Supporting Information

KI-Mediated Three-Component Annelation for the Regioselective Synthesis of Angular Azolo[1,5-*a*]pyrimidine Derivatives

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1. General

All substrates aldehydes (**1**), 3(5)-aminoazoles (**2**), cycloketones (**3**) and reagents were commercially available and used without further purification. All aldehydes (**1**) and 3(5)-aminoazoles are known compounds. TLC analysis was performed using pre-coated glass plates. Column chromatography was performed using silica gel (200–300 mesh). ^{1}H spectra were recorded in $CDCl_3$ on 400 MHz NMR spectrometers and resonances (δ) are given in parts per million relative to tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz) and integration. ^{13}C spectra were recorded in $CDCl_3$ on 100 MHz NMR spectrometers and resonances (δ) are given in ppm. HRMS analysis of compounds was performed with a time-of-flight mass spectrometer (micrOTOF-Q, Bruker Daltonik, Germany) equipped with an electrospray ionization source. The X-ray crystal-structure determinations of **4am** were obtained on a Bruker SMART APEX CCD system. Melting points were determined using XT-4 apparatus and not corrected. All reactions were heated by a metal sand bath (WATTCAS, LAB-500, https://www.wattcas.com).

2. General procedure for the synthesis of compounds 4 (4a as an example)

Benzaldehyde **1a** (53 mg, 0.5 mmol), ethyl 3-amino-1*H*-pyrazole-4-carboxylate **2a** (77.6 mg, 0.5 mmol), cyclohexanone **3a** (147.2 mg, 1.5 mmol), KI (41.5mg, 0.25 mmol), DMSO (39 mg, 0.5 mmol) and 1,2-dichloroethane (2.5 mL) were charged into a pressure tube (35 mL) and were stirred at 120 ^{o}C for 5 h. After disappearance of the reactant (monitored by TLC), added 50 mL water to the mixture, then extracted with EtOAc 3 times (3 × 50 mL). The extract was washed with 10% $Na_2S_2O_3$ solution (w/w), dried over anhydrous Na_2SO_4 and evaporation. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 5:1) to afford the product **4a** as a light yellow solid (157 mg, 98% yield).

3. Experimental details

(1)The methodology applicable for gram-scale synthesis (**4a** as an example)

Benzaldehyde **1a** (530 mg, 5 mmol), ethyl 3-amino-1*H*-pyrazole-4-carboxylate **2a** (776 mg, 5 mmol), cyclohexanone **3a** (1472 mg, 15 mmol), KI (415mg, 2.5 mmol), DMSO (390 mg, 5 mmol) and 1,2-dichloroethane (25 mL) were charged into a pressure tube (150 mL) and were stirred at 120 ^{o}C for 96 h. After disappearance of the reactant (monitored by TLC), and added 500 mL water to the mixture, then extracted with EtOAc 3 times (3 × 500 mL). The extract was washed with 10% $Na_2S_2O_3$ solution (w/w), dried over anhydrous Na_2SO_4 and evaporation. The residue was purified by column chromatography on silica gel

(petroleum ether/EtOAc = 5:1) to afford the product **4a** as a light yellow solid (1.46 g, 91% yield).

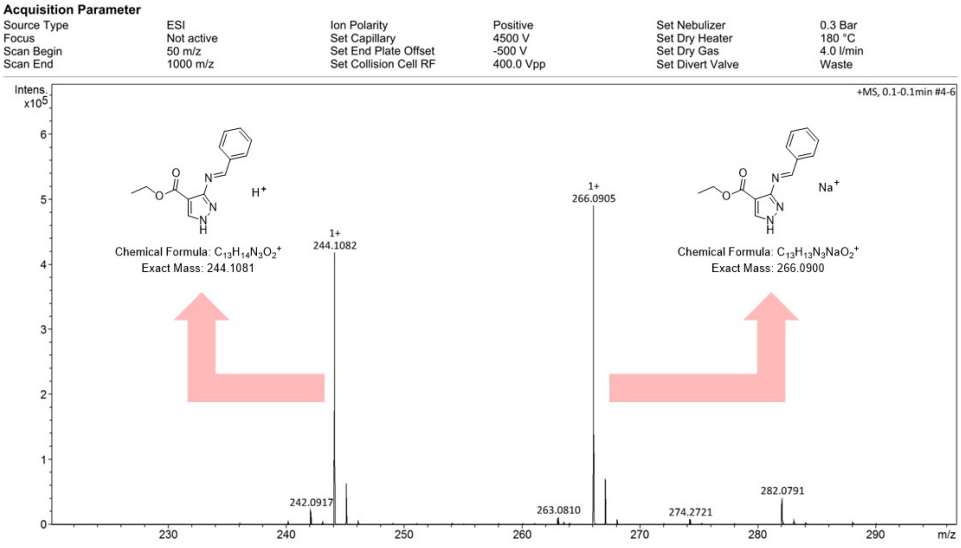
(2) The methodology applicable for **5**: (Scheme 4b)

Ethyl 5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate **4a** (321.4 mg, 1.0 mmol) and THF (4 mL) were charged into a pressure tube (15.0 mL). The mixture wasstirred at room temperature, then added LiOH (120 mg, 5.0 mmol) in water (4 mL) and stirred at same temperature for 12 h. Water was added and the solution was acidified with 6 M aqueous HCl to get precipitation, filtration and drying afforded ethyl 5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate acid as a yellow solid (275.7 mg, 94% yield). Then, the acid (58.7 mg, 0.2 mmol), estrone (54.1 mg, 0.2 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (42.2 mg, 1.1 mmol), N,N-dimethyl-4-aminopyridine (6.1 mg, 0.25 mmol) and CH_2Cl_2 (2 mL) were charged into a round-bottom flask (50 mL). After stirred at room temperature for 8 h, the reaction was quenched with 20 mL of saturated $NaHCO_3$ (aq.) and then extracted with CH_2Cl_2 (10 mL × 3). The combined organic layer was dried over Na_2SO_4, filtrated, and concentrated under reduced pressure. The residue was purified by chromatography on silica gel (petroleum ether/EtOAc = 2:1) to afford the product **5** as a white solid (91 mg, 83% yield).

4. Studying the reaction mechanism

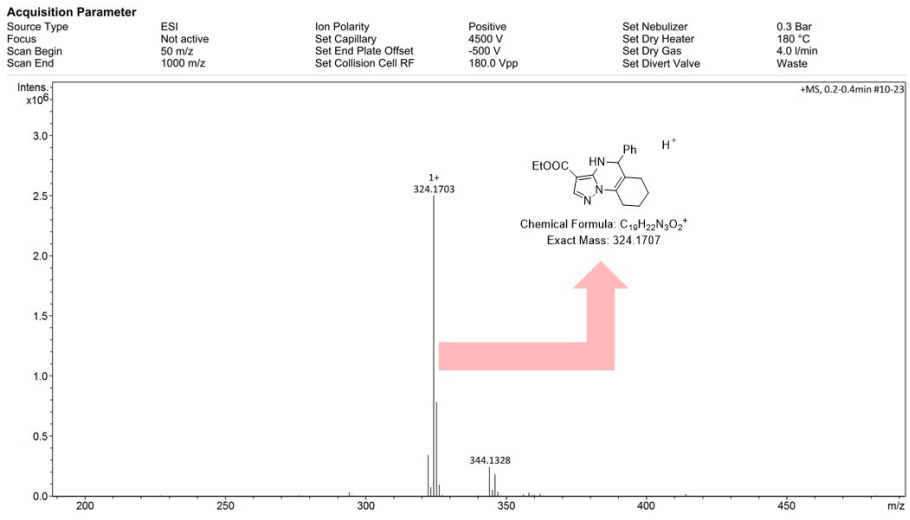
(1) The details of Scheme 5c

Benzaldehyde **1a** (530 mg, 5 mmol) and ethyl 3-amino-1*H*-pyrazole-4-carboxylate **2a** (776 mg, 5 mmol) were charged into a pressure tube (150 mL) and were stirred at 120 °C for 2 h. The imine intermediate **A** was clearly detected by HRMS. HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{13}H_{14}N_3O_2$: 244.1081; found: 244.1082, m/z $[M + Na]^+$ calcd for $C_{13}H_{14}N_3NaO_2$: 266.0900; found: 266.0905. Then, KI (41.5mg, 0.25 mmol), DMSO (390 mg, 5 mmol) and **3a** were added into the pressure tube, afterward, the mixture was stirred at 120 °C for 46 h. After disappearance of the reactant (monitored by TLC), and added 50 mL water to the mixture, then extracted with EtOAc 3 times (3 × 50 mL). The extract was washed with 10% $Na_2S_2O_3$ solution (w/w), dried over anhydrous Na_2SO_4 and evaporation. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 5:1) to afford the product **4a** as a light yellow solid (151 mg, 94% yield).

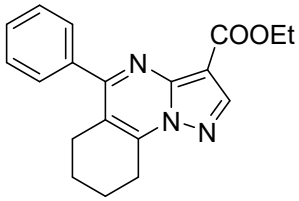


(2) The details of intermediate **C**

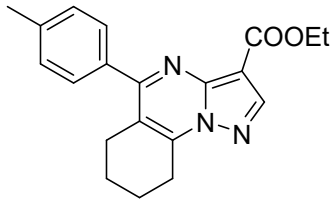
Benzaldehyde **1a** (53 mg, 0.5 mmol), ethyl 3-amino-1*H*-pyrazole-4-carboxylate **2a** (77.6 mg, 0.5 mmol), cyclohexanone **3a** (147.2 mg, 1.5 mmol), KI (8.3 mg, 0.05 mmol), DMSO (39 mg, 0.5 mmol) and 1,2-dichloroethane (2.5 mL) were charged into a pressure tube (35 mL) and were stirred at 120 °C for 5 h. The imine intermediate **C** was clearly detected by HRMS. HRMS (ESI): m/z [M + H] + calcd for $C_{19}H_{22}N_3O_2$: 324.1707; found: 324.1703.



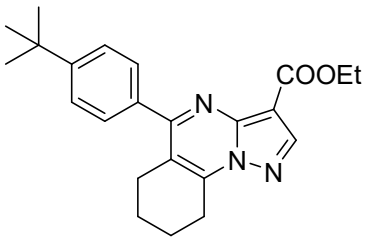
5. Characterization data for compounds



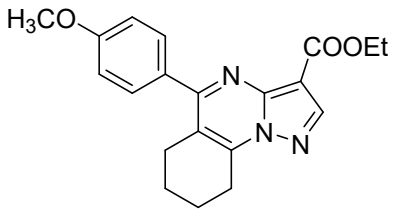
ethyl 5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4a):
Yield 98% (157.4 mg; petroleum ether/EtOAc = 15:1); light yellow solid; mp 131–133 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.53 (s, 1H), 7.69–7.64 (m, 2H), 7.48–7.43 (m, 3H), 4.39 (q, J = 7.2 Hz, 2H), 3.25 (t, J = 6.4 Hz, 2H), 2.79 (t, J = 5.6 Hz, 2H), 2.08–2.01 (m, 2H), 1.83–1.77 (m, 2H), 1.40 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 161.7, 146.6, 145.8, 145.6, 138.2, 129.2, 129.0, 128.0, 117.5, 102.6, 59.9, 26.7, 24.7, 22.2, 20.8, 14.4; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{19}H_{20}N_3O_2$: 322.1550; found: 322.1549.



ethyl 5-(p-tolyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4b):
Yield 99% (166 mg; petroleum ether/EtOAc = 8:1); yellow solid; mp 140–142 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.53 (s, 1H), 7.59 (d, J = 8.0 Hz, 2H), 7.29–7.26 (m, 2H), 4.40 (q, J = 7.2 Hz, 2H), 3.25 (t, J = 6.6 Hz, 2H), 2.81 (t, J = 5.8 Hz, 2H), 2.42 (s, 3H), 2.09–2.02 (m, 2H), 1.84–1.76 (m, 2H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.6, 161.5, 146.4, 145.7, 145.3, 139.1, 135.2, 128.9, 128.6, 117.4, 102.3, 59.7, 26.7, 24.6, 22.1, 21.1, 20.7, 14.3; HRMS (ESI): m/z [M + Na]$^+$ calcd for $C_{20}H_{21}N_3NaO_2$: 358.1526; found: 358.1527.

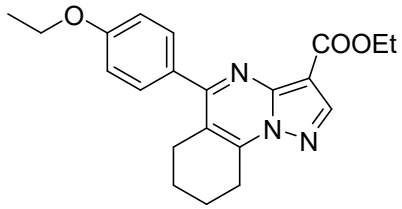


ethyl 5-(4-(*tert*-butyl)phenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4c):
Yield 98% (185 mg; petroleum ether/EtOAc = 10:1); yellow solid; mp 130–132 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.52 (s, 1H), 7.70–7.58 (m, 2H), 7.51–7.45 (m, 2H), 4.39 (q, J = 7.2 Hz, 2H), 3.24 (t, J = 6.6 Hz, 2H), 2.84 (t, J = 6.0 Hz, 2H), 2.08–2.00 (m, 2H), 1.83–1.75 (m, 2H), 1.41 (t, J = 7.2 Hz, 3H), 1.36 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 161.7, 152.4, 146.5, 145.8, 145.4, 135.3, 128.9, 125.0, 117.5, 102.5, 59.9, 34.6, 31.1, 26.8, 24.7, 22.3, 20.9, 14.4; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{23}H_{28}N_3O_2$: 378.2176; found: 378.2175.



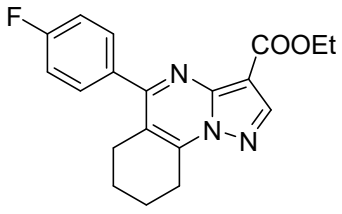
ethyl 5-(4-methoxyphenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4d):

Yield 99% (174 mg; petroleum ether/EtOAc = 8:1); yellow solid; mp 142–144 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm); 8.51 (s, 1H), 7.67 (d, J = 8.8 Hz, 2H), 6.97 (d, J = 8.8 Hz, 2H), 4.40 (q, J = 7.2 Hz, 2H), 3.86 (s, 3H), 3.23 (t, J = 6.6 Hz, 2H), 2.82 (t, J = 6.0 Hz, 2H), 2.08–2.00 (m, 2H), 1.84–1.75 (m, 2H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm); 162.8, 161.2, 160.5, 146.5, 145.8, 145.4, 130.8, 130.6, 117.4, 113.4, 102.3, 59.8, 55.2, 26.9, 24.8, 22.3, 20.8, 14.3. HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{20}H_{22}N_3O_3$: 352.1656; found: 352.1654.



ethyl 5-(4-ethoxyphenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4e):

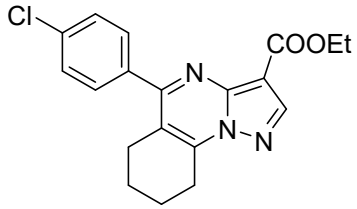
Yield 97% (177 mg; petroleum ether/EtOAc = 8:1); yellow solid; mp 131–133 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.51 (s, 1H), 7.69–7.64 (m, 2H), 6.98–6.93 (m, 2H), 4.39 (q, J = 7.2 Hz, 2H), 4.09 (q, J = 7.2 Hz, 2H), 3.22 (t, J = 6.4 Hz, 2H), 2.82 (t, J = 6.0 Hz, 2H), 2.07–2.00 (m, 2H), 1.82–1.75 (m, 2H), 1.47–1.39 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 161.1, 159.8, 146.4, 145.8, 145.3, 130.7, 130.4, 117.3, 113.8, 102.2, 63.3, 59.8, 26.9, 24.7, 22.3, 20.8, 14.6, 14.3; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{21}H_{24}N_3O_3$: 366.1812; found: 366.1809.



ethyl 5-(4-fluorophenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4f):

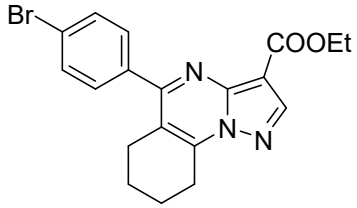
Yield 97% (164.6 mg; petroleum ether/EtOAc = 8:1); yellow solid; mp 163–165 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.53 (s, 1H), 7.71–7.66 (m, 2H), 7.18–7.12 (m, 2H), 4.39 (q, J = 7.2 Hz, 2H), 3.25 (t, J = 6.6 Hz, 2H), 2.78 (t, J = 5.8 Hz, 2H), 2.09–2.01 (m, 2H), 1.85–1.78 (m, 2H), 1.40 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 163.3 (d, C-F, $^1J_{C\text{-}F}$ = 248.1 Hz), 162.6, 160.5, 146.6, 145.7, 134.2 (d, C-F, $^4J_{C\text{-}F}$ = 3.3 Hz), 131.1 (d, C-F, $^3J_{C\text{-}F}$ = 8.5

Hz), 117.3, 115.1 (d, C-F, $^{2}J_{C\text{-}F}$ = 21.7 Hz), 102.5, 59.9, 26.7, 24.7, 22.2, 20.7, 14.3; HRMS (ESI): m/z [M + H]$^{+}$ calcd for $C_{19}H_{19}FN_3O_2$: 340.1456; found: 340.1457.



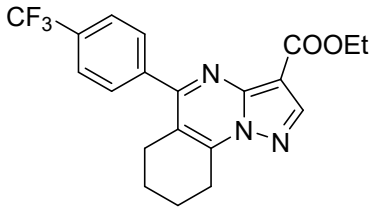
ethyl 5-(4-chlorophenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4g):

Yield 97% (172.6 mg; petroleum ether/EtOAc = 8:1); light yellow solid; mp 160–162 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.53 (s, 1H), 7.65–7.60 (m, 2H), 7.45–7.41 (m, 2H), 4.39 (q, J = 7.2 Hz, 2H), 3.24 (t, J = 6.6 Hz, 2H), 2.77 (t, J = 5.8 Hz, 2H), 2.08–2.01 (m, 2H), 1.85–1.78 (m, 2H), 1.40 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.5, 160.3, 146.6, 145.8, 145.7, 136.5, 135.3, 130.4, 128.2, 117.2, 102.6, 59.9, 26.6, 24.7, 22.1, 20.7, 14.3; HRMS (ESI): m/z [M + H]$^{+}$ calcd for $C_{19}H_{19}ClN_3O_2$: 356.1160; found: 356.1164.



ethyl 5-(4-bromophenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4h):

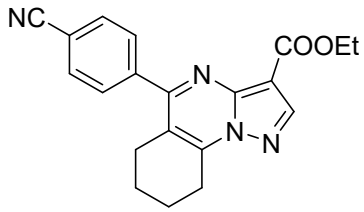
Yield 97% (194 mg; petroleum ether/EtOAc = 8:1); yellow solid; mp 171–173 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.52 (s, 1H), 7.60–7.53 (m, 4H), 4.38 (q, J = 7.2 Hz, 2H), 3.23 (t, J = 6.4 Hz, 2H), 2.76 (t, J = 5.8 Hz, 2H), 2.08–2.01 (m, 2H), 1.83–1.77 (m, 2H), 1.40 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.5, 160.3, 146.6, 145.8, 145.6, 136.9, 131.1, 130.7, 123.6, 117.2, 102.5, 59.9, 26.5, 24.7, 22.1, 20.7, 14.3; HRMS (ESI): m/z [M + H]$^{+}$ calcd for $C_{19}H_{19}BrN_3O_2$: 400.0655; found: 400.0658.



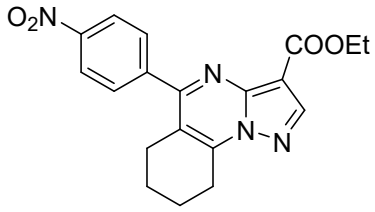
ethyl 5-(4-(trifluoromethyl)phenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4i):

Yield 98% (190.7 mg; petroleum ether/EtOAc = 8:1); light yellow solid; mp 172–174 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.55 (d, J = 0.4 Hz, 1H), 7.80 (d, J = 8.0 Hz, 2H), 7.73 (d, J = 8.0 Hz, 2H), 4.39 (q, J = 7.2 Hz, 2H), 3.26 (t, J = 6.4 Hz, 2H), 2.76 (t, J = 5.8 Hz, 2H),

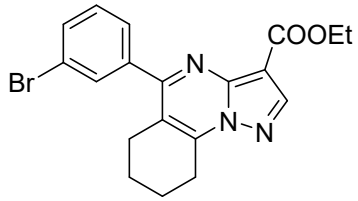
2.11–2.03 (m, 2H), 1.86–1.79 (m, 2H), 1.40 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.5, 160.1, 146.7, 146.1, 145.7, 141.6 (q, C-F, $^{4}J_{C\text{-}F}$ = 1.1 Hz), 131.0 (q, C-F, $^{2}J_{C\text{-}F}$ = 32.6 Hz), 129.4, 125.0 (q, C-F, $^{3}J_{C\text{-}F}$ = 3.6 Hz), 123.8 (q, C-F, $^{1}J_{C\text{-}F}$ = 270.6 Hz), 117.2, 102.8, 60.0, 26.4, 24.7, 22.1, 20.7, 14.3; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{20}H_{19}F_3N_3O_2$: 390.1424; found: 390.1419.



ethyl 5-(4-cyanophenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4j): Yield 97% (168 mg; petroleum ether/EtOAc = 5:1); light yellow solid; mp 218–220 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.56 (s, 1H), 7.82–7.76 (m, 4H), 4.39 (q, J = 7.2 Hz, 2H), 3.29 (t, J = 6.4 Hz, 2H), 2.76 (t, J = 6.0 Hz, 2H), 2.12–2.05 (m, 2H), 1.88–1.82 (m, 2H), 1.40 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.4, 159.4, 146.8, 146.3, 145.7, 142.5, 131.9, 129.8, 118.3, 117.1, 112.8, 103.0, 60.1, 26.4, 24.8, 22.1, 20.7, 14.3; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{20}H_{18}N_4NaO_2$: 369.1322; found: 369.1319.

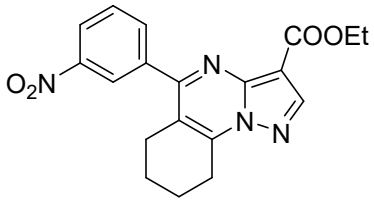


ethyl 5-(4-nitrophenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4k): Yield 96% (175.8 mg; petroleum ether/EtOAc = 8:1); light yellow solid; mp 160–162 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.56 (s, 1H), 8.33 (d, J = 8.4 Hz, 2H), 7.90–7.84 (m, 2H), 4.40 (q, J = 7.2 Hz, 2H), 3.30 (t, J = 6.4 Hz, 2H), 2.77 (t, J = 5.8 Hz, 2H), 2.13–2.05 (m, 2H), 1.90–1.83 (m, 2H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.4, 159.1, 148.0, 146.9, 146.4, 145.7, 144.3, 130.2, 123.3, 117.1, 103.1, 60.1, 26.4, 24.8, 22.1, 20.7, 14.3; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{19}H_{18}N_4NaO_4$: 389.1220; found: 389.1221.

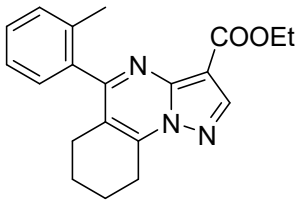


ethyl 5-(3-bromophenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4l): Yield 97% (194 mg; petroleum ether/EtOAc = 8:1); white solid; mp 168–170 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.54 (s, 1H), 7.82 (t, J = 1.6 Hz, 1H), 7.58 (dd, J = 8.0, 1.6 Hz, 2H), 7.33 (t, J = 8.0 Hz, 1H), 4.40 (q, J = 7.2 Hz, 2H), 3.26 (t, J = 6.4 Hz, 2H), 2.76 (t, J = 5.8

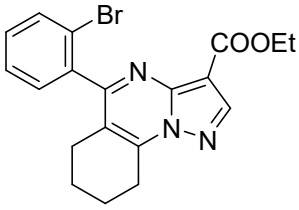
Hz, 2H), 2.09–2.02 (m, 2H), 1.86–1.79 (m, 2H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.5, 160.0, 146.7, 145.9, 145.7, 140.1, 132.1, 131.9, 129.6, 127.6, 122.2, 117.3, 102.8, 60.0, 26.5, 24.8, 22.1, 20.7, 14.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{19}H_{19}BrN_3O_2$: 400.0655; found: 400.0653.



ethyl 5-(3-nitrophenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4m): Yield 68% (126.6 mg; petroleum ether/EtOAc = 5:1); white solid; mp 190–192^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.56 (s, 1H), 8.55 (t, J = 2.0 Hz, 1H), 8.35–8.28 (m, 1H), 8.09–8.04 (m, 1H), 7.69 (t, J = 8.0 Hz, 1H), 4.40 (q, J = 7.2 Hz, 2H), 3.29 (t, J = 6.6 Hz, 2H), 2.81 (t, J = 6.0 Hz, 2H), 2.13–2.06 (m, 2H), 1.89–1.83 (m, 2H), 1.42 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.4, 158.7, 147.8, 146.8, 146.5, 145.6, 139.7, 135.2, 129.3, 124.0, 123.9, 117.1, 102.9, 60.0, 26.4, 24.8, 22.1, 20.6, 14.3; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{19}H_{18}N_4NaO_4$: 389.1220; found:389.1222.



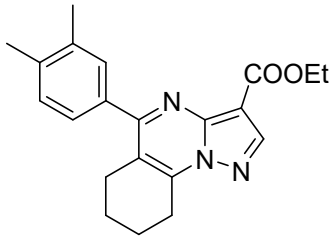
ethyl 5-(*o*-tolyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4n): Yield 91% (152.6 mg; petroleum ether/EtOAc = 10:1); light yellow solid; mp 139–141 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.54 (s, 1H), 7.34–7.30 (m, 1H), 7.28 (d, J = 6.4 Hz, 1H), 7.26–7.21 (m, 2H), 4.37 (q, J = 7.2 Hz, 2H), 3.26 (t, J = 6.4 Hz, 2H), 2.46 (s, 2H), 2.20 (s, 3H), 2.04–1.97 (m, 2H), 1.80 (d, J = 5.2 Hz, 2H), 1.37 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 162.9, 162.5, 146.4, 145.8, 145.3, 137.6, 135.3, 130.2, 128.5, 128.1, 125.3, 118.1, 102.5, 59.7, 25.2, 24.4, 21.8, 20.7, 19.5, 14.3; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{20}H_{22}N_3O_2$: 336.1707; found: 336.1709.



ethyl 5-(2-bromophenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4o):

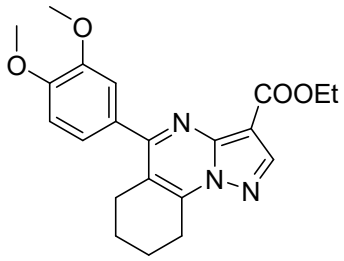
Yield 89% (178 mg; petroleum ether/EtOAc = 8:1); light yellow solid; mp 194–196 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.55 (s, 1H), 7.64 (d, J = 8.0 Hz, 1H), 7.45–7.40 (m, 1H), 7.38–7.35 (m, 1H), 7.33–7.28 (m, 1H), 4.37 (q, J = 7.2 Hz, 2H), 3.34–3.18 (m, 2H), 2.73–

2.63 (m, 1H), 2.39–2.30 (m, 1H), 2.06–1.98 (m, 2H), 1.90–1.75 (m, 2H), 1.37 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.4, 161.6, 146.5, 145.8, 145.4, 139.3, 132.4, 130.1, 130.0, 127.4, 121.7, 118.3, 102.9, 59.9, 24.8, 24.5, 21.7, 20.7, 14.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{19}H_{19}BrN_3O_2$: 400.0655; found: 400.0656.



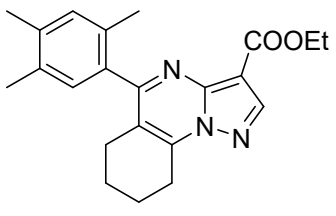
ethyl 5-(3,4-dimethylphenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4p):

Yield 95% (166 mg; petroleum ether/EtOAc = 8:1); light yellow solid; mp 145–147 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.52 (s, 1H), 7.48 (s, 1H), 7.37 (dd, J = 8.0, 1.6 Hz, 1H), 7.19 (d, J = 7.6 Hz, 1H), 4.39 (q, J = 7.2 Hz, 2H), 3.22 (t, J = 6.4 Hz, 2H), 2.79 (t, J = 5.8 Hz, 2H), 2.32 (s, 3H), 2.31 (s, 3H), 2.06–1.98 (m, 2H), 1.81–1.74 (m, 2H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.6, 161.8, 146.3, 145.7, 145.2, 137.8, 136.3, 135.6, 130.1, 128.9, 126.3, 117.4, 102.3, 59.7, 26.7, 24.6, 22.1, 20.7, 19.6, 19.4, 14.3; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{21}H_{23}N_3NaO_2$: 372.1682; found: 372.1681.



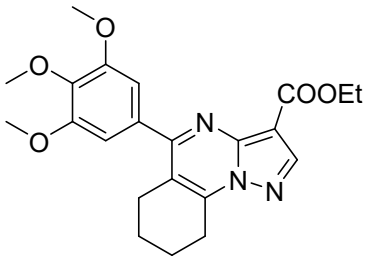
ethyl 5-(3,4-dimethoxyphenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4q):

Yield 95% (181.2 mg; petroleum ether/EtOAc = 5:1); white solid; mp 124–126 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.53 (s, 1H), 7.33 (d, J = 2.0 Hz, 1H), 7.26 (dd, J = 8.4, 2.0 Hz, 1H), 6.94 (d, J = 8.4 Hz, 1H), 4.40 (q, J = 7.2 Hz, 2H), 3.96 (s, 3H), 3.95 (s, 3H), 3.25 (t, J = 6.6 Hz, 2H), 2.85 (t, J = 6.0 Hz, 2H), 2.10–2.04 (m, 2H), 1.85–1.78 (m, 2H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 161.1, 149.9, 148.5, 146.5, 145.6, 145.4, 130.7, 122.1, 117.3, 112.4, 110.1, 102.2, 59.8, 55.8, 55.7, 26.9, 24.7, 22.3, 20.7, 14.3; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{21}H_{23}N_3NaO_4$: 404.1581; found: 404.1577.



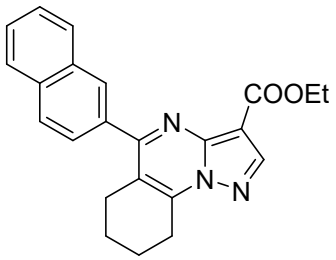
ethyl 5-(2,4,5-trimethylphenyl)-6,7,8,9-tetrahydropyrazolo[1,5-a]quinazoline-3-carboxylate (4r):

Yield 86% (156.3 mg; petroleum ether/EtOAc = 5:1); white solid; mp 207–209 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.53 (s, 1H), 7.05 (s, 1H), 7.00 (s, 1H), 4.37 (q, J = 7.2 Hz, 2H), 3.25 (t, J = 6.6 Hz, 2H), 2.48 (s, 2H), 2.28 (s, 3H), 2.24 (s, 3H), 2.12 (s, 3H), 2.04–1.98 (m, 2H), 1.83–1.76 (m, 2H), 1.37 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 163.4, 162.6, 146.4, 145.8, 145.1, 136.9, 135.2, 133.5, 132.4, 131.5, 129.2, 118.3, 102.5, 59.8, 25.3, 24.5, 21.9, 20.8, 19.4, 19.0, 18.9, 14.3; HRMS (ESI): m/z [M + Na]$^+$ calcd for $C_{22}H_{25}N_3NaO_2$: 386.1839; found: 386.1838.



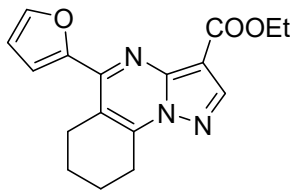
ethyl 5-(3,4,5-trimethoxyphenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4s):

Yield 94% (193.4 mg; petroleum ether/EtOAc = 5:1); white solid; mp 206–208 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.54 (s, 1H), 6.90 (s, 2H), 4.40 (q, J = 7.2 Hz, 2H), 3.91(4) (s, 6H), 3.91 (s, 3H), 3.26 (t, J = 6.4 Hz, 2H), 2.82 (t, J = 5.8 Hz, 2H), 2.10–2.04 (m, 2H), 1.87–1.80 (m, 2H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.8, 161.5, 152.9, 146.7, 145.8, 145.7, 139.1, 133.7, 117.4, 106.5, 102.6, 60.9, 60.0, 56.2, 26.9, 24.8, 22.4, 20.8, 14.4; HRMS (ESI): m/z [M + Na]$^+$ calcd for $C_{22}H_{25}N_3NaO_5$: 434.1686; found: 434.1684.

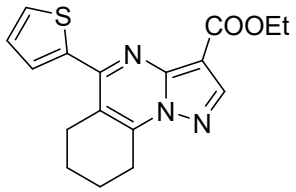


ethyl 5-(naphthalen-2-yl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4t):

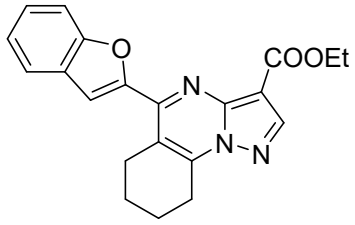
Yield 96% (178.3 mg; petroleum ether/EtOAc = 8:1); yellow solid; mp 133–135 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.56 (s, 1H), 8.13 (s, 1H), 7.89–7.82 (m, 3H), 7.76 (dd, J = 8.8, 1.6 Hz, 1H), 7.52–7.46 (m, 2H), 4.40 (q, J = 7.2 Hz, 2H), 3.22 (t, J = 6.4 Hz, 2H), 2.79 (t, J = 5.8 Hz, 2H), 2.05–1.97 (m, 2H), 1.78–1.71 (m, 2H), 1.40 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 161.5, 146.6, 145.8, 145.5, 135.5, 133.2, 132.6, 128.9, 128.3, 127.6, 127.5, 126.8, 126.24, 126.20, 117.6, 102.5, 59.9, 26.7, 24.7, 22.1, 20.7, 14.3; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{23}H_{22}N_3O_2$: 372.1707; found: 372.1710.



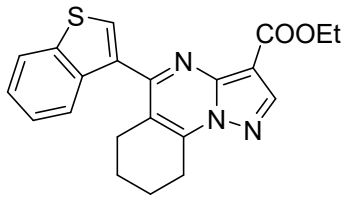
ethyl 5-(furan-2-yl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4u):
Yield 98% (152.6 mg; petroleum ether/EtOAc = 8:1); yellow solid; mp 171–173 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.51 (s, 1H), 7.67 (d, J = 0.8 Hz, 1H), 7.35 (d, J = 3.2 Hz, 1H), 6.60 (dd, J = 3.6, 1.6 Hz, 1H), 4.43 (q, J = 7.2 Hz, 2H), 3.23 (t, J = 6.4 Hz, 2H), 3.11 (t, J = 5.8 Hz, 2H), 2.06–2.00 (m, 2H), 1.96–1.89 (m, 2H), 1.45 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.9, 152.5, 149.7, 147.0, 146.0, 145.5, 145.0, 116.0, 115.4, 112.1, 60.1, 25.4, 25.0, 22.1, 20.4, 14.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{17}H_{18}N_3O_3$: 312.1343; found: 312.1345.



ethyl 5-(thiophen-2-yl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4v):
Yield 97% (158.8 mg; petroleum ether/EtOAc = 8:1); yellow solid; mp 198–200 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.51 (s, 1H), 7.66 (d, J = 4.0 Hz, 1H), 7.56 (dd, J = 4.8, 0.4 Hz, 1H), 7.17–7.12 (m, 1H), 4.43 (q, J = 7.2 Hz, 2H), 3.23 (t, J = 6.2 Hz, 2H), 3.05 (t, J = 6.0 Hz, 2H), 2.09–2.01 (m, 2H), 1.96–1.89 (m, 2H), 1.48 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 163.0, 153.8, 147.0, 145.8, 145.2, 143.2, 130.6, 129.8, 127.9, 116.0, 102.3, 60.1, 26.6, 25.0, 22.2, 20.5, 14.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{17}H_{18}N_3O_2S$: 328.1114; found: 328.1113.

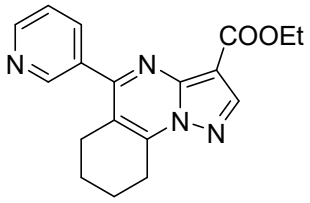


ethyl 5-(benzofuran-2-yl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4w):
Yield 92% (166 mg; petroleum ether/EtOAc = 8:1); yellow solid; mp 170–172 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.52 (s, 1H), 7.66–7.62 (m, 2H), 7.54 (d, J = 8.4 Hz, 1H), 7.39–7.34 (m, 1H), 7.29–7.24 (m, 1H), 4.45 (q, J = 7.2 Hz, 2H), 3.19 (t, J = 7.8, 4H), 2.06–1.99 (m, 2H), 1.96–1.89 (m, 2H), 1.48 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 155.4, 153.7, 149.7, 147.0, 146.2, 145.4, 127.7, 126.1, 123.3, 121.9, 116.8, 111.7, 111.2, 102.5, 60.1, 25.4, 25.0, 22.0, 20.3, 14.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{21}H_{20}N_3O_3$: 362.1499; found: 362.1502.



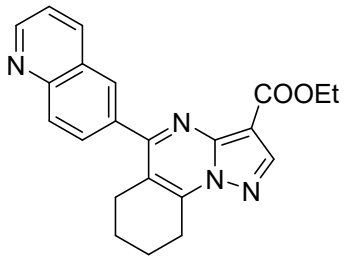
ethyl 5-(benzo[*b*]thiophen-3-yl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4x):

Yield 92% (173.6 mg; petroleum ether/EtOAc = 8:1); yellow solid; mp 192–197 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.59 (s, 1H), 8.20 (dd, J = 6.4, 2.0 Hz, 1H), 7.90 (dd, J = 7.2, 2.8 Hz, 1H), 7.75 (s, 1H), 7.45–7.37 (m, 2H), 4.40 (q, J = 7.2 Hz, 2H), 3.28 (t, J = 6.6 Hz, 2H), 2.81 (t, J = 6.0 Hz, 2H), 2.08–2.01 (m, 2H), 1.83–1.76 (m, 2H), 1.40 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.9, 156.6, 146.9, 145.9, 145.5, 139.8, 137.9, 133.3, 128.8, 124.8, 124.7, 124.2, 122.3, 118.2, 102.9, 60.0, 26.3, 24.8, 22.2, 20.8, 14.4; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{21}H_{19}N_3NaO_2S$: 400.1090; found: 400.1092.



ethyl 5-(pyridin-3-yl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4y):

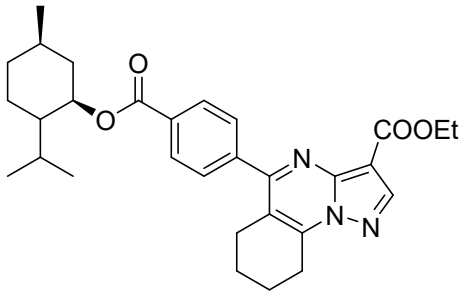
Yield 97% (156.3 mg; petroleum ether/EtOAc = 2:1); yellow solid; mp 174–176 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.92 (d, J = 2.0 Hz, 1H), 8.71 (dd, J = 4.8, 1.6 Hz, 1H), 8.56 (s, 1H), 8.05 (dt, J = 8.0, 2.0 Hz, 1H), 7.45 (dd, J = 8.0, 4.8 Hz, 1H), 4.40 (q, J = 7.2 Hz, 2H), 3.29 (t, J = 6.6 Hz, 2H), 2.82 (t, J = 6.0 Hz, 2H), 2.12–2.05 (m, 2H), 1.89–1.82 (m, 2H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 158.7, 150.2, 149.7, 146.9, 146.3, 145.9, 136.7, 134.2, 123.2, 117.4, 103.0, 60.2, 26.6, 24.9, 22.3, 20.8, 14.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{18}H_{19}N_4O_2$: 323.1503; found: 323.1505.



ethyl 5-(quinolin-6-yl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4z):

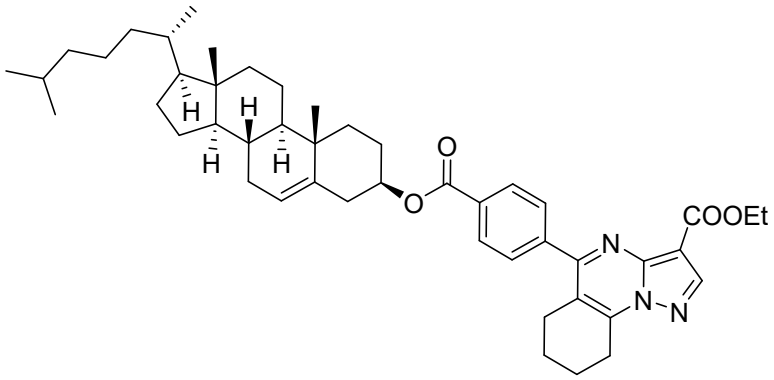
Yield 96% (178.8 mg; petroleum ether/EtOAc = 2:1); yellow solid; mp 152–154 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.95 (dd, J = 4.0, 1.6 Hz, 1H), 8.56 (s, 1H), 8.22 (dd, J = 8.4, 1.2 Hz, 1H), 8.19–8.15 (m, 2H), 8.00 (dd, J = 8.8, 2.0 Hz, 1H), 7.45 (q, J = 4.0 Hz, 1H), 4.40 (q, J = 7.2 Hz, 2H), 3.26 (t, J = 6.4 Hz, 2H), 2.82 (t, J = 5.8 Hz, 2H), 2.09–2.03 (m, 2H), 1.84–1.77 (m, 2H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.5, 160.7, 151.1, 147.9, 146.6, 145.8, 145.7, 136.5, 136.3, 129.8, 128.9, 128.8, 127.5, 121.5, 117.5,

102.6, 59.9, 26.6, 24.7, 22.1, 20.7, 14.3; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{22}H_{21}N_4O_2$: 373.1659; found: 373.1657.



ethyl 5-(4-((((1*R*,5*R*)-2-isopropyl-5-methylcyclohexyl)oxy)carbonyl)phenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4aa):

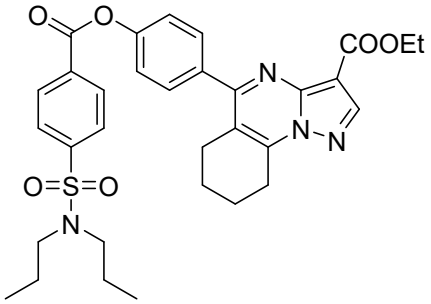
Yield 94% (236.7 mg; petroleum ether/EtOAc = 8:1); light yellow solid; mp 113–115 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.59–8.52 (m, 1H), 8.15 (d, J = 8.0 Hz, 2H), 7.74 (d, J = 8.0 Hz, 2H), 4.98 (td, J = 10.8, 4.4 Hz, 1H), 4.39 (q, J = 7.2 Hz, 2H), 3.27 (t, J = 6.0 Hz, 2H), 2.77 (t, J = 5.2 Hz, 2H), 2.17 (d, J = 11.6 Hz, 1H), 2.10–2.03 (m, 2H), 2.01–1.95 (m, 1H), 1.86–1.79 (m, 2H), 1.75 (d, J = 11.6 Hz, 2H), 1.59 (t, J =11.2 Hz, 2H), 1.40 (t, J = 7.2 Hz, 3H), 1.15 (q, J = 11.6 Hz, 2H), 0.95 (dd, J = 6.4, 3.2 Hz, 7H), 0.82 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 165.4, 162.6, 160.6, 146.7, 145.9, 145.7, 142.3, 131.2, 129.2, 129.0, 117.3, 102.8, 75.0, 60.0, 47.1, 40.8, 34.1, 31.3, 26.5, 26.4, 24.7, 23.5, 22.1, 21.9, 20.7, 20.6, 16.4, 14.3; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{30}H_{38}N_3O_4$: 504.2857; found: 504.2856.



ethyl 5-(4-((((3*R*,8*R*,9*R*,10*S*,13*S*,14*R*,17*S*)-10,13-dimethyl-17-((*S*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)carbonyl)phenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4ab):

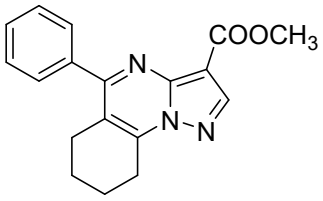
Yield 94% (345 mg; petroleum ether/EtOAc = 5:1); light yellow solid; mp 231–233 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.54 (s, 1H), 8.13 (d, J = 8.0 Hz, 2H), 7.73 (d, J = 8.0 Hz, 2H), 5.44 (d, J = 3.6 Hz, 1H), 4.95–4.83 (m, 1H), 4.39 (q, J = 7.2 Hz, 2H), 3.26 (t, J = 6.2 Hz, 2H), 2.75 (t, J = 5.4 Hz, 2H), 2.50 (d, J = 8.0 Hz, 2H), 2.08–2.01 (m, 4H), 2.00–1.90 (m, 2H), 1.87–1.72 (m, 4H), 1.62–1.45 (m, 6H), 1.42–1.34 (m, 6H), 1.27–1.12 (m, 6H), 1.10–0.95 (m, 8H), 0.93 (d, J = 6.4 Hz, 3H), 0.88 (d, J = 1.6 Hz, 3H), 0.86 (d, J = 1.6 Hz, 3H), 0.69 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 165.3, 162.6, 160.6, 146.8, 145.9, 145.7, 142.3, 139.4,

131.3, 129.3, 129.0, 122.7, 117.3, 102.9, 74.8, 60.0, 56.6, 56.0, 49.9, 42.2, 39.6, 39.4, 38.1, 36.9, 36.5, 36.1, 35.7, 31.8, 31.7, 28.1, 27.9, 27.8, 26.6, 24.8, 24.2, 23.7, 22.7, 22.5, 22.2, 20.9, 20.8, 19.3, 18.6, 14.4, 11.7; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{47}H_{64}N_3O_4$: 734.4891; found: 734.4897.



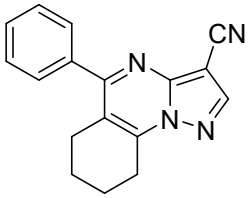
ethyl 5-(4-((4-(*N*,*N*-dipropylsulfamoyl)benzoyl)oxy)phenyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4ac):

Yield 90% (272 mg; petroleum ether/EtOAc = 5:1); light yellow solid; mp 130–132 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.54 (s, 1H), 8.35 (d, J = 8.4 Hz, 2H), 7.97 (d, J = 8.4 Hz, 2H), 7.80 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 8.4 Hz, 2H), 4.40 (q, J = 7.2 Hz, 2H), 3.27 (t, J = 6.4 Hz, 2H), 3.18–3.11 (m, 4H), 2.85 (t, J = 5.6 Hz, 2H), 2.12–2.03 (m, 2H), 1.89–1.79 (m, 2H), 1.63–1.53 (m, 4H), 1.41 (t, J = 7.2 Hz, 3H), 0.90 (t, J = 7.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 163.4, 162.5, 160.4, 151.3, 146.5, 145.8, 145.7, 144.8, 136.1, 132.4, 130.6, 130.5, 127.0, 121.2, 117.3, 102.5, 59.9, 49.7, 26.7, 24.7, 22.1, 21.7, 20.7, 14.3, 11.0; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{32}H_{36}N_4NaO_6S$: 627.2248; found: 627.2241.



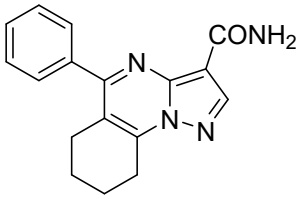
methyl 5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4ad):

Yield 98% (150.6 mg; petroleum ether/EtOAc = 8:1); brown solid; mp 161–163 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.55 (s, 1H), 7.68–7.63 (m, 2H), 7.48–7.43 (m, 3H), 3.91 (s, 3H), 3.25 (t, J = 6.4 Hz, 2H), 2.78 (t, J = 6.0 Hz, 2H), 2.08–2.01 (m, 2H), 1.83–1.77 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 163.2, 161.8, 146.8, 145.7, 145.6, 138.1, 129.2, 129.0, 128.1, 117.5, 102.3, 51.3, 26.6, 24.7, 22.2, 20.8; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{18}H_{18}N_3O_2$: 308.1394; found: 308.1392.

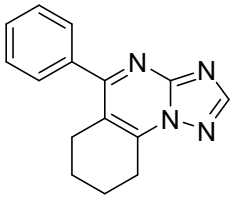


5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carbonitrile (4ae):

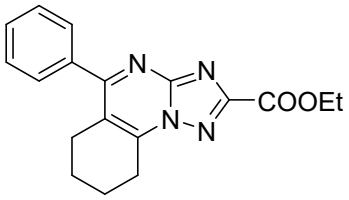
Yield 98% (134.4 mg; petroleum ether/EtOAc = 10:1); white solid; mp 230–232 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.34 (s, 1H), 7.65–7.59 (m, 2H), 7.52–7.46 (m, 3H), 3.26 (t, J = 6.6 Hz, 2H), 2.79 (t, J = 6.0 Hz, 2H), 2.10–2.03 (m, 2H), 1.86–1.79 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.4, 148.1, 146.7, 146.3, 137.5, 129.7, 128.9, 128.4, 118.7, 113.4, 82.4, 26.7, 24.8, 22.2, 20.8; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{17}H_{14}N_4Na$: 297.1111; found: 297.1108.



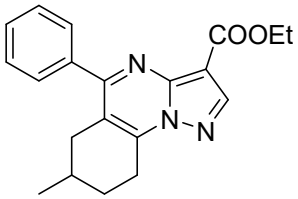
5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxamide (4af):
Yield 90% (131.5 mg; petroleum ether/EtOAc = 2:1); white solid; mp 278–280 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.65 (s, 1H), 7.98 (s, 1H), 7.63–7.58 (m, 2H), 7.55–7.49 (m, 3H), 5.62 (s, 1H), 3.29 (t, J = 6.6 Hz, 2H), 2.78 (t, J = 6.2 Hz, 2H), 2.11–2.04 (m, 2H), 1.87–1.80 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 164.3, 160.8, 146.3, 146.0, 144.6, 138.1, 129.5, 128.7, 128.4, 117.1, 26.7, 24.9, 22.4, 20.9; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{17}H_{16}N_4NaO$: 315.1216; found: 315.1214.



5-phenyl-6,7,8,9-tetrahydro-[1,2,4]triazolo[1,5-*a*]quinazoline (4ag):
Yield 98% (122.6 mg; petroleum ether/EtOAc = 5:1); yellow solid; mp 143–145 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.47 (s, 1H), 7.65–7.60 (m, 2H), 7.52–7.46 (m, 3H), 3.27 (t, J = 6.6 Hz, 2H), 2.80 (t, J = 6.0 Hz, 2H), 2.10–2.03 (m, 2H), 1.86–1.79 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 164.2, 155.5, 153.5, 146.1, 137.8, 129.5, 128.8, 128.3, 118.2, 26.6, 24.9, 22.3, 20.7; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{15}H_{15}N_4$: 251.1291; found: 251.1296.

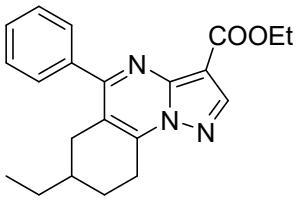


ethyl 5-phenyl-6,7,8,9-tetrahydro-[1,2,4]triazolo[1,5-*a*]quinazoline-2-carboxylate (4ah):
Yield 98% (158 mg; petroleum ether/EtOAc = 3:1); white solid; mp 186–188 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.67–7.61 (m, 2H), 7.51–7.46 (m, 3H), 4.56 (qd, J = 7.2, 0.8 Hz, 2H), 3.34 (t, J = 6.2 Hz, 2H), 2.83 (t, J = 5.8 Hz, 2H), 2.11–2.04 (m, 2H), 1.87–1.80 (m, 2H), 1.49 (td, J = 7.2, 0.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 165.5, 160.4, 156.9, 153.5, 146.6, 137.4, 129.7, 128.8, 128.2, 119.9, 62.3, 26.8, 24.9, 22.1, 20.5, 14.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{18}H_{19}N_4O_2$: 323.1503; found: 323.1505.



