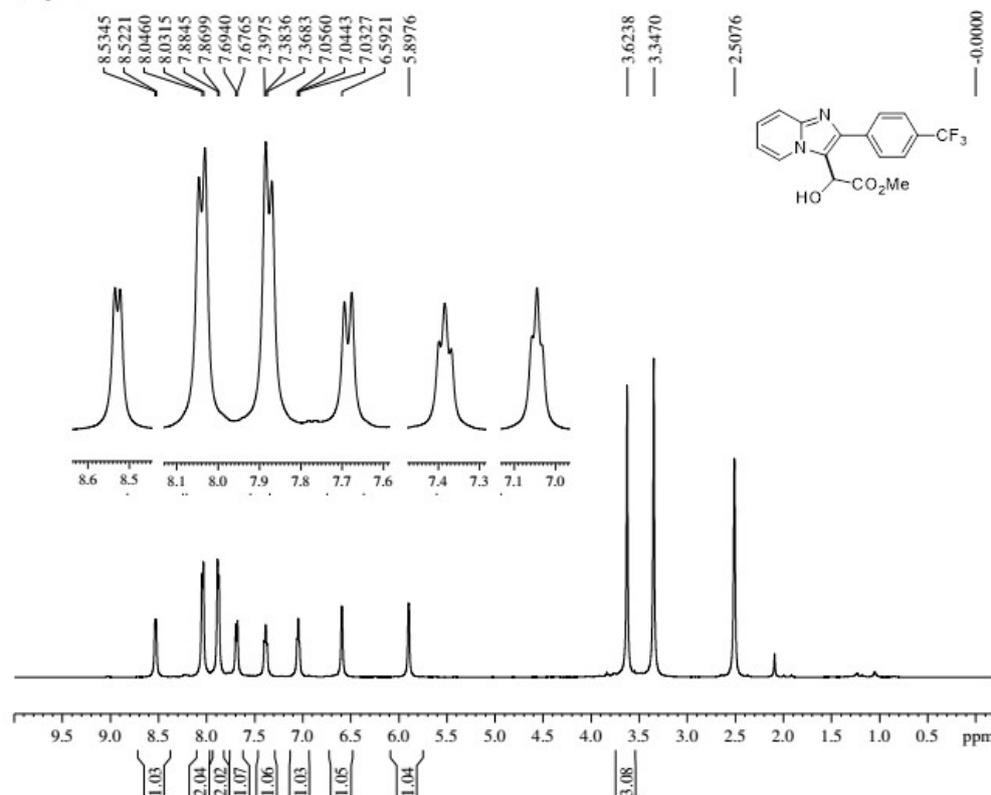


Current Data Parameters
 NAME 23-May-AN-2025
 EXPNO 330
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 125.8005351 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure S34. ¹³C NMR Spectrum of 5p

NRJP 674



Current Data Parameters
 NAME 23-MAY-AN-2025
 EXPNO 310
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250523
 Time 17.13 h
 INSTRUM Avance neo 500MHz
 PROBHD Z151574_0224 (zg30)
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2768000 sec
 RG 101
 DW 50.000 usec
 DE 11.14 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1
 SFO1 500.3030894 MHz
 NUC1 1H
 P0 2.67 usec
 P1 8.00 usec
 PLW1 24.32900047 W

F2 - Processing parameters
 SI 65536
 SF 500.3000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S35. ¹H NMR Spectrum of 5q

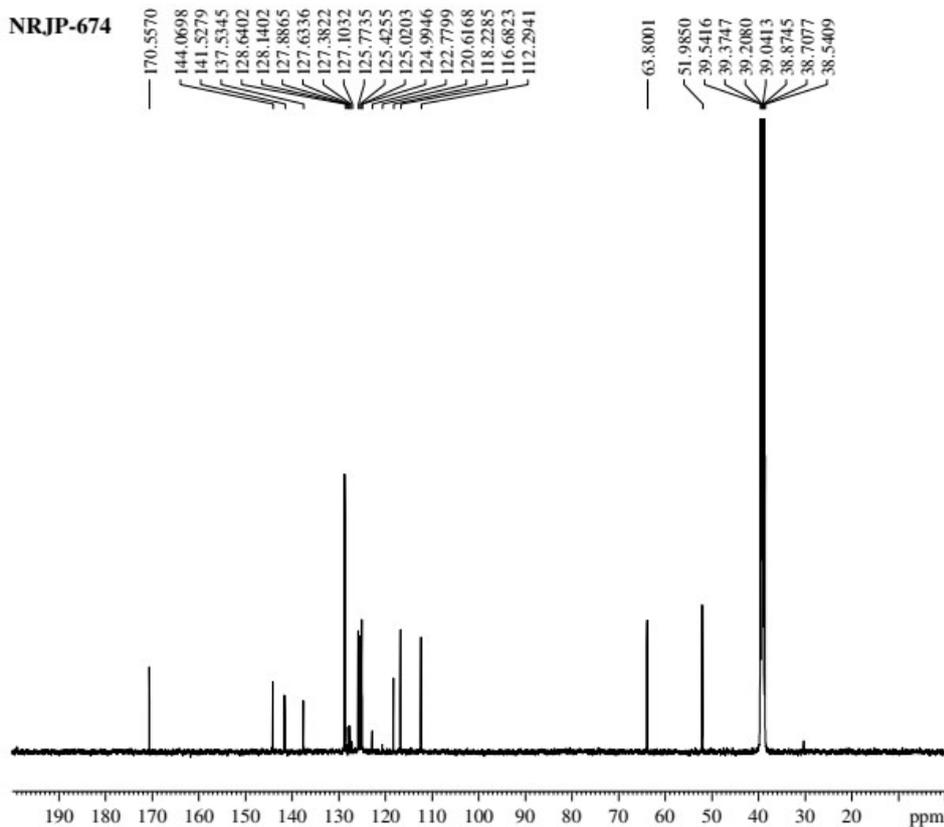


Figure S36. ¹³C NMR Spectrum of 5q



Current Data Parameters
NAME 27-MAY-AN-2025
EXPNO 330
PROCNO 1

F2 - Processing parameters
SI 32768
SF 125.8006534 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

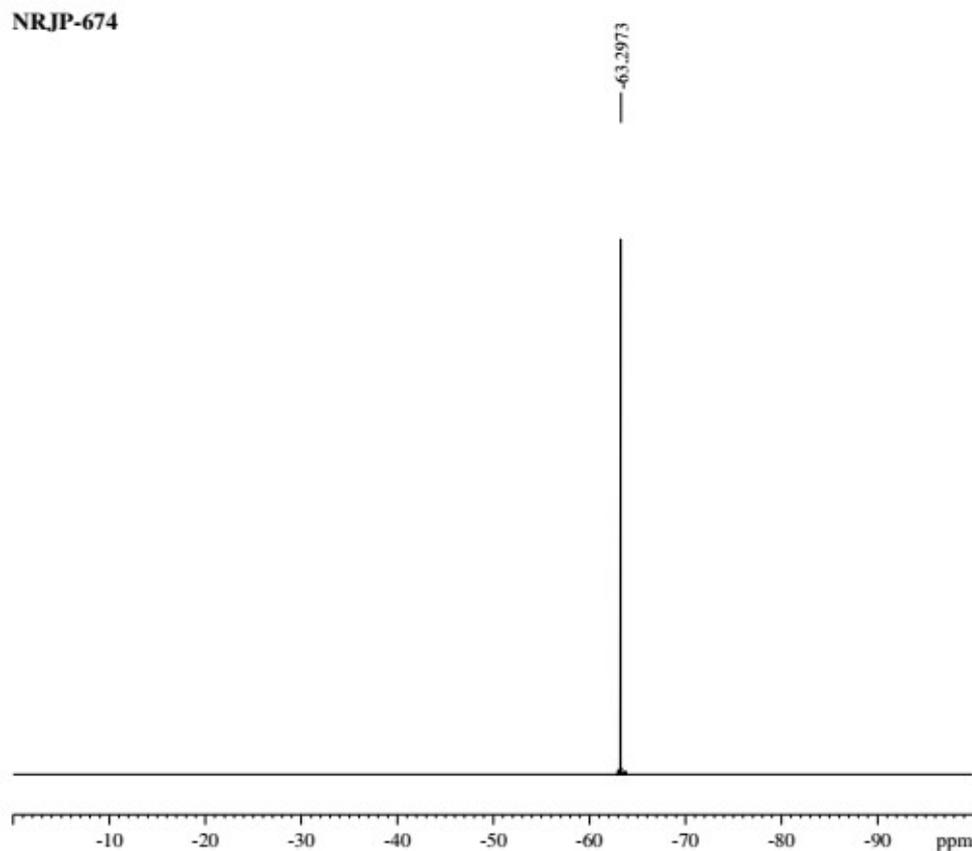


Figure S37. ¹⁹F NMR Spectrum of 5q



Current Data Parameters
NAME 24-OCT-FN-2025
EXPNO 310
PROCNO 1

F2 - Acquisition Parameters
Date_ 20251024
Time 13.34
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 201.48
DW 5.600 usec
DE 6.50 usec
TE 300.1 K
D1 1.0000000 sec
D11 0.0300000 sec
D12 0.0000200 sec
TD0 1

----- CHANNEL f1 -----
SFO1 376.4894122 MHz
NUC1 19F
P1 15.00 usec
PLW1 21.00000000 W

----- CHANNEL f2 -----
SFO2 400.1621006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.30342999 W

F2 - Processing parameters
SI 65536
SF 376.5270650 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

