A Helically Twisted Ribbon-Shaped Nanographene Constructed around a Fenestrindane Core

Xiao-Qing Sun, Wai-Shing Wong, Yuke Li, Dietmar Kuck and Hak-Fun Chow

Department of Chemistry, The Chinese University of Hong Kong, Shatin, Hong Kong

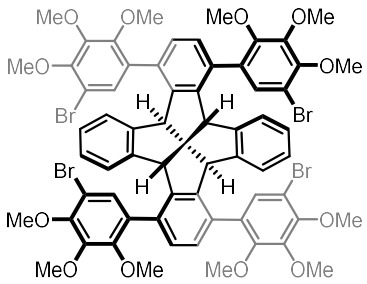
Department of Chemistry and Center for Molecular Materials (CM_2), Bielefeld University, 33615 Bielefeld, Germany

Table of Contents

1. General Information

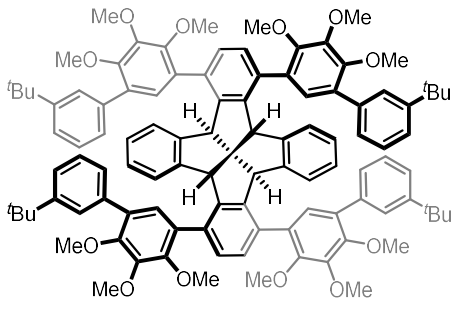
All reactions requiring anhydrous conditions were carried under nitrogen or argon. All reagents were purchased from commercial suppliers and used without further purification. Anhydrous tetrahydrofuran (THF) and dichloromethane were freshly distilled from sodium-benzophenone ketyl and CaH_2, respectively. Reactions were monitored by thin layer chromatography (TLC), using Merck pre-coated silica gel 60F254 plates. Column chromatography was performed by Merck Keiselgel 60 (230–400 mesh) or DAVISIL® LC60A (particle size 40–63 μm and pore size 60Å). ^{1}H NMR spectra were collected on a Bruker Advance III 400 spectrometer (^{1}H: 400.13 MHz; ^{13}C: 100.62 MHz) or a Bruker Advance III 500 spectrometer (^{1}H: 500.13 MHz; ^{13}C: 125.76 MHz). Chemical shifts were reported as parts per million in δ scale using the solvent residual peak as internal reference ($CDCl_3$ δ = 7.26 ppm, $C_2D_2Cl_4$ δ = 6.00 ppm). ^{13}C NMR spectra were recorded on the same spectrometer with the central resonance of the solvent peak as the internal reference ($CDCl_3$ δ = 77.16 ppm, $C_2D_2Cl_4$ δ = 73.78 ppm). High resolution mass spectra (HRMS) were obtained on a Thermo Scientific Q Exactive Focus Orbitrap using electrospray ionization (ESI). Melting points were measured on Stuart SMP50 Automatic Melting point apparatus and are uncorrected. UV-vis absorption spectra were recorded on a UV-Vis-NIR spectrophotometer. Fluorescence spectra were recorded on a Hitachi F-4500 spectrofluorometer. Cyclic voltammograms were recorded on a PAR Potentiostat/Galvanostat Model 263A.

2. Synthesis and Characterization of New Compounds



9

Compound 9: *N*-Bromosuccinimide (NBS) (179 mg, 1.01 mmol) and the zwitterionic organocatalyst **8** (2 mg, 0.005 mmol) were added to a solution of compound **6** (200 mg, 0.194 mmol) in anhydrous dichloromethane (30 mL). The reaction mixture was stirred at 20 °C in the dark for 36 h. Saturated sodium disulfite solution was then added to quench the excess NBS. The organic layer was washed with saturated NaCl solution, dried (Na_2SO_4), filtered, and the solvent was removed *in vacuo* to afford the crude product. Purification by column chromatography on silica gel (hexane/EtOAc = 4/1) afforded compound **9** (243 mg, 180 μmol, 93%) as a colorless solid. R_f: 0.65 (hexane/EtOAc = 2/1); M.p.: 228–230 °C; ^{1}H NMR (400 MHz, $C_2D_2Cl_4$, 85 °C): 7.39 (s, 4 H, ArH), 7.23 (s, 4 H, ArH), 6.84 (AA' of AA'BB', 4 H, ArH), 6.20 (BB' of AA'BB', 4 H, ArH), 5.11 (s, 4 H, CH), 4.04 (s, 12 H, OCH_3), 4.00 (s, 12 H, OCH_3), 3.41 (br s, 12 H, OCH_3); ^{13}C NMR (100 MHz, $C_2D_2Cl_4$, 85 °C): 151.2, 151.0, 147.9, 143.9, 143.2, 134.2, 132.5, 129.4, 128.4, 126.4, 125.6, 111.2, 72.9, 61.1, 61.0, 60.4, 58.3; Accurate mass (ESI-HRMS) calcd for $[M + Na]^+$: 1367.0398, $C_{65}H_{56}{}^{79}Br_4NaO_{12}{}^+$ found: 1367.0395.



5

Compound 5: Compound **9** (140 mg, 104 μmol), 3-*tert*-butylphenylboronic acid (222 mg, 1.25 mmol), $Pd_2(dba)_3$ (38 mg, 0.042 mmol), SPhos (35 mg, 0.084 mmol) and Cs_2CO_3 (542 mg, 1.66 mmol) were mixed in toluene (15 mL) and water (3 mL) in a Schlenk tube and degassed with nitrogen gas. The

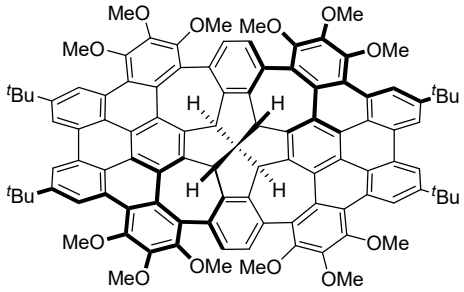
mixture was heated at 80 °C for 2 d, allowed to cool to 20 °C, and extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with saturated NaCl solution, dried (Na_2SO_4), filtered, and the solvent was removed *in vacuo* to afford the crude product. Purification by column chromatography on silica gel (hexane/EtOAc = 5/1) gave compound **5** (148 mg, 95 μmol, 91%) as a white solid. R_f: 0.25 (hexane/EtOAc = 4/1); M.p.: 213–215 °C; ^{1}H NMR (400 MHz, $C_2D_2Cl_4$, 100 °C): 7.70 (s, 4 H, ArH), 7.44–7.41 (m, 12 H, ArH), 7.38 (s, 4 H, ArH), 7.25 (s, 4 H, ArH), 6.87 (m, 4 H, ArH), 6.35 (br s, 4 H, ArH), 5.31 (s, 4 H, CH), 4.07 (s, 12 H, OCH_3), 3.87 (s, 12 H, OCH_3), 3.43 (br s, 12 H, OCH_3), 1.47 (s, 36 H, CH_3); ^{13}C NMR (100 MHz, $C_2D_2Cl_4$, 100 °C, 2 aromatic C signals overlapped, 17 out of 18 signals were found): 151.1, 150.82, 150.78, 146.9, 144.4, 143.4, 137.7, 135.1, 131.7, 131.2, 129.4, 127.7, 126.9, 126.3, 126.1, 125.7, 123.7, 72.6, 61.0, 60.8, 60.1, 59.0, 34.4, 31.3; Accurate mass (ESI-HRMS) calcd for $[M + Na]^+$: 1583.7733, $C_{105}H_{108}NaO_{12}^+$ found: 1583.7736.

Compounds 13, 14a and 3:

A solution of compound **5** (96 mg, 61 μmol) in anhydrous dichloromethane (10 mL) was stirred at 0 °C for 5 min. 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) (see Table S1 for no. of equiv.) and triflic acid (286 μL, 3.05 mmol) were subsequently added. The mixture was stirred at 0 °C for 20 min. The reaction was quenched with saturated $NaHCO_3$, washed with DCM and water. The organic layer was dried (Na_2SO_4), filtered, concentrated *in vacuo* and the residue was purified by column chromatography on silica gel (hexane/EtOAc = 10/1) to produce compounds **3**, **13** and **14a** in yields as given in Table S1.

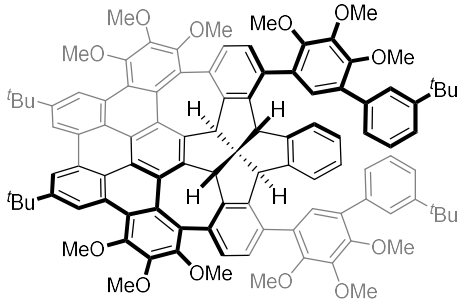
Table S1. Scholl reaction on compound **5** using different equiv. of DDQ.

Entry	DDQ (equiv.)	Starting material **5**	Compound **13**	Compound **14a**	Compound **3**
1	2.4	40%	23%	–	–
2	5.0	0	67%	–	–
3	8.0	0	38%	6%	5%
4	10.2	0	9%	32%	11%



3

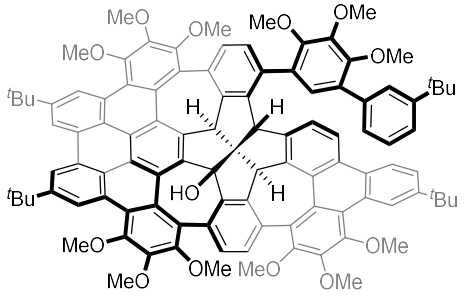
Compound 3: Yellow solid. R_f: 0.52 (hexane/EtOAc = 4/1); M.p.: > 400 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 22 °C): 9.90 (d, J = 1.4 Hz, 4 H, ArH), 9.12 (d, J = 1.6 Hz, 4 H, ArH), 7.80 (s, 4 H, ArH), 5.38 (s, 4 H, CH), 4.17 (s, 12 H, OCH_3), 3.92 (s, 12 H, OCH_3), 3.77 (s, 12 H, OCH_3), 1.72 (s, 36 H, CH_3); ^{1}H NMR (400 MHz, $C_2D_2Cl_4$, 22 °C): 9.90 (s, 4 H, ArH), 9.12 (s, 4 H, ArH), 7.81 (s, 4 H, ArH), 5.40 (s, 4 H, CH), 4.15 (s, 12 H, OCH_3), 3.96 (s, 12 H, OCH_3), 3.82 (s, 12 H, OCH_3), 1.74 (s, 36 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$; 22 °C): 152.7, 151.7, 148.6, 146.1, 142.3, 139.0, 130.1, 129.2, 129.1, 128.9, 128.7, 128.0, 124.8, 124.7, 124.2, 124.1, 123.1, 118.1, 67.0, 64.5, 61.8, 61.7, 61.3, 35.8, 32.0; Accurate mass (ESI-HRMS) calcd for $[M]^{+\bullet}$: 1540.6270, $C_{105}H_{88}O_{12}^{+\bullet}$ found: 1540.6274.



13

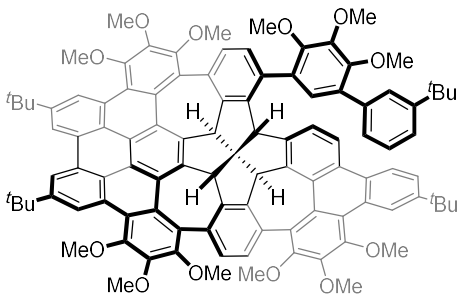
Compound 13: Yellow solid. R_f: 0.48 (hexane/EtOAc = 4/1); M.p.: > 400 °C; ^{1}H NMR (400 MHz, $C_2D_2Cl_4$, 100 °C): 10.07 (s, 2 H, ArH), 9.03 (s, 2 H, ArH), 7.66 (s, 2 H, ArH), 7.49 (d, J = 7.8 Hz, 2 H, ArH), 7.45–7.32 (m, 6 H, ArH), 7.33 (d, J = 7.9 Hz, 2 H, ArH), 7.28 (s, 2 H, ArH), 6.93 (AA' of AA'BB', 2 H, ArH), 6.21 (BB' of AA'BB', 2 H, ArH), 5.82 (s, 2 H, CH), 5.32 (s, 2 H, CH), 4.29 (s, 6 H, OCH_3), 4.24 (s, 6 H, OCH_3), 4.07 (s, 6 H, OCH_3), 4.05 (s, 6 H, OCH_3), 3.85 (s, 6 H, OCH_3), 3.59 (s, 6 H, OCH_3), 1.80 (s, 18 H, CH_3), 1.42 (s, 18 H, CH_3); ^{13}C NMR (100 MHz, $C_2D_2Cl_4$, 100 °C, 2 aromatic and 2 methoxy C signals overlapped, 35 out of 36 aromatic signals were found, 5 out of 6 methoxy signals were found): 151.6, 151.5, 151.2, 150.9, 150.8, 149.0, 147.0, 146.3, 145.9, 144.6, 139.4, 139.0, 137.6, 135.2, 131.8, 131.0, 130.1, 129.7, 129.0, 128.8, 128.7, 127.6, 127.5, 126.7, 126.2,

126.1, 125.7, 123.7, 123.29, 123.26, 123.0, 122.8, 122.7, 122.6, 118.7, 68.4, 65.3, 64.7, 61.5, 61.1, 60.9, 60.8, 60.6, 35.5, 34.4, 31.8, 31.2; Accurate mass (ESI-HRMS) calcd for $[M + H]^+$: 1551.7131, $C_{105}H_{99}O_{12}^+$, found 1551.7090.



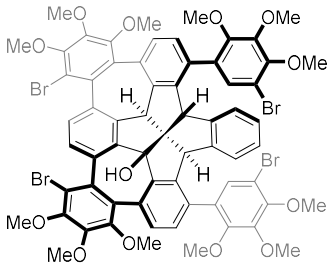
14a

Compound 14a: Yellow solid. R_f: 0.48 (hexane/EtOAc = 4/1); M.p.: > 400 °C; ^{1}H NMR (400 MHz, $CDCl_3$, 22 °C): 9.98 (d, *J* = 1.5 Hz, 1 H, ArH), 9.93 (d, *J* = 1.5 Hz, 1 H, ArH), 9.41 (d, *J* = 1.84 Hz, 1 H, ArH), 9.06 (s, 1 H, ArH), 9.04 (d, *J* = 1.4 Hz, 1 H, ArH), 8.28 (d, *J* = 8.8 Hz, 1 H, ArH), 8.18 (d, *J* = 8.6 Hz, 1 H, ArH), 7.63 (s, 1 H, ArH), 7.60 (s, 1 H, ArH), 7.58 (s, 1 H, ArH), 7.42 (d, *J* = 8.3 Hz, 1 H, ArH), 7.38–7.36 (m, 3 H, ArH), 7.24–7.20 (m, 2 H, ArH), 7.09 (s, 1 H, ArH), 6.36 (d, *J* = 8.4 Hz, 1 H, ArH), 6.04 (s, 1 H, CH), 5.31 (s, 1 H, CH), 5.22 (s, 1 H, OH), 4.91 (s, 1 H, CH), 4.17 (s, 6 H, OCH_3), 4.05 (s, 3 H, OCH_3), 4.03 (s, 3 H, OCH_3), 4.00 (s, 6 H, OCH_3), 3.99 (s, 3 H, OCH_3), 3.93 (s, 3 H, OCH_3), 3.78 (s, 3 H, OCH_3), 3.77 (s, 3 H, OCH_3), 3.76 (s, 3 H, OCH_3), 3.63 (s, 3 H, OCH_3), 1.711 (s, 9 H, CH_3), 1.706 (s, 9 H, CH_3), 1.47 (s, 9 H, CH_3), 1.30 (s, 9 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, 22 °C, some aromatic C signals overlapped, 63 out of 72 signals were found): 152.12, 152.07, 151.9, 151.8, 151.5, 151.2, 151.1, 150.2, 149.9, 148.9, 148.8, 147.7, 147.6, 146.2, 145.9, 145.2, 145.0, 143.3, 142.9, 141.6, 141.4, 141.0, 137.9, 137.5, 134.6, 132.6, 132.2, 131.7, 131.3, 131.0, 129.6, 129.52, 129.45, 129.2, 129.1, 129.0, 128.9, 128.8, 128.5, 128.3, 128.1, 128.0, 127.5, 127.4, 127.1, 126.6, 126.4, 125.8, 125.6, 124.8, 124.4, 124.0, 123.9, 123.8, 123.7, 123.6, 123.5, 123.4, 123.22, 123.18, 123.1, 122.9, 118.4, 95.7, 62.6, 62.4, 61.9, 61.8, 61.7, 61.6, 61.4, 61.2, 56.1, 35.8, 35.3, 34.9, 32.1, 31.7, 31.5, 29.9; Accurate mass (ESI-HRMS) calcd for $[M + H - H_2O]^+$: 1545.6662, $C_{105}H_{93}O_{12}^+$ found: 1545.6662.



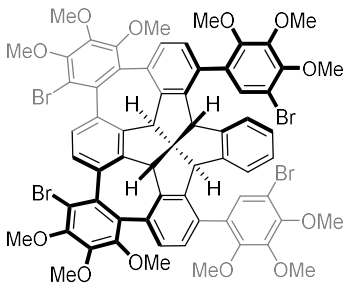
14b

Compound 14b: Trifluoroacetic acid (TFA) (150 µL, 2.0 mmol) and Et_3SiH (320 µL, 2.0 mmol) were added to a solution of compound **14a** (31 mg, 20µmol) in anhydrous dichloromethane (10 mL) at 0 °C. The reaction mixture was allowed to warm to room temperature and stirred for another hour. The mixture was quenched with saturated $NaHCO_3$ and extracted with dichloromethane (3 × 10 mL). The combined organic layers were dried (Na_2SO_4), filtered, concentrated *in vacuo* and the residue was purified by column chromatography on silica gel (hexane/EA = 7/1) to afford compound **14b** (30 mg, 19 µmol, 96%) as a yellow solid. R_f: 0.48 (hexane/EtOAc = 4/1); M.p.: >400 °C; ^{1}H NMR (400 MHz, $C_2D_2Cl_4$, 100 °C): 10.11 (br s, 1 H, ArH), 10.06 (br s, 1 H, ArH), 9.51 (br s, 1 H, ArH), 9.11 (br s, 2 H, ArH), 8.41 (d, J = 7.0 Hz, 1 H, ArH), 8.25 (d, J = 6.6 Hz, 1 H, ArH), 7.80–7.60 (m, 5 H, ArH), 7.50–7.32 (m, 5 H, ArH), 6.48 (br s, 1 H, ArH), 6.02 (br s, 1 H, CH), 5.41 (br s, 1 H, CH), 5.36 (br s, 1 H, CH), 5.08 (br s, 1 H, CH), 4.29 (s, 6 H, OCH_3), 4.19 (s, 9 H, OCH_3), 4.15 (s, 3 H, OCH_3), 4.06 (s, 3 H, OCH_3), 4.00 (s, 6 H, OCH_3), 3.88 (s, 3 H, OCH_3), 3.80 (s, 3 H, OCH_3), 3.69 (s, 3 H, OCH_3), 1.84 (s, 9 H, CH_3), 1.83 (s, 9 H, CH_3), 1.60 (s, 9 H, CH_3), 1.44 (s, 9 H, CH_3); ^{13}C NMR (100 MHz, $C_2D_2Cl_4$, 100 °C, some aromatic and methoxy C signals overlapped, 58 out of 72 aromatic signals were found, 9 out of 12 methoxy signals were found): 152.2, 151.8, 151.6, 151.5, 151.4, 151.1, 150.8, 149.8, 148.9, 148.8, 147.2, 147.0, 146.2, 145.9, 145.3, 143.9, 141.7, 141.1, 140.9, 139.0, 138.5, 137.6, 131.9, 131.2, 130.7, 130.6, 130.1, 129.8, 129.6, 129.3, 129.1, 128.9, 128.8, 128.3, 128.0, 127.84, 127.80, 127.75, 127.7 127.33, 127.28, 126.8, 126.3, 126.2, 125.3, 124.4, 123.8, 123.62, 123.57, 123.49, 123.45, 123.4, 123.1, 123.0, 122.8, 122.6, 122.5, 118.5, 68.3, 66.2, 66.0, 63.3, 62.9, 61.5, 61.3, 61.2, 61.13, 61.08, 60.92, 60.88, 60.7, 60.6, 35.5, 34.9, 34.5, 31.8, 31.4, 31.3, 30.4, 29.4; Accurate mass (ESI-HRMS) calcd for $[M]^{+\bullet}$: 1546.6740, $C_{105}H_{94}O_{12}^{+\bullet}$ found: 1546.6729.



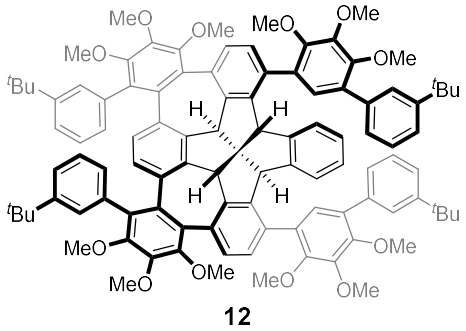
10

Compound 10a: Triflic acid (690 μL, 7.4 mmol) and DDQ (78 mg, 340 μmol) were added to a solution of compound **9** (100 mg, 73 μmol) in anhydrous dichloromethane (20 mL) at 0 °C. The reaction mixture was stirred at 0 °C for 15 min. Then the reaction was quenched with saturated $NaHCO_3$ solution. The organic layer was washed with water, saturated NaCl solution, dried (Na_2SO_4) and filtered. The solvent was removed *in vacuo* and the residue was purified by column chromatography (hexane/EtOAc = 2/1) on silica gel to afford product **10a** (62 mg, 46 μmol, 61%) as a colorless solid. R_f: 0.21 (hexane/EtOAc = 2/1); M.p.: >400 °C. ^{1}H NMR (400 MHz, $CDCl_3$; 22 °C): 8.00–7.92 (m, 2 H, ArH), 7.87 (d, J = 7.9 Hz, 1 H, ArH), 7.76 (d, J = 8.0 Hz, 1 H, ArH), 7.46 (s, 1 H, ArH), 7.22 (s, 1 H, ArH), 7.18 (d, J = 7.8 Hz, 1 H, ArH), 7.13 (d, J = 7.9 Hz, 1 H, ArH), 6.93–6.90 (m, 2 H, ArH), 6.09 (d, J = 7.4 Hz, 1 H, ArH), 5.99 (d, J = 6.7 Hz, 1 H, ArH), 5.37 (s, 1 H, CH), 5.26 (s, 1 H, CH), 4.71 (s, 1 H, OH), 4.41 (s, 1 H, CH), 4.08 (s, 3 H, OCH_3), 4.05 (s, 3 H, OCH_3), 4.03 (s, 3 H, OCH_3), 4.02 (s, 6 H, OCH_3), 3.96 (s, 3 H, OCH_3), 3.95 (s, 3 H, OCH_3), 3.91 (s, 3 H, OCH_3), 3.71 (s, 3 H, OCH_3), 3.49 (s, 3 H, OCH_3), 3.43 (s, 3 H, OCH_3), 3.40 (s, 3 H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$; 22 °C, some aromatic C signals overlapped, 40 out of 48 were found): 152.10, 152.06, 151.6, 151.2, 151.0, 150.83, 150.75, 150.2, 149.8, 148.2, 147.0, 146.9, 146.5, 144.8, 144.3, 141.3, 133.9, 133.8, 133.7, 133.1, 132.9, 132.7, 131.5, 131.4, 131.0, 130.3, 129.8, 129.6, 129.5, 129.3, 129.1, 128.9, 128.8, 127.6, 126.5, 125.0, 115.3, 115.0, 112.0, 111.9, 94.9, 73.8, 62.4, 62.1, 61.8, 61.7, 61.6, 61.5, 61.44, 61.39, 61.3, 61.08, 61.05, 60.8, 60.7, 53.9; Accurate mass (ESI-HRMS) calcd for $[M + H - H_2O]^+$: $C_{65}H_{51}{}^{79}Br_4O_{12}{}^+$ 1339.0109, found: 1339.0096.



10b

Compound 10b: The synthetic procedure was similar to that of **14b**. Starting from compound **10a**, the product **10b** was obtained as a white solid (95%). R_f: 0.67 (hexane/EtOAc = 2/1); M.p.:>400 °C; ^{1}H NMR (400 MHz, $CDCl_3$; 45 °C): 7.91 (s, 2 H, ArH), 7.80 (d, J = 8.0 Hz, 2 H, ArH), 7.45 (s, 2 H, ArH), 7.20 (d, J = 8.0 Hz, 2 H, ArH), 6.83 (AA' of AA'BB', 2 H, ArH), 5.97 (BB' of AA'BB', 2 H, ArH), 5.46 (s, 2 H, CH), 4.43 (s, 2 H, CH), 4.07 (s, 6 H, OCH_3), 4.03 (s, 6 H, OCH_3), 3.98 (s, 6 H, OCH_3), 3.94 (s, 6 H, OCH_3), 3.52 (s, 6 H, OCH_3), 3.47 (s, 6 H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$; 45 °C, two aromatic C signals overlapped, 23 out of 24 signals were found): 152.2, 151.7, 151.3, 151.2, 149.6, 148.3, 147.0, 144.9, 144.0, 139.5, 134.6, 133.9, 133.0, 131.6, 131.3, 130.1, 129.5, 129.0, 128.4, 127.2, 125.7, 115.0, 111.8, 68.0, 64.5, 63.8, 61.6, 61.5, 61.4, 61.3, 61.1, 60.7; Accurate mass (ESI-HRMS) calcd for $[M + Na]^+$: 1363.0084, $C_{65}H_{52}{}^{79}Br_4NaO_{12}{}^+$ found: 1363.0046.



12

Compound 12: The synthetic procedure was similar to that of compound **5**. Starting from compound **10b** and 3-*tert*-butylphenylboronic acid, the product **12** was obtained as a white solid (89%). R_f: 0.30 (hexane/EtOAc = 4/1); M.p.: 221–223 °C; ^{1}H NMR (400 MHz, $C_2D_2Cl_4$, 100 °C): 7.88 (d, J = 1.6 Hz, 2 H, ArH), 7.65 (br s, 2 H, ArH), 7.39–7.27 (m, 12 H, ArH), 7.06 (s, 4 H, ArH), 6.89–6.87 (m, 2 H, ArH), 6.39 (br s, 2 H, ArH), 6.18 (br s, 2 H, ArH), 5.94 (br s, 2 H, ArH), 5.67 (s, 2 H, CH), 4.59 (s, 2 H, CH), 4.12 (s, 6 H, OCH_3), 4.05 (s, 6 H, OCH_3), 3.82 (s, 6 H, OCH_3), 3.71 (s, 9 H, OCH_3), 3.70 (s, 9 H, OCH_3), 1.38 (br s, 24 H, CH_3), 0.64 (br s, 12 H, CH_3); ^{13}C NMR (100 MHz, $C_2D_2Cl_4$, 100 °C,

some aromatic and methoxy C signals overlapped, 29 out of 36 aromatic signals were found, 4 out of 6 methoxy signals were found): 151.6, 151.1, 150.8, 150.5, 149.8, 149.2, 146.9, 145.9, 145.2, 143.6, 137.6, 135.3, 132.5, 131.7, 131.3, 130.9, 130.5, 129.1, 129.0, 128.9, 127.9, 127.6, 126.62, 126.56, 126.2, 126.1, 125.5, 123.7, 122.2, 67.5, 64.7, 64.1, 61.1, 60.9, 60.7, 60.4, 34.4, 33.6, 31.2, 30.5. Accurate mass (ESI-HRMS) calcd for $[M + H]^+$: 1557.7601, $C_{105}H_{105}O_{12}^+$ found 1557.7591.

Scholl reactions with compounds **12**, **13** and **14b**.

The synthesis procedure was similar to the Scholl reaction on compound **5**. The results were tabulated in Table S2.

Table S2. Scholl reactions on compounds **12**, **13** and **14b**.

	DDQ (eq.)	Products		
		Compound **13**	Compound **14a**	Compound **3**
13	5.0	–	42%	16%
14b	3.0	–	45%	18%
12	8.0	9%	35%	13%

3. X-ray Crystal Structure of Compound 3

A single crystal of **3** suitable for X-ray diffraction analysis was obtained by diffusion of ethanol into a solution of **3** in 1,2-dichlorobenzene. Crystallographic data was collected on a Bruker D8 VENTURE diffractometer with MoK_α radiation (λ = 0.71073 Å) from a sealed-tube generator. Data collection, reduction, and empirical absorption corrections were performed using *APEX2* software.[1] The crystal structure of **3** was solved by direct methods with *SHELXS* program,[2] and all non-hydrogen atoms were anisotropically refined against F^2 with full-matrix least-squares techniques using SHELXL-97 program. Highly disordered solvent molecules (1,2-dichlorobenzene) were found in the void of the crystal structure and SQUEEZE routine in PLATON has been applied during the structural refinement.

Table S3. Crystallographic Data of **3** • 2 *o*-$C_6H_4Cl_2$.

Empirical formula	$C_{117}H_{94}Cl_4O_{12}$	Z	2
Molecular weight	1833.72	D_c (g/cm^3)	1.190
Crystal system	Triclinic	*F* (000)	1920
Space group	P-1	R_{int}	0.0773
Temperature (K)	298(2)	GOF	1.044
a / Å	13.2261(7)	Measured reflection	186121
b / Å	19.8587(9)	Independent reflection	18524
c / Å	20.3668(10)	*R*1 ($I > 2\sigma(I)$) [a]	0.1022
α / °	73.2178(15)	*R*1 (all data)	0.1467
β / °	89.2654(17)	*wR*2 ($I > 2\sigma(I)$)[b]	0.2997
γ / °	88.1548(15)	CCDC number	2003039
V / Å^3	5118.9(4)		

[a] $R1 = \sum||F_o|-|F_c||/\sum|F_o|$

[b] $wR = \{\sum[w(F_o^2 - F_c^2)^2]/\sum w(F_o^2)^2\}^{1/2}$

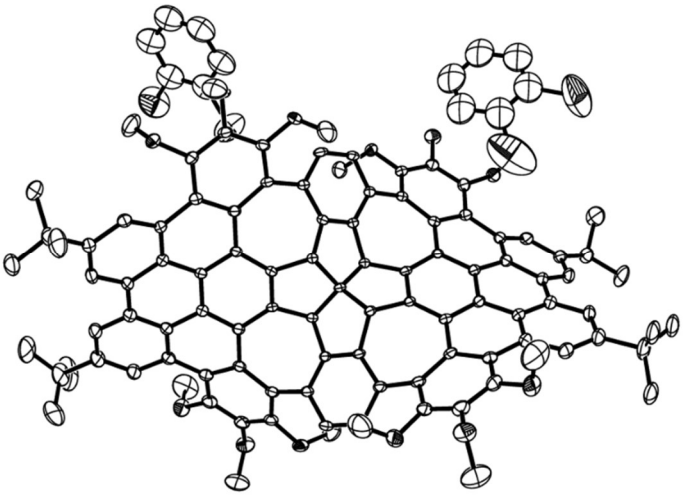


Figure S1. X-ray crystal structure of compound **3** with two co-crystallized 1,2-dichlorobenzene molecules.

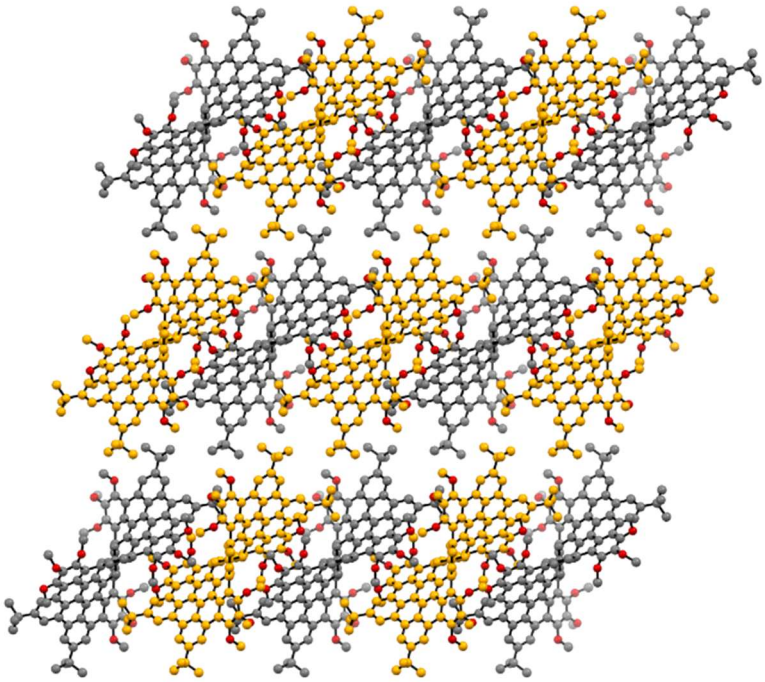


Figure S2. Molecular packing of compound **3**, viewed along the *a*-axis, (*P*)- and (*M*)-enantiomers are colored in grey and orange, respectively. The solvent molecules were omitted for clarity.

4. Structural Characterization of Compounds 14a and 10a.

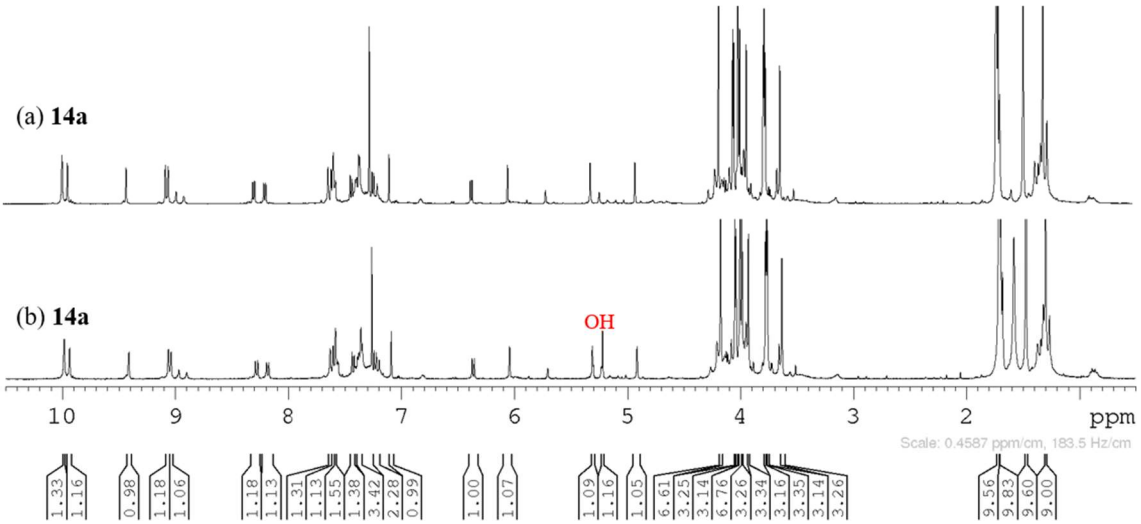


Figure S3. Stacked ^{1}H NMR spectra (400 MHz, $CDCl_3$, 22 °C) of compound **14a** (a) after and (b) before addition of D_2O.

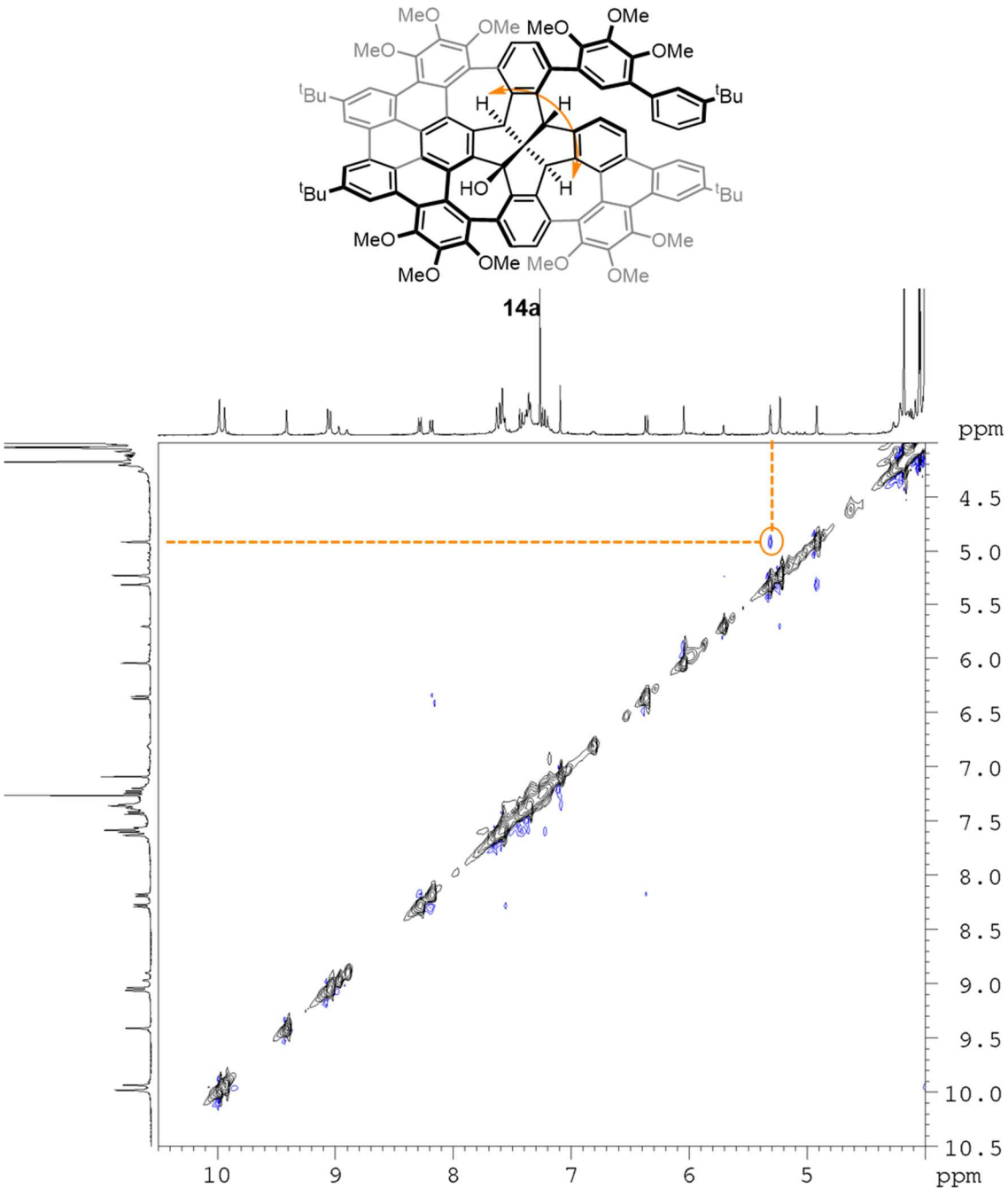


Figure S4. 2D ROSEY NMR spectrum of compound **14a** (400 MHz, $CDCl_3$, 22 °C).

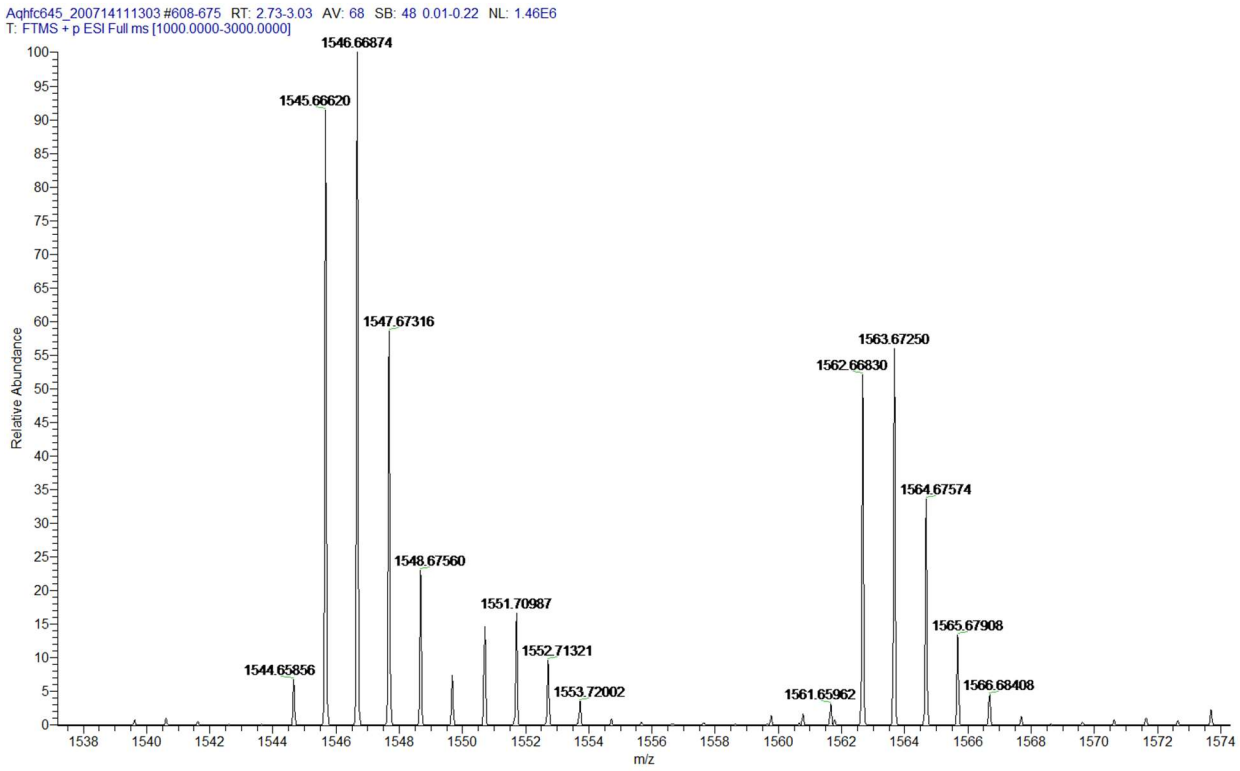


Figure S5. ESI mass spectrum of compound **14a**.