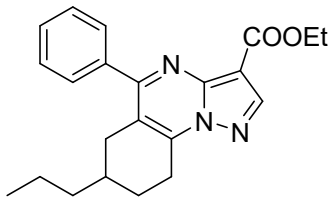
ethyl 7-methyl-5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4ai):

Yield 98% (164.3 mg; petroleum ether/EtOAc = 10:1); white solid; mp 116–118 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.54 (s, 1H), 7.70–7.64 (m, 2H), 7.51–7.45 (m, 3H), 4.48–4.32 (m, 2H), 3.46 (dd, J = 19.6, 5.2 Hz, 1H), 3.19–3.08 (m, 1H), 2.77 (dd, J = 16.4, 4.0 Hz, 1H), 2.50 (dd, J = 16.4, 10.4 Hz, 1H), 2.18–2.10 (m, 1H), 1.86–1.76 (m, 1H), 1.69–1.58 (m, 1H), 1.40 (t, J = 7.0 Hz, 3H), 1.09 (d, J = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 161.7, 146.7, 145.9, 145.4, 138.2, 129.3, 129.1, 128.1, 117.1, 102.6, 60.0, 34.9, 28.9, 28.8, 24.9, 21.2, 14.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{20}H_{22}N_3O_2$: 336.1707; found: 336.1706.



ethyl 7-ethyl-5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4aj):

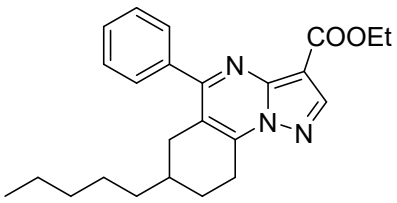
Yield 98% (171 mg; petroleum ether/EtOAc = 8:1); white solid; mp 115–117 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.53 (s, 1H), 7.71–7.65 (m, 2H), 7.51–7.44 (m, 3H), 4.47–4.31 (m, 2H), 3.52–3.41 (m, 1H), 3.19–3.06 (m, 1H), 2.81 (dd, J = 16.0, 3.2 Hz, 1H), 2.51 (dd, J = 16.4, 9.2 Hz, 1H), 2.26–2.16 (m, 1H), 1.67–1.55 (m, 2H), 1.47–1.37 (m, 5H), 0.93 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 161.8, 146.7, 145.9, 145.6, 138.2, 129.3, 129.1, 128.1, 117.1, 102.6, 60.0, 35.4, 32.9, 28.2, 26.4, 24.9, 14.4, 11.3; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{21}H_{24}N_3O_2$: 350.1863; found: 350.1865.



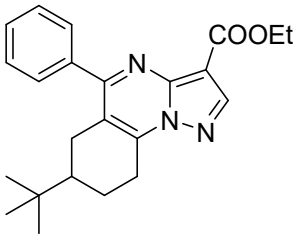
ethyl 5-phenyl-7-propyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4ak):

Yield 98% (178 mg; petroleum ether/EtOAc = 10:1); white solid; mp 135–137 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.53 (s, 1H), 7.71–7.65 (m, 2H), 7.50–7.43 (m, 3H), 4.47–4.32 (m, 2H), 3.49–3.39 (m, 1H), 3.17–3.05 (m, 1H), 2.84–2.75 (m, 1H), 2.50 (dd, J = 16.0, 9.6 Hz, 1H), 2.22–2.14 (m, 1H), 1.71–1.54 (m, 2H), 1.40 (t, J = 7.0 Hz, 3H), 1.38–1.27 (m, 4H), 0.92–0.85 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.6, 161.6, 146.5, 145.8, 145.5,

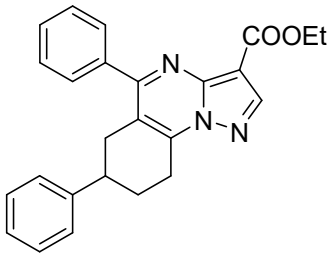
138.1, 129.1, 129.0, 128.0, 117.0, 102.5, 59.8, 37.6, 33.3, 33.1, 26.6, 24.7, 19.8, 14.3, 14.0; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{22}H_{26}N_3O_2$: 364.2020; found: 364.2023.



ethyl 7-pentyl-5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4al):
Yield 98% (191.8 mg; petroleum ether/EtOAc = 8:1); white solid; mp 100–102 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.53 (s, 1H), 7.71–7.65 (m, 2H), 7.51–7.44 (m, 3H), 4.47–4.32 (m, 2H), 3.51–3.40 (m, 1H), 3.19–3.06 (m, 1H), 2.85–2.75 (m, 1H), 2.51 (dd, J = 16.4, 9.2 Hz, 1H), 2.25–2.14 (m, 1H), 1.70–1.55 (m, 2H), 1.43–1.33 (m, 6H), 1.31–1.20 (m, 5H), 0.86 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 161.7, 146.7, 145.9, 145.6, 138.2, 129.2, 129.1, 128.1, 117.1, 102.6, 59.9, 35.4, 33.7, 33.3, 31.8, 26.7, 26.4, 24.8, 22.4, 14.4, 13.9; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{24}H_{29}N_3NaO_2$: 414.2152; found: 414.2155.

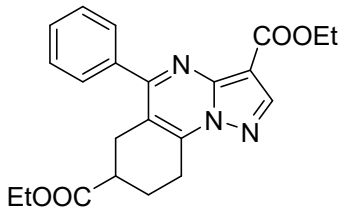


ethyl 7-(*tert*-butyl)-5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4am):
Yield 97% (183 mg; petroleum ether/EtOAc = 8:1); white solid; mp 159–161 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.53 (s, 1H), 7.72–7.67 (m, 2H), 7.51–7.45 (m, 3H), 4.48–4.31 (m, 2H), 3.56 (dd, J = 19.2, 5.2 Hz, 1H), 3.11–3.00 (m, 1H), 2.76 (d, J = 15.2 Hz, 1H), 2.66–2.56 (m, 1H), 2.30–2.23 (m, 1H), 1.57 (qd, J = 12.5, 5.6 Hz, 1H), 1.40 (t, J = 7.0 Hz, 4H), 0.93 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 161.9, 146.6, 145.8, 145.5, 138.2, 129.3, 129.0, 128.1, 117.6, 59.9, 44.1, 32.2, 28.2, 27.1, 26.0, 22.2, 14.4; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{23}H_{27}N_3NaO_2$: 400.1995; found: 400.1997.

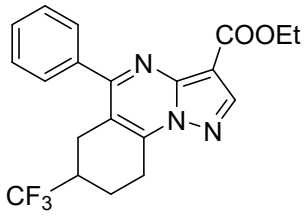


ethyl 5,7-diphenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4an):
Yield 98% (194.7 mg; petroleum ether/EtOAc = 8:1); light yellow solid; mp 180–182 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.55 (s, 1H), 7.68–7.62 (m, 2H), 7.42–7.36 (m, 3H), 7.32–7.27 (m, 2H), 7.23–7.18 (m, 3H), 4.46–4.30 (m, 2H), 3.55 (dd, J = 19.6, 5.2 Hz, 1H), 3.29–

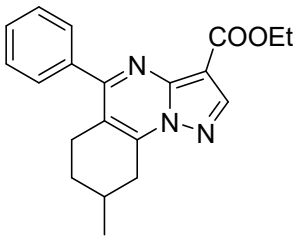
3.17 (m, 1H), 3.02–2.92 (m, 2H), 2.91–2.84 (m, 1H), 2.38–2.30 (m, 1H), 2.16 (qd, *J* = 12.0, 6.0 Hz, 1H), 1.39 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.5, 161.4, 146.6, 145.8, 145.0, 144.2, 137.9, 129.1, 128.9, 128.4, 128.0, 126.6, 116.9, 102.6, 59.8, 39.8, 34.5, 27.5, 25.4, 14.3; HRMS (ESI): m/z [M + H]$^+$ calcd for $C_{25}H_{24}N_3O_2$: 398.1863; found: 398.1861.



diethyl 5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3,7-dicarboxylate (4ao):
Yield 98% (192.8 mg; petroleum ether/EtOAc = 5:1); yellow solid; mp 158–160 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.54 (s, 1H), 7.70–7.65 (m, 2H), 7.51–7.45 (m, 3H), 4.47–4.33 (m, 2H), 4.21–4.09 (m, 2H), 3.55–3.46 (m, 1H), 3.28–3.09 (m, 2H), 2.98 (dd, *J* = 16.8, 4.4 Hz, 1H), 2.77–2.69 (m, 1H), 2.47–2.40 (m, 1H), 2.23–2.12 (m, 1H), 1.40 (t, *J* = 7.0 Hz, 3H), 1.24 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 173.8, 162.7, 161.7, 146.9, 145.9, 144.5, 137.9, 129.5, 129.1, 128.3, 115.6, 103.0, 60.9, 60.1, 39.1, 28.7, 24.0, 23.6, 14.4, 14.1; HRMS (ESI): m/z [M + Na]$^+$ calcd for $C_{22}H_{23}N_3NaO_4$: 416.1581; found: 416.1583.

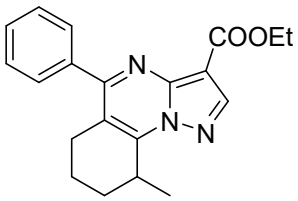


ethyl 5-phenyl-7-(trifluoromethyl)-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4ap):
Yield 97% (188.8 mg; petroleum ether/EtOAc = 8:1); white solid; mp 165–167 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.55 (s, 1H), 7.70–7.61 (m, 2H), 7.55–7.46 (m, 3H), 4.48–4.32 (m, 2H), 3.65 (dd, *J* = 19.2, 5.6 Hz, 1H), 3.25–3.13 (m, 1H), 2.97 (d, *J* = 7.6 Hz, 2H), 2.52–2.39 (m, 2H), 1.99 (qd, J = 12.6, 6.2 Hz, 1H), 1.40 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.6, 161.6, 147.1, 146.0, 144.2, 137.6, 129.7, 129.0, 128.5, 114.3, 103.2, 60.2, 38.8, 38.5, 25.7, 25.63, 25.60, 24.0, 20.1, 20.04, 20.01, 14.4; HRMS (ESI): m/z [M + Na]$^+$ calcd for $C_{20}H_{18}F_3N_3NaO_2$: 412.1243; found: 412.1243.



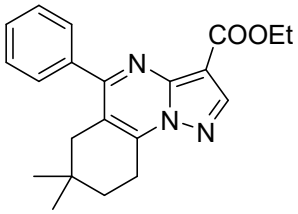
ethyl 8-methyl-5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4aq):

Yield 90% (151 mg; petroleum ether/EtOAc = 8:1); light yellow solid; mp 144–146 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.53 (s, 1H), 7.69–7.64 (m, 2H), 7.48–7.43 (m, 3H), 4.48–4.32 (m, 2H), 3.52 (dd, J = 19.2, 5.6 Hz, 1H), 2.93–2.84 (m, 1H) 2.82–2.67 (m, 2H), 2.17–2.07 (m, 1H), 1.99–1.92 (m, 1H), 1.40 (t, J = 7.2 Hz, 3H), 1.38–1.30 (m, 1H), 1.22 (d, J = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 161.7, 146.6, 146.0, 145.4, 138.3, 129.2, 129.0, 128.1, 117.1, 102.7, 60.0, 32.8, 30.5, 27.5, 26.6, 21.5, 14.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{20}H_{22}N_3O_2$: 336.1707; found: 336.1703.



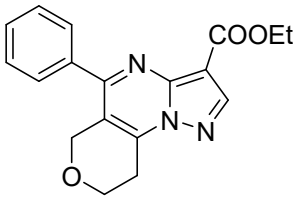
ethyl 9-methyl-5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4ar):

Yield 87% (146 mg; petroleum ether/EtOAc = 8:1); light yellow solid; mp 167–169 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.54 (s, 1H), 7.65–7.60 (m, 2H), 7.48–7.43 (m, 3H), 4.43–4.35 (m, 2H), 3.81–3.73 (m, 1H), 2.81–2.71 (m, 2H), 2.09–2.02 (m, 1H), 1.90 (dd, J = 6.8, 4.0 Hz, 1H), 1.87–1.80 (m, 2H), 1.51 (d, J = 6.8 Hz, 3H), 1.39 (t, J = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 162.2, 149.6, 146.4, 146.3, 138.5, 129.1, 128.9, 128.1, 116.8, 102.4, 59.9, 28.8, 28.7, 26.9, 18.2, 18.1, 14.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{20}H_{22}N_3O_2$: 336.1707; found: 336.1715.



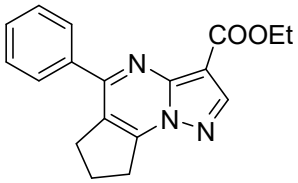
ethyl 7,7-dimethyl-5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (4as):

Yield 99% (173 mg; petroleum ether/EtOAc = 8:1); light yellow solid; mp 175–177 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.55 (s, 1H), 7.69–7.64 (m, 2H), 7.51–7.45 (m, 3H), 4.40 (q, J = 7.2 Hz, 2H), 3.27 (t, J = 6.8 Hz, 2H), 2.60 (s, 2H), 1.81 (t, J = 6.8 Hz, 2H), 1.41 (t, J = 7.2 Hz, 3H), 0.98 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 162.0, 146.7, 145.8, 144.9, 138.2, 129.2, 129.1, 128.1, 116.3, 102.7, 60.0, 39.9, 33.2, 29.4, 27.4, 22.6, 14.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{21}H_{24}N_3O_2$: 350.1863; found: 350.1864.



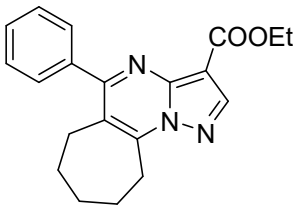
ethyl 5-phenyl-8,9-dihydro-6*H*-pyrano[3,4-*e*]pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4at):

Yield 99% (160 mg; petroleum ether/EtOAc = 5:1); light yellow solid; mp 224–226 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.57 (s, 1H), 7.66–7.61 (m, 2H), 7.53–7.46 (m, 3H), 4.80 (s, 2H), 4.41 (q, J = 7.2 Hz, 2H), 4.23 (t, J = 5.8 Hz, 2H), 3.36 (t, J = 5.8 Hz, 2H), 1.42 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.6, 158.9, 147.3, 146.3, 142.7, 137.1, 130.0, 128.7, 128.5, 116.0, 103.3, 65.4, 63.7, 60.2, 24.4, 14.4; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{18}H_{17}N_3NaO_3$: 346.1162; found: 346.1164.



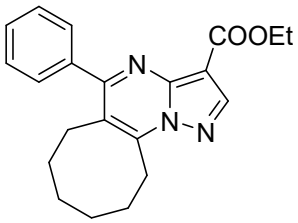
ethyl 5-phenyl-7,8-dihydro-6*H*-cyclopenta[*e*]pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4au):

Yield 97% (149 mg; petroleum ether/EtOAc = 8:1); white solid; mp 148–150 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.59 (s, 1H), 8.07–8.00 (m, 2H), 7.54–7.46 (m, 3H), 4.43 (q, J = 7.2 Hz, 2H), 3.49 (t, J = 7.8 Hz, 2H), 3.37 (t, J = 7.4 Hz, 2H), 2.43–2.34 (m, 2H), 1.45 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.9, 157.3, 151.7, 148.0, 147.5, 137.8, 130.2, 128.9, 128.5, 122.4, 102.5, 60.1, 32.2, 29.9, 22.9, 14.5; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{18}H_{18}N_3O_2$: 308.1394; found: 308.1393.



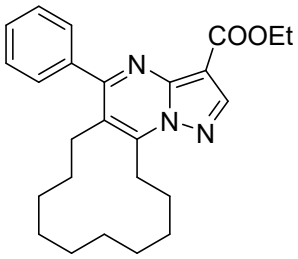
ethyl 5-phenyl-7,8,9,10-tetrahydro-6*H*-cyclohepta[*e*]pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4av):

Yield 98% (164.3 mg; petroleum ether/EtOAc = 10:1); light yellow solid; mp 131–133 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.54 (s, 1H), 7.62–7.57 (m, 2H), 7.51–7.45 (m, 3H), 4.39 (q, J = 7.2 Hz, 2H), 3.66 (t, J = 5.0 Hz 2H), 2.98–2.93 (m, 2H), 2.01–1.95 (m, 2H), 1.91–1.84 (m, 2H), 1.75–1.68 (m, 2H), 1.40 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.8, 161.9, 152.0, 146.8, 146.1, 138.9, 129.3, 129.1, 128.2, 122.7, 102.5, 60.0, 31.8, 29.3, 27.9, 26.9, 24.7, 14.5; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{20}H_{22}N_3O_2$: 336.1707; found: 336.1706.



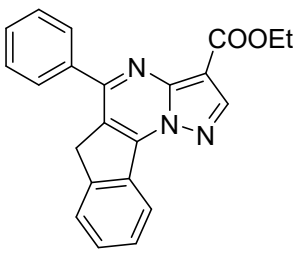
ethyl 5-phenyl-6,7,8,9,10,11-hexahydrocycloocta[*e*]pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4aw):

Yield 96% (167.7 mg; petroleum ether/EtOAc = 10:1); light yellow solid; mp 160–162 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.55 (s, 1H), 7.58–7.54 (m, 2H), 7.48–7.44 (m, 3H), 4.38 (q, J = 7.2 Hz, 2H), 3.51 (t, J = 6.2 Hz, 2H), 2.89 (t, J = 6.2 Hz, 2H), 2.00–1.94 (m, 2H), 1.63–1.56 (m, 2H), 1.52–1.45 (m, 2H), 1.44–1.37 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.72, 162.65, 149.1, 146.9, 146.1, 139.1, 128.8, 128.7, 128.1, 120.5, 102.4, 60.0, 31.1, 27.1, 26.6, 26.4, 25.7, 14.5; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{21}H_{24}N_3O_2$: 350.1863; found: 350.1862.



ethyl 5-phenyl-6,7,8,9,10,11,12,13,14,15-decahydrocyclododeca[*e*]pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4ax):

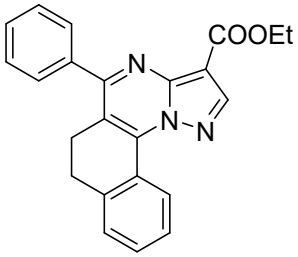
Yield 92% (186.5 mg; petroleum ether/EtOAc = 8:1); white solid; mp 172–174 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.53 (s, 1H), 7.59–7.54 (m, 2H), 7.48–7.41 (m, 3H), 4.38 (q, J = 7.2 Hz, 2H), 3.35 (t, J = 7.6 Hz, 2H), 2.85–2.75 (m, 2H), 2.03 (d, J = 4.0 Hz, 2H), 1.64–1.57 (m, 2H), 1.56–1.51 (m, 2H), 1.45 (d, J = 6.0 Hz, 4H), 1.42–1.33 (m, 7H), 1.28 (d, J = 4.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) δ 163.3, 162.5, 148.7, 146.5, 145.8, 139.5, 128.7, 128.3, 128.0, 120.8, 102.2, 59.8, 27.9, 27.2, 26.7, 26.3, 26.1, 25.9, 25.7, 24.1, 22.4, 21.9, 14.3; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{25}H_{31}N_3NaO_2$: 428.2308; found: 428.2309.



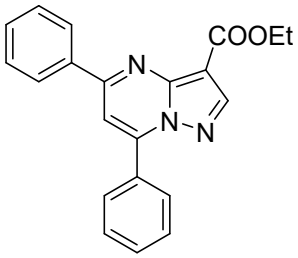
ethyl 5-phenyl-6*H*-indeno[2,1-*e*]pyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4ay):

Yield 94% (167 mg; petroleum ether/EtOAc = 8:1); yellow solid; mp 172–175 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.65–8.58 (m, 2H), 8.14–8.09 (m, 2H), 7.57–7.52 (m, 1H), 7.51–7.43 (m, 5H), 4.45 (q, J = 7.0 Hz, 2H), 4.15 (d, J = 2.8 Hz, 2H), 1.47 (t, J = 7.0 Hz, 3H); ^{13}C

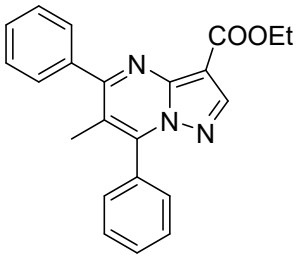
NMR (100 MHz, $CDCl_3$): δ (ppm) 162.9, 156.0, 148.0, 147.8, 146.3, 144.3, 137.5, 133.0, 130.7, 130.2, 128.8, 128.6, 127.7, 125.3, 124.5, 120.5, 102.1, 60.0, 36.5, 14.5; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{22}H_{17}N_3NaO_2$: 378.1213; found: 378.1213.



ethyl 5-phenyl-6,7-dihydrobenzo[*h*]pyrazolo[1,5-*a*]quinazoline-3-carboxylate (4az):
Yield 94% (173.6 mg; petroleum ether/EtOAc = 10:1); light yellow solid; mp 130–132 °C; ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.23–9.18 (m, 1H), 8.62 (s, 1H), 7.74–7.70 (m, 2H), 7.51–7.45 (m, 5H), 7.35–7.31 (m, 1H), 4.42 (q, J = 7.2 Hz, 2H), 3.02 (t, J = 7.0 Hz, 2H), 2.83 (t, J = 7.0 Hz, 2H), 1.43 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 160.8, 147.7, 146.9, 141.4, 140.2, 138.1, 131.4, 129.54, 129.49, 129.3, 128.2, 127.6, 126.7, 126.2, 117.5, 102.3, 60.0, 28.6, 25.4, 14.4; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{23}H_{19}N_3NaO_2$: 392.1369; found: 392.1368.

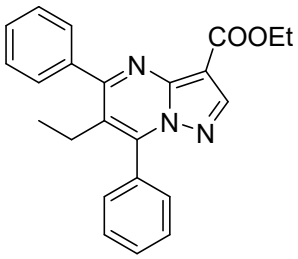


ethyl 5,7-diphenylpyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4ba):
Yield 96% (164.8 mg; petroleum ether/EtOAc = 10:1); yellow solid; mp 92–95 °C; ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.60 (s, 1H), 8.29–8.25 (m, 2H), 8.05–8.00 (m, 2H), 7.63–7.58 (m, 3H), 7.54–7.51 (m, 4H), 4.47 (q, J = 7.2 Hz, 2H), 1.48 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.8, 158.9, 148.8, 147.8, 147.7, 136.5, 131.3, 131.1, 130.7, 129.4, 128.9, 128.8, 127.6, 106.3, 103.0, 60.2, 14.5; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{21}H_{18}N_3O_2$: 344.1394; found: 344.1393.



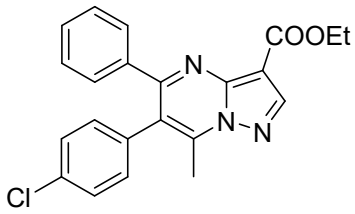
ethyl 6-methyl-5,7-diphenylpyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4bb):

Yield 95% (169.8 mg; petroleum ether/EtOAc = 8:1); yellow solid; mp 136–138 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.47 (s, 1H), 7.75–7.69 (m, 2H), 7.65–7.57 (m, 3H), 7.55–7.52 (m, 2H), 7.51–7.46 (m, 3H), 4.40 (q, J = 7.2 Hz, 2H), 2.22 (s, 3H), 1.40 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 163.4, 162.6, 147.1, 146.6, 146.3, 138.8, 130.3, 130.2, 129.3, 129.2, 129.1, 128.9, 128.2, 116.2, 102.6, 60.0, 17.1, 14.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{22}H_{20}N_3O_2$: 358.1550; found: 358.1547.



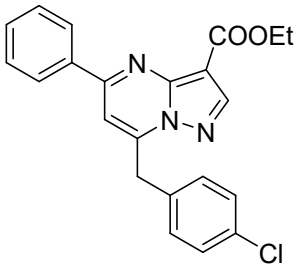
ethyl 6-ethyl-5,7-diphenylpyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4bc):

Yield 96% (178.3 mg; petroleum ether/EtOAc = 8:1); white solid; mp 136–138 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.48 (s, 1H), 7.69–7.65 (m, 2H), 7.63–7.57 (m, 3H), 7.52–7.45 (m, 5H), 4.39 (q, J = 7.2 Hz, 2H), 2.67 (q, J = 7.6 Hz, 2H), 1.38 (t, J = 7.0 Hz, 3H), 0.78 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 163.5, 162.4, 146.9, 146.1, 138.8, 129.92, 129.90, 128.80, 128.76, 128.7, 128.4, 128.0, 122.6, 102.4, 59.8, 21.5, 14.4, 14.2; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{23}H_{22}N_3O_2$: 372.1707; found: 372.1706.

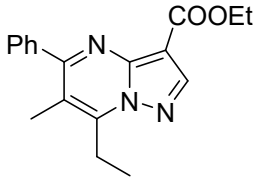


ethyl 6-(4-chlorophenyl)-7-methyl-5-phenylpyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4bd):

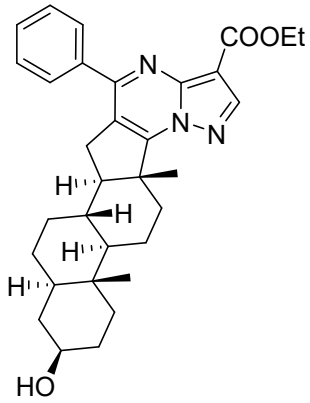
Yield 56% (109.7 mg; petroleum ether/EtOAc = 10:1); yellow solid; mp 185–187 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.62 (s, 1H), 7.40–7.36 (m, 2H), 7.36–7.32 (m, 2H), 7.30–7.19 (m, 3H), 7.12–7.08 (m, 2H), 4.43 (q, J = 7.2 Hz, 2H), 2.72 (s, 3H), 1.43 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.6, 160.2, 147.5, 146.5, 145.7, 138.1, 134.2, 133.6, 132.2, 130.0, 129.1, 128.9, 127.8, 121.3, 103.2, 60.2, 15.6, 14.4; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{22}H_{18}ClN_3NaO_2$: 414.0980; found: 414.0976.



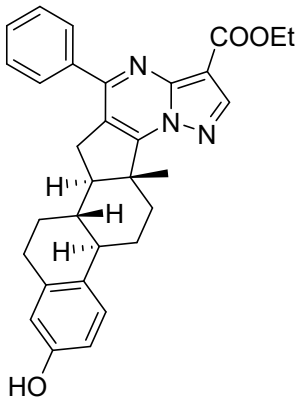
ethyl 7-(4-chlorobenzyl)-5-phenylpyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4bd'):
Yield 42% (82.3 mg; petroleum ether/EtOAc = 10:1); light yellow solid; mp 128–131 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.58 (s, 1H), 8.12–8.07 (m, 2H), 7.50–7.44 (m, 3H), 7.37–7.29 (m, 4H), 7.04 (s, 1H), 4.53 (s, 2H), 4.44 (q, J = 7.2 Hz, 2H), 1.46 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.7, 158.7, 149.1, 147.9, 147.5, 136.4, 133.6, 132.7, 131.0, 130.9, 129.1, 128.9, 127.6, 105.6, 103.2, 60.2, 35.9, 14.5; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{22}H_{18}ClN_3NaO_2$: 414.0980; found: 414.0979.



ethyl 7-ethyl-6-methyl-5-phenylpyrazolo[1,5-*a*]pyrimidine-3-carboxylate (4be)
Yield 95% (146.8 mg; petroleum ether/EtOAc = 5:1); white solid; mp 118–120 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.54 (s, 1H), 7.65–7.60 (m, 2H), 7.50–7.44 (m, 3H), 4.39 (q, J = 7.2 Hz, 2H), 3.36 (q, J = 7.6 Hz, 2H), 2.39 (s, 3H), 1.42–1.36 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.8, 162.7, 149.9, 146.8, 146.1, 139.0, 129.2, 129.1, 128.1, 114.7, 102.4, 60.0, 21.5, 15.1, 14.4, 10.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{18}H_{20}N_3O_2$: 310.1550; found: 310.1552.

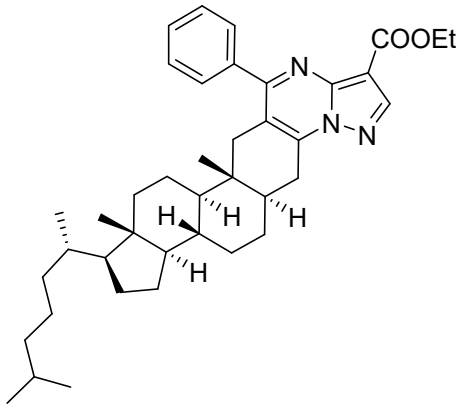


ethyl (2a*R*,4*R*,6a*R*,6b*R*,8a*R*,15a*R*,15b*S*)-4-hydroxy-6a,8a-dimethyl-14-phenyl-2,2a,3,4,5,6,6a,6b,7,8,8a,15,15a,15b-tetradecahydro-1*H*-naphtho[2',1':4,5]indeno[2,1-*e*]pyrazolo[1,5-*a*]pyrimidine-12-carboxylate (4bf):
Yield 80% (205.5 mg; petroleum ether/EtOAc = 5:1); light yellow solid; mp 147–150 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.56 (s, 1H), 8.00–7.96 (m, 2H), 7.53–7.48 (m, 3H), 4.49–4.36 (m, 2H), 3.64–3.56 (m, 1H), 3.02 (dd, J = 14.4, 5.6 Hz, 1H), 2.93–2.85 (m, 2H), 1.90–1.72 (m, 8H), 1.64–1.57 (m, 2H), 1.43 (t, J = 7.2 Hz, 4H), 1.40–1.33 (m, 3H), 1.30 (s, 3H), 1.20–1.14 (m, 1H), 1.07–0.97 (m, 2H), 0.92 (s, 3H), 0.87–0.81 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 163.0, 159.0, 157.7, 148.2, 147.9, 137.8, 130.1, 129.0, 128.5, 120.6, 101.9, 71.1, 60.0, 56.3, 54.3, 47.2, 44.9, 38.0, 36.6, 35.7, 33.8, 33.7, 31.7, 31.5, 31.4, 28.3, 20.6, 15.0, 14.5, 12.3; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{32}H_{40}N_3O_3$: 514.3064; found: 514.3071.



ethyl (6b*R*,8a*R*,15a*R*,15b*S*)-4-hydroxy-8a-methyl-14-phenyl-2,6b,7,8,8a,15,15a,15b-octahydro-1*H*-naphtho[2',1':4,5]indeno[2,1-*e*]pyrazolo[1,5-*a*]pyrimidine-12-carboxylate (4bg):

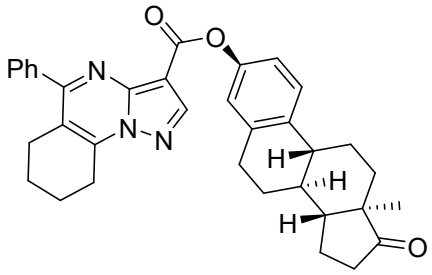
Yield 81% (200 mg; petroleum ether/EtOAc = 5:1); white solid; mp 305–308 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.59 (s, 1H), 8.03–7.97 (m, 2H), 7.54–7.48 (m, 3H), 7.17 (d, J = 8.4 Hz, 1H), 6.68 (dd, J = 8.4, 2.4 Hz, 1H), 6.61 (d, J = 2.4 Hz, 1H), 5.23 (s, 1H), 4.50–4.37 (m, 2H), 3.14 (dd, J = 14.4, 6.4 Hz, 1H), 3.02 (dd, J = 14.4, 12.0 Hz, 2H), 2.95–2.83 (m, 2H), 2.55–2.49 (m, 1H), 2.42–2.34 (m, 1H), 2.10–2.00 (m, 3H), 1.92–1.77 (m, 2H), 1.55–1.48 (m, 1H), 1.44 (t, J = 7.2 Hz, 3H), 1.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 163.2, 159.0, 157.9, 153.7, 148.2, 148.0, 137.8, 137.7, 131.7, 130.1, 129.0, 128.5, 126.2, 120.6, 115.3, 112.9, 102.0, 60.1, 55.5, 47.4, 43.8, 36.9, 33.7, 31.5, 29.3, 27.3, 25.9, 15.1, 14.5; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{31}H_{32}N_3O_3$: 494.2438; found: 494.2431.



ethyl (1*S*,3a*S*,3b*S*,5a*R*,13a*R*,13b*S*,15a*S*)-3b,13a,15a-trimethyl-1-((*S*)-6-methylheptan-2-yl)-12-phenyl-2,3,3a,3b,4,5,5a,6,13,13a,13b,14,15,15a-tetradecahydro-1*H*-cyclopenta[5,6]naphtho[1,2-*g*]pyrazolo[1,5-*a*]quinazoline-10-carboxylate (4bh):

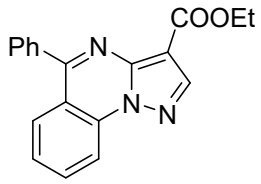
Yield 90% (274.5 mg; petroleum ether/EtOAc = 8:1); brown solid; mp 104–107 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.54 (s, 1H), 7.71–7.64 (m, 2H), 7.51–7.43 (m, 3H), 4.49–4.31 (m, 2H), 3.36 (dd, J = 14.4, 5.2 Hz, 1H), 2.80–2.70 (m, 2H), 2.54 (d, J = 16.0 Hz, 1H), 1.97 (d, J = 12.4 Hz, 1H), 1.87–1.73 (m, 4H), 1.64–1.56 (m, 1H), 1.57–1.48 (m, 1H), 1.44–1.30 (m, 10H), 1.20–0.91 (m, 10H), 0.91–0.83 (m, 10H), 0.68 (s, 3H), 0.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 162.5, 161.9, 146.6, 145.6, 144.5, 138.1, 129.1, 129.0, 127.9, 116.1, 102.5, 59.8, 56.1, 56.0, 53.2, 42.1, 40.4, 39.8, 39.5, 39.3, 35.9, 35.5, 35.1, 31.1, 29.1, 28.0,

27.8, 24.0, 23.6, 22.6, 22.4, 20.9, 18.4, 14.3, 11.7, 11.1; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{40}H_{56}N_3O_2$: 610.4367; found: 610.4355.



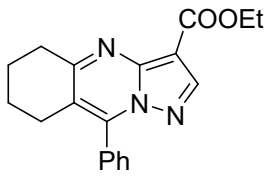
(8*S*,9*R*,13*R*,14*R*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[a]phenanthren-3-yl5-phenyl-6,7,8,9-tetrahydropyrazolo[1,5-*a*]quinazoline-3-carboxylate (5):

Yield 83% (90.6 mg; petroleum ether/EtOAc = 5:1); white solid; mp 112–114 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.67 (s, 1H), 7.69–7.64 (m, 2H), 7.45–7.41 (m, 3H), 7.29 (d, J = 8.4 Hz, 1H), 7.05–6.99 (m, 2H), 3.28 (t, J = 6.4 Hz, 2H), 2.94–2.88 (m, 2H), 2.81 (t, J = 6.0 Hz, 2H), 2.49 (dd, J = 18.8, 8.8 Hz, 1H), 2.44–2.38 (m, 1H), 2.32–2.24 (m, 1H), 2.19–2.10 (m, 1H), 2.08–1.98 (m, 4H), 1.97–1.93 (m, 1H), 1.84–1.77 (m, 2H), 1.66–1.53 (m, 3H), 1.53–1.41 (m, 3H), 0.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 220.7, 162.0, 161.0, 148.6, 147.0, 146.2, 145.8, 138.0, 137.5, 136.7, 129.3, 129.1, 128.0, 126.0, 121.9, 119.0, 117.9, 101.7, 50.2, 47.8, 44.0, 37.8, 35.7, 31.4, 29.2, 26.7, 26.2, 25.6, 24.8, 22.2, 21.4, 20.8, 13.7; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{35}H_{36}N_3O_3$: 546.2751; found: 546.2750.



ethyl 5-phenylpyrazolo[1,5-*a*]quinazoline-3-carboxylate (6):

Yield 92% (146 mg; petroleum ether/EtOAc = 8:1); light yellow solid; mp 170–172 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.60 (d, J = 8.4 Hz, 1H), 8.54 (s, 1H), 8.14 (dd, J = 8.4, 0.8 Hz, 1H), 7.98–7.93 (m, 1H), 7.86–7.81 (m, 2H), 7.59–7.53 (m, 4H), 4.43 (q, J = 7.2 Hz, 2H), 1.43 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 163.0, 162.7, 145.3, 144.3, 137.2, 136.5, 134.4, 130.2, 130.0, 129.3, 128.5, 125.8, 117.5, 115.6, 105.5, 60.3, 14.4; HRMS (ESI): m/z $[M + H]^+$ calcd for $C_{19}H_{16}N_3O_2$: 318.1237; found: 318.1235.



ethyl 9-phenyl-5,6,7,8-tetrahydropyrazolo[5,1-*b*]quinazoline-3-carboxylate (8):

Yield 51% (82 mg; petroleum ether/EtOAc = 5:1); yellow solid; mp 162–164 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.39 (s, 1H), 7.62–7.56 (m, 3H), 7.48–7.44 (m, 2H), 4.41 (q, J =

7.2 Hz, 2H), 3.19 (t, J = 6.6 Hz, 2H), 2.62 (t, J = 6.4 Hz, 2H), 1.98–1.91 (m, 2H), 1.81–1.76 (m, 2H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 164.1, 162.8, 146.9, 144.9, 130.3, 129.6, 129.0(3), 128.9(8), 118.1, 101.2, 60.0, 34.0, 26.0, 22.4, 22.1, 14.5; HRMS (ESI): m/z $[M + Na]^+$ calcd for $C_{19}H_{19}N_3NaO_2$: 344.1369; found: 344.1355.

6. Crystallographic data and molecular structure of 4am

The crystal of **4am** for X-ray diffraction study has been obtained through the dissolving of compound in $CHCl_3$, followed by slow evaporation of the solvent at room temperature. The crystal was kept at 296(2) during data collection. CCDC 2252849 contains the supplementary crystallographic data for this paper. This data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

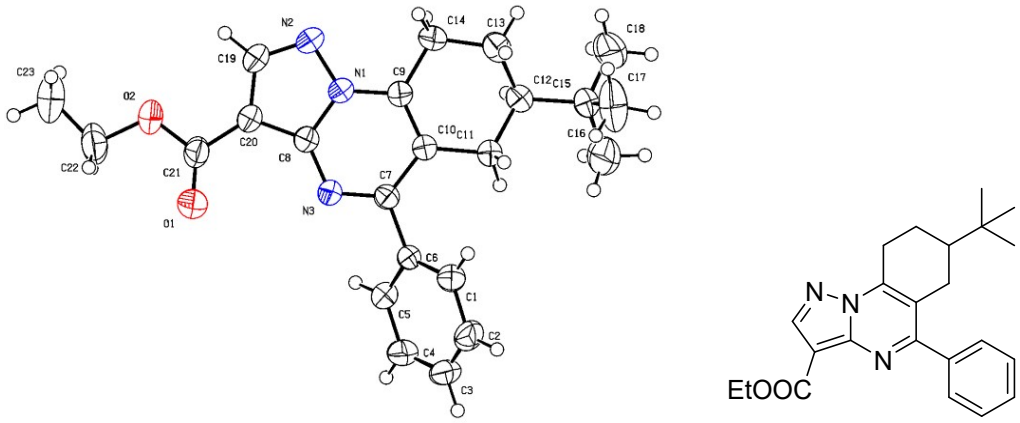
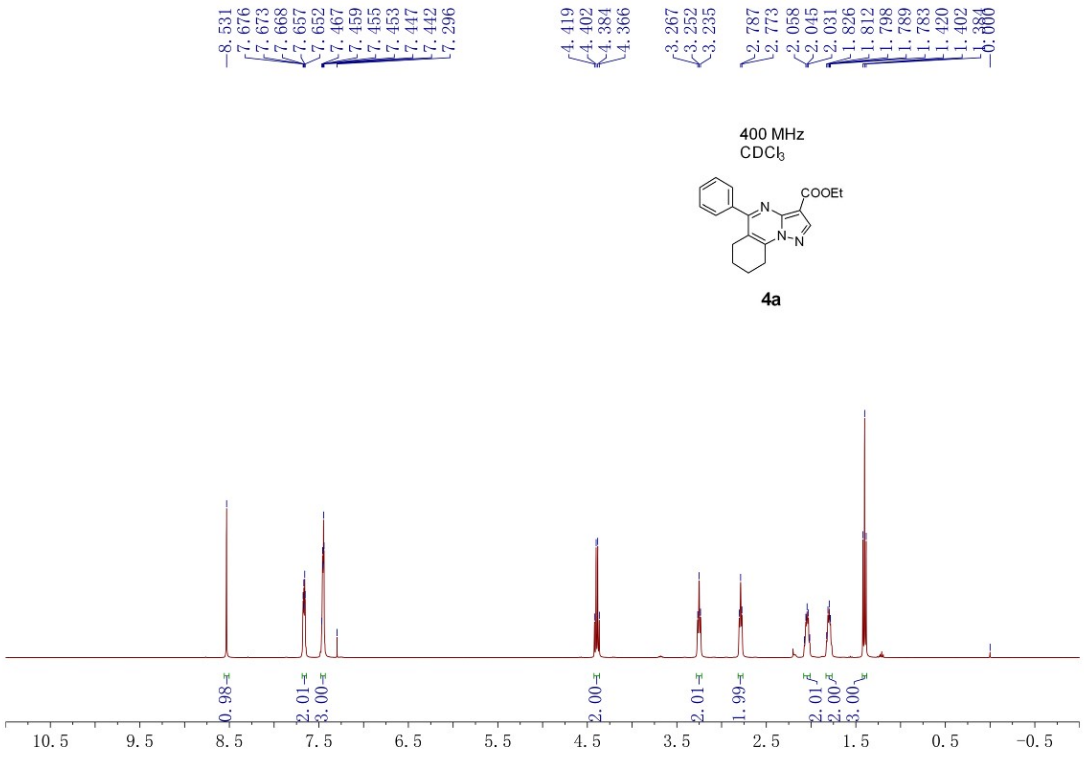
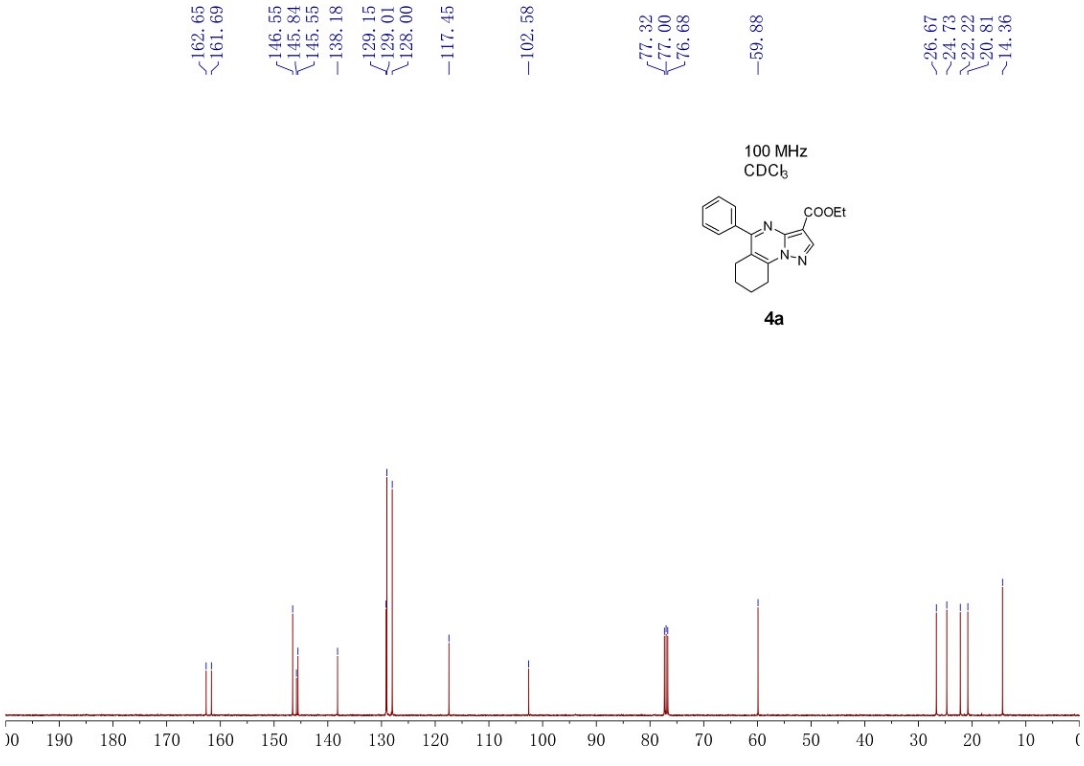


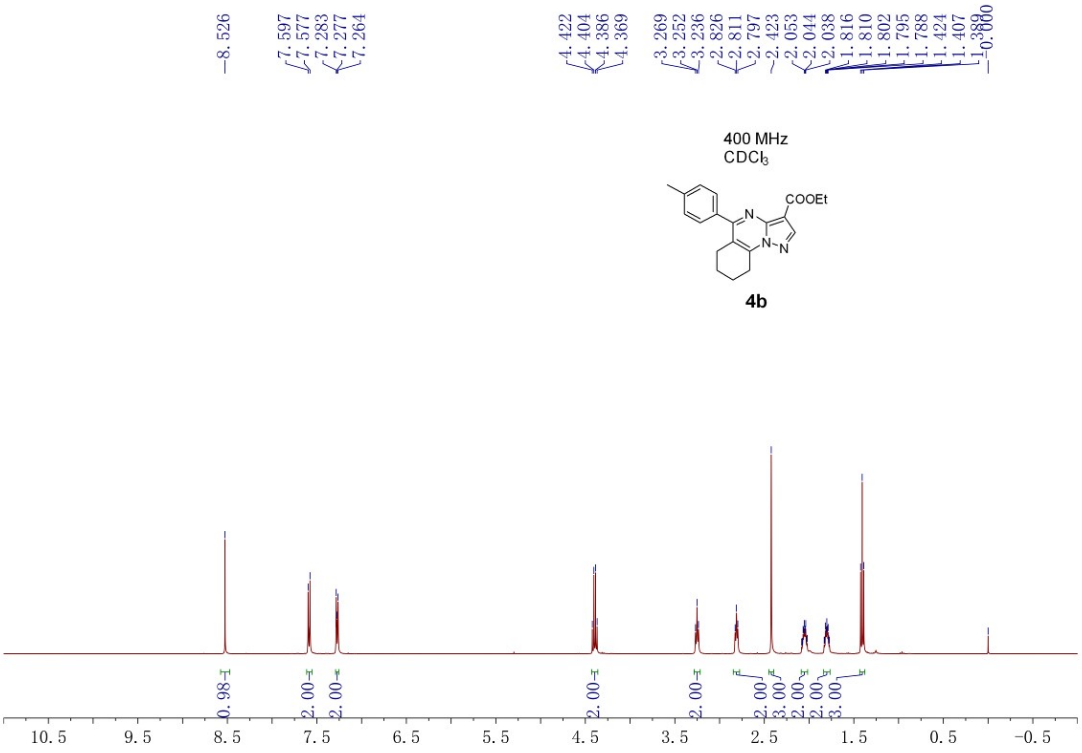
Figure S1. X-ray crystal structure of **4am**; the ellipsoids depicted at the 30% probability level.

