

Supplementing Information

Trifluoroethanol Promoted Formal Nucleophilic Substitution of Indol-2-yl

Diaryl Methanol for the Synthesis of Tetraarylmethanes

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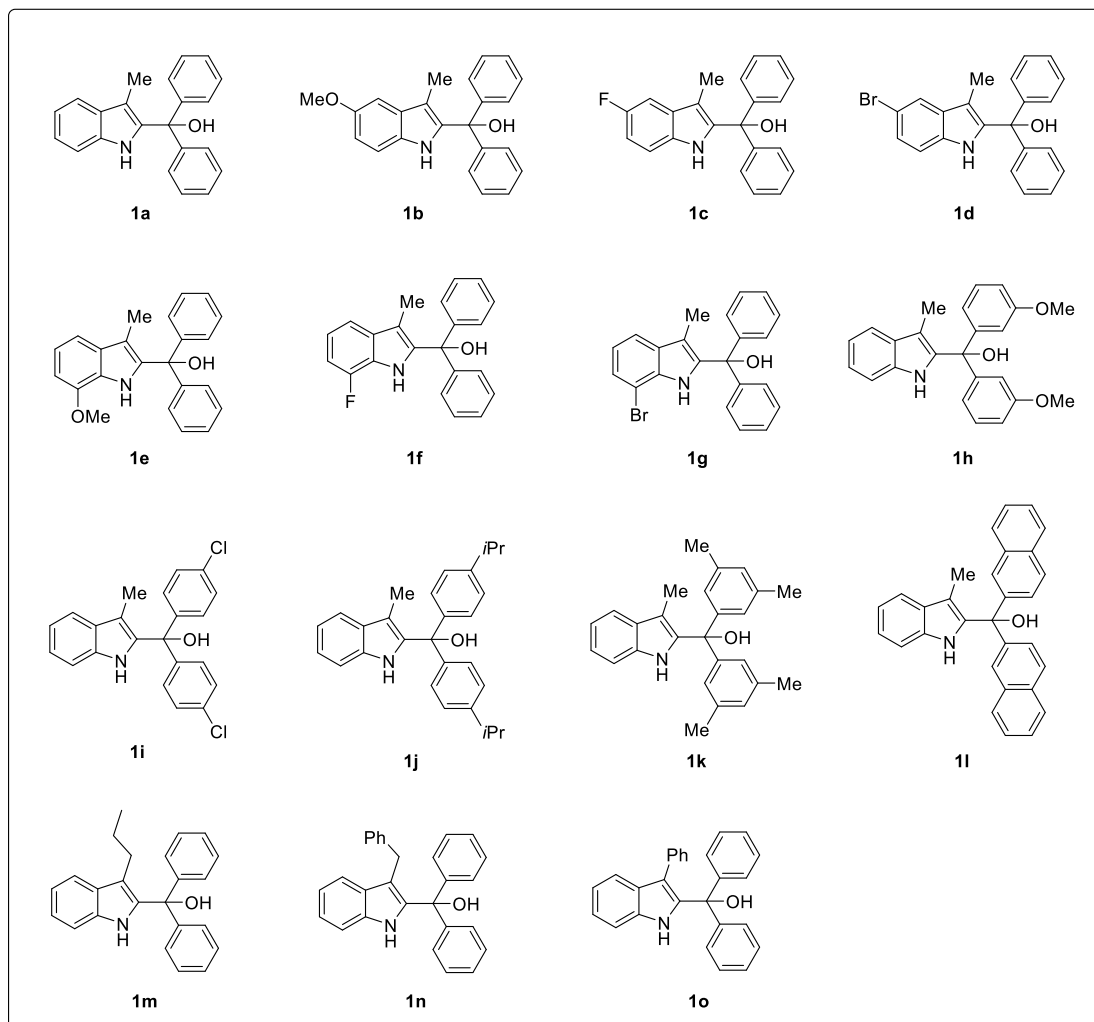
NMR spectra

I. General Information

Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co. Lit., China. All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. Anhydrous toluene, acetonitrile, dichloromethane, chloroform, dimethyl sulfoxide and tetrahydrofuran were purified by the Innovative® solvent purification system. Other anhydrous solvents and substrates **1a-1l** were purchased from J&K Scientific. ¹H, ¹³C and ¹⁹F NMR spectra were collected on a Bruker AV 400 MHz NMR spectrometer or a Bruker AV 300 MHz NMR spectrometer using residue solvent peaks as an internal standard (¹H NMR: CDCl₃ at 7.26 ppm; ¹³C NMR: CDCl₃ at 77.16 ppm). Mass spectra were collected on an Agilent GC/MS 5975C system, a MALDI Micro MX mass spectrometer, or an API QSTAR XL System. The X-ray data was collected by SuperNova, Dual, Cu at zero, Atlas diffractometer.

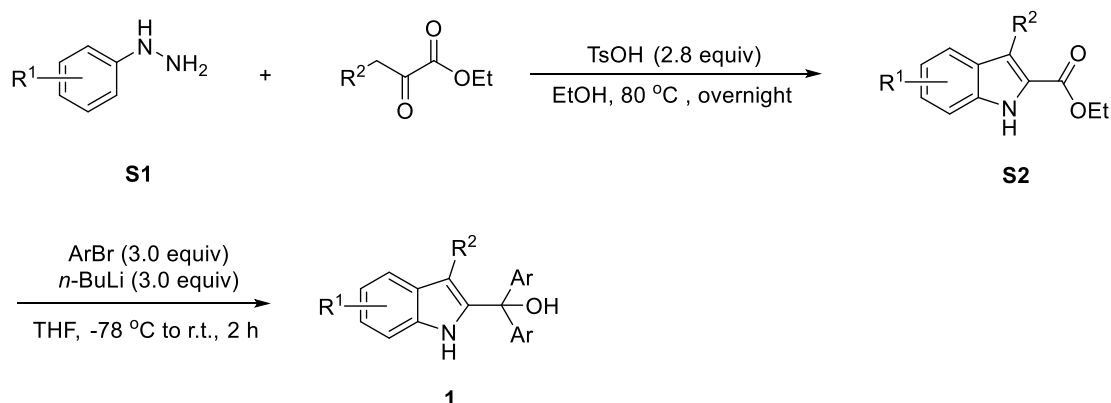
II. Preparation of Substrates

Substrates **1a-1o** were synthesized according to our previous procedure.^[1] **1m-1o** are unknown compounds,



[1] J. Wang, R. Yu, C. Nian, M. Liao, Z. Han, J. Sun and H. Huang, *Org. Lett.* 2023, **25**, 8478-8483.

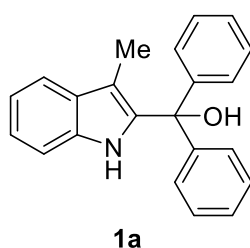
General Procedure A for the Preparation of Indol-2-yl Methanols 1a-1o.



To a solution of ethyl 2-oxobutanoate (1.43 g, 11.0 mmol, 1.1 equiv), arylhydrazines **S1** (10.0 mmol, 1.0 equiv) in anhydrous EtOH (30 mL) was added TsOH (5.33 g, 28.0 mmol, 2.8 equiv). The reaction mixture was heated to reflux on an oil bath and stirred for 12 h. The resulting precipitate was filtered off and washed with EtOH. The combined filtrate was concentrated to give a residue that was dissolved in 1:1 EtOAc: Et₂O (40 mL) and washed with 10 % aq. Na₂CO₃ (30 mL × 2), dried over Na₂SO₄ and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (eluent: petroleum ether/EtOA) to afford the desired compounds **S2**.

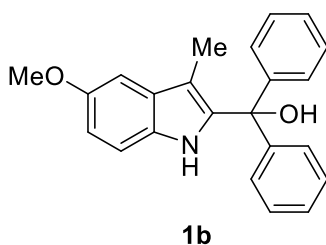
Under N₂ at -78 °C, to a solution of ArBr (18.3 mmol, 6.1 equiv) in THF (40 mL) was added a solution of *n*-BuLi (2.4 M in *n*-hexane, 7.5 mL, 18.0 mmol, 6.0 equiv) dropwise. Then the reaction mixture was stirred at -78 °C for 30 min. The solution of **S2** (3 mmol, 1.0 equiv) in anhydrous THF (10 mL) was added at -78 °C *via* syringe. Then the reaction mixture was warmed to room temperature and stirred for 1 h. The reaction mixture was quenched with aqueous NH₄Cl

solution (20 mL) and extracted with ethyl acetate (30 mL × 3). The combined organic layers were washed with water (30 mL × 2), dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/EtOAc) to afford the desired indol-2-yl methanols **1**.



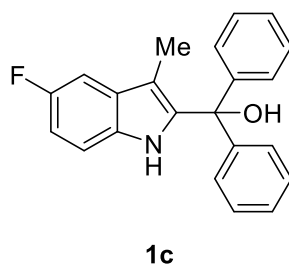
(3-Methyl-1H-indol-2-yl)diphenylmethanol (1a) was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 4:1) in 99% yield (930.8 mg).

¹H NMR (400 MHz, CDCl₃) δ 8.07 (s, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.37–7.32 (m, 10H), 7.24 (s, 1H), 7.17 (td, *J*₁ = 1.1 Hz, *J*₂ = 7.0 Hz, 1H), 7.13–7.10 (m, 1H), 2.99 (s, 1H), 1.87 (s, 3H) ppm.



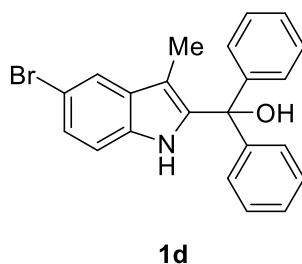
(5-Methoxy-3-methyl-1H-indol-2-yl)diphenylmethanol (1b) was prepared according to the General Procedure A as a brown solid (chromatography eluent: petroleum ether/EtOAc = 6:1) in 99% yield (1.02 g).

^1H NMR (400 MHz, CDCl_3) δ 7.94 (s, 1H), 7.37–7.31 (m, 10H), 7.24 (s, 1H), 7.15 (d, $J = 2.3$ Hz, 1H), 6.84 (dd, $J_1 = 2.4$ Hz, $J_2 = 8.8$ Hz, 1H), 3.87 (s, 3H), 3.01 (s, 1H), 1.87 (s, 3H) ppm.



(5-Fluoro-3-methyl-1H-indol-2-yl)diphenylmethanol (1c) was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 4:1) in 90% yield (894.8 mg).

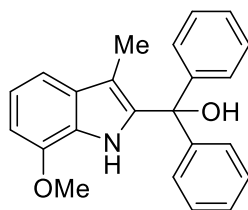
^1H NMR (400 MHz, CDCl_3) δ 8.11 (s, 1H), 7.36 (s, 10H), 7.19–7.14 (m, 2H), 6.91 (td, $J_1 = 2.4$ Hz, $J_2 = 9.2$ Hz, 1H), 3.00 (s, 1H), 1.84 (s, 3H) ppm.



(5-Bromo-3-methyl-1H-indol-2-yl)diphenylmethanol (1d) was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 4:1) in 91% yield (1071.0 mg).

^1H NMR (400 MHz, CDCl_3) δ 8.19 (s, 1H), 7.66 (d, $J = 1.6$ Hz, 1H), 7.39–7.32 (m, 10H), 7.24 (dd, $J_1 = 1.8$ Hz, $J_2 = 8.6$ Hz, 1H), 7.13 (d, $J = 8.5$ Hz, 1H), 2.99 (s, 1H),

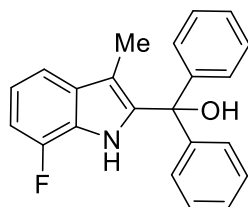
1.81 (s, 3H) ppm.



1e

(7-Methoxy-3-methyl-1H-indol-2-yl)diphenylmethanol (1e) was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 8:1) in 15% yield (154.5 mg).

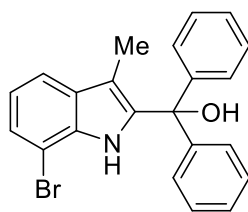
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.45 (s, 1H), 7.39–7.31 (m, 10H), 7.17 (d, $J = 8.0$ Hz, 1H), 7.05 (t, $J = 7.8$ Hz, 1H), 6.64 (d, $J = 7.6$ Hz, 1H), 3.88 (s, 3H), 3.12 (s, 1H), 1.86 (s, 3H) ppm.



1f

(7-Fluoro-3-methyl-1H-indol-2-yl)diphenylmethanol (1f) was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 5:1) in 84% yield (835.1 mg).

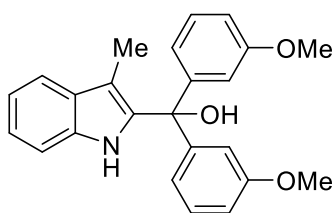
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.35 (s, 1H), 7.37 (s, 10H), 7.30 (d, $J = 7.9$ Hz, 1H), 7.05–6.99 (m, 1H), 6.89 (dd, $J_1 = 7.8$ Hz, $J_2 = 11.2$ Hz, 1H), 3.00 (s, 1H), 1.86 (s, 3H) ppm.



1g

(7-Bromo-3-methyl-1H-indol-2-yl)diphenylmethanol (1g) was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 4:1) in 91% yield (1070.9 mg).

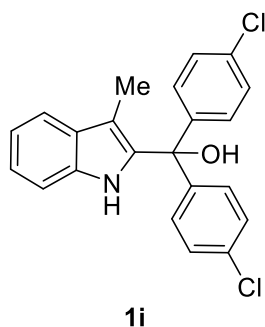
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.42 (s, 1H), 7.47 (d, $J = 7.9$ Hz, 1H), 7.39–7.32 (m, 11H), 6.99 (t, $J = 7.76$ Hz, 1H), 3.01 (s, 1H), 1.81 (s, 3H) ppm.



1h

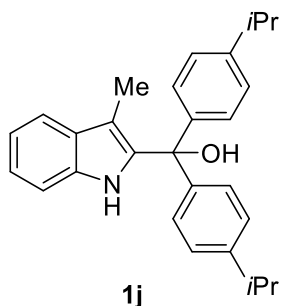
Bis(3-methoxyphenyl)(3-methyl-1H-indol-2-yl)methanol (1h) was prepared according to the General Procedure A as a pink solid (chromatography eluent petroleum ether/EtOAc = 5:1) in 99% yield (1109.1 mg).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.04 (s, 1H), 7.53 (d, $J = 7.5$ Hz, 1H), 7.25–7.22 (m, 3H), 7.16 (td, $J_1 = 1.2$ Hz, $J_2 = 7.0$ Hz, 1H), 7.12–7.08 (m, 1H), 6.98 (t, $J = 1.9$ Hz, 2H), 6.92–6.90 (m, 2H), 6.86–6.84 (m, 2H), 3.74 (s, 6H), 3.00 (s, 1H), 1.93 (s, 3H) ppm.



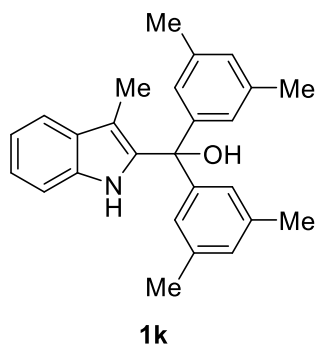
Bis(4-chlorophenyl)(3-methyl-1H-indol-2-yl)methanol (1i) was prepared according to the General Procedure A as a brown solid (chromatography eluent: petroleum ether/EtOAc = 4:1) in 43% yield (493.4 mg).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.00 (s, 1H), 7.55 (d, $J = 7.8$ Hz, 1H), 7.35–7.27 (m, 9H), 7.20 (td, $J_1 = 1.1$ Hz, $J_2 = 7.0$ Hz, 1H), 7.16–7.12 (m, 1H), 3.00 (s, 1H), 1.90 (s, 3H) ppm.

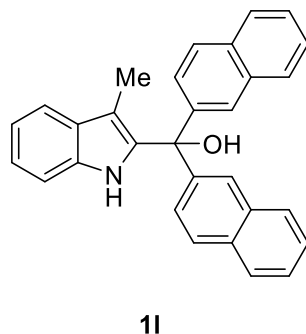


Bis(4-isopropylphenyl)(3-methyl-1H-indol-2-yl)methanol (1j) was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 6:1) in 74% yield (888.0 mg).

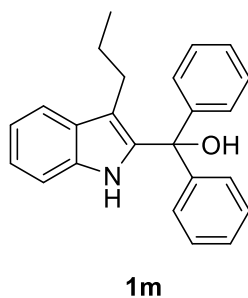
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.17 (s, 1H), 7.55 (d, $J = 7.8$ Hz, 1H), 7.28–7.09 (m, 11H), 2.96–2.84 (m, 3H), 1.87 (s, 3H), 1.27 (d, $J = 6.9$ Hz, 12H) ppm.



Bis(3,5-dimethylphenyl)(3-methyl-1H-indol-2-yl)methanol (1k) was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 4:1) in 79% yield (878.3 mg). ¹H NMR (400 MHz, CDCl₃) δ 8.03 (s, 1H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.28 (d, *J* = 7.9 Hz, 1H), 7.19 (td, *J*₁ = 1.1 Hz, *J*₂ = 7.1 Hz, 1H), 7.15-7.11 (m, 1H), 6.99 (s, 4H), 6.98 (s, 2H), 2.89 (s, 1H), 2.30 (s, 12H), 1.95 (s, 3H) ppm.



(3-Methyl-1H-indol-2-yl)di(naphthalen-2-yl)methanol (1l) was prepared according to the General Procedure A as a yellow solid (chromatography eluent: petroleum ether/EtOAc = 6:1) in 78% yield (967.4 mg). ¹H NMR (400 MHz, CDCl₃) δ 8.14 (s, 1H), 7.90-7.86 (m, 6H), 7.79 (d, *J* = 7.8 Hz, 2H), 7.64-7.60 (m, 3H), 7.57-7.49 (m, 4H), 7.29-7.17 (m, 3H), 3.26 (s, 1H), 2.00 (s, 3H) ppm.



Diphenyl(3-propyl-1H-indol-2-yl)methanol (1m) was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 30:1) in 34% yield (348.3 mg).

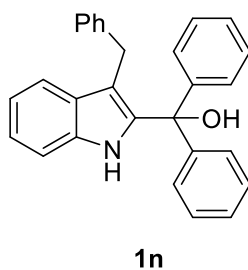
M.P. 188-189 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.04 (s, 1H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.30-7.26 (m, 10H), 7.17-7.03 (m, 3H), 3.06 (s, 1H), 2.23-2.19 (m, 2H), 1.31-1.21 (m, 2H), 0.66 (t, *J* = 7.3 Hz, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 145.3, 137.1, 134.4, 129.4, 128.3, 128.0, 127.8, 122.1, 119.4, 119.2, 114.4, 111.0, 79.5, 27.1, 23.7, 14.7 ppm.

HRMS (ES⁺) Calcd for C₂₄H₂₄NO [M + H]⁺: 342.1858, Found: 342.1852.

IR ν (KBr, cm⁻¹) 3446, 3057, 2956, 292, 2867, 1683, 1490, 144, 133, 1001.



(3-Benzyl-1H-indol-2-yl)diphenylmethanol (1n) was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 15:1) in 67% yield (782.9 mg).

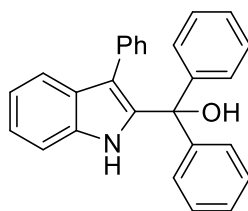
M.P. 204-205 °C.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.01 (s, 1H), 7.46-7.28 (m, 12H), 7.22-7.07 (m, 5H), 6.98 (d, $J = 6.4$ Hz, 2H), 3.85 (s, 2H), 2.88 (d, $J = 2.4$ Hz, 1H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 144.9, 141.3, 138.7, 134.3, 129.8, 128.42, 128.39, 128.30, 127.99, 127.6, 125.8, 122.3, 119.7, 119.6, 111.9, 111.1, 79.1, 30.5 ppm.

HRMS (ES+) Calcd for $\text{C}_{28}\text{H}_{24}\text{NO}$ $[\text{M} + \text{H}]^+$: 390.1858, Found: 390.1862.

IR ν (KBr, cm^{-1}) 3561, 3443, 1491, 1447, 1324, 1026.



1o

Diphenyl(3-phenyl-1H-indol-2-yl)methanol (1o) was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 8:1) in 75% yield (844.8 mg).

M.P. 233-234 °C.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.84 (s, 1H), 7.46 (d, $J = 7.9$ Hz, 1H), 7.30-7.26 (m, 11H), 7.22-7.18 (m, 4H), 7.15-7.09 (m, 3H), 3.25 (s, 1H) ppm.

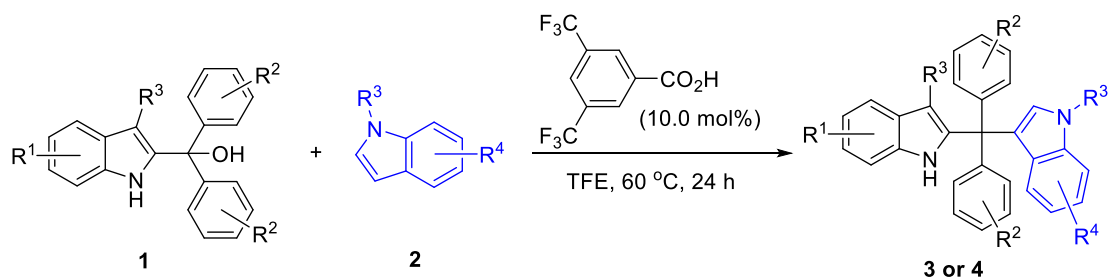
$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 145.7, 138.3, 134.7, 134.2, 130.5, 129.5, 128.5, 128.3, 128.0, 127.8, 126.8, 122.6, 120.3, 119.7, 115.1, 111.0, 79.9 ppm.

HRMS (ES+) Calcd for $\text{C}_{27}\text{H}_{22}\text{NO}$ $[\text{M} + \text{H}]^+$: 376.1701, Found: 376.1698.

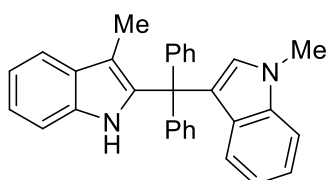
IR ν (KBr, cm^{-1}) 3540, 3465, 3056, 1489, 1450, 1329, 1282, 1172, 1158.

III. The Synthesis of Tetraarylmethanes

General Procedure B for the Synthesis of Tetraarylmethanes **3** or **4**.



To a solution of indol-2-yl methanols **1** (0.3 mmol, 1.0 equiv), indoles **2** (0.6 mmol, 2.0 equiv) in CF₃CH₂OH (3.0 mL) was added 3,5-bis(trifluoromethyl)benzoic acid (7.7 mg, 0.03 mmol, 10.0 mol%). The reaction mixture was warmed up to 60 °C and kept stirring for 24 h. The reaction mixture was directly concentrated under reduced pressure. The residue was purified by silica gel column chromatography (eluent: petroleum ether/DCM or petroleum ether/EtOAc) to afford the desired products **3** or **4**.



3a

1-Methyl-3-((3-methyl-1H-indol-2-yl)diphenylmethyl)-1H-indole (3a) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 24:1) in 88% yield (112.3 mg). M.P. 231-232 °C.

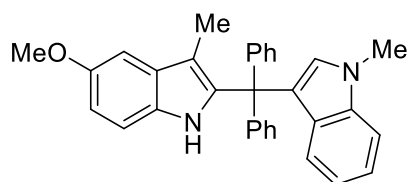
¹H NMR (400 MHz, CDCl₃) δ 8.12 (s, 1H), 7.55 (d, *J* = 5.0 Hz, 1H), 7.35-7.28 (m, 11H), 7.20 (t, *J* = 7.8 Hz, 2H), 7.16-7.12 (m, 2H), 6.85 (t, *J* = 7.8 Hz, 1H), 6.73 (s,

1H), 6.70 (d, $J = 8.2$ Hz, 1H), 3.76 (s, 3H), 1.67 (s, 3H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 144.5, 138.7, 138.0, 133.7, 130.6, 130.3, 130.1, 127.9, 127.5, 126.6, 122.0, 121.8, 121.2, 120.5, 119.4, 119.1, 118.3, 110.8, 109.4, 109.2, 55.3, 33.0, 10.3 ppm.

HRMS (ES+) Calcd for $\text{C}_{31}\text{H}_{26}\text{N}_2\text{Na}$ [$\text{M} + \text{Na}$] $^+$: 449.1994, Found: 449.1998.

IR ν (KBr, cm^{-1}) 3441, 3053, 1632, 1506, 1485, 1459, 1445, 1418, 1351.



3b

5-Methoxy-3-methyl-2-((1-methyl-1H-indol-3-yl)diphenylmethyl)-1H-indole

(**3b**) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 6:1) in 96% yield (135.6 mg).

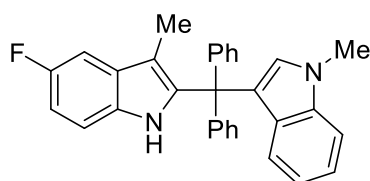
M.P. 248-250 °C.

^1H NMR (400 MHz, CDCl_3) δ 7.98 (s, 1H), 7.34-7.27 (m, 11H), 7.20-7.16 (m, 1H), 7.06 (d, $J = 8.7$ Hz, 1H), 6.96 (d, $J = 2.3$ Hz, 1H), 6.85-6.81 (m, 1H), 6.79 (dd, $J_1 = 2.4$ Hz, $J_2 = 6.3$ Hz, 1H), 6.71 (s, 1H), 6.67 (d, $J = 8.1$ Hz, 1H), 3.87 (s, 3H), 3.75 (s, 3H), 1.62 (s, 3H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 153.9, 144.5, 139.6, 138.0, 130.6, 130.5, 130.1, 128.9, 128.0, 127.5, 126.6, 122.0, 121.8, 120.5, 119.4, 111.6, 111.3, 109.4, 108.9, 100.0, 56.0, 55.4, 33.0, 10.4 ppm.

HRMS (ES+) Calcd for $\text{C}_{32}\text{H}_{28}\text{N}_2\text{ONa}$ [$\text{M} + \text{Na}$] $^+$: 479.2099, Found: 479.2094.

IR ν (KBr, cm^{-1}) 3451, 2924, 2852, 2813, 1646, 1597, 1506, 1447, 1382, 1350, 1216.



3c

5-Fluoro-3-methyl-2-((1-methyl-1H-indol-3-yl)diphenylmethyl)-1H-indole

(**3c**) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 14:1) in 99% yield (139.4 mg).

M.P. 261-262 °C.

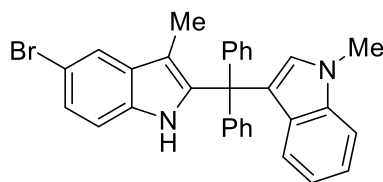
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.09 (s, 1H), 7.34-7.29 (m, 11H), 7.21-7.13 (m, 2H), 7.09-7.06 (m, 1H), 6.88-6.80 (m, 2H), 6.70 (s, 1H), 6.66 (d, $J = 8.1$ Hz, 1H), 3.75 (s, 3H), 1.59 (s, 3H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 157.8 (d, $J = 232.4$ Hz), 144.3, 140.6, 138.0, 130.7 (d, $J = 9.1$ Hz), 130.5, 130.2, 130.1, 128.0, 127.5, 126.7, 121.9 (d, $J = 1.6$ Hz), 120.3, 119.5, 114.1, 111.3, 109.50, 109.45, 109.3, 103.0 (d, $J = 13.8$ Hz), 55.4, 33.0, 10.3 ppm.

$^{19}\text{F NMR}$ (282 MHz, CDCl_3) δ -125.2 ppm.

HRMS (ES+) Calcd for $\text{C}_{31}\text{H}_{25}\text{FN}_2\text{Na}$ [$\text{M} + \text{Na}$] $^+$: 467.1899, Found: 467.1893.

IR ν (KBr, cm^{-1}) 3442, 3056, 2926, 1631, 1506, 1483, 1444, 1381, 1350.



3d

5-Bromo-3-methyl-2-((1-methyl-1H-indol-3-yl)diphenylmethyl)-1H-indole

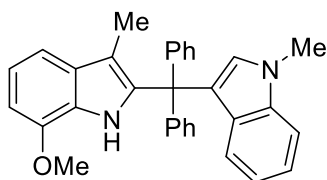
(3d) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 14:1) in 91% yield (153.1 mg). M.P. 264-265 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.15 (s, 1H), 7.64 (d, *J* = 1.8 Hz, 1H), 7.34-7.27 (m, 11H), 7.21-7.17 (m, 2H), 7.04 (d, *J* = 8.5 Hz, 1H), 6.85-6.81 (m, 1H), 6.69 (s, 1H), 6.64 (d, *J* = 8.1 Hz, 1H), 3.75 (s, 3H), 1.59 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 144.2, 140.1, 138.0, 132.3, 132.1, 130.5, 130.0, 128.1, 127.4, 126.8, 123.9, 121.9, 121.8, 120.9, 120.2, 119.5, 112.4, 112.3, 109.5, 109.1, 55.3, 33.0, 10.2 ppm.

HRMS (ES⁺) Calcd for C₃₁H₂₅BrN₂Na [M + Na]⁺: 527.1099, Found: 527.1105.

IR ν (KBr, cm⁻¹) 3480, 3420, 1613, 1601, 1382, 1350.



3e

7-Methoxy-3-methyl-2-((1-methyl-1H-indol-3-yl)diphenylmethyl)-1H-indole

(3e) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 12:1) in 88% yield (120.3 mg).

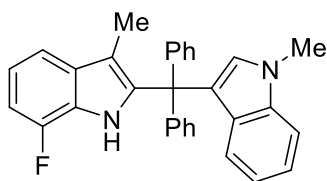
M.P. 213-214 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.24 (s, 1H), 7.33-7.27 (m, 11H), 7.19-7.14 (m, 2H), 7.04 (t, *J* = 15.6 Hz, 1H), 6.83 (t, *J* = 15.0 Hz, 1H), 6.72 (s, 1H), 6.69 (d, *J* = 8.1 Hz, 1H), 6.60 (d, *J* = 7.6 Hz, 1H), 3.85 (s, 3H), 3.74 (s, 3H), 1.63 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 145.8, 144.7, 138.2, 138.0, 131.7, 130.4, 130.1, 127.9 (2C), 127.6, 126.6, 124.1, 122.0, 121.6, 120.3, 119.5, 119.3, 111.2, 109.7, 109.3, 101.3, 55.3, 32.9, 10.5 ppm.

HRMS (ES⁺) Calcd for C₃₂H₂₈N₂ONa [M + Na]⁺: 479.2099, Found: 479.2090.

IR ν (KBr, cm⁻¹) 3451, 2922, 2852, 1631, 1598, 1481, 1447, 1365, 1245, 1215.



3f

7-Fluoro-3-methyl-2-((1-methyl-1H-indol-3-yl)diphenylmethyl)-1H-indole

(**3f**) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 14:1) in 93% yield (128.7 mg).

M.P. 233-234 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.24 (s, 1H), 7.34-7.28 (m, 12H), 7.19-7.16 (m, 1H), 7.01-6.98 (m, 1H), 6.86-6.81 (m, 2H), 6.71 (s, 1H), 6.68 (d, *J* = 8.1 Hz, 1H), 3.75 (s, 3H), 1.64 (s, 3H) ppm.

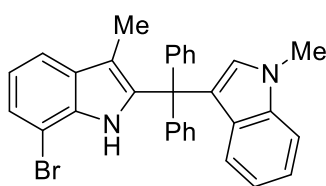
¹³C NMR (100 MHz, CDCl₃) δ 149.3 (d, *J* = 242.1 Hz), 144.3, 139.5, 138.0, 134.0 (d, *J* = 5.4 Hz), 130.4, 130.1, 128.1, 127.4, 126.8, 122.0, 121.9, 121.8, 120.1, 119.5,

119.2 (d, $J = 6.3$ Hz), 114.1 (d, $J = 3.2$ Hz), 110.2, 109.5, 106.2 (d, $J = 16.2$ Hz), 55.3, 33.0, 10.5 ppm.

^{19}F NMR (282 MHz, CDCl_3) δ -135.8 ppm.

HRMS (ES+) Calcd for $\text{C}_{31}\text{H}_{25}\text{FN}_2\text{Na}$ [$\text{M} + \text{Na}$] $^+$: 467.1899, Found: 467.1893.

IR ν (KBr, cm^{-1}) 3452, 3055, 2923, 2851, 1631, 1536, 1445, 1384, 1350, 1327, 1255.



3g

7-Bromo-3-methyl-2-((1-methyl-1H-indol-3-yl)diphenylmethyl)-1H-indole

(**3g**) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 14:1) in 97% yield (149.8 mg).

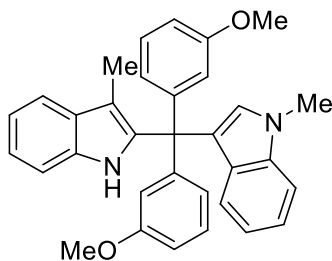
M.P. 226-228 °C.

^1H NMR (400 MHz, CDCl_3) δ 8.36 (s, 1H), 7.45 (d, $J = 7.9$ Hz, 1H), 7.34-7.30 (m, 11H), 7.25-7.17 (m, 2H), 6.97 (t, $J = 7.7$ Hz, 1H), 6.88-6.85 (m, 1H), 6.73 (d, $J = 8.0$ Hz, 1H), 6.68 (s, 1H), 3.75 (s, 3H), 1.62 (s, 3H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 144.2, 139.4, 138.0, 132.5, 131.3, 130.5, 130.0, 128.1 (2C), 127.4, 126.8, 123.5, 121.9, 121.8, 120.2, 119.5, 117.5, 110.5, 109.5, 104.4, 55.4, 33.0, 10.5 ppm.

HRMS (ES+) Calcd for $\text{C}_{31}\text{H}_{25}\text{BrN}_2\text{Na}$ [$\text{M} + \text{Na}$] $^+$: 527.1099, Found: 527.1104.

IR ν (KBr, cm^{-1}) 3431, 163, 158, 1382, 1350, 1150.



3h

2-(Bis(3-methoxyphenyl)(1-methyl-1H-indol-3-yl)methyl)-3-methyl-1H-

indole (3h) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 7:2) in 67% yield (98.2 mg).

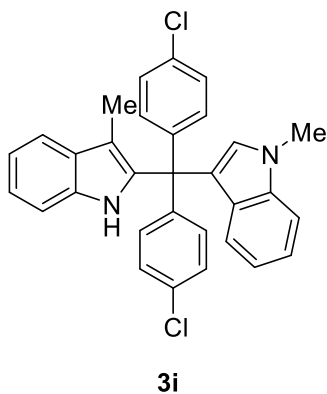
M.P. 277-278 °C.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.12(s, 1H), 7.54-7.52 (m, 1H), 7.31 (d, $J = 4.1$ Hz, 1H), 7.22-7.08 (m, 6H), 6.94-6.80 (m, 7H), 6.75-6.74 (m, 2H), 3.74 (s, 3H), 3.68 (s, 6H), 1.71 (s, 3H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.4, 146.2, 138.3, 138.0, 133.7, 130.5, 130.3, 128.7, 127.6, 123.0, 122.0, 121.7, 121.2, 120.1, 119.4, 118.9, 118.3, 116.6, 111.3, 110.8, 109.4, 109.2, 55.34, 55.25, 32.9, 10.4 ppm.

HRMS (ES+) Calcd for $\text{C}_{33}\text{H}_{30}\text{N}_2\text{O}_2\text{Na}$ $[\text{M} + \text{Na}]^+$: 509.2205, Found: 509.2209.

IR ν (KBr, cm^{-1}) 3444, 3368, 1631, 1601, 1484, 1461, 1426, 1350, 1286, 1246, 1187, 1048.



2-(Bis(4-chlorophenyl)(1-methyl-1H-indol-3-yl)methyl)-3-methyl-1H-indole

(3i) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 16:1) in 59% yield (87.9 mg).

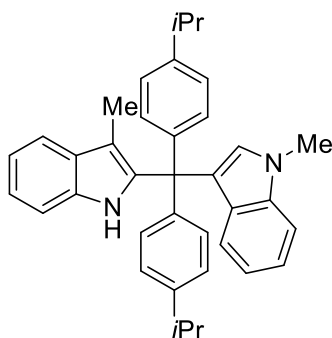
M.P. 243-245 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.04(s, 1H), 7.53-7.50 (m, 1H), 7.33 (d, *J* = 8.2 Hz, 1H), 7.25-7.18 (m, 9H), 7.16-7.08 (m, 3H), 6.85 (t, *J* = 7.6 Hz, 1H), 6.66 (d, *J* = 8.0 Hz, 1H), 6.62 (s, 1H), 3.73 (s, 3H), 1.64 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 142.6, 138.1, 137.7, 133.8, 132.7, 131.3, 130.4, 130.1, 128.2, 126.9, 122.1, 121.7, 121.6, 119.84, 119.81, 119.3, 118.4, 110.9, 109.7, 109.2, 54.5, 33.0, 10.5 ppm.

HRMS (ES⁺) Calcd for C₃₁H₂₄Cl₂N₂Na [M+ Na]⁺: 517.1214, Found: 517.1216.

IR ν (KBr, cm⁻¹) 3442, 1631, 1488, 1448, 1350, 1152, 1031.



3j

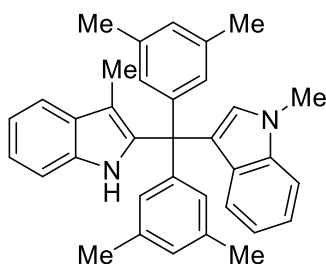
2-(Bis(4-isopropylphenyl)(1-methyl-1H-indol-3-yl)methyl)-3-methyl-1H-indole (3j) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 20:1) in 68% yield (104.2 mg). M.P. 222-223 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.01 (s, 1H), 7.54-7.52 (m, 1H), 7.33 (d, *J* = 8.2 Hz, 1H), 7.23-7.10 (m, 12H), 6.83 (t, *J* = 7.3 Hz, 1H), 6.74 (s, 1H), 6.69 (d, *J* = 8.1 Hz, 1H), 3.75 (s, 3H), 2.96-2.89 (m, 2H), 1.65 (s, 3H), 1.28 (d, *J* = 6.9 Hz, 12H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 146.9, 142.1, 139.1, 138.0, 133.7, 130.45, 130.36, 130.0, 127.8, 125.9, 122.2, 121.6, 121.0, 120.8, 119.2, 118.9, 118.2, 110.7, 109.3, 109.0, 54.6, 33.6, 32.9, 24.1, 10.3 ppm.

HRMS (ES⁺) Calcd for C₃₇H₃₈N₂Na [M + Na]⁺: 533.2932, Found: 533.2933.

IR ν (KBr, cm⁻¹) 3451, 2959, 2924, 1631, 1599, 1459, 1418, 1350.



3k

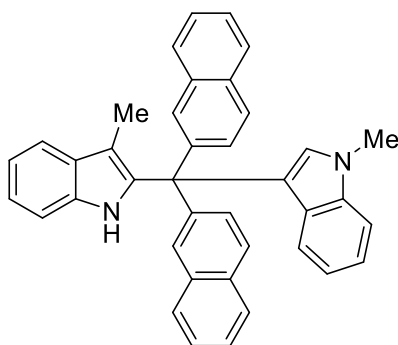
2-(Bis(3,5-dimethylphenyl)(1-methyl-1*H*-indol-3-yl)methyl)-3-methyl-1*H*-indole (3k) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 16:1) in 73% yield (105.7 mg). M.P. 251-252 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.11 (s, 1H), 7.56-7.53 (m, 1H), 7.32 (d, *J* = 8.2 Hz, 1H), 7.22-7.10 (m, 4H), 6.92 (s, 6H), 6.82 (t, *J* = 7.6 Hz, 1H), 6.71 (d, *J* = 7.5 Hz, 2H), 3.76 (s, 3H), 2.24 (s, 12H), 1.66 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 144.5, 138.8, 137.9, 137.0, 133.6, 130.4, 130.3, 128.1, 128.0, 127.8, 122.2, 121.5, 120.9, 120.8 (2C), 119.2, 118.8, 118.3, 110.7, 109.2, 55.1, 33.0, 21.8, 10.4 ppm.

HRMS (ES⁺) Calcd for C₃₅H₃₄N₂Na [M + Na]⁺: 505.2620, Found: 505.2626.

IR ν (KBr, cm⁻¹) 3447, 2915, 1631, 1596, 1458, 1408, 1350.



3l

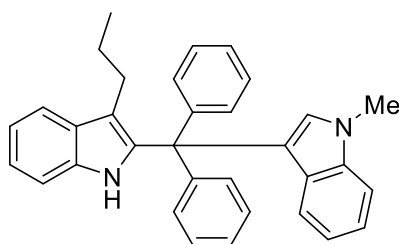
1-Methyl-3-((3-methyl-1*H*-indol-2-yl)di(naphthalen-2-yl)methyl)-1*H*-indole (3l) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 16:1) in 35% yield (55.5 mg). M.P. 278-279 °C.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.25 (s, 1H), 7.88 (s, 2H), 7.86 (d, $J = 7.9$ Hz, 2H), 7.74 (t, $J = 9.0$ Hz, 4H), 7.60-7.58 (m, 1H), 7.52-7.42 (m, 6H), 7.35 (d, $J = 8.6$ Hz, 1H), 7.23-7.13 (m, 4H), 6.79-6.75 (m, 3H), 3.76 (s, 3H), 1.71 (s, 3H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 141.8, 138.1, 138.0, 133.9, 133.2, 132.3, 130.5, 130.4, 129.3, 128.7, 128.0, 127.5, 127.4, 127.3, 126.1, 126.0, 121.9, 121.8, 121.3, 120.0, 119.6, 119.1, 118.4, 110.9, 109.7, 109.5, 55.5, 33.0, 10.3 ppm.

HRMS (ES+) Calcd for $\text{C}_{39}\text{H}_{30}\text{N}_2\text{Na}$ [$\text{M} + \text{Na}$] $^+$: 549.2307, Found: 549.2305

IR ν (KBr, cm^{-1}) 3442, 1631, 1599, 1457, 1418, 1381, 1350.



3m

3-(Diphenyl(3-propyl-1H-indol-2-yl)methyl)-1-methyl-1H-indole (3m) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 15:1) in 64% yield (87.2 mg).

M.P. 202-203 °C.

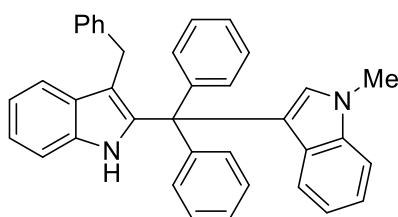
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.12 (s, 1H), 7.61 (d, $J = 6.5$ Hz, 1H), 7.37-7.29 (m, 11H), 7.20-7.13 (m, 4H), 6.85-6.81 (m, 2H), 6.74 (d, $J = 7.9$ Hz, 1H), 3.78 (s, 3H), 2.28 (t, $J = 7.8$ Hz, 2H), 0.93-0.89 (m, 2H), 0.55 (t, $J = 6.9$ Hz, 3H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 144.6, 138.0, 137.9, 134.0, 130.4, 130.3, 129.8, 127.8, 127.5, 126.6, 122.0, 121.8, 121.1, 120.6, 119.4, 119.2, 119.0, 114.1, 110.9, 109.4, 55.4,

32.9, 29.0, 21.8, 14.9 ppm.

HRMS (ES+) Calcd for C₃₃H₃₁N₂ [M+H]⁺: 455.2487, Found: 455.2479.

IR ν (KBr, cm⁻¹) 3443, 2960, 2911, 1637, 1588, 1431, 1453, 1411, 1350, 1201.



3n

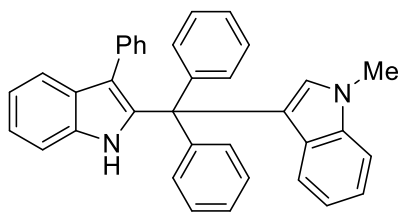
3-Benzyl-2-((1-methyl-1H-indol-3-yl)diphenylmethyl)-1H-indole (3n) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 15:1) in 98% yield (148.9 mg). M.P. 225-226 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.26 (s, 1H), 7.40-7.38 (m, 4H), 7.26-7.24 (m, 9H), 7.19-7.12 (m, 2H), 7.06-6.99 (m, 4H), 6.85 (t, *J* = 7.7 Hz, 1H), 6.77 (d, *J* = 9.7 Hz, 2H), 6.70 (d, *J* = 6.4 Hz, 2H), 3.71 (s, 2H), 3.62 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 144.4, 140.6, 139.5, 137.9, 133.9, 130.4, 130.18, 130.15, 128.4, 128.0, 127.63, 127.58, 126.6, 125.1, 121.9, 121.7, 121.3, 120.1, 119.8, 119.34, 119.29, 111.3, 110.9, 109.5, 55.5, 32.8, 31.8 ppm.

HRMS (ES+) Calcd for C₃₇H₃₁N₂ [M+H]⁺: 503.2487, Found: 503.2486.

IR ν (KBr, cm⁻¹) 3451, 2903, 1611, 1574, 1457, 1421, 1409, 1297, 1203.



3o

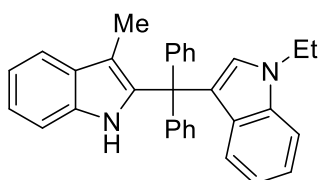
3-(Diphenyl(3-phenyl-1H-indol-2-yl)methyl)-1-methyl-1H-indole (3o) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 10:1) in 95% yield (138.8 mg). M.P. 239-241 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.42 (s, 1H), 7.35-7.28 (m, 6H), 7.23-7.13 (m, 9H), 7.08 (t, *J* = 7.2 Hz, 1H), 6.94 (t, *J* = 6.3 Hz, 1H), 6.87-6.78 (m, 4H), 6.70 (d, *J* = 6.7 Hz, 2H), 6.57 (s, 1H), 3.56 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 145.3, 137.8, 137.4, 135.3, 133.9, 131.2, 130.5, 130.3, 128.2, 127.8 (2C), 126.7, 126.5, 124.9, 122.0, 121.9, 121.5, 119.74, 119.70, 119.4, 119.3, 116.4, 110.7, 109.2, 55.9, 32.6 ppm.

HRMS (ES⁺) Calcd for C₃₆H₂₉N₂ [M + H]⁺: 489.2331, Found: 489.2239.

IR ν (KBr, cm⁻¹) 3438, 2913, 1703, 1619, 1433, 1416, 1398, 1292, 1197.



4a

1-Ethyl-3-((3-methyl-1H-indol-2-yl)diphenylmethyl)-1H-indole (4a) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 14:1) in 90% yield (118.4 mg).

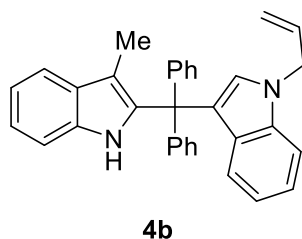
M.P. 231-233 °C.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.12 (s, 1H), 7.56-7.53 (m, 1H), 7.28-7.29 (m, 11H), 7.21-7.12 (m, 4H), 6.85 (t, $J = 7.7$ Hz, 1H), 6.79 (s, 1H), 6.70 (d, $J = 8.0$ Hz, 1H), 4.14 (dd, $J_1 = 7.2$ Hz, $J_2 = 14.4$ Hz, 2H), 1.66 (s, 3H), 1.44 (t, $J = 7.2$ Hz, 3H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 144.5, 138.8, 137.0, 133.7, 130.3, 130.1, 129.0, 127.9, 127.7, 126.6, 122.1, 121.6, 121.2, 120.5, 119.3, 119.0, 118.3, 110.8, 109.5, 109.2, 55.4, 41.1, 15.7, 10.2 ppm.

HRMS (ES+) Calcd for $\text{C}_{32}\text{H}_{28}\text{N}_2\text{Na}$ [$\text{M} + \text{Na}$] $^+$: 463.2150, Found: 463.2155.

IR ν (KBr, cm^{-1}) 3449, 3052, 2982, 2929, 2809, 1631, 1566, 1489, 1484, 1472, 1457, 1444, 1418 138, 1350.



1-Allyl-3-((3-methyl-1H-indol-2-yl)diphenylmethyl)-1H-indole (4b) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 12:1) in 80% yield (108.6 mg).

