

Supporting Information

Photocatalytic Intramolecular [2+2] Cycloaddition of Indole Derivatives *via* Energy Transfer: A Method for Late-Stage Skeletal Transformation

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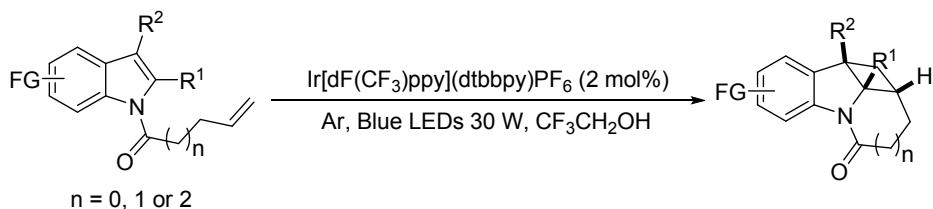
1. General information

All reactions were carried out under Argon atmosphere in Schlenk tubes. Anhydrous solvent (including DCM, DCE, DMF, THF, DMSO, DME, CH₃CN, MeOH, Water < 0.005%) were purchased from Energy, and used as received. Solvent (including TFE and EtOH, reagent grade) and commercially available compounds were purchased from Aldrich, Energy, J&K and TCI Chemical Company as reagent grade and used without further purification unless otherwise stated. ¹H NMR and ¹³C NMR spectra were obtained in CDCl₃ or DMSO-d₆ on bruker advance 400 with TMS as internal standard at room temperature. ¹⁹F NMR spectra were recorded on bruker advance 400 and referenced relative to CFCl₃. Chemical shifts (δ) were quoted in parts per million (ppm). HRMS were performed on a SCIEX UPLC (EXion) – QTOF (X500R). Cyclic voltammetry tests were carried out with a CHI700E electrochemical workstation. Melting points were obtained with a Hanon melting point apparatus (MP470). Flash column chromatography was carried out on silica gel (100-200 mesh).

Substrates **1a-1u**, **1w** and **1aa-1ag** were synthesized according to the literature procedures.¹ Substrate **1v** was synthesized according to the literature procedure.² Substrate **1x** was synthesized according to the literature procedure.³

2. Typical experimental procedure

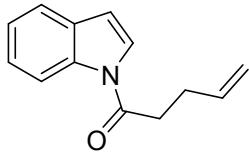
General procedure for visible-light promoted intramolecular dearomatic [2+2] cycloaddition of indole derivatives.



An oven-dried Schlenk tube (10 mL) containing a stirring bar was charged with the substrates (0.1 mmol) and photosensitizer (2 mol%). The Schlenk tube was then connected to a vacuum line where it was evacuated and back-filled with argon for 3 times. Then trifluoroethanol (1 mL), which was bubbled with argon for 5 minutes, was added under argon flow. Finally, the reaction mixture in sealed tube was placed at a distance of 2 ~ 3 cm from a 30 W blue LED and stirred at room temperature for 12 ~ 36 h. Then, the mixture was concentrated in vacuo and purified by silica gel flash chromatography (petroleum ether/ethyl acetate 10/1 ~ 1/1 or CH₂Cl₂/MeOH 100/1 ~ 20/1) to afford the corresponding product.

3. Characterization data for substrates and products

1-(1*H*-indol-1-yl)pent-4-en-1-one (1a**)**



Colorless liquid.

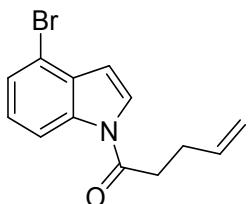
¹H NMR (400 MHz, CDCl₃) δ 8.47 (d, *J* = 8.2 Hz, 1H), 7.60 – 7.52 (m, 1H), 7.45 (d, *J* = 3.8 Hz, 1H), 7.38 – 7.32 (m, 1H), 7.30 – 7.24 (m, 1H), 6.68 – 6.60 (m, 1H), 5.94 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.19 – 5.10 (m, 1H), 5.10 – 5.02 (m, 1H), 3.07 – 2.97 (m, 2H), 2.65 – 2.54 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 170.8, 136.5, 135.6, 130.3, 125.2, 124.5, 123.7, 120.9, 116.6, 116.0, 109.2, 35.1, 28.5.

HRMS (ESI) calcd for C₁₃H₁₄NO [M+H]⁺: 200.1070. Found: 200.1064.

Analytical data for compound **1a** was consistent with the literature except for the chemical shift of a unsaturated carbon.⁴

1-(4-bromo-1*H*-indol-1-yl)pent-4-en-1-one (1b**)**



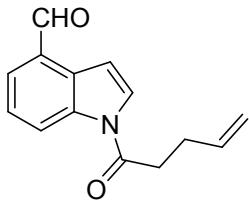
White solid, m.p. = 53.0–54.9 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.43 (d, *J* = 8.3 Hz, 1H), 7.51 (d, *J* = 3.8 Hz, 1H), 7.44 (dd, *J* = 7.8, 0.7 Hz, 1H), 7.21 (t, *J* = 8.1 Hz, 1H), 6.72 (dd, *J* = 3.8, 0.6 Hz, 1H), 5.93 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.18 – 5.11 (m, 1H), 5.10 – 5.05 (m, 1H), 3.08 – 2.97 (m, 2H), 2.66 – 2.53 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 170.8, 136.2, 135.9, 130.9, 126.6, 126.2, 125.0, 116.2, 115.7, 114.6, 108.9, 35.0, 28.3.

HRMS (ESI) calcd for C₁₃H₁₃BrNO [M+H]⁺: 278.0175. Found: 278.0177.

1-pent-4-enoyl-1*H*-indole-4-carbaldehyde (1c**)**



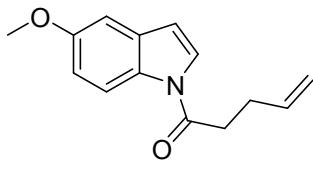
White solid, m.p. = 90.1–90.9 °C.

¹H NMR (400 MHz, CDCl₃) δ 10.23 (s, 1H), 8.77 (d, *J* = 8.3 Hz, 1H), 7.76 (d, *J* = 7.3 Hz, 1H), 7.65 (d, *J* = 3.7 Hz, 1H), 7.55 – 7.44 (m, 2H), 5.94 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.20 – 5.12 (m, 1H), 5.12 – 5.05 (m, 1H), 3.07 (t, *J* = 7.4 Hz, 2H), 2.66 – 2.55 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 192.7, 171.0, 136.24, 136.16, 129.8, 128.6, 128.2, 127.5, 124.9, 122.5, 116.3, 108.5, 35.1, 28.3.

HRMS (ESI) calcd for C₁₄H₁₄NO₂ [M+H]⁺: 228.1019. Found: 228.1018.

1-(5-methoxy-1*H*-indol-1-yl)pent-4-en-1-one (1d**)**



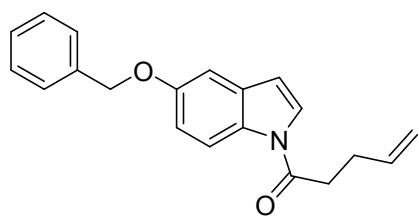
White solid, m.p. = 65.4–66.6 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.35 (d, *J* = 8.9 Hz, 1H), 7.43 (d, *J* = 3.6 Hz, 1H), 7.02 (d, *J* = 2.5 Hz, 1H), 6.95 (dd, *J* = 9.0, 2.5 Hz, 1H), 6.57 (d, *J* = 3.7 Hz, 1H), 5.93 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.17 – 5.10 (m, 1H), 5.09 – 5.04 (m, 1H), 3.85 (s, 3H), 3.04 – 2.93 (m, 2H), 2.62 – 2.54 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 170.4, 156.4, 136.6, 131.3, 130.4, 125.2, 117.4, 116.0, 113.5, 109.0, 103.5, 55.7, 34.8, 28.5.

HRMS (ESI) calcd for C₁₄H₁₆NO₂ [M+H]⁺: 230.1176. Found: 230.1169.

1-(5-(benzyloxy)-1*H*-indol-1-yl)pent-4-en-1-one (1e)



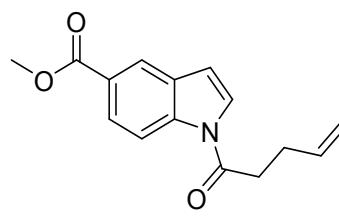
White solid, m.p. = 124.3–125.0 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.37 (d, *J* = 8.6 Hz, 1H), 7.54 – 7.30 (m, 6H), 7.10 (d, *J* = 2.4 Hz, 1H), 7.04 (dd, *J* = 9.0, 2.2 Hz, 1H), 6.56 (d, *J* = 3.7 Hz, 1H), 5.94 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.24 – 5.01 (m, 4H), 3.08 – 2.91 (m, 2H), 2.63 – 2.54 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 170.4, 155.6, 137.2, 136.6, 131.3, 130.6, 128.6, 127.9, 127.5, 125.2, 117.4, 116.0, 114.3, 109.1, 105.0, 70.5, 34.9, 28.5.

HRMS (ESI) calcd for C₂₀H₂₀NO₂ [M+H]⁺: 306.1489. Found: 306.1483.

methyl 1-pent-4-enoyl-1*H*-indole-5-carboxylate (1f)



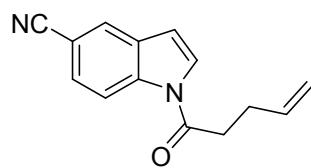
White solid, m.p. = 124.5–125.2 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.50 (d, *J* = 8.7 Hz, 1H), 8.29 (d, *J* = 1.1 Hz, 1H), 8.05 (dd, *J* = 8.7, 1.6 Hz, 1H), 7.53 (d, *J* = 3.8 Hz, 1H), 6.71 (d, *J* = 3.8 Hz, 1H), 5.94 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.20 – 5.11 (m, 1H), 5.11 – 5.05 (m, 1H), 3.94 (s, 3H), 3.03 (t, *J* = 7.4 Hz, 2H), 2.65 – 2.55 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 170.8, 167.4, 138.2, 136.3, 130.1, 126.5, 125.7, 125.5, 123.1, 116.30, 116.25, 109.6, 52.2, 35.1, 28.3.

HRMS (ESI) calcd for C₁₅H₁₆NO₃ [M+H]⁺: 258.1125. Found: 258.1125.

1-pent-4-enoyl-1*H*-indole-5-carbonitrile (1g)



White solid, m.p. = 99.7–100.7 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.58 (dd, *J* = 8.6, 0.9 Hz, 1H), 7.90 (d, *J* = 1.8 Hz, 1H), 7.64 – 7.57 (m, 2H), 6.71 (dd, *J* = 3.8, 0.8 Hz, 1H), 5.93 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.20 – 5.12 (m, 1H), 5.12 – 5.06 (m, 1H), 3.05 (t, *J* = 7.4 Hz, 2H), 2.66 – 2.56 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 170.8, 137.3, 136.0, 130.2, 128.3, 126.6, 125.6, 119.6, 117.4, 116.4, 108.7, 107.0, 35.1, 28.1.

HRMS (ESI) calcd for C₁₄H₁₃N₂O [M+H]⁺: 225.1022. Found: 225.1019.

1-(5-fluoro-1*H*-indol-1-yl)pent-4-en-1-one (1h)



White solid, m.p. = 54.1–54.8 °C.

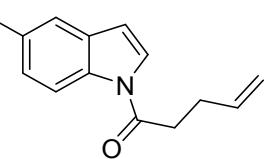
¹H NMR (400 MHz, CDCl₃) δ 8.43 (dd, *J* = 9.0, 4.7 Hz, 1H), 7.50 (d, *J* = 3.8 Hz, 1H), 7.21 (dd, *J* = 8.7, 2.6 Hz, 1H), 7.07 (td, *J* = 9.1, 2.6 Hz, 1H), 6.60 (d, *J* = 3.8 Hz, 1H), 5.93 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.18 – 5.11 (m, 1H), 5.10 – 5.05 (m, 1H), 3.07 – 2.96 (m, 2H), 2.65 – 2.54 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 170.5, 159.6 (d, *J* = 240.0 Hz), 136.4, 132.0, 131.3 (d, *J* = 10.1 Hz), 126.0, 117.6 (d, *J* = 9.0 Hz), 116.1, 112.8 (d, *J* = 24.7 Hz), 108.8 (d, *J* = 4.0 Hz), 106.4 (d, *J* = 23.8 Hz), 34.8, 28.4.

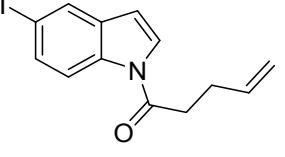
¹⁹F NMR (376 MHz, CDCl₃) δ -119.35.

HRMS (ESI) calcd for C₁₃H₁₃FNO [M+H]⁺: 218.0976. Found: 218.0975.

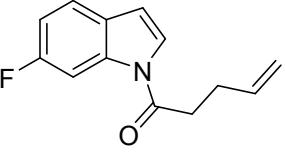
1-(5-chloro-1*H*-indol-1-yl)pent-4-en-1-one (1i)


White solid, m.p. = 53.1–53.9 °C.
¹H NMR (400 MHz, CDCl₃) δ 8.39 (d, *J* = 8.8 Hz, 1H), 7.52 (d, *J* = 2.1 Hz, 1H), 7.47 (d, *J* = 3.7 Hz, 1H), 7.30 (dd, *J* = 8.8, 2.1 Hz, 1H), 6.57 (d, *J* = 3.7 Hz, 1H), 5.93 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.18 – 5.11 (m, 1H), 5.10 – 5.05 (m, 1H), 3.00 (t, *J* = 7.4 Hz, 2H), 2.64 – 2.53 (m, 2H).
¹³C NMR (101 MHz, CDCl₃) δ 170.6, 136.3, 134.0, 131.5, 129.2, 125.7, 125.2, 120.4, 117.6, 116.2, 108.4, 34.9, 28.3.
HRMS (ESI) calcd for C₁₃H₁₃ClNO [M+H]⁺: 234.0680. Found: 234.0680.

1-(5-iodo-1*H*-indol-1-yl)pent-4-en-1-one (1j)


White solid, m.p. = 73.5–73.9 °C.
¹H NMR (400 MHz, CDCl₃) δ 8.23 (d, *J* = 8.7 Hz, 1H), 7.90 (d, *J* = 1.6 Hz, 1H), 7.61 (dd, *J* = 8.7, 1.6 Hz, 1H), 7.42 (d, *J* = 3.8 Hz, 1H), 6.56 (d, *J* = 3.8 Hz, 1H), 5.92 (ddt, *J* = 16.9, 10.2, 6.5 Hz, 1H), 5.18 – 5.11 (m, 1H), 5.10 – 5.04 (m, 1H), 3.00 (t, *J* = 7.4 Hz, 2H), 2.63 – 2.54 (m, 2H).
¹³C NMR (101 MHz, CDCl₃) δ 170.6, 136.3, 134.8, 133.6, 132.5, 129.7, 125.2, 118.4, 116.2, 108.1, 87.8, 35.0, 28.3.
HRMS (ESI) calcd for C₁₃H₁₃INO [M+H]⁺: 326.0036. Found: 326.0035.

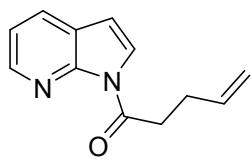
1-(6-fluoro-1*H*-indol-1-yl)pent-4-en-1-one (1k)


White solid, m.p. = 34.2–35.2 °C.
¹H NMR (400 MHz, CDCl₃) δ 8.22 (dd, *J* = 10.3, 1.8 Hz, 1H), 7.56 – 7.40 (m, 2H), 7.03 (td, *J* = 8.9, 2.3 Hz, 1H), 6.61 (d, *J* = 3.8 Hz, 1H), 5.93 (ddt, *J* = 16.9, 10.2, 6.5 Hz, 1H), 5.19 – 5.11 (m, 1H), 5.11 – 5.05 (m, 1H), 3.00 (t, *J* = 7.4 Hz, 2H), 2.64 – 2.54 (m, 2H).
¹³C NMR (101 MHz, CDCl₃) δ 170.7, 161.3 (d, *J* = 240.7 Hz), 136.3, 135.7 (d, *J* = 13.1 Hz), 126.4, 124.7 (d, *J* = 4.0 Hz), 121.3 (d, *J* = 9.9 Hz), 116.1, 111.9 (d, *J* = 24.3 Hz), 108.9, 104.1 (d, *J* = 28.7 Hz), 34.9, 28.3.
¹⁹F NMR (376 MHz, CDCl₃) δ -116.47.
HRMS (ESI) calcd for C₁₃H₁₃FNO [M+H]⁺: 218.0976. Found: 218.0974.

methyl 1-pent-4-enoyl-1*H*-indole-6-carboxylate (1l)


White solid, m.p. = 95.2–95.7 °C.
¹H NMR (400 MHz, CDCl₃) δ 9.14 (s, 1H), 8.00 – 7.95 (m, 1H), 7.64 – 7.55 (m, 2H), 6.67 (d, *J* = 3.6 Hz, 1H), 5.94 (ddt, *J* = 16.8, 10.1, 6.5 Hz, 1H), 5.19 – 5.12 (m, 1H), 5.11 – 5.05 (m, 1H), 3.94 (s, 3H), 3.03 (t, *J* = 7.4 Hz, 2H), 2.65 – 2.56 (m, 2H).
¹³C NMR (101 MHz, CDCl₃) δ 170.6, 167.6, 136.3, 135.0, 134.0, 127.3, 126.8, 124.9, 120.5, 118.3, 116.2, 108.9, 52.1, 35.0, 28.2.
HRMS (ESI) calcd for C₁₅H₁₆NO₃ [M+H]⁺: 258.1125. Found: 258.1121.

1-(1*H*-pyrrolo[2,3-*b*]pyridin-1-yl)pent-4-en-1-one (1m)



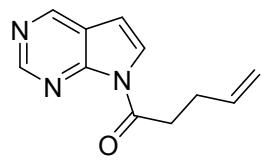
Colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 8.37 (dd, *J* = 4.8, 1.4 Hz, 1H), 8.00 (d, *J* = 4.1 Hz, 1H), 7.88 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.19 (dd, *J* = 7.8, 4.8 Hz, 1H), 6.59 (d, *J* = 4.1 Hz, 1H), 5.99 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.19 – 5.12 (m, 1H), 5.07 – 5.02 (m, 1H), 3.68 (t, *J* = 7.4 Hz, 2H), 2.64 – 2.57 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 171.5, 147.6, 143.8, 137.1, 129.3, 125.5, 123.8, 118.6, 115.5, 105.7, 37.1, 28.5.

HRMS (ESI) calcd for C₁₂H₁₃N₂O [M+H]⁺: 201.1022. Found: 201.1022.

1-(7*H*-pyrrolo[2,3-*d*]pyrimidin-7-yl)pent-4-en-1-one (1n)



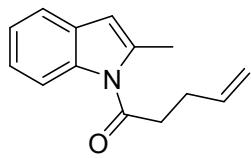
White solid, m.p. = 48.6–49.0 °C.

¹H NMR (400 MHz, CDCl₃) δ 9.07 – 8.92 (m, 2H), 8.02 – 7.96 (m, 1H), 6.69 – 6.64 (m, 1H), 5.95 (ddt, *J* = 12.9, 10.1, 6.5 Hz, 1H), 5.21 – 5.09 (m, 1H), 5.09 – 5.02 (m, 1H), 3.69 – 3.59 (m, 2H), 2.66 – 2.54 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 171.0, 152.7, 151.3, 150.0, 136.6, 126.3, 121.7, 115.9, 104.1, 37.3, 28.3.

HRMS (ESI) calcd for C₁₁H₁₂N₃O [M+H]⁺: 202.0975. Found: 202.0975.

1-(2-methyl-1*H*-indol-1-yl)pent-4-en-1-one (1o)



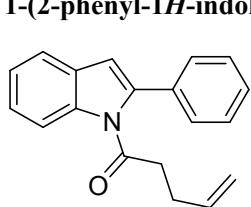
White solid, m.p. = 36.0–37.5 °C.

¹H NMR (400 MHz, CDCl₃) δ 7.96 – 7.87 (m, 1H), 7.48 – 7.38 (m, 1H), 7.25 – 7.16 (m, 2H), 6.45 – 6.23 (m, 1H), 5.92 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.23 – 4.95 (m, 2H), 3.03 (t, *J* = 7.3 Hz, 2H), 2.60 (s, 3H), 2.59 – 2.54 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 172.7, 137.4, 136.7, 136.2, 129.8, 123.4, 123.0, 119.9, 115.8, 115.1, 109.6, 38.0, 28.8, 17.7.

HRMS (ESI) calcd for C₁₄H₁₆NO [M+H]⁺: 214.1226. Found: 214.1219.

1-(2-phenyl-1*H*-indol-1-yl)pent-4-en-1-one (1p)



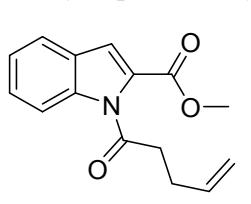
White solid, m.p. = 21.1–22.2 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.30 (d, *J* = 8.3 Hz, 1H), 7.58 – 7.53 (m, 1H), 7.52 – 7.38 (m, 5H), 7.38 – 7.31 (m, 1H), 7.27 (td, *J* = 7.6, 0.9 Hz, 1H), 6.62 (s, 1H), 5.58 (ddt, *J* = 16.5, 10.3, 6.2 Hz, 1H), 4.84 – 4.79 (m, 1H), 4.79 – 4.72 (m, 1H), 2.41 – 2.33 (m, 2H), 2.33 – 2.25 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 174.2, 139.4, 137.6, 136.3, 134.2, 128.9, 128.8, 128.7, 128.6, 125.0, 123.5, 120.4, 115.6, 115.4, 111.4, 38.8, 29.0.

HRMS (ESI) calcd for C₁₉H₁₈NO [M+H]⁺: 276.1383. Found: 276.1378.

methyl 1-pent-4-enoyl-1*H*-indole-2-carboxylate (1q)



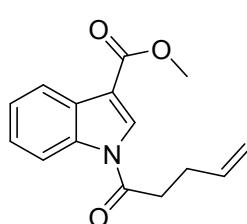
Colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 8.04 (d, *J* = 8.5 Hz, 1H), 7.62 (d, *J* = 7.9 Hz, 1H), 7.47 – 7.39 (m, 1H), 7.33 (s, 1H), 7.30 – 7.30 (m, 1H), 5.81 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.07 – 4.99 (m, 1H), 4.98 – 4.93 (m, 1H), 3.93 (s, 3H), 2.96 (t, *J* = 7.4 Hz, 2H), 2.58 – 2.50 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 173.8, 162.1, 138.2, 136.3, 129.0, 127.8, 127.1, 123.6, 122.5, 118.0, 115.9, 114.8, 52.6, 38.8, 29.4.

HRMS (ESI) calcd for C₁₅H₁₆NO₃ [M+H]⁺: 258.1125. Found: 258.1122.

methyl 1-pent-4-enoyl-1*H*-indole-3-carboxylate (**1r**)



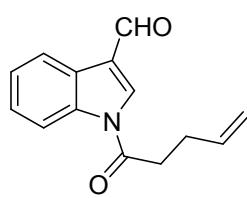
White solid, m.p. = 82.0-82.8 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.49 – 8.42 (m, 1H), 8.24 – 8.09 (m, 2H), 7.51 – 7.32 (m, 2H), 5.93 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.21 – 5.12 (m, 1H), 5.12 – 5.06 (m, 1H), 3.95 (s, 3H), 3.06 (t, *J* = 7.4 Hz, 2H), 2.67 – 2.54 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 170.9, 164.4, 135.99, 135.96, 130.5, 127.2, 126.0, 124.8, 121.5, 116.5, 116.4, 113.7, 51.7, 34.9, 28.2.

HRMS (ESI) calcd for C₁₅H₁₆NO₃ [M+H]⁺: 258.1125. Found: 258.1123.

1-pent-4-enoyl-1*H*-indole-3-carbaldehyde (**1s**)



White solid, m.p. = 100.7-101.2 °C.

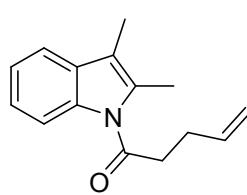
¹H NMR (400 MHz, CDCl₃) δ 10.11 (s, 1H), 8.44 – 8.39 (m, 1H), 8.33 – 8.22 (m, 1H), 8.10 (s, 1H), 7.52 – 7.35 (m, 2H), 5.94 (ddt, *J* = 16.9, 10.2, 6.5 Hz, 1H), 5.22 – 5.14 (m, 1H), 5.14 – 5.08 (m, 1H), 3.10 (t, *J* = 7.4 Hz, 2H), 2.67 – 2.58 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 185.6, 170.7, 136.4, 135.8, 134.5, 126.9, 125.9, 125.4, 122.7, 121.9, 116.6, 116.5, 35.1, 28.1.

HRMS (ESI) calcd for C₁₄H₁₄NO₂ [M+H]⁺: 228.1019. Found: 228.1016.

Analytical data for compound **1s** was consistent with the literature.⁵

1-(2,3-dimethyl-1*H*-indol-1-yl)pent-4-en-1-one (**1t**)



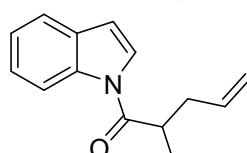
White solid, m.p. = 31.9-33.0 °C.

¹H NMR (400 MHz, CDCl₃) δ 7.93 – 7.87 (m, 1H), 7.47 – 7.40 (m, 1H), 7.29 – 7.20 (m, 2H), 5.94 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.16 – 5.09 (m, 1H), 5.08 – 5.03 (m, 1H), 3.13 – 3.05 (m, 2H), 2.64 – 2.55 (m, 2H), 2.55 (d, *J* = 0.3 Hz, 3H), 2.19 (d, *J* = 0.6 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 172.7, 136.8, 135.3, 132.7, 131.2, 123.6, 122.7, 118.2, 115.8, 115.3, 114.8, 38.2, 29.0, 14.5, 8.7.

HRMS (ESI) calcd for C₁₅H₁₈NO [M+H]⁺: 228.1383. Found: 228.1379.

1-(1*H*-indol-1-yl)-2-methylpent-4-en-1-one (**1u**)



Colorless liquid.

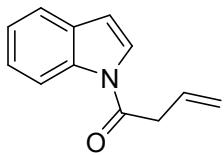
¹H NMR (400 MHz, CDCl₃) δ 8.52 (d, *J* = 8.3 Hz, 1H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.49 (d, *J* = 3.7 Hz, 1H), 7.39 – 7.33 (m, 1H), 7.31 – 7.25 (m, 1H), 6.65 (d, *J* = 3.8 Hz, 1H), 5.82 (ddt, *J* = 17.1, 10.0, 7.0 Hz, 1H), 5.16 – 5.08 (m, 1H), 5.08 – 5.03 (m, 1H), 3.33 – 3.20 (m, 1H), 2.72 – 2.60 (m, 1H), 2.38 – 2.27 (m, 1H), 1.35 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 174.8, 135.8, 135.1, 130.5, 125.2, 124.5, 123.7, 120.8, 117.5, 116.9, 109.2, 39.0, 37.9, 17.5.

HRMS (ESI) calcd for C₁₄H₁₆NO [M+H]⁺: 214.1226. Found: 214.1225.

Analytical data for compound **1u** was consistent with the literature.⁶

1-(1*H*-indol-1-yl)but-3-en-1-one (1v**)**



White solid, m.p. = 24.4–25.4 °C.

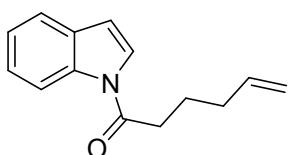
¹H NMR (400 MHz, CDCl₃) δ 8.46 (d, *J* = 8.2 Hz, 1H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.42 (d, *J* = 3.7 Hz, 1H), 7.38 – 7.32 (m, 1H), 7.30 – 7.25 (m, 1H), 6.63 (d, *J* = 3.7 Hz, 1H), 6.10 (ddt, *J* = 16.9, 10.3, 6.6 Hz, 1H), 5.33 – 5.24 (m, 2H), 3.72 – 3.65 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 169.4, 135.7, 130.3, 129.8, 125.3, 124.7, 123.8, 120.9, 119.6, 116.7, 109.5, 40.9.

HRMS (ESI) calcd for C₁₂H₁₂NO [M+H]⁺: 186.0913. Found: 186.0911.

Analytical data for compound **1v** was consistent with the literature.⁷

1-(1*H*-indol-1-yl)hex-5-en-1-one (1w**)**



Colorless liquid.

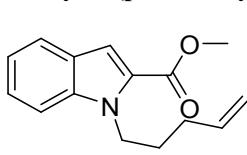
¹H NMR (400 MHz, CDCl₃) δ 8.39 (d, *J* = 8.2 Hz, 1H), 7.48 (brd, *J* = 7.7 Hz, 1H), 7.35 (d, *J* = 3.8 Hz, 1H), 7.31 – 7.23 (m, 1H), 7.21 – 7.16 (m, 1H), 6.54 (d, *J* = 3.8 Hz, 1H), 5.75 (ddt, *J* = 17.0, 10.2, 6.7 Hz, 1H), 5.05 – 4.92 (m, 2H), 2.81 (t, *J* = 7.4 Hz, 2H), 2.17 – 2.09 (m, 2H), 1.86 (p, *J* = 7.4 Hz, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 171.4, 137.6, 135.6, 130.3, 125.1, 124.6, 123.6, 120.8, 116.6, 115.8, 109.0, 34.9, 33.0, 23.5.

HRMS (ESI) calcd for C₁₄H₁₆NO [M+H]⁺: 214.1226. Found: 214.1223.

Analytical data for compound **1w** was consistent with the literature.⁷

methyl 1-(pent-4-enyl)-1*H*-indole-2-carboxylate (1x**)**



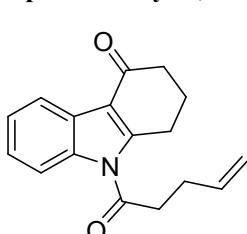
Colorless liquid.

¹H NMR (400 MHz, CDCl₃) δ 7.71 – 7.67 (m, 1H), 7.42 – 7.38 (m, 1H), 7.38 – 7.32 (m, 1H), 7.31 (d, *J* = 0.7 Hz, 1H), 7.15 (ddd, *J* = 7.9, 6.8, 1.1 Hz, 1H), 5.85 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.05 – 4.99 (m, 2H), 4.64 – 4.53 (m, 2H), 3.92 (s, 3H), 2.20 – 2.08 (m, 2H), 1.97 – 1.85 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 162.4, 139.0, 137.7, 127.0, 125.9, 124.9, 122.7, 120.5, 115.2, 110.6, 110.5, 51.6, 44.2, 31.0, 29.5.

HRMS (ESI) calcd for C₁₅H₁₈NO₂ [M+H]⁺: 244.1332. Found: 244.1328.

9-pent-4-enoyl-2,3-dihydro-1*H*-carbazol-4(9*H*)-one (1aa**)**



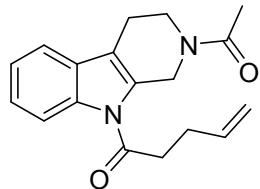
White solid, m.p. = 102.0–102.3 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.38 – 8.28 (m, 1H), 7.86 – 7.75 (m, 1H), 7.40 – 7.29 (m, 2H), 5.92 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.19 – 5.06 (m, 2H), 3.26 (t, *J* = 6.0 Hz, 2H), 3.13 (t, *J* = 7.2 Hz, 2H), 2.71 – 2.52 (m, 4H), 2.30 – 2.16 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 195.7, 173.0, 151.8, 136.1, 135.2, 126.2, 125.0, 124.6, 122.0, 117.4, 116.4, 114.3, 38.5, 37.8, 28.7, 26.4, 23.5.

HRMS (ESI) calcd for C₁₇H₁₈NO₂ [M+H]⁺: 268.1332. Found: 268.1326.

1-(2-acetyl-3,4-dihydro-1*H*-pyrido[3,4-*b*]indol-9(2*H*)-yl)pent-4-en-1-one (1ab)



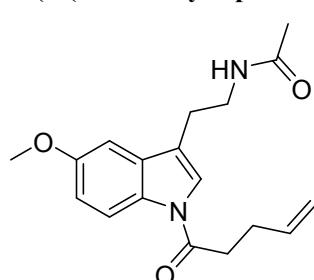
White solid, m.p. = 53.3–55.1 °C.

¹H NMR (400 MHz, DMSO-*d*₆, 353 K) δ 7.95 (d, *J* = 8.1 Hz, 1H), 7.55 – 7.46 (m, 1H), 7.36 – 7.25 (m, 2H), 5.98 (ddt, *J* = 16.8, 10.2, 6.4 Hz, 1H), 5.19 – 5.10 (m, 1H), 5.08 – 5.02 (m, 1H), 4.96 – 4.91 (m, 2H), 3.84 – 3.72 (m, 2H), 3.19 (t, *J* = 7.1 Hz, 2H), 2.76 (brs, 2H), 2.59 – 2.51 (m, 2H), 2.14 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 172.2, 171.6, 169.9, 169.5, 136.6, 136.5, 135.0, 134.6, 133.1, 132.7, 129.9, 129.5, 124.4, 124.3, 123.3, 123.1, 118.9, 118.3, 117.4, 116.13, 116.06, 115.6, 114.9, 114.4, 47.1, 43.5, 42.8, 38.6, 37.8, 37.7, 28.5, 28.4, 22.2, 22.1, 21.6, 20.9.

HRMS (ESI) calcd for C₁₈H₂₁N₂O₂ [M+H]⁺: 297.1598. Found: 297.1599.

***N*-(2-(5-methoxy-1-pent-4-enoyl-1*H*-indol-3-yl)ethyl)acetamide (1ac)**



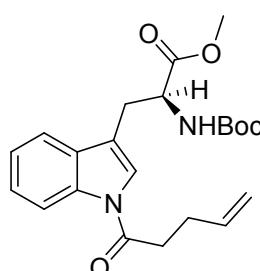
White solid, m.p. = 100.5–100.8 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.22 (d, *J* = 7.8 Hz, 1H), 7.16 (s, 1H), 6.89 (d, *J* = 2.3 Hz, 1H), 6.88 – 6.83 (m, 1H), 6.03 (brs, 1H), 5.81 (ddt, *J* = 23.5, 10.3, 6.5 Hz, 1H), 5.07 – 4.99 (m, 1H), 4.99 – 4.94 (m, 1H), 3.77 (s, 3H), 3.51 (q, *J* = 6.7 Hz, 2H), 2.87 – 2.72 (m, 4H), 2.47 – 2.34 (m, 2H), 1.90 (s, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 170.3, 170.1, 156.4, 136.5, 131.3, 130.6, 122.5, 119.4, 117.6, 116.0, 113.5, 101.7, 55.7, 38.9, 34.7, 28.4, 25.3, 23.4.

HRMS (ESI) calcd for C₁₈H₂₃N₂O₃ [M+H]⁺: 315.1703. Found: 315.1704.

(S)-methyl 2-(tert-butoxycarbonylamino)-3-(1-pent-4-enoyl-1*H*-indol-3-yl)propanoate (1ad)



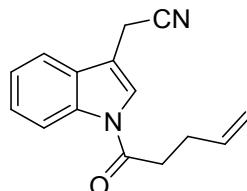
White solid, m.p. = 131.7–132.8 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.44 (d, *J* = 8.2 Hz, 1H), 7.49 (d, *J* = 7.7 Hz, 1H), 7.39 – 7.27 (m, 3H), 5.93 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.23 – 5.00 (m, 3H), 4.76 – 4.64 (m, 1H), 3.70 (s, 3H), 3.27 (dd, *J* = 15.0, 5.6 Hz, 1H), 3.16 (dd, *J* = 15.0, 6.3 Hz, 1H), 2.98 (t, *J* = 7.4 Hz, 2H), 2.63 – 2.54 (m, 2H), 1.43 (s, 9H).

¹³C NMR (101 MHz, CDCl₃) δ 172.3, 170.4, 155.1, 136.4, 135.8, 130.4, 125.4, 123.6, 122.6, 118.7, 117.2, 116.7, 116.0, 80.1, 53.4, 52.5, 35.1, 28.4, 28.3, 28.0.

HRMS (ESI) calcd for C₂₂H₂₈N₂NaO₅ [M+Na]⁺: 423.1890. Found: 423.1886.

2-(1-pent-4-enoyl-1*H*-indol-3-yl)acetonitrile (1ae)



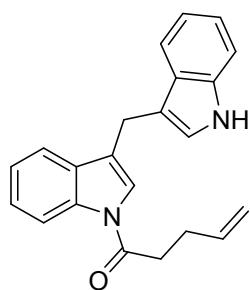
White solid, m.p. = 86.4–87.9 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.51 (d, *J* = 8.3 Hz, 1H), 7.58 – 7.50 (m, 2H), 7.48 – 7.42 (m, 1H), 7.40 – 7.34 (m, 1H), 5.96 (ddt, *J* = 16.9, 10.2, 6.5 Hz, 1H), 5.22 – 5.15 (m, 1H), 5.14 – 5.09 (m, 1H), 3.84 – 3.81 (m, 2H), 3.05 (t, *J* = 7.4 Hz, 2H), 2.67 – 2.58 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 170.5, 136.2, 136.0, 128.3, 126.2, 124.0, 122.8, 118.1, 117.1, 117.0, 116.3, 111.6, 35.1, 28.3, 14.6.

HRMS (ESI) calcd for C₁₅H₁₅N₂O [M+H]⁺: 239.1179. Found: 239.1177.

1-(3-((1*H*-indol-3-yl)methyl)-1*H*-indol-1-yl)pent-4-en-1-one (1af)



White solid, m.p. = 157.2–157.9 °C.

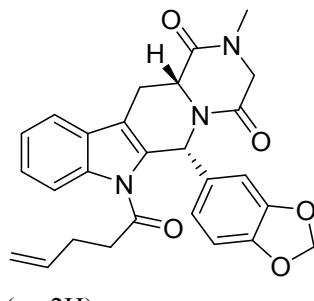
¹H NMR (400 MHz, CDCl₃) δ 8.47 (d, *J* = 8.1 Hz, 1H), 8.01 (s, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.41 – 7.32 (m, 2H), 7.29 – 7.19 (m, 2H), 7.16 (s, 1H), 7.12 (t, *J* = 7.4 Hz, 1H), 6.98 (d, *J* = 1.9 Hz, 1H), 5.87 (ddt, *J* = 16.9, 10.2, 6.6 Hz, 1H), 5.12 – 5.04 (m, 1H), 5.04 – 4.98 (m, 1H), 4.18 (s, 2H), 2.88 (t, *J* = 7.4 Hz, 2H), 2.57 – 2.48 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 170.6, 136.6, 136.4, 136.2, 130.6, 127.3, 125.3, 123.4, 122.4, 122.25, 122.21, 122.0, 119.5, 119.3, 119.0, 116.8,

115.9, 113.7, 111.3, 35.1, 28.5, 21.2.

HRMS (ESI) calcd for C₂₂H₂₁N₂O [M+H]⁺: 329.1648. Found: 329.1642.

(6*R*,12*aR*)-6-(benzo[*d*][1,3]dioxol-5-yl)-2-methyl-7-(pent-4-enoyl)-2,3,6,7,12,12*a*-hexahydropyrazino[1',2':1,6]pyrido[3,4-*b*]indole-1,4-dione (1ag)



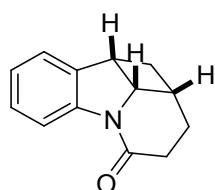
White solid, m.p. = 233.0–234.4 °C.

¹H NMR (400 MHz, CDCl₃) δ 7.71 – 7.61 (m, 2H), 7.39 – 7.31 (m, 2H), 7.20 (s, 1H), 6.88 – 6.79 (m, 2H), 6.63 (d, *J* = 8.0 Hz, 1H), 5.86 (d, *J* = 3.2 Hz, 2H), 5.75 (ddt, *J* = 16.8, 10.2, 6.5 Hz, 1H), 5.06 – 4.94 (m, 2H), 4.29 (dd, *J* = 11.5, 4.2 Hz, 1H), 4.15 (d, *J* = 17.3 Hz, 1H), 3.93 (d, *J* = 17.3 Hz, 1H), 3.72 (dd, *J* = 16.4, 4.5 Hz, 1H), 3.17 (dd, *J* = 16.1, 11.9 Hz, 1H), 3.03 (s, 3H), 3.01 – 2.90 (m, 2H), 2.51 – 2.39 (m, 2H).

¹³C NMR (101 MHz, CDCl₃) δ 171.5, 166.4, 166.2, 147.2, 146.9, 136.2, 135.4, 133.8, 128.4, 125.0, 123.3, 122.5, 119.2, 115.9, 115.6, 114.8, 109.2, 107.8, 101.0, 56.2, 55.1, 52.3, 37.9, 33.6, 28.4, 23.0.

HRMS (ESI) calcd for C₂₇H₂₆N₃O₅ [M+H]⁺: 472.1867. Found: 472.1848.

(1*a*β,1*a*¹β,9*b*β)-1,1*a*,1*a*¹,2,3,9*b*-hexahydro-4*H*-benzo[*b*]cyclobuta[*hi*]indolizin-4-one (2a)



White solid, 96% yield, m.p. = 86.0–87.2 °C.

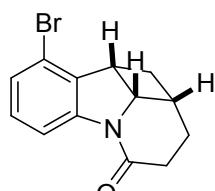
¹H NMR (400 MHz, CDCl₃) δ 7.88 (d, *J* = 7.9 Hz, 1H), 7.18 (t, *J* = 7.7 Hz, 1H), 7.08 (d, *J* = 7.2 Hz, 1H), 6.98 (t, *J* = 7.4 Hz, 1H), 4.61 (td, *J* = 6.1, 2.9 Hz, 1H), 3.61 (dd, *J* = 14.5, 7.4 Hz, 1H), 3.14 – 2.98 (m, 1H), 2.83 (tdt, *J* = 11.7, 8.8, 2.9 Hz, 1H), 2.52 – 2.38 (m, 1H), 2.30 – 2.14 (m, 2H), 1.90 (dt, *J* = 12.2, 8.3 Hz, 1H), 1.62 – 1.48 (m, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 171.5, 145.5, 136.1, 127.4, 124.0, 123.3, 117.4, 63.4, 37.8, 37.3, 34.9, 29.9, 26.9.

HRMS (ESI) calcd for C₁₃H₁₄NO [M+H]⁺: 200.1070. Found: 200.1067.

Analytical data for compound **2a** was consistent with the literature.⁷

(1*a*β,1*a*¹β,9*b*β)-9-bromo-1,1*a*,1*a*¹,2,3,9*b*-hexahydro-4*H*-benzo[*b*]cyclobuta[*hi*]indolizin-4-one (2b)



White solid, 90% yield, m.p. = 91.9–93.2 °C.

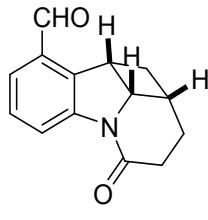
¹H NMR (400 MHz, CDCl₃) δ 7.84 – 7.77 (m, 1H), 7.12 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.06 (t, *J* = 7.9 Hz, 1H), 4.64 (td, *J* = 6.2, 2.9 Hz, 1H), 3.77 – 3.70 (m,

1H), 3.15 – 3.03 (m, 1H), 2.92 (dtd, J = 12.0, 8.8, 2.9 Hz, 1H), 2.46 (ddd, J = 14.1, 3.4, 2.4 Hz, 1H), 2.33 – 2.24 (m, 1H), 2.23 – 2.14 (m, 1H), 1.93 (ddd, J = 12.2, 8.5, 7.5 Hz, 1H), 1.56 (tdd, J = 13.5, 6.0, 3.4 Hz, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.7, 146.4, 136.8, 129.1, 126.9, 117.7, 116.1, 62.7, 38.8, 36.2, 34.8, 30.1, 26.7.

HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{13}\text{BrNO} [\text{M}+\text{H}]^+$: 278.0175. Found: 278.0173.

(1a β ,1a $^1\beta$,9b β)-4-oxo-1a,1a 1 ,2,3,4,9b-hexahydro-1*H*-benzo[*b*]cyclobuta[*hi*]indolizin-9-carbaldehyde (2c)



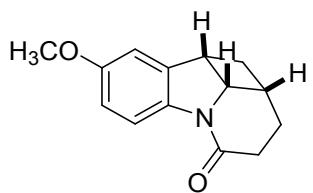
White solid, 75% yield, m.p. = 147.2–148.0 °C.

^1H NMR (400 MHz, CDCl_3) δ 9.94 (s, 1H), 8.06 (dd, J = 7.8, 0.8 Hz, 1H), 7.38 (dd, J = 7.7, 1.1 Hz, 1H), 7.31 (t, J = 7.7 Hz, 1H), 4.59 (td, J = 6.2, 2.9 Hz, 1H), 4.24 – 4.11 (m, 1H), 3.14 – 3.00 (m, 1H), 2.93 (dtd, J = 11.9, 8.8, 2.9 Hz, 1H), 2.46 – 2.34 (m, 1H), 2.28 – 2.11 (m, 2H), 1.87 – 1.74 (m, 1H), 1.54 – 1.42 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 192.0, 171.8, 147.0, 137.5, 131.5, 128.2, 127.0, 122.3, 63.5, 37.0, 36.8, 34.9, 30.0, 26.7.

HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{14}\text{NO}_2 [\text{M}+\text{H}]^+$: 228.1019. Found: 228.1018.

(1a β ,1a $^1\beta$,9b β)-8-methoxy-1,1a,1a 1 ,2,3,9b-hexahydro-4*H*-benzo[*b*]cyclobuta[*hi*]indolizin-4-one (2d)



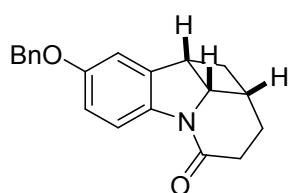
White solid, 83% yield, m.p. = 67.0–68.1 °C.

^1H NMR (400 MHz, CDCl_3) δ 7.77 (d, J = 8.5 Hz, 1H), 6.78 – 6.59 (m, 2H), 4.65 – 4.55 (m, 1H), 3.76 (s, 3H), 3.61 – 3.52 (m, 1H), 3.09 – 2.96 (m, 1H), 2.89 – 2.76 (m, 1H), 2.46 – 2.36 (m, 1H), 2.29 – 2.10 (m, 2H), 1.90 (dt, J = 11.9, 8.2 Hz, 1H), 1.60 – 1.47 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.1, 156.7, 139.2, 137.8, 117.8, 111.2, 110.3, 63.8, 55.8, 38.0, 37.3, 34.7, 30.0, 27.1.

HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{16}\text{NO}_2 [\text{M}+\text{H}]^+$: 230.1176. Found: 230.1174.

(1a β ,1a $^1\beta$,9b β)-8-(benzyloxy)-1,1a,1a 1 ,2,3,9b-hexahydro-4*H*-benzo[*b*]cyclobuta[*hi*]indolizin-4-one (2e)



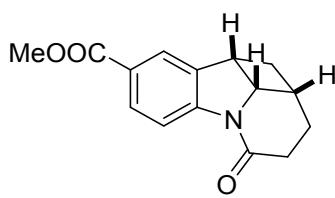
Colorless liquid, 89% yield.

^1H NMR (400 MHz, CDCl_3) δ 7.78 (d, J = 8.5 Hz, 1H), 7.47 – 7.28 (m, 5H), 6.83 – 6.71 (m, 2H), 5.01 (s, 2H), 4.60 (td, J = 6.1, 2.9 Hz, 1H), 3.61 – 3.52 (m, 1H), 3.09 – 2.97 (m, 1H), 2.82 (dtd, J = 11.8, 8.7, 2.9 Hz, 1H), 2.49 – 2.36 (m, 1H), 2.31 – 2.11 (m, 2H), 1.96 – 1.88 (m, 1H), 1.61 – 1.46 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.1, 155.8, 139.3, 137.8, 137.1, 128.6, 128.0, 127.5, 117.7, 112.3, 111.2, 70.5, 63.7, 37.9, 37.2, 34.6, 29.8, 27.0.

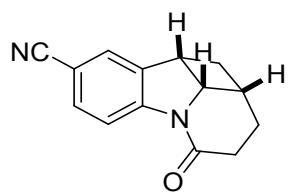
HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{20}\text{NO}_2 [\text{M}+\text{H}]^+$: 306.1489. Found: 306.1486.

methyl (1a β ,1a $^1\beta$,9b β)-4-oxo-1a,1a 1 ,2,3,4,9b-hexahydro-1*H*-benzo[*b*]cyclobuta[*hi*]indolizin-8-carboxylate (2f)



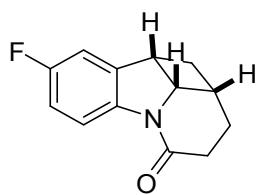
White solid, 93% yield, m.p. = 128.1-128.4 °C.
¹**H NMR** (400 MHz, CDCl₃) δ 8.00 – 7.87 (m, 2H), 7.76 (s, 1H), 4.68 (td, *J* = 6.1, 2.8 Hz, 1H), 3.88 (s, 3H), 3.72 – 3.65 (m, 1H), 3.16 – 3.03 (m, 1H), 2.87 (dtd, *J* = 11.6, 8.8, 2.8 Hz, 1H), 2.54 – 2.43 (m, 1H), 2.33 – 2.17 (m, 2H), 1.92 (dt, *J* = 12.2, 8.0 Hz, 1H), 1.63 – 1.49 (m, 1H).
¹³**C NMR** (101 MHz, CDCl₃) δ 171.8, 166.8, 149.4, 136.4, 130.1, 125.7, 124.7, 116.5, 63.8, 52.0, 37.4, 37.3, 35.0, 30.1, 26.7.
HRMS (ESI) calcd for C₁₅H₁₆NO₃ [M+H]⁺: 258.1125. Found: 258.1122.

(1aβ,1a¹β,9bβ)-4-oxo-1a,1a¹,2,3,4,9b-hexahydro-1H-benzo[b]cyclobuta[hi]indolizin-8-carbonitrile (2g)



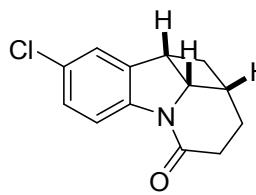
White solid, 94% yield, m.p. = 147.5-148.2 °C.
¹**H NMR** (400 MHz, CDCl₃) δ 7.95 (d, *J* = 8.2 Hz, 1H), 7.51 (d, *J* = 8.1 Hz, 1H), 7.34 (s, 1H), 4.75 – 4.64 (m, 1H), 3.77 – 3.64 (m, 1H), 3.21 – 3.06 (m, 1H), 2.98 – 2.83 (m, 1H), 2.58 – 2.44 (m, 1H), 2.37 – 2.17 (m, 2H), 1.93 (dt, *J* = 12.2, 8.1 Hz, 1H), 1.66 – 1.49 (m, 1H).
¹³**C NMR** (101 MHz, CDCl₃) δ 171.8, 149.2, 137.3, 132.8, 126.9, 119.3, 117.3, 106.8, 63.6, 37.3, 37.2, 34.9, 30.2, 26.6.
HRMS (ESI) calcd for C₁₄H₁₃N₂O [M+H]⁺: 225.1022. Found: 225.1018.

(1aβ,1a¹β,9bβ)-8-fluoro-1,1a,1a¹,2,3,9b-hexahydro-4H-benzo[b]cyclobuta[hi]indolizin-4-one (2h)



White solid, 92% yield, m.p. = 92.3-92.7 °C.
¹**H NMR** (400 MHz, CDCl₃) δ 7.80 (dd, *J* = 8.6, 4.8 Hz, 1H), 6.85 (td, *J* = 8.9, 2.6 Hz, 1H), 6.78 (dd, *J* = 8.1, 2.5 Hz, 1H), 4.64 (td, *J* = 6.1, 3.0 Hz, 1H), 3.63 – 3.54 (m, 1H), 3.12 – 2.98 (m, 1H), 2.84 (dtd, *J* = 11.9, 8.8, 3.0 Hz, 1H), 2.48 – 2.39 (m, 1H), 2.30 – 2.13 (m, 2H), 1.98 – 1.87 (m, 1H), 1.61 – 1.50 (m, 1H).
¹³**C NMR** (101 MHz, CDCl₃) δ 171.2, 159.6 (d, *J* = 242.1 Hz), 141.6 (d, *J* = 2.0 Hz), 138.1 (d, *J* = 8.2 Hz), 117.9 (d, *J* = 8.5 Hz), 113.3 (d, *J* = 23.0 Hz), 110.9 (d, *J* = 24.2 Hz), 63.9, 37.7 (d, *J* = 1.7 Hz), 37.1, 34.6, 30.0, 26.8.
¹⁹**F NMR** (376 MHz, CDCl₃) δ -119.05.
HRMS (ESI) calcd for C₁₃H₁₃FNO [M+H]⁺: 218.0976. Found: 218.0975.

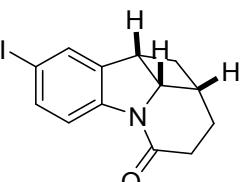
(1aβ,1a¹β,9bβ)-8-chloro-1,1a,1a¹,2,3,9b-hexahydro-4H-benzo[b]cyclobuta[hi]indolizin-4-one (2i)



White solid, 92% yield, m.p. = 132.2-132.4 °C.
¹**H NMR** (400 MHz, CDCl₃) δ 7.79 (d, *J* = 8.4 Hz, 1H), 7.18 – 7.10 (m, 1H), 7.04 (s, 1H), 4.69 – 4.57 (m, 1H), 3.66 – 3.53 (m, 1H), 3.12 – 2.98 (m, 1H), 2.90 – 2.77 (m, 1H), 2.50 – 2.38 (m, 1H), 2.31 – 2.12 (m, 2H), 1.91 (dt, *J* = 11.9, 8.1 Hz, 1H), 1.60 – 1.49 (m, 1H).
¹³**C NMR** (101 MHz, CDCl₃) δ 171.4, 144.1, 138.0, 128.8, 127.1, 123.7, 118.1, 63.7, 37.6, 37.2, 34.7, 30.0, 26.8.

HRMS (ESI) calcd for C₁₃H₁₃ClNO [M+H]⁺: 234.0680. Found: 234.0681.

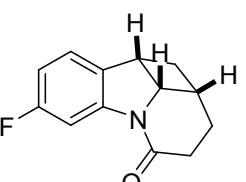
(1a β ,1a¹ β ,9b β)-8-iodo-1,1a,1a¹,2,3,9b-hexahydro-4H-benzo[b]cyclobuta[hi]indolin-4-one (2j)

White solid, 95% yield, m.p. = 146.1–146.6 °C.

¹**H NMR** (400 MHz, CDCl₃) δ 7.65 (d, *J* = 8.3 Hz, 1H), 7.48 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.39 (d, *J* = 1.6 Hz, 1H), 4.62 (td, *J* = 6.1, 3.0 Hz, 1H), 3.64 – 3.56 (m, 1H), 3.12 – 2.99 (m, 1H), 2.83 (dtd, *J* = 11.9, 8.8, 3.0 Hz, 1H), 2.49 – 2.40 (m, 1H), 2.31 – 2.22 (m, 1H), 2.22 – 2.13 (m, 1H), 1.96 – 1.86 (m, 1H), 1.54 (tdd, *J* = 12.6, 5.4, 3.1 Hz, 1H).

¹³**C NMR** (101 MHz, CDCl₃) δ 171.4, 145.4, 138.7, 136.2, 132.3, 119.1, 86.9, 63.5, 37.5, 37.3, 34.8, 30.0, 26.8.

HRMS (ESI) calcd for C₁₃H₁₃INO [M+H]⁺: 326.0036. Found: 326.0040.

(1a β ,1a¹ β ,9b β)-7-fluoro-1,1a,1a¹,2,3,9b-hexahydro-4H-benzo[b]cyclobuta[hi]indolin-4-one (2k)

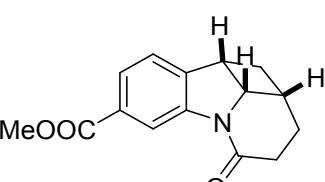
White solid, 97% yield, m.p. = 75.7–76.7 °C.

¹**H NMR** (400 MHz, CDCl₃) δ 7.56 (dd, *J* = 9.7, 2.4 Hz, 1H), 6.91 (dd, *J* = 8.1, 5.5 Hz, 1H), 6.60 (td, *J* = 9.0, 2.4 Hz, 1H), 4.60 (td, *J* = 6.1, 3.0 Hz, 1H), 3.57 – 3.48 (m, 1H), 3.04 – 2.92 (m, 1H), 2.77 (dtd, *J* = 11.9, 8.8, 2.9 Hz, 1H), 2.43 – 2.35 (m, 1H), 2.25 – 2.07 (m, 2H), 1.87 – 1.77 (m, 1H), 1.53 – 1.44 (m, 1H).

¹³**C NMR** (101 MHz, CDCl₃) δ 171.5, 162.2 (d, *J* = 243.4 Hz), 146.8 (d, *J* = 12.3 Hz), 131.5 (d, *J* = 2.7 Hz), 123.6 (d, *J* = 9.9 Hz), 110.1 (d, *J* = 22.7 Hz), 105.8 (d, *J* = 27.9 Hz), 64.4, 37.4, 37.2, 34.8, 29.9, 26.8.

¹⁹**F NMR** (376 MHz, CDCl₃) δ -114.50.

HRMS (ESI) calcd for C₁₃H₁₃FNO [M+H]⁺: 218.0976. Found: 218.0973.

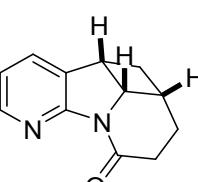
methyl (1a β ,1a¹ β ,9b β)-4-oxo-1a,1a¹,2,3,4,9b-hexahydro-1H-benzo[b]cyclobuta[hi]indolin-7-carboxylate (2l)

White solid, 93% yield, m.p. = 169.9–170.5 °C.

¹**H NMR** (400 MHz, CDCl₃) δ 8.41 – 8.37 (m, 1H), 7.66 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.06 (d, *J* = 7.7 Hz, 1H), 4.60 (td, *J* = 6.0, 3.0 Hz, 1H), 3.83 (s, 3H), 3.64 – 3.56 (m, 1H), 3.10 – 2.96 (m, 1H), 2.80 (dtd, *J* = 12.0, 8.9, 2.9 Hz, 1H), 2.46 – 2.35 (m, 1H), 2.25 – 2.09 (m, 2H), 1.87 – 1.82 (m, 1H), 1.54 – 1.42 (m, 1H).

¹³**C NMR** (101 MHz, CDCl₃) δ 171.5, 167.0, 145.7, 141.4, 129.6, 126.3, 123.1, 117.7, 63.6, 52.1, 37.8, 37.2, 34.8, 30.1, 26.7.

HRMS (ESI) calcd for C₁₅H₁₆NO₃ [M+H]⁺: 258.1125. Found: 258.1123.

(1a β ,1a¹ β ,9b β)-1,1a,1a¹,2,3,9b-hexahydro-4H-cyclobuta[hi]pyrido[3,2-b]indolin-4-one (2m)

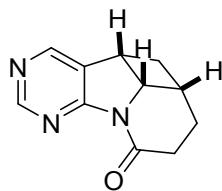
White solid, 79% yield, m.p. = 144.9–145.6 °C.

¹**H NMR** (400 MHz, CDCl₃) δ 8.26 (dd, *J* = 5.1, 1.4 Hz, 1H), 7.38 (dd, *J* = 7.3, 1.2 Hz, 1H), 6.90 (dd, *J* = 7.3, 5.2 Hz, 1H), 4.68 (td, *J* = 6.2, 2.8 Hz, 1H), 3.68 – 3.61 (m, 1H), 3.17 – 3.06 (m, 1H), 2.87 (dtd, *J* = 11.8, 8.8, 2.8 Hz, 1H),

2.59 – 2.52 (m, 1H), 2.33 – 2.27 (m, 1H), 2.25 – 2.16 (m, 1H), 2.03 – 1.94 (m, 1H), 1.68 – 1.57 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 170.8, 159.2, 146.7, 131.8, 129.6, 118.9, 61.8, 36.8, 35.6, 35.5, 30.4, 26.6.

HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{13}\text{N}_2\text{O} [\text{M}+\text{H}]^+$: 201.1022. Found: 201.1018.

(1a β ,1a $^1\beta$,9b β)-1,1a,1a 1 ,2,3,9b-hexahydro-4*H*-cyclobuta[*hi*]pyrimido[5,4-*b*]indolin-4-one (2n)



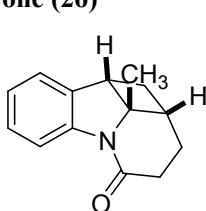
White solid, 65% yield, m.p. = 162.9–164.1 °C.

^1H NMR (400 MHz, CDCl_3) δ 8.89 (s, 1H), 8.34 (s, 1H), 4.71 (td, J = 6.3, 2.8 Hz, 1H), 3.81 – 3.73 (m, 1H), 3.25 – 3.14 (m, 1H), 2.95 (dtd, J = 12.0, 8.9, 2.8 Hz, 1H), 2.67 – 2.58 (m, 1H), 2.39 – 2.30 (m, 1H), 2.30 – 2.21 (m, 1H), 2.03 (ddd, J = 12.5, 8.5, 7.5 Hz, 1H), 1.64 (tdd, J = 13.3, 6.3, 3.0 Hz, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 170.8, 165.4, 157.6, 150.4, 127.0, 61.7, 37.0, 35.8, 33.7, 30.7, 26.3.

HRMS (ESI) calcd for $\text{C}_{11}\text{H}_{12}\text{N}_3\text{O} [\text{M}+\text{H}]^+$: 202.0975. Found: 202.0974.

(1a β ,1a $^1\beta$,9b β)-1a 1 -methyl-1,1a,1a 1 ,2,3,9b-hexahydro-4*H*-benzo[*b*]cyclobuta[*hi*]indolin-4-one (2o)



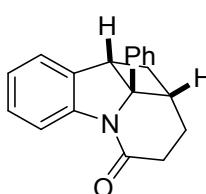
Colorless liquid, 87% yield.

^1H NMR (400 MHz, CDCl_3) δ 7.89 (d, J = 7.9 Hz, 1H), 7.20 (td, J = 7.7, 1.3 Hz, 1H), 7.10 (brd, J = 6.7 Hz, 1H), 7.01 (td, J = 7.4, 1.0 Hz, 1H), 3.23 – 3.16 (m, 1H), 2.83 – 2.69 (m, 2H), 2.47 – 2.34 (m, 2H), 2.33 – 2.25 (m, 1H), 1.69 – 1.55 (m, 2H), 1.43 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.0, 144.6, 135.1, 127.3, 124.2, 123.8, 117.9, 70.5, 43.2, 35.4, 34.3, 32.9, 27.5, 25.3.

HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{16}\text{NO} [\text{M}+\text{H}]^+$: 214.1226. Found: 214.1222.

(1a β ,1a $^1\beta$,9b β)-1a 1 -phenyl-1,1a,1a 1 ,2,3,9b-hexahydro-4*H*-benzo[*b*]cyclobuta[*hi*]indolin-4-one (2p)



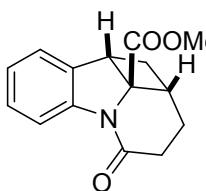
White solid, 97% yield, m.p. = 98.5–99.6 °C.

^1H NMR (400 MHz, CDCl_3) δ 8.04 (d, J = 7.9 Hz, 1H), 7.40 – 7.31 (m, 4H), 7.27 – 7.21 (m, 2H), 7.09 – 6.98 (m, 2H), 3.58 – 3.44 (m, 2H), 2.89 (dt, J = 11.9, 9.0 Hz, 1H), 2.39 – 2.29 (m, 2H), 2.14 (td, J = 14.4, 6.0 Hz, 1H), 1.86 (dt, J = 12.0, 8.1 Hz, 1H), 1.77 – 1.67 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.7, 145.2, 142.2, 134.7, 128.8, 127.6, 127.5, 125.1, 124.5, 123.7, 117.7, 75.1, 46.8, 35.6, 34.4, 33.5, 27.7.

HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{18}\text{NO} [\text{M}+\text{H}]^+$: 276.1383. Found: 276.1379.

methyl (1a β ,1a $^1\beta$,9b β)-4-oxo-1,1a,2,3,4,9b-hexahydro-1a ^1H -benzo[*b*]cyclobuta[*hi*]indolizine - 1a 1 -carboxylate (2q)



Colorless liquid, 91% yield.

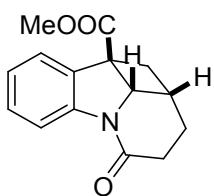
^1H NMR (400 MHz, CDCl_3) δ 7.93 (d, J = 7.9 Hz, 1H), 7.23 (t, J = 7.7 Hz, 1H), 7.10 (d, J = 7.0 Hz, 1H), 7.03 (t, J = 7.4 Hz, 1H), 3.88 (t, J = 8.0 Hz,

1H), 3.74 (s, 3H), 3.47 – 3.36 (m, 1H), 2.85 (dt, J = 12.0, 9.0 Hz, 1H), 2.47 – 2.40 (m, 1H), 2.35 – 2.23 (m, 2H), 1.86 – 1.78 (m, 1H), 1.66 – 1.53 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.5, 171.3, 145.0, 133.9, 127.8, 124.5, 123.3, 117.7, 72.0, 52.9, 41.7, 34.4, 33.8, 33.2, 27.1.

HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{16}\text{NO}_3$ [$\text{M}+\text{H}]^+$: 258.1125. Found: 258.1125.

methyl (1a β ,1a $^1\beta$,9b β)-4-oxo-1a,2,3,4-tetrahydro-1*H*-benzo[*b*]cyclobuta[*hi*]indolizine-9b(1a 1H)-carboxylate (2r)



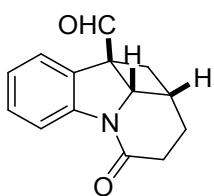
White solid, 84% yield, m.p. = 113.5–114.4 °C.

^1H NMR (400 MHz, CDCl_3) δ 7.92 (dt, J = 8.0, 0.8 Hz, 1H), 7.33 – 7.29 (m, 1H), 7.28 – 7.20 (m, 1H), 7.05 (td, J = 7.6, 1.1 Hz, 1H), 4.83 (dd, J = 6.2, 3.4 Hz, 1H), 3.85 (s, 3H), 3.26 – 3.14 (m, 1H), 3.09 (ddd, J = 12.5, 9.2, 3.4 Hz, 1H), 2.52 – 2.44 (m, 1H), 2.33 – 2.17 (m, 3H), 1.62 – 1.49 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 172.3, 171.1, 145.3, 132.9, 128.4, 124.3, 123.3, 117.5, 65.0, 52.7, 52.1, 41.5, 34.8, 29.2, 26.3.

HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{16}\text{NO}_3$ [$\text{M}+\text{H}]^+$: 258.1125. Found: 258.1124.

(1a β ,1a $^1\beta$,9b β)-4-oxo-1a,2,3,4-tetrahydro-1*H*-benzo[*b*]cyclobuta[*hi*]indolizine-9b(1a 1H)-carbaldehyde (2s)



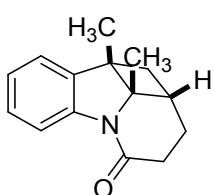
Colorless liquid, 75% yield.

^1H NMR (400 MHz, CDCl_3) δ 9.92 (s, 1H), 7.95 (d, J = 7.9 Hz, 1H), 7.35 – 7.29 (m, 1H), 7.12 – 7.05 (m, 2H), 4.80 (dd, J = 6.4, 3.2 Hz, 1H), 3.23 (ddd, J = 12.4, 9.4, 3.1 Hz, 1H), 3.08 – 2.96 (m, 1H), 2.55 – 2.46 (m, 1H), 2.37 – 2.28 (m, 1H), 2.27 – 2.18 (m, 1H), 2.07 (dd, J = 12.3, 8.7 Hz, 1H), 1.60 (tdd, J = 13.5, 6.2, 3.3 Hz, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 197.6, 171.3, 146.3, 131.7, 129.0, 124.6, 123.1, 117.9, 63.2, 58.0, 36.5, 34.8, 28.6, 26.4.

HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{14}\text{NO}_2$ [$\text{M}+\text{H}]^+$: 228.1019. Found: 228.1017.

(1a β ,1a $^1\beta$,9b β)-1a 1 ,9b-dimethyl-1,1a,1a 1 ,2,3,9b-hexahydro-4*H*-benzo[*b*]cyclobuta[*hi*]indolizin-4-one (2t)



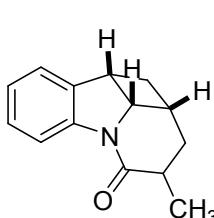
White solid, 88% yield, m.p. = 82.9–83.4 °C.

^1H NMR (400 MHz, CDCl_3) δ 7.93 – 7.85 (m, 1H), 7.25 – 7.15 (m, 1H), 7.12 – 6.99 (m, 2H), 2.77 (dtd, J = 10.0, 8.9, 5.1 Hz, 1H), 2.49 – 2.39 (m, 2H), 2.35 – 2.26 (m, 2H), 1.85 (dd, J = 11.8, 8.9 Hz, 1H), 1.65 – 1.54 (m, 1H), 1.44 (s, 3H), 1.29 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 170.9, 143.9, 139.1, 127.4, 124.2, 121.7, 117.7, 72.4, 45.6, 41.8, 33.5, 33.0, 26.7, 20.6, 17.0.

HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{18}\text{NO}$ [$\text{M}+\text{H}]^+$: 228.1383. Found: 228.1382.

(1a β ,1a $^1\beta$,9b β)-3-methyl-1,1a,1a 1 ,2,3,9b-hexahydro-4*H*-benzo[*b*]cyclobuta[*hi*]indolizin-4-one (2u)



White solid, 94% yield, m.p. = 139.6–139.9 °C.

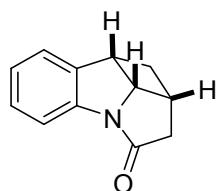
^1H NMR (400 MHz, CDCl_3) δ 7.90 (d, J = 7.9 Hz, 1H), 7.19 (t, J = 7.7 Hz,

1H), 7.08 (d, J = 7.2 Hz, 1H), 6.98 (t, J = 7.4 Hz, 1H), 4.66 (td, J = 6.1, 2.9 Hz, 1H), 3.67 – 3.59 (m, 1H), 3.06 (tdd, J = 15.4, 9.3, 6.2 Hz, 1H), 2.81 (td, J = 11.7, 8.8, 2.8 Hz, 1H), 2.30 (tt, J = 12.8, 6.5 Hz, 1H), 2.22 – 2.13 (m, 1H), 1.89 (dt, J = 12.1, 8.1 Hz, 1H), 1.35 (td, J = 13.4, 6.1 Hz, 1H), 1.20 (d, J = 6.7 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 174.0, 145.6, 136.4, 127.3, 123.9, 123.3, 117.4, 63.2, 38.3, 38.1, 37.3, 35.7, 29.9, 14.4.

HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{16}\text{NO} [\text{M}+\text{H}]^+$: 214.1226. Found: 214.1221.

(1a β ,1a $^1\beta$,8b β)-1a,1a 1 ,2,8b-tetrahydrobenzo[*b*]cyclobuta[*gh*]pyrrolizin-3(1*H*)-one (2v)



White solid, 77% yield, m.p. = 76.3–77.2 °C.

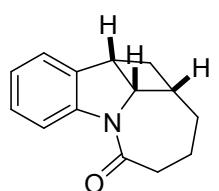
^1H NMR (400 MHz, CDCl_3) δ 7.49 (d, J = 7.7 Hz, 1H), 7.23 (td, J = 7.5, 1.7 Hz, 1H), 7.14 – 7.05 (m, 2H), 4.83 (td, J = 4.9, 2.1 Hz, 1H), 3.48 (dt, J = 9.1, 5.7 Hz, 1H), 3.22 – 3.10 (m, 1H), 3.00 – 2.88 (m, 2H), 2.34 (d, J = 17.3 Hz, 1H), 1.86 (dt, J = 13.0, 6.4 Hz, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 182.4, 146.6, 138.8, 127.4, 125.4, 123.7, 118.3, 70.1, 40.4, 38.2, 34.4, 31.3.

HRMS (ESI) calcd for $\text{C}_{12}\text{H}_{12}\text{NO} [\text{M}+\text{H}]^+$: 186.0913. Found: 186.0911.

Analytical data for compound **2v** was consistent with the literature except for the chemical shift of the carbonyl carbon.⁷

(1a β ,1a $^1\beta$,9b β)-1a,1a 1 ,2,3,4,9b-hexahydro-5a-azabeno[*a*]cyclobuta[*cd*]azulen-5(1*H*)-one (2w)



White solid, 65% yield, m.p. = 113.2–113.5 °C.

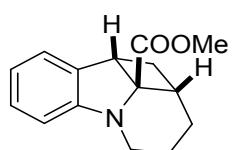
^1H NMR (400 MHz, CDCl_3) δ 8.17 (d, J = 8.1 Hz, 1H), 7.21 (t, J = 7.7 Hz, 1H), 7.08 (d, J = 7.2 Hz, 1H), 6.99 (t, J = 7.4 Hz, 1H), 4.83 – 4.77 (m, 1H), 3.91 – 3.83 (m, 1H), 2.83 – 2.71 (m, 2H), 2.55 – 2.38 (m, 2H), 2.00 – 1.90 (m, 1H), 1.79 – 1.68 (m, 2H), 1.64 – 1.49 (m, 2H).

^{13}C NMR (101 MHz, CDCl_3) δ 171.2, 144.3, 136.8, 127.7, 123.73, 123.67, 116.9, 62.1, 37.3, 35.3, 35.2, 34.7, 28.0, 21.8.

HRMS (ESI) calcd for $\text{C}_{14}\text{H}_{16}\text{NO} [\text{M}+\text{H}]^+$: 214.1226. Found: 214.1224.

Analytical data for compound **2w** was consistent with the literature.⁷

methyl (1a β ,1a $^1\beta$,9b β)-1,1a,2,3,4,9b-hexahydro-1a 1 H-benzo[*b*]cyclobuta[*hi*]indolizine-1a 1 -carboxylate (2x)



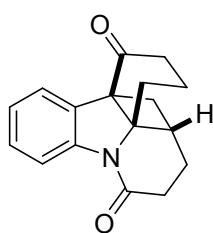
White solid, 49% yield, m.p. = 41.1–41.5 °C.

^1H NMR (400 MHz, CDCl_3) δ 7.00 (td, J = 7.7, 0.9 Hz, 1H), 6.89 – 6.83 (m, 1H), 6.61 – 6.54 (m, 2H), 3.81 (dd, J = 8.7, 6.5 Hz, 1H), 3.66 (s, 3H), 3.61 – 3.53 (m, 1H), 3.13 – 2.96 (m, 2H), 2.43 (ddd, J = 12.0, 10.3, 8.9 Hz, 1H), 1.78 – 1.56 (m, 3H), 1.50 – 1.44 (m, 1H), 1.38 – 1.31 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 173.7, 153.3, 135.4, 127.7, 122.6, 118.6, 110.0, 66.5, 52.1, 45.2, 42.2, 33.8, 31.0, 24.6, 18.5.

HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{18}\text{NO}_2 [\text{M}+\text{H}]^+$: 244.1332. Found: 244.1330.

(4a β ,5 β ,13b β)-3,4,6,7-tetrahydro-5,13b-methanopyrido[2,1-*k*]carbazole-1,8(2*H*,5*H*)-dione (2aa)



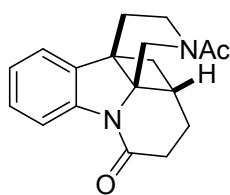
White solid, 94% yield, m.p. = 183.4–183.7 °C.

¹H NMR (400 MHz, CDCl₃) δ 7.94 (d, *J* = 7.9 Hz, 1H), 7.27 (td, *J* = 7.9, 1.4 Hz, 1H), 7.03 (td, *J* = 7.4, 0.8 Hz, 1H), 6.98 (dd, *J* = 7.4, 0.9 Hz, 1H), 3.01 (dd, *J* = 11.8, 9.3 Hz, 1H), 2.98 – 2.88 (m, 1H), 2.53 – 2.44 (m, 2H), 2.43 – 2.24 (m, 3H), 2.11 – 2.00 (m, 3H), 1.90 – 1.84 (m, 2H), 1.72 – 1.60 (m, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 209.7, 170.6, 145.2, 131.7, 128.7, 124.7, 122.7, 118.2, 75.9, 55.7, 39.22, 39.18, 33.1, 32.5, 31.6, 27.0, 20.6.

HRMS (ESI) calcd for C₁₇H₁₈NO₂ [M+H]⁺: 268.1332. Found: 268.1326.

(4a β ,5 β ,13b β)-3-acetyl-1,2,3,4,6,7-hexahydro-5,13b-methanodipyrido[1,2-*a*:3',4'-*b*]indol-8(5*H*)-one (2ab)



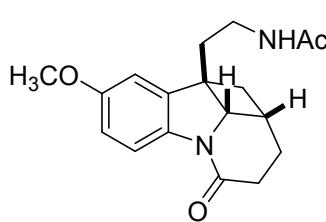
Colorless liquid, 75% yield.

¹H NMR (400 MHz, CDCl₃) δ 7.93 – 7.87 (m, 1H), 7.27 – 7.22 (m, 1H), 7.14 – 7.04 (m, 2H), 4.68 (d, *J* = 13.8 Hz, 0.7H), 4.31 – 4.22 (m, 0.3H), 3.83 – 3.68 (m, 1H), 3.27 (d, *J* = 14.0 Hz, 0.3H), 3.03 – 2.87 (m, 1.7H), 2.75 (d, *J* = 13.8 Hz, 0.7H), 2.70 – 2.61 (m, 0.3H), 2.52 – 2.32 (m, 4.3H), 2.17 (s, 2H), 2.14 (s, 1H), 2.12 – 1.99 (m, 1.7H), 1.98 – 1.90 (m, 1H), 1.74 – 1.58 (m, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 170.9, 170.5, 169.8, 169.3, 144.9, 144.7, 136.0, 135.9, 128.2, 128.1, 125.0, 124.7, 122.1, 121.8, 118.3, 118.1, 69.1, 50.5, 45.6, 44.1, 44.0, 43.0, 42.3, 41.6, 38.9, 33.2, 33.0, 30.8, 29.2, 29.1, 26.5, 21.7, 21.6.

HRMS (ESI) calcd for C₁₈H₂₁N₂O₂ [M+H]⁺: 297.1598. Found: 297.1596.

N-(2-((1a β ,1a $^1\beta$,9b β)-8-methoxy-4-oxo-1a,2,3,4-tetrahydro-1*H*-benzo[*b*]cyclobuta[*hi*]indolizin-9b(1a 1H)-yl)ethyl)acetamide (2ac)



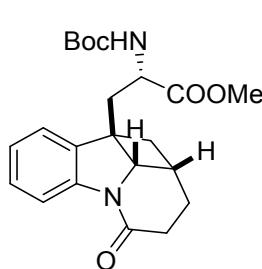
Colorless liquid, 89% yield.

¹H NMR (400 MHz, CDCl₃) δ 7.71 (d, *J* = 8.6 Hz, 1H), 6.62 (dd, *J* = 8.6, 2.5 Hz, 1H), 6.55 (d, *J* = 2.6 Hz, 1H), 5.88 (brs, 1H), 4.35 (dd, *J* = 6.0, 3.2 Hz, 1H), 3.70 (s, 3H), 3.32 – 3.19 (m, 1H), 3.15 – 3.03 (m, 1H), 3.01 – 2.87 (m, 1H), 2.44 – 2.30 (m, 2H), 2.23 – 2.07 (m, 4H), 1.92 (dd, *J* = 12.0, 9.1 Hz, 1H), 1.86 (s, 3H), 1.49 – 1.37 (m, 1H).

¹³C NMR (101 MHz, CDCl₃) δ 171.3, 170.3, 156.8, 139.0, 138.9, 117.8, 111.2, 108.7, 64.9, 55.7, 46.7, 42.4, 36.2, 34.7, 32.7, 28.1, 26.3, 23.2.

HRMS (ESI) calcd for C₁₈H₂₃N₂O₃ [M+H]⁺: 315.1703. Found: 315.1700.

methyl (S)-2-((tert-butoxycarbonyl)amino)-3-((1a β ,1a $^1\beta$,9b β)-4-oxo-1a,2,3,4-tetrahydro-1*H*-benzo[*b*]cyclobuta[*hi*]indolizin-9b(1a 1H)-yl)propanoate (2ad)



White solid, 81% yield, m.p. = 40.1–40.4 °C.

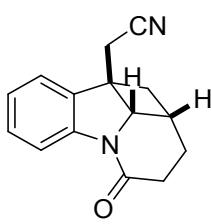
¹H NMR (400 MHz, CDCl₃) δ 7.95 – 7.84 (m, 1H), 7.22 – 7.14 (m, 1H), 7.09 – 6.97 (m, 2H), 5.30 – 5.14 (m, 0.4H), 5.13 – 4.92 (m, 0.6H), 4.71 – 4.13 (m, 2H), 3.68 (s, 1.8H), 3.37 (s, 1.2H), 3.19 – 2.96 (m, 1H), 2.59 – 2.30 (m, 4H), 2.26 – 2.13 (m, 2H), 2.03 (dd, *J* = 12.2, 9.0 Hz, 1H), 1.58 – 1.28 (m, 10H).

¹³C NMR (101 MHz, CDCl₃) δ 173.2, 173.0, 171.6, 171.5, 155.0, 154.9,

145.4, 145.1, 137.5, 136.5, 127.7, 127.5, 124.1, 124.0, 121.6, 121.4, 117.3, 80.2, 80.0, 64.52, 64.48, 52.5, 52.1, 51.1, 51.0, 46.8, 46.6, 43.8, 43.0, 35.8, 35.7, 34.95, 34.92, 28.3, 28.2, 28.1, 28.0, 26.1, 26.0.

HRMS (ESI) calcd for $C_{22}H_{29}N_2O_5$ [M+H]⁺: 401.2071. Found: 401.2068.

2-((1a β ,1a $^1\beta$,9b β)-4-oxo-1a,2,3,4-tetrahydro-1H-benzo[b]cyclobuta[hi]indolizin-9b(1a 1H)-yl)acetonitrile (2ae)



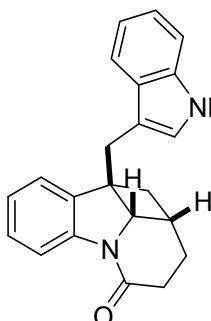
White solid, 97% yield, m.p. = 106.4-106.9 °C.