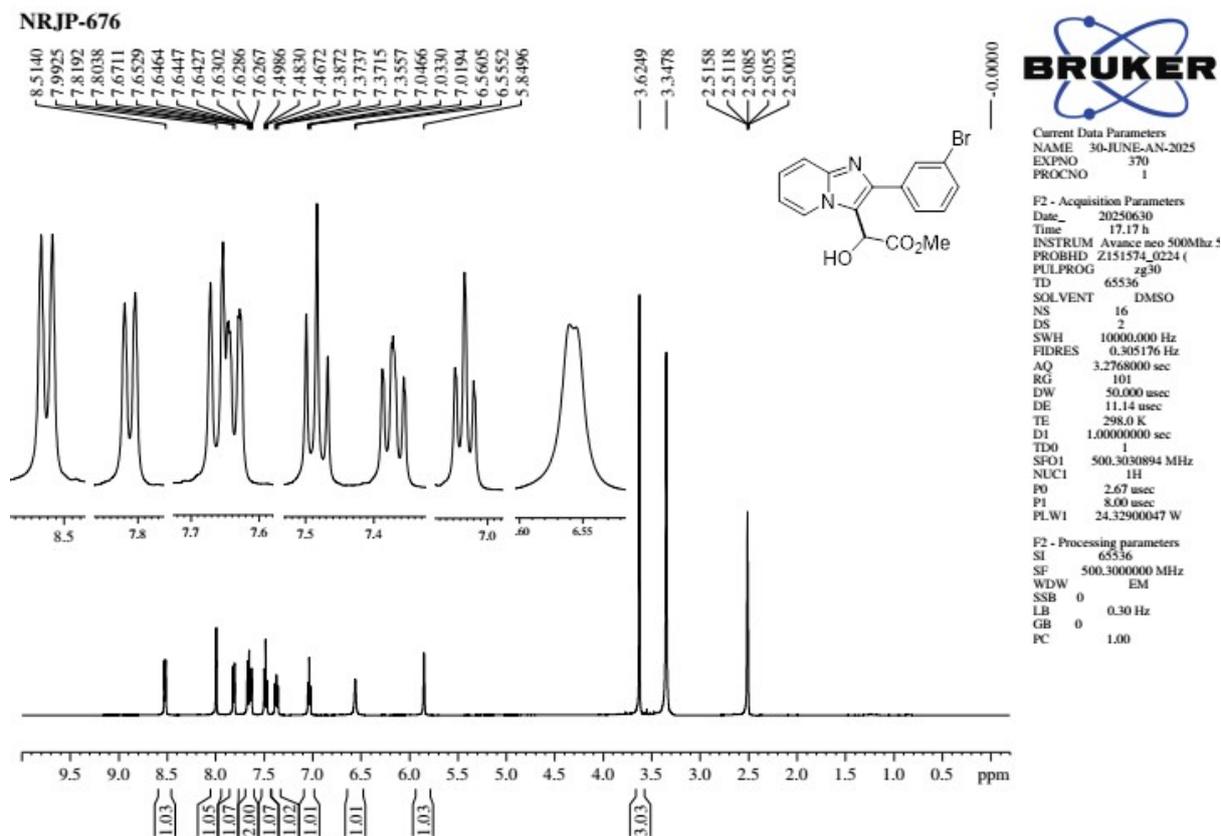


Figure S38. ¹H NMR Spectrum of 5r

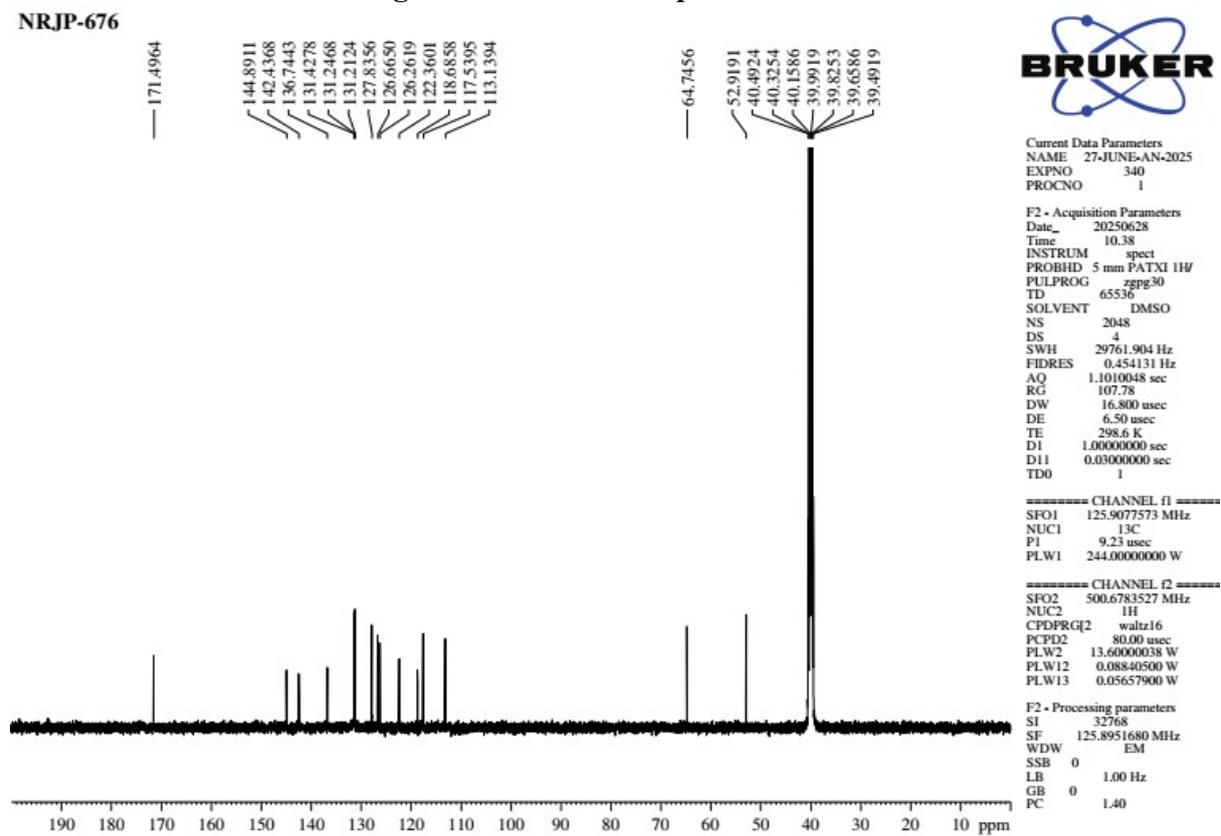
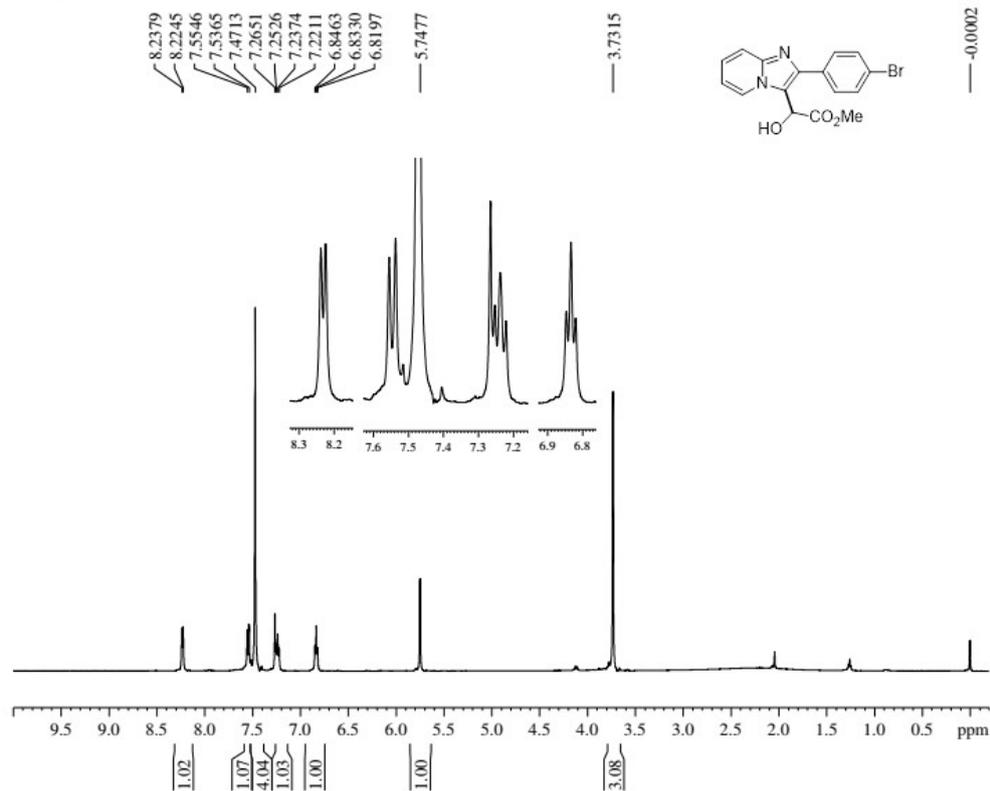


Figure S39. ¹³C NMR Spectrum of 5r

NRJP-658



Current Data Parameters
 NAME 20-MAY-AN-2025
 EXPNO 330
 PROCNO 1

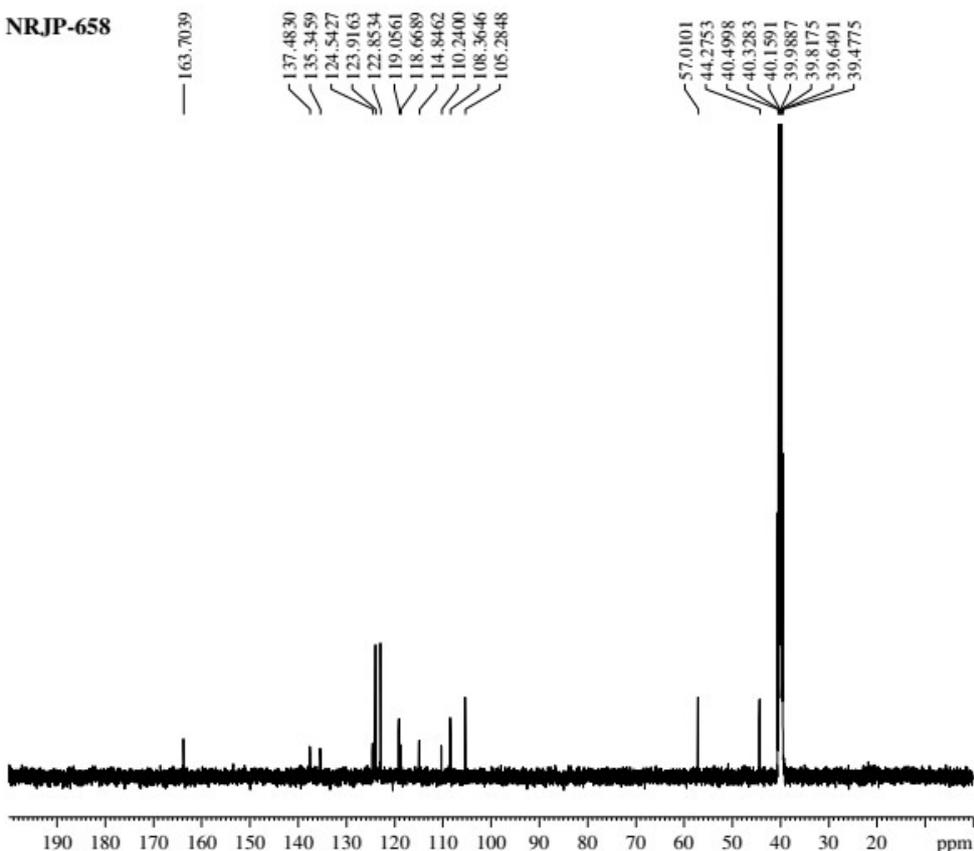
F2 - Acquisition Parameters
 Date_ 20250520
 Time 14.35
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 10026.738 Hz
 FIDRES 0.152996 Hz
 AQ 3.2680619 sec
 RG 201.78
 DW 49.867 usec
 DE 6.50 usec
 TE 298.4 K
 D1 6.5000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 500.6794419 MHz
 NUC1 1H
 P1 6.45 usec
 PLW1 13.60000038 W

F2 - Processing parameters
 SI 65536
 SF 500.6763607 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S40. ¹H NMR Spectrum of 5s

NRJP-658



Current Data Parameters
 NAME 22-MAY-FN-2025
 EXPNO 320
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250522
 Time 10.39
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 107.78
 DW 16.800 usec
 DE 6.50 usec
 TE 299.6 K
 D1 1.0000000 sec
 D11 0.03000000 sec
 TDO 1

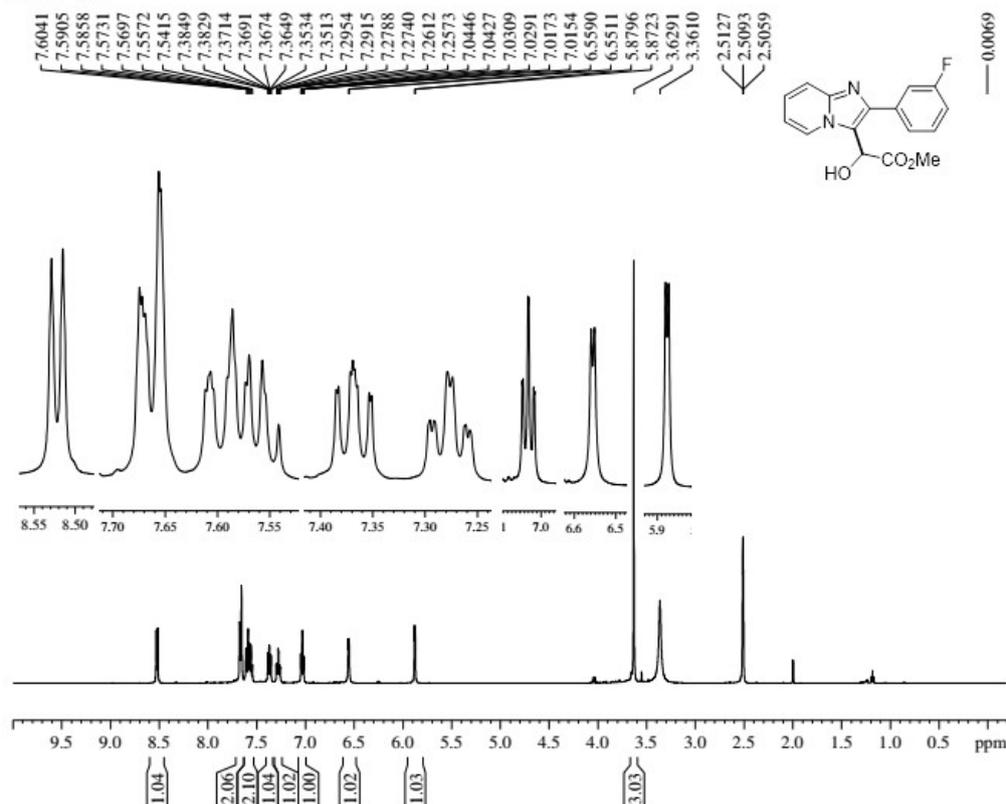
===== CHANNEL f1 =====
 SFO1 125.9077573 MHz
 NUC1 13C
 P1 9.23 usec
 PLW1 244.00000000 W

===== CHANNEL f2 =====
 SFO2 500.6783527 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 13.60000038 W
 PLW12 0.08840500 W
 PLW13 0.05657900 W

F2 - Processing parameters
 SI 32768
 SF 125.8962224 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure S41. ¹³C NMR Spectrum of 5s

