Supporting Information

for

Synthesis of indolo[1,2-*c*]quinazolines from 2-alkynylaniline derivatives through Pd-catalyzed indole formation/cyclization with *N*,*N*-dimethylformamide dimethyl acetal

Antonio Arcadi[1], Sandro Cacchi[2], Giancarlo Fabrizi[2], Francesca Ghirga[3], Antonella Goggiamani[2], Antonia Iazzetti*[2] and Fabio Marinelli*[1]

Address: [1]Dipartimento di Scienze Fisiche e Chimiche, Università di L'Aquila, Via Vetoio, 671010 Coppito (AQ), Italy, [2]Dipartimento di Chimica e Tecnologie del Farmaco, Sapienza, Università di Roma, P.le A. Moro 5, 00185, Rome, Italy and [3]Center for Life Nano Science@Sapienza, Istituto Italiano di Tecnologia, Viale Regina Elena 291, 00161 Rome, Italy

*Corresponding author

Email: Fabio Marinelli - fabio.marinelli@univaq.it

Experimental procedures, characterization data and copies of NMR spectra

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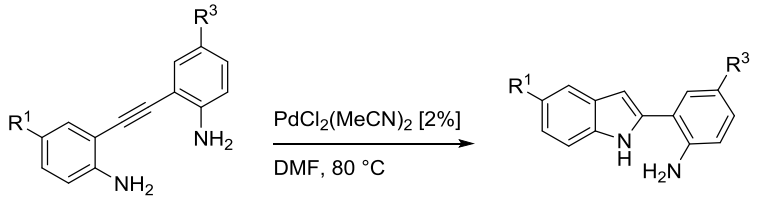
General information

Melting points are uncorrected. All of the reagents, catalysts, and solvents are commercially available and were used as purchased, without further purification. Starting materials were purified on axially compressed columns, packed with SiO_2 25–40 μm, connected to a preparative pump for solvent delivery and to a refractive index detector, and eluting with *n*-hexane/EtOAc mixtures. Reaction products were purified by flash chromatography using SiO_2 as stationary phase, eluting with *n*-hexane/ethyl acetate or MeOH/$CHCl_3$ mixtures. ^{1}H NMR (400.13 MHz), ^{13}C NMR (100.6 MHz) and ^{19}F NMR (376.5 MHz) spectra were recorded with a Bruker Avance 400 spectrometer. Splitting patterns are designed as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), or bs (broad singlet). IR spectra were recorded with a Jasco FT/IR-430 spectrometer. HRMS spectra were recorded with Orbitrap Exactive Mass spectrometer with ESI source.

The appropriate *o*-(*o*-aminophenylethynyl) trifluoroacetanilides **5** and *o*-(*o*-aminophenylethynyl)anilines **15** were prepared, usually in high yields, via a Sonogashira cross-coupling of 2-iodotrifluoroacetanilides or 2-iodoaniline with 2-ethynylanilines.[1]

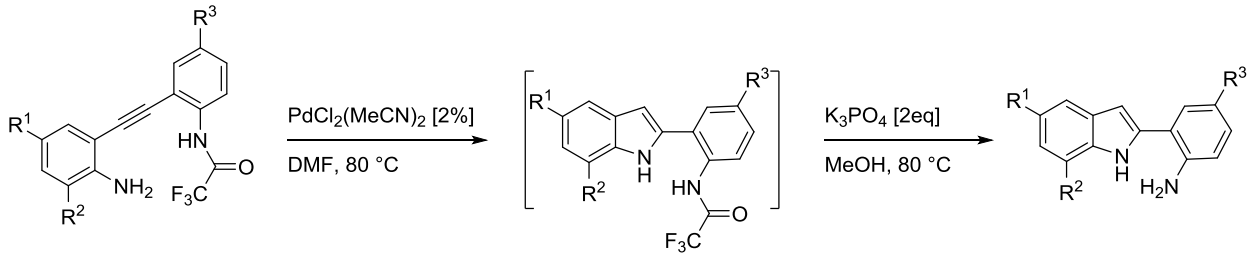
2-(*o*-Aminophenyl)indoles **14** were synthesized through two different procedures depending on the substitution of the indole derivatives: indoles **14a–c** ($R^1 = R^3$, R^2 = H) were prepared via palladium-catalyzed cyclization of the corresponding *o*-(*o*-aminophenylethynyl)aniline **15a–c** (Scheme 1). [2] Indoles **14d**,**e** ($R^1 \neq R^3$) were obtained by cyclization of the corresponding *o*-(*o*-aminophenylethynyl) trifluoroacetanilides **5** with $PdCl_2(MeCN)_2$ [2] followed by hydrolysis of -$COCF_3$ on the crude (Scheme 2).



15a ($R^1 = R^3$ = H)
15b ($R^1 = R^3$ = Me)
15c ($R^1 = R^3$ = COOMe)

14a-c

Scheme S1: Preparation of **14a–c**.



5b (R^1, R^2 = H; R^3 = Me)
5e (R^1, R^2 = Me; R^3 = H)

16

14d-e

Scheme S2: Preparation of **14d,e**.

Experimental procedures

Typical procedure for preparation of 12-(4-methoxyphenyl)indolo[1,2-*c*]quinazolines 10a–p. Preparation of 10a.

In a 50 mL Carousel Tube Reactor (Radely Discovery Technology) containing a magnetic stirring bar $Pd(OAc)_2$ (4.0 mg, 0.018 mmol) and dppp (7.4 mg, 0.018 mmol) were dissolved at room temperature with 1 mL of anhydrous MeOH. Then 2-((2-aminophenyl)ethynyl))trifluoroacetanilide (**5a**, 105.0 mg, 0.345 mmol), 4-methoxyphenyl-boronic acid (**12a**, 104.8 mg, 0.690 mmol), K_3PO_4 (146.4 mg, 0.690 mmol) and 1.0 mL of MeOH were added. The mixture was stirred at 60 °C under oxygen atmosphere until conversion of *o*-(*o*-aminophenylethynyl) trifluoroacetanilide (**5a**) into indole **11a** was completed (3 h). Then, in order to allow complete hydrolysis of **11a** to **9a**, the reaction mixture was warmed at 100 °C for 16 h, cooled to room temperature, diluted with ether and washed with a satured solution of $NaHCO_3$. The organic extract was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was dissolved in 2 mL of DMF and DMFDMA (230 μL, 1.725 mmol) was added. The mixture was stirred at 100 °C for 8 h, cooled to room temperature, diluted with ether, washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (silica gel, *n*-hexane/EtOAc 85:15 v/v) to afford 12-(4-methoxyphenyl)indolo[1,2-*c*]quinazoline **10a** (85.0 mg, 76%).

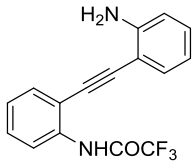
Typical procedure for preparation of indolo[1,2-*c*]quinazolines 13a-d. Preparation of 13d.

To a solution of 2-(1*H*-indol-2-yl)-4-methylaniline (**14d**, 76.7 mg, 0.345 mmol) in 2 mL of DMF, DMFDMA (91 μL, 0.690 mmol) was added; the mixture was stirred at 100 °C. After 25 h, the reaction mixture was cooled to room temperature, diluted with ether and washed with a saturated solution of $NaHCO_3$. The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (silica gel, *n*-hexane/EtOAc 85/15 v/v) to afford 2-methylindolo[1,2-*c*]quinazoline **13d** (76.1 mg, 95%).

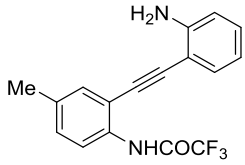
Sequential preparation of indolo[1,2-*c*]quinazoline 13a from 15a

To a stirred solution of $PdCl_2(MeCN)_2$ (6.2 mg, 0.024 mmol) in 2 mL of DMF *o*-(*o*-aminophenylethynyl)aniline (**15a**, 100 mg, 0.481 mmol) and DMFDMA (128 μL, 0.962 mmol) were added; the mixture was stirred at 100 °C under N_2 atmosphere for 24 h. Then the reaction mixture was cooled to room temperature, diluted with ether and washed with a saturated solution of $NaHCO_3$. The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash chromatography (silica gel, *n*-hexane/EtOAc 80/20v/v) to afford indolo[1,2-*c*]quinazoline **13a** (74.8 mg, 71%).

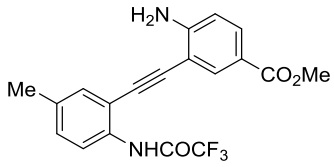
Characterization data (5a–d; 14a–e; 9a)



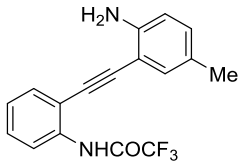
***N*-(2-((2-Aminophenyl)ethynyl)phenyl)-2,2,2-trifluoroacetamide (5a)** [3]
Pale yellow powder, **yield**: 82%; mp: 100-102 °C; **^{1}H NMR ($CDCl_3$):** δ 8.87 (bs, 1H), 8.39 (d, *J* = 7.6 Hz, 1H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.46-7.43 (m, 2H), 7.36-7.23 (m, 2H), 6.77 (d, *J* = 4.0 Hz, 2H), 4.29 (bs, 2H); **^{13}C NMR ($CDCl_3$):** δ 154.5 (q, J_{CF} = 37 Hz), 147.9, 135.8, 132.2, 131.7, 130.8, 129.8, 126.2, 120.9, 119.8, 116.0 (q, J_{CF} = 241 Hz), 114.3, 113.7, 106.3, 94.7, 88.1; **^{19}F NMR ($CDCl_3$):** δ -75.7.



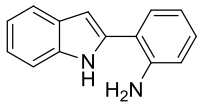
***N*-(2-((2-Aminophenyl)ethynyl)-4-methylphenyl)-2,2,2-trifluoroacetamide (5b)**[1b]
White powder, **yield**: 67%; mp: 141-143 °C; **^{1}H NMR (DMSO-*d_6*):** δ 11.17 (bs, 1H), 7.57 (s, 1H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 1 H), 7.18 (d, *J* = 7.2 Hz, 1H), 7.09 (t, *J* = 7.2 Hz, 1H), 6.73 (d, *J* = 8.4 Hz, 1H), 6.55 (t, *J* = 7.2 Hz, 1H), 5.56 (bs, 2H), 2.35 (s, 3H); **^{13}C NMR (DMSO-*d_6*):** δ 155.7 (q, J_{CF} = 36 Hz), 150.2, 137.6, 133.1, 132.9, 132.2, 130.6, 130.0, 126.9, 120.5, 116.6 (q, J_{CF} = 287 Hz), 116.2, 114.4, 105.5, 92.3, 90.5, 20.8. **^{19}F NMR (DMSO-*d_6*):** δ: -75.6.



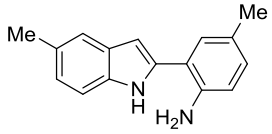
Methyl 4-amino-3-((5-methyl-2-(2,2,2-trifluoroacetamido)phenyl)ethynyl)benzoate (5c)
Pale yellow powder, **yield**: 37%; mp: 161-163 °C; **^{1}H NMR ($CDCl_3$):** δ 8.71 (bs, 1H), 8.20 (d, *J* = 8.4 Hz, 1H), 8.07 (d, *J* = 2.0 Hz, 1H), 7.88 (dd, J_1 = 8.8 Hz, J_2 = 1.8 Hz, 1H), 7.39 (s, 1H), 7.25 (d, *J* = 8.4 Hz, 1H), 6.75 (d, *J* = 8.4 Hz, 1H), 4.72 (bs, 2H), 3.90 (s, 3 H), 2.38 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 166.3, 154.5 (q, J_{CF} = 37 Hz), 151.4, 135.7, 134.6, 133.4, 132.3, 132.2, 130.8, 120.1, 119.8, 115.8 (q, J_{CF} = 287 Hz), 113.7, 113.5, 105.6, 92.8, 88.8, 51.9, 20.8.



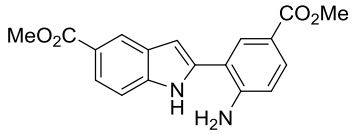
***N*-(2-((2-Amino-5-methylphenyl)ethynyl)phenyl)-2,2,2-trifluoroacetamide (5d)** [1b]
White powder, **yield**: 70%; mp :137-139 °C; **^{1}H NMR ($CDCl_3$):** δ 8.88 (bs, 1 H), 8.39 (d, *J* = 8,4 Hz, 1H), 7.57 (dd, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.50-7.38 (m, 1H), 7.32-7.22 (m, 1H), 7.18 (s, 1H), 7.05 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 6.70 (d, *J* = 8.0 Hz, 1H), 4.15 (bs, 2H), 2.28 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 154.5 (q, *J* = 37.5 Hz), 145.6, 135.7, 132.2, 131.8, 131.7, 129.7, 127.6, 125.6, 119.8, 115.7 (q, *J* = 287 Hz), 115.0, 113.8, 106.3, 95.0, 87.8, 20.3. **^{19}F NMR ($CDCl_3$):** δ -75.7.



2-(1*H*-Indol-2-yl)aniline (14a) [4]
Pale yellow powder, **yield**: 82%; lit [4] mp: 163-165 °C; mp: 166-168 °C; **^{1}H NMR ($CDCl_3$):** δ 8.47 (bs, 1H), 7.67 (d, *J* = 7.2 Hz, 1H), 7.44-7.40 (m, 2H), 7.25-7.15 (m, 3H), 6.91-6.83 (m, 2H), 6.75 (s, 1H), 4.12 (bs, 2H); **^{13}C NMR ($CDCl_3$):** δ 144.0, 136.1, 135.9, 129.2, 129.1, 128.9, 122.1, 120.4, 120.2, 119.1, 118.8, 116.6, 110.8, 101.6.

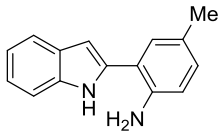


4-Methyl-2-(5-methyl-1*H*-indol-2-yl)aniline (14b) [5]
Beige powder, **yield**: 63%; lit [5] mp: 195-197 °C; mp: 194-196 °C; **^{1}H NMR ($CDCl_3$):** δ 8.33 (bs, 1H), 7.34 (s, 1H), 7.20 (t, *J* = 7.8 Hz, 1H), 7.13 (d, *J* = 1.6 Hz, 1H), 6.95 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 6.91 (dd, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 6.55 (s, 1H), 3.84 (bs, 2H), 2.38 (s, 3H), 1.22 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 141.3, 136.2, 134.5, 129.54, 129.49, 129.3, 129.2, 128.5, 123.7, 120.0, 119.1, 116.9, 110.4, 101.0, 21.5, 20.5.



Methyl 2-(2-amino-5-(methoxycarbonyl)phenyl)-1*H*-indole-5-carboxylate (14c)
Pale yellow powder, **yield**: 82%; mp: 198-200 °C; **^{1}H NMR ($CDCl_3$):** δ 8.71 (bs, 1H), 8.42 (s, 1H), 8.08 (d, *J* = 1.6 Hz, 1H), 7.95 (dd, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1H), 7.87 (dd, J_1 = 8.4

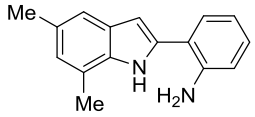
Hz, J_2 = 2.0 Hz, 1H), 7.45 (d, J = 8.4 Hz, 1H), 6.85-6.80 (m, 2H), 4.62 (bs, 2H), 3.96 (s, 3H), 3.90 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 168.1, 166.9, 148.5, 138.8, 135.9,131.16, 131.11, 128.4, 123.9, 123.4, 122.4, 120.1, 116.9, 115.3, 110.6, 102.9, 51.9, 51.8.



2-(1*H*-Indol-2-yl)-4-methylaniline (14d) [5]

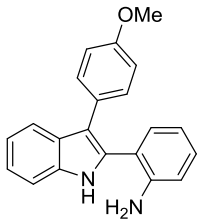
Off-white powder, **yield**: 72%; lit [5] mp: 162-163 °C; mp: 165-167 °C; **^{1}H NMR (DMSO d_6):** δ 11.2 (s, 1H), 7.52 (d, J = 7.6, Hz 1H), 7.38 (d, J = 8.0 Hz, 1H), 7.20 (s, 1H), 7.05 (t, J = 7.4 Hz, 1H), 7.00 (t, J = 7.4 Hz 1H), 6.89 (d, J = 8.0 Hz, 1H), 6.74 (d, J = 8.4 Hz, 1H), 6.66 (s, 1H), 4.98 (s, 2H), 2.23 (s, 3H); **^{13}C NMR (DMSO d_6):** δ 143.6, 136.69, 136.68, 129.4, 129.1, 125.4, 121.4, 120.1, 119.4, 117.5, 116.5, 111.5, 100.4, 20.6.

2-(5,7-Dimethyl-1*H*-indol-2-yl)aniline (14e)



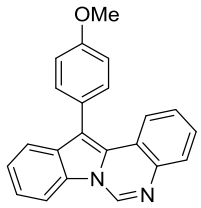
Beige powder, **yield**: 80%; mp: 192-194 °C; **^{1}H NMR ($CDCl_3$):** δ 8.27 (bs, 1H), 7.43 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.32 (s, 1H), 7.21 (td, J_1 = 7.7 Hz, J_2 = 1.2 Hz, 1H), 6.92-6.88 (m, 2H), 6.84 (d, J = 8.0 Hz, 1H), 6.67 (s, 1H), 4.13 (bs, 2H), 2.52 (s, 3H), 2.47 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 144.1, 135.6, 134.1, 129.7, 129.2, 128.9, 128.7, 124.5, 119.7, 119.1, 118.9, 117.7, 116.4, 101.7, 21.4, 16.7.

2-(3-(4-Methoxyphenyl)-1*H*-indol-2-yl)aniline (9a)

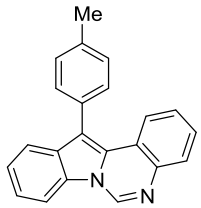


Brown oil, **yield**: 70%; mp: 155-157 °C; **^{1}H NMR ($CDCl_3$):** δ 8.29 (bs, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.41(d, J = 8.8 Hz, 3H),7.42-7.26 (m, 2H), 7.23-7.19 (m, 2H), 6.92 (d, J = 8.8 Hz, 2H), 6.82 (t, J = 7.2 Hz, 1H), 6.71 (d, J = 8.0 Hz, 1H), 3.84 (s, 3H), 3.75 (bs, 2H); **^{13}C NMR ($CDCl_3$):** δ.158.0, 144.6, 136.0, 131.7, 131.3, 129.9, 129.6, 127.7, 127.3, 122.5, 120.3, 119.5, 118.6, 118.4, 116.1, 114.9, 114.1, 111.0, 55.2.

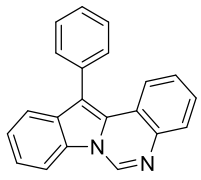
Characterization data (10a–p; 13a–e)



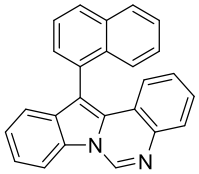
12-(4-Methoxyphenyl)indolo[1,2-*c*]quinazoline (10a)
Pale yellow powder, **yield**: 76%, mp: 135-136 °C; **IR (KBr)**: 2930, 2858, 2828, 1614, 1556, 1455 cm^{-1}; **^{1}H NMR ($CDCl_3$)**: δ 9.16 (s, 1H), 8.02 (d, *J* = 7.9 Hz, 1H), 7.82 (t, *J* = 7.0 Hz, 2H), 7.63 (d, *J* = 7.7 Hz, 1H), 7.65-7.41 (m, 5H), 7.28-7.22 (m, 1H), 7.13 (d, J_1 = 7.9 Hz, 2H), 3.96 (s, 3H); **^{13}C NMR ($CDCl_3$)**: δ 159.2, 139.4, 137.5, 131.7, 130.8, 129.4, 128.9, 127.7, 127.31, 127.29, 126.0, 124.3, 123.7, 123.0, 121.8, 119.8, 114.5, 112.6, 109.7, 55.4; **HRMS [M+H]$^+$**: calcd for $C_{22}H_{17}N_2O$ 325.1335, found 325.1335.



12-(*p*-Tolyl)indolo[1,2-*c*]quinazoline (10b)
Off-white powder, **yield**: 61%, mp: 192-193 °C; **IR (KBr):** 3060, 2931, 2847, 1740, 1560,1450 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 8.92 (s, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.53-7.49 (m, 1H), 7.40-7.26 (m, 7H), 7.15-7.09 (m, 1H), 2.40 (s, 3H); **^{13}C NMR ($CDCl_3$):** 140.1, 137.4, 137.3, 131.2, 130.54, 130.50, 129.8, 129.4, 128.8, 128.1, 127.4, 127.1, 124.0, 123.7, 122.8, 121.9, 119.8, 112.5, 109.5, 21.4; **HRMS [M+H]$^+$**: calcd for $C_{22}H_{17}N_2$ 309.1386, found 309.1385.

