Supporting Information for

Regioselective π-Extension of Indoles With Rhodium Enalcarbenoids- Synthesis of Substituted Carbazoles

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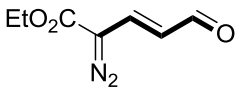
Contents:

1. General Methods:

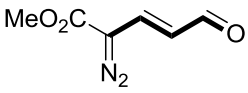
All the reactions were performed in an oven-dried glassware under argon atmosphere. Solvents were dried using standard methods. Tetrahydrofuran and diethyl ether were dried over sodium-benzophenone ketyl. Acetonitrile, dichloromethane and toluene were distilled over calcium hydride. Unless otherwise stated, all the commercial reagents were used as received. Progress of the reaction was monitored by thin layer chromatography (Merck Silicagel 60 F-254, 0.25 nm, precoated plates on alumina). Column chromatographic purifications were performed on Merck silica gel (100-200 mesh). Melting points were recorded on a digital melting point apparatus and are uncorrected.

Spectroscopic characterizations were carried at the Central Instrumentation Facility (CIF), Indian Institute of Science Education and Research (IISER) Bhopal. ^{1}H-NMR spectra were recorded on Bruker Avance III FT-NMR spectrometers at 400 MHz, 500 or 700 MHz and ^{13}C-NMR spectra were recorded at 101 MHz, 126 MHz or 176 MHz. 1H-NMR chemical shifts are reported in ppm relative to the TMS (δ=0) and are abbreviated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), br (broad). ^{13}CNMR chemical shifts are reported in ppm relative to the residual $CDCl_3$ signal (δ= 77.16). IR spectra were recorded on a Perkin Elmer FT-IR spectrometer. HRMS data was obtained on a Bruker microTOFQII or Agilent 5975C high resolution mass spectrometers.

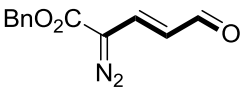
2. Preparation of Enaldiazo Esters 14a-c:



14a



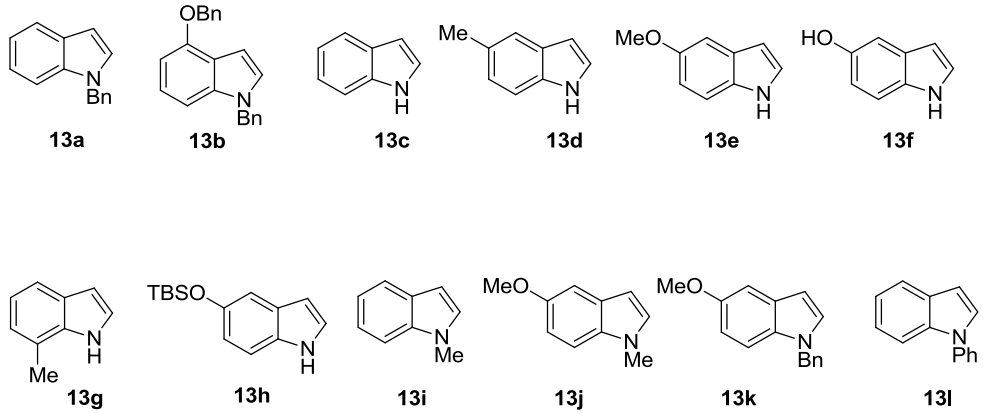
14b



14c

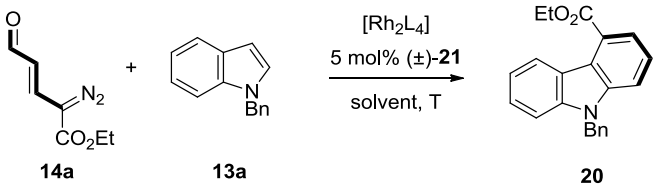
Synthesis of enaldiazo esters **14a-c** was previously reported by us.[1]

3. Preparation of Substituted Indole Starting Materials:



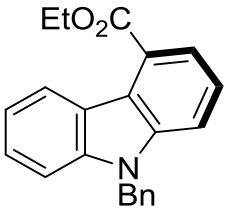
Indoles **13c-13g** were purchased from Sigma-Aldrich. Known indoles **13a, 13b and 13h-l** were prepared according to the literature procedures.[2]

4. Optimization of π-Extension of Indoles:



Entry	Rh_2L_4 (mol %)	**14a/13a**	T (^oC)	Solvent	Yield (%)
1.	$Rh_2(OAc)_4$(2)	1.5/1	40	CH_2Cl_2	42
2.	$Rh_2(Oct)_4$(2)	1.5/1	40	CH_2Cl_2	31
3.	$Rh_2(esp)_4$(2)	1.5/1	40	CH_2Cl_2	26
4.	$Rh_2(TFA)_4$(2)	1.5/1	40	CH_2Cl_2	14
5.	$Rh_2(DOSP)_4$(2)	1.5/1	40	CH_2Cl_2	20
6.	$Rh_2(OAc)_4$(2)	1.5/1	40	CH_2Cl_2	32
7.	**$Rh_2(OAc)_4$(2)**	**2.5/1**	**40**	**CH_2Cl_2**	**68**
8.	$Rh_2(OAc)_4$(2)	3/1	40	CH_2Cl_2	69
9.	$Rh_2(OAc)_4$(2)	2.5/1	40	CH_2Cl_2	45
10.	$Rh_2(OAc)_4$(2)	2.5/1	61	$CHCl_3$	10
11.	$Rh_2(OAc)_4$(2)	2.5/1	84	$C_2H_4Cl_2$	<5
12.	$Rh_2(OAc)_4$(2)	2.5/1	40	toluene	15

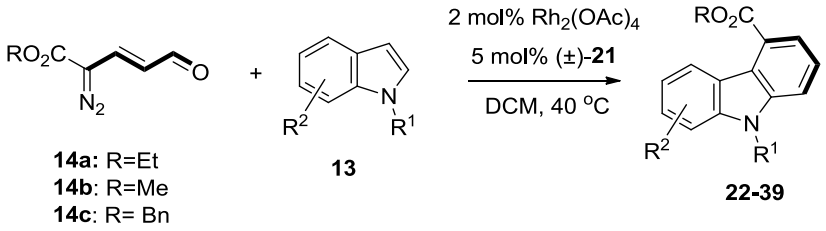
A 0.15 M solution of **14a** (0.6 mmol) was added slowly with a flow rate of 1 ml/h using a syringe pump to a solution of indole **13a** (0.24 mmol), Rh^{II} catalyst and 5 mol% (±)-BINOL phosphoric acid **21** in appropriate solvent (2 ml) at temperature T. The reaction was continued for an additional 2 h. The solvent was evaporated under reduced pressure and the product was purified by silica gel flash column chromatography using ethyl acetate-petroleum ether as the eluent.



Ethyl 9-benzyl-9H-carbazole-4-carboxylate (20): Obtained as a yellow solid. Yield = 68%; R_f=0.42 (Ethyl Acetate/Hexane : 4/96); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (d, *J* = 8.1 Hz, 1H), 7.77 (d, *J* = 7.4 Hz, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 8.1

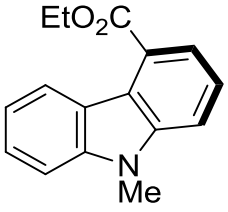
Hz, 1H), 7.34 (t, *J* = 7.9 Hz, 1H), 7.29 (d, *J* = 8.2 Hz, 1H), 7.19 (t, *J* = 8.0 Hz, 1H). 7.14 (d, *J* = 5.9 Hz, 2H), 7.01 – 6.96 (m, 2H), 5.44 (s, 2H), 4.46 (q, *J* = 7.1 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.2, 141.5, 141.4, 136.9, 129.0, 127.7, 127.0, 126.4, 126.0, 125.9, 124.9, 122.4, 121.7, 121.7, 119.7, 113.0, 108.7, 61.2, 46.5, 14.6; IR (neat): 3063, 2922, 2850, 1725, 1714, 1616, 1594 cm^{-1}; HRMS (APCI) *m/z* Calc. for $C_{22}H_{19}NO_2$ [M+H] 330.1489, Found 330.1510.

5. Carbazole Synthesis by π-Extension of Indoles (Table 2):



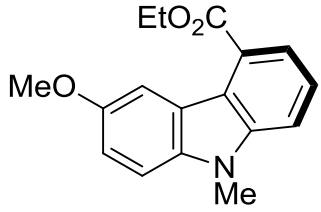
General procedure:

An oven dried 10 ml round-bottom flask containing a stir bar under inert atmosphere was charged with Indole **13** (0.24 mmol), $Rh_2(OAc)_4$ (0.0048 mmol), **21** (0.012 mmol) and CH_2Cl_2 (2 ml) and heated to reflux. To the gently refluxing contents was added a solution of enaldiazo ester **14** (0.6 mmol) in CH_2Cl_2 (4 ml) over 4 h using a syringe pump. The reaction was continued at reflux for another 2 h, and the solvent was evaporated under reduced pressure. The crude material was purified by a silica gel flash column chromatography using ethyl acetate-petroleum ether as the eluent to furnish carbazole.

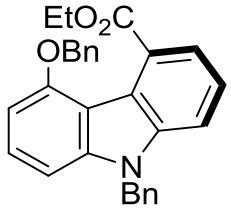


Ethyl 9-methyl-9H-carbazole-4-carboxylate (22): Obtained as a black solid. Yield = 64%; R_f=0.33 (Ethyl Acetate/Hexane : 3/97); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (d, *J* = 8.1 Hz, 1H), 7.86 (dd, *J* = 7.4, 0.6 Hz, 1H), 7.55 (t, *J* = 8.7 Hz, 2H), 7.51 – 7.46 (m, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.27 (dd, *J* = 11.6, 4.3 Hz, 1H), 4.55 (q, *J* = 7.1 Hz, 2H), 3.83 (s, 3H), 1.50 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.2, 141.8, 141.7,

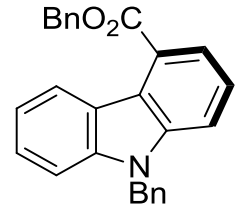
126.7, 125.8, 125.8, 124.6, 122.1, 121.5, 121.4, 119.3, 112.6, 108.3, 61.2, 29.2, 14.5; IR (neat): 3062, 2928, 2857, 1725, 1610, 1570 cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{16}H_{15}NO_2$ [M+H] 254.1176, Found: 254.1186.



Ethyl 6-methoxy-9-methyl-9H-carbazole-4-carboxylate (23): Obtained as a yellow solid. Yield = 50%; R_f=0.35 (Ethyl Acetate/Hexane : 8/92); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 2.4 Hz, 1H), 7.83 (d, *J* = 7.2 Hz, 1H), 7.55 (d, *J* = 8.1 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.32 (d, *J* = 8.9 Hz, 1H), 7.19 (dd, *J* = 8.9, 2.5 Hz, 1H), 4.53 (q, *J* = 7.1 Hz, 2H), 3.95 (s, 3H), 3.84 (s, 3H), 1.48 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.2, 153.6, 142.3, 137.1, 125.8, 124.5, 121.8, 121.8, 121.3, 116.6, 112.8, 108.9, 108.5, 61.2, 56.30, 29.41, 14.6; IR (neat): 3059, 2925, 2848, 1751, 1714, 1596, 1575, 1537 cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{17}H_{17}NO_3$ [M+H] 284.1281, Found:284.1286.

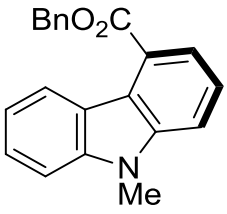


Ethyl 9-benzyl-5-(benzyloxy)-9H-carbazole-4-carboxylate (24): Obtained as a yellow solid. Yield = 70%; R_f=0.77 (Ethyl Acetate/Hexane : 2/98); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.4 Hz, 2H), 7.43 – 7.22 (series of m, 10H), 7.12 – 7.07 (m, 2H), 6.96 (d, *J* = 8.2 Hz, 1H), 6.66 (d, *J* = 8.0 Hz, 1H), 5.45 (s, 2H), 5.39 (s, 2H), 4.14 (q, *J* = 7.1 Hz, 2H), 1.28 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 155.1, 142.9, 140.6, 137.4, 136.9, 129.8, 129.0, 128.7, 127.9, 127.7, 127.3, 126.5, 124.8, 119.0, 117.9, 111.6, 110.3, 102.9, 102.1, 70.6, 61.0, 46.8, 14.4; IR (neat): 3060,2922,2856,1728 cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{29}H_{25}NO_3$ [M+H] 436.1907, Found: 436.1907.

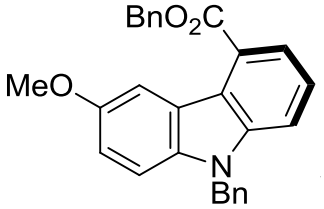


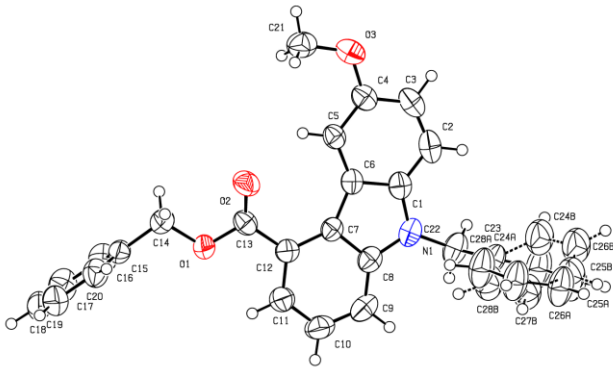
Benzyl 9-benzyl-9H-carbazole-4-carboxylate (25): Obtained as a white solid. Yield = 67%; R_f=0.63 (Ethyl Acetate/Hexane : 4/96); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.97 (d, *J* = 8.2 Hz, 1H), 7.96 (dd, *J* = 7.6, 0.9 Hz, 1H), 7.60 – 7.38 (series of m, 9H), 7.31 - 7.25 (m, 4H), 7.15 – 7.10 (m, 2H), 5.59 (s, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.9, 141.5, 141.4, 136.8, 136.2, 129.0, 128.7, 128.5, 128.4, 127.7, 127.0, 126.3, 126.0, 125.5, 124.9,

122.7, 121.9, 121.7, 119.7, 113.3, 108.7, 67.0, 46.5; IR (neat): 3033, 2920, 2849, 1715, 1617, 1593, 1571cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{27}H_{21}NO_2$ [M+H] 392.1645, Found: 392.1669.

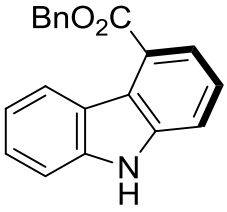


Benzyl 9-methyl-9H-carbazole-4-carboxylate (26): Obtained as a white solid. Yield = 66%; R_f=0.76 (Ethyl Acetate/Hexane : 5/95); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 (d, *J* = 8.1 Hz, 1H), 7.90 (dd, *J* = 7.5, 0.6 Hz, 1H), 7.59 (d, *J* = 7.7 Hz, 1H), 7.55 – 7.45 (m, 4H), 7.43 – 7.31 (m, 4H), 7.23 – 7.19 (m, 1H), 5.52 (s, 2H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.9, 141.8, 141.8, 136.3, 128.8, 128.5, 128.4, 126.8, 126.0, 125.4, 124.7, 122.4, 121.6, 121.5, 119.4, 112.8, 108.3, 67.0, 29.3; IR (neat): 3063, 2922, 2852, 1722, 1714, 1616, 1594, 1574 cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{21}H_{17}NO_2$ [M+H] 354.0891 , Found: 354.0911.

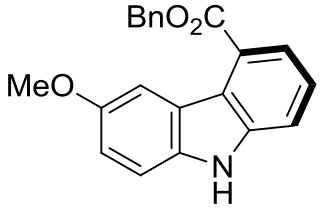


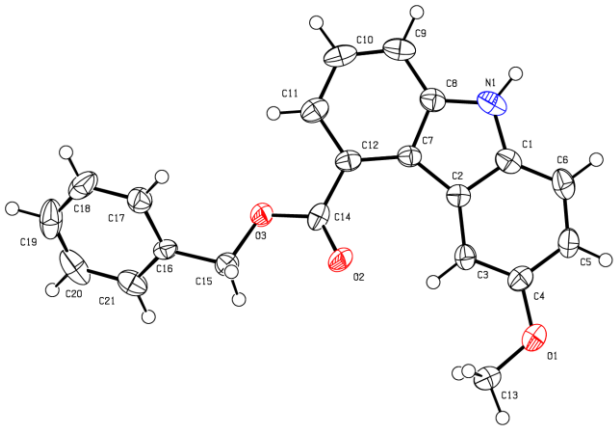


Benzyl 9-benzyl-6-methoxy-9H-carbazole-4-carboxylate (27): Obtained as a pale yellow solid. Yield = 68%; R_f=0.65 (Ethyl Acetate/Hexane : 10/90); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 2.4 Hz, 1H), 7.89 (d, *J* = 7.2 Hz, 1H), 7.55 – 7.52 (m, 3H), 7.44 – 7.33 (m, 4H), 7.28 – 7.20 (m, 4H), 7.13 (dd, *J* = 8.9, 2.5 Hz, 1H), 7.07 – 7.04 (m, 2H), 5.54 (s, 2H), 5.51 (s, 2H), 3.88 (s, 3H);^{13}C NMR (101 MHz, $CDCl_3$) δ 167.9, 153.8, 141.9, 137.0, 136.6, 136.3, 128.9, 128.8, 128.5, 128.3, 127.7, 126.3, 125.4, 124.7, 122.4, 122.0, 121.6, 116.9, 113.4, 109.3, 108.4, 66.9, 56.1, 46.7; IR (neat): 3033, 2928, 2857, 1715, 1623, 1597, 1575 cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{28}H_{23}NO_3$ [M+H] 422.1751, Found:422.1769. CCDC 1005568 contains crystallographic data.

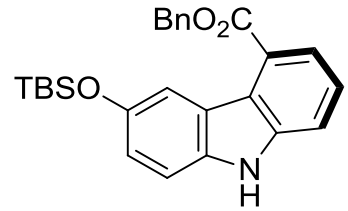


Benzyl 9H-carbazole-4-carboxylate (28): Obtained as a yellow solid. Yield = 62%; R_f=0.50 (Ethyl Acetate/Hexane : 2/98); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 (d, *J* = 8.2 Hz, 1H), 8.28 (s, 1H), 7.91 (d, *J* = 7.5 Hz, 1H), 7.55 - 7.33 (series of m, 9H) 7.21 (d, *J* = 7.9 Hz, 1H), 5.53 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.9, 140.4, 140.3, 136.2, 128.8, 128.5, 128.4, 126.9, 125.9, 125.3, 124.8, 122.9, 122.1, 122.0, 119.8, 115.2, 110.4, 66.9; IR (neat): 3035, 2926, 2854, 1727, 1714, 1698, 1605, 1573 cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{20}H_{15}NO_2$ [M+H] 302.1176, Found: 302.1160;



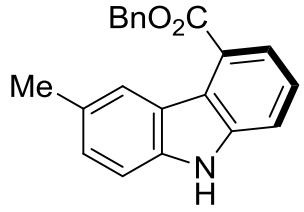


Benzyl 6-methoxy-9H-carbazole-4-carboxylate (29): Obtained as a yellow solid. Yield = 58%; R_f=0.43 (Ethyl Acetate/Hexane : 10/90); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 2.4 Hz, 1H), 8.15 (s, 1H), 7.89 (dd, *J* = 7.5, 0.6 Hz, 1H), 7.59 (dd, *J* = 8.0, 0.6 Hz, 1H), 7.51 (d, *J* = 7.2 Hz, 2H), 7.42 – 7.31 (m, 5H), 7.12 (dd, *J* = 8.8, 2.5 Hz, 1H), 5.51 (s, 2H), 3.86 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.8, 153.9, 141.1, 136.4, 135.3, 128.8, 128.4, 125.3, 124.7, 122.8, 122.5, 122.2, 117.1, 115.3, 111.0, 108.2, 66.9, 56.1; IR (neat): 3036, 2929, 2835, 1714, 1701, 1606, 1596 cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{21}H_{17}NO_3$ [M+H] 332.1281, Found: 332.1268. CCDC 1005570 contains crystallographic data.

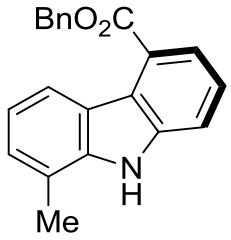


Benzyl 6-((tert-butyldimethylsilyl)oxy)-9H-carbazole-4-carboxylate (30): Obtained as a black solid. Yield = 52%; R_f=0.80 (Ethyl Acetate/Hexane : 2/98); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 2.3 Hz, 1H), 8.11 (s, 1H), 7.84 (dd, *J* = 7.5, 0.6 Hz, 1H), 7.55 – 7.31 (series of m, 7H) 7.27 (d, *J* = 8.7 Hz, 1H), 7.03 (dd, *J* = 8.6, 2.4 Hz,

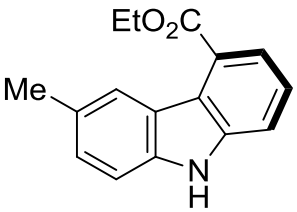
1H), 5.50 (s, 2H), 1.02 (s, 9H), 0.25 (s, 6H**)**; ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.6, 149.2, 141.2, 136.5, 135.7, 128.7, 128.4, 128.3, 125.5, 124.8, 122.7, 122.6, 122.1, 120.7, 115.7, 115.1, 110.6, 66.8, 29.8, 26.0, 18.5, -4.2; IR (neat): 3035, 2929, 2857, 1723, 1715, 1619, 1622, 1572, 1500 cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{26}H_{29}NO_3Si$ [M+H] 432.1989, Found: 432.2015.



Benzyl 6-methyl-9H-carbazole-4-carboxylate (31): Obtained as a pink solid. Yield = 67%; R_f=0.64 (Ethyl Acetate/Hexane : 4/96); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (s, 1H), 8.15 (s, 1H), 7.88 (dd, *J* = 7.6, 0.6 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 7.1 Hz, 2H), 7.43 – 7.30 (m, 5H), 7.27 (dd, *J* = 8.4, 1.0 Hz, 1H), 5.52 (s, 2H), 2.46 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 140.7, 138.6, 136.3, 129.1, 128.8, 128.5, 128.4, 128.4, 125.6, 125.4, 124.7, 122.9, 122.2, 121.9, 115.1, 110.1, 67.0, 21.8; IR (neat): 3046, 2925, 2855, 1724, 1714, 1605, 1573cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{21}H_{17}NO_2$ [M+H] 316.1332, Found: 316.1346.

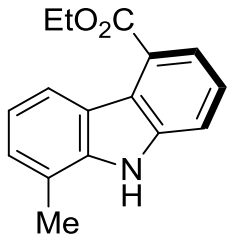


Benzyl 7-methyl-9H-carbazole-4-carboxylate (32): Obtained as a pink solid. Yield = 66%; R_f=0.72 (Ethyl Acetate/Hexane : 3/97); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 8.2 Hz, 1H), 8.18 (s, 1H), 7.92 – 7.88 (m, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.52 (d, *J* = 7.1 Hz, 2H), 7.44 – 7.31 (m, 4H), 7.27 (d, *J* = 7.2 Hz, 1H), 7.14 (t, *J* = 7.7 Hz, 1H), 5.52 (s, 2H), 2.56 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.8, 140.3, 139.7, 136.3, 128.8, 128.5, 128.4, 127.5, 125.5, 124.7, 123.6, 123.0, 122.7, 121.6, 119.9, 119.3, 115.2, 66.9, 17.0; IR (neat): 3028, 2924, 2854, 1714, 1700, 1607 cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{21}H_{17}NO_2$ [M+H]316.1332, Found : 316.1343.



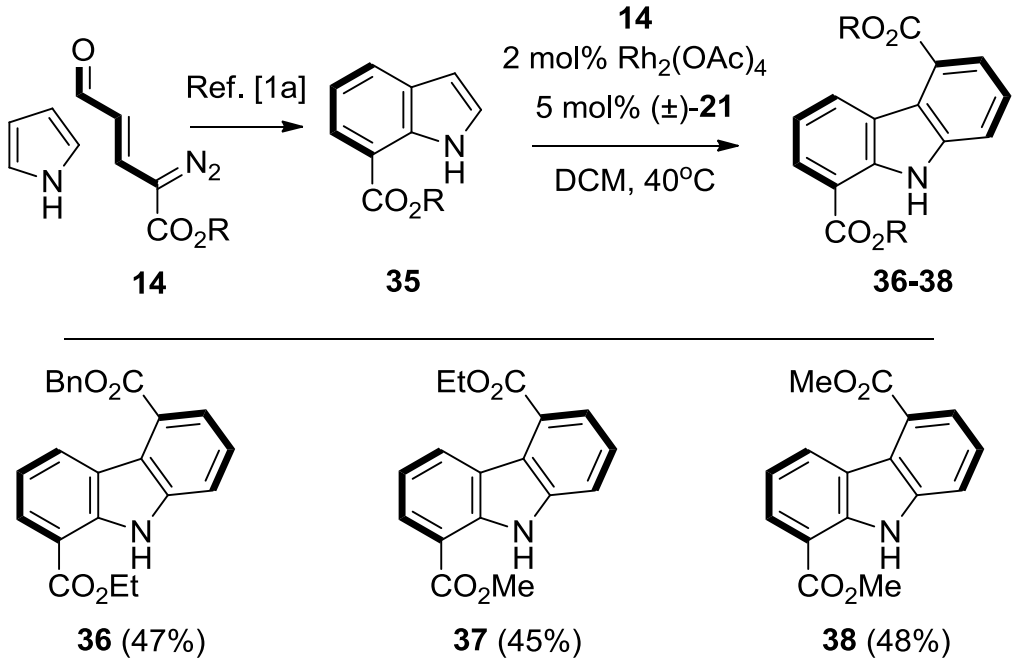
Ethyl 6-methyl-9H-carbazole-4-carboxylate (33): Obtained as a pink solid. Yield = 60%; R_f=0.75 (Ethyl Acetate/Hexane : 4/96); ^{1}H NMR (400 MHz, $CDCl_3$)

δ 8.64 (s, 1H), 8.15 (s, 1H), 7.83 (dd, *J* = 7.5, 0.7 Hz, 1H), 7.57 (dd, *J* = 8.0, 0.6 Hz, 1H), 7.40 (t, *J* = 7.8 Hz, 1H), 7.33 (d, *J* = 8.2 Hz, 1H), 7.28 (dd, *J* = 8.3, 1.0 Hz, 1H), 4.54 (q, *J* = 7.1 Hz, 2H), 2.53 (s, 3H), 1.49 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$ δ 168.2, 140.7, 138.6, 129.1, 128.4, 125.8, 125.5, 124.7, 122.6, 122.3, 121.8, 114.8, 110.1, 61.2, 21.9, 14.6; IR (neat): 3032, 2921, 2857, 1696, 1649, 1605; HRMS (LC) *m/z* Calc. for $C_{16}H_{15}NO_2$ [M+H]254.1176, Found : 256.1194.

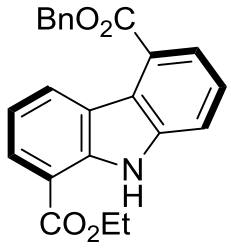


Ethyl 7-methyl-9H-carbazole-4-carboxylate (34): Obtained as a pink solid. Yield =61%; R_f=0.72 (Ethyl Acetate/Hexane : 4/96); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 8.2 Hz, 1H), 8.17 (s, 1H), 7.85 (dd, *J* = 7.5, 0.5 Hz, 1H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.27 (d, *J* = 7.1 Hz, 1H), 7.17 (t, *J* = 7.7 Hz, 1H), 4.53 (q, *J* = 7.1 Hz, 2H), 2.56 (s, 3H), 1.48 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.2, 140.3, 139.7, 127.4, 126.0, 124.7, 123.4, 122.8, 122.5, 121.6, 119.9, 119.3, 115.0, 61.2, 17.0, 14.6; IR (neat): 3054, 2925, 2855, 1717, 1696, 1606, 1590 cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{16}H_{15}NO_2$ [M+H] 254.1176, Found : 256.1162.

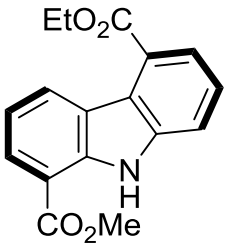
6. Carbazole Synthesis by Twofold π-Extension of Pyrroles (Table 3):



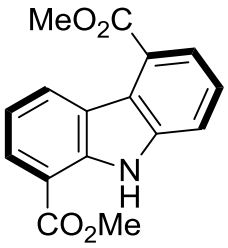
The first π-extension of pyrrole to 7-substituted indole **35** was carried according to our reported procedure.[1a] The 2nd π-extension in **35** was carried according to the general procedure described for table 2 (page# S5). The yields reported are for the 2nd π-extension of indole **35** to 4,8-disubstituted carbazoles **36-38**.

