

**Supporting Information of ‘Electron and Steric Effects on The Three-fold
Scholl-Type Cycloheptatriene Ring Formation Around A Tribenzotriquinacene
Core’**

Ho-Wang Ip,^[a] Hak-Fun Chow,^{*[a]} and Dietmar Kuck^{*[b]}

*^aDepartment of Chemistry, Institute of Molecular Functional Materials, and The
Center of Novel Functional Molecules*

The Chinese University of Hong Kong, Shatin (Hong Kong)

E-mail: hfchow@cuhk.edu.hk

^bDepartment of Chemistry and Center for Molecular Materials (CM₂)

Bielefeld University, 33615 Bielefeld (Germany)

E-mail: dietmar.kuck@uni-bielefeld.de

Contents

1. Synthesis	S3
2. X-ray Crstallography	S17
3. References.....	S19
4. 2D COSY Spectra of 7a , 7b , 10 , 16 and 17	S20
5. List of NMR and mass spectra.....	S26

1. Synthesis

General: All reagents were purchased from commercial suppliers and used without further purification. Dichloromethane was freshly distilled from calcium hydride. All reactions were carried out under nitrogen atmosphere unless otherwise stated. All reactions were monitored by thin layer chromatographic analysis on pre-coated silica gel plates, which were visualized by UV lamp at 254 or 365 nm and/or stained using 5% (w/v) dodecamolybdophosphoric acid in ethanol followed by heating. Flash column chromatography was performed on glass column of silica gel (230–400 mesh) and solvent ratios were expressed in volume to volume. ^1H , ^{13}C , COSY NMR spectra for structural characterization were recorded either on a Bruker Avance DPX 400 spectrometer or a Bruker Avance III 400 spectrometer (^1H : 400 MHz; ^{13}C : 100 MHz) or a Bruker Avance III 700 spectrometer (^1H : 700 MHz; ^{13}C : 176 MHz) as specified. Unless otherwise stated, all NMR measurements were conducted in CDCl_3 at 22 °C. The residual signals of the deuterated solvents or TMS were used as the internal standards. Chemical shifts were reported as parts per million in δ scale using the solvent residual peak as internal standard for ^1H and ^{13}C NMR. Coupling constants (J) were reported in Hertz (Hz). All mass spectra were obtained on a ThermoFinnigan MAT 95 XL double focusing sector mass spectrometer or on a Bruker Solarix 9.4 T FT-ICR mass spectrometer with electron spray ionization (ESI) technique, or on a Bruker Daltonics Autoflex MALDI-TOF mass spectrometer using 2,5-dihydroxybenzoic acid (DHB) as matrices, or on a Fisons VG Autospec X double-focusing mass spectrometer (EI, 70 eV). The reported molecular masses, given as m/z values, were monoisotopic mass unless otherwise stated. Melting points were measured on an Electrothermal[®] 9100 digital melting point apparatus or a Stuart[®] automatic melting point apparatus SMP40 and were uncorrected.

Compound 6a: Compound **5** (100 mg, 0.136 mmol), palladium(II) acetate (21.3 mg, 0.095 mmol), 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (56 mg, 0.136 mmol), cesium fluoride (372 mg, 2.448 mmol), phenylboronic acid (300 mg, 2.448 mmol) were mixed in dioxane (4 mL) in a Schlenk tube and degassed. The reaction mixture was stirred at 100 °C for 5 d. The mixture was filtered through Celite, concentrated under reduced pressure and the residue was purified by flash column chromatography (hexane/EtOAc = 80/1) to afford compound **6a** (68 mg, 0.130 mmol, 97%) as a colorless solid. M.p.: 298–300 °C; R_f : 0.23 (hexane/EtOAc = 80/1); ^1H NMR (400 MHz): 7.66 (d, J = 7.2 Hz, 2 H, ArH), 7.61–7.37 (m, 13 H, ArH), 7.31–7.29 (m, 2 H, ArH), 7.01 (d, J = 7.6 Hz, 1 H, ArH), 6.81 (t, J = 7.6 Hz, 1 H, ArH), 6.58–6.53 (m, 2 H, ArH), 5.80 (d, J = 8 Hz, 1 H, ArH), 5.65–5.59 (m, 2 H, ArH), 5.24 (s, 1 H, CH), 5.09 (s, 1 H, CH), 4.96 (s, 1 H, CH), 1.82 (s, 3 H, CH₃); ^{13}C NMR (100 MHz): 146.0, 145.9, 144.7, 144.1, 143.4, 143.3, 142.9, 142.8, 142.7, 139.1, 138.84, 138.82, 130.13, 130.10, 129.4, 129.2, 129.1, 129.0, 127.6, 127.5, 127.4, 127.3, 126.85, 126.83, 125.3, 125.0, 124.9, 62.6, 62.4, 61.8, 59.6, 29.0; MS (EI): m/z (%) 522.3 (100, $[\text{M}]^+$), 507.2 (15, $[\text{M} - \text{CH}_3]^+$), 406.2 (27); MS (ESI): m/z (%) 545.2 (100, $[\text{M} + \text{Na}]^+$). Accurate mass ($[\text{M} + \text{Na}]^+$, ESI) calcd for C₄₁H₃₀Na⁺: 545.2240, found: 545.2246.

Compound 6b: The synthetic procedure was similar to that yielding compound **6a**, using 4-*tert*-butylphenylboronic acid instead of phenylboronic acid. The crude product was purified by flash column chromatography (hexane/EtOAc = 20/1) to afford compound **6b** (84 mg, 0.122 mmol, 89%) as a colorless solid. M.p.: 226–229 °C; R_f : 0.17 (hexane/EtOAc = 20/1); ^1H NMR (400 MHz): 7.58 (s, 4 H, ArH), 7.55–7.47 (m, 6 H, ArH), 7.37 (d, J = 8.3 Hz, 2 H, ArH), 7.31–7.27 (m, 2 H, ArH), 6.99 (d, J = 7.4 Hz, 1 H, ArH), 6.75 (t, J = 7.7 Hz, 1 H, ArH), 6.51–6.47 (m, 2 H, ArH), 5.64

(d, $J = 7.9$ Hz, 1 H, ArH), 5.47–5.46 (m, 2 H, ArH), 5.21 (s, 1 H, CH), 5.05 (s, 1 H, CH), 4.92 (s, 1 H, CH), 1.79 (s, 3 H, CH₃), 1.43 (s, 9 H, C(CH₃)₃), 1.40 (s, 9 H, C(CH₃)₃), 1.38 (s, 9 H, C(CH₃)₃); ¹³C NMR (100 MHz): 150.64, 150.55, 150.4, 146.0, 145.9, 144.8, 144.1, 143.6, 143.4, 139.9, 139.81, 139.76, 139.1, 138.6, 129.9, 129.8, 129.11, 129.07, 128.9, 127.4, 126.6, 126.1, 126.0, 125.8, 125.4, 125.1, 124.9, 62.58, 62.57, 61.9, 59.6, 34.82, 34.79, 34.7, 31.64, 31.61, 31.59, 29.0; MS (EI): m/z (%) 690.4 (100, [M]⁺), 675.4 (9, [M – CH₃]⁺), 633.4 (22, [M – CH₃ – C₃H₆]⁺), 574.4 (13), 337.7 (6, [M – CH₃]^{2+(•)}), 330.2 (30, [M – 2 CH₃]²⁺), 57.1 (74, C₄H₉⁺); MS (ESI): m/z (%) 713.4 (100, [M + Na]⁺). Accurate mass ([M + Na]⁺, ESI) calcd for C₅₃H₅₄Na⁺: 713.4118, found: 713.4138.

Compound 6c: The synthetic procedure was similar to that yielding compound **6a**, using 2-methoxyphenylboronic acid instead of phenylboronic acid. The crude product was purified by flash column chromatography (hexane/EtOAc = 9/1) to afford compound **6c** (68 mg, 0.112 mmol, 82%) as a colorless solid. M.p.: 243–245 °C (dec.); R_f : 0.25 (hexane/EtOAc = 9/1); ¹H NMR (400 MHz, 1,1,2,2-tetrachloroethane-*d*₂, 60 °C): 7.54–7.41 (m, 5 H, ArH), 7.33 (d, $J = 7.3$ Hz, 1 H, ArH), 7.27 (s, 2 H, ArH), 7.25–7.06 (m, 6 H, ArH), 7.02 (d, $J = 7.4$ Hz, 1 H, ArH), 6.87 (t, $J = 7.6$ Hz, 1 H, ArH), 6.65–6.64 (m, 2 H, ArH), 5.93 (d, $J = 7.7$ Hz, 1 H, ArH), 5.81–5.80 (m, 2 H, ArH), 4.94 (s, 1 H, CH), 4.81 (s, 1 H, CH), 4.67 (s, 1 H, CH), 3.93 (s, 3 H, OCH₃), 3.88 (s, 3 H, OCH₃), 3.81 (s, 3 H, OCH₃), 1.77 (s, 3 H, CH₃); ¹³C NMR (100 MHz, 1,1,2,2-tetrachloroethane-*d*₂, 60 °C): 156.5, 146.3, 145.7, 145.3, 144.9, 135.3, 134.8, 131.8, 131.6, 131.4, 131.3, 129.7, 129.1, 128.8, 128.75, 128.66, 126.6, 126.13, 126.06, 125.2, 125.0, 124.6, 121.0, 120.9, 120.8, 111.8, 111.5, 63.4, 63.1, 62.5, 59.4, 55.5, 55.4, 55.3, 28.2; MS (MALDI): m/z (%) 635.3 (100, [M + Na]⁺). Accurate mass ([M + Na]⁺, MALDI) calcd for C₄₄H₃₆NaO₃⁺: 635.2562, found: 635.2556.

Compound 6d: The synthetic procedure was similar to that yielding compound **6a**, using 3-methoxyphenylboronic acid instead of phenylboronic acid. The crude product was purified by flash column chromatography (hexane/EtOAc = 20/1) to afford compound **6d** (76 mg, 0.124 mmol, 91%) as a colorless solid. M.p.: 130–133 °C; R_f : 0.33 (hexane/EtOAc = 10/1); ^1H NMR (400 MHz): 7.52–7.44 (m, 2 H, ArH), 7.40 (t, J = 8 Hz, 1 H, ArH), 7.32–7.27 (m, 3 H, ArH), 7.23–7.22 (m, 2 H, ArH), 7.18–7.15 (m, 1 H, ArH), 7.11 (d, J = 7.6 Hz, 1 H, ArH), 7.07–6.96 (m, 5 H, ArH), 6.88 (t, J = 7.6, 1 H, ArH), 6.67–6.63 (m, 2 H, ArH), 5.95 (d, J = 7.8 Hz, 1 H, ArH), 5.81–5.76 (m, 2 H, ArH), 5.26 (s, 1 H, CH), 5.12 (s, 1 H, CH), 5.00 (s, 1 H, CH), 3.92 (s, 3 H, OCH₃), 3.89 (s, 3 H, OCH₃), 3.86 (s, 3 H, OCH₃), 1.84 (s, 3 H, CH₃); ^{13}C NMR (100 MHz): 160.3, 160.2, 160.1, 146.0, 145.9, 144.7, 144.14, 144.11, 144.08, 144.0, 143.4, 143.3, 138.9, 138.8, 138.7, 130.25, 130.16, 130.01, 129.99, 129.9, 129.1, 127.6, 126.9, 125.4, 125.1, 121.9, 121.8, 115.2, 115.1, 112.9, 112.7, 62.6, 62.5, 61.9, 59.6, 55.53, 55.52, 55.48, 29.0; MS (EI): m/z (%) 612.3 (100, $[\text{M}]^{+\bullet}$), 597.3 (13, $[\text{M} - \text{CH}_3]^+$), 496.2 (33), 390.2 (7), 306.1 (12, $[\text{M}]^{2+}$); MS (MALDI): m/z (%) 635.3 (100, $[\text{M} + \text{Na}]^+$). Accurate mass ($[\text{M} + \text{Na}]^+$, MALDI) calcd for $\text{C}_{44}\text{H}_{36}\text{NaO}_3^+$: 635.2562, found: 635.2554.

Compound 6e: The synthetic procedure was similar to that yielding compound **6a**, using 4-methoxyphenylboronic acid instead of phenylboronic acid. The crude product was purified by flash column chromatography (hexane/EtOAc = 9/1) to afford compound **6e** (77 mg, 0.126 mmol, 93%) as a colorless solid. M.p.: 165–168 °C; R_f : 0.24 (hexane/EtOAc = 9/1); ^1H NMR (400 MHz): 7.56 (d, J = 8.4 Hz, 2H, ArH), 7.50 (d, J = 8.8 Hz, 2 H, ArH), 7.38 (d, J = 8.4 Hz, 2 H, ArH), 7.23 (A of AB system, d, J = 7.8 Hz, 1 H, ArH), 7.22 (B of AB system, d, J = 7.8 Hz, 1 H, ArH), 7.08 (d, J = 8.7 Hz, 2 H, ArH), 7.05 (d, J = 8.7 Hz, 2 H, ArH), 7.00 (d, J = 8.7 Hz, 2 H, ArH), 6.97 (d, J =

7.2 Hz, 1 H, ArH), 6.81 (t, J = 7.6 Hz, 1 H, ArH), 6.62–6.57 (m, 2 H, ArH), 5.89 (d, J = 7.6 Hz, 1 H, ArH), 5.78–5.72 (m, 2 H, ArH), 5.19 (s, 1 H, CH), 5.05 (s, 1 H, CH), 4.94 (s, 1 H, CH), 3.91 (s, 3 H, OCH₃), 3.89 (s, 3 H, OCH₃), 3.87 (s, 3 H, OCH₃), 1.80 (s, 3 H, CH₃); ¹³C NMR (100 MHz): 159.1, 159.0, 158.9, 146.02, 146.98, 144.8, 144.0, 143.4, 138.7, 138.12, 138.08, 135.3, 135.25, 135.17, 130.4, 130.12, 130.09, 129.1, 127.7, 126.9, 125.3, 125.0, 124.6, 114.6, 114.5, 114.4, 62.7, 62.4, 61.8, 59.4, 55.52, 55.47, 55.4, 29.0; MS (EI): m/z (%) 612.3 (100, [M]⁺), 597.2 (11, [M – CH₃]⁺), 496.2 (18), 390.2 (7), 306.1 (12, [M]²⁺); MS (MALDI): m/z (%) 635.3 (100, [M + Na]⁺). Accurate mass ([M + Na]⁺, MALDI) calcd for C₄₄H₃₆NaO₃⁺: 635.2562, found: 635.2562.

Compound 6g: The synthetic procedure was similar to that yielding compound **6a**, using 2,4-dimethoxyphenylboronic acid instead of phenylboronic acid. The crude product was purified by flash column chromatography (hexane/EtOAc = 5/1) to afford compound **6g** (95 mg, 0.135 mmol, 99%) as a colorless solid. M.p.: 203–205 °C (dec.); R_f: 0.23 (hexane/EtOAc = 5/1); ¹H NMR (400 MHz, 1,1,2,2-tetrachloroethane-*d*₂, 60 °C): 7.44 (d, J = 8 Hz, 1 H, ArH), 7.38 (d, J = 8.1 Hz, 1 H, ArH), 7.27–7.23 (m, 3 H, ArH), 7.02 (d, J = 7.4 Hz, 1 H, ArH), 6.91 (t, J = 7.6 Hz, 1 H, ArH), 6.79–6.69 (m, 8 H, ArH), 6.05 (d, J = 7.6 Hz, 1 H, ArH), 5.96–5.95 (m, 2 H, ArH), 4.94 (s, 1 H, CH), 4.81 (s, 1 H, CH), 4.68 (s, 1 H, CH), 3.99 (s, 3 H, OCH₃), 3.96 (s, 3 H, OCH₃), 3.94 (s, 3 H, OCH₃), 3.93 (s, 3 H, OCH₃), 3.89 (s, 3 H, OCH₃), 3.83 (s, 3 H, OCH₃), 1.78 (s, 3 H, CH₃); ¹³C NMR (100 MHz, 1,1,2,2-tetrachloroethane-*d*₂, 60 °C): 160.7, 160.6, 160.5, 157.43, 157.38, 157.2, 146.4, 145.7, 145.4, 145.1, 144.9, 144.2, 135.1, 134.4, 134.3, 132.2, 132.1, 130.0, 129.4, 126.6, 126.2, 126.1, 125.3, 125.1, 124.5, 124.4, 124.33, 124.27, 105.4, 105.3, 105.2, 99.5, 99.3, 63.4, 63.1, 62.5, 59.2, 55.51, 55.47, 55.3, 28.2; MS (MALDI): m/z

(%) 741.3 (100, $[M + K]^+$). Accurate mass ($[M + K]^+$, MALDI) calcd for $C_{47}H_{42}KO_6^+$: 741.2613, found: 741.2602.

Compound 6h: The synthetic procedure was similar to that yielding compound **6a**, using 2,5-dimethoxyphenylboronic acid instead of phenylboronic acid. The crude product was purified by flash column chromatography (hexane/EtOAc = 5/1) to afford compound **6h** (78 mg, 0.112 mmol, 82%) as a colorless solid. M.p.: 182-185 °C; R_f : 0.33 (hexane/EtOAc = 3/1); 1H NMR (400 MHz, 1,1,2,2-tetrachloroethane- d_2 , 60 °C): 7.29–7.25 (m, 2 H, ArH), 7.12–7.11 (m, 1 H, ArH), 7.08–7.03 (m, 6 H, ArH), 7.01–6.98 (m, 2 H, ArH), 6.93–6.88 (m, 2 H, ArH), 6.71–6.66 (m, 2 H, ArH), 6.02 (s, 1 H, ArH), 5.89–5.87 (m, 2 H, ArH), 4.95 (s, 1 H, CH), 4.82 (s, 1 H, CH), 4.70 (s, 1 H, CH), 3.90 (s, 3 H, OCH₃), 3.864 (s, 3 H, OCH₃), 3.855 (s, 3 H, OCH₃), 3.83 (s, 3 H, OCH₃), 3.81 (s, 3 H, OCH₃), 3.75 (s, 3 H, OCH₃), 1.75 (s, 3 H, CH₃); ^{13}C NMR (100 MHz, 1,1,2,2-tetrachloroethane- d_2 , 60 °C): 154.1, 154.0, 153.9, 151.0, 150.8, 146.2, 145.7, 145.3, 144.8, 135.2, 134.9, 134.8, 132.4, 132.20, 132.18, 129.7, 129.1, 126.6, 126.2, 126.1, 125.4, 125.2, 124.9, 117.8, 117.7, 114.3, 114.2, 113.2, 113.0, 63.3, 63.1, 62.5, 59.5, 56.2, 56.1, 56.10, 56.04, 28.2; MS (EI): m/z (%) 702.3 (100, $[M]^+$), 687.3 (7, $[M - CH_3]^+$), 671.3 (28, $[M - OCH_3]^+$), 351.1 (10, $[M]^{2+}$), 343.6 (7, $[M - CH_3]^{2+}$); MS (ESI): m/z (%) 725.3 (100, $[M + Na]^+$). Accurate mass ($[M + Na]^+$, ESI) calcd for $C_{47}H_{42}NaO_6^+$: 725.2874, found: 725.2886.

Compound 6j: The synthetic procedure was similar to that yielding compound **6a**, using 3,5-dimethoxyphenylboronic acid instead of phenylboronic acid. The crude product was purified by flash column chromatography (hexane/EtOAc = 7/1) to afford compound **6j** (92 mg, 0.131 mmol, 96%) as a colorless solid. M.p.: 260 °C (dec.); R_f : 0.43 (hexane/EtOAc = 4/1); 1H NMR (400 MHz): 7.27 (A of AB system, d,

$J = 7.8$ Hz, 1 H, ArH), 7.26 (B of AB system, d, $J = 7.8$ Hz, 1 H, ArH), 7.03 (d, $J = 7.2$ Hz, 1 H, ArH), 6.88 (t, $J = 7.6$ Hz, 1 H, ArH), 6.79 (d, $J = 2.4$ Hz, 2 H, ArH), 6.73 (d, $J = 2.4$ Hz, 2 H, ArH), 6.68–6.64 (m, 2 H, ArH), 6.63 (d, $J = 2$ Hz, 2 H, ArH), 6.57 (t, $J = 2.4$ Hz, 1 H, ArH), 6.54 (t, $J = 2$ Hz, 1 H, ArH), 6.51 (t, $J = 2$ Hz, 1 H, ArH), 6.04 (d, $J = 8$ Hz, 1 H, ArH), 5.92–5.87 (m, 2 H, ArH), 5.19 (s, 1 H, CH), 5.06 (s, 1 H, CH), 4.96 (s, 1 H, CH), 3.87 (s, 6 H, OCH₃), 3.84 (s, 6 H, OCH₃), 3.81 (s, 6 H, OCH₃), 1.78 (s, 3 H, CH₃); ¹³C NMR (100 MHz): 161.5, 161.4, 161.2, 146.0, 145.8, 144.68, 144.66, 144.5, 144.0, 143.3, 143.2, 139.0, 138.9, 129.8, 129.7, 128.9, 127.6, 126.9, 125.6, 125.4, 125.3, 107.7, 107.6, 99.5, 99.3, 62.7, 62.5, 62.0, 59.6, 55.68, 55.67, 55.6, 29.0; MS (EI): m/z (%) 702.3 (100, [M]⁺), 687.3 (12, [M – CH₃]⁺), 671.3 (9, [M – OCH₃]⁺), 586.2 (19), 351.1 (20, [M]²⁺); MS (MALDI): m/z (%) 725.3 (100, [M + Na]⁺). Accurate mass ([M + Na]⁺, MALDI) calcd for C₄₇H₄₂NaO₆⁺: 725.2874, found: 725.2876.

Compound 6k: The synthetic procedure was similar to that yielding compound **6a**, using 2,3,4-trimethoxyphenylboronic acid instead of phenylboronic acid. The crude product was purified by flash column chromatography (hexane/EtOAc = 2/1) to afford compound **6k** (106 mg, 0.134 mmol, 99%) as a colorless solid. M.p.: 114–116 °C; R_f: 0.41 (hexane/EtOAc = 2/1); ¹H NMR (400 MHz, 1,1,2,2-tetrachloroethane-*d*₂, 60 °C): 7.27–7.25 (m, 2 H, ArH), 7.22 (d, $J = 8.4$ Hz, 1 H, ArH), 7.16 (d, $J = 8.4$ Hz, 1 H, ArH), 7.03 (s, 1 H, ArH), 7.01 (s, 1 H, ArH), 6.92 (d, $J = 8.4$ Hz, 1 H, ArH), 6.89–6.86 (m, 2 H, ArH), 6.81 (d, $J = 8.8$ Hz, 1 H, ArH), 6.69–6.64 (m, 2 H, ArH), 6.01 (s, 1 H, ArH), 5.90–5.88 (m, 1 H, ArH), 5.85–5.83 (m, 1 H, ArH), 5.03 (s, 1 H, CH), 4.92 (s, 1 H, CH), 4.80 (s, 1 H, CH), 4.02 (s, 6 H, OCH₃), 3.98 (s, 3 H, OCH₃), 3.97 (s, 3 H, OCH₃), 3.96 (s, 3 H, OCH₃), 3.94 (s, 3 H, OCH₃), 3.68 (s, 3 H, OCH₃), 3.64 (s, 3 H, OCH₃), 3.56 (s, 3 H, OCH₃), 1.76 (s, 3 H, CH₃); ¹³C NMR (100 MHz,

1,1,2,2-tetrachloroethane- d_2 , 60 °C): 153.42, 153.38, 153.3, 151.43, 151.38, 151.3, 146.1, 145.9, 145.36, 143.3, 143.1, 135.0, 134.6, 134.53, 134.49, 129.79, 129.75, 129.3, 129.2, 129.1, 129.0, 126.4, 126.1, 125.5, 125.3, 125.2, 124.7, 108.43, 108.39, 108.36, 108.2, 63.2, 62.9, 62.4, 61.04, 61.01, 60.9, 60.8, 60.6, 59.4, 56.44, 56.38, 28.5; MS (ESI): m/z (%) 815.3 (100, $[M + Na]^+$). Accurate mass ($[M + Na]^+$, ESI) calcd for $C_{50}H_{48}NaO_9^+$: 815.3191, found: 815.3193.

Compound 6l: The synthetic procedure was similar to that yielding compound **6a**, using 3,4,5-trimethoxyphenylboronic acid instead of phenylboronic acid. The crude product was purified by flash column chromatography (hexane/EtOAc = 2/1) to afford compound **6l** (106 mg, 0.134 mmol, 99%) as a colorless solid. M.p.: 253–255 °C; R_f : 0.41 (hexane/EtOAc = 2/1); 1H NMR (400 MHz): 7.29 (A of AB system, d, J = 8 Hz, 1 H, ArH), 7.29 (B of AB system, d, J = 8 Hz, 1 H, ArH), 7.05 (d, J = 7.6 Hz, 1 H, ArH), 6.89 (t, J = 8 Hz, 1 H, ArH), 6.84 (s, 2 H, ArH), 6.78 (s, 2 H, ArH), 6.68–6.66 (m, 4 H, ArH), 5.93 (d, J = 7.6 Hz, 1 H, ArH), 5.79–5.74 (m, 2 H, ArH), 5.17 (s, 1 H, CH), 5.04 (s, 1 H, CH), 4.92 (s, 1 H, CH), 3.97 (s, 3 H, OCH₃), 3.95 (s, 3 H, OCH₃), 3.93 (s, 9 H, OCH₃), 3.89 (s, 6 H, OCH₃), 3.85 (s, 6 H, OCH₃), 1.82 (s, 3 H, CH₃); ^{13}C NMR (100 MHz): 154.0, 153.9, 153.7, 145.8, 145.5, 144.5, 143.9, 143.3, 142.9, 139.2, 139.0, 138.1, 137.97, 137.93, 137.8, 129.8, 129.7, 129.0, 127.6, 127.04, 127.00, 125.7, 125.4, 125.3, 106.7, 62.8, 62.4, 61.38, 61.36, 61.3, 59.6, 56.5, 56.50, 56.46, 29.1; MS (ESI): m/z (%) 815.3 (100, $[M + Na]^+$). Accurate mass ($[M + Na]^+$, ESI) calcd for $C_{50}H_{48}NaO_9^+$: 815.3191, found: 815.3184.

Compound 7a: Compound **6a** (68 mg, 0.130 mmol) was dissolved in anhydrous CH_2Cl_2 (10 mL) and cooled to 0 °C. 2,3-Dichloro-5,6-dicyano-*p*-benzoquinone (148 mg, 0.65 mmol) was added in one portion and the mixture was stirred for 5 min.

Trifluoromethanesulfonic acid (0.2 mL) was added and the mixture was stirred for 1 h. The reaction mixture was quenched by washing with saturated aqueous sodium carbonate (20 mL) and then concentrated under reduced pressure. The residue was purified by flash column chromatography (hexane/EtOAc = 6/1) to afford compound **7a** (24 mg, 0.046 mmol, 35%) as a colorless solid. M.p.: >300 °C; *R*_f: 0.19 (hexane/EtOAc = 6/1); ¹H NMR (400 MHz): 7.90–7.86 (m, 2 H, ArH), 7.60–7.52 (m, 12 H, ArH), 7.50–7.45 (m, 2 H, ArH), 7.35 (d, *J* = 7.8 Hz, 2 H, ArH), 6.59–6.55 (m, 2 H, ArH), 5.59–5.55 (m, 2 H, ArH), 5.22 (s, 2 H, CH), 2.12 (s, 1 H, OH), 1.76 (s, 3 H, CH₃); ¹³C NMR (100 MHz): 147.6, 144.7, 142.0, 140.3, 139.0, 136.5, 133.8, 131.0, 130.0, 129.5, 129.2, 129.1, 128.0, 127.7, 127.2, 125.6, 89.6, 64.3, 62.8, 22.9; MS (ESI): *m/z* (%) 559.2 (34, [M + Na]⁺), 519.2 (100, [M + H – H₂O]⁺). Accurate mass ([M + Na]⁺, ESI) calcd for C₄₁H₂₈NaO⁺: 559.2032, found: 559.2057.

Compound 7b: The synthetic procedure was similar to that yielding compound **7a**, using **6b** (84 mg, 0.122 mmol) as the starting material. The crude product was purified by flash column chromatography (hexane/EtOAc = 20/1) to afford compound **7b** (31 mg, 0.044 mmol, 36%) as a colorless solid. M.p.: >300 °C; *R*_f: 0.17 (hexane/EtOAc = 20/1); ¹H NMR (400 MHz): 7.87 (d, *J* = 1.6 Hz, 1 H, ArH), 7.79 (d, *J* = 8 Hz, 1 H, ArH), 7.57–7.53 (m, 7 H, ArH), 7.49–7.47 (m, 4 H, ArH), 7.34 (d, *J* = 5.6 Hz, 1 H, ArH), 7.32 (d, *J* = 5.6 Hz, 1 H, ArH), 6.53–6.49 (m, 2 H, ArH), 5.46–5.42 (m, 2 H, ArH), 5.19 (s, 2 H, CH), 2.19 (s, 1 H, OH), 1.74 (s, 3 H, CH₃), 1.45 (s, 9 H, C(CH₃)₃), 1.41 (s, 18 H, C(CH₃)₃); ¹³C NMR (100 MHz): 150.72, 150.70, 150.66, 147.41, 147.36, 144.6, 140.14, 140.12, 138.9, 138.7, 138.5, 135.9, 133.9, 133.5, 133.3, 130.49, 130.47, 129.4, 129.0, 128.9, 128.7, 126.9, 126.8, 125.9, 125.5, 125.0, 89.4, 64.0, 62.7, 34.8, 34.7, 31.5, 31.4, 22.8; MS (ESI): *m/z* (%) 727.4 (100, [M + Na]⁺). Accurate mass ([M + Na]⁺, ESI) calcd for C₅₃H₅₂NaO⁺: 727.3910, found: 727.3915.

Compound 10: 2,3-Dichloro-5,6-dicyano-*p*-benzoquinone (37 mg, 0.163 mmol) was added in one portion to a solution of compound **6e** (100 mg, 0.163 mmol) in anhydrous CH₂Cl₂ (10 mL) at 0 °C. After 5 min, trifluoromethanesulfonic acid (0.2 mL) was added and the mixture was stirred for 1 h. It was then quenched by washing with saturated sodium carbonate solution (20 mL) and concentrated under reduced pressure. The residue was purified by flash column chromatography (hexane/EtOAc = 9/1) to afford a mixture containing compound **10** and compound **11e** in 0.87:1 ratio. Compound **10** (7 mg, 0.011 mmol, 7%) was further purified by crystallization from a hexane/EtOAc mixture as colorless solid. M.p.: >300 °C; *R*_f: 0.51 (hexane/EtOAc = 7/1); ¹H NMR (700 MHz): 7.71 (d, *J* = 9.1 Hz, 1 H, ArH), 7.49–7.46 (m, 5 H, ArH), 7.42 (d, *J* = 7.7 Hz, 1 H, ArH), 7.29 (s, 1 H, ArH), 7.23 (d, *J* = 7.7 Hz, 1 H, ArH), 7.21 (d, *J* = 7.7 Hz, 1 H, ArH), 7.06–7.05 (m, 5 H, ArH), 6.62–6.59 (m, 2 H, ArH), 5.72–5.70 (m, 2 H, ArH), 5.14 (s, 2 H, CH), 4.17 (s, 1 H, CH), 3.94 (s, 3 H, OCH₃), 3.90 (s, 6 H, OCH₃), 1.78 (s, 3 H, CH₃); ¹³C NMR (176 MHz): 159.1, 159.0, 158.7, 147.5, 147.0, 145.3, 145.2, 140.7, 140.5, 139.1, 138.6, 137.8, 134.7, 134.6, 133.7, 133.6, 131.1, 130.8, 130.3, 129.4, 127.7, 127.4, 126.84, 126.81, 125.3, 114.5, 114.4, 114.3, 113.6, 63.8, 63.7, 60.8, 59.2, 55.5, 55.4, 27.9; MS (MALDI): *m/z* (%) 610.3 (100, [M]⁺). Accurate mass ([M]⁺, MALDI) calcd for C₄₄H₃₄O₃⁺: 610.2502, found: 610.2505.

Compound 11c: The synthetic procedure was similar to that yielding compound **10**, using **6c** (56 mg, 0.091 mmol) as the starting material. The crude product was purified by flash column chromatography (hexane/EtOAc = 9/1) to afford compound **11c** (2.2 mg, 0.004 mmol, 4%) as a colorless solid. M.p.: 201–203 °C; *R*_f: 0.33 (hexane/EtOAc = 9/1); ¹H NMR (400 MHz, 1,1,2,2-tetrachloroethane-*d*₂, 60 °C): 7.52–7.37 (m, 4 H,

ArH), 7.36–7.24 (m, 4 H, ArH), 7.23–7.00 (m, 6 H, ArH), 6.97 (t, $J = 7.2$ Hz, 2 H, ArH), 6.92 (d, $J = 7.8$ Hz, 2 H, ArH), 6.82 (t, $J = 7.4$ Hz, 1 H, ArH), 6.06 (s, 1 H, ArH), 5.83 (d, $J = 7.6$ Hz, 1 H, ArH), 4.95 (s, 1 H, CH), 4.91 (s, 1 H, CH), 4.34 (s, 1 H, CH), 3.90 (s, 3 H, OCH₃), 3.90–3.68 (m, 6 H, OCH₃), 1.78 (s, 3 H, CH₃); ¹³C NMR (176 MHz, 1,1,2,2-tetrachloroethane-*d*₂, 60 °C): 155.9, 146.2, 145.0, 144.6, 136.9, 135.1, 132.2, 131.12, 131.06, 131.0, 130.1, 129.8, 129.0, 128.6, 128.0, 126.9, 126.8, 126.1, 123.8, 122.9, 120.9, 120.3, 120.2, 111.4, 110.6, 99.4, 62.5, 60.3, 60.1, 59.4, 55.4, 55.2, 55.1, 28.0; MS (MALDI): m/z (%) 635.3 (100, [M + Na]⁺). Accurate mass ([M + Na]⁺, MALDI) calcd for C₄₄H₃₆NaO₃⁺: 635.2562, found: 635.2559.

Compound 11d: The synthetic procedure was similar to that yielding compound **10**, using **6d** (134 mg, 0.219 mmol) as the starting material. The crude product was purified by flash column chromatography (hexane/EtOAc = 12/1) to afford compound **11d** (14 mg, 0.023 mmol, 11%) as a colorless solid. M.p.: 198–199 °C; R_f : 0.4 (hexane/EtOAc = 6/1); ¹H NMR (700 MHz, CD₂Cl₂): 7.49–7.45 (m, 2 H, ArH), 7.39 (d, $J = 7.7$ Hz, 1 H, ArH), 7.35 (d, $J = 7.0$ Hz, 1 H, ArH), 7.30–7.27 (m, 4 H, ArH), 7.25 (t, $J = 8.4$ Hz, 1 H, ArH), 7.22 (d, $J = 7.7$ Hz, 1 H, ArH), 7.16 (s, 1 H, ArH), 7.13 (s, 1 H, ArH), 7.06 (t, $J = 7.7$ Hz, 1 H, ArH), 7.02 (d, $J = 8.4$ Hz, 1 H, ArH), 6.98 (d, $J = 7.7$ Hz, 1 H, ArH), 6.82 (d, $J = 8.4$ Hz, 1 H, ArH), 6.77–6.75 (m, 2 H, ArH), 6.72 (d, $J = 7.7$ Hz, 1 H, ArH), 6.16 (s, 1 H, ArH), 5.80 (d, $J = 7.7$ Hz, 1 H, ArH), 5.24 (s, 1 H, CH), 5.19 (s, 1 H, CH), 4.37 (s, 1 H, CH), 3.88 (s, 3 H, OCH₃), 3.83 (s, 3 H, OCH₃), 3.75 (s, 3 H, OCH₃), 1.8 (s, 3 H, CH₃); ¹³C NMR (176 MHz, CD₂Cl₂): 160.8, 160.6, 160.1, 146.5, 146.0, 145.7, 144.9, 144.3, 144.14, 144.05, 143.9, 142.8, 140.2, 139.13, 139.08, 130.7, 130.4, 130.170, 130.167, 129.6, 127.7, 127.2, 126.8, 126.0, 124.8, 124.4, 124.2, 122.0, 121.7, 119.9, 115.33, 115.26, 113.24, 113.21, 113.15, 112.2, 62.91, 62.85, 62.7, 60.7, 55.8, 55.6, 55.5, 28.5; MS (EI): m/z (%) 612.3 (100, [M]⁺),

597.3 (15, $[M - CH_3]^+$), 496.2 (8), 390.2 (9), 306.1 (10, $[M]^{2+}$). Accurate mass ($[M]^+$, EI): calcd for $C_{44}H_{36}O_3^{+}$: 612.2659, found: 612.2654.

Compound 11e: R_f : 0.51 (hexane/EtOAc = 7/1); 1H NMR (400 MHz): 7.37–7.33 (m, 2 H, ArH), 6.86 (d, $J = 8.7$ Hz, 2 H, ArH), 6.77 (t, $J = 7.6$ Hz, 1 H, ArH), 6.09 (s, 1 H, ArH), 5.84 (d, $J = 7.8$ Hz, 1 H, ArH), 5.21 (s, 1 H, CH), 5.17 (s, 1 H, CH), 4.35 (s, 1 H, CH), 3.92 (s, 3 H, OCH_3), 3.89 (s, 3 H, OCH_3), 3.84 (s, 3 H, OCH_3), 1.79 (s, 3 H, CH_3)

Note: Some signals of compound **11e** were overlapped by those of compound **10**, making the full characterization of compound **11e** impossible.

Compound 16: The synthetic procedure was similar to that yielding compound **10**, using **6k** (80 mg, 0.100 mmol) as the starting material. The crude product was purified by flash column chromatography (hexane/EtOAc = 2/1) to afford compound **16** (60 mg, 0.075 mmol, 75%) as a colorless solid. M.p.: 150–152 °C; R_f : 0.4 (hexane/EtOAc = 2/1); 1H NMR (400 MHz, 1,1,2,2-tetrachloroethane- d_2 , 60 °C): 7.64 (d, $J = 8$ Hz, 1 H, ArH), 7.51 (d, $J = 8$ Hz, 1 H, ArH), 7.28 (d, $J = 7.8$ Hz, 1 H, ArH), 7.24 (d, $J = 7.9$ Hz, 1 H, ArH), 7.14–7.12 (m, 3 H, ArH), 6.86 (d, $J = 8.5$ Hz, 2 H, ArH), 6.68–6.64 (m, 2 H, ArH), 5.74–5.70 (m, 2 H, ArH), 5.04 (s, 1 H, CH), 5.01 (s, 1 H, CH), 4.13 (s, 1 H, CH), 4.05 (s, 6 H, OCH_3), 3.98 (s, 12 H, OCH_3), 3.86 (s, 3 H, OCH_3), 3.62 (s, 6 H, OCH_3), 1.81 (s, 3 H, CH_3); ^{13}C NMR (100 MHz, 1,1,2,2-tetrachloroethane- d_2 , 60 °C): 153.5, 153.4, 152.2, 151.8, 151.5, 151.4, 147.9, 147.8, 145.4, 143.20, 143.18, 141.9, 141.5, 140.8, 134.6, 134.3, 134.0, 133.4, 129.8, 129.1, 128.7, 128.42, 128.38, 126.4, 126.14, 126.10, 125.6, 125.50, 125.46, 124.9, 109.4, 108.3, 108.2, 64.8, 64.6, 61.0, 60.8, 60.7, 60.6, 60.3, 59.1, 56.38, 56.36, 56.15, 27.65; MS (ESI): m/z (%) 813.3 (100, $[M + Na]^+$). Accurate mass ($[M + Na]^+$, ESI)

calcd for $C_{50}H_{46}NaO_9^+$: 813.3034, found: 813.3033.

Compound 17: The synthetic procedure was similar to that yielding compound **10**, using **6l** (50 mg, 0.063 mmol) as the starting material. The crude product was purified by flash column chromatography (hexane/EtOAc = 2/1) to afford compound **17** (20 mg, 0.025 mmol, 40%) as a colorless solid. M.p.: 205–207 °C; R_f : 0.27 (hexane/EtOAc = 2/1); 1H NMR (400 MHz): 7.58 (d, J = 7.9 Hz, 1 H, ArH), 7.43 (d, J = 7.8 Hz, 1 H, ArH), 7.22 (d, J = 7.8 Hz, 1 H, ArH), 7.16 (d, J = 8 Hz, 1 H, ArH), 7.02 (s, 1 H, ArH), 6.76–6.74 (m, 4 H, ArH), 6.67–6.63 (m, 2 H, ArH), 5.71–5.65 (m, 2 H, ArH), 5.08 (s, 1 H, CH), 5.05 (s, 1 H, CH), 4.13 (s, 1 H, CH), 4.01 (s, 3 H, OCH₃), 4.00 (s, 3 H, OCH₃), 3.96 (s, 3 H, OCH₃), 3.95 (s, 3 H, OCH₃), 3.87 (s, 12 H, OCH₃), 3.81 (s, 3 H, OCH₃), 1.79 (s, 3 H, CH₃); ^{13}C NMR (100 MHz): 153.8, 153.7, 152.5, 151.9, 148.4, 148.3, 145.0, 144.9, 141.9, 140.1, 139.5, 138.8, 138.2, 138.1, 137.9, 137.8, 137.7, 134.4, 134.2, 130.1, 129.2, 128.9, 128.1, 127.4, 127.0, 126.9, 125.8, 125.6, 124.8, 108.8, 106.6, 64.4, 64.3, 61.3, 61.2, 61.1, 60.4, 59.6, 56.4, 56.2, 28.0; MS (ESI): m/z (%) 813.3 (100, $[M + Na]^+$). Accurate mass ($[M + Na]^+$, ESI) calcd for $C_{50}H_{46}NaO_9^+$: 813.3034, found: 813.3028.