NRJP-706



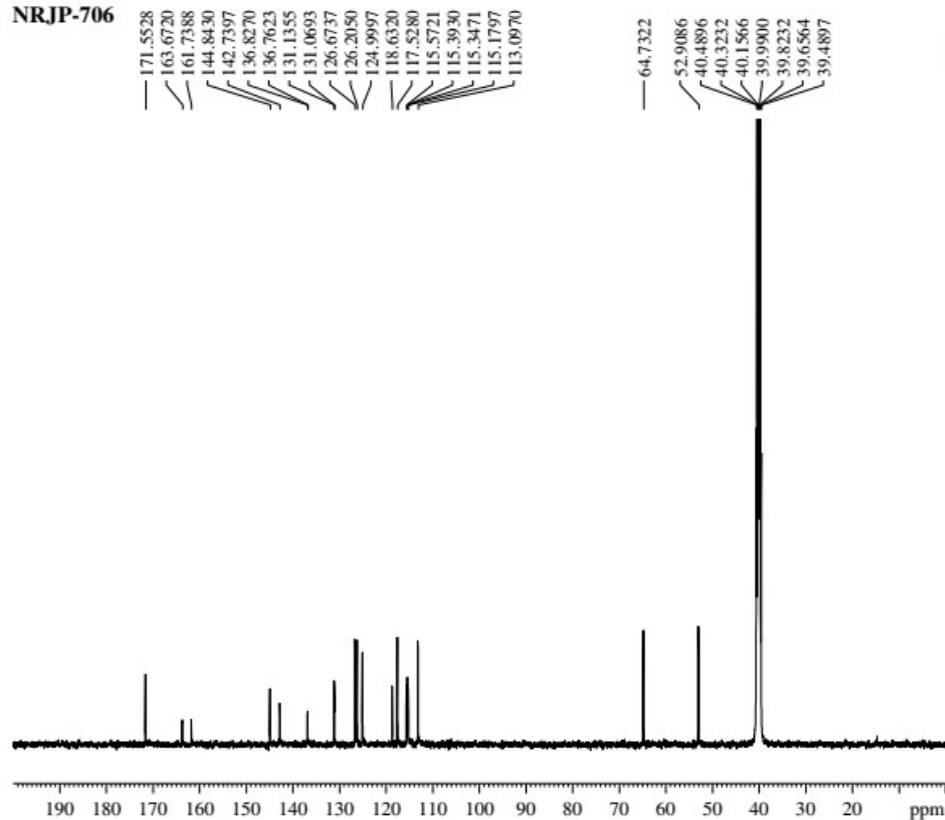
Current Data Parameters
 NAME 25-JUNE-AN-2025
 EXPNO 420
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250625
 Time 18.00 h
 INSTRUM Avance neo 500Mhz
 PROBHD Z151574_0224 (zg30)
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2768000 sec
 RG 101
 DW 50.000 usec
 DE 11.14 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1
 SFO1 500.3030894 MHz
 NUC1 1H
 PC 2.67 usec
 P1 8.00 usec
 PLW1 24.32900047 W

F2 - Processing parameters
 SI 65536
 SF 500.3000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S42. ¹H NMR Spectrum of 5t

NRJP-706

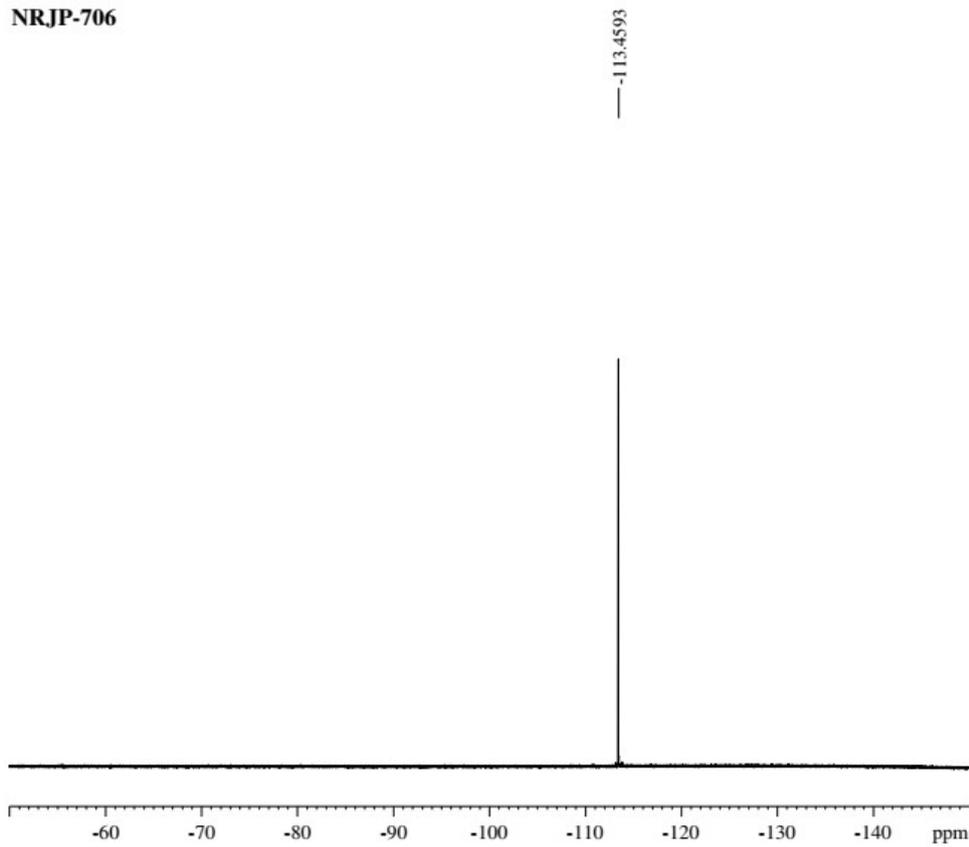


Current Data Parameters
 NAME 20-JUNE-FN-2025
 EXPNO 400
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 125.8005351 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Figure S43. ¹³C NMR Spectrum of 5t

NRJP-706



Current Data Parameters
 NAME 27-OCT-FN-2025
 EXPNO 390
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251027
 Time 11.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 201.48
 DW 5.600 usec
 DE 6.50 usec
 TE 300.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

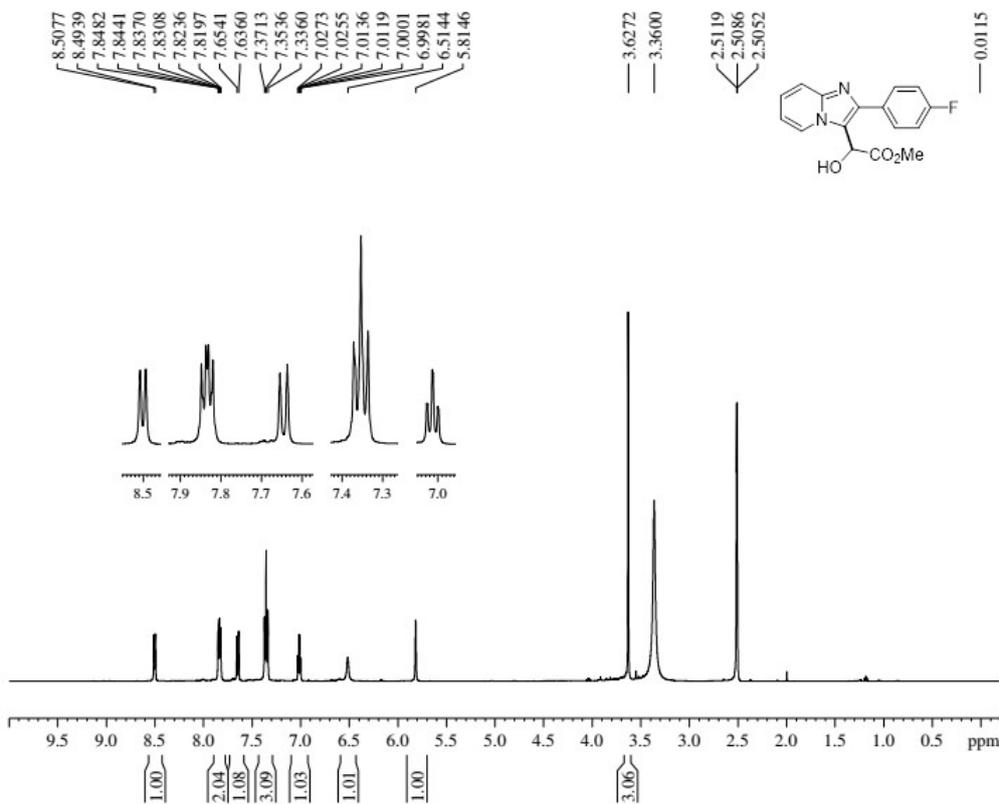
==== CHANNEL f1 ====
 SFO1 376.4894122 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 21.00000000 W

==== CHANNEL f2 ====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.00000000 W
 PLW12 0.30342999 W

F2 - Processing parameters
 SI 65536
 SF 376.5270650 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S44. ¹⁹F NMR Spectrum of 5t

NRJP-693



Current Data Parameters
 NAME 03-JUNE-FN-2025
 EXPNO 310
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250603
 Time 12.17 h
 INSTRUM Avance neo 500MHz :
 PROBHD Z151574_0224 (:
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2768000 sec
 RG 101
 DW 50.000 usec
 DE 11.14 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.3030894 MHz
 NUC1 1H
 P1 2.67 usec
 P2 8.00 usec
 PLW1 24.32500047 W

F2 - Processing parameters
 SI 65536
 SF 500.3000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S45. ¹H NMR Spectrum of 5u

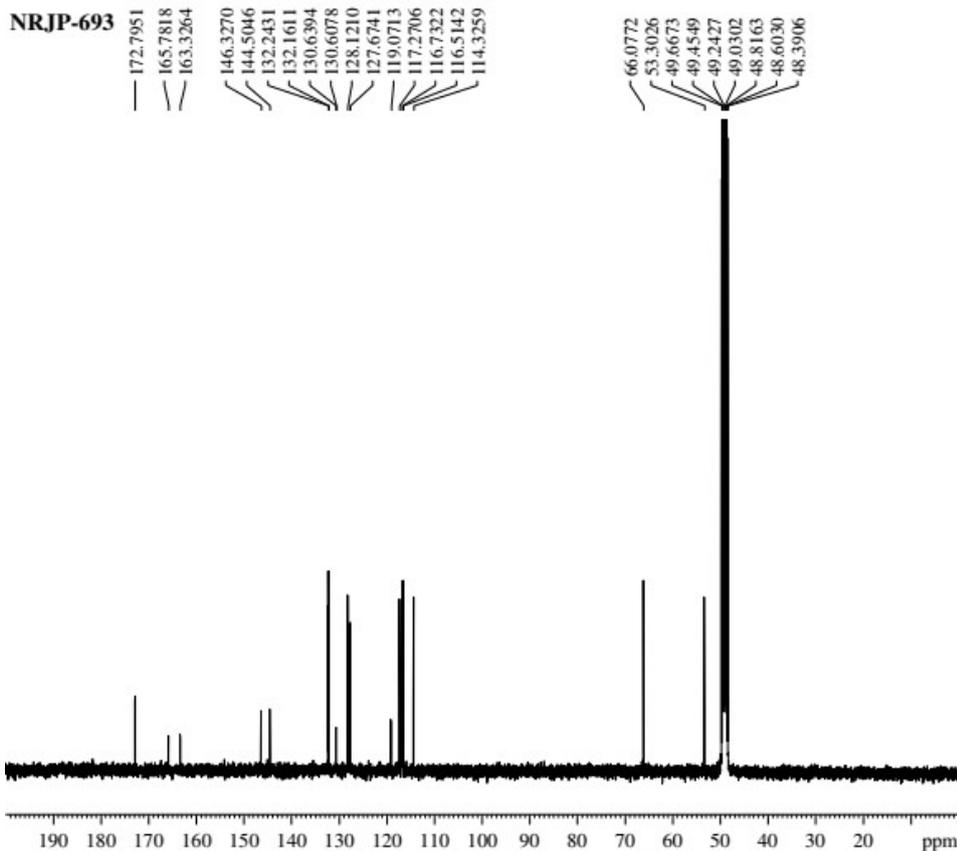


Figure S46. ¹³C NMR Spectrum of 5u



Current Data Parameters
NAME 05-MAY-AN-2025
EXPNO 330
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250505
Time 16.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT MeOD
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 300.0 K
D1 1.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6304993 MHz
NUC1 13C
P1 9.25 usec
PLW1 53.0000000 W

===== CHANNEL f2 =====
SFO2 400.1621006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 13.0000000 W
PLW12 0.30342999 W
PLW13 0.24578001 W

F2 - Processing parameters
SI 32768
SF 100.6202938 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