1H NMR (400 MHz, CDCl₃) δ 7.98 – 7.84 (m, 1H), 7.32 – 7.22 (m, 1H), 7.17 – 7.11 (m, 1H), 7.07 (td, J = 7.5, 1.1 Hz, 1H), 4.47 (dd, J = 6.3, 3.3 Hz, 1H), 3.29 – 3.16 (m, 1H), 3.00 (d, J = 17.0 Hz, 1H), 2.91 (d, J = 17.0 Hz, 1H), 2.72 (ddd, J = 12.6, 9.2, 3.3 Hz, 1H), 2.49 (ddd, J = 14.2, 3.5, 2.4 Hz, 1H), 2.38 – 2.28 (m, 1H), 2.27 – 2.14 (m, 2H), 1.57 (tdd, J = 13.7, 6.1, 3.4 Hz, 1H).

^{13}C NMR (101 MHz, CDCl₃) δ 171.2, 144.9, 135.3, 128.7, 124.5, 121.3, 117.6, 117.1, 65.6, 44.9, 40.7, 34.8, 27.7, 26.1, 23.2.

HRMS (ESI) calcd for $C_{15}H_{15}N_2O$ [M+H]⁺: 239.1179. Found: 239.1178.

(1a β ,1a $^1\beta$,9b β)-9b-((1H-indol-3-yl)methyl)-1,1a,1a 1 ,2,3,9b-hexahydro-4H-benzo[b]cyclobuta[hi]indolizin-4-one (2af)



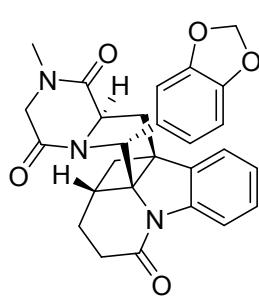
White solid, 71% yield, m.p. = 121.7-122.9 °C.

1H NMR (400 MHz, CDCl₃) δ 8.35 (s, 1H), 7.95 – 7.85 (m, 1H), 7.63 (d, J = 7.7 Hz, 1H), 7.35 – 7.30 (m, 1H), 7.22 – 7.10 (m, 4H), 7.07 – 7.01 (m, 1H), 6.75 (d, J = 2.2 Hz, 1H), 4.31 (dd, J = 6.1, 3.3 Hz, 1H), 3.43 – 3.31 (m, 2H), 2.71 – 2.51 (m, 2H), 2.40 – 2.28 (m, 1H), 2.13 – 1.97 (m, 3H), 1.46 – 1.34 (m, 1H).

^{13}C NMR (101 MHz, CDCl₃) δ 171.9, 145.3, 139.1, 135.8, 128.3, 127.5, 124.2, 122.9, 122.02, 122.00, 119.5, 118.5, 117.3, 111.5, 111.4, 65.6, 48.7, 41.8, 34.9, 28.6, 28.0, 26.2.

HRMS (ESI) calcd for $C_{22}H_{21}N_2O$ [M+H]⁺: 329.1648. Found: 329.1646.

(1R,9bR,10aR,16R,16aR)-16-(benzo[d][1,3]dioxol-5-yl)-12-methyl-2,3,10,10a,12,13-hexahydro-16H-1,9b-methanopyrazino[1',2':1,6]pyrido[3,4-b]pyrido[1,2-a]indole-4,11,14(1H)-trione (2ag)



White solid, 83% yield, m.p. = 227.3-228.3 °C.

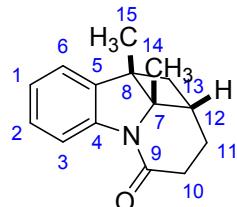
1H NMR (400 MHz, CDCl₃) δ 7.55 (d, J = 7.8 Hz, 1H), 7.08 – 6.91 (m, 3H), 6.53 – 6.47 (m, 1H), 6.45 – 6.38 (m, 2H), 5.82 – 5.76 (m, 2H), 5.53 (s, 1H), 4.59 (dd, J = 13.3, 2.9 Hz, 1H), 4.28 (d, J = 16.9 Hz, 1H), 3.95 (d, J = 16.9 Hz, 1H), 3.10 (s, 3H), 3.00 (dd, J = 14.8, 3.5 Hz, 1H), 2.91 – 2.77 (m, 1H), 2.64 (dd, J = 12.6, 9.6 Hz, 1H), 2.59 – 2.51 (m, 2H), 2.49 – 2.36 (m, 2H), 2.07 (dd, J = 12.6, 8.5 Hz, 1H), 1.73 – 1.60 (m, 1H).

^{13}C NMR (101 MHz, CDCl₃) δ 171.1, 166.4, 166.0, 147.2, 146.7, 144.5, 138.0, 130.0, 127.8, 124.7, 121.6, 121.0, 117.2, 107.8, 107.7, 101.0, 70.2, 58.9, 52.32, 52.29, 42.5, 38.0, 34.2, 33.3, 32.8, 30.4, 28.1.

HRMS (ESI) calcd for $C_{27}H_{26}N_3O_5$ [M+H]⁺: 472.1867. Found: 472.1846.

4. 2D NMR data of selected products

4.1 2D NMR data of **2t**



No.	δ_H (400 MHz, CDCl ₃)	δ_C (101 MHz, CDCl ₃)
1	7.04 (m, 1H)	124.2
2	7.20 (m, 1H)	127.4
3	7.89 (m, 1H)	117.7
4		143.9
5		139.1
6	7.04 (m, 1H)	121.7
7		72.4
8		45.6
9		170.9
10	2.44 (m, 2H)	33.0
11	2.31 (m, 1H) 1.59 (m, 1H)	26.7
12	2.77 (dtd, <i>J</i> = 10.0, 8.9, 5.1 Hz, 1H)	33.5
13	2.31 (m, 1H) 1.85 (dd, <i>J</i> = 11.8, 8.9 Hz, 1H)	41.8
14	1.29 (s, 3H)	20.6
15	1.44 (s, 3H)	17.0

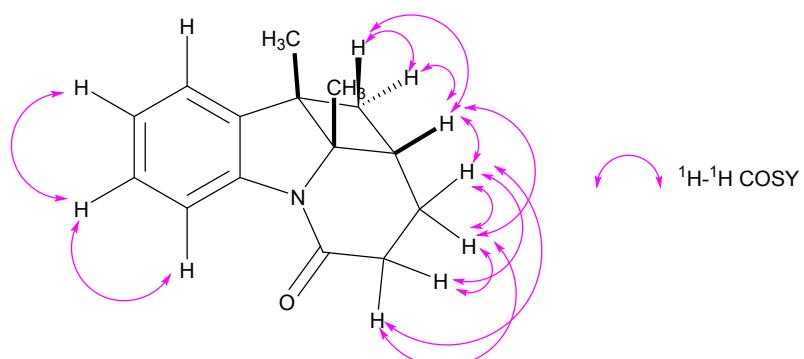


Figure S1. The main ^1H - ^1H COSY correlations of **2t**

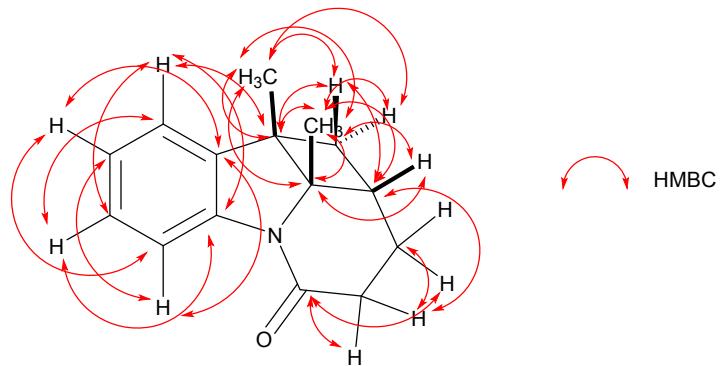


Figure S2. The main HMBC correlations of **2t**

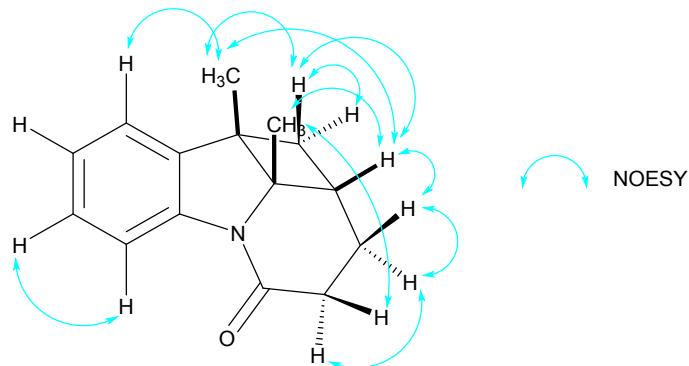
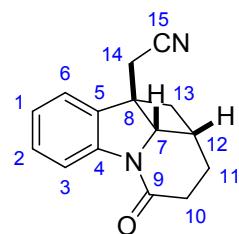


Figure S3. The main NOESY correlations of **2t**

4.2 2D NMR data of 2ae



No.	δ_{H} (400 MHz, CDCl_3)	δ_{C} (101 MHz, CDCl_3)
1	7.07 (td, $J = 7.5, 1.1$ Hz, 1H)	124.5
2	7.27 (m, 1H)	128.7
3	7.92 (m, 1H)	117.6
4		144.9
5		135.3
6	7.14 (m, 1H)	121.3
7	4.47 (dd, $J = 6.3, 3.3$ Hz, 1H)	65.6
8		44.9
9		171.2
10	2.49 (ddd, $J = 14.2, 3.5, 2.4$ Hz, 1H) 2.23 (m, 1H)	34.8
11	2.33 (m, 1H) 1.57 (tdd, $J = 13.7, 6.1, 3.4$ Hz, 1H)	26.1

12	3.22 (m, 1H)	27.7
13	2.72 (ddd, $J = 12.6, 9.2, 3.3$ Hz, 1H) 2.19 (m, 1H)	40.7
14	3.00 (d, $J = 17.0$ Hz, 1H) 2.91 (d, $J = 17.0$ Hz, 1H)	23.2
15		117.1

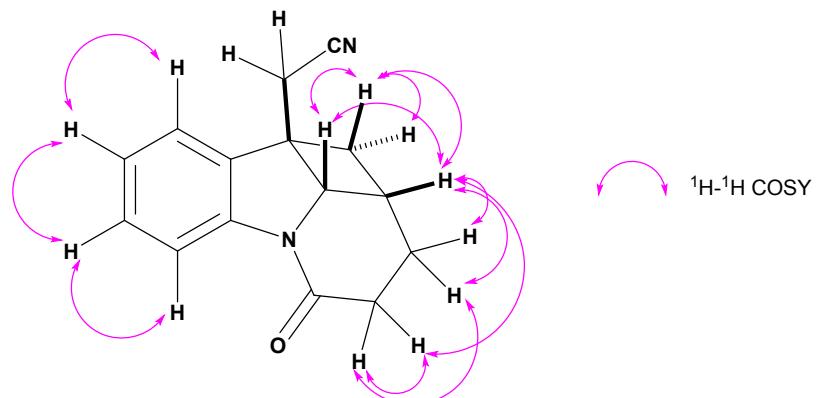


Figure S4. The main ${}^1\text{H}$ - ${}^1\text{H}$ COSY correlations of **2ae**

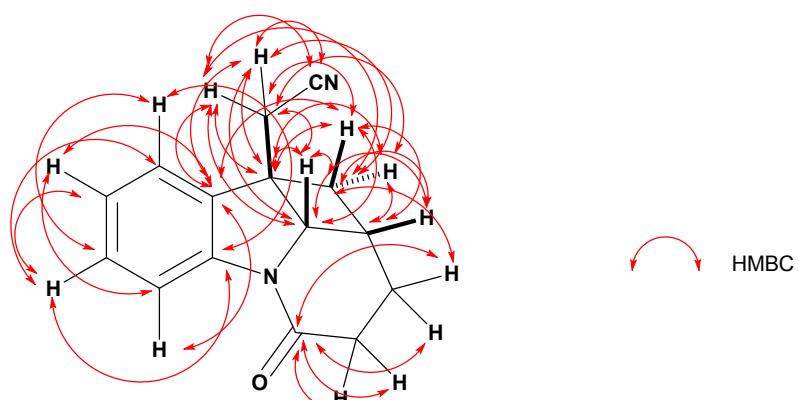


Figure S5. The main HMBC correlations of **2ae**

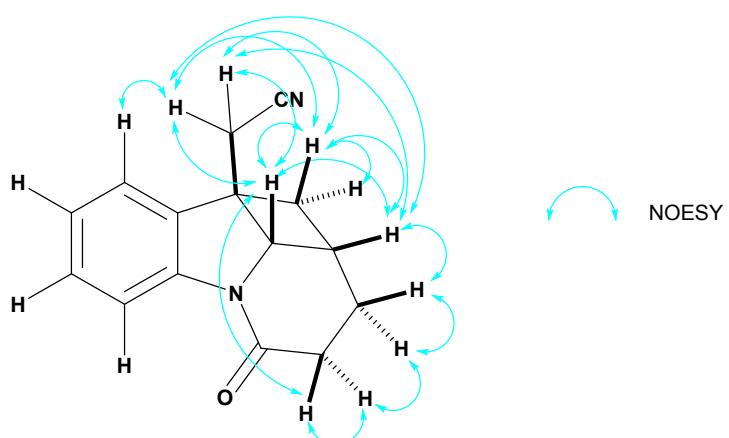
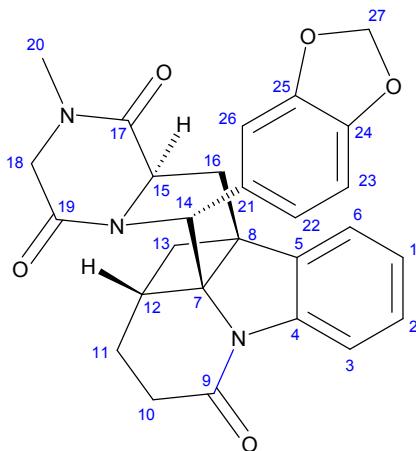


Figure S6. The main NOESY correlations of **2ae**

4.3 2D NMR data of 2ag



No.	δ_{H} (400 MHz, CDCl_3)	δ_{C} (101 MHz, CDCl_3)
1	6.95 (m, 1H)	124.7
2	7.04 (m, 1H)	127.8
3	7.55 (d, $J = 7.8$ Hz, 1H)	117.2
4		144.5
5		138.0
6	7.00 (m, 1H)	121.6
7		70.2
8		42.5
9		171.1
10	2.56 (m, 2H)	33.3
11	2.42 (m, 1H) 1.67 (m, 1H)	28.1
12	2.84 (m, 1H)	32.8
13	2.64 (dd, $J = 12.6, 9.6$ Hz, 1H) 2.07 (dd, $J = 12.6, 8.5$ Hz, 1H)	38.0
14	5.53 (s, 1H)	58.9
15	4.59 (dd, $J = 13.3, 2.9$ Hz, 1H)	52.29
16	3.00 (dd, $J = 14.8, 3.5$ Hz, 1H) 2.44 (m, 1H)	30.4
17		166.4
18	4.28 (d, $J = 16.9$ Hz, 1H) 3.95 (d, $J = 16.9$ Hz, 1H)	52.32
19		166.0
20	3.10 (s, 3H)	34.2
21		130.0
22	6.43 (m, 1H)	121.0
23	6.49 (m, 1H)	107.7
24		147.2
25		146.7
26	6.43 (m, 1H)	107.8
27	5.79 (m, 2H)	101.0

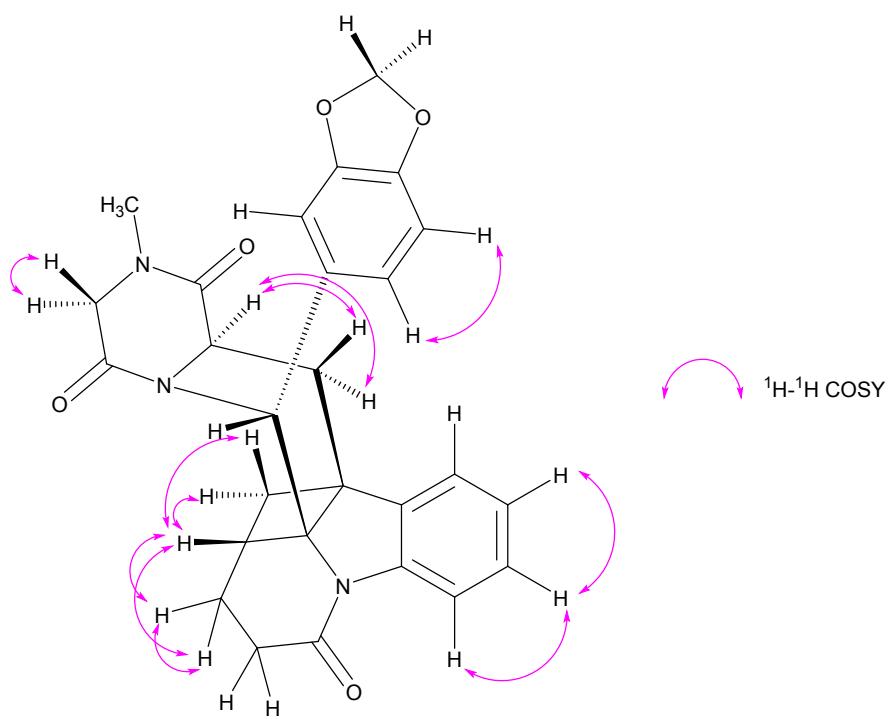


Figure S7. The main ${}^1\text{H}$ - ${}^1\text{H}$ COSY correlations of **2ag**

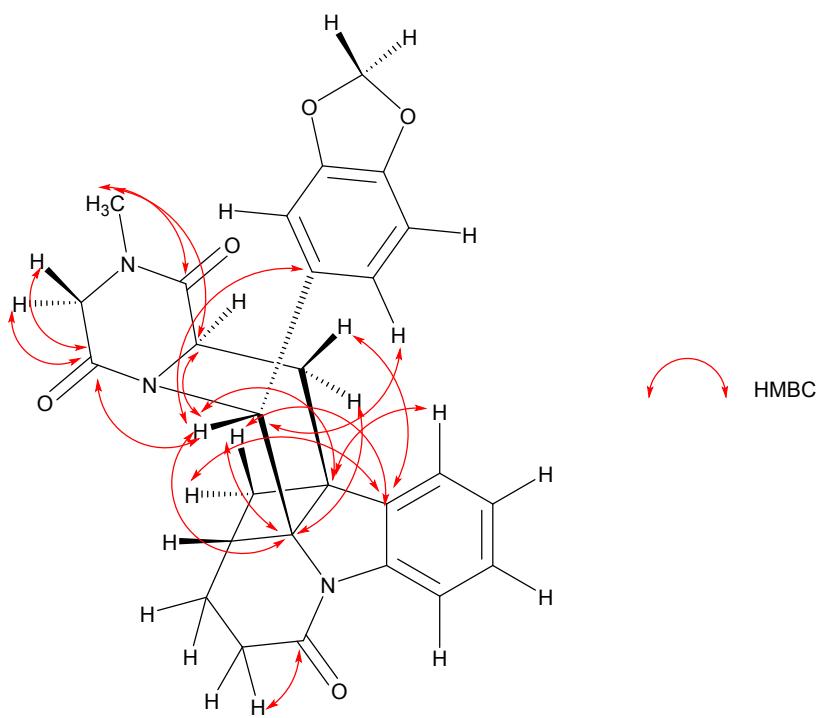


Figure S8. The main HMBC correlations of **2ag**

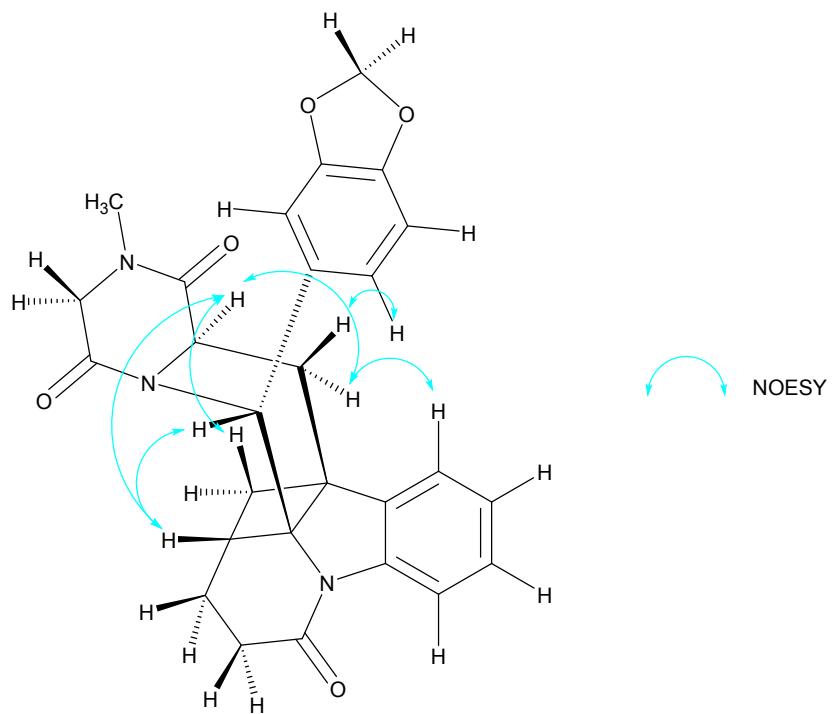


Figure S9. The main NOESY correlations of **2ag**

5. Preliminary mechanistic studies

5.1 Stern-Volmer quenching studies

Stern-Volmer experiments were conducted on a Hitachi F7000 Fluorescence Spectrophotometer. Each component was prepared in $\text{CF}_3\text{CH}_2\text{OH}$ prior to each set of experiments. The solutions were irradiated at 440 nm and the luminescence measured at 505 nm. Linear regression of I_0/I against concentration was performed in Origin.

Species	Concentration (mM)
$\text{Ir}[\text{dF}(\text{CF}_3)\text{ppy}]_2(\text{dtbbpy})\text{PF}_6$	0.1
1a	Varied

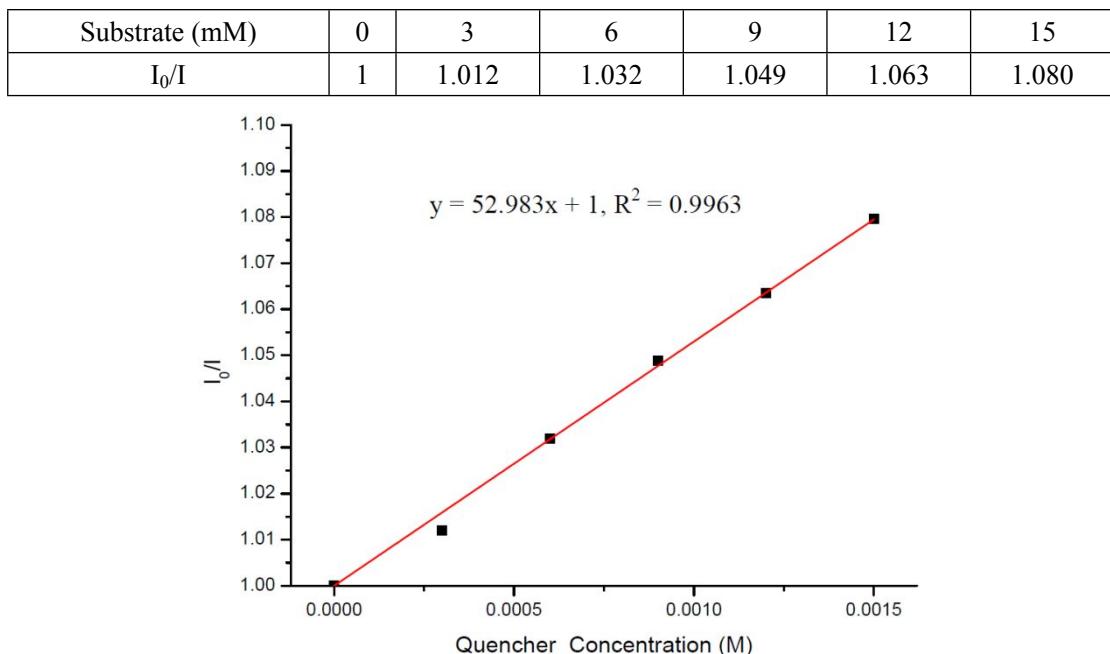
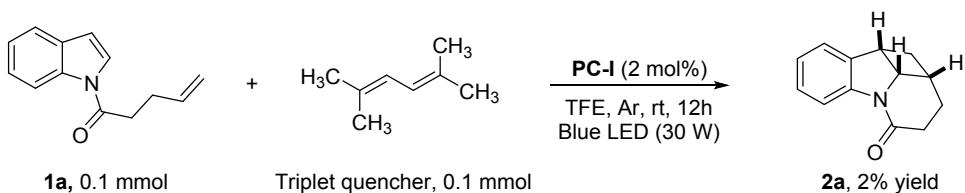


Figure S10. Stern-Volmer quenching experiments with PC-I (0.1 mM, $\lambda_{\text{ex}} = 440$ nm, $\lambda_{\text{em}} = 505$ nm).

5.2 Control experiment with triplet quencher



An oven-dried Schlenk tube (10 mL) containing a stirring bar was charged with the indole derivative **1a** (19.9 mg, 0.1 mmol) and PC-I (2.4 mg, 2 mol%). The Schlenk tube was then connected to a vacuum line where it was evacuated and back-filled with argon for 3 times. Then TFE (1 mL), which bubbled with argon for 5 minutes, and 2,5-dimethylhexa-2,4-diene (known as a

triplet quencher⁸, 14.3 μL , 0.1 mmol), were added to the reaction in sequence under argon flow. Finally, the reaction mixture in sealed tube was placed at a distance of 2 ~ 3 cm from a 30 W blue LED and stirred at room temperature for 12 h. Then, the mixture was concentrated in vacuo. The yield of the product was determined by ¹H-NMR spectroscopy using dimethyl terephthalate (19.4 mg, 0.1 mmol) as internal standard. The model reaction was significantly inhibited in the presence of 1.0 equivalent of 2,5-dimethylhexa-2,4-diene.

5.3 Cyclic voltammetry test

Cyclic voltammetry test was performed in a three-electrode cell under argon at room temperature. All cyclic voltammograms were measured using Ag/Ag⁺ (0.01 M AgNO₃ in MeCN) reference electrode, a platinum (Pt) wire counter electrode and a glassy carbon working electrode. The conditions of the experiments were as follows: testing compounds are in solution of 0.1 M tetrabutylammonium tetrafluoroborate (ⁿBu₄NBF₄) in CH₃CN or CF₃CH₂OH at a scan rate of 50 mV/s; Prior to each measurement, solutions were purged with argon (Ar) for 10 minutes to ensure the oxygen-free conditions.

Measuring the Fc/Fc⁺ redox couple afforded $E_{1/2} = +0.10$ V vs Ag/Ag⁺ under our experimental conditions. The obtained value was referenced to Ag/Ag⁺ and converted to SCE by subtracting 0.32 V, providing a value of +0.42 V for the Fc/Fc⁺ couple.⁹ The oxidation half-peak potential of **1a** in CF₃CH₂OH and MeCN was measured as +1.38 V and +1.30 V (vs Ag/Ag⁺), and calculated to +1.70 V and +1.62 V (vs SCE), respectively. The corresponding reductive peak was not observed.

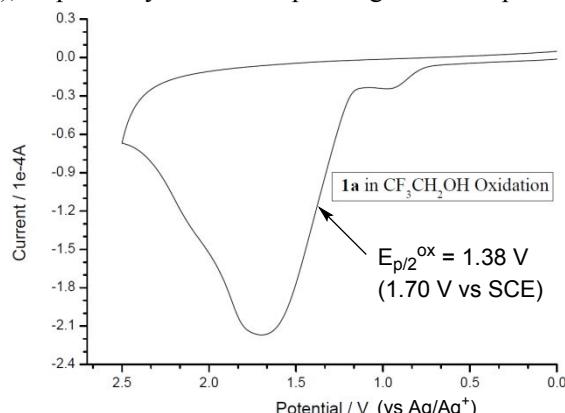


Figure S11. Cyclic voltammetry of **1a** (0.01 M) in CF₃CH₂OH (vs Ag/Ag⁺) with ⁿBu₄NBF₄ (0.1 M) under argon at a glassy carbon electrode at a scan rate of 50 mV/s.

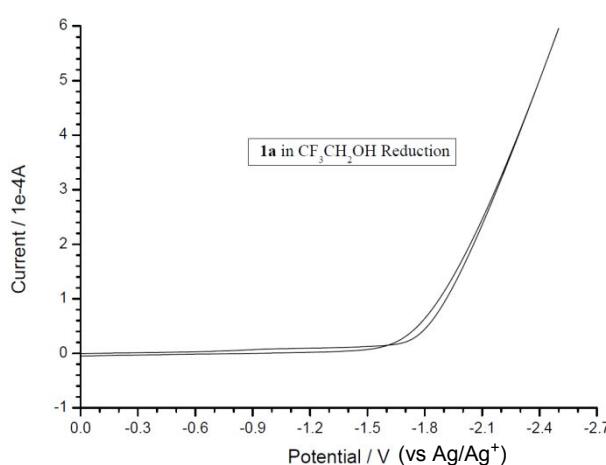


Figure S12. Cyclic voltammetry of **1a** (0.01 M) in CF₃CH₂OH (vs Ag/Ag⁺) with ⁿBu₄NBF₄ (0.1 M) under argon at S26

a glassy carbon electrode at a scan rate of 50 mV/s.

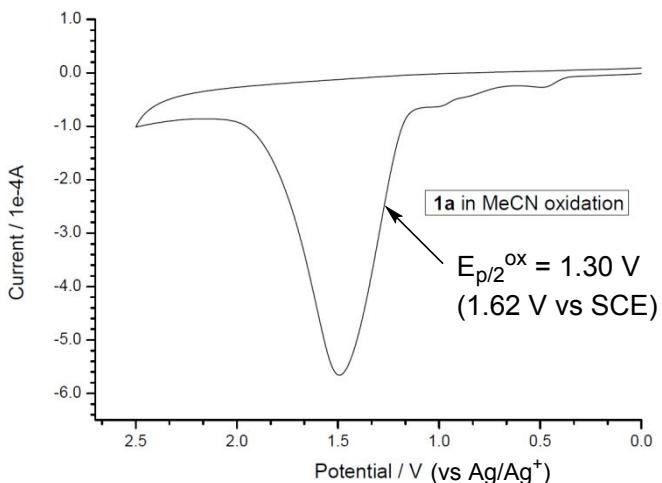


Figure S13. Cyclic voltammetry of **1a** (0.01 M) in CH₃CN (vs Ag/Ag⁺) with "Bu₄NBF₄ (0.1 M) under argon at a glassy carbon electrode at a scan rate of 50 mV/s.

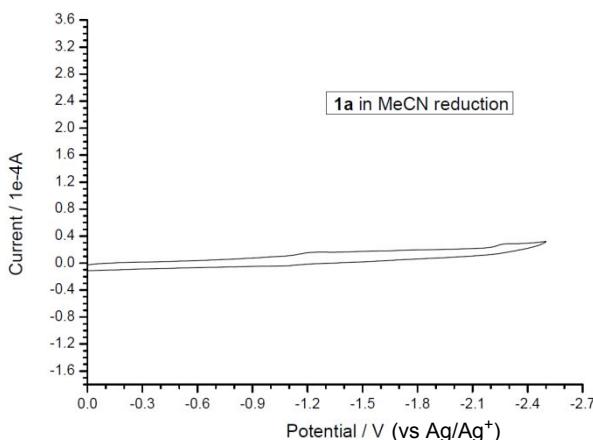


Figure S14. Cyclic voltammetry of **1a** (0.01 M) in CH₃CN (vs Ag/Ag⁺) with "Bu₄NBF₄ (0.1 M) under argon at a glassy carbon electrode at a scan rate of 50 mV/s.

5.4 *In situ* ¹³C-NMR spectroscopy

A NMR tube containing indole derivative **1a** (15 mg) dissolved in CDCl₃ (0.5 mL) was tested by ¹³C-NMR spectroscopy. The spectra showed a signal at 170.78 ppm, which was assigned to signal of the carbonyl carbon of substrate **1a**. Then, different amounts of CF₃CH₂OH (5, 5, 10, 10 and 30 μL) was added and mixed well. After each mixing, the sample was tested and analyzed. As shown in Figure S15, the downfield moving of the chemical shift of carbonyl carbon atom and line broadening were observed under ¹³C-NMR spectroscopy.

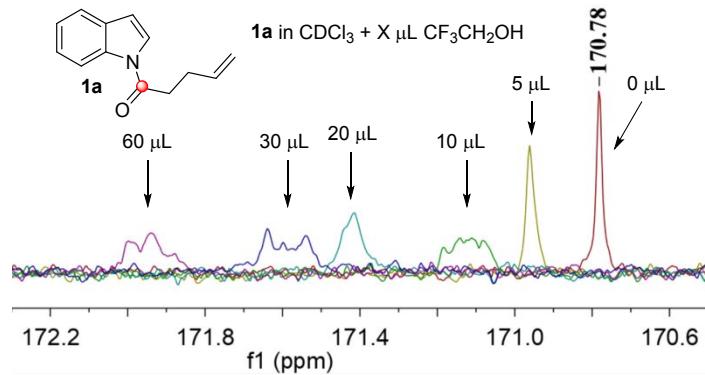


Figure S15. Chemical shift changes of carbonyl carbon of *in situ* ^{13}C NMR spectroscopy of **1a** with different amounts of $\text{CF}_3\text{CH}_2\text{OH}$.

5.5 Emission spectra of PC-I

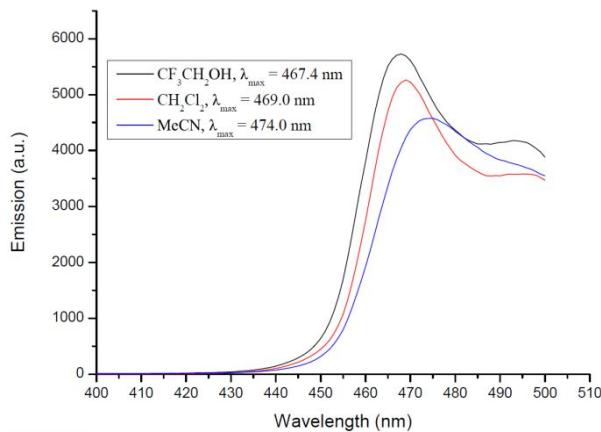


Figure S16. Emission spectra of photocatalyst PC-I (excited at 380 nm) 5 μM in solvent ($\text{CF}_3\text{CH}_2\text{OH}$, CH_2Cl_2 , MeCN).

Table S1. The photophysical properties of PC-I

	In Vacuum	$\text{CF}_3\text{CH}_2\text{OH}$	CH_2Cl_2	MeCN
Absorption (λ_{max}) / nm	—	380	380	380
Emission (λ_{max}) / nm	—	467.4	469.0	474.0
Experimental triplet state energy / kcal mol⁻¹	—	61.2	61.0	60.3 (60.1) ^a ¹⁰
Calculated triplet state energy^b / kcal mol⁻¹	62.0	61.9		

^aLiterature value in parentheses. ^bComputational method: (U)B3LYP / def2-SVP / PCM ($\text{CF}_3\text{CH}_2\text{OH}$)

5.6 Computational studies

DFT calculations were performed using the Gaussian 16 quantum chemistry software package.¹¹ All energy profiles for the reaction were calculated at the (U)B3LYP/def2-TZVPP level if not specified.¹² The solvent effect (in 2,2,2-trifluoroethanol, TFE) was taken account by the Polarizable Continuum Model.¹³ The hydrogen bond effect for the S₀-T₁ energy gap (in TFE solvent) has been investigated at the (U)B3LYP-D3(BJ)/def2-SVP level.¹⁴ All the optimized transition states were confirmed to have only one imaginary frequency. The searching for minimal energy crossing points was conducted using a modified version of Harvey's code¹⁵ (sobMECP¹⁶) interfaced with Gaussian 16.

5.6.1 The calculated results for the reaction

Table S2. Calculated results of triplet-singlet energy gaps of **1a**^a

	In vacuum	CF ₃ CH ₂ OH	CH ₂ Cl ₂	CH ₃ CN
1a -PCM	63.3	62.5 (58.2) ^b	62.2	62.5

^a Computational method: (U)B3LYP-D3(BJ) / def2-TZVPP / PCM (Solvent). The free energies are in kcal mol⁻¹.

¹. ^b the S₀-T₁ gap of substrate **1a** with 2 H-bonds with dimers of the fluorinated solvent, values in parentheses calculated at (U)B3LYP-D3(BJ) / def2-SVP / PCM level.

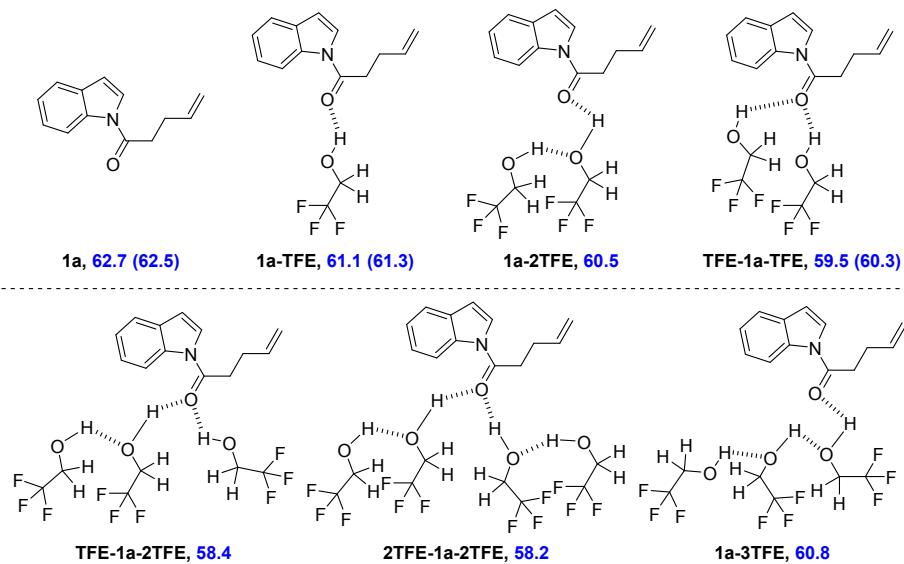


Figure S17. Proposed chemical structures based on different modes of H-bonds and calculated result of triplet-singlet energy gaps of different modes of H-bonds. Computational method: (U)B3LYP-D3(BJ)/def2-SVP/PCM (CF₃CH₂OH) (values in parentheses calculated at (U)B3LYP-D3(BJ) / def2-TZVPP / PCM (CF₃CH₂OH) level. The free energies are in kcal mol⁻¹.

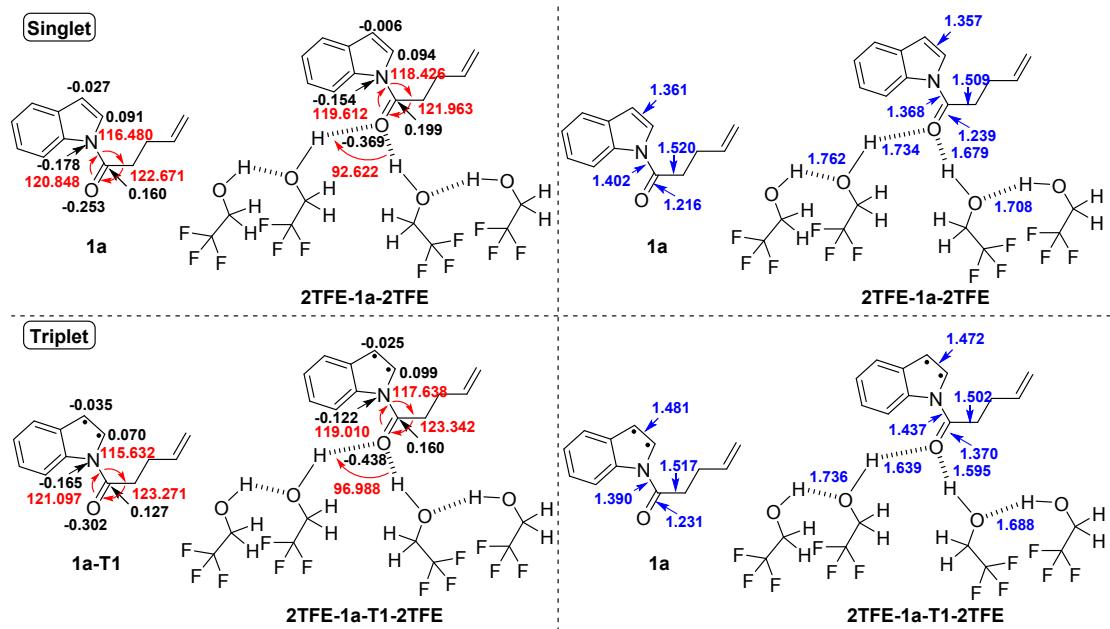


Figure S18. Mulliken spin population (black), bond angels (red) and bonds length (blue). The bond distances are in angstrom.

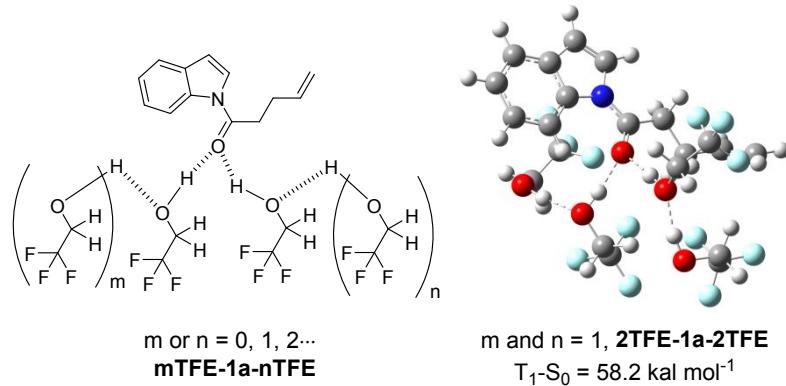
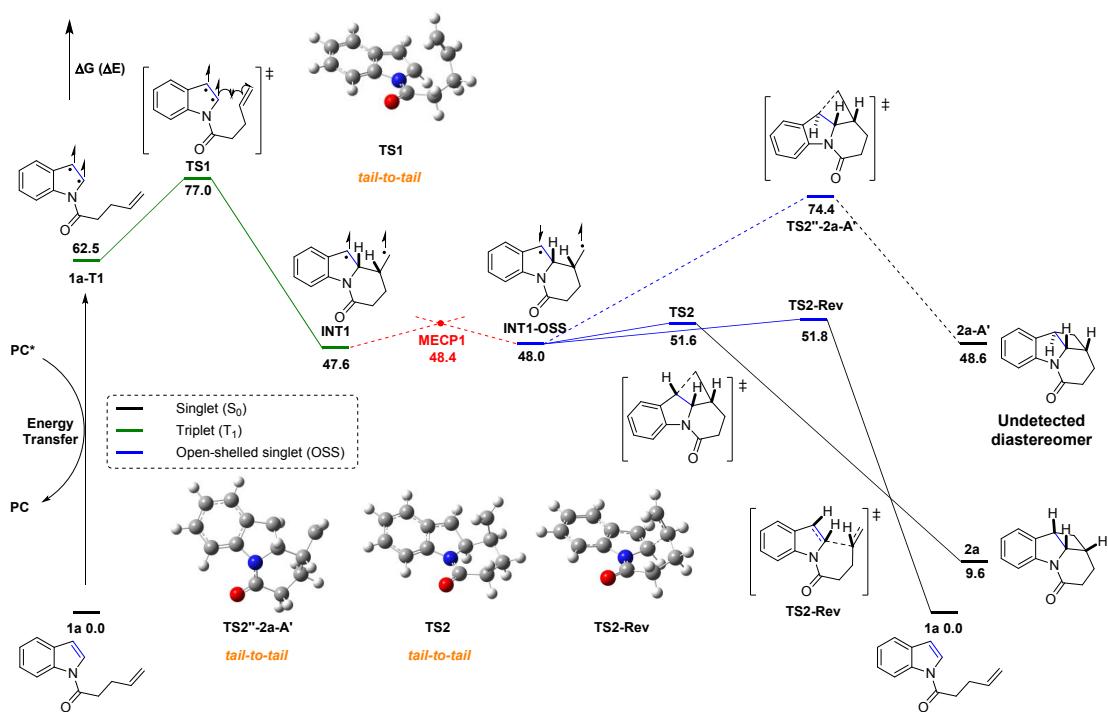
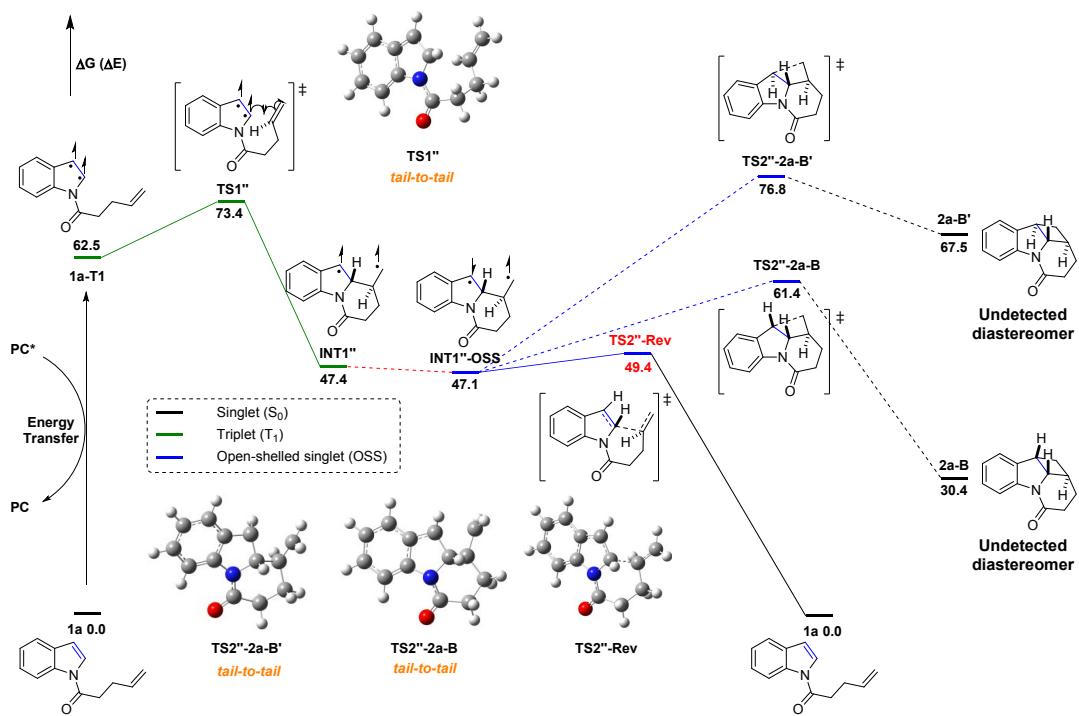


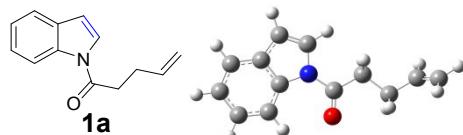
Figure S19. Proposed structure for H-bond(s) between **1a** and trifluoroethanol solvents in actual reaction conditions: aggregation-induced cooperative H-bonding enhancement (left). Calculated triplet-singlet energy gap for **2TFE-1a-TFE** (right).



to **1a**, and the optimized structures of **TS1**, **TS2**, **TS2"-2a-A'**and **TS2-Rev**. Computational Method: (U)B3LYP / def2-TZVPP / PCM ($\text{CF}_3\text{CH}_2\text{OH}$).

5.6.2 Cartesian coordinates and energies of all optimized structures

(1) At (U)B3LYP / def2-TZVPP / PCM ($\text{CF}_3\text{CH}_2\text{OH}$) level of theory

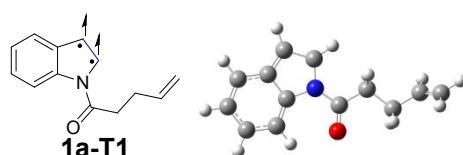


SCF Done: E(RB3LYP) = -633.432107019 A.U.

Zero-point correction = 0.228754 (Hartree/Particle)

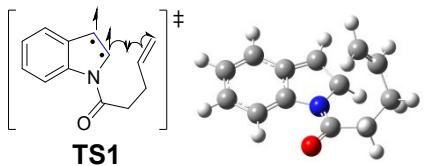
Sum of electronic and thermal Free Energies = -633.244284

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C,0,2.0921873666,1.4495346444,0.0340060031
C,0,3.4729220141,1.6010552368,0.0925825283
C,0,4.3317105893,0.4953485525,0.1192265936
C,0,3.825875707,-0.7954163248,0.0878020575
C,0,1.6068355214,-2.1470900422,-0.0129432531
C,0,0.3216202963,-1.7312358178,-0.0609881397
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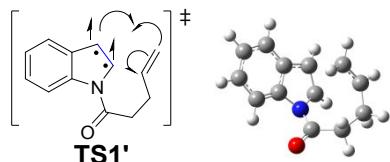


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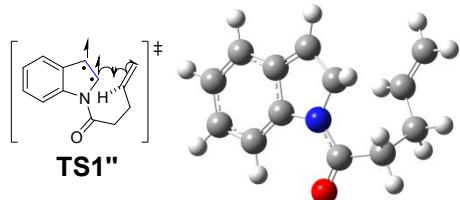
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 N, 0, 0.3478533433, 0.5994993737, 0.7836416576
 C, 0, 1.1613657972, 1.5475910018, 0.1640802681
 O, 0, 0.7659752822, 2.6936332417, 0.0089553628
 C, 0, 2.4599906749, 1.1119583018, -0.5101329917
 H, 0, 2.2013634027, 1.1919552622, -1.5725251959
 C, 0, 3.159229377, -0.2304315517, -0.2639570772
 H, 0, 4.0154831084, -0.2473840003, -0.9546097148
 C, 0, 2.4148945454, -1.5266001119, -0.418428998
 H, 0, 2.9344544357, -2.3734671717, 0.018194785
 C, 0, 1.1831808753, -1.8003514328, -1.0220525565
 H, 0, 0.6728532192, -1.0456882005, -1.6054964571
 H, 0, 3.1811757166, 1.9107345269, -0.335328244
 H, 0, 3.6178464486, -0.2236668733, 0.7286210489
 H, 0, 0.9448599242, -2.8229385154, -1.2803920945

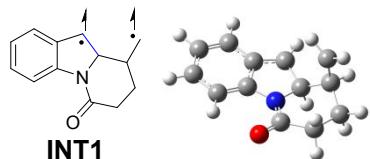


SCF Done: E(UB3LYP) = -633.312205548 A.U.
 Zero-point correction= 0.224518 (Hartree/Particle)
 Sum of electronic and thermal Free Energies= -633.127288

Imaginary Frequency = -260.26 cm⁻¹

C, 0, 1.5046395643, -1.0638491432, 0.3121199653
 C, 0, 1.1601361698, 0.3268734355, 0.1630080811
 C, 0, 2.0748990213, 1.2639601744, -0.2408597856
 C, 0, 3.383508847, 0.8204064729, -0.539579056
 C, 0, 3.7455861006, -0.5270877427, -0.413890255
 C, 0, 2.8328754808, -1.474170323, 0.0092031674
 C, 0, 0.3903119295, -1.7547591392, 0.7435440612
 C, 0, -0.720083256, -0.7891922978, 0.9019283093
 H, 0, 1.8031131941, 2.3014505934, -0.3389590729
 H, 0, 4.1152559716, 1.5408526694, -0.8778821374
 H, 0, 4.7578560824, -0.826946467, -0.6503597001
 H, 0, 3.1128035862, -2.5138224428, 0.1103916633
 H, 0, 0.313233389, -2.8072450503, 0.9596056562
 H, 0, -1.4092637257, -0.8262287544, 1.7344822393

N, 0, -0.2127579632, 0.4687915735, 0.5025101974
 C, 0, -1.0111493711, 1.5666541128, 0.2759873104
 O, 0, -0.5485929317, 2.6501679753, -0.0759843841
 C, 0, -2.4848077593, 1.3079724951, 0.4712786768
 H, 0, -2.6641019214, 0.9230857617, 1.4776000231
 C, 0, -3.1012543411, 0.3298603462, -0.5648361254
 H, 0, -4.1325785931, 0.1465319506, -0.2600591468
 C, 0, -2.4124095457, -0.9950728637, -0.7897596814
 H, 0, -1.5115388063, -0.9741545779, -1.3928070807
 C, 0, -3.0346222506, -2.1864435363, -0.6179549088
 H, 0, -4.0027739183, -2.2531624879, -0.1369614985
 H, 0, -2.9909532042, 2.2676529941, 0.3957731152
 H, 0, -3.1453068418, 0.8520270363, -1.5244393831
 H, 0, -2.5646639069, -3.114403765, -0.9143042504



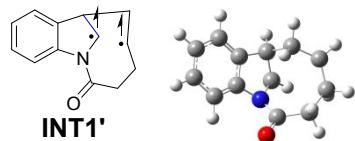
SCF Done: E(UB3LYP) = -633.355415467 A.U.
 Zero-point correction = 0.226440 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -633.168462

C, 0, -1.3971787587, -0.9609564179, 0.2281574608
 C, 0, -0.9821283964, 0.4070339426, 0.1678591223
 C, 0, -1.8958607316, 1.4311636415, -0.0048039948
 C, 0, -3.2495482251, 1.0920565252, -0.1255951461
 C, 0, -3.6769427418, -0.2402113802, -0.0736536741
 C, 0, -2.7685812014, -1.2694494196, 0.1018251547
 C, 0, -0.2777097517, -1.7702278005, 0.4144972776
 C, 0, 0.9331675913, -0.915332872, 0.5857890867
 H, 0, -1.5730123798, 2.4574560683, -0.0459762209
 H, 0, -3.9774483669, 1.8808251663, -0.2595120943
 H, 0, -4.7311323908, -0.4648052572, -0.1683140005
 H, 0, -3.0966280488, -2.299417112, 0.1450381151
 H, 0, -0.2661375351, -2.8414658672, 0.5360862012
 H, 0, 1.2302938539, -0.9310160001, 1.6451958379
 N, 0, 0.417366903, 0.447813555, 0.2803915535
 C, 0, 1.223186156, 1.5229654314, 0.0219873309
 O, 0, 0.7716668458, 2.6508013717, -0.1440302682
 C, 0, 2.7129470573, 1.2618273965, -0.143129397
 H, 0, 2.912340716, 1.5210989143, -1.1860791657
 C, 0, 3.2304705331, -0.1475462436, 0.1622170203
 H, 0, 4.1693029902, -0.3131082979, -0.3671217706

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C, 0, 2.2033273958, -1.2264784498, -0.2193695984
H, 0, 2.5787164292, -2.1881048218, 0.1626370093
C, 0, 1.9764474939, -1.3403926714, -1.6854241178
H, 0, 1.0266462114, -1.6719546253, -2.0802934158
H, 0, 3.2363556184, 2.0095750002, 0.4532474134
H, 0, 3.4480430773, -0.2416272717, 1.2278193309
H, 0, 2.8053529055, -1.2310389045, -2.3709804703

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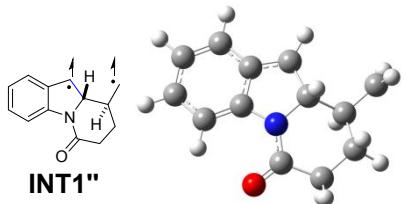


SCF Done: E(UB3LYP) = -633.305691628 A.U.
 Zero-point correction = 0.227522 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -633.116954

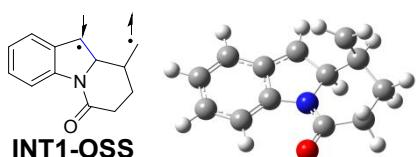
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C, 0, -1.2125118836, -0.9190662083, 0.202202021
C, 0, -0.9860526812, 0.4478201081, 0.4149119896
C, 0, -1.9581022315, 1.4019178066, 0.188928225
C, 0, -3.2071417922, 0.9545571228, -0.2550001215
C, 0, -3.453700709, -0.3979872032, -0.4613794461
C, 0, -2.4499832294, -1.3473204838, -0.2402252308
C, 0, 0.0878744268, -1.6592428654, 0.4552352867
C, 0, 0.7824107989, -0.6556108703, 1.3092312808
H, 0, -1.7634768877, 2.4498460315, 0.3561886451
H, 0, -3.9941380688, 1.6760682403, -0.4295006569
H, 0, -4.431146037, -0.7201553546, -0.794786818
H, 0, -2.6427956294, -2.397947729, -0.4149383201
H, 0, -0.0206086072, -2.6450095377, 0.9011914841
H, 0, 1.7076860397, -0.7671332745, 1.8416645407
N, 0, 0.3739228532, 0.6141353395, 0.8637430858
C, 0, 1.2190922866, 1.5012533809, 0.1900586296
O, 0, 0.8536171982, 2.6391996002, -0.0502077559
C, 0, 2.56236803, 1.0211904594, -0.3742967546
H, 0, 2.4552765675, 1.2597204014, -1.4365181335
C, 0, 3.1554985242, -0.3978117588, -0.2432005223
H, 0, 4.0913592271, -0.3599763186, -0.8143102494
C, 0, 2.4052665504, -1.6177125754, -0.7047925788
H, 0, 3.0026337418, -2.5206551906, -0.7527304736
C, 0, 0.9311657237, -1.7500332145, -0.8989718218
H, 0, 0.5638605171, -0.9502731914, -1.5494705169
H, 0, 3.3095369288, 1.7266113605, -0.0056614734
H, 0, 3.497197484, -0.5509770521, 0.7888081965
H, 0, 0.6937060991, -2.6908958228, -1.3953527316

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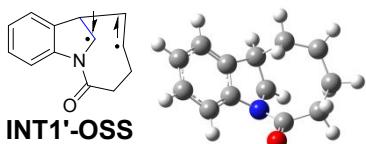
SCF Done: E(UB3LYP) = -633.356350915 A.U.
 Zero-point correction= 0.226342
Sum of electronic and thermal Free Energies= -633.168757
 C, 0, 1.4955210054, -0.9921639518, 0.0306300997
 C, 0, 1.1212292615, 0.3852986273, 0.1203320542
 C, 0, 2.059925567, 1.3963863188, 0.0237275206
 C, 0, 3.3984239229, 1.0343227415, -0.1758258108
 C, 0, 3.786024344, -0.3074362058, -0.2734177457
 C, 0, 2.8521334705, -1.323925201, -0.1728349832
 C, 0, 0.3585947806, -1.7848080801, 0.1776357676
 C, 0, -0.8204163846, -0.9175497395, 0.4730284671
 H, 0, 1.7678602307, 2.429923215, 0.0987126287
 H, 0, 4.1458982254, 1.8122984951, -0.2529774304
 H, 0, 4.8294545125, -0.5501237658, -0.4253356137
 H, 0, 3.1492237111, -2.3616642119, -0.2446912158
 H, 0, 0.3192184479, -2.8614712618, 0.2011803696
 H, 0, -1.0904525515, -1.0283939083, 1.534889246
 N, 0, -0.2740867045, 0.453245221, 0.2788105718
 C, 0, -1.0500171479, 1.5704916289, 0.135069677
 O, 0, -0.5680995187, 2.6961433447, 0.0729229836
 C, 0, -2.5445337313, 1.364655586, -0.0460937721
 H, 0, -3.0490973931, 2.0826844933, 0.6009882706
 C, 0, -3.1019701656, -0.0467740657, 0.1508380289
 H, 0, -3.3120016113, -0.2252790362, 1.2084871147
 C, 0, -2.1209216172, -1.1291486594, -0.3321564202
 H, 0, -1.8857212668, -0.9696666368, -1.3882467081
 C, 0, -2.6617314673, -2.5024802587, -0.1440036293
 H, 0, -3.1212192699, -2.7814697708, 0.7952671839
 H, 0, -2.7354722896, 1.7014075223, -1.0690551275
 H, 0, -4.0511667913, -0.1375568134, -0.3771709868
 H, 0, -2.557400569, -3.2581226269, -0.9079935405



SCF Done: E(UB3LYP) = -633.355665558 A.U.
 Zero-point correction = 0.226388 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -633.167777

C,0,-1.3939563989,-0.9631245427,0.2359662605
C,0,-0.9805401424,0.4048649674,0.1688204498
C,0,-1.8944319724,1.4264982432,-0.0163179522
C,0,-3.2471678593,1.0846297264,-0.141952436
C,0,-3.673025099,-0.2474994435,-0.0825578358
C,0,-2.7638774344,-1.2743577797,0.1050182879
C,0,-0.2734158184,-1.769960423,0.4322645059
C,0,0.9360328111,-0.9133829524,0.5948477619
H,0,-1.5727232625,2.4529968483,-0.0620214722
H,0,-3.9753661751,1.8715108796,-0.2850651061
H,0,-4.7263852044,-0.4743229587,-0.1809202298
H,0,-3.0907827248,-2.304439984,0.1537969495
H,0,-0.2606161161,-2.8401417327,0.5623632501
H,0,1.2439458899,-0.926379799,1.650597173
N,0,0.4183184674,0.4485508944,0.2902782504
C,0,1.2250381989,1.5232618312,0.0339670975
O,0,0.7749161982,2.6520970878,-0.1289889976
C,0,2.7144401196,1.2601859932,-0.1367064506
H,0,2.9093410095,1.5249616249,-1.1792190358
C,0,3.2336280675,-0.1517382864,0.1564819251
H,0,4.1668380443,-0.3153822682,-0.3832006003
C,0,2.1993739642,-1.2270250638,-0.221971607
H,0,2.5730486395,-2.1904329977,0.1550734669
C,0,1.9610171128,-1.3314267721,-1.6859752149
H,0,0.9812936741,-1.5513478601,-2.0849478507
H,0,3.2411984966,2.0042453309,0.4612628559
H,0,3.4612710752,-0.2525615549,1.2193549728
H,0,2.7959096885,-1.2907954084,-2.3717838382



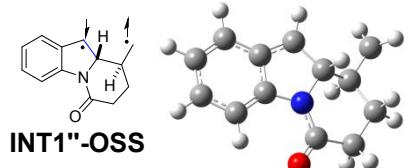
SCF Done: E(UB3LYP) = -633.307677214 A.U.

Zero-point correction = 0.226256 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -633.121135

C,0,-1.192832487,-0.9172217489,0.3457218264
C,0,-1.036197566,0.4762398991,0.3638816806
C,0,-2.0497765102,1.3382290091,-0.003926457
C,0,-3.2701419481,0.7693400237,-0.3834768824
C,0,-3.447403295,-0.610065683,-0.3951134786
C,0,-2.4010878178,-1.4676617967,-0.039561475
C,0,0.1443503593,-1.5353574206,0.6882121036

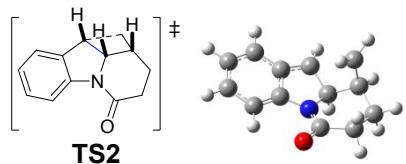
C, 0, 0.765675022, -0.421470824, 1.4033922369
 H, 0, -1.9087277645, 2.4077728557, 0.0107641924
 H, 0, -4.0902617455, 1.4176038994, -0.6619217177
 H, 0, -4.404571209, -1.0245775549, -0.6822419041
 H, 0, -2.5388122252, -2.5407844358, -0.0673514159
 H, 0, 0.1271664445, -2.4956882277, 1.1929656605
 H, 0, 1.6719393557, -0.4123793774, 1.9786516477
 N, 0, 0.3070563412, 0.7657820963, 0.7975160959
 C, 0, 1.1263848751, 1.5649185975, -0.01221593
 O, 0, 0.7077953482, 2.6196983564, -0.4567409119
 C, 0, 2.5276625195, 1.0909772879, -0.4252967899
 H, 0, 2.5421294401, 1.318918422, -1.4935797793
 C, 0, 3.1088559481, -0.3256220696, -0.2058318855
 H, 0, 4.1058140474, -0.2962937053, -0.6567466496
 C, 0, 2.4134167302, -1.5501129711, -0.7125711194
 H, 0, 3.0352942054, -2.4333043379, -0.7946336805
 C, 0, 0.963957978, -1.7070041859, -0.771803895
 H, 0, 0.5101717233, -0.9228431228, -1.383222298
 H, 0, 3.2274020299, 1.8005308856, 0.0225708356
 H, 0, 3.3163668548, -0.4644377028, 0.8650191693
 H, 0, 0.6676063455, -2.6697871683, -1.184006179



SCF Done: E(UB3LYP) = -633.357404939 A.U.
 Zero-point correction = 0.226581 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -633.169282

C, 0, 1.4969480459, -0.9919706892, 0.0429714305
 C, 0, 1.1224650297, 0.3851285283, 0.1249999784
 C, 0, 2.0591121952, 1.3964015182, 0.0075735892
 C, 0, 3.396378017, 1.0332816748, -0.196190039
 C, 0, 3.7843772834, -0.3089983505, -0.2831816683
 C, 0, 2.8515547192, -1.3250959009, -0.1675380623
 C, 0, 0.3579220443, -1.7831880403, 0.1904399286
 C, 0, -0.8172980593, -0.9190499503, 0.4813736167
 H, 0, 1.767056259, 2.4304408854, 0.0750312244
 H, 0, 4.1430921993, 1.8109372669, -0.2834353014
 H, 0, 4.8270295513, -0.5525401793, -0.4390242941
 H, 0, 3.1486100473, -2.363293352, -0.2328125394
 H, 0, 0.3144990047, -2.8598919793, 0.1843812502
 H, 0, -1.1061294873, -1.0261639636, 1.5364768797

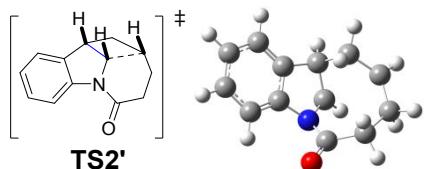
N, 0, -0.2715524408, 0.4519548862, 0.2931470843
 C, 0, -1.0483357413, 1.5703037712, 0.1561621808
 O, 0, -0.566844552, 2.6962462811, 0.1039109795
 C, 0, -2.5415280448, 1.3643694098, -0.0333788868
 H, 0, -3.0499543417, 2.0780439404, 0.6153399133
 C, 0, -3.1016964448, -0.0470892072, 0.1510893772
 H, 0, -3.3153560316, -0.2325058451, 1.2068581858
 C, 0, -2.1287755715, -1.1313157115, -0.3367893948
 H, 0, -1.8785786478, -0.9644012035, -1.3885402172
 C, 0, -2.6698395009, -2.4986459159, -0.1614170502
 H, 0, -3.2722643652, -2.7414569706, 0.7039704664
 H, 0, -2.7265774665, 1.7085464737, -1.0550664941
 H, 0, -4.050635255, -0.1292783276, -0.3789242222
 H, 0, -2.3844794457, -3.3019460494, -0.8247109152



SCF Done: E(UB3LYP) = -633.351808929 A.U.
 Zero-point correction = 0.227054 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -633.162033
 Imaginary Frequency = -289.35 cm⁻¹

C, 0, 1.3978698347, -1.0017549183, -0.1877542408
 C, 0, 1.0146135119, 0.3701776229, -0.22454947
 C, 0, 1.9400700862, 1.3830955043, -0.0482649485
 C, 0, 3.273383344, 1.0206774977, 0.1786351304
 C, 0, 3.6679849968, -0.3190112508, 0.2256207419
 C, 0, 2.7416196496, -1.3358918603, 0.0452769097
 C, 0, 0.2543557671, -1.7987950205, -0.4017558558
 C, 0, -0.8803241995, -0.9060328102, -0.8147619858
 H, 0, 1.6409441039, 2.4172335819, -0.0793003497
 H, 0, 4.0115143272, 1.7991622985, 0.3175958325
 H, 0, 4.7074713622, -0.5633915477, 0.3992020399
 H, 0, 3.0442030996, -2.3740817345, 0.0784289034
 H, 0, 0.2433135323, -2.8639032075, -0.5673622212
 H, 0, -1.024068435, -0.8889916847, -1.9044788463
 N, 0, -0.3814544296, 0.4387909757, -0.4074638181
 C, 0, -1.1850631361, 1.4812012993, -0.0378474955
 O, 0, -0.7378569986, 2.6014232319, 0.1855710733
 C, 0, -2.6541417037, 1.1772599896, 0.2162412314
 H, 0, -2.7570142465, 1.2969966504, 1.2989833791
 C, 0, -3.1913978735, -0.1900394783, -0.2153813286

H, 0, -4.0862189776, -0.4295688263, 0.3600954637
 C, 0, -2.1389273097, -1.3013276646, -0.072231415
 H, 0, -2.5256364738, -2.20458844, -0.5470911496
 C, 0, -1.6726464689, -1.6516764231, 1.3156512739
 H, 0, -1.2331899183, -0.8949950655, 1.950669895
 H, 0, -3.2348053373, 1.9867131654, -0.225666954
 H, 0, -3.4928335917, -0.1517066537, -1.2647901474
 H, 0, -2.0070365154, -2.5605052316, 1.795482352



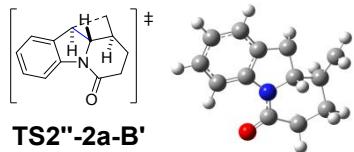
SCF Done: E(UB3LYP) = -633.302848879 A.U.
 Zero-point correction = 0.226121 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -633.114186

Imaginary Frequency = -433.27 cm⁻¹

C, 0, -1.2073360383, -0.9412455889, 0.2449059969
 C, 0, -1.0166413592, 0.4408666459, 0.3803905652
 C, 0, -2.0122521363, 1.3545441745, 0.0936433523
 C, 0, -3.2450301276, 0.8515321159, -0.3358705273
 C, 0, -3.4556189414, -0.5160846162, -0.4684182112
 C, 0, -2.4303518913, -1.4241518467, -0.1828560682
 C, 0, 0.0999254132, -1.6402450887, 0.560021454
 C, 0, 0.8041804339, -0.5534502728, 1.3162232882
 H, 0, -1.8458590877, 2.4148856154, 0.2039146333
 H, 0, -4.0475337908, 1.5422787552, -0.5580430913
 H, 0, -4.4206139063, -0.8818854293, -0.7929208692
 H, 0, -2.5948133011, -2.487815501, -0.2979491134
 H, 0, -0.0057508214, -2.5755797134, 1.1055655237
 H, 0, 1.6051814717, -0.6033275494, 2.0300996436
 N, 0, 0.3368627869, 0.6770311829, 0.8179158382
 C, 0, 1.1324790147, 1.5827245517, 0.1046681546
 O, 0, 0.7417425, 2.7193537166, -0.0965214346
 C, 0, 2.4022511702, 1.0944654597, -0.5948186867
 H, 0, 2.0856847928, 1.0862050995, -1.6443354588
 C, 0, 3.1419032625, -0.2185647871, -0.2878955981
 H, 0, 3.9771355018, -0.2466367536, -1.003277964
 C, 0, 2.4286342132, -1.5424327804, -0.3300599509
 H, 0, 2.9956288574, -2.369821084, 0.0824690551
 C, 0, 1.0054479982, -1.8317943919, -0.7215018216
 H, 0, 0.6603693613, -1.1473908575, -1.4993066017
 H, 0, 3.1192334298, 1.9127551012, -0.5248422534

H, 0, 3.6341188541, -0.1292577625, 0.6869498466

H, 0, 0.9010013398, -2.8431603953, -1.1175887015



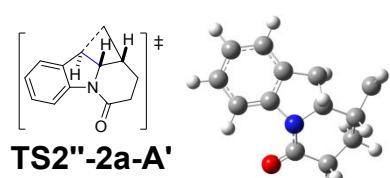
SCF Done: E(UB3LYP) = -633.314479894 A.U.