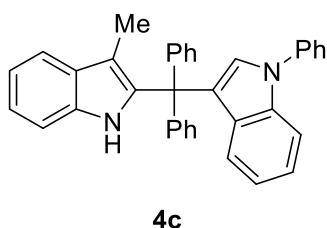
M.P. 241-242 °C.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.11 (s, 1H), 7.56-7.54 (m, 1H), 7.36-7.29 (m, 11H), 7.22-7.11 (m, 4H), 6.87-6.82 (m, 1H), 6.79 (s, 1H), 6.71 (d, $J = 8.1$ Hz, 1H), 6.03-5.94 (m, 1H), 5.19 (d, $J = 10.2$ Hz, 1H), 5.05 (d, $J = 17.0$ Hz, 1H), 4.70 (d, $J = 4.7$ Hz, 2H), 1.67 (s, 3H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 144.5, 138.6, 137.4, 133.7, 133.5, 130.3, 130.1, 129.7, 128.0, 127.8, 126.6, 122.1, 121.8, 121.2, 120.8, 119.5, 119.1, 118.3, 117.1, 110.8, 109.9, 109.2, 55.3, 48.9, 10.3 ppm.

HRMS (ES+) Calcd for $\text{C}_{33}\text{H}_{28}\text{N}_2\text{Na}$ $[\text{M} + \text{Na}]^+$: 475.2150, Found: 475.2146.

IR ν (KBr, cm^{-1}) 3445, 1631, 1602, 1472, 1382, 1350.



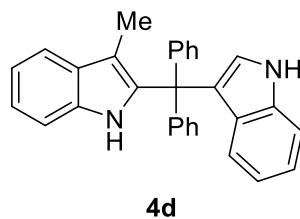
2-(Diphenyl(1-phenyl-1H-indol-3-yl)methyl)-3-methyl-1H-indole (4c) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 24:1) in 65% yield (94.6 mg). M.P. 256-257 °C.

^1H NMR (400 MHz, CDCl_3) δ 8.12 (s, 1H), 7.59-7.49 (m, 6H), 7.38-7.28 (m, 11H), 7.24-7.10 (m, 4H), 7.05 (s, 1H), 6.89 (t, $J = 7.7$ Hz, 1H), 6.76 (d, $J = 8.0$ Hz, 1H), 1.70 (s, 3H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 144.3, 139.6, 138.3, 137.2, 133.8, 130.3, 130.2, 129.7, 129.6, 128.5, 128.1, 126.8, 126.7, 124.6, 122.9, 122.6, 122.3, 121.3, 120.4, 119.1, 118.3, 110.8, 110.7, 109.4, 55.4, 10.3 ppm.

HRMS (ES+) Calcd for $\text{C}_{36}\text{H}_{28}\text{N}_2\text{Na}$ $[\text{M} + \text{Na}]^+$: 511.2150, Found: 511.2152.

IR ν (KBr, cm^{-1}) 3448, 3089, 1506, 1499, 1457, 1457, 1418, 1235, 1156.



2-((1H-indol-3-yl)diphenylmethyl)-3-methyl-1H-indole (4d) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 8:1) in 52% yield (64.2 mg).

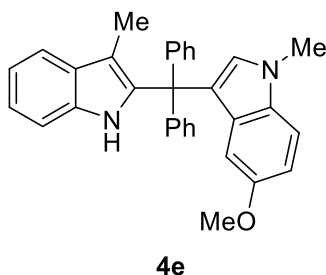
M.P. 253-254 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.05 (s, 1H), 7.96 (s, 1H), 7.52-7.50 (m, 1H), 7.35-7.23 (m, 11H), 7.14-7.08 (m, 4H), 6.82-6.79 (m, 2H), 6.67 (d, *J* = 8.0 Hz, 1H), 1.62 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 144.4, 138.5, 137.2, 133.8, 130.3, 130.1, 128.0, 127.2, 126.7, 125.9, 122.25, 122.17, 121.9, 121.3, 119.9, 119.1, 118.3, 111.4, 110.8, 109.3, 55.3, 10.3 ppm.

HRMS (ES⁺) Calcd for C₃₀H₂₄N₂Na [M + Na]⁺: 435.1837, Found: 435.1827.

IR ν (KBr, cm⁻¹) 3442, 3365, 3055, 1613, 1597, 1457, 1418, 1350.



5-Methoxy-1-methyl-3-((3-methyl-1H-indol-2-yl)diphenylmethyl)-1H-indole (4e) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 8:1) in 93% yield (127.2 mg).

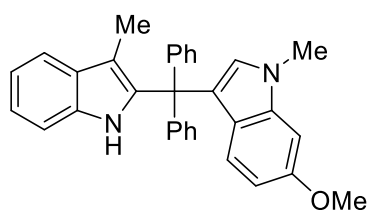
M.P. 239-241 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.12 (s, 1H), 7.55-7.53 (m, 1H), 7.32-7.28 (m, 10H), 7.21-7.11 (m, 4H), 6.83 (dd, *J*₁ = 1.8 Hz, *J*₂ = 7.0 Hz, 1H), 6.70 (s, 1H), 6.00 (s, 1H), 3.72 (s, 3H), 3.31 (s, 3H), 1.66 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 153.6, 144.4, 138.8, 133.7, 133.3, 130.9, 130.3, 130.2, 128.0, 127.7, 126.6, 121.2, 120.1, 119.1, 118.2, 112.4, 110.8, 110.2, 109.2, 103.0, 55.4, 55.3, 33.1, 10.3 ppm.

HRMS (ES⁺) Calcd for C₃₂H₂₈N₂ONa [M + Na]⁺: 479.2099, Found: 479.2090.

IR ν (KBr, cm⁻¹) 3451, 3377, 3054, 3018, 2938, 1631, 1588, 1490, 1444, 1424, 1380, 1224.



4f

6-Methoxy-1-methyl-3-((3-methyl-1H-indol-2-yl)diphenylmethyl)-1H-indole

(**4f**) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 12:1) in 76% yield (104.1 mg).

M.P. 259-260 °C.

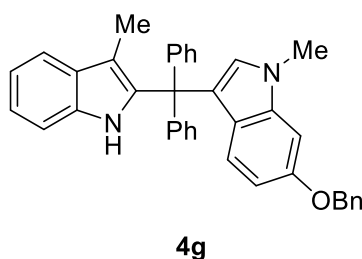
¹H NMR (400 MHz, CDCl₃) δ 8.10 (s, 1H), 7.51 (s, 1H), 7.27-7.10 (m, 13H), 6.74 (s, 1H), 6.56-6.48 (m, 3H), 3.83 (s, 3H), 3.02 (s, 3H), 1.63 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 156.2, 144.4, 138.7, 138.6, 133.6, 130.2, 130.0, 128.1, 129.4, 127.8, 126.5, 122.6, 121.8, 121.1, 120.5, 119.0, 110.7, 109.2, 109.1, 92.7, 55.6,

55.2, 32.9, 10.2 ppm.

HRMS (ES+) Calcd for C₃₂H₂₈N₂ONa [M + Na]⁺: 479.2099, Found: 479.2095.

IR ν (KBr, cm⁻¹) 3442, 3068, 2931, 1688, 1490, 1458, 1420, 1418, 1332, 1254, 1227, 1205, 1172, 1119, 1108, 1034.



6-(Benzyloxy)-1-methyl-3-((3-methyl-1H-indol-2-yl)diphenylmethyl)-1H-

indole (4g) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 8:1) in 84% yield (134.2 mg).

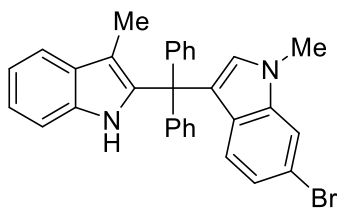
M.P. 226-227 °C.

¹H NMR (400 MHz, CDCl₃) δ 8.13 (s, 1H), 7.55-7.53 (m, 1H), 7.48 (d, *J* = 7.2 Hz, 2H), 7.41 (t, *J* = 7.1 Hz, 2H), 7.37-7.28 (m, 11H), 7.20-7.18 (m, 1H), 7.15-7.10 (m, 2H), 6.86 (d, *J* = 1.6 Hz, 1H), 6.61-6.58 (m, 2H), 6.55 (d, *J* = 8.8 Hz, 1H), 5.10 (s, 2H), 3.68 (s, 3H), 1.66 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 155.5, 144.5, 138.72, 138.70, 137.4, 133.7, 130.3, 130.1, 129.7, 128.7, 128.1, 127.9, 127.7, 126.6, 122.7, 122.1, 121.2, 120.6, 119.0, 118.3, 110.8, 109.7, 109.2, 94.1, 70.6, 55.2, 33.0, 10.3 ppm.

HRMS (ES+) Calcd for C₃₈H₃₂N₂ONa [M + Na]⁺: 555.2412, Found: 555.2411.

IR ν (KBr, cm⁻¹) 3441, 1631, 1588, 1489, 1472, 1382, 1350, 1332.



4h

6-Bromo-1-methyl-3-((3-methyl-1H-indol-2-yl)diphenylmethyl)-1H-indole

(4h) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 24:1) in 64% yield (97.1 mg).

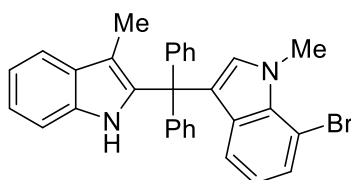
M.P. 276-277 °C.

¹H NMR (400 MHz, CDCl₃) δ 7.97 (s, 1H), 7.54-7.49 (m, 2H), 7.29 (s, 10H), 7.21-7.12 (m, 3H), 6.92 (d, *J* = 8.5 Hz, 1H), 6.71 (s, 1H), 6.50 (d, *J* = 8.6 Hz, 1H), 3.17 (s, 3H), 1.64 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 144.3, 138.8, 138.2, 133.7, 131.0, 130.3, 130.1, 128.1, 126.8, 126.5, 123.2, 122.7, 121.4, 120.8, 119.2, 118.3, 115.6, 112.6, 110.8, 109.4, 55.1, 33.1, 10.3 ppm.

HRMS (ES⁺) Calcd for C₃₁H₂₅BrN₂Na [M + Na]⁺: 527.1099, Found: 527.1097.

IR ν (KBr, cm⁻¹) 3450, 2811, 1632, 1578, 1445, 1418, 1382, 1350.



4i

7-Bromo-1-methyl-3-((3-methyl-1H-indol-2-yl)diphenylmethyl)-1H-indole

(4i) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 30:1) in 56% yield (84.9 mg).

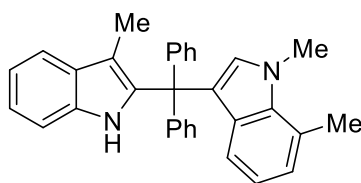
M.P. 273-274 °C.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.00 (s, 1H), 7.55-7.53 (m, 1H), 7.34-7.29 (m, 11H), 7.22-7.12 (m, 3H), 6.68 (s, 1H), 6.61-6.60 (m, 2H), 4.12 (s, 3H), 1.65 (s, 3H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 144.2, 138.1, 134.3, 133.7, 133.6, 130.6, 130.3, 130.1, 128.1, 126.9, 121.5, 121.4, 120.5, 120.1, 119.2, 118.3, 110.8, 109.4, 55.1, 104.0, 55.2, 37.2, 10.3 ppm.

HRMS (ES+) Calcd for $\text{C}_{31}\text{H}_{25}\text{BrN}_2\text{Na}$ $[\text{M} + \text{Na}]^+$: 527.1099, Found: 527.1100.

IR ν (KBr, cm^{-1}) 3451, 1631, 1489, 1457, 1418, 1381, 1350.



4j

1,7-Dimethyl-3-((3-methyl-1H-indol-2-yl)diphenylmethyl)-1H-indole (4j)

was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM = 16:1) in 95% yield (132.0 mg).

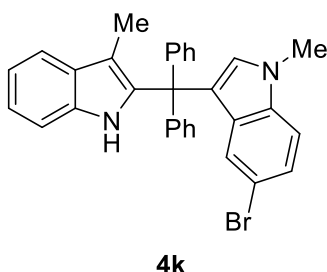
M.P. 231-232 °C.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.13 (s, 1H), 7.55-7.53 (m, 1H), 7.30-7.28 (m, 10H), 7.19-7.11 (m, 3H), 6.87 (d, $J = 6.9$ Hz, 1H), 6.68 (t, $J = 7.7$ Hz, 1H), 6.59 (s, 1H), 6.53 (d, $J = 8.0$ Hz, 1H), 4.01 (s, 3H), 2.80 (s, 3H), 1.66 (s, 3H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 144.4, 138.8, 136.8, 133.7, 132.4, 130.3, 130.1, 128.5, 127.9, 126.6, 124.5, 121.3, 121.2, 120.2, 120.0, 119.6, 119.0, 118.2, 110.8, 109.1, 55.3, 37.1, 20.0, 10.3 ppm.

HRMS (ES+) Calcd for C₃₂H₂₈N₂Na [M + Na]⁺: 463.2150, Found: 463.2157.

IR ν (KBr, cm⁻¹) 3450, 1630, 1620, 1489, 1459, 1407, 1418, 1380, 1350.



5-Bromo-1-methyl-3-((3-methyl-1H-indol-2-yl)diphenylmethyl)-1H-indole

(**4k**) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/DCM =12:1) in 75% yield (114.4 mg).

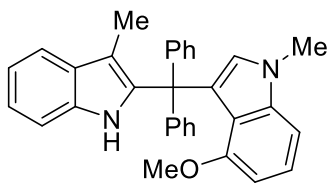
M.P. 244-246 °C.

¹H NMR (400 MHz, CDCl₃) δ 7.97 (s, 1H), 7.55-7.53 (m, 1H), 7.30-7.29 (m, 10H), 7.24-7.16 (m, 3H), 7.15-7.10 (m, 2H), 6.75 (s, 1H), 6.73 (d, *J* = 1.7 Hz, 1H), 3.72 (s, 3H), 1.65 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 144.1, 138.4, 136.6, 133.7, 131.6, 130.3, 130.1, 129.2, 128.1, 126.8, 124.8, 124.3, 121.4, 120.1, 119.2, 118.3, 112.8, 111.0, 110.9, 109.2, 55.1, 33.1, 10.3 ppm.

HRMS (ES+) Calcd for C₃₁H₂₅BrN₂Na [M + Na]⁺: 527.1099, Found: 527.1096.

IR ν (KBr, cm⁻¹) 3453, 3055, 1631, 1589, 1474, 1418, 1382, 1350.



4I

4-Methoxy-1-methyl-3-((3-methyl-1H-indol-2-yl)diphenylmethyl)-1H-indole

(4I) was prepared according to the General Procedure B as a white solid (chromatography eluent: petroleum ether/EtOAc = 100:1) in 76% yield (103.8 mg).

M.P. 235-236 °C.

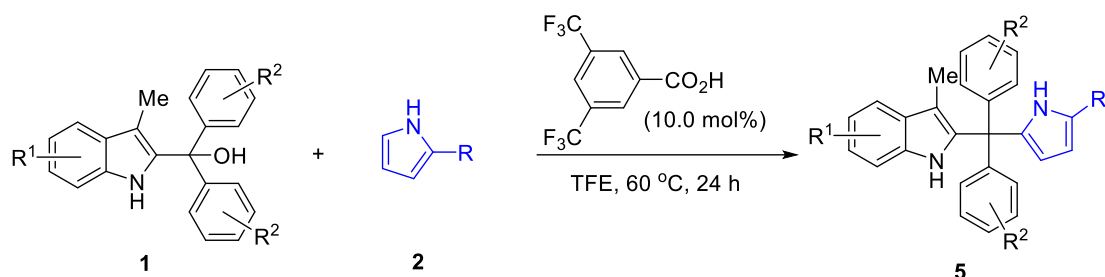
¹H NMR (400 MHz, CDCl₃) δ 8.07 (s, 1H), 7.50-7.48 (m, 1H), 7.24-7.12 (m, 12H), 7.10-7.05 (m, 2H), 6.93 (d, *J* = 8.2 Hz, 1H), 6.45 (s, 1H), 6.30 (d, *J* = 7.8 Hz, 1H), 3.66 (s, 3H), 2.95 (s, 3H), 1.61 (s, 3H) ppm.

¹³C NMR (100 MHz, CDCl₃) δ 158.3, 145.9, 139.9, 133.7, 130.3, 130.2, 130.1, 130.0, 127.3 (2C), 125.9, 122.9, 120.7, 118.6, 118.0, 117.9, 110.5, 108.5, 102.4, 100.4, 56.0, 54.3, 33.1, 10.4 ppm.

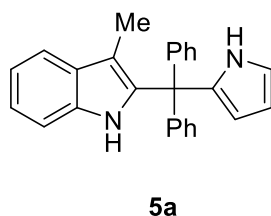
HRMS (ES⁺) Calcd for C₃₂H₂₈N₂O [M + Na]⁺: 527.1099, Found: 527.1096.

IR ν (KBr, cm⁻¹) 3461, 2962, 2812, 1631, 1588, 1498, 1458, 1382, 1350, 1262, 1094, 1026.

General Procedure C for the Synthesis of Tetraarylmethanes 5.



To a solution of indol-2-yl methanols **1** (0.3 mmol, 1.0 equiv), pyrroles **2** (0.6 mmol, 2.0 equiv) in $\text{CF}_3\text{CH}_2\text{OH}$ (3.0 mL) was added 3,5-bis(trifluoromethyl)benzoic acid (7.7 mg, 0.03 mmol, 10.0 mol%). The reaction mixture was warmed up to 60 °C and kept stirring for 24 h. The reaction mixture was directly concentrated under reduced pressure. The residue was purified by silica gel column chromatography (eluent: petroleum ether/DCM) to afford the desired products **5**.



2-(Diphenyl(1H-pyrrol-2-yl)methyl)-3-methyl-1H-indole (5a) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/DCM = 8:1) in 65% yield (70.2 mg).

M.P. 187-188 °C.

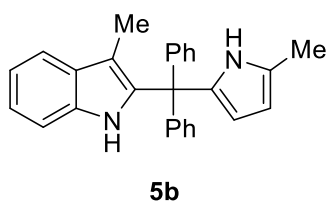
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.00 (s, 1H), 7.77 (s, 1H), 7.57 (d, $J = 7.0$ Hz, 1H), 7.36-7.28 (m, 6H), 7.25-7.12 (m, 7H), 6.76 (d, $J = 1.4$ Hz, 1H), 6.24-6.22 (m, 1H), 6.05 (s, 1H), 1.71 (s, 3H) ppm.

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 144.5, 137.0, 135.2, 134.1, 130.3, 129.7, 128.3, 127.2,

121.8, 119.4, 118.5, 117.4, 110.9, 110.1, 110.0, 108.5, 56.4, 9.8 ppm.

HRMS (ES+) Calcd for C₂₆H₂₂N₂Na [M + Na]⁺: 385.1681, Found: 385.1684.

IR ν (KBr, cm⁻¹) 3448, 3398, 3054, 2915, 1457, 1421, 1331, 1034.



3-Methyl-2-((5-methyl-1H-pyrrol-2-yl)diphenylmethyl)-1H-indole (5b) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/DCM = 20:1) in 91% yield (102.3 mg). M.P. 179-181 °C.

¹H NMR (400 MHz, CDCl₃) δ 7.82 (s, 1H), 7.67 (s, 1H), 7.59-7.57 (m, 1H), 7.35-7.28 (m, 7H), 7.25-7.23 (m, 4H), 7.19-7.13 (m, 2H), 5.88 (d, *J* = 2.5 Hz, 2H), 2.24 (s, 3H), 1.73 (s, 3H) ppm.

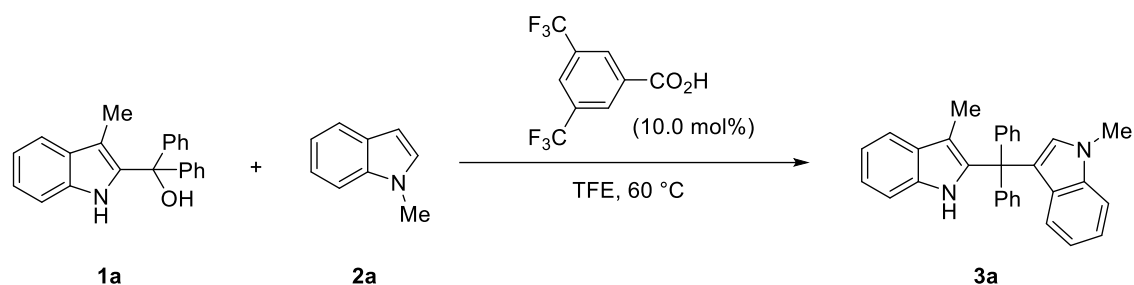
¹³C NMR (100 MHz, CDCl₃) δ 144.6, 137.2, 134.0, 133.6, 130.3, 129.7, 128.2, 127.5, 127.1, 121.7, 119.4, 118.5, 110.9, 110.3, 109.9, 106.2, 56.4, 13.4, 9.9 ppm.

HRMS (ES+) Calcd for C₂₇H₂₄N₂Na [M + Na]⁺: 399.1837, Found: 399.1834.

IR ν (KBr, cm⁻¹) 3449, 3434, 1598, 1489, 1472, 1457, 1444.

IV. Gram-scale Synthesis and Bioactivity of Products

Gram-scale synthesis:



To a solution of 2-indolylmethanol **1a** (1.25 g, 4.0 mmol, 1.0 equiv), arene **2a** (1.05 g, 8.0 mmol, 2.0 equiv) in $\text{CF}_3\text{CH}_2\text{OH}$ (40 mL) was added 3,5-bis(trifluoromethyl)benzoic acid (103.3 mg, 0.4 mmol, 10.0 mol%). The reaction mixture was warmed up to 60 °C and kept stirring for 24 h. The reaction mixture was directly concentrated under reduced pressure. The residue was purified by silica gel column chromatography (eluent: petroleum ether/DCM = 24:1) to afford the desired products **3a** in 83% yield (1.42 g).

Bioactivity of Products

Cell lines and cell culture conditions

L929, 4T1, HeLa and HepG2 cells were cultured in DMEM with 10% FBS and 50 U/mL penicillin and streptomycin.

Cell viability test

MTT assay was applied to examine the cell viability. Cells (5×10^3 cells/well) were cultured in 96-well plates overnight. Then, the culture medium was removed, cells were washed with PBS, and the fresh medium containing various concentrations of the compounds was added to incubate with the cells for 24 h. After incubation, the medium was added with 20 μ L of MTT (5 mg/mL). After 4 h of incubation at 37 °C, the medium was aspirated, and 200 μ L DMSO was added into each well. The 96-well plates were placed on a shaker at 100 rpm for 10 min, then the absorptions at 570 nm were measured by a microplate reader (Multiskan FC, Thermo-Fisher, USA).

Table S1. Anticancer activity of selected products

TAMs	IC ₅₀ value (μ M) ^a			
	L929	4T1	Hela	HepG2
3c	>50	>50	>50	>50
3d	>50	22.4	49.0	>50
3f	>50	>50	>50	>50

3g	>50	42.7	>50	>50
3h	>50	>50	27.8	>50
4e	>50	>50	27.4	>50
4f	>50	24.2	>50	>50
4g	>50	>50	>50	>50
Doxorubicin	>50	1.9	2.0	11.4

^a The half maximal inhibitory concentration (IC₅₀) was determined by MTT assay in 24h. Data were calculated from three independent experiments using OriginLab 2019 software.

V. Determination of Product Structure

The structure of product **3b** was determined by X-ray diffraction. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2363600). The data can be obtained free of charge via the internet at <https://www.ccdc.cam.ac.uk/structures/>. The measurements were taken in a Bruker D8 Venture CCD diffractometer. The data were integrated by Bruker D8 Venture with λ and ω scans absorption corrections. The structure solution and refinement were processed by ShelXL (Rigaku OD, 2021).

Method of crystallization: A solution of **3b** in DCM and petroleum ether was evaporated the solvent slowly at room temperature.

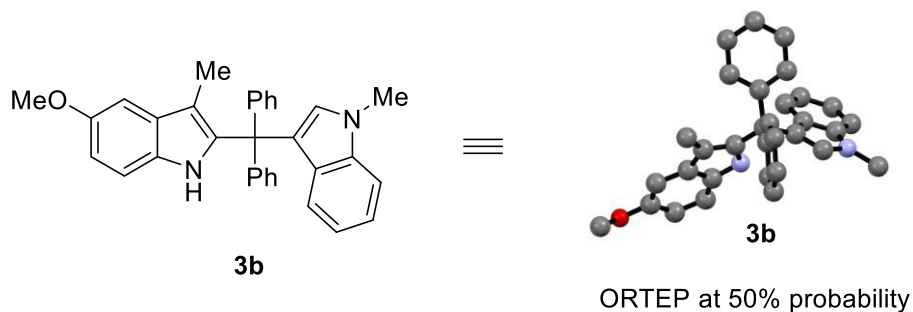
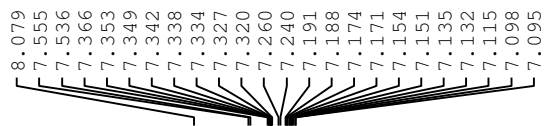
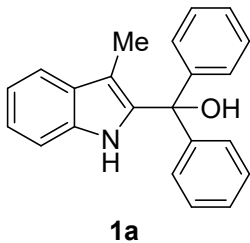


Table S2 Crystal data and structure refinement for 3b.

Identification code	3b
Empirical formula	C ₃₂ H ₂₈ N ₂ O ₅
Formula weight	456.56
Temperature/K	296.5
Crystal system	monoclinic
Space group	P21/n
a/Å	21.5474(10)
b/Å	11.3765(4)
c/Å	22.1803(10)

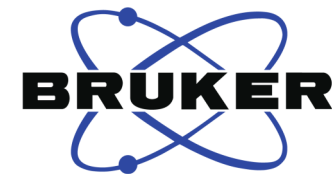
$\alpha/^\circ$	90
$\beta/^\circ$	113.870(5)
$\gamma/^\circ$	90
Volume/ \AA^3	4972.1(4)
Z	8
$\rho_{\text{calc}}/\text{g}/\text{cm}^3$	1.220
μ/mm^{-1}	0.074
F(000)	1936
Crystal size/ mm^3	$0.12 \times 0.15 \times 0.1$
Radiation	GaK α ($\lambda = 0.71073$)
2Θ range for data collection/ $^\circ$	2.002 to 27.9470
Index ranges	$-27 \leq h \leq 30, -16 \leq k \leq 15, -31 \leq l \leq 31$
Reflections collected	49527
Independent reflections	14788 [$R_{\text{int}} = 0.0557, R_{\text{sigma}} = 0.0820$]
Data/restraints/parameters	14788/0/631
Goodness-of-fit on F^2	1.129
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.1169, wR_2 = 0.3338$
Final R indexes [all data]	$R_1 = 0.2195, wR_2 = 0.3914$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	0.766/-0.473

wj-4-70-1



2.988

1.874

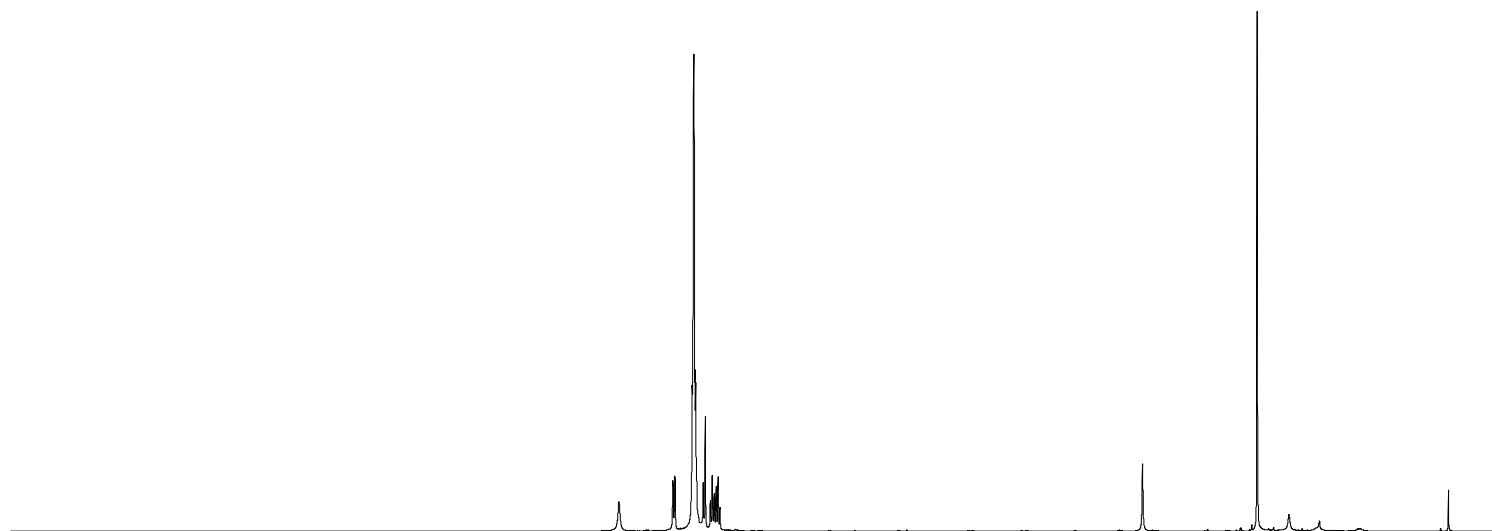


Current Data Parameters
NAME 20230725-400M
EXPNO 37
PROCNO 1

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Time 0.47
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PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 90.23
DW 60.800 usec
DE 6.50 usec
TE 292.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900275 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



0.89
1.08
10.29
0.92
1.09
1.08

0.91

3.00

wj-4-70-10

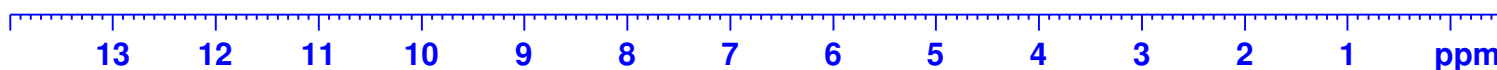
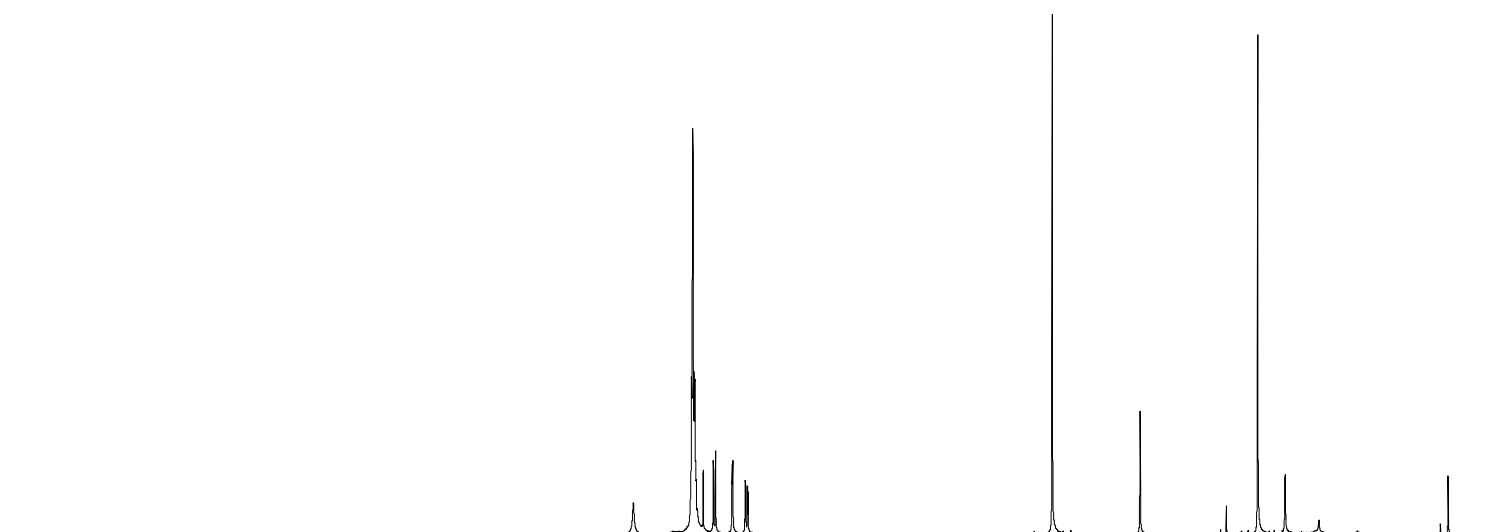
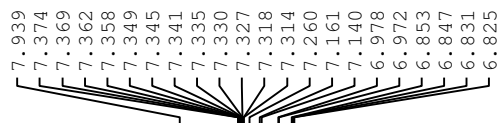
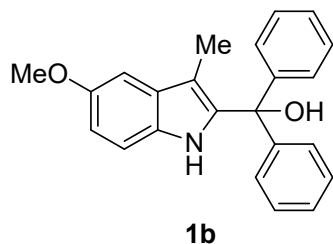


Current Data Parameters
NAME 20230725-400M
EXPNO 55
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230725
Time 4.12
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.67
DW 60.800 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



wj-4-70-6

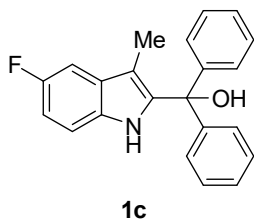


Current Data Parameters
NAME 20230725-400M
EXPNO 47
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230725
Time 2.41
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 292.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

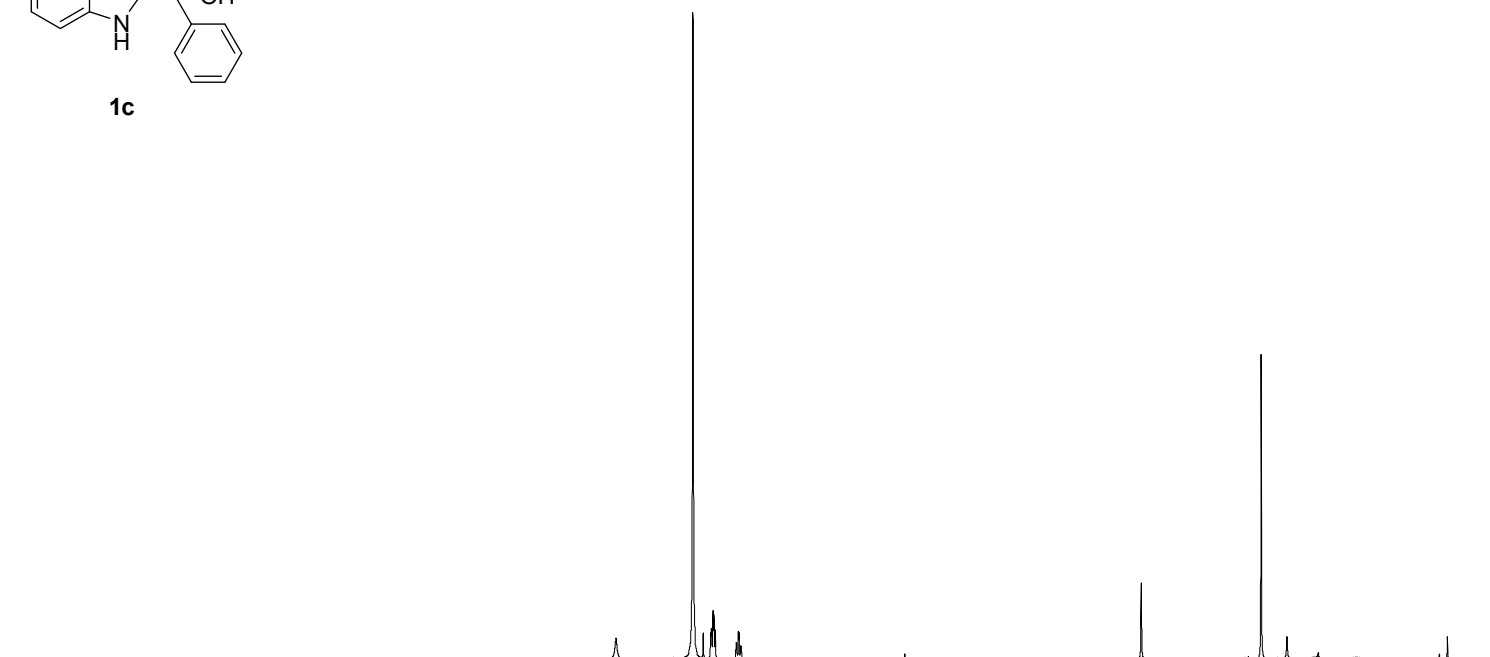
F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



8.108
7.360
7.260
7.188
7.182
7.177
7.165
7.156
7.144
6.940
6.934
6.918
6.912
6.895
6.889

3.001

1.836



13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.84

10.07

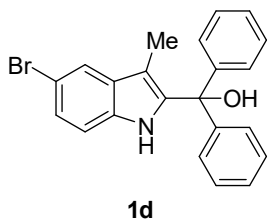
2.10

1.02

0.92

3.00

wj-4-70-8



8.189
7.658
7.654
7.390
7.386
7.381
7.373
7.371
7.368
7.361
7.351
7.344
7.333
7.322
7.315
7.260
7.255
7.251
7.234
7.229
7.140
7.119

2.985

1.815

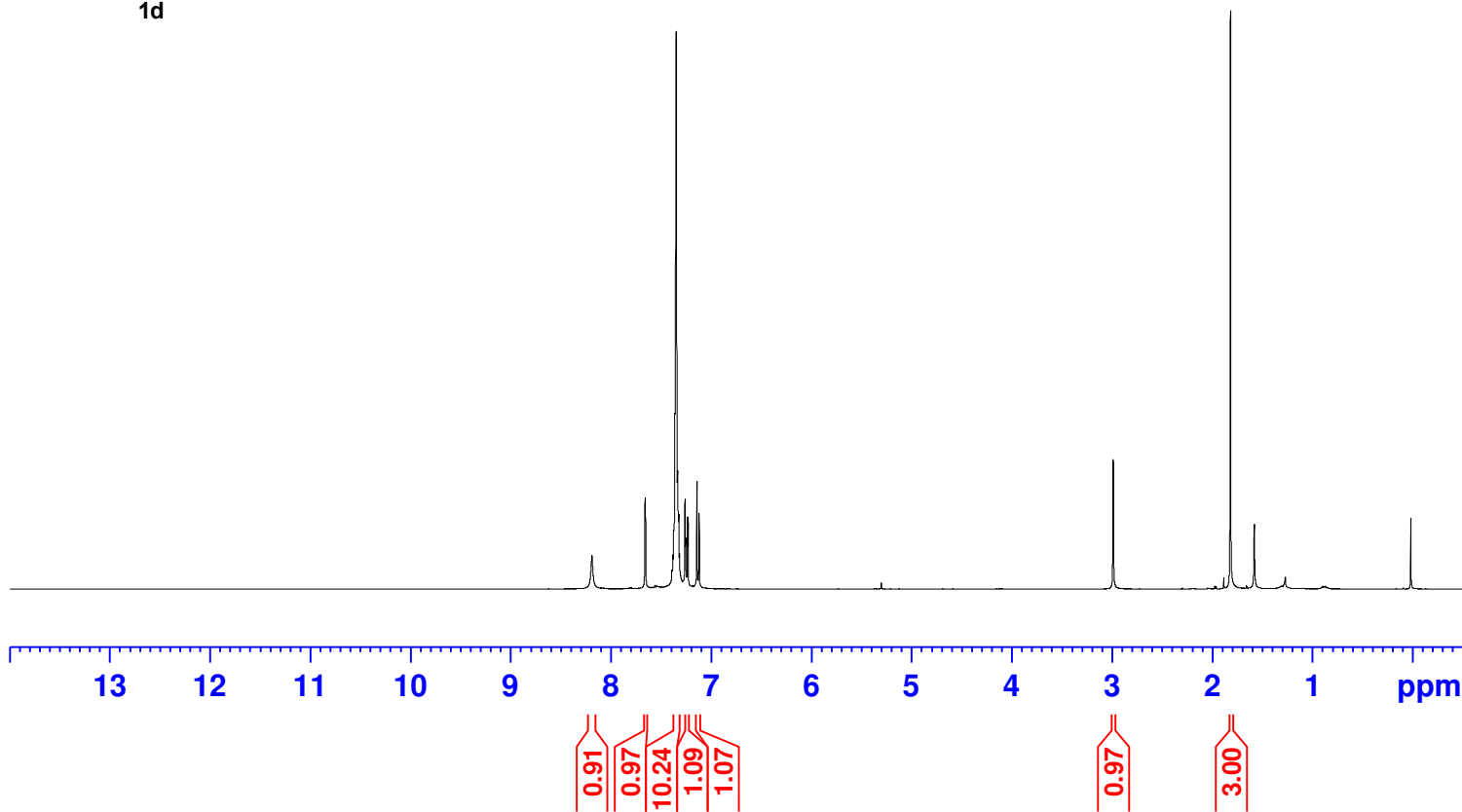


Current Data Parameters
NAME 20230725-400M
EXPNO 51
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230725
Time 3.26
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 125.76
DW 60.800 usec
DE 6.50 usec
TE 292.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



wj-4-70-11

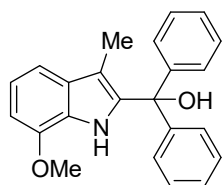
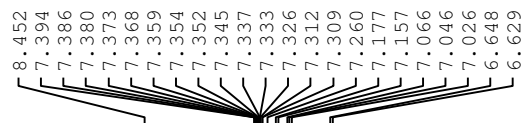


Current Data Parameters
NAME 20230725-400M
EXPNO 57
PROCNO 1

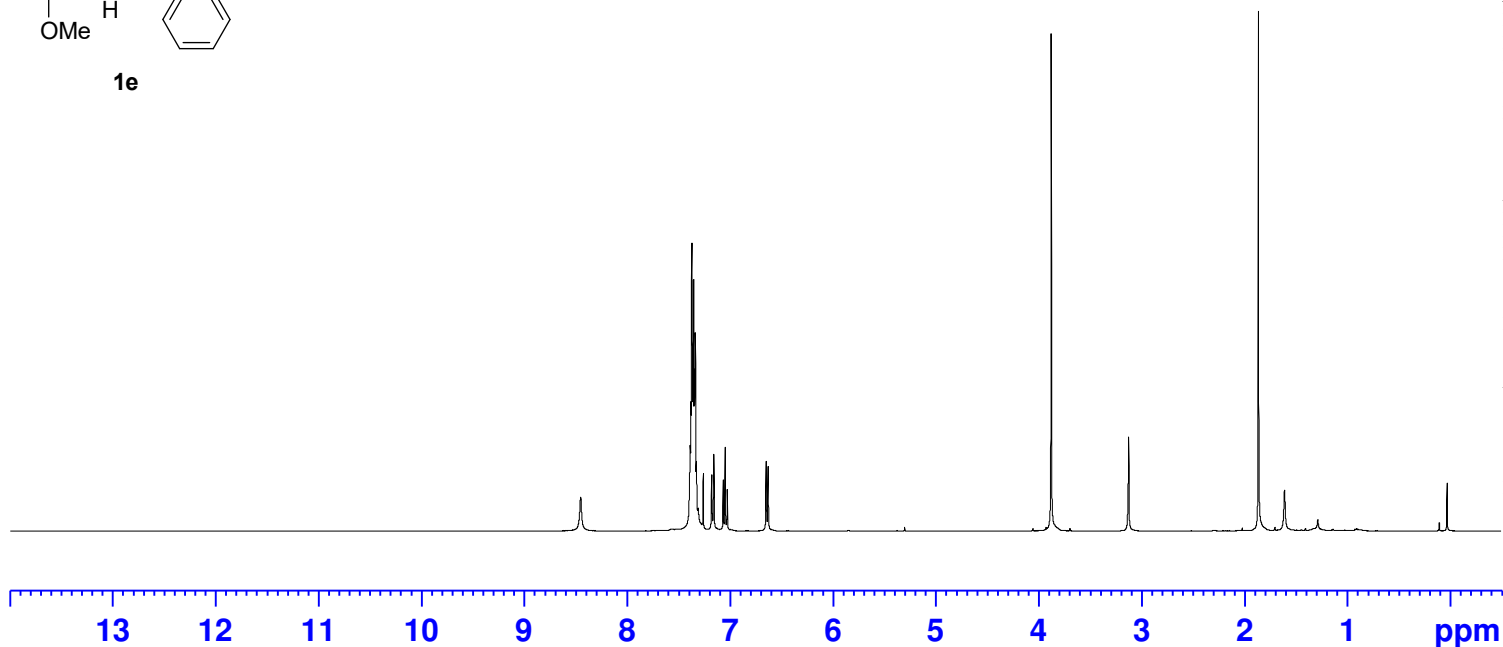
F2 - Acquisition Parameters
Date_ 20230725
Time 7.55
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1e



0.91

10.37

1.08

1.03

1.03

3.04

1.01

3.00

wj-4-70-13

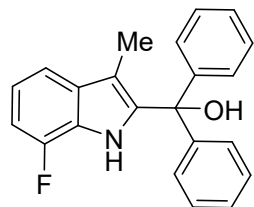


Current Data Parameters
NAME 20230730-400M
EXPNO 52
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230729
Time 19.45
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 125.76
DW 60.800 usec
DE 6.50 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

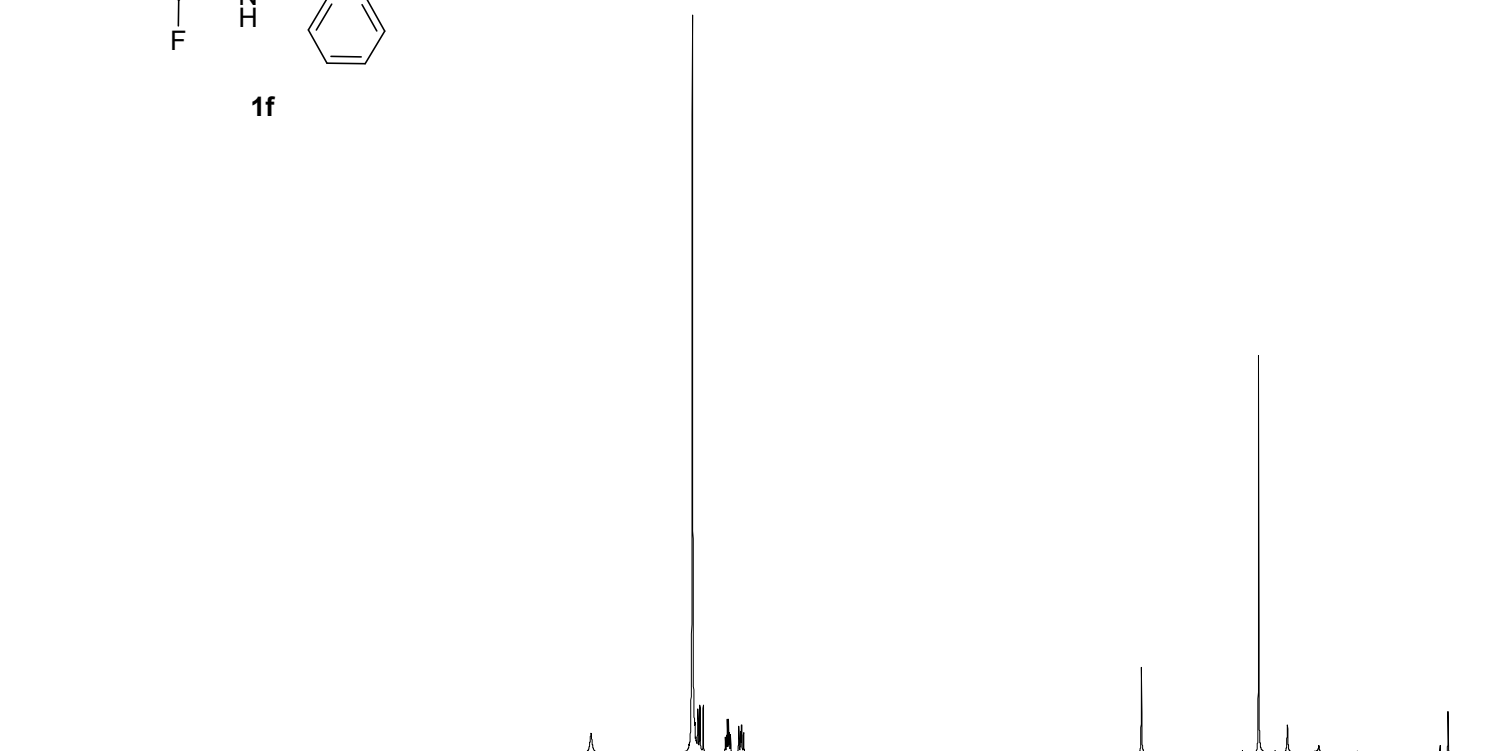


1f

8.351
7.365
7.312
7.292
7.260
7.046
7.034
7.026
7.014
7.006
6.994
6.915
6.895
6.887
6.867