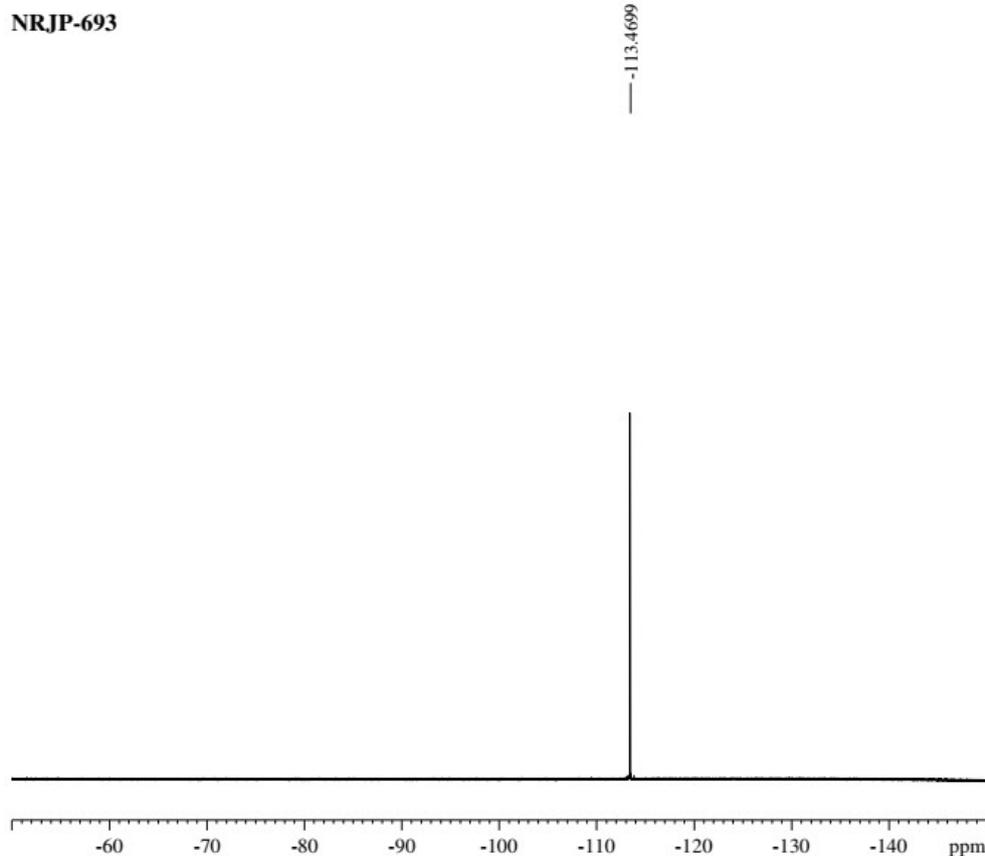


Figure S47. ¹⁹F NMR Spectrum of 5u



Current Data Parameters
NAME 22-OCT-AN-2025
EXPNO 320
PROCNO 1

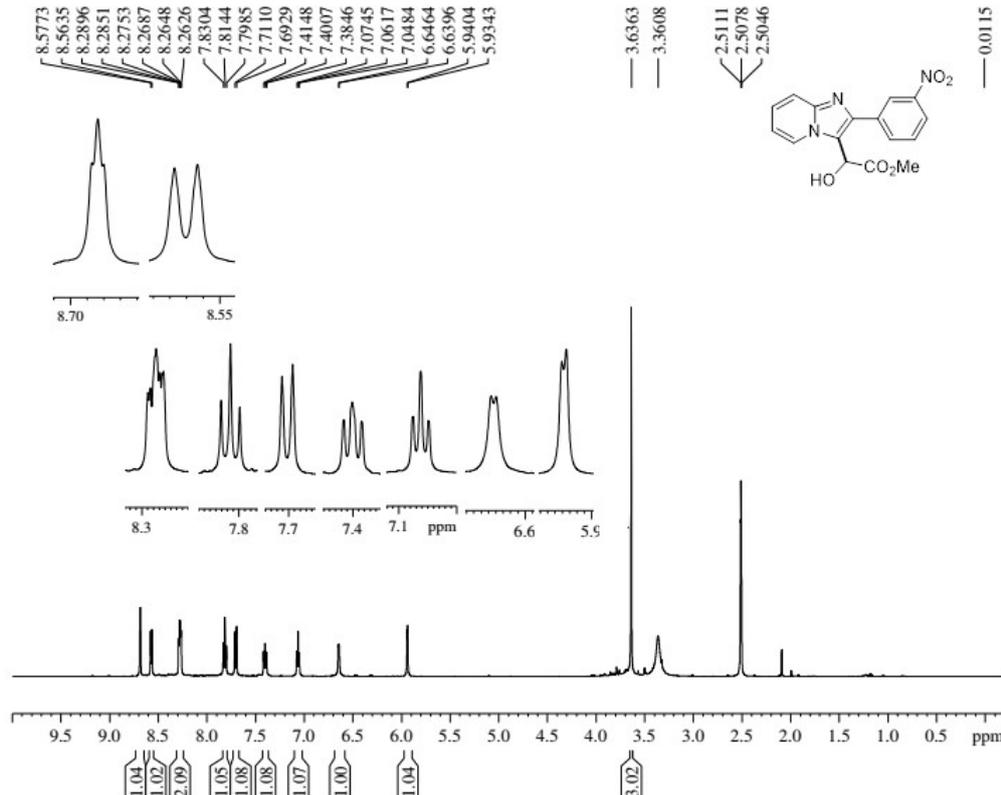
F2 - Acquisition Parameters
Date_ 20251022
Time 16.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflgqz.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 201.48
DW 5.600 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
D11 0.0300000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 376.4894122 MHz
NUC1 19F
P1 15.00 usec
PLW1 21.0000000 W

===== CHANNEL f2 =====
SFO2 400.1621006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 13.0000000 W
PLW12 0.30342999 W

F2 - Processing parameters
SI 65536
SF 376.5270650 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRJP-697



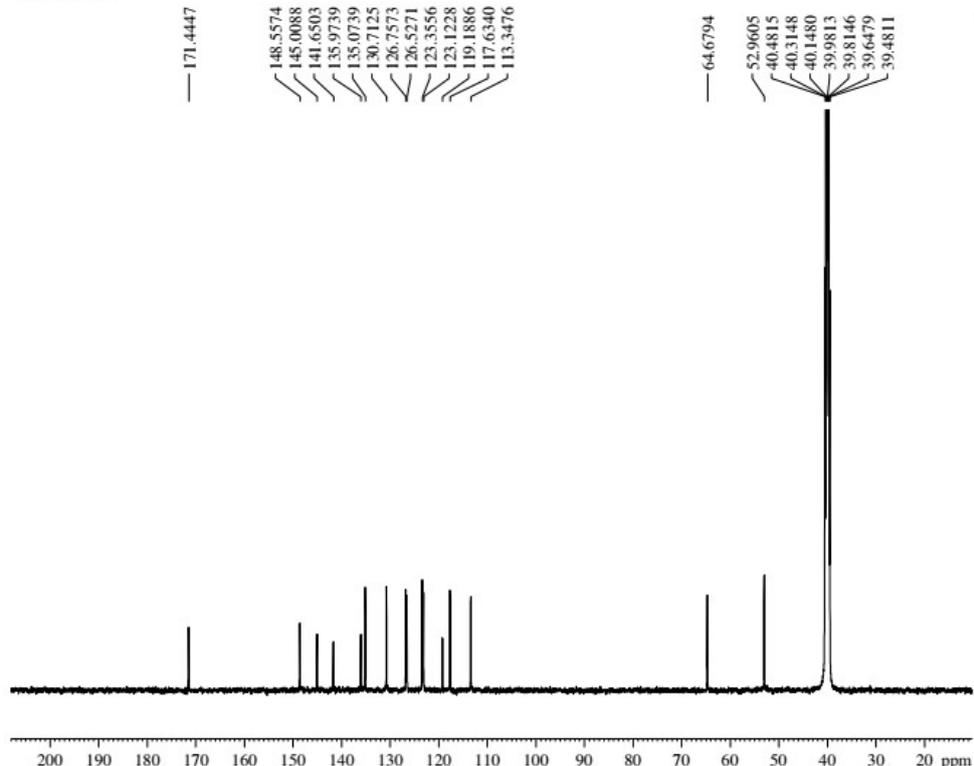
Current Data Parameters
 NAME 26-MAY-AN-2025
 EXPNO 350
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250526
 Time 22.01 h
 INSTRUM Avance neo 500Mhz !
 PROBHD Z151574_0224 (!
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2768000 sec
 RG 101
 DW 50.000 usec
 DE 11.14 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.3030894 MHz
 NUC1 1H
 PO 2.67 usec
 PI 8.00 usec
 PLW1 24.32900047 W

F2 - Processing parameters
 SI 65536
 SF 500.3000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S48. ¹H NMR Spectrum of 5v

NRJP-697

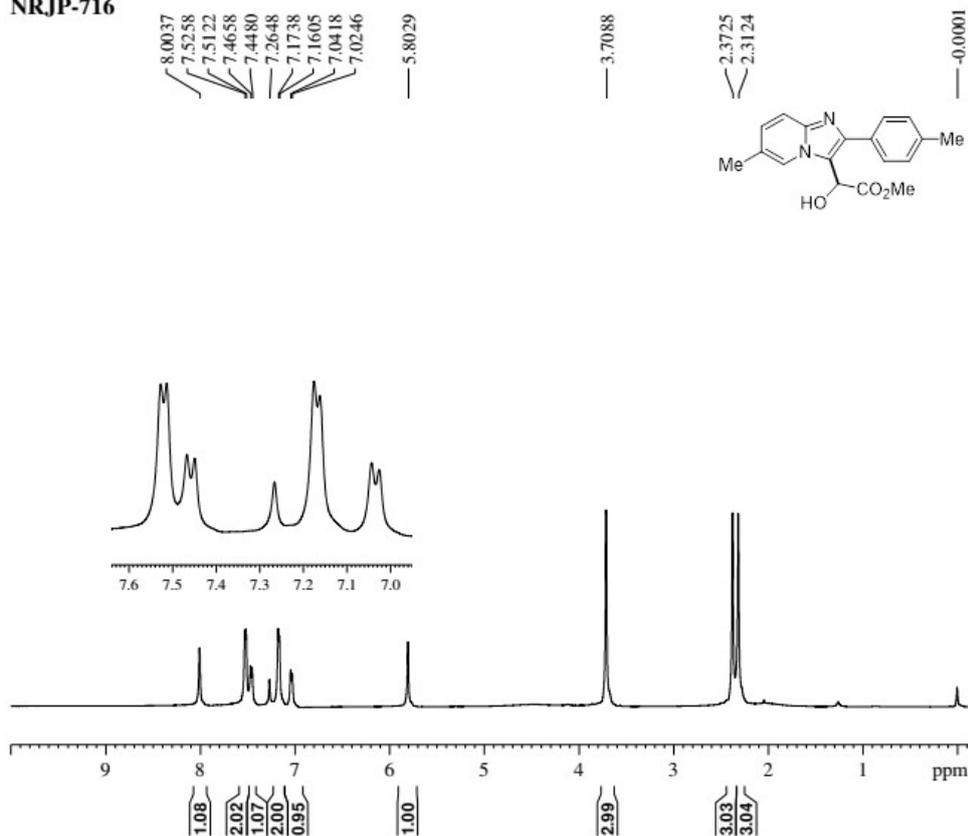


Current Data Parameters
 NAME 22-MAY-AN-2025
 EXPNO 370
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 125.8005351 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Figure S49. ¹³C NMR Spectrum of 5v

NRJP-716



Current Data Parameters
 NAME 14-OCT-FN-2025
 EXPNO 360
 PROCNO 1

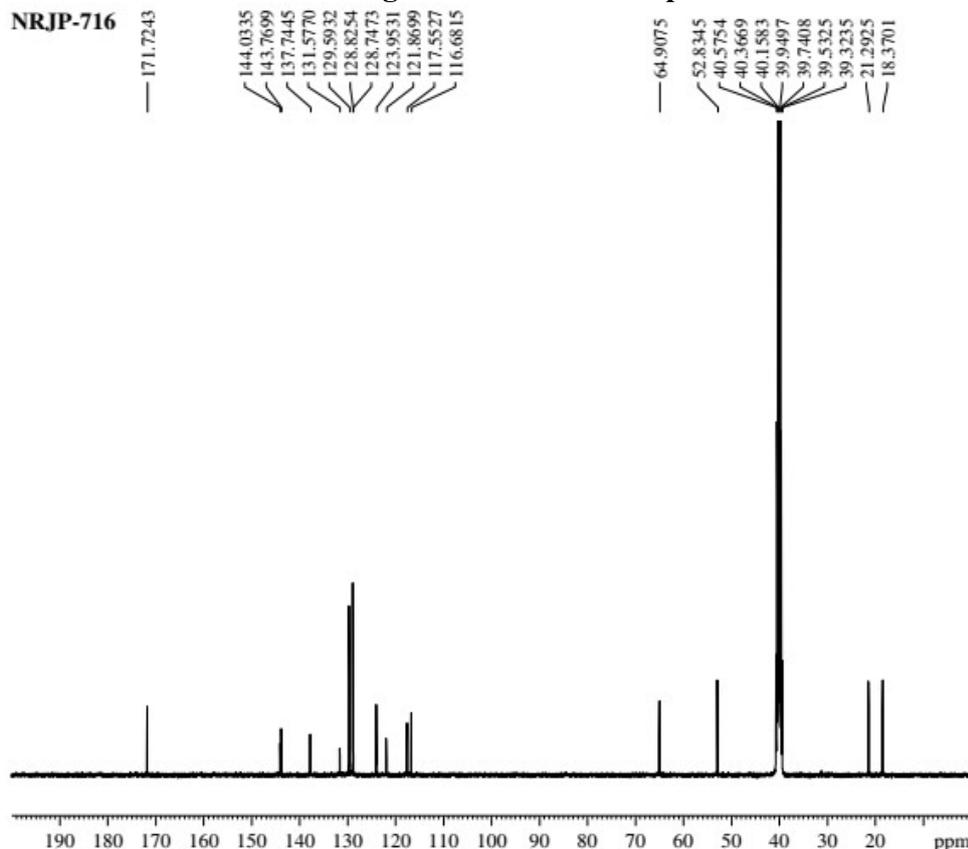
F2 - Acquisition Parameters
 Date_ 20251014
 Time 7.43
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10026.738 Hz
 FIDRES 0.152996 Hz
 AQ 3.2680619 sec
 RG 121.1
 DW 49.867 usec
 DE 6.50 usec
 TE 298.0 K
 D1 6.5000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.6794419 MHz
 NUC1 1H
 P1 6.45 usec
 PLW1 13.60000038 W

F2 - Processing parameters
 SI 65536
 SF 500.6763594 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S50. ¹H NMR Spectrum of 5w