Empirical formula	$C_{23}H_{27}N_3O_2$		Absorption coefficient	0.078 mm^{-1}
Formula weight	377.47		F(000)	404.0
Temperature	296(2) K		Crystal size	0.18 × 0.16 × 0.15 mm^3
Crystal system	triclinic		Theta range for data collection	40184 to 54.938°
Space group	P-1		Reflections collected	6262
Unit cell dimensions	a = 10.097(4) Å	α = 108.552(5)°	Independent reflections	4579 [R(int) = 0.0198, R(sigma) = 0.0446]
	b = 10.892(4) Å	β = 110.723(4)°	Data / restraints / parameters	4579/0/257
	c = 11.599(4) Å	γ = 103.618(5)°	Goodness-of-fit on F^2	1.089
Volume	1040.2(7) $Å^3$		Final R indices [I>2sigma(I)]	R_1 = 0.0746, wR_2 = 0.2475
Z	2		R indices (all data)	R_1 = 0.1018, wR_2 = 0.2829
Density (calculated)	1.205 g/cm^3		Largest diff. peak and hole	0.61/-0.33 e.$Å^{-3}$

7. NMR spectra



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COOEt
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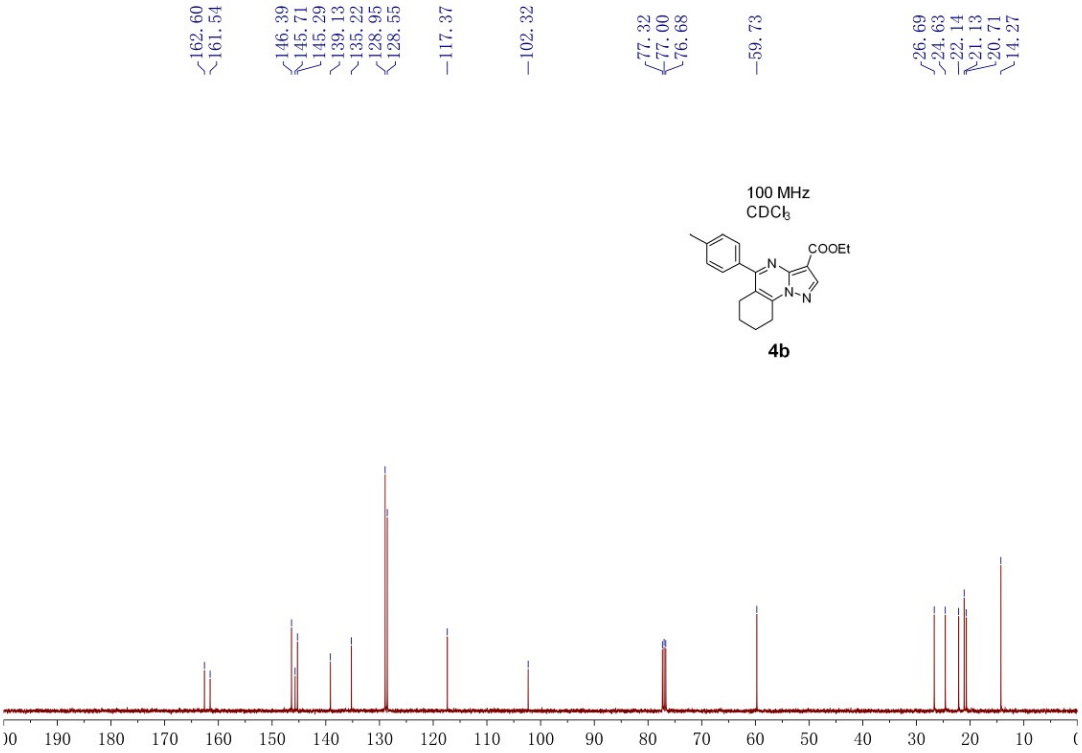
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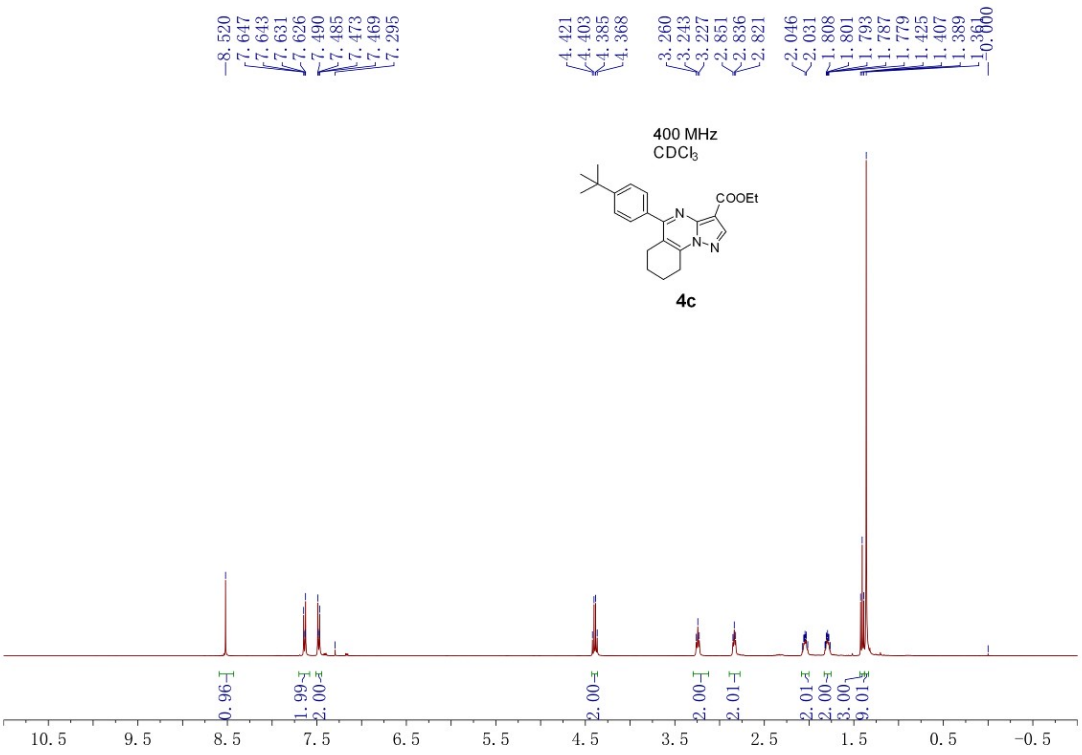
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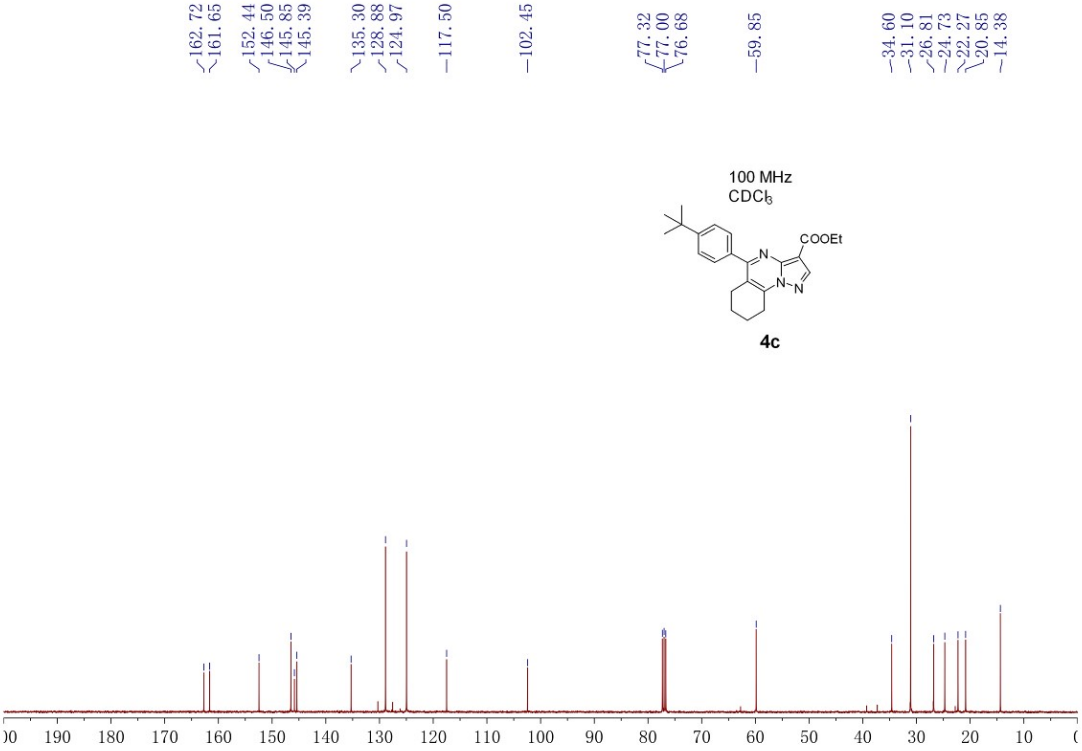
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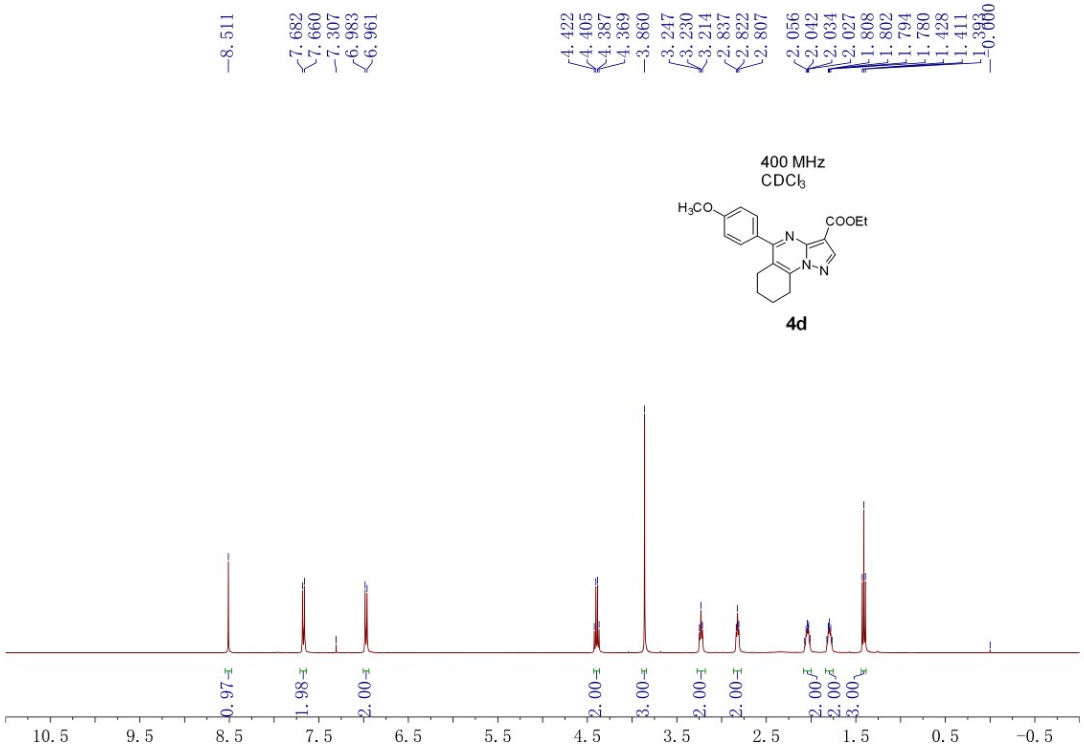
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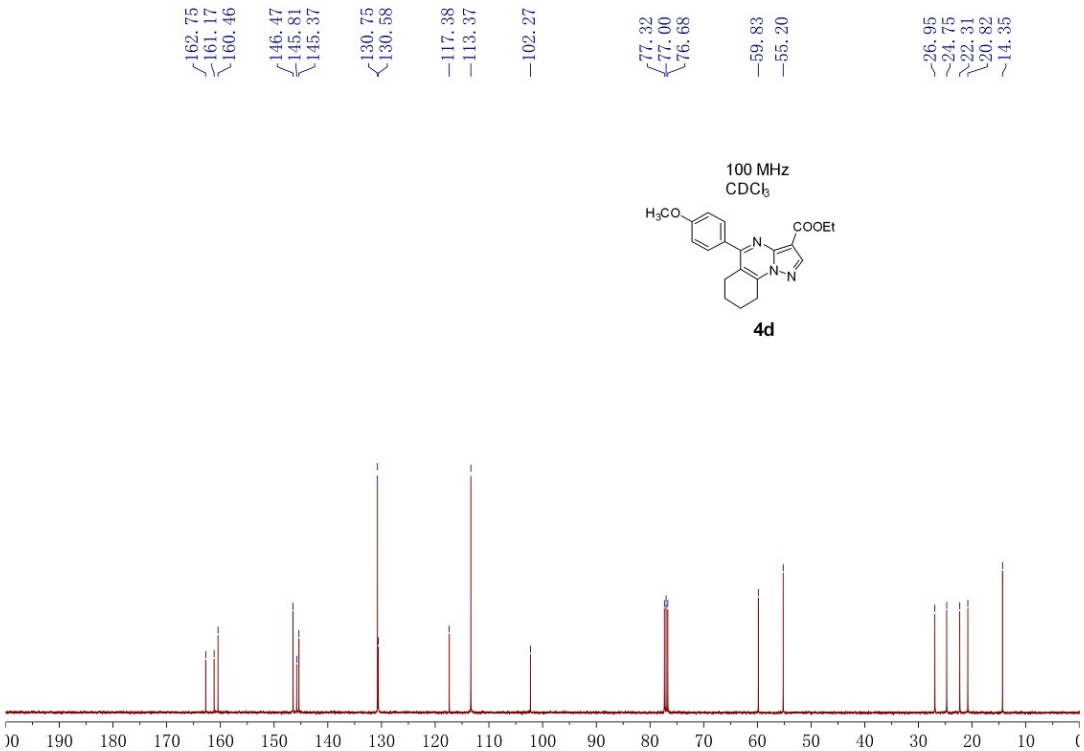
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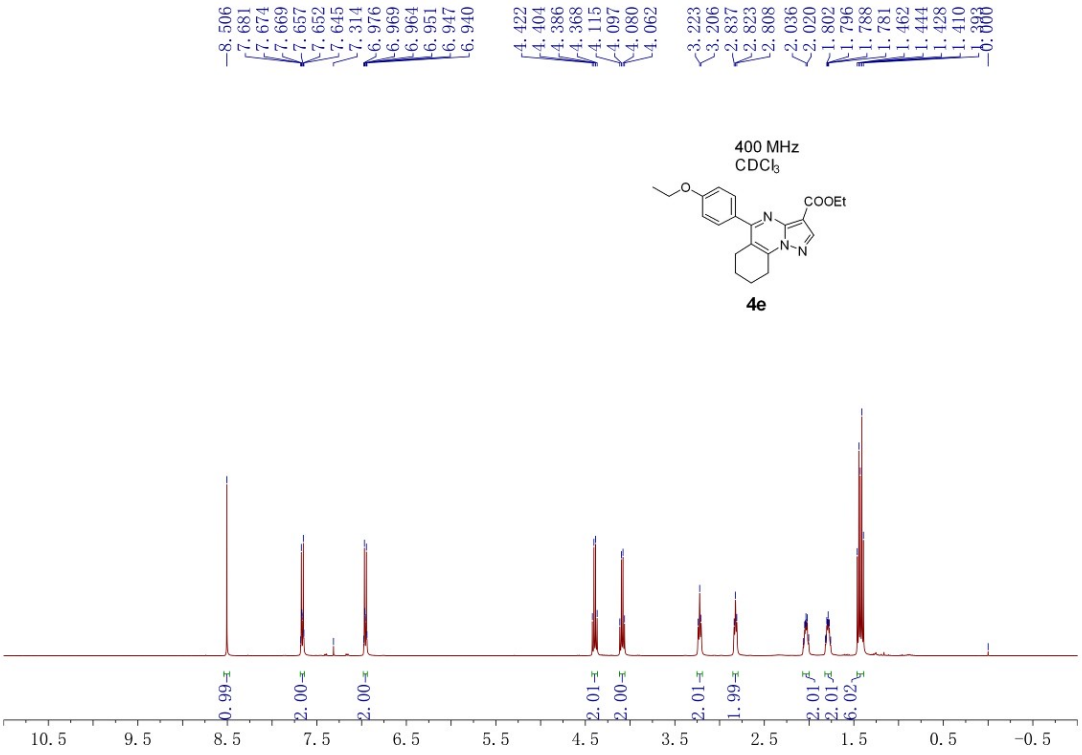
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1.781
1.462
1.444
1.428
1.410
400 MHz
CDCl3
COOEt
4e
0.99
2.00
2.00
2.01
2.00
2.01
1.99
2.01
2.01
6.02
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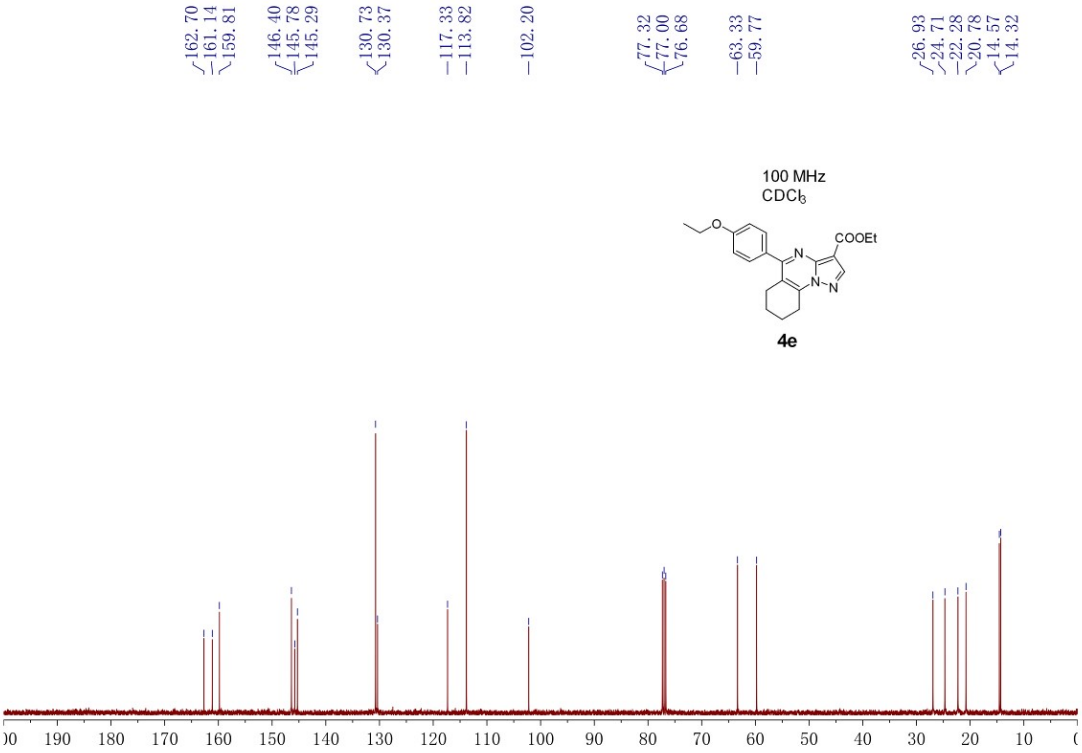
-0.5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113.82
102.20
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77.00
76.68
63.33
59.77
26.93
24.71
22.28
20.78
14.57
14.32
100 MHz
CDCl3
COOEt
4e
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80
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20
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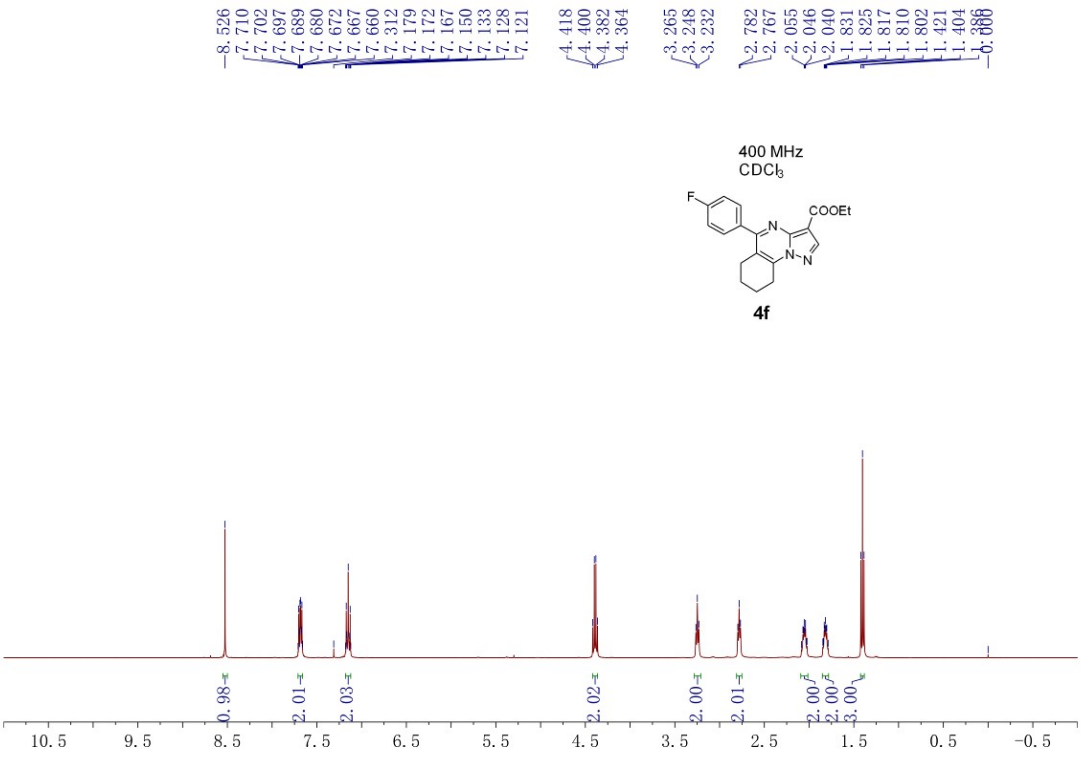
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7.667
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7.179
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7.167
7.150
7.133
7.128
7.121
4.418
4.400
4.382
4.364
3.265
3.248
3.232
2.782
2.767
2.055
2.046
2.040
1.831
1.825
1.817
1.810
1.802
1.421
1.404
1.386
0.000
400 MHz
CDCl3
F
COOEt
N
N-N
4f
0.98
2.01
2.03
2.02
2.00
2.01
2.00
2.00
3.00
10.5
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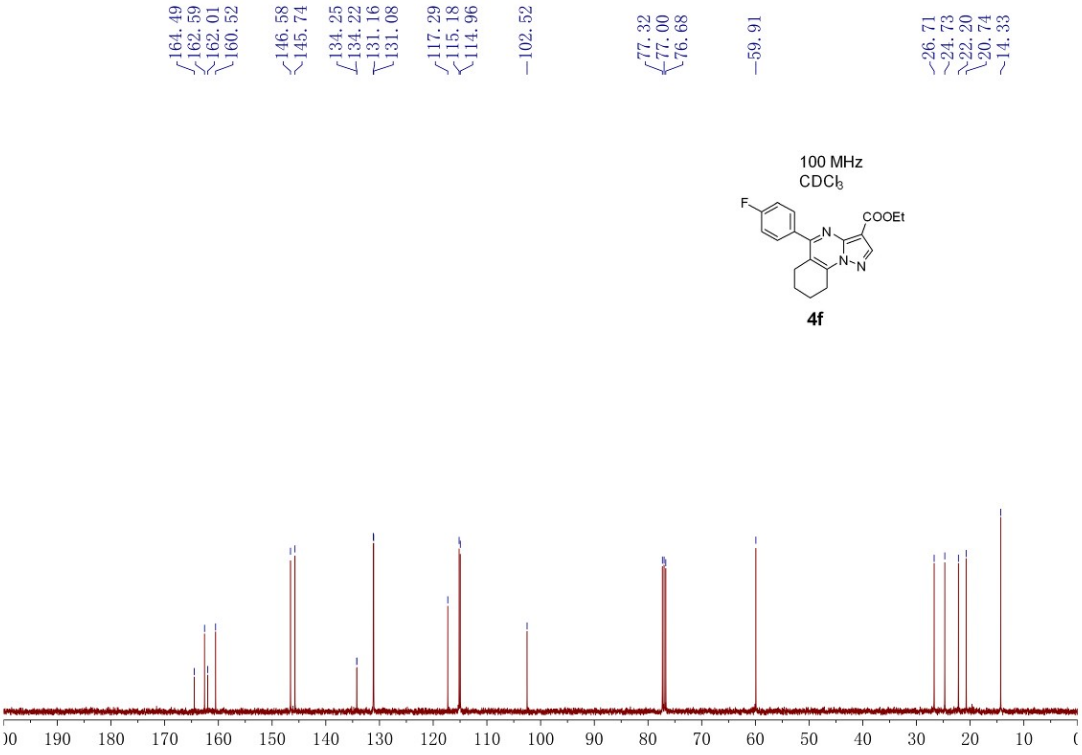
-0.5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134.22
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131.08
117.29
115.18
114.96
102.52
77.32
77.00
76.68
59.91
26.71
24.73
22.20
20.74
14.33
100 MHz
CDCl3
F
COOEt
N
N-N
4f
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80
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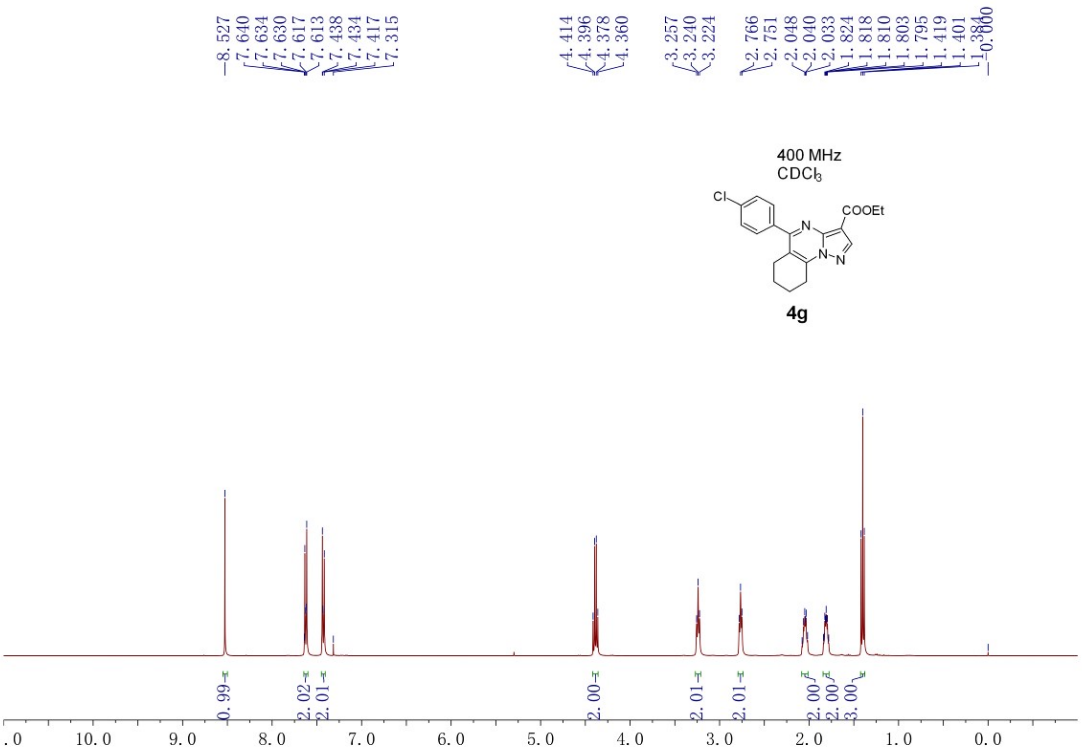
40
30
20
10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7.434
7.417
7.315
4.414
4.396
4.378
4.360
3.257
3.240
3.224
2.766
2.751
2.048
2.040
2.033
1.824
1.818
1.810
1.803
1.795
1.419
1.401
1.384
0.000
400 MHz
CDCl3
Cl
COOEt
N
N-N
4g
0.99
2.02
2.01
2.00
2.01
2.01
2.00
2.00
3.00
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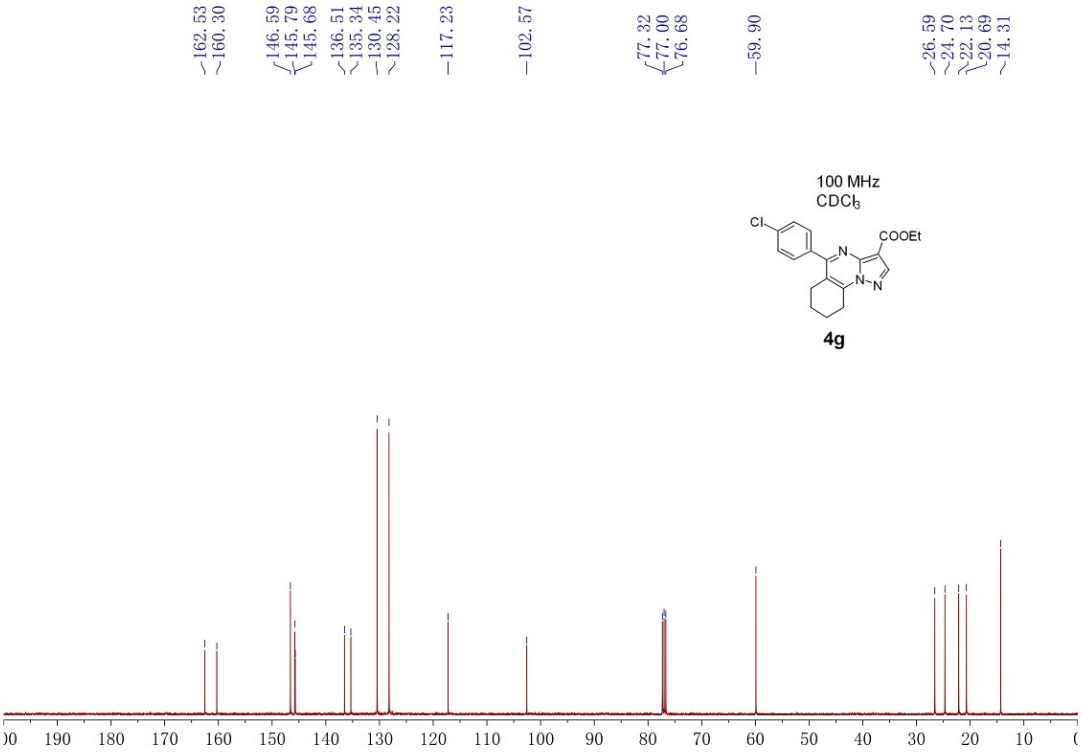
0.0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117.23
102.57
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77.00
76.68
59.90
26.59
24.70
22.13
20.69
14.31
100 MHz
CDCl3
Cl
COOEt
N
N-N
4g
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160
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80
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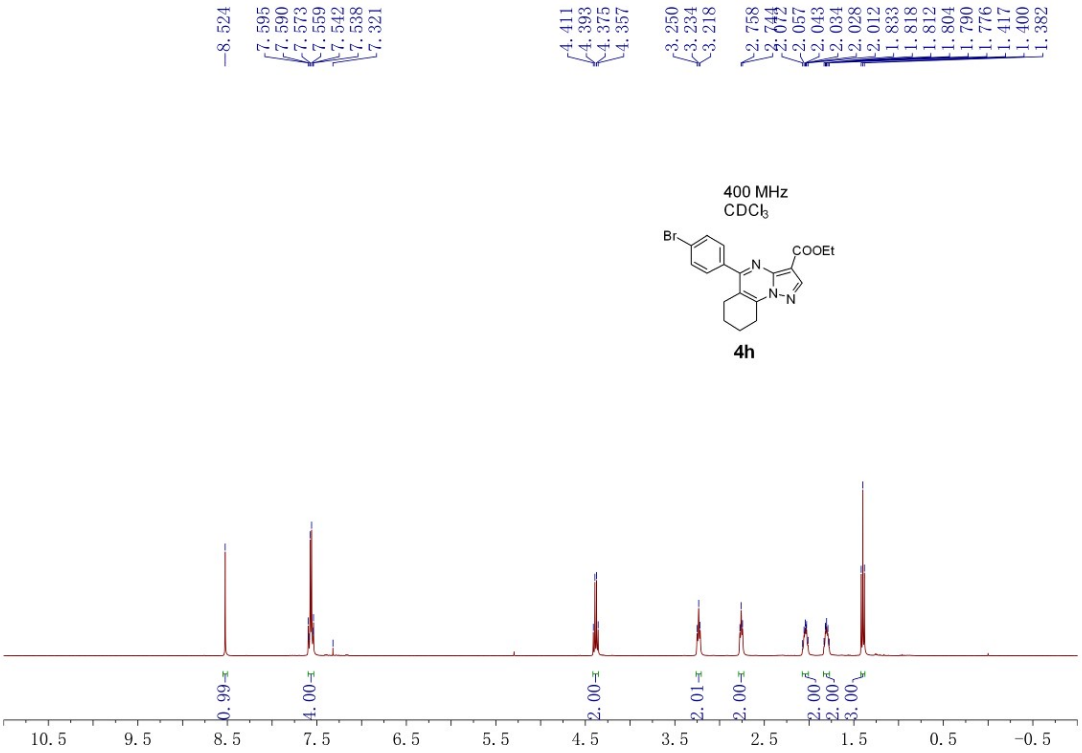
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7.542
7.538
7.321
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4.393
4.375
4.357
3.250
3.234
3.218
2.758
2.744
2.072
2.057
2.043
2.034
2.028
2.012
1.833
1.818
1.812
1.804
1.790
1.776
1.417
1.400
1.382
400 MHz
CDCl3
Br
COOEt
N
N
N
4h
0.99
4.00
2.00
2.01
2.00
2.00
2.00
3.00
10.5
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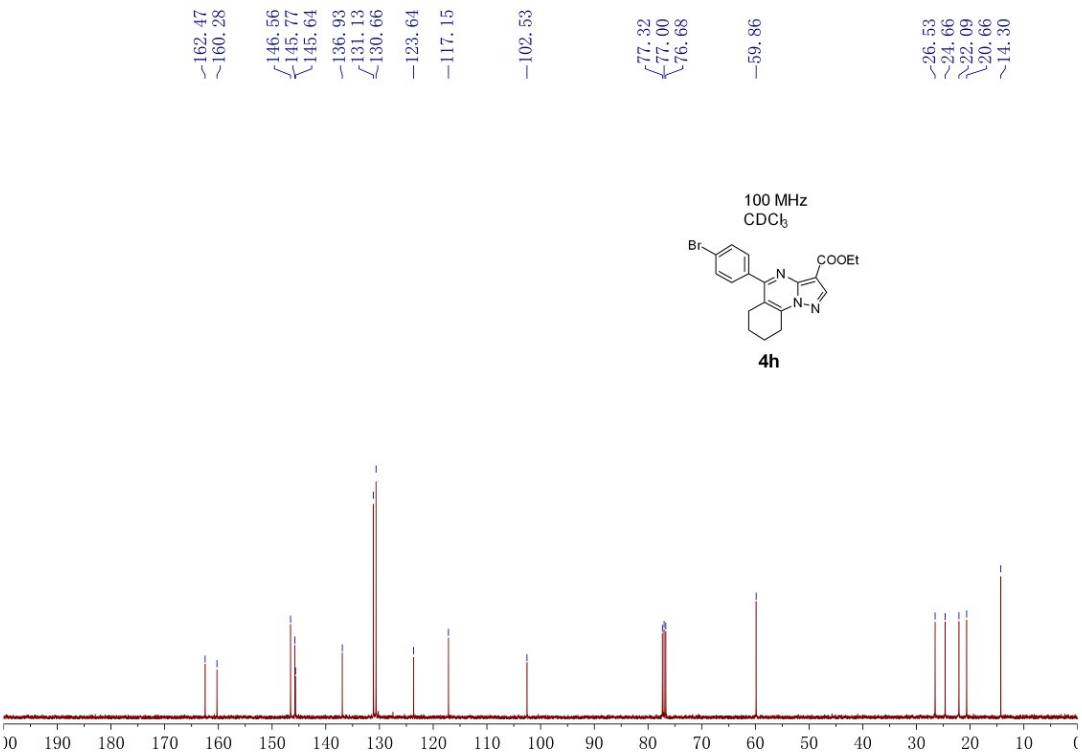
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5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145.64
136.93
131.13
130.66
123.64
117.15
102.53
77.32
77.00
76.68
59.86
26.53
24.66
22.09
20.66
14.30
100 MHz
CDCl3
Br
COOEt
N
N
N
4h
190
180
170
160
150
140
130
120
110
100
90
80
70
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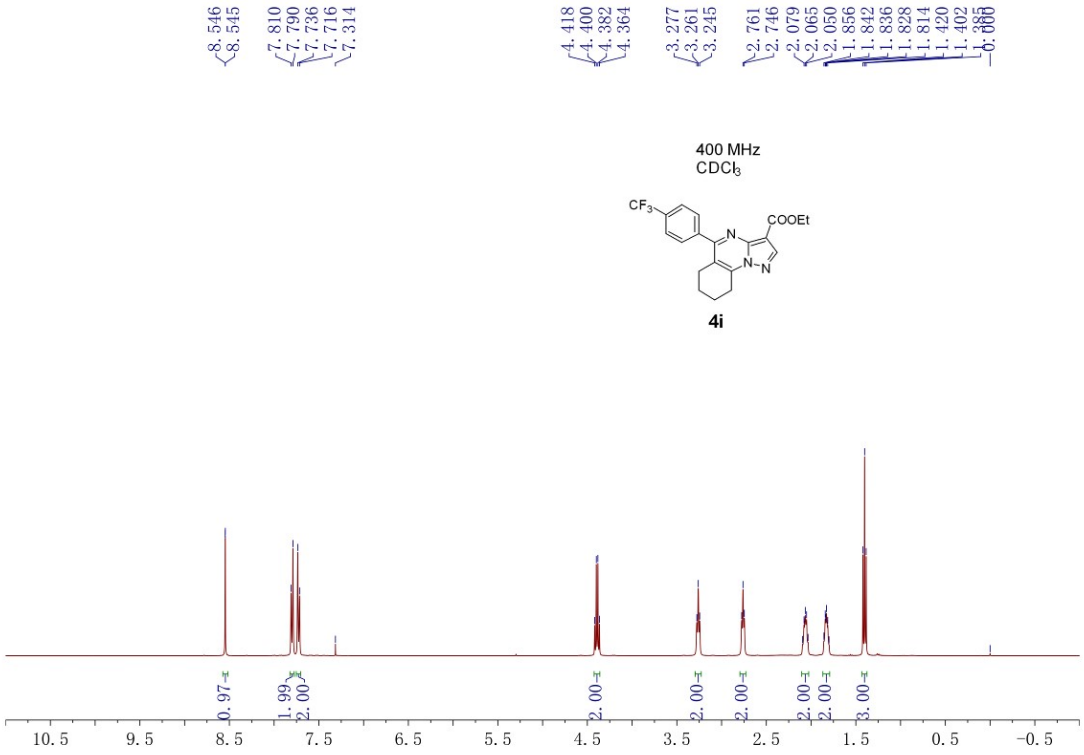
50
40
30
20
10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7.810
7.790
7.736
7.716
7.314
4.418
4.400
4.382
4.364
3.277
3.261
3.245
2.761
2.746
2.079
2.065
2.050
1.856
1.842
1.836
1.828
1.814
1.420
1.402
400 MHz
CDCl3
CF3
COOEt
N
N
N
4i
0.97
1.99
2.00
2.00
2.00
2.00
2.00
2.00
3.00
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7.5
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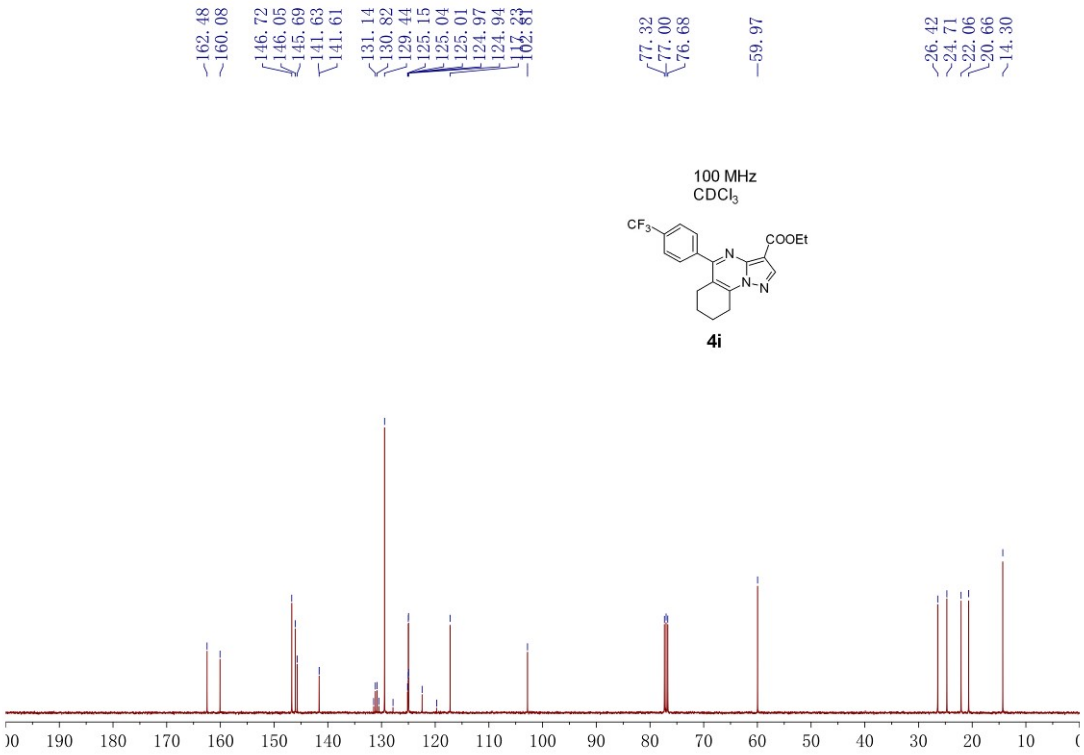
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141.61
131.14
130.82
129.44
125.15
125.04
125.01
124.97
124.94
77.32
77.00
76.68
59.97
26.42
24.71
22.06
20.66
14.30
100 MHz
CDCl3
CF3
COOEt
N
N
N
4i
190
180
170
160
150
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120
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100
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80
70
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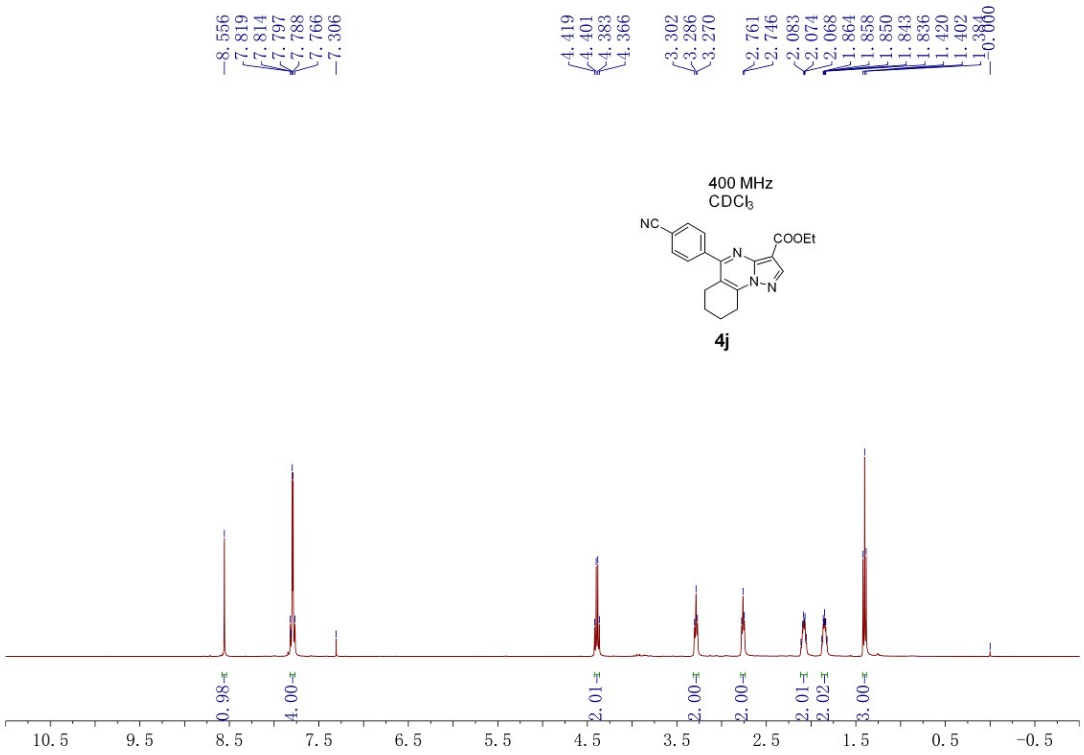
20
10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7.766
7.306
4.419
4.401
4.383
4.366
3.302
3.286
3.270
2.761
2.746
2.083
2.074
2.068
1.864
1.858
1.850
1.843
1.836
1.420
1.402
1.384
0.000
400 MHz
CDCl3
NC
COOEt
N
N-N
4j
0.98
4.00
2.01
2.00
2.00
2.01
2.02
3.00
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7.5
6.5
5.5
4.5
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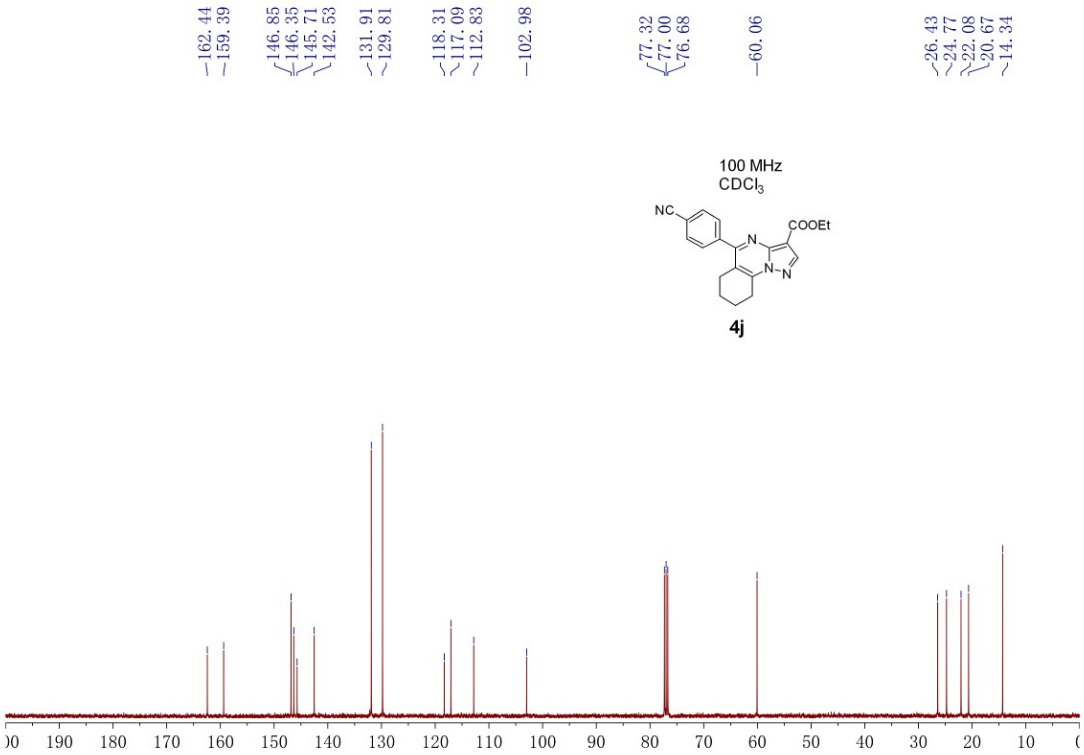
0.5
-0.5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129.81
118.31
117.09
112.83
102.98
77.32
77.00
76.68
60.06
26.43
24.77
22.08
20.67
14.34
100 MHz
CDCl3
NC
COOEt
N
N-N
4j
190
180
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160
150
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120
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100
90
80
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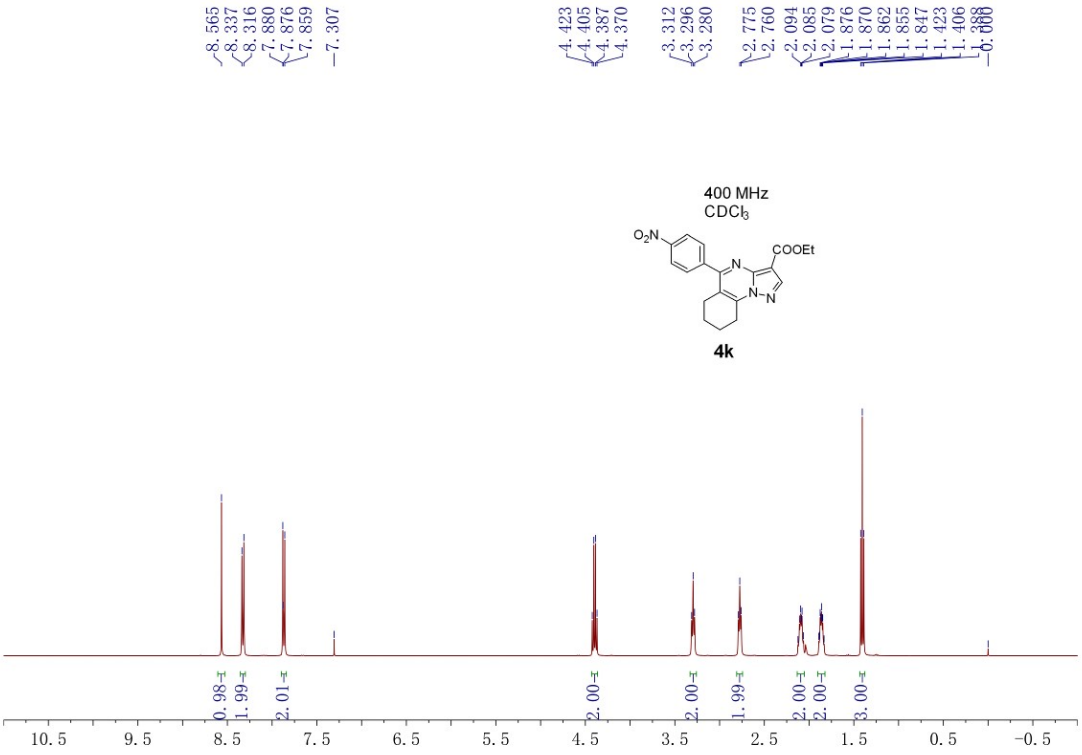
20
10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7.859
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4.423
4.405
4.387
4.370
3.312
3.296
3.280
2.775
2.760
2.094
2.085
2.079
1.876
1.870
1.862
1.855
1.847
1.423
1.406
1.388
0.000
400 MHz
CDCl3
O2N
COOEt
N
N-N
4k
0.98
1.99
2.01
2.00
2.00
1.99
2.00
2.00
3.00
10.5
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5.5
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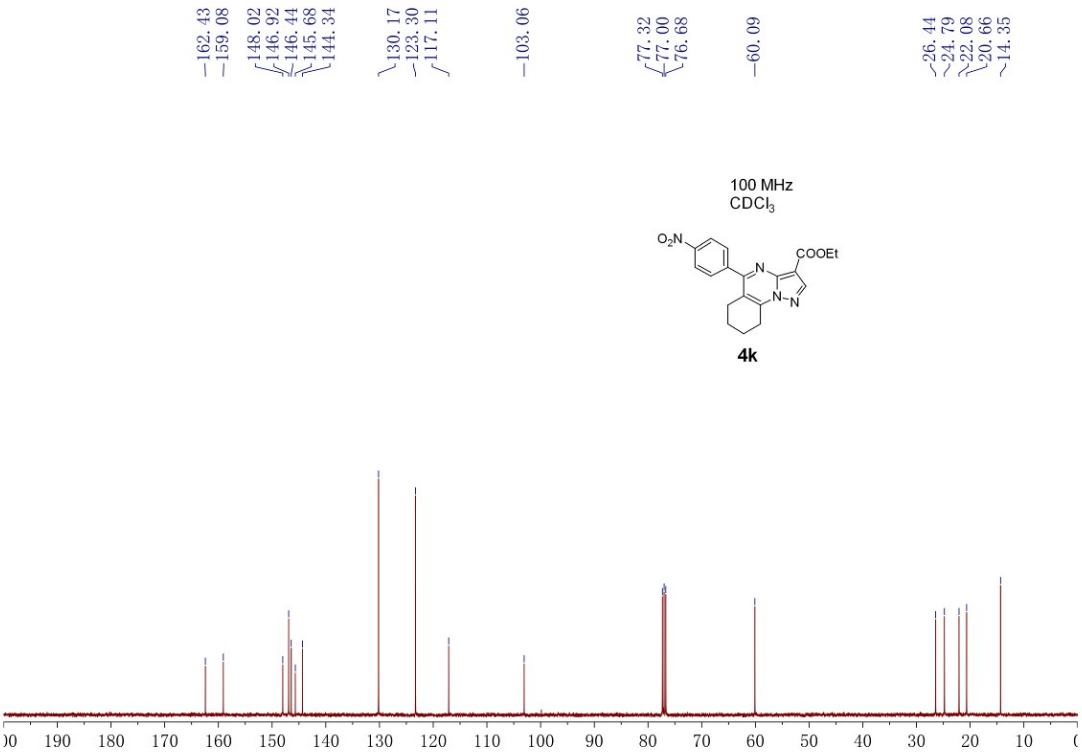
-0.5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130.17
123.30
117.11
103.06
77.32
77.00
76.68
60.09
26.44
24.79
22.08
20.66
14.35
100 MHz
CDCl3
O2N
COOEt
N
N-N
4k
190
180
170
160
150
140
130
120
110
100
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80
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20
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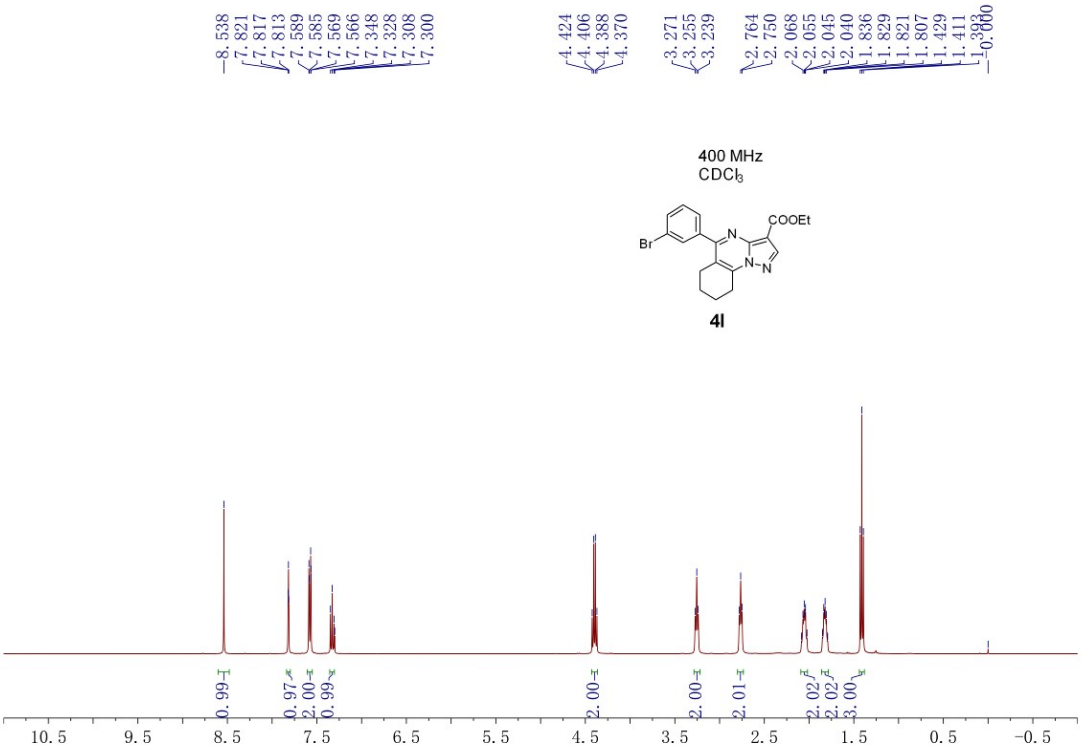
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7.566
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7.328
7.308
7.300
4.424
4.406
4.388
4.370
3.271
3.255
3.239
2.764
2.750
2.068
2.055
2.045
2.040
1.836
1.829
1.821
1.807
1.429
1.411
1.393
10.000
400 MHz
CDCl3
Br
COOEt
N
N-N
4l
0.99
0.97
2.00
0.99
2.00
2.00
2.01
2.02
2.02
3.00
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5.5
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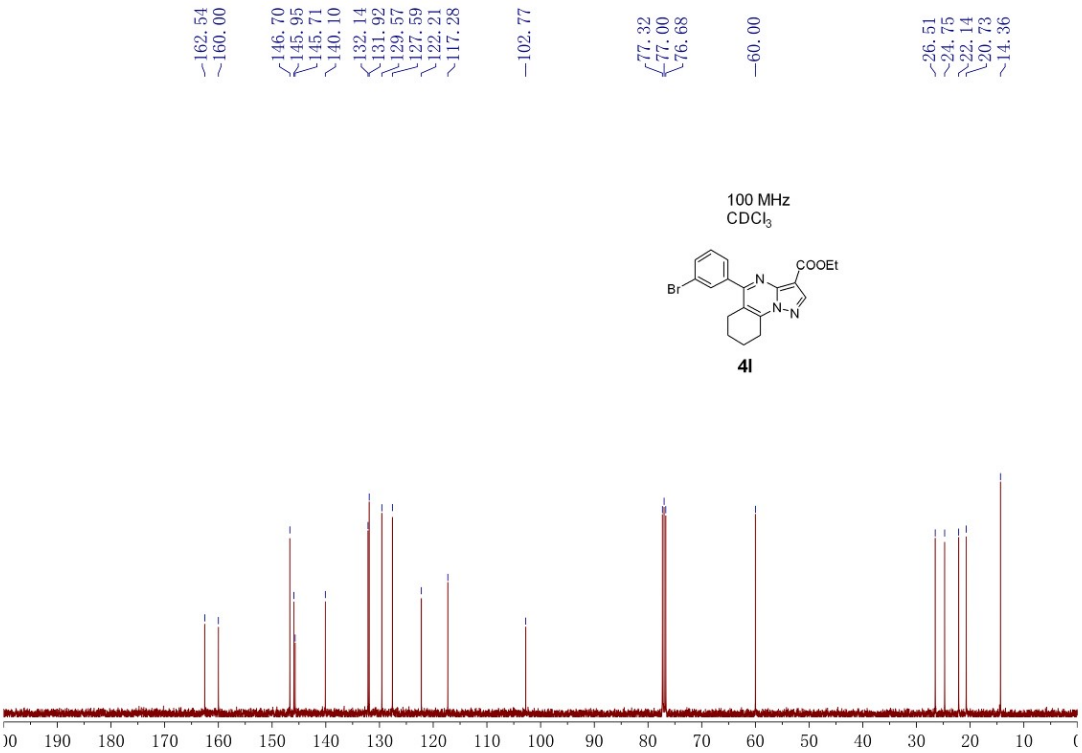
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131.92
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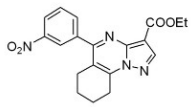
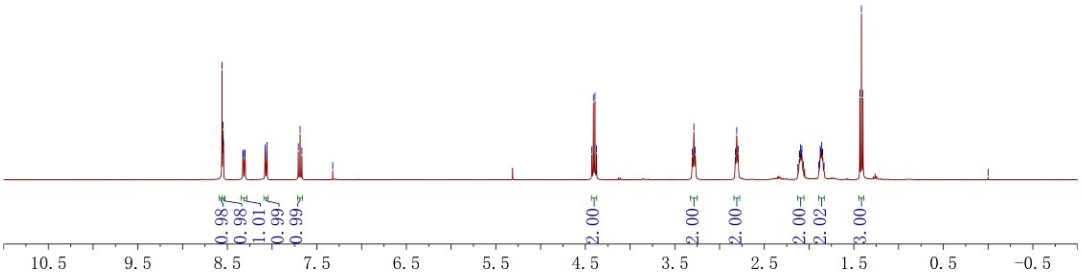
127.59
122.21
117.28
102.77
77.32
77.00
76.68
60.00
26.51
24.75
22.14
20.73
14.36
100 MHz
CDCl3
Br
COOEt
N
N-N
4l
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