3.000

1.860



13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.93

10.06

1.06

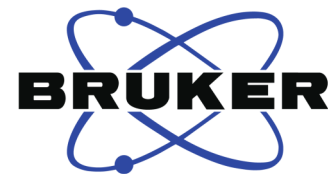
1.02

0.99

0.94

3.00

wj-4-70-9

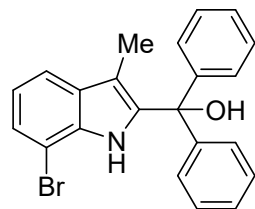


Current Data Parameters
NAME 20230725-400M
EXPNO 53
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230725
Time 3.49
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 140.02
DW 60.800 usec
DE 6.50 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

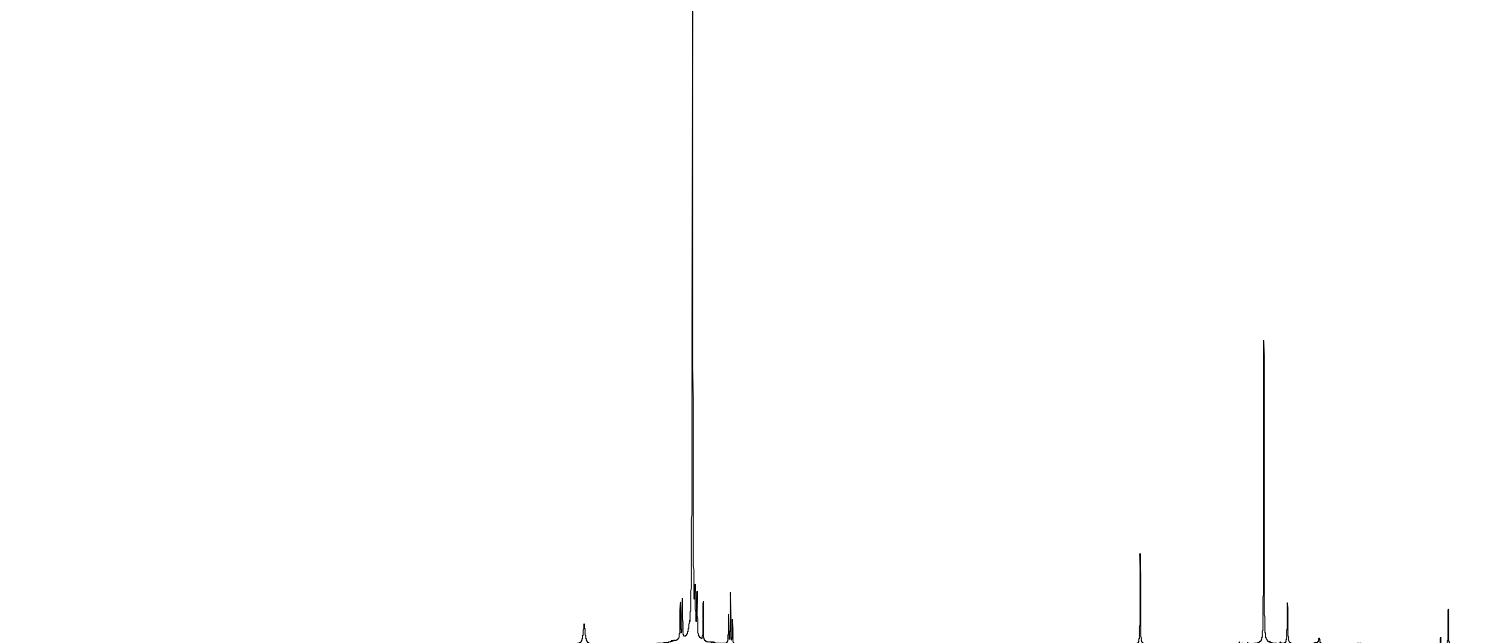


1g

8.418
7.483
7.463
7.394
7.363
7.345
7.339
7.329
7.320
7.260
7.014
6.995
6.975

3.011

1.809



13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.81

1.08

11.21

1.01

0.91

3.00

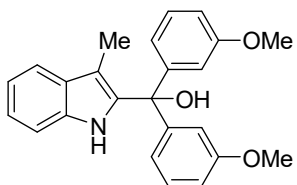
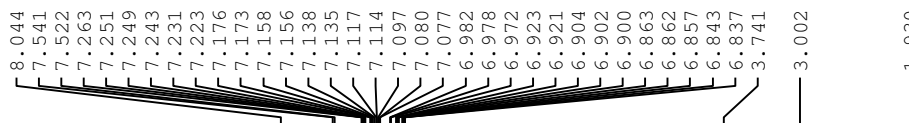


Current Data Parameters
 NAME 20230726-400M
 EXPNO 20
 PROCNO 1

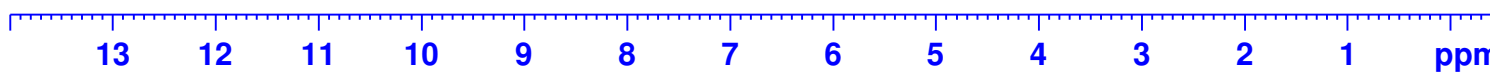
F2 - Acquisition Parameters
 Date_ 20230726
 Time 7.41
 INSTRUM spect
 PROBHD 5 mm PADUL 13C
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 6
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 113.67
 DW 60.800 usec
 DE 6.50 usec
 TE 292.9 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 9.90 usec
 PLW1 23.00000000 W
 SFO1 400.1924713 MHz

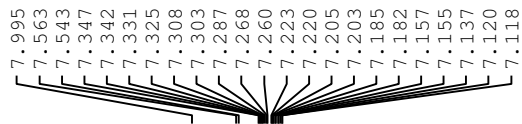
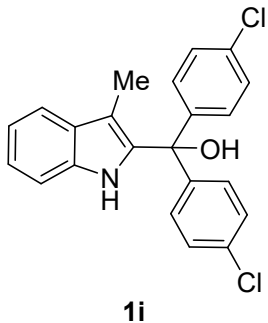
F2 - Processing parameters
 SI 65536
 SF 400.1900204 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



1h



wj-4-70-14



— 2.996

— 1.897

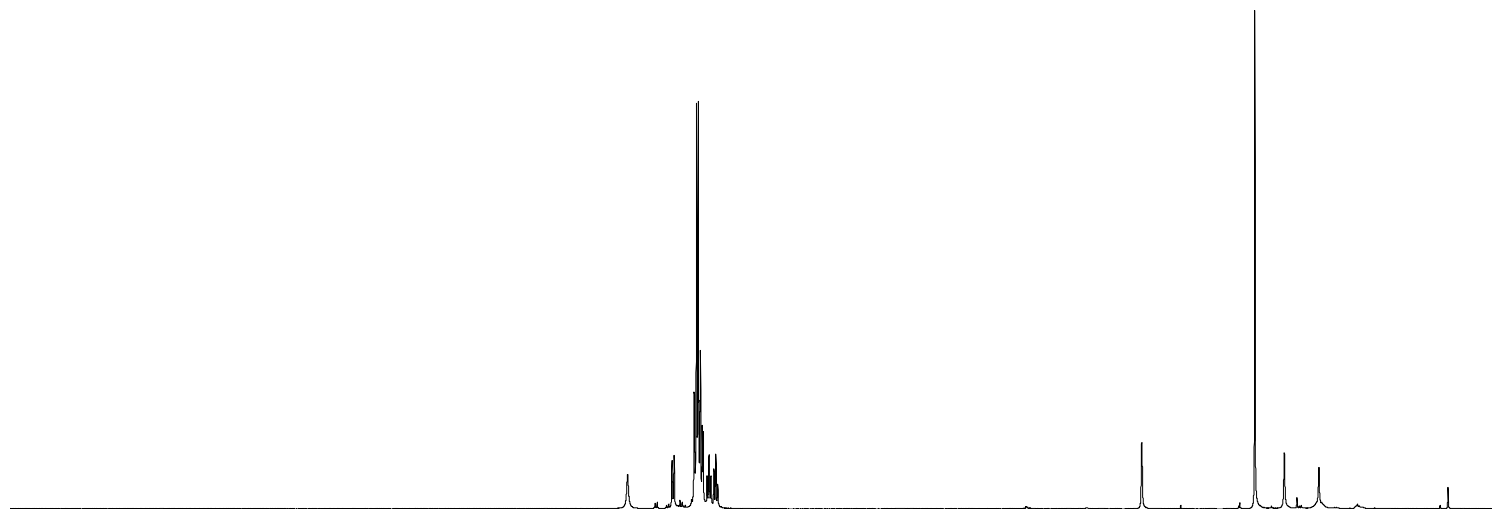


Current Data Parameters
NAME 20230730-400M
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230729
Time 21.15
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.67
DW 60.800 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

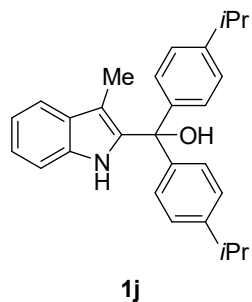


0.94
1.02
9.15
1.10
1.02

0.99

3.00

wj-4-70-7



8.165
7.556
7.536
7.281
7.260
7.210
7.190
7.172
7.170
7.153
7.150
7.134
7.132
7.114
7.096
7.091

2.965
2.948
2.931
2.913
2.896
2.879
2.862
2.844
1.872
1.276
1.258

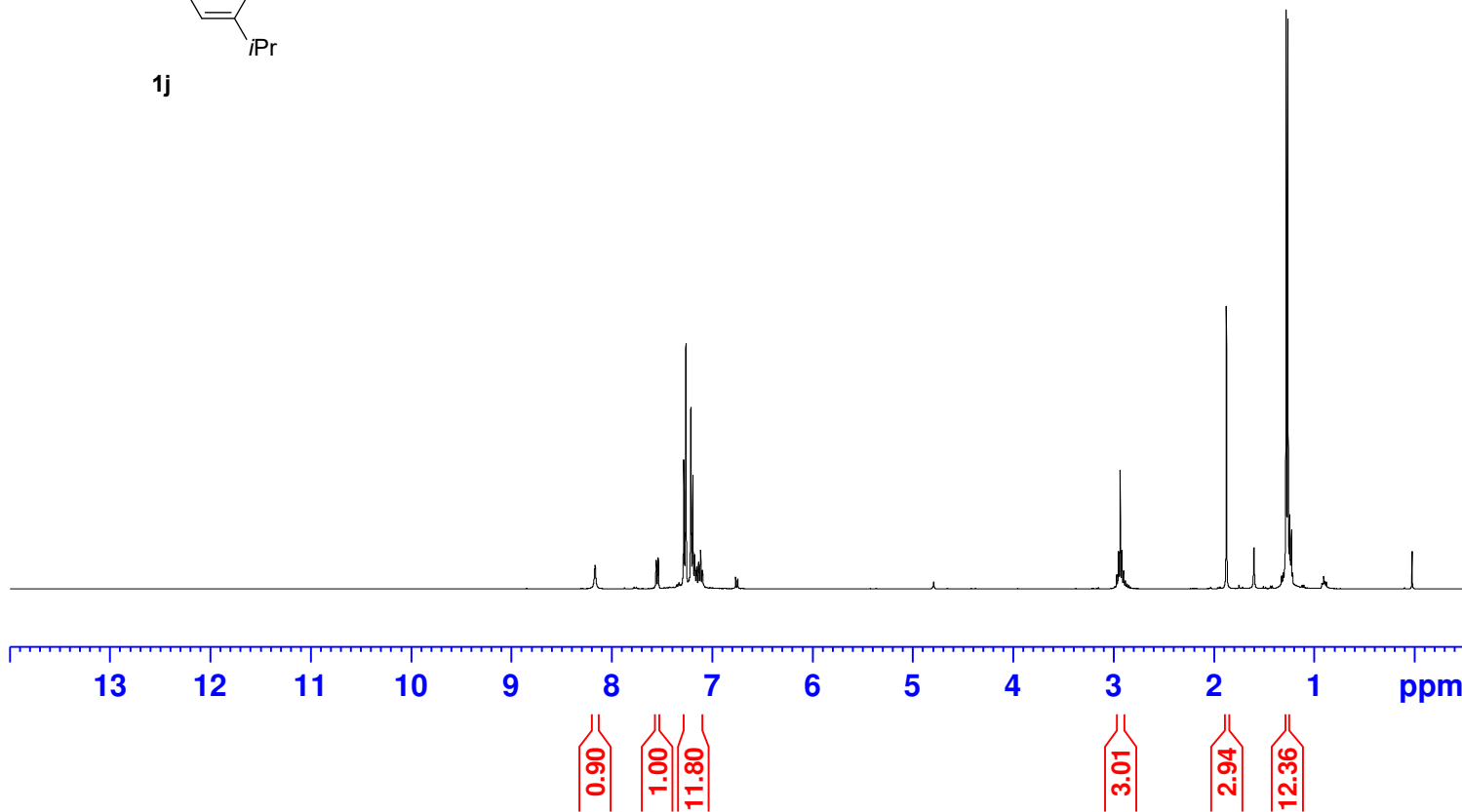


Current Data Parameters
NAME 20230725-400M
EXPNO 49
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230725
Time 3.03
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 90.23
DW 60.800 usec
DE 6.50 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



wj-4-70-5



Current Data Parameters
NAME 20230725-400M
EXPNO 45
PROCNO 1

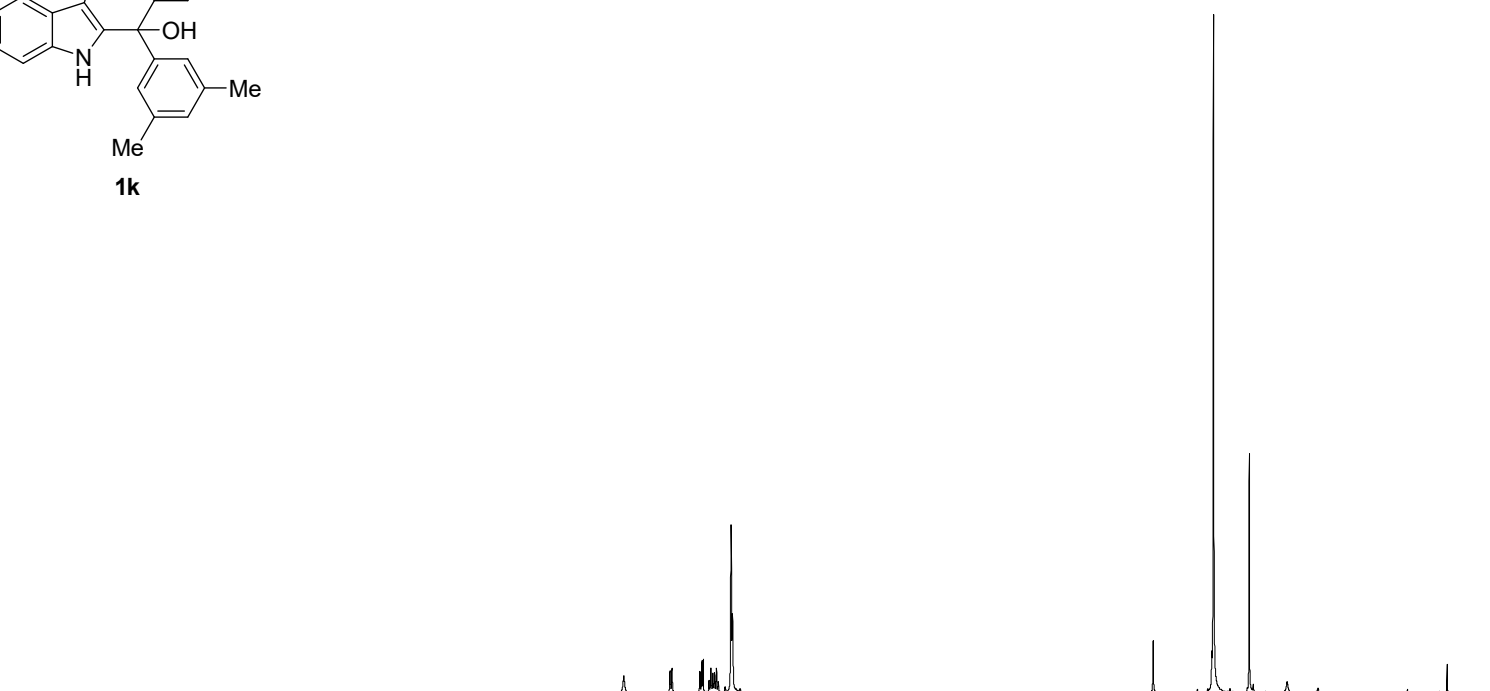
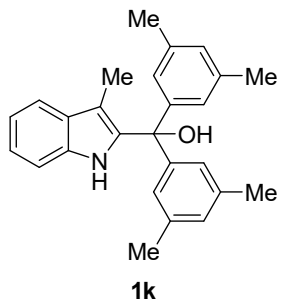
F2 - Acquisition Parameters
Date_ 20230725
Time 2.18
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.032
7.583
7.564
7.292
7.272
7.260
7.204
7.202
7.187
7.184
7.167
7.164
7.152
7.149
7.132
7.115
6.989
6.976

2.885
2.299
1.951



13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.93
1.00
1.00
1.10
1.04
4.02
2.03
0.93
12.23
3.00

wj-5-54-2

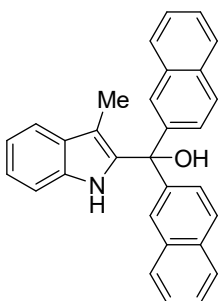
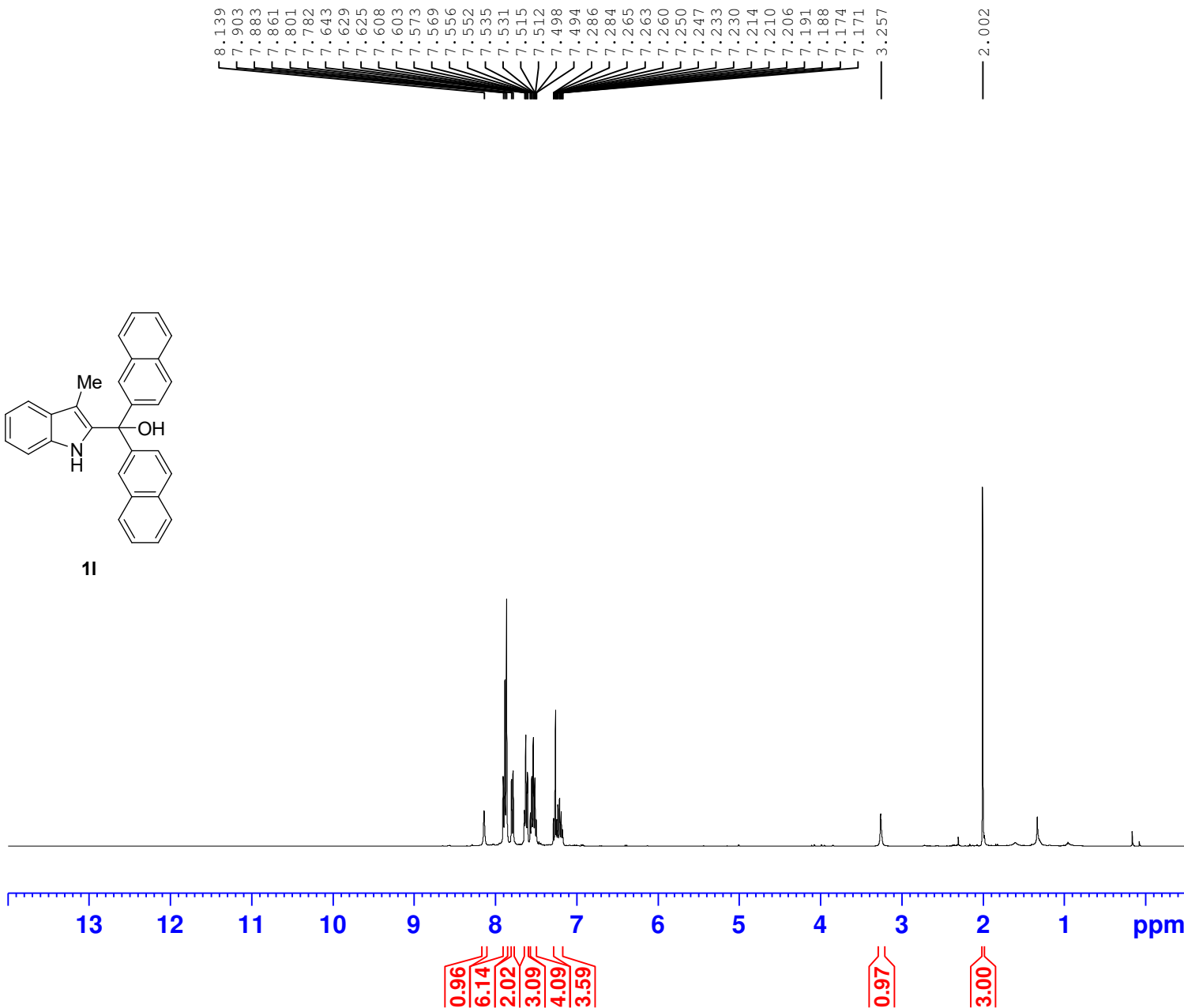


Current Data Parameters
NAME 20231101-400
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231101
Time 0.42
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 61.19
DW 60.800 usec
DE 6.50 usec
TE 291.9 K
D1 1.00000000 sec
TD0 1

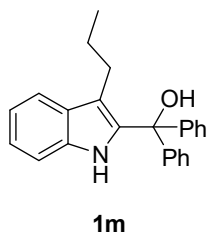
==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



11

ncc-5-18



8.037
7.542
7.523
7.298
7.281
7.279
7.260
7.169
7.149
7.140
7.122
7.120
7.105
7.103
7.086
7.068
7.048
7.031

3.061
2.226
2.206
2.200
2.185
1.313
1.294
1.275
1.255
1.237
1.217
0.680
0.662
0.643

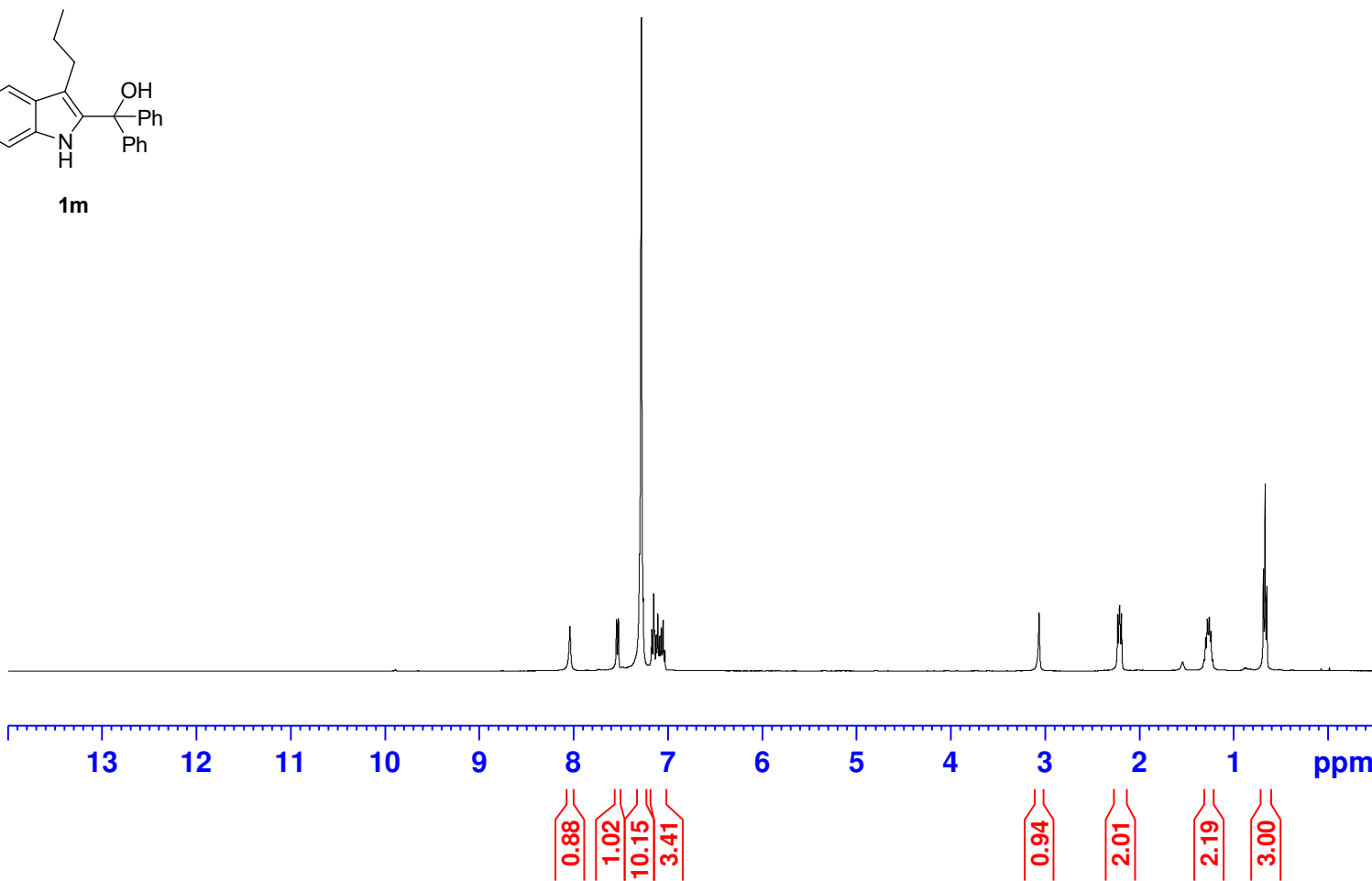


Current Data Parameters
NAME 20240702-400M
EXPNO 24
PROCNO 1

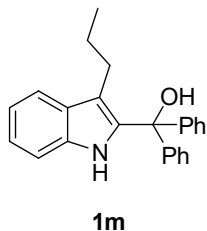
F2 - Acquisition Parameters
Date_ 20240702
Time 6.09
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 29.75
DW 60.800 usec
DE 6.50 usec
TE 291.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900617 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



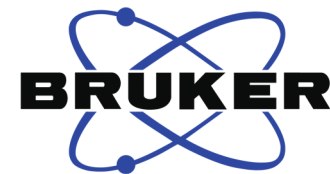
ncc-5-18



145.25
137.08
134.44
129.41
128.30
127.98
127.76
122.06
119.36
119.22
114.42
111.03

79.46
77.48
77.16
76.84

27.14
23.68
14.65



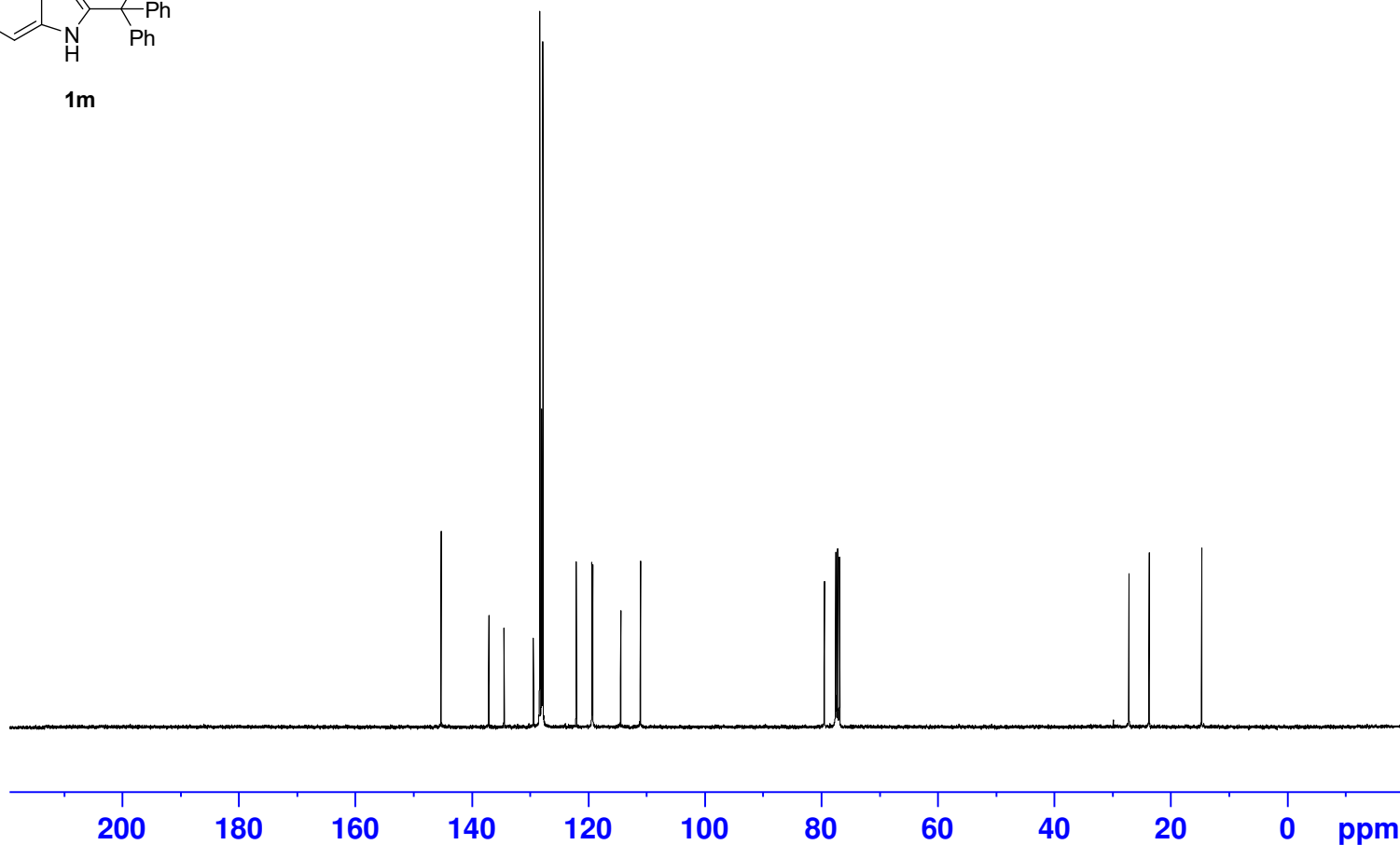
Current Data Parameters
NAME 20240702-400M
EXPNO 25
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240702
Time 6.39
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 292.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

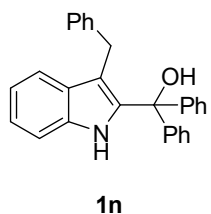
==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278573 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



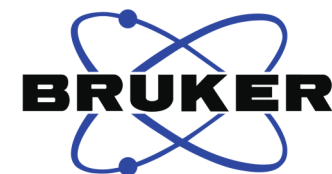
ncc-5-15-a



8.013
7.465
7.445
7.397
7.389
7.386
7.383
7.340
7.333
7.325
7.300
7.279
7.260
7.221
7.203
7.177
7.159
7.139
7.110
7.092
7.073
6.993
6.977

3.855

2.882
2.876

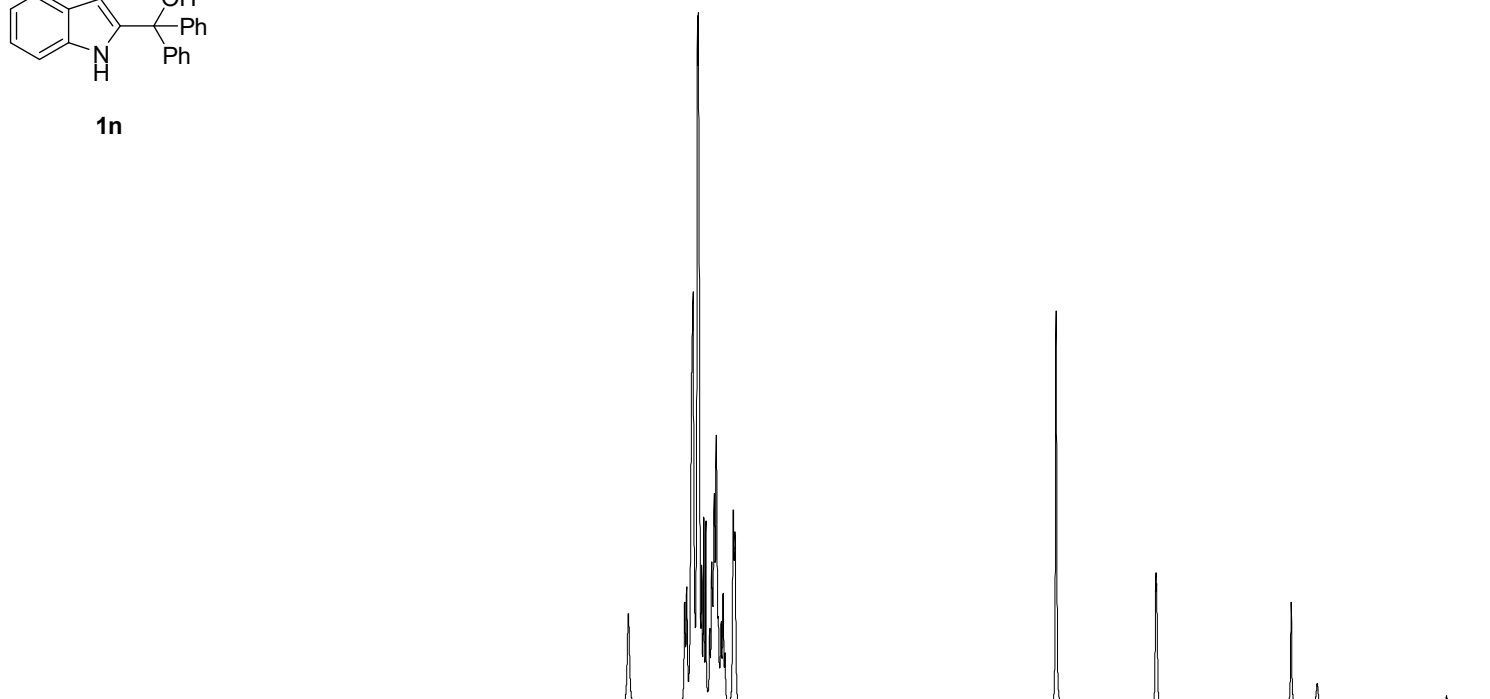


Current Data Parameters
NAME 20240625-400M
EXPNO 17
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240624
Time 23.53
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 61.19
DW 60.800 usec
DE 6.50 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

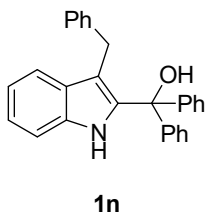


13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.93
12.50
5.25
2.01

2.00
1.02

ncc-5-15-a



144.86
141.30
138.73
134.33
129.79
128.42
128.39
128.30
127.99
127.56
125.84
122.30
119.72
119.59
111.88
111.07

79.13
77.47
77.15
76.84

30.50



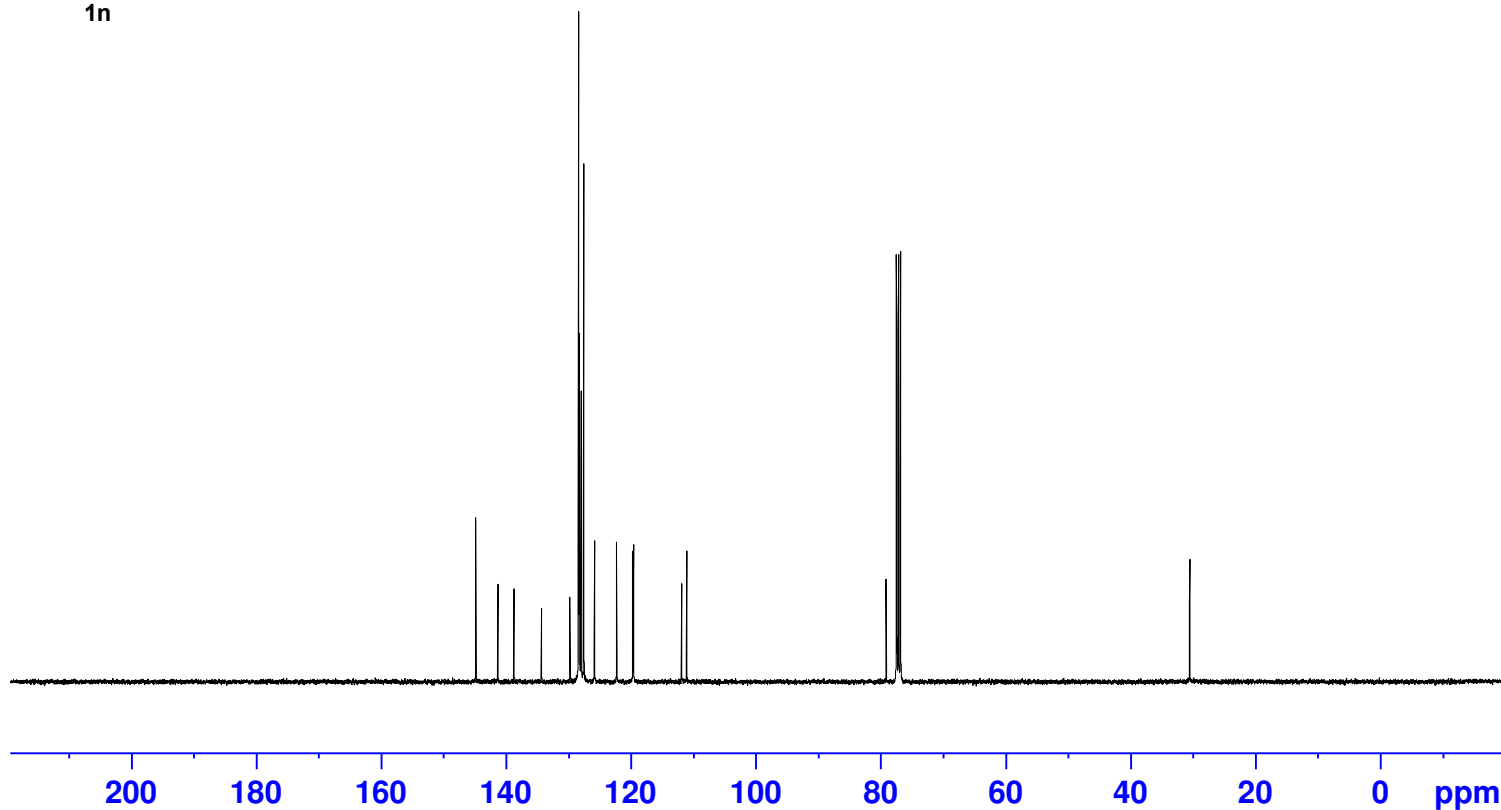
Current Data Parameters
NAME 20240625-400M
EXPNO 18
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240625
Time 0.40
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 800
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 50.16
DW 20.800 usec
DE 6.50 usec
TE 292.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

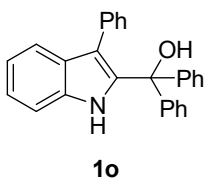
==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278529 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

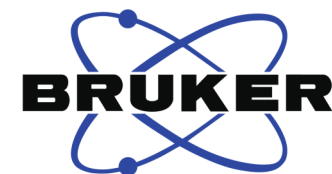


ncc-5-16



7.843
7.465
7.446
7.295
7.260
7.224
7.211
7.208
7.182
7.152
7.146
7.133
7.128
7.105
7.087

3.247

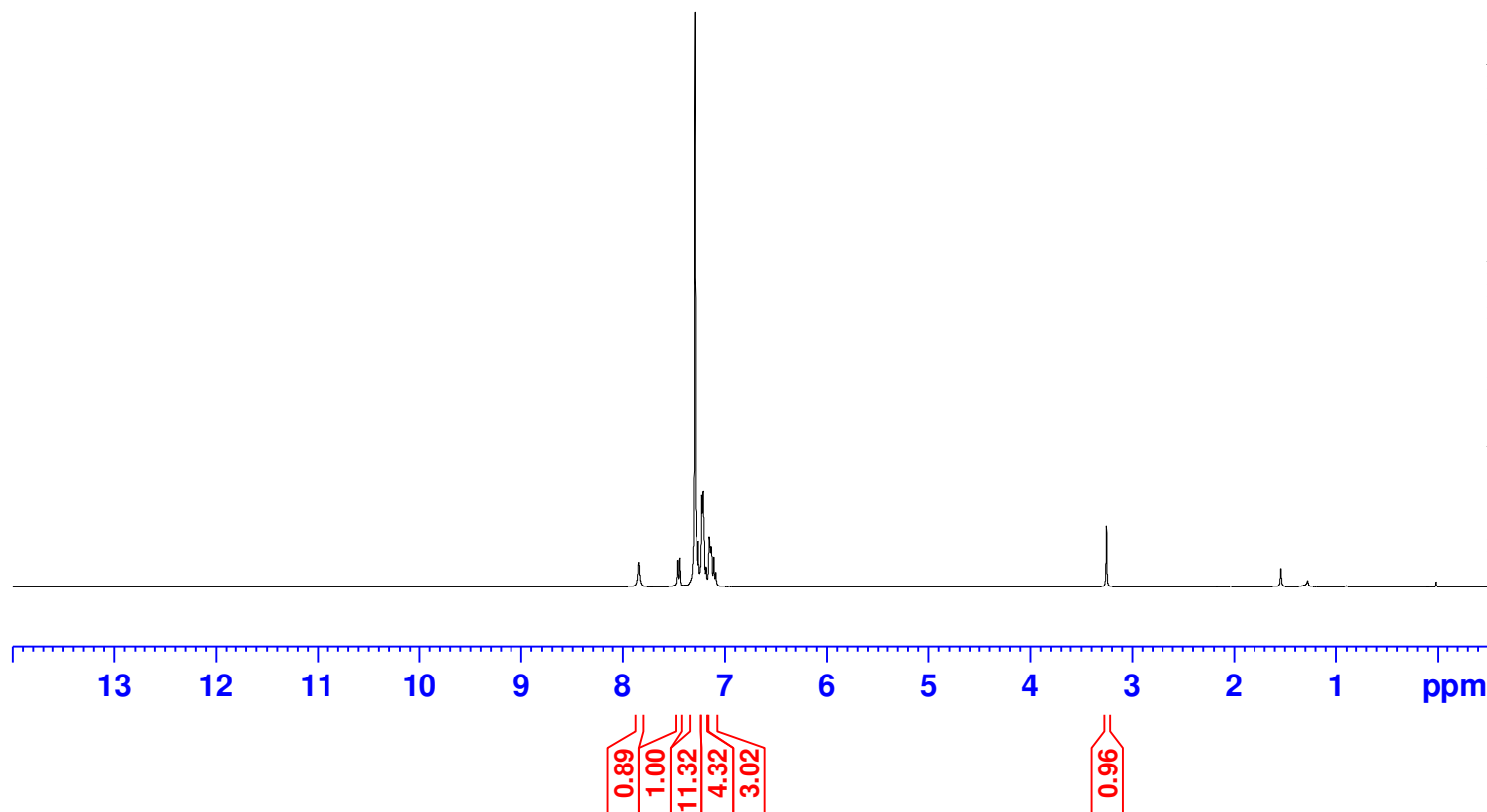


Current Data Parameters
NAME 20240628-400M
EXPNO 20
PROCNO 1

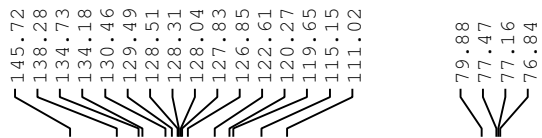
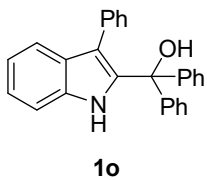
F2 - Acquisition Parameters
Date_ 20240627
Time 22.59
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 68.24
DW 60.800 usec
DE 6.50 usec
TE 291.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900285 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ncc-5-16



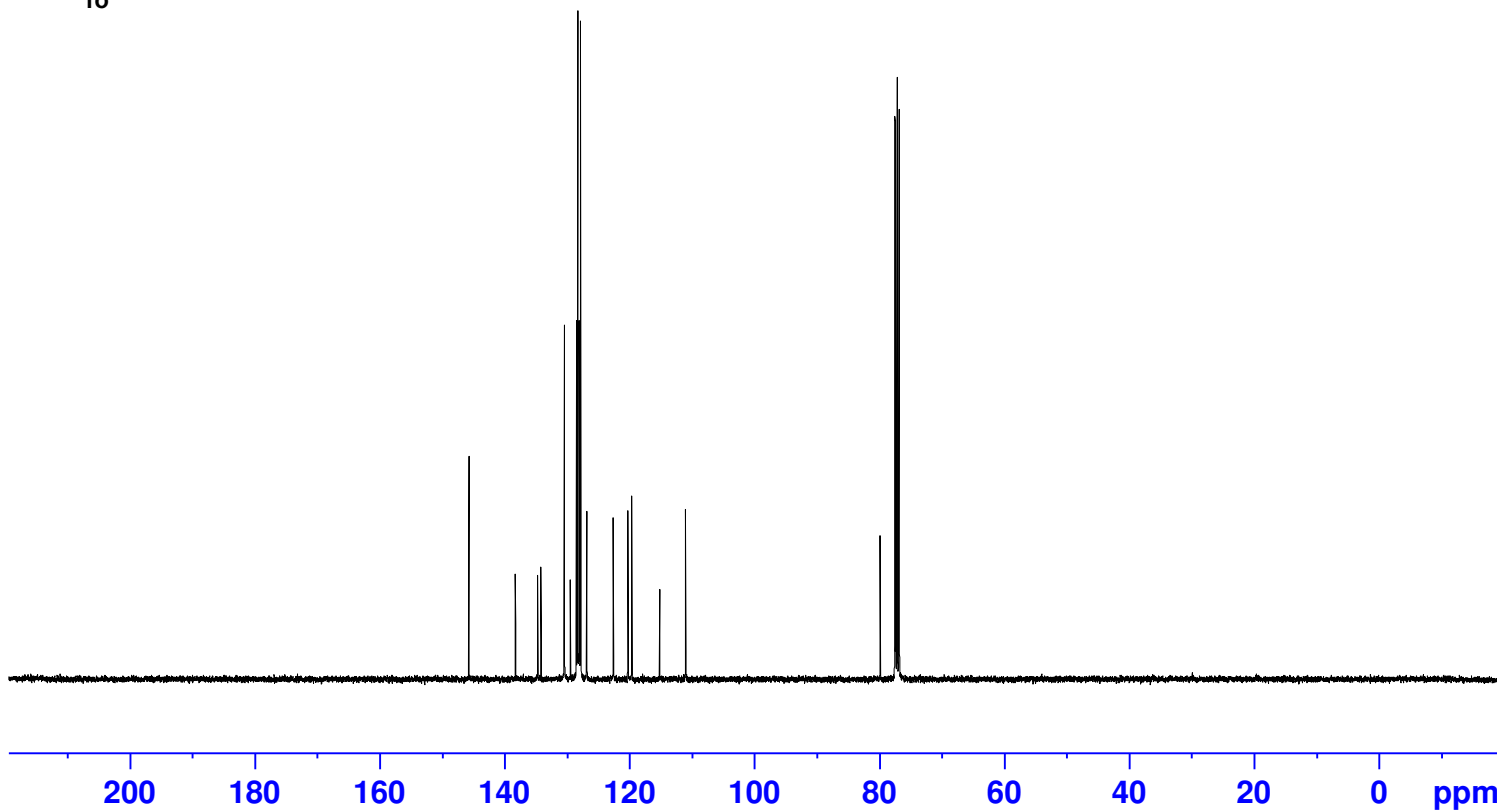
Current Data Parameters
NAME 20240628-400M
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240627
Time 23.29
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 35.06
DW 20.800 usec
DE 6.50 usec
TE 292.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

