Supporting Information

An Unusual Formal Migrative Cycloaddition of Aurone-derived Azadienes: Synthesis of Benzofuran-fused Nitrogen Heterocycles

Qiang Feng,[a,†] An Wu,[a,†] Xinhao Zhang,[b] Lijuan Song,[c,*] and Jianwei Sun [a,d,*]

[a] *Department of Chemistry and Shenzhen Research Institute, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong SAR, China*

[b] *Shenzhen Bay Laboratory, State Key Laboratory of Chemical Oncogenomics, Peking University Shenzhen Graduate School, Shenzhen, China*

[c] *School of Science, Harbin Institute of Technology (Shenzhen), Shenzhen, 518055 China*

[d] *The Hong Kong Branch of Chinese National Engineering Research Centre for Tissue Restoration & Reconstruction, Clear Water Bay, Kowloon, Hong Kong SAR, China*

[†] *These authors contributed equally to this work.*

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I. General Information

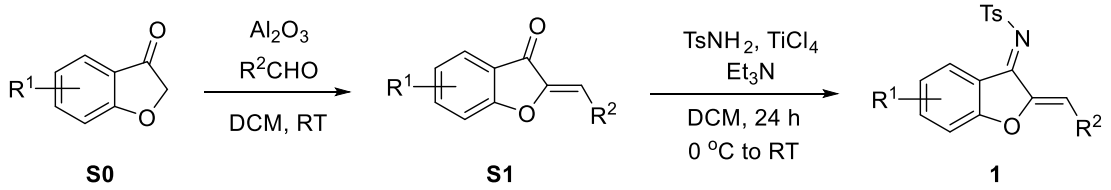
All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using dry solvents. Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co., China. Anhydrous DCM was distilled with calcium hydride, and anhydrous 1,2-dichloroethane was purchased from Sigma-Aldrich® Scientific Ltd. Siloxy alkynes were prepared according to the procedures in the literatures and the characterization data match the reported data.[1] ^{1}H and ^{13}C NMR spectra were collected on a Bruker AV 400 MHz NMR spectrometer using residue solvent peaks as an internal standard (^{1}H NMR: $CDCl_3$ at 7.26 ppm, ^{13}C NMR: $CDCl_3$ at 77.0 ppm). The ESI-TOF mass spectra was run by a WatersR Xevo G2-XS TOF instrument with an ESI source. The MALDI-TOF mass spectra were run by a WatersR MicromassR MALDI micro MXTM Mass Spectrometer operated on the reflectron mode. The DCTB matrix was used. The CI mass spectrum was run by a WatersR MicromassR GCTTM Premier Mass Spectrometer operated on the positive ion mode with NH_3/CH_4 as the reagent gas.

[1] A. Wu, Q. Feng, H. H. Y. Sung, I. D. Williams and J. Sun , *Angew. Chem. Int. Ed.,* 2019**, 58**, 6776–6780.

II. Substrate Preparation

Substrates **1** were prepared according to the General Procedure A, which was modified from the literature procedure.[2,3]

General Procedure A.



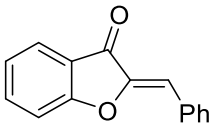
At room temperature, to an oven-dried round-bottom flask charged with a solution of the benzofuran-3(*2H*)-one **S0** (1 equiv) and the aldehyde (1.2 equiv) in DCM (0.1 M) was added basic Al_2O_3 (5 equiv, activated by heating at 130 °C in oven for 2 h). The mixture was stirred at room temperature and the progress was monitored by TLC. Upon completion, the reaction mixture was filtered, and the filtrate was concentrated under the reduced pressure. The residue was purified by silica gel flash column chromatography or recrystallization to give the desired product **S1**.

Under N_2 at 0 °C, to a solution of the enone **S1** (1 equiv) and 4-methylbenzenesulfonamide (1.5 equiv) in DCM (0.1 M) were sequentially added Et_3N (2 equiv) and $TiCl_4$ (1 equiv). The mixture was stirred at room temperature for ~12 h and then quenched with water. The layers were separated, and the aqueous layer was extracted with DCM (3 times). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel flash column

[2] Z.-P. Wang, S. Xiang, P.-L. Shao and Y. He, *J. Org. Chem.*, 2018, **83**, 10995–11007.

[3] Z.-Q. Rong, M. Wang, C. H. E. Chow and Y. Zhao, *Chem. Eur. J.*, 2016, **22**, 9483–9487.

chromatography to give desired product **1**.



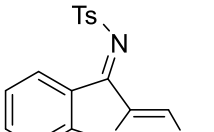
S1a

(*Z*)-2-Benzylidenebenzofuran-3(2*H*)-one (S**1a**) was prepared as a yellow solid from benzofuran-3(*2H*)-one (20 mmol) and benzaldehyde (24 mmol, 1.2 equiv) according to the General Procedure A (purification by recrystallization from DCM/hexanes) in 91% yield (4.04 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 – 7.91 (m, 2H), 5.80 (dd, J = 7.6, 0.8 Hz, 1H), 7.66 – 7.62 (m, 1H), 7.47 – 7.37 (m, 3H), 7.32 (d, J = 8.3 Hz, 1H), 7.21 (t, J = 7.5 Hz, 1H), 6.89 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 184.7, 166.1, 146.8, 136.8, 132.2, 131.5, 129.8, 128.9, 124.6, 123.4, 121.6, 113.0, 112.9.

This is a known compound. The spectral data are identical to those reported in the literature.[2]



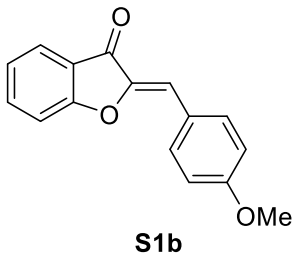
1a

***N*-((*E*)-2-((*Z*)-Benzylidene)benzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide** (**1a**) was prepared as a light yellow solid from **S1a** (870 mg, 3 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/DCM = 1:1) in 62% yield (0.82 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, J = 8.0 Hz, 1H), 8.01 (d, J = 8.2 Hz, 2H), 7.88 (d, J = 7.1 Hz, 2H), 7.68 (t, J = 7.4 Hz, 1H), 7.45 – 7.26 (m, 7H), 7.11 (s, 1H), 2.47 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 164.7, 149.6, 143.3, 138.9, 137.6, 132.3, 131.6, 131.0, 130.2, 129.4, 128.9, 127.0, 123.7, 118.2, 115.6, 112.3, 21.6.

This is a known compound. The spectral data are identical to those reported in the literature.[3]



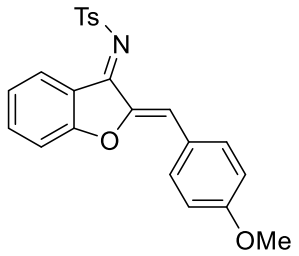
S1b

(*Z*)-2-(4-Methoxybenzylidene)benzofuran-3(2*H*)-one (**S1b**) was prepared as a yellow solid from benzofuran-3(2*H*)-one (5 mmol) and 4-methoxybenzaldehyde (6 mmol, 1.2 equiv) according to the General Procedure A (purification by recrystallization from DCM/hexanes) in 77% yield (0.97 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.85 (m, 2H), 7.80 (dd, J = 7.6, 0.7 Hz, 1H), 7.70 – 7.56 (m, 1H), 7.32 (d, J = 8.3 Hz, 1H), 7.20 (t, J = 7.4 Hz, 1H), 7.02 – 6.94 (m, 2H), 6.88 (s, 1H), 3.87 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 184.5, 165.8, 161.0, 145.8, 136.5, 133.4, 125.0, 124.5, 123.2, 121.9, 114.5, 113.4, 112.8, 55.4.

This is a known compound. The spectral data are identical to those reported in the literature.[2]



1b

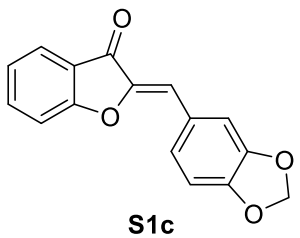
***N*-((*E*)-2-((*Z*)-4-Methoxybenzylidene)benzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide** (**1b**) was prepared as a light yellow solid from

S1b (756 mg, 3 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/ethyl acetate = 1:1) in 48% yield (0.58 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, J = 8.0 Hz, 1H), 8.07 (d, J = 8.1 Hz, 2H), 7.85 (d, J = 8.6 Hz, 2H), 7.67 (t, J = 7.7 Hz, 1H), 7.41 (d, J = 8.0 Hz, 2H), 7.37 – 7.22 (m, 2H), 7.12 (s, 1H), 6.95 (d, J = 8.7 Hz, 2H), 3.85 (s, 3H), 2.49 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 164.2, 161.3, 148.0, 143.0, 139.1, 137.0, 133.6, 130.6, 129.3, 126.8, 125.0, 123.3, 118.4, 116.4, 114.4, 112.1, 55.2, 21.4.

This is a known compound. The spectral data are identical to those reported in the literature.[3]



S1c

(*Z*)-2-(Benzo[d][1,3]dioxol-5-ylmethylene)benzofuran-3(2*H*)-one (**S1c**) was prepared as a yellow solid from benzofuran-3(2*H*)-one (5 mmol) and benzo[d][1,3]dioxole-5-carbaldehyde (6 mmol, 1.2 equiv) according to the General Procedure A (purification by recrystallization from DCM/hexanes) in 72% yield (0.95 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, J = 7.6 Hz, 1H), 7.63 (t, J = 7.8 Hz, 1H), 7.58 (s, 1H), 7.31 (d, J = 8.3 Hz, 2H), 7.20 (t, J = 7.5 Hz, 1H), 6.87 (d, J = 8.1 Hz, 1H), 6.82 (s, 1H), 6.03 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 184.4, 165.8, 149.2, 148.2, 145.8, 136.6, 127.6, 126.6, 124.5, 123.3, 121.8, 113.4, 112.9, 110.6, 108.8, 101.6.

This is a known compound. The spectral data are identical to those reported in the literature.[4]

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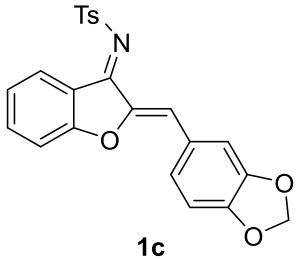
[4] M. Morimoto, H. Fukumoto, T. Nozoe, A. Hagiwara and K. Komai, *J. Agric.*



1c

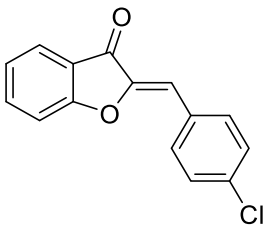
***N*-((2*Z*,3*E*)-2-(Benzo[*d*][1,3]dioxol-5-ylmethylene)benzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide** (**1c**) was prepared as a light yellow solid from **S1c** (772 mg, 2.9 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/DCM = 3:2) in 41% yield (0.5 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (d, J = 8.0 Hz, 1H), 7.99 (d, J = 8.2 Hz, 2H), 7.74 – 7.61 (m, 1H), 7.56 (d, J = 1.4 Hz, 1H), 7.44 – 7.17 (m, 5H), 7.04 (s, 1H), 6.83 (d, J = 8.1 Hz, 1H), 6.02 (s, 2H), 2.46 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 157.3, 142.7, 141.3 (2C), 136.2, 132.1, 130.2, 123.8, 122.4, 121.2, 119.9, 119.8, 116.6, 111.5, 109.3, 105.2, 103.5, 101.8, 94.7, 14.6.

IR (thin film) 3227, 2900, 1653, 1608, 1534, 1491, 1446, 1343, 1299, 1260, 1201, 1149, 1086, 1034 cm^{-1}.

HRMS (CI) calculated for: $C_{23}H_{18}NO_5S$ $[M+H]^+$ 420.0900, found: 420.0916.



S1d

(*Z*)-2-(4-Chlorobenzylidene)benzofuran-3(2*H*)-one (**S1d**) was prepared as a yellow solid from benzofuran-3(2*H*)-one (5 mmol) and 4-chlorobenzaldehyde (6 mmol, 1.2 equiv) according to the General Procedure A (purification by

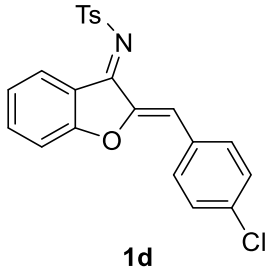
Food Chem., 2007, **55**, 700–705.

recrystallization from DCM/hexanes) in 79% yield (1.01 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.78 (m, 3H), 7.67 – 7.63 (m, 1H), 7.42 – 7.39 (m, 2H), 7.31 (d, *J* = 8.3 Hz, 1H), 7.24 – 7.20 (m, 1H), 6.81 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 184.5, 166.0, 146.9, 137.0, 135.8, 132.6, 130.8, 129.1, 124.7, 123.6, 121.5, 112.9, 111.5.

This is a known compound. The spectral data are identical to those reported in the literature.[5]



1d

***N*-((*E*)-2-((*Z*)-4-Chlorobenzylidene)benzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide** (**1d**) was prepared as a light yellow solid from **S1d** (768 mg, 3 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/DCM = 3:1) in 56% yield (0.69 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 8.0 Hz, 1H), 7.99 (d, *J* = 8.3 Hz, 2H), 7.80 (d, *J* = 8.6 Hz, 2H), 7.70 – 7.66 (m, 1H), 7.40 – 7.37 (m, 4H), 7.32 – 7.26 (m, 2H), 7.02 (s, 1H), 2.47 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 164.6, 149.8, 143.5, 138.8, 137.7, 136.2, 132.7, 131.1, 131.0, 129.5, 129.2, 127.0, 123.9, 118.2, 114.0, 112.3, 21.6.

This is a known compound. The spectral data are identical to those reported in the literature.[3]

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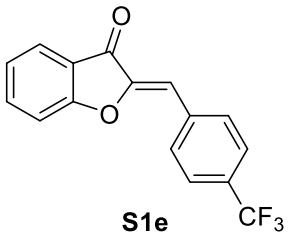
[5] H. Harkat, A. Blanc, J.-M. Weibel and P. Pale, *J. Org. Chem.*, 2008, **73**, 1620–1623.



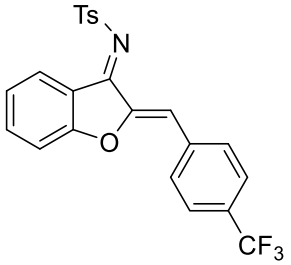
S1e

(*Z*)-2-(4-(Trifluoromethyl)benzylidene)benzofuran-3(2*H*)-one (**S1e**) was prepared as a yellow solid from benzofuran-3(2*H*)-one (5 mmol) and 4-formylbenzonitrile (6 mmol, 1.2 equiv) according to the General Procedure A (purification by recrystallization from DCM/hexanes) in 91% yield (1.12 g).

1H NMR (400 MHz, CDCl3) δ 8.01 (d, J = 8.2 Hz, 2H), 7.82 (dd, J = 7.6, 0.8 Hz, 1H), 7.68 (dd, J = 11.3, 4.5 Hz, 3H), 7.35 (d, J = 8.3 Hz, 1H), 7.25 (t, J = 7.6, 1H), 6.87 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 184.7, 166.3, 147.8, 137.3, 135.7, 131.4, 131.2, 125.7 (q, J = 3.8 Hz), 124.9, 123.9 (q, J = 271 Hz), 123.8, 121.3, 113.0, 110.7.

This is a known compound. The spectral data are identical to those reported in the literature.[6]



1e

4-Methyl-*N*-((*E*)-2-((Z)-4-(trifluoromethyl)benzylidene)benzofuran-3(2*H*)-ylidene)benzenesulfonamide (**1e**) was prepared as a light yellow solid from **S1e** (870 mg, 3 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/DCM = 1:1) in 62% yield (0.82 g).

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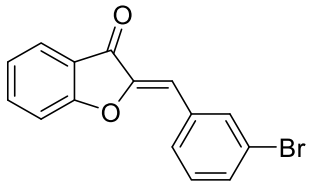
[6] K. M. Taylor, Z. E. Taylor and S. T. Handy, *Tetrahedron Lett.*, 2017, **58**, 240–241.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, J = 8.0 Hz, 1H), 7.98 (m, 4H), 7.83 – 7.55 (m, 3H), 7.33 (m, 4H), 7.04 (s, 1H), 2.48 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 164.8, 150.8, 143.6, 138.6, 138.0, 135.7, 131.4, 131.3, 130.9, 129.5, 127.1, 125.7 (q, J = 3.9 Hz), 124.1, 123.8 (q, J = 270 Hz), 118.0, 112.8, 112.3, 21.6.

This is a known compound. The spectral data are identical to those reported in the literature.[7]



S1f

(*Z*)-2-(3-Bromobenzylidene)benzofuran-3(2*H*)-one (**S1f**) was prepared as a light yellow solid from benzofuran-3(*2H*)-one (5 mmol) and 3-bromobenzaldehyde (6 mmol, 1.2 equiv) according to the General Procedure A (purification by recrystallization from DCM/hexanes) in 79% yield (1.18 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (t, J = 1.7 Hz, 1H), 7.84 – 7.75 (m, 2H), 7.67 (ddd, J = 8.6, 7.4, 1.4 Hz, 1H), 7.51 (ddd, J = 8.0, 1.8, 0.9 Hz, 1H), 7.39 – 7.28 (m, 2H), 7.25 – 7.20 (m, 1H), 6.77 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 184.6, 166.1, 147.3, 137.1, 134.3, 133.8, 132.6, 130.3, 130.0, 124.7, 123.7, 122.9, 121.3, 113.0, 111.0.

This is a known compound. The spectral data are identical to those reported in the literature.[8]

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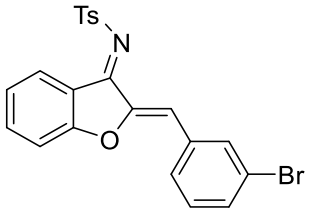
[7] J. Chen and Y. Huang, *Org. Lett.*, 2017, **19**, 5609–5612.

[8] M. P. Carrasco, A. S. Newton, L. Gonçalves, A. Góis, M. Machado, J. Gut, F. Nogueira, T. Hänscheid, R. C. Guedes, D. J. V. A. dos Santos, P. J. Rosenthal and R. Moreira, *Eur. J. Med. Chem.*, 2014, **80**, 523–534.



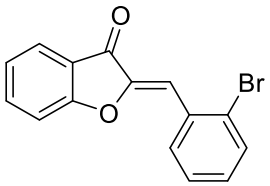
1f

***N*-((*E*)-2-((*Z*)-3-Bromobenzylidene)benzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide** (**1f**) was prepared as a light yellow solid from **S1f** (900 mg, 3 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/DCM = 1:1) in 52% yield (0.71 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (d, J = 7.9 Hz, 1H), 7.99 (d, J = 7.8 Hz, 3H), 7.83 – 7.60 (m, 2H), 7.47 (d, J = 7.9 Hz, 1H), 7.44 – 7.10 (m, 5H), 6.95 (s, 1H), 2.47 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 164.6, 150.2, 143.5, 138.7, 137.8, 134.3, 133.8, 132.8, 131.1, 130.3, 129.9, 129.5, 127.0, 124.0, 122.9, 118.0, 113.2, 112.3, 21.6.

This is a known compound. The spectral data are identical to those reported in the literature.[2]



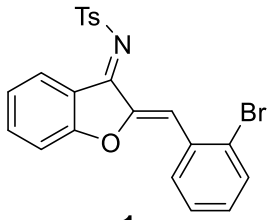
S1g

(*Z*)-2-(2-Bromobenzylidene)benzofuran-3(2*H*)-one (**S1g**) was prepared as a yellow solid from benzofuran-3(2*H*)-one (5 mmol) and 2-bromobenzaldehyde (6 mmol, 1.2 equiv) according to the General Procedure A (purification by recrystallization from DCM/hexanes) in 68% yield (1.02 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (dd, J = 7.9, 1.6 Hz, 1H), 7.81 (dd, J = 7.6, 0.8 Hz, 1H), 7.71 – 7.60 (m, 2H), 7.42 (ddd, J = 8.1, 7.5, 0.8 Hz, 1H), 7.31 (t, J = 4.2 Hz, 2H), 7.25 – 7.19 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 184.5, 166.2, 147.5, 137.1, 133.4, 132.3, 132.0, 130.7, 127.6, 126.5, 124.8, 123.7, 121.4, 112.9, 110.7.

This is a known compound. The spectral data are identical to those reported in the literature.[8]



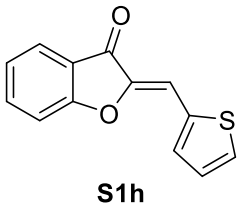
1g

***N*-((*E*)-2-((*Z*)-2-Bromobenzylidene)benzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide** (**1g**) was prepared as a light yellow solid from **S1g** (900 mg, 3 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/DCM = 1:1) in 55% yield (0.74 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, J = 7.7 Hz, 1H), 8.28 (dd, J = 7.9, 1.3 Hz, 1H), 8.02 (d, J = 8.2 Hz, 2H), 7.72 – 7.63 (m, 1H), 7.63 – 7.56 (m, 1H), 7.53 (s, 1H), 7.38 m, 3H), 7.27 (m, 2H), 7.18 (td, J = 8.0, 1.5 Hz, 1H), 2.46 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 164.7, 150.4, 143.3, 138.7, 137.7, 133.3, 132.4, 131.9, 131.1, 130.9, 129.4, 127.7, 126.9, 126.4, 123.9, 118.1, 112.9, 112.2, 21.6.

This is a known compound. The spectral data are identical to those reported in the literature.[3]



S1h

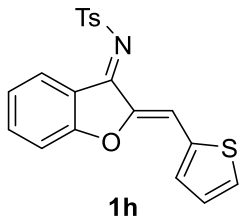
(*Z*)-2-(Thiophen-2-ylmethylene)benzofuran-3(2*H*)-one (**S1h**)was prepared as a yellow solid from benzofuran-3(*2H*)-one (5 mmol) and thiophene-2-carbaldehyde (6 mmol, 1.2 equiv) according to the General Procedure A

(purification by recrystallization from DCM/hexanes) in 77% yield (0.88 g).

^{1}H NMR (400 MHz, $CDCl_3$) 7.77 (d, *J* = 7.4 Hz, 1H), 7.66 – 7.56 (m, 2H), 7.52 (d, *J* = 3.6 Hz, 1H), 7.31 (d, *J* = 8.3 Hz, 1H), 7.15 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 183.7, 165.5, 145.2, 136.6, 135.4, 133.0 131.7, 128.0, 124.4, 123.4, 122.1, 112.9, 106.9.

This is a known compound. The spectral data are identical to those reported in the literature.[2]



1h

4-Methyl-*N*-((2*Z*,3*E*)-2-(thiophen-2-ylmethylene)benzofuran-3(2*H*)-ylidene)benzenesulfonamide (**1h**) was prepared as a light yellow solid from **S1h** (684 mg, 3 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/ethyl acetate/DCM = 20:4:1) in 51% yield (0.58 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, *J* = 7.7 Hz, 1H), 8.00 (d, *J* = 8.3 Hz, 2H), 7.70 – 7.57 (m, 2H), 7.50 (d, *J* = 3.7 Hz, 1H), 7.44 – 7.21 (m, 5H), 7.11 (dd, *J* = 5.0, 3.8 Hz, 1H), 2.46 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 163.9, 147.8, 143.2, 139.0, 137.2, 135.9, 133.6, 132.8, 130.7, 129.4, 128.2, 126.9, 123.7, 119.0, 112.3, 110.1, 21.5.

This is a known compound. The spectral data are identical to those reported in the literature.[9]

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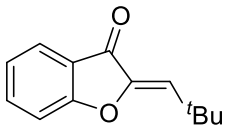
[9] H. Ni, X. Tang, W. Zheng, W. Yao, N. Ullah and Y. Lu, *Angew. Chem., Int. Ed.*, 2017, **56**, 14222–14226.



S1i

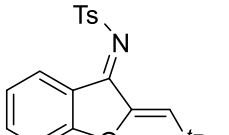
(*Z*)-2-(2,2-Dimethylpropylidene)benzofuran-3(2*H*)-one (**S1i**) was prepared as a light yellow solid from benzofuran-3(2*H*)-one (5 mmol) and pivalaldehyde (6 mmol, 1.2 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/DCM = 2:1) in 44% yield (0.44 g).

^{1}H NMR (400 MHz, $CDCl_3$) 7.74 (dd, *J* = 7.7, 0.6 Hz, 1H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.21 (d, *J* = 8.3 Hz, 1H), 7.15 (t, *J* = 7.5 Hz, 1H), 6.12 (s, 1H), 1.31 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 185.0, 166.2, 146.6, 136.9, 126.1, 124.6, 122.9, 121.6, 112.9, 32.6, 29.8.

IR (thin film) 3056, 2961, 2871, 1710, 1662, 1605, 1464, 1328, 1298, 1265, 1119, 1108 cm^{-1}.

HRMS (CI) calculated for $C_{13}H_{14}O_2$ $[M]^+$: 202.0994, found: 202.0999.



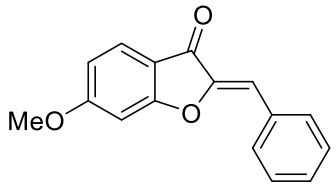
1i

***N*-((2*Z*,3*E*)-2-(2,2-Dimethylpropylidene)benzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide** (**1i**) was prepared as a light yellow solid from **S1i** (388 mg, 1.92 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/ethyl acetate = 5:1) in 44% yield (0.3 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (d, *J* = 8.0 Hz, 1H), 7.96 (d, *J* = 8.3 Hz, 2H), 7.80 – 7.52 (m, 1H), 7.36 (d, *J* = 8.1 Hz, 2H), 7.24 – 7.14 (m, 2H), 6.36 (s, 1H), 2.46 (s, 3H), 1.28 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 164.9, 149.2, 143.2, 139.0, 137.7, 131.0, 129.4, 129.1, 127.0, 123.2, 118.2, 112.2, 33.1, 29.9, 21.6.

This is a known compound. The spectral data are identical to those reported in the literature.[10]



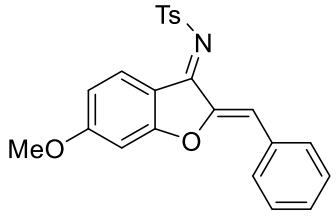
S1j

(*Z*)-2-Benzylidene-6-methoxybenzofuran-3(2*H*)-one (**S1j**) was prepared as a light yellow solid from 6-methoxybenzofuran-3(2*H*)-one (5 mmol) and benzaldehyde (6 mmol, 1.2 equiv) according to the General Procedure A (purification by recrystallization from DCM/hexanes) in 83% yield (1.05 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.81 (m, 2H), 7.68 (d, J = 8.4 Hz, 1H), 7.50 – 7.31 (m, 3H), 6.80 (s, 1H), 6.77 – 6.60 (m, 2H), 3.90 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 182.9, 168.5, 167.4, 147.8, 132.4, 131.2, 129.5, 128.8, 125.7, 114.7, 112.1, 111.8, 96.6, 56.0.

This is a known compound. The spectral data are identical to those reported in the literature.[2]



1j

***N*-((*E*)-2-((*Z*)-Benzylidene)-6-methoxybenzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide** (**1j**) was prepared as a light yellow solid from **S1j** (756 mg, 3 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent:

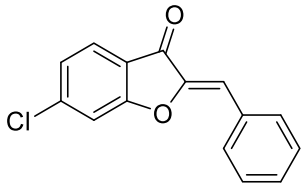
[10] Y.-N. Wang, L.-C. Yang, Z.-Q. Rong, T.-L. Liu, R. Liu and Y. Zhao, *Angew. Chem., Int. Ed.*, 2018, **57**, 1596–1600.

hexanes/DCM = 1:1) in 42% yield (0.51 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, J = 9.0 Hz, 1H), 7.99 (d, J = 8.0 Hz, 2H), 7.85 (d, J = 7.3 Hz, 2H), 7.39 (m, 5H), 7.02 (s, 1H), 6.79 (m, 2H), 3.94 (s, 3H), 2.46 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.0, 167.6, 163.7, 150.6, 143.1, 139.2, 132.4, 131.4, 129.9, 129.4, 128.8 (2C), 126.9, 114.5, 112.8, 111.7, 95.8, 56.2, 21.6.

This is a known compound. The spectral data are identical to those reported in the literature.[9]



S1k

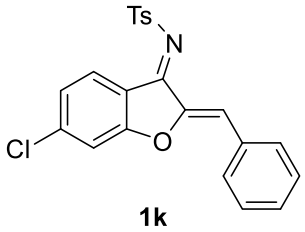
(*Z*)-2-Benzylidene-6-chlorobenzofuran-3(2*H*)-one (**S1k**) was prepared as a light red solid from 6-chlorobenzofuran-3(2*H*)-one (3 mmol) and benzaldehyde (3.6 mmol, 1.2 equiv) according to the General Procedure A (purification by recrystallization from DCM/hexanes) in 74% yield (0.57 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, J = 6.5 Hz, 2H), 7.70 (d, J = 7.9 Hz, 1H), 7.54 – 7.29 (m, 4H), 7.17 (d, J = 7.8 Hz, 1H), 6.87 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 183.1, 166.1, 146.8, 142.8, 131.9, 131.5, 130.1, 128.9, 125.3, 124.3, 120.2, 113.8, 113.5.

This is a known compound. The spectral data are identical to those reported in the literature.[11]

[11] T. Yatabe, X. Jin, N. Mizuno and K. Yamaguchi, *ACS Catal.*, 2018, **8**, 4969–4978.



1k

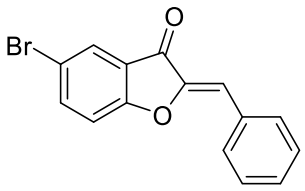
***N*-((*E*)-2-((*Z*)-Benzylidene)-6-chlorobenzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide** (**1k**) was prepared as a light yellow solid from **S1k** (506 mg, 3 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/ethyl acetate = 5:1) in 54% yield (0.48 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 8.6 Hz, 1H), 7.99 (d, *J* = 8.2 Hz, 2H), 7.83 (d, *J* = 6.7 Hz, 2H), 7.53 – 7.29 (m, 6H), 7.22 (dd, *J* = 8.6, 1.5 Hz, 1H), 7.08 (s, 1H), 2.47 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) *δ* 164.7, 163.6, 149.6, 143.6, 143.5, 138.6, 132.0, 131.8, 131.7, 130.4, 129.4, 128.9, 127.0, 124.5, 116.9, 116.2, 112.8, 21.6.

IR (thin film) 3057, 1657, 1600, 1547, 1432, 1304, 1186, 1081 cm^{-1}.

HRMS (CI) calculated for $C_{22}H_{17}ClNO_3S$ $[M+H]^+$: 410.0612, found: 410.0609.



S1l

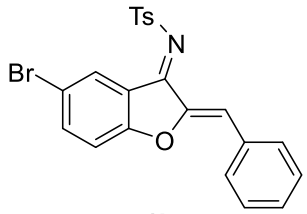
(*Z*)-2-Benzylidene-5-bromobenzofuran-3(2*H*)-one (**S1l**) was prepared as a light yellow solid from 5-bromobenzofuran-3(2*H*)-one (5 mmol) and benzaldehyde (6 mmol, 1.2 equiv) according to the General Procedure A (purification by recrystallization from DCM/hexanes) in 83% yield (1.05 g).

^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.90 (dd, *J* = 6.1, 4.6 Hz, 3H), 7.73 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.50 – 7.38 (m, 3H), 7.24 (d, *J* = 8.7 Hz, 1H), 6.91 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) *δ* 183.22, 164.7, 146.8, 139.3, 131.9, 131.7, 130.2, 129.0,

127.3, 123.3, 116.3, 114.7, 114.1.

This is a known compound. The spectral data are identical to those reported in the literature.[6]



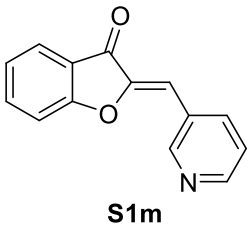
1l

***N*-((*E*)-2-((*Z*)-Benzylidene)-5-bromobenzofuran-3(2*H*)-ylidene)-4-methylbenzenesulfonamide** (**1l**) was prepared as a light yellow solid from **S1l** (860 mg, 2.86 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/ethyl acetate = 5:1) in 40% yield (0.52 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (s, 1H), 7.99 (d, J = 8.3 Hz, 2H), 7.96 – 7.80 (m, 2H), 7.76 (dd, J = 8.8, 2.1 Hz, 1H), 7.42 (ddd, J = 14.9, 8.8, 5.5 Hz, 5H), 7.32 – 7.19 (m, 1H), 7.13 (s, 1H), 2.48 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.5, 163.4, 149.4, 143.6, 140.1, 138.5, 133.1, 132.0, 131.8, 130.6, 129.5, 129.0, 127.1, 120.0, 116.6, 116.4, 113.9, 21.6.