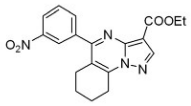
400 MHz
$CDCl_3$



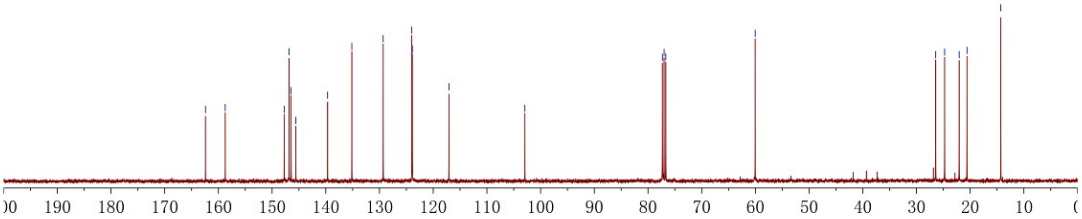
4m

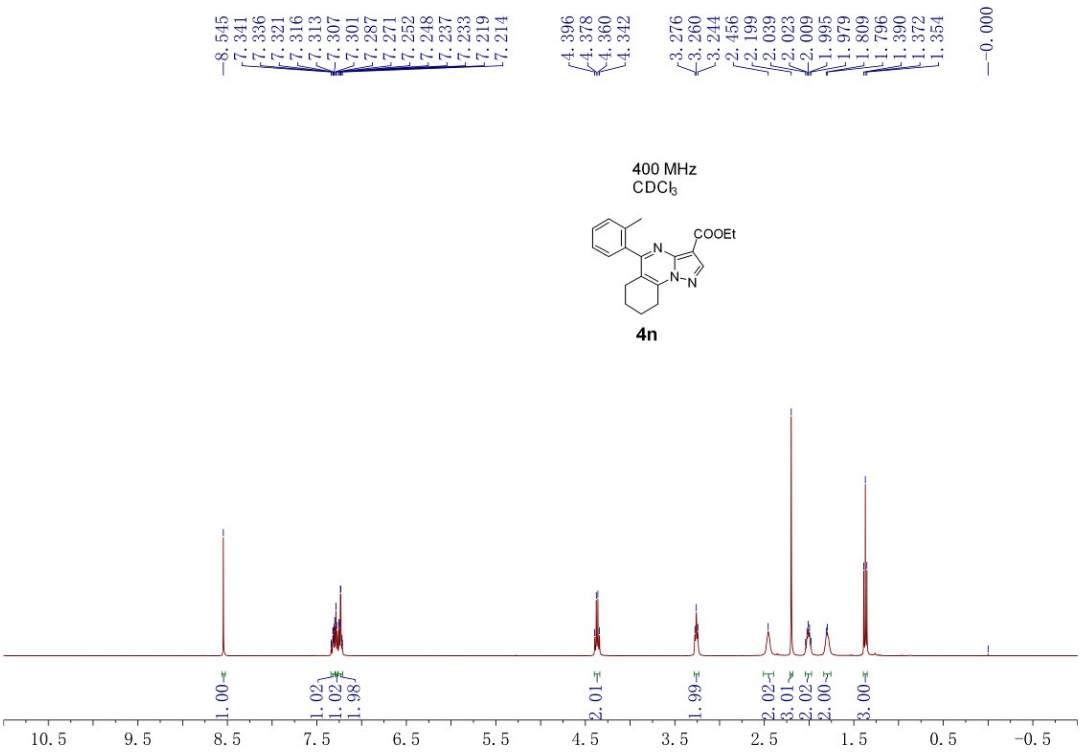


100 MHz
$CDCl_3$



4m

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7.313
7.307
7.301
7.287
7.271
7.252
7.248
7.237
7.233
7.219
7.214
4.396
4.378
4.360
4.342
3.276
3.260
3.244
2.456
2.199
2.039
2.023
2.009
1.995
1.979
1.809
1.796
1.390
1.372
1.354
0.000
400 MHz
CDCl3
COOEt
4n
1.00
1.02
1.02
1.98
2.01
1.99
2.02
3.01
2.02
2.00
3.00
10.5
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5.5
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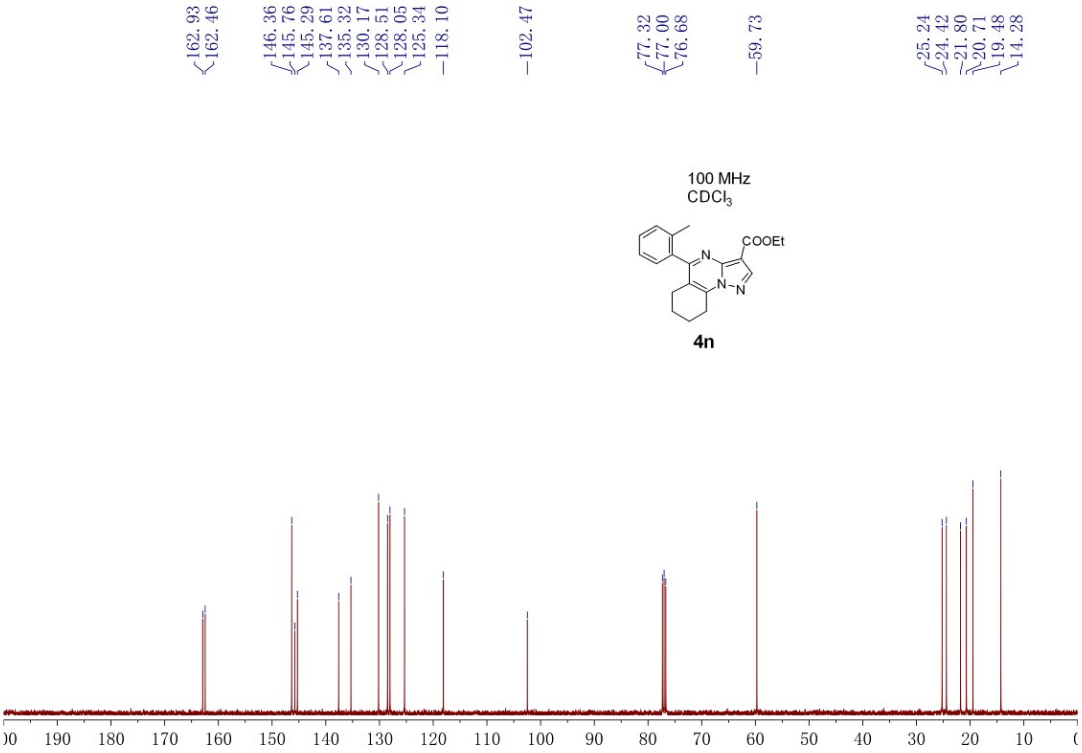
-0.5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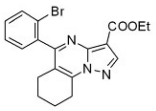
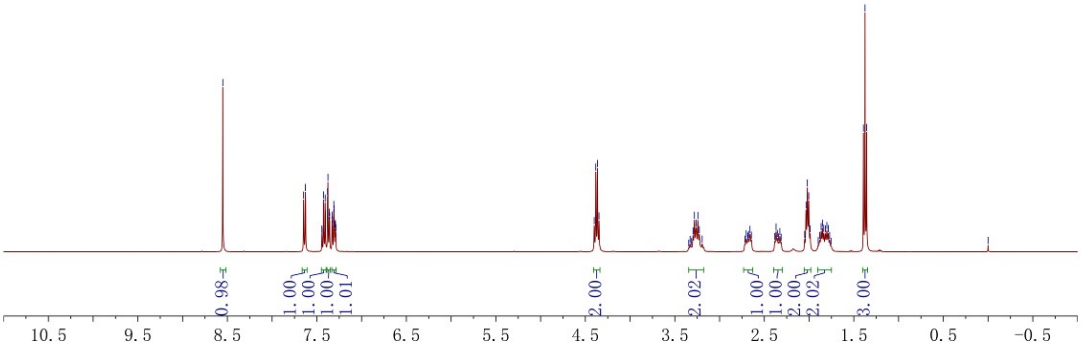
130.17
128.51
128.05
125.34
118.10
102.47
77.32
77.00
76.68
59.73
25.24
24.42
21.80
20.71
19.48
14.28
100 MHz
CDCl3
COOEt
4n
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