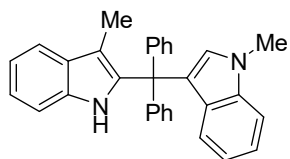
==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.4000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

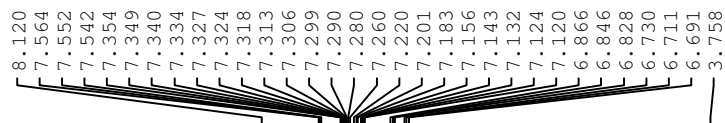
F2 - Processing parameters
SI 32768
SF 100.6278521 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



ncc-2-34



3a



1.672

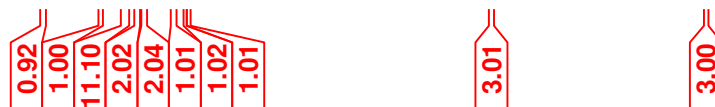
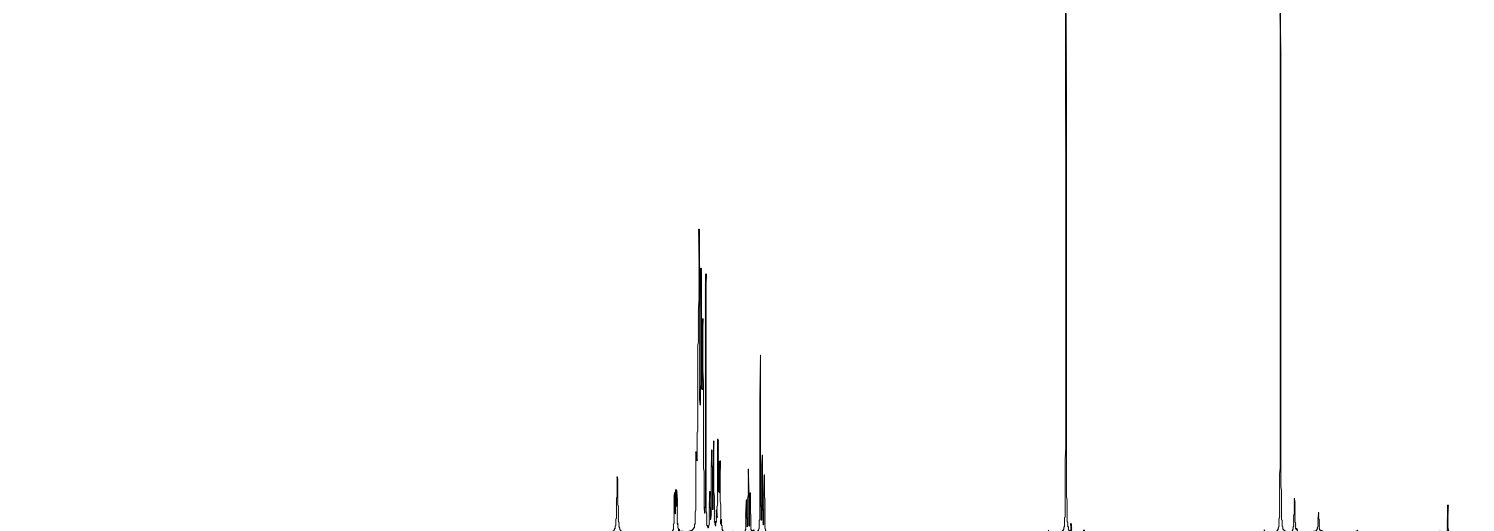


Current Data Parameters
NAME 20231021-400M
EXPNO 28
PROCNO 1

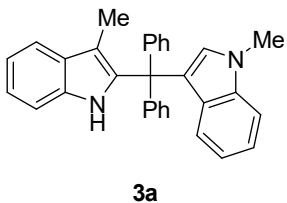
F2 - Acquisition Parameters
Date_ 20231020
Time 23.41
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 90.23
DW 60.800 usec
DE 6.50 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ncc-2-34



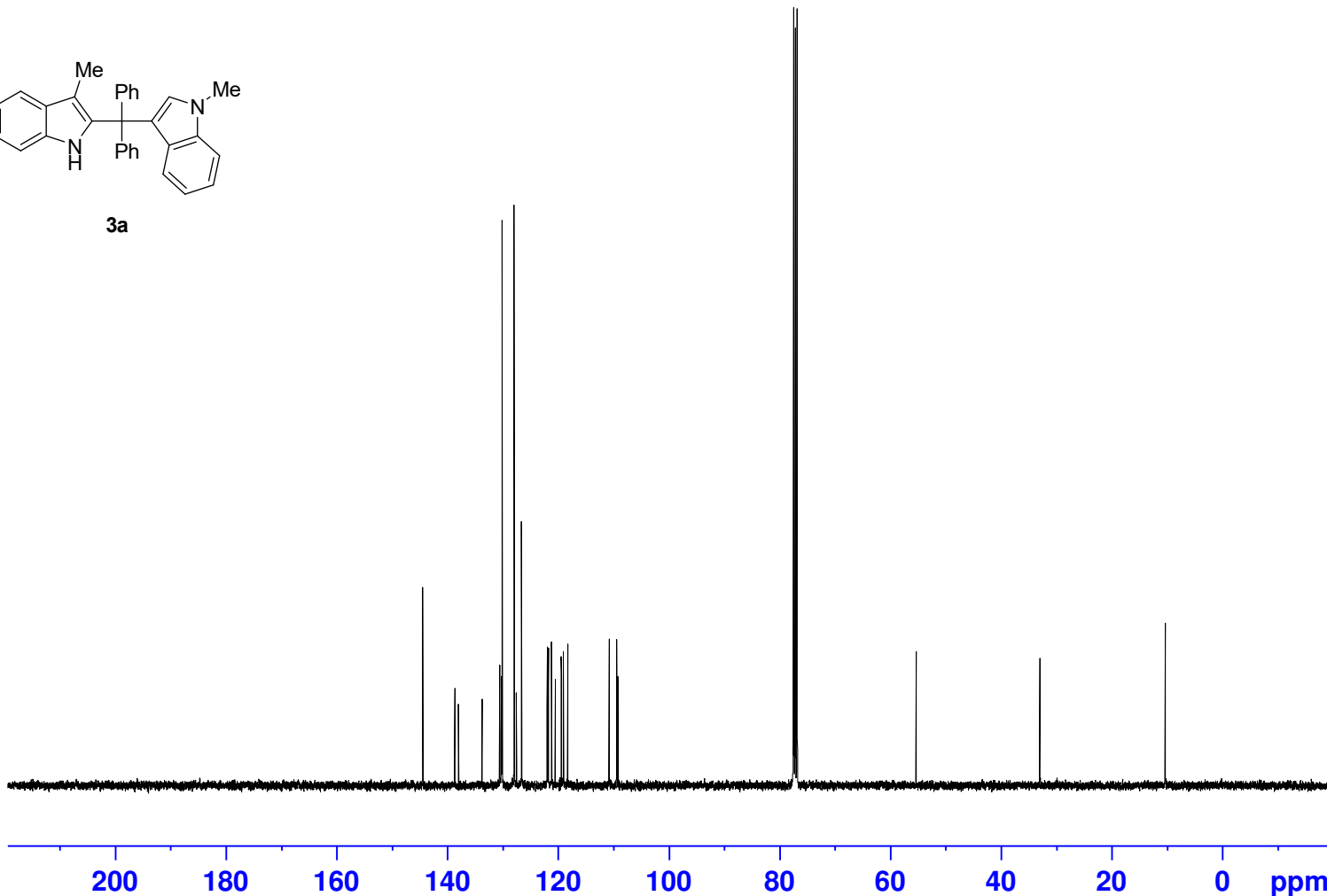
144.50
138.69
138.03
133.72
130.56
130.29
130.13
127.95
127.54
126.62
121.99
121.78
121.21
120.53
119.43
119.06
118.26
110.79
109.43
109.18

77.47
77.15
76.84

55.32

32.96

10.31



Current Data Parameters
NAME 20231021-400M
EXPNO 29
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231021
Time 0.06
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 35.06
DW 20.800 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278499 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ncc-2-42

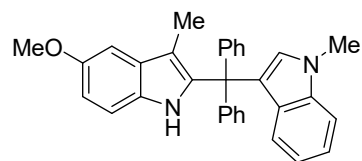


Current Data Parameters
NAME 20230831-400M
EXPNO 17
PROCNO 1

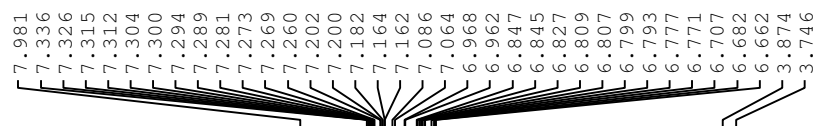
F2 - Acquisition Parameters
Date_ 20230831
Time 4.02
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 292.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

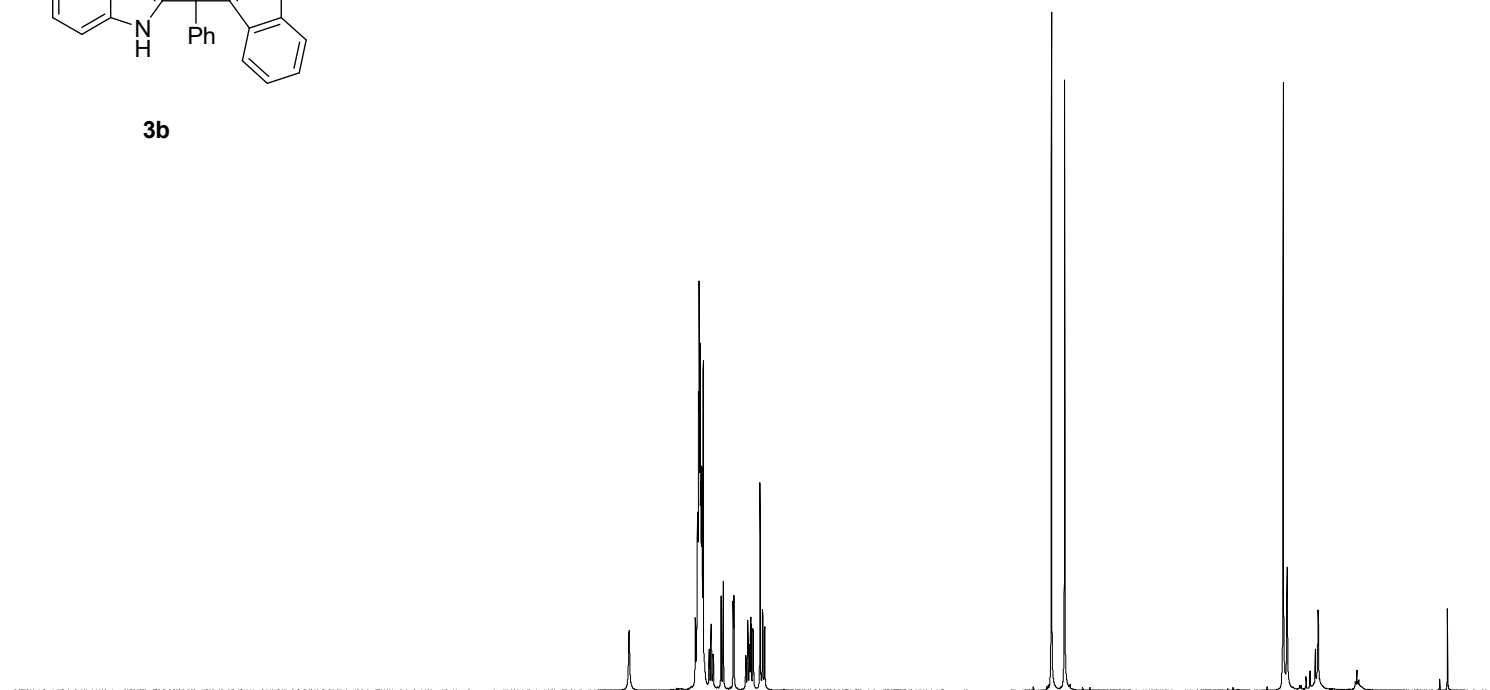
F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3b



1.621



ncc-2-42



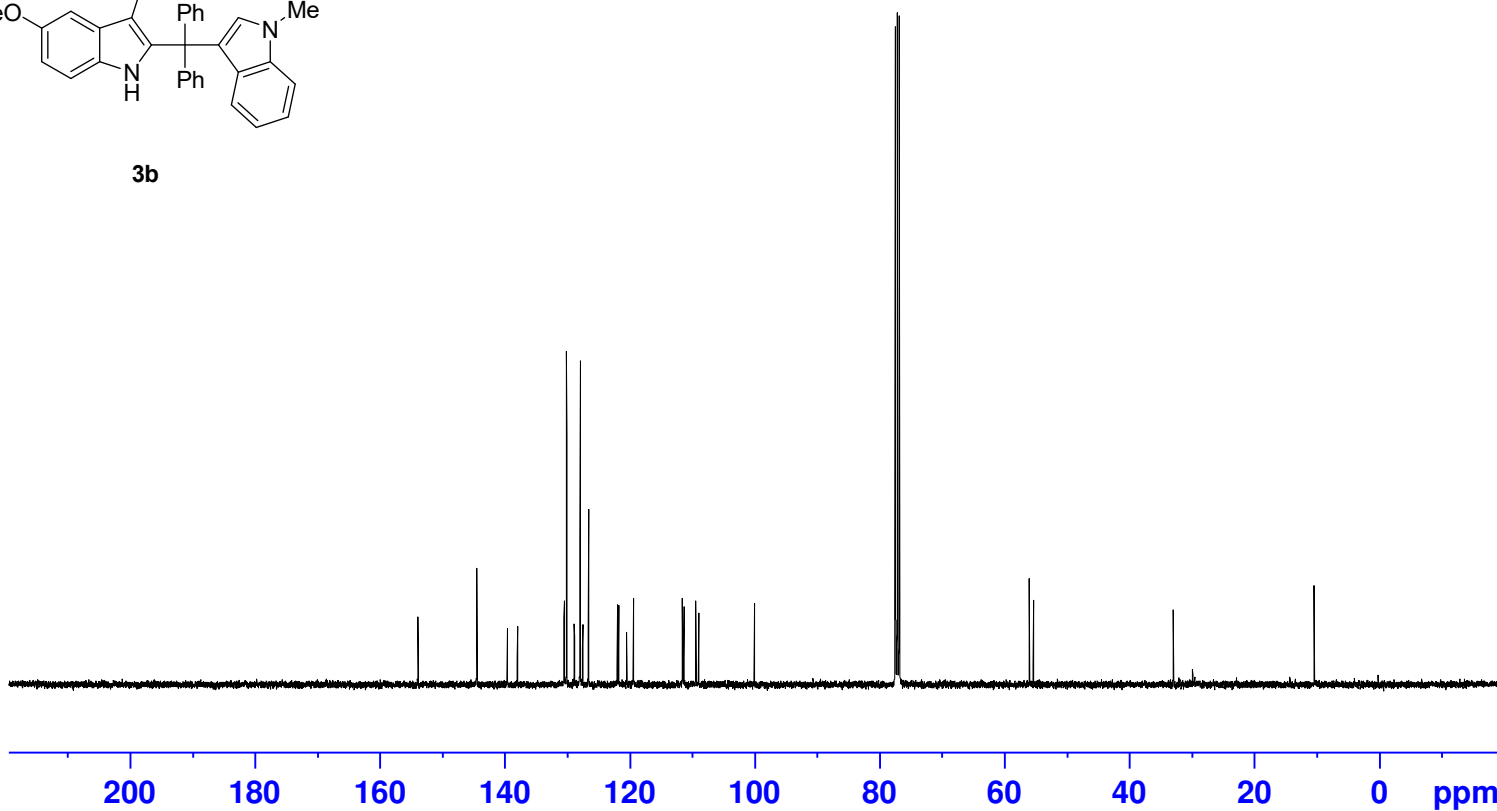
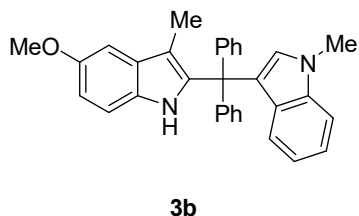
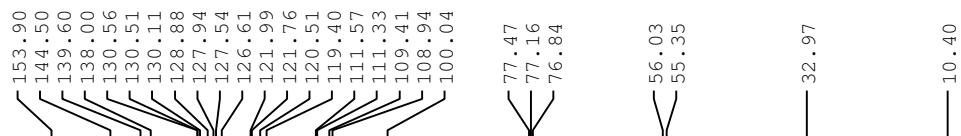
Current Data Parameters
NAME 20230831-400M
EXPNO 18
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230831
Time 4.32
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

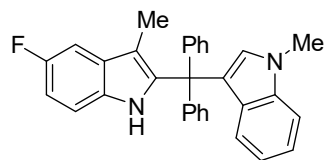
=====
CHANNEL f1
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

=====
CHANNEL f2
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

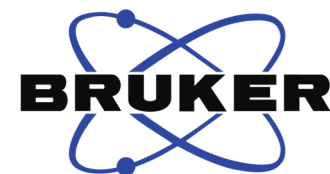
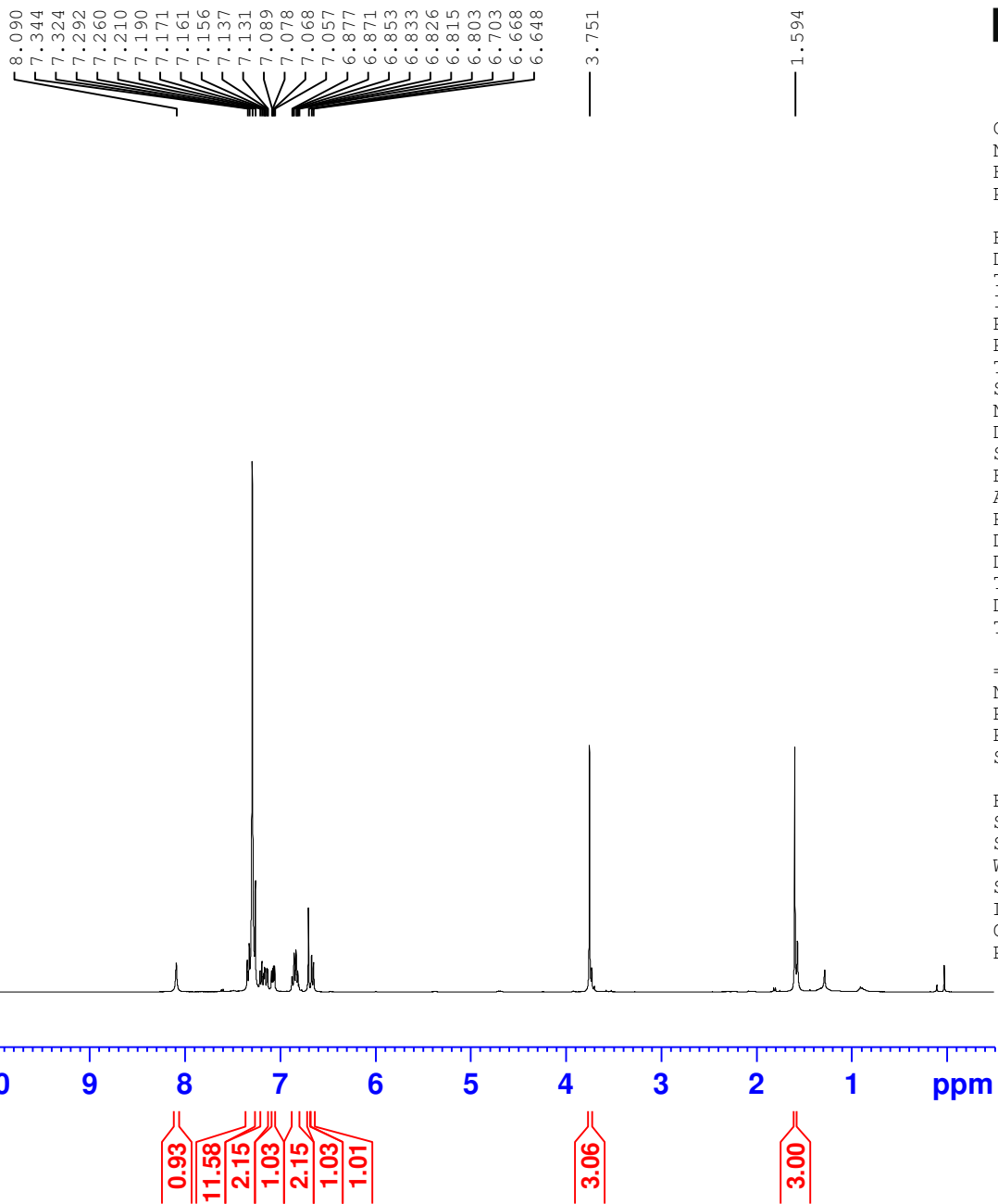
F2 - Processing parameters
SI 32768
SF 100.6278484 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



ncc-2-44



3c



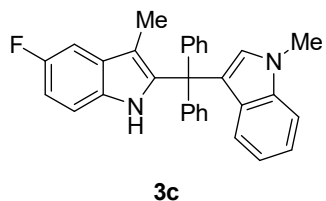
Current Data Parameters
NAME 20230901-400M
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230831
Time 21.55
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 292.1 K
D1 1.00000000 sec
TD0 1

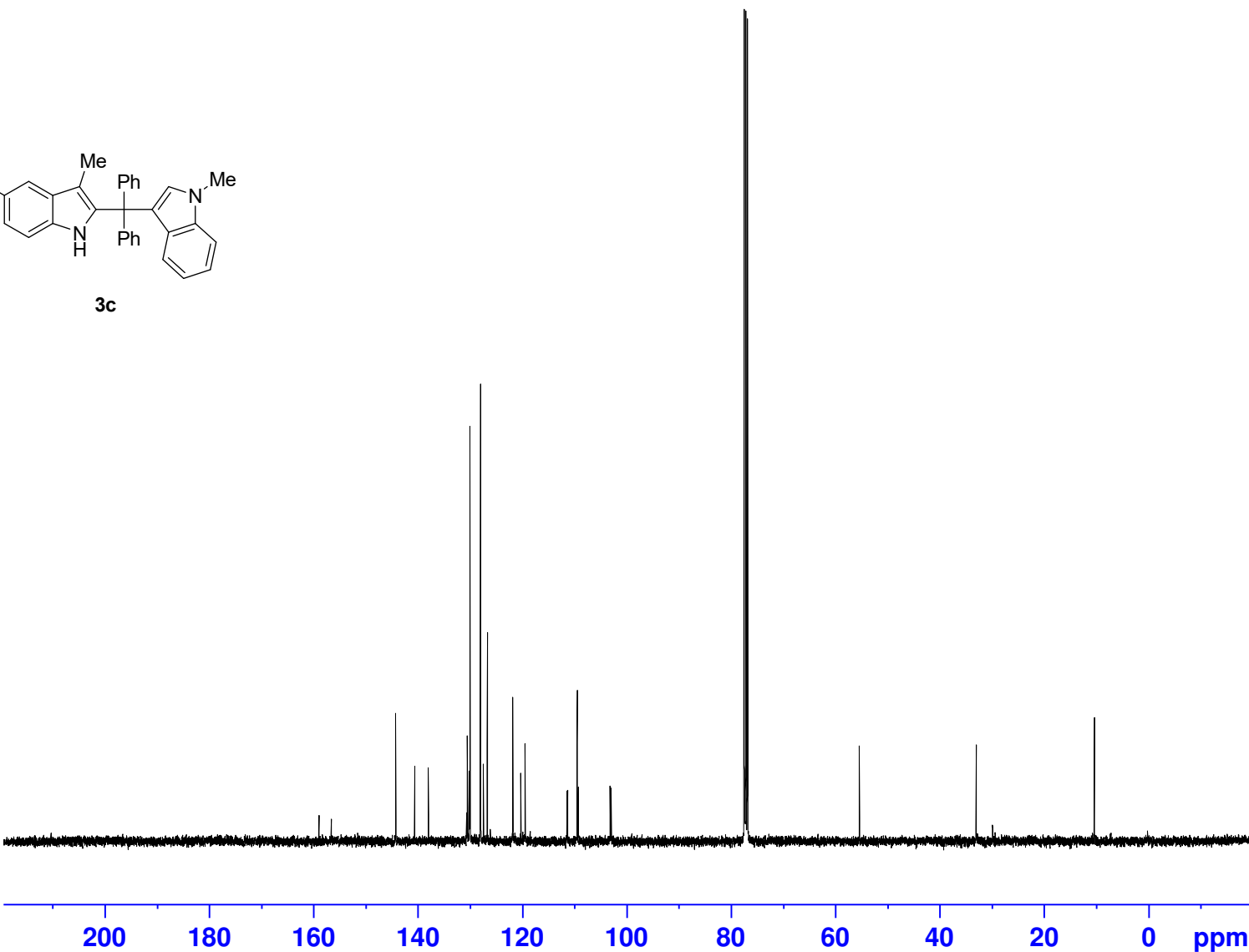
==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ncc-2-44



158.97
156.65
144.28
140.64
138.02
130.70
130.61
130.54
130.20
130.06
128.03
127.47
126.73
121.85
120.31
119.49
111.42
111.32
109.50
109.45
109.26
103.20
102.97
77.48
77.16
76.84



Current Data Parameters
NAME 20230901-400M
EXPNO 11
PROCNO 1

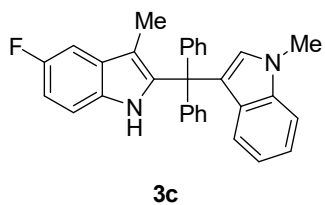
F2 - Acquisition Parameters
Date_ 20230831
Time 22.19
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 35.06
DW 20.800 usec
DE 6.50 usec
TE 292.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278477 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ncc-2-44



— -125.18



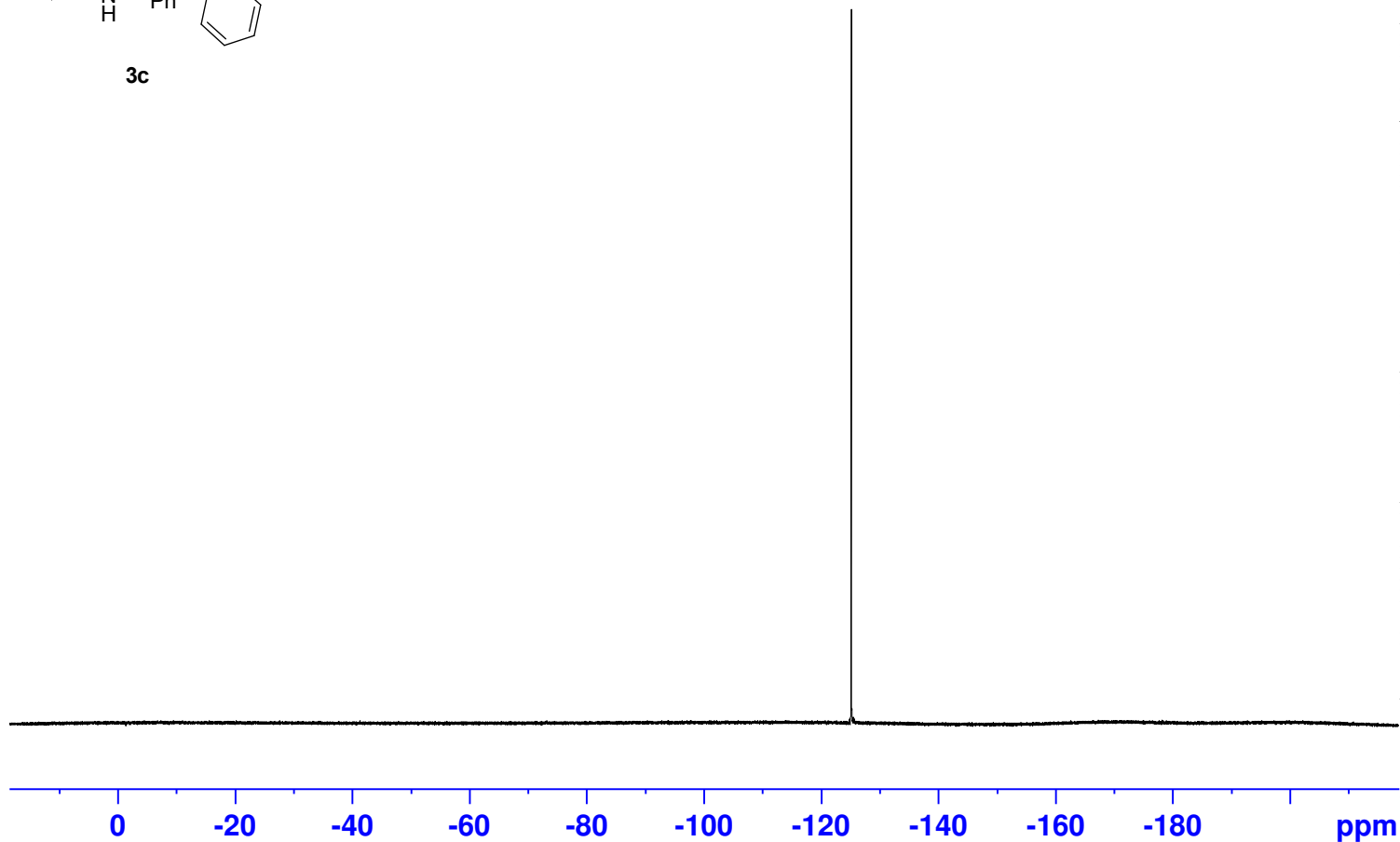
Current Data Parameters
NAME 20230901-300M
EXPNO 466
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230901
Time 13.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

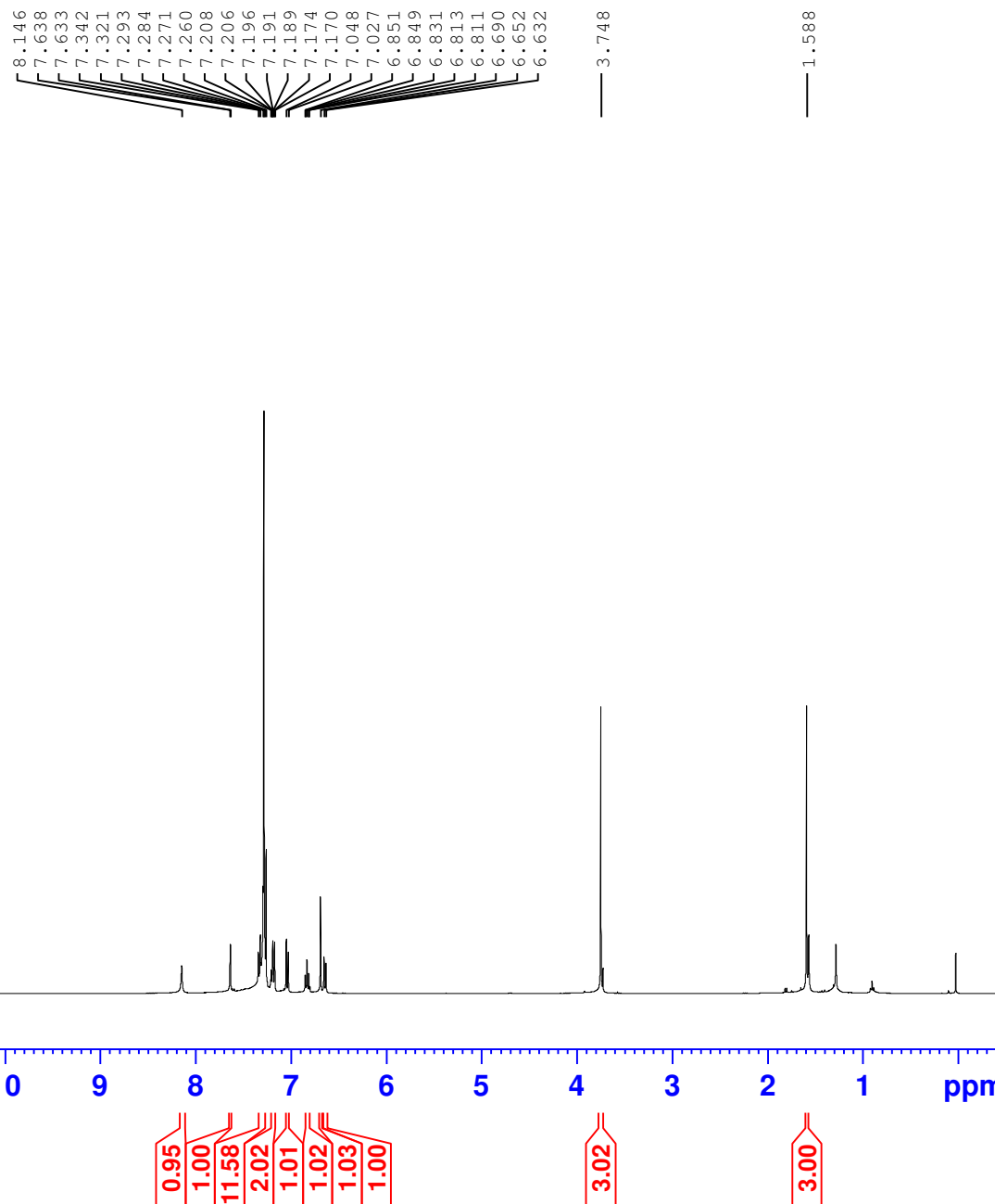
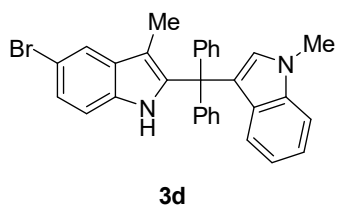
==== CHANNEL f1 =====
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

==== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ncc-2-46



Current Data Parameters
NAME 20230831-400M
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230831
Time 7.27
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ncc-2-46



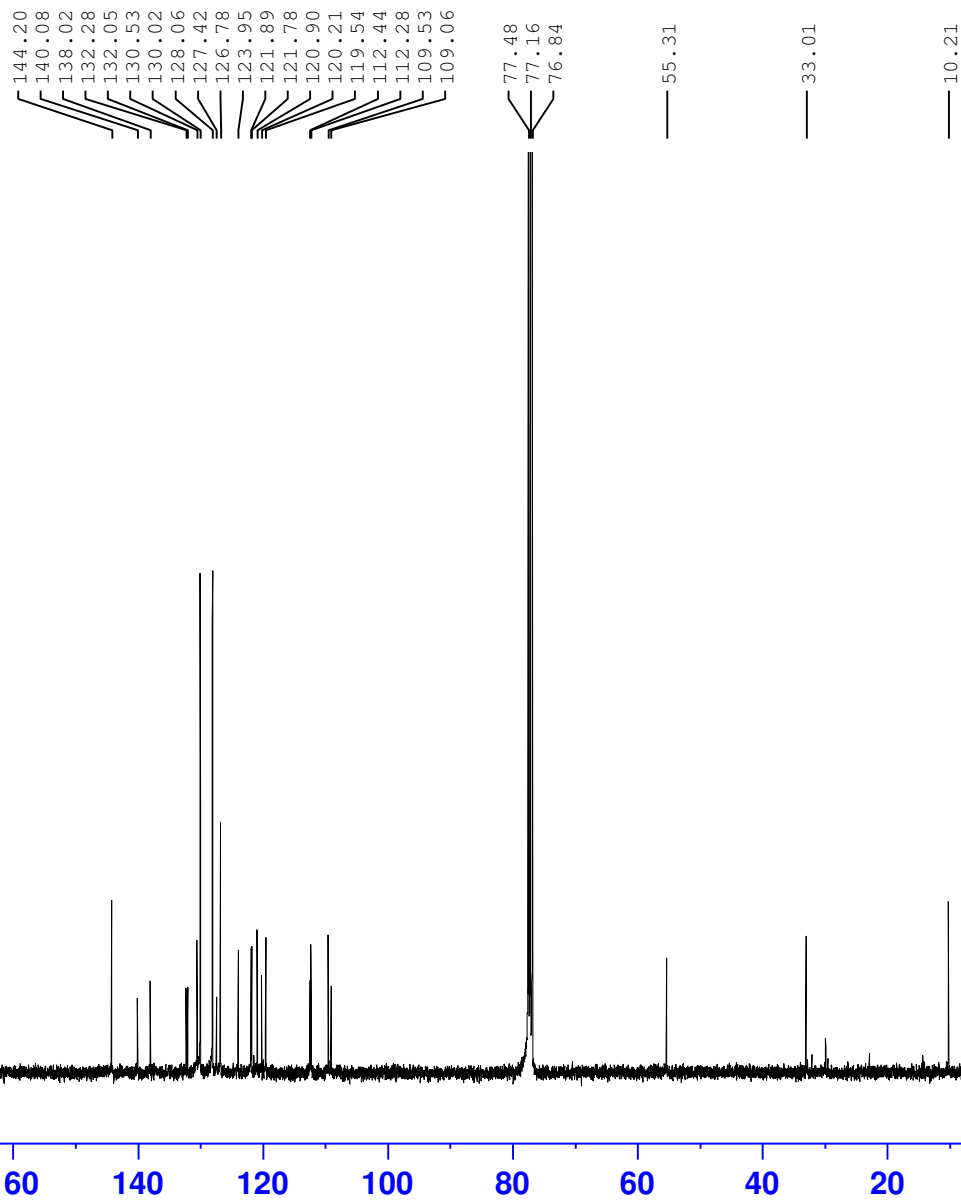
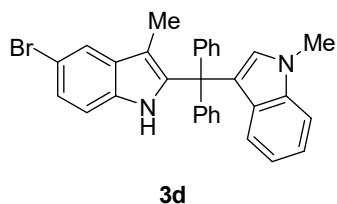
Current Data Parameters
NAME 20230831-400M
EXPNO 27
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230831
Time 7.57
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 293.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

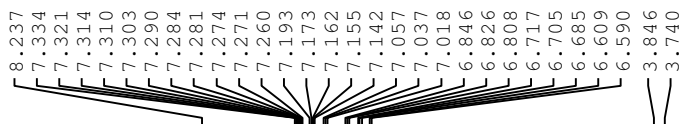
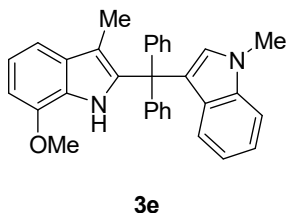
=====
CHANNEL f1
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

=====
CHANNEL f2
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278477 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



ncc-2-41



1.634

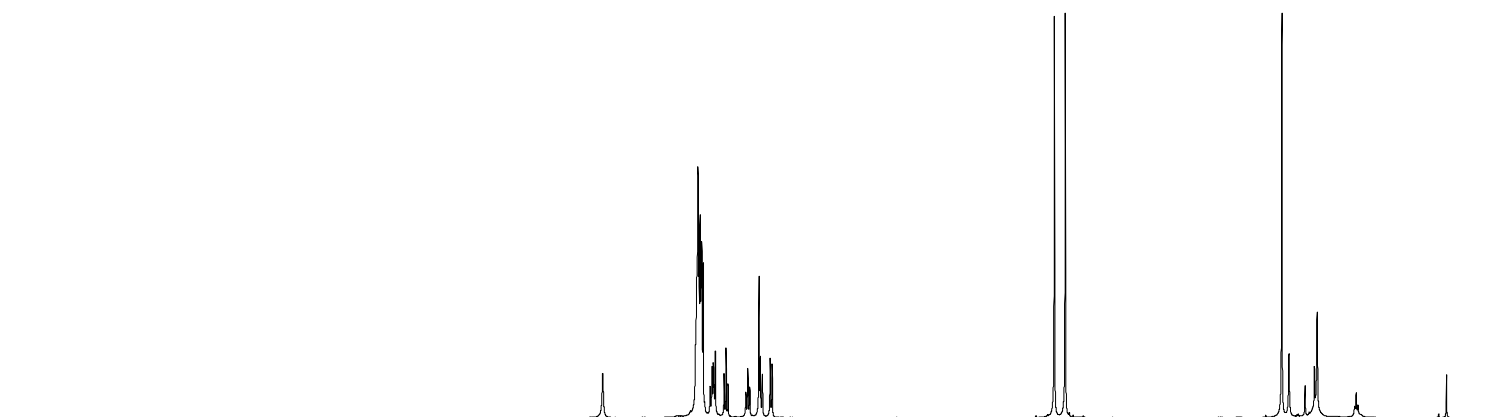


Current Data Parameters
NAME 20230831-400M
EXPNO 15
PROCNO 1

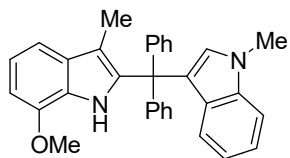
F2 - Acquisition Parameters
Date_ 20230831
Time 3.27
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 90.23
DW 60.800 usec
DE 6.50 usec
TE 292.3 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

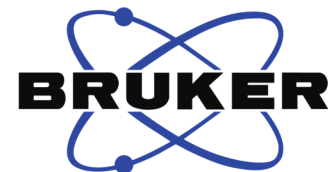
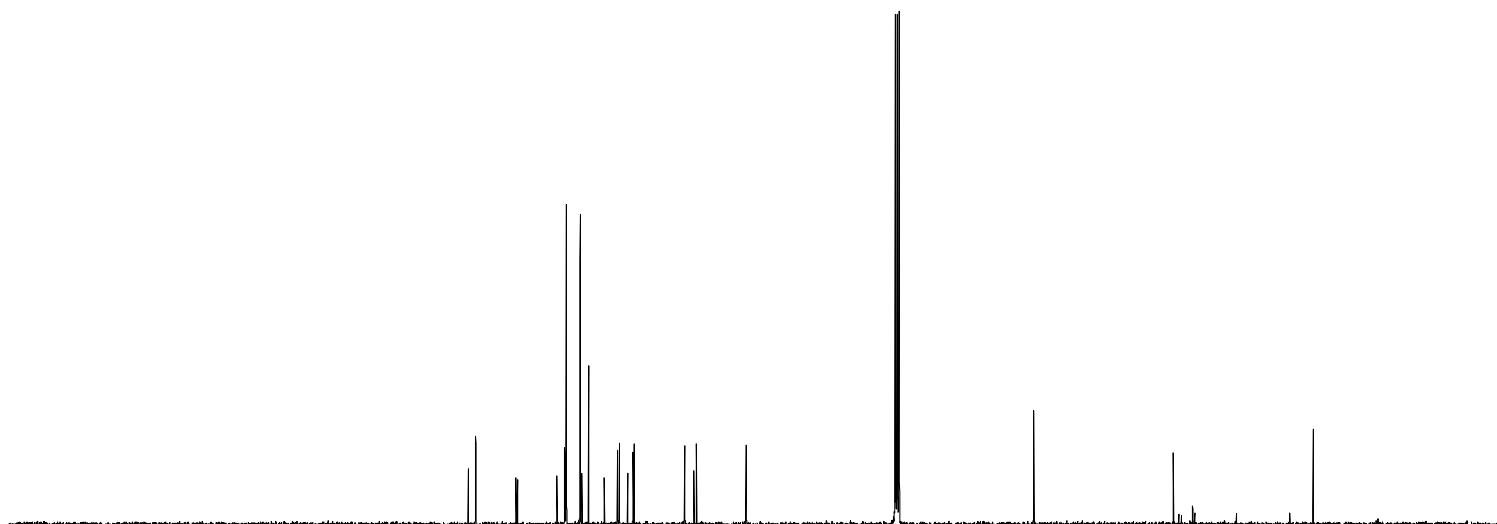
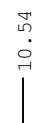
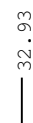
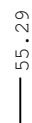
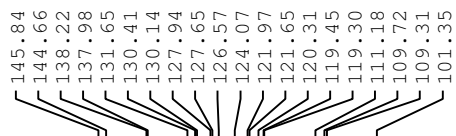
F2 - Processing parameters
SI 65536
SF 400.1900138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ncc-2-41



3e



Current Data Parameters
NAME 20230831-400M
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230831
Time 3.57
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 293.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

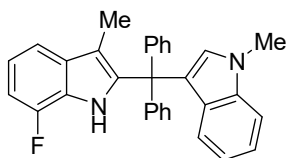
==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

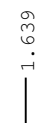
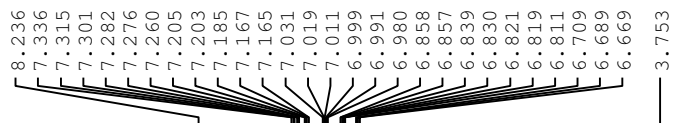
F2 - Processing parameters
SI 32768
SF 100.6278491 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

ncc-2-43



3f

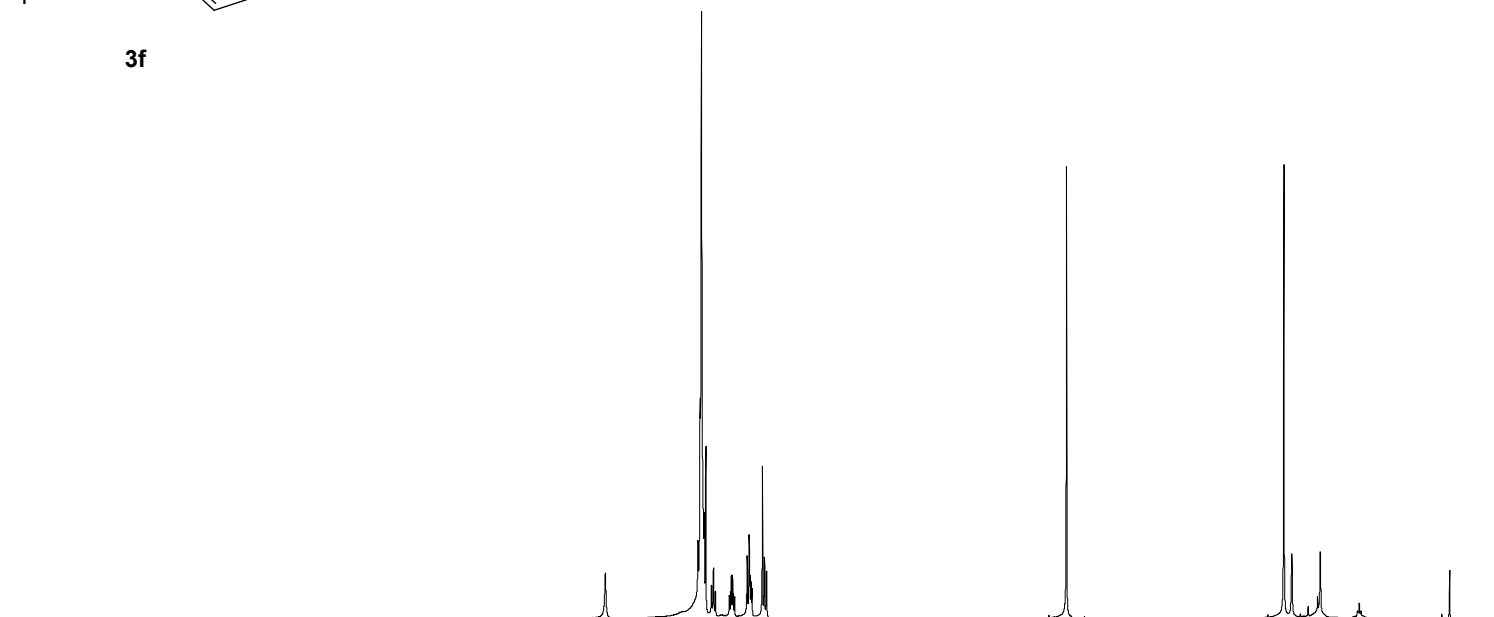


Current Data Parameters
NAME 20230831-400M
EXPNO 19
PROCNO 1

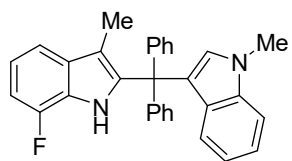
F2 - Acquisition Parameters
Date_ 20230831
Time 4.36
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 292.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ncc-2-43



