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Supporting Information for

Palladium–catalyzed amidation of carbazole derivatives *via* hydroamination of isocyanates

Meng-Yuan Li,[‡] Peng Chen,[‡] Ming-Xia Pan, Hao-Lan Hu, and Yi-Jun Jiang[*]

E-mail: jiangyijun@nbu.edu.cn

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1. General

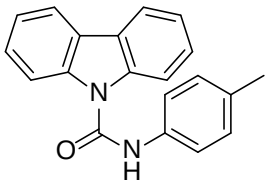
All commercially available reagents were directly used as received without further purification. All reactions were monitored by thin–layer chromatography (TLC) on gel F_{254} plates using UV light as visualizing agent (if applicable), and a solution of phosphomolybdic acid hydrate (50 g/L) in EtOH followed by heating as developing agents.

^{1}H NMR and ^{13}C NMR spectra were recorded in DMSO-*d*6 or $CDCl_3$ solution on a Bruker Ascend 500 MHz instrument. Chemical shifts were denoted in ppm (δ), and calibrated by using residual undeuterated solvent (DMSO-*d*6 (2.50 ppm) or $CHCl_3$ (7.26 ppm) or tetramethylsilane (0.00 ppm) as internal reference for ^{1}H NMR and the deuterated solvent ($CDCl_3$ (77.16 ppm) or DMSO-*d*6 (39.52 ppm)) as internal standard for ^{13}C NMR. The coupling constants were reported in Hz. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dt = double triplet, m = multiplet. High–resolution mass spectral analysis (HRMS) data were measured on a Thermo Scientific TM Q Exactive PlusTM mass spectrometer by means of the HESI–Orbitrap technique.

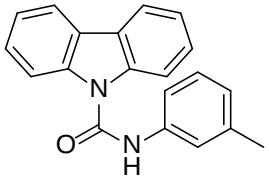
2. The experimental details and the analytical data for the products

The general experimental procedure was described as follows:

A mixture of carbazole or its derivative (0.25 mmol), isocyanate substrate (0.3 mmol), $Pd(PPh_3)_4$ (14.4 mg, 0.05 mmol) and DCM (2.0 mL) were added into a 15 mL pressure tube from LH LABWARE. The reaction mixture was stirred at 80℃ for 0.5 h to 4 h (monitored by thin layer chromatography until the carbazole or its derivative had disappeared or the system no longer changed). Then the reaction mixture was cooled to room temperature. The cooled reaction system was added to *n*–hexane (20.0 mL). After stirring for 10 min, a white precipitate formed. The pure product could be obtained by filtering and washing with acetonitrile (4.0 mL).

3aa: 

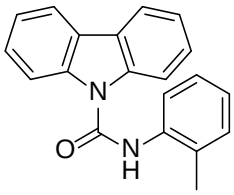
The general experimental procedure was followed to afford product **3aa** as a white solid (75.5 mg, 96% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.04 (d, J = 10.0 Hz, 4H), 7.53–7.44 (m, 5H), 7.37 (t, J = 10.0 Hz, 2H), 7.23 (d, J = 7.5 Hz, 2H), 2.38 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 150.3, 138.3, 134.6, 130.0, 127.2, 125.4, 122.7, 120.4, 120.2, 113.6, 21.0. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{12}N_2O$ 301.1335; Found 301.1332.

3ab: 

The general experimental procedure was followed to afford product **3ab** as a white solid (67.8 mg, 88% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.90 (d, J = 8.5 Hz, 2H), 7.87 (d, J = 7.5 Hz, 2H), 7.55 (s, 1H), 7.40–7.34 (m, 3H), 7.34–7.29 (m, 1H), 7.28–7.19 (m, 3H), 6.96 (d,

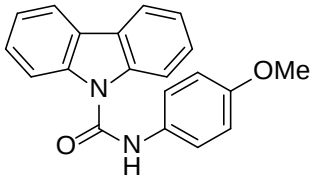
J =7.5 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 150.2, 139.4, 138.1, 137.2, 129.2, 127.0, 125.6, 125.2, 122.6, 120.6, 120.2, 117.1, 113.5, 21.6. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{12}N_2O$ 301.1335; Found 301.1340.

3ac:



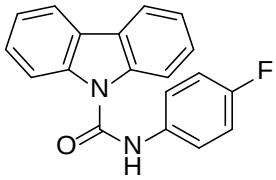
The general experimental procedure was followed to afford product **3ac** as a white solid (66.0 mg, 84% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 10.05 (s, 1H), 8.24 (d, *J* = 5.0 Hz, 2H), 8.06 (d, *J* = 10.0 Hz, 2H), 7.57–7.51 (m, 2H), 7.46 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.36–7.32 (m, 1H), 7.28 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.22 (dt, *J* = 7.5, 1.5 Hz, 1H), 2.37 (s, 3H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 150.6, 138.1, 136.1, 133.2, 130.7, 126.8, 126.4, 126.1, 125.5, 124.1, 122.0, 120.3, 113.9, 18.4. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{12}N_2O$ 301.1335; Found 301.1333.

3ad:



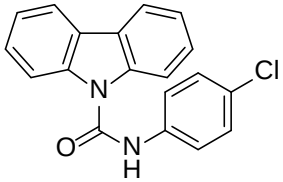
The general experimental procedure was followed to afford product **3ad** as a white solid (69.3 mg, 88% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.04 (d, *J* =9.0 Hz, 4H), 7.53–7.43 (m, 5H), 7.37 (t, *J* = 7.5 Hz, 2H), 6.96 (d, *J* = 9.0 Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 157.1, 150.6, 138.3, 130.1, 127.2, 125.4, 122.7, 122.2, 120.4, 114.7, 113.6, 55.7. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{17}N_2O_2$ 317.1285; Found 317.1287.

3ae:



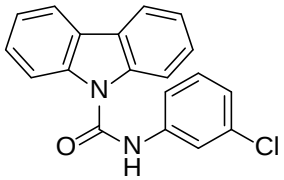
The general experimental procedure was followed to afford product **3ae** as a white solid (65.4 mg, 86% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.01 (t, *J* = 14.5 Hz, 4H), 7.60–7.51 (m, 3H), 7.47 (t, *J* = 16.0 Hz, 2H), 7.37 (t, *J* = 15.0 Hz, 2H), 7.12 (t, *J* = 17.5 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 159.8 (d, $^1J_{C-F}$ = 244.8 Hz), 150.4, 138.2, 133.2 (d, $^4J_{C-F}$ = 2.8 Hz), 127.3, 125.4, 122.8, 122.1 (d, $^3J_{C-F}$ = 8.3 Hz), 120.5, 116.2 (d, $^2J_{C-F}$ = 22.8 Hz), 113.6. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{14}FN_2O$ 305.1085; Found 305.1081.

3af:



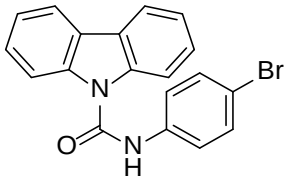
The general experimental procedure was followed to afford product **3af** as a white solid (76.3 mg, 89% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 10.70 (s, 1H), 8.24 (d, J = 7.5 Hz, 2H), 7.94 (d, J = 9.0 Hz, 2H), 7.93 (t, J = 9.0 Hz, 2H), 7.53 (t, J = 15.5 Hz, 2H), 7.48 (d, J = 8.5 Hz, 2H), 7.39 (t, J = 7.5 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 150.1, 137.9, 137.5, 128.9, 127.6, 126.9, 124.2, 122.2, 121.6, 120.4, 113.8. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{14}ClN_2O$ 321.0789; Found 321.0789.

3ag:



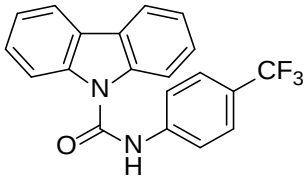
The general experimental procedure was followed to afford product **3ag** as a white solid (48.6 mg, 61% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 10.74 (s, 1H), 8.23 (d, J = 7.5 Hz, 2H), 7.95 (d, J = 8.0 Hz, 2H), 7.88–7.84 (m, 1H), 7.65 (dd, J = 8.0, 2.0 Hz, 1H), 7.54 (t, J = 8.0 Hz, 2H), 7.45 (t, J = 8.0 Hz, 1H), 7.39 (t, J = 7.5 Hz, 2H), 7.23 (dd, J = 8.0, 2.5 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 150.1, 140.0, 137.8, 133.3, 130.6, 126.9, 124.2, 123.6, 122.2, 120.4, 119.5, 118.4, 113.9. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{14}ClN_2O$ 321.0789; Found 321.0788.

3ah:

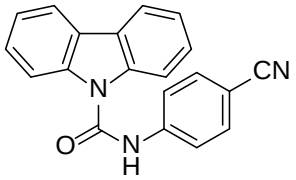


The general experimental procedure was followed to afford product **3ah** as a white solid (67.7 mg, 74% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 10.69 (s, 1H), 8.23 (d, J = 7.5 Hz, 2H), 7.93 (d, J = 8.0 Hz, 2H), 7.72–7.56 (m, 4H), 7.53 (t, J = 8.0 Hz, 2H), 7.39 (t, J = 15.0 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 150.0, 137.9, 137.9, 131.8, 126.9, 124.2, 122.2, 122.0, 120.4, 115.6, 113.8. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{14}BrN_2O$ 365.0284; Found 365.0281.

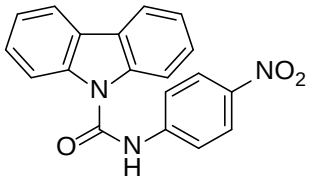
3ai:



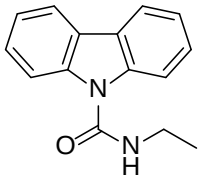
The general experimental procedure was followed to afford product **3ai** as a white solid (78.8 mg, 89% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 10.93 (s, 1H), 8.24 (d, J = 7.5 Hz, 2H), 7.95 (d, J = 8.0 Hz, 2H), 7.91 (d, J = 8.5 Hz, 2H), 7.79 (d, J = 8.5 Hz, 2H), 7.57–7.50 (m, 2H), 7.43–7.37 (m, 2H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 150.6, 142.7, 138.3, 127.4, 126.7 (q, $^3J_{C-F}$ = 3.7 Hz), 124.8 (q, $^1J_{C-F}$ = 272.2 Hz), 124.7, 124.3 (q, $^2J_{C-F}$ = 33.8 Hz), 122.8, 120.9, 120.3, 114.4. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{14}F_3N_2O$ 355.1053; Found 355.1051.

3aj: 

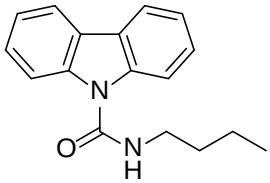
The general experimental procedure was followed to afford product **3aj** as a white solid (54.5 mg, 70% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 10.98 (s, 1H), 8.23 (d, *J* = 8.0 Hz, 2H), 7.96 (d, *J* = 8.5 Hz, 2H), 7.92–7.86 (m, 4H), 7.54 (t, *J* = 10.5 Hz, 2H), 7.40 (t, *J* = 15.0 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 150.0, 143.0, 137.8, 133.4, 126.9, 124.3, 122.5, 120.4, 120.0, 119.1, 114.0, 105.5. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{14}N_3O$ 312.1131; Found 312.1129.

3ak: 

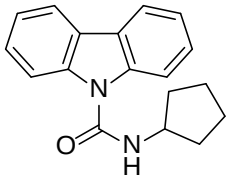
The general experimental procedure was followed to afford product **3ak** as a white solid (67.0 mg, 81% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 11.17 (s, 1H), 8.32 (d, *J* = 8.5 Hz, 2H), 8.24 (d, *J* = 8.0 Hz, 2H), 7.97 (d, *J* = 7.5 Hz, 2H), 7.94 (d, *J* = 9.0 Hz, 2H), 7.54 (t, *J* = 15.5 Hz, 2H), 7.41 (t, *J* = 15.0 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 150.1, 145.0, 142.7, 137.8, 127.0, 125.1, 124.4, 122.6, 120.5, 119.6, 114.1. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{14}N_3O_3$ 332.1030; Found 332.1033.

3al: 

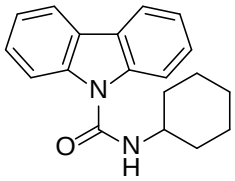
The general experimental procedure was followed to afford product **3al** as a white solid (53.0 mg, 89% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.92 (t, *J* = 16.0 Hz, 4H), 7.40 (dt, *J* = 7.0, 1.0 Hz, 2H), 7.26 (t, *J* = 7.5 Hz, 2H), 5.78 (s, 1H), 3.51 (dt, *J* = 7.0, 5.5 Hz, 2H), 1.29 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 152.8, 138.3, 126.8, 125.0, 122.1, 120.2, 113.5, 35.9, 15.1. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{15}N_2O$ 239.1179; Found 239.1177.

3am: 

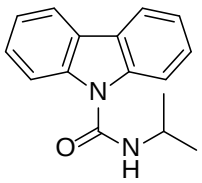
The general experimental procedure was followed to afford product **3am** as a white solid (65.9 mg, 99% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 8.33 (t, *J* = 11.0 Hz, 1H), 8.18 (d, *J* = 7.5 Hz, 2H), 7.93 (d, *J* = 8.5 Hz, 2H), 7.51 (t, *J* = 8.0 Hz, 2H), 7.34 (t, *J* = 15.0 Hz, 2H), 3.43–3.37 (m, 2H), 1.70–1.62 (m, 2H), 1.50–1.40 (m, 2H), 0.97 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 152.2, 138.1, 126.5, 123.8, 121.5, 120.2, 113.5, 40.1, 31.2, 19.8, 13.7. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{17}H_{19}N_2O$ 267.1492; Found 267.1493.

3an: 

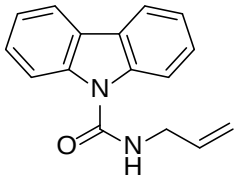
The general experimental procedure was followed to afford product **3an** as a white solid (63.3 mg, 92% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.98 (d, J = 7.5 Hz, 2H), 7.95 (d, J = 8.5 Hz, 2H), 7.45 (t, J = 8.5 Hz, 2H), 7.31 (t, J = 7.5 Hz, 2H), 5.76 (d, J = 7.5 Hz, 1H), 4.44–4.30 (m, 1H), 2.23–2.10 (m, 2H), 1.83–1.68 (m, 4H), 1.67–1.57 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 152.3, 138.4, 126.9, 125.0, 122.1, 120.2, 113.4, 52.9, 33.3, 23.8. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{18}H_{19}N_2O$ 279.1492; Found 279.1491.

3ao: 

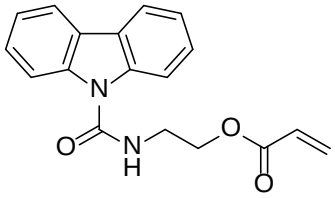
The general experimental procedure was followed to afford product **3ao** as a white solid (40.9 mg, 56% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.00 (dd, J = 12.0, 7.5 Hz, 4H), 7.47 (t, J = 8.0 Hz, 2H), 7.32 (t, J = 7.5 Hz, 2H), 5.66 (d, J = 7.5 Hz, 1H), 4.06–3.95 (m, 1H), 2.23–2.12 (m, 2H), 1.86–1.76 (m, 2H), 1.74–1.65 (m, 1H), 1.55–1.43 (m, 2H), 1.42–1.32 (m, 2H), 1.31–1.20 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 151.9, 138.5, 126.9, 125.1, 122.2, 120.3, 113.5, 50.1, 33.4, 25.6, 25.0. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{19}H_{21}N_2O$ 293.1648; Found 293.1647.

3ap: 

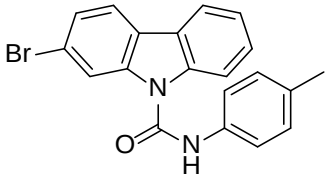
The general experimental procedure was followed to afford product **3ap** as a white solid (43.3mg, 69% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.29 (d, J = 7.5 Hz, 1H), 8.19 (d, J = 7.5 Hz, 2H), 7.90 (d, J = 8.5 Hz, 2H), 7.50 (t, J = 7.5 Hz, 2H), 7.33 (t, J = 7.5 Hz, 2H), 4.15–4.05 (m, 1H), 1.31 (d, J = 6.5 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 151.3, 138.0, 126.5, 123.7, 121.5, 120.3, 113.5, 42.7, 22.3. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{17}N_2O$ 253.1335; Found 253.1334.

3ar: 

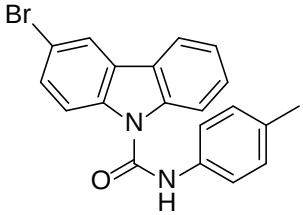
The general experimental procedure was followed to afford product **3ar** as a white solid (58.9 mg, 94% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.54 (s, 1H), 8.19 (d, J = 8.0 Hz, 2H), 7.96 (d, J = 6.0 Hz, 2H), 7.51 (t, J = 8.0 Hz, 2H), 7.34 (t, J = 7.5 Hz, 2H), 6.10–6.00 (m, 1H), 5.33 (d, J = 17.0 Hz, 1H), 5.20 (d, J = 10.5 Hz, 1H), 4.04 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 152.2, 138.0, 135.0, 126.6, 123.9, 121.7, 120.3, 116.0, 113.7, 42.8. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{15}N_2O$ 251.1179; Found 251.1172.

3as: 

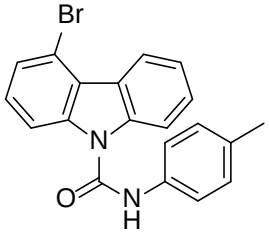
The general experimental procedure was followed to afford product **3as** as a white solid (56.0 mg, 73% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.53 (s, 1H), 8.19 (d, J = 8.0 Hz, 2H), 7.94 (d, J = 8.5 Hz, 2H), 7.49 (t, J = 8.0 Hz, 2H), 7.34 (t, J = 7.5 Hz, 2H), 6.46–6.38 (m, 1H), 6.29-6.20(m, 1H),6.02-5.96(m, 1H), 4.41 (t, J = 5.5 Hz, 2H), 3.75-3.65 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 165.6, 152.3, 137.9, 131.9, 128.4, 126.6, 123.9, 121.7, 120.3, 113.6, 62.7, 39.4. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{18}H_{17}N_2O_3$ 309.1234; Found 309.1234.

3ca: 

The general experimental procedure was followed to afford product **3ca** as a white solid (58.09 mg, 61% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 10.56 (s, 1H), 8.25 (d, J = 7.5 Hz, 1H), 8.21 (d, J = 8.0 Hz, 1H), 8.07 (s, 1H), 7.94–7.86 (m, 1H), 7.60–7.49 (m, 4H), 7.43–7.35 (m, 1H), 7.23 (d, J = 7.5 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 149.6, 138.8, 138.1, 135.6, 133.2, 129.4, 127.3, 124.8, 123.3, 123.2, 122.4, 122.2, 120.6, 120.2, 119.3, 116.4, 113.8, 20.5. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{16}N_2BrO$ 379.0441; Found 379.0439.

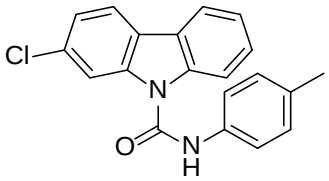
3da: 

The general experimental procedure was followed to afford product **3da** as a white solid (71.2 mg, 70% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 10.51 (s, 1H), 8.51 (d, J = 3.0 Hz, 1H), 8.29 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 8.5 Hz, 1H), 7.87 (dd, J = 9.0, 2.5 Hz, 1H), 7.66 (d, J = 8.5 Hz, 1H), 7.61–7.53 (m, 3H), 7.42–7.36 (m, 1H), 7.22 (d, J =8.0 Hz, 2H), 2.31 (s, 3H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 149.6, 138.3, 136.9, 135.7, 133.1, 129.4, 129.2, 127.6, 126.1, 123.1, 122.9, 122.3, 121.0, 120.1, 115.7, 114.2, 113.7, 20.5. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{16}N_2BrO$ 379.0441; Found 379.0439.

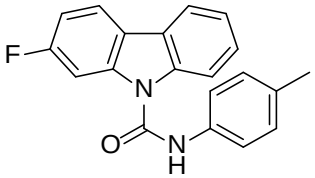
3ea: 

The general experimental procedure was followed to afford product **3ea** as a white solid (84.4 mg, 89% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 10.68 (s, 1H), 8.74 (d, J = 8.0 Hz,

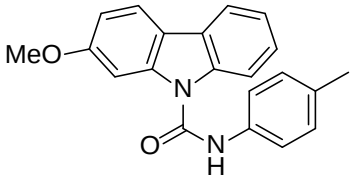
1H), 7.96 (d, J = 8.0 Hz, 2H), 7.64–7.57 (m, 4H), 7.47 (t, J = 8.0 Hz, 2H), 7.24 (d, J = 8.0 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 149.3, 139.4, 138.3, 135.6, 133.3, 129.4, 127.7, 127.5, 125.9, 123.0, 122.0, 121.9, 121.8, 120.1, 115.4, 113.3, 112.7, 20.5. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{16}N_2BrO$ 379.0441; Found 379.0439.

3fa: 

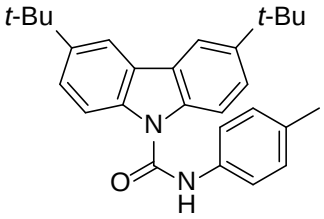
The general experimental procedure was followed to afford product **3fa** as a white solid (76.2 mg, 91% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 10.55 (s, 1H), 8.27 (t, J = 5.0 Hz, 2H), 7.92–7.88 (m, 2H), 7.61–7.52 (m, 3H), 7.45–7.32 (m, 2H), 7.23 (d, J = 8.0 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 149.6, 138.5, 138.3, 135.6, 133.2, 131.0, 129.4, 127.2, 123.3, 122.9, 122.4, 122.2, 121.8, 120.6, 120.2, 113.8, 113.6, 20.5. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{16}N_2ClO$ 335.0946; Found 335.0942.

3ga: 

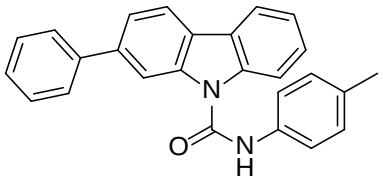
The general experimental procedure was followed to afford product **3ga** as a white solid (70.5 mg, 89% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 10.54 (s, 1H), 8.27–8.21 (m, 2H), 7.90 (d, J = 8.5 Hz, 1H), 7.68 (d, J = 10.0 Hz, 1H), 7.60 (d, J = 8.0 Hz, 2H), 7.53–7.49 (m, 1H), 7.41–7.35 (m, 1H), 7.28–7.17 (m, 3H), 2.31 (s, 3H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 161.4 (d, $^1J_{C–F}$ = 241.9 Hz), 149.8, 138.7 (d, $^3J_{C–F}$ = 12.6 Hz), 138.4, 135.7, 133.2, 129.4, 126.5, 123.6, 122.3, 121.9 (d, $^3J_{C–F}$ = 12.6 Hz), 120.7, 120.3, 120.2, 113.7, 109.9 (d, $^2J_{C–F}$ = 23.9 Hz), 101.0 (d, $^2J_{C–F}$ = 27.7 Hz), 20.5. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{16}FN_2O$ 319.1241; Found 319.1241.

3ha: 

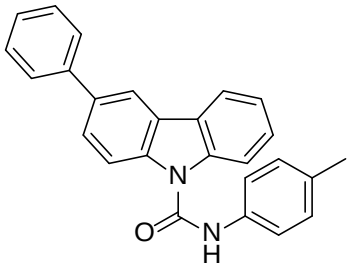
The general experimental procedure was followed to afford product **3ha** as a white solid (58.1 mg, 70% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.76 (d, J = 8.0 Hz, 2H), 7.67 (d, J = 8.5 Hz, 1H), 7.56 (s, 1H), 7.47 (s, 1H), 7.40 (d, J = 8.0 Hz, 2H), 7.28 (t, J = 7.5 Hz, 1H), 7.20 (t, J = 7.5 Hz, 1H), 7.14 (d, J = 8.0 Hz, 2H), 6.80 (d, J = 8.5 Hz, 1H), 3.77 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 159.6, 150.4, 139.7, 137.8, 134.6, 134.5, 129.9, 125.6, 125.5, 122.6, 120.6, 120.2, 119.6, 118.4, 112.9, 111.1, 98.2, 55.7, 21.0. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{21}H_{19}N_2O_2$ 331.1441; Found 331.1439.

3ja: 

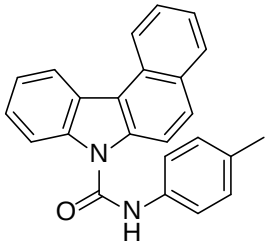
The general experimental procedure was followed to afford product **3ja** as a white solid (89.0 mg, 87% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.10–8.02 (m, 2H), 7.96 (d, J = 8.5 Hz, 2H), 7.55 (s, 1H), 7.53 (d, J = 2.0 Hz, 1H), 7.51 (d, J = 1.5 Hz, 1H), 7.48 (d, J = 9.0 Hz, 2H), 7.21 (d, J = 8.0 Hz, 2H), 2.38 (s, 3H), 1.48 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 150.5, 145.7, 136.7, 134.8, 134.3, 129.9, 125.5, 124.8, 120.1, 116.4, 113.3, 34.9, 31.9, 21.0. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{33}N_2O$ 413.2587; Found 413.2581.

3ka: 

The general experimental procedure was followed to afford product **3ka** as a white solid (65.9 mg, 70% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.31-8.28 (m, 1H), 8.03 (t, J = 10.0 Hz, 2H), 7.98 (d, J = 8.5 Hz, 1H), 7.68 (d, J = 7.5 Hz, 2H), 7.59 (d, J = 8.0 Hz, 1H), 7.56 (s, 1H), 7.49–7.42 (m, 5H), 7.39–7.34 (m, 2H), 7.23 (d, J = 8.0 Hz, 2H), 2.38 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 150.4, 141.4, 140.6, 139.1, 138.6, 134.7, 134.6, 130.0, 129.0, 127.6, 127.5, 127.2, 125.3, 124.4, 122.8, 122.2, 120.6, 120.5, 120.3, 113.4, 112.4, 21.0. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{26}H_{21}N_2O$ 377.1648; Found 377.1647.

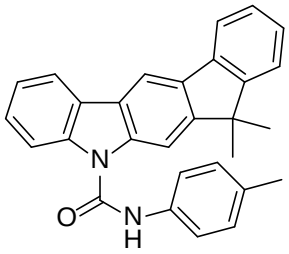
3la: 

The general experimental procedure was followed to afford product **3la** as a white solid (73.3 mg, 78% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.18 (d, J = 1.5 Hz, 1H), 8.05 (t, J = 8.5 Hz, 2H), 8.01 (d, J = 8.5 Hz, 1H), 7.71–7.67 (m, 3H), 7.55 (s, 1H), 7.51–7.45 (m, 5H), 7.41–7.33 (m, 2H), 7.24 (d, J = 8.5 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 150.3, 141.2, 138.7, 137.7, 136.0, 134.7, 134.6, 130.0, 129.0, 127.43, 127.36, 127.2, 126.5, 125.9, 125.4, 122.8, 120.5, 120.2, 118.7, 113.9, 113.7, 21.1. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{26}H_{21}N_2O$ 377.1648; Found 377.1645.

3ma: 

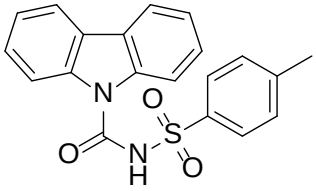
The general experimental procedure was followed to afford product **3ma** as a white solid (73.6 mg, 84% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.75 (d, J = 8.0 Hz, 1H), 8.54 (d, J = 8.0 Hz, 1H), 8.23 (d, J = 9.0 Hz, 1H), 8.07 (d, J = 8.5 Hz, 1H), 8.0 (d, J = 8.0 Hz, 1H), 7.90 (d, J = 9.0 Hz, 1H), 7.71 (t, J = 7.5 Hz, 1H), 7.60 (s, 1H), 7.56–7.43 (m, 5H), 7.26–7.22 (m, 2H), 2.38 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 149.9, 137.6, 136.4, 134.9, 134.5, 130.4, 130.0, 129.4, 129.3, 128.5, 127.4, 125.9, 125.8, 124.4, 123.6, 123.0, 122.6, 120.2, 117.9, 113.9, 113.2, 21.1. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{24}H_{19}N_2O$ 351.1492; Found 351.1491.

3na:



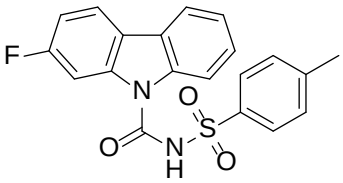
The general experimental procedure was followed to afford product **3na** as a white solid (102.05 mg, 98% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.11 (d, J = 2.5 Hz, 1H), 8.07 (d, J = 2.0 Hz, 1H), 7.97 (d, J = 7.5 Hz, 1H), 7.79 (dd, J = 8.0, 2.0 Hz, 1H), 7.75 (d, J = 7.5 Hz, 1H), 7.54 (s, 1H), 7.45 (d, J = 7.5 Hz, 2H), 7.41 (d, J = 7.5 Hz, 1H), 7.36 (t, J = 7.5 Hz, 2H), 7.31–7.25 (m, 2H), 7.21–7.15 (m, 2H), 2.33 (s, 3H), 1.50 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 154.0, 153.8, 150.4, 139.1, 138.6, 138.2, 134.7, 134.6, 134.5, 129.9, 127.2, 127.0, 126.6, 125.7, 124.5, 122.8, 122.6, 120.4, 120.1, 119.8, 113.0, 111.0, 108.5, 47.1, 27.8, 21.0. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{29}H_{25}N_2O$ 417.1961; Found 417.1967.

3at:



The general experimental procedure was followed to afford product **3at** as a white solid (71.5 mg, 79% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 8.72 (d, J = 8.5 Hz, 2H), 8.06 (d, J = 7.5 Hz, 2H), 7.84 (d, J = 8.0 Hz, 2H), 7.40 (t, J = 7.5 Hz, 2H), 7.26–7.22 (m, 4H), 2.32 (s, 3H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 156.3, 143.0, 139.9, 139.3, 128.4, 127.0, 126.1, 124.2, 121.1, 119.3, 117.1, 21.0. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{17}N_2O_3S$ 365.0954; Found 365.0957.

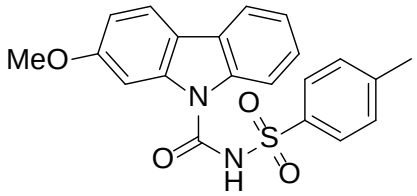
3gt:



The general experimental procedure was followed to afford product **3gt** as a white solid (40.0 mg, 40% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 8.66 (d, J = 8.5 Hz, 1H), 8.49 (dd, J = 12.0, 2.5 Hz, 1H), 8.08 (dd, J = 8.5, 6.0 Hz, 1H), 8.04 (dd, J = 8.0, 1.5 Hz, 1H), 7.81(dd, J = 6.0, 1.5 Hz, 1H), 7.37 (ddd, J = 8.5, 7.0, 1.5 Hz, 1H), 7.27–7.21 (m, 3H), 7.09 (td, J = 9.0, 3.0 Hz, 1H), 2.32 (s, 3H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 161.1 (d, $^1J_{C-F}$ = 238.1 Hz), 155.9, 142.8, 139.86 (d, $^3J_{C-F}$ = 11.3 Hz), 139.88, 139.81, 128.3, 126.9, 125.7, 123.6, 121.3,

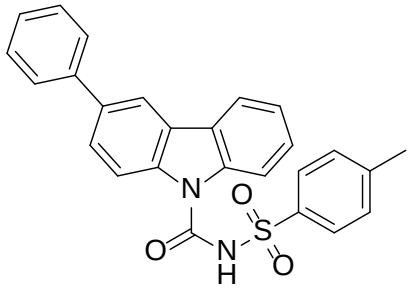
120.7, 120.4 (d, $^{3}J_{C–F}$ = 10.1 Hz), 119.1, 116.9, 108.7 (d, $^{2}J_{C–F}$ = 25.2 Hz), 103.8 (d, $^{2}J_{C–F}$ = 29.0 Hz), 20.9. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{20}H_{16}FN_2O_3S$ 383.0860; Found 383.0859.