NRJP-716



Current Data Parameters
 NAME 29-SEP-AN-2025
 EXPNO 330
 PROCNO 1

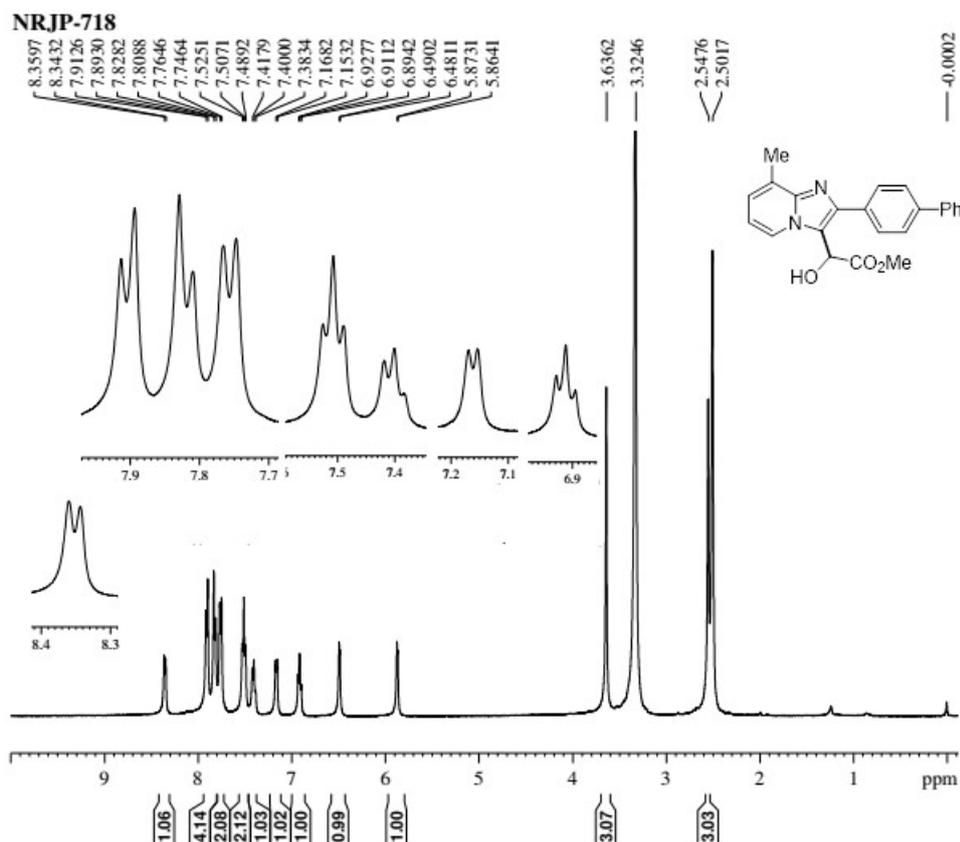
F2 - Acquisition Parameters
 Date_ 20250930
 Time 9.10
 INSTRUM spect
 PROBHD 5 mm FAPBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 201.48
 DW 20.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6304993 MHz
 NUC1 13C
 P1 9.25 usec
 PLW1 53.0000000 W

===== CHANNEL f2 =====
 SFO2 400.1621006 MHz
 NUC2 1H
 CFPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.0000000 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 S51. ¹³C NMR Spectrum of 5w



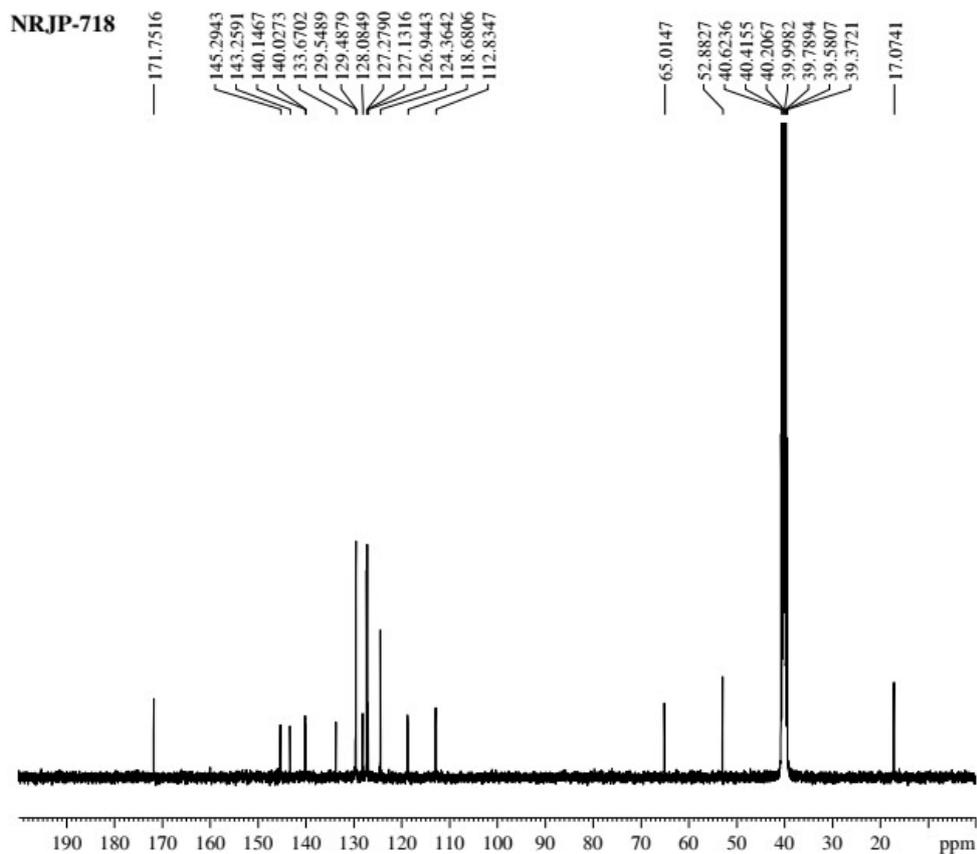
Current Data Parameters
 NAME 29-SEP-AN-2025
 EXPNO 340
 PROCNO 1

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 4.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1629712 MHz
 NUC1 1H
 PI 13.75 usec
 PLW1 13.0000000 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. ¹H NMR Spectrum of 5x



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 1.0000000 sec
 D11 0.0300000 sec
 TD0 1

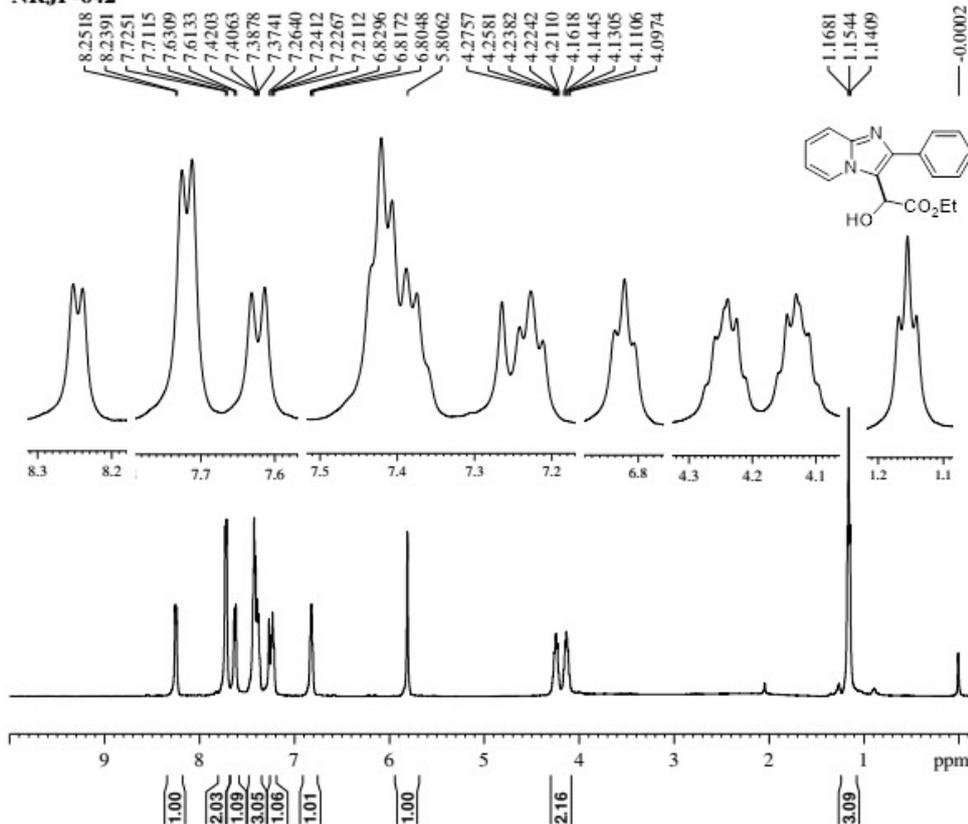
==== CHANNEL f1 =====
 SFO1 100.6304993 MHz
 NUC1 13C
 PI 9.25 usec
 PLW1 53.0000000 W

==== CHANNEL f2 =====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.0000000 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. ¹³C NMR Spectrum of 5x

NRJP-642



Current Data Parameters
 NAME 26-DEC-FN-2025
 EXPNO 430
 PROCNO 1

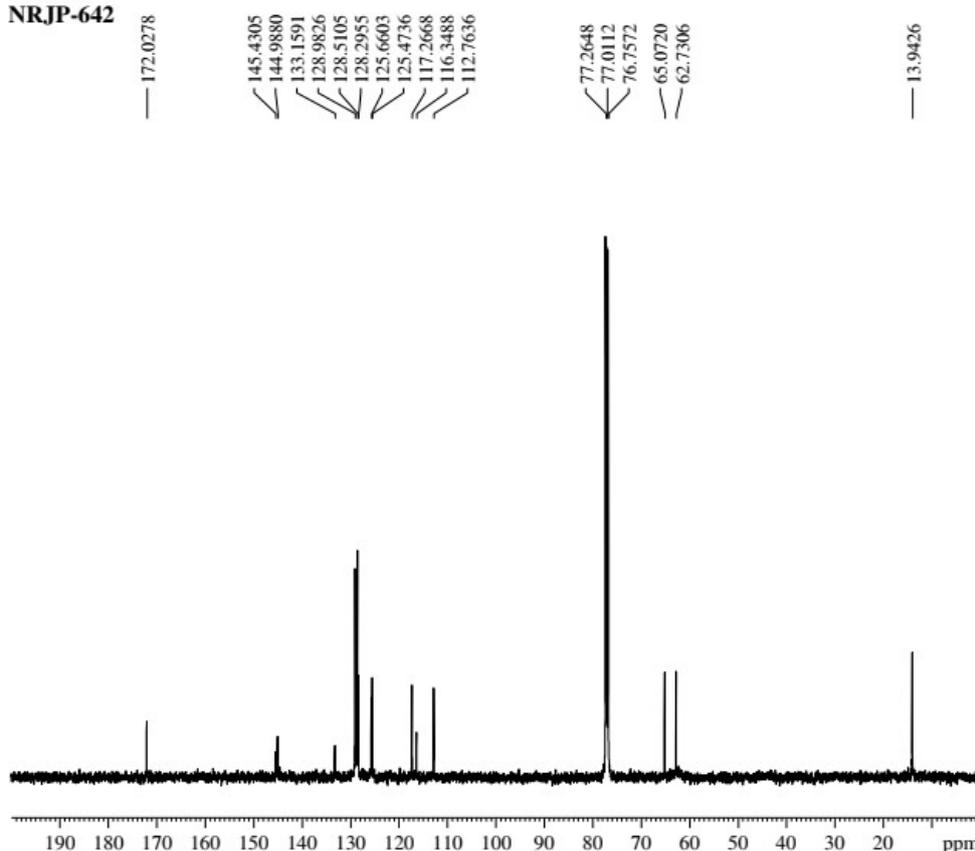
F2 - Acquisition Parameters
 Date_ 20241226
 Time 8.25
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 10026.738 Hz
 FIDRES 0.152996 Hz
 AQ 3.2680619 sec
 RG 136.78
 DW 49.867 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 ====
 SFO1 500.6794419 MHz
 NUC1 1H
 P1 6.45 usec
 PLW1 13.60000038 W

F2 - Processing parameters
 SI 65536
 SF 500.6763601 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S54. ¹H NMR Spectrum of 5y