Table S4. Summary of characteristic molecular ions from compound **14a**.

Assignment	$[M]^{+\bullet}$	$[M + H - H_2O]^+$
Molecular formula	$[C_{105}H_{94}O_{13}]^{+\bullet}$	$[C_{105}H_{93}O_{12}]^+$
Experimental mass	1562.6683	1545.6662
Theoretical mass	1562.6689	1545.6662
Error (ppm)	−0.4	0

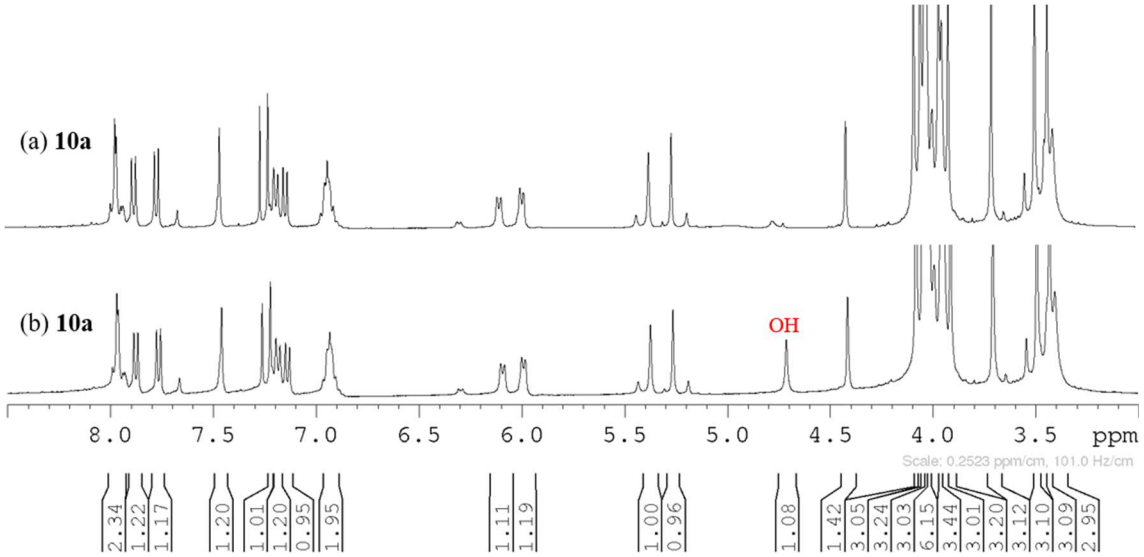


Figure S6. Stacked ^{1}H NMR spectra (400 MHz, $CDCl_3$, 22 °C) of compound **10a** (a) after and (b) before addition of D_2O.

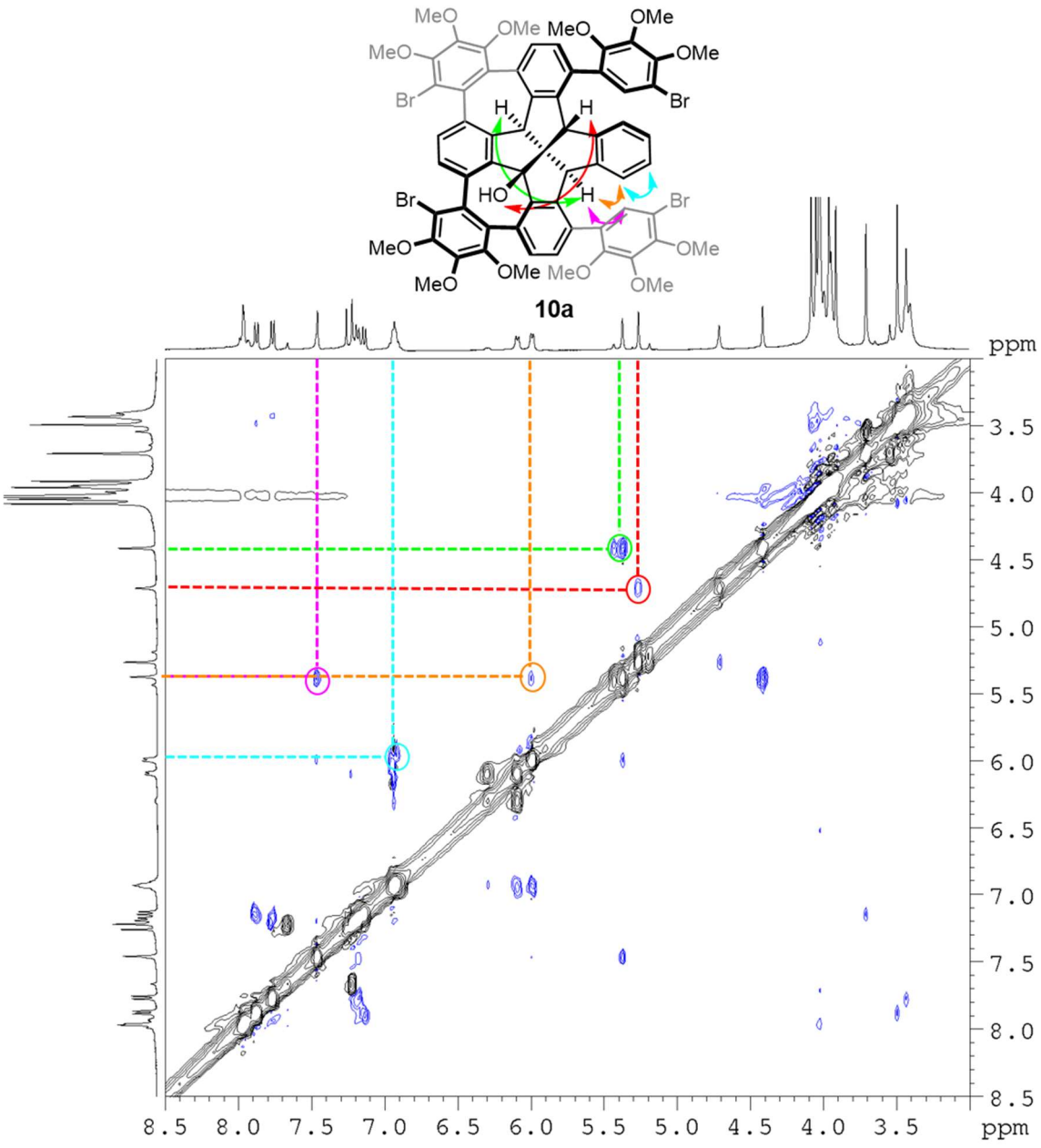


Figure S7. 2D ROESY NMR spectrum of compound **10a** (400 MHz, $CDCl_3$, 22 °C).

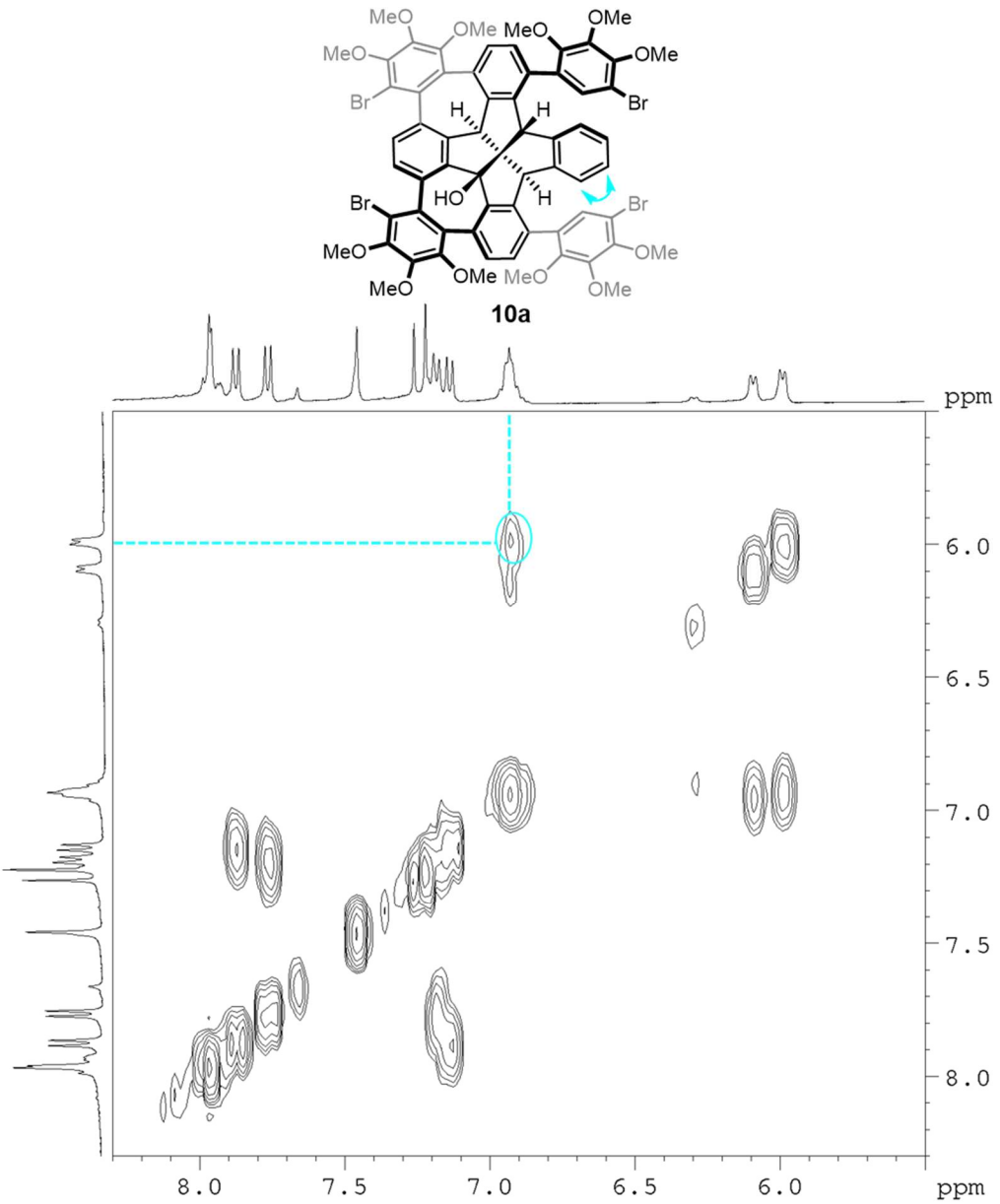


Figure S8. 2D COSY NMR spectrum of **10a** (400 MHz, $CDCl_3$, 22 °C).

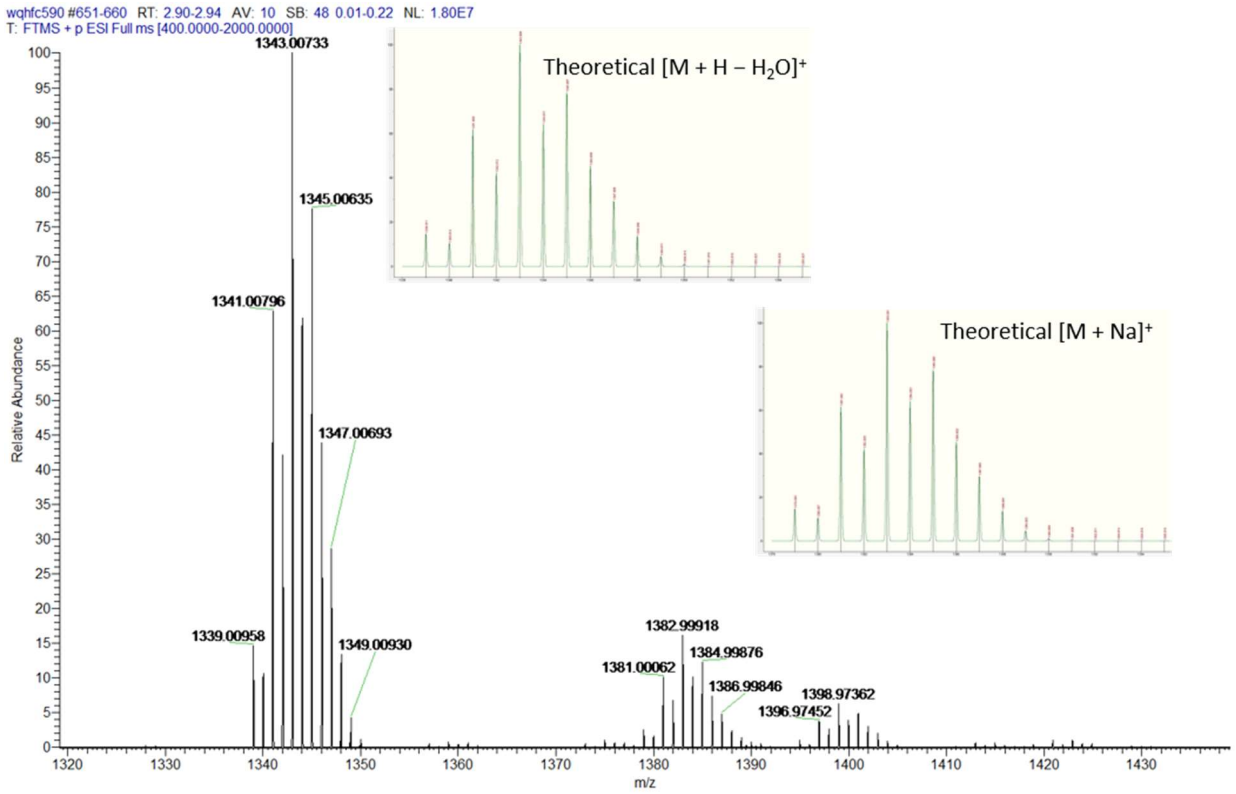


Figure S9. Partial ESI mass spectrum of compound **10a**.

Table S5. Summary of characteristic molecular ions from compound **10a.**

Assignment	$[M + Na]^+$	$[M + H - H_2O]^+$
Molecular formula	$[C_{65}H_{52}Br_4O_{13} + Na]^+$	$[C_{65}H_{51}Br_4O_{12}]^+$
Experimental mass ($^{79}Br_4$)	1379.0015	1339.0096
Theoretical mass ($^{79}Br_4$)	1379.0034	1339.0109
Error (ppm)	−1.4	−0.9

5. 2D NMR Spectra of Compounds 9, 13 and 3

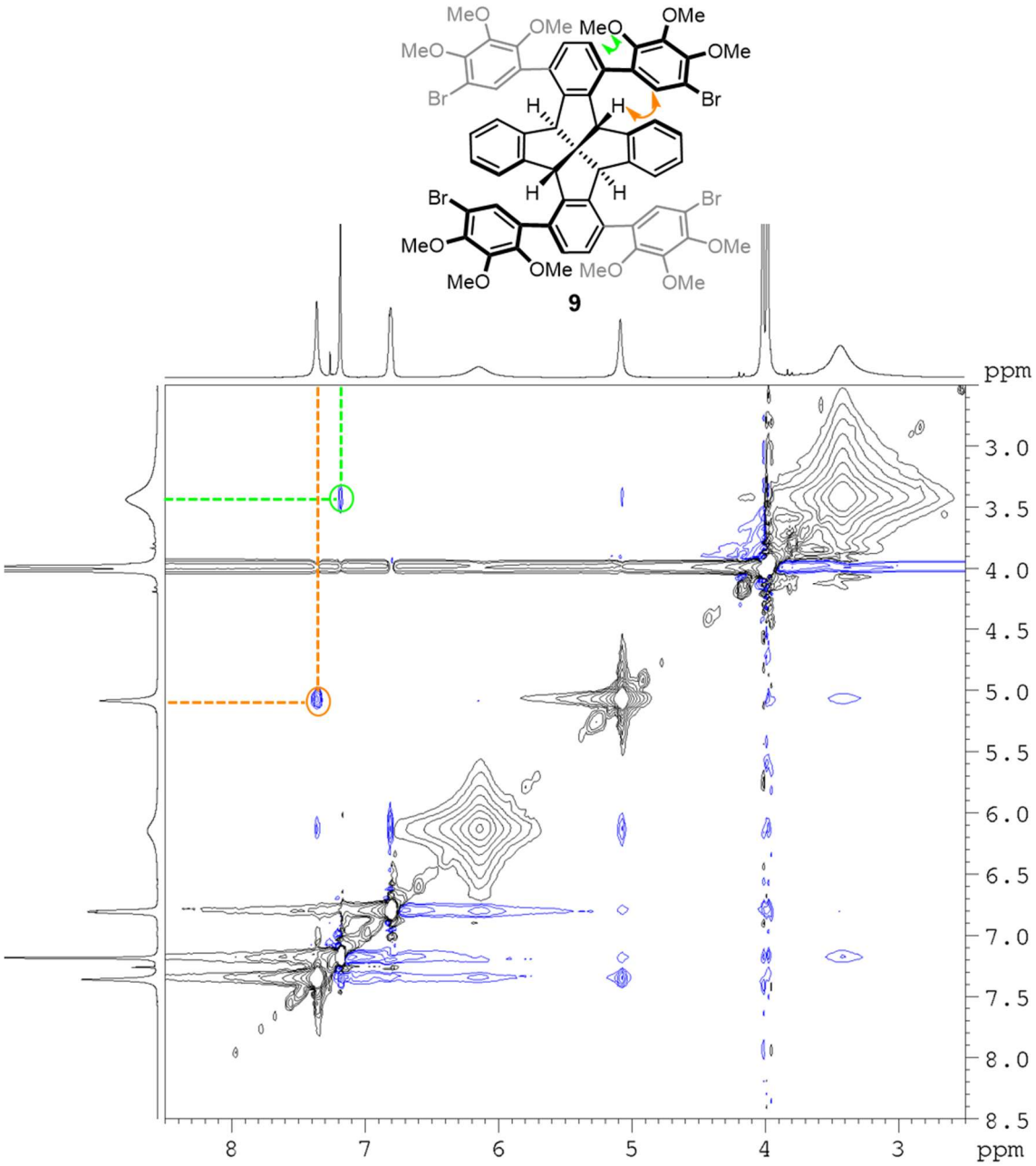


Figure S10. 2D ROESY NMR spectrum of **9** (400 MHz, $CDCl_3$, 45 °C).

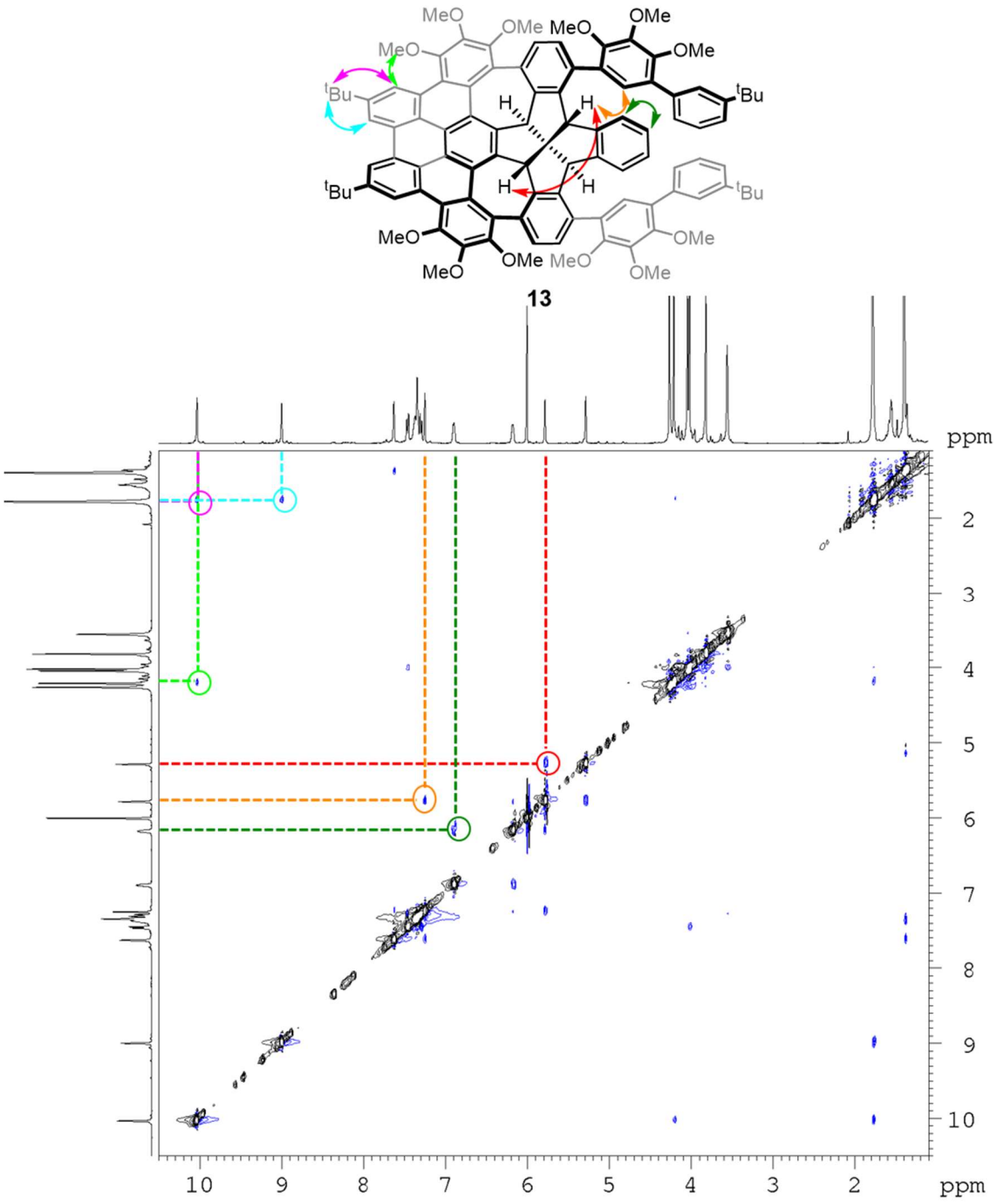


Figure S11. 2D ROESY NMR spectrum of **13** (400 MHz, $C_2D_2Cl_4$, 100 °C).

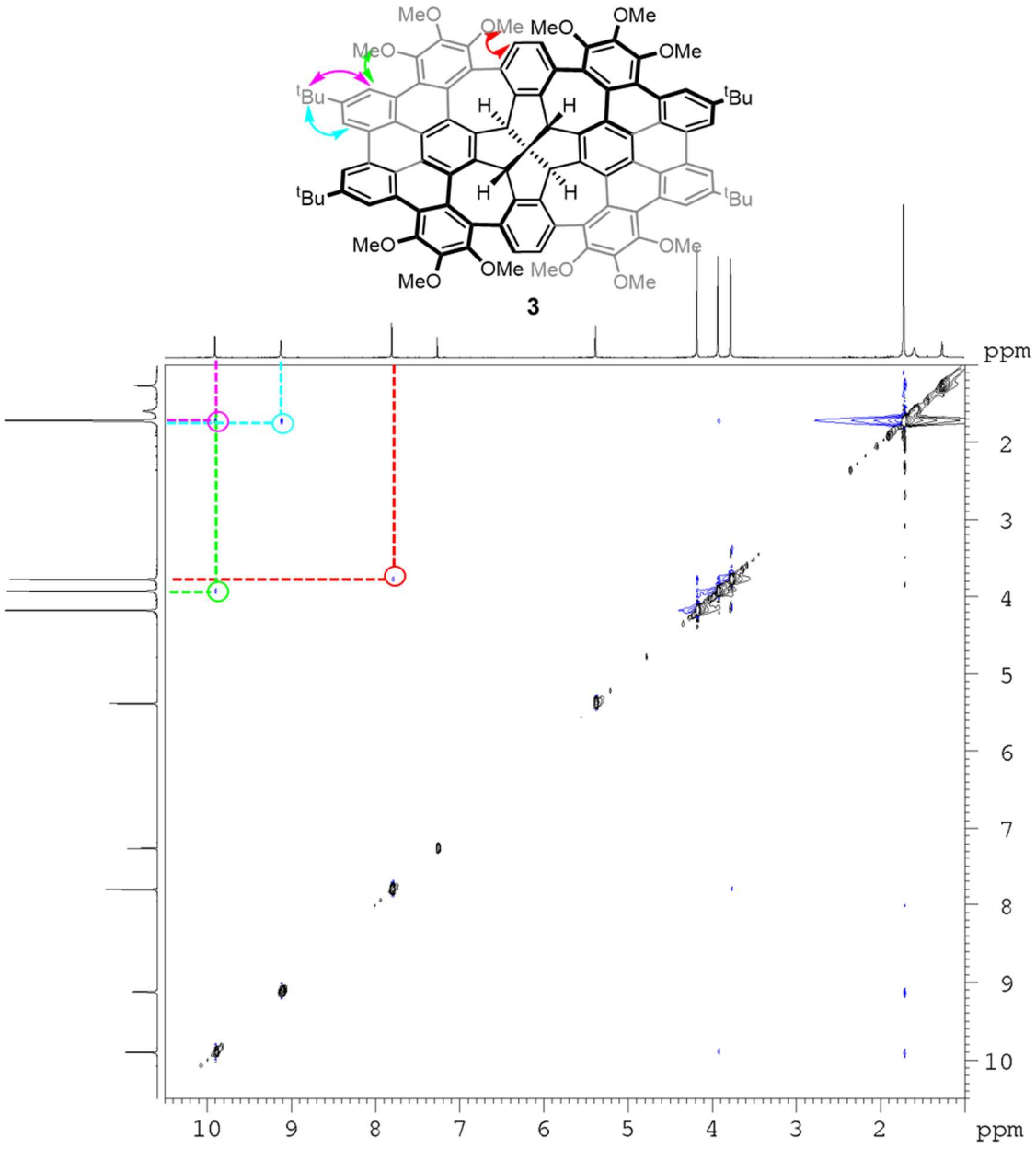


Figure S12. 2D ROESY NMR spectrum of **3** (400 MHz, $CDCl_3$, 22 °C).

6. Temperature-dependent NMR Spectra of Compounds 9, 5, 13, 14b, 10b and 12.

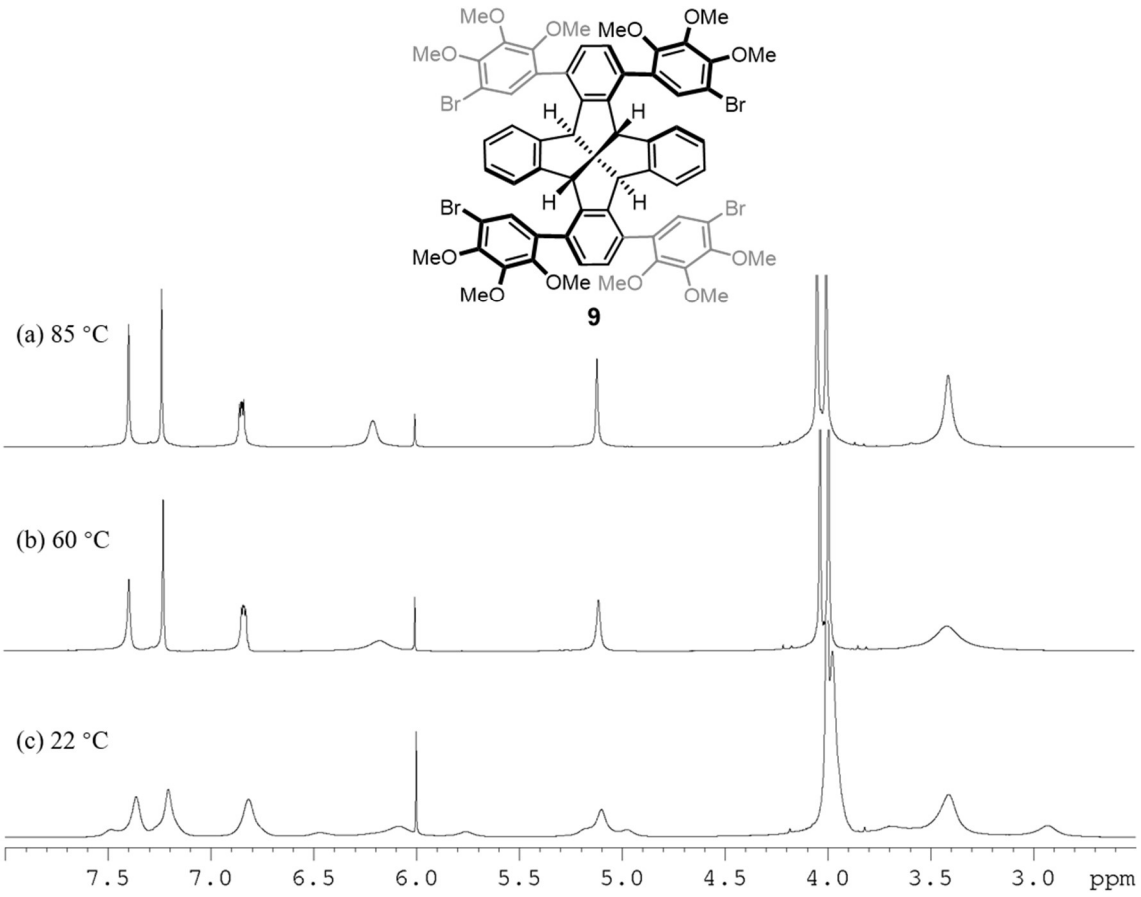


Figure S13. Stacked variable temperature ^{1}H NMR spectra (400 MHz, $C_2D_2Cl_4$) of compound **9** at (a) 85 °C, (b) 60 °C and (c) 22 °C.

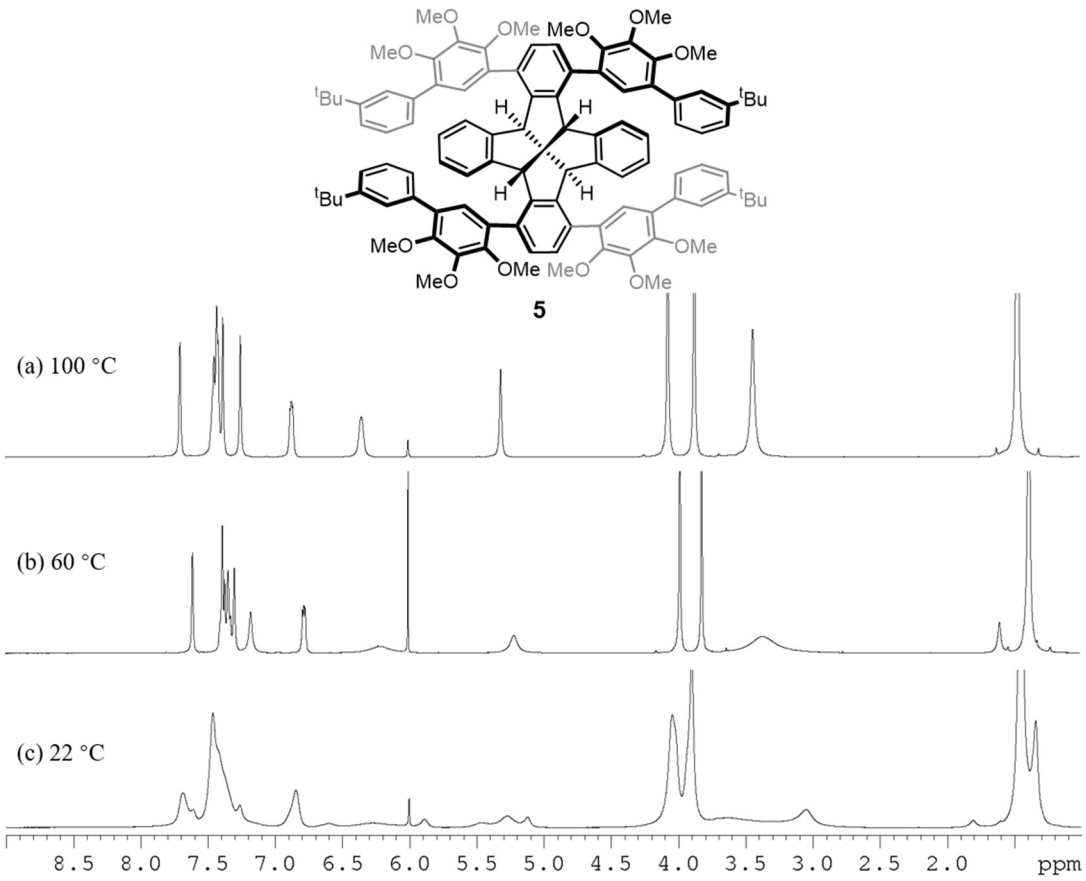


Figure S14. Stacked variable temperature ^{1}H NMR spectra (400 MHz, $C_2D_2Cl_4$) of compound **5** at (a) 100 °C, (b) 60 °C and (c) 22 °C.

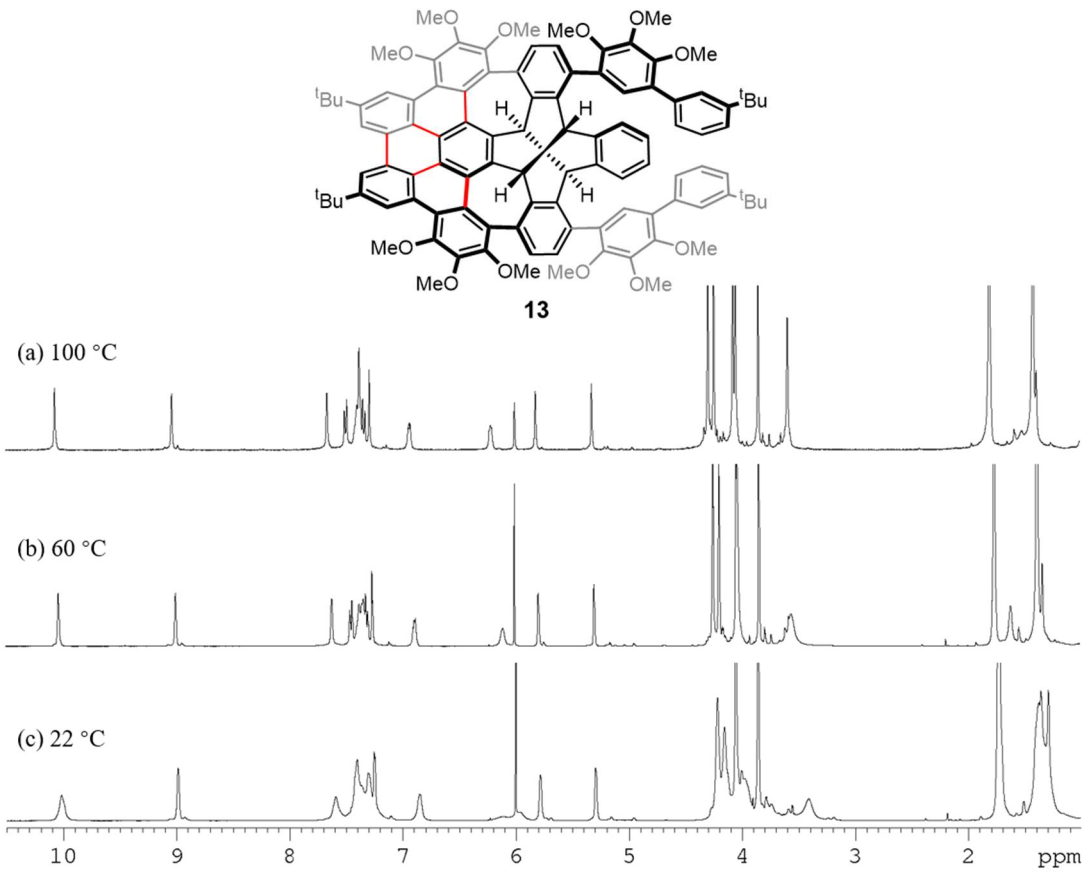


Figure S15. Stacked variable temperature ^{1}H NMR spectra (400 MHz, $C_2D_2Cl_4$) of compound **13** at (a) 100 °C, (b) 60 °C and (c) at 22 °C.

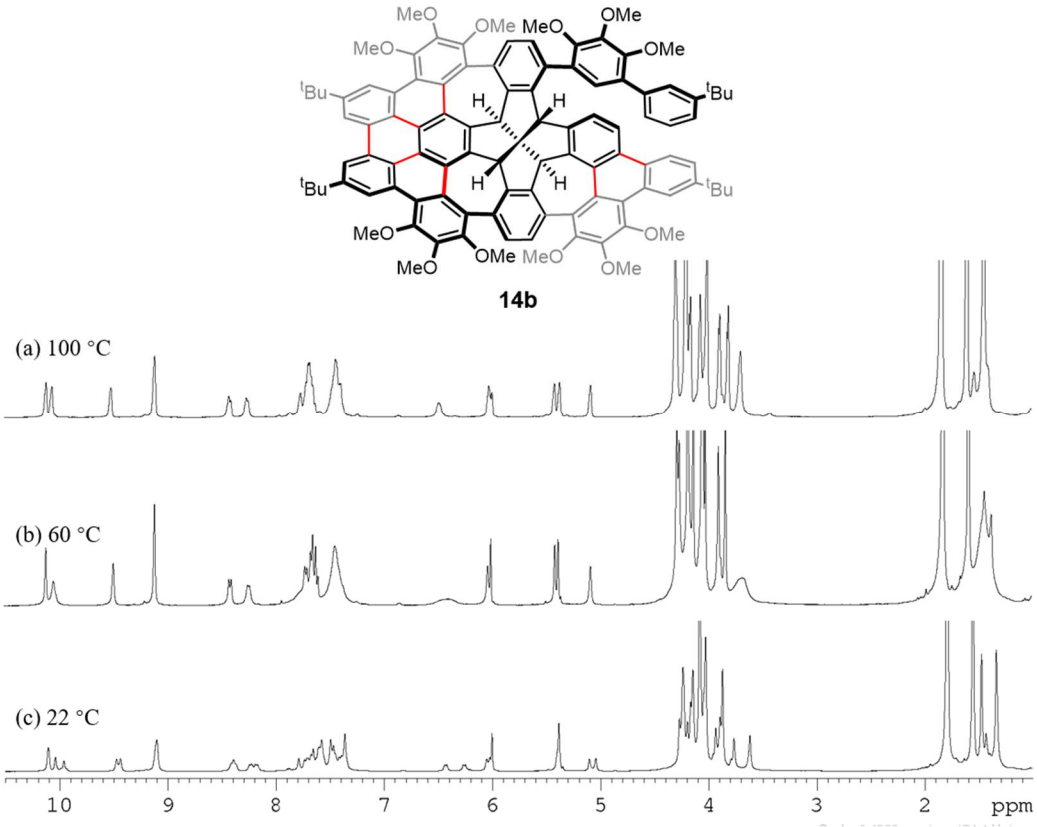


Figure S16. Stacked variable temperature ^{1}H NMR spectra (400 MHz, $C_2D_2Cl_4$) of compound **14b** at (a) 100 °C, (b) 60 °C and (c) at 22 °C.

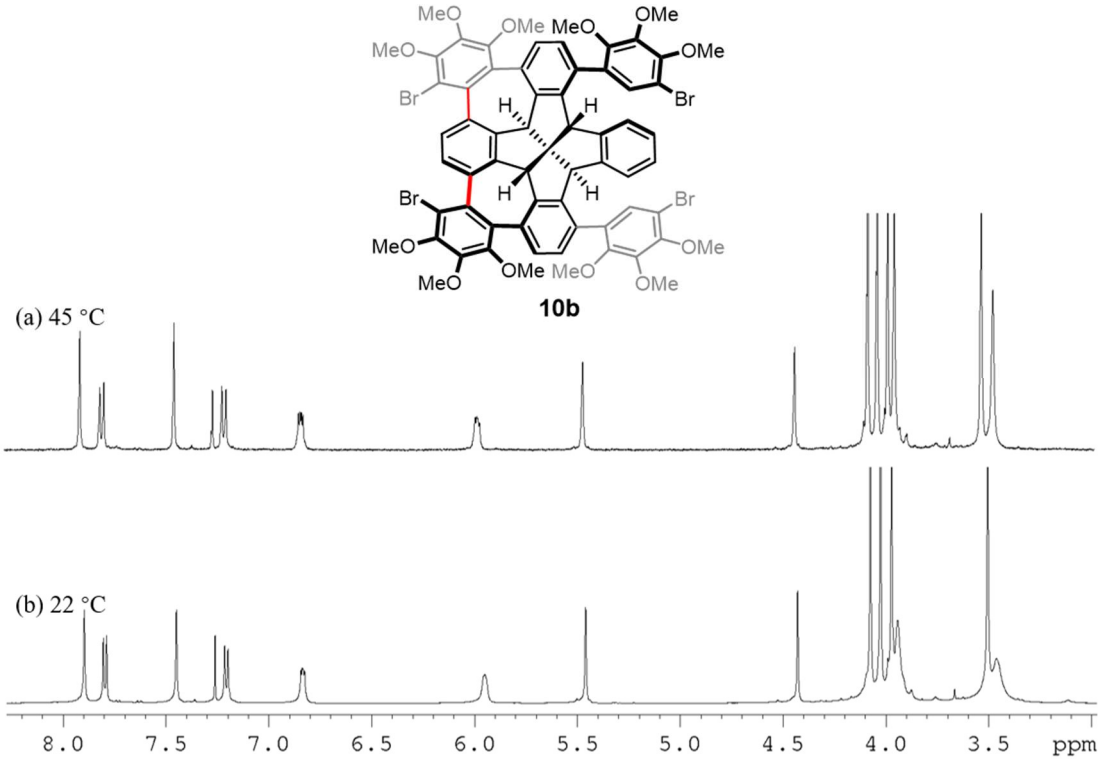


Figure S17. Stacked variable temperature ^{1}H NMR spectra (400 MHz, $CDCl_3$) of compound **10b** at (a) 45 °C and (c) 22 °C.