This is a known compound. The spectral data are identical to those reported in the literature.[12]



S1m

(*Z*)-2-(Pyridin-3-ylmethylene)benzofuran-3(2H)-one (**S1m**) was prepared as a light yellow solid from benzofuran-3(2*H*)-one (5 mmol) and nicotinaldehyde

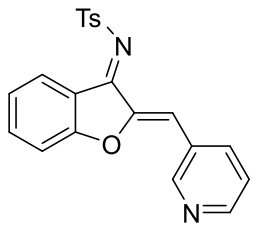
[12] R. Zeng, C. Shan, M. Liu, K. Jiang, Y. Ye, T.-Y. Liu and Y.-C. Chen, *Org. Lett.*, 2019, **21**, 2312–2316.

(5.5 mmol, 1.1 equiv) according to the General Procedure A (purification by recrystallization from Et_2O/hexanes) in 49% yield (551 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.02 (d, J = 1.9 Hz, 1H), 8.58 (dd, J = 4.8, 1.5 Hz, 1H), 8.27 (dt, J = 8.0, 1.9 Hz, 1H), 7.79 (dd, J = 7.6, 0.8 Hz, 1H), 7.66 (ddd, J = 8.6, 7.4, 1.4 Hz, 1H), 7.38 (dd, J = 8.0, 4.8 Hz, 1H), 7.31 (d, J = 8.3 Hz, 1H), 7.23 (t, J = 7.5 Hz, 1H), 6.82 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 184.3, 166.1, 152.2, 150.0, 148.0, 137.6, 137.3, 128.5, 124.8, 123.8, 123.7, 121.3, 112.9, 108.8.

This is a known compound. The spectral data are identical to those reported in the literature.[2]



1m

4-Methyl-*N*-((2*Z*,3*E*)-2-(pyridin-3-ylmethylene)benzofuran-3(2H)-ylidene)benzenesulfonamide (**1m**) was prepared as a light yellow solid from **S1m** (516 mg, 2.3 mmol) and 4-methylbenzenesulfonamide (1.5 equiv) according to the General Procedure A (purified by silica gel chromatography, eluent: hexanes/ethyl acetate = 3:1 → 1:1) in 42% yield (0.36 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (d, J = 1.7 Hz, 1H), 8.77 (d, J = 7.9 Hz, 1H), 8.57 (dd, J = 4.8, 1.4 Hz, 1H), 8.31 – 8.23 (m, 1H), 7.99 (d, J = 8.3 Hz, 2H), 7.74 – 7.65 (m, 1H), 7.38 (t, J = 7.5 Hz, 3H), 7.34 – 7.27 (m, 2H), 7.02 (s, 1H), 2.47 (s, 3H).

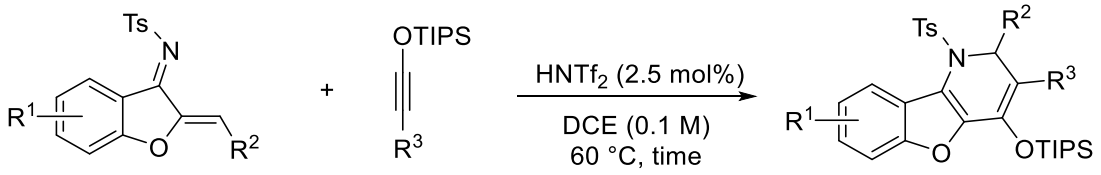
^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7, 164.6, 152.2, 151.0, 150.2, 143.6, 138.6, 137.9, 137.6, 131.2, 129.5, 128.6, 127.1, 124.1, 123.8, 118.8, 112.3, 111.1, 21.6.

IR (thin film) 3057, 1657, 1600, 1547, 1432, 1304, 1186, 1081 cm^{-1}.

HRMS (CI) calculated for $C_{21}H_{17}N_2O_3S$ $[M+H]^+$: 377.0954, found: 377.0958.

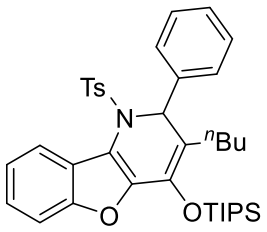
III. $HNTf_2$-Catalyzed Annulation of Azadiene with Siloxy Alkynes

General Procedure B.



1 2 **3**

Under N_2, to an oven-dried 4-mL vial were sequentially added the siloxy alkyne **2** (0.75 mmol, 2.5 equiv), $HNTf_2$ (2.1 mg, 7.5 μmol, 2.5 mol%), and DCE (3 mL). After stirring for 5 min, the azadiene **1** (0.3 mmol) was added into the solution. The reaction mixture was stirred at 60 °C for 20 h before it was concentrated under reduced pressure. The residue was purified by silica gel flash column chromatography to give the pure product **3**.



3a

3-Butyl-2-phenyl-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro [3,2-*b*]pyridine (**3a**) was prepared as light yellow solid from **1a** (112.5 mg, 0.3 mmol) and (hex-1-yn-1-yloxy)triisopropylsilane **2a** (190.5 mg, 0.75 mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 3:1→1:1) in 70% yield (132 mg).

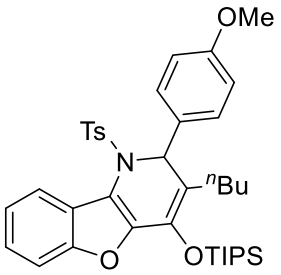
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, J = 6.2, 2.9 Hz, 1H), 7.51 (d, J = 8.2 Hz, 2H), 7.42 – 7.37 (m, 3H), 7.27 – 7.22 (m, 5H), 7.12 (d, J = 8.1 Hz, 2H), 5.86 (s, 1H), 2.37 – 2.31 (m, 4H), 1.86 – 1.79 (m, 1H), 1.37 – 1.23 (m, 7H), 1.08 (d, J = 7.5 Hz, 9H), 1.02 (d, J = 7.5 Hz, 9H), 0.88 (t, J = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 144.3, 143.6, 138.7, 136.9, 135.2, 129.3, 128.3,

128.0, 127.8, 127.3, 124.5, 124.3, 123.5, 121.8, 116.3, 115.9, 111.1, 63.9, 30.3, 28.3, 23.1, 21.4, 17.9 13.9, 13.4.

IR (thin film) 2943, 2864, 1597, 1459, 1360, 1316, 1264, 1208, 1165, 1091, 1021 cm^{-1}.

HRMS (CI) calculated for $C_{37}H_{47}NO_4SSi$ $[M + H]^+$: 630.3068, found: 630.3081.



3b

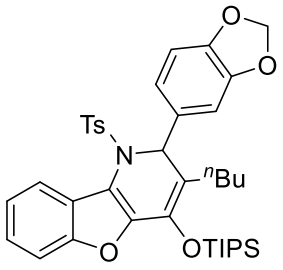
3-Butyl-2-(4-methoxyphenyl)-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3b**) was prepared as a light yellow solid from **1b** (122 mg, 0.3 mmol) and (hex-1-yn-1-yloxy)triisopropylsilane **2a** (190.5 mg, 0.75 mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 2:1→1:1) in 61% yield (121 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.95 (m, 1H), 7.52 (d, J = 8.2 Hz, 2H), 7.41 – 7.38 (m, 1H), 7.34 (d, J = 8.7 Hz, 2H), 7.29 – 7.24 (m, 2H), 7.14 (d, J = 8.1 Hz, 2H), 6.80 (d, J = 8.7 Hz, 2H), 5.83 (s, 1H), 3.75 (s, 3H), 2.36 – 2.28 (m, 4H), 1.88 – 1.81 (m, 1H), 1.39 – 1.23 (m, 7H), 1.10 (d, J = 7.5 Hz, 9H), 1.04 (d, J = 7.5 Hz, 9H), 0.90 (t, J = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 153.3, 144.3, 143.6, 136.7, 135.3, 130.7, 129.3, 129.0, 127.3, 124.6, 124.2, 123.5, 121.7, 116.6, 115.7, 113.7, 111.1, 63.5, 55.1, 30.3, 28.3, 23.1, 21.4, 17.9, 13.9, 13.3.

IR (thin film) 2950, 2867, 1722, 1631, 1479, 1446, 1360, 1314, 1261, 1165, 1091, 1035 cm^{-1}.

HRMS (CI) calculated for $C_{38}H_{49}NO_5SSi$ $[M]^+$: 659.3101, found: 659.3123.



3c

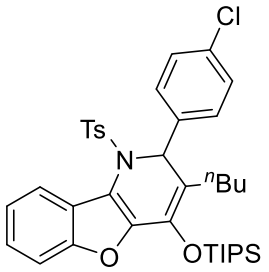
2-(Benzo[*d*][1,3]dioxol-5-yl)-3-butyl-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3c**) was prepared as a light yellow solid from **1c** (126 mg, 0.3 mmol) and (hex-1-yn-1-yloxy)triisopropylsilane **2a** (190.5 mg, 0.75 mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 2:1→1:1) in 56% yield (113 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.97 (m, 1H), 7.50 (d, J = 8.3 Hz, 2H), 7.41 – 7.37 (m, 1H), 7.29 – 7.27 (m, 2H), 7.13 (d, J = 8.1 Hz, 2H), 6.92 (d, J = 1.6 Hz, 1H), 6.87 (dd, J = 8.0, 1.6 Hz, 1H), 6.68 (d, J = 8.0 Hz, 1H), 5.90 (dd, J = 4.1, 1.3 Hz, 2H), 5.77 (s, 1H), 2.36 – 2.28 (m, 4H), 1.85 – 1.78 (m, 1H), 1.47 – 1.22 (m, 7H), 1.08 (d, J = 7.6 Hz, 9H), 1.01 (d, J = 7.6 Hz, 9H), 0.90 (t, J = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 147.7, 147.4, 144.2, 143.6, 136.8, 135.3, 132.6, 129.3, 127.3, 124.5, 124.3, 123.6, 121.8, 121.4, 116.4, 115.8, 111.1, 108.4, 107.9, 101.0, 63.8, 30.3, 28.2, 23.1, 21.4, 17.9, 13.9, 13.3.

IR (thin film) 2949, 2866, 1629, 1508, 1458, 1430, 1360, 1312, 1166, 1092, 1028 cm^{-1}.

HRMS (CI) calculated for $C_{38}H_{47}NO_6SSi$ $[M]^+$: 673.2893, found: 673.2863.



3d

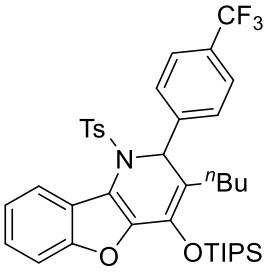
3-Butyl-2-(4-chlorophenyl)-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3d**) was prepared as a light yellow solid from **1d** (123 mg, 0.3 mmol) and (hex-1-yn-1-yloxy)triisopropylsilane **2a** (190.5 mg, 0.75 mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 2:1) in 77% yield (153 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.93 (m, 1H), 7.51 (d, J = 8.3 Hz, 2H), 7.40 – 7.35 (m, 3H), 7.27 – 7.22 (m, 4H), 7.13 (d, J = 8.1 Hz, 2H), 5.83 (s, 1H), 2.37 – 2.29 (m, 4H), 1.88 – 1.80 (m, 1H), 1.37 – 1.25 (m, 7H), 1.08 (d, J = 7.5 Hz, 9H), 1.02 (d, J = 7.5 Hz, 9H), 0.89 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 144.1, 143.8, 137.3, 137.2, 135.1, 133.9, 129.3, 129.2, 128.5, 127.3, 124.5, 124.3, 123.6, 121.7, 115.9, 115.6, 111.1, 63.2, 30.3, 28.3, 23.1, 21.4, 17.9, 13.9, 13.3.

IR (thin film) 2949, 2866, 1631, 1595, 1478, 1458, 1428, 1360, 1316, 1264, 1208, 1165, 1091, 1021 cm^{-1}.

HRMS (CI) calculated for $C_{37}H_{46}ClNO_4SSi$ $[M]^+$: 663.2605, found: 663.2623.



3e

3-Butyl-1-tosyl-2-(4-(trifluoromethyl)phenyl)-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3e**) was prepared as white solid from **1e**

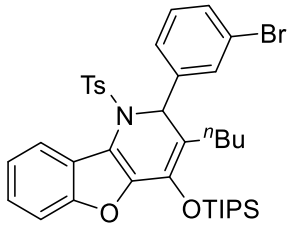
(133 mg, 0.3 mmol) and (hex-1-yn-1-yloxy)triisopropylsilane **2a** (190.5 mg, 0.75 mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 2:1) in 61% yield (128 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.94 (m, 1H), 7.40 – 7.38 (m, 6H), 7.40 – 7.38 (m, 1H), 7.29 – 7.24 (m, 2H), 7.13 (d, J = 8.1 Hz, 2H) 5.88 (s, 1H), 2.38 – 2.31 (m, 4H), 1.85 – 1.78 (m, 1H), 1.36 – 1.21 (m, 7H), 1.07 (d, J = 7.6 Hz, 9H), 1.00 (d, J = 7.6 Hz, 9H), 0.88 (t, J = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 144.1, 144.0, 142.9, 137.4, 135.0, 130.2 (q, J = 32.2 Hz), 129.4, 128.2, 127.4, 125.4 (q, J = 3.6 Hz), 124.7, 124.2, 123.7, 122.6, 121.7, 116.0, 115.2, 111.2, 63.3, 30.3, 28.3, 23.1, 21.4, 17.9, 13.9, 13.4.

IR (thin film) 2950, 2867, 1628, 1459, 1422, 1361, 1321, 1264, 1200, 1166, 1126, 1065, 1021 cm^{-1}.

HRMS (CI) calculated for $C_{38}H_{46}F_3NO_4SSi$ $[M]^+$: 697.2869, found: 697.2866.



3f

2-(3-Bromophenyl)-3-butyl-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3f**) was prepared as a white solid from **1f** (136 mg, 0.3 mmol) and (hex-1-yn-1-yloxy) triisopropylsilane **2a** (190.5 mg, 0.75 mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 2:1) in 71% yield (151 mg).

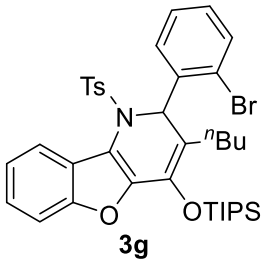
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.94 (m, 1H), 7.50 – 7.46 (m, 3H), 7.40 – 7.37 (m, 2H), 7.35 – 7.33 (m, 1H), 7.27 – 7.25 (m, 2H), 7.14 – 7.10 (m, 3H), 5.80 (s, 1H), 2.35 – 2.28 (m, 4H), 1.83 – 1.76 (m, 1H), 1.37 – 1.21 (m, 7H), 1.08 (d, J = 7.5 Hz, 9H), 1.01 (d, J = 7.5 Hz, 9H), 0.88 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 144.1, 143.9, 141.1, 137.3, 134.9, 131.2, 130.8,

130.0, 129.3, 127.3, 126.7, 124.5, 124.3, 123.7, 122.4, 121.8, 116.0, 115.2, 111.2, 63.3, 30.2, 28.3, 23.1, 21.4, 17.9, 13.9, 13.4.

IR (thin film) 2949, 2866, 1630, 1594, 1462, 1462, 1426, 1360, 1316, 1265, 1208, 1165, 1092, 1030 cm^{-1}.

HRMS (CI) calculated for $C_{37}H_{46}BrNO_4SSi$ $[M]^+$: 707.2100, found: 707.2087.



3g

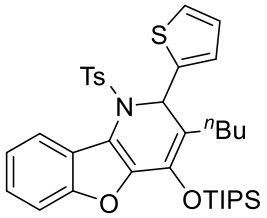
2-(2-Bromophenyl)-3-butyl-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3g**) was prepared as a white solid from **1g** (136 mg, 0.3 mmol) and (hex-1-yn-1-yloxy) triisopropylsilane **2a** (190.5 mg, 0.75 mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 2:1) in 63% yield (133 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (m, 1H), 7.58 – 7.51 (m, 3H), 7.43 (d, J = 4.5 Hz, 1H), 7.30 – 7.27 (m, 2H), 7.13 – 7.00 (m, 5H), 6.38 (s, 1H), 2.35 (s, 3H), 2.26-2.20 (m, 1H), 1.80 – 1.75 (m, 1H), 1.33 – 1.29 (m, 7H), 1.06 (d, J = 7.3 Hz, 9H), 1.01 (d, J = 7.3 Hz, 9H), 0.87 (t, J = 6.6 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.4, 144.5, 143.8, 138.5, 135.9, 134.5, 133.2, 129.8, 129.2, 128.9, 127.8, 127.7, 124.7, 124.4, 123.7, 122.8, 121.8, 119.3, 116.8, 111.2, 63.1, 30.3, 27.3, 23.0, 21.4, 17.9, 13.9, 13.2.

IR (thin film) 2951, 2866, 1630, 1595, 1460, 1429, 1362, 1318, 1264, 1199, 1167, 1092, 1023 cm^{-1}.

HRMS (CI) calculated for $C_{37}H_{46}BrNO_4SSi$ $[M]^+$: 707.2100, found: 707.2109.



3h

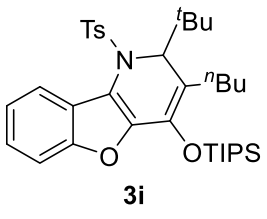
3-Butyl-2-(thiophen-2-yl)-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3h**) was prepared as a white solid from **1h** (114 mg, 0.3 mmol) and (hex-1-yn-1-yloxy) triisopropylsilane **2a** (190.5 mg, 0.75 mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 2:1) in 51% yield (97 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.99 (m, 1H), 7.49 (d, J = 8.3 Hz, 2H), 7.41 – 7.38 (m, 1H), 7.30 – 7.25 (m, 2H), 7.11 (dd, J = 4.6, 3.4 Hz, 3H), 7.03 (d, J = 3.5 Hz, 1H), 6.85 (dd, J = 5.0, 3.6 Hz, 1H), 6.06 (s, 1H), 2.38 – 2.31 (m, 4H), 1.97 – 1.89 (m, 1H), 1.35 – 1.25 (m, 7H), 1.06 (d, J = 7.5 Hz, 9H), 1.00 (d, J = 7.5 Hz, 9H), 0.90 (t, J = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 144.1, 143.8, 143.6, 136.5, 135.2, 129.3, 127.3, 126.4, 125.9, 125.5, 124.5, 123.6, 121.7, 117.2, 116.0, 111.2, 60.2, 30.4, 28.1, 23.1, 21.4, 17.9 (2C), 13.9, 13.3.

IR (thin film) 2947, 2865, 1630, 1600, 1459, 1428, 1361, 1319, 1265, 1164, 1092, 1025 cm^{-1}.

HRMS (CI) calculated for $C_{35}H_{45}NO_4S_2Si$ $[M]^+$: 635.2559, found: 635.2566.



3i

2-(*tert*-Butyl)-3-butyl-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3i**) was prepared as a white solid from **1i** (107 mg, 0.3 mmol) and (hex-1-yn-1-yloxy)triisopropylsilane **2a** (190.5 mg, 0.75

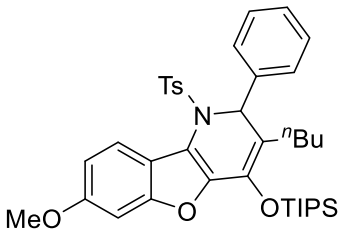
mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 3:1→1:1) in 61% yield (112 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 – 8.62 (m, 1H), 7.90 (d, J = 8.3 Hz, 2H), 7.60 (ddd, J = 8.5, 7.3, 1.3 Hz, 1H), 7.29 – 7.26 (m, 2H), 7.13 – 7.05 (m, 2H), 2.56 (s, 1H), 2.41 (s, 3H), 2.35 – 2.28 (m, 1H), 1.95 – 1.88 (m, 1H), 1.43 – 0.89 (m, 34H), 0.64 (t, J = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 180.4, 169.8, 142.7, 141.4, 139.2, 138.5, 130.9, 129.0, 128.1, 126.8, 121.9, 117.8, 112.3, 97.6, 60.9, 33.8, 28.1, 25.6, 21.9, 21.4, 17.5 (2C), 13.6, 12.6.

IR (thin film) 2950, 2867, 1699, 1595, 1466, 1353, 1311, 1267, 1213, 1198, 1151, 1087, 1052, 1006 cm^{-1}.

HRMS (CI) calculated for $C_{35}H_{52}NO_4SSi$ $[M+H]^+$: 610.3381, found: 610.3382.



3j

3-Butyl-7-methoxy-2-phenyl-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3j**) was prepared as a white solid from **1j** (122mg, 0.3 mmol) and (hex-1-yn-1-yloxy)triisopropylsilane **2a** (190.5 mg, 0.75 mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 1:1) in 57% yield (112 mg).

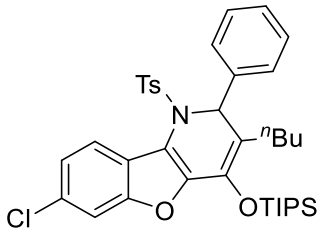
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 9.4 Hz, 1H), 7.51 (d, J = 8.2 Hz, 2H), 7.41 (d, J = 7.0 Hz, 2H), 7.27 – 7.21 (m, 3H), 7.12 (d, J = 8.0 Hz, 2H), 6.89 – 6.88 (m, 2H), 5.83 (s, 1H), 3.84 (s, 3H), 2.34 – 2.29 (m, 4H), 1.85 – 1.78 (m, 1H), 1.35 – 1.21 (m, 7H), 1.07 (d, J = 7.5 Hz, 9H), 1.01 (d, J = 7.5 Hz, 9H), 0.88 (t, J = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 154.3, 143.6, 143.3, 138.9, 136.9, 135.3, 129.3,

128.3, 127.9, 127.8, 127.3, 121.9, 118.0, 115.9, 114.3, 112.2, 95.9, 63.9, 55.7, 30.3, 28.2, 23.1, 21.4, 17.9, 13.9, 13.3.

IR (thin film) 2951, 2866, 1626, 1494, 1460, 1427, 1363, 1267m 1156, 1095, 1027 cm^{-1}.

HRMS (CI) calculated for $C_{38}H_{49}NO_5SSi$ $[M]^+$: 659.3101, found: 659.3089.



3k

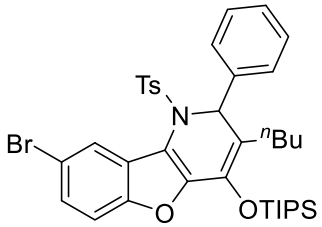
3-Butyl-7-chloro-2-phenyl-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3k**) was prepared as a white solid from **1k** (123 mg, 0.3 mmol) and (hex-1-yn-1-yloxy)triisopropylsilane **2a** (190.5 mg, 0.75 mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 2:1) in 71% yield (142 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.6 Hz, 1H), 7.51 (d, J = 8.2 Hz, 2H), 7.40 (dd, J = 4.1, 2.3 Hz, 3H), 7.28 – 7.21 (m, 4H), 7.14 (d, J = 8.1 Hz, 2H), 5.86 (s, 1H), 2.35 – 2.31 (s, 4H), 1.87 – 1.80 (m, 1H), 1.35 – 1.23 (m, 7H), 1.07 (d, J = 7.5 Hz, 9H), 1.01 (d, J = 7.5 Hz, 9H), 0.88 (t, J = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.2, 144.9, 143.8, 138.5, 136.6, 135.1, 130.1, 129.4, 128.4, 128.1, 127.7, 127.3, 124.3, 123.2, 122.3, 116.8, 115.7, 11.6, 63.9, 30.2, 23.1, 21.4, 17.9, 13.9, 13.3.

IR (thin film) 2951, 1866, 1630, 1462, 1425, 1359, 1301, 1265, 1163, 1097, 1025 cm^{-1}.

HRMS (CI) calculated for $C_{37}H_{46}ClNO_4SSi$ $[M]^+$: 663.2605, found: 663.2620.



3l

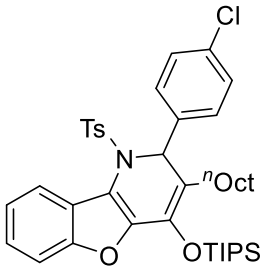
8-Bromo-3-butyl-2-phenyl-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3l**) was prepared as a white solid from **1l** (136mg, 0.3 mmol) and (hex-1-yn-1-yloxy)triisopropylsilane **2a** (190.5 mg, 0.75 mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 1:1) in 68% yield (144 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 2.0 Hz, 1H), 7.52 (d, J = 8.3 Hz, 2H), 7.39 (dd, J = 7.8, 1.2 Hz, 2H), 7.32 (dd, J = 8.7, 2.0 Hz, 1H), 7.29 – 7.22 (m, 4H), 7.14 (d, J = 8.1 Hz, 2H), 5.84 (s, 1H), 2.36 – 2.30 (m, 4H), 1.87 – 1.80 (m, 1H), 1.34 – 1.21 (m, 7H), 1.06 (d, J = 7.5 Hz, 9H), 1.00 (d, J = 7.5 Hz, 9H), 0.87 (t, J = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 145.5, 143.9, 138.4, 136.6, 135.1, 129.4, 128.4, 128.2, 127.7, 127.4, 127.3, 126.3, 124.2, 117.6, 116.9, 115.2, 112.5, 63.8, 30.2, 28.3, 23.1, 21.4, 17.9, 13.9, 13.3.

IR (thin film) 2951, 2866, 1630, 1458, 1449, 1412, 1350, 1305, 1265, 1210, 1165, 1098, 1024 cm^{-1}.

HRMS (CI) calculated for $C_{37}H_{46}BrNO_4SSi$ $[M]^+$: 707.2100, found: 707.2090.



3m

2-(4-Chlorophenyl)-3-octyl-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-

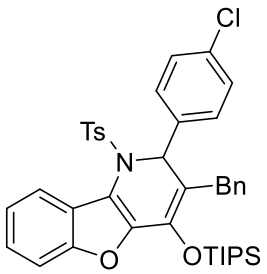
dihydrobenzofuro[3,2-*b*]pyridine (**3m**) was prepared as a white solid from **1d** (82 mg, 0.2 mmol) and (dec-1-yn-1-yloxy)triisopropylsilane (155 mg, 0.5 mmol, 2.5 equiv) according to the General Procedure B (catalyst loading: 10 mol%, purified by silica gel chromatography, eluent: hexanes/DCM = 1:1) in 66% yield (96 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.93 (m, 1H), 7.48 (d, J = 8.2 Hz, 2H), 7.39 – 7.32 (m, 3H), 7.27 – 7.21 (m, 4H), 7.11 (d, J = 8.2 Hz, 2H), 5.80 (s, 1H), 2.34 – 2.26 (m, 4H), 1.84 – 1.77 (m, 1H), 1.35 – 1.24 (m, 15H), 1.06 (d, J = 7.5 Hz, 9H), 1.00 (d, J = 7.5 Hz, 9H), 0.91 (t, J = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 144.1, 143.8, 137.3, 137.2, 135.1, 133.9, 129.4, 129.2, 128.6, 127.3, 124.5, 124.3, 123.7, 121.7, 115.9, 115.8, 111.2, 63.3, 31.8, 30.0, 29.4, 29.2, 28.6, 28.2, 22.6, 21.4, 17.9, 14.1, 13.4.

IR (thin film) 2931, 2862, 1631, 1595, 1459, 1429, 1361, 1316, 1266, 1204, 1166, 1092, 1017 cm^{-1}.

HRMS (CI) calculated for $C_{41}H_{54}ClNO_4SSi$ $[M]^+$: 719.3231, found: 719.3228.



3n

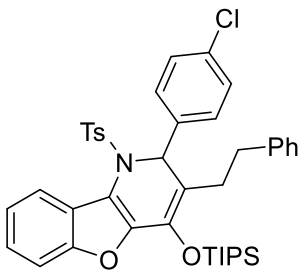
3-Benzyl-2-(4-chlorophenyl)-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3n**) was prepared as a white solid from **1d** (82 mg, 0.2 mmol) and triisopropyl((3-phenylprop-1-yn-1-yl) oxy)silane (144 mg, 0.5 mmol, 2.5 equiv) according to the General Procedure B (catalyst loading: 10 mol%, purified by silica gel chromatography, eluent: hexanes/DCM = 1:1) in 74% yield (103 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 -7.98 (m, 1H), 7.32 – 7.09 (m, 10H), 7.10 (dd, *J* = 13.5, 11.9 Hz, 2H), 6.94 (s, 4H), 5.87 (s, 1H), 3.99 (d, *J* = 14.4 Hz, 1H), 2.93 (d, *J* = 14.4 Hz, 1H), 2.32 (s, 3H), 1.44 – 1.37 (m, 3H), 1.12 (d, *J* = 7.5 Hz, 9H), 1.04 (d, *J* = 7.5 Hz, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.4, 143.5, 143.3, 138.3, 137.1 (2C), 134.5, 134.0, 129.4, 129.3, 129.2, 128.7 (2C), 127.1, 126.5, 124.7, 124.1, 123.7, 121.9, 115.9, 114.7, 111.2, 62.4, 33.4, 21.4, 18.0, 13.5.

IR (thin film) 2950, 2868, 1631, 1597, 1486, 1457, 1425, 1360, 1318, 1265, 1209, 1165, 1090, 1041, 1010 cm^{-1}.

HRMS (CI) calculated for $C_{40}H_{44}ClNO_4SSi$ $[M]^+$: 697.2449, found: 697.2458.



3o

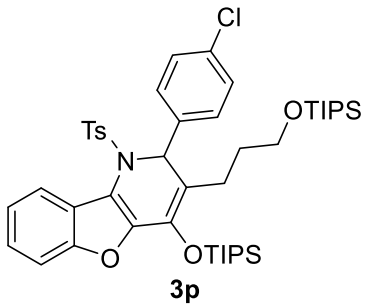
2-(4-Chlorophenyl)-3-phenethyl-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3o**) was prepared as a white solid from **1d** (123 mg, 0.3 mmol) and triisopropyl((4-phenylbut-1-yn-1- yl)oxy)silane (226 mg, 0.75 mmol, 2.5 equiv) according to the General Procedure B (purified by silica gel chromatography, eluent: hexanes/DCM = 1:1) in 53% yield (112 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.98 (m, 1H), 7.53 (d, *J* = 8.3 Hz, 2H), 7.43 – 7.38 (m, 3H), 7.33 – 7.20 (m, 7H), 7.14 (d, *J* = 8.0 Hz, 4H), 5.94 (s, 1H), 2.66 – 2.51 (m, 2H), 2.41 – 2.35 (m, 4H), 2.25 – 2.18 (m, 1H), 1.42 – 1.30 (m, 3H), 1.11 (d, *J* = 7.8 Hz, 9H), 1.04 (d, *J* = 7.5 Hz, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.4, 143.9 (2C), 141.2, 137.8, 137.1, 135.0, 134.0, 129.4, 129.2, 128.6, 128.4, 128.0, 127.3, 126.1, 124.7, 124.3, 123.7, 121.8, 116.3, 114.2, 111.2, 63.4, 34.1, 20.7, 21.4, 17.9, 13.4.

IR (thin film) 2947, 2866, 1631, 1598, 1484, 1459, 1428, 1361, 1317, 1266, 1207, 1165, 1091, 1043, 1009 cm^{-1}.

HRMS (CI) calculated for $C_{41}H_{46}ClNO_4SSi$ $[M]^+$: 711.2605, found: 711.2631.



3p

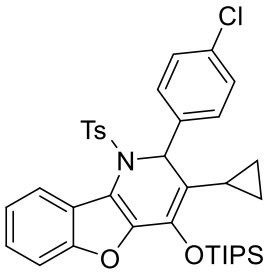
2-(4-Chlorophenyl)-1-tosyl-4-((triisopropylsilyl)oxy)-3-(3-((triisopropyl silyl)oxy)propyl)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3p**) was prepared as white solid from **1d** (82 mg, 0.2 mmol) and 3,3,11,11- tetraisopropyl-2,12-dimethyl-4,10-dioxa-3,11-disilatridec-5-yne (206 mg, 0.5 mmol, 2.5 equiv) according to the General Procedure B (catalyst loading: 10 mol%, purified by silica gel chromatography, eluent: hexanes/ethyl acetate = 3:2) in 64% yield (105 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.93 (m, 1H), 7.49 (d, J = 8.2 Hz, 2H), 7.42 – 7.38 (m, 1H), 7.34 (d, J = 8.5 Hz, 2H), 7.30 – 7.26 (m, 2H), 7.23 (d, J = 8.5 Hz, 2H), 7.13 (d, J = 8.2 Hz, 2H), 5.82 (s, 1H), 3.63 (t, J = 6.3 Hz, 2H), 2.35 – 2.27 (m, 4H), 2.04 – 1.96 (m, 1H), 1.55 – 1.46 (m, 1H), 1.37 – 1.29 (m, 4H), 1.10 – 1.00 (m, 39H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 144.2, 143.8, 137.4, 137.3, 134.9, 133.9, 129.4, 129.2, 128.6, 127.3, 124.6, 124.4, 123.7, 121.8, 116.0, 115.0, 111.2, 63.4, 63.3, 31.3, 25.1, 21.4, 18.0, 17.9, 13.4, 11.9.