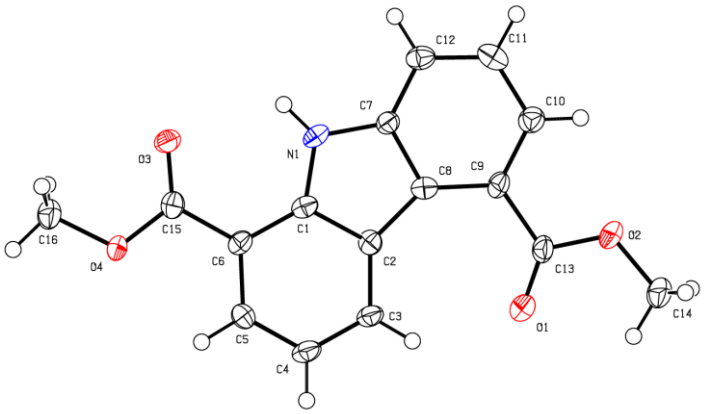


5-benzyl 1-ethyl 9H-carbazole-1,5-dicarboxylate (36): Obtained as a white solid. Yield = 47%; R_f=0.63; (Ethyl Acetate/Hexane: 3/97). ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.36 (s, 1H), 9.20 (d, *J* = 8.0 Hz, 1H), 8.17 (dd, *J* = 7.6, 1.0 Hz, 1H), 8.01 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.74 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.57 (d, *J* = 7.3 Hz, 2H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.45 (dd, *J* = 10.1, 4.6 Hz, 2H), 7.42 – 7.38 (m, 1H), 7.29 (d, *J* = 4.5 Hz, 1H), 5.55 (s, 2H), 4.52 (q, *J* = 7.1 Hz, 2H), 1.51 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.8, 167.5, 141.0, 140.6, 136.2, 131.7, 128.8, 128.5, 128.5, 128.4, 125.5, 125.4, 123.6, 123.3, 121.4, 118.9, 115.8, 111.6, 67.0, 61.1, 14.6; IR (neat): 3417, 3042, 2919, 2857, 1664 cm^{-1}; HRMS (LC) *m/z* calc. for $C_{23}H_{19}NO_4$ [M+H] 374.1387, Found: 374.1399.



5-ethyl 1-methyl 9H-carbazole-1,5-dicarboxylate (37): Obtained as a white solid. Yield = 45%; R_f=0.64; (Ethyl Acetate/Hexane : 4/94). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.27 (s, 1H), 9.17 (d, *J* = 8.0 Hz, 1H), 8.11 (d, *J* = 7.6 Hz, 1H), 7.92 (d, *J* = 7.5 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 1H), 7.28 (d, *J* = 7.9 Hz, 1H), 4.52 (q, *J* = 7.1 Hz, 2H), 4.01 (s, 3H), 1.48 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.2, 167.8, 140.9, 140.6, 131.7, 128.5, 125.9, 125.6, 123.4, 123.4, 121.3, 118.9, 115.6, 111.3, 61.3, 52.1, 14.6; IR (neat): 3417, 2928, 2857, 1690, 1570 cm^{-1}; HRMS (LC) *m/z* calc. for $C_{17}H_{15}NO4$ [M+H] 298.1074, Found: 298.1098.

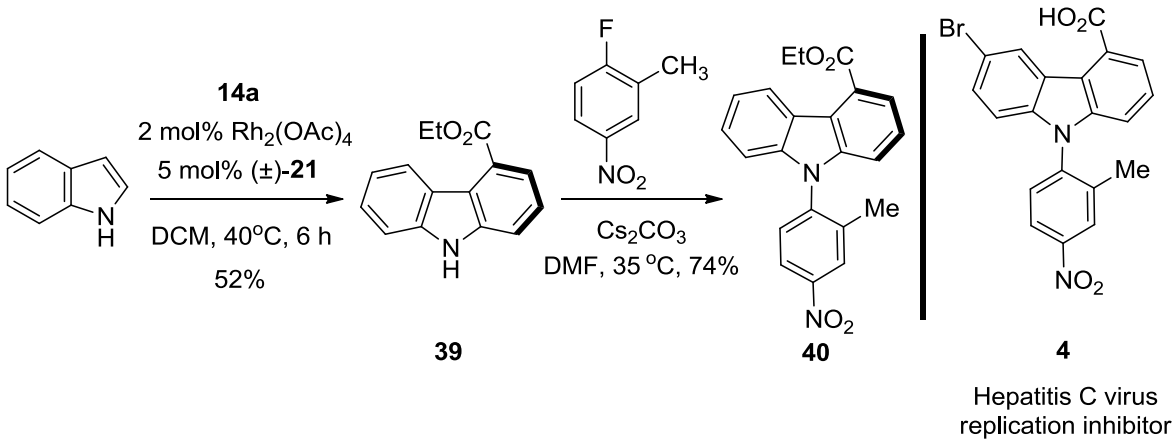




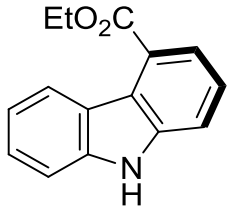
Dimethyl 9H-carbazole-1,5-dicarboxylate (38): Obtained as a white solid. Yield = 48%; R_f=0.55; (Ethyl Acetate/Hexane: 3/97). ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.31 (s, 1H), 9.18 (d, *J* = 8.1 Hz, 1H), 8.17 – 8.13 (m, 1H), 7.95 (d, *J* = 7.6 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.31 (t, *J* = 7.9 Hz, 1H), 4.09 (s, 3H), 4.05 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.2, 168.1, 140.9, 140.5, 131.6, 128.5, 125.6, 125.4, 123.5, 123.3, 121.2, 119.0, 115.7, 111.3, 52.3, 52.1; IR (neat): 3410, 2925, 2857, 1680 cm^{-1}; HRMS (LC) *m/z* calc. for $C_{16}H_{13}NO_4$ [M+H] 284.0917, Found: 284.0935. CCDC 1005569 contains crystallographic data.

7. Synthetic Applications of π-Extension:

A: Synthesis of 40-an analogue of hepatitis C virus replication inhibitor 4:



Scheme S1: Synthesis of an analogue **40** of hepatitis C virus replication inhibitor **4** via π-extension of indole



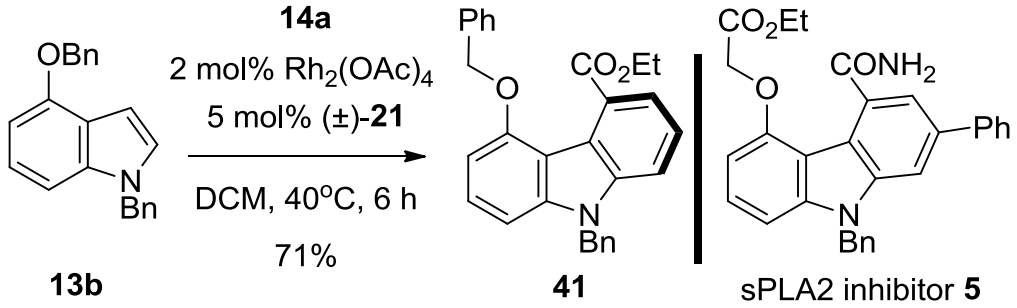
Ethyl 9H-carbazole-4-carboxylate (39): Prepared by following the general procedure of π-extension. Obtained as a pale yellow liquid. Yield = 52%; R_f=0.53 (Ethyl Acetate/Hexane : 3/97); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.95 – 8.91 (m, 1H), 8.40 (s, 1H), 7.91 (dd, *J* = 7.5, 1.1 Hz, 1H), 7.53 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.49 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H), 7.46 – 7.42 (m, 1H), 7.40 – 7.36 (m, 1H), 7.32 – 7.27 (m, 1H), 4.60 (q, *J* = 7.1 Hz, 2H), 1.54 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.3, 140.4, 140.3, 126.8, 125.7, 125.6, 124.8, 122.6, 122.0, 121.8, 119.7, 115.0, 110.5, 61.3, 14.5; IR (neat): 3029, 2921, 2718, 1726, 1715, 1697 cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{15}H_{13}NO_2$ $[M+H]^+$ 240.1019, Found: 240.1002.

Preparation of 40:

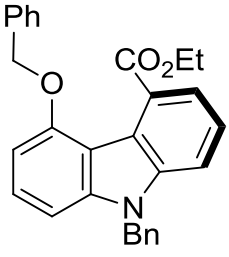
Prepared using the literature procedure reported by Beigelman et. al.[3] A solution of carbazole **39** (0.4 mmol), 3-nitro-5-fluorotoluene (0.4 mmol) and anhydrous cesium carbonate (0.5 mmol) in dry DMF (5 mL) was stirred at 35 ^{0}C for 14 h. The reaction mixture was extracted with ethyl acetate and washed with water, brine and dried over anhydrous sodium sulfate. Purification by silica gel column chromatography using 5% ethyl acetate-hexane gave N-

arylcarbazole **40** as a white solid. Yield = 74%; R_f=0.65; (Ethyl Acetate/Hexane : 80/20); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (d, *J* = 8.1 Hz, 1H), 8.37 (d, *J* = 2.2 Hz, 1H), 8.27 (dd, *J* = 8.5, 2.4 Hz, 1H), 7.94 – 7.91 (m, 1H), 7.53 (d, *J* = 8.6 Hz, 1H), 7.44 (dt, *J* = 16.0, 4.4 Hz, 2H), 7.33 (dd, *J* = 11.3, 4.0 Hz, 1H), 7.15 (d, *J* = 7.7 Hz, 1H), 6.98 (d, *J* = 8.1 Hz, 1H), 4.57 (q, *J* = 7.1 Hz, 2H), 2.06 (s, 3H), 1.51 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 148.0, 141.9, 141.4, 141.4, 139.8, 130.8, 127.5, 127.0, 126.4, 126.2, 125.5, 123.6, 122.9, 122.3, 122.3, 120.9, 113.7, 109.4, 61.5, 18.1, 14.6; IR (neat): 3020, 2926, 2900, 1630, 1425 cm^{-1}; HRMS (LC) *m/z* calc. for $C_{22}H_{18}N_2O_4$ [M+H] 375.1339, Found: 1375.1323.

B: Synthesis of 41- an analogue of sPLA2 inhibitor 5:



The sPLA2 inhibitor **5**[4] analogue **41** was prepared by π-extension of **13b** with **14a** according to the general procedure of π-extension.

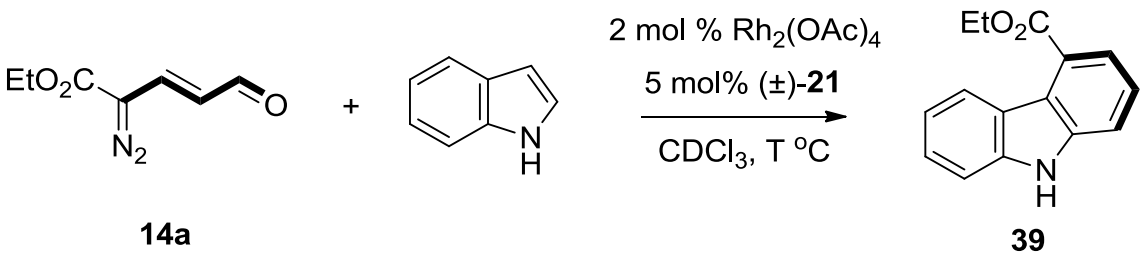


Ethyl 9-benzyl-5-(benzyloxy)-9H-carbazole-4-carboxylate (41): Prepared by following the general procedure of π-extension. Obtained as a yellow solid. Yield = 71%; R_f=0.77 (Ethyl Acetate/Hexane : 2/98); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.4 Hz, 2H), 7.43 – 7.35 (m, 3H), 7.32 (dd, J = 9.1, 2.9 Hz, 2H), 7.29 – 7.25 (m, 2H), 7.24 (s, 2H), 7.12 – 7.07 (m, 2H), 6.96 (d, *J* = 8.2 Hz, 1H), 6.66 (d, *J* = 8.0 Hz, 1H), 5.45 (s, 2H), 5.39 (s, 2H), 4.14 (q, *J* = 7.1 Hz, 2H), 1.28 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 155.1, 142.9, 140.6, 137.4, 136.9, 129.8, 129.0, 128.7, 127.9, 127.7, 127.3, 126.5,

124.8, 119.0, 117.9, 111.6, 110.3, 102.9, 102.1, 70.6, 61.0, 46.8, 14.4; IR (neat):3060,2922,2856,1728 cm^{-1}; HRMS (LC) *m/z* Calc. for $C_{29}H_{25}NO_3$ [M+H] 436.1907, Found: 436.1907.

8. Mechanistic Studies

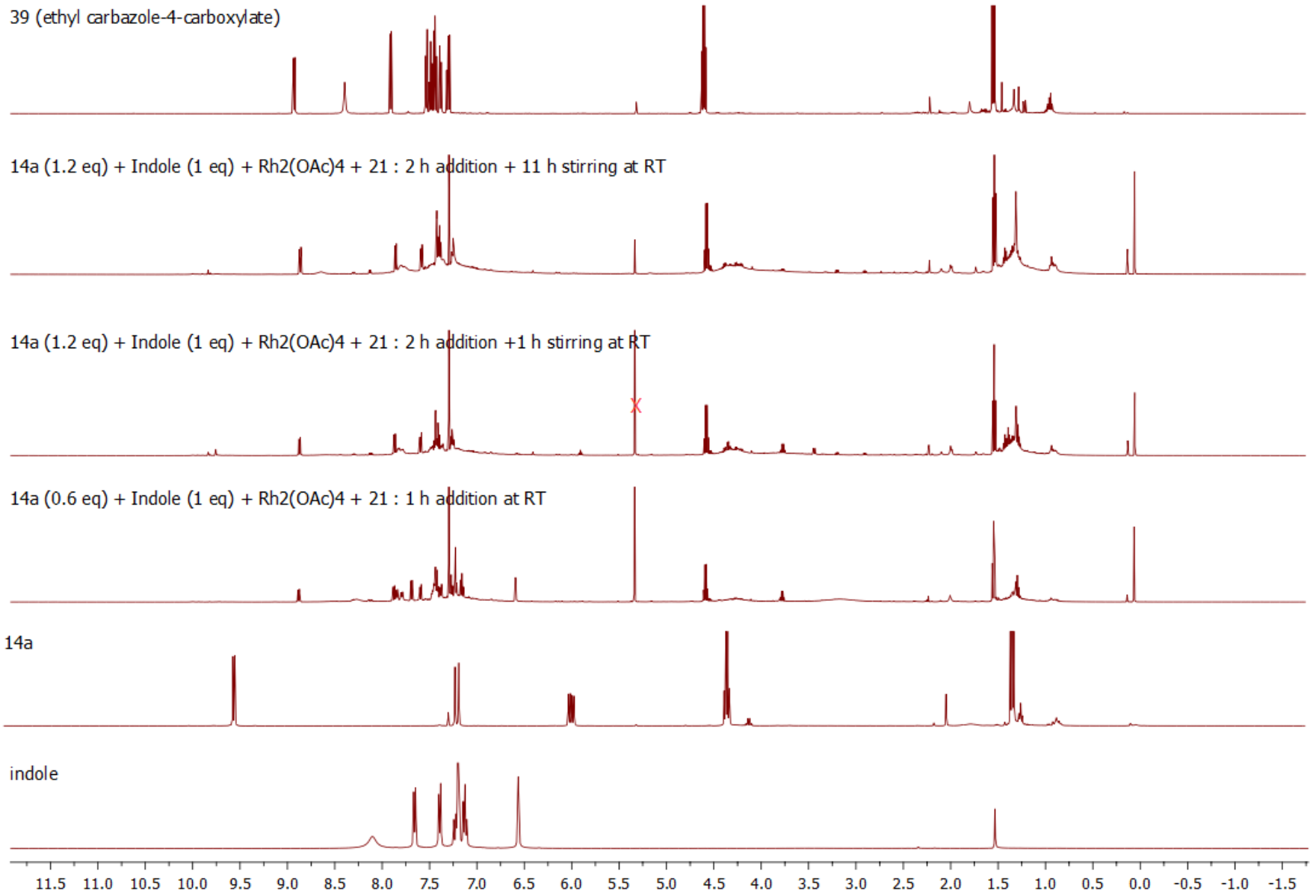
To probe the mechanism of the reaction, the π-extension was carried with indole, enaldiazo ester **14a**, 2 mol% $Rh_2(OAc)_4$ and 5 mol % (±)-**21** at different temperatures in $CDCl_3$ solvent and progress of the reaction was monitored by thin layer chromatography (TLC) and ^{1}H-NMR data. At 10 ^{o}C, the reaction did not proceed even after 10 hours. However, the reaction was proceeded at room temperature (25 ^{o}C) as well as at 40 ^{o}C. But, no intermediate formation was detected by ^{1}H-NMR studies and by TLC analysis.

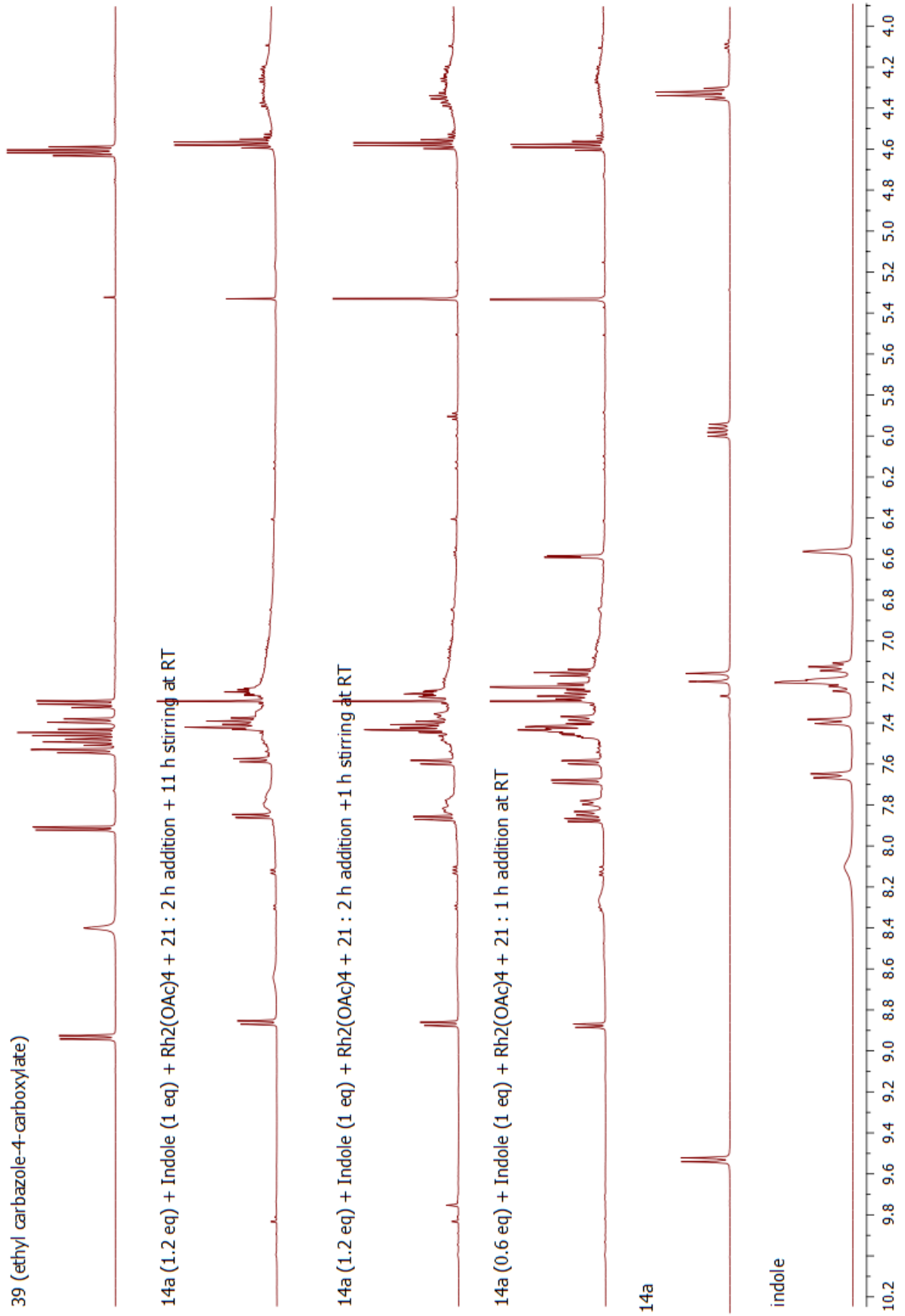


14a **39**

(a) NMR study at room temperature (25 ^{o}C):

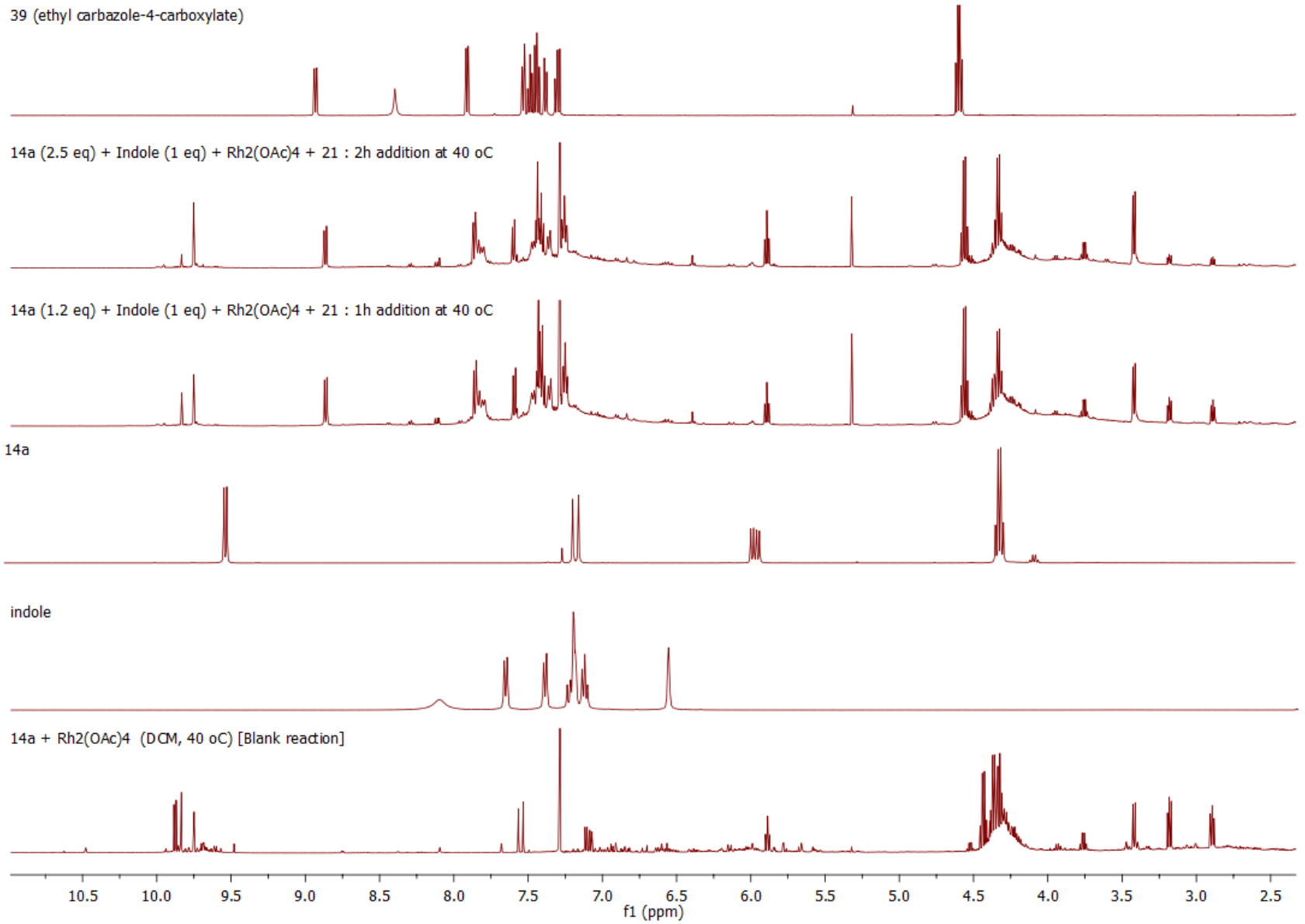
An oven dried 10 ml round-bottom flask containing a stir bar under inert atmosphere was charged with Indole (0.24 mmol), $Rh_2(OAc)_4$ (0.0048 mmol), (±)-**21** (0.012 mmol) and $CDCl_3$ (2 ml). To the gently stirring contents at rt (25 ^{o}C) was added a solution of enaldiazo ester **14a** (0.3 mmol) in $CDCl_3$ (2 ml) with a flow rate of 1 ml/h using a syringe pump. The reaction was monitored by thin layer chromatography (TLC) and ^{1}H-NMR data. As shown in the below NMR spectral data no intermediate was detected after 0.6 eq. as well as 1.2 eq. of **14a** addition.