Zero-point correction= 0.229260 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -633.121900

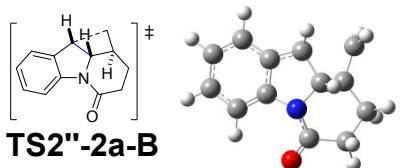
Imaginary Frequency = -548.49 cm⁻¹

C, 0, 1.4397672983, -0.9490259911, -0.0198493868
C, 0, 1.0844282775, 0.4395144191, 0.0535319945
C, 0, 2.0521557717, 1.4312956501, 0.0775519478
C, 0, 3.3930806007, 1.0453270295, 0.0639257377
C, 0, 3.7567679413, -0.2975017477, 0.0036674906
C, 0, 2.7830807535, -1.2950925576, -0.0497927831
C, 0, 0.1815738133, -1.7052387681, -0.2533699282
C, 0, -0.8160969419, -0.7664233443, 0.2608337624
H, 0, 1.7670880361, 2.4716791682, 0.1152686911
H, 0, 4.1607181035, 1.8066260838, 0.1046896385
H, 0, 4.8036779148, -0.5695174315, -0.0065804053
H, 0, 3.0716752409, -2.3361561514, -0.1123235337
H, 0, 0.0592795804, -2.079412741, -1.2620924536
H, 0, -0.8812850003, -0.8823882336, 1.3515033128
N, 0, -0.32074035, 0.5802170655, 0.0437954953
C, 0, -1.1989060063, 1.6145912235, -0.0114543795
O, 0, -0.8660177366, 2.7929434072, -0.073103378
C, 0, -2.6932958597, 1.2086475343, -0.0853364869
H, 0, -3.2332667752, 1.944528199, 0.5094495931
C, 0, -3.1549000132, -0.2282671064, 0.2993816193
H, 0, -3.1972671344, -0.3288378446, 1.3851860907
C, 0, -2.1361196564, -1.2274136688, -0.2670888498
H, 0, -2.1512130961, -1.1826490757, -1.3582477389
C, 0, -1.8517196627, -2.6399386299, 0.1683971368
H, 0, -1.8734027726, -2.8757294939, 1.2238555786
H, 0, -2.9702355378, 1.406894077, -1.1250522705
H, 0, -4.1633516251, -0.3873140493, -0.0824889832
H, 0, -1.9863501637, -3.4652000223, -0.5161185117



SCF Done: E(UB3LYP) = -633.317464684 A.U.
 Zero-point correction= 0.228464 (Hartree/Particle)
 Sum of electronic and thermal Free Energies= -633.125662
 Imaginary Frequency = -465.20 cm⁻¹

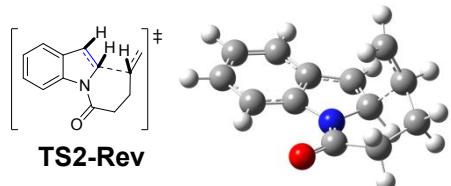
 C, 0, -1.2320051121, -1.0341266477, 0.0942573334
 C, 0, -1.0970444262, 0.3228511782, -0.3142236163
 C, 0, -2.1903764227, 1.166053176, -0.3855007708
 C, 0, -3.4490506676, 0.6427970728, -0.0771989148
 C, 0, -3.5989460932, -0.6837525189, 0.3155625322
 C, 0, -2.4895249363, -1.5243014546, 0.4161326663
 C, 0, 0.1381980563, -1.5648682432, 0.234150872
 C, 0, 0.9164403679, -0.6954905149, -0.6917764105
 H, 0, -2.0715937084, 2.1992589816, -0.6733905575
 H, 0, -4.318566797, 1.2824479504, -0.1494053021
 H, 0, -4.5839016837, -1.0665137431, 0.5472297173
 H, 0, -2.6077768655, -2.5504070222, 0.738616303
 H, 0, 0.4744644081, -1.6874109209, 1.2548386375
 H, 0, 0.7259125621, -1.0209608633, -1.7174367836
 N, 0, 0.2773904763, 0.6366712796, -0.5503668744
 C, 0, 0.9455700186, 1.6947034081, 0.0132568691
 O, 0, 0.3832519725, 2.7325577521, 0.3393531402
 C, 0, 2.4456096118, 1.4908704432, 0.2179399666
 H, 0, 2.9517452789, 1.7247942709, -0.7236595515
 C, 0, 2.8417890944, 0.0728962736, 0.6734519487
 H, 0, 3.9202067679, 0.022870934, 0.8268253661
 C, 0, 2.3945236445, -0.914212713, -0.4036677046
 H, 0, 2.9861155801, -0.7335939916, -1.3030637761
 C, 0, 2.3108156109, -2.3866768628, -0.1131390103
 H, 0, 2.3957881629, -3.0816784358, -0.9367598569
 H, 0, 2.7578216493, 2.2431433905, 0.939240612
 H, 0, 2.3718437223, -0.1542610297, 1.6326041391
 H, 0, 2.4969817279, -2.7763461494, 0.8770040259



SCF Done: E(UB3LYP) = -633.337650089 A.U.
 Zero-point correction= 0.228033 (Hartree/Particle)
 Sum of electronic and thermal Free Energies= -633.146393
 Imaginary Frequency = -478.83 cm⁻¹

 C, 0, -1.327863123, -0.9587327913, -0.2567242969
 C, 0, -0.9982776447, 0.4258111788, -0.2321217787

C, 0, -1.9451274082, 1.3894330075, 0.072205152
 C, 0, -3.2439048709, 0.96472268, 0.3656073649
 C, 0, -3.5901434445, -0.3872547979, 0.3372969031
 C, 0, -2.641377866, -1.3521500009, 0.0236014165
 C, 0, -0.1797562703, -1.7205416362, -0.6541804403
 C, 0, 0.9578739723, -0.7410604935, -0.7412952701
 H, 0, -1.6838850063, 2.435300988, 0.0788763801
 H, 0, -3.995137275, 1.7032853323, 0.6115377968
 H, 0, -4.6064057967, -0.6842006228, 0.55879867
 H, 0, -2.9080415701, -2.4005780091, 0.0013086718
 H, 0, -0.2411395743, -2.6090794187, -1.2604397269
 H, 0, 1.5350274505, -0.8102672592, -1.6656630543
 N, 0, 0.3600965993, 0.5987887565, -0.5797390698
 C, 0, 1.2023660776, 1.6000707083, -0.1489112334
 O, 0, 0.8008857955, 2.6968686241, 0.2162169313
 C, 0, 2.6871189147, 1.2256074629, -0.1811776919
 H, 0, 2.9830814774, 1.2127364843, -1.2333475131
 C, 0, 3.0531862194, -0.1528581494, 0.4658475481
 H, 0, 3.8352283458, -0.6283572568, -0.1271922293
 C, 0, 1.7831789667, -1.012525649, 0.4992543989
 H, 0, 1.1725017222, -0.6407162726, 1.3274852207
 C, 0, 1.7278332367, -2.5102627932, 0.597228328
 H, 0, 1.7226514999, -2.998496725, 1.5634871421
 H, 0, 3.2272349787, 2.0434626786, 0.288226313
 H, 0, 3.4479474925, -0.0024110072, 1.4699731919
 H, 0, 2.0796381008, -3.1061680184, -0.2357471245

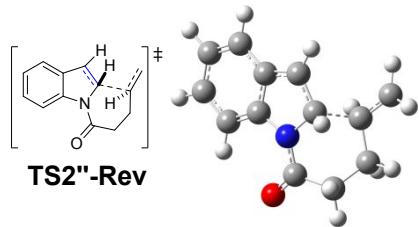


SCF Done: E(UB3LYP) = -633.349800171 A.U.
 Zero-point correction= 0.226152 (Hartree/Particle)
 Sum of electronic and thermal Free Energies= -633.161687

Imaginary Frequency = -675.24 cm⁻¹

C, 0, 1.4558017423, -0.9835824235, -0.3895082887
 C, 0, 0.9955162895, 0.3517702881, -0.1920094916
 C, 0, 1.8432873244, 1.3537909214, 0.2557407191
 C, 0, 3.1745860301, 1.015539514, 0.505814138
 C, 0, 3.6486923361, -0.2893160384, 0.3137268738
 C, 0, 2.8048026929, -1.2924191989, -0.1293916952
 C, 0, 0.3782694567, -1.7572927421, -0.8472016056
 C, 0, -0.8200446455, -0.9592135002, -0.8247416365
 H, 0, 1.4881002328, 2.3615118667, 0.390860002

H, 0, 3.8547105388, 1.7831962914, 0.8496030695
 H, 0, 4.6882106216, -0.5115530759, 0.5152159492
 H, 0, 3.1683113899, -2.3007379675, -0.2760170788
 H, 0, 0.4023391772, -2.7983314677, -1.1249875097
 H, 0, -1.4318198628, -1.013148262, -1.7227574076
 N, 0, -0.3688405993, 0.3900664754, -0.5240301083
 C, 0, -1.2352213867, 1.422960596, -0.2510702285
 O, 0, -0.8359441527, 2.5589398257, -0.0413144123
 C, 0, -2.7192297634, 1.097943018, -0.1501604835
 H, 0, -3.0285489749, 1.6009042134, 0.7668874226
 C, 0, -3.1669894751, -0.3770265589, -0.140427839
 H, 0, -4.05447188, -0.4684723856, 0.4858010898
 C, 0, -2.0844099772, -1.3489450878, 0.3434679402
 H, 0, -2.3037013319, -2.3733871579, 0.0476969358
 C, 0, -1.6836882071, -1.2375951303, 1.708890243
 H, 0, -1.1442299363, -2.0377691828, 2.1958298815
 H, 0, -3.2190675146, 1.6379477875, -0.9564227035
 H, 0, -3.4657794824, -0.6750167029, -1.1460261651
 H, 0, -1.7666026425, -0.304102915, 2.2494613896

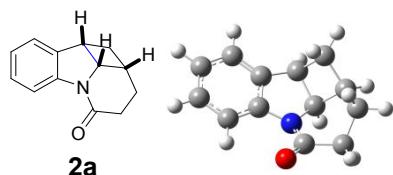


SCF Done: E(UB3LYP) = -633.354103803 A.U.
 Zero-point correction= 0.226313 (Hartree/Particle)
 Sum of electronic and thermal Free Energies= -633.165536

Imaginary Frequency = -660.80 cm⁻¹

C, 0, -1.4102068057, -1.0376773616, -0.304174704
 C, 0, -1.0964857633, 0.3426008052, -0.1378933721
 C, 0, -2.0513485884, 1.2683644858, 0.2521545158
 C, 0, -3.3534779391, 0.8085920172, 0.4585300389
 C, 0, -3.6881047552, -0.5421885089, 0.2883707894
 C, 0, -2.7326987888, -1.4705435358, -0.0867092709
 C, 0, -0.2366165585, -1.7167975914, -0.6682391588
 C, 0, 0.871914578, -0.7917716461, -0.6789787809
 H, 0, -1.7982099599, 2.3081648453, 0.3761993179
 H, 0, -4.1199782004, 1.5140881092, 0.7494746377
 H, 0, -4.7087745569, -0.8605602327, 0.4543646699
 H, 0, -2.9910337377, -2.5135330184, -0.2126020539
 H, 0, -0.1400307357, -2.7734993496, -0.8555841553
 H, 0, 1.5143841333, -0.7941017233, -1.5535547662

N, 0, 0.2652288807, 0.5055961811, -0.4215381188
 C, 0, 1.0336449601, 1.6325277179, -0.2384994195
 O, 0, 0.553405144, 2.7255518676, 0.0221039937
 C, 0, 2.5105581854, 1.3617403511, -0.3702722927
 H, 0, 2.7203627371, 1.1241326296, -1.4161415372
 C, 0, 2.9997026181, 0.204572022, 0.5312806988
 H, 0, 3.9808067447, -0.1052138186, 0.1717084646
 C, 0, 2.0766418256, -1.0260785484, 0.6159906444
 H, 0, 1.394990681, -0.96270564, 1.4624136669
 C, 0, 2.7311629384, -2.289533457, 0.5296791547
 H, 0, 2.2431397265, -3.1949017262, 0.8631553745
 H, 0, 3.0415814586, 2.2807896333, -0.1360445413
 H, 0, 3.145324404, 0.5863118294, 1.5424607318
 H, 0, 3.6596593742, -2.3971413368, -0.0153635272

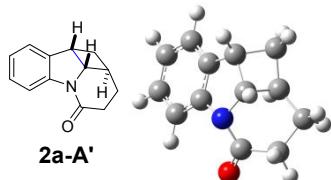


SCF Done: E(RB3LYP) = -633.426052148 A.U.
 Zero-point correction = 0.233497 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -633.228966

C, 0, 1.4954183053, -0.1105786863, -0.2236092337
 C, 0, 0.1037133859, 0.0519703725, -0.2813759037
 C, 0, -0.4974132904, 1.2702391695, -0.0002100095
 C, 0, 0.3312957474, 2.341540474, 0.3435146614
 C, 0, 1.7128144985, 2.1959405772, 0.3984723389
 C, 0, 2.3026021481, 0.9607557925, 0.1134670269
 C, 0, 1.8390590017, -1.5347381275, -0.5542453463
 C, 0, 0.5265391228, -2.1247140107, -1.1131876158
 H, 0, -1.5683765662, 1.3833556947, -0.0461906267
 H, 0, -0.1157012316, 3.3022100998, 0.5631467898
 H, 0, 2.3343875716, 3.0418602274, 0.6597639993
 H, 0, 3.3780078834, 0.8449004181, 0.1581318258
 H, 0, 2.7071307547, -1.646609553, -1.1983811008
 H, 0, 0.4256081589, -2.2839684175, -2.1865371518
 N, 0, -0.5034402112, -1.180204739, -0.6317323538
 C, 0, -1.7289076497, -1.626609938, -0.2241152031
 O, 0, -2.6114290013, -0.881852439, 0.1899052014
 C, 0, -1.8554408332, -3.1381236351, -0.2487639232
 H, 0, -2.8016024848, -3.3975469353, 0.2205478459
 C, 0, -0.6558699897, -3.7797170654, 0.479388161
 H, 0, -0.6644527293, -3.460295656, 1.5236979111

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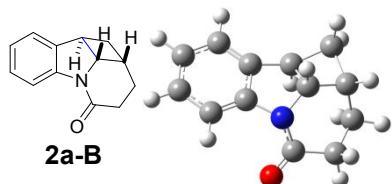
C,0,0.6550875164,-3.359406072,-0.1985534808
H,0,1.0790889982,-4.1864512402,-0.7668639571
C,0,1.7747751658,-2.6104696002,0.5887621347
H,0,1.4295760819,-2.1968427303,1.535849327
H,0,-1.8892721167,-3.4904667599,-1.2835718057
H,0,-0.7691899905,-4.8635267158,0.4826261014
H,0,2.693016814,-3.1670251346,0.7626340373
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SCF Done: E(RB3LYP) = -633.392912906 A.U.
 Zero-point correction= 0.233324 (Hartree/Particle)
 Sum of electronic and thermal Free Energies= -633.195797