IR (thin film) 2945, 2866, 1711, 1631, 1461, 1431, 1363, 1265, 1209, 1167, 1098, 1012 cm^{-1}.

HRMS (CI) calculated for $C_{45}H_{64}ClNO_5SSi_2$ $[M]^+$: 821.3732, found: 821.3721.



3q

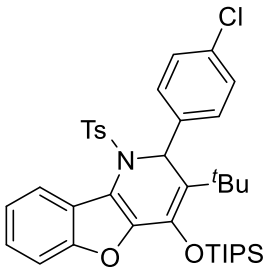
2-(4-Chlorophenyl)-3-cyclopropyl-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-dihydrobenzofuro[3,2-*b*]pyridine (**3q**) was prepared as a white solid from **1d** (82 mg, 0.2 mmol) and ((cyclopropylethynyl)oxy) triisopropylsilane (119 mg, 0.5 mmol, 2.5 equiv) according to the General Procedure B (catalyst loading: 10 mol%, purified by silica gel chromatography, eluent: hexanes/DCM = 2:1) in 58% yield (75 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.90 (m, 1H), 7.48 (d, J = 8.2 Hz, 2H), 7.38 – 7.34 (m, 3H), 7.26 – 7.19 (m, 4H), 7.11 (d, J = 8.2 Hz, 2H), 5.40 (s, 1H), 2.34 (s, 3H), 1.89 – 1.83 (m, 1H), 1.32 – 1.22 (m, 3H), 1.05 (d, J = 7.5 Hz, 9H), 1.00 (d, J = 7.5 Hz, 9H), 0.80 – 0.74 (m, 1H), 0.66 – 0.56 (m, 2H), 0.34 – 0.29 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 144.9, 143.8, 138.7, 137.8, 134.7, 133.8, 129.2, 129.1, 128.4, 127.3, 124.5, 124.3, 123.6, 121.3, 115.7, 115.0, 111.2, 59.9, 21.5, 17.9, 13.2, 10.2, 6.0, 4.7.

IR (thin film) 2949, 2867, 1622, 1481, 1458, 1424, 1363, 1315, 1266, 1196, 1164, 1092, 1043, 1017 cm^{-1}.

HRMS (CI) calculated for $C_{36}H_{43}ClNO_4SSi$ $[M+H]^+$: 648.2365, found: 648.2401.



3r

3-(*tert*-Butyl)-2-(4-chlorophenyl)-1-tosyl-4-((triisopropylsilyl)oxy)-1,2-

dihydrobenzofuro[3,2-*b*]pyridine (**3r**) was prepared as a white solid from **1d** (82 mg, 0.2 mmol) and ((3,3-dimethylbut-1-yn-1-yl)oxy) triisopropylsilane (127 mg, 0.5 mmol, 2.5 equiv) according to the General Procedure B (catalyst loading: 10 mol%, purified by silica gel chromatography, eluent: hexanes/DCM = 1:1) in 62% yield (78 mg).

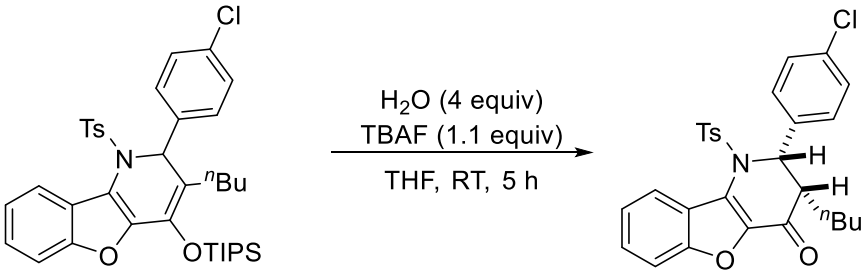
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.90 (m, 1H), 7.51 (d, J = 8.3 Hz, 2H), 7.38 – 7.35 (m, 3H), 7.26 – 7.20 (m, 4H), 7.13 (d, J = 8.1 Hz, 2H), 6.09 (s, 1H), 2.33 (s, 3H), 1.45 – 1.7 (m, 3H), 1.10 (d, J = 7.5 Hz, 9H), 1.06 (s, 9H), 1.00 (d, J = 7.5 Hz, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.1, 144.3, 143.8, 138.0, 137.8, 135.5, 133.9, 129.6 (2C), 128.6, 127.3, 124.7, 124.1, 123.7, 121.9, 119.5, 115.9, 111.1, 62.0, 33.7, 29.1, 21.4, 18.1, 14.2.

IR (thin film) 2954, 2869, 1609, 1567, 1480, 1458, 1422, 1355, 1315, 1266, 1210, 1164, 1089, 1046, 1012 cm^{-1}.

HRMS (CI) calculated for $C_{37}H_{46}ClNO_4SSi$ $[M]^+$: 663.2605, found: 663.2588.

IV. Product Derivatizations



3d **4a**

***Cis*-3-Butyl-2-(4-chlorophenyl)-1-tosyl-2,3-dihydrobenzofuro[3,2-b]pyridin-4(1H)-one (4a).** At room temperature, to an oven-dried round-bottom flask with a magnetic stir bar were sequentially added **3d** (66.3 mg, 0.1 mmol), H_2O (4 equiv, ~ 7 μL), and THF (0.5 mL) followed by TBAF (110 μL, 0.11 mmol, 1.1 equiv, 1 M in THF). The mixture was stirred at room temperature and the progress was monitored by TLC. Upon completion (~ 5 h), the mixture was concentrated under reduced pressure, and the residue was purified by silica gel chromatography (eluent: hexanes/ethyl acetate = 8:1) in 91% yield (46 mg). The relative stereochemistry was determined by nOe study.

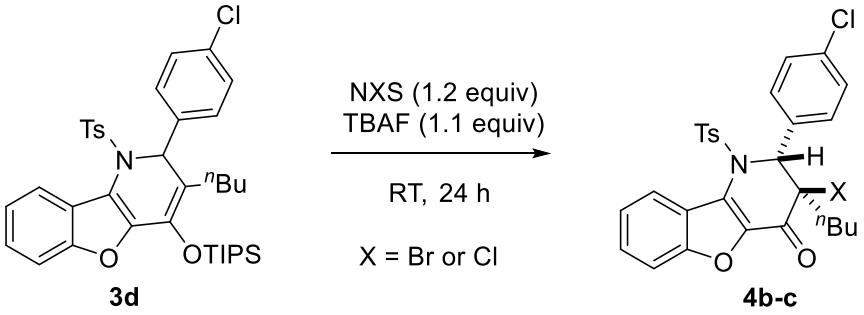
^{1}H NMR (400 MHz, $CDCl_3$) δ 8,23 (d, J = 8.2 Hz, 1H), 7.65 (d, J = 8.3 Hz, 2H), 7.53 – 7.49 (m, 2H), 7.35 – 7.28 (m, 3H), 7.28 (s, 4H), 5.60 (d, J = 5.2 Hz, 1H), 2.43

(s, 3H), 2.41 – 2.37 (m, 1H), 2.11 – 2.04 (m, 1H), 1.17 (m, 5H), 0.83 (t, J = 7.0 Hz, 3H).

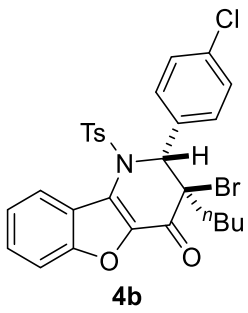
^{13}C NMR (100 MHz, $CDCl_3$) δ 184.9, 155.9, 145.4, 139.6, 135.8, 134.7, 133.2, 132.2, 130.4, 130.0 (2C), 128.9, 127.1, 125.7, 124.3, 122.4, 112.7, 64.9, 46.8, 30.0, 24.5, 22.3, 21.7, 13.8.

IR (thin film) 2964, 2930, 2864, 1680, 1602, 1563, 1490, 1446, 1409, 1362, 1296, 1168, 1095, 1006 cm^{-1}.

HRMS (ESI) calculated for $C_{28}H_{27}ClNO_4S$ $[M+H]^+$: 508.1344, found: 508.1350.



At room temperature, to an oven-dried round-bottom flask with a magnetic stir bar were sequentially added **3d** (66.3 mg, 0.1 mmol), NBS or NCS (1.2 equiv), THF (1 mL) followed by TBAF (110 μL, 1.1 equiv, 1 M in THF). The mixture was stirred at room temperature and the progress was monitored by TLC. Upon completion (~ 24 h), the mixture was concentrated under reduced pressure, and the residue was purified by silica gel flash column chromatography to give the product.



***Trans*-3-Bromo-3-butyl-2-(4-chlorophenyl)-1-tosyl-2,3-dihydrobenzofuro**

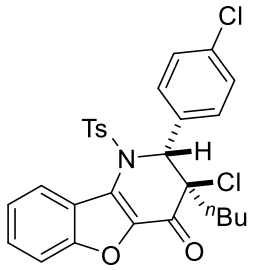
[3,2-*b*]pyridin-4(*1H*)-one (**4b**) was prepared as a colorless foam (purified by silica gel chromatography, eluent: hexanes/ethyl acetate = 8:1) in 74% yield (43 mg). The stereochemistry was determined by X-ray crystallography.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, J = 8.4 Hz, 1H), 7.645 – 7.51 (m, 4H), 7.29 – 7.25 (m, 1H), 7.16 (d, J = 7.4 Hz, 6H), 5.94 (s, 1H), 2.52 – 2.45 (m, 1H), 2.35 (s, 3H), 1.75 – 1.72 (m, 1H), 1.49 – 1.41 (m, 1H), 1.29 – 1.14 (m, 3H), 0.81 (t, J = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 177.1, 156.5, 144.7, 136.5, 135.6, 135.3, 133.5, 132.3, 130.4, 129.6, 129.4, 129.1, 127.4, 125.7, 124.2, 119.6, 113.1, 72.3, 67.4, 33.3, 26.6, 22.4, 21.5, 13.7.

IR (thin film) 3058, 2961, 2931, 2869, 1673, 1606, 1587, 1554, 489, 1419, 1356, 1266, 1169, 1090, 1012 cm^{-1}.

HRMS (CI) calculated for$C_{28}H_{25}BrClNO_4S$ $[M]^+$: 585.0376, found: 585.0365.



4c

***Trans*-3-Butyl-3-chloro-2-(4-chlorophenyl)-1-tosyl-2,3-dihydrobenzofuro**

[3,2-*b*]pyridin-4(*1H*)-one (**4c**) was prepared as a colorless foam (purified by silica gel chromatography, eluent: hexanes/ethyl acetate = 8:1) in 81% yield (44 mg). The stereochemistry was determined by X-ray crystallography.

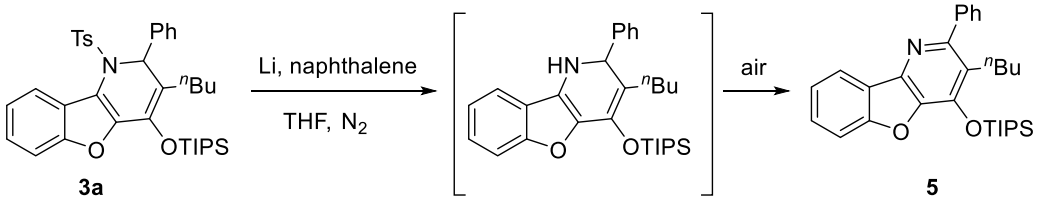
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, J = 8.4 Hz, 1H), 7.66 (d, J = 8.2 Hz, 2H), 7.59 – 7.52 (m, 2H), 7.30 (t, J = 7.5 Hz, 1H), 7.19 – 7.16 (m, 6H), 5.89 (s, 1H), 2.42 – 2.35 (m, 4H), 1.75 – 1.67 (m, 1H), 1.54 – 1.46 (m, 1H), 1.31 – 1.14 (m, 3H), 0.81 (t, J = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 177.0, 156.6, 144.8, 136.0, 135.7, 135.5, 133.8, 132.5,

130.6, 129.6, 129.4, 129.2, 127.6, 125.9, 124.3, 119.9, 113.0, 71.9, 71.3, 32.5, 25.0, 22.4, 21.5, 13.7.

IR (thin film) 3058, 2960, 2932, 2869, 1678, 1606, 1588, 1489, 1418, 1355, 1267, 1169, 1090, 1011 cm^{-1}.

HRMS (CI) calculated for $C_{28}H_{25}Cl_2NO_4S$ [M]$^+$: 541.0881, found: 541.0894.



3-Butyl-2-phenyl-4-((triisopropylsilyl)oxy)benzofuro[3,2-b]pyridine (5). At room temperature under N_2, to an oven-dried 25-mL round-bottom flask charged with a magnetic stirring bar, naphthalene (410 mg, 3.2 mmol, 8 equiv) and lithium powder (22 mg, 2.4 mmol, 8 equiv) was added anhydrous THF (10 mL). After stirring vigorously for about 5 minutes, the reaction turned dark green. Next, the mixture was allowed to stir at the same temperature for 1 h before slow addition of a solution of **3a** (252 mg, 0.4 mmol) in anhydrous THF (5 mL) at –78 °C. The mixture was allowed to warm to room temperature and the progress was monitored by TLC. Upon completion (~ 1 h), a saturated aqueous NH_4Cl (10 mL) was added at 0 °C. The layers were separated, and the aqueous layer was extracted with diethyl ether (10 mL × 2). The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by silica gel flash column chromatography (eluent: hexanes/ethyl acetate = 1:0→20:1) to give the desired product **5** as a light yellow oil in 70% yield (133 mg).

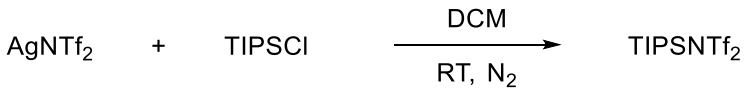
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, J = 7.7 Hz, 1H), 7.59 (d, J = 8.2 Hz, 1H), 7.54 – 7.50 (m, 3H), 7.49 – 7.45 (m, 2H), 7.43 – 7.37 (m, 2H), 2.76 – 2.72 (m, 2H), 1.63 – 1.48 (m, 5H), 1.27 – 1.18 (m, 20H), 0.78 (t, J = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 156.6, 146.0, 142.5, 141.6, 139.5, 129.1, 128.2, 128.0, 127.6, 126.3, 124.2, 123.3, 121.4, 111.7, 32.2, 27.3, 22.8, 18.0, 13.8, 13.7.

IR (thin film) 2949, 2866, 1630, 1589, 1560, 1461, 1434, 1381, 1328, 1256, 1204, 1156, 1107, 1074, 1009 cm^{-1}.

HRMS (ESI) calculated for $C_{30}H_{40}NO_2Si$ $[M+H]^+$: 474.2823, found: 474.2842.

V. Mechanistic Studies

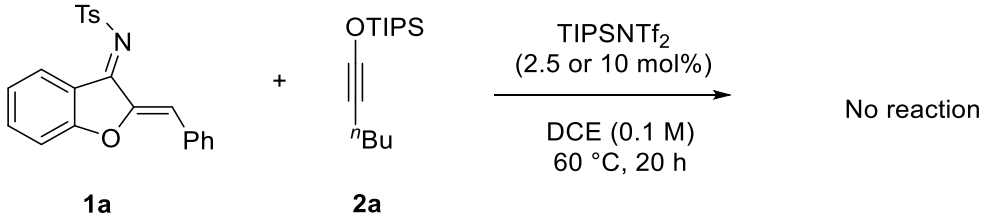


At room temperature under N_2 atmosphere, to an oven-dried round-bottom flask charged with a solution of TIPSCl (964 mg, 5.0 mmol) in DCM (150 mL) was added $AgNTf_2$ (1.94g, 5.0 mmol, 1 equiv). The mixture was stirred at room temperature for 36 h and it was filtered under N_2 atomsphere, and the filtrate was concentrated under the reduced pressure. The resulting brown oil was subjected to bulb-to-bulb distillation (m.p. 150 ^oC at 1 Torr) to give the pure $TIPSNTf_2$.

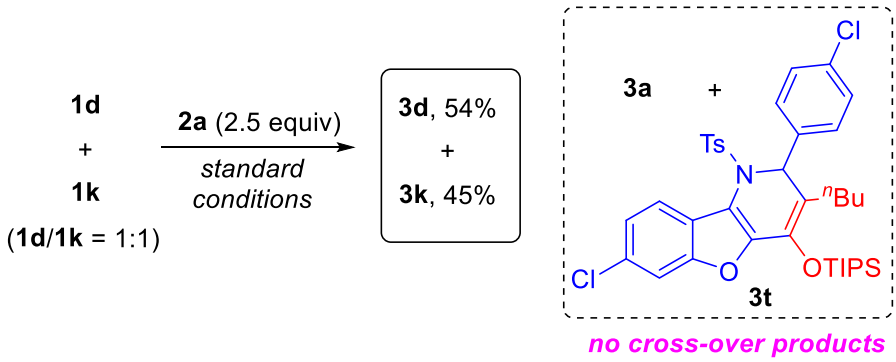
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.06 – 1.01 (m, 21H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 18.1, 17.9, 13.4, 12.8.

^{19}F NMR (100 MHz, $CDCl_3$) δ –75.6.



The reaction was conducted according to the General Procedure B except that $TIPSNTf_2$ was used as catalyst. However, no reaction was observed.



Under N_2, to an oven-dried 4-mL vial were sequentially added the siloxy alkyne **2a** (127 mg, 0.5 mmol, 2.5 equiv), $HNTf_2$ (1.4 mg, 5.0 μmol, 2.5 mol%), and DCE (2 mL). After stirring for 5 min, azadiene **1d** (82 mg, 0.2 mmol) and **1k** (82 mg, 0.2 mmol) were added. The reaction mixture was stirred at 60 °C for 20 h before it was concentrated under reduced pressure. The residue was analyzed by ^{1}H NMR, which indicated the exclusive formation of **3d** and **3k** in 54% and 45% yields, respectively.

VI. DFT Calculations

All the DFT calculations were carried out with the Gaussian 16 package.[13] All molecular geometries were optimized with the M06-2X/6-31G(d) including dispersion correction.[14] Frequency analysis were then performed on the optimized structure. Single point energies were calculated in dichloromethane solution using the SMD solvation model with the optimized structure by using 6-311G(d,p) basis set.[15] All energies discussed are Gibbs free relative energies at 298.15 K and 1 atm in kcal mol^{-1}.

Attempts to locate the transition state of C−N bond formation form intermediate **II** failed, which may be due to two reasons. First, the relatively bulky siloxy group obstructs the approaching of nitrogen atom. Second, the flexibility of the molecule increases the complexity in locating an accurate transition state. The scanning of C−N bond in Figure S2(a) suggested a flat

(13) M. J. T. Frisch, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. , *Gaussian, Inc., Wallingford CT,* **2016**.

(14) (a) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.,* **2010**, 132, 154104; (b) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.,* **2011**, 32, 1456-1465.

(15) A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B,* **2009**, 113, 6378-6396.

energy surface, which also indicates an untypical transition state. In addition, another neutral pathway by releasing $TMSNTf_2$ was also considered (Figure S2b). However, the extremely high energy barrier precludes this mechanism.

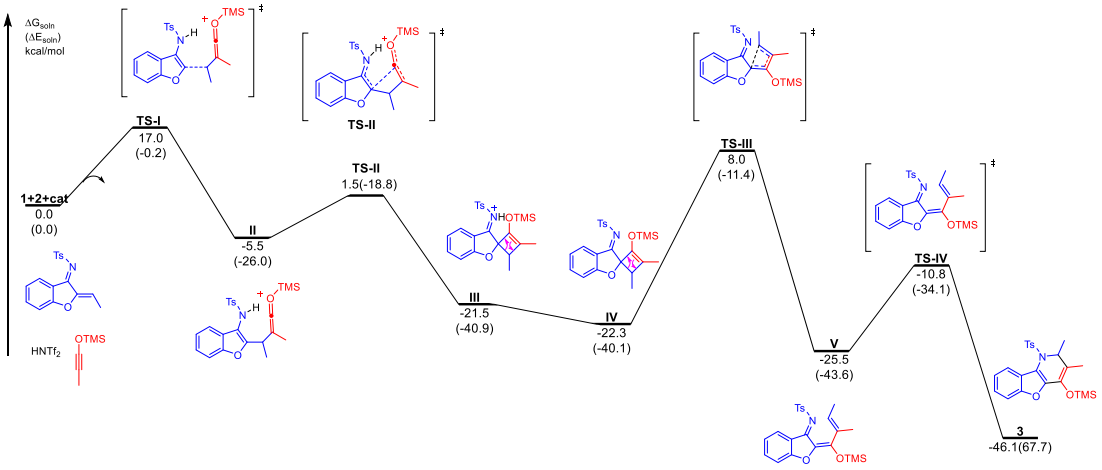


Figure S1. The potential energy surface of migrative cycloaddition of aurone-derived azadienes with siloxy alkynes (kcal/mol).

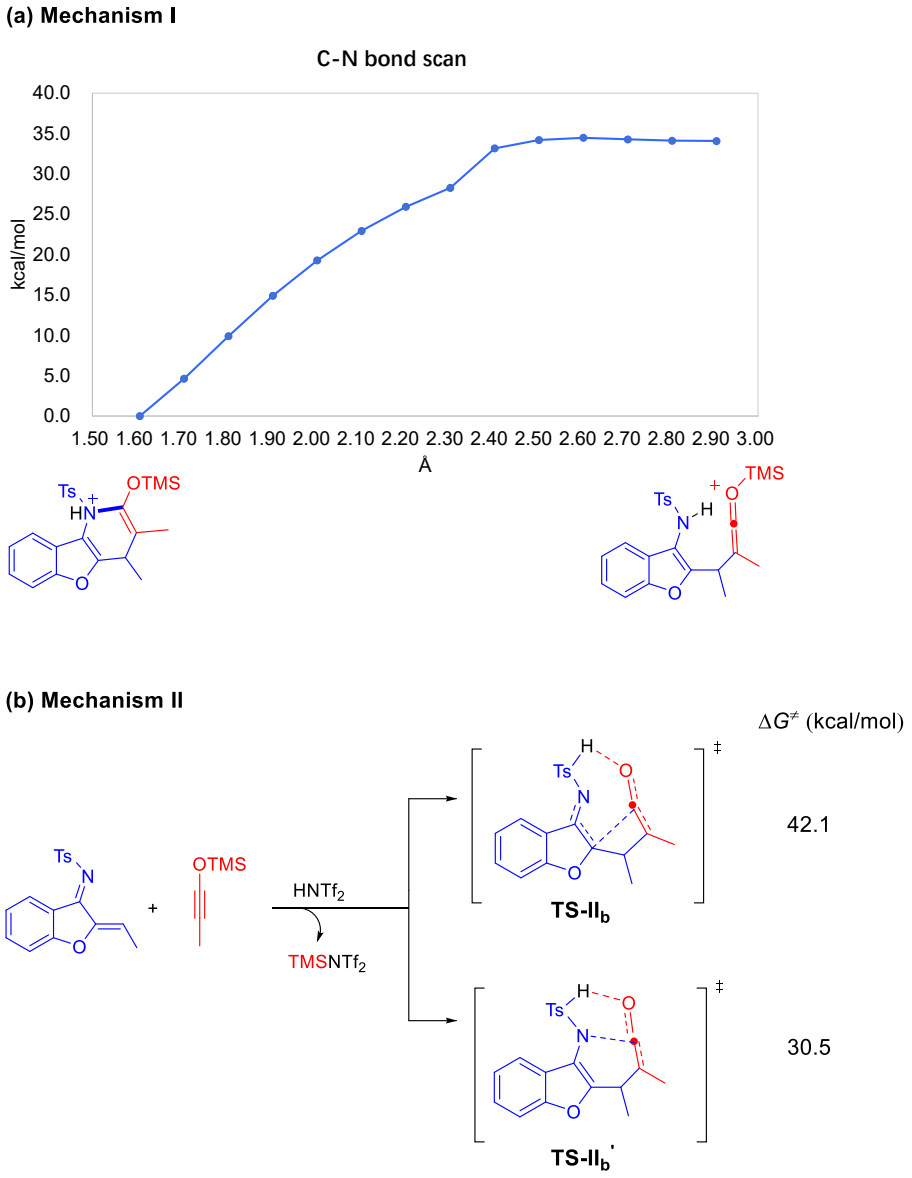


Figure S2. Scan of C–N bond formation toward the [4+2] product.

Cartesian coordinates and energies

TS-I (IF: -124.7365)

E = -1935.720411 G = -1935.31882 ZPE = -1935.252377 Esol=-1936.189588

S	-0.535319	1.177640	-2.125637
Si	3.625478	-1.495944	-0.743748
O	-1.919743	1.477601	-2.437838
O	0.496051	1.149633	-3.148099
O	-2.164508	-0.995424	1.676551
O	2.043211	-2.269916	-0.315780
C	0.919879	-2.282586	1.897920
C	1.549787	-2.352662	0.819964
C	-1.079266	-0.694123	0.913359
C	-1.391252	-0.669766	-0.418989
C	-2.797709	-0.944377	-0.516047
C	-3.210872	-1.152852	0.808684
C	-4.517755	-1.460564	1.164597
H	-4.803172	-1.613420	2.198725
C	-5.423677	-1.551752	0.118977
H	-6.459420	-1.788422	0.338206
C	-5.039996	-1.334950	-1.221433
H	-5.791310	-1.403563	-2.000383
C	-3.735442	-1.026784	-1.557737
H	-3.443496	-0.828400	-2.583305
C	1.211221	4.573682	2.575062
H	2.199387	4.280900	2.938312
H	0.502391	4.511680	3.404340
H	1.270074	5.623834	2.269677
C	0.776371	3.718672	1.414783
C	1.721713	3.190880	0.525057
H	2.776713	3.398000	0.684406
C	1.327667	2.434324	-0.572756
H	2.052269	2.053947	-1.288089
C	-0.030474	2.195348	-0.768746
C	-0.996232	2.709518	0.091350
H	-2.048870	2.527993	-0.104894
C	-0.581080	3.469842	1.180941
H	-1.323999	3.887609	1.854823
C	3.271720	-0.850210	-2.440464
H	2.386271	-0.204642	-2.464299
H	4.122044	-0.268061	-2.811893

H	3.107780	-1.674326	-3.141860
C	3.863118	-0.213100	0.587023
H	4.855256	0.240056	0.483161
H	3.126498	0.594955	0.524239
H	3.813517	-0.655693	1.587845
C	4.831656	-2.902810	-0.649344
H	4.904990	-3.306140	0.365344
H	4.544489	-3.714599	-1.324063
H	5.830674	-2.564257	-0.944021
C	0.451052	-2.912288	3.151794
H	0.751078	-3.961011	3.183888
H	0.869554	-2.400033	4.021871
H	-0.640366	-2.855485	3.203037
C	0.194701	-0.452983	1.542009
H	0.911508	-0.043571	0.831674
N	-0.421643	-0.375495	-1.408090
H	-0.382117	-1.055823	-2.170352
C	0.232624	0.172804	2.907321
H	-0.080575	1.217758	2.785302
H	-0.461161	-0.310300	3.597980
H	1.243296	0.165724	3.320994

II

E = -1935.75674913 G = -1935.349865 ZPE = -1935.285075 Esol= -1936.23073

S	-0.293037	0.176181	-2.242101
Si	4.067721	-1.251908	-0.192790
O	-1.561242	0.315299	-2.931068
O	0.921780	-0.199787	-2.950956
O	-2.554573	-0.322293	1.798674
O	2.322426	-1.845957	0.122522
C	0.793562	-1.191319	1.994015
C	1.590161	-1.507157	1.028805
C	-1.373132	-0.390761	1.138839
C	-1.531431	-0.858438	-0.126468
C	-2.944308	-1.091453	-0.313810
C	-3.517399	-0.751603	0.917743
C	-4.877320	-0.833519	1.182860
H	-5.283145	-0.561608	2.150346
C	-5.674377	-1.277396	0.136941
H	-6.745524	-1.359797	0.286680
C	-5.128151	-1.613213	-1.116087

H	-5.791937	-1.941064	-1.908724
C	-3.767618	-1.523969	-1.361234
H	-3.351949	-1.754435	-2.336419
C	0.728182	4.956347	1.327494
H	1.734422	4.928558	1.751885
H	0.005715	4.989986	2.147007
H	0.630290	5.890965	0.765131
C	0.477032	3.777399	0.425887
C	1.540887	3.107551	-0.190821
H	2.558033	3.447826	-0.014112
C	1.311198	2.029221	-1.040029
H	2.128613	1.517482	-1.541217
C	-0.000400	1.627023	-1.274436
C	-1.083126	2.295116	-0.706683
H	-2.097639	1.981636	-0.935806
C	-0.831636	3.360486	0.150976
H	-1.665559	3.888566	0.605063
C	4.029589	-1.031205	-2.025538
H	3.086992	-0.586043	-2.364637
H	4.853550	-0.384677	-2.346023
H	4.142623	-1.993703	-2.533277
C	4.135856	0.284710	0.850181
H	5.080392	0.809285	0.668420
H	3.322227	0.977979	0.610642
H	4.090539	0.052722	1.918787
C	5.054307	-2.683240	0.449671
H	4.922528	-2.824206	1.526533
H	4.784032	-3.611565	-0.062200
H	6.120228	-2.506279	0.268102
C	0.657651	-2.075751	3.216996
H	1.268000	-2.976902	3.149166
H	0.945016	-1.517655	4.111224
H	-0.392619	-2.370625	3.308288
C	-0.116116	0.049055	1.824611
H	0.397866	0.754118	1.162683
N	-0.421825	-1.001253	-1.003494
H	-0.381479	-1.911465	-1.470195
C	-0.369757	0.743654	3.161514
H	-0.964389	1.642424	2.980862
H	-0.927305	0.107600	3.852380
H	0.574715	1.040130	3.624598

TS-II (IF: -259.5155)

E = -1935.75356508 G = -1935.34708 ZPE = -1935.282738 Esol=-1936.219217

S	0.975106	-1.384306	-1.480856
Si	-3.509810	-0.797621	-1.115523
O	0.773770	-0.534537	-2.637369
O	0.714667	-2.810576	-1.507548
O	-0.328984	2.002228	1.872201
O	-3.134098	0.107291	0.454561
C	-1.920984	-0.788427	2.460078
C	-2.377278	-0.206626	1.370203
C	-0.319204	0.669514	1.608148
C	-0.135013	0.428340	0.259875
C	-0.063337	1.725351	-0.380188
C	-0.173705	2.640566	0.678744
C	-0.152488	4.019636	0.521950
H	-0.243831	4.680971	1.375449
C	-0.008251	4.484202	-0.775520
H	0.019132	5.553450	-0.956495
C	0.101485	3.597486	-1.863591
H	0.208809	4.001175	-2.864427
C	0.075500	2.224606	-1.690560
H	0.167855	1.554295	-2.535343
C	6.407524	-0.298784	0.934483
H	6.582955	-0.908775	1.823608
H	6.526337	0.753093	1.205003
H	7.187765	-0.543232	0.205561
C	5.047221	-0.562896	0.347460
C	4.435879	-1.812790	0.500060
H	4.944812	-2.590647	1.061798
C	3.196568	-2.079505	-0.067632
H	2.730365	-3.055285	0.026690
C	2.570133	-1.072017	-0.798461
C	3.150974	0.182738	-0.974454
H	2.651885	0.942976	-1.569072
C	4.388354	0.425901	-0.392745
H	4.858471	1.396059	-0.524481
C	-2.926422	-2.541369	-0.826684
H	-1.904287	-2.710770	-1.175666
H	-2.990673	-2.825144	0.230598
H	-3.586406	-3.223749	-1.373848
C	-5.356014	-0.608338	-1.088805
H	-5.789650	-1.055987	-1.989603
H	-5.803626	-1.105280	-0.223054
H	-5.644990	0.446512	-1.068781

C	-2.662522	0.188605	-2.433155
H	-2.738211	1.261904	-2.230439
H	-1.608138	-0.082311	-2.535796
H	-3.156789	-0.002098	-3.392587
C	-2.720323	-1.740029	3.310024
H	-3.699155	-1.950535	2.874559
H	-2.175859	-2.683045	3.421172
H	-2.871921	-1.310636	4.304719
C	-0.519919	-0.293195	2.753817
H	0.203543	-1.118675	2.682316
N	-0.152511	-0.850887	-0.306606
C	-0.392771	0.371670	4.123967
H	-1.118020	1.181984	4.228215
H	-0.564199	-0.363285	4.913846
H	0.609970	0.785872	4.251324
H	-0.268210	-1.600125	0.375164