3ht:



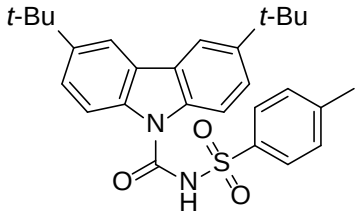
The general experimental procedure was followed to afford product **3ht** as a white solid (87.0 mg, 88% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 8.65 (d, *J* = 8.5 Hz, 1H), 8.29 (s, 1H), 7.93 (t, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.18 (t, *J* = 7.5 Hz, 1H), 6.85 (dd, *J* = 8.5, 2.5 Hz, 1H), 3.79 (s, 3H), 2.32 (s, 3H).^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 158.5, 156.2, 143.1, 140.7, 139.8, 139.4, 128.4,126.9, 124.7, 124.3, 121.0, 119.8, 118.4, 117.8, 116.9, 109.2, 101.5, 55.2, 20.9. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{21}H_{19}N_2O_4S$ 395.1060; Found 395.1058.

3lt:



The general experimental procedure was followed to afford product **3lt** as a white solid (95.8 mg, 87% yield). ^{1}H NMR (500 MHz, DMSO-*d*6): δ (ppm) = 8.78 (d, *J* = 8.5 Hz, 1H), 8.72 (d, *J* = 8.0 Hz, 1H), 8.42 (s, 1H), 8.20 (d, *J* = 7.5 Hz, 1H), 7.85 (d, *J* = 7.5 Hz, 2H), 7.81 (d, *J* = 8.0 Hz, 2H), 7.73 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.49 (t, *J* = 8.0 Hz, 2H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.29–7.24 (m, 3H), 2.33 (s, 3H). ^{13}C NMR (126 MHz, DMSO-*d*6): δ (ppm) = 156.2, 143.0, 140.7, 139.9, 139.8, 138.9, 133.2, 129.0, 128.4, 127.0, 126.8, 126.8, 126.3, 124.9, 124.8, 124.3, 121.2, 119.6, 117.5, 117.3, 117.1, 21.0. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{26}H_{21}N_2O_3S$ 441.1267; Found 441.1270.

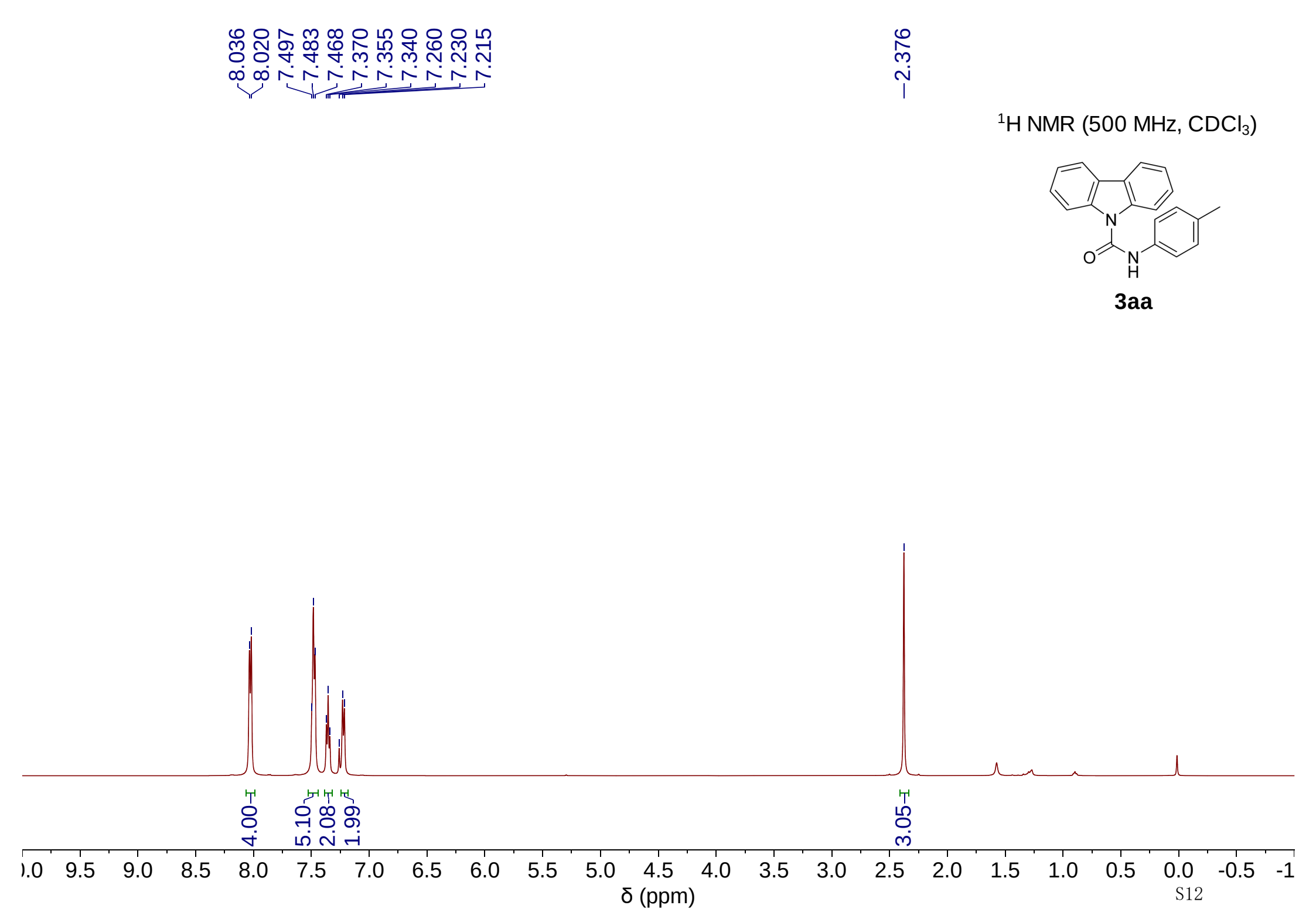
3jt:

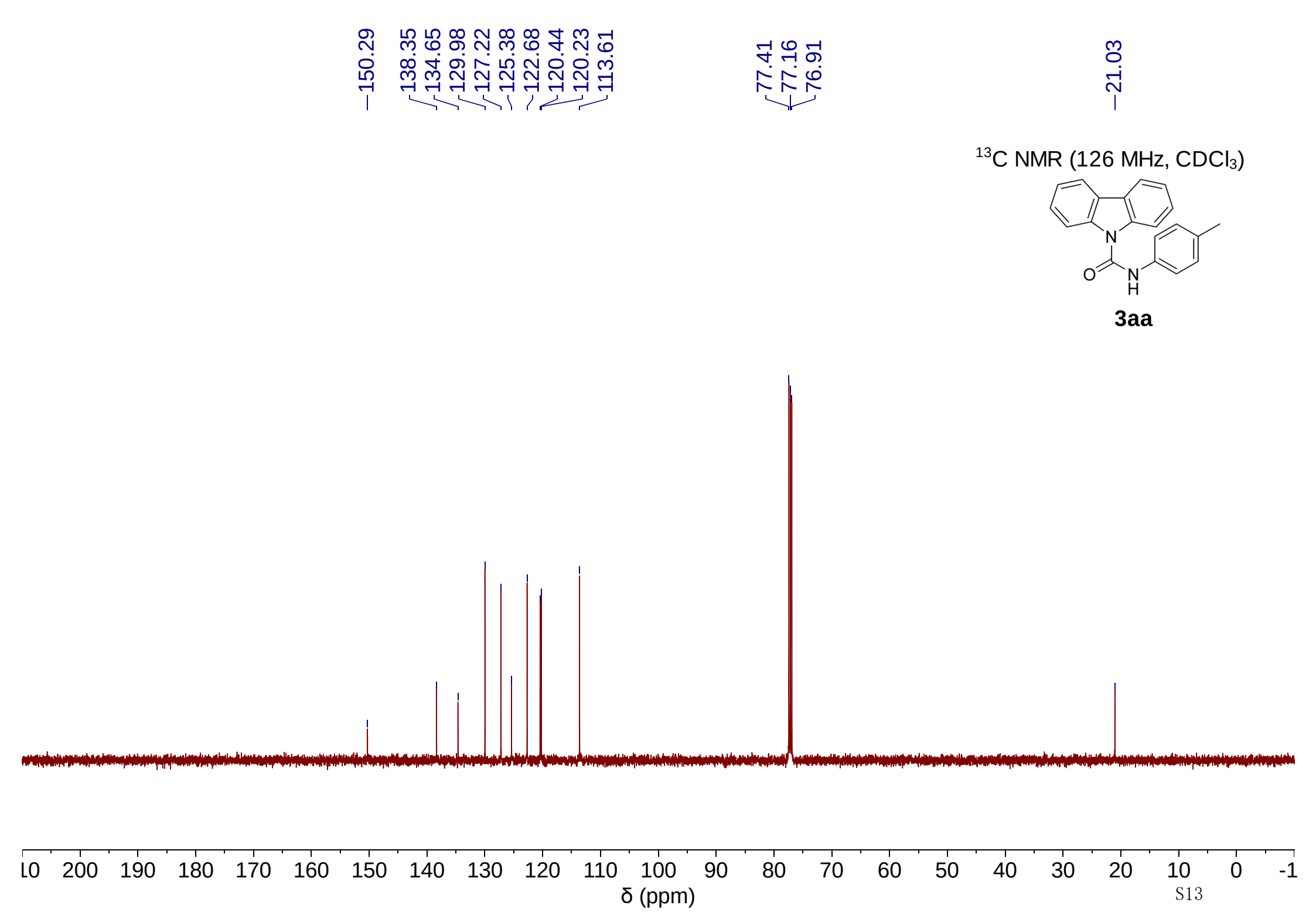


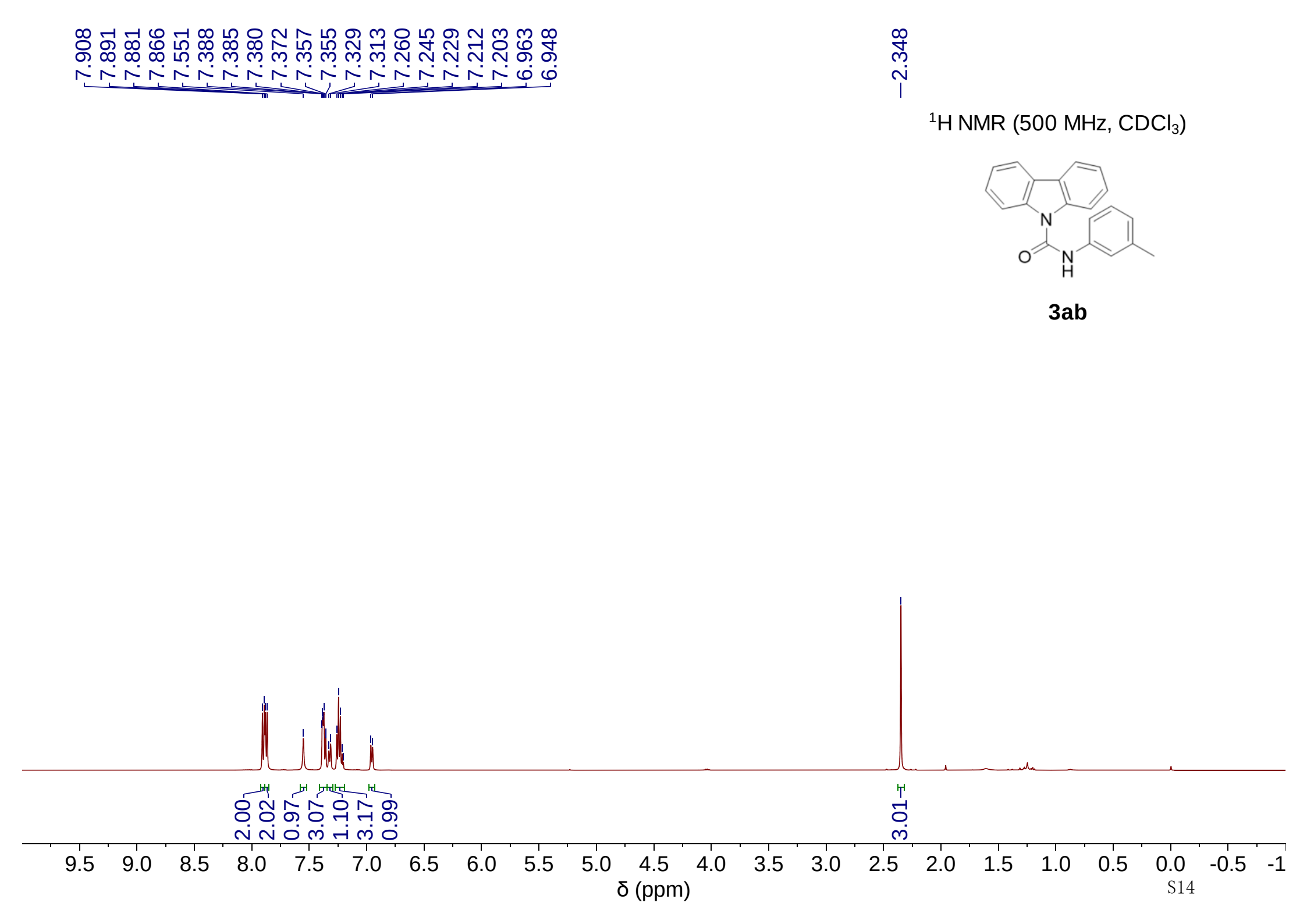
The general experimental procedure was followed to afford product **3jt** as a white solid (114.3 mg, 96% yield). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.54 (d, *J* = 9.0 Hz, 2H), 8.09 (s, 2H), 7.79 (d, *J* = 8.5 Hz, 2H), 7.43-7.38 (dt, *J* = 9.0, 2.0 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 2.32 (s, 3H), 1.39 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$): δ (ppm) = 156.3, 143.3, 143.2, 139.7, 137.7, 128.3, 126.9, 124.2, 123.4, 116.5, 115.4, 34.4, 31.8, 21.0. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{28}H_{33}N_2O_3S$ 477.2206; Found 477.2201.

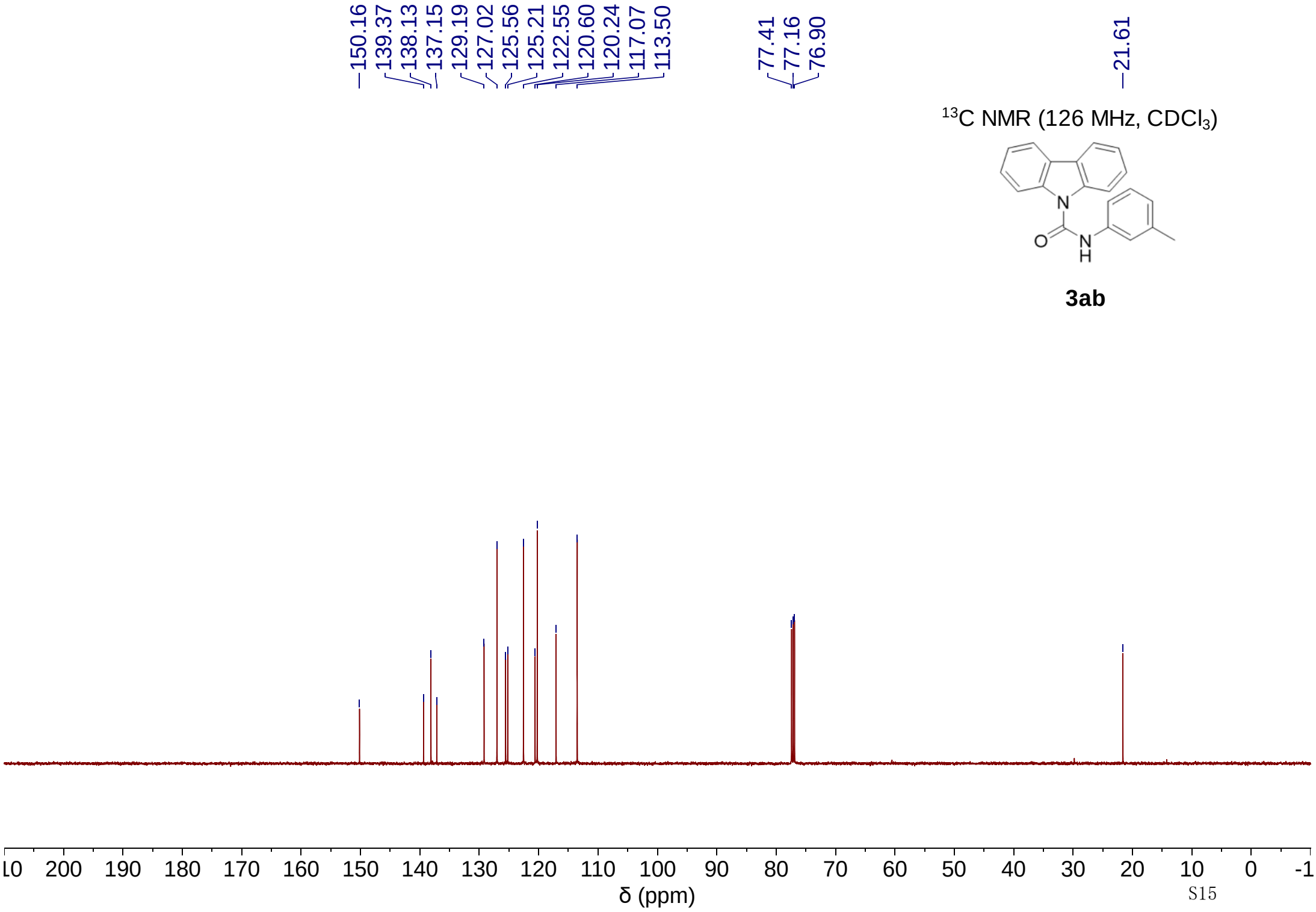
3. Copies of NMR spectra

See the next page!


8.036
8.020
7.497
7.483
7.468
7.370
7.355
7.340
7.260
7.230
7.215
2.376
^{1}H NMR (500 MHz, $CDCl_3$)
N
O
N
H
3aa
4.00
5.10
2.08
1.99
3.05
δ (ppm)

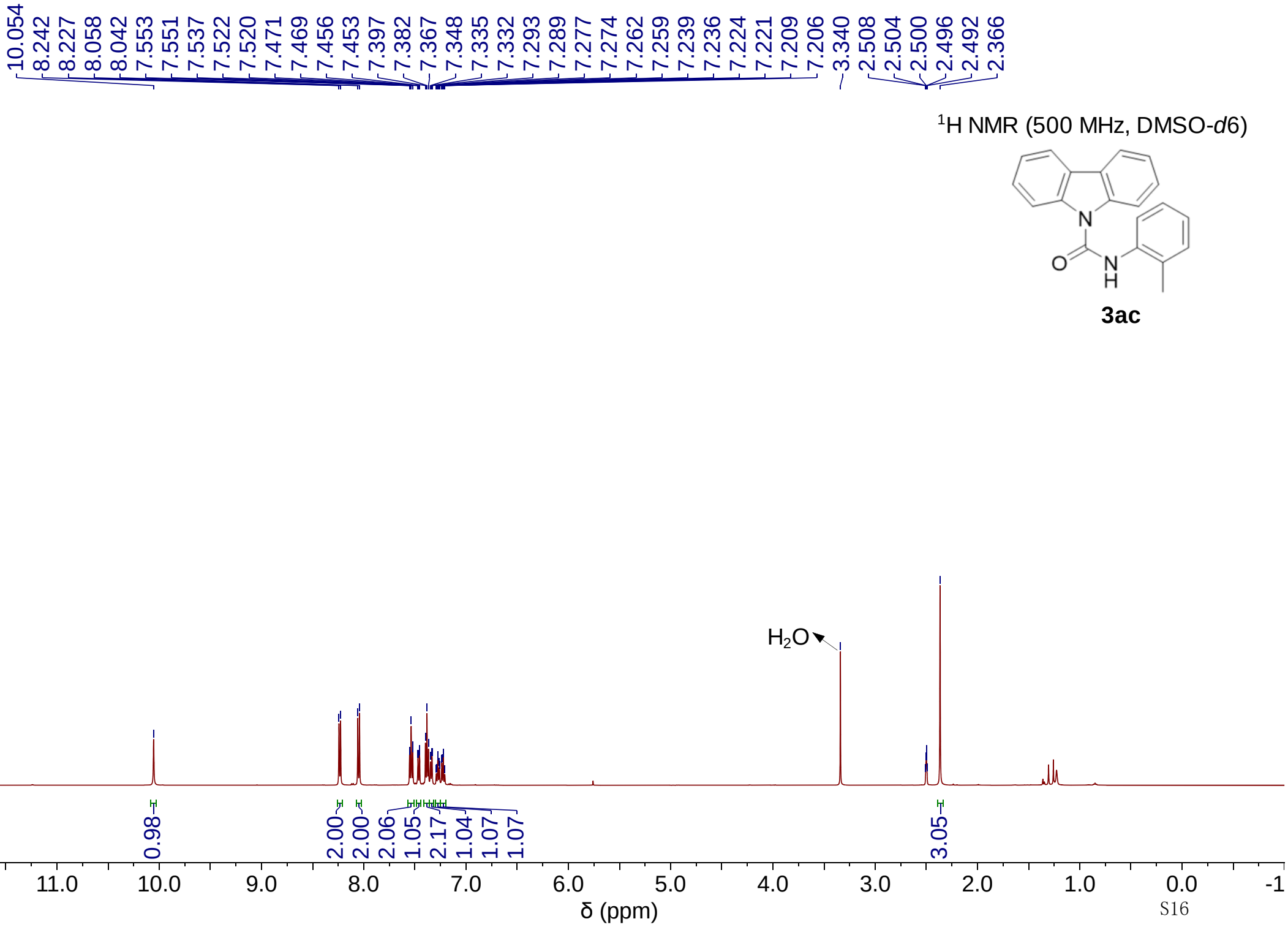

150.29
138.35
134.65
129.98
127.22
125.38
122.68
120.44
120.23
113.61
77.41
77.16
76.91
21.03
13C NMR (126 MHz, CDCl3)
N
O
N
H
3aa
δ (ppm)


7.908
7.891
7.881
7.866
7.551
7.388
7.385
7.380
7.372
7.357
7.355
7.329
7.313
7.260
7.245
7.229
7.212
7.203
6.963
6.948
2.348
1H NMR (500 MHz, CDCl3)
N
O
N
H
3ab
2.00
2.02
0.97
3.07
1.10
3.17
0.99
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
δ (ppm)

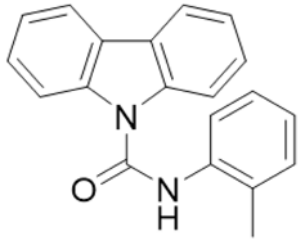


^{13}C NMR (126 MHz, $CDCl_3$)

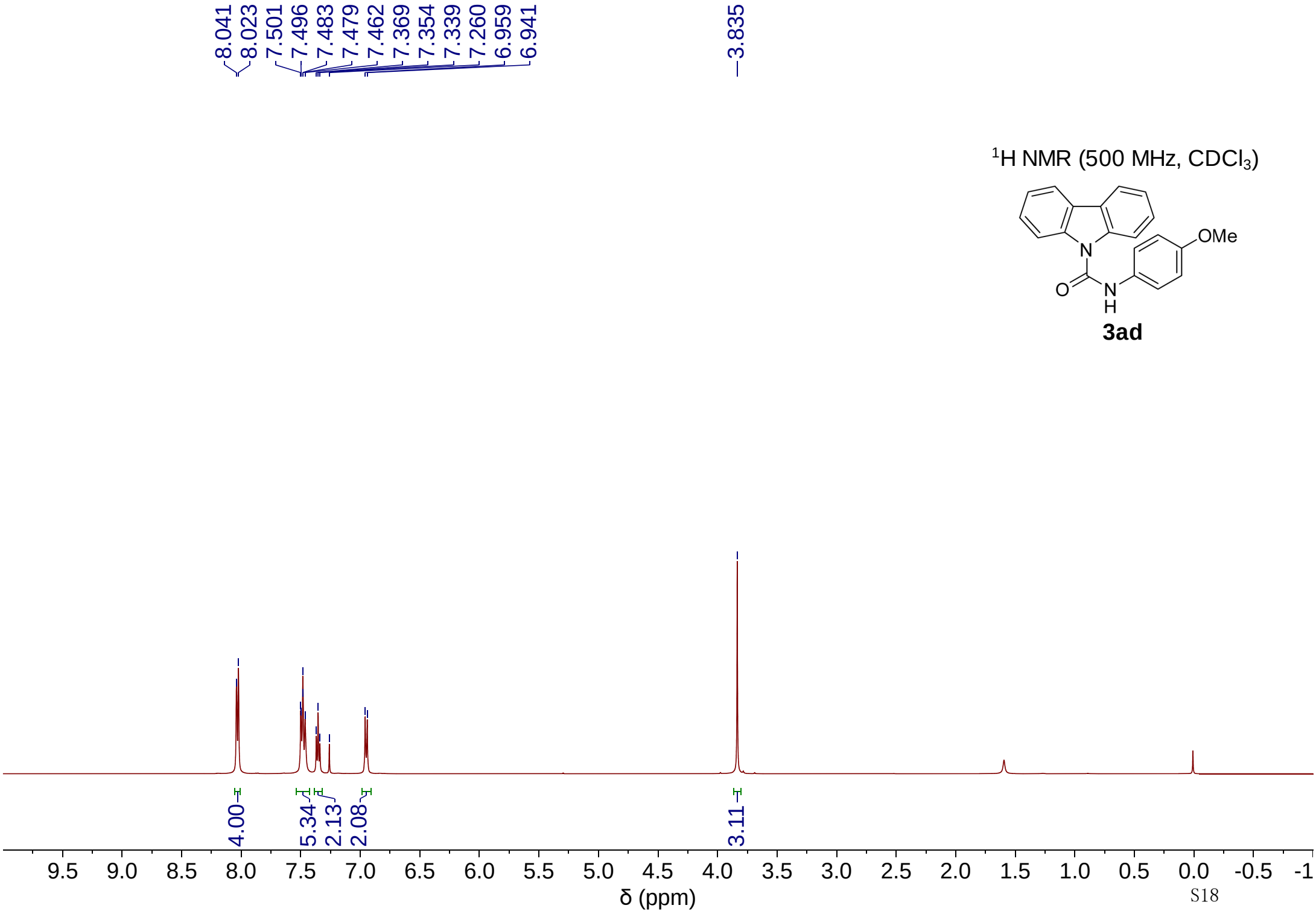
3ab


10.054
8.242
8.227
8.058
8.042
7.553
7.551
7.537
7.522
7.520
7.471
7.469
7.456
7.453
7.397
7.382
7.367
7.348
7.335
7.332
7.293
7.289
7.277
7.274
7.262
7.259
7.239
7.236
7.224
7.221
7.209
7.206
3.340
2.508
2.504
2.500
2.496
2.492
2.366
^{1}H NMR (500 MHz, DMSO-*d*6)
N
O
N
H
3ac
H2O
0.98
2.00
2.00
2.06
1.05
2.17
1.04
1.07
1.07
3.05
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
δ (ppm)

^{13}C NMR (126 MHz, DMSO-*d*6)



3ac

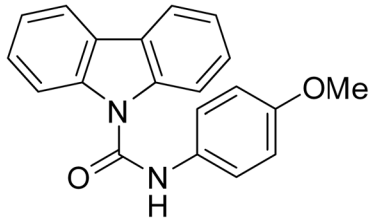


^{1}H NMR (500 MHz, $CDCl_3$)

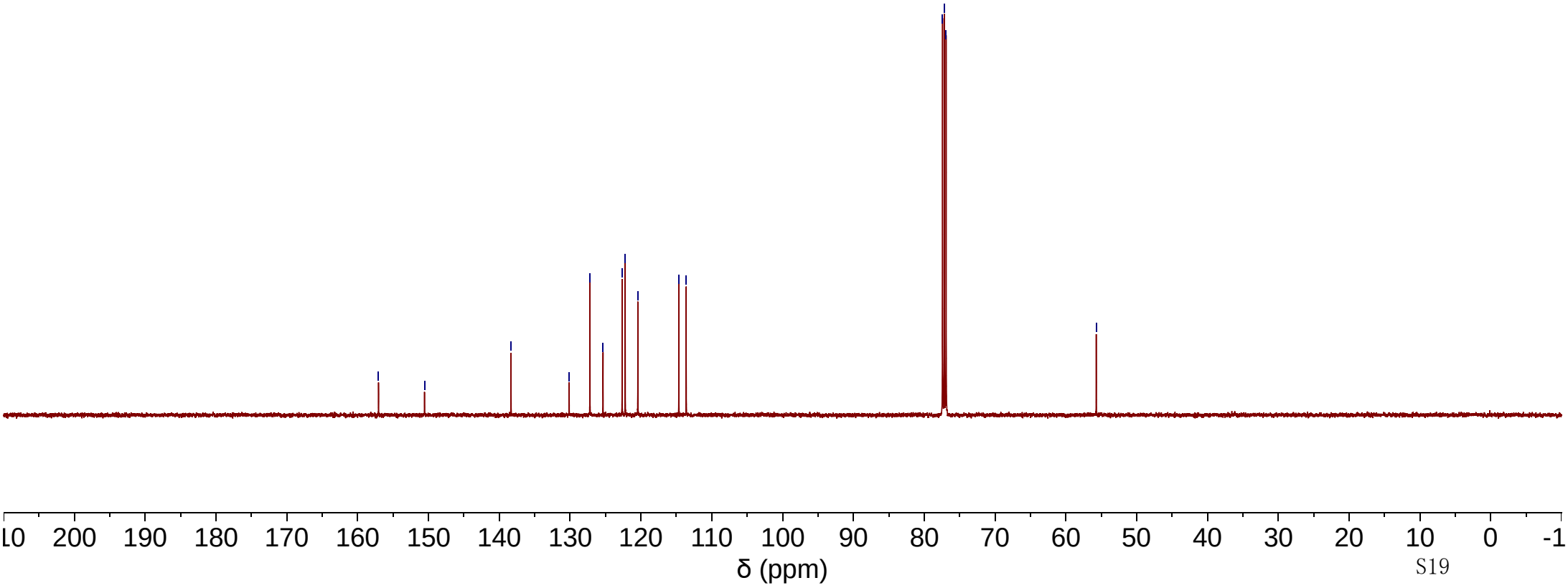
3ad

157.05
150.56
138.34
130.13
127.20
125.35
122.66
122.22
120.44
114.65
113.61
77.41
77.16
76.91
55.71

^{13}C NMR (126 MHz, $CDCl_3$)



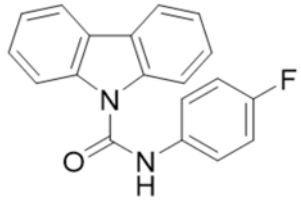
3ad



8.013
7.999
7.984
7.562
7.553
7.544
7.540
7.535
7.526
7.485
7.468
7.453
7.365
7.350
7.335
7.260
7.121
7.104
7.086

1.579

^{1}H NMR (500 MHz, $CDCl_3$)



3ae

H_2O

4.00
2.99
2.04
2.01
1.98

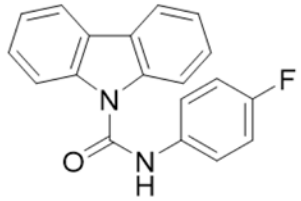
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

δ (ppm)

