

## **Supporting Information**

### **Synthesis and Structure of Corona[6](het)arenes Containing Mixed Bridge Units**

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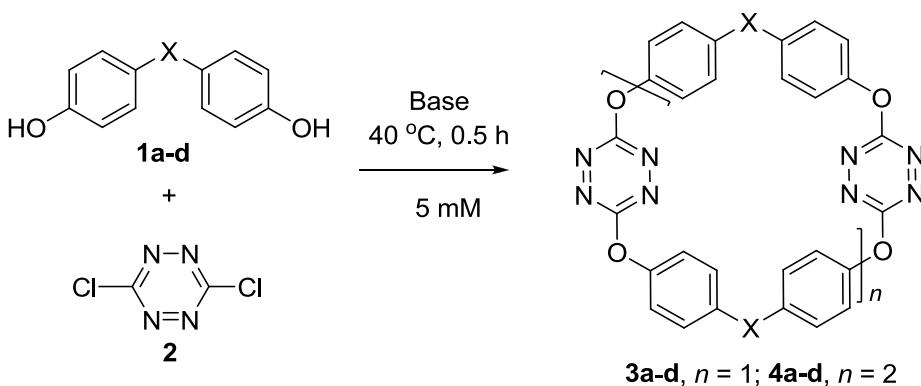
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## 1. General Information

All commercially available reagents were used as received. TLC analysis was performed on pre-coated, glass-backed silica gel plates and visualized with UV light. Flash column chromatography was performed on silica gel (100-200). Anhydrous acetonitrile and dichloromethane was dried by 4 Å molecular sieve.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded using 400 MHz spectrometers (JEOL ECX-400). Chemical shifts are reported in ppm versus tetramethylsilane with either tetramethylsilane or the residual solvent resonance used as an internal standard. Abbreviations are used in the description of NMR data as follows: chemical shift ( $\delta$ , ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constant ( $J$ , Hz). Infrared spectra were recorded using a FT-IR spectrum (PerkinElmer Spectrum 100) with KBr discs in the 4000-400  $\text{cm}^{-1}$  region. UV-vis spectra were recorded using a UV-vis spectrophotometer (PerkinElmer Lambda 35). Mass and elemental analysis was performed at the Institute of Chemistry, CAS. Melting points are uncorrected.

## 2. Experimental Procedures and Characterization of Products

### 2.1. General Procedure for the Synthesis of **3a-3d** and **4a-d**

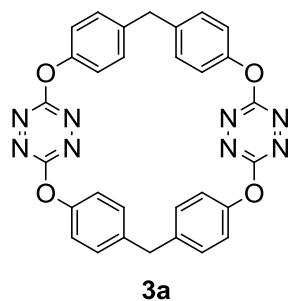


**Scheme S1** Synthesis of corona[4]arene[2]tetrazines **3a-d** and **4a-d**

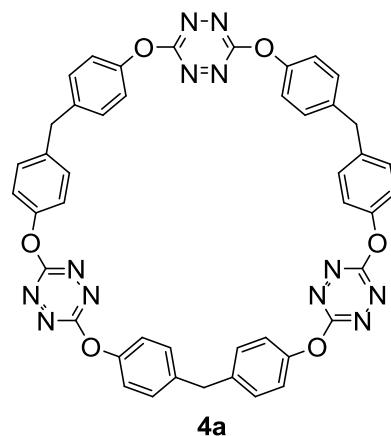
To a solution of  $\text{Et}_3\text{N}$  or DIPEA (2.1 mmol) in acetonitrile (150 mL) which was pre-heated to 40 °C was added dropwise a solution of 1,4-dihydroxybenzene derivatives **1a-1d** (1 mmol) and 3,6-dichlorotetrazine **2** (1 mmol) in acetonitrile (50 mL) during 30 min. The mixture was then cooled gradually to room temperature,

water (300 mL) was added. The resulting mixture was extracted with ethyl acetate ( $4 \times 100$  mL). The combined organic phase was washed with brine ( $3 \times 300$  mL), and dried over anhydrous  $\text{MgSO}_4$ . After filtration and removal of solvent, the residue was chromatographed on a silica gel column with a mixture of petroleum ether and ethyl acetate as the mobile phase to give pure product **3a-d** and **4a-d**. X-ray quality single crystals **3a-d** and **4a-d** were obtained by diffusing hexane into the solution of **3a-d** and **4a-d** in chloroform or acetone.

Characterization data of all products are listed below.

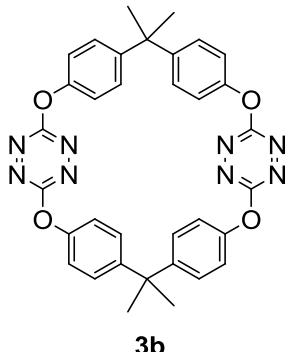


**3a** (150 mg, yield 54%): red solid, m.p.> 300 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ , TMS):  $\delta_{\text{H}}$  7.43(d,  $J=8.4$  Hz, 8H), 7.17(d,  $J=8.4$  Hz, 8H), 3.92(s, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ , TMS):  $\delta_{\text{C}}$  167.0, 150.6, 140.0, 129.9, 121.1; IR (KBr)  $\nu$ : 1508, 1478, 1391, 1332, 1202, 1167, 1066, 1020, 960, 895, 834, 783, 575, 493  $\text{cm}^{-1}$ ; HRMS (APCI) Calcd. for  $\text{C}_{30}\text{H}_{21}\text{N}_8\text{O}_4$   $[\text{M}+\text{H}]^+$  557.1680. Found: 557.1678  $[\text{M}+\text{H}]^+$ .  $R_f = 0.35$  (PE:DCM = 1:3).

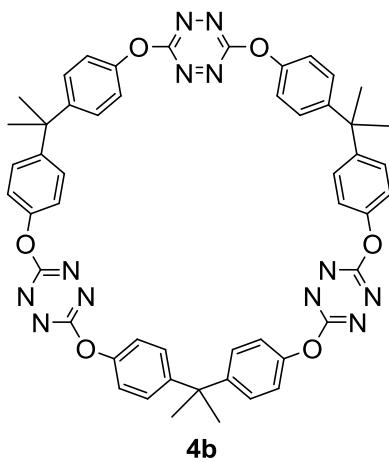


**4a** (14 mg, yield 5%): red solid, m.p.> 300 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ , TMS):  $\delta_{\text{H}}$  7.32(d,  $J=8.8$  Hz, 12H), 7.26(d,  $J=8.8$  Hz, 12H), 4.02(s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ , TMS):  $\delta_{\text{C}}$  166.8, 151.1, 139.1, 130.1, 120.6; IR (KBr)  $\nu$ : 1506, 1473, 1382,

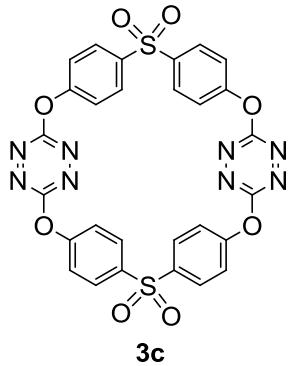
1196, 1165, 1063, 1018, 958, 897, 832, 565, 494  $\text{cm}^{-1}$ ; HRMS (APCI) Calcd. for  $\text{C}_{45}\text{H}_{31}\text{N}_{12}\text{O}_6$   $[\text{M}+\text{H}]^+$  835.2484. Found: 835.2477  $[\text{M}+\text{H}]^+$ .  $R_f = 0.35$  (DCM).



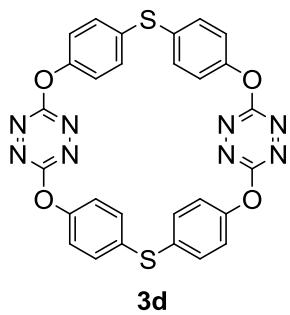
**3b** (224 mg, yield 73%): red solid, m.p.> 300 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ , TMS):  $\delta_{\text{H}}$  7.34(d,  $J= 8.0$  Hz, 8H), 7.21(d,  $J= 8.0$  Hz, 8H), 1.71(s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ , TMS):  $\delta_{\text{C}}$  166.7, 150.1, 147.6, 127.6, 119.9, 41.4, 29.3; IR (KBr)  $\nu$ : 2976, 1506, 1470, 1392, 1332, 1201, 1168, 1066, 1019, 943, 987, 845, 586, 557  $\text{cm}^{-1}$ ; HRMS (APCI) Calcd. for  $\text{C}_{34}\text{H}_{29}\text{N}_8\text{O}_4$   $[\text{M}+\text{H}]^+$  613.2306. Found: 613.2302  $[\text{M}+\text{H}]^+$ .  $R_f = 0.60$  (PE:DCM = 1:3).



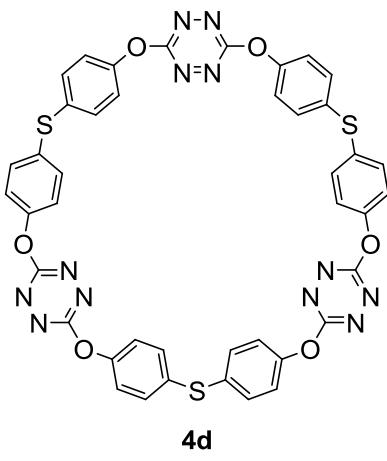
**4b** (40 mg, yield 13%): red solid, m.p.> 300 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ , TMS):  $\delta_{\text{H}}$  7.30(d,  $J=8.8$  Hz, 12H), 7.25(d,  $J=8.8$  Hz, 12H), 1.68(s, 18H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ , TMS):  $\delta_{\text{C}}$  166.8, 150.5, 148.0, 128.1, 120.4, 42.3, 30.5. IR (KBr)  $\nu$ : 2967, 1508, 1471, 1380, 1206, 1172, 1063, 1015, 951, 893, 847  $\text{cm}^{-1}$ ; MS (APCI),  $m/z$ (%), 919.6 $[\text{M}+\text{H}]^+$  Anal. Calcd. for  $\text{C}_{51}\text{H}_{42}\text{N}_{12}\text{O}_6$ : C, 66.66; N, 18.29; H, 4.61. Found: C, 66.37; N, 18.27; H, 4.73.  $R_f = 0.50$  (DCM).



**3c** (194 mg, yield 59%): red solid, m.p.> 300 °C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>, TMS): δ<sub>H</sub> 8.15(d, *J*=8.8 Hz, 8H), 7.57(d, *J*=8.8 Hz, 8H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, TMS): δ<sub>C</sub> 166.9, 156.0, 138.9, 130.1, 122.6. IR (KBr) *v*: 1591, 1492, 1379, 1328, 1297, 1211, 1155, 1109, 1065, 1017, 953, 897, 708, 579 cm<sup>-1</sup>. MS (ESI), *m/z* (%), 673.19[M+OH]<sup>-</sup>(100); Anal. Calcd. for C<sub>28</sub>H<sub>16</sub>N<sub>8</sub>O<sub>8</sub>S<sub>2</sub>: C, 51.22; N, 17.07; H, 2.46. Found: C, 51.15; N, 17.09; H, 2.59. R<sub>f</sub> = 0.30 (DCM:EA = 20:1).



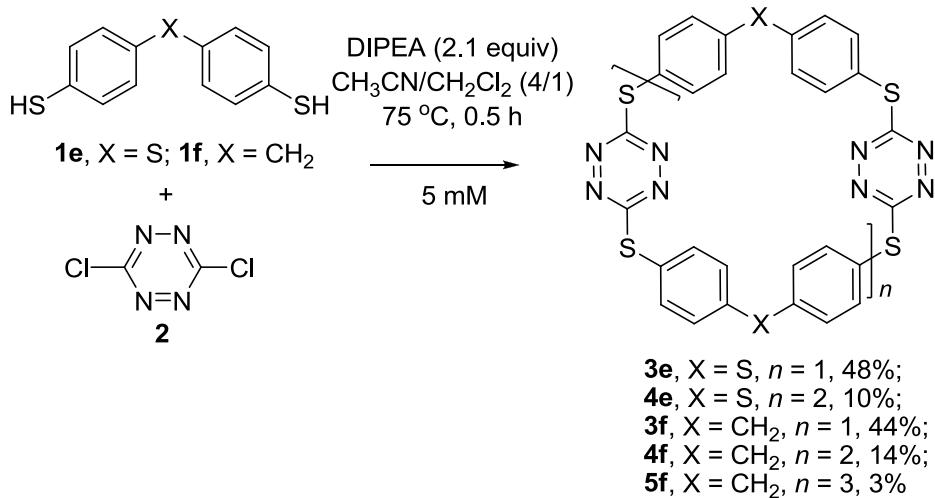
**3d** (219 mg, yield 74%): red solid, m.p.> 300 °C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>, TMS): δ<sub>H</sub> 7.55(d, *J*=8.8 Hz, 8H), 7.36(d, *J*=8.8 Hz, 8H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, TMS): δ<sub>C</sub> 166.9, 154.2, 148.2, 122.4, 119.7; IR (KBr) *v*: 1477, 1388, 1333, 1199, 1163, 1066, 1016, 958, 895, 866, 841, 565 cm<sup>-1</sup>; HRMS (APCI) Calcd. for C<sub>28</sub>H<sub>17</sub>N<sub>8</sub>O<sub>4</sub>S<sub>2</sub> 593.0809 [M+H]<sup>+</sup>, Found 593.0804 [M+H]<sup>+</sup>. R<sub>f</sub> = 0.30 (PE:DCM = 1:5).



**4d**

**4d** (36 mg, yield 12%): red solid, m.p.> 300 °C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>, TMS): δ<sub>H</sub> 7.45(d, *J*=8.8 Hz, 12H), 7.38(d, *J*=8.8 Hz, 12H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, TMS): δ<sub>C</sub> 166.8, 152.0, 132.5, 132.4, 122.1; IR (KBr) *v*: 1488, 1379, 1199, 1161, 1064, 1013, 951, 837, 562 cm<sup>-1</sup>; HRMS (APCI) Calcd. for C<sub>42</sub>H<sub>25</sub>N<sub>12</sub>O<sub>6</sub>S<sub>3</sub> 889.1177 [M+H]<sup>+</sup>, Found: 889.1185 [M+H]<sup>+</sup>. Rf = 0.30 (DCM).

## 2.2. General Procedure for the Synthesis of **3e**, **3f**, **4e**, **4f** and **5f**

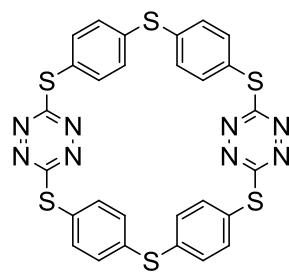


**Scheme S2** Synthesis of **3e**, **3f**, **4e**, **4f** and **5f**

To a solution of DIPEA (2.1 mmol) in acetonitrile (150 mL) which was pre-heated to 75 °C was added dropwise a solution of 1,4-benzenedithiol derivatives **1e** or **1f** (1 mmol) and 3,6-dichlorotetrazine **2** (1 mmol) in acetonitrile (10 mL) and dichloromethane (40 mL) during 30 min. The mixture was then cooled gradually to room temperature, and hydrochloric acid solution (0.1 M, 150 mL) was added. The resulting mixture was extracted with dichloromethane (4 × 150 mL). The combined organic phase was washed with brine (3 × 250 mL), and dried over anhydrous MgSO<sub>4</sub>.

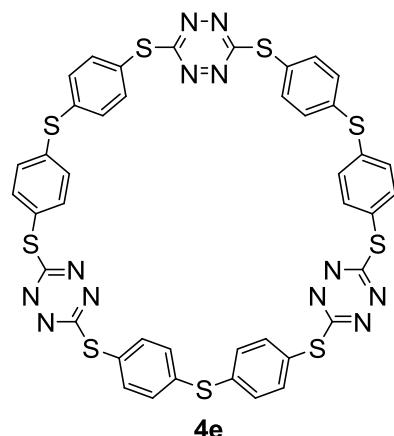
After filtration, silica gel (100-200 mesh) was added and then the solvent was removed. The residue was chromatographed on a silica gel column with a mixture of petroleum ether and dichloromethane as the mobile phase to give pure products **3e**, **3f**, **4e**, **4f** and **5f**. X-ray quality single crystals **3e**, **3f**, **4f** and **5f** were obtained by diffusing hexane into the solution of **3e**, **3f**, **4f** and **5f** in chloroform or dichloromethane.

Characterization data of all products are listed below.



**3e**

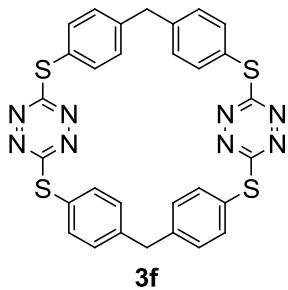
**3e** (158 mg, yield 48%): red solid, m.p. 227 °C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>, TMS): δ<sub>H</sub> 7.60 (d, *J* = 8.3 Hz, 8H), 7.44 (d, *J* = 8.7 Hz, 8H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, TMS): δ<sub>C</sub> 173.3, 136.8, 135.0, 132.0, 125.2; IR (KBr, v/cm<sup>-1</sup>) 1570, 1475, 1388, 1234, 1182, 1099, 1048, 1012, 879, 813 cm<sup>-1</sup>; MS (APCI) *m/z* 657 [M+H]<sup>+</sup> Anal. Calcd. for C<sub>28</sub>H<sub>16</sub>N<sub>8</sub>S<sub>6</sub>: C, 51.20; H, 2.46; N, 17.06; Found: C, 51.00; H, 2.52; N, 17.03. R<sub>f</sub> = 0.45 (PE:DCM = 1:1).



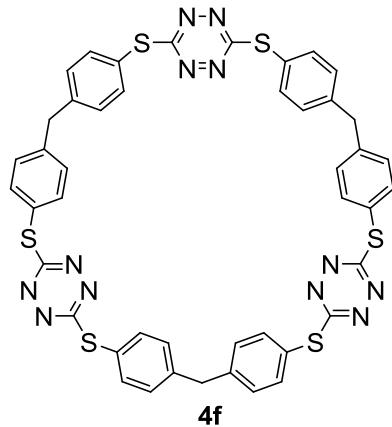
**4e**

**4e** (33 mg, yield 10%): red solid, m.p. 233 °C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>, TMS): δ<sub>H</sub> 7.69(d, *J* = 8.2 Hz, 12H), 7.46 (d, *J* = 8.2 Hz, 12H); <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>, TMS): δ<sub>C</sub> 172.8, 136.8, 136.0, 131.6, 125.2; IR (KBr, v/cm<sup>-1</sup>) 1571, 1475, 1389, 1236, 1095, 1048, 1012, 878, 815, 743 cm<sup>-1</sup>; MS (APCI), *m/z* 985 [M+H]<sup>+</sup>; Anal. Calcd. for C<sub>42</sub>H<sub>24</sub>N<sub>12</sub>S<sub>9</sub>: C, 51.20; H, 2.46; N, 17.06; H, 4.61. Found: C, 50.93; H, 2.48;

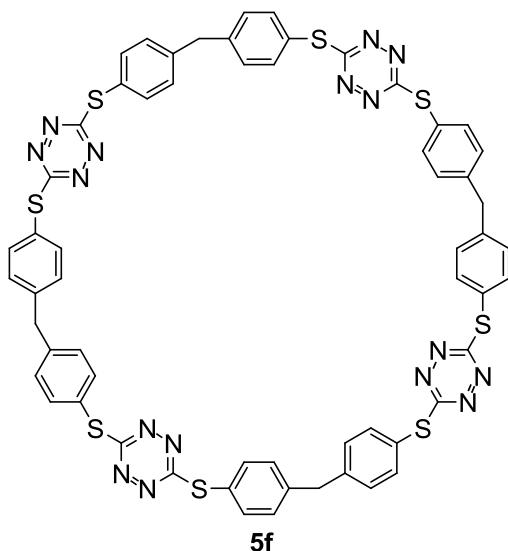
N, 17.03. R<sub>f</sub> = 0.40 (PE:DCM = 1:3).



**3f** (137 mg, yield 44%): red solid, m.p. 227 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS): δ<sub>H</sub> 7.53 (d, *J* = 8.2 Hz, 8H), 7.28 (d, *J* = 8.2 Hz, 8H), 3.93 (s, 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, TMS): δ<sub>C</sub> 173.7, 142.0, 135.0, 130.2, 123.6, 41.8; IR (KBr, ν/cm<sup>-1</sup>) 2924, 1570, 1475, 1388, 1234, 1182, 1099, 1074, 1048, 1012, 879, 813, 742 cm<sup>-1</sup>; MS (APCI) *m/z* 621 [M+H]<sup>+</sup> Anal. Calcd. for C<sub>30</sub>H<sub>20</sub>N<sub>8</sub>S<sub>4</sub>: C, 58.04; H, 3.25; N, 18.05; Found: C, 58.02; H, 3.24; N, 17.97. R<sub>f</sub> = 0.40 (PE:DCM = 1:2).

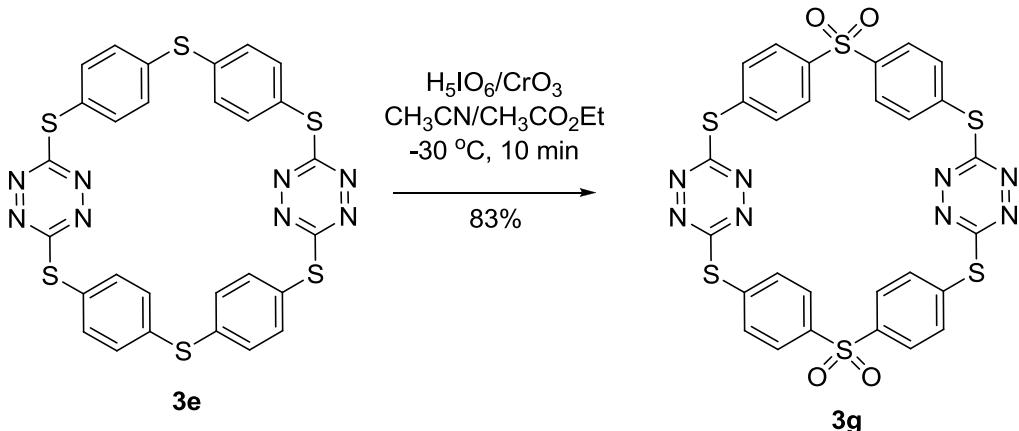


**4f** (43 mg, yield 14%): red solid, m.p. 167 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS): δ<sub>H</sub> 7.53 (d, *J* = 8.2 Hz, 12H), 7.23 (d, *J* = 8.2 Hz, 12H), 4.0 (s, 6H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, TMS): δ<sub>C</sub> 174.0, 142.6, 135.9, 130.5, 123.5, 41.3; IR (KBr, ν/cm<sup>-1</sup>) 2919, 1591, 1491, 1404, 1234, 1182, 1046, 1015, 875, 803, 786 cm<sup>-1</sup>; MS (APCI), *m/z* 931 [M+H]<sup>+</sup>; Anal. Calcd. for C<sub>45</sub>H<sub>30</sub>N<sub>12</sub>S<sub>6</sub>: C, 58.04; H, 3.25; N, 18.05; H, 4.61; Found: C, 58.01; H, 3.27; N, 17.89. R<sub>f</sub> = 0.30 (PE:DCM = 1:5).



**5f** (10 mg, yield 3%): red solid, m.p. 209 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS): δ<sub>H</sub> 7.54 (d, *J* = 8.2 Hz, 16H), 7.23 (d, *J* = 8.2 Hz, 16H), 4.0 (s, 8H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, TMS): δ<sub>C</sub> 174.0, 142.6, 135.9, 130.5, 123.5, 41.3; IR (KBr, v/cm<sup>-1</sup>) 2922, 1591, 1491, 1404, 1234, 1182, 1046, 1016, 877, 804, 786 cm<sup>-1</sup>; MS (APCI), *m/z* 1241 [M+H]<sup>+</sup>; Anal. Calcd. for C<sub>45</sub>H<sub>30</sub>N<sub>12</sub>S<sub>6</sub>:C<sub>60</sub>H<sub>40</sub>N<sub>16</sub>S<sub>8</sub>: C, 58.04; H, 3.25; N, 18.05; Found: C, 58.17; H, 3.23; N, 17.79. R<sub>f</sub> = 0.50 (DCM).

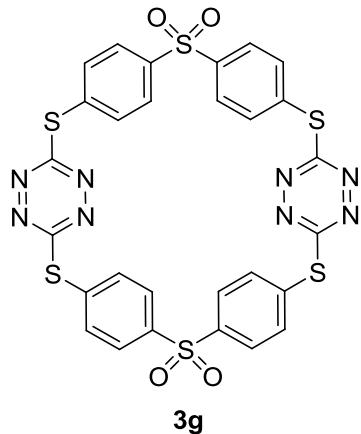
### 2.3. The Synthesis of 3g



**Scheme S3** Synthesis of 3g

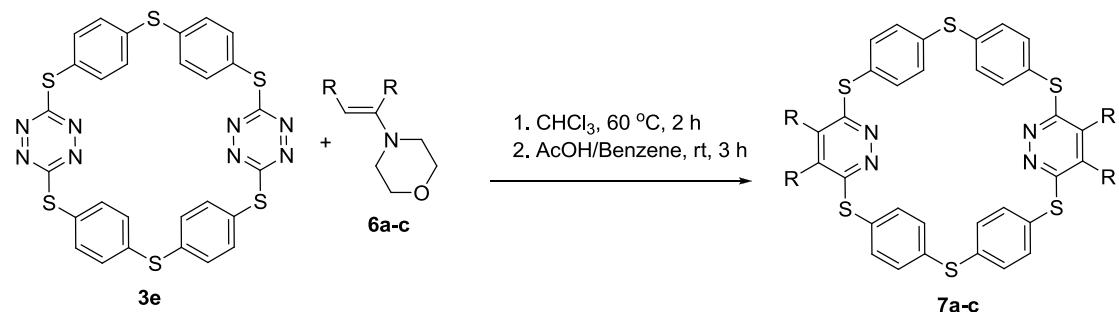
A solution of H<sub>5</sub>IO<sub>6</sub> (7.5 mmol) in acetonitrile (20 mL) was stirred for 30 min room temperature, then CrO<sub>3</sub> (0.75 mmol) was added and stirred for 10 min. The resulting solution was added dropwise to the solution of **3e** (0.5 mmol) in ethyl acetate (30 mL) at -30 °C. Then the mixture was stirred constantly for 10 min at the same temperature before a saturated sodium carbonate solution (50 mL) was added to quench the

reaction. The resulting mixture was extracted with dichloromethane ( $100\text{ mL} \times 3$ ), the combined organic phase was washed by brine ( $150\text{ mL} \times 3$ ) and dried over anhydrous  $\text{Na}_2\text{SO}_4$ . After filtration and removal of solvent, The residue was chromatographed on a silica gel column with a mixture of petroleum ether and dichloromethane as the mobile phase to give the pure product **3g**. X-ray quality single crystal **3g** was obtained by diffusing hexane into the solution of **3g** in chloroform.



**3g** (299 mg, yield 83%): red solid, m.p. 237–238 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ , TMS):  $\delta_{\text{H}}$  8.01 (d,  $J = 8.2$  Hz, 8H), 7.92 (d,  $J = 8.2$  Hz, 8H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ , TMS):  $\delta_{\text{C}}$  172.6, 141.6, 135.0, 134.2, 129.2; IR (KBr,  $\nu/\text{cm}^{-1}$ ) 1578, 1476, 1392, 1322, 1279, 1236, 1159, 1084, 1012, 768, 632, 584  $\text{cm}^{-1}$ ; HRMS(APCI) Calc.Mass: 720.9692 [M+H] $^+$ , Found Mass: 720.9674 [M+H] $^+$ .  $R_f = 0.60$  (DCM:Acetone = 25:1).

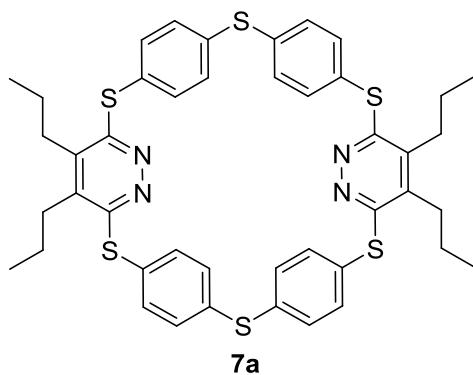
#### 2.4. General Procedure for the Synthesis of **7a-c**



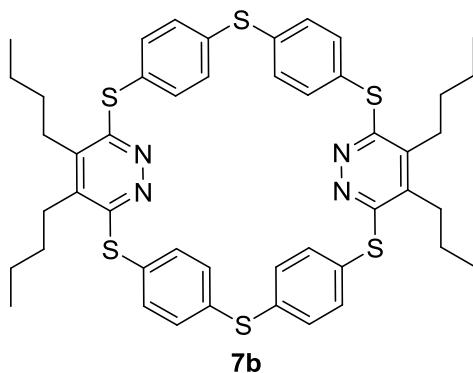
**Scheme S4** Synthesis of **7a-c**

A solution of  $S_6$ -corona[3]arene[3]tetrazine **3e** (0.5 mmol) in dry chloroform (25 mL) was added dropwise N-(1-Cyclopenten-1-yl)morpholine (2.25 mmol) **6a**, **6b** or **6c** at ambient temperature, and the resulting solution was stirred constantly refluxed for 2 h.

After the starting material disappeared which was monitored by TLC, the solvent was removed, benzene (5 mL) and glacial acetic acid (0.5 mL) was added. The resulting reaction mixture was stirred for 3 h at room temperature. After filtration and removal of solvent, the residue was chromatographed on a silica gel column with a mixture of dichloromethane and petroleum ether as the mobile phase to give pure products **7a-c**. X-ray quality single crystal **7a** was obtained by diffusing hexane into the solution of **7a** in chloroform. Characterization data of all products are listed below.

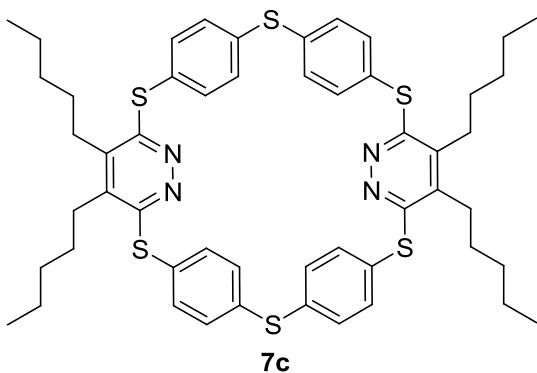


**7a** (349 mg, yield 85%): white solid, m.p. 255 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS): δ<sub>H</sub> 7.43 (d, *J* = 8.2 Hz, 8H), 7.31 (d, *J* = 8.3 Hz, 8H), 2.82-2.71 (m, 8H), 1.67-1.59 (m, 8H), 1.27 (t, *J* = 7.3 Hz, 3H), 1.10 (t, *J* = 7.3 Hz, 6H), 1.00 (t, *J* = 6.9 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, TMS): δ<sub>C</sub> 159.6, 159.4, 140.0, 138.9, 138.8, 135.0, 133.4, 131.2, 130.1, 31.2, 31.0, 28.7, 23.2, 22.6, 22.2, 14.6, 13.8, 13.4; IR (KBr, v/cm<sup>-1</sup>) 2959, 2930, 2871, 1574, 1526, 1474, 1389, 1307, 1182, 1085, 1012, 811 cm<sup>-1</sup>; HRMS (APCI), *m/z* 821.1954 [M+H]<sup>+</sup>; Anal. Calcd. for C<sub>44</sub>H<sub>44</sub>N<sub>4</sub>S<sub>6</sub>: C, 64.35; H, 5.40; N, 6.82; Found: C, 64.35; H, 5.22; N, 6.88. R<sub>f</sub> = 0.35 (PE:DCM = 1:1).



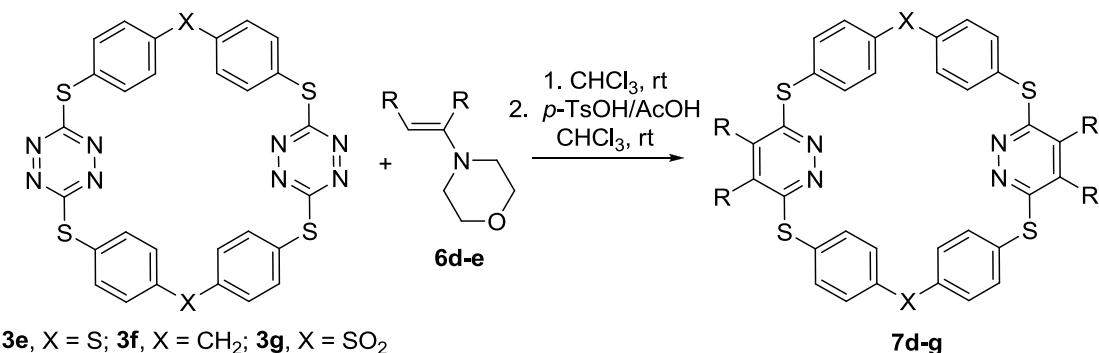
**7b** (382 mg, yield 87%): white solid, m.p. 151-152 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS): δ<sub>H</sub> 7.42 (d, *J* = 8.2 Hz, 8H), 7.31 (d, *J* = 8.2 Hz, 8H), 2.77-2.72 (m, 8H),

1.70-1.49 (m, 16H), 1.09 (t,  $J$  = 7.3 Hz, 3H), 1.00 (t,  $J$  = 7.3 Hz, 6H), 0.94 (t,  $J$  = 6.9 Hz, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , TMS):  $\delta_{\text{C}}$  159.6, 139.1, 139.0, 138.8, 135.0, 133.5, 131.2, 130.1, 32.2, 31.1, 29.1, 28.8, 23.2, 22.6, 22.3, 14.6, 14.0, 13.7; IR (KBr,  $\nu/\text{cm}^{-1}$ ) 2957, 2928, 2869, 1574, 1526, 1476, 1388, 1308, 1179, 1094, 1012, 810  $\text{cm}^{-1}$ ; HRMS (APCI) Calcd. for  $\text{C}_{48}\text{H}_{53}\text{N}_4\text{S}_6$  877.2589 [M+H] $^+$ , Found Mass 877.2577 [M+H] $^+$ .  $R_f$  = 0.30 (PE:DCM = 1:3).



**7c** (350 mg, yield 75%): white solid, m.p. 141 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , TMS):  $\delta_{\text{H}}$  7.42 (d,  $J$  = 8.3 Hz, 8H), 7.31 (d,  $J$  = 8.7 Hz, 8H), 2.76-2.72 (m, 8H), 1.60-1.58 (m, 8H), 1.46-1.25 (m, 8H), 1.00-0.92 (m, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , TMS):  $\delta_{\text{C}}$  159.6, 139.0, 135.0, 133.4, 131.2, 130.1, 32.2, 31.3, 31.2, 29.7, 29.0, 28.8, 23.2, 22.5, 22.3, 14.0, 14.0, 13.7; IR (KBr,  $\nu/\text{cm}^{-1}$ ) 2954, 2926, 2856, 1575, 1527, 1474, 1388, 1307, 1178, 1096, 1012, 810  $\text{cm}^{-1}$ ; HRMS (APCI),  $m/z$  933.3207 [M+H] $^+$ , 955.3017 [M+Na] $^+$ ; Anal. Calcd. for  $\text{C}_{52}\text{H}_{60}\text{N}_4\text{S}_6$ : C, 66.91; H, 6.48; N, 6.00; Found: C, 66.93; H, 6.67; N, 5.68.  $R_f$  = 0.30 (PE:DCM = 1:3).

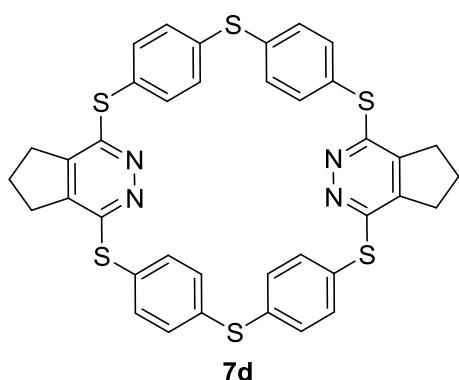
## 2.5. General Procedure for the Synthesis of 7d-g



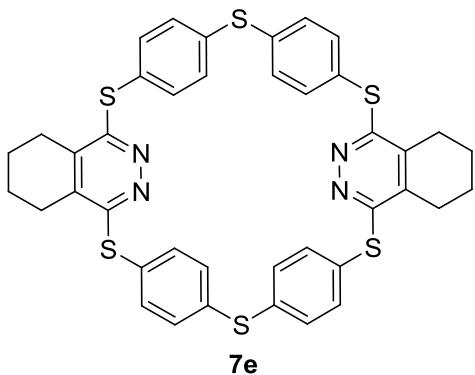
**Scheme S5** Synthesis of 7d-g

A solution of  $\text{S}_6$ -corona[3]arene[3]tetrazine **3e**, **3f**, or **3g** (0.5 mmol) in dry chloroform (25 mL) was added dropwise **6d** (2.25 mmol) or **6e** (2.25 mmol) at

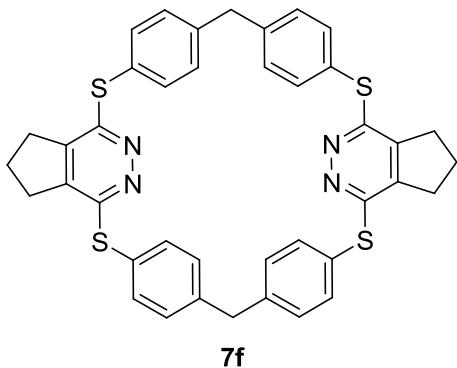
ambient temperature, and the resulting solution was stirred constantly for 1 h (**6d**) or 5 h (**6e**). After the starting material disappeared which was monitored by TLC, a catalytic amount of 4-methylbenzenesulfonic acid (10 mg) and an equivalent amount of glacial acetic acid (1 mL) was added. The resulting reaction mixture was stirred for 2 h (**6d**) or 12 h (**6e**) at room temperature before 50 mL saturated sodium carbonate solution was added to quench the reaction. The resulting mixture was extracted with dichloromethane ( $3 \times 100$  mL). The combined organic phase was washed with brine ( $3 \times 150$  mL), and dried over anhydrous  $\text{MgSO}_4$ . After filtration and removal of solvent, the residue was chromatographed on a silica gel column with a mixture of dichloromethane and ethyl acetate as the mobile phase to give pure products **7d-g**. X-ray quality single crystals **7d**, **7e** or **7f** were obtained by diffusing hexane into the solution of **7d**, **7e** or **7f** in chloroform. Characterization data of all products are listed below.



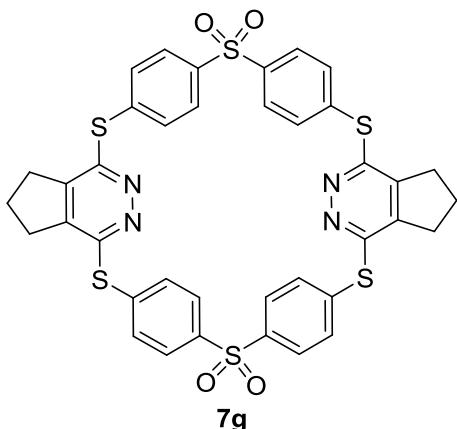
**7d** (330 mg, yield 90%): white solid, m.p. 288 °C (decomposition);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ , TMS)  $\delta$  (ppm) 7.44 (d,  $J = 8.2$  Hz, 8H), 7.31 (d,  $J = 8.2$  Hz, 8H), 2.90 (t,  $J = 7.6$  Hz, 8H), 2.20-2.14 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ , TMS)  $\delta$  (ppm) 156.8, 143.9, 135.2, 133.2, 131.5, 129.4, 31.6, 22.6; IR (KBr,  $\nu/\text{cm}^{-1}$ ) 2954, 1571, 1473, 1429, 1389, 1293, 1262, 1172, 1098, 1013, 955, 908, 811, 731 $\text{cm}^{-1}$ ; HRMS(APCI) 733.0700 [ $\text{M}+\text{H}]^+$ , 755.0520 [ $\text{M}+\text{Na}]^+$ ; Anal. Calcd. for  $\text{C}_{38}\text{H}_{28}\text{N}_4\text{S}_6$ : C, 62.26; H, 3.85; N, 7.64; Found: C, 61.99; H, 3.89; N, 7.53.  $R_f = 0.30$  (DCM).



**7e** (285 mg, yield 75%): white solid, m.p.: >300 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS) δ (ppm) 7.45 (d, *J* = 8.2 Hz, 8H), 7.32 (d, *J* = 8.2 Hz, 8H), 2.69 (t, *J* = 2.3 Hz, 8H), 1.83 (t, *J* = 2.3 Hz, 8H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, TMS) δ (ppm) 159.3, 135.8, 135.4, 133.8, 131.4, 129.6, 25.5, 21.5; IR (KBr, v/cm<sup>-1</sup>) 3060, 2937, 2856, 1573, 1532, 1474, 1421, 1389, 1350, 1281, 1239, 1184, 1099, 1075, 1012, 958, 911, 814, 743 cm<sup>-1</sup>; HRMS(APCI) 737.1011 [M+H]<sup>+</sup>; Anal. Calcd. for C<sub>40</sub>H<sub>32</sub>N<sub>4</sub>S<sub>6</sub>: C, 63.12; H, 4.24; N, 7.36; Found: C, 61.99; H, 3.89; N, 7.53. R<sub>f</sub> = 0.40 (DCM:EA = 30:1).

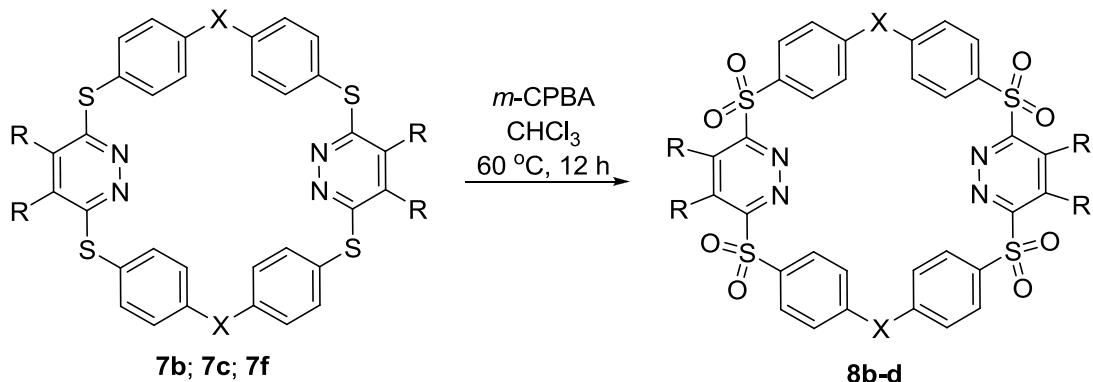


**7f** (207 mg, yield 99%): white solid, m.p. >300 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS) δ (ppm) 7.41 (d, *J* = 7.6 Hz, 6H), 7.14 (d, *J* = 7.6 Hz, 6H), 3.90 (s, 4H), 2.79 (t, *J* = 7.6 Hz, 8H), 2.12-2.06 (m, 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, TMS) δ (ppm) 157.6, 144.2, 140.6, 133.3, 130.0, 128.1, 41.4, 31.7, 22.7; IR (KBr, v/cm<sup>-1</sup>) 3019, 2951, 2901, 1594, 1548, 1489, 1428, 1403, 1290, 1261, 1172, 1104, 1016, 802 cm<sup>-1</sup>; HRMS(APCI) 697.1567 [M+H]<sup>+</sup>; Anal. Calcd. for C<sub>40</sub>H<sub>32</sub>N<sub>4</sub>S<sub>4</sub>: C, 68.93; H, 4.63; N, 8.04; Found: C, 68.82; H, 4.77; N, 8.04. R<sub>f</sub> = 0.30 (DCM:Acetone = 40:1).