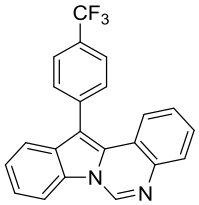


12-Phenylindolo[1,2-*c*]quinazoline (10c)
Yellow powder, **yield**: 75%,mp: 155-156 °C; **IR (KBr):** 3066, 2934, 2853, 1740, 1579,1450 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 8.90 (s, 1H), 7.83 (d, *J* = 7.6 Hz, 1H), 7.67 (t, *J* = 8.4 Hz, 2H), 7.54-7.26 (m, 9H), 7.10 (d, J_1 = 7.6 Hz, J_2 = 0.8 Hz, 1H); **^{13}C NMR ($CDCl_3$):**140.2, 137.2, 134.3, 130.7, 130.4, 129.4, 129.0, 128.9, 128.2, 127.7, 127.5, 127.2, 124.2, 123.7, 122.9, 121.8, 119.7, 112.5, 109.5; **HRMS [M+H]$^+$**: calcd for $C_{21}H_{15}N_2$ 295.1230, found 295.1229.



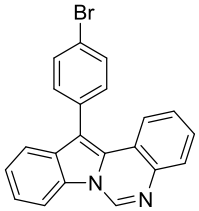
12-(Naphthalen-1-yl)indolo[1,2-*c*]quinazoline (10d)

Pale yellow powder, **yield**: 60%, mp: 192-193 °C; **IR (KBr):** 3042, 2925, 1618, 1469, 1445 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.07 (s, 1H), 8.00-7.90 (m, 3H), 7.70 (d, *J* = 7.7 Hz, 1H), 7.59 (s, 1H), 7.58 (d, *J* = 1.3 Hz, 1H), 7.52 (d, *J* = 8.3 Hz, 1H), 7.46-7.36 (m, 2H), 7.34-7.25 (m, 3H), 7.24-7.18 (m, 1H), 7.13 (dd, J_1 = 8.0 Hz, J_2 = 0.9 Hz, 1H), 6.98-6.90 (m, 1H); **^{13}C NMR ($CDCl_3$):** δ 140.2, 137.3, 134.1, 132.7, 131.8, 131.1, 129.6, 129.0, 128.8, 128.7, 128.5, 128.4, 128.0, 127.3, 126.4, 126.20, 126.19, 126.0, 124.2, 122.9, 121.7, 120.2, 109.9, 109.6; **HRMS [M+H]$^+$**: calcd for $C_{25}H_{17}N_2$ 345.1386, found 345.1385.



12-(4-(Trifluoromethyl)phenyl)indolo[1,2-*c*]quinazoline (10e)

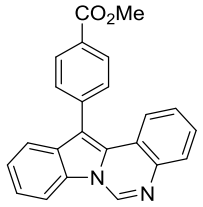
Yellow powder, **yield**: 69%, mp: 188-189 °C; **IR (KBr):** 2924, 2855, 1616, 1473(cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.00 (s, 1H), 7.93 (d, *J* = 7.8 Hz, 1H), 7.80-7.63 (m, 6H), 7.54-7.50 (m, 1H), 7.47-7.33 (m, 3H), 7.22-7.15 (m, 1H); **^{13}C NMR ($CDCl_3$):** δ 140.3 (q, J_{C-F} = 1.5 Hz, 1H), 138.5, 137.0, 131.0, 129.9, 129.8 (q, J_{CF} = 32 Hz, 1H), 129.6, 129.3, 128.5, 127.9, 127.4, 126.0 (q, J_{CF} = 4 Hz), 124.3 (q, J_{CF} = 272 Hz), 124.5, 123.5, 123.2, 121.3, 119.3, 110.8, 109.7; **^{19}F NMR ($CDCl_3$):** δ -63.33. **HRMS [M+H]$^+$**: calcd for $C_{22}H_{14}F_3N_2$ 363.1104, found 363.1101.



12-(4-Bromophenyl)indolo[1,2-*c*]quinazoline (10f)

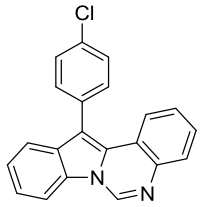
beige powder, **yield**: 60%, mp: 207-208 °C; **IR (KBr):** 3042, 2921, 1629, 1457 cm^{-1}; **^{1}H NMR ($CDCl_3$):** δ 8.96 (s, 1H), 7.89 (d, *J* = 7.4 Hz, 1H), 7.66-7.62 (m, 2H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.55-7.46 (m, 1H), 7.44-7.30 (m 5H), 7.21-7.14 (m, 1H); **^{13}C NMR ($CDCl_3$):** δ 140.2, 137.1, 133.4, 132.4, 132.3, 130.1, 129.5, 129.1, 128.3, 127.7, 127.3, 124.3, 123.6,

123.0, 121.8, 121.5, 119.4, 111.0, 109.7; **HRMS [M+H]$^+$**: calcd for $C_{21}H_{14}BrN_2$ 373.0345, found 373.0334.



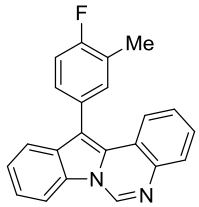
Methyl 4-(indolo[1,2-*c*]quinazolin-12-yl)benzoate (10g)

Pale yellow powder, **yield**: 59%, mp: 170-171 °C; **IR (KBr):** 3404, 3048, 2923, 1637, 1475 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.03 (s, 1H), 8.26 (d, *J* = 8.4 Hz, 2H), 8.02-7.99 (m, 1H), 7.80 (td, J_1 = 8.3 Hz, J_2 = 1.1 Hz, 2H), 7.72 (d, *J* = 8.4 Hz, 2H), 7.65-7.61 (m, 1H), 7.54-7.42 (m, 3H), 7.28-7.22 (m, 1H), 4.00 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 167.02, 140.3, 139.6, 137.1, 130.7, 130.3, 129.9, 129.6, 129.4, 129.3, 128.4, 127.9, 127.3, 124.4, 123.6, 123.1, 121.4, 119.4, 111.4, 109.7, 52.3; **HRMS [M+H]$^+$**: calcd for $C_{23}H_{17}N_2O_2$ 353.1285, found 353.1276.



12-(4-Chlorophenyl)indolo[1,2-*c*]quinazoline (10h)

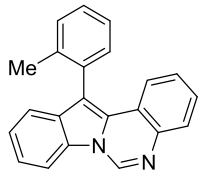
Off-white powder, **yield**: 52%, mp: 236-237 °C; **IR (KBr):** 3048, 2921, 1619, 1474 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.03(s, 1H), 7.97 (d, *J* = 7.2 Hz, 1H), 7.77 (t, *J* = 8.2 Hz, 2H), 7.60-7.40 (m, 8H), 7.26-7.22 (m, 1H); **^{13}C NMR ($CDCl_3$):** δ 140.2, 137.1, 133.6, 132.9, 132.0, 130.1, 129.4, 129.3, 129.1, 128.3, 127.7, 127.3, 124.3, 123.5, 123.0, 121.5, 119.4, 111.1, 109.7; **HRMS [M+H]$^+$**: calcd for $C_{21}H_{14}ClN_2$ 329.0840, found 329.0839.



12-(4-Fluoro-3-methylphenyl)indolo[1,2-*c*]quinazoline (10i)

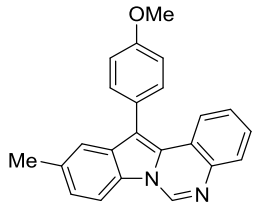
Pale yellow powder, **yield**: 65%, mp: 165-166 °C; **IR (KBr):** 3034, 2943, 1625, 1445 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.02 (s, 1H), 7.95 (d, *J* = 7.4 Hz, 1H), 7.75 (t, *J* = 8.4 Hz, 2H), 7.59-7.54 (m, 1H), 7.48-7.30 (m, 5H), 7.27-7.14 (m, 2H), 2.37 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 161.0 (d, J_{CF} = 244 Hz), 140.2, 137.2, 133.6 (d, J_{CF} =5 Hz),130.4, 129.9 (d, J_{CF} = 4 Hz),

129.6, 129.4, 128.9, 128.2, 127.6, 127.2, 125.6 (d, J_{CF} = 17 Hz), 124.1, 123.6, 122.9, 121.8, 119.6, 115.7 (d, J_{CF} = 23 Hz), 111.6, 109.7, 14.7; **^{19}F NMR ($CDCl_3$):** δ -118.7; **HRMS [M+H]$^+$**: calcd for $C_{22}H_{16}FN_2$, 327.1292, found 327.1297.



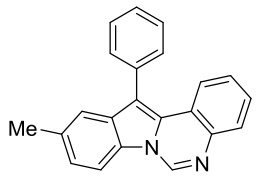
12-(*o*-Tolyl)indolo[1,2-*c*]quinazoline (10j)

Beige powder, **yield**: 56%, mp: 195-196 °C; **IR (KBr):** 3055, 3014, 1617, 1604, 1469, 1449 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.00 (s, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.41-7.25 (m, 9H), 7.16-7.10 (m, 1H), 2.02 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 140.0, 138.3, 137.3, 135.4, 133.5, 131.3, 130.5, 130.2, 129.1, 128.8, 128.2, 128.0, 127.5, 126.4, 124.1, 123.5, 122.8, 122.1, 119.9, 111.4, 109.6, 20.0; **HRMS [M+H]$^+$**: calcd for $C_{22}H_{17}N_2$ 309.1386, found 309.1384.



12-(4-Methoxyphenyl)-10-methylindolo[1,2-*c*]quinazoline (10k)

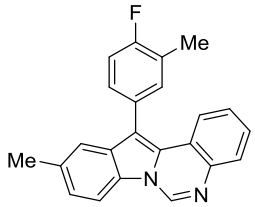
Pale yellow powder, **yield**: 63%**,** mp: 177-178 °C**; IR (KBr):** 2930, 2858, 2828, 1614, 1556, 1455 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.01 (s, 1H), 8.86 (d, *J* = 8.4 Hz, 1H), 7.84-7.75 (m, 2H), 7.52 (d, *J* = 8.6 Hz, 2H), 7.49-7.41 (m, 1H), 7.39 (s, 1H), 7.30-7.20 (m, 2H), 7.14 (d, *J* = 8.6 Hz, 2H), 3.96 (s, 3H), 2.51 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 159.2, 140.1, 137.3, 133.9, 131.8, 130.9, 128.7, 128.0, 127.7, 127.6, 127.1, 126.5, 124.4, 123.6, 122.0, 119.3, 114.5, 111.8, 109.2, 55.4, 21.7; **HRMS [M+H]$^+$**: calcd for $C_{23}H_{19}N_2O$ 339.1492, found 339.1493.



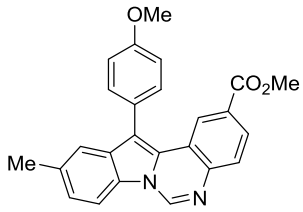
10-Methyl-12-phenylindolo[1,2-*c*]quinazoline (10l)

Off-white powder, **yield**: 72%, mp: 173-174 °C; **IR (KBr):** 3056, 2921, 2853, 1740, 1599,1450 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 8.94 (s, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.55-7.46 (m, 4H), 7.45-7.34 (m, 2H), 7.30 (s, 1H), 7.21-7.09 (m, 2H), 2.41 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 140.2, 137.3, 134.5, 134.0, 130.71, 130.68, 129.0, 128.8, 128.1,

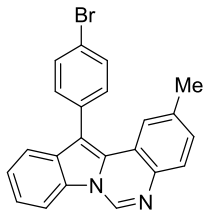
127.8, 127.7, 127.6, 127.1, 124.5, 123.7, 121.9, 119.2, 112.1, 109.2, 21.7; **HRMS [M+H]$^+$**: calcd for $C_{22}H_{17}N_2$ 309.1386, found 309.1392.



12-(4-Fluoro-3-methylphenyl)-10-methylindolo[1,2-*c*]quinazoline (10m)
Pale yellow powder, **yield**: 76%, mp: 170-171 °C; **IR (KBr):** 3058, 2922, 1639, 1445 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.01 (s, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.44-7.33 (m, 3H), 7.32-7.18 (m, 3H), 2.52 (s, 3H), 2.42 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 161.0 (d, J_{CF} = 245 Hz), 140.1, 137.3, 134.0, 133.6 (d, J_{CF} = 5 Hz), 130.7, 130.0 (d, J_{CF} = 4 Hz), 129.64, 129.56, 128.8, 128.2, 127.7, 121.1, 125.6 (d, J_{CF} = 17 Hz), 124.5, 123.5, 121.8, 119.1, 115.7 (d, J_{CF} = 23 Hz), 111.2, 109.3, 21.8, 14.8 (d, J_{CF} = 3 Hz); **^{19}F NMR ($CDCl_3$):** δ -118.7; **HRMS [M+H]$^+$**: calcd for $C_{23}H_{18}FN_2$ 341.1449, found 341.1448.

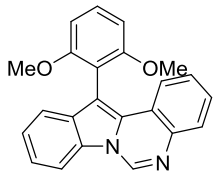


Methyl 12-(4-methoxyphenyl)-10-methylindolo[1,2-c]quinazoline-2-carboxylate (10n)
Beige powder, **yield**: 60%, mp: 187.0-188 °C; **IR (KBr):** 3400, 2935, 1634, 1450 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.04 (s, 1H), 8.55 (d, *J* = 1.7 Hz, 1H), 8.07 (dd, J_1 = 8.4, J_2 = 1.7 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.54 (dd, J_1 = 8.7, J_2 = 1.9 Hz, 2H), 7.44 (s, 1H), 7.31 (dd, J_1 = 8.4, J_2 = 0.9 Hz, 1H), 7.17 (d, *J* = 8.7 Hz 1H), 3.97 (s, 3H), 3.85 (s, 3H), 2.52 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 166.3, 159.4, 143.3, 138.9, 134.3, 131.5, 130.8, 129.2, 128.2, 128.0, 127.8, 126.9, 125.7, 125.4, 124.9, 121.8, 119.5, 114.6, 113.0, 109.3, 55.4, 52.1, 21.7; **HRMS [M+H]$^+$**: calcd for $C_{25}H_{21}N_2O_3$ 397.1547, found 397.1556.



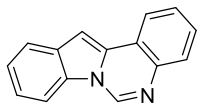
12-(4-Bromophenyl)-2-methylindolo[1,2-*c*]quinazoline (10o)

Light brown powder, **yield**: 58%, mp: 221-222 °C; **IR (KBr):** 3056, 2922, 1620, 1559, 1469, 1221 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 8.95 (s, 1H), 7.91 (d, *J* = 7.3 Hz, 1H), 7.64-7.58 (m, 3H), 7.58-7.49 (m, 2H), 7.46-7.32 (m, 4H), 7.24 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 2.23 (s, 3H); **^{13}C NMR ($CDCl_3$):** 138.1, 137.4, 136.5, 133.5, 132.3, 132.1, 130.4, 130.0, 129.5, 128.2, 127.7, 124.2, 123.6, 123.0, 121.7, 121.3, 119.4, 110.8, 109.7, 21.7; **HRMS $[M+H]^+$**: calcd for $C_{22}H_{16}BrN_2$ 387.0491, found 387.0492.



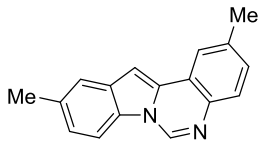
12-(2,6-Dimethoxyphenyl)indolo[1,2-*c*]quinazoline (10p)

Off-white powder, **yield**: 12%, mp: 210-211 °C; **IR (KBr):** 3022**,** 2925, 1618, 1470(cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.07 (s, 1H), 7.98 (d, *J* = 7.3 Hz, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.59 (dd, J_1 = 8.1 Hz, J_2 = 0.9 Hz, 1H), 7.50-7.34 (m, 5H), 7.26-7.21 (m, 1H), 6.78 (d, *J* = 8.4 Hz, 2H), 3.66 (s, 6H); **^{13}C NMR ($CDCl_3$):** δ 159.1, 140.0, 137.4, 130.2, 129.71, 129.70, 128.67, 128.4, 127.5, 127.0, 123.9, 123.7, 122.7, 122.2, 120.5, 111.1, 109.6, 104.3, 103.7, 55.9; **HRMS $[M+H]^+$**: calcd for $C_{23}H_{19}N_2O_2$ 355.1441, found 355.1436.



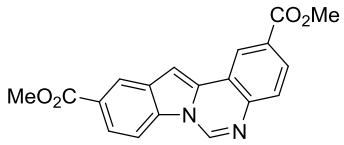
Indolo[1,2-*c*]quinazoline (13a)

White powder, **yield**: 86%, mp: 205-206 °C; **IR (KBr):** 2922, 1593, 1458 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.0 (s, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.86-7.78 (m, 2H), 7.60-7.38 (m, 4H), 7.12 (s, 1H); **^{13}C NMR ($CDCl_3$):** δ 139.4, 137.0, 132.9, 130.3, 129.7, 129.1, 128.1, 127.7, 124.1, 123.1, 122.2, 121.3, 120.9, 109.9, 94.7 **HRMS $[M+H]^+$**: calcd for $C_{15}H_{11}N_2$ 219.0917, found 219.0918.



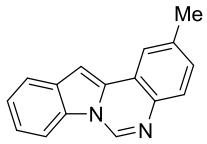
2,10-Dimethylindolo[1,2-*c*]quinazoline (13b)

Light brown powder, **yield**: 87%, mp: 202.0-203.3 °C; **IR (KBr):** 2922, 1540, 1370 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 8.86 (s, 1H), 7.77-7.71 (m, 2H), 7.61 (d, J = 8.2 Hz, 1H), 7.51 (s, 1H), 7.27 (dd, J_1 = 8.2 Hz, J_2 = 1.5 Hz, 1H), 7.14 (dd, J_1 = 8.4 Hz, J_2 = 1.1 Hz, 1H), 6.93 (s, 1H), 2.47 (s, 3H), 2.45 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 137.6, 137.4, 136.5, 133.7, 133.1, 130.3, 130.0, 128.7, 127.9, 123.7, 123.0, 121.1, 120.5, 109.5, 93.9, 21.8, 21.6; **HRMS [M+H]$^+$**: calcd for $C_{17}H_{15}N_2$ 247.1230, found 247.1230.



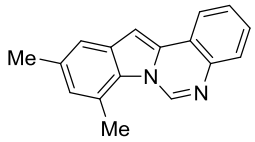
Dimethyl indolo[1,2-*c*]quinazoline-2,10-dicarboxylate (13c)

Yellow powder, **yield**: 81%, mp: 207-208 °C; **IR (KBr):** 2916, 1701, 1386 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.01 (s, 1H), 8.69 (d, J = 1.8 Hz, 1H), 8.53 (d, J = 1.0 Hz, 1H), 8.14 (dd, J_1 = 8.4 Hz, J_2 = 1.8 Hz, 1H), 8.08 (dd, J_1 = 8.7 Hz, J_2 = 1.5 Hz, 1H), 7.93 (d, J = 8.7 Hz, 1H), 7.78 (d, J = 8.5 Hz, 1H), 7.26 (s, 1H), 3.95 (s, 3H), 3.93 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 167.3, 166.3, 142.6, 138.4, 133.5, 132.6, 130.2, 129.3, 129.28, 128.5, 126.4, 125.3, 123.9, 123.8, 121.0, 109.8, 96.7, 52.5, 52.2; **HRMS [M+H]$^+$**: calcd for $C_{19}H_{15}N_2O_4$ 335.1026, found 335.1022.



2-Methylindolo[1,2-*c*]quinazoline (13d)

Off-white powder, **yield**: 95%, mp: 145-146 °C; **IR (KBr):** 2916, 2857, 1617, 1488, 1376 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 8.89 (s, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.78-7.72 (m, 2H), 7.61 (d, J = 8.0 Hz, 1H), 7.39-7.26 (m, 3H), 7.01 (s, 1H), 2.45 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 137.8, 137.4, 136.4, 133.0, 130.4, 130.3, 129.7, 127.9, 123.9, 123.0, 122.1, 121.1, 120.9, 109.8, 94.3, 21.62; **HRMS [M+H]$^+$**: calcd for $C_{16}H_{13}N_2$ 233.1073, found 233.1073.



8,10-Dimethylindolo[1,2-*c*]quinazoline (13e)

Pale yellow powder, **yield**: 73%, mp: 196-197 °C; **IR (KBr):** 2926, 1460,1383 (cm^{-1}); **^{1}H NMR ($CDCl_3$):** δ 9.22 (s, 1H), 7.94 (dd, J_1 = 7.7 Hz, J_2 = 1.1 Hz, 1H), 7.68 (d, J = 8.1 Hz, 1H), 7.48-7.34 (m, 3H), 6.99 (s, 1H), 6.91 (s, 1H), 2.77 (s, 3H), 2.42 (s, 3H); **^{13}C NMR ($CDCl_3$):** δ 139.3, 138.8, 133.4, 133.2, 130.6, 128.9, 128.0, 127.7, 127.4, 127.0, 122.9, 122.2, 121.5, 118.3, 95.1, 21.4, 21.3; **HRMS [M+H]$^{+}$**: calcd for $C_{17}H_{15}N_2$ 247.1232, found 247.1230.

References

[1] (a) Cacchi, S.; Fabrizi, G.; Pace, P. *J. Org. Chem.* **1998**, *63*, 1001-1011; (b) Arcadi, A.; Cacchi, S.; Fabrizi, G.; Ghirga, F.; Goggiamani, A.; Iazzetti, A.; Marinelli, F. *Synthesis* **2018**, 50, 1133-1140.