Compound 18: Compound **16** (60 mg, 0.075 mmol) was dissolved in anhydrous CH_2Cl_2 (10 mL) and cooled to 0 °C. 2,3-Dichloro-5,6-dicyano-*p*-benzoquinone (34 mg, 0.152 mmol) was added in one portion and the mixture was stirred for 5 min. Trifluoromethanesulfonic acid (0.2 mL) was added and the resulting mixture was stirred for 1 h. The reaction mixture was quenched and washed with saturated sodium carbonate solution (20 mL), concentrated under reduced pressure and the residue was purified by flash column chromatography (hexane/EtOAc = 2/1) to afford compound **18** (34 mg, 0.043 mmol, 57%) as a colorless solid. M.p.: 253 °C (dec.); R_f : 0.4

(hexane/EtOAc = 2/1); ^1H NMR (400 MHz): 7.43 (d, $J = 8$ Hz, 1 H, ArH), 7.391 (A of AB system, d, $J = 8.5$ Hz, 1 H, ArH), 7.386 (B of AB system, d, $J = 8.3$ Hz, 1 H, ArH), 7.33–7.29 (m, 2 H, ArH), 7.24 (d, $J = 8$ Hz, 1 H, ArH), 7.04 (s, 1 H, ArH), 7.02 (s, 2 H, ArH), 4.443 (s, 1 H, CH), 4.438 (s, 1 H, CH), 4.422 (s, 1 H, CH), 4.01 (s, 12 H, OCH_3), 3.98 (s, 6 H, OCH_3), 3.89 (s, 3 H, OCH_3), 3.87 (s, 3 H, OCH_3), 3.86 (s, 3 H, OCH_3), 1.84 (s, 3 H, CH_3); ^{13}C NMR (100 MHz): 152.5, 152.42, 152.39, 151.93, 151.87, 151.8, 145.3, 145.1, 145.0, 144.92, 144.85, 144.6, 141.9, 141.8, 141.7, 134.41, 134.37, 134.13, 134.09, 134.06, 133.9, 130.4, 129.5, 129.4, 129.2, 129.1, 128.8, 127.8, 126.9, 124.8, 124.6, 124.5, 108.4, 108.2, 62.7, 62.63, 62.55, 61.4, 61.3, 61.2, 58.9, 56.2, 26.1; MS (ESI): m/z (%) 809.3 (100, $[\text{M} + \text{Na}]^+$). Accurate mass ($[\text{M} + \text{Na}]^+$, ESI) calcd for $\text{C}_{50}\text{H}_{42}\text{NaO}_9^+$: 809.2721, found: 809.2726.

2. X-ray Crystallography

Crystal data were collected on a Bruker D8 venture diffractometer or Bruker Kappa ApexII Duo diffractometer with Mo-K α radiation ($\lambda = 0.71073$ Å). The crystal structures were solved by direct methods using SHELXS-97¹ and all the non-hydrogen atoms were anisotropically refined by full-matrix least-squares on F^2 using the SHELXL-97 program.² The highly disordered co-crystallized solvent molecules were removed by the standard SQUEEZE³ protocol incorporated in PLATON.⁴

X-ray crystal structure of compound **7a**

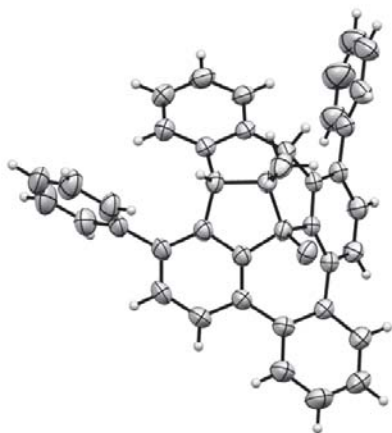


Figure S1. X-ray crystal structure of compound **7a**.

A single crystal of **7a** was obtained from a chloroform solution by slow evaporation.

X-ray crystal data for **7a**: C₄₁H₂₇O; $M = 535.62$; monoclinic; $a = 23.6823(14)$, $b = 14.1831(8)$, $c = 19.4393(10)$ Å; $\beta = 101.9212(17)$; $V = 6388.6(6)$ Å³; space group $C2/c$; $Z = 8$; $\rho_{\text{calcd}} = 1.114$ Mg m⁻³; $T = 296(2)$ K; λ (MoK α) = 1.54178 Å; 63194 reflections collected; 5781 independent reflections; $R_{\text{int}} = 0.0613$; observed data with I

$\geq 2\sigma(I) = 4070$; $R_1 = 0.0864$, $wR_2 = 0.1598$ [$I \geq 2\sigma(I)$]. CCDC-1478751 contains the supplementary crystallographic data for **7a**.

3. References

- (1) G. M. Sheldrick, *SHELXS-97, Program for Crystal Structure Solution*, University of Göttingen, Göttingen, Germany, 1997.
- (2) G. M. Sheldrick, *SHELXL-97, Program for the Refinement of Crystal Structures from Diffraction Data*, University of Göttingen, Göttingen, Germany, 1997.
- (3) P. A. van der Sluis, A. L. Spek, *Acta Crystallogr. A* **1990**, A46, 194.
- (4) A. L. Spek, *PLATON, A Multipurpose Crystallographic Tool*, Utrecht University, Utrecht, The Netherlands, 2000.

4. 2D COSY Spectra of 7a, 7b, 10, 16 and 17



Current Data Parameters
NAME Eric_8a_un_mono_OH_data
EXPNO 555
PROCNO 1

F2 - Acquisition Parameters

Date_ 20160202
Time_ 13:01
INSTRUM spect
PROBHD Z824601_0021 (cosygmrf)
PULPROG 2048
TD CDC13
SOLVENT NS
NS 4
DS 16
SWH 8012.820 Hz
FIDRES 3.912510 Hz
AQ 0.1277952 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 294.5 K
D0 0.00000300 sec
D1 2.00000000 sec
d13 0.00000400 sec
D16 0.00020000 sec
in0 0 sec

STICNT 0
deorig 0.00000300 sec
philoop 0
t1loop 0
SF01 400.1324008 MHz
NUC1 1H
P1 15.00 usec
PLW1 8.31000042 W
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition Parameters

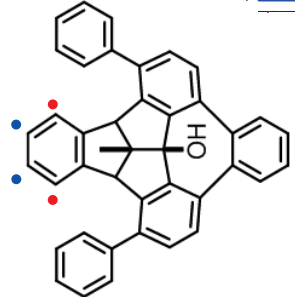
TD 128
SF01 400.1324 MHz
FIDRES 62.500000 Hz
SW 19.993 ppm
FnMODE QF

F2 - Processing parameters

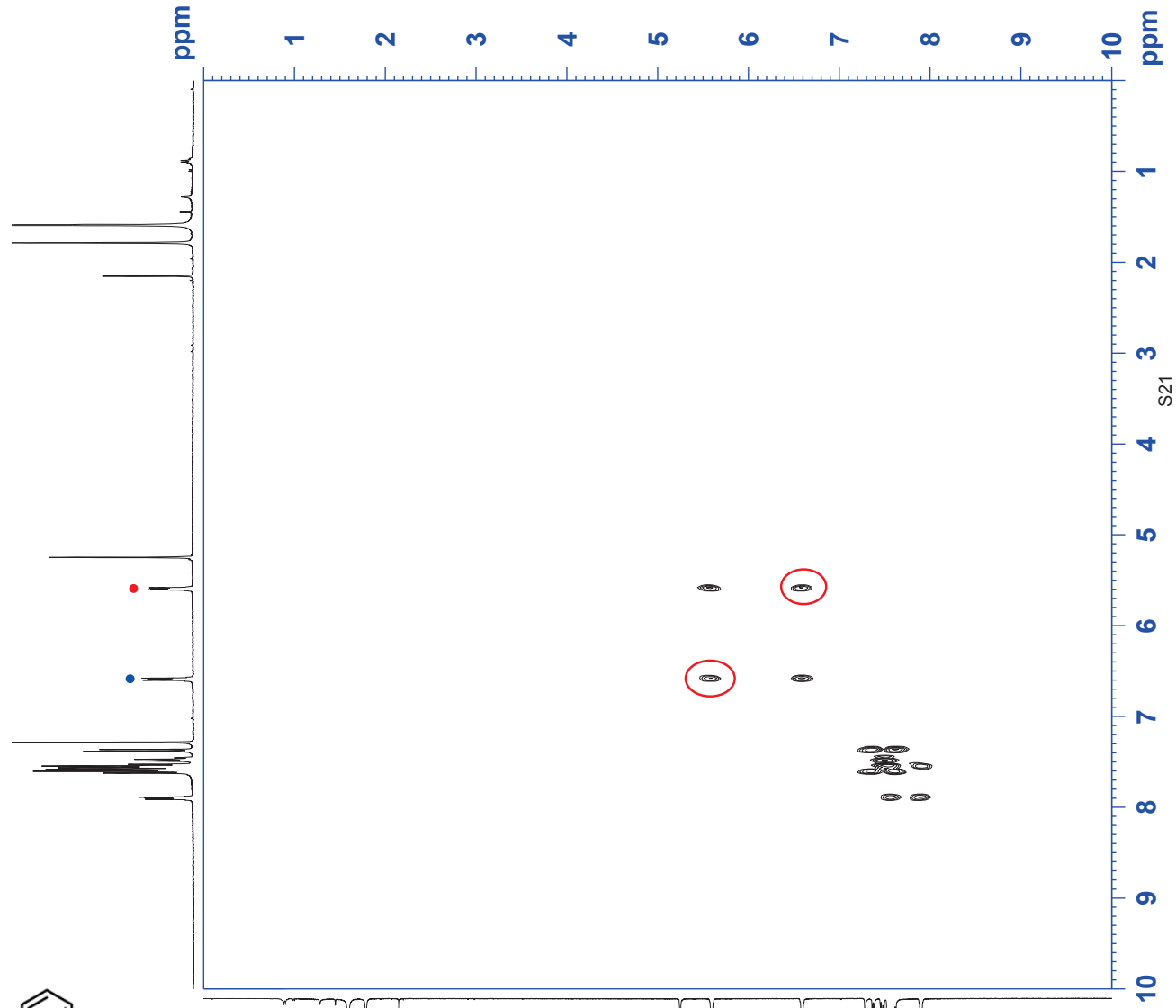
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

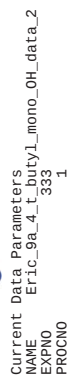
F1 - Processing parameters

SI 1024
MC2 QF
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0



7a





F2 - Acquisition Parameters

Date_ 20160212
Time 11.36

```
INSTRUM spect
PROBHD Z108618 0257 (
```

PULPROG	cosygmfqf
TD	2018

SOLVENT

NS	4
DS	16

SWH	8012.820 HZ
FIDRES	3.912510 HZ

AQ 0.1277952 sec
BC 2050

RD	DW	2050	62.400 usec

DE	6.50 usec
TE	294.3 K

D0	0.00000300 sec
D1	2.00000000 sec

Iteration	Time (sec)
d1	0.00000000
d13	0.00000400
d16	0.00000000

```
DT0 0.0002000 SEC
in0 0 sec
```

```
ST1CNT      0
dorig      0.00000300 sec
```

Loop	Time (s)
ph1loop	0.0
t1loop	0.0

SF01 400.2324014 MHZ

NUCL	TH
P1	12.80 usec

```
PLW1      13.56000042 W
GPNAM[1]  SMS010.100
```

```
GPNAME[2] SMSQ10.100
GPNAME[3] SMSQ10.100
```

GPZ1	16.00 %
GPZ2	16.00 %

GPZ2	GPZ3
12.00 %	40.00 %

P16 1000.00 usec

F1 - Acquisition parameters	128
TD	

400.2324 MHZ

FIDRES
SW
62.500000 HZ
19.988 ppm

FnMODE QF

F2 - Processing parameters
1024

SI
SF
400.230000 MHz
1024

WDW SSB 0 SINE

LB 0 Hz
GB 0

1.40 PC

F1 - Processing parameters

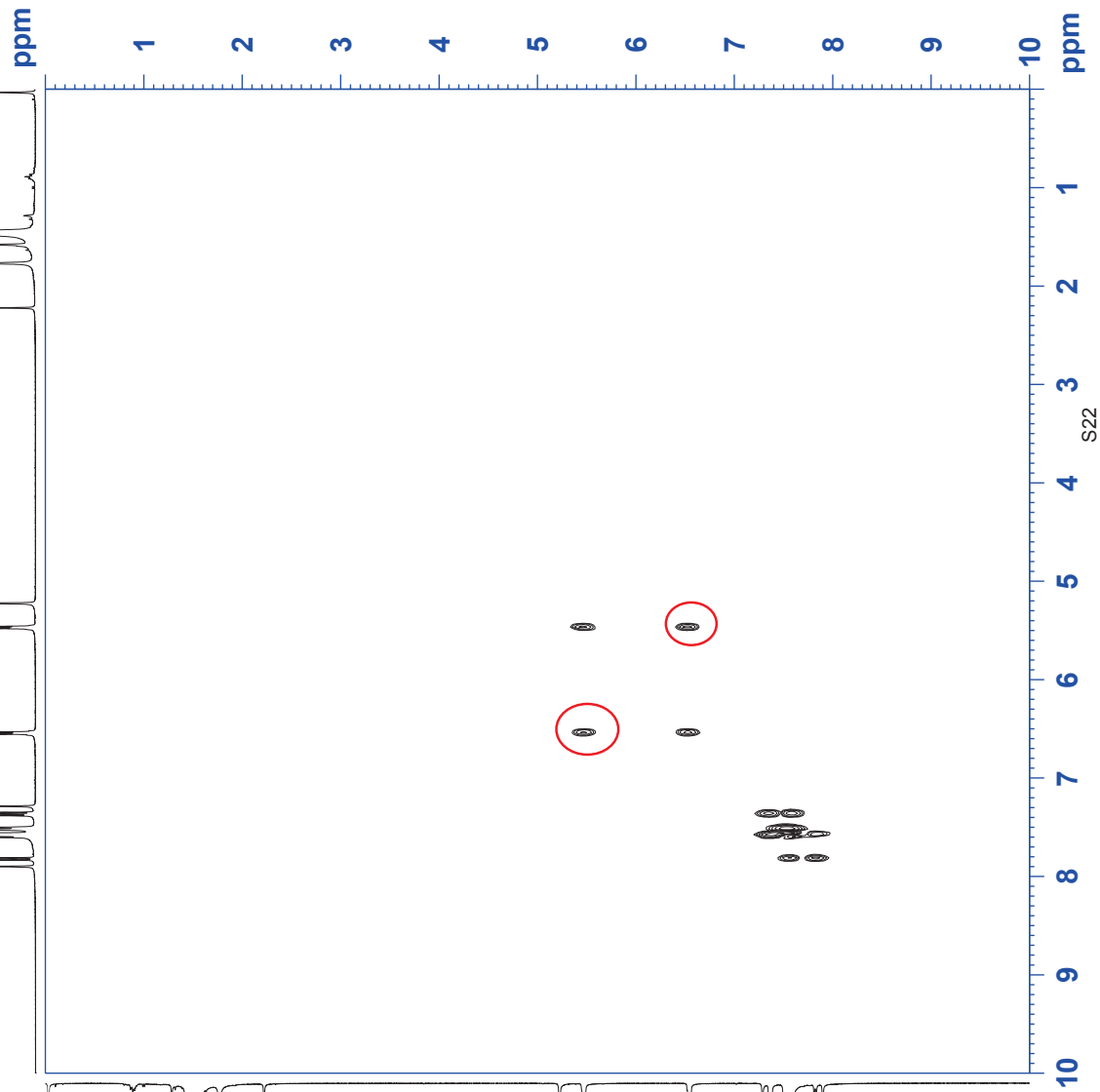
SI MC2
1024 QF

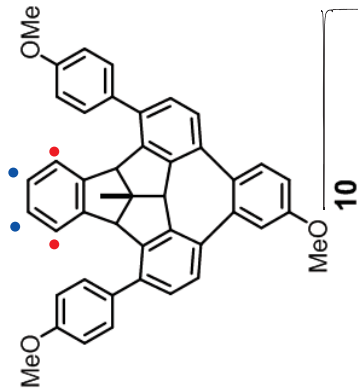
SF 400.2300000 MHz
WDW STNF

BSS

GB
00

HZ
00





Current Data Parameters
 NAME Eric_9a_4_OME_data
 EXPNO 222
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20160126
 Time_ 17.02
 INSTRUM Spect
 PROBHD 5 mm CPTCI 1H-
 PULPROG cosygmrfqf
 TD 2048
 SOLVENT CDCl3
 NS 4
 DS 16
 SWH 14097.744 Hz
 FIDRES 0.883664 Hz
 AQ 0.9726357 sec
 RG 203
 DW 35.467 usec
 DE 10.00 usec
 TE 298.0 K
 D0 0.00000300 sec
 D1 2.00000000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00007140 sec

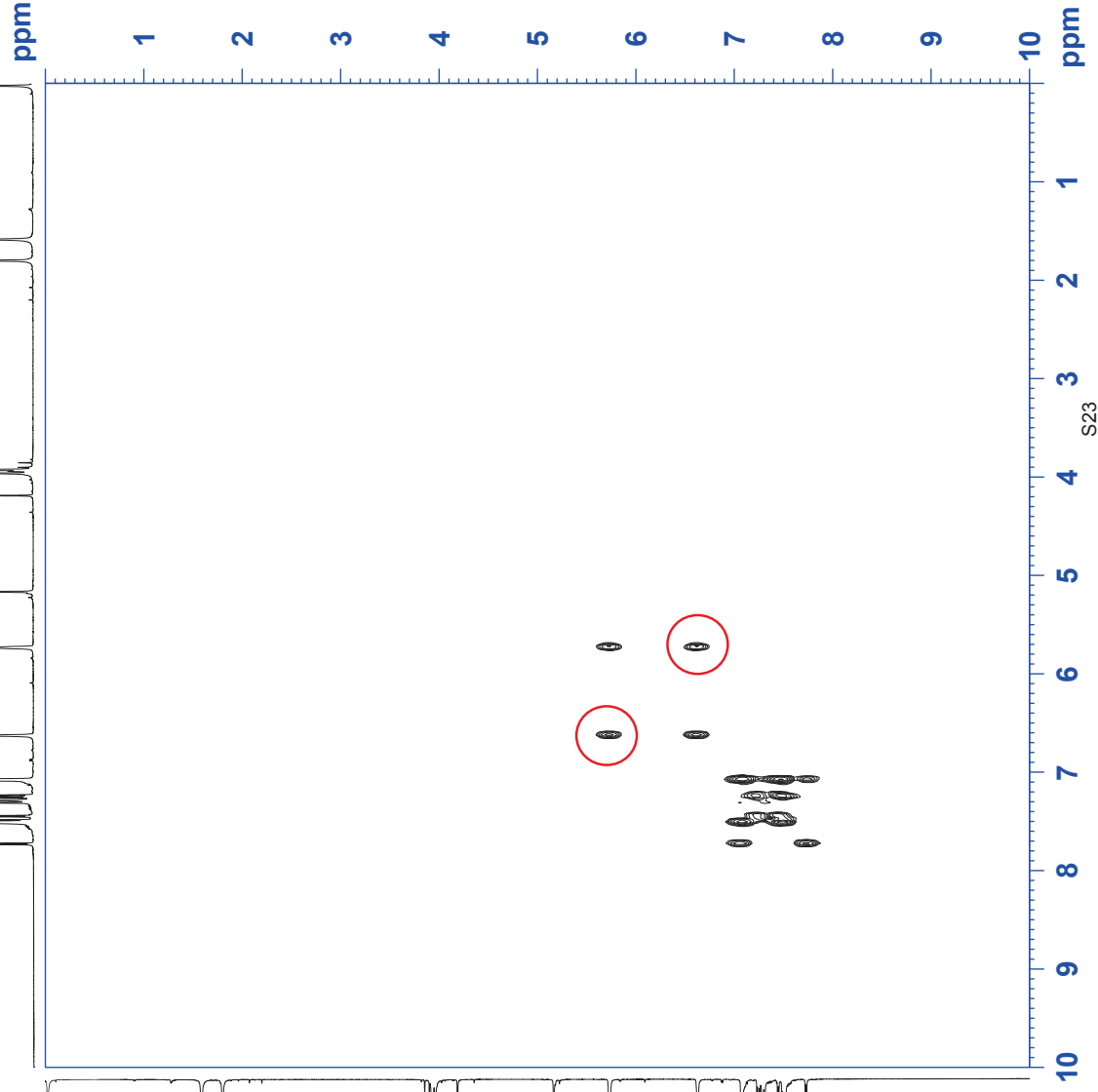
===== CHANNEL f1 =====
 SF01 700.1642010 MHz
 NUC1 1H
 P1 8.45 usec
 PLW1 7.00000000 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPZ1 16.00 %
 GPZ2 12.00 %
 GPZ3 40.00 %
 P16 1000.00 usec

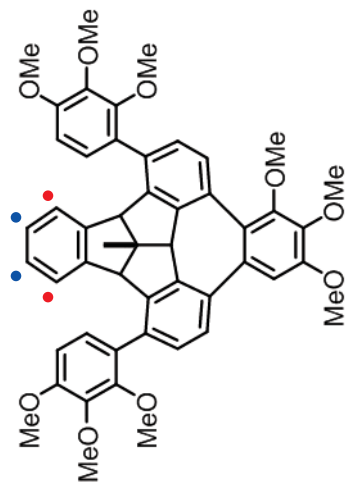
F1 - Acquisition parameters
 TD 128
 SF01 700.1642 MHz
 FIDRES 109.418770 Hz
 SW 20.003 ppm
 FnmODE QF

F2 - Processing parameters
 SI 1024
 SF 700.1600000 MHz
 WDW SINE
 SSB 0 Hz
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 700.1600000 MHz
 WDW SINE
 SSB 0 Hz
 LB 0 Hz
 GB 0



60 °C



Current Data Parameters
NAME Eric_9a_2_3_4_0Me_mono_data
EXPNO 333
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170126
Time_ 15:37

INSTRUM spect
PROBHD Z824601_0021 (cosygmrf)
PULPROG zgpg30
TD 2048
SOLVENT CDCl3
NS 4
DS 16

SWH 8012.820 Hz
FIDRES 3.912510 Hz
AQ 0.1277952 sec
RG 203

DW 62.400 usec
DE 6.50 usec
TE 333.2 K

D1 0.00000300 sec
D13 2.00000000 sec
D16 0.00000400 sec
in0 0.00020000 sec

STICNT 0
d0orig 0.00000300 sec
philoop 0
t1loop 0

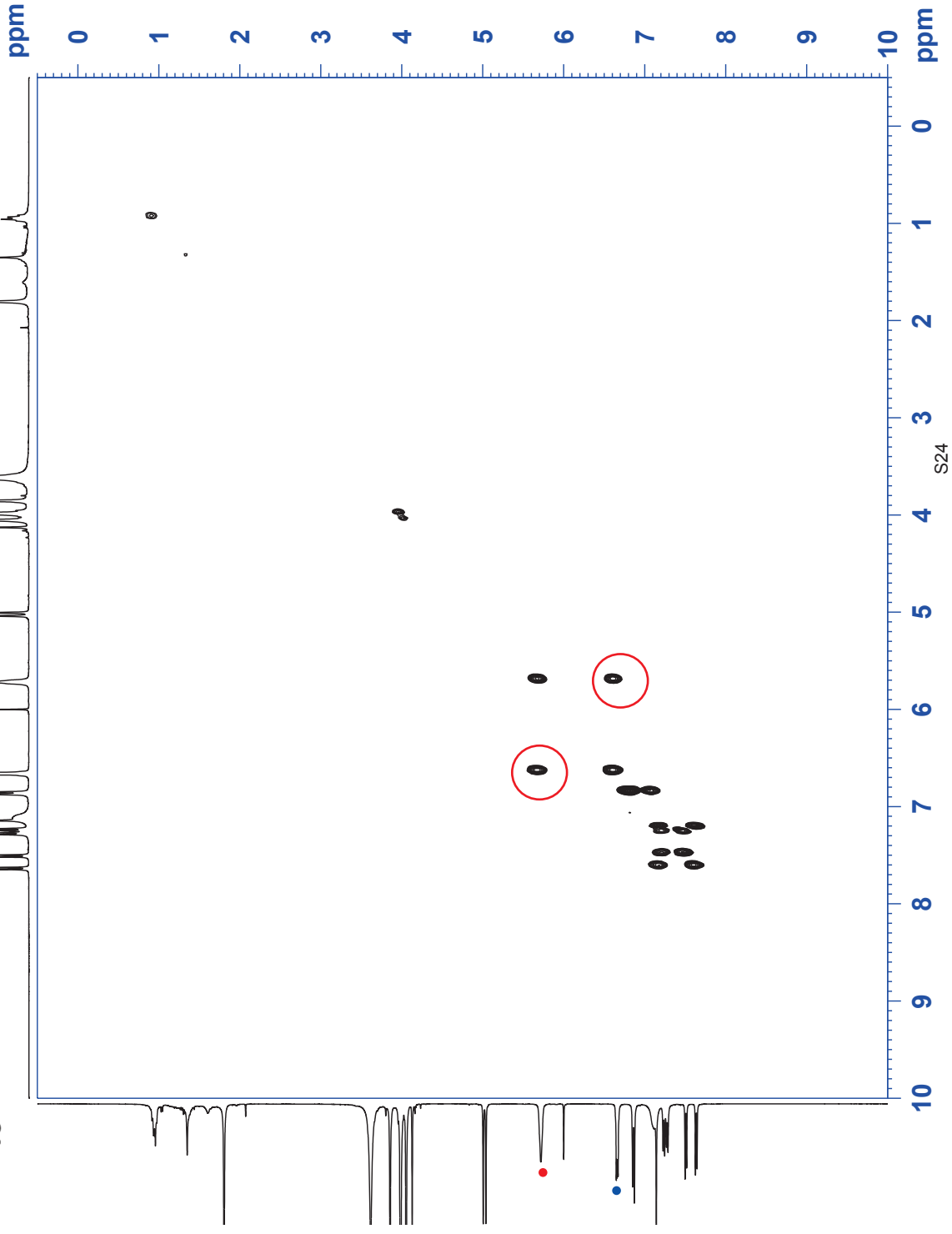
SF01 400.1324008 MHz
NUC1 1H
P1 15.00 usec

PLW1 8.31000042 W
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

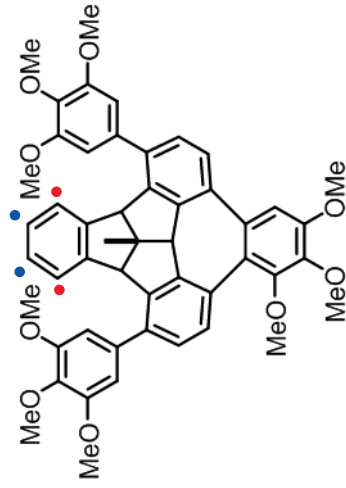
F1 - Acquisition parameters
TD 128
SF01 400.1324 MHz
FIDRES 62.500000 Hz
SW 19.993 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1305184 MHz
WDW SINE
SSB 0 Hz
LB 0
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 OF
SF 400.1305228 MHz
WDW SINE
SSB 0 Hz
LB 0
GB 0



16



Current Data Parameters
 NAME Eric_8a_3_4_5_0Me_mono_data
 EXPNO 222
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20170118
 Time_ 18.17
 INSTRUM spect
 PROBH1D Z824601_0021 (cosygmrf)
 PULPROG 2048
 TD CDC13
 SOLVENT 4
 NS 16
 DS 4
 SWH 8012.820 Hz
 FIDRES 3.912510 Hz
 AQ 0.1277952 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 295.1 K
 D1 0.00000300 sec
 d13 2.00000000 sec
 D0 0.00000400 sec
 D16 0.00020000 sec
 in0 0 sec

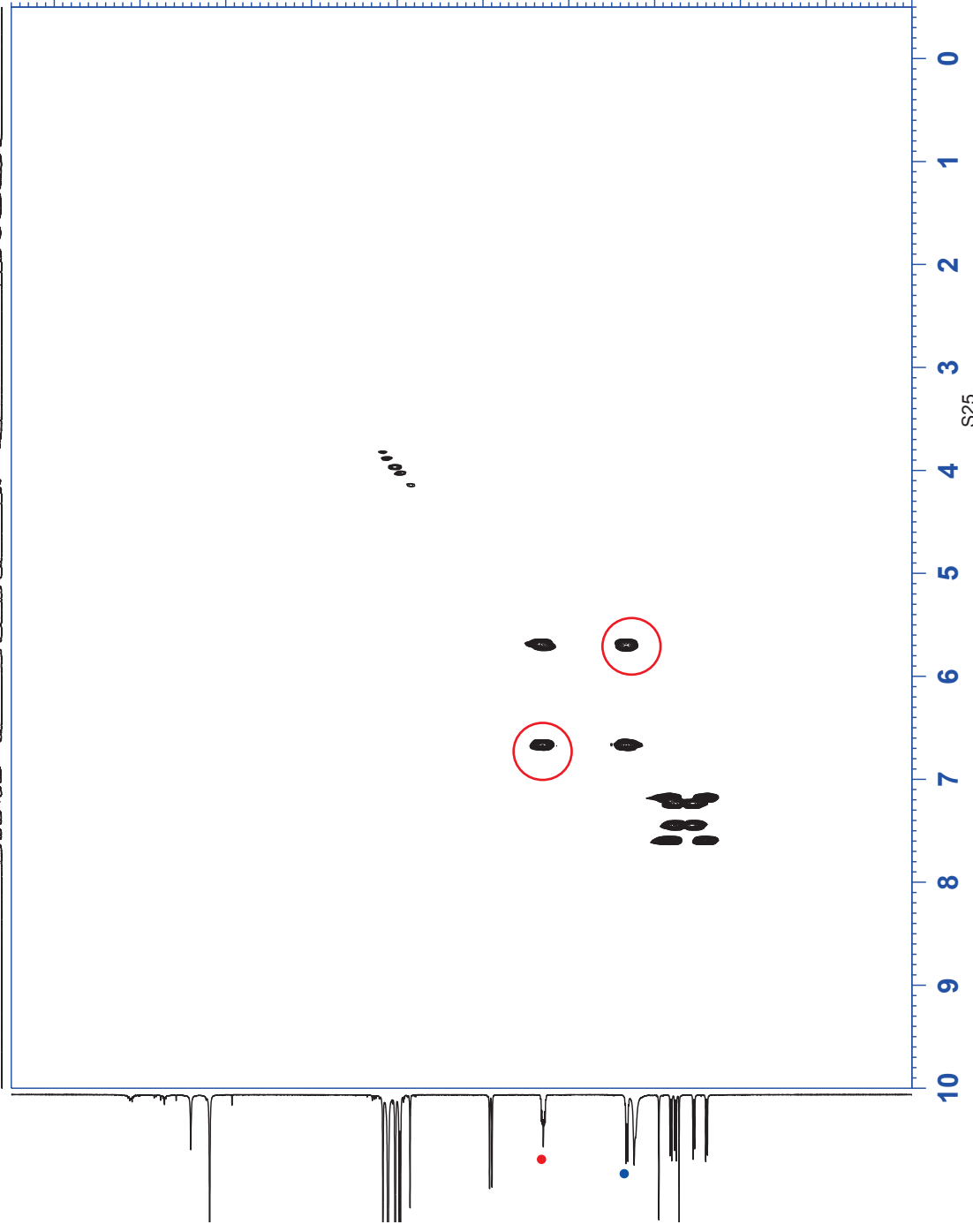
STICNT 0
 doorig 0.00000300 sec
 philoop 0
 tiloop 0
 SF01 400.1324008 MHz
 NUC1 1H
 PLW1 15.00 usec
 GPNAM[1] 8.31000042 W
 SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPZ1 16.00 %
 GPZ2 12.00 %
 GPZ3 40.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SF01 400.1324 MHz
 FIDRES 62.500000 Hz
 SW 19.993 ppm
 FnmODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300000 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

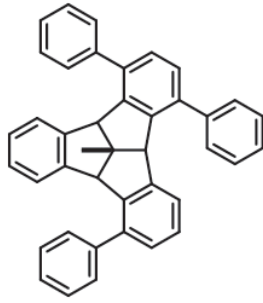
F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 400.1300000 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0

ppm



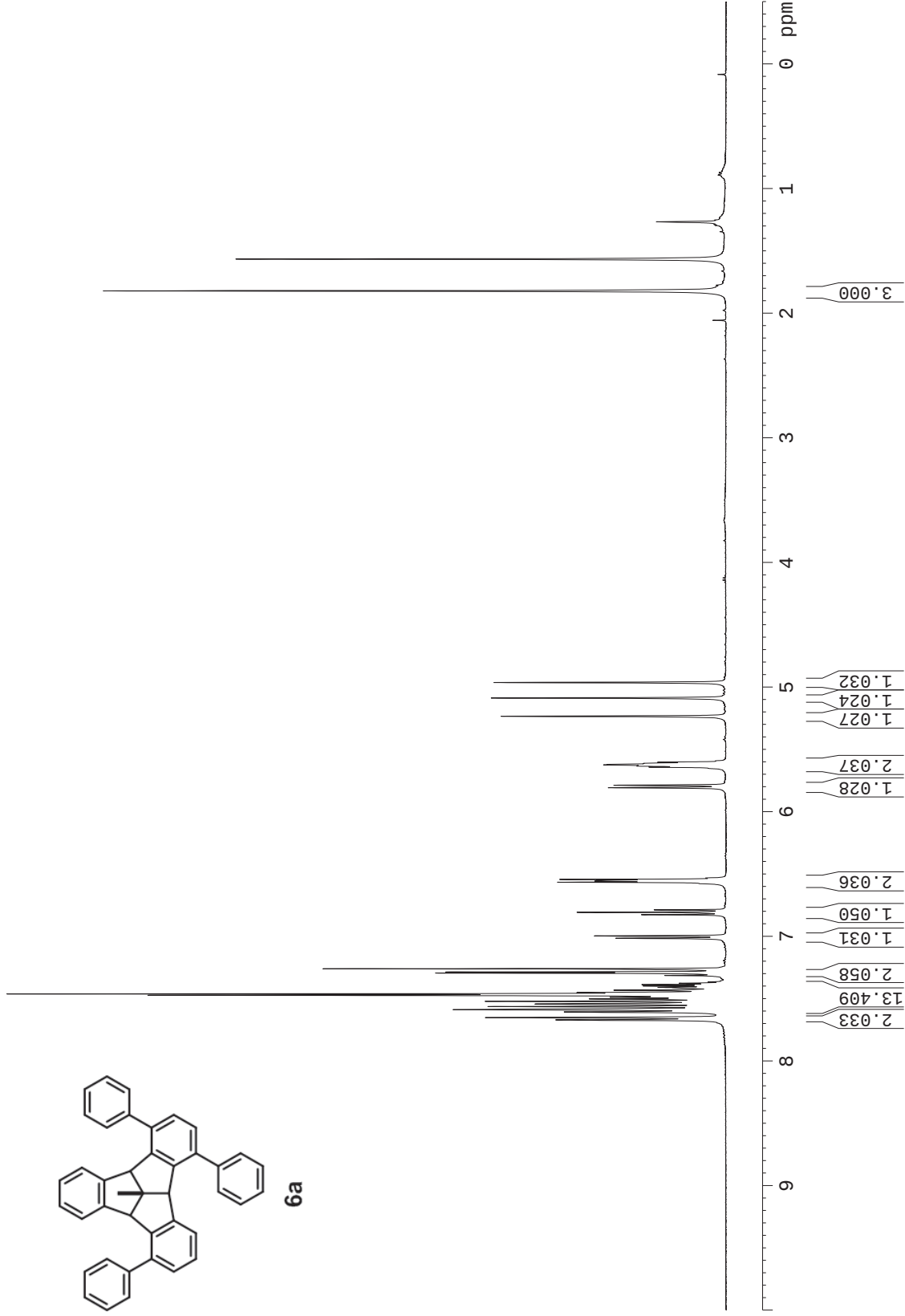
ppm

5. List of NMR and mass spectra



1.8212

1.5658





Current Data Parameters
NAME Eric_8a_un_data
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160112
Time_ 13.19 h
INSTRUM Spect
PROBHD Z824601_0021
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 162
DS 4

SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203

DW 20.800 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec

TD0 1
SF01 100.6228298 MHz
NUC1 13C

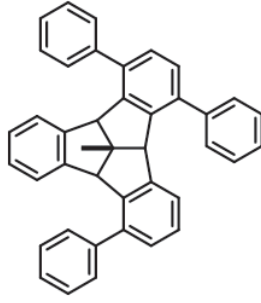
P1 9.50 usec
PLW1 41.25000000 W
SF02 400.1316005 MHz
NUC2 1H

CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLW12 0.23083000 W
PLW13 0.11611000 W

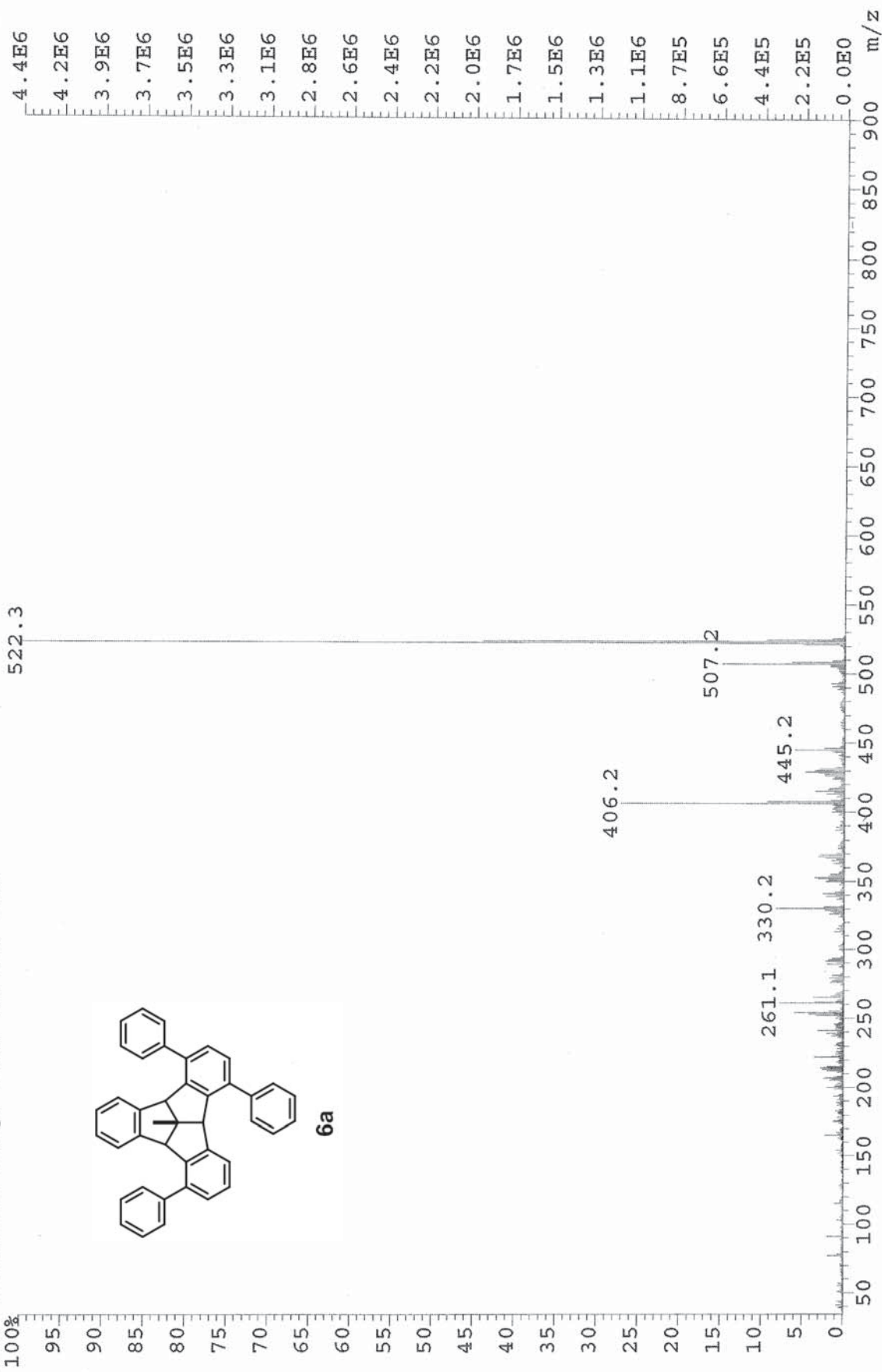
F2 - Processing parameters
SI 32768
SF 100.6127581 MHz
WDW EM
SSB 0

LB 1.00 Hz
GB 0
PC 1.40

145.985
145.904
144.700
144.132
143.447
143.337
142.850
142.759
142.681
139.144
138.842
138.817
130.133
130.101
129.393
129.219
129.128
128.981
127.620
127.498
127.429
127.267
126.849
126.833
125.258
124.996
124.884
77.477
77.160
76.842
62.596
62.411
61.783
59.647
28.978



File:EI2016_069 Ident:165_194 Win 500PPM Acq:15-FEB-2016 20:00:24 +18:34 Cal:EI_POS_CAL_900
AutoSpec EI+ Magnet BpM:522 BpI:4370330 TIC:25930646 Flags:HALL
File Text:Er. Wang, OCl, Er-07, HWP



Bruker 9.4T FTICR MS Analysis Report

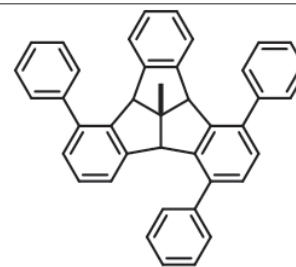
Faculty of Science, The Chinese University of Hong Kong