**7g** (191 mg, yield 80%): white solid, m.p.>300 °C; <sup>1</sup>H NMR (400 MHz, CF<sub>3</sub>COOD + CDCl<sub>3</sub>, TMS) δ (ppm) 8.01 (d, *J* = 7.8 Hz, 8H), 7.68 (d, *J* = 7.8 Hz, 8H), 3.26 (t, *J* = 7.3 Hz, 8H), 2.53 (t, *J* = 7.3 Hz, 4H); <sup>13</sup>C NMR (100 MHz, CF<sub>3</sub>COOD + CDCl<sub>3</sub>, TMS) δ (ppm) 157.4, 151.4, 142.0, 134.0, 131.4, 129.4, 32.3, 22.6; IR (KBr, v/cm<sup>-1</sup>) 2811, 1577, 1477, 1429, 1391, 1319, 1280, 1158, 1110, 1085, 1012, 767, 743 cm<sup>-1</sup>; HRMS (ESI) Calcd. for C<sub>38</sub>H<sub>27</sub>N<sub>4</sub>O<sub>4</sub>S<sub>6</sub> 795.0362 [M-H]<sup>-</sup>, Found Mass 795.0365 [M-H]<sup>-</sup>. Rf = 0.30 (DCM:Acetone = 40:1).

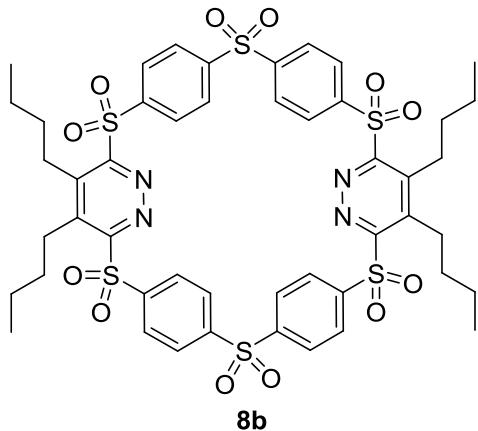
## 2.6. General Procedure for the Synthesis of 8b-d



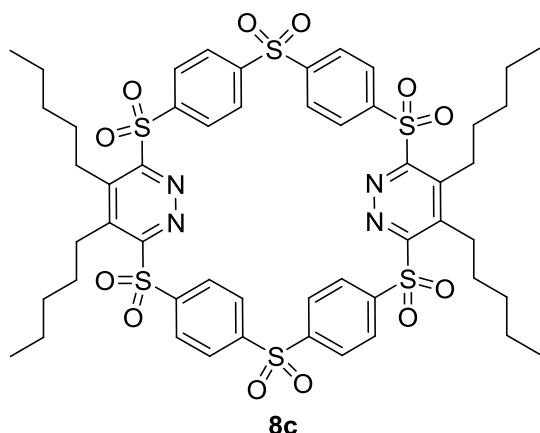
**Scheme S6** Synthesis of **8b-d**

A solution of S<sub>6</sub>-corona[3]arene[3]pyridazine **7b**, **7c**, or **7f** (0.5 mmol) in dry chloroform (30 mL) was added 3-chlorobenzoperoxoic acid at ambient temperature, and the resulting solution was refluxed for 12 h. After the starting material was consumed, which was monitored TLC, a saturated sodium carbonate solution (50 mL) was added to quench the reaction. The resulting mixture was extracted with dichloromethane (3 × 100 mL). The combined organic phase was washed with brine (3 × 150 mL), and dried over anhydrous MgSO<sub>4</sub>. After filtration and removal of

solvent, the residue was chromatographed on a silica gel column with a mixture of dichloromethane and ethyl acetate as the mobile phase to give pure products **8b-d**. X-ray quality single crystal **8d** was obtained by diffusing hexane into the solution of **8d** in chloroform. Characterization data of all products are listed below.

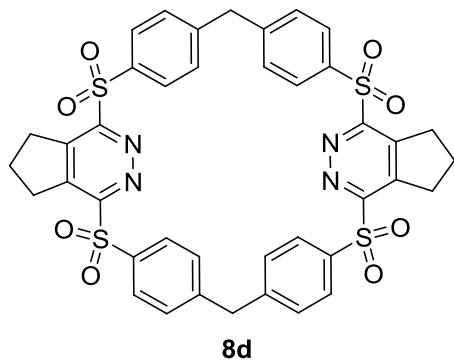


**8b** (427 mg, yield 80%): white solid, m.p. >300 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS) δ (ppm) 8.14-8.09 (m, 16H), 3.35-3.13 (m, 8H), 1.90-1.78 (m, 8H), 1.67-1.60 (m, 8H), 1.22 (t, *J* = 6.8 Hz, 3H), 1.01 (t, *J* = 7.4 Hz, 6H), 0.99 (t, *J* = 7.3 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, TMS) δ (ppm) 162.9, 145.3, 145.2, 145.0, 144.0, 130.6, 128.7, 33.4, 32.4, 31.1, 29.2, 27.1, 27.0, 25.0, 23.4, 22.2, 14.8, 13.9, 13.6; IR (KBr, v/cm<sup>-1</sup>) 3095, 2961, 2933, 2873, 1497, 1466, 1392, 1332, 1292, 1161, 1102, 1075, 638, 620 cm<sup>-1</sup>; HRMS(ESI) 1067.1834 [M-H]<sup>-</sup>; Anal. Calcd. for C<sub>48</sub>H<sub>52</sub>N<sub>4</sub>O<sub>12</sub>S<sub>6</sub>: C, 53.91; H, 4.90; N, 5.24; Found: C, 54.01; H, 5.05; N, 5.06. R<sub>f</sub> = 0.30 (PE:DCM = 5:1).



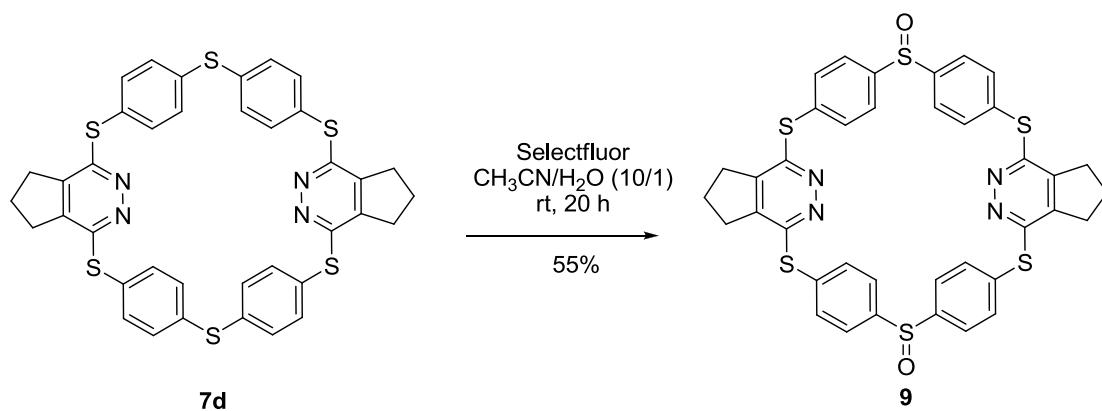
**8c** (472 mg, yield 84%): white solid, m.p. >300 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS) δ (ppm) 8.14-8.09 (m, 8H), 3.35-3.32 (m, 8H), 1.80-1.76 (m, 8H), 1.61-1.456 (m, 16H), 1.07-0.97 (m, 12H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, TMS) δ (ppm) 162.6, 145.2,

145.0, 143.7, 130.5, 128.7, 33.3, 32.4, 31.3, 31.2, 31.1, 30.0, 27.2, 27.0, 23.4, 22.5, 22.2, 14.0, 13.9, 13.6; IR (KBr,  $\nu/\text{cm}^{-1}$ ) 3096, 2958, 2932, 2872, 1497, 1467, 1391, 1334, 1291, 1160, 1102, 1076, 640, 620  $\text{cm}^{-1}$ ; HRMS(ESI) 1123.2468 [M-H] $^-$ ; Anal. Calcd. for  $\text{C}_{52}\text{H}_{60}\text{N}_4\text{O}_{12}\text{S}_6$ : C, 55.49; H, 5.37; N, 4.98; Found: C, 55.48; H, 5.53; N, 4.95.  $R_f = 0.60$  (DCM).



**8d** (163 mg, yield 99%): white solid, m.p.  $>300^\circ\text{C}$ ;  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ , 100  $^\circ\text{C}$ , TMS)  $\delta$  (ppm) 7.94 (d,  $J = 8.2$  Hz, 8H), 7.36 (d,  $J = 8.2$  Hz, 8H), 4.20 (s, 4H), 3.54 (t,  $J = 7.6$  Hz, 8H), 2.31-2.25 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ , 100  $^\circ\text{C}$ , TMS)  $\delta$  (ppm) 160.0, 148.2, 146.6, 135.3, 129.6, 129.0, 31.0, 22.9; IR (KBr,  $\nu/\text{cm}^{-1}$ ) 3093, 3056, 2962, 1592, 1513, 1409, 1390, 1324, 1191, 1161, 1146, 1081, 685  $\text{cm}^{-1}$ ; HRMS (APCI) Calcd. for  $\text{C}_{40}\text{H}_{33}\text{N}_4\text{O}_8\text{S}_4$  825.1176 [M+H] $^+$ , Found Mass 825.1167 [M+H] $^+$ .  $R_f = 0.60$  (DCM:Acetone = 40:1).

## 2.7. The Synthesis of 9



**Scheme S7** Synthesis of **9**

A solution of **7d** (0.1 mmol) in the mixture of acetonitrile (5 mL) and water (0.5 mL) was added Selectfluor (0.35 mmol) slowly at room temperature, and the resulting

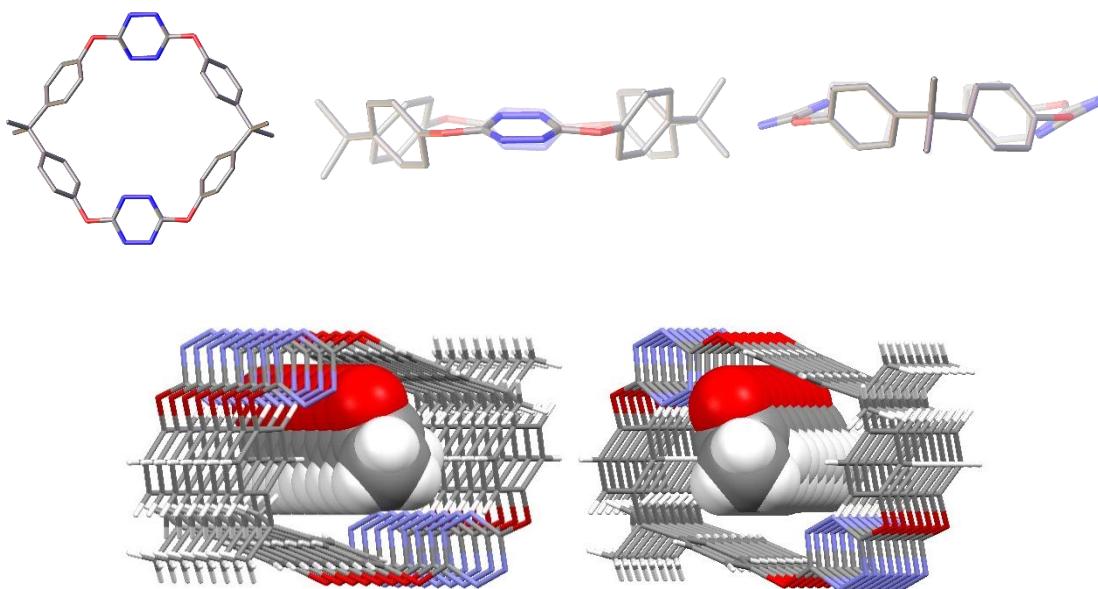
solution was stirred for 20 h at the same temperature. Water (10 mL) was added and the resulting mixture was extracted with dichloromethane (20 mL×3). The combined organic phase was washed with brine (30 mL×3), and dried over anhydrous MgSO<sub>4</sub>. After filtration and removal of solvent, the residue was chromatographed on a silica gel column with a mixture of dichloromethane and acetone as the mobile phase to give pure product **9**.

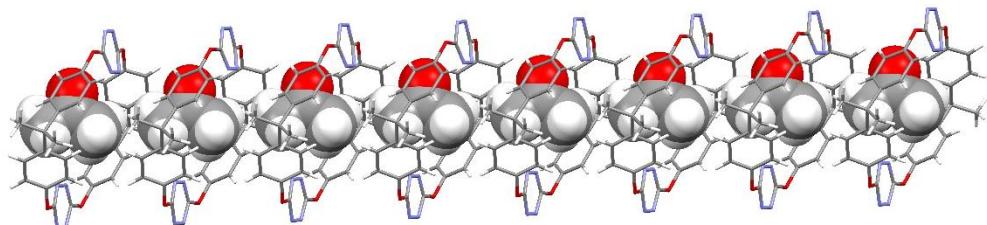
**9** (42 mg, yield 55%): white solid, m.p. >300 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS) δ (ppm) 7.60-7.55 (m, 16H), 2.94 (t, *J* = 7.8 Hz, 8H), 2.21-2.18 (m, 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, TMS) δ (ppm) 156.2, 144.5, 144.2, 134.9, 132.6, 125.7, 31.7, 22.5; IR (KBr, v/cm<sup>-1</sup>) 3071, 2925, 1574, 1474, 1429, 1386, 1317, 1286, 1263, 1176, 1098, 1075, 1052, 1011, 910, 820, 740 cm<sup>-1</sup>; HRMS (ESI) Calcd. for C<sub>38</sub>H<sub>29</sub>N<sub>4</sub>O<sub>2</sub>S<sub>6</sub> 765.0609 [M+H]<sup>+</sup>, Found Mass 765.0603 [M+H]<sup>+</sup>. R<sub>f</sub> = 0.30 (DCM:EA = 3:1).

### 3. X-ray Molecular Structures

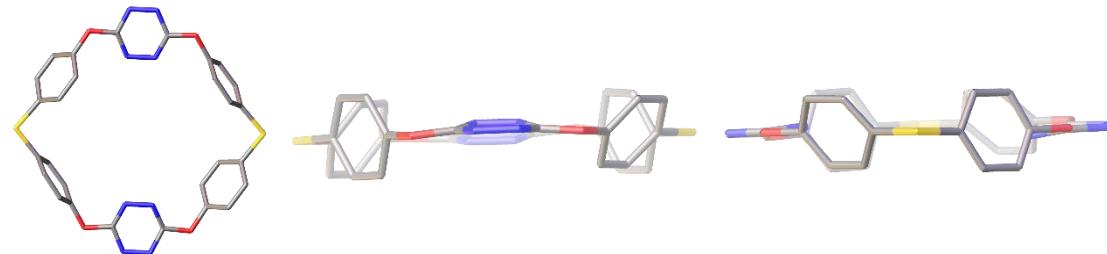


**Figure S1.** X-ray molecular structures of **3a** with top (left) and side (middle and right) views.

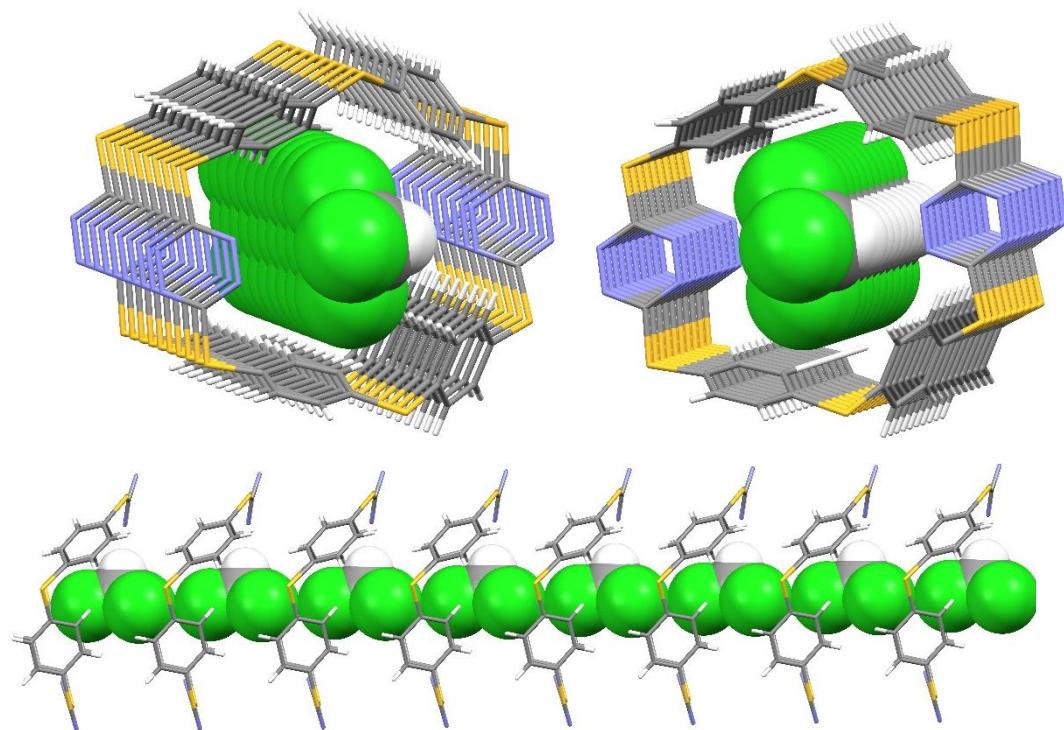




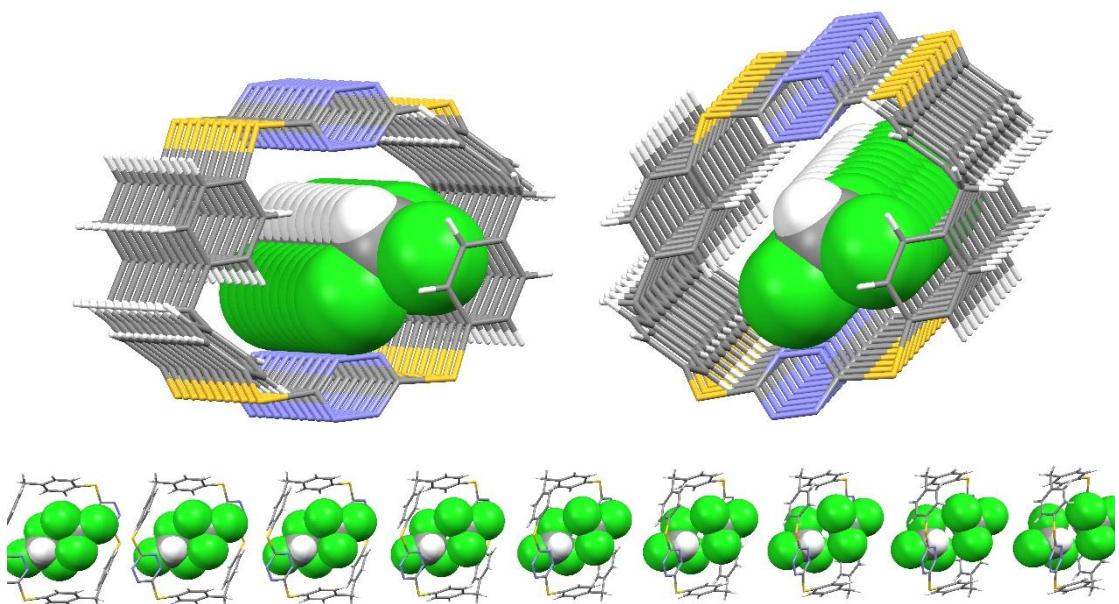
**Figure S2.** X-ray molecular structures of **3b** with top (up left), side (up middle and right) views and the packing model with acetone (down).



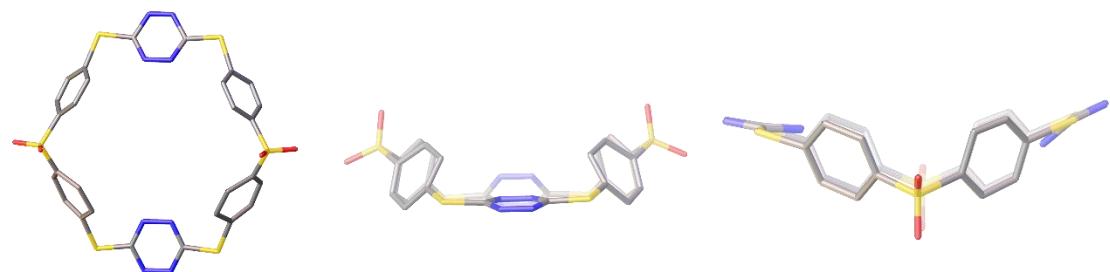
**Figure S3.** X-ray molecular structures of **3d** with top (left) and side (middle and right) views.



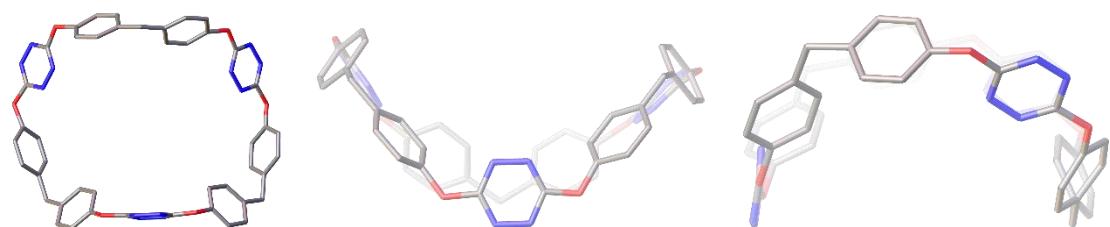
**Figure S4.** X-ray molecular structures of **3e** in the packing model with  $\text{CHCl}_3$ .



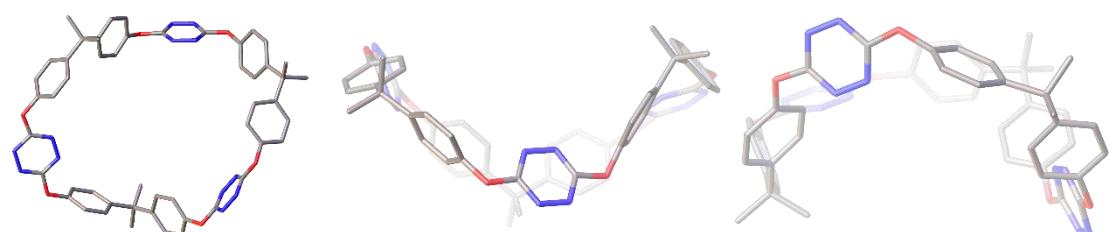
**Figure S5.** X-ray molecular structures of **3f** in the packing model with  $\text{CHCl}_3$ .



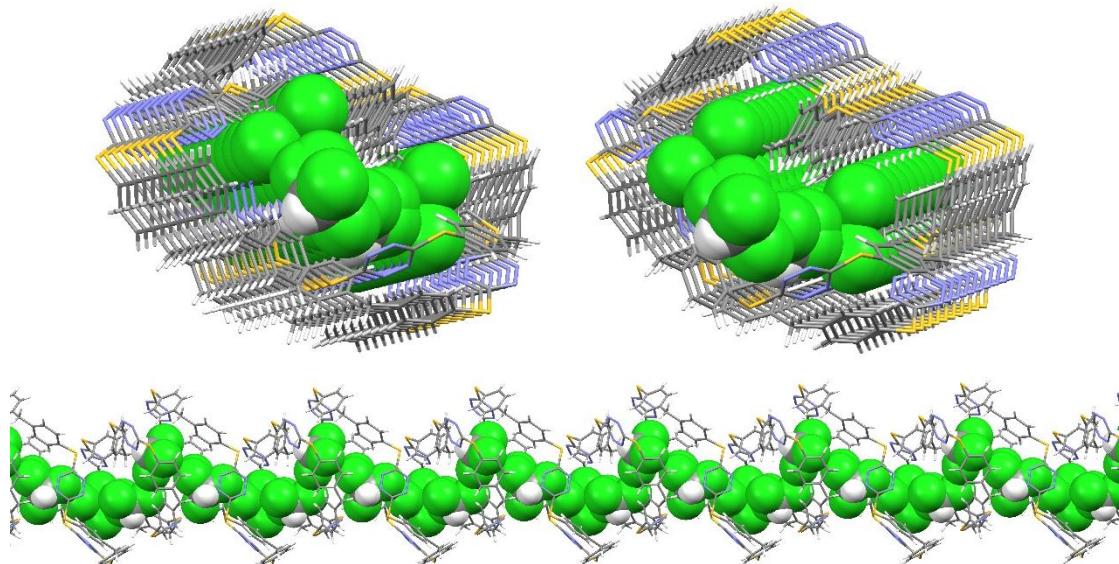
**Figure S6.** X-ray molecular structures of **3g** with top (left) and side (middle and right) views.



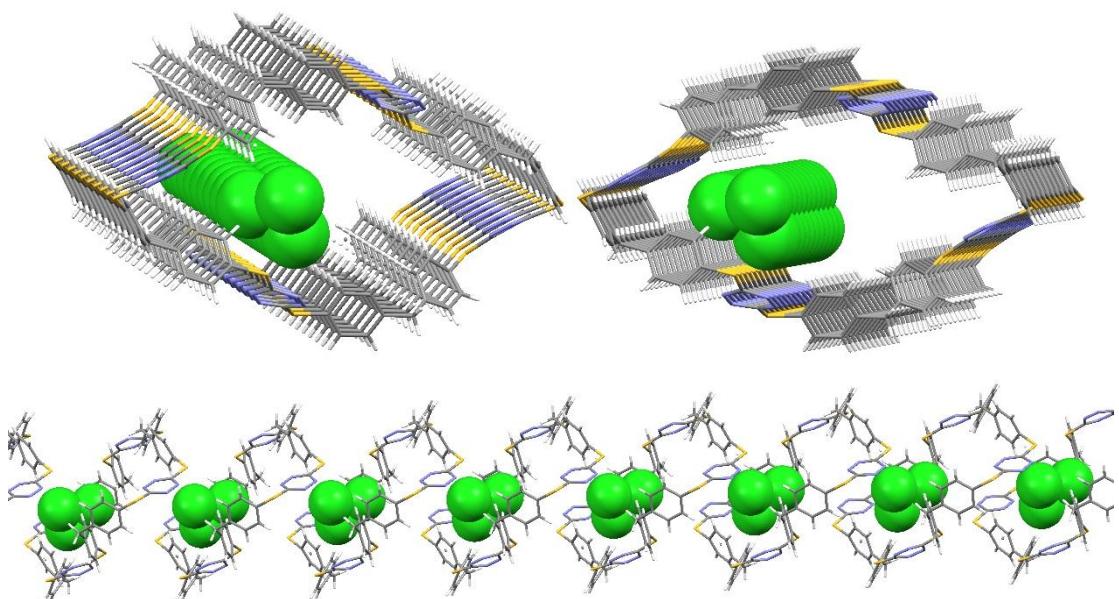
**Figure S7.** X-ray molecular structures of **4a** with top (left) and side (middle and right) views.



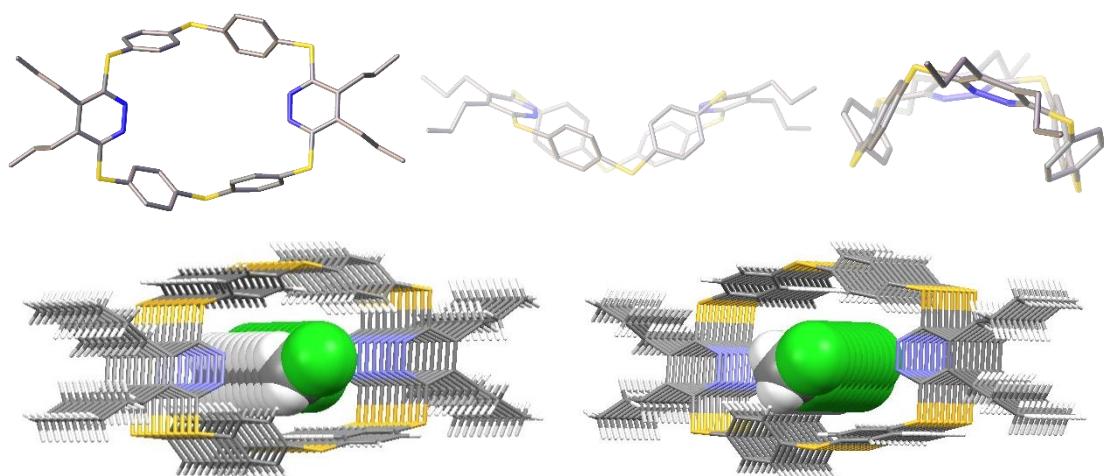
**Figure S8.** X-ray molecular structures of **4b** with top (left) and side (middle and right) views.

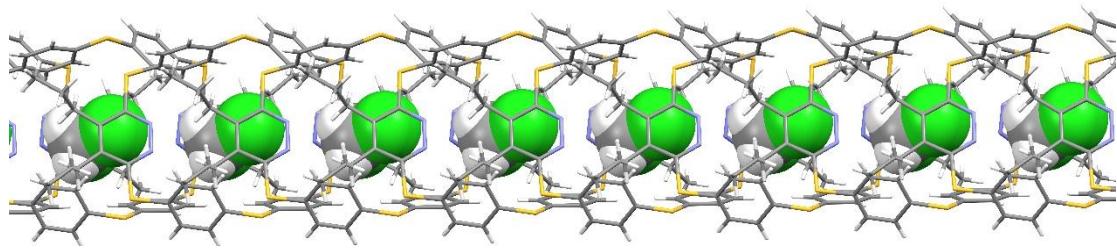


**Figure S9.** X-ray molecular structures of **4f** in the packing model with  $\text{CHCl}_3$ .

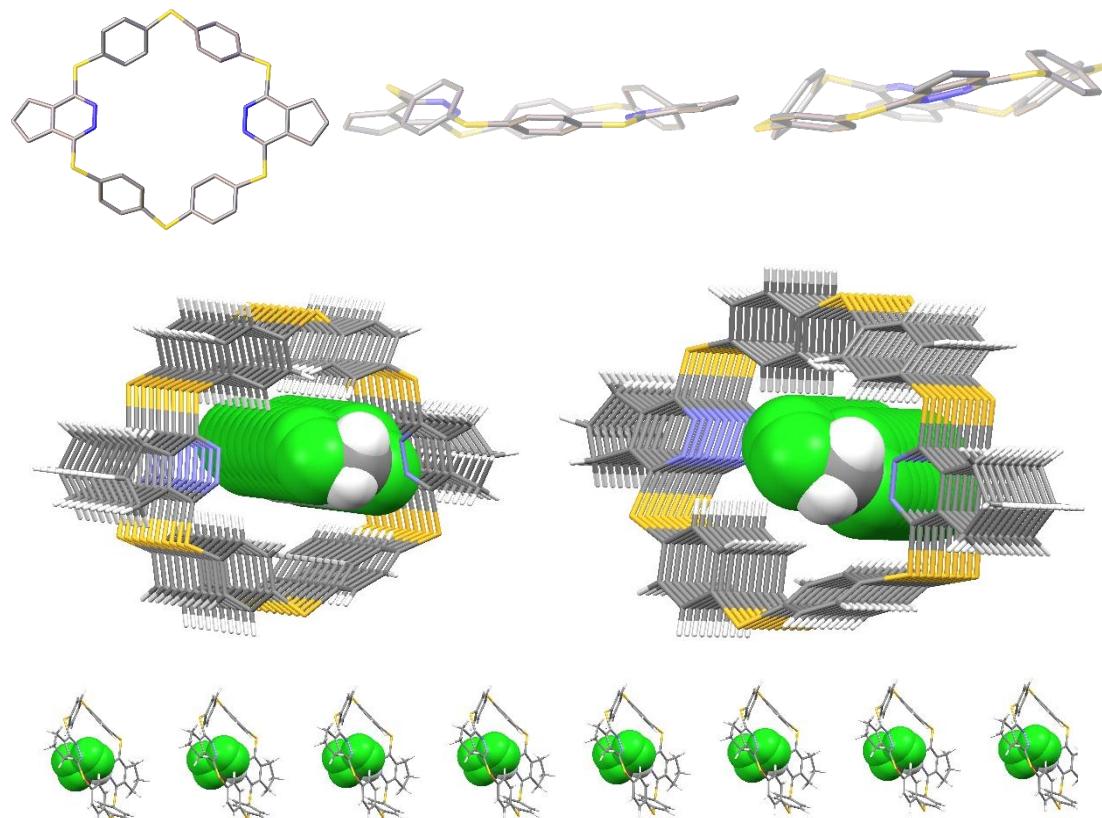


**Figure S10.** X-ray molecular structures of **5f** in the packing model with  $\text{CHCl}_3$ .

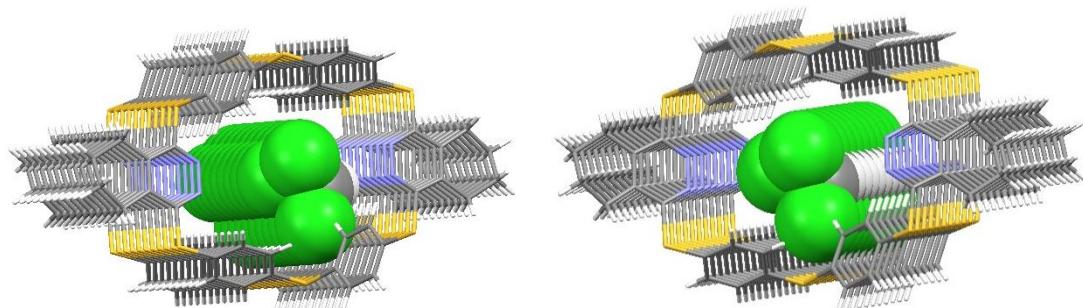


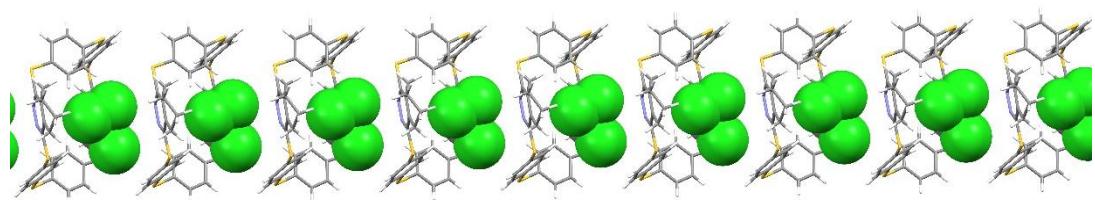


**Figure S11.** X-ray molecular structures of **7a** with top (up left), side (up middle and right) views and the packing model with CHCl<sub>3</sub> (down).

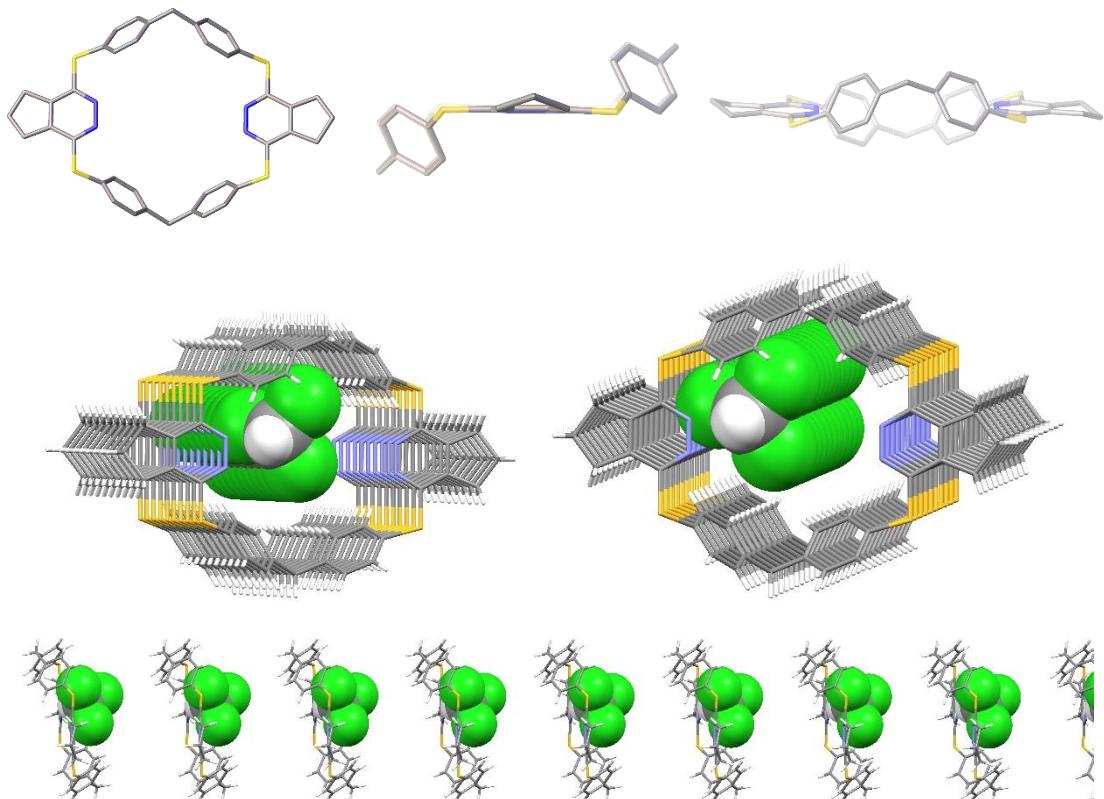


**Figure S12.** X-ray molecular structures of **7d** with top (up left), side (up middle and right) views and the packing model with CHCl<sub>3</sub> (down).

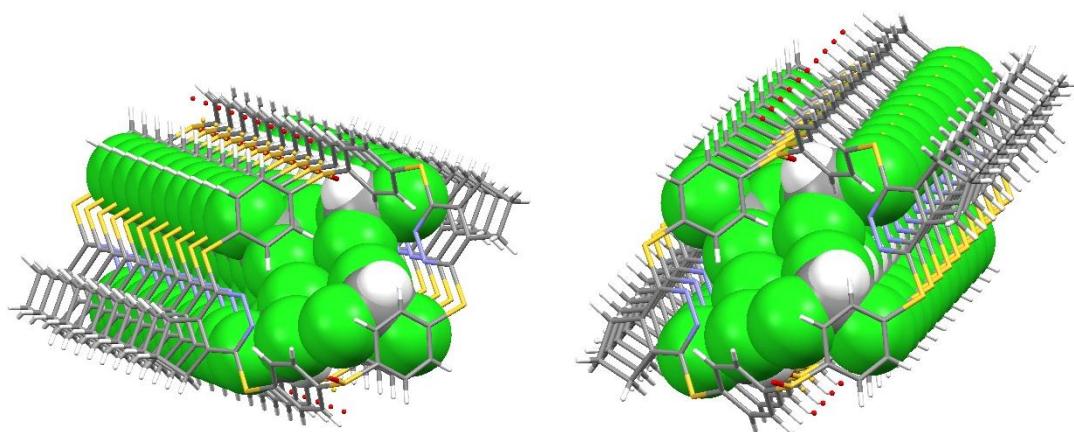


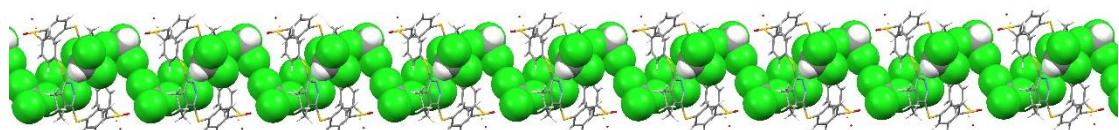


**Figure S13.** X-ray molecular structures of **7e** in the packing model with  $\text{CHCl}_3$ .



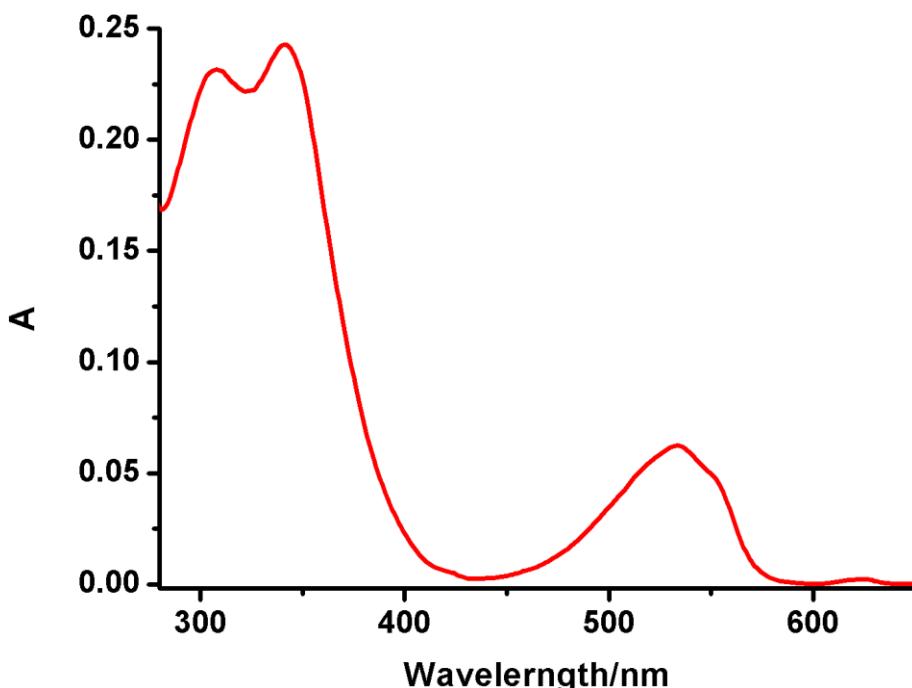
**Figure S14.** X-ray molecular structures of **7f** with top (up left), side (up middle and right) views and the packing model with  $\text{CHCl}_3$  (down).