III

E = -1935.79040164 G = -1935.384103 ZPE = -1935.318278 Esol= -1936.25147

S	1.309047	-0.975610	-1.567846
Si	-3.537892	-0.915764	-1.169510
O	1.108908	0.071273	-2.541856
O	1.005685	-2.365453	-1.808415
O	-1.596927	1.764681	1.659829
O	-3.422279	-0.599417	0.513393
C	-1.843010	-1.399729	2.244090
C	-2.345883	-0.604828	1.283629
C	-1.231319	0.424411	1.374672
C	-0.295102	0.516357	0.201355
C	-0.145084	1.881618	-0.135817
C	-0.964423	2.565475	0.799560
C	-1.101764	3.952996	0.801496
H	-1.735234	4.442361	1.531214
C	-0.404598	4.644559	-0.169787
H	-0.488056	5.726342	-0.205744
C	0.403403	3.990685	-1.132892
H	0.907116	4.582087	-1.888625
C	0.539431	2.624433	-1.134308
H	1.116819	2.121823	-1.897751
C	6.672036	-0.460651	1.145131
H	6.706997	-1.033275	2.074915
H	6.920963	0.579483	1.366157

H	7.450463	-0.856422	0.483730
C	5.326136	-0.574693	0.483949
C	4.591577	-1.765137	0.570984
H	4.994902	-2.601177	1.134521
C	3.365283	-1.898816	-0.062670
H	2.808662	-2.829771	-0.019141
C	2.872696	-0.813302	-0.788960
C	3.577450	0.383505	-0.902281
H	3.189462	1.200134	-1.501213
C	4.803427	0.490182	-0.258946
H	5.371246	1.411785	-0.343516
C	-2.707826	-2.559387	-1.500975
H	-1.613500	-2.518092	-1.477288
H	-3.042754	-3.322027	-0.790272
H	-2.980321	-2.907761	-2.503492
C	-5.371985	-0.960398	-1.462736
H	-5.596125	-1.157318	-2.515857
H	-5.845078	-1.744568	-0.864573
H	-5.834281	-0.006287	-1.192588
C	-2.715299	0.482040	-2.113935
H	-2.917170	1.454250	-1.650478
H	-1.632704	0.363787	-2.230445
H	-3.135857	0.516205	-3.125458
C	-2.246833	-2.690354	2.860059
H	-3.127372	-3.098546	2.359102
H	-1.438666	-3.427318	2.806517
H	-2.489052	-2.548741	3.918986
C	-0.716746	-0.432121	2.597845
H	0.302359	-0.815549	2.446582
N	0.183662	-0.621870	-0.268331
C	-0.828745	0.274163	3.939263
H	-1.832294	0.684464	4.077291
H	-0.631845	-0.439200	4.744762
H	-0.103151	1.087956	4.021208
H	-0.185458	-1.475814	0.162484

V

E = -1935.41266924 G = -1935.018889 ZPE = -1934.953253 Esol= -1935.826724

S	1.093998	-1.061924	-1.565534
Si	-3.524751	-0.697577	-1.142188
O	0.996120	-0.039815	-2.606514
O	0.840464	-2.450878	-1.903425

O	-1.272588	1.822829	1.748787
O	-3.453294	-0.189228	0.483166
C	-2.057163	-1.238388	2.241380
C	-2.402803	-0.357066	1.296117
C	-1.129037	0.448316	1.390771
C	-0.223996	0.423380	0.166365
C	0.042670	1.823212	-0.158381
C	-0.606185	2.563758	0.845211
C	-0.564997	3.954693	0.896390
H	-1.079389	4.486525	1.688043
C	0.144938	4.603516	-0.101393
H	0.194742	5.688268	-0.094647
C	0.788354	3.891658	-1.126591
H	1.317437	4.432576	-1.903424
C	0.741425	2.508451	-1.167700
H	1.198867	1.960885	-1.979887
C	6.496350	-0.681032	1.162312
H	6.391945	-0.805282	2.244311
H	6.983199	0.278579	0.973699
H	7.162787	-1.473079	0.804706
C	5.157131	-0.761245	0.476744
C	4.285901	-1.822462	0.757196
H	4.583149	-2.579306	1.478423
C	3.056434	-1.924000	0.124127
H	2.382461	-2.750871	0.326210
C	2.691251	-0.943233	-0.798196
C	3.534717	0.117202	-1.100364
H	3.236193	0.853197	-1.839002
C	4.767894	0.198827	-0.457636
H	5.438441	1.021596	-0.689219
C	-2.818085	-2.422344	-1.263699
H	-1.759333	-2.446437	-0.985035
H	-3.364699	-3.115611	-0.615199
H	-2.895142	-2.792120	-2.292103
C	-5.357539	-0.657144	-1.510822
H	-5.557443	-0.964091	-2.542685
H	-5.905702	-1.329906	-0.844452
H	-5.759460	0.351810	-1.375415
C	-2.625125	0.529880	-2.239002
H	-2.774286	1.554562	-1.880516
H	-1.548975	0.346045	-2.315292
H	-3.034386	0.475176	-3.254441
C	-2.652773	-2.486240	2.786239
H	-3.632601	-2.672810	2.339000

H	-2.007223	-3.346629	2.575882
H	-2.775003	-2.424598	3.873427
C	-0.751194	-0.522262	2.562728
H	0.147887	-1.105241	2.325384
N	0.089772	-0.747484	-0.264399
C	-0.644801	0.136450	3.929058
H	-1.531608	0.742426	4.133771
H	-0.558688	-0.627431	4.708556
H	0.235145	0.784181	3.988625

TS-III (-314.3923)

E = -1935.361931 G = -1934.967757 ZPE = -1934.90466 Esol= -1935.778858

S	1.092502	-0.740906	-1.885259
Si	-3.747494	-0.773412	-0.845617
O	1.145910	0.445052	-2.739337
O	0.839463	-2.038673	-2.485900
O	-1.593694	1.725285	1.469471
O	-3.399138	-0.847613	0.820515
C	-1.484548	-1.484906	2.175153
C	-2.172039	-0.690183	1.351772
C	-1.258884	0.445607	1.069678
C	-0.302950	0.502233	-0.049173
C	0.067278	1.926080	-0.124405
C	-0.751600	2.571894	0.814275
C	-0.712111	3.937491	1.054546
H	-1.365343	4.386645	1.793435
C	0.190853	4.677436	0.302885
H	0.252452	5.750686	0.454346
C	1.016847	4.067100	-0.651286
H	1.703770	4.675205	-1.229744
C	0.961697	2.699725	-0.878525
H	1.572490	2.238925	-1.641649
C	6.230887	-1.094705	1.332192
H	6.011329	-1.125684	2.404046
H	6.890837	-0.244534	1.144790
H	6.779102	-2.009516	1.084536
C	4.963347	-0.993992	0.523739
C	3.952346	-1.952976	0.679391
H	4.094982	-2.766910	1.385774
C	2.782463	-1.883918	-0.061556
H	2.002890	-2.633291	0.042578
C	2.613978	-0.832699	-0.964289

C	3.601764	0.124199	-1.145981
H	3.458431	0.913304	-1.876776
C	4.774614	0.035201	-0.397622
H	5.555420	0.777928	-0.535913
C	-2.951544	-2.229403	-1.700207
H	-1.860520	-2.193396	-1.608805
H	-3.305570	-3.175231	-1.277119
H	-3.195557	-2.226499	-2.768481
C	-5.614146	-0.868293	-0.877009
H	-5.988633	-0.874156	-1.905955
H	-5.967488	-1.778801	-0.383767
H	-6.057540	-0.011452	-0.360396
C	-3.162143	0.863831	-1.561398
H	-3.176612	1.659294	-0.807018
H	-2.154583	0.802417	-1.984680
H	-3.838095	1.169580	-2.367854
C	-1.782300	-2.864093	2.661659
H	-2.729056	-3.213373	2.242232
H	-0.990215	-3.559289	2.359870
H	-1.852056	-2.899234	3.754660
C	-0.259545	-0.673054	2.460318
H	0.687308	-1.026036	2.041801
N	-0.027301	-0.601720	-0.670938
C	-0.175800	0.184545	3.684883
H	-1.133618	0.677417	3.872871
H	0.060721	-0.434660	4.562511
H	0.610038	0.939851	3.591823

V

E = -1935.413798 G = -1935.021707 ZPE = -1934.955231 Esol= -1935.830188

S	2.073288	1.546146	-0.453242
Si	-4.140043	-1.720993	-0.250013
O	2.238840	2.606989	0.539127
O	1.909577	1.922753	-1.854185
O	-2.606000	0.623410	0.683416
O	-2.664145	-2.037455	0.549713
C	-0.344683	-2.352430	0.277003
C	-1.473346	-1.422982	0.468015
C	-1.411012	-0.064390	0.495838
C	-0.342510	0.879822	0.167084
C	-1.021422	2.182025	0.101538
C	-2.358761	1.933912	0.422482

C	-3.329915	2.924264	0.460471
H	-4.356651	2.689555	0.718114
C	-2.912665	4.212521	0.149281
H	-3.638009	5.020149	0.162687
C	-1.579244	4.491405	-0.184093
H	-1.291366	5.508861	-0.424335
C	-0.621428	3.487699	-0.211551
H	0.407261	3.713138	-0.463128
C	6.818610	-2.194951	0.073075
H	6.501019	-3.202947	0.357039
H	7.531781	-1.839031	0.820291
H	7.345445	-2.275718	-0.883638
C	5.637308	-1.266595	-0.043455
C	4.527160	-1.634396	-0.816192
H	4.524161	-2.598524	-1.318629
C	3.435987	-0.788839	-0.948261
H	2.568193	-1.076897	-1.533782
C	3.453307	0.440104	-0.289327
C	4.535092	0.830098	0.486333
H	4.508402	1.787068	0.996929
C	5.625304	-0.030659	0.601886
H	6.477117	0.263011	1.209027
C	-3.836211	-0.647250	-1.756407
H	-3.944829	0.417779	-1.534242
H	-2.825286	-0.802530	-2.150884
H	-4.541893	-0.906945	-2.552489
C	-4.694077	-3.431415	-0.770838
H	-5.691450	-3.404146	-1.222611
H	-4.004094	-3.859439	-1.505492
H	-4.731882	-4.108326	0.088482
C	-5.360374	-0.990553	0.961477
H	-5.516019	-1.667551	1.807266
H	-5.006260	-0.033281	1.350922
H	-6.330505	-0.833009	0.477373
C	-0.602579	-3.405348	-0.776251
H	-0.869883	-2.946321	-1.735584
H	0.287063	-4.020956	-0.928116
H	-1.431344	-4.056607	-0.481774
C	0.776924	-2.348380	1.012311
H	1.513434	-3.115274	0.769137
N	0.875439	0.485531	-0.020408
C	1.142831	-1.458124	2.151732
H	0.324948	-0.796995	2.444386
H	1.438222	-2.063215	3.016078

H	2.000402	-0.833817	1.874396

TS-IV (IF: -355.1250)

E = -1935.395884 G = -1934.999784 ZPE = -1934.937644 Esol= -1935.810754

S	-1.424744	-1.079711	0.890364
Si	4.200836	0.127738	0.699753
O	-0.902890	-0.162050	1.900243
O	-1.419394	-2.517396	1.143433
O	2.113061	1.301026	-1.253813
O	3.637701	-0.861933	-0.577119
C	1.782894	-2.323620	-0.754815
C	2.351860	-1.075206	-0.904412
C	1.517933	0.063624	-1.128787
C	0.193493	0.178274	-0.712419
C	-0.021196	1.597755	-0.509538
C	1.177676	2.214527	-0.887240
C	1.359070	3.592842	-0.891874
H	2.301663	4.032755	-1.198028
C	0.278156	4.358991	-0.480649
H	0.373245	5.439854	-0.456993
C	-0.938494	3.766089	-0.095966
H	-1.761636	4.400802	0.214829
C	-1.104182	2.391415	-0.110283
H	-2.046079	1.937613	0.177400
C	-7.195046	0.469277	-0.194590
H	-7.287512	0.984903	-1.156116
H	-7.587900	1.129654	0.581982
H	-7.831121	-0.420304	-0.238455
C	-5.761480	0.094077	0.078647
C	-5.100415	-0.813751	-0.759629
H	-5.634170	-1.246192	-1.602063
C	-3.779368	-1.167489	-0.529748
H	-3.265636	-1.870791	-1.178136
C	-3.106244	-0.600275	0.550713
C	-3.736937	0.297176	1.402173
H	-3.184460	0.718333	2.236660
C	-5.065414	0.639561	1.157364
H	-5.568019	1.340789	1.817846
C	2.760365	0.576075	1.806366
H	2.158080	1.403566	1.418567
H	2.084098	-0.273601	1.958502
H	3.136215	0.874118	2.791618

C	5.424725	-0.959810	1.609483
H	5.971307	-0.383674	2.363949
H	4.922523	-1.786869	2.121348
H	6.157226	-1.386275	0.916852
C	5.091239	1.606268	-0.018456
H	5.901768	1.283508	-0.679600
H	4.411458	2.236947	-0.595829
H	5.532365	2.210957	0.781407
C	2.411730	-3.364748	0.137329
H	3.296065	-2.966863	0.638729
H	1.685782	-3.678813	0.896426
H	2.717386	-4.255381	-0.421459
C	0.470880	-2.539441	-1.255598
H	-0.095532	-3.326671	-0.758056
N	-0.657758	-0.886135	-0.581785
C	0.106628	-2.320303	-2.694675
H	0.636005	-1.470701	-3.128343
H	0.400088	-3.221841	-3.248098
H	-0.969749	-2.180857	-2.807143

3

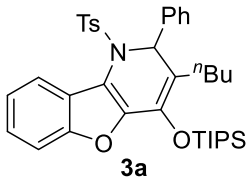
E = -1935.45648963 G = -1935.058709 ZPE = -1934.994934 Esol= -1935.868677

S	-2.550267	-1.432638	0.534611
Si	3.494371	1.220647	0.175258
O	-3.557881	-0.692549	-0.203658
O	-2.898342	-2.446232	1.515603
O	0.373109	2.019403	-0.522744
O	2.343207	-0.016303	0.037490
N	-1.646119	-0.256607	1.370132
C	-0.585135	-0.766893	2.280087
C	0.783882	-0.899700	1.620667
C	1.141907	-0.012675	0.672656
C	0.122601	0.926052	0.247141
C	-1.196629	0.806723	0.554703
C	-1.873344	1.902828	-0.091521
C	-0.846572	2.610875	-0.737243
C	-1.060188	3.759875	-1.483814
H	-0.238117	4.277040	-1.966013
C	-2.375023	4.198505	-1.576560
H	-2.596515	5.091927	-2.151192
C	-3.423670	3.505181	-0.947128
H	-4.437997	3.876603	-1.050284

C	-3.192907	2.356063	-0.206429
H	-3.999776	1.802671	0.259647
C	1.870628	-3.449408	-3.055264
H	2.059906	-4.520437	-2.948117
H	2.775986	-2.917057	-2.742736
H	1.708182	-3.231822	-4.114192
C	0.696554	-3.012065	-2.219548
C	0.328617	-3.726826	-1.075541
H	0.867935	-4.633957	-0.816150
C	-0.709396	-3.288171	-0.262373
H	-0.998246	-3.831023	0.632743
C	-1.393273	-2.127892	-0.613545
C	-1.076997	-1.416551	-1.769190
H	-1.646333	-0.530487	-2.034225
C	-0.028926	-1.867060	-2.562887
H	0.235864	-1.317242	-3.461825
C	5.100618	0.351197	0.586098
H	5.037494	-0.150073	1.557355
H	5.334741	-0.407033	-0.168058
H	5.937642	1.056270	0.624067
C	3.624050	2.101391	-1.468398
H	4.398244	2.875587	-1.439759
H	3.882149	1.397180	-2.265730
H	2.672099	2.573114	-1.726503
C	2.972709	2.367478	1.561754
H	2.071156	2.930390	1.301176
H	2.767666	1.801857	2.477530
H	3.767954	3.086988	1.783740
C	1.692291	-1.986218	2.103744
H	2.683737	-1.891420	1.656385
H	1.793036	-1.963971	3.195999
H	1.288772	-2.971589	1.837653
H	-0.925508	-1.754144	2.607363
C	-0.512417	0.154324	3.499855
H	-1.482995	0.194330	3.999899
H	0.238804	-0.215995	4.203809
H	-0.227000	1.164937	3.192000

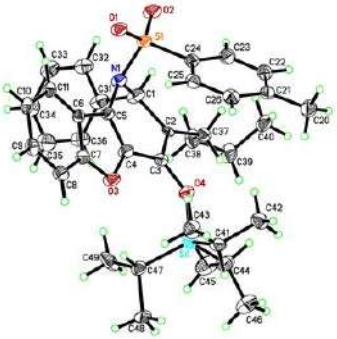
VII. Product Structure Determination

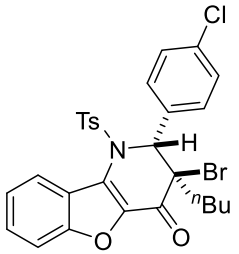
The structure of products **3a**, **4b** and **4c** were determined by X-ray crystallography. The X-ray data of **3a** (CCDC 2045484), **4b** (CCDC 2079164) and **4c** (CCDC 2079165) have been deposited at the Cambridge Crystallographic Data Center. The relative stereochemistry of **4a** was determined by analogy and nOe study. The correlation observed in NMR is shown below.



3a

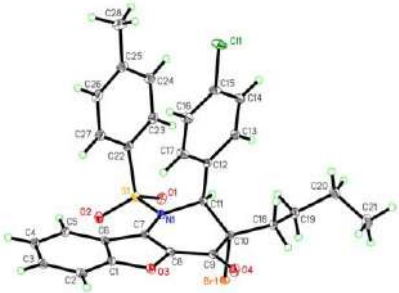
≡

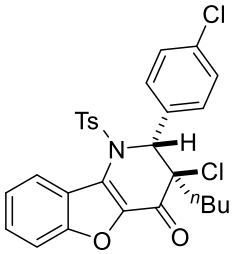




4b

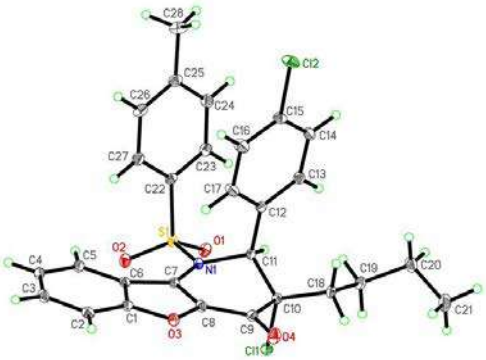
≡

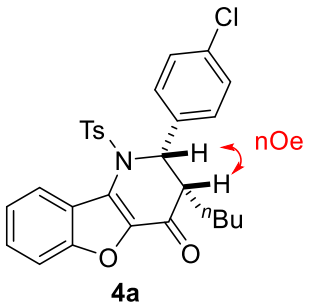




4c

≡





4a

Table S1. Crystal data and structure refinement for 3a.

Identification code	**3a**
Empirical formula	$C_{37}H_{47}NO_4SSi$
Formula weight	629.90
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	16.6691(10)
b/Å	10.8205(5)
c/Å	20.3333(13)
α/°	90
β/°	112.297(7)
γ/°	90
Volume/Å^3	3393.3(4)
Z	4
ϱ_{calc}g/cm^3	1.233
μ/mm^{-1}	1.495
F(000)	1352.0
Crystal size/mm^3	0.15 × 0.12 × 0.02
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.684 to 134.982
Index ranges	-19 ≤ h ≤ 19, -12 ≤ k ≤ 12, -24 ≤ l ≤ 23
Reflections collected	18730
Independent reflections	6094 [R_{int} = 0.0647, R_{sigma} = 0.0517]
Data/restraints/parameters	6094/179/565
Goodness-of-fit on F^2	1.002
Final R indexes [I>=2σ (I)]	R_1 = 0.0624, wR_2 = 0.1655
Final R indexes [all data]	R_1 = 0.0726, wR_2 = 0.1728

Largest diff. peak/hole / e Å^{-3} 0.37/-0.55

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3a. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	7014.6(5)	6644.6(7)	2194.6(4)	30.9(2)
Si1	4099(2)	6751(3)	3664.5(16)	29.6(6)
Si1A	3947(3)	6969(4)	3469(2)	22.0(8)
O1	7100.6(14)	7800.2(19)	1887.2(12)	34.5(5)
O2	7449.1(15)	5569(2)	2082.1(12)	40.4(6)
O3	4449.1(14)	8156.0(19)	2300.4(12)	34.5(5)
O4	4822(3)	6196(5)	3369(2)	37.4(11)
O4A	4456(4)	5995(5)	3116(3)	29.6(14)
N1	5955.2(16)	6309(2)	1842.5(13)	28.0(5)
C1	5692(2)	5057(3)	2007.2(17)	34.1(7)
C2	5486(3)	5113(5)	2695(3)	21.7(11)
C2A	5177(6)	4982(7)	2502(5)	19.9(16)
C3	5072(5)	6135(8)	2814(4)	28.6(19)
C3A	4840(8)	5974(9)	2643(6)	21(3)
C4	4944(2)	7140(3)	2315.7(16)	31.3(6)
C5	5400.7(18)	7277(2)	1892.6(15)	24.9(6)
C6	5195.0(17)	8475(2)	1565.9(14)	23.2(5)
C7	4617.4(18)	8980(3)	1844.7(15)	28.4(6)
C8	4257(2)	10138(3)	1685.6(17)	33.1(7)
C9	4485(2)	10830(3)	1208.8(16)	32.2(6)
C10	5050.4(19)	10352(3)	908.2(15)	29.1(6)
C11	5413.3(18)	9188(2)	1082.1(14)	25.2(6)
C20	7985(2)	7371(3)	5352.8(17)	41.1(8)
C21	7724.8(18)	7170(3)	4563.5(16)	32.0(6)
C22	7860(2)	6040(3)	4294.8(17)	37.3(7)
C23	7650(2)	5863(3)	3572.2(18)	37.7(7)
C24	7293.5(18)	6851(3)	3112.6(16)	29.5(6)
C25	7137.8(18)	7985(3)	3359.5(16)	30.1(6)
C26	7356.3(19)	8137(3)	4085.7(16)	32.4(6)

C31	5053(2)	4514(3)	1318.6(18)	35.3(7)
C32	5378(2)	3957(3)	847.1(18)	35.5(7)
C33	4826(2)	3499(3)	200.4(19)	40.2(7)
C34	3939(2)	3587(3)	8(2)	45.5(8)
C35	3608(2)	4130(3)	473(2)	48.5(9)
C36	4166(2)	4586(3)	1126(2)	42.2(8)
C37	5679(3)	3999(4)	3171(2)	29.9(9)
C37A	5101(5)	3718(7)	2780(4)	23.1(15)
C38	5276(3)	2779(4)	2823(3)	38.5(11)
C38A	5951(5)	3240(8)	3323(4)	24.7(15)
C39	5309(4)	1772(5)	3367(3)	44.3(12)
C39A	5798(7)	2064(9)	3662(5)	33.1(18)
C40	6217(4)	1374(6)	3830(3)	45.0(12)
C40A	6629(7)	1525(9)	4211(6)	34(2)
C41	4604(4)	8022(6)	4330(4)	34.8(11)
C41A	4719(4)	8271(5)	3931(3)	28.3(12)
C42	5464(4)	7570(8)	4911(4)	38.5(14)
C42A	5498(5)	7883(7)	4575(4)	42.4(17)
C43	4749(5)	9185(7)	3996(4)	42.5(14)
C43A	4251(5)	9366(6)	4107(4)	36.7(14)
C44	3940(5)	5388(7)	4183(4)	38.9(14)
C44A	3801(7)	5872(8)	4134(5)	28.3(17)
C45	3473(5)	4282(7)	3698(4)	55.4(18)
C45A	3239(7)	4750(8)	3773(5)	38(2)
C46	3522(5)	5631(8)	4709(4)	56.1(16)
C46A	3532(5)	6405(8)	4717(4)	32.2(14)
C47	3089(6)	7299(8)	2943(5)	30(2)
C47A	2924(9)	7551(11)	2771(7)	25(3)
C48	2368(7)	7717(12)	3237(7)	35(2)
C48A	2300(16)	7940(20)	3064(12)	48(5)
C49	2700(6)	6433(11)	2296(5)	51(3)
C49A	2493(10)	6593(15)	2167(9)	41(4)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	35.0(4)	30.5(4)	35.8(4)	12.2(3)	22.9(3)	14.7(3)
Si1	25.2(11)	34.7(14)	28.4(14)	-4.5(9)	9.7(11)	0.8(9)
Si1A	31(2)	17.4(14)	23.9(19)	0.5(12)	17.1(18)	1.9(11)
O1	36.6(11)	34.3(11)	40.9(12)	14.0(9)	24.2(10)	11.3(9)
O2	49.4(13)	36.7(12)	48.4(13)	12.6(10)	33.4(11)	23.3(10)
O3	40.3(12)	29.9(11)	45.4(12)	12.1(9)	29.9(10)	14.8(9)
O4	37(2)	51(2)	32(2)	10.6(17)	21.3(19)	16.8(19)
O4A	51(4)	15(2)	37(3)	3(2)	32(3)	3(3)
N1	36.2(13)	21.6(11)	32.7(13)	6.3(9)	20.3(11)	9.7(9)
C1	50.9(18)	20.8(13)	43.9(16)	10.0(11)	33.1(14)	12.6(12)
C2	9(2)	30(2)	24(2)	2.5(16)	4(2)	-3.5(17)
C2A	23(4)	13(2)	25(3)	-4(2)	11(3)	-5(2)
C3	24(4)	35(3)	30(3)	3(2)	12(3)	6(3)
C3A	31(6)	13(2)	25(5)	-2(2)	18(5)	-6(3)
C4	38.0(16)	27.1(15)	35.0(16)	8.1(12)	21.0(13)	10.3(12)
C5	27.6(14)	23.7(13)	27.3(14)	5.1(11)	14.7(11)	7.3(10)
C6	24.9(13)	21.8(13)	21.9(13)	2.7(10)	7.6(10)	2.2(10)
C7	30.4(14)	26.5(14)	30.4(15)	6.3(11)	13.7(12)	3.9(11)
C8	34.4(16)	27.7(15)	38.9(17)	3.5(12)	15.8(13)	9.4(12)
C9	36.9(16)	22.5(14)	32.4(15)	3.9(11)	7.7(13)	3.7(11)
C10	35.9(15)	24.1(14)	24.2(14)	4.2(11)	8.0(12)	-2.2(11)
C11	28.1(14)	23.0(13)	23.2(13)	1.4(10)	8.2(11)	-2.1(10)
C20	35.5(17)	53(2)	33.3(17)	4.1(15)	11.0(13)	-9.7(14)
C21	20.8(13)	42.9(17)	32.5(15)	5.7(13)	10.2(11)	-4.9(12)
C22	33.6(16)	40.8(18)	38.0(17)	16.1(14)	14.2(13)	11.7(13)
C23	38.7(17)	37.1(17)	41.5(18)	12.5(14)	20.0(14)	15.9(13)
C24	27.2(14)	32.3(15)	31.6(15)	9.4(12)	14.0(12)	7.3(11)
C25	26.4(14)	26.3(14)	37.7(16)	7.7(12)	12.0(12)	1.2(11)
C26	29.0(15)	29.5(15)	38.0(16)	0.5(12)	11.7(13)	-4.5(11)
C31	49.8(19)	20.2(14)	49.8(19)	9.7(13)	34.6(16)	7.9(12)
C32	42.2(17)	22.0(14)	51.6(19)	5.0(13)	28.4(15)	1.4(12)
C33	56(2)	26.1(15)	47.8(19)	2.8(14)	30.0(16)	0.9(14)

C34	53(2)	30.9(16)	53(2)	13.9(15)	21.7(17)	0.1(14)
C35	47(2)	38.3(18)	67(2)	23.7(17)	30.4(19)	12.5(15)
C36	46.5(19)	29.3(16)	62(2)	13.8(15)	32.7(17)	10.8(14)
C37	28(2)	31.7(18)	33(2)	7.7(15)	15.0(17)	4.7(15)
C37A	27(3)	16(2)	25(3)	-3(2)	8(3)	-6(2)
C38	42(2)	32(2)	36(2)	10.1(16)	8.6(18)	-6.4(16)
C38A	27(3)	25(3)	26(3)	-1(2)	14(3)	2(2)
C39	53(3)	35(2)	43(3)	13.4(19)	16(2)	-3.1(19)
C39A	33(4)	29(3)	35(4)	6(3)	10(3)	0(3)
C40	56(3)	48(3)	40(3)	21(2)	29(2)	12(2)
C40A	34(4)	37(4)	34(4)	5(3)	15(3)	5(3)
C41	27(2)	45(2)	36(3)	-3.6(19)	16(2)	4.7(18)
C41A	31(2)	25(2)	28(2)	-3.1(19)	9.8(19)	-11.1(18)
C42	31(3)	45(3)	36(3)	-10(2)	8(2)	0(2)
C42A	38(4)	47(4)	42(4)	10(3)	16(3)	-4(3)
C43	46(4)	41(3)	37(3)	-9(2)	11(3)	-1(2)
C43A	36(4)	34(3)	35(3)	-11(3)	9(3)	-12(3)
C44	45(3)	45(3)	33(2)	2(2)	22(2)	4(2)
C44A	44(4)	19(3)	30(3)	6(2)	22(3)	3(3)
C45	67(4)	53(3)	58(3)	-8(3)	36(3)	-13(3)
C45A	63(5)	25(3)	36(3)	-1(2)	32(3)	-10(3)
C46	69(4)	61(4)	52(3)	-3(3)	37(3)	0(3)
C46A	39(2)	33(2)	31.3(19)	-0.4(15)	19.8(16)	-3.5(16)
C47	31(4)	31(4)	30(4)	3(3)	15(3)	-4(3)
C47A	30(6)	21(5)	23(6)	12(4)	10(4)	8(4)
C48	28(4)	45(6)	40(6)	4(5)	21(4)	-13(4)
C48A	69(9)	43(8)	49(10)	31(6)	43(7)	14(6)
C49	25(4)	62(5)	49(5)	-19(4)	-5(3)	4(4)
C49A	41(4)	39(4)	42(4)	-1.5(19)	15(2)	-1(2)

Table S4. Bond Lengths for 3a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	O1	1.429(2)	C9	C10	1.402(4)
S1	O2	1.434(2)	C10	C11	1.384(4)

S1	N1	1.674(3)	C20	C21	1.511(4)
S1	C24	1.758(3)	C21	C22	1.392(5)
Si1	O4	1.650(5)	C21	C26	1.401(4)
Si1	C41	1.889(7)	C22	C23	1.388(5)
Si1	C44	1.889(8)	C23	C24	1.395(4)
Si1	C47	1.861(9)	C24	C25	1.387(4)
Si1A	O4A	1.675(6)	C25	C26	1.390(4)
Si1A	C41A	1.899(7)	C31	C32	1.404(4)
Si1A	C44A	1.883(9)	C31	C36	1.381(5)
Si1A	C47A	1.866(13)	C32	C33	1.380(5)
O3	C4	1.368(3)	C33	C34	1.382(5)
O3	C7	1.389(3)	C34	C35	1.393(5)
O4	C3	1.346(7)	C35	C36	1.390(6)
O4A	C3A	1.343(9)	C37	C38	1.528(7)
N1	C1	1.501(4)	C37A	C38A	1.517(11)
N1	C5	1.426(3)	C38	C39	1.539(6)
C1	C2	1.562(6)	C38A	C39A	1.515(12)
C1	C2A	1.552(9)	C39	C40	1.509(8)
C1	C31	1.519(5)	C39A	C40A	1.527(13)
C2	C3	1.372(9)	C41	C42	1.551(9)
C2	C37	1.503(7)	C41	C43	1.492(10)
C2A	C3A	1.293(12)	C41A	C42A	1.512(9)
C2A	C37A	1.504(11)	C41A	C43A	1.534(9)
C3	C4	1.446(9)	C44	C45	1.558(10)
C3A	C4	1.467(11)	C44	C46	1.505(9)
C4	C5	1.356(4)	C44A	C45A	1.539(12)
C5	C6	1.437(4)	C44A	C46A	1.531(11)
C6	C7	1.400(4)	C47	C48	1.598(19)
C6	C11	1.402(4)	C47	C49	1.543(13)
C7	C8	1.373(4)	C47A	C48A	1.44(3)
C8	C9	1.387(4)	C47A	C49A	1.56(2)

Table S5. Bond Angles for 3a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°