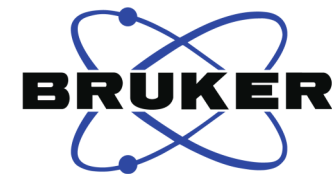
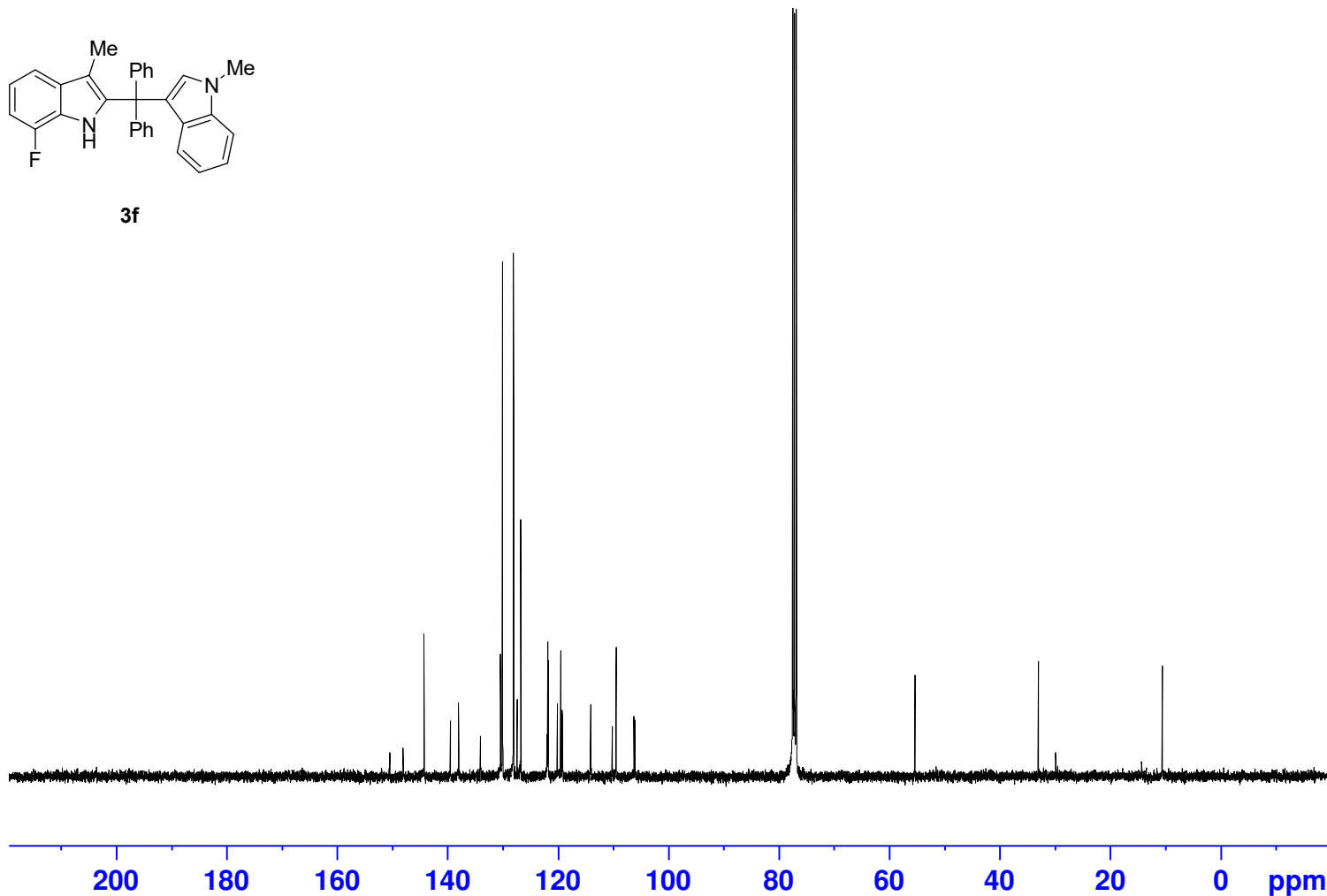
3f

150.49
148.07
144.27
139.50
138.01
134.07
134.01
130.42
130.05
128.06
127.43
126.76
122.00
121.89
121.77
120.11
119.52
119.27
119.21
114.11
114.07
110.18
109.49
106.24
106.08
77.47
77.16
76.84

55.32

32.98

10.51



Current Data Parameters
NAME 20230831-400M
EXPNO 20
PROCNO 1

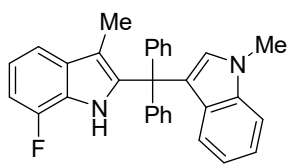
F2 - Acquisition Parameters
Date_ 20230831
Time 5.05
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 292.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

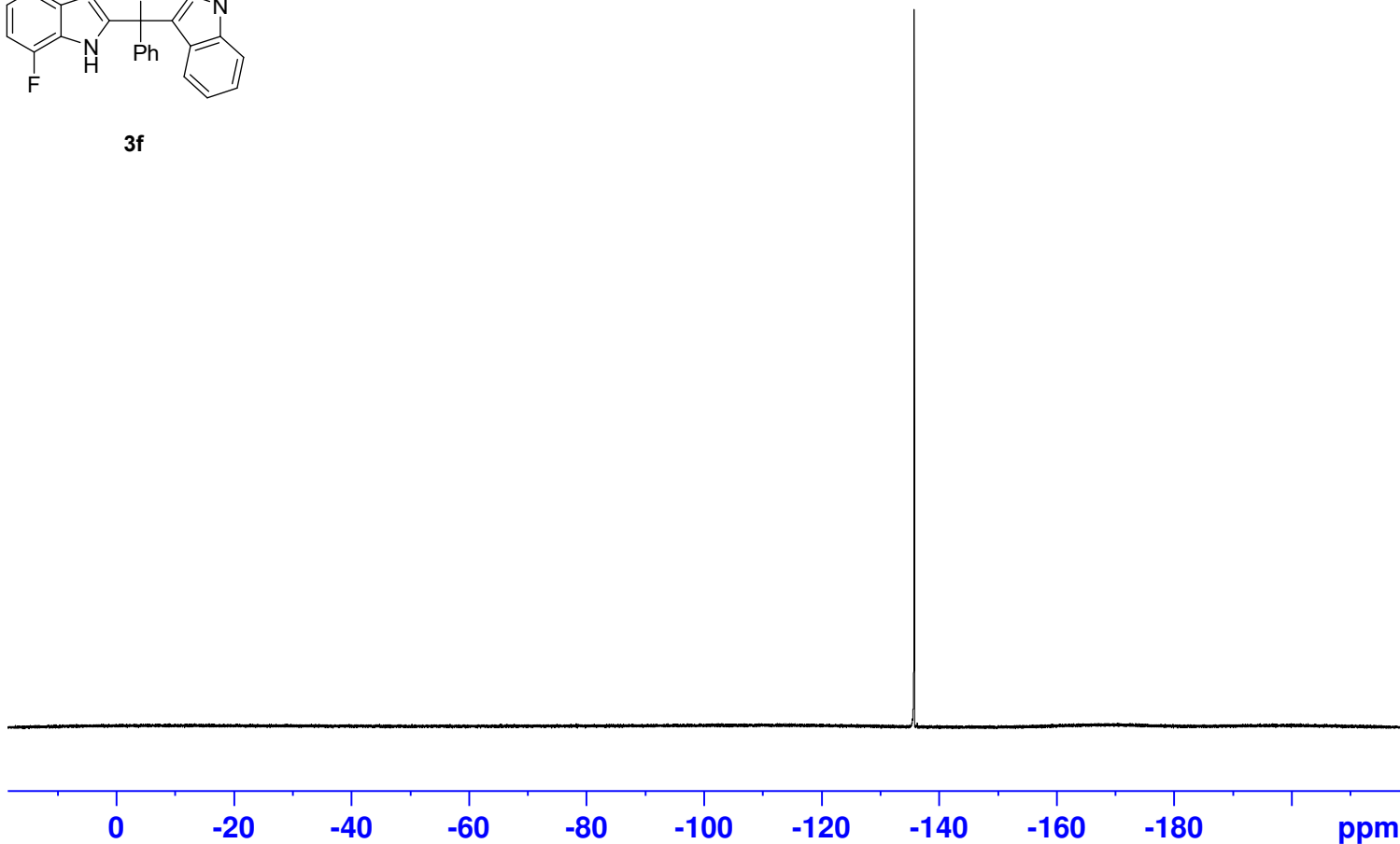
F2 - Processing parameters
SI 32768
SF 100.6278481 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ncc-2-43



3f

-135.82



Current Data Parameters
NAME 20230831-300M
EXPNO 460
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230831
Time 11.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

==== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ncc-2-45



Current Data Parameters
NAME 20230901-400M
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230831
Time 22.24
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.67
DW 60.800 usec
DE 6.50 usec
TE 292.1 K
D1 1.00000000 sec
TD0 1

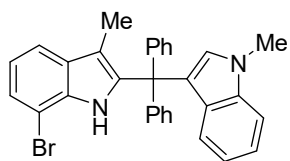
==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

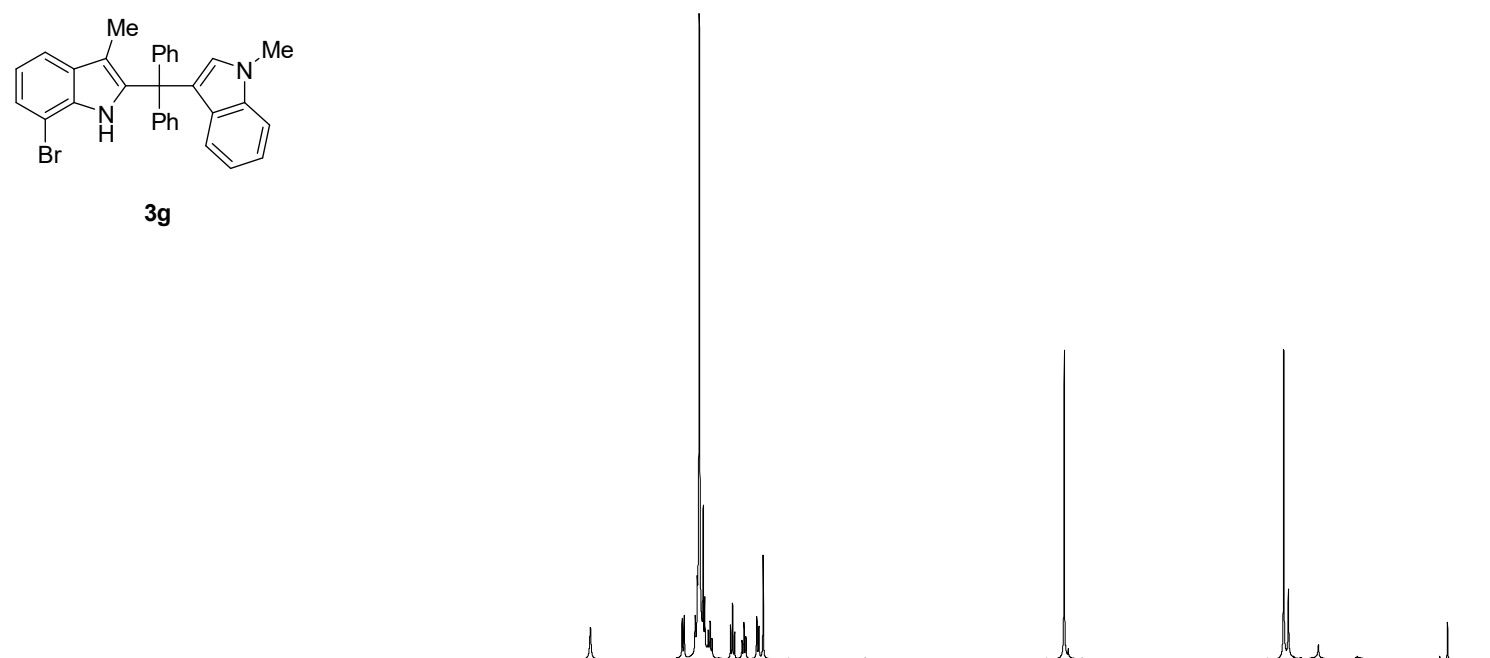
8.357
7.464
7.445
7.338
7.316
7.298
7.260
7.245
7.212
7.192
7.174
6.994
6.974
6.955
6.884
6.882
6.864
6.846
6.739
6.718
6.677

3.750

1.616



3g



13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.99
1.13
11.23
2.31
1.02
1.03
1.03
1.00
3.02
3.00

ncc-2-45



Current Data Parameters
NAME 20230901-400M
EXPNO 13
PROCNO 1

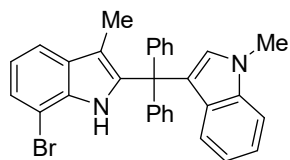
F2 - Acquisition Parameters
Date_ 20230831
Time 22.48
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 292.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

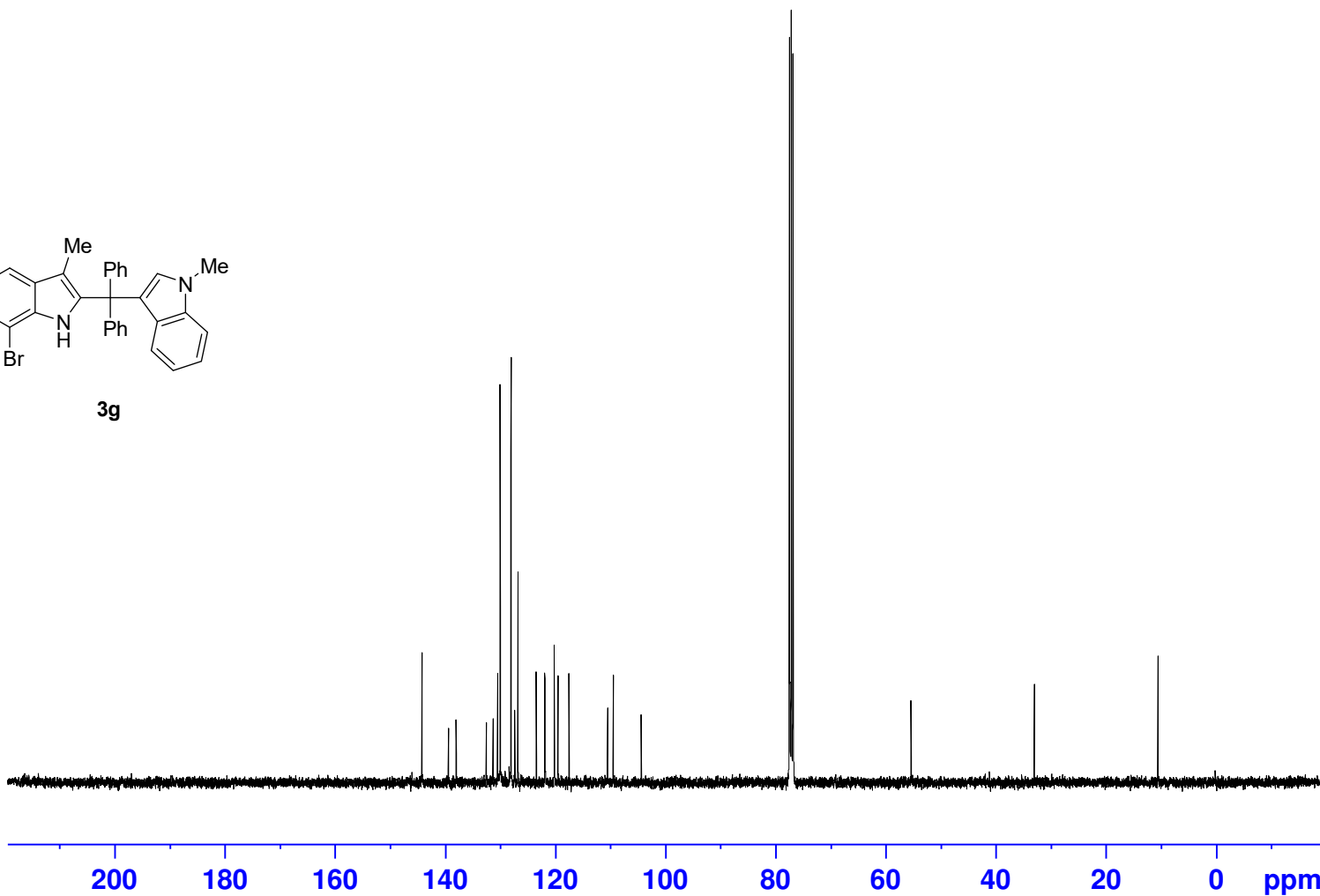
==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278477 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

144.23
139.42
138.02
132.54
131.29
130.50
130.02
128.06
127.38
126.80
123.46
121.92
121.85
120.19
119.51
117.52
110.52
109.48
104.42
77.48
77.16
76.84
55.38
33.00
10.52



3g



ncc-2-82

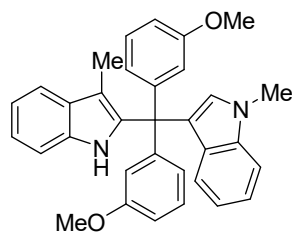
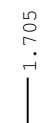
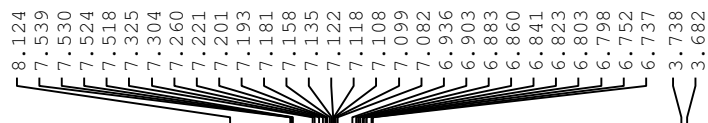


Current Data Parameters
NAME 20231010-400M
EXPNO 22
PROCNO 1

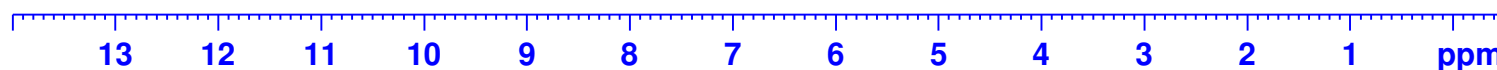
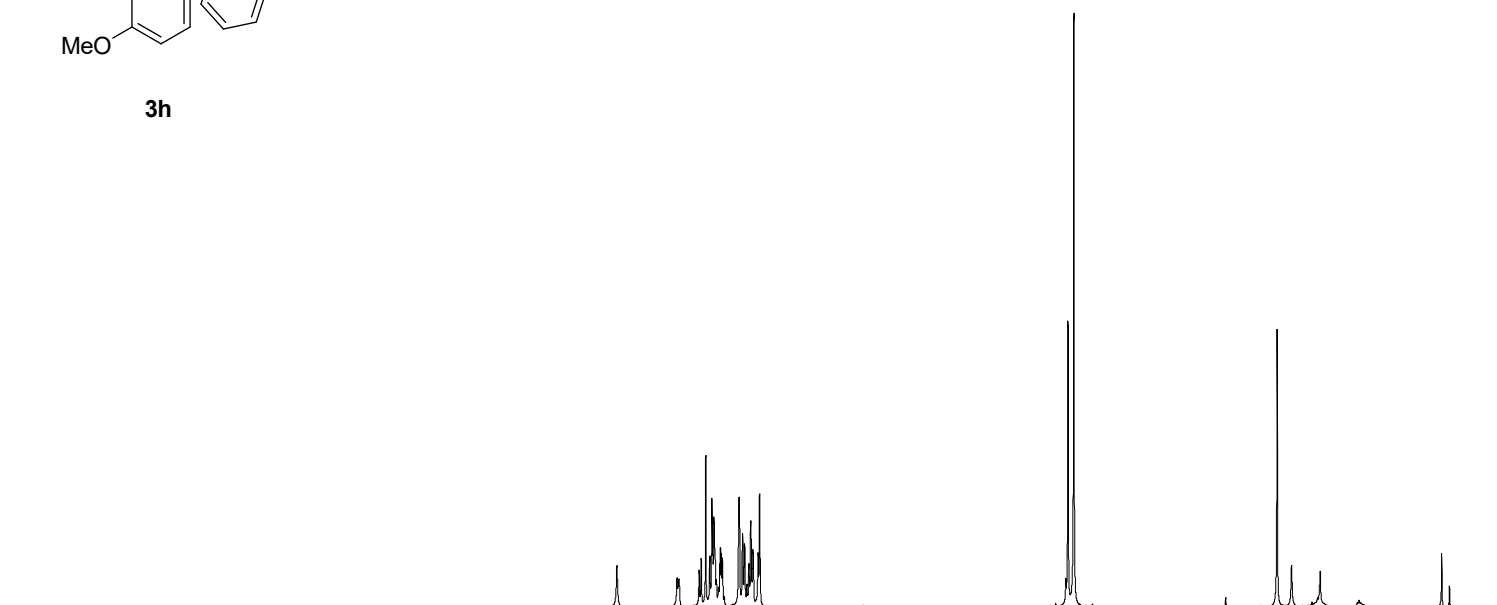
F2 - Acquisition Parameters
Date_ 20231010
Time 1.23
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 75.43
DW 60.800 usec
DE 6.50 usec
TE 293.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3h



ncc-2-82



Current Data Parameters
NAME 20231010-400M
EXPNO 23
PROCNO 1

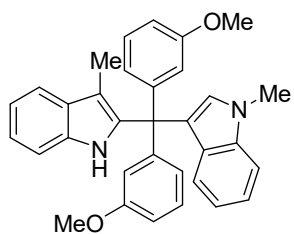
F2 - Acquisition Parameters
Date_ 20231010
Time 1.53
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 61.19
DW 20.800 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

=====
CHANNEL f1
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

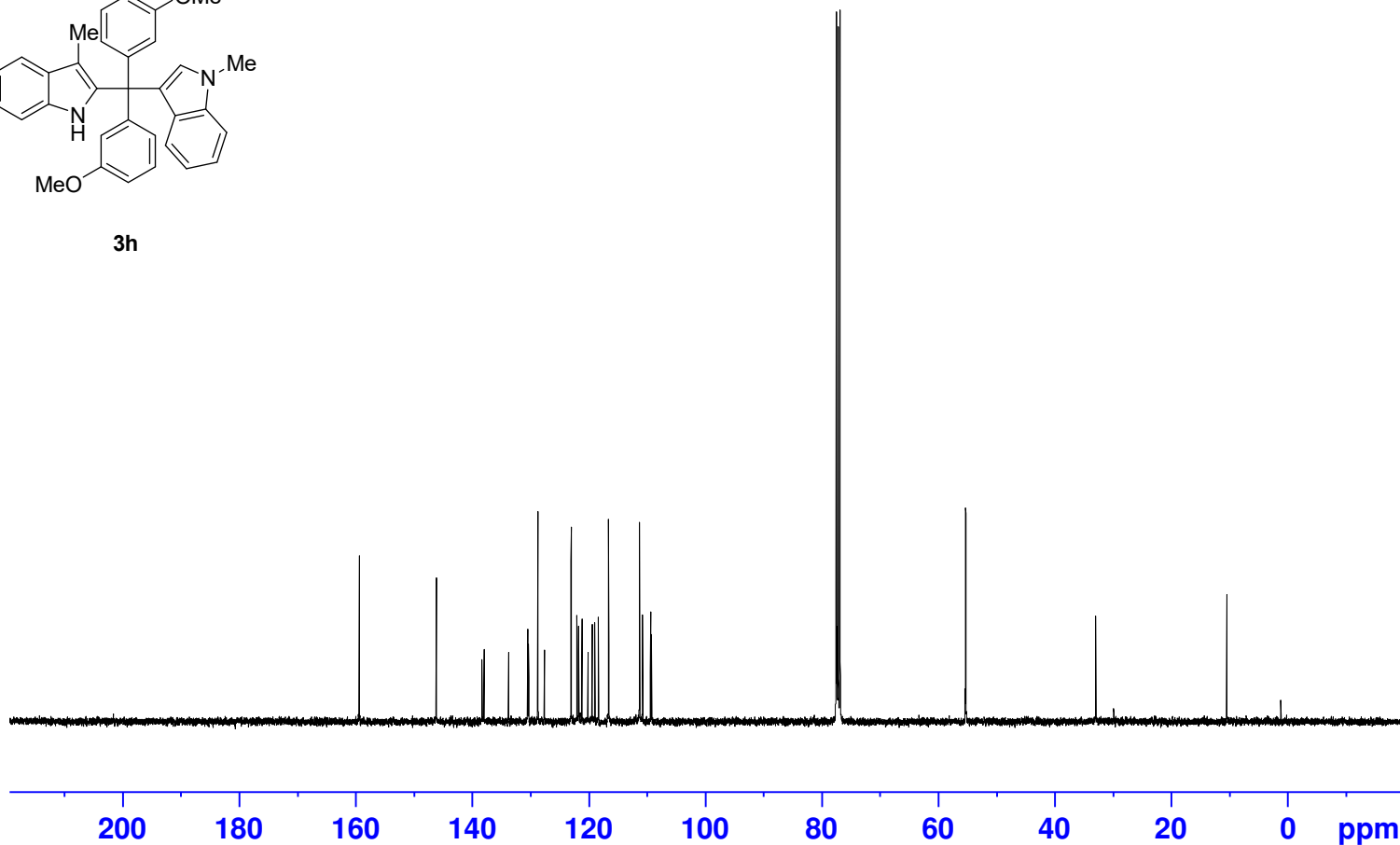
=====
CHANNEL f2
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278491 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

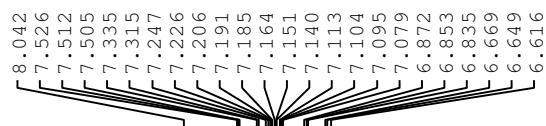
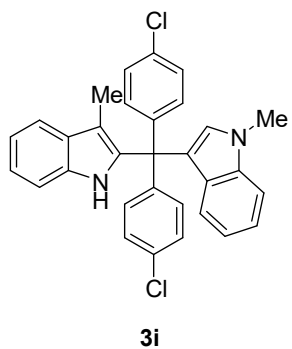
159.37
146.17
138.33
137.97
133.73
130.46
130.31
128.73
127.60
123.02
122.01
121.72
121.16
120.12
119.40
118.95
118.33
116.57
111.28
110.76
109.38
109.20
77.47
77.15
76.84
55.34
55.25
32.95
10.42



3h

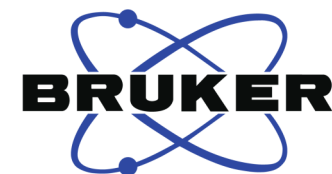


ncc-2-51-2



3.734

1.644

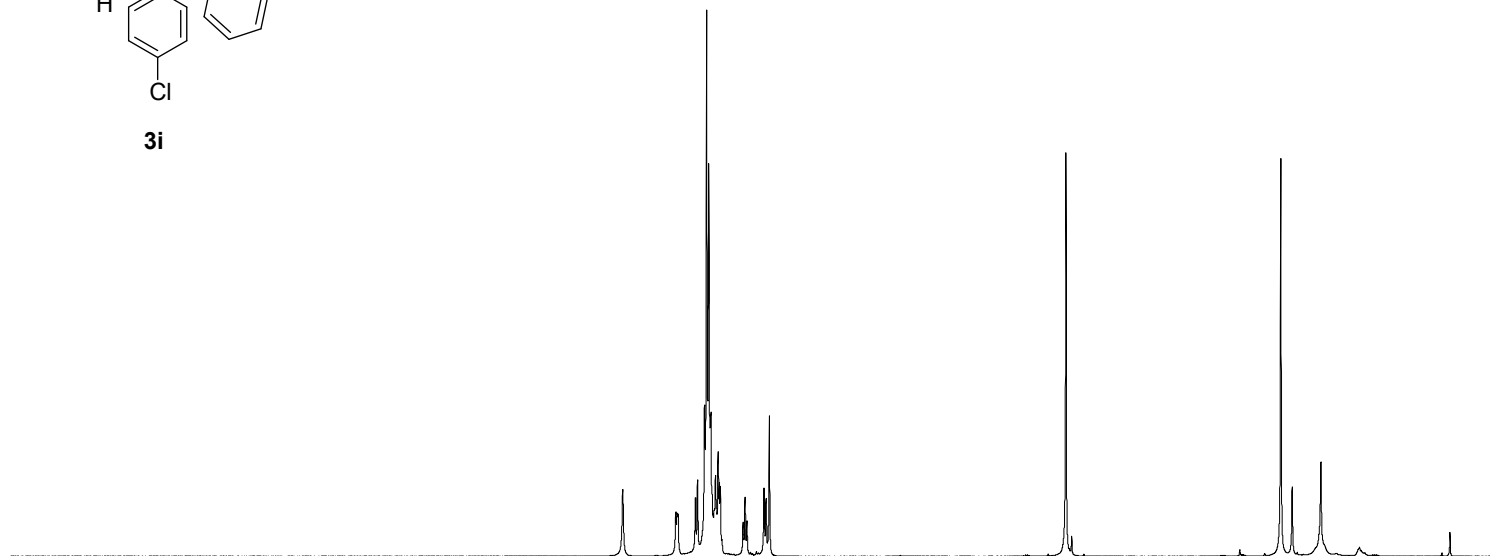


Current Data Parameters
NAME 20230917-400M
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230916
Time 22.40
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 10
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 75.43
DW 60.800 usec
DE 6.50 usec
TE 290.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900270 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ncc-2-51-2



Current Data Parameters
NAME 20230917-400M
EXPNO 10
PROCNO 1

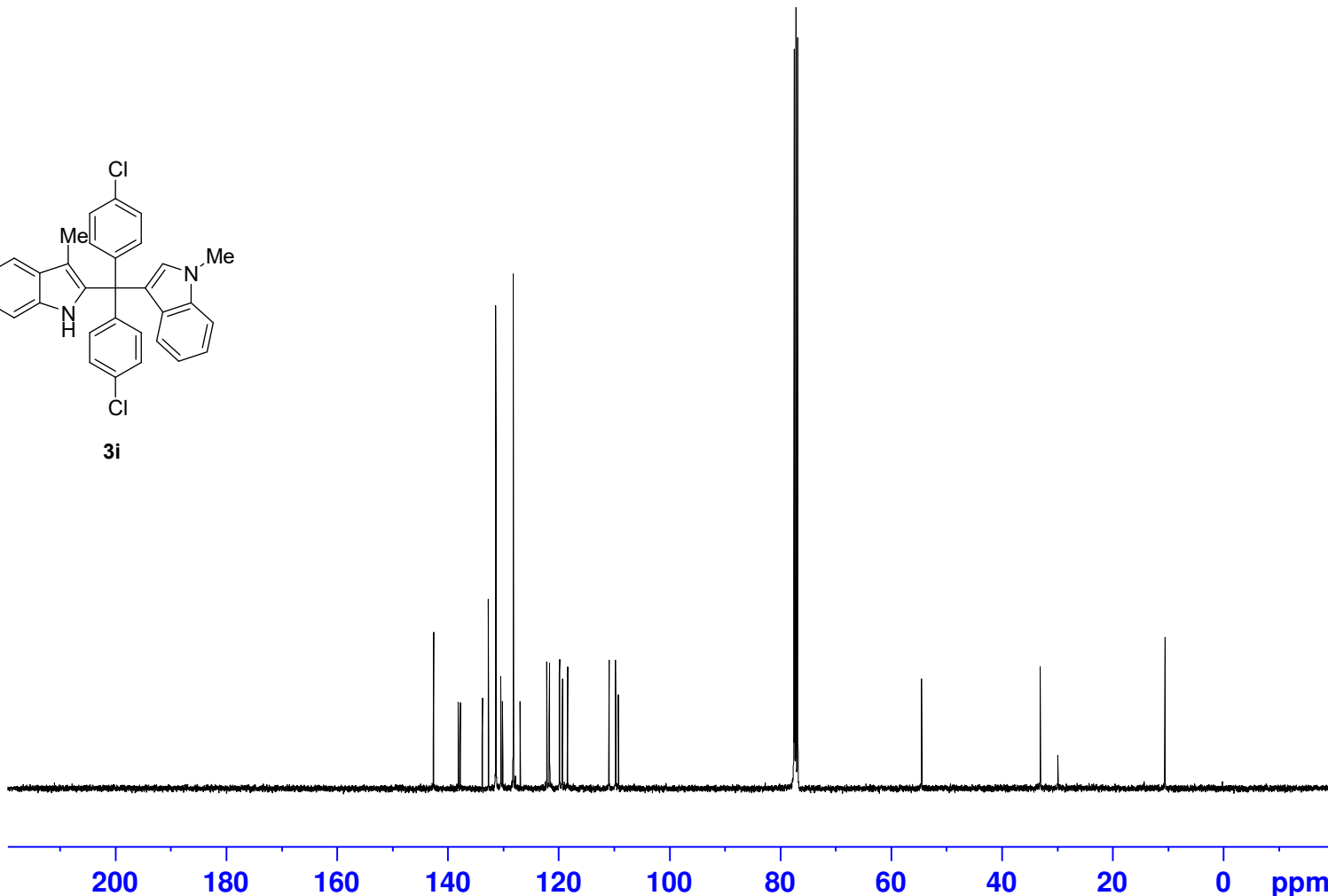
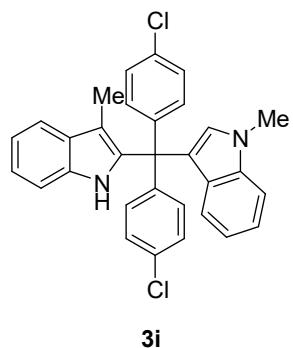
F2 - Acquisition Parameters
Date_ 20230916
Time 23.38
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 50.16
DW 20.800 usec
DE 6.50 usec
TE 291.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

=====
CHANNEL f1
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

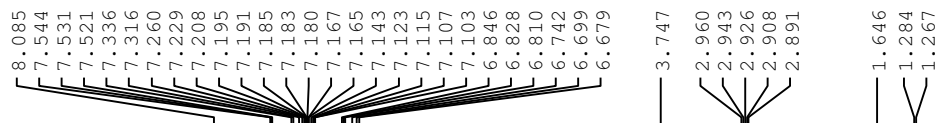
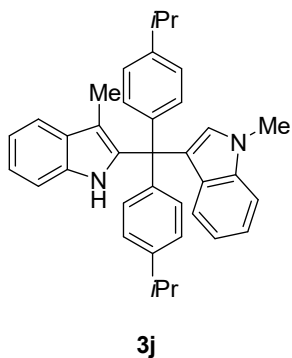
=====
CHANNEL f2
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278499 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

142.58
138.10
137.74
133.78
132.66
131.32
130.42
130.11
128.19
126.95
122.14
121.67
121.61
119.84
119.81
119.31
118.37
110.90
109.70
109.21
77.47
77.16
76.84
54.47
33.04
10.49



ncc-2-98-2

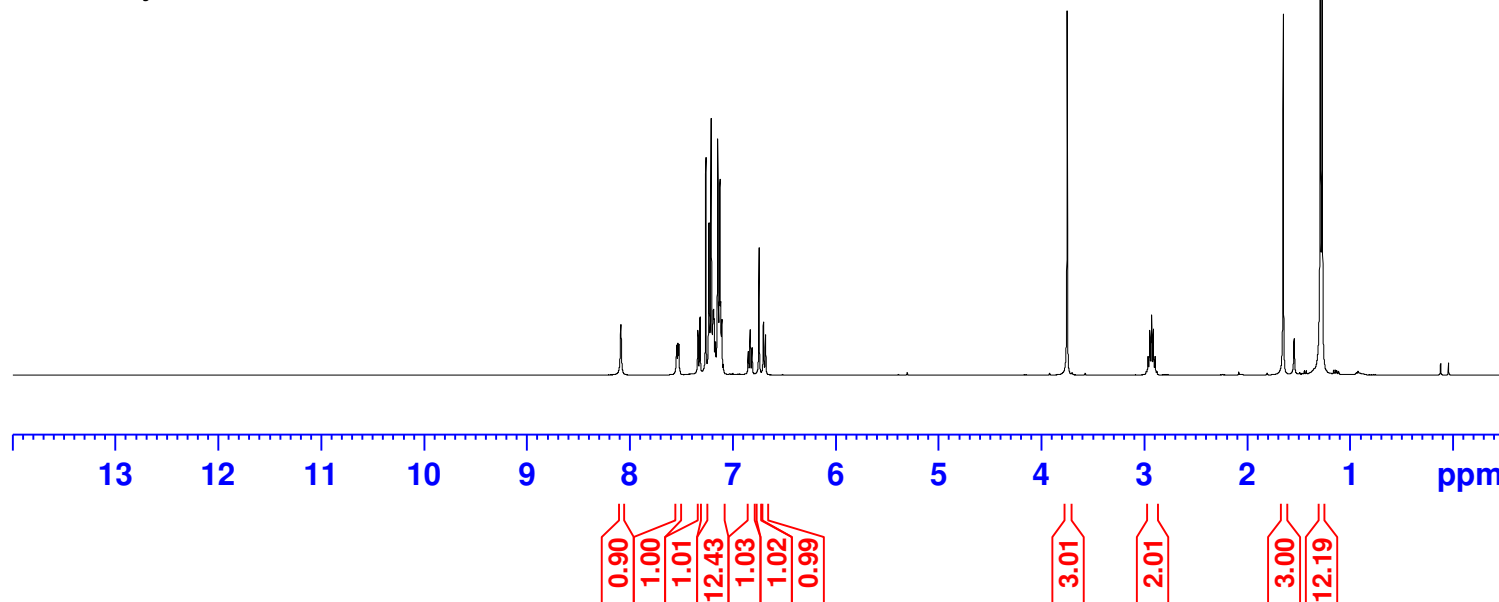


Current Data Parameters
NAME 20231104-400M
EXPNO 27
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231103
Time 23.16
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 68.24
DW 60.800 usec
DE 6.50 usec
TE 291.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ncc-2-98-2



Current Data Parameters
NAME 20231104-400M
EXPNO 28
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231103
Time 23.40
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 292.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278492 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

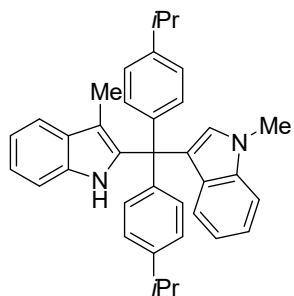
146.91
142.10
139.10
137.95
133.66
130.45
130.36
129.97
127.75
125.86
122.19
121.57
121.00
120.77
119.20
118.92
118.19
110.74
109.29
108.99

77.48
77.16
76.84

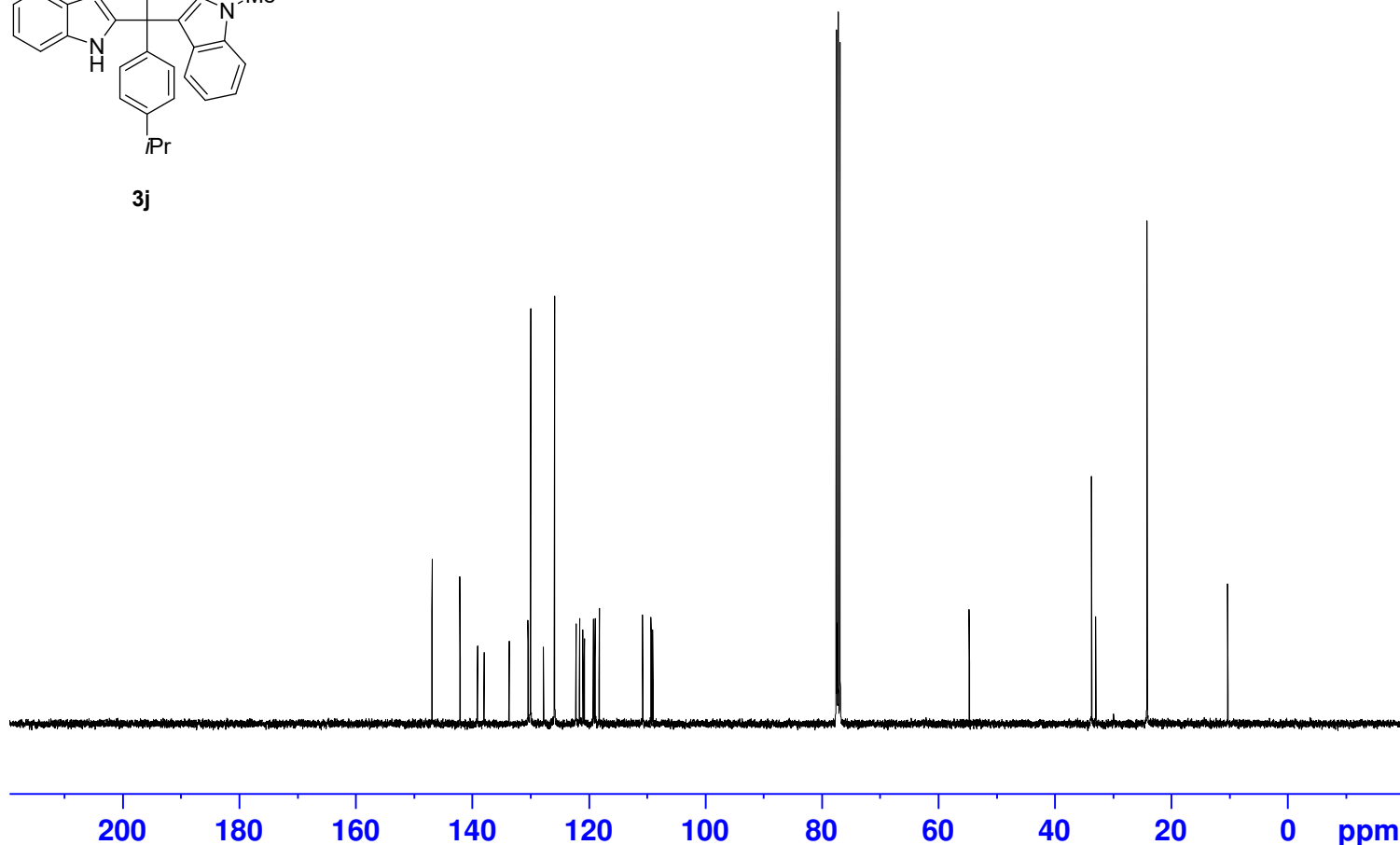
54.64

33.65
32.94
24.13

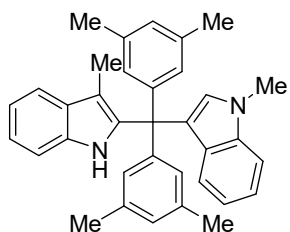
10.25



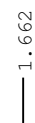
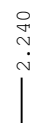
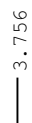
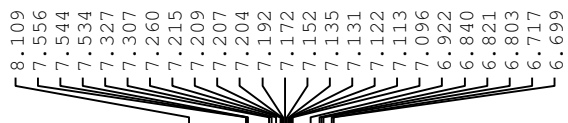
3j



ncc-2-99



3k

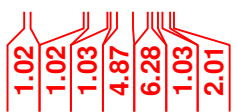
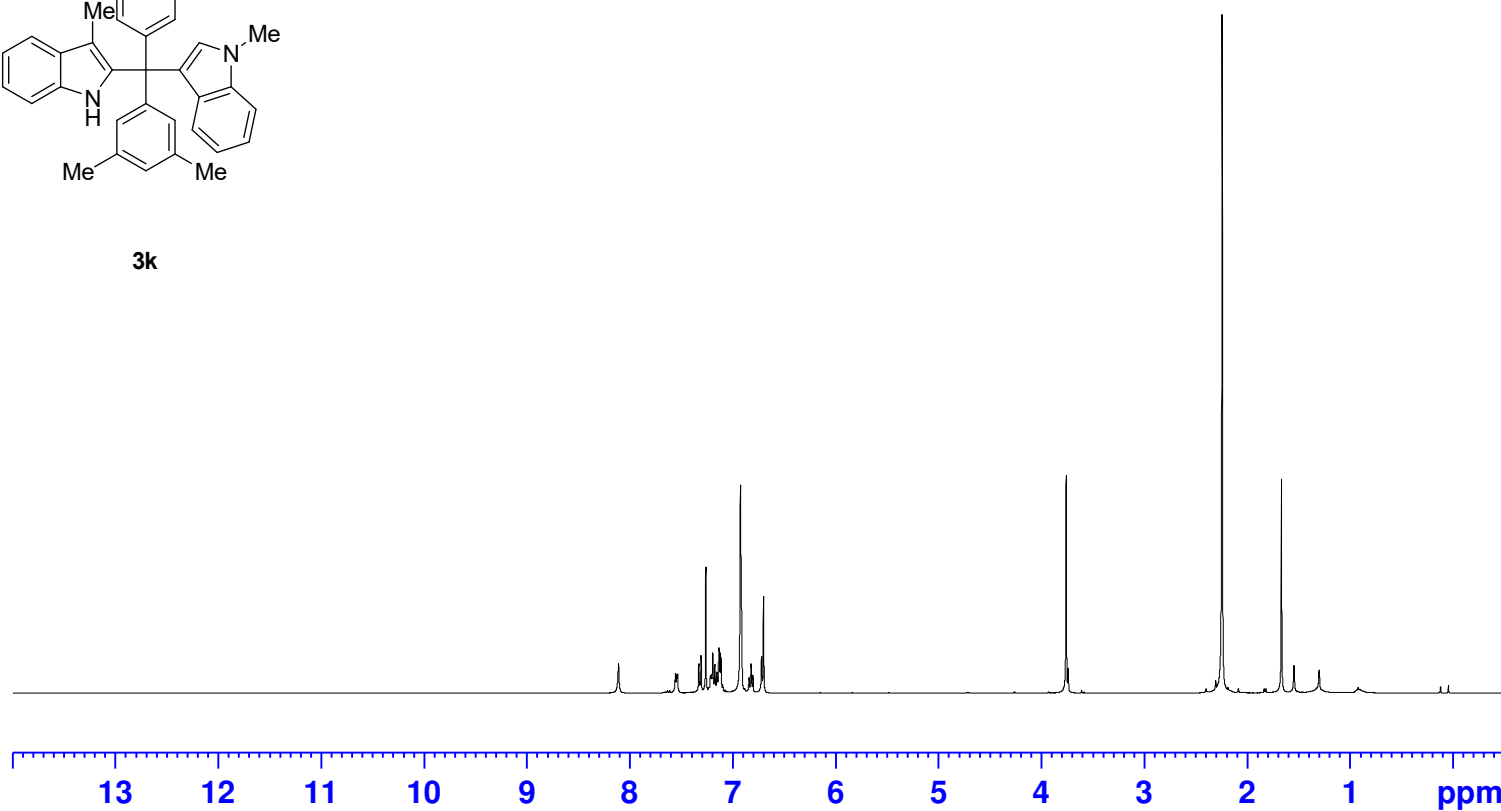


Current Data Parameters
NAME 20231103-400M
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231103
Time 1.03
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 68.24
DW 60.800 usec
DE 6.50 usec
TE 292.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ncc-2-99



Current Data Parameters
NAME 20231103-400M
EXPNO 33
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231103
Time 1.33
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 35.06
DW 20.800 usec
DE 6.50 usec
TE 292.7 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.4000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.0000000 W
PLW12 0.3071200 W
PLW13 0.2487700 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278492 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

144.53
138.81
137.94
137.02
133.62
130.43
130.33
128.14
128.01
127.81
122.16
121.51
120.87
120.78
119.21
118.76
118.33
110.72
109.20