Analysis Info

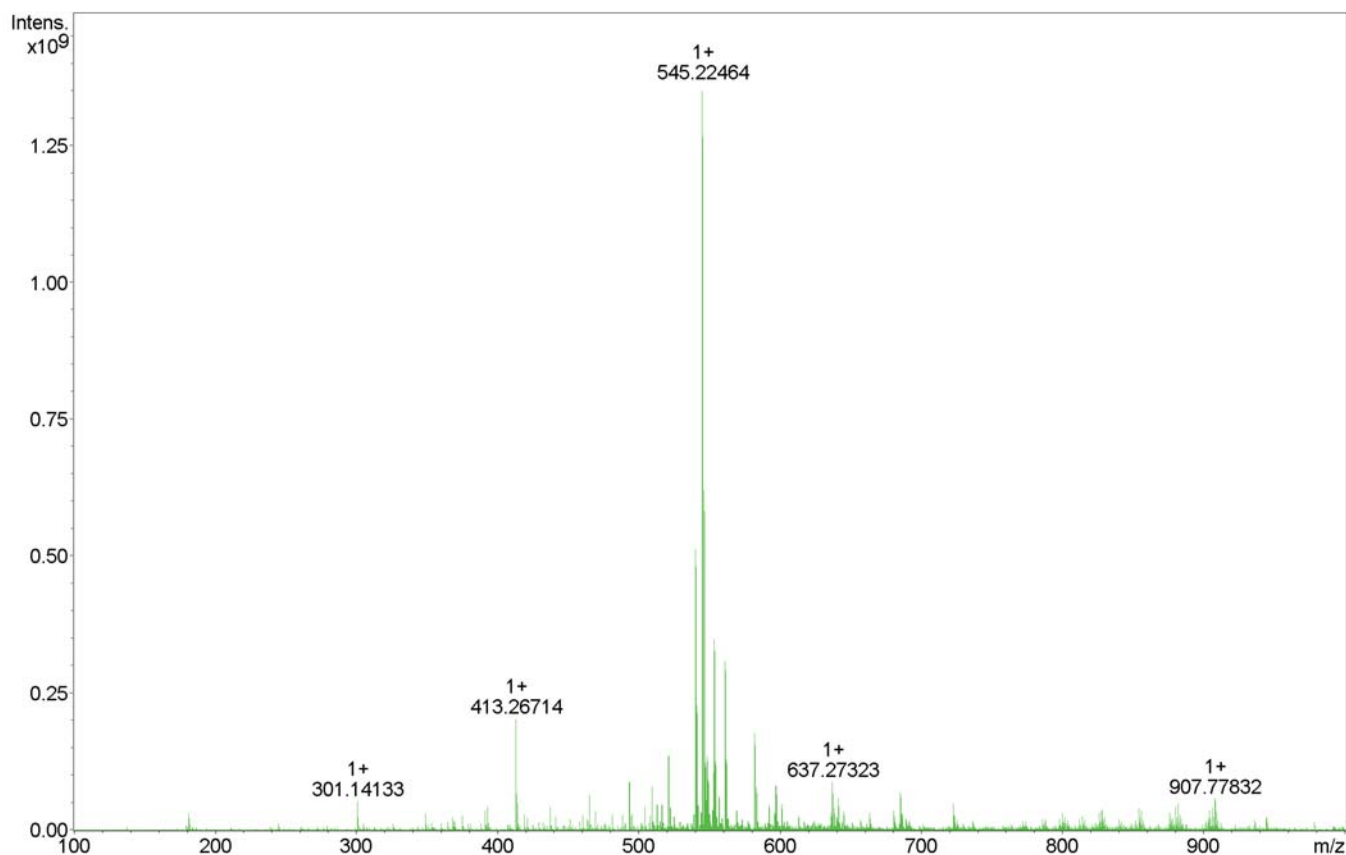
Sample Name :	Eric_8a_un	Reference No. :	xhfc042
Applicant Name :	Ip Ho Wang	Analysis Date :	4/2/2016 11:18:37
Analysis Path :	xhfc042_000001.d		
Instrument :	solarix	Polarity	Positive
Method	4_17_mass_range_pos_7T	Acquired Scans	11
Comment :	4.4kV, 120ml/hr, 1.0 nebulizer gas		

Accurate Mass Measurement

Molecular formula :	C ₄₁ H ₃₀
Abundant Isotopic (theoretical) [M+Na] ⁺ :	545.223972
Monoisotopic (theoretical) [M+Na] ⁺ :	545.223972
(experimental) [M+Na] ⁺ :	545.22464
error (ppm) :	1.2



6a



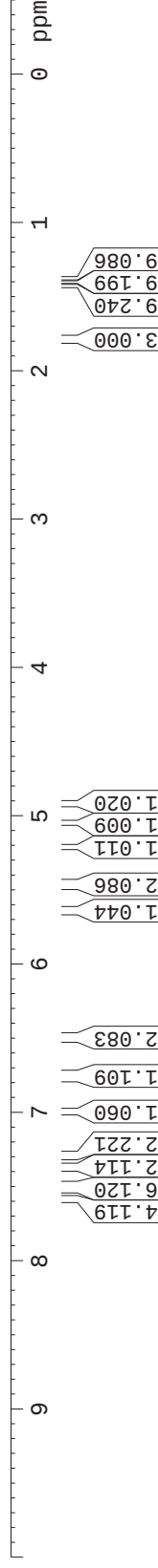
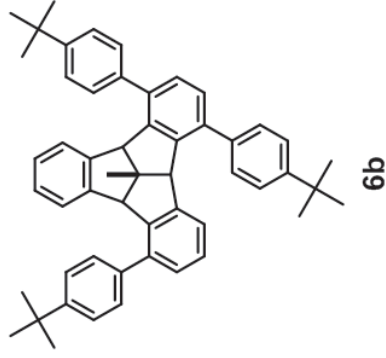
AV400Q NMR

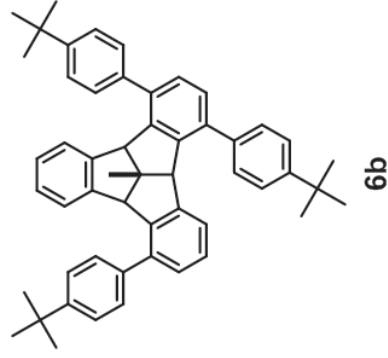


Current Data Parameters
NAME Eric_Ba_4_t_butyl_data
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111111
Time 11:33 h
INSTRUM spect
PROBHD zgpg30
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2
DS 2
SWH 8612.850 Hz
FIDRES 0.244532 Hz
AQ 2.0447523 sec
RG 203
DW 62.400 usec
DE 19.59 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO 400.1324705 MHz
NUC1 1H
P1 15.00 usec
PLW1 8.31000042 W
F2 - Processing parameters
SI 65536
SF 400.1324705 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1.7857
1.5531
1.4267
1.4011
1.3756

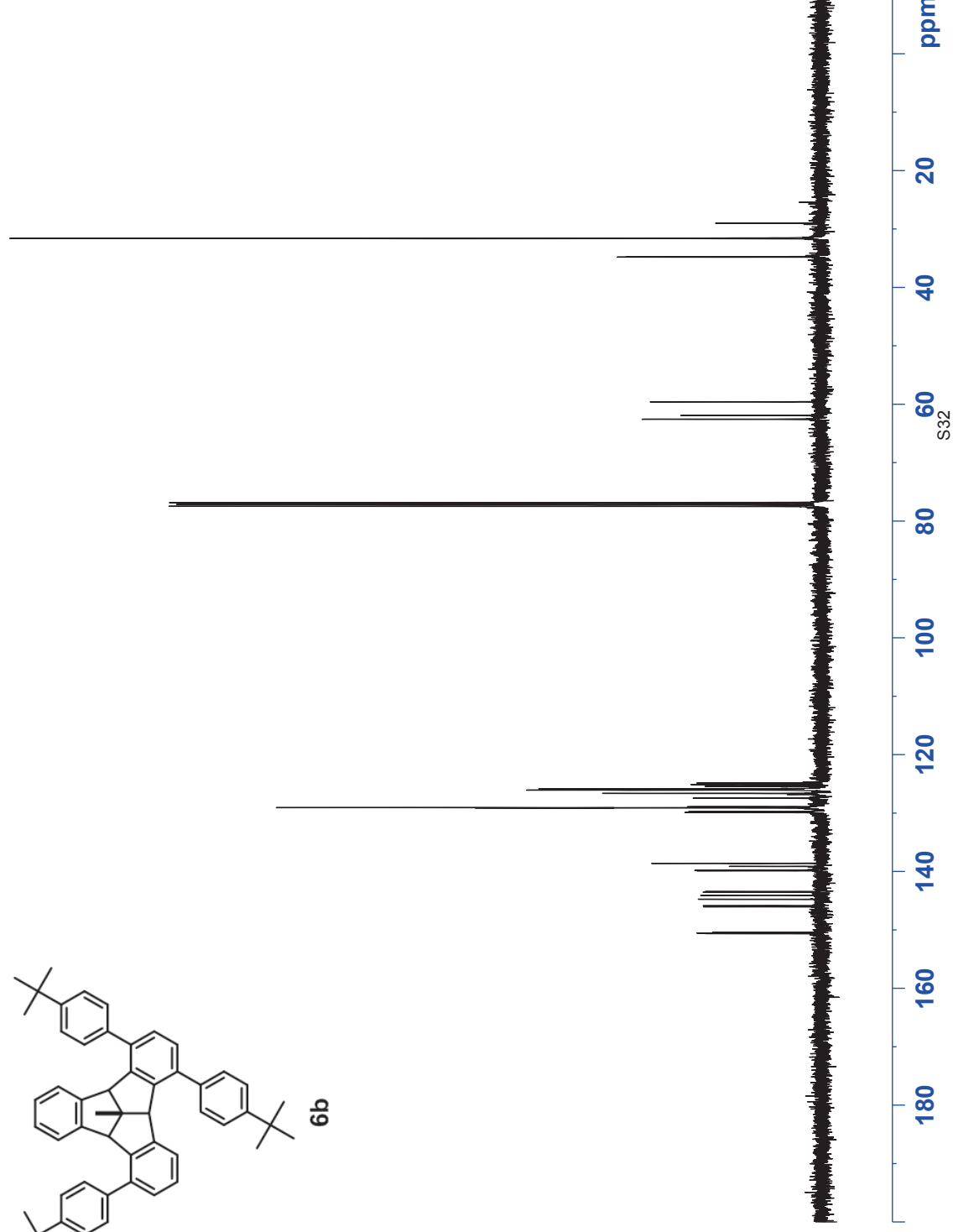
7.5760
7.5470
7.5261
7.5104
7.4933
7.4728
7.3798
7.3591
7.3081
7.2888
7.2721
7.2600
7.0029
6.9845
6.7735
6.7543
6.7351
6.5148
6.5059
6.4976
6.4913
6.4832
6.4734
5.6494
5.6297
5.4717
5.4647
5.4576
5.2102
5.0463
4.9192



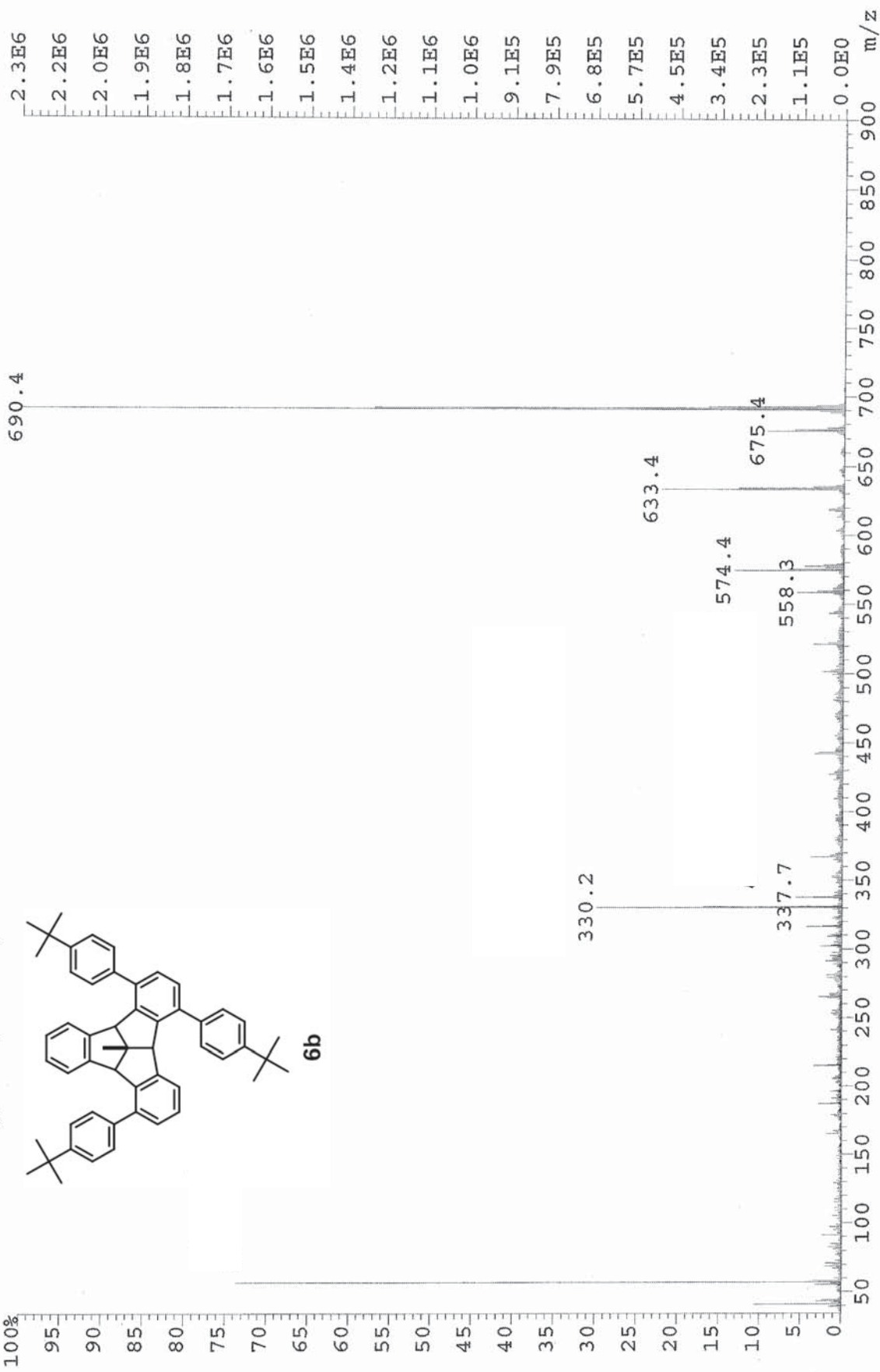


150.636
150.550
150.399
146.041
145.864
144.754
144.068
143.565
143.433
139.876
139.810
139.760
139.127
138.603
129.887
129.756
129.114
129.068
128.906
127.444
126.629
126.065
125.959
125.824
125.435
125.119
124.864
77.477
77.160
76.842
62.580
62.569
61.932
59.586
34.822
34.786
34.736
31.636
31.612
31.594
29.023

Current Data Parameters
NAME Eric_Ba_4_t_butyl_data
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111211
Time 11:16:11
INSTRUM spect
PROBHD ZB24601.0021
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 105
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
TE 293.2 K
DE 0.59 usec
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SF01 100.6228298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SF02 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLWI2 0.23083000 W
PLWI3 0.11611000 W
F2 - Processing parameters
SI 32768
SF 100.6127624 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



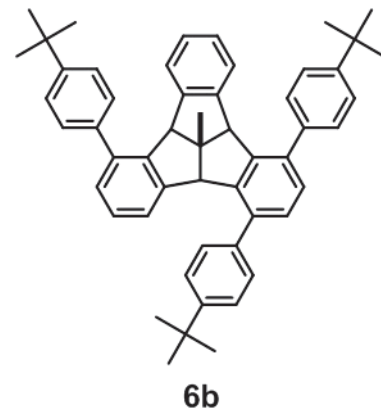
File:EI2016_071 Ident:141_214 Win 500PPM Acq:15-FEB-2016 21:07:16 +18:22 Cal:EI_POS_CAL_900
AutoSpec EI+ Magnet BpM:690 BpI:2265448 TIC:18898798 Flags:HALL
File Text:Er. Wang, OCl, Er-09, HWP



9.4T FTICR MS Analysis Report

Faculty of Science, The Chinese University of Hong Kong

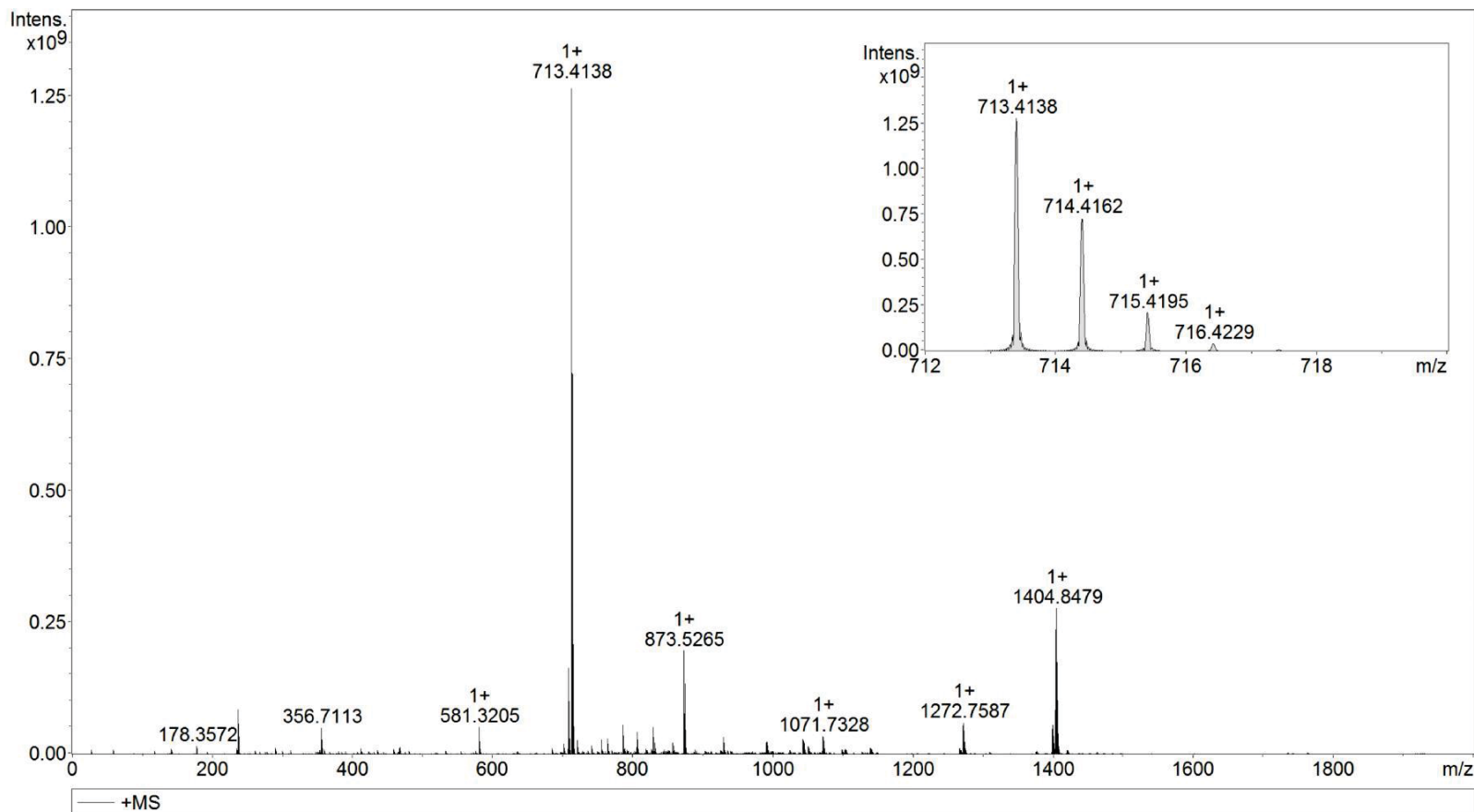
Sample No.	Eric02
Reference No.	CHF0024
Applicant name	Ip Ho Wang
Analysis Path	\\192.168.0.1\Data\Service\MSonly\20160509\Eric02_000004.d
Instrument	solariX
Polarity	Positive
Acquired Scans	4
Operator	Winnie
Analysis Date	5/9/2016 3:25:05 PM



Molecular Formula: C₅₃H₅₄

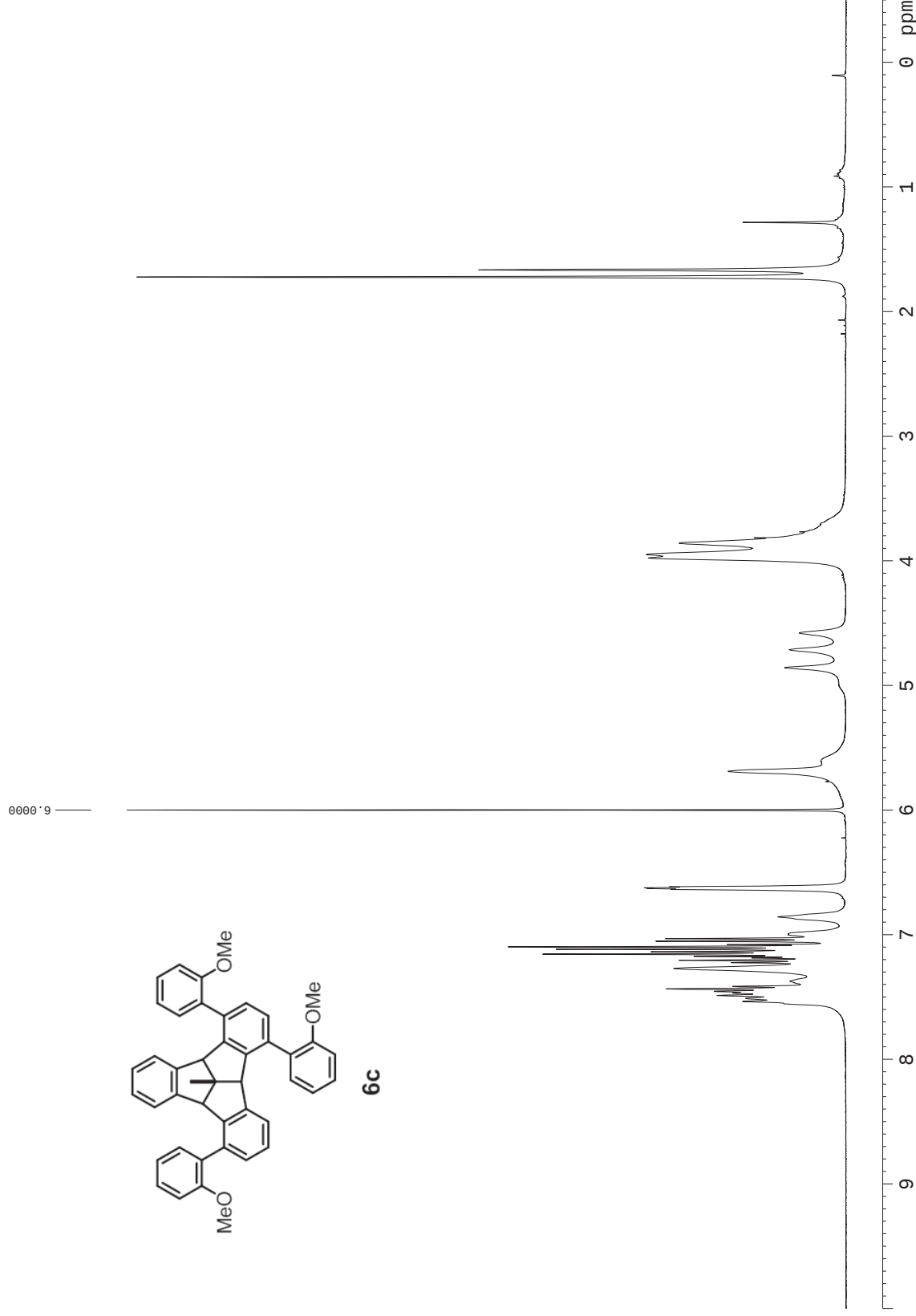
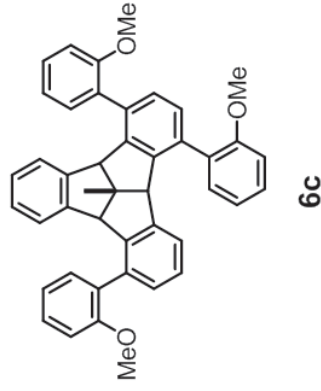
Abundant Isotopic (theoretical)[M+Na]⁺: 713.4118

Monoisotopic (theoretical)[M+Na]⁺: 713.4118(experimental)[M+Na]⁺: 713.4138 error(ppm): 2.80



22 °C

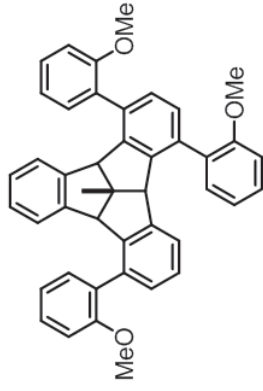
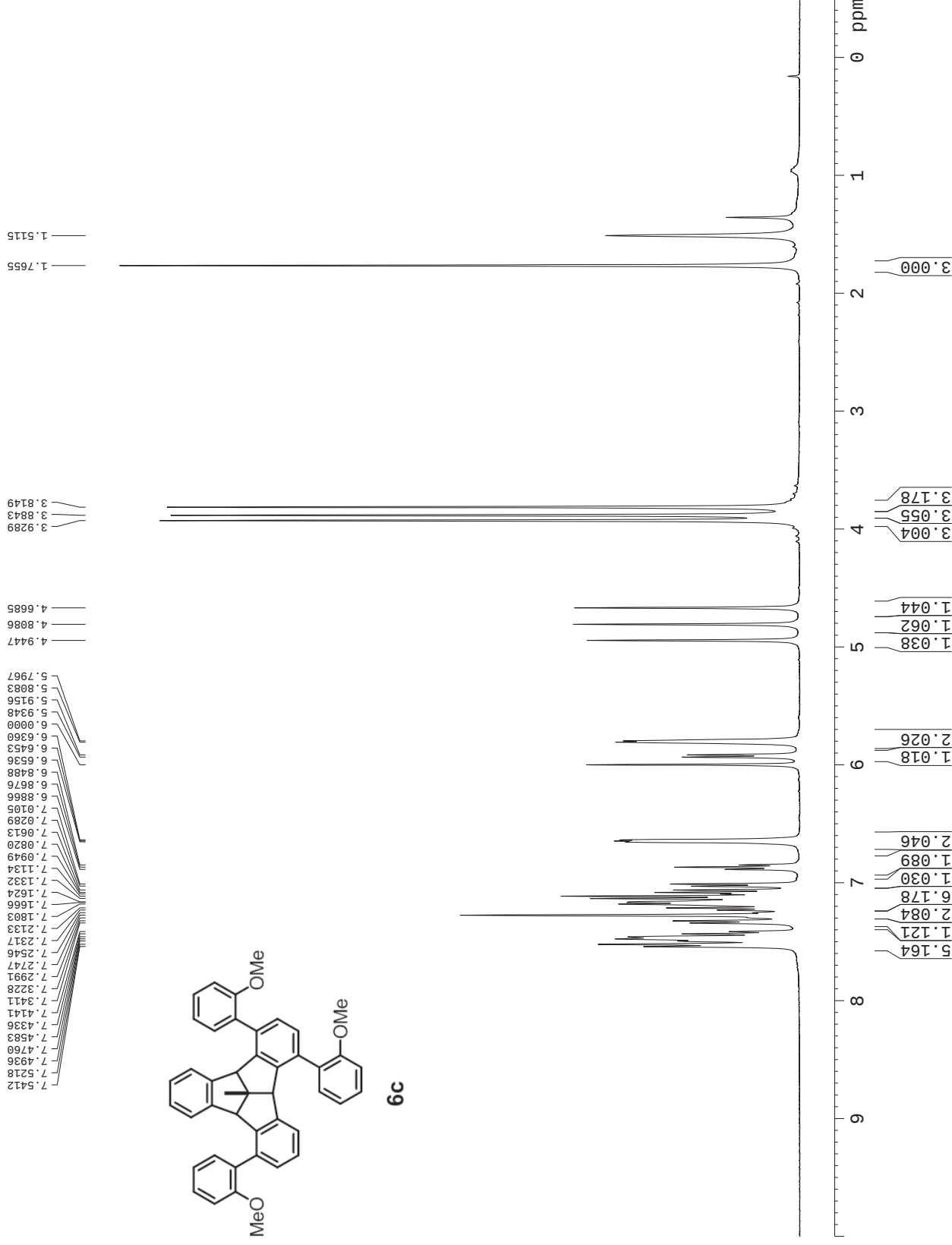
AV400Q NMR



Current Data Parameters
 NAME Eric_8a_2_Ome_rbd
 EXPNO 3
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20160418
 Time 9.07 h
 INSTRUM spect
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl₃
 NS 17
 DS 4
 SWH 8012.826 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 181
 DW 62.160 usec
 DE 6.160 usec
 TE 294.9 K
 D1 1.00000000 sec
 TDO 1
 SFO 400.1324701 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 8.31000042 W
 F2 - Processing parameters
 SI 65536
 SF 400.1305146 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

60 °C

AV400Q NMR

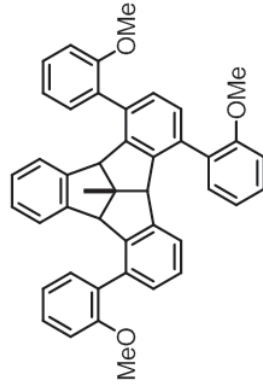
**6c**

Current Data Parameters
NAME Eric_8a_2_0Me_rh
EXPNO 1
PROCNO 1

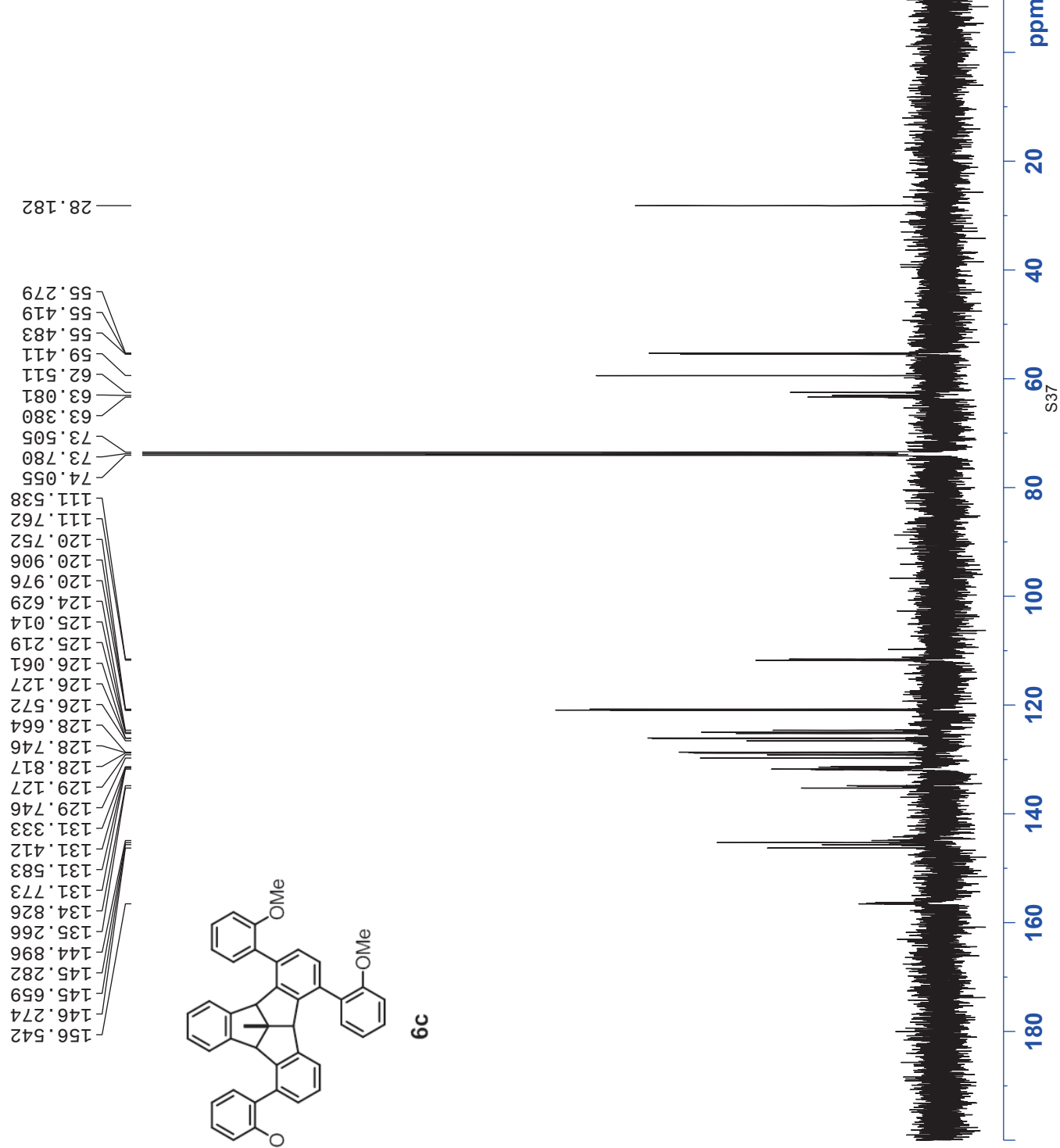
F2 - Acquisition Parameters
Date_ 20160415
Time 16.10 h
INSTRUM spect
PROBHD 5mm
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 21
DS 4
SWH 8012.826 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 203
RW 62.69 usec
DE 6.69 usec
TE 334.5 K
D1 1.00000000 sec
D0 1
SFO 400.132470 MHz
NUC1 1H
P1 15.00 usec
PLW1 8.31000042 W

F2 - Processing parameters
SI 65536
SF 400.1305124 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

60 °C



6c



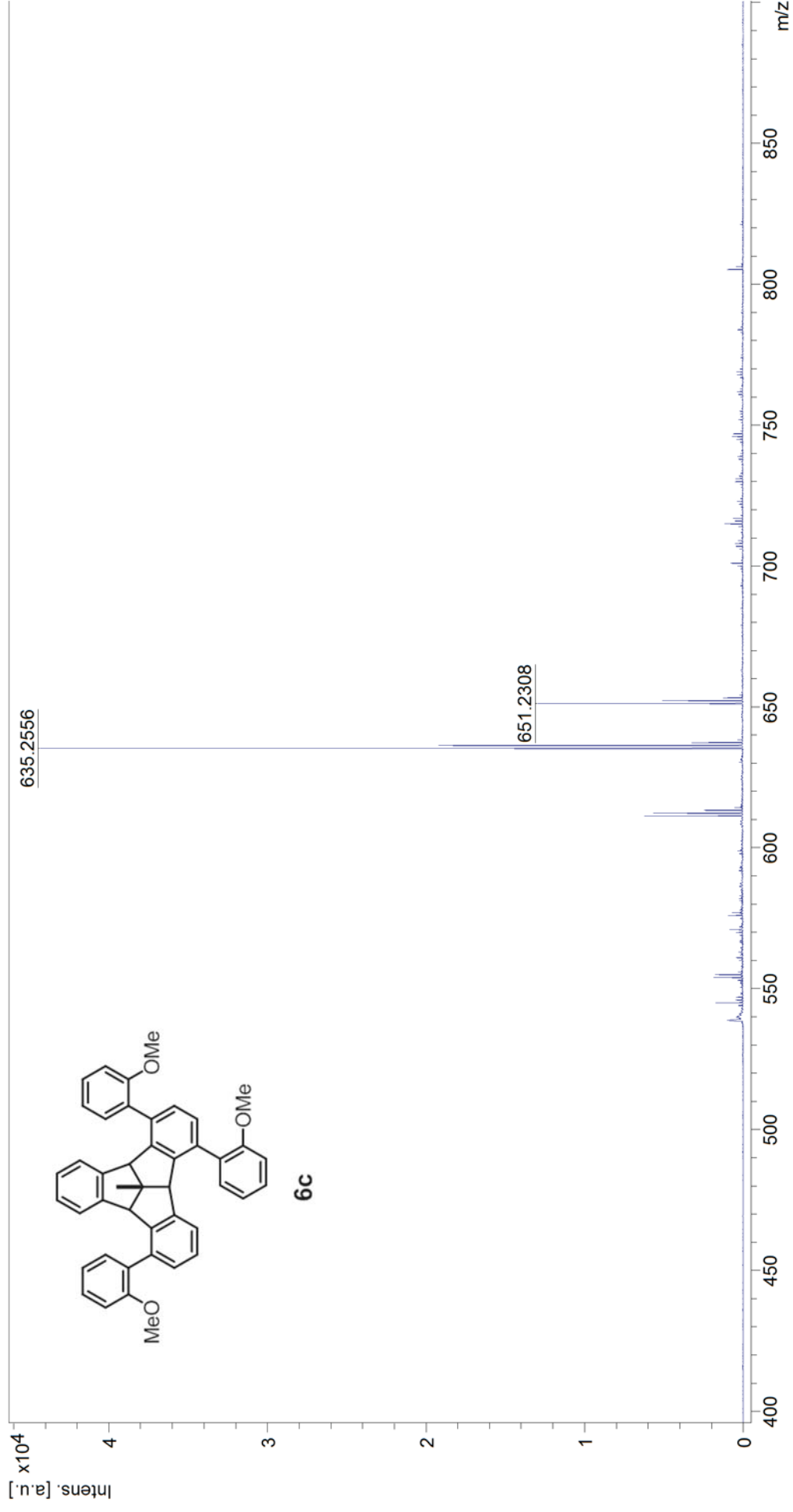
Current Data Parameters
NAME Eric_8a_2_Ome_rb
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160415
Time 16.15 h
INSTRUM Spect
PROBHD Z824601_0021
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
DS 551
NS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
TE 333.6 K
DE 6.50 usec
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SF01 100.6228298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SF02 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLW12 0.23083000 W
PLW13 0.11611000 W

F2 - Processing parameters
SI 32768
SF 100.6129235 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Comment 1

Comment 2



AV400Q NMR

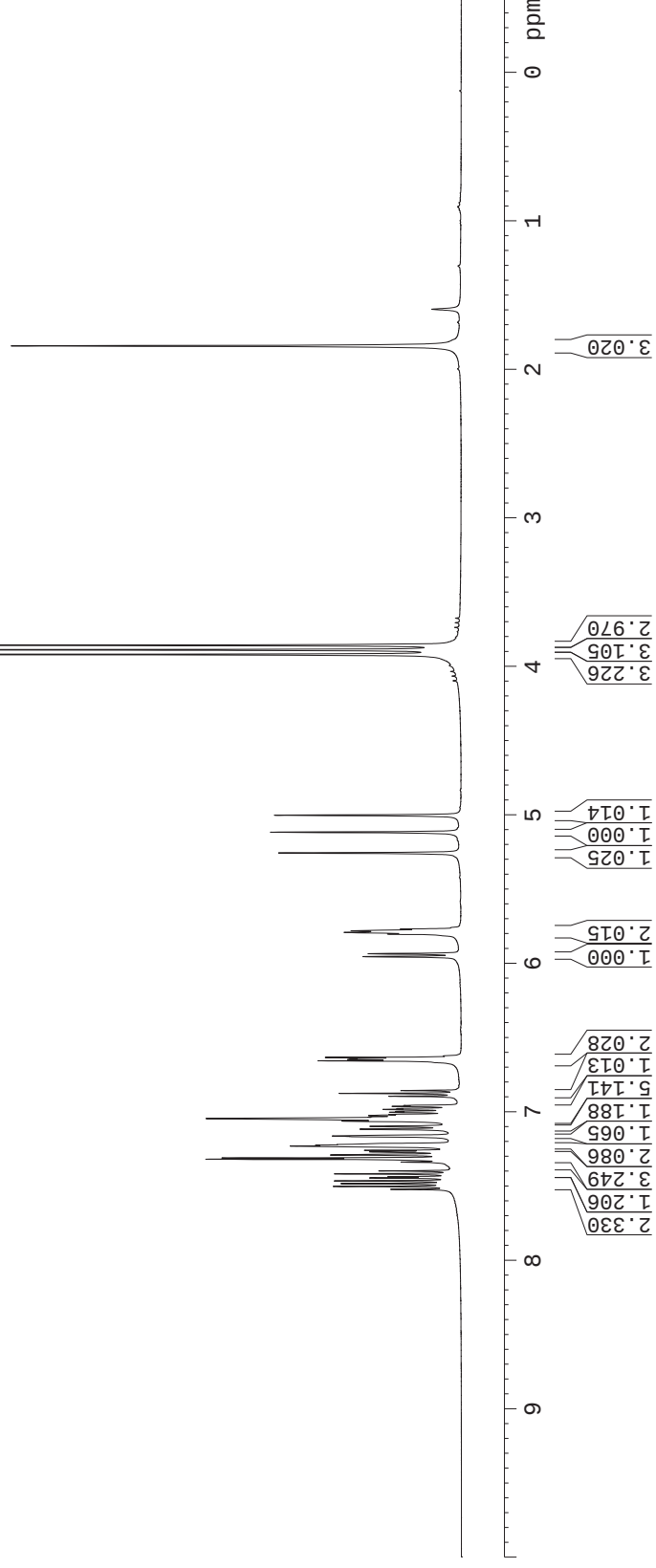
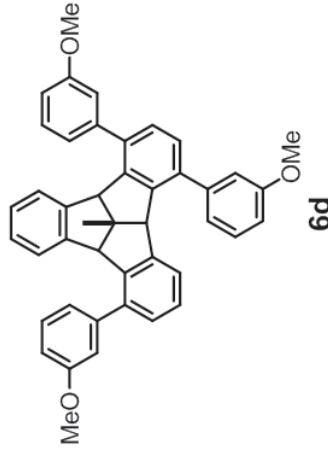