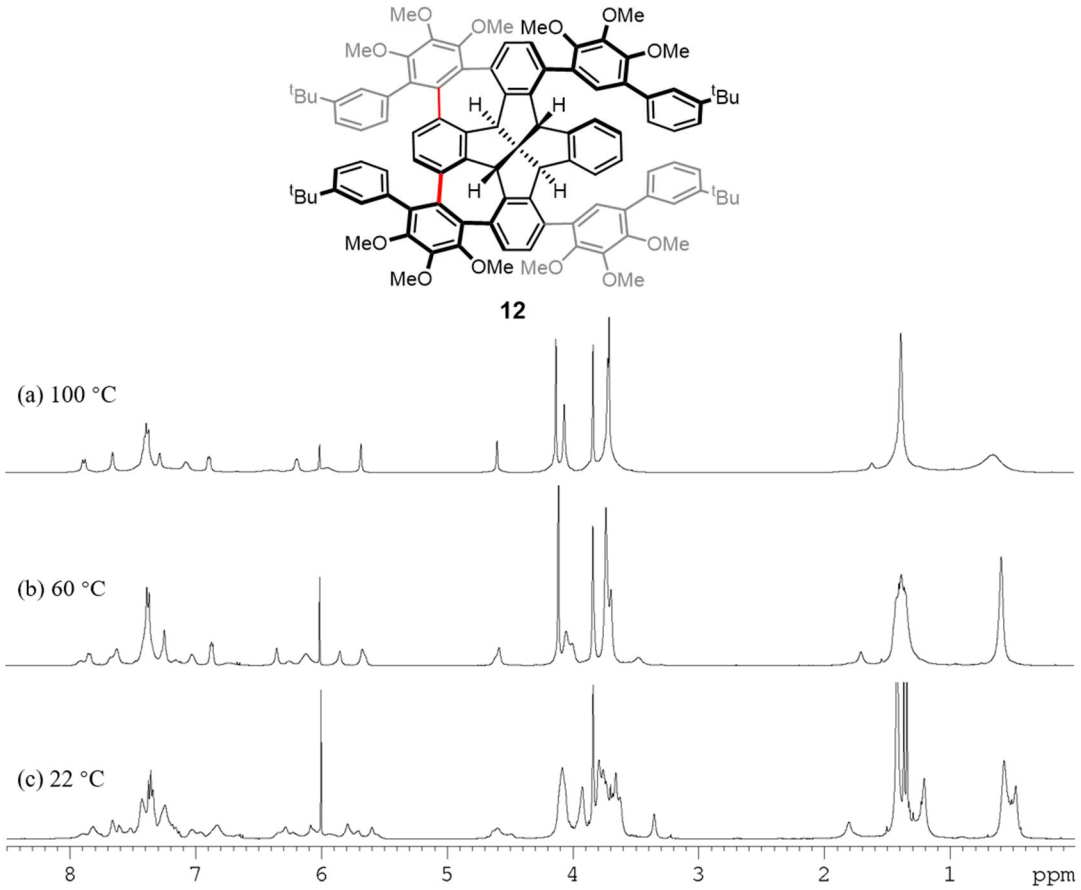


Figure S18. Stacked variable temperature ^{1}H NMR spectra (400 MHz, $C_2D_2Cl_4$) of compound **12** at (a) 100 °C, (b) 60 °C and (c) 22 °C.

7. Cyclic Voltammetry of Compound 3

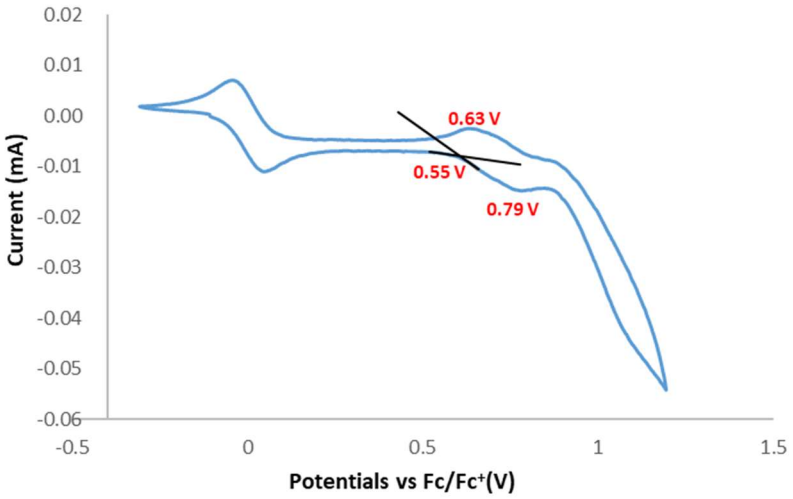


Figure S19. Cyclic voltammogram of compound **3.** (Scan rate: 20 mV s^{-1}, supporting electrolyte: 0.1 M $^{n}Bu_4NPF_6$ in CH_2Cl_2, working electrode: platinum bead, auxiliary electrode: platinum wire, pseudo-reference: silver wire).

Table S6. Electrochemical and Estimated Electronic Data for Compound **3**.

Compound	E_{ox1} (V)	E_{ox1}^{onset} (V)	HOMO level (eV) [a]	HOMO–LUMO gap (eV) [b]	LUMO level (eV) [c]
3	0.71	0.55	−5.65	2.92	−2.73

[a]Estimated by $E_{HOMO} = -(5.10 + E_{ox1}^{onset})$ (eV).[3]

[b]Approximated by the optical gap (E_{opt}) from UV–Vis spectroscopy.[4]

[c]Estimated by $E_{LUMO} = E_{HOMO} + E_{opt}$.

8. Density Functional Theory (DFT) Calculations

All the calculations were performed using the Gaussian 09 programs.[5] The 6-31G(d) basis set was used.[6–7] All of the structures were fully optimized with the B3LYP method in dichloromethane solvent employing the Polarizable Continuum Model (PCM).[8] Grimmes's DFT-D3 dispersion correction was used to describe the van der Waals interaction.[9] Vibrational frequency calculations were performed to ensure that a transition state has only one imaginary frequency and a local minimum has no imaginary frequency. Transition states connecting relevant minima were further examined by running intrinsic reaction coordinate (IRC) calculations.

Cartesian coordinates and free energy for all of the calculated structures

Structure G'

G = -4495.140777 Hartree

C	-3.22359	-1.86641	-1.31169
C	-4.50464	-1.91431	0.74985
C	-4.39617	-2.18139	-0.61857
C	2.39723	-0.96572	0.29730
C	2.27208	0.36585	-0.10739
C	-2.24887	-1.06524	0.75564
C	-2.15562	-1.27884	-0.62879
C	0.02604	-0.55351	0.11464
C	-0.25119	-1.19160	2.44300
C	0.85699	-1.88765	1.95175
C	0.33761	-1.94430	4.64728
C	1.43417	-2.63850	4.14140
C	-0.70627	0.45933	-1.95887
C	0.15723	1.37171	-1.33576
C	-0.35578	3.01856	-3.00904
C	-1.15359	2.08924	-3.67467

C	-1.33961	0.79507	-3.16637
C	4.77049	-0.72960	0.50145
C	4.66355	0.58448	0.04002
C	1.06676	-1.63699	0.48580
C	0.80458	0.77409	-0.10689
H	0.97839	-2.55803	-0.10662
H	0.66366	1.44889	0.74263
H	-0.35264	-1.64814	-1.77351
H	-1.16239	0.58001	1.57371
C	-0.97084	-0.46447	1.30878
C	-0.79710	-0.84651	-1.17216
C	1.72038	-2.63361	2.76234
C	3.62481	-1.53904	0.64073
C	3.41730	1.14857	-0.25936
C	0.31401	2.67714	-1.82521
C	-0.52840	-1.20802	3.81790
C	-3.42681	-1.35713	1.44390
C	1.15386	3.69463	-1.13847
C	-2.18594	-0.17059	-3.91323
C	-1.68068	-0.45607	4.37828
C	2.82991	-3.43016	2.15717
C	2.23660	4.27806	-1.80653
C	3.06947	5.22671	-1.20210
C	2.76542	5.64762	0.11042
C	1.66701	5.09446	0.79600
C	0.88072	4.10438	0.17480
C	-1.64355	-1.37288	-4.39379
C	-2.45745	-2.29315	-5.06576
C	-3.83208	-2.05066	-5.20709

C	-4.39484	-0.84190	-4.75454
C	-3.54560	0.07993	-4.12457
C	2.99489	-4.76623	2.58677
C	3.95479	-5.61470	2.02282
C	4.79074	-5.13631	1.01003
C	4.64305	-3.81988	0.54378
C	3.69000	-2.94827	1.12737
C	-1.83021	0.91112	4.11964
C	-2.96496	1.63156	4.50223
C	-3.99300	0.95327	5.19200
C	-3.84588	-0.41185	5.50317
C	-2.69092	-1.10804	5.10090
C	4.27490	5.70115	-1.93358
C	5.44085	-3.42945	-0.64794
C	-5.83996	-0.53613	-4.91501
C	-3.04155	3.08475	4.19781
C	5.53477	5.72356	-1.31107
C	6.68479	6.12170	-1.99840
C	6.56481	6.50000	-3.34442
C	5.32276	6.48304	-3.97786
C	4.18114	6.08688	-3.27917
C	4.79864	-2.86694	-1.77897
C	5.47593	-2.51424	-2.96619
C	6.81470	-2.77170	-3.07451
C	6.79583	-3.66190	-0.74217
C	-4.16245	3.64483	3.56401
C	-3.12473	5.81827	3.56888
C	-2.00519	5.27845	4.20073
C	-1.95666	3.91901	4.50852

C	-6.82654	-1.48807	-4.60732
C	-8.18857	-1.19639	-4.72623
C	-8.56556	0.07943	-5.17139
C	-7.59977	1.03675	-5.48082
C	-6.24351	0.73462	-5.35332
C	7.57062	-3.37964	-1.96420
C	-4.21845	5.00423	3.23882
H	-3.15240	-2.08837	-2.36900
H	-5.42452	-2.14815	1.27953
H	-5.22910	-2.63058	-1.15346
H	0.14422	-1.96213	5.71497
H	2.07503	-3.18607	4.82144
H	-0.24923	4.02428	-3.40640
H	-1.64641	2.36596	-4.60289
H	5.74404	-1.12341	0.77628
H	5.56164	1.18850	-0.05551
H	3.34795	2.18476	-0.57296
H	-3.50762	-1.14851	2.50500
H	2.47625	3.93173	-2.80719
H	-3.96957	0.99699	-3.72747
H	-1.04368	1.43353	3.58466
H	7.45018	6.81005	-3.89488
H	5.24085	6.78266	-5.01937
H	3.21264	6.08627	-3.77168
H	3.72445	-2.71575	-1.73576
H	4.91779	-2.07683	-3.78651
H	7.35405	-2.54802	-3.99047
H	7.33671	-4.07371	0.10196
H	-5.00167	3.00206	3.31746

H	-3.15216	6.87810	3.32573
H	-1.16628	5.91784	4.45970
H	-1.08351	3.50305	5.00294
H	-6.51997	-2.47213	-4.26866
H	-9.62101	0.32009	-5.27708
H	-7.90286	2.02000	-5.83099
H	-5.49348	1.47709	-5.61147
H	5.61055	5.42853	-0.26908
O	-5.12460	1.65309	5.50969
O	-4.88344	-1.06750	6.12422
O	-2.56154	-2.44459	5.41027
O	2.21397	-5.28877	3.58866
O	4.03456	-6.92975	2.39886
O	5.75207	-5.95238	0.46515
O	1.32798	5.41662	2.08010
O	-0.14270	3.52569	0.88891
O	3.55519	6.55461	0.78432
O	-0.32224	-1.69518	-4.17367
O	-1.90046	-3.42466	-5.61092
O	-4.60470	-3.02893	-5.79055
C	-4.70165	-2.91527	-7.21776
H	-3.71175	-3.00561	-7.67958
H	-5.34007	-3.73663	-7.54947
H	-5.15843	-1.95876	-7.49976
C	-1.95471	-4.56125	-4.73604
H	-1.39911	-4.36185	-3.81160
H	-2.99398	-4.81518	-4.49851
H	-1.48772	-5.38888	-5.27447
C	0.56757	-1.23068	-5.19756

H	0.32016	-1.68936	-6.16198
H	0.52368	-0.13800	-5.28368
H	1.57222	-1.53268	-4.89280
C	-1.38441	4.24434	0.84823
H	-2.07884	3.69732	1.48755
H	-1.26133	5.25770	1.24279
H	-1.76904	4.28439	-0.17867
C	1.20874	6.80139	2.43020
H	0.58357	6.82909	3.32467
H	2.18272	7.24514	2.64590
H	0.71433	7.36563	1.63015
C	3.54200	7.89942	0.27698
H	2.53631	8.32992	0.34898
H	4.22851	8.46524	0.90960
H	3.88423	7.94165	-0.76077
C	5.25206	-6.96757	-0.42612
H	4.57379	-7.64290	0.10201
H	4.73704	-6.50678	-1.27813
H	6.12741	-7.51556	-0.77897
C	-3.31396	-3.32996	4.56463
H	-4.37857	-3.07316	4.58051
H	-2.93829	-3.29120	3.53583
H	-3.17038	-4.33333	4.97058
C	-4.60153	-1.58649	7.43699
H	-4.31486	-0.77515	8.11674
H	-5.53200	-2.04002	7.78399
H	-3.80871	-2.33713	7.40181
C	-5.56464	1.65059	6.87503
H	-6.16407	0.76477	7.09709

H	-4.70980	1.69788	7.56007
H	-6.17277	2.55013	6.99584
C	4.69869	-7.14898	3.65694
H	4.16684	-6.64109	4.46709
H	4.68415	-8.22782	3.82196
H	5.73586	-6.79705	3.60811
C	1.03899	-5.96907	3.11618
H	0.38679	-5.27508	2.57300
H	1.31630	-6.80995	2.47127
H	0.52273	-6.33727	4.00436
C	-9.23496	-2.22289	-4.35736
H	-9.65421	-2.01868	-3.36342
H	-10.07018	-2.21383	-5.06670
H	-8.81585	-3.23399	-4.33659
C	-5.43956	5.58953	2.56754
H	-6.09244	6.08376	3.29898
H	-5.16238	6.34281	1.82162
H	-6.03249	4.81643	2.06846
C	8.02753	6.16353	-1.30594
H	8.81903	5.75360	-1.94361
H	8.31214	7.19573	-1.06369
H	8.01529	5.59707	-0.36939
C	8.37731	-4.64305	-2.43018
H	9.01361	-4.38087	-3.27835
H	9.00360	-4.99903	-1.60943
H	7.68655	-5.43595	-2.72514
H	8.34685	-2.64095	-1.67554

$TS_{G'\rightarrow I'}$

G = -4495.122806 Hartree

C	-3.33955	-1.88604	-1.33149
C	-4.62182	-1.84206	0.72899
C	-4.52107	-2.14732	-0.63200
C	2.32064	-1.06104	0.28702
C	2.20190	0.25581	-0.18748
C	-2.33977	-1.06850	0.71640
C	-2.25475	-1.31385	-0.66218
C	-0.04973	-0.63385	0.06057
C	-0.35336	-1.29474	2.38710
C	0.73732	-2.00790	1.88791
C	0.16651	-2.17914	4.56052
C	1.24711	-2.88922	4.04150
C	-0.78504	0.37894	-2.01453
C	0.10213	1.28191	-1.41312
C	-0.40881	2.92971	-3.08023
C	-1.23532	2.01162	-3.72563
C	-1.43554	0.72257	-3.21071
C	4.72414	-0.82948	0.37496
C	4.57940	0.49532	-0.16365
C	0.98125	-1.72577	0.43822
C	0.74911	0.67352	-0.18849
H	0.91623	-2.63223	-0.17799
H	0.64628	1.36546	0.65728
H	-0.46623	-1.73517	-1.81847
H	-1.18500	0.53184	1.54312
C	-1.03794	-0.51617	1.26433
C	-0.88983	-0.92144	-1.21838

C	1.56662	-2.81056	2.67263
C	3.53859	-1.60798	0.67098
C	3.34584	1.03182	-0.45889
C	0.27702	2.58310	-1.90711
C	-0.64994	-1.36018	3.75691
C	-3.52655	-1.30480	1.41080
C	1.15141	3.58785	-1.24545
C	-2.31785	-0.22722	-3.93512
C	-1.75834	-0.56339	4.34125
C	2.69539	-3.56522	2.05493
C	2.21167	4.16528	-1.95519
C	3.08061	5.09950	-1.38002
C	2.83668	5.51485	-0.05301
C	1.76276	4.96782	0.67507
C	0.93998	3.99032	0.08166
C	-1.80969	-1.43918	-4.42624
C	-2.65763	-2.34548	-5.07597
C	-4.03000	-2.07729	-5.18482
C	-4.55857	-0.85694	-4.72036
C	-3.67765	0.04929	-4.11287
C	2.82875	-4.93013	2.38157
C	3.83520	-5.71810	1.81687
C	4.80076	-5.13965	0.97931
C	4.72925	-3.77847	0.64665
C	3.64729	-2.99813	1.15597
C	-1.82538	0.81603	4.11557
C	-2.90729	1.59776	4.52776
C	-3.96972	0.96888	5.21303
C	-3.90573	-0.41067	5.48958

C	-2.80059	-1.16876	5.05865
C	4.26158	5.56208	-2.15761
C	5.76281	-3.14733	-0.21850
C	-6.00210	-0.52653	-4.84096
C	-2.88848	3.06011	4.26110
C	5.54570	5.56261	-1.58622
C	6.67317	5.94421	-2.31865
C	6.50446	6.32954	-3.65750
C	5.23759	6.33573	-4.23974
C	4.11901	5.95467	-3.49675
C	5.33726	-2.01438	-1.06625
C	6.34734	-1.32885	-1.86782
C	7.64057	-1.69192	-1.82762
C	7.07599	-3.46264	-0.15768
C	-3.97757	3.71568	3.66467
C	-2.78336	5.80761	3.69826
C	-1.69439	5.17238	4.29406
C	-1.73992	3.80594	4.56865
C	-6.99534	-1.45912	-4.49675
C	-8.35477	-1.14343	-4.57428
C	-8.72271	0.13684	-5.01492
C	-7.75037	1.07458	-5.36071
C	-6.39619	0.74861	-5.27412
C	8.14661	-2.81224	-0.97780
C	-3.93997	5.08348	3.37295
H	-3.27513	-2.13664	-2.38250
H	-5.54896	-2.03231	1.26321
H	-5.36730	-2.58300	-1.15684
H	-0.05048	-2.24431	5.62157

H	1.85342	-3.49736	4.70203
H	-0.29255	3.93141	-3.48435
H	-1.74124	2.29423	-4.64481
H	5.60401	-0.98990	0.98946
H	5.48140	1.07576	-0.33093
H	3.25529	2.03847	-0.84938
H	-3.59995	-1.07068	2.46687
H	2.40477	3.82422	-2.96765
H	-4.07475	0.97440	-3.70683
H	-1.01163	1.30096	3.58627
H	7.37160	6.62689	-4.24275
H	5.11821	6.64095	-5.27592
H	3.13151	5.97136	-3.94960
H	4.37338	-2.11545	-1.55975
H	6.00782	-0.53680	-2.52795
H	8.36160	-1.19678	-2.47417
H	7.40211	-4.25932	0.49981
H	-4.86622	3.14230	3.42044
H	-2.73824	6.87241	3.48096
H	-0.80675	5.74231	4.55296
H	-0.89097	3.31571	5.03655
H	-6.69583	-2.44658	-4.16159
H	-9.77652	0.39614	-5.08801
H	-8.04665	2.06134	-5.70678
H	-5.64131	1.47621	-5.55920
H	5.65892	5.26408	-0.54862
O	-5.04855	1.73348	5.55858
O	-4.97709	-1.01541	6.10436
O	-2.74986	-2.51737	5.33360

O	1.96173	-5.53683	3.25604
O	3.86636	-7.06687	2.03556
O	5.81565	-5.93504	0.51372
O	1.48221	5.28415	1.97375
O	-0.05393	3.41320	0.83780
O	3.66354	6.40677	0.59381
O	-0.48900	-1.77883	-4.23250
O	-2.13952	-3.49064	-5.63081
O	-4.83651	-3.04200	-5.74235
C	-4.96518	-2.93659	-7.16780
H	-3.98906	-3.05324	-7.65247
H	-5.63010	-3.74537	-7.47751
H	-5.40653	-1.97180	-7.44627
C	-2.09768	-4.59649	-4.71604
H	-1.46185	-4.35935	-3.85491
H	-3.10781	-4.85178	-4.37522
H	-1.67217	-5.43770	-5.26735
C	0.35876	-1.47556	-5.35025
H	0.03177	-2.02134	-6.24191
H	0.35877	-0.39705	-5.55178
H	1.36439	-1.79580	-5.06940
C	-1.29130	4.14257	0.86867
H	-1.95755	3.59152	1.53384
H	-1.13872	5.14832	1.27135
H	-1.72471	4.19937	-0.13742
C	1.39295	6.66871	2.33708
H	0.79479	6.69815	3.24949
H	2.37942	7.09658	2.52600
H	0.88292	7.24471	1.55584

C	3.64943	7.75569	0.09564
H	2.65338	8.19884	0.21028
H	4.36827	8.30695	0.70453
H	3.95112	7.80009	-0.95439
C	5.46311	-6.75265	-0.61581
H	4.64818	-7.43574	-0.35752
H	5.17374	-6.12498	-1.46741
H	6.35919	-7.32228	-0.86816
C	-3.58218	-3.33427	4.49251
H	-4.62699	-3.01097	4.54617
H	-3.23432	-3.29580	3.45408
H	-3.49067	-4.35331	4.87338
C	-4.71880	-1.58654	7.40054
H	-4.38161	-0.81254	8.10023
H	-5.67232	-1.99459	7.74108
H	-3.97143	-2.38079	7.33921
C	-5.50723	1.70119	6.91769
H	-6.18121	0.85905	7.08922
H	-4.66164	1.64373	7.61301
H	-6.03963	2.64199	7.07559
C	4.41546	-7.45469	3.30931
H	3.81923	-7.03931	4.12723
H	4.37464	-8.54490	3.33530
H	5.45638	-7.12170	3.39204
C	0.80870	-6.11990	2.62389
H	0.21963	-5.34908	2.11307
H	1.11357	-6.89439	1.91182
H	0.21509	-6.56391	3.42465
C	-9.40846	-2.14874	-4.16965

H	-9.83980	-1.89624	-3.19225
H	-10.23507	-2.17109	-4.88904
H	-8.99300	-3.15882	-4.09685
C	-5.12839	5.77221	2.74235
H	-5.72885	6.29331	3.49954
H	-4.81259	6.52226	2.00868
H	-5.78577	5.05676	2.23806
C	8.04386	5.96038	-1.68229
H	8.79908	5.52986	-2.34968
H	8.36049	6.98738	-1.45871
H	8.05823	5.39922	-0.74259
C	8.89618	-3.86484	-1.83853
H	9.72183	-3.39643	-2.38399
H	9.30614	-4.65371	-1.19998
H	8.21252	-4.32154	-2.56097
H	8.89340	-2.39714	-0.27819

Structure I'

G = -4495.127502 Hartree

C	-3.40887	-1.86407	-1.35851
C	-4.66526	-1.79838	0.71725
C	-4.58589	-2.10576	-0.64463
C	2.28649	-1.14392	0.16554
C	2.17223	0.16845	-0.32128
C	-2.37125	-1.06286	0.67725
C	-2.30700	-1.31005	-0.70219
C	-0.08329	-0.66942	-0.00720
C	-0.36473	-1.31629	2.32358
C	0.71177	-2.04003	1.81034

C	0.18048	-2.20766	4.48747
C	1.24783	-2.92489	3.95316
C	-0.83111	0.36544	-2.06599
C	0.07465	1.25434	-1.47169
C	-0.44599	2.92335	-3.11174
C	-1.28882	2.01847	-3.75458
C	-1.49549	0.72671	-3.24918
C	4.73999	-0.97499	0.03917
C	4.53414	0.37098	-0.54632
C	0.93561	-1.77600	0.35810
C	0.73765	0.61771	-0.26848
H	0.84258	-2.68600	-0.24915
H	0.68587	1.30606	0.58755
H	-0.54041	-1.75546	-1.88560
H	-1.17907	0.52017	1.48704
C	-1.05400	-0.53108	1.20876
C	-0.94350	-0.93848	-1.27603
C	1.54571	-2.84905	2.57775
C	3.51476	-1.71382	0.47940
C	3.30742	0.93619	-0.69594
C	0.25395	2.55991	-1.95200
C	-0.64244	-1.38163	3.69680
C	-3.55340	-1.27889	1.38585
C	1.13728	3.55399	-1.28671
C	-2.39946	-0.20721	-3.96717
C	-1.74023	-0.58322	4.29765
C	2.67256	-3.60320	1.95976
C	2.17786	4.15772	-2.00424
C	3.04683	5.09010	-1.42624

C	2.82587	5.47262	-0.08534
C	1.77474	4.89565	0.65277
C	0.94800	3.92558	0.05284
C	-1.91430	-1.42384	-4.47006
C	-2.78437	-2.31666	-5.10968
C	-4.15382	-2.02798	-5.20094
C	-4.65873	-0.80153	-4.72614
C	-3.75751	0.08923	-4.12594
C	2.82106	-4.94937	2.32970
C	3.88821	-5.72208	1.85163
C	4.91505	-5.12884	1.10320
C	4.83591	-3.77957	0.72251
C	3.65604	-3.03546	1.07296
C	-1.80082	0.79903	4.08772
C	-2.87559	1.58028	4.51853
C	-3.93850	0.94852	5.20038
C	-3.88034	-0.43462	5.46011
C	-2.78050	-1.19211	5.01497
C	4.20427	5.58748	-2.21766
C	5.92900	-3.13523	-0.04430
C	-6.09846	-0.44929	-4.82833
C	-2.84986	3.04716	4.27864
C	5.50021	5.59386	-1.67364
C	6.60604	6.00905	-2.42059
C	6.40286	6.42355	-3.74588
C	5.12378	6.42475	-4.30078
C	4.02709	6.00941	-3.54359
C	5.52059	-1.98026	-0.93622
C	6.66141	-1.34001	-1.67161

C	7.93443	-1.70765	-1.51569
C	7.22631	-3.44001	0.13781
C	-3.92881	3.71493	3.67783
C	-2.73276	5.80396	3.77018
C	-1.65496	5.15660	4.37330
C	-1.70576	3.78466	4.61956
C	-7.10146	-1.36712	-4.47214
C	-8.45649	-1.03013	-4.53078
C	-8.81038	0.25686	-4.96396
C	-7.82848	1.17972	-5.32169
C	-6.47831	0.83234	-5.25419
C	8.37738	-2.80527	-0.59173
C	-3.88450	5.08756	3.41134
H	-3.36135	-2.11514	-2.41030
H	-5.58891	-1.97299	1.26261
H	-5.44541	-2.52744	-1.15911
H	-0.02043	-2.27118	5.55173
H	1.86143	-3.53385	4.60597
H	-0.32888	3.92862	-3.50636
H	-1.80476	2.31480	-4.66373
H	5.42357	-0.84909	0.89294
H	5.42695	0.91676	-0.83411
H	3.18680	1.93834	-1.08930
H	-3.61081	-1.04296	2.44242
H	2.35344	3.84236	-3.02820
H	-4.13629	1.01823	-3.71139
H	-0.98782	1.28665	3.55938
H	7.25285	6.74731	-4.34215
H	4.97764	6.75256	-5.32655

H	3.02997	6.02205	-3.97498
H	4.77064	-2.30936	-1.66905
H	6.40227	-0.56852	-2.39227
H	8.70996	-1.22477	-2.10768
H	7.49517	-4.21863	0.84163
H	-4.81444	3.14727	3.40985
H	-2.68344	6.87275	3.57447
H	-0.77326	5.72177	4.66171
H	-0.86554	3.28348	5.09163
H	-6.81286	-2.35951	-4.14202
H	-9.86093	0.53288	-5.02127
H	-8.11382	2.17187	-5.66144
H	-5.71607	1.54880	-5.54775
H	5.64017	5.27300	-0.64610
O	-5.01054	1.71603	5.55831
O	-4.95160	-1.04221	6.07170
O	-2.73326	-2.54384	5.27390
O	1.92469	-5.56955	3.16330
O	3.92885	-7.06285	2.08028
O	5.98981	-5.91389	0.77813
O	1.52088	5.17351	1.96534
O	-0.03032	3.32287	0.80984
O	3.65587	6.35958	0.56359
O	-0.59563	-1.77949	-4.29386
O	-2.29193	-3.46991	-5.67131
O	-4.98207	-2.97879	-5.74975
C	-5.11620	-2.87759	-7.17512
H	-4.14519	-3.01540	-7.66434
H	-5.79830	-3.67478	-7.47734

H	-5.54038	-1.90571	-7.45561
C	-2.23764	-4.57151	-4.75180
H	-1.57901	-4.33574	-3.90770
H	-3.24156	-4.81575	-4.38540
H	-1.83330	-5.41925	-5.30891
C	0.23240	-1.53828	-5.44191
H	-0.12548	-2.11198	-6.30322
H	0.24882	-0.46873	-5.68578
H	1.23749	-1.86758	-5.17005
C	-1.25016	4.07414	0.93112
H	-1.91112	3.48895	1.57162
H	-1.06346	5.04267	1.40300
H	-1.70898	4.21418	-0.05518
C	1.42592	6.54606	2.37151
H	0.85395	6.53985	3.30077
H	2.41243	6.98033	2.54452
H	0.88604	7.13752	1.62264
C	3.60964	7.72024	0.09985
H	2.61167	8.14631	0.25484
H	4.33911	8.26611	0.70083
H	3.87932	7.79413	-0.95722
C	5.82227	-6.67392	-0.43088
H	4.97477	-7.36089	-0.33685
H	5.67356	-6.00581	-1.28747
H	6.74572	-7.24003	-0.56366
C	-3.57396	-3.34814	4.42868
H	-4.61714	-3.02168	4.49260
H	-3.23249	-3.29864	3.38861
H	-3.48363	-4.37173	4.79731

C	-4.69135	-1.62945	7.36040
H	-4.35029	-0.86466	8.06825
H	-5.64505	-2.03901	7.69848
H	-3.94628	-2.42487	7.28749
C	-5.47487	1.66296	6.91501
H	-6.15594	0.82323	7.06897
H	-4.63246	1.58674	7.61231
H	-6.00040	2.60507	7.08717
C	4.36414	-7.44833	3.40008
H	3.69334	-7.03873	4.16044
H	4.32931	-8.53854	3.41912
H	5.39087	-7.10716	3.57228
C	0.76278	-6.09019	2.49320
H	0.19699	-5.28159	2.01601
H	1.05550	-6.83611	1.74605
H	0.15160	-6.55847	3.26624
C	-9.52185	-2.02006	-4.11888
H	-9.99578	-1.72031	-3.17537
H	-10.31733	-2.08412	-4.87056
H	-9.10602	-3.02269	-3.97831
C	-5.06088	5.79010	2.77355
H	-5.66328	6.31296	3.52792
H	-4.73165	6.54105	2.04670
H	-5.71994	5.08326	2.25948
C	7.98999	6.02923	-1.81368
H	8.73460	5.61683	-2.50404
H	8.30140	7.05574	-1.58081
H	8.03035	5.45328	-0.88373
C	9.18182	-3.88277	-1.35888

H	10.05327	-3.43793	-1.85218
H	9.53625	-4.66149	-0.67465
H	8.55403	-4.35421	-2.12272
H	9.06124	-2.37629	0.15959

Structure H'

G = -4495.155267 Hartree

C	-3.91526	1.22271	0.67413
C	-5.22646	-0.80720	0.86987
C	-5.13980	0.58827	0.90398
C	1.76811	-0.85986	-0.29067
C	1.65171	-0.86798	1.09953
C	-2.87466	-0.95504	0.34525
C	-2.78900	0.44668	0.40470
C	-0.53751	-0.37005	0.18270
C	-1.12918	-2.26534	-1.22424
C	0.01977	-1.67982	-1.76941
C	-0.99118	-3.95478	-2.92966
C	0.18298	-3.39235	-3.42712
C	-0.65832	1.88586	0.97136
C	0.27745	1.23103	1.78655
C	0.91817	3.36033	2.72418
C	0.02019	4.00897	1.87840
C	-0.76869	3.28329	0.97399
C	3.95554	-1.80015	-0.20162
C	3.82134	-1.90769	1.18541
C	0.48617	-0.49737	-0.96671
C	0.30297	-0.27156	1.50063
H	0.57213	0.41374	-1.57424

H	-0.15535	-0.81733	2.33524
H	-1.38512	1.28927	-0.95613
H	-1.30328	-2.31157	0.89925
C	-1.50727	-1.58734	0.09890
C	-1.38582	0.91276	0.07086
C	0.72847	-2.23383	-2.84458
C	2.90834	-1.27152	-0.97307
C	2.68412	-1.42808	1.85284
C	1.06689	1.96687	2.68061
C	-1.65497	-3.42369	-1.81088
C	-4.09564	-1.58388	0.59822
C	2.08187	1.31613	3.55168
C	-1.63817	4.00536	0.00625
C	-2.84905	-4.10862	-1.24572
C	1.98343	-1.58398	-3.32869
C	3.45212	1.49872	3.31505
C	4.53374	0.92948	4.02594
C	4.20969	0.13479	5.11273
C	2.75928	-0.20481	5.45554
C	1.71808	0.46458	4.58263
C	-1.37123	3.93283	-1.36756
C	-2.15919	4.64231	-2.29326
C	-3.24830	5.40868	-1.83467
C	-3.54426	5.47238	-0.45575
C	-2.71388	4.78617	0.43913
C	2.16262	-1.39651	-4.71380
C	3.26340	-0.69556	-5.21916
C	4.21321	-0.15969	-4.34265
C	4.05940	-0.30304	-2.95409

C	2.98308	-1.07331	-2.45054
C	-2.77354	-4.78464	-0.02542
C	-3.89588	-5.35833	0.58701
C	-5.14305	-5.25424	-0.06960
C	-5.23673	-4.58629	-1.30560
C	-4.08936	-4.02059	-1.88825
C	5.91416	1.14514	3.49466
C	4.93162	0.50815	-2.05049
C	-4.73979	6.18541	0.06949
C	-3.74192	-6.05506	1.89100
C	6.53231	0.11522	2.77889
C	7.82372	0.26105	2.25746
C	8.48945	1.47369	2.47167
C	7.87012	2.52072	3.16017
C	6.58062	2.36528	3.66908
C	4.33401	1.43859	-1.18304
C	5.12138	2.24761	-0.36701
C	6.51288	2.15027	-0.41364
C	6.32923	0.42599	-2.08805
C	-4.62367	-5.81948	2.95880
C	-3.37143	-7.31112	4.37568
C	-2.48537	-7.55774	3.32692
C	-2.66646	-6.93525	2.09143
C	-6.00334	6.00483	-0.51698
C	-7.14417	6.63261	-0.00762
C	-7.00764	7.46510	1.11300
C	-5.76045	7.65549	1.70803
C	-4.63025	7.02016	1.19233
C	7.13357	1.24355	-1.28287

C	-4.45518	-6.43813	4.20155
H	-3.84014	2.30576	0.70525
H	-6.17757	-1.29750	1.06052
H	-6.02451	1.18261	1.11726
H	-1.39126	-4.85130	-3.39495
H	0.68411	-3.85730	-4.26733
H	1.52658	3.93989	3.41327
H	-0.05314	5.09264	1.89570
H	4.86516	-2.13968	-0.68790
H	4.61458	-2.37854	1.75941
H	2.61382	-1.53113	2.93046
H	-4.17348	-2.66363	0.59828
H	3.71688	2.12133	2.46443
H	-2.94616	4.81446	1.49935
H	-1.81572	-4.83682	0.48341
H	9.49858	1.60485	2.08933
H	8.39900	3.45814	3.30680
H	6.10166	3.17252	4.21581
H	3.25172	1.51690	-1.14413
H	4.64950	2.96601	0.29917
H	7.12153	2.77709	0.23153
H	6.79682	-0.27905	-2.76893
H	-5.45375	-5.13583	2.81396
H	-3.22407	-7.79870	5.33680
H	-1.65099	-8.23950	3.47017
H	-1.98160	-7.14122	1.27349
H	-6.09037	5.36639	-1.39060
H	-7.88343	7.96791	1.51673
H	-5.66555	8.30856	2.57157

H	-3.65724	7.18306	1.64762
H	5.99328	-0.81314	2.61842
H	2.59976	0.15564	6.48669
O	-6.24607	-5.77601	0.55002
O	-6.47661	-4.41721	-1.87407
O	-4.19531	-3.34781	-3.08559
O	1.25021	-1.89215	-5.61883
O	3.36876	-0.44465	-6.56585
O	5.28474	0.53065	-4.85850
O	2.53121	-1.59815	5.34976
O	0.44240	0.23180	4.77119
O	4.99455	-0.44477	5.99300
O	-0.34734	3.13424	-1.82862
O	-1.82920	4.47841	-3.60833
O	-4.04009	6.03090	-2.77580
C	-4.00355	7.46777	-2.77534
H	-2.99531	7.82854	-3.01076
H	-4.69773	7.78608	-3.55529
H	-4.32332	7.87768	-1.81315
C	-1.74700	5.63131	-4.45700
H	-2.73348	5.94092	-4.80761
H	-1.26170	6.46569	-3.93667
H	-1.12878	5.32951	-5.30556
C	0.87999	3.82477	-2.09070
H	0.75044	4.56667	-2.88683
H	1.24906	4.31645	-1.18165
H	1.59728	3.06511	-2.41037
C	-0.08082	-0.61753	5.82341
H	-1.13416	-0.35153	5.88813

H	0.04380	-1.66152	5.54022
H	0.41836	-0.41256	6.77333
C	2.79679	-2.39087	6.51838
H	2.38601	-3.37689	6.29618
H	3.86846	-2.46692	6.71379
H	2.28950	-1.97032	7.39577
C	6.43545	-0.28550	6.05936
H	6.69778	0.77222	6.03910
H	6.70975	-0.73705	7.01129
H	6.90707	-0.81052	5.22876
C	4.98626	1.88819	-5.21577
H	4.21836	1.92342	-5.99603
H	4.65258	2.45238	-4.33586
H	5.91660	2.31817	-5.59286
C	-4.63937	-1.98632	-2.94830
H	-5.61229	-1.94387	-2.44700
H	-3.90934	-1.39949	-2.37982
H	-4.72577	-1.59129	-3.96254
C	-6.67090	-5.03547	-3.15925
H	-6.53571	-6.12151	-3.08664
H	-7.70235	-4.81608	-3.44201
H	-5.98301	-4.62441	-3.90130
C	-7.06330	-6.69809	-0.18450
H	-7.78993	-6.17335	-0.80895
H	-6.44621	-7.35372	-0.81028
H	-7.58366	-7.30049	0.56390
C	3.86460	-1.55507	-7.32954
H	3.20051	-2.42007	-7.23016
H	3.88741	-1.22476	-8.37017

H	4.87818	-1.82236	-7.00655
C	0.25521	-0.93540	-6.01519
H	-0.32855	-0.60546	-5.14722
H	0.72323	-0.07260	-6.50169
H	-0.39980	-1.44876	-6.72194
C	-8.49937	6.39498	-0.63306
H	-9.03947	5.59528	-0.10922
H	-9.12498	7.29288	-0.58461
H	-8.41015	6.09586	-1.68246
C	-5.43400	-6.18902	5.32630
H	-6.19736	-6.97737	5.36468
H	-4.93194	-6.17843	6.30007
H	-5.95653	-5.23515	5.20010
C	8.44354	-0.86077	1.46149
H	7.95626	-0.94269	0.48221
H	9.51103	-0.69412	1.29078
H	8.32156	-1.82425	1.96895
C	8.64009	1.18261	-1.38323
H	9.11163	1.43817	-0.42907
H	8.98569	0.18719	-1.68029
H	9.01100	1.89427	-2.13257

$TS_{H'\rightarrow J'}$

G = -4495.12144 Hartree

C	-3.85518	1.52173	-0.24444
C	-5.26964	-0.44338	-0.35752
C	-5.12668	0.94622	-0.30739
C	1.85587	-0.68357	-0.51714
C	1.70629	-0.63742	0.85171