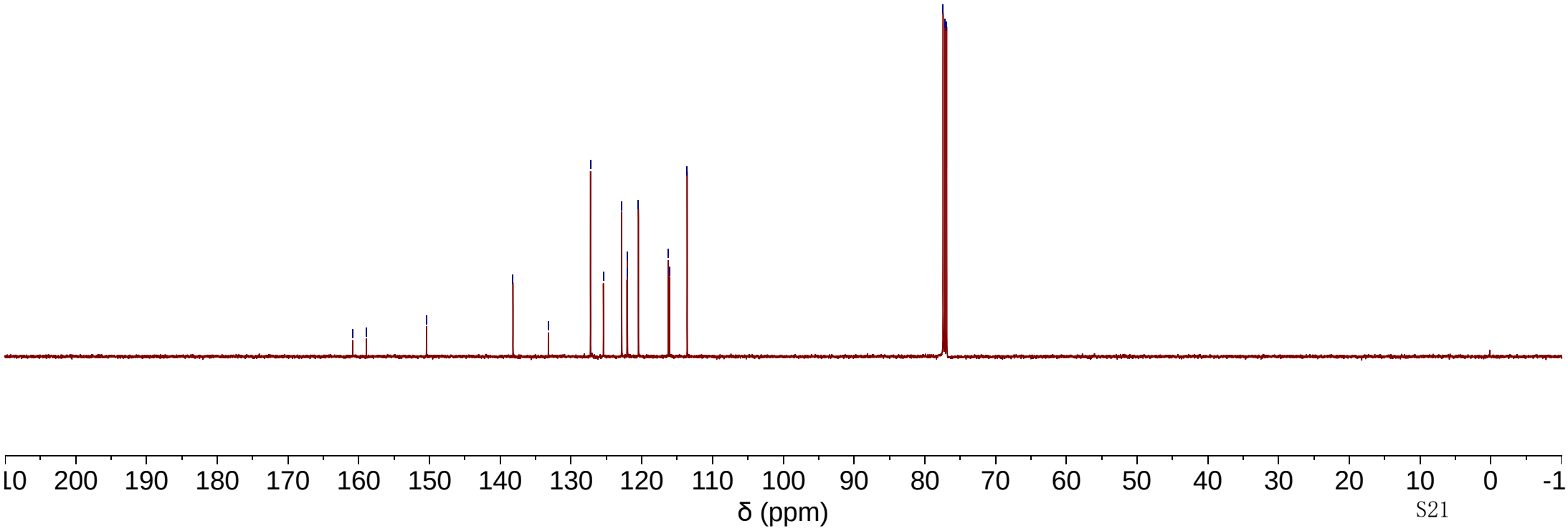
160.86
158.91
150.43
138.21
133.20
133.18
127.25
125.42
122.84
122.09
122.03
120.47
116.27
116.09
113.58

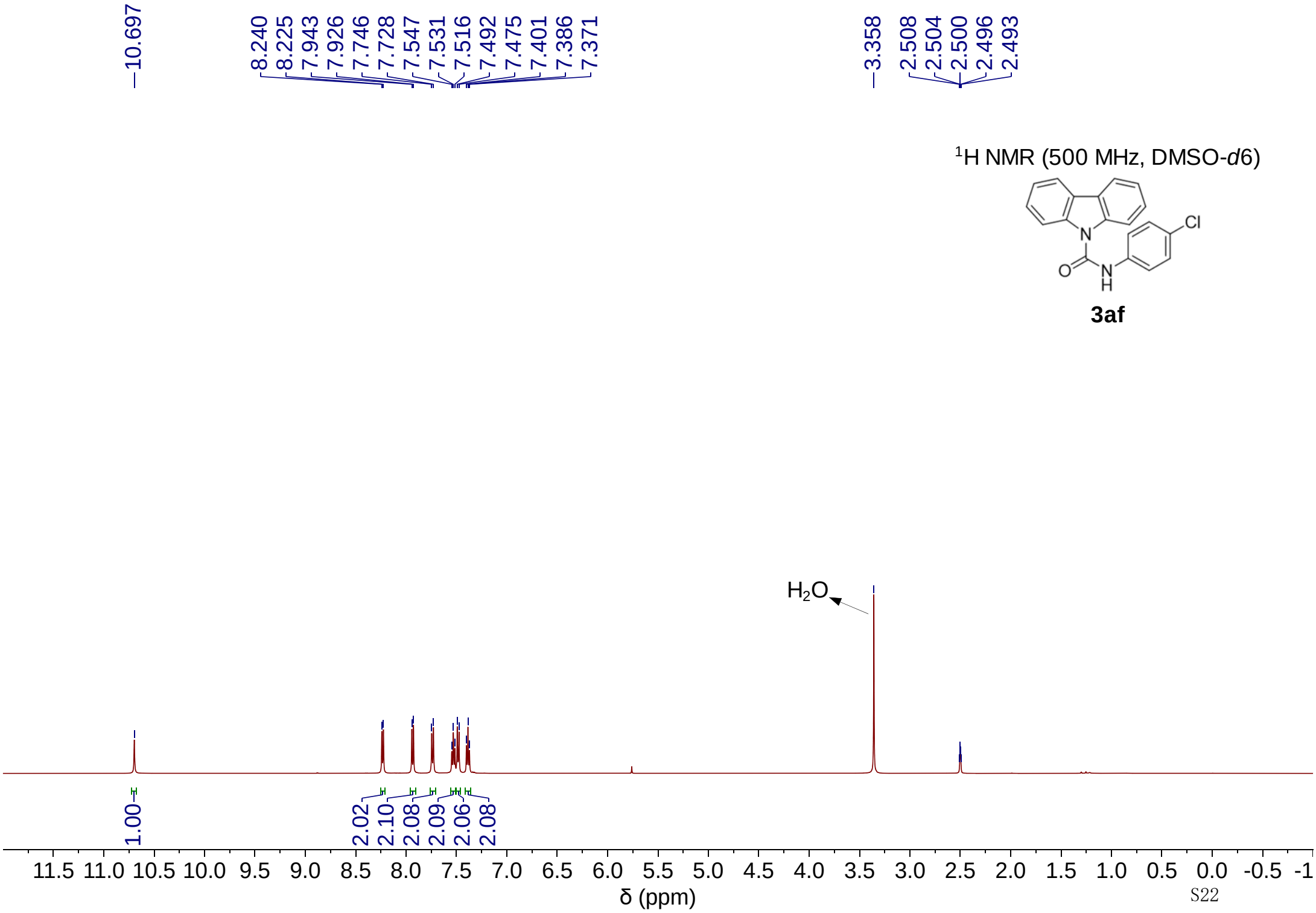
77.41
77.16
76.91

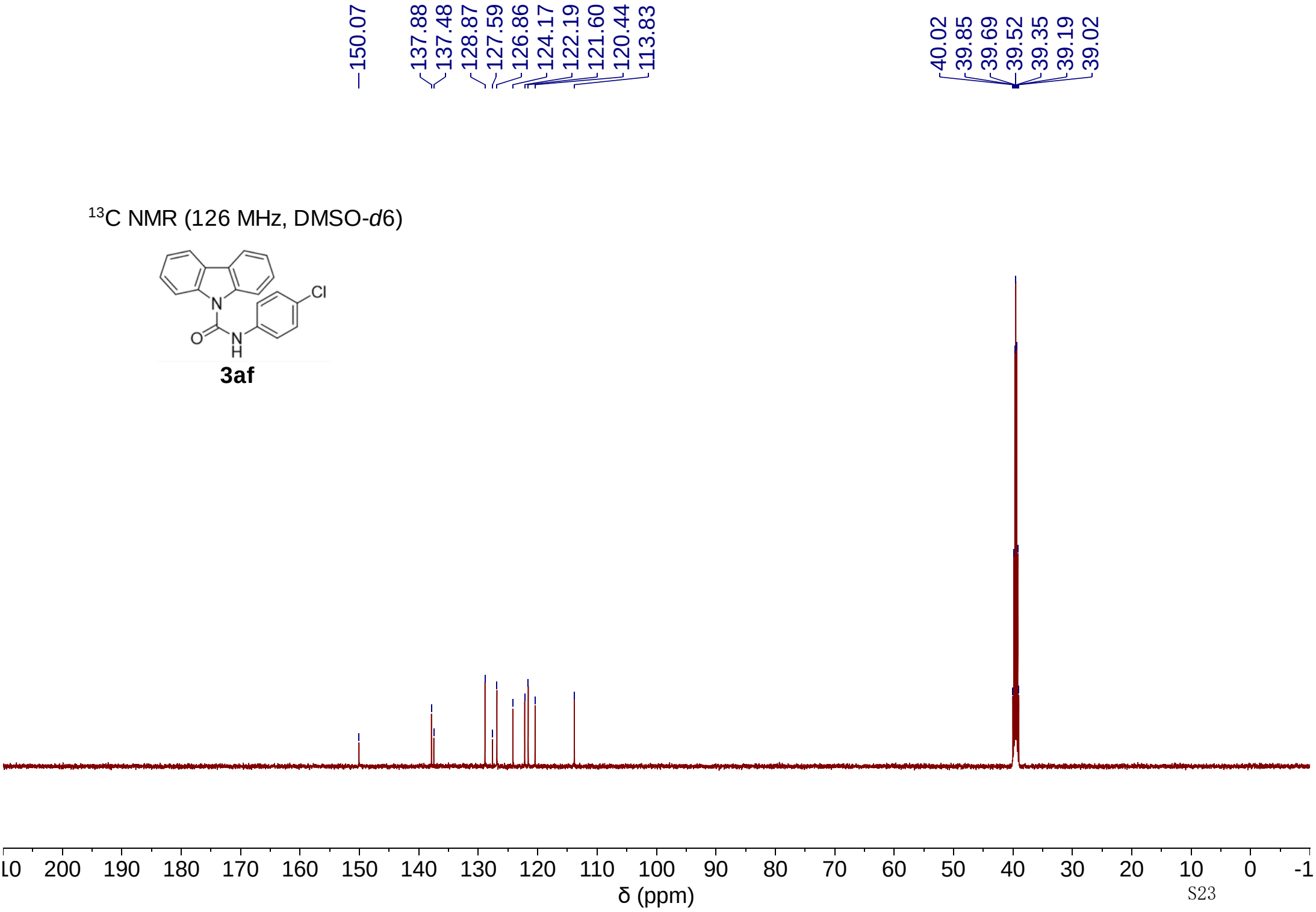
^{13}C NMR (126 MHz, $CDCl_3$)



3ae




10.697
8.240
8.225
7.943
7.926
7.746
7.728
7.547
7.531
7.516
7.492
7.475
7.401
7.386
7.371
3.358
2.508
2.504
2.500
2.496
2.493
1H NMR (500 MHz, DMSO-d6)
Cl
N
O
N
H
3af
H2O
1.00
2.02
2.10
2.08
2.09
2.06
2.08
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
δ (ppm)

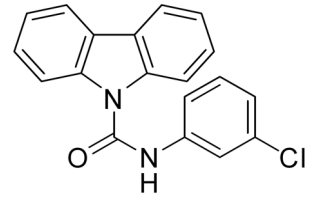


^{13}C NMR (126 MHz, DMSO-*d*6)

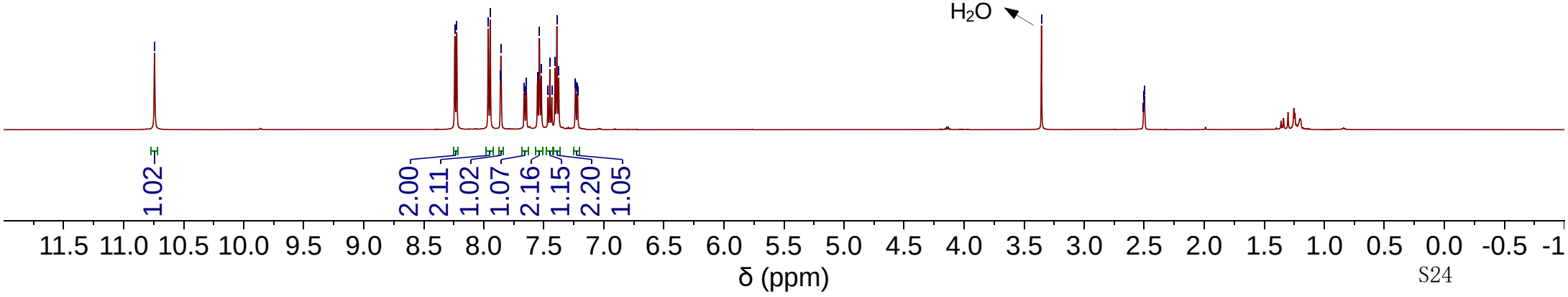
3af

10.743
8.242
8.226
7.964
7.947
7.862
7.858
7.854
7.665
7.661
7.649
7.645
7.554
7.537
7.522
7.466
7.450
7.434
7.407
7.392
7.377
7.238
7.234
7.222
7.218
3.356
2.507
2.504
2.500
2.496

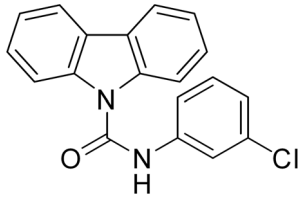
^{1}H NMR (500 MHz, DMSO-*d*6)



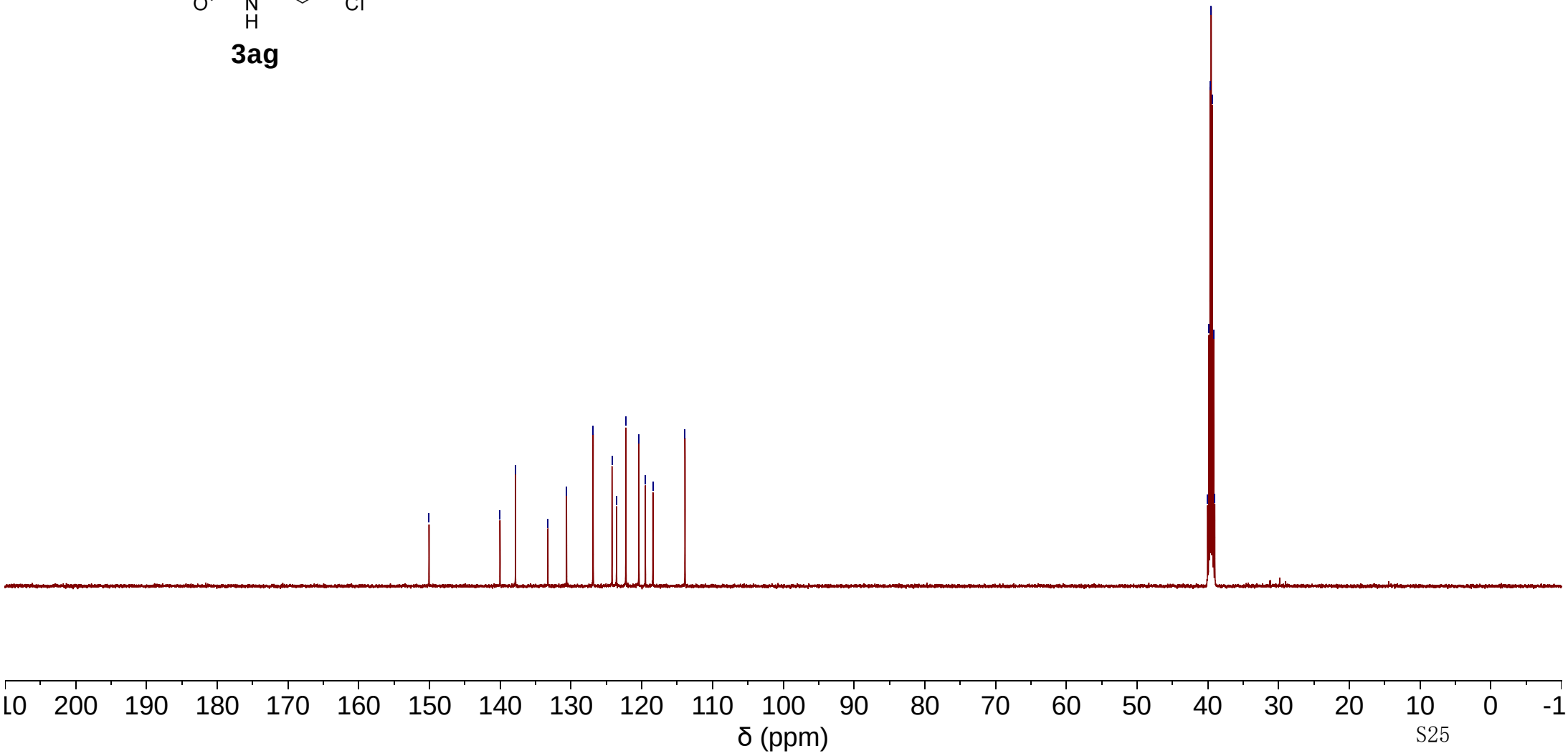
3ag

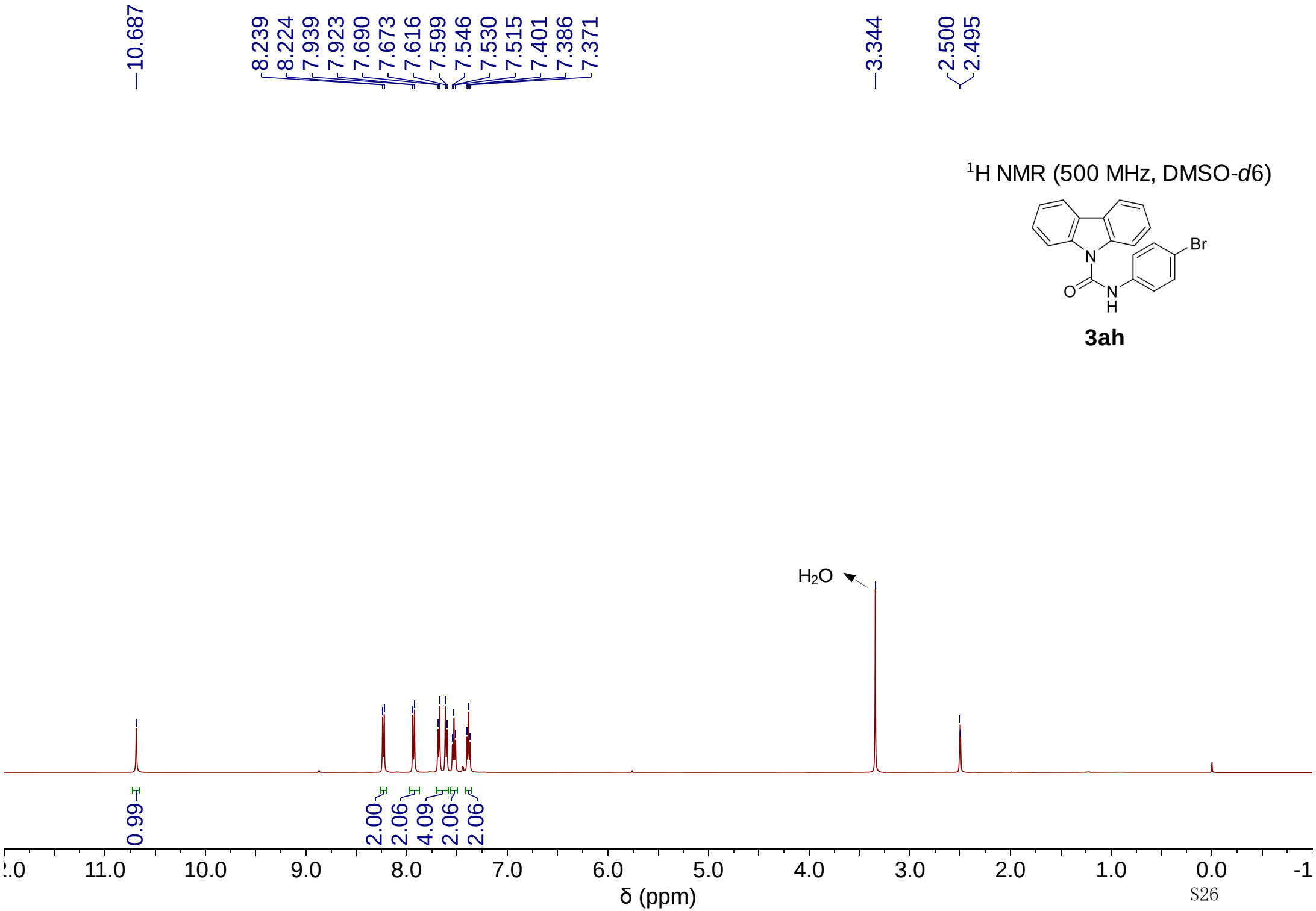


^{1}H NMR (500 MHz, DMSO-*d*6)



3ag

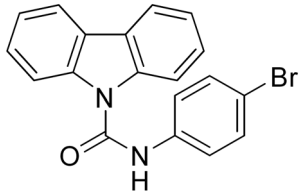



10.687
8.239
8.224
7.939
7.923
7.690
7.673
7.616
7.599
7.546
7.530
7.515
7.401
7.386
7.371
3.344
2.500
2.495
^{1}H NMR (500 MHz, DMSO-*d*6)
Br
N
O
N
H
3ah
H_2O
0.99
2.00
2.06
4.09
2.06
2.06
δ (ppm)

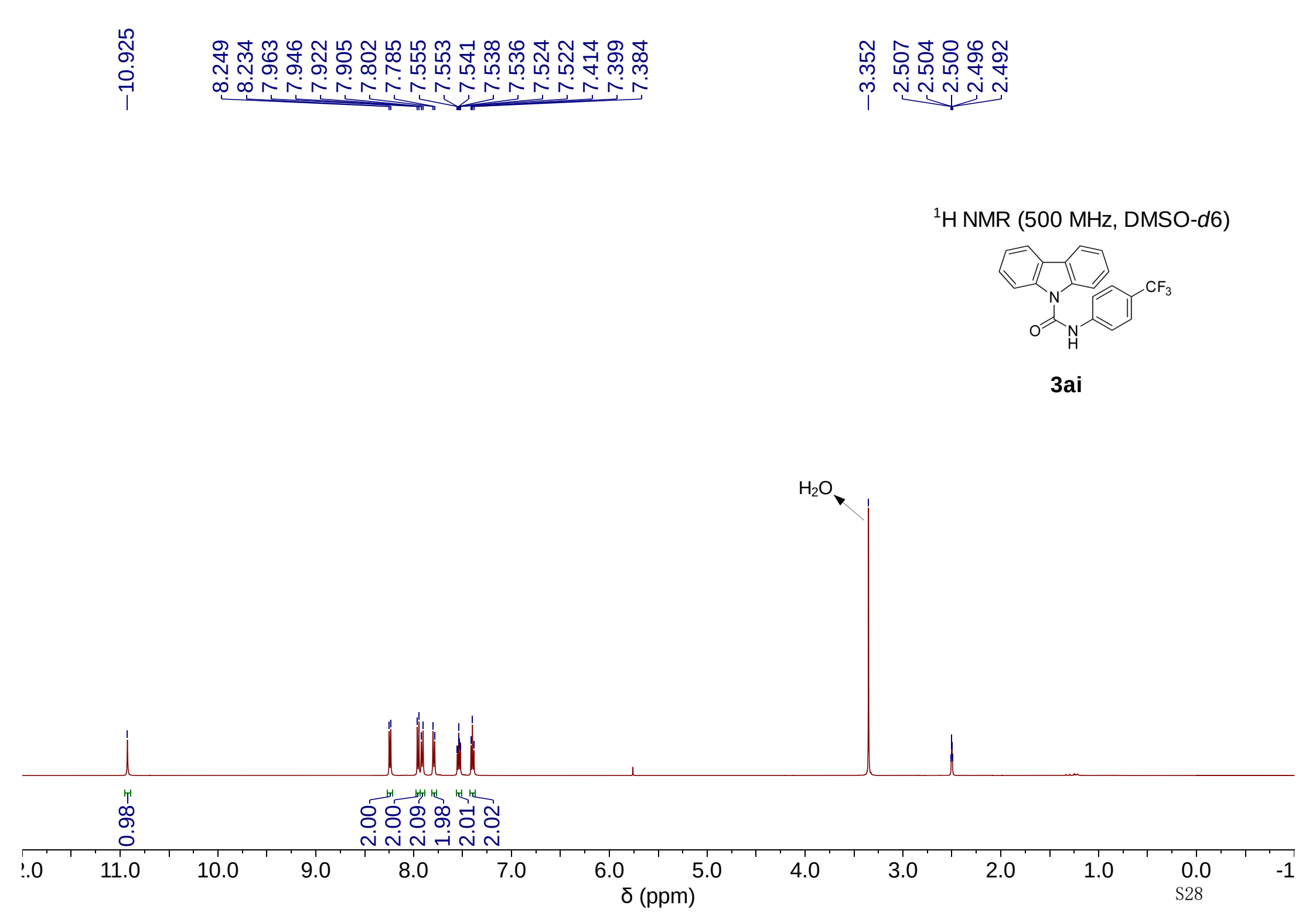
150.03
137.90
137.87
131.76
126.85
124.16
122.18
121.95
120.42
115.62
113.81

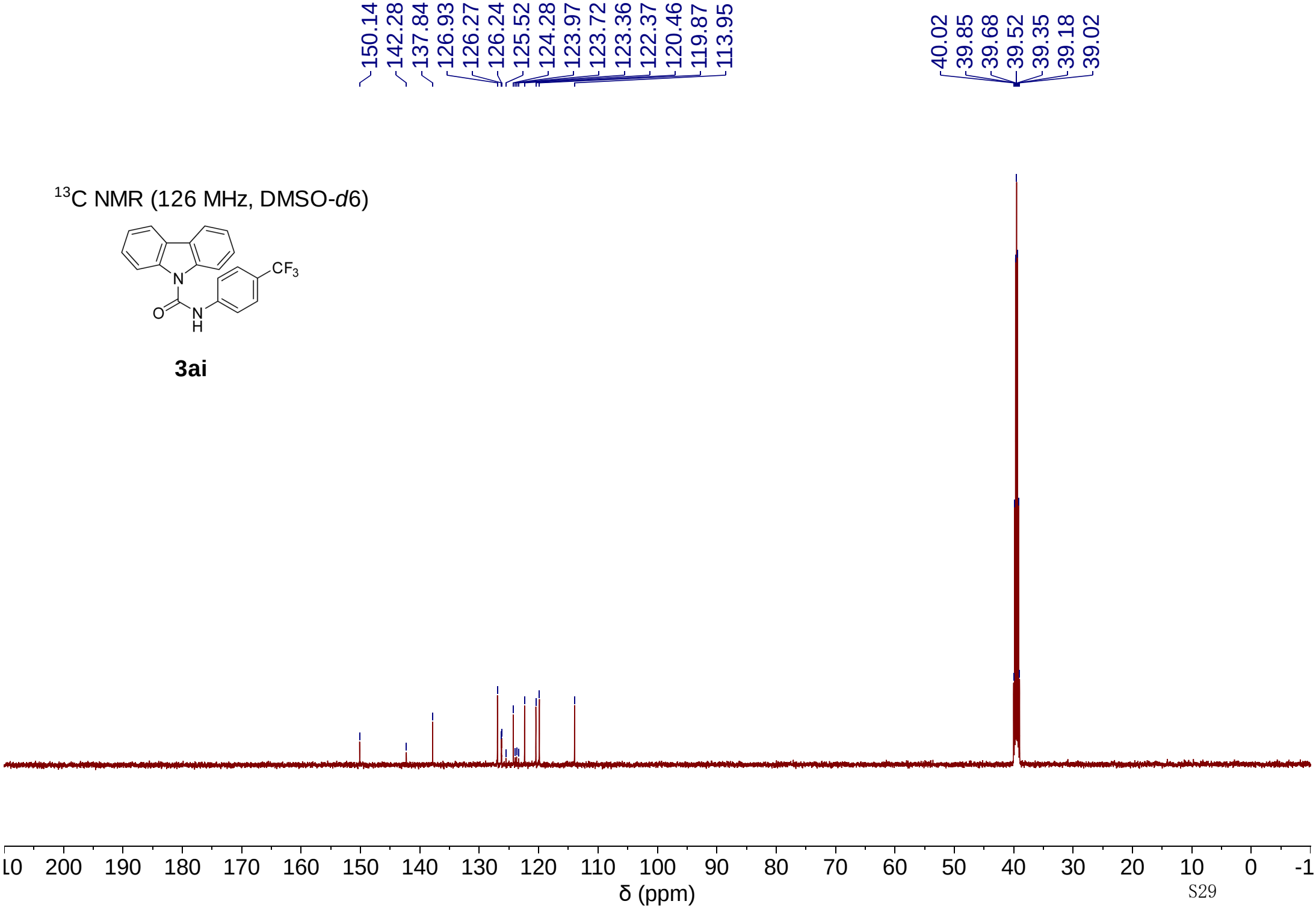
40.02
39.86
39.69
39.52
39.35
39.19
39.02

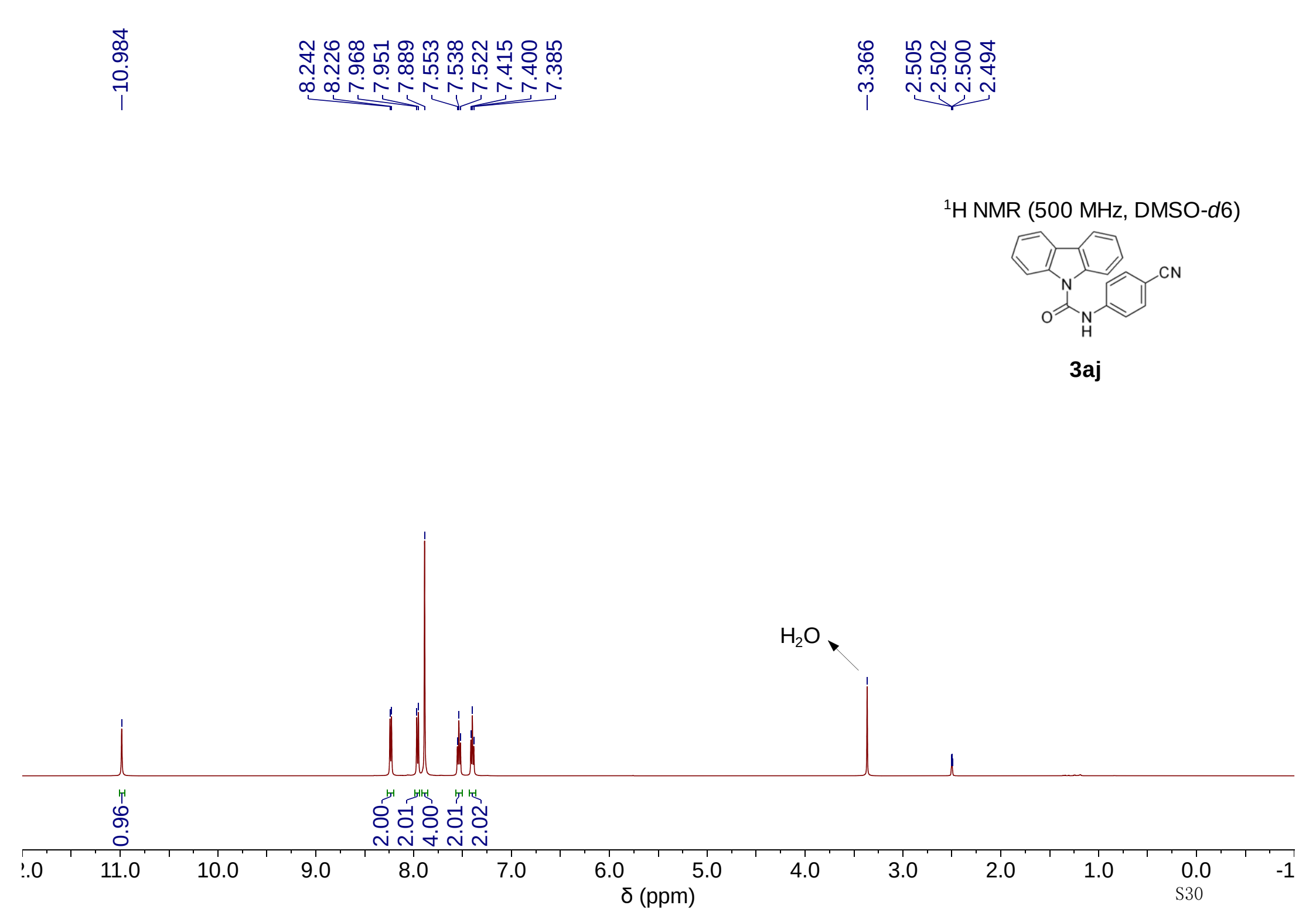
^{13}C NMR (126 MHz, DMSO-*d*6)



3ah


10.925
8.249
8.234
7.963
7.946
7.922
7.905
7.802
7.785
7.555
7.553
7.541
7.538
7.536
7.524
7.522
7.414
7.399
7.384
3.352
2.507
2.504
2.500
2.496
2.492
1H NMR (500 MHz, DMSO-d6)
CF3
N
O
N
H
3ai
H2O
0.98
2.00
2.00
2.09
1.98
2.01
2.02
δ (ppm)

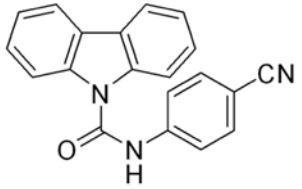

150.14
142.28
137.84
126.93
126.27
126.24
125.52
124.28
123.97
123.72
123.36
122.37
120.46
119.87
113.95
40.02
39.85
39.68
39.52
39.35
39.18
39.02
13C NMR (126 MHz, DMSO-d6)
CF3
N
O
N
H
3ai
δ (ppm)