[2] Arcadi, A.; Cacchi, S.; Fabrizi, G.; Ghirga, F.; Marinelli, F.; Parisi L. M. *Heterocycles.* **2004**, *64,* 475.

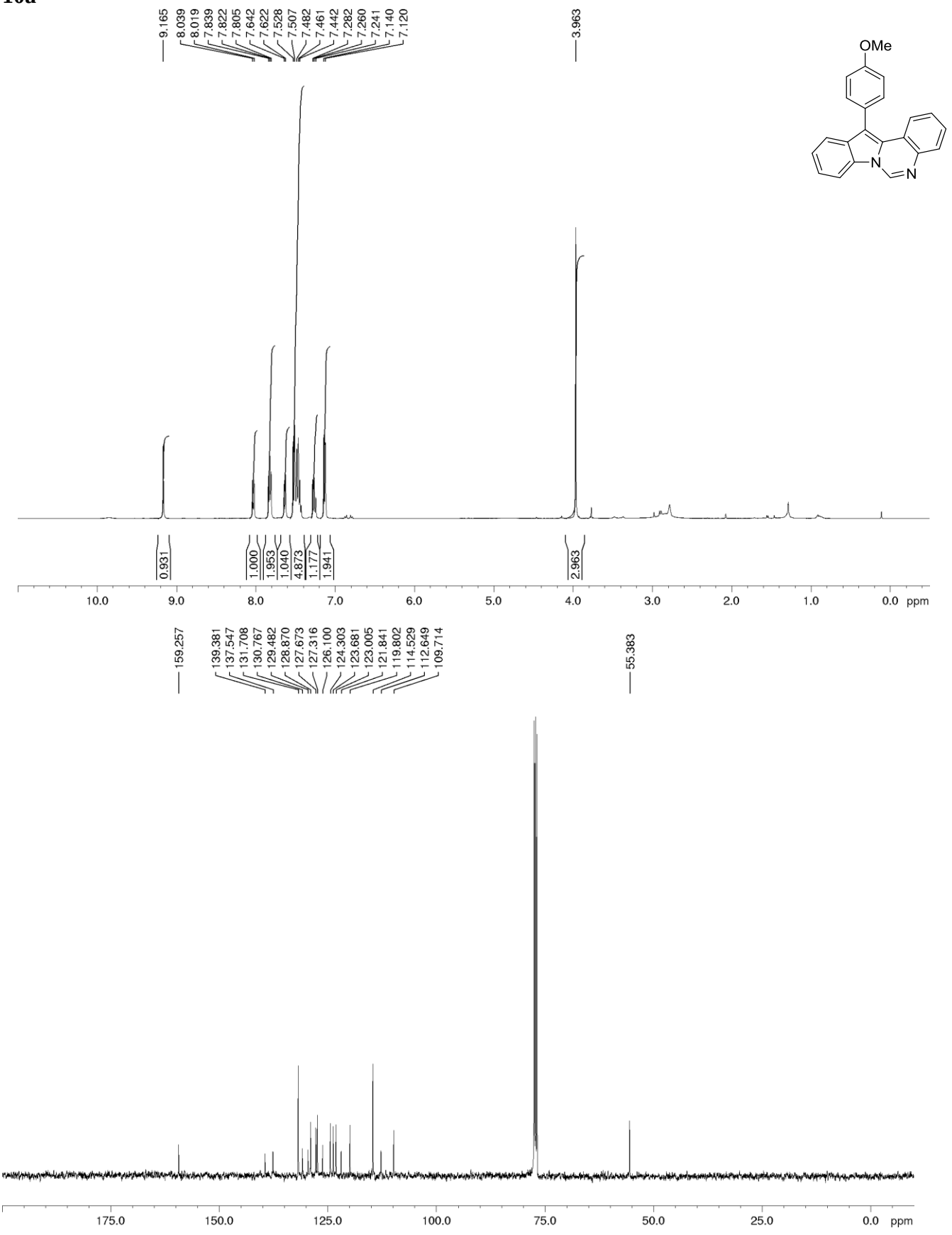
[3] Cacchi, S.; Fabrizi, G.; Pace, P. Marinelli, F. *Synlett* **1999**, 620.

[4] Kumar, K. S; Ramulu, M. S.; Rajesham, B.; Kumar, N. P.; Voorab, V.; Kanchab, R. K. *Org. Biomol. Chem*., **2017**,*15*, 4468.

[5] Nitin T. Patil, Rahul D. Kavthe, Vivek S. Raut, Vaddu V. N. Reddy *J. Org. Chem.* **2009**, 6315.

NMR Spectra

10a



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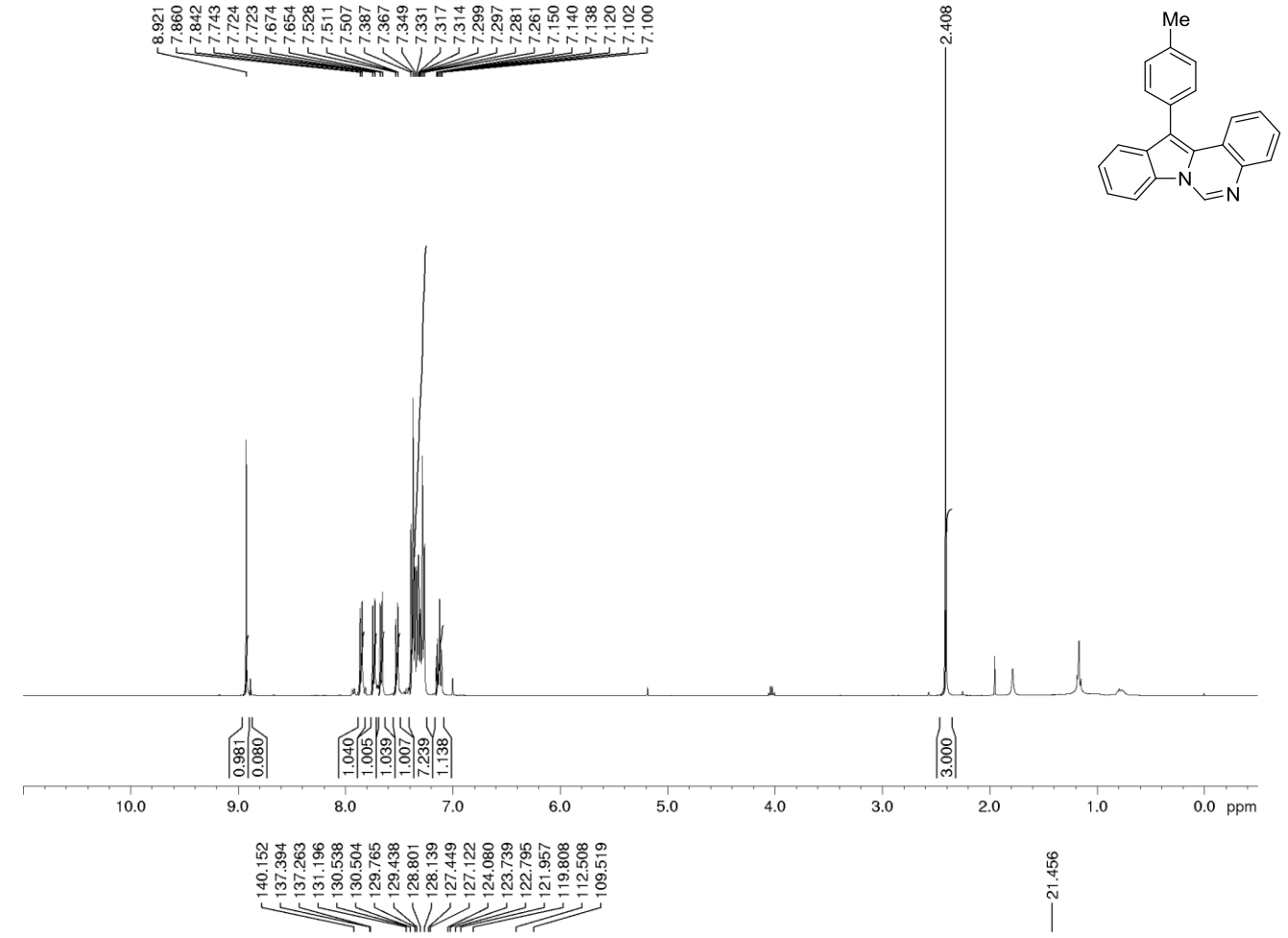
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7.507
7.387
7.367
7.349
7.331
7.317
7.314
7.299
7.297
7.281
7.261
7.150
7.140
7.138
7.120
7.102
7.100
2.408
Me
N
N
0.981
0.080
1.040
1.005
1.039
1.007
7.239
1.138
3.000
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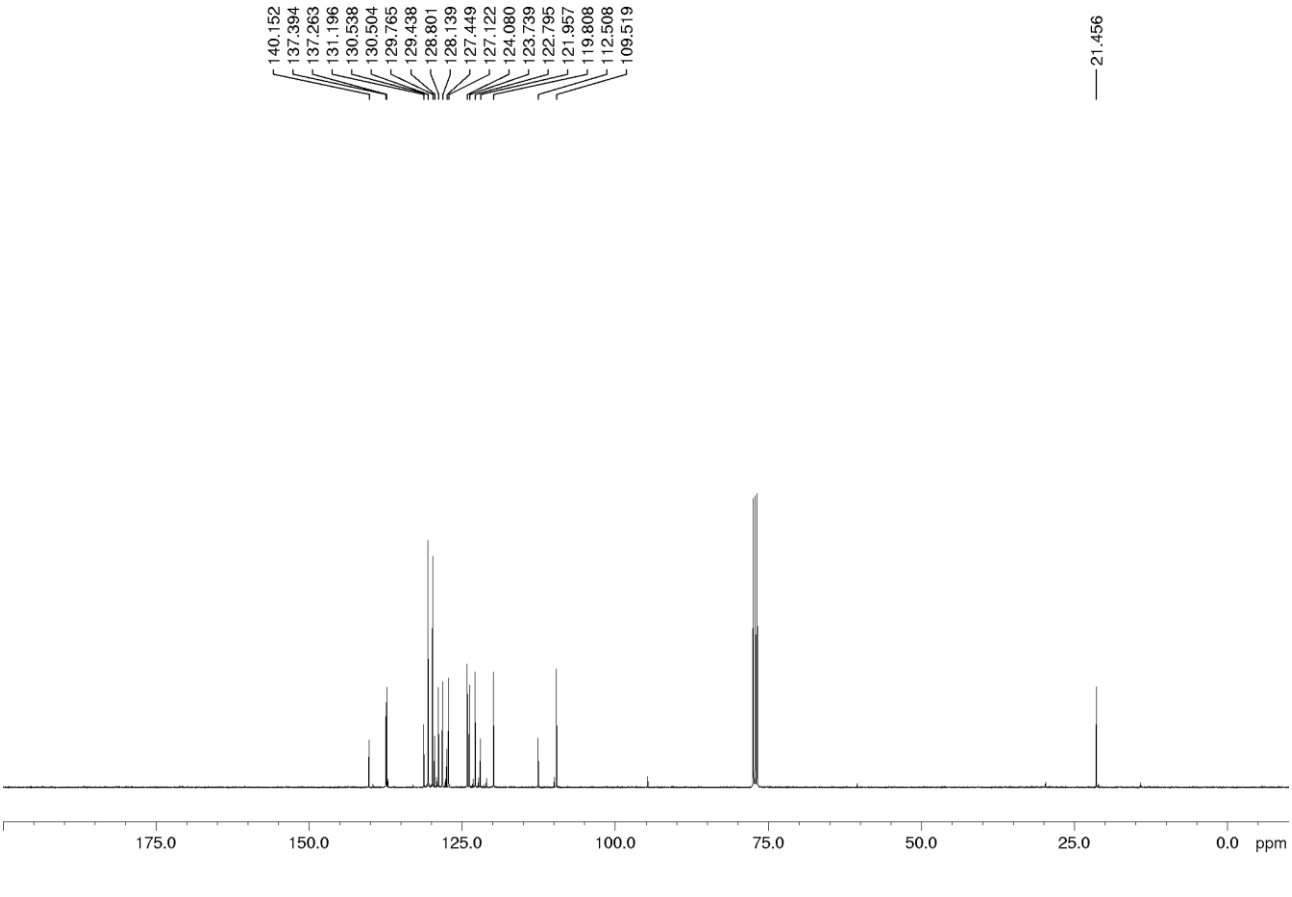
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm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128.139
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124.080
123.739
122.795
121.957
119.808
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21.456
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125.0
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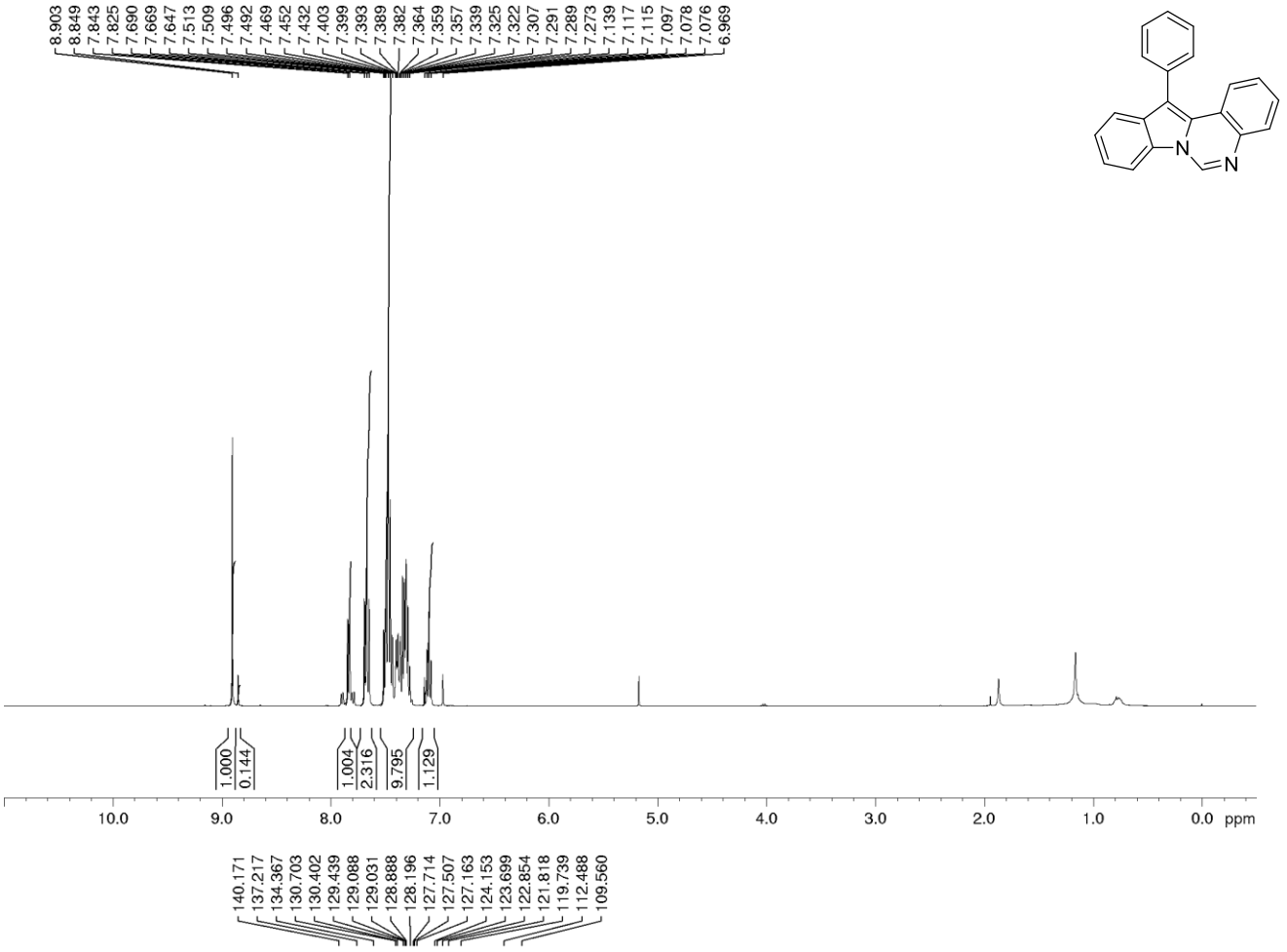
75.0
50.0
25.0
0.0 ppm

10c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7.513
7.509
7.496
7.492
7.469
7.452
7.432
7.403
7.399
7.393
7.389
7.382
7.364
7.359
7.357
7.339
7.325
7.322
7.307
7.291
7.289
7.273
7.139
7.117
7.115
7.097
7.078
7.076
6.969
1.000
0.144
1.004
2.316
9.795
1.129
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9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm

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134.367
130.703
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129.439
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129.031
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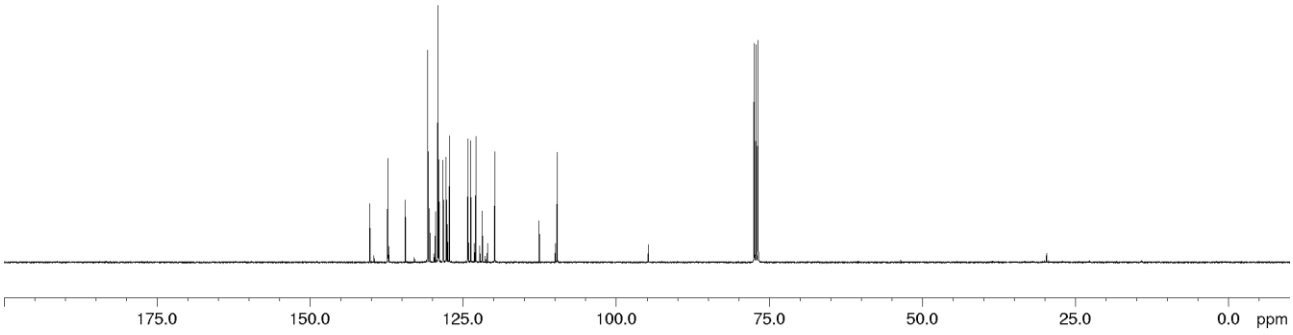
109.560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10d


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7.505
7.452
7.449
7.432
7.414
7.406
7.401
7.393
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7.283
7.280
7.272
7.235
7.232
7.215
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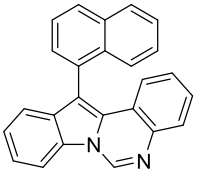
6.956
6.938
6.920
6.918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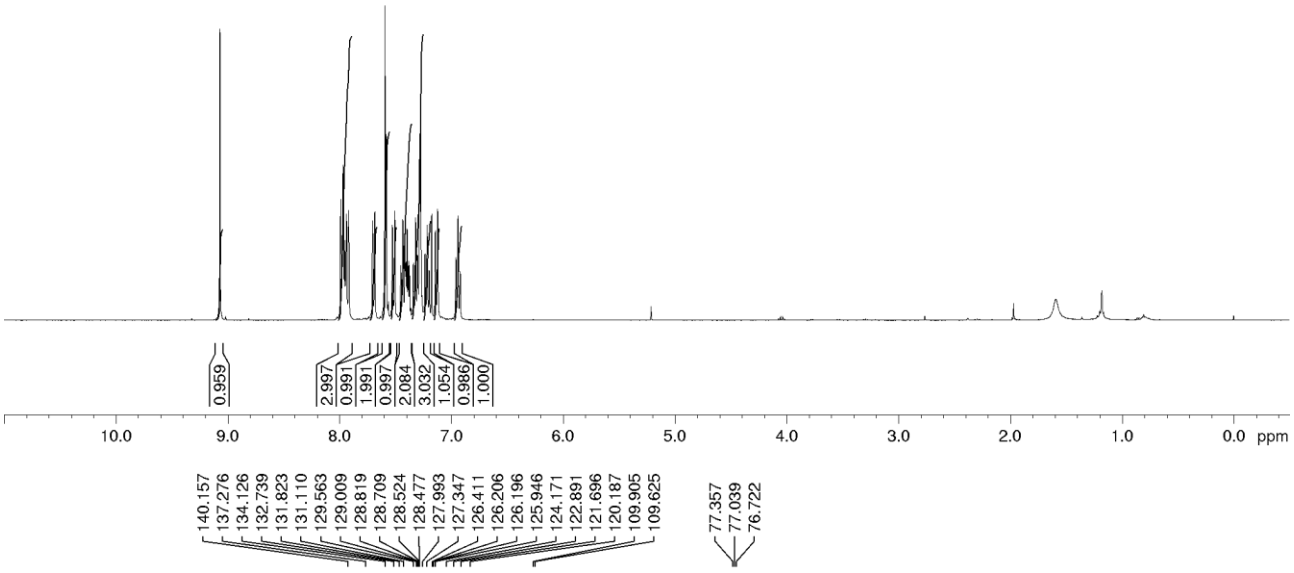
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127.347
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126.196
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109.625