C	-2.86890	-0.69772	-0.30843
C	-2.72825	0.69712	-0.23130
C	-0.49095	-0.23454	-0.12182
C	-1.00227	-2.25952	-1.39323
C	0.16564	-1.71167	-1.93227
C	-0.69781	-4.14989	-2.84712
C	0.47908	-3.60538	-3.35159
C	-0.69000	1.96529	0.89081
C	0.21483	1.23629	1.66641
C	0.70985	3.15639	3.00716
C	-0.19486	3.89675	2.24452
C	-0.88600	3.33002	1.15982
C	4.15872	-1.38666	-0.29302
C	4.01741	-1.39923	1.07188
C	0.56568	-0.43923	-1.24126
C	0.30829	-0.20885	1.22064
H	0.64478	0.40776	-1.93512
H	-0.11295	-0.86930	1.98931
H	-1.04875	1.61112	-1.17934
H	-1.50708	-2.01973	0.67223
C	-1.52154	-1.40447	-0.23565
C	-1.26652	1.11209	-0.22937
C	0.94574	-2.35632	-2.89928
C	3.06581	-1.03912	-1.13951
C	2.80284	-0.95615	1.73577
C	0.94227	1.80859	2.71091
C	-1.45372	-3.50570	-1.85207
C	-4.14299	-1.27017	-0.35413
C	1.95187	0.98448	3.42781

C	-1.78649	4.18393	0.34164
C	-2.66421	-4.16212	-1.29254
C	2.19245	-1.72927	-3.42631
C	3.19773	0.61830	2.73448
C	4.36643	0.24400	3.57832
C	4.10829	-0.28010	4.79368
C	2.69486	-0.50642	5.28546
C	1.70311	0.44151	4.64690
C	-1.55394	4.37172	-1.02639
C	-2.42067	5.16266	-1.80454
C	-3.55405	5.74603	-1.20580
C	-3.80774	5.55727	0.17054
C	-2.90014	4.80164	0.92128
C	2.42888	-1.78213	-4.81436
C	3.57066	-1.20897	-5.39140
C	4.51546	-0.56244	-4.58426
C	4.30669	-0.45582	-3.20358
C	3.17383	-1.07543	-2.61282
C	-2.74102	-4.49730	0.06248
C	-3.90267	-5.01701	0.64575
C	-5.03005	-5.22985	-0.17969
C	-4.96716	-4.91879	-1.55184
C	-3.78640	-4.38816	-2.10051
C	5.74158	0.50307	3.08500
C	5.19665	0.45109	-2.42399
C	-5.04300	6.06350	0.82732
C	-3.91277	-5.33432	2.09802
C	6.72938	-0.49552	3.13180
C	8.03804	-0.24858	2.70985

C	8.36273	1.04193	2.26326
C	7.39614	2.04516	2.22101
C	6.08476	1.77812	2.61433
C	4.64276	1.58650	-1.81177
C	5.46680	2.48623	-1.13712
C	6.83956	2.25432	-1.06053
C	6.57768	0.23094	-2.33536
C	-4.96848	-4.92808	2.93003
C	-3.85861	-5.85195	4.85742
C	-2.80070	-6.26407	4.04642
C	-2.82447	-6.00852	2.67533
C	-6.30437	5.85070	0.24719
C	-7.47920	6.28028	0.87154
C	-7.37957	6.94274	2.10417
C	-6.13488	7.16056	2.69490
C	-4.96988	6.72345	2.06307
C	7.41156	1.11381	-1.64277
C	-4.95843	-5.17943	4.30596
H	-3.75133	2.59932	-0.20707
H	-6.26024	-0.88868	-0.39734
H	-6.00563	1.58563	-0.31283
H	-1.03442	-5.11624	-3.20994
H	1.04423	-4.15551	-4.09316
H	1.25475	3.63036	3.81853
H	-0.34737	4.94932	2.46657
H	5.09240	-1.70342	-0.74199
H	4.83850	-1.74862	1.68553
H	2.53747	-1.51227	2.63489
H	-4.26784	-2.34486	-0.37479

H	3.45337	1.28283	1.91254
H	-3.10908	4.62199	1.97123
H	-1.87690	-4.32115	0.69515
H	9.38119	1.25935	1.95080
H	7.66480	3.04240	1.88612
H	5.33940	2.56819	2.58744
H	3.57379	1.76863	-1.88586
H	5.03927	3.37338	-0.67776
H	7.47802	2.96238	-0.54103
H	7.00285	-0.64575	-2.81524
H	-5.80902	-4.39894	2.49309
H	-3.83319	-6.05291	5.92608
H	-1.95497	-6.78910	4.48298
H	-2.00491	-6.34343	2.04549
H	-6.36325	5.34472	-0.71158
H	-8.28295	7.29065	2.59984
H	-6.06996	7.68028	3.64717
H	-3.99975	6.90614	2.51693
H	6.46687	-1.47709	3.51542
H	2.70969	-0.38543	6.37757
O	-6.17314	-5.70230	0.40177
O	-6.10345	-5.05121	-2.31351
O	-3.74616	-4.04829	-3.43444
O	1.53800	-2.39663	-5.66176
O	3.73157	-1.18934	-6.74799
O	5.63694	-0.02373	-5.15774
O	2.19998	-1.81912	4.95834
O	0.51993	0.67877	5.23650
O	5.07601	-0.69979	5.66524

O	-0.48035	3.75667	-1.63222
O	-2.11539	5.25398	-3.13234
O	-4.42538	6.44126	-2.01559
C	-4.52089	7.85484	-1.77226
H	-3.55726	8.34429	-1.95623
H	-5.26343	8.23100	-2.47838
H	-4.84970	8.06536	-0.75085
C	-2.16163	6.53609	-3.77338
H	-3.18192	6.80692	-4.05139
H	-1.73697	7.31261	-3.12588
H	-1.54488	6.43981	-4.66984
C	0.66708	4.59937	-1.79315
H	0.44289	5.44508	-2.45294
H	1.01381	4.97062	-0.82044
H	1.44405	3.97845	-2.24528
C	0.19671	0.07051	6.49919
H	-0.85111	0.31559	6.67188
H	0.32460	-1.01359	6.45070
H	0.80632	0.49274	7.30476
C	2.89583	-2.88757	5.60833
H	2.34818	-3.79831	5.35816
H	3.93034	-2.97059	5.25648
H	2.90056	-2.74699	6.69747
C	5.75851	0.34310	6.39049
H	5.04864	0.91970	6.99521
H	6.47163	-0.16279	7.04258
H	6.28955	1.00982	5.70418
C	5.42788	1.25042	-5.79095
H	4.69771	1.16424	-6.60199

H	5.08935	1.99102	-5.05640
H	6.39648	1.55140	-6.19423
C	-4.38133	-2.79123	-3.72934
H	-5.44317	-2.82138	-3.46254
H	-3.88889	-1.97633	-3.18635
H	-4.27236	-2.63999	-4.80504
C	-6.02944	-5.99172	-3.40097
H	-5.81535	-6.99867	-3.02290
H	-7.01499	-5.98143	-3.87023
H	-5.26614	-5.69714	-4.12458
C	-6.81682	-6.84436	-0.18146
H	-7.48910	-6.55015	-0.99034
H	-6.07625	-7.55837	-0.56046
H	-7.38664	-7.31096	0.62549
C	4.12050	-2.44716	-7.33170
H	3.36839	-3.21555	-7.13159
H	4.19428	-2.26919	-8.40583
H	5.09561	-2.76110	-6.94173
C	0.57084	-1.49883	-6.23325
H	-0.03745	-1.03810	-5.44582
H	1.06984	-0.72358	-6.82459
H	-0.06457	-2.10724	-6.87904
C	-8.82863	6.01031	0.24687
H	-9.28466	5.10609	0.67112
H	-9.52443	6.83730	0.42591
H	-8.74715	5.85945	-0.83444
C	-6.12108	-4.75417	5.17334
H	-6.86302	-5.55925	5.25803
H	-5.79444	-4.50599	6.18897

H	-6.63453	-3.88172	4.75585
C	9.07964	-1.34217	2.71836
H	9.30272	-1.67614	1.69688
H	10.02145	-0.99130	3.15497
H	8.74320	-2.21442	3.28720
C	8.88733	0.83374	-1.49177
H	9.09537	0.40033	-0.50463
H	9.24480	0.12814	-2.24820
H	9.47945	1.75216	-1.57076

Structure J'

G = -4495.124743 Hartree

C	-3.73915	1.64390	-0.54999
C	-5.20307	-0.28301	-0.69304
C	-5.01967	1.10266	-0.68585
C	1.90482	-0.69937	-0.57939
C	1.76946	-0.58626	0.78026
C	-2.82078	-0.60040	-0.46636
C	-2.64041	0.79049	-0.41965
C	-0.43611	-0.20861	-0.19126
C	-0.98143	-2.26266	-1.40567
C	0.19752	-1.75286	-1.95584
C	-0.69412	-4.20663	-2.79081
C	0.49229	-3.69680	-3.30815
C	-0.66729	1.95901	0.90515
C	0.22222	1.20382	1.66904
C	0.60166	3.01546	3.17787
C	-0.29181	3.78688	2.43170
C	-0.91359	3.29361	1.27120

C	4.22966	-1.36872	-0.33701
C	4.12019	-1.27419	1.01685
C	0.61307	-0.46542	-1.30821
C	0.36319	-0.20800	1.14895
H	0.70527	0.35666	-2.02978
H	-0.02680	-0.91851	1.89038
H	-0.86777	1.70571	-1.20142
H	-1.55113	-1.91948	0.63487
C	-1.50527	-1.34586	-0.29819
C	-1.17137	1.16646	-0.29739
C	0.97246	-2.43762	-2.89852
C	3.11964	-1.06839	-1.19545
C	2.89155	-0.81320	1.70576
C	0.89390	1.70417	2.78578
C	-1.44940	-3.51679	-1.82543
C	-4.10495	-1.13948	-0.58215
C	1.91507	0.84979	3.44151
C	-1.80111	4.18784	0.48431
C	-2.68042	-4.13034	-1.26389
C	2.22628	-1.84338	-3.44453
C	3.16367	0.51491	2.65436
C	4.37416	0.24876	3.52374
C	4.16038	-0.32818	4.71796
C	2.76680	-0.67830	5.19661
C	1.73621	0.28582	4.65193
C	-1.51960	4.48386	-0.85513
C	-2.38227	5.30114	-1.61051
C	-3.55869	5.80171	-1.01967
C	-3.86099	5.50312	0.32706

C	-2.95830	4.72415	1.05916
C	2.47144	-1.96540	-4.82583
C	3.63142	-1.44630	-5.42226
C	4.58838	-0.78077	-4.64174
C	4.37652	-0.60695	-3.27059
C	3.22274	-1.17236	-2.65635
C	-2.80171	-4.38251	0.10580
C	-3.98456	-4.85824	0.68330
C	-5.09035	-5.10874	-0.16093
C	-4.98391	-4.87880	-1.54676
C	-3.78030	-4.39722	-2.09037
C	5.71658	0.66608	3.04913
C	5.28018	0.30709	-2.51867
C	-5.14266	5.91154	0.96228
C	-4.03672	-5.09424	2.15019
C	6.81135	-0.21428	3.08008
C	8.08166	0.18100	2.65080
C	8.25760	1.50188	2.21245
C	7.18441	2.39191	2.18816
C	5.91525	1.97670	2.58776
C	4.74129	1.45359	-1.91399
C	5.57419	2.33474	-1.22528
C	6.93941	2.07402	-1.12993
C	6.65811	0.06230	-2.41976
C	-5.11022	-4.63441	2.93035
C	-4.05823	-5.45764	4.93443
C	-2.98391	-5.92265	4.17580
C	-2.97012	-5.74363	2.79233
C	-6.36829	5.68943	0.31265

C	-7.58594	6.02087	0.91386
C	-7.56698	6.59420	2.19433
C	-6.35896	6.82014	2.85363
C	-5.15010	6.48044	2.24425
C	7.49809	0.92586	-1.71289
C	-5.13767	-4.80862	4.31773
H	-3.60901	2.71815	-0.55100
H	-6.20174	-0.70129	-0.78684
H	-5.87460	1.76720	-0.78041
H	-1.04213	-5.18013	-3.12152
H	1.05296	-4.28146	-4.02610
H	1.09462	3.43981	4.04752
H	-0.48892	4.81337	2.72870
H	5.15456	-1.71386	-0.78162
H	4.96247	-1.55901	1.63526
H	2.60423	-1.55350	2.46978
H	-4.25864	-2.21081	-0.57625
H	3.38266	1.31820	1.94817
H	-3.20476	4.45681	2.08187
H	-1.95431	-4.17930	0.75254
H	9.24209	1.83271	1.89041
H	7.33575	3.41498	1.85588
H	5.08751	2.68026	2.57263
H	3.67663	1.65558	-1.99677
H	5.15776	3.22555	-0.76338
H	7.58331	2.76128	-0.59036
H	7.07071	-0.82451	-2.89128
H	-5.93456	-4.12459	2.44276
H	-4.06204	-5.59842	6.01297

H	-2.15452	-6.42906	4.66280
H	-2.13773	-6.11978	2.20392
H	-6.36391	5.25379	-0.68193
H	-8.50482	6.86563	2.67359
H	-6.35690	7.26934	3.84326
H	-4.20880	6.66827	2.75339
H	6.66204	-1.22400	3.45085
H	2.77989	-0.66375	6.29452
O	-6.25356	-5.53436	0.41533
O	-6.09922	-5.03816	-2.33331
O	-3.70046	-4.14600	-3.44234
O	1.57138	-2.59284	-5.65168
O	3.80248	-1.49058	-6.77310
O	5.72293	-0.29393	-5.23072
O	2.34552	-1.98639	4.75285
O	0.60447	0.54759	5.35398
O	5.18098	-0.67810	5.57077
O	-0.40610	3.94218	-1.45826
O	-2.03011	5.49672	-2.91538
O	-4.42095	6.52691	-1.81263
C	-4.57530	7.91410	-1.46840
H	-3.62313	8.44685	-1.57656
H	-5.30383	8.31888	-2.17325
H	-4.94874	8.03553	-0.44780
C	-2.09789	6.81914	-3.46689
H	-3.11569	7.07454	-3.76775
H	-1.72809	7.56133	-2.74936
H	-1.44304	6.80795	-4.34117
C	0.71302	4.83309	-1.54082

H	0.47242	5.71001	-2.15196
H	1.02623	5.15411	-0.53924
H	1.52059	4.26891	-2.01325
C	0.24724	-0.29675	6.45761
H	-0.79419	-0.05931	6.67903
H	0.33897	-1.35370	6.19127
H	0.85902	-0.07904	7.34049
C	3.11156	-3.05735	5.30757
H	2.64202	-3.98037	4.96092
H	4.15512	-3.02771	4.97186
H	3.09293	-3.02668	6.40578
C	5.54262	0.34829	6.51019
H	4.68966	0.62645	7.14247
H	6.33521	-0.07038	7.13251
H	5.91158	1.23534	5.98283
C	5.54528	0.94222	-5.94620
H	4.82306	0.81851	-6.75906
H	5.21332	1.73321	-5.26334
H	6.52432	1.19796	-6.35485
C	-4.25158	-2.87436	-3.82679
H	-5.31074	-2.81252	-3.55411
H	-3.70028	-2.05680	-3.34826
H	-4.14292	-2.81011	-4.91122
C	-6.01339	-6.04368	-3.35997
H	-5.82484	-7.02914	-2.91729
H	-6.98689	-6.04743	-3.85391
H	-5.22807	-5.80406	-4.08015
C	-6.90930	-6.68908	-0.12821
H	-7.55825	-6.41970	-0.96418

H	-6.17664	-7.43540	-0.45700
H	-7.50531	-7.10503	0.68744
C	4.10843	-2.78998	-7.31933
H	3.30816	-3.50125	-7.09968
H	4.19532	-2.64551	-8.39715
H	5.06095	-3.15229	-6.91668
C	0.61653	-1.69931	-6.25240
H	0.01542	-1.20535	-5.47998
H	1.12719	-0.95107	-6.86794
H	-0.02691	-2.31960	-6.87828
C	-8.89577	5.74192	0.21350
H	-9.35355	4.81748	0.58929
H	-9.61732	6.54947	0.37998
H	-8.75671	5.62461	-0.86599
C	-6.31663	-4.32707	5.13195
H	-7.03947	-5.13763	5.29408
H	-6.00320	-3.97134	6.11956
H	-6.84737	-3.51290	4.62767
C	9.23444	-0.79512	2.63447
H	9.40252	-1.18402	1.62139
H	10.16672	-0.31736	2.95473
H	9.04590	-1.65193	3.28893
C	8.96906	0.62954	-1.54602
H	9.19856	0.40822	-0.49570
H	9.28053	-0.22889	-2.14872
H	9.58437	1.49009	-1.83353

DDQ

G = -1485.098249 Hartree

C	0.90611	-1.67144	0.00174
C	2.40011	-1.71011	0.00221
C	3.12212	-0.39257	0.00177
C	2.44425	0.78175	0.00082
C	0.94281	0.81585	0.00005
C	0.22850	-0.49720	0.00068
Cl	-1.48884	-0.40009	0.00002
Cl	0.13039	-3.20691	0.00265
C	3.10405	2.04737	0.00043
C	4.54813	-0.45354	0.00236
O	0.35701	1.88021	-0.00058
O	3.02867	-2.74978	0.00331
N	3.64226	3.07709	0.00010
N	5.70905	-0.50113	0.00284

DDQ anion

G = -1485.871733 Hartree

C	0.99074	-1.59172	-0.04856
C	2.44716	-1.72717	0.02693
C	3.13521	-0.45442	0.01162
C	2.45248	0.79231	-0.06428
C	1.06128	0.85317	-0.13034
C	0.34476	-0.36790	-0.12105
Cl	-1.41310	-0.25447	-0.20584
Cl	0.08564	-3.08609	-0.04177
C	3.18895	2.01504	-0.07418
C	4.55138	-0.48509	0.07771
O	3.02758	-2.83429	0.09653
N	3.80104	3.00577	-0.08208

N	5.71746	-0.50836	0.13149
O	0.46759	2.07929	-0.20036
H	-0.49786	1.96804	-0.23521

Structure 5"

G = -2964.832106 Hartree

C	-1.50514	0.64518	3.32595
C	-0.34282	-0.65148	5.01318
C	-1.28249	0.32523	4.66885
C	1.38867	-1.15166	-1.78239
C	2.10657	-0.05153	-1.28567
C	0.14769	-1.02294	2.68029
C	-0.78402	-0.02722	2.34111
C	0.40151	-0.57927	0.32899
C	0.35880	-2.92885	0.88495
C	-0.10232	-2.79675	-0.43527
C	-0.21583	-5.26492	0.82533
C	-0.73301	-5.11473	-0.45956
C	-0.73842	1.53010	0.25609
C	0.57491	1.77199	-0.17884
C	-0.05153	4.02273	-0.75299
C	-1.36665	3.76167	-0.37304
C	-1.73758	2.50816	0.13831
C	3.00418	-1.43912	-3.54118
C	3.73552	-0.35814	-3.03823
C	0.14210	-1.39437	-0.95348
C	1.44123	0.51843	-0.03503
H	-0.71700	-0.99612	-1.50140

H	2.18084	0.66748	0.76189
H	-1.77568	-0.36678	0.48103
H	1.92288	-1.59378	1.57114
C	0.83452	-1.58124	1.43580
C	-0.86892	0.13683	0.83492
C	-0.68834	-3.87555	-1.11720
C	1.82484	-1.84582	-2.90895
C	3.29515	0.33662	-1.90662
C	0.94388	3.03798	-0.65617
C	0.34418	-4.18052	1.52025
C	0.37855	-1.32718	4.02319
C	2.34706	3.35523	-1.03409
C	-3.15377	2.24496	0.51490
C	0.92063	-4.39093	2.87429
C	-1.28730	-3.72082	-2.47024
C	2.67558	3.66097	-2.35889
C	4.00295	3.89951	-2.74813
C	5.00587	3.85349	-1.76481
C	4.68578	3.57512	-0.43571
C	3.36399	3.32142	-0.06859
C	-3.87556	1.19762	-0.07978
C	-5.19513	0.95346	0.29868
C	-5.81411	1.75004	1.26177
C	-5.12107	2.81658	1.85827
C	-3.79205	3.04898	1.46780
C	-0.93284	-4.56947	-3.52950
C	-1.49997	-4.38660	-4.79237
C	-2.41647	-3.35961	-5.01668
C	-2.79677	-2.50170	-3.96977

C	-2.23218	-2.71302	-2.70475
C	2.26577	-4.08548	3.11808
C	2.83591	-4.23735	4.39105
C	2.02164	-4.71604	5.43264
C	0.68678	-5.04304	5.19635
C	0.13586	-4.88803	3.92395
C	4.33763	4.16324	-4.17024
C	-3.74558	-1.37898	-4.18599
C	-5.76902	3.67375	2.88320
C	4.25976	-3.88963	4.62923
C	5.49766	3.61828	-4.74759
C	5.80964	3.85536	-6.08632
C	4.96696	4.64135	-6.87635
C	3.80977	5.18796	-6.31554
C	3.49876	4.95145	-4.97651
C	-4.65829	-0.99441	-3.18707
C	-5.51793	0.08713	-3.37950
C	-5.48954	0.80446	-4.57790
C	-3.73003	-0.64869	-5.38688
C	4.65659	-3.25887	5.82106
C	6.96092	-3.21903	5.08002
C	6.58007	-3.84440	3.89008
C	5.24369	-4.17645	3.66735
C	-6.63413	3.12086	3.84330
C	-7.24025	3.92554	4.80811
C	-6.99322	5.30047	4.83391
C	-6.13517	5.86339	3.88569
C	-5.53008	5.05852	2.92051
C	-4.59370	0.42931	-5.58179

C	5.99302	-2.92770	6.04461
H	-2.22463	1.41152	3.05315
H	-0.16400	-0.88665	6.05928
H	-1.83466	0.84598	5.44700
H	-0.24228	-6.23917	1.30619
H	-1.18739	-5.96500	-0.96108
H	0.21606	5.00558	-1.13193
H	-2.12320	4.53451	-0.47934
H	3.35834	-1.97179	-4.42004
H	4.65701	-0.05237	-3.52721
H	1.25759	-2.69307	-3.28426
H	3.88150	1.16123	-1.51934
H	1.11537	-2.06971	4.30534
H	1.89009	3.64990	-3.10879
H	6.03671	4.05727	-2.03981
H	5.47011	3.55715	0.31600
H	3.11509	3.09275	0.96388
H	-3.41136	0.59271	-0.85325
H	-5.74908	0.14278	-0.16670
H	-6.84875	1.56227	1.53357
H	-3.22569	3.84524	1.94261
H	-0.20238	-5.35663	-3.36410
H	-1.22258	-5.04774	-5.60884
H	-2.85511	-3.23548	-6.00247
H	-2.52256	-2.06826	-1.88182
H	2.87158	-3.69511	2.30573
H	2.44434	-4.85730	6.42310
H	0.07254	-5.42003	6.00949
H	-0.90938	-5.12318	3.74496

H	6.14525	2.98378	-4.14866
H	6.70732	3.41768	-6.51488
H	5.20900	4.82522	-7.91948
H	3.15073	5.80601	-6.91943
H	2.60774	5.39841	-4.54427
H	-4.70977	-1.55918	-2.26017
H	-6.21263	0.36851	-2.59328
H	-6.15788	1.64791	-4.72685
H	-3.01496	-0.90890	-6.16207
H	3.90815	-3.00470	6.56656
H	8.00186	-2.96059	5.25368
H	7.32565	-4.08193	3.13598
H	4.96208	-4.68344	2.74858
H	-6.81291	2.04920	3.84793
H	-7.89962	3.47611	5.54585
H	-7.46468	5.92725	5.58583
H	-5.94208	6.93281	3.89181
H	-4.88290	5.50983	2.17353
H	-4.55682	0.98473	-6.51510
H	6.27680	-2.43337	6.96988

$TS_{5''\rightarrow K''}$

G = -4449.899564 Hartree

C	2.45013	-2.93107	-1.42770
C	0.97116	-4.81401	-1.05488
C	2.08149	-4.25233	-1.69307
C	-0.29314	1.34228	2.06207
C	-0.83317	1.52218	0.76311
C	0.60881	-2.75945	0.15499

C	1.70402	-2.19243	-0.51020
C	0.63012	-0.40097	0.70225
C	0.17335	-1.88117	2.58227
C	0.80448	-0.74081	3.09312
C	0.19821	-2.85863	4.77758
C	0.91474	-1.76290	5.26097
C	1.92245	0.27083	-1.21362
C	0.67463	0.94209	-1.31920
C	1.54171	2.23088	-3.15837
C	2.78083	1.60668	-3.01169
C	3.00160	0.62895	-2.02564
C	-1.79626	3.00904	2.91740
C	-2.33516	3.19098	1.63688
C	0.85270	0.34529	2.04149
C	-0.17104	0.58517	-0.16884
H	1.79378	0.90428	2.02277
H	-1.28485	-0.17065	-0.63774
H	2.80548	-0.66456	0.52765
H	-1.13339	-1.73769	0.88499
C	-0.06501	-1.75653	1.08117
C	1.90862	-0.74664	-0.09452
C	1.22559	-0.67457	4.43086
C	-0.76860	2.08314	3.13519
C	-1.86486	2.45057	0.55549
C	0.46419	1.91425	-2.32611
C	-0.19842	-2.93608	3.43397
C	0.22773	-4.07176	-0.13303
C	-0.83402	2.60192	-2.50459
C	4.36135	0.04430	-1.85771

C	-1.03385	-4.05937	2.93188
C	2.00445	0.48386	4.94217
C	-0.93484	3.98545	-2.31198
C	-2.16947	4.64421	-2.40912
C	-3.30749	3.88780	-2.74394
C	-3.20864	2.51740	-2.97981
C	-1.97896	1.87064	-2.85486
C	5.05634	0.17240	-0.64516
C	6.32598	-0.38715	-0.50814
C	6.91720	-1.06936	-1.57075
C	6.24878	-1.19690	-2.79998
C	4.97110	-0.62740	-2.92426
C	1.61566	1.18335	6.09406
C	2.35469	2.28787	6.52347
C	3.48066	2.70673	5.81497
C	3.89995	2.01259	4.66655
C	3.15476	0.89902	4.25730
C	-2.24174	-3.76249	2.28649
C	-2.99896	-4.74846	1.64257
C	-2.55186	-6.07900	1.70592
C	-1.38831	-6.39810	2.40886
C	-0.62530	-5.39705	3.01548
C	-2.27255	6.09904	-2.13514
C	5.08770	2.44454	3.88621
C	6.86914	-1.91900	-3.93943
C	-4.19484	-4.35102	0.85504
C	-3.36959	6.61926	-1.42733
C	-3.46379	7.98516	-1.16099
C	-2.46302	8.85707	-1.59725

C	-1.36685	8.35214	-2.30141
C	-1.27212	6.98629	-2.56716
C	5.96238	1.50138	3.31736
C	7.06453	1.91099	2.56650
C	7.31351	3.27099	2.36449
C	5.35320	3.80888	3.67960
C	-4.36918	-4.81941	-0.45828
C	-6.37903	-3.49160	-0.70208
C	-6.22379	-3.03076	0.60802
C	-5.13813	-3.45067	1.37700
C	7.62878	-3.08247	-3.72746
C	8.20952	-3.76185	-4.79835
C	8.04169	-3.29256	-6.10357
C	7.28855	-2.13746	-6.32858
C	6.70883	-1.45773	-5.25753
C	6.45373	4.21795	2.92587
C	-5.44776	-4.38879	-1.23208
H	3.29787	-2.48443	-1.93680
H	0.67491	-5.83503	-1.28065
H	2.65103	-4.83784	-2.40989
H	-0.06657	-3.66834	5.45233
H	1.23538	-1.74417	6.29898
H	1.40461	2.97960	-3.93268
H	3.60273	1.88991	-3.66296
H	-2.18045	3.59048	3.75062
H	-3.13962	3.90440	1.48500
H	-0.34236	1.95006	4.12493
H	-2.32763	2.56459	-0.41371
H	-0.64241	-4.51356	0.33394

H	-0.05071	4.53985	-2.01260
H	-4.26883	4.38220	-2.84524
H	-4.09191	1.95392	-3.26365
H	-1.88194	0.81105	-3.05756
H	4.61620	0.72528	0.18002
H	6.86243	-0.27653	0.42938
H	7.91512	-1.48236	-1.45695
H	4.42017	-0.74411	-3.85322
H	0.72726	0.87135	6.63624
H	2.04887	2.82725	7.41566
H	4.05184	3.56134	6.16581
H	3.46898	0.34615	3.37716
H	-2.57206	-2.73192	2.23278
H	-3.12390	-6.86170	1.21555
H	-1.06060	-7.43253	2.46384
H	0.30804	-5.64451	3.51327
H	-4.14032	5.94562	-1.06305
H	-4.31595	8.36712	-0.60547
H	-2.53656	9.92102	-1.39005
H	-0.58732	9.02339	-2.65131
H	-0.42727	6.60554	-3.13444
H	5.79260	0.44172	3.48675
H	7.73970	1.16763	2.15164
H	8.17070	3.58890	1.77769
H	4.67733	4.55337	4.09105
H	-3.63386	-5.49732	-0.88308
H	-7.21607	-3.14995	-1.30473
H	-6.94459	-2.33598	1.02957
H	-5.02084	-3.08309	2.39236

H	7.74390	-3.47063	-2.71926
H	8.78644	-4.66396	-4.61331
H	8.49329	-3.82235	-6.93771
H	7.15797	-1.75973	-7.33907
H	6.14474	-0.54751	-5.44129
H	6.63448	5.27817	2.77068
H	-5.55418	-4.74477	-2.25312
C	-5.50912	0.13220	-0.08410
C	-6.16069	-0.01438	-1.40163
C	-5.30525	-0.55756	-2.46707
C	-3.96418	-0.83033	-2.25057
C	-3.36185	-0.66092	-0.96161
C	-4.20052	-0.21530	0.12913
Cl	-3.51202	-0.20819	1.72154
Cl	-6.53575	0.68415	1.19597
C	-3.14671	-1.36724	-3.29436
C	-5.92165	-0.80742	-3.72464
O	-2.12317	-1.01232	-0.79618
O	-7.34703	0.25933	-1.59518
N	-2.48720	-1.79394	-4.15127
N	-6.42481	-1.01242	-4.75411

Structure K"

G = -2964.046179 Hartree

C	4.05458	-2.10859	-0.63844
C	2.86772	-4.20580	-0.36027
C	4.00647	-3.49886	-0.76063
C	0.62805	1.71893	2.59673
C	0.01828	2.02211	1.33985

C	1.83224	-2.15010	0.33960
C	2.95003	-1.43816	-0.11054
C	1.50733	0.17928	0.99099
C	0.53879	-1.53682	2.45306
C	1.20276	-0.62441	3.28242
C	-0.13841	-2.78730	4.38324
C	0.59760	-1.93051	5.19841
C	2.19658	0.70969	-1.24421
C	0.88987	1.25063	-1.04546
C	0.77741	1.90644	-3.34685
C	2.08933	1.45204	-3.51748
C	2.82452	0.84540	-2.48277
C	-0.64833	3.47963	3.60433
C	-1.24994	3.78893	2.36810
C	1.64573	0.58889	2.47876
C	0.63706	1.20762	0.35497
H	2.64627	0.95511	2.71941
H	3.60452	0.58822	0.41828
H	-0.12799	-1.23962	0.39458
C	0.79339	-1.24085	0.98520
C	2.72996	0.05299	0.03646
C	1.27058	-0.81582	4.67248
C	0.29147	2.45378	3.72708
C	-0.92222	3.07511	1.22988
C	0.13690	1.80856	-2.11210
C	-0.19805	-2.60421	2.99313
C	1.77547	-3.53677	0.19873
C	-1.28277	2.16945	-1.94282
C	4.21113	0.36705	-2.72130

C	-1.05231	-3.49035	2.15982
C	2.00663	0.10243	5.58029
C	-1.76369	3.40530	-2.39950
C	-3.09801	3.78660	-2.19392
C	-3.95395	2.88588	-1.53412
C	-3.49206	1.64241	-1.10380
C	-2.16330	1.27865	-1.30384
C	5.28350	0.89623	-1.98987
C	6.56788	0.38473	-2.17565
C	6.78771	-0.65535	-3.07910
C	5.72795	-1.19143	-3.83068
C	4.44435	-0.65558	-3.64644
C	1.38942	0.60397	6.73788
C	2.07747	1.48405	7.57349
C	3.38336	1.86902	7.27226
C	4.03019	1.36940	6.12885
C	3.32532	0.48451	5.29933
C	-1.99873	-2.93141	1.29067
C	-2.80681	-3.72924	0.46902
C	-2.65523	-5.12453	0.53691
C	-1.73618	-5.69470	1.41769
C	-0.94065	-4.88719	2.23176
C	-3.58801	5.10949	-2.65551
C	5.42404	1.76438	5.80147
C	5.94737	-2.31711	-4.77286
C	-3.79806	-3.10611	-0.44446
C	-4.49516	5.85126	-1.87977
C	-4.95436	7.09472	-2.31365
C	-4.51579	7.62010	-3.53166

C	-3.61428	6.89232	-4.31242
C	-3.15444	5.64919	-3.87853
C	6.33188	0.83416	5.26630
C	7.63865	1.20892	4.95373
C	8.06495	2.52165	5.17065
C	5.86612	3.08156	6.01447
C	-3.97343	-3.58980	-1.75173
C	-5.67750	-1.92462	-2.18070
C	-5.51791	-1.43867	-0.88043
C	-4.58365	-2.01957	-0.02203
C	6.82256	-3.36672	-4.44497
C	7.02107	-4.43132	-5.32411
C	6.34865	-4.46715	-6.54826
C	5.47540	-3.42999	-6.88591
C	5.27634	-2.36580	-6.00659
C	7.17309	3.45623	5.70267
C	-4.90160	-3.00301	-2.61239
H	4.93743	-1.56494	-0.95261
H	2.83537	-5.28644	-0.46777
H	4.85743	-4.02948	-1.17853
H	-0.68785	-3.61149	4.82922
H	0.64268	-2.11630	6.26757
H	0.23668	2.31144	-4.19628
H	2.55970	1.55401	-4.49132
H	-0.91580	4.06016	4.48248
H	-1.97300	4.59585	2.31037
H	0.75307	2.24381	4.68447
H	-1.37979	3.31406	0.27979
H	0.90656	-4.09332	0.52907

H	-1.07220	4.10028	-2.86610
H	-4.99638	3.15103	-1.38618
H	-4.17263	0.94452	-0.62819
H	-1.81244	0.30198	-0.98461
H	5.11099	1.70208	-1.28252
H	7.40160	0.79941	-1.61651
H	7.79284	-1.04151	-3.21988
H	3.60200	-1.08507	-4.18049
H	0.36536	0.32145	6.96434
H	1.59360	1.87008	8.46623
H	3.91543	2.53900	7.94092
H	3.81371	0.08322	4.41660
H	-2.10751	-1.85137	1.25209
H	-3.27981	-5.76286	-0.08116
H	-1.63969	-6.77542	1.47083
H	-0.21093	-5.33261	2.90183
H	-4.82422	5.46232	-0.92015
H	-5.64969	7.65641	-1.69599
H	-4.87418	8.58822	-3.86997
H	-3.27448	7.28878	-5.26523
H	-2.47309	5.08018	-4.50492
H	6.01924	-0.19570	5.11793
H	8.32693	0.47183	4.54903
H	9.08307	2.81335	4.92844
H	5.17438	3.82247	6.40557
H	-3.36182	-4.41696	-2.10131
H	-6.40255	-1.46929	-2.84928
H	-6.13091	-0.61295	-0.52879
H	-4.48253	-1.64872	0.99439

H	7.33161	-3.35969	-3.48510
H	7.69578	-5.23734	-5.04881
H	6.50348	-5.29633	-7.23292
H	4.95335	-3.44521	-7.83876
H	4.61179	-1.55323	-6.28722
H	7.49259	4.48145	5.86891
H	-5.01473	-3.38591	-3.62294

Structure 13"

G = -2958.974115 Hartree

C	3.19915	0.67117	-1.27968
C	4.93548	-0.95975	-0.55753
C	4.56860	0.29901	-1.13200
C	-1.91261	-2.37134	0.51285
C	-1.85445	-2.62264	-0.86465
C	2.61704	-1.46941	-0.22971
C	2.25715	-0.25218	-0.79059
C	0.17941	-1.43768	-0.29031
C	1.28980	-2.45428	1.59399
C	0.09121	-1.94585	2.10176
C	2.06796	-3.01129	3.76634
C	0.87959	-2.51494	4.29547
C	0.12876	0.27529	-1.98813
C	-0.82102	-0.67035	-2.37864
C	-1.28033	0.70853	-4.29214
C	-0.25219	1.58120	-3.93702
C	0.46583	1.39625	-2.73957
C	-3.82238	-3.83276	0.69088
C	-3.74507	-4.10522	-0.67838

C	-0.77731	-1.45232	0.94593
C	-0.67299	-1.92581	-1.50640
H	-1.16553	-0.44517	1.12385
H	-0.11244	-2.65058	-2.11472
H	0.55898	0.72352	0.05964
H	1.44119	-3.27637	-0.39309
C	1.40549	-2.30037	0.11125
C	0.77028	-0.05776	-0.68674
C	-0.15400	-1.99256	3.48899
C	-2.90395	-2.96976	1.29552
C	-2.75640	-3.50482	-1.46038
C	-1.59944	-0.42174	-3.51920
C	2.29845	-3.01095	2.37747
C	3.95307	-1.81836	0.00623
C	-2.81438	-1.22361	-3.83328
C	1.52972	2.35359	-2.32649
C	3.53904	-3.60233	1.80061
C	-1.44951	-1.60564	4.11077
C	-3.92458	-1.05786	-2.99783
C	-5.10673	-1.78551	-3.18000
C	-5.16626	-2.68596	-4.25764
C	-4.07555	-2.84169	-5.11415
C	-2.89866	-2.11491	-4.90885
C	1.25384	3.70320	-2.57180
C	2.22169	4.69367	-2.41412
C	3.52108	4.32347	-2.12327
C	3.86272	2.97545	-1.89123
C	2.83534	1.98436	-1.83664
C	-1.97582	-2.36800	5.17025

C	-3.23426	-2.08032	5.69847
C	-4.01498	-1.06107	5.15372
C	-3.52205	-0.29244	4.08787
C	-2.22604	-0.54595	3.62004
C	4.35176	-2.99752	0.78006
C	5.66137	-3.51622	0.55674
C	6.05072	-4.71424	1.18691
C	5.20460	-5.36711	2.06579
C	3.97866	-4.79103	2.39503
C	-6.23496	-1.61722	-2.23033
C	-4.37783	0.70677	3.40020
C	5.27316	2.57887	-1.78831
C	6.62724	-2.74443	-0.23769
C	-7.56993	-1.66544	-2.66626
C	-8.62252	-1.49727	-1.76573
C	-8.36167	-1.27427	-0.41102
C	-7.03895	-1.22629	0.03682
C	-5.98737	-1.39957	-0.86230
C	-4.40762	0.74739	1.99433
C	-5.23745	1.64544	1.32334
C	-6.05093	2.52205	2.04597
C	-5.20420	1.58886	4.11475
C	7.90113	-3.24358	-0.55077
C	8.56355	-1.12177	-1.49040
C	7.29957	-0.58102	-1.21274
C	6.30276	-1.41508	-0.63681
C	6.31263	3.48737	-2.04943
C	7.64350	3.08714	-2.02174
C	7.97365	1.76424	-1.75197

C	6.97384	0.81537	-1.49749
C	5.61085	1.22784	-1.49523
C	-6.03066	2.49065	3.44313
C	8.84990	-2.44724	-1.18420
H	2.83525	-3.37814	4.44172
H	0.75216	-2.51603	5.37402
H	-1.86200	0.90620	-5.18873
H	-0.01065	2.41329	-4.59167
H	-4.59593	-4.30077	1.29383
H	-4.45948	-4.78133	-1.13970
H	-2.95355	-2.78742	2.36216
H	-2.69925	-3.71385	-2.52397
H	-3.85343	-0.34841	-2.17937
H	-6.05916	-3.28580	-4.40956
H	-4.13704	-3.54639	-5.93908
H	-2.04545	-2.24983	-5.56774
H	0.25353	3.98006	-2.88918
H	1.96769	5.73881	-2.56454
H	4.28019	5.09389	-2.06993
H	-1.41578	-3.21475	5.55485
H	-3.62654	-2.68511	6.51146
H	-5.02238	-0.88851	5.52166
H	-1.82843	0.09268	2.84237
H	7.03741	-5.12629	1.01516
H	5.51304	-6.29795	2.53277
H	3.34586	-5.27011	3.13536
H	-7.78397	-1.81081	-3.72165
H	-9.64771	-1.52989	-2.12516
H	-9.18191	-1.13912	0.28880

H	-6.81921	-1.05551	1.08687
H	-4.96640	-1.40134	-0.49449
H	-3.80499	0.04220	1.42735
H	-5.26317	1.64384	0.23725
H	-6.69998	3.22029	1.52475
H	-5.18526	1.57628	5.20132
H	8.16471	-4.26683	-0.31199
H	9.31982	-0.51968	-1.98135
H	6.09465	4.51834	-2.29823
H	8.42830	3.81239	-2.21657
H	9.01900	1.47957	-1.71453
H	-6.65804	3.17174	4.01194
H	9.82265	-2.86206	-1.43215

$TS_{13"\rightarrow L"}$

G = -4444.054484 Hartree

C	3.14370	0.66675	-1.01686
C	4.84657	-1.06181	-0.41968
C	4.50162	0.25854	-0.87617
C	-1.92913	-2.59428	0.35623
C	-1.92082	-2.66181	-1.04275
C	2.52922	-1.59259	-0.18125
C	2.18449	-0.31070	-0.64797
C	0.10982	-1.54769	-0.37012
C	1.14833	-2.77081	1.44296
C	0.00284	-2.17993	1.98489
C	1.86959	-3.49122	3.58272
C	0.76877	-2.85346	4.14624
C	0.03156	0.41541	-1.75805