O1	S1	O2	119.98(13)	C11	C6	C5	137.7(3)
O1	S1	N1	105.50(12)	O3	C7	C6	111.3(2)
O1	S1	C24	108.86(14)	C8	C7	O3	124.2(3)
O2	S1	N1	105.69(14)	C8	C7	C6	124.5(3)
O2	S1	C24	109.03(14)	C7	C8	C9	116.5(3)
N1	S1	C24	107.01(13)	C8	C9	C10	120.9(3)
O4	Si1	C41	109.7(3)	C11	C10	C9	121.7(3)
O4	Si1	C44	101.2(3)	C10	C11	C6	118.4(3)
O4	Si1	C47	113.3(4)	C22	C21	C20	121.3(3)
C44	Si1	C41	106.7(3)	C22	C21	C26	118.5(3)
C47	Si1	C41	110.9(4)	C26	C21	C20	120.2(3)
C47	Si1	C44	114.3(4)	C23	C22	C21	121.6(3)
O4A	Si1A	C41A	108.7(4)	C22	C23	C24	118.4(3)
O4A	Si1A	C44A	97.8(4)	C23	C24	S1	119.2(2)
O4A	Si1A	C47A	110.6(6)	C25	C24	S1	119.1(2)
C44A	Si1A	C41A	111.1(4)	C25	C24	C23	121.7(3)
C47A	Si1A	C41A	112.2(5)	C24	C25	C26	118.7(3)
C47A	Si1A	C44A	115.3(6)	C25	C26	C21	121.2(3)
C4	O3	C7	105.0(2)	C32	C31	C1	118.6(3)
C3	O4	Si1	145.6(5)	C36	C31	C1	122.7(3)
C3A	O4A	Si1A	140.7(6)	C36	C31	C32	118.7(3)
C1	N1	S1	116.79(19)	C33	C32	C31	121.0(3)
C5	N1	S1	114.67(19)	C32	C33	C34	120.0(3)
C5	N1	C1	113.2(2)	C33	C34	C35	119.6(4)
N1	C1	C2	110.3(3)	C36	C35	C34	120.3(3)
N1	C1	C2A	118.2(3)	C31	C36	C35	120.5(3)
N1	C1	C31	107.8(2)	C2	C37	C38	116.5(4)
C31	C1	C2	121.7(3)	C2A	C37A	C38A	113.3(7)
C31	C1	C2A	102.1(4)	C37	C38	C39	112.9(4)
C3	C2	C1	119.0(5)	C39A	C38A	C37A	110.2(7)
C3	C2	C37	122.2(5)	C40	C39	C38	113.8(5)
C37	C2	C1	118.6(4)	C38A	C39A	C40A	113.0(8)
C3A	C2A	C1	119.6(7)	C42	C41	Si1	110.4(5)
C3A	C2A	C37A	124.4(8)	C43	C41	Si1	113.2(5)
C37A	C2A	C1	116.0(6)	C43	C41	C42	110.5(6)

O4	C3	C2	121.6(7)	C42A	C41A	Si1A	114.9(5)
O4	C3	C4	122.7(6)	C42A	C41A	C43A	111.0(5)
C2	C3	C4	115.7(5)	C43A	C41A	Si1A	112.3(4)
O4A	C3A	C4	118.7(7)	C45	C44	Si1	112.9(5)
C2A	C3A	O4A	122.6(9)	C46	C44	Si1	117.4(5)
C2A	C3A	C4	118.5(7)	C46	C44	C45	109.2(6)
O3	C4	C3	123.3(4)	C45A	C44A	Si1A	112.1(6)
O3	C4	C3A	121.8(5)	C46A	C44A	Si1A	118.4(6)
C5	C4	O3	112.1(2)	C46A	C44A	C45A	111.2(7)
C5	C4	C3	123.9(4)	C48	C47	Si1	112.3(7)
C5	C4	C3A	125.0(4)	C49	C47	Si1	116.1(7)
N1	C5	C6	132.6(2)	C49	C47	C48	111.0(8)
C4	C5	N1	120.0(2)	C48A	C47A	Si1A	112.3(11)
C4	C5	C6	107.4(2)	C48A	C47A	C49A	109.3(15)
C7	C6	C5	104.2(2)	C49A	C47A	Si1A	112.9(9)
C7	C6	C11	118.1(2)				

Table S6. Torsion Angles for 3a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	N1	C1	C2	90.4(3)	C4	C5	C6	C7	1.0(3)
S1	N1	C1	C2A	110.4(4)	C4	C5	C6	C11	-179.0(3)
S1	N1	C1	C31	-134.6(2)	C5	N1	C1	C2	-46.1(4)
S1	N1	C5	C4	-112.3(3)	C5	N1	C1	C2A	-26.1(5)
S1	N1	C5	C6	67.8(4)	C5	N1	C1	C31	88.9(3)
S1	C24	C25	C26	179.7(2)	C5	C6	C7	O3	-1.5(3)
Si1	O4	C3	C2	-148.5(8)	C5	C6	C7	C8	179.0(3)
Si1	O4	C3	C4	32.9(14)	C5	C6	C11	C10	-179.7(3)
Si1A	O4A	C3A	C2A	-179.7(8)	C6	C7	C8	C9	0.7(5)
Si1A	O4A	C3A	C4	5.4(18)	C7	O3	C4	C3	169.7(5)
O1	S1	N1	C1	172.8(2)	C7	O3	C4	C3A	-169.4(6)
O1	S1	N1	C5	-51.3(2)	C7	O3	C4	C5	-0.7(3)
O1	S1	C24	C23	-150.3(2)	C7	C6	C11	C10	0.3(4)
O1	S1	C24	C25	31.0(3)	C7	C8	C9	C10	0.4(4)
O2	S1	N1	C1	44.7(2)	C8	C9	C10	C11	-1.1(4)

O2	S1	N1	C5	-179.35(19)	C9	C10	C11	C6	0.7(4)
O2	S1	C24	C23	-17.7(3)	C11	C6	C7	O3	178.5(2)
O2	S1	C24	C25	163.5(2)	C11	C6	C7	C8	-1.0(4)
O3	C4	C5	N1	179.9(3)	C20	C21	C22	C23	-177.7(3)
O3	C4	C5	C6	-0.2(4)	C20	C21	C26	C25	177.9(3)
O3	C7	C8	C9	-178.8(3)	C21	C22	C23	C24	-0.2(5)
O4	Si1	C41	C42	-51.7(6)	C22	C21	C26	C25	-0.8(4)
O4	Si1	C41	C43	72.7(5)	C22	C23	C24	S1	-179.5(2)
O4	Si1	C44	C45	-68.8(6)	C22	C23	C24	C25	-0.8(5)
O4	Si1	C44	C46	162.8(6)	C23	C24	C25	C26	0.9(4)
O4	Si1	C47	C48	174.8(6)	C24	S1	N1	C1	-71.4(2)
O4	Si1	C47	C49	45.6(9)	C24	S1	N1	C5	64.5(2)
O4	C3	C4	O3	-10.0(10)	C24	C25	C26	C21	-0.1(4)
O4	C3	C4	C5	159.2(6)	C26	C21	C22	C23	1.0(5)
O4A	Si1A	C41A	C42A	-66.3(6)	C31	C1	C2	C3	-89.7(6)
O4A	Si1A	C41A	C43A	165.7(5)	C31	C1	C2	C37	85.0(5)
O4A	Si1A	C44A	C45A	-61.6(8)	C31	C1	C2A	C3A	-104.3(9)
O4A	Si1A	C44A	C46A	166.8(7)	C31	C1	C2A	C37A	75.1(7)
O4A	Si1A	C47A	C48A	155.5(12)	C31	C32	C33	C34	0.1(5)
O4A	Si1A	C47A	C49A	31.4(12)	C32	C31	C36	C35	-0.8(4)
O4A	C3A	C4	O3	-20.4(12)	C32	C33	C34	C35	-0.5(5)
O4A	C3A	C4	C5	172.4(7)	C33	C34	C35	C36	0.2(5)
N1	S1	C24	C23	96.2(3)	C34	C35	C36	C31	0.5(5)
N1	S1	C24	C25	-82.6(3)	C36	C31	C32	C33	0.5(4)
N1	C1	C2	C3	38.0(6)	C37	C2	C3	O4	0.5(11)
N1	C1	C2	C37	-147.3(4)	C37	C2	C3	C4	179.2(5)
N1	C1	C2A	C3A	13.7(11)	C37	C38	C39	C40	-64.7(6)
N1	C1	C2A	C37A	-166.9(5)	C37A	C2A	C3A	O4A	6.9(17)
N1	C1	C31	C32	80.9(3)	C37A	C2A	C3A	C4	-178.2(8)
N1	C1	C31	C36	-96.7(3)	C37A	C38A	C39A	C40A	179.5(8)
N1	C5	C6	C7	-179.1(3)	C41	Si1	O4	C3	-107.8(10)
N1	C5	C6	C11	0.9(6)	C41	Si1	C44	C45	176.4(5)
C1	N1	C5	C4	25.2(4)	C41	Si1	C44	C46	48.1(6)
C1	N1	C5	C6	-154.7(3)	C41	Si1	C47	C48	-61.2(8)
C1	C2	C3	O4	175.0(6)	C41	Si1	C47	C49	169.6(7)

C1	C2	C3	C4	-6.3(9)	C41A	Si1A	O4A	C3A	-60.1(12)
C1	C2	C37	C38	-54.6(6)	C41A	Si1A	C44A	C45A	-175.2(6)
C1	C2A	C3A	O4A	-173.8(8)	C41A	Si1A	C44A	C46A	53.2(8)
C1	C2A	C3A	C4	1.2(14)	C41A	Si1A	C47A	C48A	-82.9(14)
C1	C2A	C37A	C38A	70.4(9)	C41A	Si1A	C47A	C49A	153.0(10)
C1	C31	C32	C33	-177.1(3)	C44	Si1	O4	C3	139.7(9)
C1	C31	C36	C35	176.7(3)	C44	Si1	C41	C42	57.2(6)
C2	C1	C31	C32	-150.4(3)	C44	Si1	C41	C43	-178.4(5)
C2	C1	C31	C36	32.1(5)	C44	Si1	C47	C48	59.5(8)
C2	C3	C4	O3	171.4(5)	C44	Si1	C47	C49	-69.7(9)
C2	C3	C4	C5	-19.4(9)	C44A	Si1A	O4A	C3A	-175.6(12)
C2	C37	C38	C39	-165.5(4)	C44A	Si1A	C41A	C42A	40.3(7)
C2A	C1	C31	C32	-153.9(4)	C44A	Si1A	C41A	C43A	-87.7(6)
C2A	C1	C31	C36	28.6(4)	C44A	Si1A	C47A	C48A	45.7(14)
C2A	C3A	C4	O3	164.5(8)	C44A	Si1A	C47A	C49A	-78.4(12)
C2A	C3A	C4	C5	-2.8(13)	C47	Si1	O4	C3	16.8(11)
C2A	C37A	C38A	C39A	171.2(7)	C47	Si1	C41	C42	-177.7(6)
C3	C2	C37	C38	119.9(7)	C47	Si1	C41	C43	-53.3(7)
C3	C4	C5	N1	9.6(6)	C47	Si1	C44	C45	53.4(7)
C3	C4	C5	C6	-170.5(5)	C47	Si1	C44	C46	-74.9(7)
C3A	C2A	C37A	C38A	-110.2(11)	C47A	Si1A	O4A	C3A	63.5(13)
C3A	C4	C5	N1	-11.7(7)	C47A	Si1A	C41A	C42A	171.1(7)
C3A	C4	C5	C6	168.1(6)	C47A	Si1A	C41A	C43A	43.1(7)
C4	O3	C7	C6	1.3(3)	C47A	Si1A	C44A	C45A	55.6(9)
C4	O3	C7	C8	-179.1(3)	C47A	Si1A	C44A	C46A	-76.0(9)

Table S7. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 3a.

Atom	*x*	*y*	*z*	U(eq)
H1A	6224	4534	2135	41
H1B	6214	4513	2198	41
H8	3873	10448	1891	40
H9	4255	11638	1084	39
H10	5188	10840	577	35
H11	5801	8879	879	30

H20A	8064	6569	5594	62
H20B	7531	7838	5439	62
H20C	8531	7835	5538	62
H22	8101	5374	4613	45
H23	7747	5088	3395	45
H25	6887	8644	3039	36
H26	7254	8910	4261	39
H32	5987	3895	975	43
H33	5056	3123	-113	48
H34	3557	3278	-438	55
H35	2999	4189	344	58
H36	3935	4950	1441	51
H37A	5479	4171	3562	36
H37B	6316	3890	3387	36
H37C	4891	3132	2377	28
H37D	4665	3746	3001	28
H38A	5587	2480	2525	46
H38B	4664	2925	2508	46
H38C	6361	3075	3087	30
H38D	6210	3875	3694	30
H39A	5016	2084	3676	53
H39B	4982	1041	3109	53
H39C	5528	1442	3286	40
H39D	5386	2239	3895	40
H40A	6480	941	3538	68
H40B	6194	819	4203	68
H40C	6565	2103	4047	68
H40D	7045	1365	3986	52
H40E	6496	750	4397	52
H40F	6880	2114	4602	52
H41	4194	8217	4569	42
H41A	4955	8588	3578	34
H42A	5341	6899	5183	58
H42B	5740	8257	5231	58
H42C	5853	7270	4687	58

H42D	5880	8596	4761	64
H42E	5815	7232	4440	64
H42F	5304	7570	4943	64
H43A	5203	9049	3808	64
H43B	4930	9843	4354	64
H43C	4210	9426	3608	64
H43D	3957	9086	4417	55
H43E	3822	9703	3667	55
H43F	4674	10008	4351	55
H44	4537	5083	4472	47
H44A	4391	5520	4395	34
H45A	2852	4462	3468	83
H45B	3556	3532	3987	83
H45C	3717	4156	3334	83
H45D	2635	5014	3529	57
H45E	3271	4129	4133	57
H45F	3451	4392	3427	57
H46A	3852	6265	5047	84
H46B	3515	4867	4965	84
H46C	2926	5918	4456	84
H46D	3869	7154	4912	48
H46E	3643	5793	5097	48
H46F	2913	6608	4517	48
H47	3256	8068	2754	36
H47A	3077	8292	2549	30
H48A	2136	6987	3390	53
H48B	1897	8144	2860	53
H48C	2628	8276	3642	53
H48D	2090	7219	3242	72
H48E	1811	8349	2694	72
H48F	2576	8520	3456	72
H49A	3122	6309	2073	76
H49B	2171	6804	1952	76
H49C	2559	5634	2453	76
H49D	2943	6174	2050	61

H49E	2093	7019	1745	61
H49F	2173	5982	2328	61

Table S8. Atomic Occupancy for 3a.

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
Si1	0.6	Si1A	0.4	O4	0.6
O4A	0.4	H1A	0.6	H1B	0.4
C2	0.6	C2A	0.4	C3	0.6
C3A	0.4	C37	0.6667	H37A	0.6667
H37B	0.6667	C37A	0.3333	H37C	0.3333
H37D	0.3333	C38	0.6667	H38A	0.6667
H38B	0.6667	C38A	0.3333	H38C	0.3333
H38D	0.3333	C39	0.6667	H39A	0.6667
H39B	0.6667	C39A	0.3333	H39C	0.3333
H39D	0.3333	C40	0.6667	H40A	0.6667
H40B	0.6667	H40C	0.6667	C40A	0.3333
H40D	0.3333	H40E	0.3333	H40F	0.3333
C41	0.5	H41	0.5	C41A	0.5
H41A	0.5	C42	0.5	H42A	0.5
H42B	0.5	H42C	0.5	C42A	0.5
H42D	0.5	H42E	0.5	H42F	0.5
C43	0.5	H43A	0.5	H43B	0.5
H43C	0.5	C43A	0.5	H43D	0.5
H43E	0.5	H43F	0.5	C44	0.6
H44	0.6	C44A	0.4	H44A	0.4
C45	0.6	H45A	0.6	H45B	0.6
H45C	0.6	C45A	0.4	H45D	0.4
H45E	0.4	H45F	0.4	C46	0.6
H46A	0.6	H46B	0.6	H46C	0.6
C46A	0.4	H46D	0.4	H46E	0.4
H46F	0.4	C47	0.6	H47	0.6
C47A	0.4	H47A	0.4	C48	0.6
H48A	0.6	H48B	0.6	H48C	0.6
C48A	0.4	H48D	0.4	H48E	0.4

H48F	0.4	C49	0.6	H49A	0.6
H49B	0.6	H49C	0.6	C49A	0.4
H49D	0.4	H49E	0.4	H49F	0.4

Table S9. Crystal data and structure refinement for 4b.

Identification code	**4b**
Empirical formula	$C_{28}H_{25}BrClNO_4S$
Formula weight	586.91
Temperature/K	99.97(16)
Crystal system	triclinic
Space group	P-1
a/Å	10.7962(5)
b/Å	10.9702(4)
c/Å	11.8384(5)
α/°	78.442(4)
β/°	65.815(4)
γ/°	79.502(4)
Volume/Å^3	1245.21(10)
Z	2
ϱ_{calc}g/cm^3	1.565
μ/mm^{-1}	4.326
F(000)	600.0
Crystal size/mm^3	0.2 × 0.1 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.268 to 153.63
Index ranges	-13 ≤ h ≤ 11, -13 ≤ k ≤ 13, -14 ≤ l ≤ 14
Reflections collected	7889
Independent reflections	5020 [R_{int} = 0.0176, R_{sigma} = 0.0241]
Data/restraints/parameters	5020/0/327
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0229, wR_2 = 0.0580
Final R indexes [all data]	R_1 = 0.0242, wR_2 = 0.0588
Largest diff. peak/hole / e Å^{-3}	0.43/-0.48

Table S10. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for 4b. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Br1	4557.7(2)	4957.1(2)	3679.0(2)	13.74(5)
Cl1	-1917.0(4)	3539.3(4)	1631.6(4)	21.68(9)
S1	5159.5(3)	2604.6(3)	1092.3(3)	10.82(7)
O1	5711.4(11)	3761.7(10)	468.9(9)	14.7(2)
O2	6044.8(11)	1527.3(10)	1306.3(10)	15.1(2)
O3	2487.1(11)	1491.7(9)	5683.3(9)	13.2(2)
O4	1514.0(12)	4029.4(10)	5924.4(10)	18.9(2)
N1	4002.1(12)	2887.6(11)	2492.3(11)	10.5(2)
C1	3150.8(15)	425.8(14)	5176.2(14)	12.7(3)
C2	3073.0(15)	-756.4(14)	5871.6(14)	15.5(3)
C3	3793.3(16)	-1751.3(14)	5227.6(15)	16.9(3)
C4	4579.3(16)	-1548.4(14)	3936.0(15)	16.2(3)
C5	4652.2(15)	-366.8(14)	3255.8(14)	13.9(3)
C6	3911.2(14)	668.7(13)	3877.2(13)	11.7(3)
C7	3657.8(14)	2020.0(13)	3589.6(13)	10.9(3)
C8	2817.4(14)	2444.4(13)	4699.3(13)	11.8(3)
C9	2270.1(15)	3718.3(14)	4912.0(13)	12.5(3)
C10	2777.5(14)	4662.7(13)	3717.3(13)	10.8(3)
C11	3077.3(14)	4079.5(13)	2527.3(13)	10.2(3)
C12	1777.0(14)	3919.6(13)	2373.2(13)	11.2(3)
C13	1255.1(15)	4890.1(14)	1672.3(14)	14.4(3)
C14	105.3(15)	4790.7(14)	1463.0(14)	15.3(3)
C15	-514.5(15)	3702.0(15)	1937.0(14)	15.2(3)
C16	-11.7(17)	2715.9(15)	2624.3(15)	19.7(3)
C17	1127.9(16)	2833.6(15)	2839.3(15)	17.9(3)
C18	1838.2(15)	5895.3(13)	3827.7(13)	12.6(3)
C19	2396.4(15)	6979.8(13)	2790.2(14)	14.9(3)
C20	1289.4(17)	8073.1(15)	2781.5(16)	20.4(3)
C21	847.4(18)	8824.0(17)	3863.8(18)	26.3(4)
C22	4199.8(15)	2269.4(14)	320.5(13)	12.6(3)
C23	3856.7(16)	3209.1(14)	-515.1(14)	15.8(3)
C24	2991.4(16)	2983.6(15)	-1036.8(14)	18.1(3)

C25	2448.5(16)	1848.6(15)	-718.5(14)	17.2(3)
C26	2825.7(17)	913.7(15)	112.1(14)	18.3(3)
C27	3695.3(17)	1114.0(14)	633.4(14)	16.8(3)
C28	1459.8(19)	1623.9(18)	-1235.9(17)	25.9(4)

Table S11. Anisotropic Displacement Parameters ($Å^2×10^3$) for 4b. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br1	13.39(8)	12.60(8)	18.14(8)	-2.81(5)	-8.77(6)	-1.33(5)
Cl1	15.89(17)	28.9(2)	23.94(18)	4.30(15)	-12.75(14)	-7.99(14)
S1	9.82(15)	11.04(16)	9.88(15)	-2.60(11)	-1.54(12)	-1.31(12)
O1	13.5(5)	14.5(5)	13.2(5)	-2.1(4)	-1.3(4)	-3.9(4)
O2	12.1(5)	13.5(5)	17.3(5)	-4.0(4)	-3.7(4)	1.5(4)
O3	14.8(5)	11.8(5)	11.0(5)	0.5(4)	-4.1(4)	-1.1(4)
O4	21.5(6)	17.8(5)	12.3(5)	-3.7(4)	-2.2(4)	1.3(4)
N1	10.2(5)	9.5(5)	9.6(5)	-1.6(4)	-2.3(4)	0.6(4)
C1	11.5(6)	12.9(7)	15.2(7)	-2.2(5)	-6.5(5)	-1.3(5)
C2	15.3(7)	15.7(7)	15.9(7)	1.9(5)	-7.6(6)	-3.6(5)
C3	18.7(7)	10.7(7)	24.3(8)	2.7(6)	-13.2(6)	-2.8(5)
C4	16.0(7)	12.2(7)	23.8(8)	-4.0(6)	-11.0(6)	-0.2(5)
C5	13.2(7)	13.4(7)	16.8(7)	-3.5(5)	-7.2(5)	-0.4(5)
C6	10.9(6)	11.6(7)	13.9(7)	0.1(5)	-6.8(5)	-1.7(5)
C7	9.3(6)	11.7(6)	12.5(6)	-1.6(5)	-5.1(5)	-1.2(5)
C8	11.8(6)	12.2(7)	10.8(6)	0.0(5)	-4.3(5)	-1.9(5)
C9	11.7(6)	14.0(7)	12.0(6)	-2.0(5)	-5.0(5)	-0.3(5)
C10	9.8(6)	11.0(6)	12.2(6)	-2.9(5)	-4.1(5)	-1.2(5)
C11	10.9(6)	9.1(6)	10.2(6)	-1.2(5)	-4.2(5)	0.1(5)
C12	9.9(6)	13.7(7)	9.5(6)	-3.6(5)	-2.9(5)	-0.1(5)
C13	15.7(7)	13.0(7)	14.6(7)	-1.5(5)	-6.2(5)	-1.6(5)
C14	15.8(7)	16.4(7)	14.7(6)	-2.2(5)	-8.0(5)	1.3(5)
C15	10.6(7)	22.6(8)	13.9(7)	-2.7(6)	-5.9(5)	-2.4(6)
C16	18.1(7)	19.2(7)	23.7(8)	4.3(6)	-10.9(6)	-8.2(6)
C17	17.4(7)	17.3(7)	20.4(7)	4.2(6)	-11.1(6)	-3.9(6)
C18	12.8(6)	11.0(6)	13.4(6)	-3.5(5)	-4.3(5)	0.6(5)
C19	17.0(7)	11.3(6)	15.7(7)	-1.8(5)	-5.8(6)	-1.1(5)
C20	23.1(8)	13.9(7)	23.6(8)	0.8(6)	-11.0(6)	0.1(6)
C21	22.6(8)	20.4(8)	33.7(9)	-8.9(7)	-9.3(7)	4.9(6)
C22	12.6(6)	14.9(7)	10.3(6)	-4.5(5)	-3.2(5)	-1.1(5)
C23	17.2(7)	14.6(7)	13.2(7)	-2.5(5)	-3.3(6)	-1.8(5)
C24	20.3(8)	19.3(7)	14.1(7)	-1.9(6)	-7.2(6)	0.0(6)

C25	16.4(7)	23.1(8)	12.1(7)	-7.6(6)	-3.6(6)	-0.7(6)
C26	21.5(8)	16.7(7)	17.0(7)	-4.0(6)	-5.8(6)	-5.2(6)
C27	21.8(7)	15.0(7)	14.1(7)	-1.5(5)	-7.3(6)	-2.9(6)
C28	29.7(9)	31.0(9)	24.3(8)	-5.3(7)	-15.6(7)	-6.8(7)

Table S12. Bond Lengths for 4b.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Br1	C10	1.9872(14)	C9	C10	1.5358(19)
Cl1	C15	1.7401(15)	C10	C11	1.5527(18)
S1	O1	1.4321(11)	C10	C18	1.5285(19)
S1	O2	1.4287(11)	C11	C12	1.5320(19)
S1	N1	1.6651(12)	C12	C13	1.396(2)
S1	C22	1.7587(15)	C12	C17	1.392(2)
O3	C1	1.3655(18)	C13	C14	1.388(2)
O3	C8	1.3726(17)	C14	C15	1.380(2)
O4	C9	1.2165(19)	C15	C16	1.386(2)
N1	C7	1.4033(18)	C16	C17	1.387(2)
N1	C11	1.4901(17)	C18	C19	1.5351(19)
C1	C2	1.386(2)	C19	C20	1.533(2)
C1	C6	1.411(2)	C20	C21	1.525(2)
C2	C3	1.384(2)	C22	C23	1.390(2)
C3	C4	1.406(2)	C22	C27	1.392(2)
C4	C5	1.379(2)	C23	C24	1.390(2)
C5	C6	1.412(2)	C24	C25	1.390(2)
C6	C7	1.4542(19)	C25	C26	1.399(2)
C7	C8	1.371(2)	C25	C28	1.506(2)
C8	C9	1.444(2)	C26	C27	1.384(2)

Table S13. Bond Angles for 4b.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	S1	N1	106.34(6)	C11	C10	Br1	107.47(9)
O1	S1	C22	107.97(7)	C18	C10	Br1	108.95(9)
O2	S1	O1	119.67(6)	C18	C10	C9	111.62(11)
O2	S1	N1	106.50(6)	C18	C10	C11	114.26(11)
O2	S1	C22	110.88(7)	N1	C11	C10	110.69(11)
N1	S1	C22	104.30(6)	N1	C11	C12	112.23(11)
C1	O3	C8	105.13(11)	C12	C11	C10	112.94(11)
C7	N1	S1	125.74(10)	C13	C12	C11	118.20(13)
C7	N1	C11	116.72(11)	C17	C12	C11	123.53(13)
C11	N1	S1	116.47(9)	C17	C12	C13	118.19(13)
O3	C1	C2	123.19(13)	C14	C13	C12	121.19(14)
O3	C1	C6	112.41(12)	C15	C14	C13	119.22(14)
C2	C1	C6	124.40(14)	C14	C15	Cl1	119.77(12)
C3	C2	C1	116.70(14)	C14	C15	C16	120.97(14)
C2	C3	C4	120.70(14)	C16	C15	Cl1	119.23(12)
C5	C4	C3	122.01(14)	C15	C16	C17	119.21(14)
C4	C5	C6	118.87(14)	C16	C17	C12	121.21(14)
C1	C6	C5	117.30(13)	C10	C18	C19	115.40(12)
C1	C6	C7	103.69(12)	C20	C19	C18	112.31(12)
C5	C6	C7	139.02(14)	C21	C20	C19	113.77(14)
N1	C7	C6	135.18(13)	C23	C22	S1	118.91(11)
C8	C7	N1	118.37(13)	C23	C22	C27	120.97(14)
C8	C7	C6	106.32(12)	C27	C22	S1	119.86(11)
O3	C8	C9	119.65(12)	C22	C23	C24	119.01(14)
C7	C8	O3	112.45(12)	C25	C24	C23	121.18(14)
C7	C8	C9	127.90(13)	C24	C25	C26	118.56(15)
O4	C9	C8	124.51(13)	C24	C25	C28	121.28(15)
O4	C9	C10	122.89(13)	C26	C25	C28	120.15(15)
C8	C9	C10	112.58(12)	C27	C26	C25	121.19(15)
C9	C10	Br1	101.76(9)	C26	C27	C22	119.05(14)
C9	C10	C11	111.90(11)				

Table S14. Torsion Angles for 4b.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Br1	C10	C11	N1	58.74(12)	C5	C6	C7	C8	-179.15(17)
Br1	C10	C11	C12	-174.47(9)	C6	C1	C2	C3	-0.3(2)
Br1	C10	C18	C19	57.33(14)	C6	C7	C8	O3	-0.65(16)
Cl1	C15	C16	C17	178.31(13)	C6	C7	C8	C9	-179.92(14)
S1	N1	C7	C6	-13.4(2)	C7	N1	C11	C10	48.29(16)
S1	N1	C7	C8	171.39(11)	C7	N1	C11	C12	-78.89(14)
S1	N1	C11	C10	-142.86(10)	C7	C8	C9	O4	179.15(15)
S1	N1	C11	C12	89.96(12)	C7	C8	C9	C10	-2.4(2)
S1	C22	C23	C24	-174.00(11)	C8	O3	C1	C2	-179.70(13)
S1	C22	C27	C26	173.36(12)	C8	O3	C1	C6	0.13(15)
O1	S1	N1	C7	-149.35(12)	C8	C9	C10	Br1	-84.41(12)
O1	S1	N1	C11	42.93(11)	C8	C9	C10	C11	30.05(16)
O1	S1	C22	C23	-14.03(14)	C8	C9	C10	C18	159.53(12)
O1	S1	C22	C27	171.64(12)	C9	C10	C11	N1	-52.16(15)
O2	S1	N1	C7	-20.68(13)	C9	C10	C11	C12	74.63(14)
O2	S1	N1	C11	171.61(10)	C9	C10	C18	C19	168.91(12)
O2	S1	C22	C23	-146.93(11)	C10	C11	C12	C13	91.81(15)
O2	S1	C22	C27	38.73(14)	C10	C11	C12	C17	-91.63(16)
O3	C1	C2	C3	179.53(13)	C10	C18	C19	C20	166.47(12)
O3	C1	C6	C5	179.37(12)	C11	N1	C7	C6	154.29(15)
O3	C1	C6	C7	-0.50(16)	C11	N1	C7	C8	-20.93(18)
O3	C8	C9	O4	-0.1(2)	C11	C10	C18	C19	-62.87(16)
O3	C8	C9	C10	178.38(12)	C11	C12	C13	C14	177.98(13)
O4	C9	C10	Br1	94.07(15)	C11	C12	C17	C16	-177.00(14)
O4	C9	C10	C11	-151.47(14)	C12	C13	C14	C15	-1.3(2)
O4	C9	C10	C18	-22.00(19)	C13	C12	C17	C16	-0.4(2)
N1	S1	C22	C23	98.80(12)	C13	C14	C15	Cl1	-177.53(11)
N1	S1	C22	C27	-75.54(13)	C13	C14	C15	C16	0.5(2)
N1	C7	C8	O3	175.84(12)	C14	C15	C16	C17	0.3(2)
N1	C7	C8	C9	-3.4(2)	C15	C16	C17	C12	-0.3(2)
N1	C11	C12	C13	-142.22(13)	C17	C12	C13	C14	1.2(2)
N1	C11	C12	C17	34.34(18)	C18	C10	C11	N1	179.76(11)
C1	O3	C8	C7	0.34(16)	C18	C10	C11	C12	-53.45(16)

C1	O3	C8	C9	179.68(12)	C18	C19	C20 C21	72.59(17)
C1	C2	C3	C4	1.2(2)	C22	S1	N1 C7	96.66(12)
C1	C6	C7	N1	-174.95(15)	C22	S1	N1 C11	-71.06(11)
C1	C6	C7	C8	0.67(15)	C22	C23	C24 C25	1.2(2)
C2	C1	C6	C5	-0.8(2)	C23	C22	C27 C26	-0.9(2)
C2	C1	C6	C7	179.32(14)	C23	C24	C25 C26	-2.1(2)
C2	C3	C4	C5	-1.0(2)	C23	C24	C25 C28	177.12(15)
C3	C4	C5	C6	-0.2(2)	C24	C25	C26 C27	1.5(2)
C4	C5	C6	C1	1.0(2)	C25	C26	C27 C22	0.0(2)
C4	C5	C6	C7	-179.19(16)	C27	C22	C23 C24	0.3(2)
C5	C6	C7	N1	5.2(3)	C28	C25	C26 C27	-177.73(15)

Table S15. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 4b.