10.984
8.242
8.226
7.968
7.951
7.889
7.553
7.538
7.522
7.415
7.400
7.385
3.366
2.505
2.502
2.500
2.494
1H NMR (500 MHz, DMSO-d6)
CN
N
O
N
H
3aj
H2O
0.96
2.00
2.01
4.00
2.01
2.02
δ (ppm)

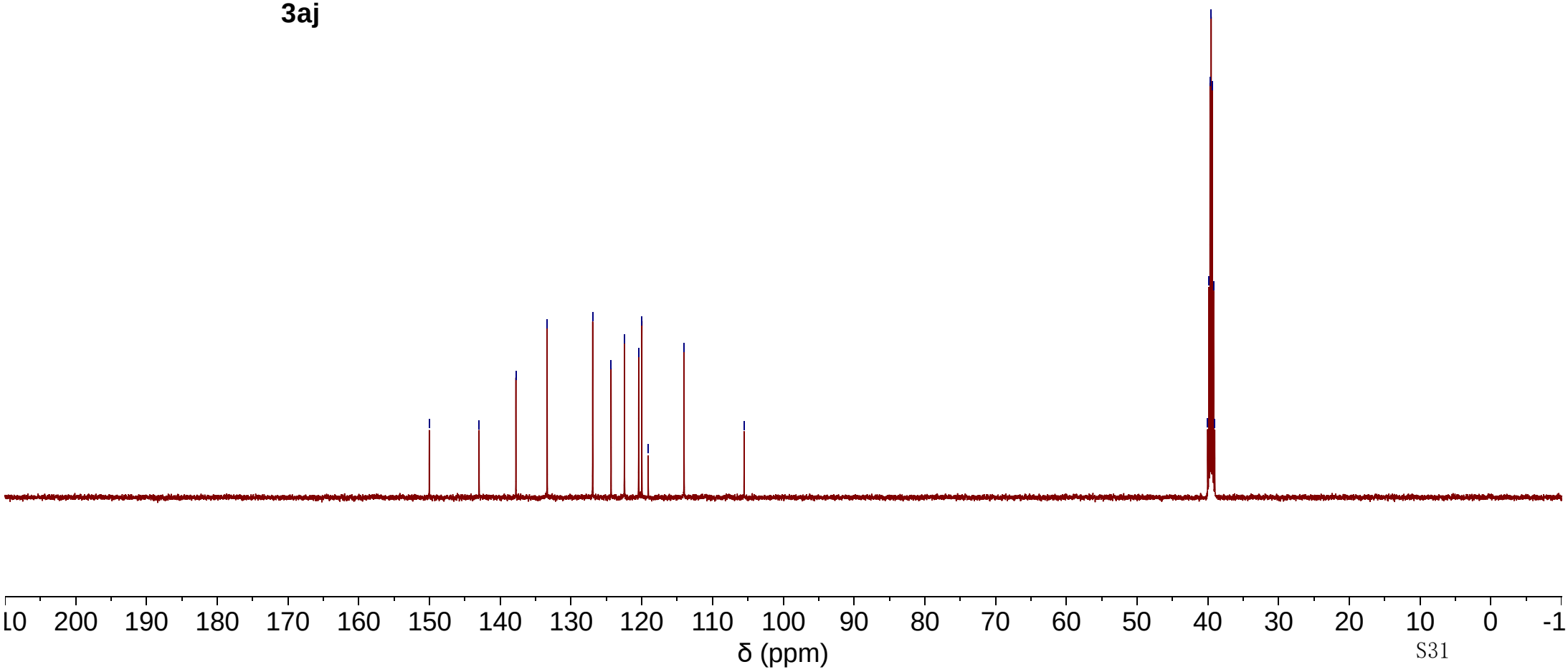
150.03
142.99
137.79
133.37
126.94
124.34
122.45
120.44
119.99
119.09
114.03
105.54

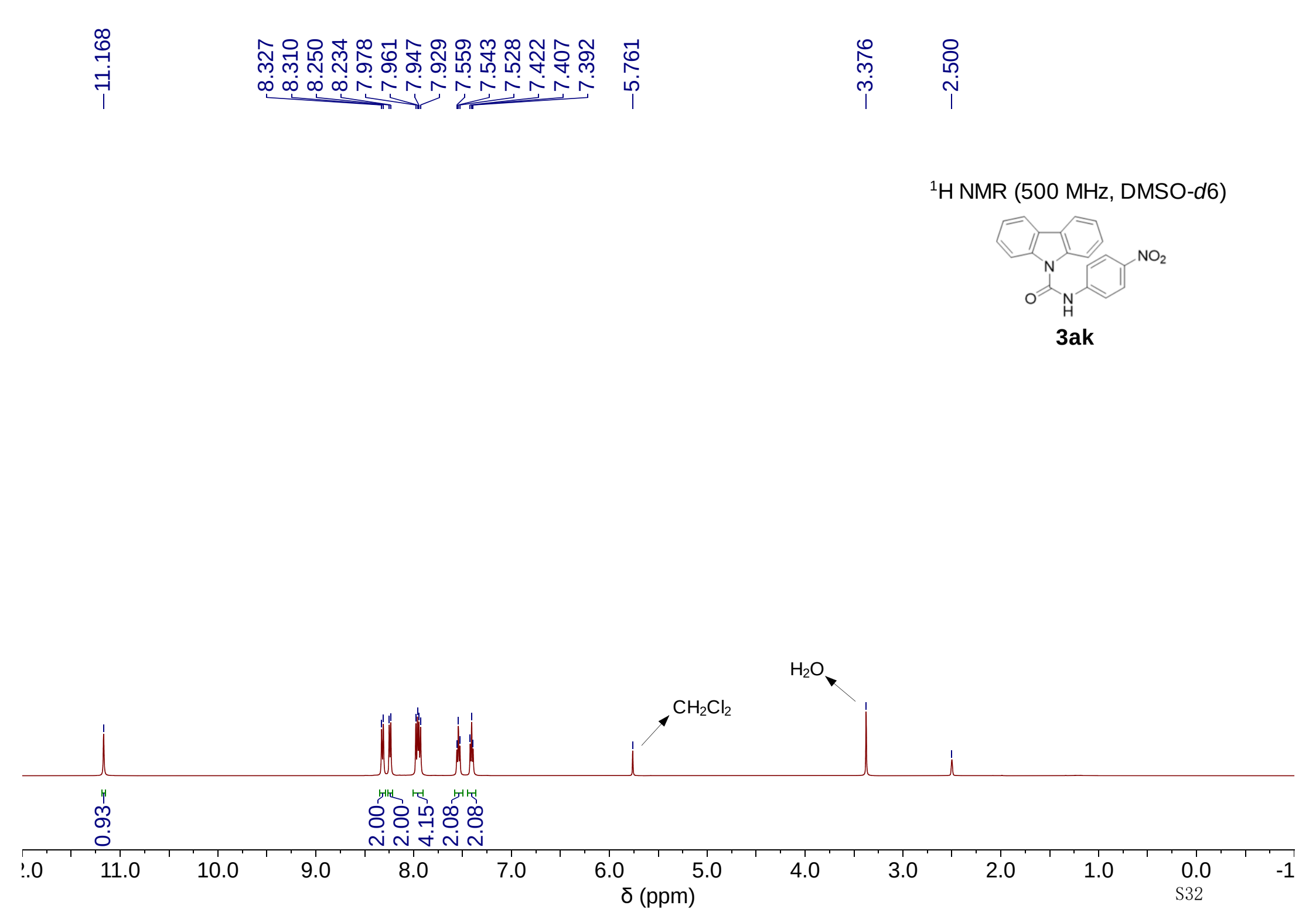
40.02
39.85
39.69
39.52
39.35
39.19
39.02

^{13}C NMR (126 MHz, DMSO-*d*6)



3aj

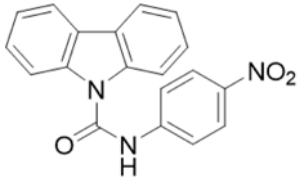



11.168
8.327
8.310
8.250
8.234
7.978
7.961
7.947
7.929
7.559
7.543
7.528
7.422
7.407
7.392
5.761
3.376
2.500
^{1}H NMR (500 MHz, DMSO-*d*6)
NO2
N
O
N
H
3ak
H2O
CH2Cl2
0.93
2.00
2.00
4.15
2.08
2.08
δ (ppm)

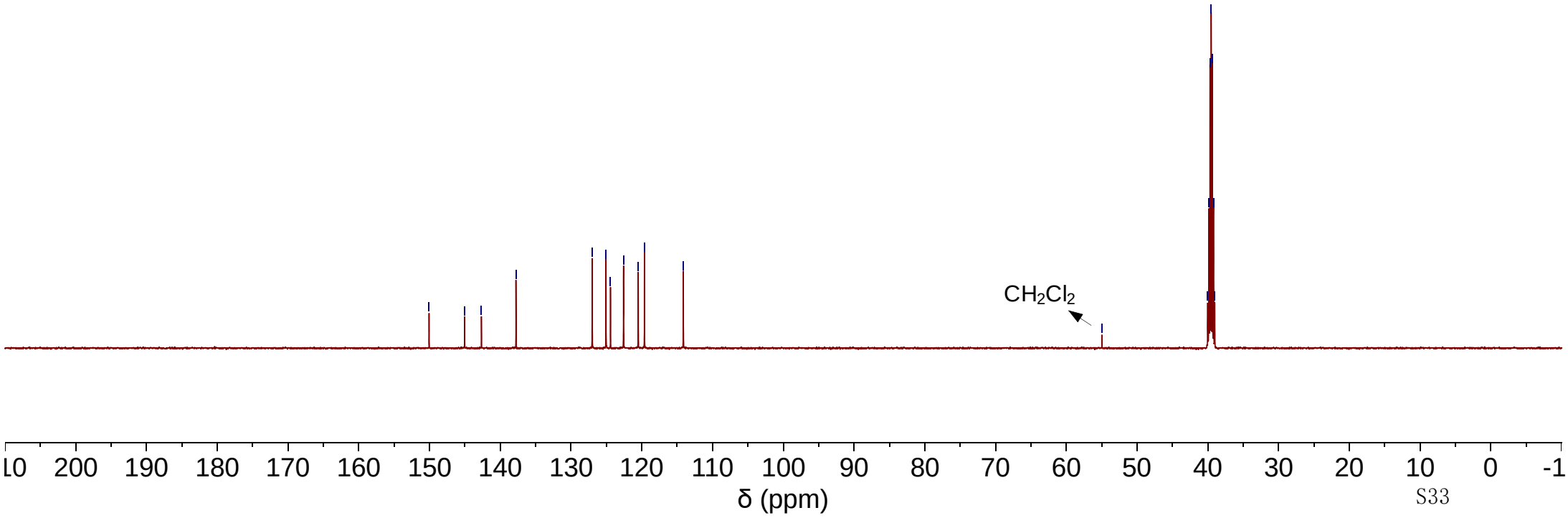
150.06
145.04
142.66
137.78
127.01
125.06
124.42
122.58
120.50
119.62
114.13

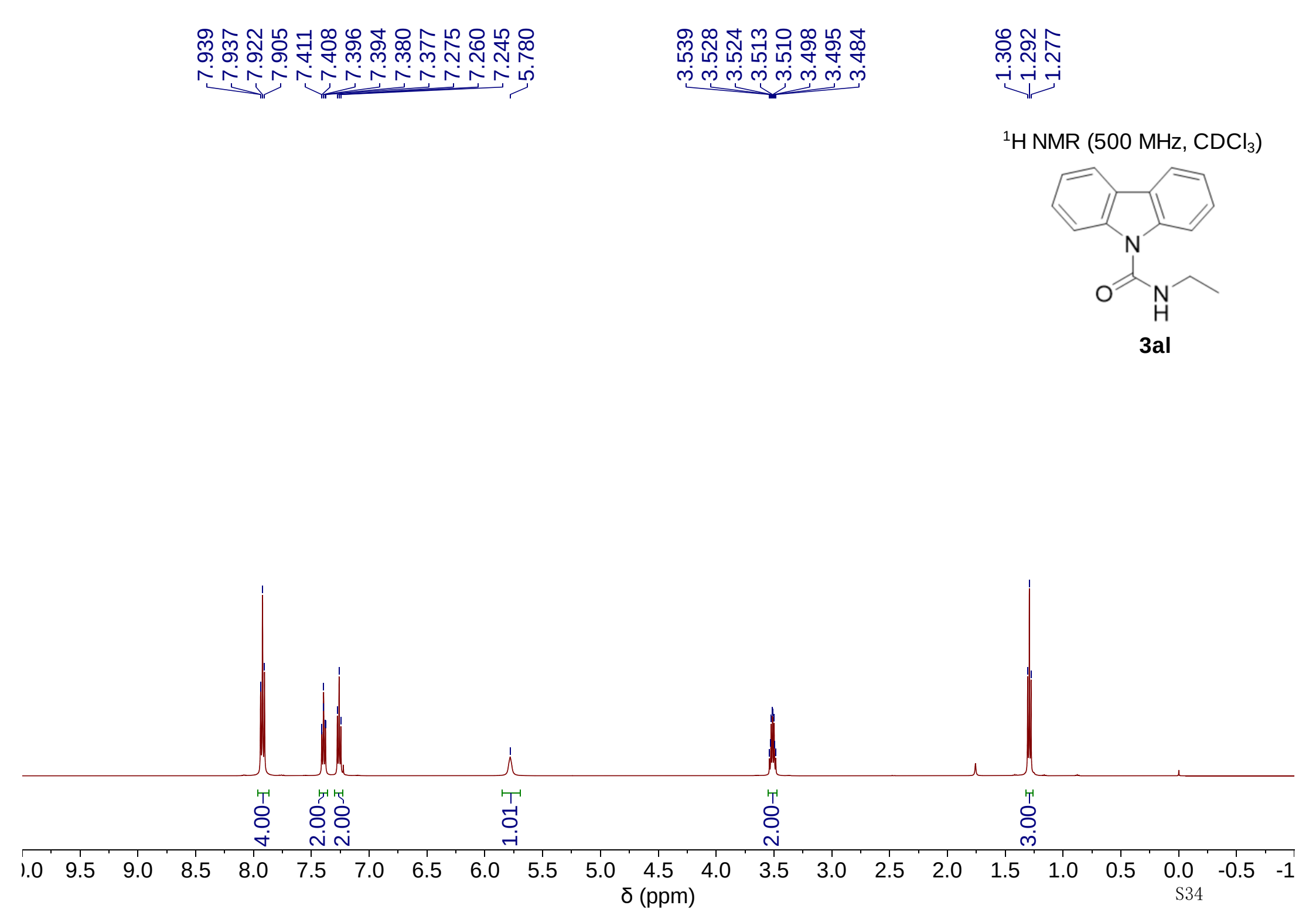
54.96
40.02
39.85
39.69
39.52
39.35
39.19
39.02

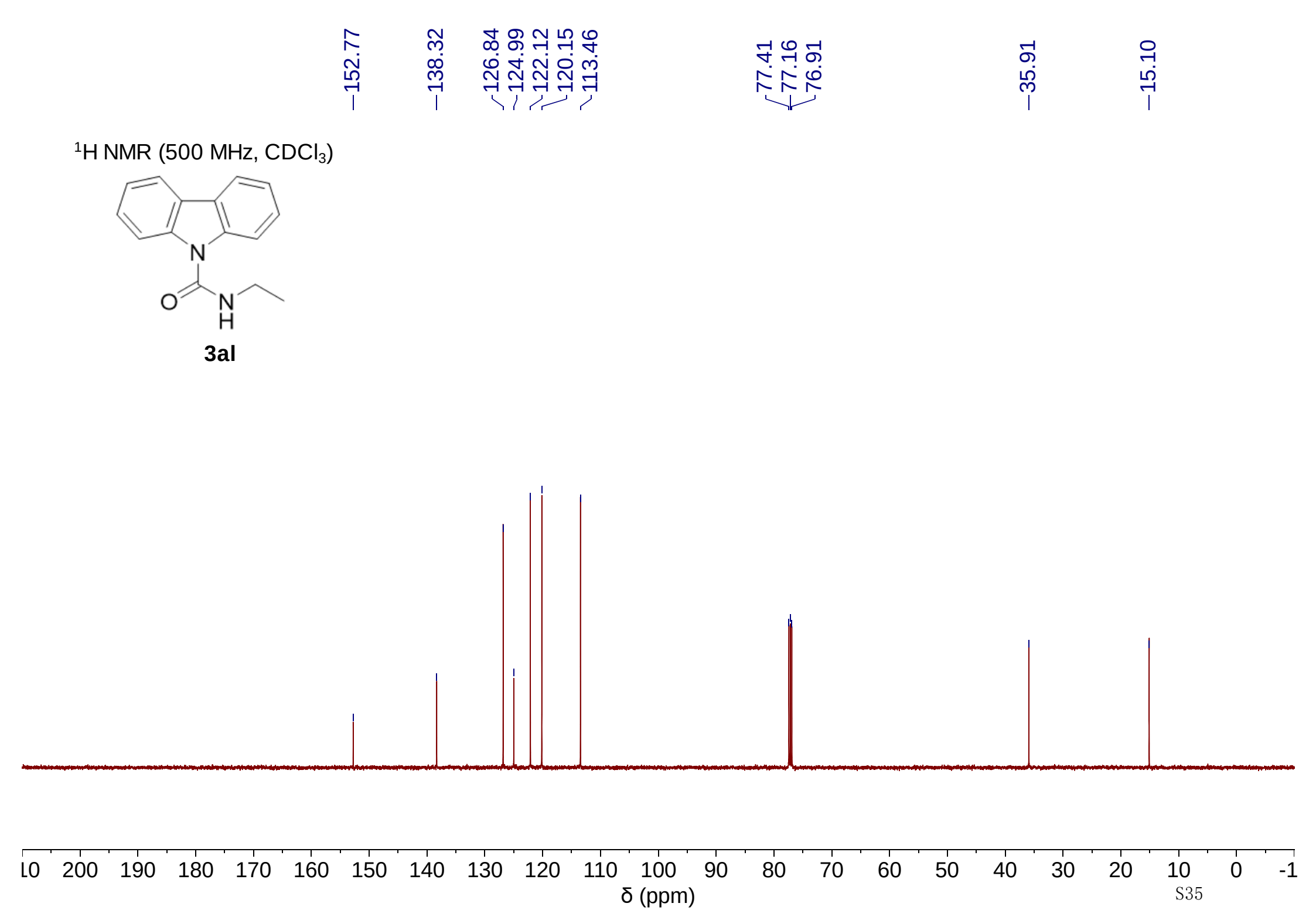
^{13}C NMR (126 MHz, DMSO-*d*6)



3ak

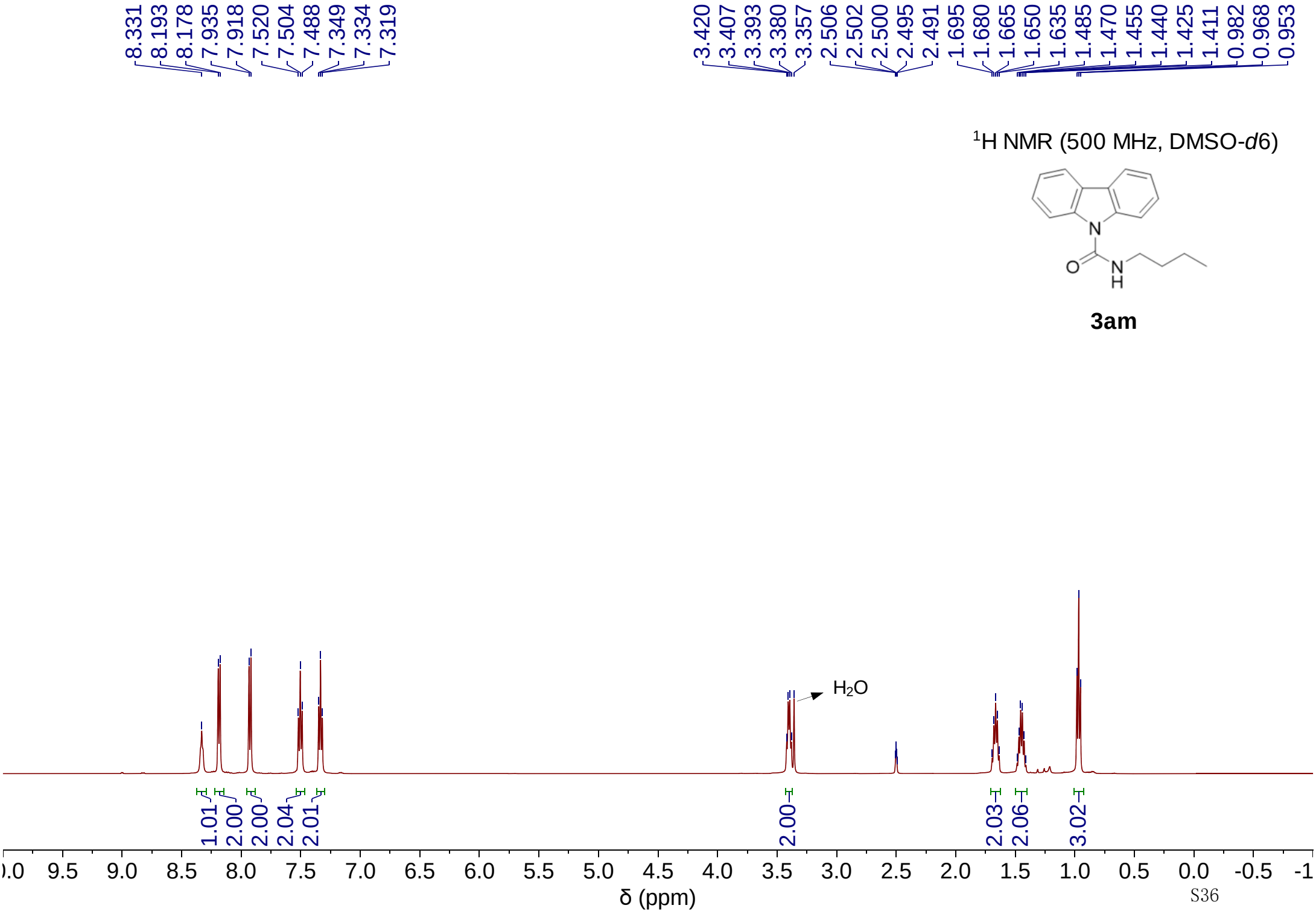


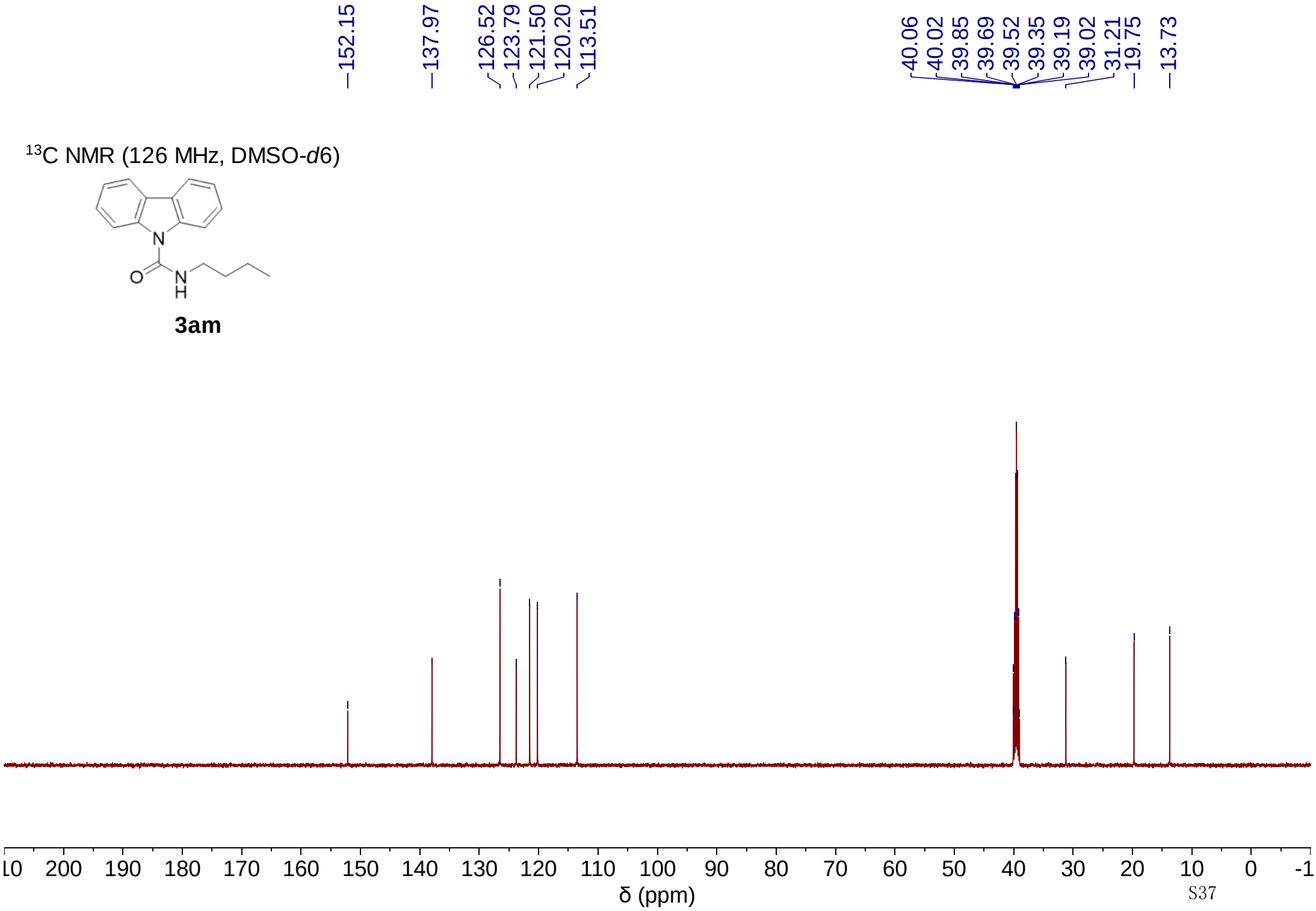

7.939
7.937
7.922
7.905
7.411
7.408
7.396
7.394
7.380
7.377
7.275
7.260
7.245
5.780
3.539
3.528
3.524
3.513
3.510
3.498
3.495
3.484
1.306
1.292
1.277
1H NMR (500 MHz, CDCl3)
N
O
N
H
3al
4.00
2.00
2.00
1.01
2.00
3.00
δ (ppm)



^{1}H NMR (500 MHz, $CDCl_3$)

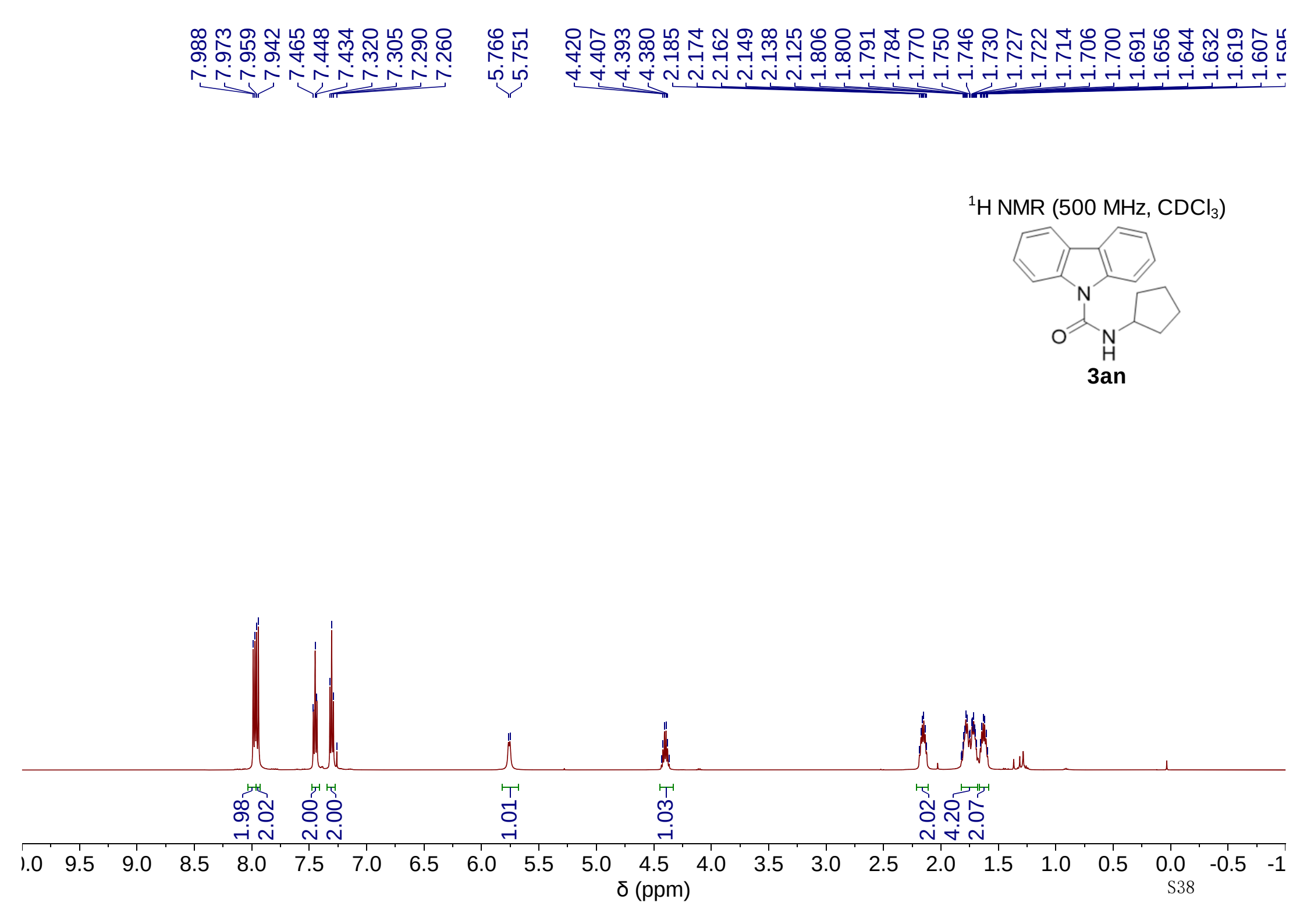
3al


8.331
8.193
8.178
7.935
7.918
7.520
7.504
7.488
7.349
7.334
7.319
3.420
3.407
3.393
3.380
3.357
2.506
2.502
2.500
2.495
2.491
1.695
1.680
1.665
1.650
1.635
1.485
1.470
1.455
1.440
1.425
1.411
0.982
0.968
0.953
1H NMR (500 MHz, DMSO-d6)
N
O
N
H
3am
H2O
1.01
2.00
2.00
2.04
2.01
2.00
2.03
2.06
3.02
δ (ppm)



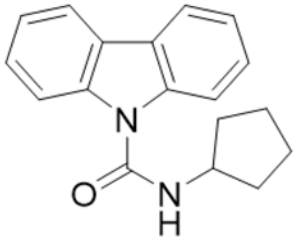
^{13}C NMR (126 MHz, DMSO-*d*6)