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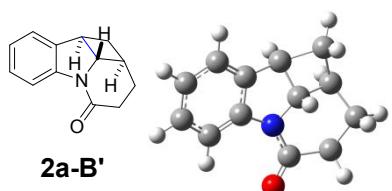
C,0,1.1766390779,-0.9293060433,0.3591275634
C,0,0.9339400121,0.4609747657,0.36212629
C,0,1.9032721855,1.3645493428,-0.0479448301
C,0,3.1354925794,0.8639177107,-0.4703668042
C,0,3.3901926715,-0.5034144546,-0.478719464
C,0,2.4093046836,-1.4036594728,-0.0586952728
C,0,-0.0059836278,-1.6924335203,0.924700438
C,0,-1.0218702241,-0.5522294061,1.0231716447
H,0,1.7044013508,2.424765167,-0.0425820794
H,0,3.9033107078,1.5550686216,-0.7921696625
H,0,4.3536681885,-0.8707626171,-0.8057260473
H,0,2.6099991845,-2.4675932275,-0.0598759809
H,0,0.259867314,-2.2323647699,1.8324174975
H,0,-1.6854089715,-0.5651781721,1.8848133596
N,0,-0.3988322918,0.7501666249,0.7915052858
C,0,-1.2524242405,1.6152234877,0.104937274
O,0,-0.8693728013,2.6584631489,-0.3973598557
C,0,-2.7269493732,1.158467895,0.0363584455
H,0,-3.1353081688,1.2669786435,1.0438243239
C,0,-2.9880416841,-0.3248039727,-0.4560698076
H,0,-3.7746318446,-0.7683142063,0.1551490674
C,0,-1.6489719811,-1.0117228048,-0.2821524934
H,0,-1.0059364127,-0.6121263604,-1.0710904691
C,0,-1.0496320385,-2.425293375,-0.0149525884
H,0,-1.6832843082,-3.0757204208,0.5872380991
H,0,-3.2399155251,1.8806287153,-0.5929832788
H,0,-3.330682651,-0.3182193766,-1.4900790531
H,0,-0.6774149412,-2.974939283,-0.8772101016
```



SCF Done: E(RB3LYP) = -633.364122457 A.U.
Zero-point correction= 0.233374 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -633.166900

C,0,1.244580604,-0.8854633234,0.0542091494
C,0,1.011268751,0.5011389787,0.3150692255
C,0,2.0307299165,1.4266436623,0.2434688575
C,0,3.3162284808,0.9721570205,-0.0743850055
C,0,3.5594415023,-0.3735116866,-0.3119068465
C,0,2.5184054794,-1.3101196594,-0.2620354608
C,0,-0.1510292952,-1.4766609219,0.0521109014
C,0,-0.796275108,-0.5971432478,1.0830046096
H,0,1.8446850946,2.4718581117,0.4431132634
H,0,4.1310073584,1.6821874975,-0.1216870955
H,0,4.5632203983,-0.7042414999,-0.5434828764
H,0,2.7128432631,-2.3528239883,-0.4755463157
H,0,-0.5316369088,-1.136223247,-0.9173404405
H,0,-0.4025419921,-0.8107033214,2.0781073934
N,0,-0.3747267954,0.7426153179,0.6790517874
C,0,-1.266237214,1.4943728047,-0.0546363592
O,0,-0.9336076726,2.466090621,-0.717807793
C,0,-2.7183310792,1.0101515143,0.0310281355
H,0,-3.10085213,1.2574535207,1.025707193
C,0,-2.9081612833,-0.5092144454,-0.2192011583
H,0,-3.9709936586,-0.7471434779,-0.180941943
C,0,-2.1323361019,-1.2959331563,0.8486850288
H,0,-2.7445811249,-1.4408661958,1.7364391716
C,0,-1.2319985004,-2.5500270562,0.43655947
H,0,-0.9950507536,-3.1481406455,1.3142245075
H,0,-3.2847451563,1.598054445,-0.6878682978
H,0,-2.5742143031,-0.7536800729,-1.228340797
H,0,-1.5821360909,-3.1912079488,-0.3685424345



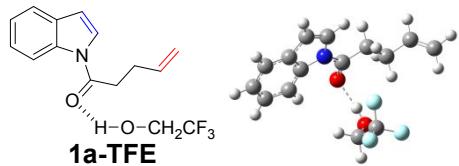
SCF Done: E(RB3LYP) = -633.332277860 A.U.

Zero-point correction = 0.232316 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -633.136772

C, 0, 1.3706316463, -0.9269547847, -0.0511865413
C, 0, 1.0508465597, 0.480762193, -0.0844819859
C, 0, 2.0389797529, 1.4452399993, -0.0112213649
C, 0, 3.3659390907, 1.0250941565, 0.1134869616
C, 0, 3.6909868455, -0.3246289519, 0.1573428225
C, 0, 2.6941222385, -1.30304012, 0.0633689741
C, 0, 0.0601458963, -1.6655286963, -0.3649445731
C, 0, -0.8335216858, -0.6309067431, 0.1563490883
H, 0, 1.7859126902, 2.4951392831, -0.0378310536
H, 0, 4.149244352, 1.7680986578, 0.182677682
H, 0, 4.7254310459, -0.6245780163, 0.2580895692
H, 0, 2.9605247953, -2.3517706637, 0.0781584876
H, 0, -0.0041659562, -1.7051702039, -1.4571303472
H, 0, -0.7837957645, -0.7124958604, 1.2544380516
N, 0, -0.3665294038, 0.6650677375, -0.1773094733
C, 0, -1.3187724675, 1.6371417813, -0.0648638746
O, 0, -1.1018499729, 2.8387848935, -0.0972299813
C, 0, -2.7961767379, 1.0923205907, 0.0102411784
H, 0, -3.3216124615, 1.790805903, 0.6601578747
C, 0, -3.1586921958, -0.3923349761, 0.4231675341
H, 0, -3.1205986333, -0.4901744035, 1.508925489
C, 0, -2.0914749133, -1.2733830741, -0.236533333
H, 0, -2.2232187532, -1.2695499062, -1.3199907084
C, 0, -1.2081691328, -2.6050918943, 0.1023529901
H, 0, -1.2017399393, -2.8655402574, 1.156657612
H, 0, -3.1844762844, 1.2728373629, -0.9962089817
H, 0, -4.1830854135, -0.593780763, 0.1094663768
H, 0, -1.3897710201, -3.4756297312, -0.5189263398

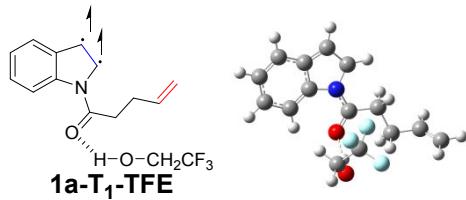
(2) At (U)B3LYP-D3(BJ)/def2-TZVPP/PCM (CF₃CH₂OH) level of theory



SCF Done: E(RB3LYP) = -1086.49079759 A.U.
Zero-point correction = 0.287852 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -1086.256987

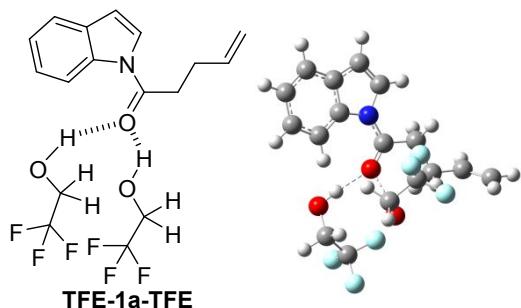
C, 0, -2.5049495334, 0.7902258655, 0.6063666692
C, 0, -1.8346090364, -0.1117332558, -0.2490986676
C, 0, -2.5272987729, -0.9825995362, -1.0822759409
C, 0, -3.9167989445, -0.9362981555, -1.0420410476

C, 0, -4.5961103437, -0.0494568636, -0.2001726747
 C, 0, -3.8990338501, 0.818398418, 0.6276981434
 C, 0, -1.4980490034, 1.533494545, 1.3240969513
 C, 0, -0.2895397497, 1.0895894784, 0.9173377486
 H, 0, -2.0110545944, -1.6625764062, -1.7370287304
 H, 0, -4.4813620928, -1.6024847421, -1.6798105334
 H, 0, -5.6774984216, -0.0419129608, -0.1968095285
 H, 0, -4.4229488467, 1.5042481748, 1.2794207517
 H, 0, -1.6701708211, 2.3053052014, 2.054792253
 H, 0, 0.691190913, 1.4012320718, 1.2218622809
 N, 0, -0.4512956903, 0.078410439, -0.0487821761
 C, 0, 0.5658686993, -0.6241078731, -0.6624336342
 O, 0, 0.3092890808, -1.4625133751, -1.5152133629
 C, 0, 1.9760356265, -0.3058832841, -0.2253735633
 H, 0, 2.0387917549, -0.4031218255, 0.8597013018
 C, 0, 3.0208584168, -1.1993813197, -0.8936143934
 H, 0, 2.9139111484, -1.1137891634, -1.9774268471
 C, 0, 4.4105543888, -0.8125697788, -0.4899994525
 H, 0, 4.7176437092, 0.1977994161, -0.7464875287
 C, 0, 5.2609841, -1.6057701322, 0.1500143186
 H, 0, 4.9900814223, -2.6182823606, 0.4257291281
 H, 0, 2.1761807707, 0.7448198166, -0.4500470133
 H, 0, 2.8363750658, -2.2417411945, -0.6353596879
 H, 0, 6.2552996721, -1.2732960157, 0.4171434225
 C, 0, 0.4936348444, -4.2137883812, 1.1222404926
 C, 0, -0.0830314235, -4.474356717, -0.2596703193
 H, 0, -0.3066632394, -5.5393210697, -0.3167337099
 H, 0, -1.0199157028, -3.9170237269, -0.330445881
 O, 0, 0.8245592381, -4.1438589078, -1.2758135217
 H, 0, 0.753682557, -3.1883928334, -1.4527843211
 F, 0, 0.783386661, -2.9057972759, 1.3181422907
 F, 0, 1.6333081597, -4.8978789462, 1.342121367
 F, 0, -0.3838344221, -4.5726004255, 2.083011546



SCF Done: E(UB3LYP) = -1086.38646437 A.U.
 Zero-point correction = 0.282694 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -1086.159221
 C, 0, -2.4009381333, 0.6581054398, 0.8538178119
 C, 0, -1.7409390085, -0.1483834306, -0.1507457846

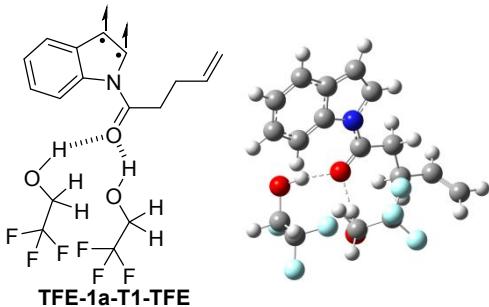
C, 0, -2.4368923375, -0.9160372554, -1.0344672641
 C, 0, -3.8564369721, -0.9143383861, -0.9382843368
 C, 0, -4.526618667, -0.1470686251, 0.0273227502
 C, 0, -3.8320887997, 0.6367783098, 0.9196715727
 C, 0, -1.4501345618, 1.3174678511, 1.5822109472
 C, 0, -0.1333152888, 0.9337634303, 1.0504237971
 H, 0, -1.9366712603, -1.5025312557, -1.784314615
 H, 0, -4.4238622938, -1.5208517142, -1.6290042812
 H, 0, -5.6068831847, -0.1743975538, 0.0651554103
 H, 0, -4.3433258733, 1.2312591064, 1.6632471296
 H, 0, -1.5990608845, 1.9985027366, 2.4023981038
 H, 0, 0.8410370697, 1.270540903, 1.3430180165
 N, 0, -0.3270023546, 0.0436863265, 0.0072431778
 C, 0, 0.648478802, -0.5869873969, -0.7237911137
 O, 0, 0.3380587891, -1.3526335509, -1.6563361318
 C, 0, 2.0684009812, -0.3072949689, -0.3135138311
 H, 0, 2.1698586258, -0.4862070919, 0.7613976116
 C, 0, 3.0839014566, -1.1557881942, -1.079334641
 H, 0, 2.9485224236, -0.9812138241, -2.1492608594
 C, 0, 4.4901939768, -0.8242291248, -0.6860946966
 H, 0, 4.806104112, 0.2000109631, -0.8665067651
 C, 0, 5.3467441826, -1.6781648925, -0.1384512022
 H, 0, 5.0682214146, -2.7065103914, 0.0607705412
 H, 0, 2.2800456173, 0.7582508912, -0.4583463201
 H, 0, 2.8872912379, -2.2135768716, -0.9032500237
 H, 0, 6.3529688895, -1.381783694, 0.1268768382
 C, 0, 0.2366641643, -4.0897885809, 1.0888458874
 C, 0, -0.3601267442, -4.2843769906, -0.2952575086
 H, 0, -0.6712267793, -5.3269271216, -0.363244787
 H, 0, -1.2498885704, -3.6523473667, -0.3535690454
 O, 0, 0.5673442044, -4.0127066939, -1.3077971663
 H, 0, 0.5581484674, -3.0482881973, -1.4879182689
 F, 0, 0.6305355421, -2.8135694789, 1.3038640653
 F, 0, 1.3172098306, -4.867933187, 1.2983683275
 F, 0, -0.6668463333, -4.3914432192, 2.0471127843



SCF Done: E(RB3LYP) = -1539.49287827 A.U.
 Zero-point correction= 0.346433 (Hartree/Particle)
 Sum of electronic and thermal Free Energies= -1539.214395

C, 0, -3.3926307288, -0.3235050354, -1.1587194037
 C, 0, -2.4330946921, -0.3261667455, -0.1237360218
 C, 0, -2.5978469399, 0.4344022518, 1.0268387552
 C, 0, -3.7549080555, 1.2002488268, 1.1273935184
 C, 0, -4.717283667, 1.2096332993, 0.1135921645
 C, 0, -4.5446441714, 0.4507952026, -1.0352117829
 C, 0, -2.9078816192, -1.1955110388, -2.2022932617
 C, 0, -1.715476176, -1.6878984254, -1.8103368889
 H, 0, -1.8696883223, 0.4343471085, 1.8177336687
 H, 0, -3.9088181023, 1.7998814519, 2.0138081449
 H, 0, -5.6047878961, 1.8166747554, 0.2277968851
 H, 0, -5.2853802369, 0.4592992016, -1.8229592894
 H, 0, -3.403933805, -1.4184486622, -3.1314953199
 H, 0, -1.0562968685, -2.3678694942, -2.3147603526
 N, 0, -1.3847834476, -1.1816912023, -0.535411461
 C, 0, -0.2362582759, -1.4590950342, 0.1587658546
 O, 0, -0.0722620636, -1.0140636957, 1.2939344723
 C, 0, 0.801547372, -2.3128258629, -0.5255117697
 H, 0, 1.0241914143, -1.8829984471, -1.5033201082
 C, 0, 2.0853086877, -2.4621101091, 0.2916135116
 H, 0, 1.830201535, -2.8483032778, 1.2804421278
 C, 0, 3.0536900673, -3.3870663851, -0.3794670332
 H, 0, 2.7145107242, -4.4095870508, -0.5215636378
 C, 0, 4.2624170494, -3.0390161266, -0.8032340114
 H, 0, 4.6336874435, -2.0280326062, -0.6822109275
 H, 0, 0.3603550777, -3.2944246415, -0.7175280061
 H, 0, 2.5477559315, -1.4862210843, 0.4380392277
 H, 0, 4.92220866, -3.7506297605, -1.2815069685
 C, 0, 1.8683960389, 2.0101060816, 0.0249229927
 C, 0, 1.4239187644, 1.9003431257, 1.4739281635
 H, 0, 1.8305102866, 2.7610768879, 2.0029210222
 H, 0, 0.3336143762, 1.9655987424, 1.4863093877
 O, 0, 1.9055773878, 0.7295390641, 2.0787636421
 H, 0, 1.3280491733, -0.0090196224, 1.8188521189
 F, 0, 1.4007177877, 0.9871964735, -0.7294701937
 F, 0, 3.2089971612, 2.003242033, -0.1038913443
 F, 0, 1.4147982555, 3.1525272872, -0.5308887504
 C, 0, 1.0443684827, -1.6245435995, 5.028098531
 C, 0, -0.0779906163, -0.6665642173, 4.6677858851
 H, 0, -0.5259384872, -0.3262580545, 5.6005200848
 H, 0, 0.377382515, 0.1876890103, 4.1624748308

O, 0, -1.0682458244, -1.2945039271, 3.8946166661
 H, 0, -0.786416398, -1.2925250101, 2.9661847852
 F, 0, 1.6711365124, -2.1068352808, 3.93260649
 F, 0, 0.6076333271, -2.6913503354, 5.7274984108
 F, 0, 1.9775838826, -1.005054831, 5.7825739009

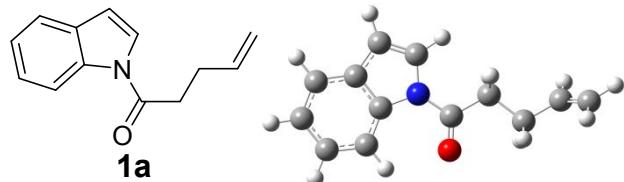


SCF Done: E(UB3LYP) = -1539.39132171 A.U.
 Zero-point correction= 0.341608 (Hartree/Particle)
Sum of electronic and thermal Free Energies= -1539.118341

C, 0, -3.3910012056, -0.2863171666, -1.1768411996
 C, 0, -2.4157779668, -0.3027078752, -0.1081262027
 C, 0, -2.5823281337, 0.4254013257, 1.0328009715
 C, 0, -3.7565042903, 1.2113362184, 1.1480602263
 C, 0, -4.7246125661, 1.2473111702, 0.128629195
 C, 0, -4.565980708, 0.5167906937, -1.0237864364
 C, 0, -2.9507173114, -1.096950301, -2.1866585897
 C, 0, -1.6580430531, -1.6563508142, -1.7723301505