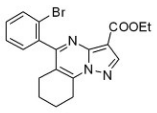
400 MHz
$CDCl_3$



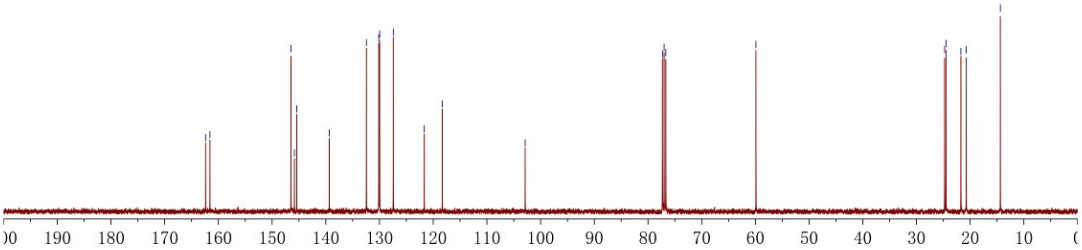
4o

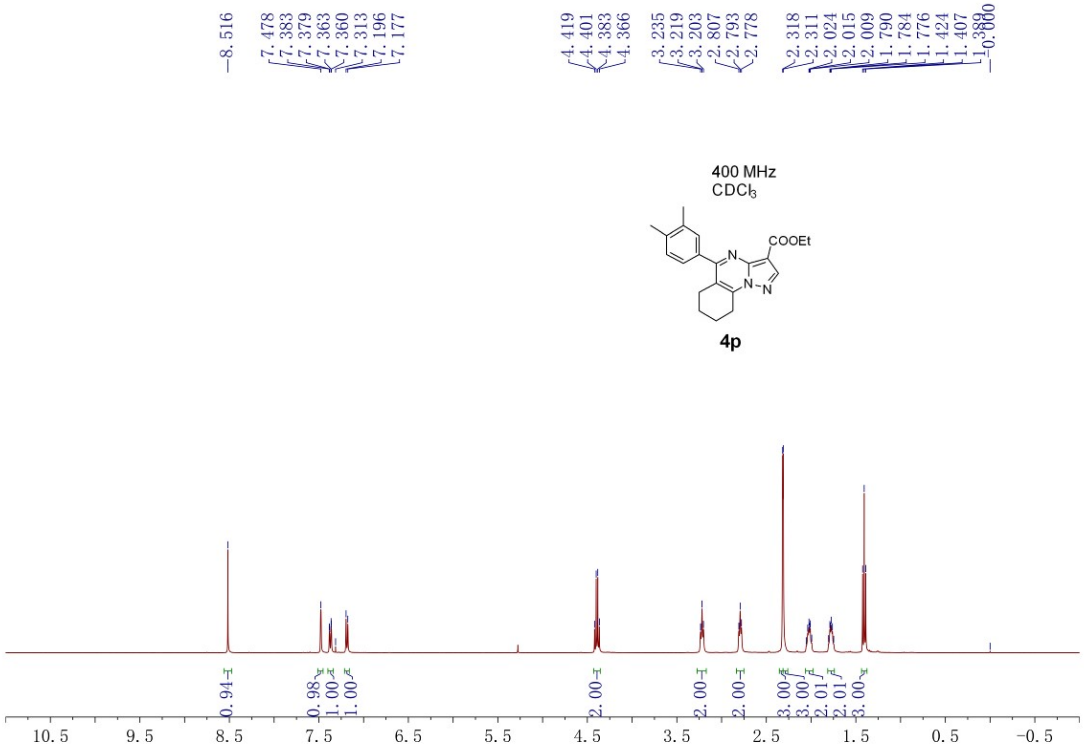


100 MHz
$CDCl_3$



4o

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7.383
7.379
7.363
7.360
7.313
7.196
7.177
4.419
4.401
4.383
4.366
3.235
3.219
3.203
2.807
2.793
2.778
2.318
2.311
2.024
2.015
2.009
1.790
1.784
1.776
1.424
1.407
1.389
0.000
400 MHz
CDCl3
COOEt
4p
0.94
0.98
1.00
1.00
2.00
2.00
2.00
3.00
3.00
2.01
2.01
3.00
10.5
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5.5
4.5
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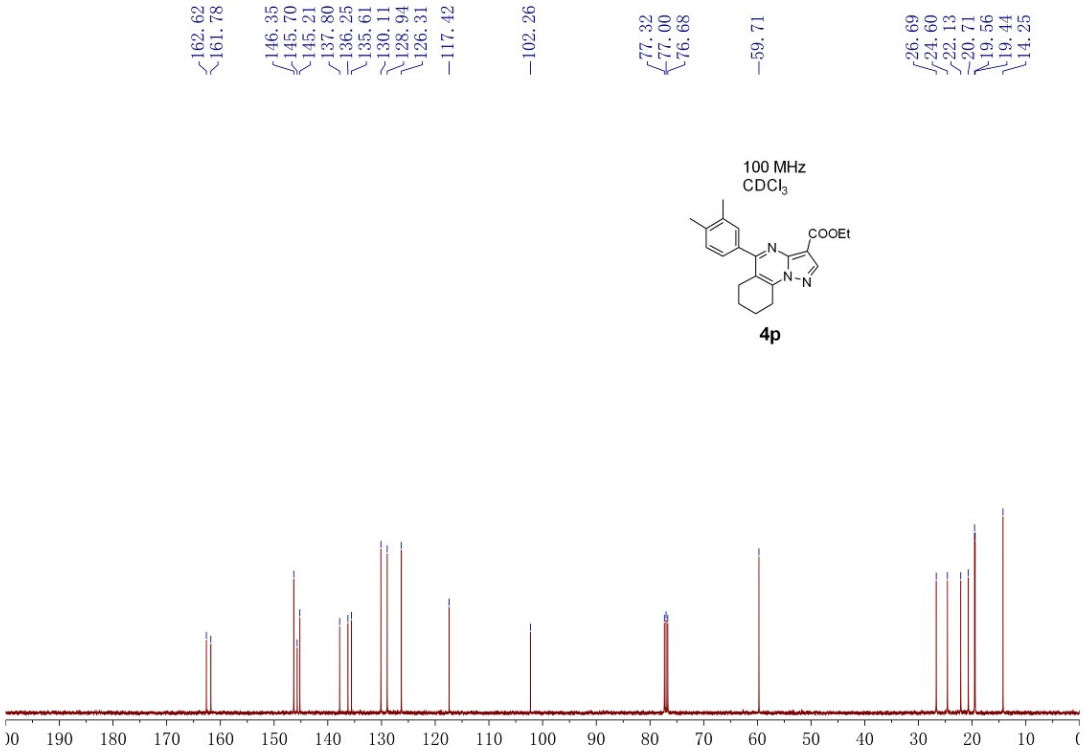
-0.5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126.31
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102.26
77.32
77.00
76.68
59.71
26.69
24.60
22.13
20.71
19.56
19.44
14.25
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COOEt
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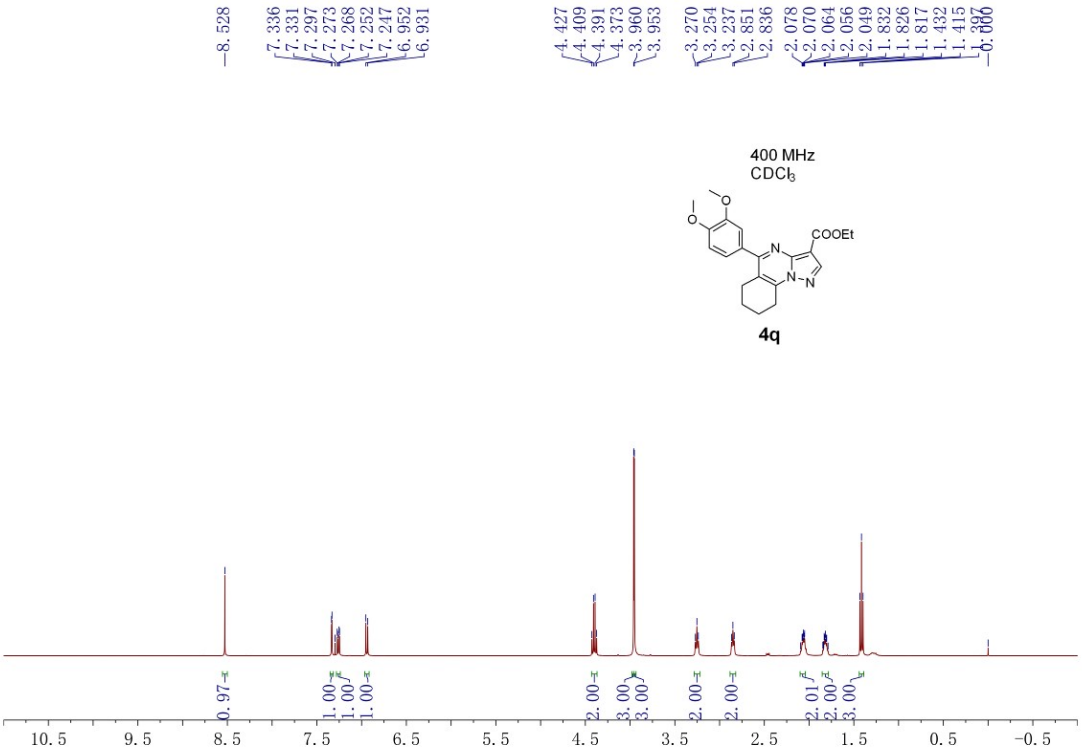
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3.960
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2.049
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1.415
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COOEt
4q
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3.00
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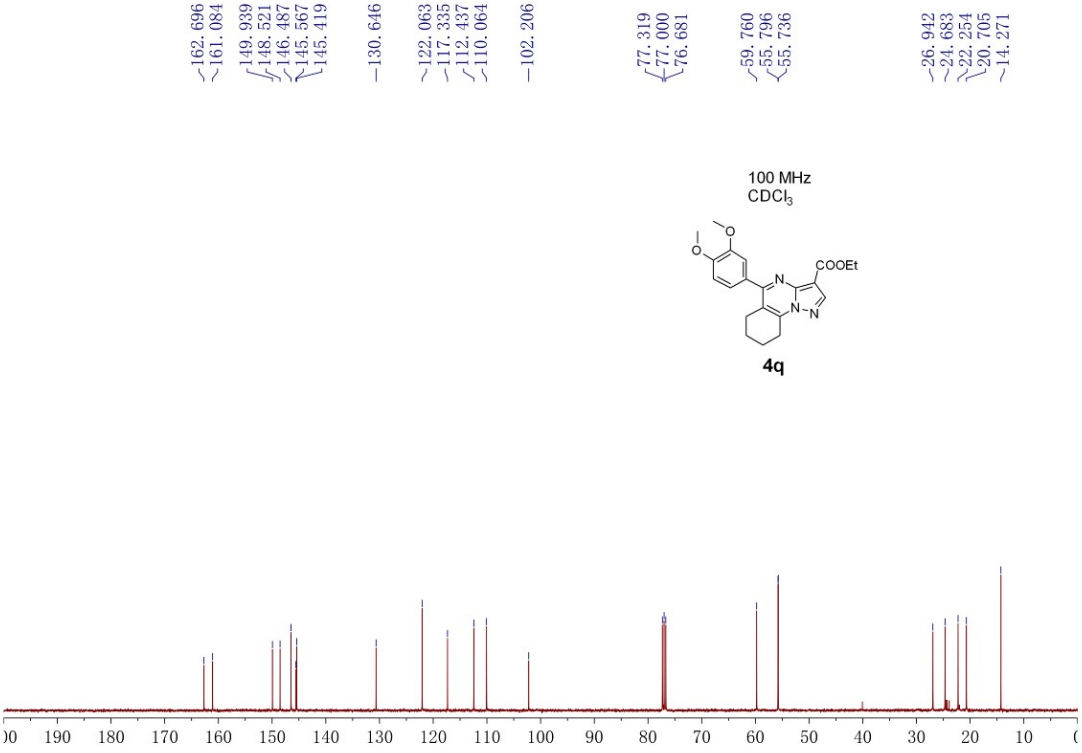
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COOEt
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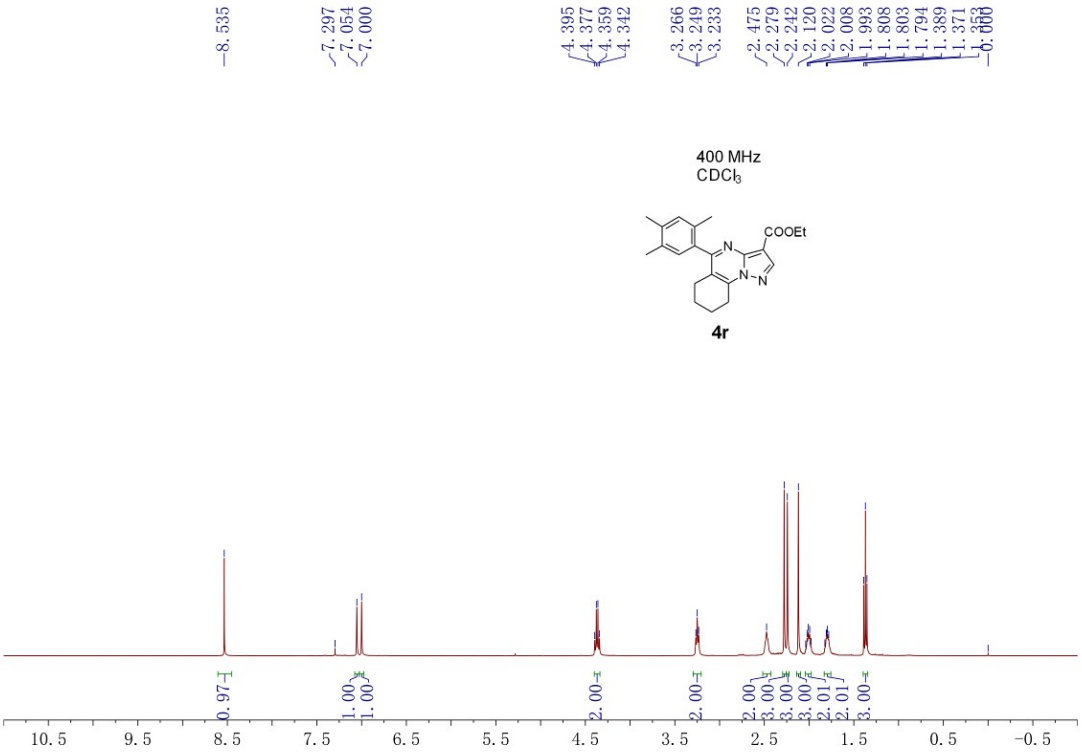
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1.803
1.794
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400 MHz
CDCl3
COOEt
4r
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1.00
2.00
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2.00
3.00
3.00
3.00
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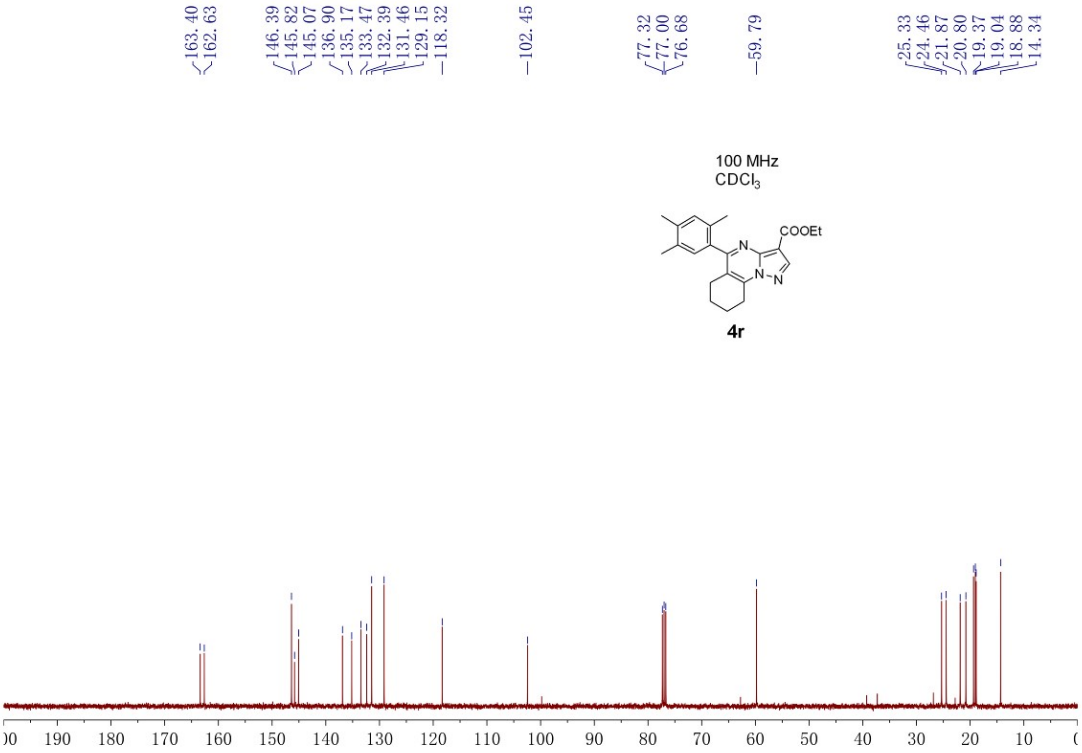
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77.00
76.68
59.79
25.33
24.46
21.87
20.80
19.37
19.04
18.88
14.34
100 MHz
CDCl3
COOEt
4r
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120
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20
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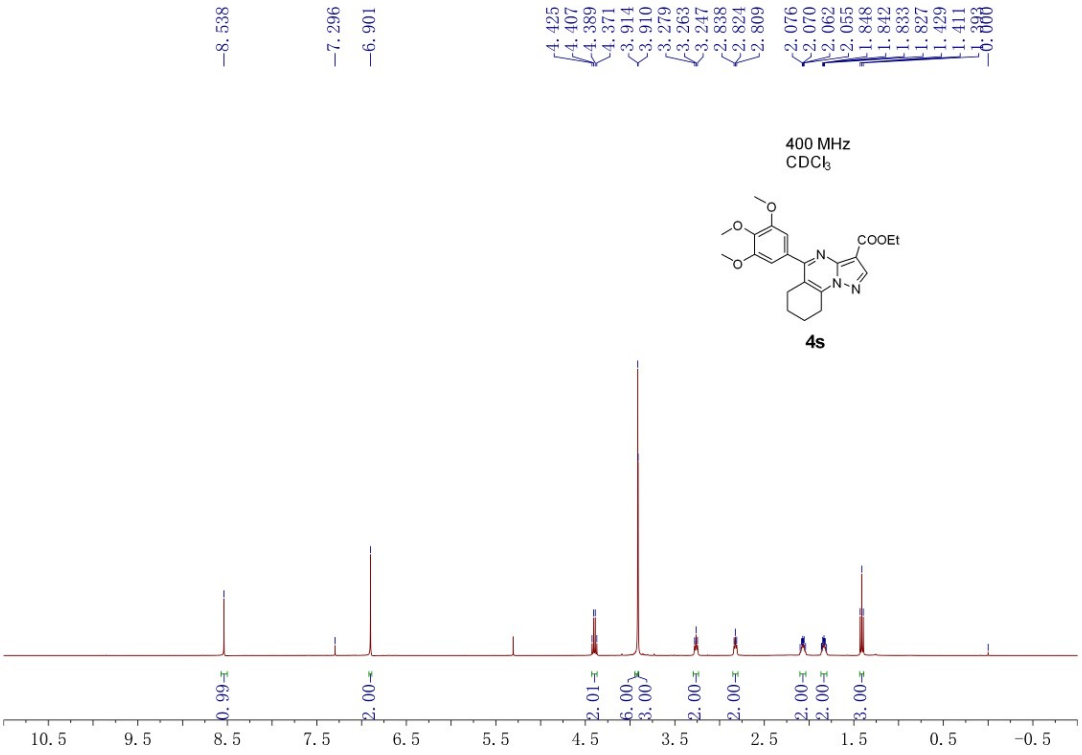
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COOEt
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6.00
3.00
2.00
2.00
2.00
2.00
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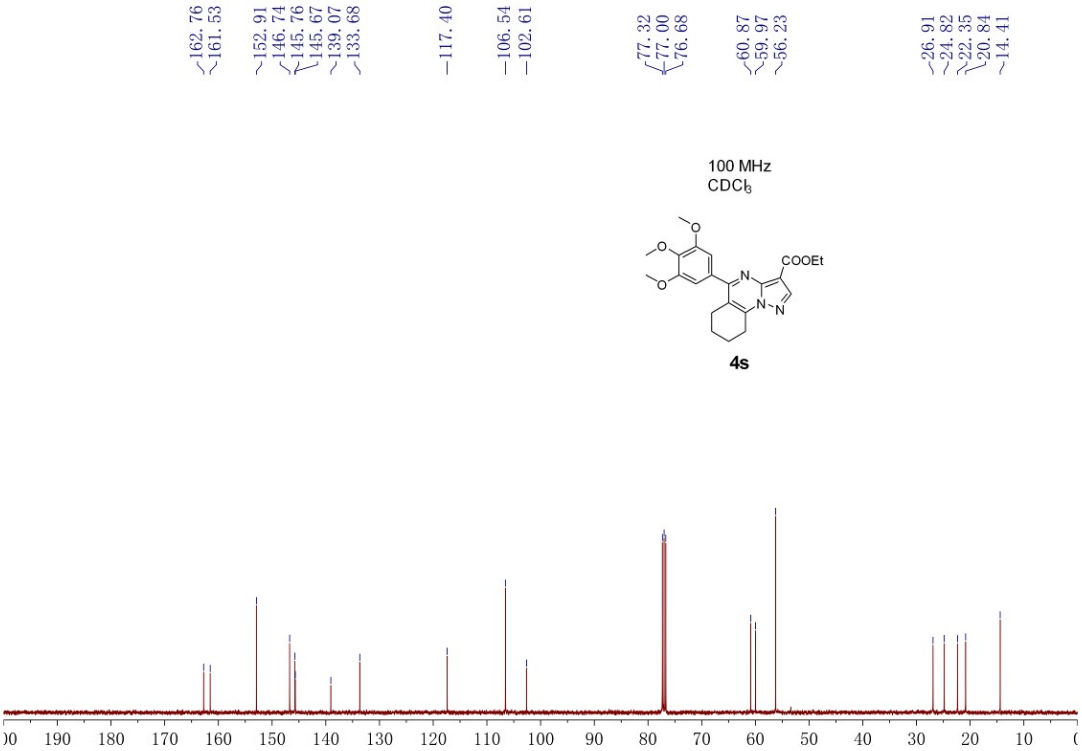
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26.91
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22.35
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14.41
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COOEt
4s
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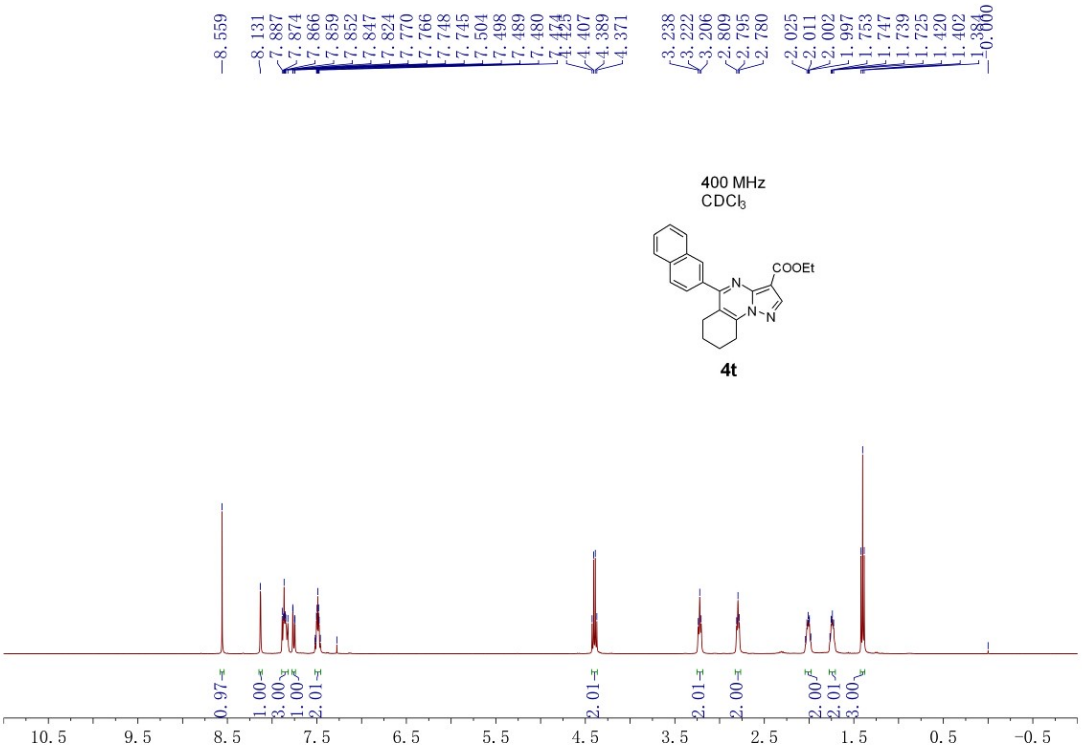
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7.745
7.504
7.498
7.489
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400 MHz
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COOEt
4t
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1.00
2.01
2.01
2.01
2.00
2.00
2.01
3.00
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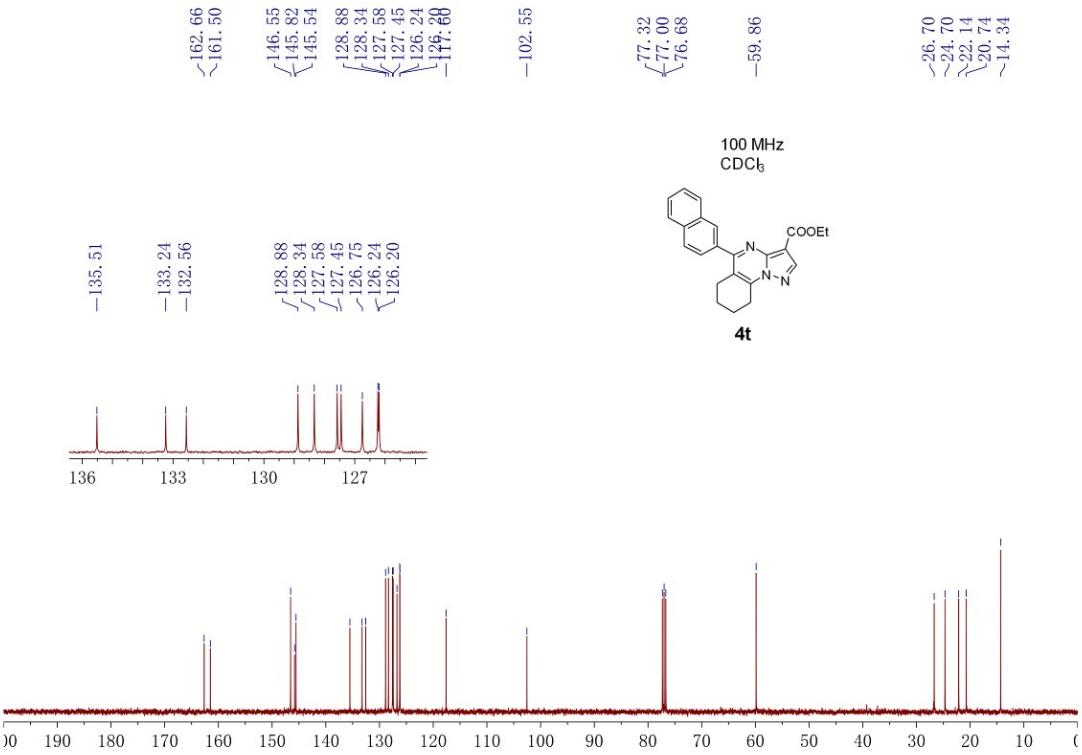
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100 MHz
CDCl3
COOEt
4t
135.51
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127.58
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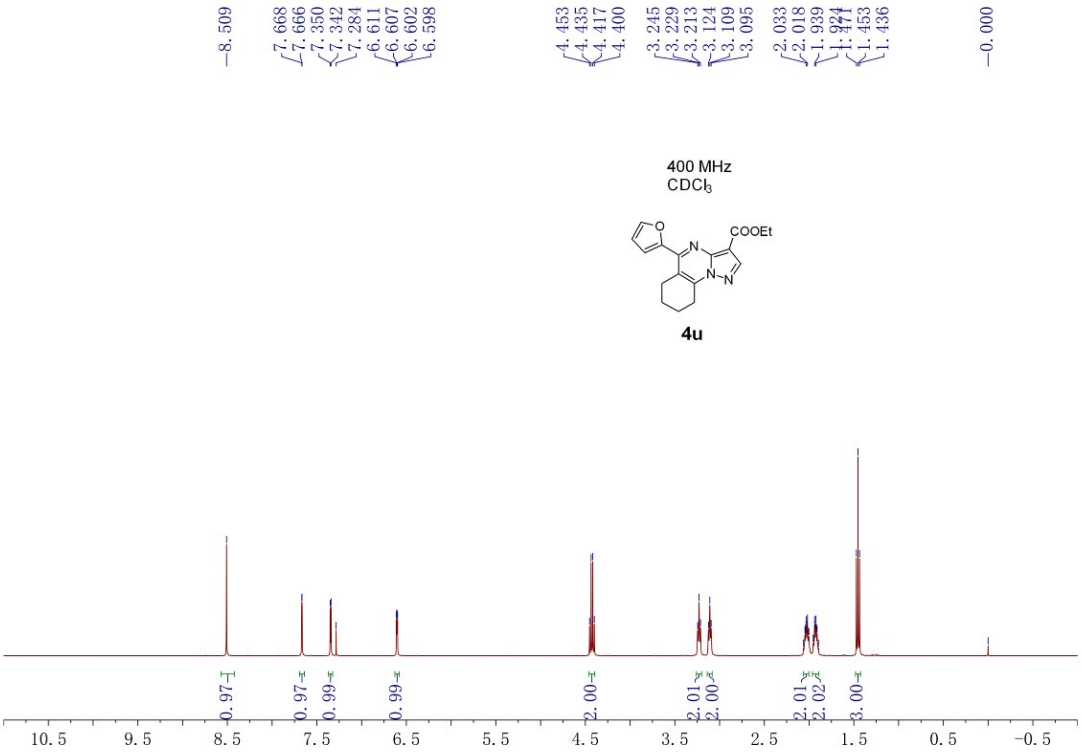
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3.229
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3.095
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2.018
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1.436
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400 MHz
CDCl3
COOEt
4u
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0.97
0.99
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2.00
2.01
2.02
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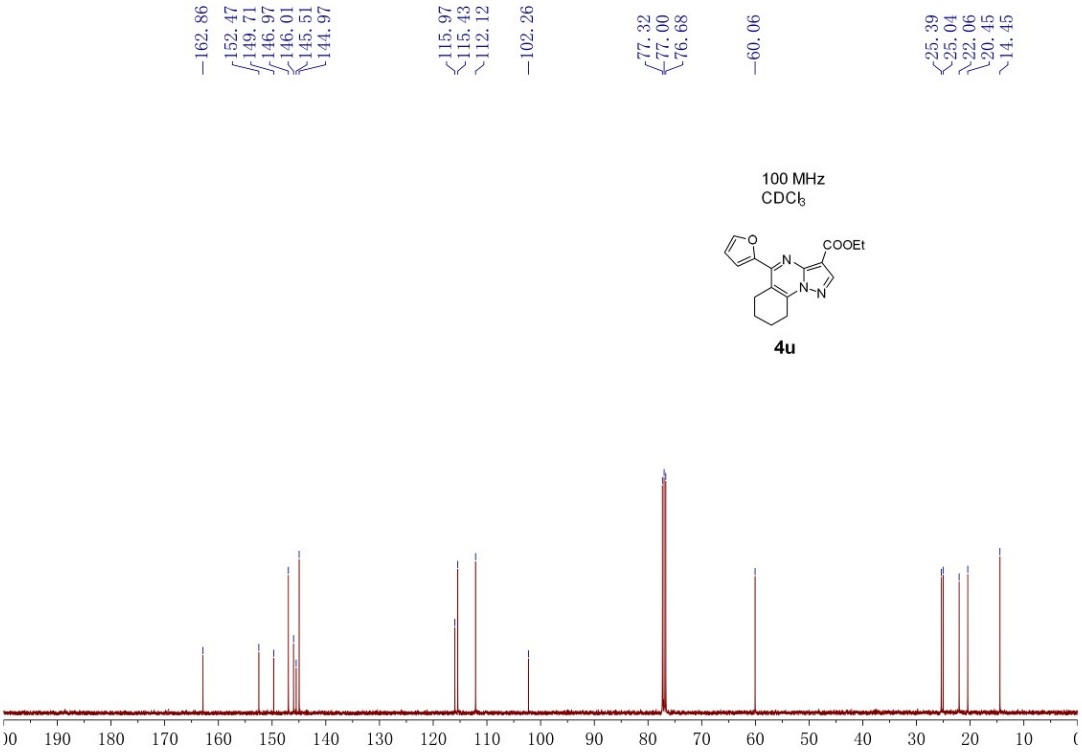
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25.39
25.04
22.06
20.45
14.45
100 MHz
CDCl3
COOEt
4u
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150
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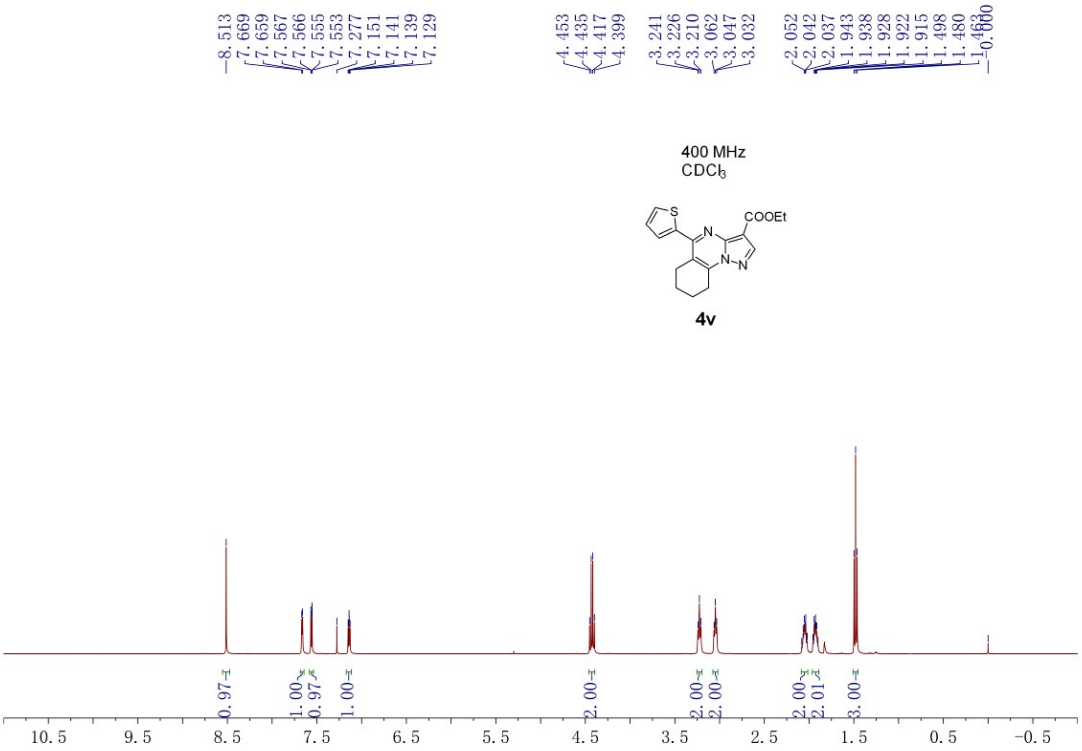
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400 MHz
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S
N
N
N
COOEt
4v
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0.97
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2.00
2.00
2.00
2.01
3.00
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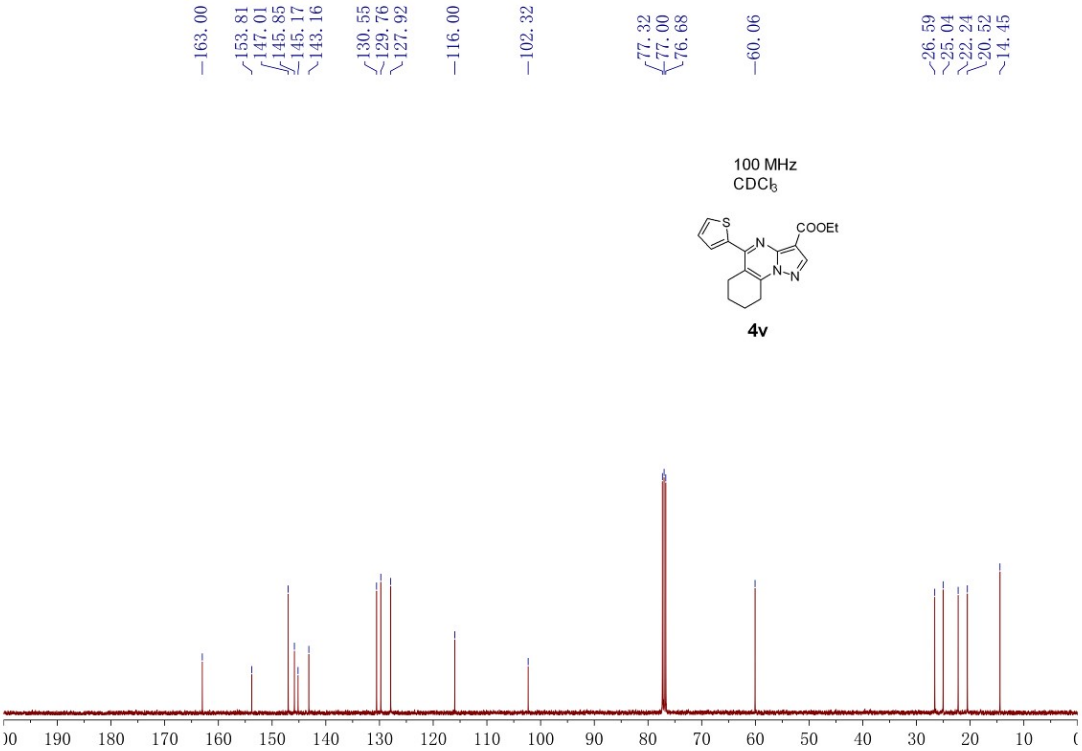
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26.59
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22.24
20.52
14.45
100 MHz
CDCl3
S
N
N
N
COOEt
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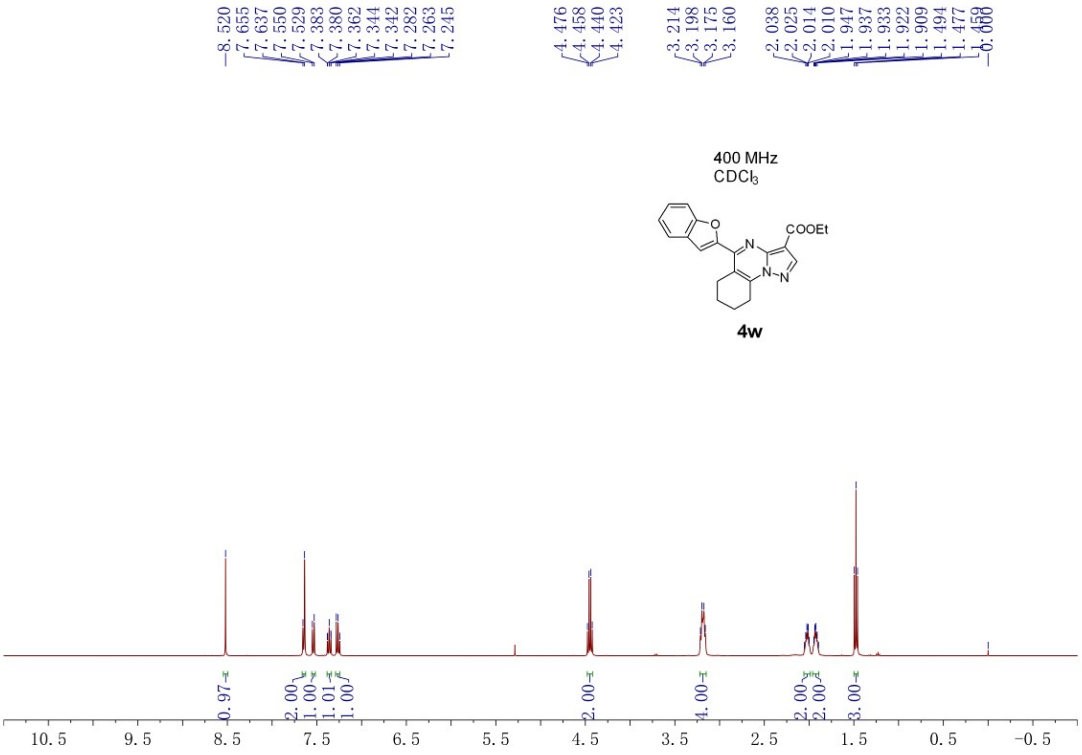
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COOEt
4w
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2.00
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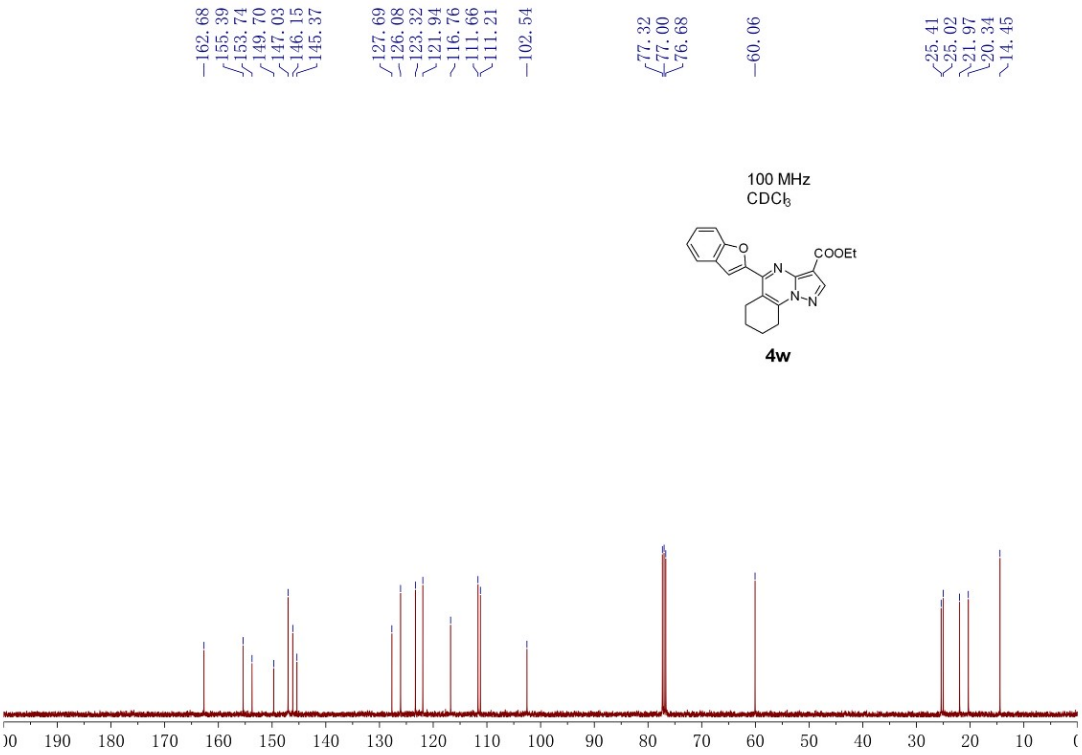
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76.68
60.06
25.41
25.02
21.97
20.34
14.45
100 MHz
CDCl3
COOEt
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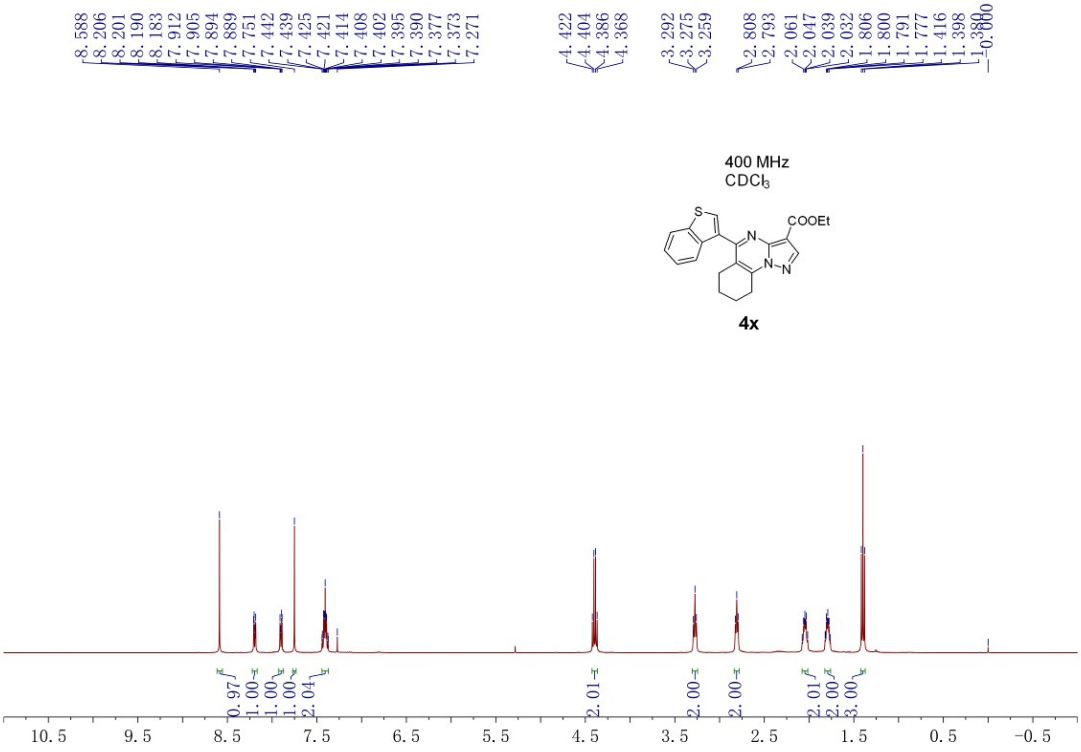
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COOEt
4x
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2.00
2.00
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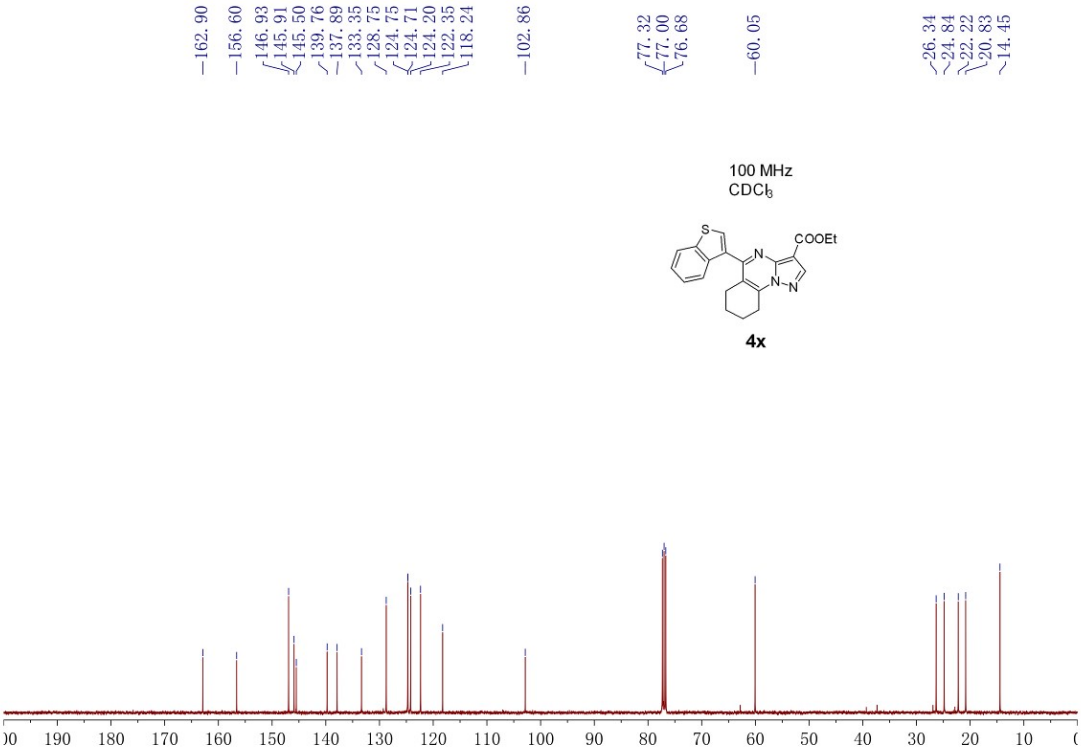
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26.34
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22.22
20.83
14.45
100 MHz
CDCl3
COOEt
4x
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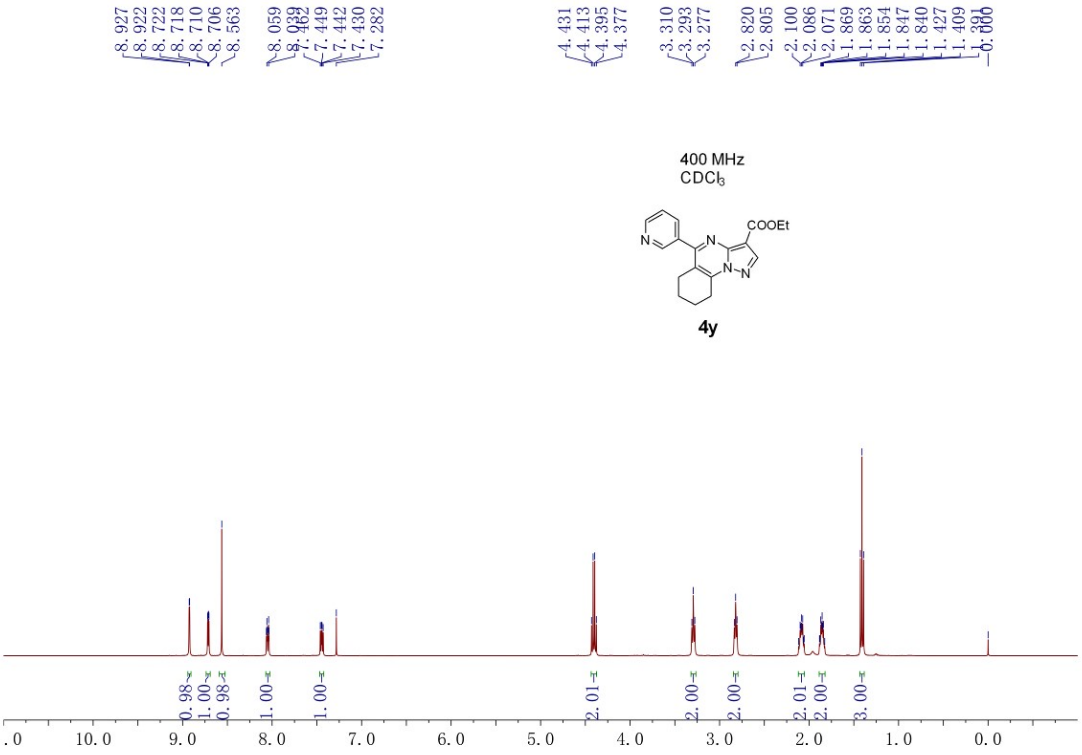
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1.391
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400 MHz
CDCl3
COOEt
4y
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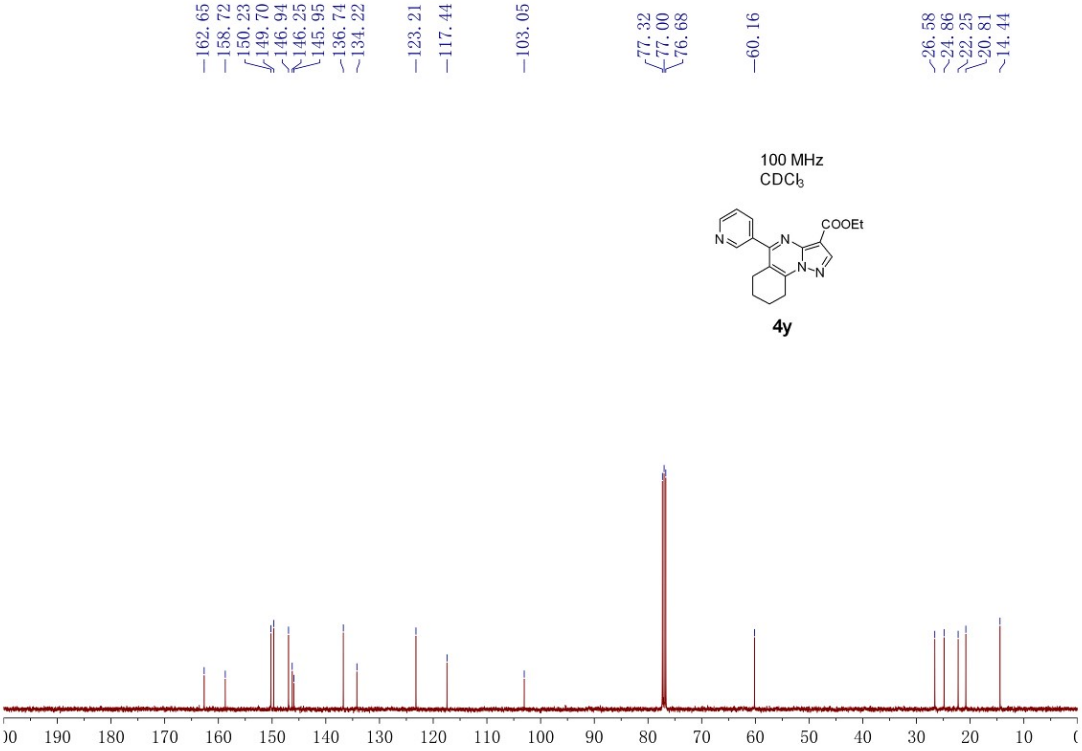
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26.58
24.86
22.25
20.81
14.44
100 MHz
CDCl3
COOEt
4y
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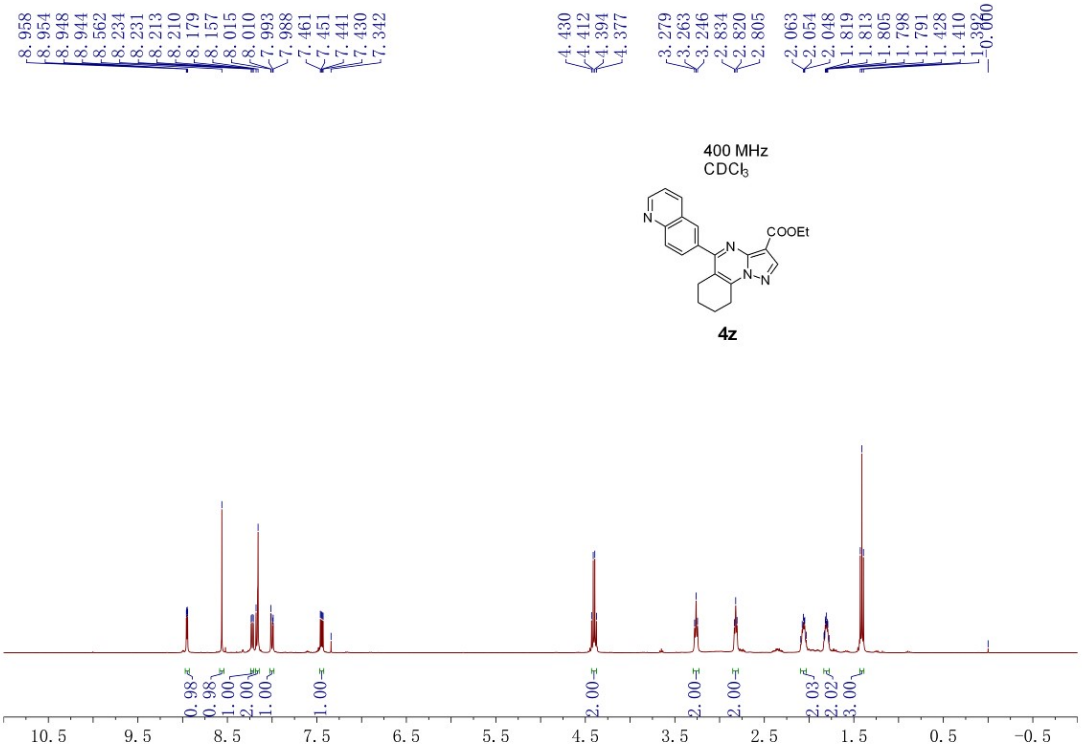
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COOEt
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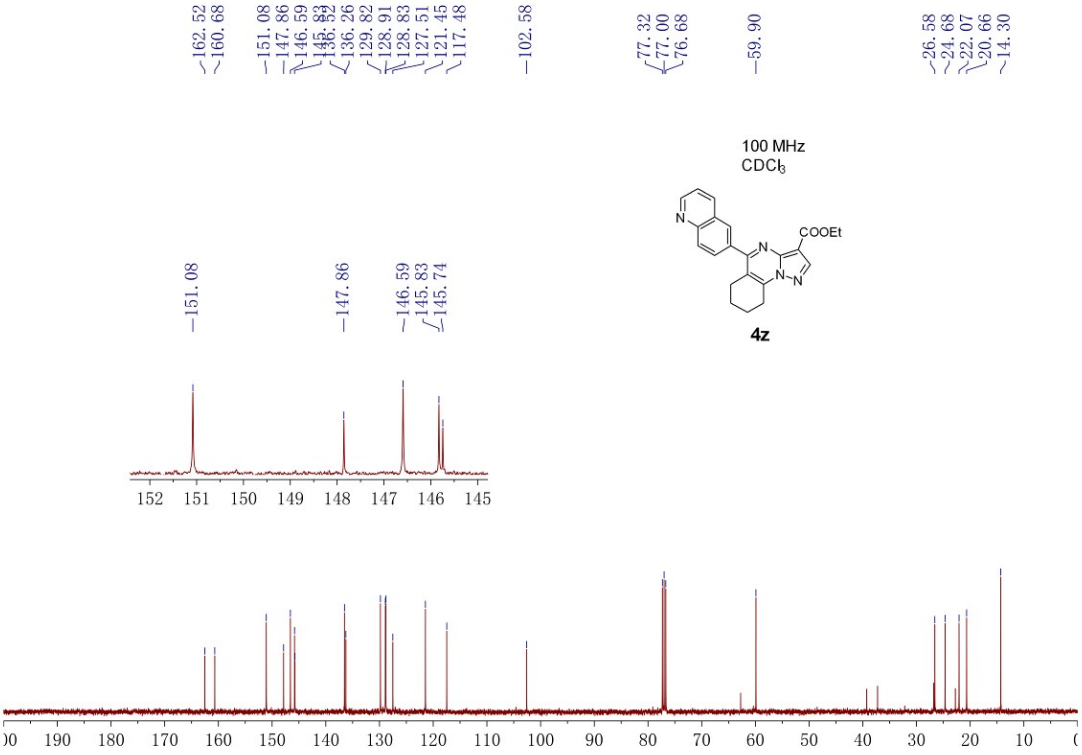
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24.68
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14.30
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CDCl3
COOEt
4z
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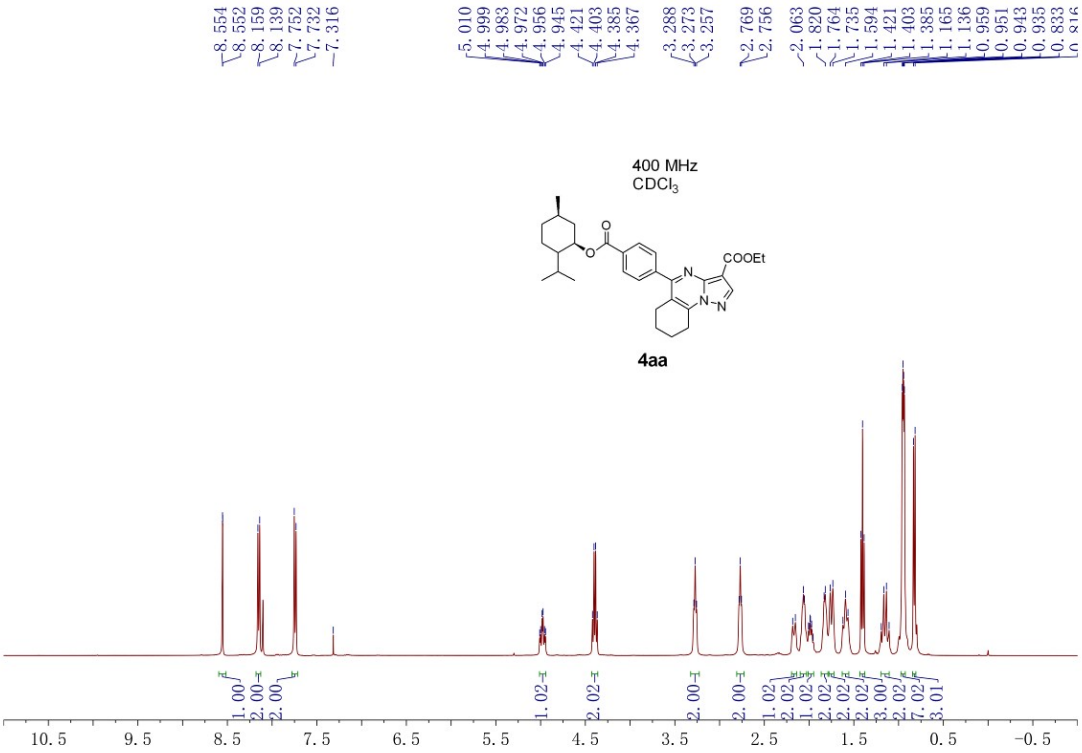
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400 MHz
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COOEt
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2.02
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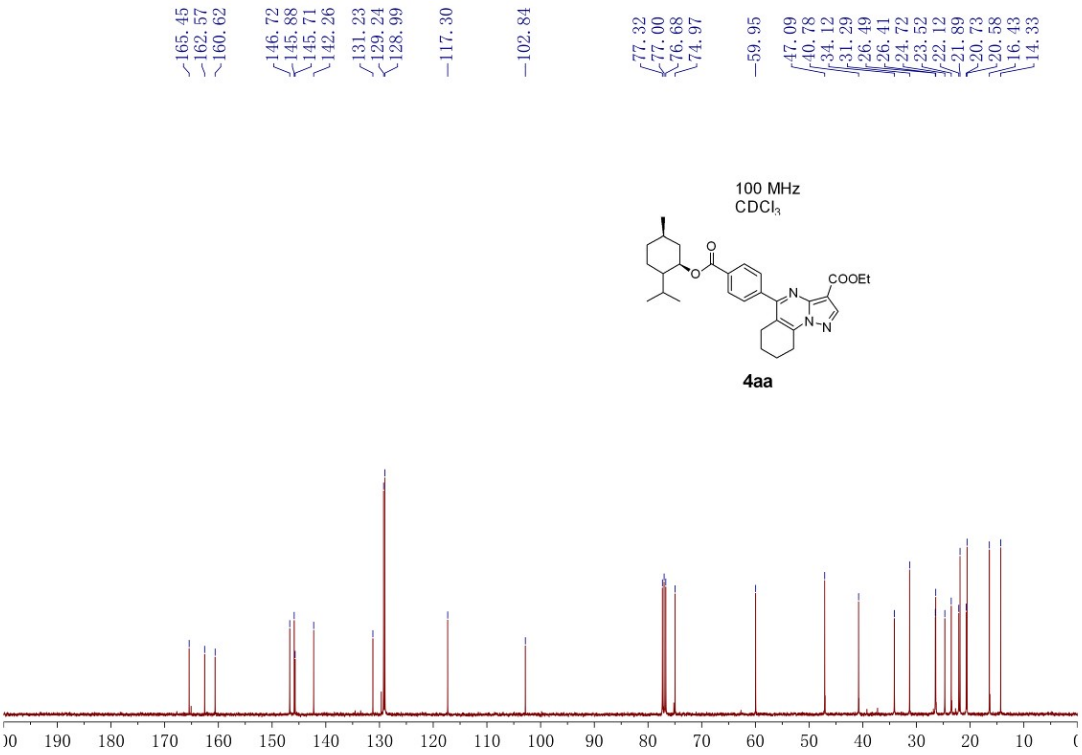
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77.32
77.00
76.68
74.97
59.95
47.09
40.78
34.12
31.29
26.49
26.41
24.72
23.52
22.12
21.89
20.73
20.58
16.43
14.33
100 MHz
CDCl3
COOEt
4aa
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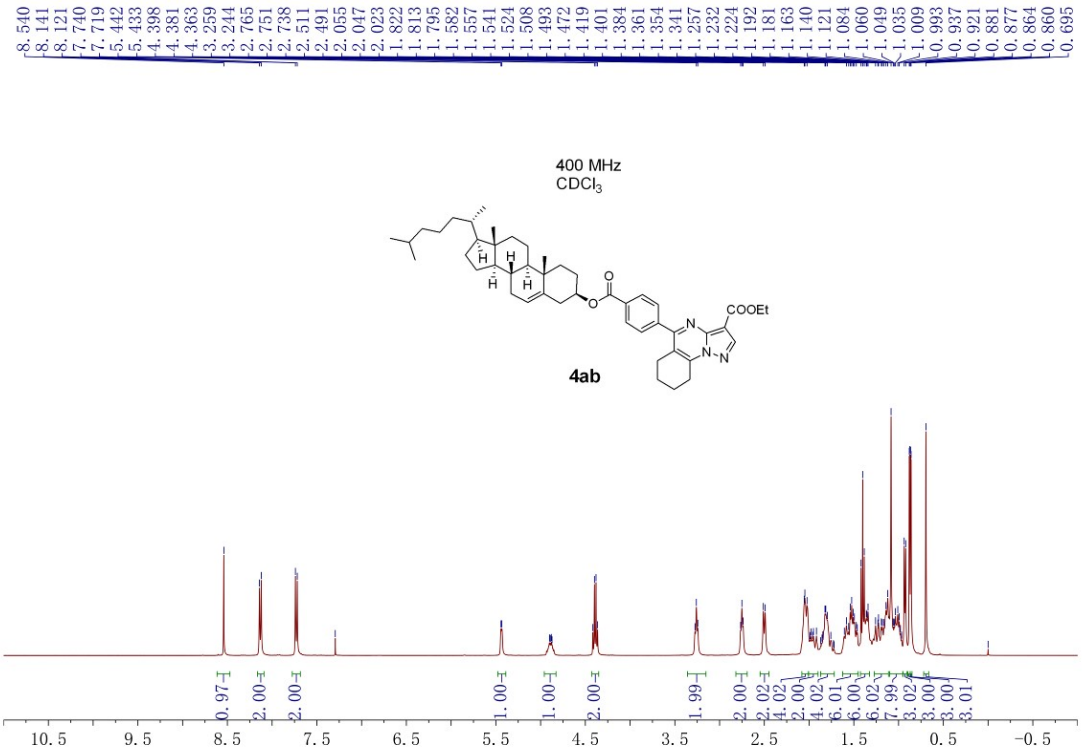
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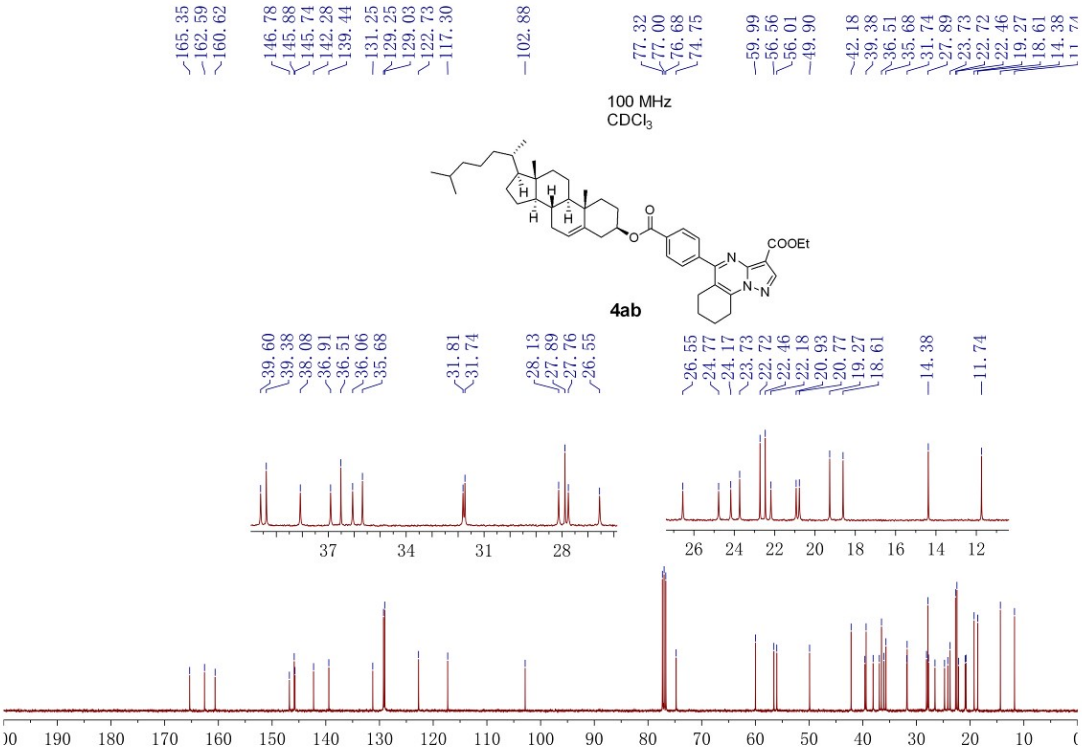
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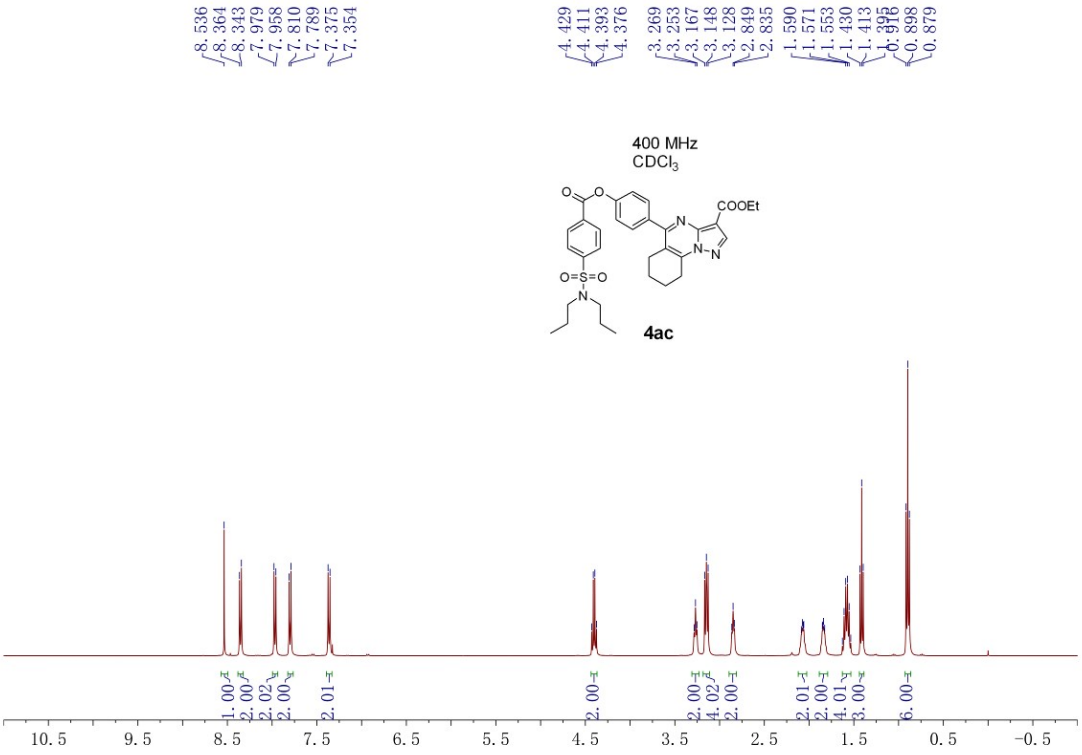
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4.411
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4.376
3.269
3.253
3.167
3.148
3.128
2.849
2.835
1.590
1.571
1.553
1.430
1.413
0.916
0.898
0.879
400 MHz
CDCl3
COOEt
4ac
1.00
2.00
2.02
2.00
2.01
2.00
2.00
4.02
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4.01
3.00
6.00
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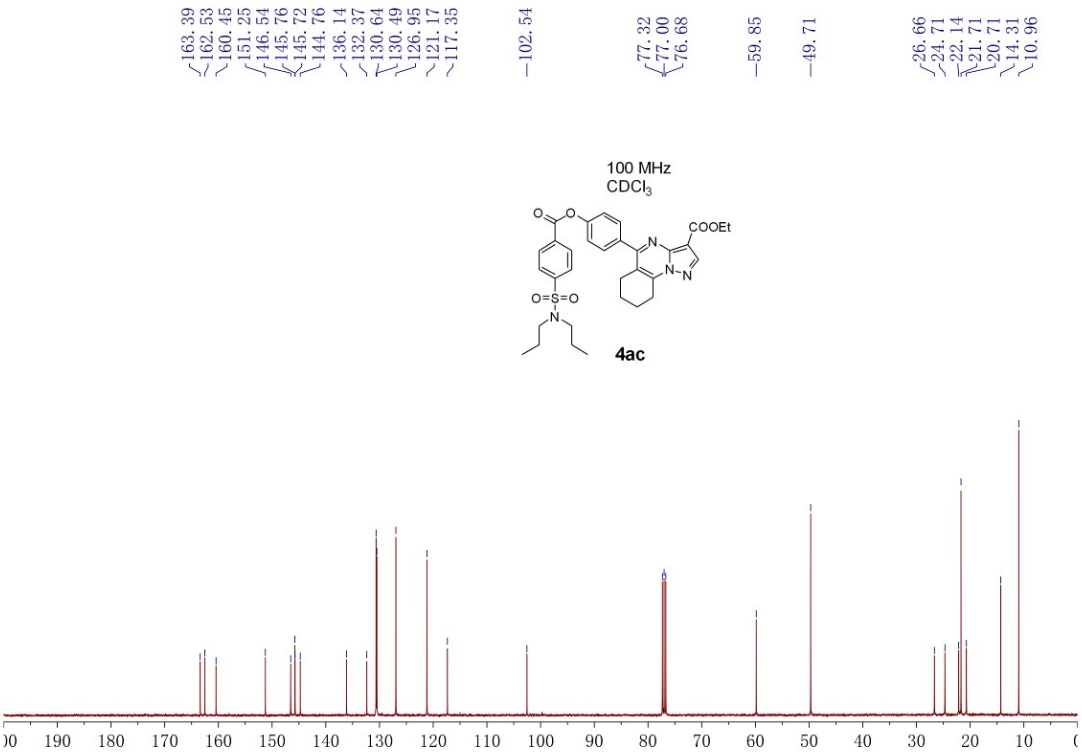
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117.35
102.54
77.32
77.00
76.68
59.85
49.71
26.66
24.71
22.14
21.71
20.71
14.31
10.96
100 MHz
CDCl3
COOEt
4ac
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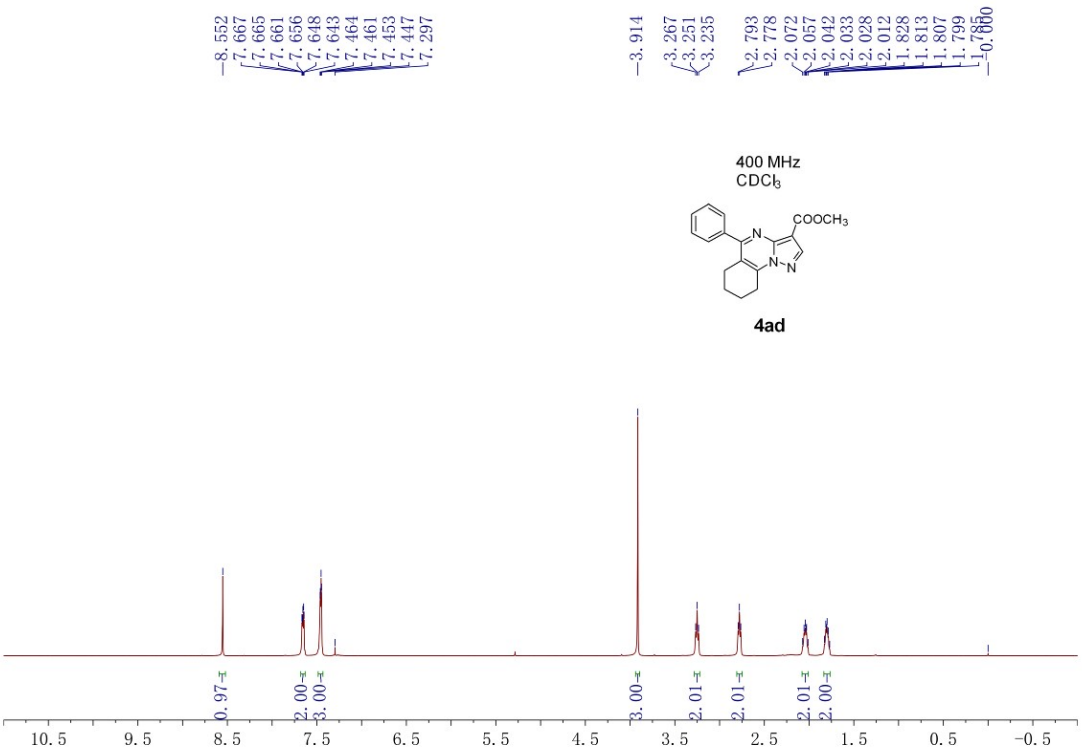
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7.453
7.447
7.297
3.914
3.267
3.251
3.235
2.793
2.778
2.072
2.057
2.042
2.033
2.028
2.012
1.828
1.813
1.807
1.799
1.785
1.000
400 MHz
CDCl3
COOCH3
4ad
0.97
2.00
3.00
3.00
2.01
2.01
2.01
2.00
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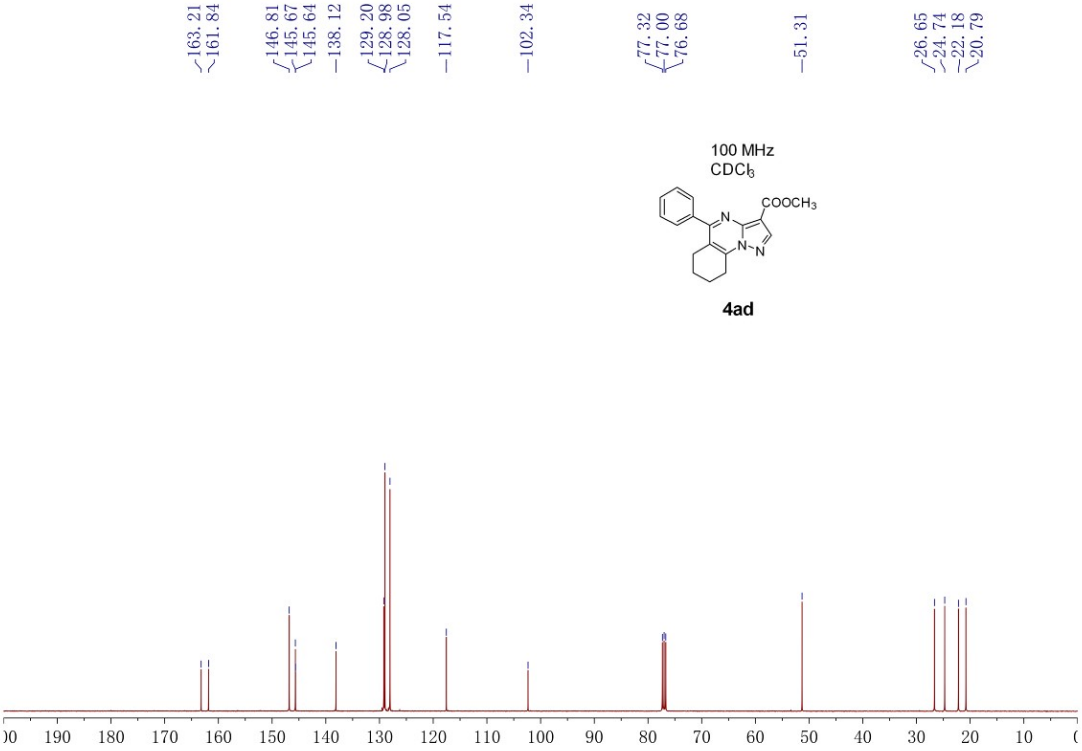
-0.5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76.68
51.31
26.65
24.74
22.18
20.79
100 MHz
CDCl3
COOCH3
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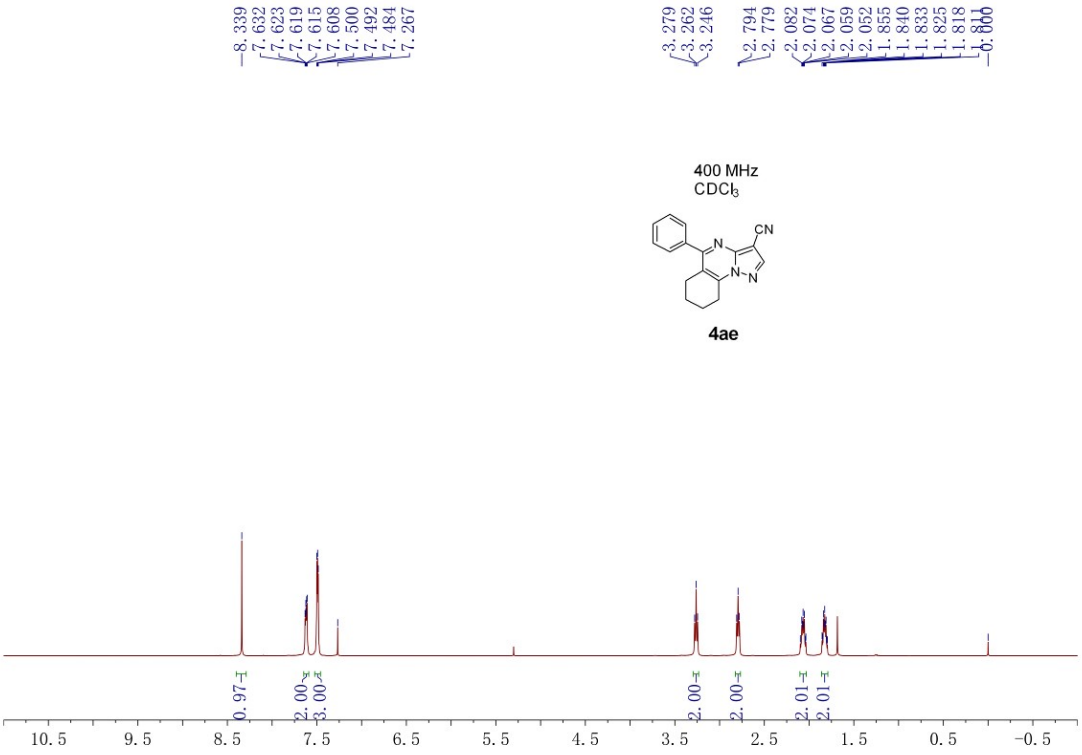
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7.619
7.615
7.608
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7.492
7.484
7.267
3.279
3.262
3.246
2.794
2.779
2.082
2.074
2.067
2.059
2.052
1.855
1.840
1.833
1.825
1.818
1.811
0.000
400 MHz
CDCl3
CN
N
N
N
4ae
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3.00
2.00
2.00
2.01
2.01
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4.5
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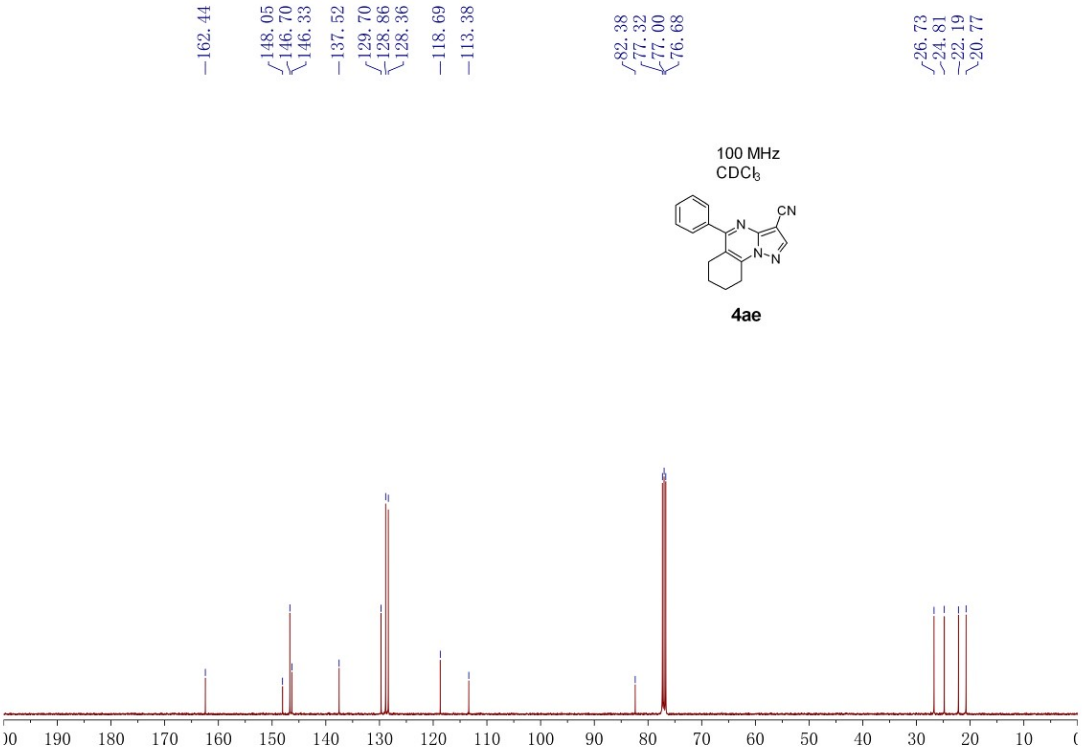
-0.5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113.38
82.38
77.32
77.00
76.68
26.73
24.81
22.19
20.77
100 MHz
CDCl3
CN
N
N
N
4ae
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180
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160
150
140
130
120
110
100
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80
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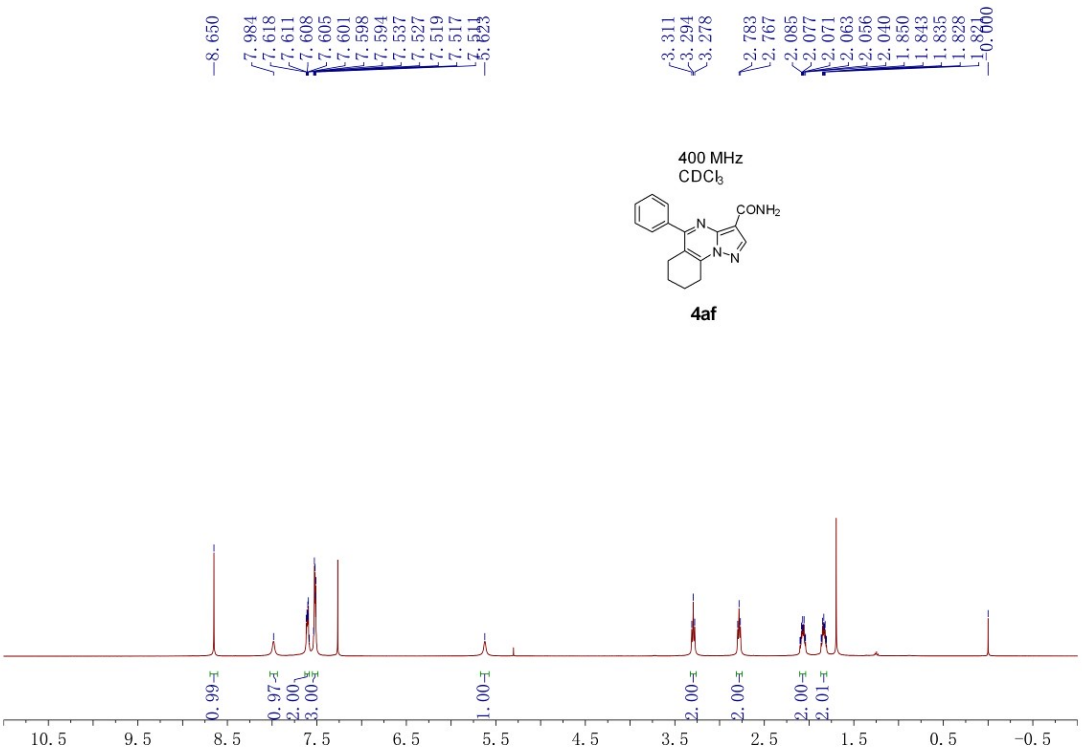
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7.598
7.594
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7.527
7.519
7.517
7.511
5.623
3.311
3.294
3.278
2.783
2.767
2.085
2.077
2.071
2.063
2.056
2.040
1.850
1.843
1.835
1.828
1.821
0.000
400 MHz
CDCl3
CONH2
4af
0.99
0.97
2.00
3.00
1.00
2.00
2.00
2.00
2.01
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7.5
6.5
5.5
4.5
3.5
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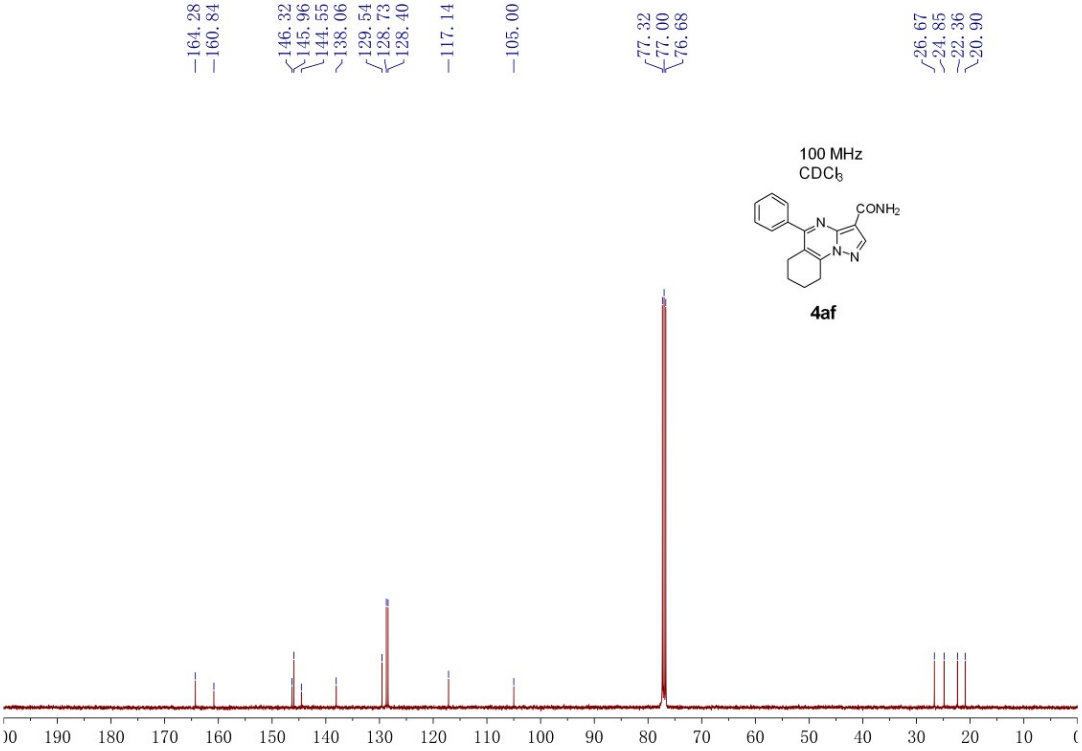
0.5
-0.5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117.14
105.00
77.32
77.00
76.68
26.67
24.85
22.36
20.90
100 MHz
CDCl3
CONH2
4af
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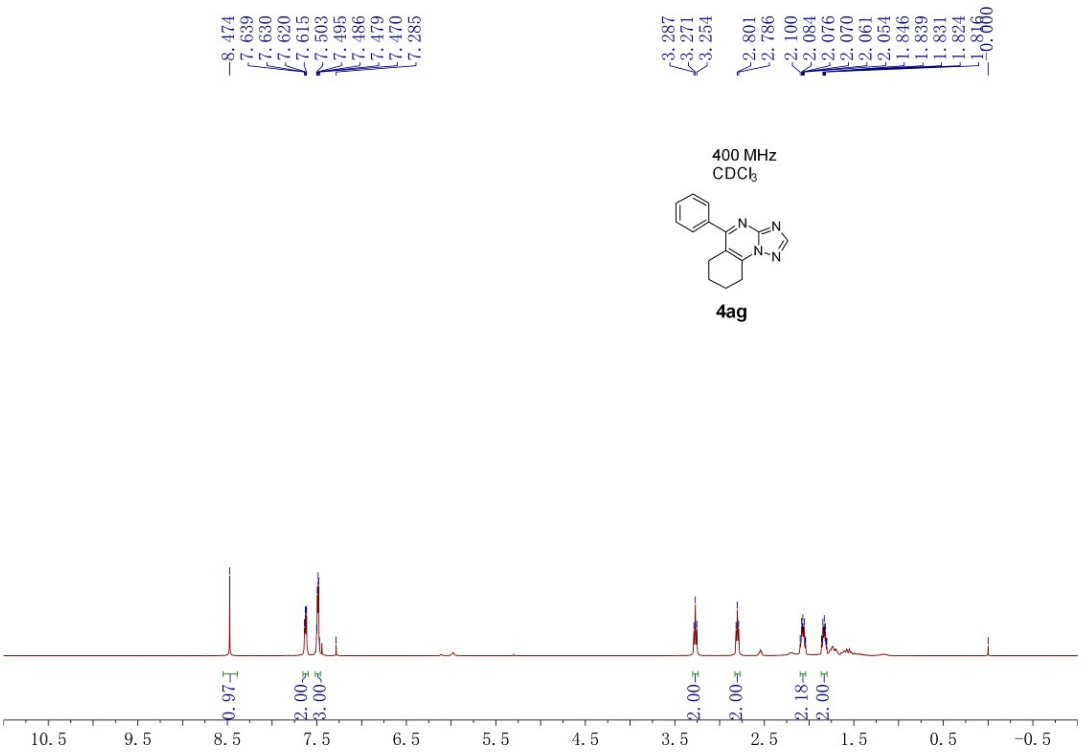
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10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2.100
2.084
2.076
2.070
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2.054
1.846
1.839
1.831
1.824
1.816
10.000
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CDCl3
4ag
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3.00
2.00
2.00
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2.00
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5.5
4.5
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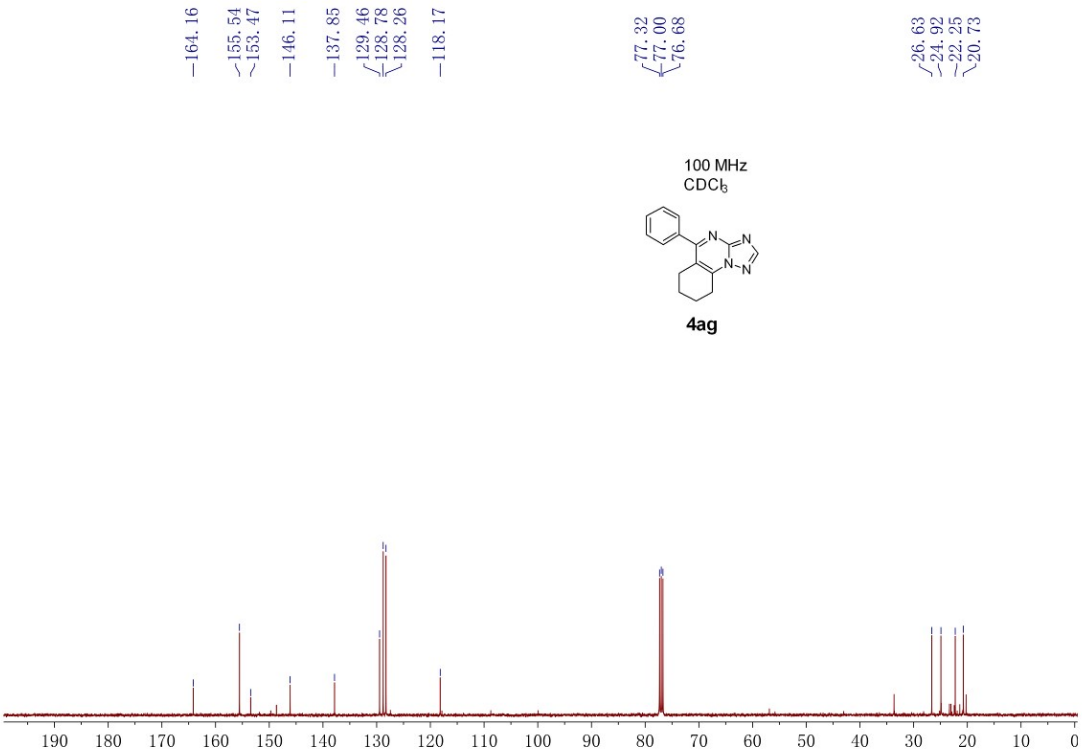
-0.5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24.92
22.25
20.73
100 MHz
CDCl3
4ag
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