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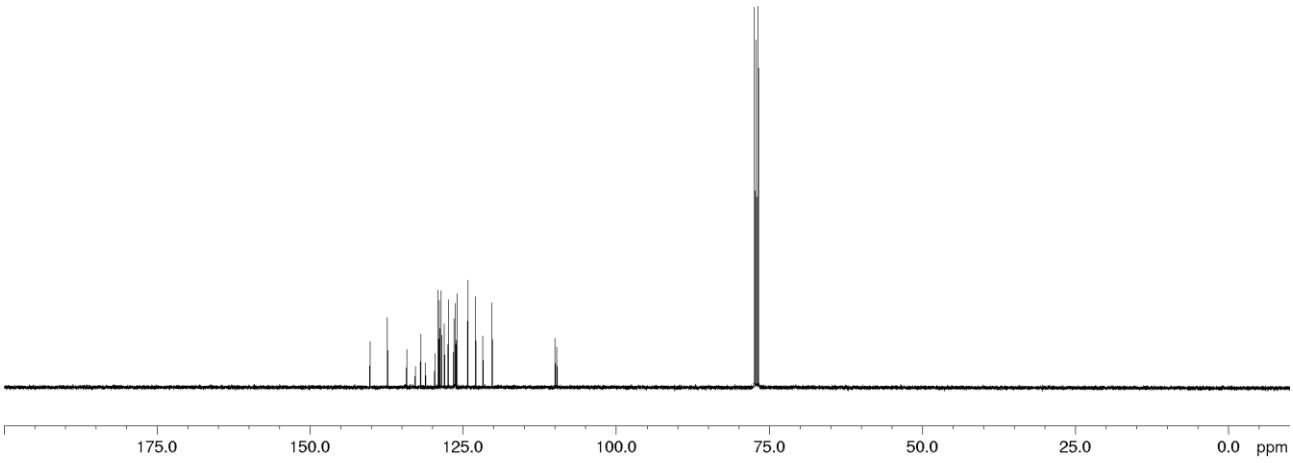
77.039
76.722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0.0 ppm

10e


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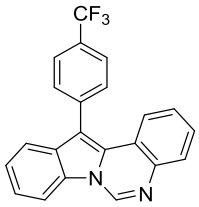
7.180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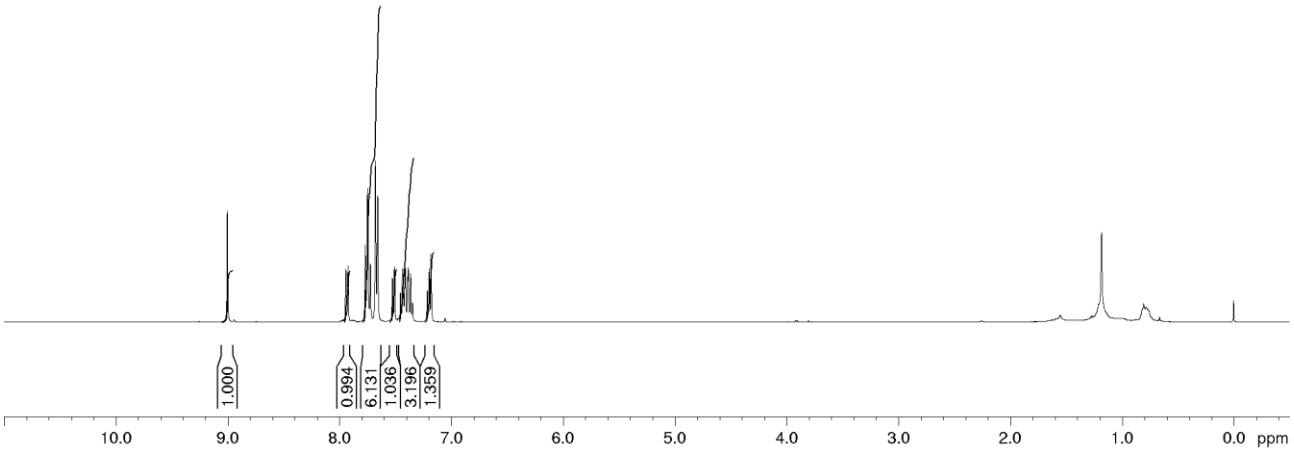
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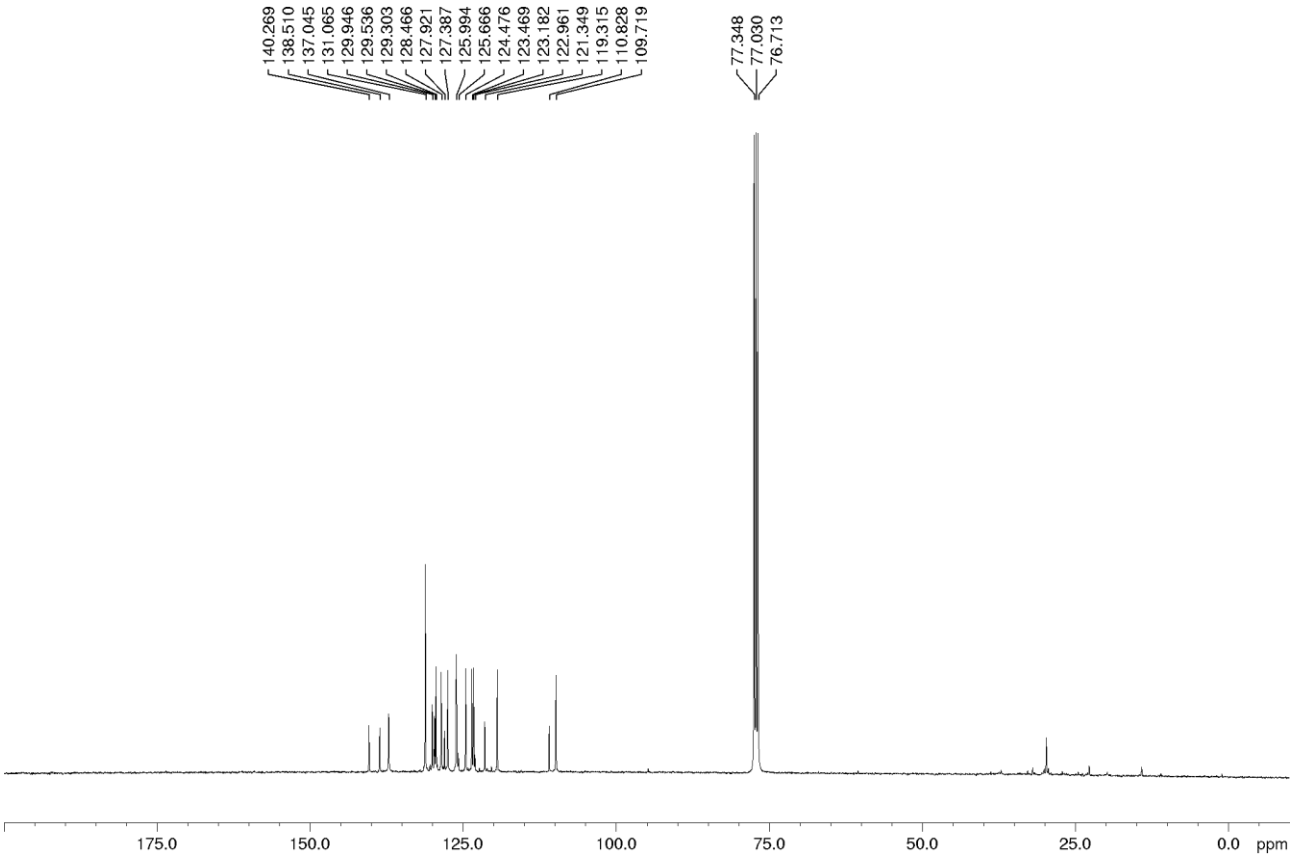
0.0 ppm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123.469
123.182
122.961
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119.315
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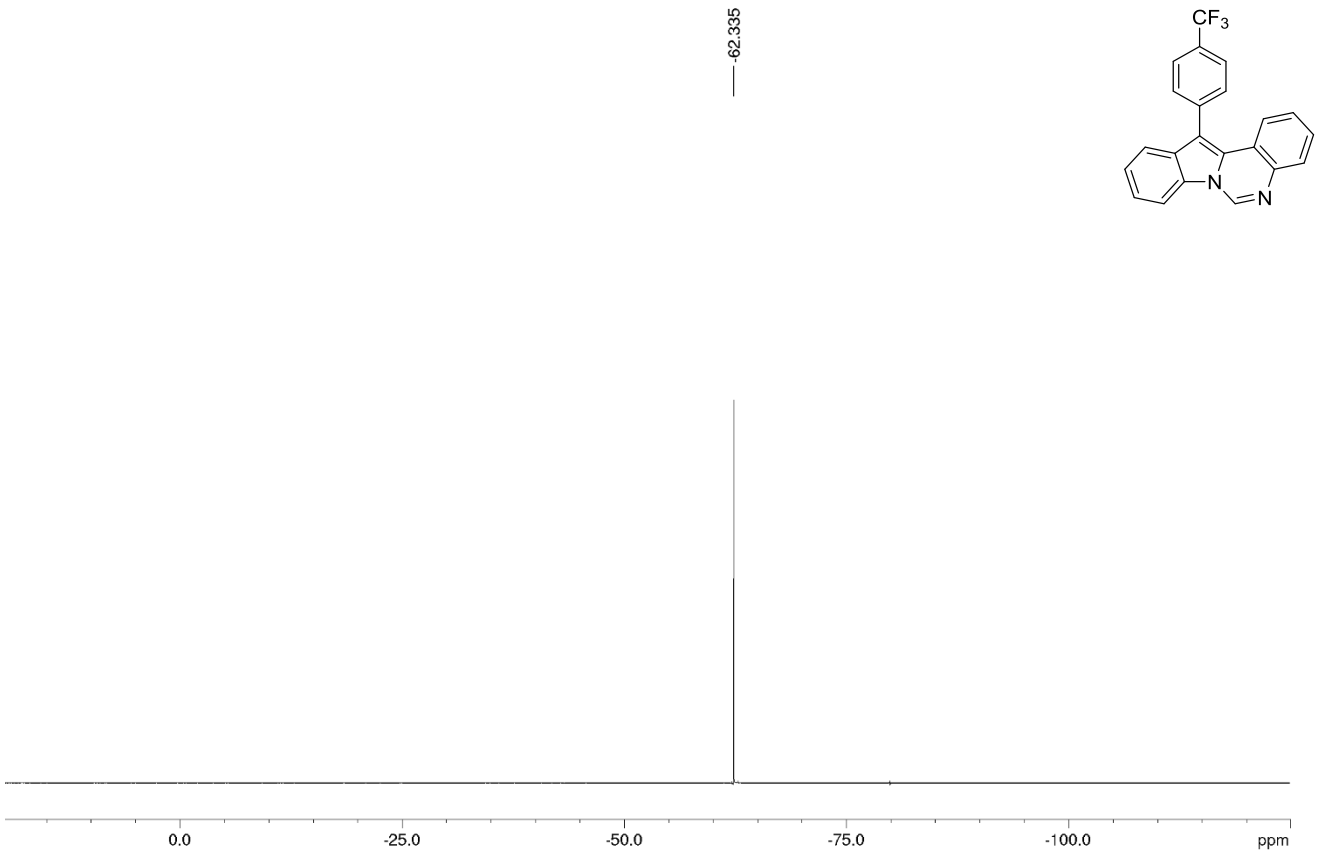
10e



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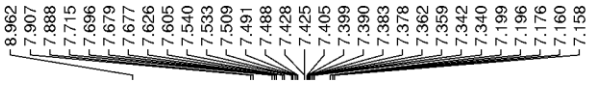
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7.540
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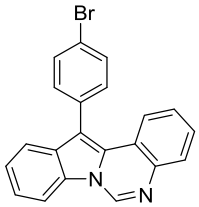
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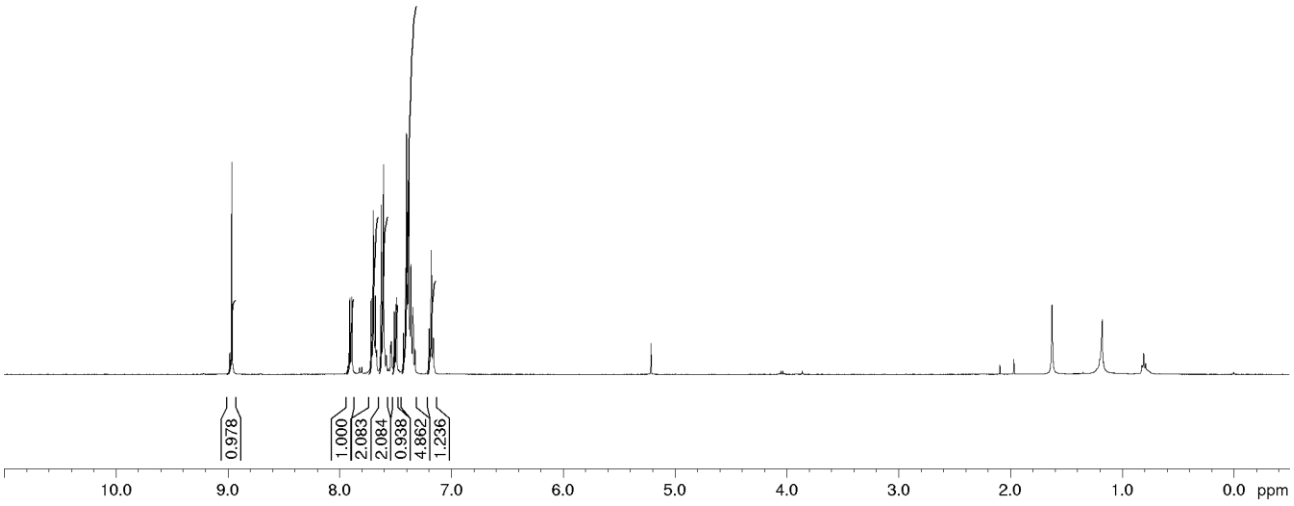
N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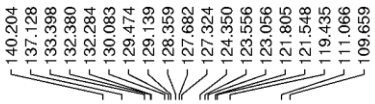
0.0 ppm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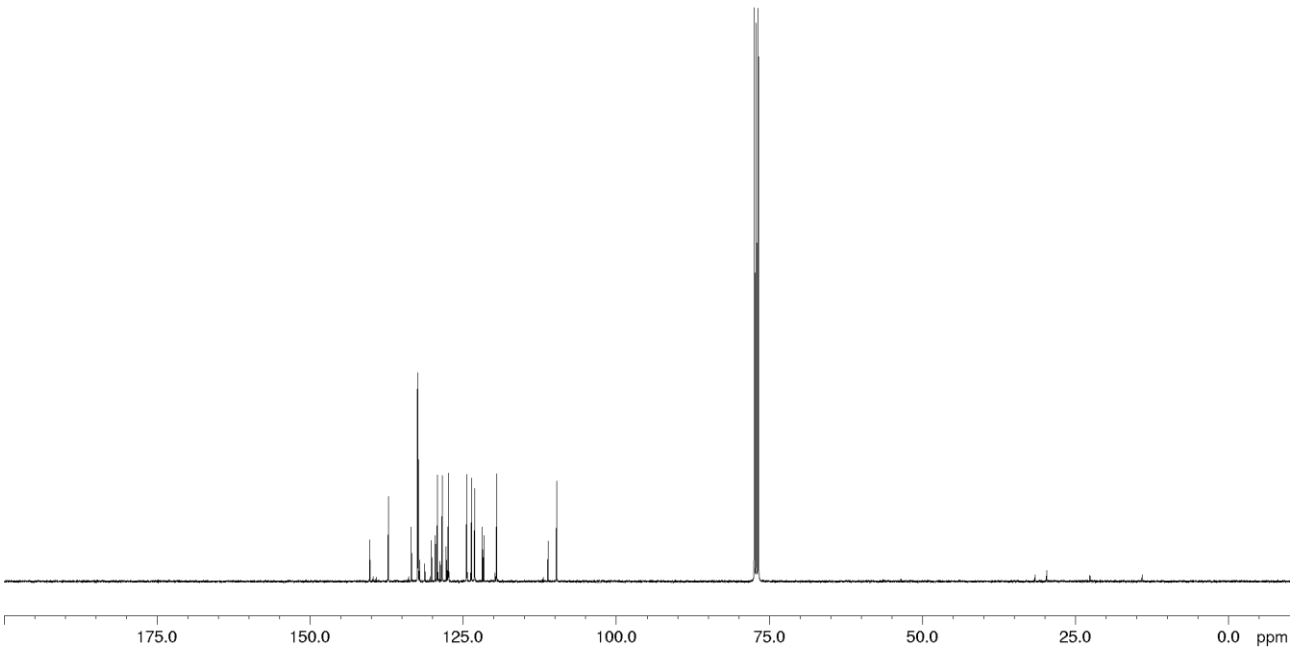
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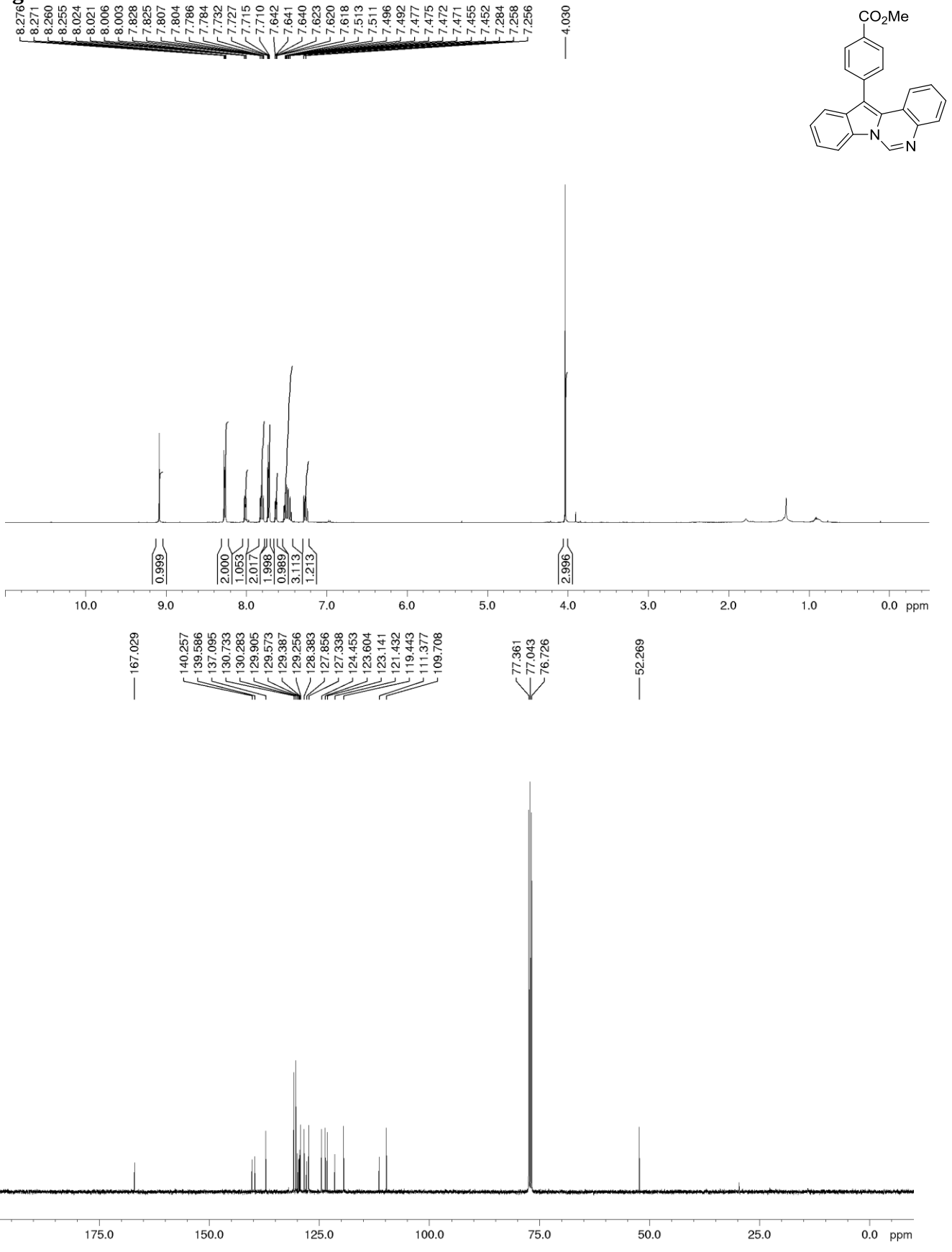
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7.825
7.807
7.804
7.786
7.784
7.732
7.727
7.715
7.710
7.642
7.641
7.640
7.623
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7.618
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7.511
7.496
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7.471
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7.284
7.258
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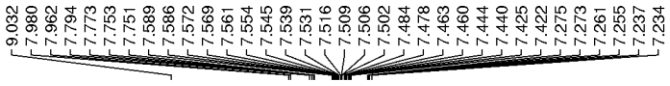
10h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7.545
7.539
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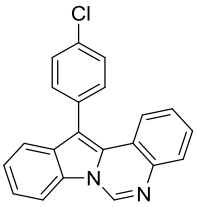
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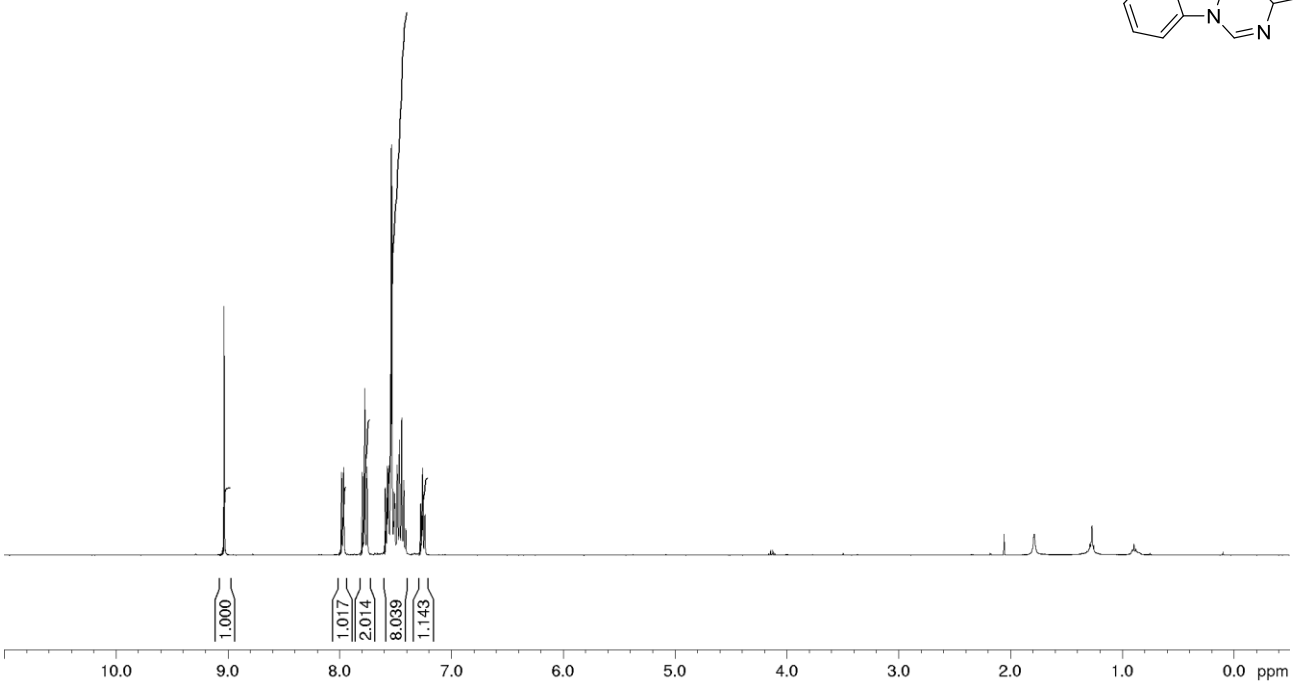
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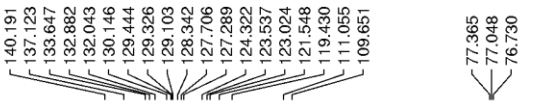
0.0 ppm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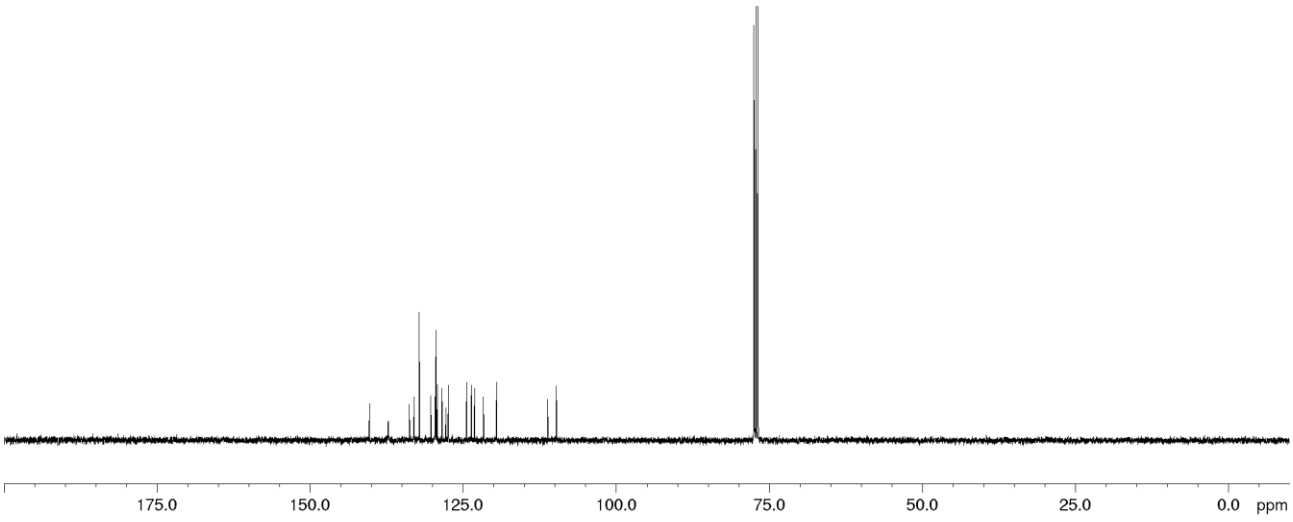
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0.0 ppm