3am

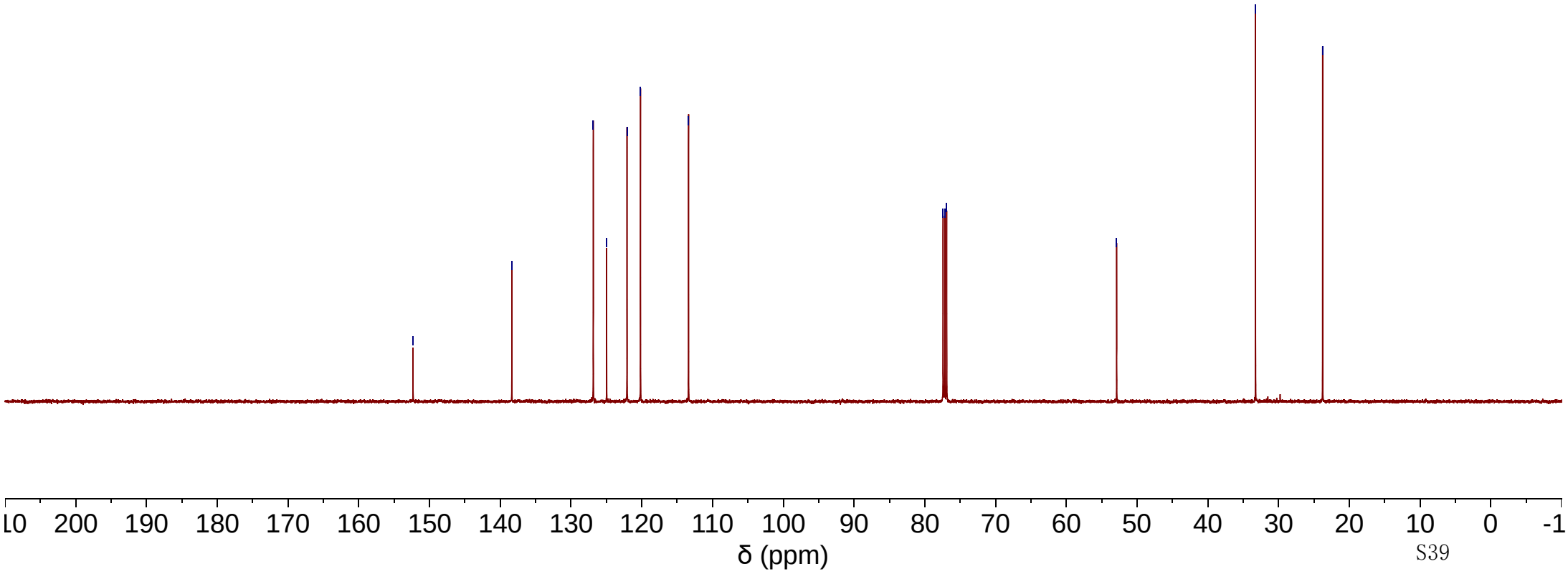

7.988
7.973
7.959
7.942
7.465
7.448
7.434
7.320
7.305
7.290
7.260
5.766
5.751
4.420
4.407
4.393
4.380
2.185
2.174
2.162
2.149
2.138
2.125
1.806
1.800
1.791
1.784
1.770
1.750
1.746
1.730
1.727
1.722
1.714
1.706
1.700
1.691
1.656
1.644
1.632
1.619
1.607
1.595
1H NMR (500 MHz, CDCl3)
N
O
N
H
3an
1.98
2.02
2.00
2.00
1.01
1.03
2.02
4.20
2.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
δ (ppm)

152.33
138.36
126.85
124.97
122.09
120.18
113.39
77.41
77.16
76.91
52.88
33.26
23.78

^{13}C NMR (126 MHz, $CDCl_3$)

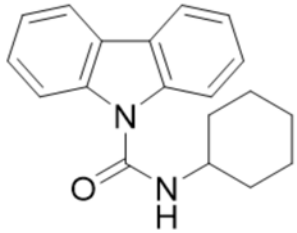


3an

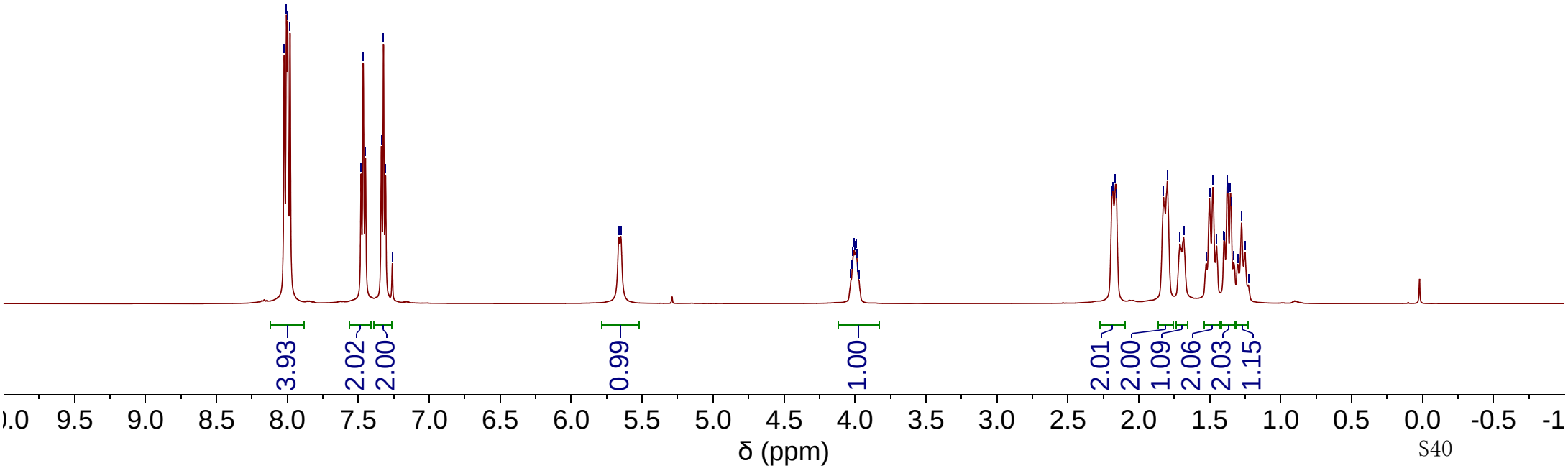


8.022 8.007 7.998 7.981 7.481 7.465 7.449 7.338 7.323 7.308 7.261 5.664 5.649 4.029 4.021 4.014 4.007 4.000 3.992 3.985 3.978 3.970 2.190 2.180 2.165 2.156 1.826 1.798 1.710 1.683 1.501 1.477 1.451 1.401 1.395 1.378 1.371 1.355 1.348 1.275

^{1}H NMR (500 MHz, $CDCl_3$)

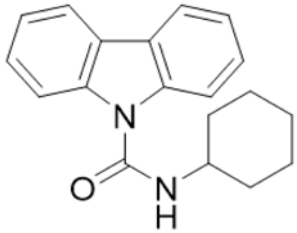


3ao

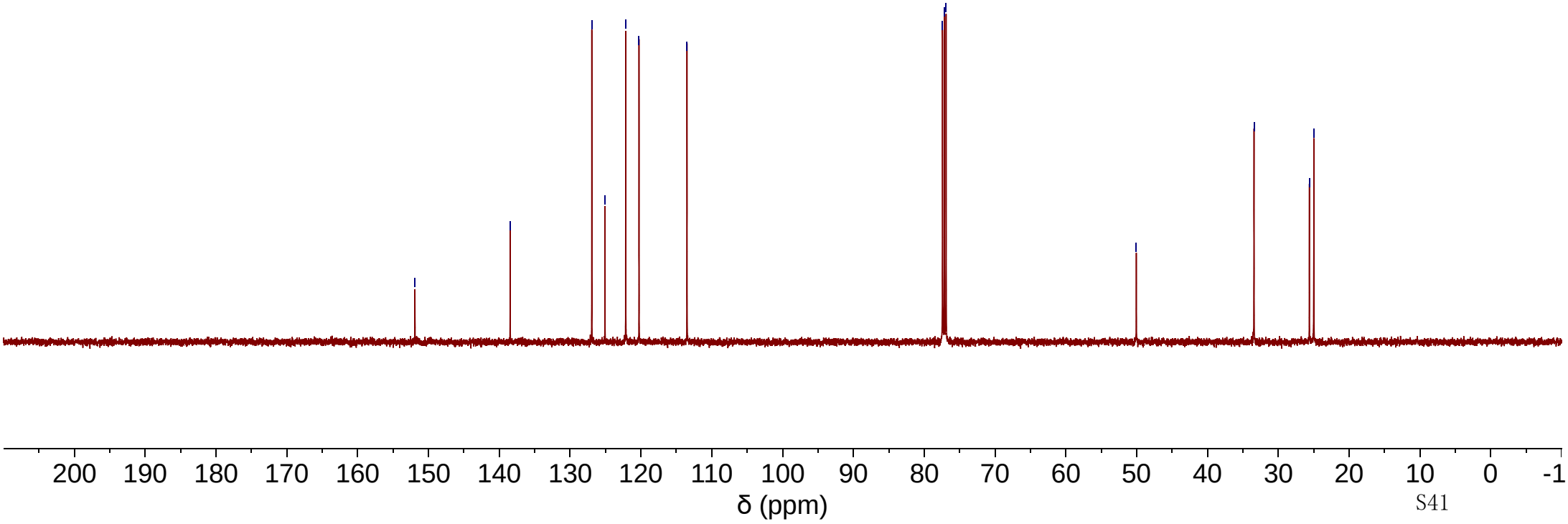


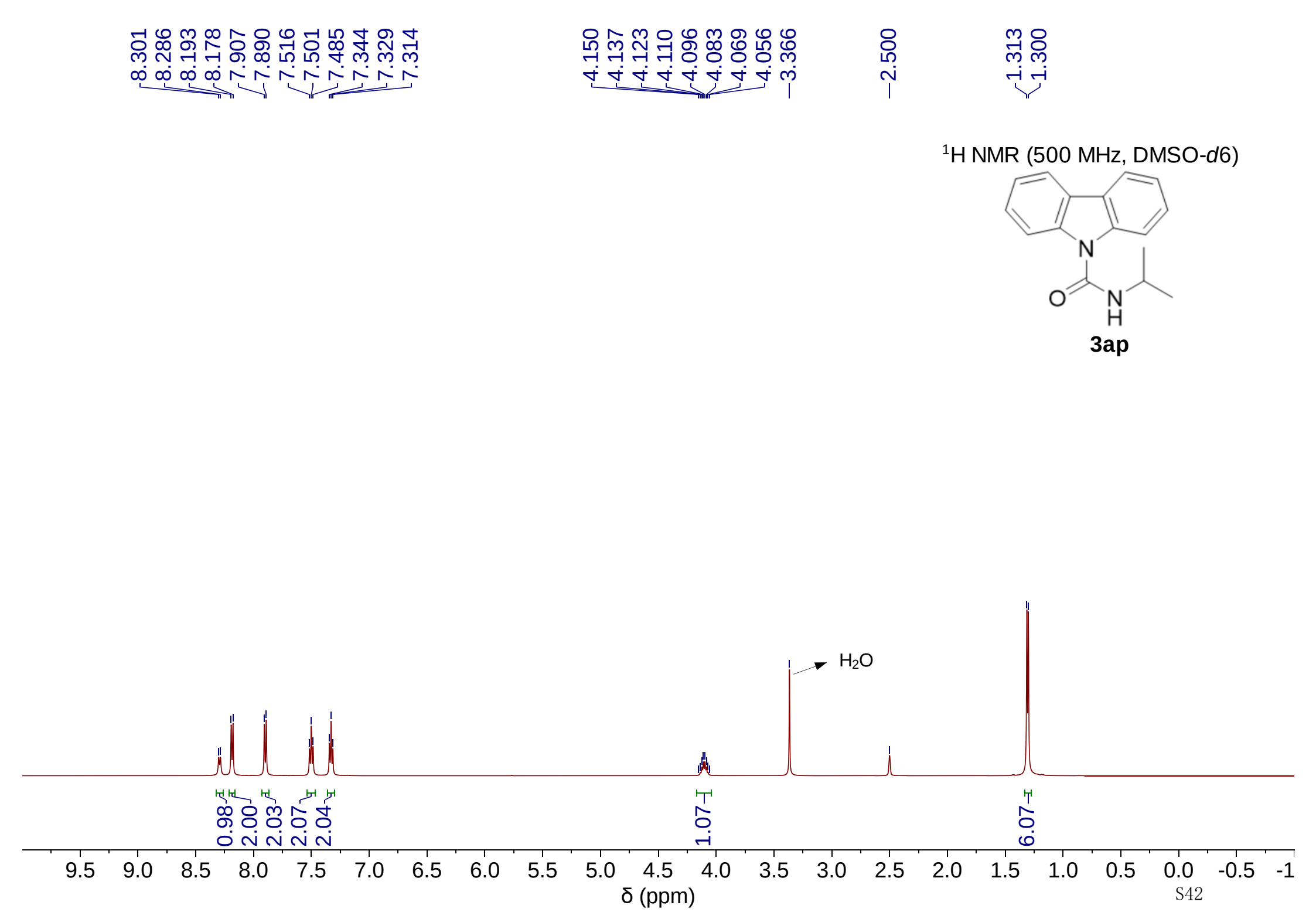
151.91
138.47
126.93
125.07
122.15
120.27
113.49
77.42
77.16
76.91
50.05
33.43
25.61
24.98

^{13}C NMR (126 MHz, $CDCl_3$)



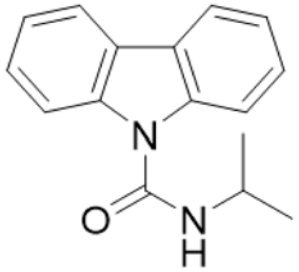
3ao



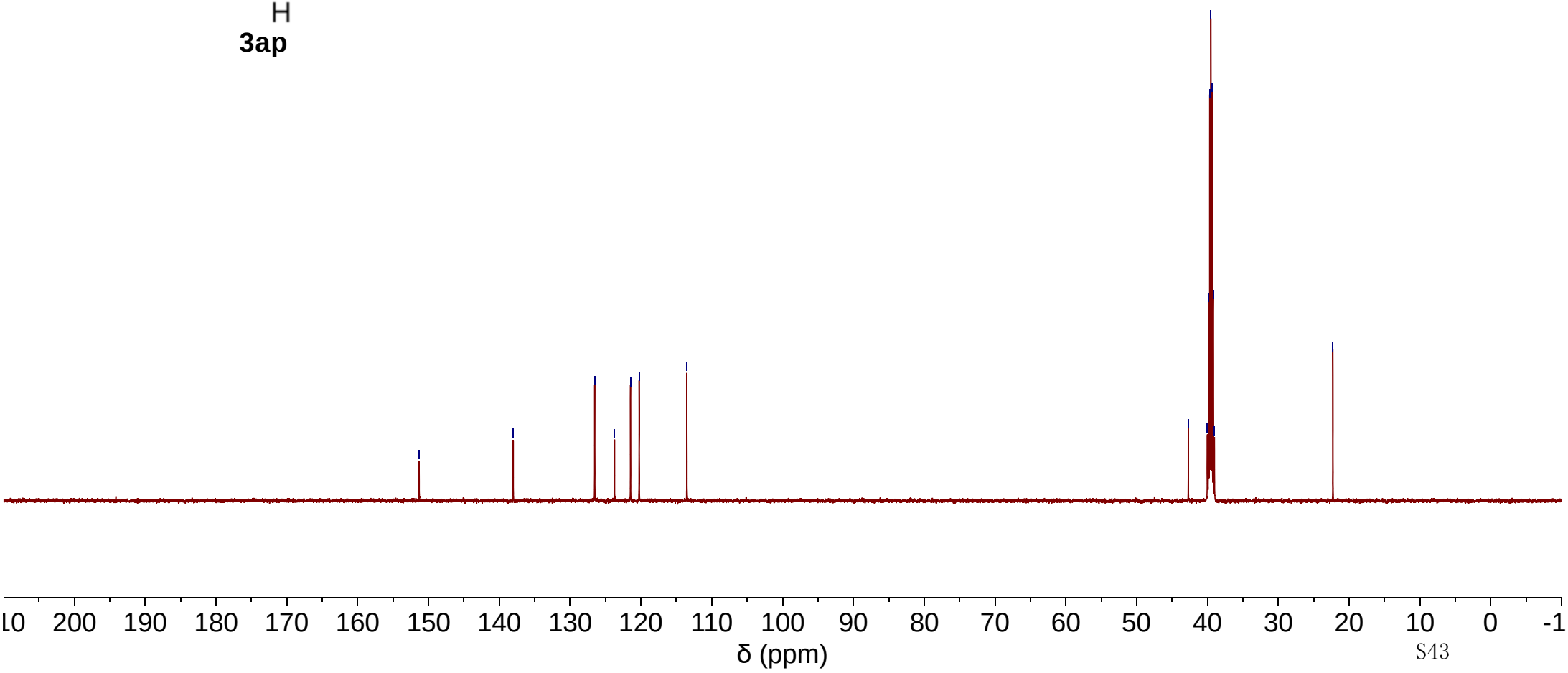

8.301
8.286
8.193
8.178
7.907
7.890
7.516
7.501
7.485
7.344
7.329
7.314
4.150
4.137
4.123
4.110
4.096
4.083
4.069
4.056
3.366
2.500
1.313
1.300
1H NMR (500 MHz, DMSO-d6)
N
O
N
H
3ap
H2O
0.98
2.00
2.03
2.07
2.04
1.07
6.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
δ (ppm)

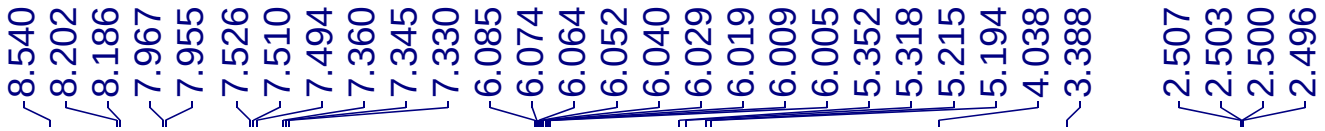
151.31
138.03
126.54
123.73
121.48
120.25
113.51
42.71
40.02
39.85
39.69
39.52
39.35
39.19
39.02
22.29

^{13}C NMR (126 MHz, DMSO-*d*6)

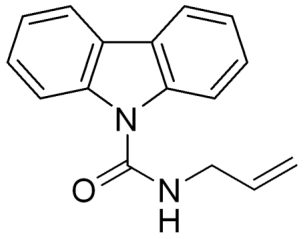


3ap

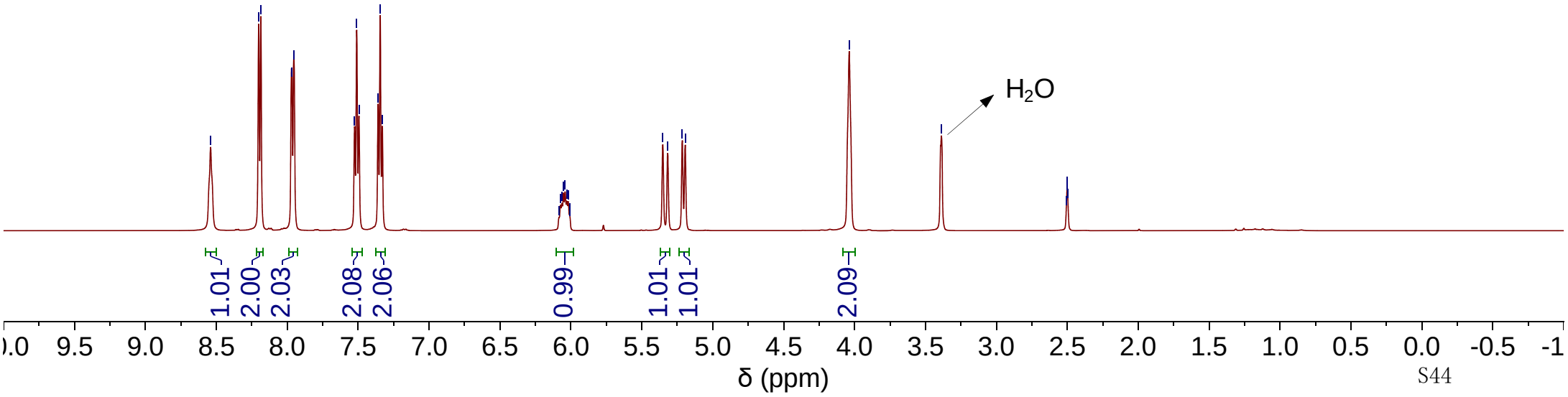


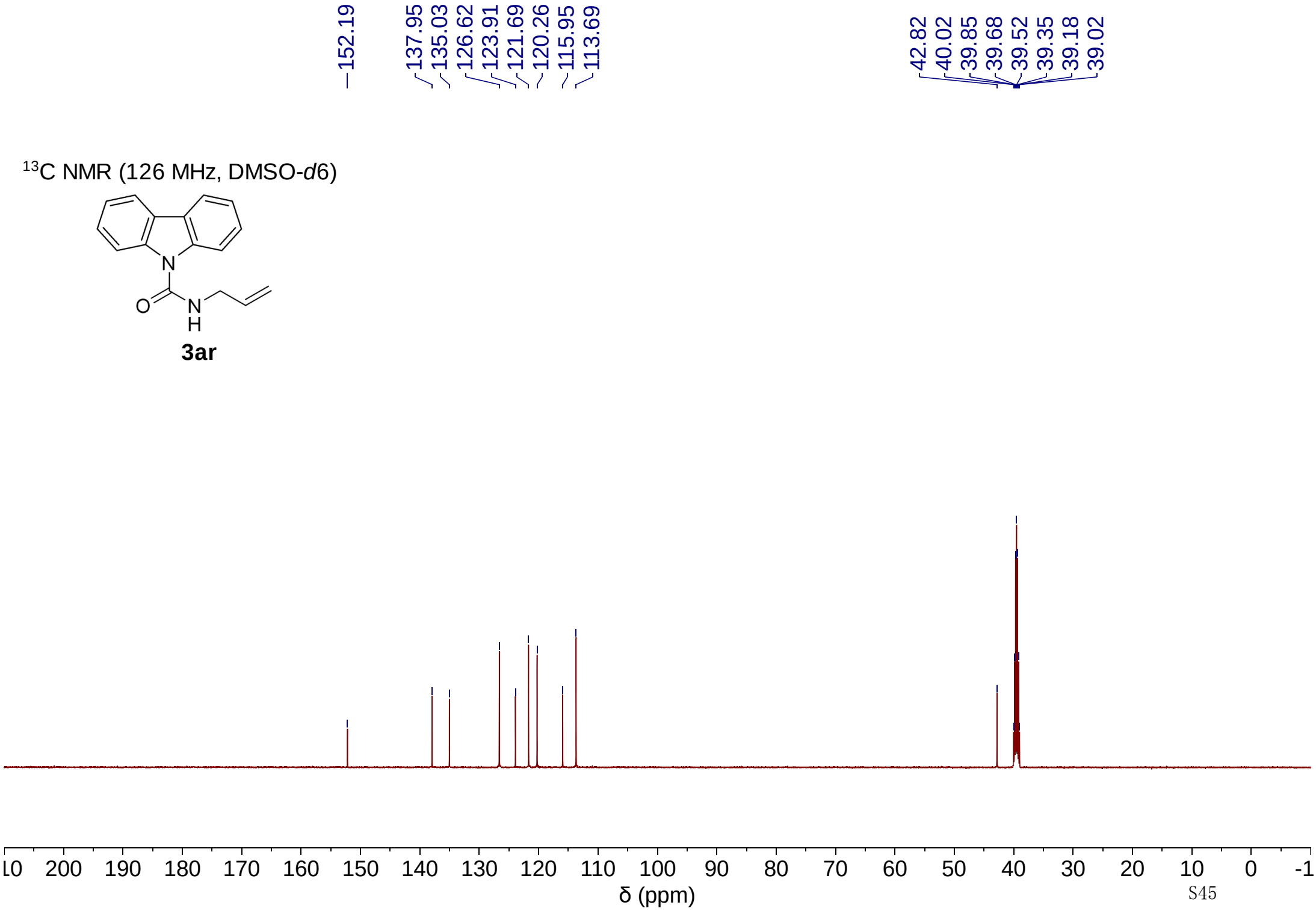


^{1}H NMR (500 MHz, DMSO-*d*6)



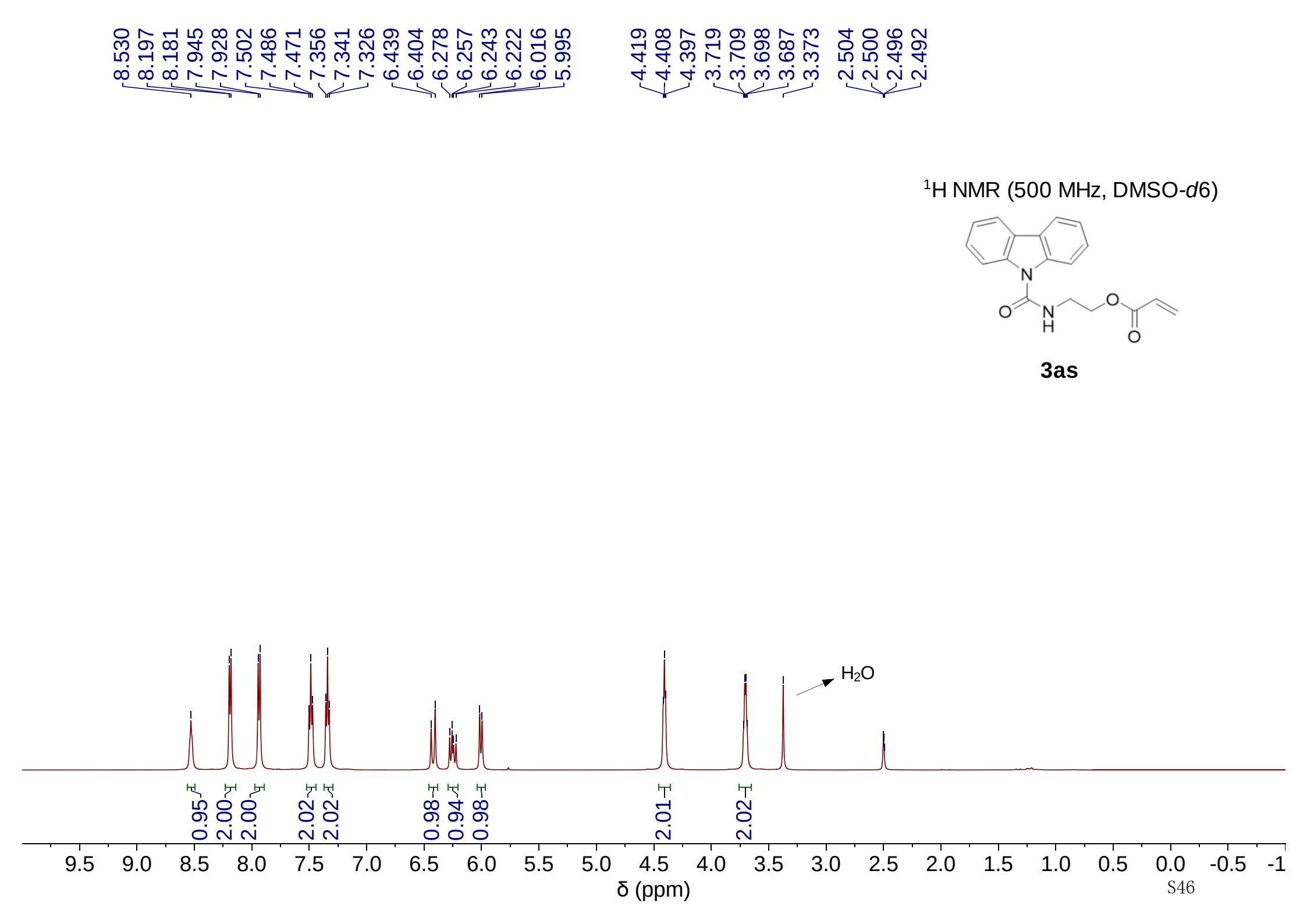
3ar

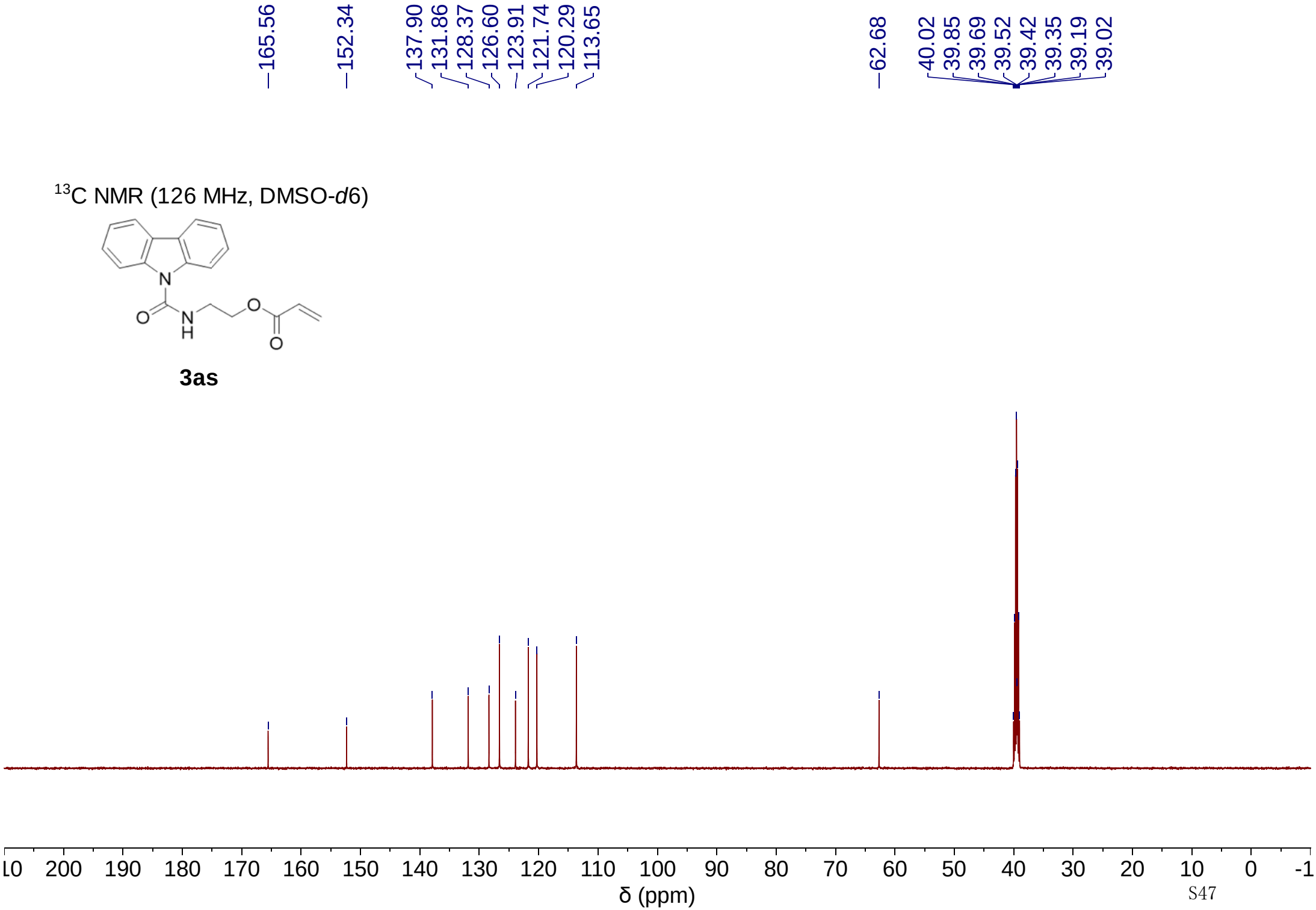


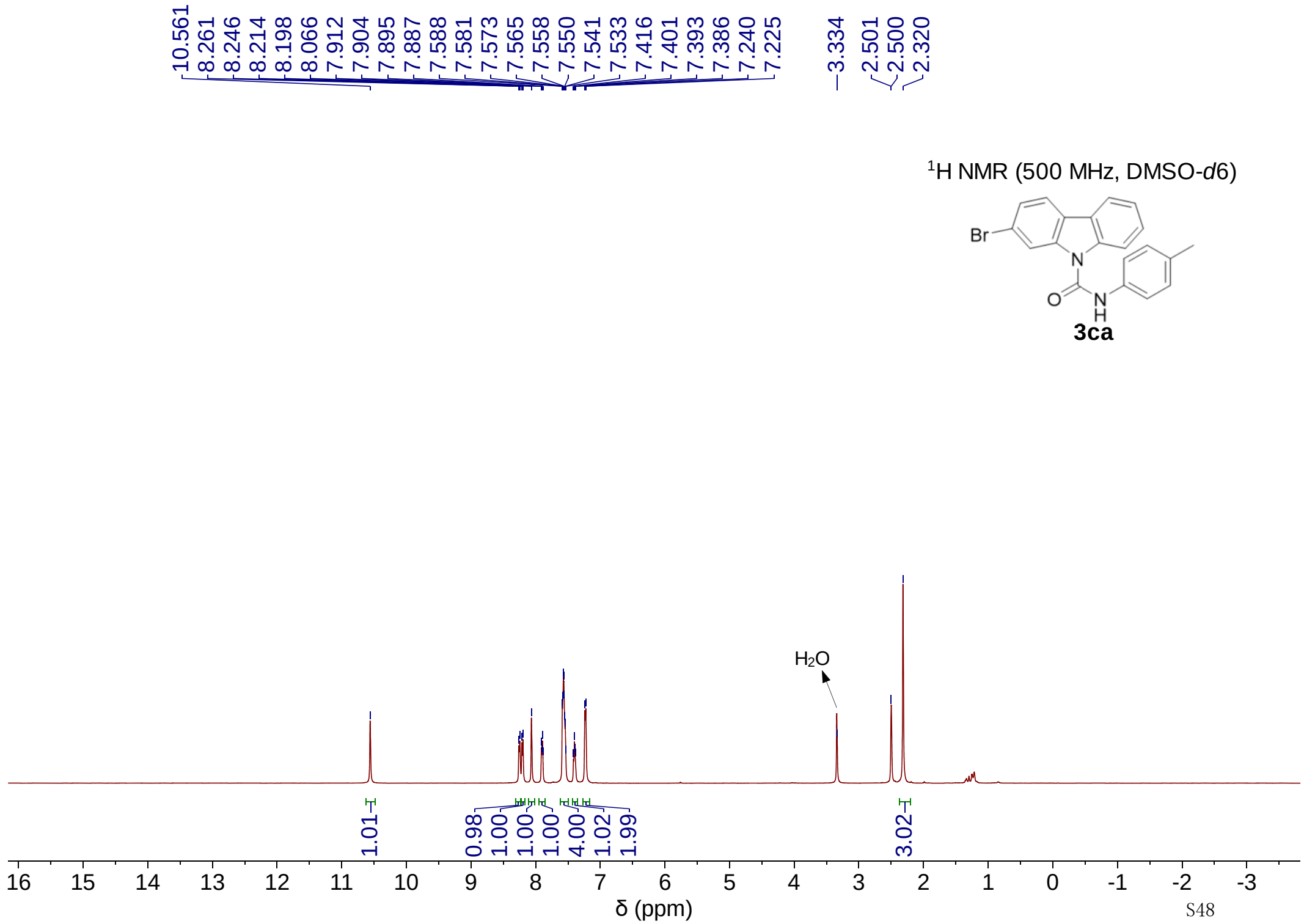


^{13}C NMR (126 MHz, DMSO-*d*6)