C	-0.99086	-0.43978	-2.22668
C	-1.55303	1.27743	-3.79561
C	-0.48999	2.07167	-3.37252
C	0.34577	1.66175	-2.31302
C	-3.68973	-4.23595	0.41888
C	-3.67699	-4.30509	-0.97805
C	-0.85311	-1.64110	0.86142
C	-0.78995	-1.83662	-1.61273
H	-1.29381	-0.67517	1.09850
H	-0.23750	-2.41822	-2.36499
H	0.43538	0.60938	0.37083
H	1.38095	-3.37077	-0.63909
C	1.30864	-2.46870	-0.01737
C	0.74798	-0.20094	-0.67127
C	-0.16886	-2.12009	3.38040
C	-2.80969	-3.38443	1.09489
C	-2.78582	-3.52177	-1.71664
C	-1.82993	0.00499	-3.24384
C	2.12459	-3.40825	2.19895
C	3.84774	-1.96921	0.05046
C	-2.97845	-0.79700	-3.74871
C	1.48416	2.49935	-1.85065
C	3.37306	-3.95389	1.60164
C	-1.12164	-1.19037	4.05379
C	-4.11087	-0.95240	-2.94130
C	-5.20799	-1.71736	-3.36303
C	-5.15038	-2.31976	-4.63194
C	-4.03334	-2.15401	-5.45058
C	-2.94628	-1.39259	-5.01624

C	1.25992	3.87753	-1.93480
C	2.26390	4.81221	-1.69812
C	3.55260	4.36992	-1.48176
C	3.85254	2.99572	-1.40870
C	2.79521	2.02807	-1.44051
C	-0.73928	-0.59806	5.27521
C	-1.51882	0.39049	5.87057
C	-2.67731	0.84906	5.24634
C	-3.08456	0.28910	4.02641
C	-2.32193	-0.74917	3.47026
C	4.21708	-3.24023	0.68290
C	5.52347	-3.74343	0.42441
C	5.89515	-5.00389	0.92992
C	5.02763	-5.74193	1.71686
C	3.79464	-5.20125	2.07580
C	-6.37588	-1.92280	-2.46880
C	-4.24902	0.83791	3.28541
C	5.25055	2.56384	-1.34721
C	6.50293	-2.90292	-0.27688
C	-7.67759	-2.03294	-2.98872
C	-8.76760	-2.26944	-2.15096
C	-8.57791	-2.40943	-0.77381
C	-7.29009	-2.29714	-0.24373
C	-6.20142	-2.04467	-1.07843
C	-5.16003	0.00594	2.61642
C	-6.20635	0.55073	1.87157
C	-6.35874	1.93535	1.77699
C	-4.41647	2.23027	3.18666
C	7.76686	-3.38934	-0.63828

C	8.47087	-1.19675	-1.36297
C	7.21670	-0.66363	-1.03519
C	6.20155	-1.53159	-0.54181
C	6.30703	3.47242	-1.54121
C	7.62907	3.04899	-1.54054
C	7.93476	1.70317	-1.37085
C	6.91778	0.75628	-1.19370
C	5.56332	1.19108	-1.15689
C	-5.45992	2.77491	2.43838
C	8.73161	-2.55023	-1.18751
H	2.57774	-3.99481	4.23415
H	0.64762	-2.90024	5.22374
H	-2.18440	1.63346	-4.60475
H	-0.29788	3.00488	-3.89067
H	-4.37756	-4.85831	0.98467
H	-4.36211	-4.97198	-1.49328
H	-2.78991	-3.36912	2.18072
H	-2.76901	-3.58148	-2.80069
H	-4.12763	-0.47099	-1.97001
H	-5.97246	-2.94457	-4.96896
H	-4.00414	-2.63150	-6.42617
H	-2.07026	-1.27244	-5.64763
H	0.26264	4.23075	-2.17104
H	2.03828	5.87317	-1.71436
H	4.33572	5.10466	-1.34895
H	0.20102	-0.87374	5.74014
H	-1.20194	0.82822	6.81329
H	-3.26718	1.63965	5.70099
H	-2.66711	-1.17487	2.53957

H	6.88331	-5.40203	0.73706
H	5.32465	-6.71778	2.08929
H	3.14204	-5.75310	2.74496
H	-7.84005	-1.91251	-4.05625
H	-9.76577	-2.34202	-2.57452
H	-9.42437	-2.60410	-0.12095
H	-7.12760	-2.42196	0.82372
H	-5.20723	-1.97540	-0.65180
H	-5.04550	-1.07327	2.67667
H	-6.89601	-0.10604	1.35110
H	-7.16375	2.35723	1.18199
H	-3.70047	2.88891	3.67073
H	8.01182	-4.43582	-0.50617
H	9.23904	-0.56501	-1.79313
H	6.10842	4.52139	-1.71792
H	8.42684	3.77211	-1.68084
H	8.97471	1.39860	-1.35661
H	-5.55786	3.85327	2.35388
H	9.69703	-2.95639	-1.47433
C	-0.08805	4.85685	1.02467
C	-1.44518	5.13357	0.51612
C	-2.27569	3.94602	0.26578
C	-1.80461	2.66132	0.49673
C	-0.48477	2.43332	1.00967
C	0.36548	3.58048	1.23288
Cl	1.97693	3.24565	1.77903
Cl	0.91066	6.24512	1.29826
C	-2.63291	1.52807	0.23021
C	-3.58900	4.17699	-0.22991

O	-0.07346	1.23646	1.28777
O	-1.86186	6.27645	0.30547
N	-3.30322	0.60998	-0.00986
N	-4.66206	4.36909	-0.63848

Structure L"

G = -2958.190857 Hartree

C	3.18512	0.60818	-1.08030
C	4.92107	-1.07099	-0.43003
C	4.54659	0.24144	-0.90117
C	-1.86777	-2.50674	0.37996
C	-1.93187	-2.69041	-1.00541
C	2.62923	-1.69231	-0.23432
C	2.25287	-0.42143	-0.74674
C	0.23350	-1.71496	-0.52140
C	1.26398	-2.81828	1.38361
C	0.15317	-2.14841	1.90781
C	1.97404	-3.48149	3.54267
C	0.88277	-2.81070	4.08273
C	0.06897	0.27249	-1.83055
C	-0.99396	-0.57135	-2.25473
C	-1.69025	1.22797	-3.65311
C	-0.61465	2.02595	-3.25643
C	0.32102	1.56983	-2.30900
C	-3.76150	-3.97139	0.64369
C	-3.82843	-4.14215	-0.74268
C	-0.68473	-1.61318	0.76505
C	-0.78295	-1.99016	-1.68396
H	-1.01105	-0.57980	0.92412

H	-0.33131	-2.60352	-2.47359
H	1.54994	-3.53234	-0.66785
C	1.42898	-2.60651	-0.09430
C	0.88671	-0.46231	-0.96929
C	-0.02886	-2.05682	3.30411
C	-2.77420	-3.16134	1.21523
C	-2.90392	-3.50849	-1.57689
C	-1.91326	-0.08316	-3.17289
C	2.23312	-3.44419	2.16044
C	3.94745	-2.00848	0.04619
C	-3.05669	-0.89933	-3.67184
C	1.45059	2.40841	-1.84108
C	3.49420	-3.98868	1.59281
C	-1.01513	-1.16506	3.98720
C	-4.24728	-0.95531	-2.93962
C	-5.32108	-1.75420	-3.36032
C	-5.18045	-2.48785	-4.55053
C	-4.00131	-2.42681	-5.29186
C	-2.93608	-1.63605	-4.85667
C	1.19066	3.78433	-1.85174
C	2.17844	4.73129	-1.60193
C	3.48656	4.31679	-1.44573
C	3.82359	2.95085	-1.43399
C	2.78909	1.95619	-1.47681
C	-0.78852	-0.76065	5.32012
C	-1.66840	0.10011	5.97105
C	-2.78459	0.61319	5.31281
C	-3.02667	0.26547	3.97577
C	-2.14540	-0.62755	3.34800

C	4.34224	-3.26064	0.69309
C	5.66525	-3.72579	0.46230
C	6.06035	-4.97098	0.98706
C	5.19467	-5.72544	1.76173
C	3.93822	-5.21869	2.08936
C	-6.55822	-1.85720	-2.54666
C	-4.16162	0.84971	3.21356
C	5.23210	2.55520	-1.39808
C	6.62680	-2.86132	-0.23387
C	-7.82301	-1.90896	-3.15647
C	-8.98176	-2.03049	-2.38897
C	-8.89863	-2.10775	-0.99644
C	-7.64664	-2.06030	-0.37805
C	-6.48783	-1.93222	-1.14487
C	-4.83366	0.11717	2.21772
C	-5.86888	0.69412	1.48175
C	-6.26213	2.01155	1.72975
C	-4.56851	2.17485	3.45004
C	7.91003	-3.31350	-0.56752
C	8.55797	-1.11156	-1.32204
C	7.28437	-0.61041	-1.02413
C	6.28856	-1.50178	-0.52765
C	6.25971	3.48788	-1.62769
C	7.59239	3.09936	-1.62928
C	7.93686	1.76765	-1.42333
C	6.94848	0.79745	-1.21509
C	5.58446	1.19722	-1.18408
C	-5.60876	2.74889	2.71953
C	8.85593	-2.45318	-1.11609

H	2.66846	-3.98179	4.21081
H	0.75080	-2.85568	5.15749
H	-2.37864	1.62161	-4.39555
H	-0.49518	2.99635	-3.72425
H	-4.46941	-4.48609	1.28695
H	-4.59766	-4.77527	-1.17446
H	-2.70107	-3.07736	2.29436
H	-2.94448	-3.64868	-2.65259
H	-4.33354	-0.37847	-2.02343
H	-5.99016	-3.13226	-4.88009
H	-3.90660	-3.00708	-6.20527
H	-2.01166	-1.59572	-5.42563
H	0.17885	4.12481	-2.03701
H	1.92714	5.78641	-1.56621
H	4.25480	5.06530	-1.30239
H	0.09611	-1.09052	5.85210
H	-1.47318	0.38237	7.00183
H	-3.46661	1.27528	5.83739
H	-2.36307	-0.88357	2.32532
H	7.06214	-5.34533	0.81906
H	5.51116	-6.68863	2.15001
H	3.28784	-5.78167	2.75139
H	-7.89949	-1.83320	-4.23768
H	-9.95082	-2.05972	-2.87963
H	-9.80053	-2.20635	-0.39892
H	-7.56875	-2.13117	0.70359
H	-5.51818	-1.92665	-0.65757
H	-4.55754	-0.91658	2.02642
H	-6.37406	0.11206	0.71758

H	-7.06932	2.45804	1.15570
H	-4.04700	2.77145	4.19292
H	8.18642	-4.34859	-0.41220
H	9.31557	-0.46640	-1.75001
H	6.02890	4.52514	-1.83333
H	8.36900	3.83839	-1.79973
H	8.98512	1.49421	-1.41150
H	-5.89991	3.77709	2.91689
H	9.83828	-2.83360	-1.37906

Structure 14b"

G = -2956.627413 Hartree

C	-1.73096	0.16184	3.49119
C	-0.28273	-1.42882	4.67916
C	-1.34223	-0.49494	4.64830
C	0.02256	-0.47034	-2.36789
C	0.58804	0.77142	-2.11602
C	0.05185	-0.96971	2.33678
C	-1.00031	-0.05592	2.31991
C	-0.09475	-0.12307	0.05237
C	0.73548	-2.36558	0.41058
C	0.06205	-2.38345	-0.79955
C	1.21946	-4.66972	0.18015
C	0.61999	-4.66496	-1.08202
C	-1.13245	2.00981	0.64118
C	-0.08702	2.26786	-0.24666
C	-0.60123	4.58652	-0.31035
C	-1.63925	4.35801	0.59284
C	-1.94339	3.07064	1.07167

C	0.45392	-0.22641	-4.70949
C	1.05011	1.05325	-4.44930
C	-0.54719	-1.06021	-1.11060
C	0.66067	1.04104	-0.63559
H	-1.64071	-1.14308	-1.19445
H	1.71380	1.10990	-0.32551
H	-2.22074	0.15827	0.58221
H	1.78742	-0.64276	1.12056
C	0.75352	-1.00311	1.01443
C	-1.23710	0.50905	0.92045
C	0.01251	-3.50341	-1.61543
C	-0.01390	-1.05284	-3.64585
C	1.06649	1.60631	-3.13673
C	0.20696	3.52631	-0.76369
C	1.30190	-3.49949	0.97112
C	0.40344	-1.74351	3.46757
C	1.32166	3.75693	-1.72764
C	-3.09223	2.86652	1.99298
C	1.97161	-3.46224	2.29898
C	-0.64829	-3.47591	-2.94857
C	1.61147	2.94910	-2.88730
C	2.47166	3.49779	-3.88618
C	3.19334	4.67739	-3.61254
C	3.02344	5.36296	-2.42463
C	2.06011	4.92656	-1.51725
C	-4.16210	2.03242	1.63534
C	-5.20696	1.81071	2.53231
C	-5.19295	2.40822	3.79259
C	-4.13818	3.25685	4.16983

C	-3.10393	3.48538	3.24864
C	-1.34276	-4.63938	-3.29783
C	-1.88712	-4.82081	-4.56665
C	-1.65697	-3.86864	-5.54094
C	-0.95465	-2.68004	-5.25512
C	-0.54293	-2.40391	-3.91456
C	1.47864	-2.76028	3.46282
C	2.06182	-3.09475	4.72714
C	3.23700	-3.87282	4.76919
C	3.78844	-4.41223	3.62270
C	3.12473	-4.24763	2.41020
C	2.53331	2.88501	-5.22076
C	-0.57005	-1.77659	-6.34944
C	-4.10066	3.87469	5.51941
C	1.39288	-2.71746	5.98336
C	1.72458	1.75001	-5.51843
C	1.65602	1.25492	-6.85025
C	2.45627	1.84013	-7.84117
C	3.28958	2.90966	-7.53682
C	3.31700	3.43366	-6.24954
C	0.24147	-0.63825	-6.07626
C	0.75969	0.14046	-7.14850
C	0.38926	-0.17184	-8.46373
C	-0.91584	-2.04343	-7.68487
C	1.88465	-3.13580	7.24211
C	-0.05045	-2.24521	8.36861
C	-0.54416	-1.80686	7.15239
C	0.16813	-2.00281	5.94741
C	-5.27084	4.36805	6.12110

C	-5.23326	4.94249	7.39176
C	-4.02455	5.03466	8.08665
C	-2.85401	4.54583	7.50078
C	-2.89183	3.97087	6.23043
C	-0.45468	-1.24446	-8.72459
C	1.18780	-2.90023	8.41511
H	-2.56642	0.84908	3.51879
H	-1.86796	-0.25053	5.56334
H	1.62909	-5.60251	0.55683
H	0.63348	-5.58075	-1.66584
H	-0.44439	5.59063	-0.69324
H	-2.26118	5.19104	0.90938
H	3.89003	5.07409	-4.33985
H	3.60302	6.25837	-2.21999
H	1.87457	5.50559	-0.61833
H	-4.17299	1.56186	0.65669
H	-6.02955	1.15789	2.25376
H	-5.99060	2.19722	4.49899
H	-2.28079	4.14129	3.51712
H	-1.46195	-5.41811	-2.55159
H	-2.44788	-5.72122	-4.79977
H	-2.01873	-4.06269	-6.54229
H	3.72614	-4.07051	5.71418
H	4.70463	-4.99324	3.67380
H	3.51506	-4.72849	1.51913
H	2.45697	1.44103	-8.84910
H	3.96061	4.28349	-6.06082
H	0.73111	0.44321	-9.28844
H	-1.55205	-2.88271	-7.93499

H	2.82081	-3.67531	7.31266
H	-0.62122	-2.07973	9.27795
H	-1.50560	-1.30746	7.13754
H	-6.21145	4.32085	5.57925
H	-6.14817	5.32517	7.83615
H	-3.99533	5.48211	9.07631
H	-1.91052	4.60348	8.03692
H	-1.98192	3.56832	5.79363
H	-0.75131	-1.46534	-9.74588
H	1.59506	-3.24101	9.36279
H	3.91817	3.34413	-8.30878

$TS_{14b"\rightarrow E"}$

G = -4441.711038 Hartree

C	4.35349	-0.22260	-0.22958
C	5.38924	1.87353	0.52750
C	5.46867	0.57636	-0.02695
C	-1.65696	0.73709	0.62576
C	-1.41065	-0.22217	1.62779
C	3.02428	1.50246	0.79329
C	3.11278	0.24216	0.21182
C	0.76921	0.55183	0.85086
C	1.03906	2.93193	0.55011
C	-0.14310	2.58482	-0.11106
C	0.71519	5.18540	-0.06611
C	-0.51193	4.85378	-0.64935
C	1.44882	-1.78410	0.57657
C	0.53897	-1.72349	1.63029
C	0.50741	-4.09313	1.83656

C	1.42158	-4.17557	0.78679
C	1.89185	-3.03229	0.11469
C	-4.02424	0.43960	0.87008
C	-3.76797	-0.50837	1.92146
C	-0.40259	1.17533	0.08542
C	0.07036	-0.33443	1.91610
H	0.28213	-0.02477	2.94912
H	1.51383	-0.36286	-1.02897
H	1.61000	1.95132	2.36406
C	1.63355	1.77242	1.27917
C	1.73913	-0.39165	0.03864
C	-0.99460	3.52713	-0.68506
C	-2.96332	1.14568	0.22868
C	-2.43458	-0.91320	2.26112
C	0.02329	-2.84545	2.27191
C	1.52685	4.22542	0.58703
C	4.11020	2.40155	0.87750
C	-1.00033	-2.74791	3.34680
C	2.79313	-3.17289	-1.05835
C	2.76917	4.57956	1.32531
C	-2.30708	3.16829	-1.28419
C	-2.19766	-1.95804	3.26601
C	-3.24883	-2.22917	4.18792
C	-3.00782	-3.07940	5.28392
C	-1.79206	-3.72379	5.43571
C	-0.82035	-3.59499	4.44614
C	2.45450	-2.59795	-2.29383
C	3.33350	-2.69462	-3.37172
C	4.54975	-3.36348	-3.23460

C	4.90297	-3.96353	-2.01385
C	4.00570	-3.86333	-0.93842
C	-2.67819	3.95812	-2.37660
C	-3.94636	3.89890	-2.94665
C	-4.88716	3.05098	-2.40368
C	-4.56611	2.17746	-1.34495
C	-3.24068	2.17029	-0.78706
C	3.98132	3.79249	1.35451
C	5.16840	4.42500	1.84375
C	5.07465	5.67300	2.49254
C	3.87257	6.34722	2.59461
C	2.74473	5.82118	1.97189
C	-4.60065	-1.71951	3.91981
C	-5.62149	1.33180	-0.78728
C	6.19791	-4.67269	-1.85537
C	6.49154	3.82979	1.59227
C	-4.86202	-0.99833	2.71386
C	-6.20420	-0.69576	2.34563
C	-7.24810	-1.01596	3.22535
C	-6.97947	-1.63886	4.43609
C	-5.67618	-1.99901	4.77229
C	-5.37774	0.60107	0.40395
C	-6.45326	-0.05150	1.06551
C	-7.71891	-0.07254	0.46409
C	-6.89446	1.24131	-1.37990
C	7.68364	4.46534	2.01122
C	9.03428	2.84213	0.85089
C	7.88399	2.18543	0.45013
C	6.59998	2.63818	0.82943

C	7.36711	-4.18057	-2.46088
C	8.58475	-4.84392	-2.30933
C	8.65894	-6.01298	-1.54785
C	7.50459	-6.51288	-0.93978
C	6.28695	-5.84978	-1.09233
C	-7.92410	0.53869	-0.76667
C	8.93249	3.98325	1.65814
H	4.46044	-1.19820	-0.68843
H	6.43411	0.16745	-0.29840
H	1.03656	6.22161	-0.10485
H	-1.11186	5.65743	-1.06283
H	0.12779	-5.00649	2.28472
H	1.74748	-5.15296	0.44198
H	-3.78259	-3.26367	6.01706
H	-1.61679	-4.36461	6.29458
H	0.10149	-4.16284	4.52158
H	1.50306	-2.08652	-2.40844
H	3.06534	-2.25342	-4.32762
H	5.21917	-3.44441	-4.08599
H	4.27659	-4.28221	0.02654
H	-1.94954	4.64301	-2.79399
H	-4.19562	4.52684	-3.79552
H	-5.88754	3.06446	-2.81266
H	5.95686	6.13611	2.91474
H	3.81810	7.29786	3.11662
H	1.81619	6.38181	1.99569
H	-8.26872	-0.74363	2.98263
H	-5.51683	-2.50962	5.71331
H	-8.53447	-0.61387	0.92976

H	-7.08904	1.69519	-2.34147
H	7.64295	5.36289	2.61528
H	10.00720	2.46873	0.54440
H	7.98600	1.30342	-0.17072
H	7.32514	-3.25881	-3.03453
H	9.47805	-4.44215	-2.78003
H	9.60738	-6.52958	-1.42928
H	7.54970	-7.42569	-0.35182
H	5.39075	-6.25972	-0.63488
H	-8.89243	0.47037	-1.25257
H	9.82614	4.50042	1.99551
H	-7.79064	-1.85807	5.12393
H	-0.42364	0.53089	-1.14047
C	-2.56746	-1.33004	-2.01397
C	-1.68162	-0.32936	-2.55926
C	-2.17522	0.52550	-3.59257
C	-3.49306	0.45232	-4.01455
C	-4.45638	-0.46504	-3.38650
C	-3.88993	-1.37979	-2.38265
Cl	-4.99916	-2.51706	-1.68901
Cl	-1.87941	-2.45447	-0.88305
C	-3.98607	1.28282	-5.05900
C	-1.26099	1.46710	-4.16143
O	-5.65266	-0.45950	-3.69668
O	-0.46795	-0.16318	-2.11608
N	-4.38795	1.96524	-5.91199
N	-0.51805	2.22671	-4.63292

Structure E"

G = -2955.843991 Hartree

C	-1.42678	0.27756	3.48310
C	-0.15184	-1.36077	4.79770
C	-1.11778	-0.33648	4.68799
C	0.29067	-0.48965	-2.25180
C	0.93477	0.75397	-2.02031
C	0.29881	-1.03943	2.45430
C	-0.67419	-0.05203	2.35182
C	0.41643	-0.19509	0.15102
C	0.67214	-2.54642	0.60114
C	0.06269	-2.42959	-0.66450
C	0.50869	-4.88523	0.41043
C	-0.05555	-4.77163	-0.86684
C	-0.71120	1.94668	0.62893
C	0.40410	2.21366	-0.16271
C	-0.13421	4.52562	-0.29034
C	-1.23202	4.28935	0.53492
C	-1.57318	2.99828	0.98025
C	0.55288	-0.24295	-4.61416
C	1.26854	0.99031	-4.36945
C	0.09550	-1.07731	-1.01116
C	1.15865	0.98193	-0.53828
H	2.22989	1.03150	-0.30752
H	-1.76769	0.06913	0.51960
H	2.12950	-1.10101	1.27419
C	1.04282	-1.20662	1.16450
C	-0.82184	0.45339	0.91983
C	-0.29629	-3.52038	-1.47029
C	0.08272	-1.05482	-3.54686

C	1.37284	1.56257	-3.05770
C	0.70046	3.46751	-0.69111
C	0.90832	-3.76988	1.19317
C	0.49483	-1.82114	3.61364
C	1.79986	3.67826	-1.67025
C	-2.81297	2.80049	1.77478
C	1.57555	-3.89536	2.51415
C	-0.92209	-3.35458	-2.80044
C	2.01520	2.86288	-2.83349
C	2.87223	3.35119	-3.85873
C	3.62854	4.51781	-3.63230
C	3.50928	5.22964	-2.45162
C	2.57212	4.83182	-1.50053
C	-3.78929	1.87574	1.37388
C	-4.91922	1.66638	2.16358
C	-5.09037	2.37410	3.35298
C	-4.13736	3.32105	3.76607
C	-3.00846	3.52555	2.95728
C	-1.83395	-4.36135	-3.13861
C	-2.43084	-4.43107	-4.39218
C	-2.03546	-3.54808	-5.37726
C	-1.10143	-2.52697	-5.11921
C	-0.62520	-2.31412	-3.78134
C	1.31872	-3.04156	3.64862
C	1.81200	-3.46265	4.92248
C	2.68753	-4.56421	4.99819
C	3.03560	-5.29226	3.87501
C	2.44812	-4.98052	2.65241
C	2.88878	2.69064	-5.16987

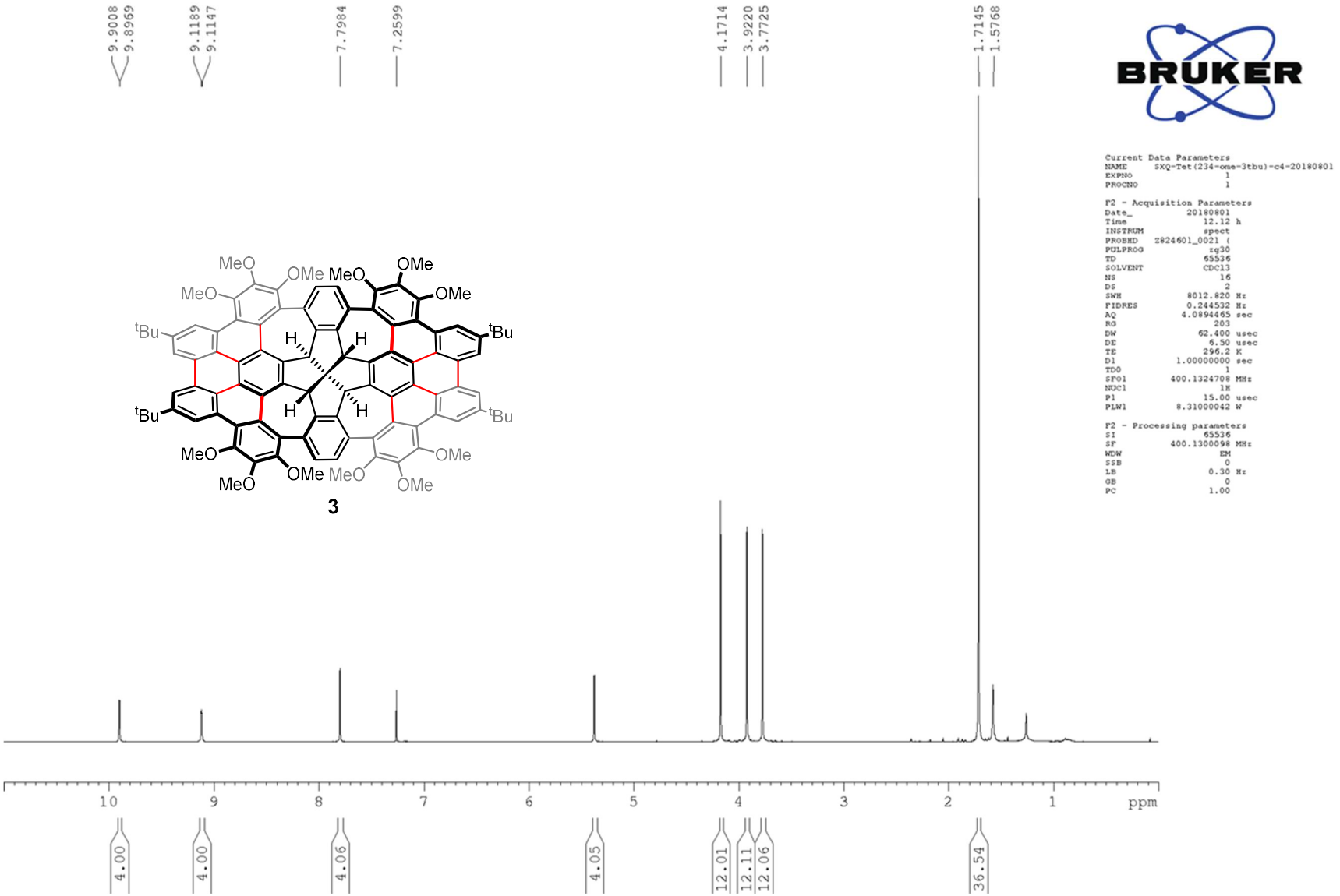
C	-0.59314	-1.71675	-6.22869
C	-4.30733	4.07785	5.03216
C	1.33586	-2.81814	6.15661
C	1.98715	1.61487	-5.44667
C	1.88317	1.09788	-6.77115
C	2.73865	1.58702	-7.76574
C	3.66590	2.57946	-7.47343
C	3.73223	3.13175	-6.19905
C	0.30181	-0.64348	-5.97435
C	0.89944	0.05905	-7.05552
C	0.53529	-0.26658	-8.36765
C	-0.91326	-2.01757	-7.56538
C	1.85516	-3.16564	7.42431
C	0.21426	-1.79716	8.53871
C	-0.28892	-1.41145	7.30821
C	0.26790	-1.88443	6.09901
C	-4.83575	3.45669	6.17685
C	-4.99212	4.16658	7.36731
C	-4.62242	5.51213	7.43762
C	-4.09537	6.14167	6.30714
C	-3.93952	5.43173	5.11673
C	-0.37017	-1.29188	-8.61640
C	1.31216	-2.66635	8.59620
H	-2.20774	1.02486	3.44869
H	-1.64918	-0.00113	5.57022
H	0.64992	-5.88489	0.80981
H	-0.28267	-5.68651	-1.40245
H	0.03930	5.52718	-0.67209
H	-1.88324	5.11726	0.80024

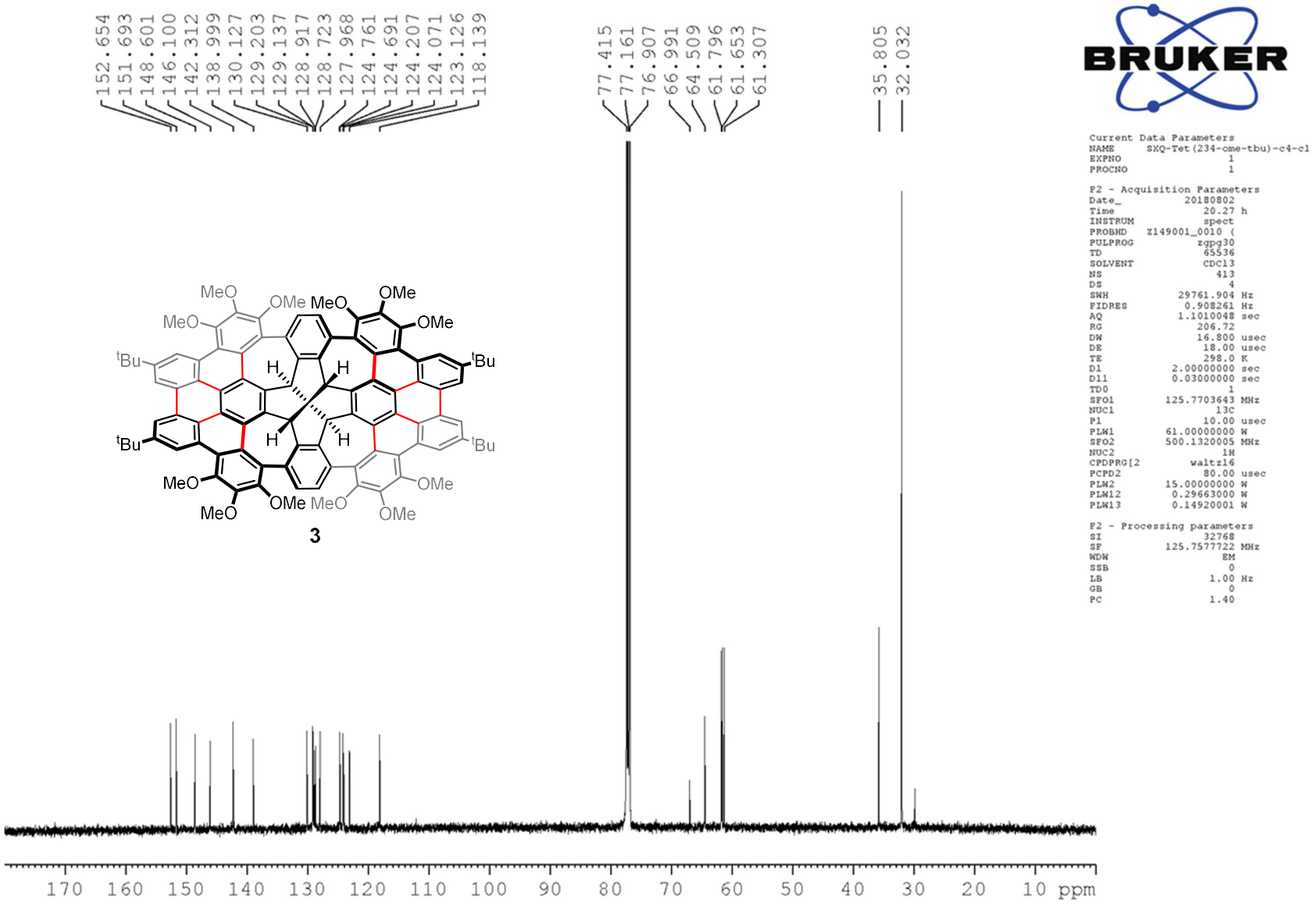
H	4.30332	4.89202	-4.39105
H	4.11119	6.11803	-2.28721
H	2.42842	5.42839	-0.60544
H	-3.66722	1.32983	0.44325
H	-5.67550	0.95390	1.84657
H	-5.98112	2.21245	3.95267
H	-2.23727	4.21890	3.27979
H	-2.10616	-5.09455	-2.38858
H	-3.17357	-5.19376	-4.60295
H	-2.47113	-3.65035	-6.36189
H	3.08337	-4.88018	5.95470
H	3.72434	-6.12775	3.95450
H	2.67432	-5.59031	1.78365
H	2.71208	1.17035	-8.76527
H	4.45845	3.91349	-6.01996
H	0.94127	0.29030	-9.20365
H	-1.57878	-2.83564	-7.80627
H	2.70202	-3.83621	7.50242
H	-0.23149	-1.41239	9.45135
H	-1.12028	-0.71713	7.28887
H	-5.10341	2.40432	6.13985
H	-5.39563	3.66548	8.24304
H	-4.74385	6.06510	8.36487
H	-3.81207	7.18989	6.34899
H	-3.55100	5.93691	4.23680
H	-0.64542	-1.53541	-9.63786
H	1.73585	-2.95469	9.55379
H	4.34166	2.93164	-8.24682

9. References

1. *APEX2 Data Collection Software*, version 2012. 4; Bruker AXS: Delft, The Netherlands, 2012.
2. G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr.* 2008, **64**, 112–122.
3. C. M. Cardona, W. Li, A. E. Kaifer, D. Stockdale and G. C. Bazan, *Adv. Mater.* 2011, **23**, 2367–2371.
4. Estimated from the crossing point of the normalized absorption and emission spectra.
5. Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
6. W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.* 1972, **56**, 2257–2261.
7. P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta* 1973, **28**, 213–222.
8. J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.* 2005, **105**, 2999–3094.
9. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104.

10. NMR and Mass Spectra of New Compounds





BRUKER

Current Data Parameters
NAME SXQ-Tet(234-ome-tbu)-c4-c1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180802
Time 20.27 h
INSTRUM spect
PROBHD Z149001_0010 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 413
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 206.72
DW 16.800 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 10.00 usec
PLW1 61.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.29663000 W
PLW13 0.14920001 W

F2 - Processing parameters
SI 32768
SF 125.7577722 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

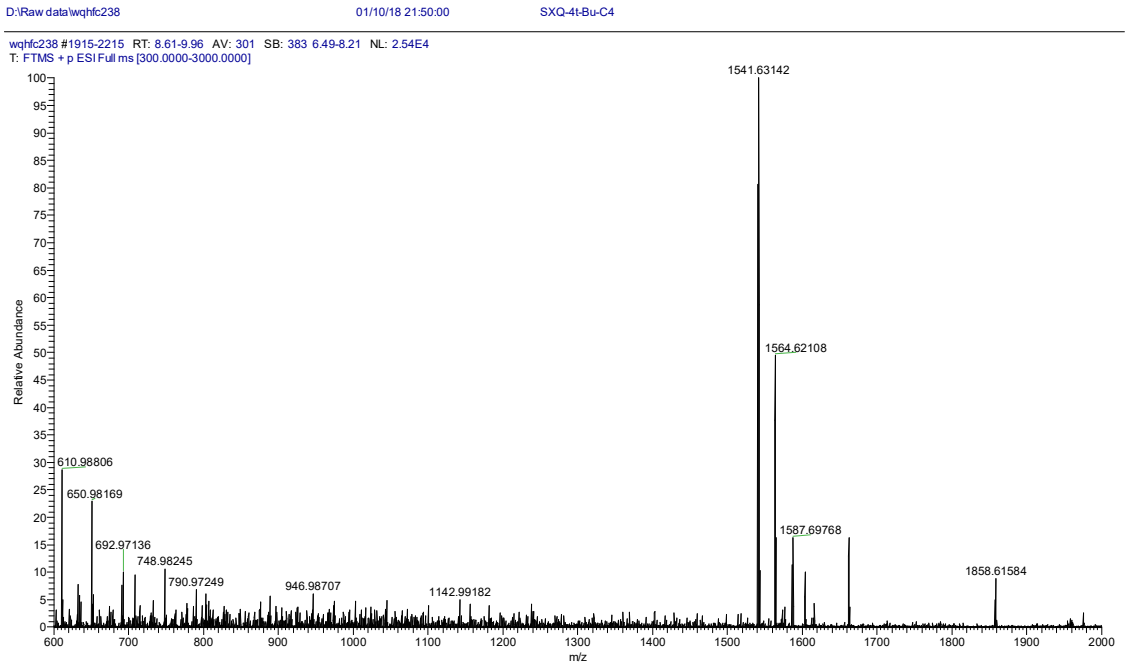
Thermo QEFMS Analysis Report of Compound 3

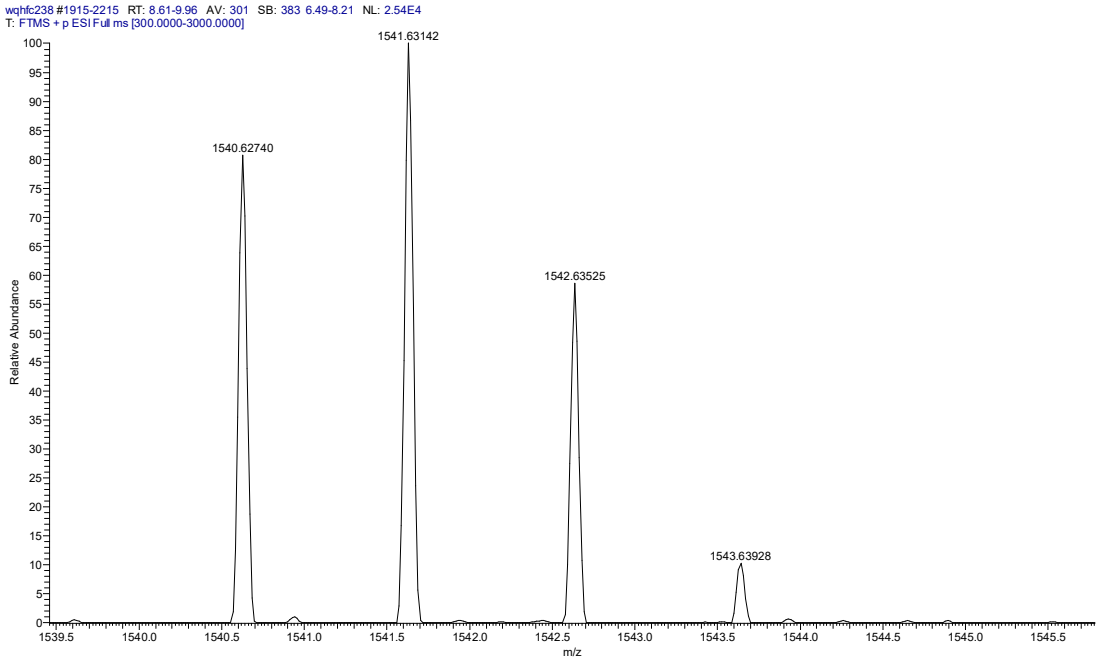
Analysis Info

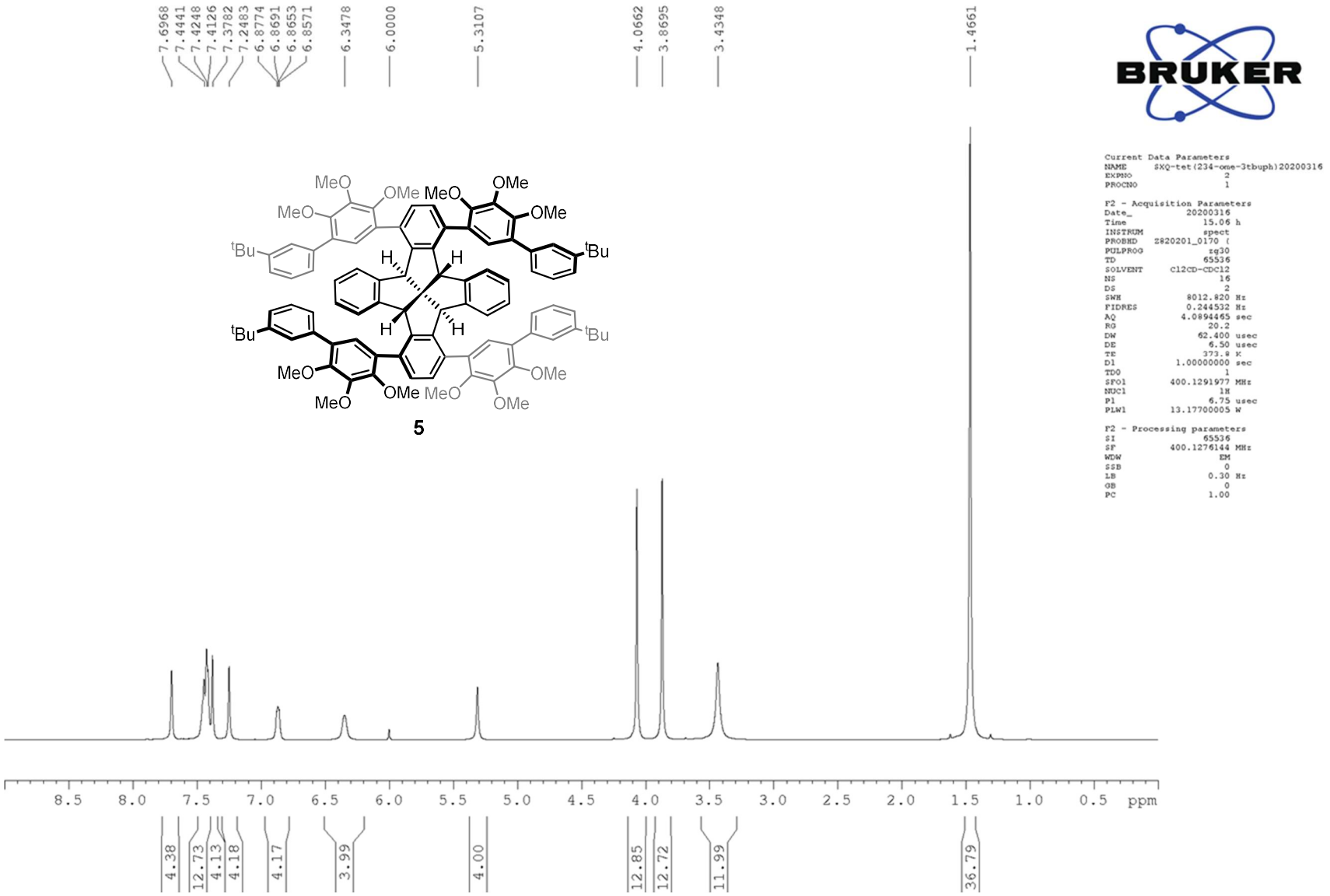
Sample Name :	SXQ-4t-Bu-C4	Reference No.:	Wqhfc238
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI pos, 3.2kV, by LC, with sheath gas		