NRJP-642



Current Data Parameters
 NAME 10-DEC-FN-2025
 EXPNO 310
 PROCNO 1

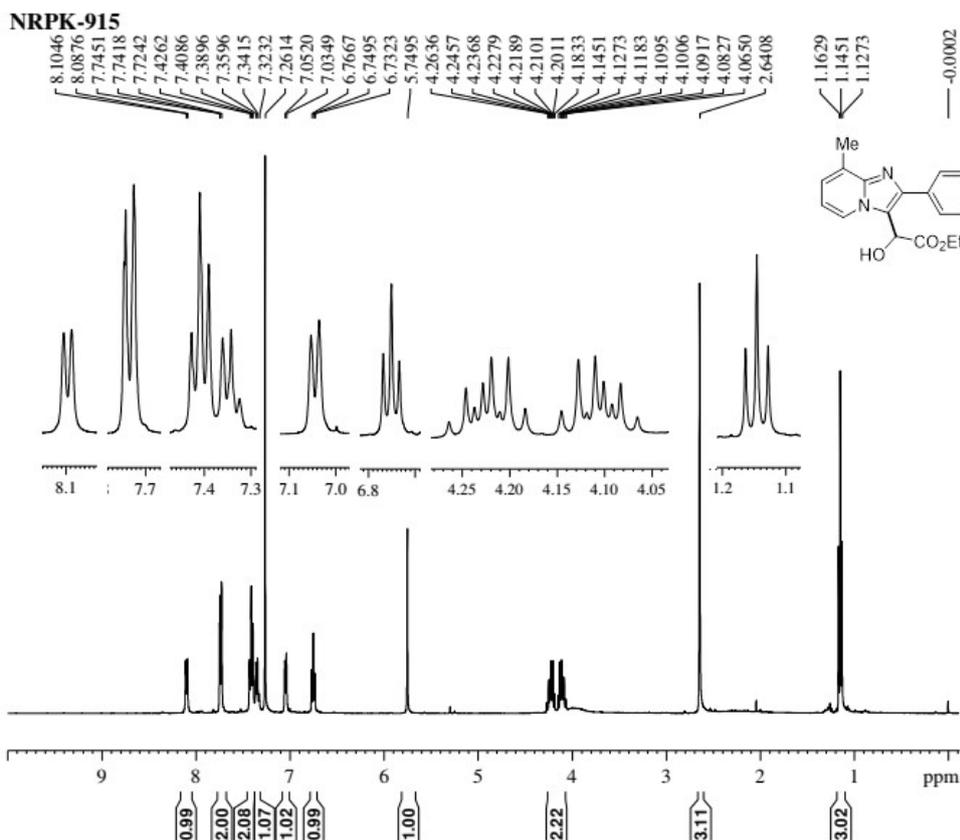
F2 - Acquisition Parameters
 Date_ 20251210
 Time 11.58
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 107.78
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.0000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 ====
 SFO1 125.9077573 MHz
 NUC1 13C
 P1 9.23 usec
 PLW1 244.00000000 W

==== CHANNEL f2 ====
 SFO2 500.6783527 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 13.60000038 W
 PLW12 0.08840500 W
 PLW13 0.05657900 W

F2 - Processing parameters
 SI 32768
 SF 125.8951728 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Figure S55. ¹³C NMR Spectrum of 5y



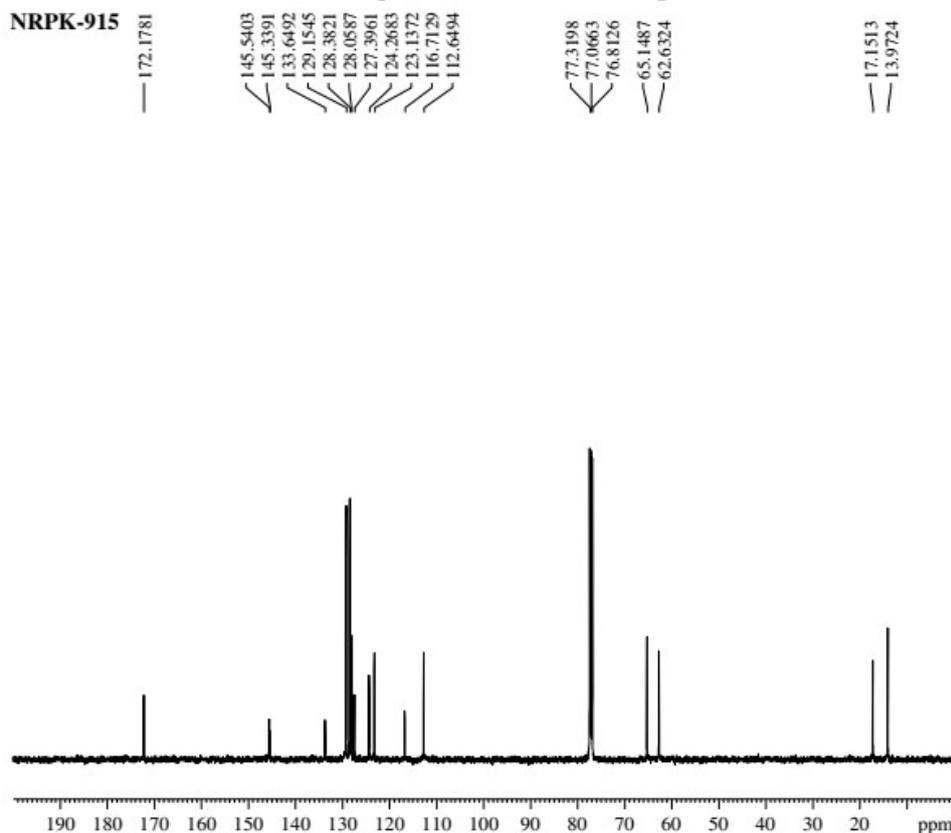
Current Data Parameters
 NAME 11-DEC-AN-2025
 EXPNO 330
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251211
 Time 22.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 129.57
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 13.75 usec
 PLW1 13.0000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1605091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S56. ¹H NMR Spectrum of 5z



Current Data Parameters
 NAME 09-DEC-AN-2025
 EXPNO 370
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251209
 Time 17.22
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 107.78
 DW 16.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.0000000 sec
 D11 0.03000000 sec
 TDO 1

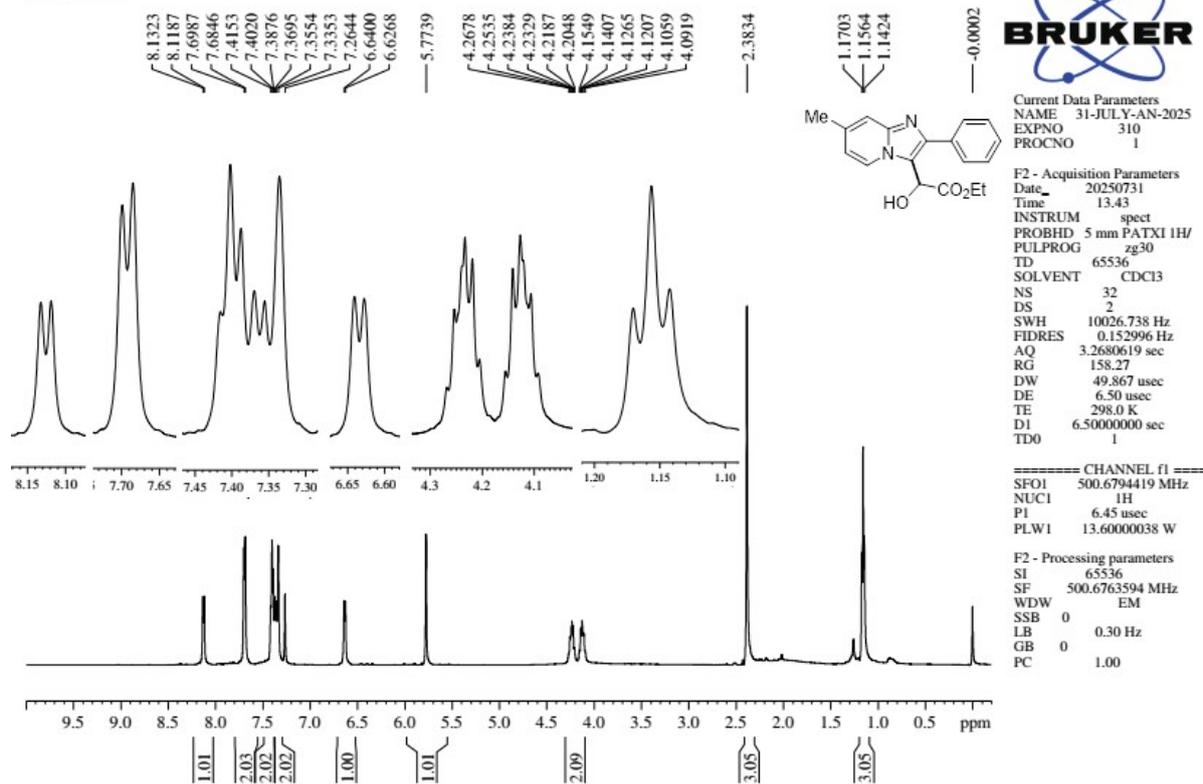
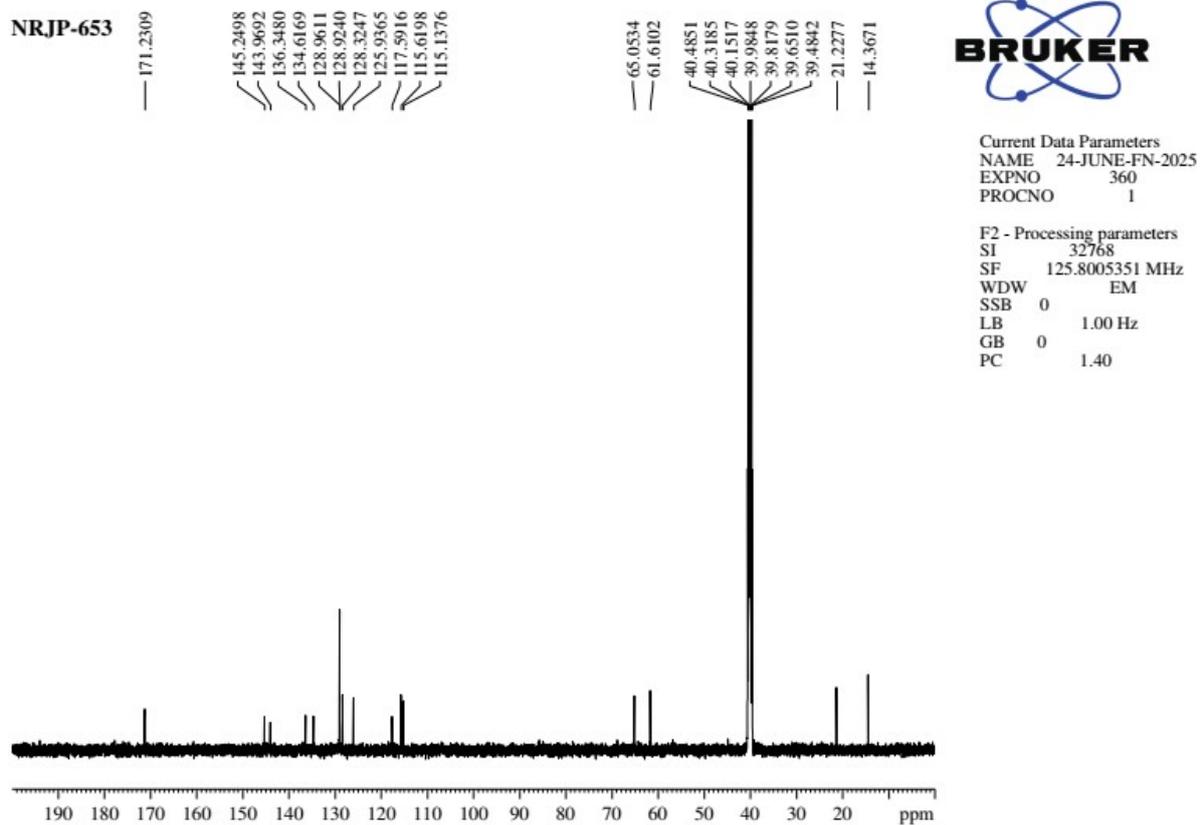
===== CHANNEL f1 =====
 SFO1 125.9077573 MHz
 NUC1 13C
 P1 9.23 usec
 PLW1 244.0000000 W

===== CHANNEL f2 =====
 SFO2 500.6783527 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 13.60000038 W
 PLW12 0.08840500 W
 PLW13 0.05657900 W

F2 - Processing parameters
 SI 32768
 SF 125.8951680 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Figure S57. ¹³C NMR Spectrum of 5z