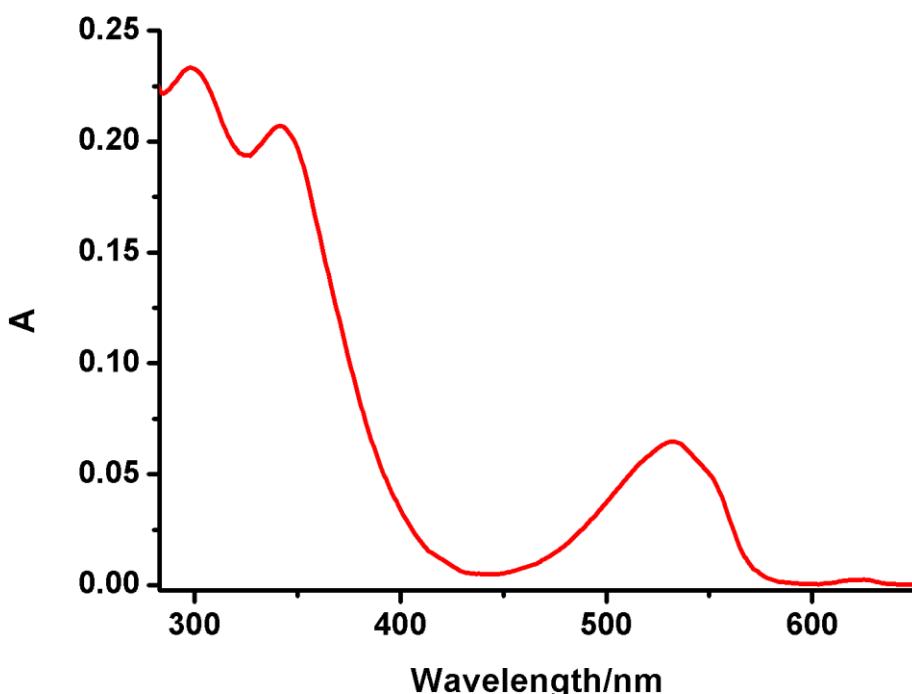


**Figure S15.** X-ray molecular structures of **9** in the packing model with CHCl<sub>3</sub>.

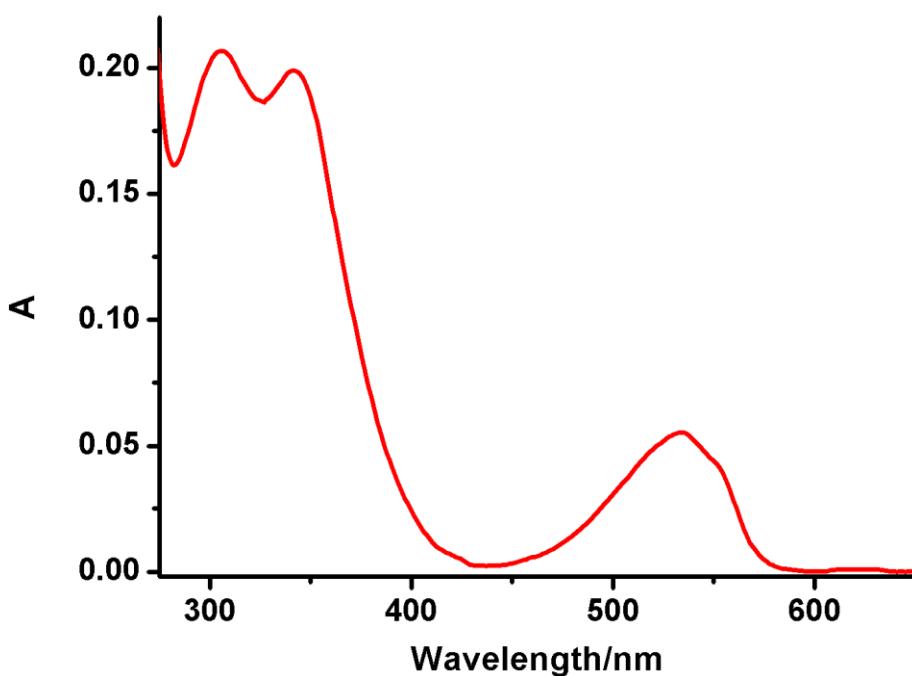
#### 4. UV/vis spectra and photophysical data of the macrocyclic compounds



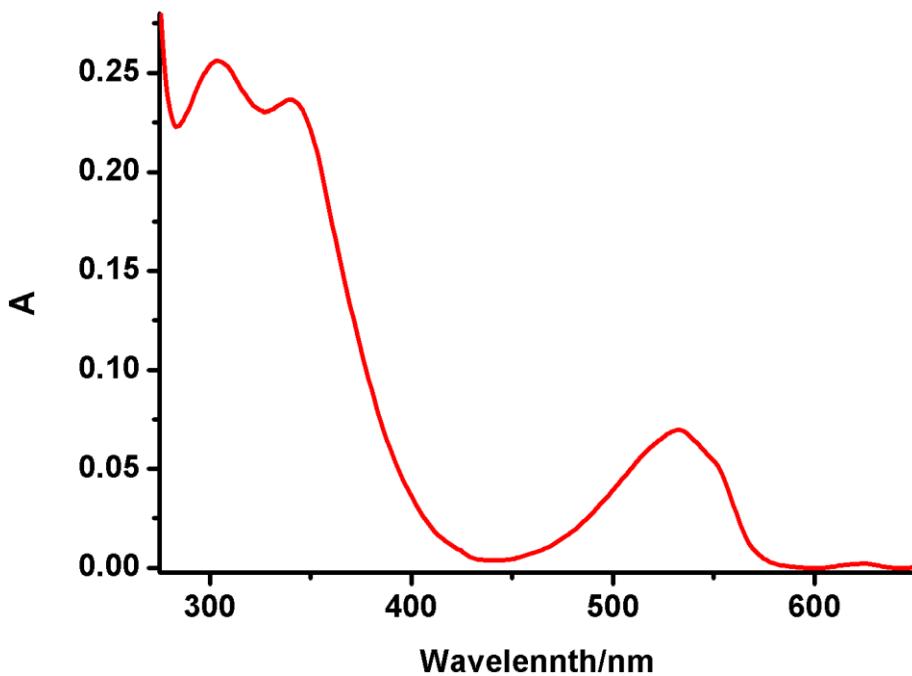
**Figure S16.** UV/vis spectra of **3a** in DCM ( $C = 4.58 \times 10^{-5}$  M) at 298K.



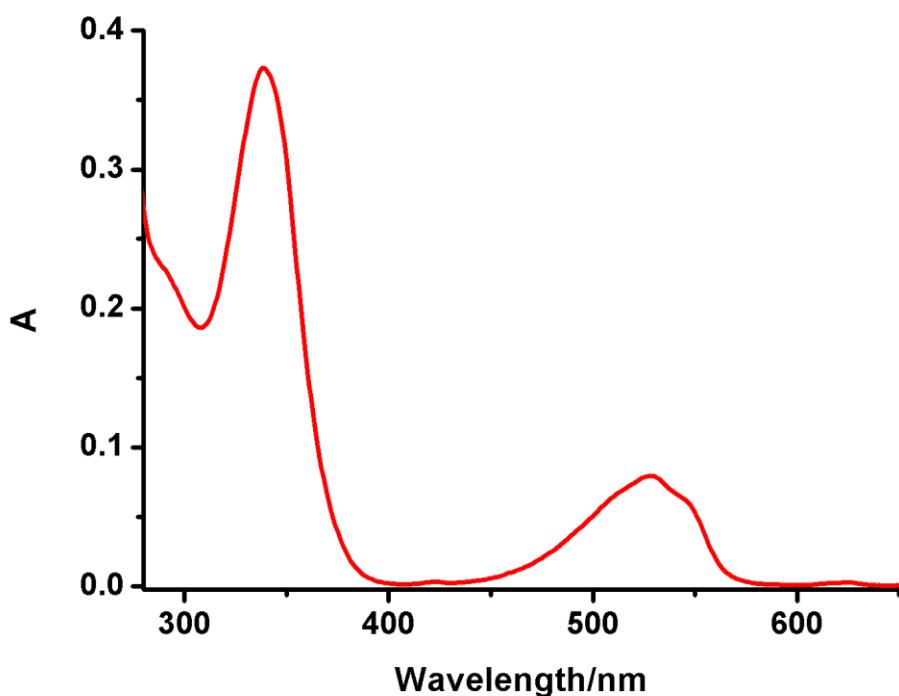
**Figure S17.** UV/vis spectra of **4a** in DCM ( $C = 3.29 \times 10^{-5}$  M) at 298K.



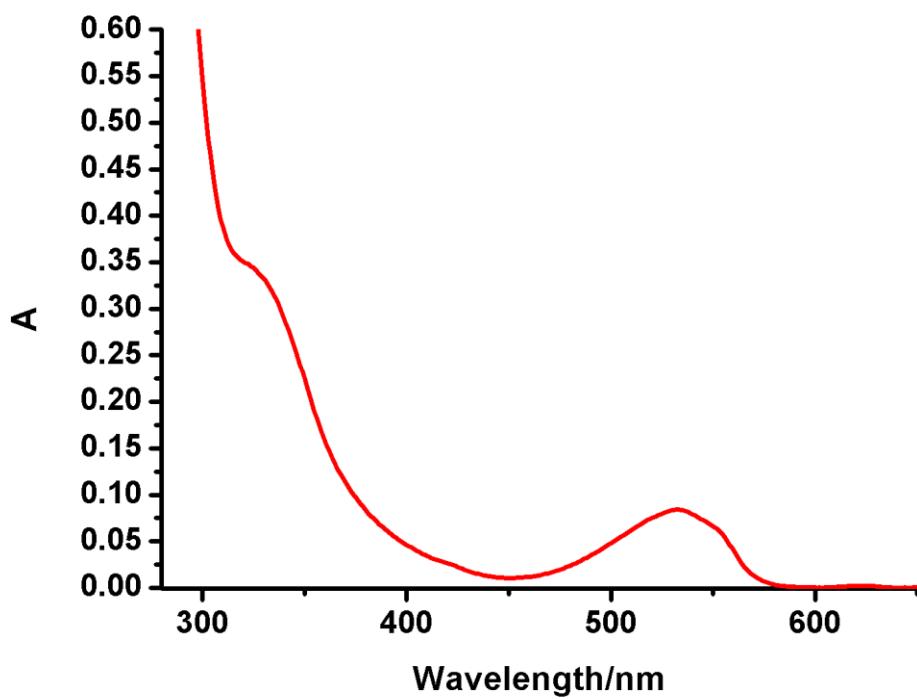
**Figure S18.** UV/vis spectra of **3b** in DCM ( $C = 4.16 \times 10^{-5}$  M) at 298K.



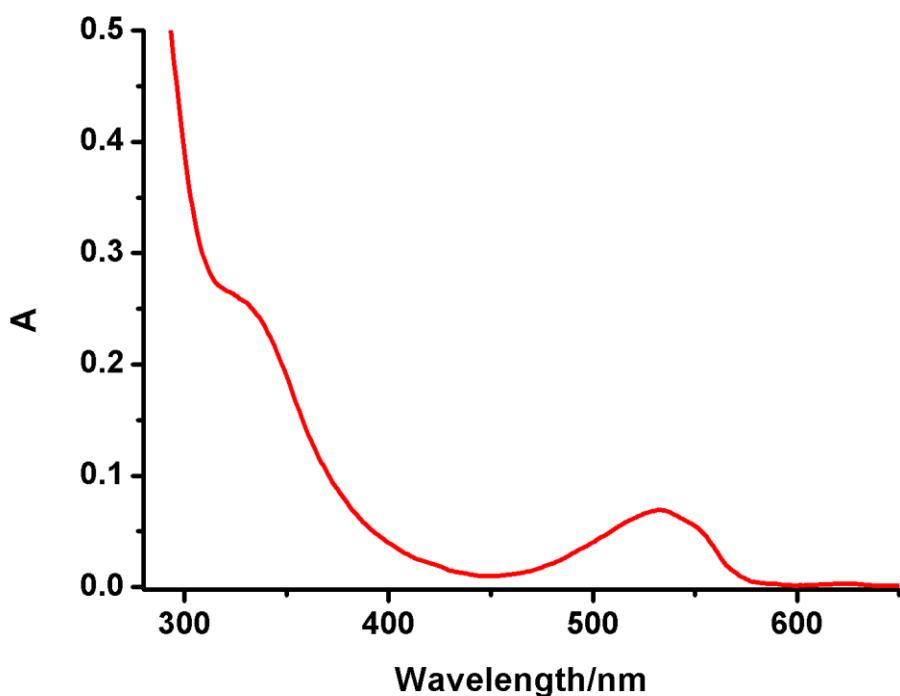
**Figure S19.** UV/vis spectra of **4b** in DCM ( $C = 6.40 \times 10^{-5}$  M) at 298K.



**Figure S20.** UV/vis spectra of **3c** in DCM ( $C = 7.17 \times 10^{-5}$  M) at 298K.



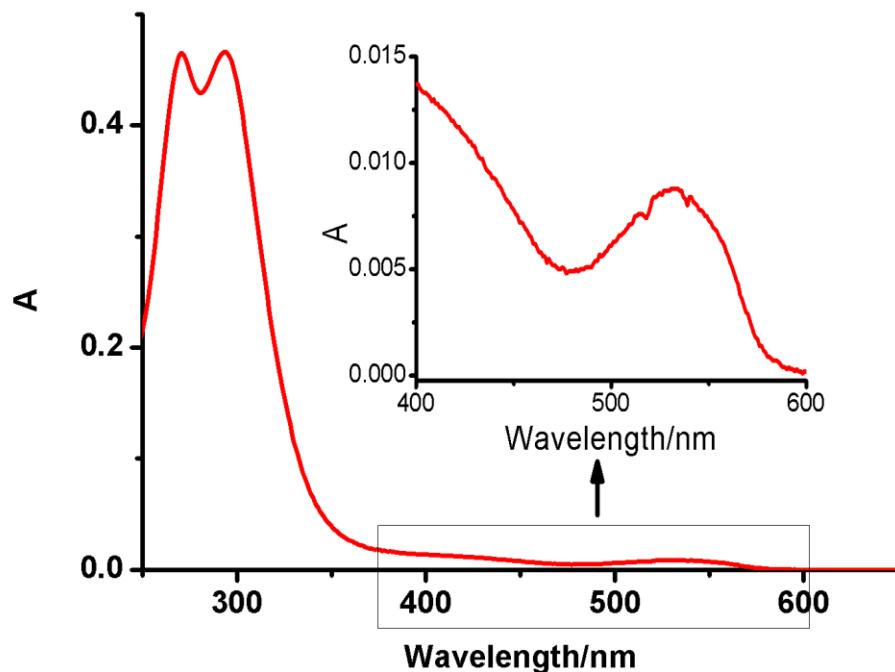
**Figure S21.** UV/vis spectra of **3d** in DCM ( $C = 7.61 \times 10^{-5}$  M) at 298K.



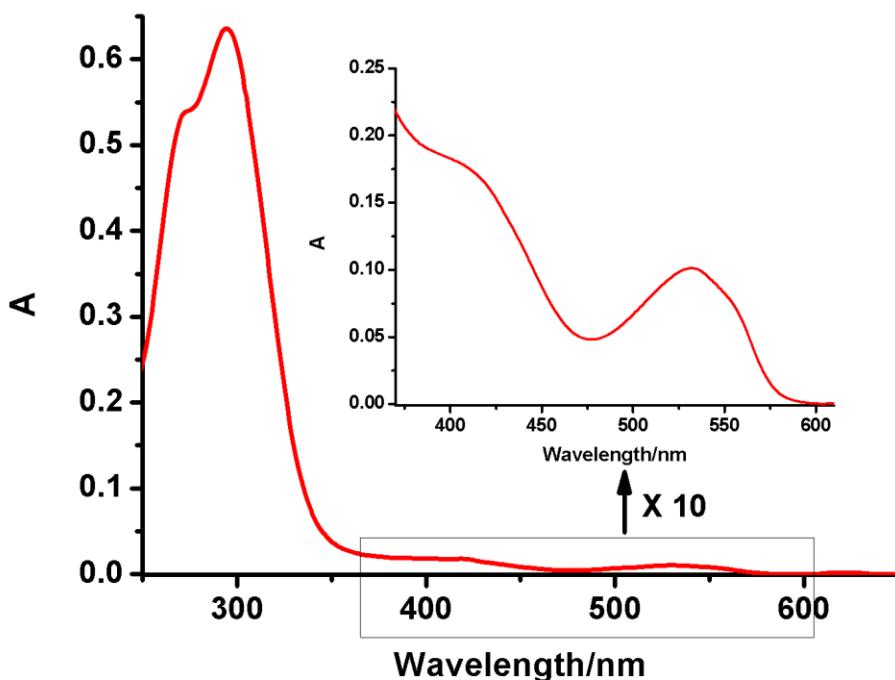
**Figure S22.** UV/vis spectra of **4d** in DCM ( $C = 3.31 \times 10^{-5}$  M) at 298K.

**Table S1** The photophysical data of macrocyclic compounds **3a-3d**, **4a**, **4b** and **4d**

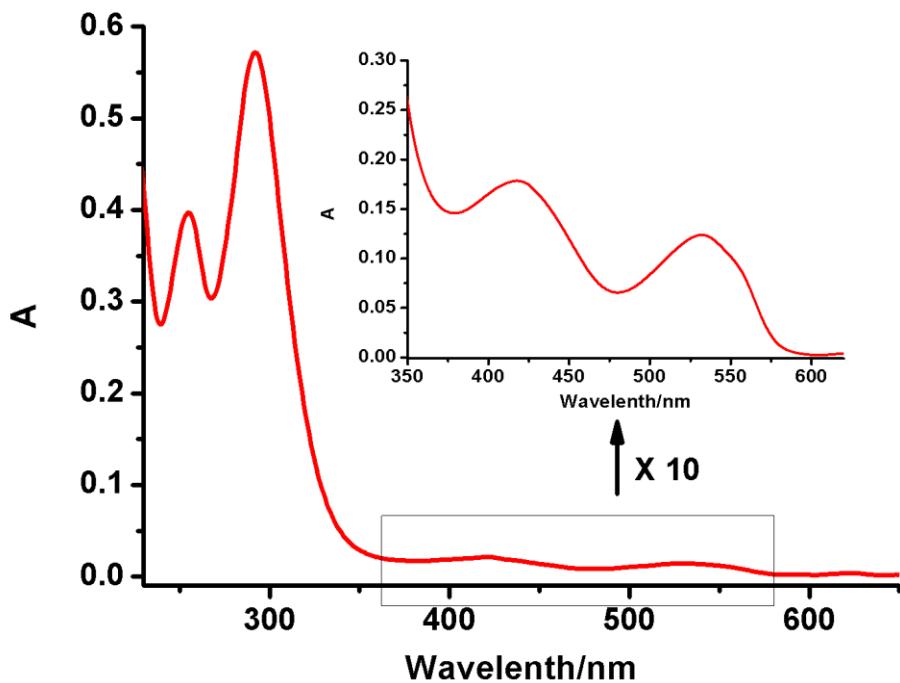
compound	C ( $10^{-5}$ mol/L)	$\lambda_1$ (nm) ( $\varepsilon_1$ [ $\times 10^3$ mol $^{-1}$ cm $^{-1}$ ] )	$\lambda_2$ (nm) ( $\varepsilon_2$ [ $\times 10^3$ mol $^{-1}$ cm $^{-1}$ ] )	$\lambda_3$ (nm) ( $\varepsilon_3$ [ $\times 10^3$ mol $^{-1}$ cm $^{-1}$ ] )
<b>3a</b>	4.58	308 (5.06)	342 (5.30)	534 (1.36)
<b>4a</b>	3.29	298 (7.10)	342 (6.29)	532 (1.97)
<b>3b</b>	4.16	306 (4.97)	342 (4.77)	554 (1.33)
<b>4b</b>	6.40	303 (4.00)	340 (3.70)	533 (1.09)
<b>3c</b>	7.17	339 (5.21)	-	528 (1.11)
<b>3d</b>	7.61	323 (4.57)	-	533 (1.11)
<b>4d</b>	3.31	324 (8.00)	-	533 (2.09)



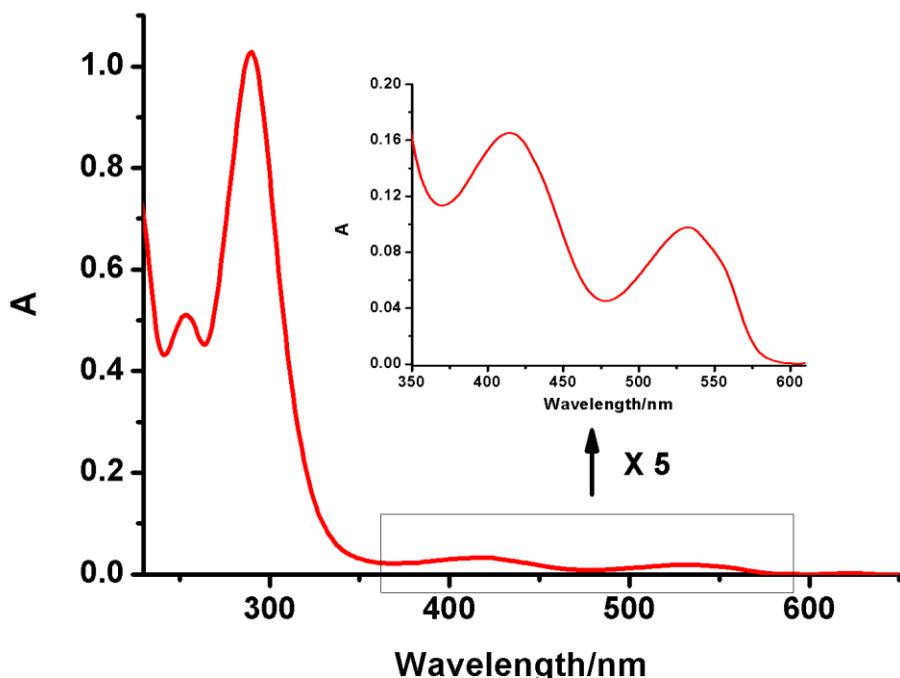
**Figure S23.** UV/vis spectra of **3e** in DCM ( $C = 8.22 \times 10^{-6}$  M) at 298K. The inset shows the UV/vis spectra from 350 to 610 nm.



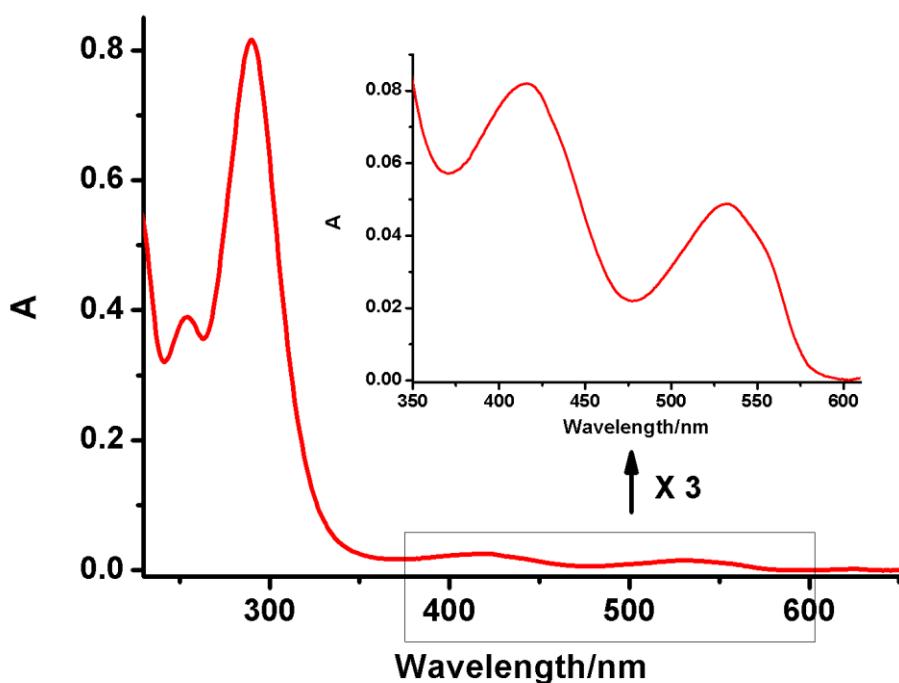
**Figure S24.** UV/vis spectra of **4e** in DCM ( $C = 6.57 \times 10^{-6}$  M) at 298K. The inset shows the UV/vis spectra from 350 to 610 nm ( $C = 6.57 \times 10^{-5}$  M).



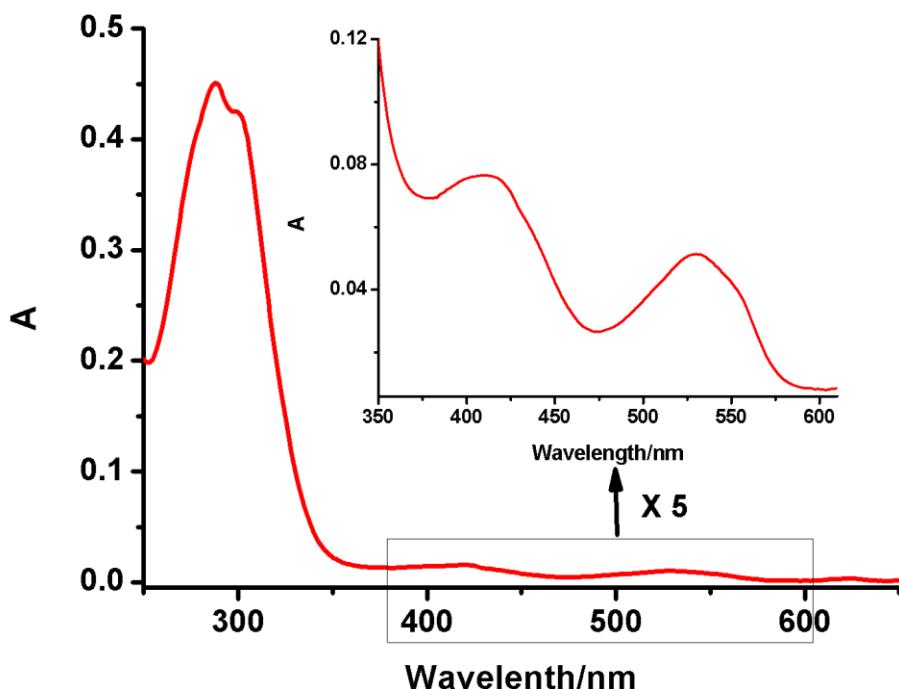
**Figure S25.** UV/vis spectra of **3f** in DCM ( $C = 1.28 \times 10^{-5}$  M) at 298K. The inset shows the UV/vis spectra from 350 to 610 nm ( $C = 1.28 \times 10^{-4}$  M).



**Figure S26.** UV/vis spectra of **4f** in DCM ( $C = 1.29 \times 10^{-5}$  M) at 298K. The inset shows the UV/vis spectra from 350 to 610 nm ( $C = 6.44 \times 10^{-5}$  M).



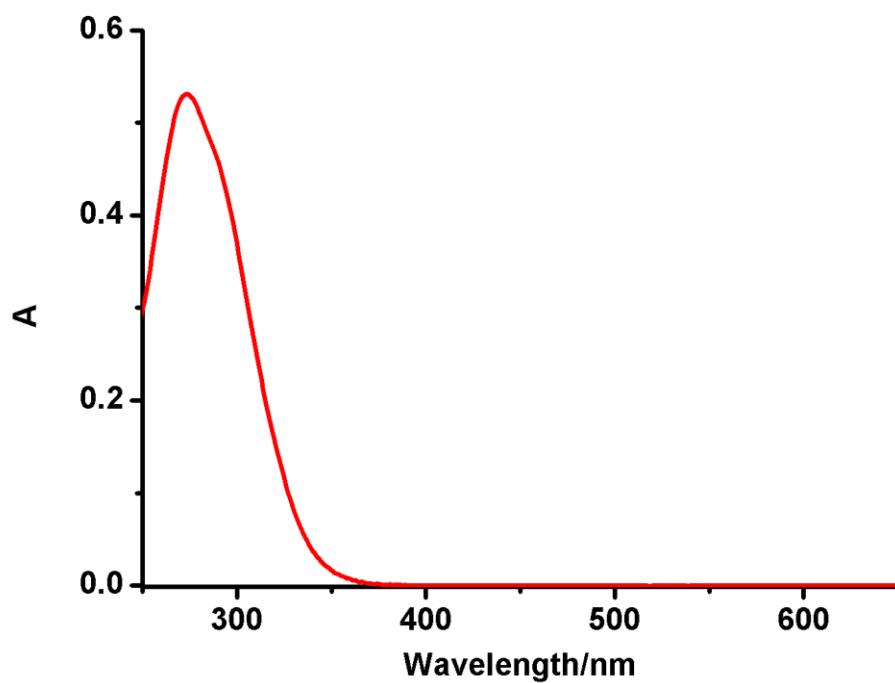
**Figure S27.** UV/vis spectra of **5f** in DCM ( $C = 1.14 \times 10^{-5}$  M) at 298K. The inset shows the UV/vis spectra from 350 to 610 nm ( $C = 3.79 \times 10^{-5}$  M).



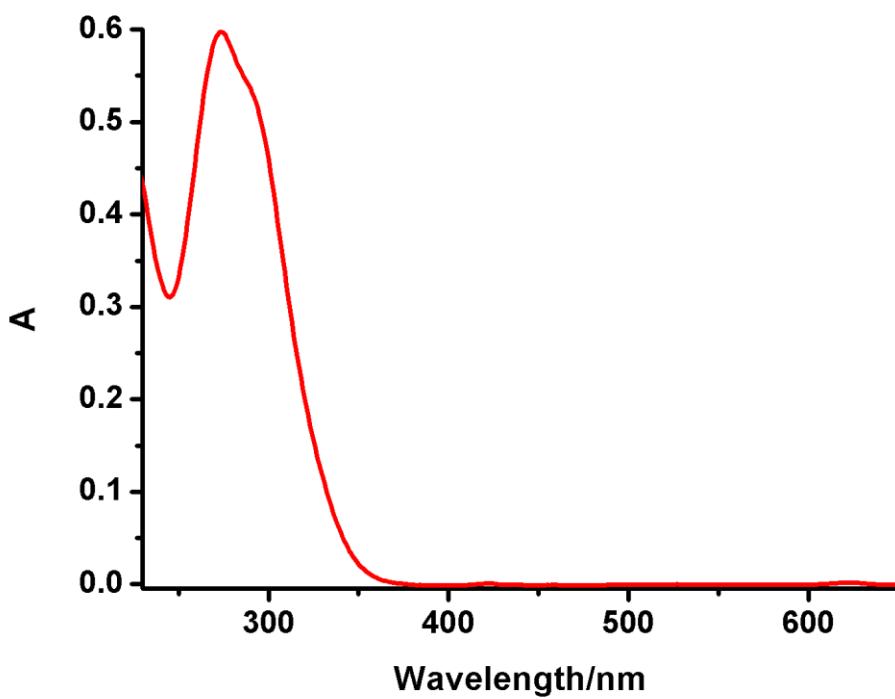
**Figure S28.** UV/vis spectra of **3g** in DCM ( $C = 8.16 \times 10^{-6}$  M) at 298K. The inset shows the UV/vis spectra from 350 to 610 nm ( $C = 4.08 \times 10^{-5}$  M).

**Table S2** The photophysical data of macrocyclic compounds **3a-f**, **4e**, **4f** and **5f**

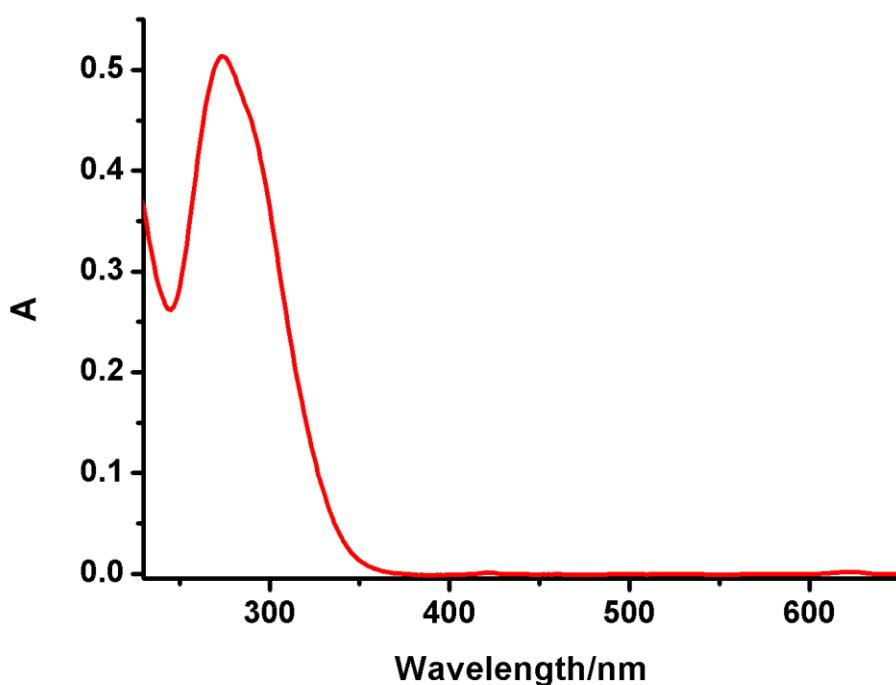
compound	C ( $10^{-6}$ mol/L)	$\lambda_1$ (nm) ( $\varepsilon_1$ [ $\times 10^3$ mol $^{-1}$ cm $^{-1}$ ] )	$\lambda_2$ (nm) ( $\varepsilon_2$ [ $\times 10^3$ mol $^{-1}$ cm $^{-1}$ ] )	$\lambda_3$ (nm) ( $\varepsilon_3$ [ $\times 10^3$ mol $^{-1}$ cm $^{-1}$ ] )	$\lambda_4$ (nm) ( $\varepsilon_3$ [ $\times 10^3$ mol $^{-1}$ cm $^{-1}$ ] )
<b>3e</b>	8.22	271 (56.56)	293 (56.73)	409 (1.57)	533 (1.08)
<b>4e</b>	6.57	272 (81.95)	294 (96.85)	403 (2.76)	532 (1.54)
<b>3f</b>	12.89	255 (30.81)	292 (44.39)	418 (1.40)	532 (0.96)
<b>4f</b>	12.89	254 (40.41)	290 (79.81)	414 (2.56)	532 (1.51)
<b>5f</b>	11.37	254 (34.24)	290 (71.76)	417 (2.17)	532 (1.29)
<b>3g</b>	8.16	288 (55.25)	299 (52.11)	412 (1.87)	531 (1.26)



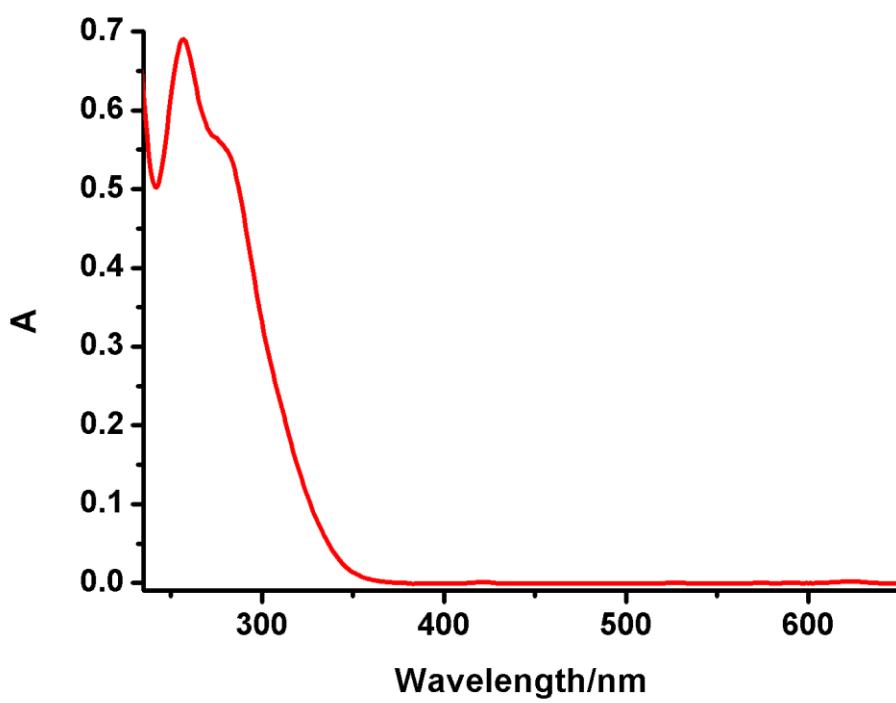
**Figure S29.** UV/vis spectra of **7b** in DCM ( $C = 9.19 \times 10^{-6}$  M) at 298K



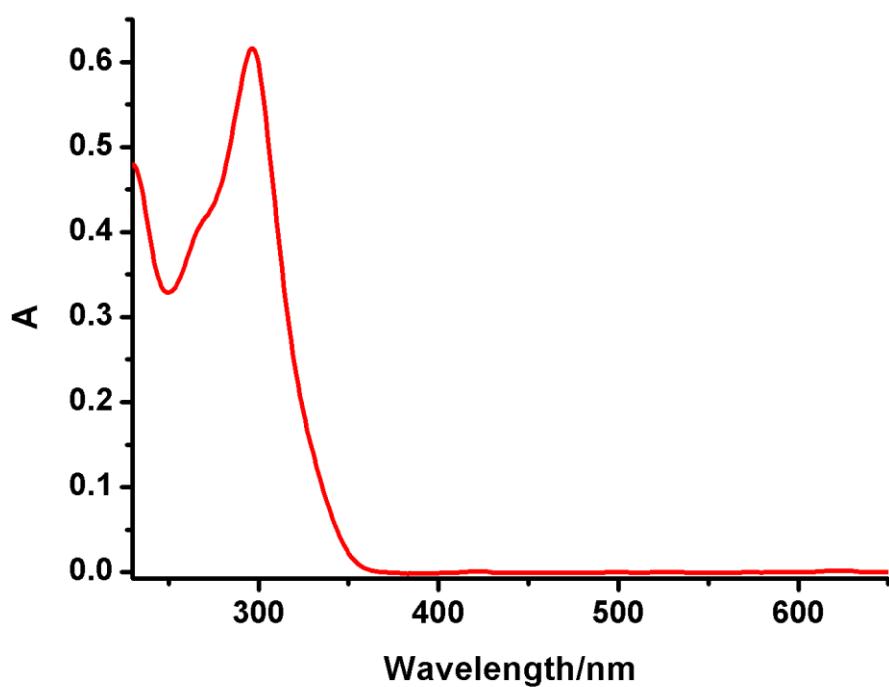
**Figure S30.** UV/vis spectra of **7d** in DCM ( $C = 3.21 \times 10^{-5}$  M) at 298K.



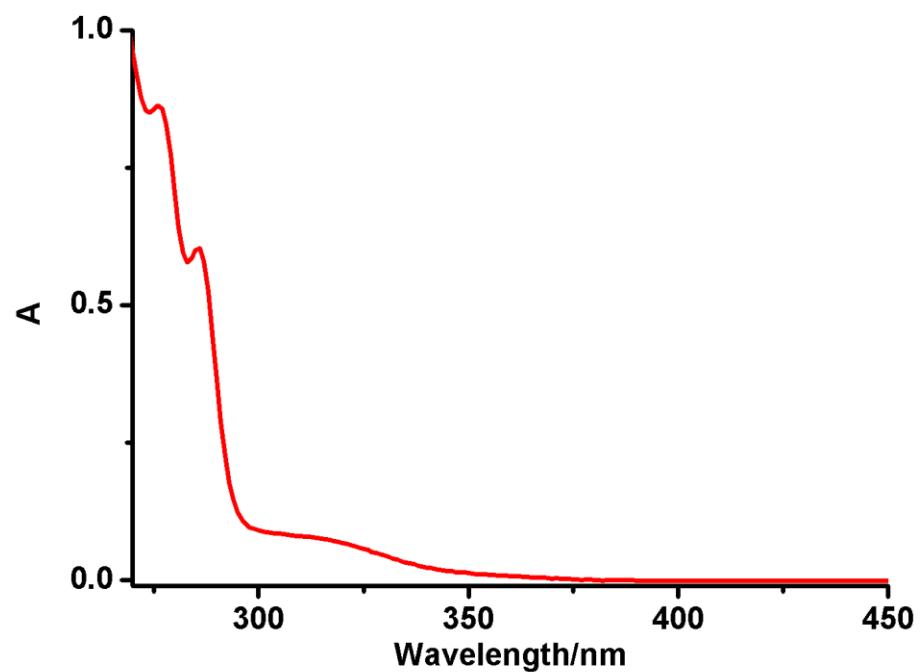
**Figure S31.** UV/vis spectra of **7e** in DCM ( $C = 7.73 \times 10^{-6}$  M) at 298K.



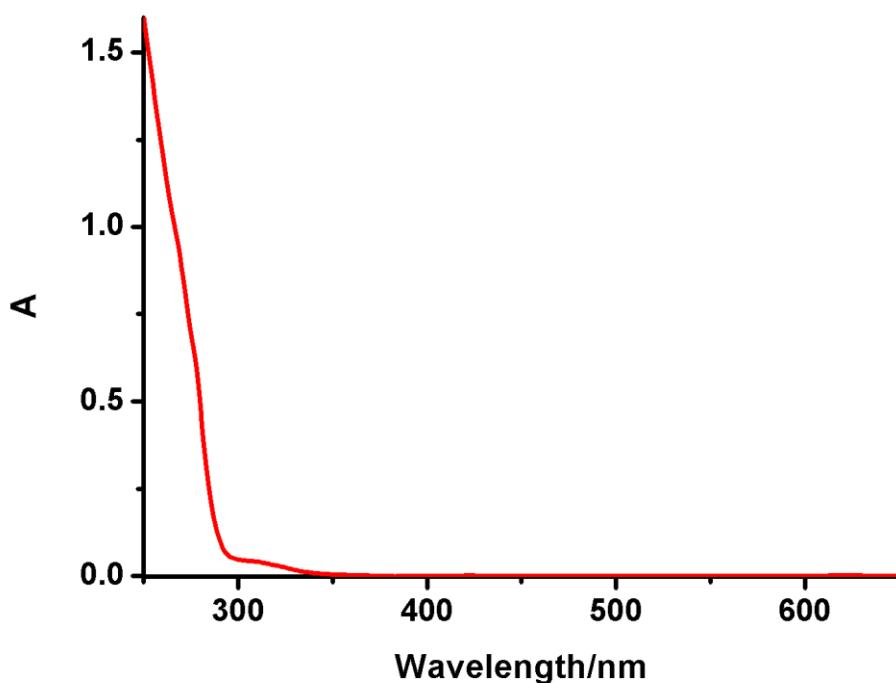
**Figure S32.** UV/vis spectra of **7f** in DCM ( $C = 1.69 \times 10^{-5}$  M) at 298K.