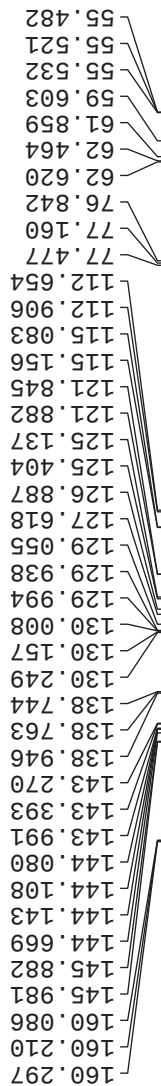
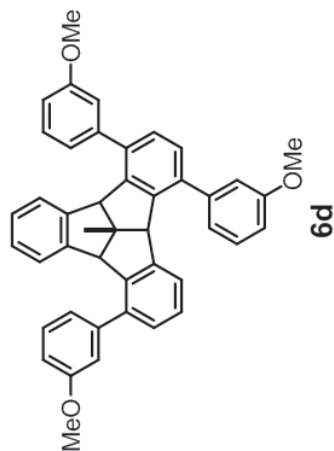
Current Data Parameters
NAME Eric_8a_3_Ome_data
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151216
Time 16.20 h
INSTRUM spect
PROBHD zgpg30
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 39
DS 2
SWH 8012.826 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 32
RW 62.432 usec
DE 6.160 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
SFO 400.222471 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2260004 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1.5953
1.8419

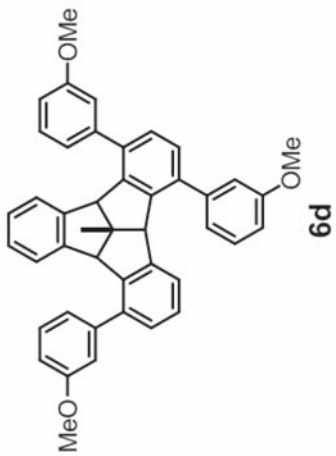
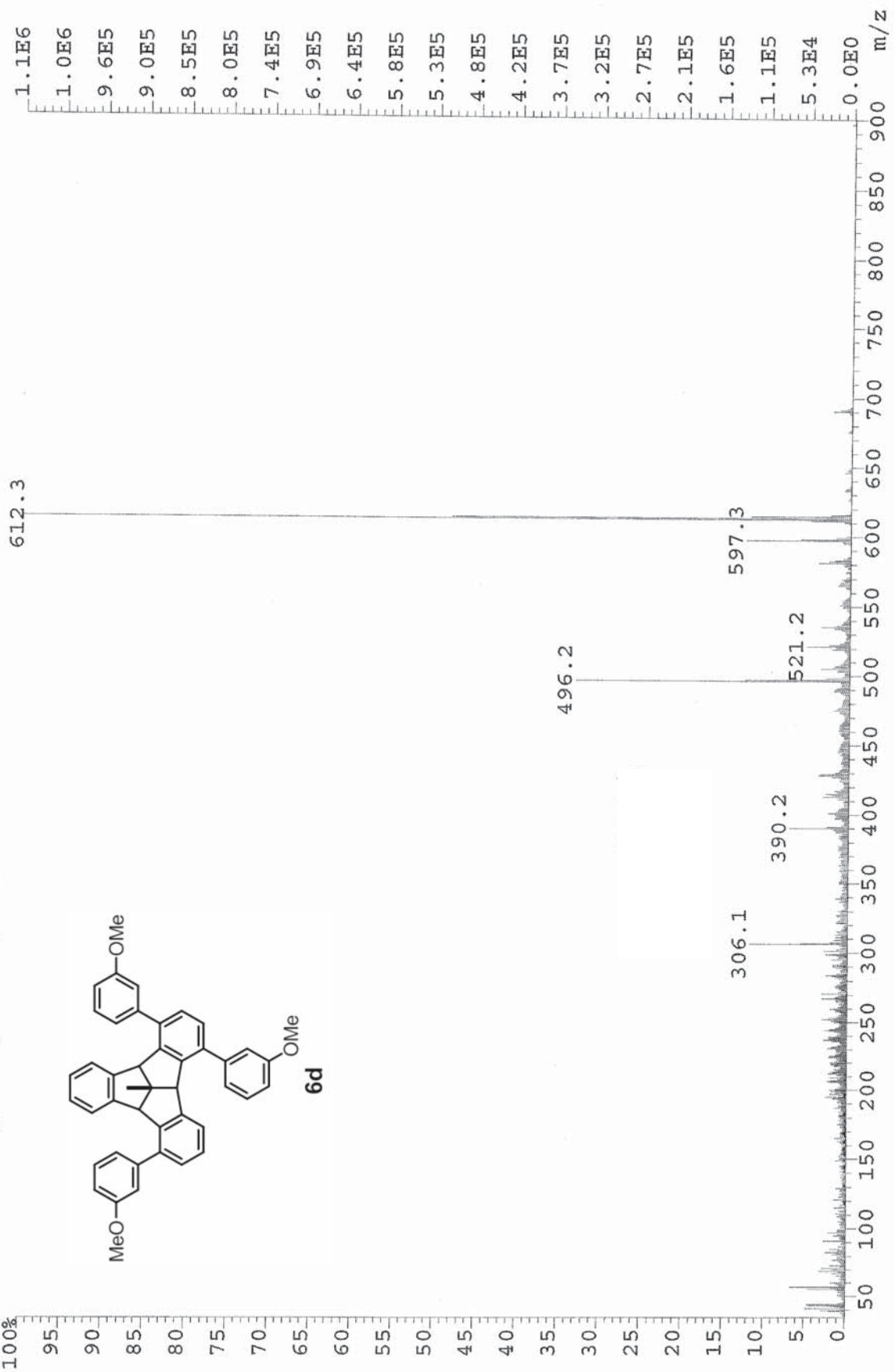
3.226
3.105
2.970
3.8578
3.9202

7.5225
7.5029
7.4841
7.4657
7.4457
7.4381
7.4184
7.3985
7.3390
7.3196
7.3114
7.2913
7.2702
7.2600
7.2314
7.2262
7.2212
7.1636
7.1173
7.0983
7.0632
7.0458
7.0361
7.0254
7.0184
7.0036
6.9977
6.9844
6.9787
6.9640
6.9582
6.8958
6.8765
6.8574
6.6980
6.6570
6.6402
6.6434
6.6345
6.6251
6.9553
6.9358
6.8145
6.8031
6.8021
6.7923
6.7812
6.7703
6.7598
6.7572
6.1175
5.0031



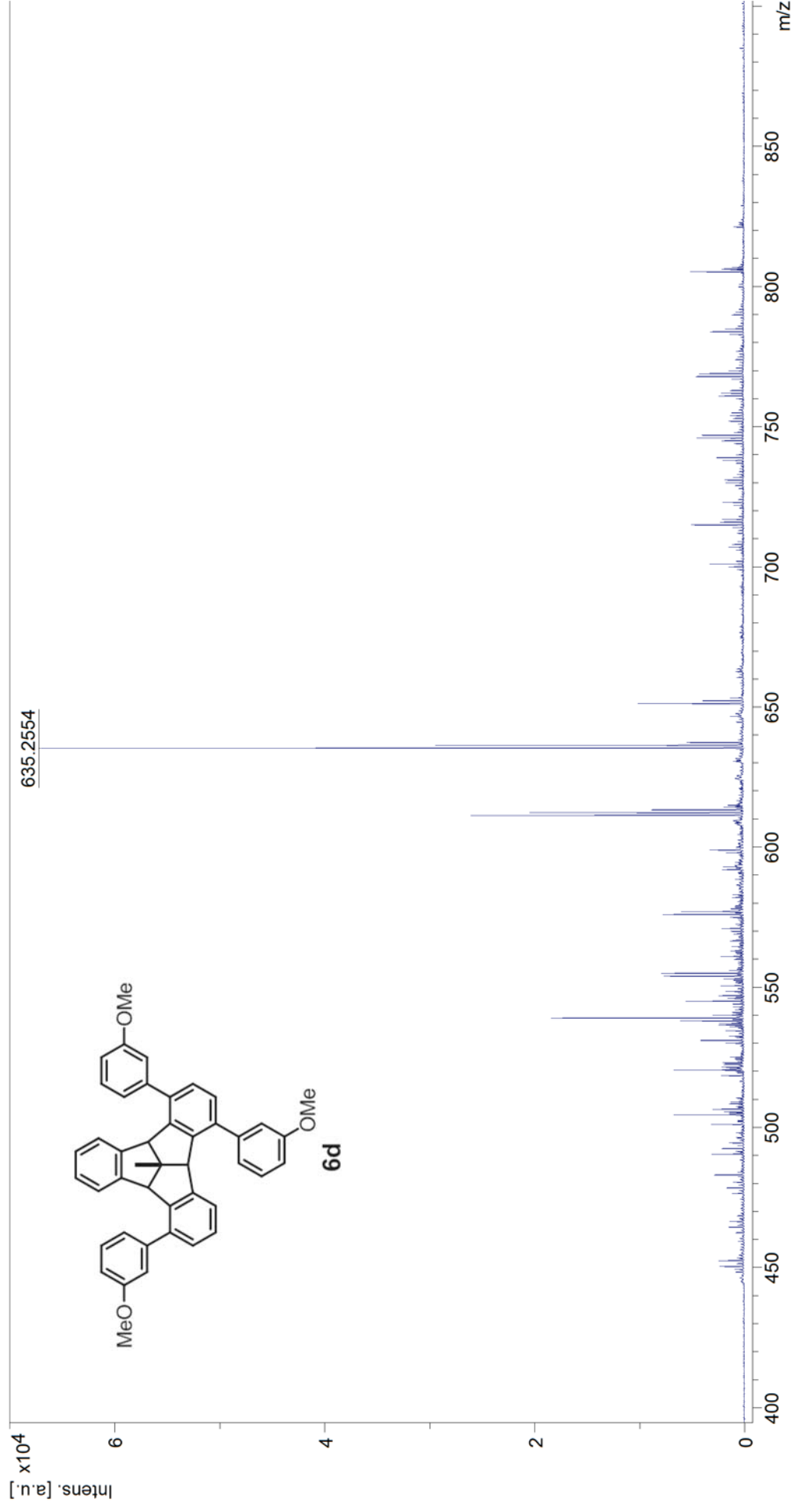


File:EI2016_072 Ident:118_129 Win 500PPM Acq:15-FEB-2016 21:55:50 +12:48 Cal:EI_POS_CAL_900
AutoSpec EI+ Magnet BpM:612 BpI:1061781 TIC:10480833 Flags:HALL
File Text:Er. Wang, OCl, Er-11, HWP



Comment 1

Comment 2



AV400Q NMR



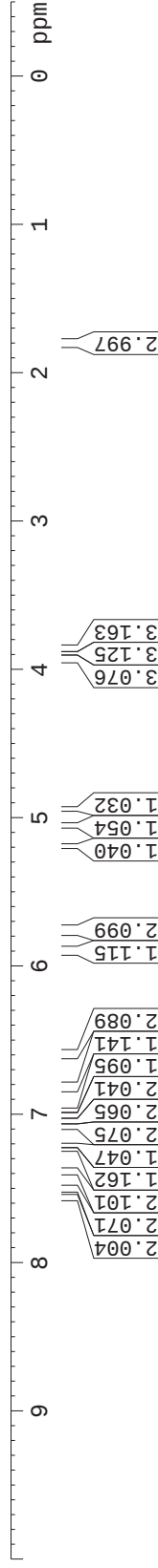
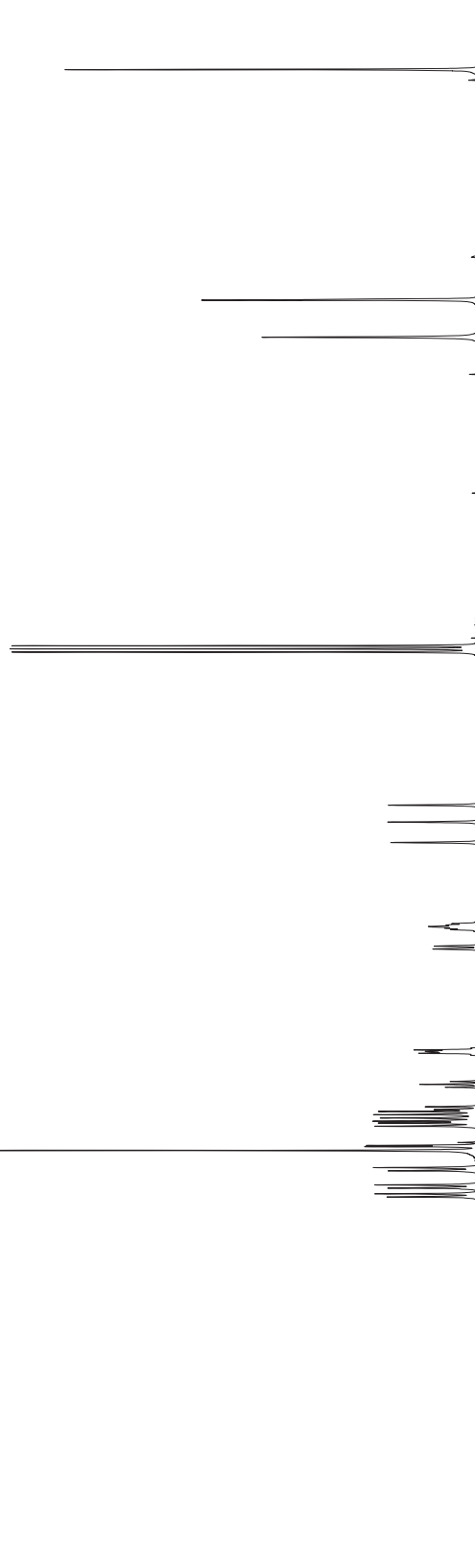
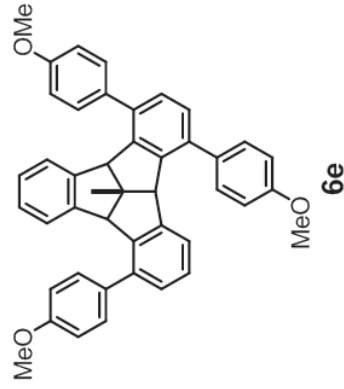
Current Data Parameters
NAME Eric_8a_4_Ome_data
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160115
Time 11.53 h
INSTRUM spect
PROBHD ZL08618_0250
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 26
DS 2
SWH 8012.826 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 161
RW 62.161 usec
DE 6.160 usec
TE 295.8 K
D1 1.00000000 sec
D0 1.00000000 sec
SFO 400.232471 MHz
NUC1 1H
P1 12.00 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2306120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

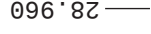
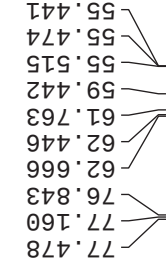
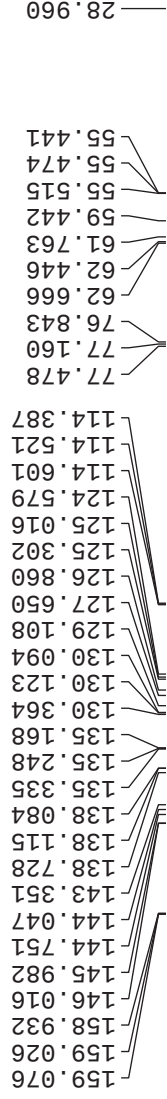
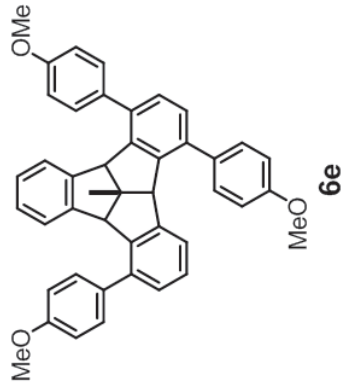
-0.0000

1.7964
1.5476

3.9101
3.8886
3.8682

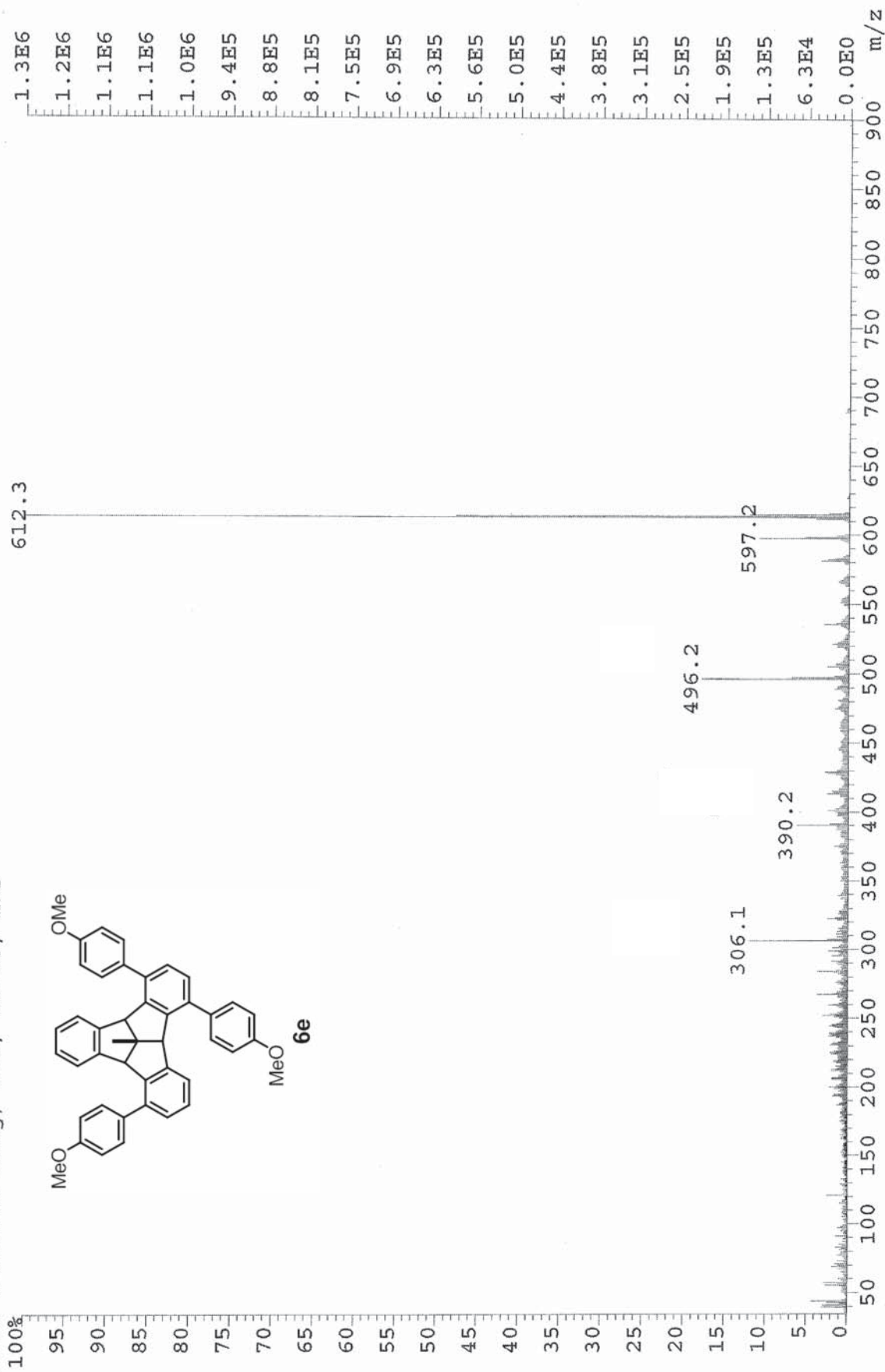
4.9384
5.0519
5.1893
5.7230
5.7340
5.7447
5.7531
5.7639
5.7739
5.7848
5.8849
5.9044
5.9684
6.5807
6.5872
6.5911
6.5974
6.6032
6.6155
6.7929
6.8120
6.8312
6.9628
6.9816
6.9938
7.0155
7.0376
7.0593
7.0716
7.0933
7.2027
7.2220
7.2302
7.2562
7.3708
7.3925
7.4871
7.5087
7.5467
7.5683





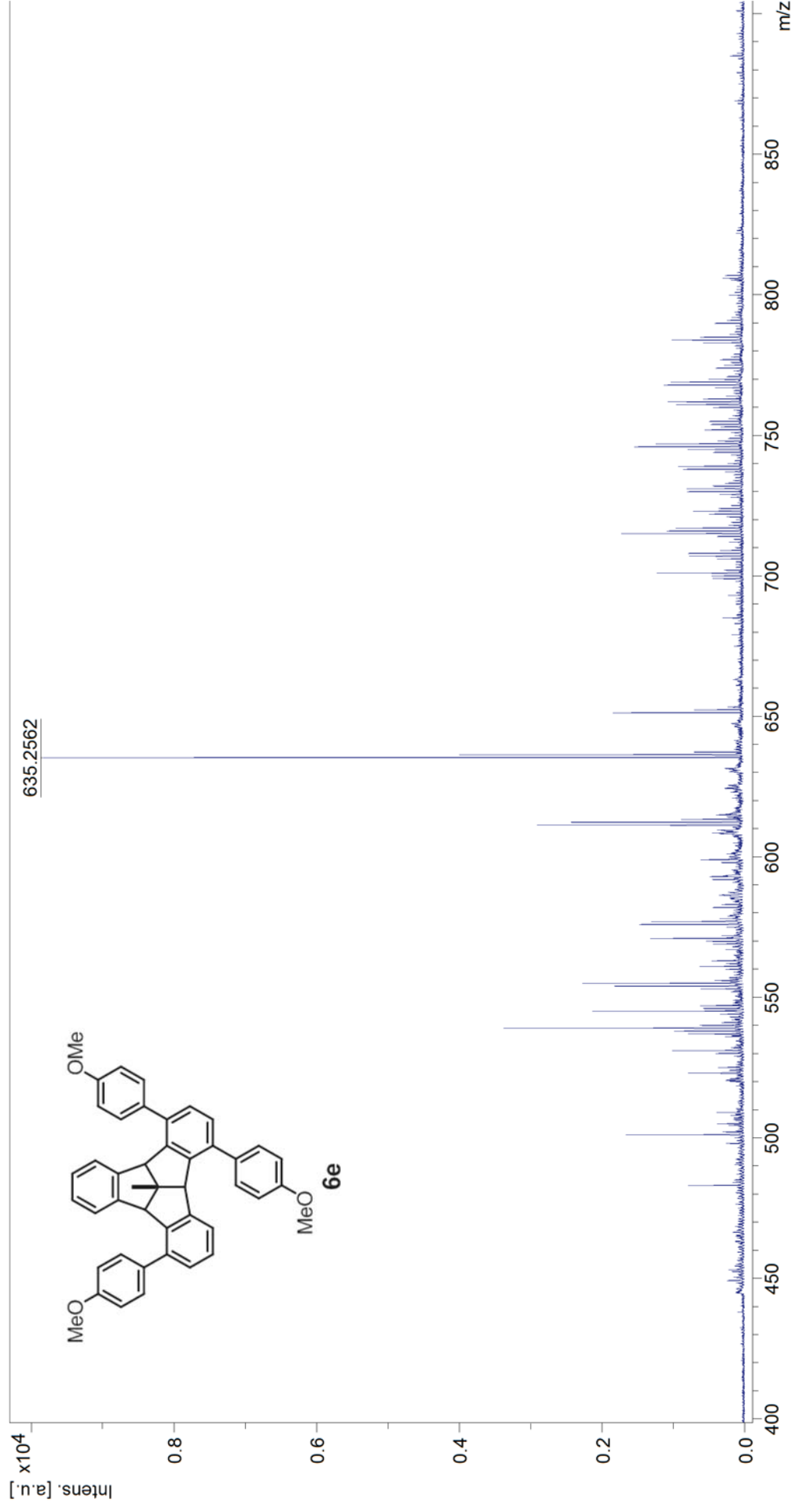
Current Data Parameters		Acquisition Parameters	
NAME	Eric_8a_4_Owe_data	Date_	20160115
EXPNO	2	Time	12.21 h
PROCNO	1	INSTRUM	spect
		PROBHD	Z108618_02957 (
		PULPROG	zgpg30
		TD	65536
		SOLVENT	CDC13
		DS	104
		NS	4
		SWH	24038.461 Hz
		FIDRES	0.366798 Hz
		AQ	1.3031488 sec
		RG	90.5
		DW	20.800 usec
		DE	6.50 usec
		TE	295.7 K
		D1	2.00000000 sec
		D11	0.03000000 sec
		TD0	1
		SF01	100.6479773 MHz
		NUC1	13C
		P1	9.50 usec
		PLW1	55.340000015 W
		SF02	400.2316009 MHz
		NUC2	1H
		CPDPRG2	waltz16
		PCPD2	90.00 usec
		PLW2	13.560000042 W
		PLW12	0.274230001 W
		PLW13	0.137956000 W
F2 - Processing parameters			
SI		32768	
SF		100.6379114 MHz	
WDW		EM	
SSB	0		
LB		1.00 Hz	
GB	0		
PC		1.40	

File:EI2016_075 Ident:165_210 Win 500PPM Acq:17-FEB-2016 20:39:52 +19:23 Cal:EI_POS_CAL_900
AutoSpec EI+ Magnet BpM:612 BpI:1252736 TIC:10374387 Flags:HALI
File Text:Er. Wang, OCl, Er-13, HWP



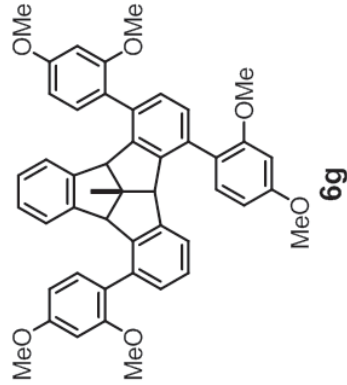
Comment 1

Comment 2



22 °C

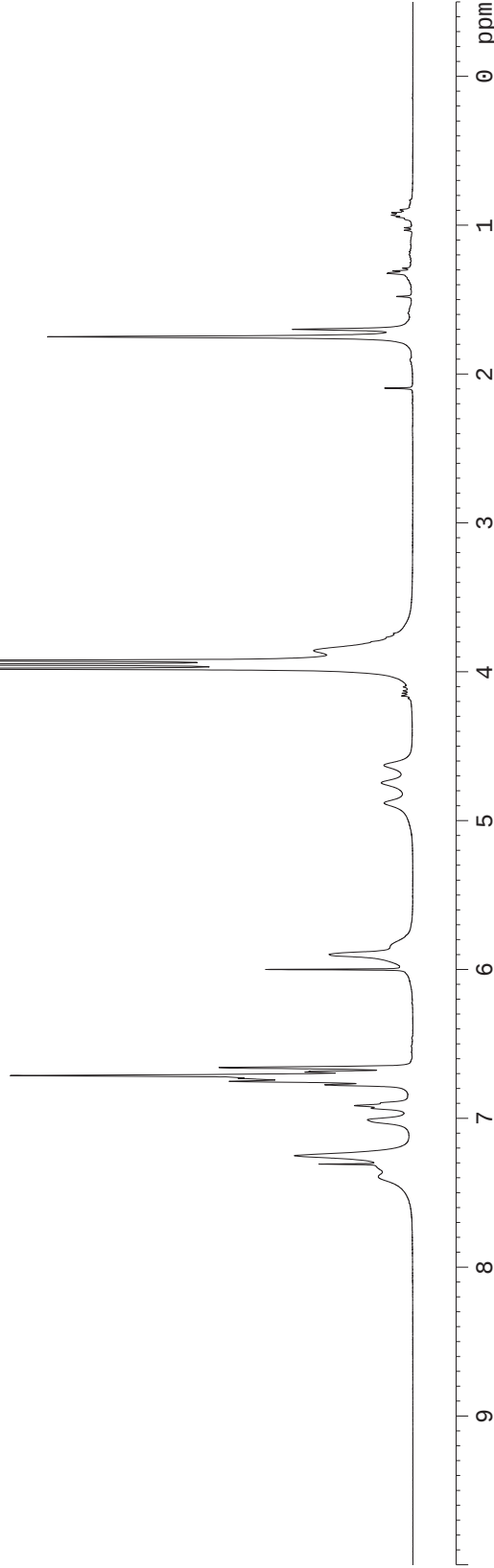
0000.9



AV400Q NMR



Current Data Parameters
NAME Eric_Ba_2_4_Ome_data_25
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Time 20.00 h
Date_ 18.08 h
INSTRUM spect
PULPROG zgpg30
TD 32768
FIDRES 0.3768
SOLVENT CDCl3
NS 15
DS 2
SWH 8012.820 Hz
FIDRES 0.3768 Hz
AQ 2.0447233 sec
RG 64
DE 62.40 usec
TE 295.2 K
D1 1.00000000 sec
T08 1
SFO1 400.1324708 MHz
NUC1 13C
P1 15.00 usec
PL1 8.31089042 W
F2 - Processing parameters
SI 65536
SF 400.1305149 MHz
WDW EN
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



60 °C

AV400Q NMR



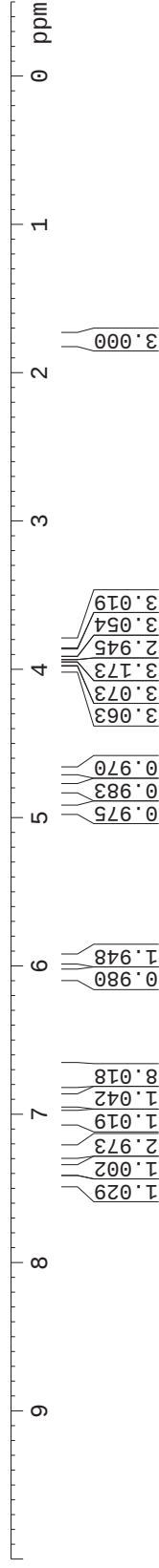
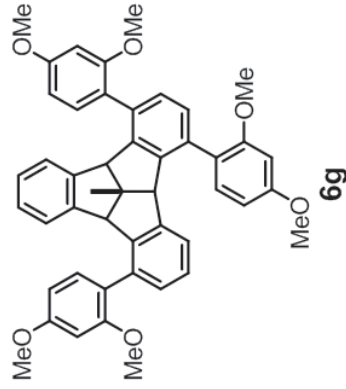
Current Data Parameters
 NAME Eric_Ba_2_4_Ome_data_60
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Time 20:54:15.48 h
 INSTRUM spect
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 2
 DS 2
 SWH 8012.8220 Hz
 FIDRES 0.001233 Hz
 AQ 2.0447233 sec
 RG 80.6
 DZ 62.0 usec
 DE 6.59 usec
 TE 333.3 K
 T1 1.0006060 sec
 T06 1
 SF01 400.1324708 MHz
 NUC1 13C
 PL1 15 dB usec
 PL11 8.31069042 W
 F2 - Processing parameters
 SI 65536
 SF 400.1305132 MHz
 WHW 0
 SSF 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1.7767
1.5556

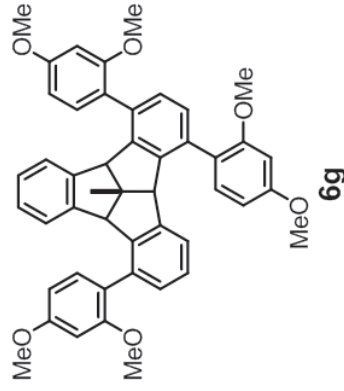
3.9916
3.9631
3.9405
3.9321
3.8907
3.8262

4.9400
4.8090
4.6799

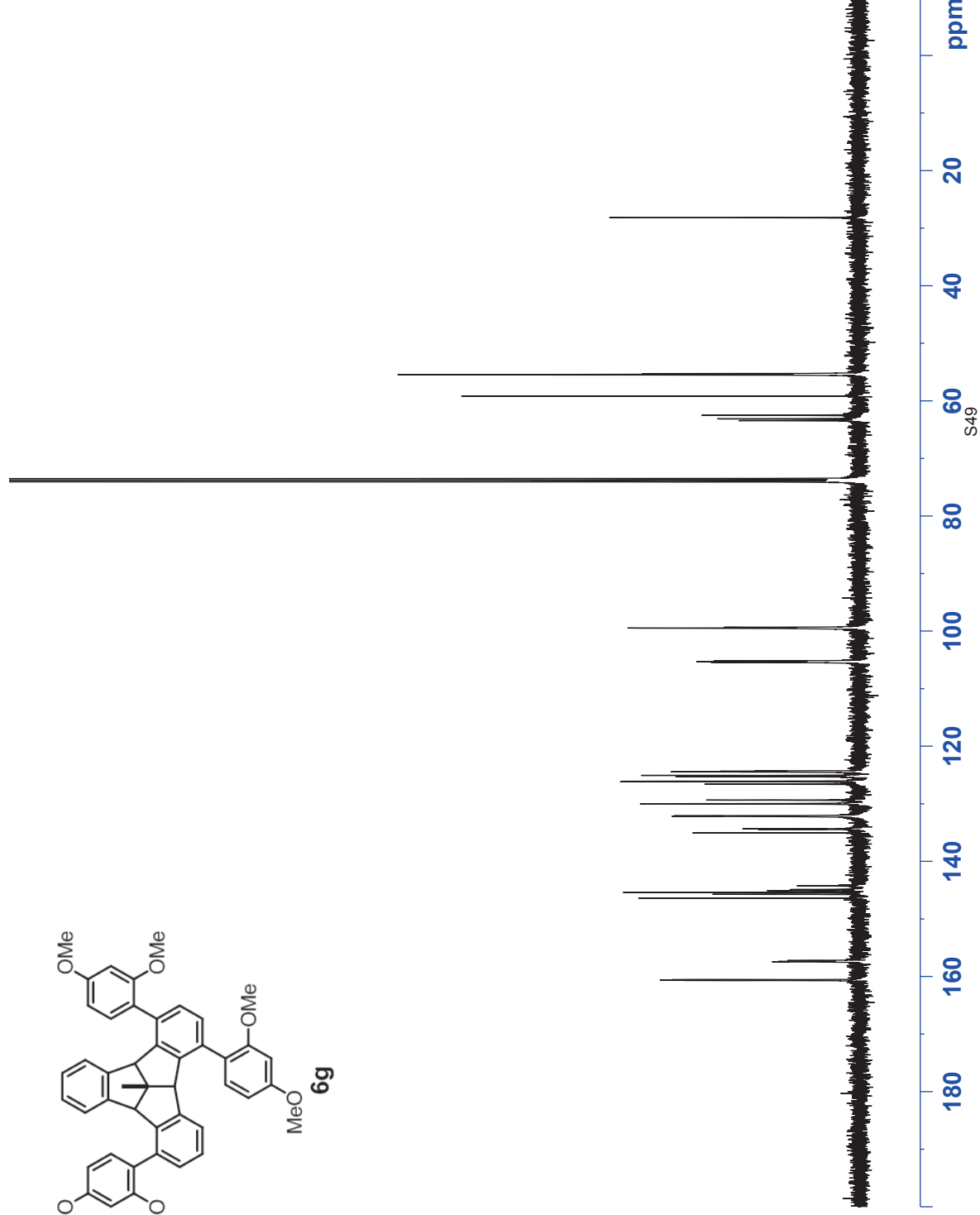
7.4525
7.4324
7.3945
7.3742
7.3227
7.2727
7.2500
7.2289
7.0339
7.0154
6.9308
6.9118
6.8930
6.7917
6.7733
6.7518
6.7325
6.7080
6.6889
6.6593
6.6402
6.6000
5.9603
5.9519



60 °C



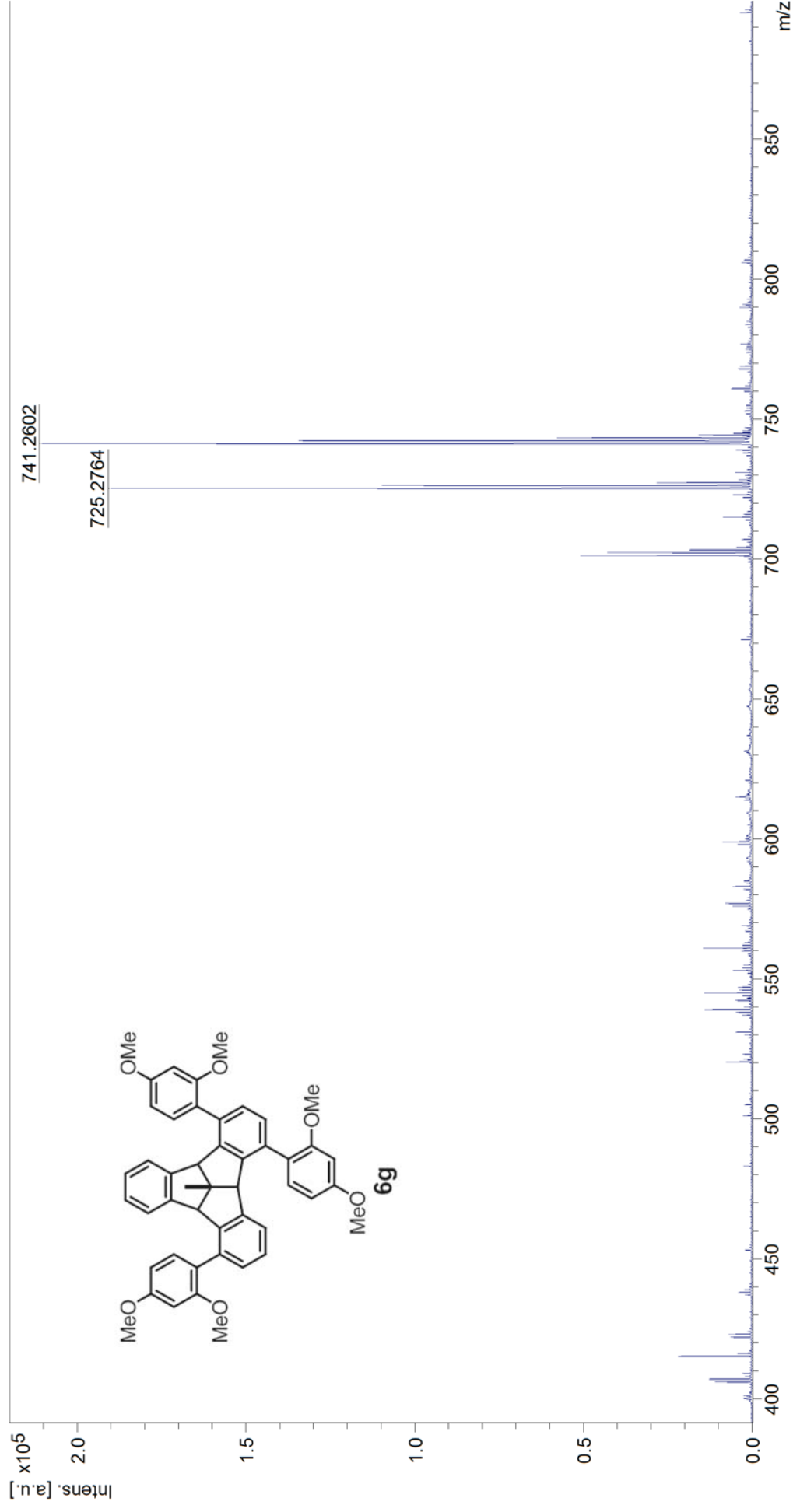
160.681
160.599
160.547
157.433
157.380
157.223
146.401
145.718
145.382
145.075
144.891
144.239
135.052
134.443
134.345
132.164
132.084
129.990
129.353
126.583
126.159
126.078
125.291
125.068
124.472
124.414
124.334
124.268
105.417
105.298
105.155
99.468
99.330
74.055
73.780
73.504
63.433
63.124
62.510
59.206
55.514
55.471
55.282
28.197



Current Data Parameters
NAME Eric_8a_2_4_OME_data_60
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160418
Time 10.09 h
INSTRUM Spect
PROBHD Z824601_0021
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 978
DS 4
SWH 24638.464 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 333.2 K
D11 2.0000000 sec
D12 0.0300000 sec
D13 0.0300000 sec
SF01 100.628298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SF02 400.1316095 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLW3 0.23000000 W
PLW4 0.11001000 W
F2 - Processing parameters
SI 32768
SF 100.6129258 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Comment 1