3ar


8.530
8.197
8.181
7.945
7.928
7.502
7.486
7.471
7.356
7.341
7.326
6.439
6.404
6.278
6.257
6.243
6.222
6.016
5.995
4.419
4.408
4.397
3.719
3.709
3.698
3.687
3.373
2.504
2.500
2.496
2.492
^{1}H NMR (500 MHz, DMSO-*d*6)
N
O
N
H
O
O
3as
H_2O
0.95
2.00
2.00
2.02
2.02
0.98
0.94
0.98
2.01
2.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
δ (ppm)

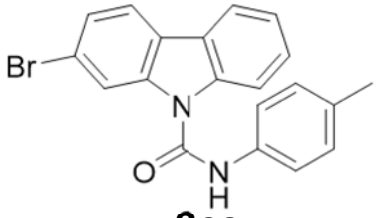

165.56
152.34
137.90
131.86
128.37
126.60
123.91
121.74
120.29
113.65
62.68
40.02
39.85
39.69
39.52
39.42
39.35
39.19
39.02
^{13}C NMR (126 MHz, DMSO-*d*6)
N
O
N
H
O
O
3as
δ (ppm)


10.561
8.261
8.246
8.214
8.198
8.066
7.912
7.904
7.895
7.887
7.588
7.581
7.573
7.565
7.558
7.550
7.541
7.533
7.416
7.401
7.393
7.386
7.240
7.225
3.334
2.501
2.500
2.320
1H NMR (500 MHz, DMSO-d6)
Br
N
O
N
H
3ca
H2O
1.01
0.98
1.00
1.00
1.00
4.00
1.02
1.99
3.02
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
δ (ppm)

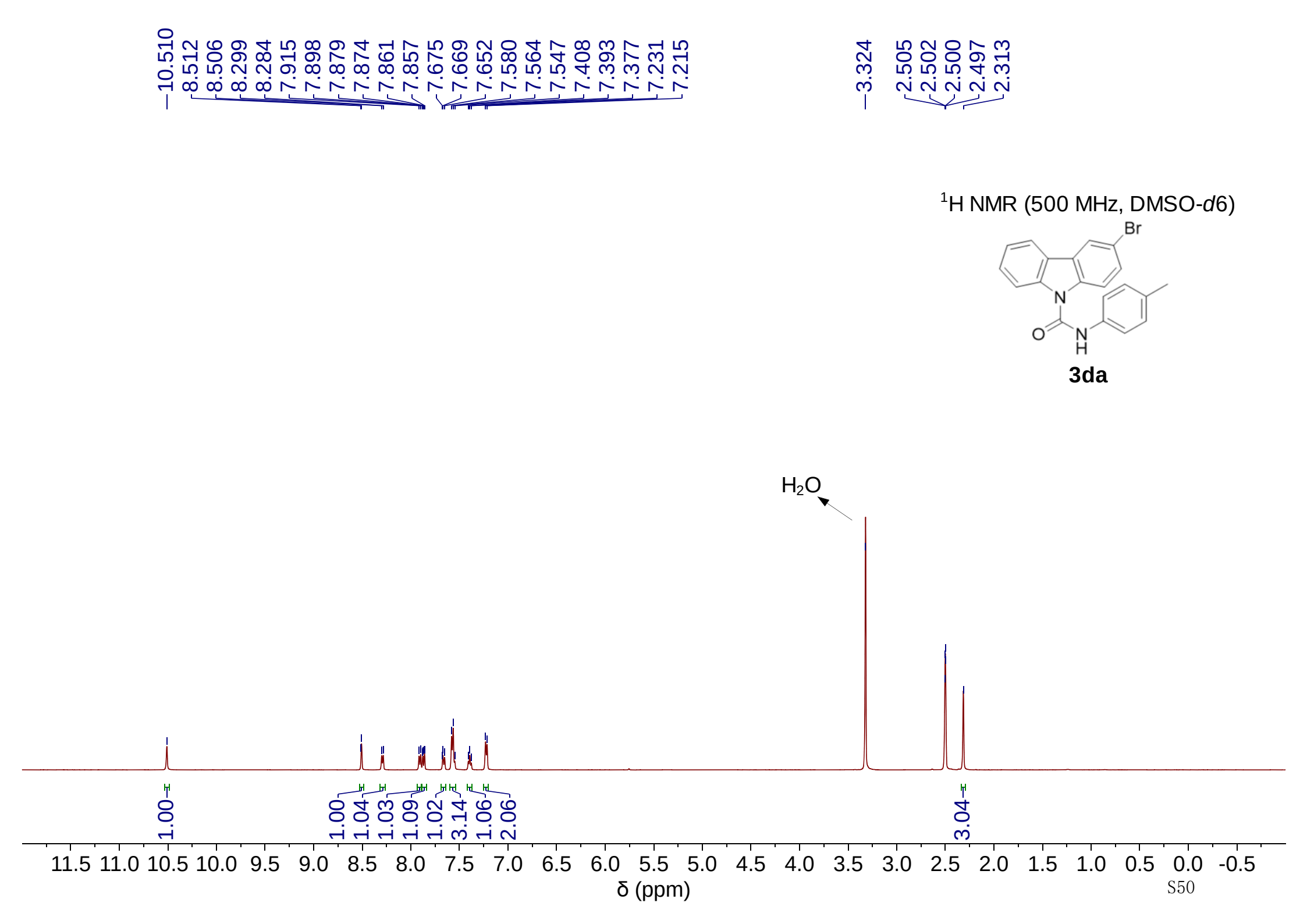
149.61
138.78
138.07
135.61
133.19
129.35
127.28
124.83
123.32
123.23
122.37
122.15
120.63
120.21
119.28
116.44
113.77

40.02
39.85
39.69
39.61
39.52
39.35
39.19
39.02
20.51

^{13}C NMR (126 MHz, DMSO-*d*6)



3ca

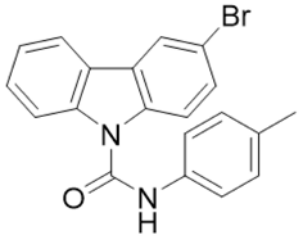

10.510
8.512
8.506
8.299
8.284
7.915
7.898
7.879
7.874
7.861
7.857
7.675
7.669
7.652
7.580
7.564
7.547
7.408
7.393
7.377
7.231
7.215
3.324
2.505
2.502
2.500
2.497
2.313
1H NMR (500 MHz, DMSO-d6)
Br
N
O
N
H
3da
H2O
1.00
1.00
1.04
1.03
1.09
1.02
3.14
1.06
2.06
3.04
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
δ (ppm)

149.639
138.290
136.851
135.688
133.102
129.346
129.169
127.554
126.078
123.048
122.929
122.250
120.966
120.095
115.673
114.217
113.728

39.854
39.685
39.520
39.356
39.188

20.531

^{13}C NMR (126 MHz, DMSO-*d*6)

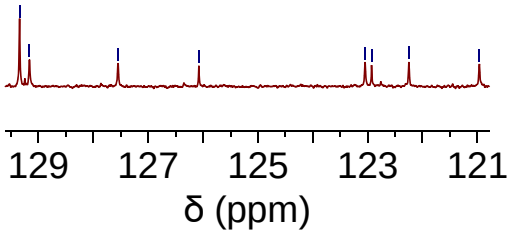


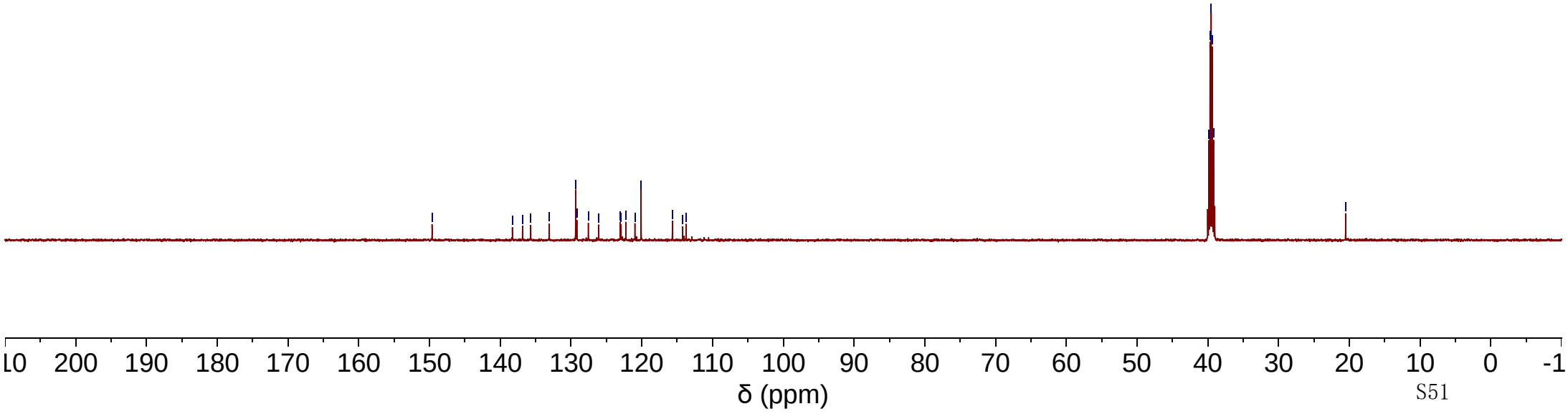
3da

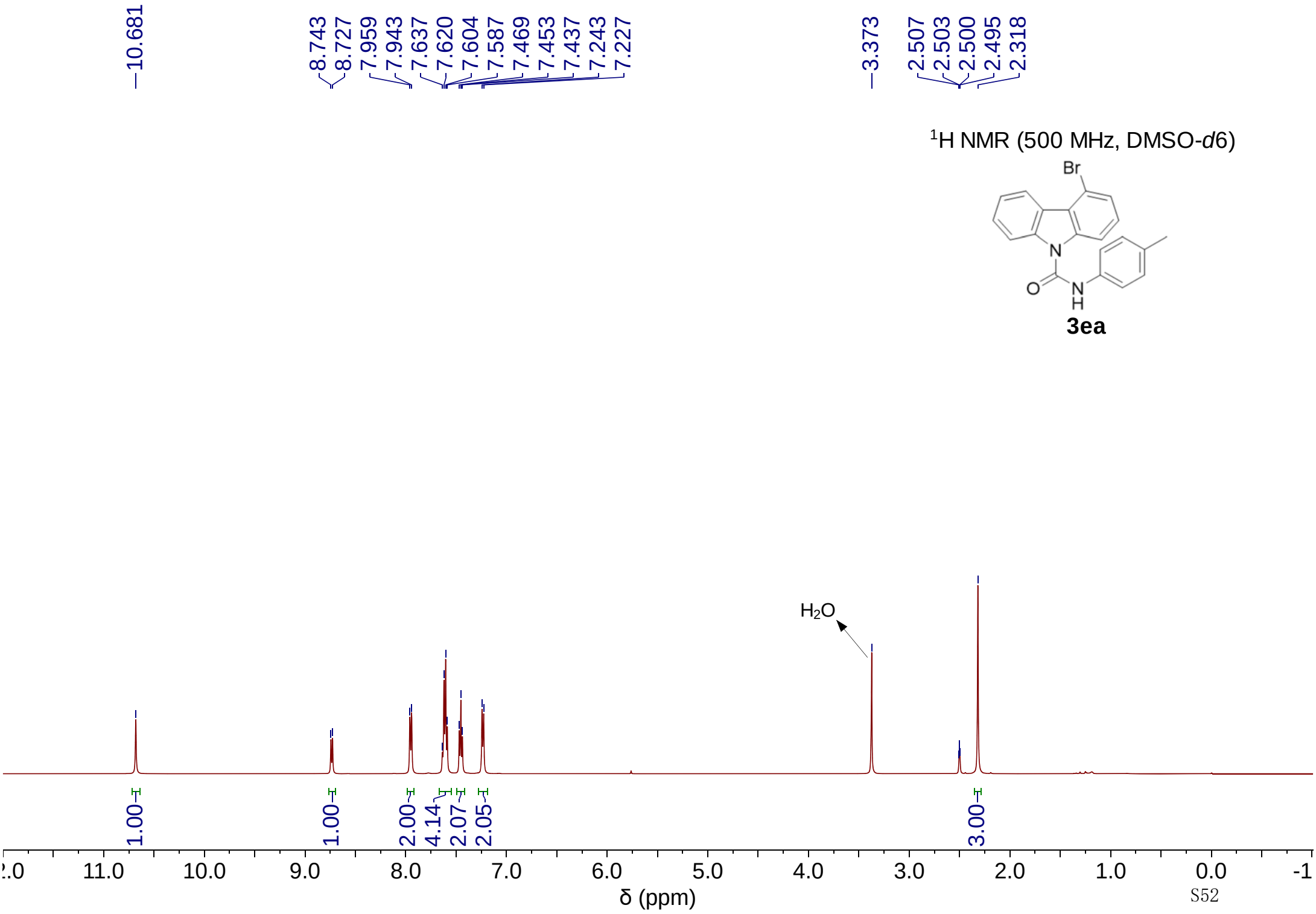
129.345
129.167
127.553

126.077

123.047
122.928
122.248
120.965





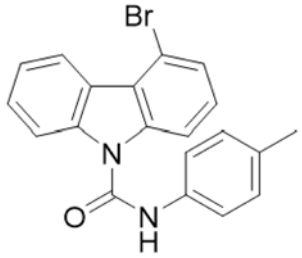

10.681
8.743
8.727
7.959
7.943
7.637
7.620
7.604
7.587
7.469
7.453
7.437
7.243
7.227
3.373
2.507
2.503
2.500
2.495
2.318
1H NMR (500 MHz, DMSO-d6)
Br
N
O
N
H
3ea
H2O
1.00
1.00
2.00
4.14
2.07
2.05
3.00
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
δ (ppm)

149.33
139.42
138.34
135.59
133.29
129.39
127.66
127.52
125.90
122.98
121.97
121.90
121.83
120.11
115.41
113.34
112.73

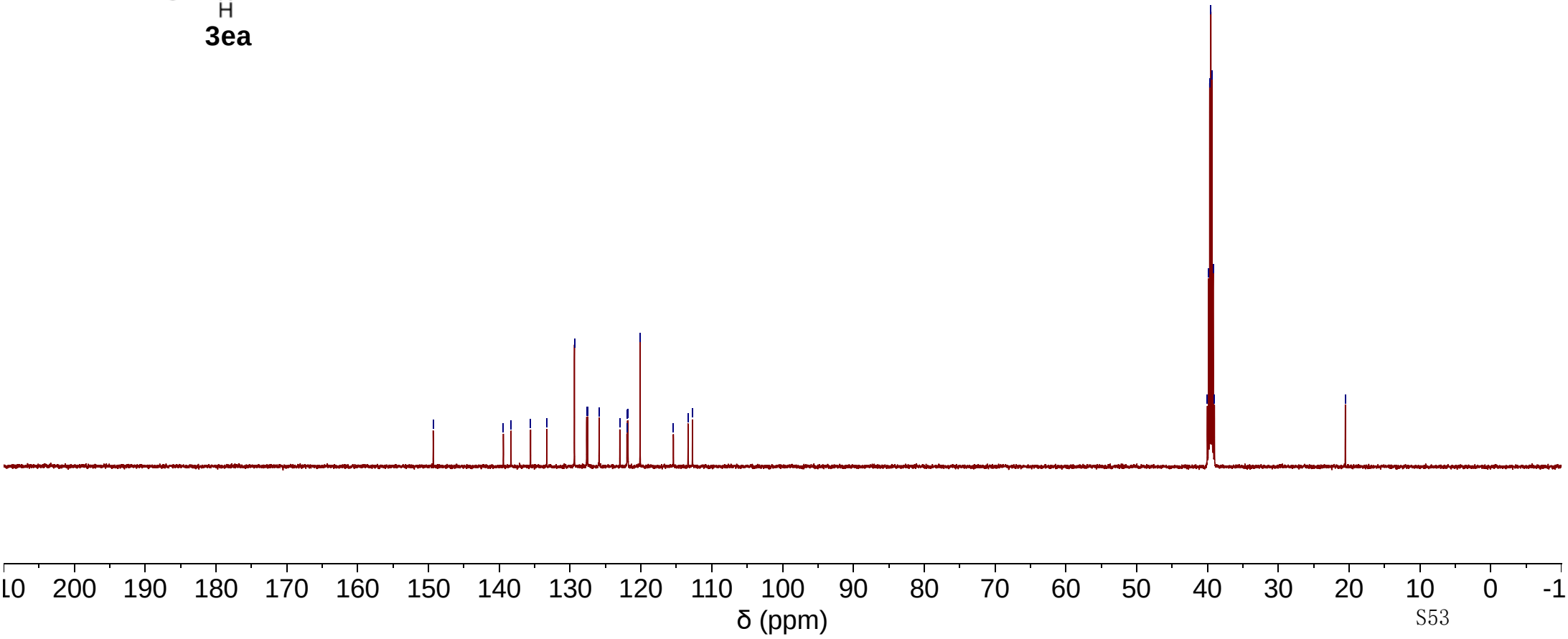
40.02
39.85
39.69
39.52
39.35
39.19
39.02

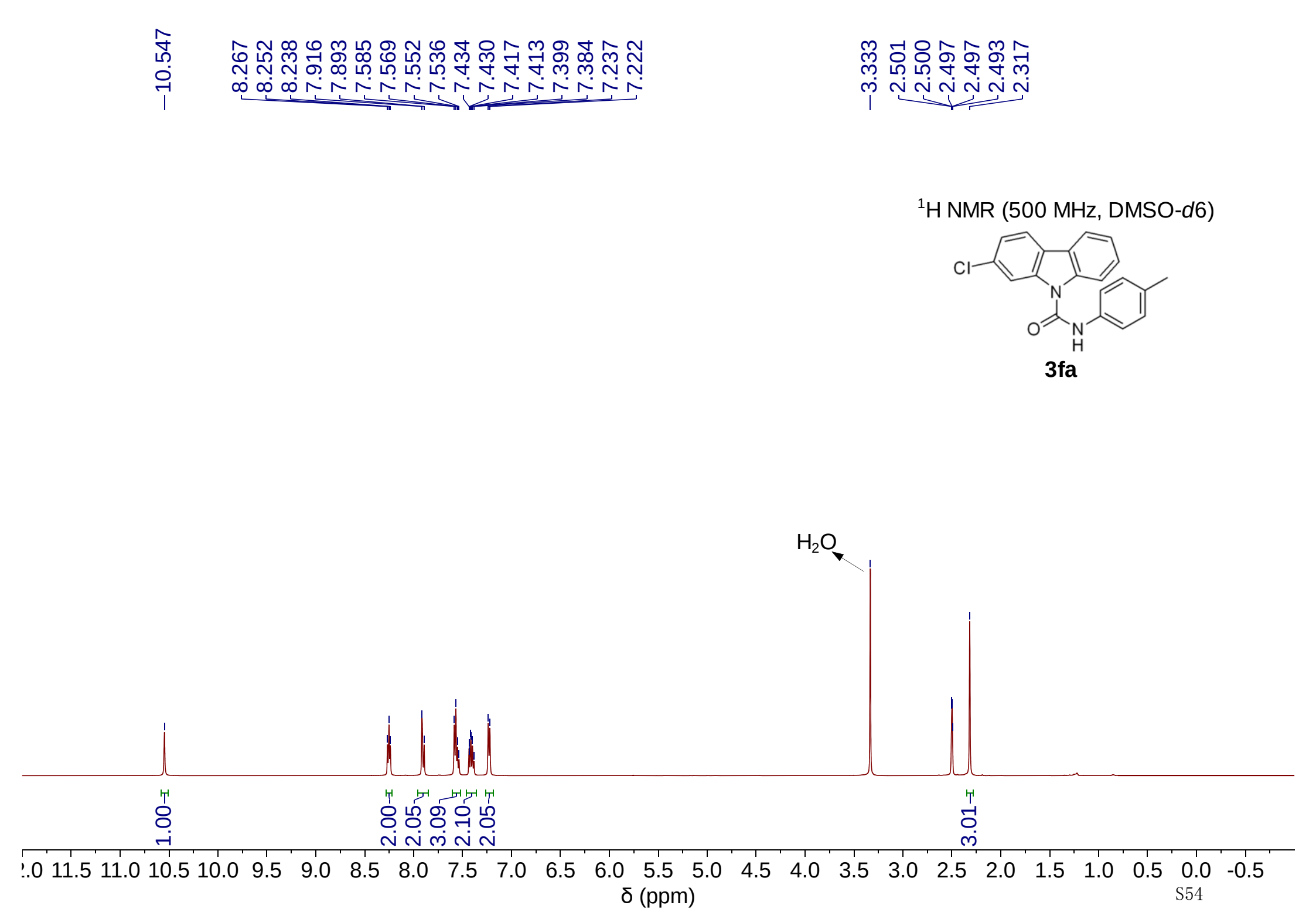
20.54

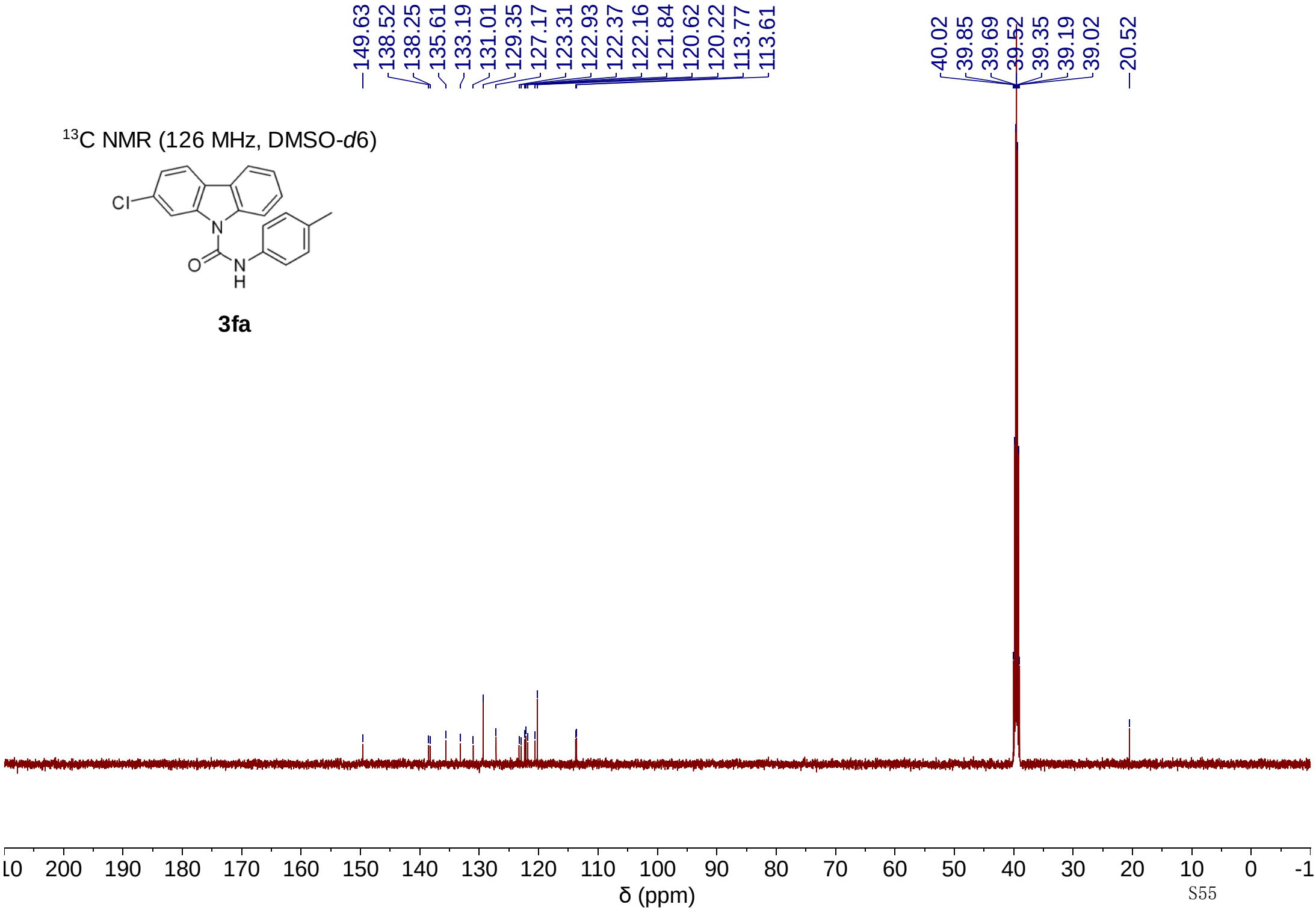
^{13}C NMR (126 MHz, DMSO-*d*6)



3ea

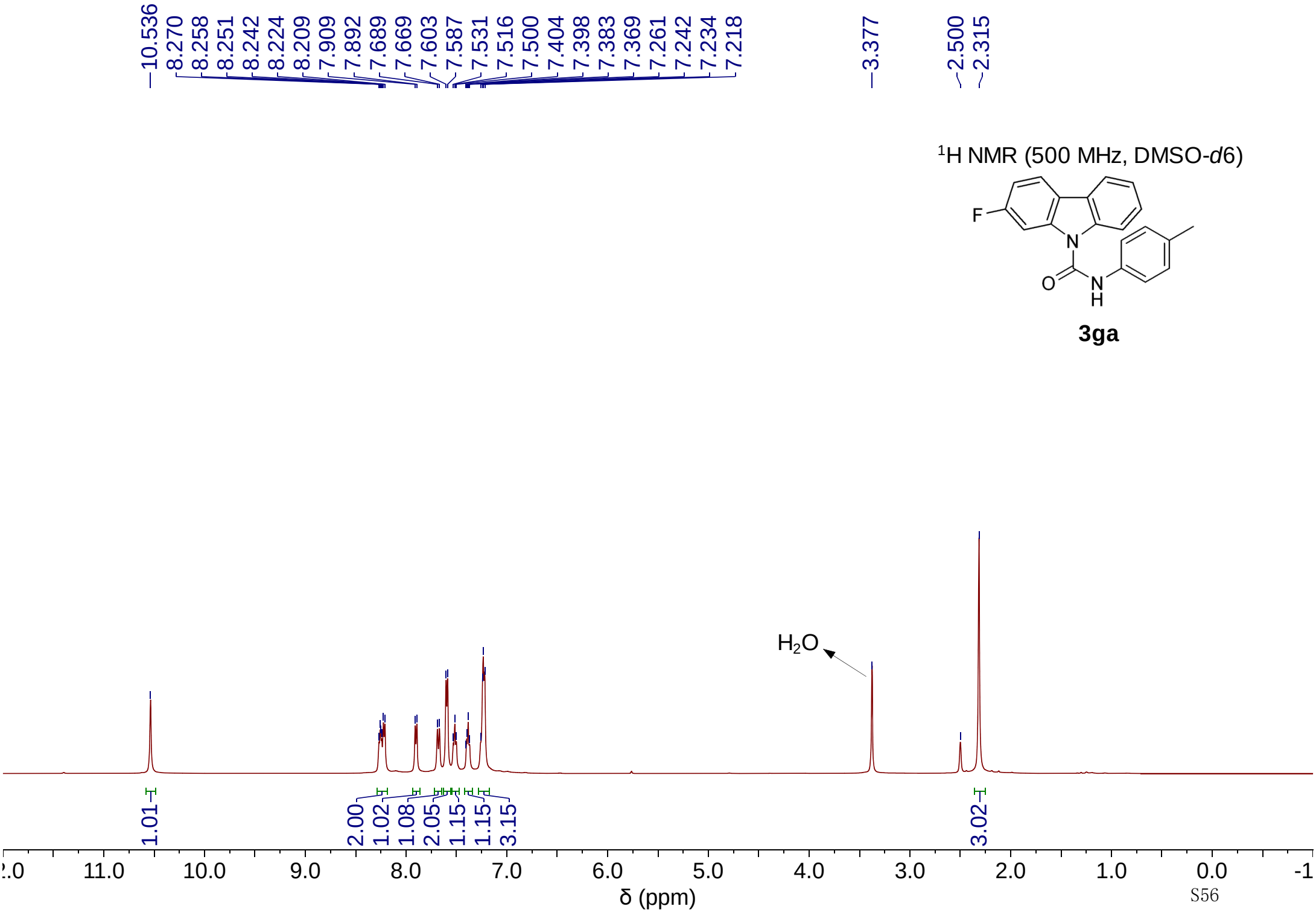



10.547
8.267
8.252
8.238
7.916
7.893
7.585
7.569
7.552
7.536
7.434
7.430
7.417
7.413
7.399
7.384
7.237
7.222
3.333
2.501
2.500
2.497
2.497
2.493
2.317
1H NMR (500 MHz, DMSO-d6)
Cl
N
O
N
H
3fa
H2O
1.00
2.00
2.05
3.09
2.10
2.05
3.01
δ (ppm)

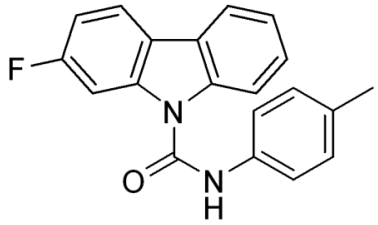


^{13}C NMR (126 MHz, DMSO-*d*6)