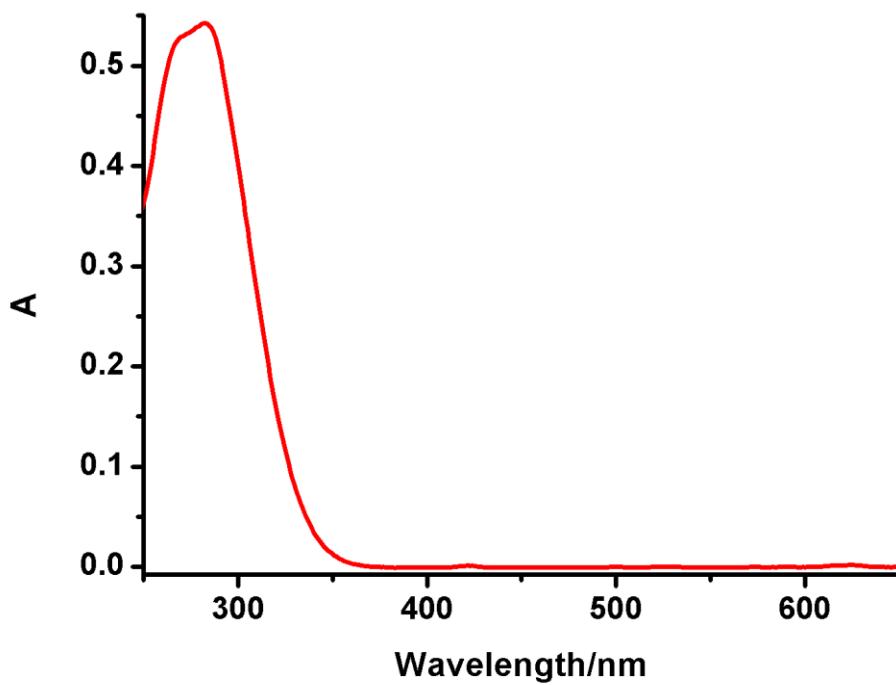
**Figure S33.** UV/vis spectra of **7g** in DCM ( $C = 1.25 \times 10^{-5}$  M) at 298K.



**Figure S34.** UV/vis spectra of **8b** in DCM ( $C = 1.23 \times 10^{-4}$  M) at 298K.



**Figure S35.** UV/vis spectra of **8d** in DCM ( $C = 5.23 \times 10^{-5}$  M) at 298K.

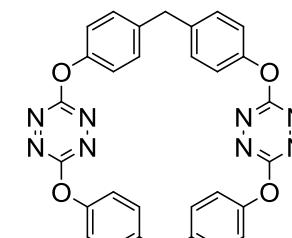
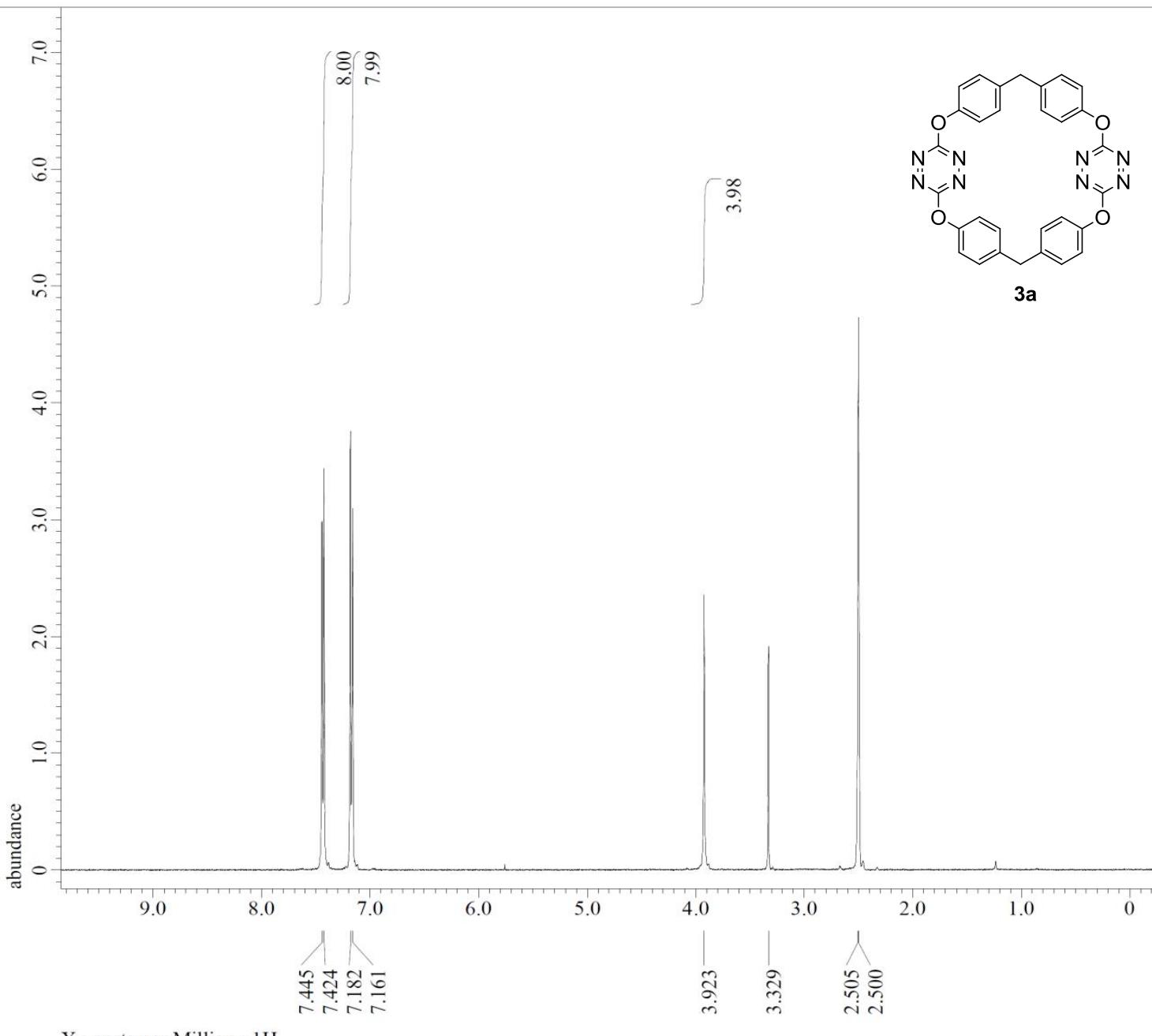


**Figure S36.** UV/vis spectra of **9** in DCM ( $C = 1.15 \times 10^{-5}$  M) at 298K.

**Table S3** The photophysical data of macrocyclic compounds **7a-g**, **8b-d** and **9**

compound	C ( $10^{-5}$ mol/L)	$\lambda_1$ (nm) ( $\epsilon_1$ [ $\times 10^3$ mol $^{-1}$ cm $^{-1}$ ] )
<b>7b</b>	0.92	273 (57.77)
<b>7d</b>	3.21	274 (65.17)
<b>7e</b>	0.77	274 (66.72)
<b>7f</b>	1.69	257 (40.88)
<b>7g</b>	1.25	297 (49.08)
<b>8b</b>	12.34	286 (4.88)
<b>8d</b>	5.23	286 (4.88)
<b>9</b>	1.15	282 (47.03)

**4. Copies of  $^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra**



**JEOL**  
**RESONANCE**

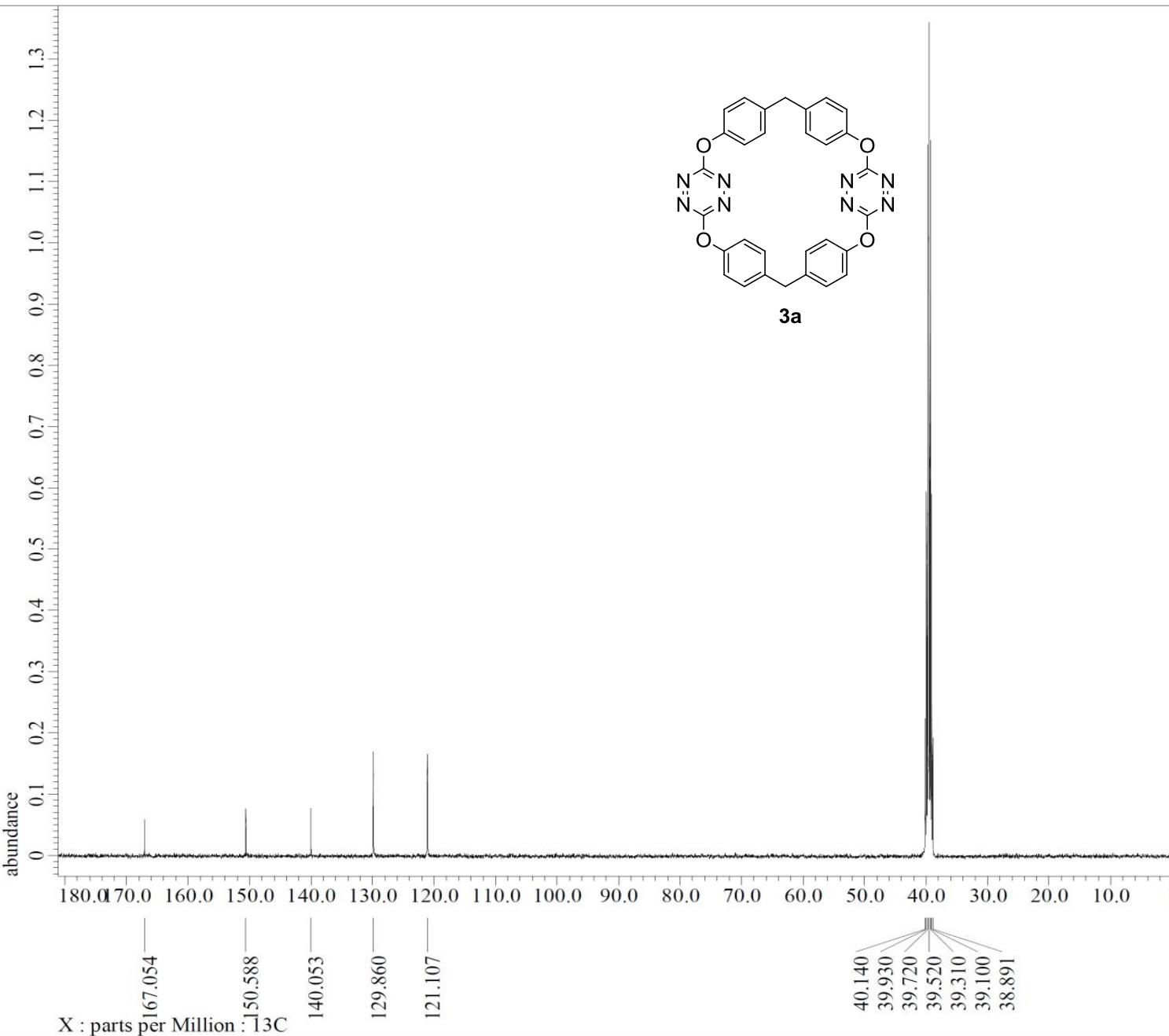
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**JEOL**  
**RESONANCE**

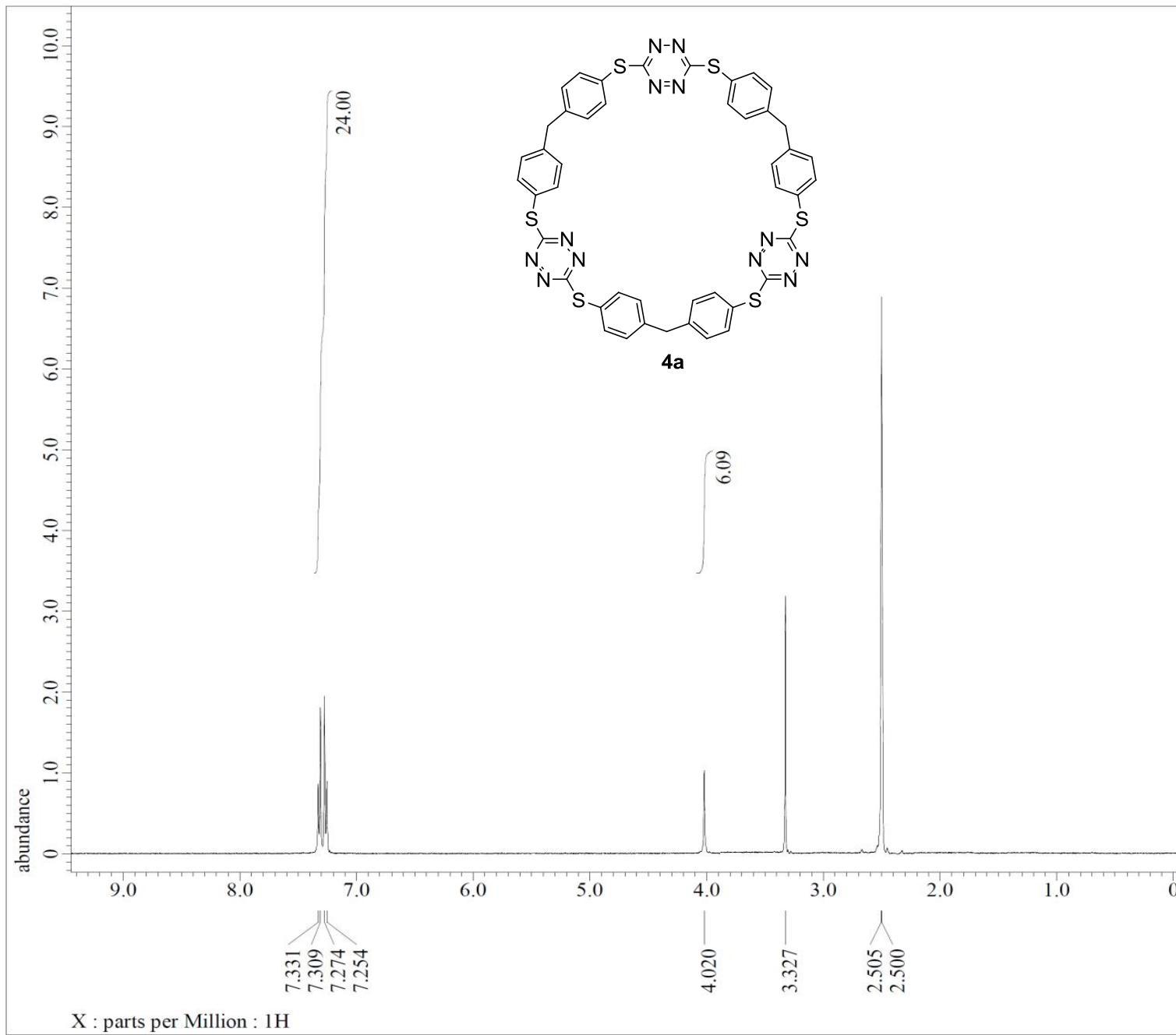
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**JEOL**  
**RESONANCE**

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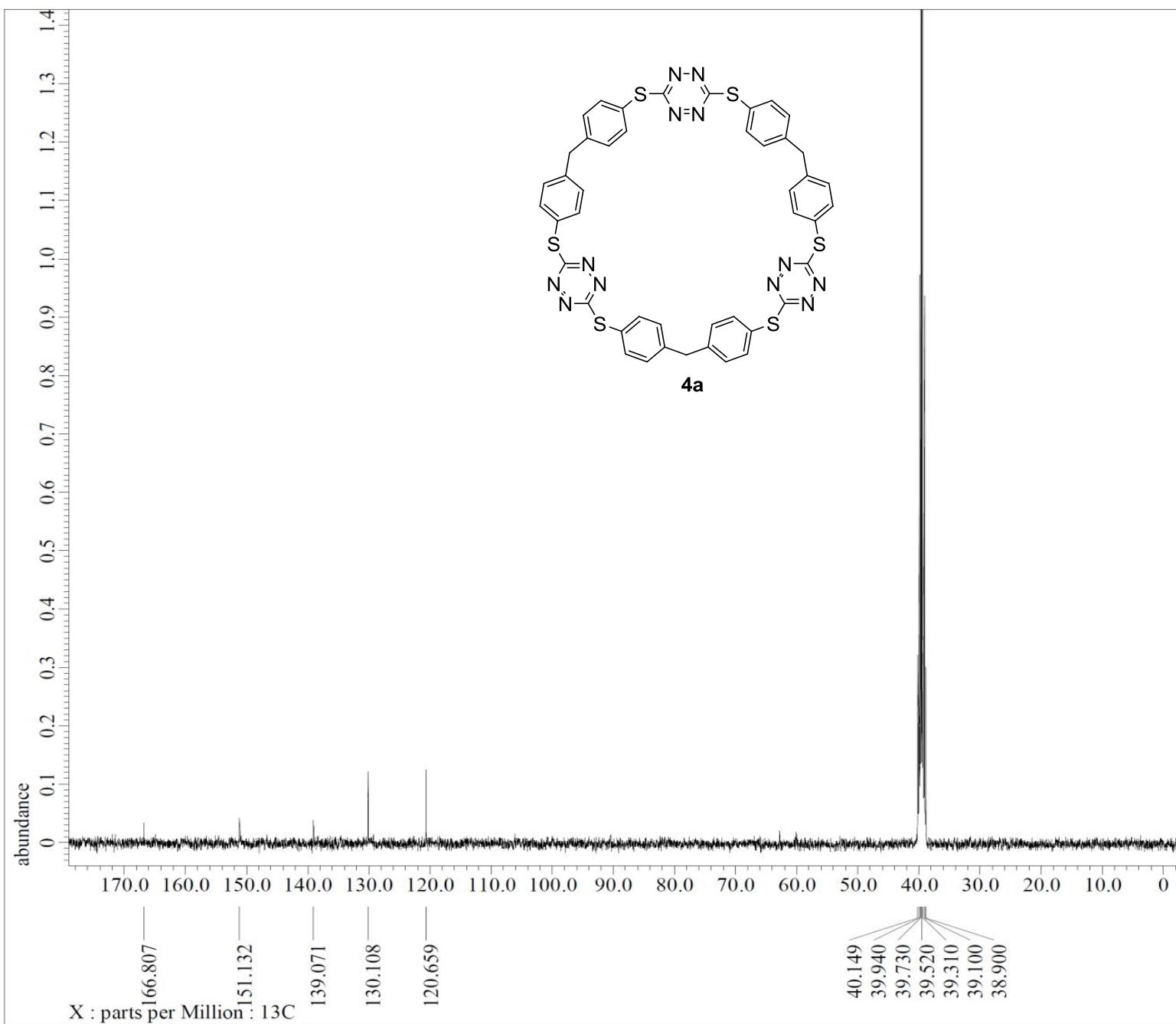
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X : parts per Million : 1H



**JEOL**  
**RESONANCE**

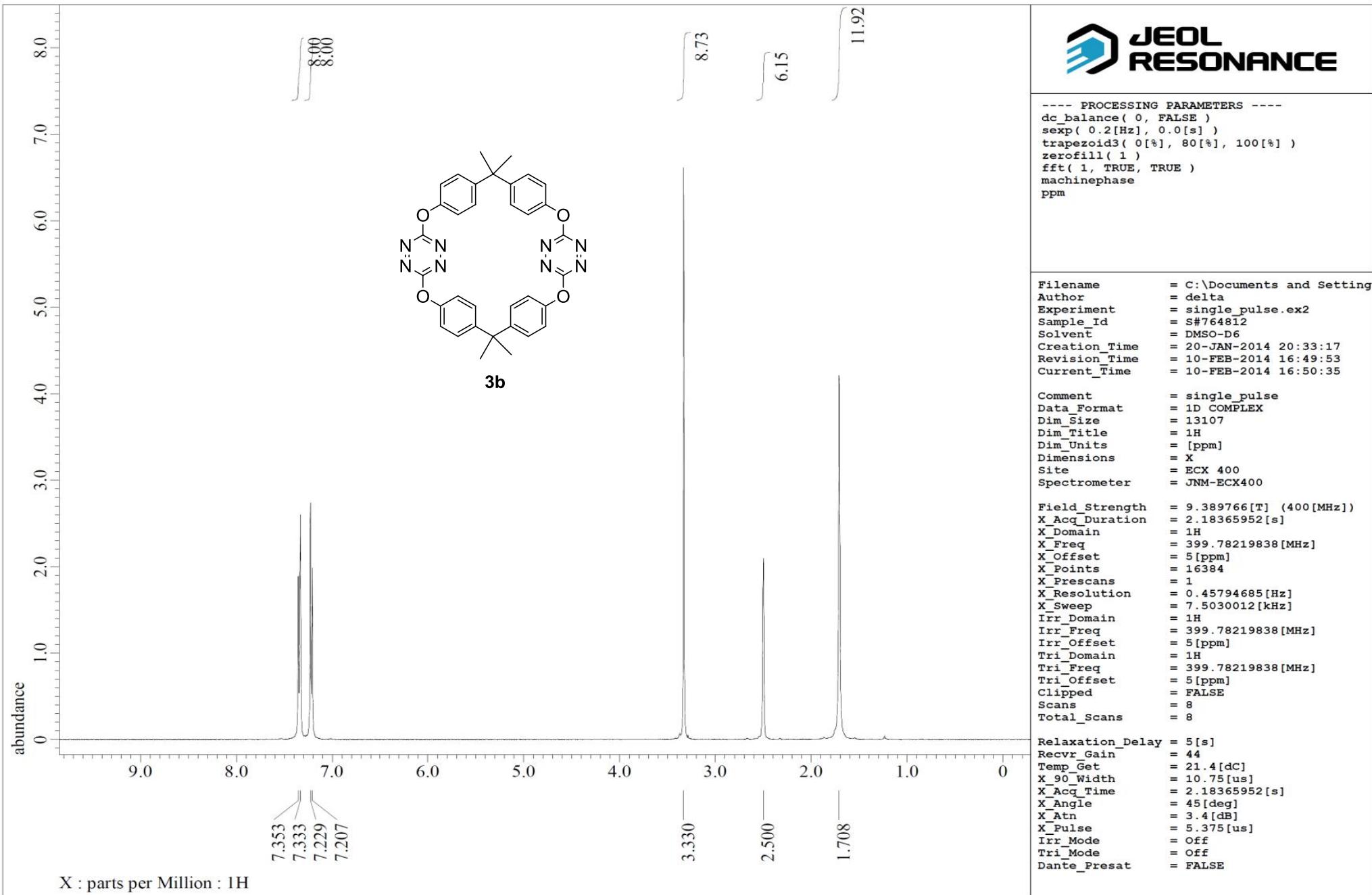
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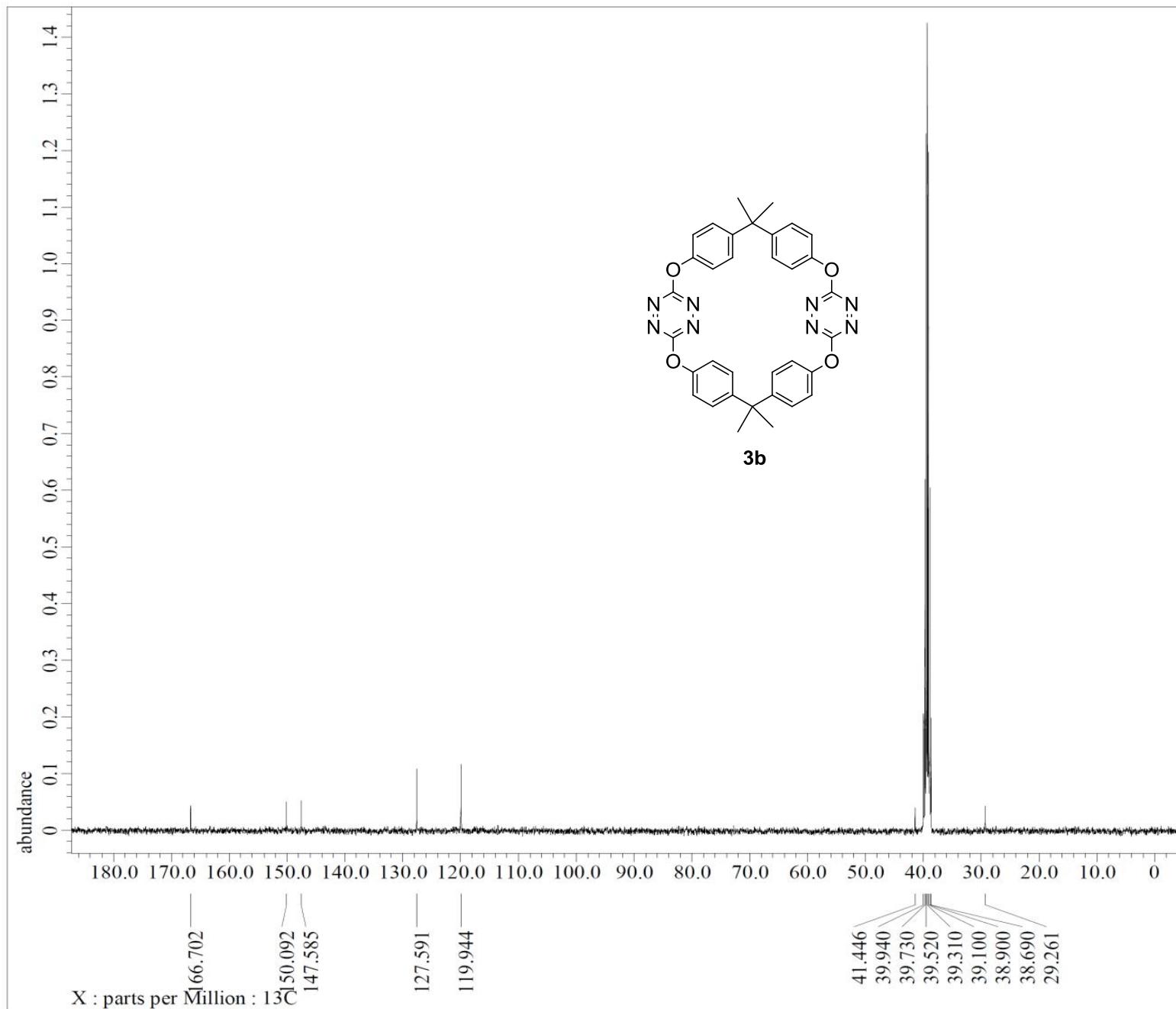
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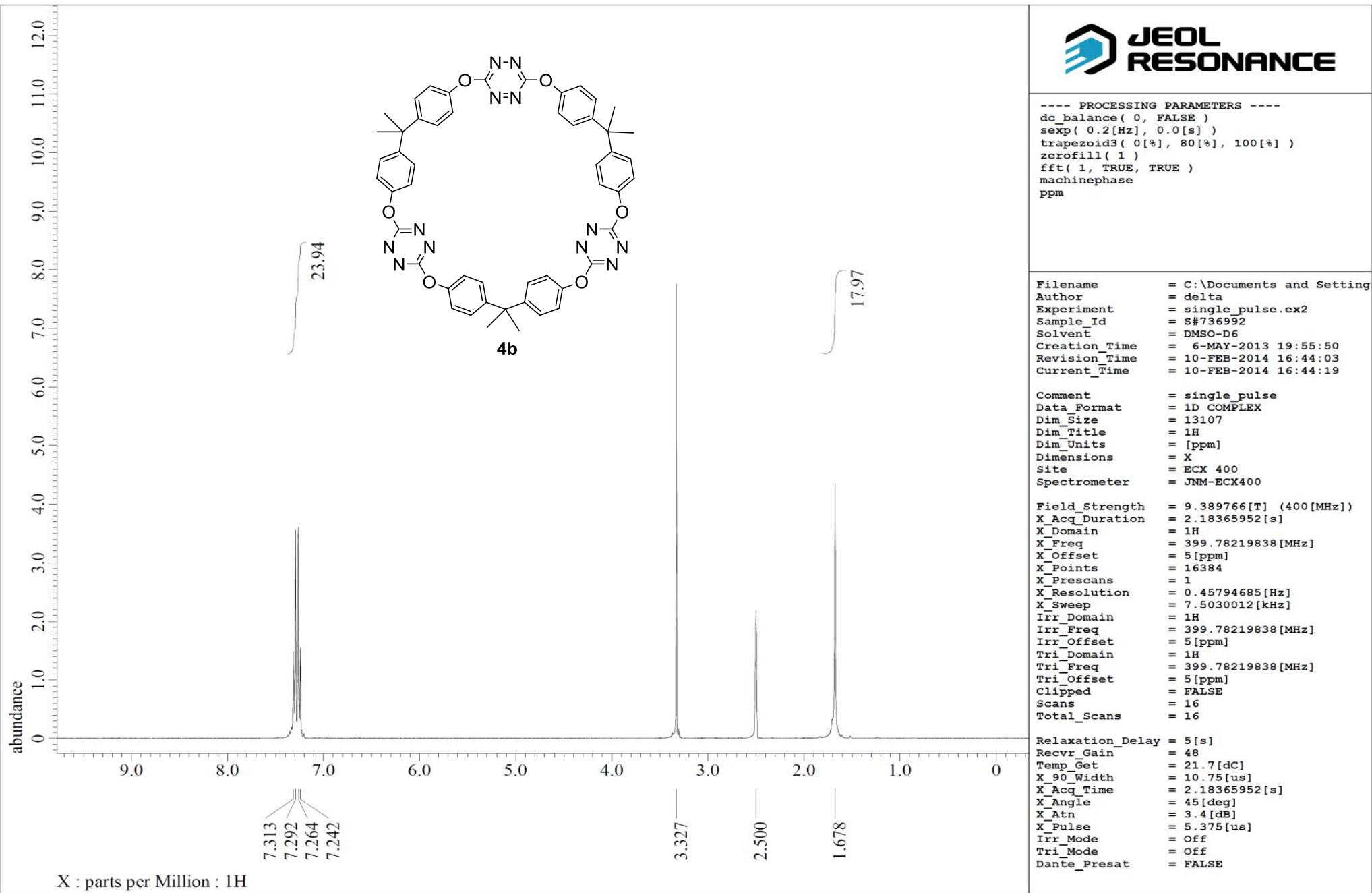


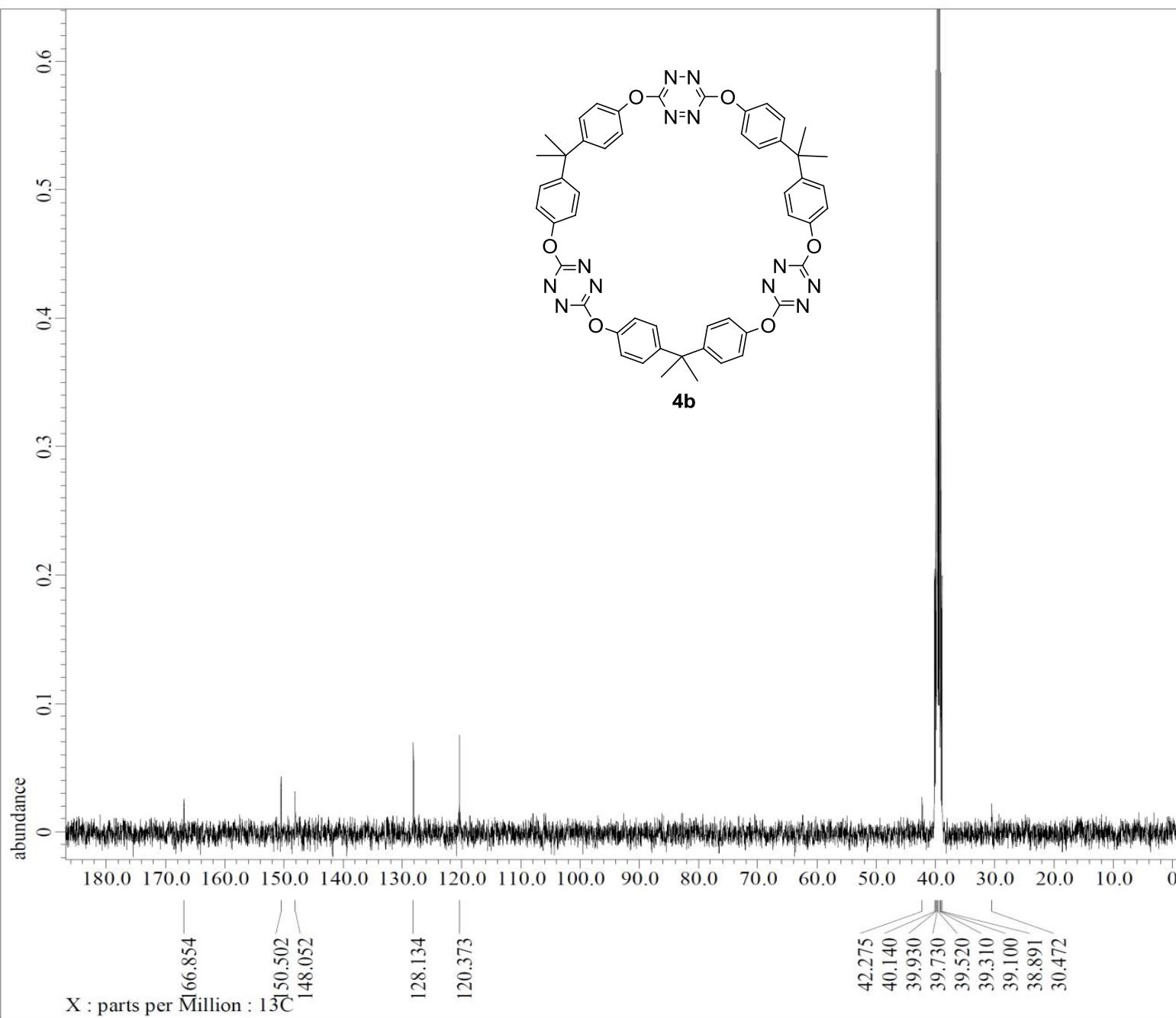


**JEOL**  
**RESONANCE**

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Scans = 253.0  
Total\_Scans = 253.0  
Relaxation\_Delay = 2[s]  
Recvr\_Gain = 54  
Temp\_Get = 21.8[dC]  
X\_90\_Width = 8.75[us]  
X\_Acq\_Time = 1.04333312[s]  
X\_Angle = 30[deg]  
X\_Atn = 7.8[dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE





**JEOL**  
**RESONANCE**

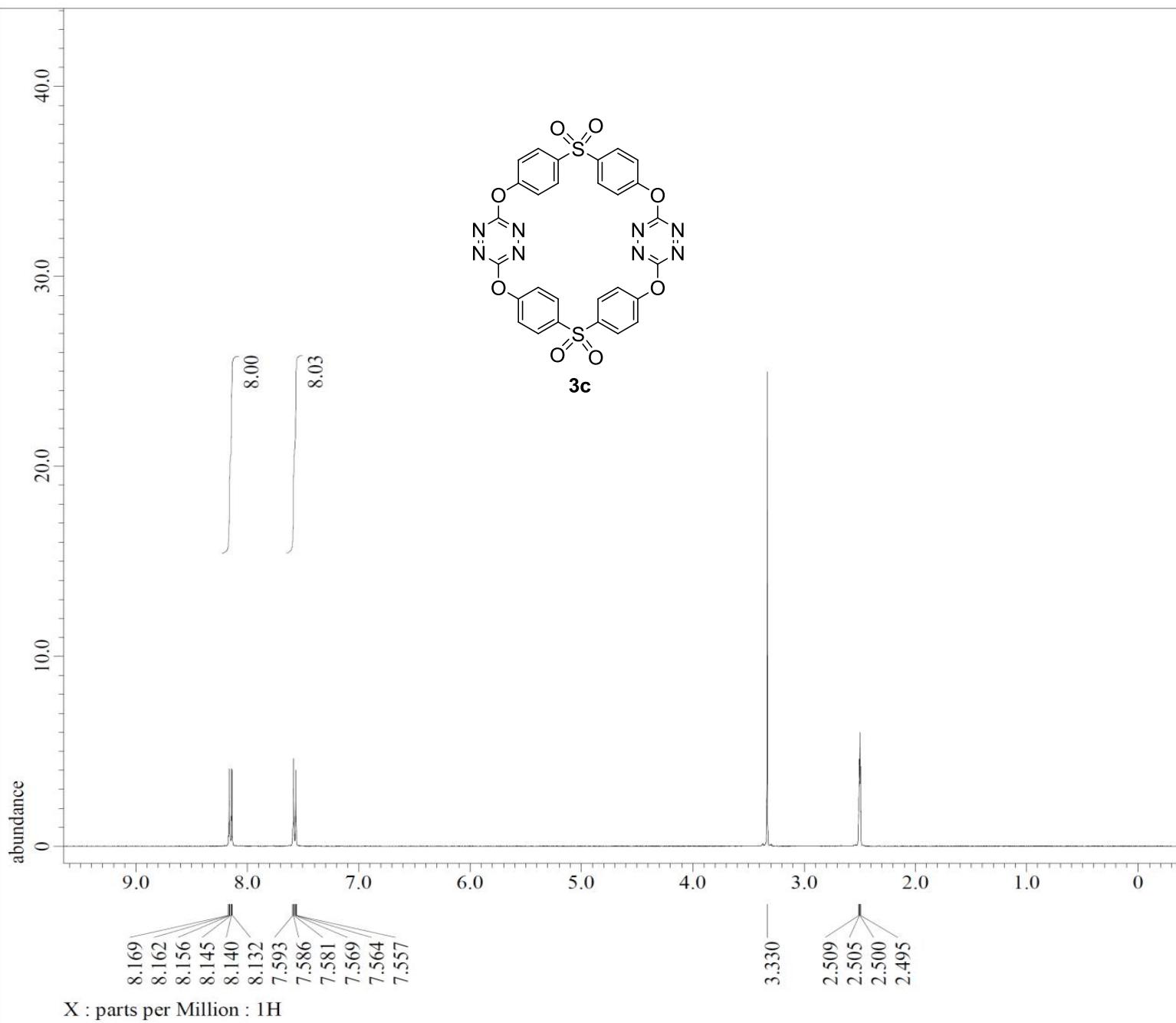
---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
sexp( 2.0[Hz], 0.0[s] )  
trapezoid3( 0[%], 80[%], 100[%] )  
zerofill( 1 )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm

Filename = C:\Documents and Setting  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_Id = S#780314  
Solvent = DMSO-D6  
Creation\_Time = 6-MAY-2013 21:10:15  
Revision\_Time = 10-FEB-2014 16:33:27  
Current\_Time = 10-FEB-2014 16:34:01

Comment = single pulse decoupled g  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
Dim\_Title =  $^{13}\text{C}$   
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 1.04333312[s]  
X\_Domain =  $^{13}\text{C}$   
X\_Freq = 100.52530333[MHz]  
X\_Offset = 100 [ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 0.95846665[Hz]  
X\_Sweep = 31.40703518[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5 [ppm]  
Clipped = FALSE  
Scans = 80  
Total\_Scans = 80

Relaxation\_Delay = 2[s]  
Recv\_Gain = 54  
Temp\_Get = 21.7[dC]  
X\_90\_Width = 8.75[us]  
X\_Acq\_Time = 1.04333312[s]  
X\_Angle = 30[deg]  
X\_Atn = 7.8[dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE



**JEOL**  
**RESONANCE**

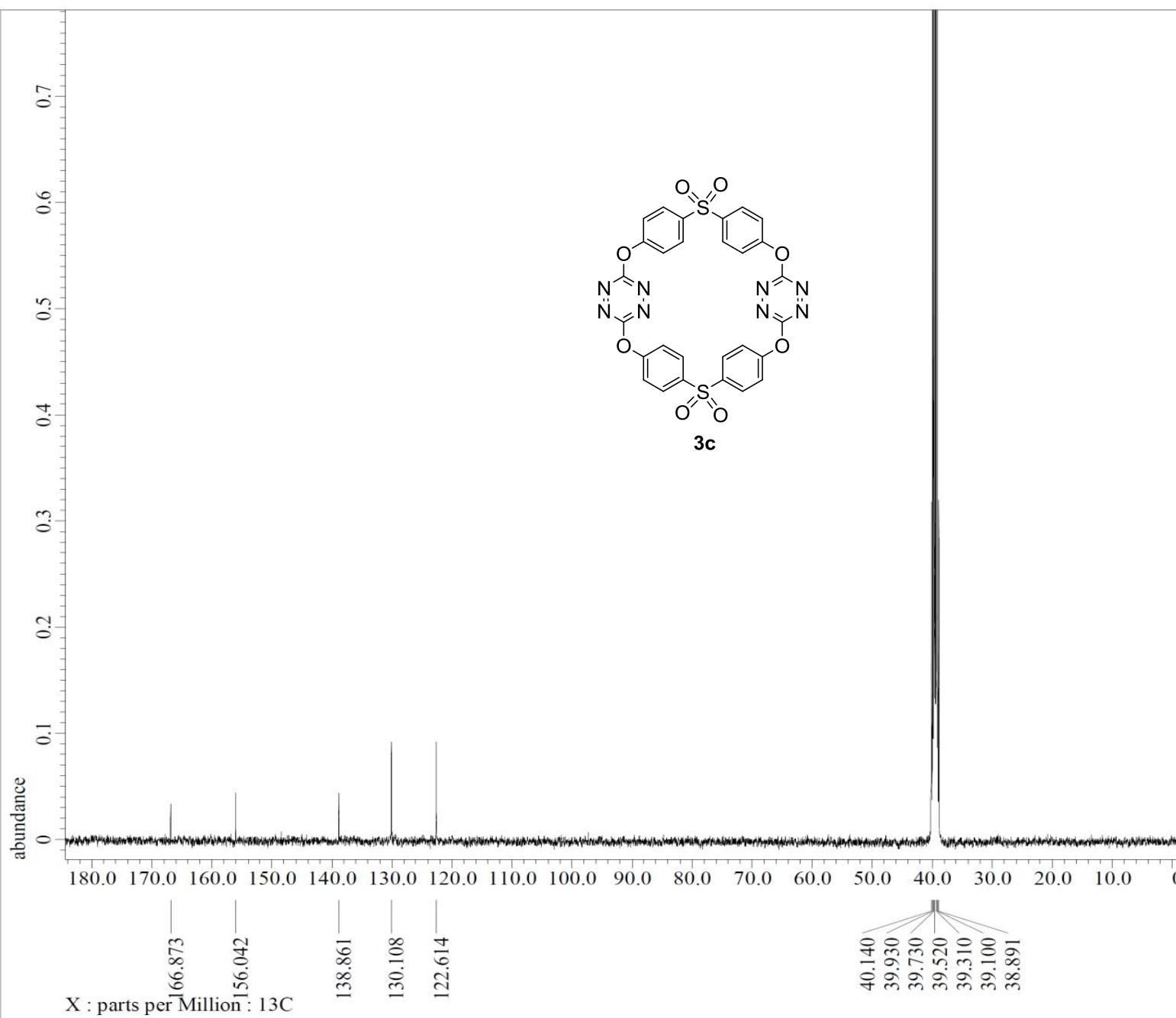
---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
sexp( 0.2[Hz], 0.0[s] )  
trapezoid3( 0[%], 80[%], 100[%] )  
zerofill( 1 )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm

Filename = C:\Documents and Setting  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#807072  
Solvent = DMSO-D6  
Creation\_Time = 5-JUN-2013 21:51:17  
Revision\_Time = 10-FEB-2014 19:32:23  
Current\_Time = 10-FEB-2014 19:33:06

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8

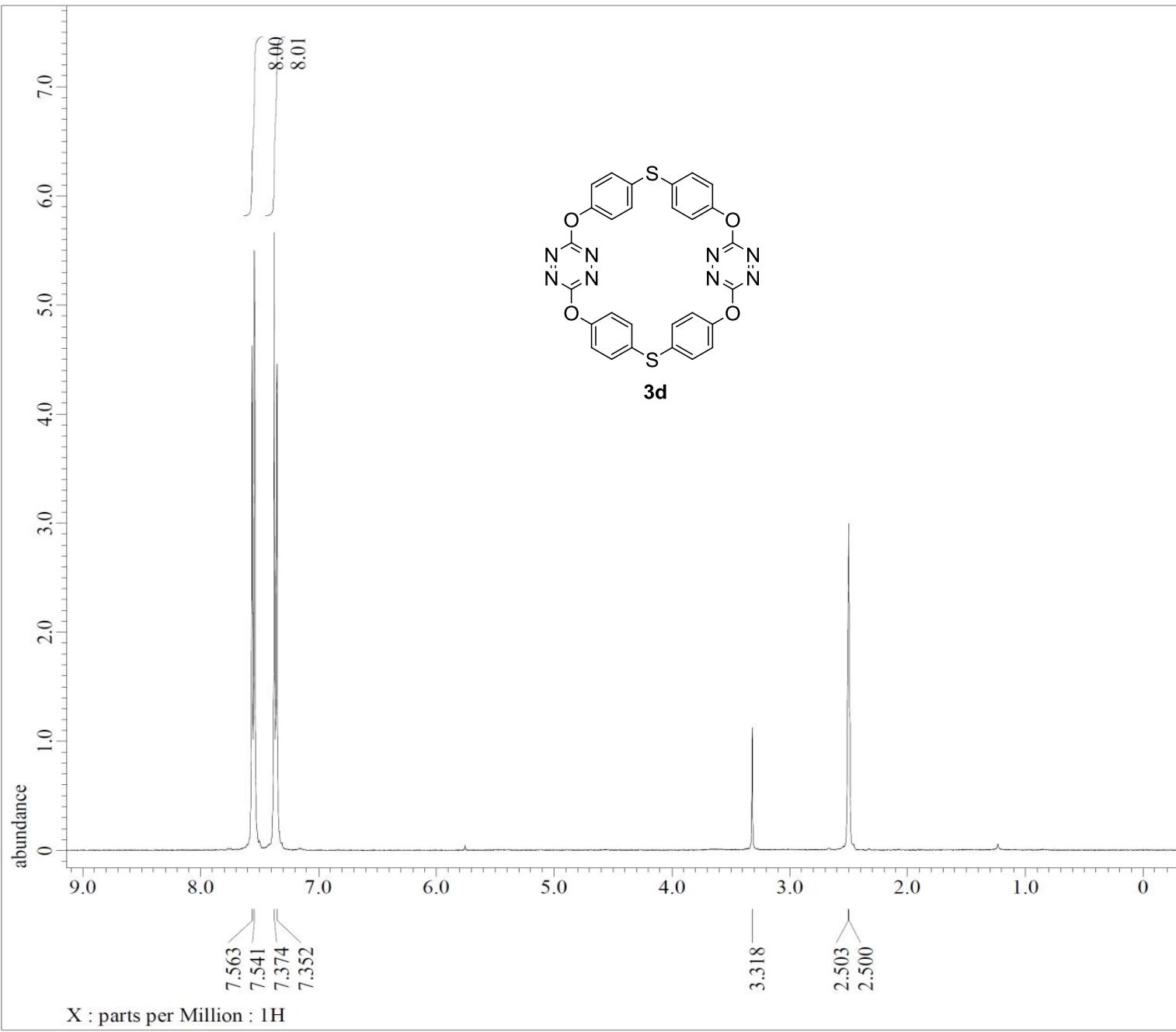
Relaxation\_Delay = 5[s]  
Recv\_Gain = 50  
Temp\_Get = 20.9[dC]  
X\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[dB]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE



**JEOL**  
**RESONANCE**

---- PROCESSING PARAMETERS ----  
dc\_balance( 0 , FALSE )  
sexp( 2.0[Hz] 0.0[s] )  
trapezoid3( 0[%], 80[%], 100[%] )  
zerofill( 1 )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm

Filename = C:\Documents and Setting  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_Id = S#808063  
Solvent = DMSO-D6  
Creation\_Time = 5-JUN-2013 22:41:23  
Revision\_Time = 10-FEB-2014 19:28:30  
Current\_Time = 10-FEB-2014 19:28:49  
Comment = single pulse decoupled g  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
Dim\_Title =  $^{13}\text{C}$   
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400  
Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 1.04333312[s]  
X\_Domain =  $^{13}\text{C}$   
X\_Freq = 100.52530333[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 0.95846665[Hz]  
X\_Sweep = 31.40703518[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 963  
Total\_Scans = 963  
Relaxation\_Delay = 2[s]  
Recv\_Gain = 58  
Temp\_Get = 20.1[dC]  
X\_90\_Width = 8.75[us]  
X\_Acq\_Time = 1.04333312[s]  
X\_Angle = 30[deg]  
X\_Atn = 7.8[dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE



**JEOL**  
**RESONANCE**

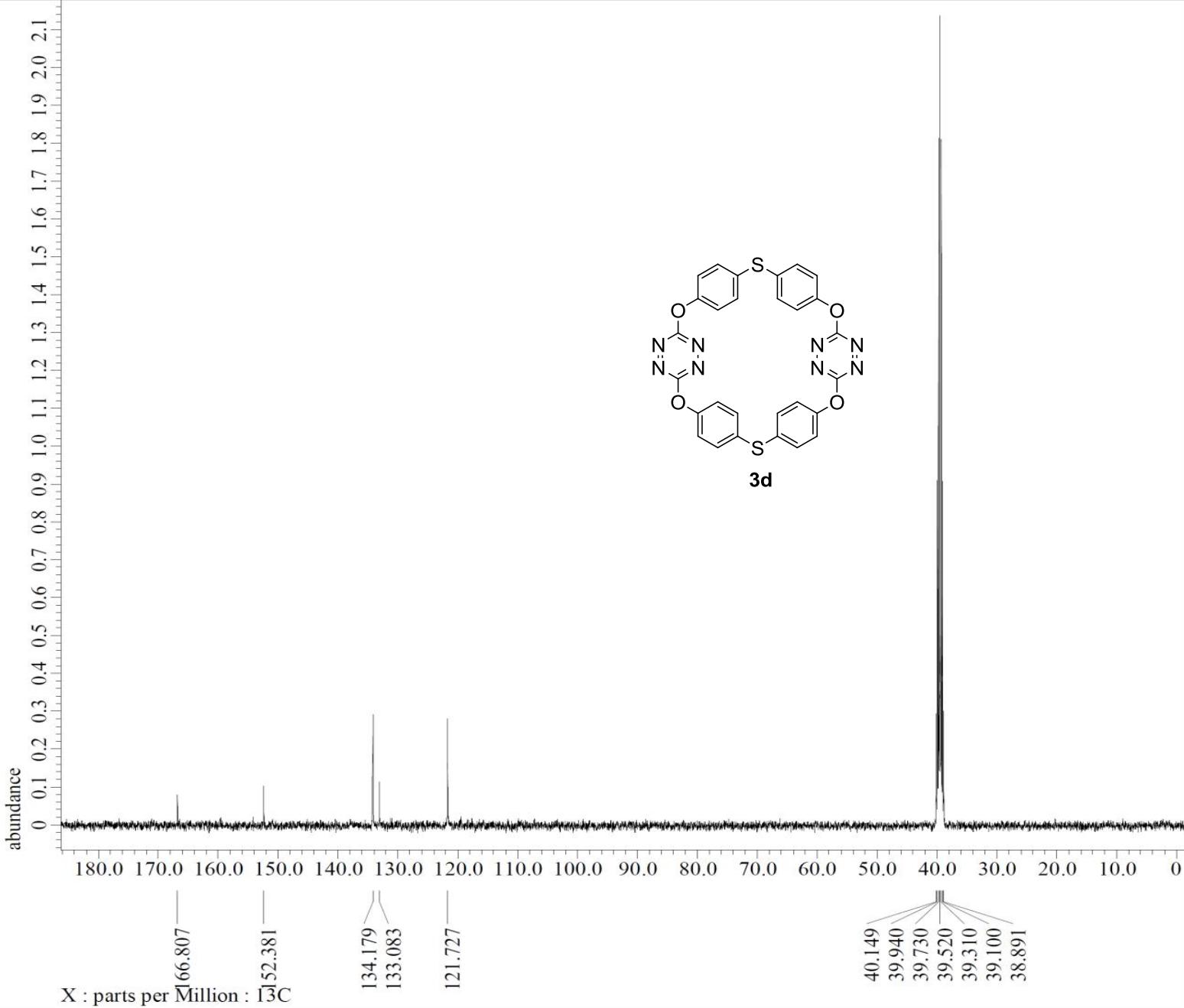
---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
sexp( 0.2[Hz], 0.0[s] )  
trapezoid3( 0[%], 80[%], 100[%] )  
zerofill( 1 )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm

Filename = C:\Documents and Setting  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#743925  
Solvent = DMSO-D6  
Creation\_Time = 19-JAN-2014 19:57:59  
Revision\_Time = 10-FEB-2014 19:36:27  
Current\_Time = 10-FEB-2014 19:36:52

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8

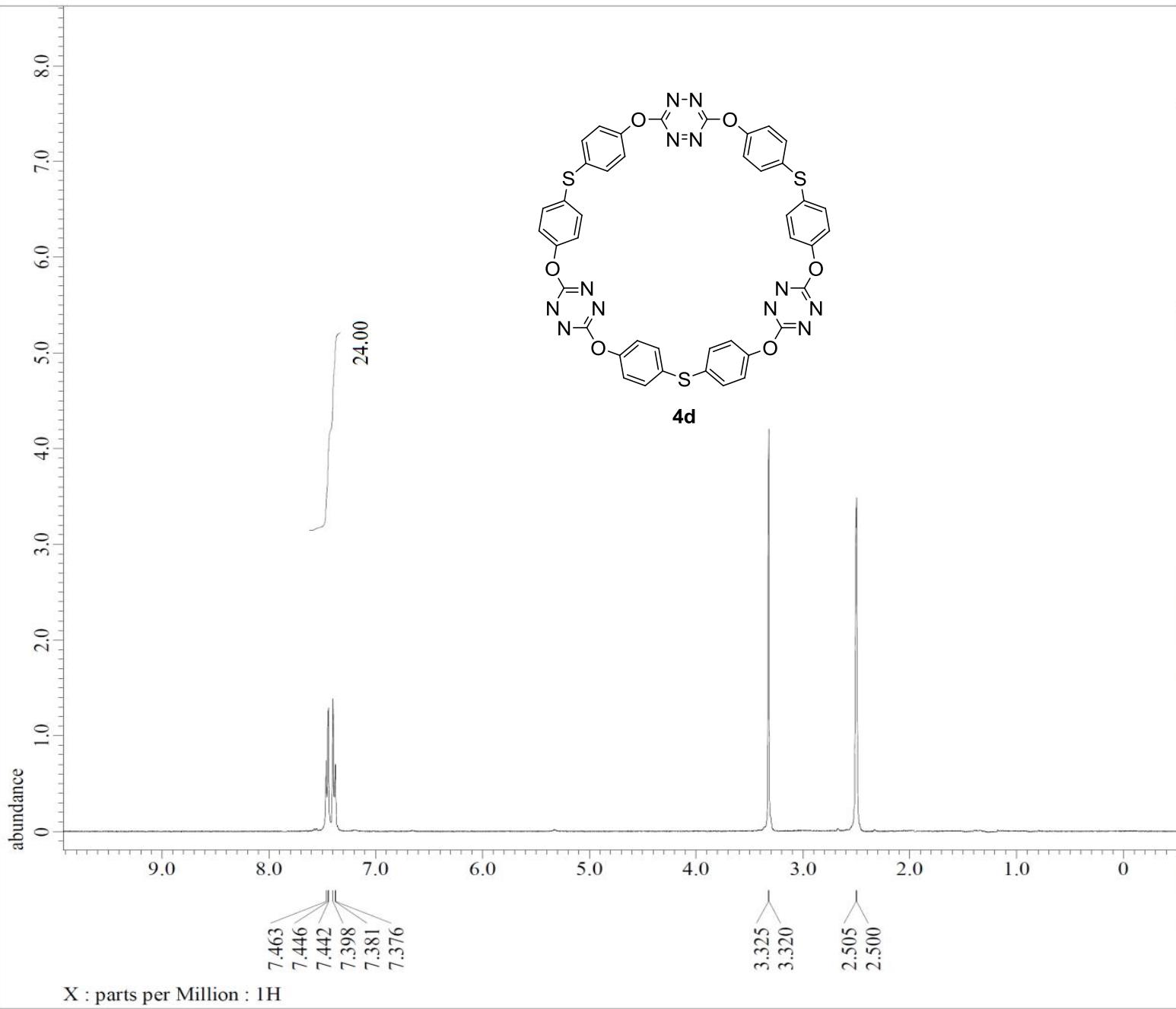
Relaxation\_Delay = 5[s]  
Recvr\_Gain = 48  
Temp\_Get = 23.1[dC]  
X\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[dB]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE



**JEOL**  
**RESONANCE**

---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
sexp( 2.0[Hz], 0.0[s] )  
trapezoid3( 0[%], 80[%], 100[%] )  
zerofill( 1 )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm

Filename = C:\Documents and Settings  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_Id = S#745045  
Solvent = DMSO-D6  
Creation\_Time = 19-JAN-2014 20:07:34  
Revision\_Time = 10-FEB-2014 19:34:08  
Current\_Time = 10-FEB-2014 19:34:31  
Comment = single pulse decoupled g  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
Dim\_Title = 13C  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400  
Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 1.04333312[s]  
X\_Domain = 13C  
X\_Freq = 100.52530333[MHz]  
X\_Offset = 100 [ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 0.95846665[Hz]  
X\_Sweep = 31.40703518[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5 [ppm]  
Clipped = FALSE  
Scans = 136  
Total\_Scans = 136  
Relaxation\_Delay = 2[s]  
Recv\_Gain = 58  
Temp\_Get = 23.1[dC]  
X\_90\_Width = 8.75[us]  
X\_Acq\_Time = 1.04333312[s]  
X\_Angle = 30[deg]  
X\_Atn = 7.8[dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE



**JEOL**  
**RESONANCE**

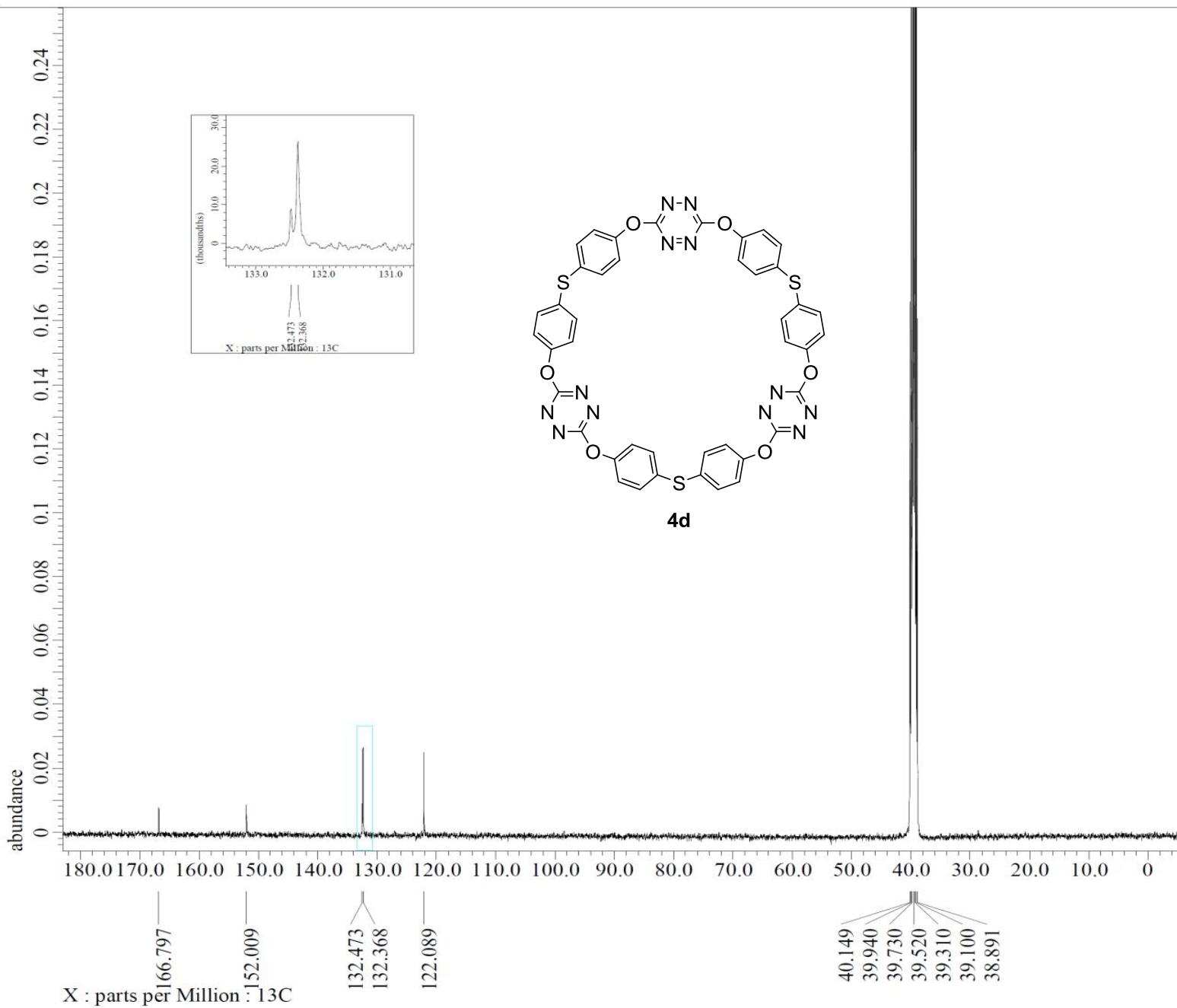
---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 0.2[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

Filename = C:\Documents and Setting  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#647324  
Solvent = DMSO-D6  
Creation\_Time = 28-JAN-2014 17:16:46  
Revision\_Time = 10-FEB-2014 19:50:59  
Current\_Time = 10-FEB-2014 19:51:21

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 50  
Temp\_Get = 22.7[dC]  
X\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[db]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE



**JEOL**  
**RESONANCE**

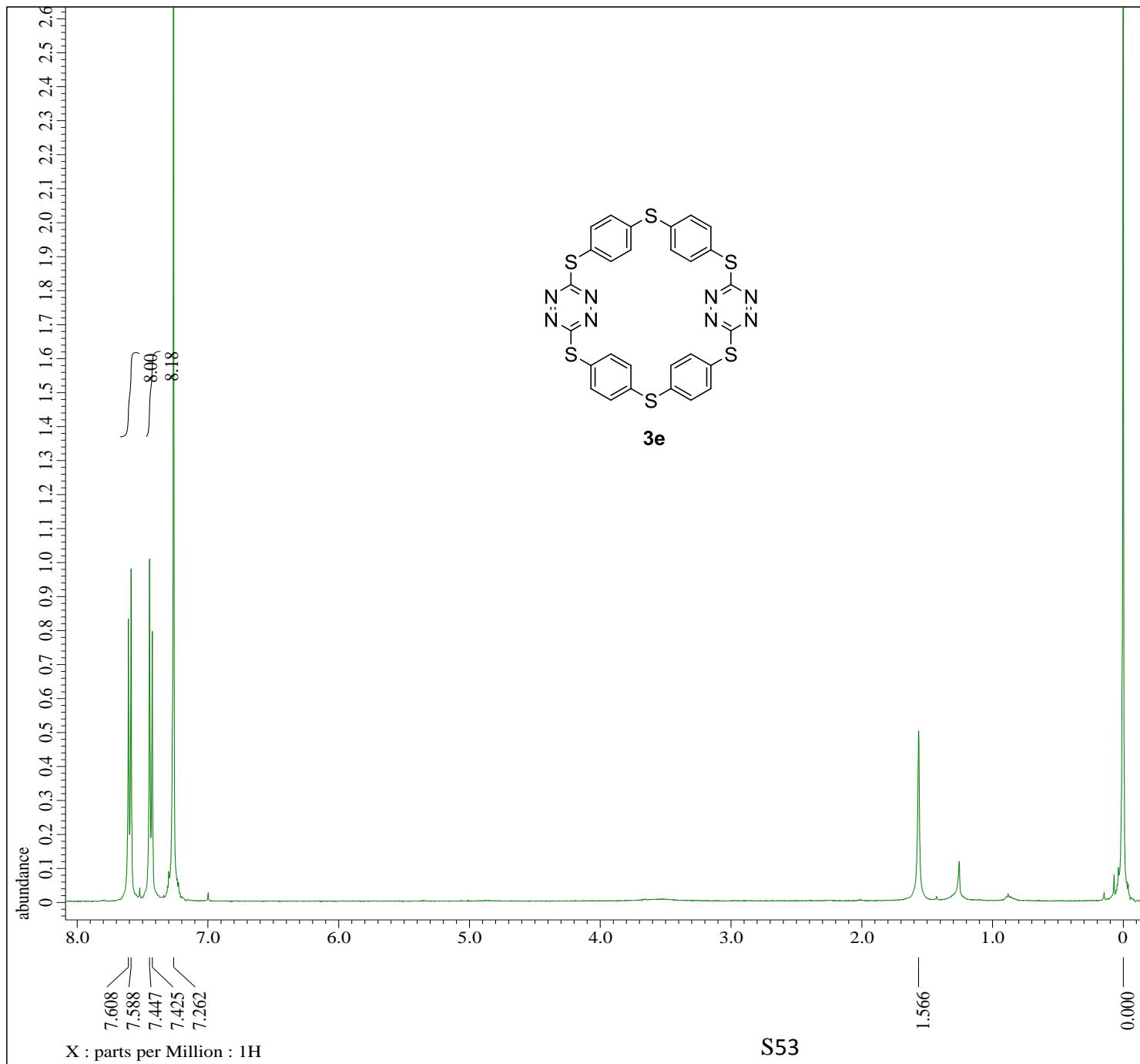
---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
sexp( 2.0[Hz], 0.0[s] )  
trapezoid3( 0[%], 80[%], 100[%] )  
zerofill( 1 )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm

Filename = C:\Documents and Settings  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_Id = S#723131  
Solvent = DMSO-D6  
Creation\_Time = 29-JAN-2014 03:49:41  
Revision\_Time = 10-FEB-2014 19:55:22  
Current\_Time = 10-FEB-2014 19:56:51

Comment = single pulse decoupled g  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
Dim\_Title = <sup>13</sup>C  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 1.04333312[s]  
X\_Domain = <sup>13</sup>C  
X\_Freq = 100.52530333[MHz]  
X\_Offset = 100 [ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 0.95846665[Hz]  
X\_Sweep = 31.40703518[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5 [ppm]  
Clipped = FALSE  
Scans = 10000  
Total\_Scans = 10000

Relaxation\_Delay = 2[s]  
Recv\_Gain = 54  
Temp\_Get = 24[dC]  
X\_90\_Width = 8.75[us]  
X\_Acq\_Time = 1.04333312[s]  
X\_Angle = 30[deg]  
X\_Atn = 7.8[dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE



**JEOL**  
Solutions for Innovation

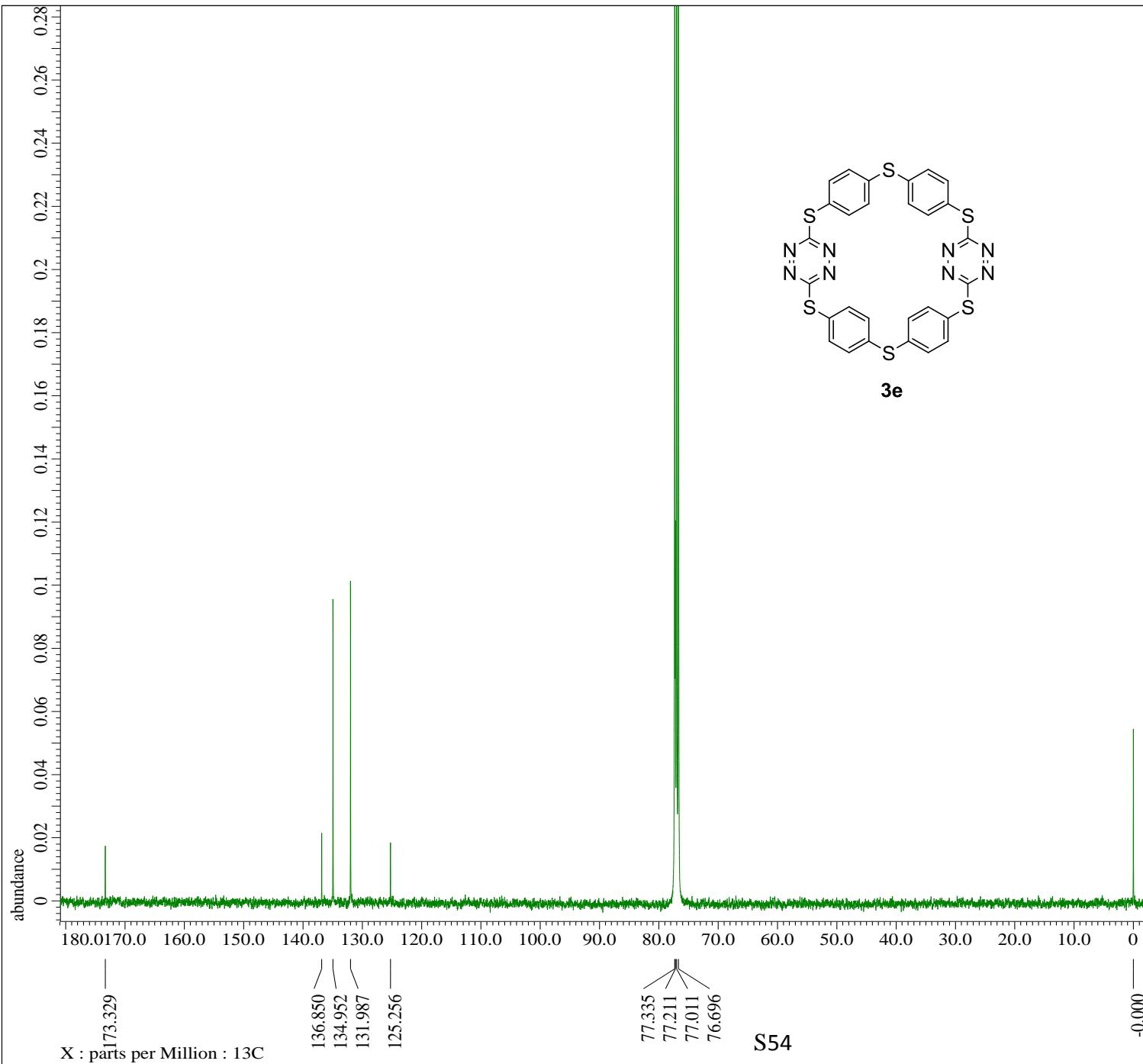
---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 0.2[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

Filename = s-ggh-221-1-20130708-4.jdf  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#755870  
Solvent = CHLOROFORM-D  
Creation\_Time = 8-JUL-2013 20:28:27  
Revision\_Time = 21-APR-2015 16:46:24  
Current\_Time = 21-APR-2015 16:46:42

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 25  
Total\_Scans = 25

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 46  
Temp\_Get = 19.5[dC]  
X\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[dB]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 7.18365952[s]



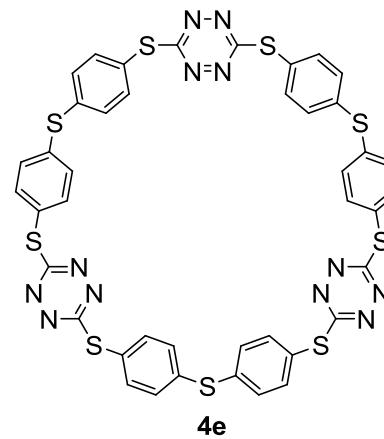
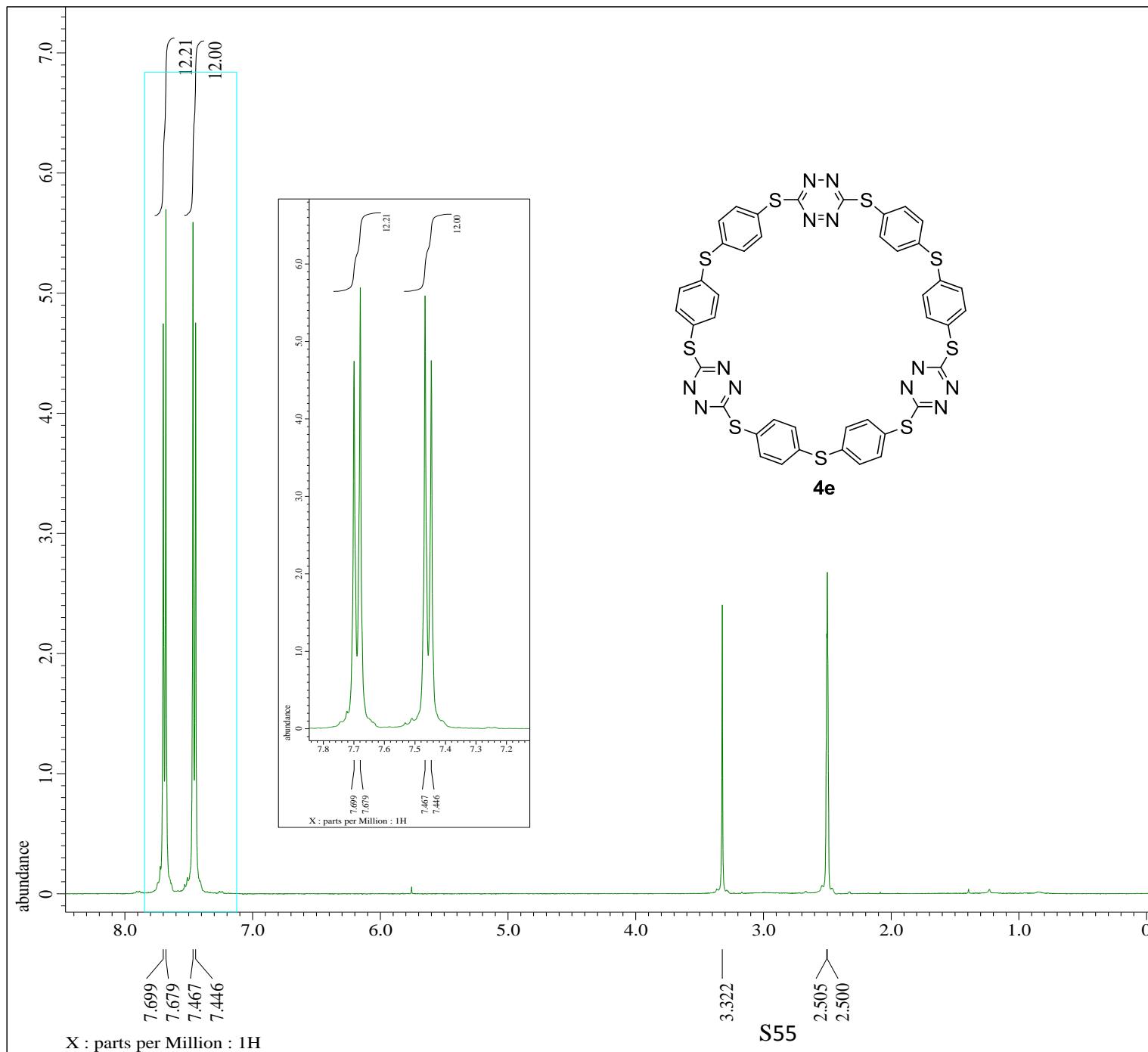
---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 2.0[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

Filename = s-ggh-221-01-C-single\_puls  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_Id = S#834480  
Solvent = CHLOROFORM-D  
Creation\_Time = 9-AUG-2013 06:33:30  
Revision\_Time = 9-AUG-2013 08:36:11  
Current\_Time = 21-APR-2015 16:45:53

Comment = single pulse decoupled gat  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
Dim\_Title = 13C  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 1.04333312[s]  
X\_Domain = 13C  
X\_Freq = 100.52530333[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 0.95846665[Hz]  
X\_Sweep = 31.40703518[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Clipped = TRUE  
Scans = 9422  
Total\_Scans = 9422

Relaxation\_Delay = 2[s]  
Recvr\_Gain = 58  
Temp\_Get = 18.7[dC]  
X\_90\_Width = 8.75[us]  
X\_Acq\_Time = 1.04333312[s]  
X\_Angle = 30[deg]  
X\_Atn = 7.8[dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE  
Noe\_Time = 2[s]  
Repetition\_Time = 3.04333312[s]



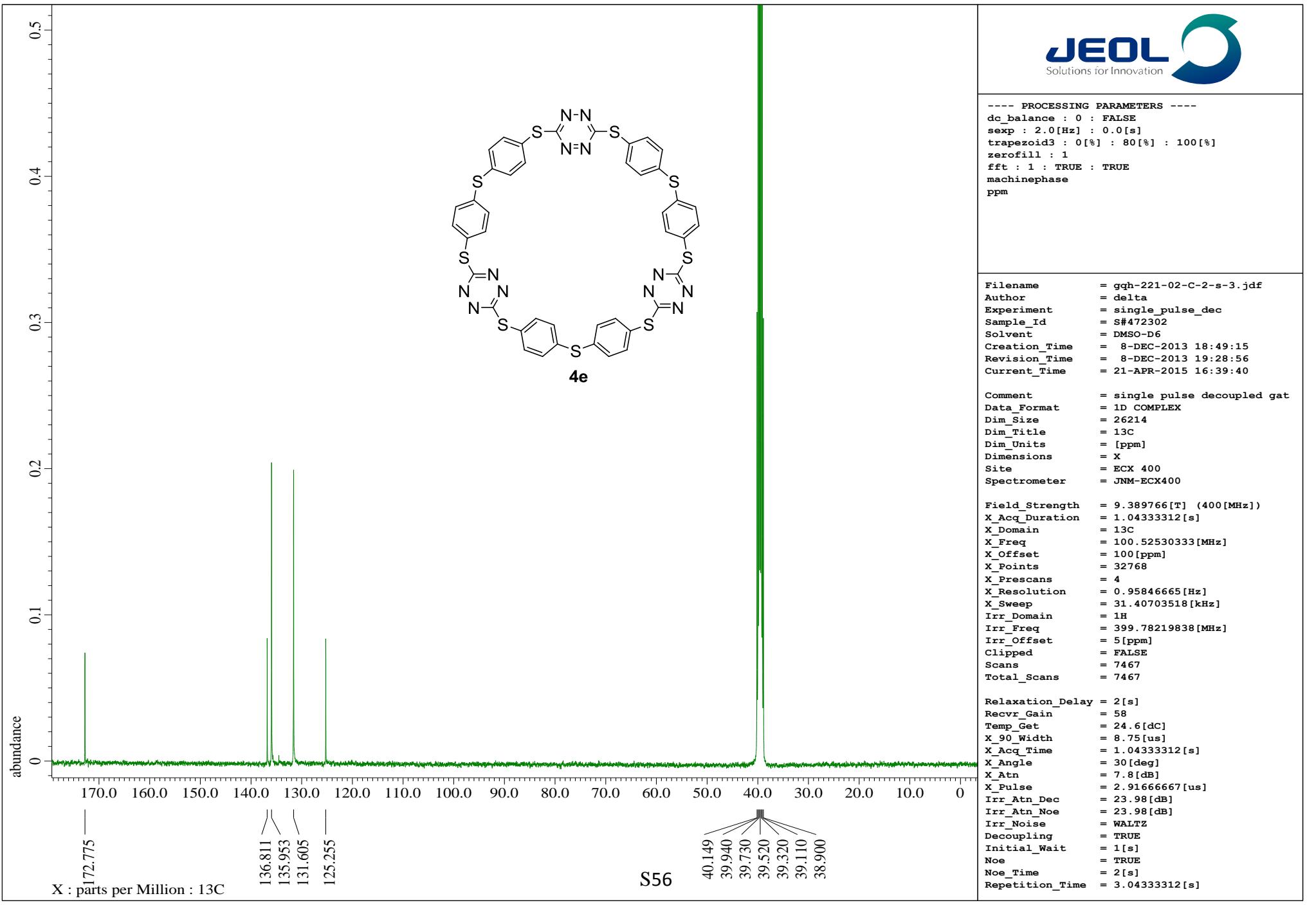
---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 0.2[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

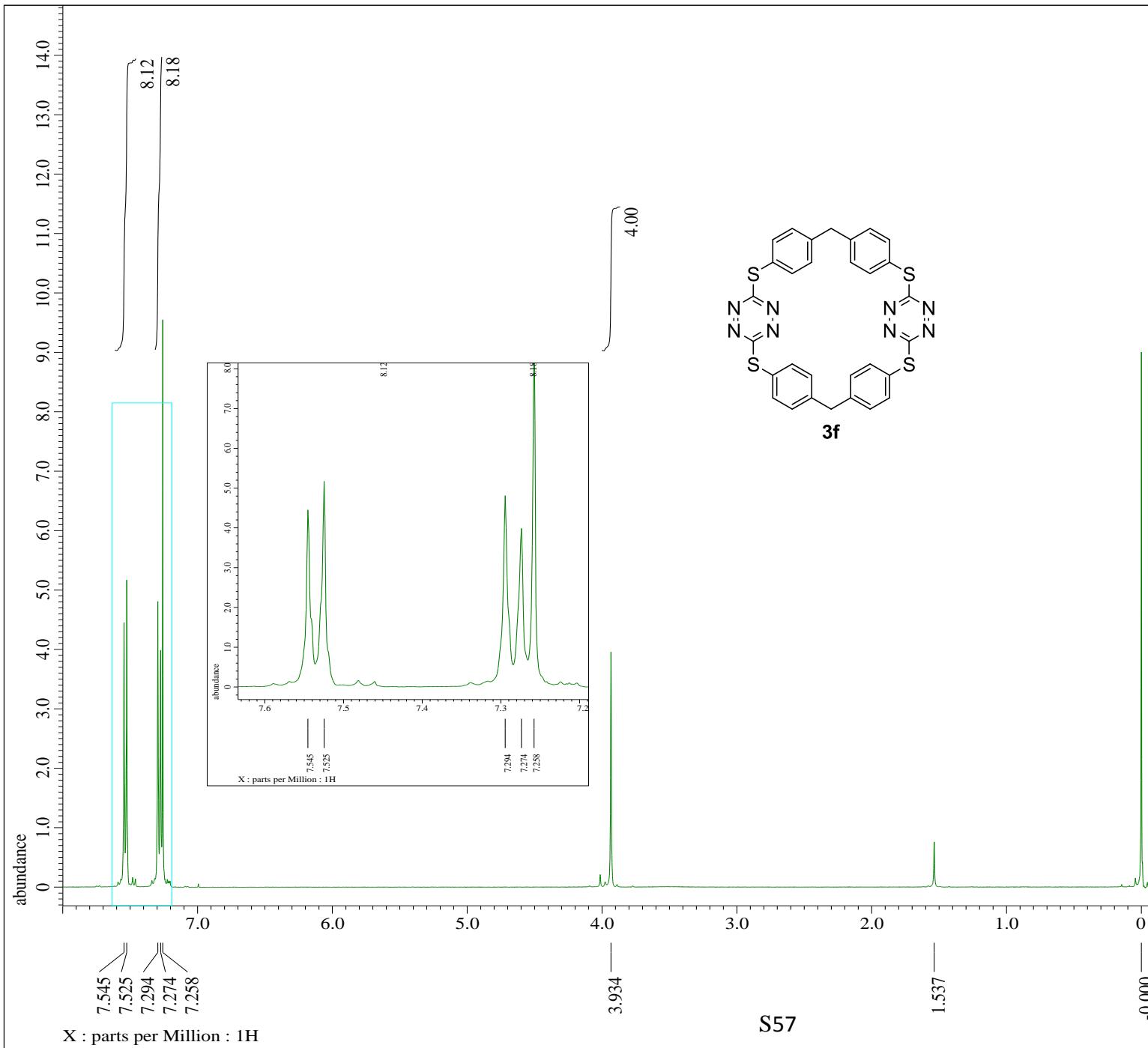
Filename = gqh-221-02-20131208-4.jdf  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#443881  
Solvent = DMSO-D6  
Creation\_Time = 8-DEC-2013 11:42:21  
Revision\_Time = 21-APR-2015 16:39:04  
Current\_Time = 21-APR-2015 16:39:08

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acc\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 48  
Temp\_Get = 23.4[dC]  
X\_90\_Width = 10.75[us]  
X\_Acc\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[dB]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 7.18365952[s]