10i


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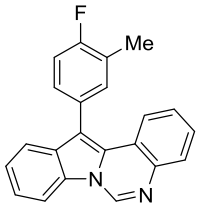
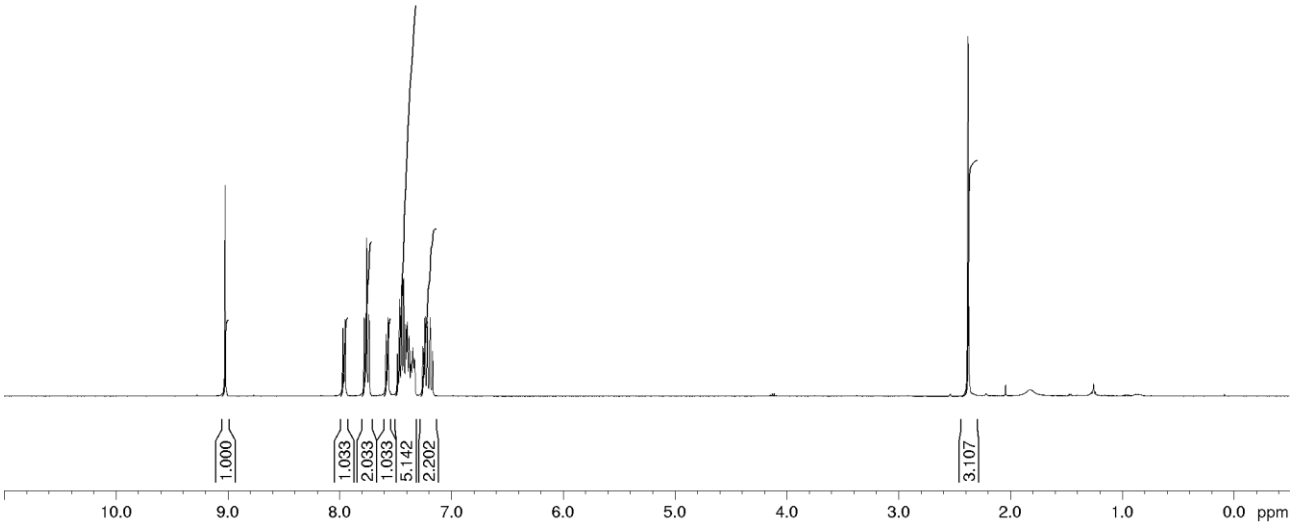
2.377


F
Me
N
N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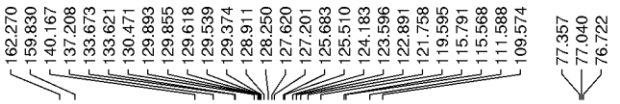
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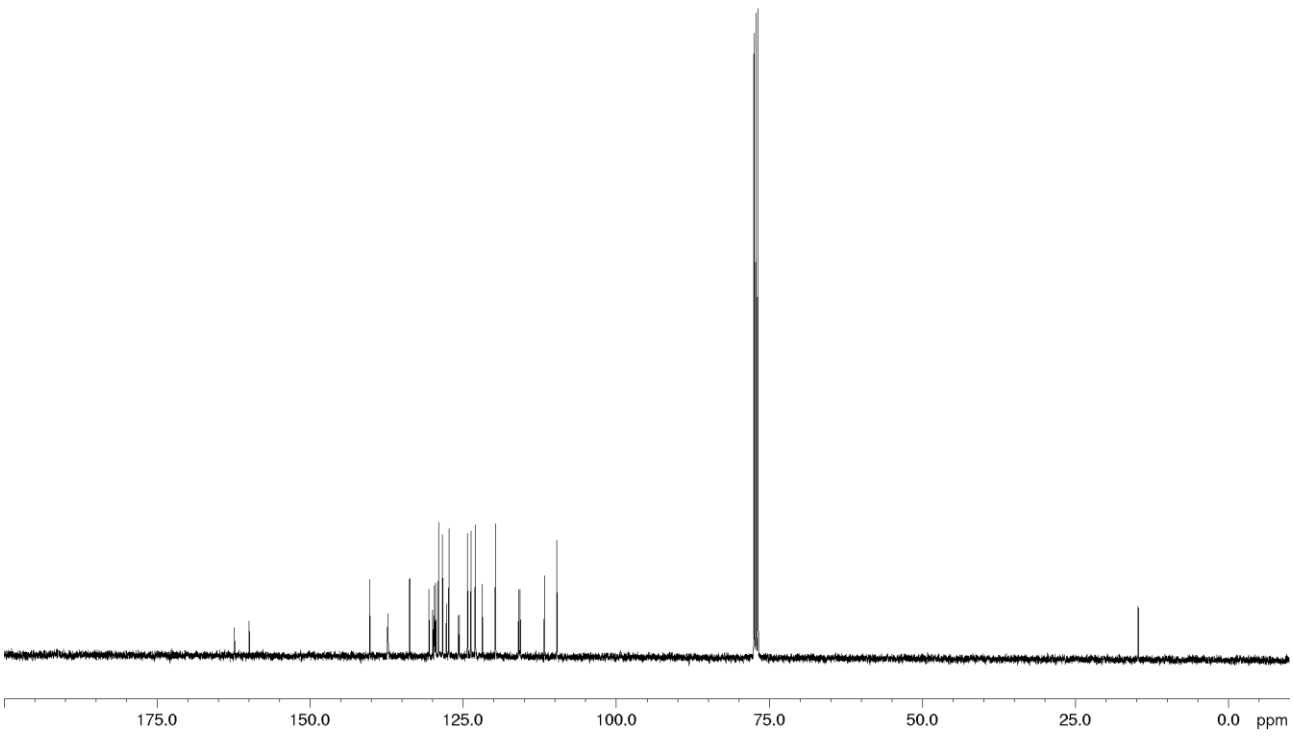
14.704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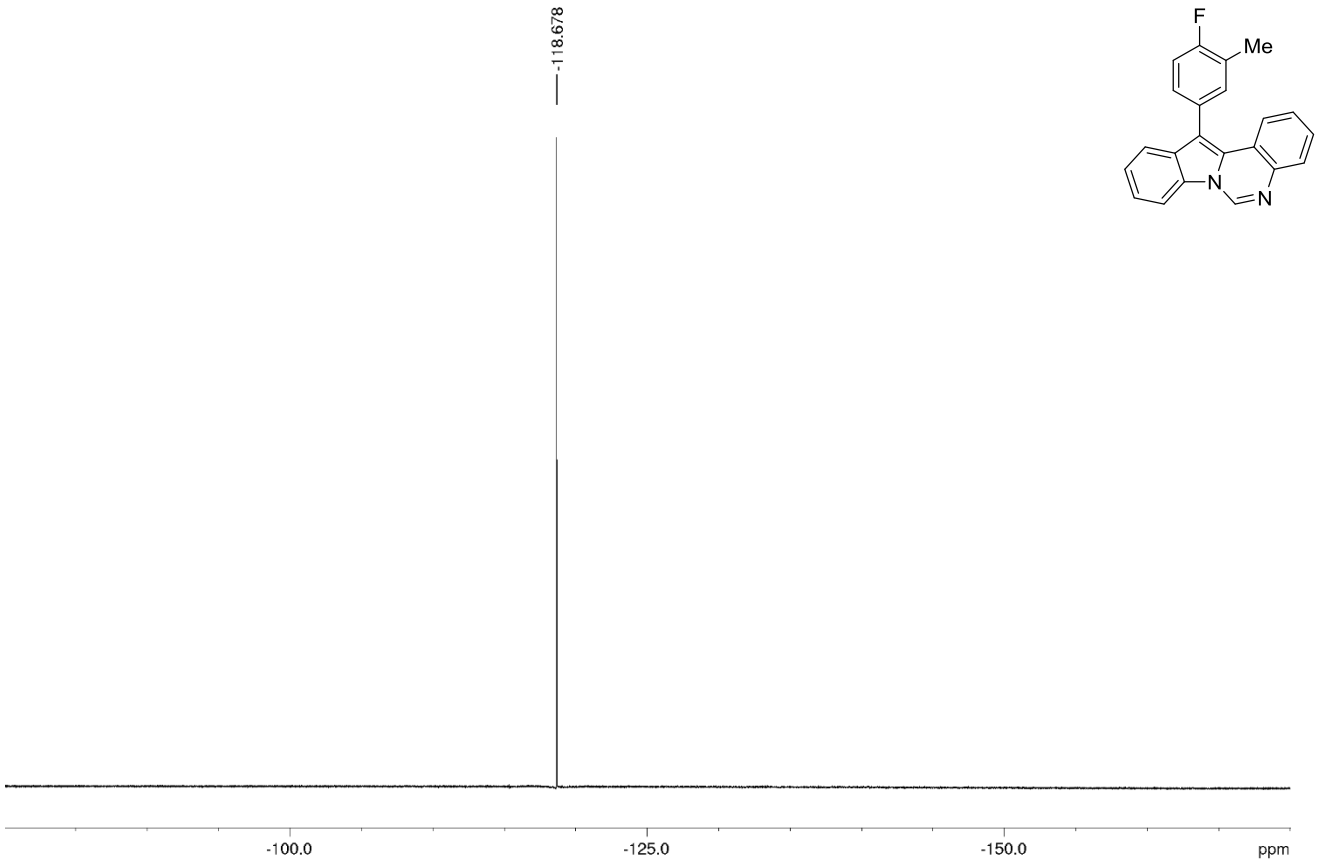
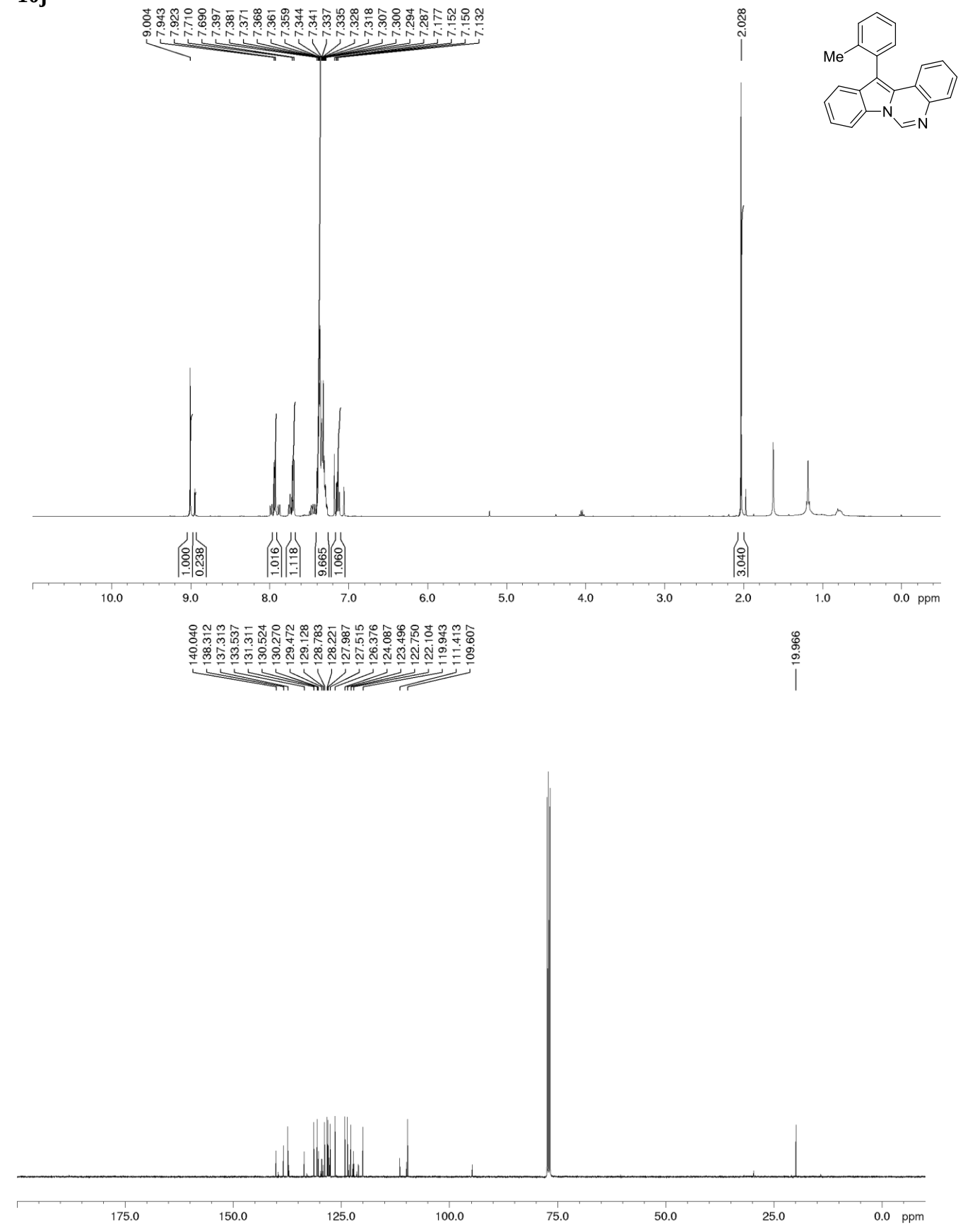
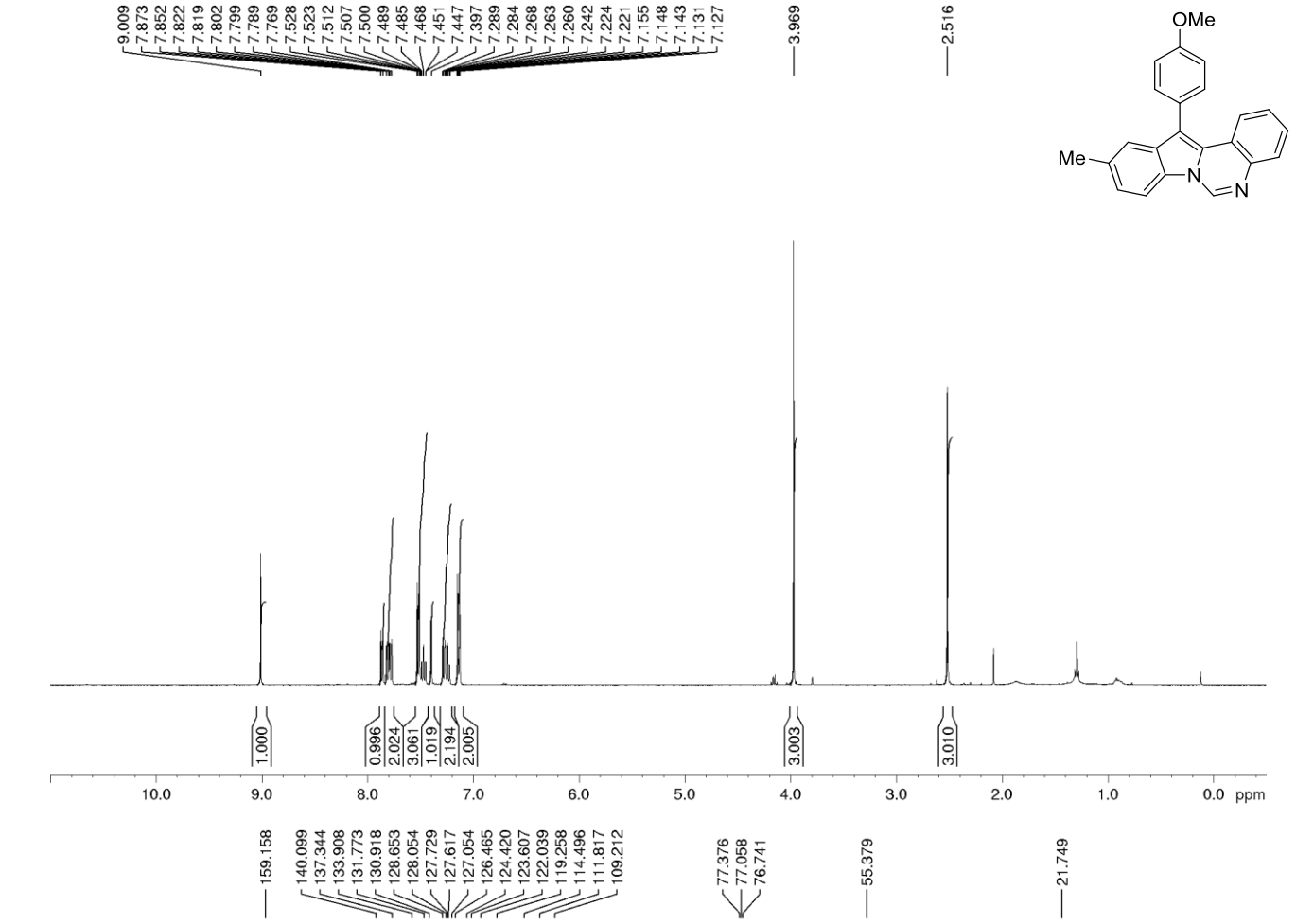
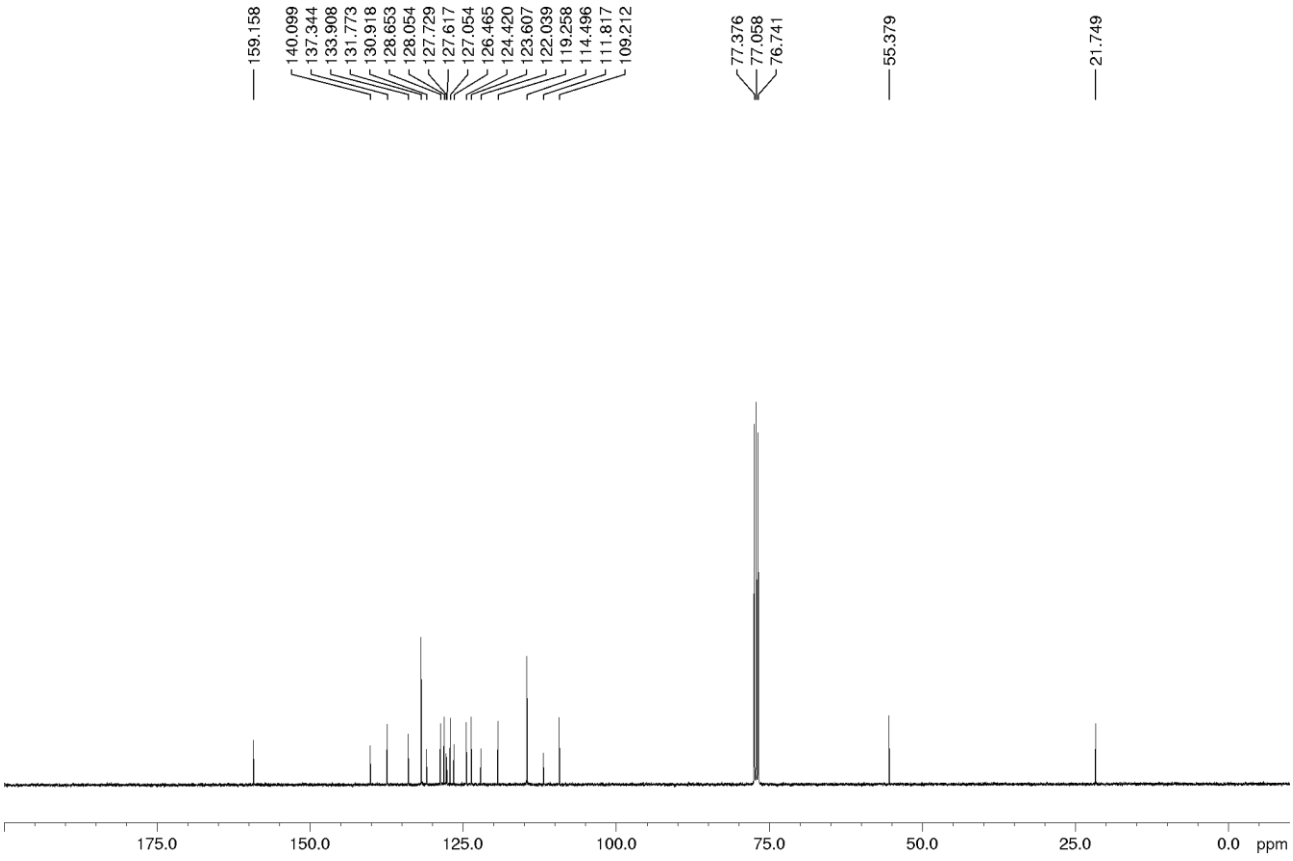