 H, 0, -1.8579547703, 0.4086097215, 1.826659435
 H, 0, -3.9036136997, 1.7940912766, 2.0456194317
 H, 0, -5.6055223189, 1.8598839669, 0.2604817032
 H, 0, -5.3056796683, 0.5383792346, -1.8111789067
 H, 0, -3.4317690186, -1.3082709707, -3.1258868998
 H, 0, -1.0223683502, -2.3461403958, -2.2911216287
 N, 0, -1.3465204493, -1.1704381489, -0.5178719407
 C, 0, -0.2144378119, -1.4444482225, 0.1999405775
 O, 0, -0.0698668821, -0.9603949305, 1.3514699518
 C, 0, 0.812328933, -2.3132413591, -0.4656909157
 H, 0, 1.0579041169, -1.8908998065, -1.4456478358
 C, 0, 2.0859867605, -2.473447492, 0.3656781418
 H, 0, 1.8156118729, -2.867956663, 1.3473036235
 C, 0, 3.0644258604, -3.392284757, -0.2978441558
 H, 0, 2.723985331, -4.4112518841, -0.4626037934
 C, 0, 4.2836285122, -3.0455551205, -0.6928287473
 H, 0, 4.6578325075, -2.0384540361, -0.549668328
 H, 0, 0.3717803793, -3.2963724177, -0.6696846482
 H, 0, 2.5448088982, -1.4987352016, 0.530887467

H, 0, 4.9491826837, -3.7536544347, -1.1686004539
 C, 0, 1.8639072564, 2.0186544184, -0.1114963898
 C, 0, 1.3434292743, 1.9882337359, 1.3158762361
 H, 0, 1.715559513, 2.8834282553, 1.8133333362
 H, 0, 0.2532751481, 2.0461628911, 1.2621847063
 O, 0, 1.7920518592, 0.8565445309, 2.0082837289
 H, 0, 1.203827474, 0.1071513635, 1.7758628093
 F, 0, 1.4399176473, 0.9543936686, -0.8313836547
 F, 0, 3.2103470964, 2.0128624182, -0.1697015944
 F, 0, 1.4384924031, 3.1274433062, -0.7548328719
 C, 0, 1.0700912421, -1.7267072895, 5.0471868842
 C, 0, -0.063932007, -0.79625391, 4.6525579196
 H, 0, -0.5424858062, -0.4654815446, 5.5743401965
 H, 0, 0.3853279286, 0.0694446958, 4.1603312181
 O, 0, -1.0119640776, -1.4471157321, 3.8498948922
 H, 0, -0.7236848193, -1.3811985283, 2.9186784065
 F, 0, 1.7472475986, -2.1920462699, 3.9754883105
 F, 0, 0.6357230532, -2.8058319904, 5.730783596
 F, 0, 1.9620830844, -1.0871343893, 5.8359510891

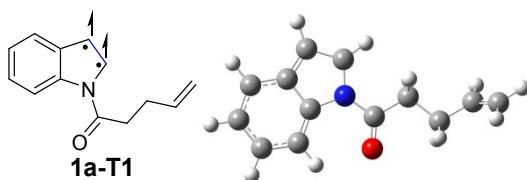
(3) At (U)B3LYP / def2-SVP / PCM (CF₃CH₂OH) level of theory



SCF Done: E(RB3LYP) = -632.734369133 A.U.
 Zero-point correction = 0.228884 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = - 632.546320

C, 0, -2.4571454795, 0.9889173764, 0.0375821329
 C, 0, -1.59058471, -0.1367515712, -0.0033222536
 C, 0, -2.0865747273, -1.4468274202, 0.0165931498
 C, 0, -3.4726764459, -1.6110904624, 0.0786926749
 C, 0, -4.3450566278, -0.5063263744, 0.1197296107
 C, 0, -3.847411967, 0.7958205338, 0.0995059167
 C, 0, -1.6247776946, 2.1703427957, 0.0039685652
 C, 0, -0.3293457485, 1.7558064204, -0.0528524029
 H, 0, -1.4125268861, -2.299188905, -0.0153692847
 H, 0, -3.8859958458, -2.6227803589, 0.095604354
 H, 0, -5.4239208649, -0.6742552545, 0.1679580808
 H, 0, -4.5231166731, 1.6541940445, 0.1315519251
 H, 0, -1.9609899619, 3.2053882537, 0.0208154511
 H, 0, 0.5780434542, 2.3504652922, -0.0907377273
 N, 0, -0.268726554, 0.351105855, -0.0594555264

C, 0, 0.8944673417, -0.4297353293, -0.1143982078
 O, 0, 0.8304259656, -1.6437567594, -0.1248515286
 C, 0, 2.2144739048, 0.3227447882, -0.1586905229
 H, 0, 2.2713190054, 0.9976361714, 0.7118599372
 C, 0, 3.4270629369, -0.6158553035, -0.1825533684
 H, 0, 3.3214822237, -1.2975802125, -1.0444514435
 C, 0, 4.7272562327, 0.1323826042, -0.2883919194
 H, 0, 4.8450340849, 0.7638142688, -1.1796850403
 C, 0, 5.721097626, 0.0843327459, 0.6044340419
 H, 0, 5.6484029639, -0.5290091061, 1.5094629604
 H, 0, 2.2166365385, 0.977385171, -1.0475206817
 H, 0, 3.4238081618, -1.2500604781, 0.7178661914
 H, 0, 6.6455357464, 0.6518972143, 0.4630439152

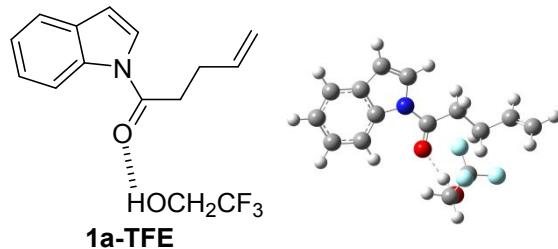


SCF Done: E(RB3LYP) = -632.734369133 A.U.
 Zero-point correction = 0.223416 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -632.446448

C, 0, -2.4704807981, 1.0234714608, 0.0447558924
 C, 0, -1.5814758546, -0.1255324971, -0.0075590965
 C, 0, -2.0538255663, -1.4115315239, 0.0063313748
 C, 0, -3.4750508281, -1.6035631314, 0.081379187
 C, 0, -4.3614616869, -0.5125958383, 0.1356451867
 C, 0, -3.8916175601, 0.7947029251, 0.1175496499
 C, 0, -1.7069622842, 2.1682292375, 0.0202323827
 C, 0, -0.2838309839, 1.7622281697, -0.0437553828
 H, 0, -1.3727667699, -2.2570446774, -0.0360695916
 H, 0, -3.8666934629, -2.6228319834, 0.0981940955
 H, 0, -5.4367729308, -0.6994656894, 0.1920750373
 H, 0, -4.5762398219, 1.6444348991, 0.1580986199
 H, 0, -2.0517084799, 3.2004567679, 0.0496340631
 H, 0, 0.5922675892, 2.3778166061, -0.2139595233
 N, 0, -0.2340504772, 0.368979137, -0.0701473299
 C, 0, 0.9041200402, -0.4262434418, -0.137403527
 O, 0, 0.8209663696, -1.6543615786, -0.1678386459
 C, 0, 2.2248117649, 0.3194055619, -0.1665088695
 H, 0, 2.2766493538, 0.9996679734, 0.703254872
 C, 0, 3.4347364004, -0.6225667398, -0.1767099118
 H, 0, 3.3315706377, -1.3075802421, -1.036426235
 C, 0, 4.74071539, 0.1159005383, -0.2749464213

H, 0, 4.8676432391, 0.7466203997, -1.1657054062
 C, 0, 5.7303565721, 0.0622875842, 0.6225073609
 H, 0, 5.6495073584, -0.5500722154, 1.5276003427
 H, 0, 2.245920281, 0.9789262499, -1.054702143
 H, 0, 3.4207586013, -1.2547331308, 0.7252999558
 H, 0, 6.6591099072, 0.6240111787, 0.4855630631

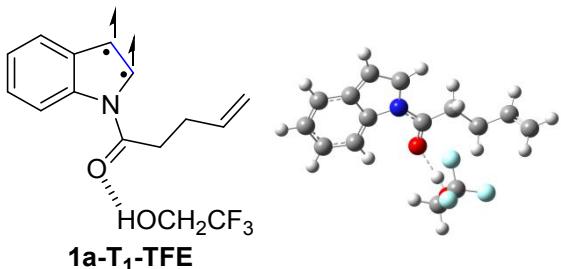
(4) At (U)B3LYP-D3(BJ)/def2-SVP/PCM ($\text{CF}_3\text{CH}_2\text{OH}$) level of theory



SCF Done: E(RB3LYP) = -1085.24831617 A.U.
 Zero-point correction= 0.288831 (Hartree/Particle)
 Sum of electronic and thermal Free Energies= -1085.012335

C, 0, -2.6083652795, 1.0116583512, 0.5494932985
 C, 0, -1.9740500138, 0.0157499593, -0.2393372799
 C, 0, -2.7064285145, -0.8654188853, -1.041200288
 C, 0, -4.0976271468, -0.730013048, -1.0403037338
 C, 0, -4.7419265653, 0.2519492179, -0.2658903152
 C, 0, -4.0063164393, 1.1273911307, 0.5323841144
 C, 0, -1.5670122135, 1.7350371259, 1.2480347399
 C, 0, -0.3742504167, 1.1911570217, 0.8878564339
 H, 0, -2.2093326895, -1.6225611877, -1.6411059233
 H, 0, -4.6951637825, -1.4046886127, -1.6577582314
 H, 0, -5.83144081, 0.3274490953, -0.2916411595
 H, 0, -4.5041807639, 1.8901398722, 1.1352419203
 H, 0, -1.7045566559, 2.5641978965, 1.9388405746
 H, 0, 0.6282109514, 1.4594737159, 1.2033593812
 N, 0, -0.5828224483, 0.1357643597, -0.0237782555
 C, 0, 0.400169401, -0.6617805629, -0.58874228
 O, 0, 0.0923958036, -1.5531975688, -1.3706420146
 C, 0, 1.8298156957, -0.378851305, -0.1786756344
 H, 0, 1.9063149901, -0.5484744953, 0.9078230049
 C, 0, 2.854171297, -1.2463361599, -0.9170724174
 H, 0, 2.8127774451, -1.0025357076, -1.9927207547
 C, 0, 4.2452789413, -1.0301297028, -0.3920816135
 H, 0, 4.684067381, -0.0383477891, -0.5631897557
 C, 0, 4.946059834, -1.9500946215, 0.2777938842
 H, 0, 4.5286167704, -2.9424957487, 0.4776628913
 H, 0, 2.0440176436, 0.690483878, -0.3374051599

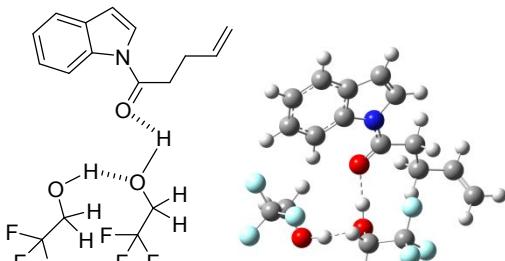
H, 0, 2.5842343211, -2.3059036694, -0.8247288294
 H, 0, 5.952616606, -1.7445389107, 0.653151609
 C, 0, 1.1227940138, -4.2683258324, 1.0351102796
 C, 0, 0.4279270946, -4.6714970701, -0.2575875913
 H, 0, 0.5057155036, -5.7685353278, -0.3204457352
 H, 0, -0.6409717831, -4.4168057225, -0.136535759
 O, 0, 1.0122279438, -4.1066275978, -1.3891616154
 H, 0, 0.7082311629, -3.1776343177, -1.4727683147
 F, 0, 0.9945689993, -2.9461244176, 1.2909063388
 F, 0, 2.4419193316, -4.5304609628, 1.0047622139
 F, 0, 0.5997861317, -4.9260855, 2.0826081073



SCF Done: E(UB3LYP) = -1085.14408690 A.U.
 Zero-point correction = 0.283654 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -1084.914977

C, 0, -2.5383626959, 0.9590014152, 0.7940638129
 C, 0, -1.9179223452, 0.0116624219, -0.1164093818
 C, 0, -2.6562744731, -0.8082773029, -0.9296265245
 C, 0, -4.080734475, -0.7075665178, -0.8596634269
 C, 0, -4.7137364809, 0.2024233467, 0.0115991192
 C, 0, -3.9746449499, 1.0352580512, 0.8363258094
 C, 0, -1.5464414969, 1.6285302171, 1.4739618284
 C, 0, -0.2473996355, 1.1046939966, 0.9988123589
 H, 0, -2.1727091973, -1.507317343, -1.6053452388
 H, 0, -4.6844974307, -1.3530495382, -1.5002043265
 H, 0, -5.8048141819, 0.2485659839, 0.0334149004
 H, 0, -4.4591835569, 1.7416568349, 1.5127155868
 H, 0, -1.659452391, 2.4037918233, 2.2287265747
 H, 0, 0.7554361938, 1.3821611079, 1.29975807
 N, 0, -0.4940313874, 0.132525489, 0.0363284604
 C, 0, 0.4438420179, -0.6116351411, -0.6458032315
 O, 0, 0.0785436155, -1.4454244684, -1.4970868017
 C, 0, 1.885249481, -0.3598557384, -0.2756992289
 H, 0, 2.0016673173, -0.5396241007, 0.8079410086
 C, 0, 2.8702454354, -1.2385302829, -1.0540099138
 H, 0, 2.8228925631, -0.9627524357, -2.1216730588
 C, 0, 4.2755757166, -1.0946930474, -0.5436502357

H, 0, 4.7560407933, -0.119200739, -0.6967586429
 C, 0, 4.9424161866, -2.0593437344, 0.0979692719
 H, 0, 4.4826521547, -3.036663901, 0.2802593975
 H, 0, 2.1193029058, 0.7103191698, -0.426128074
 H, 0, 2.5595595976, -2.2890887164, -0.9878527051
 H, 0, 5.9606040114, -1.9077071312, 0.4677848962
 C, 0, 1.0437803437, -4.2468749536, 0.8924499489
 C, 0, 0.2502139643, -4.5052402048, -0.3804707731
 H, 0, 0.1692104102, -5.6006540452, -0.4740207995
 H, 0, -0.7660823484, -4.1073026581, -0.2039959341
 O, 0, 0.8611147999, -3.9841134539, -1.5164436673
 H, 0, 0.617972639, -3.029434113, -1.5905698405
 F, 0, 1.1015501541, -2.9320616635, 1.2005837057
 F, 0, 2.3149031592, -4.6774640718, 0.7946644345
 F, 0, 0.4809853255, -4.873727655, 1.940308751

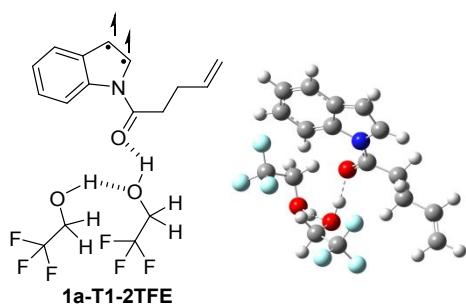


1a-2TFE

SCF Done: E(RB3LYP) = -1537.70916583 A.U.
 Zero-point correction = 0.348493 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -1537.424969

C, 0, -3.583627951, 0.768907598, -0.0247040494
 C, 0, -2.1710087901, 0.720539996, -0.1476916358
 C, 0, -1.4825644041, 1.5229654111, -1.0606930983
 C, 0, -2.2376933951, 2.3946488867, -1.8497529616
 C, 0, -3.6377699677, 2.4628009518, -1.7351598559
 C, 0, -4.3204760668, 1.6518456837, -0.8278345281
 C, 0, -3.9602475267, -0.1961065293, 0.9878960336
 C, 0, -2.8227622504, -0.7842902389, 1.4430461677
 H, 0, -0.4058031261, 1.4610130706, -1.1613658415
 H, 0, -1.7179787806, 3.0322278586, -2.568157355
 H, 0, -4.1962505486, 3.1567076796, -2.3676108919
 H, 0, -5.4083212638, 1.6987431814, -0.741893148
 H, 0, -4.969384931, -0.4182506634, 1.3284960203
 H, 0, -2.6998916072, -1.5556117326, 2.1957377092
 N, 0, -1.7026792108, -0.2442150678, 0.7747882958
 C, 0, -0.3815100707, -0.5905240122, 0.9799257857
 O, 0, 0.5049311102, -0.0158574483, 0.3526309092

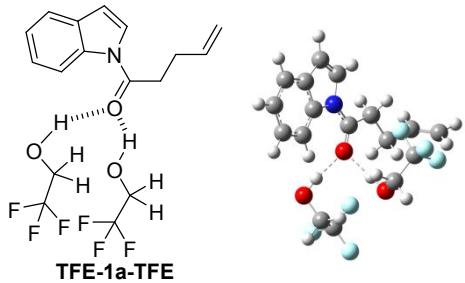
C, 0, -0.097352456, -1.6942070173, 1.9745788284
 H, 0, -0.5351568265, -2.6242032631, 1.5743015059
 C, 0, 1.3969449996, -1.8923463488, 2.2525516748
 H, 0, 1.7980459447, -0.9661962578, 2.6992981704
 C, 0, 1.6394258068, -3.0554238328, 3.1724140746
 H, 0, 1.2578201054, -2.9551180444, 4.1968965143
 C, 0, 2.2572565753, -4.1835725212, 2.8099363819
 H, 0, 2.6361282524, -4.3179693789, 1.7913185047
 H, 0, -0.6337938226, -1.4835963333, 2.9132803078
 H, 0, 1.9412304361, -2.0494930111, 1.3130282472
 H, 0, 2.4025069998, -5.0096321402, 3.5118269107
 C, 0, 1.7211450856, -3.0076088661, -1.5842493086
 C, 0, 2.2883634737, -1.6454900355, -1.9470331876
 H, 0, 3.1648679591, -1.8180668545, -2.5883570476
 H, 0, 1.5268963886, -1.1146447059, -2.541583962
 O, 0, 2.6951313525, -0.9296415574, -0.812903093
 H, 0, 1.8985607661, -0.6115762946, -0.3184752715
 F, 0, 0.5850765361, -2.8995073258, -0.8589887561
 F, 0, 2.582148123, -3.7358346823, -0.8522458232
 F, 0, 1.4261550052, -3.7071167451, -2.6892004605
 C, 0, 2.0758132782, 2.4917813298, -2.3788860264
 C, 0, 2.8740989307, 2.3273928074, -1.0954777204
 H, 0, 3.2573197635, 3.3272868477, -0.8344898941