NRJP-653

Figure S58. ¹H NMR Spectrum of 5aaFigure S59. ¹³C NMR Spectrum of 5aa

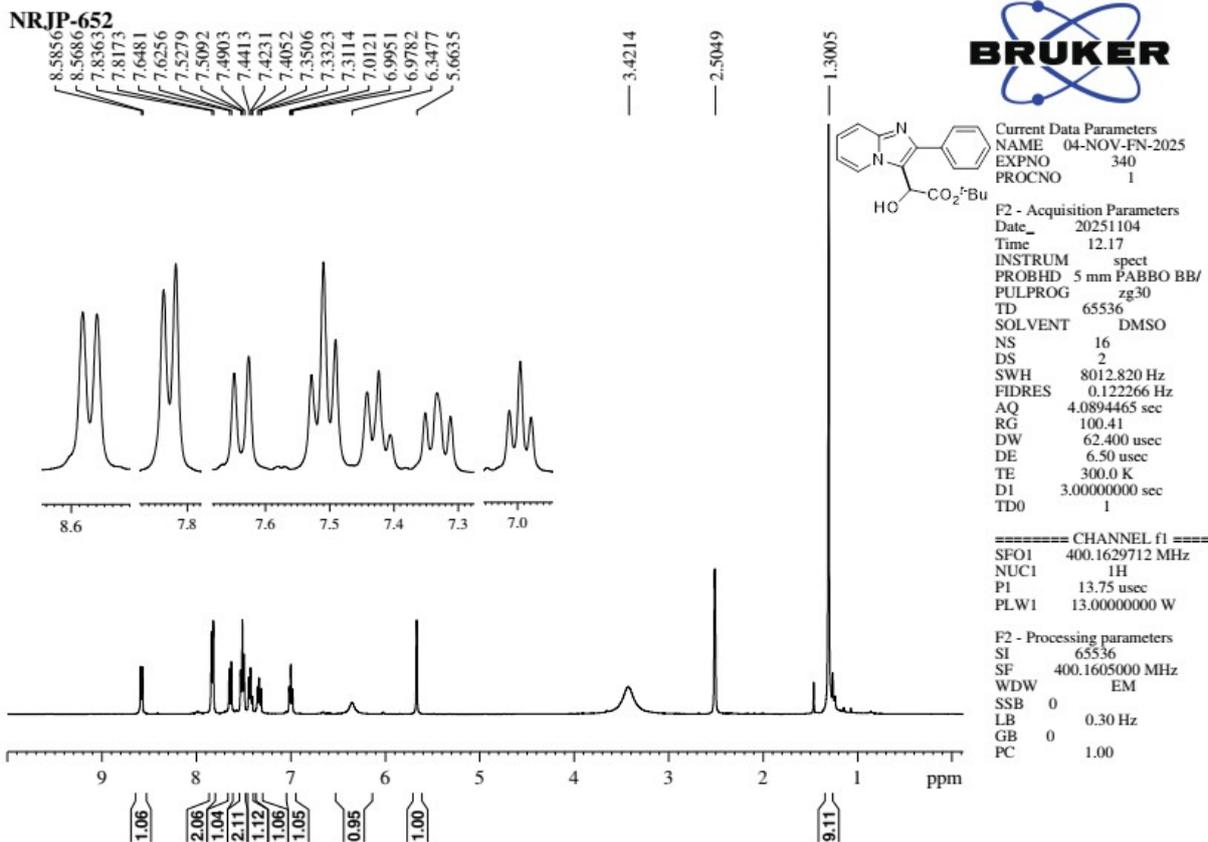


Figure S60. ¹H NMR Spectrum of 5ab

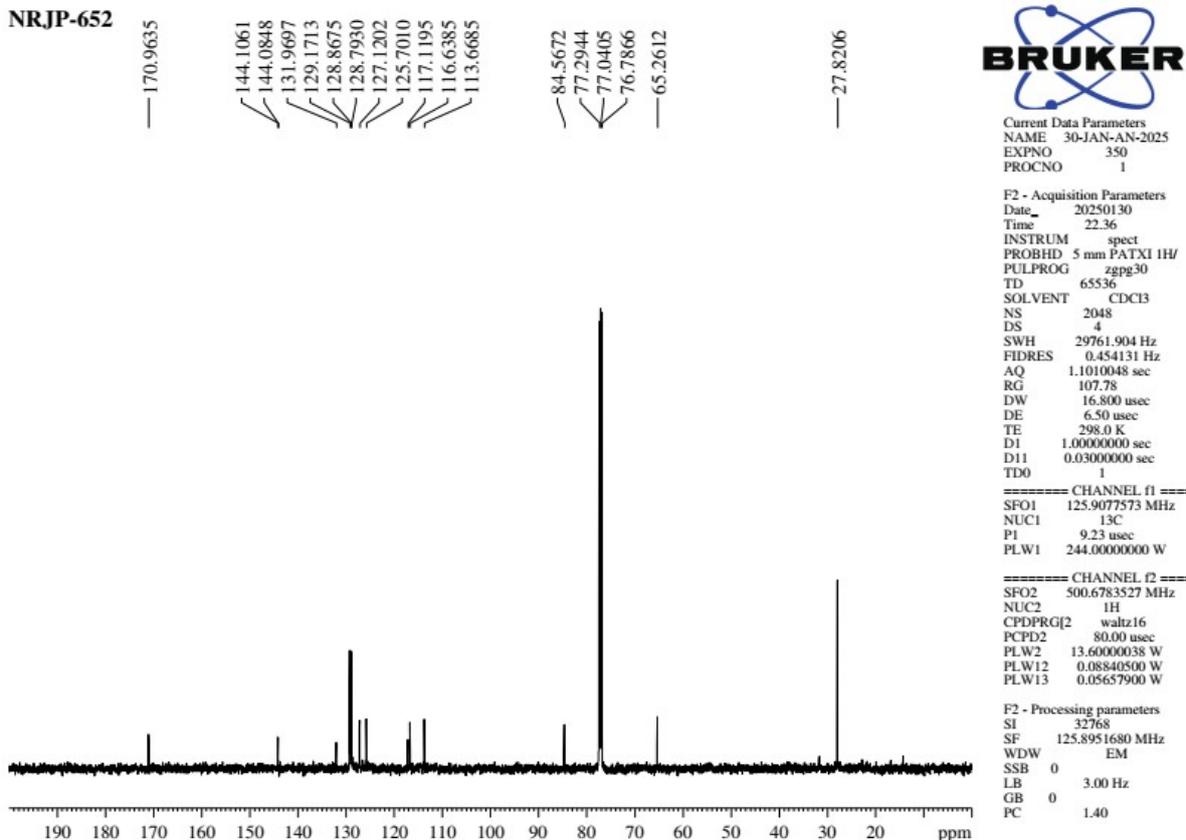
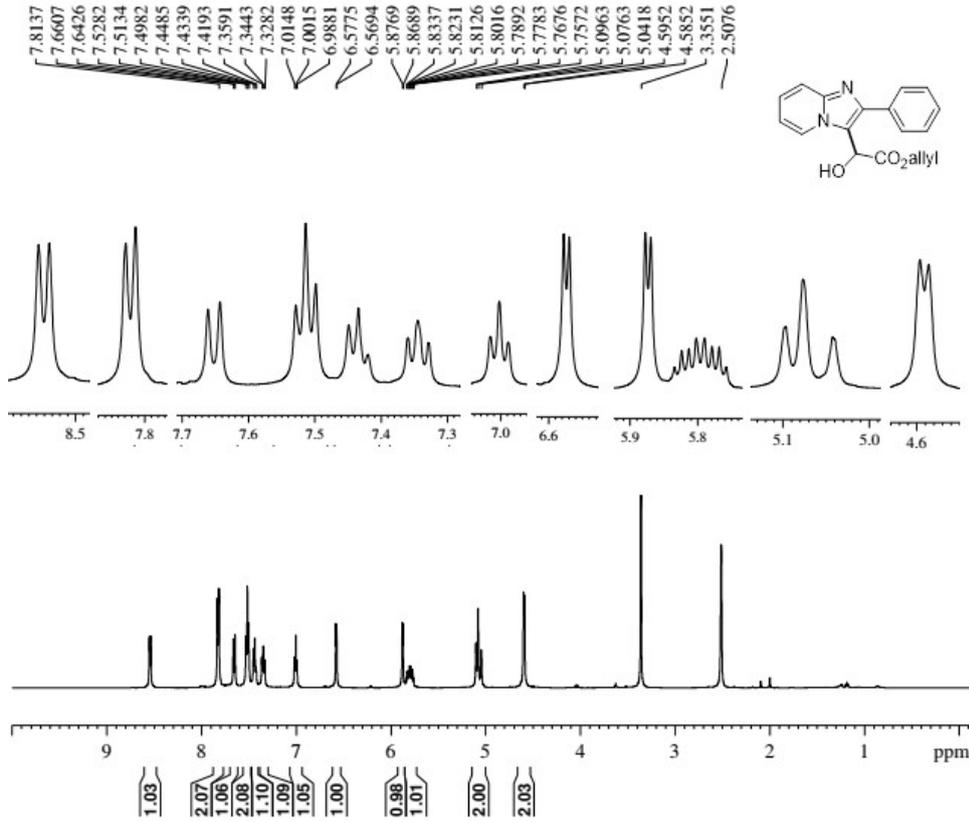


Figure S61. ¹³C NMR Spectrum of 5ab

NRJP-654



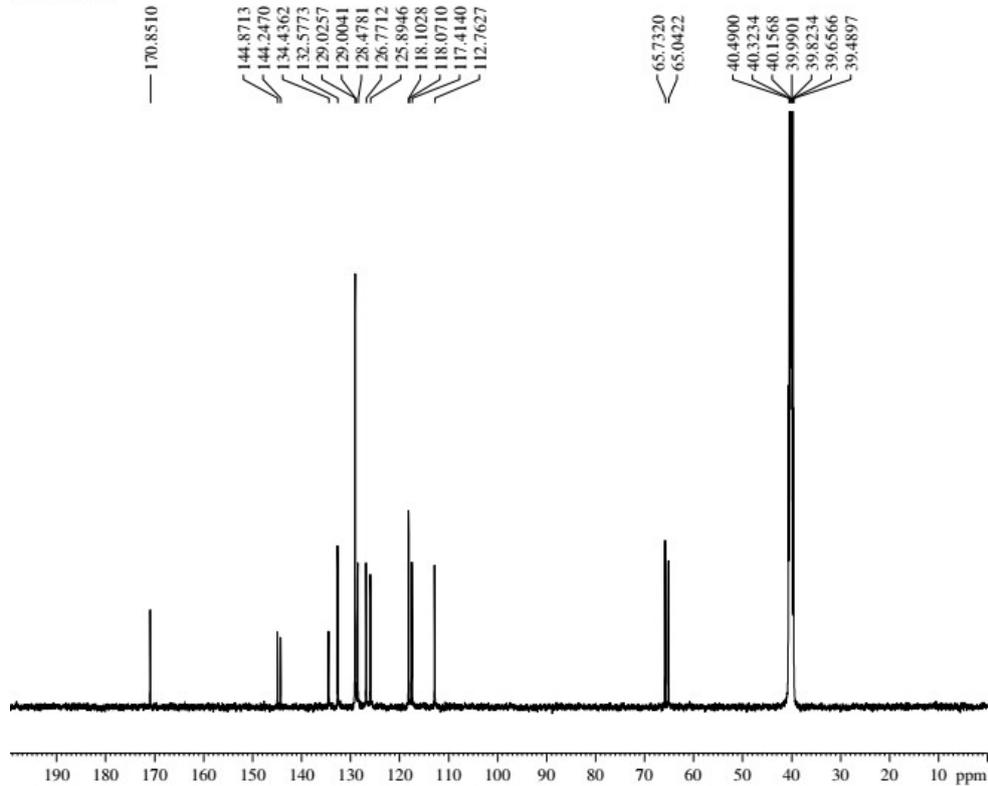
Current Data Parameters
 NAME 30-MAY-AN-2025
 EXPNO 340
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250530
 Time 16.55 h
 INSTRUM Avance neo 500Mhz :
 PROBHD Z151574_0224 (:
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2768000 sec
 RG 101
 DW 50.000 usec
 DE 11.14 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.3030894 MHz
 NUC1 1H
 P0 2.67 usec
 P1 8.00 usec
 PLW1 24.32900047 W

F2 - Processing parameters
 SI 65536
 SF 500.3000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S62. ¹H NMR Spectrum of 5ac

NRJP-654

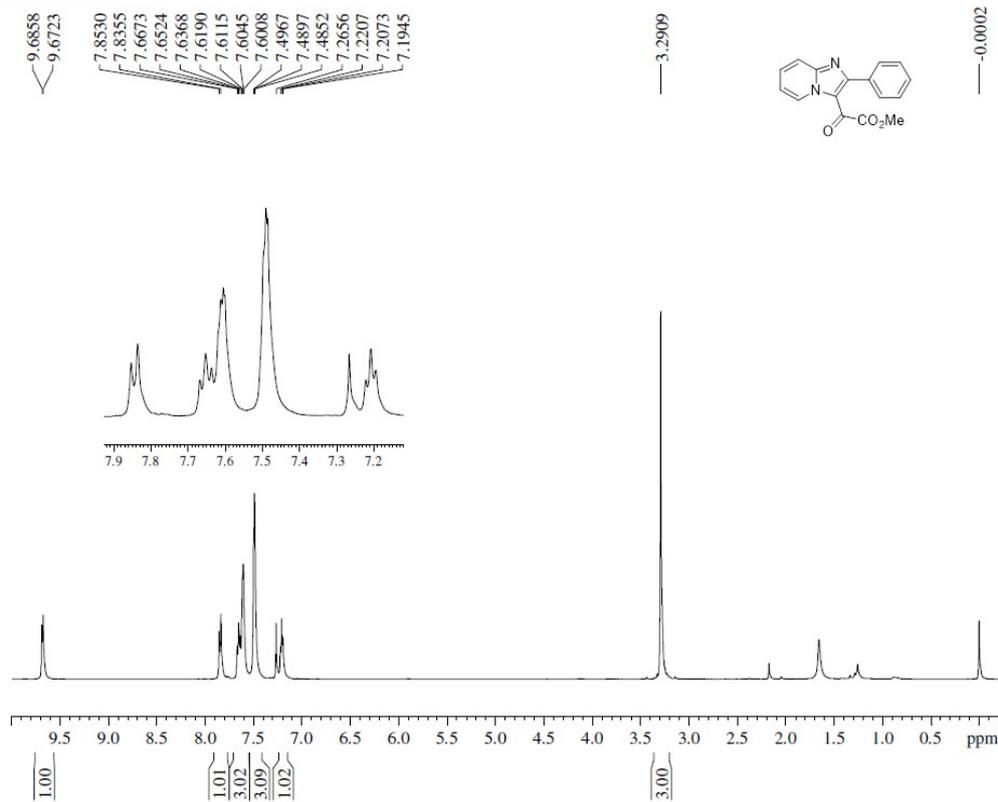


Current Data Parameters
 NAME 29-MAY-FN-2025
 EXPNO 360
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 125.8005351 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