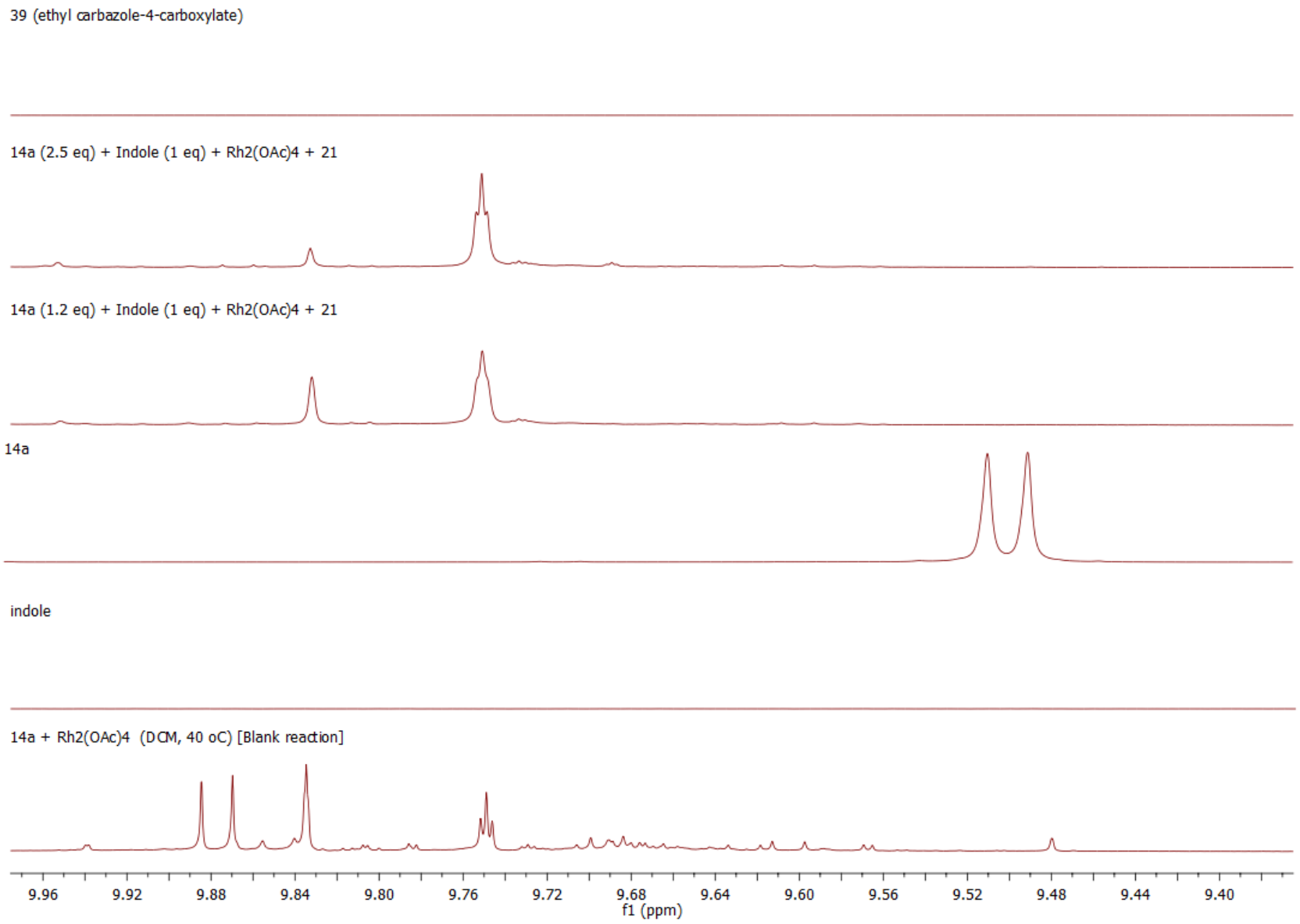

39 (ethyl carbazole-4-carboxylate)
14a (1.2 eq) + Indole (1 eq) + Rh2(OAc)4 + 21 : 2 h addition + 11 h stirring at RT
14a (1.2 eq) + Indole (1 eq) + Rh2(OAc)4 + 21 : 2 h addition +1 h stirring at RT
14a (0.6 eq) + Indole (1 eq) + Rh2(OAc)4 + 21 : 1 h addition at RT
14a
indole
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5

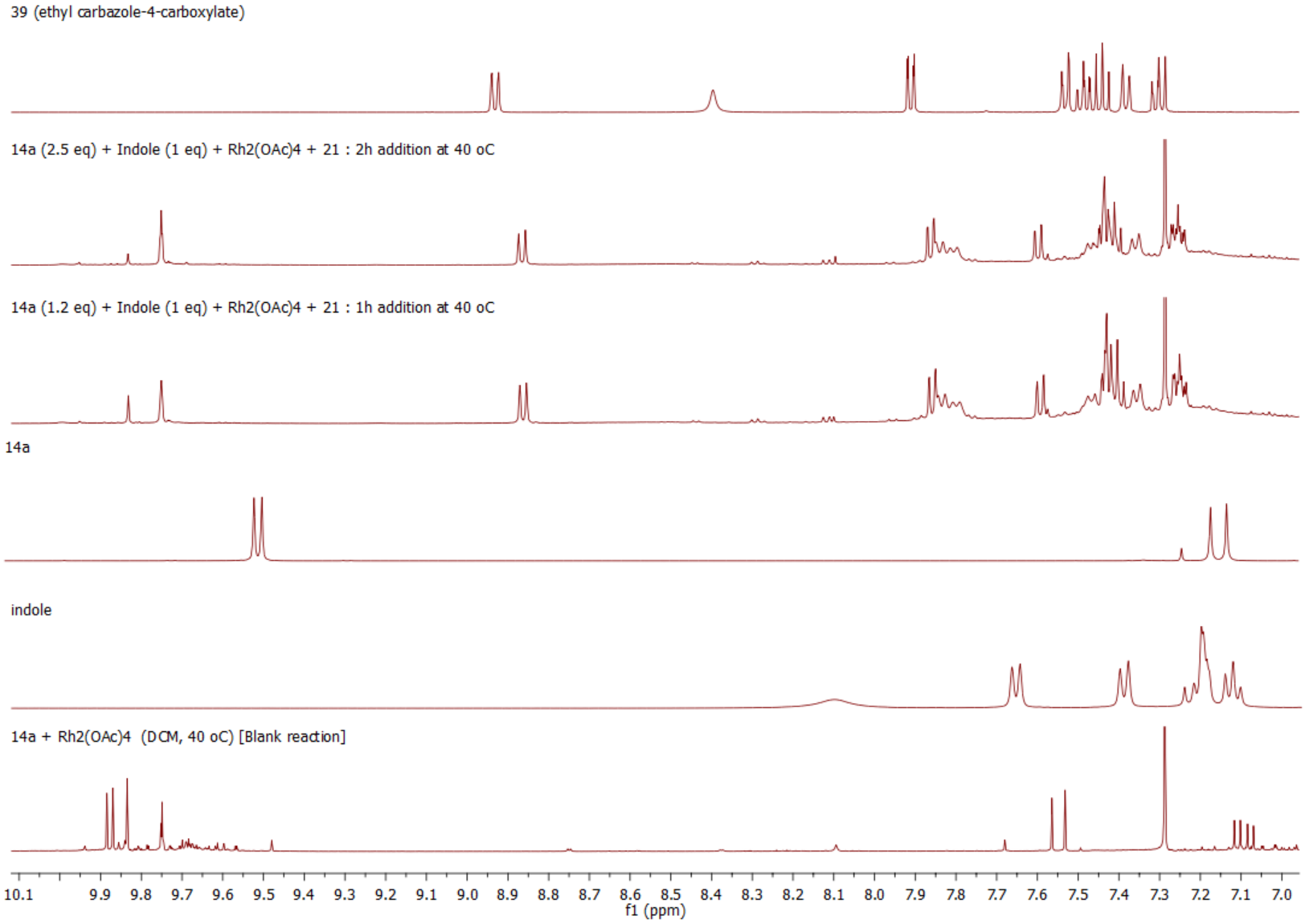

39 (ethyl carbazole-4-carboxylate)
14a (1.2 eq) + Indole (1 eq) + Rh2(OAc)4 + 21 : 2 h addition + 11 h stirring at RT
14a (1.2 eq) + Indole (1 eq) + Rh2(OAc)4 + 21 : 2 h addition +1 h stirring at RT
14a (0.6 eq) + Indole (1 eq) + Rh2(OAc)4 + 21 : 1 h addition at RT
14a
indole
10.2 9.8 9.6 9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0

(b) NMR study at 40 ^{o}C:

An oven dried 10 ml round-bottom flask containing a stir bar under inert atmosphere was charged with Indole (0.24 mmol), $Rh_2(OAc)_4$ (0.0048 mmol), (±)-**21** (0.012 mmol) and $CDCl_3$ (2 ml). To the gently stirring contents at 40 ^{o}C was added a solution of enaldiazo ester **14a** (0.3 mmol) in $CDCl_3$ (2 ml) with a flow rate of 1 ml/h using a syringe pump. The reaction was monitored by thin layer chromatography (TLC) and ^{1}H-NMR data. As shown in the below NMR spectral data no intermediate was detected after 0.6 eq. as well as 1.2 eq. of **14a** addition.


39 (ethyl carbazole-4-carboxylate)
14a (2.5 eq) + Indole (1 eq) + Rh2(OAc)4 + 21 : 2h addition at 40 oC
14a (1.2 eq) + Indole (1 eq) + Rh2(OAc)4 + 21 : 1h addition at 40 oC
14a
indole
14a + Rh2(OAc)4 (DCM, 40 oC) [Blank reaction]
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
f1 (ppm)


39 (ethyl carbazole-4-carboxylate)
14a (2.5 eq) + Indole (1 eq) + Rh2(OAc)4 + 21
14a (1.2 eq) + Indole (1 eq) + Rh2(OAc)4 + 21
14a
indole
14a + Rh2(OAc)4 (DCM, 40 oC) [Blank reaction]
9.96
9.92
9.88
9.84
9.80
9.76
9.72
9.68
9.64
9.60
9.56
9.52
9.48
9.44
9.40
f1 (ppm)


39 (ethyl carbazole-4-carboxylate)
14a (2.5 eq) + Indole (1 eq) + Rh2(OAc)4 + 21 : 2h addition at 40 oC
14a (1.2 eq) + Indole (1 eq) + Rh2(OAc)4 + 21 : 1h addition at 40 oC
14a
indole
14a + Rh2(OAc)4 (DCM, 40 oC) [Blank reaction]
10.1 9.9 9.8 9.7 9.6 9.5 9.4 9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)

9. References:

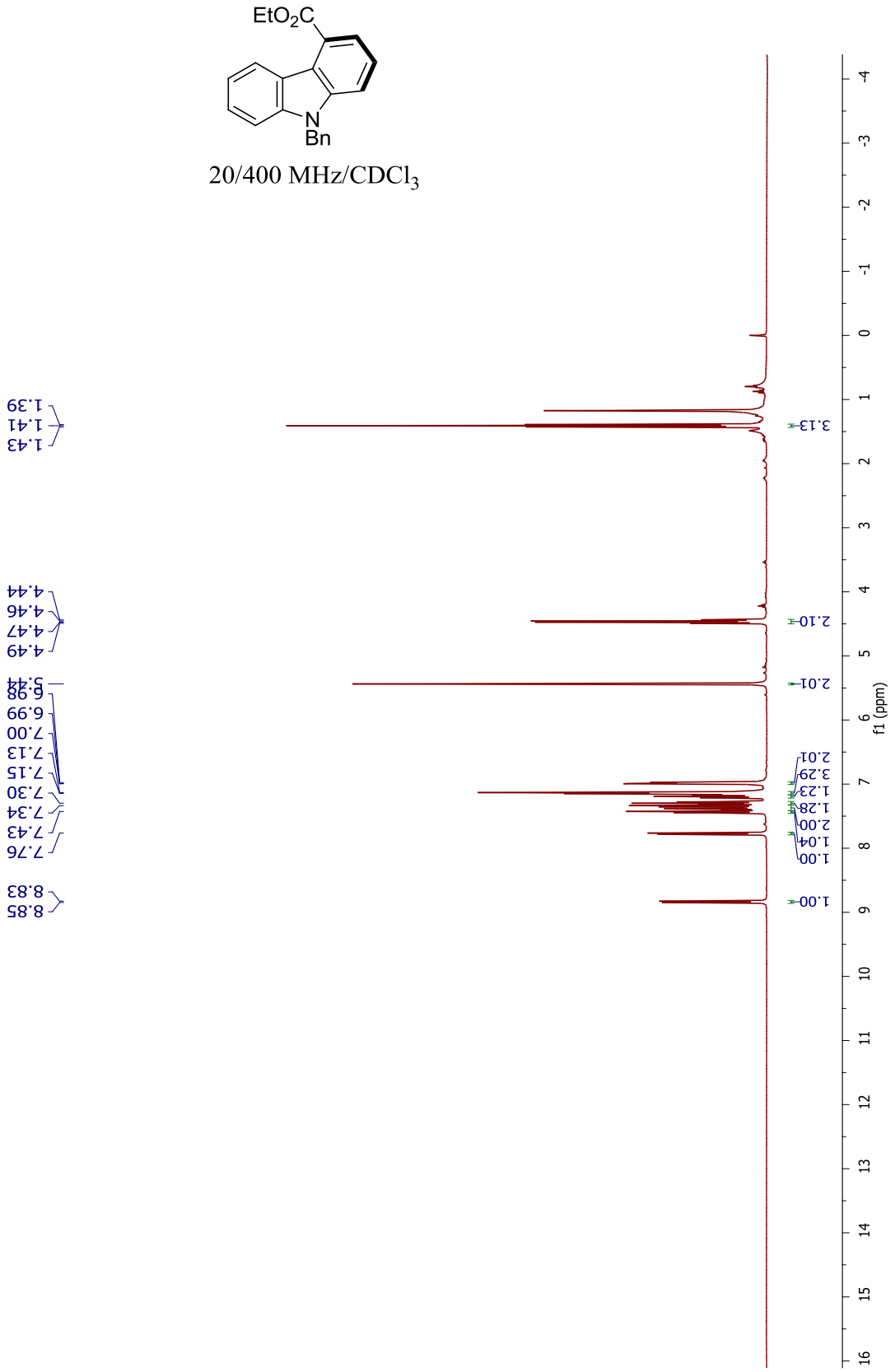
[1] a) S. G. Dawande, V. Kanchupalli, J. Kalepu, H. Chennamsetti, B. S. Lad, S. Katukojvala, *Angew. Chem. Int. Ed.* **2014**, *53*, 4076; b) S. G. Dawande, V. Kanchupalli, B. S. Lad, J. Rai, S. Katukojvala, *Org. Lett.* **2014**, *16*, 3700.

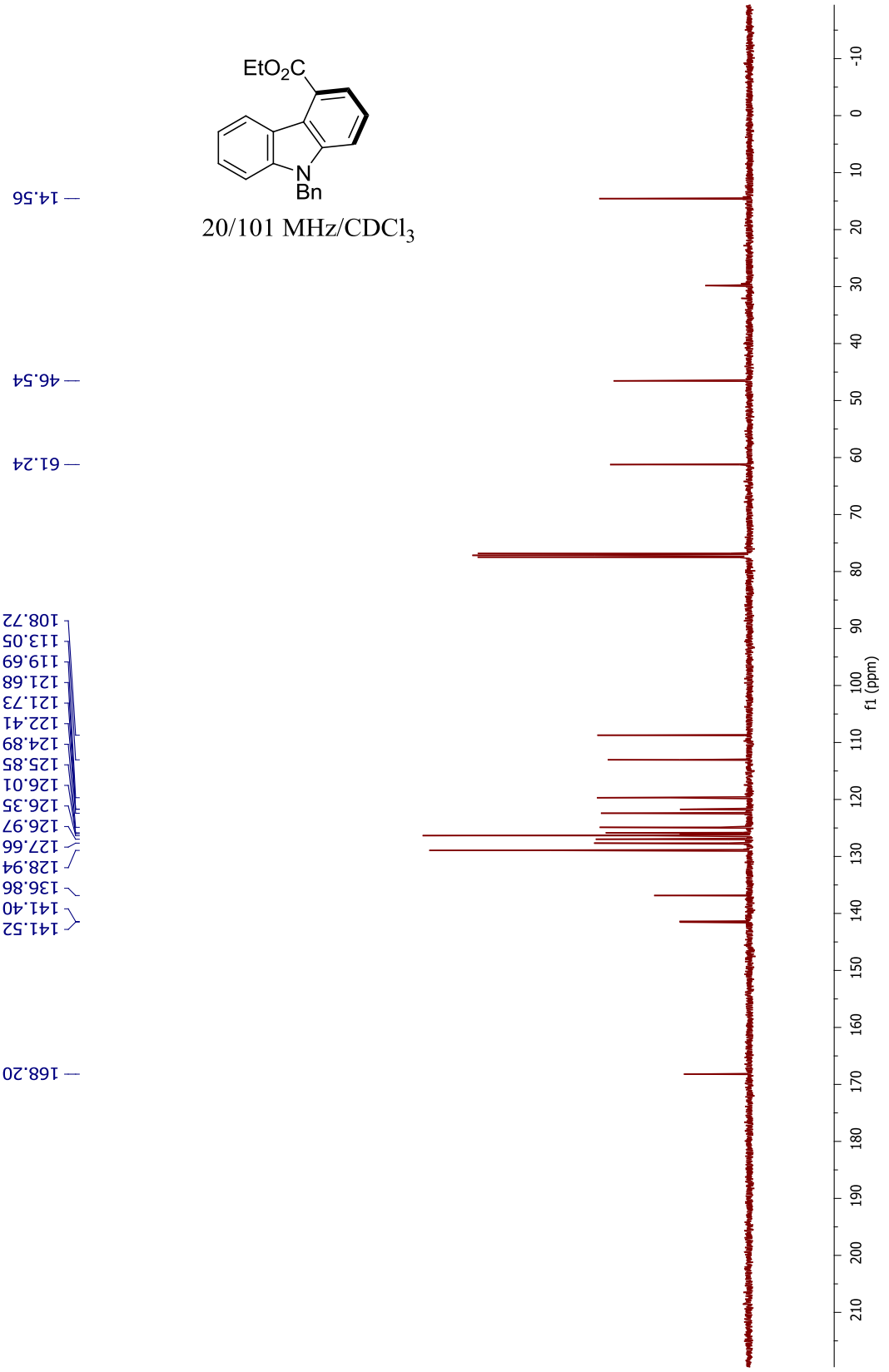
[2] a) M. Chen, Z. T. Huang, Q. Y. Zheng, *Chem. Commun*, **2012**, 48, 11686-11688; b) F. Ito, K. Shudo, K. Yamaguchi, *Tetrahedron* **2011**, 67, 1805-1811; c) D. Saha, R. Ghosh, A. Sarkar, *Tetrahedron* **2013**, 67, 1805-1811.

[3] L. Beigelman, B. Buckman, G. Wang, J. Matulic-Adamic, A. D. Stoycheva, S. W. Andrews, S. M. Misialek, P. T. R. Rajagopalan, A. M. Fryer, I. Gunawardana, et al, PCT Int. Appl. (2008), WO 2008100867 A2 20080821.

[4] B. A. Anderson, N. J. Bach, J. A. Bastian, N. K. Harn, R. W. Harper, G. A. Hite, M. D. Kinnick, H.-S. Lin, R. J. Loncharich, J. M. McGill, et al. Eur. Pat. Appl. (1999). EP 952149 A2 19991027.

10. NMR Spectra:

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Bn
20/101 MHz/CDCl3
14.56
46.54
61.24
108.72
113.05
119.69
121.68
121.73
122.41
124.89
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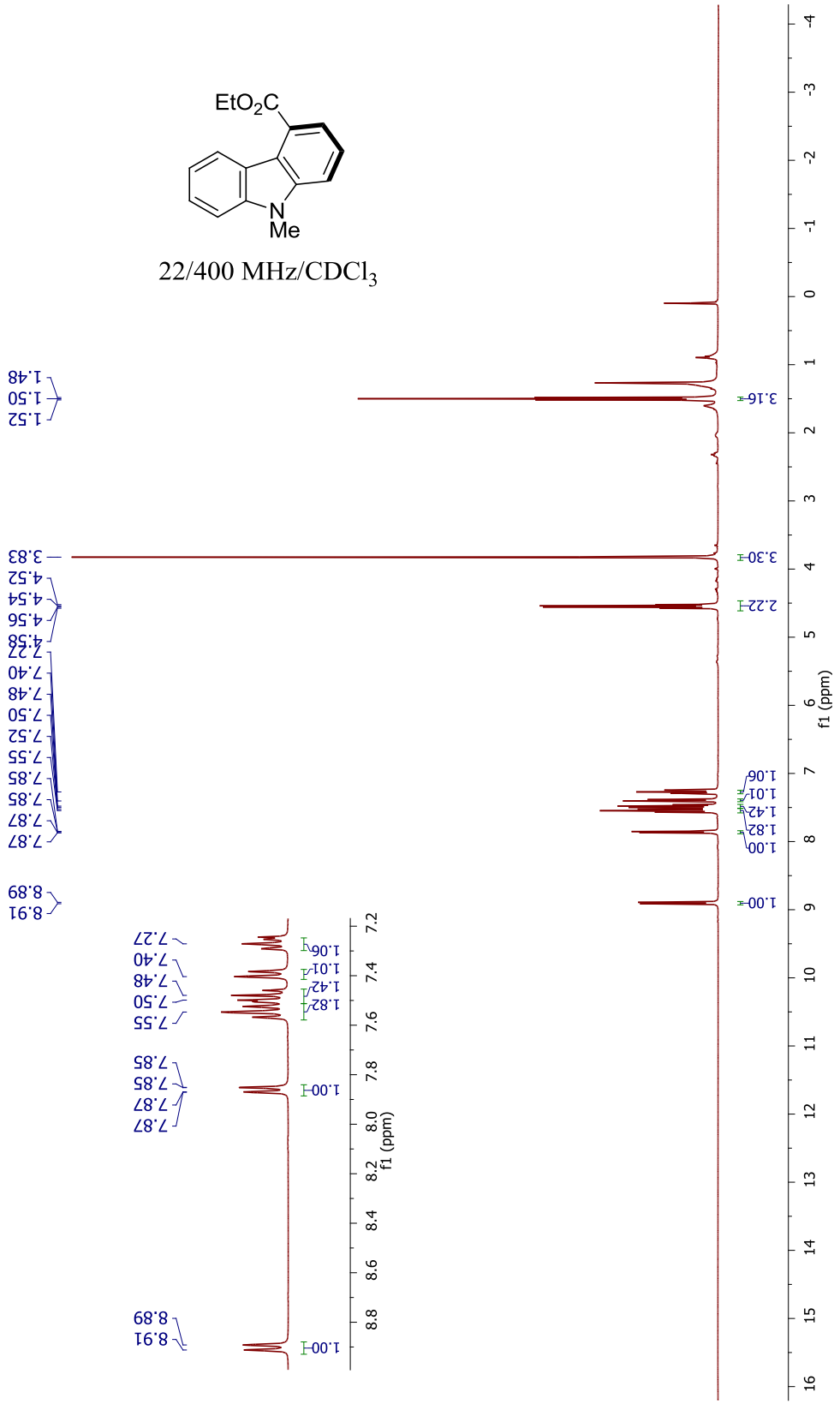
126.01
126.35
126.97
127.66
128.94
136.86
141.40
141.52
168.20
f1 (ppm)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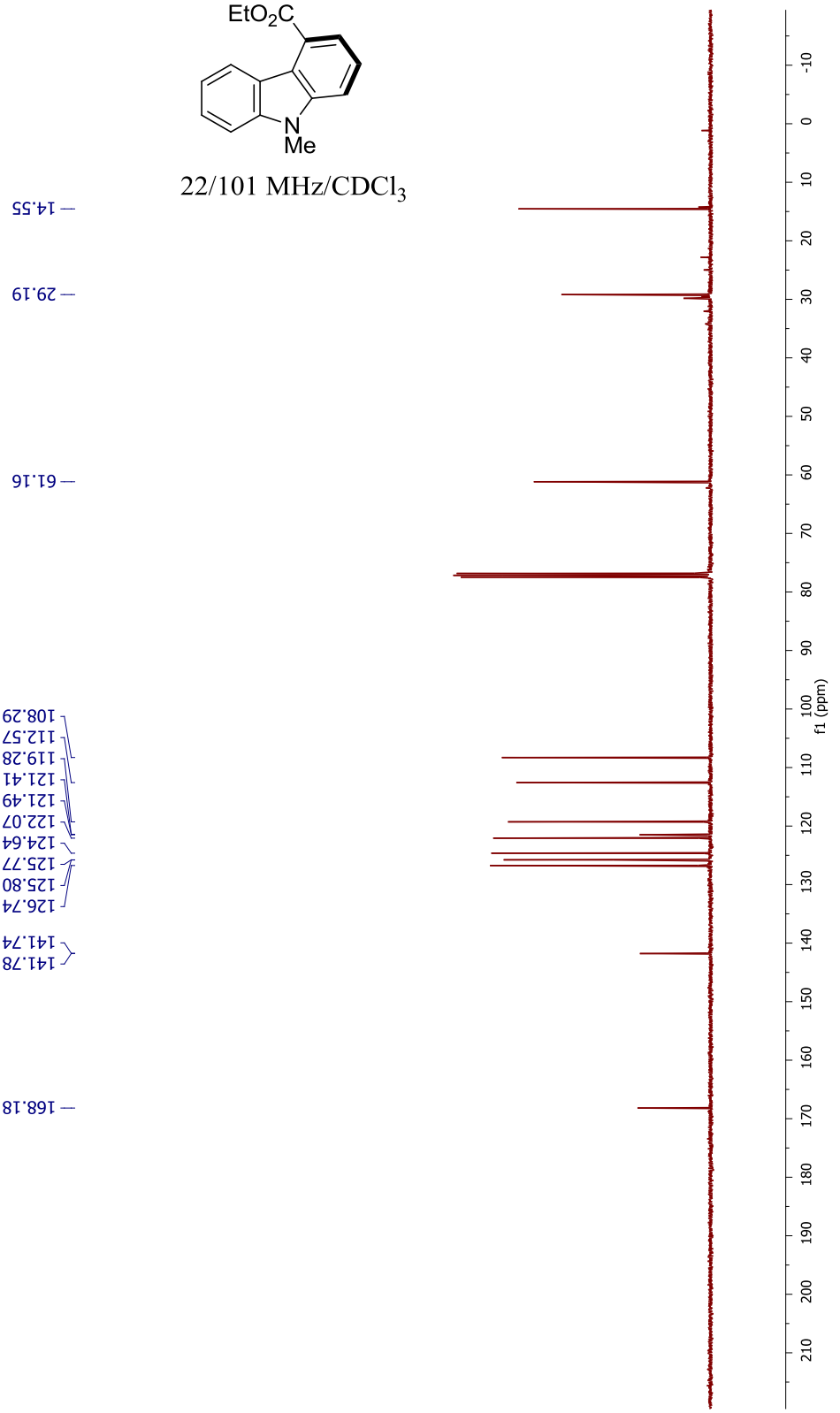
N
Me
22/400 MHz/CDCl3
f1 (ppm)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N
Me
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14.55
29.19
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125.80
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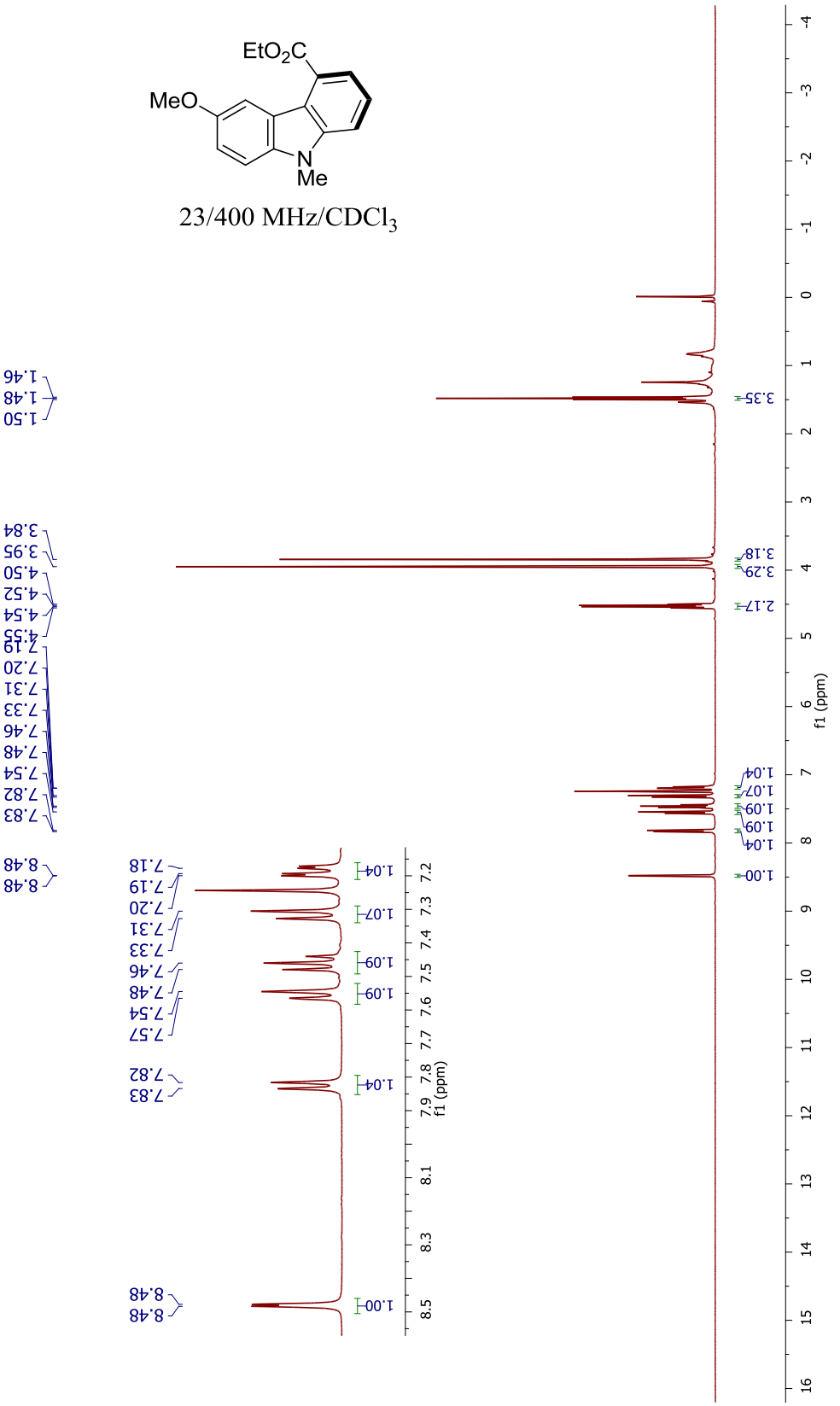
141.74
141.78
168.18
f1 (ppm)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Me
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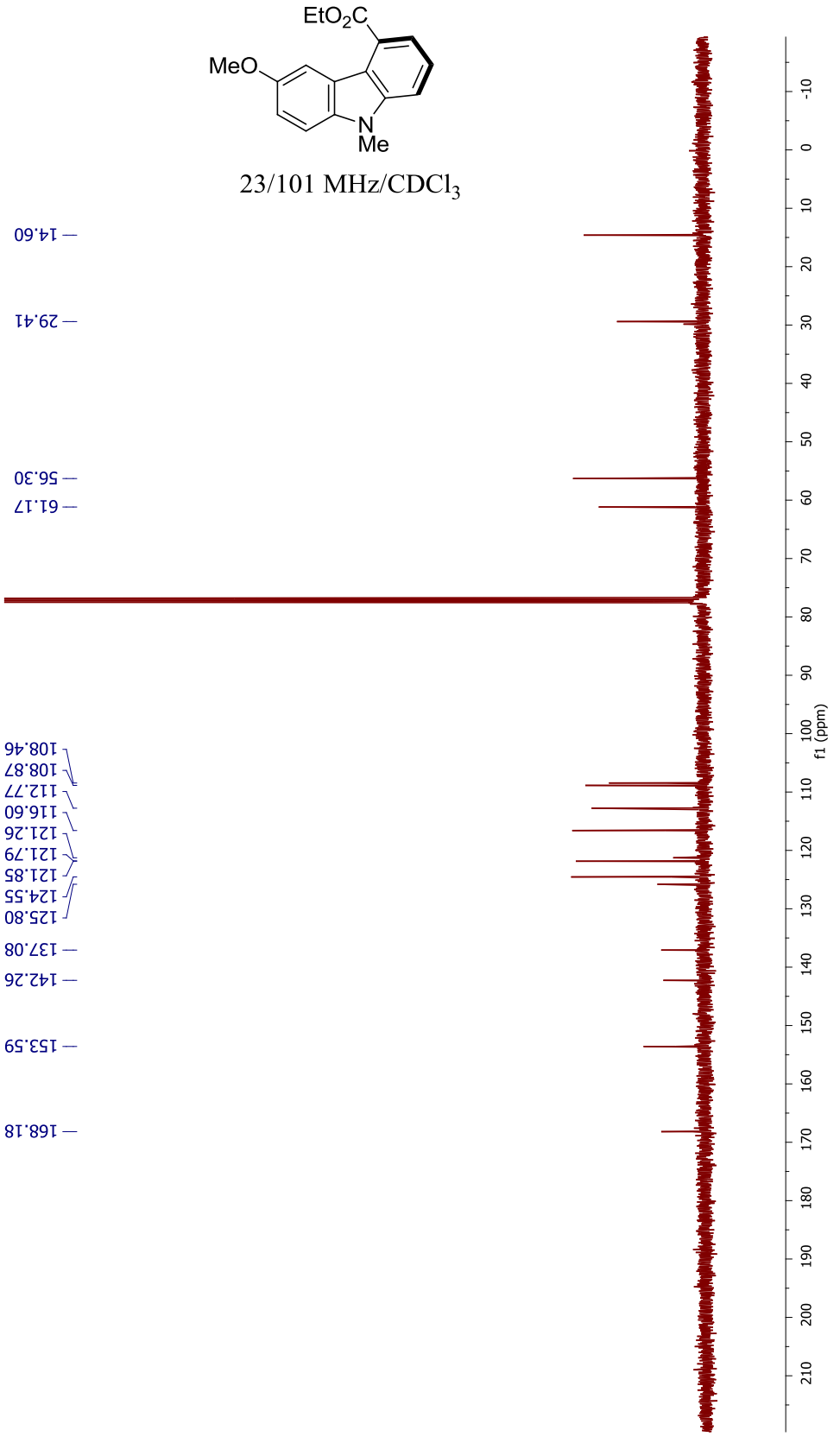
f1 (ppm)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MeO
N
Me
23/101 MHz/CDCl3
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29.41
56.30
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108.46
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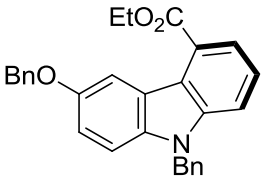
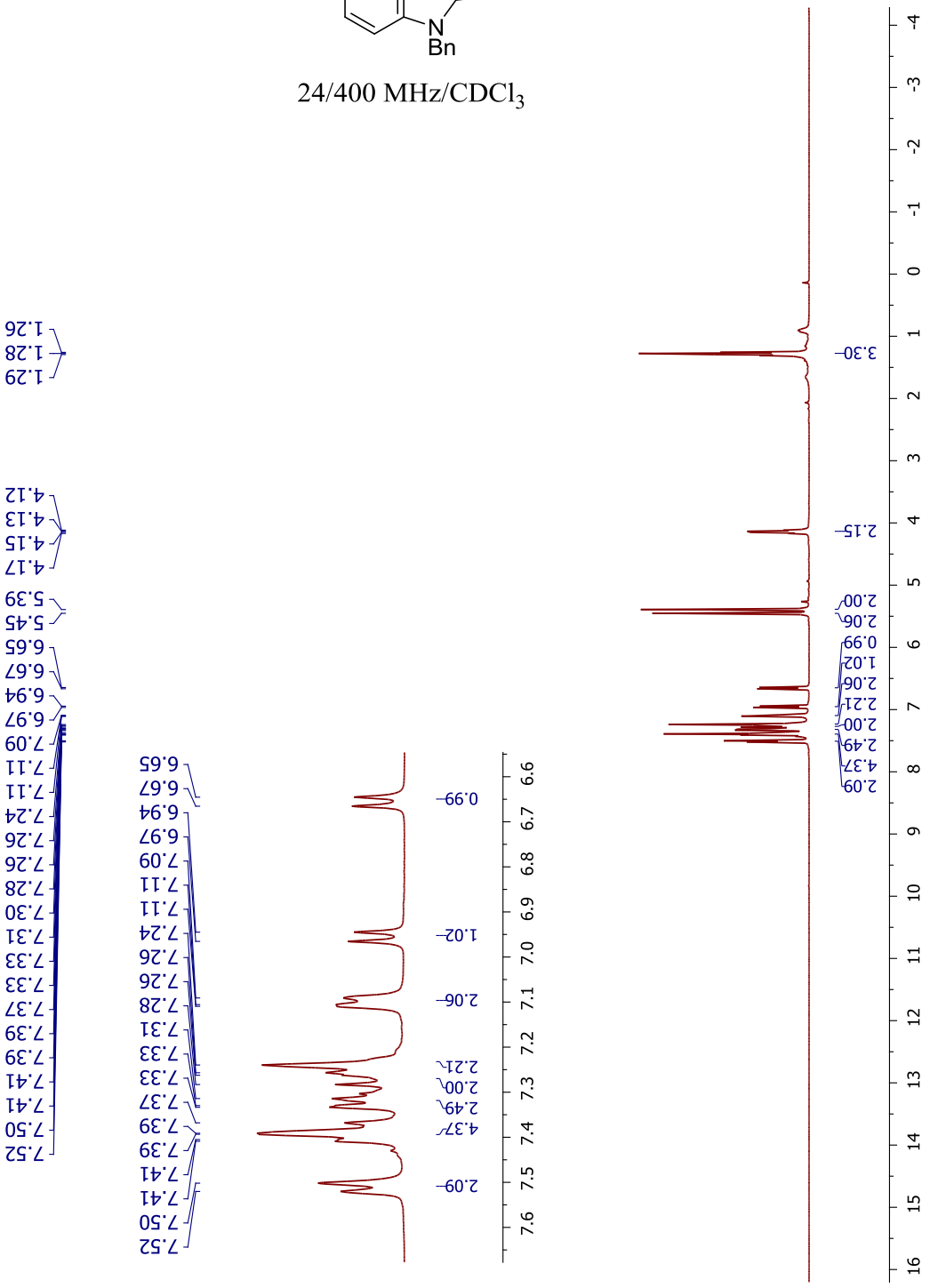
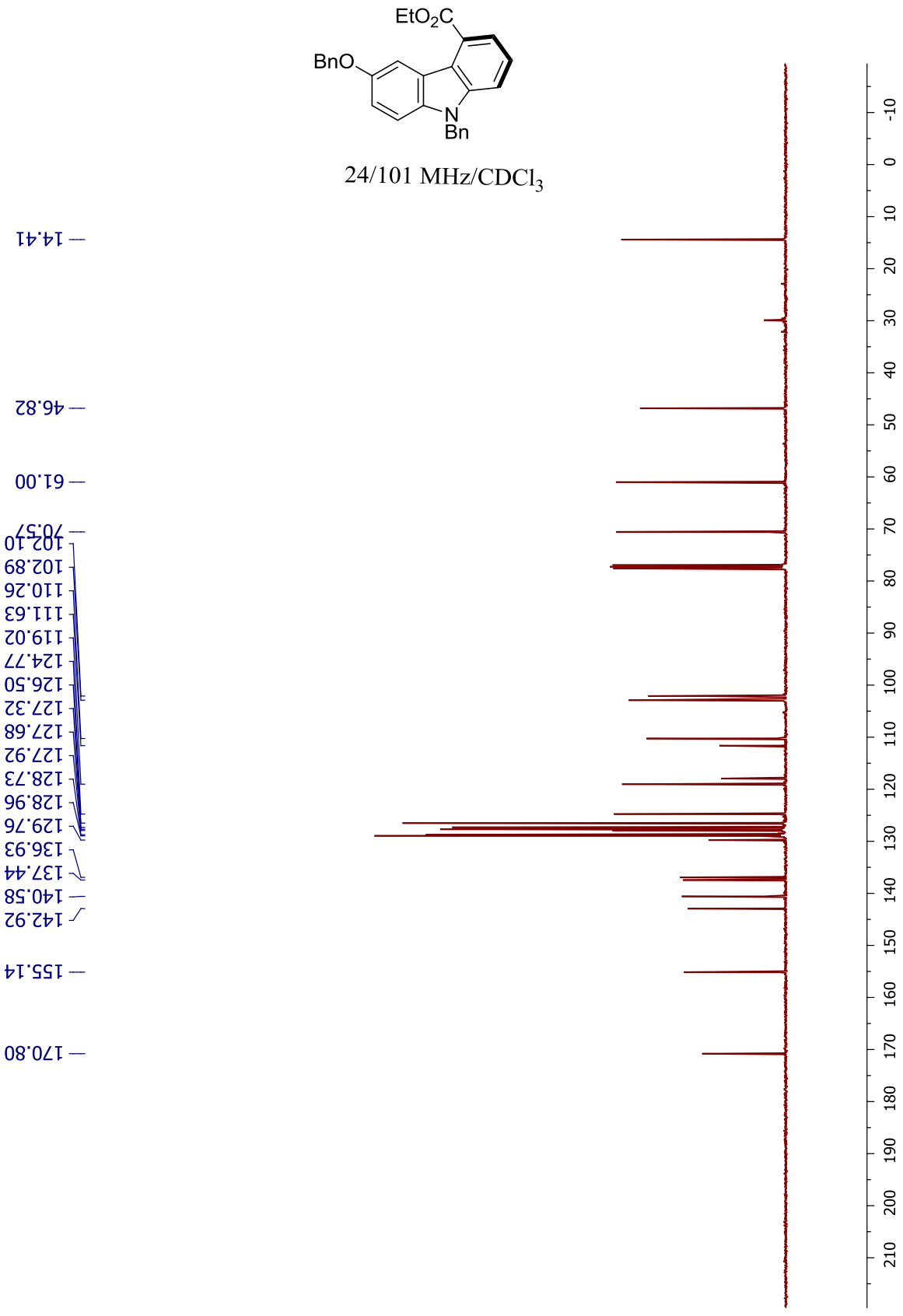
124.55
125.80
137.08
142.26
153.59
168.18
f1 (ppm)