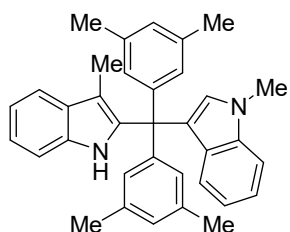
77.48
77.16
76.84

55.06

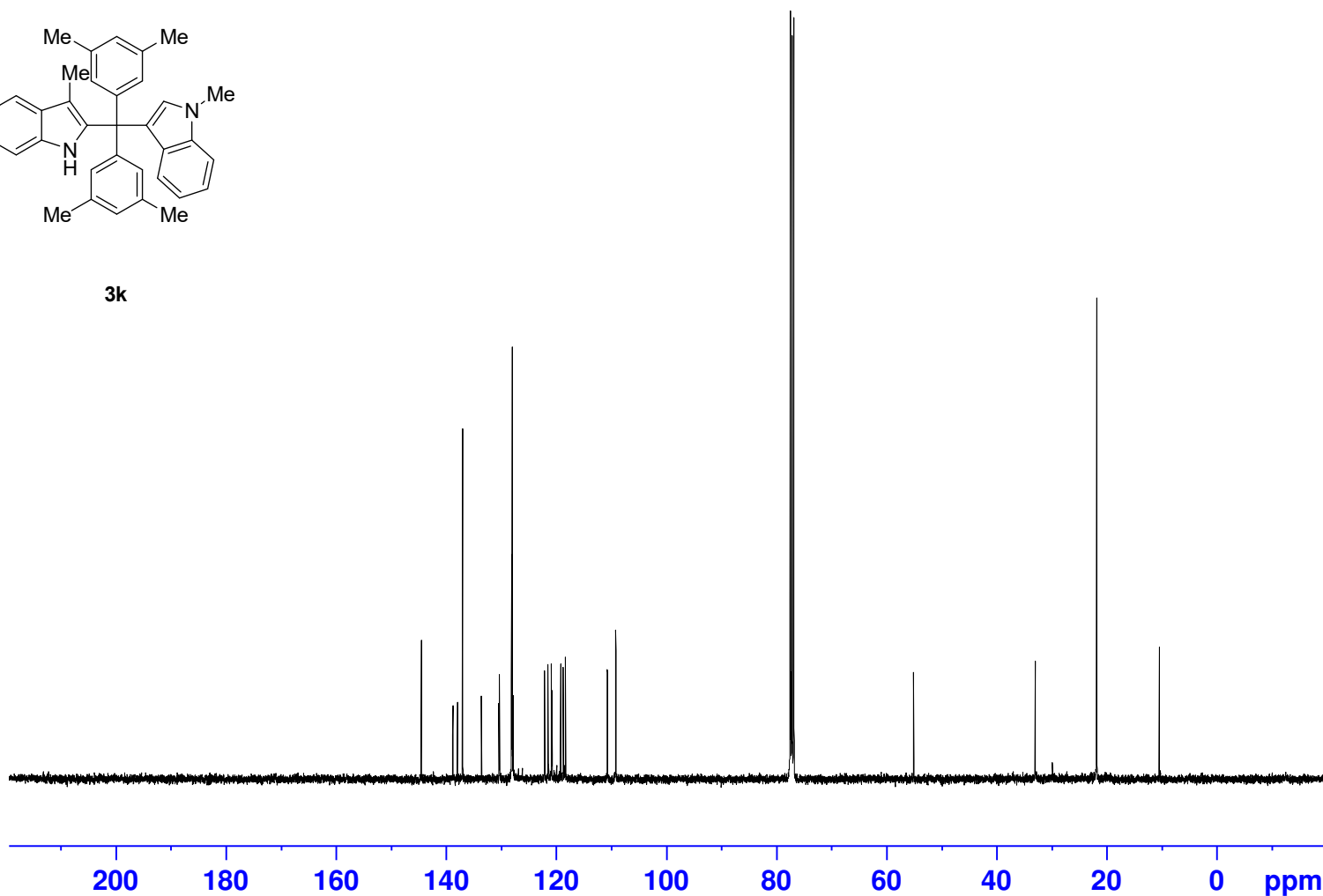
32.97

21.79

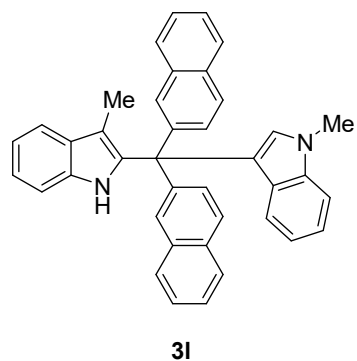
10.41



3k



ncc-3-4



8.249
7.885
7.866
7.846
7.761
7.739
7.714
7.597
7.584
7.575
7.523
7.507
7.489
7.484
7.462
7.443
7.422
7.418
7.364
7.344
7.260
7.233
7.222
7.210
7.204
7.184
7.178
7.168
7.159
7.150
7.134
6.795
6.787
6.771
6.751
3.763

1.707

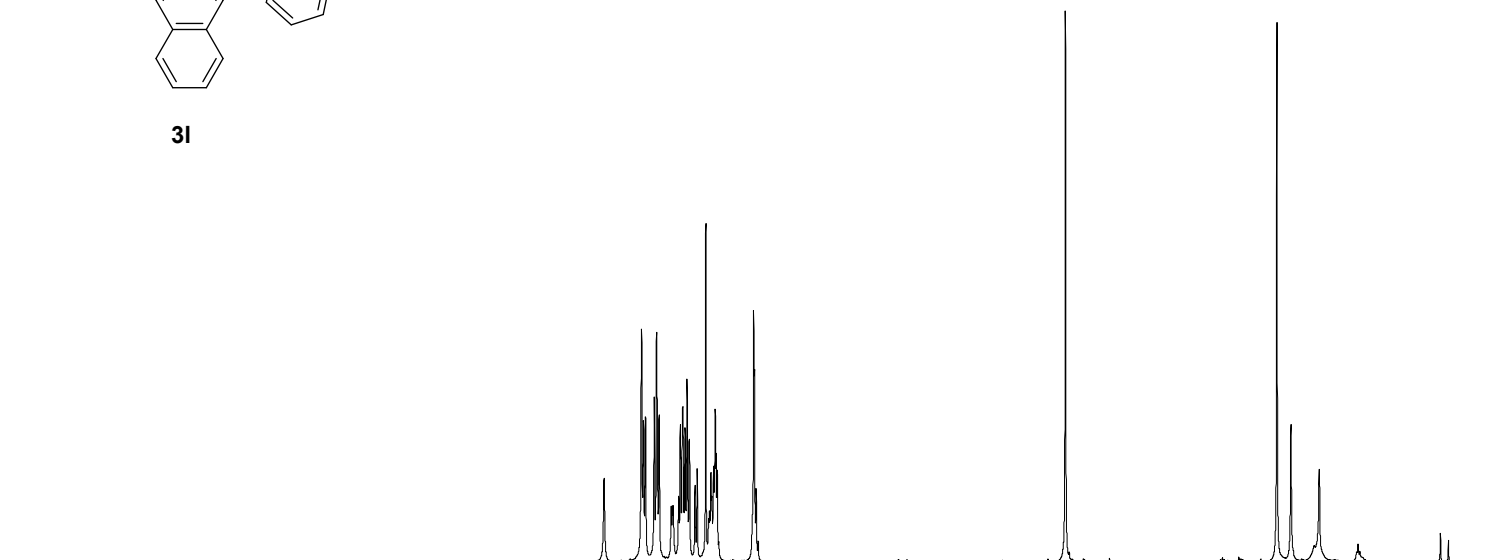


Current Data Parameters
NAME 20231104-400M-2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231104
Time 12.32
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 292.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



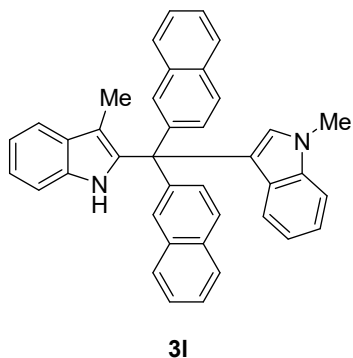
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.97
2.02
2.02
4.05
1.01
6.18
1.03
4.14
3.01

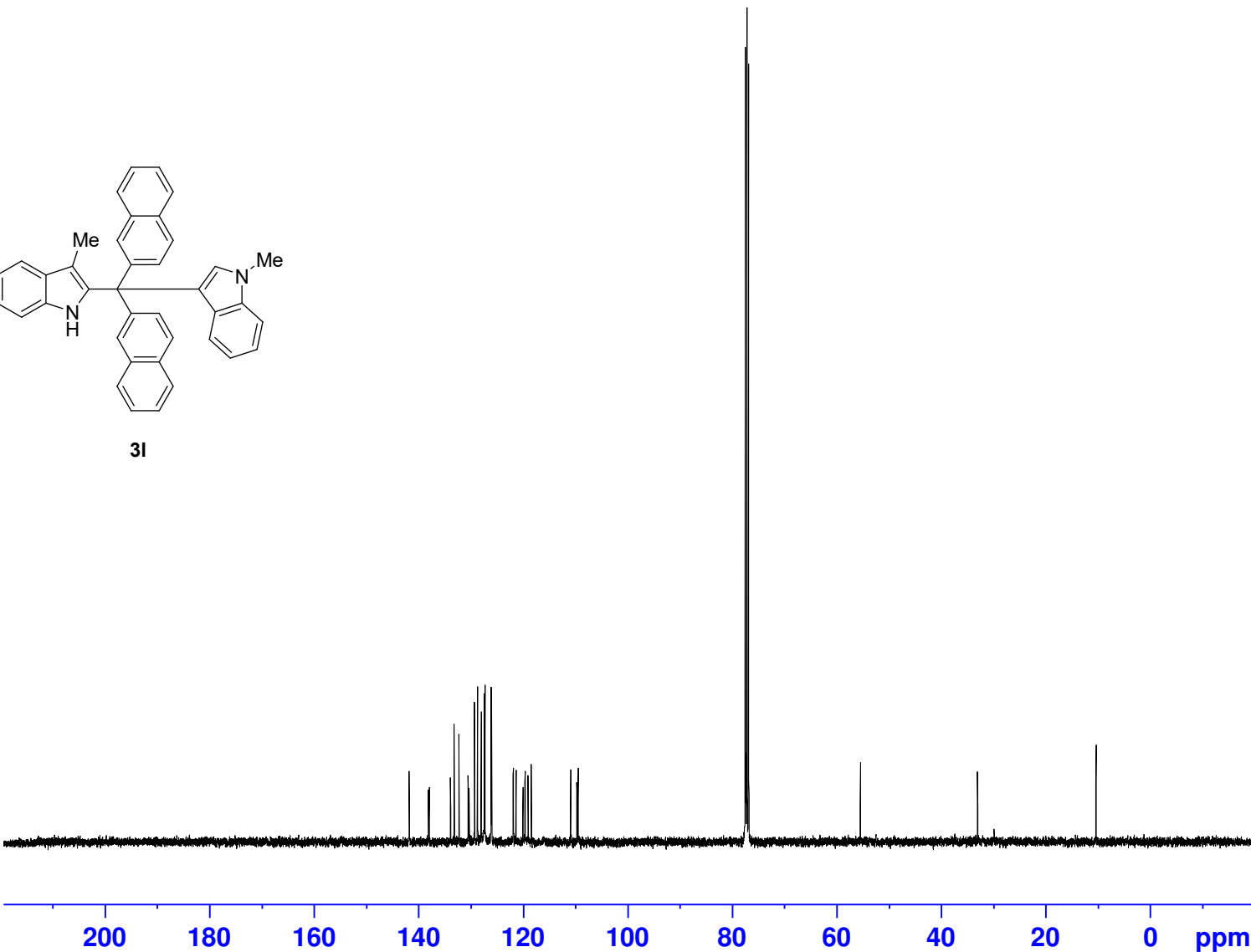
3.01

3.00

ncc-3-4



141.81
138.14
137.99
133.90
133.20
132.28
130.52
130.35
129.31
128.71
128.01
127.48
127.45
127.30
126.14
126.04
121.90
121.84
121.34
120.04
119.64
119.09
118.44
110.89
109.70
109.48
77.47
77.16
76.84



Current Data Parameters
NAME 20231104-400M-2
EXPNO 9
PROCNO 1

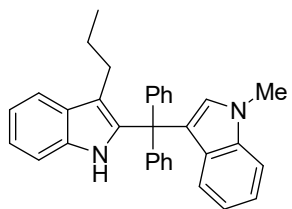
F2 - Acquisition Parameters
Date_ 20231104
Time 12.30
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 35.06
DW 20.800 usec
DE 6.50 usec
TE 293.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278492 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ncc-5-22



3m

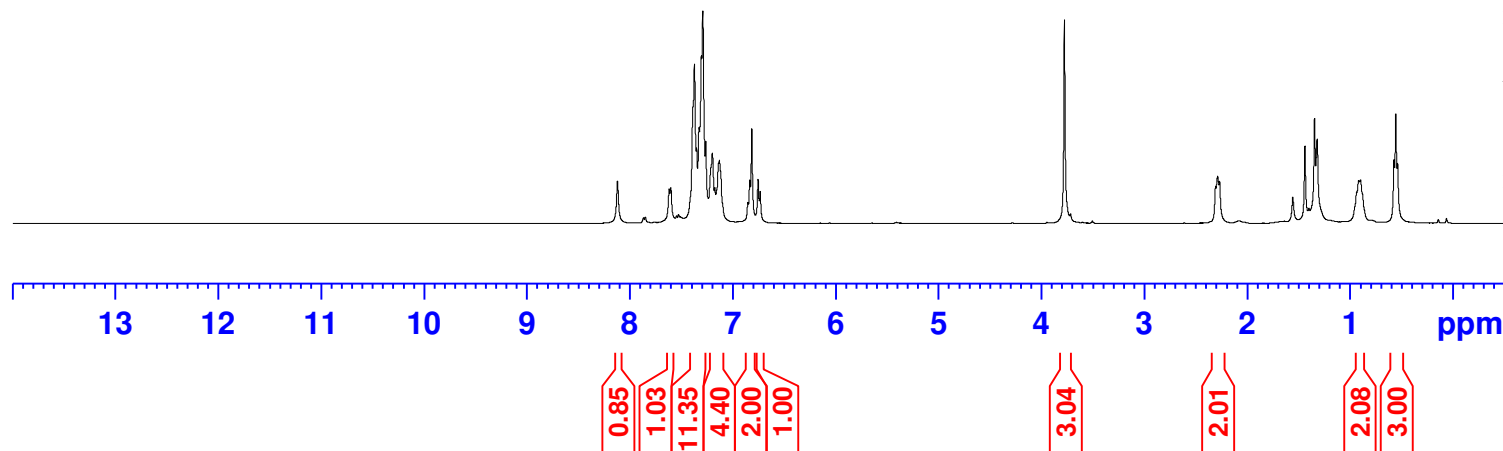


Current Data Parameters
NAME 20240705-400M
EXPNO 13
PROCNO 1

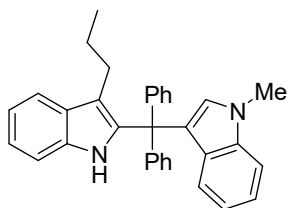
F2 - Acquisition Parameters
Date_ 20240704
Time 21.46
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 53.3
DW 60.800 usec
DE 6.50 usec
TE 292.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

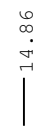
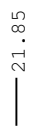
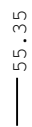
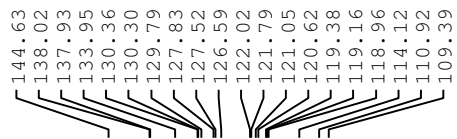
F2 - Processing parameters
SI 65536
SF 400.1900146 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ncc-5-22



3m



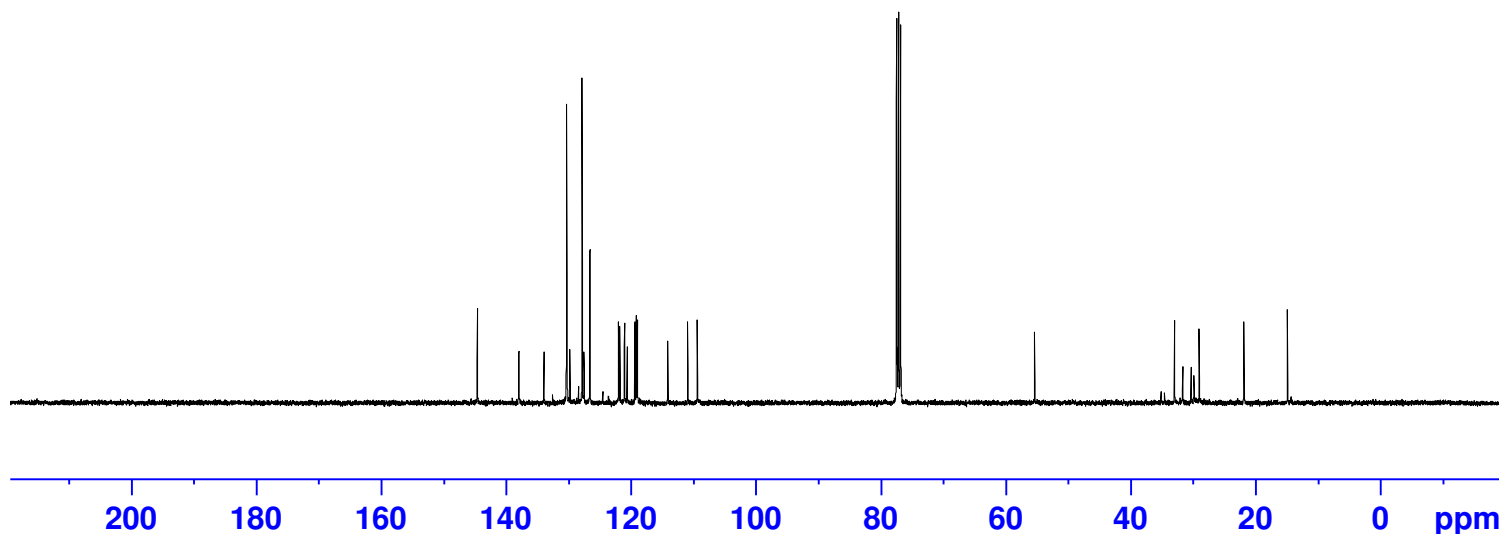
Current Data Parameters
NAME 20240705-400M
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240704
Time 22.22
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 600
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 44.2
DW 20.800 usec
DE 6.50 usec
TE 293.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278513 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



ncc-5-15

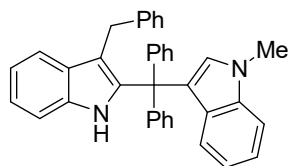
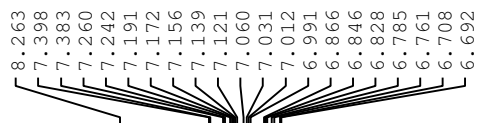


Current Data Parameters
NAME 20240702-400M
EXPNO 22
PROCNO 1

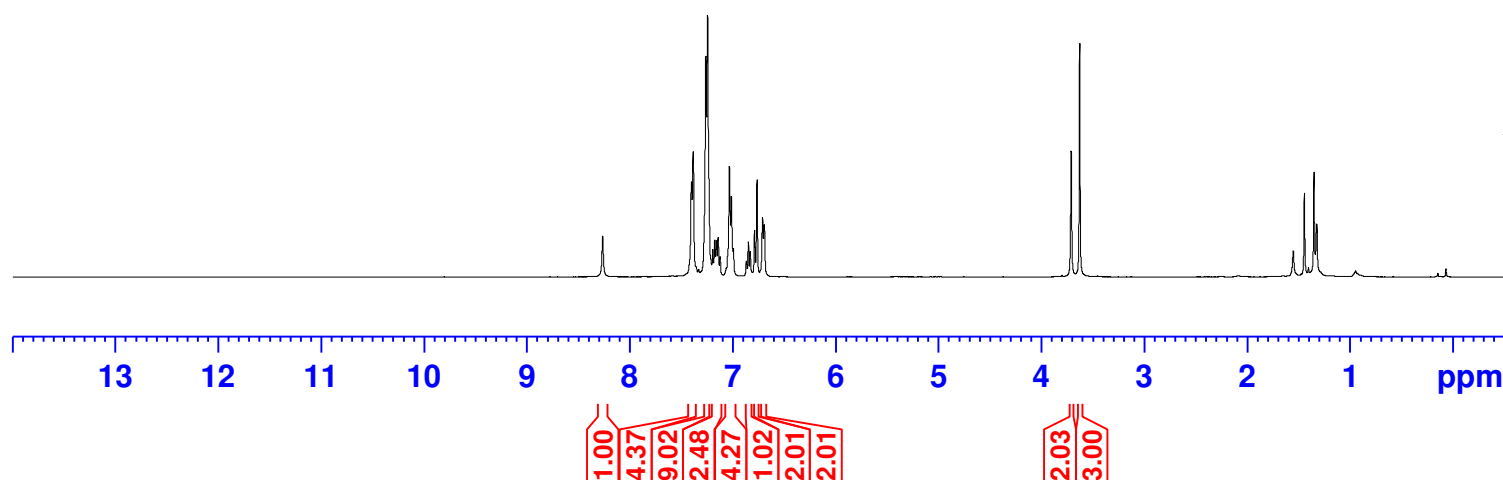
F2 - Acquisition Parameters
Date_ 20240702
Time 5.34
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 61.19
DW 60.800 usec
DE 6.50 usec
TE 291.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

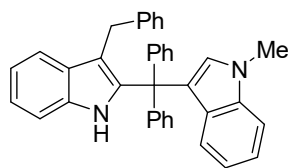
F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3n



ncc-5-15

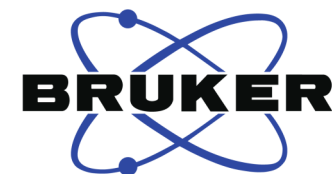
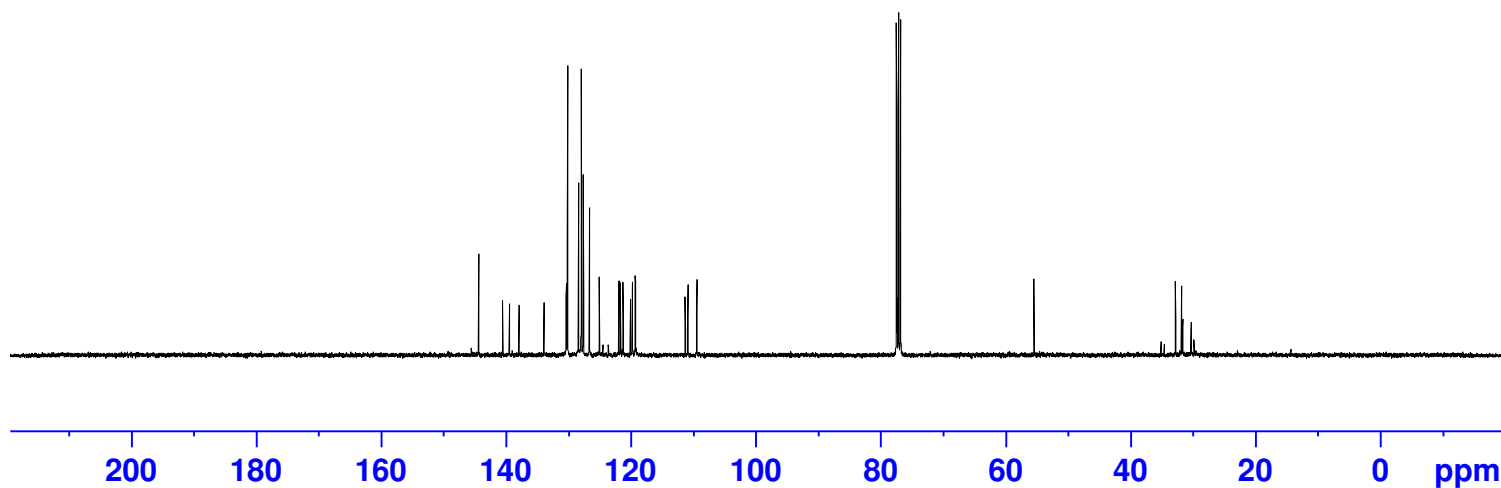


3n

144.38
140.56
139.46
137.94
133.91
130.37
130.18
130.15
128.40
127.95
127.63
127.58
126.65
125.07
121.93
121.68
121.25
120.08
119.78
119.34
119.29
111.31
110.88
109.45
77.47
77.16
76.84

55.46

32.77
31.82



Current Data Parameters
NAME 20240702-400M
EXPNO 23
PROCNO 1

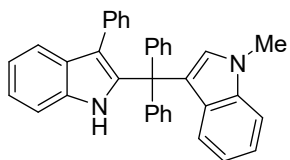
F2 - Acquisition Parameters
Date_ 20240702
Time 6.04
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 50.16
DW 20.800 usec
DE 6.50 usec
TE 292.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

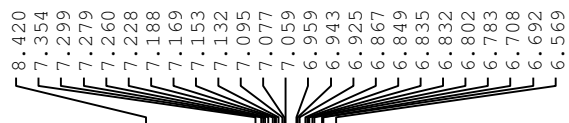
==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278528 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

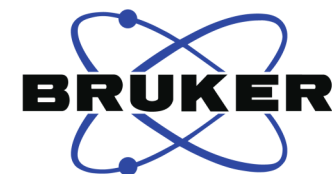
ncc-5-19



3o



3.558

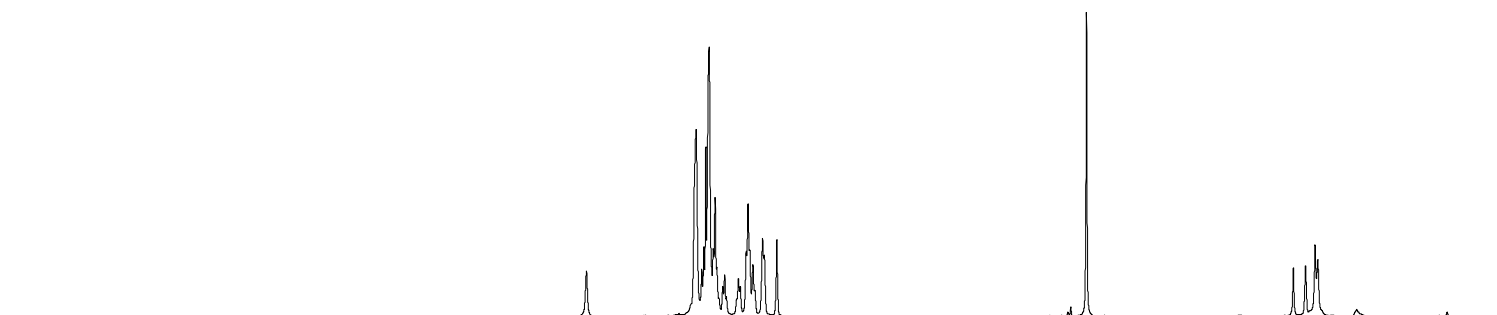


Current Data Parameters
NAME 20240706-400M
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240705
Time 22.06
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 61.19
DW 60.800 usec
DE 6.50 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.02
6.59
9.41
1.02
1.10
4.31
2.04
1.01

3.00

ncc-5-19



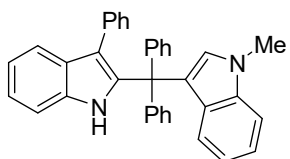
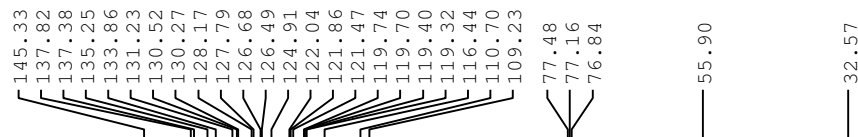
Current Data Parameters
NAME 20240706-400M
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240705
Time 22.30
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 293.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

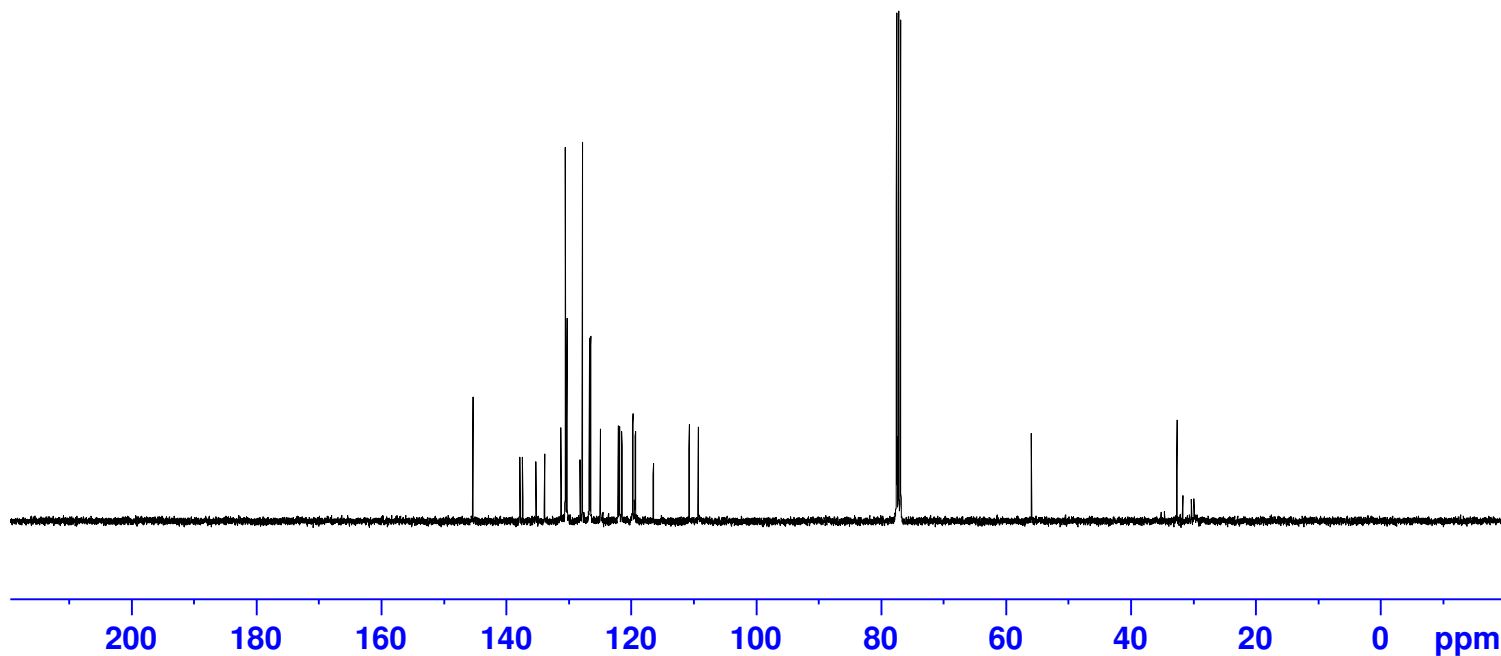
==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278507 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



3o



ncc-2-60



Current Data Parameters
NAME 20230917-400M-2
EXPNO 17
PROCNO 1

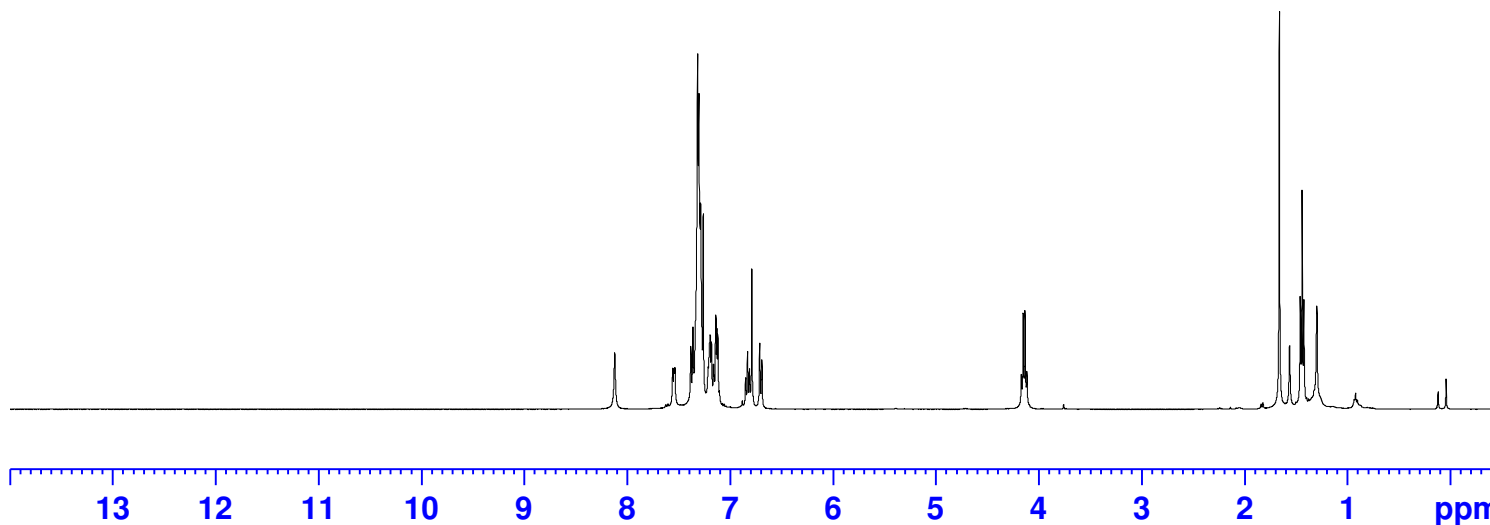
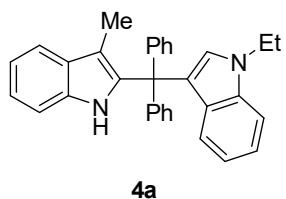
F2 - Acquisition Parameters
Date_ 20230916
Time 13.48
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 75.43
DW 60.800 usec
DE 6.50 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.120
7.556
7.544
7.535
7.380
7.360
7.313
7.302
7.294
7.286
7.260
7.214
7.192
7.180
7.160
7.153
7.137
7.128
7.119
6.848
6.828
6.810
6.787
6.710
6.690
4.167
4.149
4.131
4.113

1.658
1.456
1.438
1.420



0.94
1.02
11.14
4.17
1.01
0.98
1.00

2.03

3.00
3.01

ncc-2-60



Current Data Parameters
NAME 20230917-400M-2
EXPNO 18
PROCNO 1

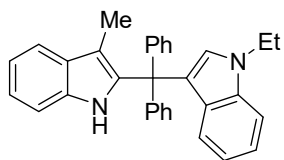
F2 - Acquisition Parameters
Date_ 20230916
Time 14.18
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 53.3
DW 20.800 usec
DE 6.50 usec
TE 291.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

=====
CHANNEL f1
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

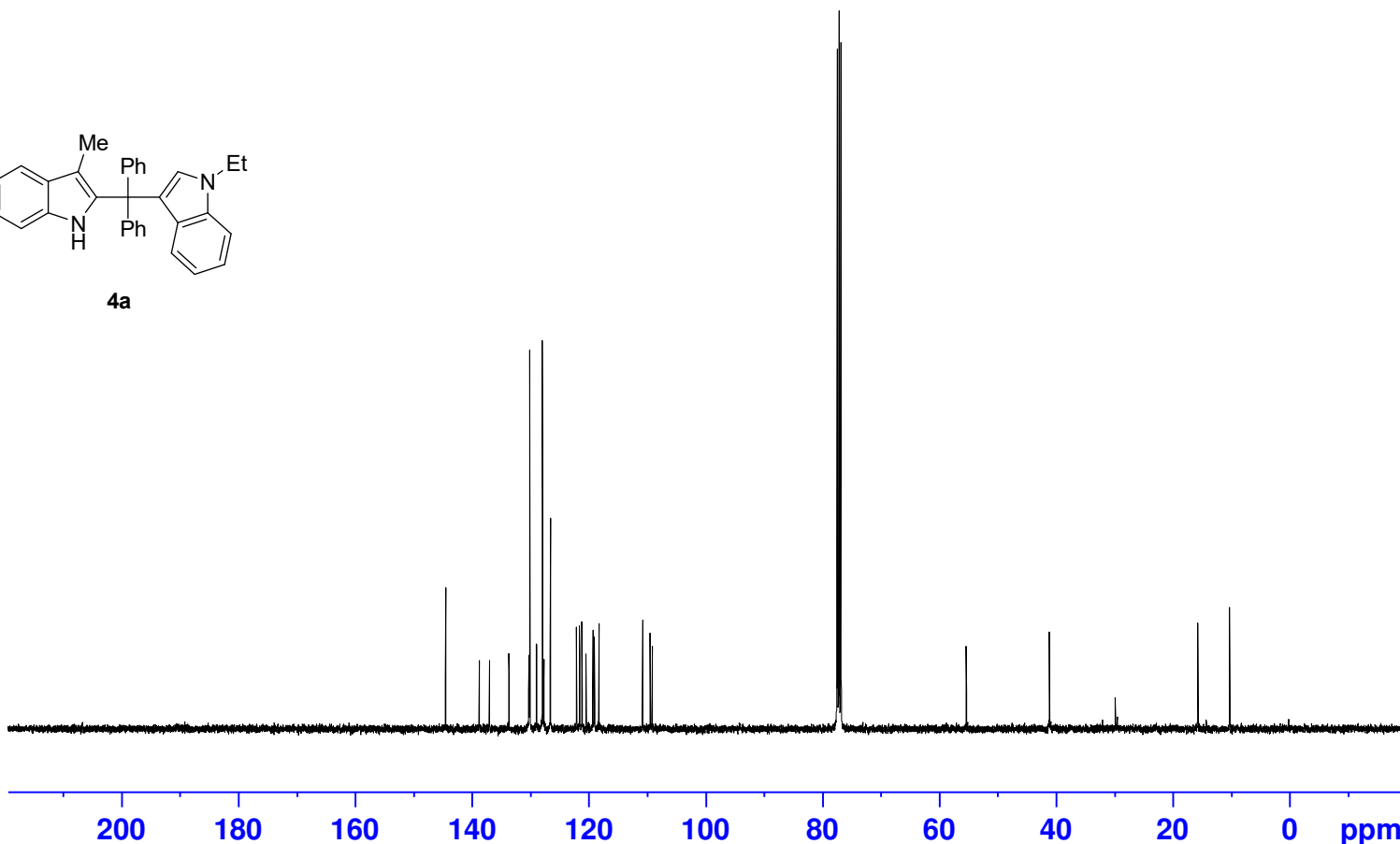
=====
CHANNEL f2
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278499 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

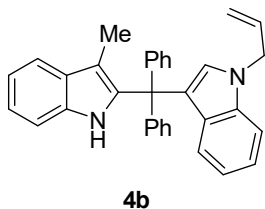
144.54
138.76
137.02
133.68
130.29
130.14
128.96
127.94
127.72
126.59
122.14
121.58
121.18
120.49
119.31
119.04
118.26
110.79
109.51
109.15
77.47
77.16
76.84
55.36
41.14
15.71
10.25



4a



ncc-2-61



8.106
7.558
7.543
7.538
7.345
7.320
7.307
7.291
7.259
7.218
7.202
7.194
7.174
7.144
7.135
7.109
6.874
6.857
6.838
6.820
6.789
6.716
6.696
6.031
6.019
6.006
5.992
5.977
5.963
5.951
5.938
5.205
5.180
5.068
5.025
4.708
4.696

1.667

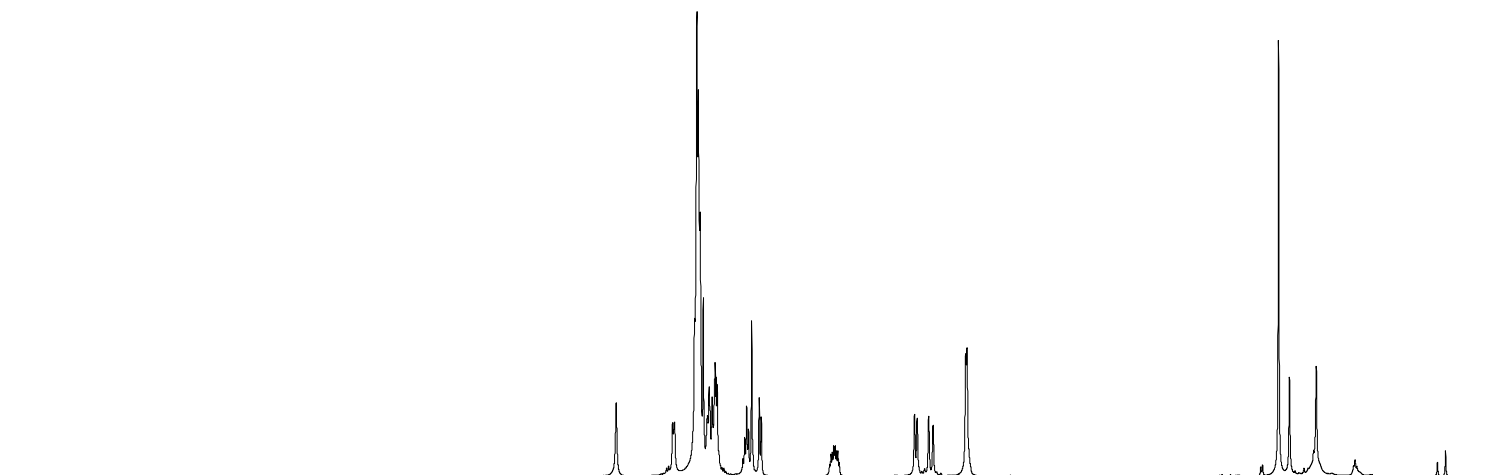


Current Data Parameters
NAME 20230915-400M
EXPNO 27
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230914
Time 23.50
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 68.24
DW 60.800 usec
DE 6.50 usec
TE 291.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

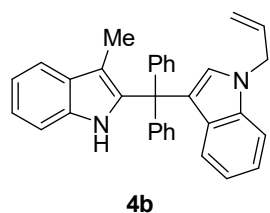
F2 - Processing parameters
SI 65536
SF 400.1900141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.89
1.02
11.23
4.18
1.00
0.99
0.98
1.01
1.03
1.00
2.06
3.00

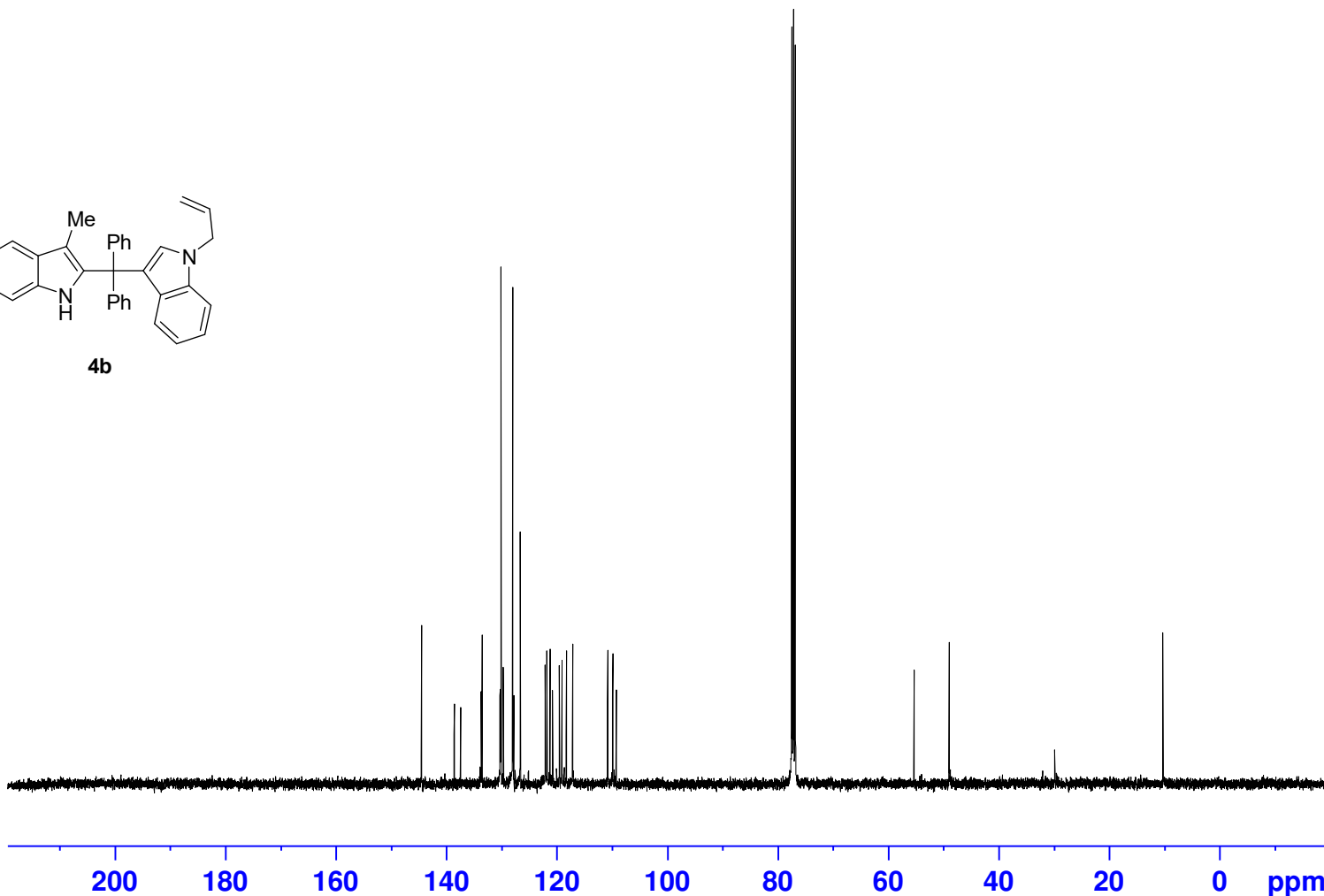
ncc-2-61



144.52
138.59
137.41
133.70
133.52
130.29
130.13
129.70
127.98
127.79
126.63
122.11
121.79
121.22
120.77
119.55
119.06
118.28
117.15
110.81
109.88
109.25
77.48
77.16
76.84

55.31
48.93

10.26



Current Data Parameters
NAME 20230915-400M
EXPNO 28
PROCNO 1

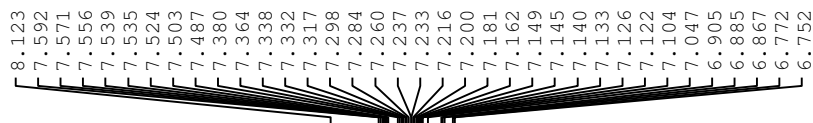
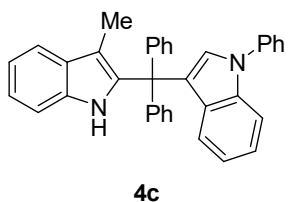
F2 - Acquisition Parameters
Date_ 20230915
Time 0.14
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 44.2
DW 20.800 usec
DE 6.50 usec
TE 291.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278507 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ncc-3-14

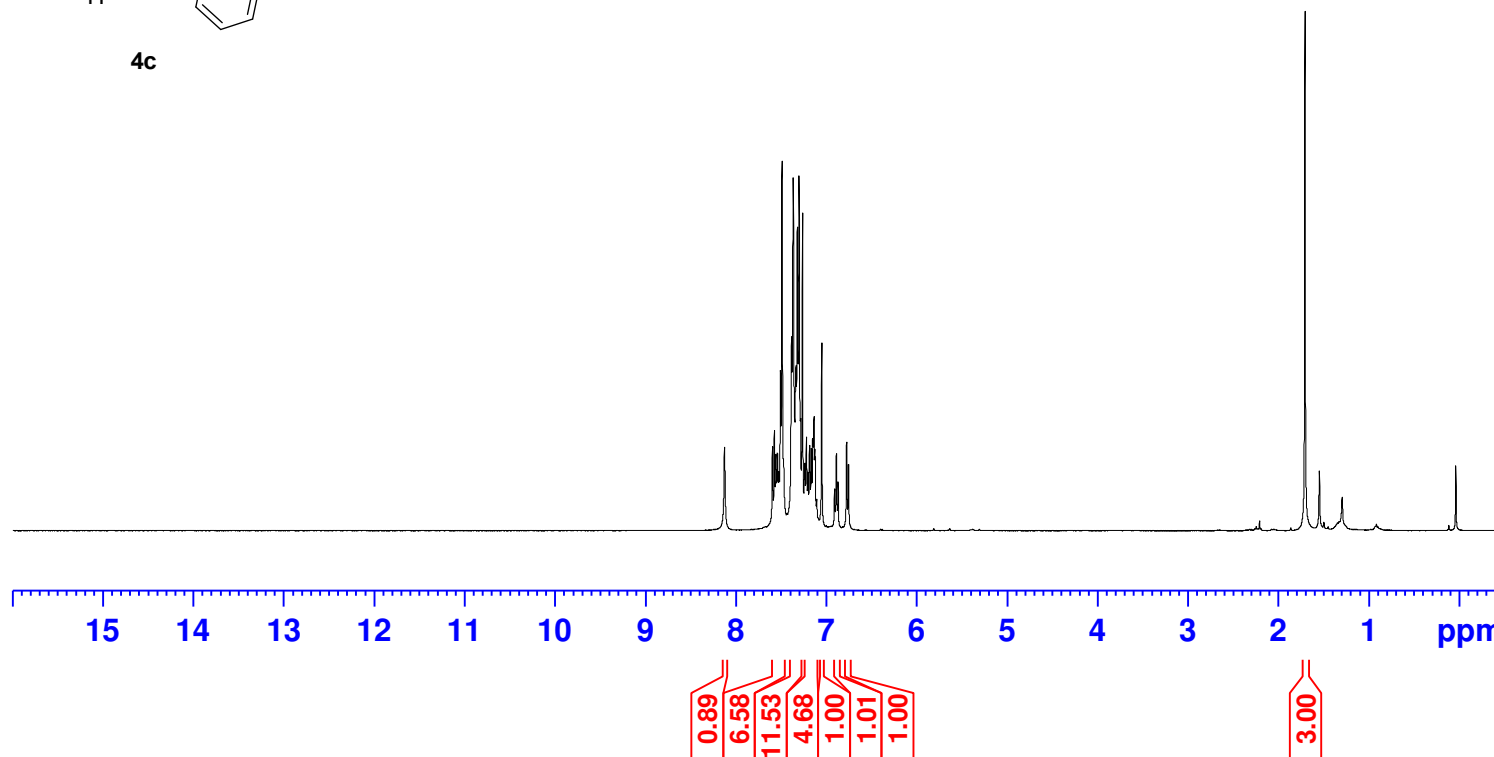


Current Data Parameters
NAME 20231115-400M
EXPNO 18
PROCNO 1

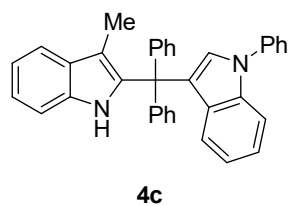
F2 - Acquisition Parameters
Date_ 20231115
Time 0.28
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