10j

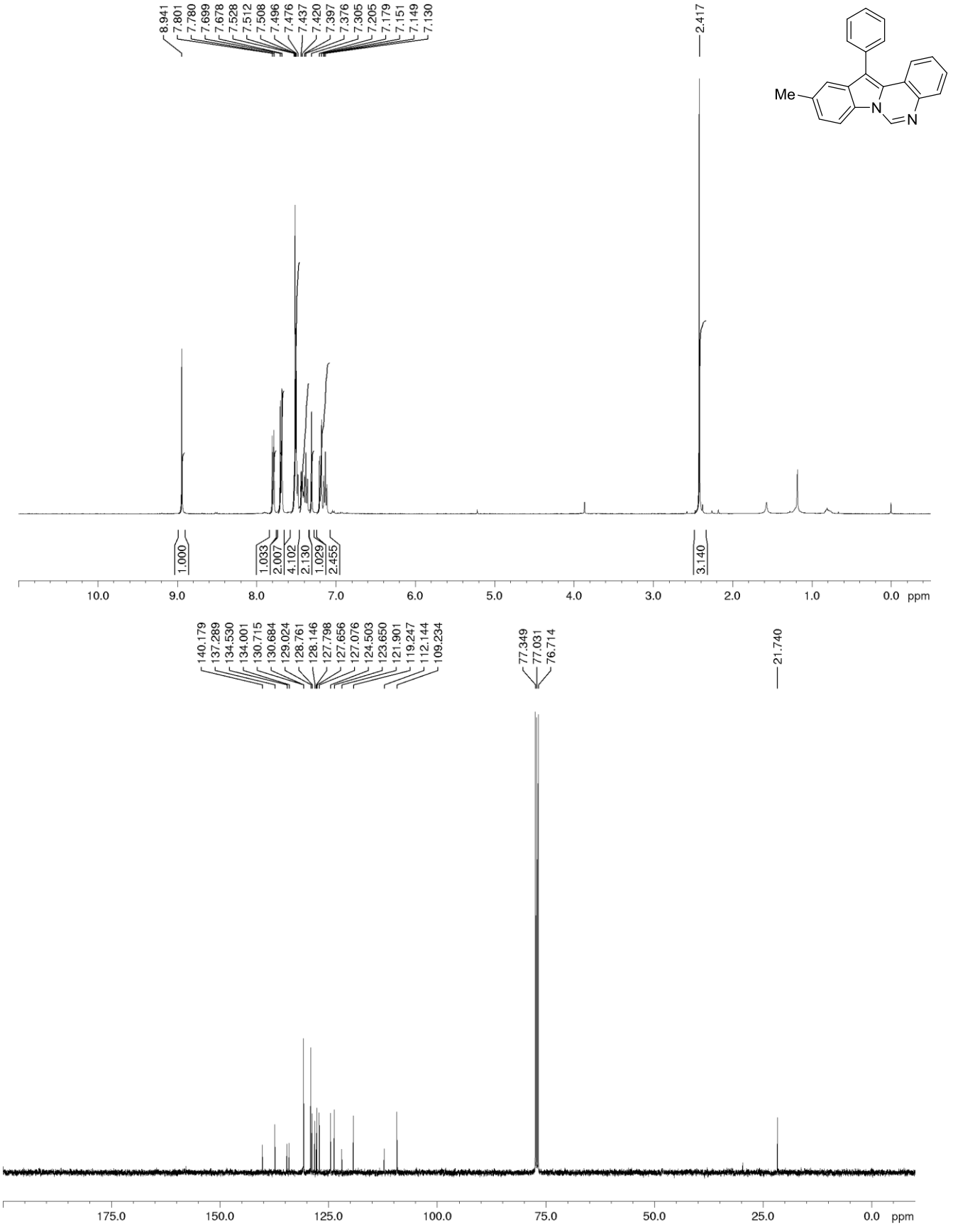

9.004
7.943
7.923
7.710
7.690
7.397
7.381
7.371
7.368
7.361
7.359
7.344
7.341
7.337
7.335
7.328
7.318
7.307
7.300
7.294
7.287
7.177
7.152
7.150
7.132
2.028
Me
N
N
1.000
0.238
1.016
1.118
9.665
1.060
3.040
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm
140.040
138.312
137.313
133.537
131.311
130.524
130.270
129.472
129.128
128.783
128.221
127.987
127.515
126.376
124.087
123.496
122.750
122.104
119.943
111.413
109.607
19.966
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0 ppm

10k

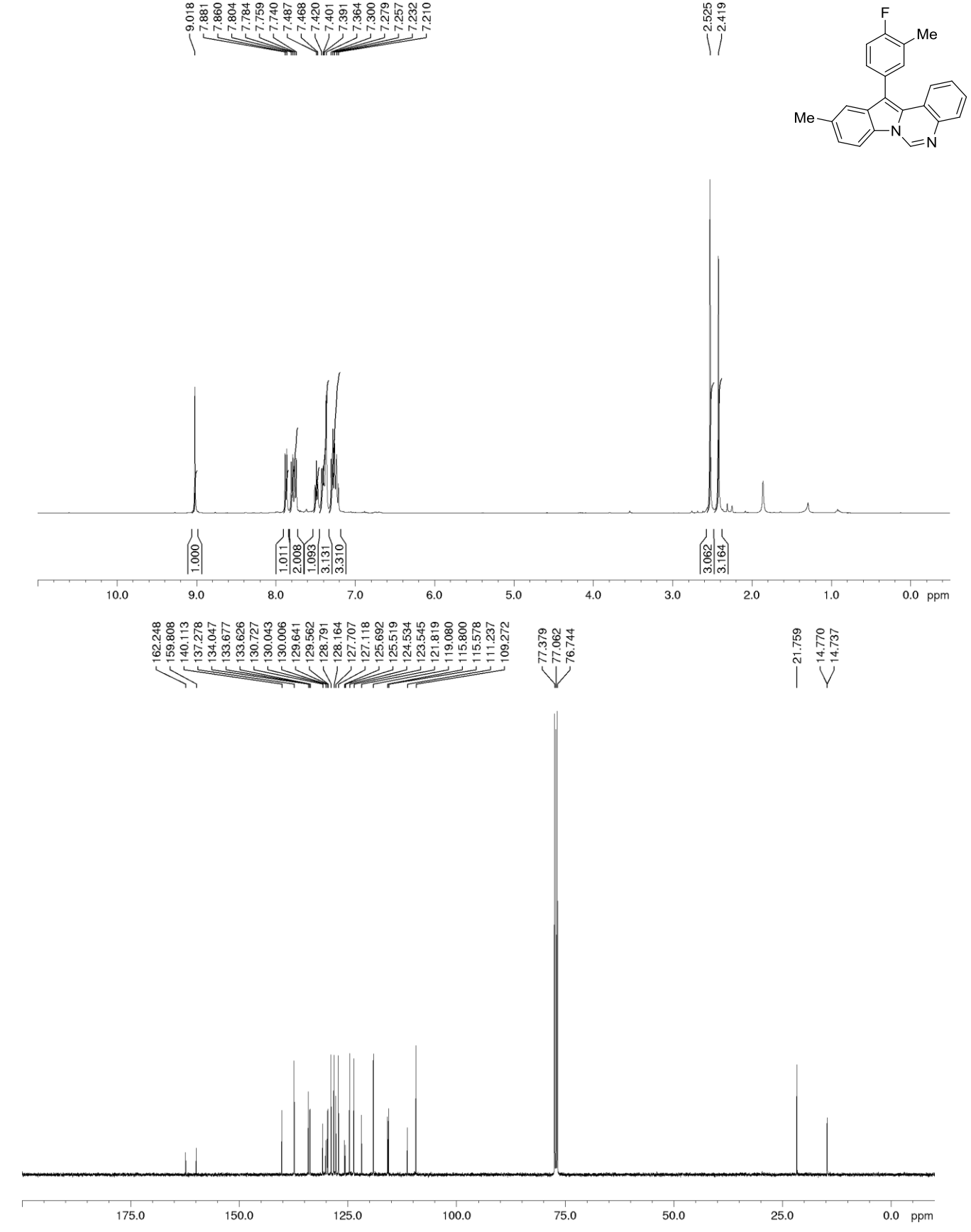

9.009
7.873
7.852
7.822
7.819
7.802
7.799
7.789
7.769
7.528
7.523
7.512
7.507
7.500
7.489
7.485
7.468
7.451
7.447
7.397
7.289
7.284
7.268
7.263
7.260
7.242
7.224
7.221
7.155
7.148
7.143
7.131
7.127
3.969
2.516
OMe
Me
N
N
1.000
0.996
2.024
3.061
1.019
2.194
2.005
3.003
3.010
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm


159.158
140.099
137.344
133.908
131.773
130.918
128.653
128.054
127.729
127.617
127.054
126.465
124.420
123.607
122.039
119.258
114.496
111.817
109.212
77.376
77.058
76.741
55.379
21.749
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0 ppm

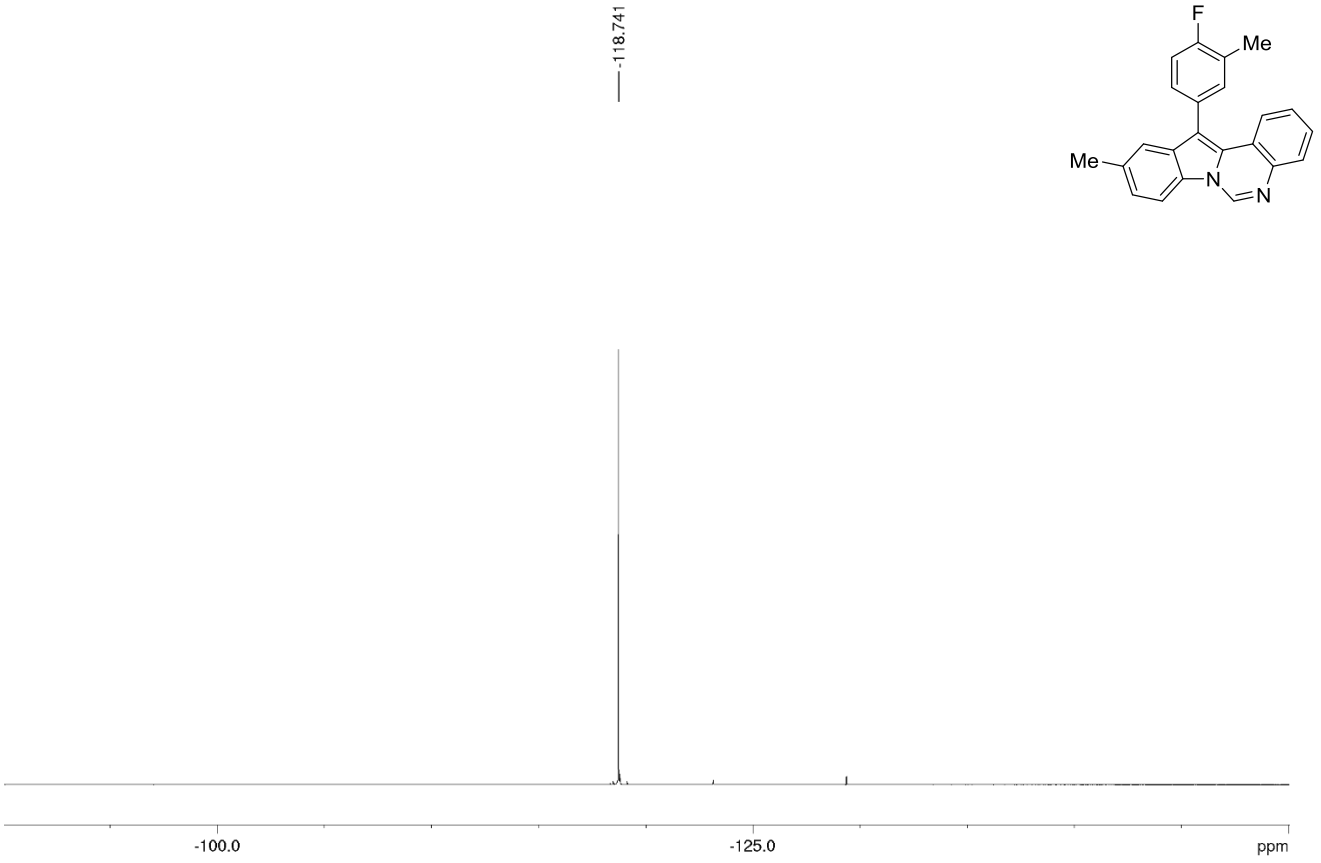
10l


8.941
7.801
7.780
7.699
7.678
7.528
7.512
7.508
7.496
7.476
7.437
7.420
7.397
7.376
7.305
7.205
7.179
7.151
7.149
7.130
2.417
Me
N
N
1.000
1.033
2.007
4.102
2.130
1.029
2.455
3.140
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm
140.179
137.289
134.530
134.001
130.715
130.684
129.024
128.761
128.146
127.798
127.656
127.076
124.503
123.650
121.901
119.247
112.144
109.234
77.349
77.031
76.714
21.740
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0 ppm

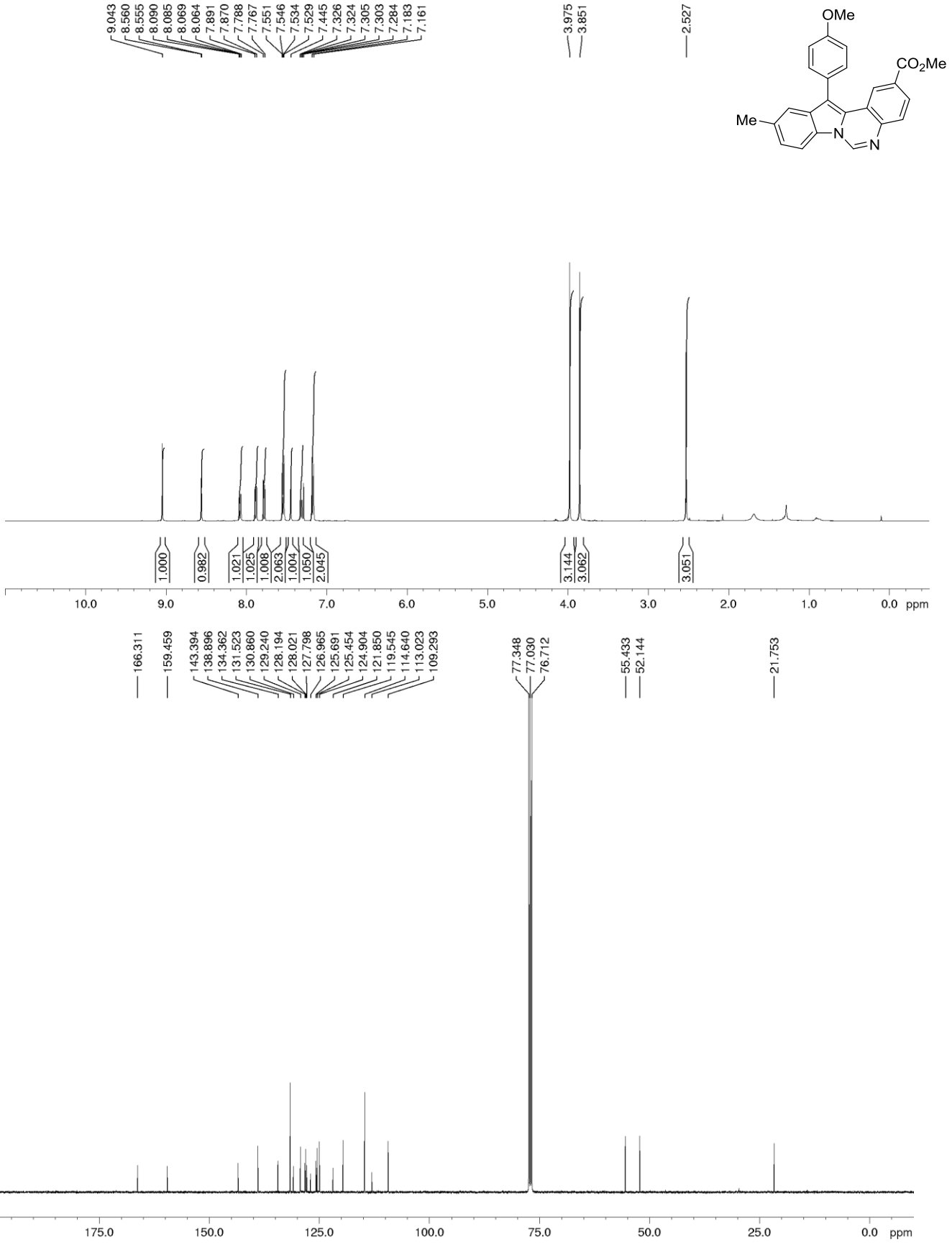
10m


9.018
7.881
7.860
7.804
7.784
7.759
7.740
7.487
7.468
7.420
7.401
7.391
7.364
7.300
7.279
7.257
7.232
7.210
2.525
2.419
F
Me
Me
N
N
1.000
1.011
2.008
1.093
3.131
3.310
3.062
3.164
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm
162.248
159.808
140.113
137.278
134.047
133.677
133.626
130.727
130.043
130.006
129.641
129.562
128.791
128.164
127.707
127.118
125.692
125.519
124.534
123.545
121.819
119.080
115.800
115.578
111.237
109.272
77.379
77.062
76.744
21.759
14.770
14.737
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0 ppm