Atom	*x*	*y*	*z*	U(eq)
H2	2551	-878	6747	19
H3	3756	-2580	5663	20
H4	5075	-2247	3519	19
H5	5192	-252	2384	17
H11	3583	4680	1793	12
H13	1695	5632	1333	17
H14	-251	5464	999	18
H16	-443	1968	2944	24
H17	1472	2161	3313	21
H18A	1645	6157	4642	15
H18B	960	5743	3833	15
H19A	3139	7282	2909	18
H19B	2790	6670	1970	18
H20A	1636	8642	1984	24
H20B	481	7741	2814	24
H21A	147	9509	3797	39
H21B	1638	9170	3831	39
H21C	473	8275	4658	39
H23	4208	3994	-727	19
H24	2767	3616	-1621	22
H26	2479	127	322	22
H27	3944	472	1197	20
H28A	523	1773	-625	39
H28B	1640	757	-1405	39
H28C	1573	2196	-2014	39

Table S16. Crystal data and structure refinement for 4c.

Identification code	**4c**
Empirical formula	$C_{28}H_{25}Cl_2NO_4S$
Formula weight	542.45
Temperature/K	100.02(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.7086(4)
b/Å	10.8936(5)
c/Å	11.8325(6)
α/°	78.430(4)
β/°	66.115(4)
γ/°	79.274(3)
Volume/Å^3	1227.97(10)
Z	2
ρ_{calc}g/cm^3	1.467
μ/mm^{-1}	3.481
F(000)	564.0
Crystal size/mm^3	0.2 × 0.1 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.252 to 153.236
Index ranges	-10 ≤ h ≤ 13, -13 ≤ k ≤ 13, -14 ≤ l ≤ 13
Reflections collected	8055
Independent reflections	4967 [R_{int} = 0.0187, R_{sigma} = 0.0297]
Data/restraints/parameters	4967/0/327
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0284, wR_2 = 0.0725
Final R indexes [all data]	R_1 = 0.0310, wR_2 = 0.0747
Largest diff. peak/hole / e Å^{-3}	0.38/-0.33

Table S17. Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for 4c. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	4490.7(3)	4941.3(3)	3649.5(3)	15.26(8)
Cl2	-1951.4(3)	3570.5(3)	1645.9(3)	21.97(9)
S1	5176.5(3)	2585.2(3)	1101.3(3)	11.65(8)
O1	5733.7(10)	3748.3(9)	475.5(9)	15.44(19)
O2	6066.8(10)	1493.7(9)	1314.9(9)	15.8(2)
O3	2513.8(9)	1471.0(9)	5685.9(9)	13.84(19)
O4	1568.8(11)	4033.9(10)	5924.6(10)	20.5(2)
N1	4026.9(11)	2872.5(10)	2500.0(10)	11.4(2)
C1	3170.8(13)	393.2(12)	5179.7(13)	13.2(2)
C2	3088.0(14)	-797.5(13)	5876.1(13)	15.6(3)
C3	3804.8(14)	-1802.8(13)	5234.4(14)	16.9(3)
C4	4591.2(14)	-1601.5(13)	3943.2(14)	16.1(3)
C5	4666.3(13)	-407.8(13)	3262.1(13)	14.5(3)
C6	3927.7(13)	636.7(12)	3885.6(12)	12.4(2)
C7	3684.7(13)	2000.3(12)	3595.2(12)	11.5(2)
C8	2854.5(13)	2431.1(12)	4703.5(12)	12.9(2)
C9	2318.3(13)	3713.9(12)	4914.1(13)	13.4(2)
C10	2828.3(13)	4667.8(12)	3719.6(12)	11.7(2)
C11	3103.5(13)	4079.8(12)	2535.9(12)	11.1(2)
C12	1784.7(13)	3933.8(12)	2382.9(12)	12.2(2)
C13	1269.5(14)	4902.7(12)	1667.8(13)	14.9(3)
C14	103.7(14)	4812.9(13)	1460.2(13)	15.9(3)
C15	-532.7(13)	3724.8(13)	1952.1(13)	15.6(3)
C16	-36.9(15)	2739.2(14)	2655.0(15)	20.9(3)
C17	1118.0(15)	2848.4(14)	2871.0(14)	19.1(3)
C18	1876.0(13)	5906.1(12)	3831.4(13)	13.8(2)
C19	2414.1(14)	6995.3(12)	2787.0(13)	15.5(3)
C20	1286.0(16)	8088.6(13)	2783.9(14)	20.8(3)
C21	851.4(16)	8851.1(15)	3857.9(16)	26.0(3)
C22	4201.4(13)	2261.4(13)	329.2(12)	13.5(2)
C23	3881.5(14)	3200.2(13)	-529.8(13)	16.1(3)
C24	3011.9(15)	2979.4(14)	-1060.4(13)	18.0(3)

C25	2436.4(14)	1849.7(14)	-722.7(13)	17.7(3)
C26	2794.3(15)	915.1(14)	129.8(14)	19.0(3)
C27	3667.6(15)	1107.8(13)	658.2(13)	17.2(3)
C28	1441.2(17)	1634.8(16)	-1251.3(16)	26.2(3)

Table S18. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 4c. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	13.10(15)	14.13(15)	21.20(16)	-3.92(11)	-8.37(12)	-2.05(11)
Cl2	16.67(16)	27.12(18)	26.06(18)	4.51(13)	-13.32(14)	-8.69(13)
S1	9.97(14)	11.22(15)	12.61(15)	-3.03(11)	-2.27(11)	-1.85(11)
O1	14.3(4)	13.5(4)	16.5(5)	-2.5(4)	-2.2(4)	-4.7(4)
O2	12.8(4)	13.9(5)	18.5(5)	-4.1(4)	-3.9(4)	0.8(4)
O3	14.3(4)	11.9(4)	14.2(4)	-0.7(3)	-5.0(4)	-1.1(3)
O4	23.8(5)	18.0(5)	14.7(5)	-4.6(4)	-2.5(4)	0.8(4)
N1	10.5(5)	10.2(5)	12.3(5)	-2.4(4)	-3.4(4)	0.4(4)
C1	11.8(6)	12.4(6)	17.2(6)	-2.8(5)	-7.2(5)	-1.3(5)
C2	15.2(6)	15.2(6)	17.5(6)	1.1(5)	-8.0(5)	-3.9(5)
C3	17.7(6)	11.0(6)	24.8(7)	2.0(5)	-12.5(6)	-3.1(5)
C4	15.3(6)	12.3(6)	23.7(7)	-4.6(5)	-10.5(5)	0.5(5)
C5	12.8(6)	13.2(6)	18.8(7)	-3.7(5)	-6.9(5)	-0.8(5)
C6	10.9(6)	11.8(6)	16.4(6)	-0.8(5)	-7.2(5)	-2.5(5)
C7	9.6(5)	11.5(6)	14.5(6)	-2.0(5)	-5.4(5)	-1.7(4)
C8	12.9(6)	11.6(6)	14.1(6)	0.2(5)	-5.6(5)	-2.0(5)
C9	12.2(6)	14.1(6)	14.5(6)	-3.5(5)	-5.5(5)	-0.7(5)
C10	9.7(5)	11.5(6)	13.8(6)	-3.0(5)	-4.0(5)	-1.4(4)
C11	10.3(6)	9.8(6)	13.0(6)	-2.4(4)	-3.8(5)	-0.9(4)
C12	9.7(6)	13.4(6)	13.5(6)	-4.0(5)	-3.7(5)	-0.7(5)
C13	14.9(6)	12.5(6)	16.9(6)	-1.6(5)	-5.6(5)	-2.2(5)
C14	15.6(6)	15.4(6)	16.9(6)	-1.3(5)	-8.0(5)	0.5(5)
C15	10.7(6)	20.9(7)	16.2(6)	-2.9(5)	-6.1(5)	-2.1(5)
C16	18.3(7)	19.1(7)	27.2(8)	5.0(6)	-11.8(6)	-8.5(5)
C17	18.4(7)	17.1(7)	24.1(7)	4.8(5)	-12.7(6)	-5.2(5)
C18	13.3(6)	11.1(6)	15.8(6)	-3.7(5)	-4.3(5)	0.4(5)
C19	17.0(6)	12.1(6)	16.8(6)	-2.1(5)	-5.3(5)	-2.6(5)
C20	23.5(7)	14.0(6)	24.3(7)	0.9(5)	-11.0(6)	-0.4(5)
C21	21.8(7)	19.2(7)	35.0(9)	-9.3(6)	-8.6(6)	3.5(6)
C22	12.6(6)	15.6(6)	12.3(6)	-5.8(5)	-3.0(5)	-1.5(5)
C23	16.7(6)	14.4(6)	15.3(6)	-2.4(5)	-3.7(5)	-2.8(5)
C24	20.4(7)	17.8(6)	14.9(6)	-2.0(5)	-7.0(5)	0.1(5)

C25	16.4(6)	21.7(7)	15.5(6)	-7.2(5)	-4.7(5)	-1.7(5)
C26	22.4(7)	17.5(7)	18.3(7)	-4.0(5)	-6.5(6)	-6.7(5)
C27	21.2(7)	14.2(6)	16.7(6)	-2.0(5)	-7.5(5)	-3.0(5)
C28	28.6(8)	31.7(8)	25.7(8)	-5.8(6)	-15.4(7)	-7.5(6)

Table S19. Bond Lengths for 4c.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C10	1.8256(13)	C9	C10	1.5404(18)
Cl2	C15	1.7416(13)	C10	C11	1.5538(17)
S1	O1	1.4342(10)	C10	C18	1.5256(17)
S1	O2	1.4280(10)	C11	C12	1.5345(17)
S1	N1	1.6634(11)	C12	C13	1.3918(18)
S1	C22	1.7574(13)	C12	C17	1.3956(19)
O3	C1	1.3659(16)	C13	C14	1.3899(19)
O3	C8	1.3745(16)	C14	C15	1.3824(19)
O4	C9	1.2170(17)	C15	C16	1.383(2)
N1	C7	1.4027(17)	C16	C17	1.3899(19)
N1	C11	1.4879(16)	C18	C19	1.5352(18)
C1	C2	1.3872(19)	C19	C20	1.5311(19)
C1	C6	1.4086(19)	C20	C21	1.524(2)
C2	C3	1.383(2)	C22	C23	1.3896(19)
C3	C4	1.409(2)	C22	C27	1.3959(19)
C4	C5	1.3831(19)	C23	C24	1.392(2)
C5	C6	1.4119(18)	C24	C25	1.393(2)
C6	C7	1.4547(17)	C25	C26	1.399(2)
C7	C8	1.3704(18)	C25	C28	1.508(2)
C8	C9	1.4386(18)	C26	C27	1.382(2)

Table S20. Bond Angles for 4c.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	S1	N1	106.46(6)	C11	C10	Cl1	107.20(8)
O1	S1	C22	107.70(6)	C18	C10	Cl1	109.27(9)
O2	S1	O1	119.75(6)	C18	C10	C9	111.35(11)
O2	S1	N1	106.27(6)	C18	C10	C11	113.79(11)
O2	S1	C22	110.96(6)	N1	C11	C10	110.58(10)
N1	S1	C22	104.57(6)	N1	C11	C12	112.19(10)
C1	O3	C8	105.11(10)	C12	C11	C10	113.38(10)
C7	N1	S1	125.94(9)	C13	C12	C11	118.42(11)
C7	N1	C11	116.72(10)	C13	C12	C17	118.37(12)
C11	N1	S1	116.28(9)	C17	C12	C11	123.12(12)
O3	C1	C2	123.10(12)	C14	C13	C12	121.31(12)
O3	C1	C6	112.28(11)	C15	C14	C13	119.02(13)
C2	C1	C6	124.62(13)	C14	C15	Cl2	119.59(11)
C3	C2	C1	116.61(13)	C14	C15	C16	121.06(13)
C2	C3	C4	120.68(12)	C16	C15	Cl2	119.33(11)
C5	C4	C3	122.02(13)	C15	C16	C17	119.34(13)
C4	C5	C6	118.69(13)	C16	C17	C12	120.88(13)
C1	C6	C5	117.36(12)	C10	C18	C19	115.47(11)
C1	C6	C7	103.97(11)	C20	C19	C18	112.25(11)
C5	C6	C7	138.67(13)	C21	C20	C19	113.73(12)
N1	C7	C6	135.30(12)	C23	C22	S1	119.17(10)
C8	C7	N1	118.44(12)	C23	C22	C27	120.91(13)
C8	C7	C6	106.12(11)	C27	C22	S1	119.71(11)
O3	C8	C9	119.68(12)	C22	C23	C24	119.08(13)
C7	C8	O3	112.51(11)	C23	C24	C25	121.12(13)
C7	C8	C9	127.79(12)	C24	C25	C26	118.46(13)
O4	C9	C8	124.57(13)	C24	C25	C28	121.12(14)
O4	C9	C10	122.66(12)	C26	C25	C28	120.42(13)
C8	C9	C10	112.75(11)	C27	C26	C25	121.40(13)
C9	C10	Cl1	103.05(8)	C26	C27	C22	118.99(13)
C9	C10	C11	111.52(10)				

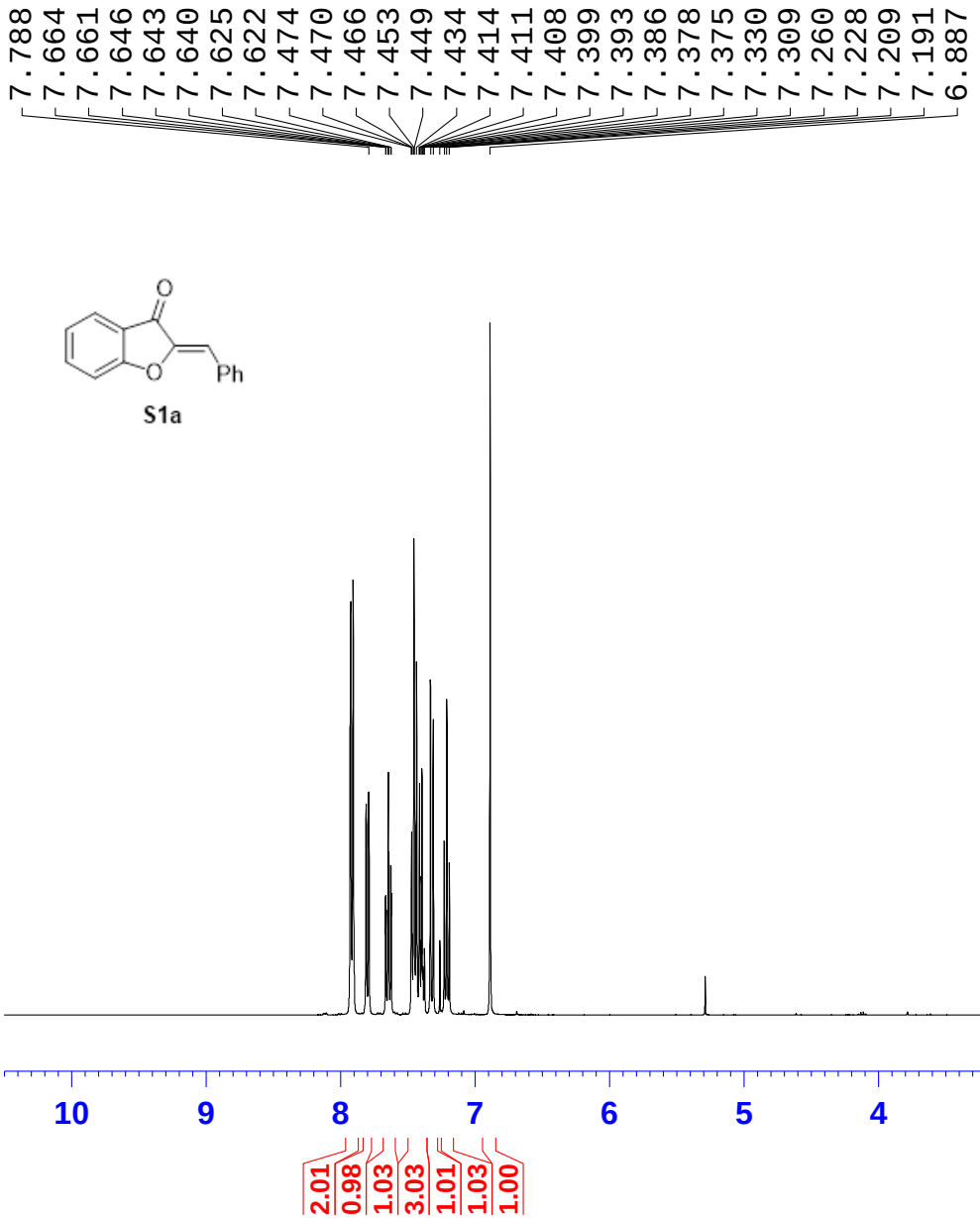
Table S21. Torsion Angles for 4c.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cl1	C10	C11	N1	59.61(11)	C5	C6	C7	C8	-178.62(15)
Cl1	C10	C11	C12	-173.39(9)	C6	C1	C2	C3	-0.2(2)
Cl1	C10	C18	C19	56.99(13)	C6	C7	C8	O3	-1.10(15)
Cl2	C15	C16	C17	178.26(12)	C6	C7	C8	C9	-179.79(12)
S1	N1	C7	C6	-13.7(2)	C7	N1	C11	C10	48.64(14)
S1	N1	C7	C8	171.23(10)	C7	N1	C11	C12	-79.02(14)
S1	N1	C11	C10	-142.44(9)	C7	C8	C9	O4	179.07(14)
S1	N1	C11	C12	89.90(11)	C7	C8	C9	C10	-2.64(19)
S1	C22	C23	C24	-174.54(10)	C8	O3	C1	C2	179.87(12)
S1	C22	C27	C26	173.80(11)	C8	O3	C1	C6	-0.21(14)
O1	S1	N1	C7	-149.51(10)	C8	C9	C10	Cl1	-84.30(11)
O1	S1	N1	C11	42.73(10)	C8	C9	C10	C11	30.38(15)
O1	S1	C22	C23	-12.40(13)	C8	C9	C10	C18	158.67(11)
O1	S1	C22	C27	172.76(11)	C9	C10	C11	N1	-52.48(13)
O2	S1	N1	C7	-20.81(12)	C9	C10	C11	C12	74.52(13)
O2	S1	N1	C11	171.43(9)	C9	C10	C18	C19	170.17(11)
O2	S1	C22	C23	-145.24(11)	C10	C11	C12	C13	92.81(14)
O2	S1	C22	C27	39.91(13)	C10	C11	C12	C17	-90.69(15)
O3	C1	C2	C3	179.75(12)	C10	C18	C19	C20	166.25(11)
O3	C1	C6	C5	179.21(11)	C11	N1	C7	C6	154.05(14)
O3	C1	C6	C7	-0.43(14)	C11	N1	C7	C8	-21.06(17)
O3	C8	C9	O4	0.5(2)	C11	C10	C18	C19	-62.77(15)
O3	C8	C9	C10	178.76(11)	C11	C12	C13	C14	177.99(12)
O4	C9	C10	Cl1	94.02(13)	C11	C12	C17	C16	-176.86(13)
O4	C9	C10	C11	-151.29(13)	C12	C13	C14	C15	-1.5(2)
O4	C9	C10	C18	-23.00(18)	C13	C12	C17	C16	-0.4(2)
N1	S1	C22	C23	100.58(11)	C13	C14	C15	Cl2	-177.32(11)
N1	S1	C22	C27	-74.27(12)	C13	C14	C15	C16	0.8(2)
N1	C7	C8	O3	175.32(10)	C14	C15	C16	C17	0.1(2)
N1	C7	C8	C9	-3.4(2)	C15	C16	C17	C12	-0.4(2)
N1	C11	C12	C13	-141.04(12)	C17	C12	C13	C14	1.3(2)
N1	C11	C12	C17	35.46(18)	C18	C10	C11	N1	-179.46(10)
C1	O3	C8	C7	0.84(14)	C18	C10	C11	C12	-52.46(14)

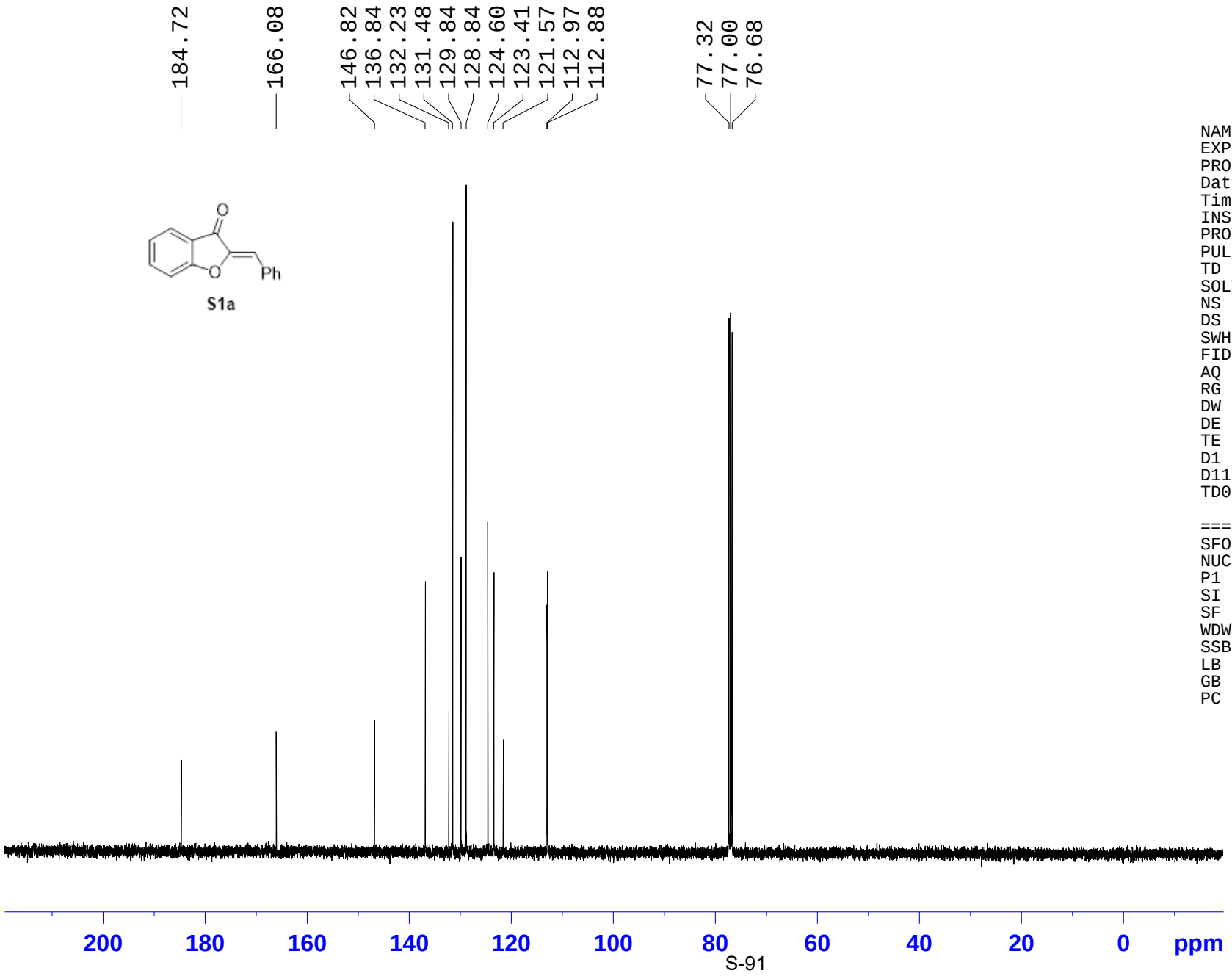
C1	O3	C8	C9	179.64(11)	C18	C19	C20 C21	72.46(16)
C1	C2	C3	C4	1.07(19)	C22	S1	N1 C7	96.64(11)
C1	C6	C7	N1	-174.63(14)	C22	S1	N1 C11	-71.12(10)
C1	C6	C7	C8	0.89(14)	C22	C23	C24 C25	1.5(2)
C2	C1	C6	C5	-0.87(19)	C23	C22	C27 C26	-1.0(2)
C2	C1	C6	C7	179.49(12)	C23	C24	C25 C26	-2.5(2)
C2	C3	C4	C5	-1.0(2)	C23	C24	C25 C28	177.04(13)
C3	C4	C5	C6	-0.1(2)	C24	C25	C26 C27	1.8(2)
C4	C5	C6	C1	0.98(18)	C25	C26	C27 C22	-0.1(2)
C4	C5	C6	C7	-179.56(14)	C27	C22	C23 C24	0.2(2)
C5	C6	C7	N1	5.9(3)	C28	C25	C26 C27	-177.77(14)

Table S22. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 4c.

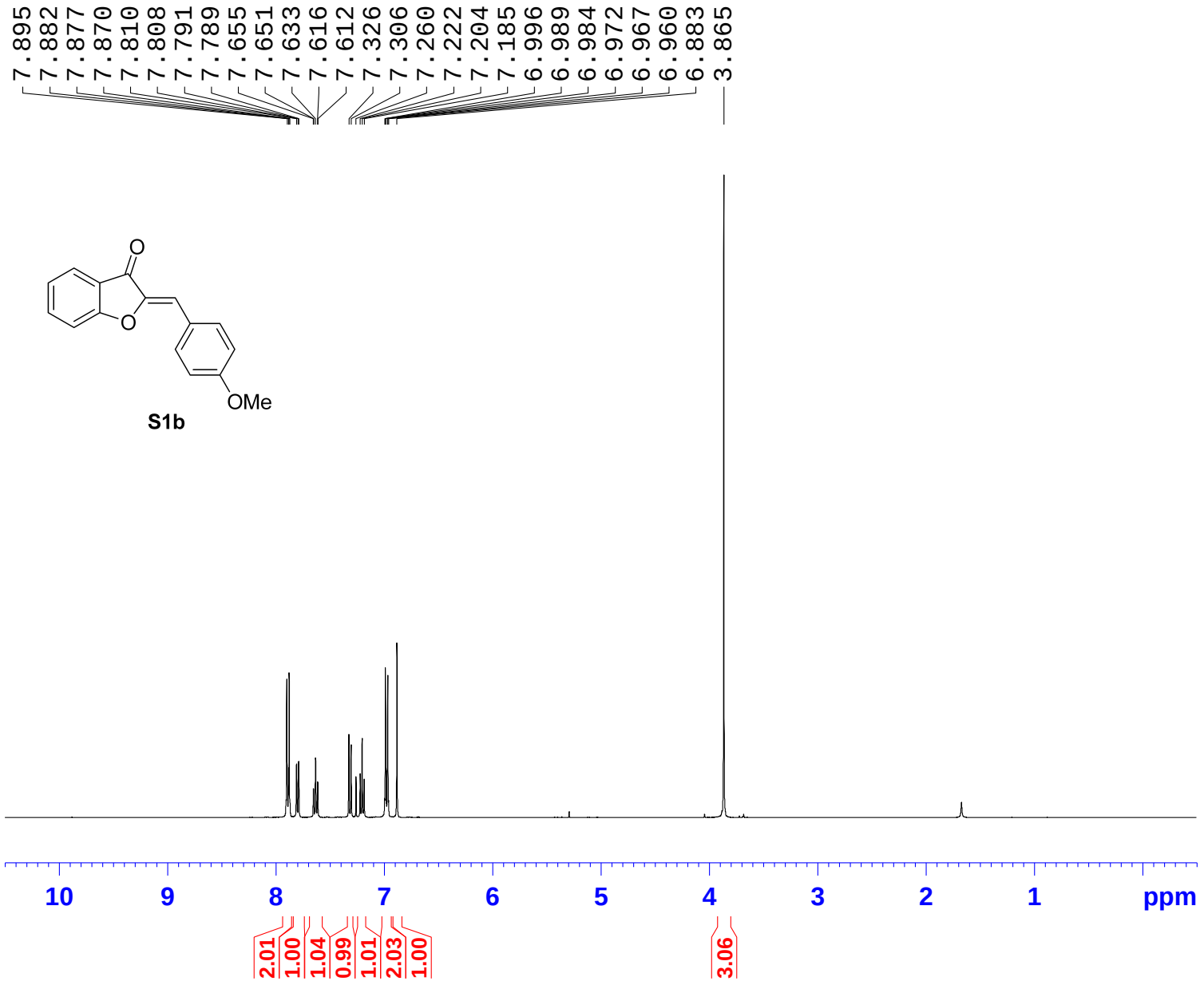
Atom	*x*	*y*	*z*	U(eq)
H2	2566	-917	6749	19
H3	3766	-2638	5669	20
H4	5085	-2307	3527	19
H5	5204	-293	2392	17
H11	3613	4678	1801	13
H13	1724	5640	1315	18
H14	-250	5489	987	19
H16	-481	1995	2987	25
H17	1458	2175	3357	23
H18A	1696	6176	4639	17
H18B	986	5748	3850	17
H19A	3165	7308	2894	19
H19B	2800	6678	1971	19
H20A	1618	8659	1985	25
H20B	471	7746	2827	25
H21A	156	9552	3781	39
H21B	1654	9185	3830	39
H21C	465	8306	4653	39
H23	4251	3982	-752	19
H24	2807	3610	-1663	22
H26	2429	131	350	23
H27	3901	465	1237	21
H28A	499	1775	-641	39
H28B	1632	766	-1438	39
H28C	1546	2224	-2019	39