 H, 0, 2.1584249556, 2.0257539793, -0.3091039181
 O, 0, 3.9384182301, 1.4426321741, -1.253462635
 H, 0, 3.5932476305, 0.5319552508, -1.1217890454
 F, 0, 1.5182537572, 1.3235984839, -2.7757039541
 F, 0, 2.8277496328, 2.9294875631, -3.3985128681
 F, 0, 1.066244687, 3.369761605, -2.210237945



SCF Done: E(UB3LYP) = -1537.60653718 A.U.
 Zero-point correction = 0.343359 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -1537.328594

C, 0, -3.5743492131, 0.7290006788, -0.0645018747
 C, 0, -2.1256311574, 0.7030186409, -0.1571182387
 C, 0, -1.4368798018, 1.4967432879, -1.036920343

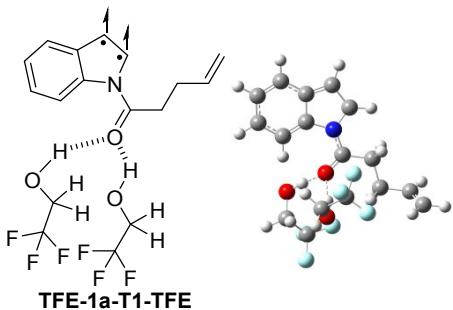
C, 0, -2.1883822327, 2.3818095433, -1.8653145931
 C, 0, -3.5964232585, 2.441954016, -1.7912985916
 C, 0, -4.3009816346, 1.6363214916, -0.9121673132
 C, 0, -3.9698738633, -0.1973372018, 0.8743344585
 C, 0, -2.7486724147, -0.8382471342, 1.4075619166
 H, 0, -0.357667708, 1.4454961501, -1.1074938994
 H, 0, -1.6477999819, 3.0217903524, -2.5644651618
 H, 0, -4.1355888951, 3.134953994, -2.4408623753
 H, 0, -5.3901618563, 1.6757971016, -0.8536399221
 H, 0, -4.9819553507, -0.4429883902, 1.1883549239
 H, 0, -2.6550275496, -1.6193870699, 2.1524708765
 N, 0, -1.6457324137, -0.269653916, 0.7860036055
 C, 0, -0.3224384193, -0.5647522932, 1.0168581999
 O, 0, 0.5690531501, 0.0541200721, 0.3915913848
 C, 0, -0.0419032087, -1.655369344, 2.0193304382
 H, 0, -0.5018652251, -2.5925711668, 1.6559621741
 C, 0, 1.4534907965, -1.8757705242, 2.2736392401
 H, 0, 1.876614959, -0.9536854957, 2.7084319447
 C, 0, 1.7011348272, -3.0396473074, 3.1902888248
 H, 0, 1.3454765905, -2.9328315072, 4.2236801332
 C, 0, 2.2925670971, -4.1782853803, 2.8158000462
 H, 0, 2.6443012152, -4.3198985951, 1.7881298295
 H, 0, -0.5584464795, -1.420812747, 2.9683571461
 H, 0, 1.9766610487, -2.0425641147, 1.3233480409
 H, 0, 2.4418126934, -5.0062841818, 3.5146979866
 C, 0, 1.6176575658, -3.0014618114, -1.5908648117
 C, 0, 2.140951177, -1.6189946266, -1.9431978628
 H, 0, 2.9612835106, -1.7575017206, -2.663340171
 H, 0, 1.3263550505, -1.0778840138, -2.4524855143
 O, 0, 2.6266405842, -0.942950146, -0.8189825882
 H, 0, 1.8544652899, -0.5925974004, -0.2871498167
 F, 0, 0.5379412985, -2.9391015358, -0.7806661096
 F, 0, 2.5389873061, -3.7456641386, -0.9538260321
 F, 0, 1.2488538386, -3.6639910054, -2.6983835097
 C, 0, 2.0723903955, 2.5118095232, -2.3507279744
 C, 0, 2.8350030871, 2.2964759977, -1.0534574586
 H, 0, 3.2191664802, 3.2839211659, -0.7491314013
 H, 0, 2.0987100746, 1.9710825309, -0.2965095166
 O, 0, 3.8953784886, 1.4076363316, -1.2178038098
 H, 0, 3.5379319302, 0.4963518691, -1.1151458434
 F, 0, 1.5251855013, 1.3620963077, -2.8090624594
 F, 0, 2.8516984486, 2.9887562172, -3.3319146617
 F, 0, 1.0580010489, 3.3850469457, -2.176021556



SCF Done: E(RB3LYP) = -1537.70554243 A.U.
 Zero-point correction = 0.348498 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -1537.421528

C, 0, -3.4756892498, -0.3378305994, -1.166167157
 C, 0, -2.5501764807, -0.3814071609, -0.0909611512
 C, 0, -2.7821560224, 0.3022514024, 1.1060745533
 C, 0, -3.9653717292, 1.0416699556, 1.2041468275
 C, 0, -4.889717989, 1.0991432095, 0.1470039652
 C, 0, -4.6548389054, 0.4098306881, -1.0428541652
 C, 0, -2.933726536, -1.1477497749, -2.2382429637
 C, 0, -1.7400095988, -1.6417195947, -1.8216286566
 H, 0, -2.0929423354, 0.2490285954, 1.9427635492
 H, 0, -4.1727784011, 1.5823519018, 2.1303174895
 H, 0, -5.8030869969, 1.6871029155, 0.2619620763
 H, 0, -5.3717748338, 0.4487908492, -1.8658416592
 H, 0, -3.3940252438, -1.3315472371, -3.2067082527
 H, 0, -1.0394086672, -2.2856168079, -2.3420807927
 N, 0, -1.4668056891, -1.1939519857, -0.50910673
 C, 0, -0.3148487457, -1.4451507926, 0.1985617074
 O, 0, -0.1815966185, -1.0087641124, 1.344004214
 C, 0, 0.7672272763, -2.2479562255, -0.4863437125
 H, 0, 1.0200303195, -1.7484849208, -1.4347446814
 C, 0, 2.0272307377, -2.4160556329, 0.3696483313
 H, 0, 1.7640654065, -2.961721862, 1.2905786867
 C, 0, 3.1107236786, -3.1398638319, -0.3778926083
 H, 0, 2.9173049126, -4.1921726591, -0.6238092352
 C, 0, 4.2567379806, -2.5742613729, -0.7685213178
 H, 0, 4.46978578, -1.5222238975, -0.5499835436
 H, 0, 0.3505120353, -3.2320590619, -0.7603715368
 H, 0, 2.3981948557, -1.4319565346, 0.6853312402
 H, 0, 5.0162607658, -3.1348197665, -1.3207679698
 C, 0, 2.1922196247, 1.5878351847, -0.0301736466
 C, 0, 1.7322357504, 1.7220144622, 1.4139800838
 H, 0, 2.3404637778, 2.5209419088, 1.8648289352
 H, 0, 0.6829078077, 2.0677492174, 1.3872634554
 O, 0, 1.913293756, 0.5490224004, 2.1483609045
 H, 0, 1.2191484583, -0.0941789474, 1.8957005783

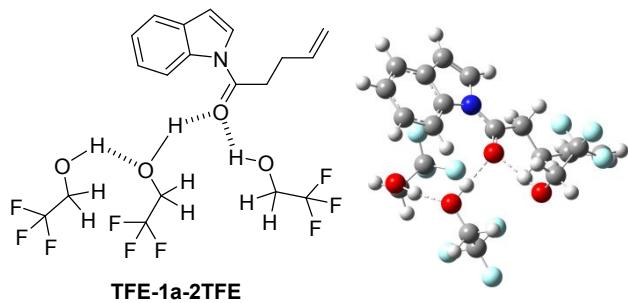
F, 0, 1.417365743, 0.7234992268, -0.7285160796
 F, 0, 3.4538585627, 1.1344217715, -0.1211044606
 F, 0, 2.1324950845, 2.7700852638, -0.6613549563
 C, 0, 0.9801224782, -1.5790667927, 4.9208246812
 C, 0, -0.0587266966, -0.503884795, 4.6508293593
 H, 0, -0.4138155228, -0.1410805199, 5.6274553685
 H, 0, 0.4688984511, 0.3208442146, 4.1418185456
 O, 0, -1.1481022464, -1.0018605846, 3.9285627527
 H, 0, -0.8681886746, -1.132315301, 3.003156453
 F, 0, 1.4773897098, -2.0849167385, 3.7713900471
 F, 0, 0.4791507743, -2.6133975379, 5.6164179347
 F, 0, 2.0141549762, -1.0800868795, 5.6206922464



SCF Done: E(UB3LYP) = -1537.60470328 A.U.
 Zero-point correction= 0.343660 (Hartree/Particle)
 Sum of electronic and thermal Free Energies= -1537.326733

C, 0, -3.4889645685, -0.3133203184, -1.1909567289
 C, 0, -2.5450492429, -0.3731746628, -0.0877625834
 C, 0, -2.7802776708, 0.264723104, 1.1053064512
 C, 0, -3.9870251078, 1.0119852006, 1.2293015283
 C, 0, -4.9195369018, 1.0995379095, 0.1718298072
 C, 0, -4.6957339292, 0.45134549, -1.0291125194
 C, 0, -2.9960504615, -1.06578452, -2.233148533
 C, 0, -1.6987474381, -1.6198768212, -1.8012561477
 H, 0, -2.0932324741, 0.1890577213, 1.9417461786
 H, 0, -4.1887967547, 1.5252392142, 2.171204177
 H, 0, -5.8309256152, 1.6846034126, 0.3118200092
 H, 0, -5.413320438, 0.5078999361, -1.8495249311
 H, 0, -3.4501091969, -1.2437231951, -3.2053244088
 H, 0, -1.0087041884, -2.2510423135, -2.3486215859
 N, 0, -1.4364230106, -1.1856495692, -0.5121279424
 C, 0, -0.2993898081, -1.4338190774, 0.2157916413
 O, 0, -0.1834733283, -0.9582190743, 1.3755756566
 C, 0, 0.7748915385, -2.2475120295, -0.4548301945
 H, 0, 1.0432173559, -1.7613717948, -1.4101008749
 C, 0, 2.0299759221, -2.4130895871, 0.4098073522

H, 0, 1.7580816656, -2.9514384903, 1.3326542925
 C, 0, 3.1192456715, -3.1443227223, -0.3209310246
 H, 0, 2.9253666812, -4.1980495213, -0.5617317255
 C, 0, 4.2713061683, -2.5866086161, -0.7060000683
 H, 0, 4.4861196472, -1.5335291179, -0.4941429329
 H, 0, 0.3646826511, -3.2374451956, -0.7310818571
 H, 0, 2.3972934087, -1.4270045563, 0.7242532057
 H, 0, 5.0336193635, -3.1540272213, -1.2475338189
 C, 0, 2.2231184215, 1.5955070884, -0.0922438907
 C, 0, 1.7171932148, 1.7679094824, 1.3326071932
 H, 0, 2.3242802818, 2.5681939397, 1.784272887
 H, 0, 0.6761852509, 2.1334622704, 1.2590217664
 O, 0, 1.8478116521, 0.6093969512, 2.0944947154
 H, 0, 1.1347774699, -0.0240289379, 1.8370739441
 F, 0, 1.4555639626, 0.7381242065, -0.8031544454
 F, 0, 3.4783034849, 1.1143604141, -0.1305019707
 F, 0, 2.2145254124, 2.7686264248, -0.7468719011
 C, 0, 0.9918872694, -1.616305742, 4.9393727631
 C, 0, -0.0613393582, -0.5705449563, 4.6153587458
 H, 0, -0.4399484925, -0.1867701417, 5.575793427
 H, 0, 0.4628636297, 0.2486589375, 4.0934272177
 O, 0, -1.1223324705, -1.1090966816, 3.8833005625
 H, 0, -0.8301582693, -1.200603258, 2.9503037943
 F, 0, 1.5381918314, -2.1372815899, 3.8211035159
 F, 0, 0.4920365319, -2.64577675, 5.6448338737
 F, 0, 1.9929917581, -1.0787340016, 5.6612040893



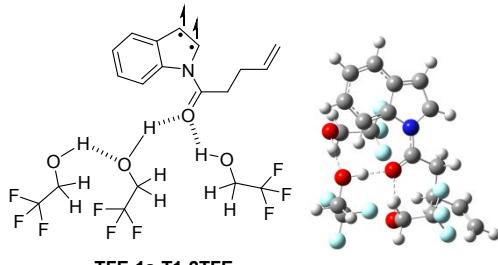
SCF Done: E(RB3LYP) = -1990.17078530 A.U.
 Zero-point correction= 0.408262 (Hartree/Particle)

Sum of electronic and thermal Free Energies= -1989.836268

C, 0, -2.7330289265, -2.901671432, -0.157495885
 C, 0, -1.666850415, -2.0435278413, -0.531364261
 C, 0, -1.5042193914, -1.6115822994, -1.849638288
 C, 0, -2.4368400281, -2.0545304919, -2.7928679871
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 C, 0, -3.6556554928, -3.3325516563, -1.1199265741

C, 0, -2.6107871738, -3.1527703834, 1.2637194715
 C, 0, -1.527914635, -2.4710663321, 1.7132335525
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 H, 0, -2.3326023561, -1.7270262436, -3.8296523571
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 H, 0, -4.4795844308, -3.9916295729, -0.8377512576
 H, 0, -3.2659850287, -3.7746672614, 1.8699644741
 H, 0, -1.1140854746, -2.4193788899, 2.7139284488
 N, 0, -0.9178654485, -1.7758103766, 0.6432069295
 C, 0, 0.1913470598, -0.9740360248, 0.7405611112
 O, 0, 0.6480294668, -0.4247585376, -0.2679319788
 C, 0, 0.8281436478, -0.8103792343, 2.0995468248
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 C, 0, 1.7982639993, 0.3737105175, 2.185382444
 H, 0, 1.2363600362, 1.2969870635, 1.9719555827
 C, 0, 2.439441993, 0.4596606761, 3.5413524692
 H, 0, 1.7716999043, 0.6869850735, 4.3827386574
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 H, 0, 2.5761100027, 0.2923994106, 1.4162124813
 H, 0, 4.1604824389, 0.3229691665, 4.780480379
 C, 0, 4.2043693211, -1.7218874424, -0.2842108719
 C, 0, 3.8216893409, -0.7872565374, -1.4215038515
 H, 0, 4.7569842617, -0.4791898617, -1.9129160876
 H, 0, 3.2376647843, -1.3846884206, -2.1454168534
 O, 0, 3.1500782711, 0.3498888679, -0.969340352
 H, 0, 2.2595364435, 0.0805129325, -0.6569150973
 F, 0, 3.1148890019, -2.1884811186, 0.3668300914
 F, 0, 4.9744455142, -1.1127478269, 0.6355530122
 F, 0, 4.8815173417, -2.7849059739, -0.7446022458
 C, 0, 0.7312931713, 3.4946703557, -1.0398902771
 C, 0, 0.7466298762, 2.4463784737, -2.1378733285
 H, 0, 0.5631849575, 2.9616219471, -3.091834083
 H, 0, 1.7554149712, 2.0022468932, -2.1576217666
 O, 0, -0.2495214419, 1.4774859272, -1.9441714032
 H, 0, 0.043151444, 0.827034791, -1.2693497116
 F, 0, 1.0024612114, 2.9587046263, 0.1652302099
 F, 0, -0.4669040305, 4.1027128951, -0.9393384777
 F, 0, 1.649243431, 4.4437077886, -1.2786372443
 C, 0, -2.6851442724, 1.5288299485, 0.9921551163
 C, 0, -3.1676034022, 2.2598393352, -0.2504174126
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 H, 0, -2.6982740317, 3.2595616653, -0.2287339107

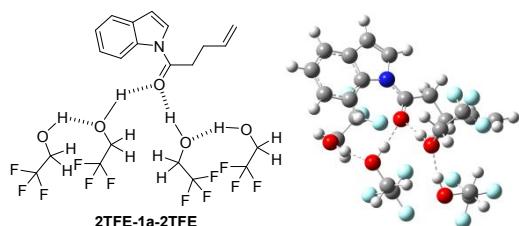
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 F, 0, -3.2009759626, 0.293675742, 1.0984489931
 F, 0, -3.0108196127, 2.2049120721, 2.1064555816



SCF Done: E(UB3LYP) = -1990.07083003 A.U.
 Zero-point correction= 0.403175 (Hartree/Particle)
 Sum of electronic and thermal Free Energies= -1989.743267

C, 0, -2.7591970293, -2.8687525724, -0.1402526804
 C, 0, -1.6459940078, -2.021193151, -0.5303021198
 C, 0, -1.4854259515, -1.5865130232, -1.8222413911
 C, 0, -2.4572387889, -1.9852018194, -2.7818334626
 C, 0, -3.5527136836, -2.8072515176, -2.4340795518
 C, 0, -3.719819611, -3.2550553092, -1.1371577359
 C, 0, -2.6555841793, -3.1398059869, 1.2050438082
 C, 0, -1.4503105568, -2.4512684262, 1.6987462199
 H, 0, -0.6602167072, -0.9466171358, -2.1143081829
 H, 0, -2.3473501306, -1.6390995135, -3.8110940245
 H, 0, -4.2744309808, -3.0881586168, -3.2039288708
 H, 0, -4.5622783972, -3.8902174795, -0.8576341758
 H, 0, -3.3194526147, -3.7411147485, 1.8219158651
 H, 0, -1.02108612, -2.4588510288, 2.6935962554
 N, 0, -0.8593537268, -1.772099489, 0.647621469
 C, 0, 0.248166491, -0.9665453721, 0.7203394991
 O, 0, 0.6951748066, -0.4289631861, -0.3320332838