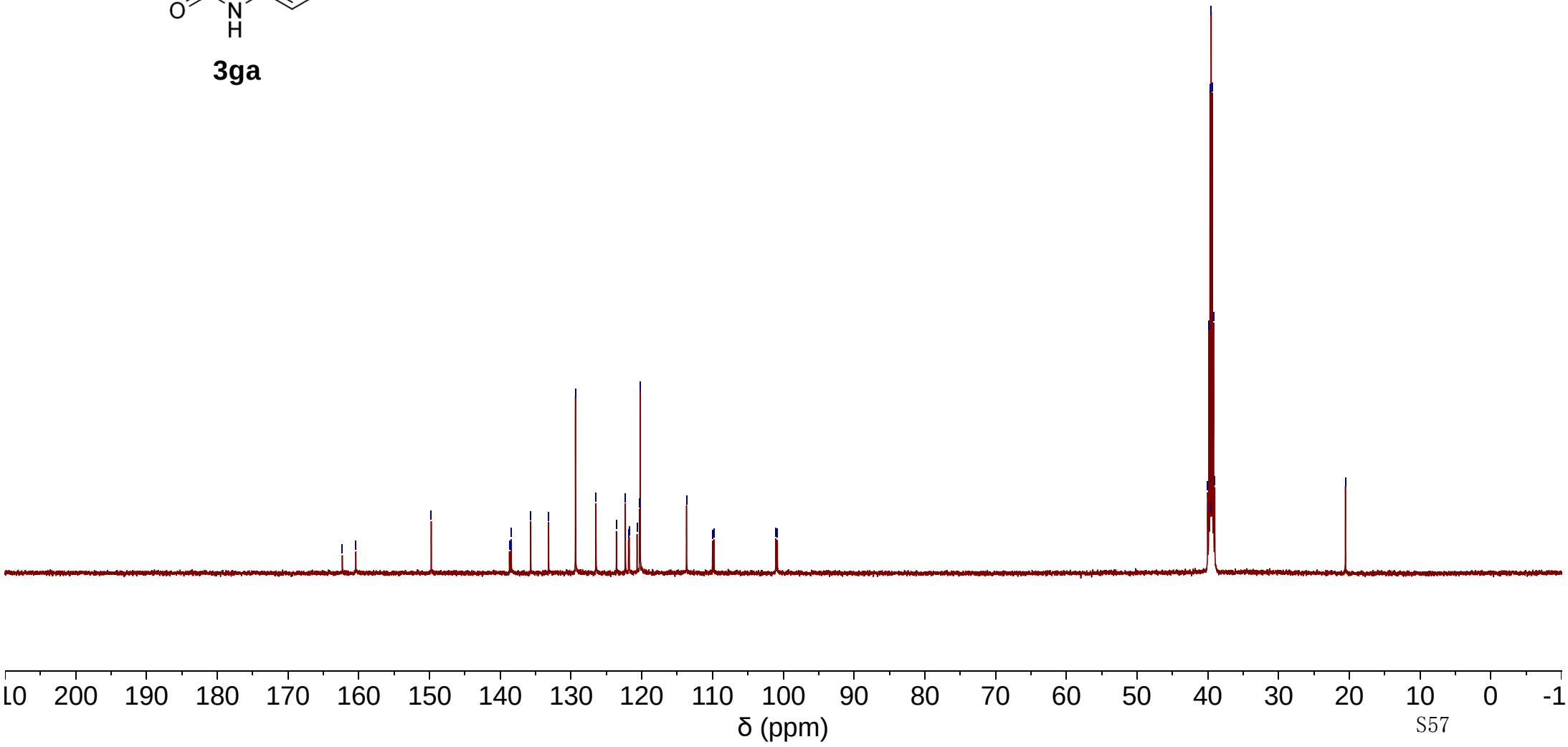
3fa

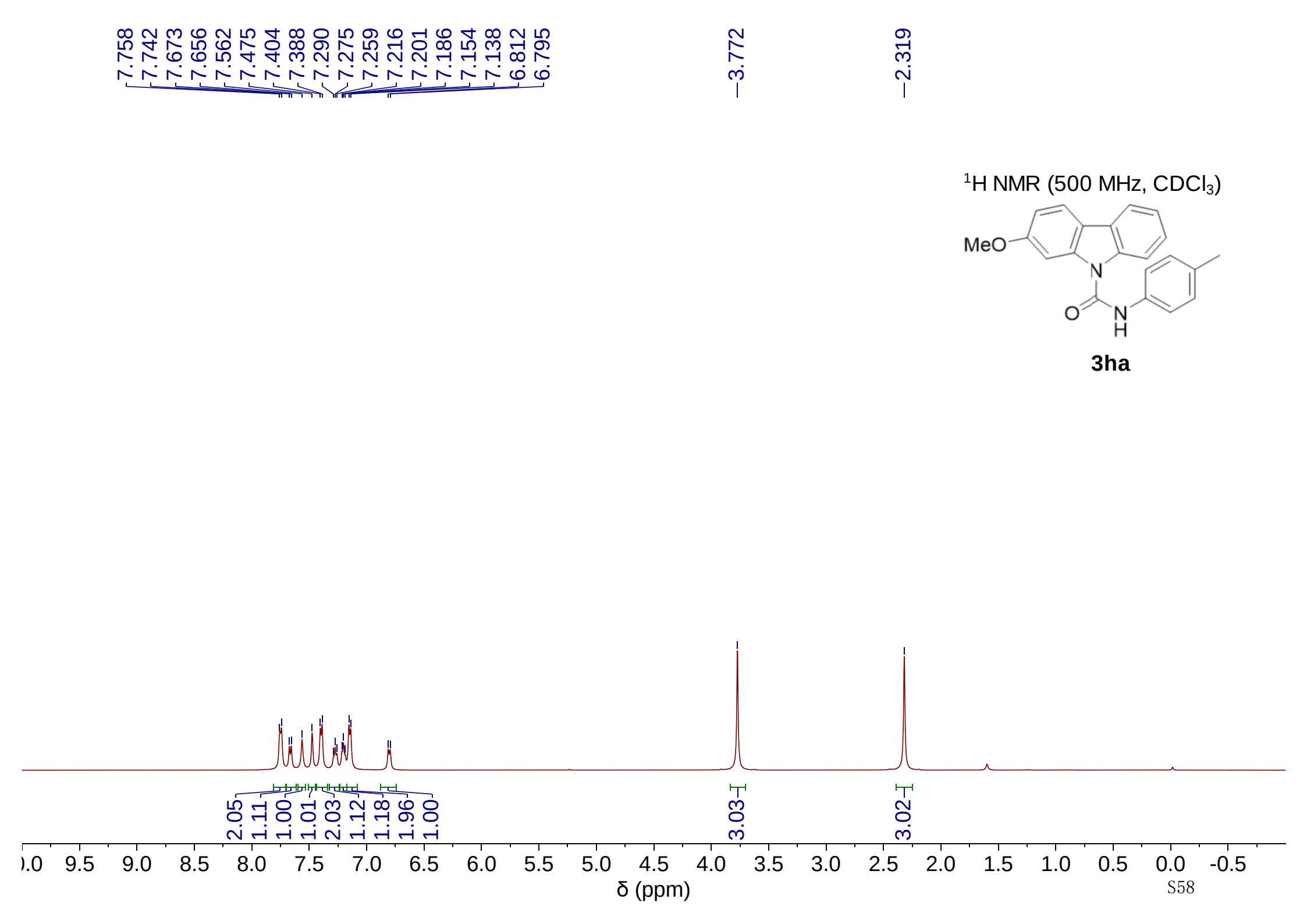

10.536
8.270
8.258
8.251
8.242
8.224
8.209
7.909
7.892
7.689
7.669
7.603
7.587
7.531
7.516
7.500
7.404
7.398
7.383
7.369
7.261
7.242
7.234
7.218
3.377
2.500
2.315
1H NMR (500 MHz, DMSO-d6)
F
N
O
N
H
3ga
H2O
1.01
2.00
1.02
1.08
2.05
1.15
1.15
3.15
3.02
δ (ppm)

^{13}C NMR (126 MHz, DMSO-*d*6)



3ga



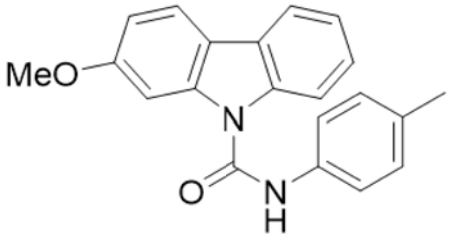


^{1}H NMR (500 MHz, $CDCl_3$)

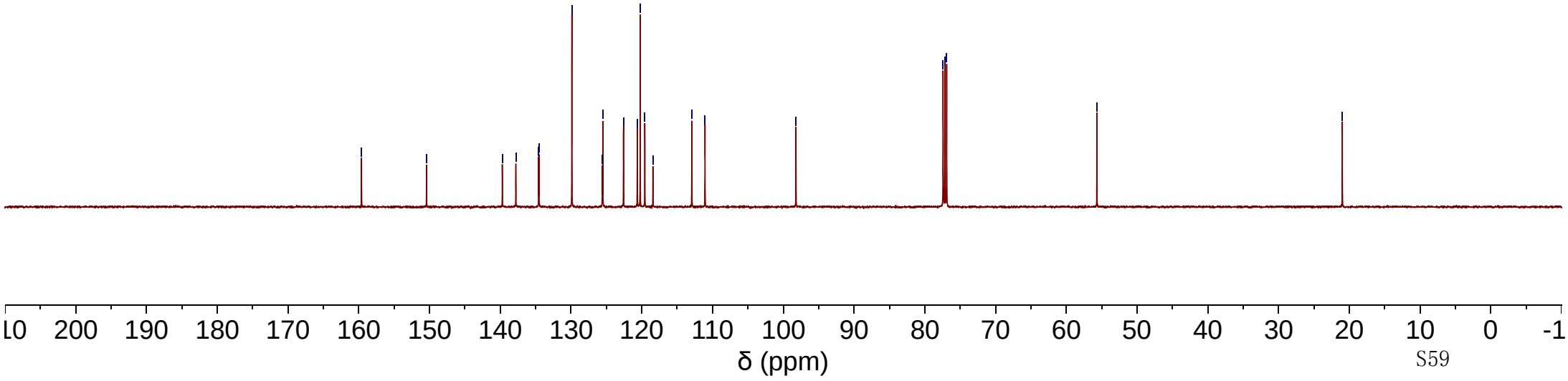
3ha

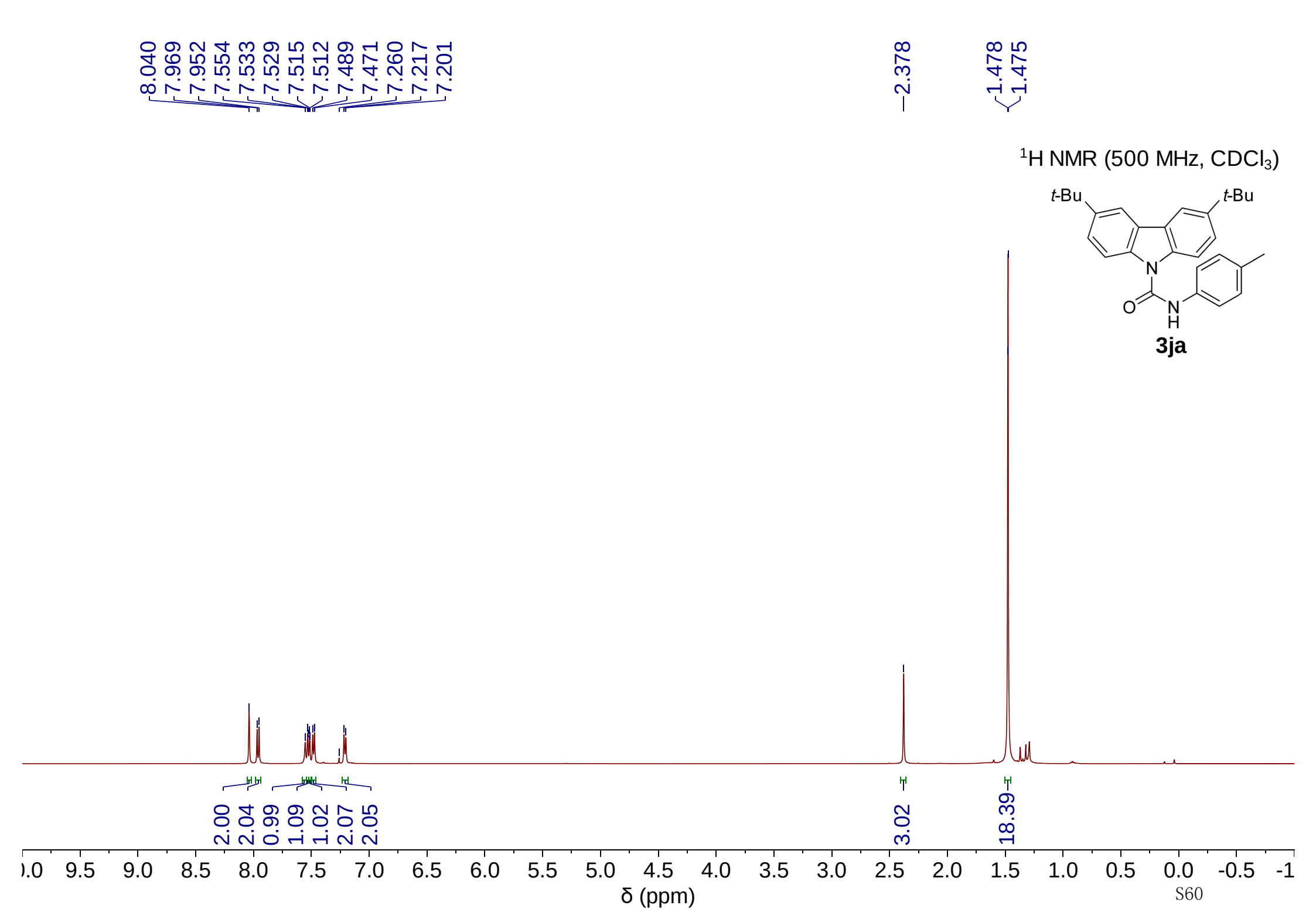
159.61
150.42
139.71
137.80
134.58
134.52
129.88
125.58
125.51
122.58
120.64
120.22
119.57
118.43
112.93
111.06
98.21
77.42
77.16
76.91
55.68
20.99

^{1}H NMR (126 MHz, $CDCl_3$)



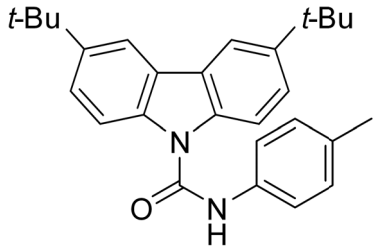
3ha



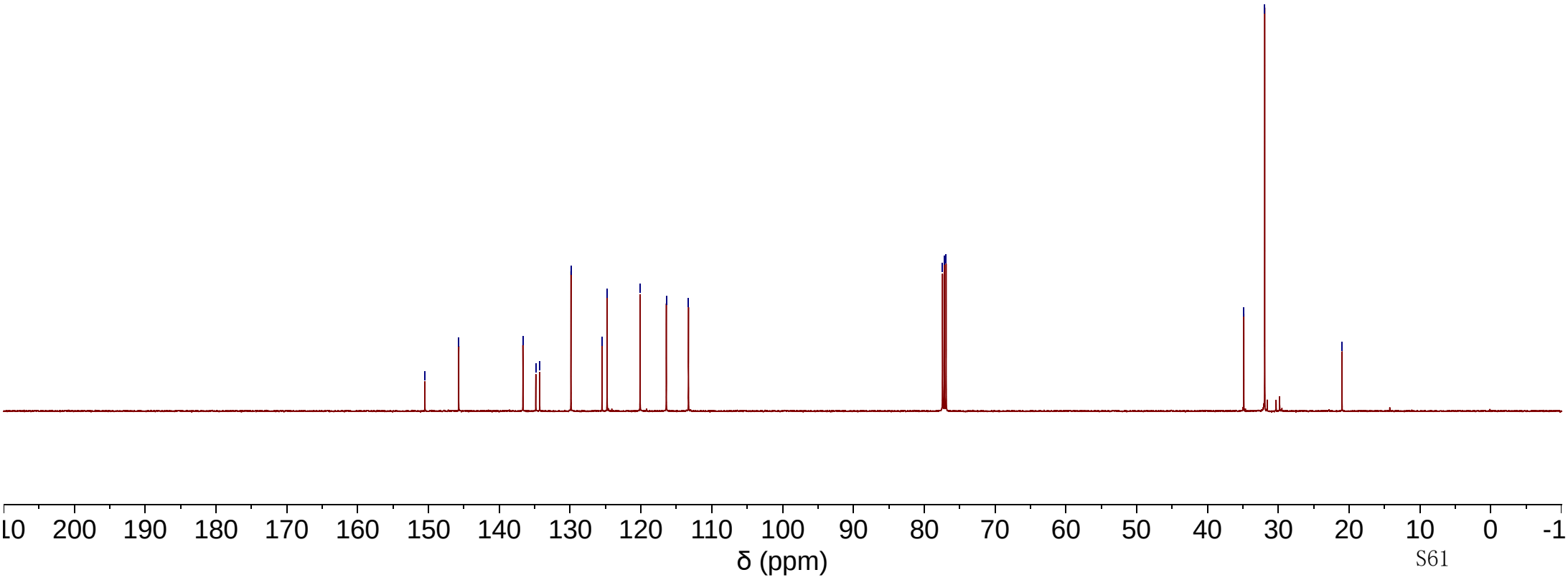

8.040
7.969
7.952
7.554
7.533
7.529
7.515
7.512
7.489
7.471
7.260
7.217
7.201
2.378
1.478
1.475
^{1}H NMR (500 MHz, $CDCl_3$)
t-Bu
t-Bu
N
O
N
H
3ja
2.00
2.04
0.99
1.09
1.02
2.07
2.05
3.02
18.39
δ (ppm)

150.51
145.73
136.66
134.84
134.29
129.88
125.49
124.78
120.12
116.42
113.29
77.41
77.16
76.91
34.87
31.91
20.99

^{13}C NMR (126 MHz, $CDCl_3$)

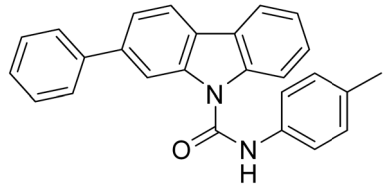


3ja

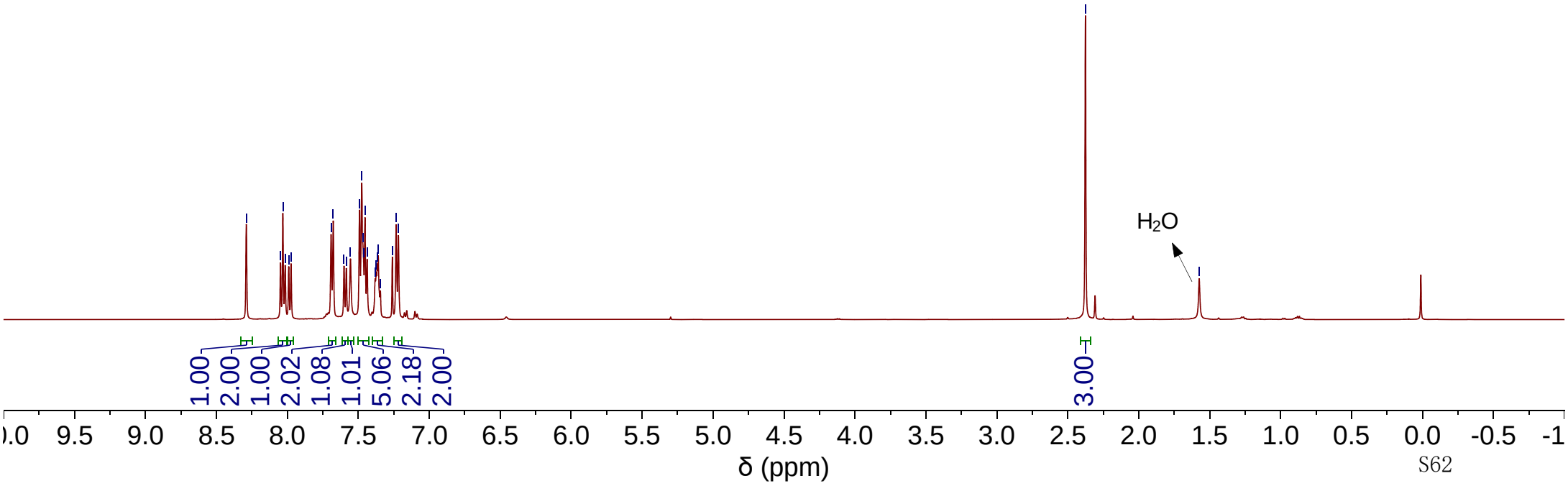


8.290
8.048
8.032
8.015
7.990
7.974
7.692
7.677
7.601
7.585
7.555
7.492
7.476
7.467
7.463
7.453
7.438
7.382
7.374
7.367
7.359
7.345
7.260
7.233
7.218
2.376
1.574

^{1}H NMR (500 MHz, $CDCl_3$)

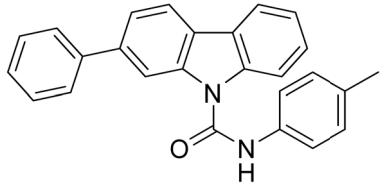


3ka

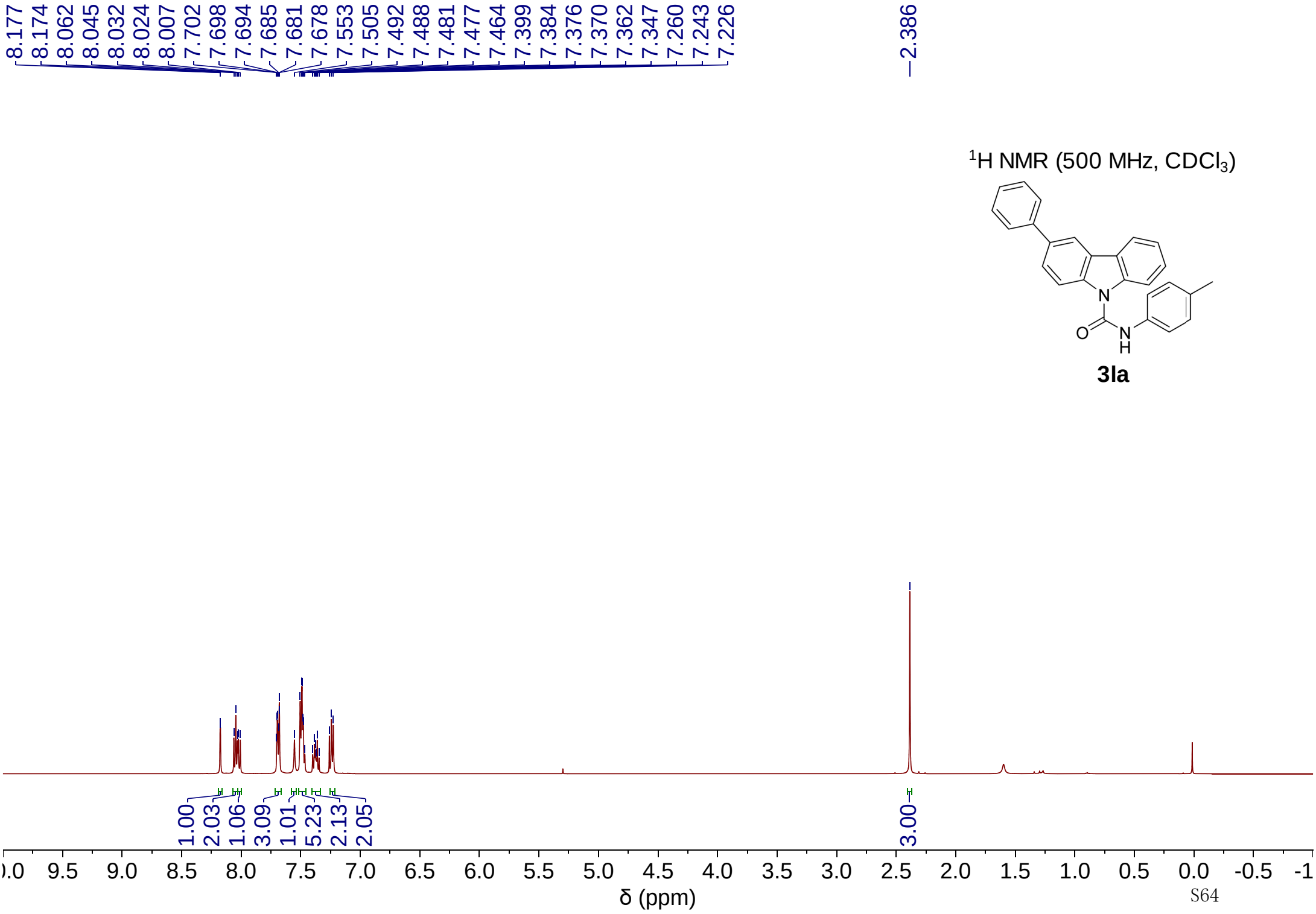


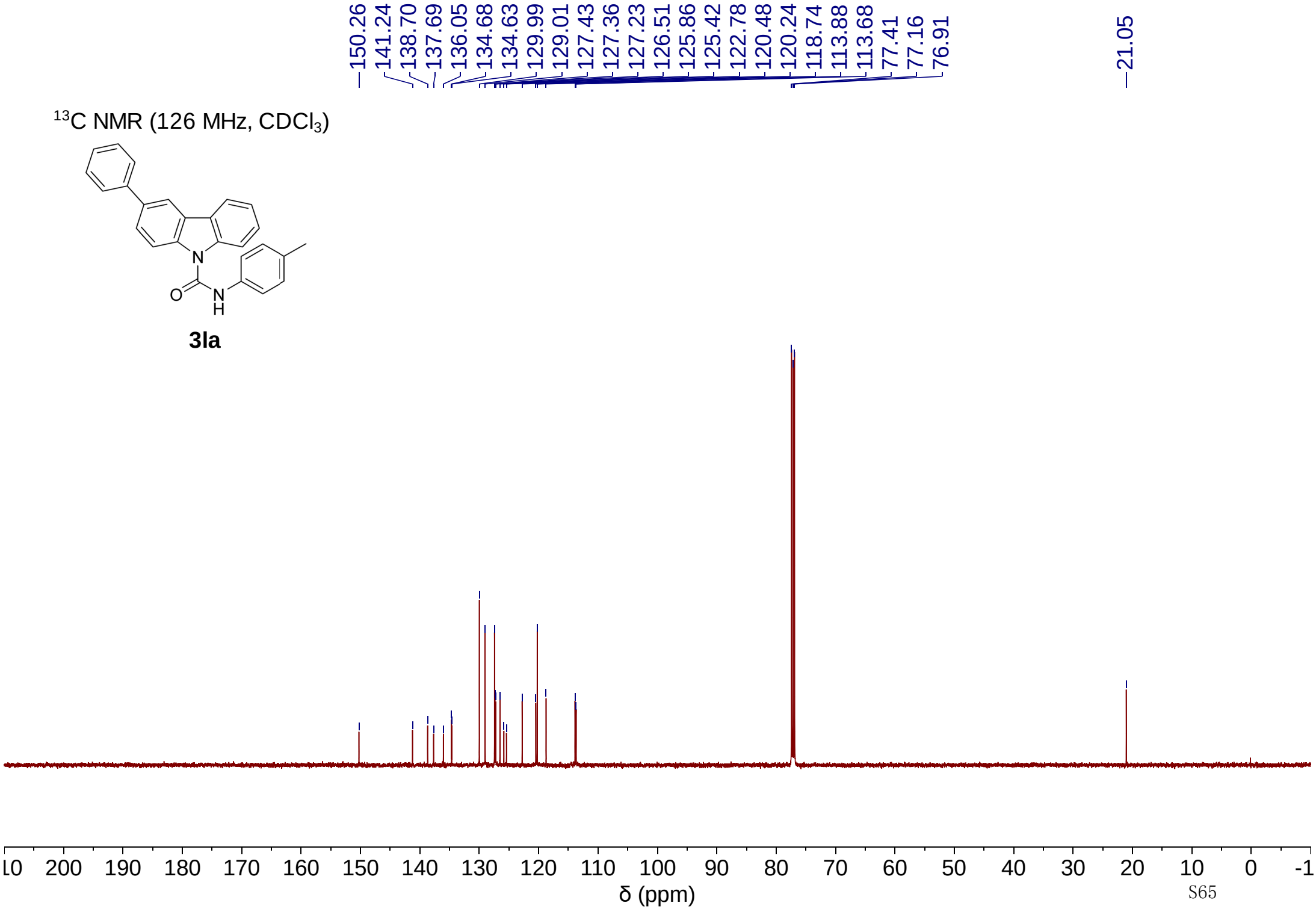
150.35
141.43
140.65
139.09
138.58
134.72
134.59
130.00
128.98
127.65
127.54
127.15
125.25
124.38
122.80
122.19
120.56
120.52
120.30
113.39
112.42
77.42
77.16
76.91
21.04

^{13}C NMR (126 MHz, $CDCl_3$)



3ka


8.177
8.174
8.062
8.045
8.032
8.024
8.007
7.702
7.698
7.694
7.685
7.681
7.678
7.553
7.505
7.492
7.488
7.481
7.477
7.464
7.399
7.384
7.376
7.370
7.362
7.347
7.260
7.243
7.226
2.386
1H NMR (500 MHz, CDCl3)
N
O
N
H
3la
1.00
2.03
1.06
3.09
1.01
5.23
2.13
2.05
3.00
δ (ppm)

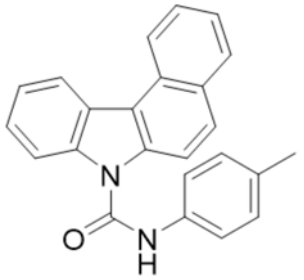


^{13}C NMR (126 MHz, $CDCl_3$)

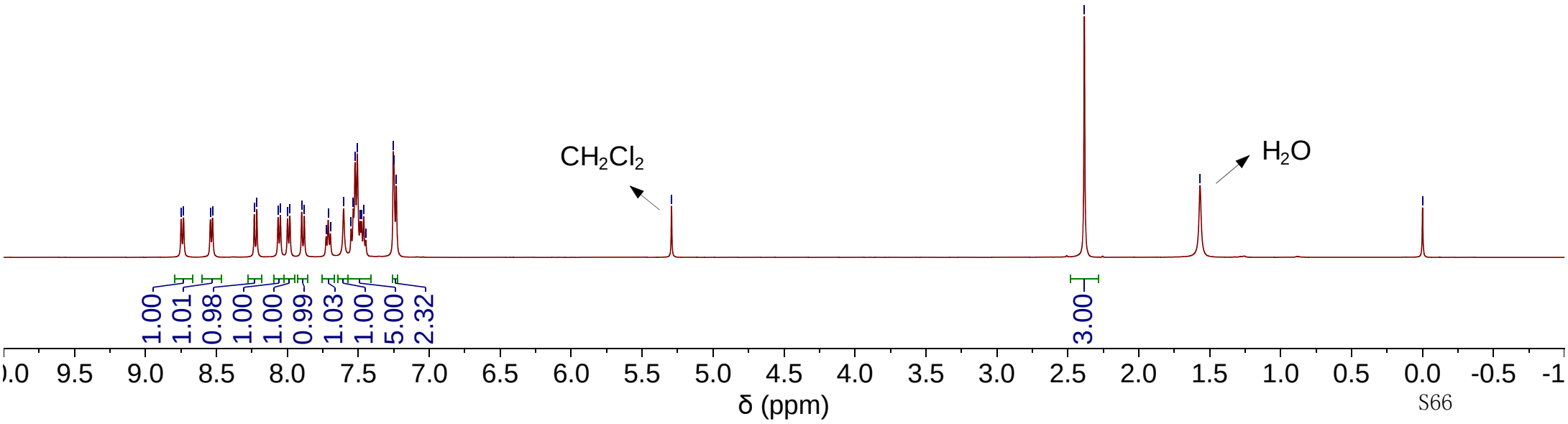
3la

8.748
8.732
8.543
8.527
8.233
8.215
8.066
8.049
7.999
7.983
7.899
7.881
7.727
7.712
7.697
7.604
7.551
7.536
7.523
7.507
7.488
7.477
7.462
7.447
7.254
7.248
7.233
5.293
2.383
1.568
0.000

^{1}H NMR (500 MHz, $CDCl_3$)

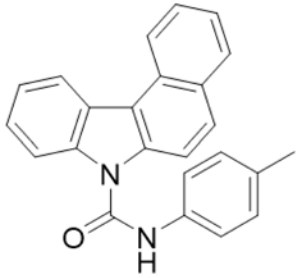


3ma



149.94
137.56
136.41
134.90
134.54
130.43
130.05
129.36
129.27
128.48
127.39
125.92
125.75
124.43
123.63
123.01
122.63
120.21
117.94
113.90
113.18
77.41
77.16
76.91
21.07

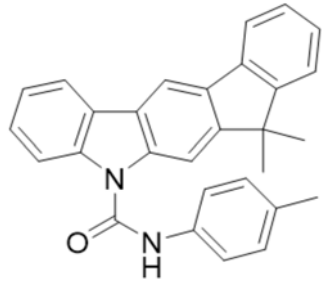
^{13}C NMR (126 MHz, $CDCl_3$)