---- PROCESSING PARAMETERS ----

```

dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

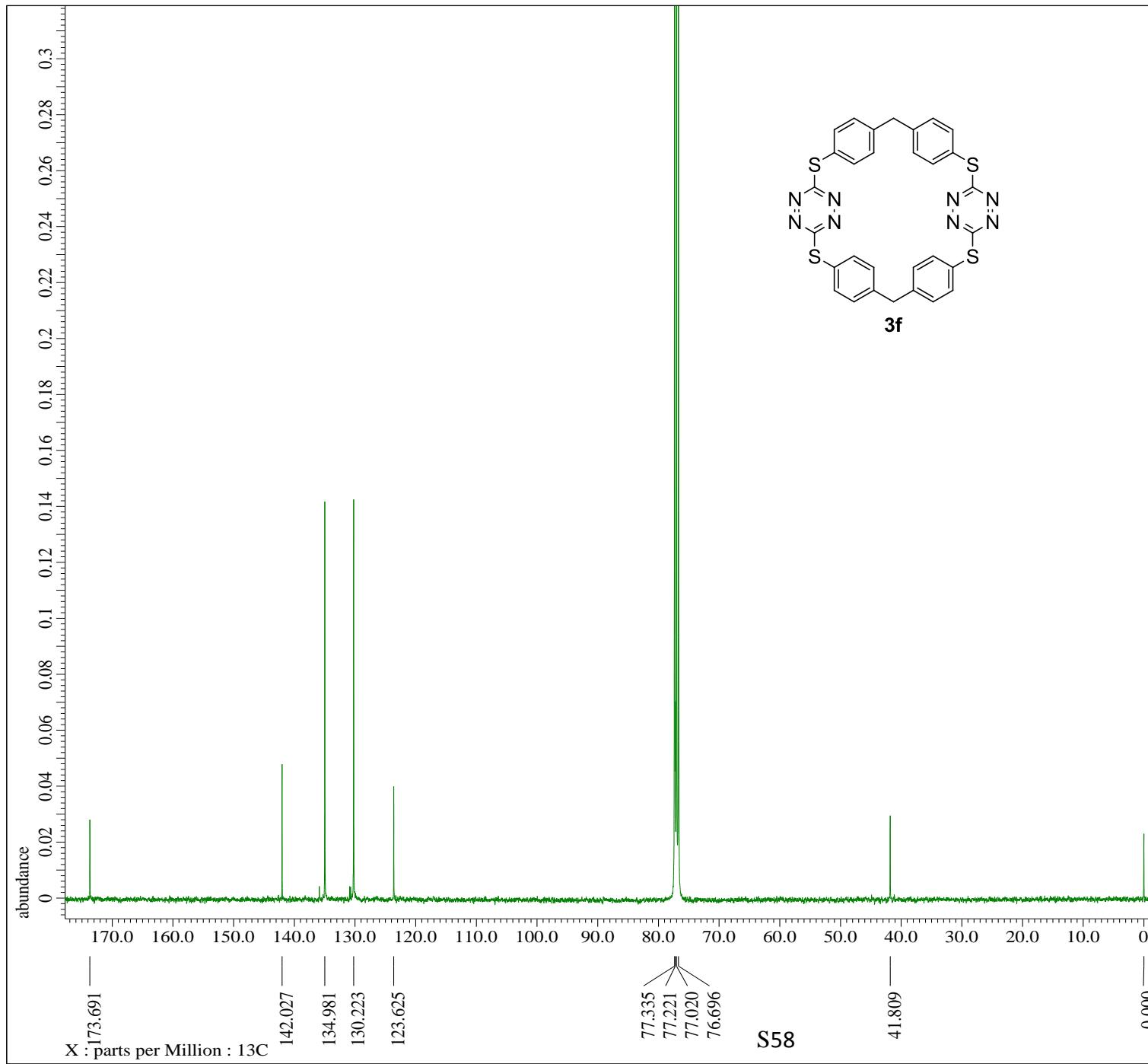
```

Filename = ggh-220-01-2013126-s-4.jdf
Author = delta
Experiment = single\_pulse.ex2
Sample\_Id = S#857175
Solvent = CHLOROFORM-D
Creation\_Time = 5-DEC-2013 23:11:11
Revision\_Time = 21-APR-2015 21:16:01
Current\_Time = 21-APR-2015 21:16:05

Comment = single\_pulse
Data\_Format = 1D COMPLEX
Dim\_Size = 13107
Dim\_Title = 1H
Dim\_Units = [ppm]
Dimensions = X
Site = ECX 400
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])
X\_Acq\_Duration = 2.18365952[s]
X\_Domain = 1H
X\_Freq = 399.78219838[MHz]
X\_Offset = 5[ppm]
X\_Points = 16384
X\_Prescans = 1
X\_Resolution = 0.45794685[Hz]
X\_Sweep = 7.5030012[kHz]
Irr\_Domain = 1H
Irr\_Freq = 399.78219838[MHz]
Irr\_Offset = 5[ppm]
Tri\_Domain = 1H
Tri\_Freq = 399.78219838[MHz]
Tri\_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total\_Scans = 8

Relaxation\_Delay = 5[s]
Recv\_Gain = 48
Temp\_Get = 23.6[dC]
X\_90\_Width = 10.75[us]
X\_Acq\_Time = 2.18365952[s]
X\_Angle = 45[deg]
X\_Atn = 3.4[dB]
X\_Pulse = 5.375[us]
Irr\_Mode = Off
Tri\_Mode = Off
Dante\_Presat = FALSE
Initial\_Wait = 1[s]
Repetition\_Time = 7.18365952[s]



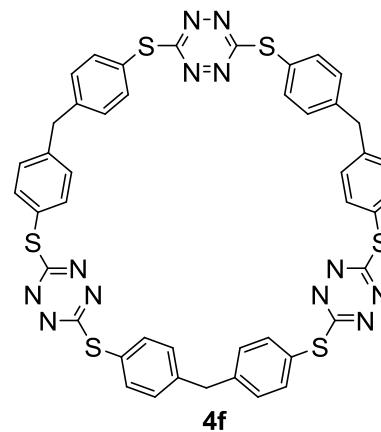
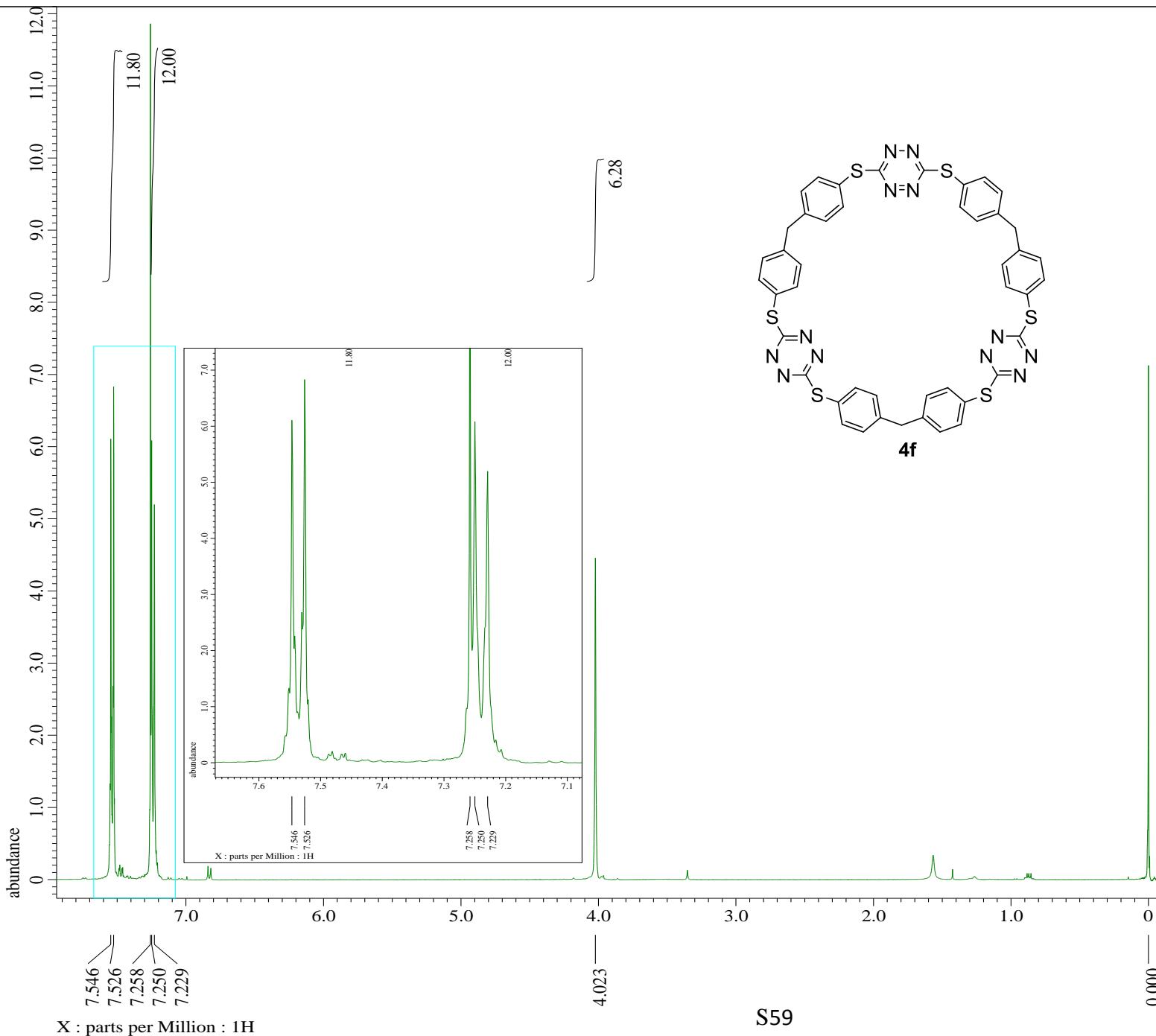
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---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 2.0[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

Filename = gqh-220-01-C-s-5.jdf  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_Id = S#858172  
Solvent = CHLOROFORM-D  
Creation\_Time = 6-DEC-2013 07:14:53  
Revision\_Time = 6-DEC-2013 09:03:14  
Current\_Time = 21-APR-2015 21:14:43

Comment = single pulse decoupled gat  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
Dim\_Title = 13C  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400  
Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 1.04333312[s]  
X\_Domain = 13C  
X\_Freq = 100.52530333[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 0.95846665[Hz]  
X\_Sweep = 31.40703518[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 9486  
Total\_Scans = 9486

Relaxation\_Delay = 2[s]  
Recvr\_Gain = 54  
Temp\_Get = 24.3[dC]  
X\_90\_Width = 8.75[us]  
X\_Acq\_Time = 1.04333312[s]  
X\_Angle = 30[deg]  
X\_Atn = 7.8[dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE  
Noe\_Time = 2[s]  
Repetition\_Time = 3.04333312[s]



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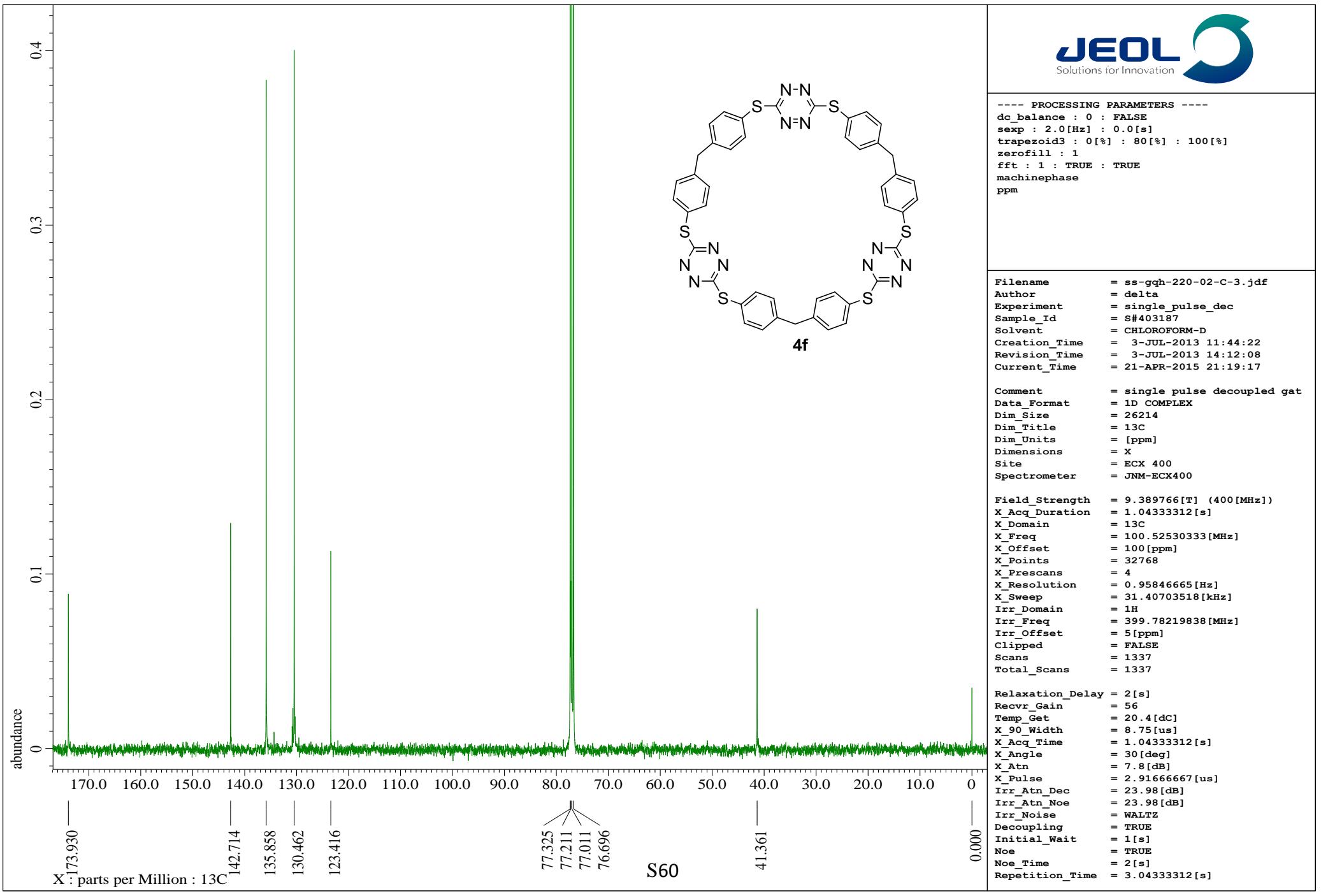
---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 0.2[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

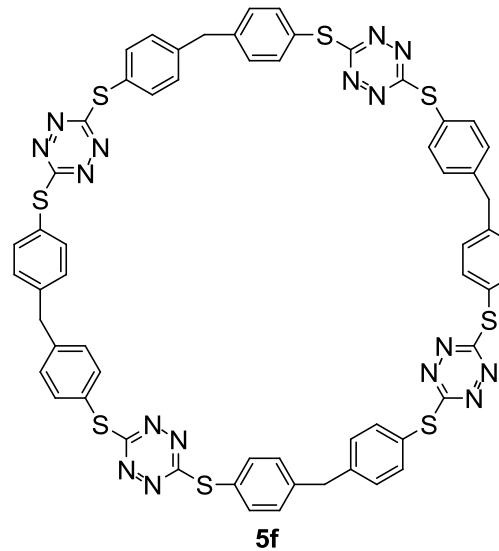
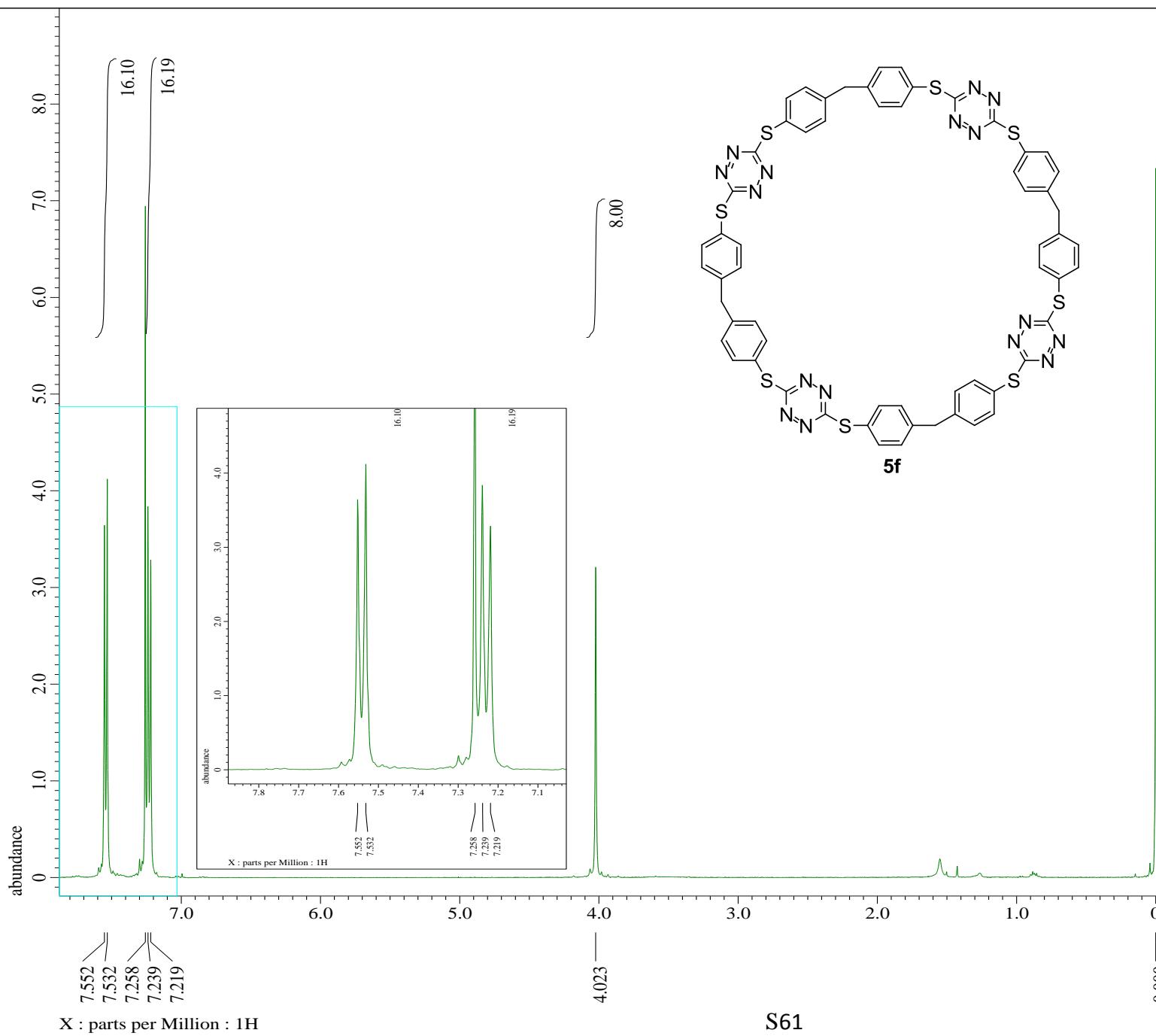
Filename = s-gqh-220-02-4.jdf  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#388774  
Solvent = CHLOROFORM-D  
Creation\_Time = 3-JUL-2013 10:13:52  
Revision\_Time = 21-APR-2015 21:25:25  
Current\_Time = 21-APR-2015 21:25:30

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 44  
Temp\_Get = 20.4[dC]  
x\_90\_Width = 10.75[us]  
x\_Acq\_Time = 2.18365952[s]  
x\_Angle = 45[deg]  
x\_Atn = 3.4[dB]  
x\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 7.18365952[s]





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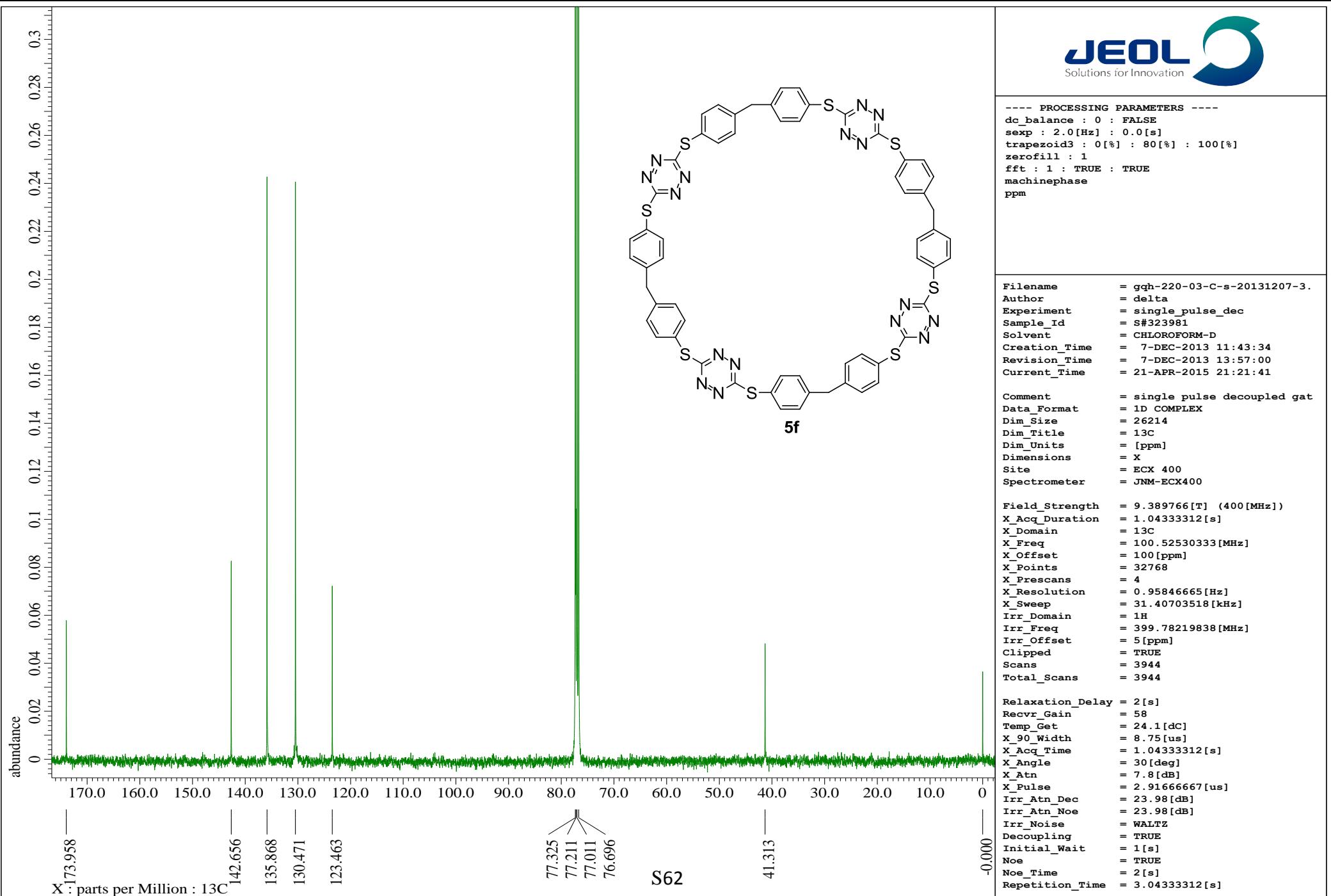
----- PROCESSING PARAMETERS -----  
dc\_balance : 0 : FALSE  
sexp : 0.2[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

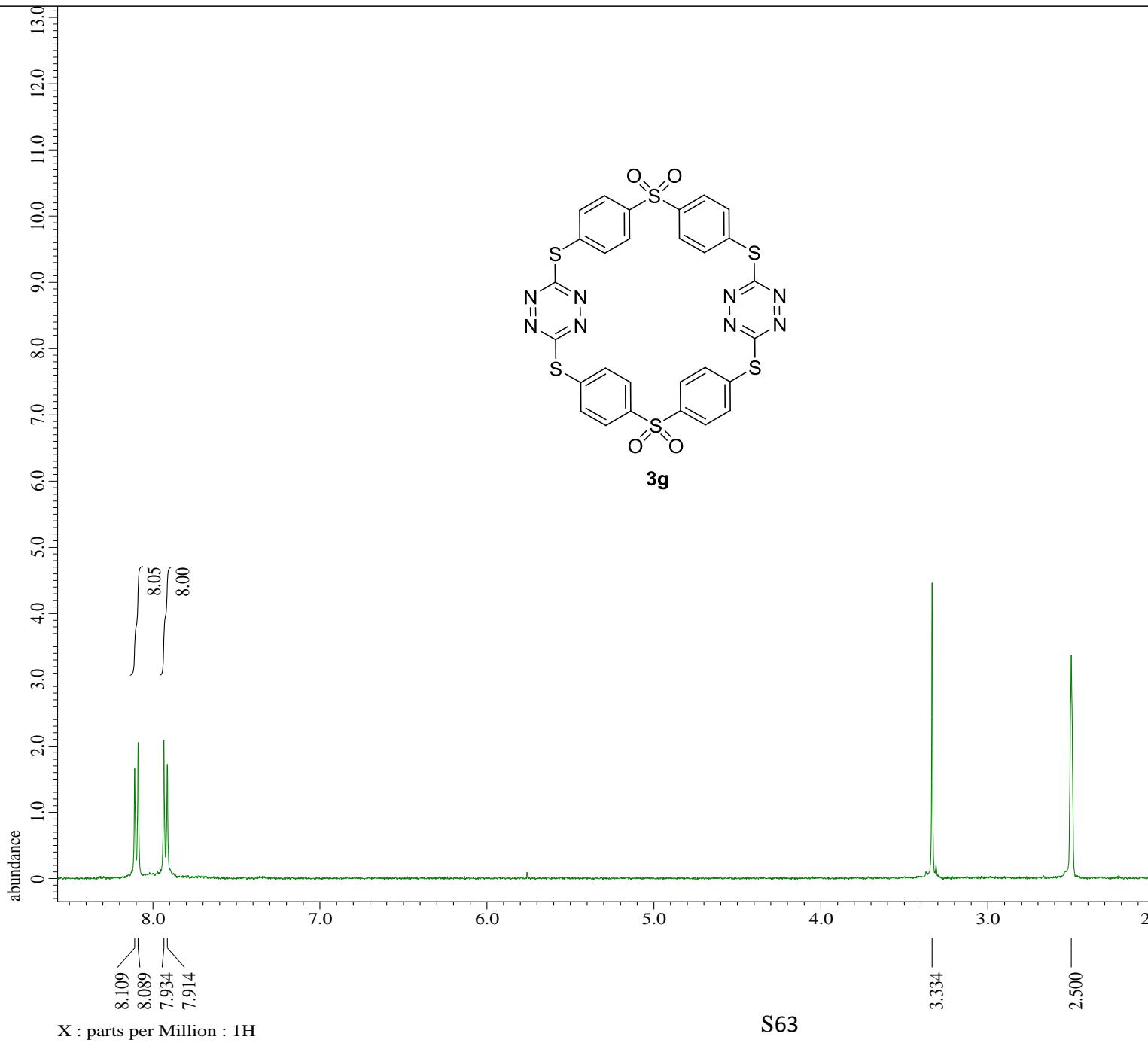
Filename = ggh-220-03-s-4.jdf  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#339665  
Solvent = CHLOROFORM-D  
Creation\_Time = 6-DEC-2013 08:49:47  
Revision\_Time = 21-APR-2015 21:22:52  
Current\_Time = 21-APR-2015 21:22:58

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 48  
Temp\_Get = 22.8[dC]  
X\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[dB]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 7.18365952[s]





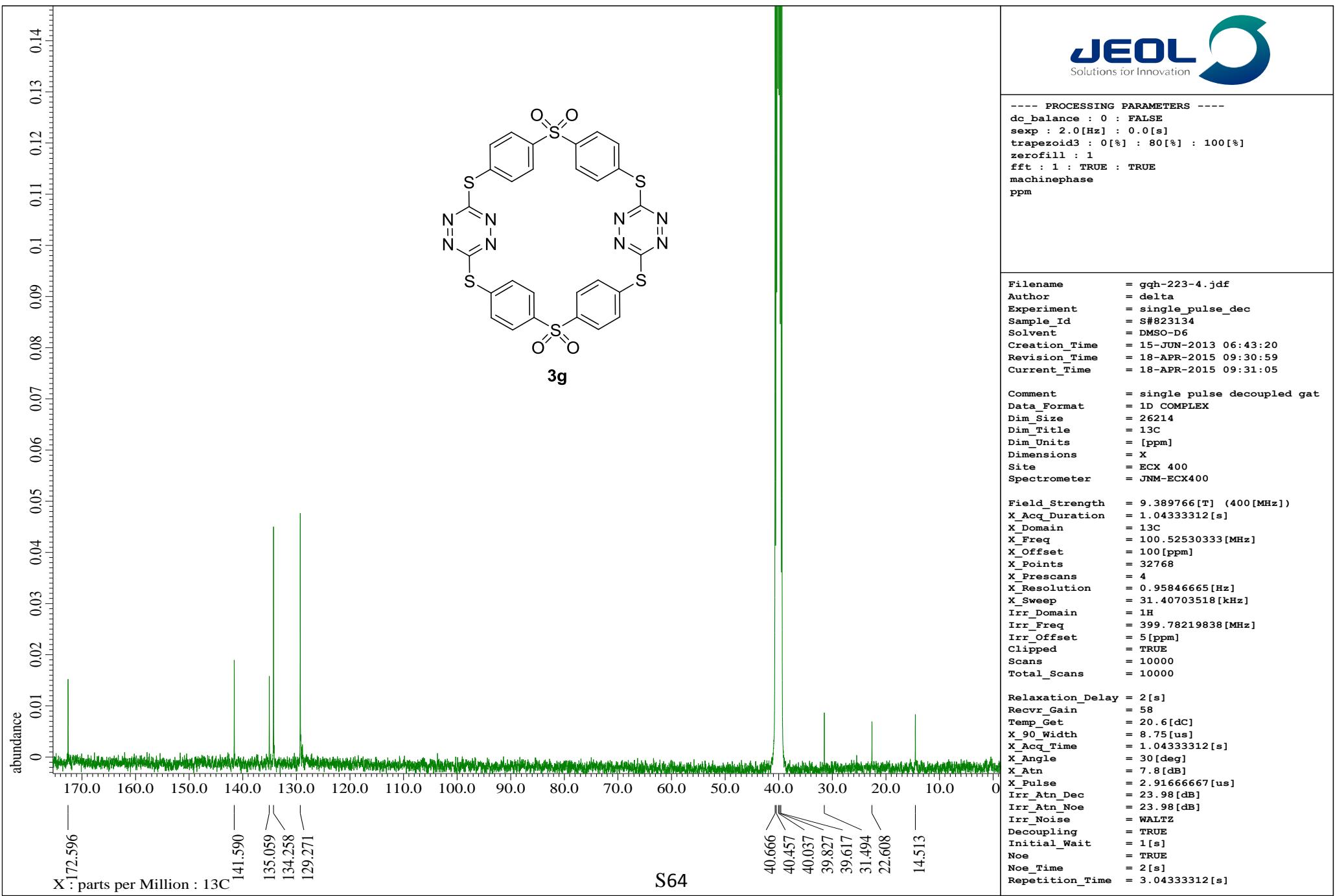
---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 0.2[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinemphase  
ppm

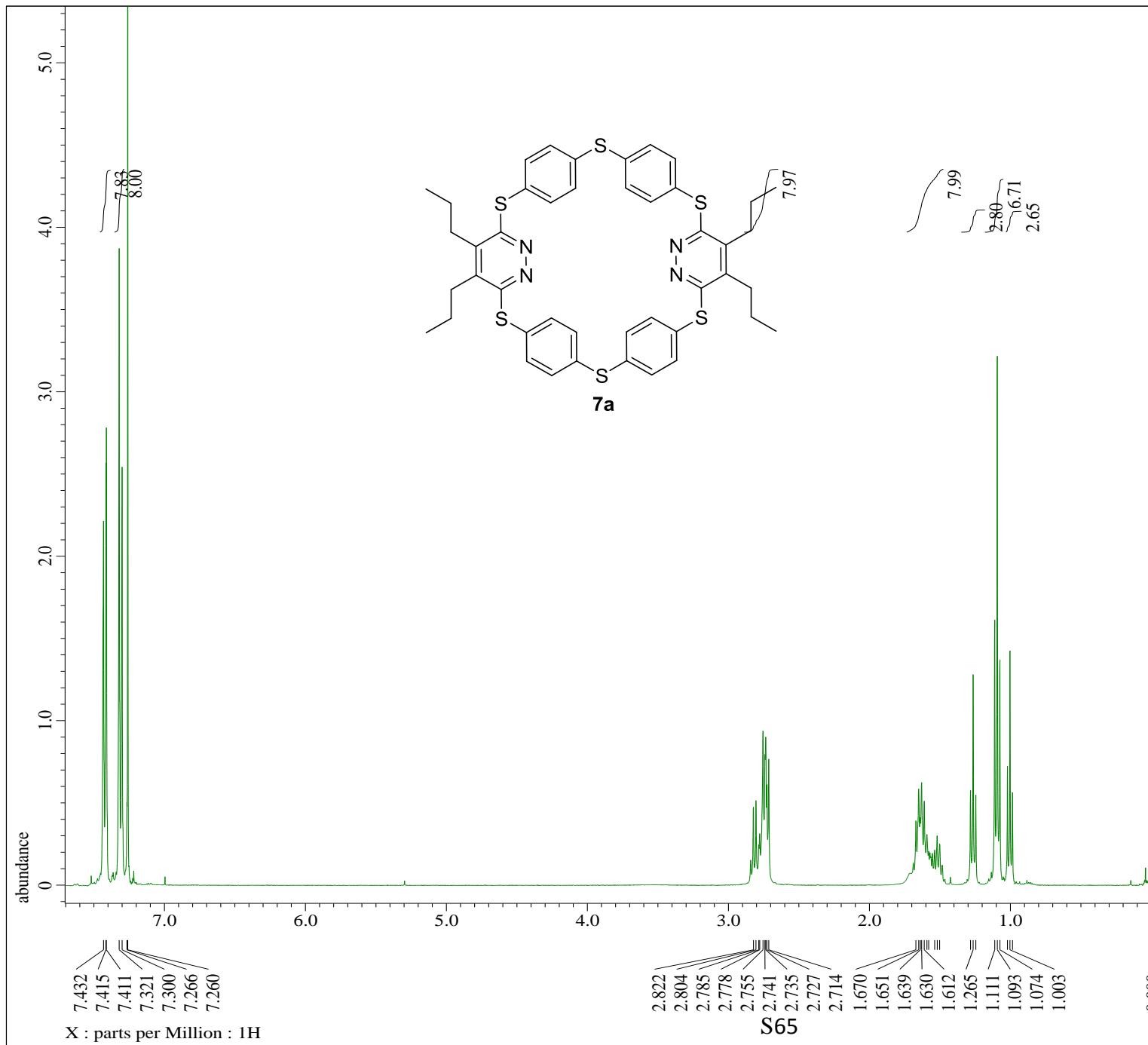
Filename = gqh-223-20130614-4.jdf  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#775215  
Solvent = DMSO-D6  
Creation\_Time = 14-JUN-2013 21:00:05  
Revision\_Time = 18-APR-2015 09:34:30  
Current\_Time = 18-APR-2015 09:36:17

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 32  
Total\_Scans = 32

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 76  
Temp\_Get = 20.4[dc]  
X\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[dB]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 7.18365952[s]





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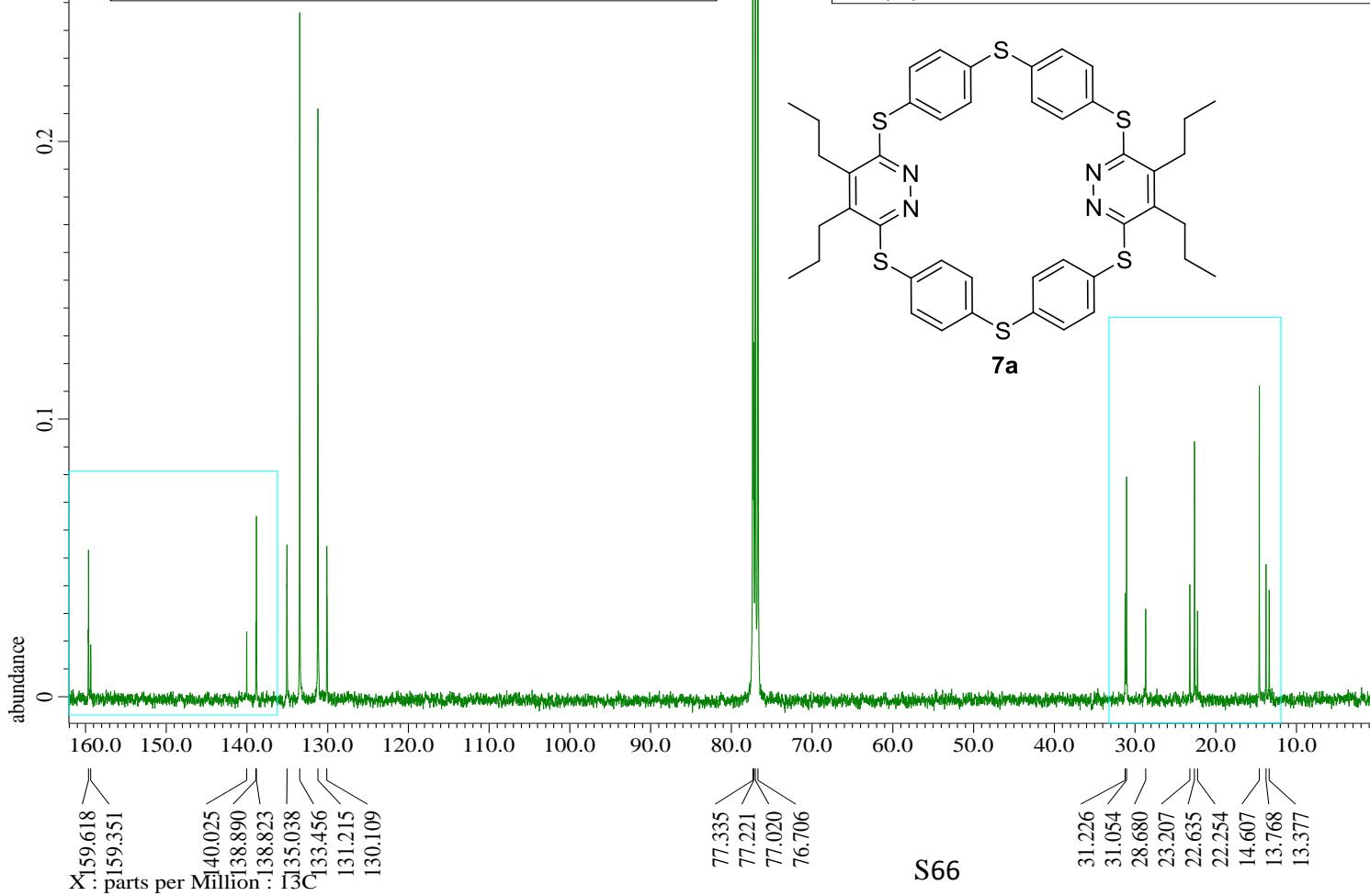
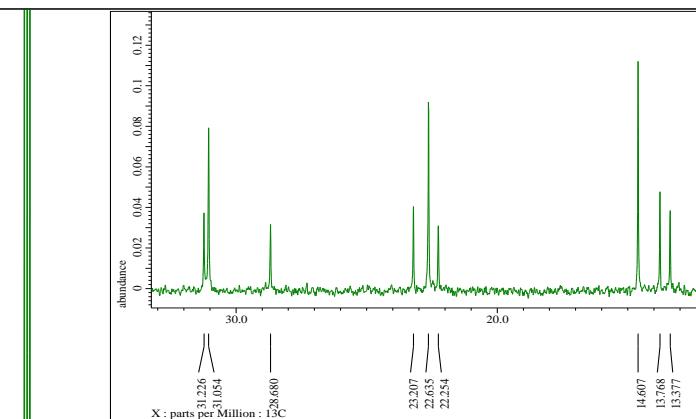
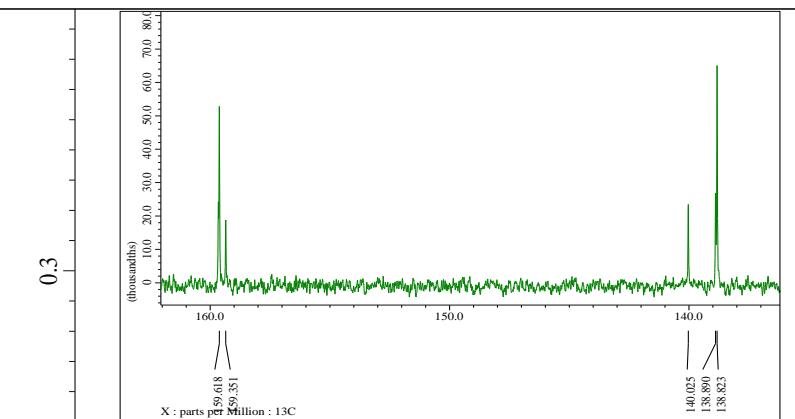
---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 0.2[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

Filename = gqh-255-20131020-4.jdf  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#470070  
Solvent = CHLOROFORM-D  
Creation\_Time = 20-OCT-2013 12:25:59  
Revision\_Time = 21-APR-2015 20:21:10  
Current\_Time = 21-APR-2015 20:21:23

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 42  
Temp\_Get = 19.3[dC]  
X\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[dB]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 7.18365952[s]



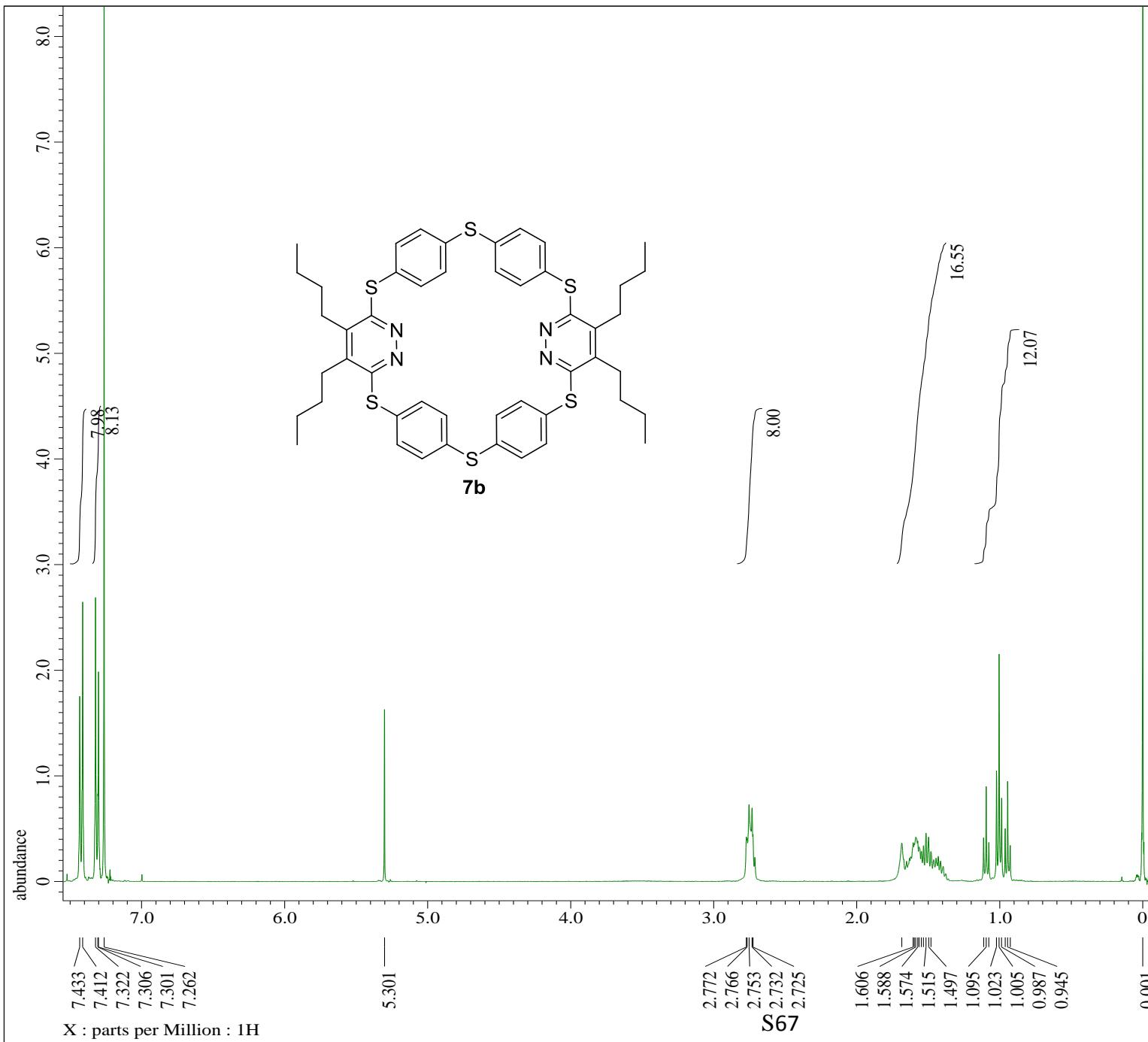
---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
sexp( 2.0[Hz], 0.0[s] )  
trapezoid3( 0[%], 80[%], 100[%] )  
zerofill( 1 )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm

Filename = ggh-255-20131020-C-6.jdf  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_Id = S#471287  
Solvent = CHLOROFORM-D  
Creation\_Time = 20-OCT-2013 15:19:58  
Revision\_Time = 21-APR-2015 20:24:31  
Current\_Time = 21-APR-2015 20:24:37

Comment = single pulse decoupled gat  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
Dim\_Title = 13C  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acc\_Duration = 1.04333312[s]  
X\_Domain = 13C  
X\_Freq = 100.52530333[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 0.95846665[Hz]  
X\_Sweep = 31.40703518[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Clipped = TRUE  
Scans = 3412  
Total\_Scans = 3412

Relaxation\_Delay = 2[s]  
Recvr\_Gain = 58  
Temp\_Get = 19.5[dC]  
X\_90\_Width = 8.75[us]  
X\_Acc\_Time = 1.04333312[s]  
X\_Angle = 30[deg]  
X\_Atn = 7.8[dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Nce = TRUE  
Noe\_Time = 2[s]  
Repetition\_Time = 3.04333312[s]



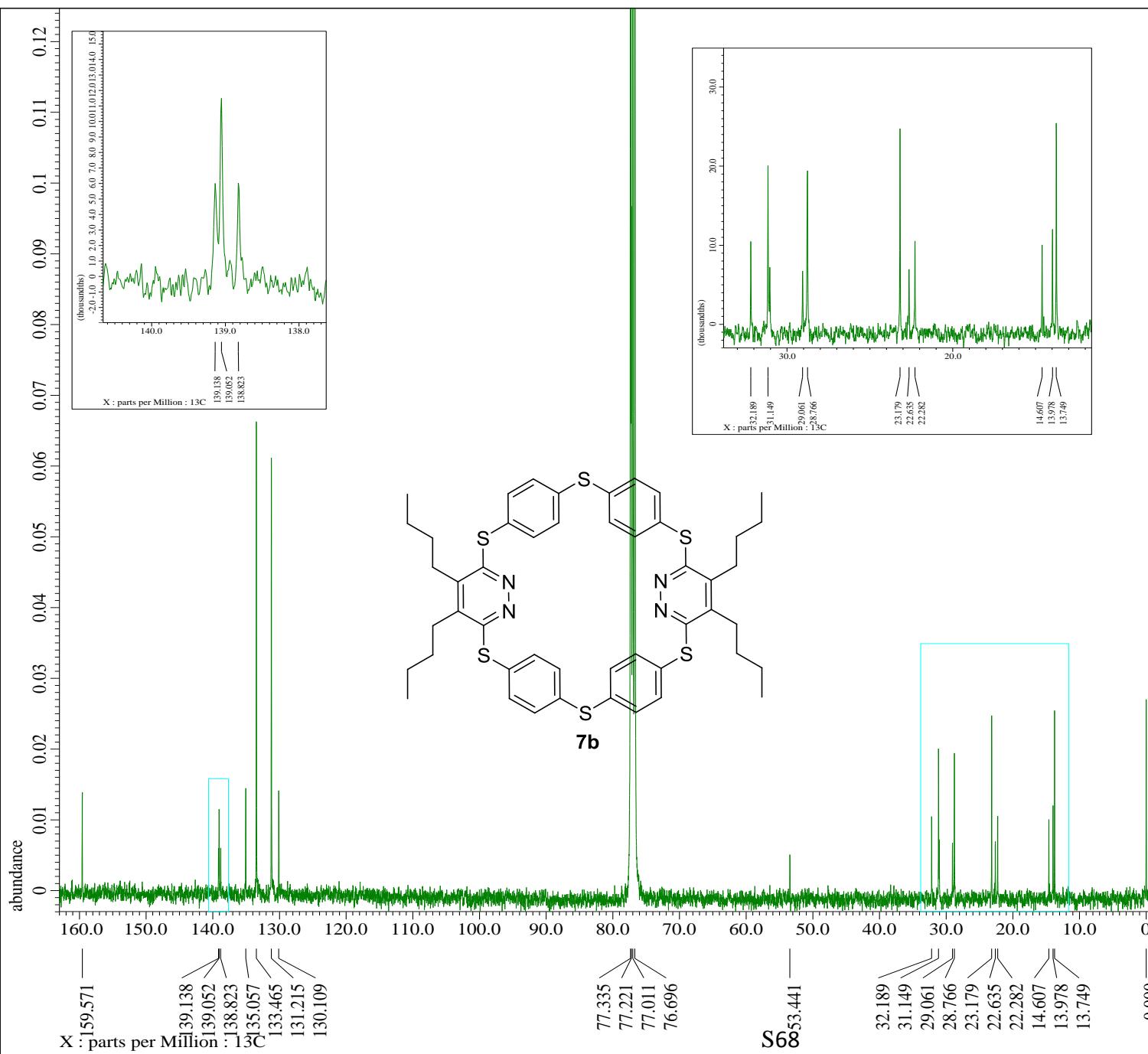
---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 0.2[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

Filename = ggh-270-4.jdf  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#795761  
Solvent = CHLOROFORM-D  
Creation\_Time = 10-OCT-2013 21:28:30  
Revision\_Time = 21-APR-2015 20:38:40  
Current\_Time = 21-APR-2015 20:38:45

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = x  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8

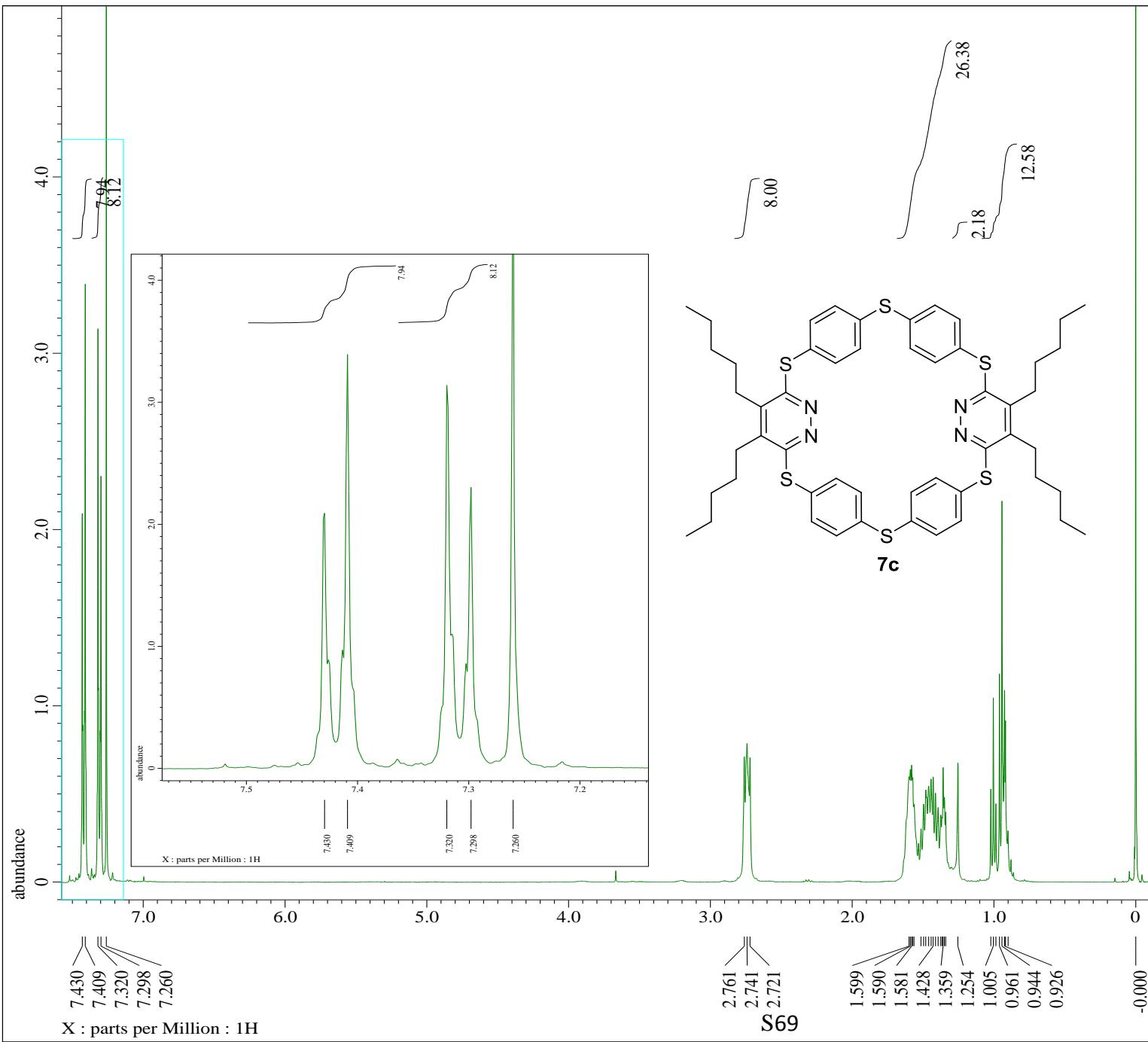
Relaxation\_Delay = 5[s]  
Recvr\_Gain = 46  
Temp\_Get = 18.7[dc]  
x\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[dB]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 7.18365952[s]



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----- PROCESSING PARAMETERS -----  
dc\_balance : 0 : FALSE  
sexp : 2.0[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

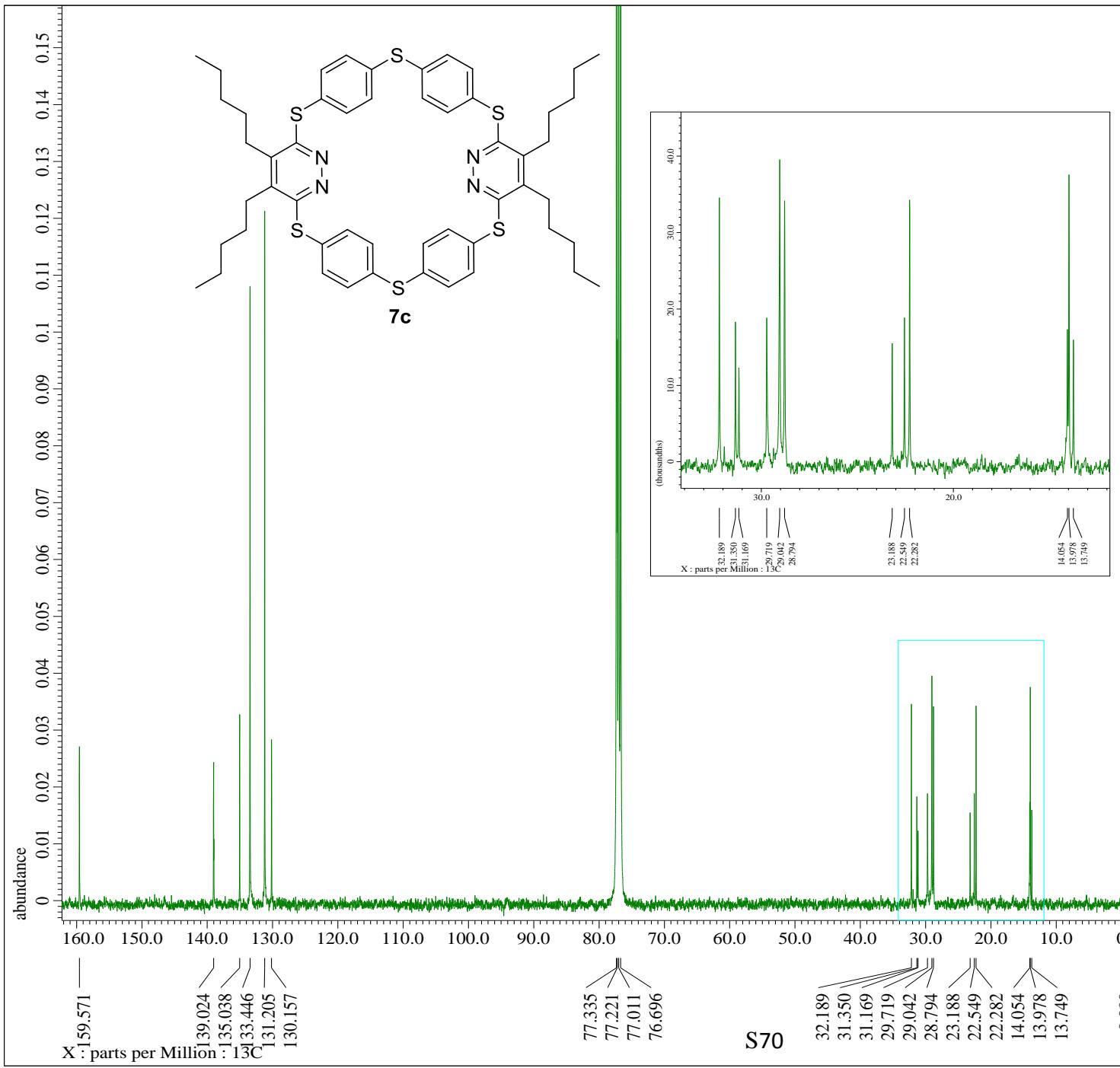
Filename = gqh-270-C-4.jdf  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_Id = S#796828  
Solvent = CHLOROFORM-D  
Creation\_Time = 11-OCT-2013 07:53:56  
Revision\_Time = 21-APR-2015 20:40:49  
Current\_Time = 21-APR-2015 20:40:57  
Comment = single pulse decoupled gat  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
Dim\_Title =  $^{13}\text{C}$   
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400  
Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acc\_Duration = 1.04333312[s]  
X\_Domain =  $^{13}\text{C}$   
X\_Freq = 100.52530333[MHz]  
X\_Offset = 100 [ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 0.95846665[Hz]  
X\_Sweep = 31.40703518[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5 [ppm]  
Clipped = TRUE  
Scans = 12315  
Total\_Scans = 12315  
Relaxation\_Delay = 2[s]  
Recv\_Gain = 58  
Temp\_Get = 42.1[dC]  
X\_90\_Width = 8.75[us]  
X\_Acc\_Time = 1.04333312[s]  
X\_Angle = 30 [deg]  
X\_Atn = 7.8 [dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE  
Noe\_Time = 2[s]  
Repetition\_Time = 3.04333312[s]



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S69  
2.761  
2.741  
2.721

1.599  
1.590  
1.581  
1.428  
1.359  
1.254  
1.005  
0.961  
0.944  
0.926



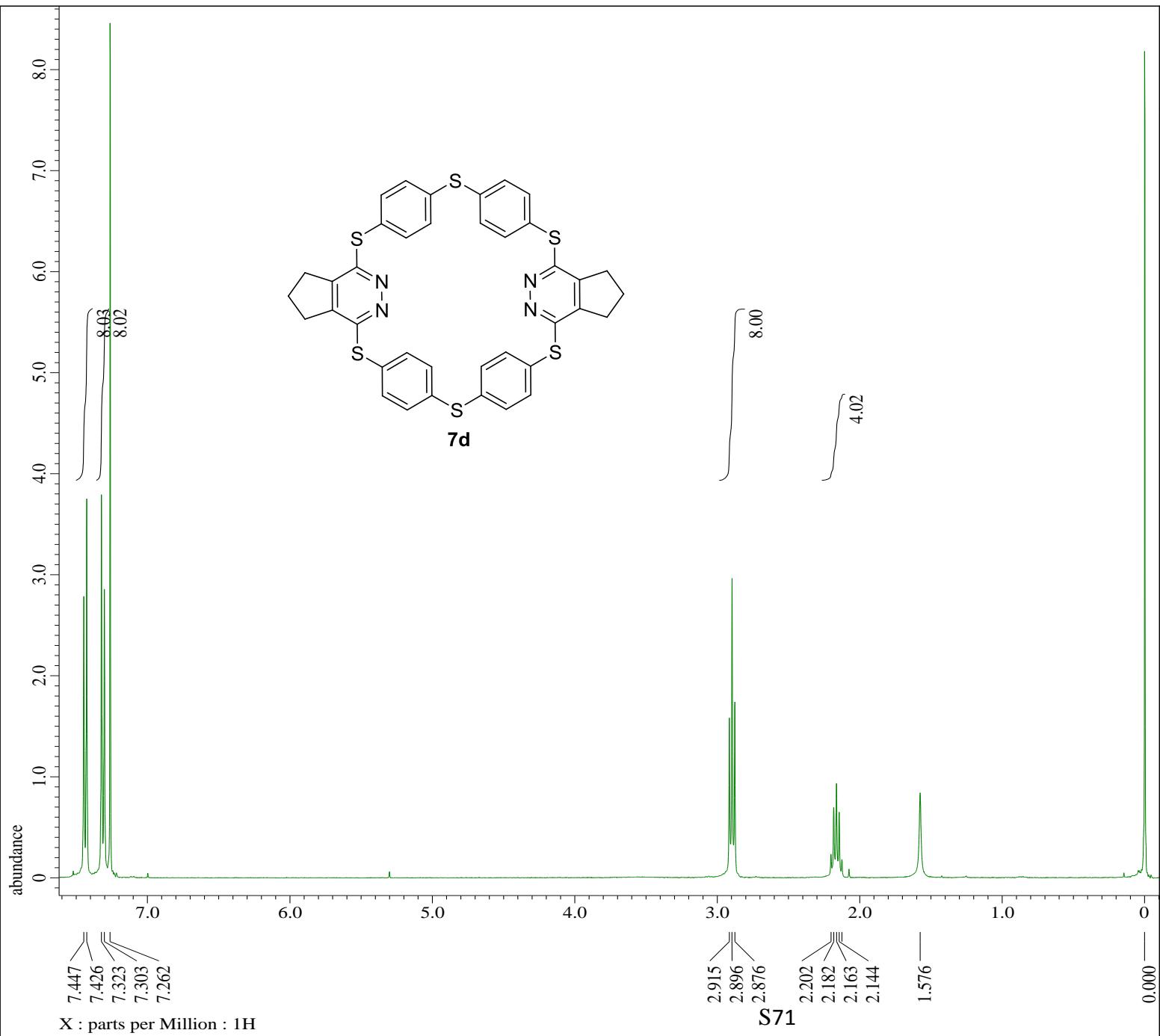
---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 2.0[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

Filename = ggh-263-C-4.jdf  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_Id = S#688388  
Solvent = CHLOROFORM-D  
Creation\_Time = 2-OCT-2013 10:34:26  
Revision\_Time = 21-APR-2015 20:30:42  
Current\_Time = 21-APR-2015 20:30:48

Comment = single pulse decoupled gat  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
Dim\_Title =  $^{13}\text{C}$   
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acc\_Duration = 1.04333312[s]  
X\_Domain =  $^{13}\text{C}$   
X\_Freq = 100.52530333[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 0.95846665[Hz]  
X\_Sweep = 31.40703518[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Clipped = TRUE  
Scans = 19003  
Total\_Scans = 19003

Relaxation\_Delay = 2[s]  
Recvr\_Gain = 58  
Temp\_Get = 20[dC]  
X\_90\_Width = 8.75[us]  
X\_Acc\_Time = 1.04333312[s]  
X\_Angle = 30[deg]  
X\_Atn = 7.8[dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE  
Noe\_Time = 2[s]  
Repetition\_Time = 3.04333312[s]



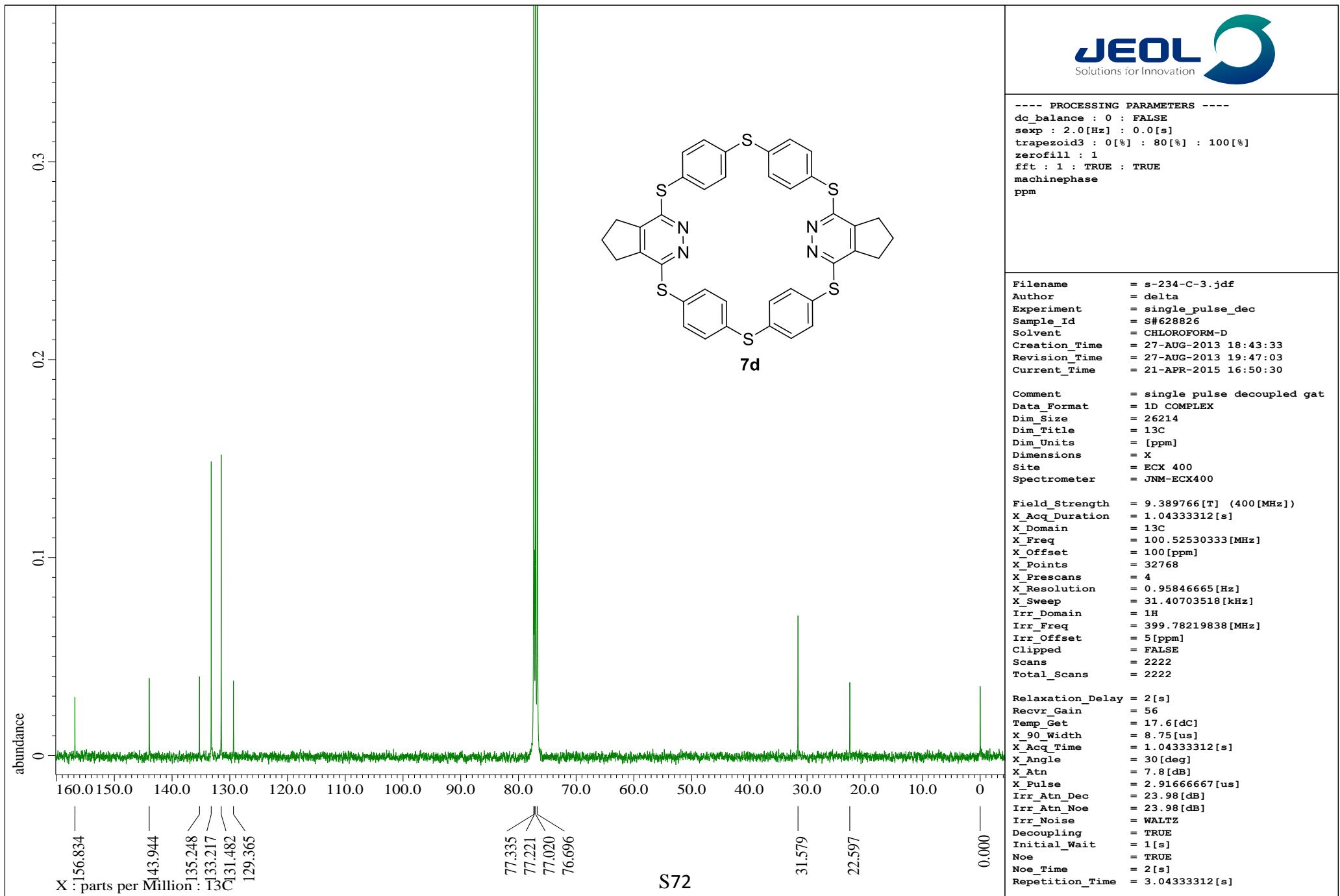
---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 0.2[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

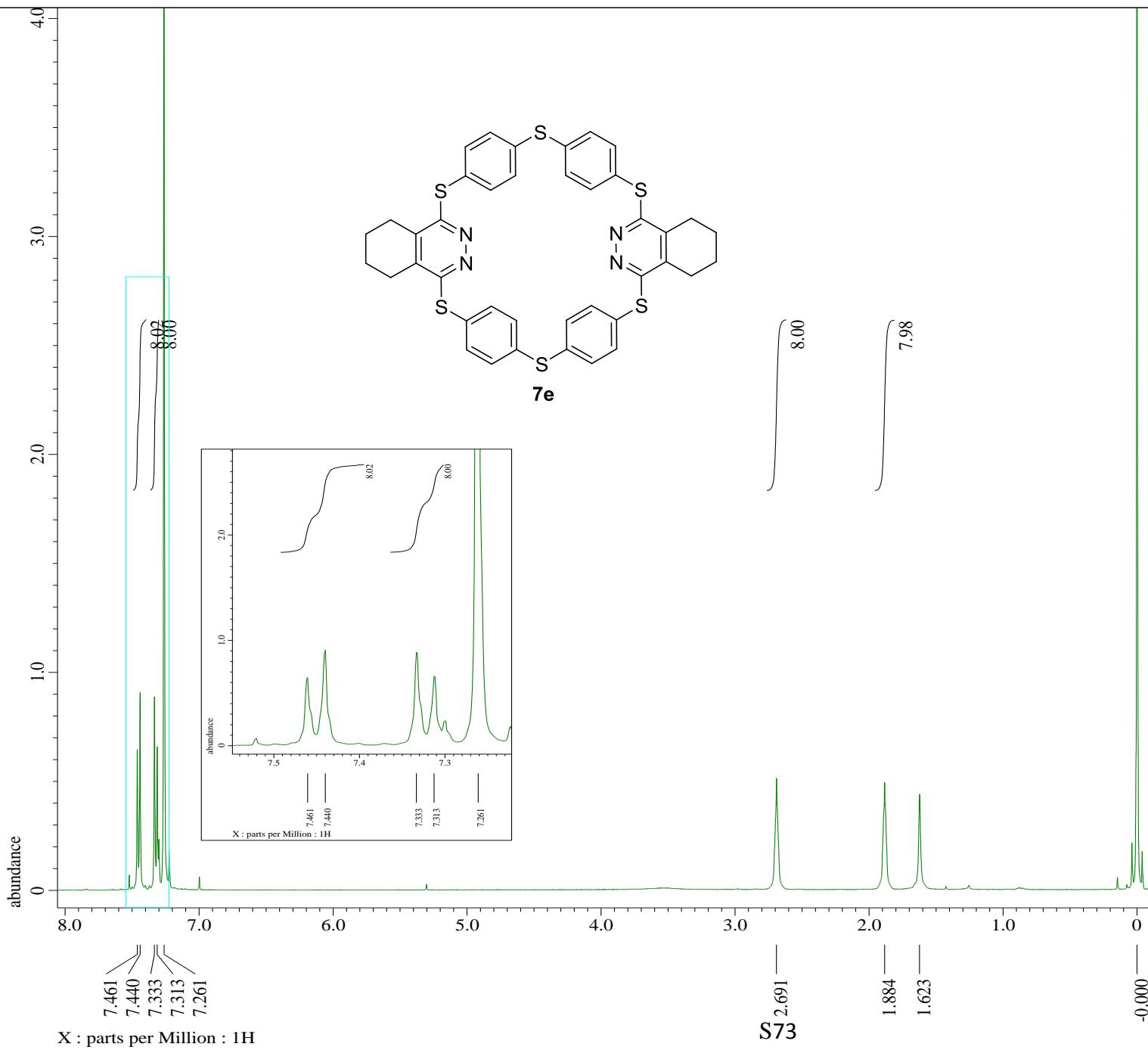
Filename = s-ggh-234-4.jdf  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#627729  
Solvent = CHLOROFORM-D  
Creation\_Time = 27-AUG-2013 16:49:54  
Revision\_Time = 21-APR-2015 16:50:57  
Current\_Time = 21-APR-2015 16:51:12

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 48  
Temp\_Get = 18.2[dC]  
X\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[dB]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 7.18365952[s]





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```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2 [Hz] : 0.0 [s]
trapezoid3 : 0 [%] : 80 [%] : 100 [%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
```

```
Filename      = ggh-237-20131020-4.jdf
Author        = delta
Experiment    = single_pulse.ex2
Sample_Id     = S#577677
Solvent       = CHLOROFORM-D
Creation_Time = 20-OCT-2013 15:35:52
Revision_Time = 21-APR-2015 16:54:40
Current_Time  = 21-APR-2015 16:54:49
```

```
Comment      = single_pulse
Data_Format = 1D COMPLEX
Dim_Size    = 13107
Dim_Title   = 1H
Dim_Units   = [ppm]
Dimensions  = X
Site        = ECX 400
Spectrometer = JNM-ECX400
```

```

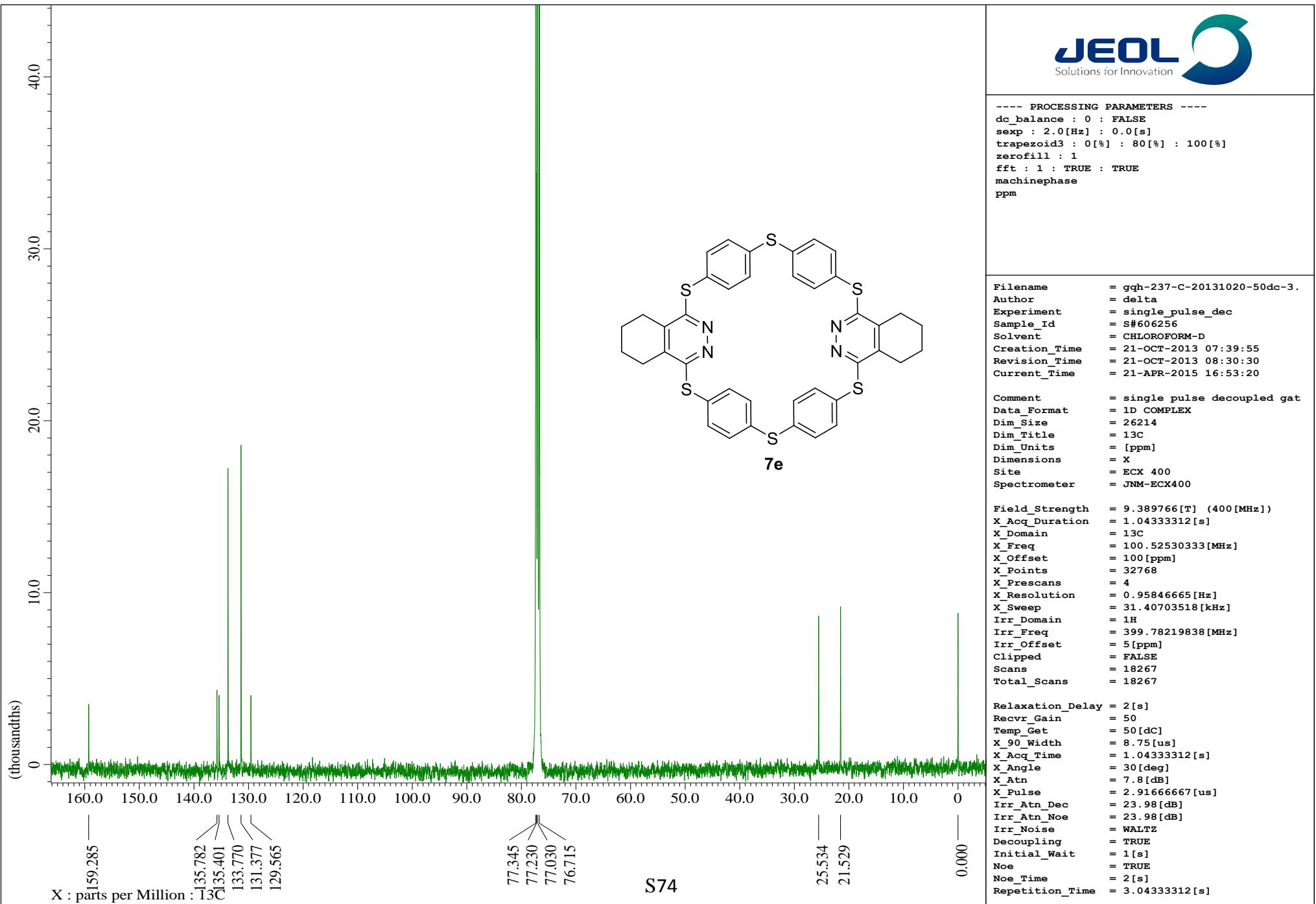
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685[Hz]
X_Sweep = 7.5030012[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 100
Total_Scans = 100

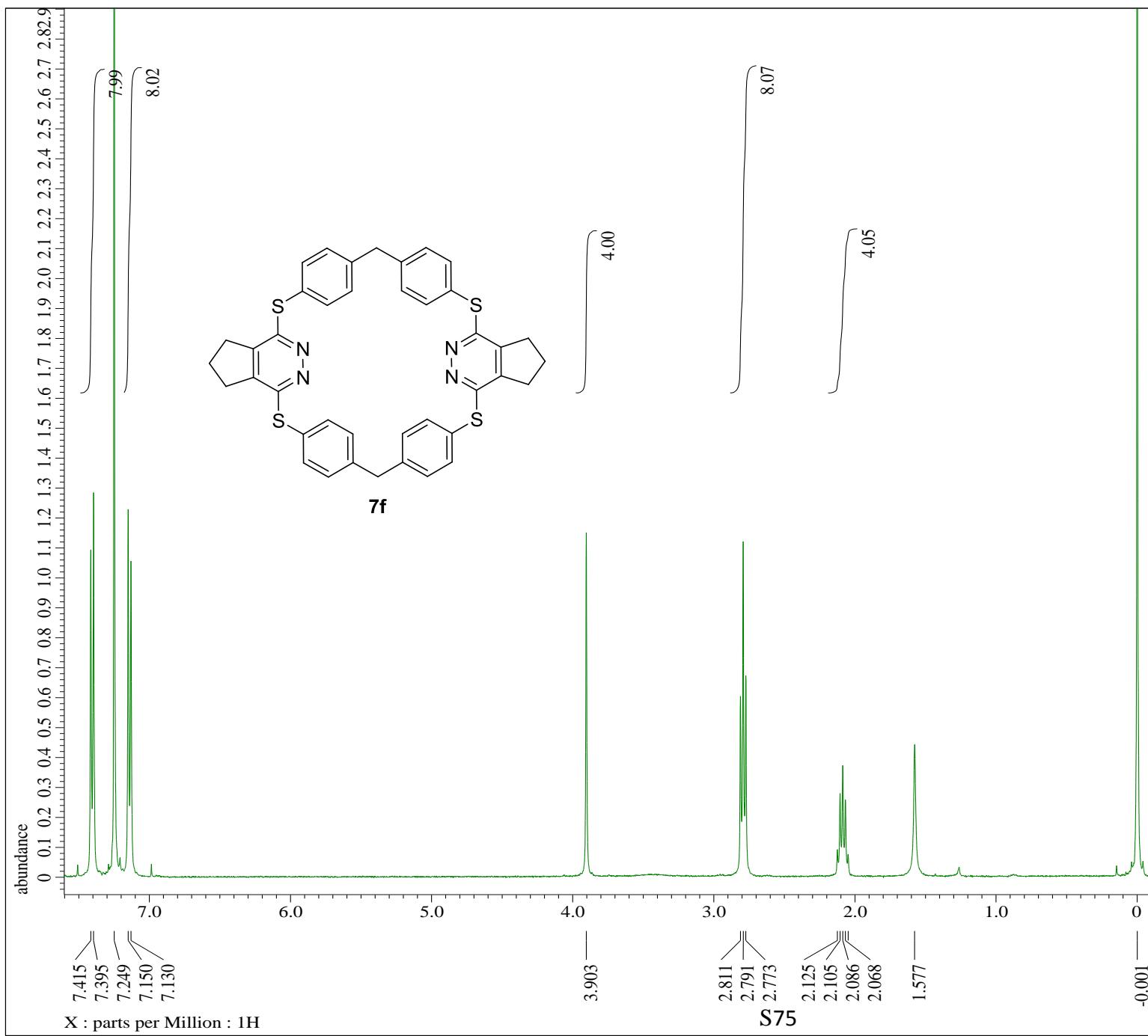
```

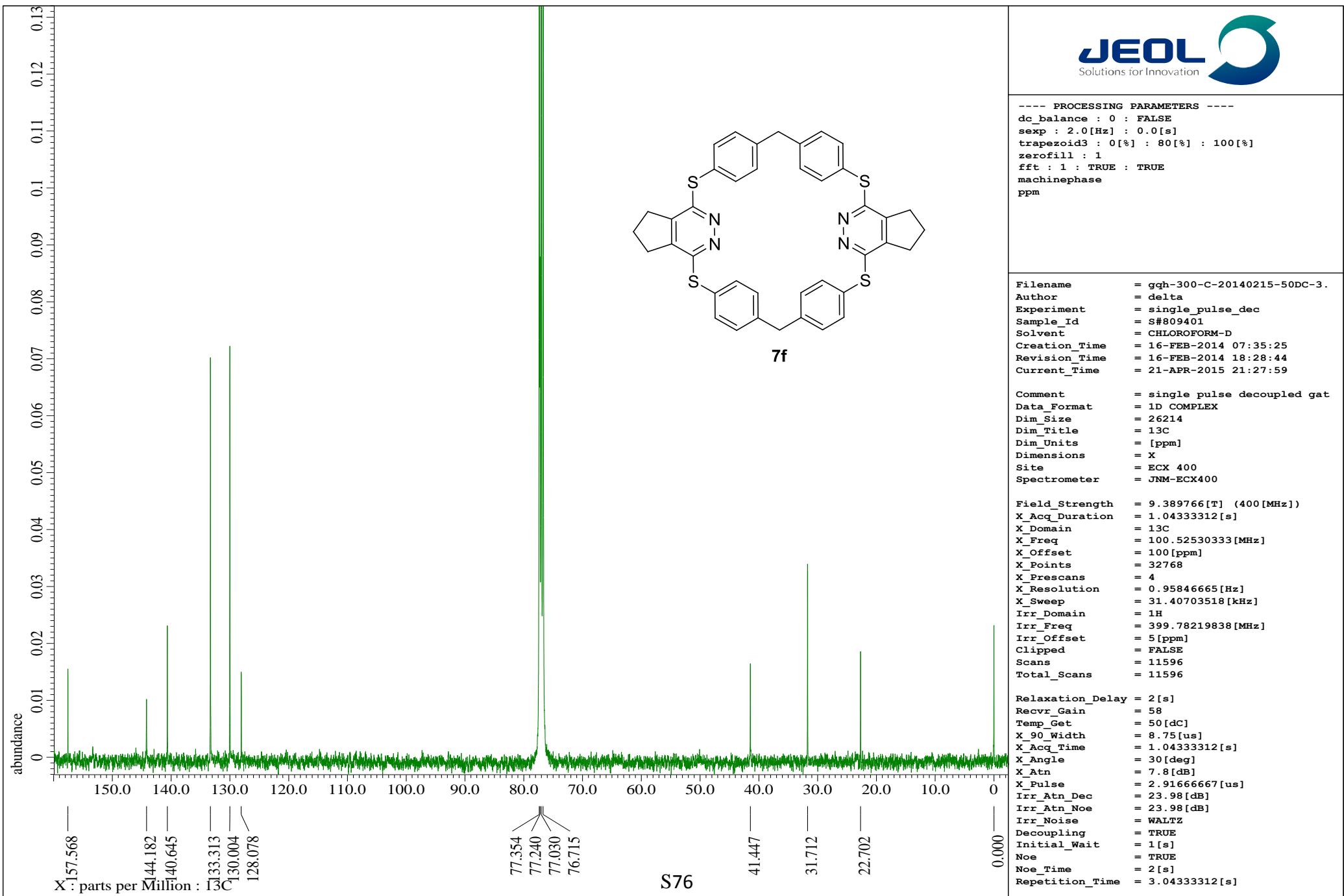
```