 C, 0, 0.8659061125, -0.7683267387, 2.0767730922
 H, 0, 1.3675617196, -1.7049050312, 2.3852616281
 C, 0, 1.8595373872, 0.3987252128, 2.1265963398
 H, 0, 1.3176985676, 1.3230534825, 1.8687115353
 C, 0, 2.4943254492, 0.5320146276, 3.4810613982
 H, 0, 1.8253327513, 0.8029572138, 4.3088336063
 C, 0, 3.7903276468, 0.3206849066, 3.731041727
 H, 0, 4.4797135453, 0.0336594776, 2.930138319
 H, 0, 0.0625509185, -0.6006917305, 2.8156034257
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 H, 0, 4.205482937, 0.4205418323, 4.7381063357

C, 0, 4.2441329548, -1.8127247527, -0.2619307615
 C, 0, 3.8526662443, -0.9130524529, -1.4247165482
 H, 0, 4.7872131965, -0.6181137416, -1.9270694481
 H, 0, 3.2729614953, -1.538451544, -2.1293020077
 O, 0, 3.1739095055, 0.2284751203, -1.0059309784
 H, 0, 2.2672777295, -0.0341713904, -0.7089694847
 F, 0, 3.1627405514, -2.2688665559, 0.4067073273
 F, 0, 5.0155009237, -1.1729758702, 0.6370929351
 F, 0, 4.9289741334, -2.8847016741, -0.6941751938
 C, 0, 0.6206264783, 3.5744902455, -0.9800917923
 C, 0, 0.7627225657, 2.4705682658, -2.0128650583
 H, 0, 0.6595198965, 2.9385290397, -3.0037669705
 H, 0, 1.779672761, 2.0539028916, -1.9234334276
 O, 0, -0.2203674988, 1.4859659011, -1.8570646195
 H, 0, 0.0791367315, 0.8135374519, -1.1916003403
 F, 0, 0.7887438807, 3.1208317681, 0.2757217645
 F, 0, -0.5982613291, 4.1501329722, -1.0281088102
 F, 0, 1.5317587233, 4.5389966035, -1.1880032971
 C, 0, -2.7603915002, 1.4514903593, 0.976321782
 C, 0, -3.2103631819, 2.1666737709, -0.287944454
 H, 0, -4.3049308942, 2.2685280791, -0.2134439904
 H, 0, -2.7723073552, 3.1800982626, -0.2460233233
 O, 0, -2.8931449319, 1.4656229584, -1.447174367
 H, 0, -1.9350208207, 1.5732551913, -1.6389789443
 F, 0, -1.4124353608, 1.3562684082, 1.0479816769
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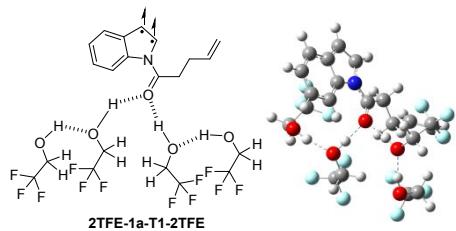


SCF Done: E(RB3LYP) = -2442.63390123 A.U.
 Zero-point correction= 0.467655 (Hartree/Particle)
 Sum of electronic and thermal Free Energies= -2442.249344

C, 0, 4.5341963581, 1.8385163432, 0.0395036863
 C, 0, 3.272143878, 1.3845370671, -0.4204580101
 C, 0, 3.0881981233, 0.9122467326, -1.7216615253
 C, 0, 4.2015947225, 0.9151065675, -2.5679641657
 C, 0, 5.4571976016, 1.370613056, -2.131816265
 C, 0, 5.6349814724, 1.8327850186, -0.8270463122
 C, 0, 4.3780145201, 2.22107579, 1.4290412411

C, 0, 3.0864140516, 1.9979349389, 1.778884363
 H, 0, 2.1261419897, 0.5452980601, -2.0653942048
 H, 0, 4.0874714338, 0.5492003175, -3.5907420966
 H, 0, 6.3037619206, 1.3572023754, -2.8219904954
 H, 0, 6.6113018013, 2.1798434248, -0.4819856626
 H, 0, 5.1536245861, 2.6152513918, 2.0822512798
 H, 0, 2.5861075125, 2.1667657735, 2.7263796005
 N, 0, 2.3714245886, 1.4915870394, 0.6692649585
 C, 0, 1.0462049645, 1.153262107, 0.6577460441
 O, 0, 0.5209674449, 0.7718715887, -0.3974004643
 C, 0, 0.2666636106, 1.2588345158, 1.9455065746
 H, 0, 0.1665298414, 2.3286712272, 2.194819813
 C, 0, -1.1112746609, 0.5990136556, 1.8460617366
 H, 0, -0.9701187122, -0.4758476111, 1.6537954527
 C, 0, -1.9294199619, 0.7897118204, 3.0897845283
 H, 0, -1.5268326988, 0.3476922395, 4.0106711683
 C, 0, -3.0874580289, 1.4550027517, 3.1338813361
 H, 0, -3.5082869794, 1.9168896468, 2.2352070315
 H, 0, 0.8553469524, 0.8040904956, 2.7566205669
 H, 0, -1.6568200609, 0.9968616128, 0.9826656219
 H, 0, -3.6517694887, 1.5644175252, 4.0643529323
 C, 0, -2.102306436, 3.6519068529, -0.6021639143
 C, 0, -1.7844299493, 2.8567935901, -1.8580401819
 H, 0, -2.5814311931, 3.0601647811, -2.5877377077
 H, 0, -0.8346648266, 3.2427542627, -2.2650020608
 O, 0, -1.7452017276, 1.4811765059, -1.6051194875
 H, 0, -0.9160959108, 1.2321483423, -1.1336478747
 F, 0, -1.1360922509, 3.5102020179, 0.3306473009
 F, 0, -3.255919432, 3.2520050887, -0.0317705128
 F, 0, -2.2124403965, 4.9574259575, -0.8772647232
 C, 0, -0.9415066026, -3.2643540127, -0.5567014918
 C, 0, -0.7875417833, -2.2466883696, -1.6731778474
 H, 0, -0.8887430656, -2.7939966562, -2.6223762589
 H, 0, -1.6230908404, -1.5340987485, -1.6007474479
 O, 0, 0.4692649184, -1.6222079897, -1.6359517382
 H, 0, 0.4430479118, -0.8271344264, -1.064068383
 F, 0, -0.8054104131, -2.7137537857, 0.6630205604
 F, 0, -0.0093779264, -4.2378475131, -0.6461433055
 F, 0, -2.1453054429, -3.8520779249, -0.6119275882
 C, 0, 2.8878830167, -2.1633556522, 1.2903530385
 C, 0, 3.014532069, -3.1671507597, 0.1559723403
 H, 0, 3.9874237089, -3.6662844468, 0.2906588782
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 O, 0, 2.9790042626, -2.5649300697, -1.0986353133

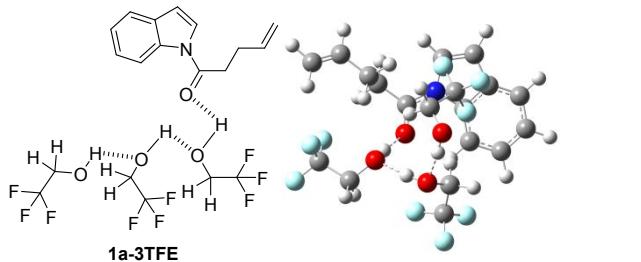
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 F, 0, 2.9682059049, -2.773398356, 2.4846620215
 C, 0, -4.4441954053, -1.0196891947, 0.0120312764
 C, 0, -4.5547186038, 0.0404556522, -1.0697292758
 H, 0, -5.6114223206, 0.0576073968, -1.387025606
 H, 0, -4.3262865899, 1.0090353049, -0.595950225
 O, 0, -3.7181147545, -0.2390066523, -2.1537955987
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 F, 0, -5.2081156135, -0.7009640632, 1.072680584



SCF Done: E(UB3LYP) = -2442.53545769 A.U.
 Zero-point correction = 0.462849 (Hartree/Particle)
 Sum of electronic and thermal Free Energies= -2442.156610

C, 0, -2.6348875633, -2.9454679969, 0.0800834344
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 C, 0, -1.7626203294, -1.48164058, -1.7088049733
 C, 0, -2.8559904312, -1.9053108999, -2.5118077904
 C, 0, -3.8137215994, -2.831337385, -2.0379620074
 C, 0, -3.7226574866, -3.3571199845, -0.7632526427
 C, 0, -2.2953455395, -3.2524749463, 1.3788739626
 C, 0, -1.0771732484, -2.491579464, 1.7022707592
 H, 0, -1.0445724848, -0.7622113682, -2.0879371986
 H, 0, -2.9536263077, -1.4972382427, -3.5193397443
 H, 0, -4.6360510738, -3.1290277267, -2.6917777823
 H, 0, -4.4587385468, -4.0693745916, -0.3863341632
 H, 0, -2.8093264015, -3.9177438717, 2.0687577696
 H, 0, -0.4955793018, -2.4911613664, 2.6170744164
 N, 0, -0.7065626119, -1.7476693501, 0.5998774602
 C, 0, 0.356838937, -0.8871272486, 0.5196118419
 O, 0, 0.5950920202, -0.304405071, -0.5820869067
 C, 0, 1.1687487126, -0.6645358145, 1.7640352454
 H, 0, 1.7223051374, -1.5893792017, 2.0120024488
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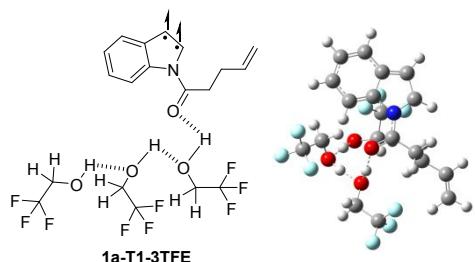
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H, 0, 4.8842981599, 0.321817719, 1.8836920023
H, 0, 0.482365887, -0.4868769354, 2.6115986
H, 0, 2.7587623642, 0.3780877954, 0.7255063677
H, 0, 4.9506900923, 0.711528336, 3.7098627963
C, 0, 4.188077112, -1.7958196741, -0.9471581618
C, 0, 3.467039306, -1.1913532027, -2.141615995
H, 0, 4.2219755578, -1.0158538311, -2.9226896359
H, 0, 2.7553011281, -1.9482915623, -2.5138159788
O, 0, 2.8495385841, 0.0186936356, -1.8209017407
H, 0, 2.0014980744, -0.1303595951, -1.3145817892
F, 0, 3.3303608225, -2.1205952114, 0.0419344234
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F, 0, 4.842252766, -2.911923618, -1.2984023928
C, 0, 0.1069051489, 3.900816053, -0.5773275064
C, 0, 0.3670717846, 2.9203085107, -1.7069226852
H, 0, 0.2028772399, 3.4689460746, -2.6475656611
H, 0, 1.4288323595, 2.6327352088, -1.6644152819
O, 0, -0.4979937965, 1.8203926475, -1.6479858759
H, 0, -0.0884432217, 1.0802295696, -1.1312313557
F, 0, 0.2725566951, 3.3462371113, 0.6367196111
F, 0, -1.1587765674, 4.3729485767, -0.6155902244
F, 0, 0.9314095779, 4.9560362757, -0.6633779773
C, 0, -2.8088745163, 1.2457201381, 1.3570548453
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H, 0, -4.4848576661, 2.081467869, 0.3777339847
H, 0, -3.0189457824, 3.0959443879, 0.3475457723
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F, 0, -1.4584003954, 1.1971884047, 1.3011338382
F, 0, -3.2422370446, -0.0278881738, 1.3506517928
F, 0, -3.1354816958, 1.7777824982, 2.5479934252
C, 0, 4.3004793862, 3.4770587249, -0.2502493819
C, 0, 4.7774437273, 2.5335747403, -1.3404202394
H, 0, 5.7306722747, 2.9455609699, -1.7151814826
H, 0, 4.9932356996, 1.56619375, -0.8582631216
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F, 0, 3.1233691766, 3.0817494653, 0.2765395228
F, 0, 4.1231113964, 4.7300994174, -0.702684051
F, 0, 5.1924401645, 3.5309506546, 0.7564473273



SCF Done: E(RB3LYP) = -1990.17350510 A.U.
 Zero-point correction = 0.408849 (Hartree/Particle)
 Sum of electronic and thermal Free Energies = -1989.838301

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C,0,-1.9315914766,2.8600379327,-2.6776735428
C,0,-2.9253027648,3.6506011234,-2.0729580989
C,0,-3.3962883948,3.3522657951,-0.7939339796
C,0,-3.1020513511,1.6725264045,1.1896408687
C,0,-2.278231958,0.6021174646,1.3316232777
H,0,-0.6197259666,1.1410884726,-2.4937298173
H,0,-1.5773022324,3.1068290688,-3.6805619588
H,0,-3.3359471451,4.5052801568,-2.6153421268
H,0,-4.1761125952,3.9585898478,-0.3279521537
H,0,-3.8160539608,2.0258664349,1.9304978138
H,0,-2.1580761041,-0.0680336999,2.1757986755
N,0,-1.4799478148,0.4547945186,0.1758046685
C,0,-0.4370631955,-0.431545764,0.0113256567
O,0,0.3279093797,-0.3021866622,-0.9450372954
C,0,-0.2494122126,-1.5424414853,1.016799807
H,0,-0.0067754102,-2.4380696794,0.4273836644
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6. X-ray crystal data of 2a and 2aa

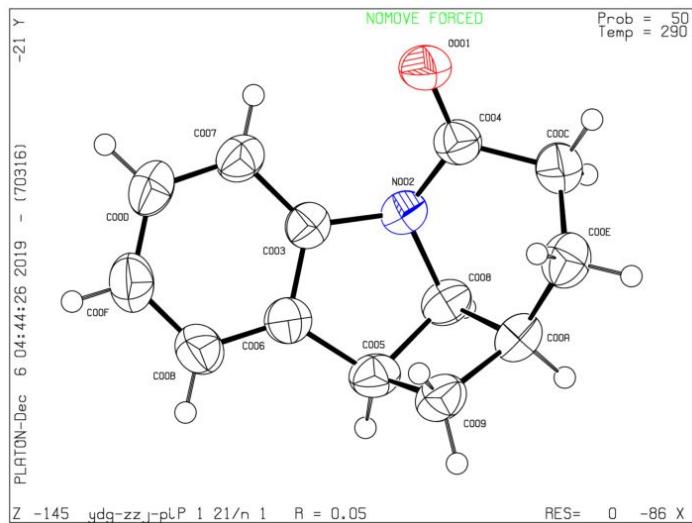


Figure S22: X-Ray crystal structure of **2a** (The crystal was obtained by slow evaporation of the solution of CH_2Cl_2 and hexane) (CCDC 1987283):

Bond precision:	C-C = 0.0020 Å	Wavelength=1.54184
Cell:	a = 8.31074(18)	b = 13.9007(3)
	alpha = 90	beta = 96.992(2)
		gamma = 90
Temperature:	290 K	
	Calculated	Reported
Volume	1016.69(4)	1016.68(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	$\text{C}_{13}\text{H}_{13}\text{NO}$	$\text{C}_{13}\text{H}_{13}\text{NO}$
Sum formula	$\text{C}_{13}\text{H}_{13}\text{NO}$	$\text{C}_{13}\text{H}_{13}\text{NO}$
Mr	199.24	199.24
D_x , g cm^{-3}	1.302	1.302
Z	4	4
μ (mm^{-1})	0.651	0.651
F000	424.0	424.0
F000'	425.19	
h, k, l_{\max}	10, 17, 10	10, 17, 10
Nref	1974	1957
T_{\min}, T_{\max}	0.768, 0.823	0.727, 1.000
T_{\min}'	0.624	
Correction method = # Reported	T Limits: $T_{\min}=0.727$ $T_{\max}=1.000$	
AbsCorr = MULTI-SCAN		
Data completeness = 0.991	Theta(max) = 71.654	
R(reflections)= 0.0550(1765)	wR2(reflections)= 0.1487(1957)	
S = 1.037	Npar= 136	

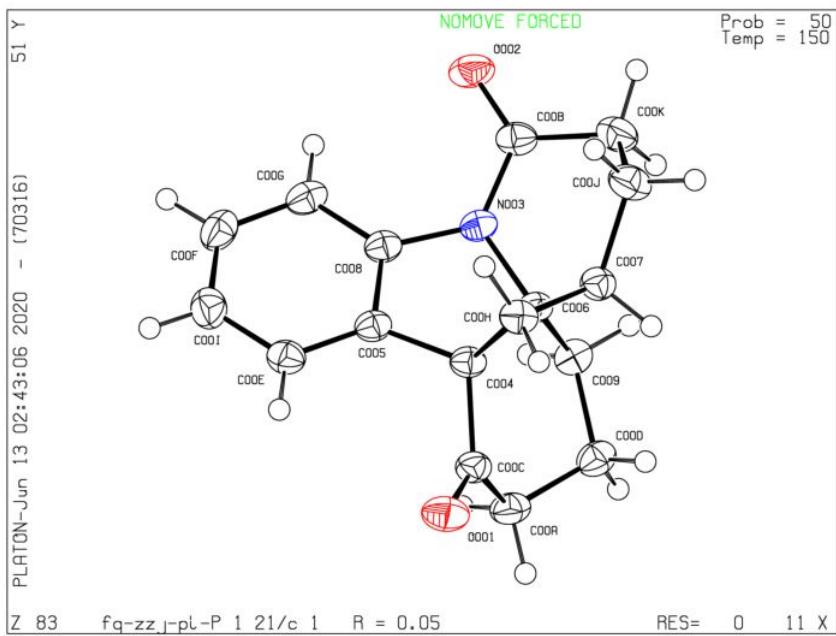


Figure S23: X-Ray crystal structure of **2aa** (The crystal was obtained by slow evaporation of the solution of CH₂Cl₂ and hexane) (CCDC 2009561):

Bond precision:	C-C = 0.0022 Å	Wavelength=1.54184
Cell:	a=11.2862(3)	b=9.2093(2)
	alpha=90	beta=109.258(3)
		gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	1286.49(6)	1286.48(5)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C ₁₇ H ₁₇ NO ₂	C ₁₇ H ₁₇ NO ₂
Sum formula	C ₁₇ H ₁₇ NO ₂	C ₁₇ H ₁₇ NO ₂
Mr	267.32	267.31
Dx,g cm ⁻³	1.380	1.380
Z	4	4
Mu (mm ⁻¹)	0.721	0.721
F000	568.0	568.0
F000'	569.67	
h,k,l _{max}	13,11,16	13,11,16
Nref	2499	2463
T _{min} ,T _{max}	0.732,0.749	0.763,1.000
T _{min'}	0.664	
Correction method= # Reported		
AbsCorr = MULTI-SCAN		
Data completeness= 0.986	Theta(max)= 71.299	
R(reflections)= 0.0547(2226)	wR2(reflections)= 0.1461(2463)	
S = 1.054	Npar= 181	

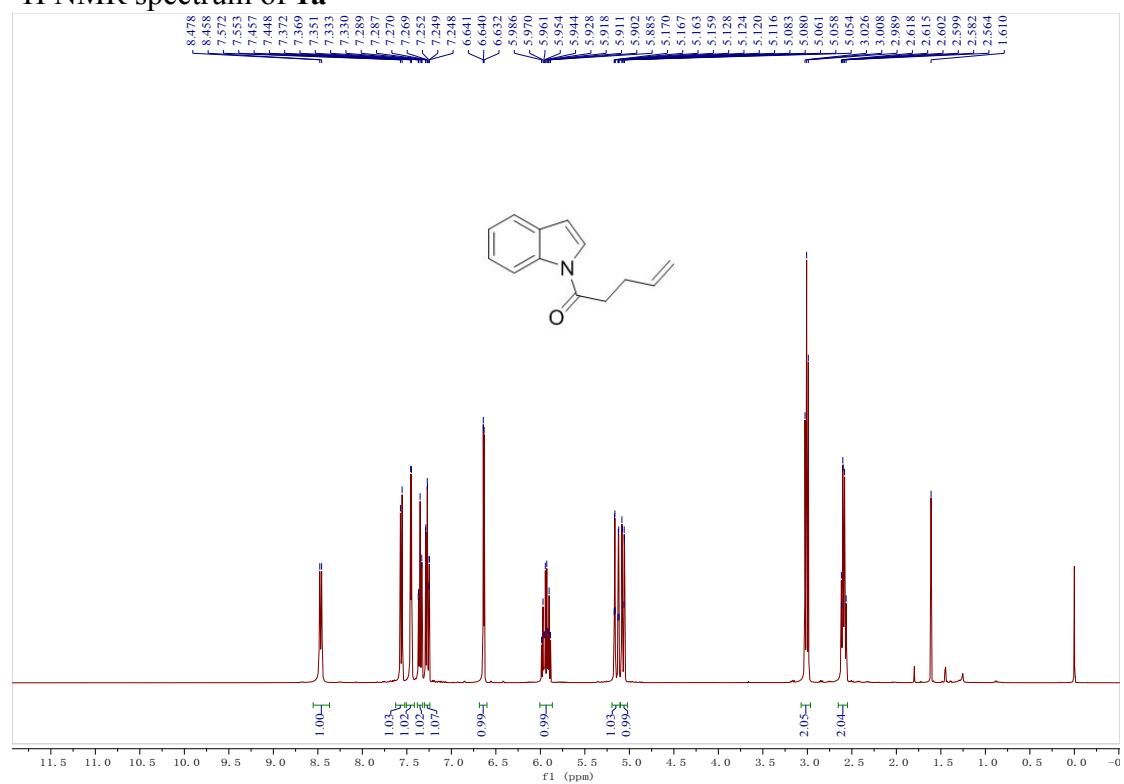
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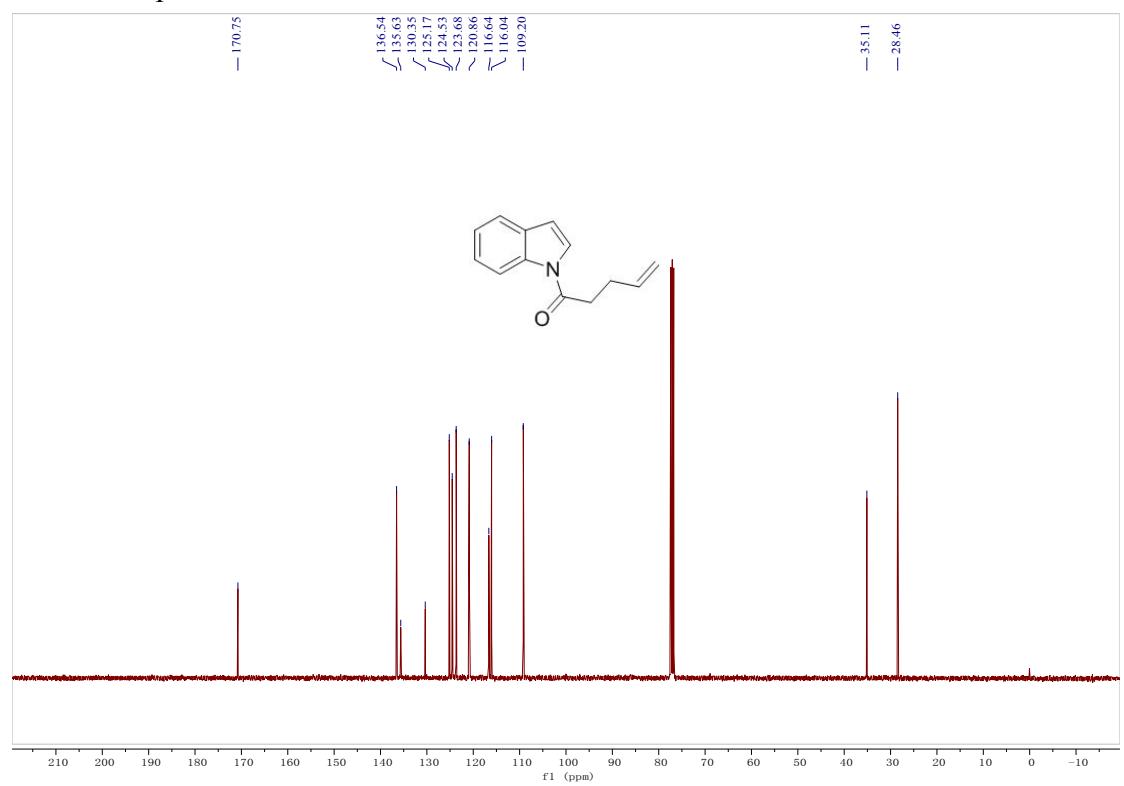
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8. Copies of NMR spectra for substrates and products

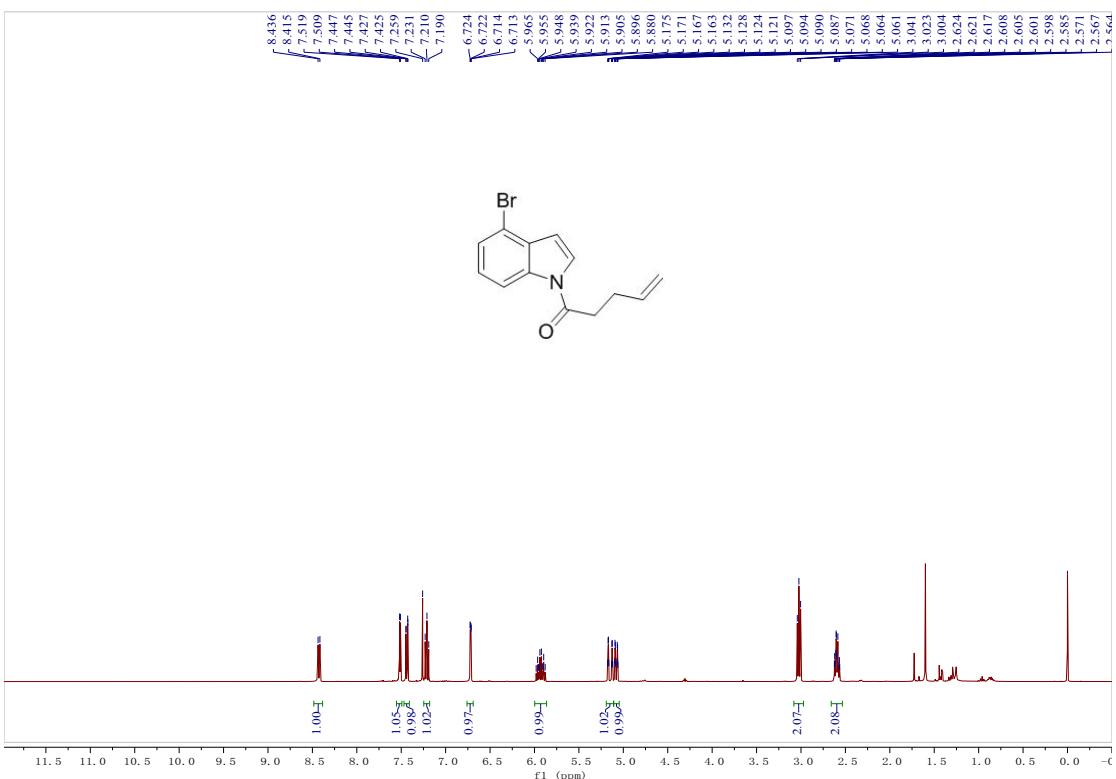
¹H NMR spectrum of **1a**