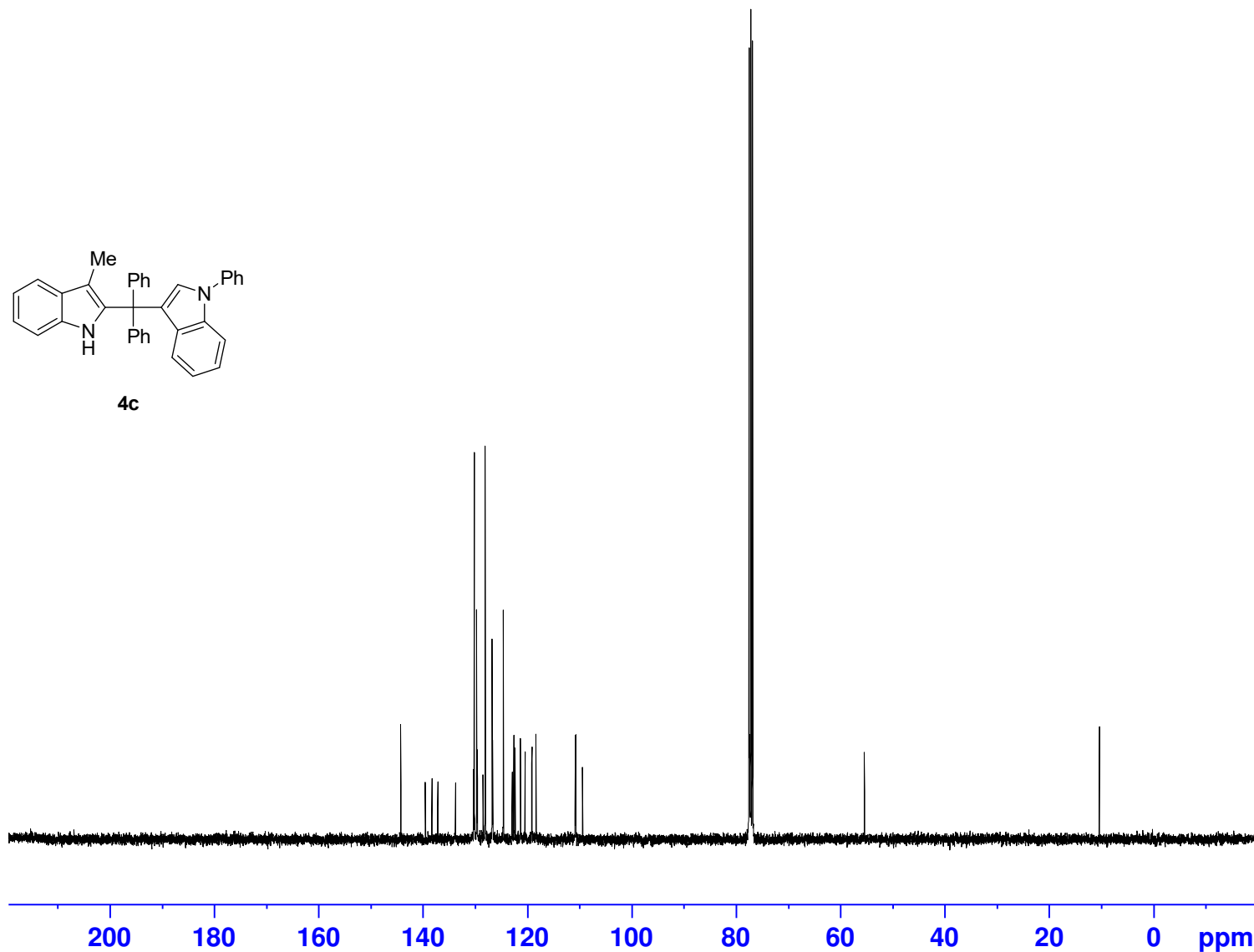
ncc-3-14



144.27
139.57
138.30
137.18
133.78
130.32
130.17
129.71
129.60
128.50
128.08
126.77
126.65
124.62
122.92
122.59
122.35
121.34
120.44
119.14
118.35
110.82
110.73
109.42
77.47
77.16
76.84

55.37

10.32



Current Data Parameters
NAME 20231115-400M
EXPNO 19
PROCNO 1

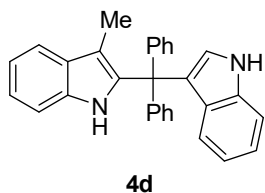
F2 - Acquisition Parameters
Date_ 20231115
Time 0.52
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

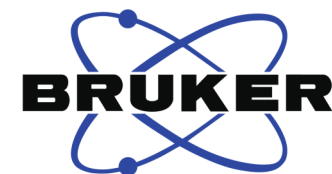
F2 - Processing parameters
SI 32768
SF 100.6278477 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NCC-2-73



8.073
7.991
7.546
7.534
7.526
7.374
7.354
7.291
7.278
7.270
7.260
7.170
7.152
7.131
7.120
7.111
6.853
6.833
6.816
6.706
6.686

1.650

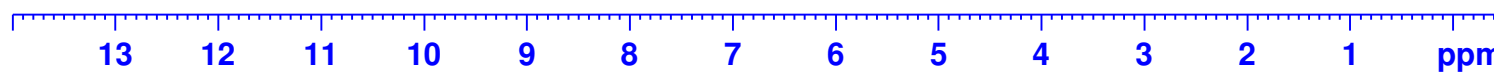
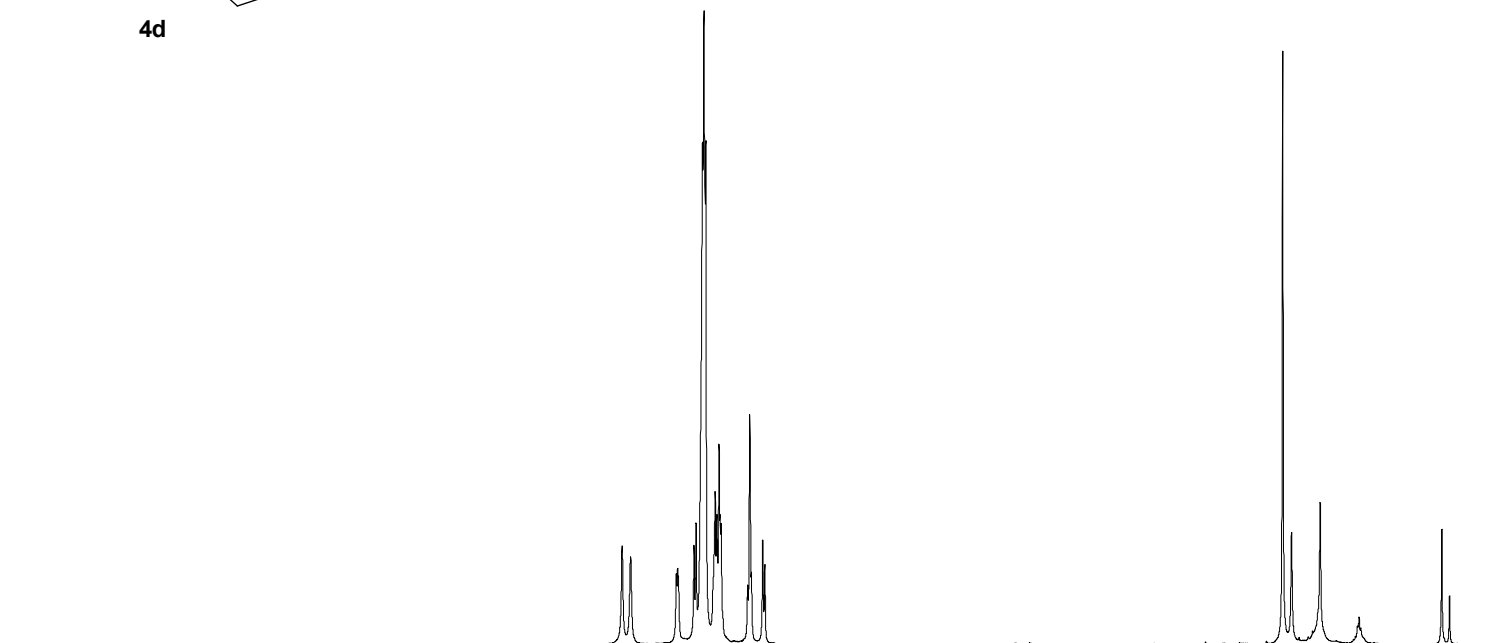


Current Data Parameters
NAME 20231008-400M
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231007
Time 23.12
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.67
DW 60.800 usec
DE 6.50 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1

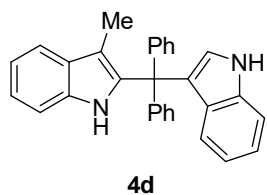
==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.00
0.97
1.01
11.74
4.27
2.01
1.00
3.00

NCC-2-73

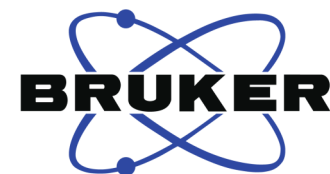
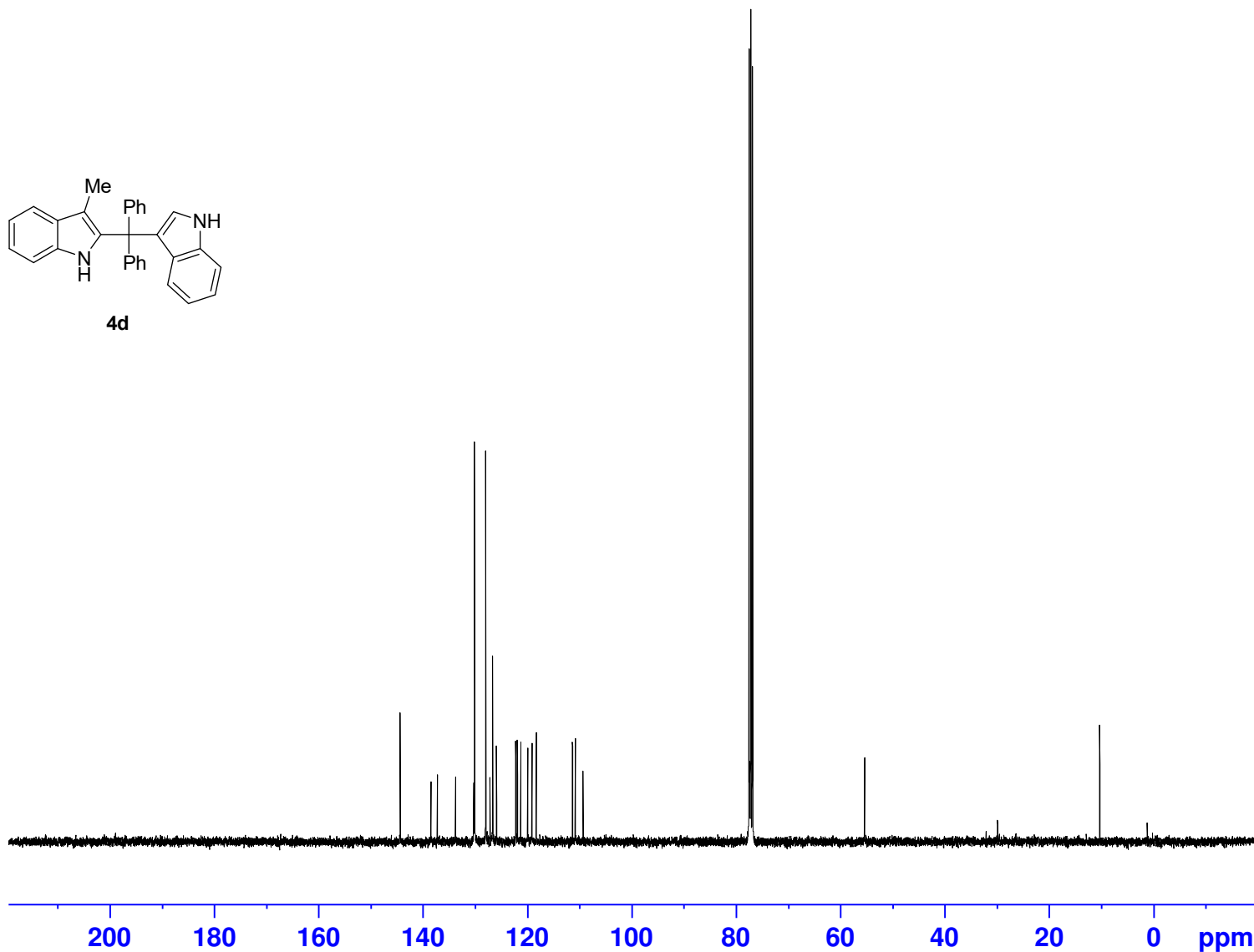


144.41
138.48
137.24
133.75
130.30
130.13
127.99
127.17
126.67
125.92
122.25
122.17
121.92
121.27
119.92
119.11
118.28
111.35
110.82
109.33

77.47
77.16
76.84

55.33

10.26



Current Data Parameters
NAME 20231008-400M
EXPNO 14
PROCNO 1

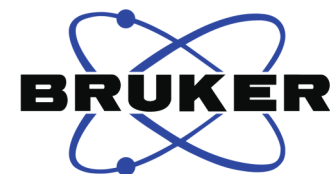
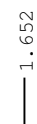
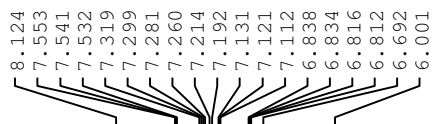
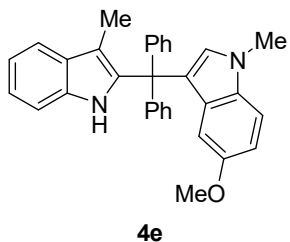
F2 - Acquisition Parameters
Date_ 20231007
Time 23.42
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 50.16
DW 20.800 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278477 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ncc-2-64

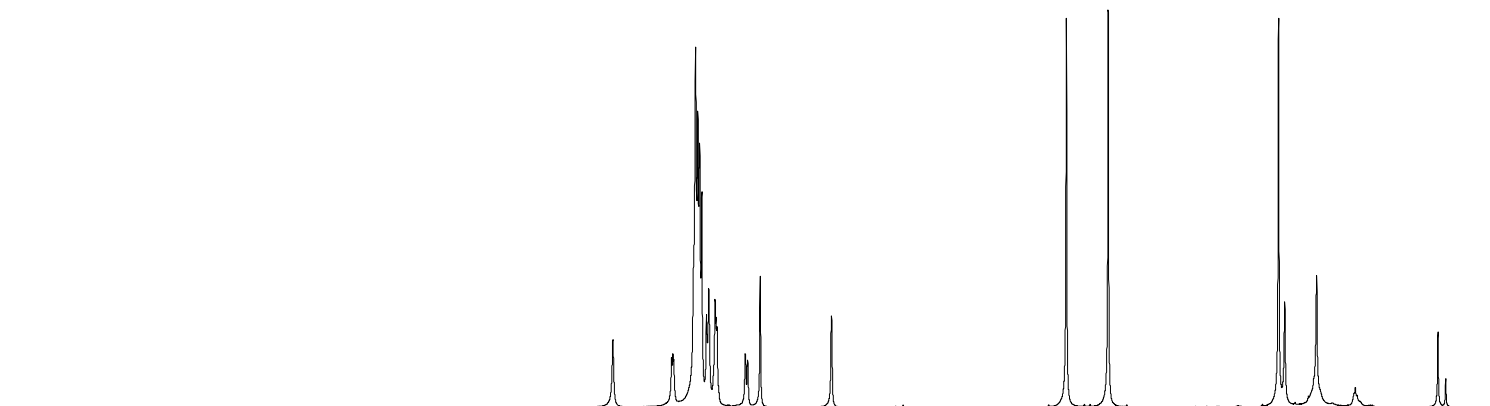


Current Data Parameters
NAME 20230921-400M
EXPNO 35
PROCNO 1

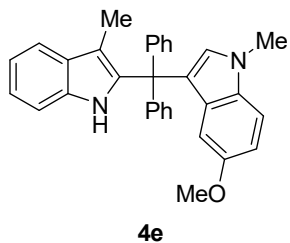
F2 - Acquisition Parameters
Date_ 20230921
Time 1.03
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 90.23
DW 60.800 usec
DE 6.50 usec
TE 290.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ncc-2-64



153.57
144.41
138.81
133.72
133.25
130.88
130.29
130.16
127.96
127.74
126.58
121.20
120.07
119.06
118.23
112.37
110.80
110.20
109.19
102.98

77.47
77.16
76.84

55.43
55.29

33.14

10.28



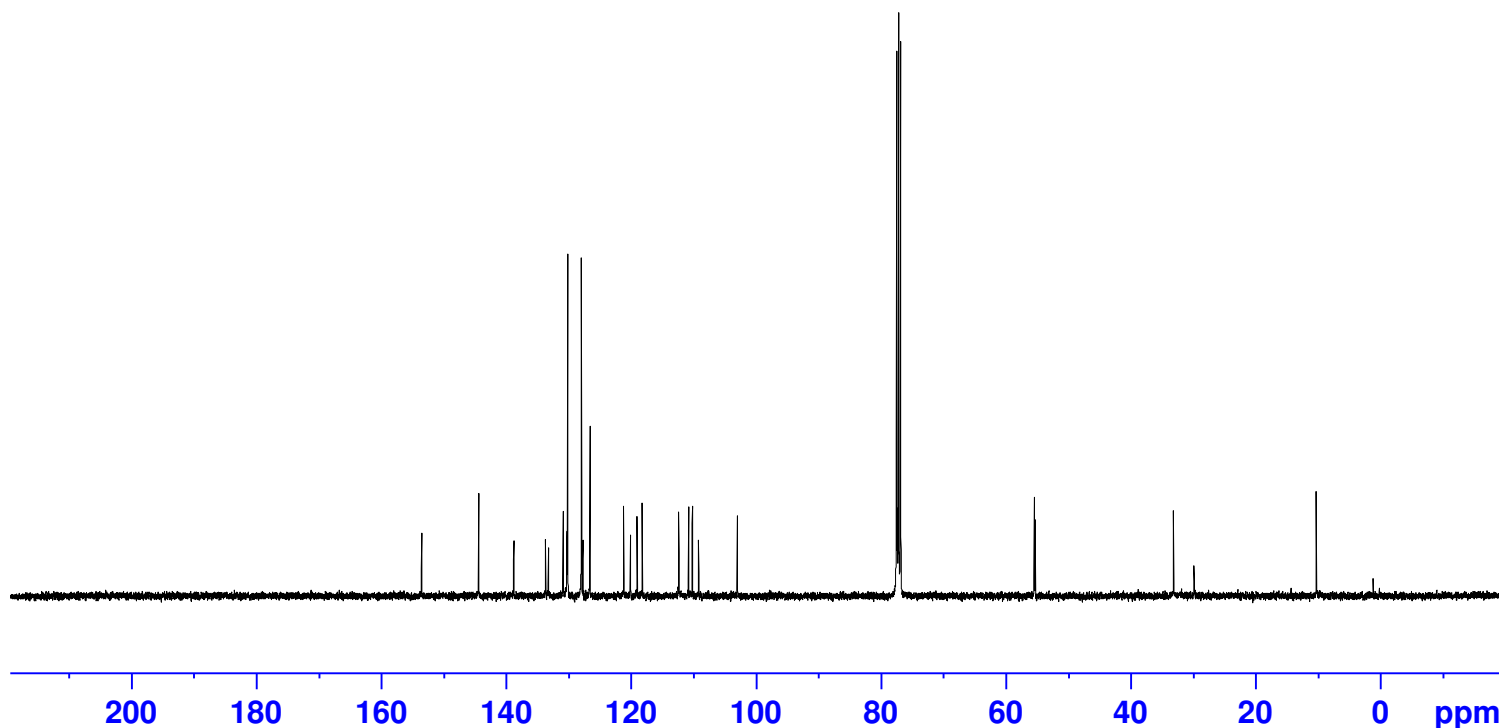
Current Data Parameters
NAME 20230921-400M
EXPNO 36
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230921
Time 1.38
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 600
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 29.75
DW 20.800 usec
DE 6.50 usec
TE 291.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278492 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



ncc-2-95



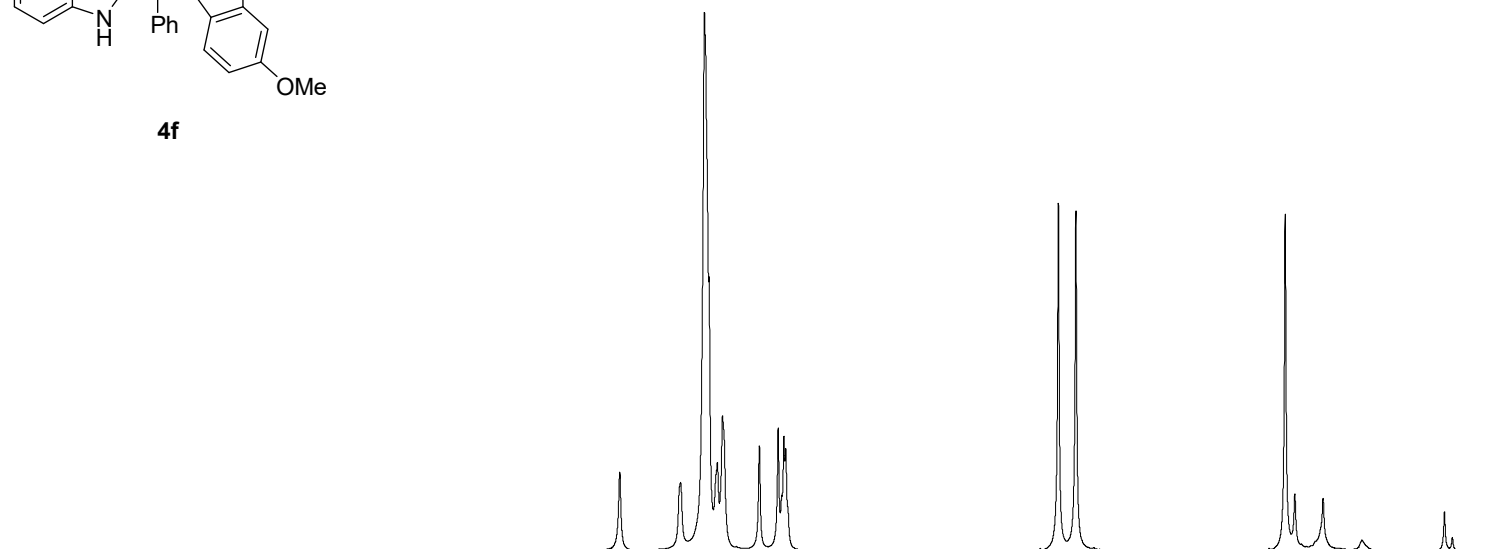
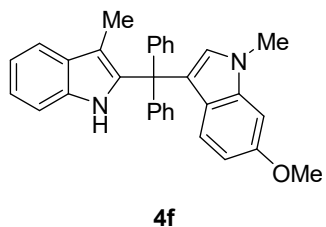
Current Data Parameters
NAME 20231028-400M-2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231028
Time 11.04
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 90.23
DW 60.800 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900272 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.096
7.506
7.273
7.228
7.147
7.097
6.739
6.556
6.521
6.500
6.483
3.832
3.661
1.626



13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.96
1.01
13.88
1.01
3.02
3.05
3.02
3.00

ncc-2-95



Current Data Parameters
NAME 20231028-400M-2
EXPNO 11
PROCNO 1

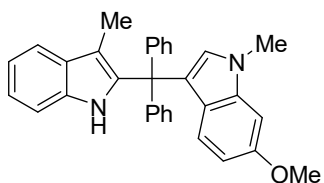
F2 - Acquisition Parameters
Date_ 20231028
Time 11.34
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 53.3
DW 20.800 usec
DE 6.50 usec
TE 293.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

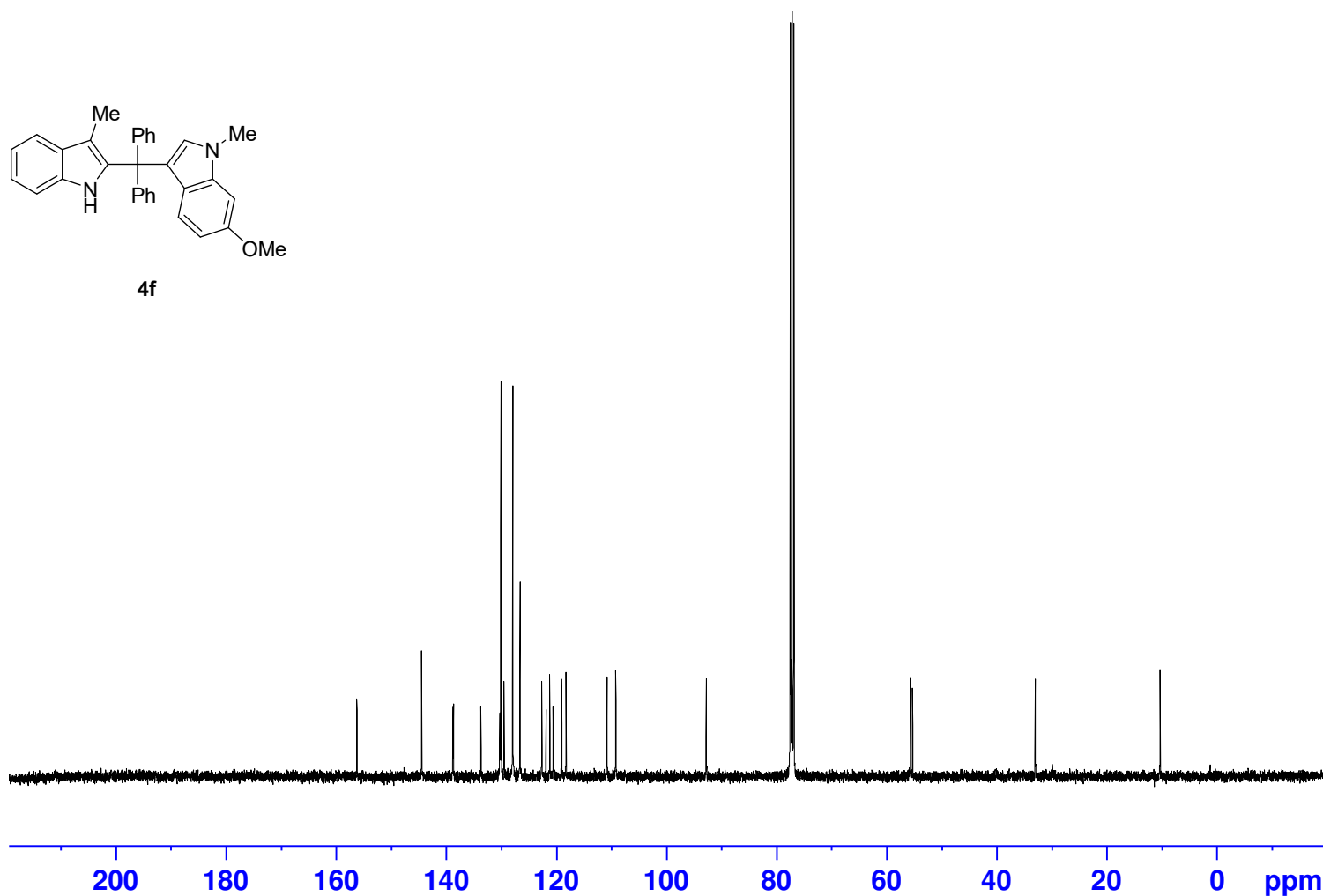
==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278491 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

156.18
144.43
138.71
138.64
133.63
130.21
130.02
129.44
127.85
126.53
122.57
121.81
121.12
120.54
118.97
118.18
110.71
109.17
109.09
92.69
77.40
77.09
76.77
55.57
55.19
32.90
10.22



4f



ncc-2-65

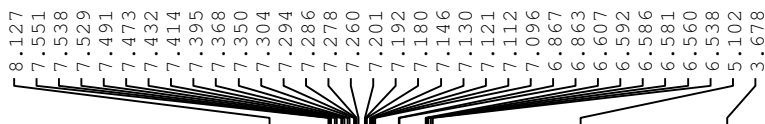


Current Data Parameters
NAME 20230921-400M
EXPNO 33
PROCNO 1

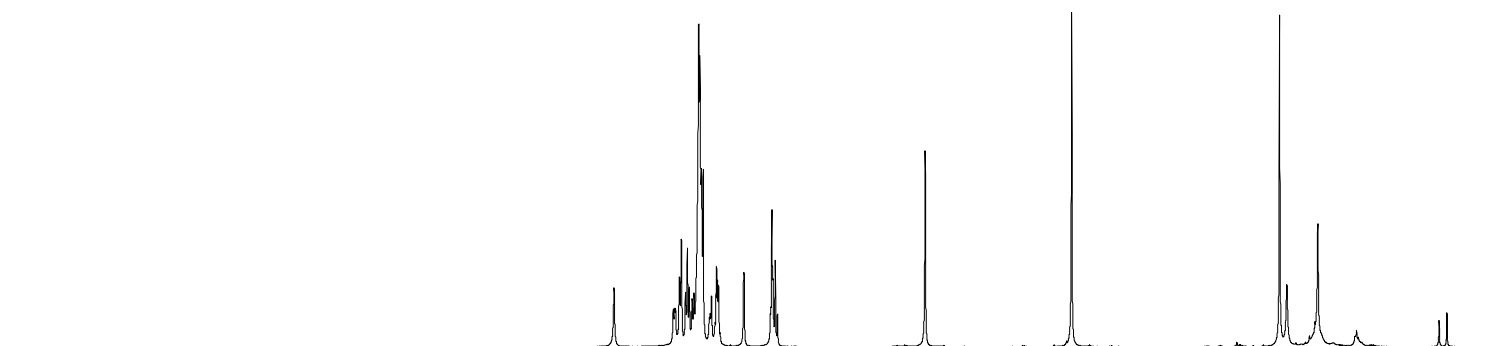
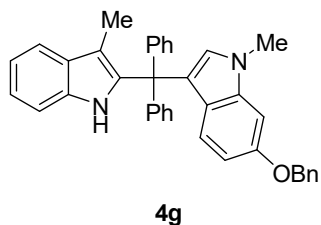
F2 - Acquisition Parameters
Date_ 20230921
Time 0.23
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 90.23
DW 60.800 usec
DE 6.50 usec
TE 290.6 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.656



ncc-2-65



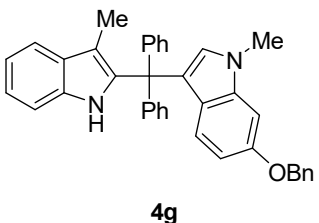
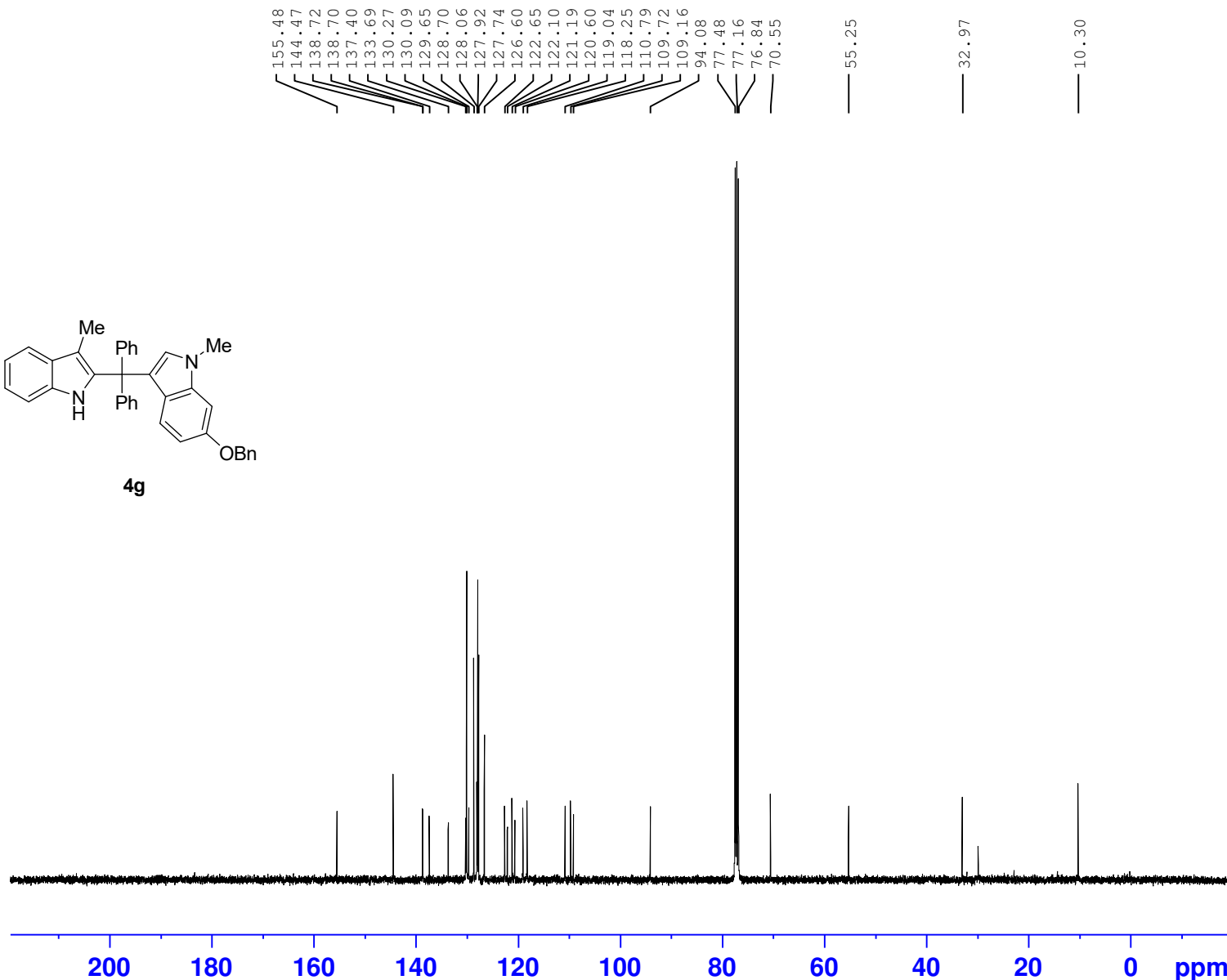
Current Data Parameters
NAME 20230921-400M
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230921
Time 0.59
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 29.75
DW 20.800 usec
DE 6.50 usec
TE 291.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



ncc-2-94



Current Data Parameters
NAME 20231027-400M
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231026
Time 22.57
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 90.23
DW 60.800 usec
DE 6.50 usec
TE 292.3 K
D1 1.00000000 sec
TD0 1

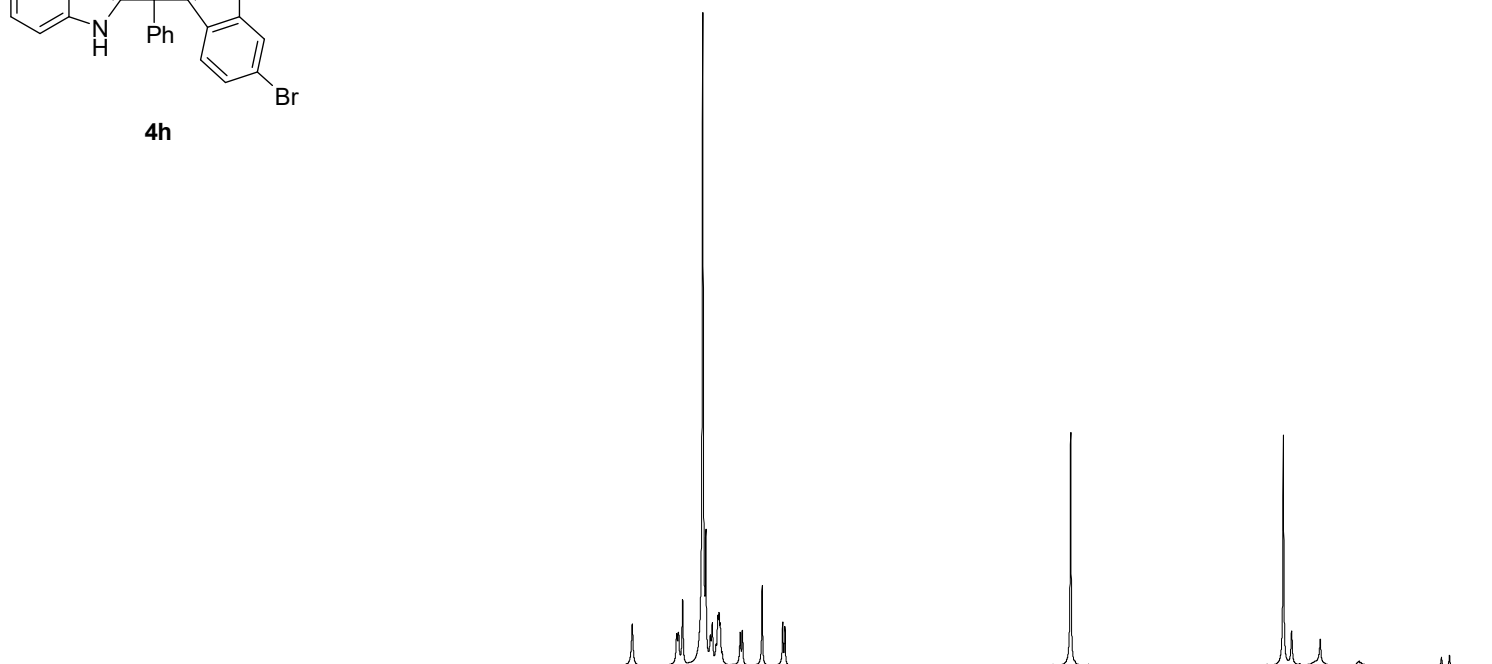
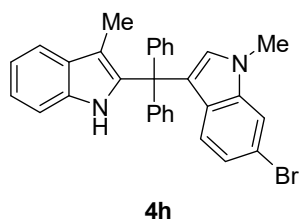
==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.975
7.543
7.527
7.486
7.289
7.259
7.213
7.196
7.159
7.141
7.131
7.121
6.926
6.905
6.712
6.512
6.490

3.712

1.644



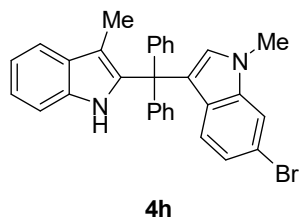
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.86
2.03
10.84
3.11
1.02
1.00
1.01

3.05

3.00

ncc-2-94



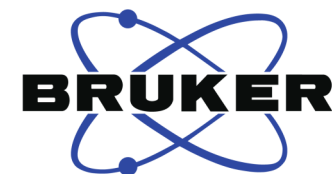
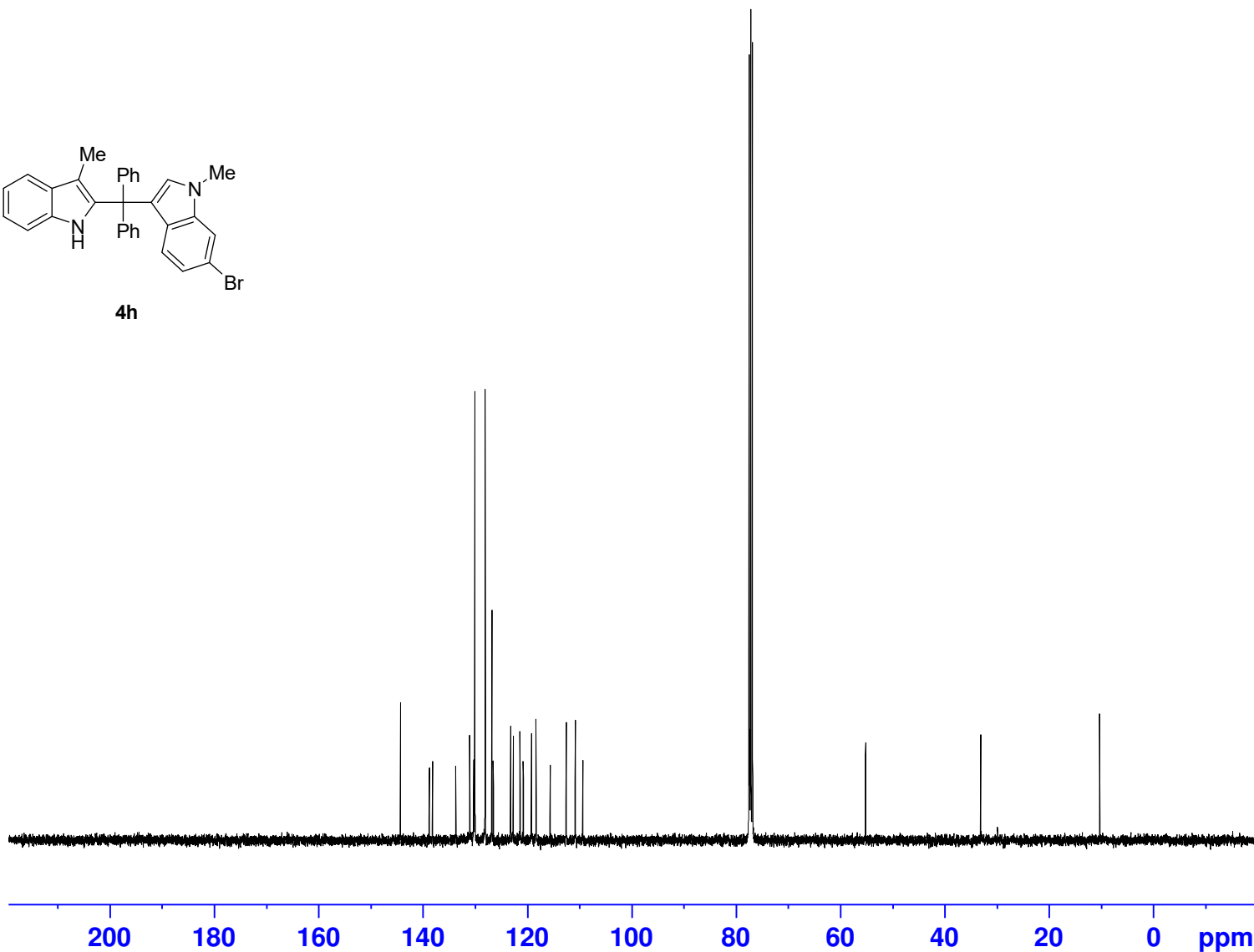
144.29
138.79
138.17
133.71
131.04
130.26
130.05
128.06
126.79
126.51
123.19
122.69
121.39
120.77
119.20
118.32
115.63
112.55
110.82
109.35

77.47
77.16
76.84

55.15

33.07

10.27



Current Data Parameters
NAME 20231027-400M
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231026
Time 23.21
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 35.06
DW 20.800 usec
DE 6.50 usec
TE 292.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278491 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ncc-2-93

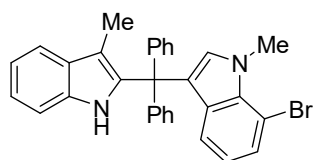
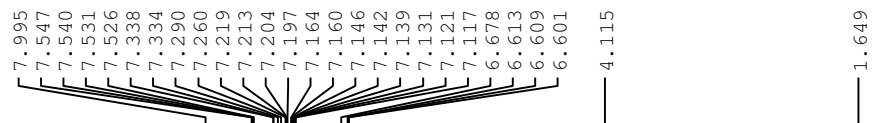


Current Data Parameters
NAME 20231027-400M
EXPNO 10
PROCNO 1

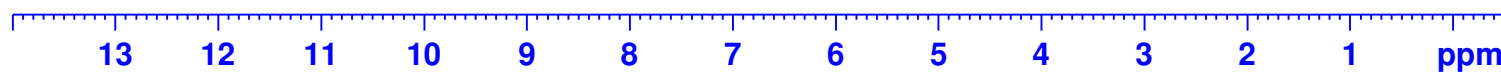
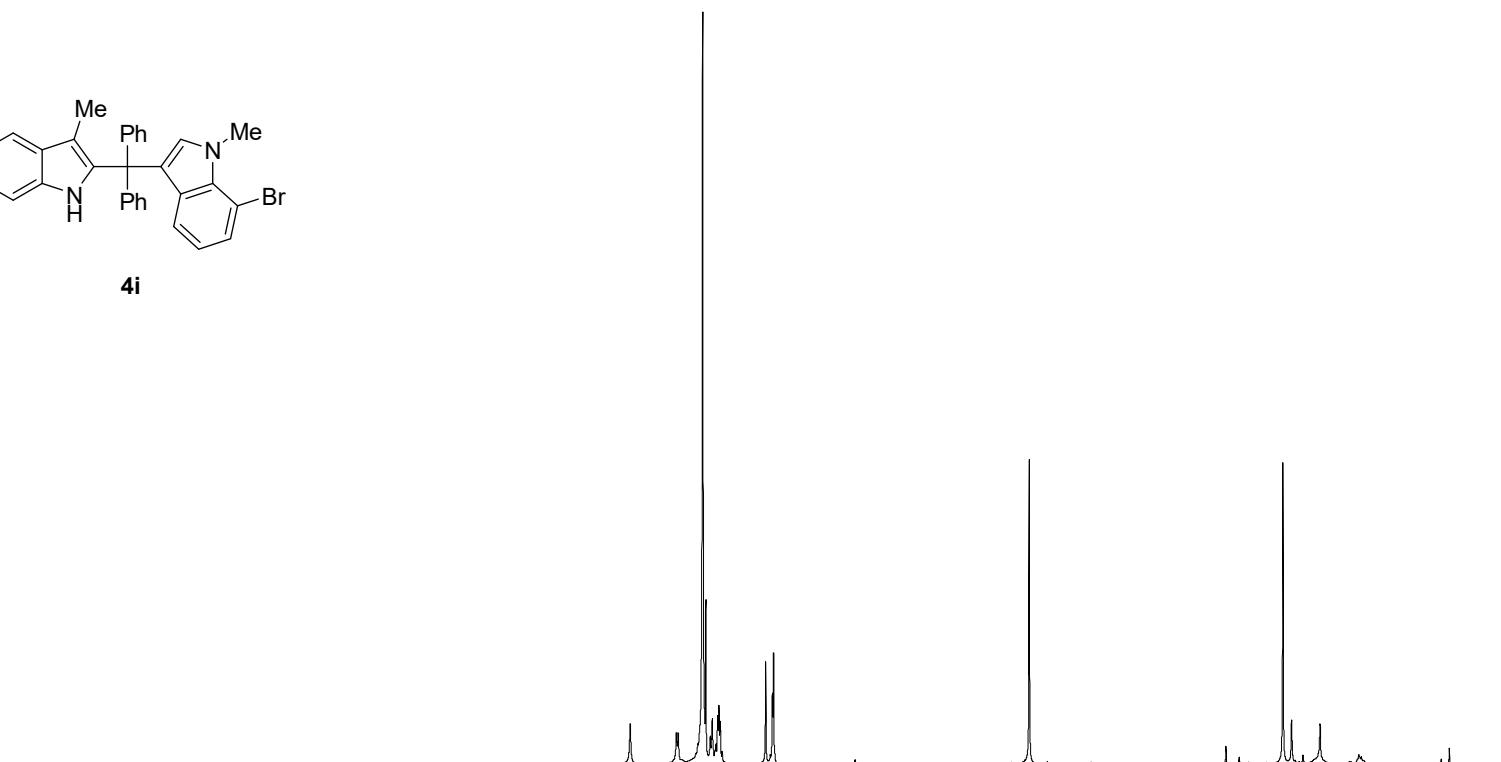
F2 - Acquisition Parameters
Date_ 20231026
Time 22.28
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 90.23
DW 60.800 usec
DE 6.50 usec
TE 291.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