24/400 MHz/$CDCl_3$

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BnO
N
Bn
24/101 MHz/CDCl3
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46.82
61.00
70.57
102.10
102.89
110.26
111.63
119.02
124.77
126.50
127.32
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137.44
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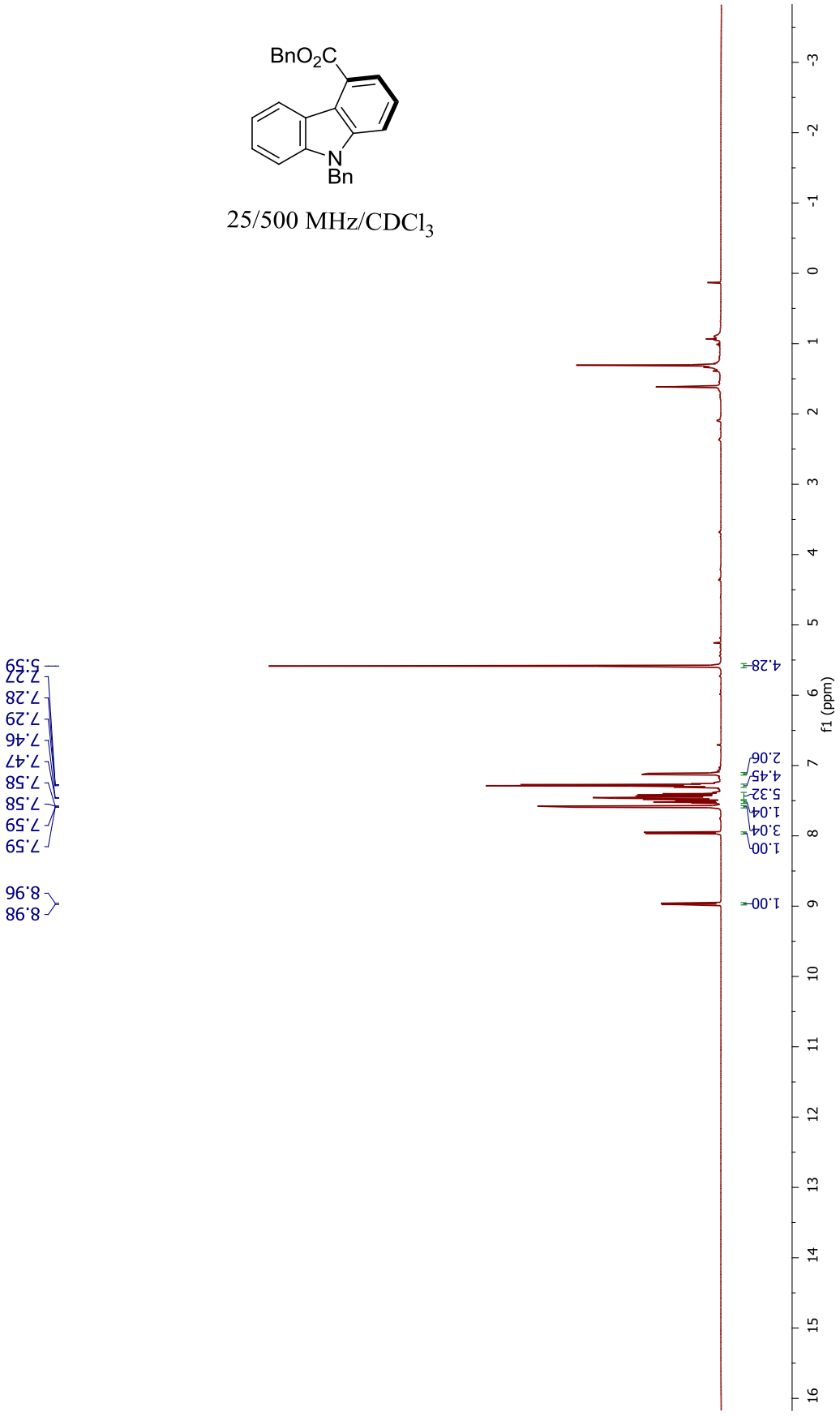
142.92
155.14
170.80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Bn
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7.59
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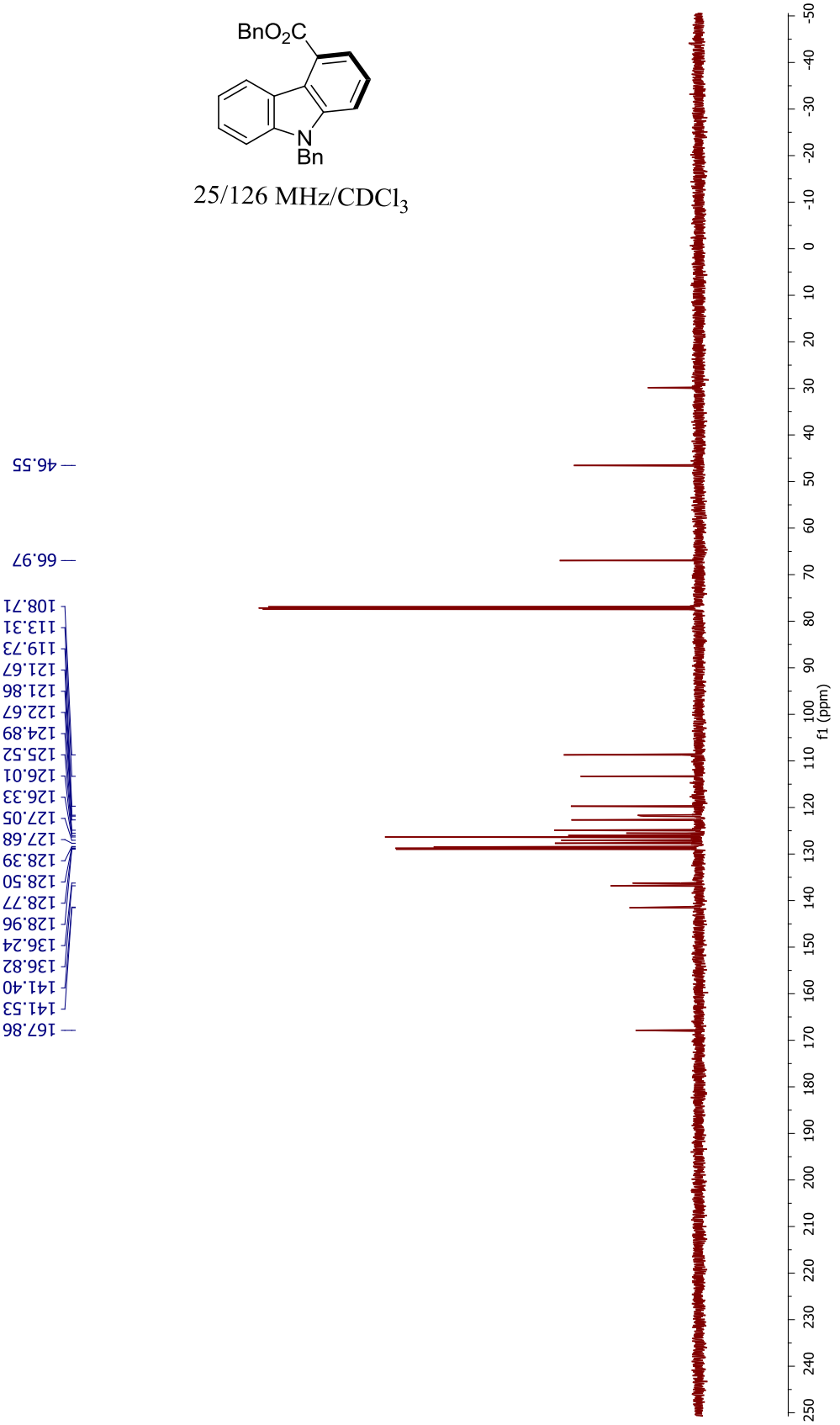
1.00
1.00
f1 (ppm)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Bn
25/126 MHz/CDCl3
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141.53
141.40
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136.24
128.96
128.77
128.50
128.39
127.68
127.05
126.33
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121.86
121.67
119.73
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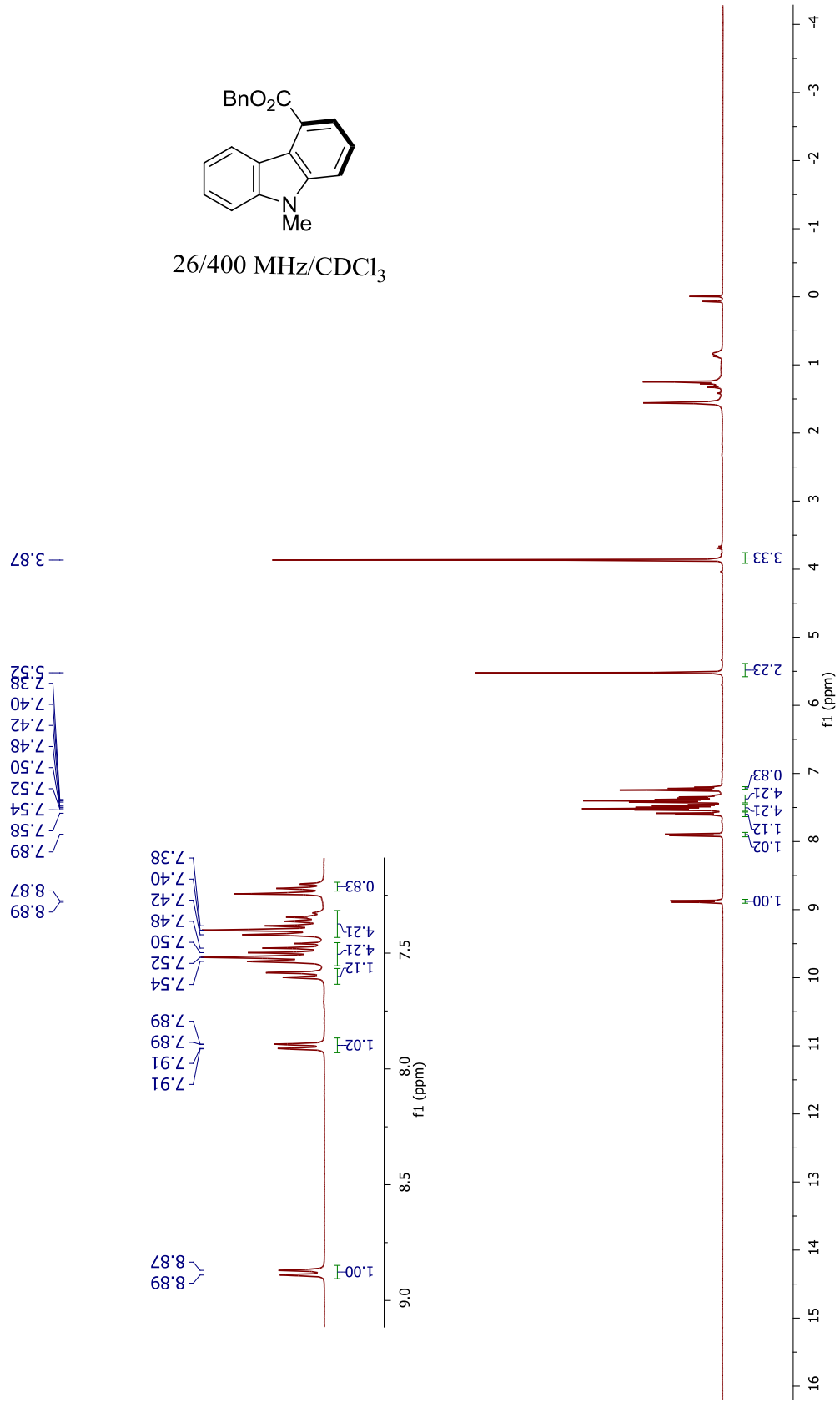
108.71
66.97
46.55
f1 (ppm)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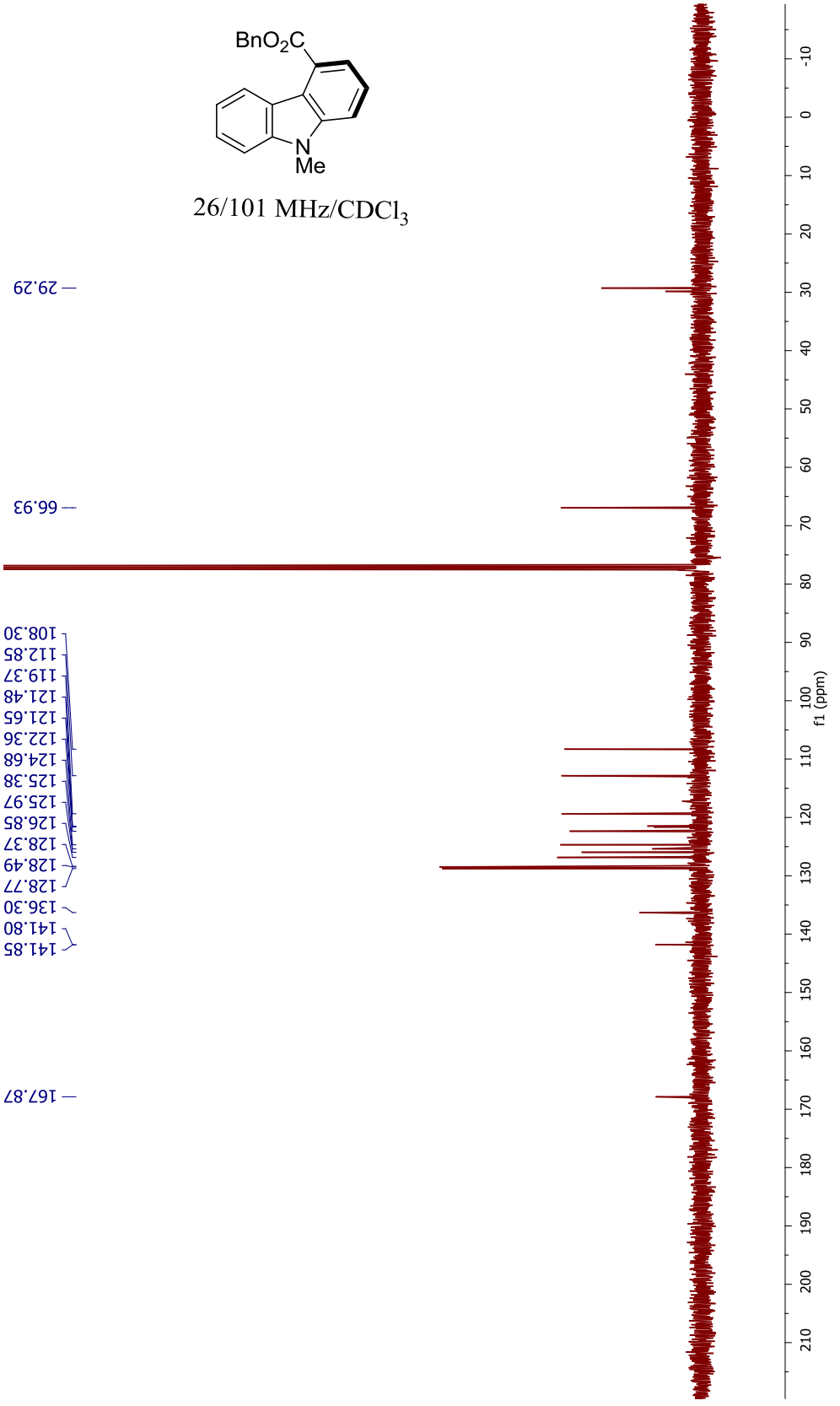
Me
26/400 MHz/CDCl3
f1 (ppm)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Me
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126.85
128.37
128.49
128.77
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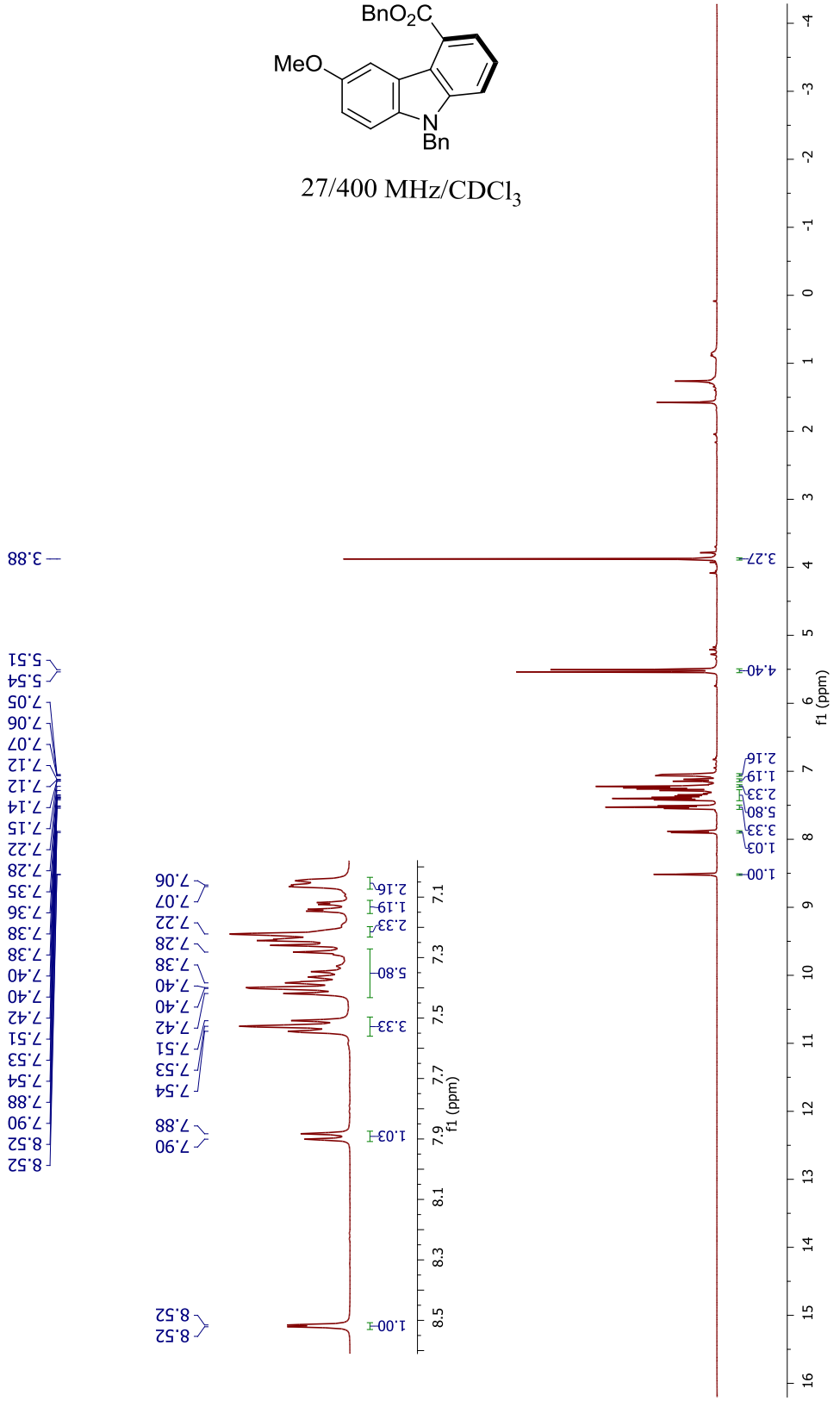
141.80
141.85
167.87
f1 (ppm)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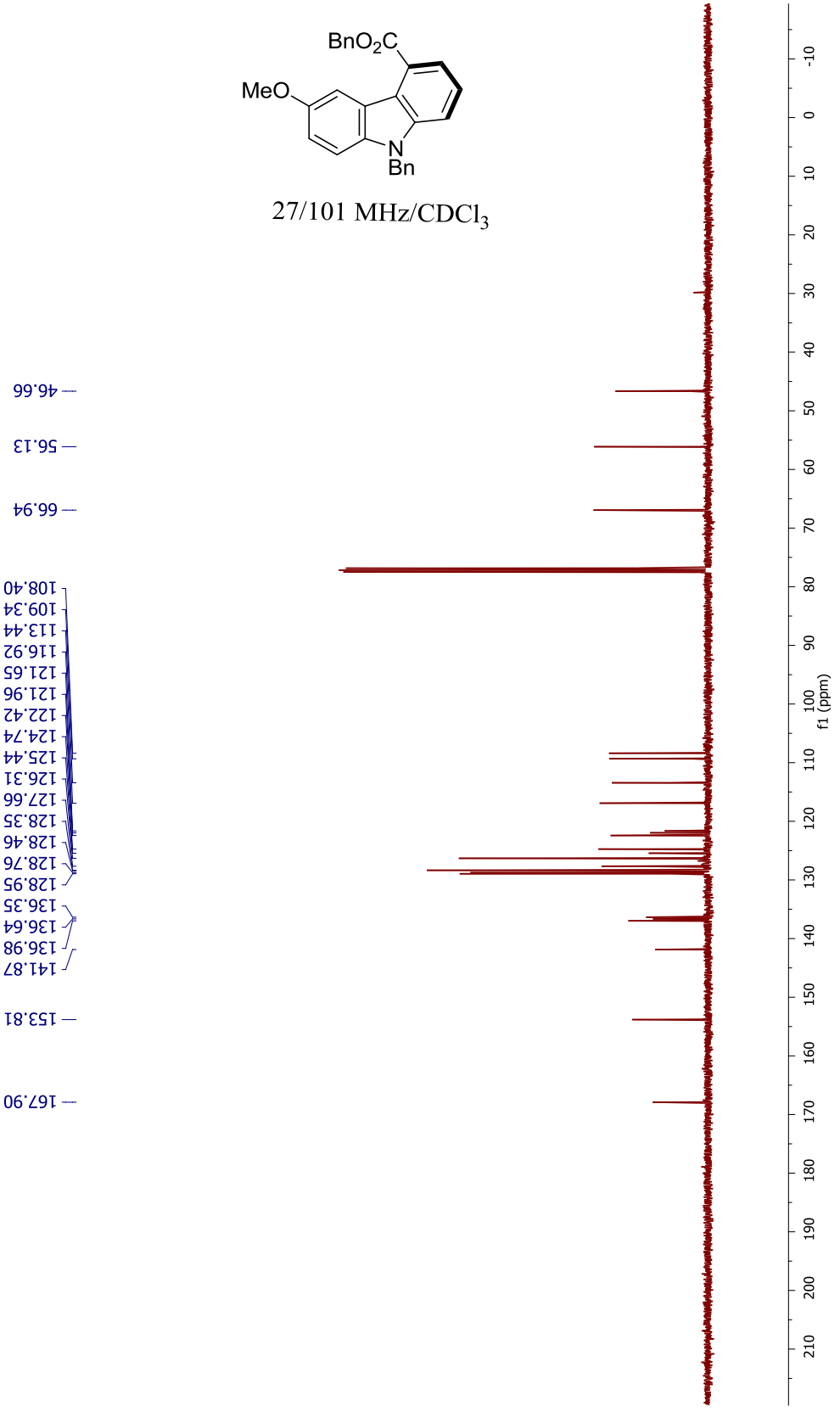
MeO
N
Bn
27/400 MHz/CDCl3
f1 (ppm)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121.65
121.96
122.42
124.74
125.44
126.31
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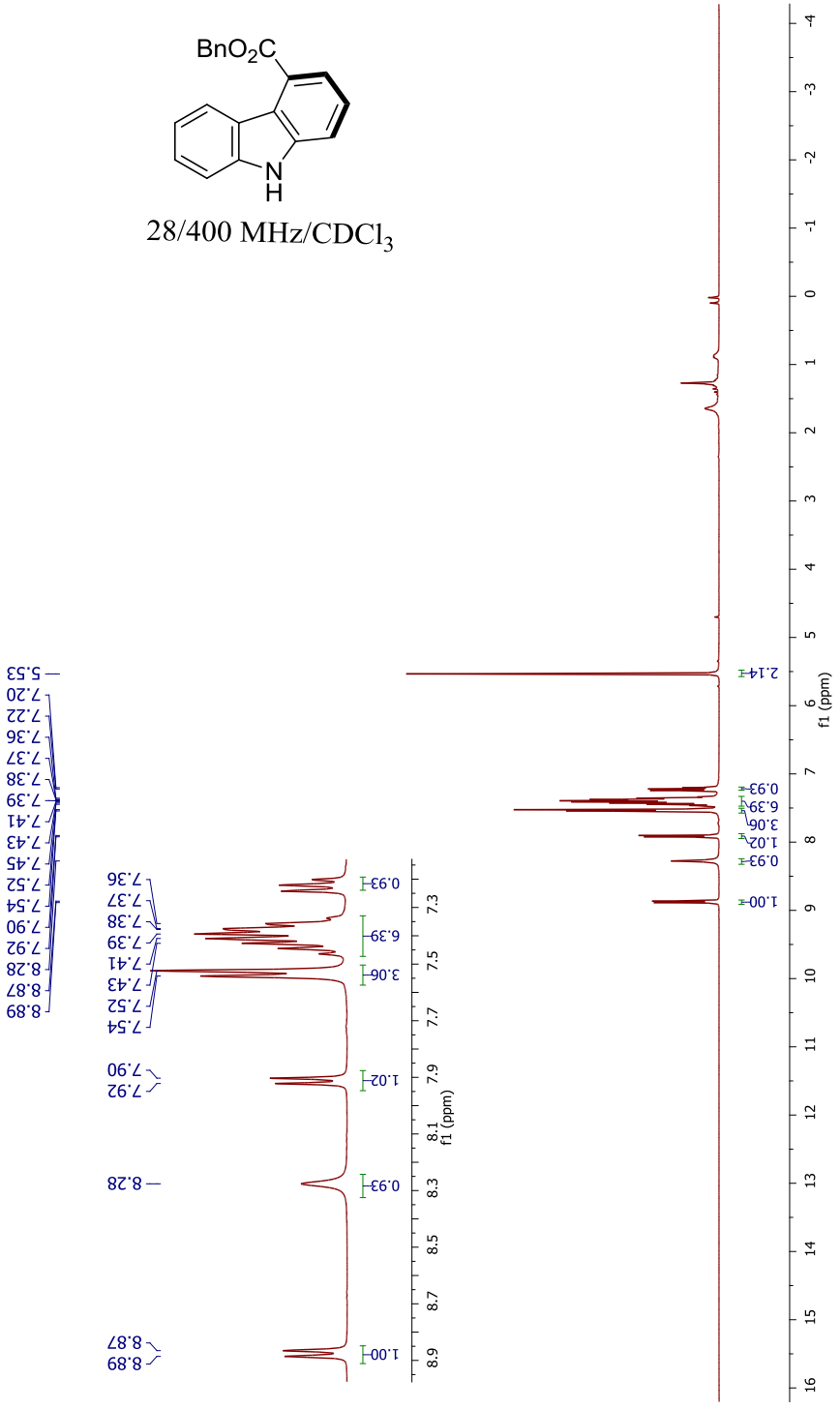