Figure S63. ¹³C NMR Spectrum of 5ac

NRJP-702



Current Data Parameters
 NAME 26-MAY-AN-2025
 EXPNO 360
 PROCNO 1

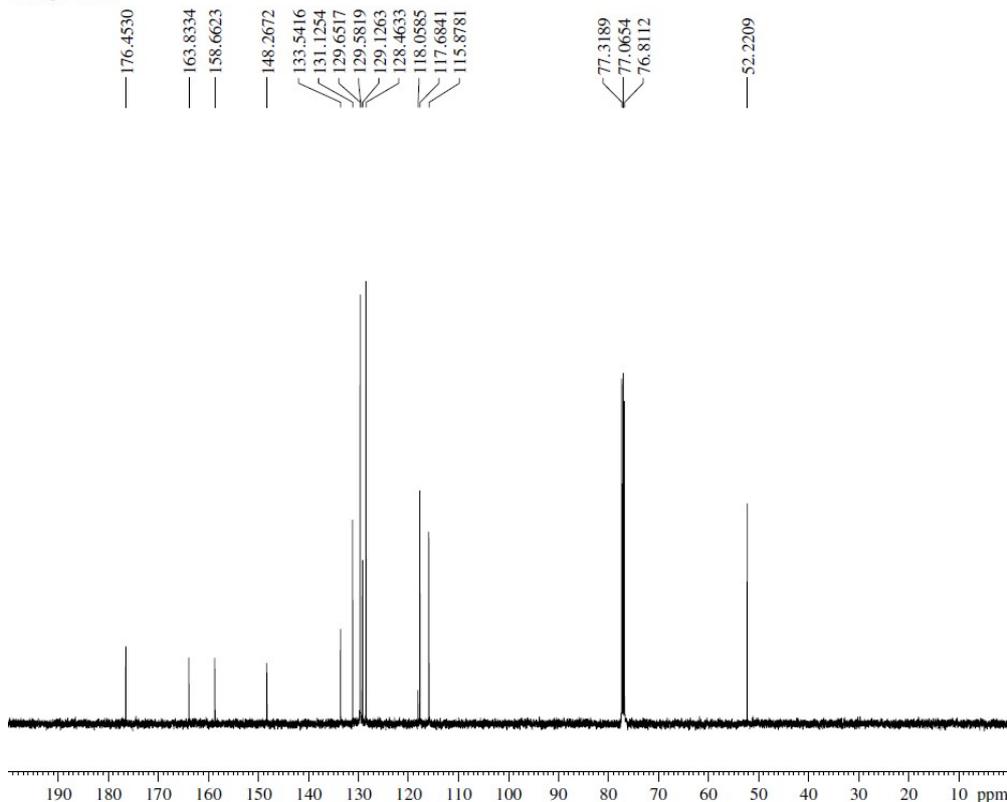
F2 - Acquisition Parameters
 Date_ 20250526
 Time 14.41
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 10026.738 Hz
 FIDRES 0.152996 Hz
 AQ 3.2680619 sec
 RG 201.78
 DW 49.867 usec
 DE 6.50 usec
 TE 298.7 K
 D1 6.5000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 500.6794419 MHz
 NUC1 1H
 P1 6.45 usec
 PLW1 13.60000038 W

F2 - Processing parameters
 SI 65536
 SF 500.6763611 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S64. ¹H NMR Spectrum of 7

NRJP-702



Current Data Parameters
 NAME 23-MAY-FN-2025
 EXPNO 450
 PROCNO 1

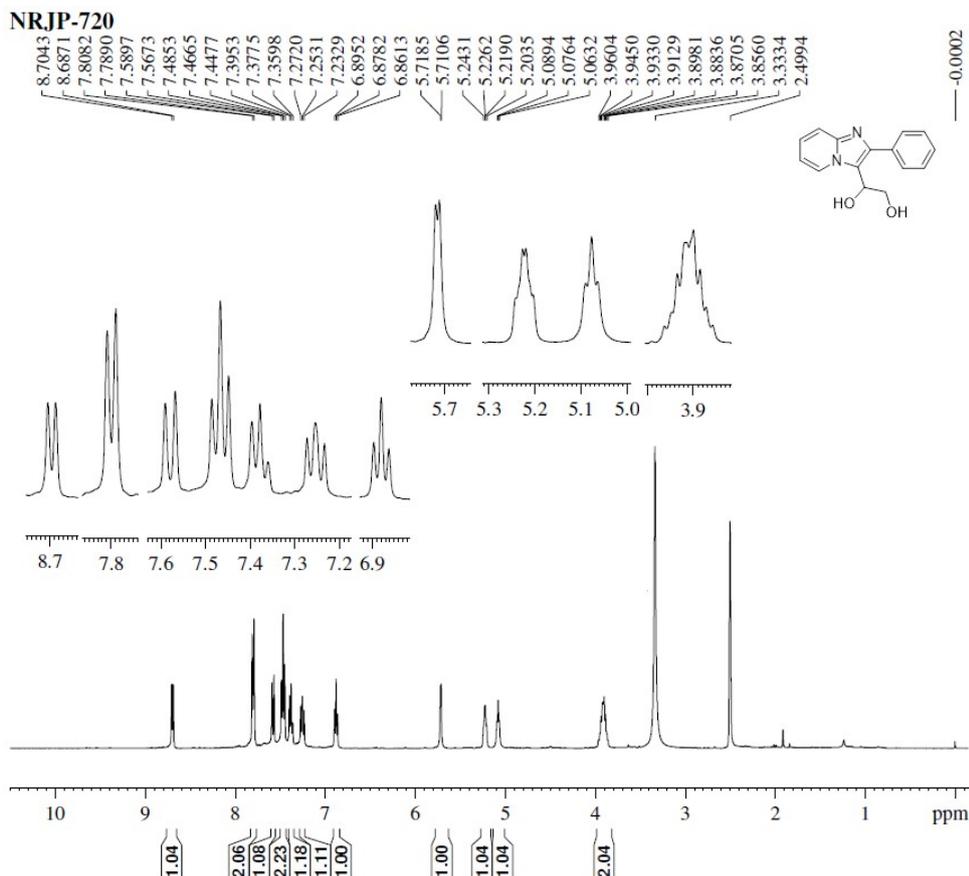
F2 - Acquisition Parameters
 Date_ 20250523
 Time 11.02
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 107.78
 DW 16.800 usec
 DE 6.50 usec
 TE 299.4 K
 D1 1.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 125.9077573 MHz
 NUC1 13C
 P1 9.25 usec
 PLW1 244.0000000 W

===== CHANNEL f2 =====
 SFO2 500.6783527 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 13.60000038 W
 PLW12 0.08840500 W
 PLW13 0.05657900 W

F2 - Processing parameters
 SI 32768
 SF 125.8951680 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure S65. ¹³C NMR Spectrum of 7



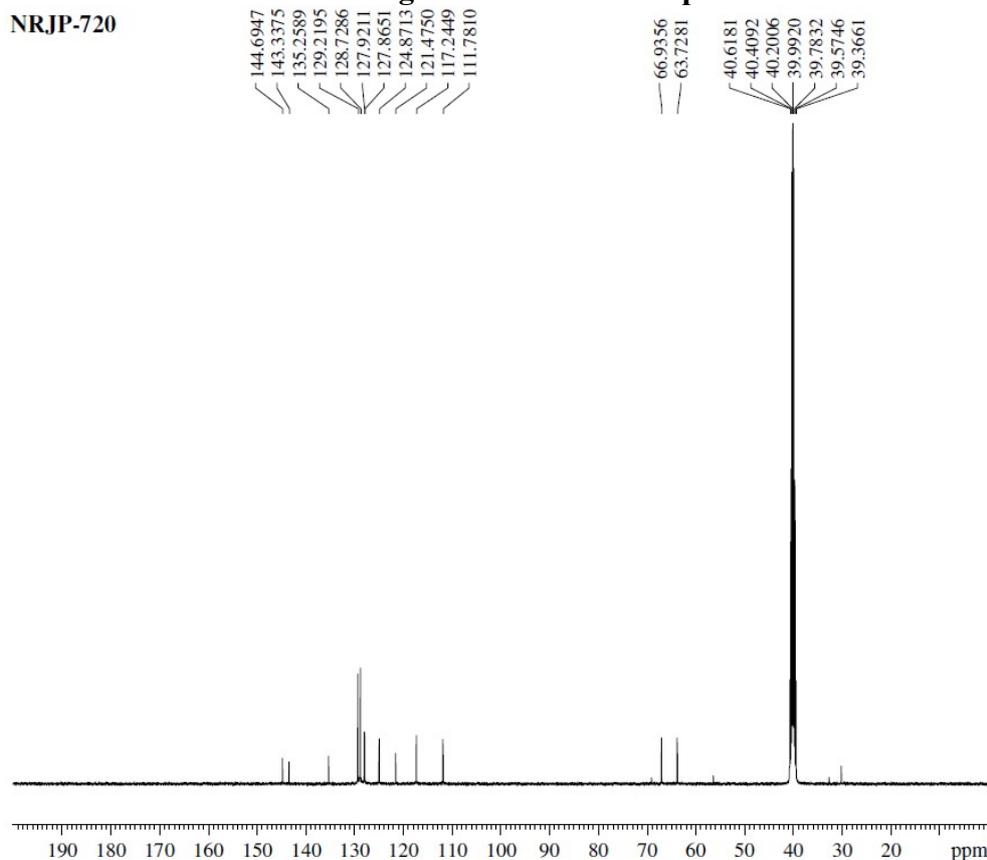
Current Data Parameters
 NAME 22-OCT-AN-2025
 EXPNO 440
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251022
 Time 17.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 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 1.50000000 sec
 TDO 1

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

F2 - Processing parameters
 SI 65536
 SF 400.1605027 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S66. ¹H NMR Spectrum of 8



Current Data Parameters
 NAME 08-OCT-AN-2025
 EXPNO 330
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251009
 Time 3.22
 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 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 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
 CPDPRG2 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 S67. ¹³C NMR Spectrum of 8

Sample: 447
 File:HRMS25130OCT25_COD
 Description:NRJP651 T

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

ID:HRMS25130OCT25
 Time:11:53:10
 Formula:

Printed: Thu Oct 30 14:36:01 2025

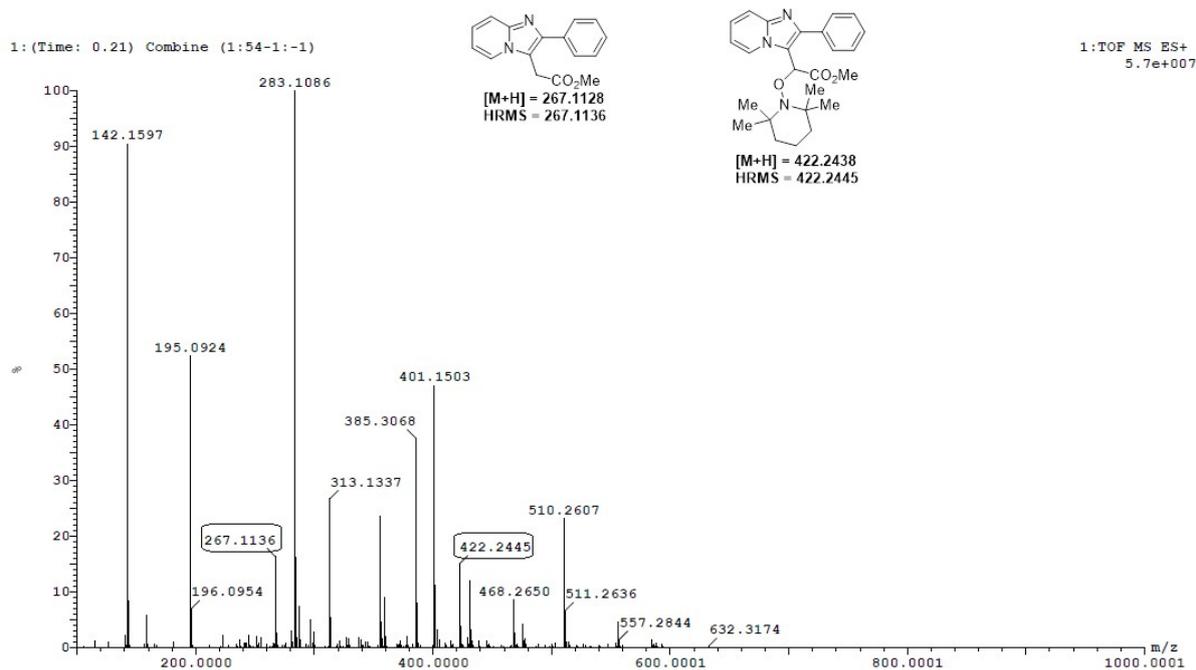


Figure S68. HRMS spectra of 6