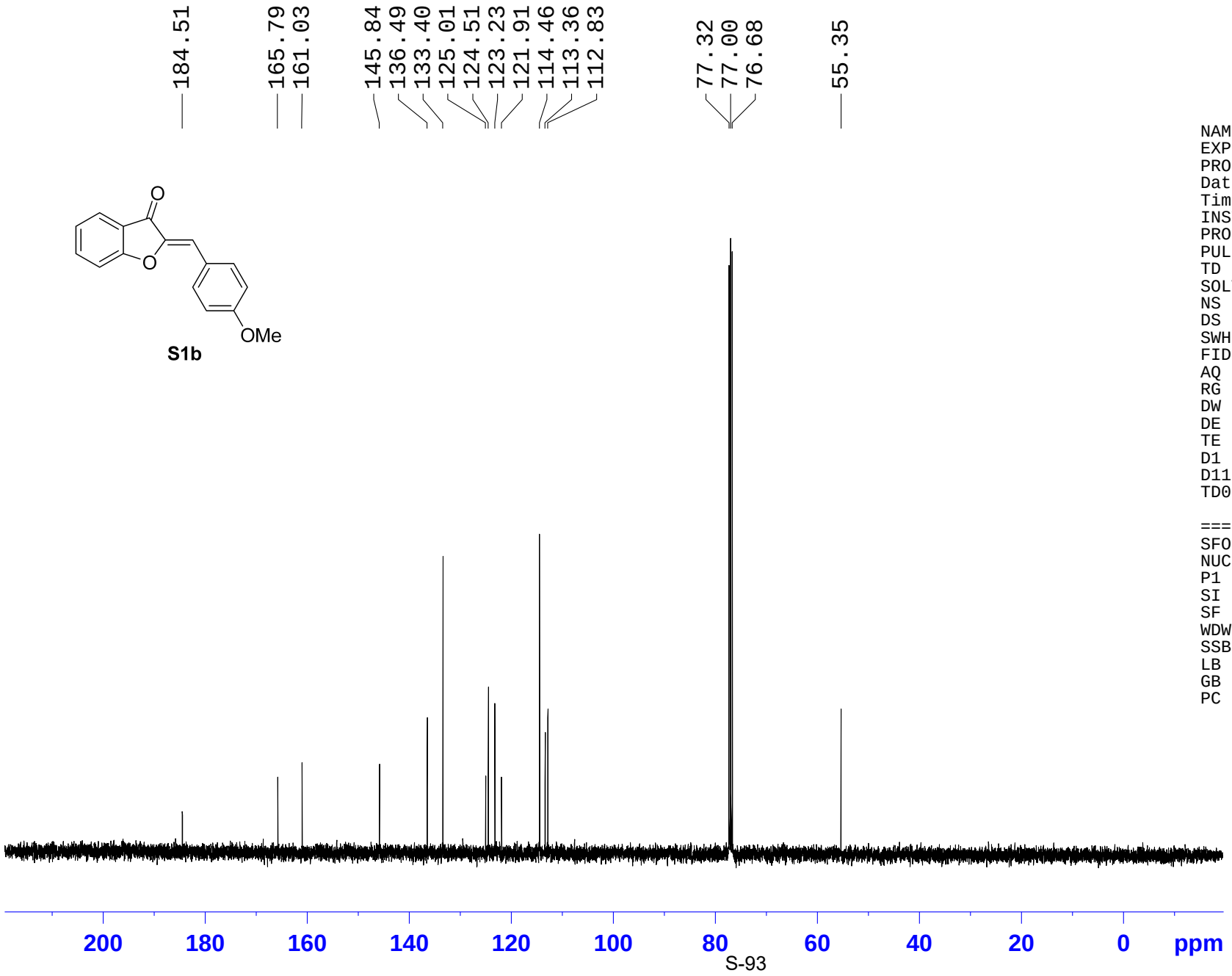

```
NAME            fq4-130
EXPNO                 1
PROCNO                1
Date_          20190120
Time              20.33
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    4
DS                    0
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ           4.0894966 sec
RG                82.92
DW               62.400 usec
DE                6.50 usec
TE                297.0 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                  1H
P1                14.50 usec
SI                65536
SF          400.1300100 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



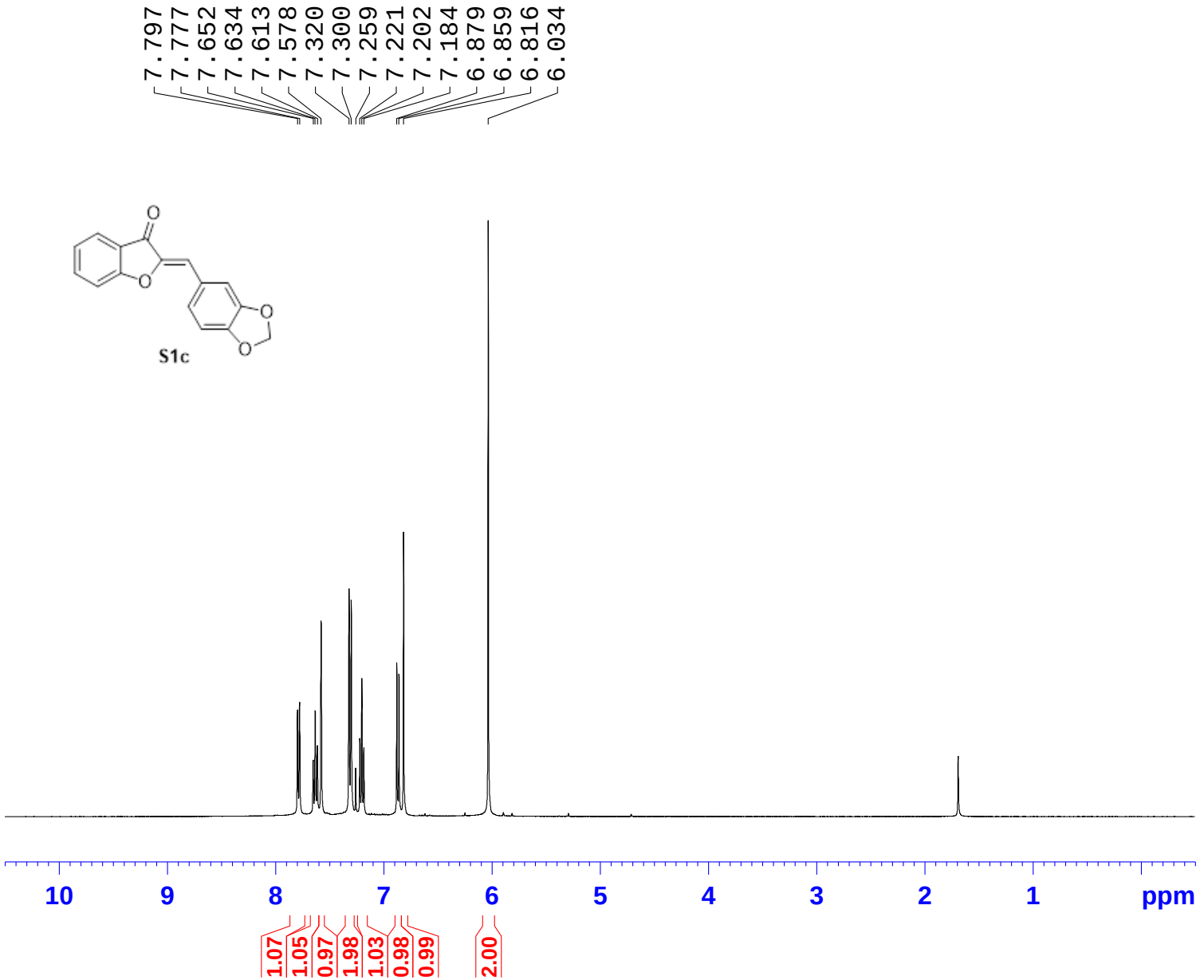
NAME	fq4-130
EXPNO	2
PROCNO	1
Date_	20190120
Time	20.38
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	80
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	297.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127766 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



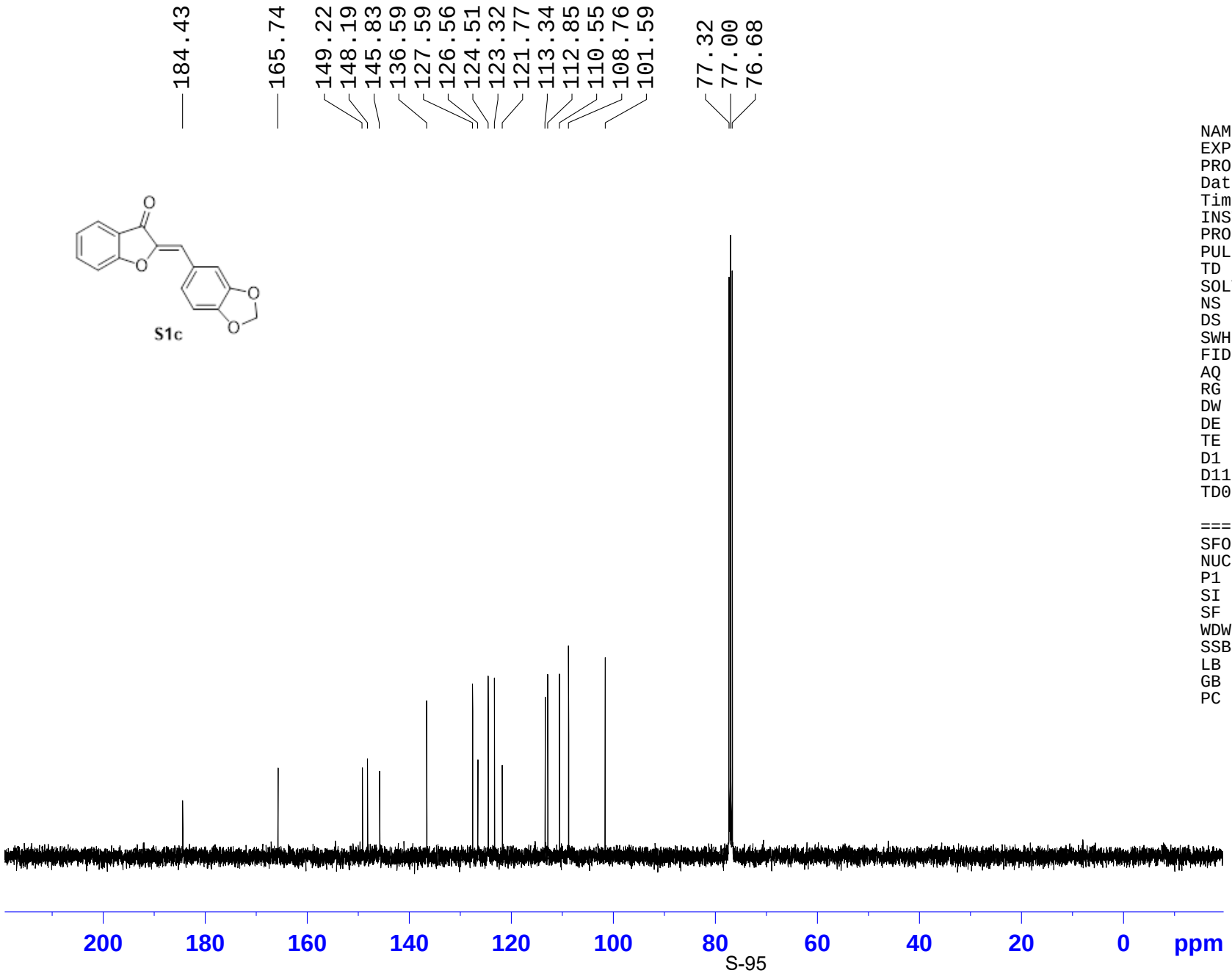
NAME	fq4-131
EXPNO	1
PROCNO	1
Date_	20190120
Time	20.42
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	4
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	126.97
DW	62.400 usec
DE	6.50 usec
TE	297.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	14.50 usec
SI	65536
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



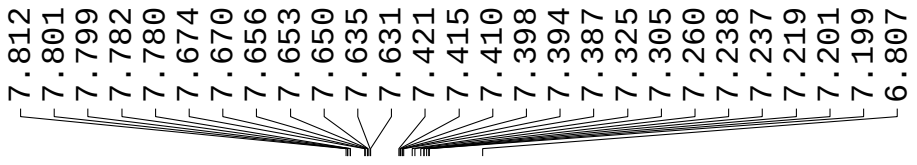

```
NAME            fq4-131
EXPNO                 2
PROCNO                1
Date_          20190120
Time              20.43
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                   60
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               297.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                9.70 usec
SI               32768
SF          100.6127736 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

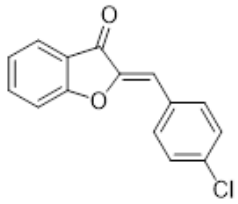



```
NAME            fq4-141
EXPNO                 1
PROCNO                1
Date_          20190130
Time              19.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    4
DS                    0
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ           4.0894966 sec
RG               126.97
DW               62.400 usec
DE                6.50 usec
TE               295.2 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                  1H
P1                14.50 usec
SI                65536
SF          400.1300105 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

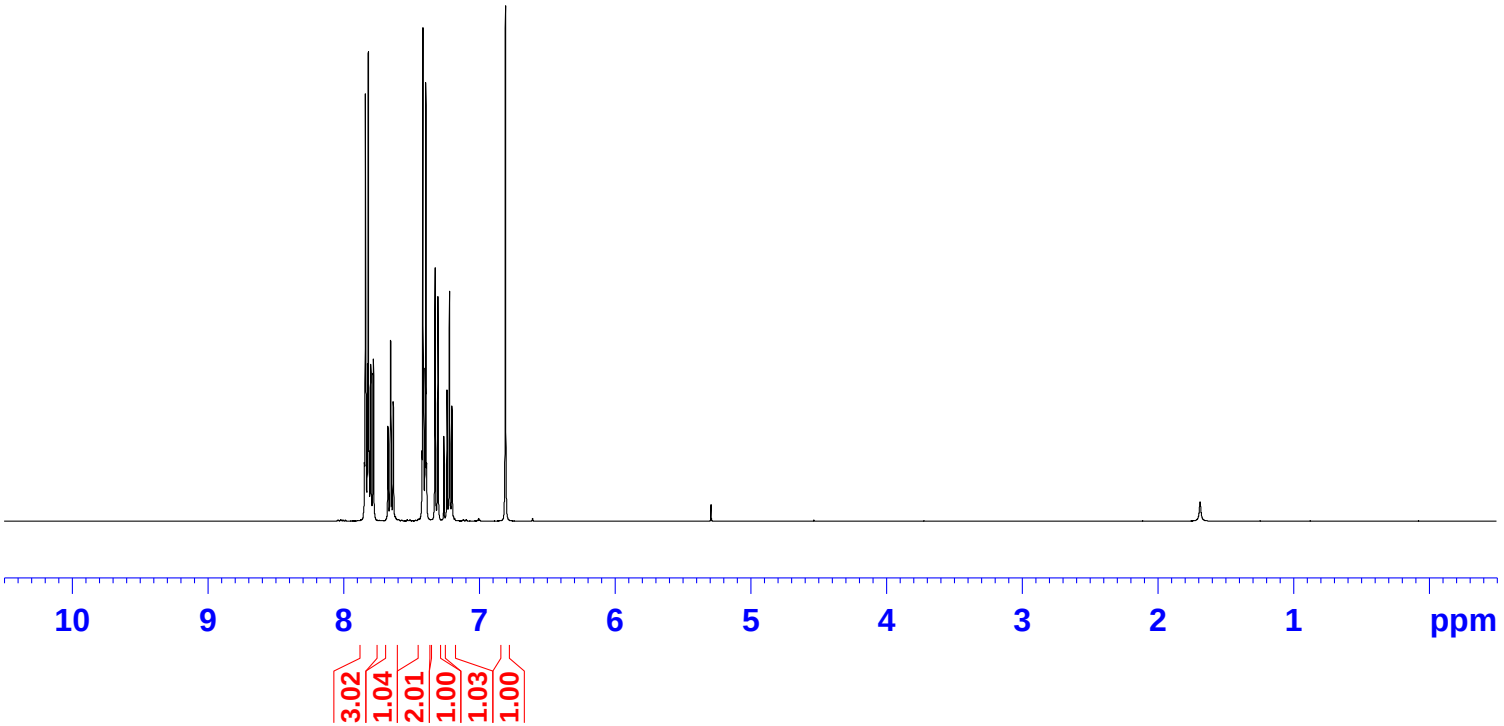


NAME	fq4-141
EXPNO	2
PROCNO	1
Date_	20190130
Time	19.16
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	100
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	296.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127744 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

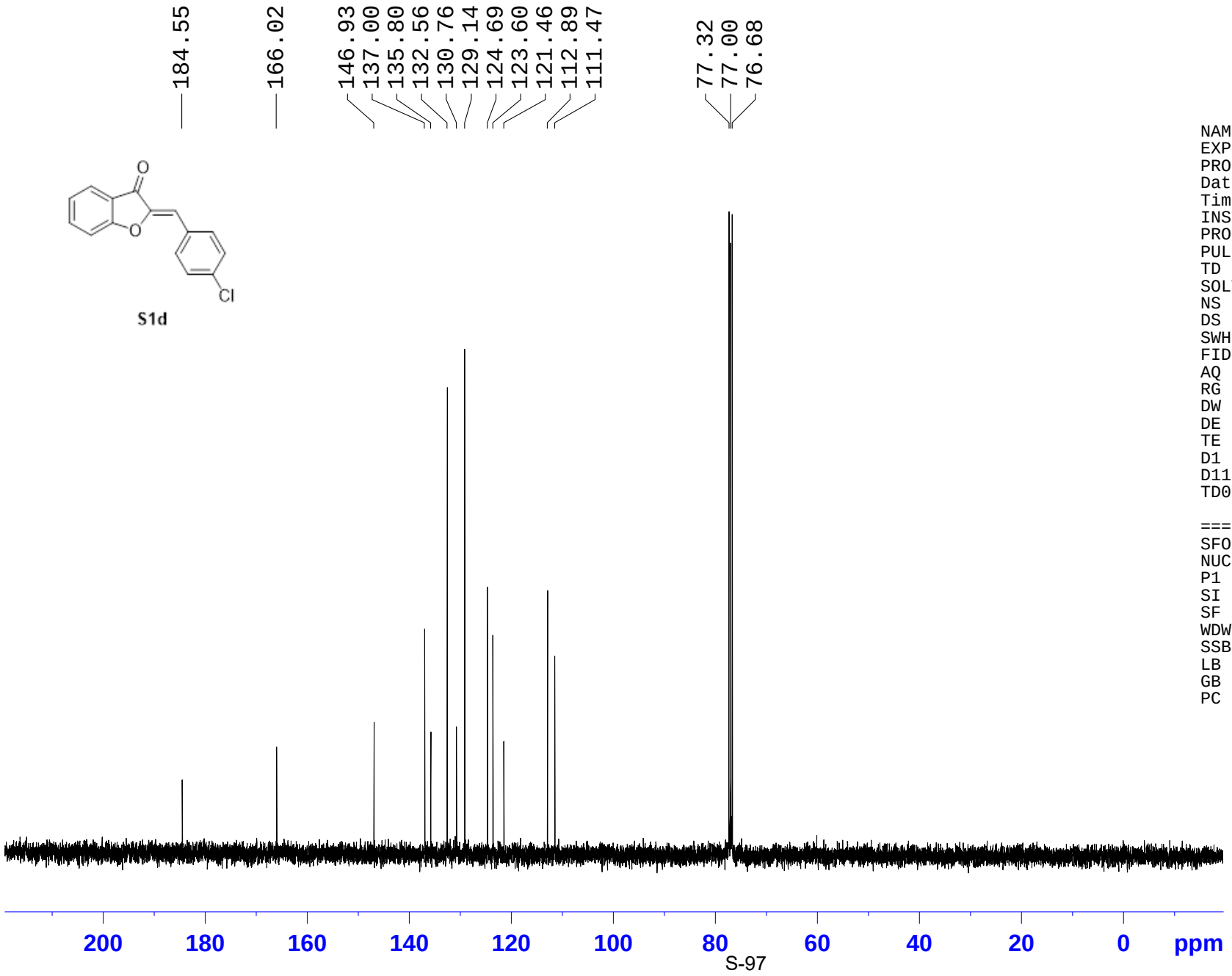




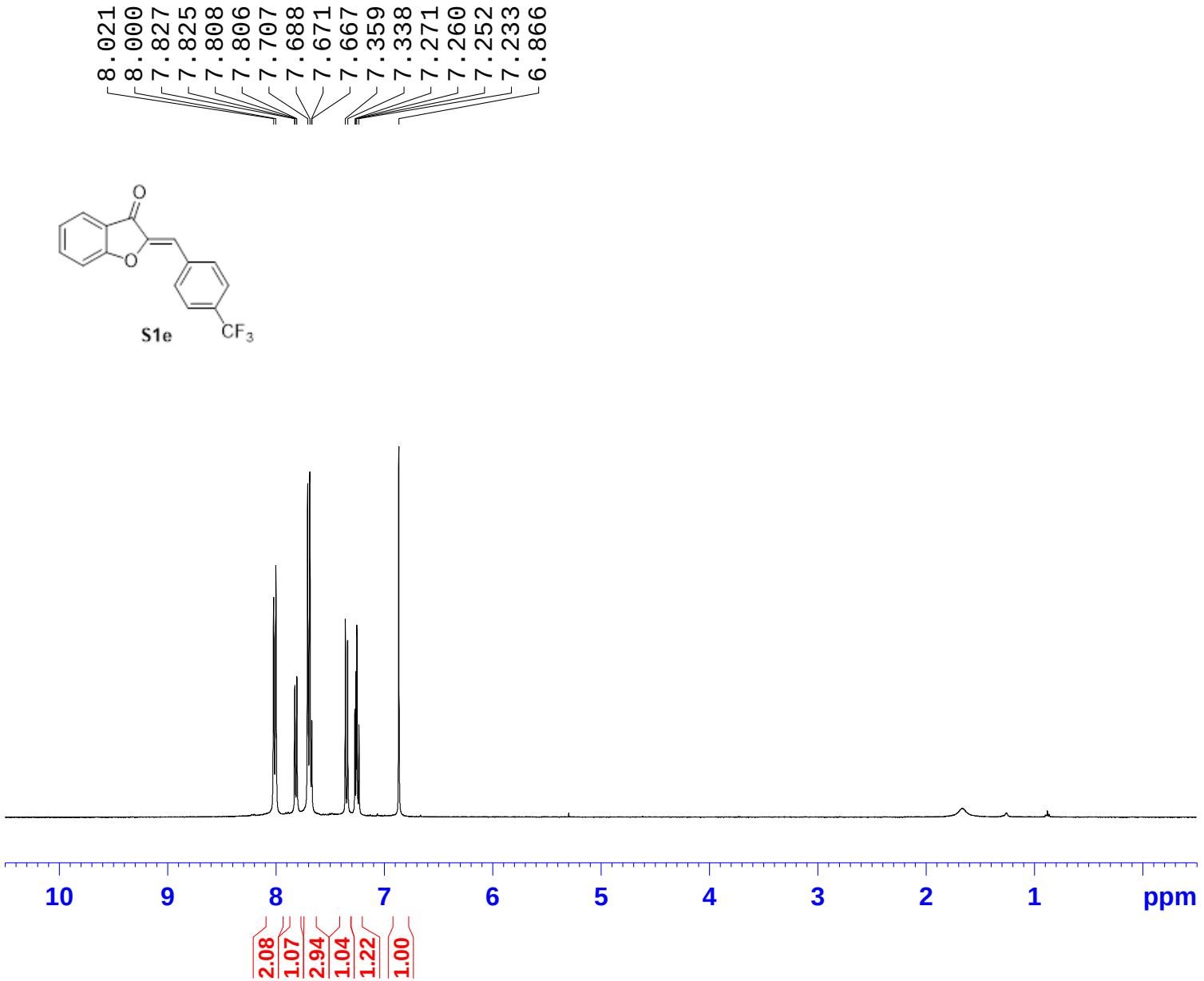
S1d



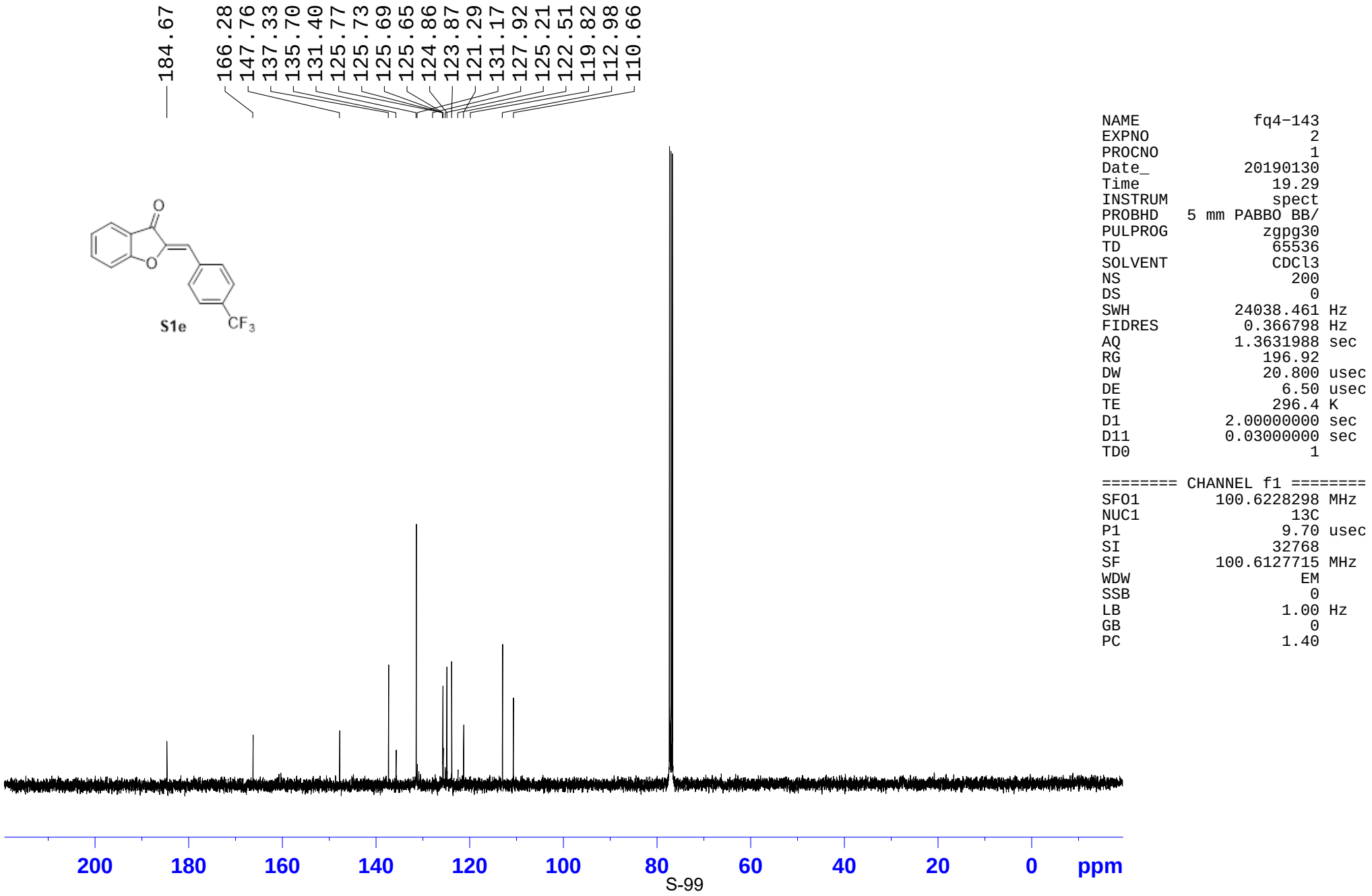
NAME	fq4-132
EXPNO	1
PROCNO	1
Date_	20190120
Time	20.49
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	4
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	126.97
DW	62.400 usec
DE	6.50 usec
TE	297.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	14.50 usec
SI	65536
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



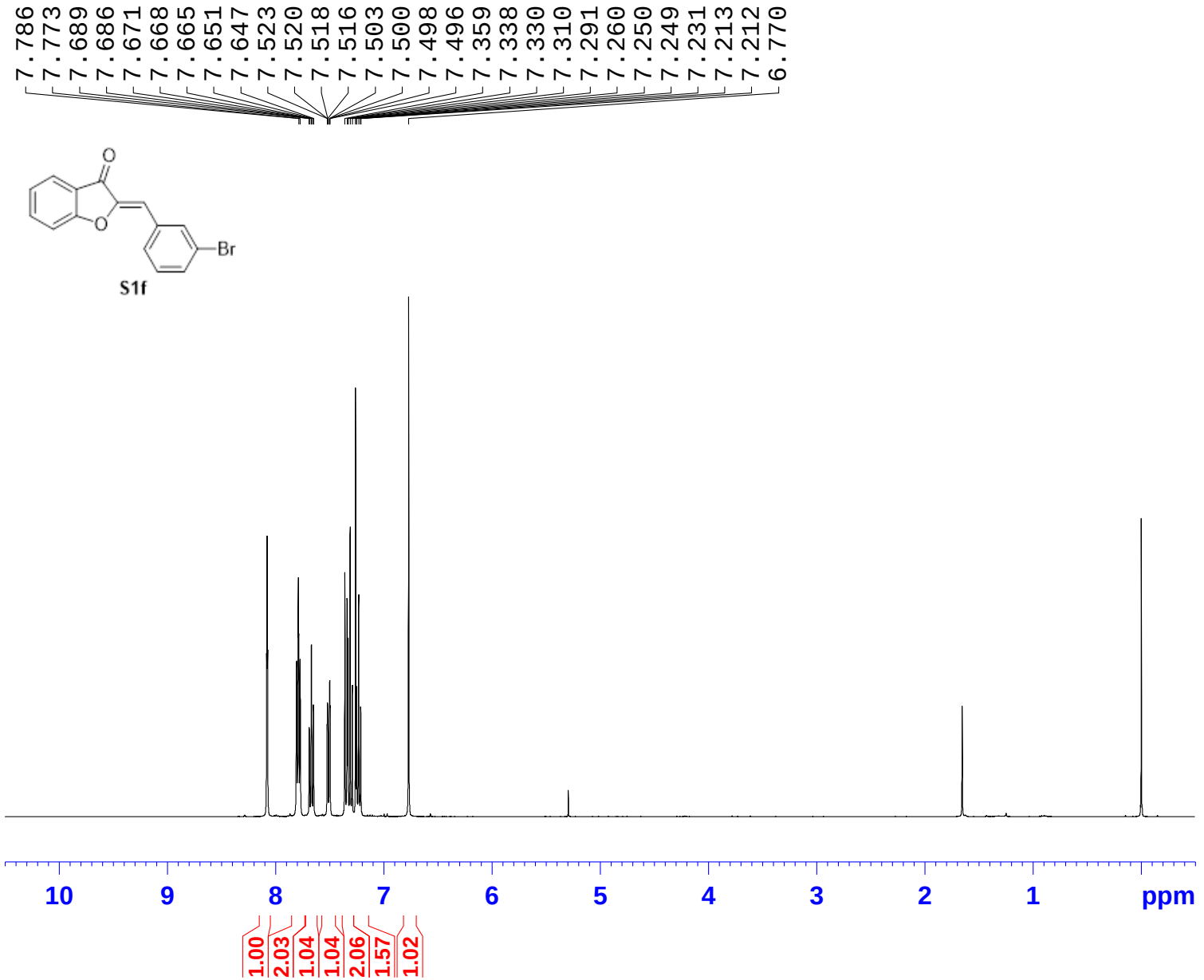

```
NAME            fq4-132
EXPNO                 2
PROCNO                1
Date_          20190120
Time              20.50
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                   40
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               297.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                9.70 usec
SI               32768
SF          100.6127740 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```



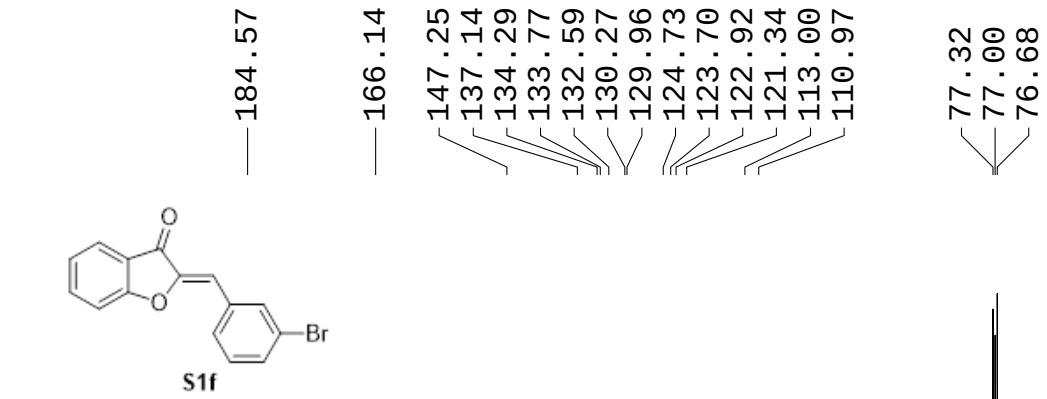

```
NAME            fq4-143
EXPNO                 1
PROCNO                1
Date_          20190130
Time              19.27
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    4
DS                    0
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ           4.0894966 sec
RG              164.33
DW              62.400 usec
DE               6.50 usec
TE              295.7 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                14.50 usec
SI                65536
SF          400.1300103 MHz
WDW                 EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



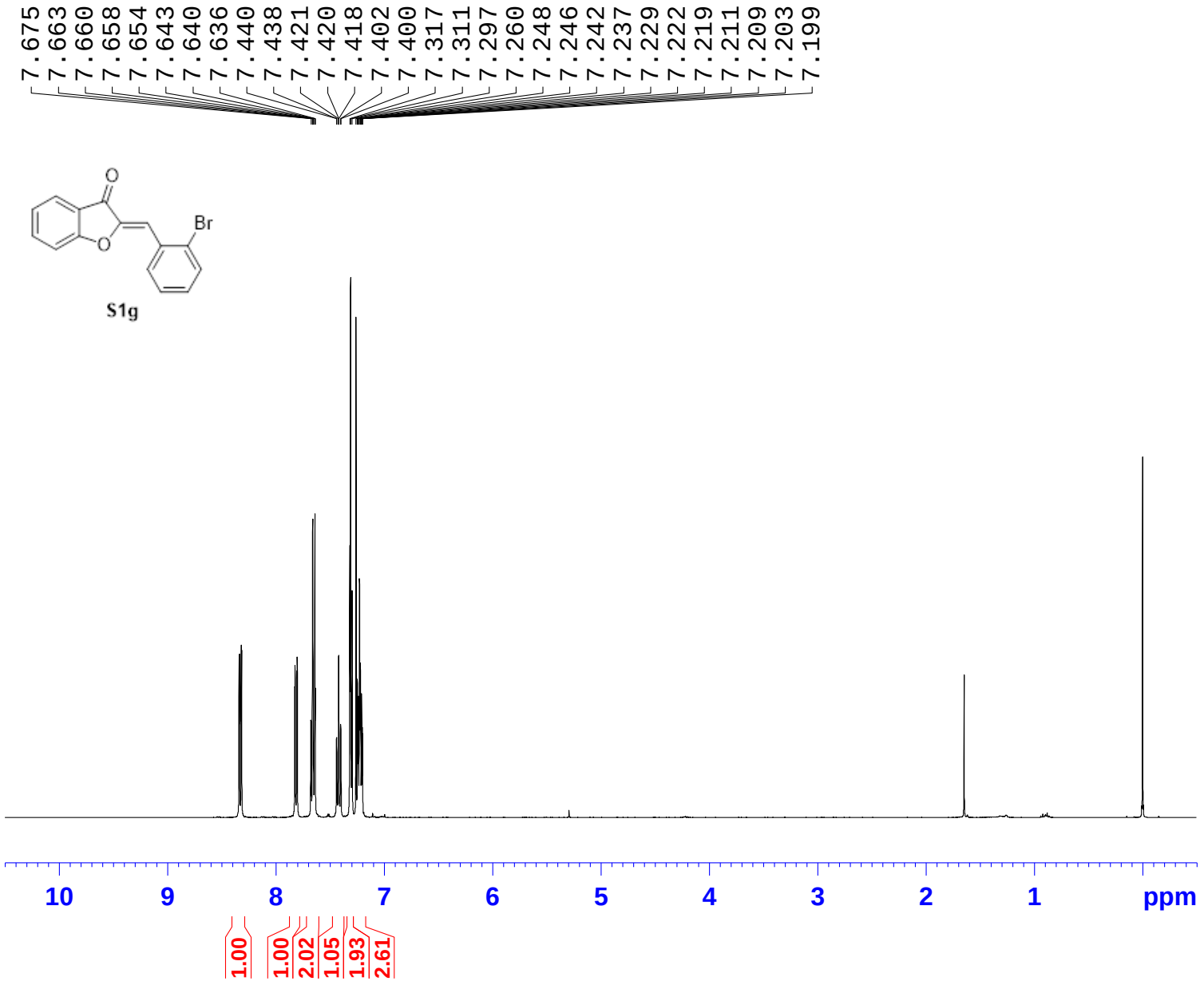