3ma

8.114
8.109
8.070
8.066
7.966
7.951
7.792
7.788
7.776
7.771
7.756
7.741
7.544
7.453
7.438
7.422
7.407
7.359
7.344
7.329
7.299
7.286
7.273
7.189
7.173
2.333
1.504

^{1}H NMR (500 MHz, $CDCl_3$)



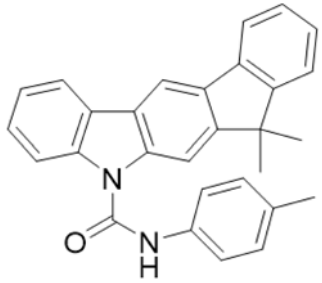
3na

1.00
1.00
1.00
1.01
1.01
1.01
2.06
1.11
2.12
2.10
2.09
2.99
6.24

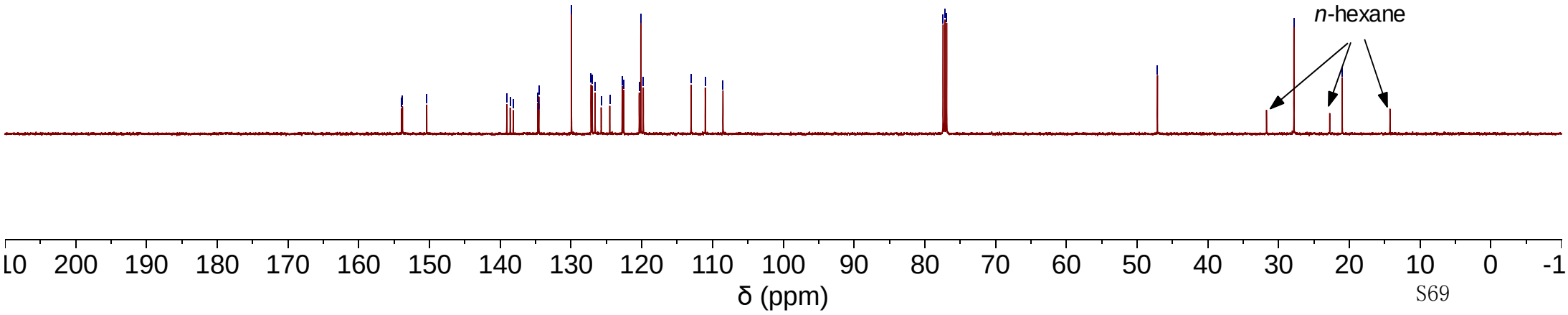
δ (ppm)

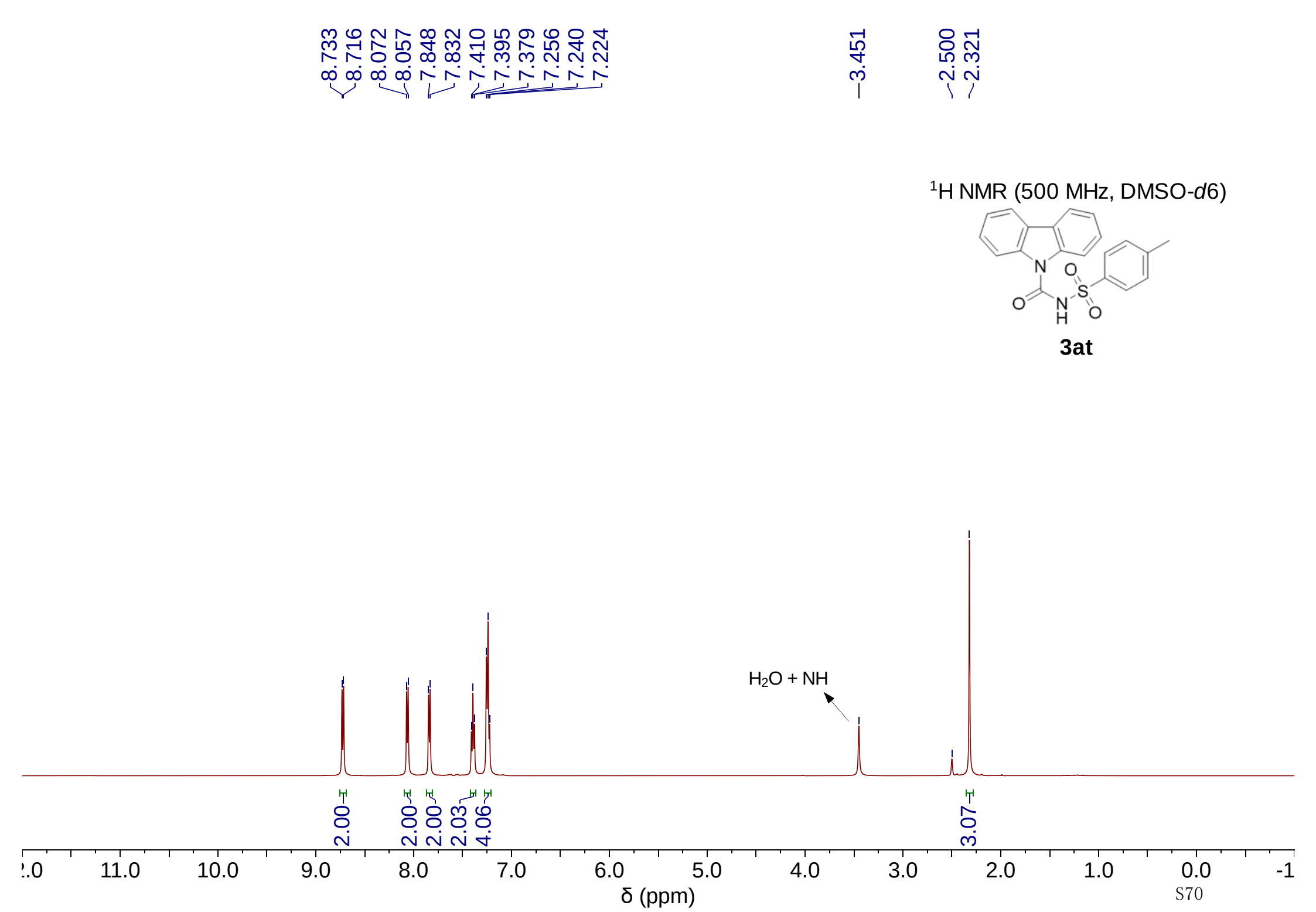
153.96
153.82
150.39
139.08
138.60
138.17
134.70
134.56
134.54
129.94
127.17
127.00
126.60
125.74
124.52
122.77
122.56
120.36
120.13
119.78
113.02
111.02
108.52
77.42
77.16
76.91
47.12
27.83
21.01

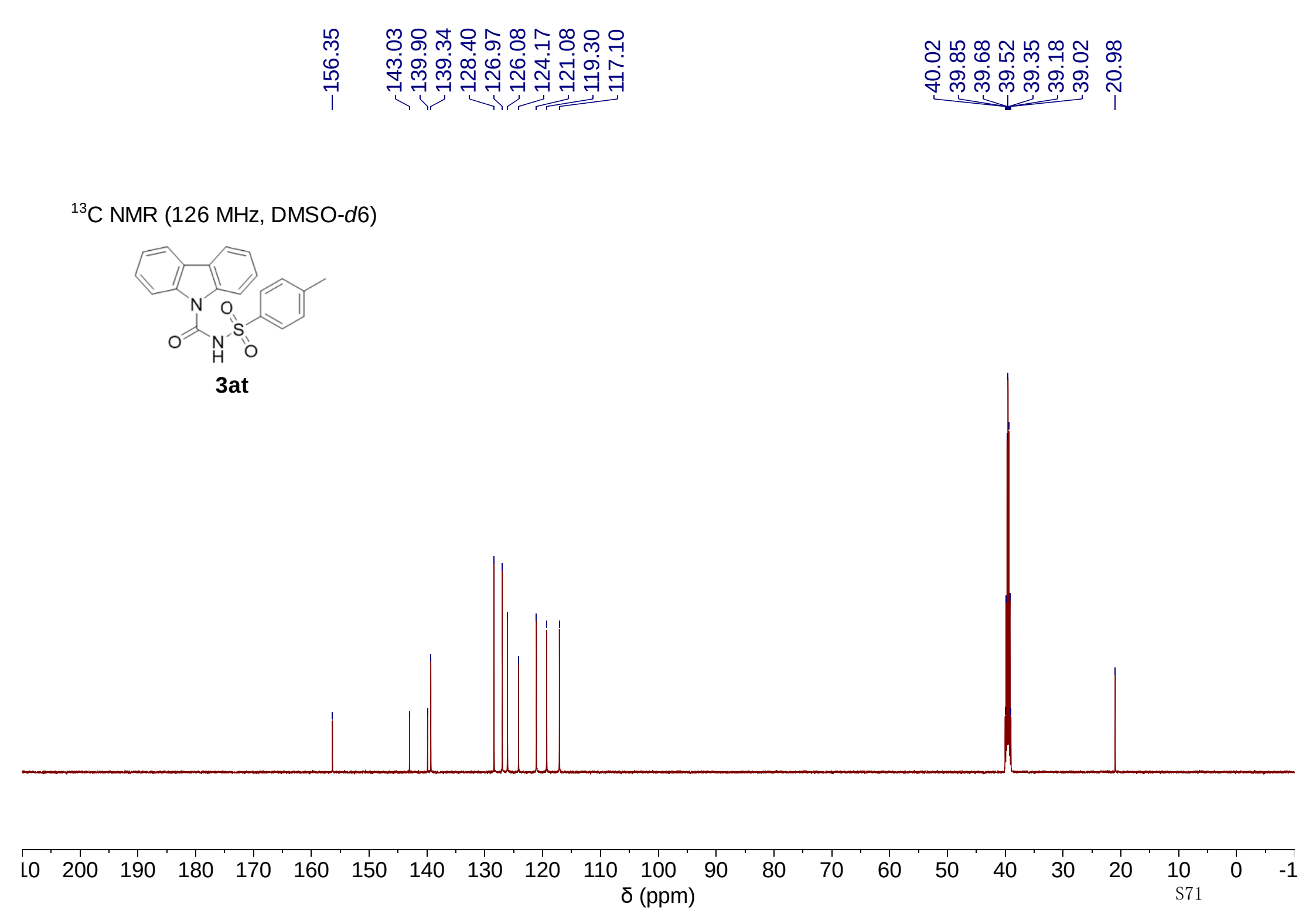
^{13}C NMR (126 MHz, $CDCl_3$)



3na

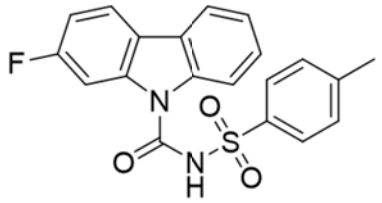



8.733
8.716
8.072
8.057
7.848
7.832
7.410
7.395
7.379
7.256
7.240
7.224
3.451
2.500
2.321
1H NMR (500 MHz, DMSO-d6)
3at
H2O + NH
2.00
2.00
2.00
2.03
4.06
3.07
δ (ppm)

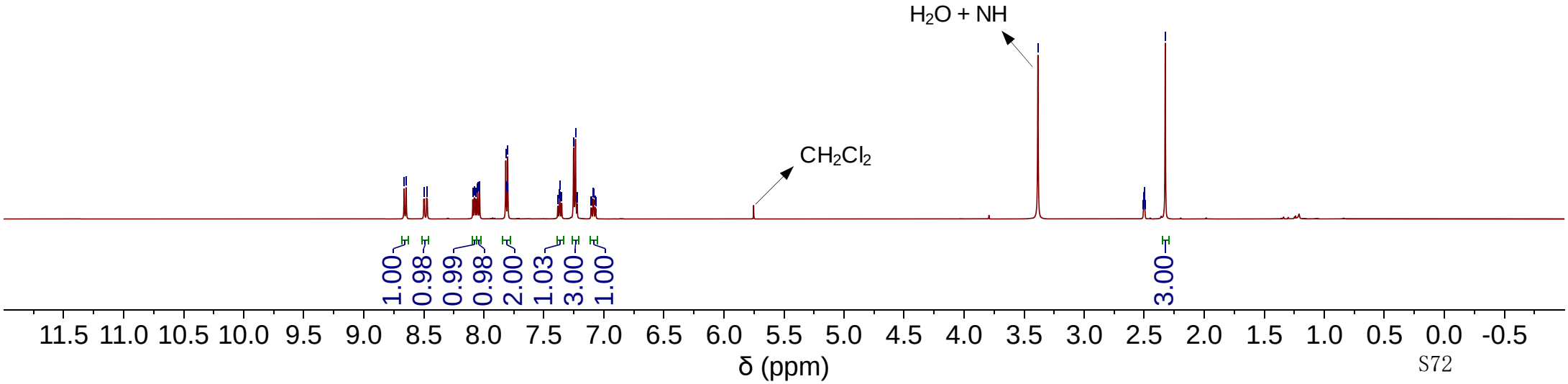

156.35
143.03
139.90
139.34
128.40
126.97
126.08
124.17
121.08
119.30
117.10
40.02
39.85
39.68
39.52
39.35
39.18
39.02
20.98
13C NMR (126 MHz, DMSO-d6)
N
O
S
O
O
N
H
O
3at
δ (ppm)

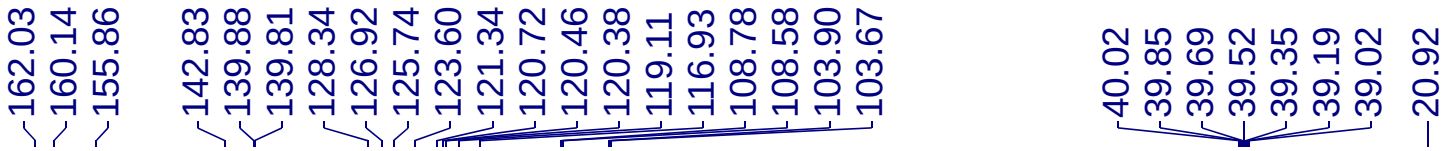
8.664 8.647 8.500 8.495 8.476 8.471 8.092 8.080 8.075 8.063 8.052 8.050 8.037 8.034 7.817 7.814 7.805 7.801 7.384 7.382 7.370 7.368 7.365 7.353 7.351 7.253 7.237 7.223 7.221 7.102 7.090 7.085 7.072 3.385 2.508 2.504 2.500 2.496 2.493 2.325

^{1}H NMR (500 MHz, DMSO-*d*6)

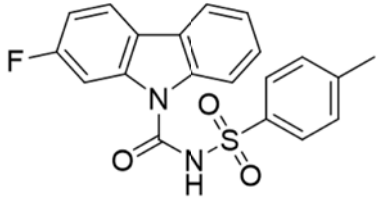


3gt

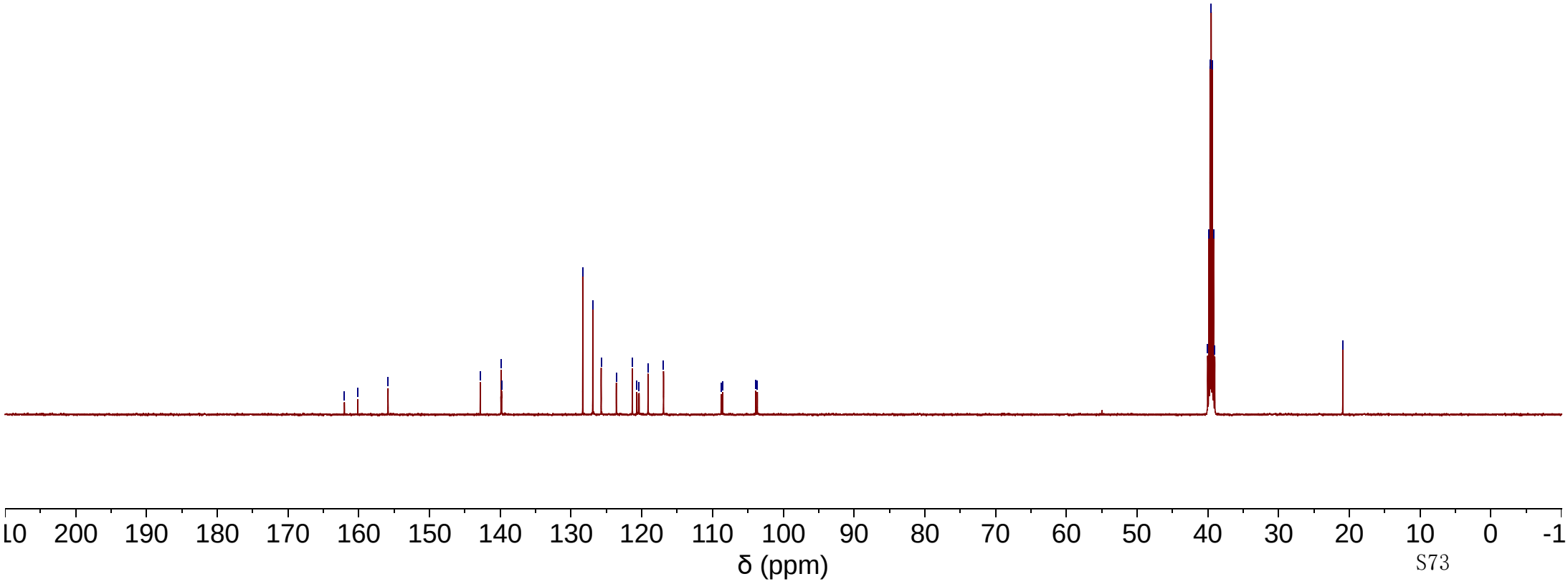


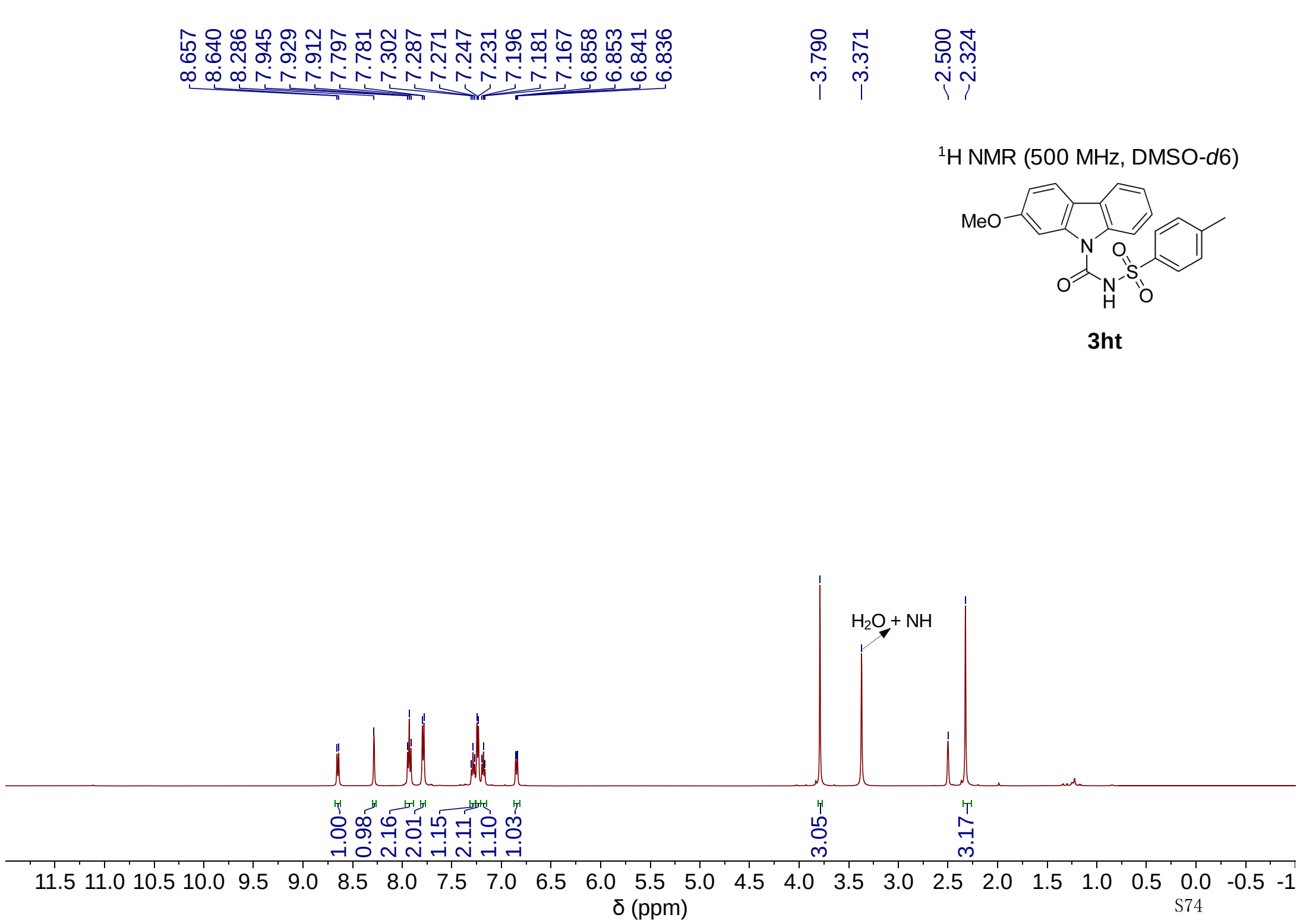


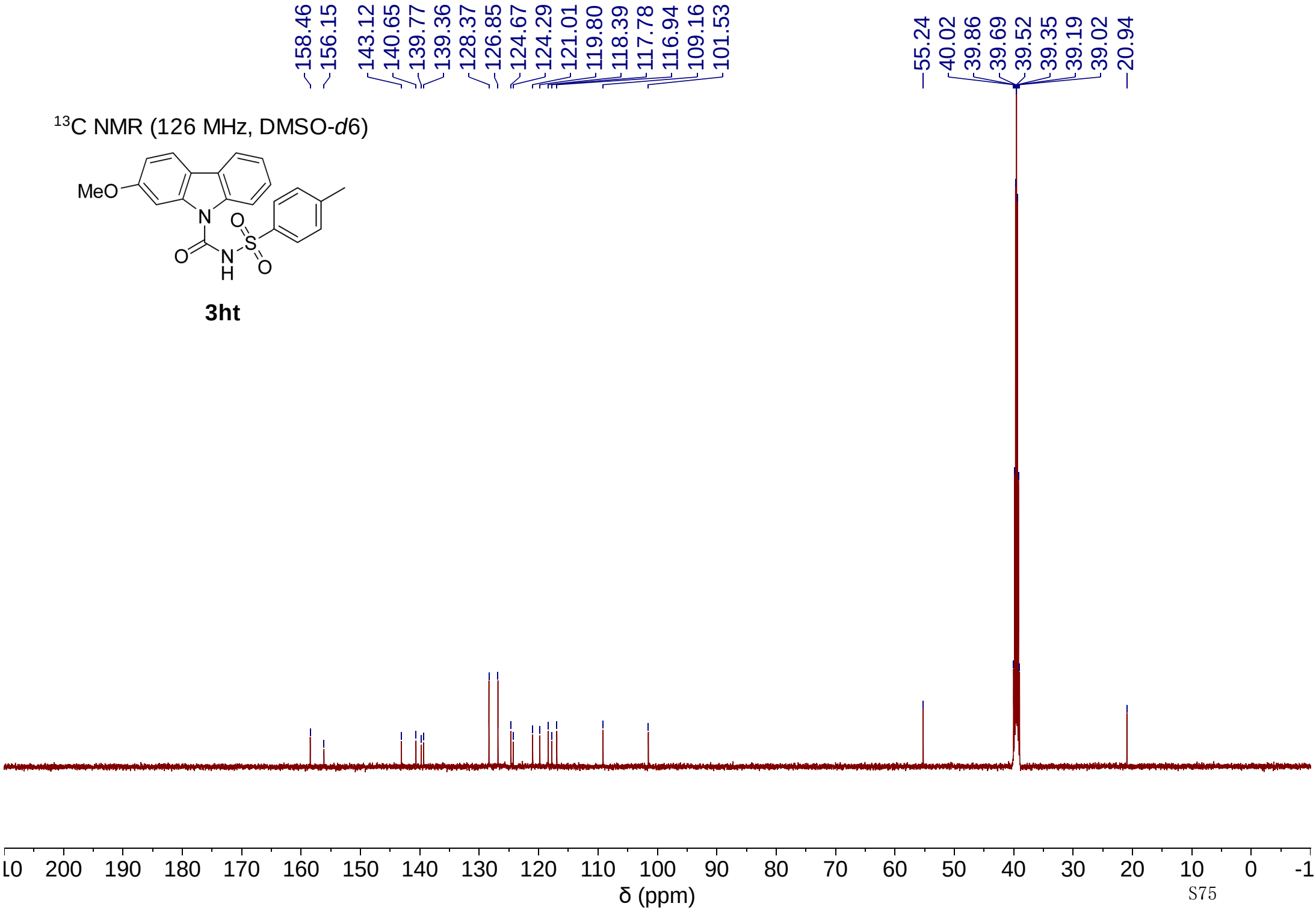
^{13}C NMR (126 MHz, DMSO-*d*6)



3gt

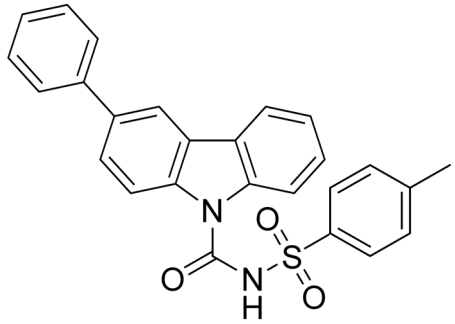



8.657
8.640
8.286
7.945
7.929
7.912
7.797
7.781
7.302
7.287
7.271
7.247
7.231
7.196
7.181
7.167
6.858
6.853
6.841
6.836
3.790
3.371
2.500
2.324
1H NMR (500 MHz, DMSO-d6)
MeO
N
O
S
O
O
N
H
O
3ht
H2O + NH
1.00
0.98
2.16
2.01
1.15
2.11
1.10
1.03
3.05
3.17
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
δ (ppm)


158.46
156.15
143.12
140.65
139.77
139.36
128.37
126.85
124.67
124.29
121.01
119.80
118.39
117.78
116.94
109.16
101.53
55.24
40.02
39.86
39.69
39.52
39.35
39.19
39.02
20.94
^{13}C NMR (126 MHz, DMSO-*d*6)
MeO
N
O
S
O
O
N
H
O
3ht
δ (ppm)

8.793 8.776 8.733 8.716 8.418 8.206 8.191 7.856 7.841 7.818 7.802 7.740 7.735 7.722 7.718 7.503 7.488 7.472 7.431 7.415 7.400 7.360 7.345 7.330 7.283 7.267 7.251 3.429 2.500 2.330

^{1}H NMR (500 MHz, DMSO-*d*6)



3lt

H_2O + NH

1.02 1.00 1.00 0.99 2.01 2.05 1.00 2.08 1.09 1.09 3.06 3.05

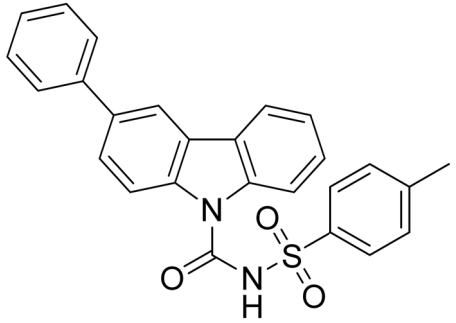
2.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1

δ (ppm)

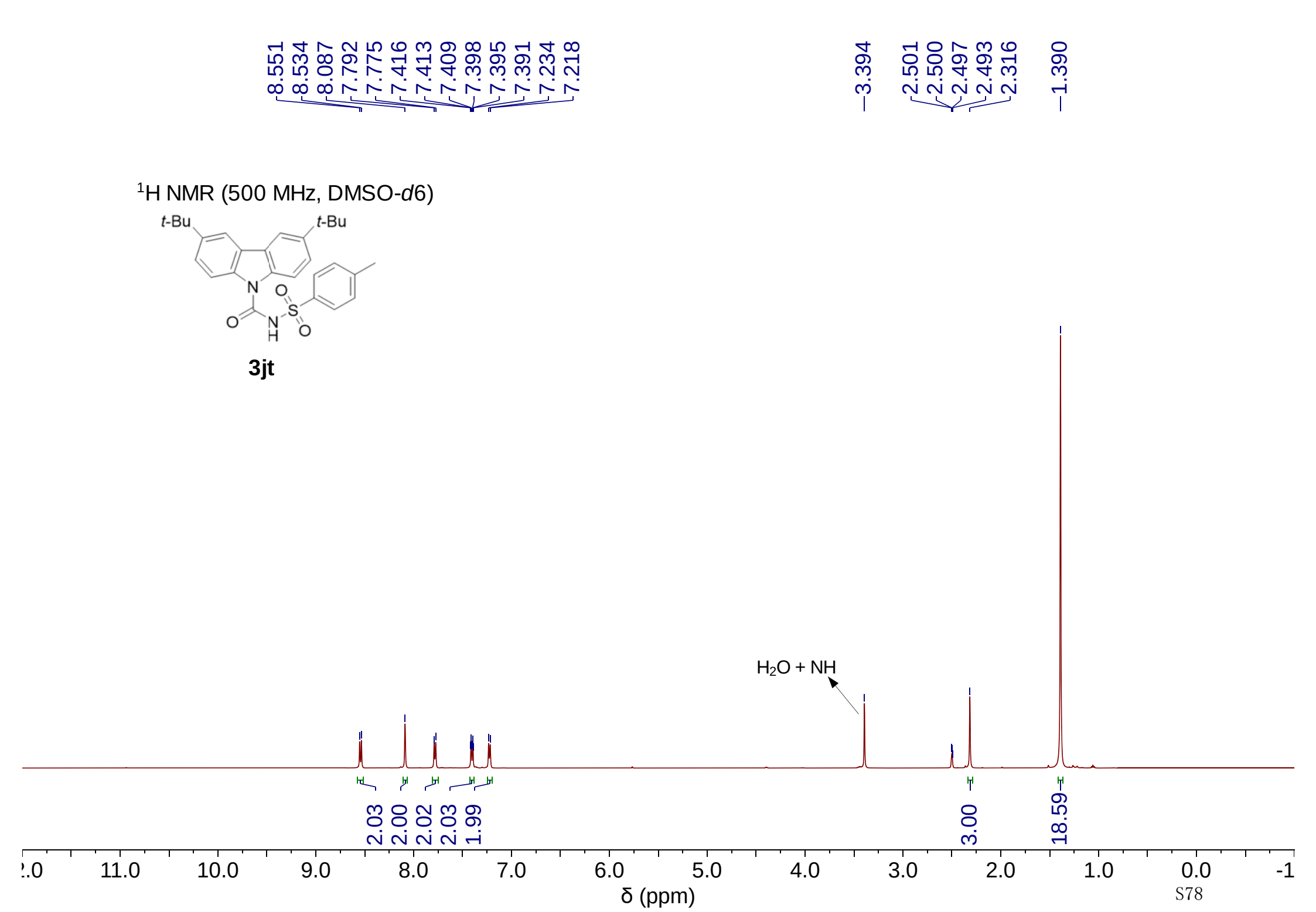
156.21
143.02
140.75
139.88
139.81
138.87
133.17
128.96
128.39
127.01
126.82
126.79
126.29
124.91
124.84
124.29
121.17
119.63
117.46
117.28
117.13

40.02
39.85
39.69
39.52
39.35
39.19
39.02
20.98

^{13}C NMR (126 MHz, DMSO-*d*6)



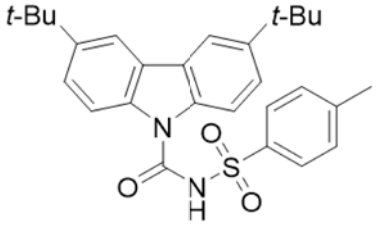
3lt


8.551
8.534
8.087
7.792
7.775
7.416
7.413
7.409
7.398
7.395
7.391
7.234
7.218
3.394
2.501
2.500
2.497
2.493
2.316
1.390
1H NMR (500 MHz, DMSO-d6)
t-Bu
t-Bu
N
O
S
O
N
H
O
O
3jt
H2O + NH
2.03
2.00
2.02
2.03
1.99
3.00
18.59
δ (ppm)

156.33
143.27
143.20
139.67
137.67
128.31
126.88
124.18
123.37
116.52
115.39

40.02
39.85
39.69
39.52
39.35
39.19
39.02
34.43
31.80
20.97

^{13}C NMR (126 MHz, DMSO-*d*6)



3jt