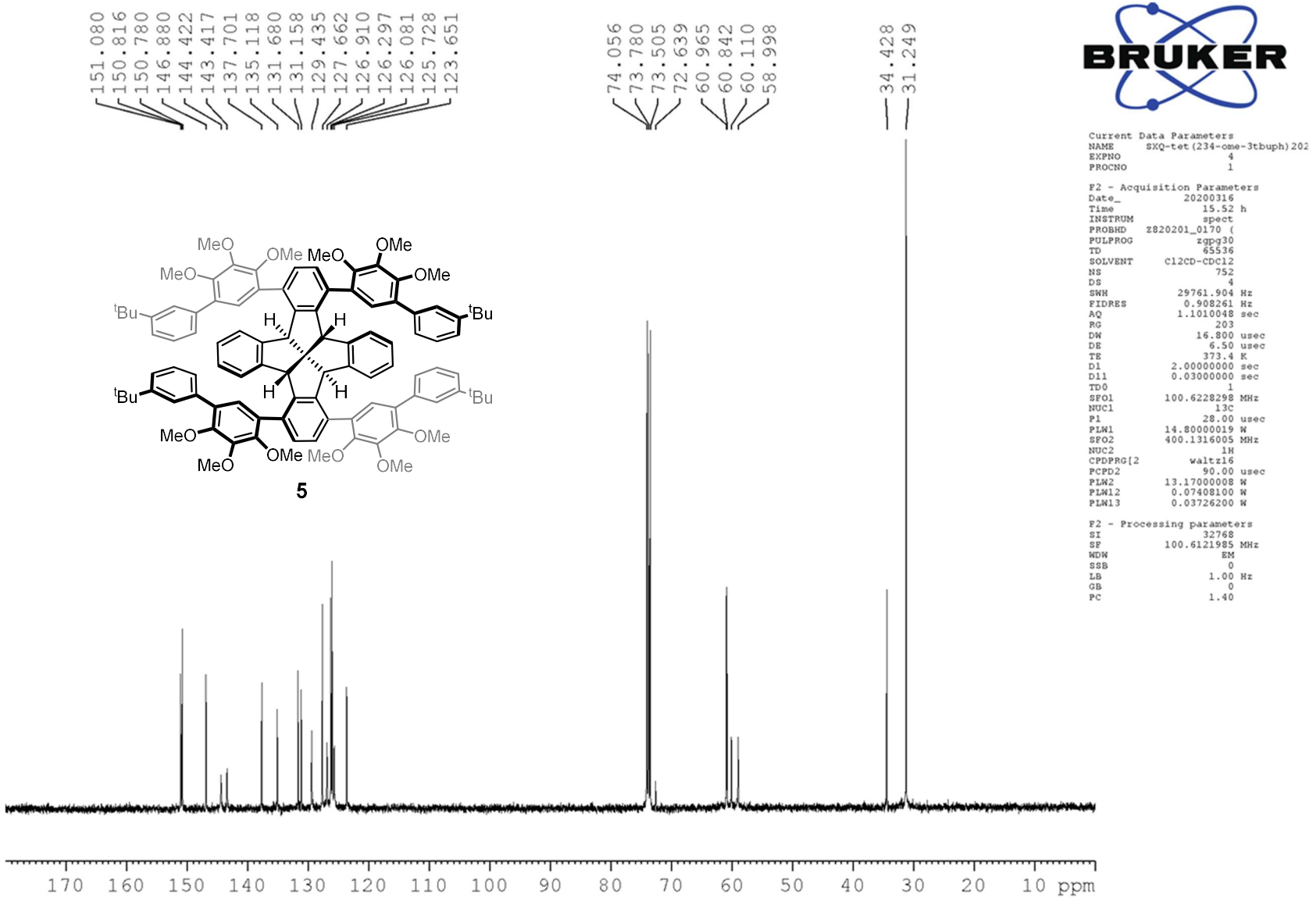
Accurate Mass Measurement

Molecular formula :	$C_{105}H_{88}O_{12}$
Experimental Mass $[M]^{+\bullet}$:	1540.62740
Theoretical Mass $[M]^{+\bullet}$:	1540.62703
Error (ppm) :	0.2






7.6968
7.4441
7.4248
7.4126
7.3782
7.2483
6.8774
6.8691
6.8653
6.8571
6.3478
6.0000
5.3107
4.0662
3.8695
3.4348
1.4661
BRUKER
MeO
OMe
tBu
H
5
Current Data Parameters
NAME SXQ-tet(234-one-3tbuph)20200316
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200316
Time 15.06 h
INSTRUM spect
PROBHD Z820201_0170 (
PULPROG zg30
TD 65536
SOLVENT C12CD-CDC12
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 20.2
DW 62.400 usec
DE 6.50 usec
TE 373.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.1291977 MHz
NUC1 1H
P1 6.75 usec
PLW1 13.17700005 W
F2 - Processing parameters
SI 65536
SF 400.1276144 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
4.38
12.73
4.13
4.18
4.17
3.99
4.00
12.85
12.72
11.99
36.79



BRUKER

Current Data Parameters
NAME SXQ-tet(234-ome-3tbuph)202
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200316
Time 15.52 h
INSTRUM spect
PROBHD Z820201_0170 (
PULPROG zgpg30
TD 65536
SOLVENT C12CD-CDC12
NS 752
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 373.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 28.00 usec
PLW1 14.80000019 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.17000008 W
PLW12 0.07408100 W
PLW13 0.03726200 W

F2 - Processing parameters
SI 32768
SF 100.6121985 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

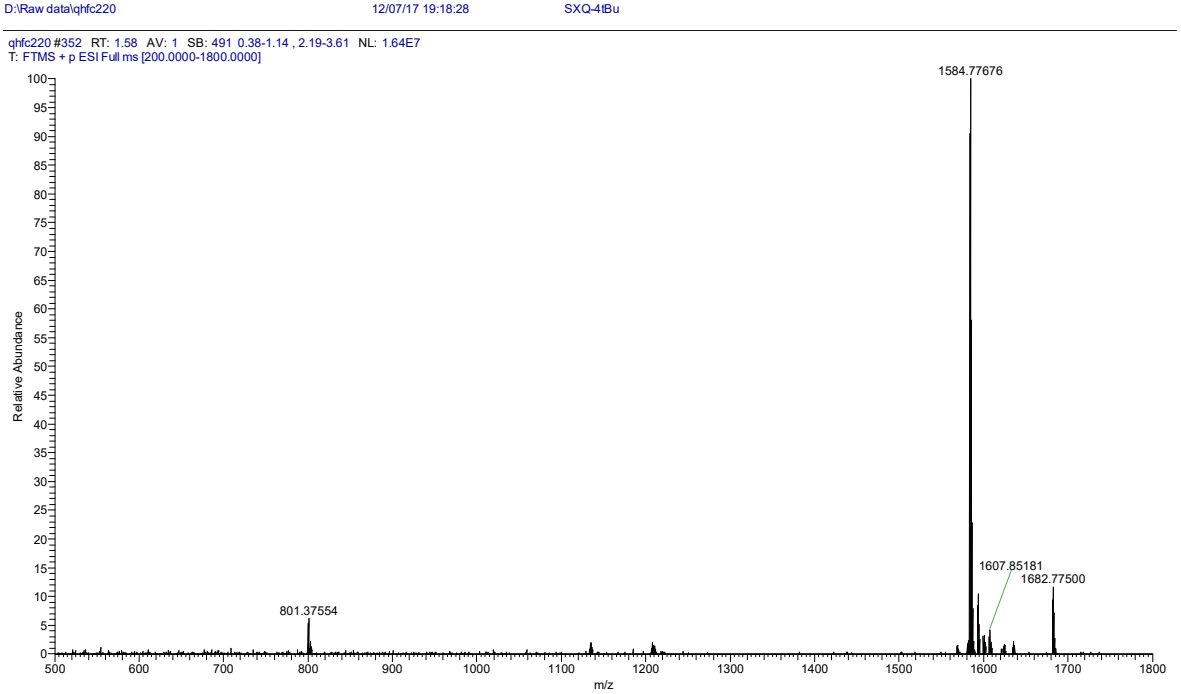
Thermo QEFMS Analysis Report of Compound 5

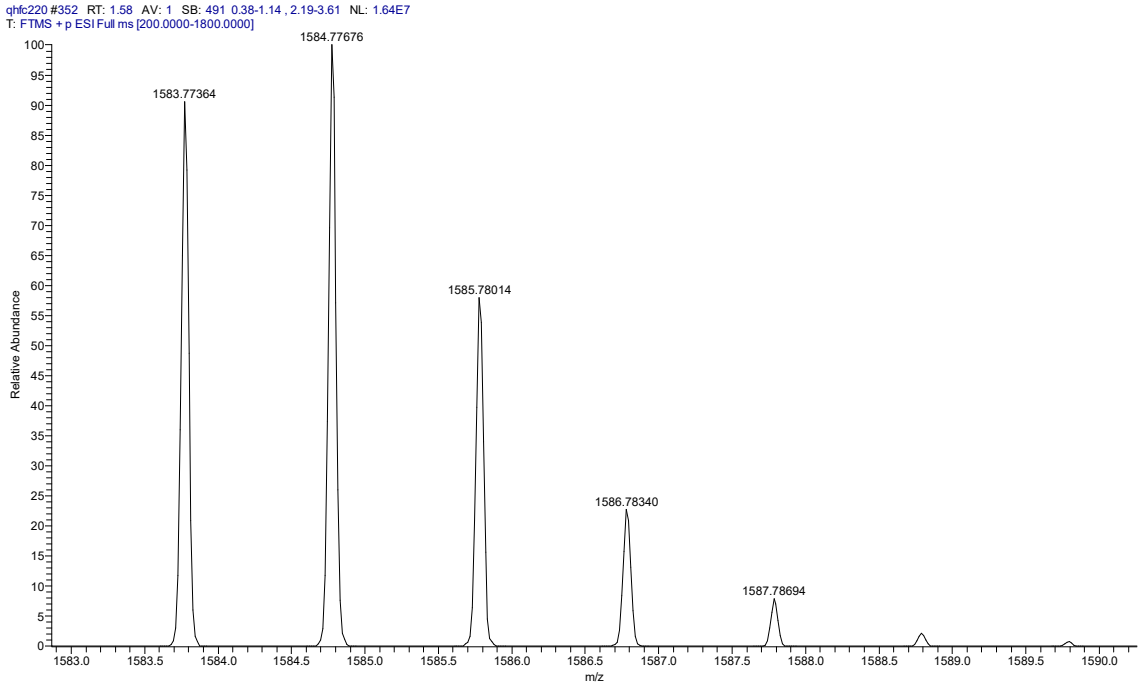
Analysis Info

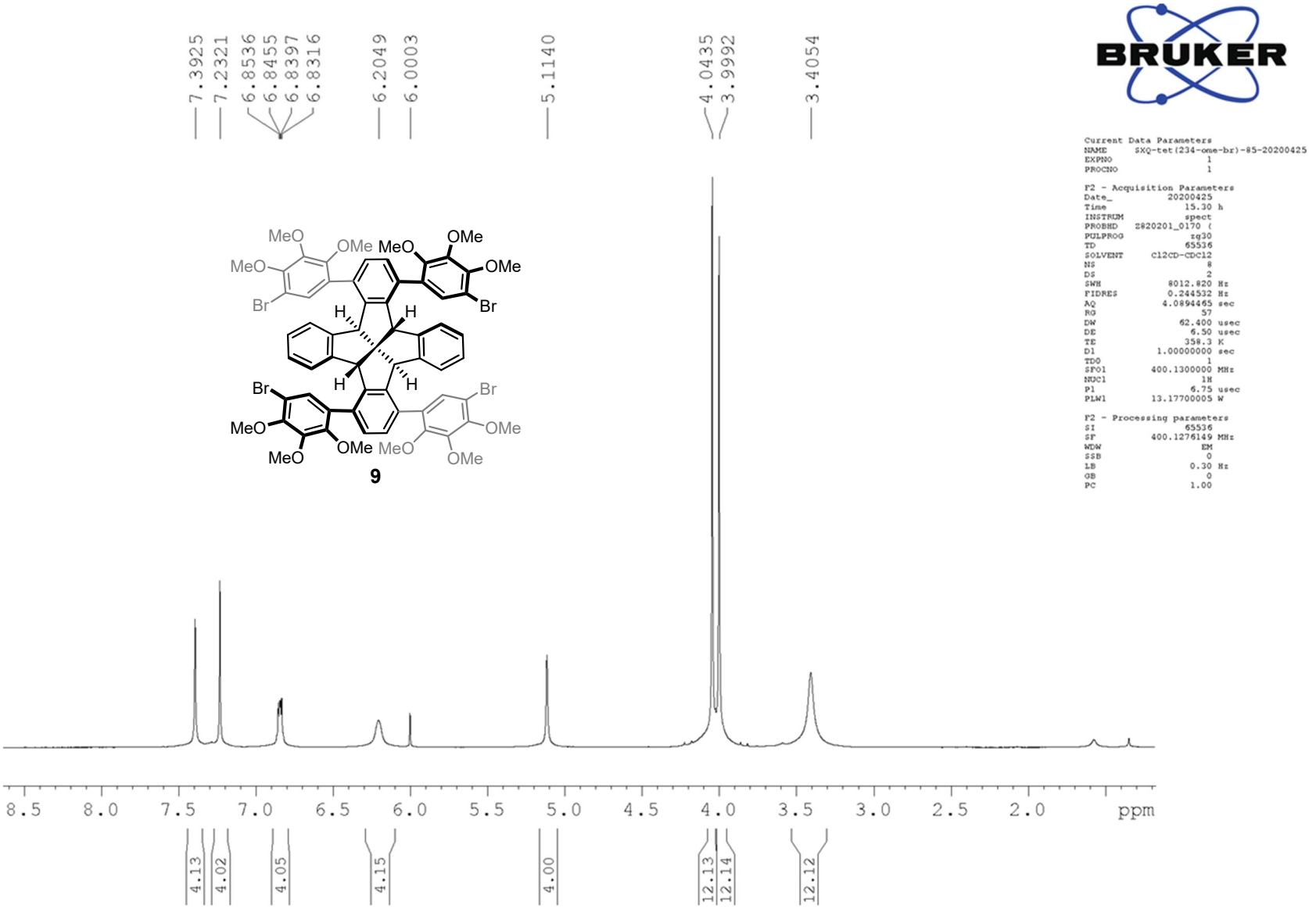
Sample Name :	SXQ-4tBu	Reference No.:	Qhfc220
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI pos, 3.5kV, by LC, with sheath gas		

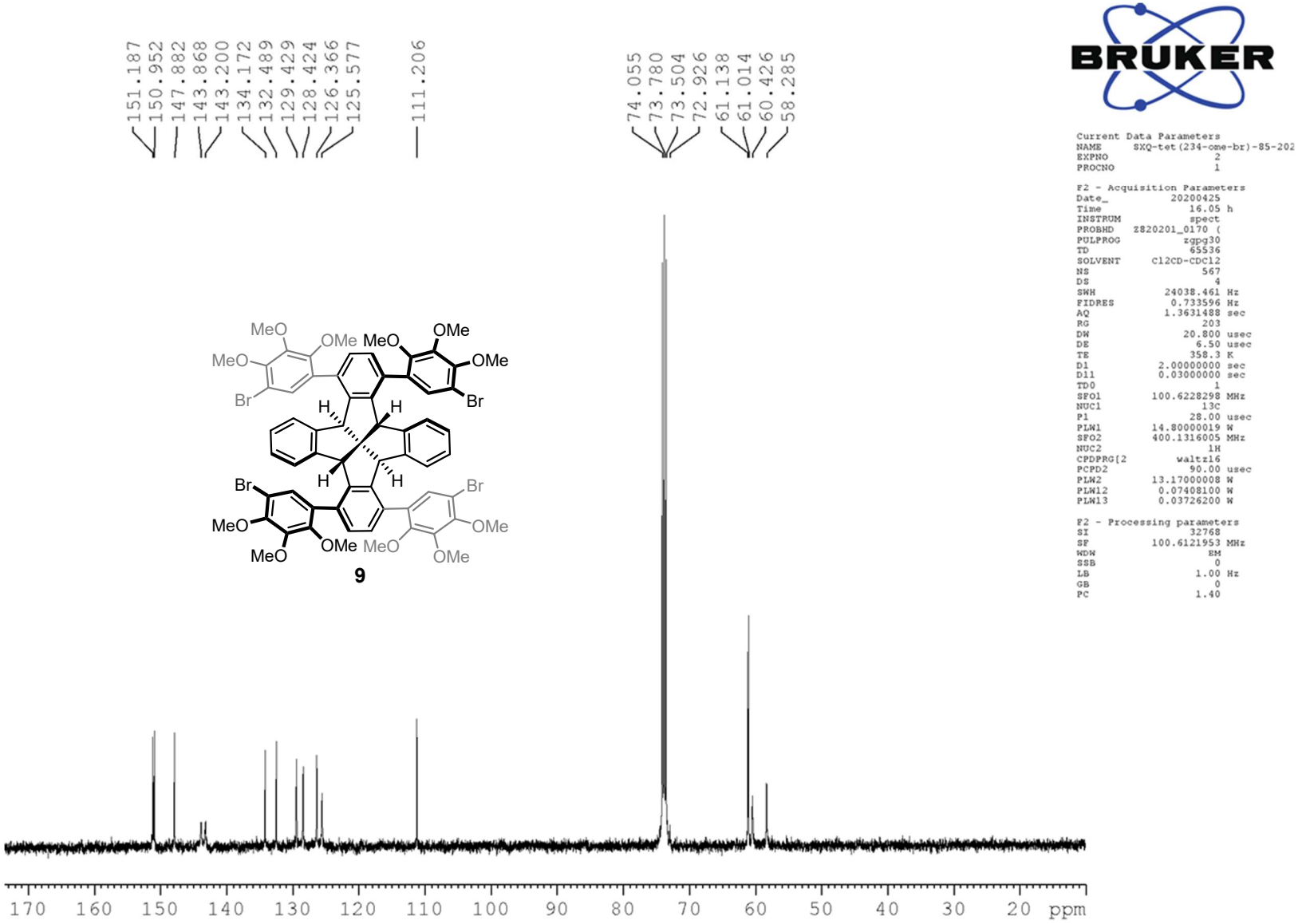
Accurate Mass Measurement

Molecular formula :	$C_{105}H_{108}O_{12}$
Experimental Mass $[M + Na]^+$:	1583.77364
Theoretical Mass $[M + Na]^+$:	1583.77330
Error (ppm) :	0.2






7.3925
7.2321
6.8536
6.8455
6.8397
6.8316
6.2049
6.0003
5.1140
4.0435
3.9992
3.4054
MeO
OMe
MeO
OMe
Br
Br
H
H
H
H
Br
Br
MeO
OMe
MeO
OMe
9
BRUKER
Current Data Parameters
NAME SXQ-tet(234-ome-br)-85-20200425
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200425
Time 15.30 h
INSTRUM spect
PROBHD Z820201_0170 (
PULPROG zg30
TD 65536
SOLVENT C12CD-CDC12
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 57
DW 62.400 usec
DE 6.50 usec
TE 358.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.1300000 MHz
NUC1 1H
P1 6.75 usec
PLW1 13.17700005 W
F2 - Processing parameters
SI 65536
SF 400.1276149 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
4.13
4.02
4.05
4.15
4.00
12.13
12.14
12.12


151.187
150.952
147.882
143.868
143.200
134.172
132.489
129.429
128.424
126.366
125.577
111.206
74.055
73.780
73.504
72.926
61.138
61.014
60.426
58.285
BRUKER
Current Data Parameters
NAME SXQ-tet(234-ome-br)-85-202
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200425
Time 16.05 h
INSTRUM spect
PROBHD Z820201_0170 (
PULPROG zgpg30
TD 65536
SOLVENT C12CD-CDC12
NS 567
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 358.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 28.00 usec
PLW1 14.80000019 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.17000008 W
PLW12 0.07408100 W
PLW13 0.03726200 W
F2 - Processing parameters
SI 32768
SF 100.6121953 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
MeO
OMe
Br
H
9
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

Thermo QEFMS Analysis Report of Compound 9

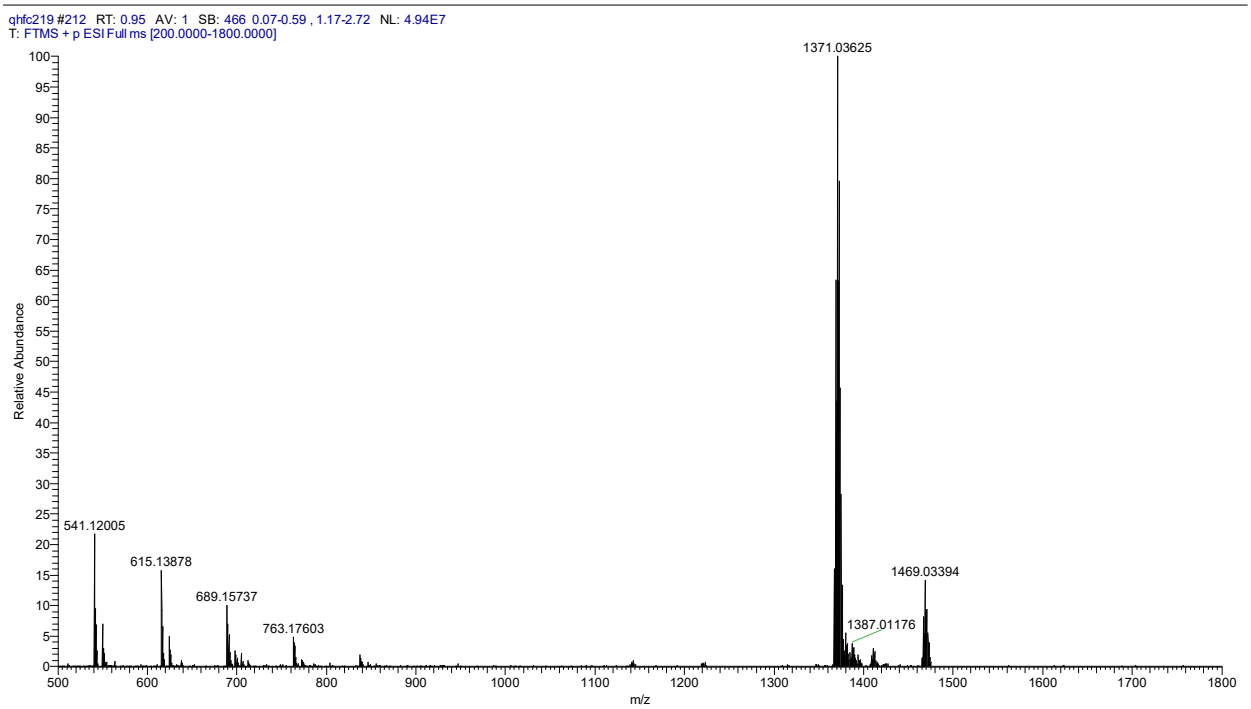
Analysis Info

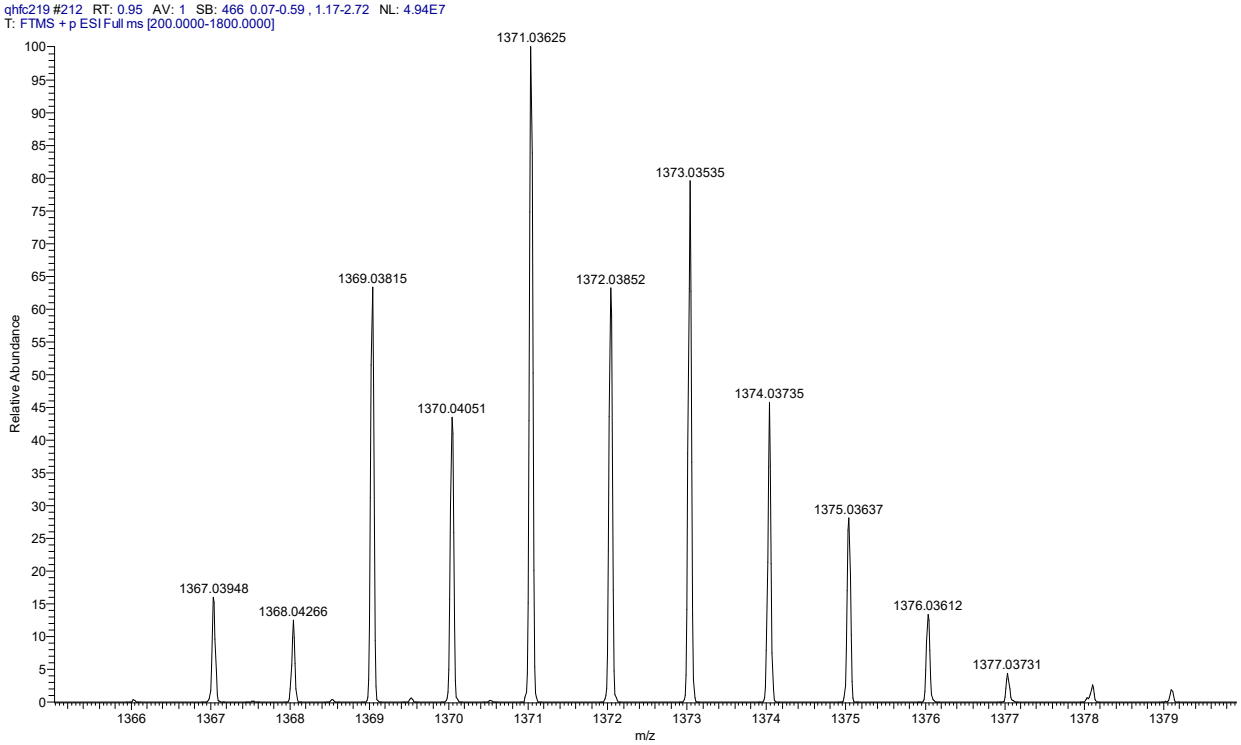
Sample Name :	SXQ-4Br	Reference No.:	Qhfc219
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI pos, 3.5kV, by LC, with sheath gas		

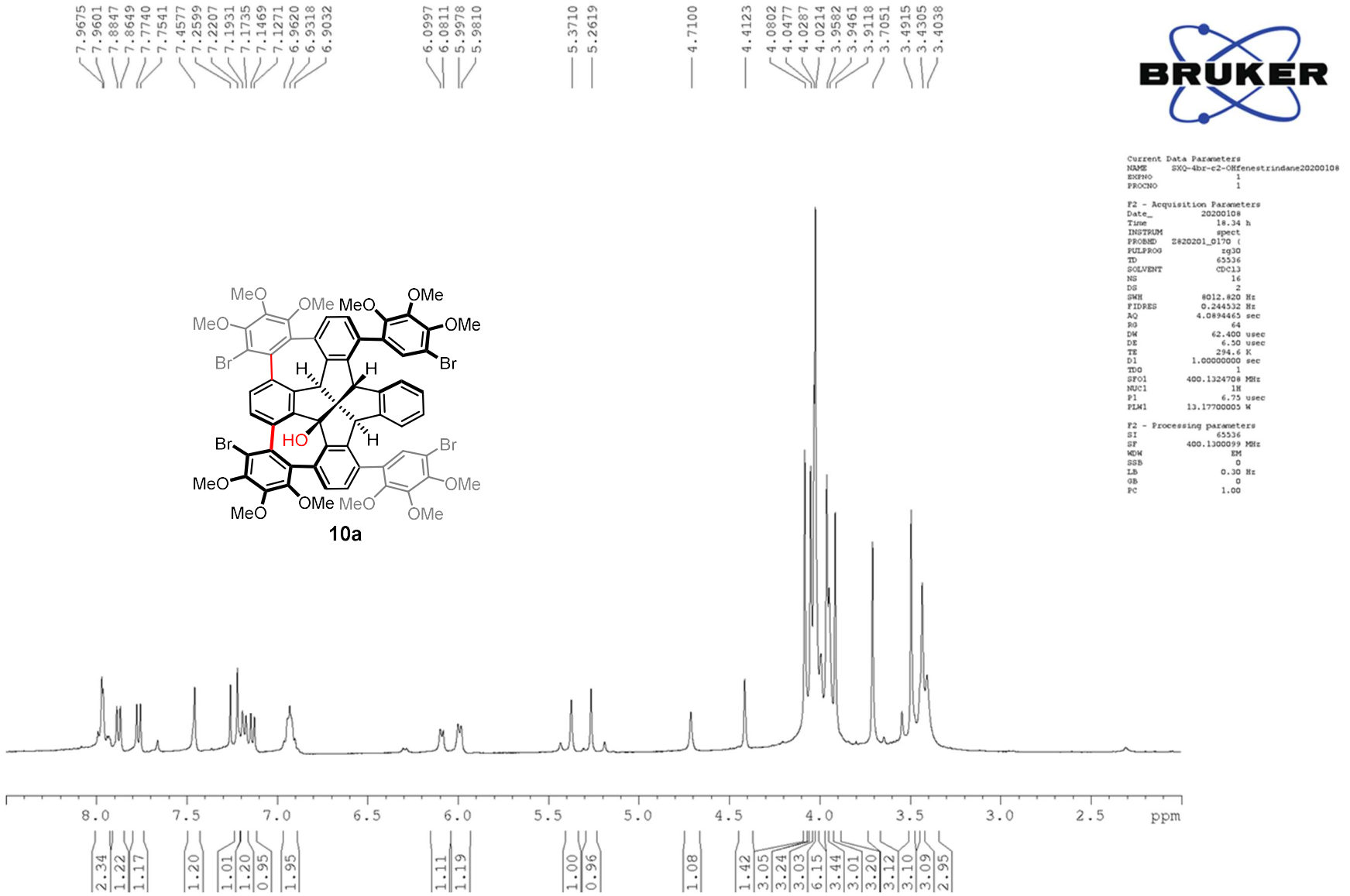
Accurate Mass Measurement

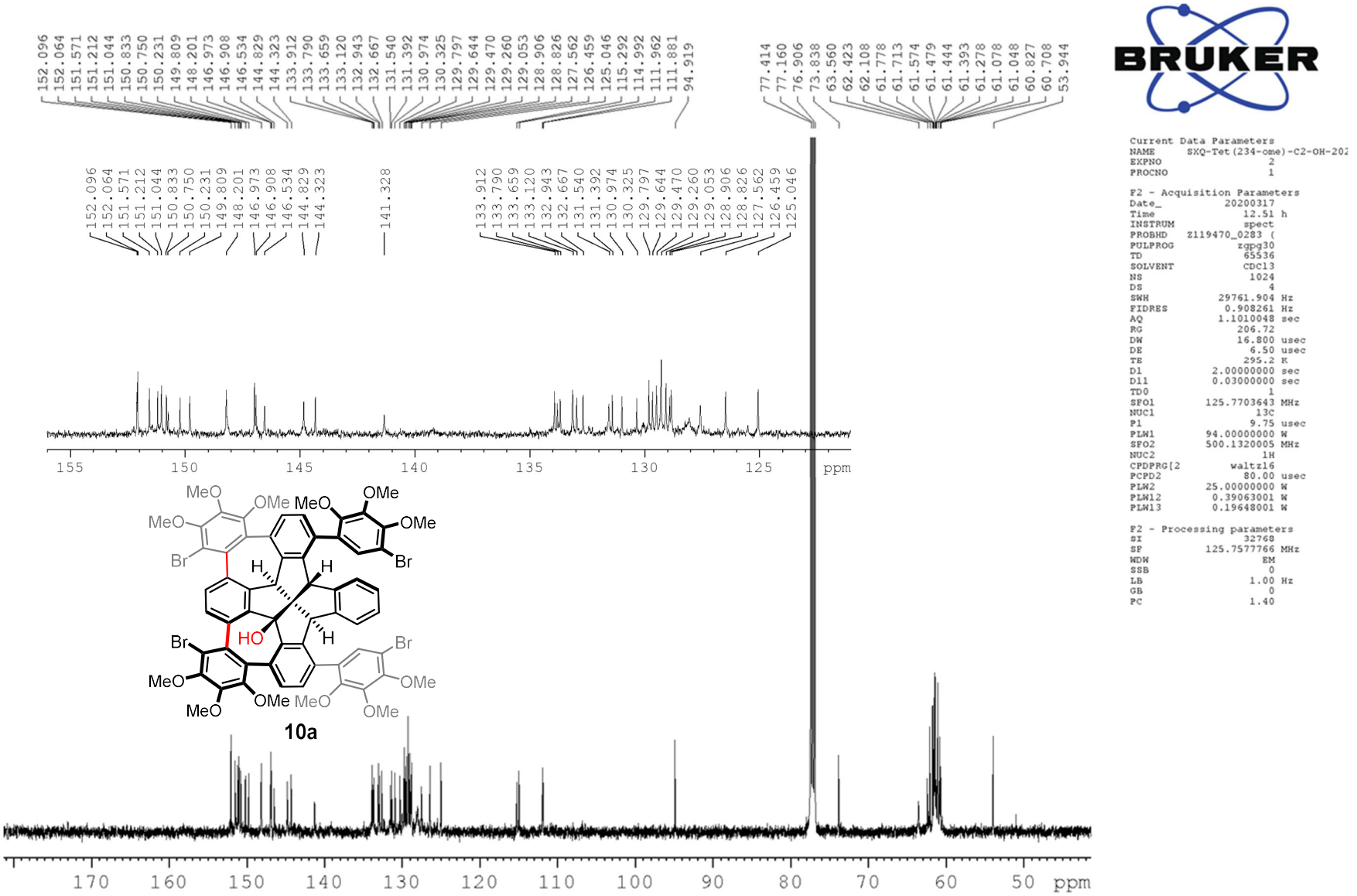
Molecular formula :	$C_{65}H_{56}Br_4O_{12}$
Experimental Mass $[M + Na]^+$:	1367.03948
Theoretical Mass $[M+ Na]^+$:	1367.03975
Error (ppm) :	−0.2

D:\Raw data\qhfc219 12/07/17 19:07:34 SXQ-4Br






7.9675
7.9601
7.8847
7.8649
7.7740
7.7541
7.4577
7.2599
7.2207
7.1931
7.1735
7.1469
7.1271
6.9620
6.9318
6.9032
6.0997
6.0811
5.9978
5.9810
5.3710
5.2619
4.7100
4.4123
4.0802
4.0477
4.0287
4.0214
3.9582
3.9461
3.9118
3.7051
3.4915
3.4305
3.4038
BRUKER
Current Data Parameters
NAME SXQ-4br-c2-OHfenestrindane20200108
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200108
Time 18.34 h
INSTRUM spect
PROBHD Z820201_0170 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 6.75 usec
PLW1 13.17700005 W
F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
OMe
Br
H
HO
10a
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
2.34
1.22
1.17
1.20
1.01
1.20
0.95
1.95
1.11
1.19
1.00
0.96
1.08
1.42
3.05
3.24
3.03
6.15
3.44
3.01
3.20
3.12
3.10
3.09
2.95