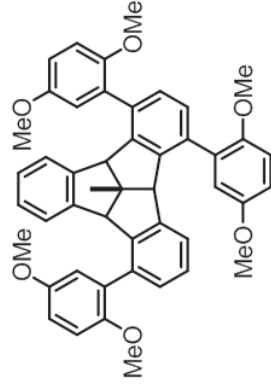
Comment 2



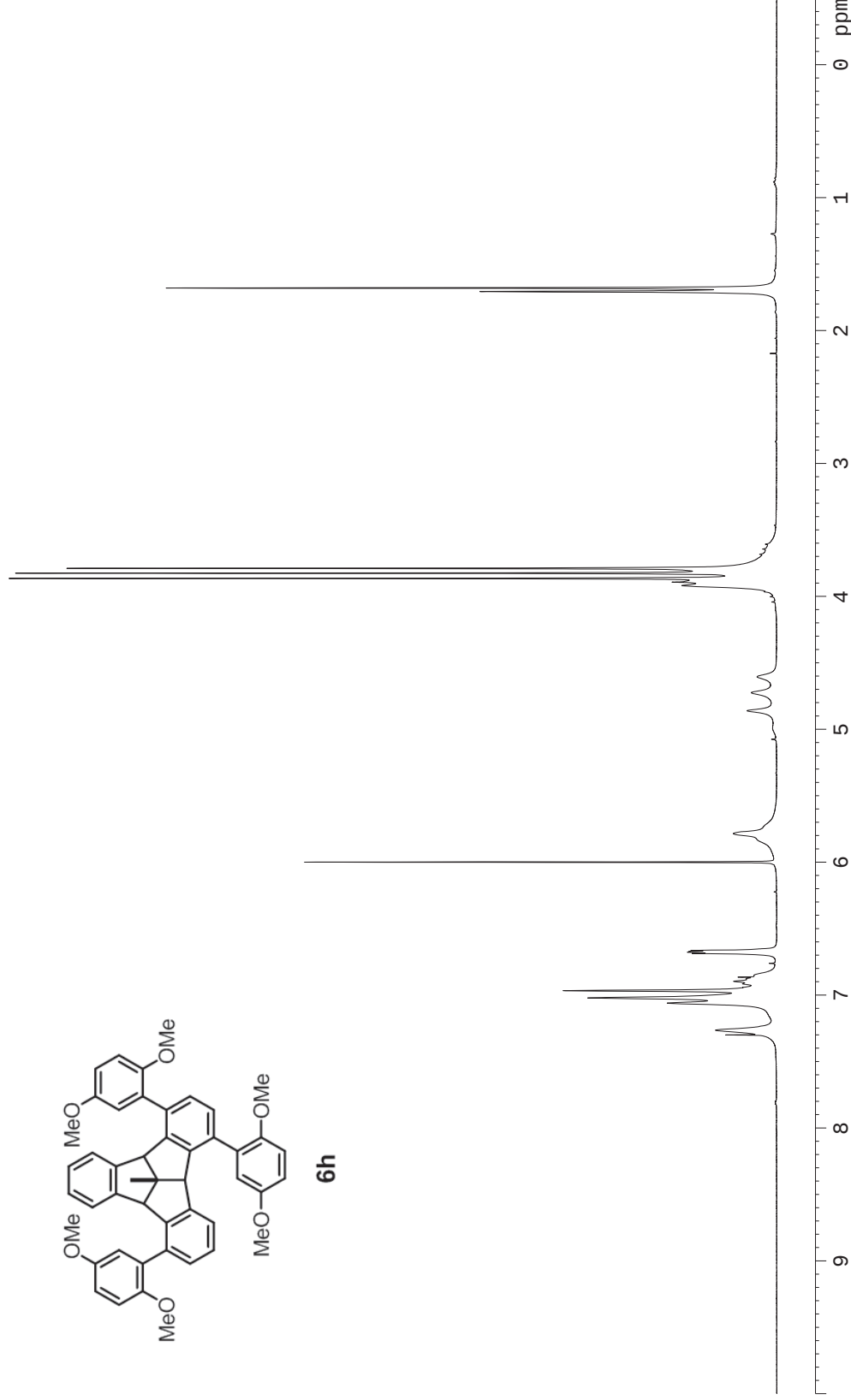
22 °C

0000.9

AV400Q NMR



6h



Current Data Parameters
NAME Eric_Ba_2_5_Ome_data_25
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Time 20.00
Time 17.47 h
INSTRUM spect
PULPROG zgpg30
TD 32768
FIDRES 0.33
SOLVENT CDCl3
NS 2
DS 8012.82 Hz
SWH 8012.82 Hz
FIDRES 0.33 Hz
AQ 2.0447233 sec
RG 283
DE 62.283 usec
TE 295.0 K
T1 1.0000000 sec
T2 1.0000000 sec
T2RHO 1
SFO1 400.1324708 MHz
NUC1 13C
P1 15.00 usec
PL1 8.31000042 W
F2 - Processing parameters
SI 65536
SF 400.1305141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

60 °C

AV400Q NMR



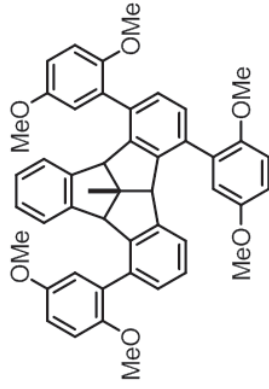
Current Data Parameters
 NAME Eric_Ba_2_5_Ome_data_60
 PROCNO 1
 F2 - Acquisition Parameters
 Time 20:00:16.20 h
 INSTRUM spect
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 2
 DS 2
 SWH 8012.8220 Hz
 FIDRES 0.344820 Hz
 AQ 2.0447233 sec
 RG 263
 DE 6.59 usec
 TE 333.6 K
 D1 1.0000000 sec
 T08 1
 SF01 400.1324708 MHz
 NUC1 13C
 PL1 15.00 usec
 F2 - Processing parameters
 SI 65536
 SF 400.1305125 MHz
 WHW 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1.5170
1.7500

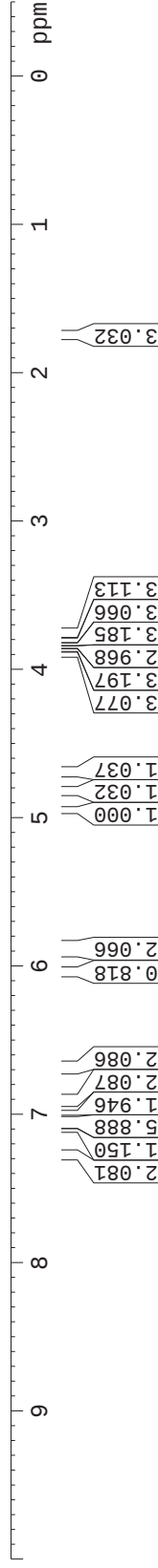
3.9023
3.8642
3.8551
3.8272
3.8137
3.7465

4.9519
4.8244
4.6956

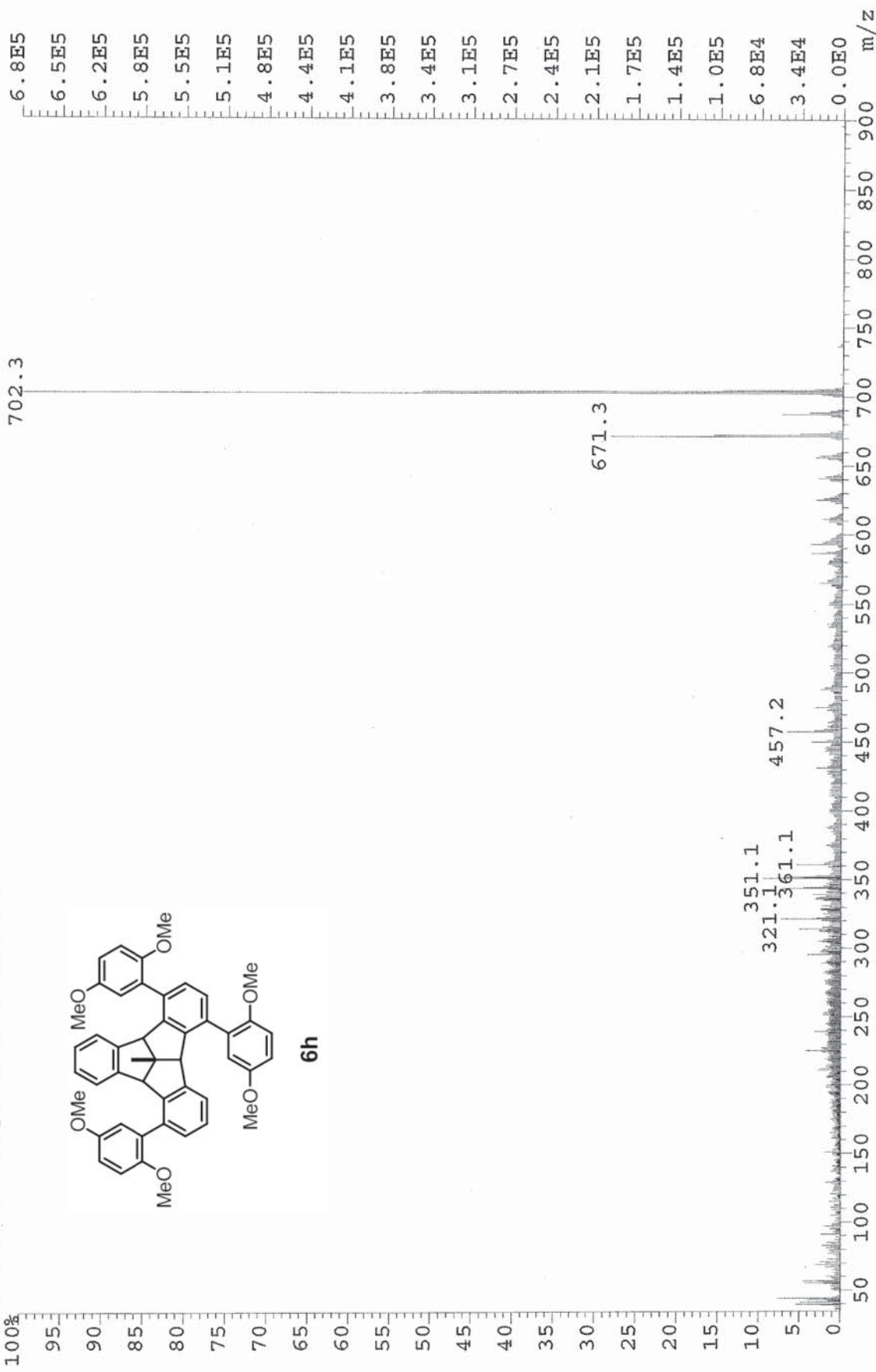
7.2933
7.2737
7.2694
7.2497
7.148
7.1083
7.0806
7.0716
7.0643
7.0510
7.0395
7.0324
7.0259
6.9925
6.9871
6.9272
6.9174
6.8979
6.8890
6.8789
6.7107
6.6977
6.6866
6.6755
6.6626
6.0231
6.0000
5.8906
5.8696



6h



File:EI2016_080 Ident:178_239 Win 500PPM Acq:18-FEB-2016 01:06:21 +21:33 Cal:EI_POS_CAL_900
 AutoSpec EI+ Magnet BpM:702 BpI:684480 TIC:8581441 Flags:HALL
 File Text:Er. Wang, OCl, Er-18, HWP



Bruker 9.4T FTICR MS Analysis Report

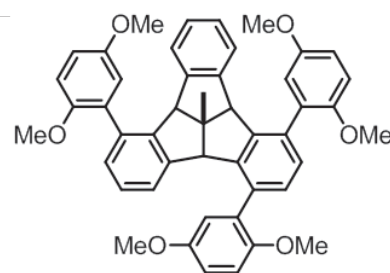
Faculty of Science, The Chinese University of Hong Kong

Analysis Info

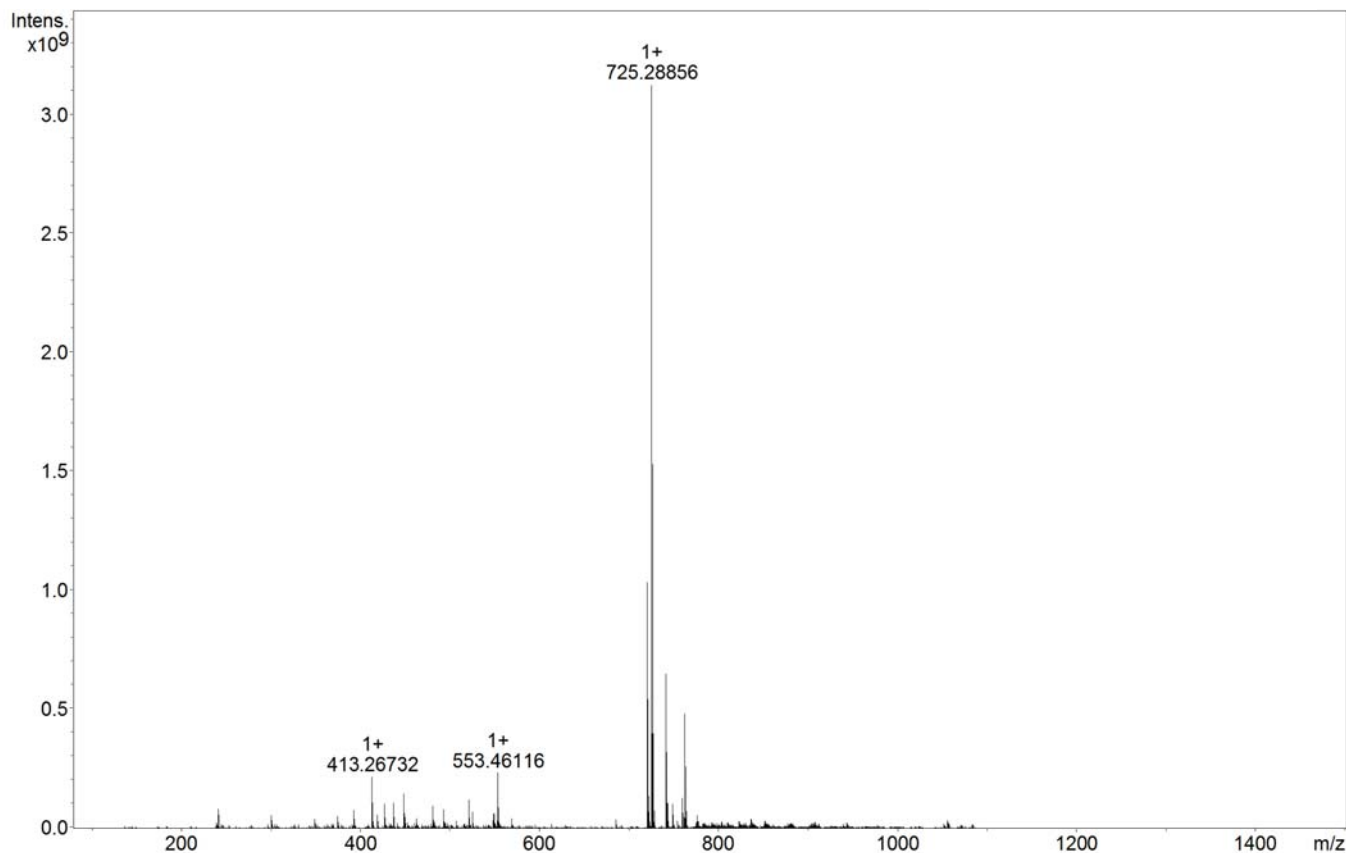
Sample Name :	Eric_8a_2_5_OMe	Reference No. :	xhfc044
Applicant Name :	Ip Ho Wang	Analysis Date :	4/2/2016 11:45:24
Analysis Path :	xhfc044_000001.d		
Instrument :	solarix	Polarity	Positive
Method	4_17_mass_range_pos_7T	Acquired Scans	9
Comment :	4.4kV, 120ml/hr, 1.0 nebulizer gas		

Accurate Mass Measurement

Molecular formula :	C ₄₇ H ₄₂ O ₆
Abundant Isotopic (theoretical) [M+Na] ⁺ :	725.287360
Monoisotopic (theoretical) [M+Na] ⁺ :	725.287360
(experimental) [M+Na] ⁺ :	725.28856
error (ppm) :	1.6



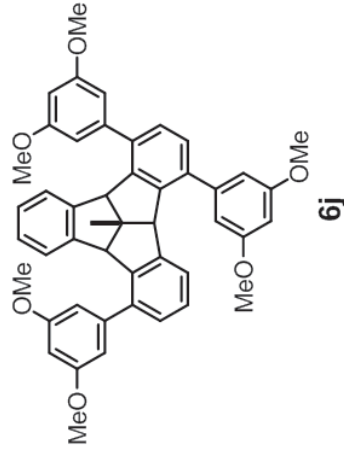
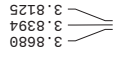
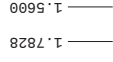
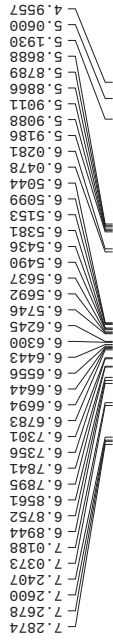
6h



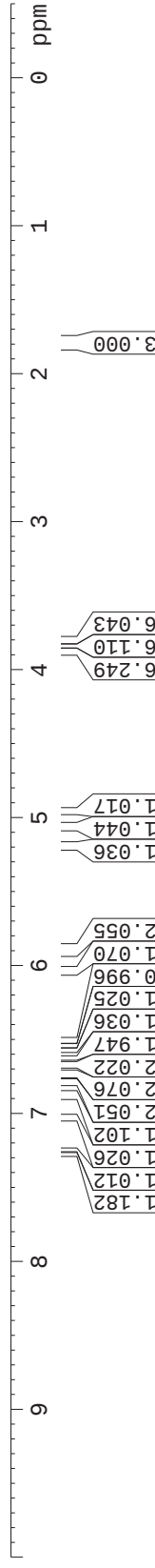
AV400Q NMR

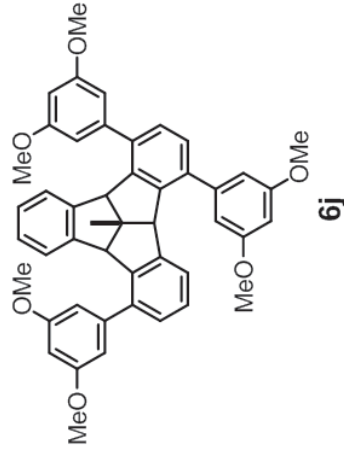


Current Data Parameters
NAME Eric_8a_3_5_Ome_data
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151216
Time 16.15 h
PULPROG zgpg30
PROBHD Z108618_0257 (1
TD 32768
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447144 sec
RG 62.400 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 13C
P1 12.00 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 32768
SF 400.2306997 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



6j





161.464
161.370
161.246
145.984
145.847
144.679
144.655
144.523
144.004
143.327
143.172
139.011
138.914
129.801
129.731
128.929
127.607
126.942
125.596
125.419
125.318
107.687
107.629
99.471
99.254

77.478
77.160
76.843
62.663
62.543
61.981
59.590
55.676
55.666
55.627

28.977

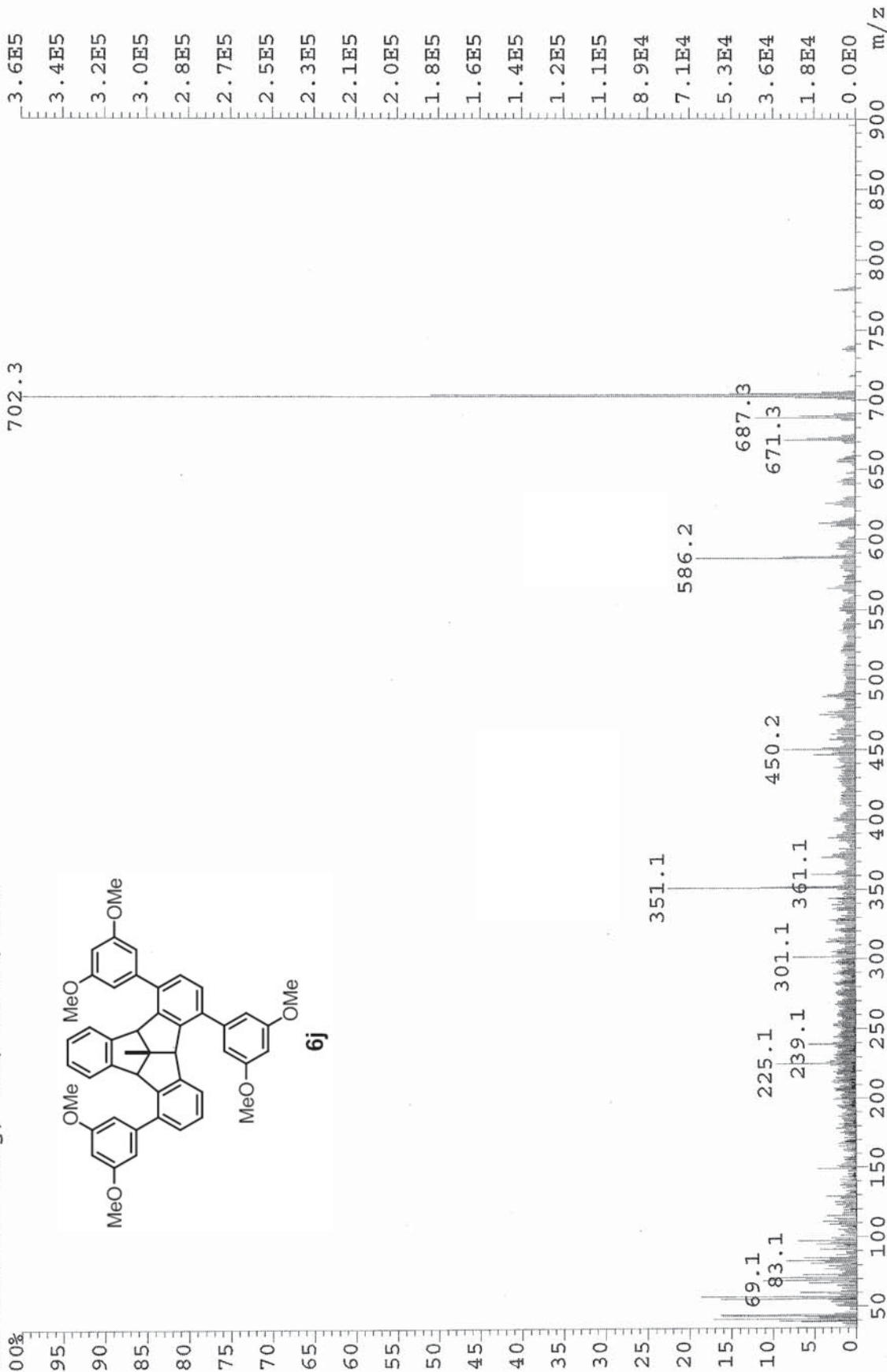
Current Data Parameters
NAME Eric_8a_3_5_OME_data
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151216
Time 16.33 h
INSTRUM spect
PROBHD Z108618_0257 (Zgpg30)
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 238
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SF01 100.6479773 MHz
NUC1 13C
P1 9.50 usec
PLW1 55.34000015 W
SF02 400.2316009 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 13.56000042 W
PLW12 0.27428001 W
PLW13 0.13796000 W

F2 - Processing parameters
SI 32768
SF 100.6379016 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

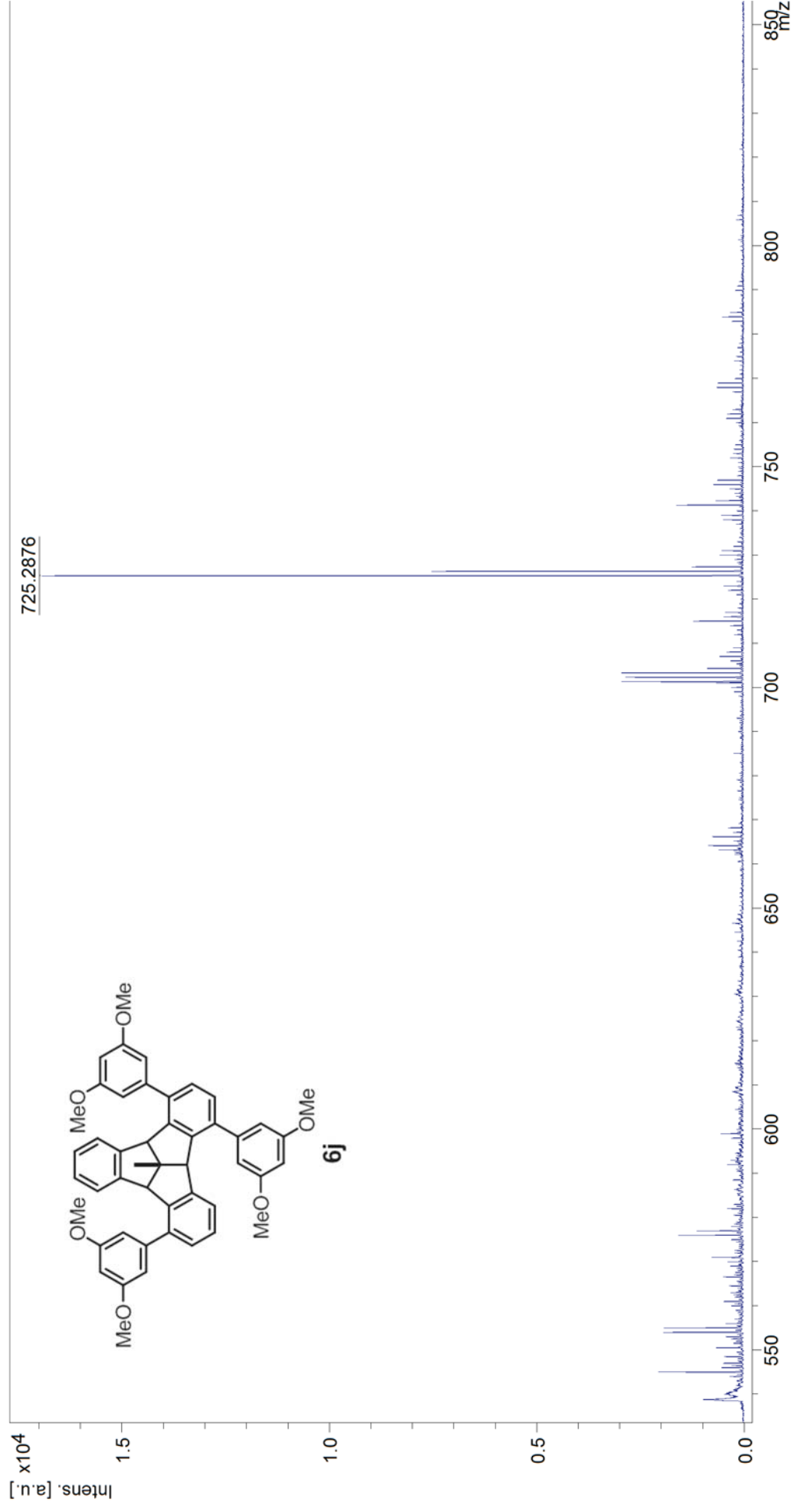


File:EI2016_081 Ident:152_191 Win 500PPM Acq:18-FEB-2016 01:56:59 +17:45 Cal:EI_POS_CAL_900
 AutoSpec EI+ Magnet BpM:702 BpI:355994 TIC:6511747 Flags:HALL
 File Text:Er. Wang, OCl, Er-19, HWP



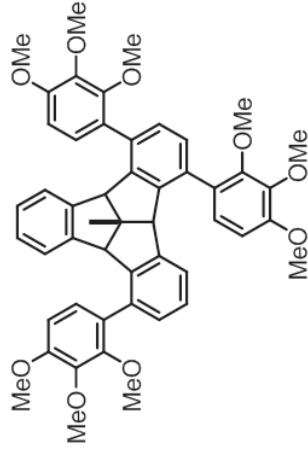
Comment 1

Comment 2



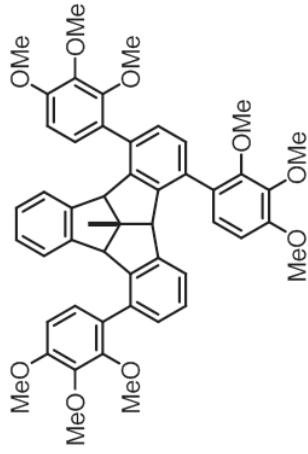
22 °C

AV400Q NMR

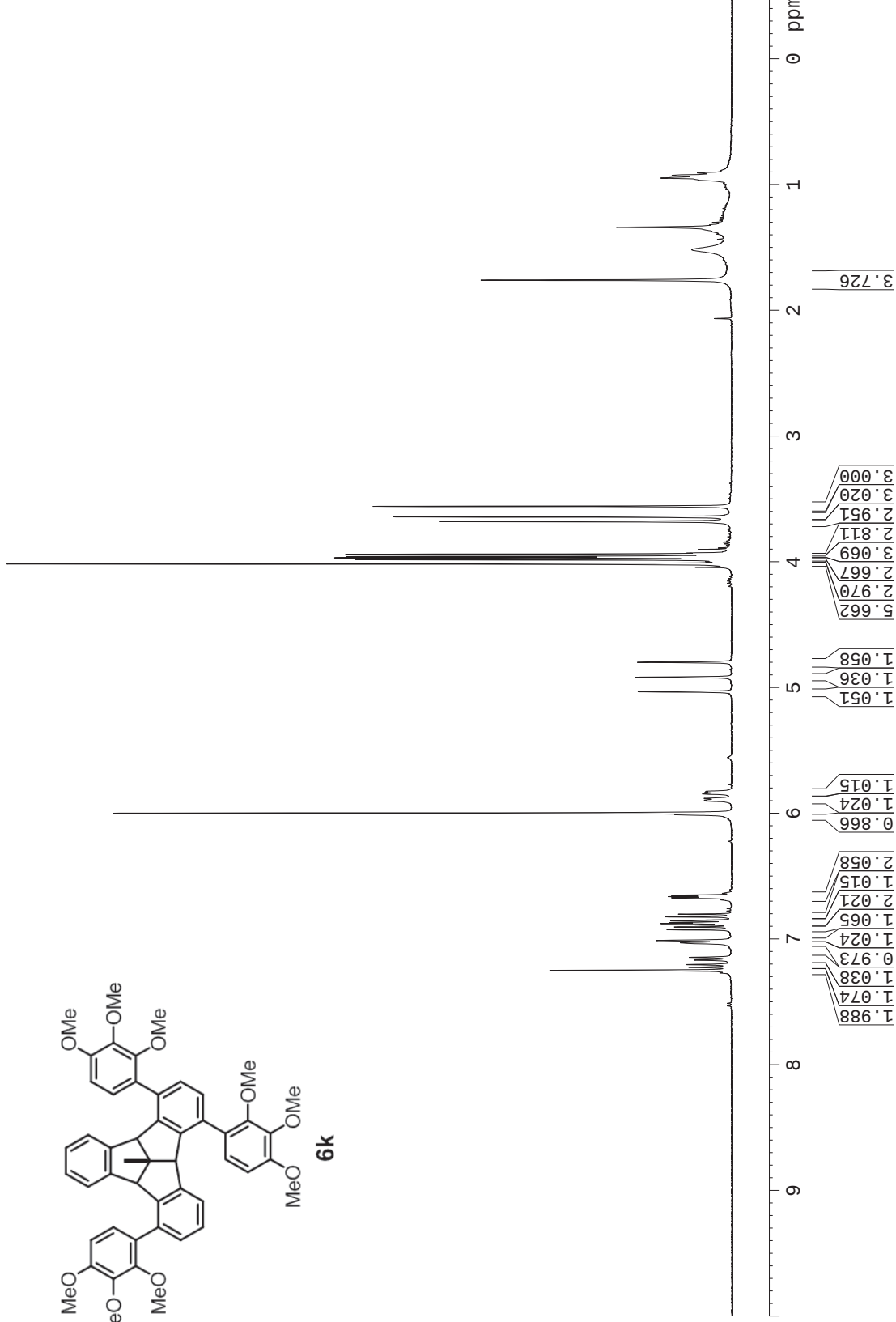
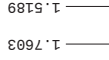
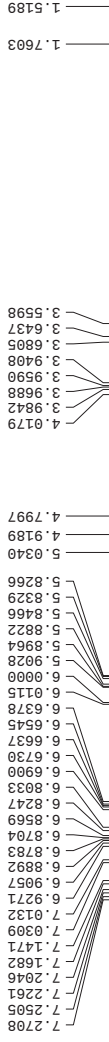


60 °C

AV400Q NMR



6k



Current Data Parameters
NAME Eric_Ba_2_3_4_Omc_data
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170515
Time 14.56 h
INSTRUM spect
PROBHD zgpg30
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
DS 2
SS 2
SWH 8612.850 Hz
FIDRES 0.244532 Hz
AQ 2.0447253 sec
RG 203
DW 62.400 usec
DE 3.50 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO 400.1324700 MHz
NUC1 1H
P1 15.00 usec
PLW1 8.31000042 W
F2 - Processing parameters
SI 65536
SF 400.1365121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

60 °C



Current Data Parameters
NAME Eric_Ba_2_3_4_0Me_data
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20110103
Time 15.03 h
INSTRUM spect
PROBHD Z824601.0021
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 342
DS 4

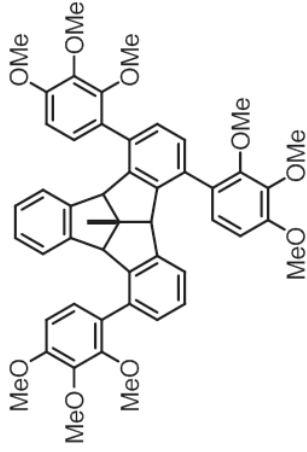
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
TE 300.2 K
DE 93.50 usec
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

SF01 100.6228298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SF02 400.1316005 MHz
NUC2 1H

CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLWI2 0.23083000 W
PLWI3 0.11611000 W

F2 - Processing parameters
SI 32768
SF 100.6129230 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

153.422
153.376
153.286
151.429
151.383
151.263
146.137
145.897
145.358
143.259
143.135
134.972
134.555
134.527
134.487
129.790
129.751
129.287
129.205
129.075
129.027
126.443
126.076
125.481
125.339
125.174
124.696
108.428
108.388
108.356
108.172
74.056
73.780
73.504
63.183
62.894
62.377
61.039
61.005
60.935
60.672
60.599
59.447
56.439
56.375
28.495



6k

180 160 140 120 100 80 60 40 20 ppm

S62

Thermo QEFMS Analysis Report

Analysis Info

Sample Name :	Eric_26	Reference No.:	Qhfc003
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI pos, 3.2kV, by LC, with sheath gas		

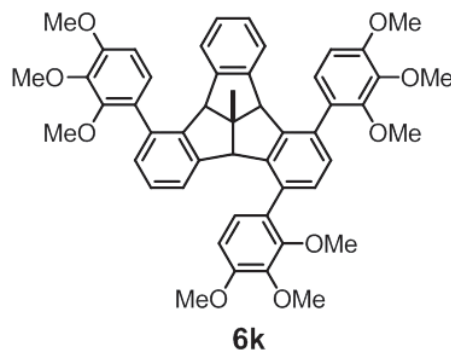
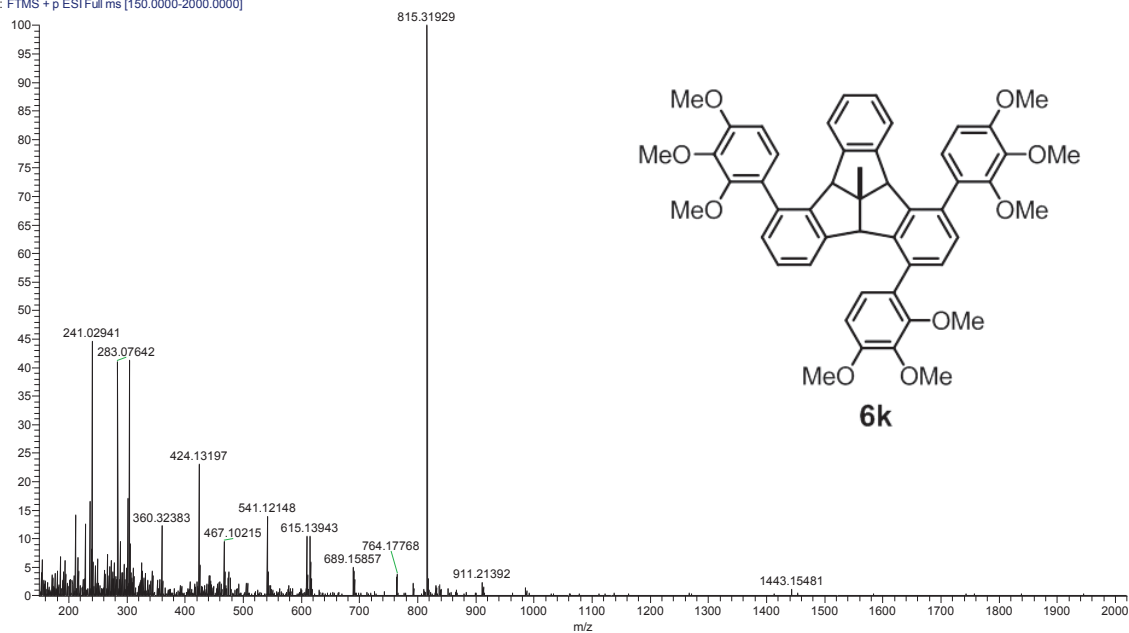
Accurate Mass Measurement

Molecular formula :	C ₅₀ H ₄₈ O ₉
Experimental Mass [M+Na] ⁺ :	815.31929
Theoretical Mass [M+Na] ⁺ :	815.31905
Error (ppm) :	0.2

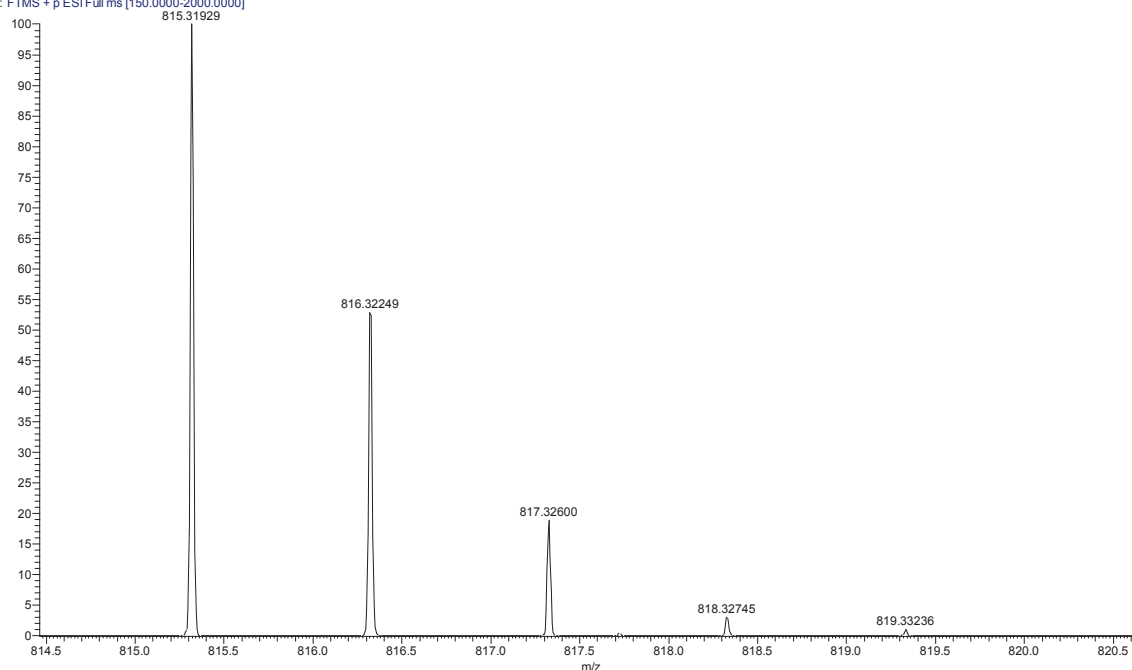
D:\Raw data\qhfc003_170208103211

02/08/17 10:33:20

qhfc003_170208103211 #193 RT: 0.87 AV: 1 SB: 66 0.53-0.74, 0.92-1
T: FTMS + p ESI Full ms [150.0000-2000.0000]



qhfc003_170208103211 #193 RT: 0.87 AV: 1 SB: 66 0.53-0.74, 0.92-0.99 NL: 8.03E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



AV400Q NMR



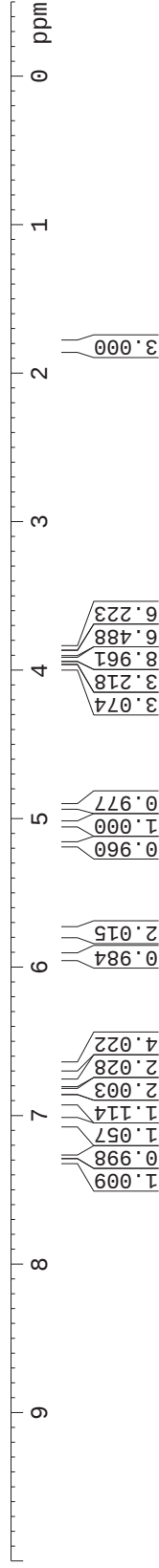
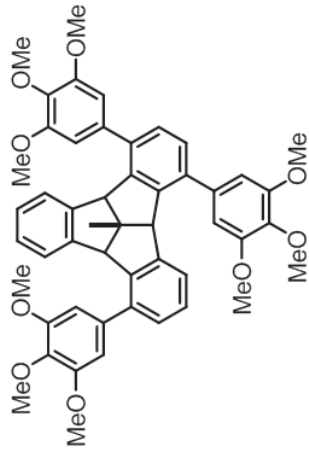
Current Data Parameters
NAME Eric_Ba_3_4_5_Ome_data
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171211
Time 17:38 h
INSTRUM spect
PROBHD zgpg30
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8612.850 MHz
FIDRES 0.244532 Hz
AQ 2.0447222 sec
RG 101
DW 62.400 usec
DE 3.150 usec
TE 296.2 usec
D1 1.00000000 sec
TD0 1
SFO 400.1324700 MHz
NUC1 1H
P1 15.00 usec
PLW1 8.31000042 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1.8179
1.6502

3.9737
3.9503
3.9304
3.8883
3.8512

5.1749
5.0368
4.9193

7.3135
7.2941
7.2859
7.2665
7.2600
7.0559
7.0374
6.9059
6.8866
6.8675
6.8380
6.7779
6.6844
6.6622
6.9373
6.9177
6.7936
6.7807
6.7726
6.7585
6.7505
6.7396



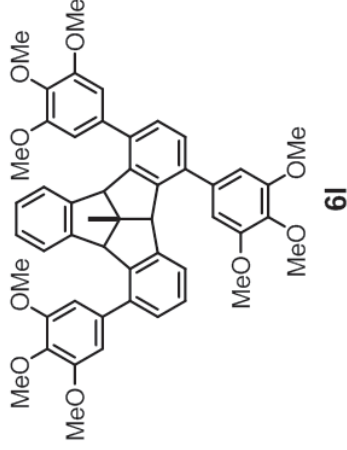


Current Data Parameters
NAME Eric_Ba_3_4_5_OME_data
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20101113
Time 17.43 h
INSTRUM spect
PROBHD Z824601.0021
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 230
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 0.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SF01 100.6228298 MHz
NUC1 13C
P1 13C
PLW1 41.25000000 W
SF02 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLWI2 0.23083000 W
PLWI3 0.11611000 W
F2 - Processing parameters
SI 32768
SF 100.6127591 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