4i



ncc-2-93



Current Data Parameters
NAME 20231027-400M
EXPNO 11
PROCNO 1

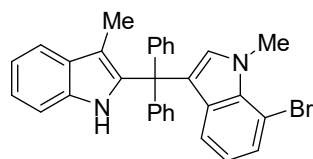
F2 - Acquisition Parameters
Date_ 20231026
Time 22.52
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 35.06
DW 20.800 usec
DE 6.50 usec
TE 292.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

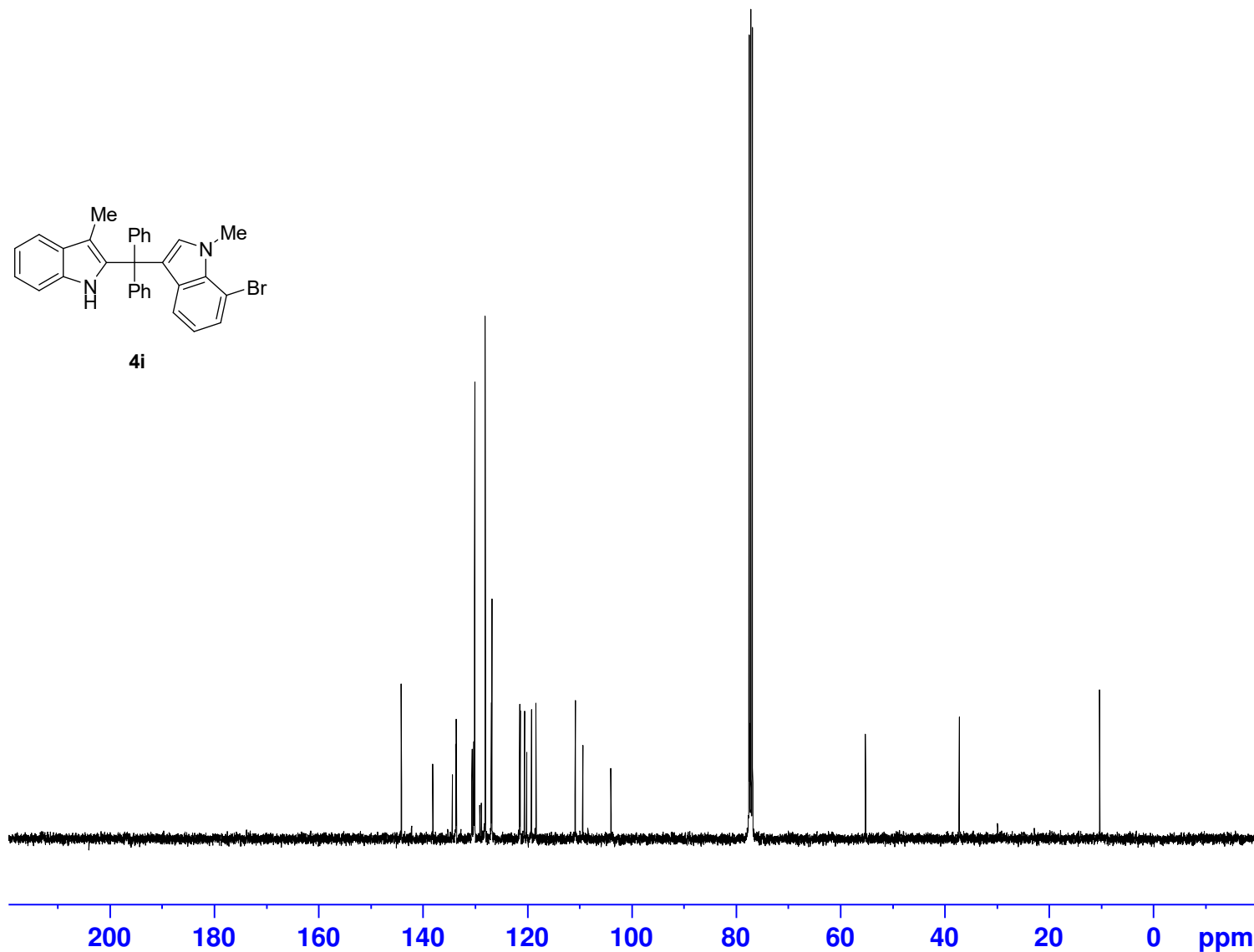
==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278491 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

144.15
138.12
134.33
133.70
133.61
130.61
130.27
130.09
128.06
126.90
126.78
121.47
121.36
120.53
120.13
119.17
118.33
110.82
109.37
103.96
77.47
77.16
76.84
55.16
37.20
10.29



4i



NCC-3-7



Current Data Parameters
NAME 20231111-400M
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231110
Time 22.24
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 90.23
DW 60.800 usec
DE 6.50 usec
TE 292.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

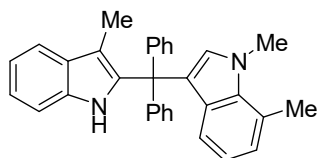
F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.132
7.551
7.539
7.531
7.304
7.293
7.277
7.260
7.189
7.178
7.130
7.120
7.112
6.878
6.861
6.698
6.678
6.660
6.587
6.543
6.523

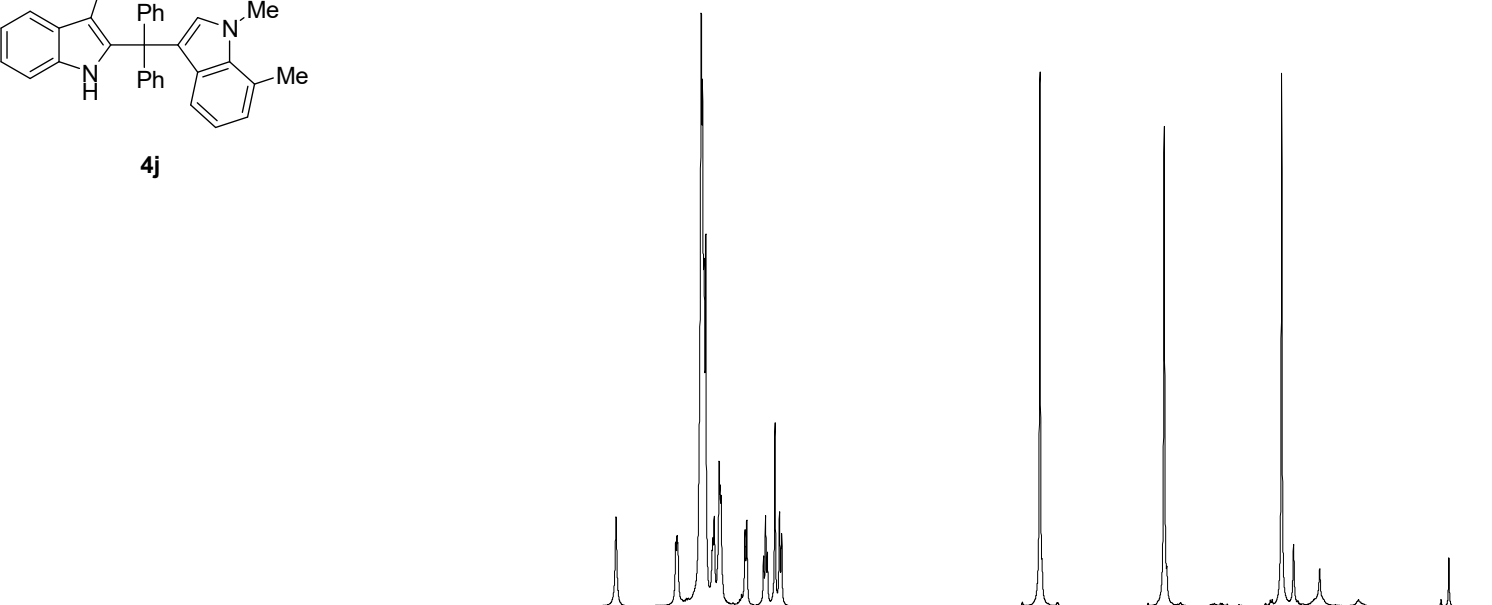
4.011

2.803

1.661



4j



13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.98
1.01
10.12
3.04
1.01
1.02
0.99
0.98

3.02

3.03

3.00

NCC-3-7



Current Data Parameters
NAME 20231111-400M
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231110
Time 22.54
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 293.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278492 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

144.41
138.76
136.82
133.68
132.37
130.27
130.14
128.51
127.92
126.57
124.49
121.34
121.16
120.24
120.05
119.58
119.02
118.24
110.79
109.12

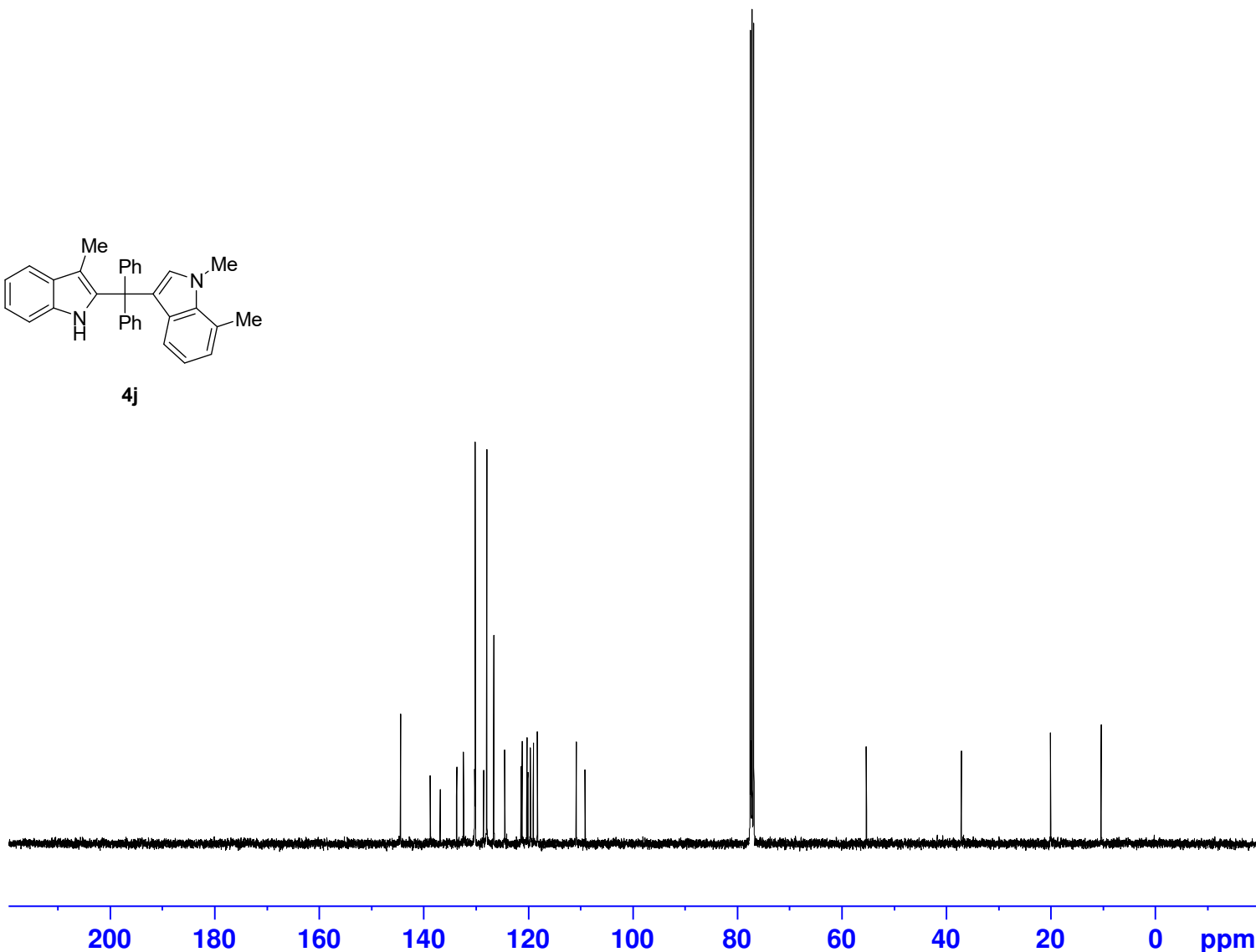
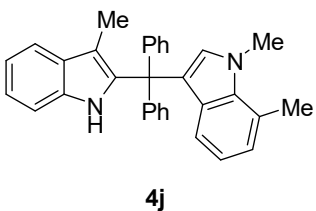
77.47
77.16
76.84

55.26

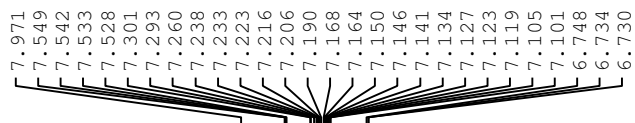
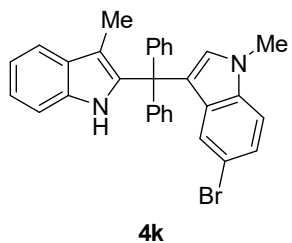
37.09

20.01

10.33

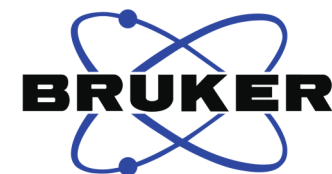


ncc-2-89-2



3.720

1.654

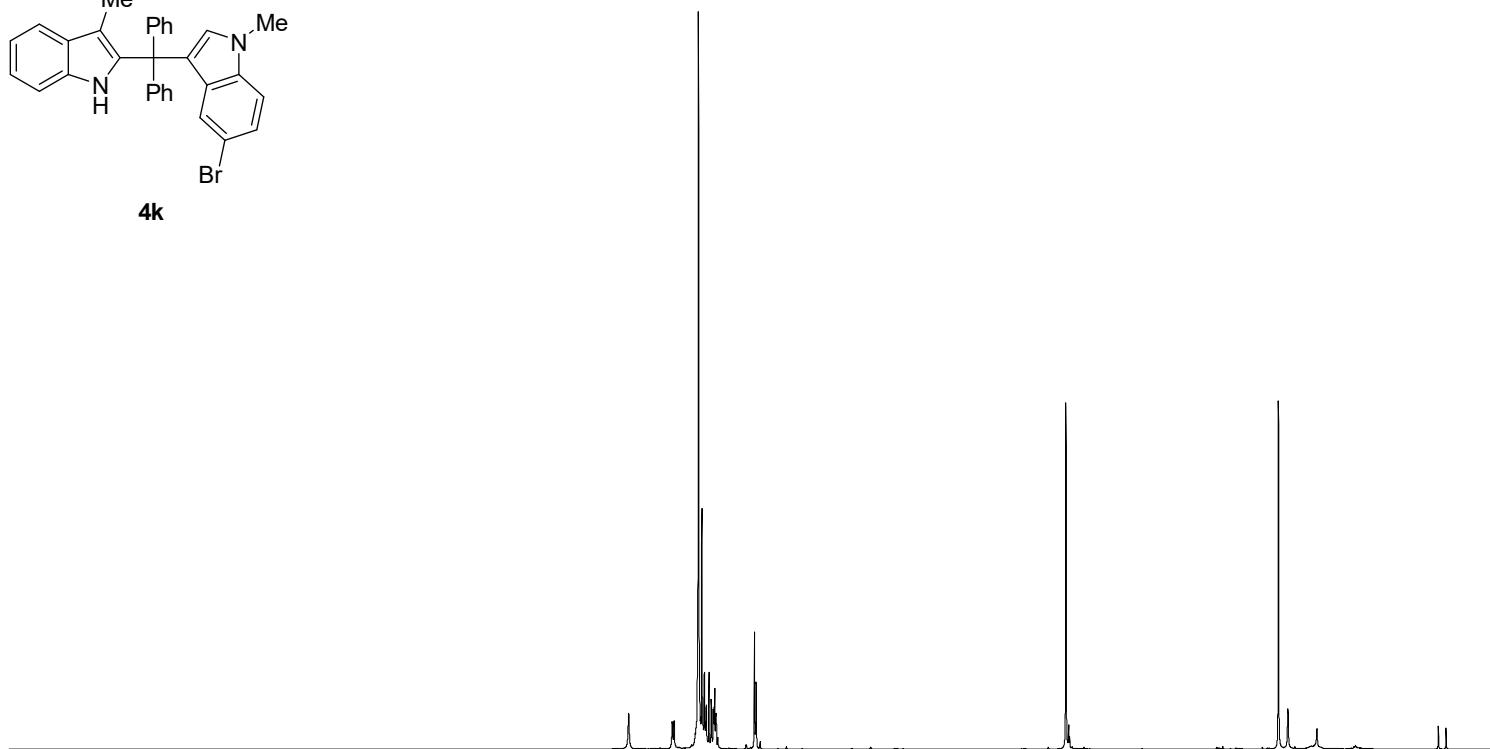


Current Data Parameters
NAME 20231101-400M
EXPNO 25
PROCNO 1

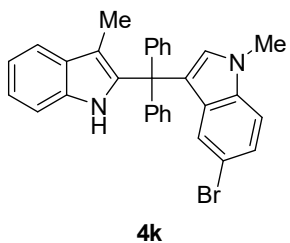
F2 - Acquisition Parameters
Date_ 20231031
Time 23.18
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.67
DW 60.800 usec
DE 6.50 usec
TE 292.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



ncc-2-89-2



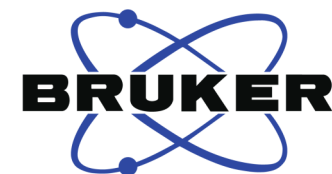
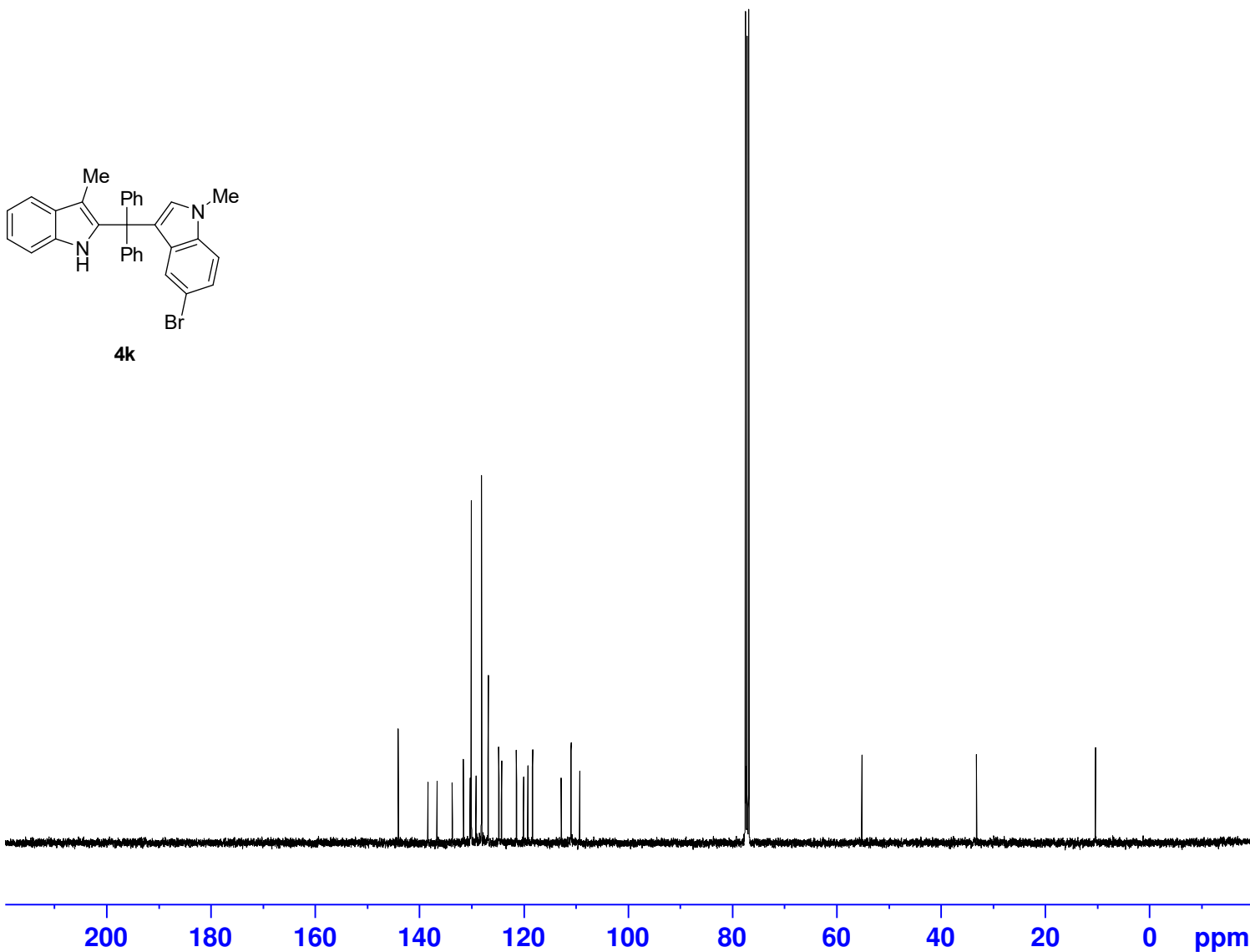
144.06
138.37
136.65
133.70
131.56
130.28
130.06
129.17
128.09
126.82
124.78
124.26
121.39
120.05
119.21
118.31
112.82
110.99
110.90
109.23

77.47
77.15
76.84

55.15

33.15

10.32



Current Data Parameters
NAME 20231101-400M
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231031
Time 23.42
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 292.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278484 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ncc-2-90-2



Current Data Parameters
NAME 20231031-400M
EXPNO 18
PROCNO 1

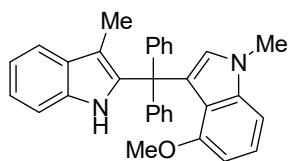
F2 - Acquisition Parameters
Date_ 20231030
Time 23.14
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.67
DW 60.800 usec
DE 6.50 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

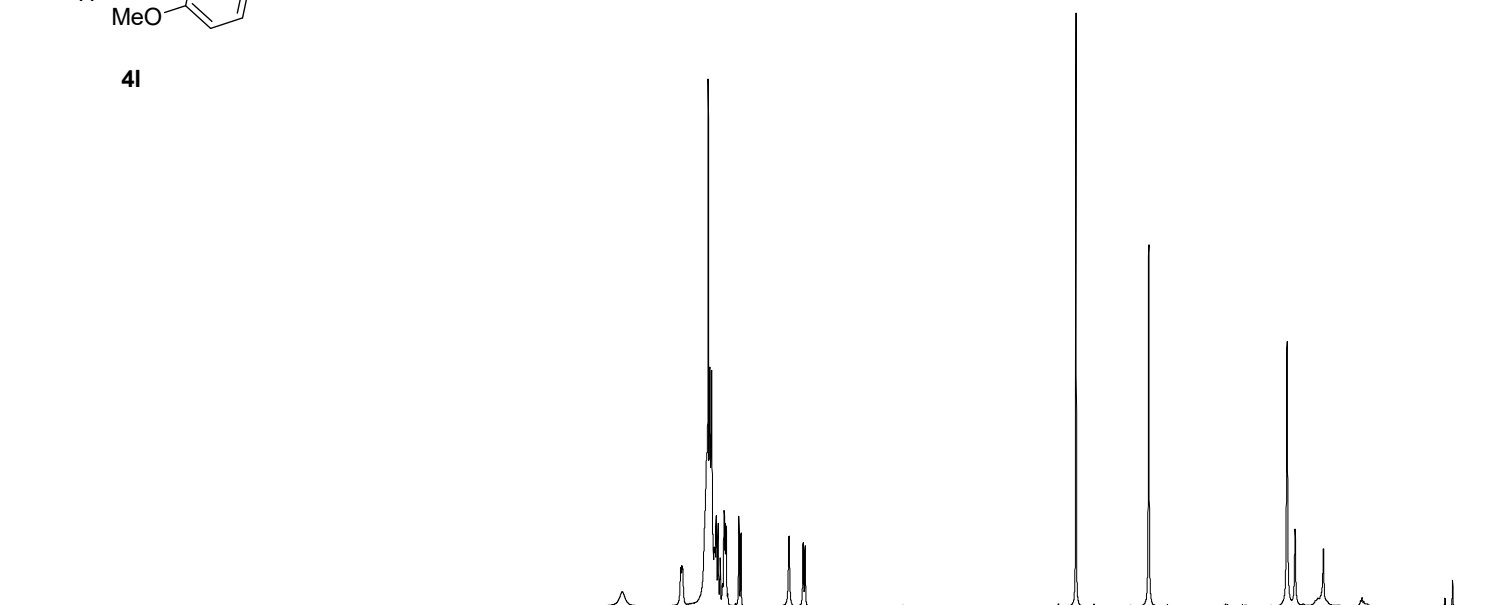
F2 - Processing parameters
SI 65536
SF 400.1900235 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.074
7.504
7.493
7.484
7.236
7.222
7.204
7.190
7.178
7.172
7.159
7.140
7.120
7.097
7.081
7.072
7.062
7.047
6.938
6.918
6.451
6.314
6.294

3.660
2.953
1.609



4I



13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.93
1.03
12.59
2.03
1.00
1.01
1.00

3.04
3.03
3.00

ncc-2-90-2



Current Data Parameters
NAME 20231031-400M
EXPNO 19
PROCNO 1

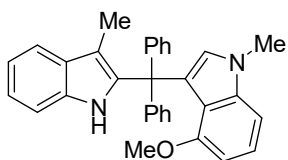
F2 - Acquisition Parameters
Date_ 20231030
Time 23.44
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 35.06
DW 20.800 usec
DE 6.50 usec
TE 293.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

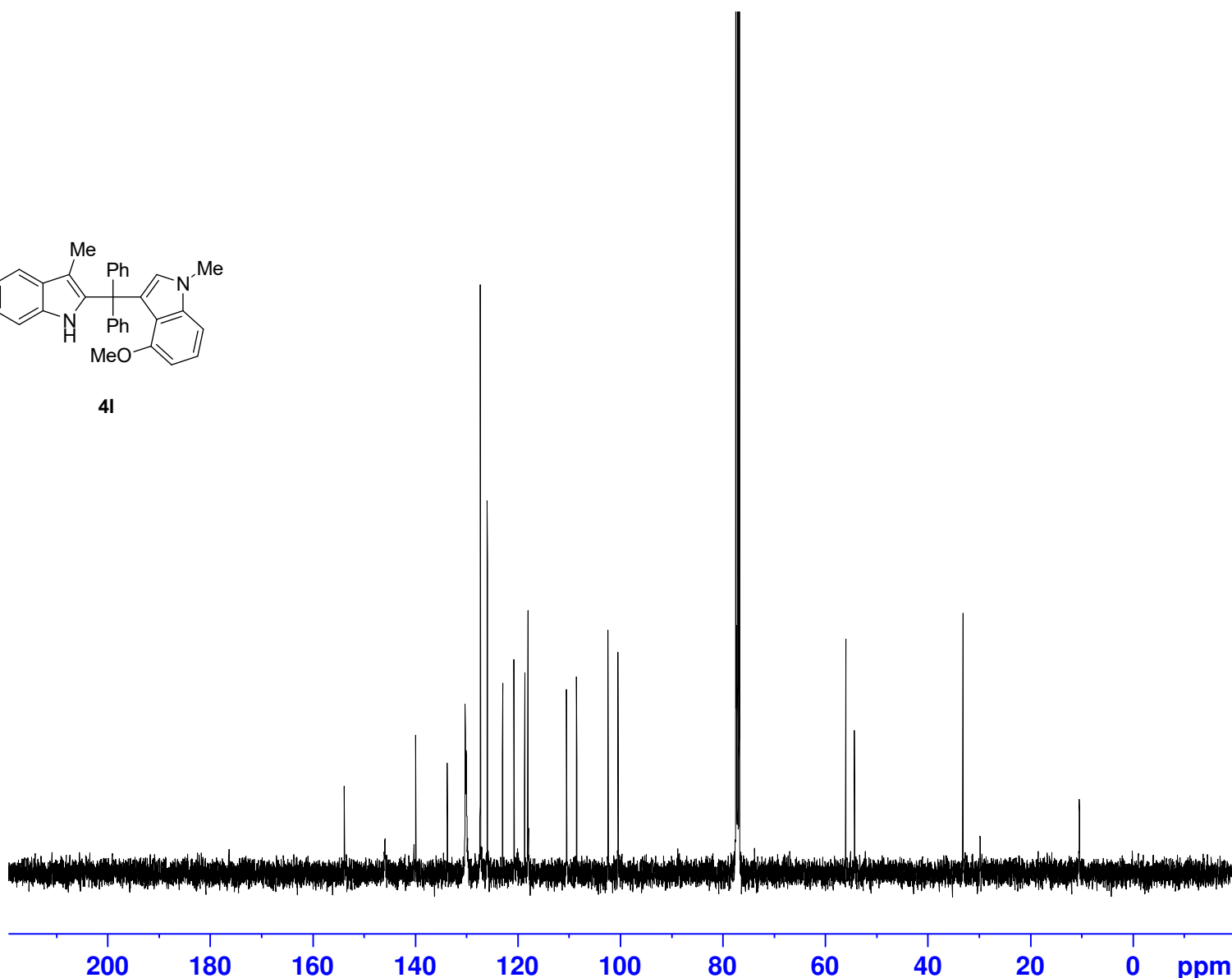
==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278560 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

153.84
145.90
139.90
133.74
130.31
130.21
130.07
130.03
127.31
125.93
122.95
120.75
118.64
117.99
117.89
110.49
108.50
102.38
100.43
77.39
77.07
76.75
55.97
54.30
33.11
10.41



4l



ncc-4-26



Current Data Parameters
NAME 20240408-400M
EXPNO 33
PROCNO 1

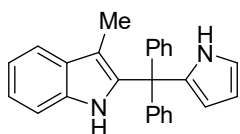
F2 - Acquisition Parameters
Date_ 20240408
Time 4.04
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.67
DW 60.800 usec
DE 6.50 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

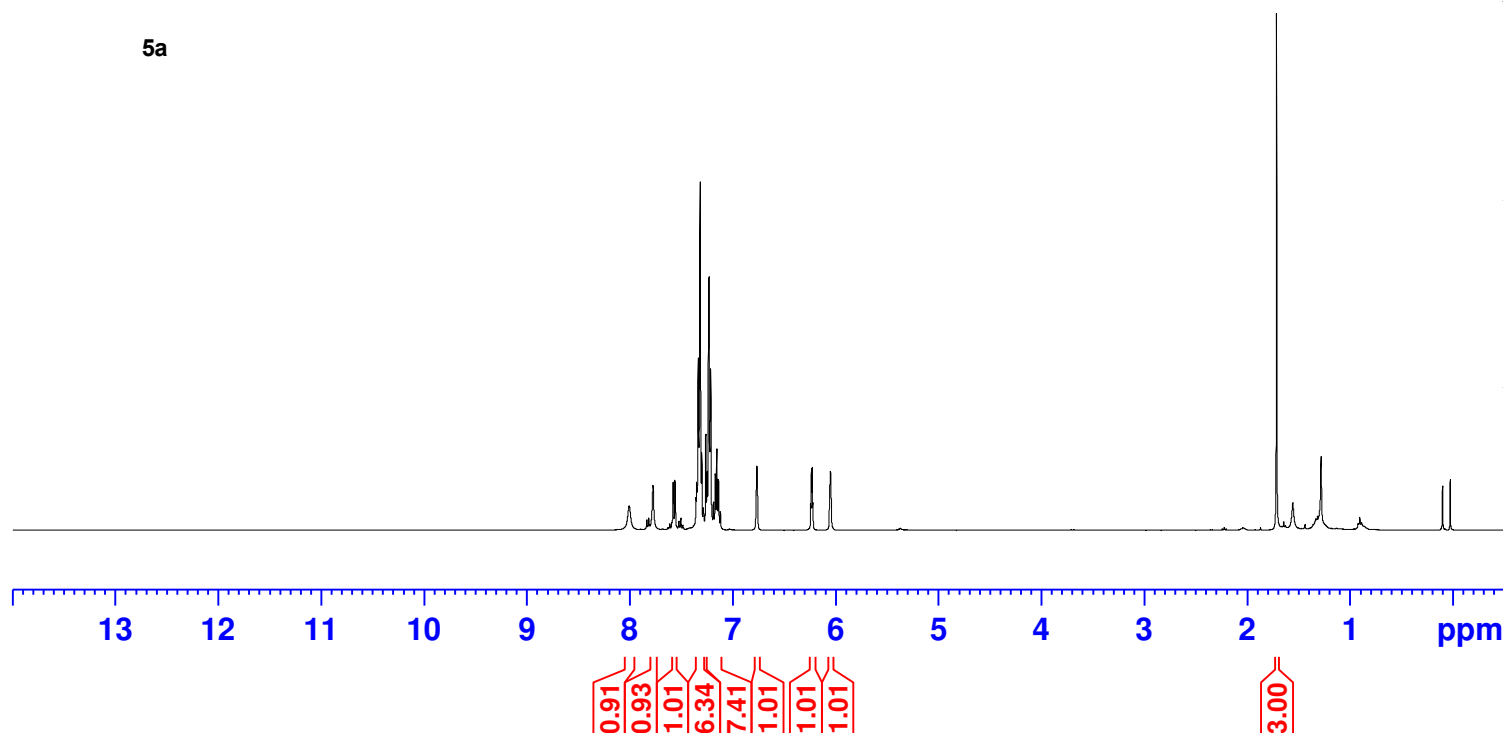
F2 - Processing parameters
SI 65536
SF 400.1900142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.004
7.773
7.578
7.560
7.355
7.348
7.334
7.315
7.300
7.285
7.281
7.260
7.246
7.233
7.229
7.214
7.183
7.169
7.166
7.155
7.151
7.137
7.134
7.119
6.765
6.761
6.240
6.232
6.225
6.218
6.048

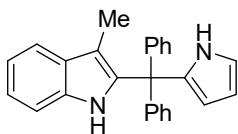
1.711



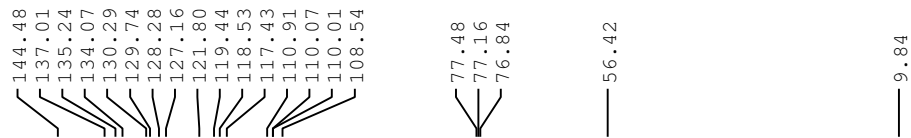
5a



ncc-4-26



5a



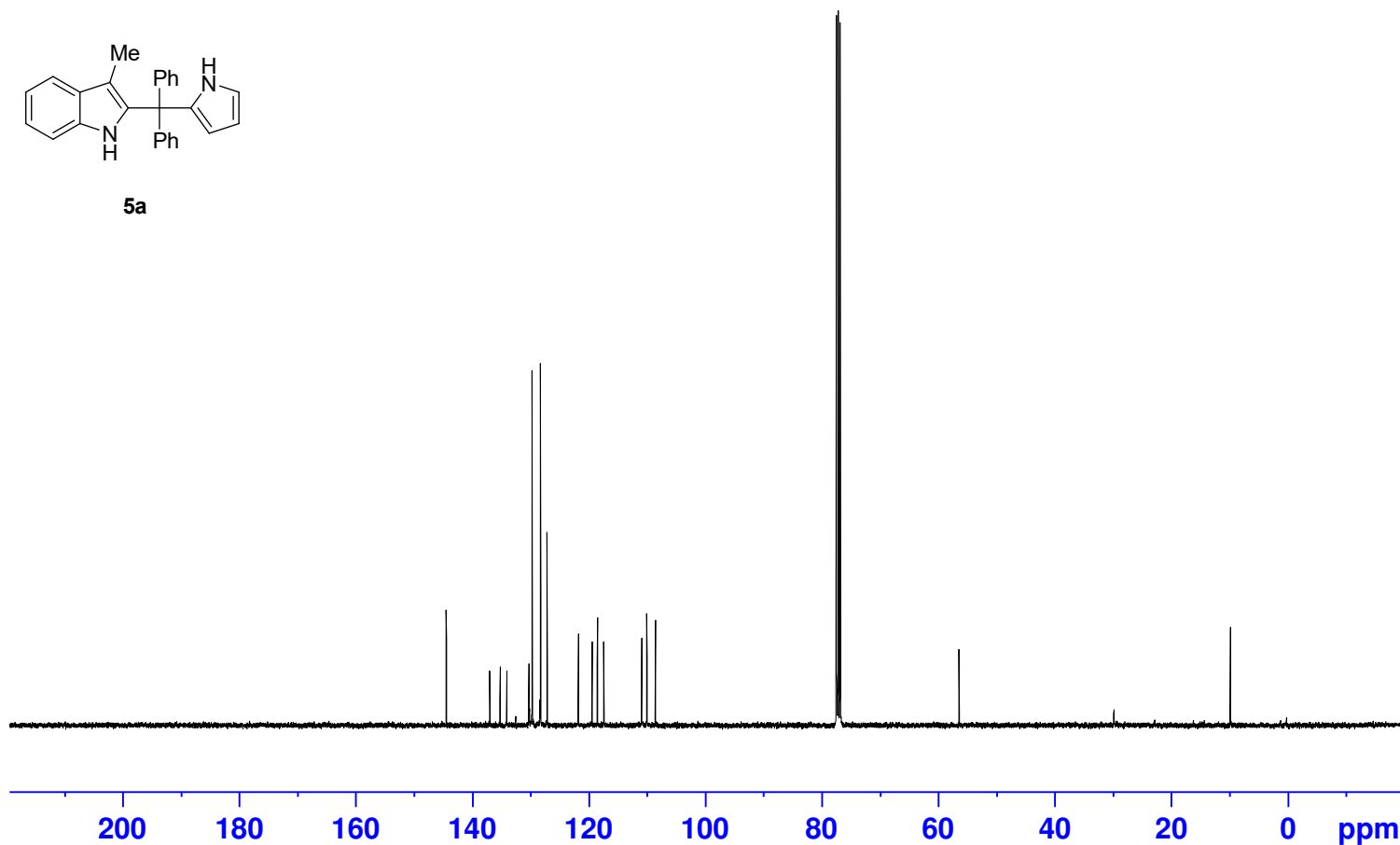
Current Data Parameters
NAME 20240408-400M
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240408
Time 4.51
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 800
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 294.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278469 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



ncc-3-90



Current Data Parameters
NAME 20240302-400M
EXPNO 18
PROCNO 1

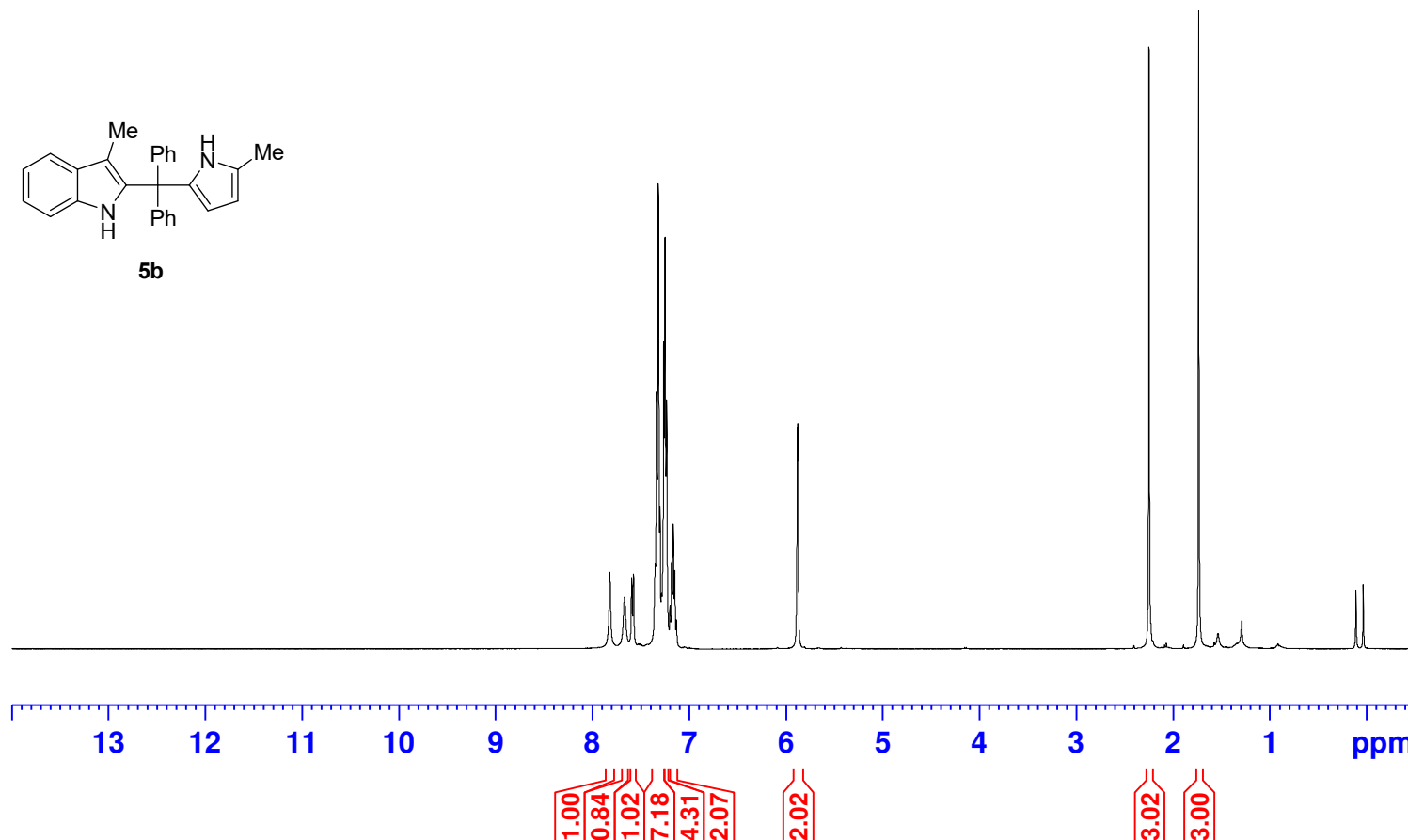
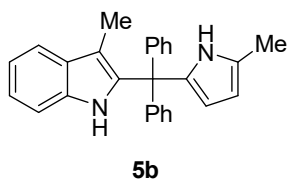
F2 - Acquisition Parameters
Date_ 20240301
Time 22.56
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

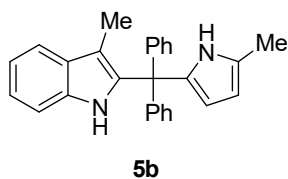
F2 - Processing parameters
SI 65536
SF 400.1900138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.818
7.665
7.593
7.575
7.573
7.351
7.336
7.317
7.300
7.285
7.281
7.260
7.248
7.232
7.194
7.180
7.177
7.162
7.148
7.145
7.130
5.880
5.874

2.244
1.731



ncc-3-90

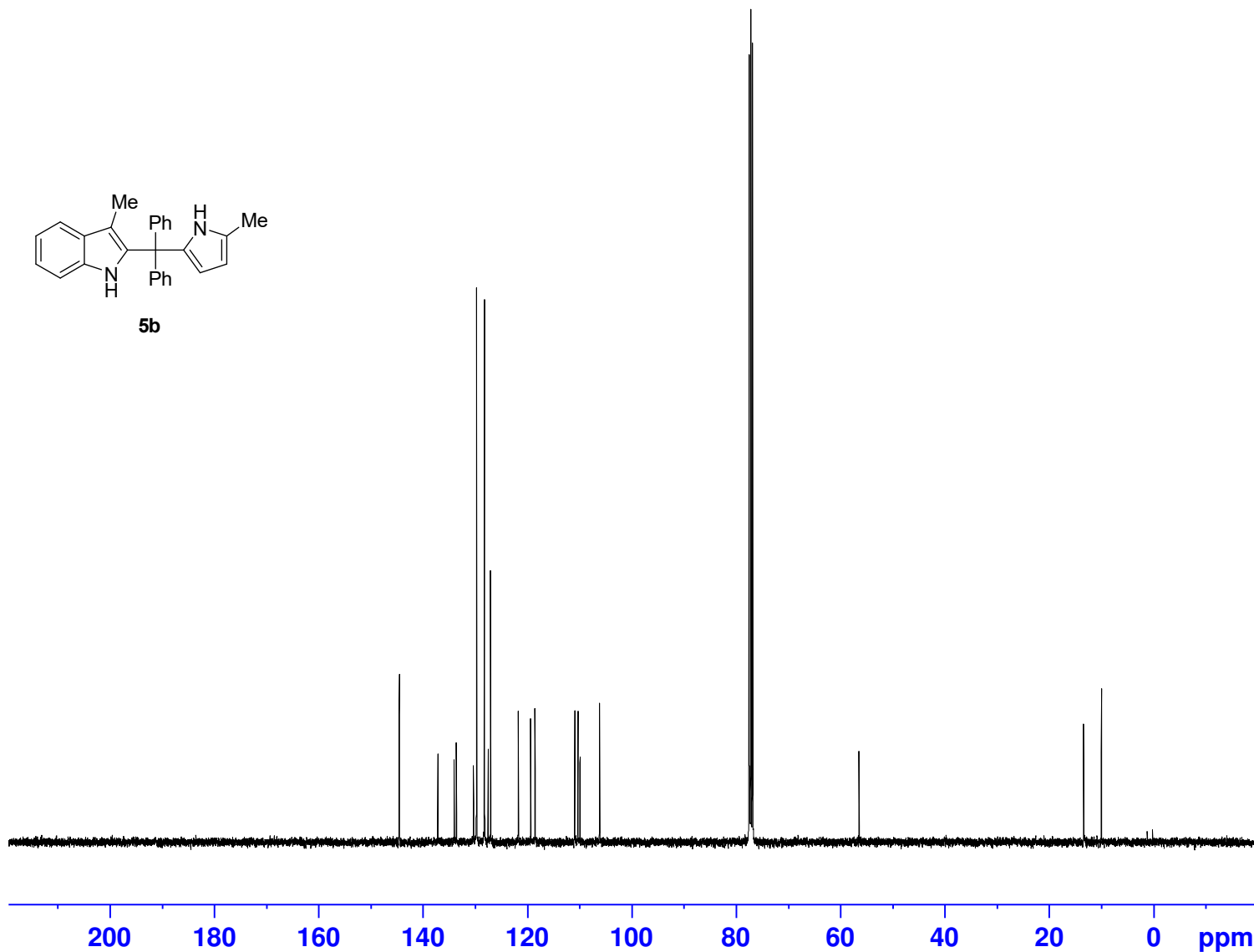


144.57
137.17
134.05
133.61
130.33
129.74
128.21
127.52
127.06
121.72
119.38
118.53
110.89
110.30
109.91
106.16

77.47
77.16
76.84

56.42

13.36
9.95



Current Data Parameters
NAME 20240302-400M
EXPNO 19
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240301
Time 23.32
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 29.75
DW 20.800 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

==== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278477 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40