f1 (ppm)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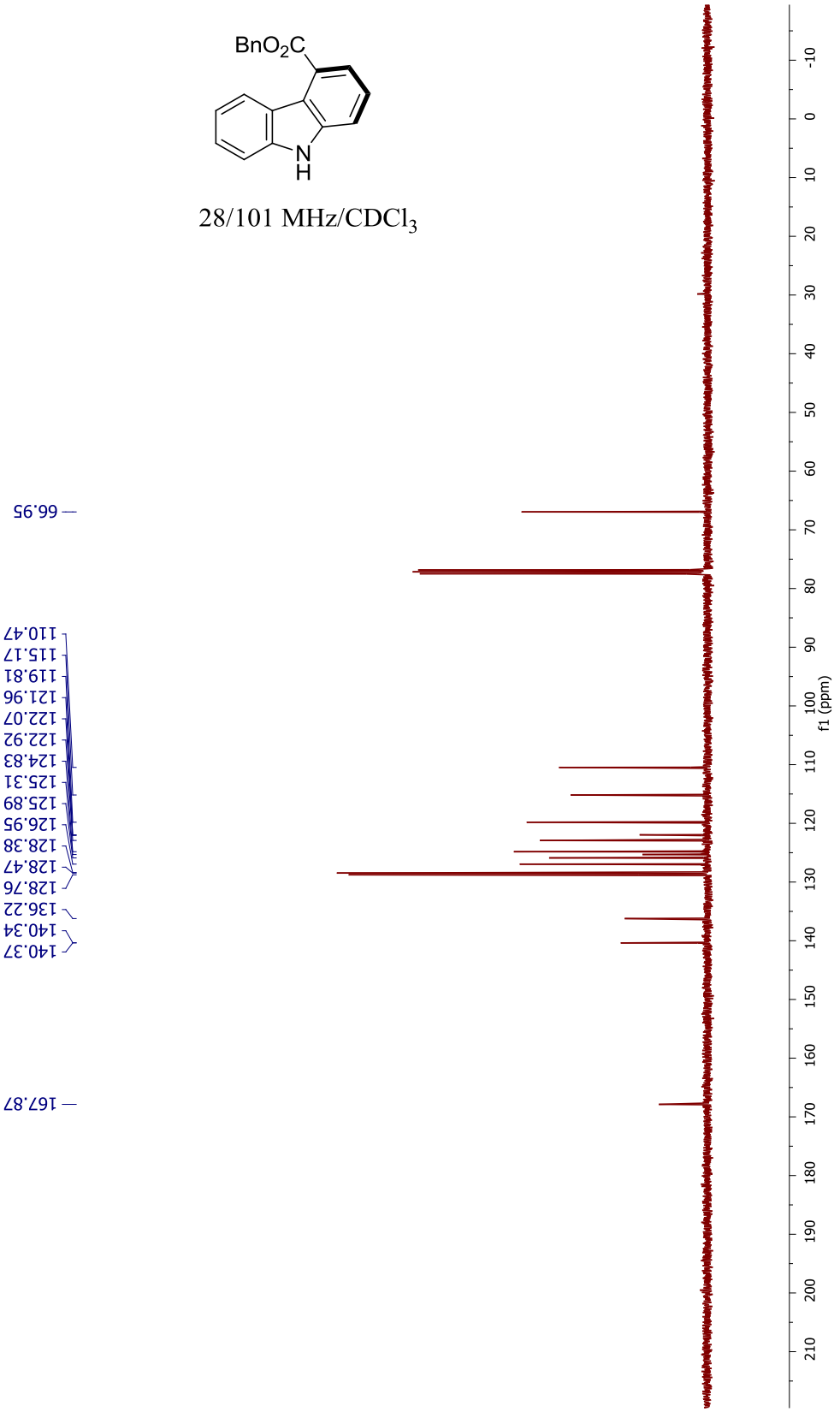
H
28/400 MHz/CDCl3
f1 (ppm)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N
H
28/101 MHz/CDCl3
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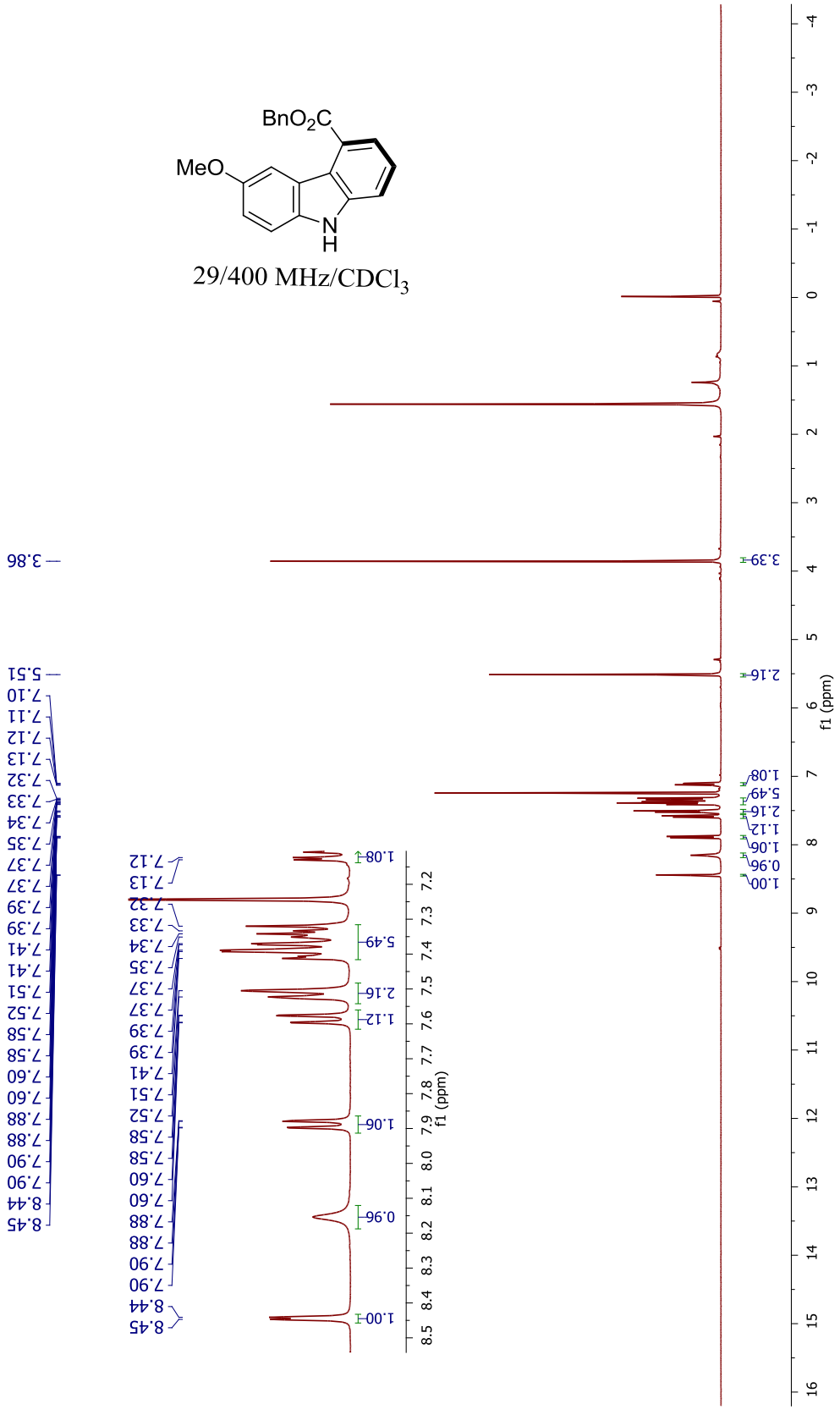
128.38
128.47
128.76
136.22
140.34
140.37
167.87
f1 (ppm)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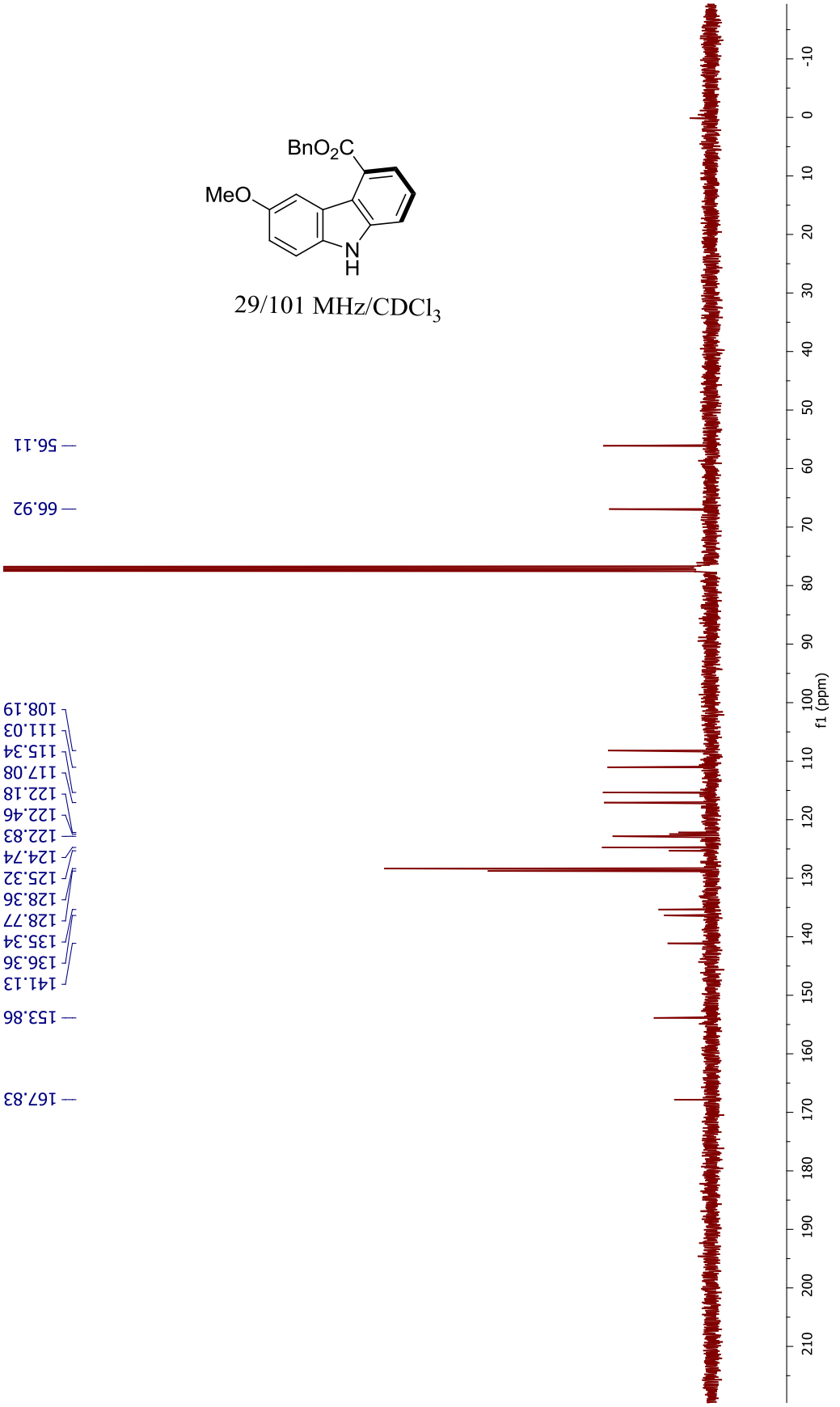
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MeO
N
H
29/101 MHz/CDCl3
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108.19
111.03
115.34
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125.32
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136.36
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153.86
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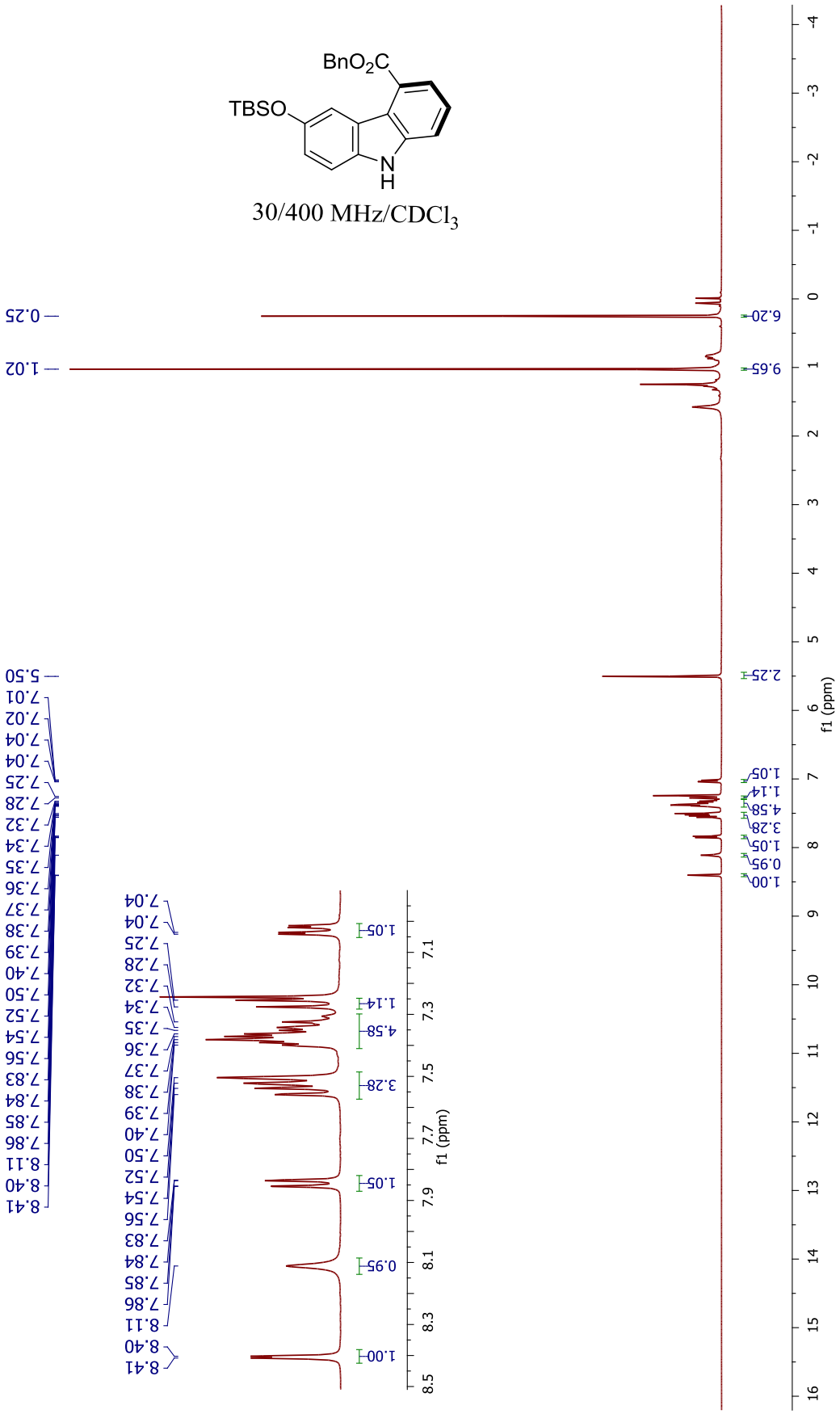
f1 (ppm)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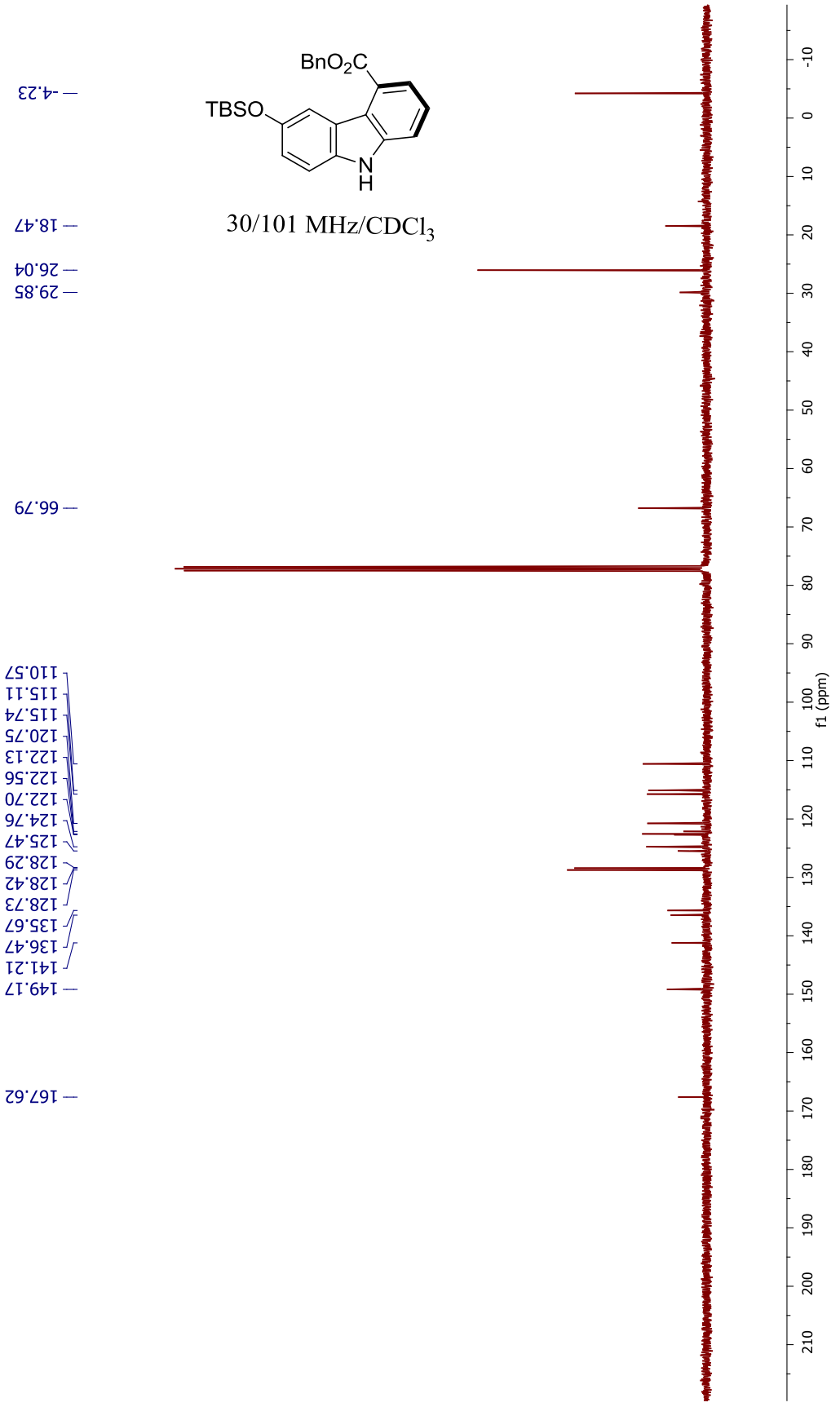
H
30/400 MHz/CDCl3
f1 (ppm)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TBSO
N
H
30/101 MHz/CDCl3
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18.47
26.04
29.85
66.79
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115.11
115.74
120.75
122.13
122.56
122.70
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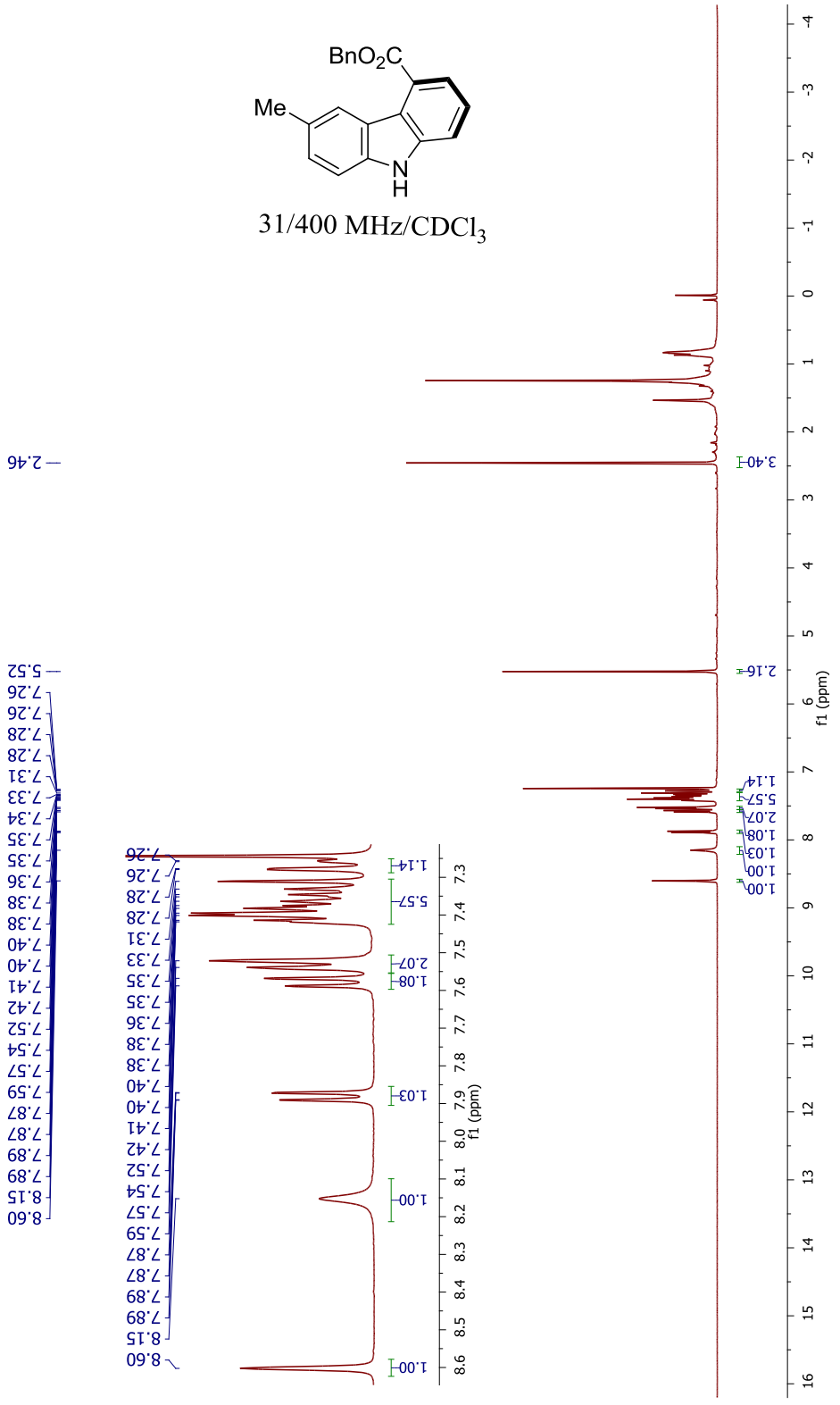
128.29
128.42
128.73
135.67
136.47
141.21
149.17
167.62
f1 (ppm)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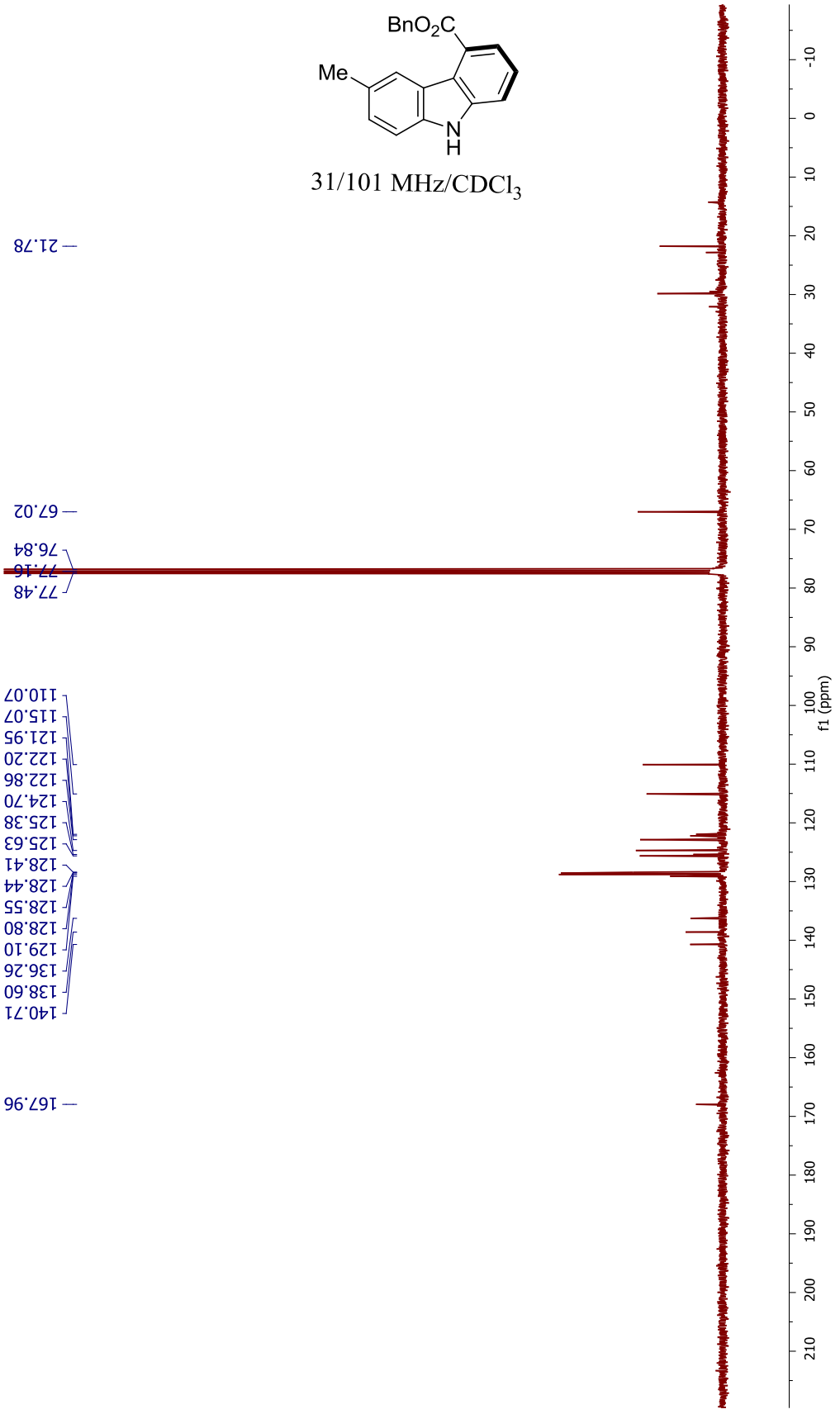
Me
N
H
31/400 MHz/CDCl3
f1 (ppm)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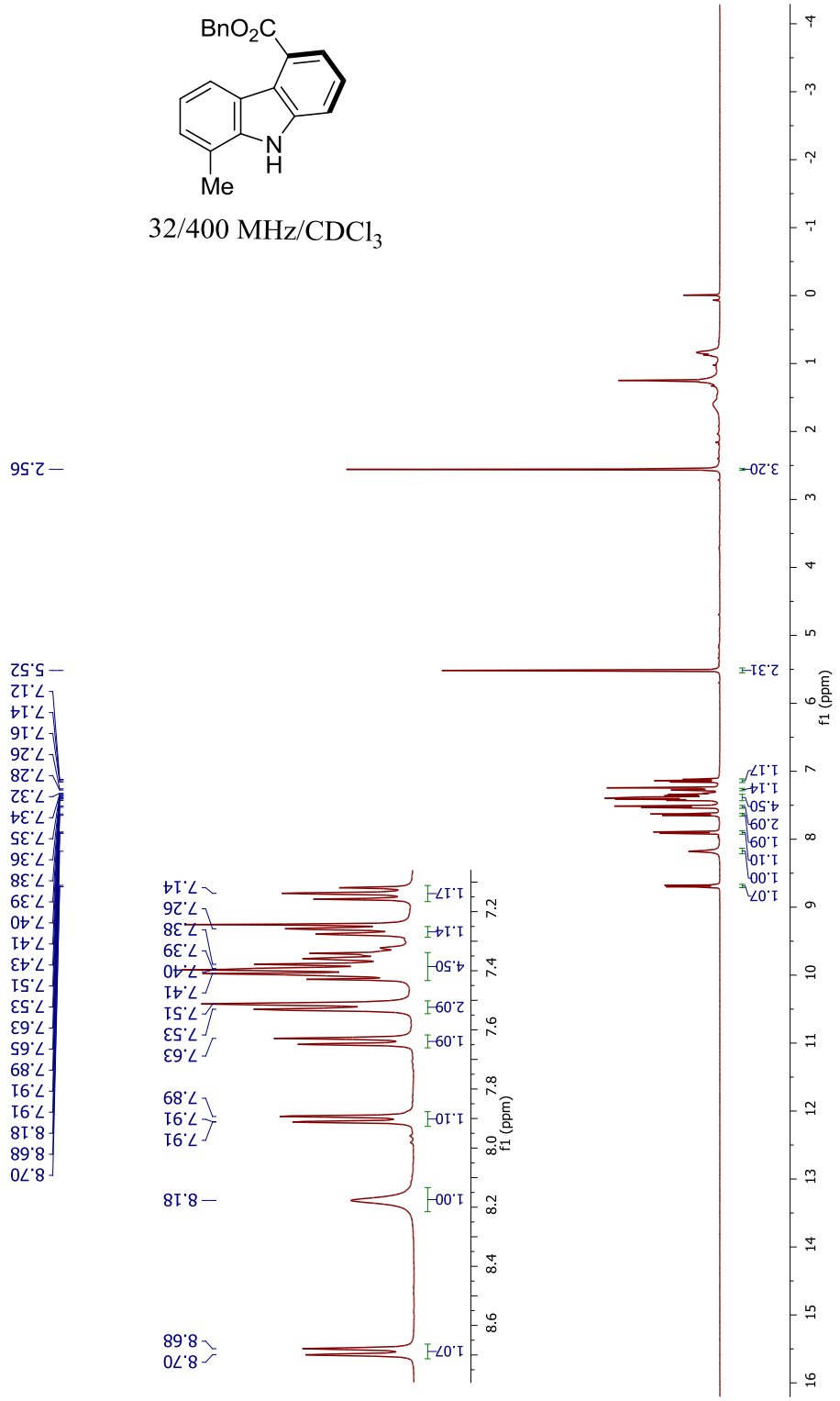
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H
Me
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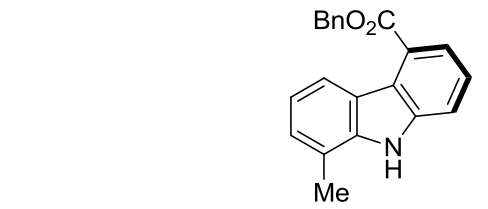
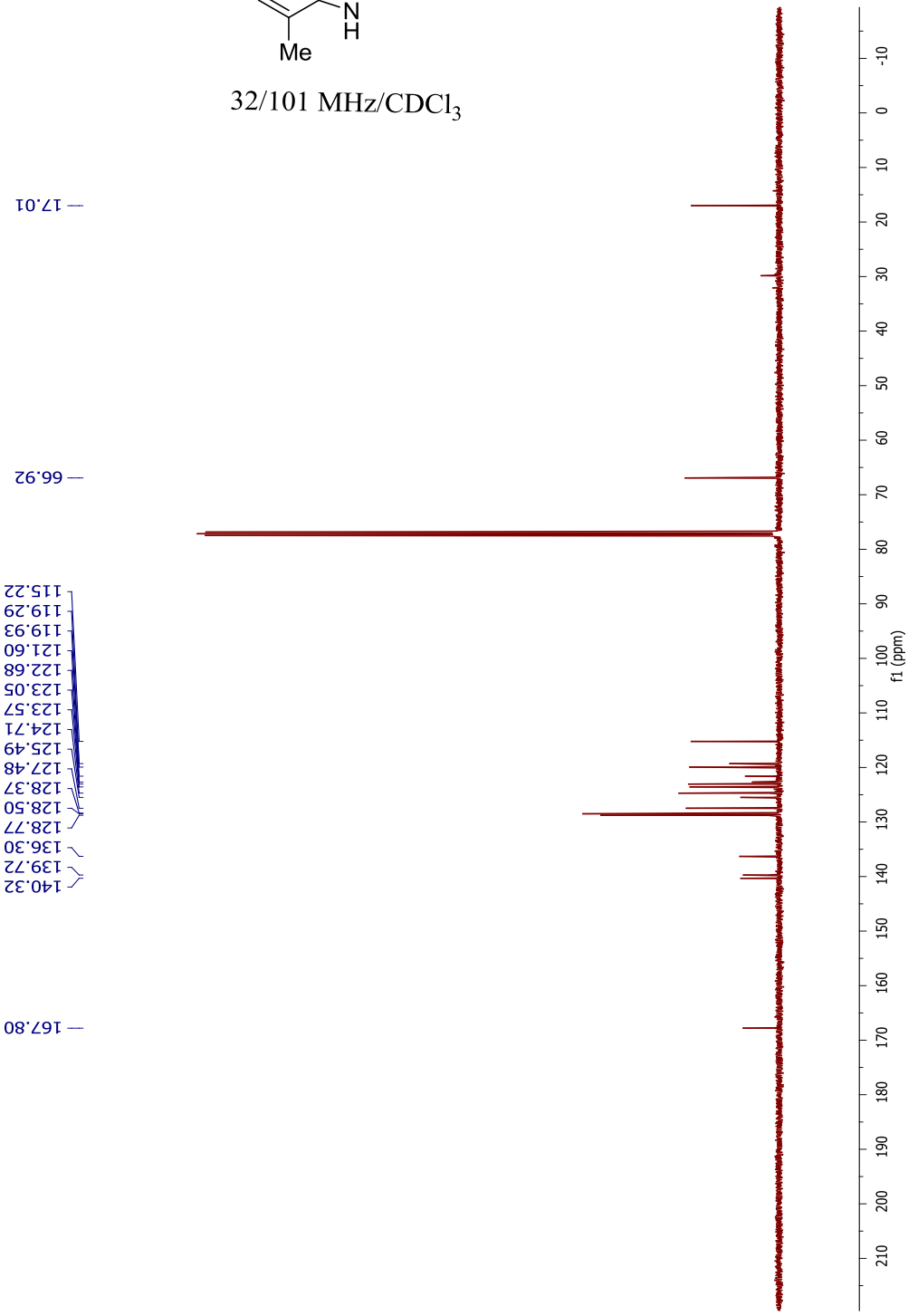
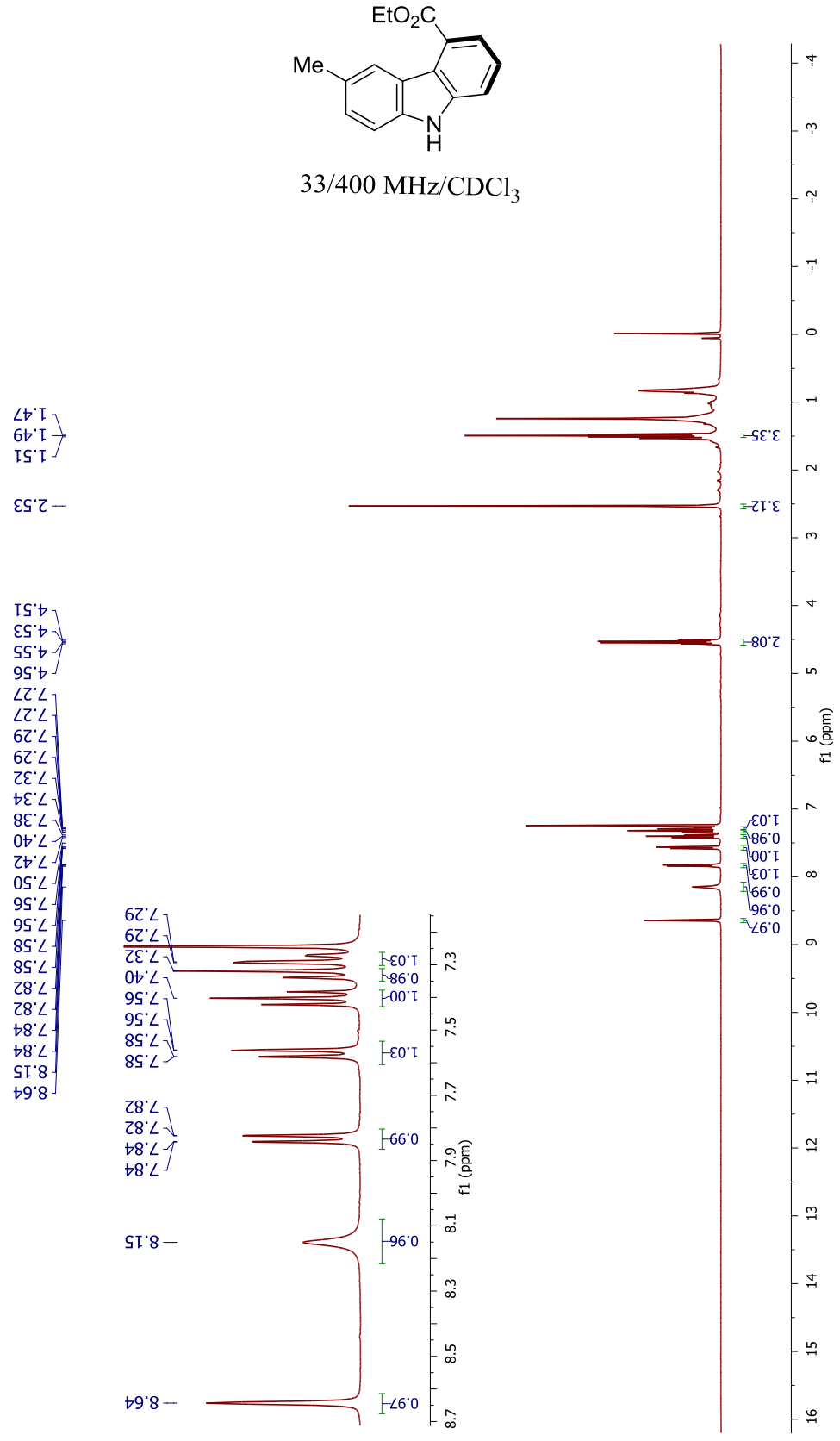