153.958
153.877
153.745
145.841
145.463
144.493
143.859
143.305
142.946
139.238
138.969
138.137
137.974
137.934
137.754
129.795
129.741
129.006
127.596
127.038
126.996
125.668
125.434
125.318
106.679
77.478
77.160
76.843
62.803
62.367
61.379
61.360
61.314
59.608
56.524
56.504
56.457
29.071



Thermo QEFMS Analysis Report

Analysis Info

Sample Name :	Eric_29	Reference No.:	Qhfc006
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI pos, 3.2kV, by LC, with sheath gas		

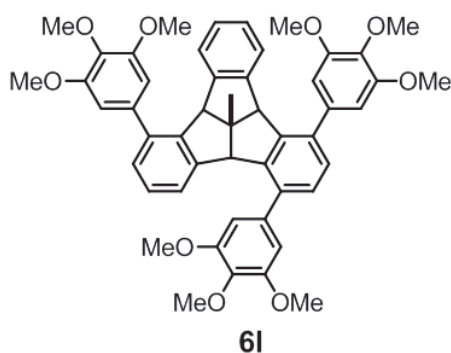
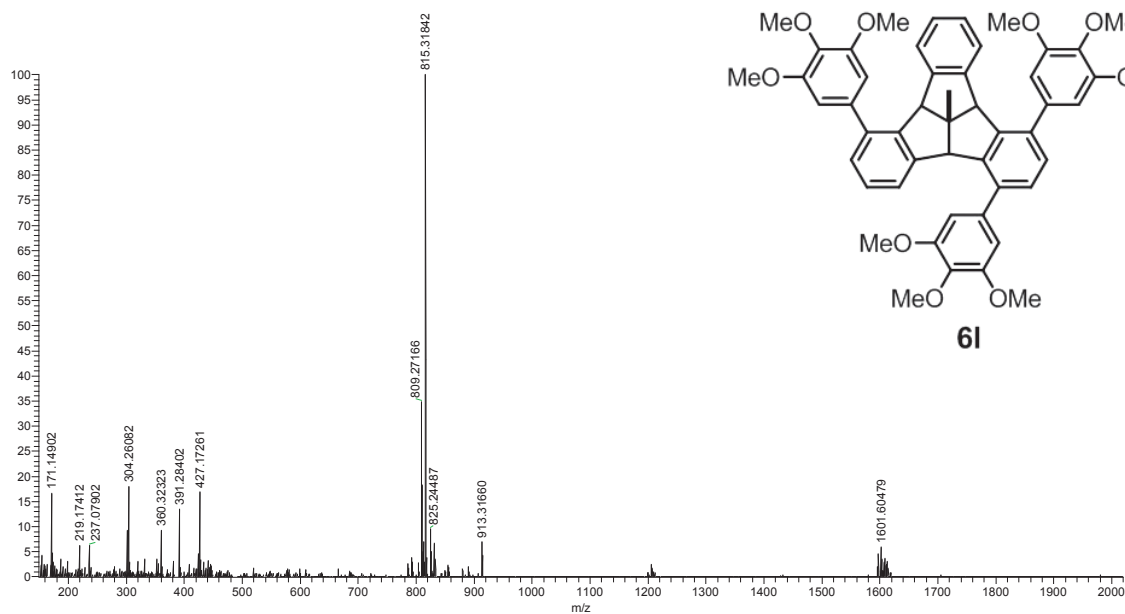
Accurate Mass Measurement

Molecular formula :	C ₅₀ H ₄₈ O ₉
Experimental Mass [M+Na] ⁺ :	815.31842
Theoretical Mass [M+Na] ⁺ :	815.31905
Error (ppm) :	0.7

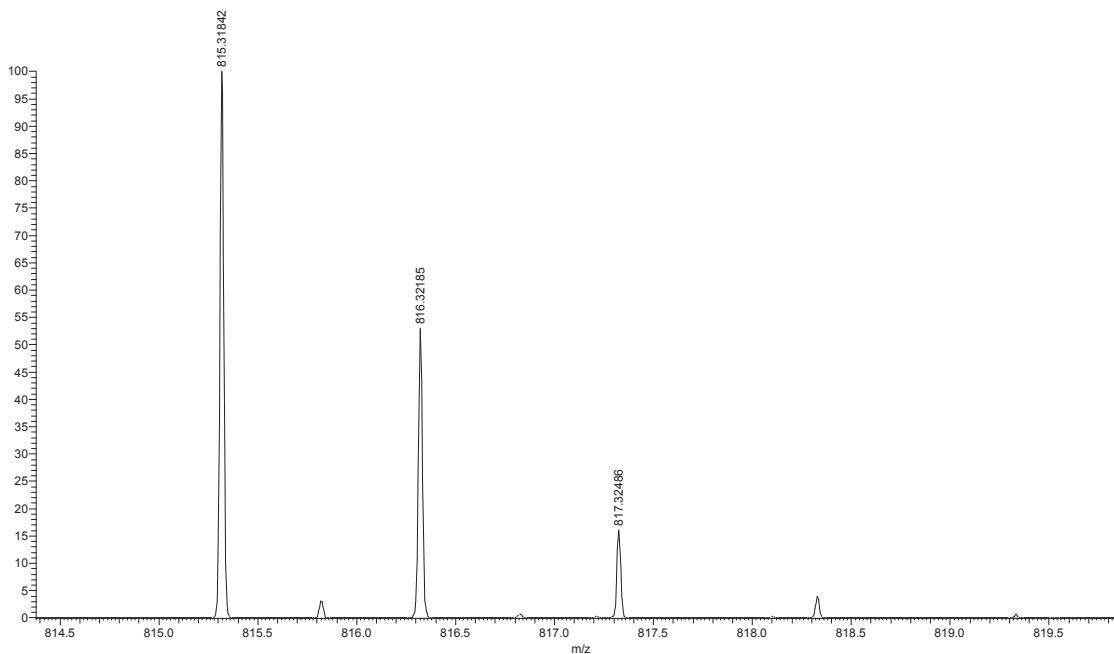
D:\Raw data\qhf006

02/08/17 10:51:49

qhf006 #198 RT: 0.90 AV: 1 SB: 73 0.51-0.75 , 0.93-1.01 NL: 4.99E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



qhf006 #198 RT: 0.90 AV: 1 SB: 73 0.51-0.75 , 0.93-1.01 NL: 4.99E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



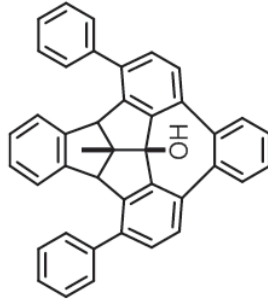
AV400Q NMR



2.1218
1.7624
1.5504

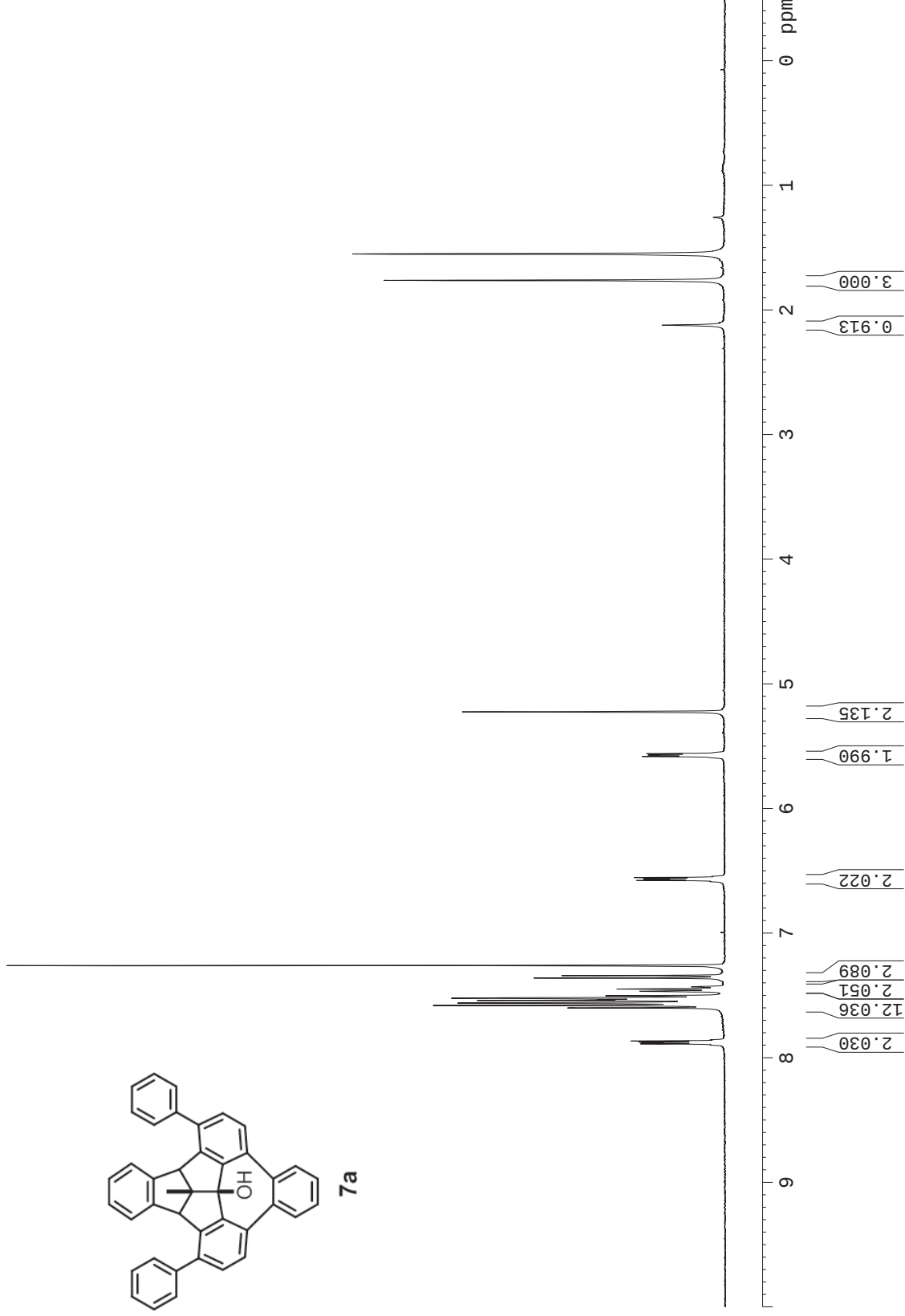
5.5923
5.5834
5.5749
5.5695
5.5609
5.5528
5.2249

7.8976
7.8885
7.8799
7.8742
7.8656
7.8565
7.6000
7.5801
7.5607
7.5405
7.5328
7.5221
7.5027
7.4664
7.4483
7.3604
7.3408
7.2600
6.5871
6.5778
6.5697
6.5633
6.5552
6.5463

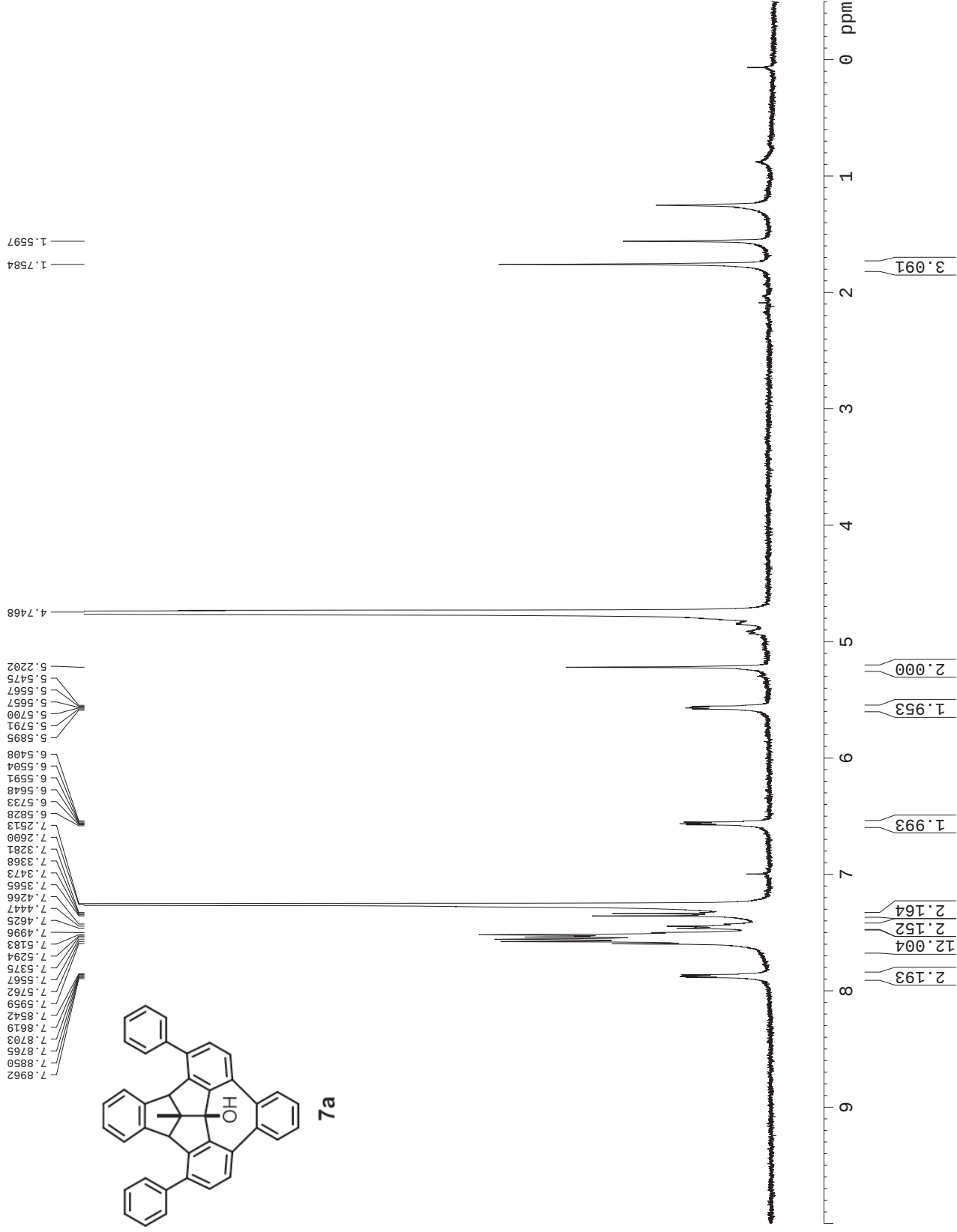


7a

Current Data Parameters
NAME Eric_Ba_un_mono_OH_data
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Time 20.52
Time 12.41 h
INSTRUM spect
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
DS 2
SWH 8012.820 Hz
FIDRES 0.344820 Hz
AQ 2.0447233 sec
RG 263
DE 62.263 usec
TE 295.2 K
T0 1.00000000 sec
T00 1
SFO1 400.1324708 MHz
NUC1 13C
P1 15.00 usec
PL1 8.31000042 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



CDCl₃/D₂O = 50/1



AV400Q NMR



Current Data Parameters
Name: Eric_9a_un_mono_0h_data.D20
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170206
Time 13:25:00
INSTRUM spect
PROBHD 5mm
PULPROG zgpg30
TD 32768
FIDRES 0.224522
SOLVENT CDCl3
NS 89
DS 2
AQ 8812.822 Hz
FIDRES 0.244522 Hz
RG 2.8447203 sec
DM 62.400 usec
DE 1.00000000 sec
TE 295.2 K
D1 1.00000000 sec
SFO1 400.2324714 MHz
N1 30
NUC1 13C
P1 12.00 usec
PL1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2324714 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME Eric_8a_un_mono_OH_data
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20151217
Time 22.46 h
INSTRUM Spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 11334
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 295.6 K
D1 2.0000000 sec
D11 0.0300000 sec
TDS 1
SF01 100.6228298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SF02 400.1316095 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLW12 0.23000000 W
PLW13 0.11001000 W

F2 - Processing parameters
SI 32768
SF 100.6127536 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

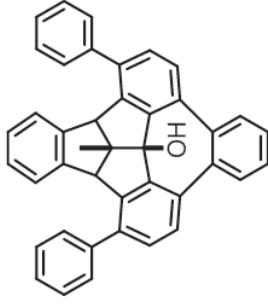
22.901

62.806
64.261

76.842
77.160
77.477

89.649

125.558
127.157
127.689
128.017
129.135
129.179
129.460
129.971
129.971
130.958
133.811
136.532
138.994
140.333
141.990
144.710
147.602



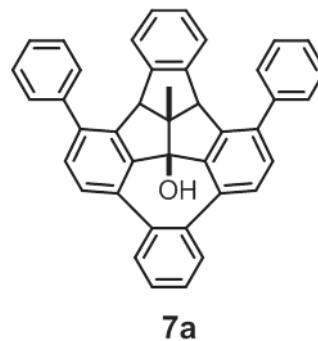
7a



9.4T FTICR MS Analysis Report

Faculty of Science, The Chinese University of Hong Kong

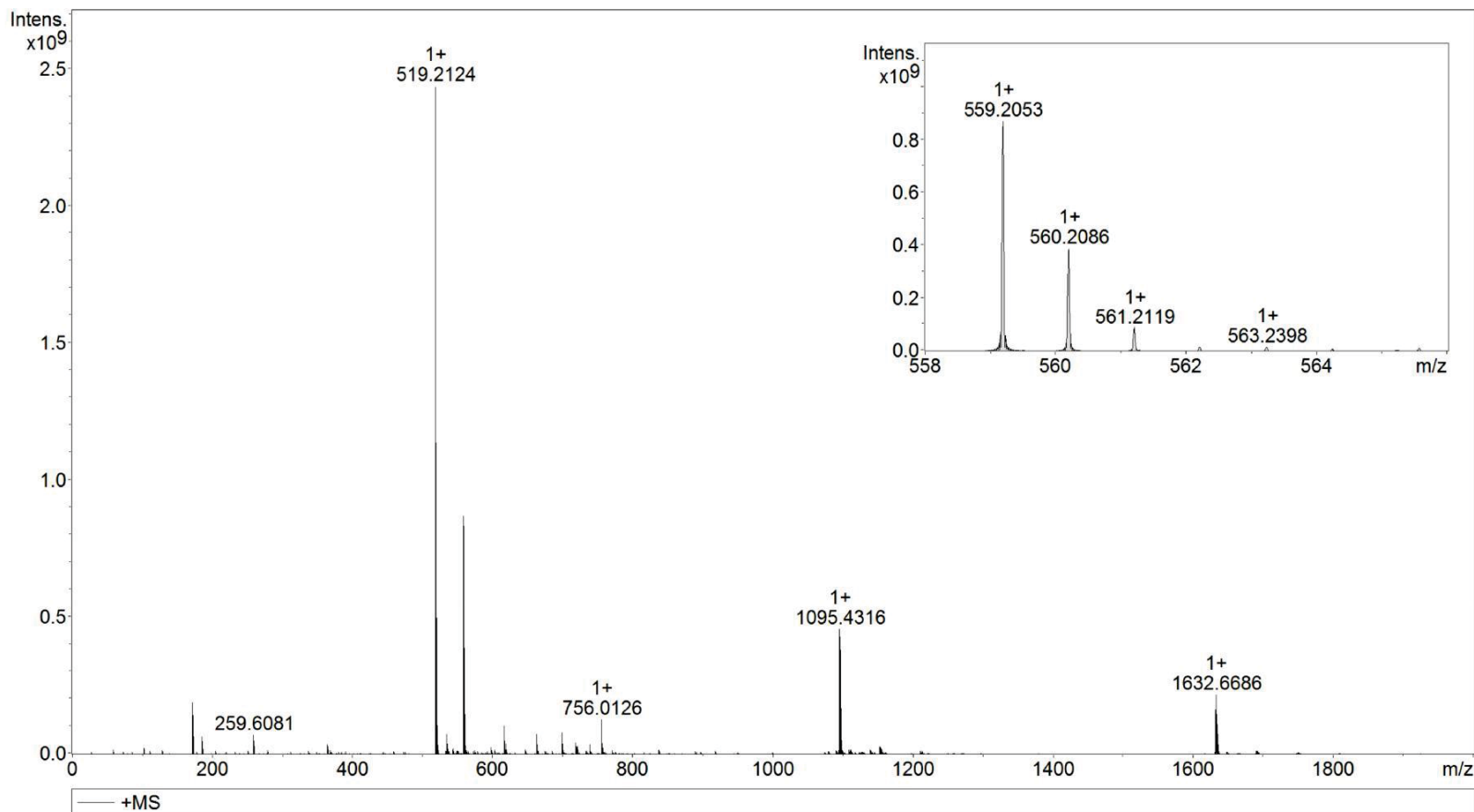
Sample No.	Eric12
Reference No.	CHF0025
Applicant name	Ip Ho Wang
Analysis Path	\\192.168.0.1\Data\Service\MSonly\20160509\Eric12_000002.d
Instrument	solariX
Polarity	Positive
Acquired Scans	4
Operator	Winnie
Analysis Date	5/9/2016 3:32:19 PM



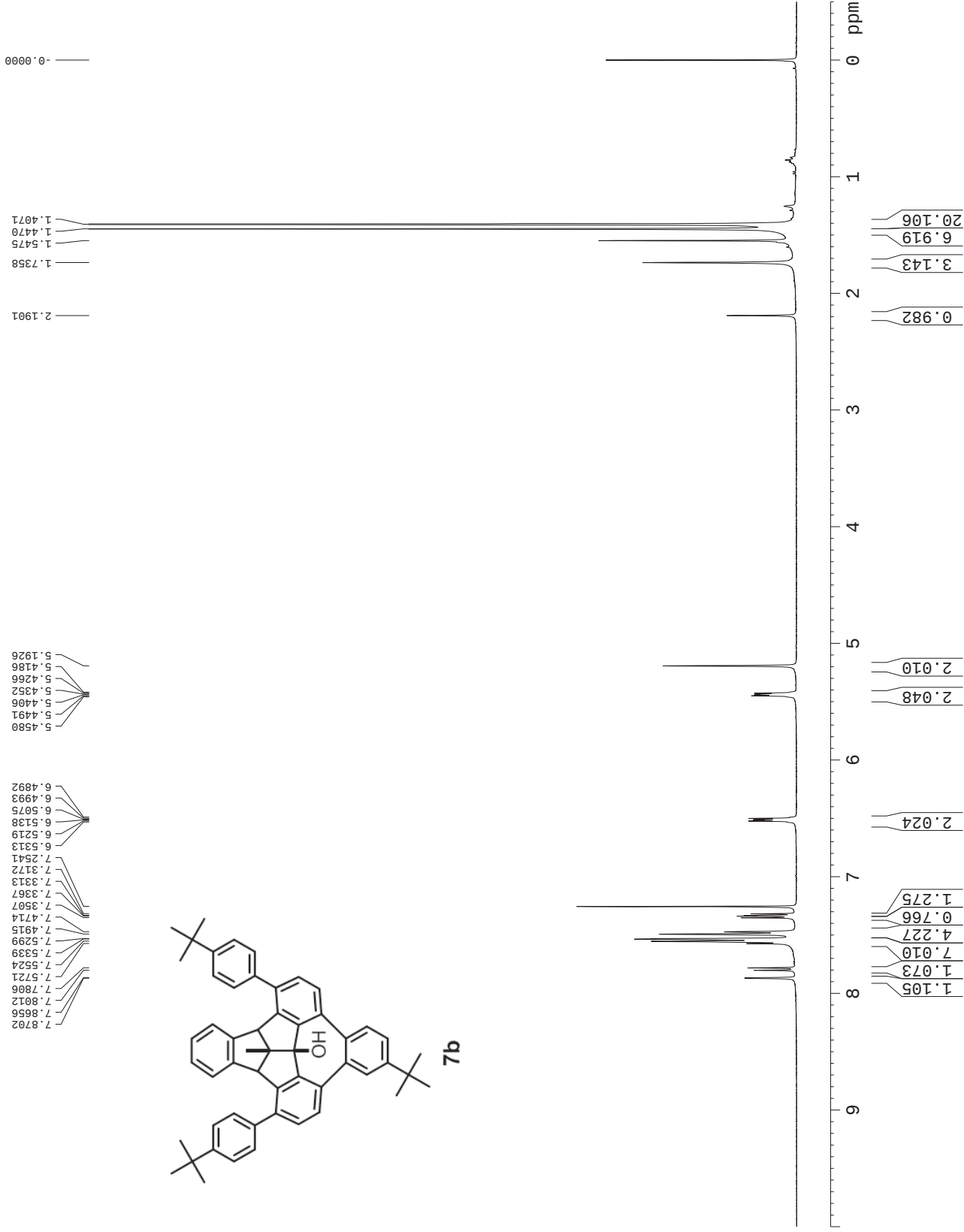
Molecular Formula: C₄₁H₂₈O

Abundant Isotopic (theoretical)[M+Na]⁺: 559.2032

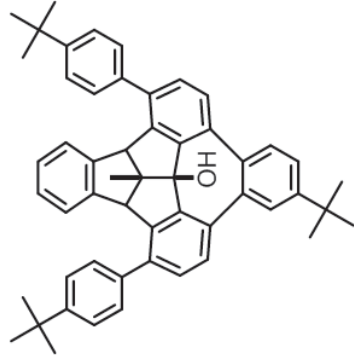
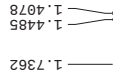
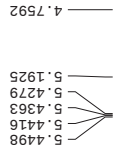
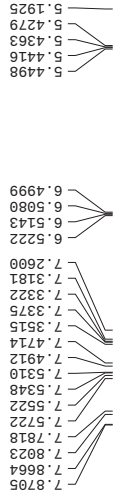
Monoisotopic (theoretical)[M+Na]⁺: 559.2032(experimental)[M+Na]⁺: 559.2057 error(ppm): 4.47



Chemical structure of compound **7b**, a phthalocyanine derivative. It features a central macrocyclic ring with four tert-butylphenyl substituents and a central hydroxyl group (OH).



CDCl₃/D₂O = 50/1

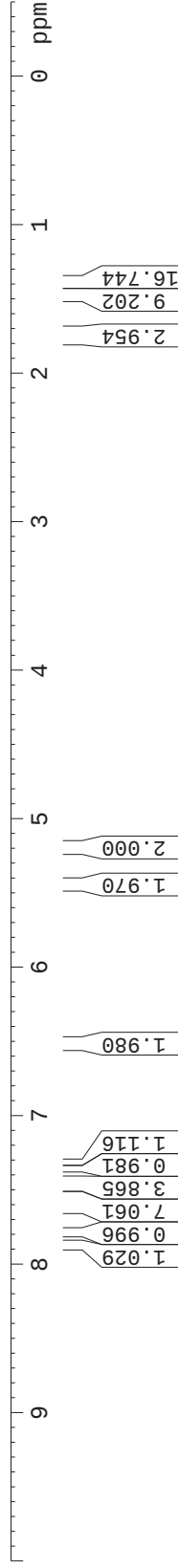


7b

AV400Q NMR



Current Data Parameters
Name: EFG_9H_1_TEMPERATURE_data_000
EXPNO 1
PROCNO 1
P2 - Acquisition Parameters
Date_ 20180227
Time 18:47 h
INSTRUM spect
PROBHD Z108618.0357 L
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
DS 2
SWH 9542.750 Hz
FIDRES 0.2245532 Hz
AQ 2.6447293 sec
RG 327.5
DM 65.480 usec
DE 2305.0 K
TE 300.2 K
T1 1.0080000 sec
T1RHO 1
T2 400.2324714 MHz
SFO1 400.1464010 MHz
P1 13.5600042 M
PC 1.00
P2 - Processing parameters
SI 400.2300117 MHz
SF 400.1464010 MHz
WDW 0
SSB 0
GB 0
PC 1.00

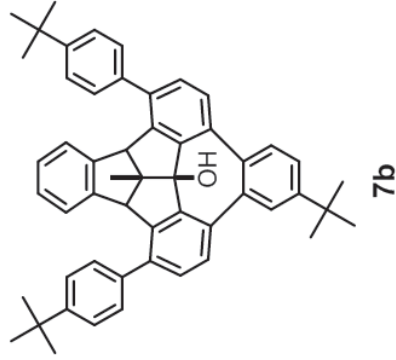




Current Data Parameters
NAME E1C_Ba_4_t-butyl_mono_OH_data_2
EXPNO 222
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160212
Time 12:25:11 h
INSTRUM spect
PROBHD Z100B18.0257 (1H/13C)
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1369
DS 4
SWH 24938.461 Hz
FIDRES 0.366788 Hz
AQ 1.33531600 sec
RG 161
GB 1
PC 1.40
DE 20.860 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
SFO1 100.647973 MHz
NUC1 13C
P1 1.50 usec
PL1 0.00 dB
PL12 55.34000015 W
SFO2 400.231609 MHz
IN 1H
NUG2 90.00 usec
PCPD2 13.56000042 W
PL2 0.00 dB
PL13 0.00 dB
PL14 0.13750000 W
PL15 0.13750000 W
F2 - Processing parameters
SI 32768
SF 100.6379179 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

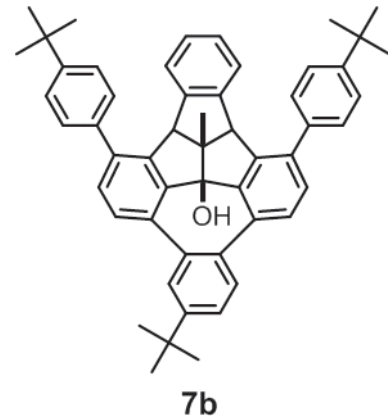
150.721
150.702
150.660
147.409
147.357
144.565
140.145
140.116
138.908
138.698
138.514
135.927
133.900
133.485
133.340
130.487
130.469
129.441
128.985
128.869
128.696
126.860
126.764
125.854
125.494
125.008
89.420
77.325
77.007
76.690
64.022
62.738
34.813
34.676
31.454
31.425
22.755
0.000



9.4T FTICR MS Analysis Report

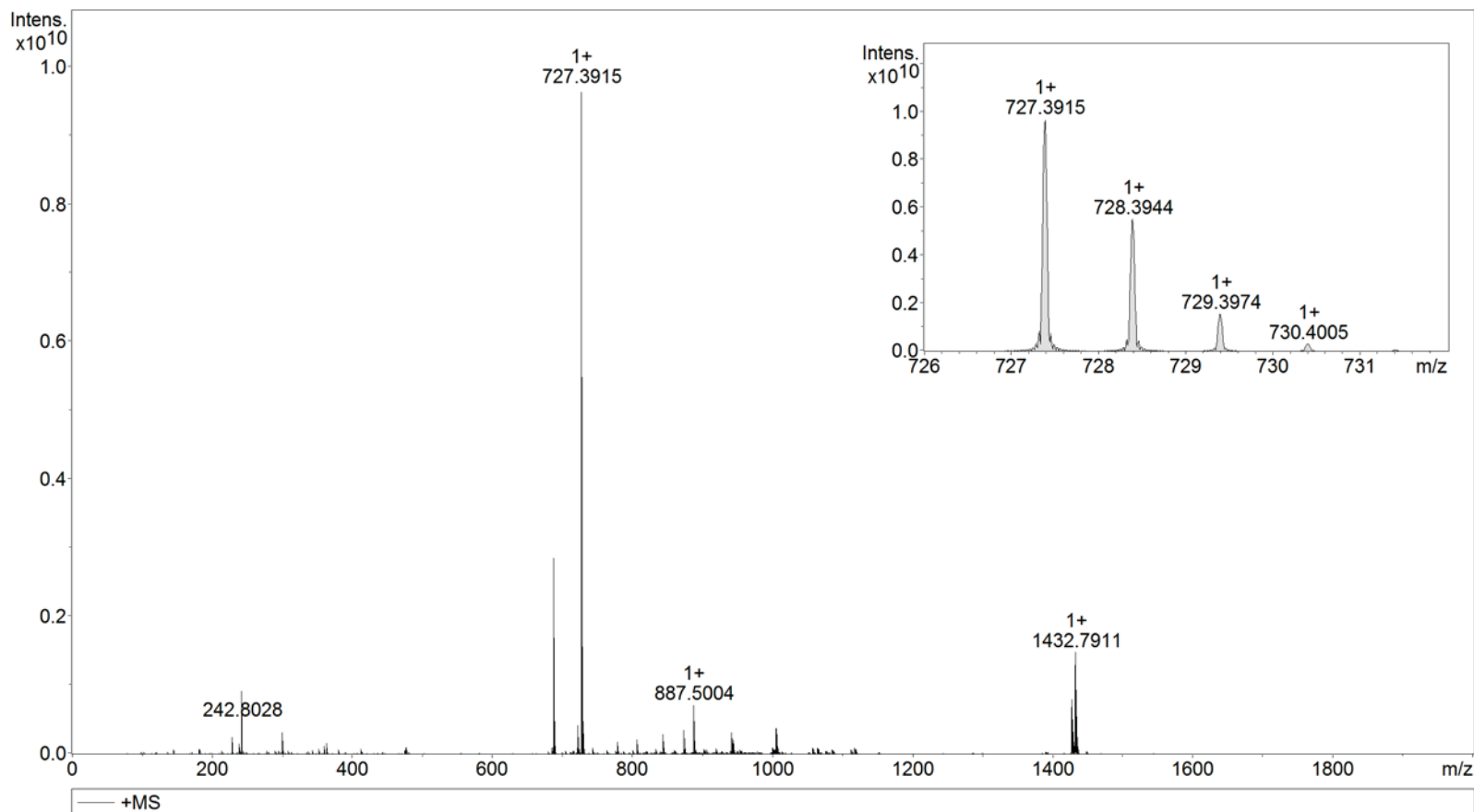
Faculty of Science, The Chinese University of Hong Kong

Sample No.	Eric03
Reference No.	CHF0026
Applicant name	Ip Ho Wang
Analysis Path	D:\Data\Service\MSonly\20160516\CHF\Eric03_000004.d
Instrument	solarix
Polarity	Positive
Acquired Scans	12
Operator	Winnie
Analysis Date	5/16/2016 2:42:22 PM



Molecular Formula: C₅₃H₅₂O

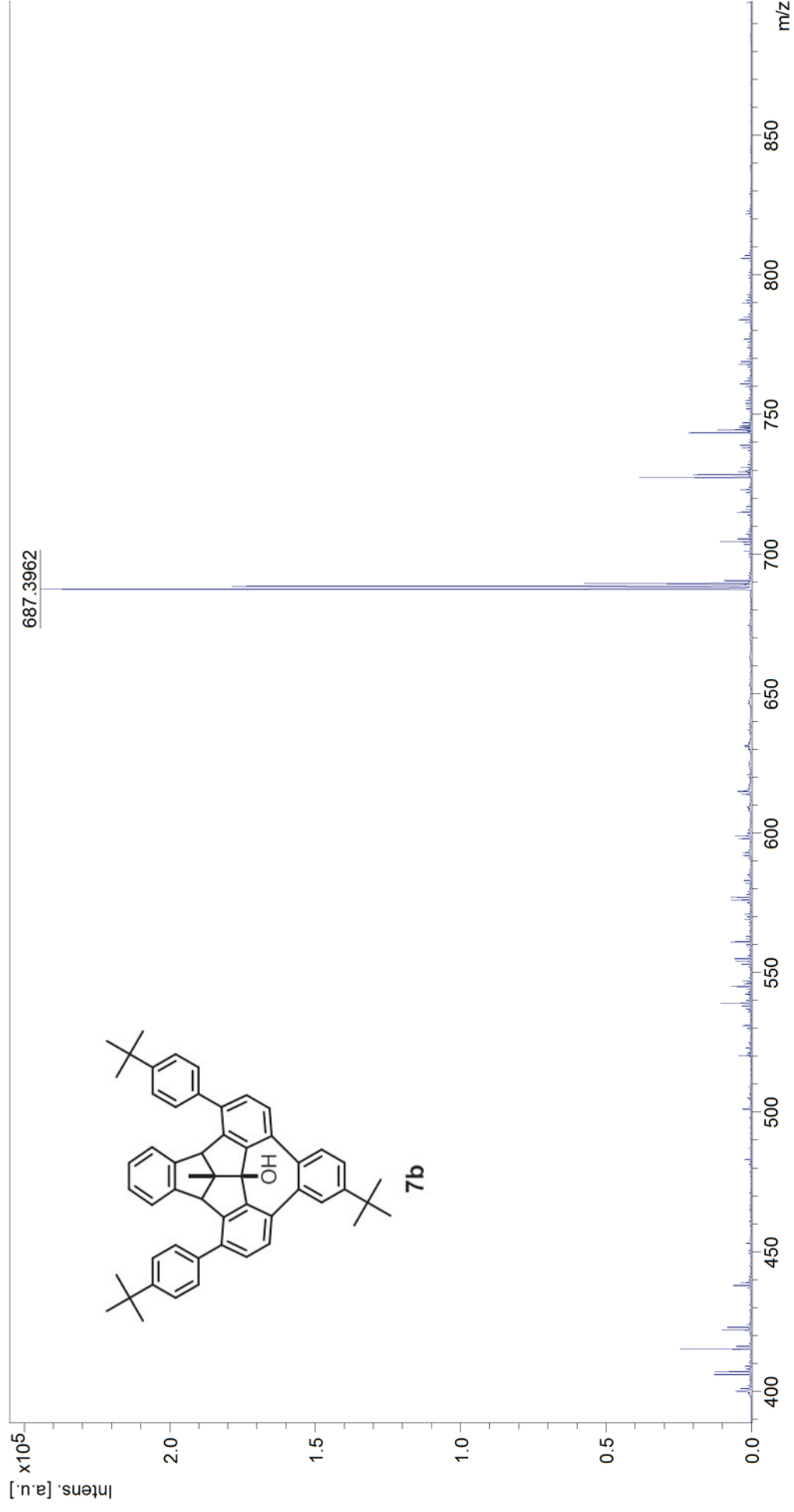
Abundant Isotopic (theoretical)[M+Na]⁺ : 727.3910 (experimental)[M+Na]⁺: 727.3915 error(ppm): 0.69
Monoisotopic (theoretical)[M+Na]⁺ : 727.3910



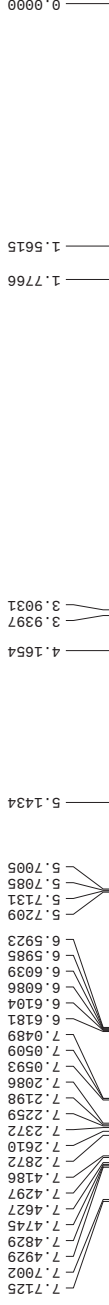
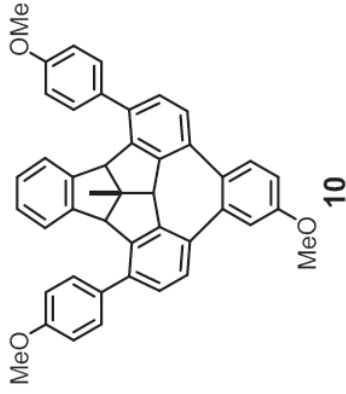
G:\MS Angew\18.Eric_9a_4tBu_mono_OH(A20) good\0_A22\11SRef

Comment 1

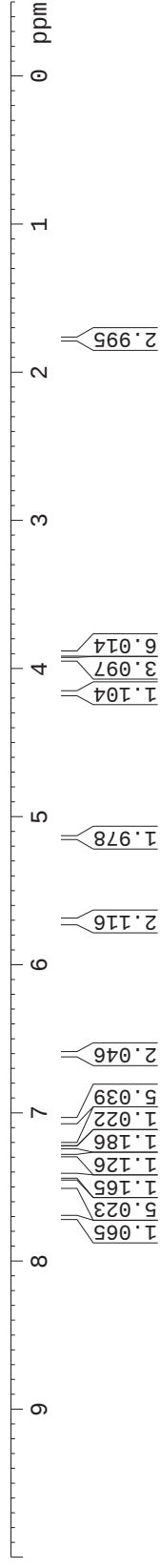
Comment 2

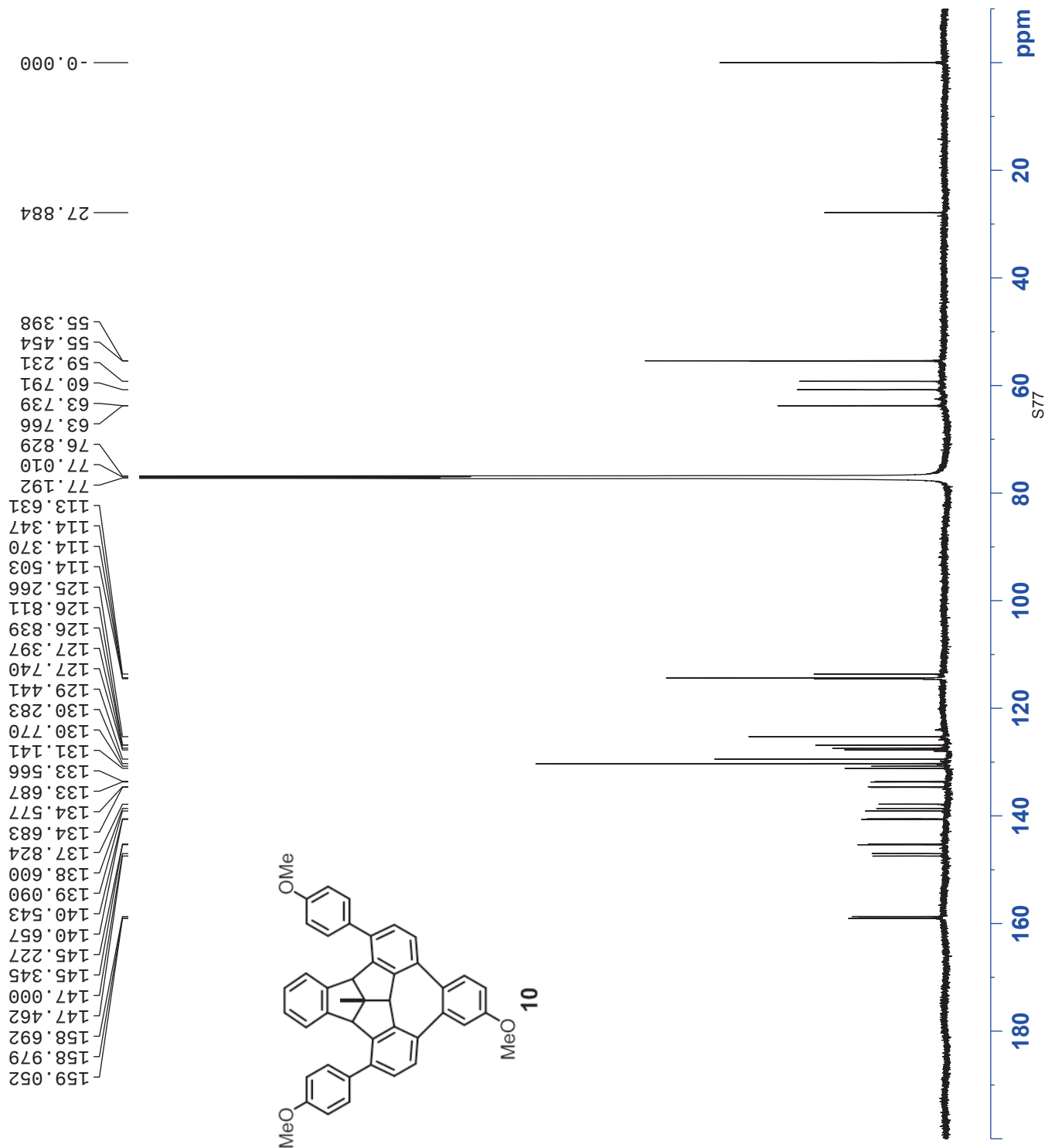
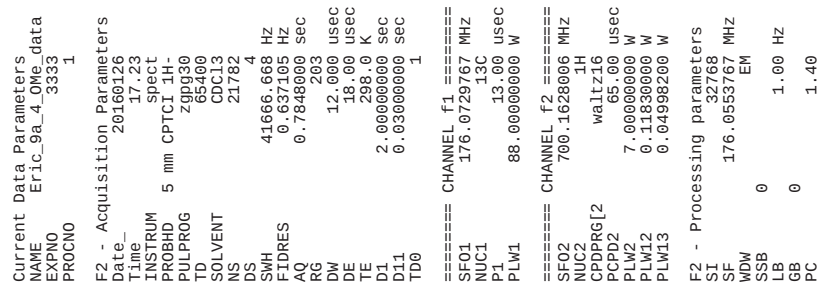