7.651
7.647
7.644
7.636
7.632
7.629
7.627
7.497
7.495
7.491
7.488
7.482
7.308
4.591
4.589
4.573
4.571
4.555
4.553
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4.536
3.353
3.338
3.322
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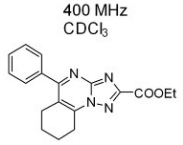
0.000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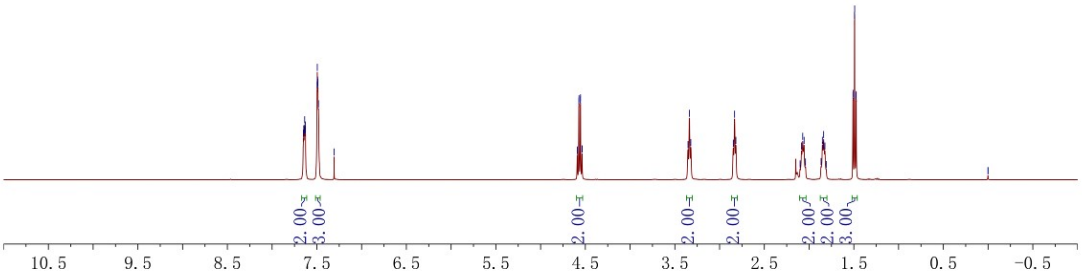
COOEt

4ah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2.00
3.00
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6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5


165.51
160.44
156.90
153.52
146.60
137.39
129.70
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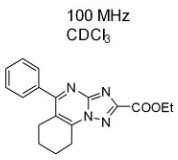
100 MHz
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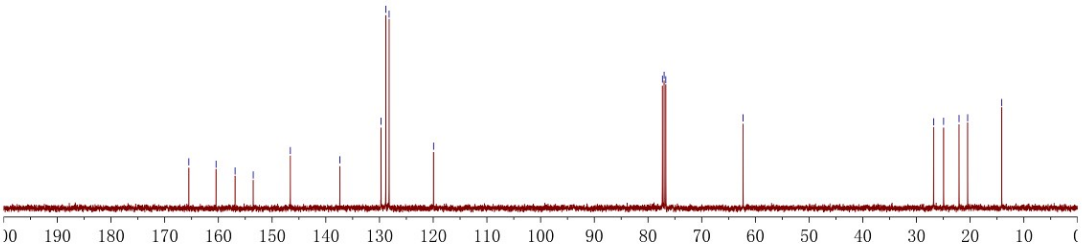
COOEt

4ah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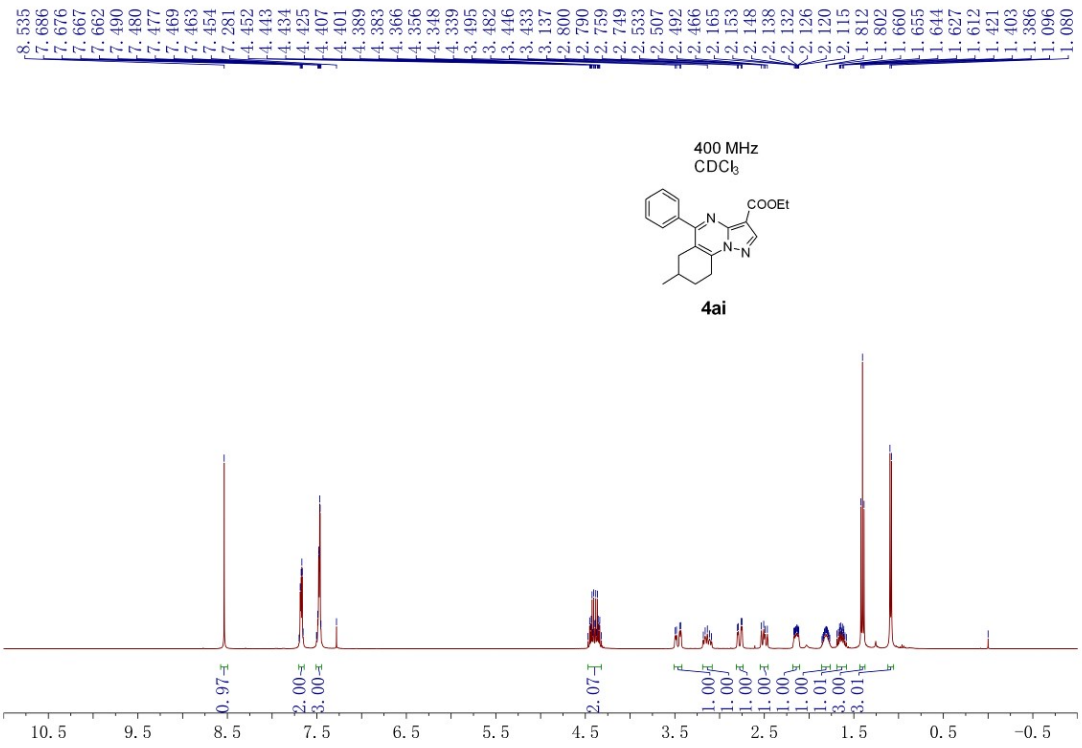
20
10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4.434
4.425
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4.401
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3.495
3.482
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3.137
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2.138
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1.655
1.644
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COOEt
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3.00
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1.00
1.00
1.00
1.00
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3.00
3.01
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5.5
4.5
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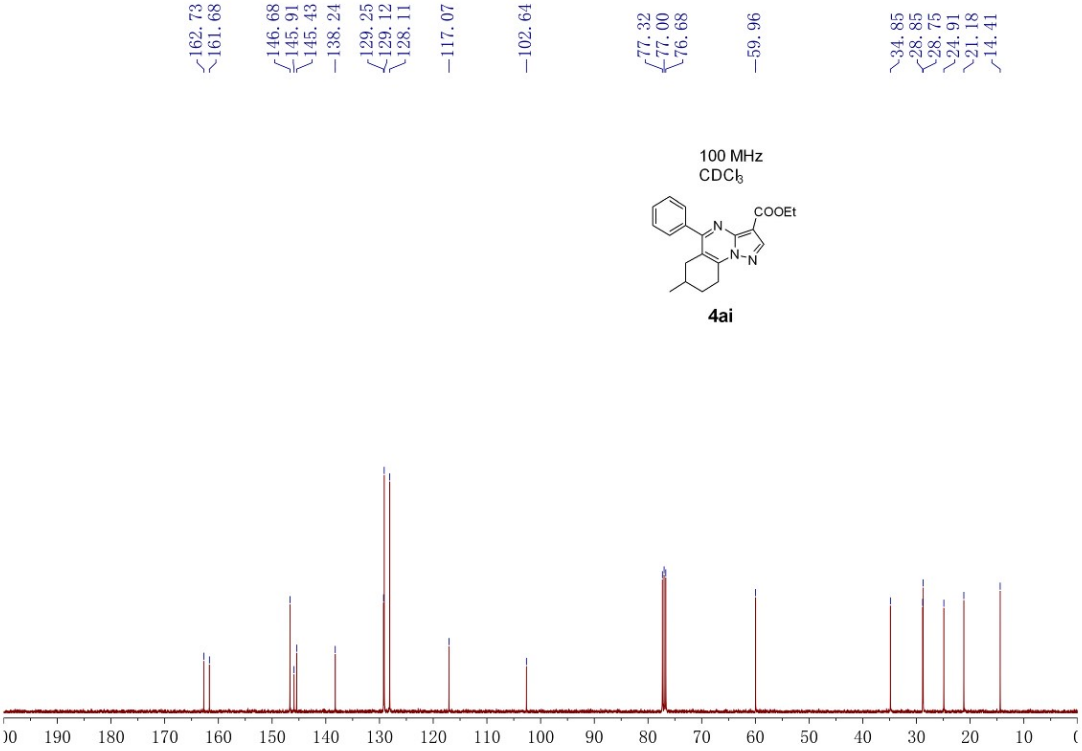
-0.5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129.12
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117.07
102.64
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77.00
76.68
59.96
34.85
28.85
28.75
24.91
21.18
14.41
100 MHz
CDCl3
COOEt
4ai
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


8.535
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7.668
7.659
7.489
7.480
7.475
7.468
7.462
7.282
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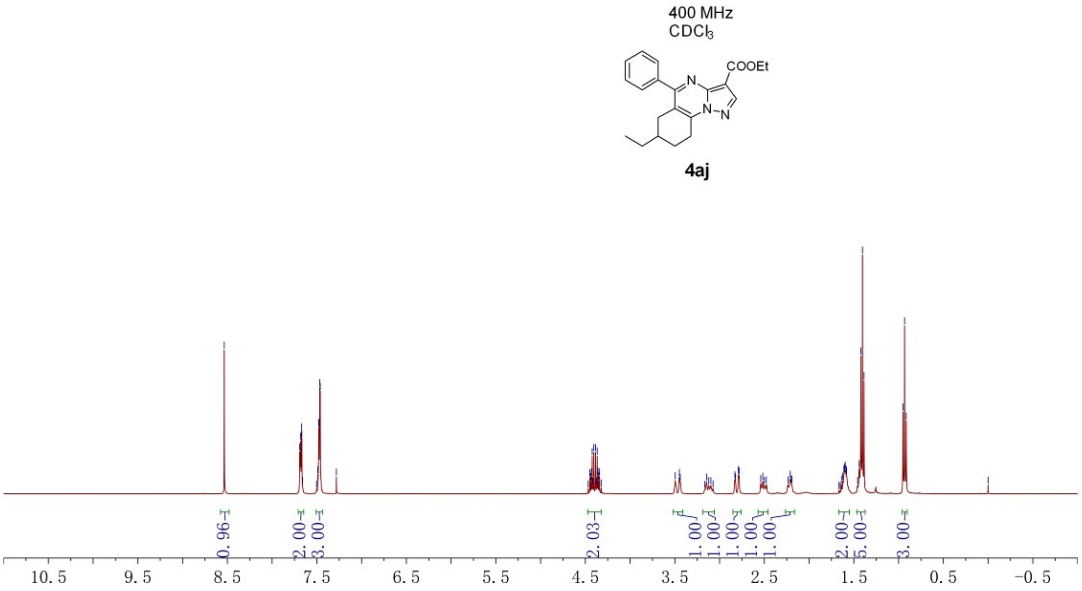
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1.00
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6.00
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5


162.73
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129.10
128.10
117.06
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26.38
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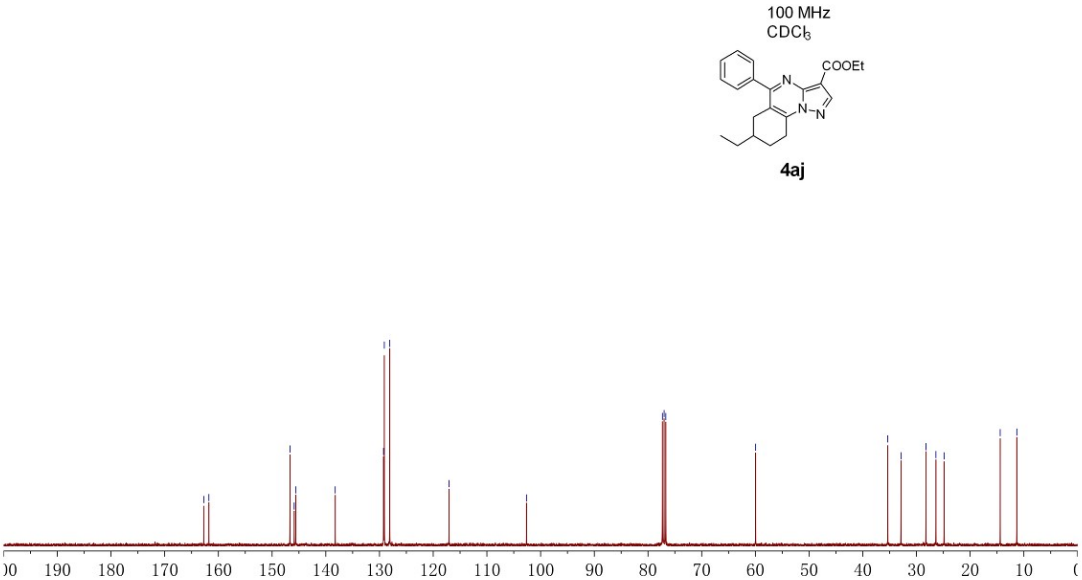
11.31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COOEt
4aj
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160
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100
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80
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50
40
30
20
10


8.530
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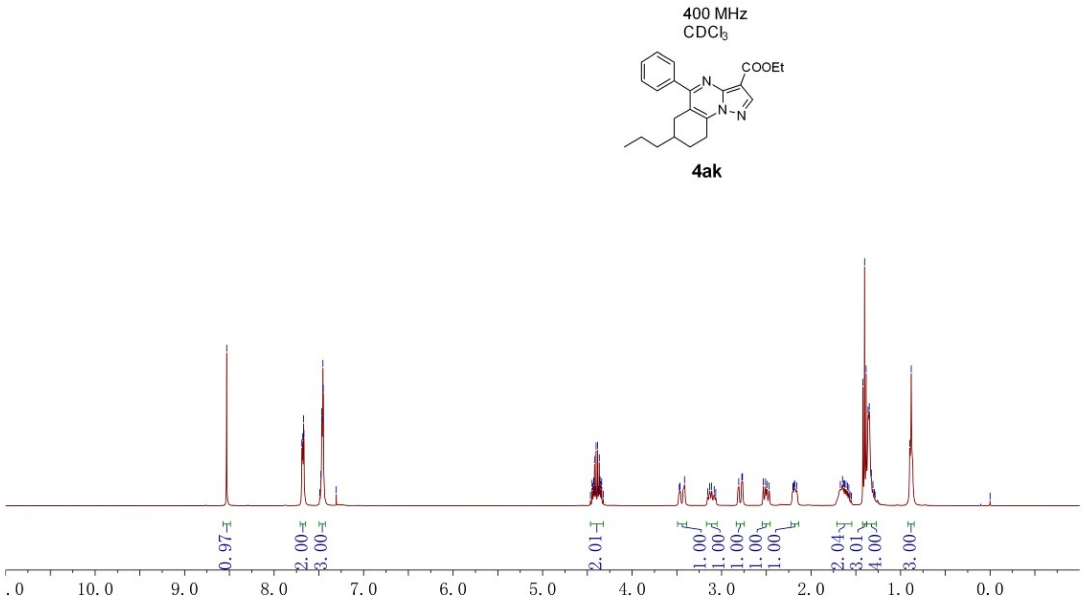
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1.00
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4.00
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


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102.48
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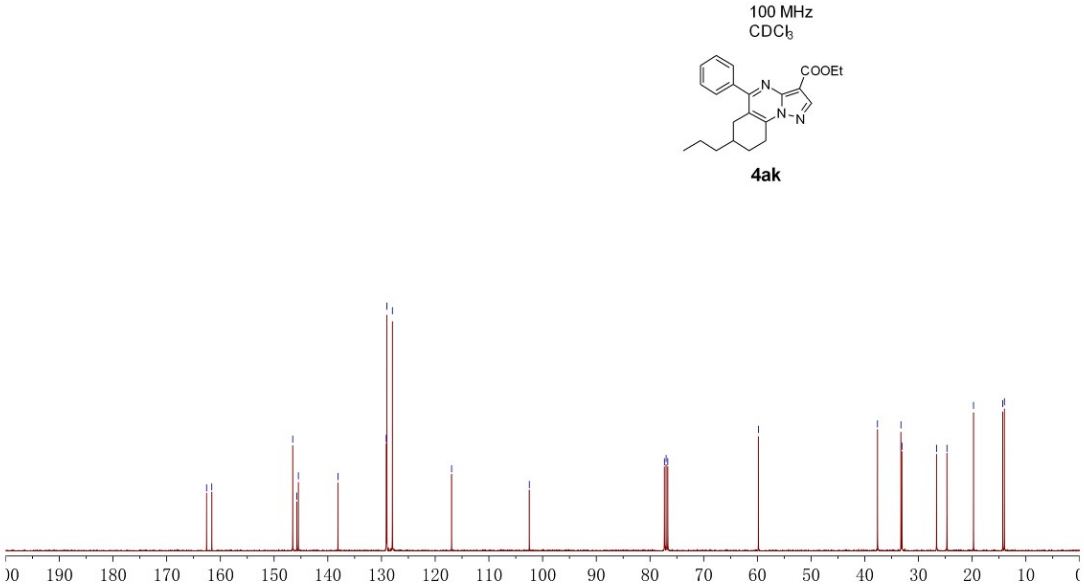
14.01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COOEt
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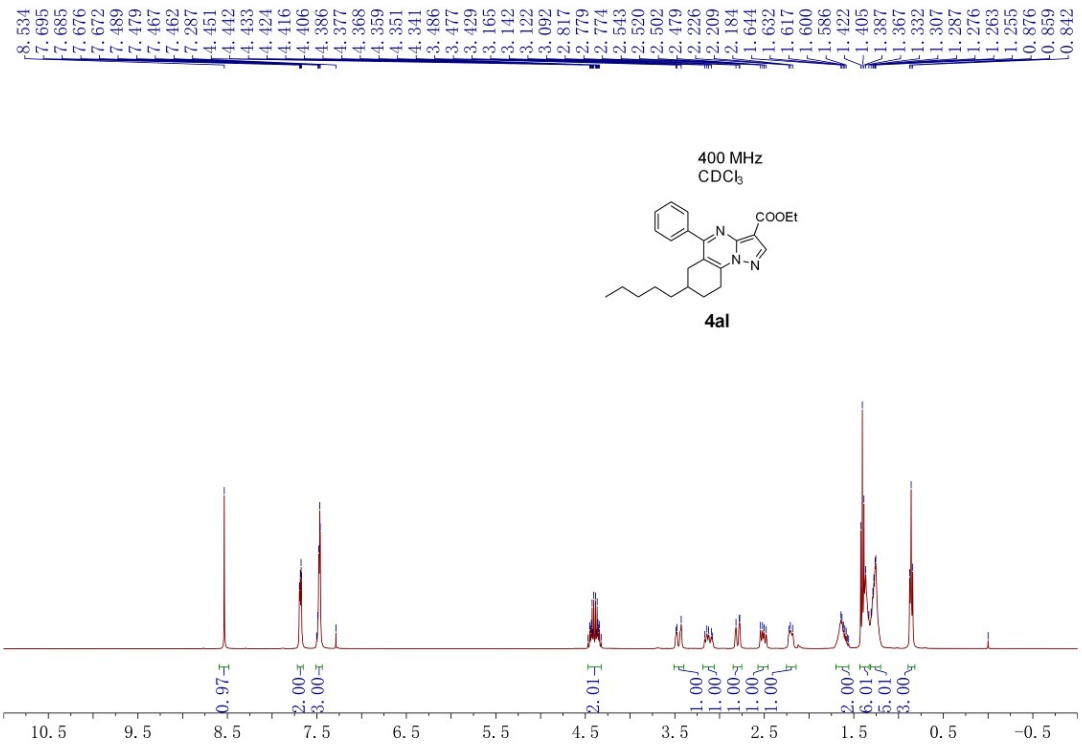
20
10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3.165
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1.422
1.405
1.387
1.367
1.332
1.307
1.287
1.276
1.263
1.255
0.876
0.859
0.842
400 MHz
CDCl3
COOEt
4al
0.97
2.00
3.00
2.01
1.00
1.00
1.00
1.00
1.00
2.00
6.01
6.01
3.00
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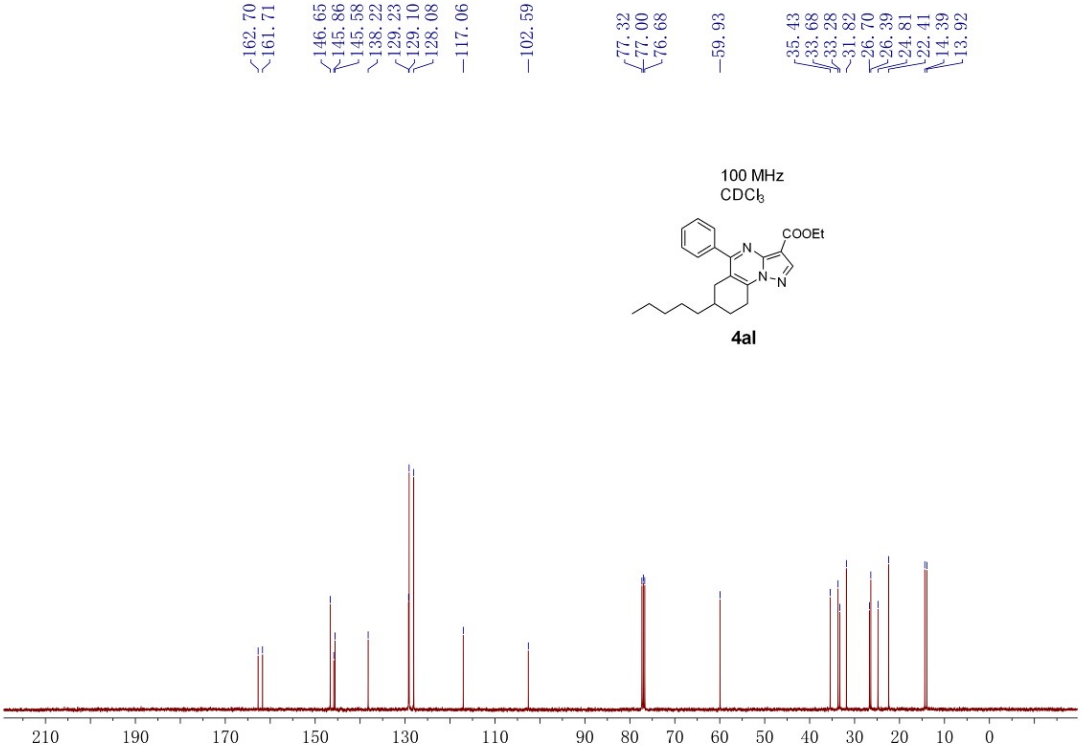
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76.68
59.93
35.43
33.68
33.28
31.82
26.70
26.39
24.81
22.41
14.39
13.92
100 MHz
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COOEt
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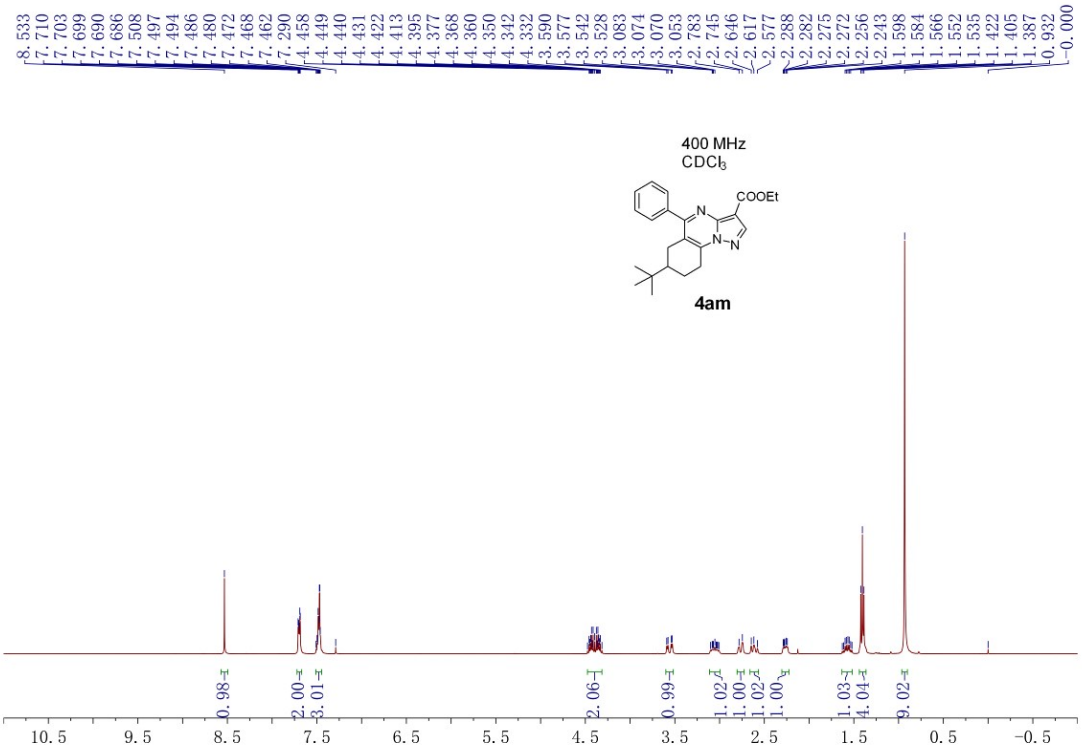
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7.462
7.290
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4.449
4.440
4.431
4.422
4.413
4.395
4.377
4.368
4.360
4.350
4.342
4.332
3.590
3.577
3.542
3.528
3.083
3.074
3.070
3.053
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2.745
2.646
2.617
2.577
2.288
2.282
2.275
2.272
2.256
2.243
1.598
1.584
1.566
1.552
1.535
1.422
1.405
1.387
0.932
0.000
400 MHz
CDCl3
COOEt
4am
0.98
2.00
3.01
2.06
0.99
1.02
1.00
1.02
1.00
1.03
4.04
9.02
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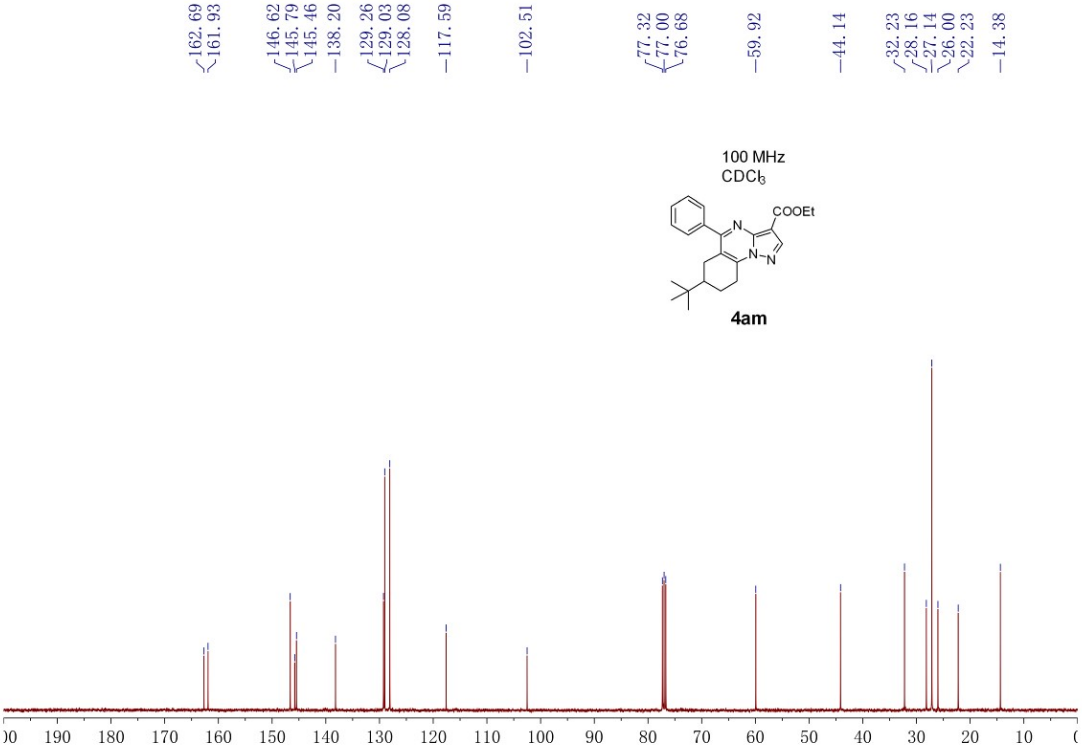
0.5
-0.5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77.00
76.68
59.92
44.14
32.23
28.16
27.14
26.00
22.23
14.38
100 MHz
CDCl3
COOEt
4am
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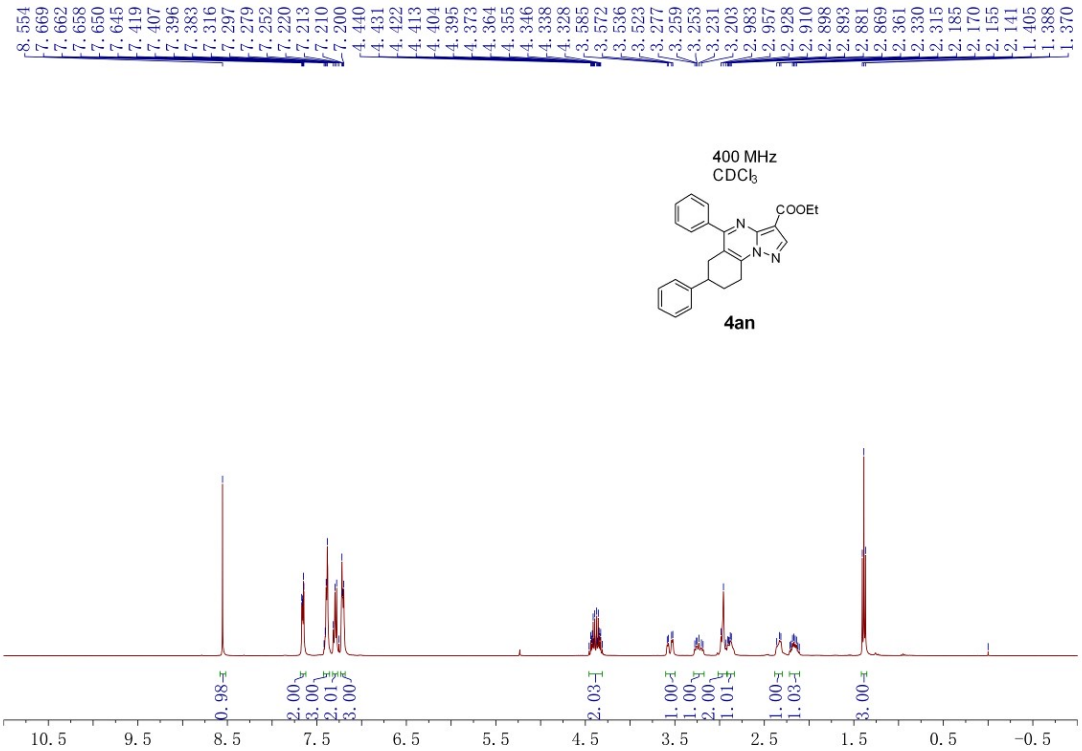
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7.279
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7.213
7.210
7.200
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4.431
4.422
4.413
4.404
4.395
4.373
4.364
4.355
4.346
4.338
4.328
3.585
3.572
3.536
3.523
3.277
3.259
3.253
3.231
3.203
2.983
2.957
2.928
2.910
2.898
2.893
2.881
2.869
2.361
2.330
2.315
2.185
2.170
2.155
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1.405
1.388
1.370
400 MHz
CDCl3
COOEt
4an
0.98
2.00
3.00
2.01
3.00
2.03
1.00
1.00
2.00
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1.00
1.03
3.00
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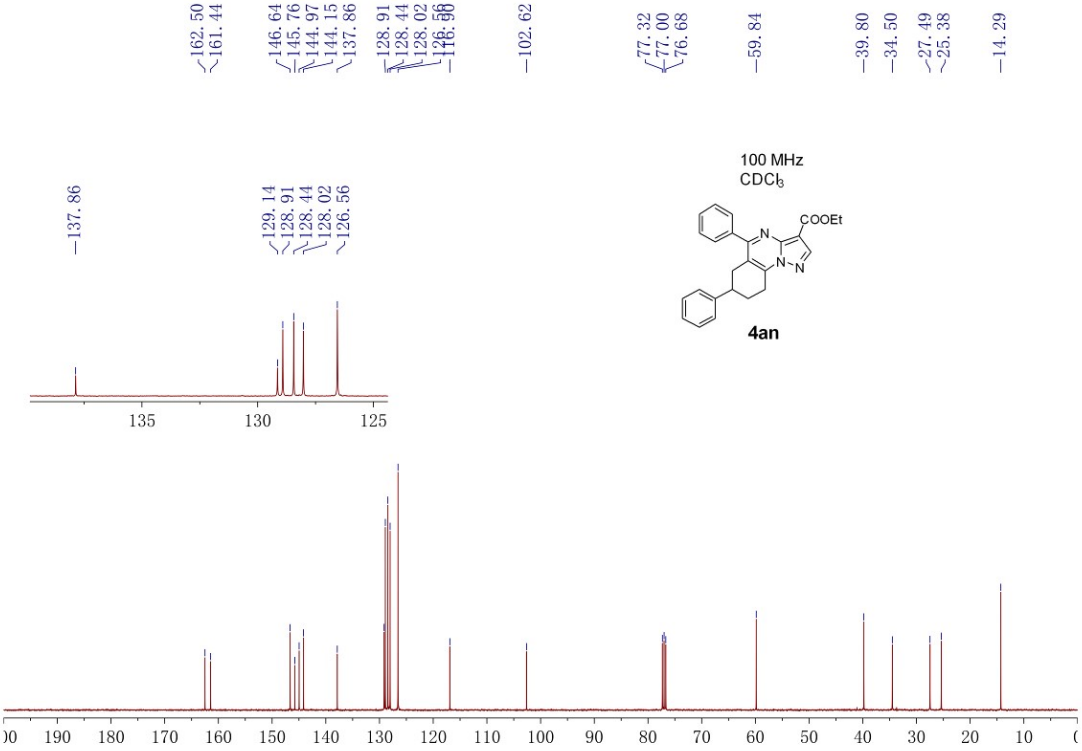
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77.00
76.68
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39.80
34.50
27.49
25.38
14.29
137.86
129.14
128.91
128.44
128.02
126.56
135
130
125
100 MHz
CDCl3
COOEt
4an
190
180
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110
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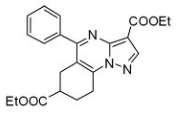
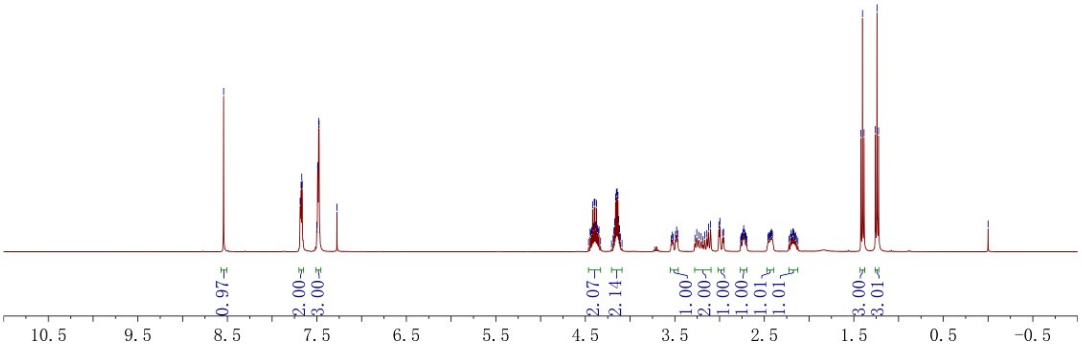
30
20
10

400 MHz
$CDCl_3$



4ao



100 MHz
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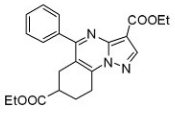

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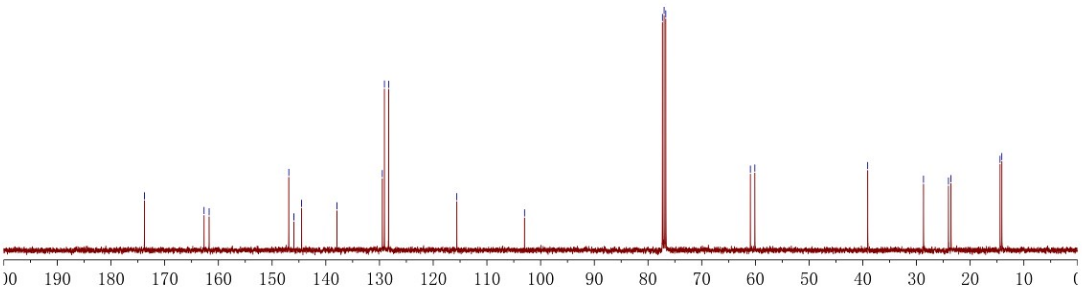

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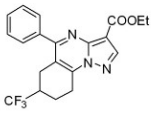

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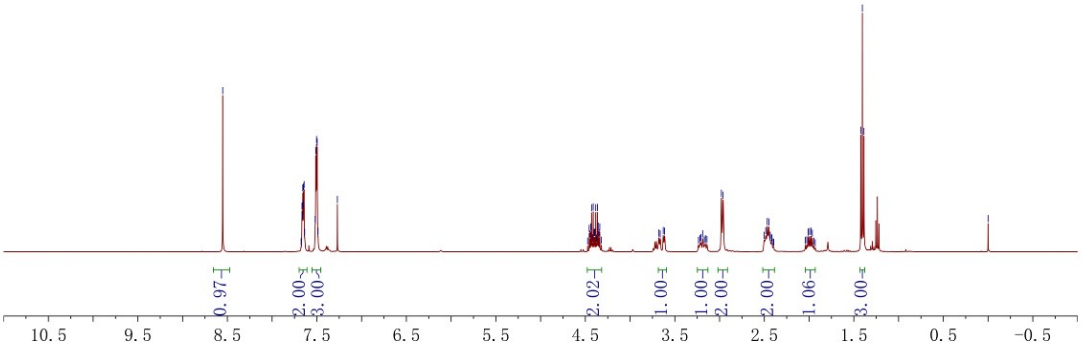

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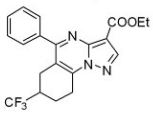

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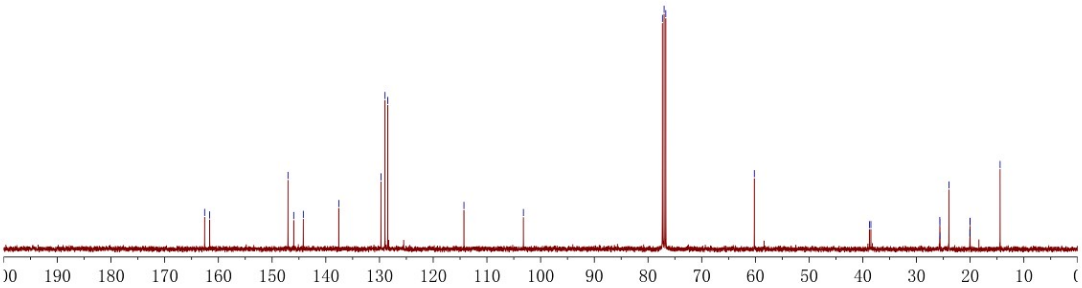

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4.440
4.432
4.422
4.414
4.404
4.385
4.375
4.367
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4.340
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2.705
2.679
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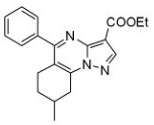
400 MHz
$CDCl_3$



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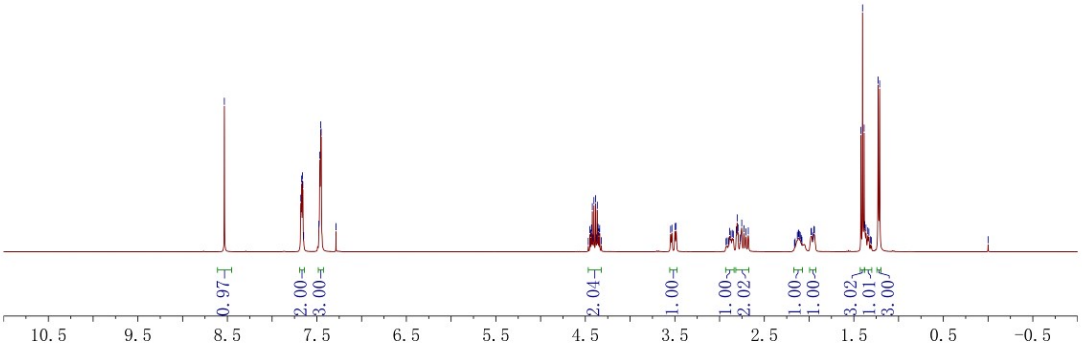

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129.04
128.07
117.10
102.65
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21.47
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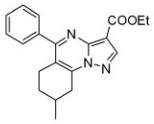
100 MHz
$CDCl_3$



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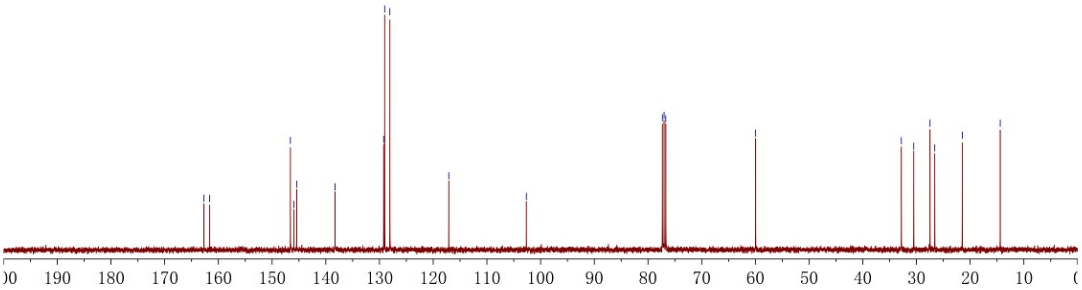

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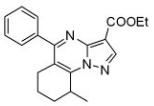

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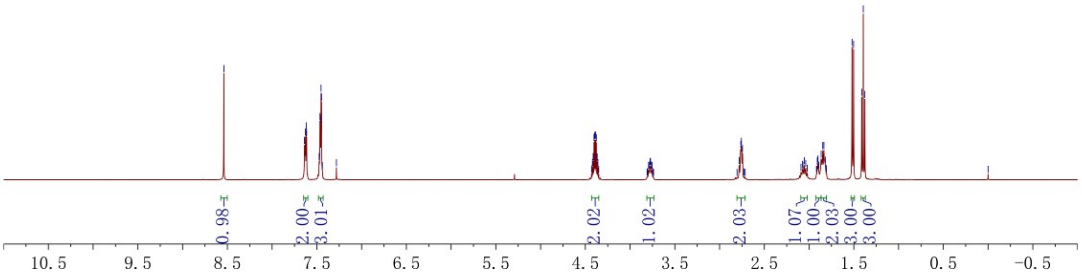

100 MHz
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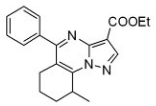

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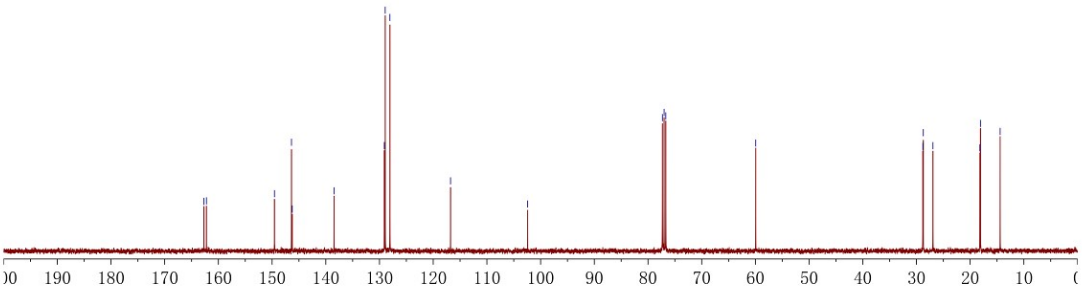