BRUKER

```
Current Data Parameters
NAME      SXQ-Tet(234-ome)-C2-OH-202
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20200317
Time              12.51 h
INSTRUM             spect
PROBHD    Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                 9.75 usec
PLW1          94.00000000 W
SFO2          500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2          25.00000000 W
PLW12          0.39063001 W
PLW13          0.19648001 W

F2 - Processing parameters
SI                32768
SF          125.7577766 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

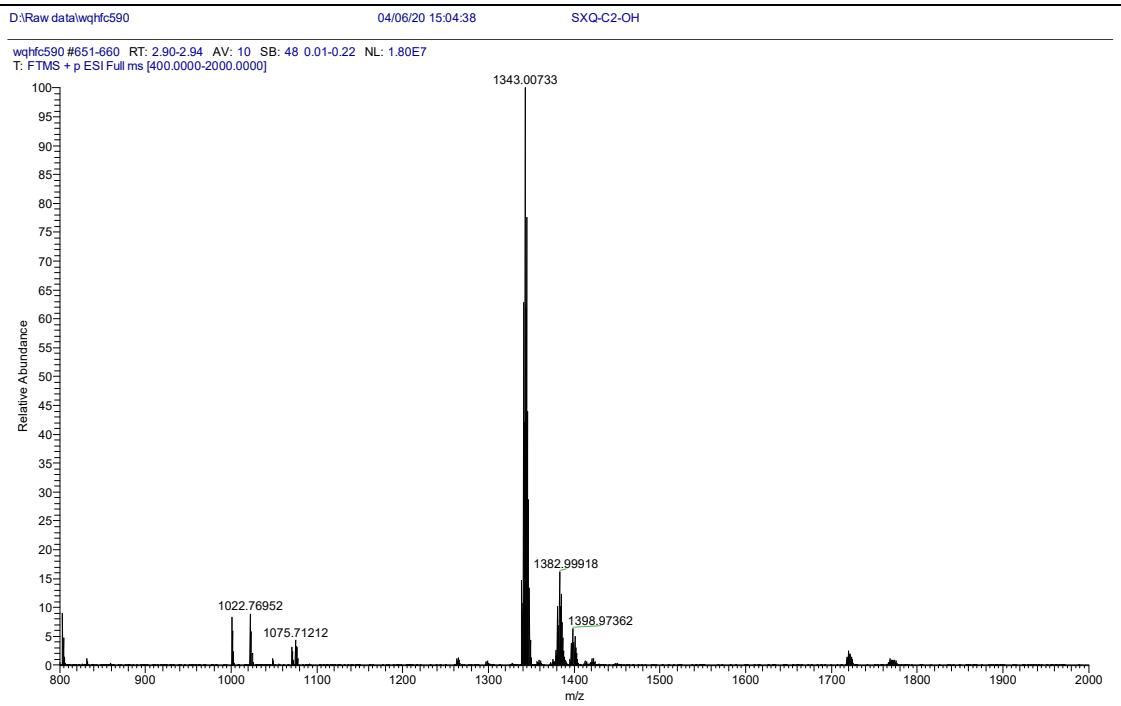
Thermo QEFMS Analysis Report of Compound 10a

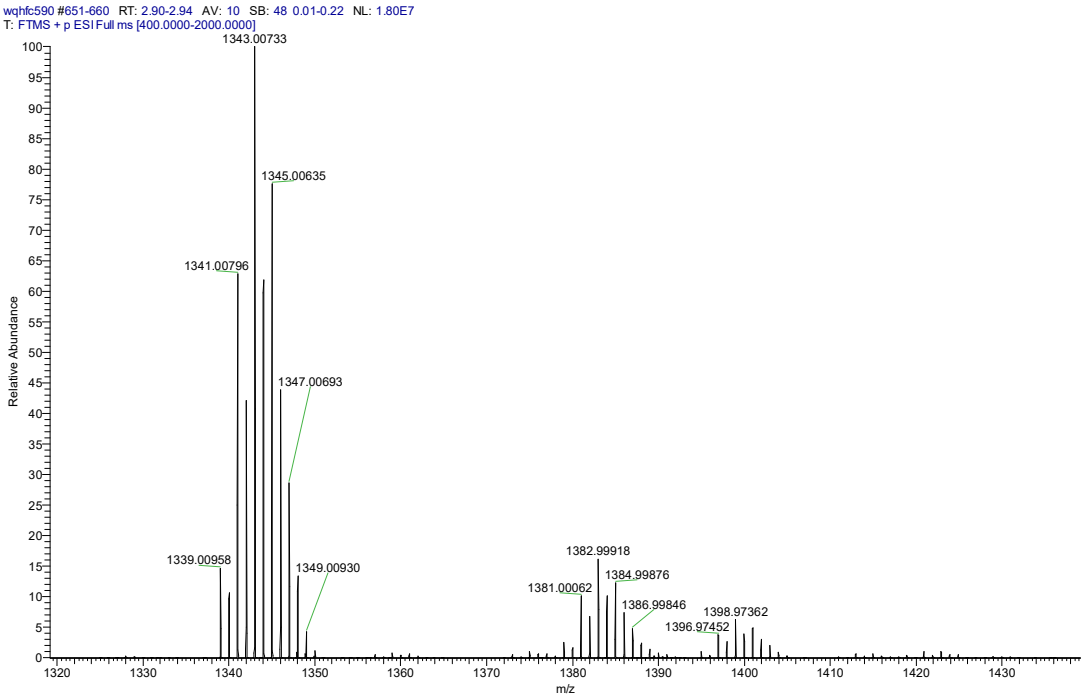
Analysis Info

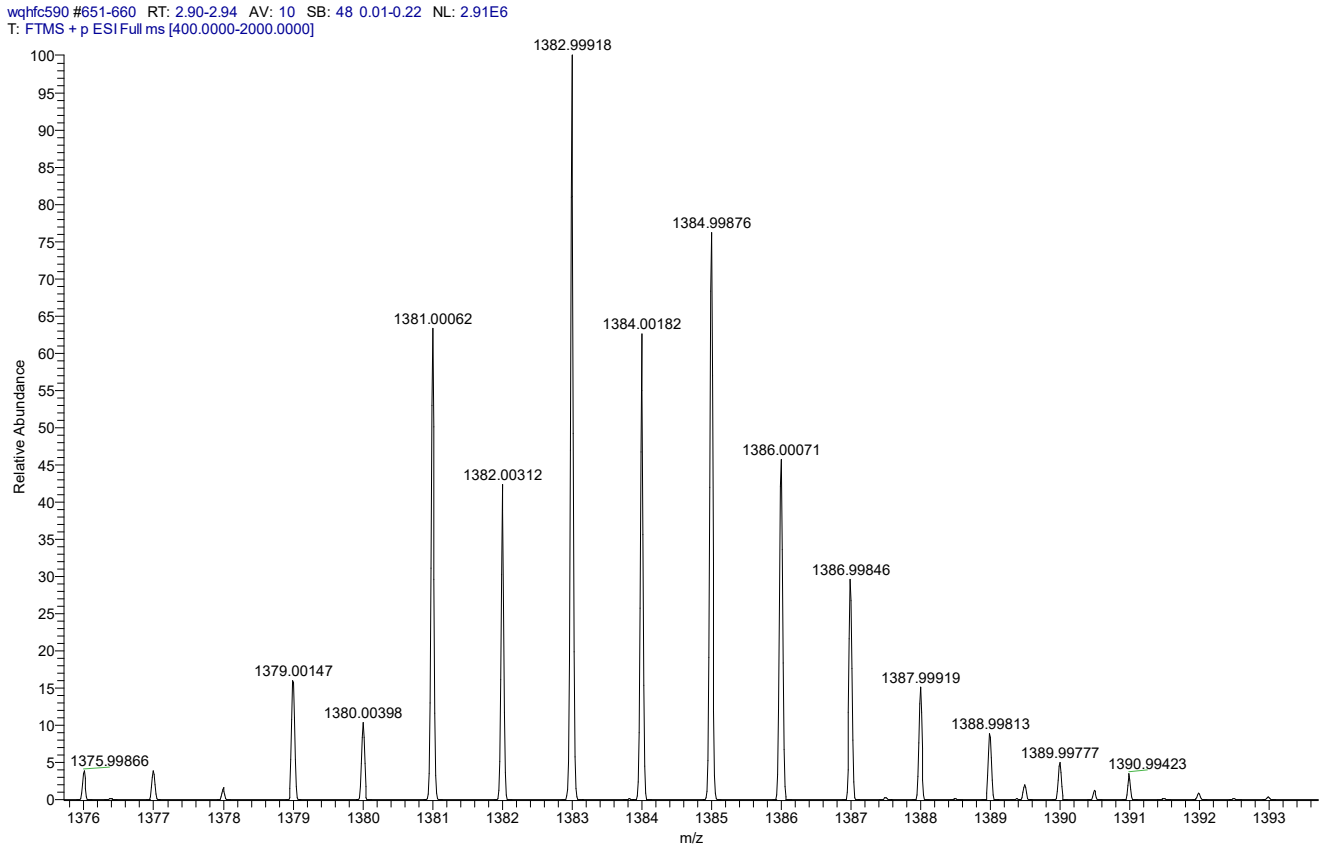
Sample Name :	SXQ-C2-OH	Reference No.:	Wqhfc590
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI, 3.5kV, by infusion, with 0.1% formic acid		

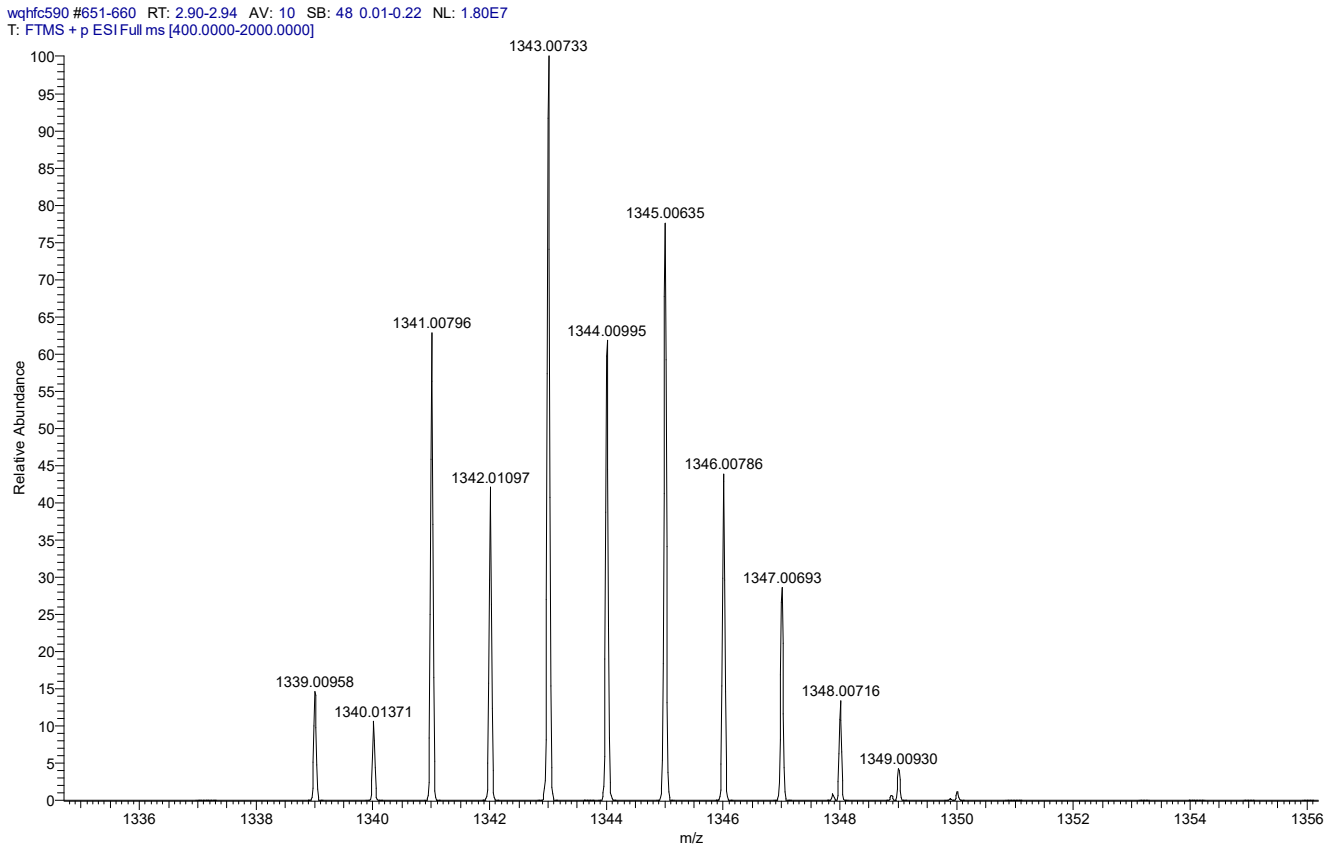
Accurate Mass Measurement

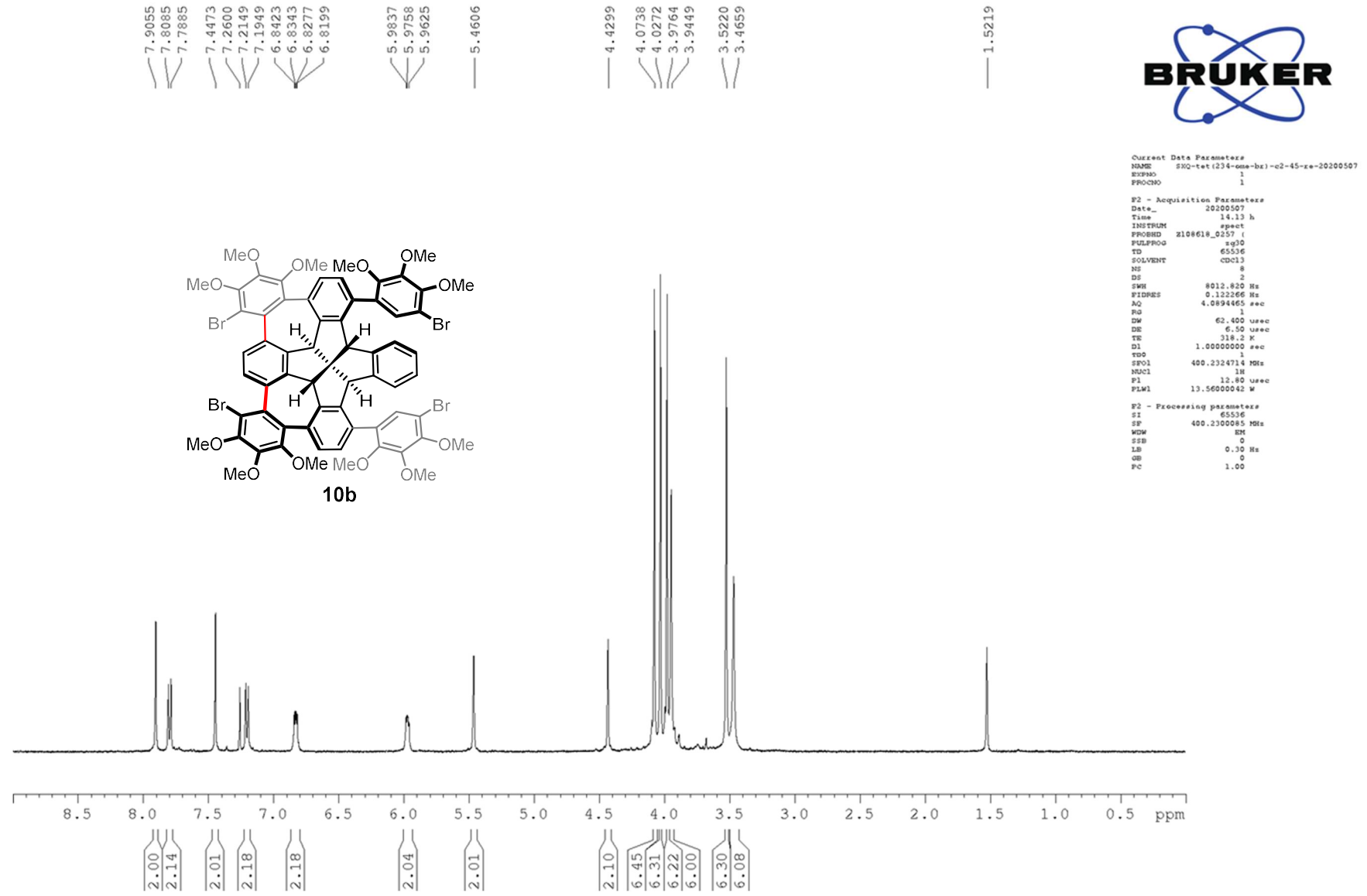
Molecular formula :	$C_{65}H_{52}Br_4O_{13}$
Experimental Mass $[M + Na]^+$, $[M + H - H_2O]^+$:	1379.00147, 1339.00958
Theoretical Mass $[M + Na]^+$, $[M + H - H_2O]^+$:	1379.00336, 1339.01085
Error (ppm) :	-1.4, -0.9

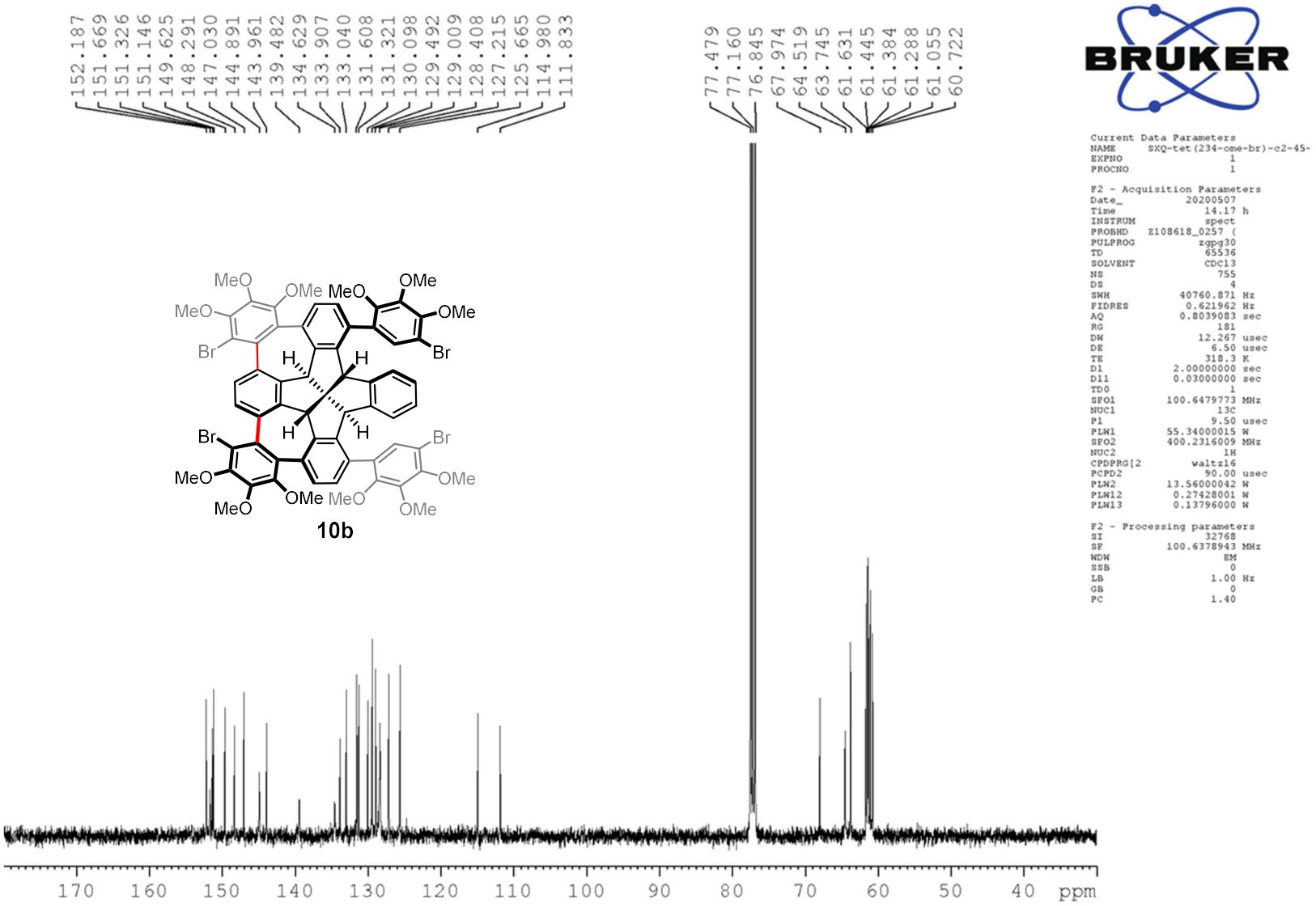





wqhfc590 #651-660 RT: 2.90-2.94 AV: 10 SB: 48 0.01-0.22 NL: 2.91E6
T: FTMS + p ESI Full ms [400.0000-2000.0000]
1382.99918
1384.99876
1381.00062
1384.00182
1386.00071
1382.00312
1386.99846
1379.00147
1387.99919
1380.00398
1388.99813
1389.99777
1375.99866
1390.99423
Relative Abundance
m/z


wqhfc590 #651-660 RT: 2.90-2.94 AV: 10 SB: 48 0.01-0.22 NL: 1.80E7
T: FTMS + p ESI Full ms [400.0000-2000.0000]
1343.00733
1345.00635
1341.00796
1344.00995
1346.00786
1342.01097
1347.00693
1339.00958
1348.00716
1340.01371
1349.00930
Relative Abundance
m/z


7.9055
7.8085
7.7885
7.4473
7.2600
7.2149
7.1949
6.8423
6.8343
6.8277
6.8199
5.9837
5.9758
5.9625
5.4606
4.4299
4.0738
4.0272
3.9764
3.9449
3.5220
3.4659
1.5219
BRUKER
Current Data Parameters
NAME SXQ-tet(234-ome-br)-c2-45-re-20200507
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200507
Time 14.13 h
INSTRUM spect
PROBHD z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 1
DW 62.400 usec
DE 6.50 usec
TE 318.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
OMe
Br
H
10b
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.00
2.14
2.01
2.18
2.18
2.04
2.01
2.10
6.45
6.31
6.22
6.00
6.30
6.08



BRUKER

```
Current Data Parameters
NAME      SXQ-tet(234-ome-br)-c2-45-
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20200507
Time              14.17 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT             CDCl3
NS                    755
DS                      4
SWH             40760.871 Hz
FIDRES          0.621962 Hz
AQ              0.8039083 sec
RG                    181
DW                12.267 usec
DE                 6.50 usec
TE                318.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1         100.6479773 MHz
NUC1                 13C
P1                 9.50 usec
PLW1         55.34000015 W
SFO2         400.2316009 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI                32768
SF           100.6378943 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Thermo QEFMS Analysis Report of Compound 10b

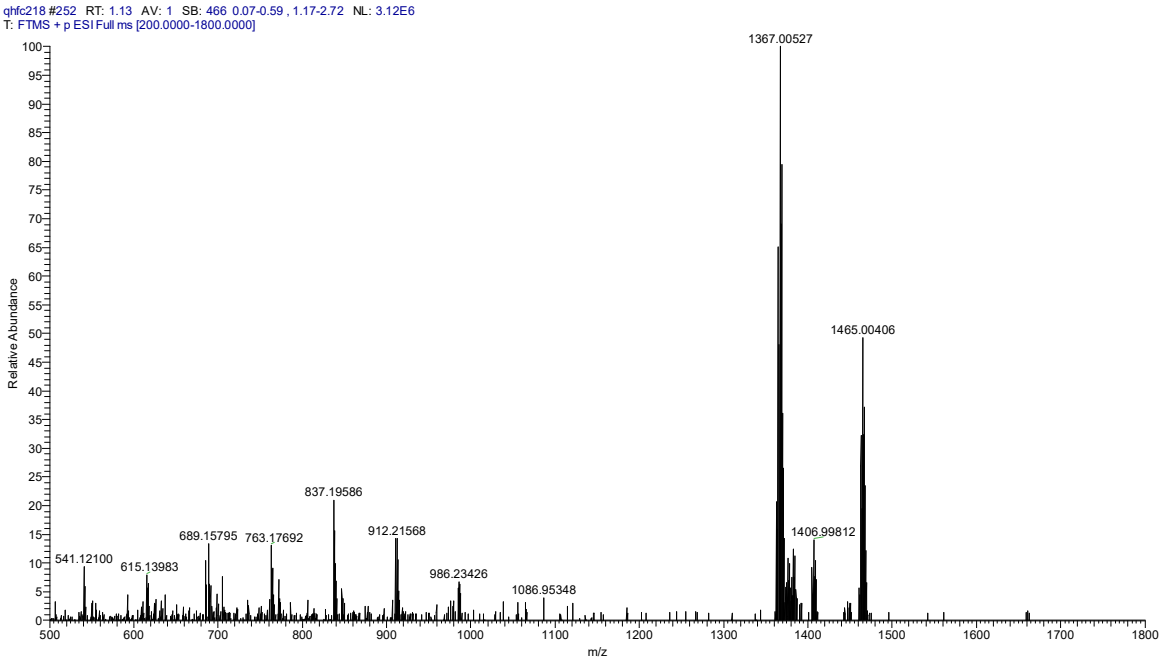
Analysis Info

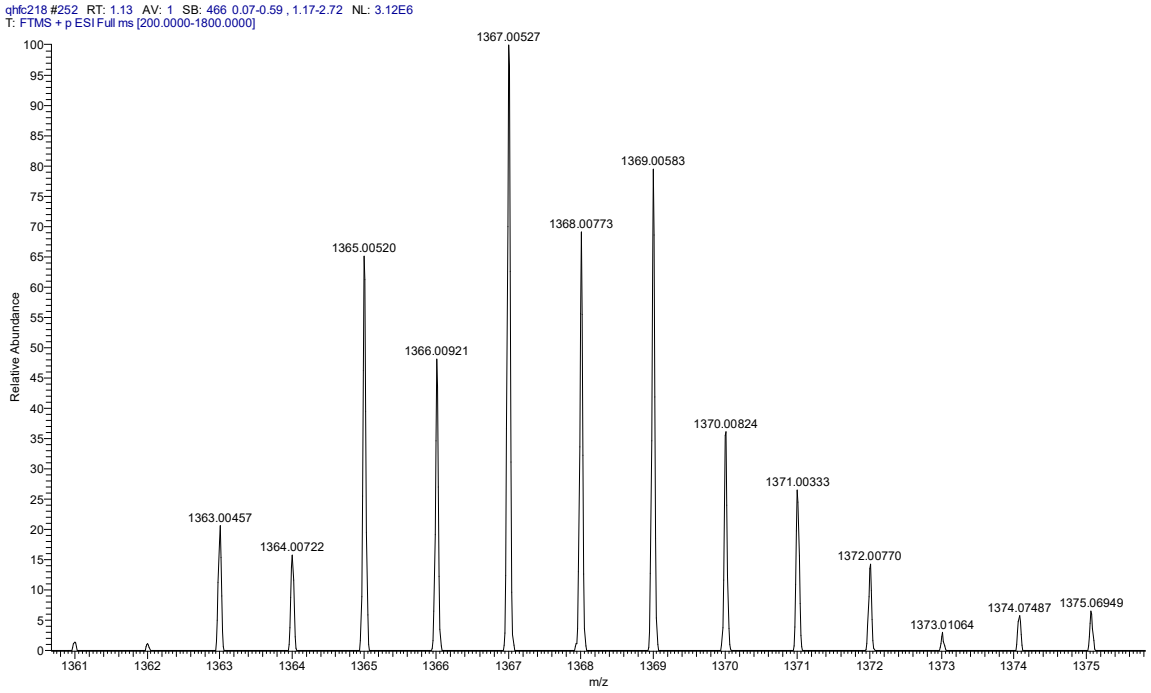
Sample Name :	SXQ-4Br-C2	Reference No.:	Qhfc218
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI pos, 3.5kV, by LC, with sheath gas		

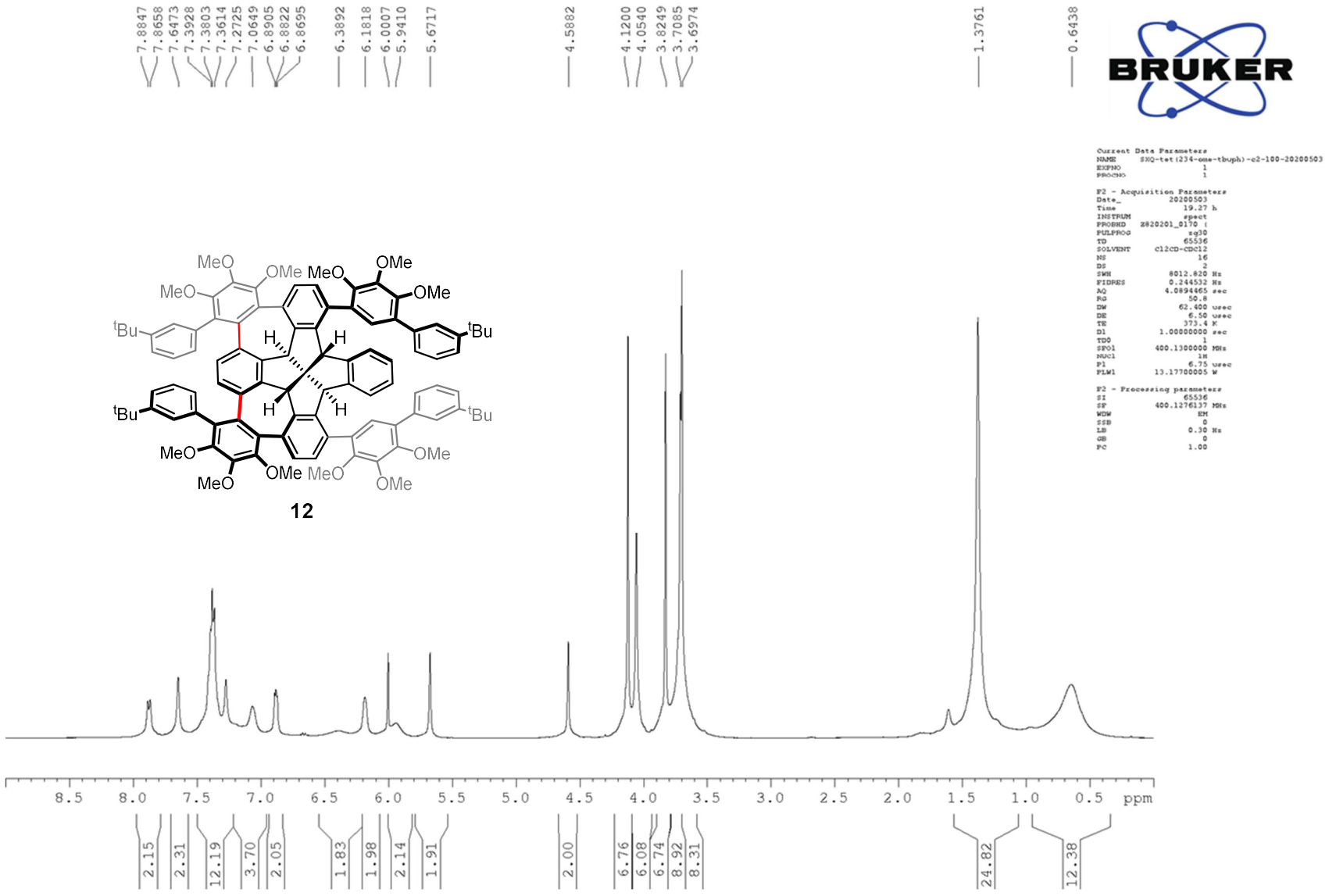
Accurate Mass Measurement

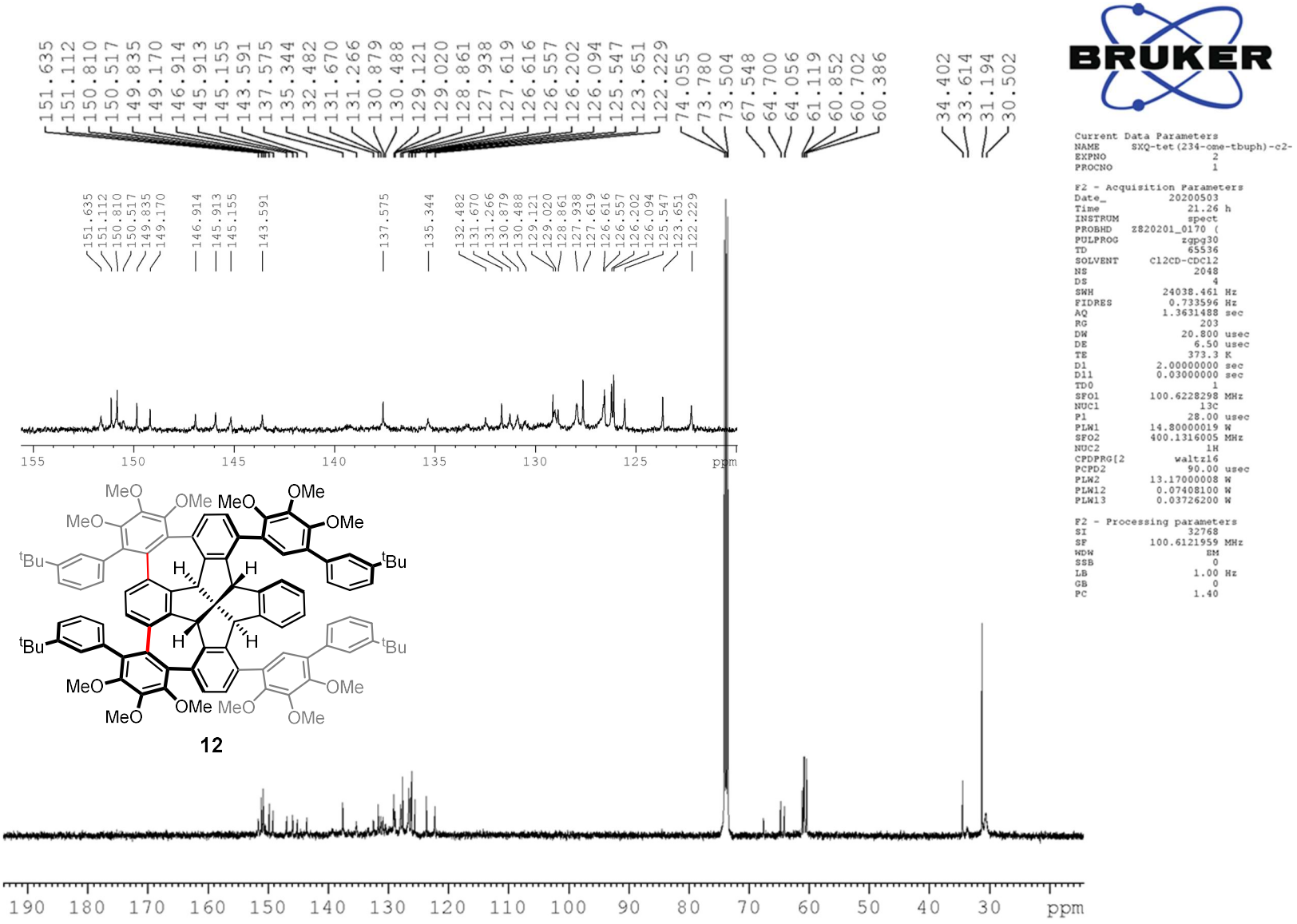
Molecular formula :	$C_{65}H_{52}Br_4O_{12}$
Experimental Mass $[M + Na]^+$:	1363.00457
Theoretical Mass $[M + Na]^+$:	1363.00845
Error (ppm) :	-2.8

D:\Raw data\qhfc218 12/07/17 18:56:38 SXQ-4Br-C2






7.8847
7.8658
7.6473
7.3928
7.3803
7.3614
7.2725
7.0649
6.8905
6.8822
6.8695
6.3892
6.1818
6.0007
5.9410
5.6717
4.5882
4.1200
4.0540
3.8249
3.7085
3.6974
1.3761
0.6438
BRUKER
Current Data Parameters
NAME SXQ-tet(234-ome-tbuph)-c2-100-20200503
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200503
Time 19.27 h
INSTRUM spect
PROBHD Z820201_0170 (
PULPROG zg30
TD 65536
SOLVENT c12CD-CDCl2
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 50.8
DW 62.400 usec
DE 6.50 usec
TE 373.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.1300000 MHz
NUC1 1H
P1 6.75 usec
PLW1 13.17700005 W
F2 - Processing parameters
SI 65536
SF 400.1276137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
OMe
tBu
H
12
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.15
2.31
12.19
3.70
2.05
1.83
1.98
2.14
1.91
2.00
6.76
6.08
6.74
8.92
8.31
24.82
12.38



BRUKER

Current Data Parameters
NAME SXQ-tet(234-ome-tbuph)-c2-
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200503
Time 21.26 h
INSTRUM spect
PROBHD Z820201_0170 (
PULPROG zgpg30
TD 65536
SOLVENT C12CD-CDC12
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 373.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 28.00 usec
PLW1 14.80000019 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.17000008 W
PLW12 0.07408100 W
PLW13 0.03726200 W

F2 - Processing parameters
SI 32768
SF 100.6121959 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

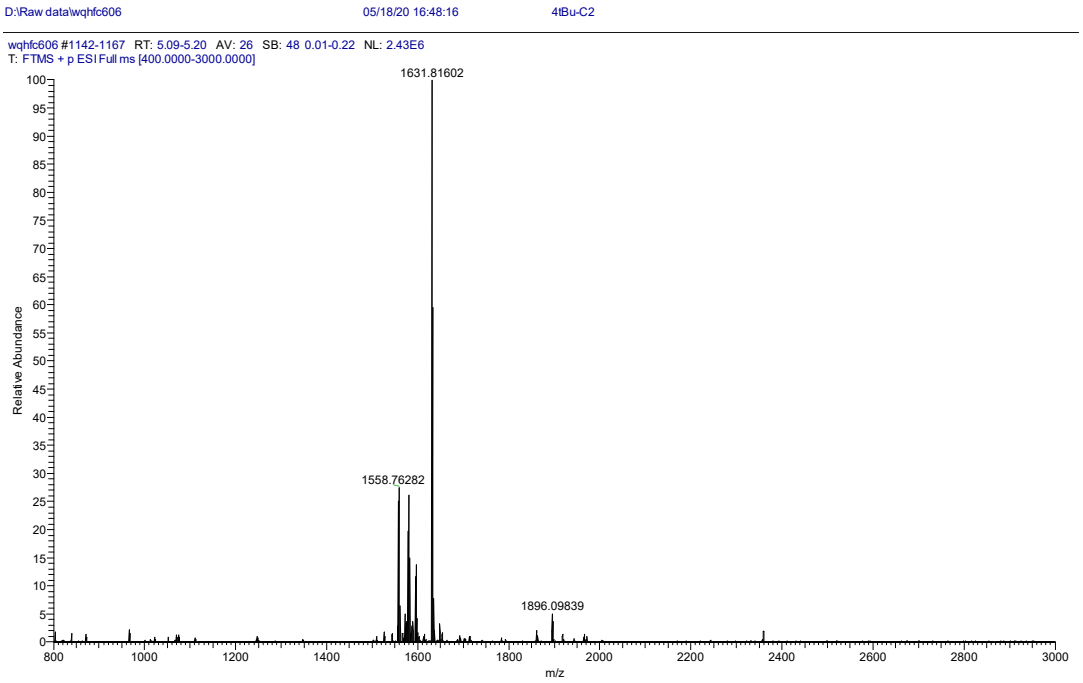
Thermo QEFMS Analysis Report of Compound 12

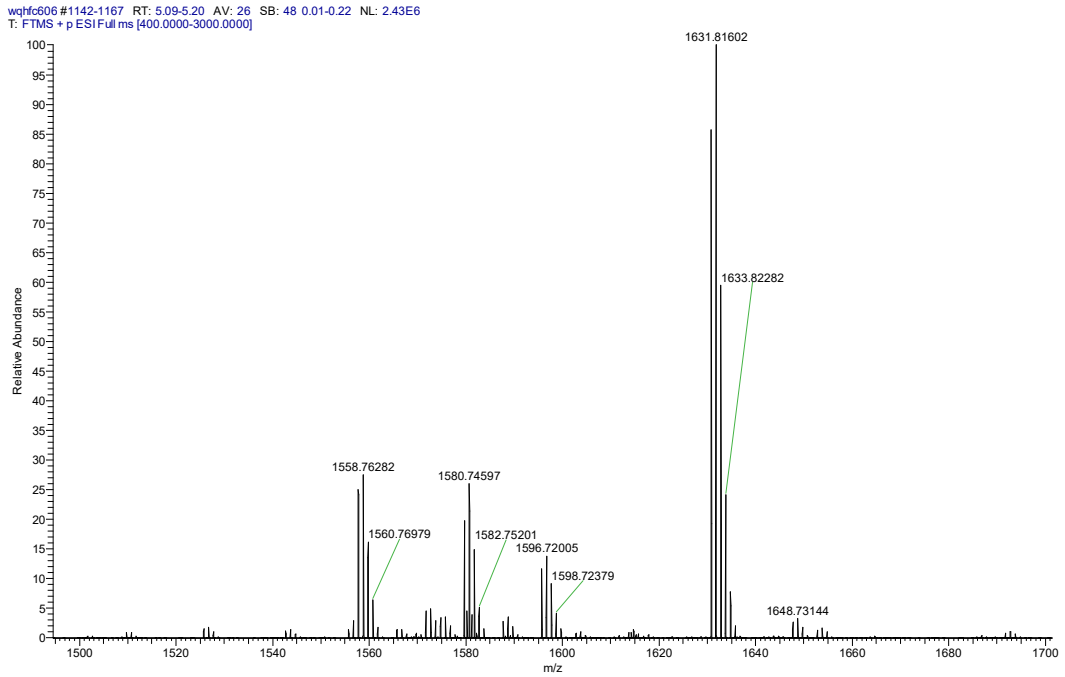
Analysis Info

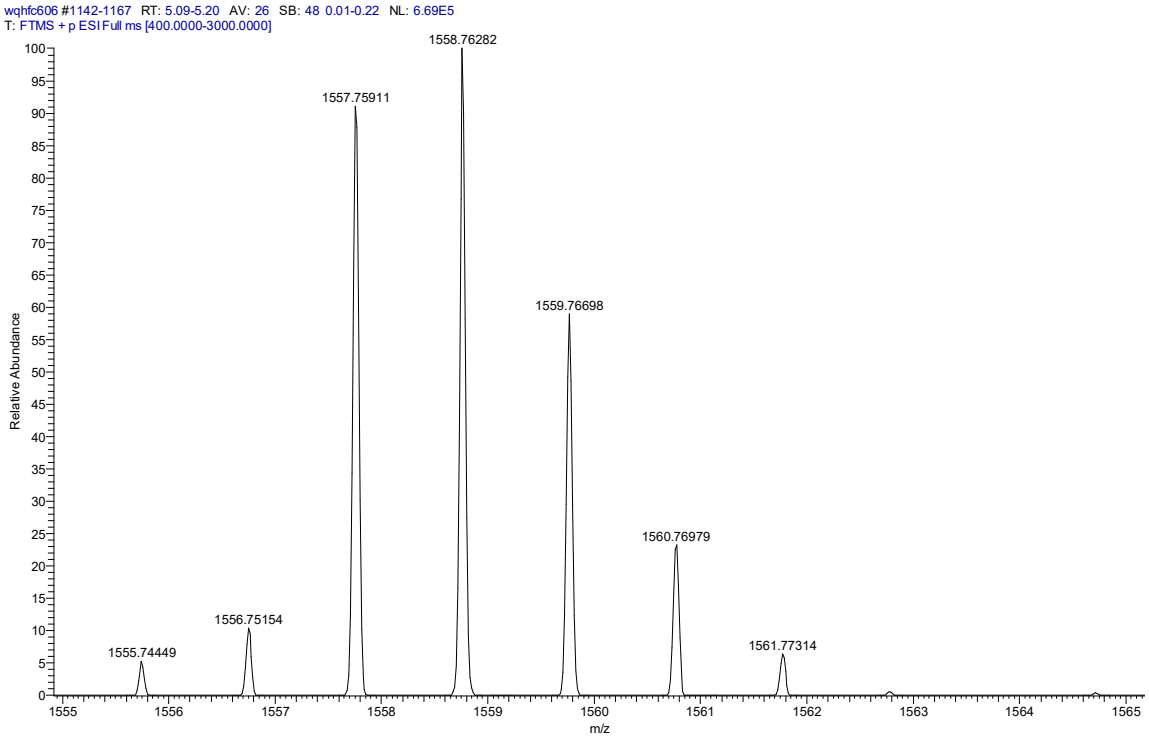
Sample Name :	4tBu-C2	Reference No.:	Wqhfc606
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI, 3.5kV, by infusion, with 0.2% formic acid		