AV400Q NMR



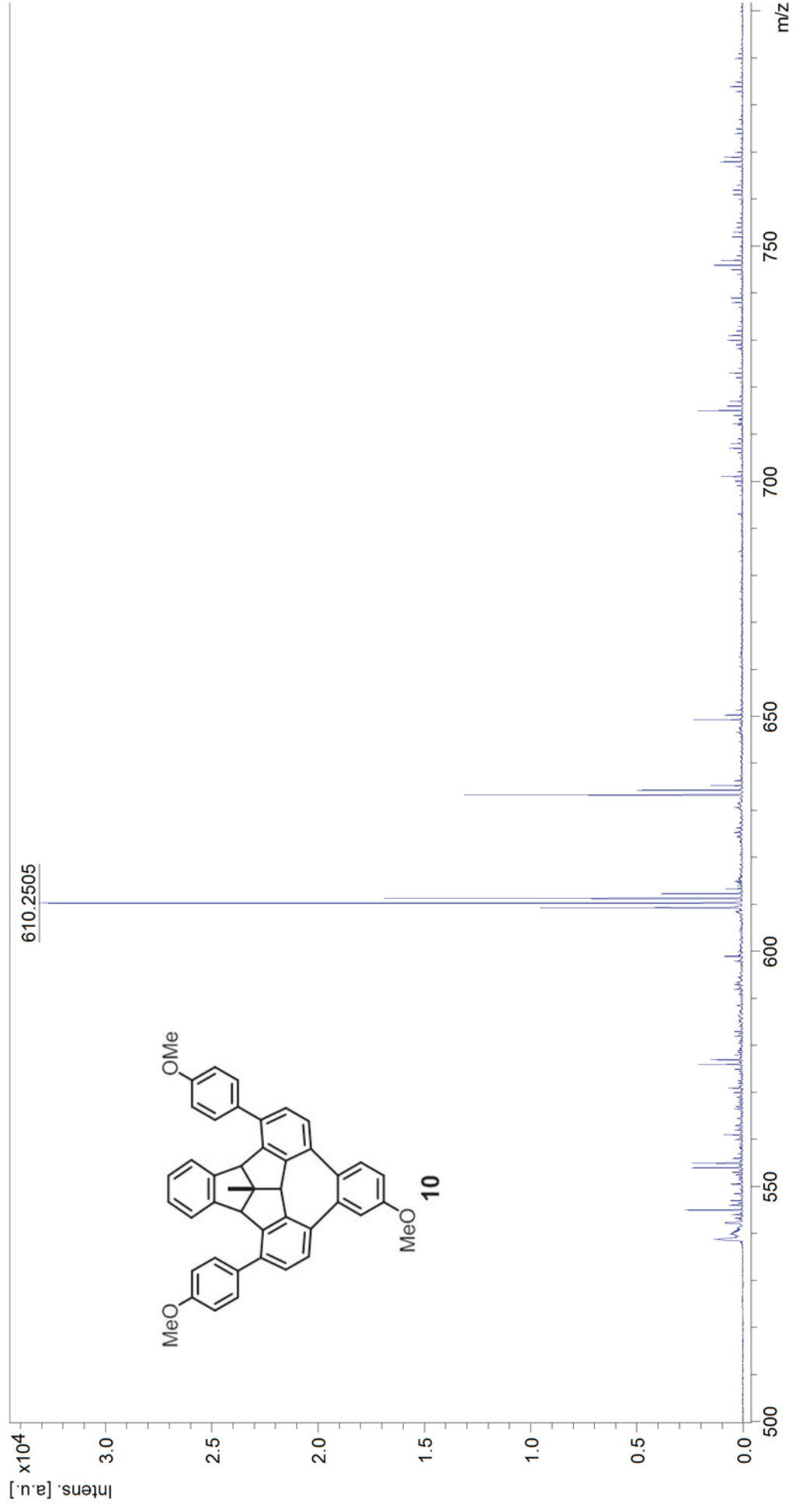
Current Data Parameters
NAME Eric_9a_4_OME_data
EXPNO 111
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160126
Time 16.56
INSTRUM spect
PROBHD 5 mm CPTCL1H1
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 41
DS 2
SWH 14007.744 Hz
FIDRES 0.436229 Hz
AQ 1.162177 sec
RG 9
RW 35.416 usec
DE 10.00 usec
TE 298.0 K
D1 1.0000000 sec
D0 1
===== CHANNEL f1 =====
SF01 700.1643238 MHz
NUC1 1H
P1 8.45 usec
PL1 7.00000000 W
F2 - Processing parameters
SI 65536
SF 700.1600158 MHz
WDW EN
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Comment 1

Comment 2

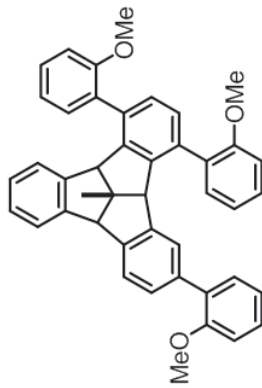
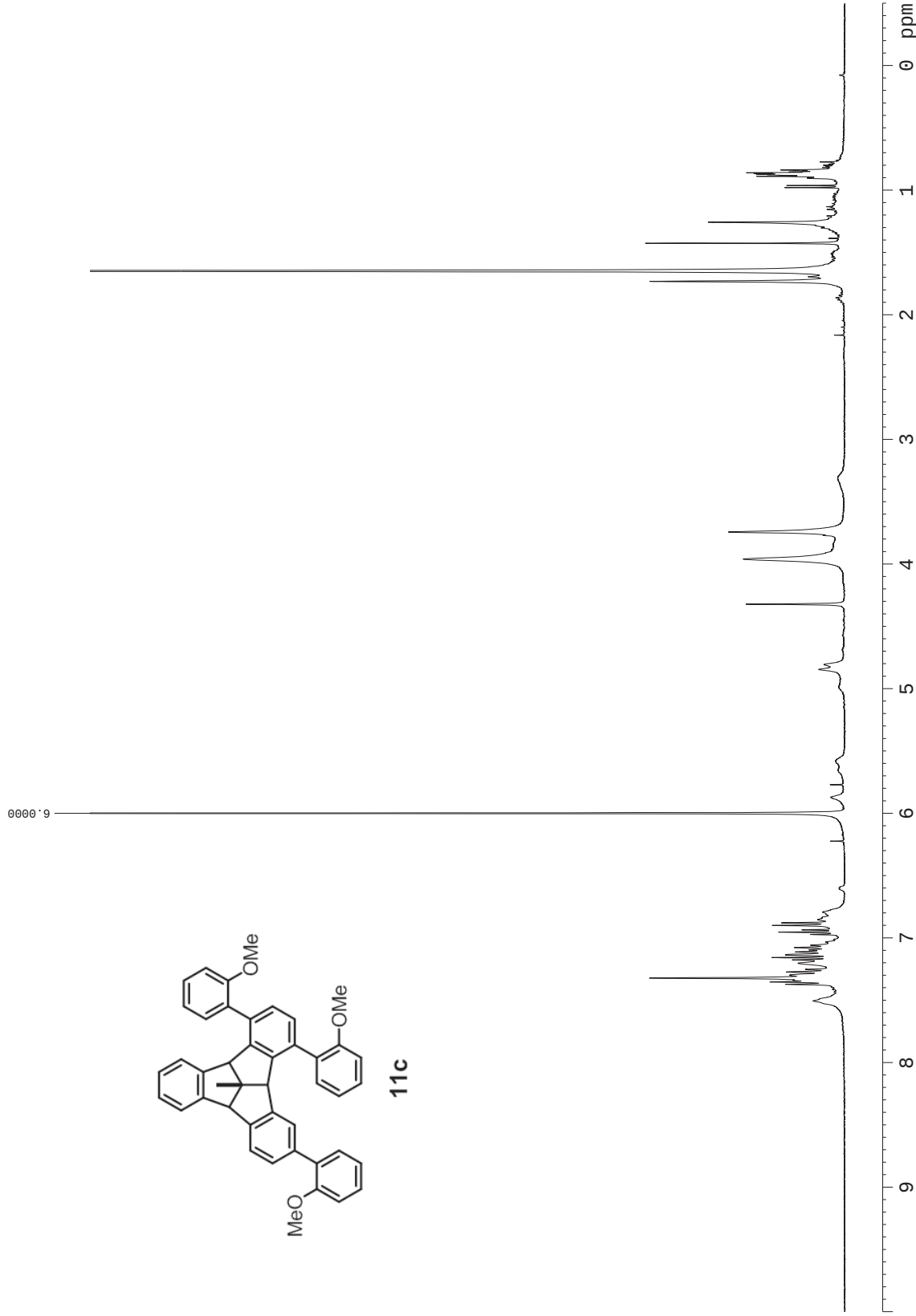


22 °C

AV400Q NMR



Current Data Parameters
NAME Eric_9a_2_OMe_data
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160419
Time 12.35 h
INSTRUM spect
PROBHD 5mm QNP 1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 51
DS 4
SWH 8012.826 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 203
RW 62.60 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
SFO 400.1324701 MHz
NUC1 1H
P1 15.00 usec
PLW1 8.31000042 W
F2 - Processing parameters
SI 65536
SF 400.1305137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

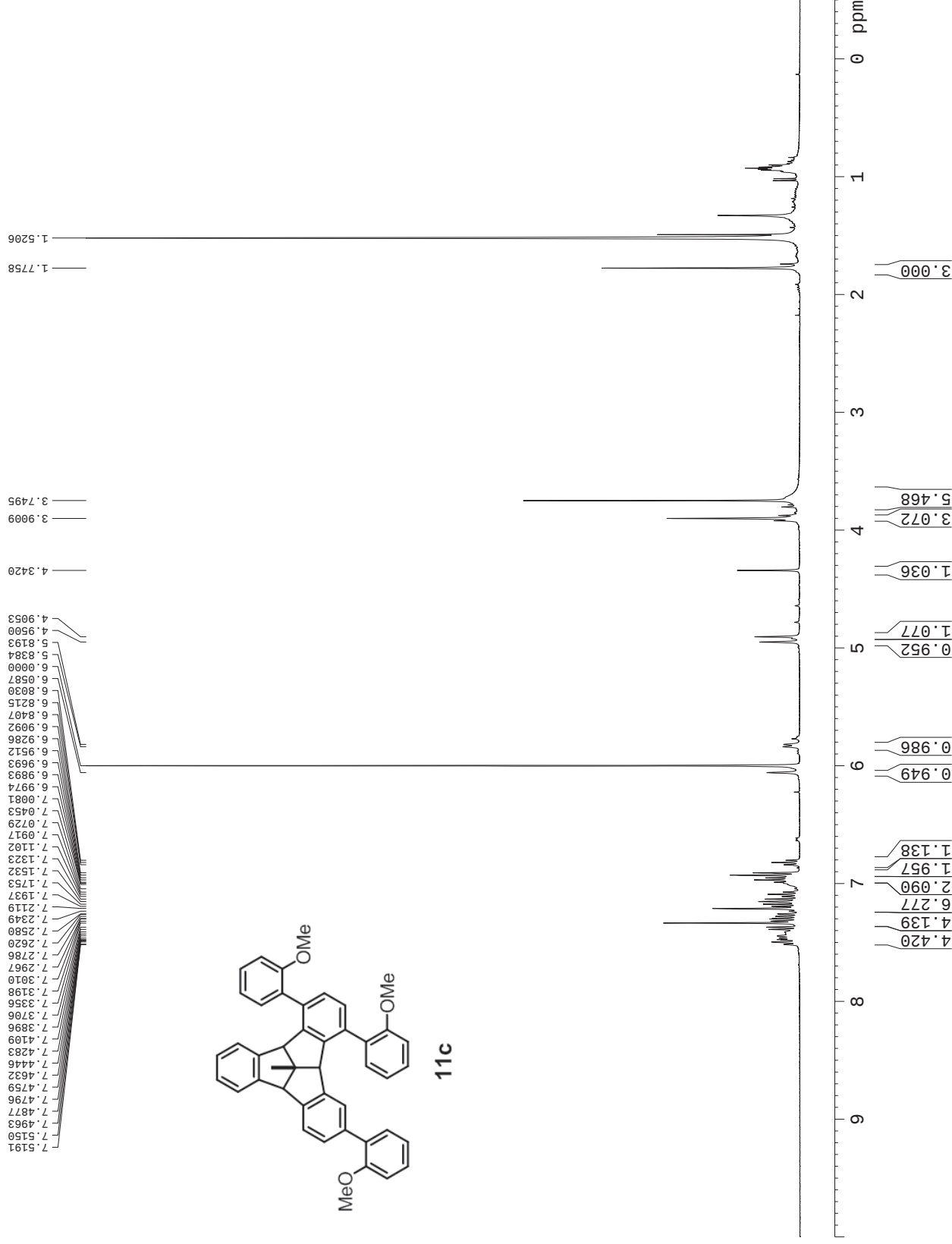


11c

AV400Q NMR



11C



60 °C



Current Data Parameters
NAME Eric_9a_2_OME_700
EXPNO 3333
PROCNO 1

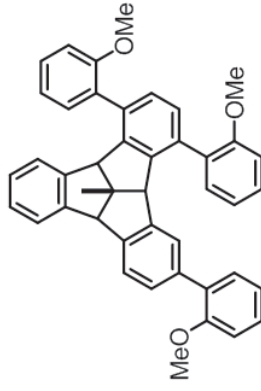
F2 - Acquisition Parameters
Date_ 20160512
Time 12.24
INSTRUM Spect
PROBHD 5 mm CPTCI-1H-
PULPROG zgpg30
TD 65400
SOLVENT CDCl3
DS 25632
NS 4
SWH 41666.668 Hz
FIDRES 0.637105 Hz
AQ 0.7848000 sec
RG 203
DW 12.000 usec
DE 18.00 usec
TE 333.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 176.0729767 MHz
NUC1 13C
P1 13.00 usec
PLW1 88.00000000 W

===== CHANNEL f2 =====
SF02 700.1628006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 65.00 usec
PLW2 7.00000000 W
PLW12 0.11830000 W
PLW13 0.04998200 W

F2 - Processing parameters
SI 32768
SF 176.0556367 MHz
WDW EM
SSB 0
LB 0 1.00 Hz
GB 0
PC 1.40

155.875
146.219
145.037
144.576
136.879
135.052
132.215
131.122
131.063
130.967
130.101
129.837
128.951
128.620
127.992
126.920
126.756
126.080
123.796
122.903
120.915
120.250
120.198
111.358
110.558
99.427
73.938
73.780
73.623
62.498
60.260
60.145
59.359
55.376
55.216
55.117



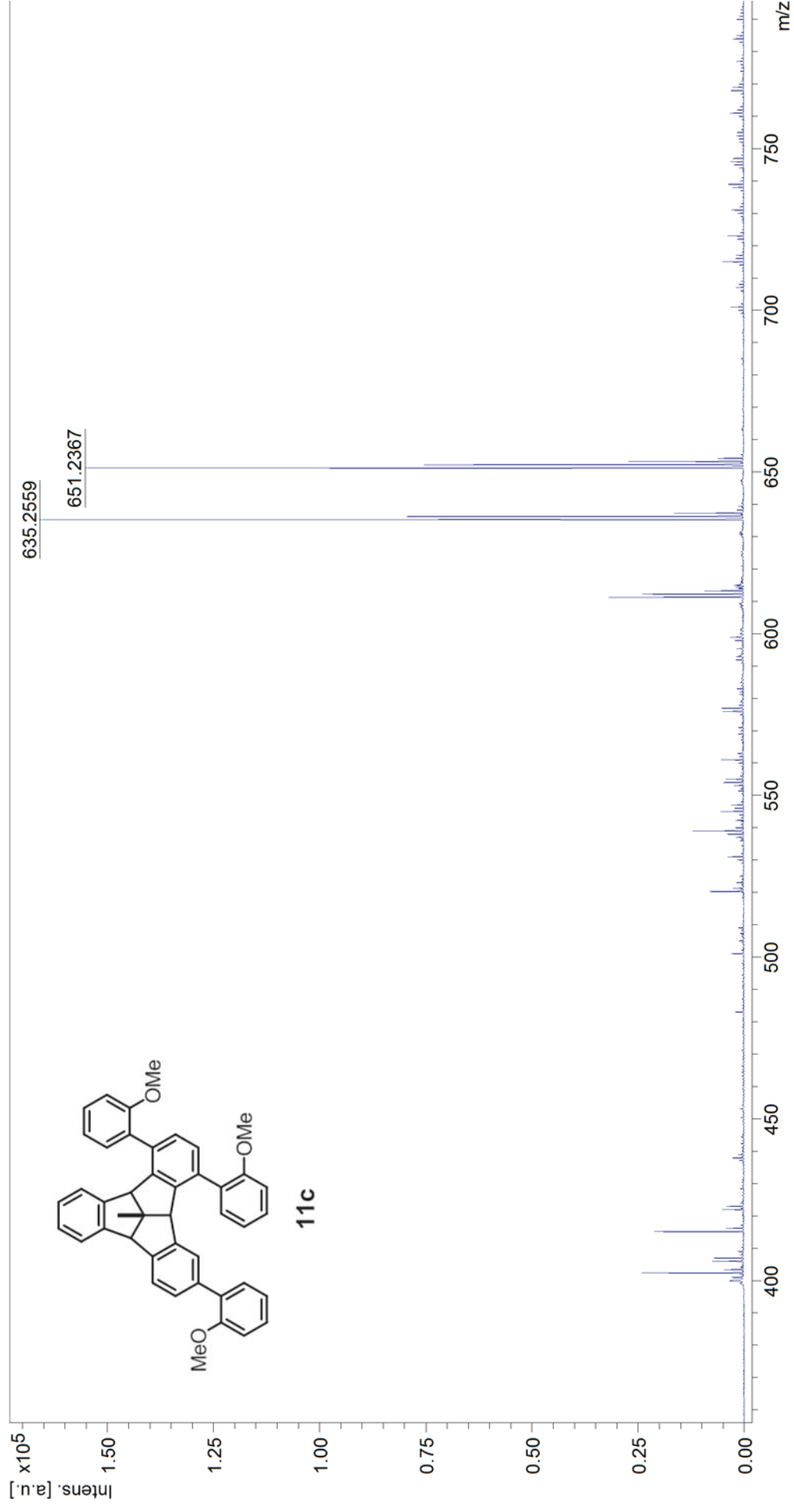
11c

180 160 140 120 100 80 60 40 20 ppm

S81

Comment 1

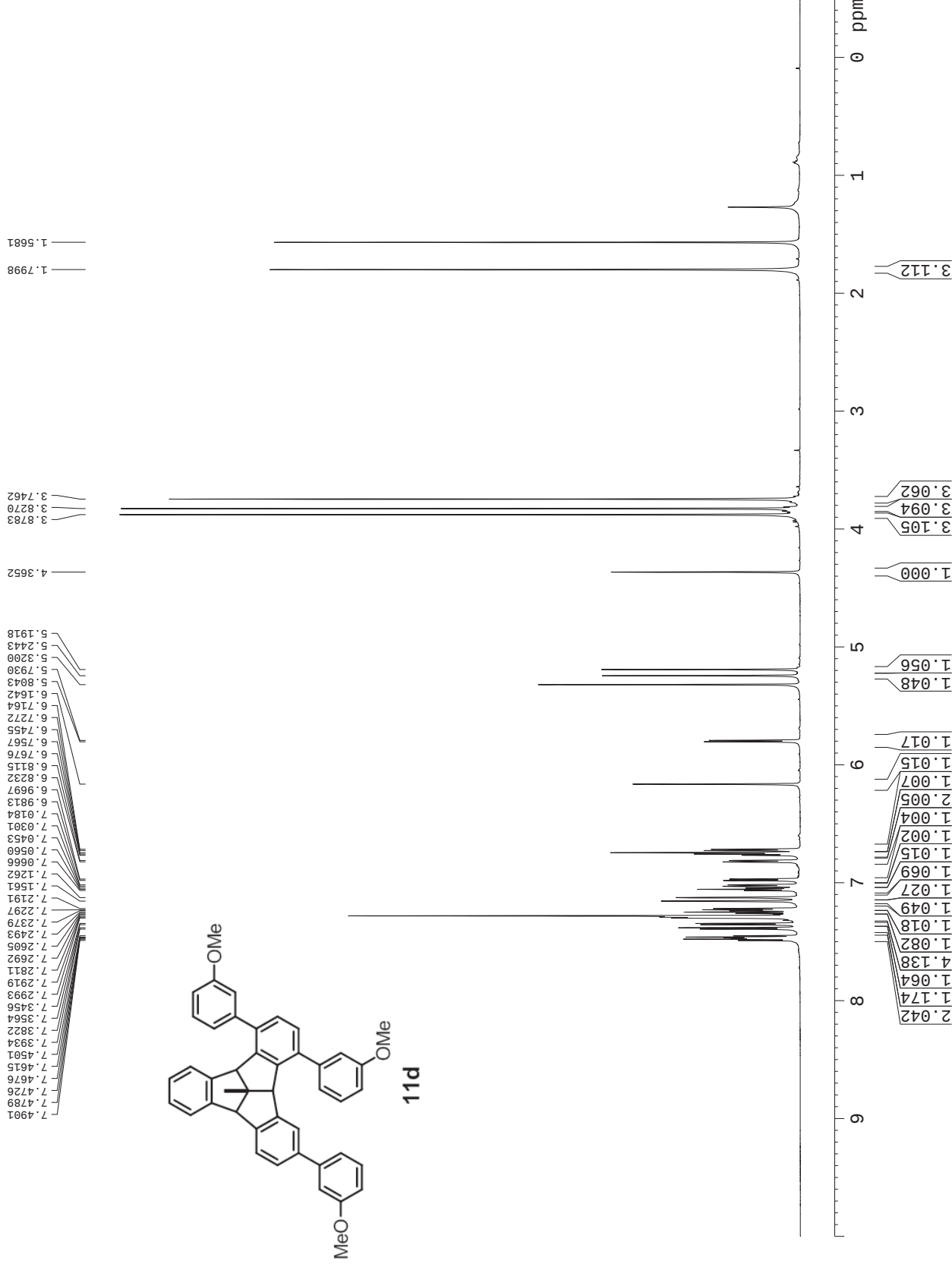
Comment 2



AV400Q NMR



Current Data Parameters
NAME Eric_9a_3_OMe_mono_data
EXPNO 111
PROCNO 1
F2 - Acquisition Parameters
Time 20.00
Time 14.39
INSTRUM spect
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 64
DS 2
SWH 14097.7 Hz
FIDRES 0.32259 Hz
AQ 1.162177 sec
RG 8
SFO 50.45 usec
DE 10.00 usec
TE 298.0 K
D1 1.50000000 sec
T00 1.00000000 sec
===== CHANNEL f1 =====
SFO1 780.164328 MHz
NUC1 1H
P1 8.45 usec
PL1 7.00000000 W
F2 - Processing parameters
SFO2 780.164328 MHz
SF 780.160268 MHz
WDW EM
SSB 0
GB 0
PC 1.00





Current Data Parameters
NAME Eric_9a_3_0Me_mono_data
EXPNO 3333
PROCNO 1

F2 - Acquisition Parameters

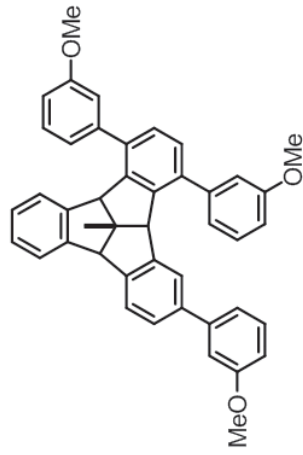
Date_ 20160112
Time_ 14.53
INSTRUM spect
PROBHD 5 mm CPTCI 1H-
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 2000
DS 4
SWH 41666.668 Hz
FIDRES 0.635783 Hz
AQ 0.7864320 sec
RG 203
DW 12.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 176.0729767 MHz
NUC1 13C
P1 13.00 usec
PL1 88.00000000 W

===== CHANNEL f2 =====
SF02 796.1628096 MHz
NUC2 1H
PCPDG[2] Waltz16
PCPD2 65.00 usec
PLW2 7.00000000 W
PLW12 0.11830000 W
PLW13 0.0498200 W

F2 - Processing parameters
SI 32768
SF 176.0553087 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

160.125
146.460
145.959
145.680
144.857
144.264
144.140
144.054
143.923
142.834
140.156
139.130
139.076
130.672
130.438
130.170
130.167
129.638
127.698
127.220
126.761
126.035
124.843
124.395
124.172
121.977
121.713
119.902
115.330
115.259
113.236
113.214
113.150
112.189
62.913
62.854
62.744
60.650
55.752
55.555
55.521
54.149
53.996
53.840
53.686
53.532
28.523



11d

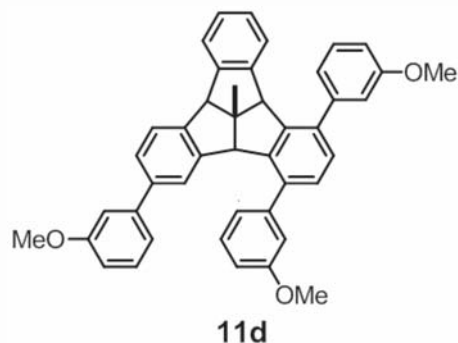
180 160 140 120 100 80 60 20 ppm

S84

Accurate Mass Measurement

Sample Name : Er-12 **Group :** OC1
Sample Supplier : Er. Wang
Sample Filename : MFB2016_026.

Instrument : Autospec
Ionisation Method : EI
Matching Method : HR with calibration PFK
Resolution : > 7000
Substance Inlet : EI Schubstange

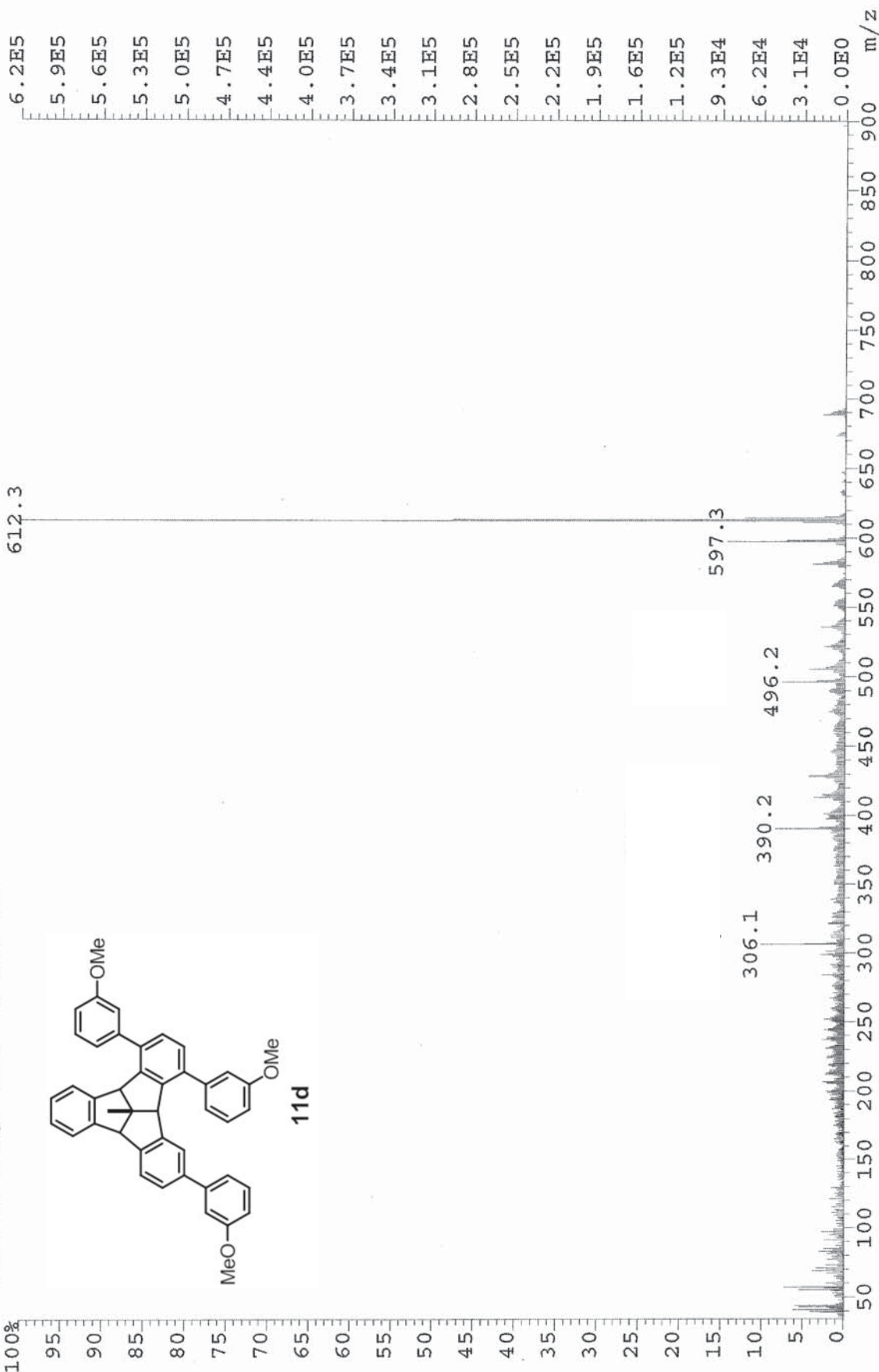


Measured PFK Mass(es) :	616,96327	Deviation [mmu] :	0,49 [mmu]
Measured Ion Mass(es) :	612,26541	Deviation [ppm] :	0,80 [ppm]
Calculated Ion Mass(es) :	612,26590		
Potential Molecular Formula :	C ₄₄ H ₃₆ O ₃ ⁺		

Comment : Measured and calculated masses are true ion masses, taking into account the mass of lost (or added) electrons.

Bielefeld, 17.02.2016

File:EI2016 074 Ident:159_181 Win 500PPM Acq:15-FEB-2016 22:50:05 +17:35 Cal:EI_POS_CAL_900
 AutoSpec EI+ Magnet BpM:612 BpI:622353 TIC:6185087 Flags:HALL
 File Text:Er. Wang, OC1, Er-12, HWP



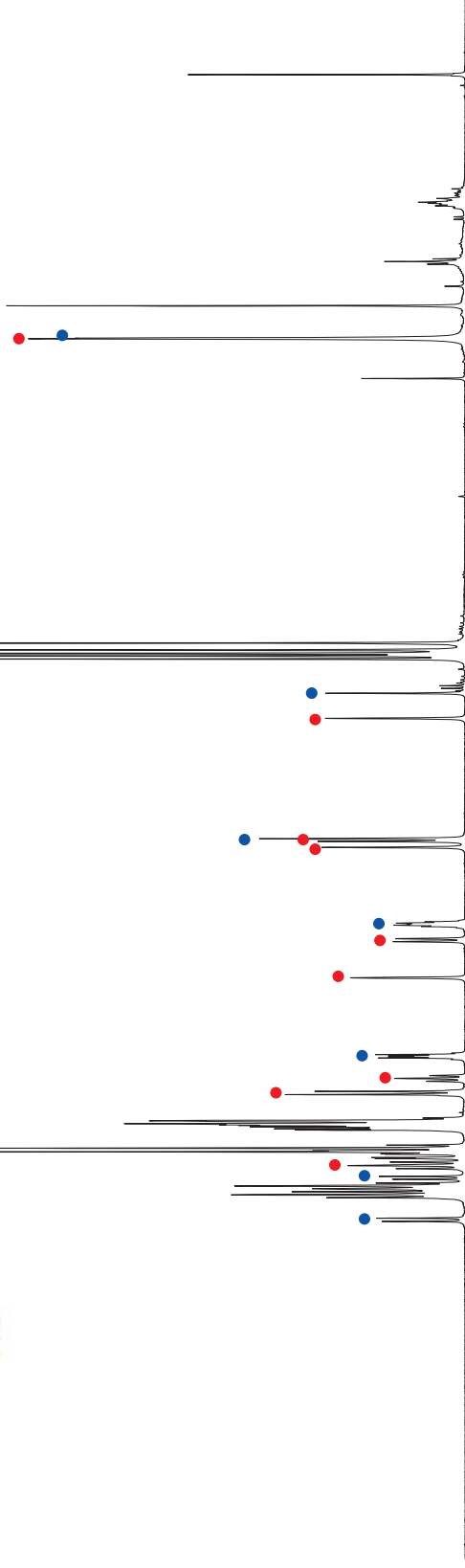
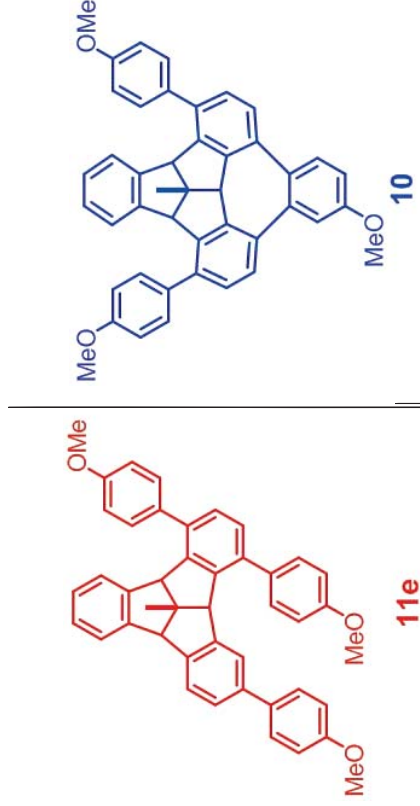
AV400Q NMR



Current Data Parameters
NAME Eric_9a_4_0Me
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160916
Time 15.22 h
INSTRUM Spect
PROBHD 5mm QNP 1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 34
DS 4
SWH 8012.826 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 99.5
DE 626.60 usec
TE 295.1 K
D1 1.00000000 sec
SFO 400.222471 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2260101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1.7918
1.7875
1.5697

7.7278
7.7062
7.6681
7.5491
7.5283
7.5079
7.4901
7.4702
7.4446
7.4249
7.3730
7.3526
7.3287
7.3050
7.2983
7.2760
7.2727
7.2599
7.2526
7.2354
7.2147
7.1131
7.1046
7.0971
7.0914
7.0826
7.0779
7.0705
7.0554
7.0512
7.0327
6.8749
6.8531
6.7848
6.7659
6.7470
6.6284
6.6202
6.6058
6.0891
5.8457
5.8261
5.7437
5.7354
5.7301
5.7213
5.7131
5.2128
5.1725
5.1548
4.3450
4.1762
3.9459
3.9249
3.9087
3.8852
3.8385



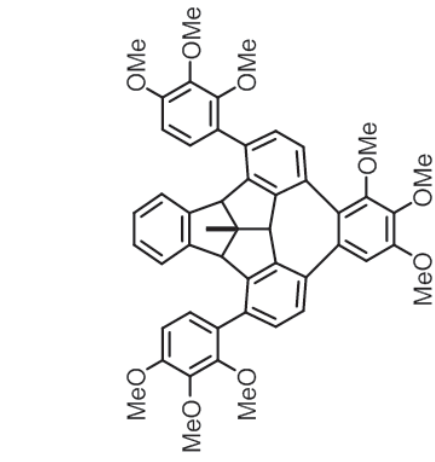
ppm

0.894
7.375
1.707
2.177
0.863
7.520
11.005
2.082
1.024
1.647
1.000
1.050
1.619
1.046
1.046
1.046
1.580
1.033
0.875
2.483
3.039
4.773
3.058
3.120
3.005
2.319

S87

22 °C

AV400Q NMR



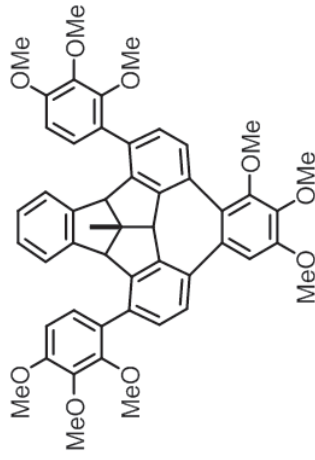
16



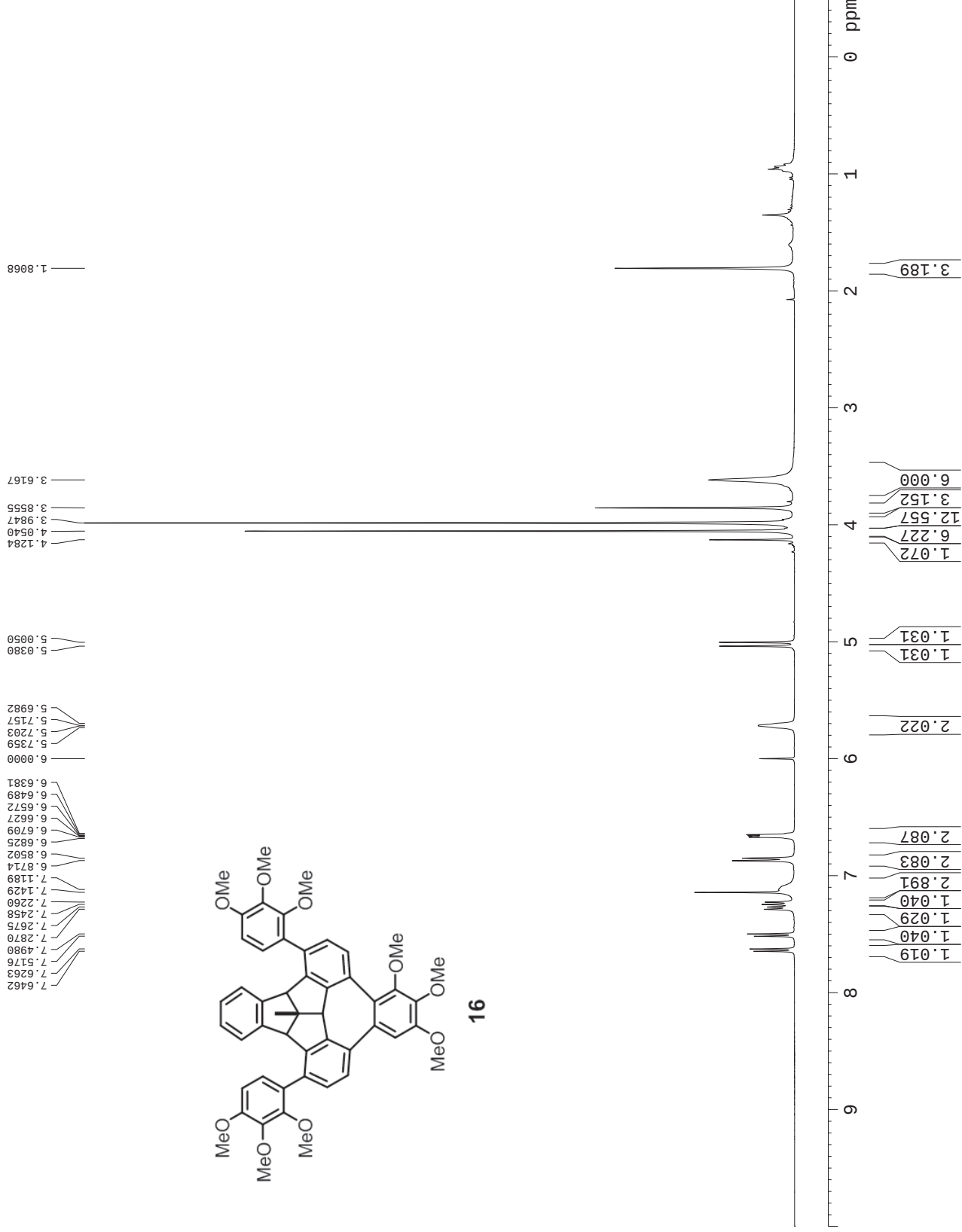
885

60 °C

AV400Q NMR



16



689

Current Data Parameters
Date_ 20170328
Time_ 14:00:00
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170328
Time_ 14:00:00
INSTRUM spect
PROBHD 5mm
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 64
DS 2
SWH 8932.822 MHz
FIDRES 0.244552 Hz
AQ 2.8447234 sec
RG 62.460 usec
DM 62.460 usec
TE 300.2 K
TE 333.2 K
D1 1.00000000 sec
SFO1 400.1324708 MHz
N1 201.2612701 MHz
P1 15.00 usec
PL1 8.31000042 W
F2 - Processing parameters
SI 32768
SF 400.1324708 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