32/101 MHz/$CDCl_3$

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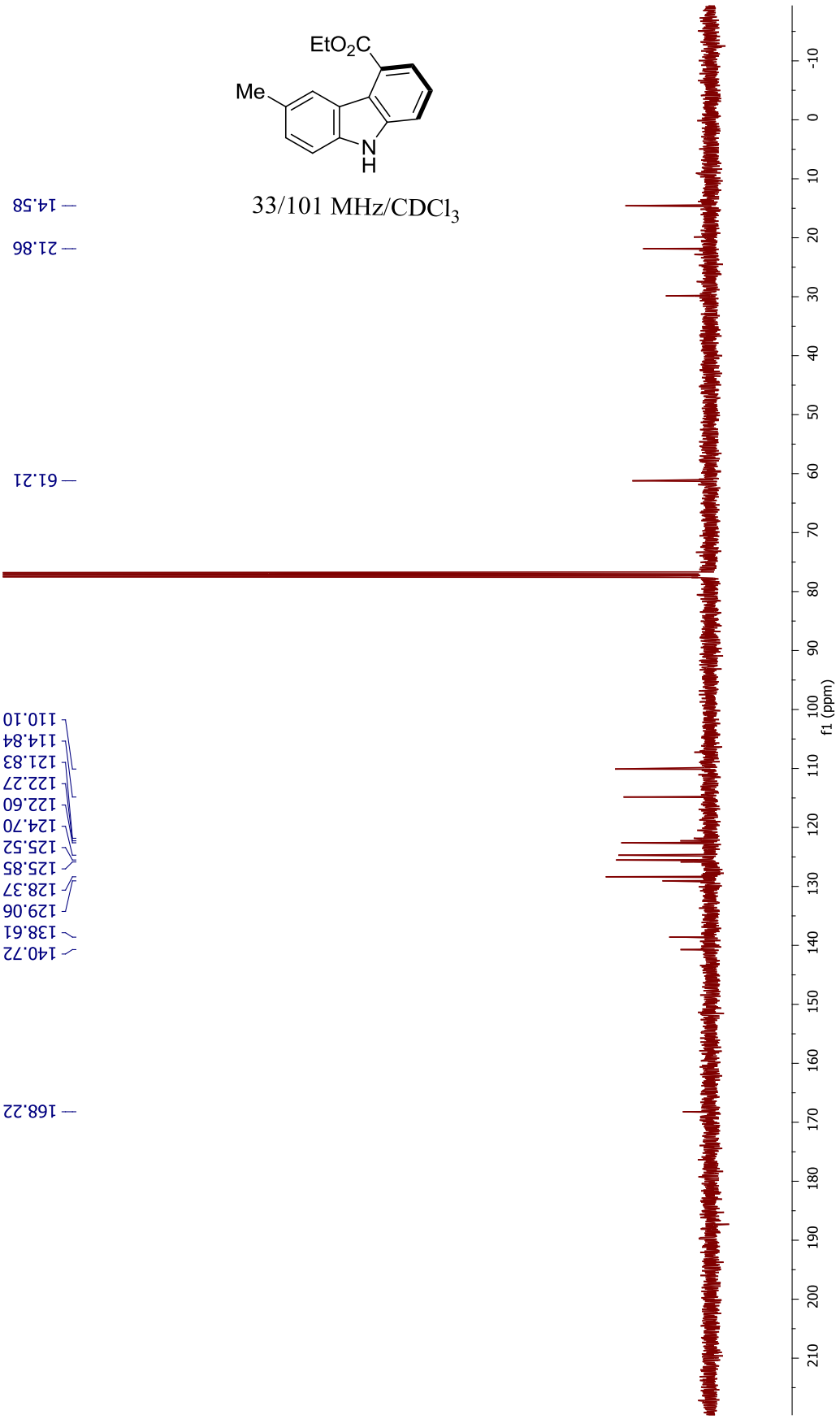
N
H
33/400 MHz/CDCl3
f1 (ppm)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H
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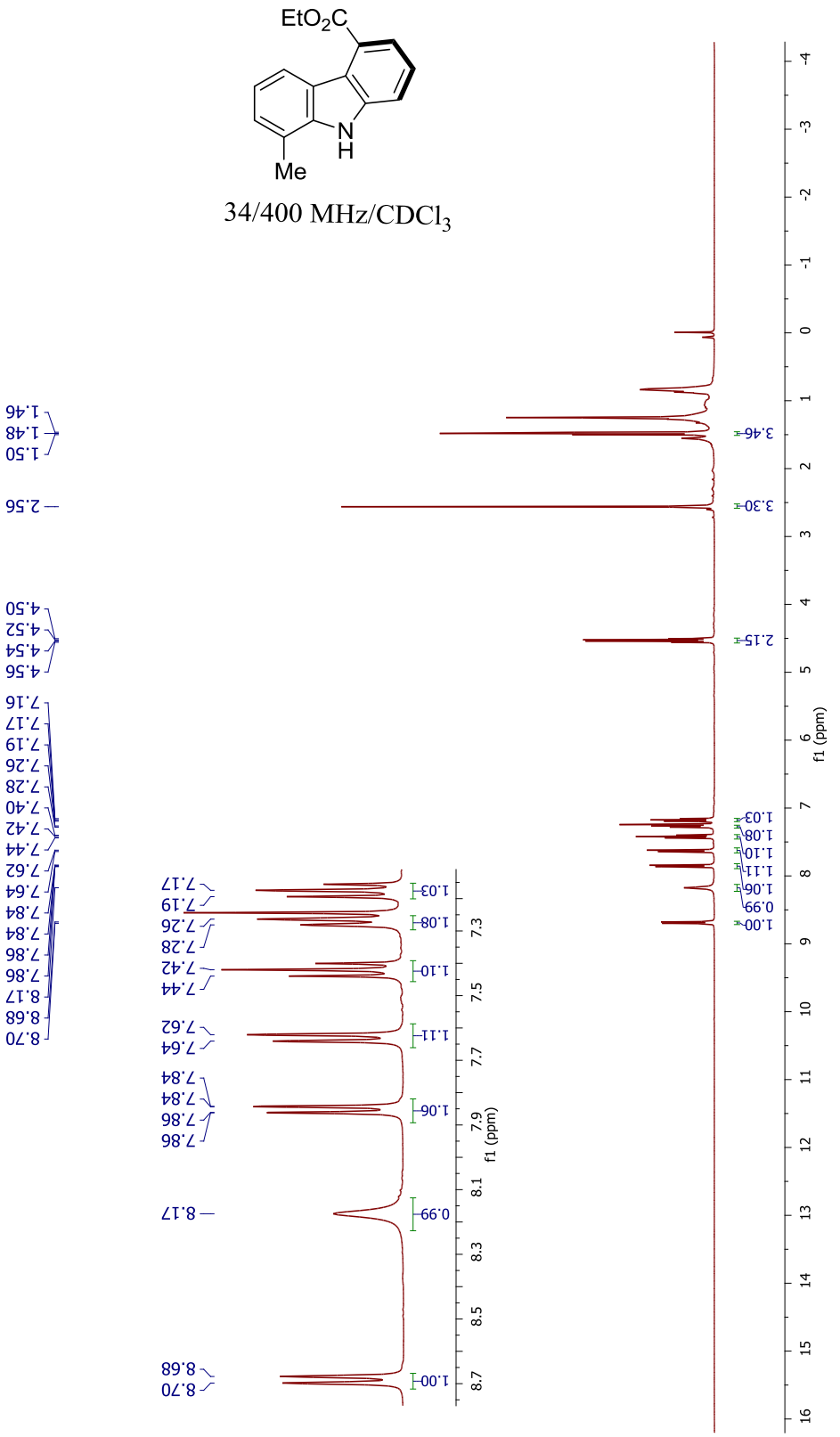
140.72
168.22
f1 (ppm)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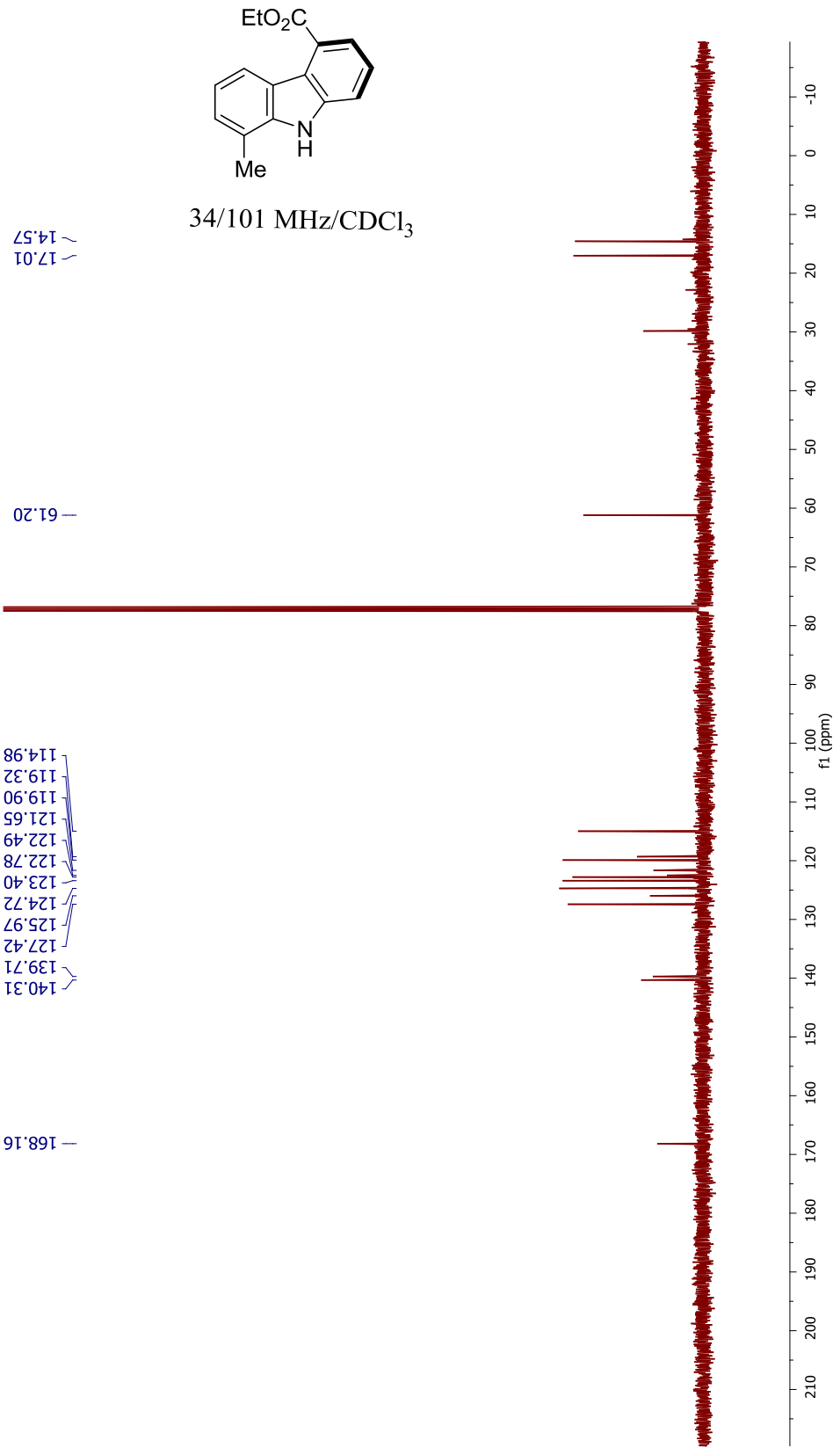
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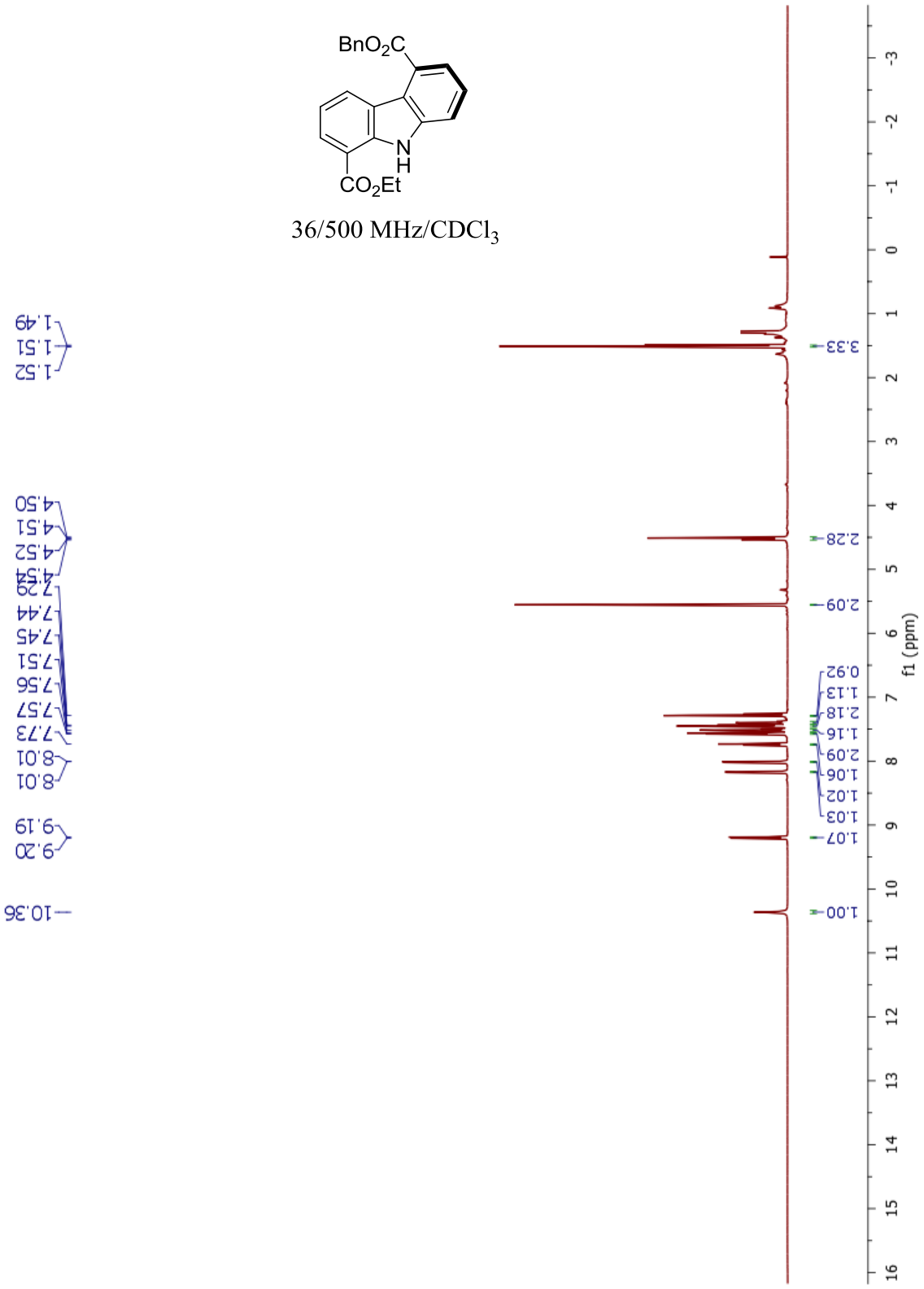
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CO2Et
36/500 MHz/CDCl3
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4.51
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4.54
7.29
7.44
7.45
7.51
7.56
7.57
7.73
8.01
8.01
9.19
9.20
10.36
3.33
2.28
2.09
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1.03
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1.06
2.09
1.16
2.18
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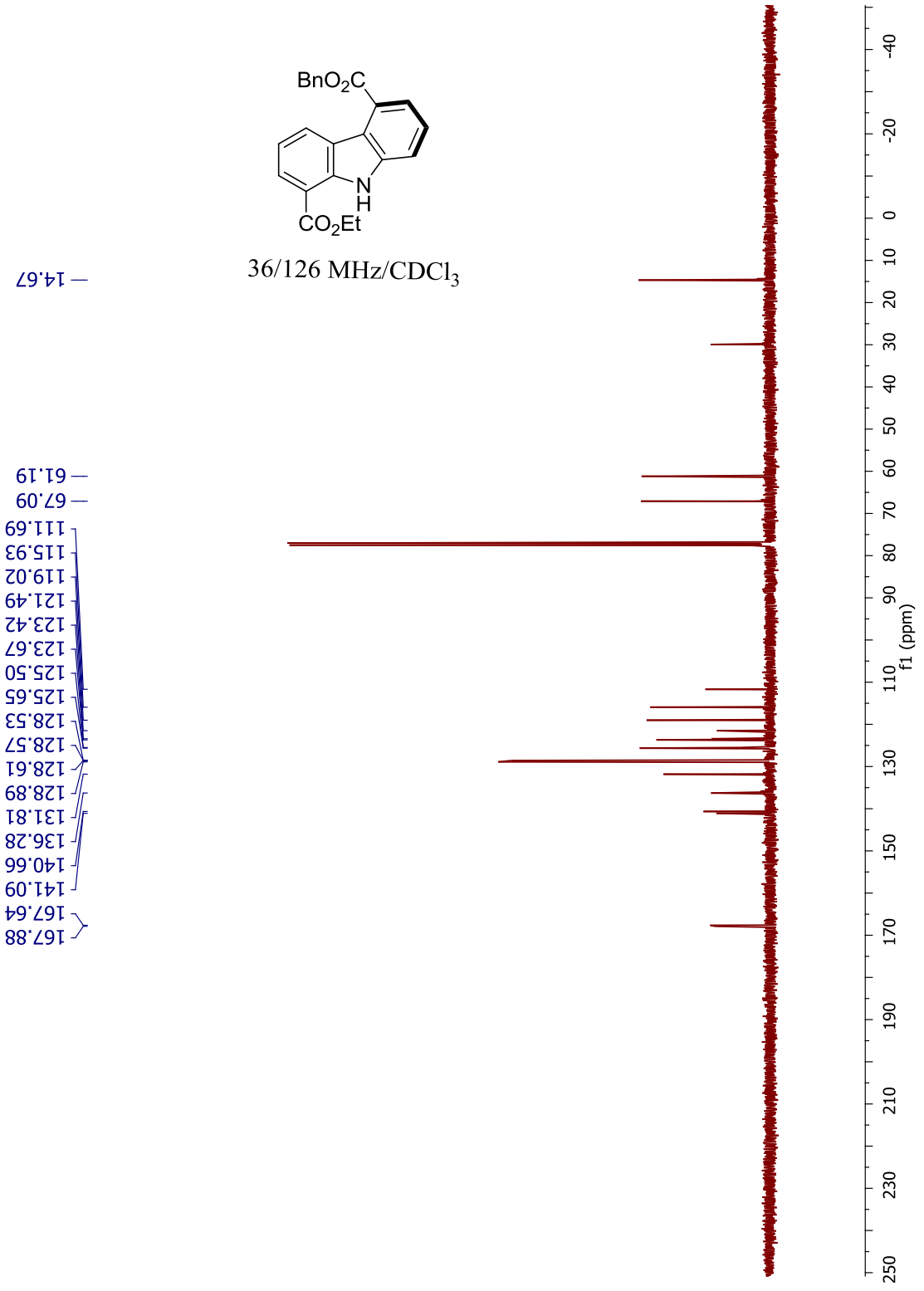
0.92
f1 (ppm)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N
H
CO2Et
36/126 MHz/CDCl3
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123.67
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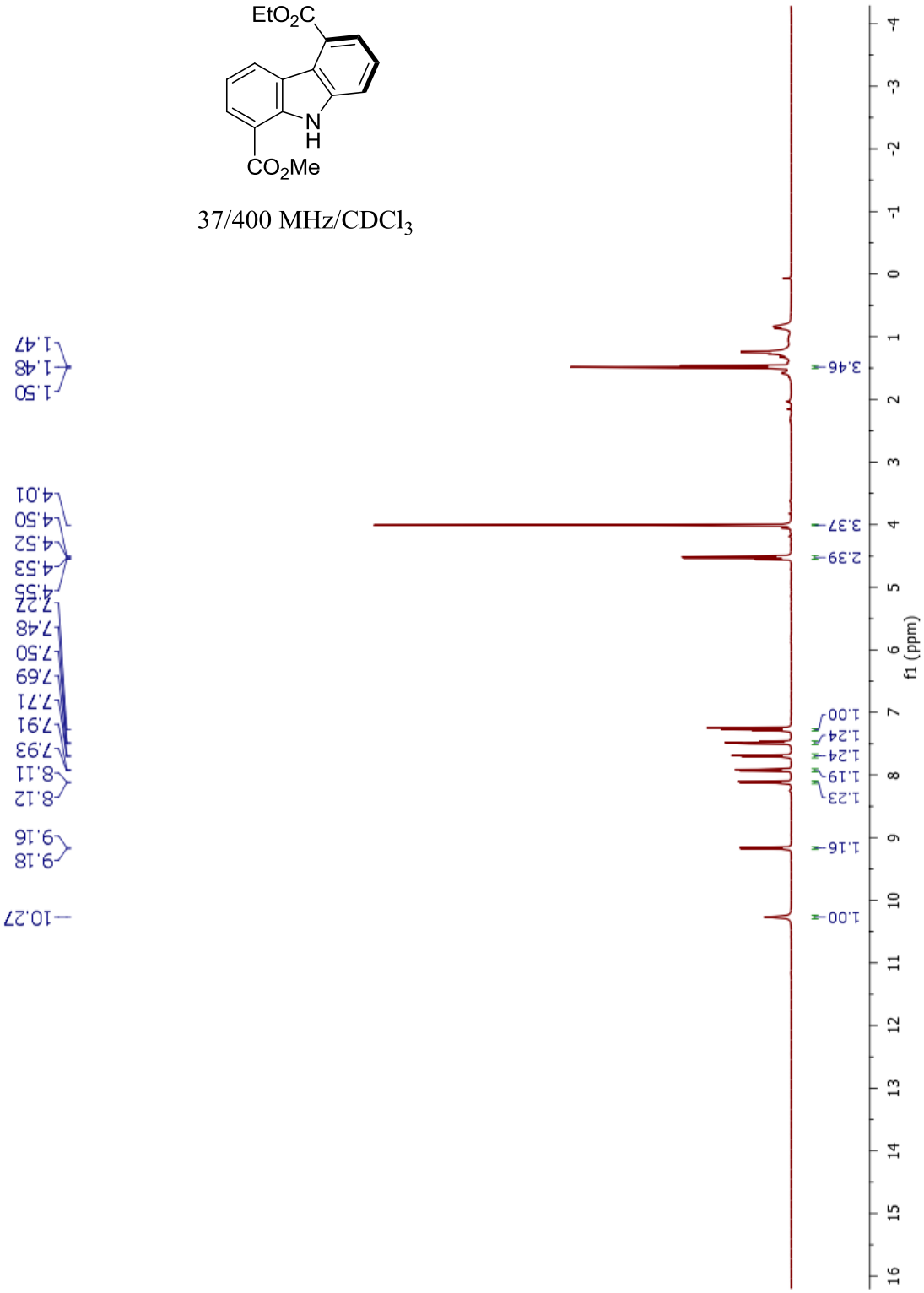