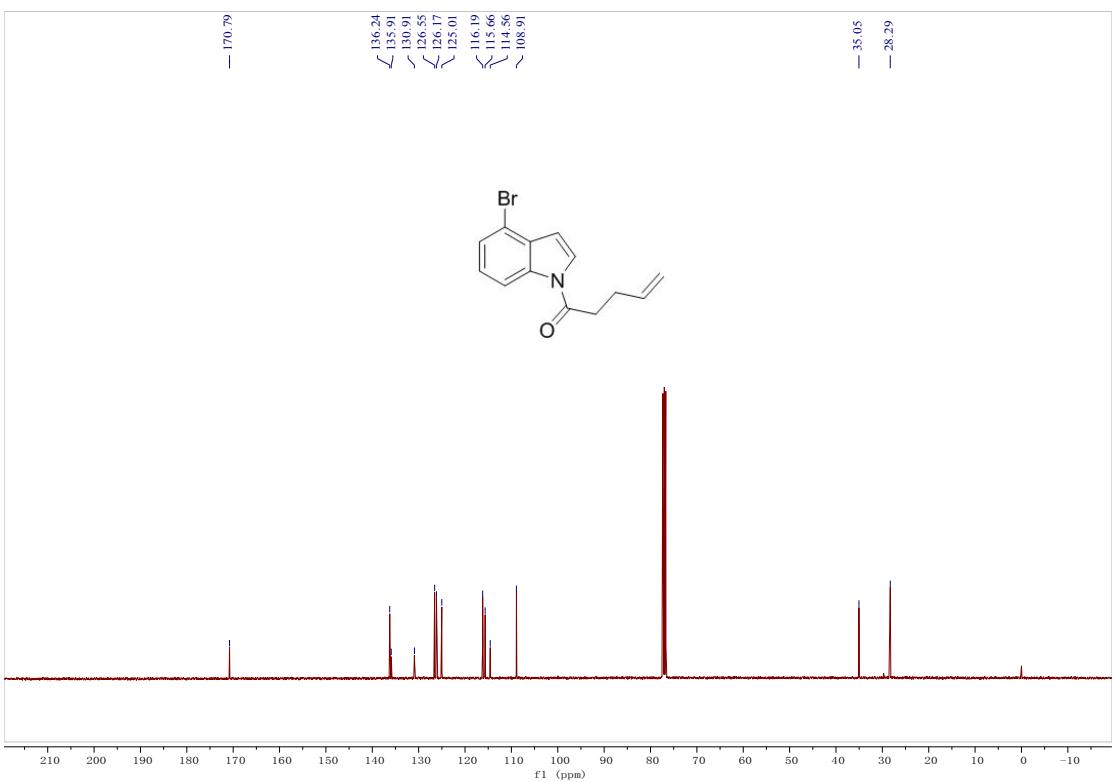
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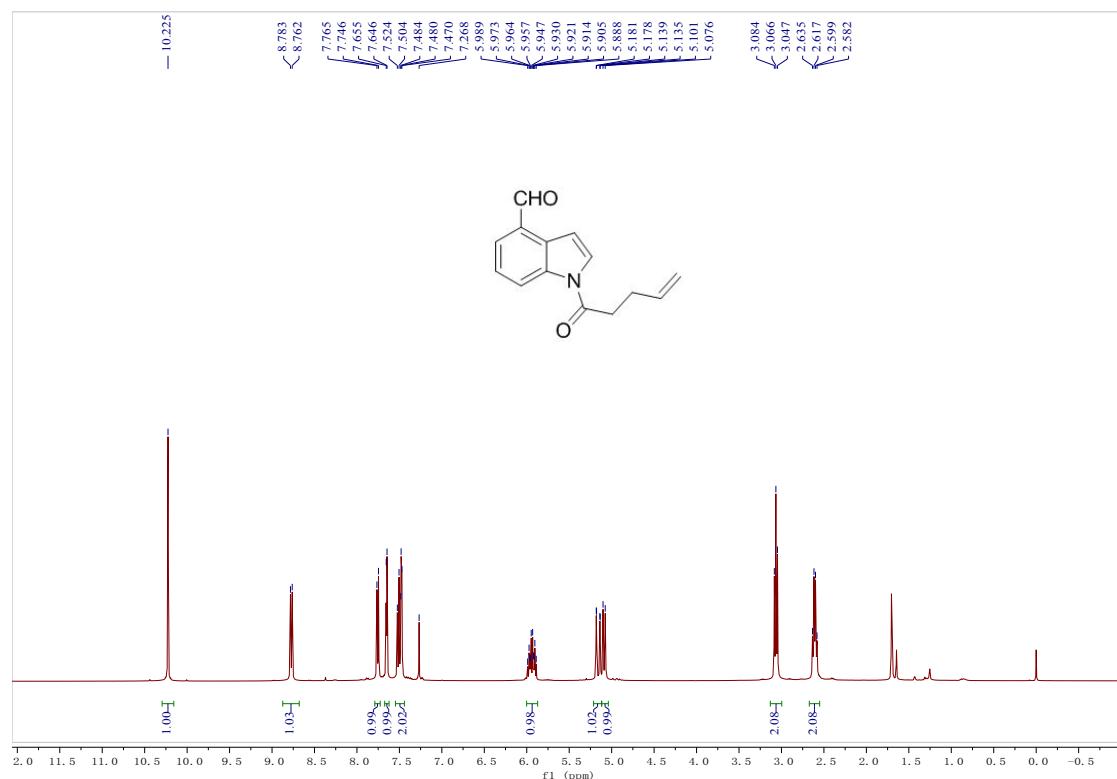
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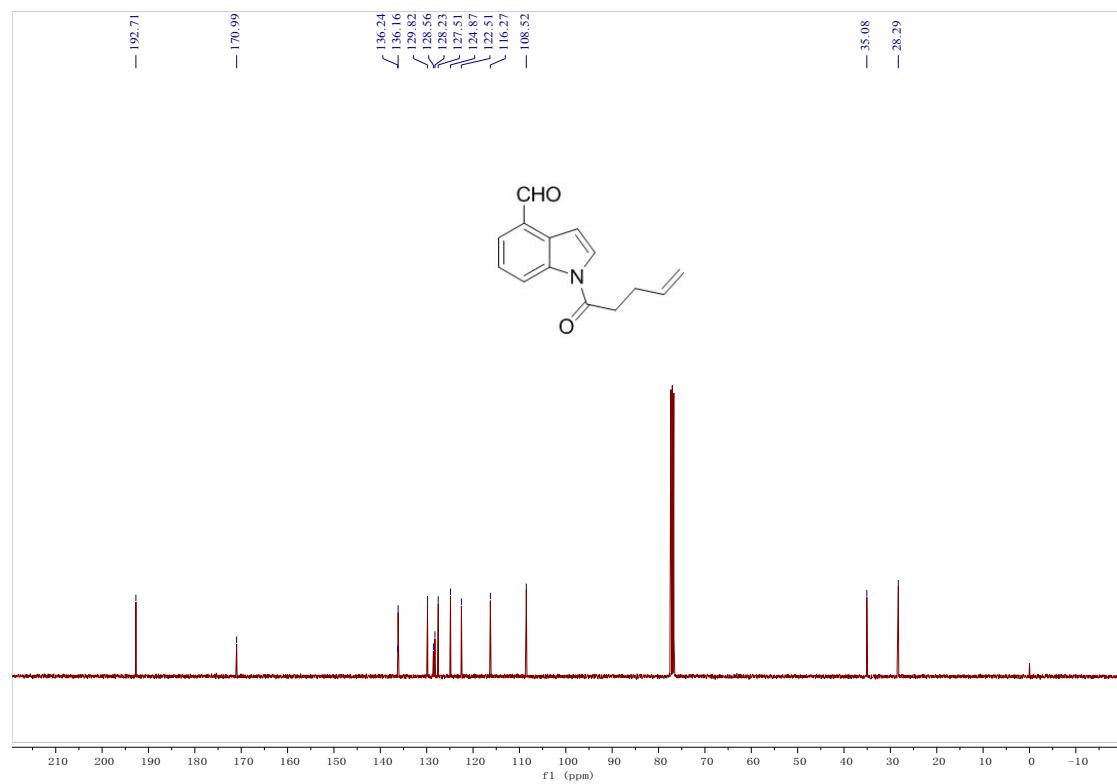
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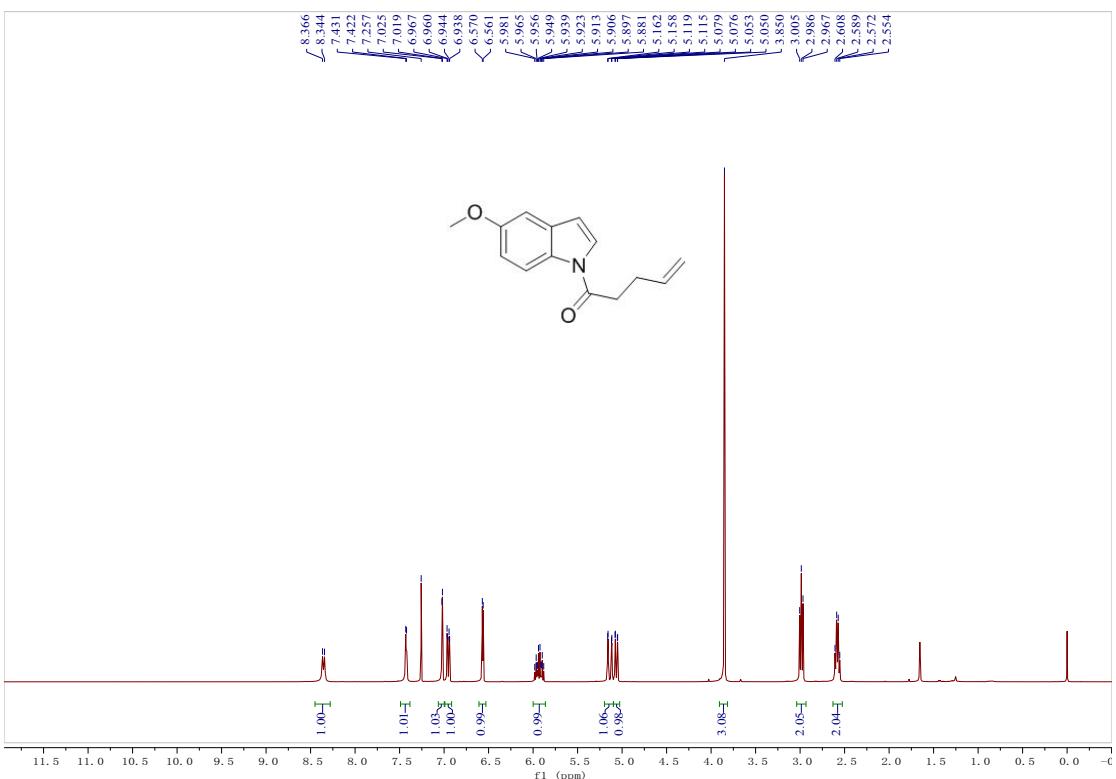
¹H NMR spectrum of **1c**



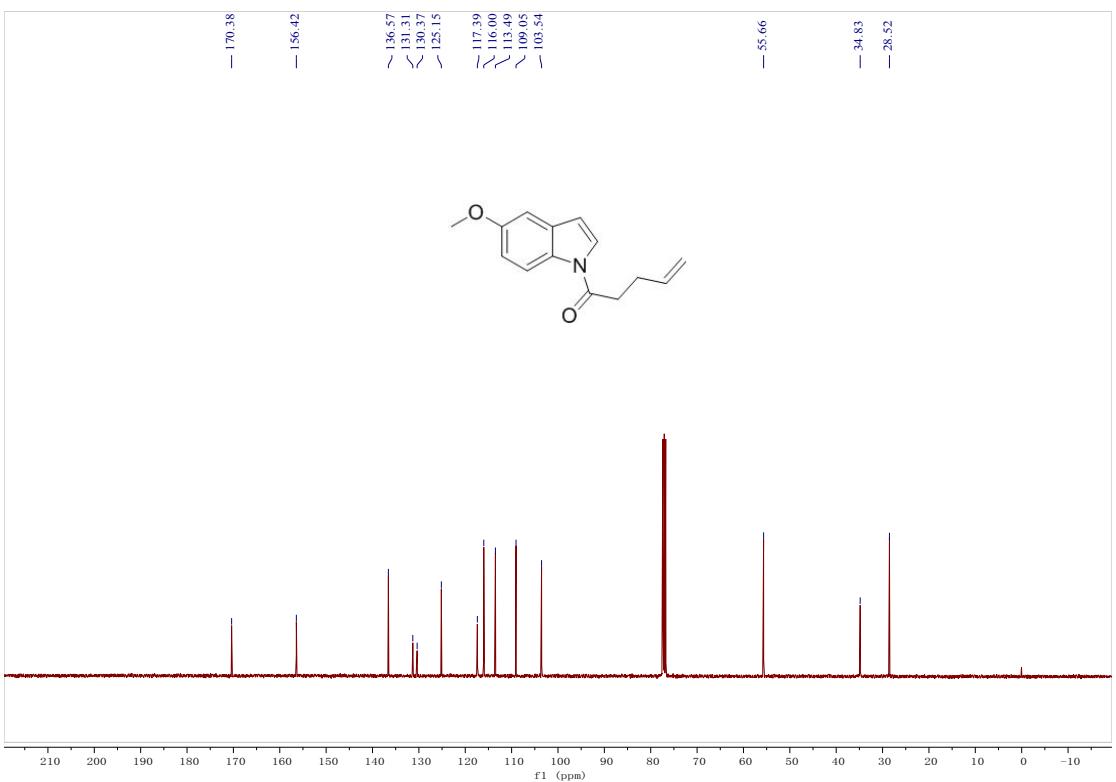
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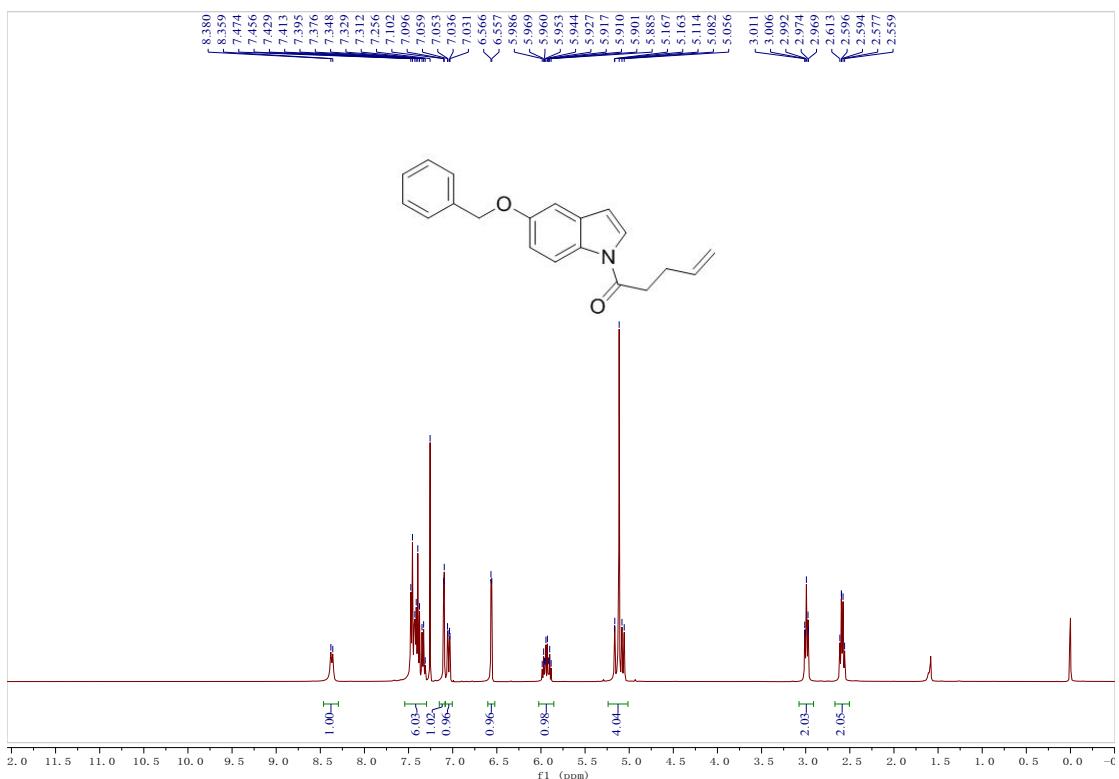
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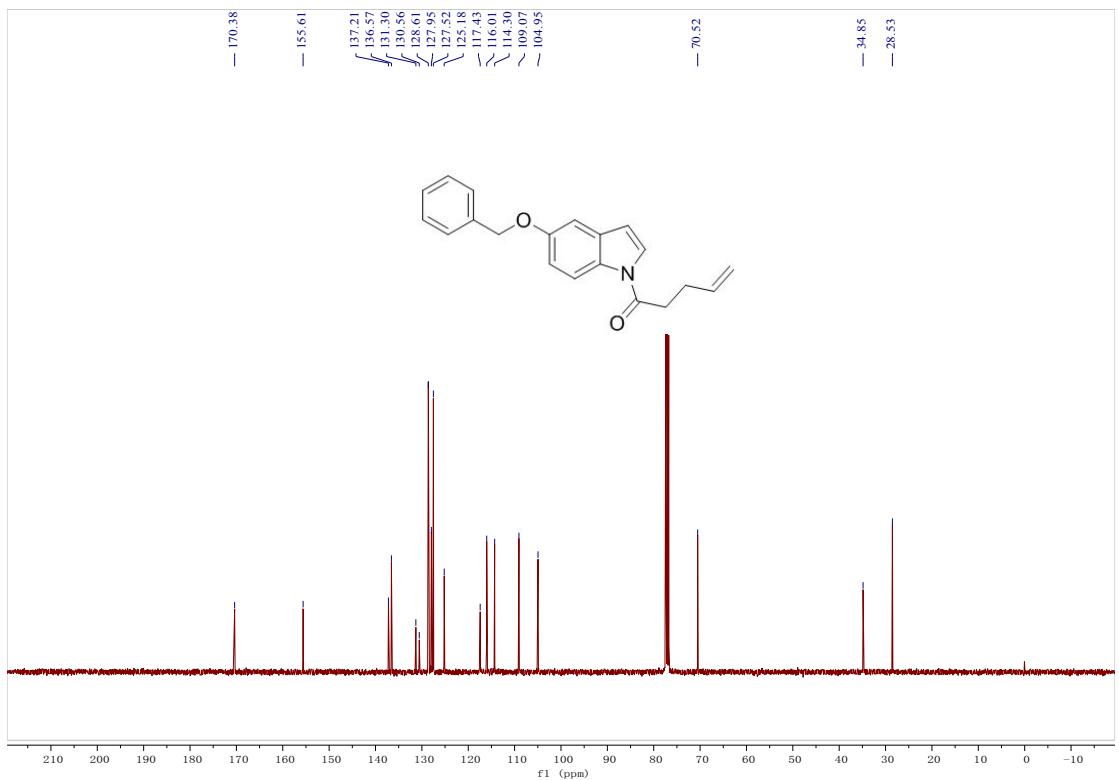
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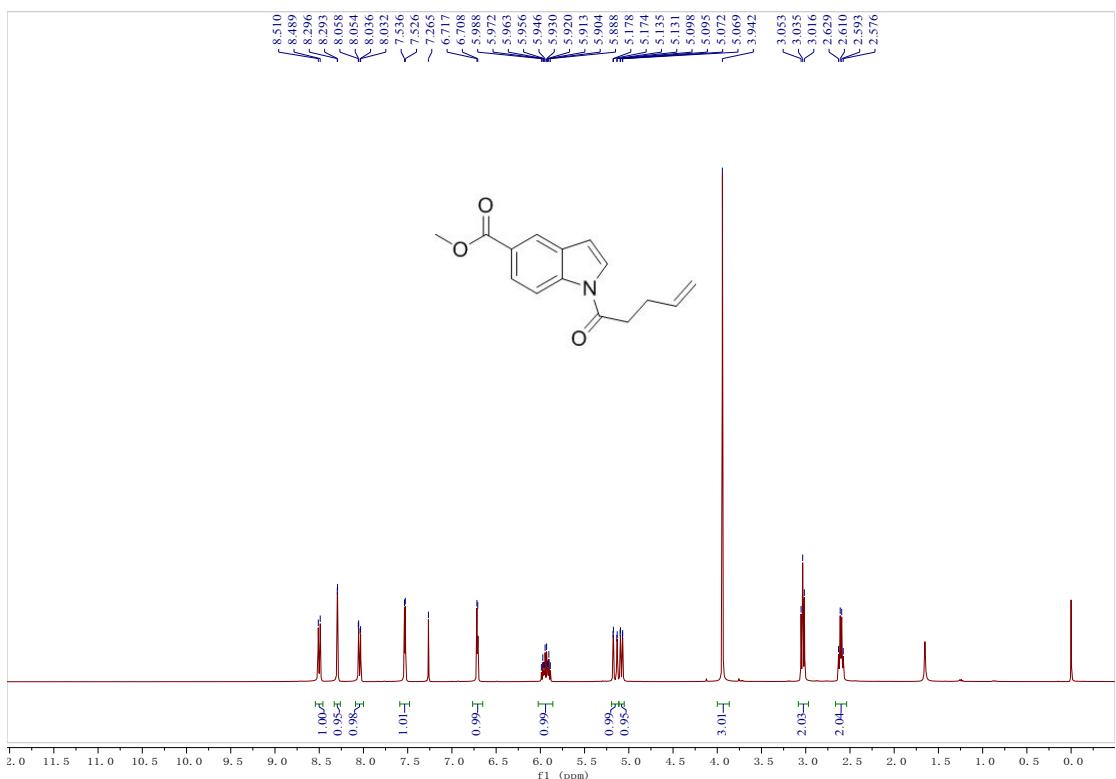
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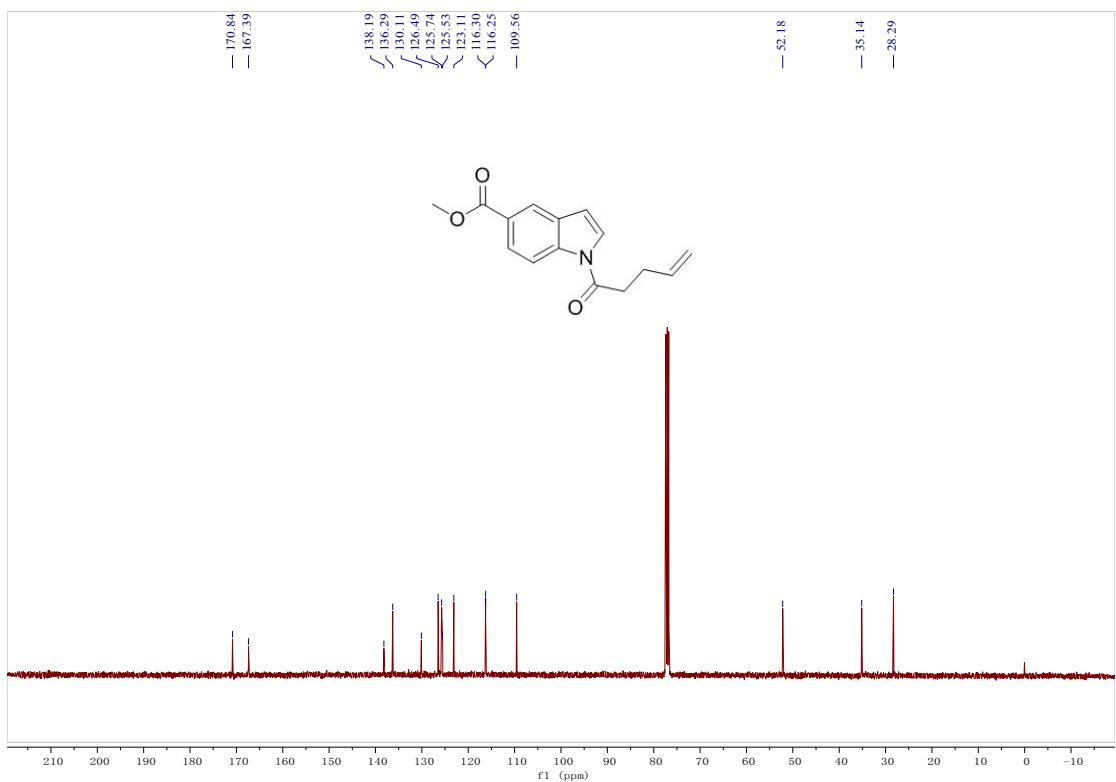
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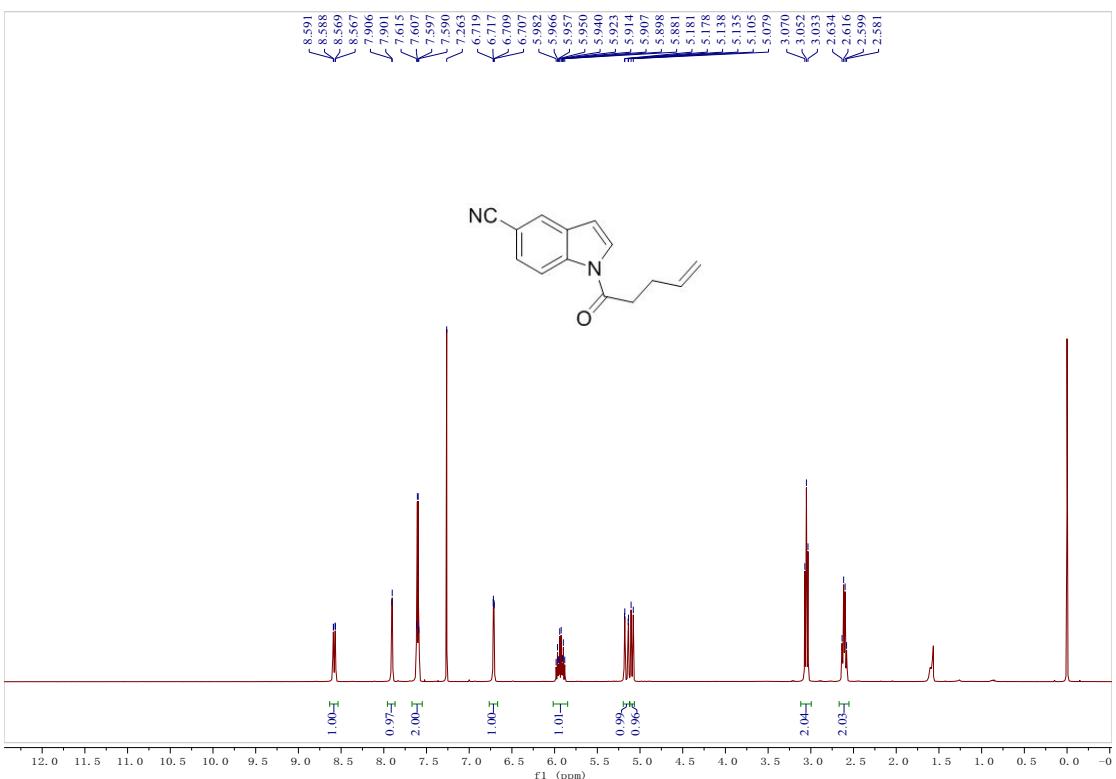
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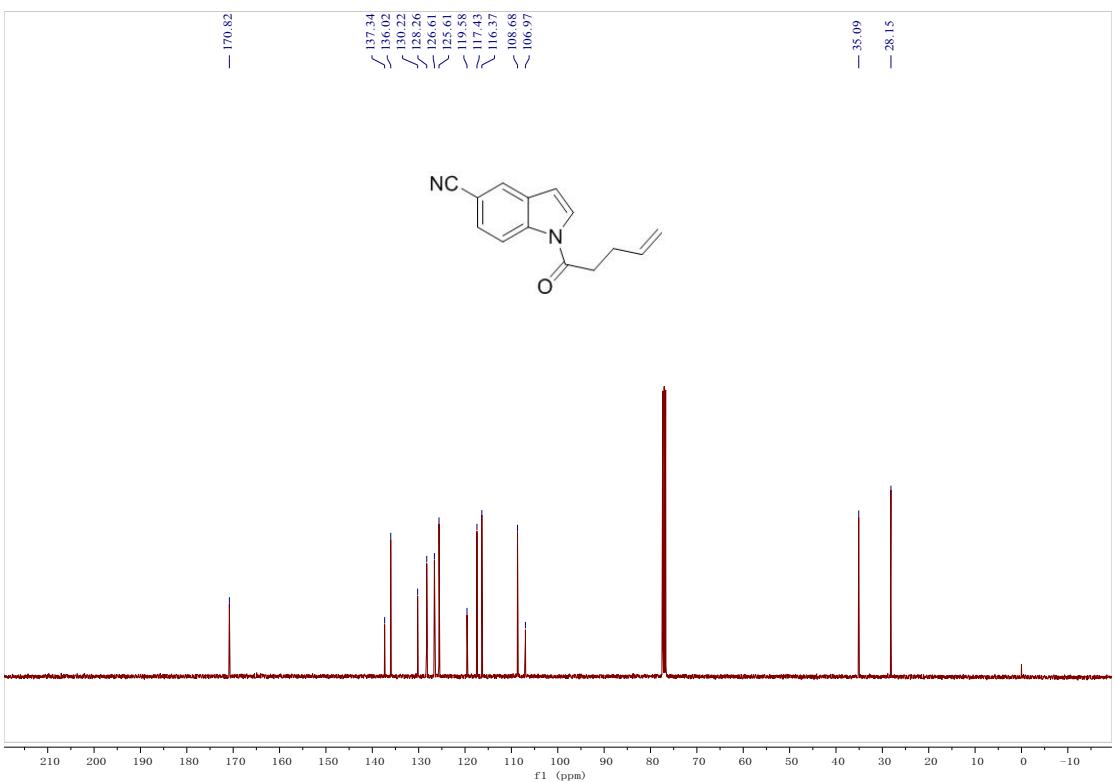
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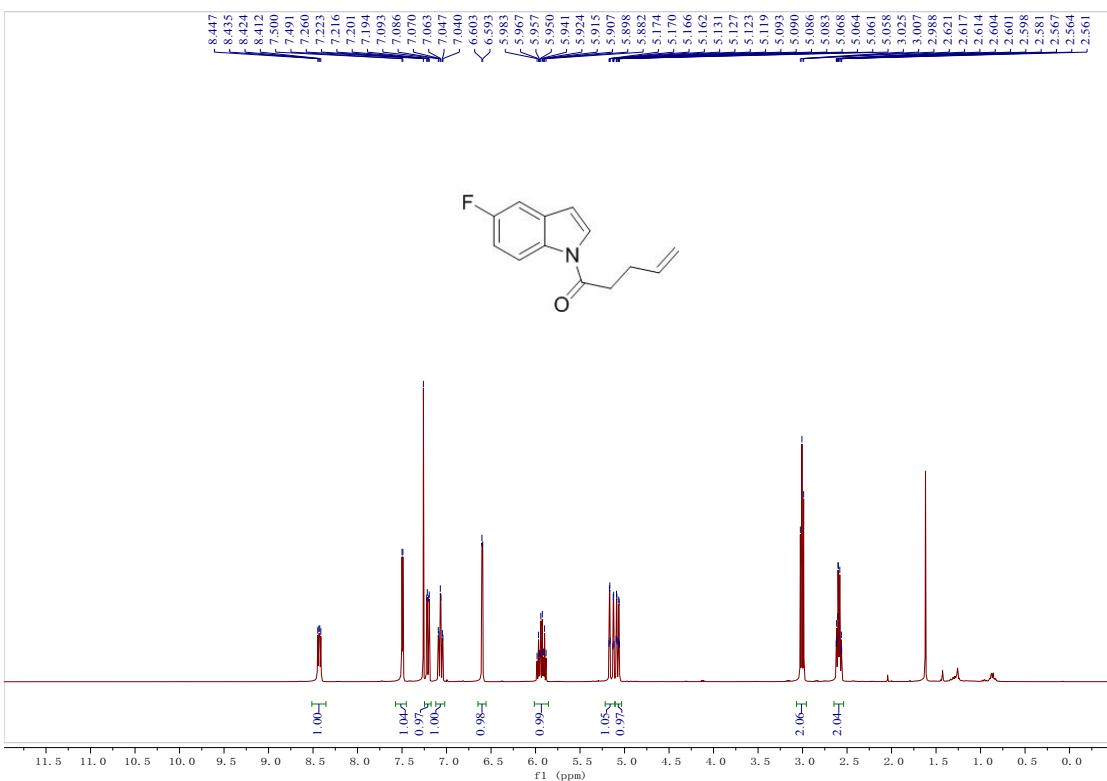
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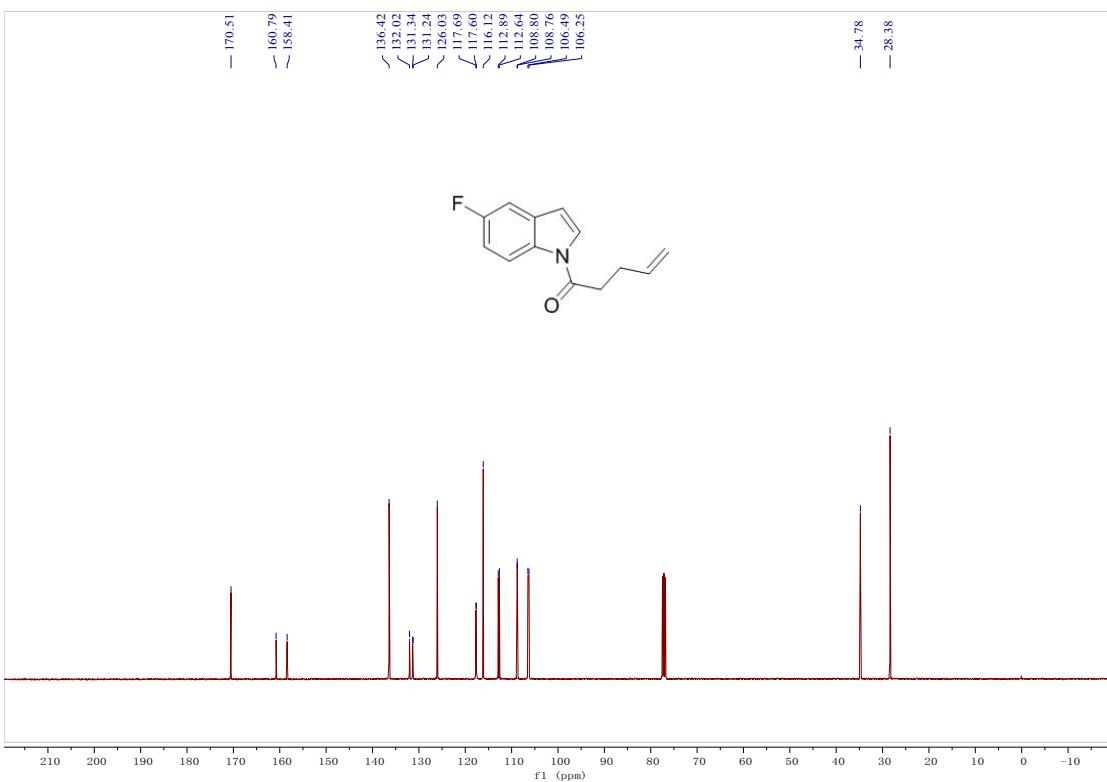
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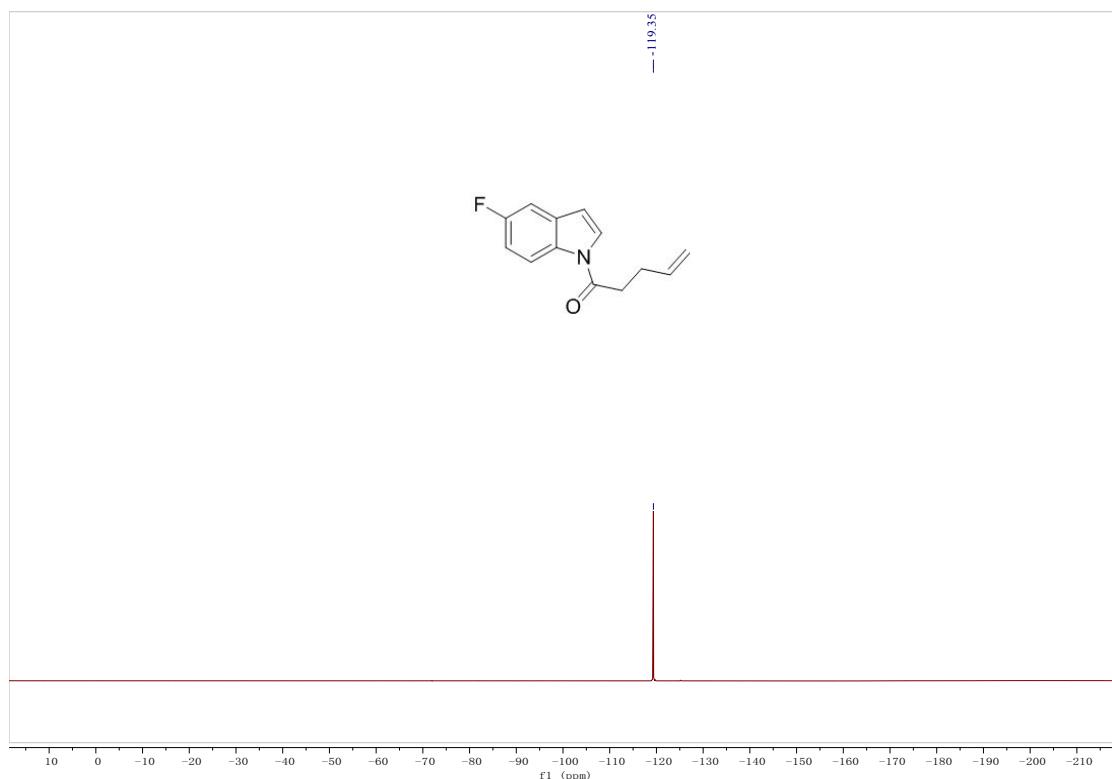
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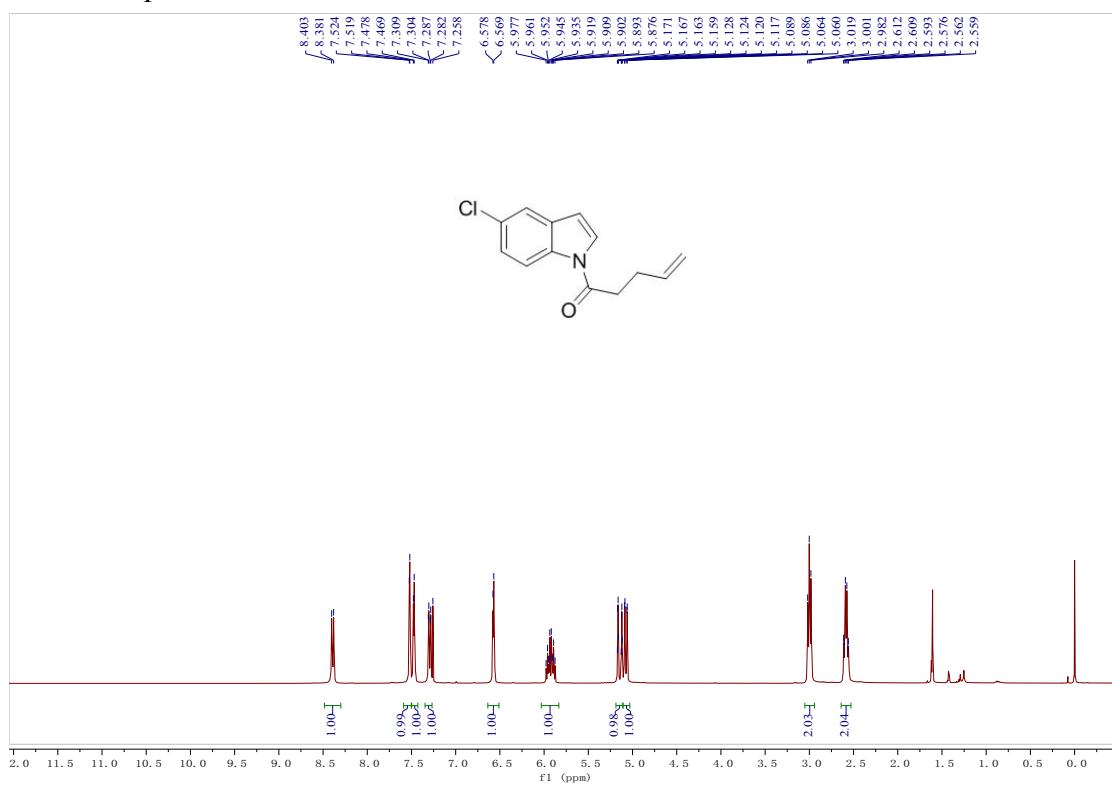
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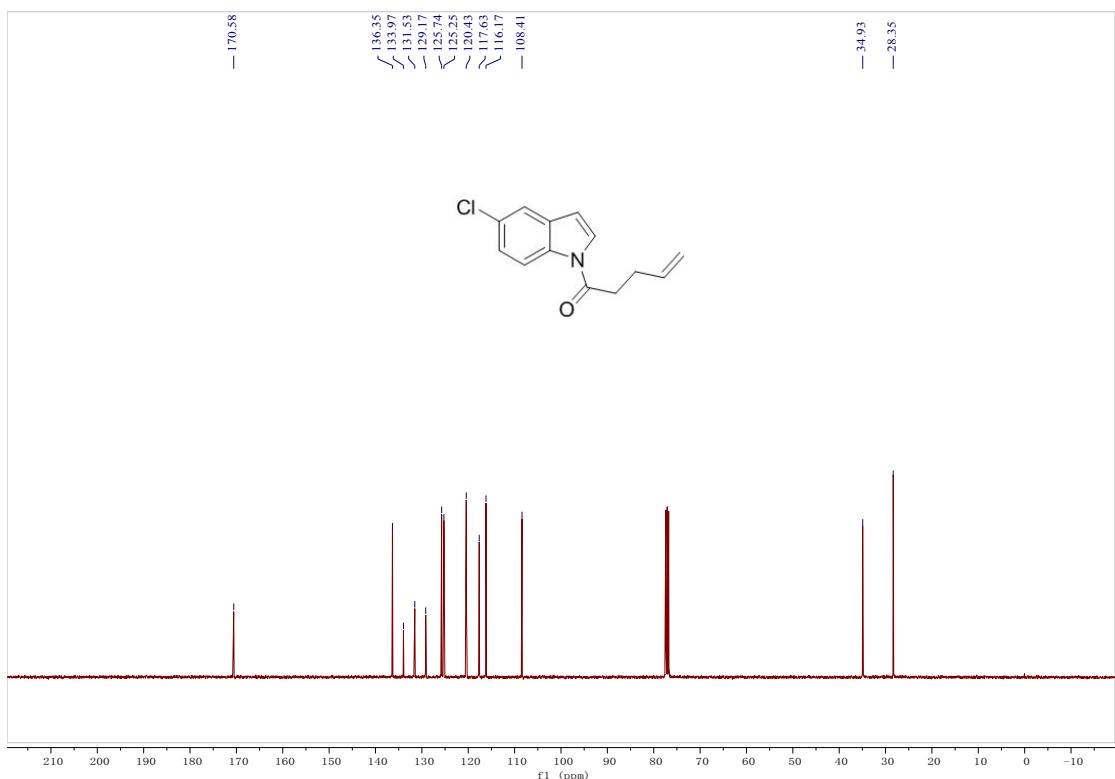
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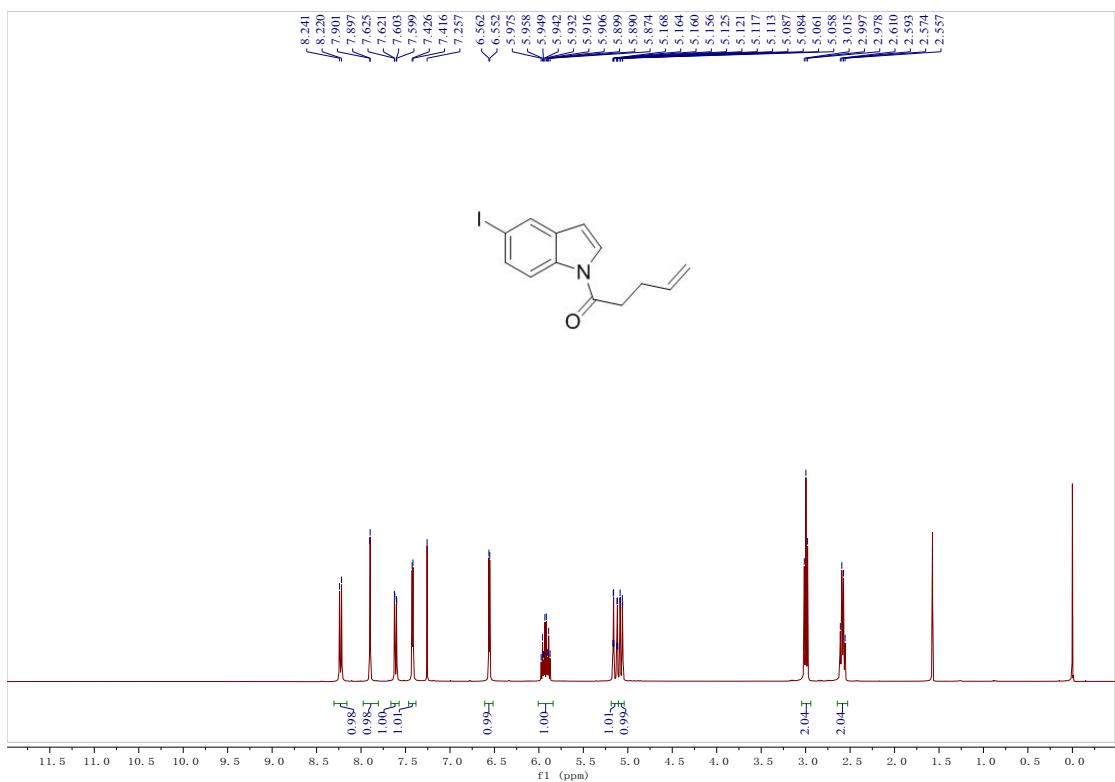
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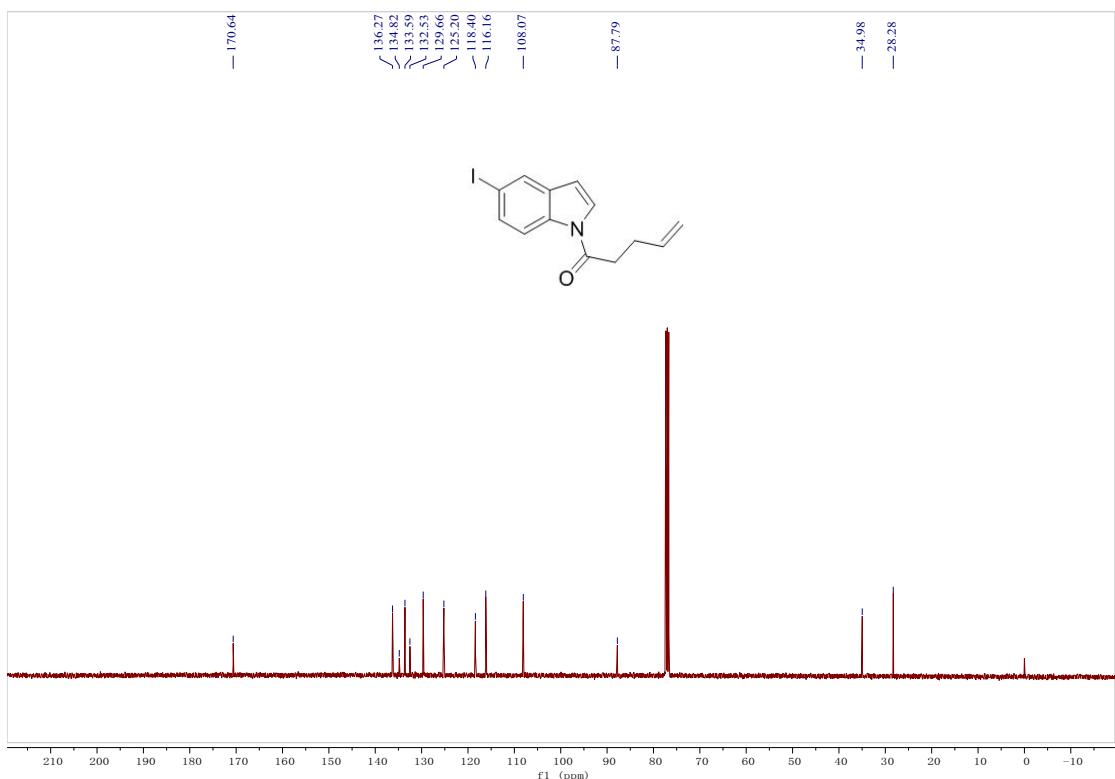
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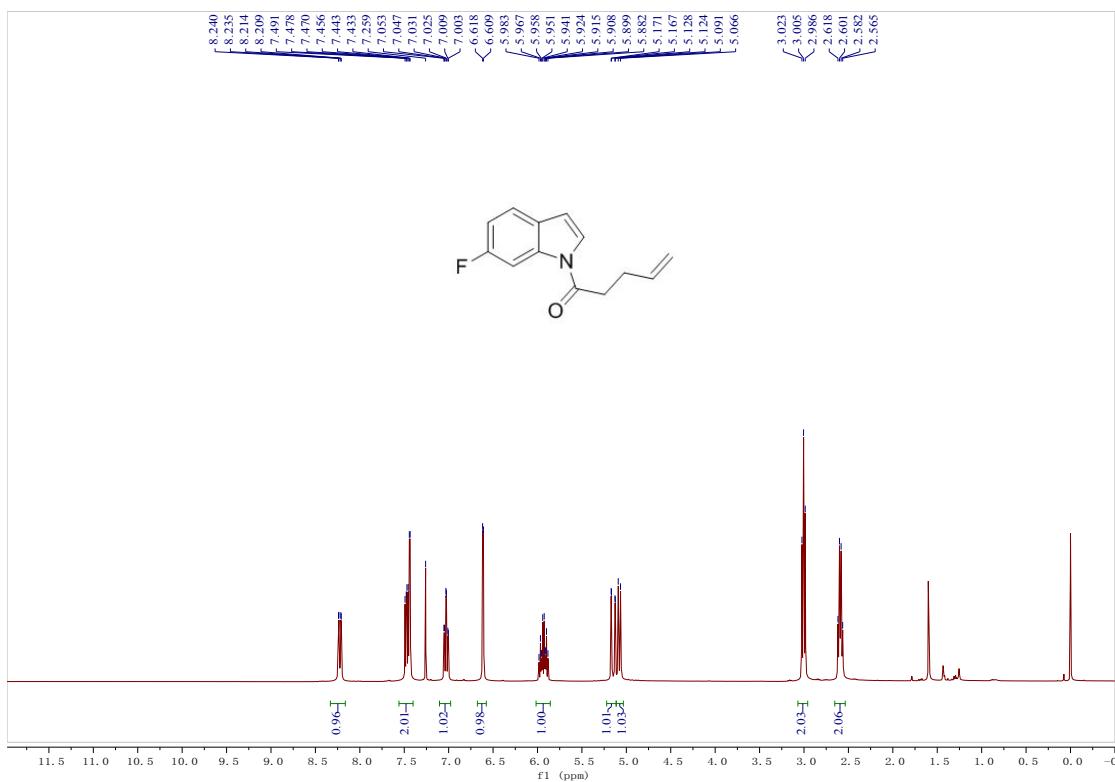
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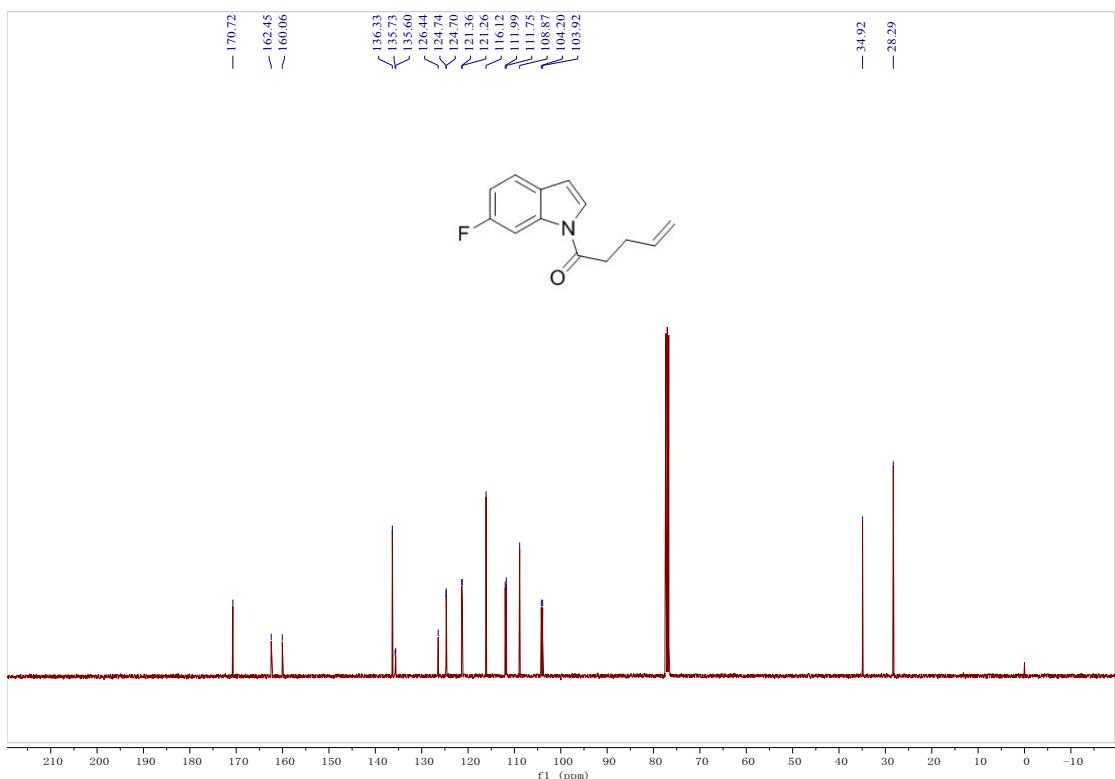
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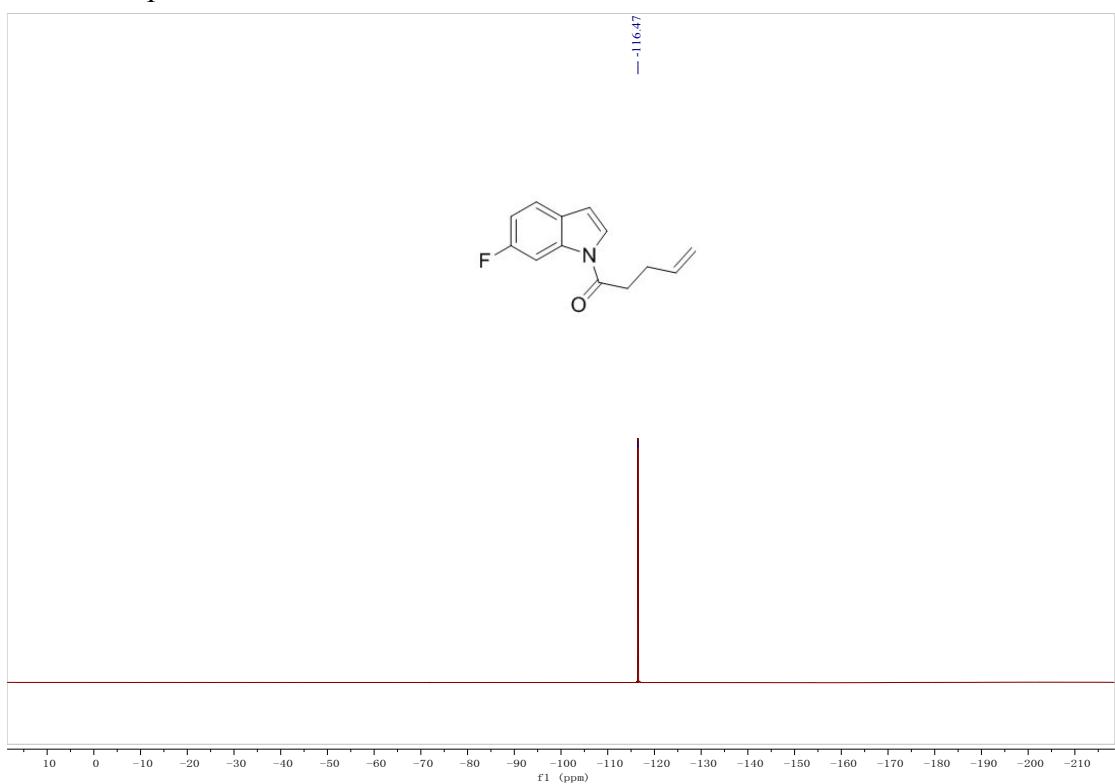
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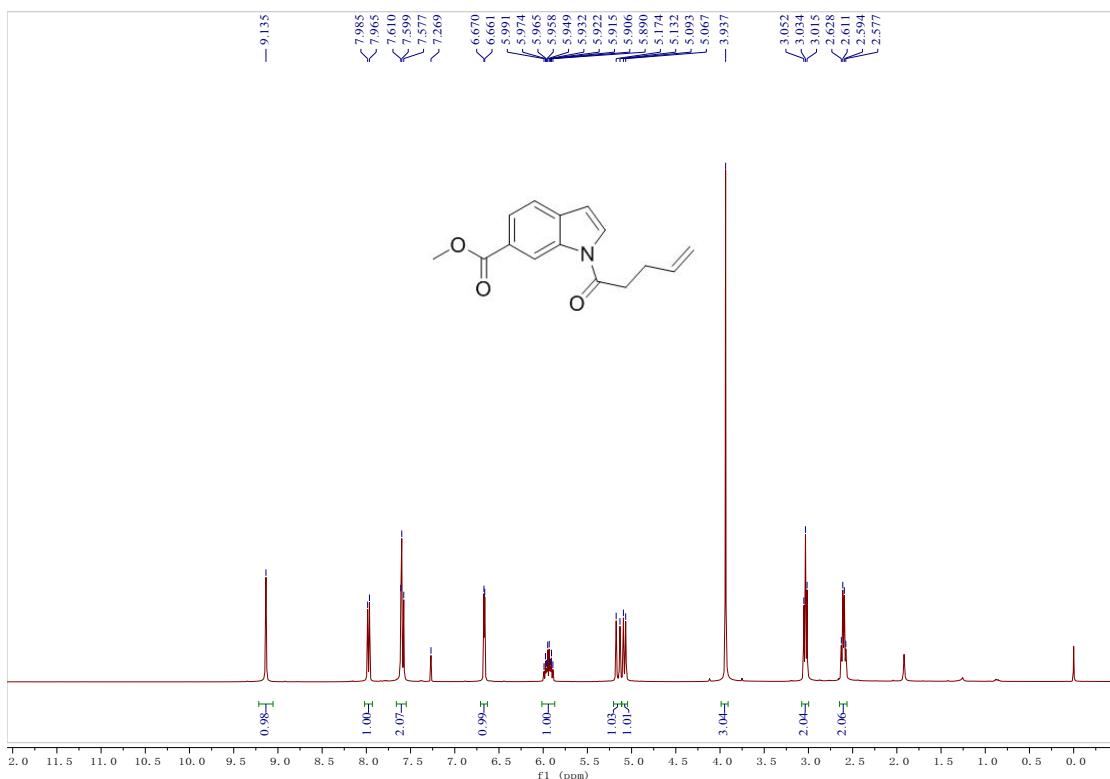
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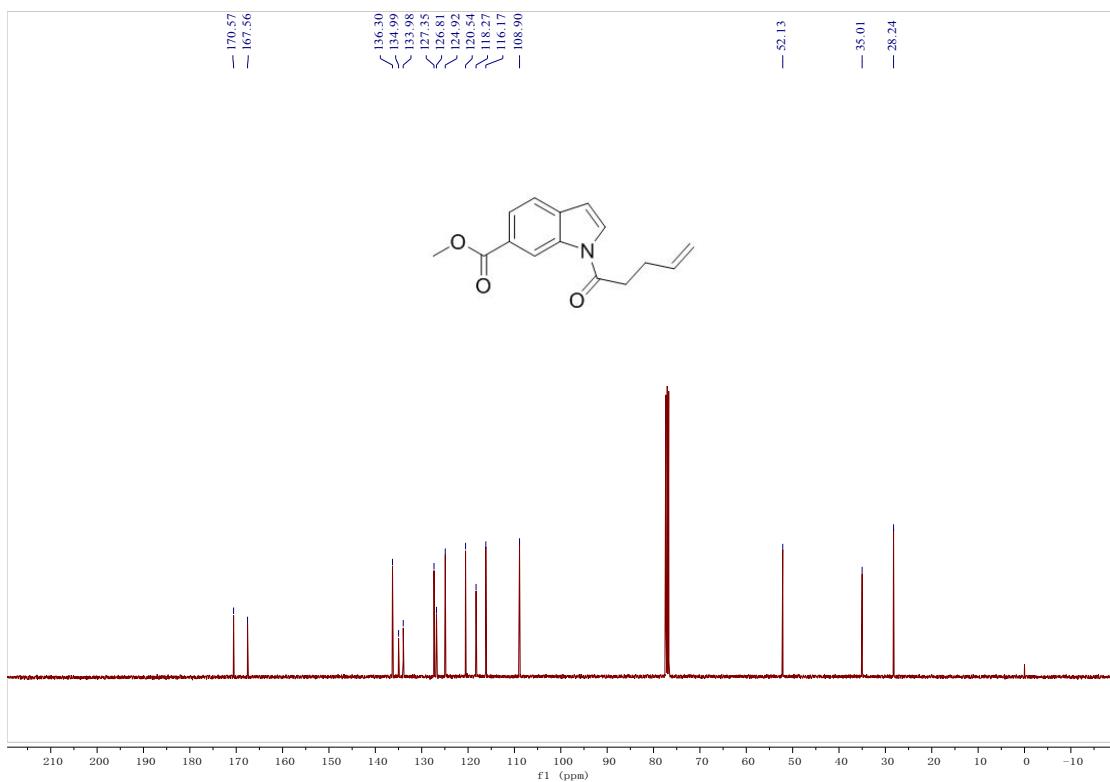
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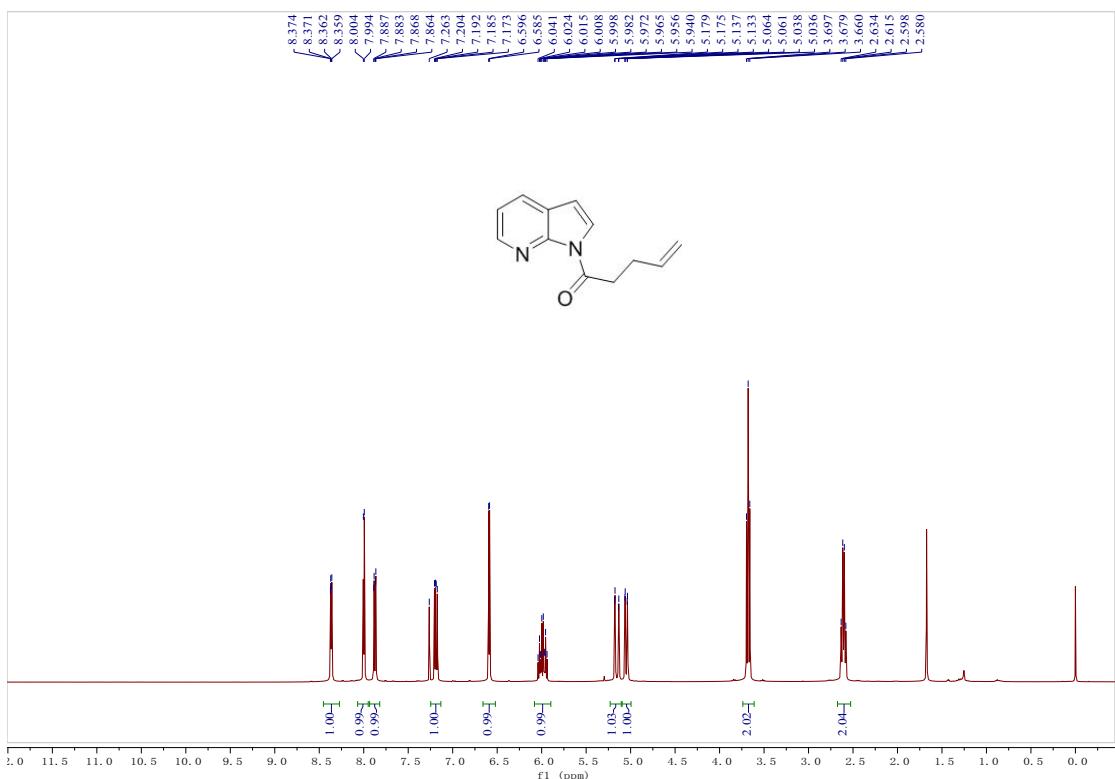
¹H NMR spectrum of **1I**



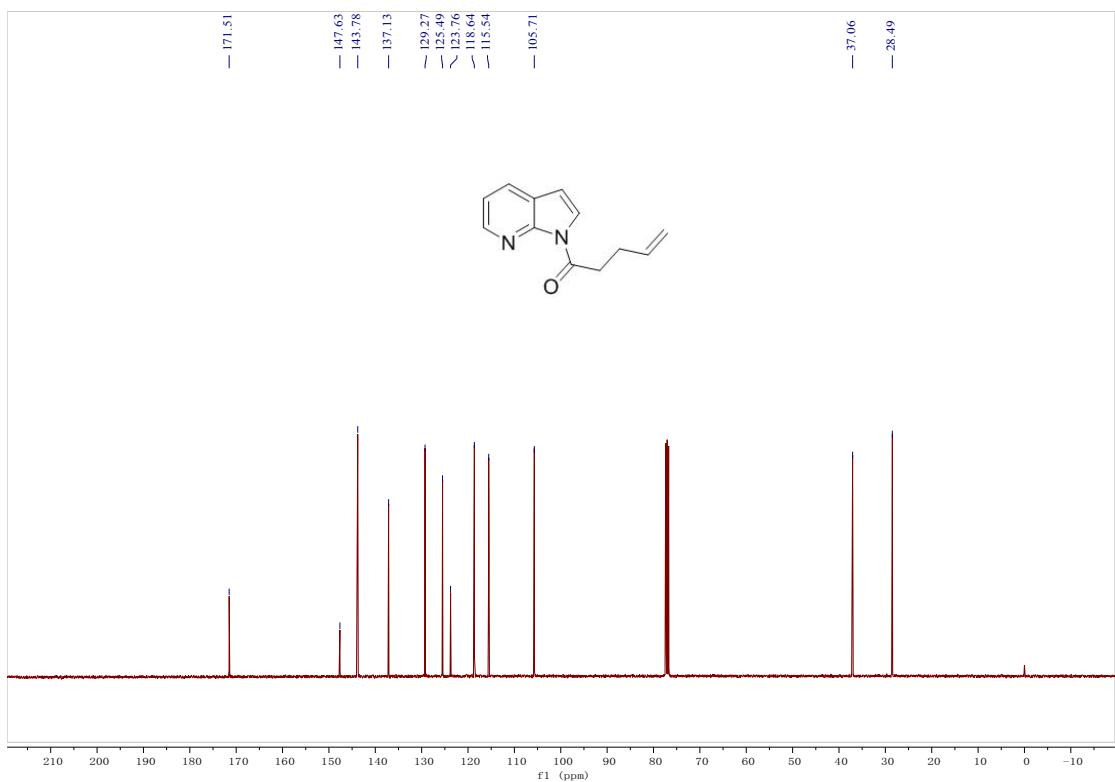
¹³C NMR spectrum of **1I**



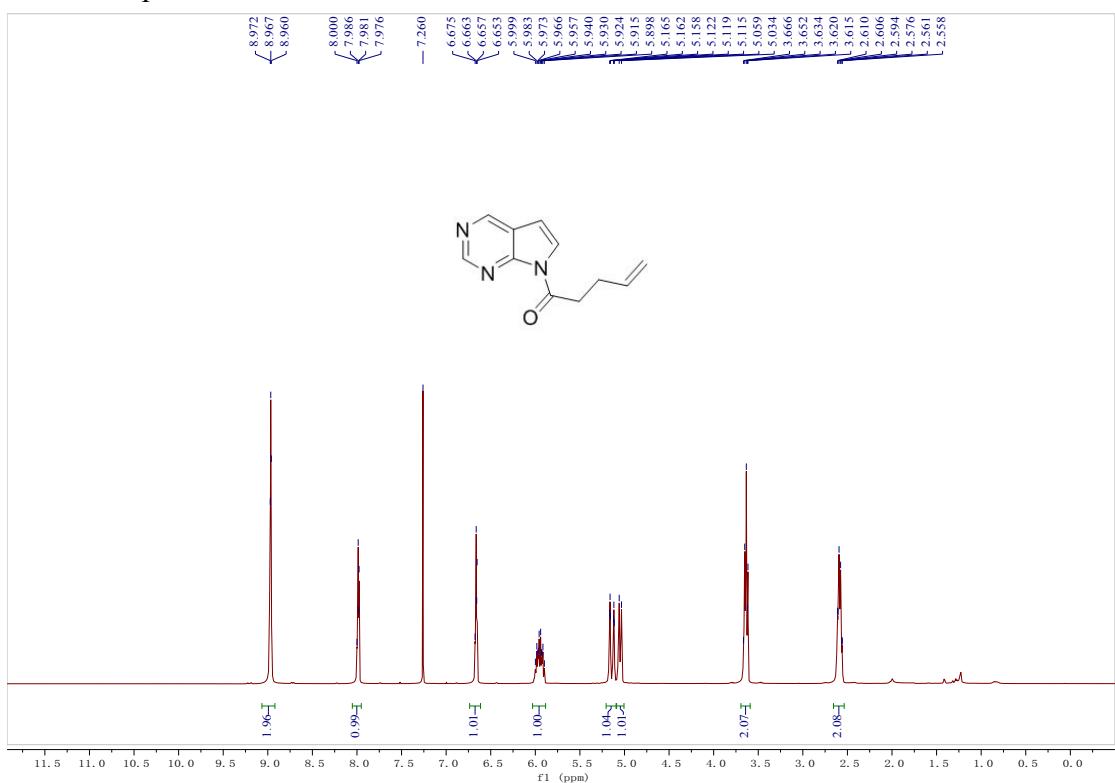
¹H NMR spectrum of **1m**



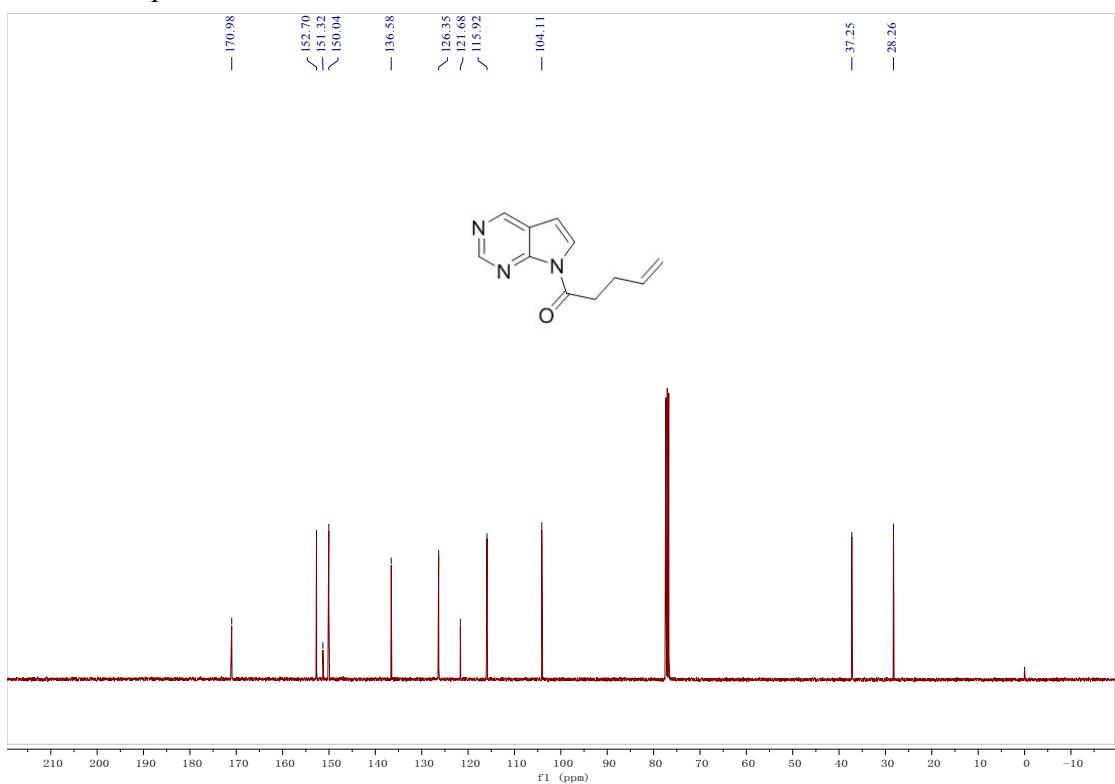
¹³C NMR spectrum of **1m**



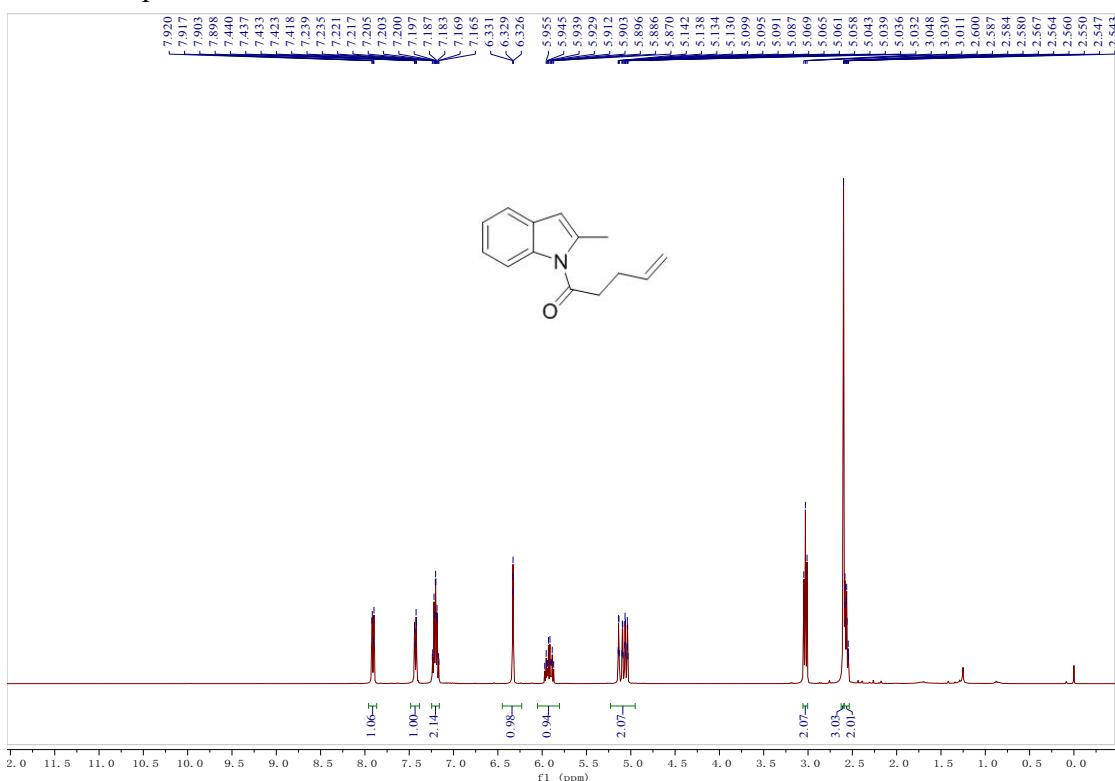
¹H NMR spectrum of **1n**



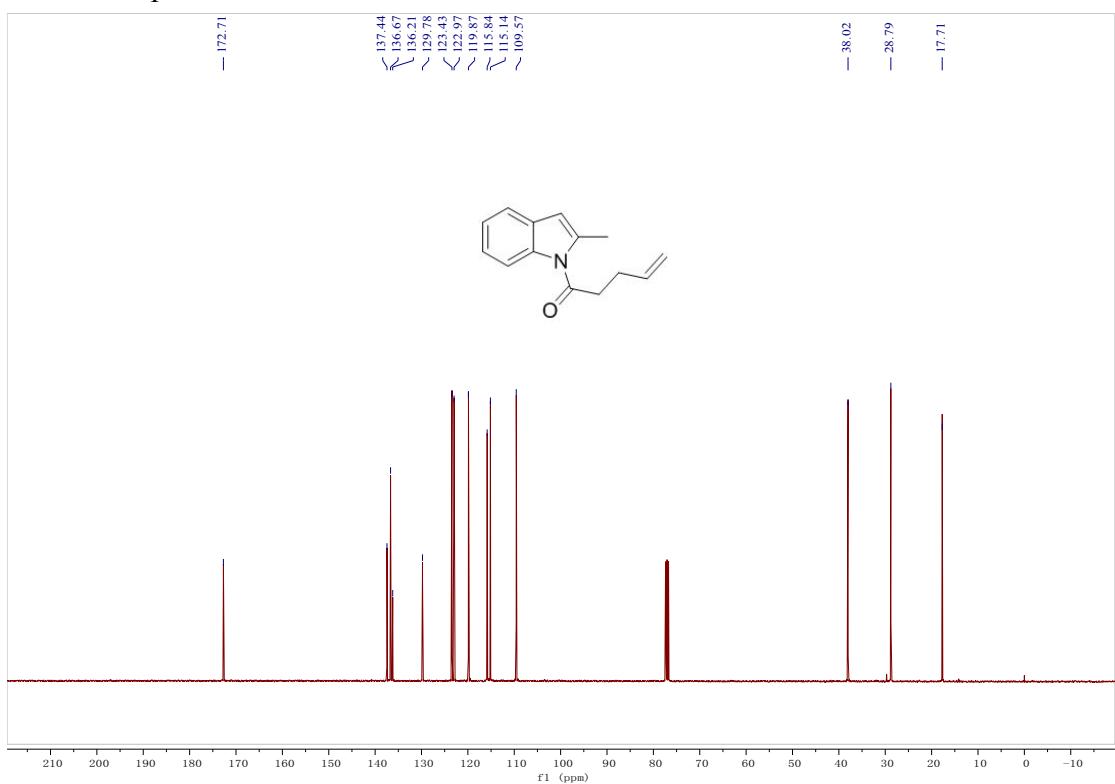
¹³C NMR spectrum of **1n**



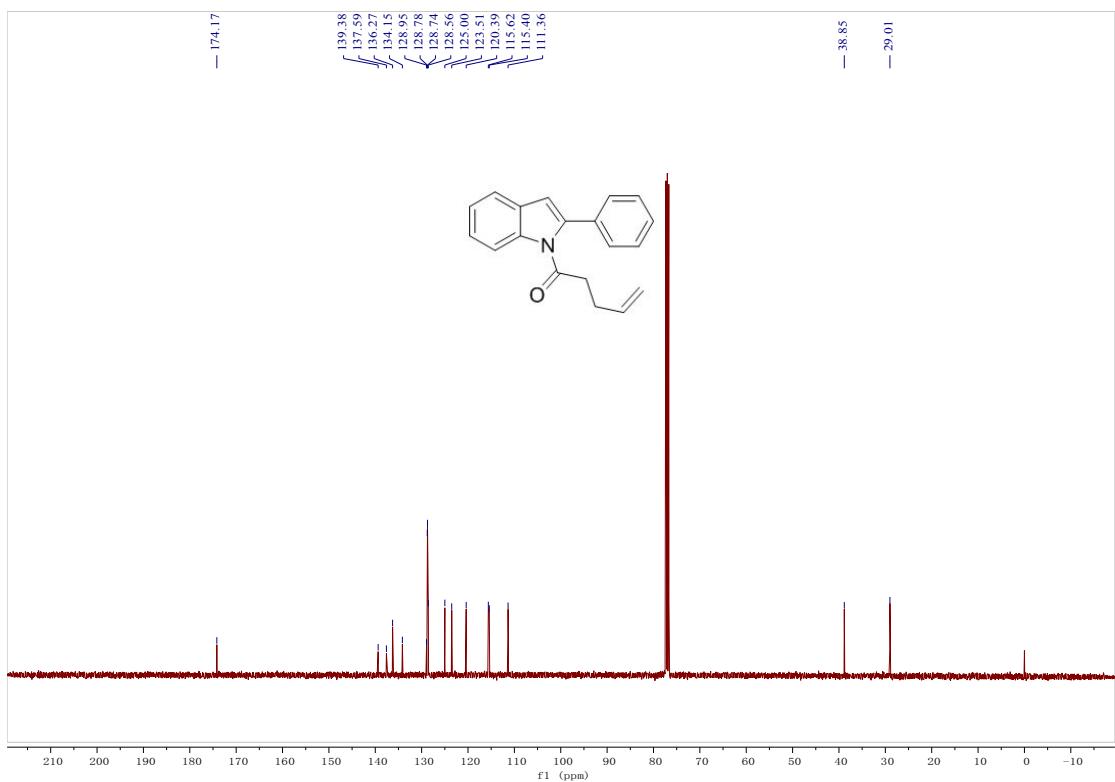
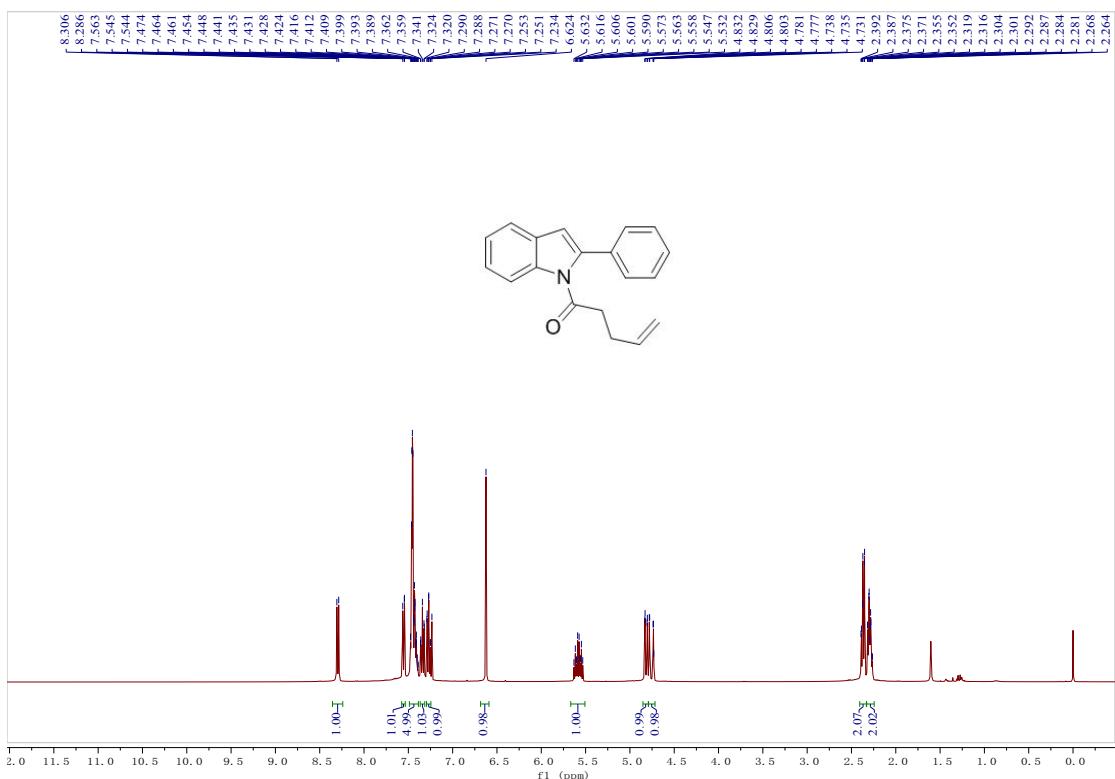
¹H NMR spectrum of **1o**



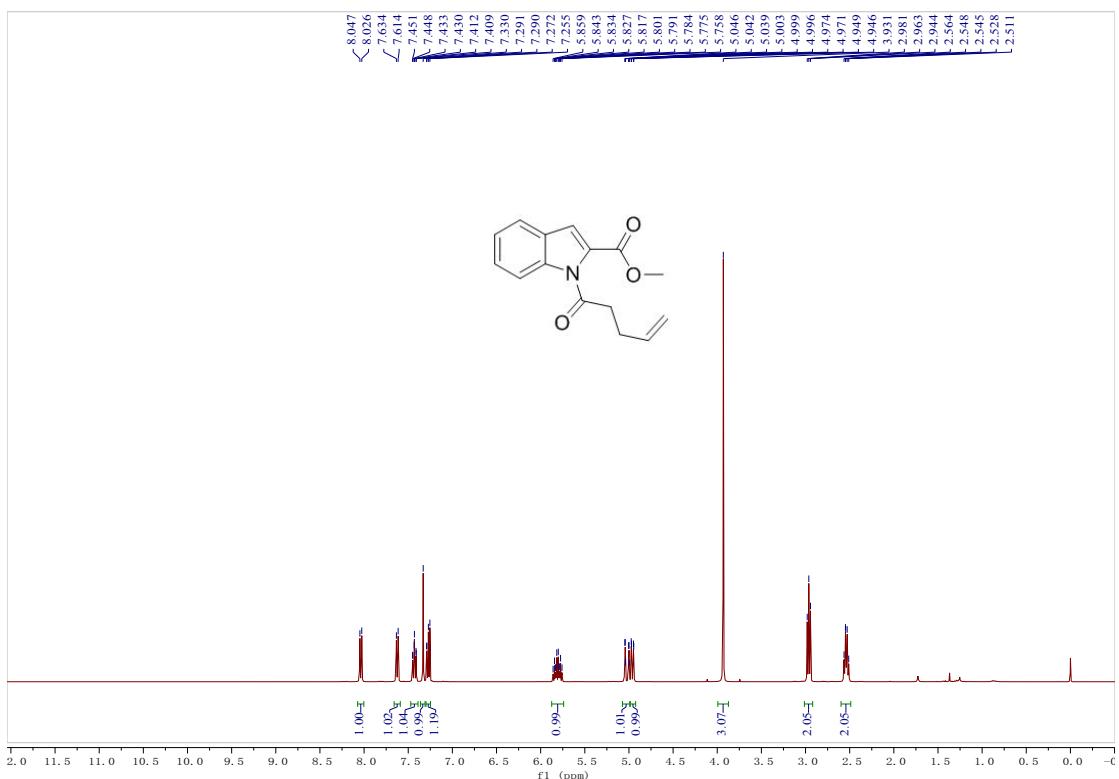
¹³C NMR spectrum of **1o**



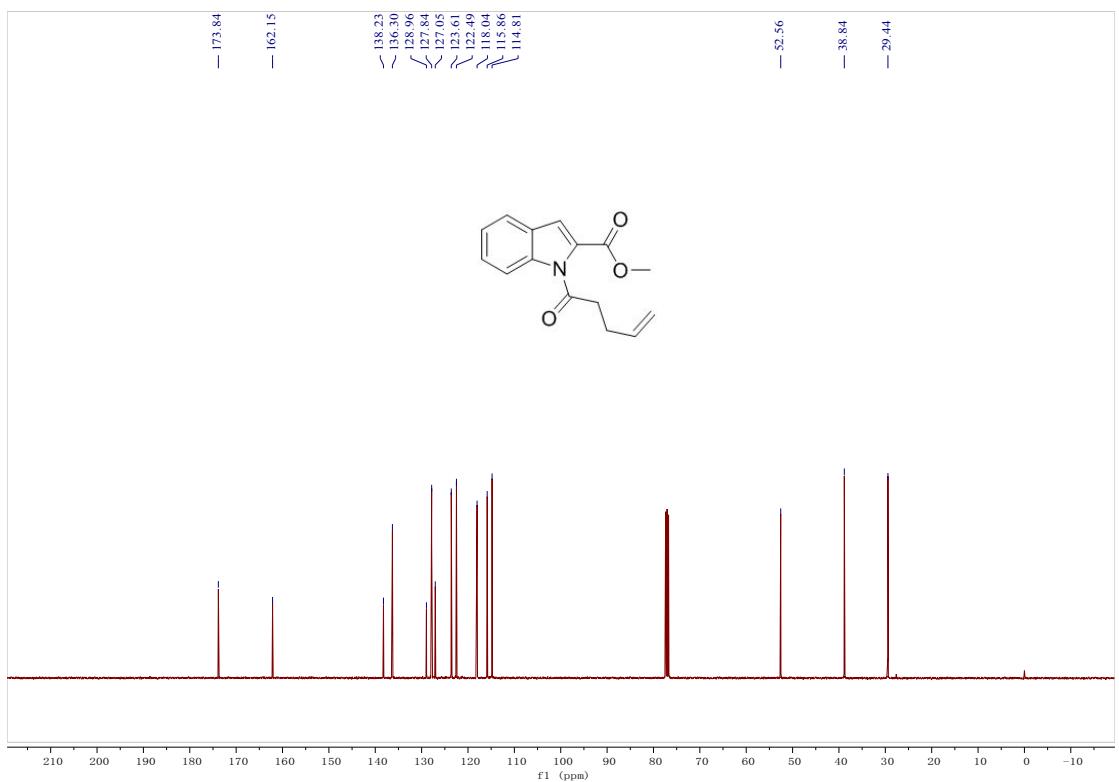
¹H NMR spectrum of **1p**



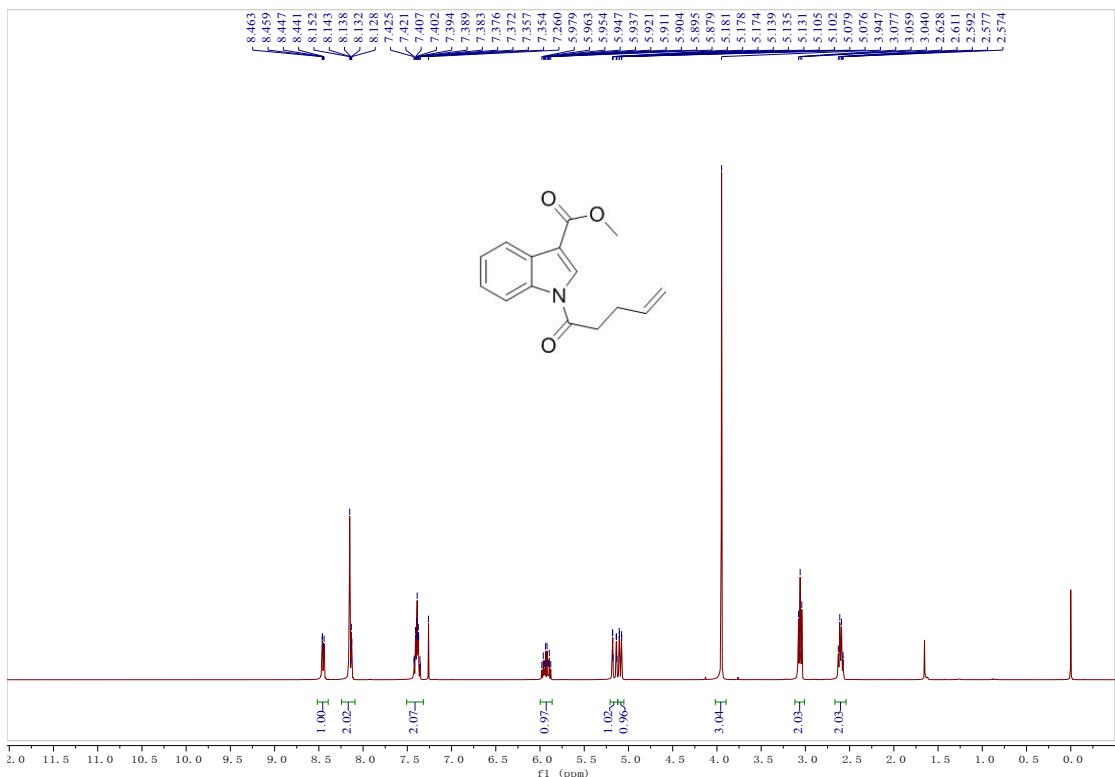
¹H NMR spectrum of **1q**



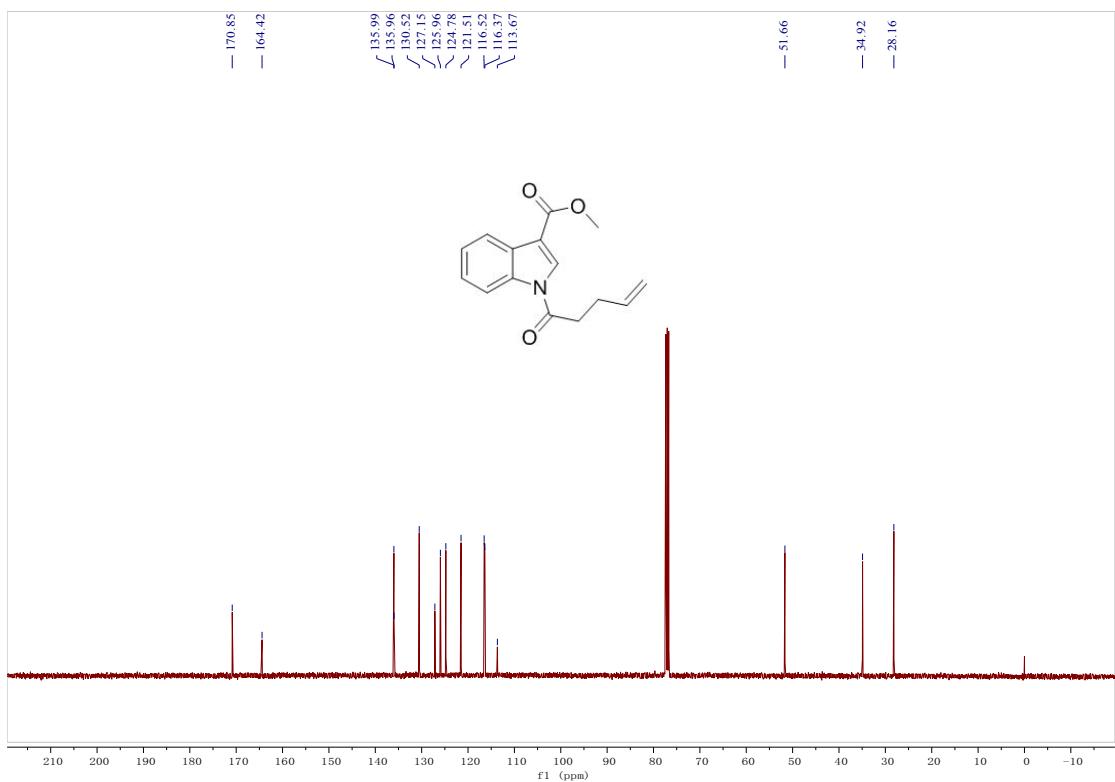
¹³C NMR spectrum of **1q**



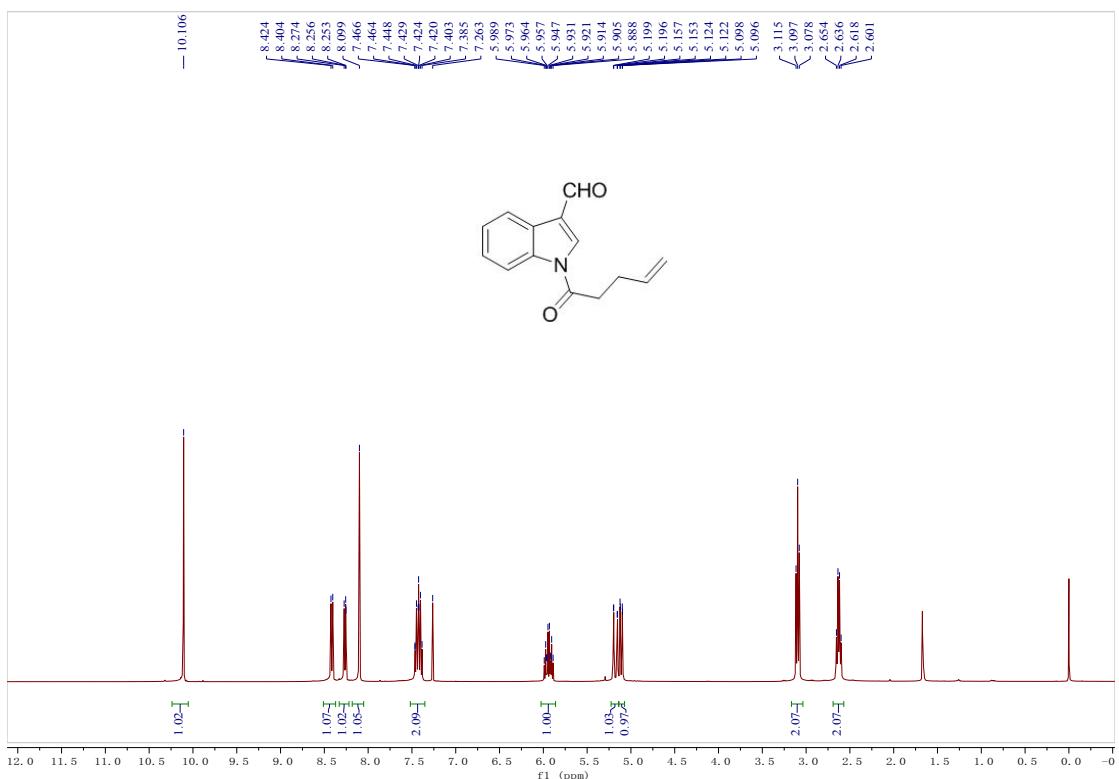
¹H NMR spectrum of **1r**



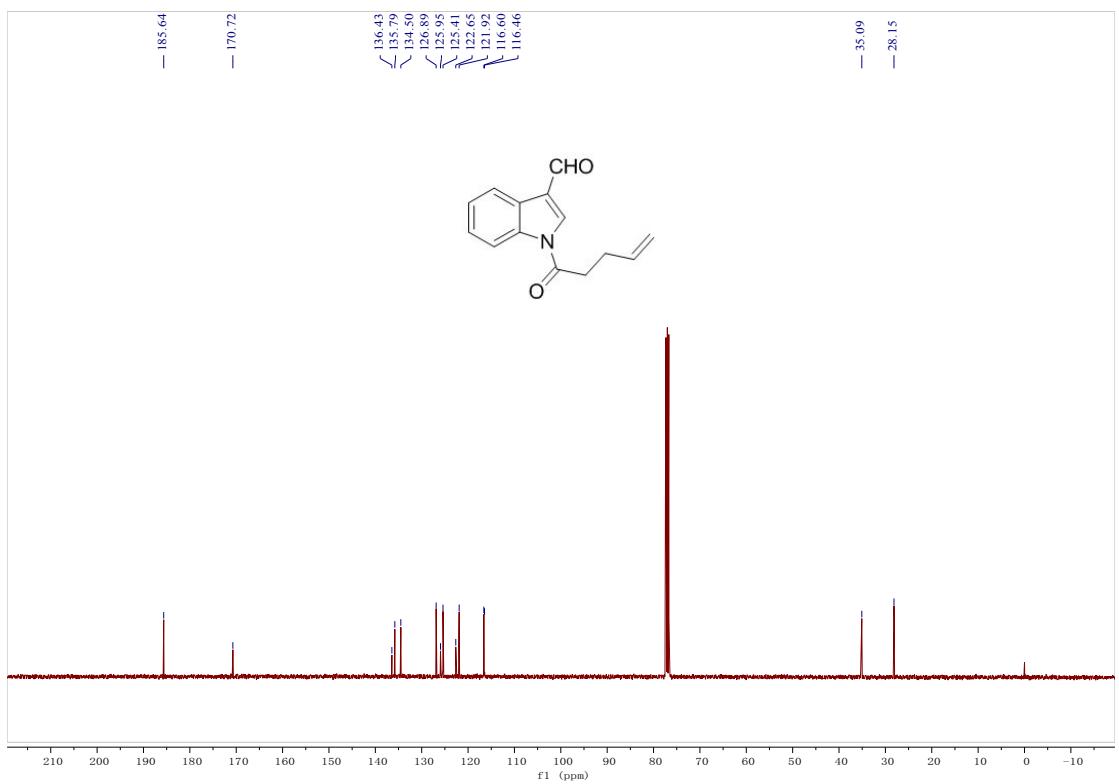
¹³C NMR spectrum of **1r**



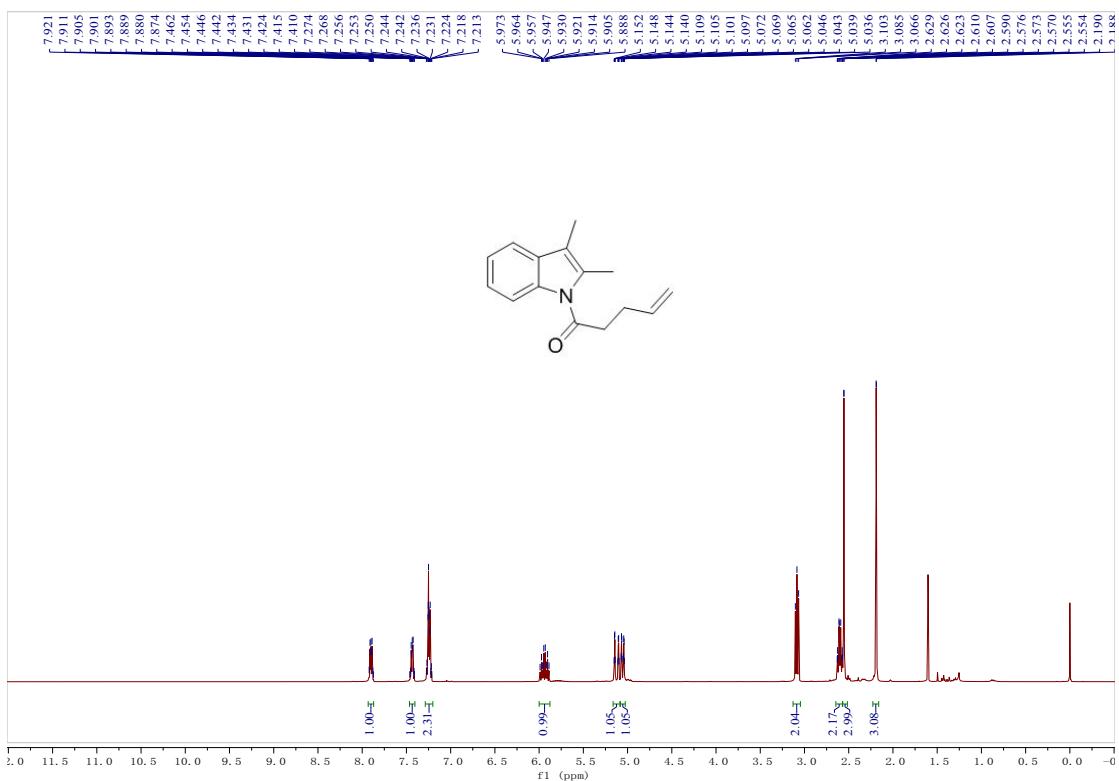
¹H NMR spectrum of **1s**



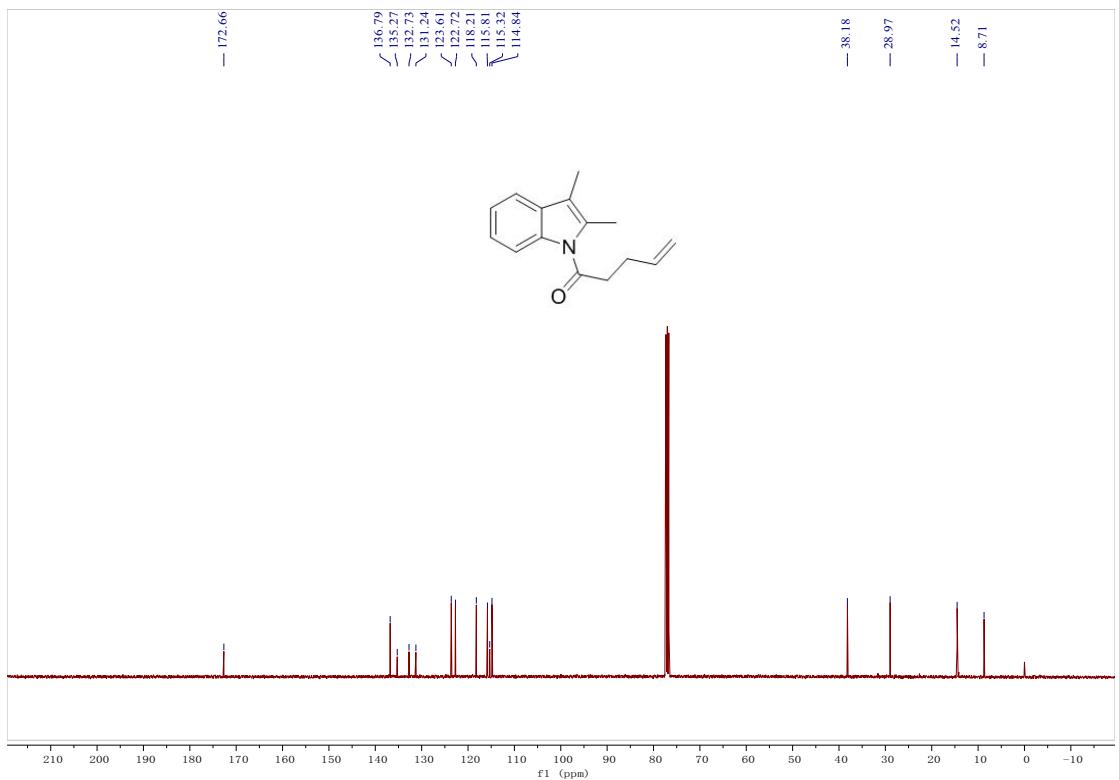
¹³C NMR spectrum of **1s**



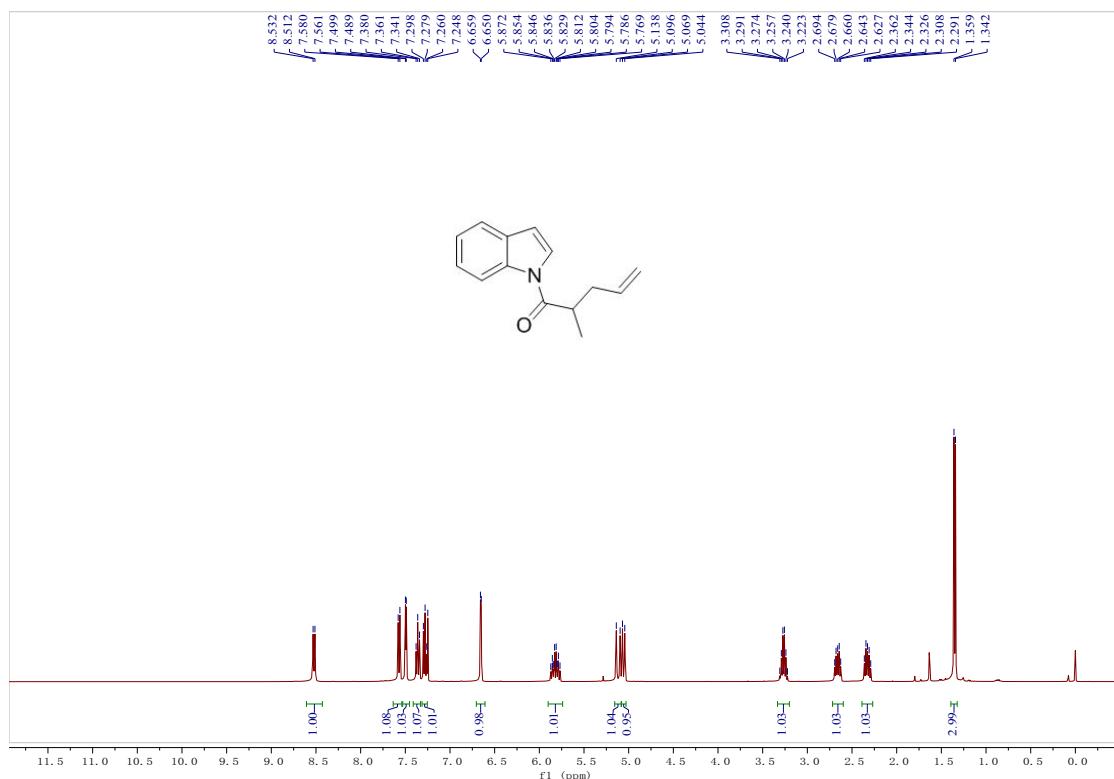
¹H NMR spectrum of **1t**



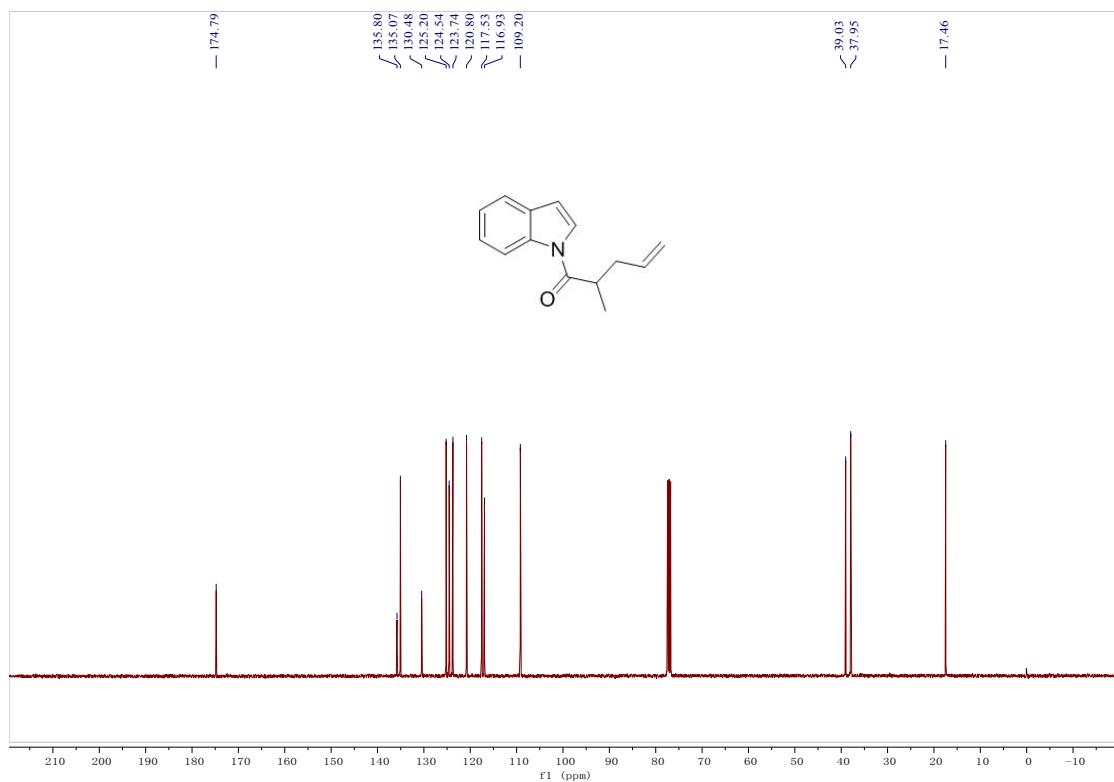
¹³C NMR spectrum of **1t**



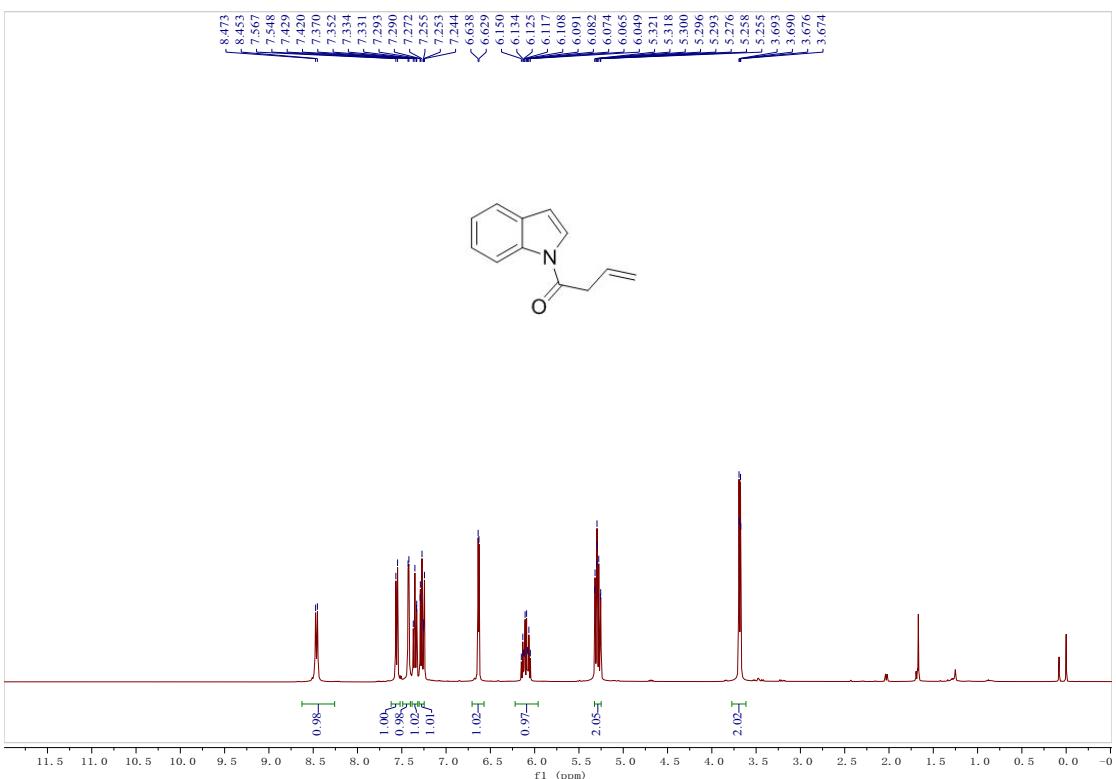
¹H NMR spectrum of **1u**



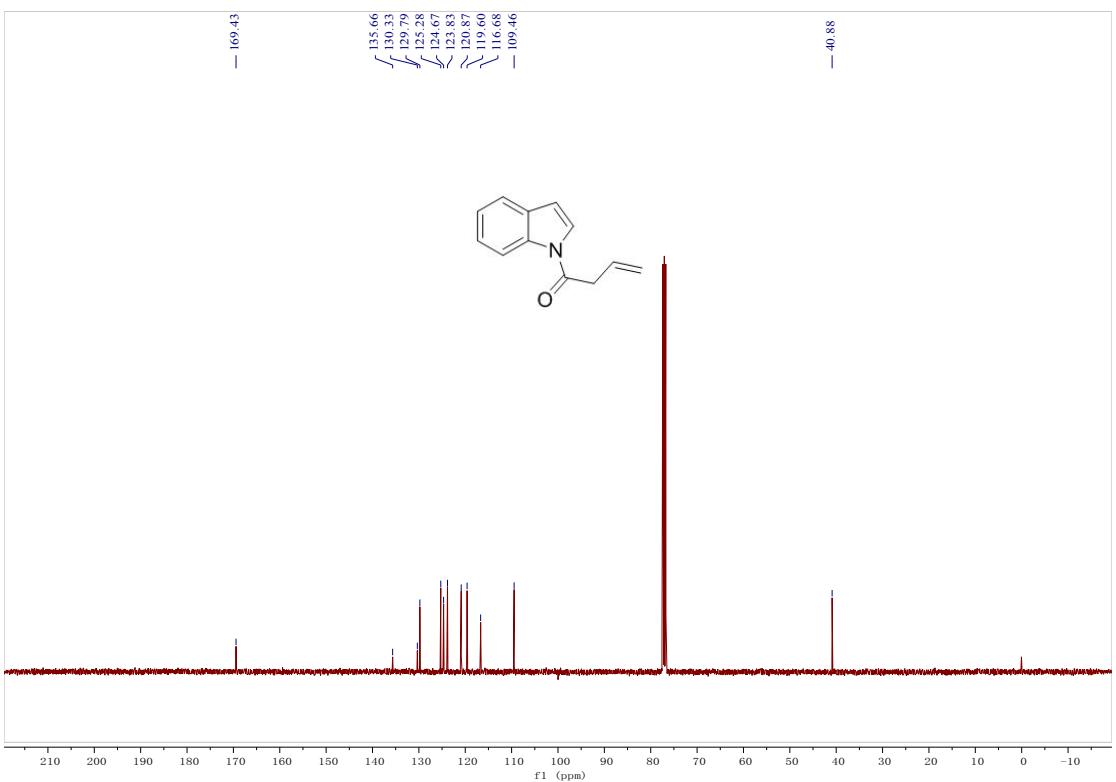
¹³C NMR spectrum of **1u**



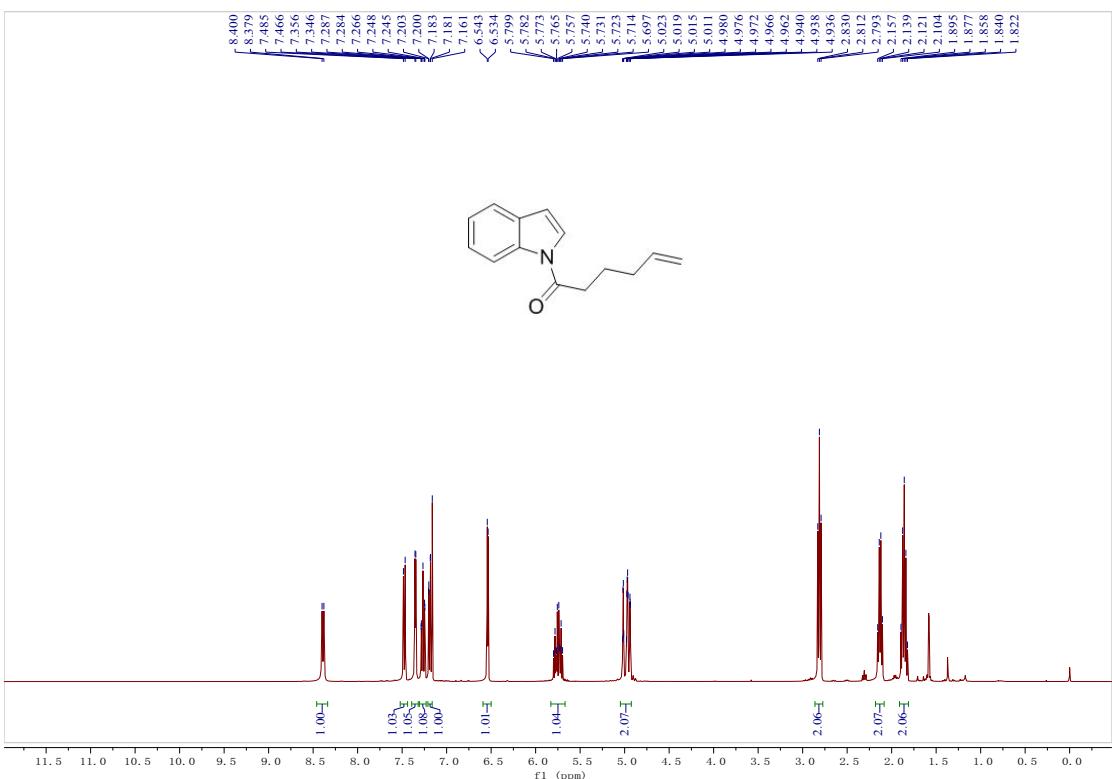
¹H NMR spectrum of **1v**



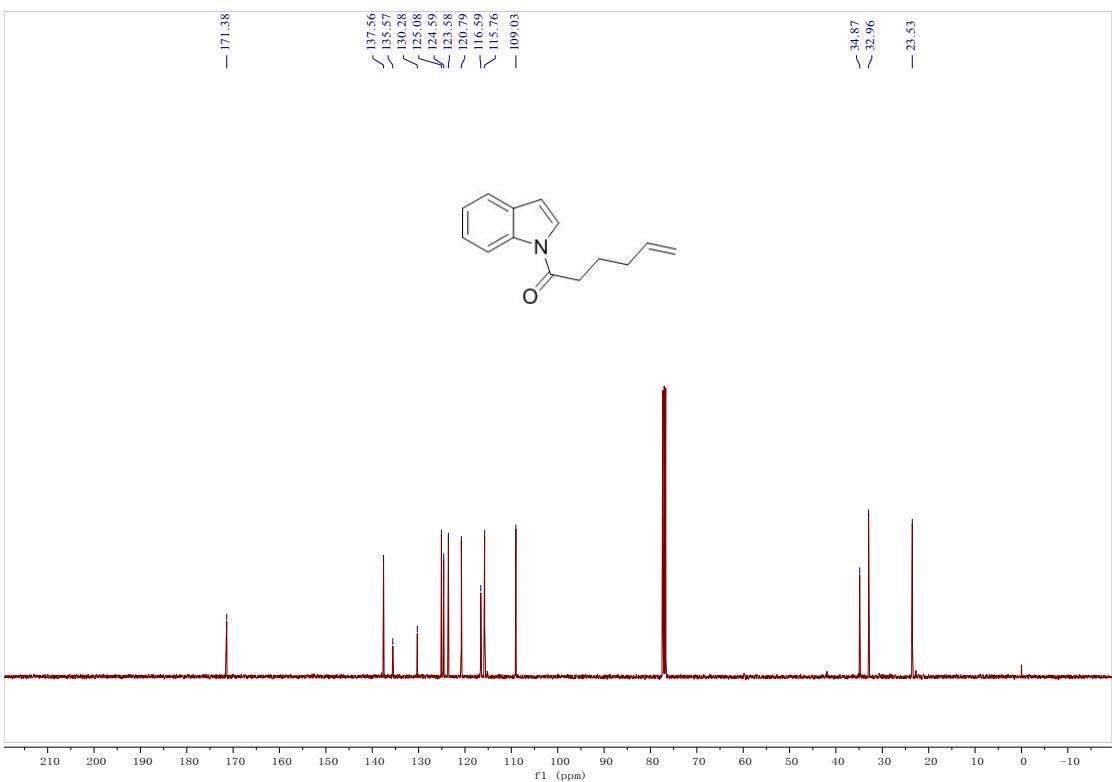
¹³C NMR spectrum of **1v**



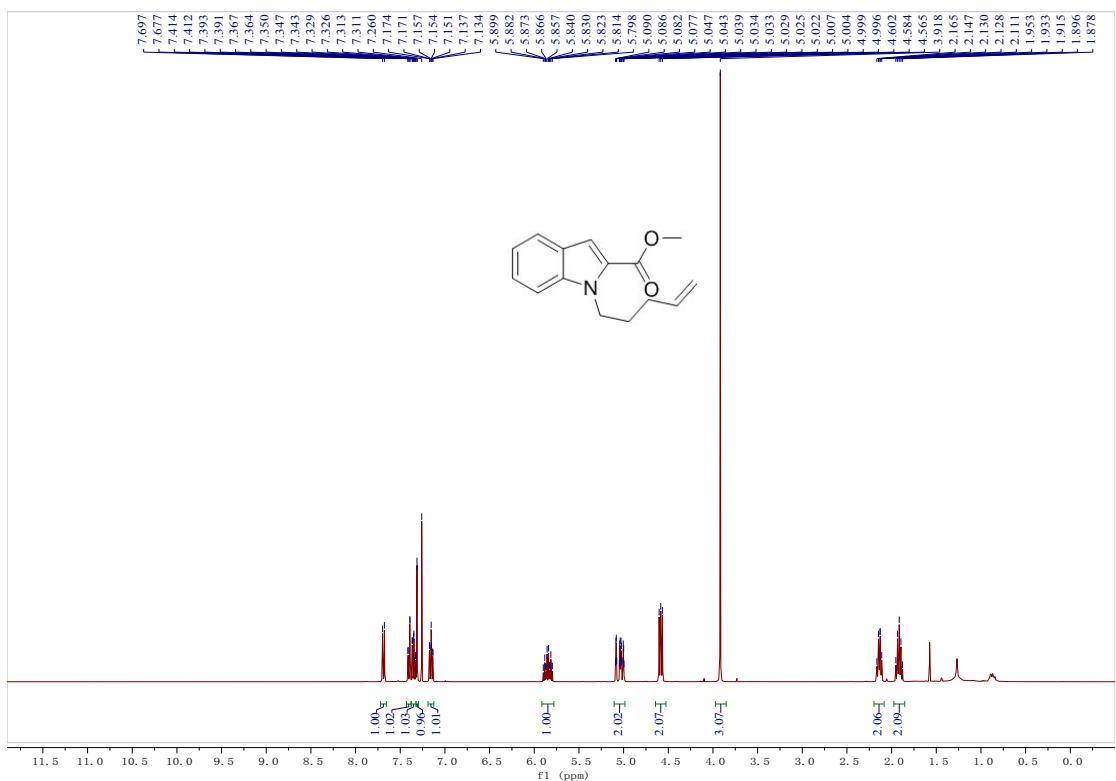
¹H NMR spectrum of **1w**



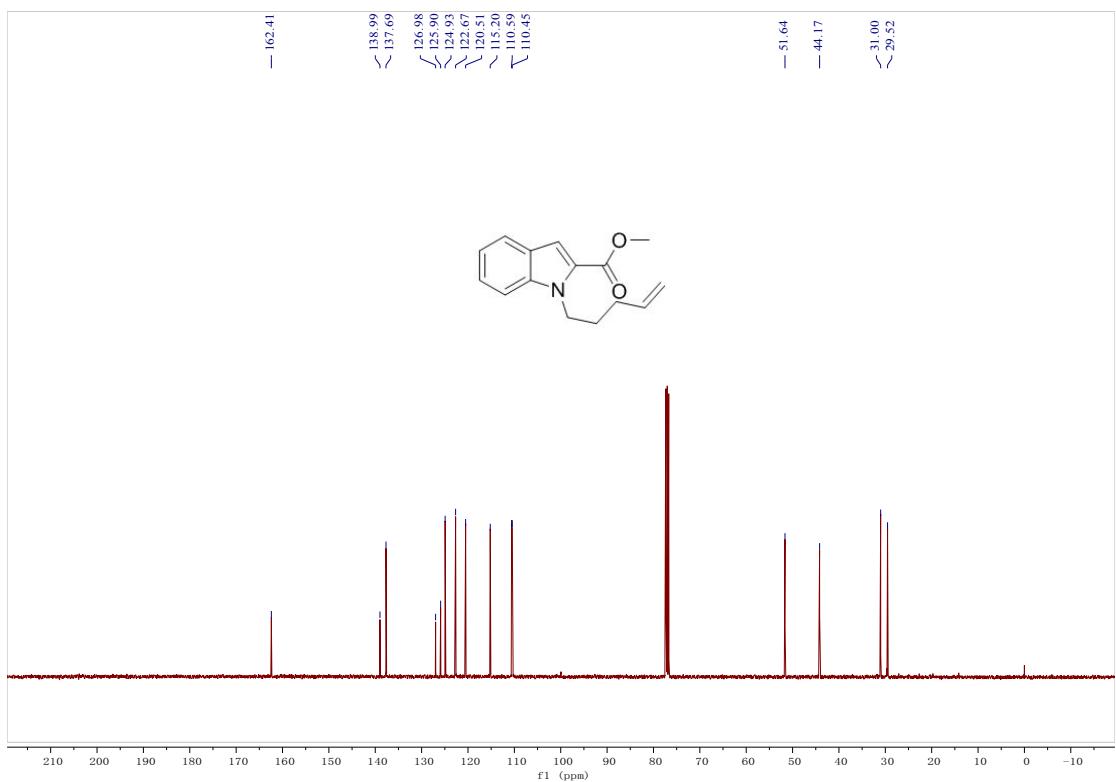
¹³C NMR spectrum of **1w**



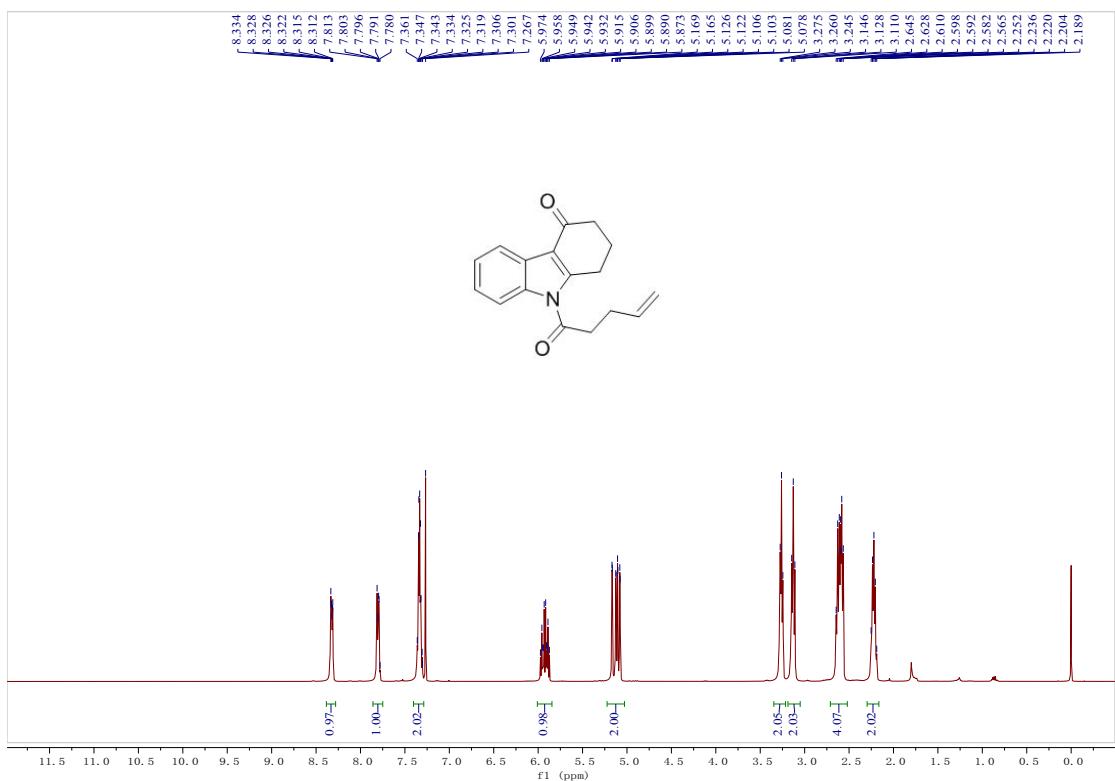
¹H NMR spectrum of **1x**



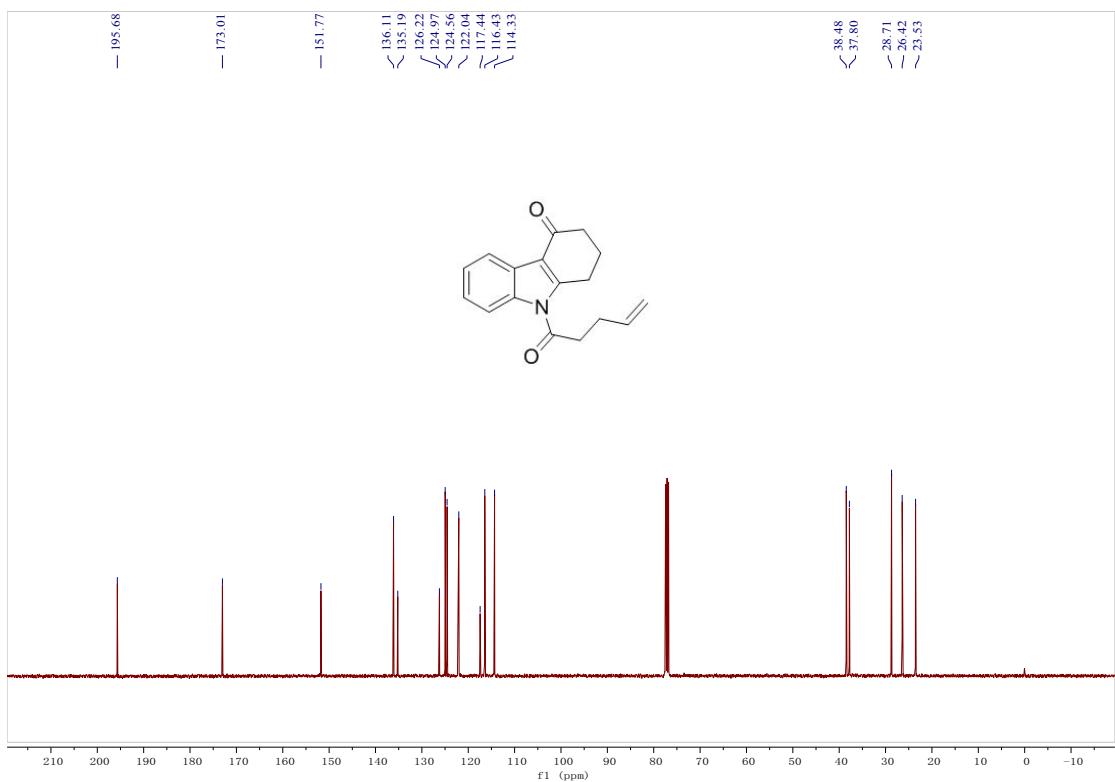
¹³C NMR spectrum of **1x**



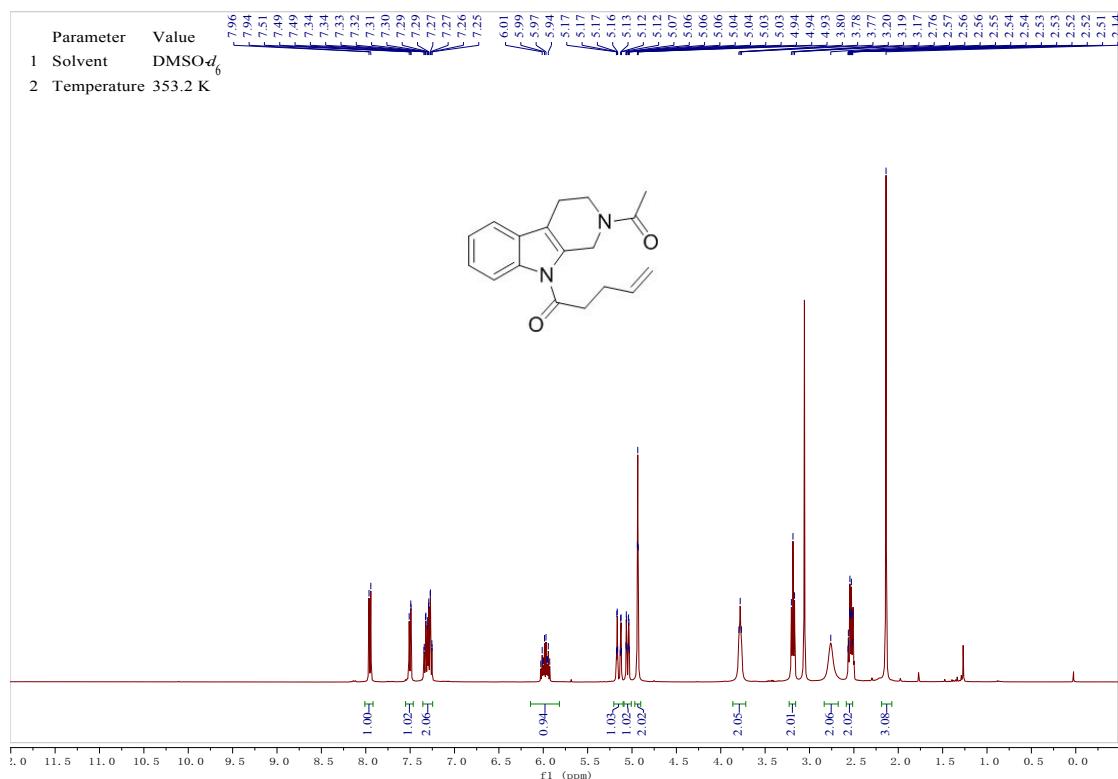
¹H NMR spectrum of 1aa



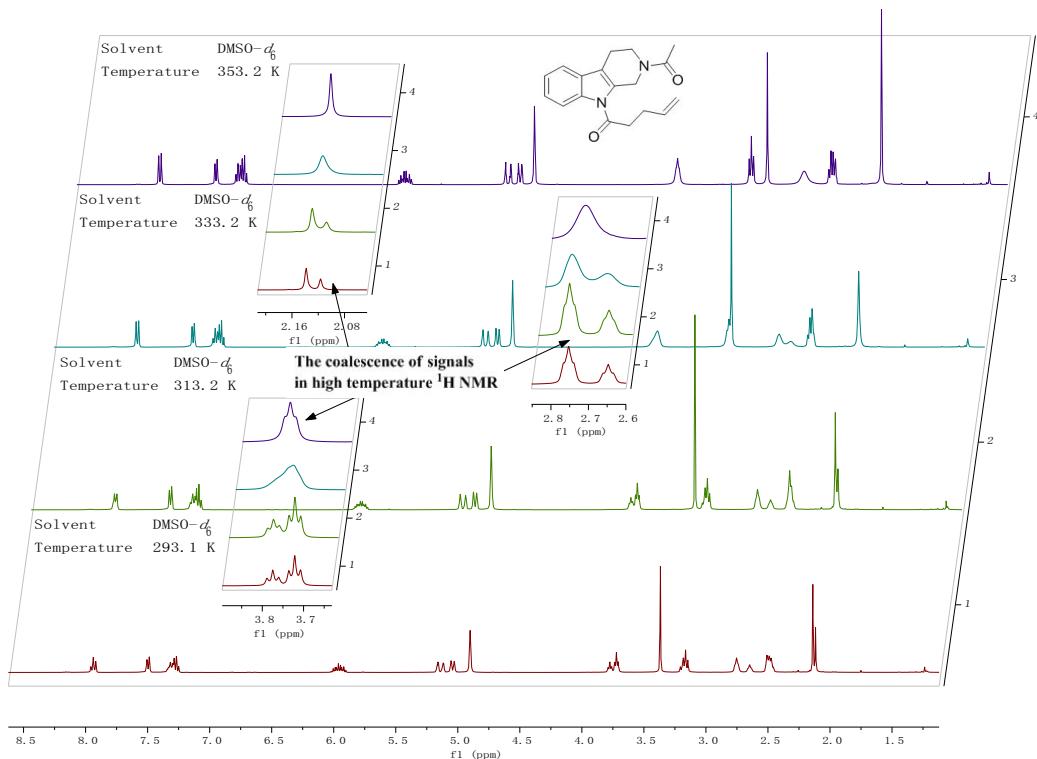
¹³C NMR spectrum of **1aa**



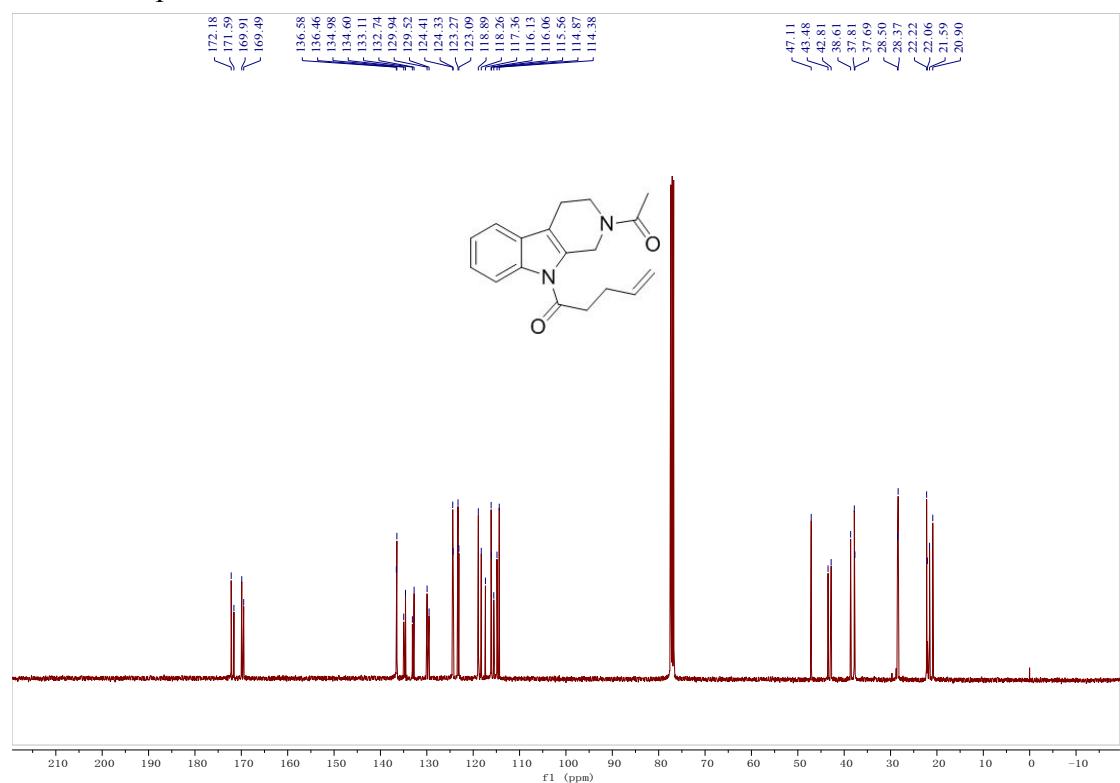
¹H NMR spectrum of **1ab**



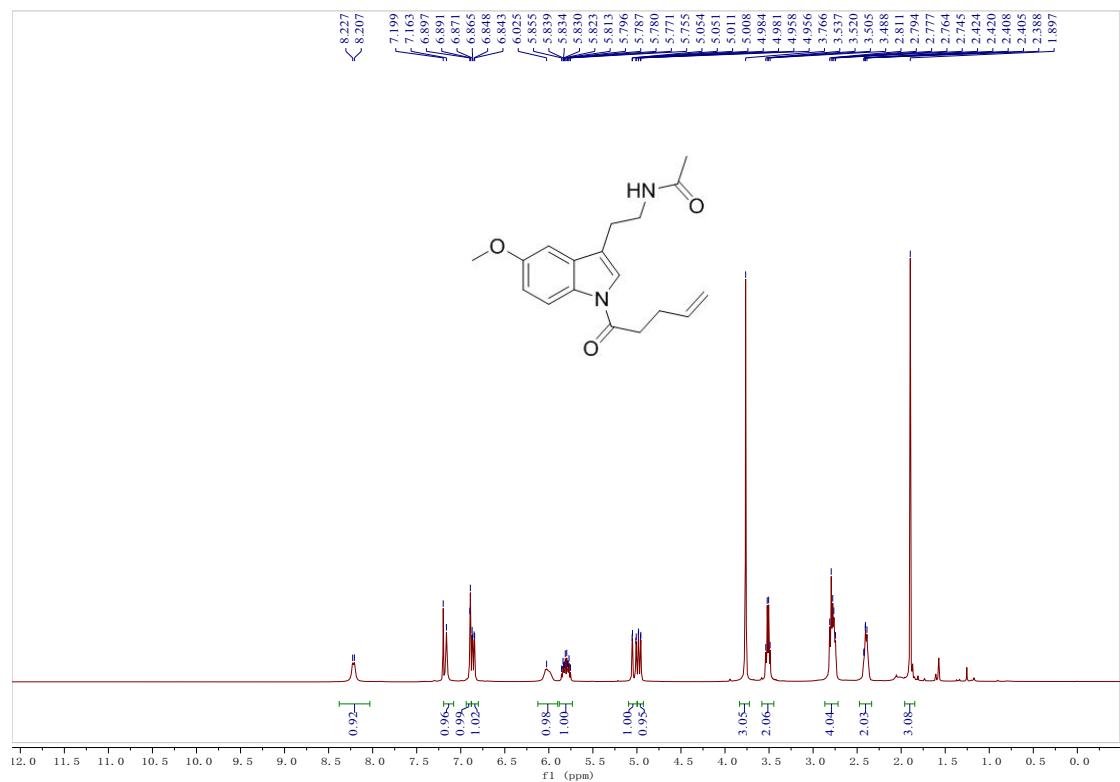
In situ variable temperature ¹H NMR spectrum of **1ab**



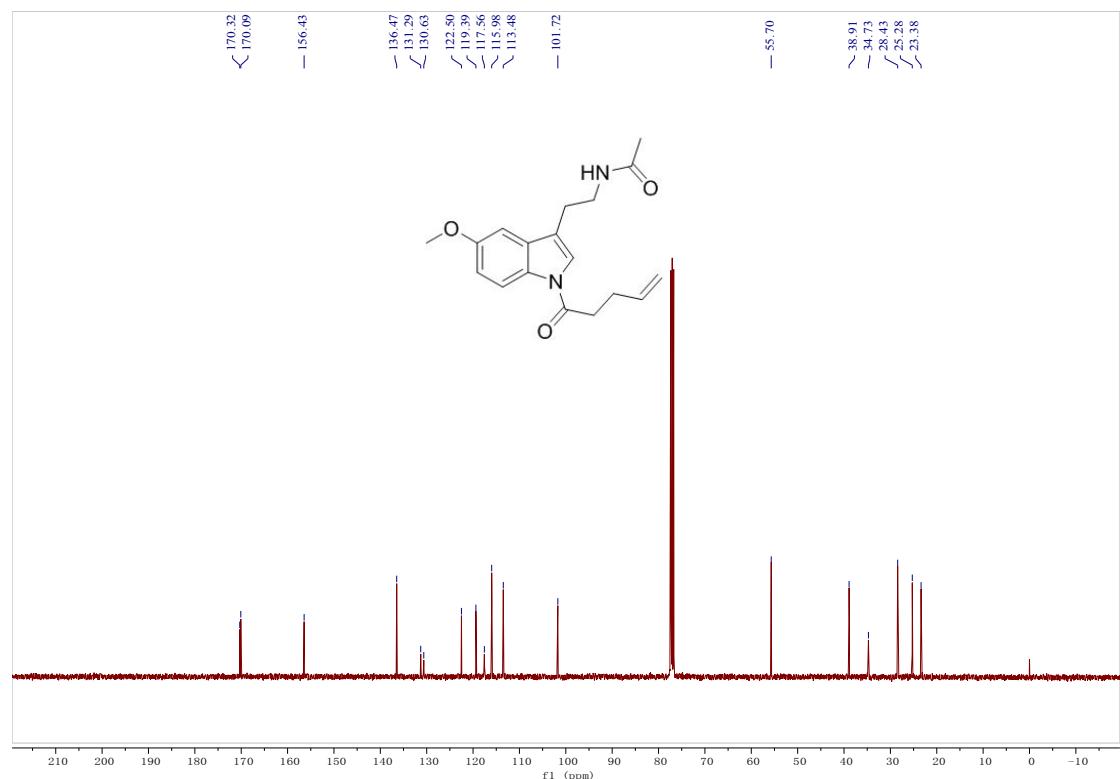
¹³C NMR spectrum of **1ab**



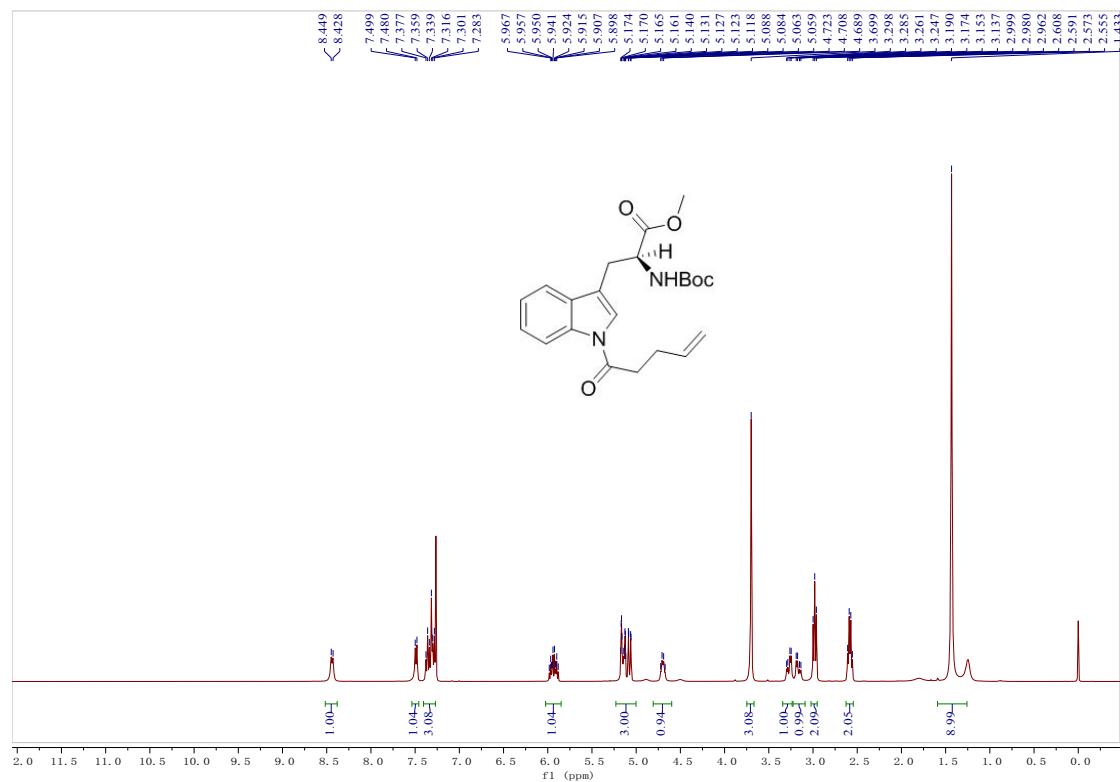
¹H NMR spectrum of **1ac**



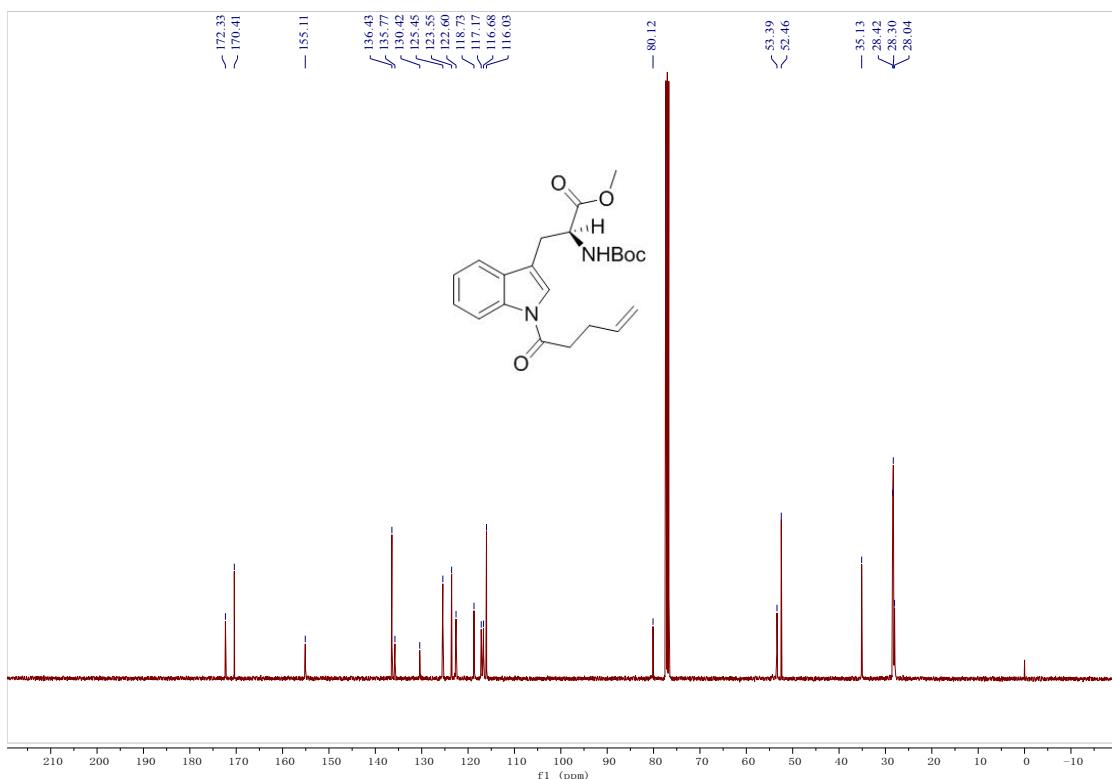
¹³C NMR spectrum of **1ac**



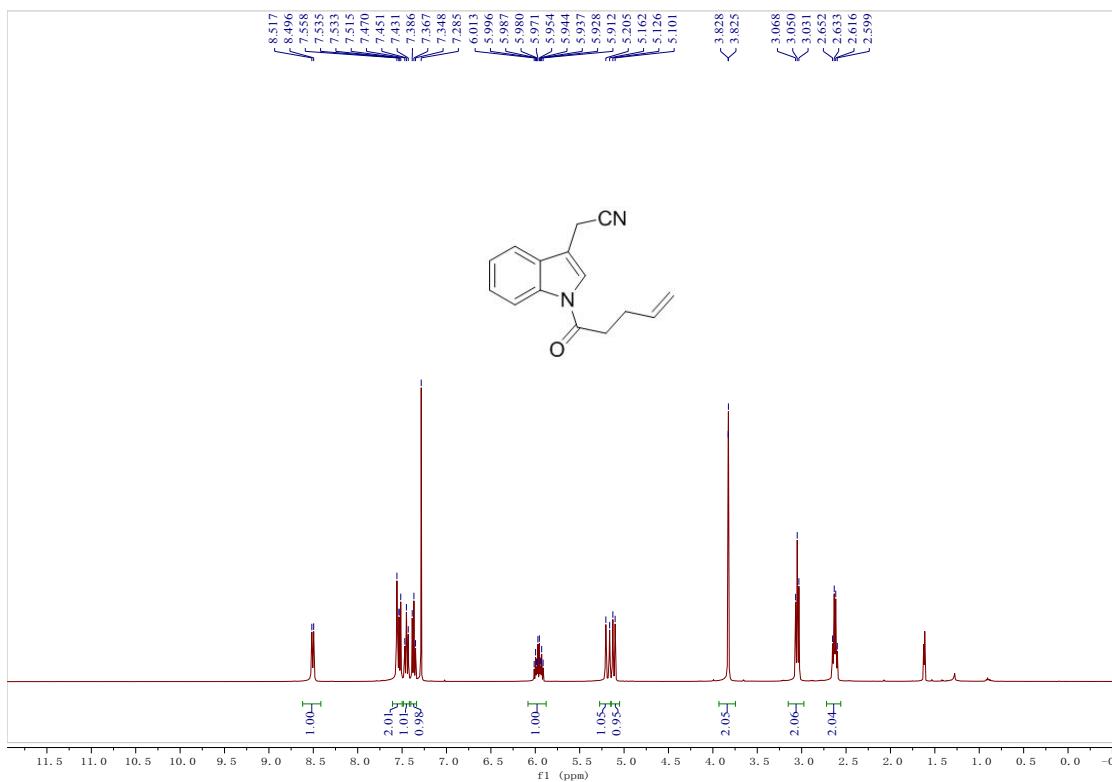
¹H NMR spectrum of **1ad**



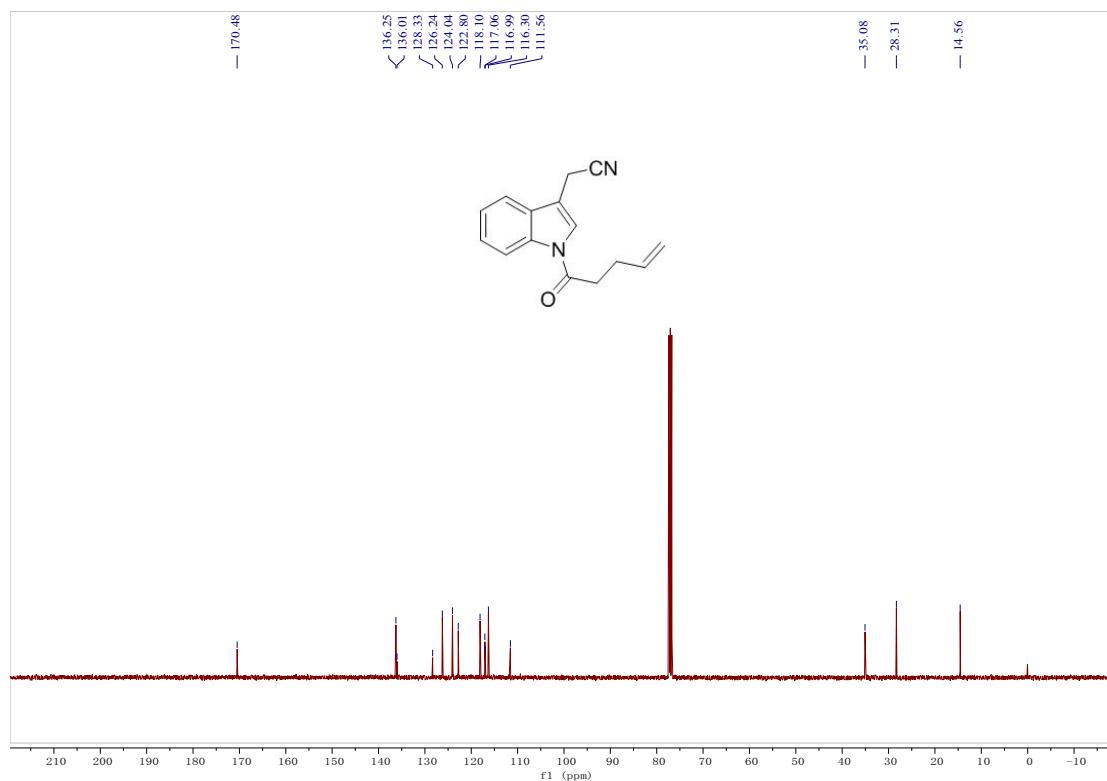
¹³C NMR spectrum of **1ad**



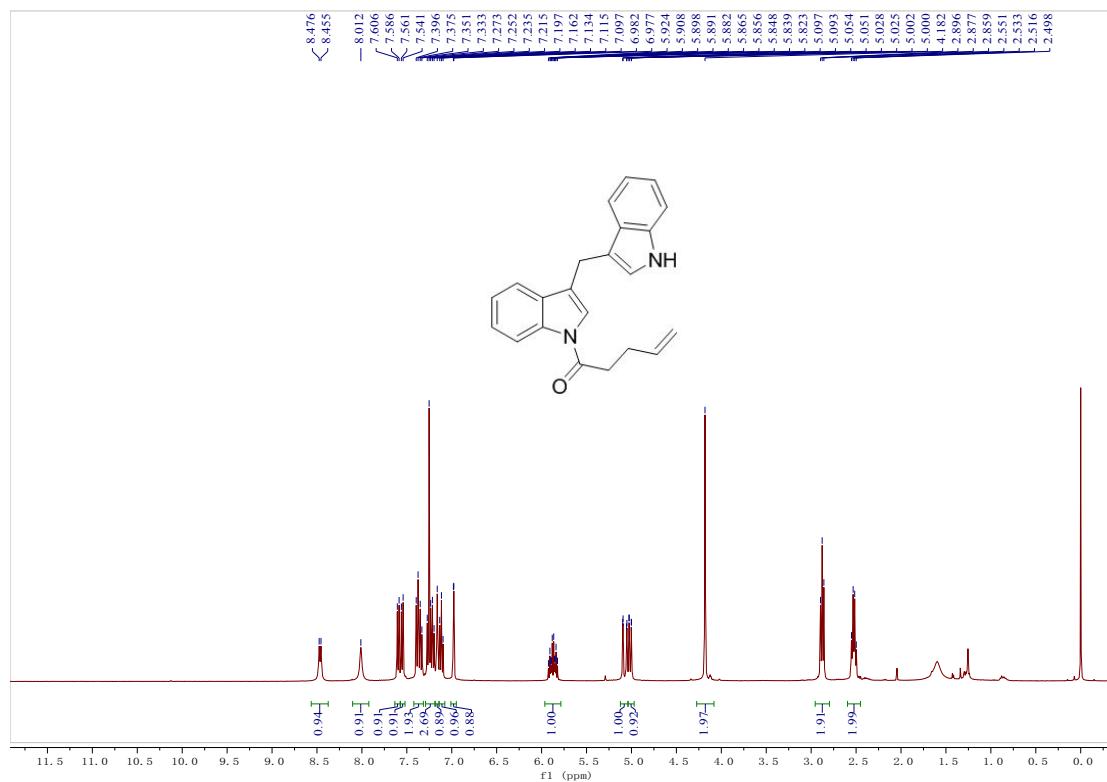
¹H NMR spectrum of **1ae**



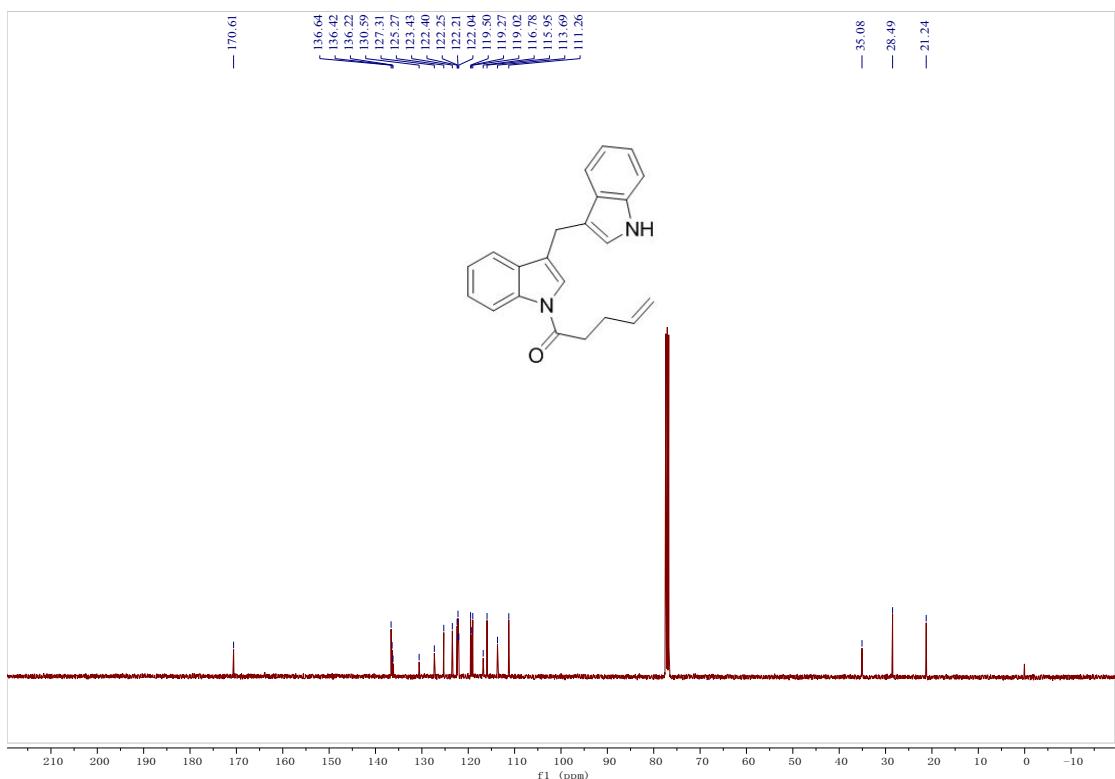
¹³C NMR spectrum of **1ae**



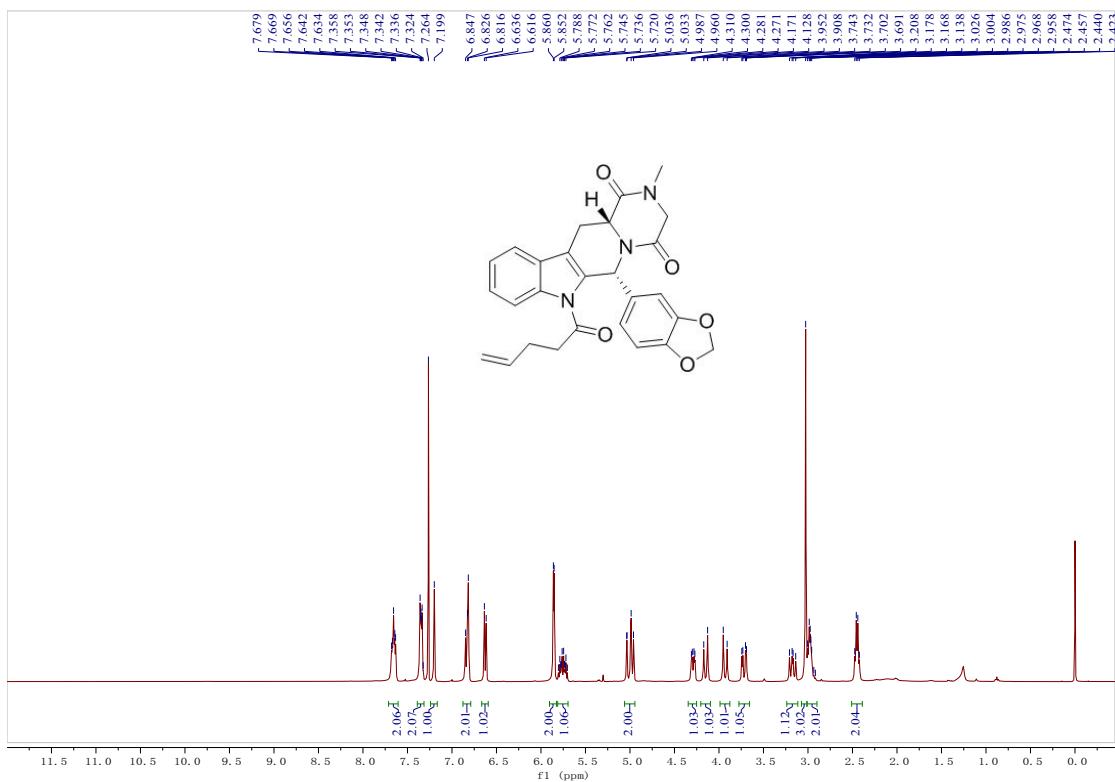
¹H NMR spectrum of **1af**



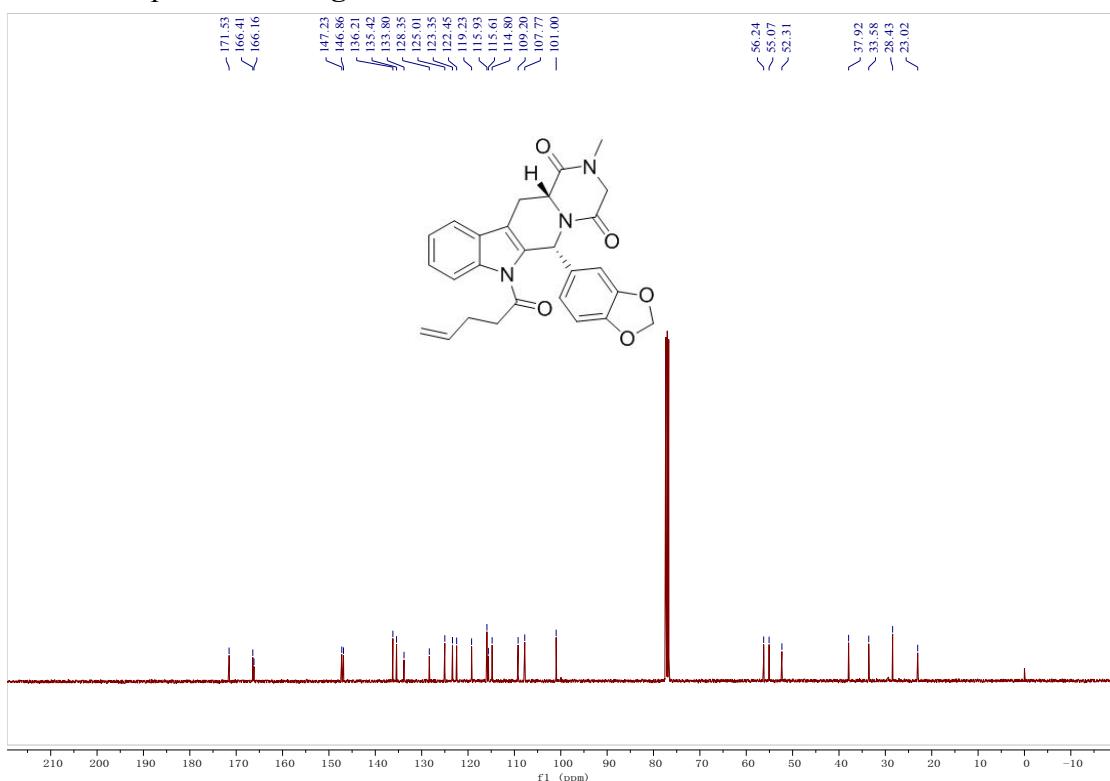
¹³C NMR spectrum of **1af**



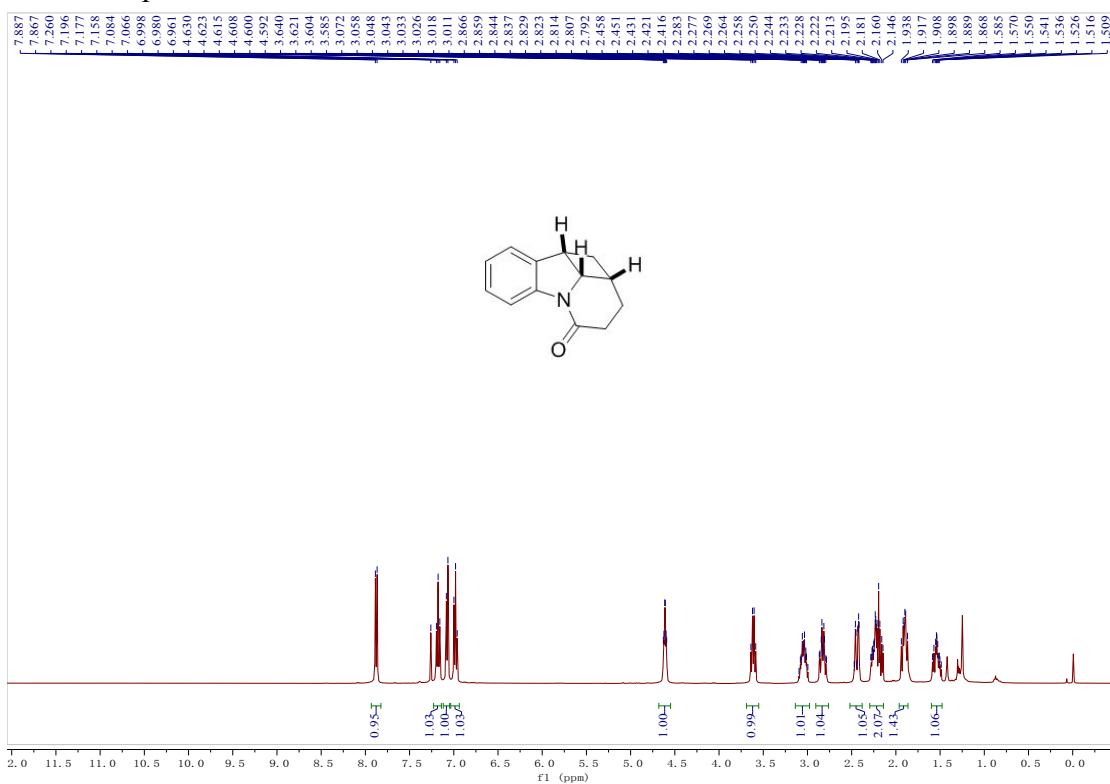
¹H NMR spectrum of **1ag**



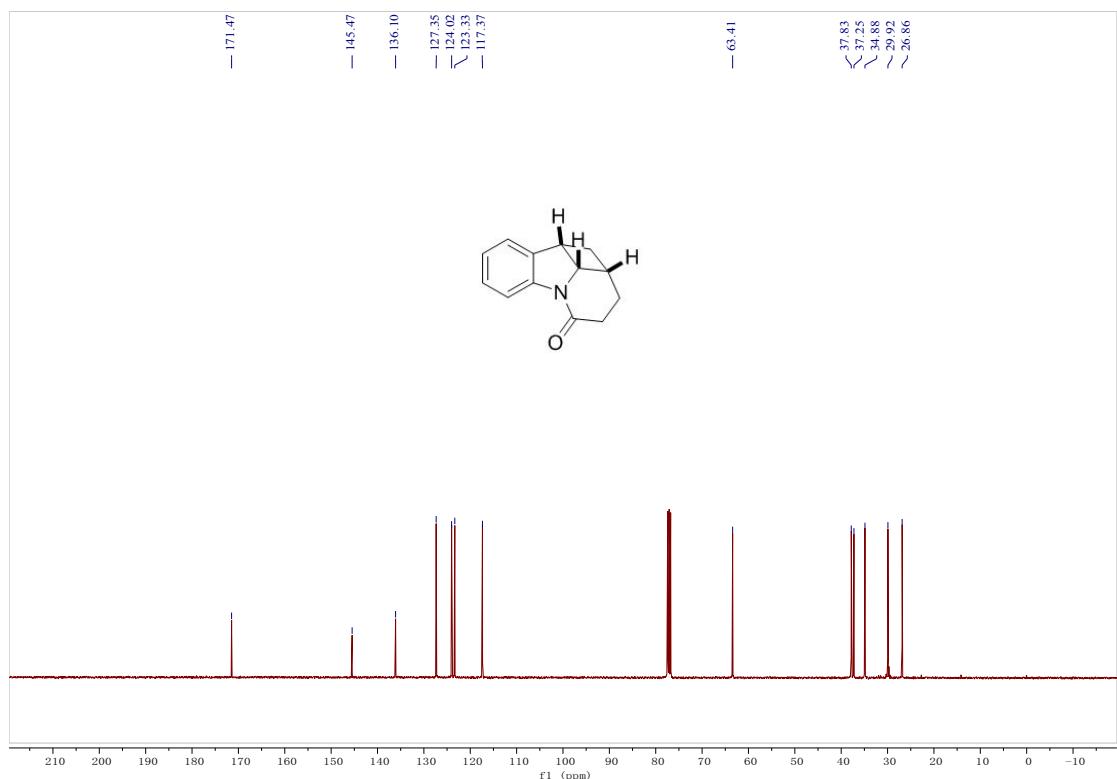
¹³C NMR spectrum of **1ag**



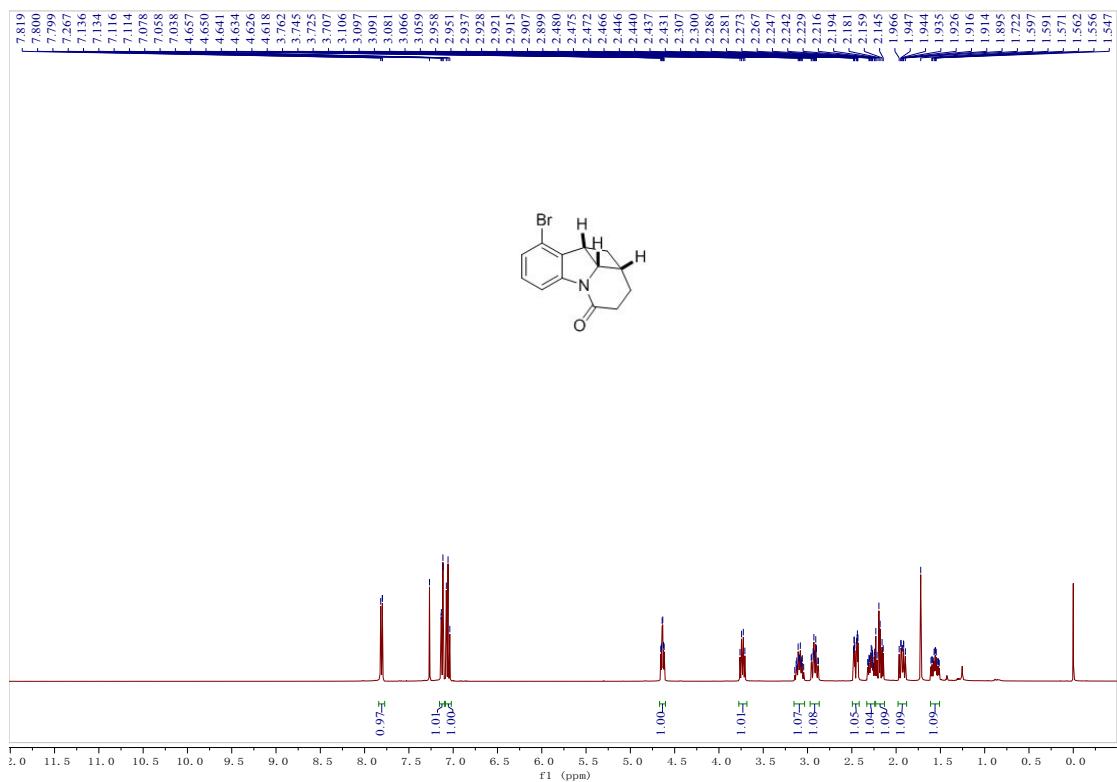
¹H NMR spectrum of **2a**



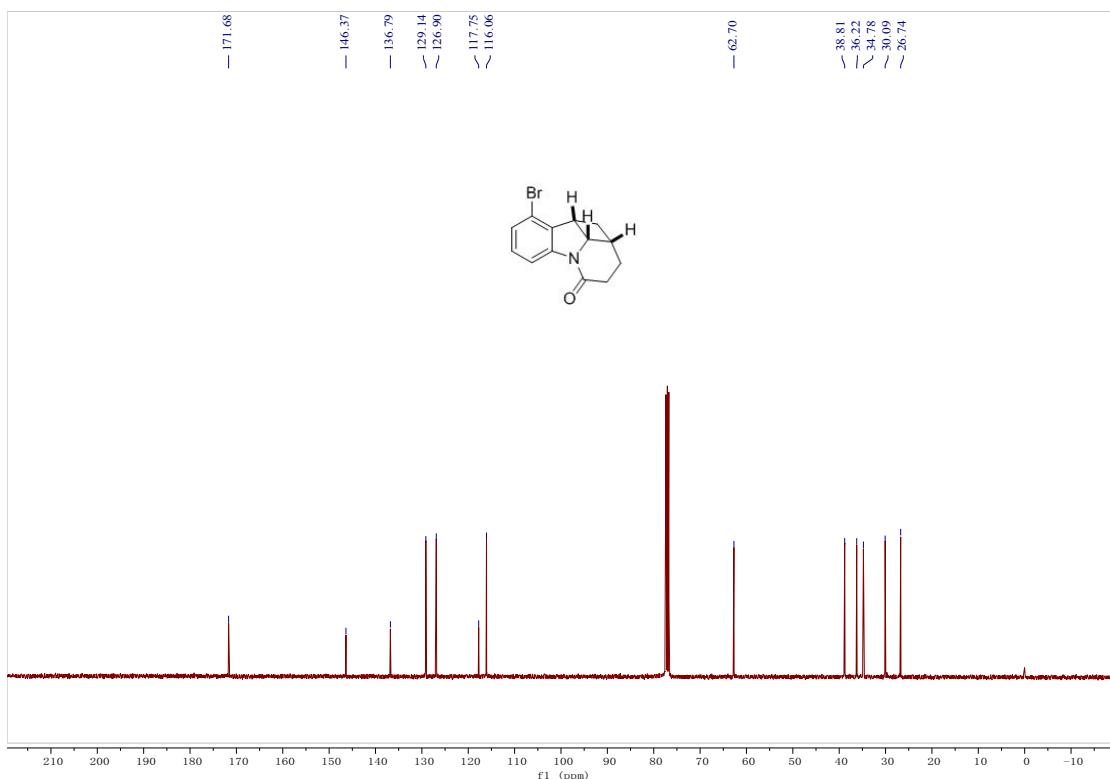
¹³C NMR spectrum of **2a**



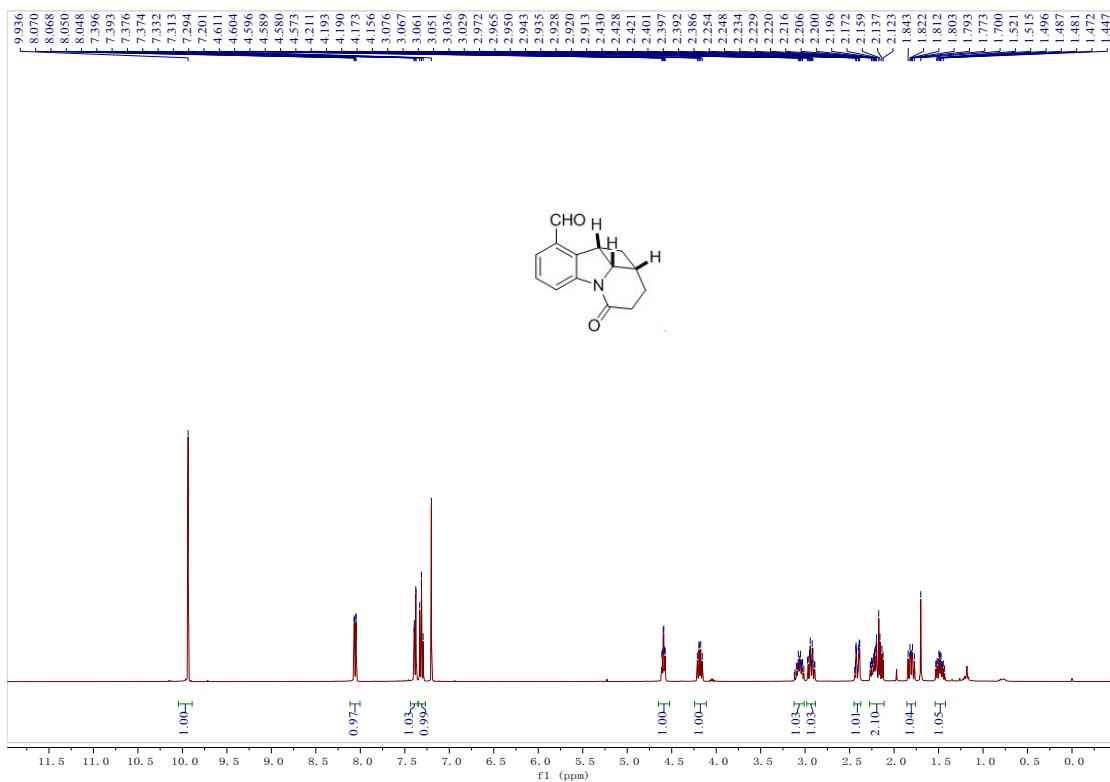
¹H NMR spectrum of **2b**



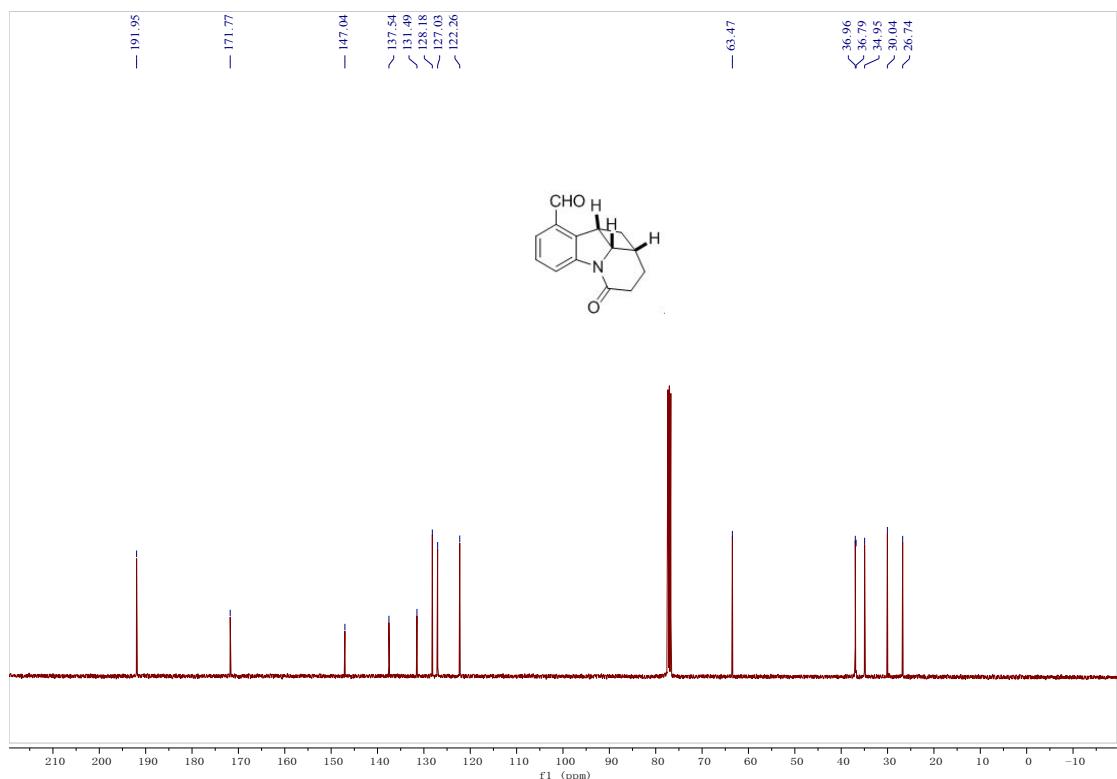
¹³C NMR spectrum of **2b**



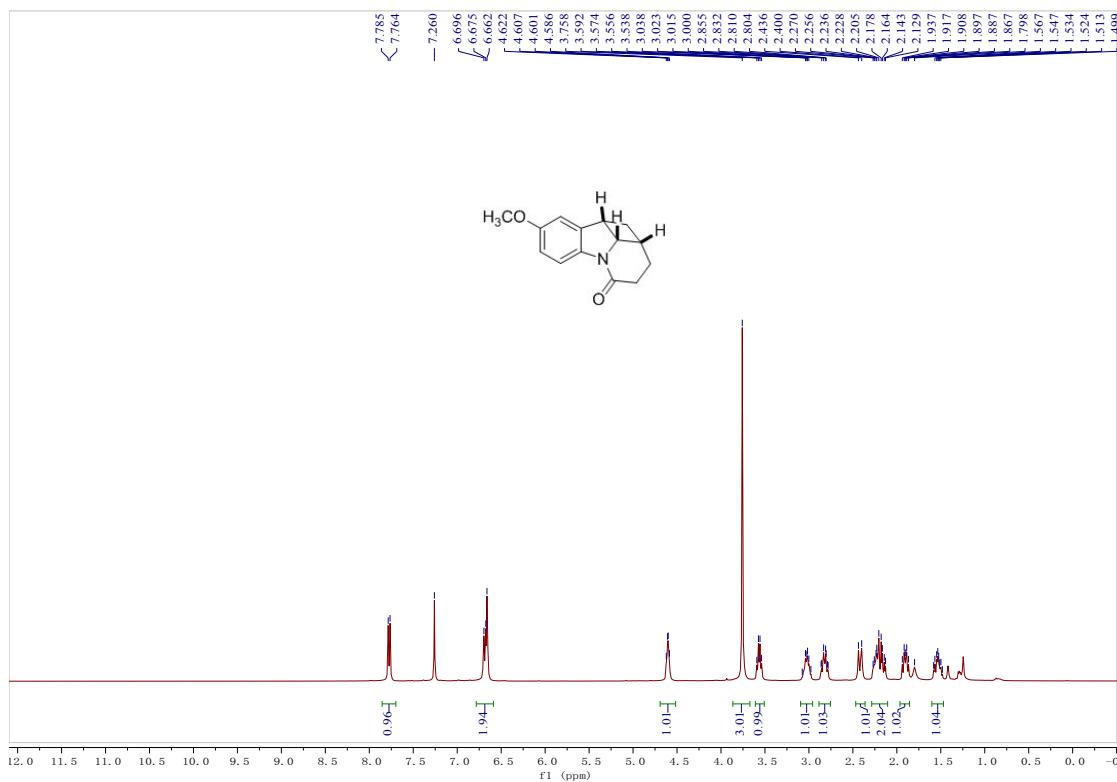
¹H NMR spectrum of **2c**



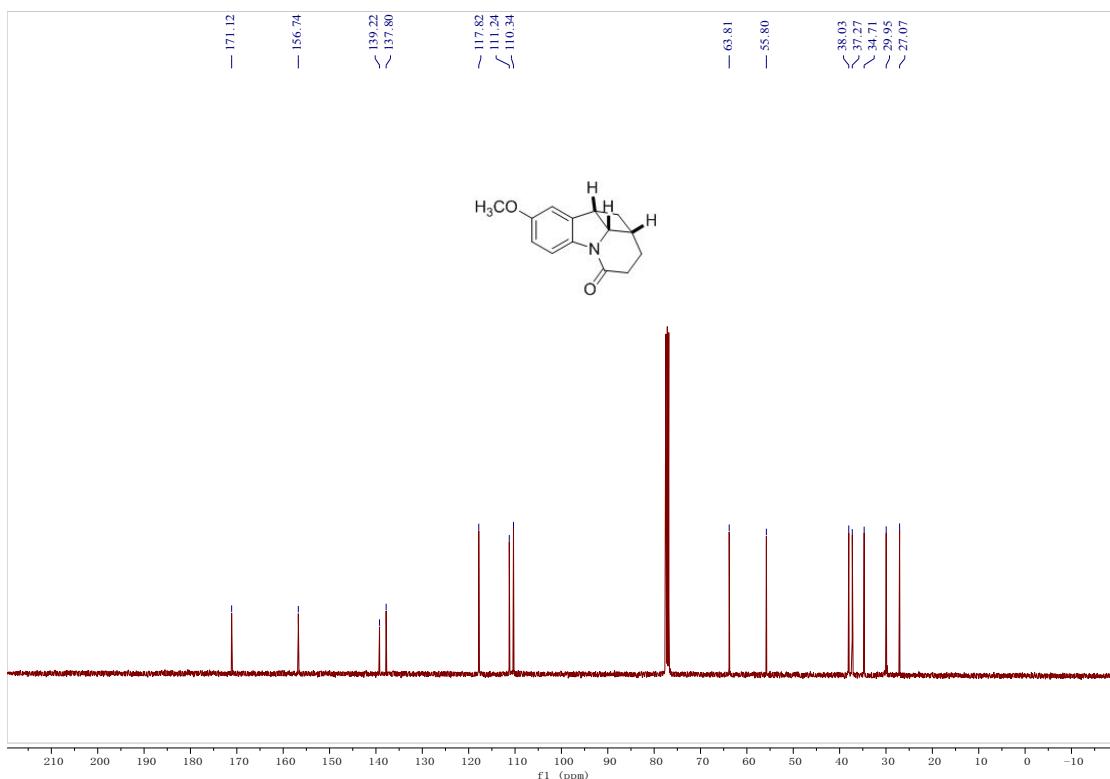
¹³C NMR spectrum of **2c**



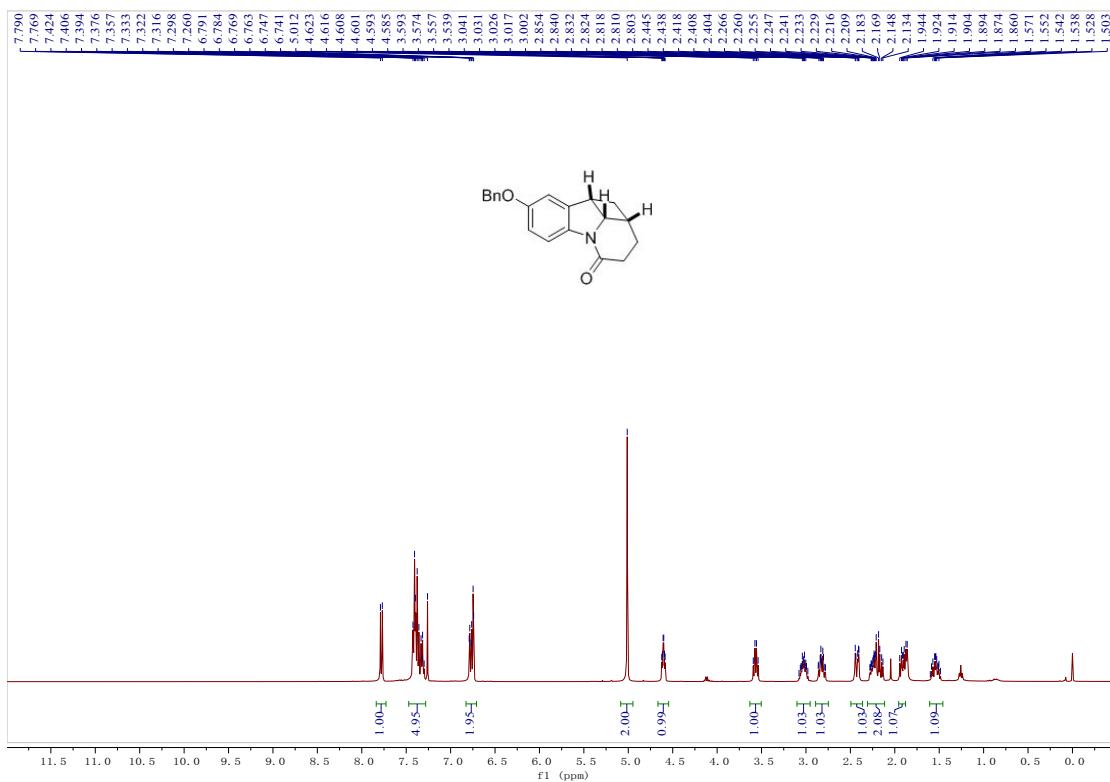
¹H NMR spectrum of **2d**



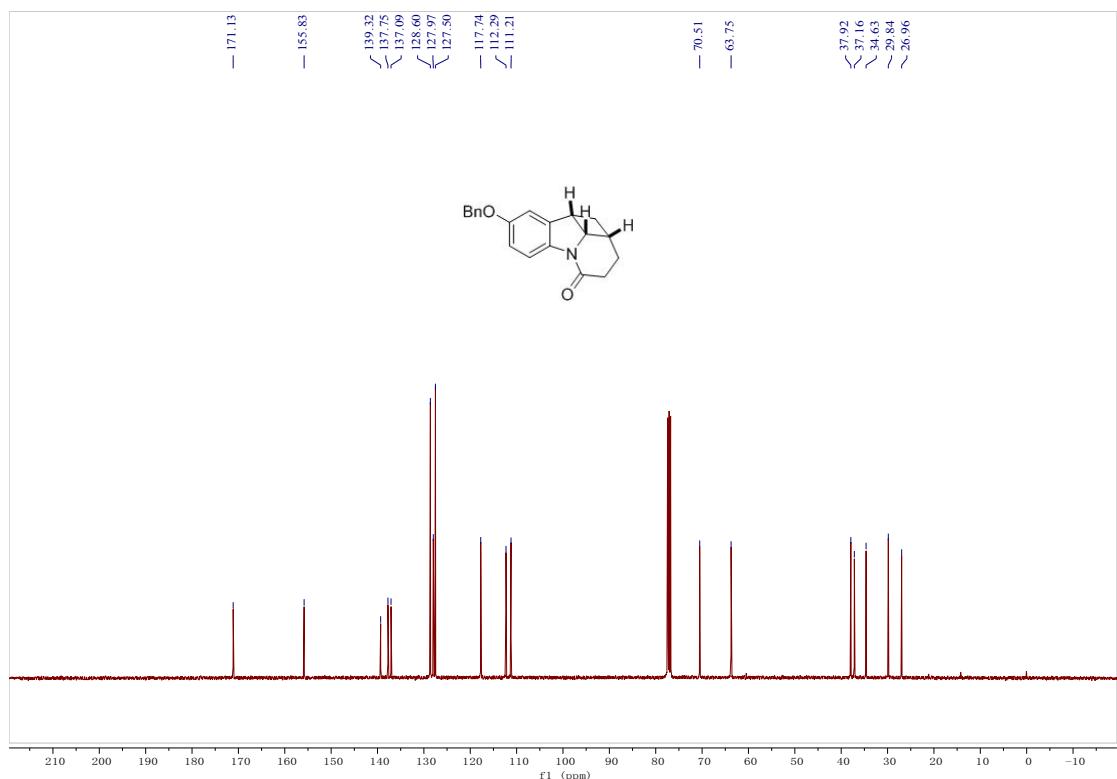
¹³C NMR spectrum of **2d**



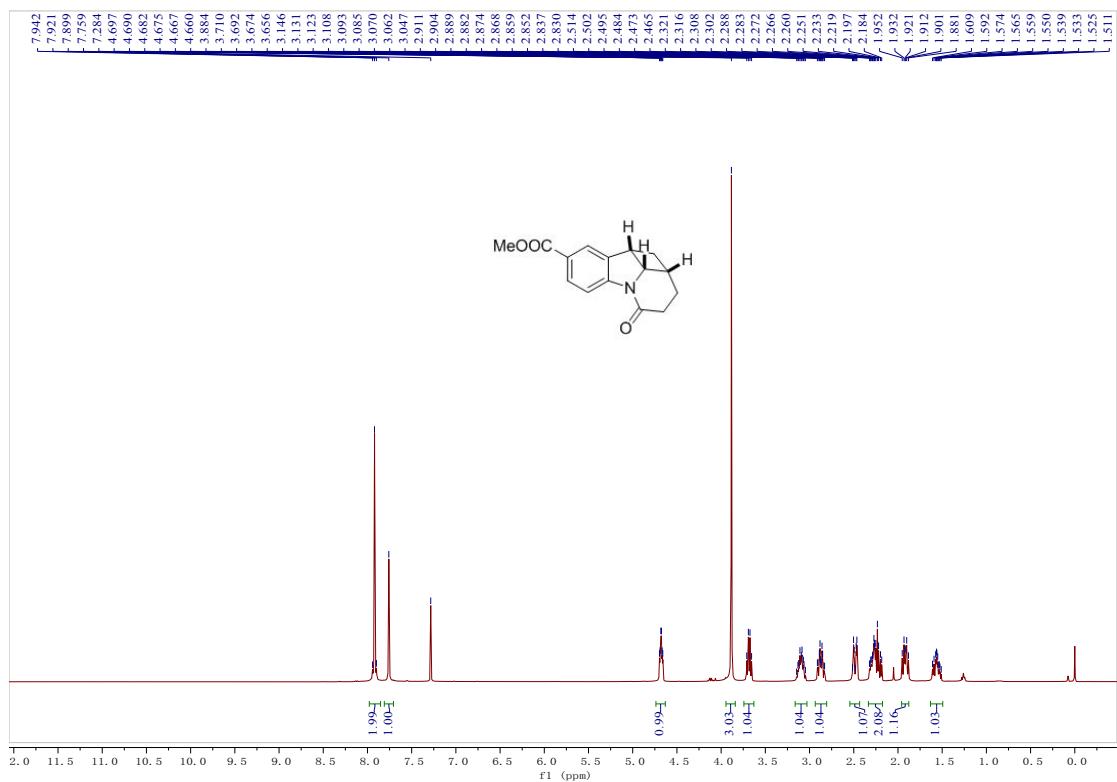
¹H NMR spectrum of **2e**



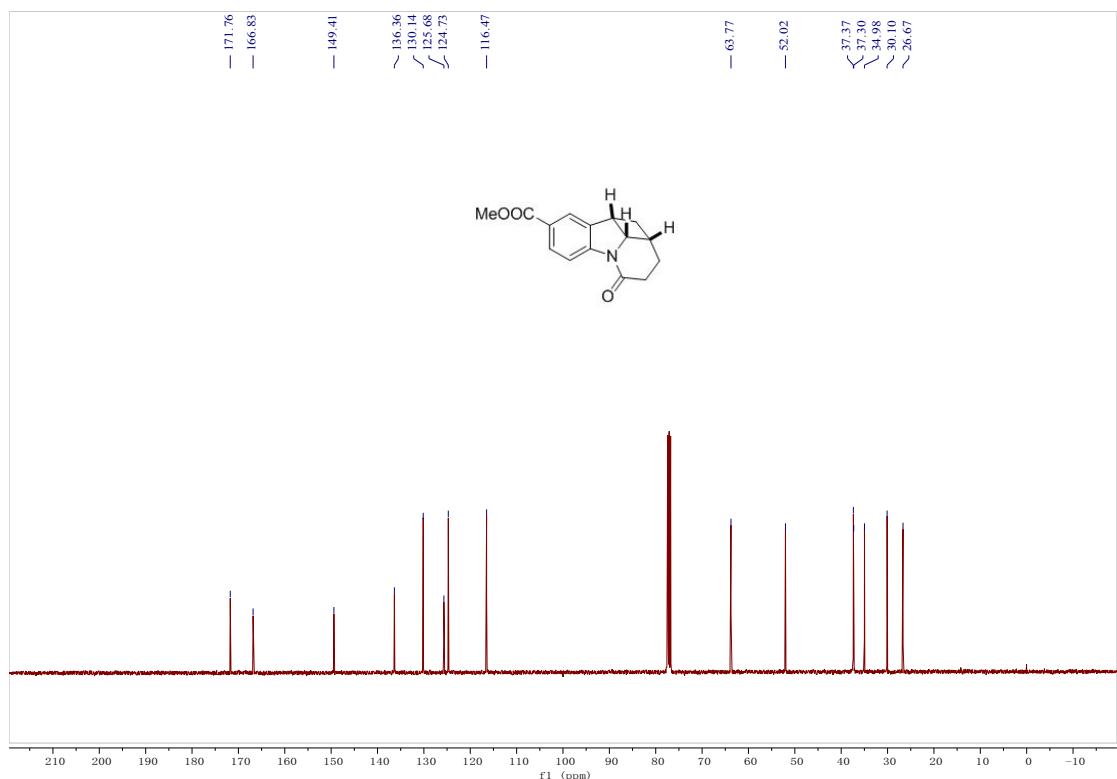
¹³C NMR spectrum of **2e**



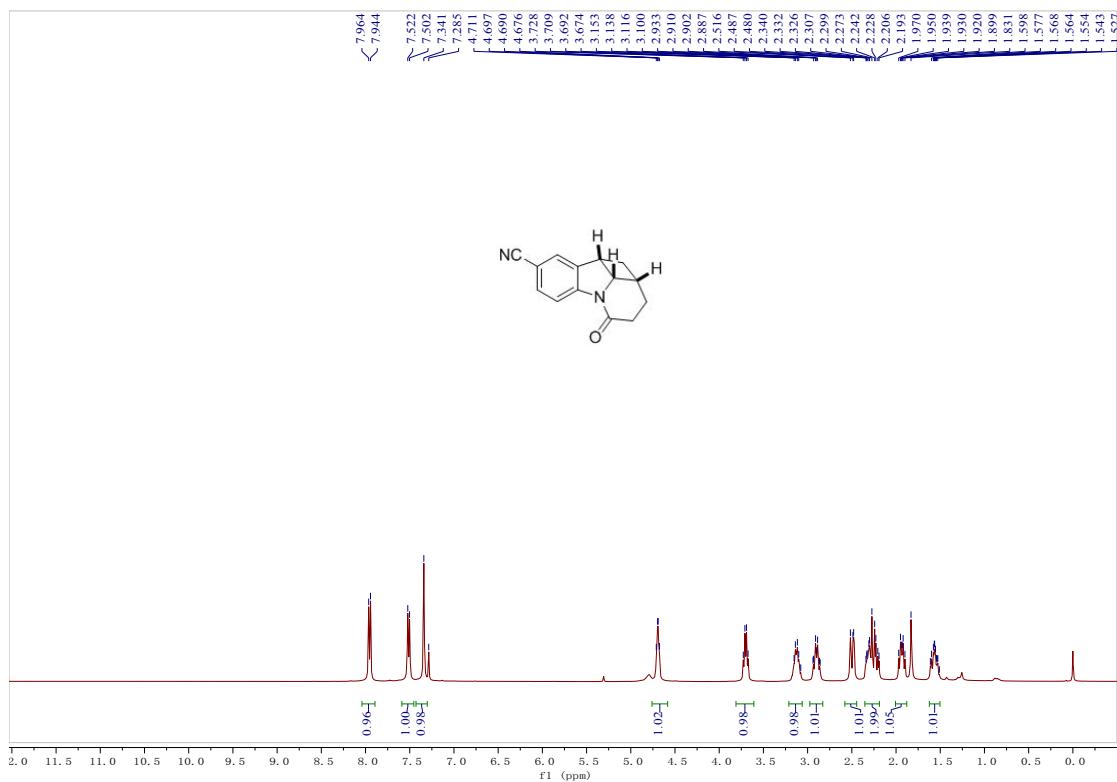
¹H NMR spectrum of **2f**



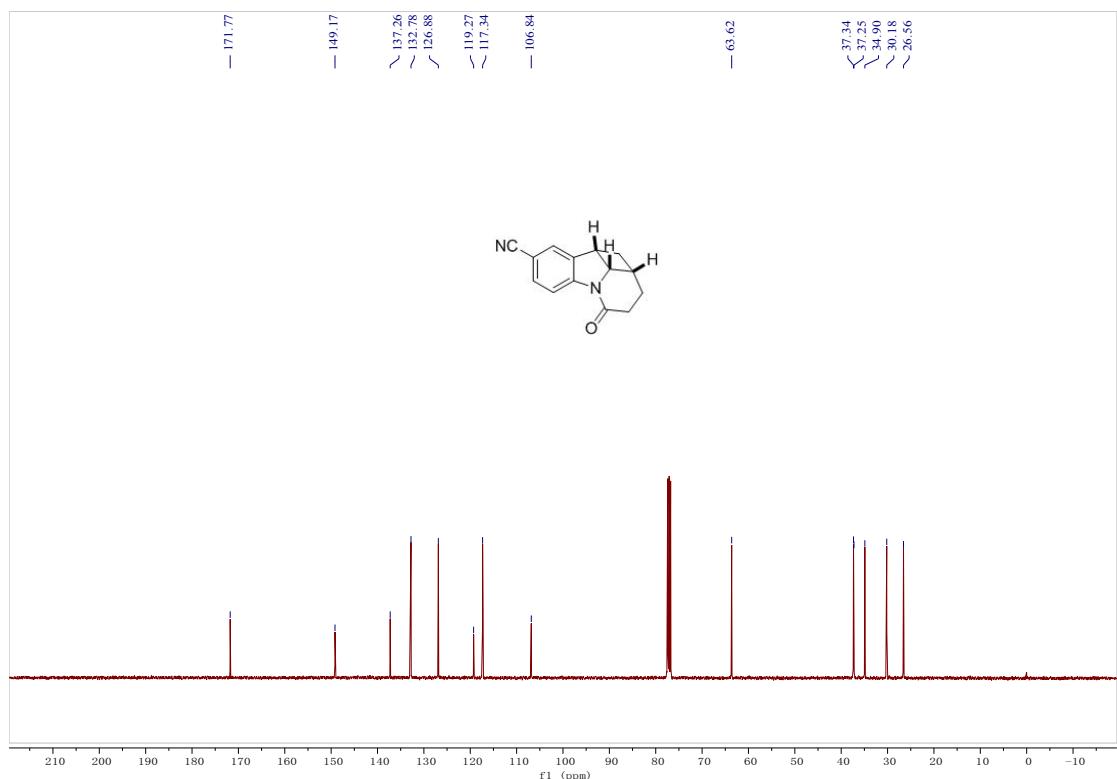
¹³C NMR spectrum of **2f**



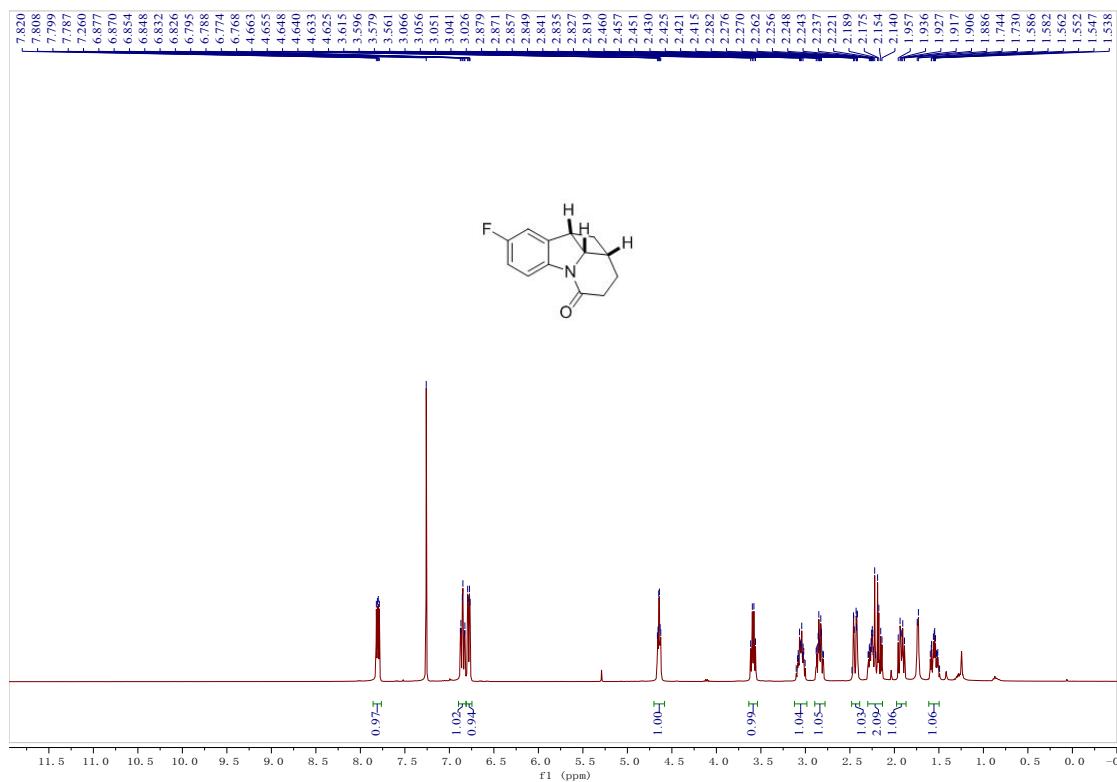
¹H NMR spectrum of **2g**



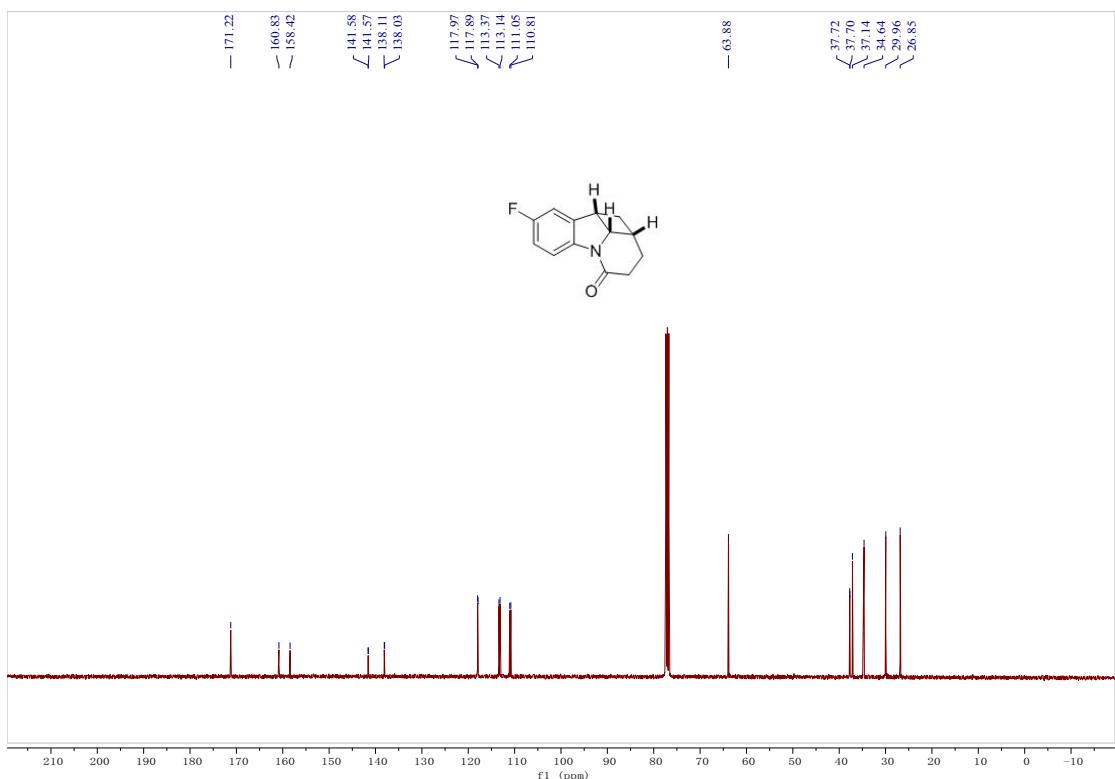
¹³C NMR spectrum of **2g**



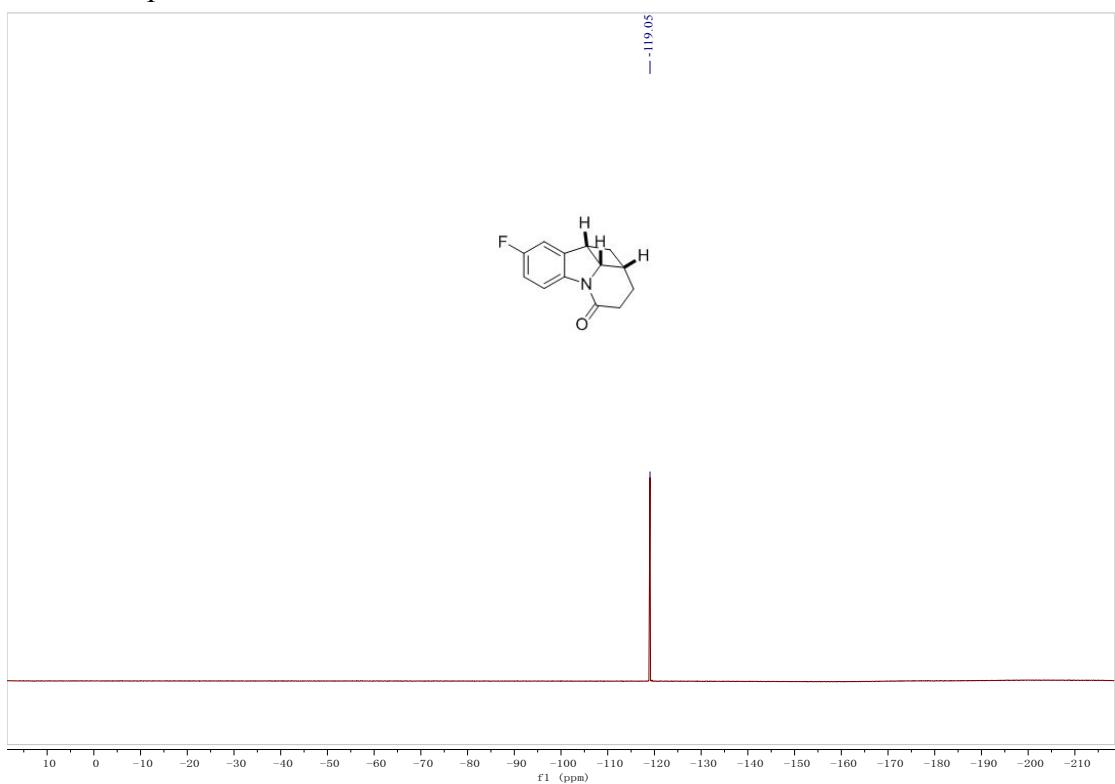
¹H NMR spectrum of **2h**



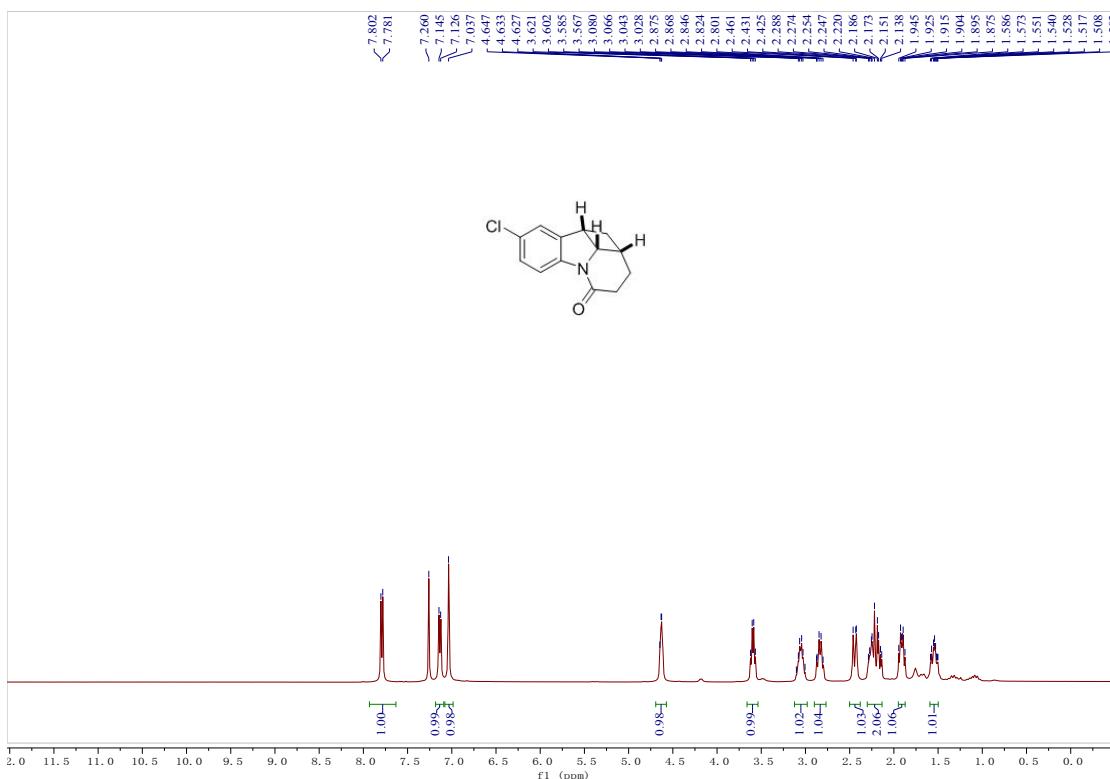
¹³C NMR spectrum of **2h**



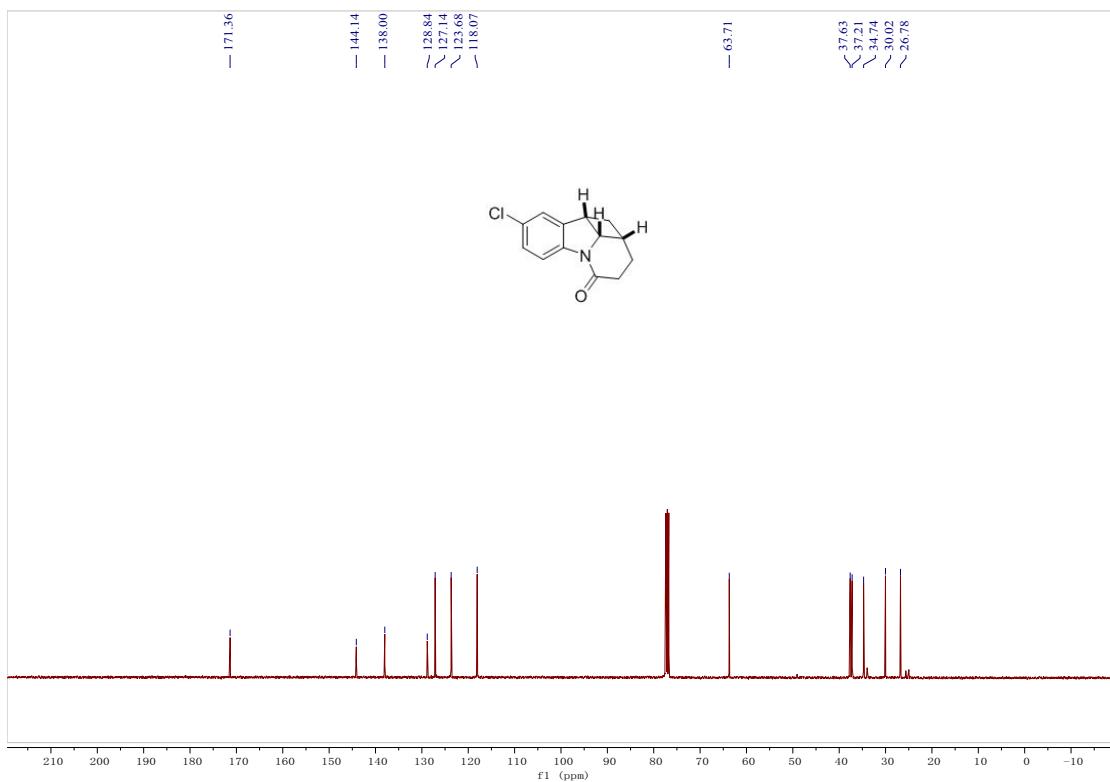
¹⁹F NMR spectrum of **2h**



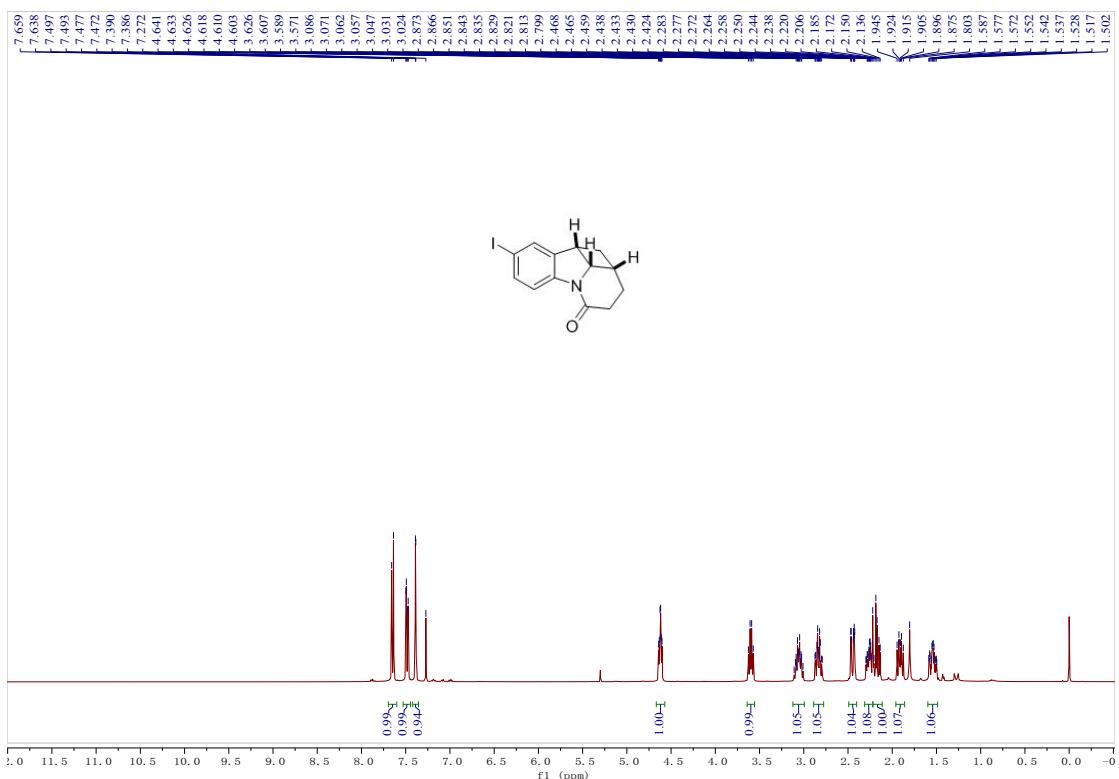
¹H NMR spectrum of **2i**



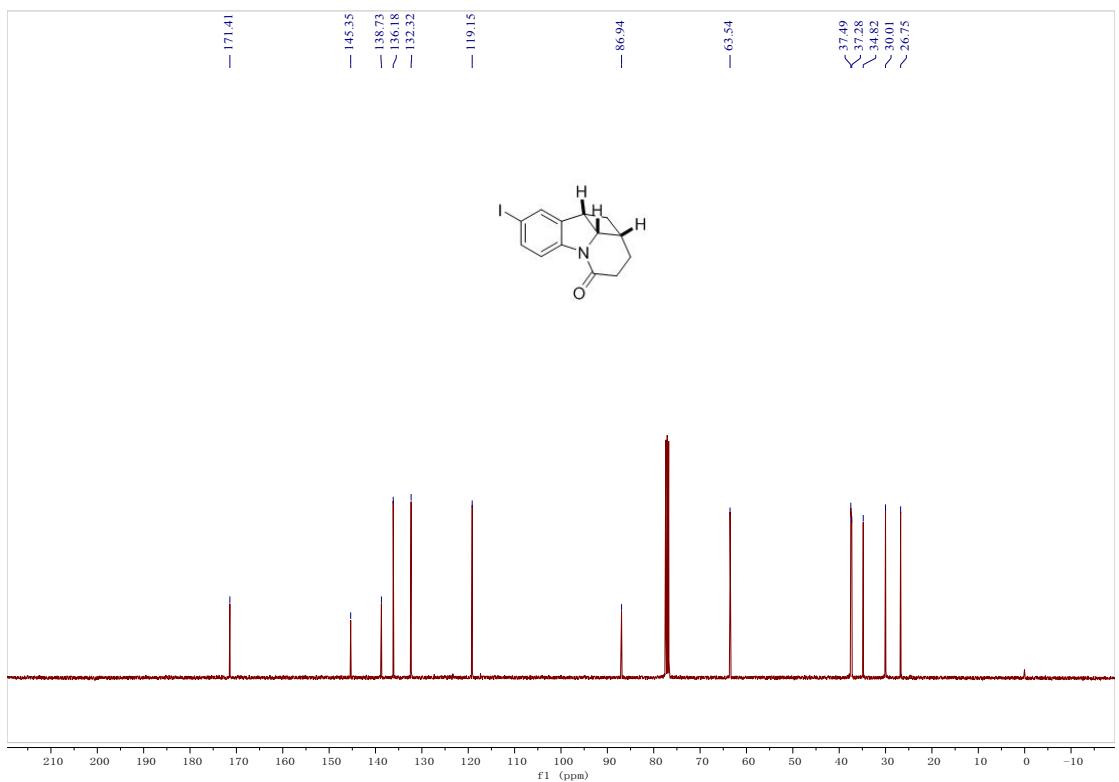
¹³C NMR spectrum of **2i**



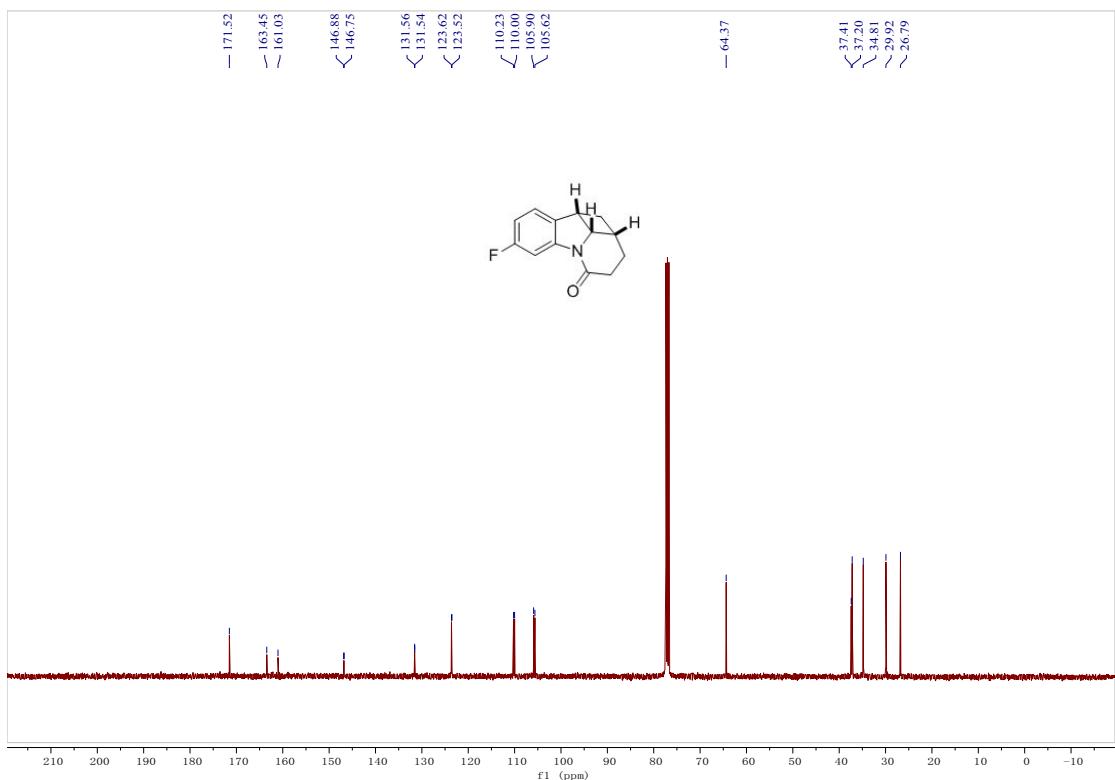
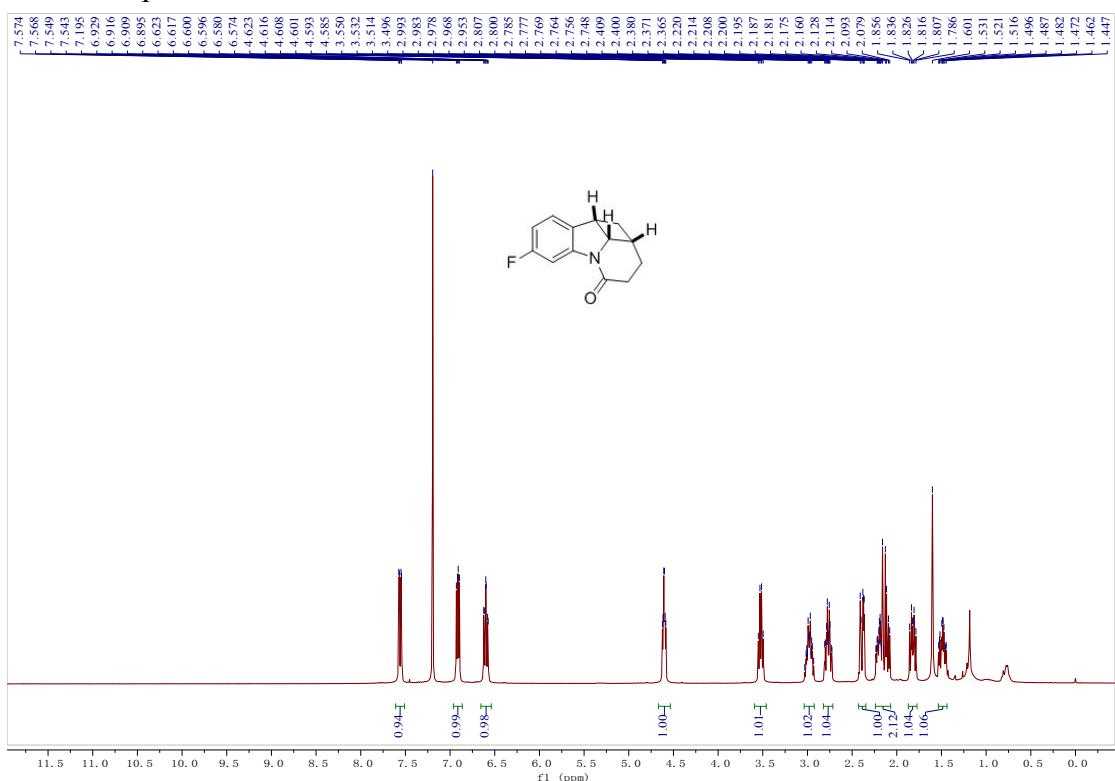
¹H NMR spectrum of **2j**



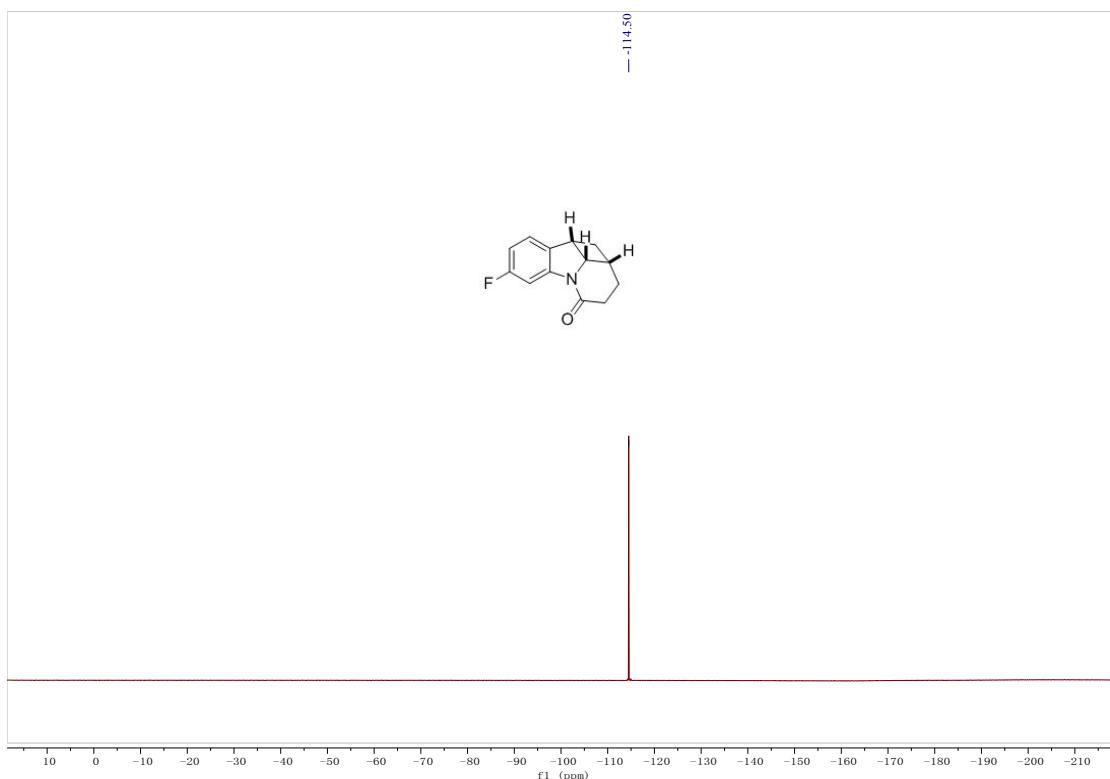
¹³C NMR spectrum of **2j**



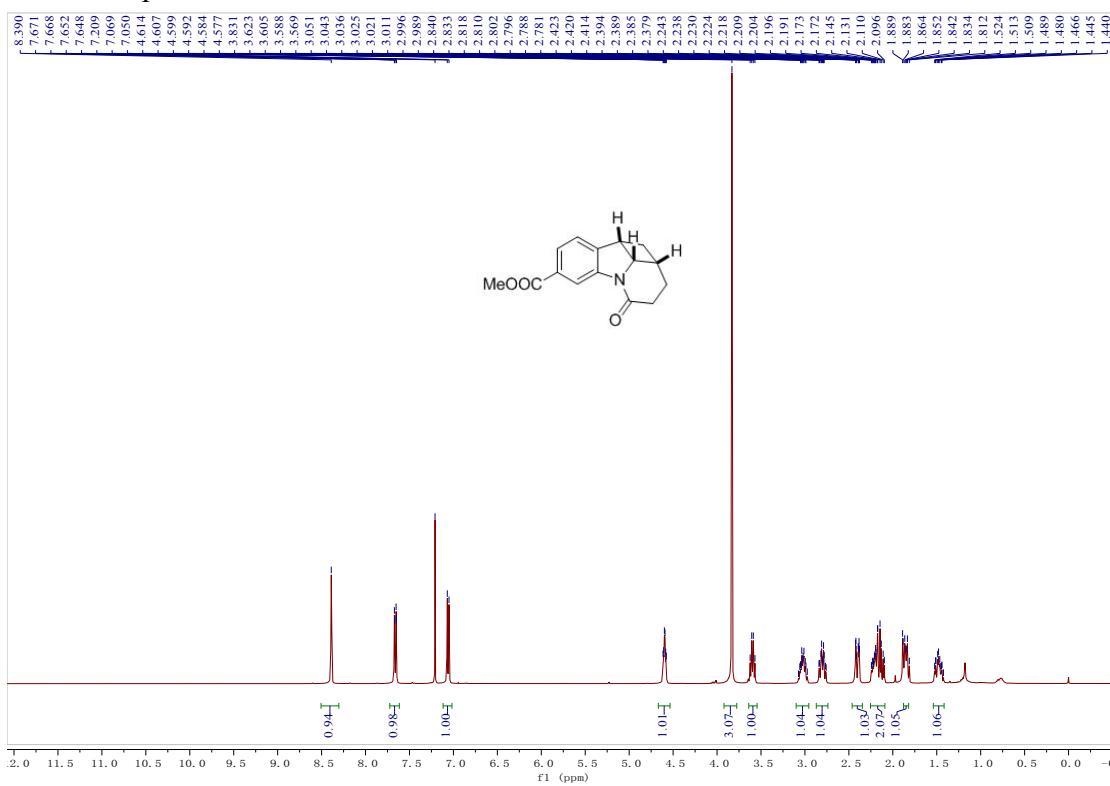
¹H NMR spectrum of **2k**



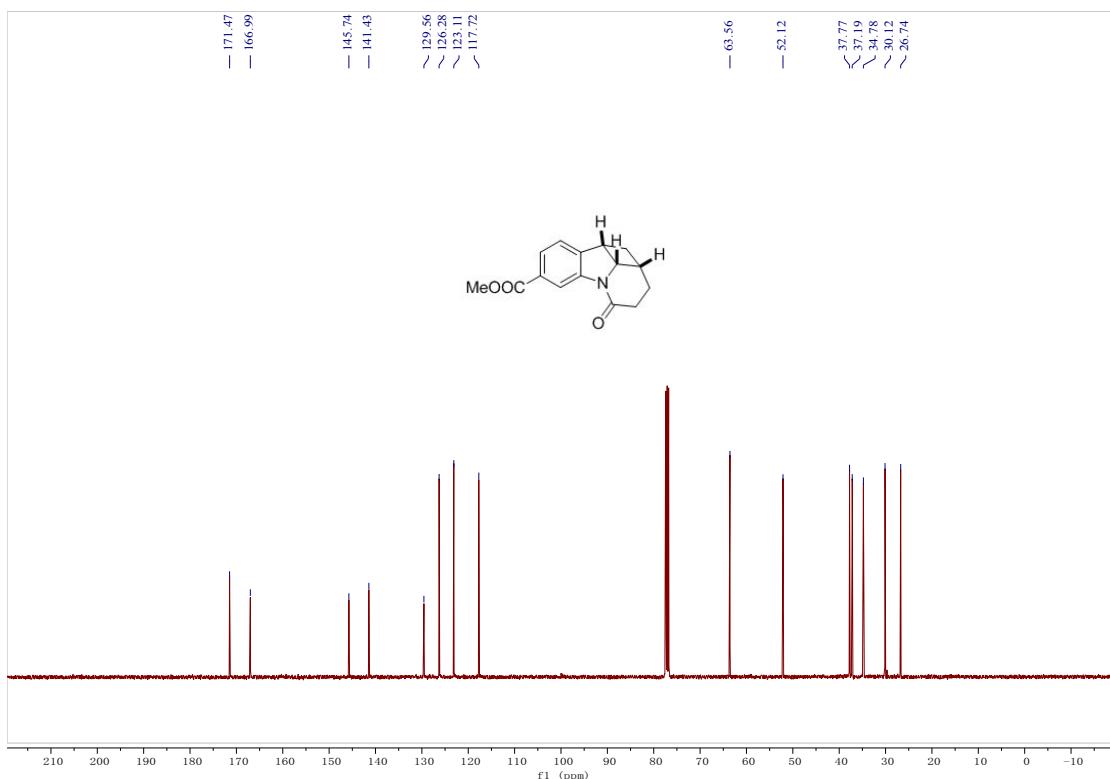
¹⁹F NMR spectrum of **2k**



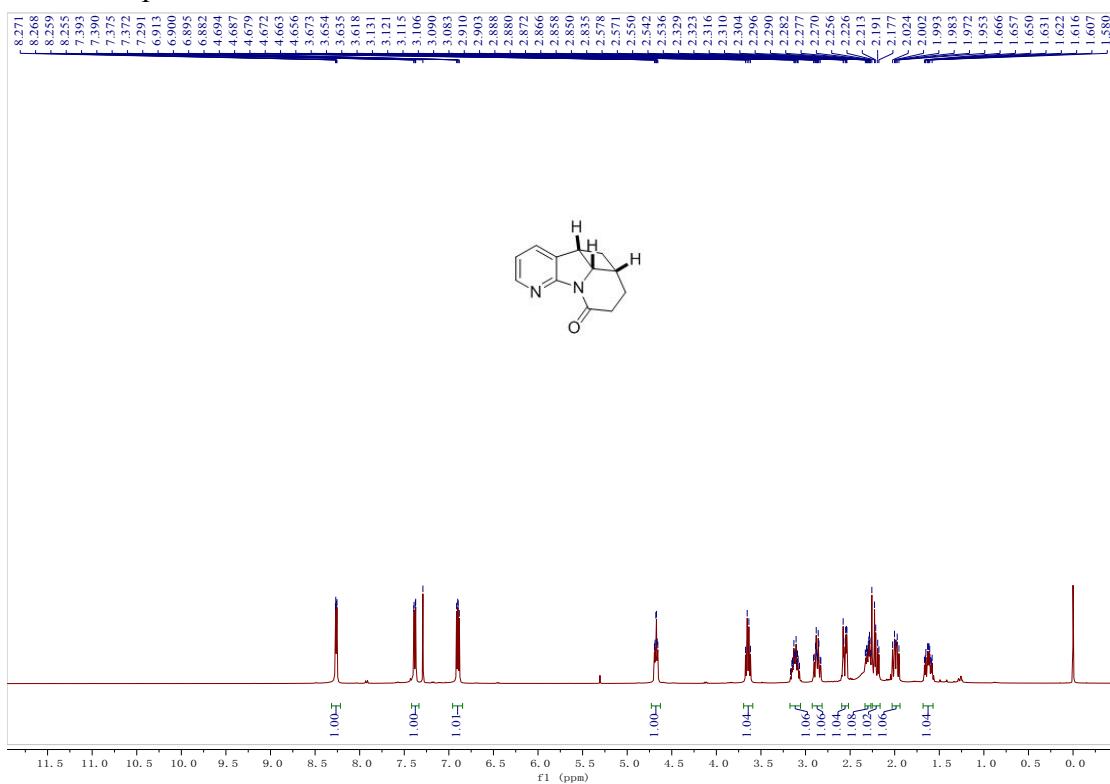
¹H NMR spectrum of **2l**



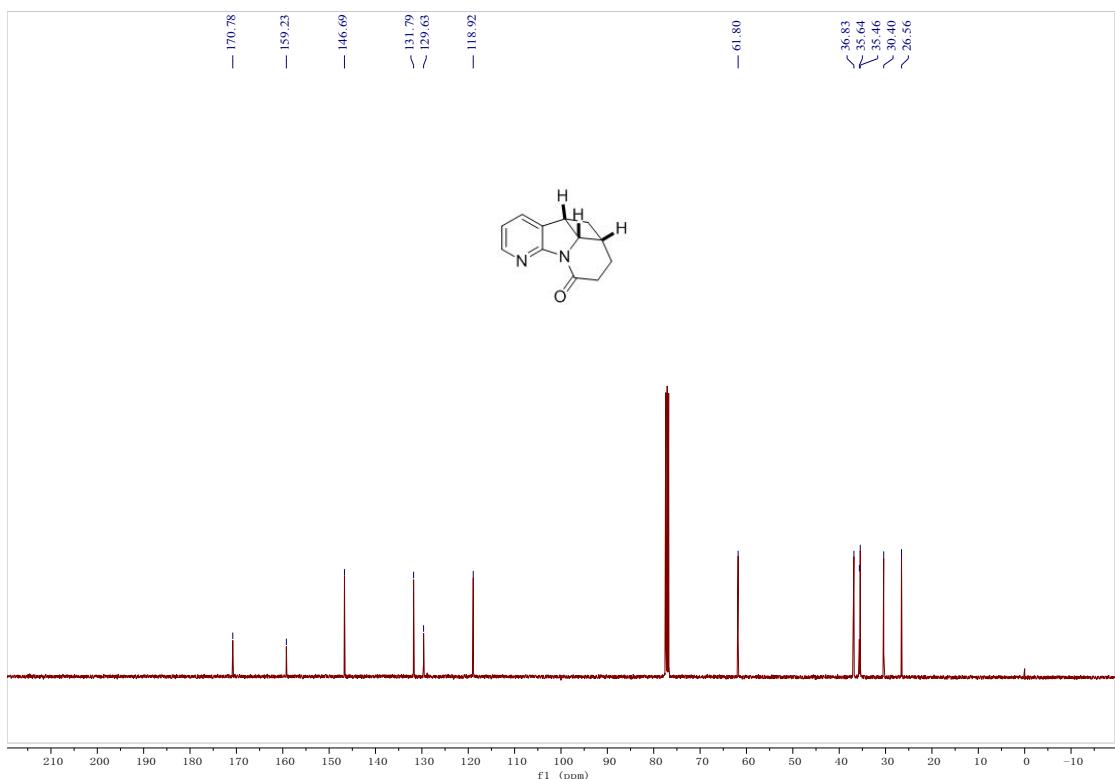
¹³C NMR spectrum of **2l**



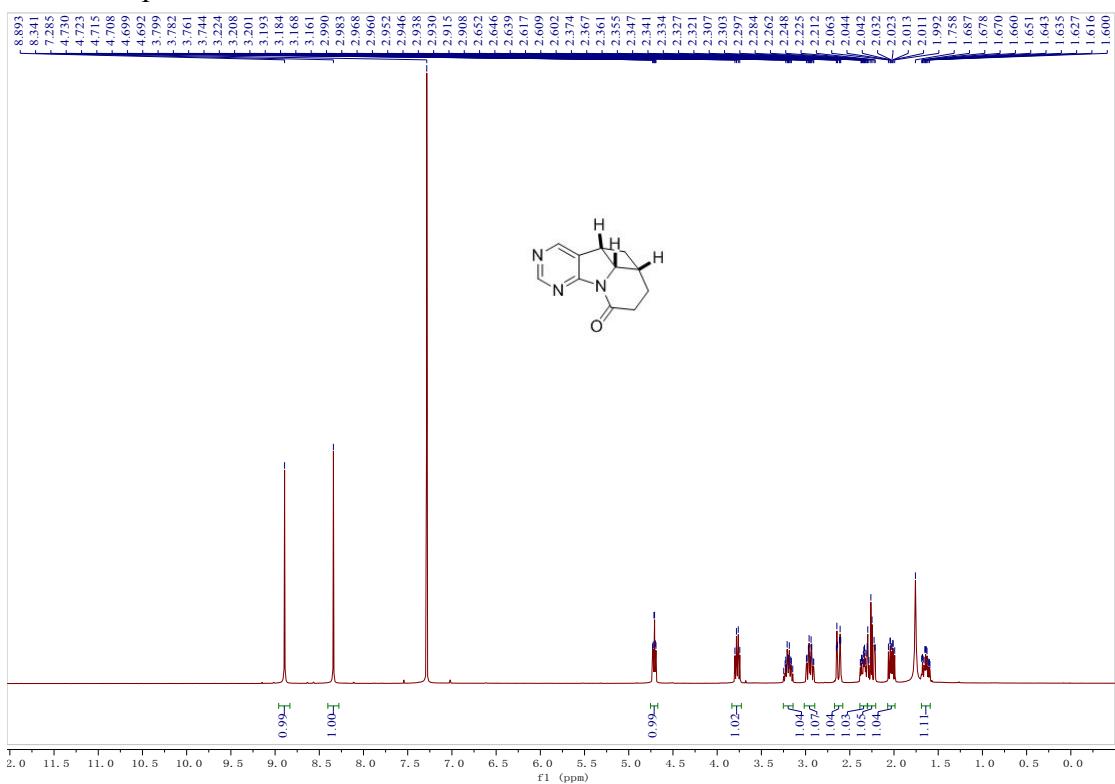
¹H NMR spectrum of **2m**



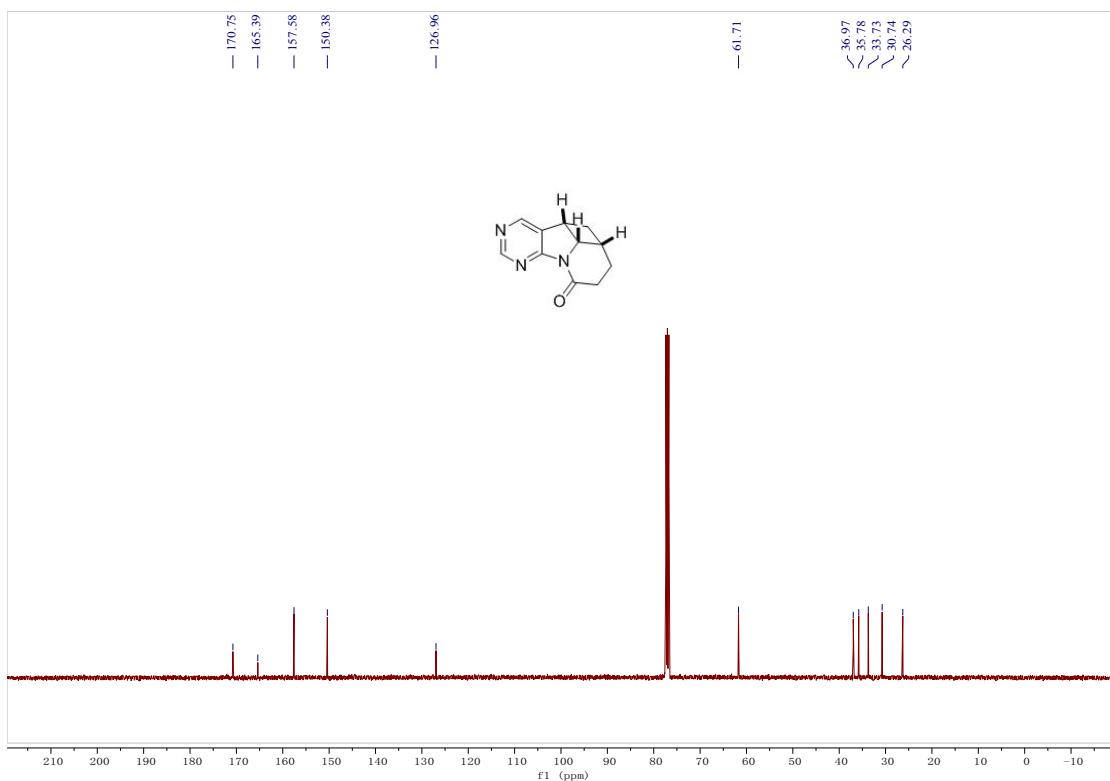
¹³C NMR spectrum of **2m**



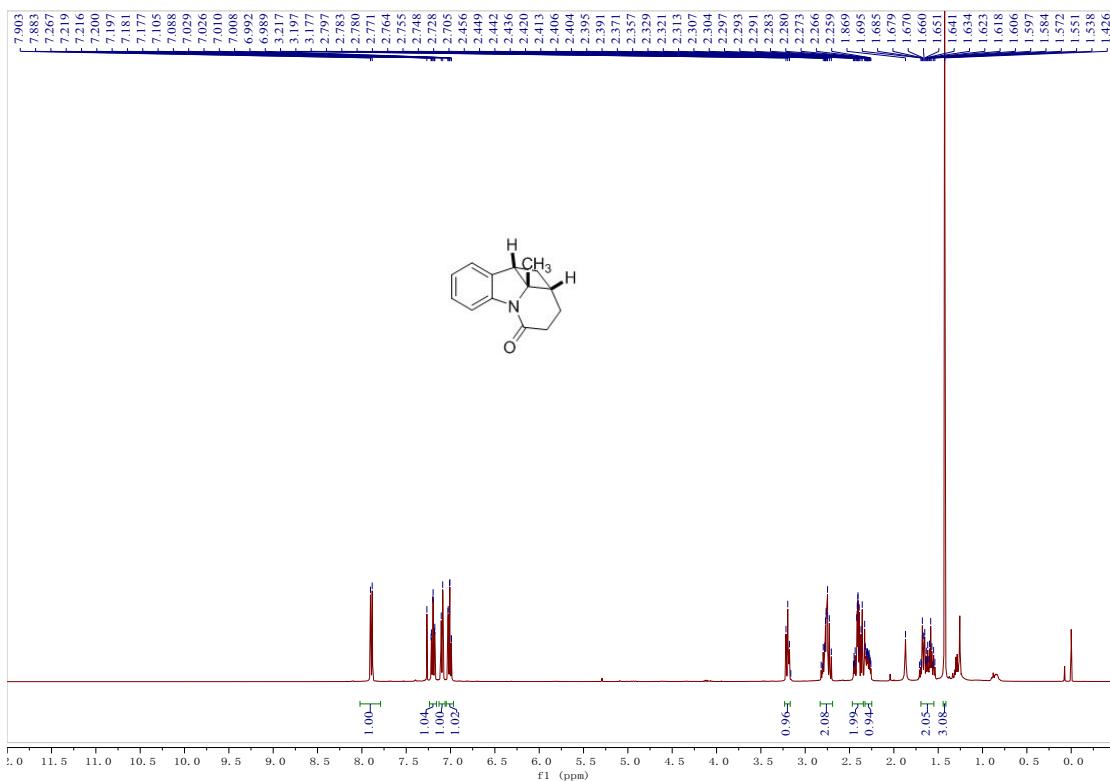
¹H NMR spectrum of **2n**



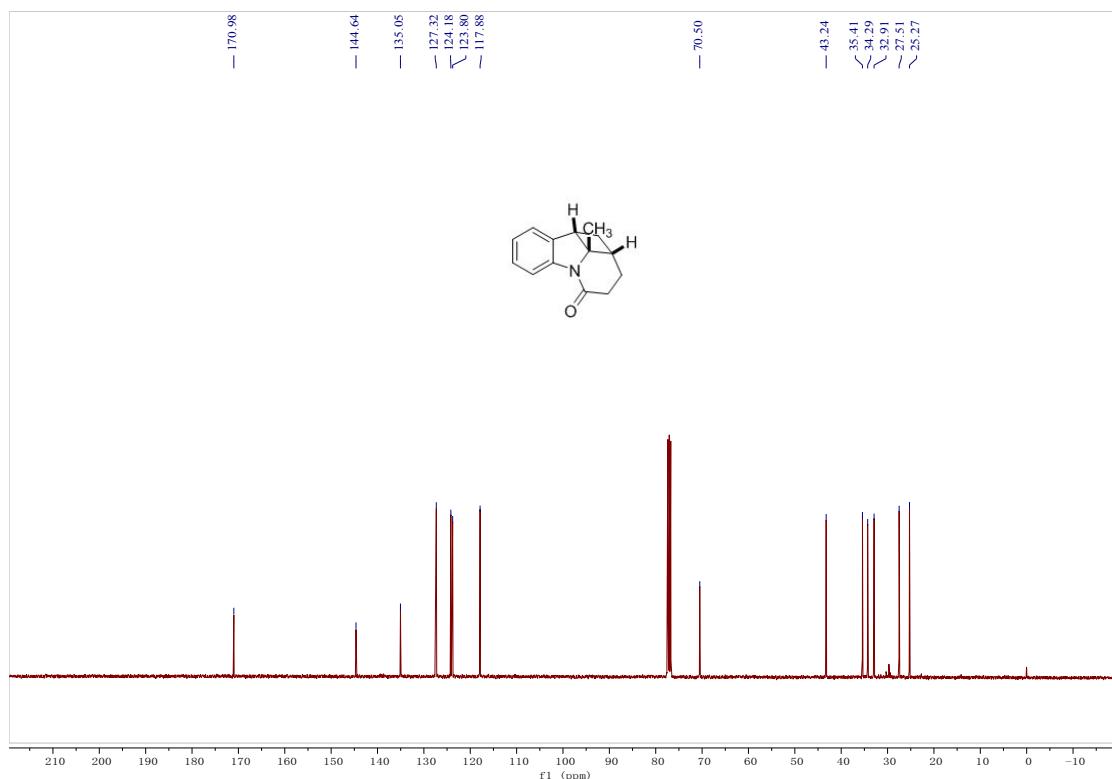
¹³C NMR spectrum of **2n**



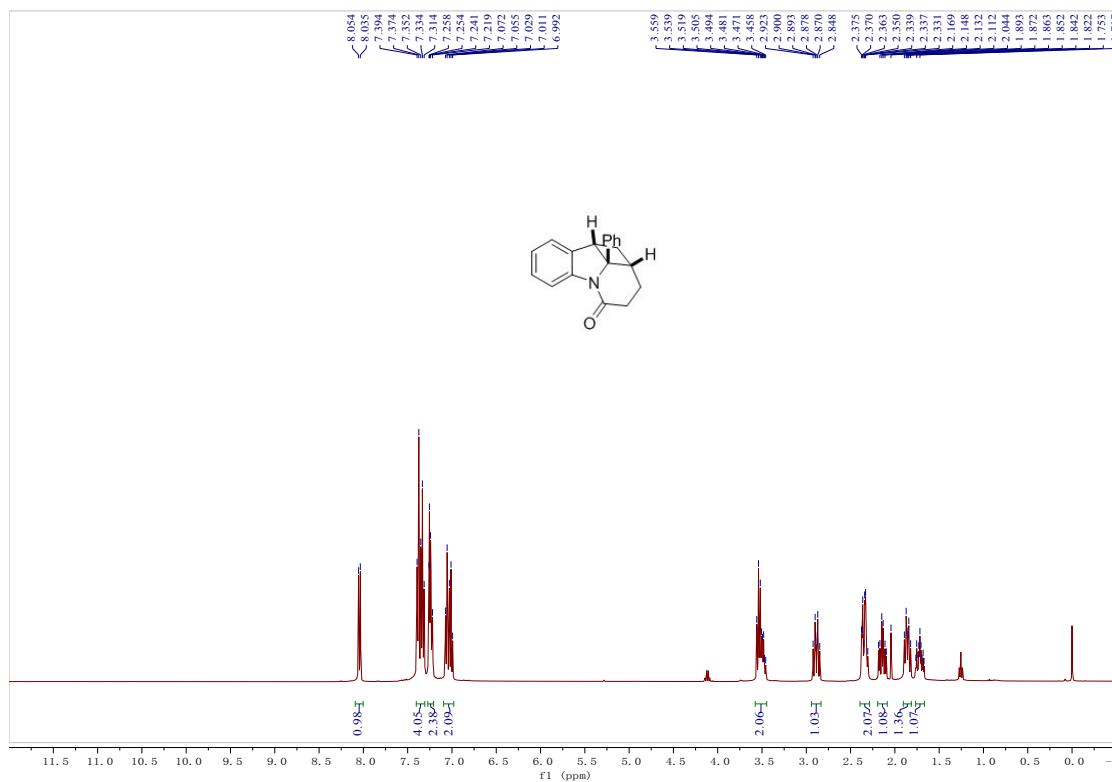
¹H NMR spectrum of 2o



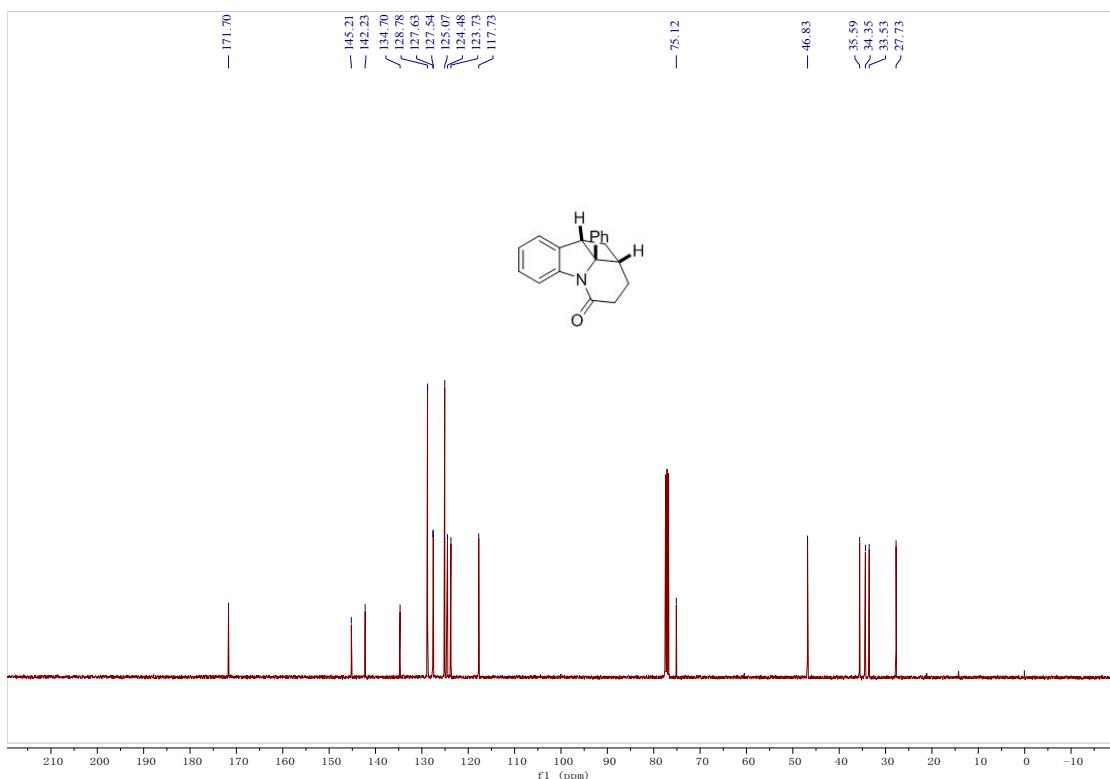
¹³C NMR spectrum of **2o**



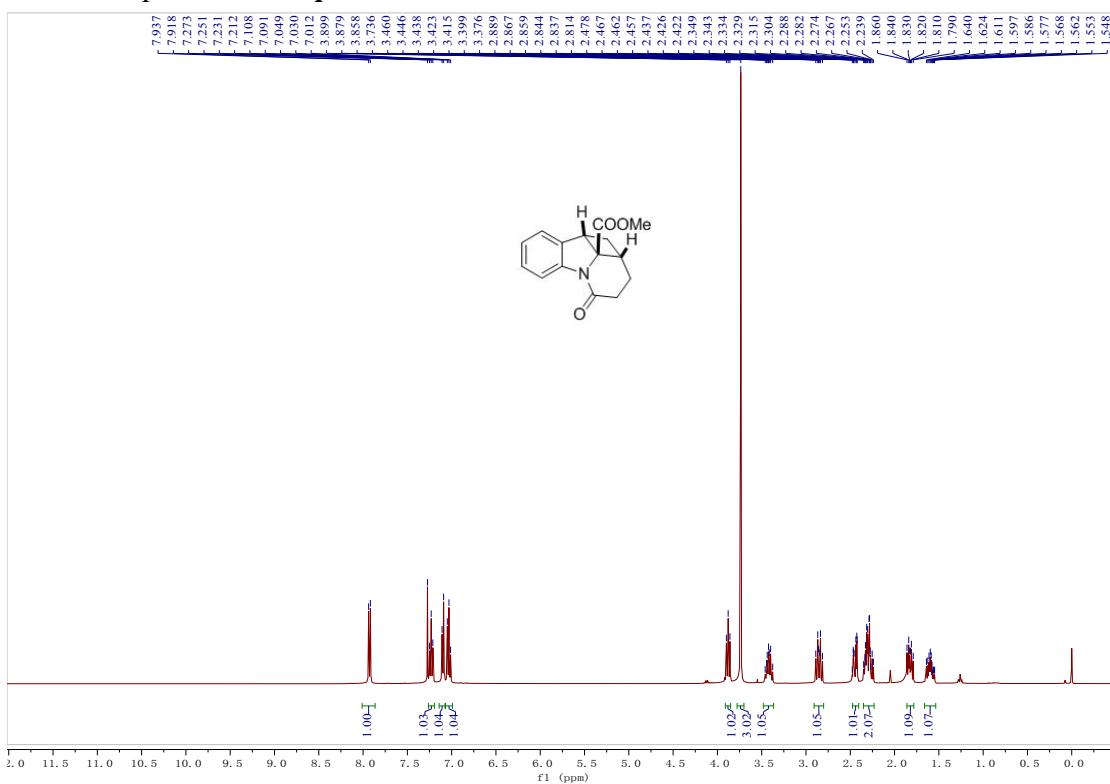
¹H NMR spectrum of **2p**



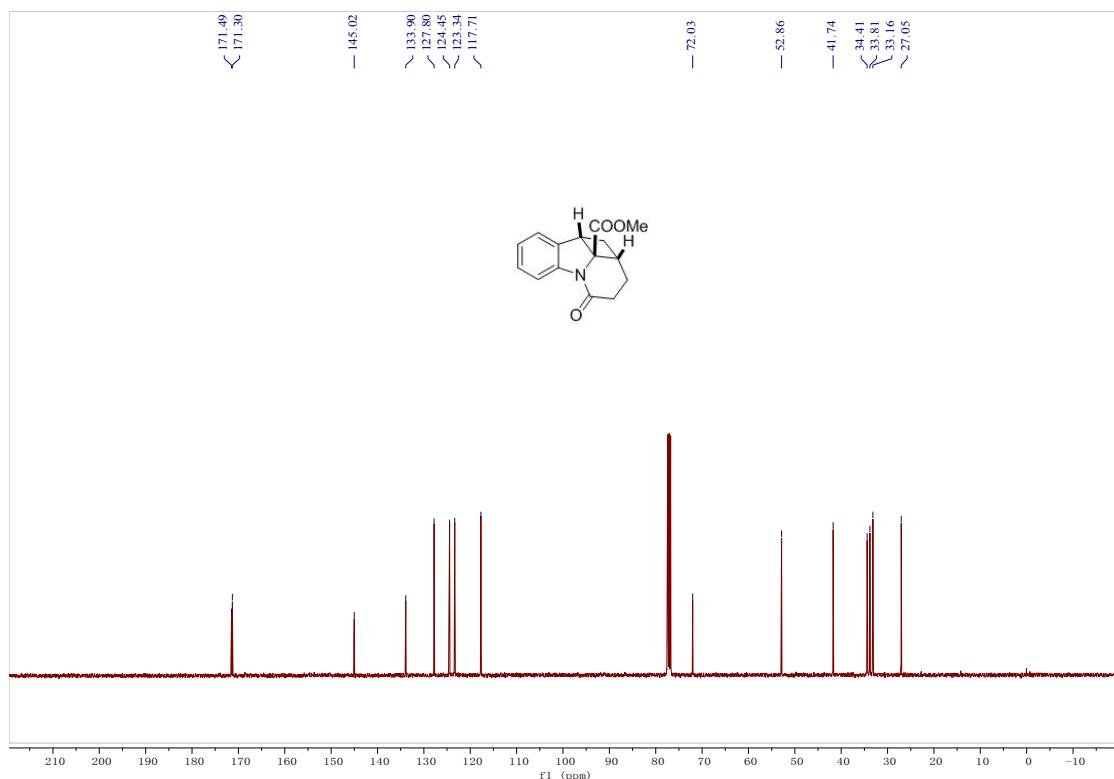
¹³C NMR spectrum of **2p**



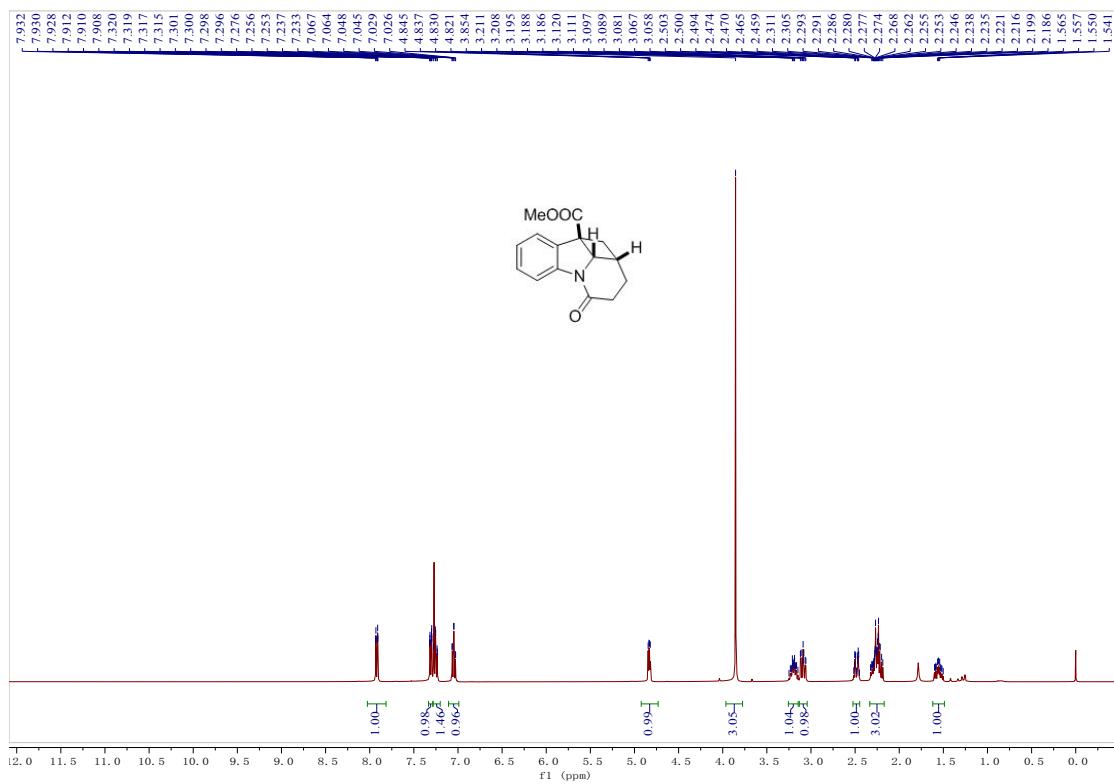
¹H NMR spectrum of **2q**



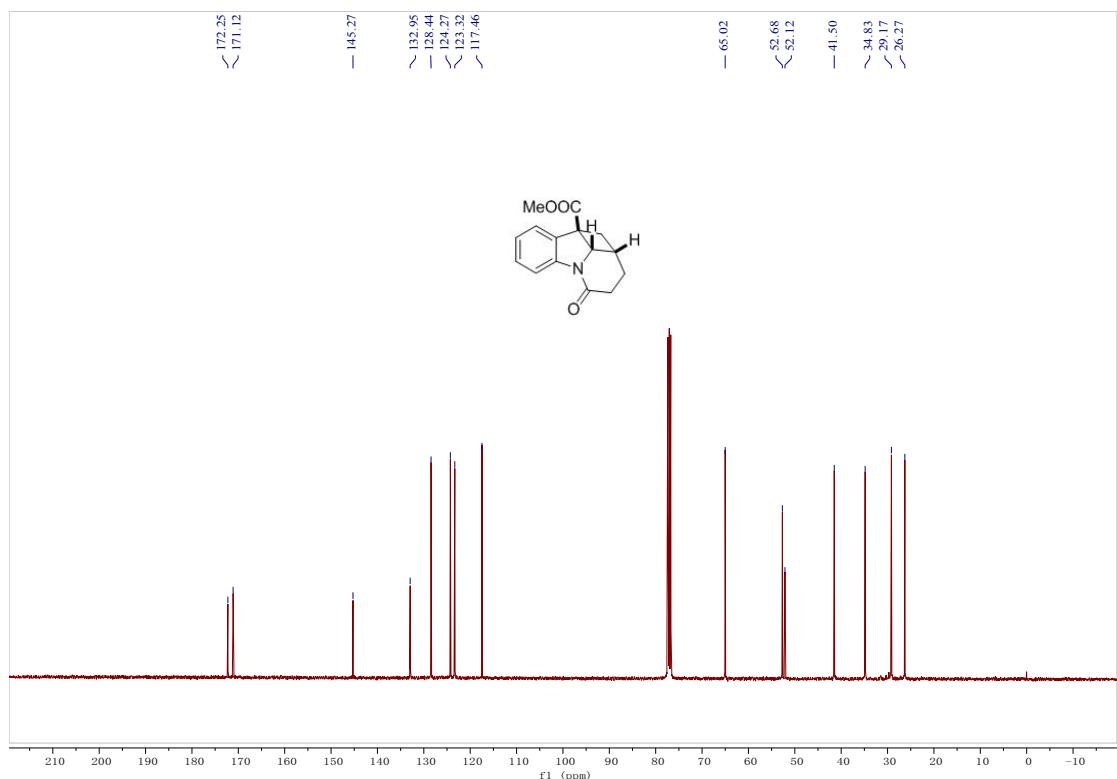
¹³C NMR spectrum of **2q**



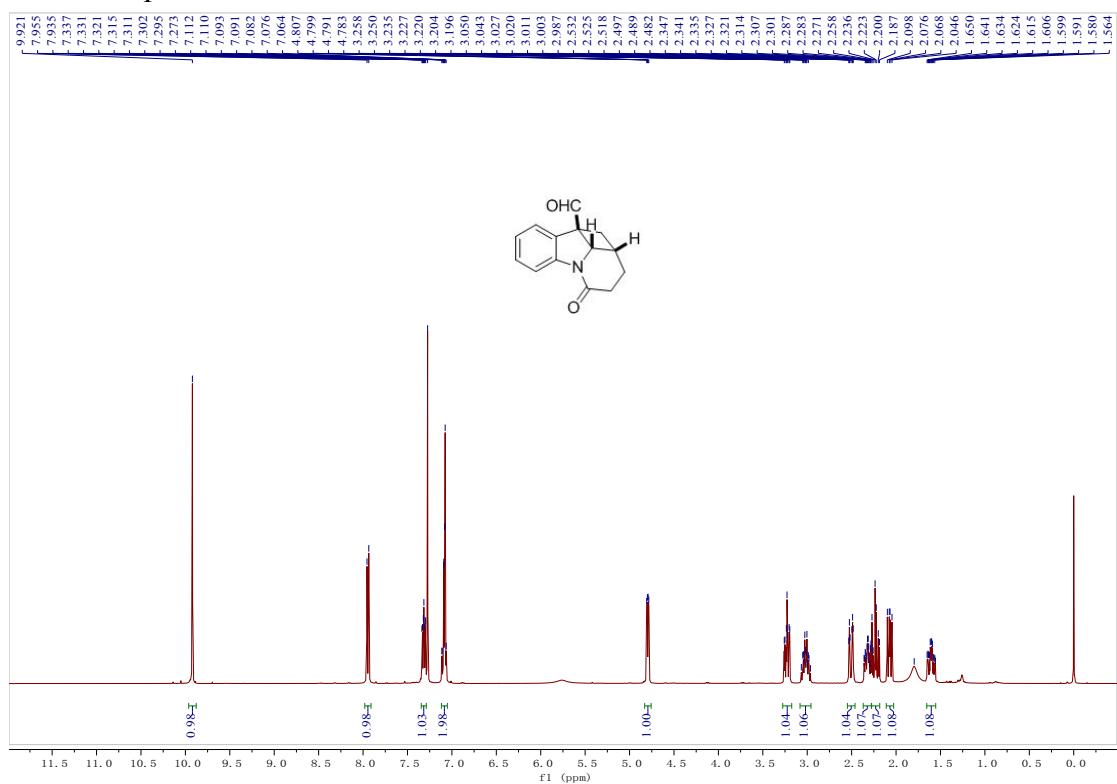
¹H NMR spectrum of **2r**



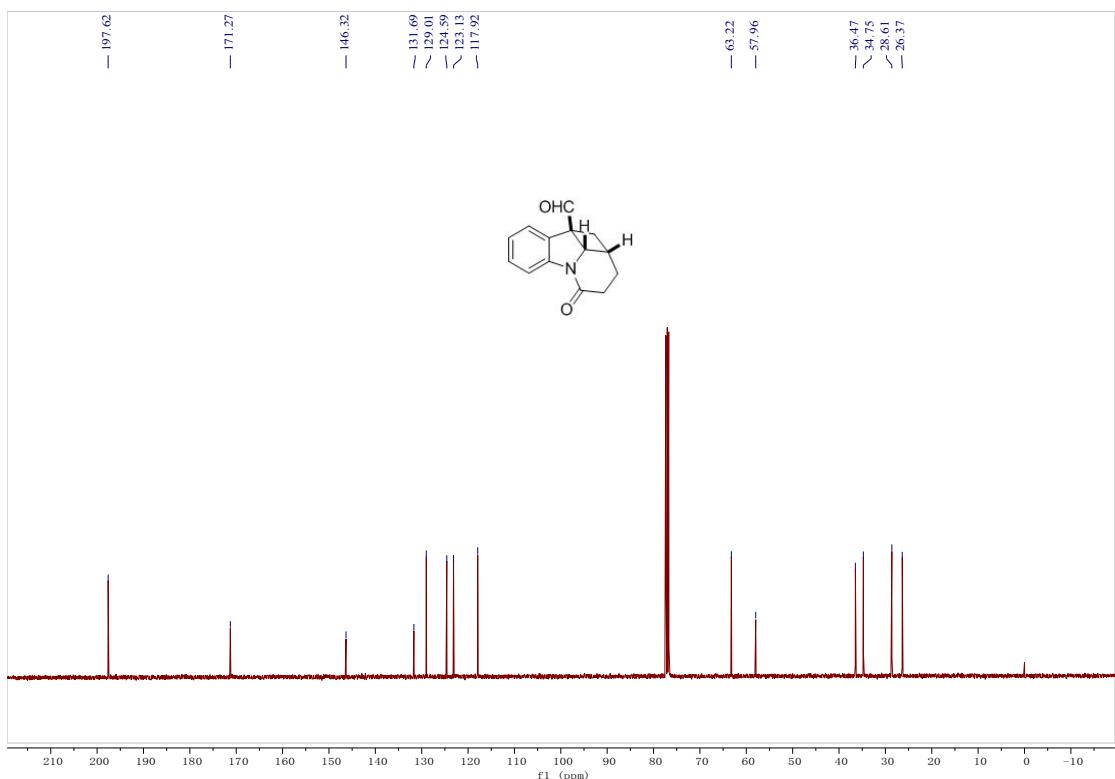
¹³C NMR spectrum of **2r**



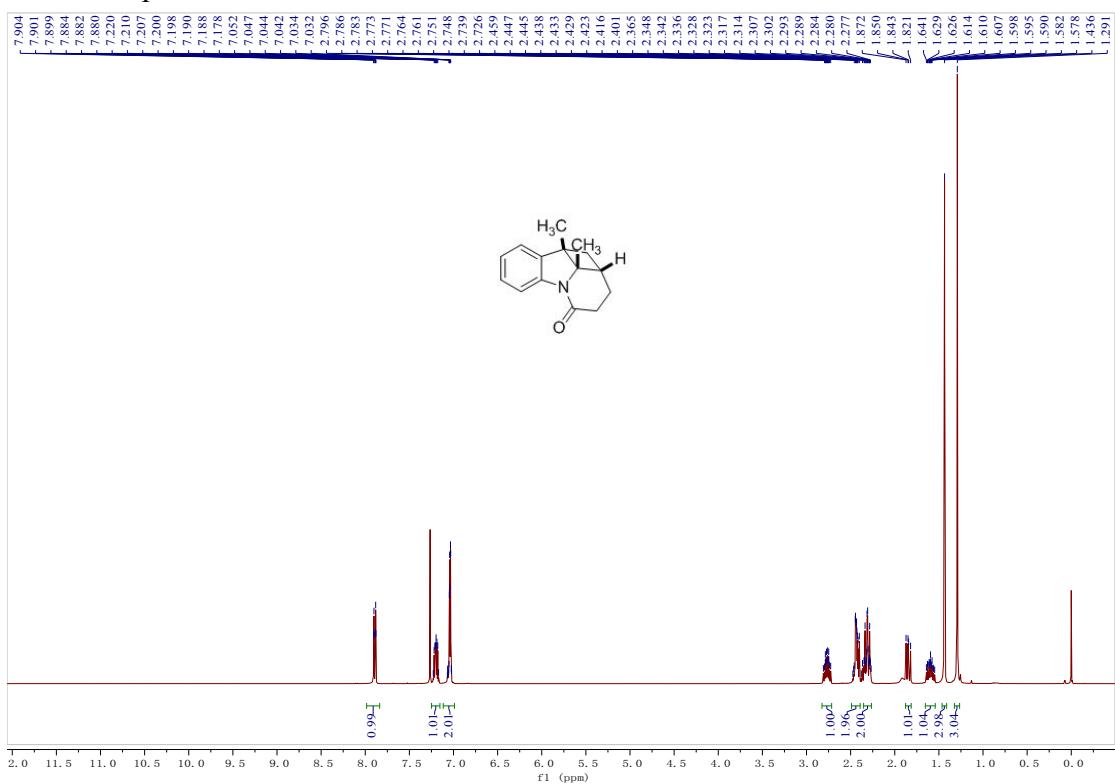
¹H NMR spectrum of **2s**



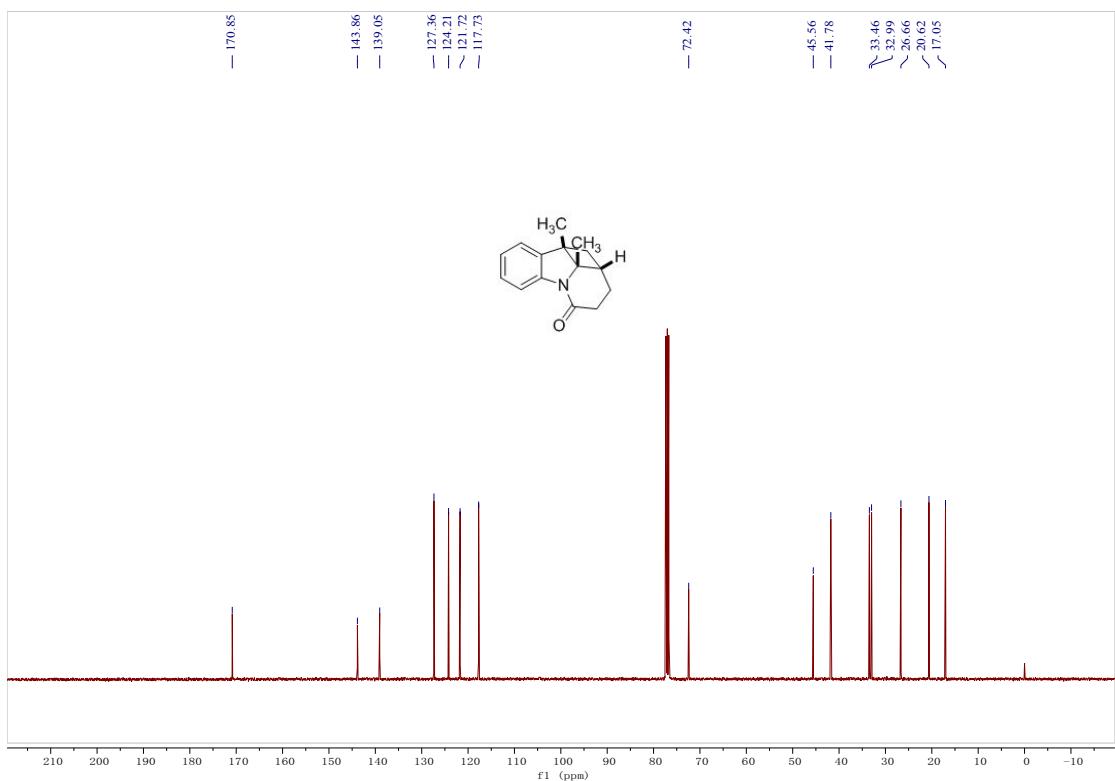
¹³C NMR spectrum of **2s**



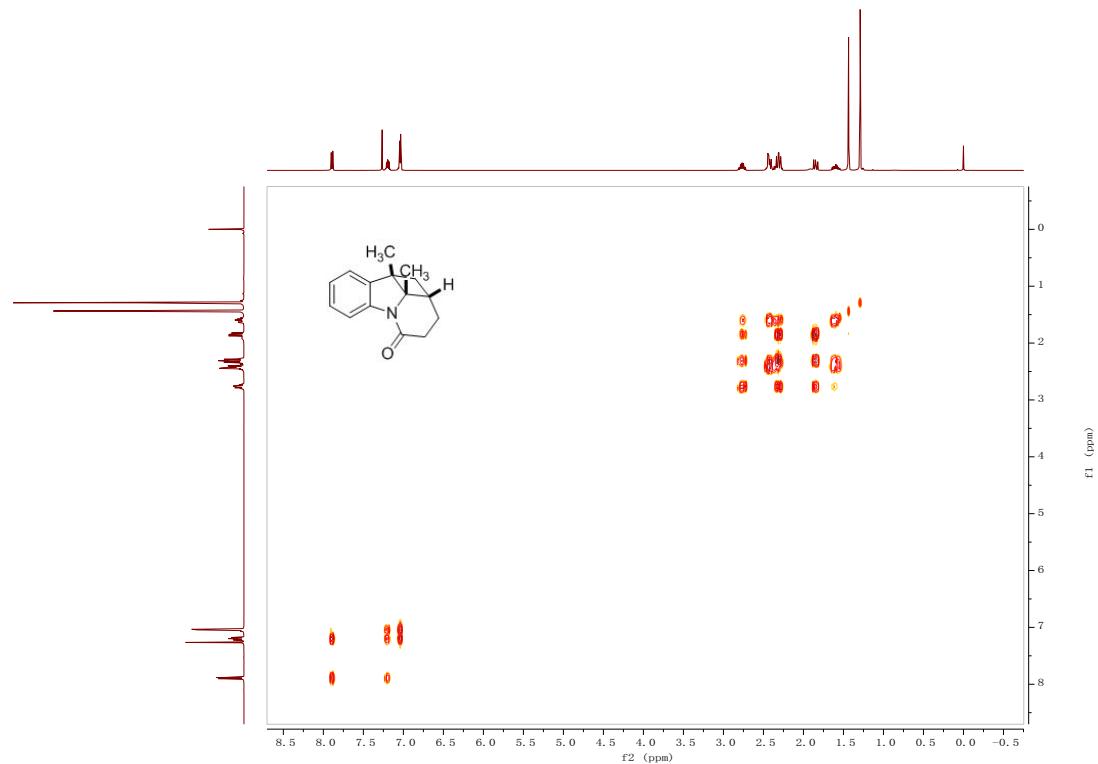
¹H NMR spectrum of 2t



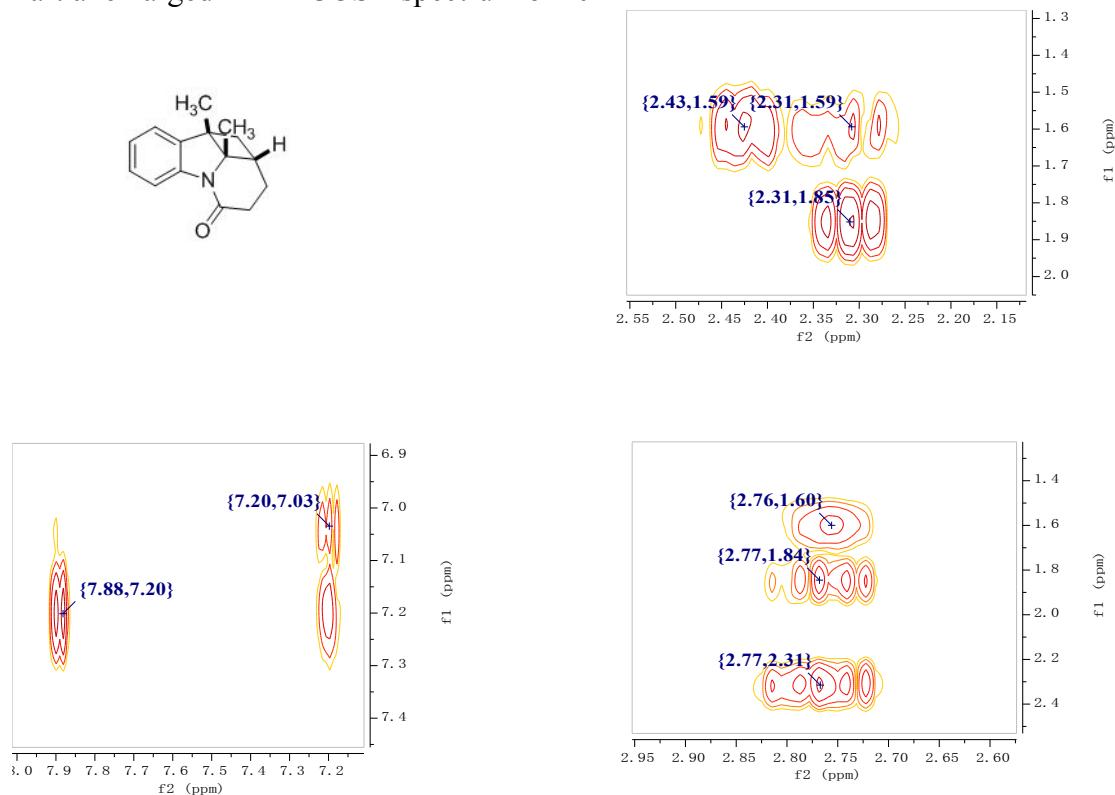
¹³C NMR spectrum of **2t**



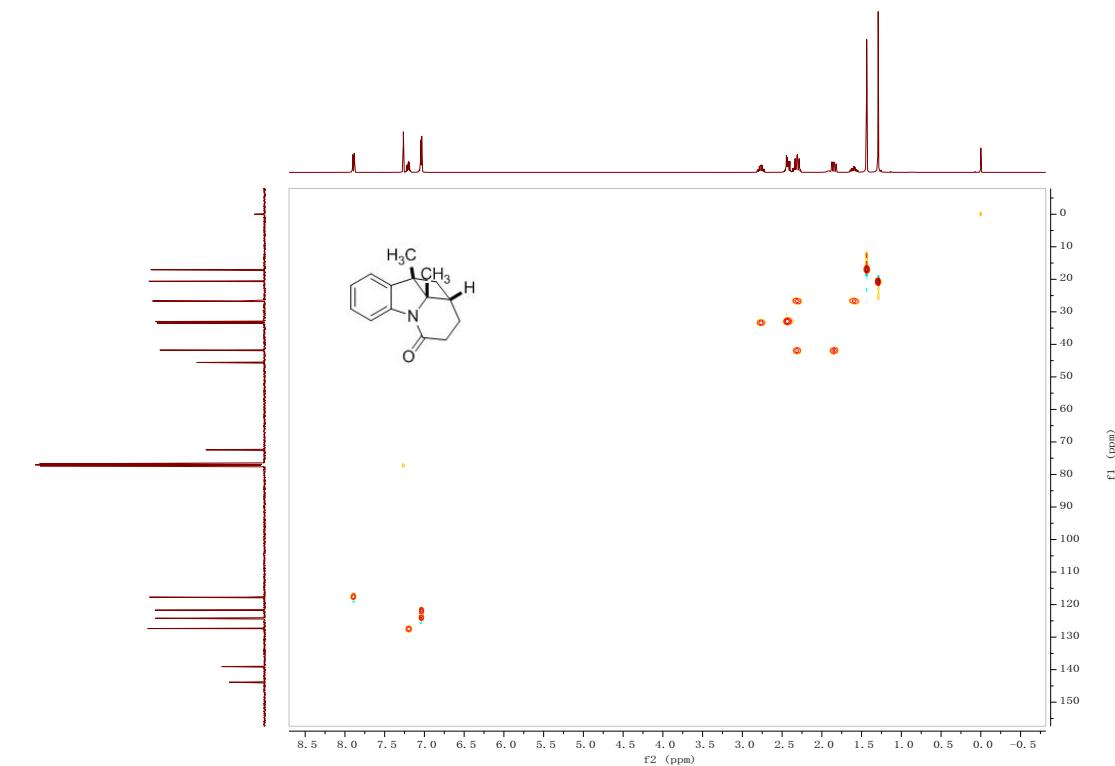
¹H-¹H COSY spectrum of **2t**



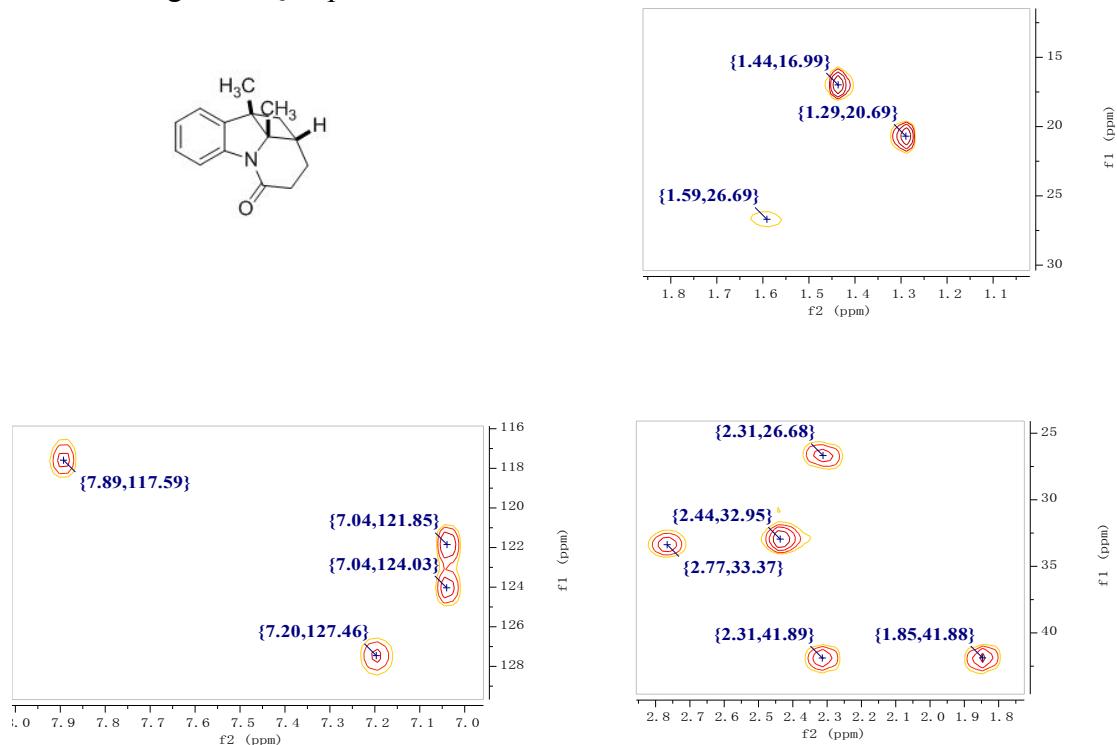
Partial enlarged ^1H - ^1H COSY spectrum of **2t**



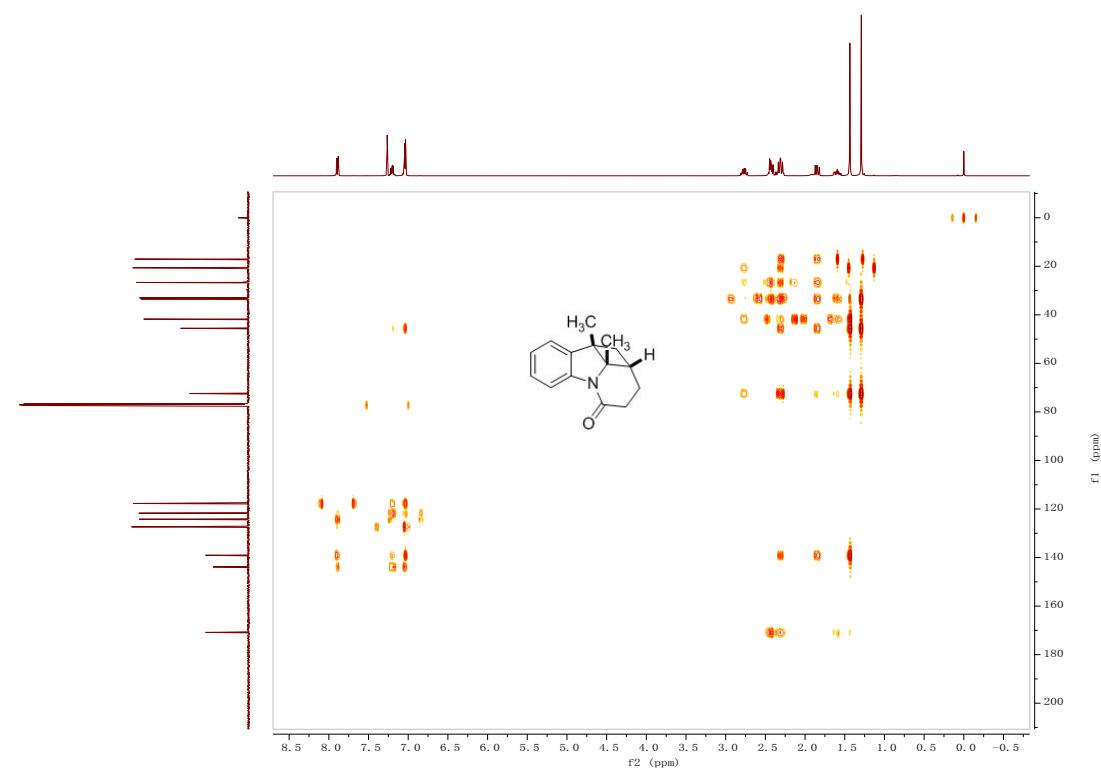
HSQC spectrum of **2t**



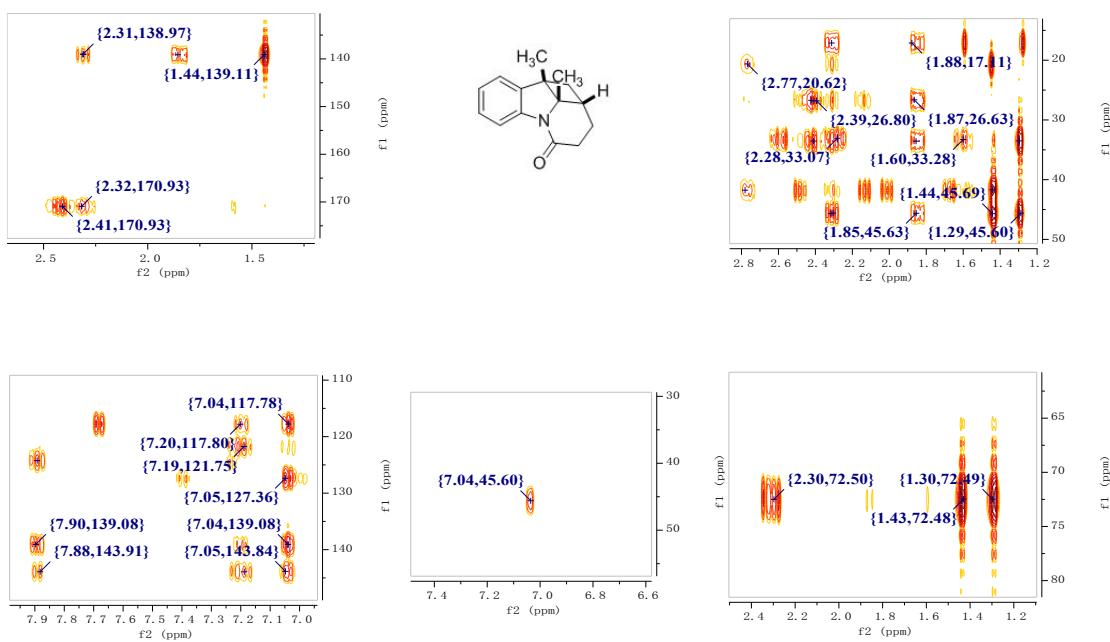
Partial enlarged HSQC spectrum of **2t**



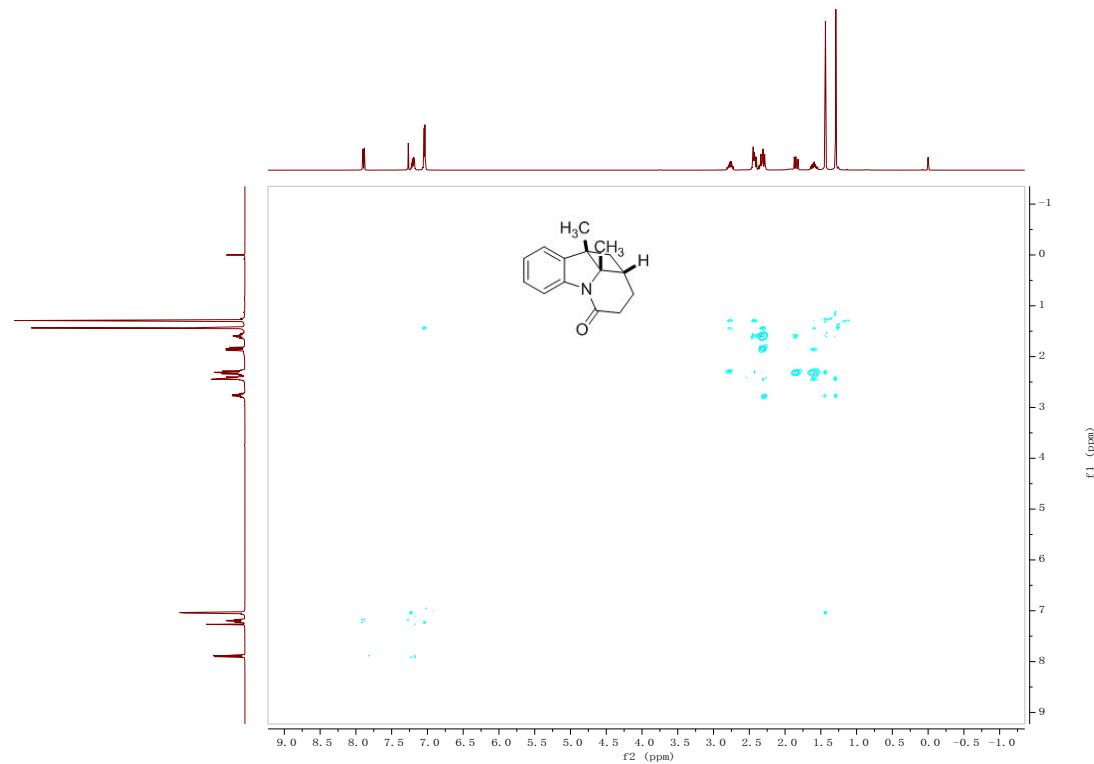
HMBC spectrum of **2t**



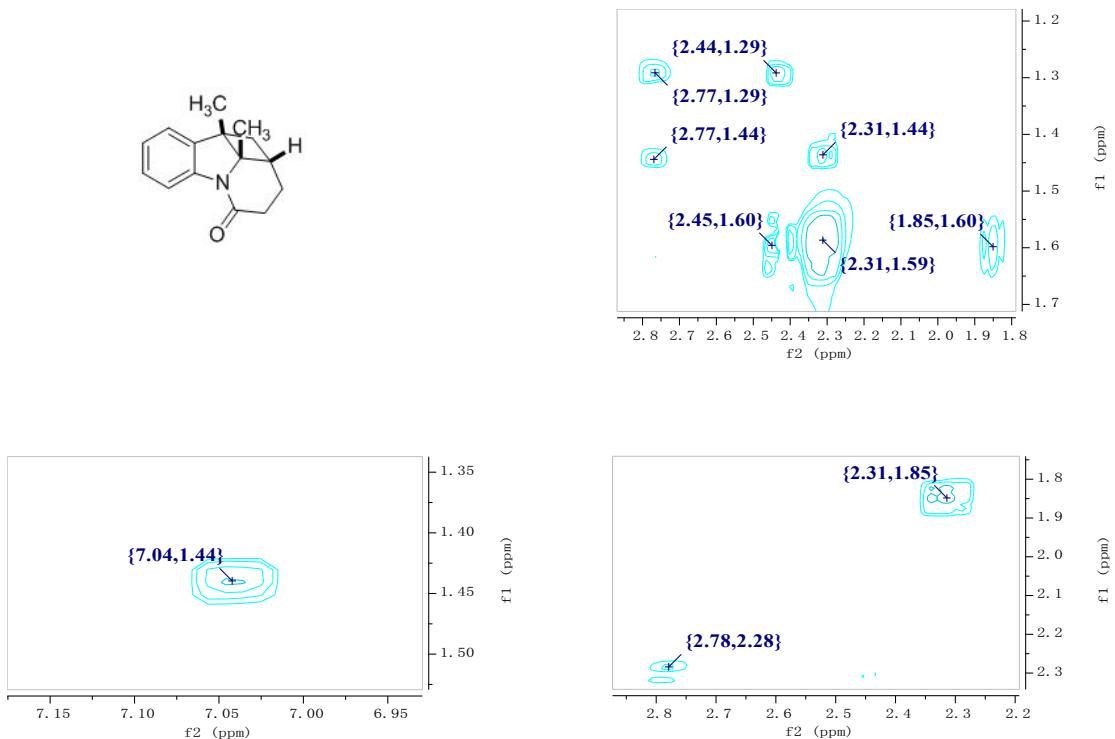
Partial enlarged HMBC spectrum of **2t**



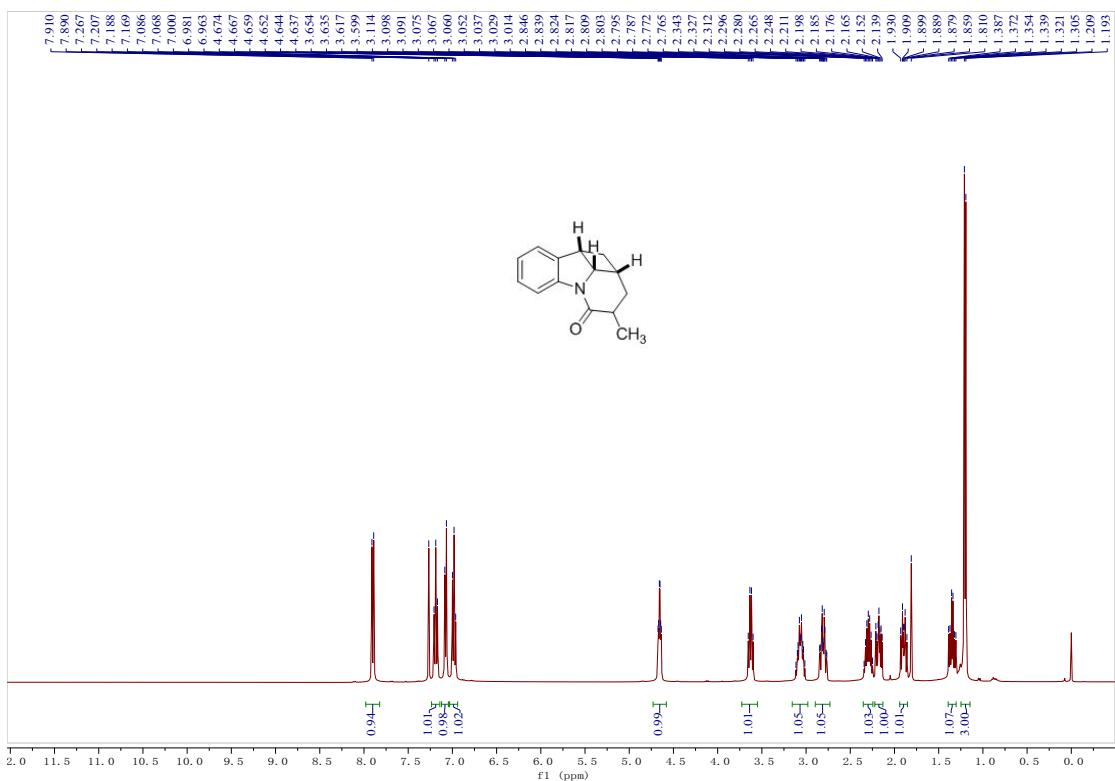
NOESY spectrum of **2t**



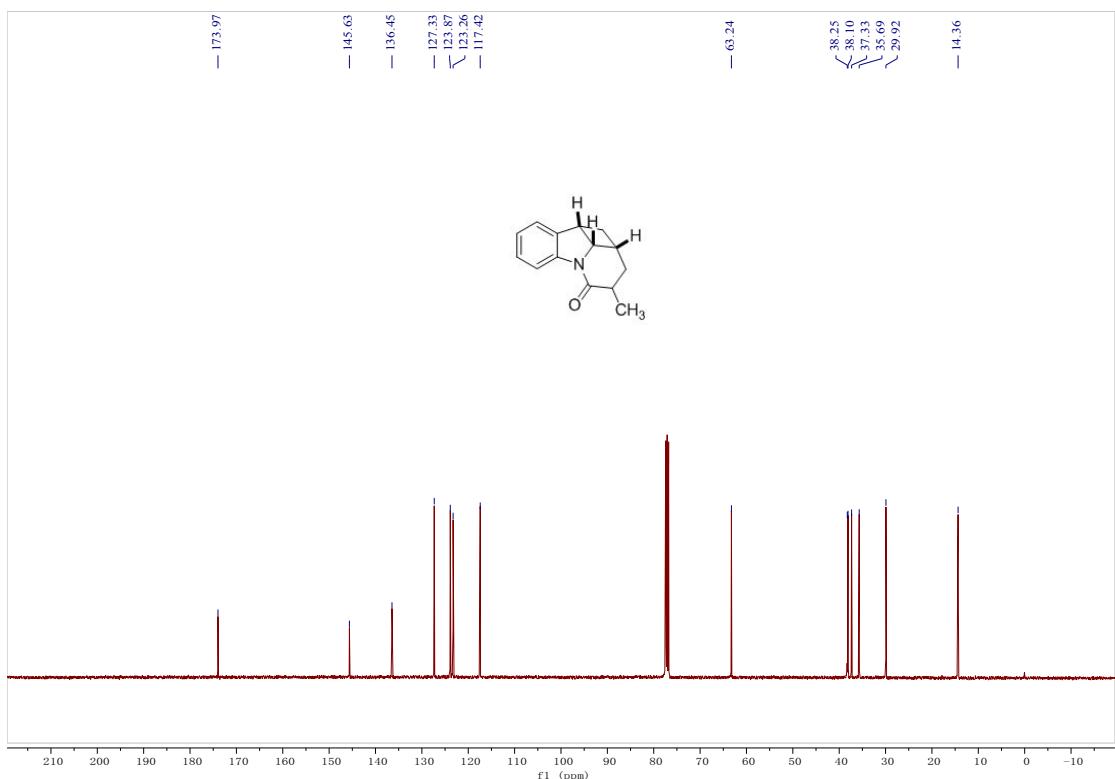
Partial enlarged NOESY spectrum of **2t**



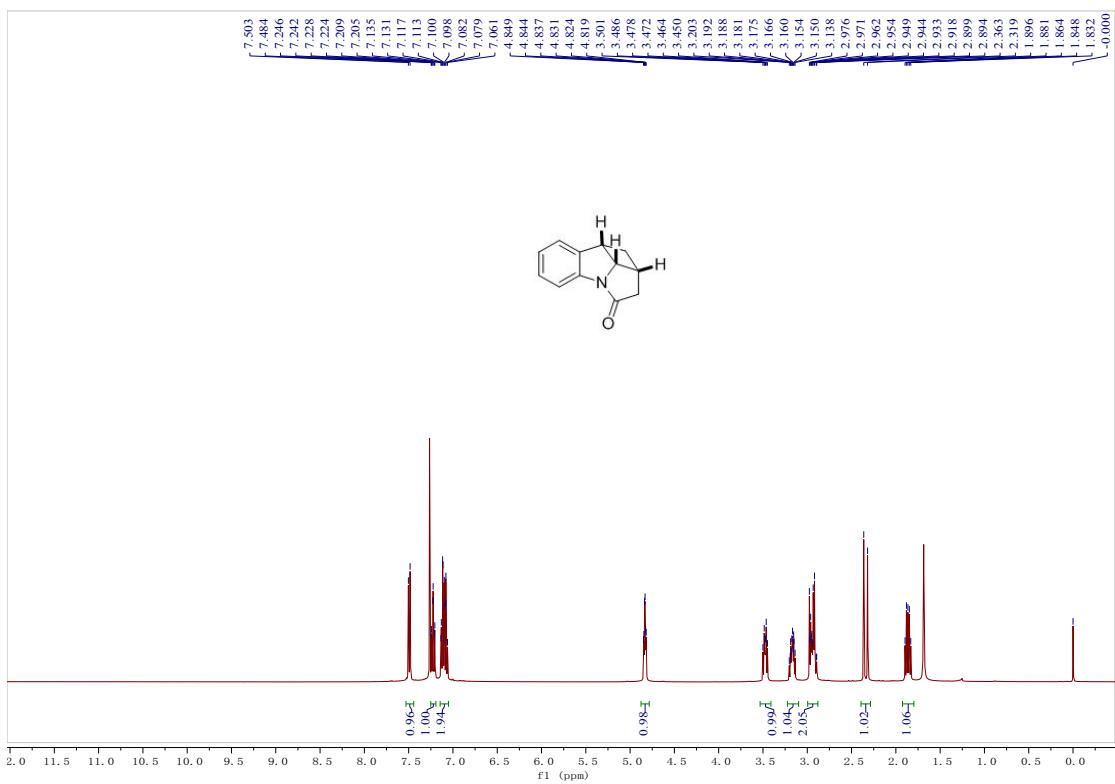
^1H NMR spectrum of **2u**



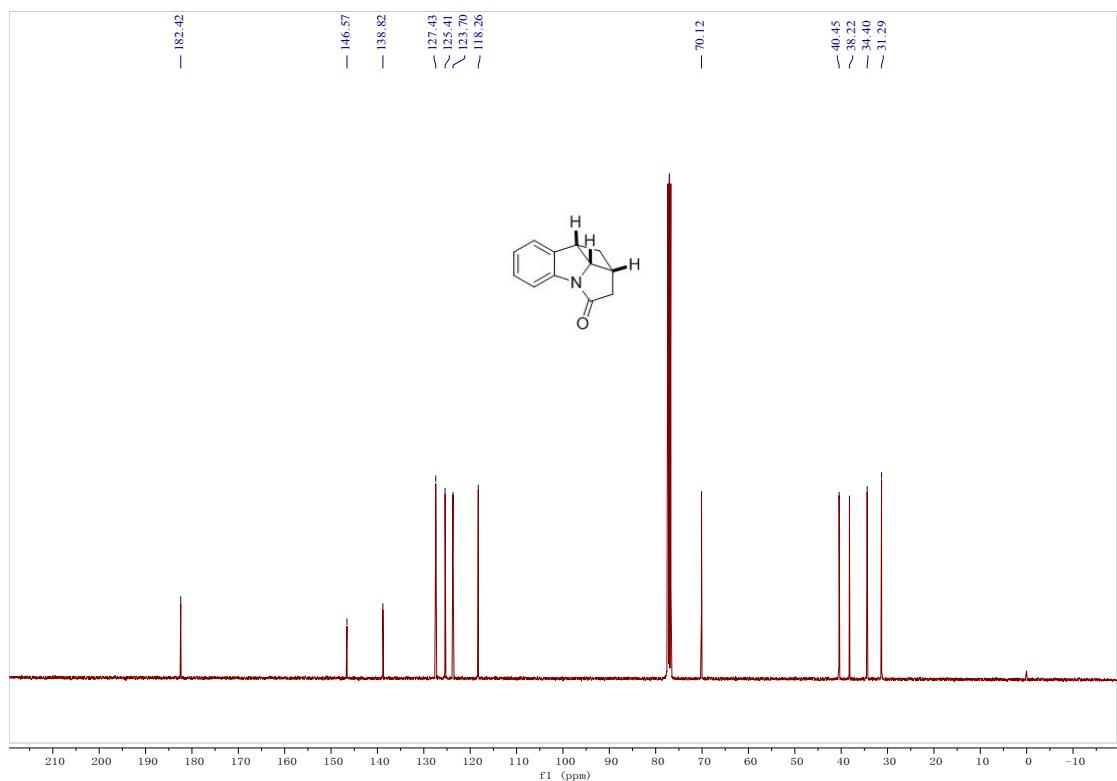
¹³C NMR spectrum of **2u**



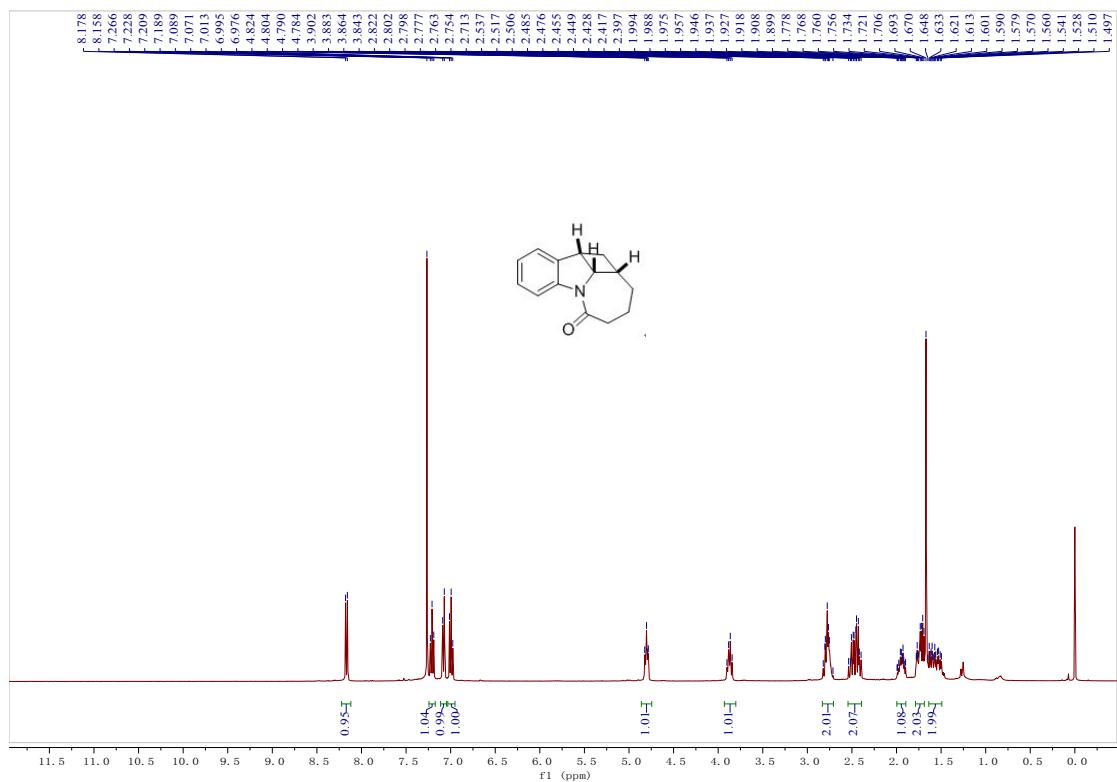
¹H NMR spectrum of **2v**



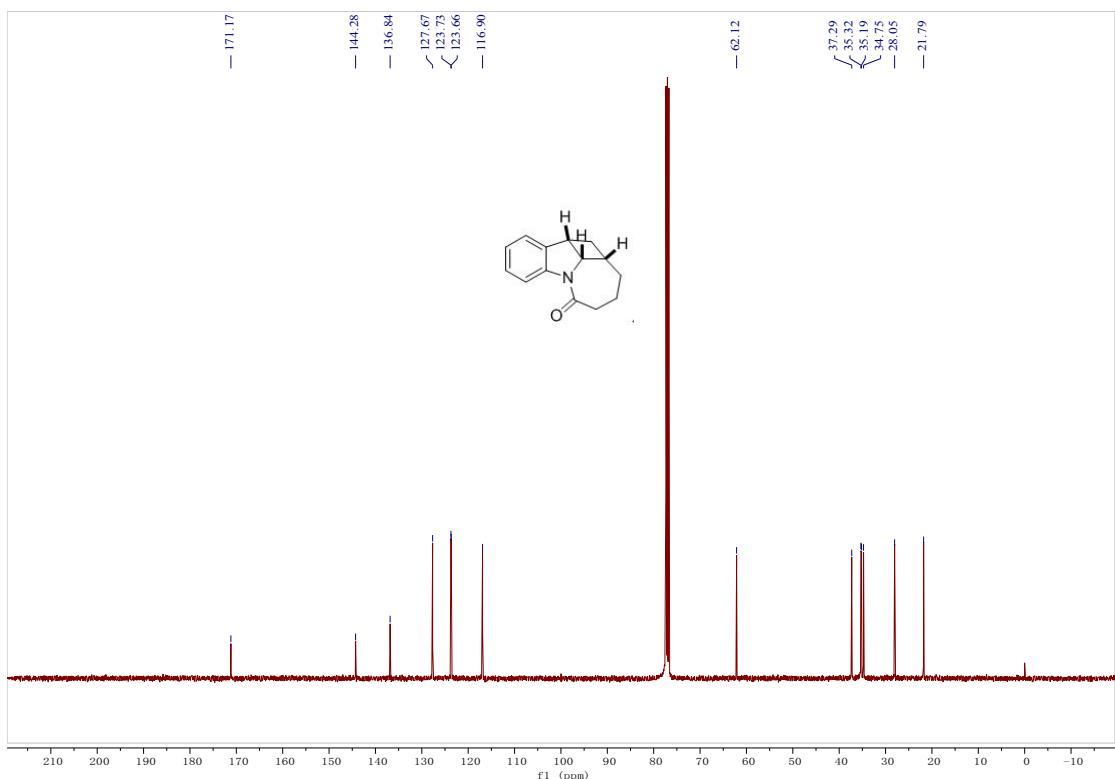
¹³C NMR spectrum of **2v**



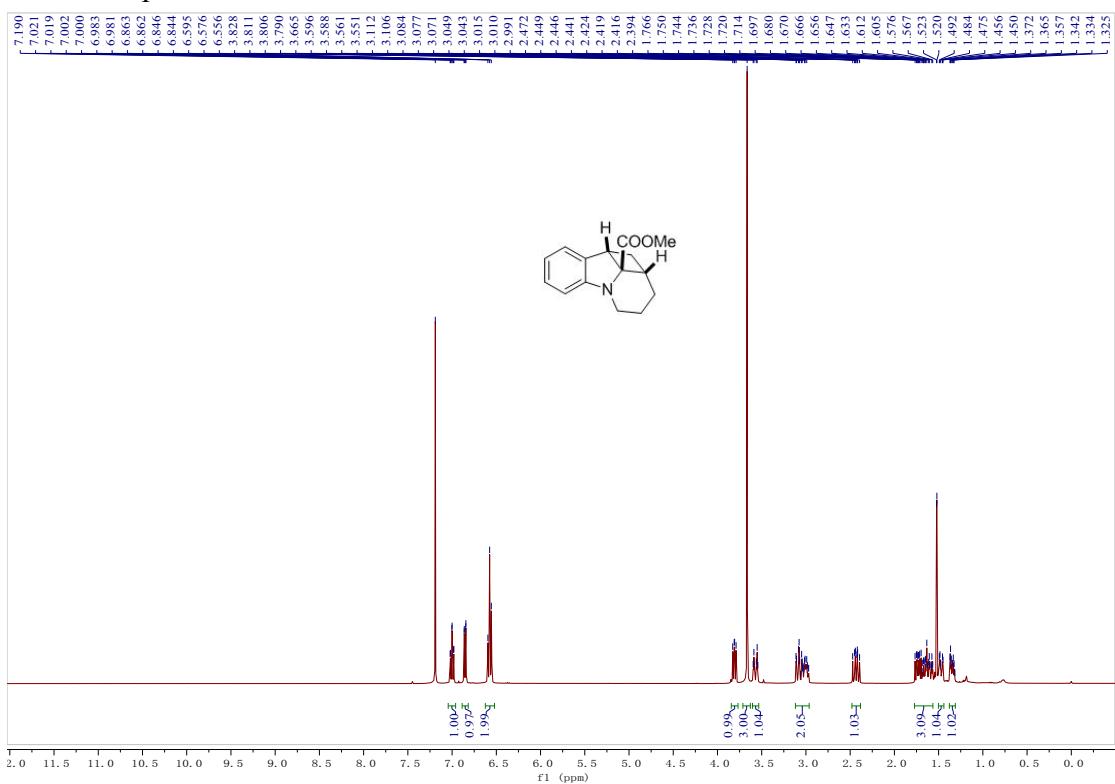
¹H NMR spectrum of **2w**



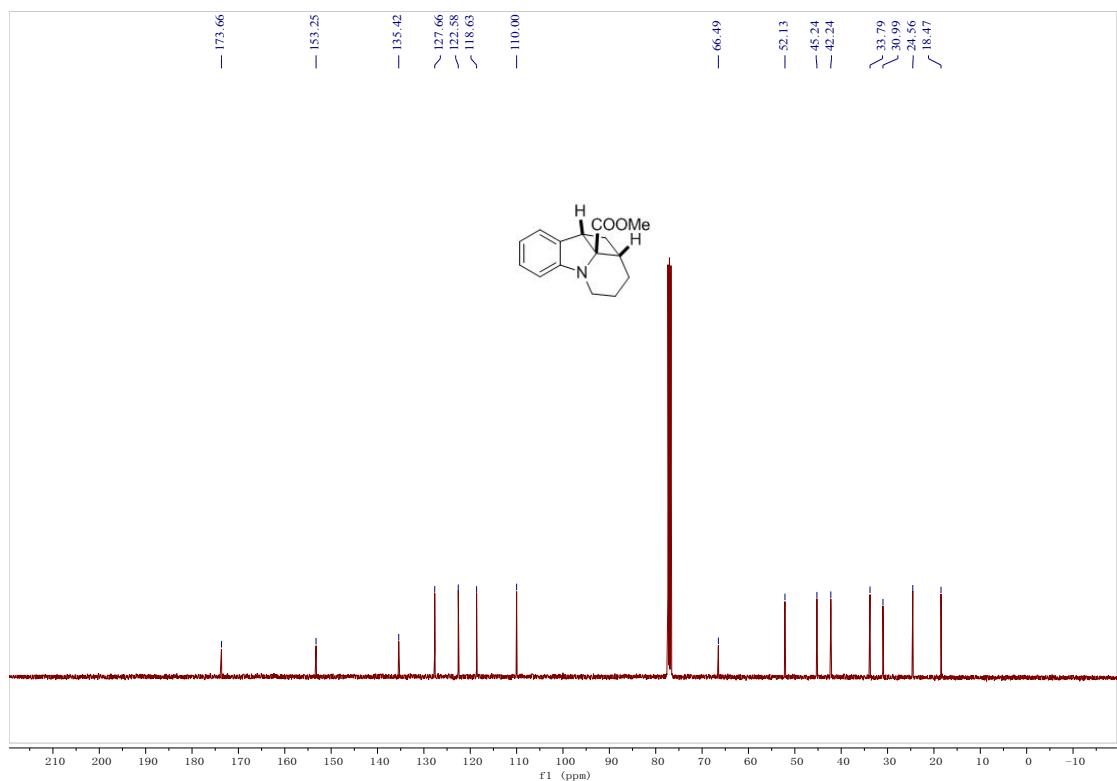
¹³C NMR spectrum of **2w**



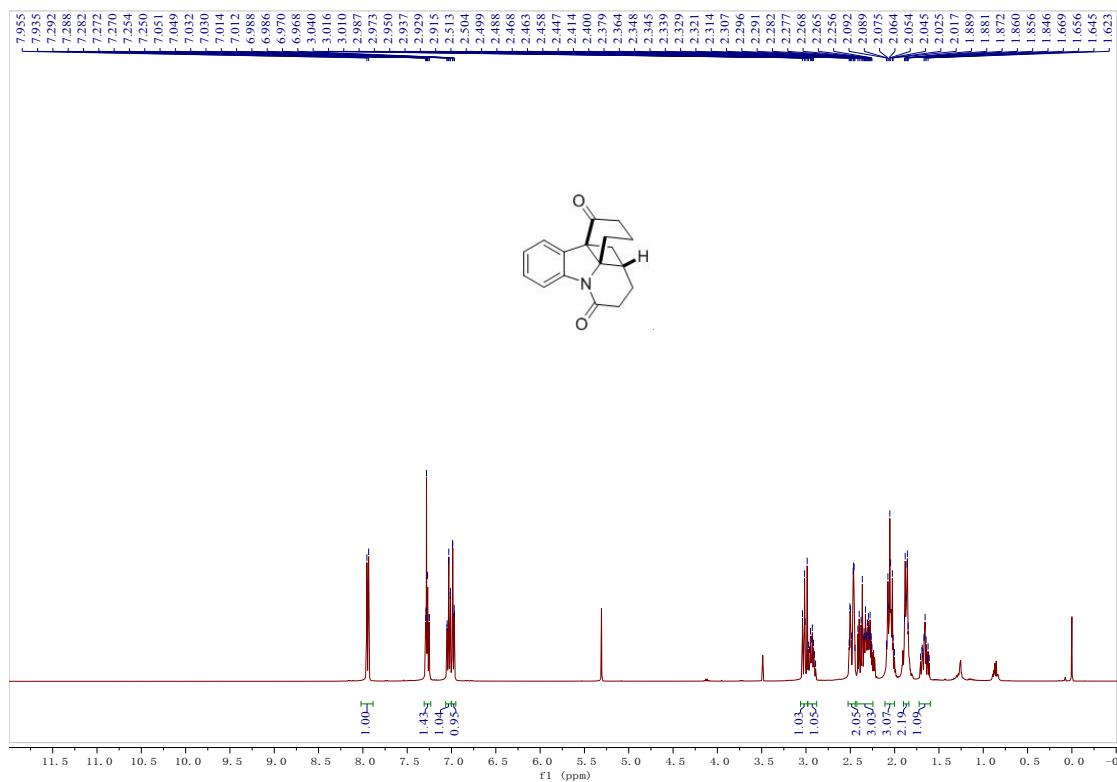
¹H NMR spectrum of **2x**



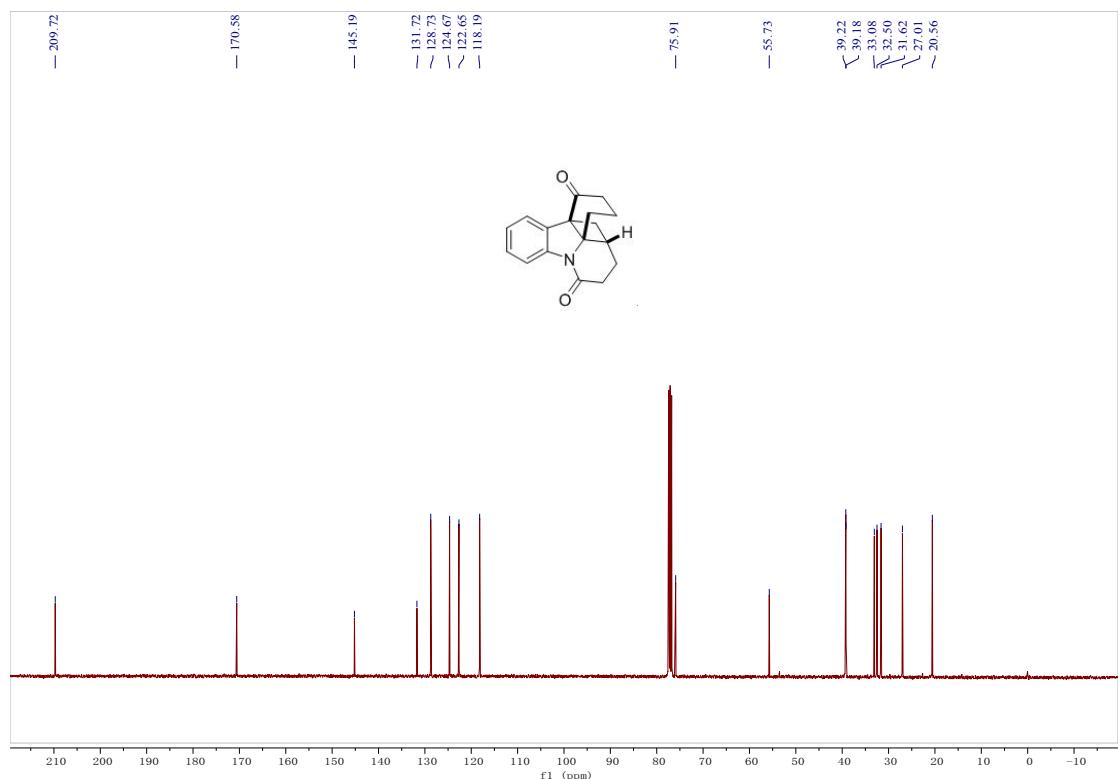
¹³C NMR spectrum of **2x**



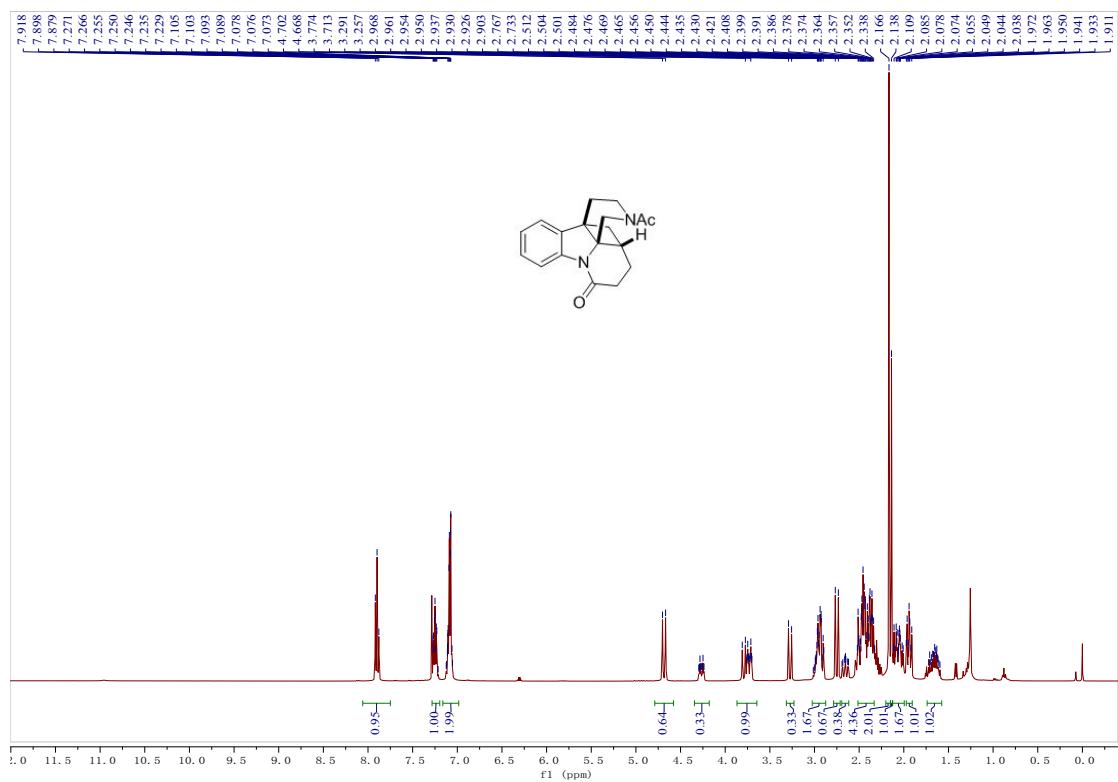
¹H NMR spectrum of **2aa**



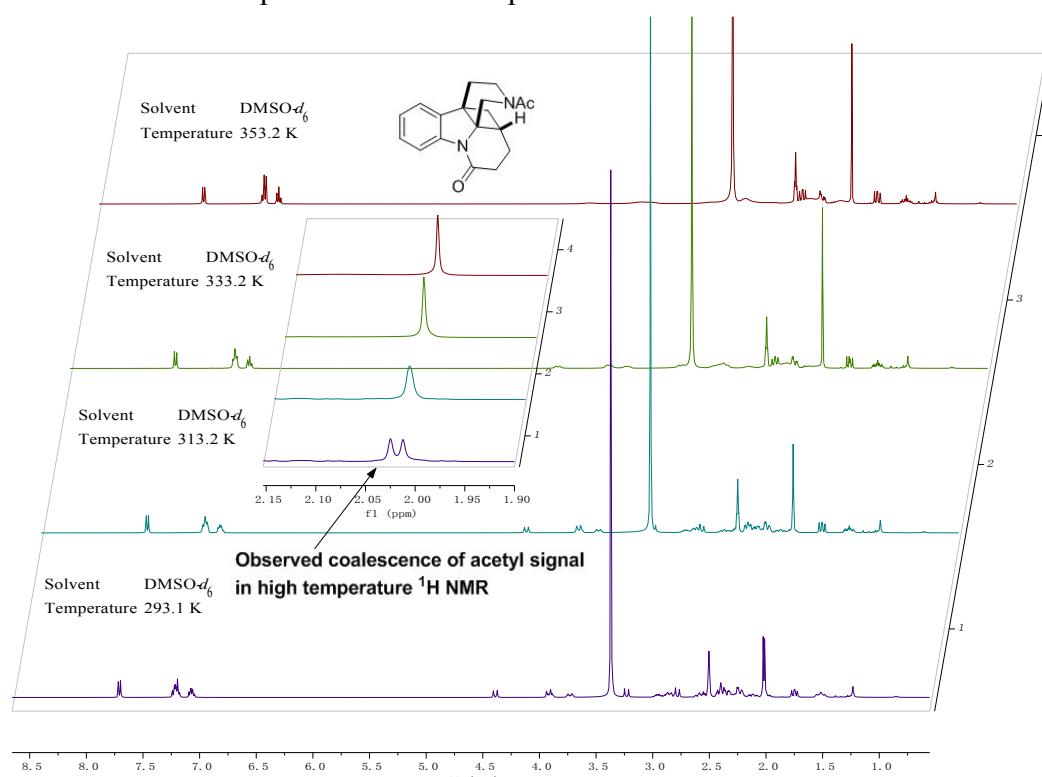
¹³C NMR spectrum of **2aa**



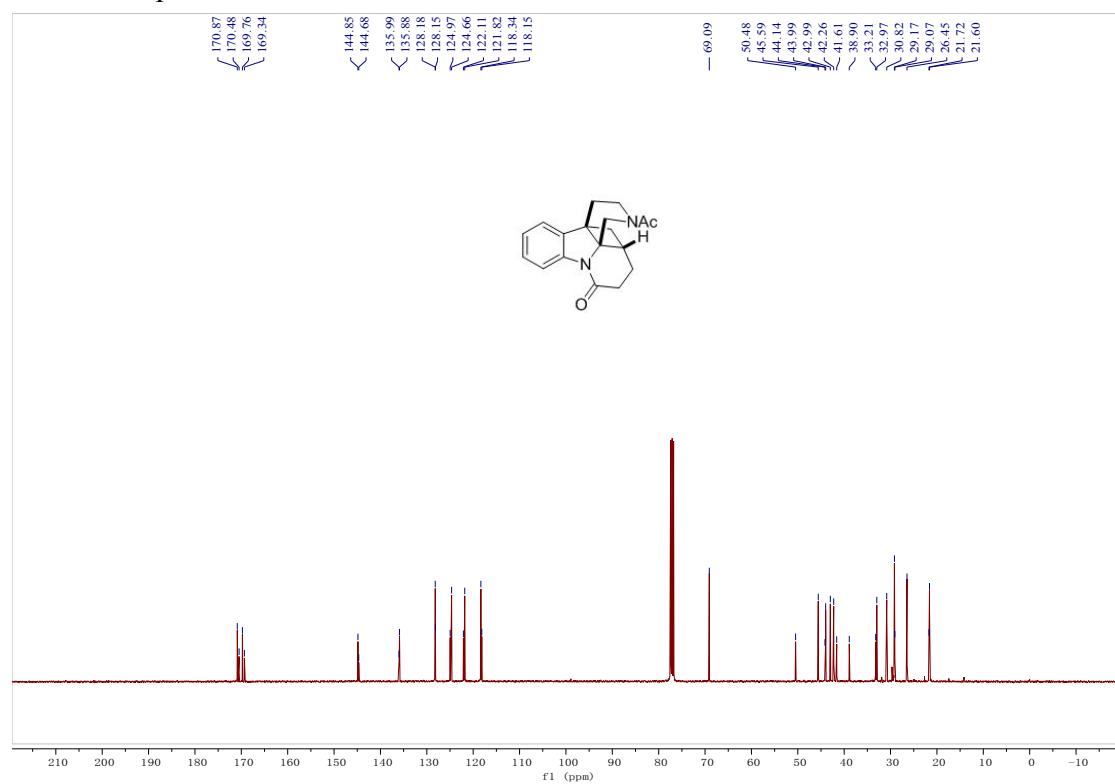
¹H NMR spectrum of **2ab**



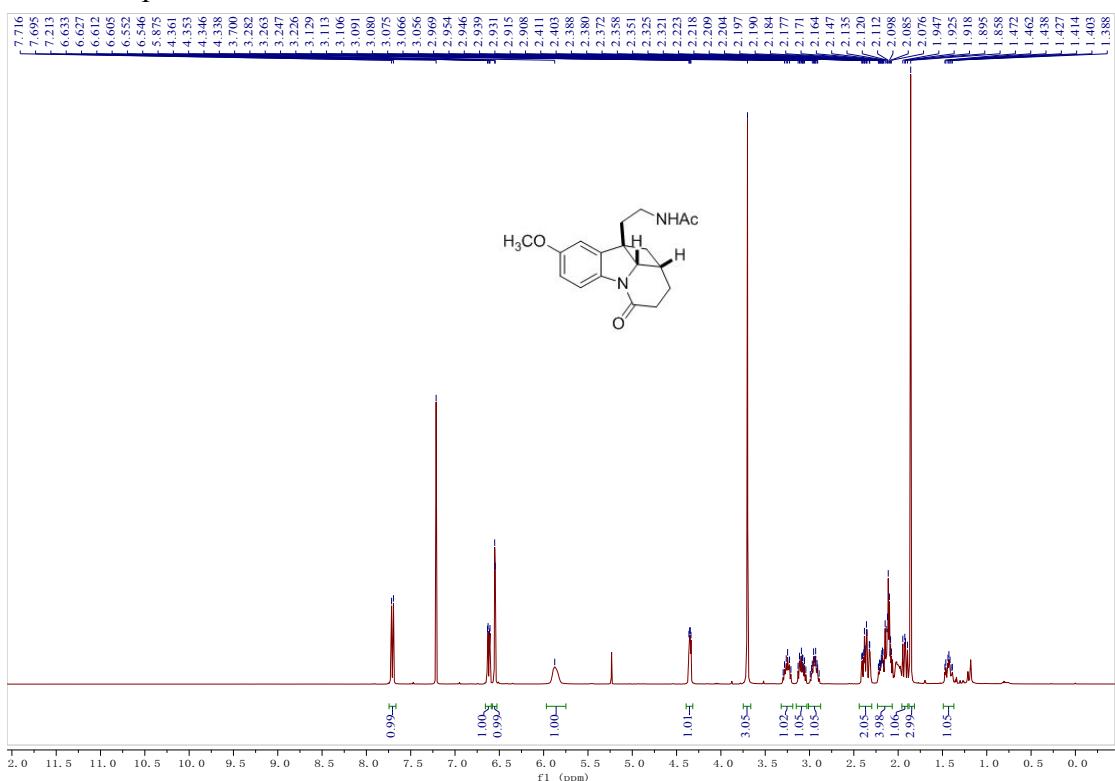
In situ variable temperature ^1H NMR spectrum of **2ab**



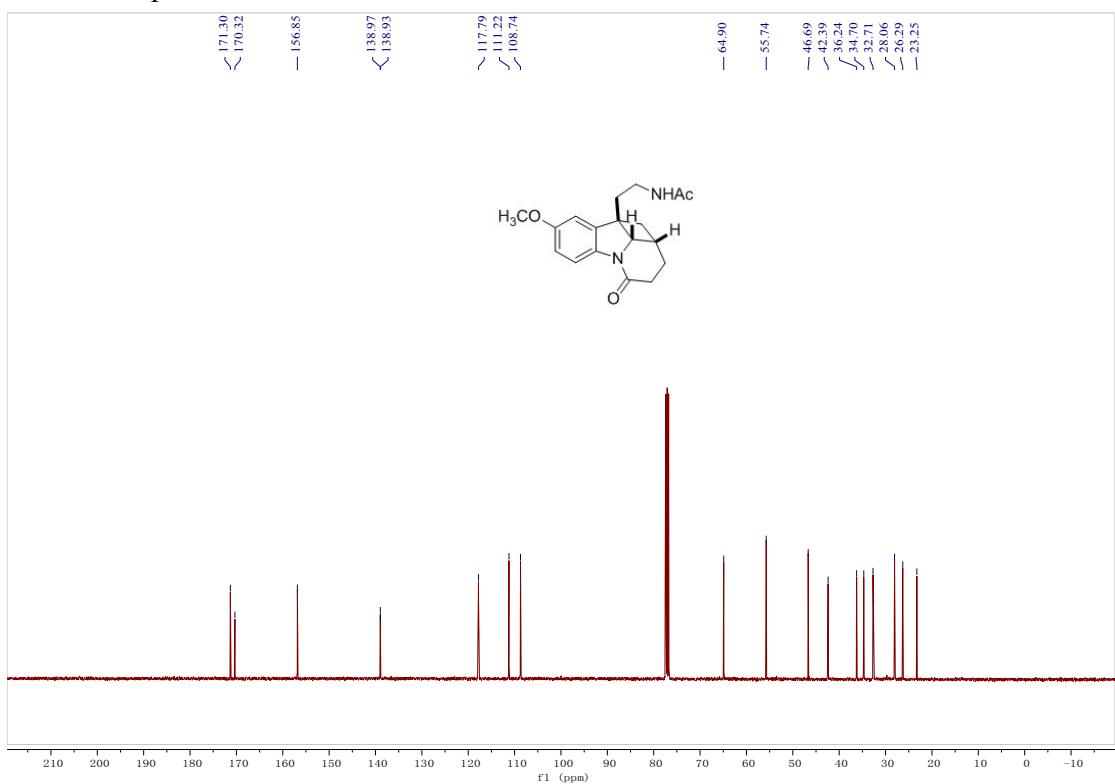
^{13}C NMR spectrum of **2ab**



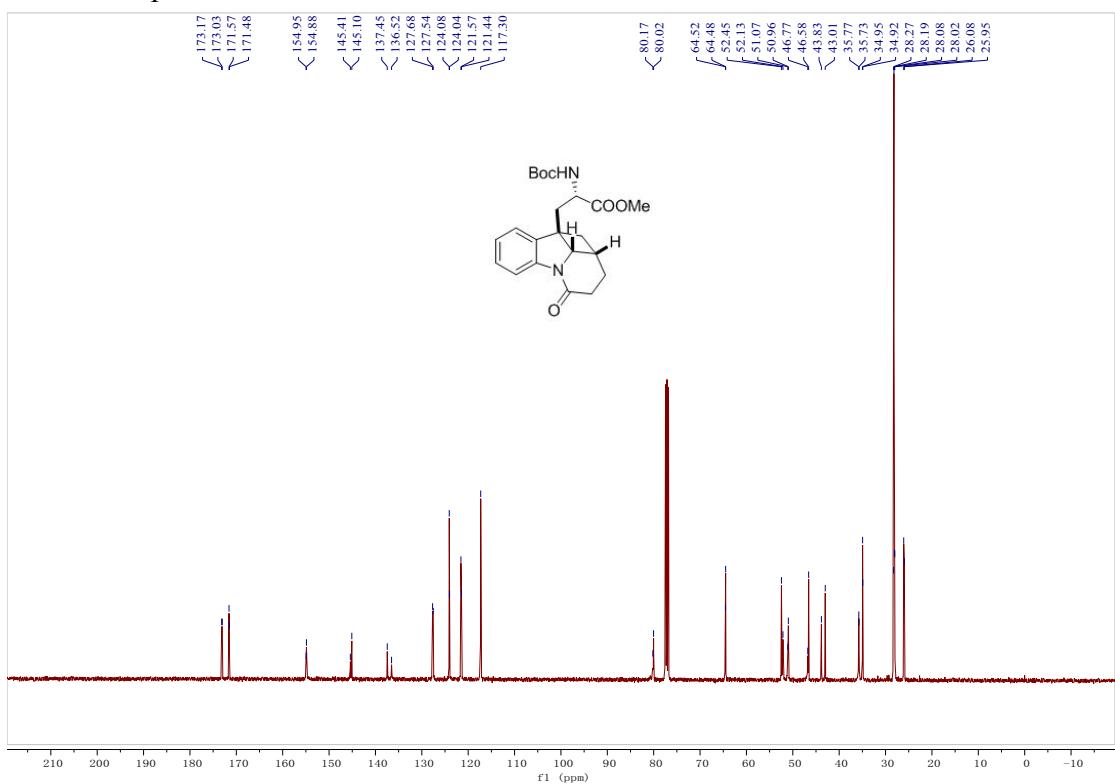
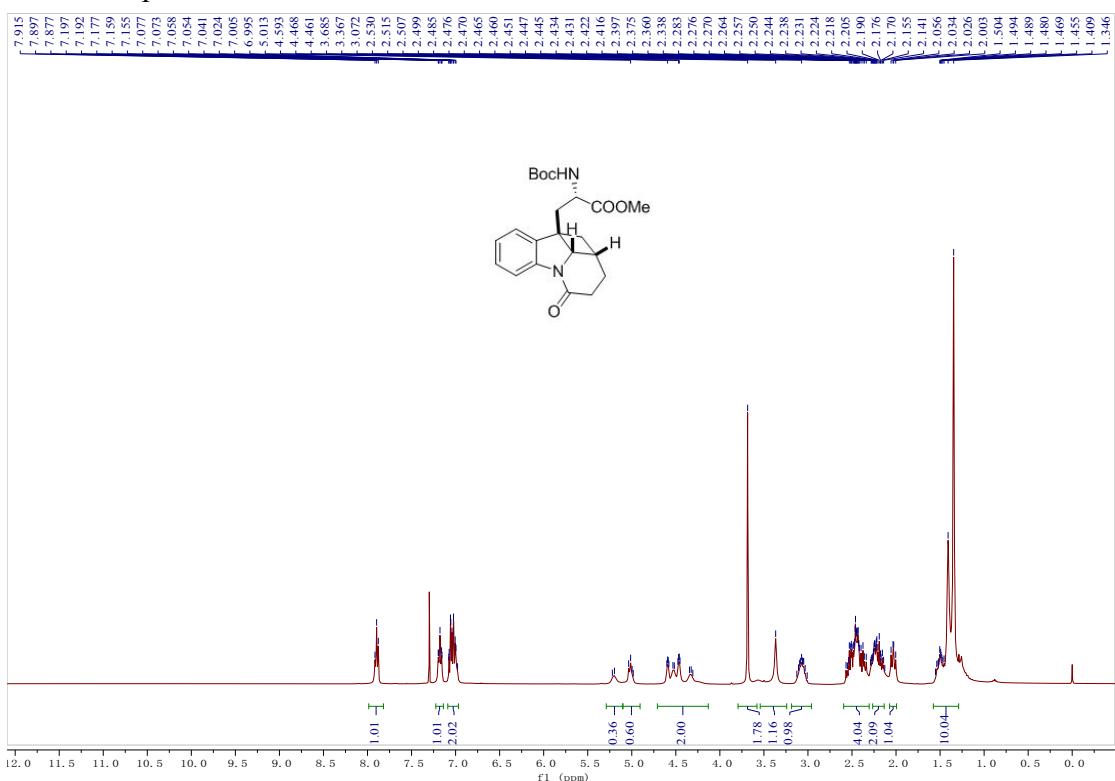
¹H NMR spectrum of **2ac**



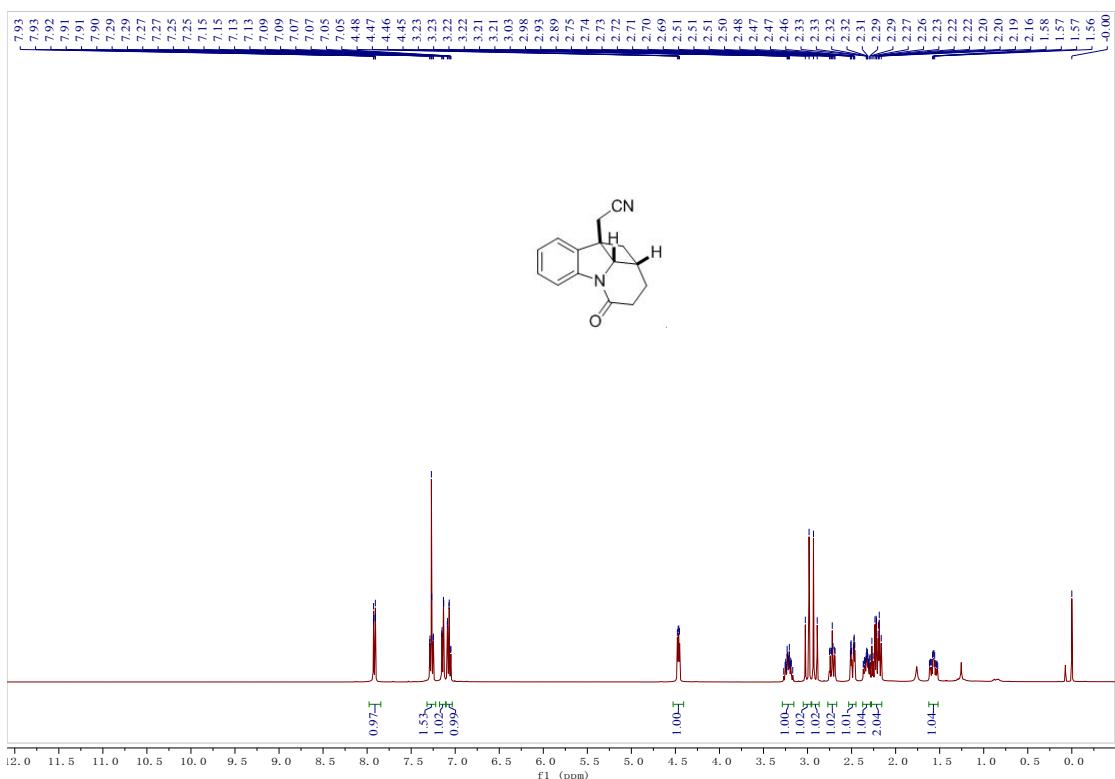
¹³C NMR spectrum of **2ac**



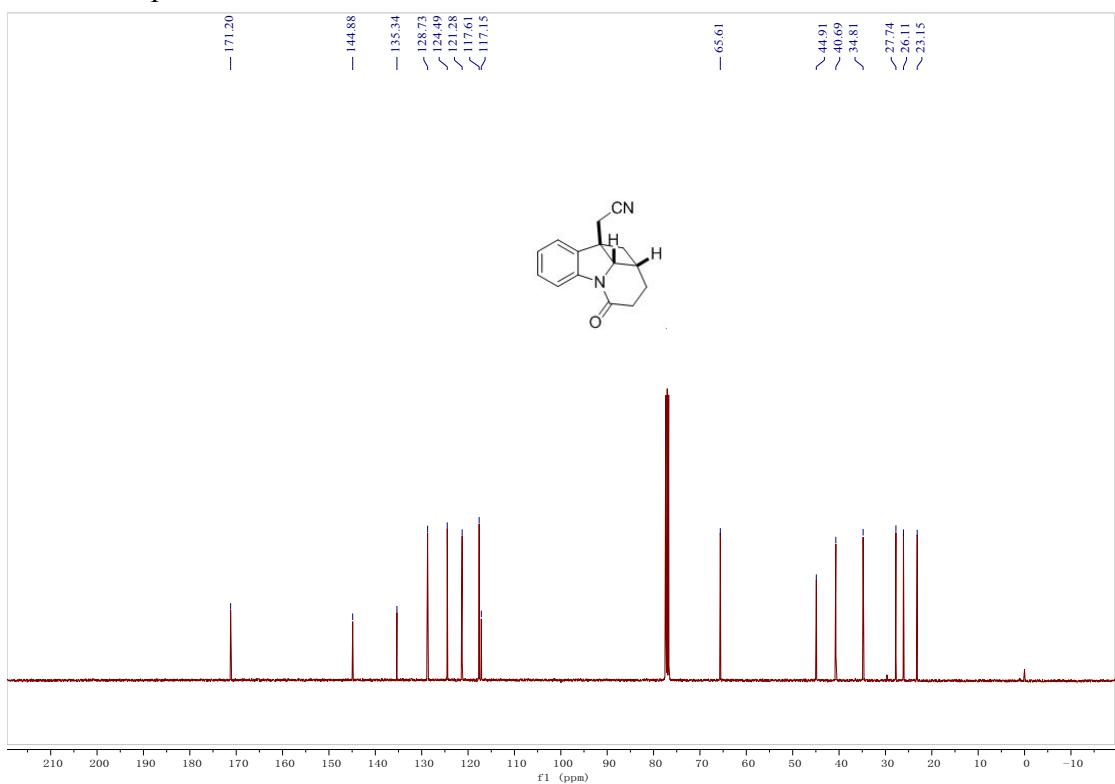
¹H NMR spectrum of **2ad**



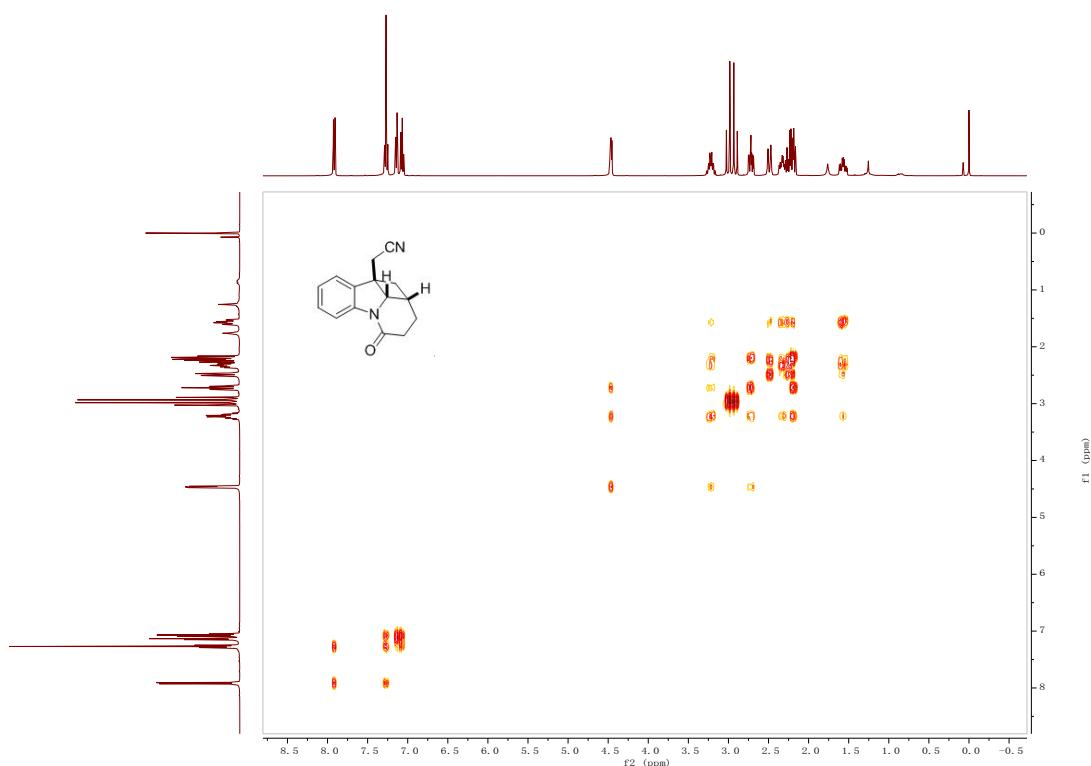
¹H NMR spectrum of **2ae**



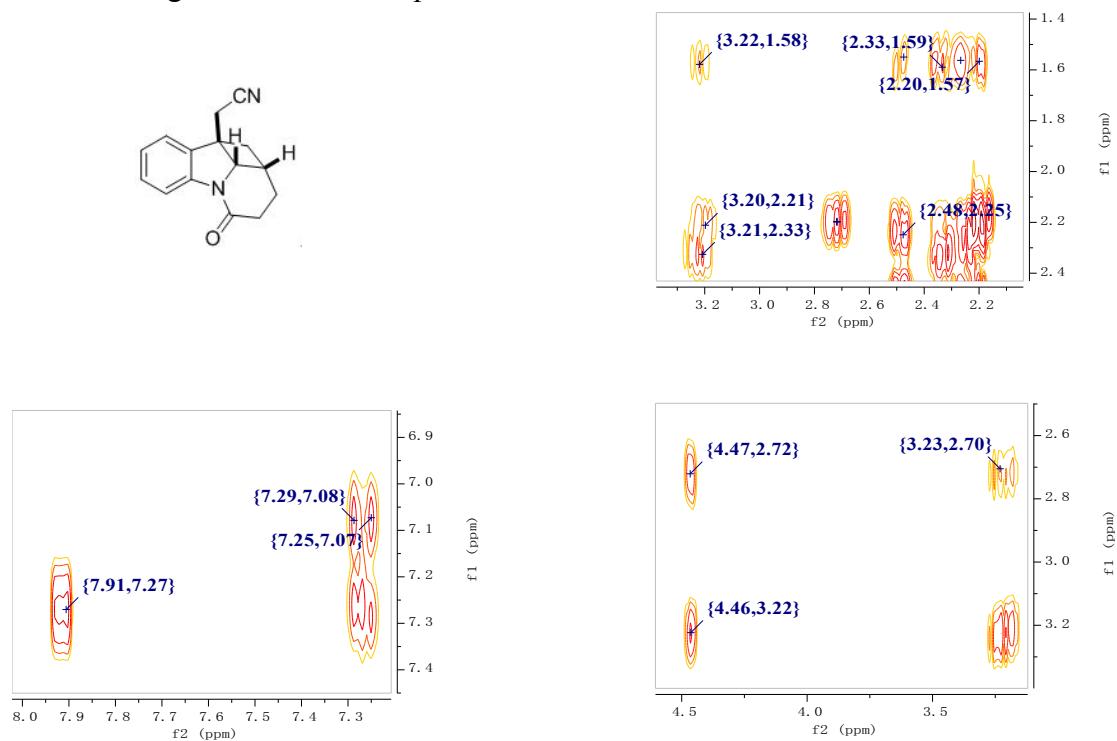
¹³C NMR spectrum of **2ae**



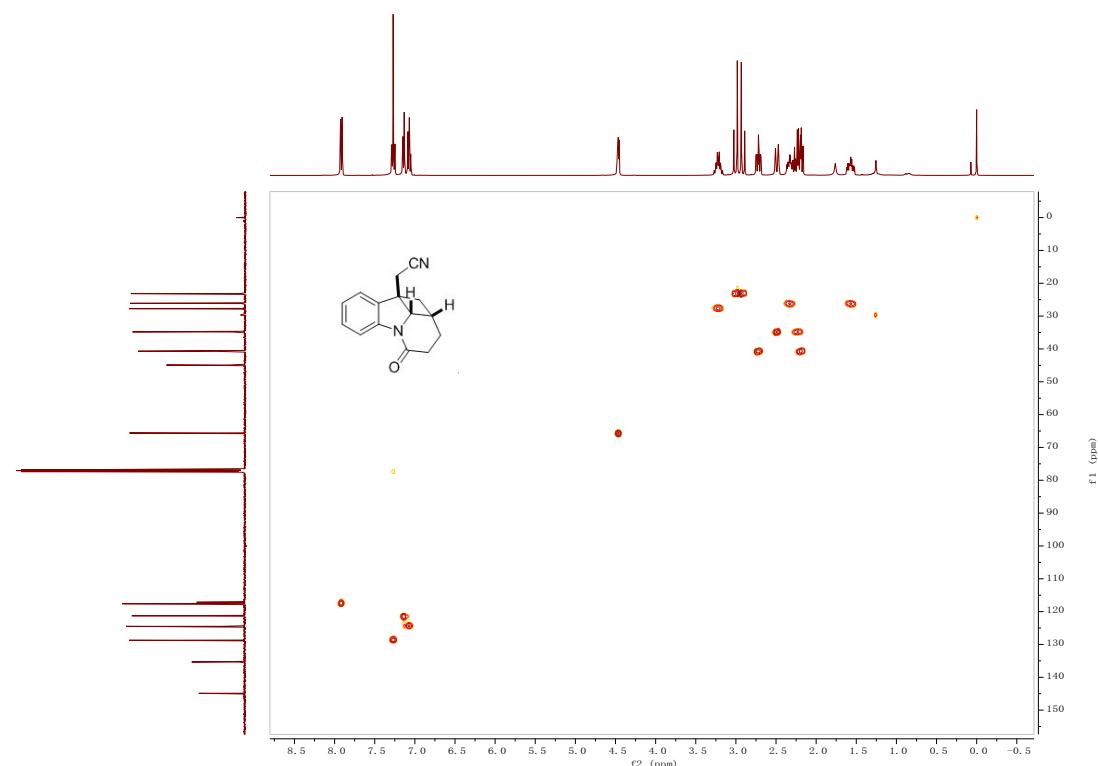
¹H-¹H COSY spectrum of **2ae**



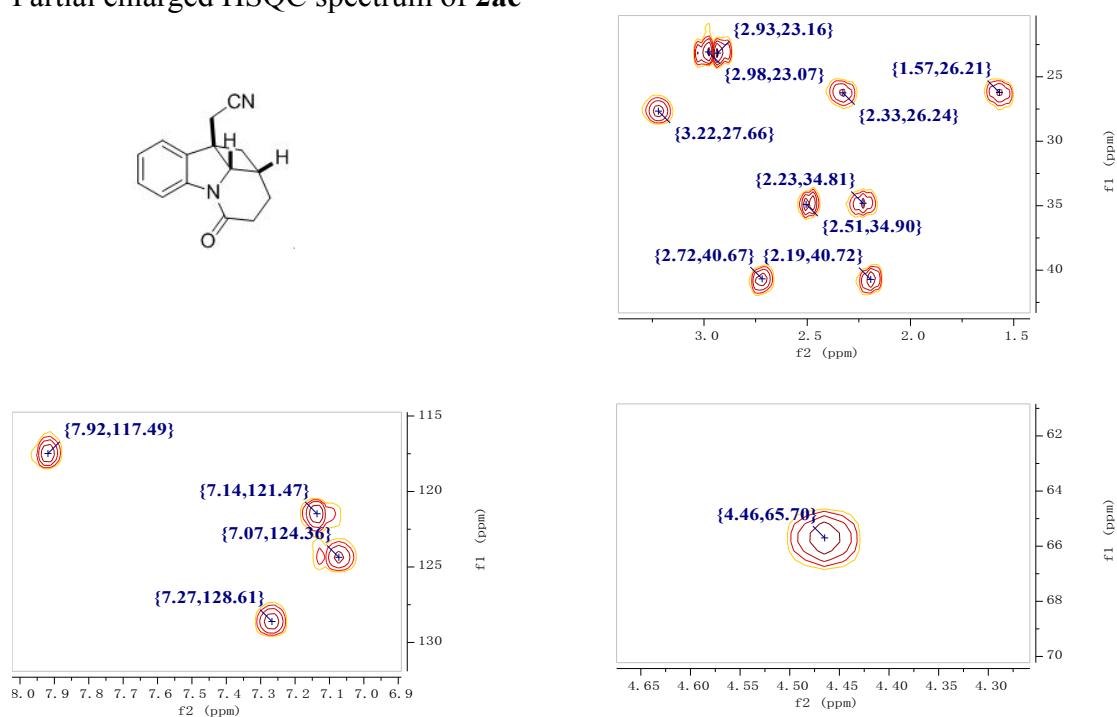
Partial enlarged ¹H-¹H COSY spectrum of **2ae**



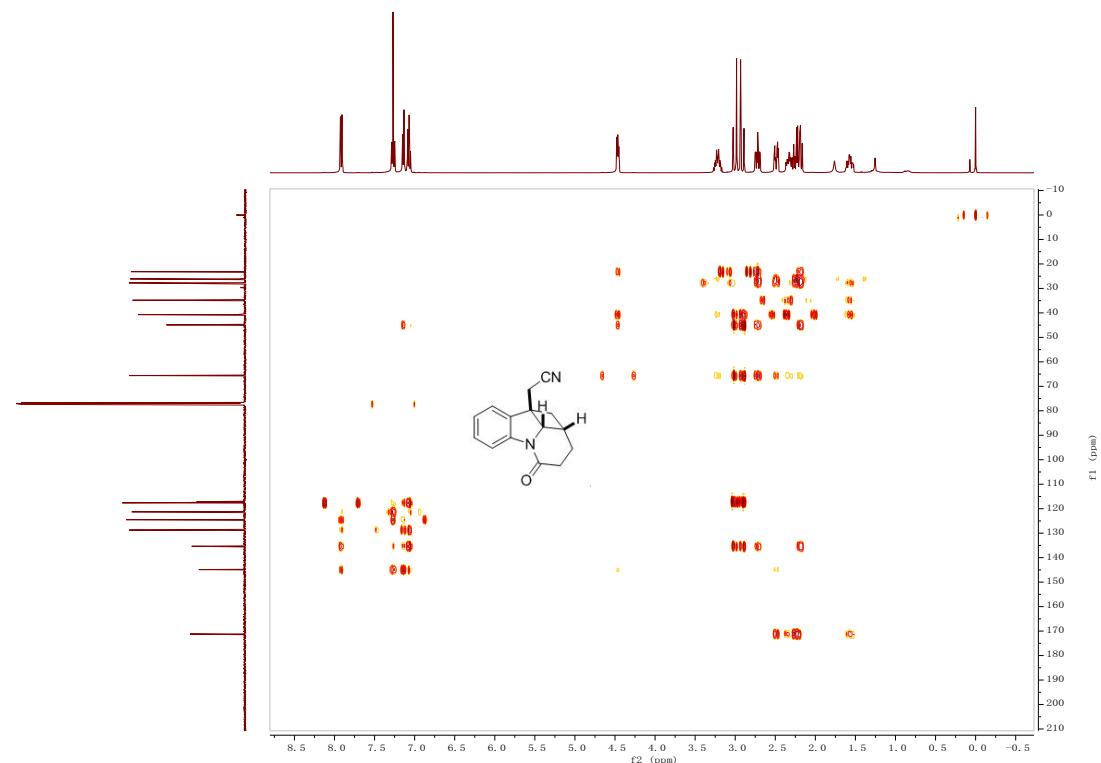
HSQC spectrum of **2ae**



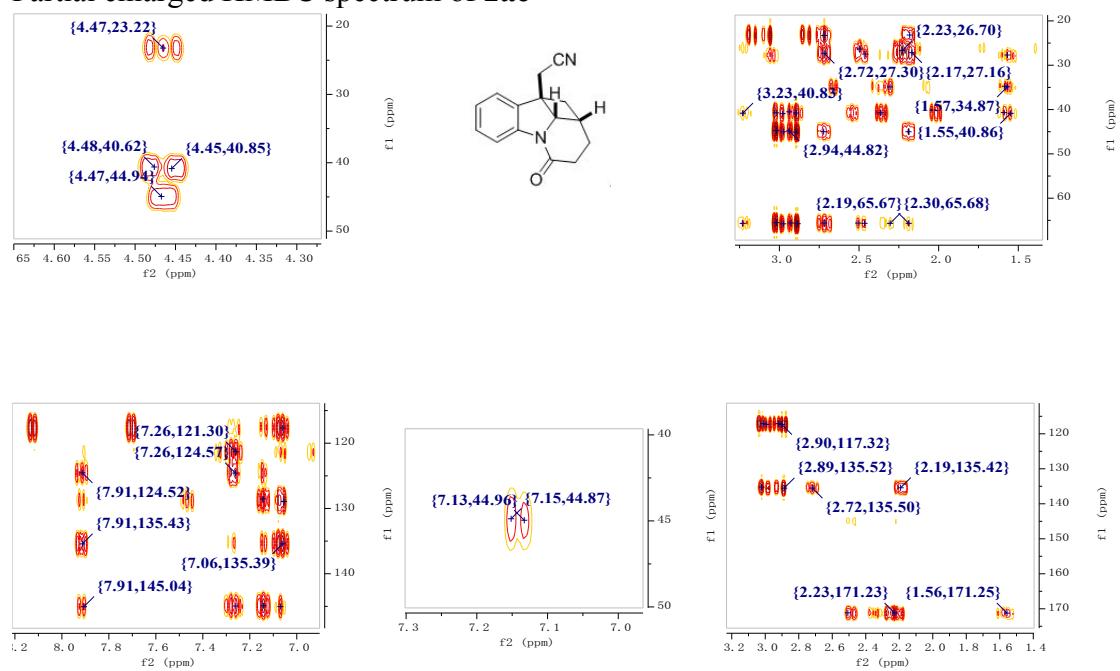
Partial enlarged HSQC spectrum of **2ae**



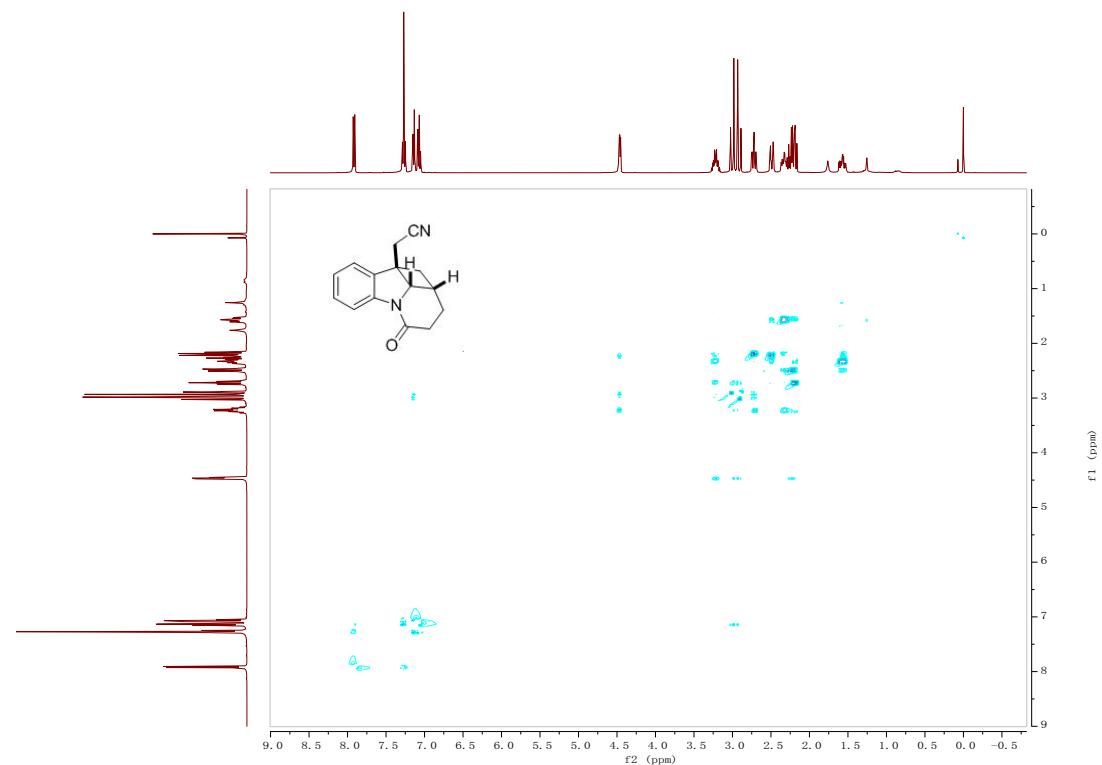
HMBC spectrum of **2ae**



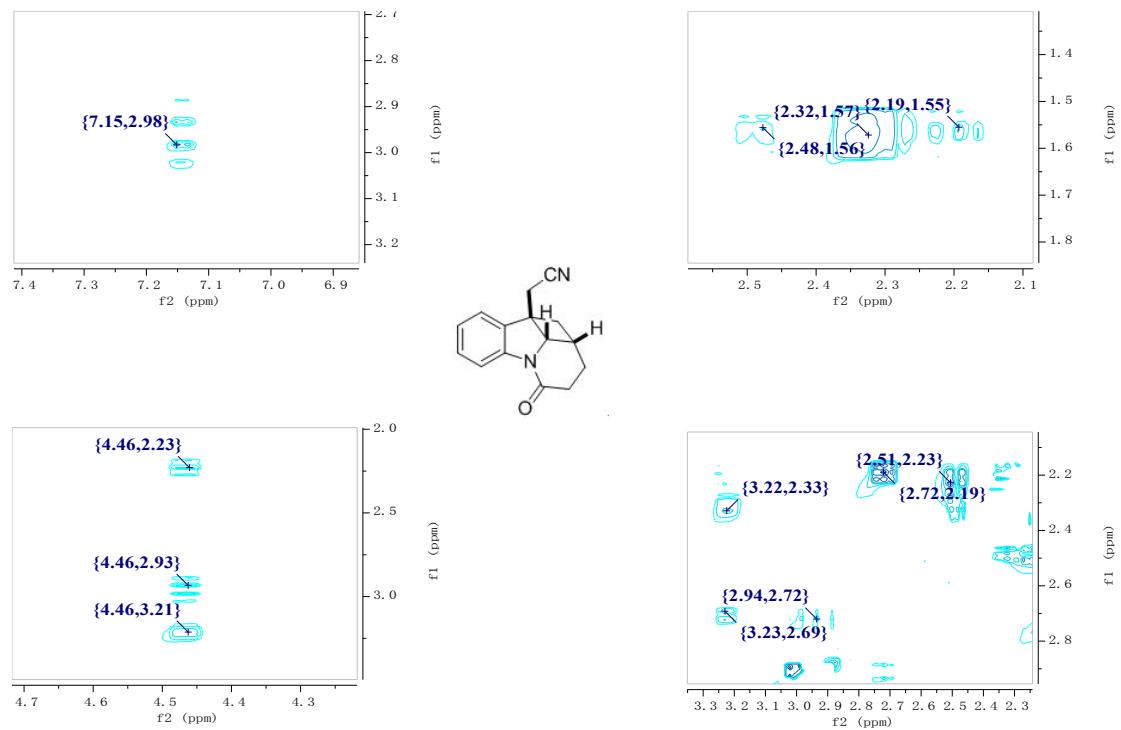
Partial enlarged HMBC spectrum of **2ae**



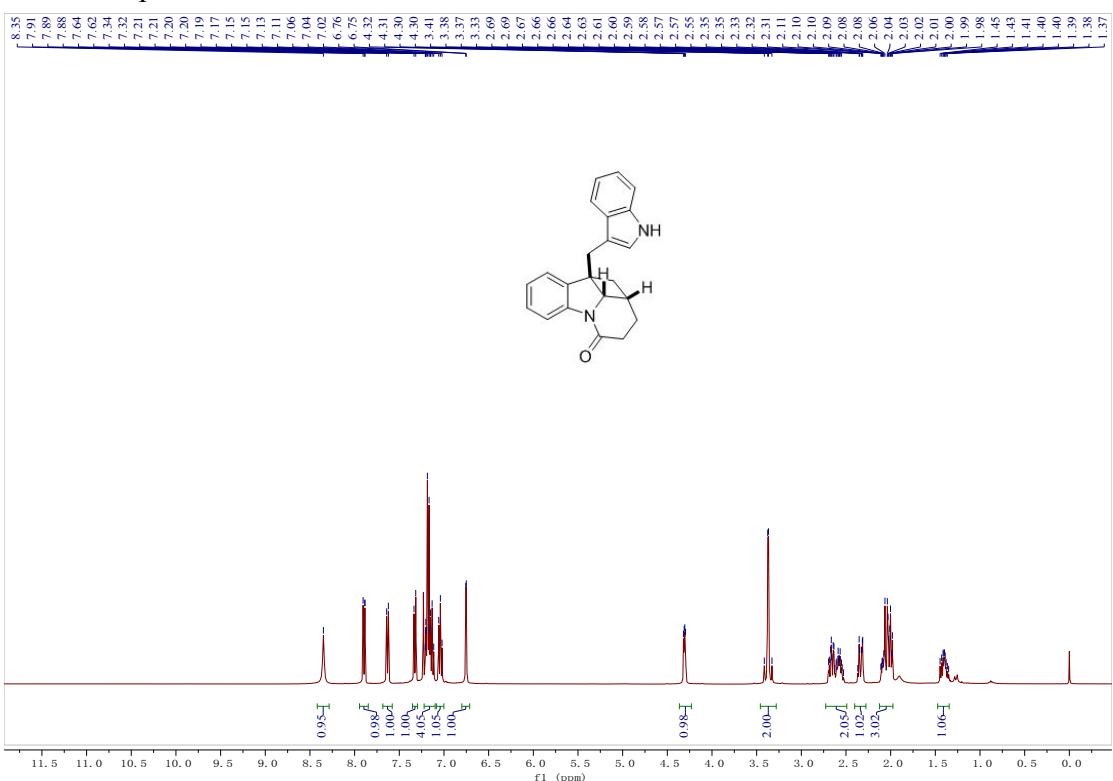
NOESY spectrum of **2ae**



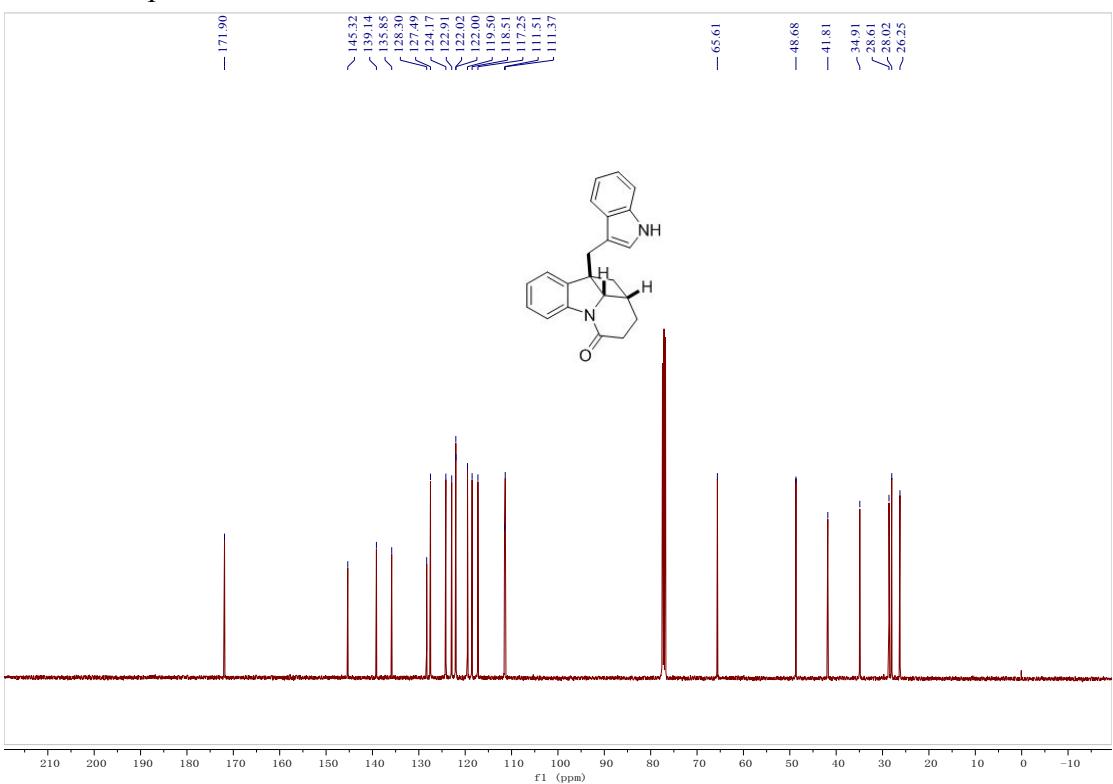
Partial enlarged NOESY spectrum of **2ae**



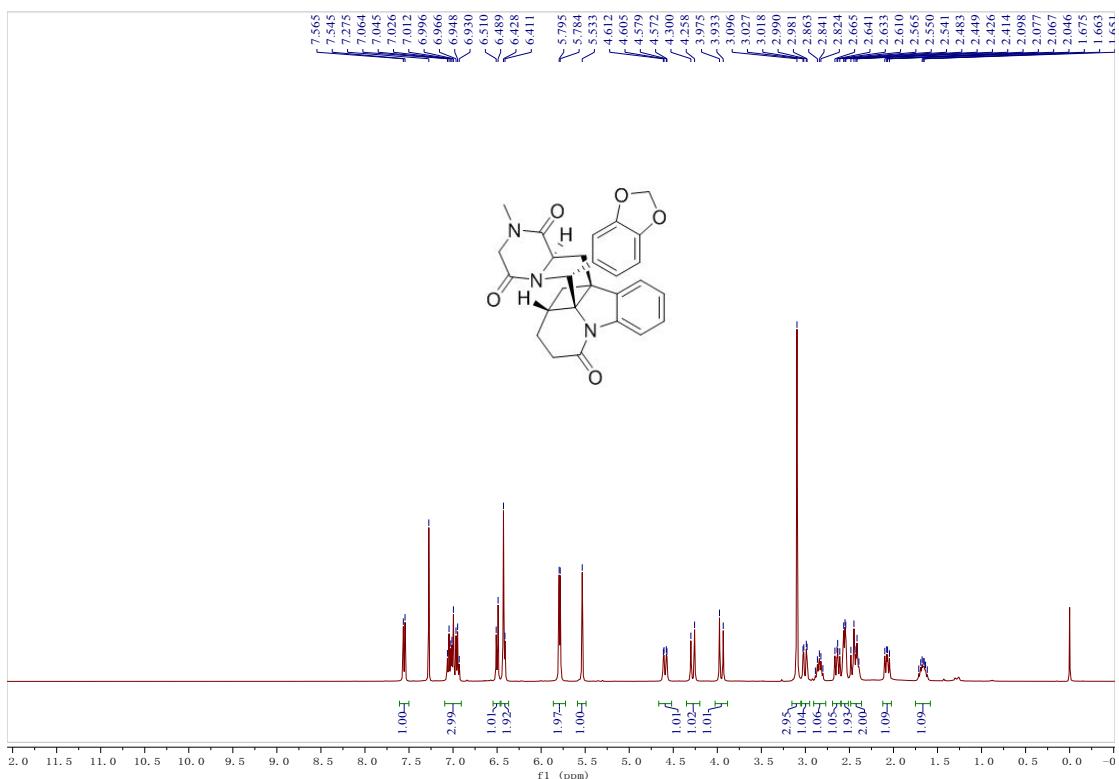
¹H NMR spectrum of 2af



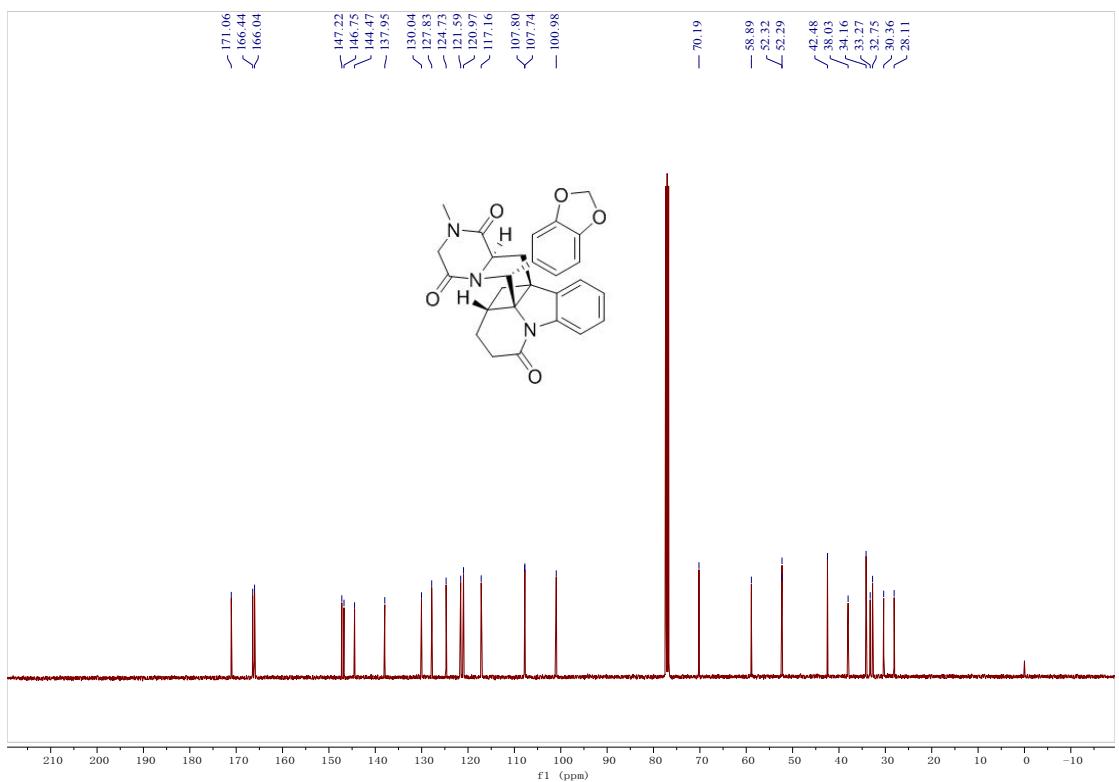
¹³C NMR spectrum of **2af**



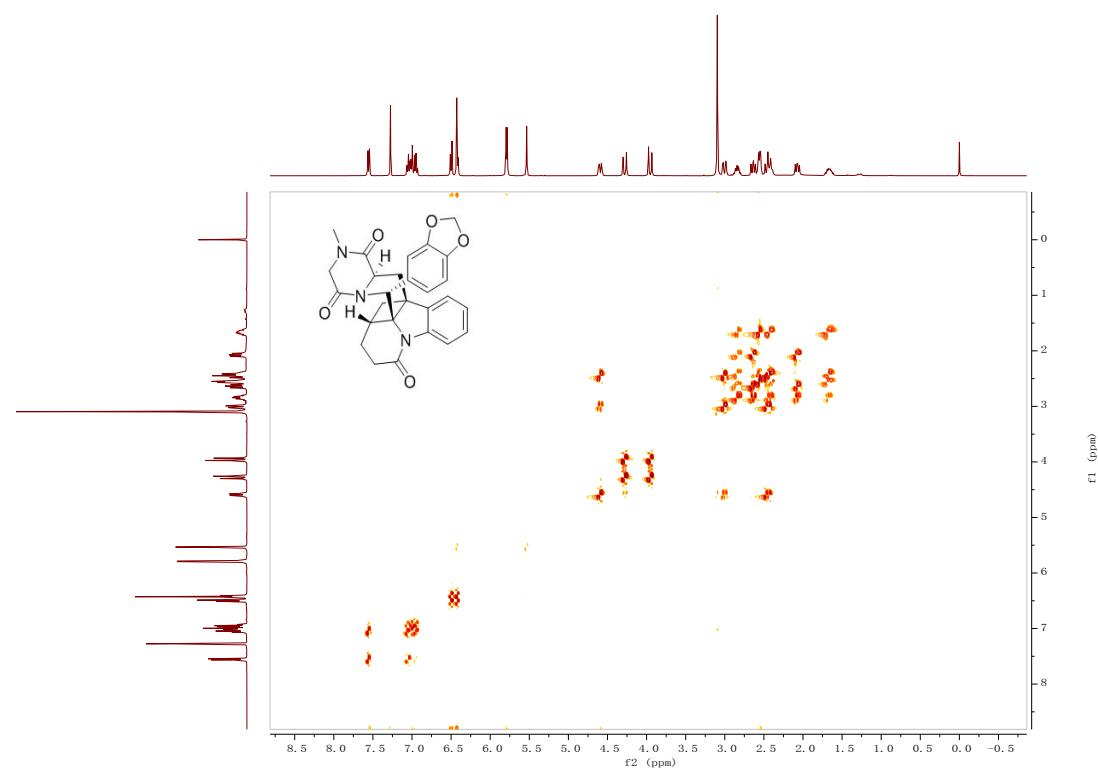
¹H NMR spectrum of **2ag**



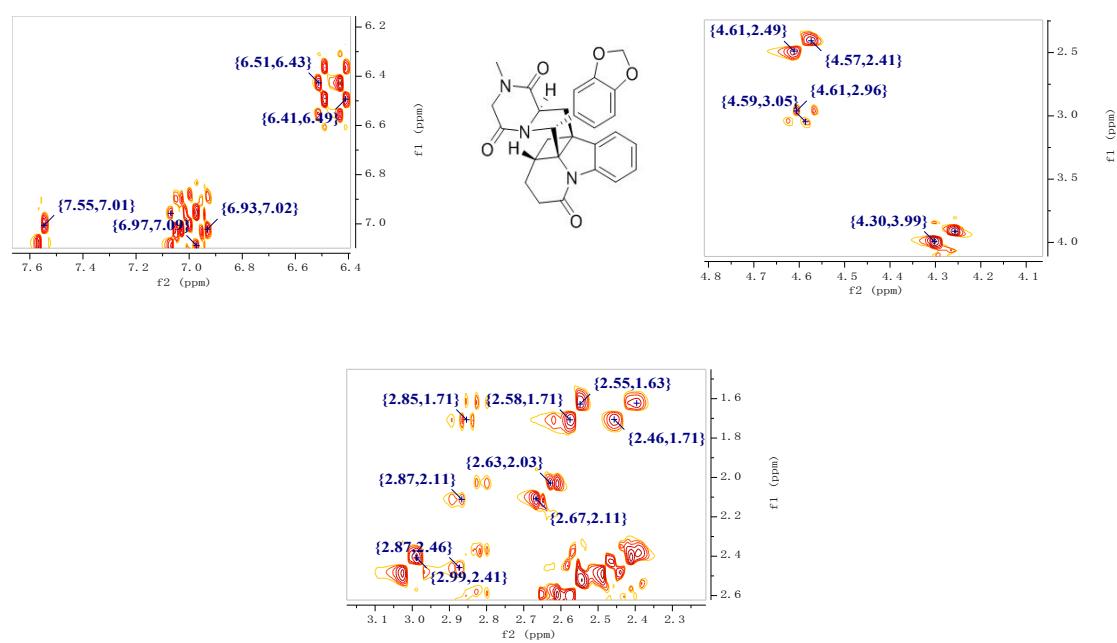
¹³C NMR spectrum of **2ag**



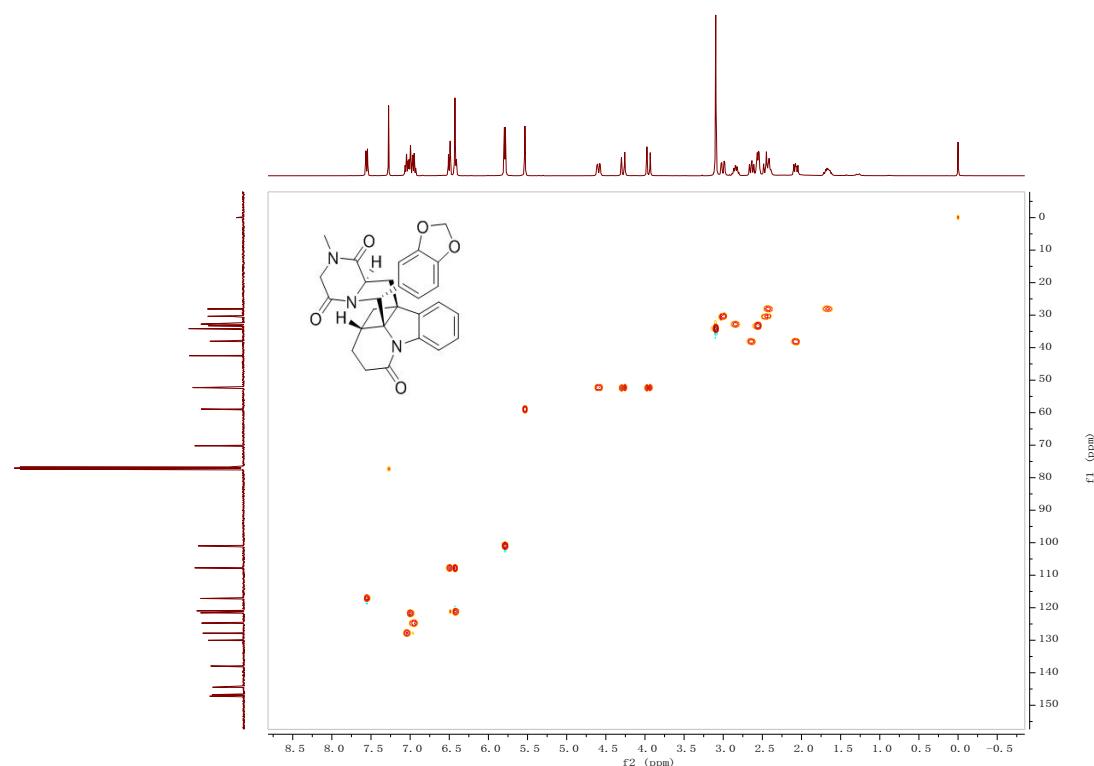
^1H - ^1H COSY spectrum of **2ag**



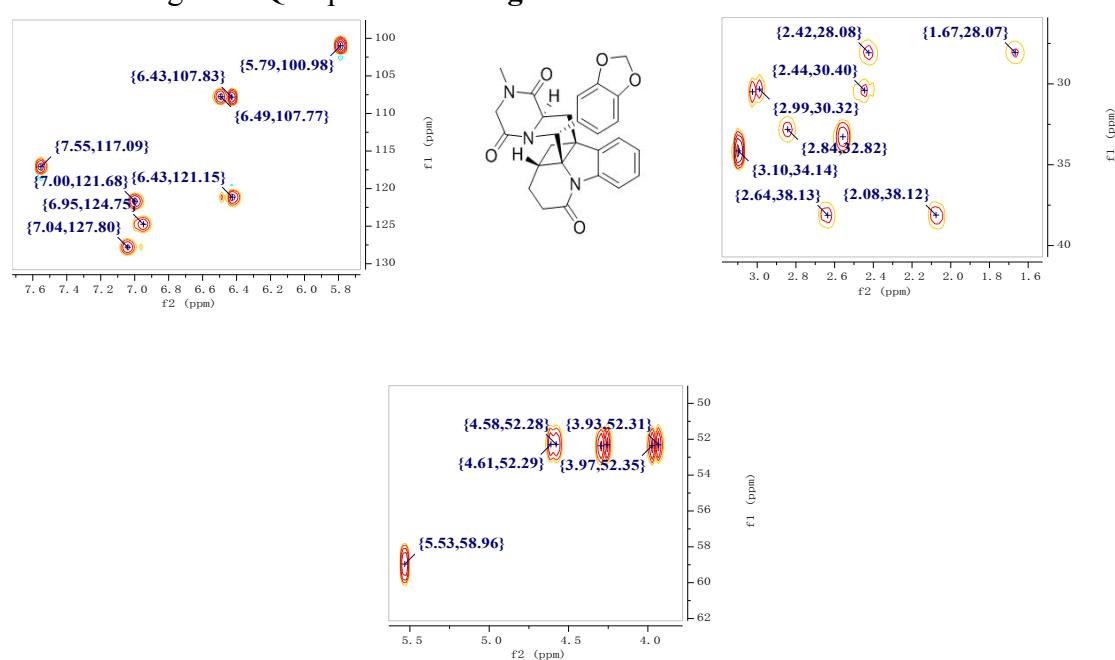
Partial enlarged ^1H - ^1H COSY spectrum of **2ag**



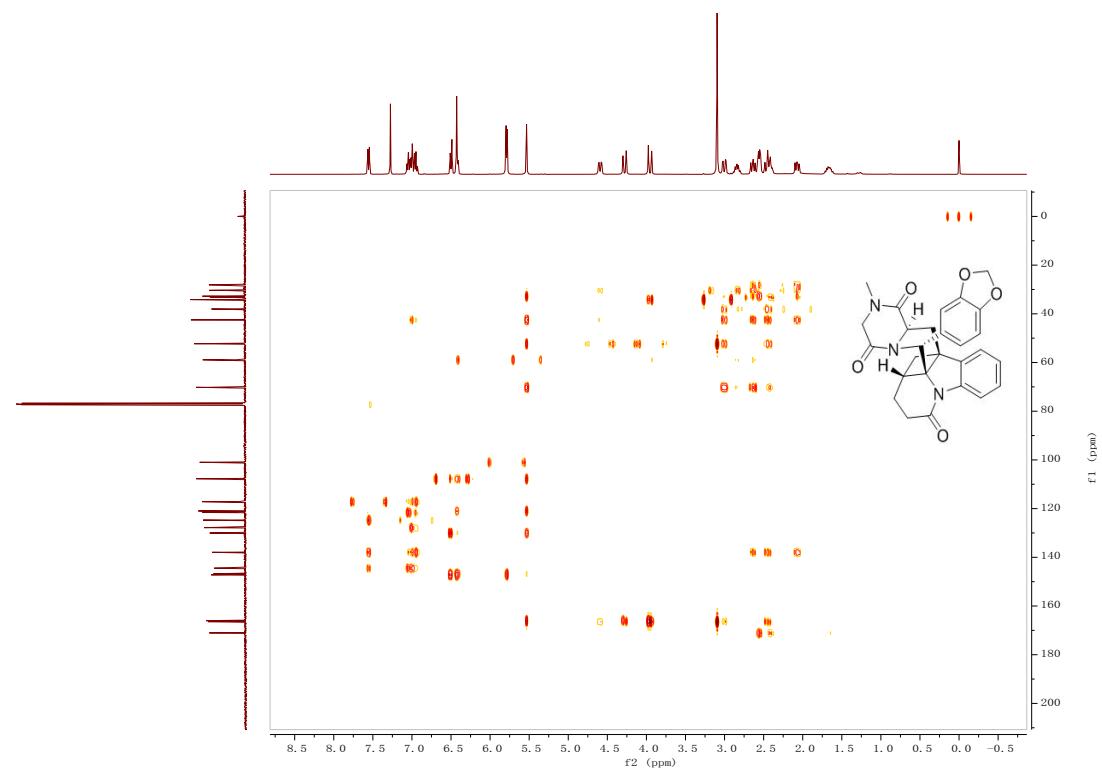
HSQC spectrum of **2ag**



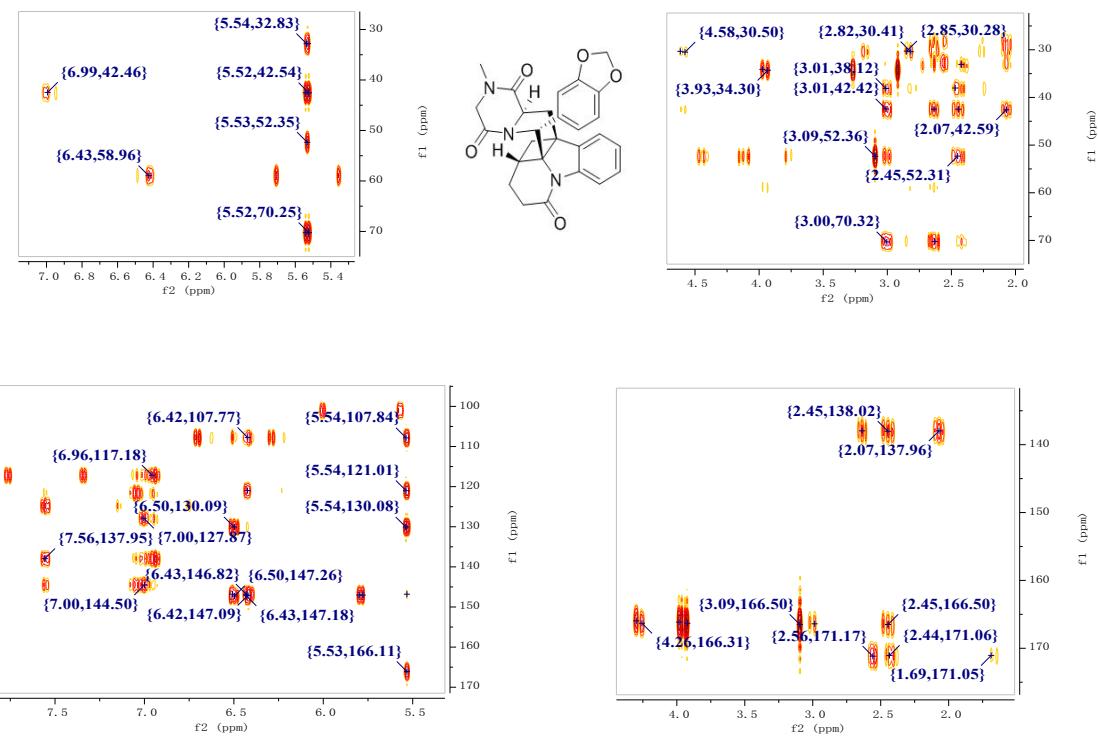
Partial enlarged HSQC spectrum of **2ag**



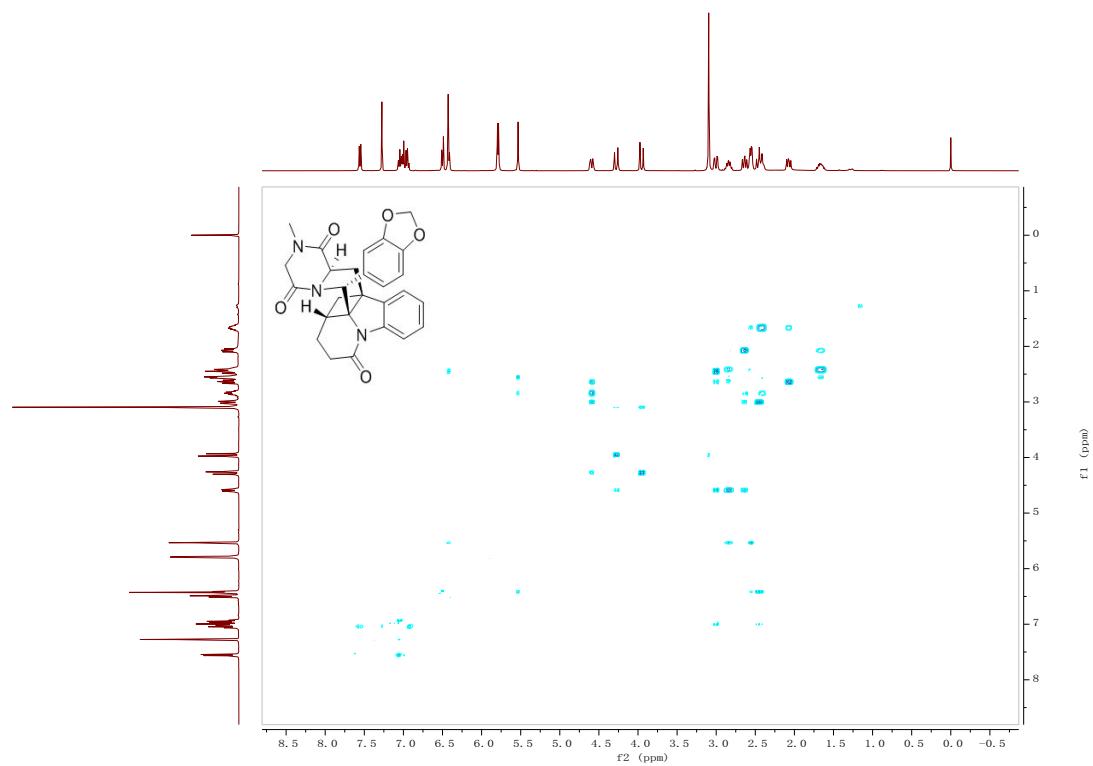
HMBC spectrum of **2ag**



Partial enlarged HMBC spectrum of **2ag**



NOESY spectrum of **2ag**



Partial enlarged NOESY spectrum of **2ag**