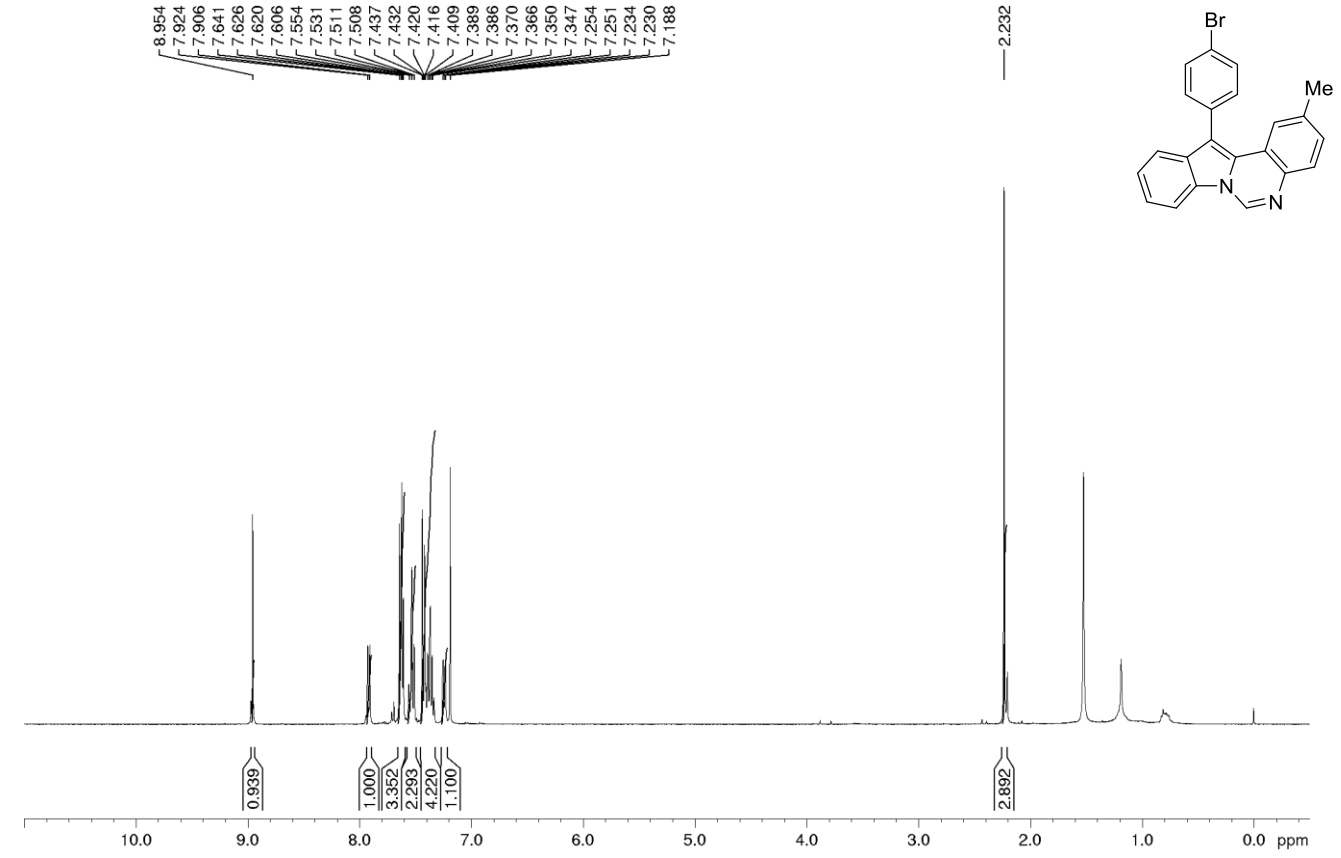
10m

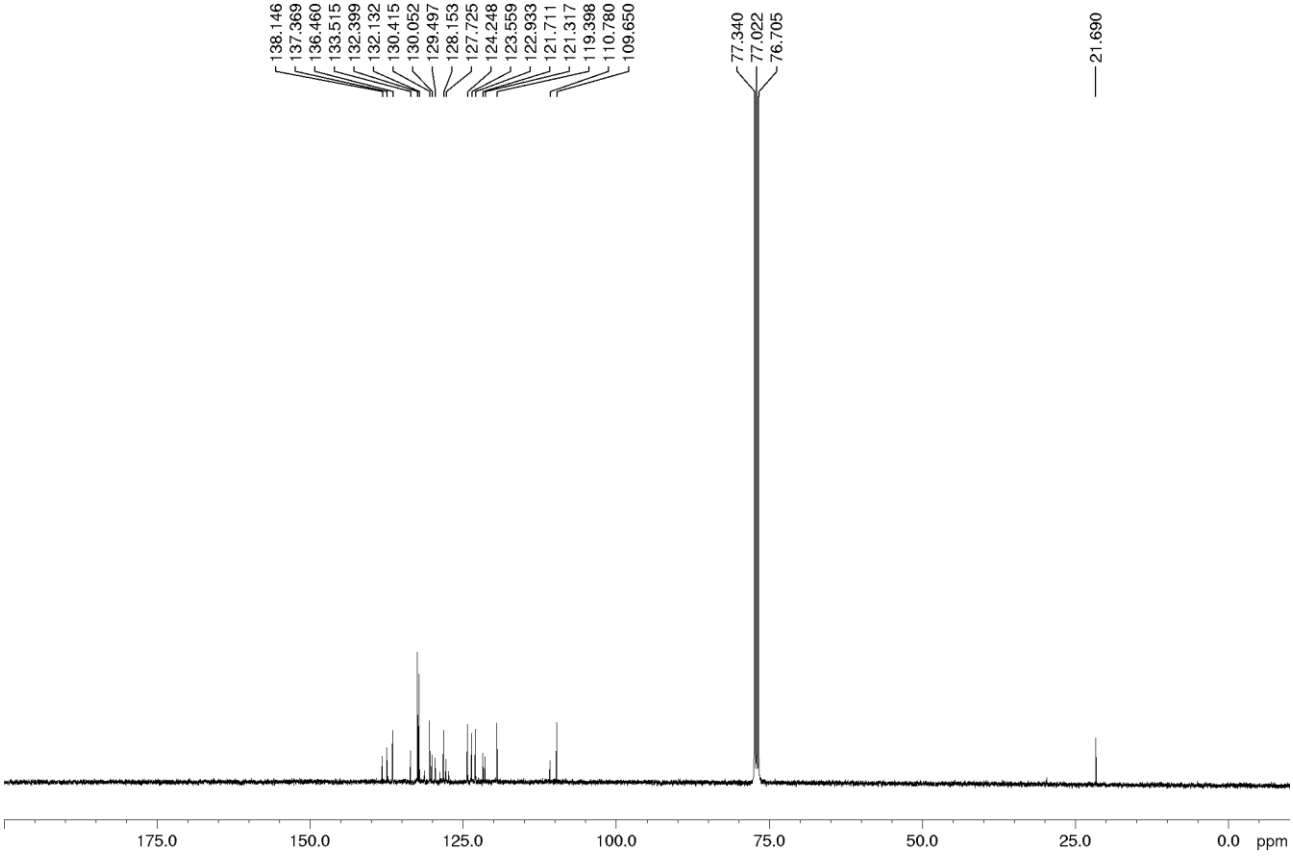


10n

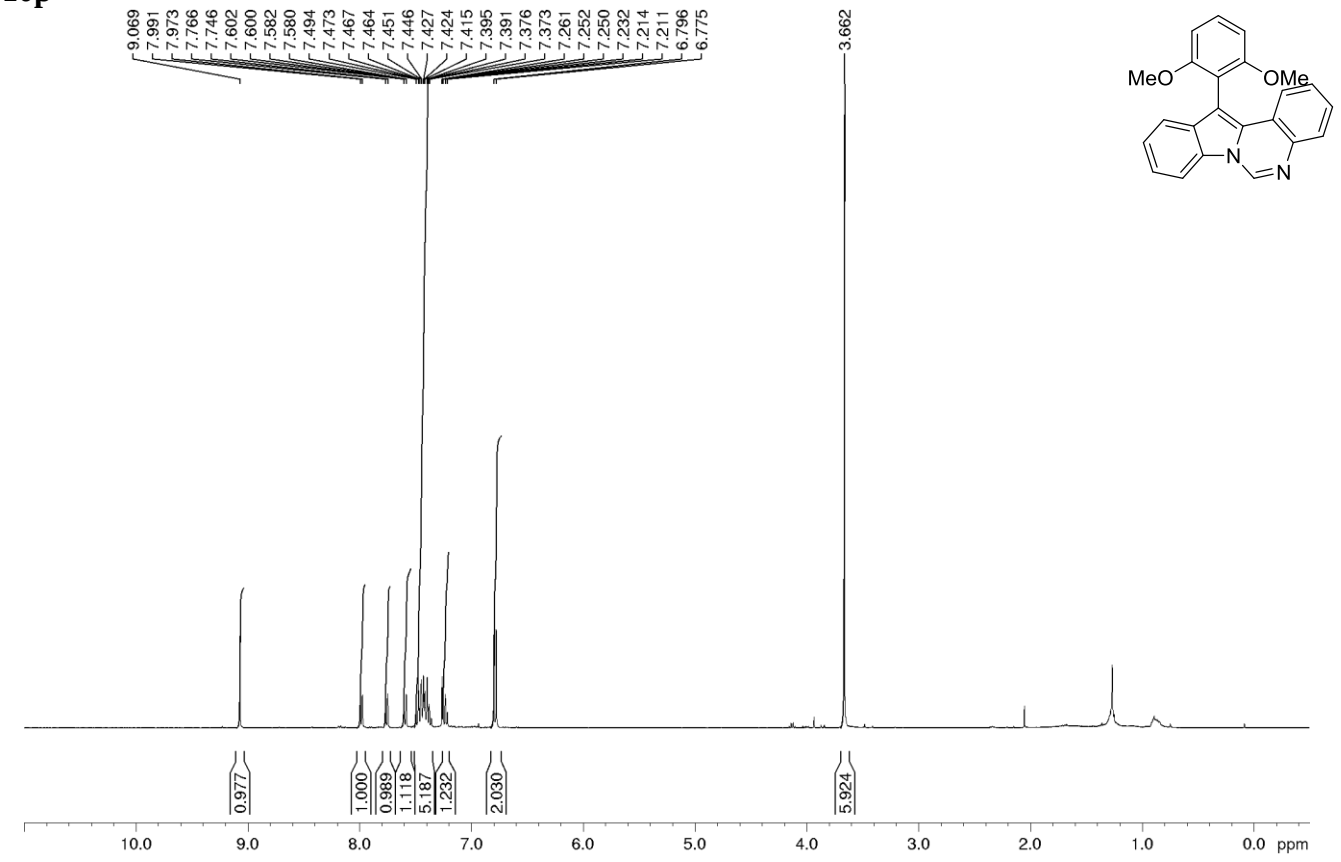

9.043
8.560
8.555
8.090
8.085
8.069
8.064
7.891
7.870
7.788
7.767
7.551
7.546
7.534
7.529
7.445
7.326
7.324
7.305
7.303
7.284
7.183
7.161
3.975
3.851
2.527
OMe
CO2Me
Me
N
N
1.000
0.982
1.021
1.025
1.008
2.063
1.004
1.050
2.045
3.144
3.062
3.051
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm
166.311
159.459
143.394
138.896
134.362
131.523
130.860
129.240
128.194
128.021
127.798
126.965
125.691
125.454
124.904
121.850
119.545
114.640
113.023
109.293
77.348
77.030
76.712
55.433
52.144
21.753
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0 ppm

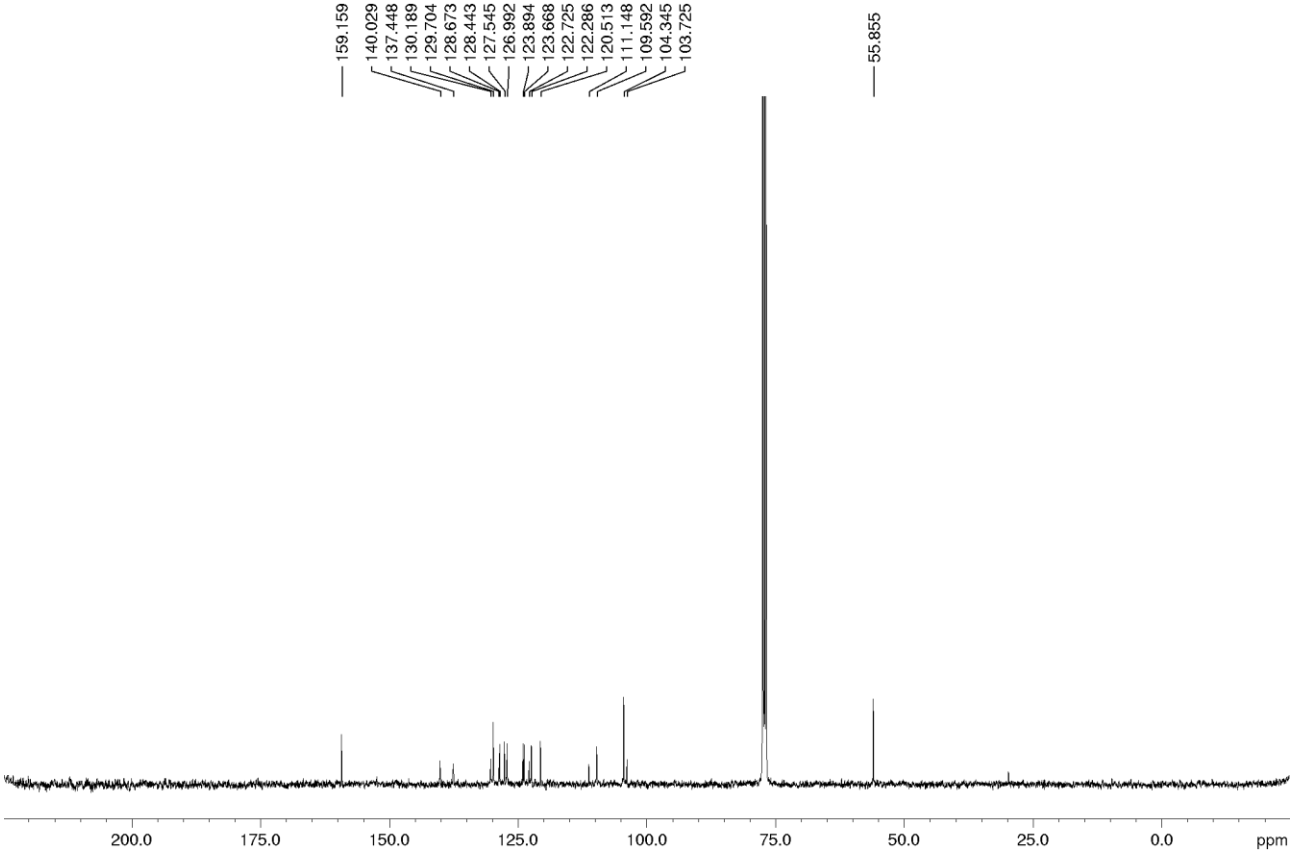
10o


8.954
7.924
7.906
7.641
7.626
7.620
7.606
7.554
7.531
7.511
7.508
7.437
7.432
7.420
7.416
7.409
7.389
7.386
7.370
7.366
7.350
7.347
7.254
7.251
7.234
7.230
7.188
2.232
Br
Me
N
N
0.939
1.000
3.352
2.293
4.220
1.100
2.892
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm


138.146
137.369
136.460
133.515
132.399
132.132
130.415
130.052
129.497
128.153
127.725
124.248
123.559
122.933
121.711
121.317
119.398
110.780
109.650
77.340
77.022
76.705
21.690
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0 ppm

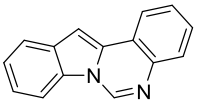
10p

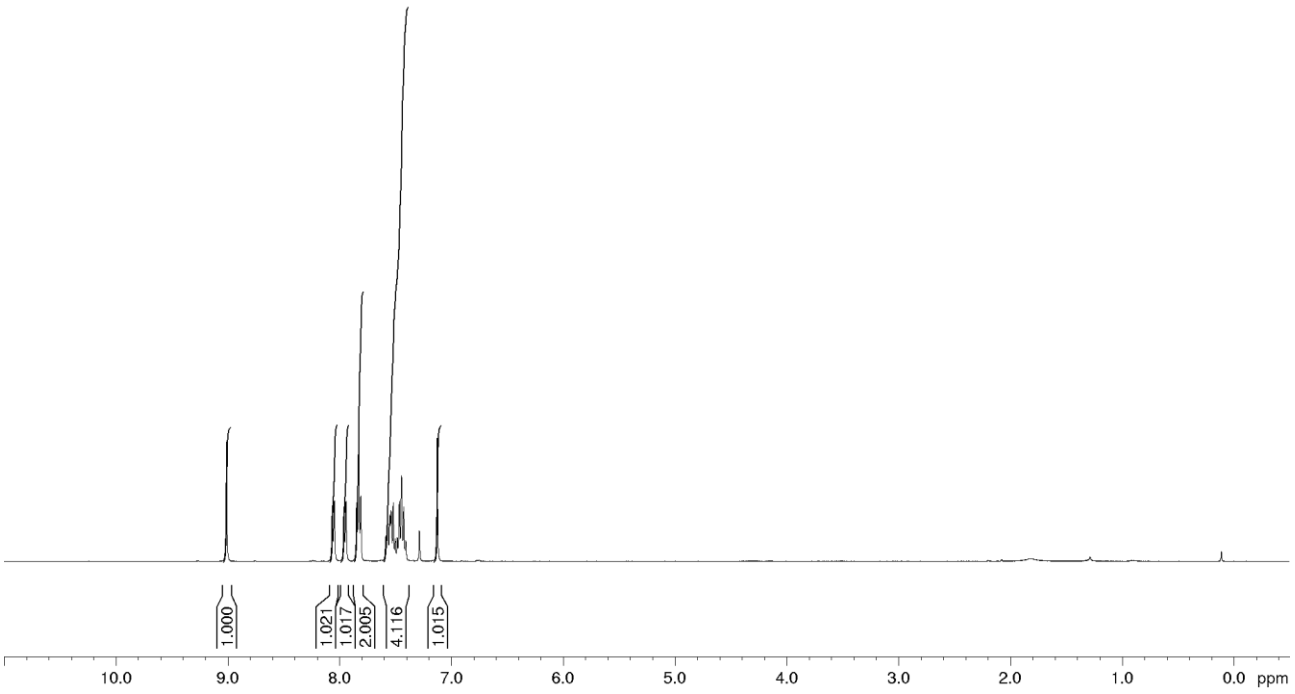

9.069
7.991
7.973
7.766
7.746
7.602
7.600
7.582
7.580
7.494
7.473
7.467
7.464
7.451
7.446
7.427
7.424
7.415
7.395
7.391
7.376
7.373
7.261
7.252
7.250
7.232
7.214
7.211
6.796
6.775
3.662
MeO
OMe
N
N
0.977
1.000
0.989
1.118
5.187
1.232
2.030
5.924
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm

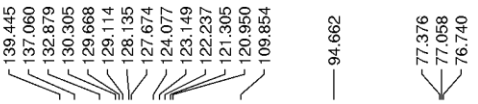

159.159
140.029
137.448
130.189
129.704
128.673
128.443
127.545
126.992
123.894
123.668
122.725
122.286
120.513
111.148
109.592
104.345
103.725
55.855
200.0
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0
ppm

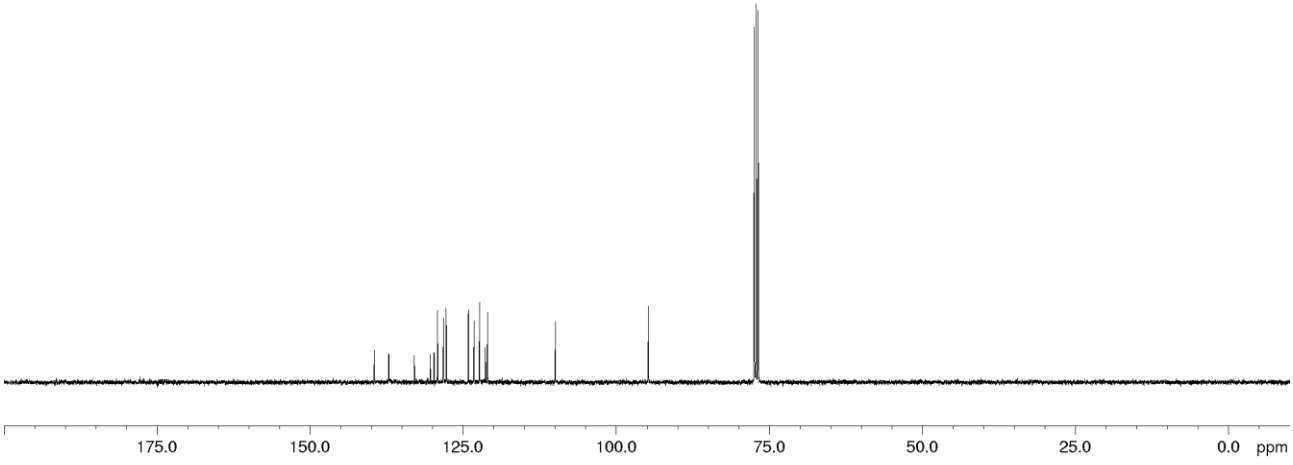
13a


9.010
8.063
8.044
7.959
7.940
7.845
7.828
7.809
7.585
7.567
7.548
7.536
7.517
7.499
7.481
7.463
7.445
7.423
7.405
7.284
7.125