140.66
141.09
167.64
167.88
f1 (ppm)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N
H
CO2Me
37/400 MHz/CDCl3
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4.55
7.22
7.48
7.50
7.69
7.71
7.91
7.93
8.11
8.12
9.16
9.18
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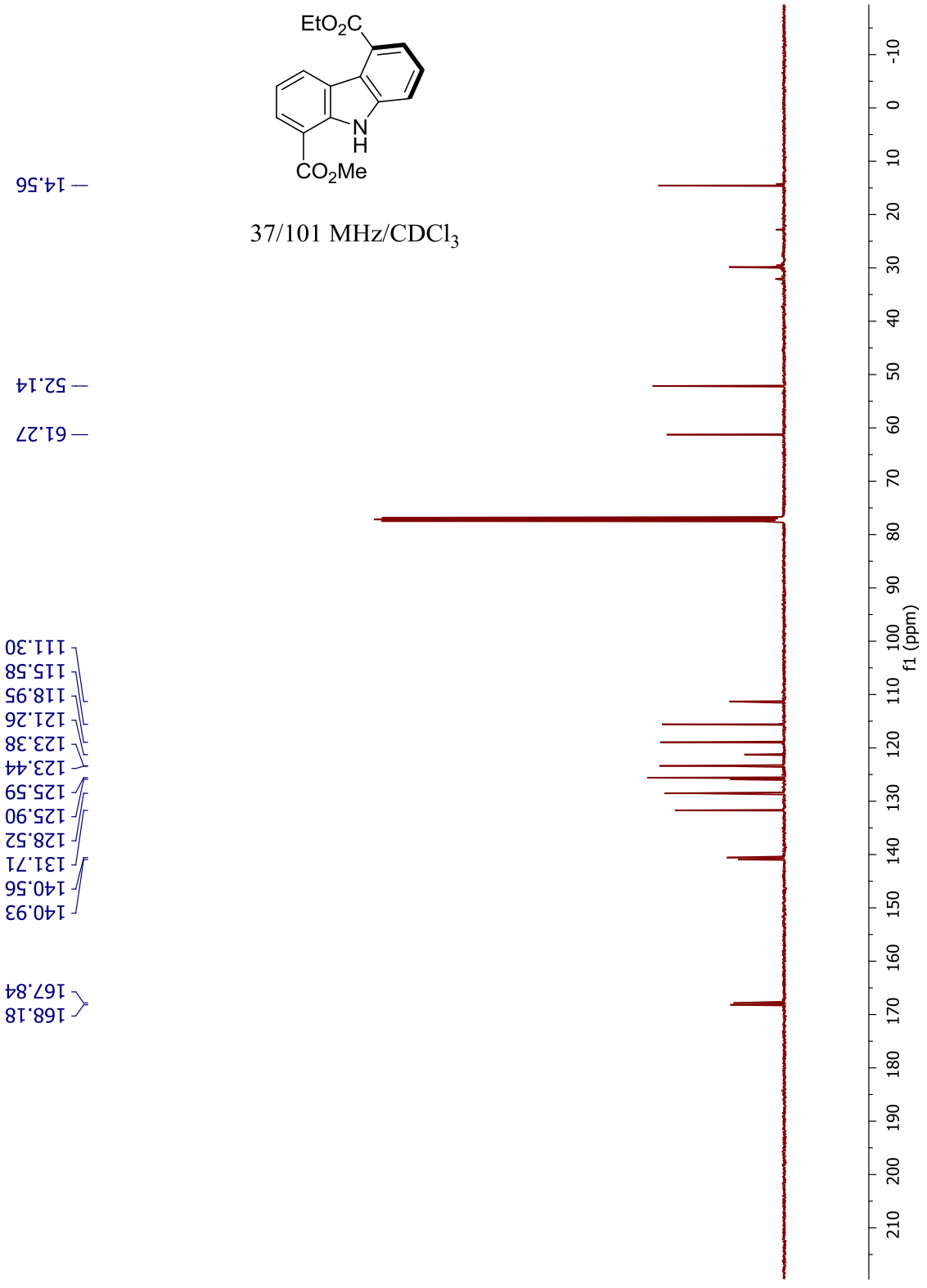
1.19
1.23
1.16
1.00
f1 (ppm)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N
H
CO2Me
37/101 MHz/CDCl3
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61.27
111.30
115.58
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131.71
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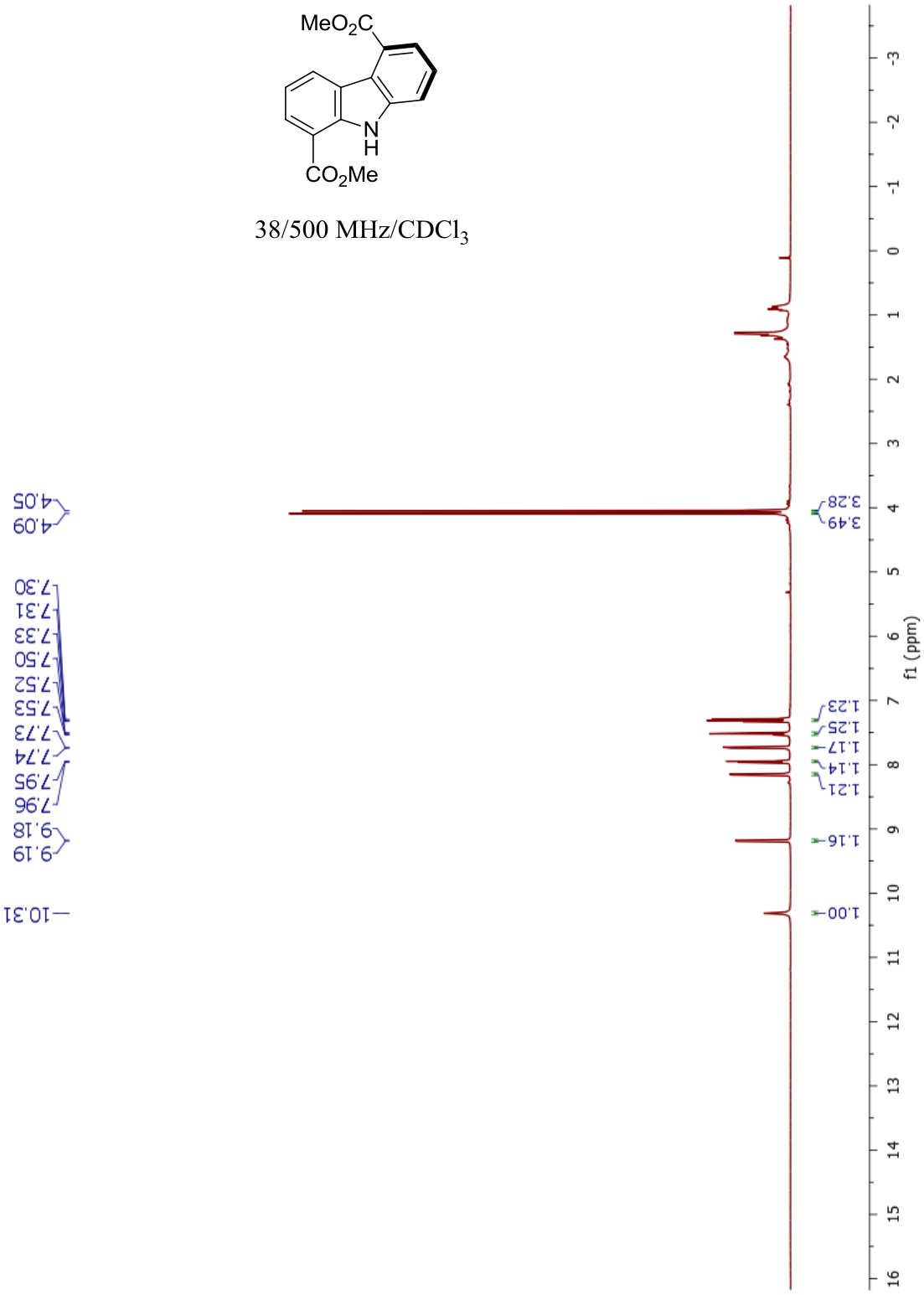
140.93
167.84
168.18
f1 (ppm)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CO2Me
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7.30
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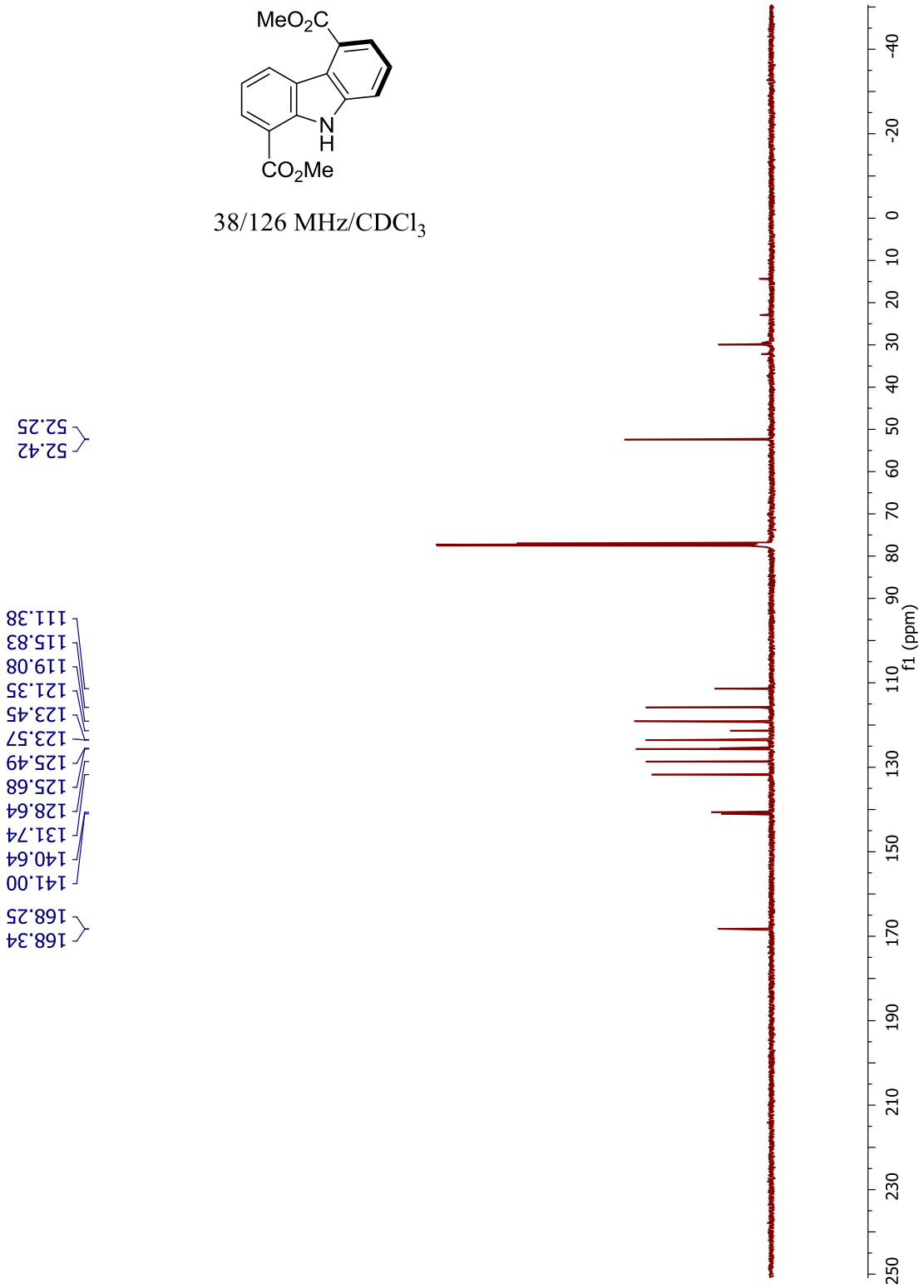
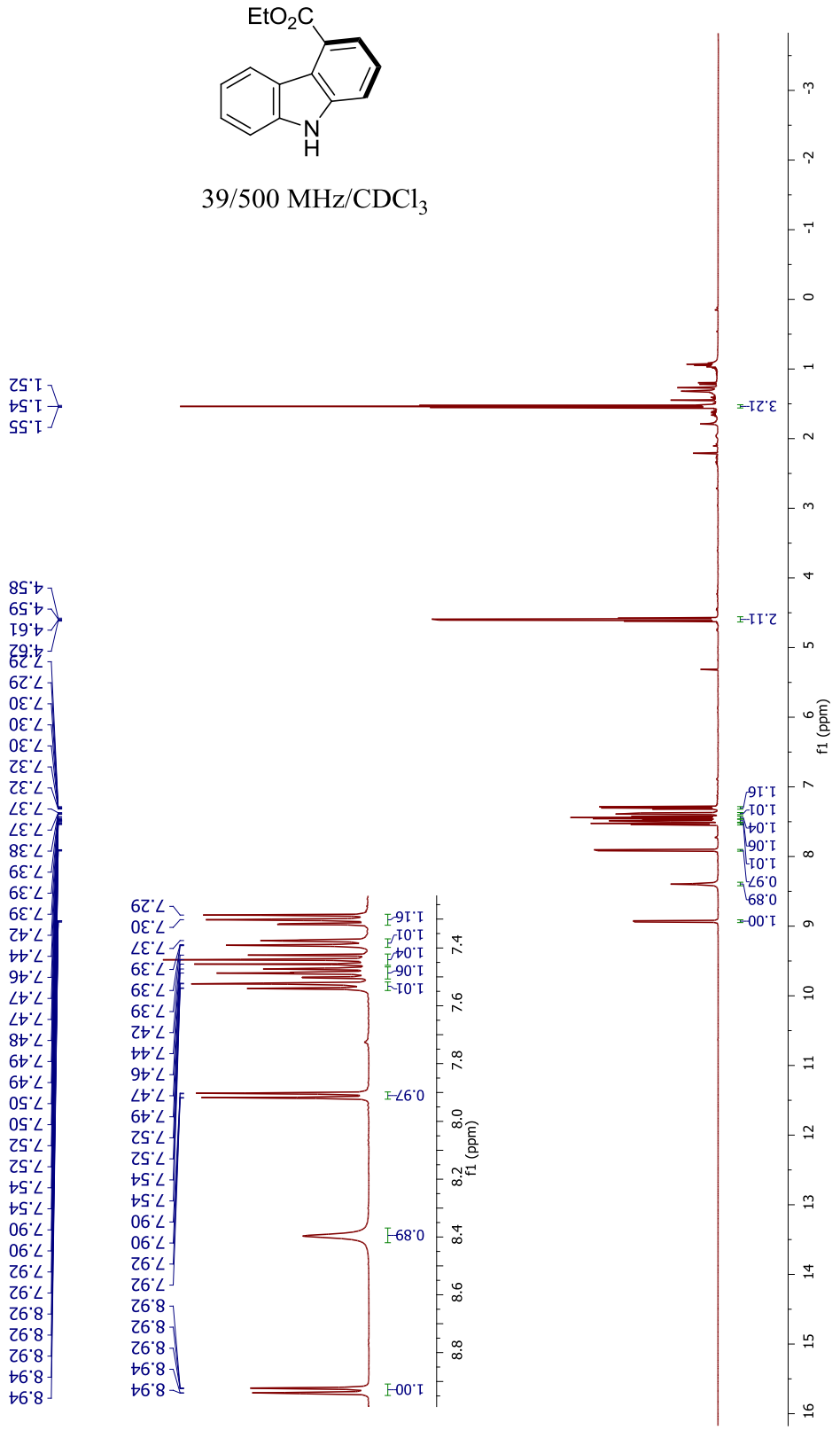
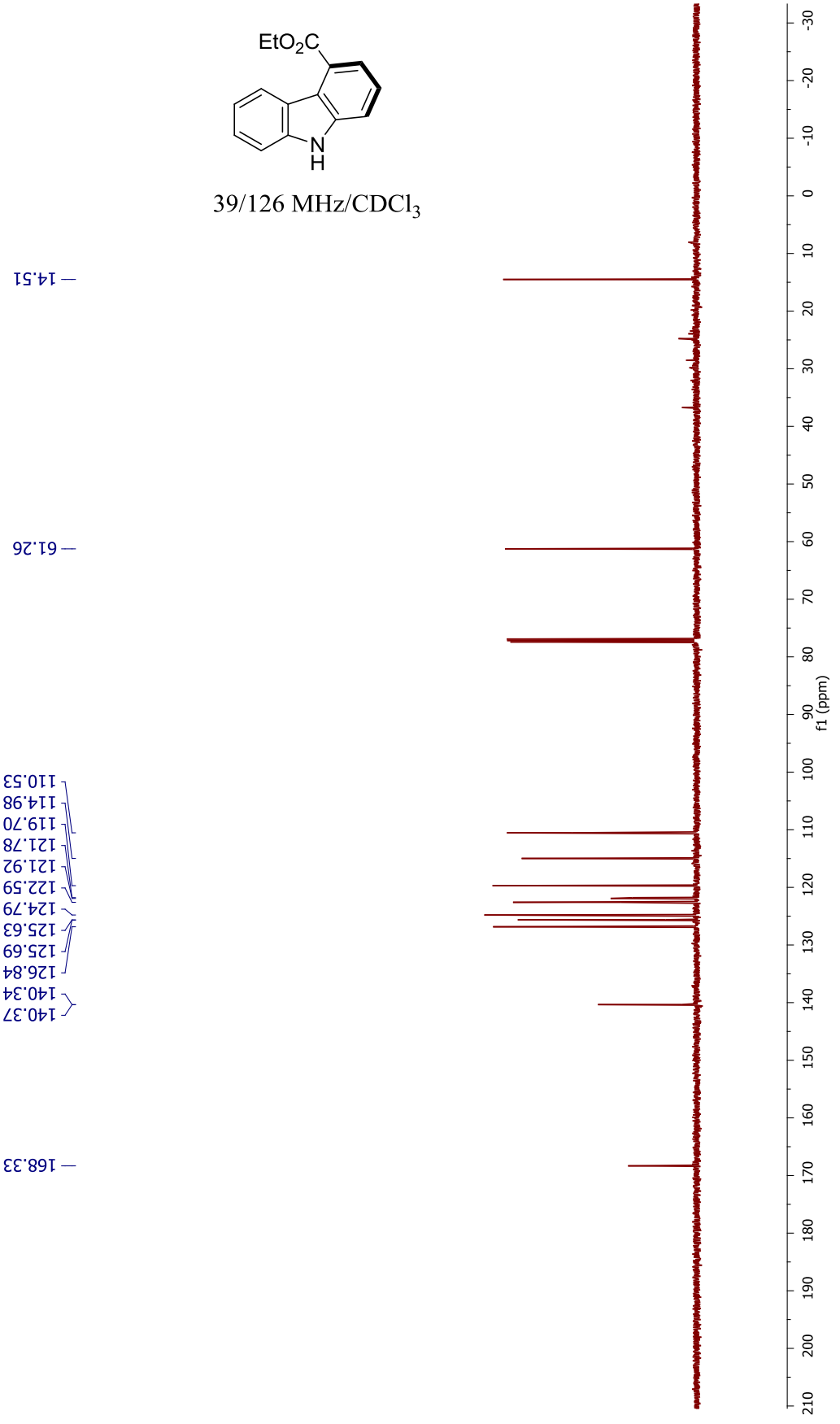
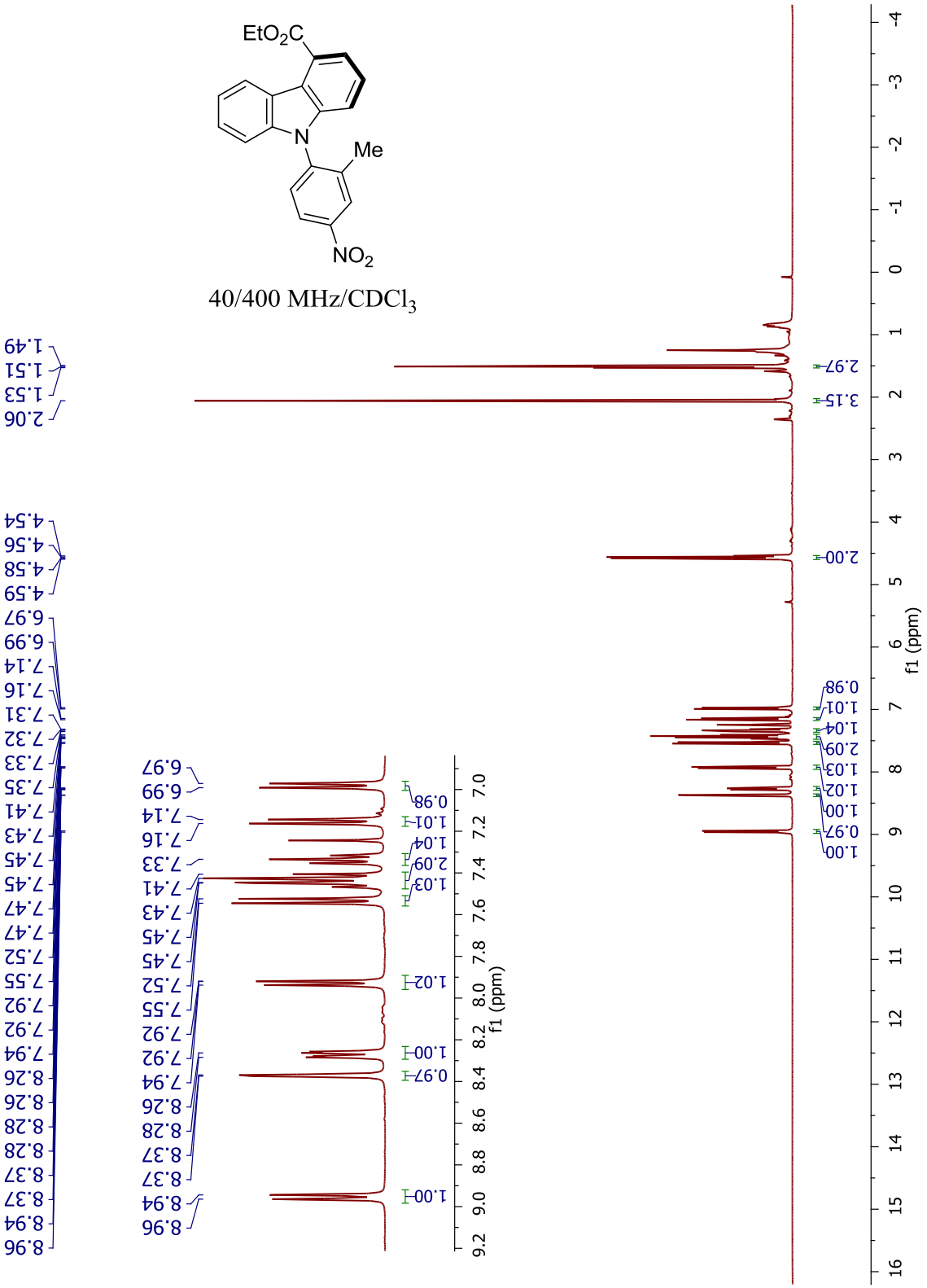
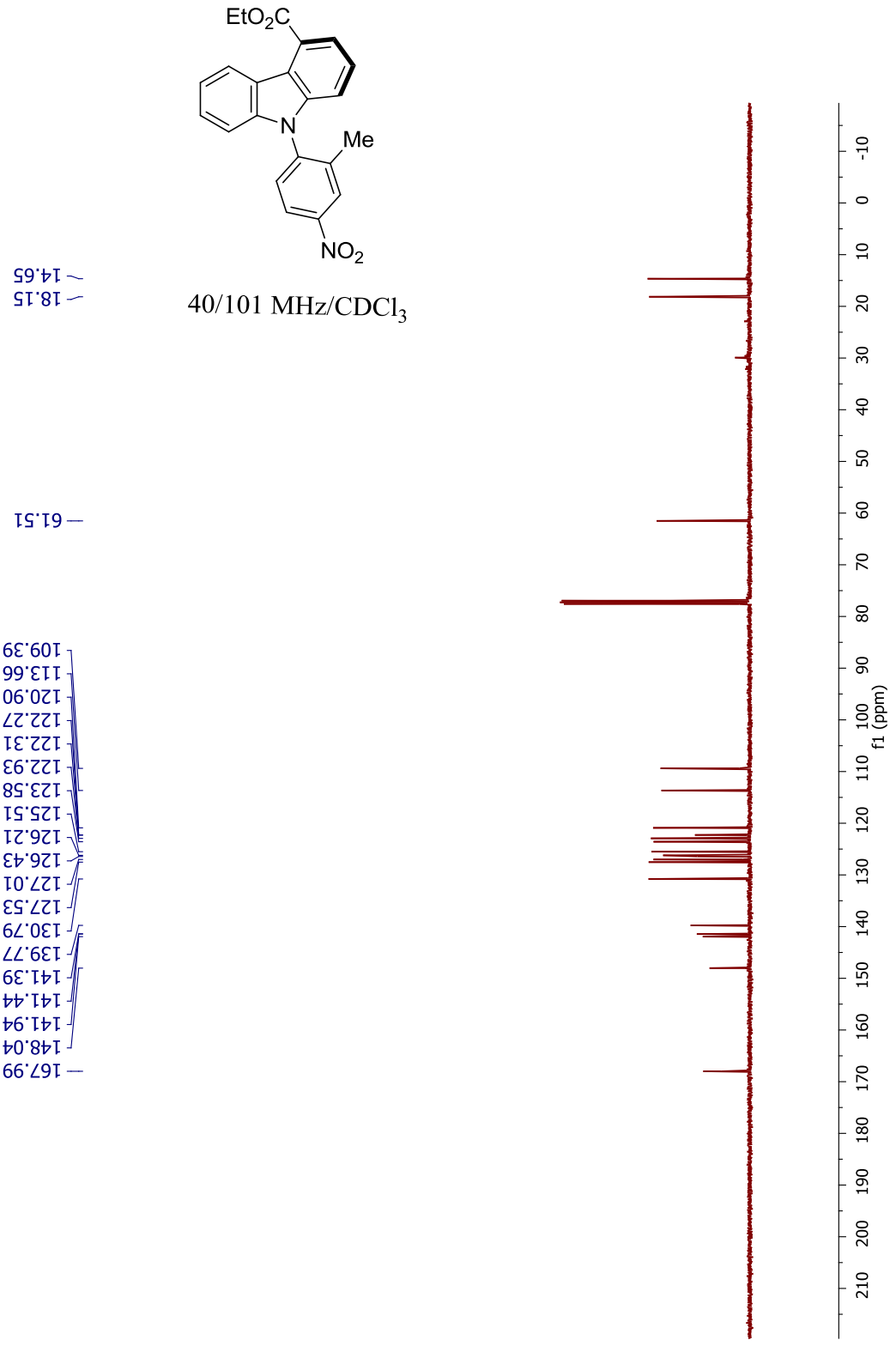
7.50
7.52
7.53
7.73
7.74
7.95
7.96
9.18
9.19
10.31
3.49
3.28
1.23
1.25
1.17
1.14
1.21
1.16
1.00
f1 (ppm)