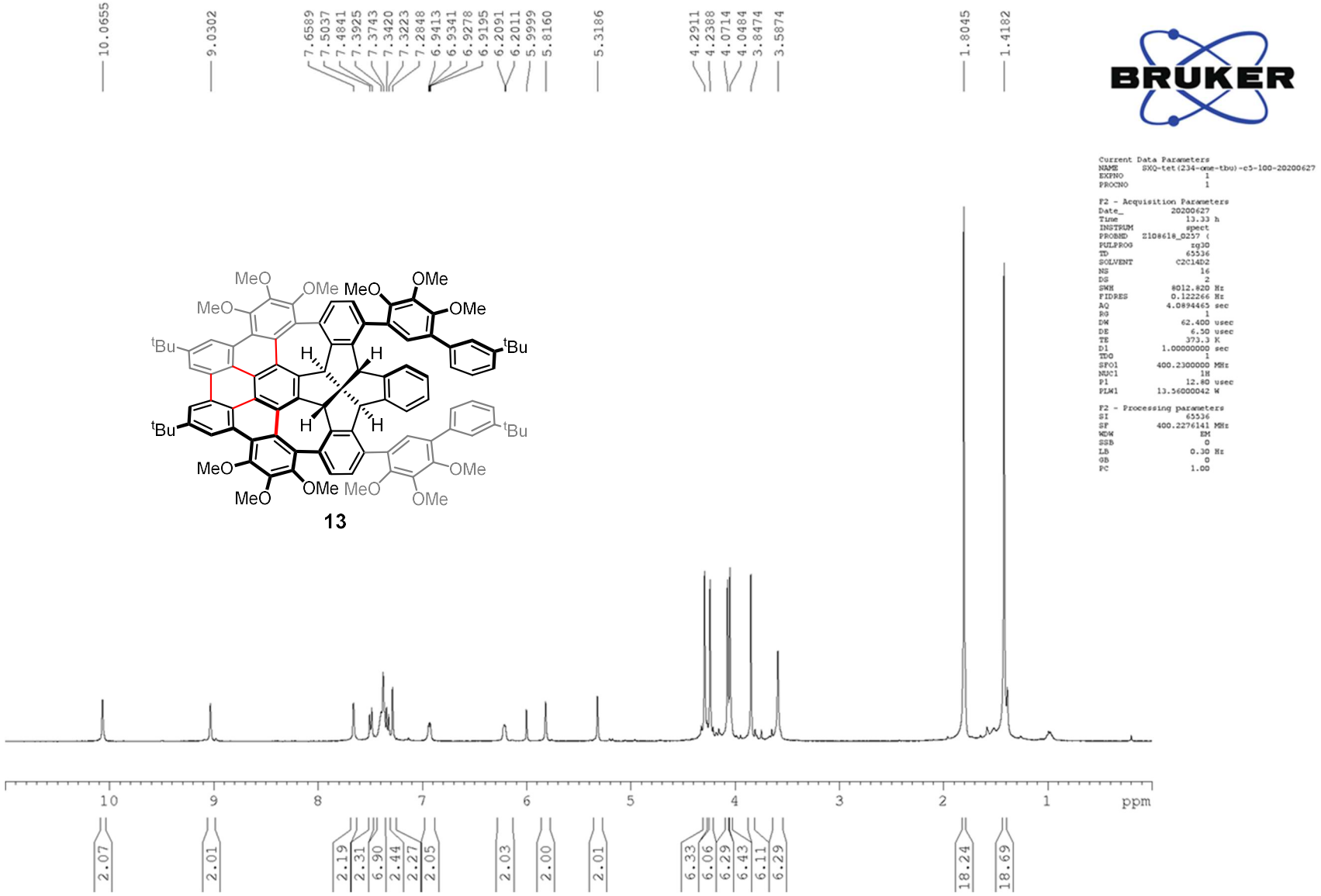
Accurate Mass Measurement

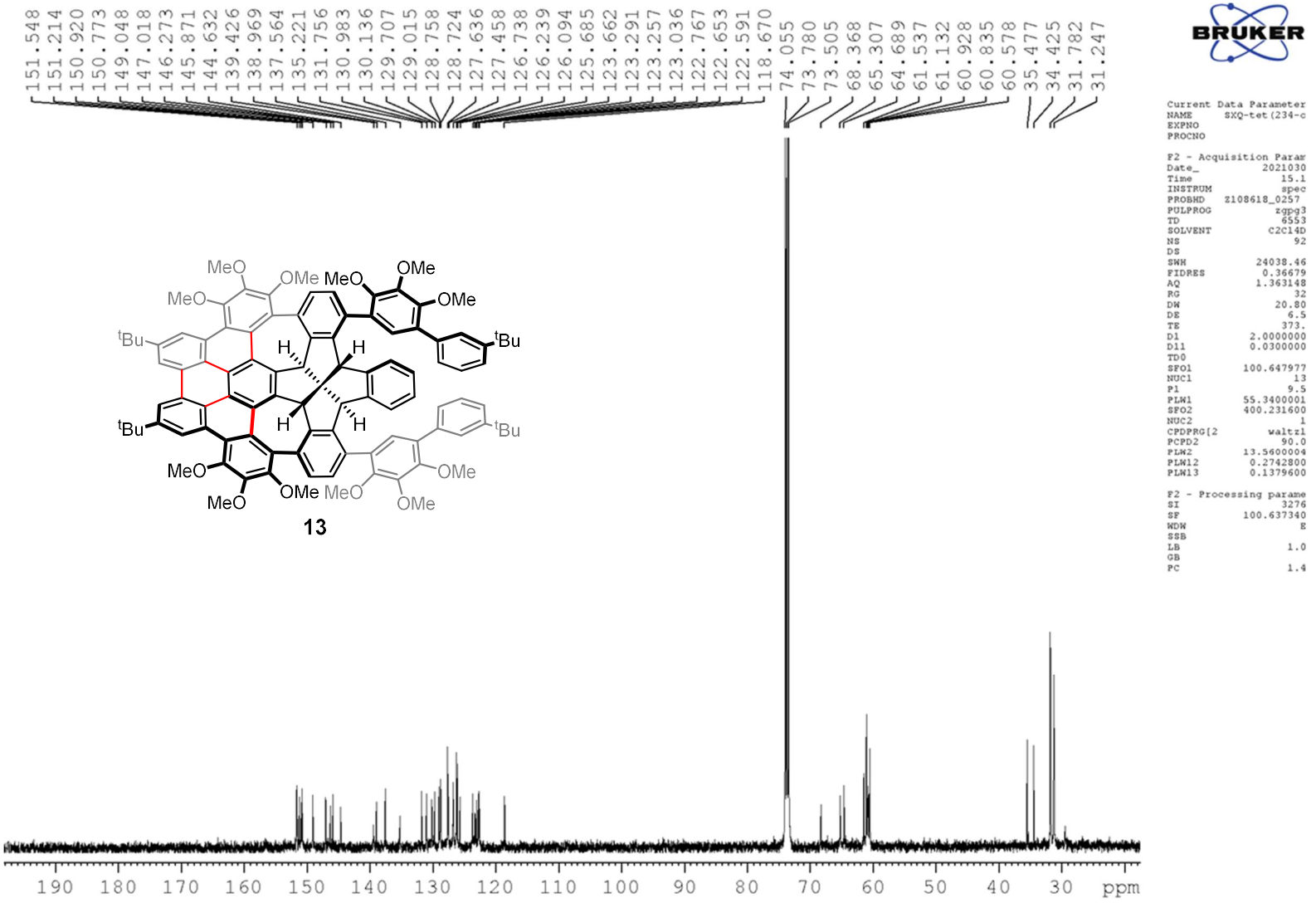
Molecular formula :	$C_{105}H_{104}O_{12}$
Experimental Mass $[M + H]^+$:	1557.75911
Theoretical Mass $[M + H]^+$:	1557.76006
Error (ppm) :	-0.6






wqhfc606 #1142-1167 RT: 5.09-5.20 AV: 26 SB: 48 0.01-0.22 NL: 6.69E5
T: FTMS + p ESI Full ms [400.0000-3000.0000]
1558.76282
1557.75911
1559.76698
1560.76979
1556.75154
1555.74449
1561.77314
Relative Abundance
m/z


10.0655
9.0302
7.6589
7.5037
7.4841
7.3925
7.3743
7.3420
7.3223
7.2848
6.9413
6.9341
6.9278
6.9195
6.2091
6.2011
5.9999
5.8160
5.3186
4.2911
4.2388
4.0714
4.0484
3.8474
3.5874
1.8045
1.4182
BRUKER
Current Data Parameters
NAME SXQ-tet(234-ome-tbu)-c5-100-20200627
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200627
Time 13.33 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT C2C14D2
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 1
DW 62.400 usec
DE 6.50 usec
TE 373.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.2300000 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2276141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
OMe
tBu
H
13
10
9
8
7
6
5
4
3
2
1
ppm
2.07
2.01
2.19
2.31
6.90
2.44
2.27
2.05
2.03
2.00
2.01
6.33
6.06
6.29
6.43
6.11
6.29
18.24
18.69



13

```
Current Data Parameter
NAME      SXQ-tet(234-c
EXPNO
PROCNO

F2 - Acquisition Parar
Date_           2021030
Time              15.1
INSTRUM           spec
PROBHD   Z108618_0257
PULPROG          zgpg3
TD                6553
SOLVENT          C2Cl4D
NS                  92
DS
SWH           24038.46
FIDRES          0.36679
AQ              1.363148
RG                  32
DW                20.80
DE                 6.5
TE                373.
D1           2.0000000
D11          0.0300000
TD0
SFO1         100.647977
NUC1                13
P1                 9.5
PLW1         55.3400001
SFO2         400.231600
NUC2                 1
CPDPRG[2         waltz1
PCPD2              90.0
PLW2         13.5600004
PLW12         0.2742800
PLW13         0.1379600

F2 - Processing parame
SI                3276
SF           100.637340
WDW                  E
SSB
LB                 1.0
GB
PC                 1.4
```

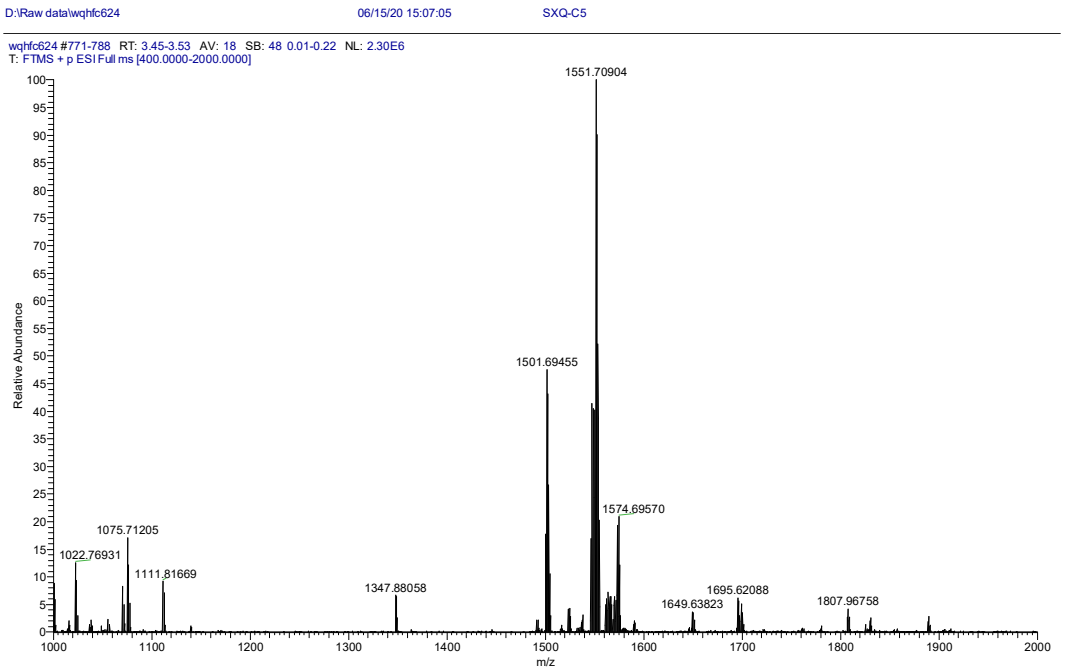
Thermo QEFMS Analysis Report of Compound 13

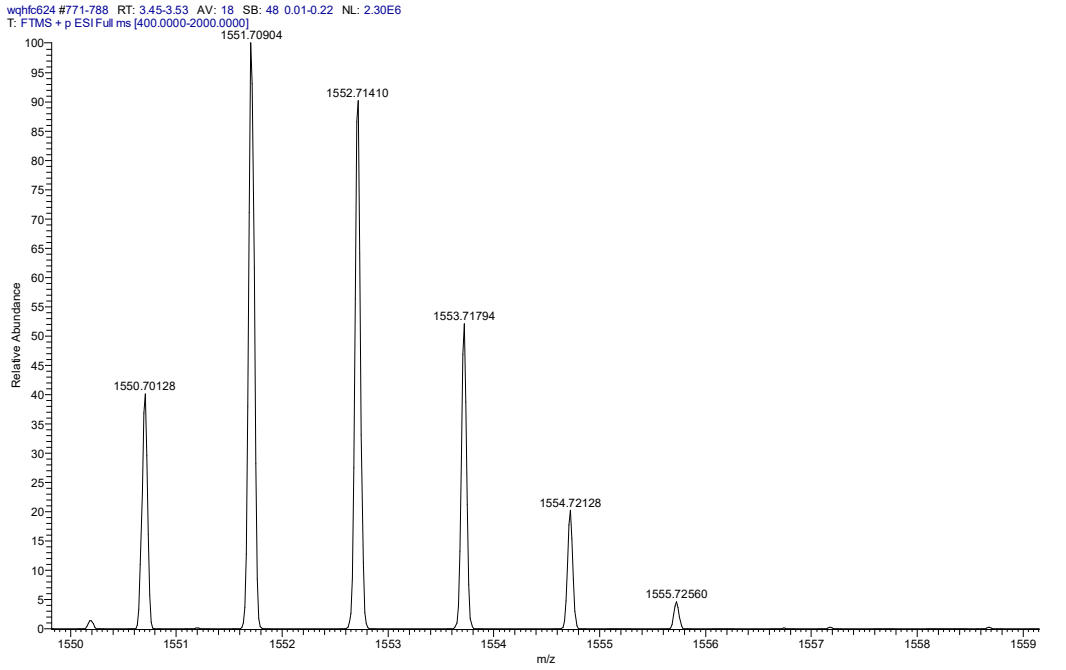
Analysis Info

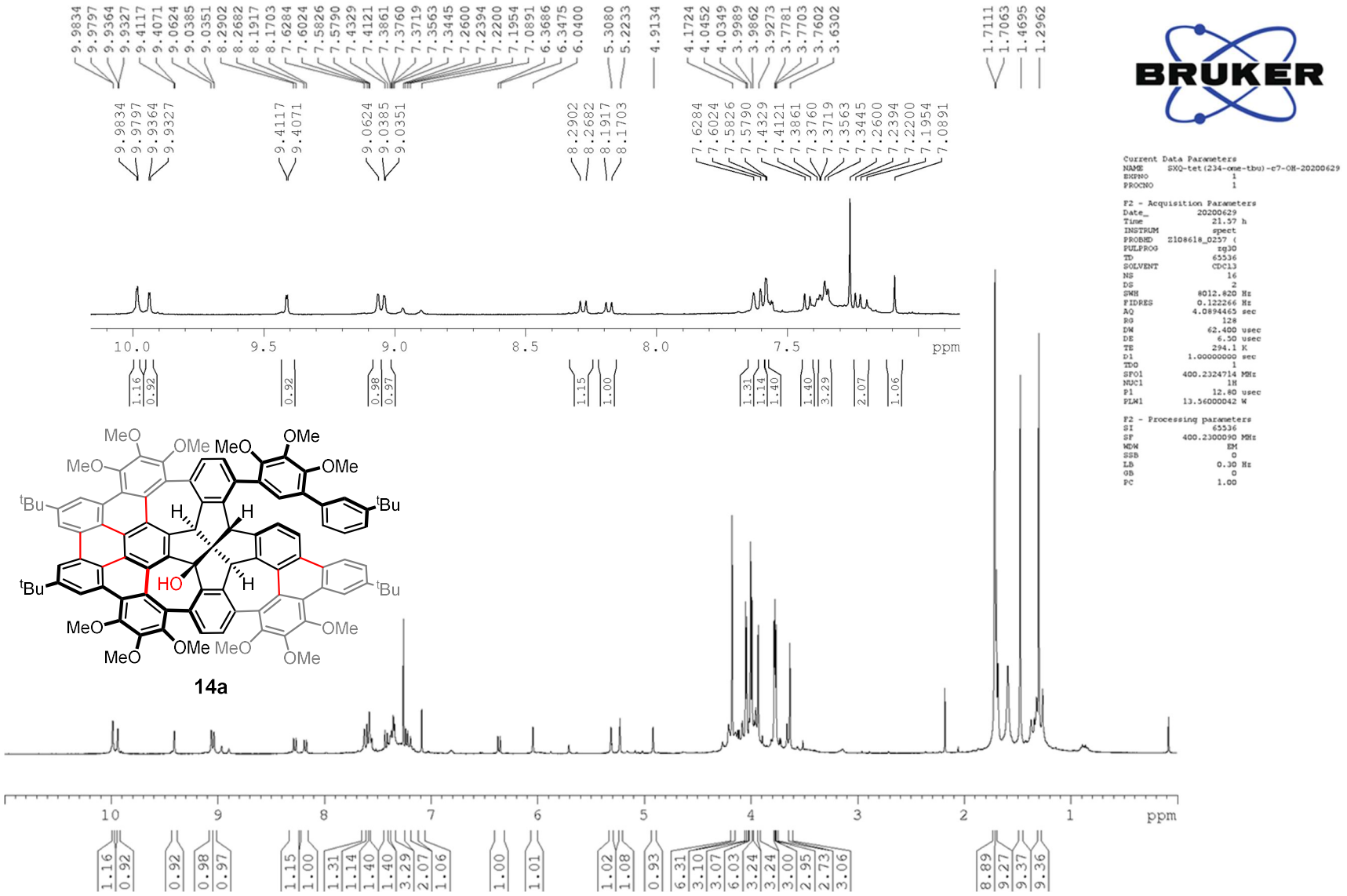
Sample Name :	SXQ-C5	Reference No.:	Wqhfc624
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI, 3.5kV, by infusion, with 0.2% formic acid		

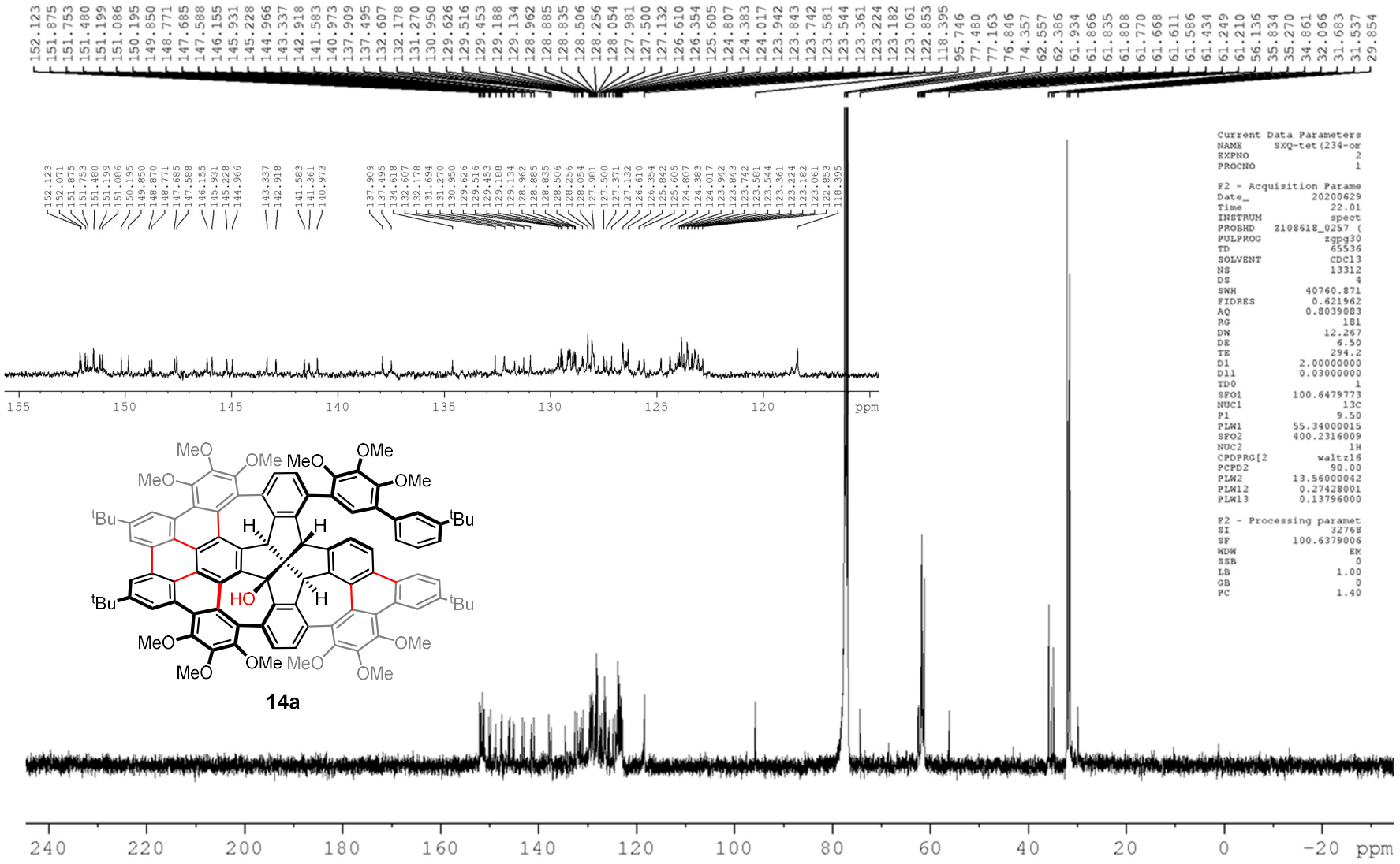
Accurate Mass Measurement

Molecular formula :	$C_{105}H_{98}O_{12}$
Experimental Mass $[M + H]^+$:	1551.70904
Theoretical Mass $[M + H]^+$:	1551.71311
Error (ppm) :	-3.5






14a


Current Data Parameters
NAME SXQ-tet(234-or
EXPNO 2
PROCNO 1
F2 - Acquisition Parame
Date_ 20200629
Time 22.01
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 13312
DS 4
SWH 40760.871
FIDRES 0.621962
AQ 0.8039083
RG 181
DW 12.267
DE 6.50
TE 294.2
D1 2.00000000
D11 0.03000000
TD0 1
SFO1 100.6479773
NUC1 13C
P1 9.50
PLW1 55.34000015
SFO2 400.2316009
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00
PLW2 13.56000042
PLW12 0.27428001
PLW13 0.13796000
F2 - Processing paramet
SI 32768
SF 100.6379006
WDW EM
SSB 0
LB 1.00
GB 0
PC 1.40
ppm
MeO
OMe
tBu
H
HO
14a

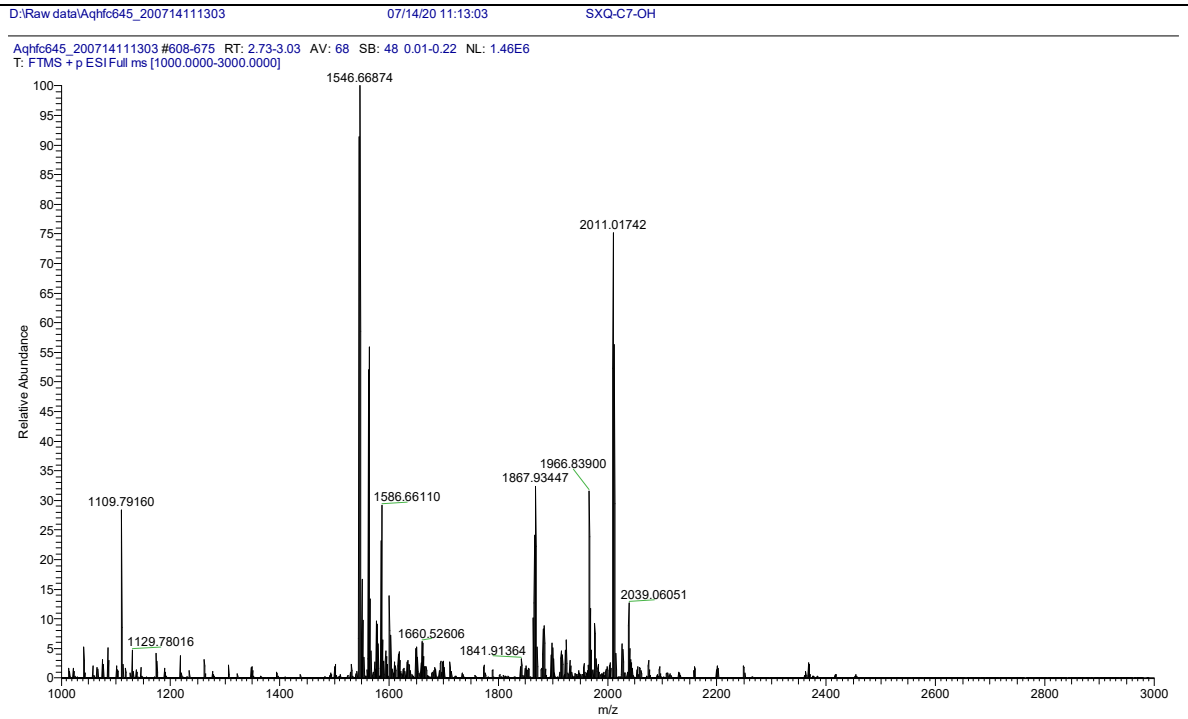
Thermo QEFMS Analysis Report of Compound 14a

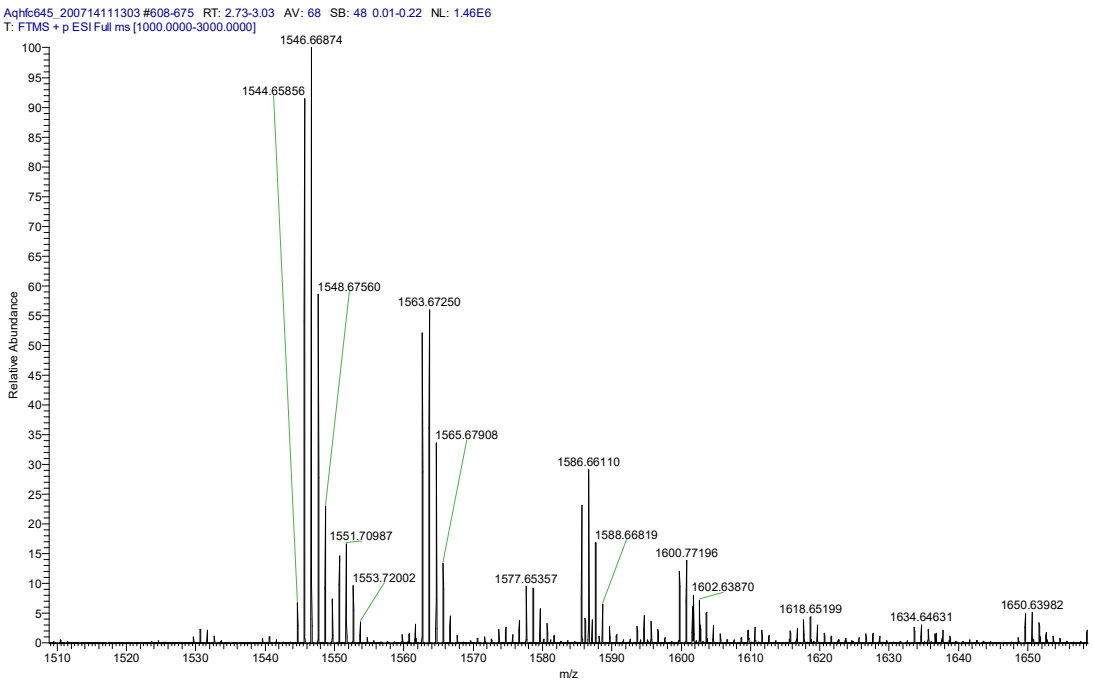
Analysis Info

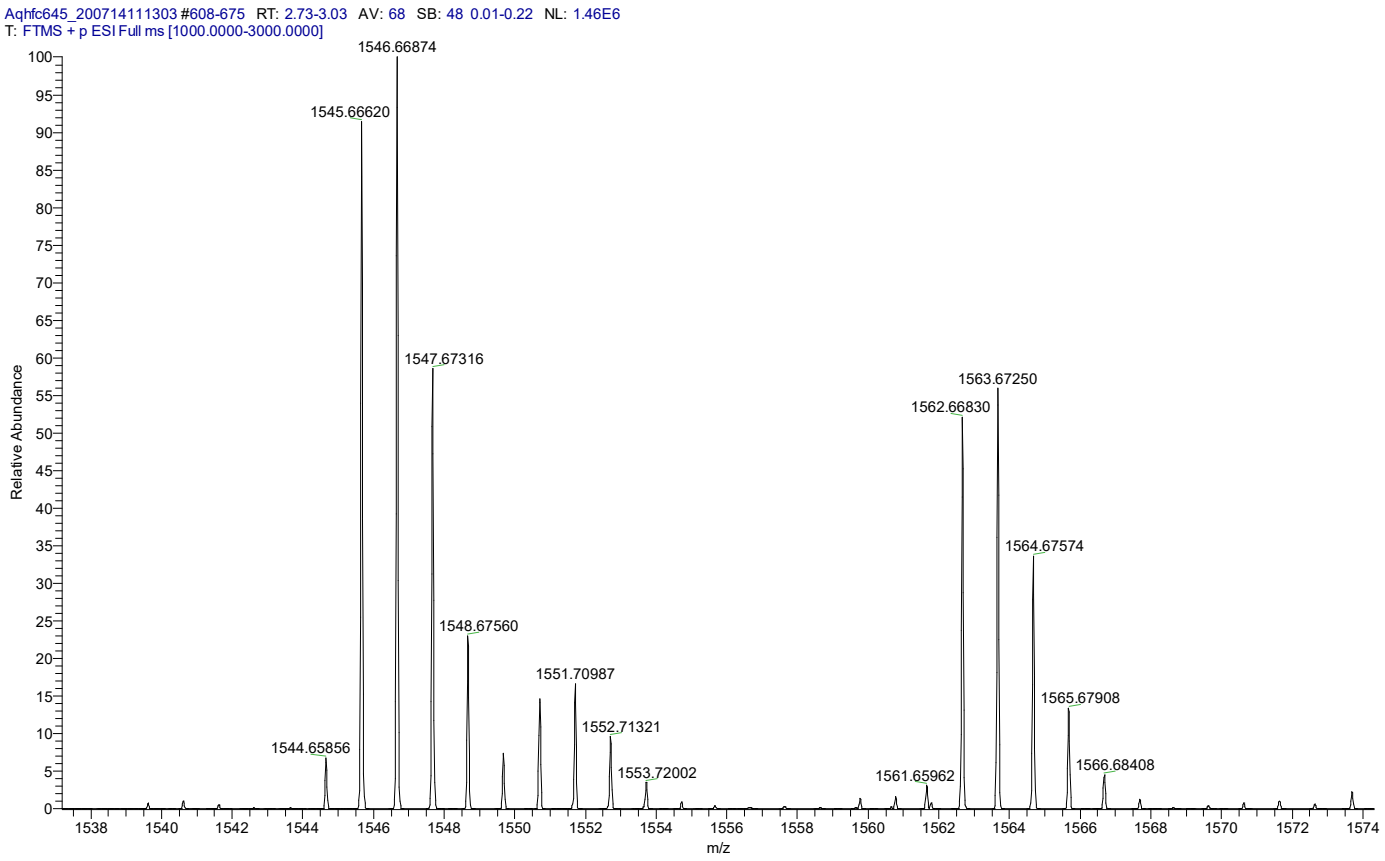
Sample Name :	SXQ-C7-OH	Reference No.:	Aqhfc645
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI, by infusion, with sheath gas		

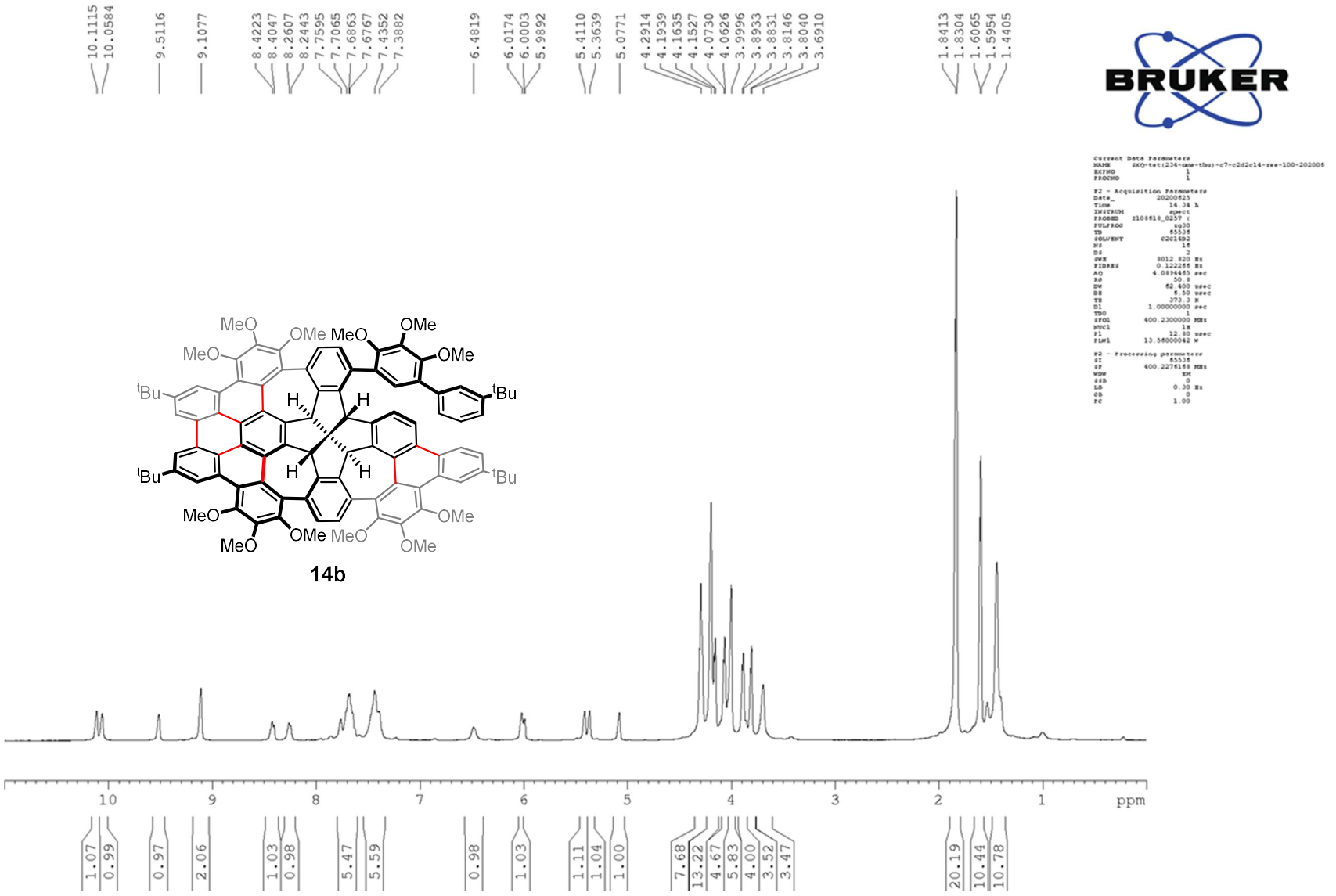
Accurate Mass Measurement

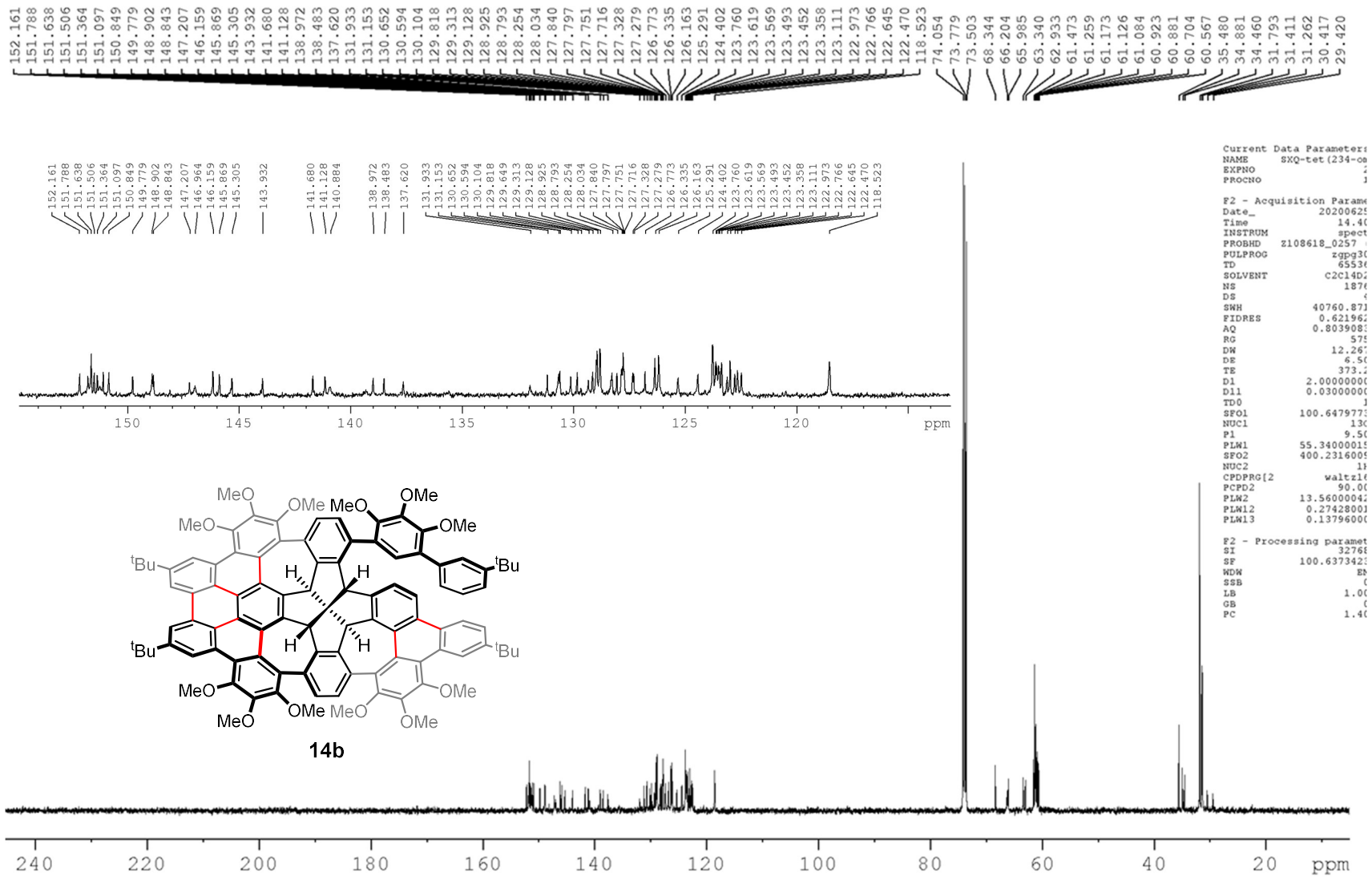
Molecular formula :	$C_{105}H_{94}O_{13}$
Experimental Mass $[M]^{+\bullet}$, $[M - H_2O + H]^+$:	1562.66830, 1545.66620
Theoretical Mass $[M]^{+\bullet}$, $[M - H_2O + H]^+$:	1562.66889, 1545.66615
Error (ppm) :	-0.4, 0.0






Aqhfc645_200714111303 #608-675 RT: 2.73-3.03 AV: 68 SB: 48 0.01-0.22 NL: 1.46E6
T: FTMS + p ESI Full ms [1000.0000-3000.0000]
1546.66874
1545.66620
1547.67316
1563.67250
1562.66830
1564.67574
1548.67560
1551.70987
1565.67908
1552.71321
1544.65856
1553.72002
1566.68408
1561.65962
Relative Abundance
m/z


10.1115
10.0584
9.5116
9.1077
8.4223
8.4047
8.2607
8.2443
7.7595
7.7065
7.6863
7.6767
7.4352
7.3882
6.4819
6.0174
6.0003
5.9892
5.4110
5.3639
5.0771
4.2914
4.1939
4.1635
4.1527
4.0730
4.0626
3.9996
3.8933
3.8831
3.8146
3.8040
3.6910
1.8413
1.8304
1.6065
1.5954
1.4405
BRUKER
MeO
OMe
tBu
H
14b
10
9
8
7
6
5
4
3
2
1
ppm
1.07
0.99
0.97
2.06
1.03
0.98
5.47
5.59
0.98
1.03
1.11
1.04
1.00
7.68
13.22
4.67
5.83
4.00
3.52
3.47
20.19
10.44
10.78


14b

Thermo QEFMS Analysis Report of Compound 14b

Analysis Info

Sample Name :	SXQ-tbu-C3	Reference No.:	Wqhfc591
Instrument :	Q Exactive Focus Orbitrap		
Source :	HESI II	Polarity :	Positive
Comment :	ESI, 3.5kV, by infusion, with 0.1% formic acid		

Accurate Mass Measurement

Molecular formula :	$C_{105}H_{94}O_{12}$
Experimental Mass $[M]^{+\bullet}$:	1546.67292
Theoretical Mass $[M]^{+\bullet}$:	1546.67398
Error (ppm) :	-0.7