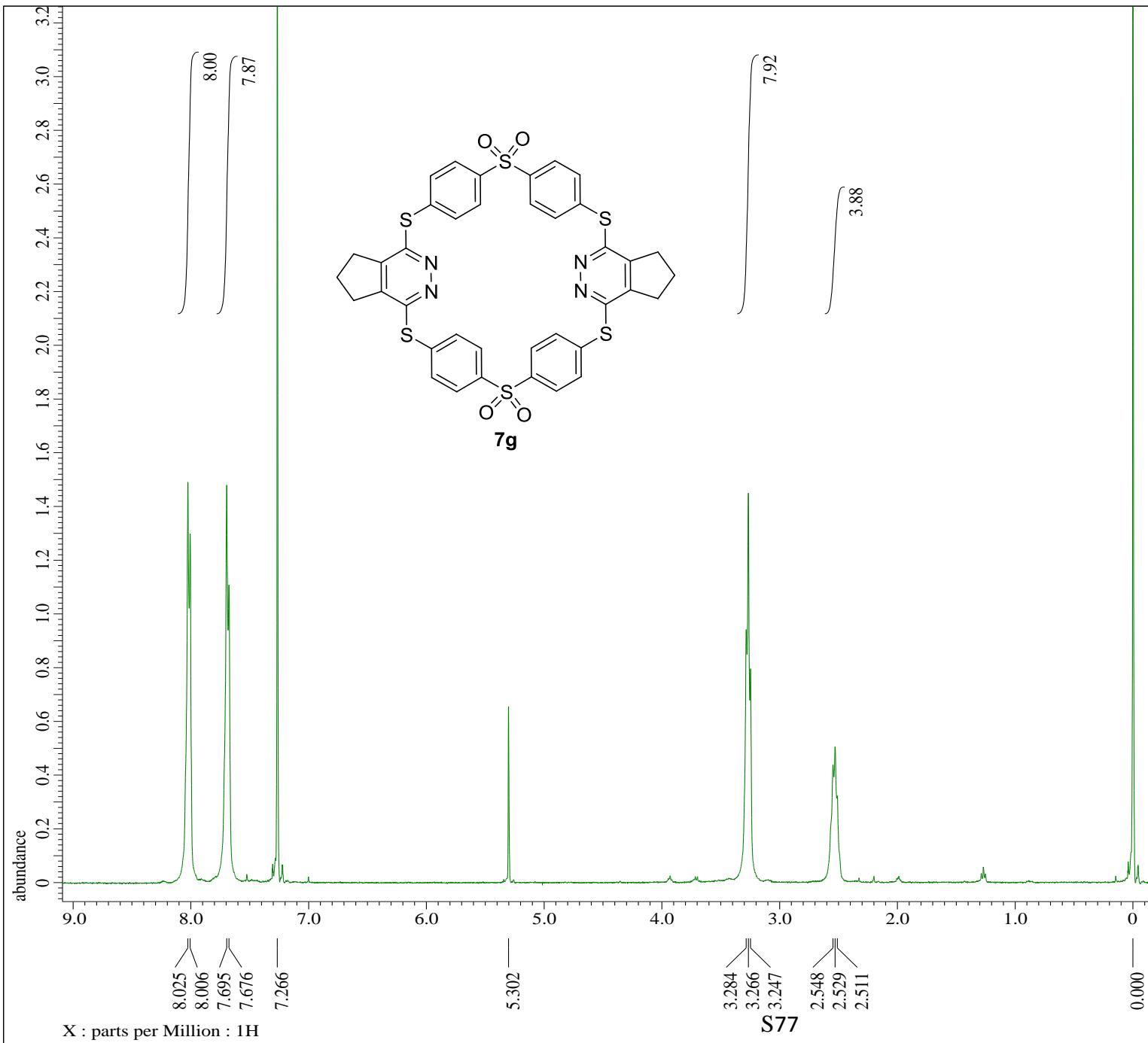
Relaxation_Delay = 5[s]
Recv_Gain        = 50
Temp_Get          = 18.9[dC]
X_90_Width       = 10.75[us]
X_Acq_Time       = 2.18365952[s]
X_Angle          = 45[deg]
X_Atn            = 3.4[dB]
X_Pulse          = 5.375[us]
Irr_Mode         = Off
Tri_Mode         = Off
Dante_Presat    = FALSE
Initial_Wait     = 1[s]
Repetition_Time  = 7.18365952[s]

```









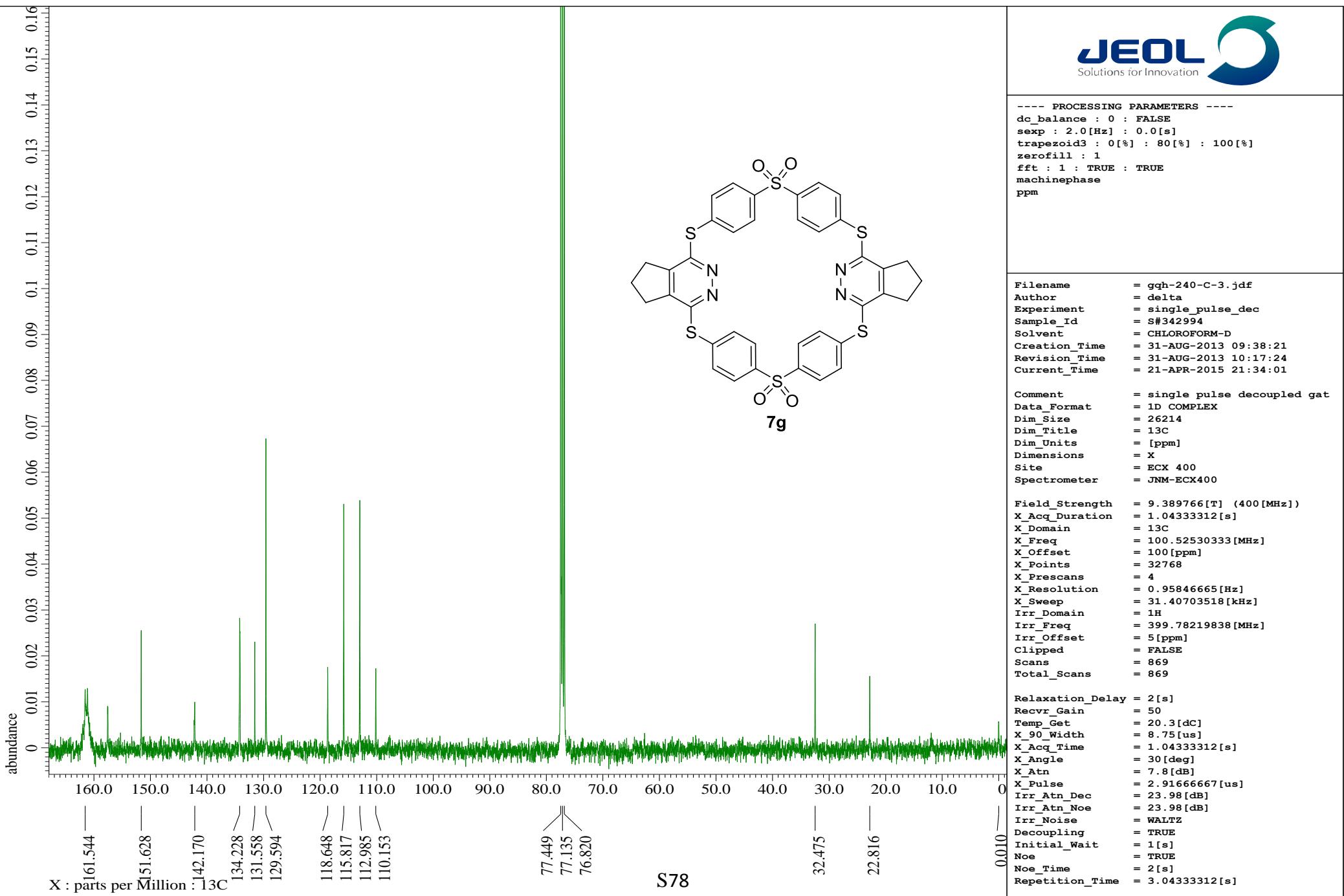
---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
sexp( 0.2[Hz], 0.0[s] )  
trapezoid3( 0[%], 80[%], 100[%] )  
zerofill( 1 )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm

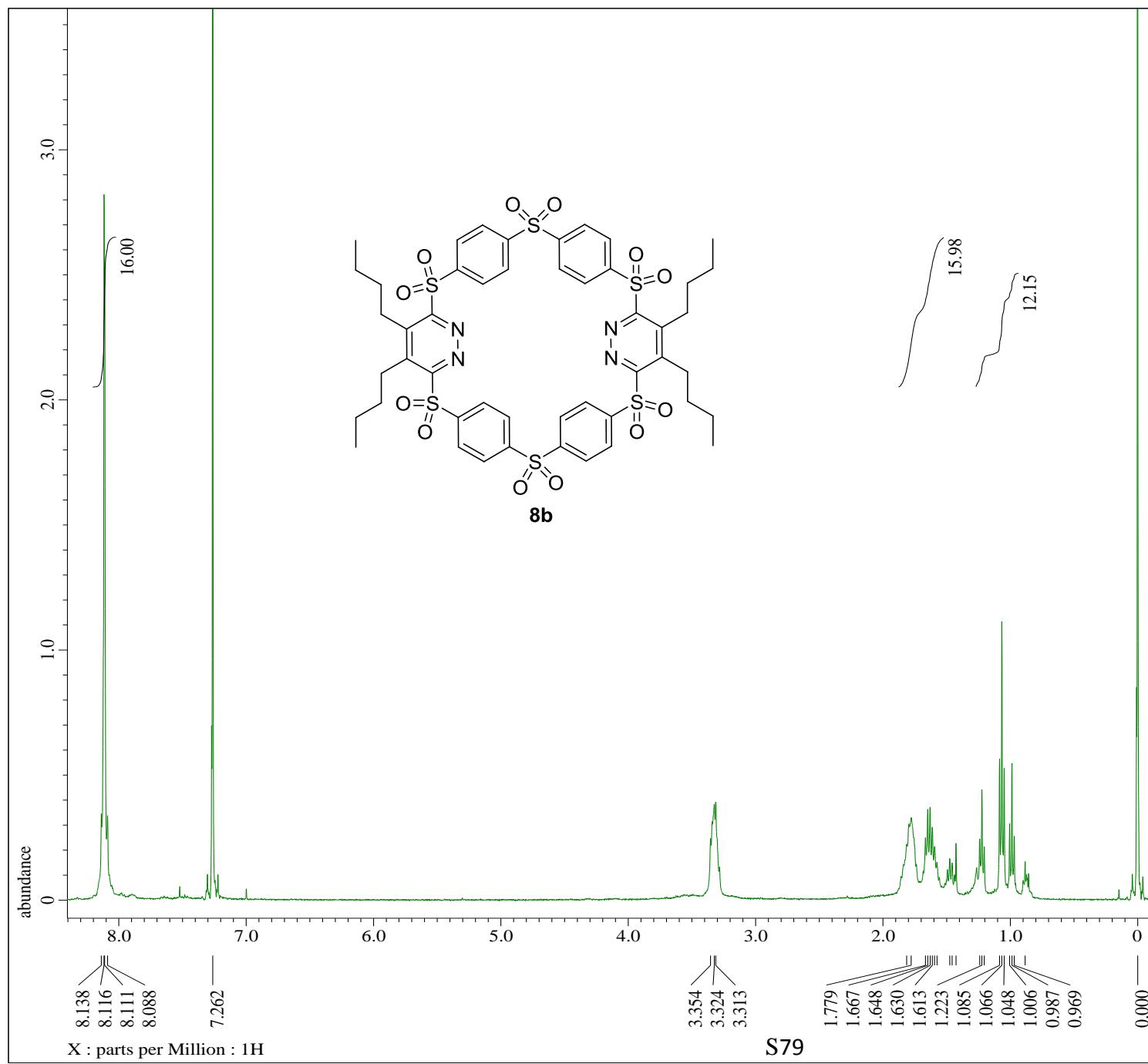
Filename = ggh-240-CF3COOH-1.5h-6.jdf  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#381751  
Solvent = CHLOROFORM-D  
Creation\_Time = 31-AUG-2013 09:59:58  
Revision\_Time = 24-JAN-2014 09:20:50  
Current\_Time = 21-APR-2015 21:34:30

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 48  
Temp\_Get = 20.1[dc]  
x\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[dB]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 7.18365952[s]





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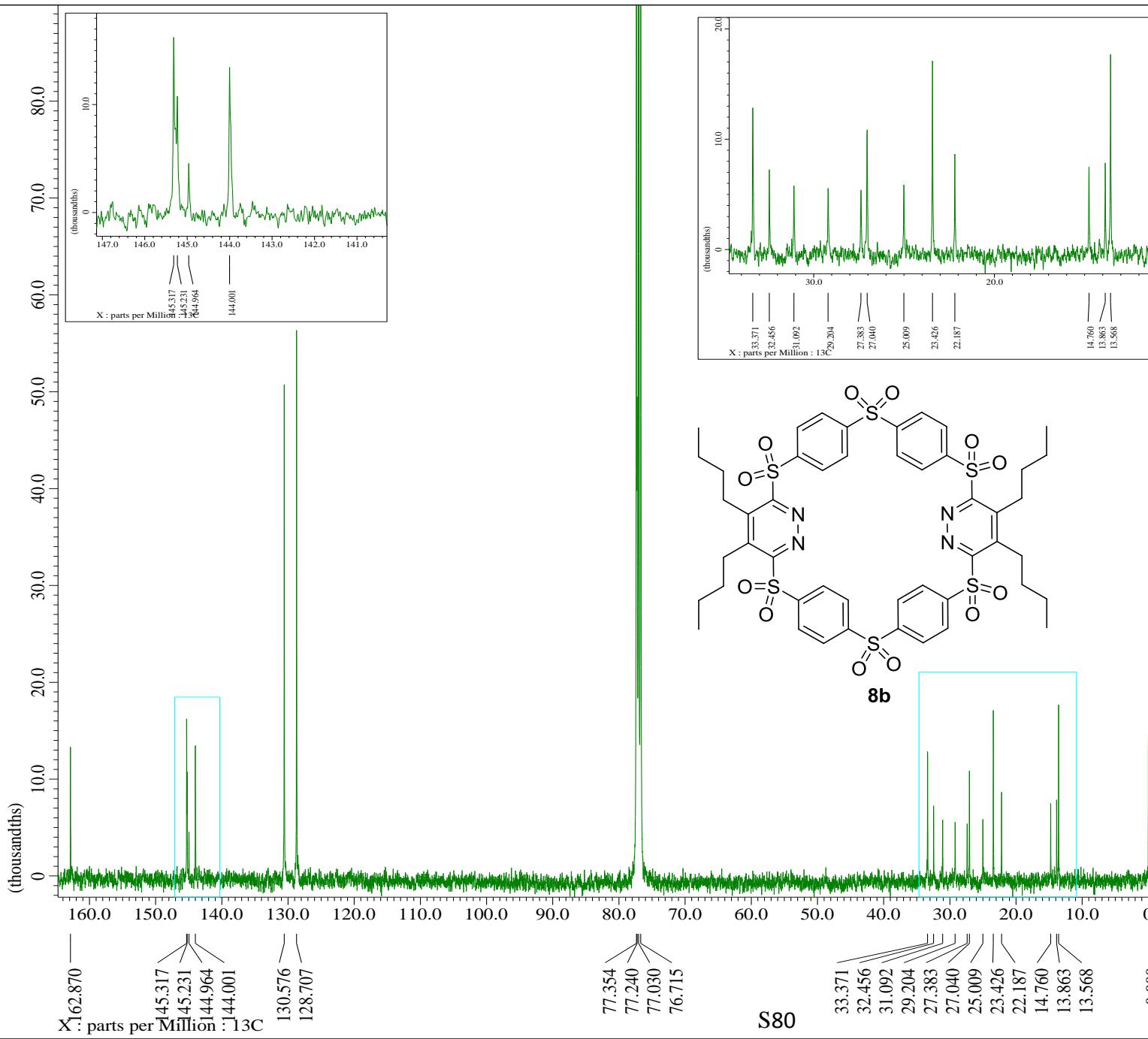
----- PROCESSING PARAMETERS -----  
dc\_balance : 0 : FALSE  
sexp : 0.2[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

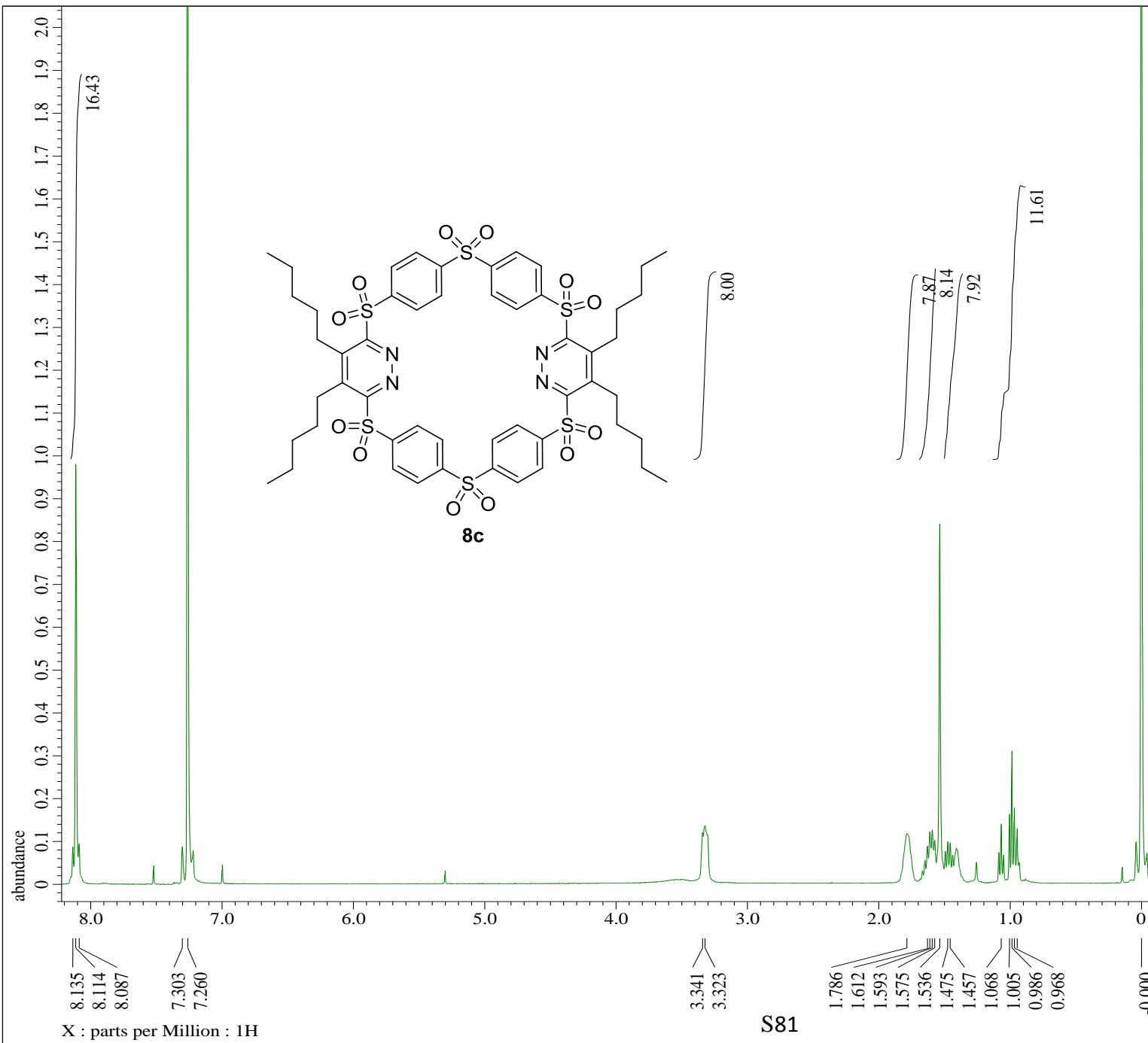
Filename = gqh-271-7.jdf  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#556198  
Solvent = CHLOROFORM-D  
Creation\_Time = 12-OCT-2013 14:49:15  
Revision\_Time = 21-APR-2015 20:44:55  
Current\_Time = 21-APR-2015 20:45:01

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 48  
Temp\_Get = 19.6[dC]  
X\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[dB]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 7.18365952[s]





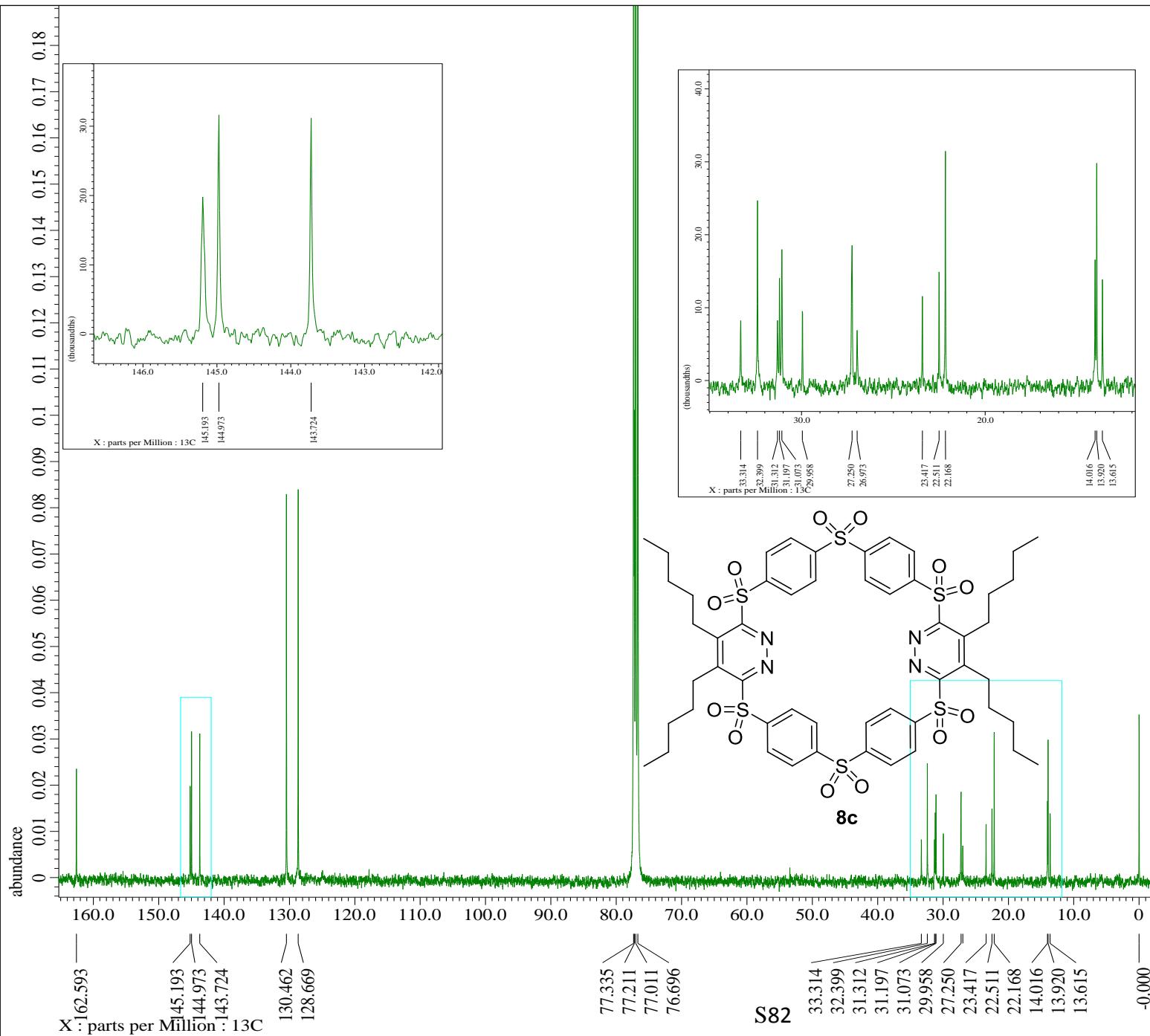
---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 0.2[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

Filename = ggh-264-20131101-3.jdf  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#817740  
Solvent = CHLOROFORM-D  
Creation\_Time = 1-NOV-2013 22:37:29  
Revision\_Time = 1-NOV-2013 23:23:12  
Current\_Time = 21-APR-2015 20:35:17

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = x  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 279  
Total\_Scans = 279

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 50  
Temp\_Get = 22[dC]  
x\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[db]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 7.18365952[s]



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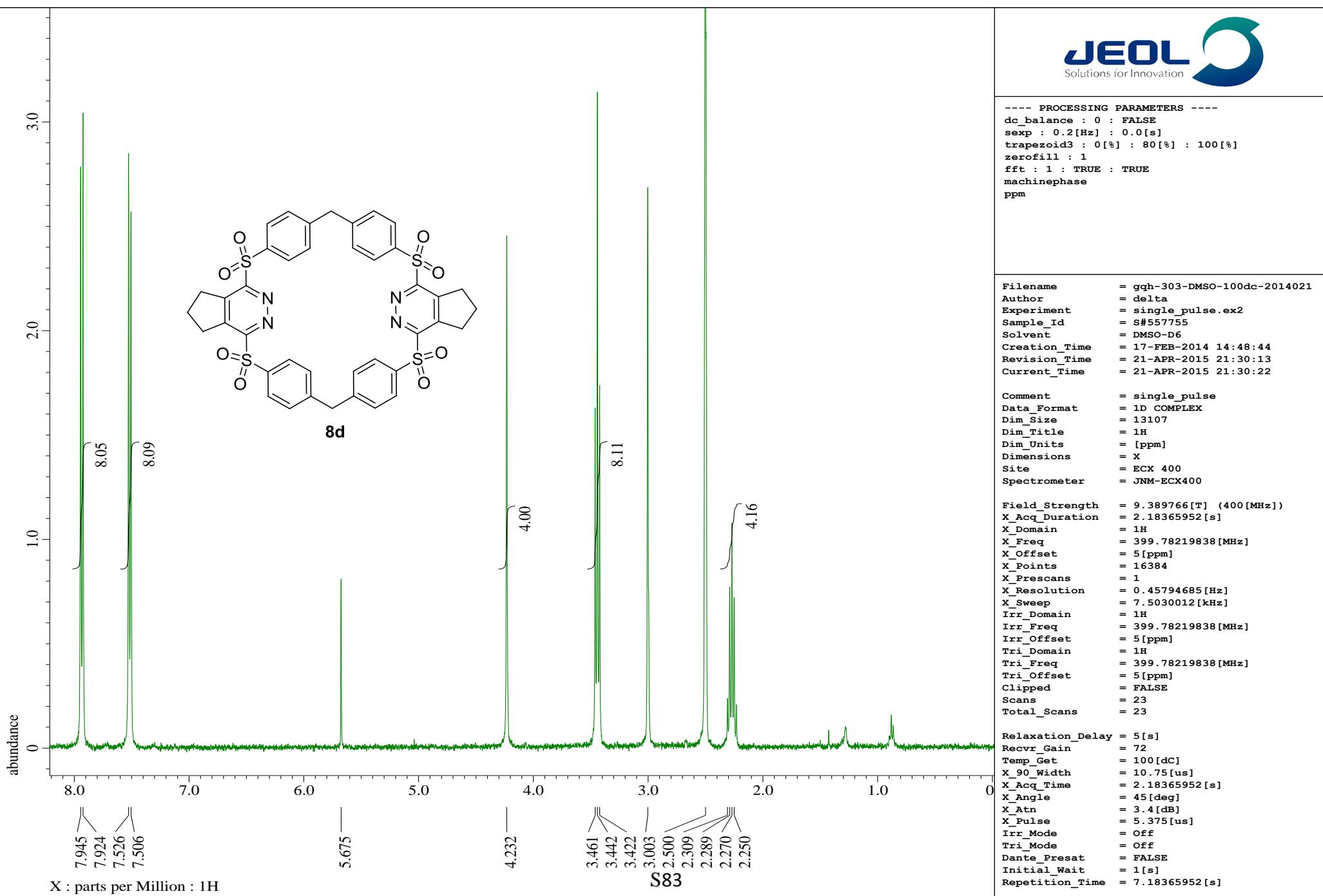
----- PROCESSING PARAMETERS -----  
dc\_balance : 0 : FALSE  
sexp : 2.0[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

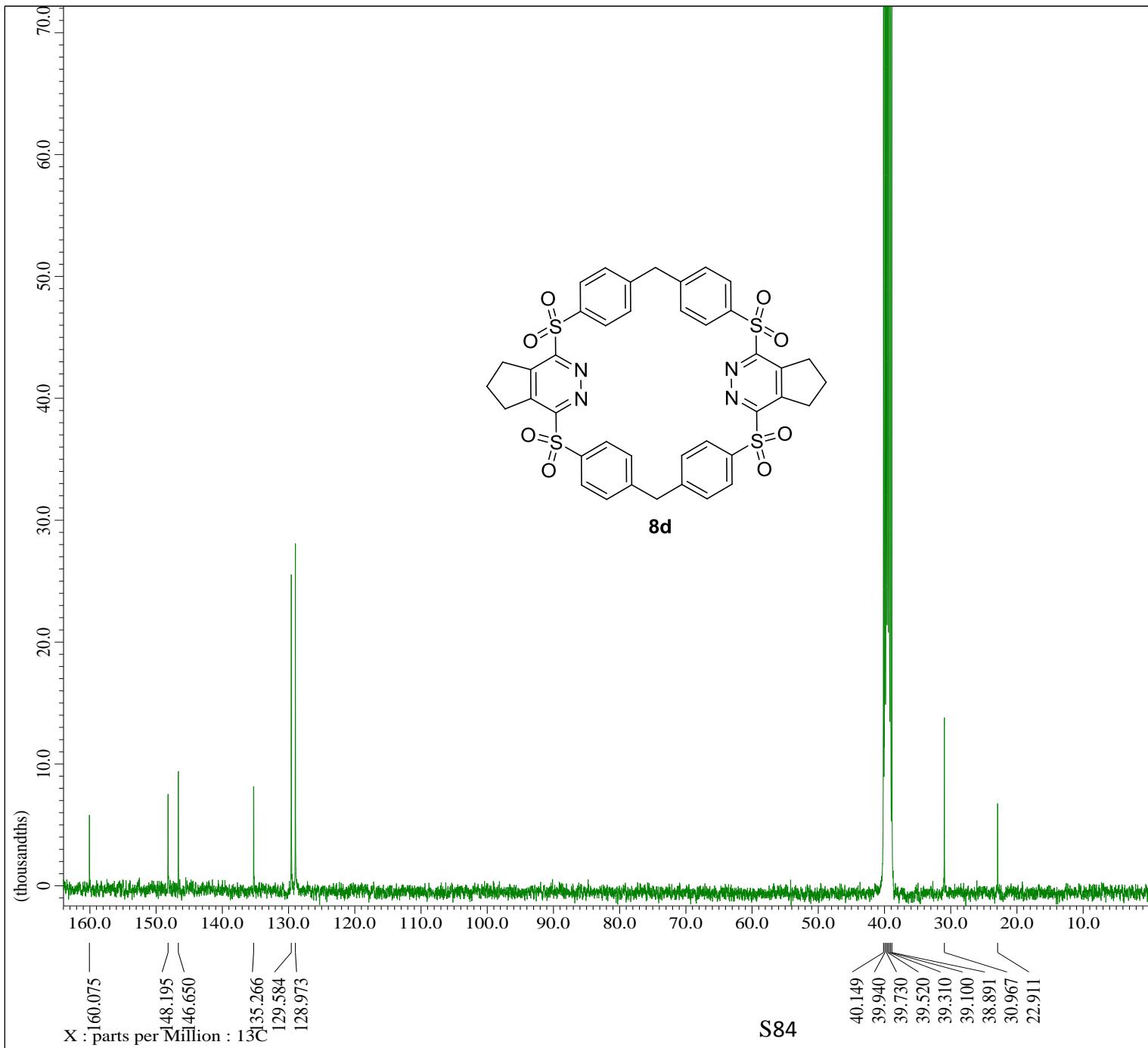
Filename = ggh-264-C-201301003\_copy-5  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_Id = S#795156  
Solvent = CHLOROFORM-D  
Creation\_Time = 4-OCT-2013 07:57:59  
Revision\_Time = 21-APR-2015 20:34:36  
Current\_Time = 21-APR-2015 20:34:41

Comment = single pulse decoupled gat  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
Dim\_Title = <sup>13</sup>C  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 1.04333312[s]  
X\_Domain = <sup>13</sup>C  
X\_Freq = 100.52530333[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 0.95846665[Hz]  
X\_Sweep = 31.40703518[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Clipped = TRUE  
Incomplete\_Copy = TRUE  
Scans = 12412  
Total\_Scans = 12412

Relaxation\_Delay = 2[s]  
Recv\_Gain = 58  
Temp\_Get = 19.8[dC]  
X\_90\_Width = 8.75[us]  
X\_Acq\_Time = 1.04333312[s]  
X\_Angle = 30[deg]  
X\_Atn = 7.8[dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe\_Time = 2[s]





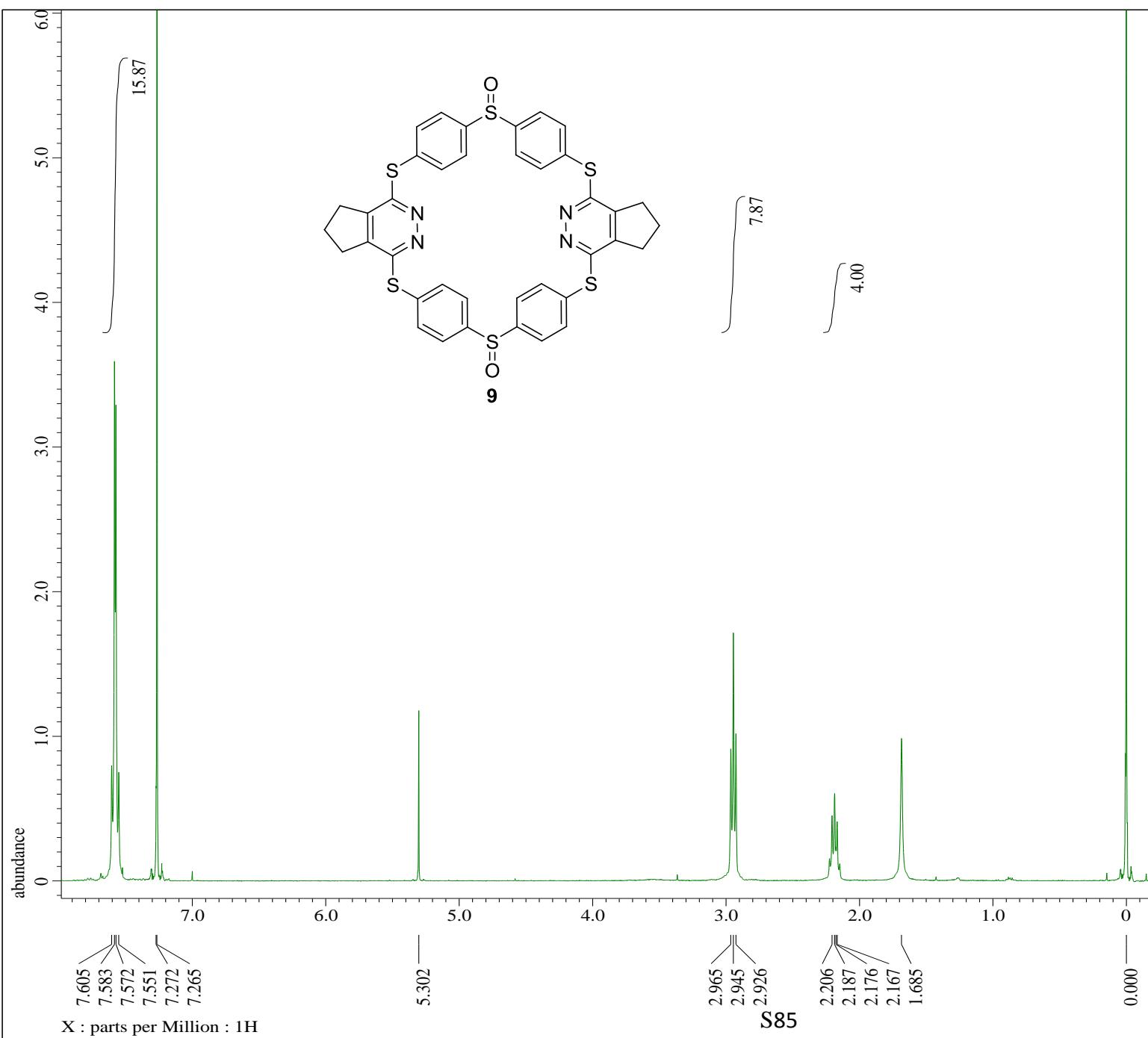
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---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 2.0[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

Filename = ggh-303-C-DMSO-20140218-10  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_Id = S#808974  
Solvent = DMSO-D6  
Creation\_Time = 18-FEB-2014 06:34:21  
Revision\_Time = 18-FEB-2014 08:27:40  
Current\_Time = 21-APR-2015 21:29:34

Comment = single pulse decoupled gat  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
Dim\_Title = 13C  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400  
Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acc\_Duration = 1.04333312[s]  
X\_Domain = 13C  
X\_Freq = 100.52530333[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 0.95846665[Hz]  
X\_Sweep = 31.40703518[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 10411  
Total\_Scans = 10411

Relaxation\_Delay = 2[s]  
Recvr\_Gain = 50  
Temp\_Get = 100[dC]  
X\_90\_Width = 8.75[us]  
X\_Acc\_Time = 1.04333312[s]  
X\_Angle = 30[deg]  
X\_Atn = 7.8[dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE  
Noe\_Time = 2[s]  
Repetition\_Time = 3.04333312[s]



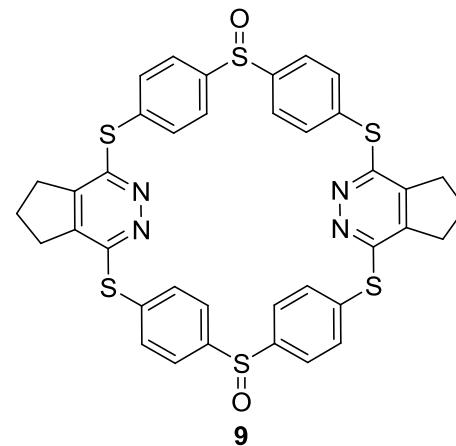
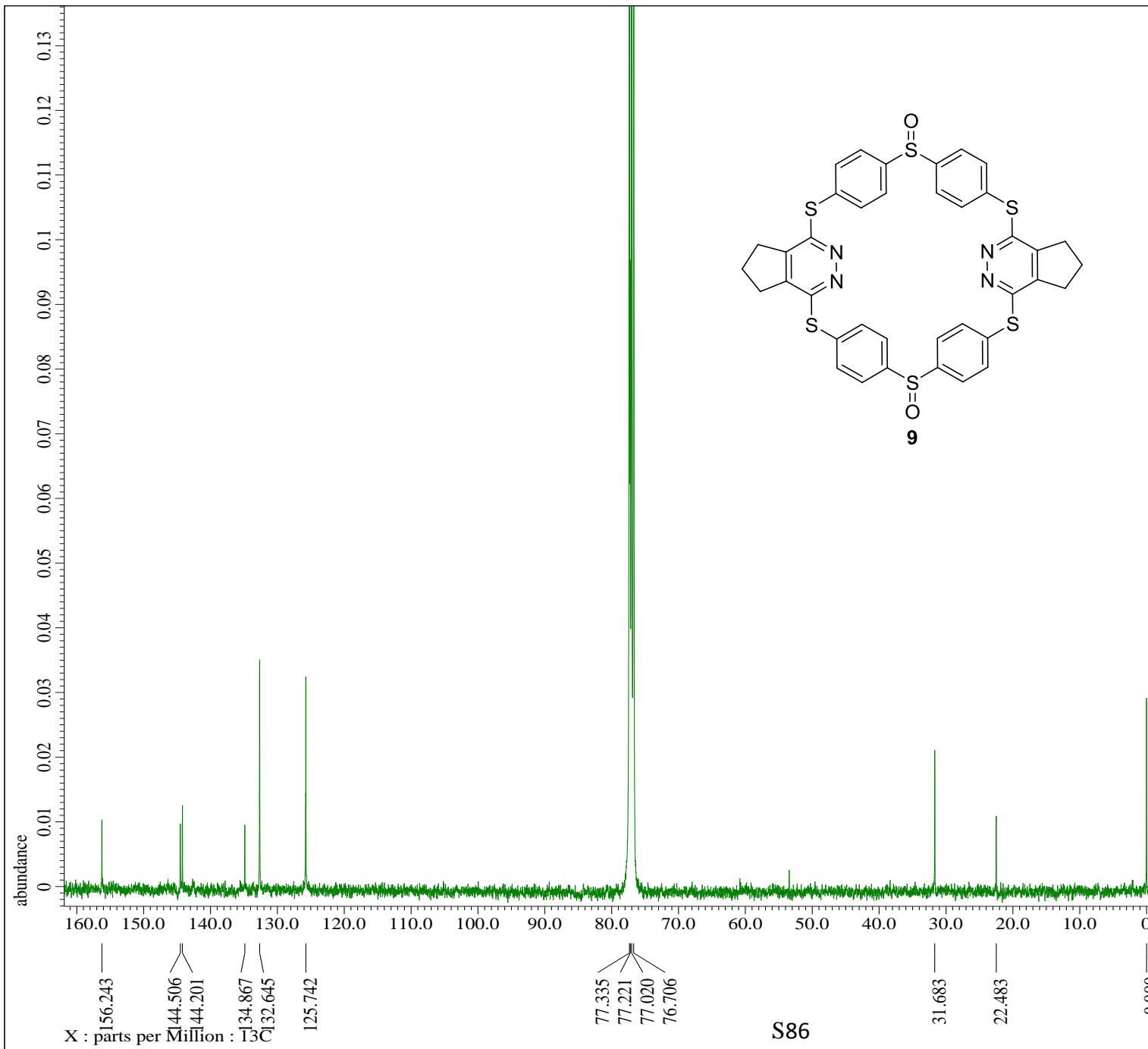
---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 0.2[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

Filename = gqh-259-02-20130926-3.jdf  
Author = delta  
Experiment = single\_pulse.ex2  
Sample\_Id = S#631150  
Solvent = CHLOROFORM-D  
Creation\_Time = 26-SEP-2013 16:56:31  
Revision\_Time = 26-SEP-2013 17:37:52  
Current\_Time = 21-APR-2015 21:36:35

Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
Dim\_Title = 1H  
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400

Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 2.18365952[s]  
X\_Domain = 1H  
X\_Freq = 399.78219838[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.45794685[Hz]  
X\_Sweep = 7.5030012[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = 1H  
Tri\_Freq = 399.78219838[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 13  
Total\_Scans = 13

Relaxation\_Delay = 5[s]  
Recvr\_Gain = 48  
Temp\_Get = 18.8[dc]  
X\_90\_Width = 10.75[us]  
X\_Acq\_Time = 2.18365952[s]  
X\_Angle = 45[deg]  
X\_Atn = 3.4[dB]  
X\_Pulse = 5.375[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 7.18365952[s]



---- PROCESSING PARAMETERS ----  
dc\_balance : 0 : FALSE  
sexp : 2.0[Hz] : 0.0[s]  
trapezoid3 : 0[%] : 80[%] : 100[%]  
zerofill : 1  
fft : 1 : TRUE : TRUE  
machinephase  
ppm

Filename = gqh-259-02-C-3.jdf  
Author = delta  
Experiment = single\_pulse\_dec  
Sample\_Id = S#17959  
Solvent = CHLOROFORM-D  
Creation\_Time = 28-SEP-2013 11:12:13  
Revision\_Time = 28-SEP-2013 22:00:13  
Current\_Time = 21-APR-2015 21:36:02  
Comment = single pulse decoupled gat  
Data\_Format = 1D COMPLEX  
Dim\_Size = 26214  
Dim\_Title =  $^{13}\text{C}$   
Dim\_Units = [ppm]  
Dimensions = X  
Site = ECX 400  
Spectrometer = JNM-ECX400  
Field\_Strength = 9.389766[T] (400[MHz])  
X\_Acq\_Duration = 1.04333312[s]  
X\_Domain =  $^{13}\text{C}$   
X\_Freq = 100.52530333[MHz]  
X\_Offset = 100[ppm]  
X\_Points = 32768  
X\_Prescans = 4  
X\_Resolution = 0.95846665[Hz]  
X\_Sweep = 31.40703518[kHz]  
Irr\_Domain = 1H  
Irr\_Freq = 399.78219838[MHz]  
Irr\_Offset = 5[ppm]  
Clipped = TRUE  
Scans = 13392  
Total\_Scans = 13392  
Relaxation\_Delay = 2[s]  
Recv\_Gain = 56  
Temp\_Get = 20.2[dc]  
x\_90\_Width = 8.75[us]  
X\_Acc\_Time = 1.04333312[s]  
X\_Angle = 30[deg]  
X\_Atn = 7.8[dB]  
X\_Pulse = 2.91666667[us]  
Irr\_Atn\_Dec = 23.98[dB]  
Irr\_Atn\_Noe = 23.98[dB]  
Irr\_Noise = WALTZ  
Decoupling = TRUE  
Initial\_Wait = 1[s]  
Noe = TRUE  
Noe\_Time = 2[s]  
Repetition\_Time = 3.04333312[s]