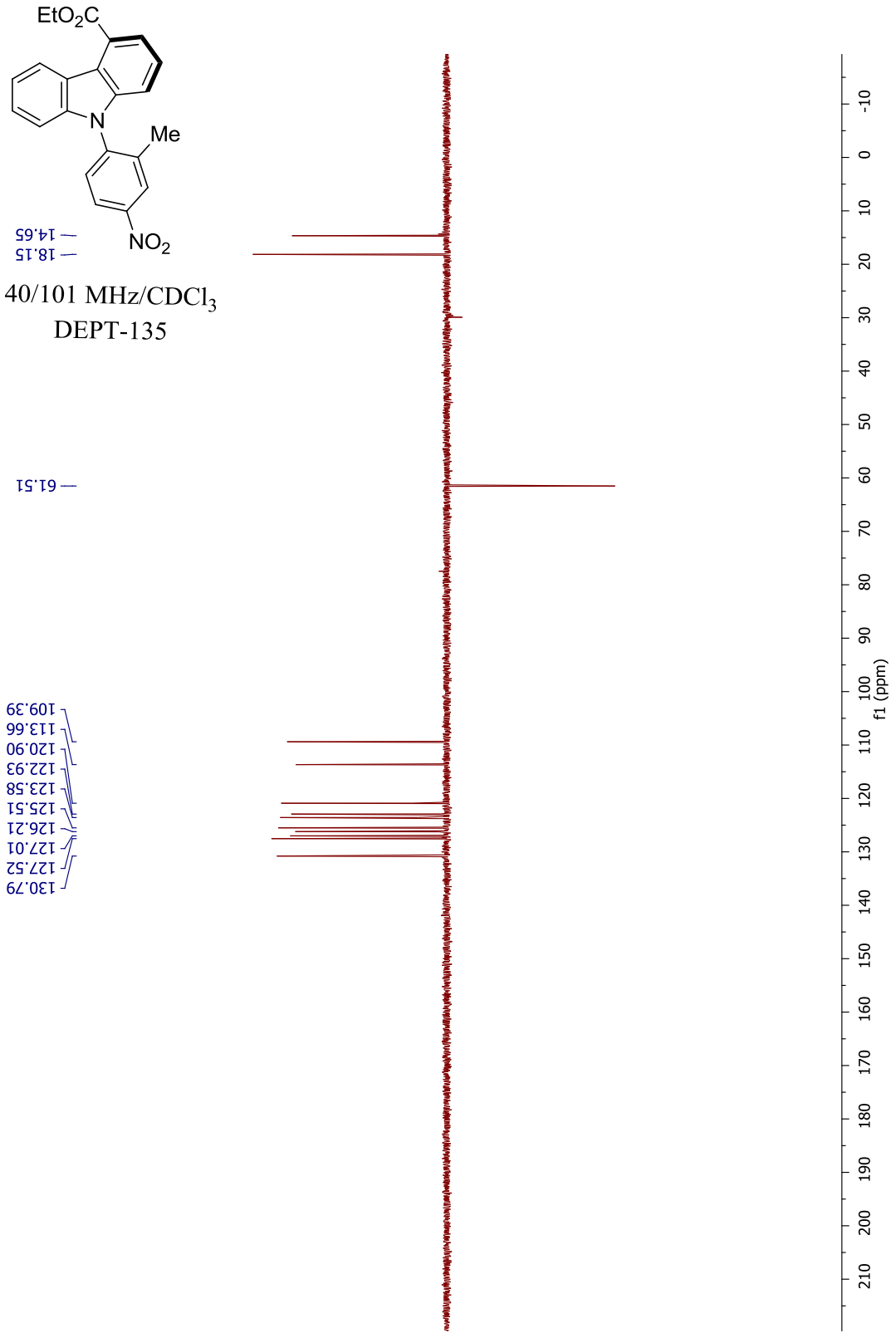

MeO2C
N
H
CO2Me
38/126 MHz/CDCl3
52.25
52.42
111.38
115.83
119.08
121.35
123.45
123.57
125.49
125.68
128.64
131.74
140.64
141.00
168.25
168.34
f1 (ppm)

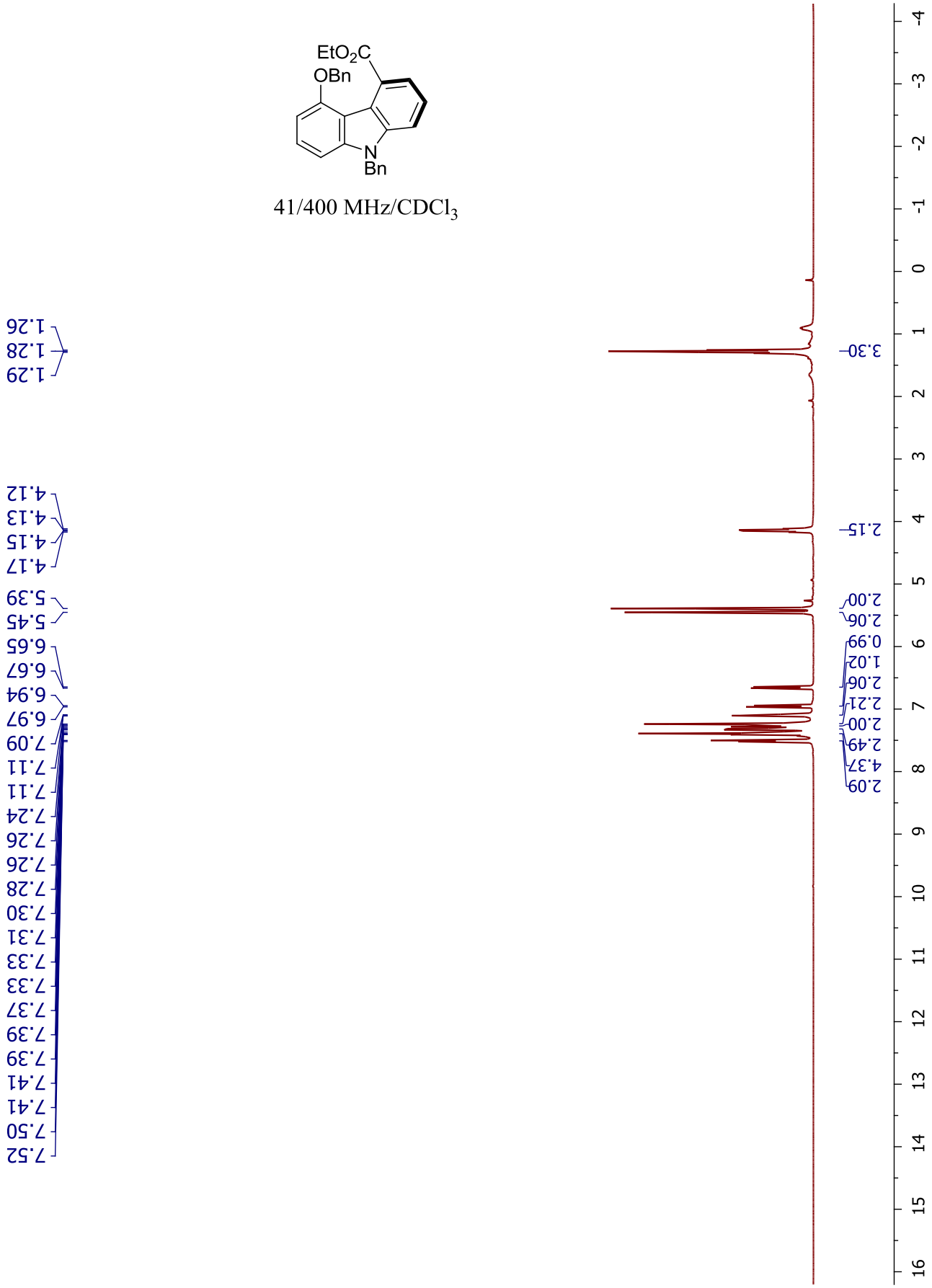

EtO2C
N
H
39/500 MHz/CDCl3
f1 (ppm)

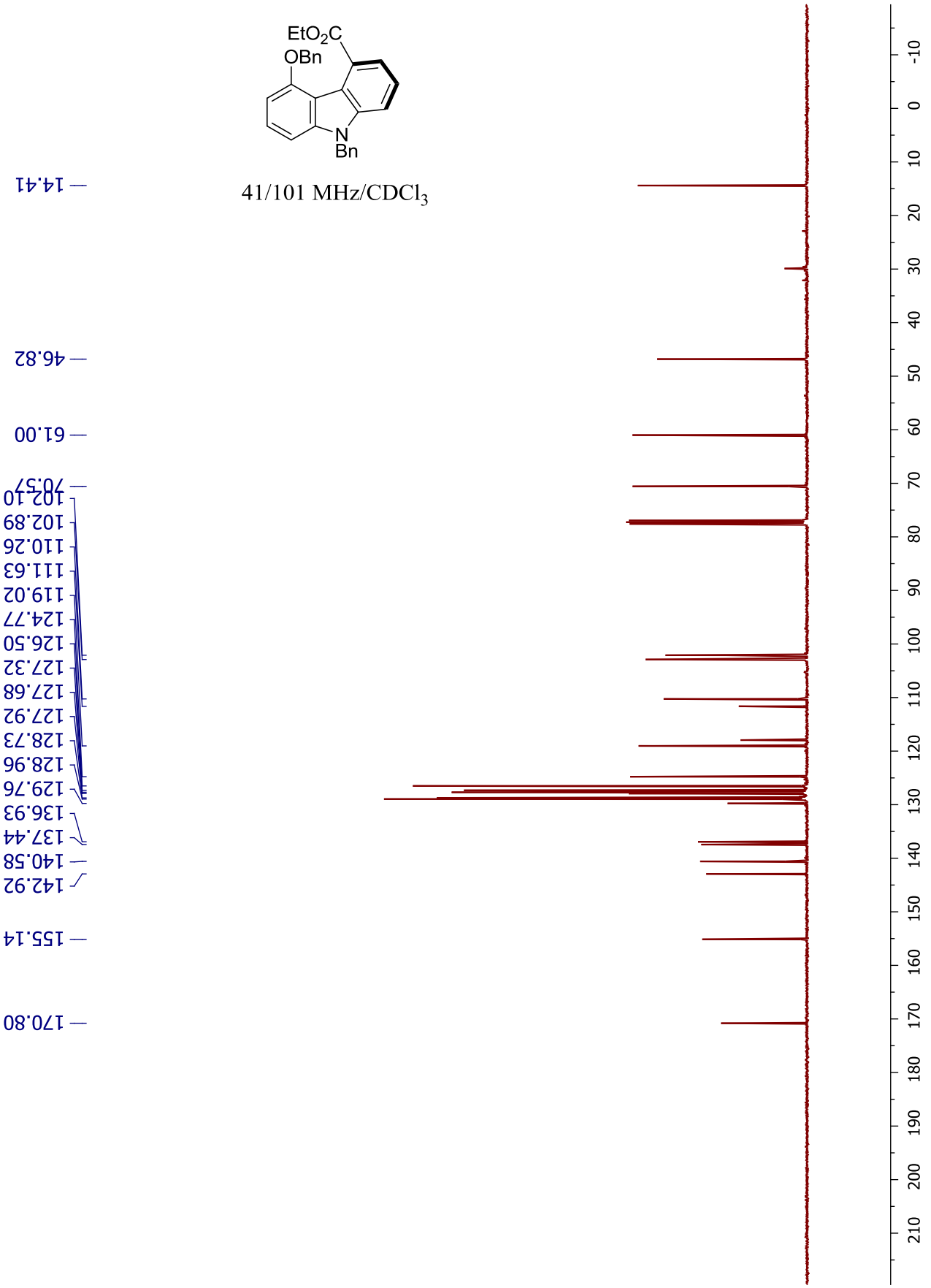

EtO2C
N
H
39/126 MHz/CDCl3
14.51
61.26
110.53
114.98
119.70
121.78
121.92
122.59
124.79
125.63
125.69
126.84
140.34
140.37
168.33
f1 (ppm)

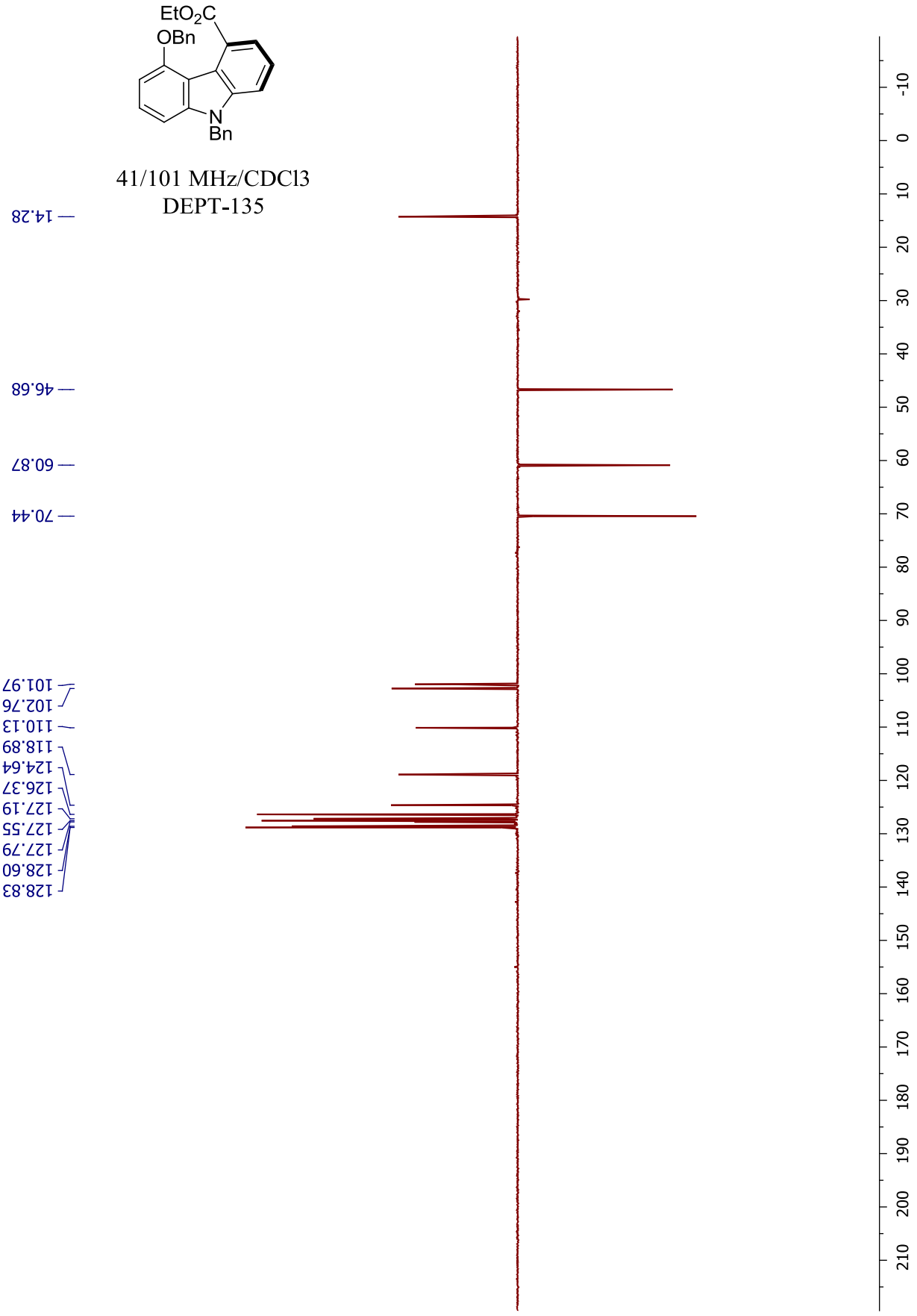

EtO2C
N
Me
NO2
40/400 MHz/CDCl3
f1 (ppm)


EtO2C
N
Me
NO2
40/101 MHz/CDCl3
14.65
18.15
61.51
109.39
113.66
120.90
122.27
122.31
122.93
123.58
125.51
126.21
126.43
127.01
127.53
130.79
139.77
141.39
141.44
141.94
148.04
167.99
f1 (ppm)


EtO2C
N
Me
NO2
14.65
18.15
40/101 MHz/CDCl3
DEPT-135
61.51
109.39
113.66
120.90
122.93
123.58
125.51
126.21
127.01
127.52
130.79
f1 (ppm)


EtO2C
OBn
N
Bn
41/400 MHz/CDCl3
1.26
1.28
1.29
4.12
4.13
4.15
4.17
5.39
5.45
6.65
6.67
6.94
6.97
7.09
7.11
7.11
7.24
7.26
7.26
7.28
7.30
7.31
7.33
7.33
7.37
7.39
7.39
7.41
7.41
7.50
7.52
3.30
2.15
2.00
2.06
0.99
1.02
2.06
2.21
2.00
2.49
4.37
2.09


EtO2C
OBn
N
Bn
41/101 MHz/CDCl3
14.41
46.82
61.00
70.57
102.10
102.89
110.26
111.63
119.02
124.77
126.50
127.32
127.68
127.92
128.73
128.96
129.76
136.93
137.44
140.58
142.92
155.14
170.80


EtO2C
OBn
N
Bn
41/101 MHz/CDCl3
DEPT-135
14.28
46.68
60.87
70.44
101.97
102.76
110.13
118.89
124.64
126.37
127.19
127.55
127.79
128.60
128.83