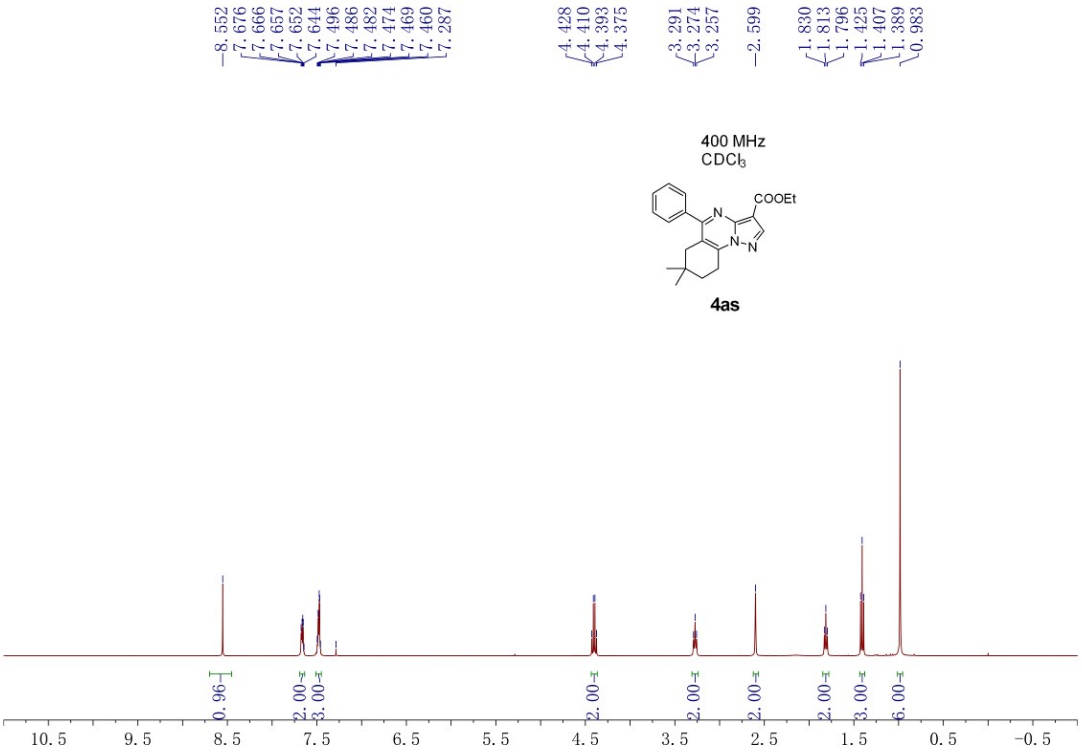
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4.393
4.375
3.291
3.274
3.257
2.599
1.830
1.813
1.796
1.425
1.407
1.389
0.983
400 MHz
CDCl3
COOEt
4as
0.96
2.00
3.00
2.00
2.00
2.00
2.00
3.00
6.00
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5.5
4.5
3.5
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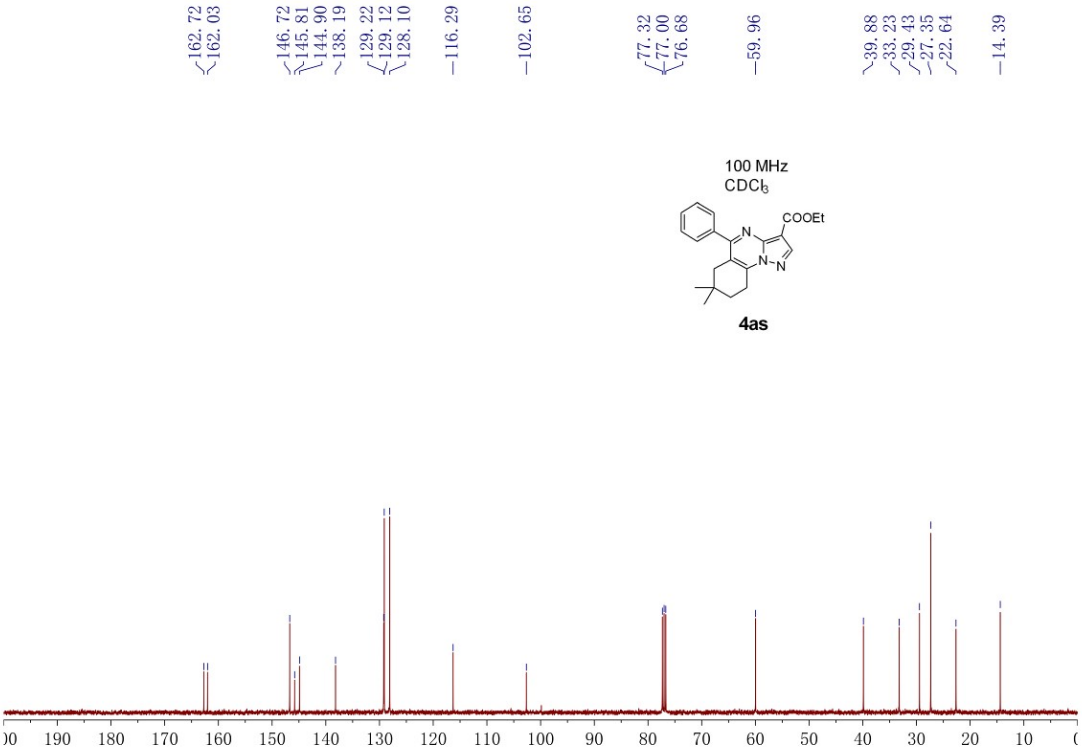
1.5
0.5
-0.5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129.12
128.10
116.29
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77.32
77.00
76.68
59.96
39.88
33.23
29.43
27.35
22.64
14.39
100 MHz
CDCl3
COOEt
4as
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180
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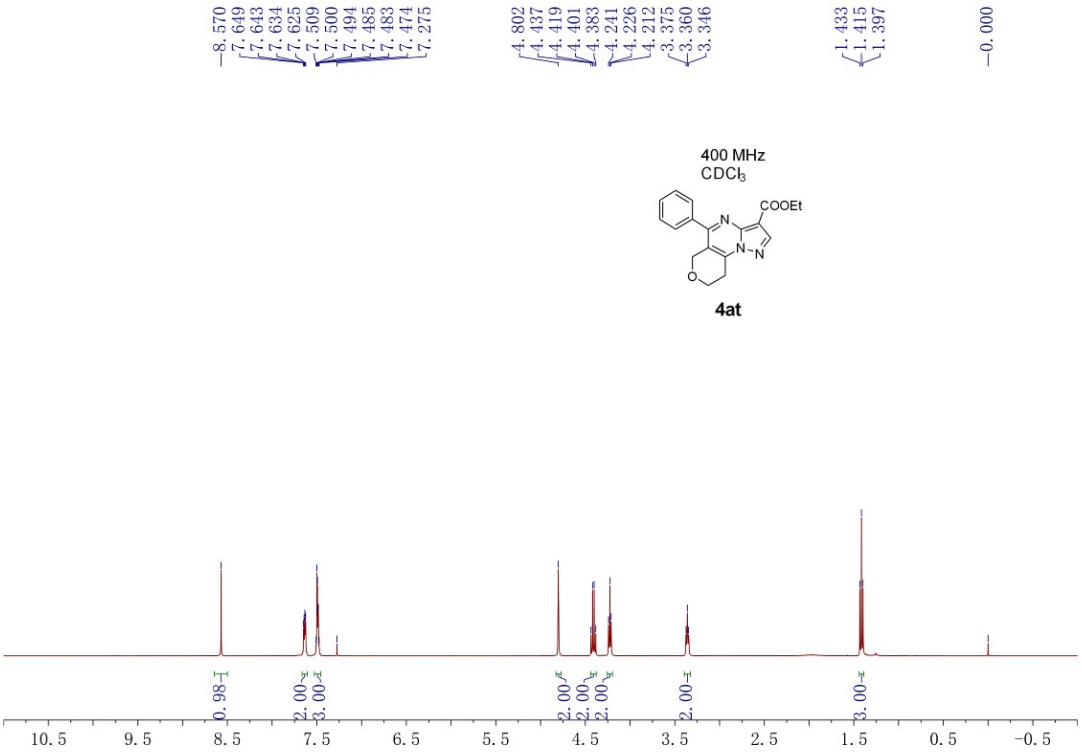
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10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7.485
7.483
7.474
7.275
4.802
4.437
4.419
4.401
4.383
4.241
4.226
4.212
3.375
3.360
3.346
1.433
1.415
1.397
0.000
400 MHz
CDCl3
COOEt
4at
0.98
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3.00
2.00
2.00
2.00
2.00
3.00
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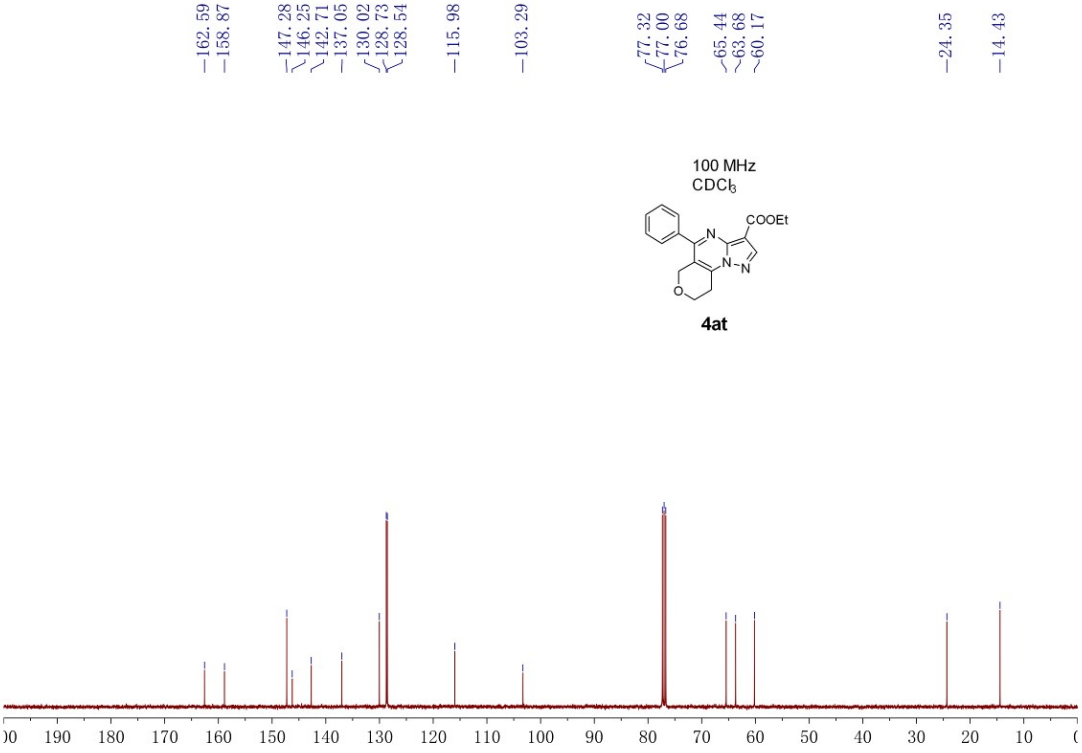
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103.29
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77.00
76.68
65.44
63.68
60.17
24.35
14.43
100 MHz
CDCl3
COOEt
4at
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30
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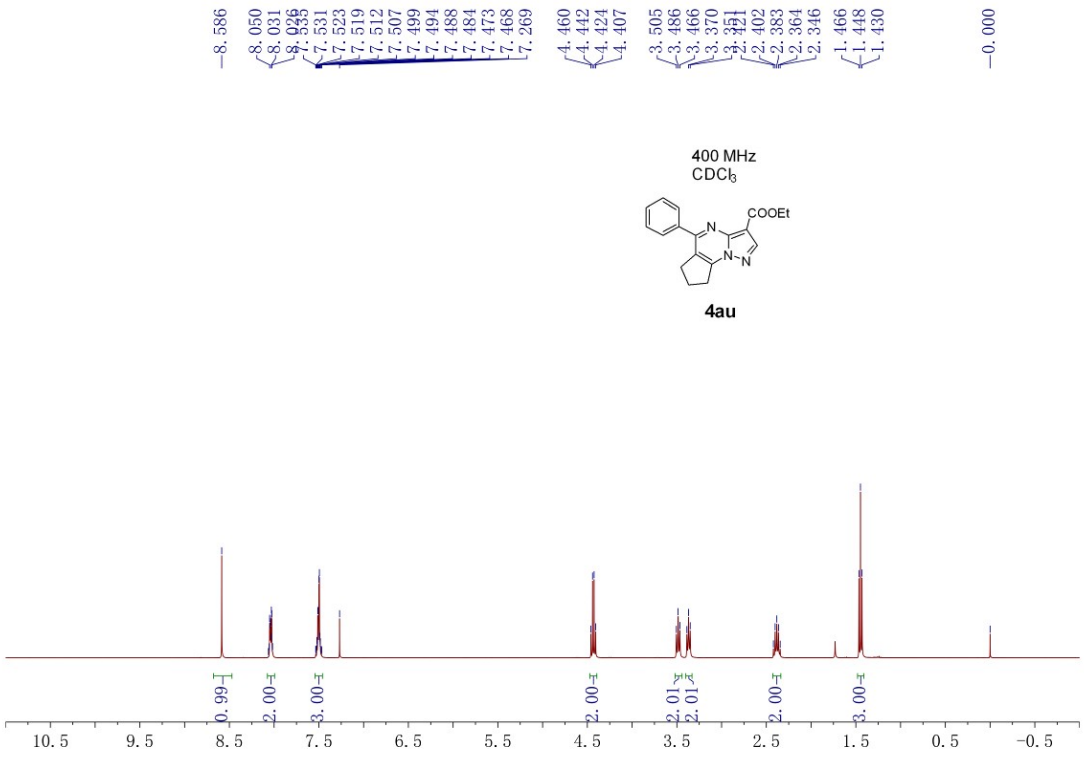
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7.269
4.460
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4.424
4.407
3.505
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3.466
3.370
2.402
2.383
2.364
2.346
1.466
1.448
1.430
0.000
400 MHz
CDCl3
COOEt
4au
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3.00
2.00
2.01
2.01
2.00
3.00
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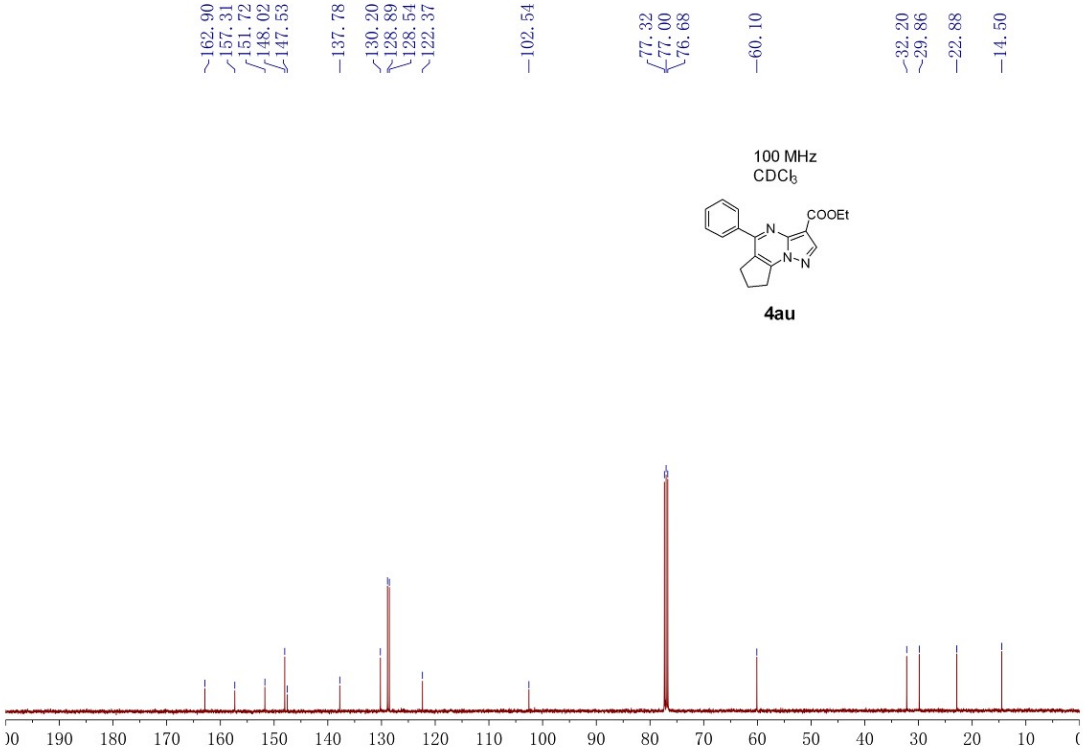
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128.54
122.37
102.54
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77.00
76.68
60.10
32.20
29.86
22.88
14.50
100 MHz
CDCl3
COOEt
4au
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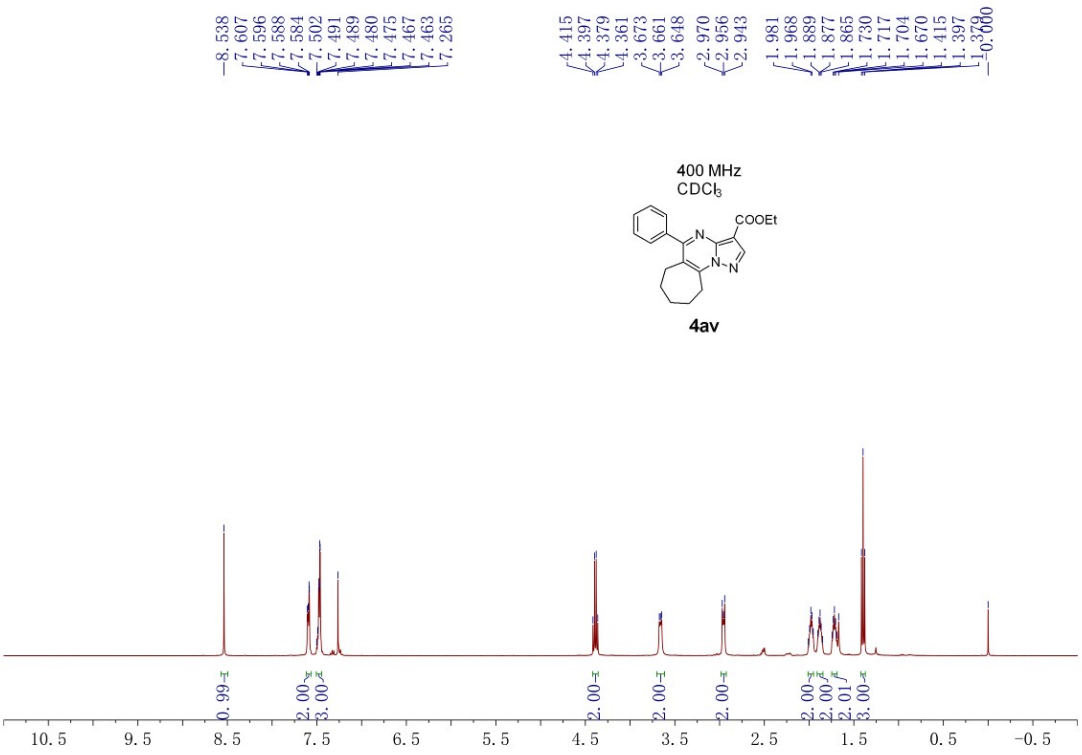
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7.265
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3.673
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2.970
2.956
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1.968
1.889
1.877
1.865
1.730
1.717
1.704
1.670
1.415
1.397
1.379
10.000
400 MHz
CDCl3
COOEt
4av
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2.00
2.00
2.00
2.00
2.01
3.00
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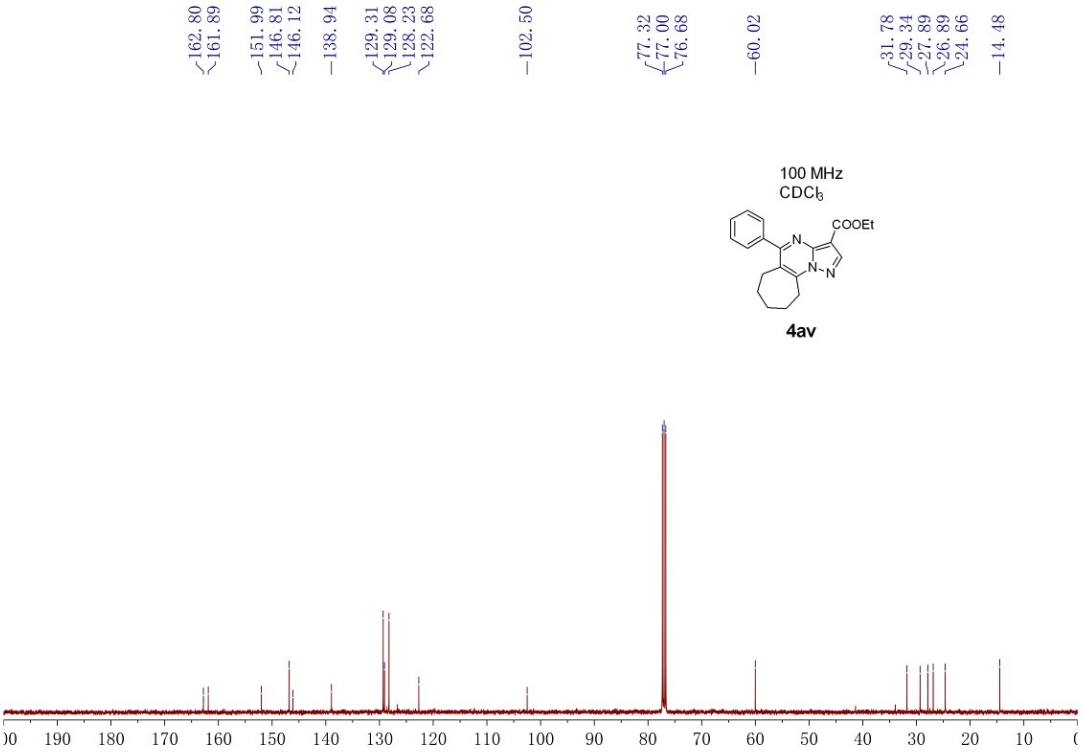
-0.5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77.00
76.68
60.02
31.78
29.34
27.89
26.89
24.66
14.48
100 MHz
CDCl3
COOEt
4av
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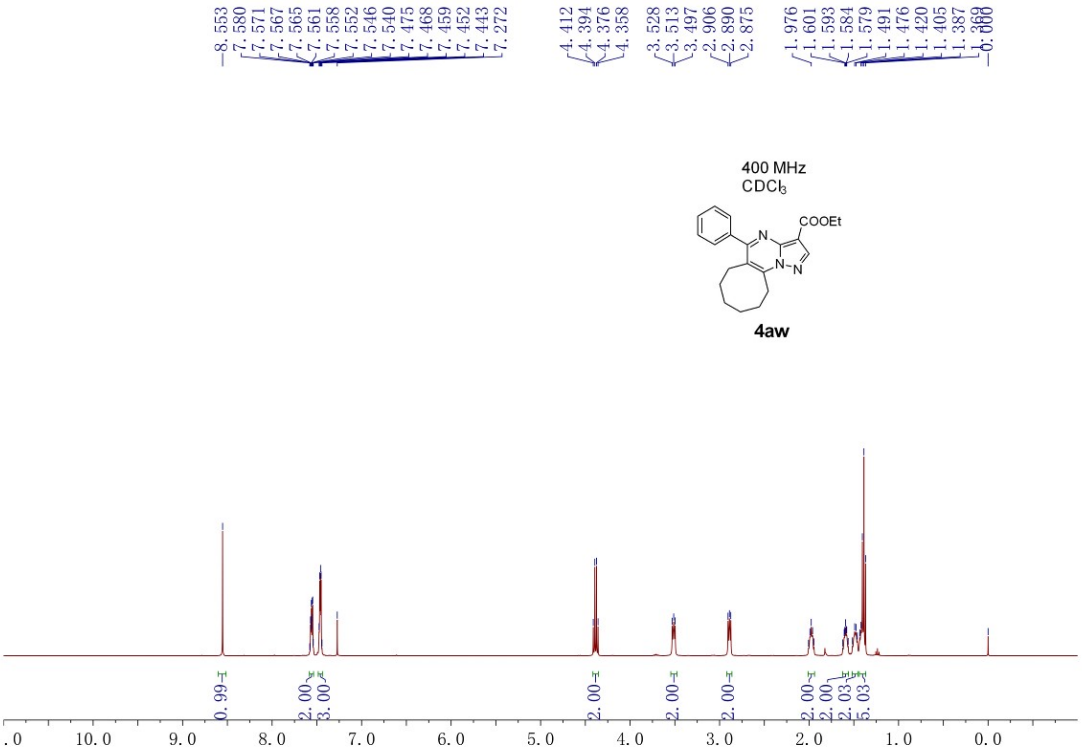
20
10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7.443
7.272
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3.497
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1.491
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1.420
1.405
1.387
1.369
0.000
400 MHz
CDCl3
COOEt
4aw
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2.00
2.00
2.00
2.00
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5.03
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9.0
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7.0
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5.0
4.0
3.0
2.0
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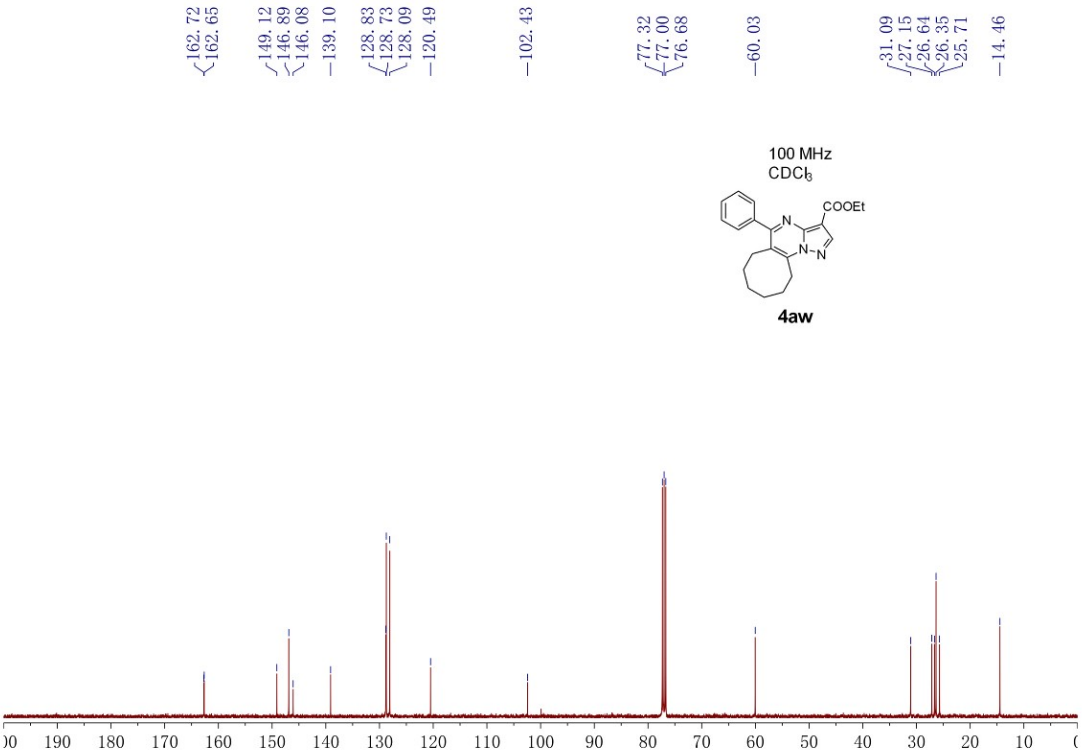
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120.49
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77.00
76.68
60.03
31.09
27.15
26.64
26.35
25.71
14.46
100 MHz
CDCl3
COOEt
4aw
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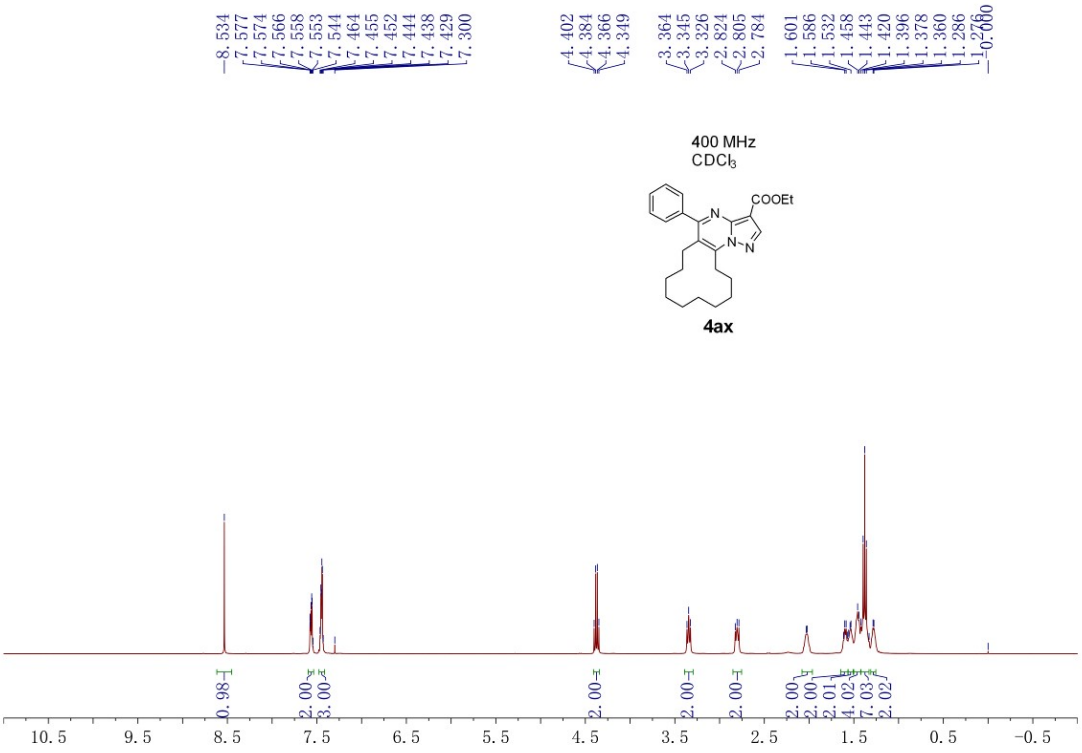
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7.429
7.300
4.402
4.384
4.366
4.349
3.364
3.345
3.326
2.824
2.805
2.784
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1.586
1.532
1.458
1.443
1.420
1.396
1.378
1.360
1.286
1.276
0.880
400 MHz
CDCl3
COOEt
4ax
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3.00
2.00
2.00
2.00
2.00
2.00
2.01
4.02
7.03
2.02
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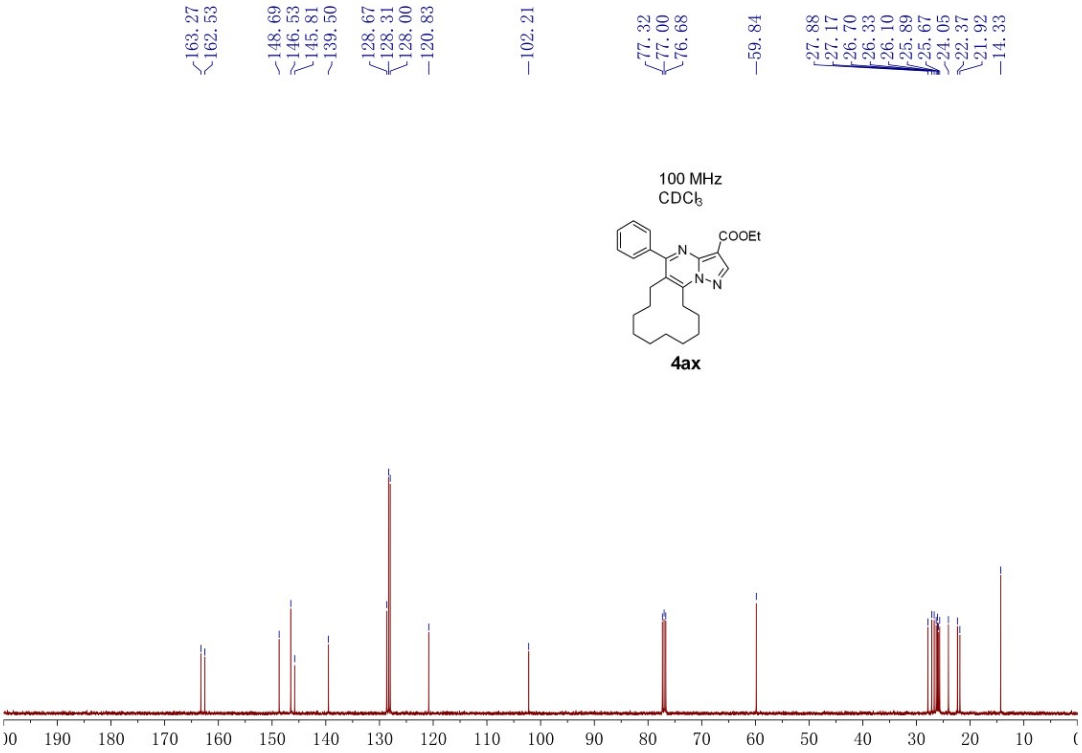
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77.00
76.68
59.84
27.88
27.17
26.70
26.33
26.10
25.89
25.67
24.05
22.37
21.92
14.33
100 MHz
CDCl3
COOEt
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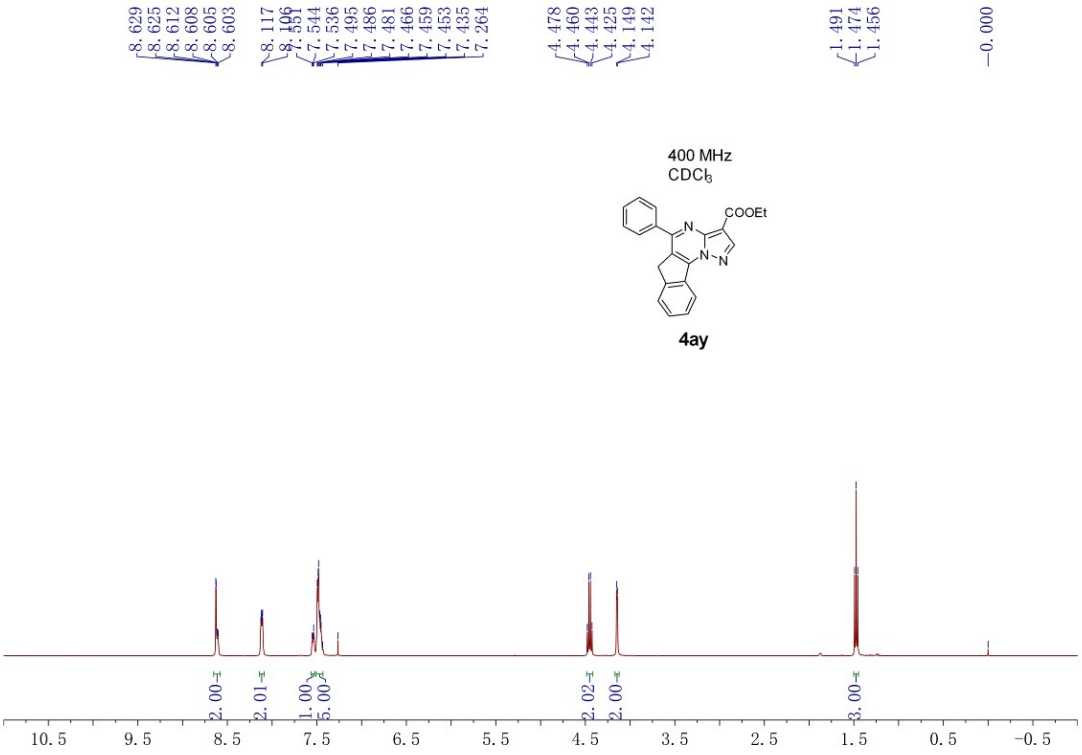
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7.495
7.486
7.481
7.466
7.459
7.453
7.435
7.264
4.478
4.460
4.443
4.425
4.149
4.142
1.491
1.474
1.456
0.000
400 MHz
CDCl3
COOEt
4ay
2.00
2.01
1.00
6.00
2.02
2.00
3.00
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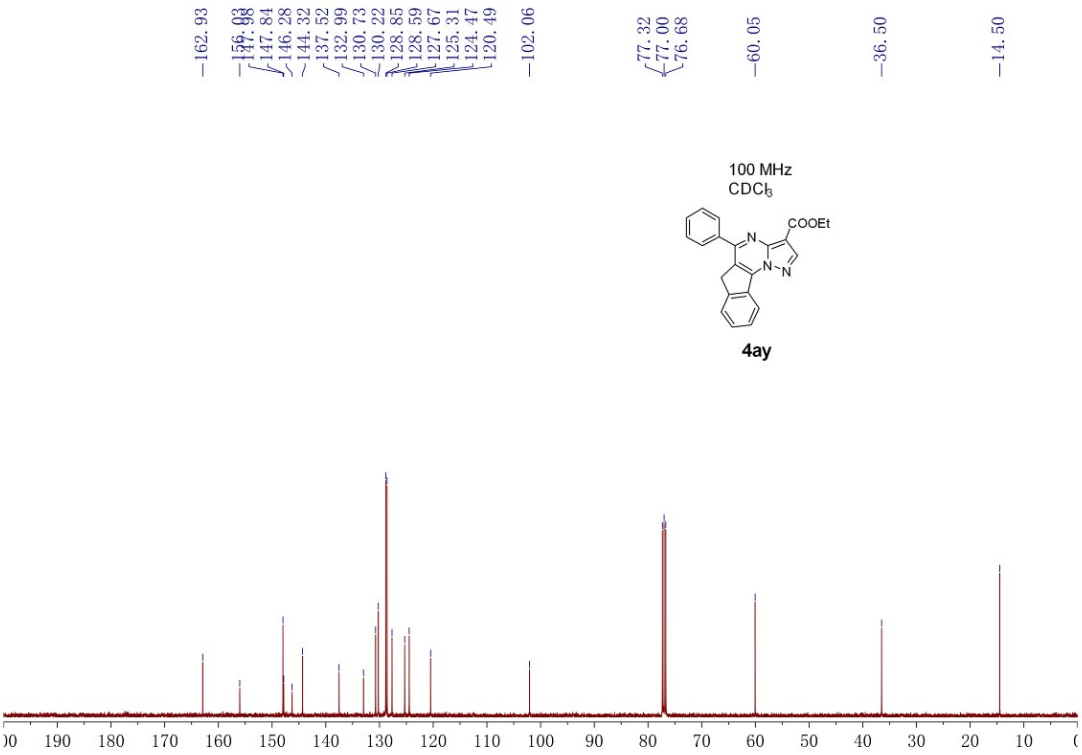
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120.49
102.06
77.32
77.00
76.68
60.05
36.50
14.50
100 MHz
CDCl3
COOEt
4ay
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120
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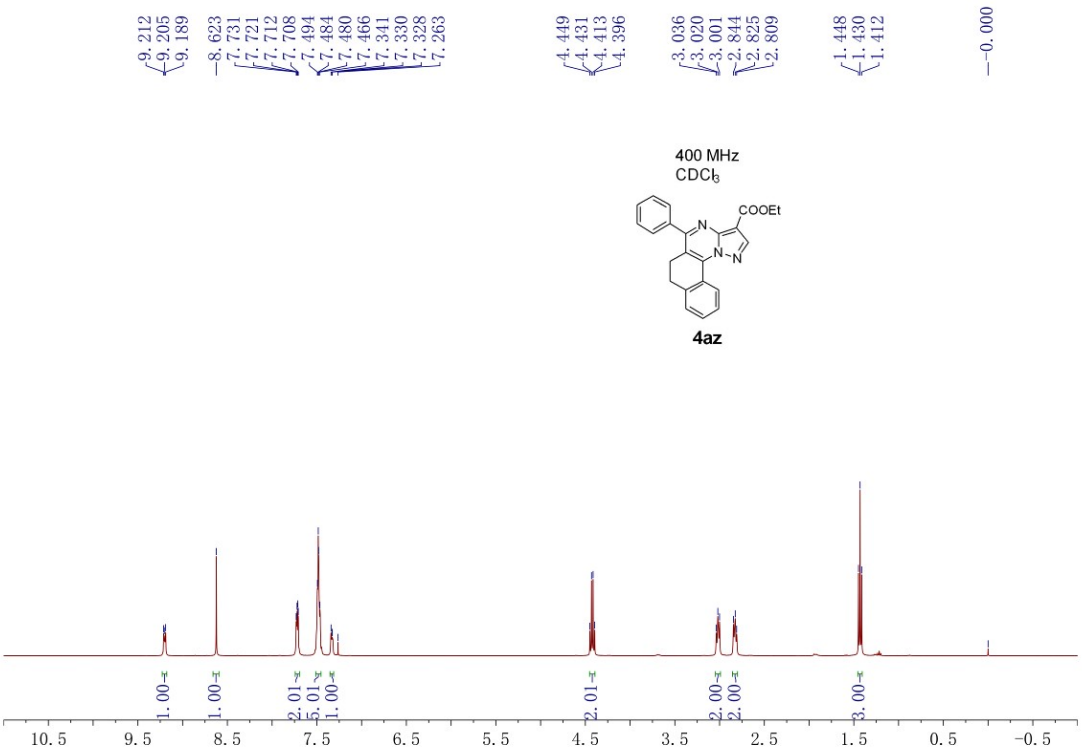
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7.466
7.341
7.330
7.328
7.263
4.449
4.431
4.413
4.396
3.036
3.020
3.001
2.844
2.825
2.809
1.448
1.430
1.412
0.000
400 MHz
CDCl3
COOEt
4az
1.00
1.00
2.01
5.01
1.00
2.01
2.00
2.00
3.00
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5.5
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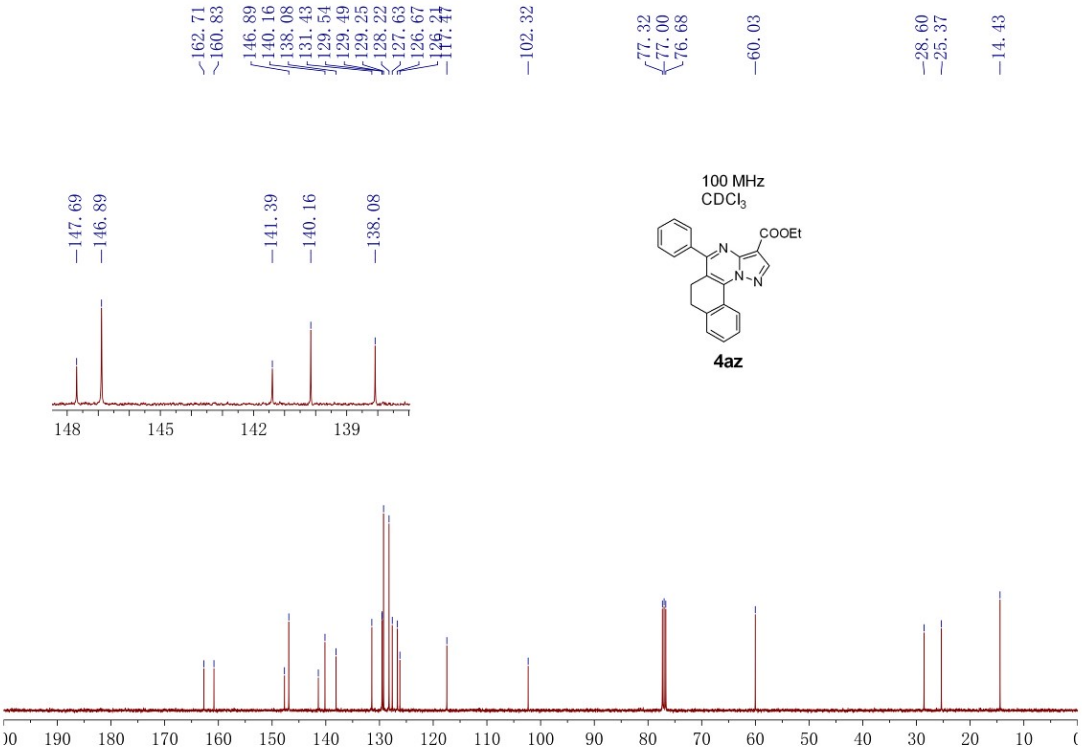
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126.67
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77.32
77.00
76.68
60.03
28.60
25.37
14.43
147.69
146.89
141.39
140.16
138.08
100 MHz
CDCl3
COOEt
4az
148
145
142
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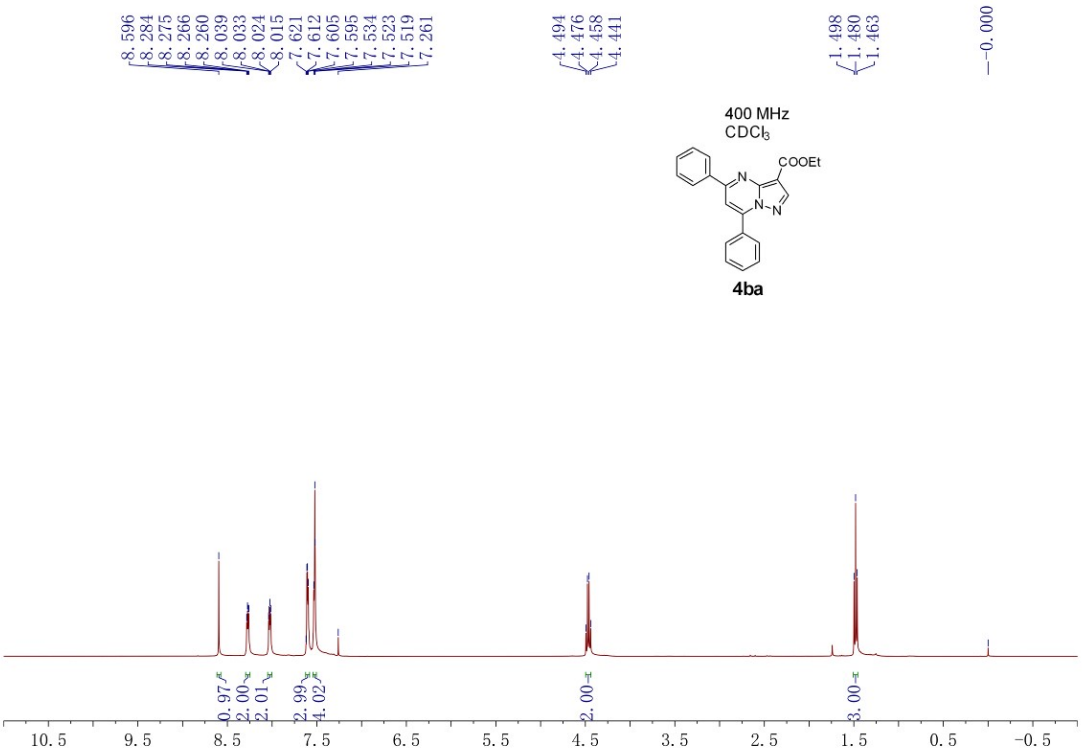
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8.033
8.024
8.015
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7.605
7.595
7.534
7.523
7.519
7.261
4.494
4.476
4.458
4.441
1.498
1.480
1.463
0.000
400 MHz
CDCl3
COOEt
4ba
0.97
2.00
2.01
2.99
4.02
2.00
3.00
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5.5
4.5
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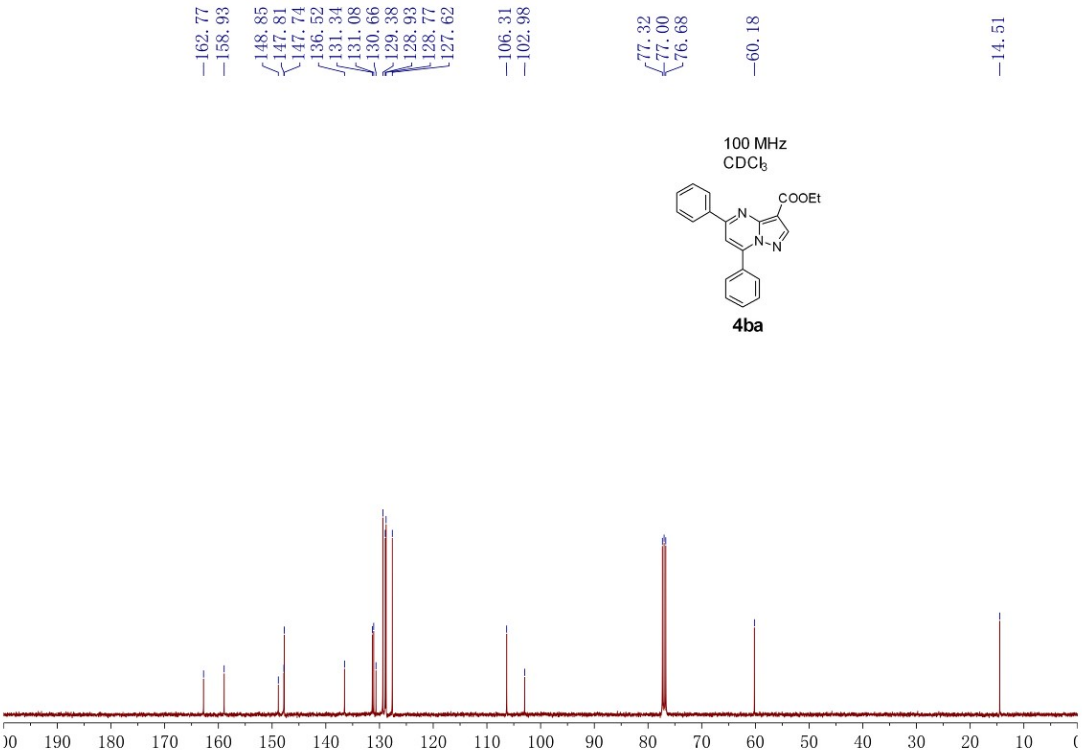
-0.5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129.38
128.93
128.77
127.62
106.31
102.98
77.32
77.00
76.68
60.18
14.51
100 MHz
CDCl3
COOEt
4ba
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180
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160
150
140
130
120
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100
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80
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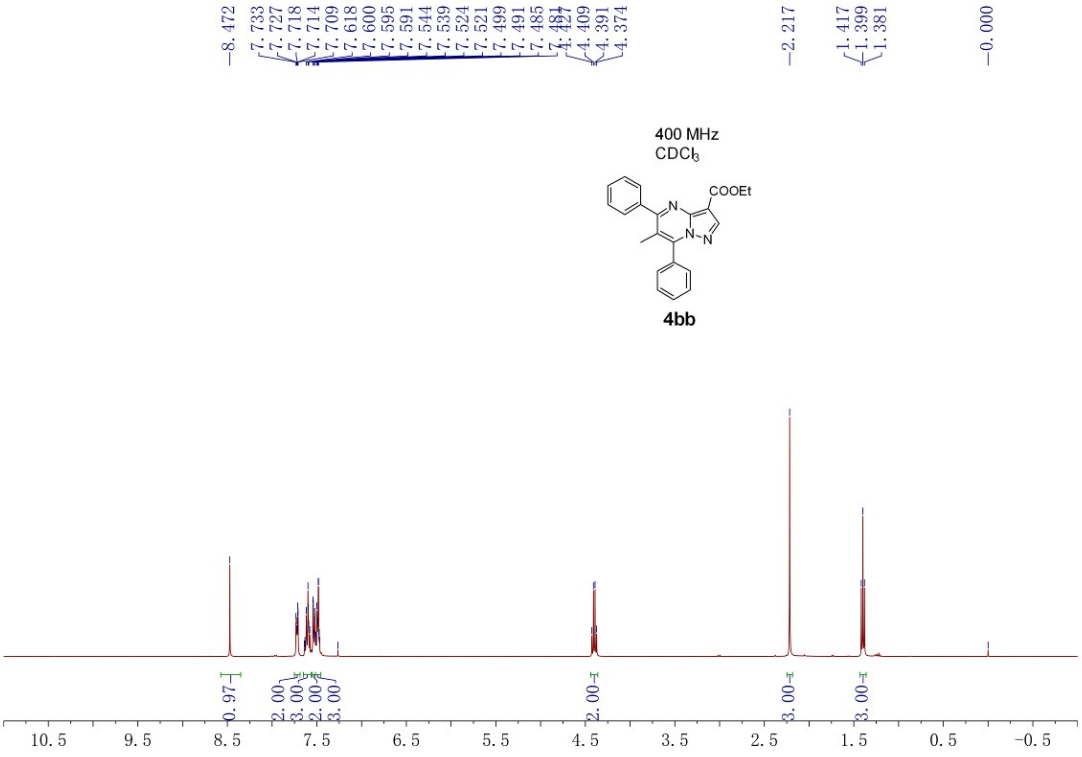
40
30
20
10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7.539
7.524
7.521
7.499
7.491
7.485
4.409
4.391
4.374
2.217
1.417
1.399
1.381
0.000
400 MHz
CDCl3
COOEt
4bb
0.97
2.00
3.00
2.00
3.00
2.00
3.00
3.00
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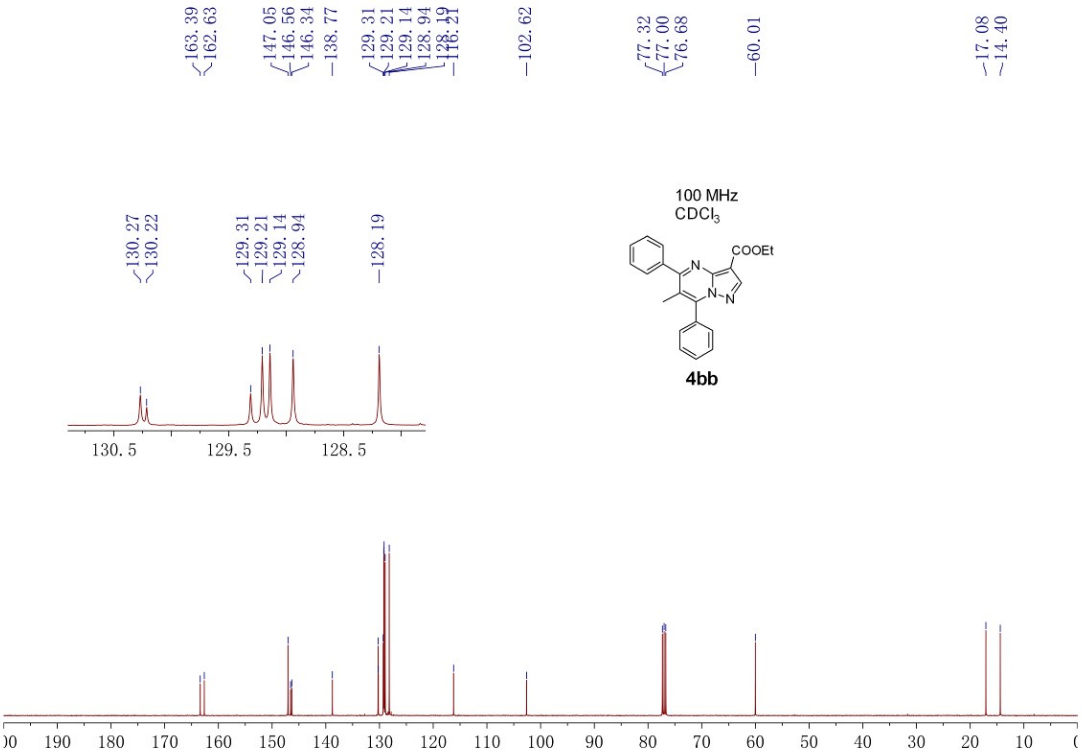
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77.00
76.68
60.01
17.08
14.40
130.27
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COOEt
4bb
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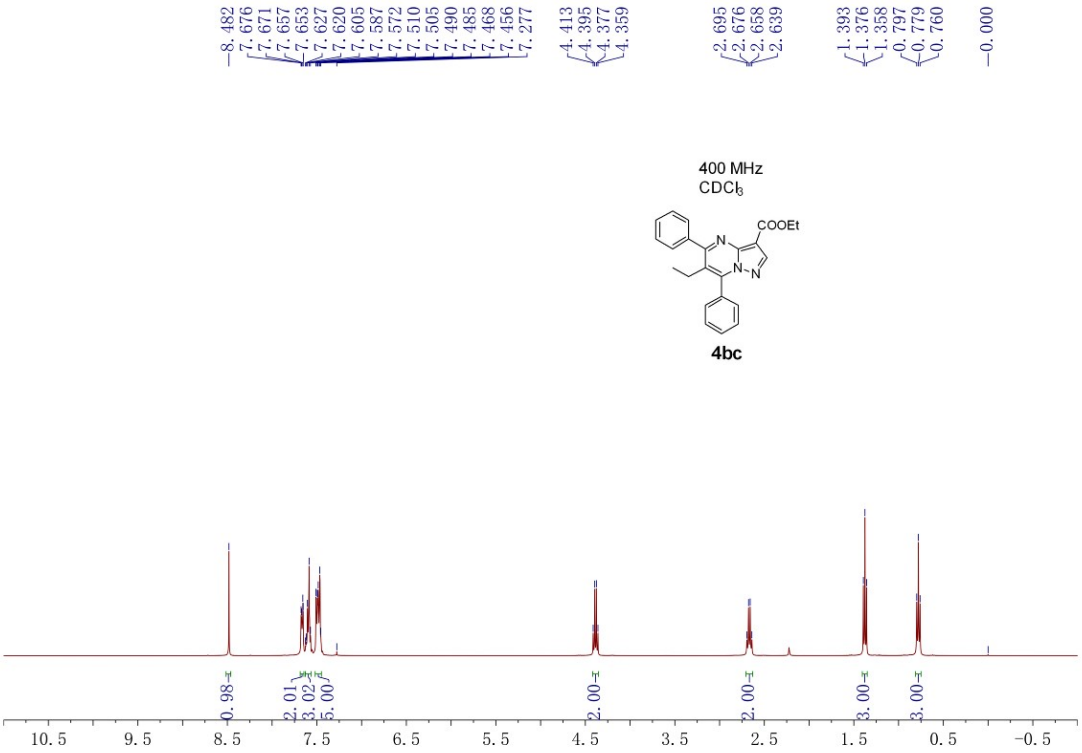
129.5
128.5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7.605
7.587
7.572
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7.490
7.485
7.468
7.456
7.277
4.413
4.395
4.377
4.359
2.695
2.676
2.658
2.639
1.393
1.376
1.358
0.797
0.779
0.760
0.000
400 MHz
CDCl3
COOEt
4bc
0.98
2.01
3.02
6.00
2.00
2.00
3.00
3.00
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7.5
6.5
5.5
4.5
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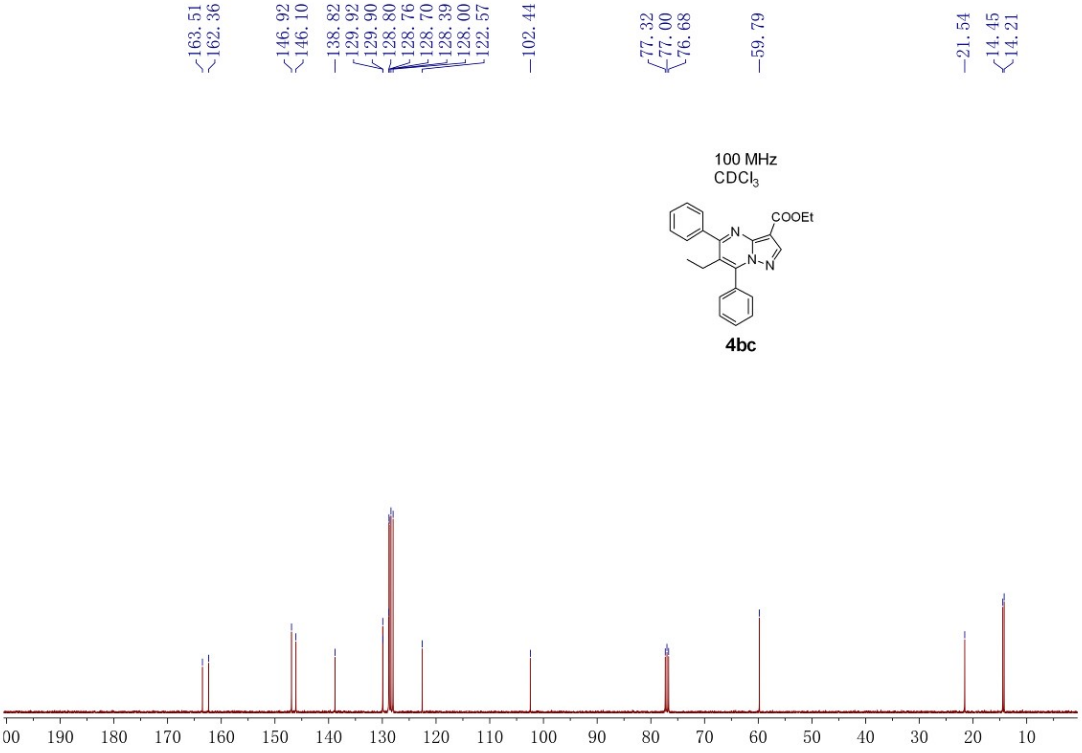
0.5
-0.5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128.80
128.76
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128.39
128.00
122.57
102.44
77.32
77.00
76.68
59.79
21.54
14.45
14.21
100 MHz
CDCl3
COOEt
4bc
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180
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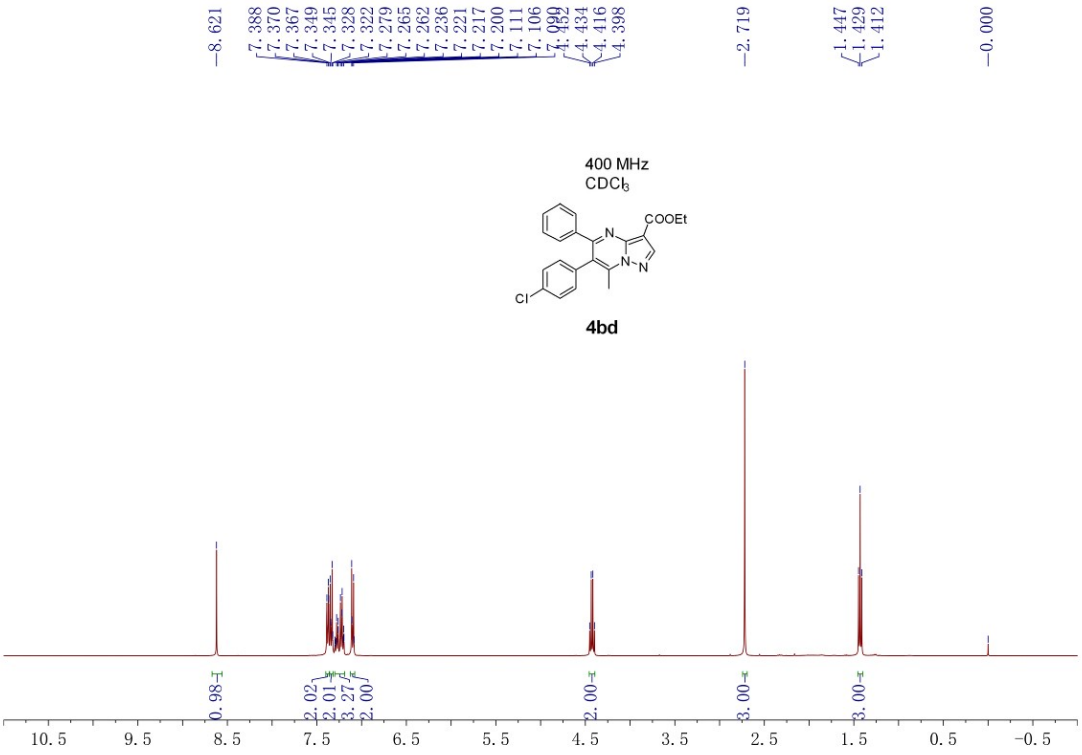
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10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7.262
7.236
7.221
7.217
7.200
7.111
7.106
4.434
4.416
4.398
2.719
1.447
1.429
1.412
0.000
400 MHz
CDCl3
COOEt
N
N
N
Cl
4bd
0.98
2.02
2.01
3.27
2.00
2.00
3.00
3.00
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7.5
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5.5
4.5
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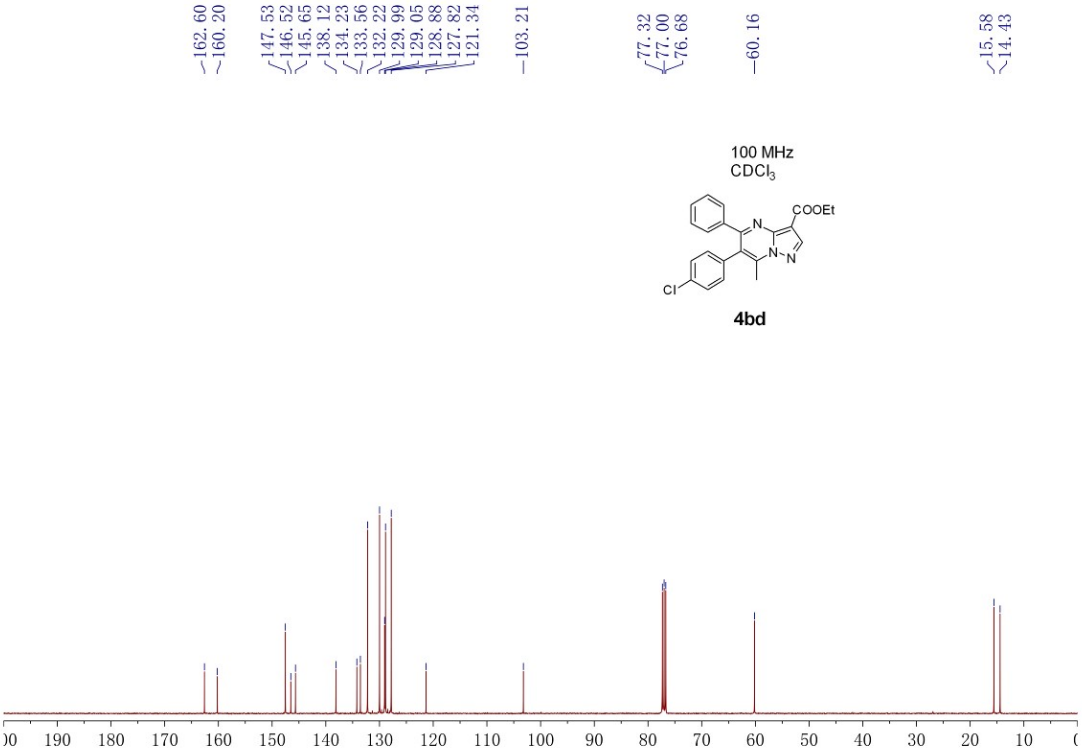
-0.5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132.22
129.99
129.05
128.88
127.82
121.34
103.21
77.32
77.00
76.68
60.16
15.58
14.43
100 MHz
CDCl3
COOEt
N
N
N
Cl
4bd
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180
170
160
150
140
130
120
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100
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80
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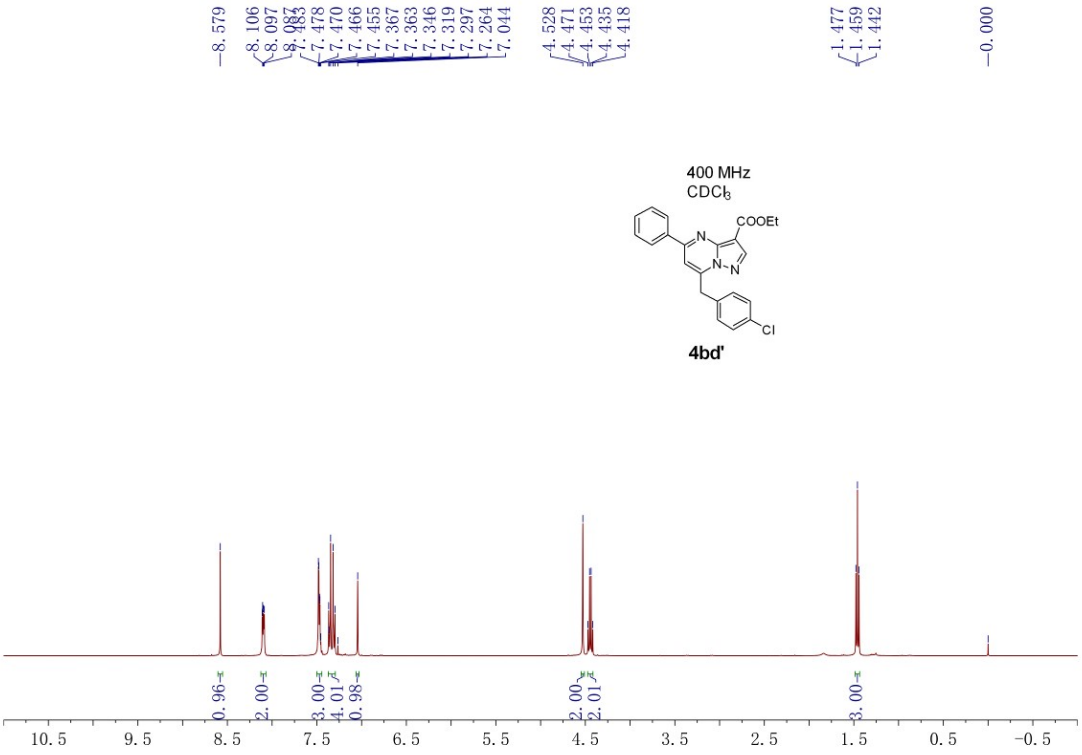
40
30
20
10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7.367
7.363
7.346
7.319
7.297
7.264
7.044
4.528
4.471
4.453
4.435
4.418
1.477
1.459
1.442
0.000
400 MHz
CDCl3
COOEt
N
N-N
Cl
4bd'
0.96
2.00
3.00
4.01
0.98
2.00
2.01
3.00
10.5
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7.5
6.5
5.5
4.5
3.5
2.5
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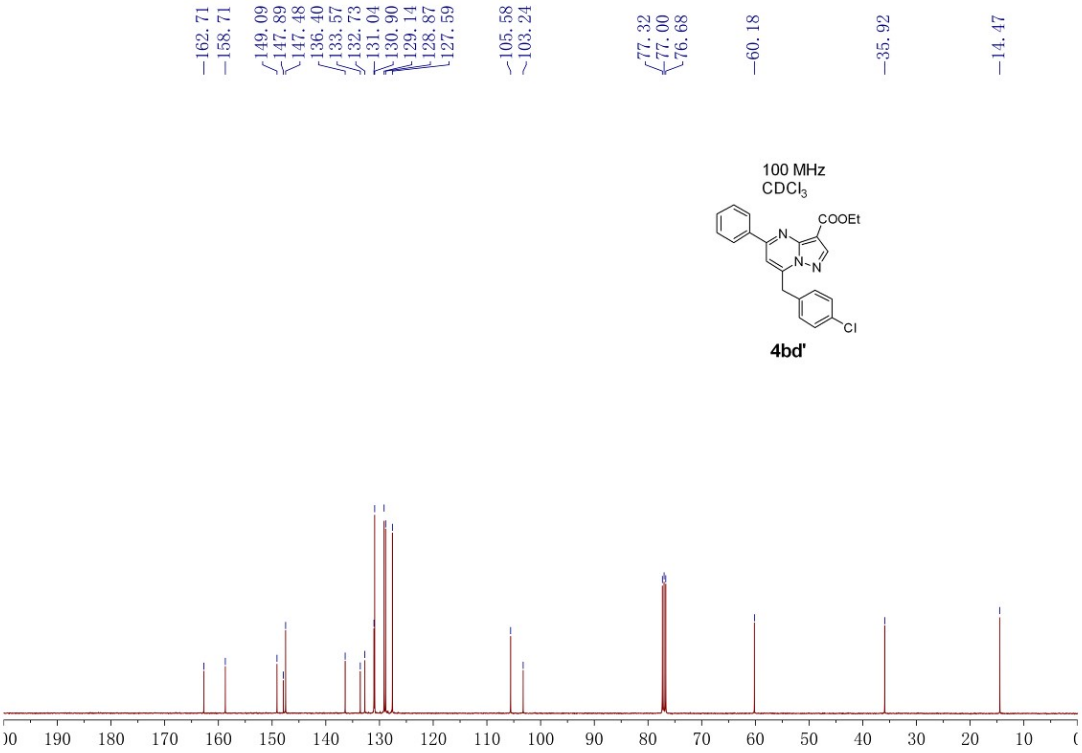
0.5
-0.5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131.04
130.90
129.14
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127.59
105.58
103.24
77.32
77.00
76.68
60.18
35.92
14.47
100 MHz
CDCl3
COOEt
N
N-N
Cl
4bd'
190
180
170
160
150
140
130
120
110
100
90
80
70
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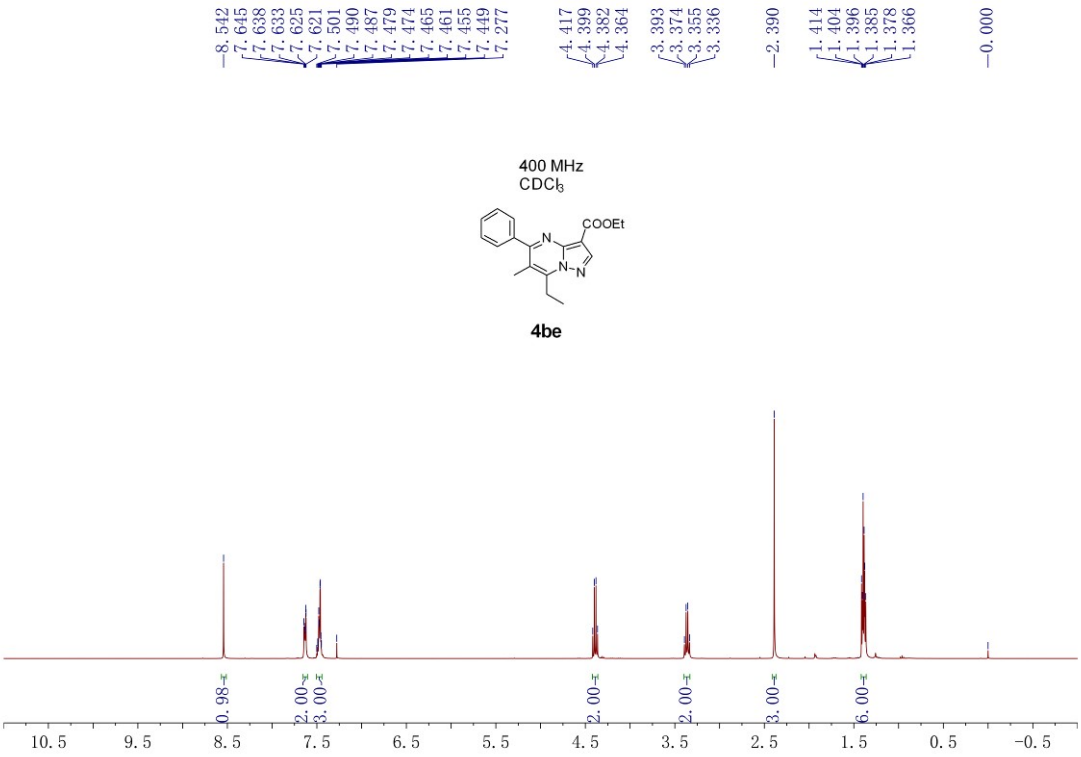
50
40
30
20
10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7.490
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7.474
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7.461
7.455
7.449
7.277
4.417
4.399
4.382
4.364
3.393
3.374
3.355
3.336
2.390
1.414
1.404
1.396
1.385
1.378
1.366
0.000
400 MHz
CDCl3
COOEt
4be
0.98
2.00
3.00
2.00
2.00
3.00
6.00
10.5
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7.5
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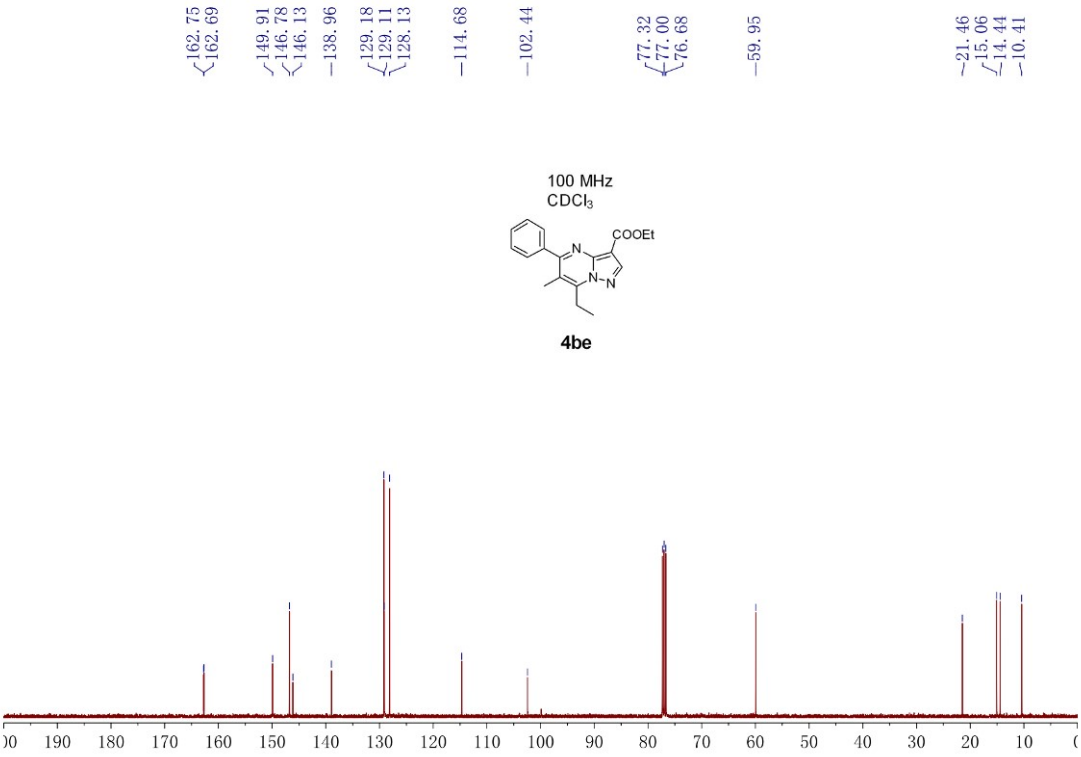
0.5
-0.5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129.11
128.13
114.68
102.44
77.32
77.00
76.68
59.95
21.46
15.06
14.44
10.41
100 MHz
CDCl3
COOEt
4be
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