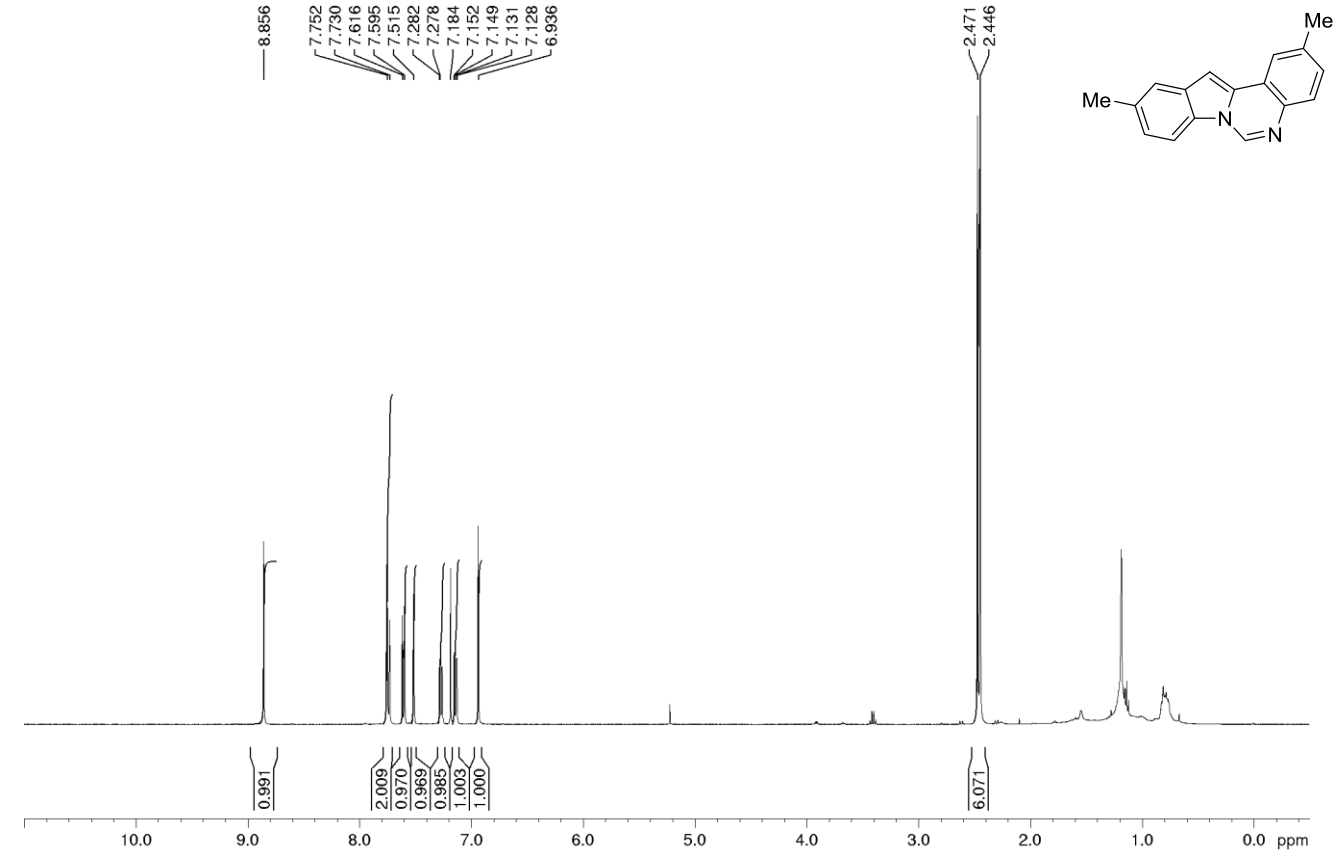

N
N

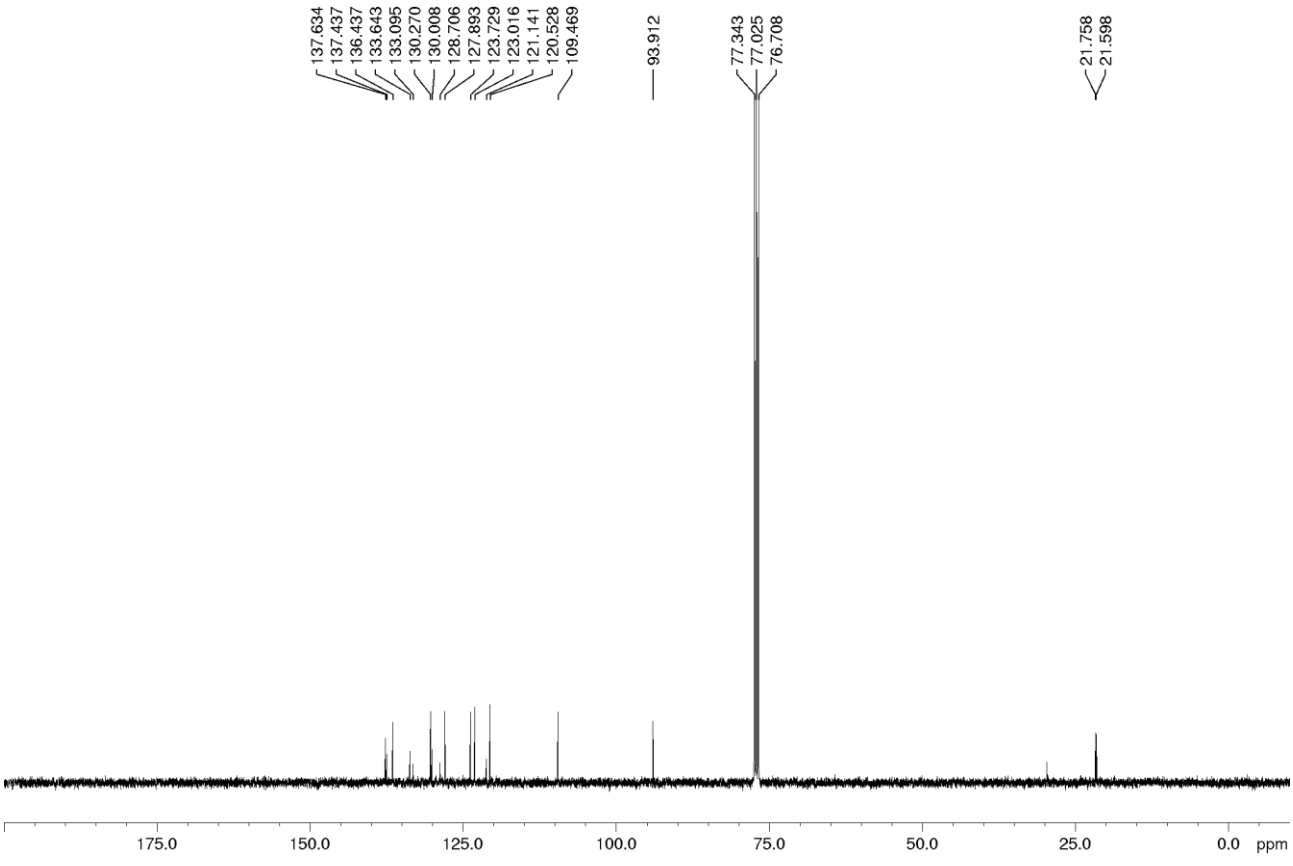

1.000
1.021
1.017
2.005
4.116
1.015
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm


139.445
137.060
132.879
130.305
129.668
129.114
128.135
127.674
124.077
123.149
122.237
121.305
120.950
109.854
94.662
77.376
77.058
76.740

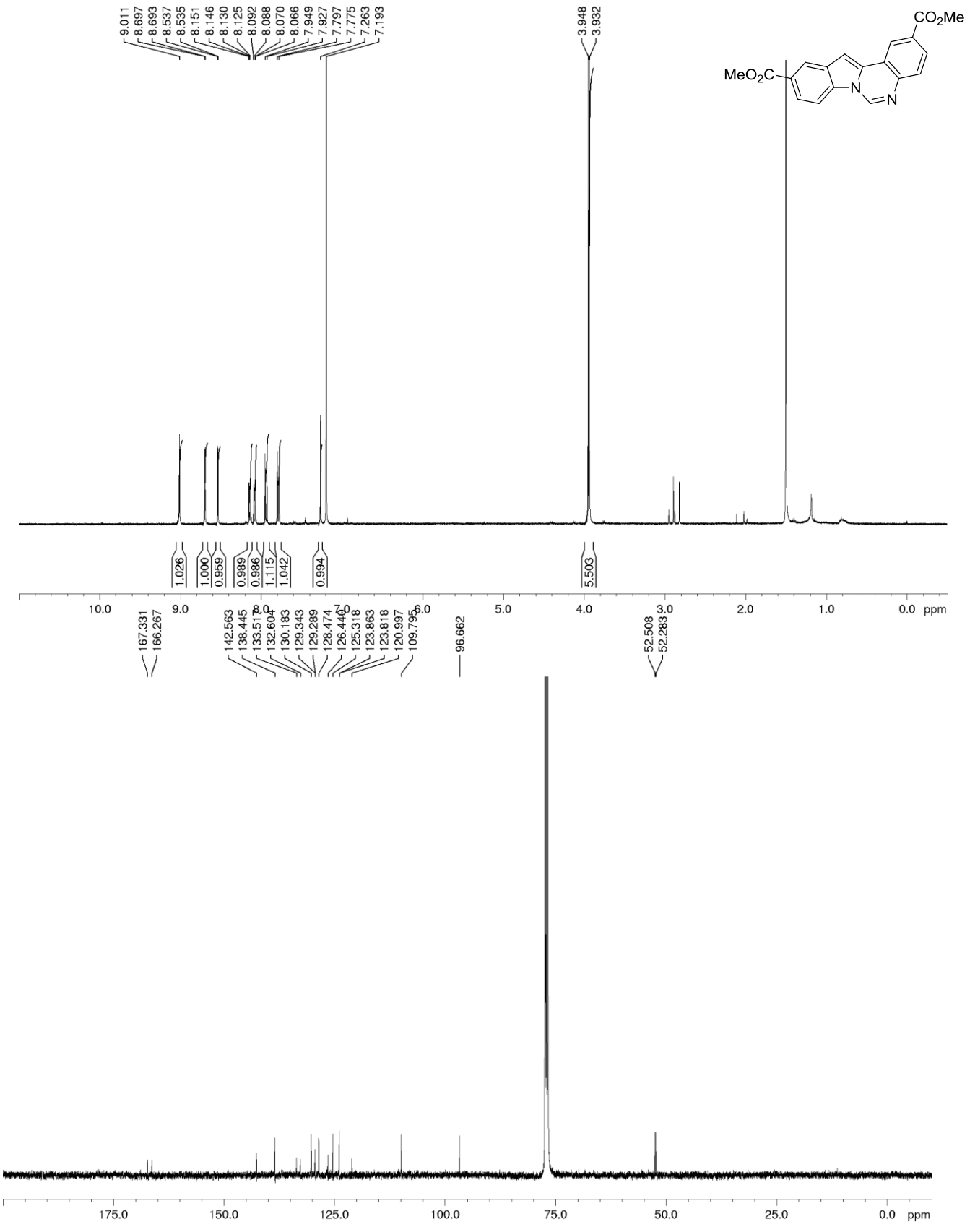

175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0 ppm

13b

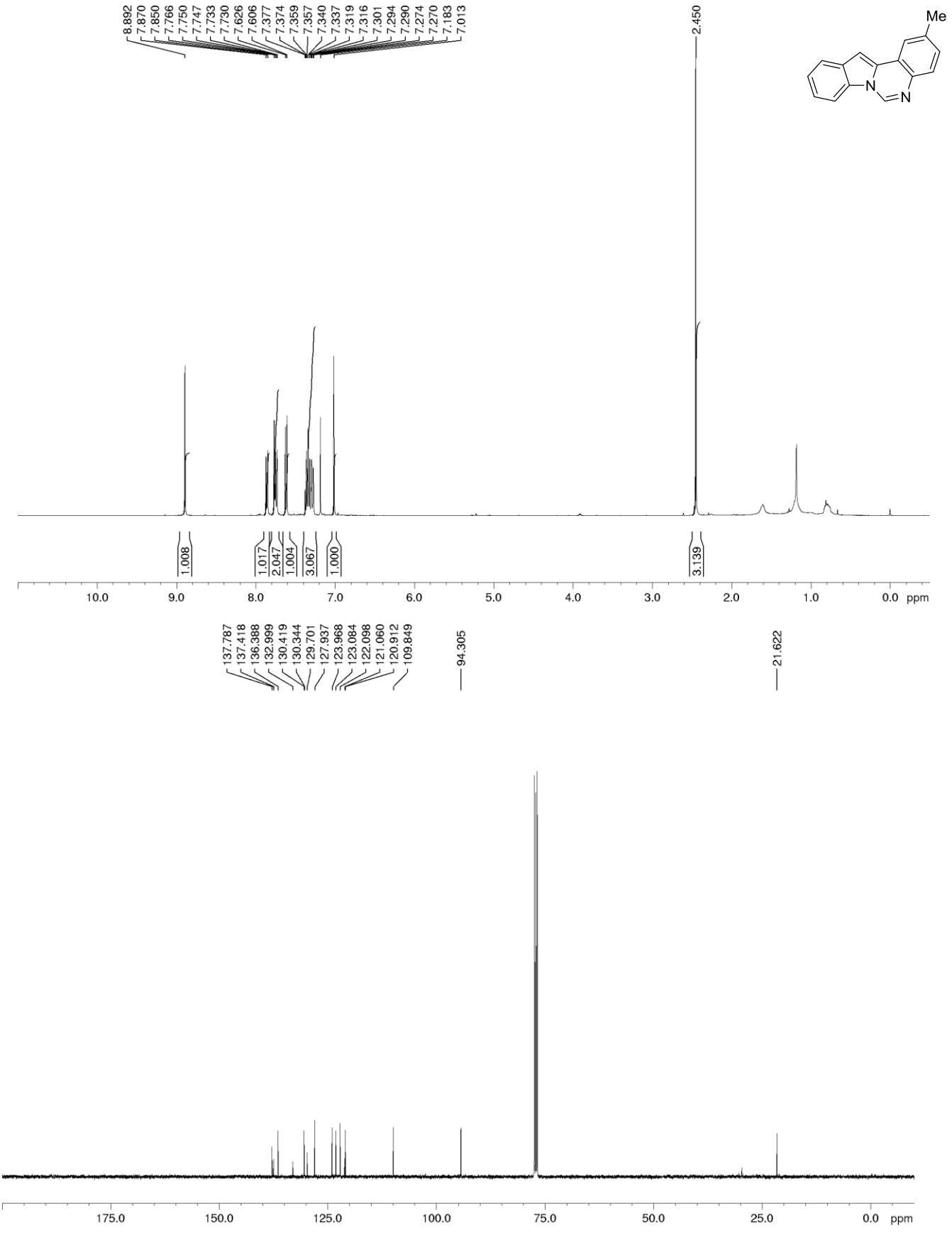

8.856
7.752
7.730
7.616
7.595
7.515
7.282
7.278
7.184
7.152
7.149
7.131
7.128
6.936
2.471
2.446
Me
Me
N
N
0.991
2.009
0.970
0.969
0.985
1.003
1.000
6.071
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm


137.634
137.437
136.437
133.643
133.095
130.270
130.008
128.706
127.893
123.729
123.016
121.141
120.528
109.469
93.912
77.343
77.025
76.708
21.758
21.598
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0 ppm

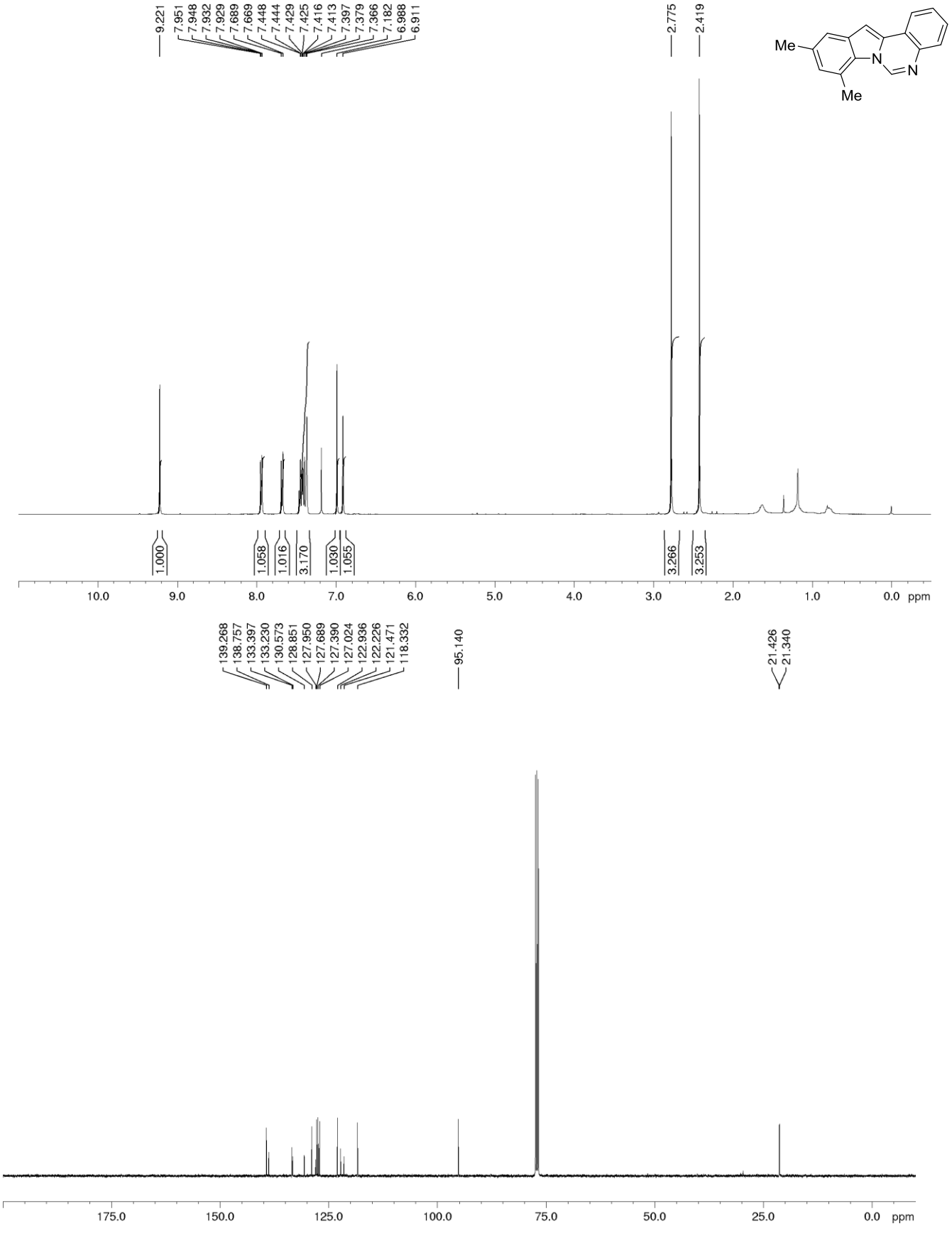
13c


9.011
8.697
8.693
8.537
8.535
8.151
8.146
8.130
8.125
8.092
8.088
8.070
8.066
7.949
7.927
7.797
7.775
7.263
7.193
3.948
3.932
CO2Me
MeO2C
N
N
1.026
1.000
0.959
0.989
0.986
1.115
1.042
0.994
5.503
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm
167.331
166.267
142.563
138.445
133.517
132.604
130.183
129.343
129.289
128.474
126.446
125.318
123.863
123.818
120.997
109.795
96.662
52.508
52.283
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0 ppm

13d


8.892
7.870
7.850
7.766
7.750
7.747
7.733
7.730
7.626
7.606
7.377
7.374
7.359
7.357
7.340
7.337
7.319
7.316
7.301
7.294
7.290
7.274
7.270
7.183
7.013
2.450
Me
N
N
1.008
1.017
2.047
1.004
3.067
1.000
3.139
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm
137.787
137.418
136.388
132.999
130.419
130.344
129.701
127.937
123.968
123.084
122.098
121.060
120.912
109.849
94.305
21.622
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0 ppm

13e


9.221
7.951
7.948
7.932
7.929
7.689
7.669
7.448
7.444
7.429
7.425
7.416
7.413
7.397
7.379
7.366
7.182
6.988
6.911
2.775
2.419
Me
N
N
Me
1.000
1.058
1.016
3.170
1.030
1.055
3.266
3.253
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm
139.268
138.757
133.397
133.230
130.573
128.851
127.950
127.689
127.390
127.024
122.936
122.226
121.471
118.332
95.140
21.426
21.340
175.0
150.0
125.0
100.0
75.0
50.0
25.0
0.0 ppm