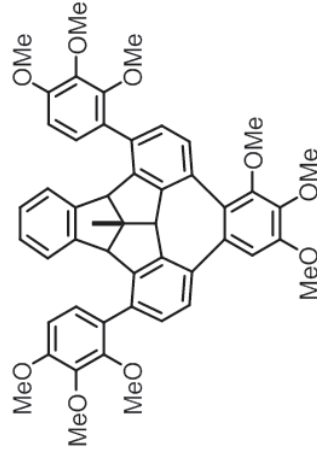
60 °C



Current Data Parameters
NAME_1 E1C_9a_2_3_0Me_mono_data
EXPNO 444
PROCNO 1

F2 - Acquisition Parameters
Date_ 2011-08-16
Time_ 16:02 h
INSTRUM spect
PROBHD Z824601_0021 (4
PULPROG zgpg30
D11 0.03000000 sec
SOLVENT CDCl3
NS 600
DS 4
SWH 24038.461 Hz
FIDRES 0.36000000 Hz
AQ 1.3631488 sec
RG 203
DW 26.800 usec
DE 6.50 usec
TE 300.2 K
D11 0.03000000 sec
TD0 1
SFO1 100.628298 MHz
N1 1
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SFO2 400.1316005 MHz
N2 1H
NUC2 1H
PCPRG2 waltz16
PCPDZ 50.00 usec
PLW2 8.31000042 W
PLW12 0.23083600 W
PLW13 0.11611000 W
F2 - Processing parameters
SI 32768
SF 100.6129249 MHz
WDW EM
SSB 0
GB 0
PC 1.40

153.533
153.439
152.166
151.766
151.489
151.423
147.917
147.833
145.397
143.204
143.182
141.887
141.498
140.832
134.620
134.271
134.028
133.433
129.828
129.116
128.655
128.418
128.381
126.359
126.144
126.099
125.579
125.504
125.458
124.939
109.410
108.262
108.201
74.055
73.780
73.504
64.757
64.593
60.977
60.812
60.718
60.630
60.281
59.127
56.378
56.355
56.153
27.645



16

ppm

Thermo QEFMS Analysis Report

Analysis Info

Sample Name :	Eric_27	Reference No.:	Qhfc004
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI pos, 3.2kV, by LC, with sheath gas		

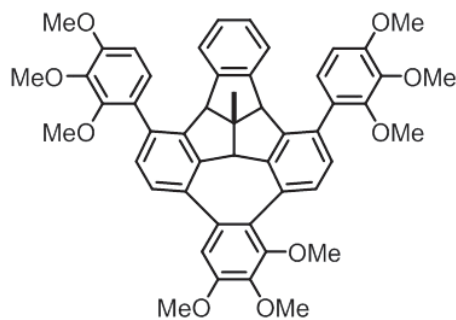
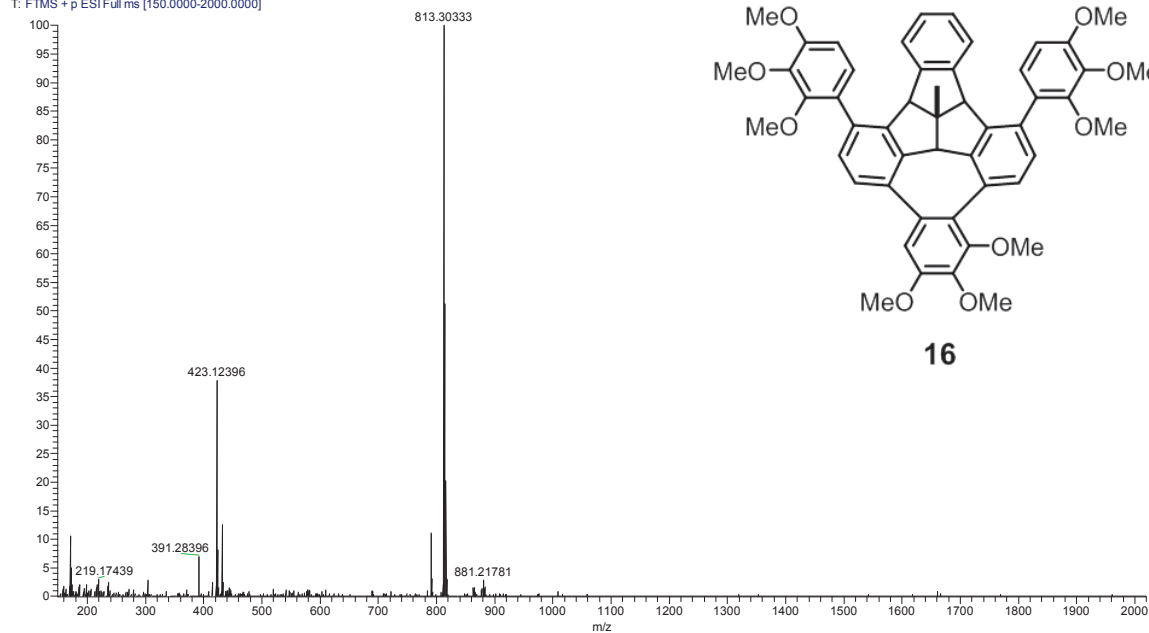
Accurate Mass Measurement

Molecular formula :	C ₅₀ H ₄₆ O ₉
Experimental Mass [M+Na] ⁺ :	813.30333
Theoretical Mass [M+Na] ⁺ :	813.30340
Error (ppm) :	0.0

D:\Raw data\qhfc004

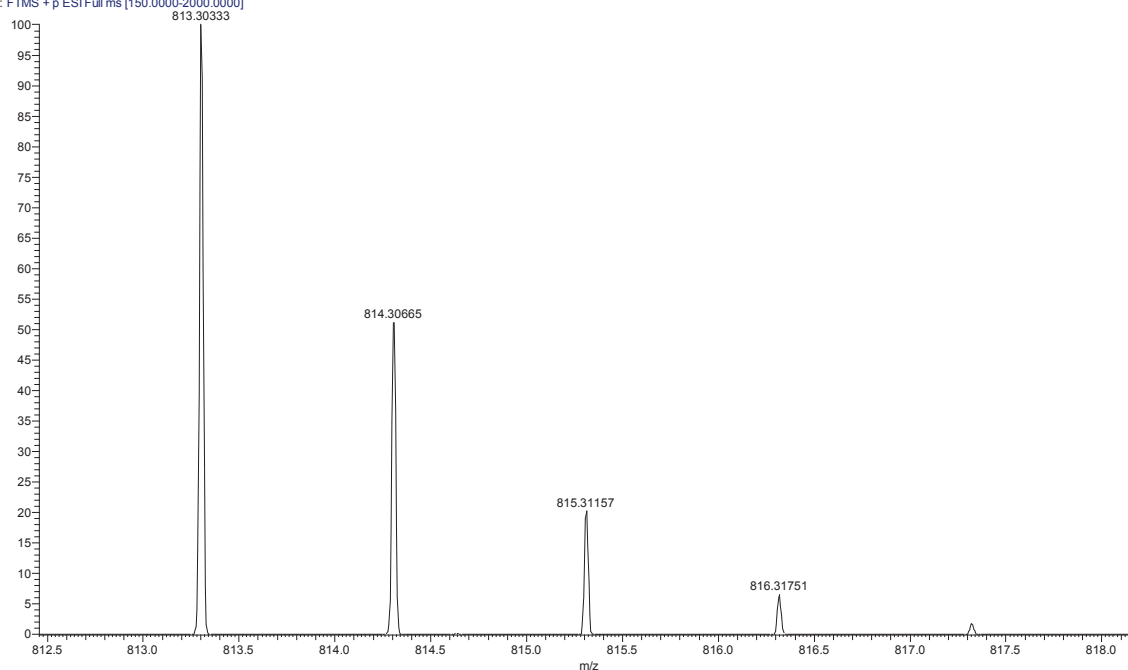
02/08/17 10:39:31

qhfc004 #193 RT: 0.87 AV: 1 SB: 64 0.53-0.74, 0.92-0.99 NL: 5.73E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



16

qhfc004 #193 RT: 0.87 AV: 1 SB: 64 0.53-0.74, 0.92-0.99 NL: 5.73E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



AV400Q NMR

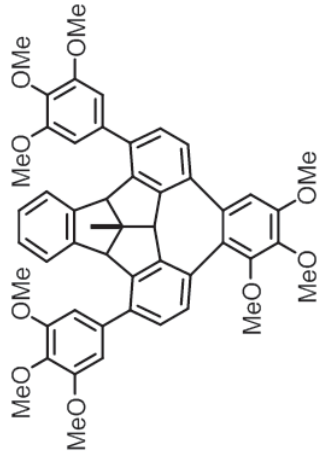


Current Data Parameters
NAME: S92
EXPNO: 1
PROCNO: 11
F2 - Acquisition Parameters
Date_: 20170118
Time: 14.11
INSTRUM: spect
PROBHD: 5mm
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 39
DS: 2
SWH: 8812.822 MHz
FIDRES: 0.244552 Hz
AQ: 2.8447203 sec
RG: 327.68
DM: 62.400 usec
DE: 1.00000000 sec
TE: 295.1 K
D1: 1.00000000 sec
SFO1: 400.1324708 MHz
N1: 13C
NUC1: 13C
PL1: 15.00 usec
PLW1: 8.31000042 W
F2 - Processing parameters
SI: 65536
SF: 400.1324708 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

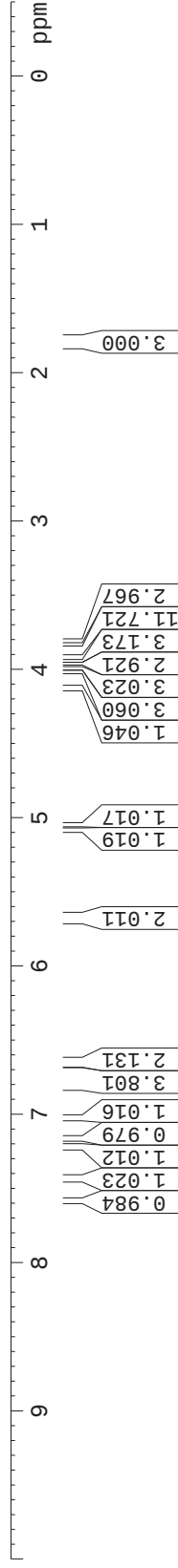
1.5690
1.7890

4.1256
4.0144
3.9984
3.9554
3.9493
3.8686
3.8095

7.5911
7.5713
7.4420
7.4224
7.2600
7.2280
7.2085
7.1747
7.1548
7.0247
6.7555
6.7355
6.6331
6.6548
6.6487
6.6405
6.6299
6.6089
6.6990
6.6907
6.6870
6.6776
6.6682
6.645
6.6561
5.6457
5.0810
5.0524

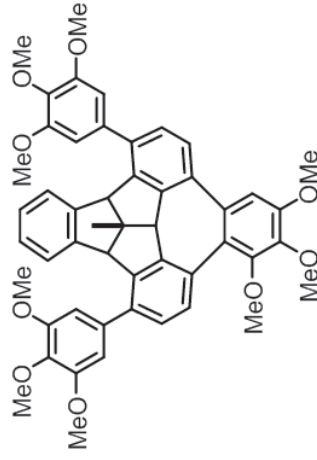


17



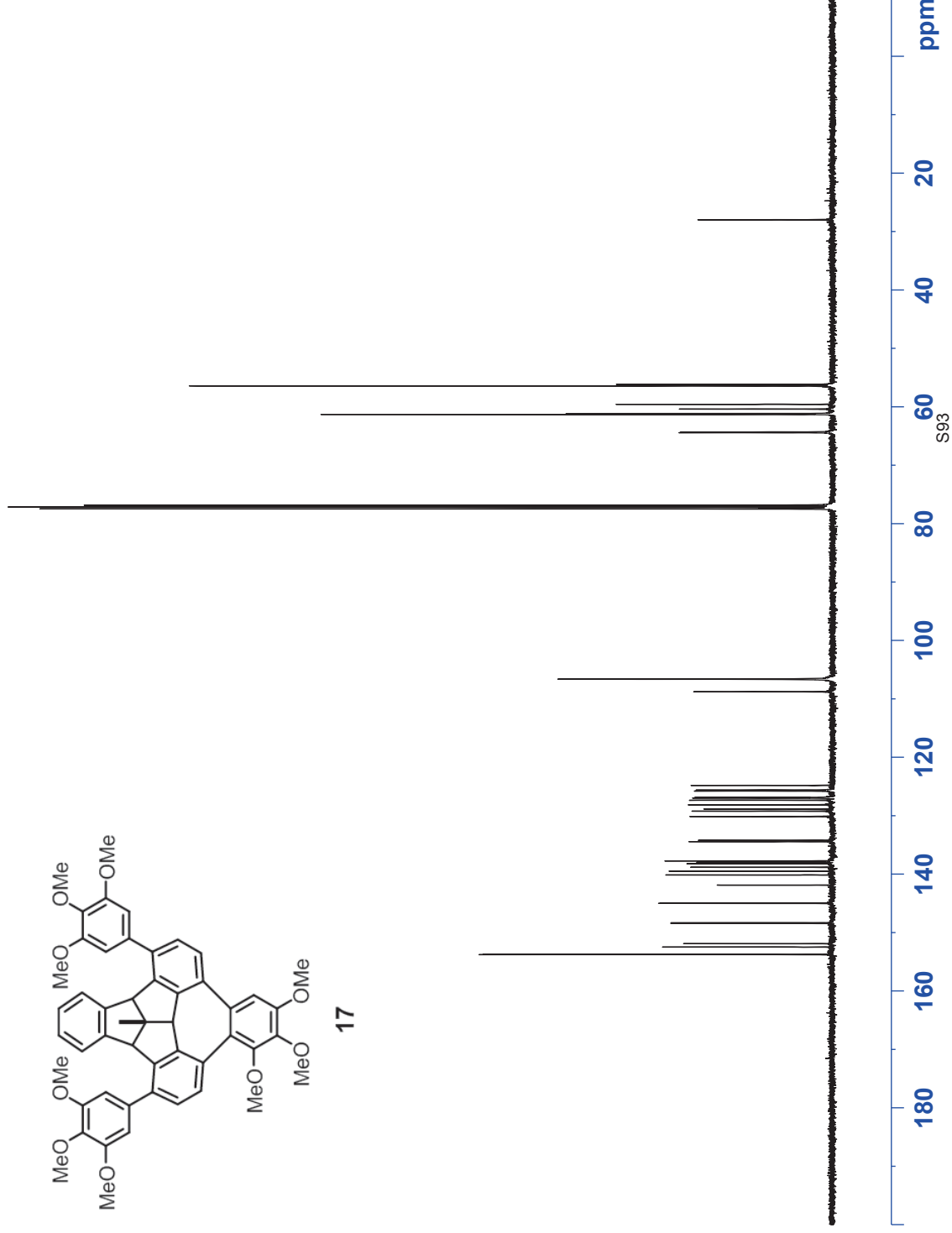


153.775
153.732
152.484
151.909
148.439
148.329
145.011
144.946
141.880
140.149
139.500
138.831
138.218
138.082
137.882
137.785
137.735
134.434
134.219
130.132
129.224
128.852
128.132
127.350
126.971
126.876
125.778
125.612
124.800
108.790
106.621
77.479
77.160
76.842
64.432
64.310
61.308
61.194
61.148
60.391
59.576
56.426
56.163
27.988



17

Current Data Parameters
NAME: E1c_8a_3_4_1_0me_mono_data
EXPNO: 3
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 20110707
Time: 17:07 h
INSTRUM: spect
PROBHD: Z824601_0021 (1H)
PULPROG: zgpg30
PCPDZ: 0.00000000 sec
SOLVENT: CDCl3
NS: 979
DS: 4
SWH: 24038.461 Hz
FIDRES: 0.00000000 Hz
AQ: 1.3631488 sec
RG: 203
DW: 26.800 usec
DE: 6.50 usec
TE: 295.2 K
D11: 2.00000000 sec
D1: 0.03000000 sec
TD0: 1
SF01: 100.6228298 MHz
NUC1: 13C
PL1: 0.50 usec
PLW1: 41.25000000 W
SF02: 400.1316005 MHz
NUC2: 1H
PCPDZ2: waitz20
PCPDZ: 0.00000000 usec
PLW2: 8.31000042 W
PLW12: 0.23083000 W
PLW13: 0.11611000 W
F2 - Processing parameters
SI: 32768
SF: 100.6127671 MHz
WDW: EM
SSB: 0
GB: 0
PC: 1.40



Thermo QEFMS Analysis Report

Analysis Info

Sample Name :	Eric_30	Reference No.:	Qhfc008
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI pos, 3.0kV, by LC, with sheath gas		

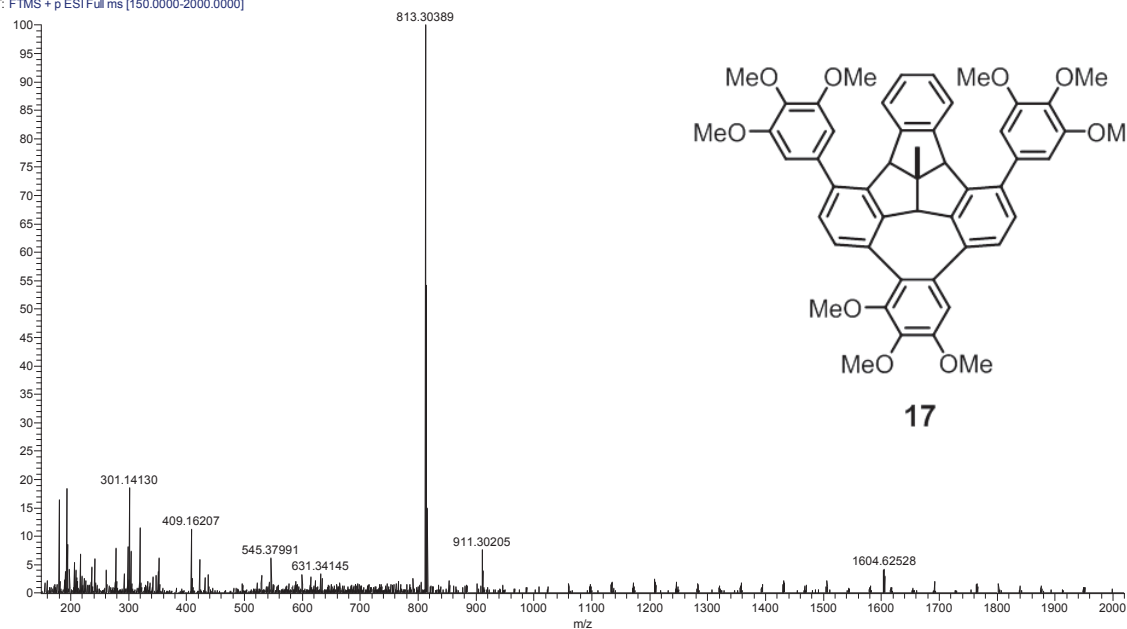
Accurate Mass Measurement

Molecular formula :	C ₅₀ H ₄₆ O ₉
Experimental Mass [M+Na] ⁺ :	813.30389
Theoretical Mass [M+Na] ⁺ :	813.30340
Error (ppm) :	0.6

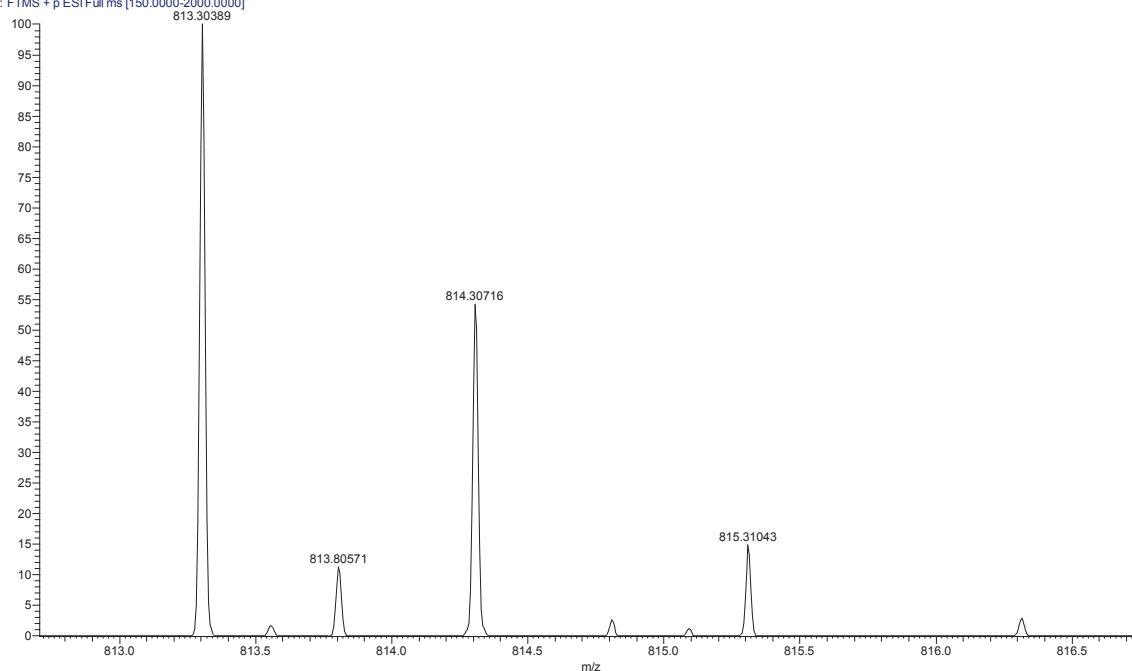
D:\Raw data\qhfc008_170210173105

02/10/17 17:39:17

qhfc008_170210173105 #197 RT: 0.89 AV: 1 SB: 94 0.60-0.80, 0.95-
T: FTMS + p ESI Full ms [150.0000-2000.0000]



qhfc008_170210173105 #197 RT: 0.89 AV: 1 SB: 94 0.60-0.80, 0.95-1.16 NL: 1.98E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



AV400Q NMR

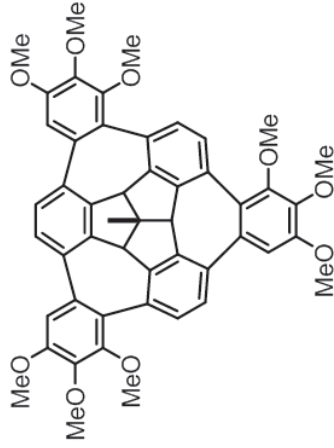


Current Data Parameters
NAME Eric_9a_2_3_4_Omc_data
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170111
Time 17:58 h
INSTRUM spect
PROBHD zgpg30
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2
DS 2
SWH 8612.850 Hz
FIDRES 0.244532 Hz
AQ 2.0447512 sec
RG 114
DW 62.400 usec
DE 3.152 usec
TE 296.2 usec
D1 1.00000000 sec
TD0 1
SFO 400.1324700 MHz
NUC1 13C
P1 15.00 usec
PLW1 8.31000042 W
F2 - Processing parameters
SI 65536
SF 400.1324700 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

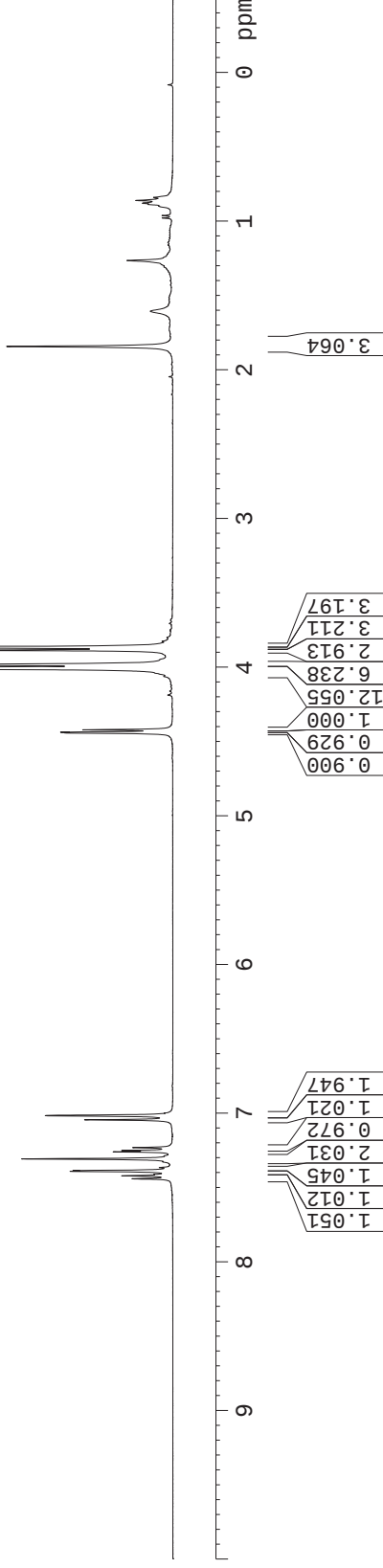
1.0693
1.8431

3.0624
3.0609
3.0594
3.0579
3.0564
4.0098
4.0083
4.0068
4.4219
4.4382
4.4427

7.0166
7.0443
7.0434
7.2314
7.2515
7.2600
7.2609
7.2869
7.3073
7.3275
7.3655
7.3863
7.3908
7.4121
7.4211
7.4410



18



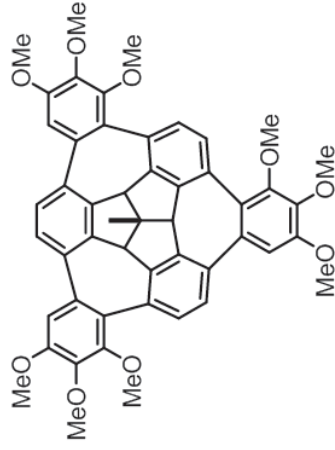
S95



Current Data Parameters
NAME Eric_9a_2_3_4_OME_data
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20110103
Time 18.03 h
INSTRUM spect
PROBHD Z824601.0021
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 185
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
TE 300.2 K
DE 95.0 usec
D1 2.00000000 sec
D11 0.03000000 sec
D12 1
D13 1
D14 1
D15 1
D16 1
D17 1
D18 1
D19 1
D20 1
D21 1
D22 1
D23 1
D24 1
D25 1
D26 1
D27 1
D28 1
D29 1
D30 1
D31 1
D32 1
D33 1
D34 1
D35 1
D36 1
D37 1
D38 1
D39 1
D40 1
D41 1
D42 1
D43 1
D44 1
D45 1
D46 1
D47 1
D48 1
D49 1
D50 1
D51 1
D52 1
D53 1
D54 1
D55 1
D56 1
D57 1
D58 1
D59 1
D60 1
D61 1
D62 1
D63 1
D64 1
D65 1
D66 1
D67 1
D68 1
D69 1
D70 1
D71 1
D72 1
D73 1
D74 1
D75 1
D76 1
D77 1
D78 1
D79 1
D80 1
D81 1
D82 1
D83 1
D84 1
D85 1
D86 1
D87 1
D88 1
D89 1
D90 1
D91 1
D92 1
D93 1
D94 1
D95 1
D96 1
D97 1
D98 1
D99 1
D100 1
D101 1
D102 1
D103 1
D104 1
D105 1
D106 1
D107 1
D108 1
D109 1
D110 1
D111 1
D112 1
D113 1
D114 1
D115 1
D116 1
D117 1
D118 1
D119 1
D120 1
D121 1
D122 1
D123 1
D124 1
D125 1
D126 1
D127 1
D128 1
D129 1
D130 1
D131 1
D132 1
D133 1
D134 1
D135 1
D136 1
D137 1
D138 1
D139 1
D140 1
D141 1
D142 1
D143 1
D144 1
D145 1
D146 1
D147 1
D148 1
D149 1
D150 1
D151 1
D152 1
D153 1
D154 1
D155 1
D156 1
D157 1
D158 1
D159 1
D160 1
D161 1
D162 1
D163 1
D164 1
D165 1
D166 1
D167 1
D168 1
D169 1
D170 1
D171 1
D172 1
D173 1
D174 1
D175 1
D176 1
D177 1
D178 1
D179 1
D180 1
D181 1
D182 1
D183 1
D184 1
D185 1
D186 1
D187 1
D188 1
D189 1
D190 1
D191 1
D192 1
D193 1
D194 1
D195 1
D196 1
D197 1
D198 1
D199 1
D200 1
D201 1
D202 1
D203 1
D204 1
D205 1
D206 1
D207 1
D208 1
D209 1
D210 1
D211 1
D212 1
D213 1
D214 1
D215 1
D216 1
D217 1
D218 1
D219 1
D220 1
D221 1
D222 1
D223 1
D224 1
D225 1
D226 1
D227 1
D228 1
D229 1
D230 1
D231 1
D232 1
D233 1
D234 1
D235 1
D236 1
D237 1
D238 1
D239 1
D240 1
D241 1
D242 1
D243 1
D244 1
D245 1
D246 1
D247 1
D248 1
D249 1
D250 1
D251 1
D252 1
D253 1
D254 1
D255 1
D256 1
D257 1
D258 1
D259 1
D260 1
D261 1
D262 1
D263 1
D264 1
D265 1
D266 1
D267 1
D268 1
D269 1
D270 1
D271 1
D272 1
D273 1
D274 1
D275 1
D276 1
D277 1
D278 1
D279 1
D280 1
D281 1
D282 1
D283 1
D284 1
D285 1
D286 1
D287 1
D288 1
D289 1
D290 1
D291 1
D292 1
D293 1
D294 1
D295 1
D296 1
D297 1
D298 1
D299 1
D300 1
D301 1
D302 1
D303 1
D304 1
D305 1
D306 1
D307 1
D308 1
D309 1
D310 1
D311 1
D312 1
D313 1
D314 1
D315 1
D316 1
D317 1
D318 1
D319 1
D320 1
D321 1
D322 1
D323 1
D324 1
D325 1
D326 1
D327 1
D328 1
D329 1
D330 1
D331 1
D332 1
D333 1
D334 1
D335 1
D336 1
D337 1
D338 1
D339 1
D340 1
D341 1
D342 1
D343 1
D344 1
D345 1
D346 1
D347 1
D348 1
D349 1
D350 1
D351 1
D352 1
D353 1
D354 1
D355 1
D356 1
D357 1
D358 1
D359 1
D360 1
D361 1
D362 1
D363 1
D364 1
D365 1
D366 1
D367 1
D368 1
D369 1
D370 1
D371 1
D372 1
D373 1
D374 1
D375 1
D376 1
D377 1
D378 1
D379 1
D380 1
D381 1
D382 1
D383 1
D384 1
D385 1
D386 1
D387 1
D388 1
D389 1
D390 1
D391 1
D392 1
D393 1
D394 1
D395 1
D396 1
D397 1
D398 1
D399 1
D400 1
D401 1
D402 1
D403 1
D404 1
D405 1
D406 1
D407 1
D408 1
D409 1
D410 1
D411 1
D412 1
D413 1
D414 1
D415 1
D416 1
D417 1
D418 1
D419 1
D420 1
D421 1
D422 1
D423 1
D424 1
D425 1
D426 1
D427 1
D428 1
D429 1
D430 1
D431 1
D432 1
D433 1
D434 1
D435 1
D436 1
D437 1
D438 1
D439 1
D440 1
D441 1
D442 1
D443 1
D444 1
D445 1
D446 1
D447 1
D448 1
D449 1
D450 1
D451 1
D452 1
D453 1
D454 1
D455 1
D456 1
D457 1
D458 1
D459 1
D460 1
D461 1
D462 1
D463 1
D464 1
D465 1
D466 1
D467 1
D468 1
D469 1
D470 1
D471 1
D472 1
D473 1
D474 1
D475 1
D476 1
D477 1
D478 1
D479 1
D480 1
D481 1
D482 1
D483 1
D484 1
D485 1
D486 1
D487 1
D488 1
D489 1
D490 1
D491 1
D492 1
D493 1
D494 1
D495 1
D496 1
D497 1
D498 1
D499 1
D500 1
D501 1
D502 1
D503 1
D504 1
D505 1
D506 1
D507 1
D508 1
D509 1
D510 1
D511 1
D512 1
D513 1
D514 1
D515 1
D516 1
D517 1
D518 1
D519 1
D520 1
D521 1
D522 1
D523 1
D524 1
D525 1
D526 1
D527 1
D528 1
D529 1
D530 1
D531 1
D532 1
D533 1
D534 1
D535 1
D536 1
D537 1
D538 1
D539 1
D540 1
D541 1
D542 1
D543 1
D544 1
D545 1
D546 1
D547 1
D548 1
D549 1
D550 1
D551 1
D552 1
D553 1
D554 1
D555 1
D556 1
D557 1
D558 1
D559 1
D560 1
D561 1
D562 1
D563 1
D564 1
D565 1
D566 1
D567 1
D568 1
D569 1
D570 1
D571 1
D572 1
D573 1
D574 1
D575 1
D576 1
D577 1
D578 1
D579 1
D580 1
D581 1
D582 1
D583 1
D584 1
D585 1
D586 1
D587 1
D588 1
D589 1
D590 1
D591 1
D592 1
D593 1
D594 1
D595 1
D596 1
D597 1
D598 1
D599 1
D600 1
D601 1
D602 1
D603 1
D604 1
D605 1
D606 1
D607 1
D608 1
D609 1
D610 1
D611 1
D612 1
D613 1
D614 1
D615 1
D616 1
D617 1
D618 1
D619 1
D620 1
D621 1
D622 1
D623 1
D624 1
D625 1
D626 1
D627 1
D628 1
D629 1
D630 1
D631 1
D632 1
D633 1
D634 1
D635 1
D636 1
D637 1
D638 1
D639 1
D640 1
D641 1
D642 1
D643 1
D644 1
D645 1
D646 1
D647 1
D648 1
D649 1
D650 1
D651 1
D652 1
D653 1
D654 1
D655 1
D656 1
D657 1
D658 1
D659 1
D660 1
D661 1
D662 1
D663 1
D664 1
D665 1
D666 1
D667 1
D668 1
D669 1
D670 1
D671 1
D672 1
D673 1
D674 1
D675 1
D676 1
D677 1
D678 1
D679 1
D680 1
D681 1
D682 1
D683 1
D684 1
D685 1
D686 1
D687 1
D688 1
D689 1
D690 1
D691 1
D692 1
D693 1
D694 1
D695 1
D696 1
D697 1
D698 1
D699 1
D700 1
D701 1
D702 1
D703 1
D704 1
D705 1
D706 1
D707 1
D708 1
D709 1
D710 1
D711 1
D712 1
D713 1
D714 1
D715 1
D716 1
D717 1
D718 1
D719 1
D720 1
D721 1
D722 1
D723 1
D724 1
D725 1
D726 1
D727 1
D728 1
D729 1
D730 1
D731 1
D732 1
D733 1
D734 1
D735 1
D736 1
D737 1
D738 1
D739 1
D740 1
D741 1
D742 1
D743 1
D744 1
D745 1
D746 1
D747 1
D748 1
D749 1
D750 1
D751 1
D752 1
D753 1
D754 1
D755 1
D756 1
D757 1
D758 1
D759 1
D760 1
D761 1
D762 1
D763 1
D764 1
D765 1
D766 1
D767 1
D768 1
D769 1
D770 1
D771 1
D772 1
D773 1
D774 1
D775 1
D776 1
D777 1
D778 1
D779 1
D780 1
D781 1
D782 1
D783 1
D784 1
D785 1
D786 1
D787 1
D788 1
D789 1
D790 1
D791 1
D792 1
D793 1
D794 1
D795 1
D796 1
D797 1
D798 1
D799 1
D800 1
D801 1
D802 1
D803 1
D804 1
D805 1
D806 1
D807 1
D808 1
D809 1
D810 1
D811 1
D812 1
D813 1
D814 1
D815 1
D816 1
D817 1
D818 1
D819 1
D820 1
D821 1
D822 1
D823 1
D824 1
D825 1
D826 1
D827 1
D828 1
D829 1
D830 1
D831 1
D832 1
D833 1
D834 1
D835 1
D836 1
D837 1
D838 1
D839 1
D840 1
D841 1
D842 1
D843 1
D844 1
D845 1
D846 1
D847 1
D848 1
D849 1
D850 1
D851 1
D852 1
D853 1
D854 1
D855 1
D856 1
D857 1
D858 1
D859 1
D860 1
D861 1
D862 1
D863 1
D864 1
D865 1
D866 1
D867 1
D868 1
D869 1
D870 1
D871 1
D872 1
D873 1
D874 1
D875 1
D876 1
D877 1
D878 1
D879 1
D880 1
D881 1
D882 1
D883 1
D884 1
D885 1
D886 1
D887 1
D888 1
D889 1
D890 1
D891 1
D892 1
D893 1
D894 1
D895 1
D896 1
D897 1
D898 1
D899 1
D900 1
D901 1
D902 1
D903 1
D904 1
D905 1
D906 1
D907 1
D908 1
D909 1
D910 1
D911 1
D912 1
D913 1
D914 1
D915 1
D916 1
D917 1
D918 1
D919 1
D920 1
D921 1
D922 1
D923 1
D924 1
D925 1
D926 1
D927 1
D928 1
D929 1
D930 1
D931 1
D932 1
D933 1
D934 1
D935 1
D936 1
D937 1
D938 1
D939 1
D940 1
D941 1
D942 1
D943 1
D944 1
D945 1
D946 1
D947 1
D948 1
D949 1
D950 1
D951 1
D952 1
D953 1
D954 1
D955 1
D956 1
D957 1
D958 1
D959 1
D960 1
D961 1
D962 1
D963 1
D964 1
D965 1
D966 1
D967 1
D968 1
D969 1
D970 1
D971 1
D972 1
D973 1
D974 1
D975 1
D976 1
D977 1
D978 1
D979 1
D980 1
D981 1
D982 1
D983 1
D984 1
D985 1
D986 1
D987 1
D988 1
D989 1
D990 1
D991 1
D992 1
D993 1
D994 1
D995 1
D996 1
D997 1
D998 1
D999 1
D1000 1



18

152.539
152.420
152.394
151.926
151.871
151.776
145.266
145.108
144.956
144.924
144.854
144.648
141.876
141.802
141.704
134.412
134.372
134.128
134.091
134.061
133.912
130.372
129.49

Thermo QEFMS Analysis Report

Analysis Info

Sample Name :	Eric_28	Reference No.:	Qhfc005
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI pos, 3.2kV, by LC, with sheath gas		

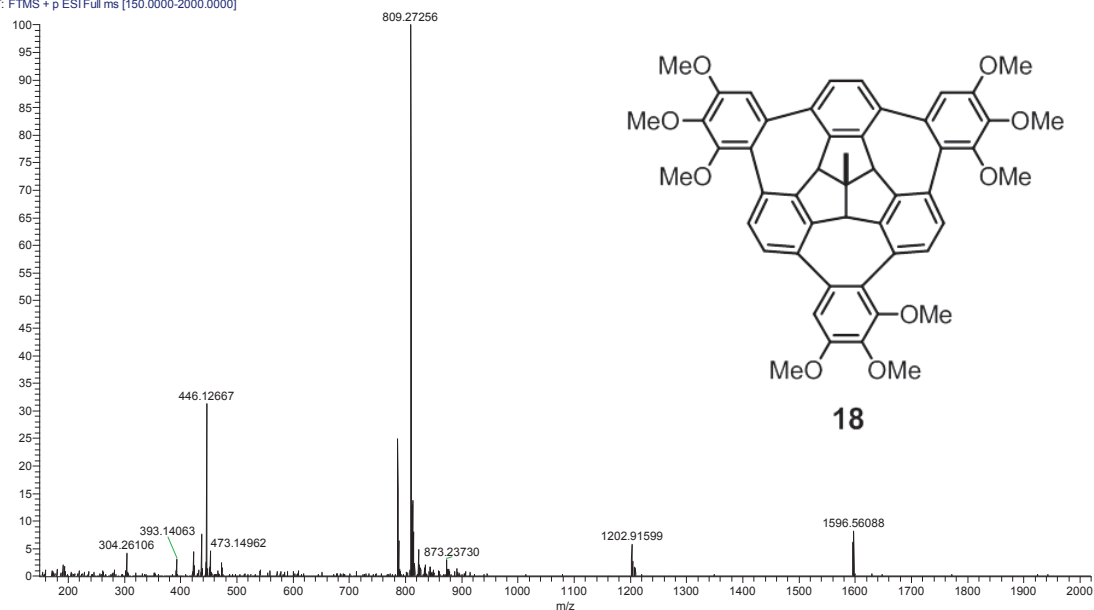
Accurate Mass Measurement

Molecular formula :	C ₅₀ H ₄₂ O ₉
Experimental Mass [M+Na] ⁺ :	809.27256
Theoretical Mass [M+Na] ⁺ :	809.27210
Error (ppm) :	0.5

D:\Raw data\qhfc005

02/08/17 10:45:30

qhfc005 #189 RT: 0.85 AV: 1 SB: 65 0.53-0.74, 0.92-0.99 NL: 1.64E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



qhfc005 #189 RT: 0.85 AV: 1 SB: 65 0.53-0.74, 0.92-0.99 NL: 1.64E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