8.557
7.993
7.986
7.982
7.973
7.969
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7.506
7.498
7.493
7.486
7.268
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4.454
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4.409
4.391
4.382
4.364
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3.011
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2.905
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2.873
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1.774
1.765
1.751
1.741
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1.581
1.450
1.432
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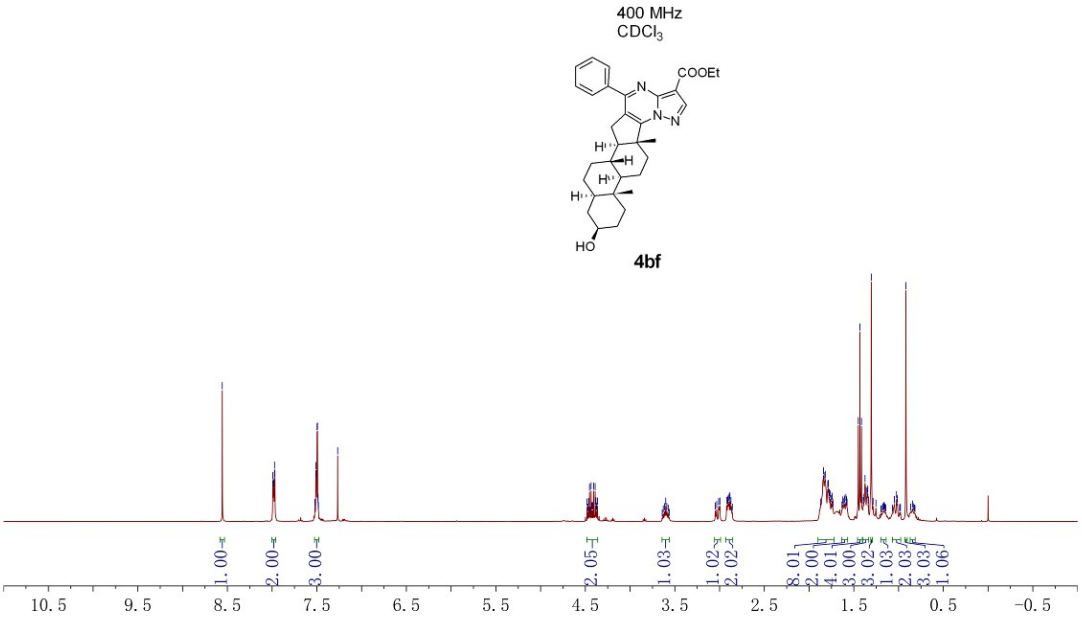
0.918


400 MHz
CDCl3
COOEt
N
N
N
H
H
H
H
HO
4bf
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2.00
3.00
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1.03
1.02
2.02
8.01
2.00
4.01
3.00
3.02
1.03
2.03
3.03
1.06
10.5
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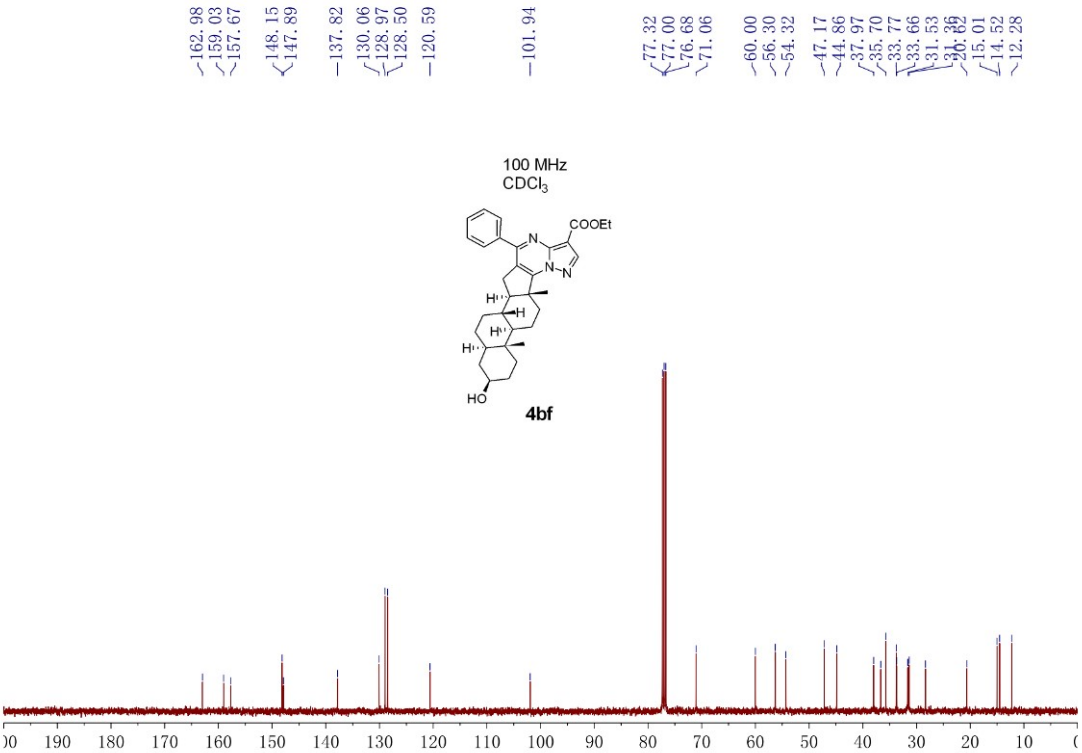
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5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137.82
130.06
128.97
128.50
120.59
101.94
77.32
77.00
76.68
71.06
60.00
56.30
54.32
47.17
44.86
37.97
35.70
33.77
33.66
31.53
15.01
14.52
12.28
100 MHz
CDCl3
COOEt
N
N
N
H
H
H
H
HO
4bf
190
180
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160
150
140
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120
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100
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80
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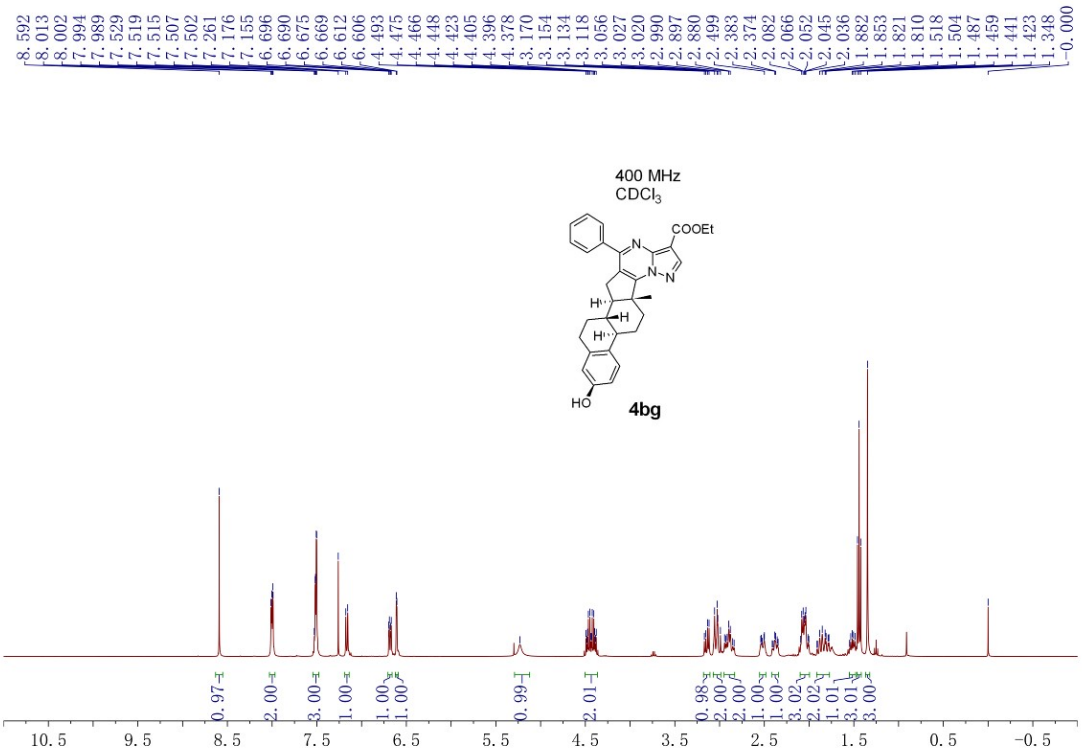
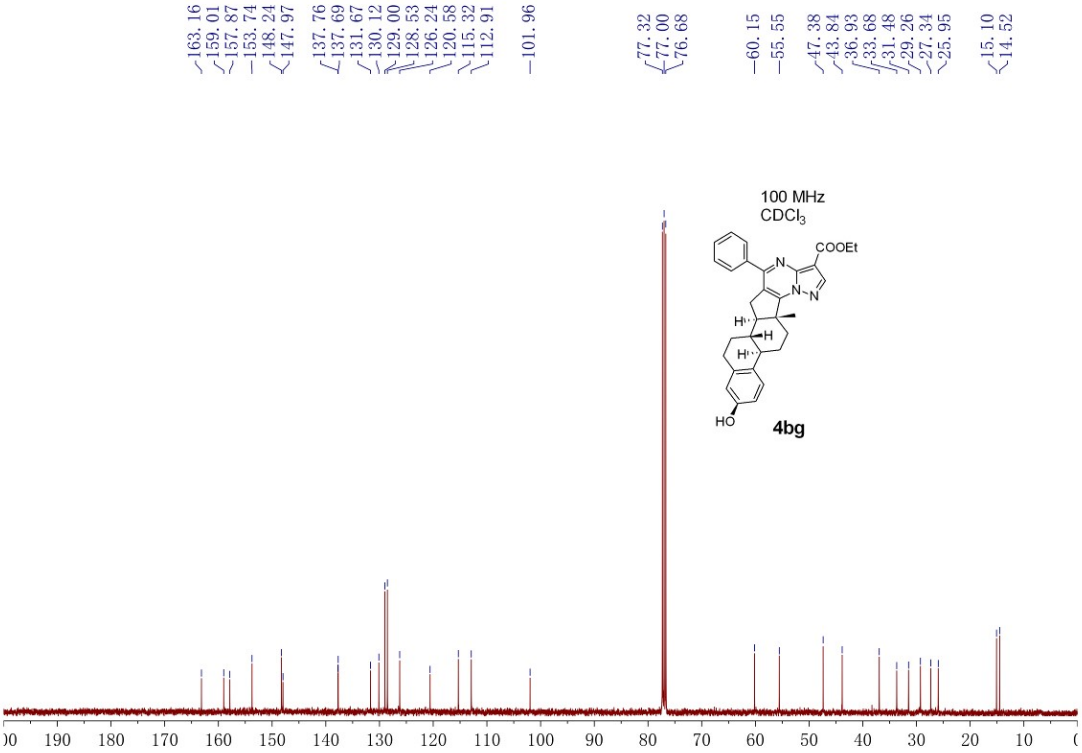
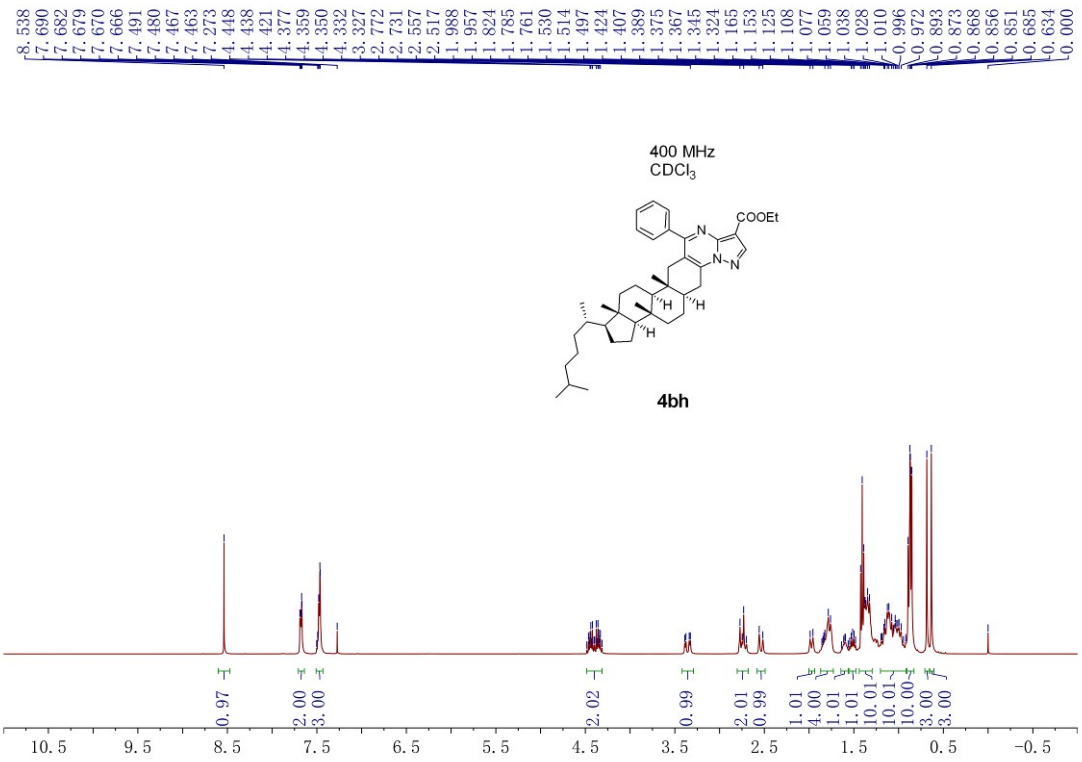
20
10


400 MHz
CDCl3
COOEt
HO
4bg


100 MHz
CDCl3
COOEt
HO
4bg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7.480
7.467
7.463
7.273
4.448
4.438
4.421
4.377
4.359
4.350
4.332
3.327
2.772
2.731
2.557
2.517
1.988
1.957
1.824
1.785
1.761
1.530
1.514
1.497
1.424
1.407
1.389
1.375
1.367
1.345
1.324
1.165
1.153
1.125
1.108
1.077
1.059
1.038
1.028
1.010
0.996
0.972
0.893
0.873
0.868
0.856
0.851
0.685
0.634
0.000
400 MHz
CDCl3
COOEt
4bh
0.97
2.00
3.00
2.02
0.99
2.01
0.99
1.01
4.00
1.01
1.01
10.01
10.01
10.00
3.00
3.00
10.5
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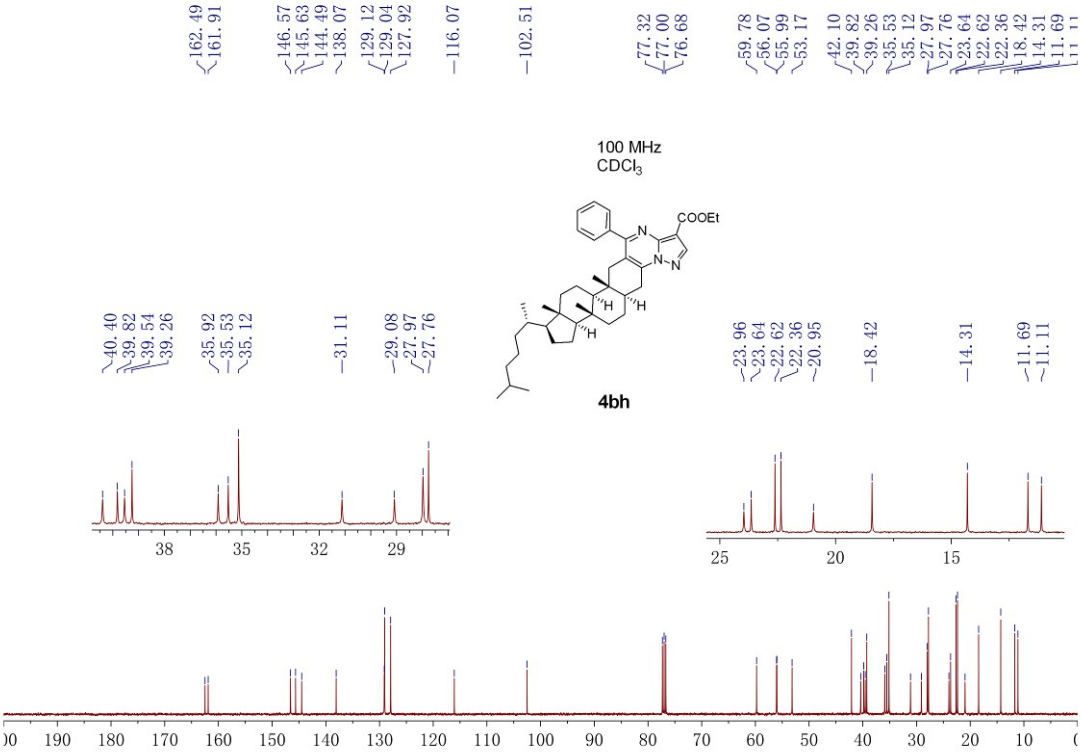
5.5
4.5
3.5
2.5
1.5
0.5
-0.5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145.63
144.49
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129.12
129.04
127.92
116.07
102.51
77.32
77.00
76.68
59.78
56.07
55.99
53.17
42.10
39.82
39.26
35.53
35.12
27.97
27.76
23.64
22.62
22.36
18.42
14.31
11.69
11.11
100 MHz
CDCl3
COOEt
4bh
40.40
39.82
39.54
39.26
35.92
35.53
35.12
31.11
29.08
27.97
27.76
23.96
23.64
22.62
22.36
20.95
18.42
14.31
11.69
11.11
38
35
32
29
25
20
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150
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130
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110
100
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80
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50
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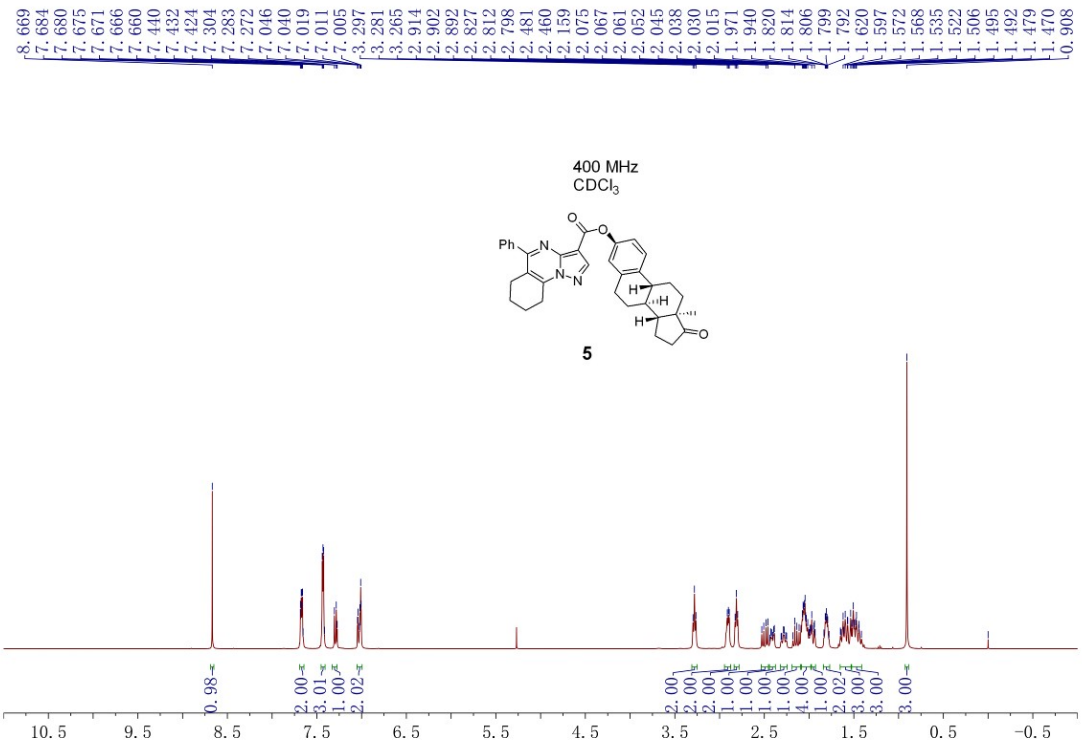
20
10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7.684
7.680
7.675
7.671
7.666
7.660
7.440
7.432
7.424
7.304
7.283
7.272
7.046
7.040
7.019
7.011
7.005
3.297
3.281
3.265
2.914
2.902
2.892
2.827
2.812
2.798
2.481
2.460
2.159
2.075
2.067
2.061
2.052
2.045
2.038
2.030
2.015
1.971
1.940
1.820
1.814
1.806
1.799
1.792
1.620
1.597
1.572
1.568
1.535
1.522
1.506
1.495
1.492
1.479
1.470
0.908
400 MHz
CDCl3
Ph
N
N
N
O
O
H
H
H
O
5
0.98
2.00
3.01
1.00
2.02
2.00
2.00
2.00
1.00
1.00
1.00
1.00
4.00
1.00
2.02
3.00
3.00
3.00
10.5
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6.5
5.5
4.5
3.5
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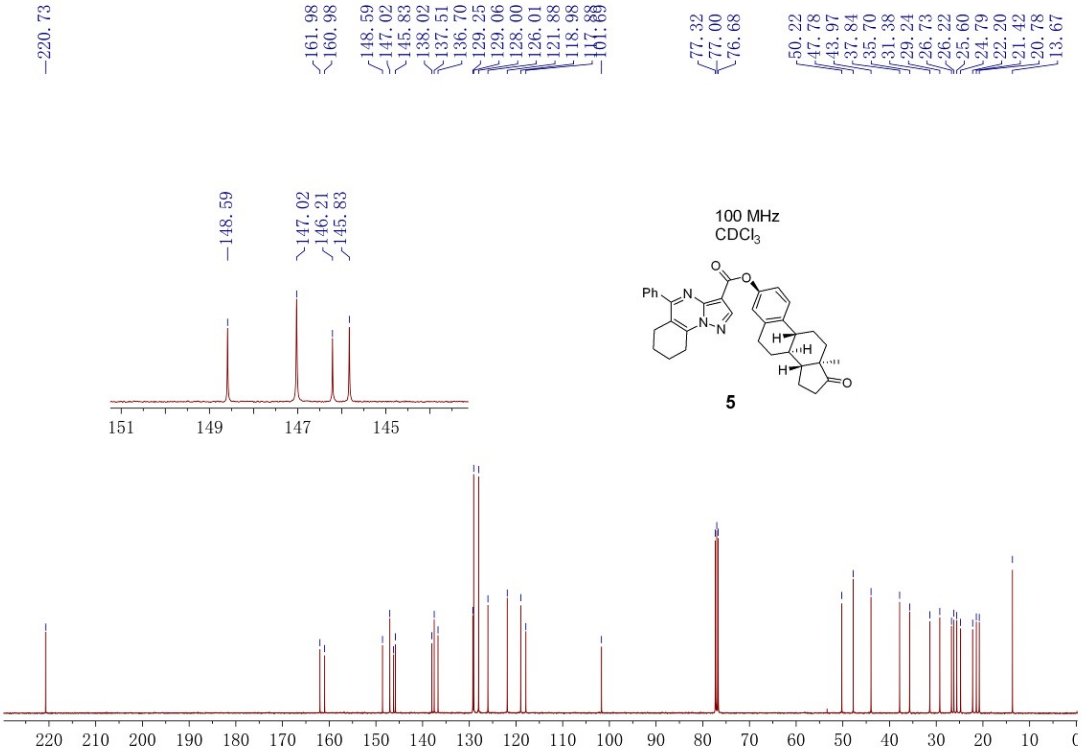
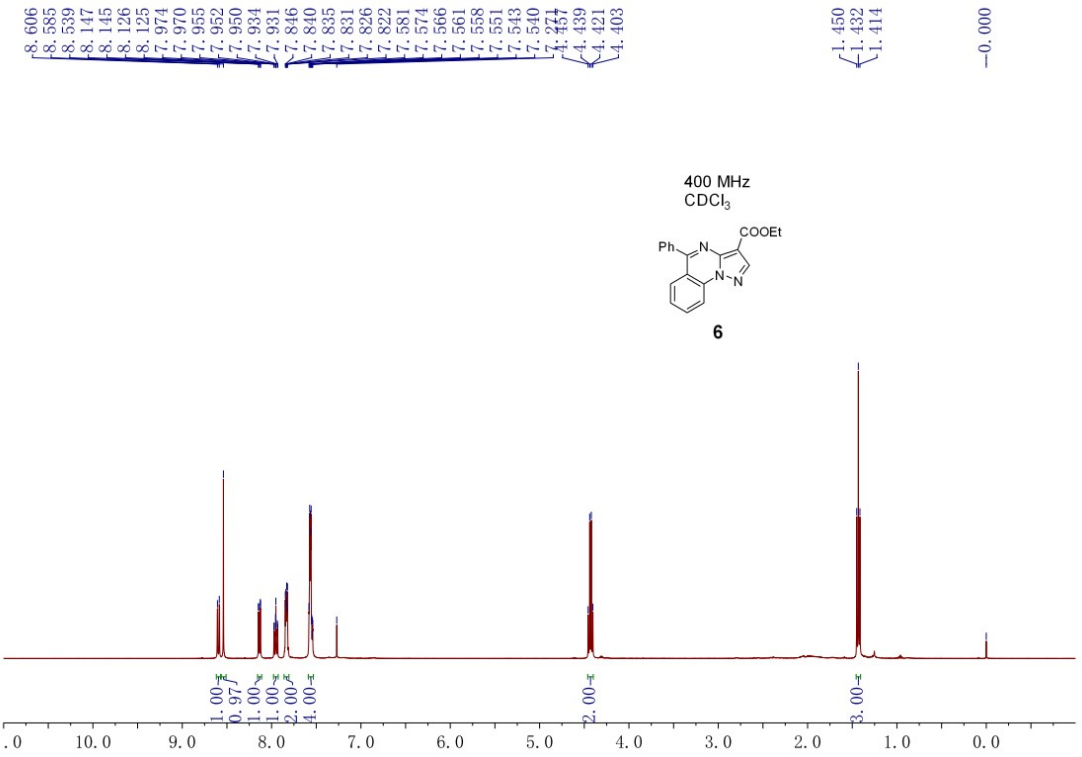
0.5
-0.5


220.73
161.98
160.98
148.59
147.02
145.83
138.02
137.51
136.70
129.25
129.06
128.00
126.01
121.88
118.98
77.32
77.00
76.68
50.22
47.78
43.97
37.84
35.70
31.38
29.24
26.73
26.22
25.60
24.79
22.20
21.42
20.78
13.67
148.59
147.02
146.21
145.83
151
149
147
145
100 MHz
CDCl3
Ph
N
N
N
O
O
H
H
H
O
5
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10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8.585
8.539
8.147
8.145
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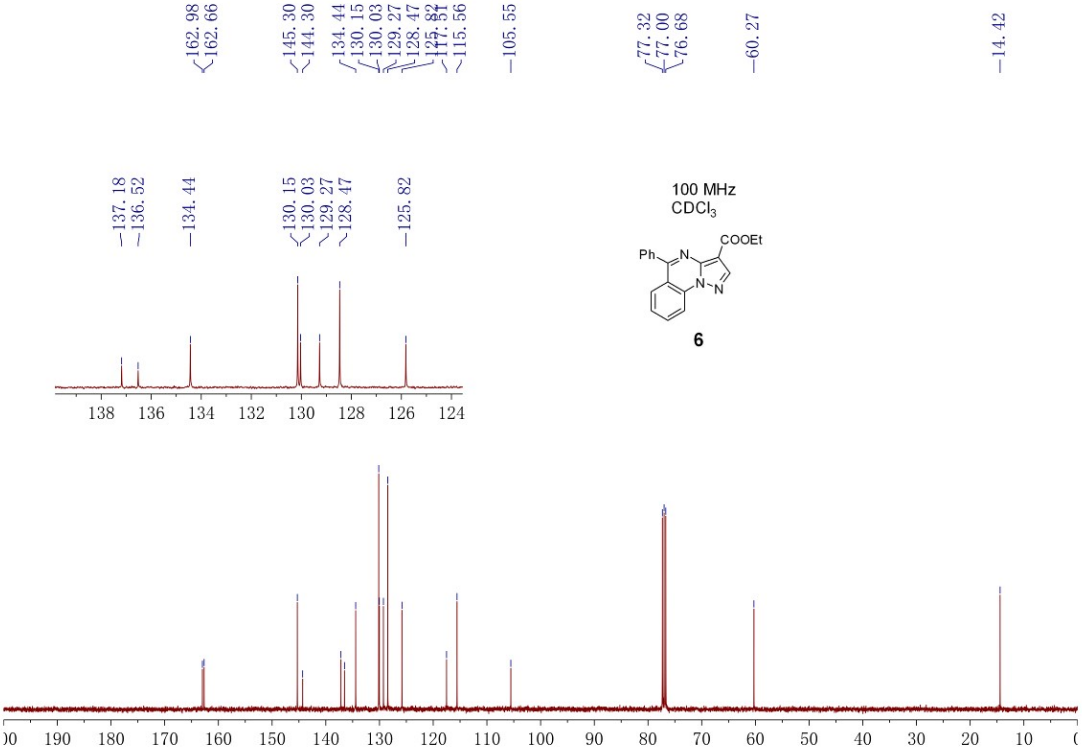
8.125
7.974
7.970
7.955
7.952
7.950
7.934
7.931
7.846
7.840
7.835
7.831
7.826
7.822
7.581
7.574
7.566
7.561
7.558
7.551
7.543
7.540
7.271
4.457
4.439
4.421
4.403
1.450
1.432
1.414
0.000
400 MHz
CDCl3
COOEt
Ph
N
N
N
6
1.00
0.97
1.00
1.00
2.00
4.00
2.00
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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162.66
145.30
144.30
134.44
130.15
130.03
129.27
128.47
125.82
117.51
115.56
105.55
77.32
77.00
76.68
60.27
14.42
137.18
136.52
134.44
130.15
130.03
129.27
128.47
125.82
100 MHz
CDCl3
COOEt
Ph
N
N
N
6
138
136
134
132
130
128
126
124
190
180
170
160
150
140
130
120
110
100
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80
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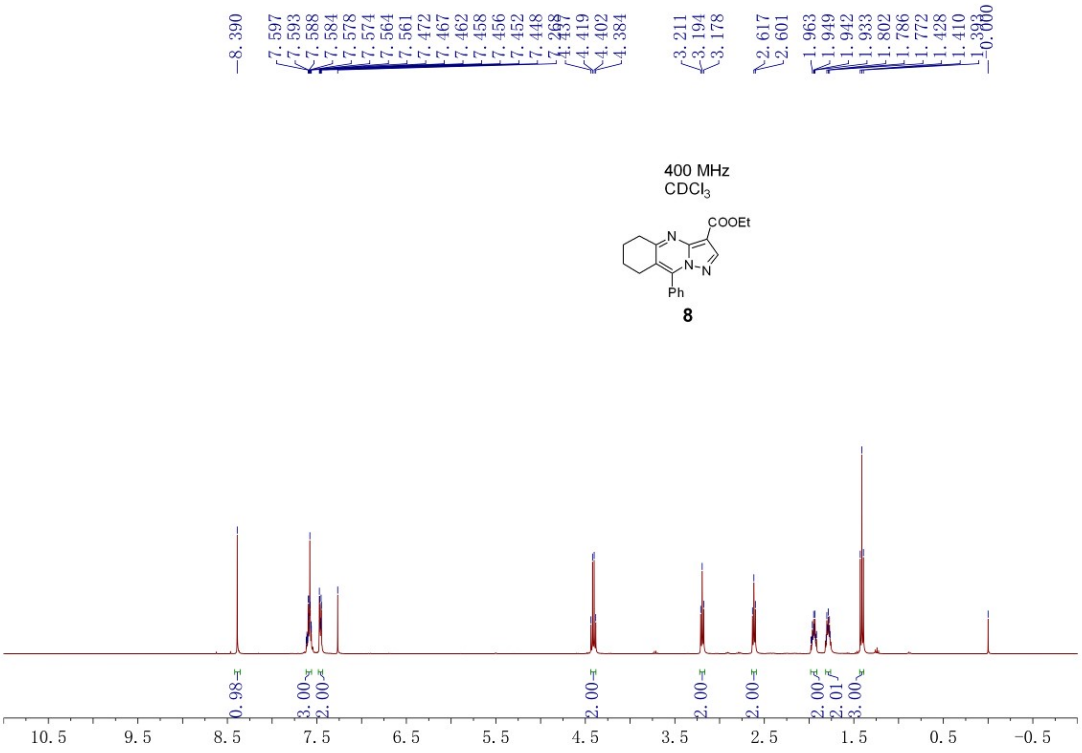
20
10


8.390
7.597
7.593
7.588
7.584
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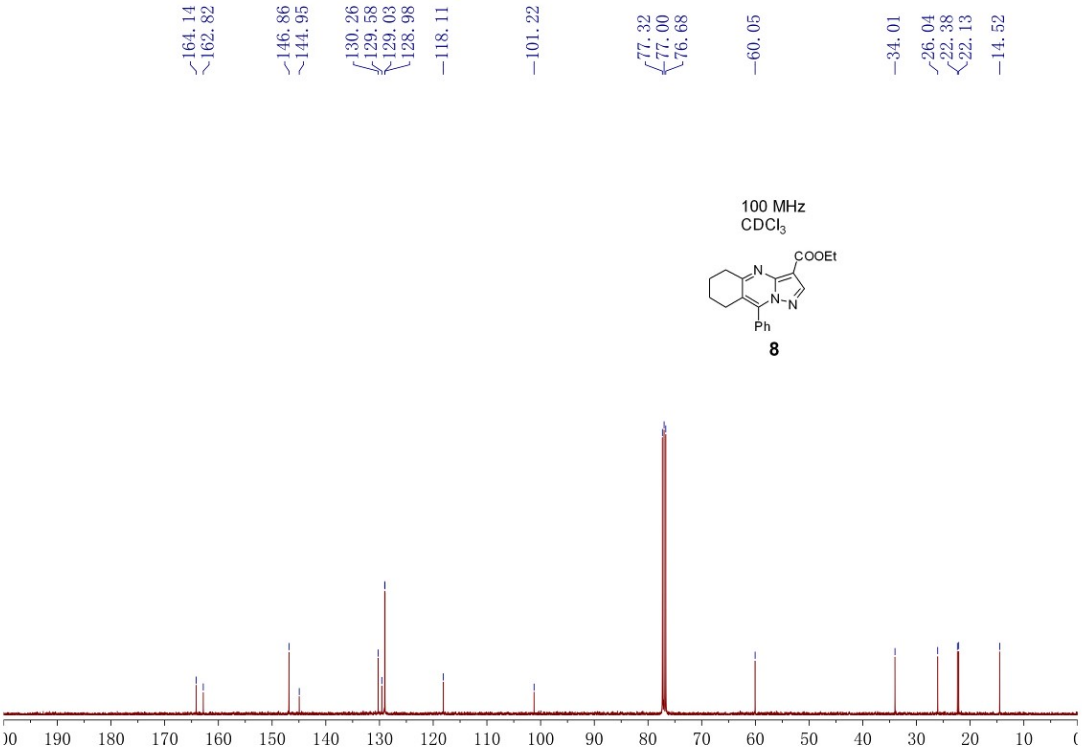
7.574
7.564
7.561
7.472
7.467
7.462
7.458
7.456
7.452
7.448
7.268
4.437
4.419
4.402
4.384
3.211
3.194
3.178
2.617
2.601
1.963
1.949
1.942
1.933
1.802
1.786
1.772
1.428
1.410
1.393
0.000
400 MHz
CDCl3
COOEt
Ph
8
0.98
3.00
2.00
2.00
2.00
2.00
2.00
2.01
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5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146.86
144.95
130.26
129.58
129.03
128.98
118.11
101.22
77.32
77.00
76.68
60.05
34.01
26.04
22.38
22.13
14.52
100 MHz
CDCl3
COOEt
Ph
8
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10