```
NAME            fq4-143
EXPNO                 2
PROCNO                1
Date_          20190130
Time              19.29
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  200
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               296.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                9.70 usec
SI               32768
SF          100.6127715 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```



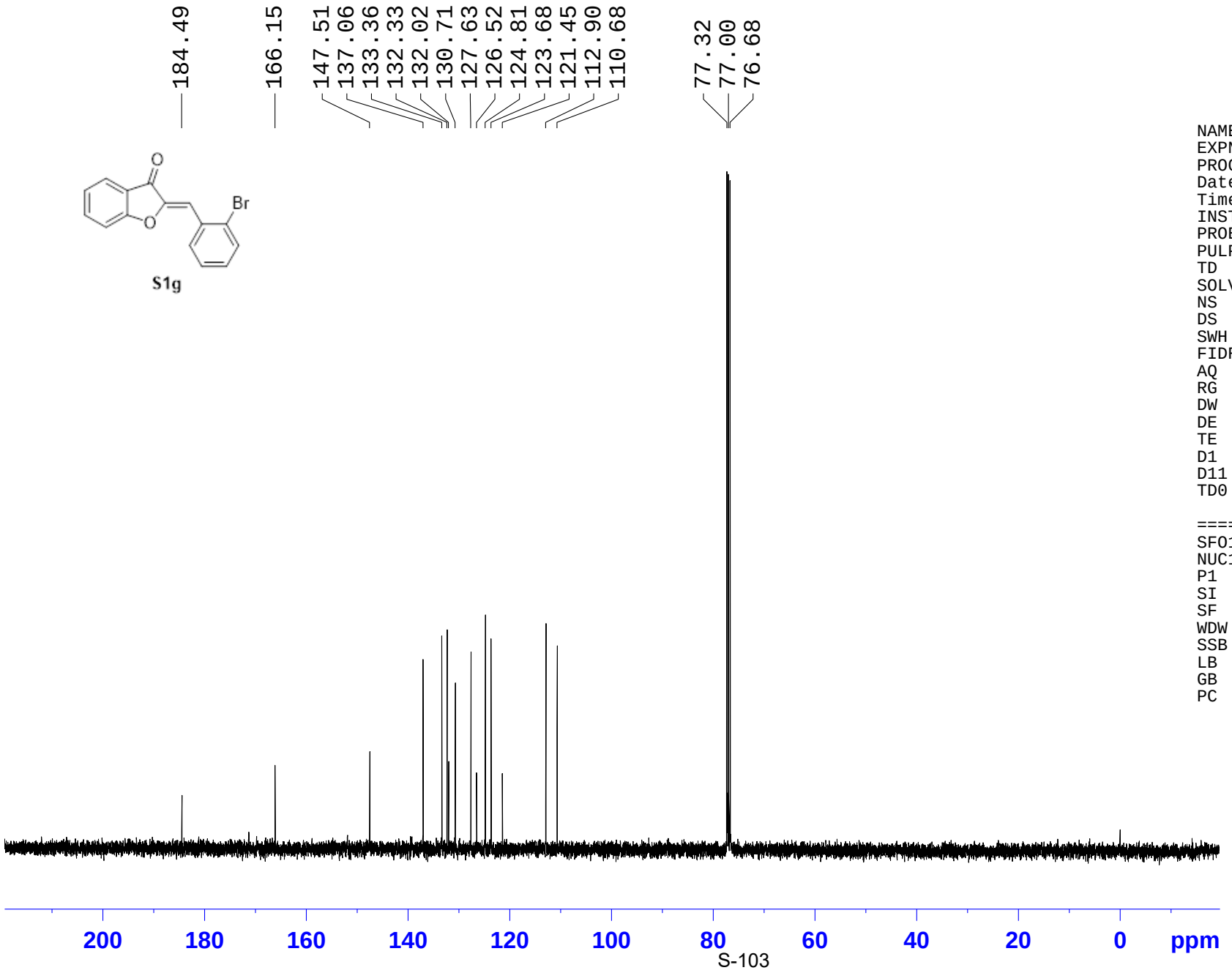

```
NAME                fq5-22
EXPNO                    1
PROCNO                   1
Date_             20190320
Time                 14.18
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ               4.0894966 sec
RG                  112.31
DW                  62.400 usec
DE                   6.50 usec
TE                  296.5 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                   14.50 usec
SI                   65536
SF            400.1300102 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



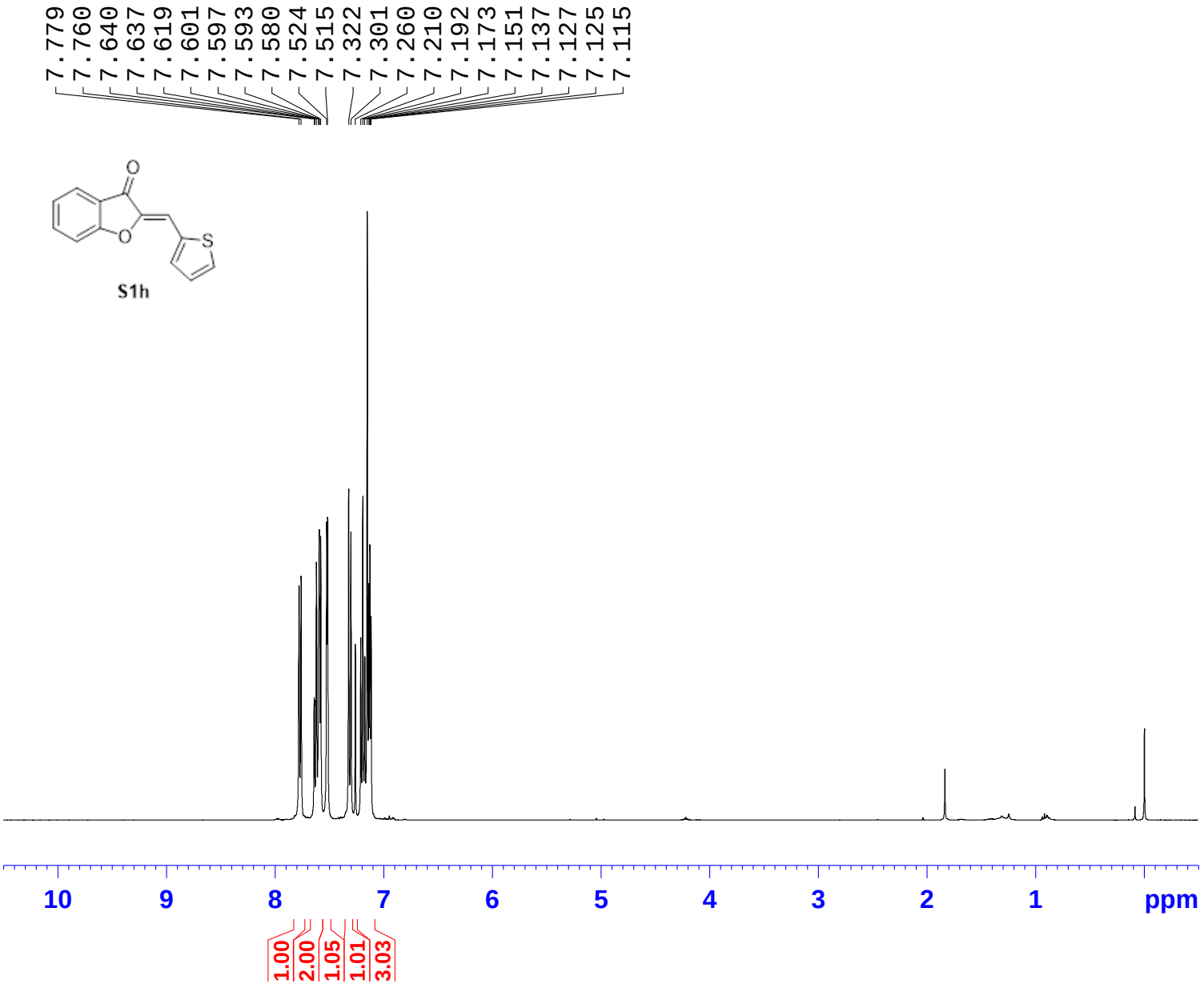

```
NAME                fq5-22
EXPNO                    2
PROCNO                   1
Date_             20190320
Time                 14.20
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       40
DS                        0
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631988 sec
RG                   196.92
DW                   20.800 usec
DE                    6.50 usec
TE                   297.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           100.6228298 MHz
NUC1                    13C
P1                    9.70 usec
SI                   32768
SF             100.6127743 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.40
```



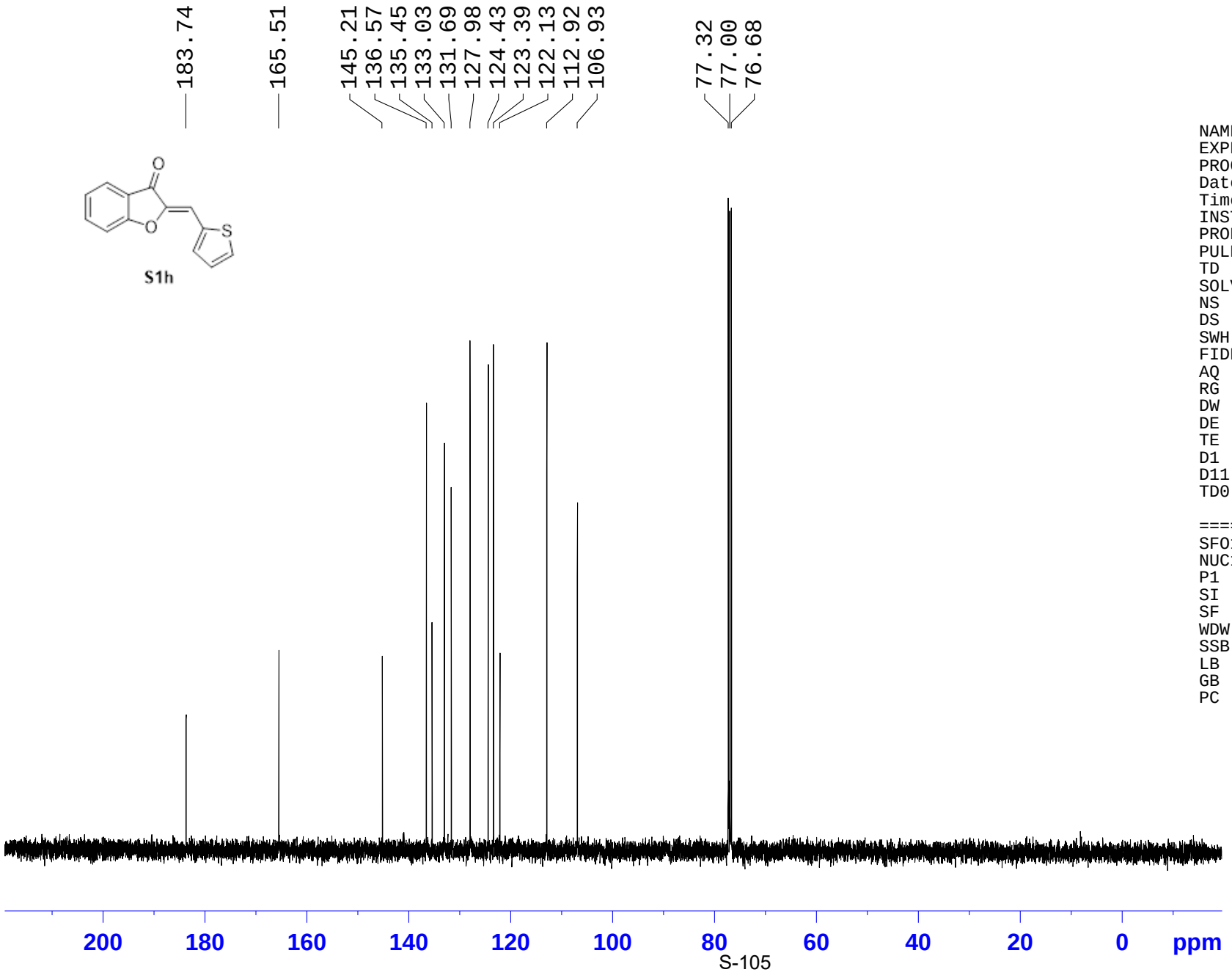

```
NAME                fq5-21
EXPNO                    1
PROCNO                   1
Date_             20190320
Time                 14.11
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ               4.0894966 sec
RG                  126.97
DW                  62.400 usec
DE                   6.50 usec
TE                  296.4 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                   14.50 usec
SI                   65536
SF            400.1300101 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



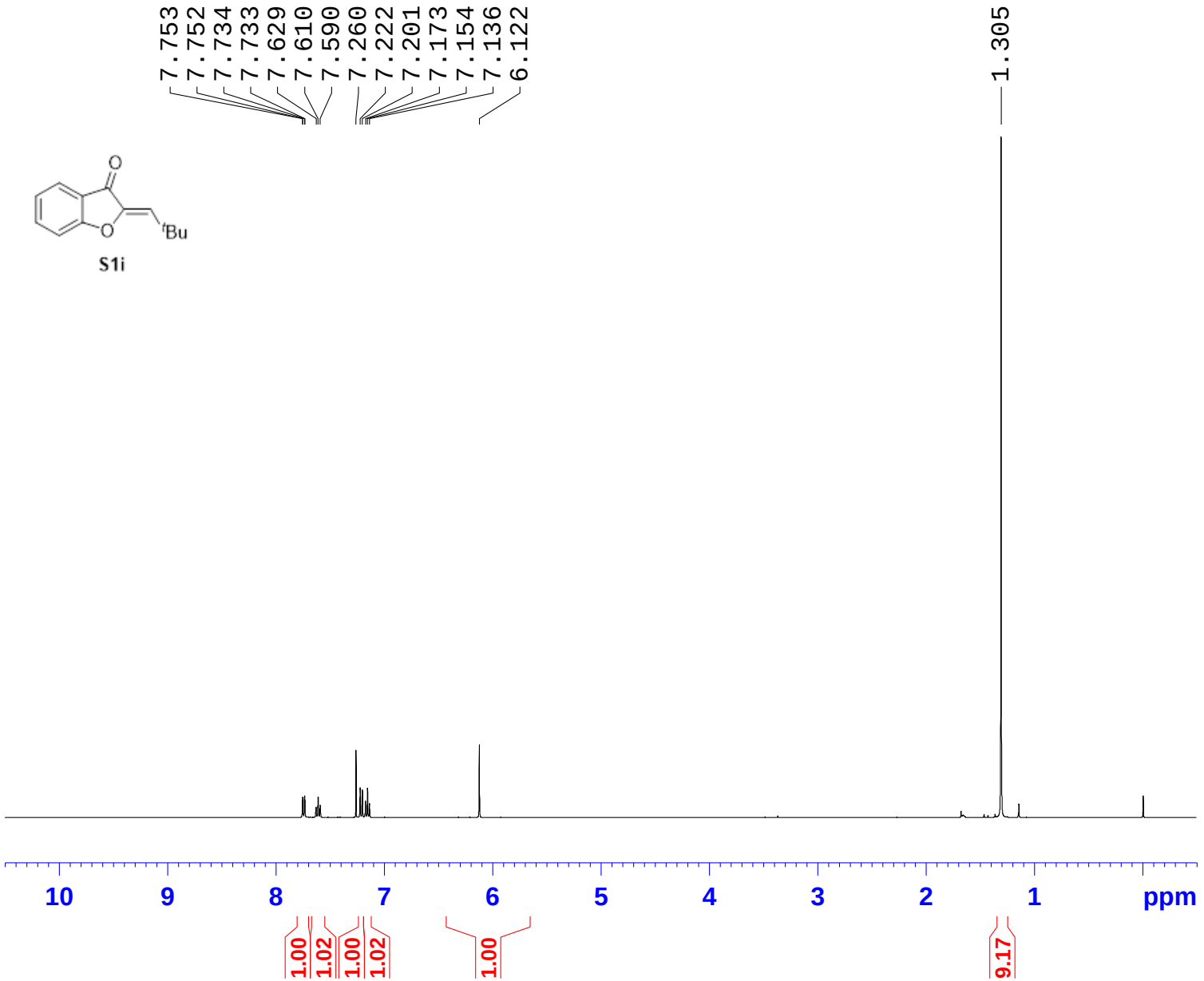
NAME	fq5-21
EXPNO	2
PROCNO	1
Date_	20190320
Time	14.14
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	60
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	297.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127736 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



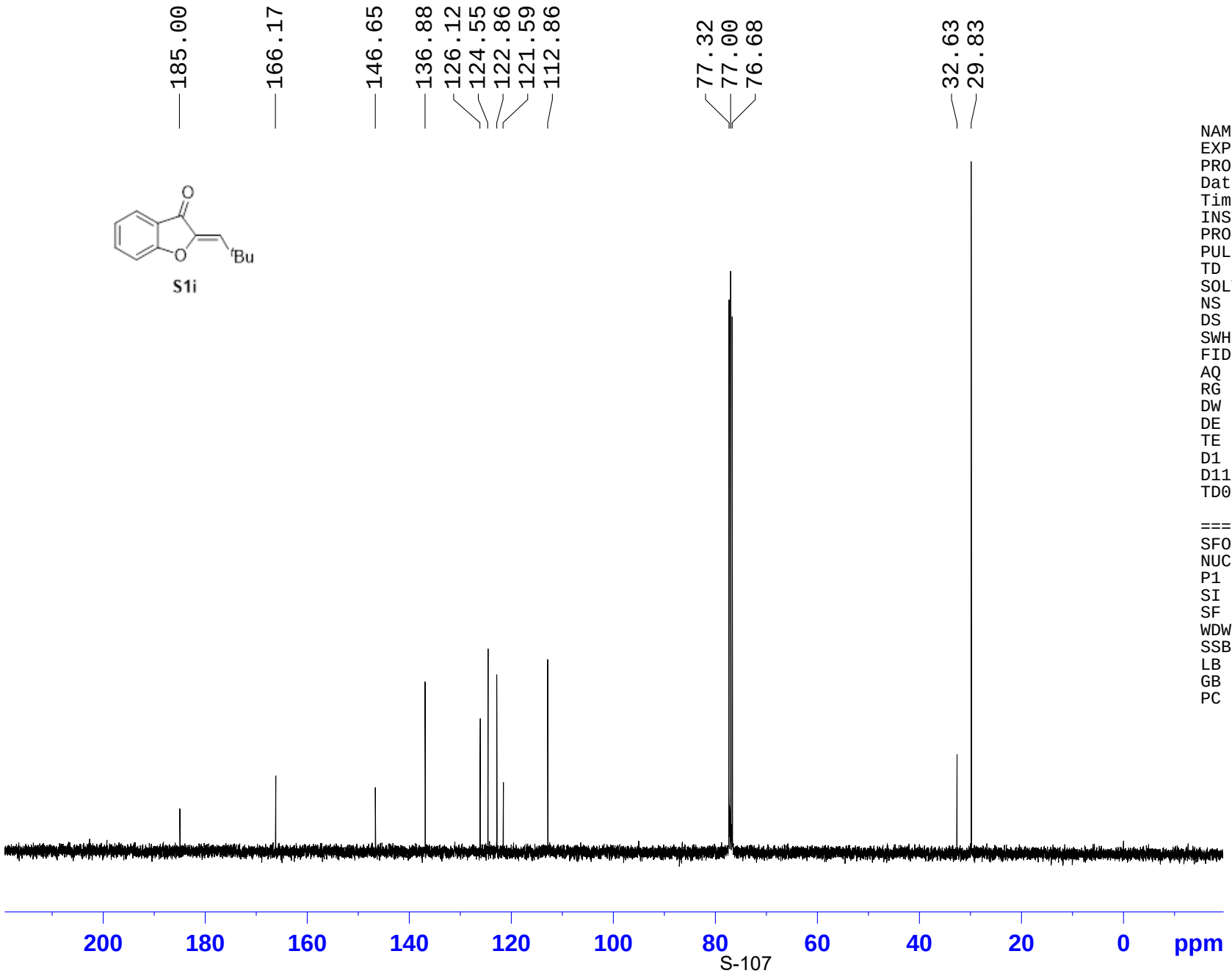

```
NAME                fq5-31
EXPNO                    1
PROCNO                   1
Date_             20190323
Time                 15.23
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ               4.0894966 sec
RG                   82.92
DW                   62.400 usec
DE                    6.50 usec
TE                   295.7 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                   14.50 usec
SI                   65536
SF            400.1300101 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



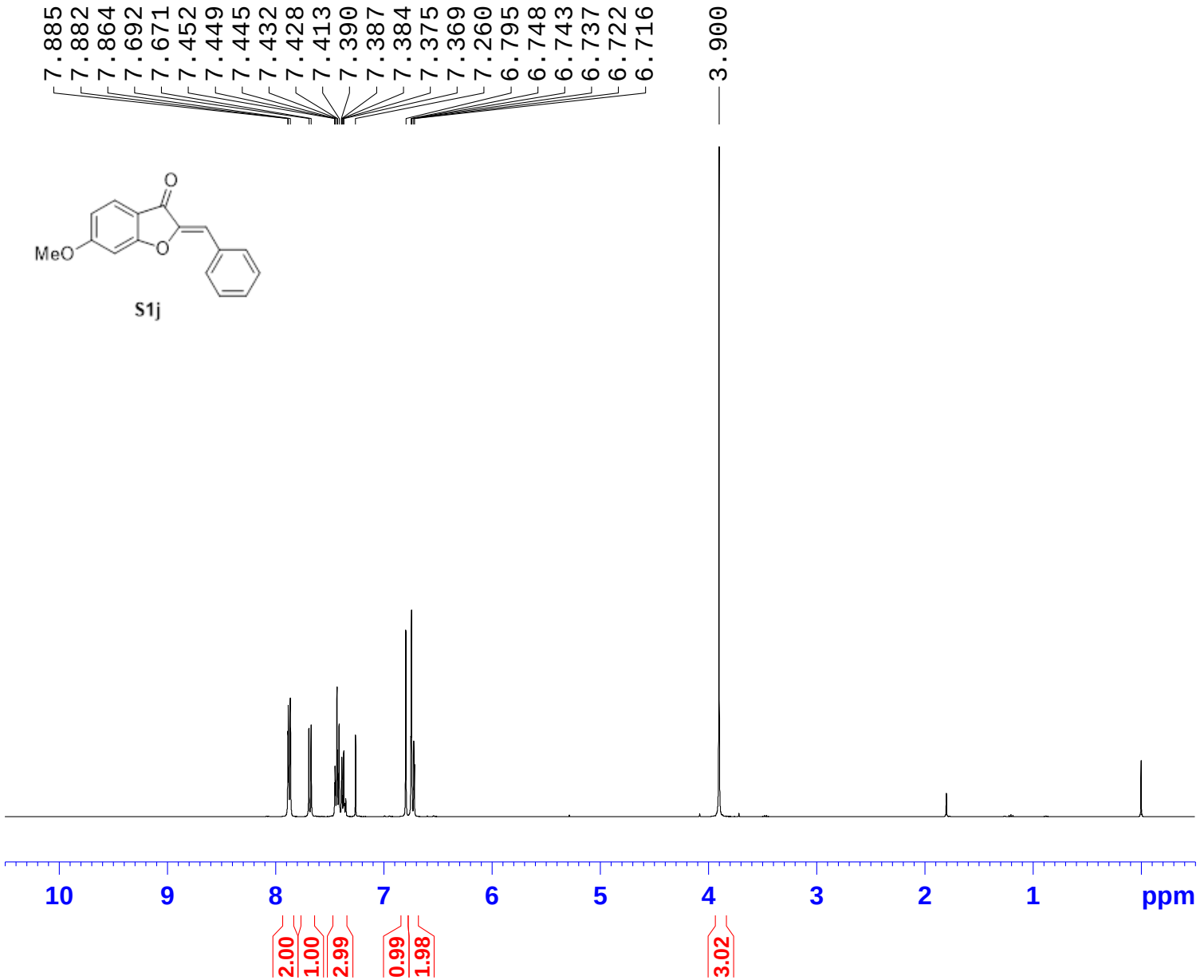
NAME	fq5-31
EXPNO	2
PROCNO	1
Date_	20190323
Time	15.25
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	40
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	296.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127785 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



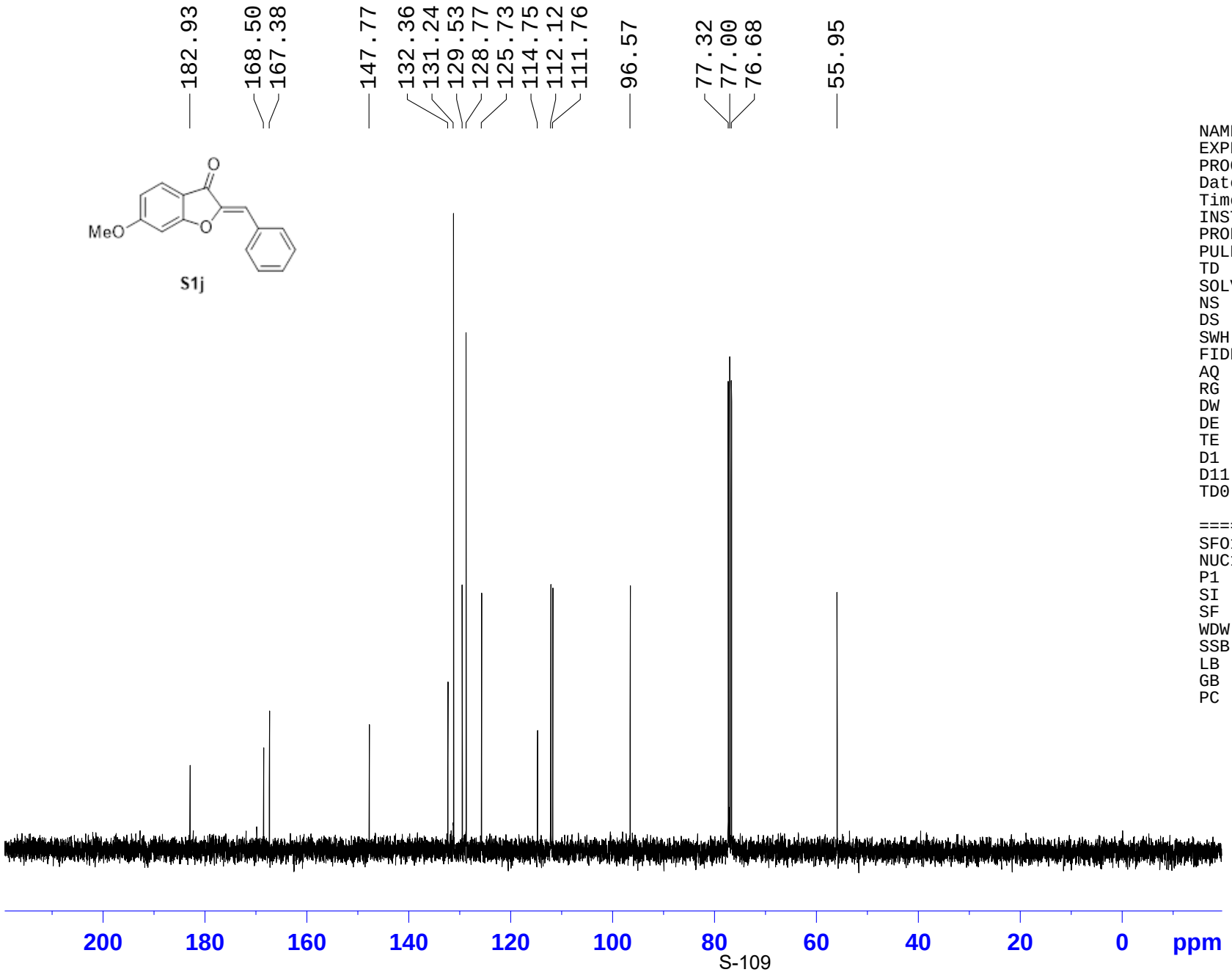
NAME	fq5-39
EXPNO	1
PROCNO	1
Date_	20190326
Time	21.26
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	103.52
DW	62.400 usec
DE	6.50 usec
TE	296.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	14.50 usec
SI	65536
SF	400.1300102 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



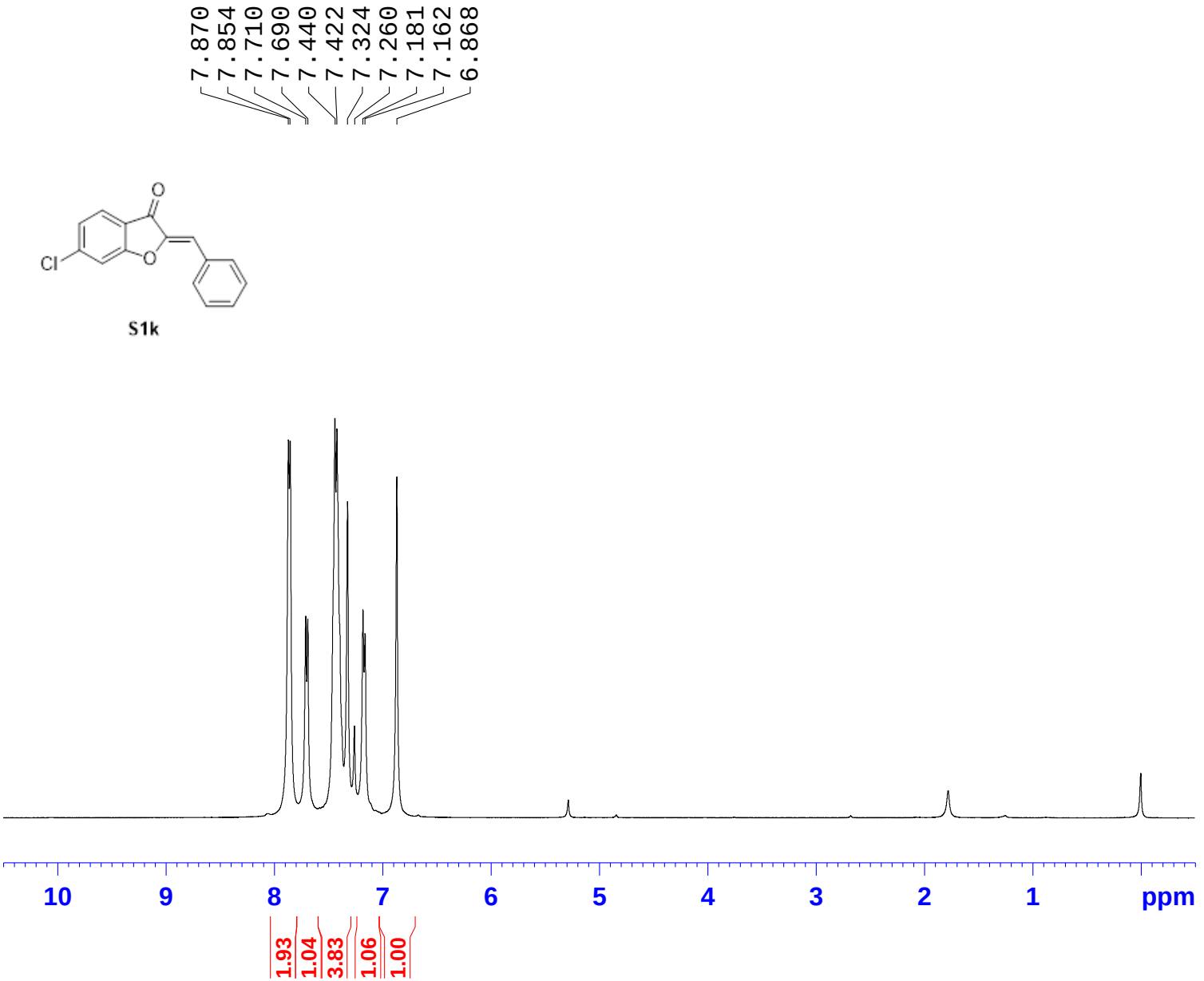
NAME	fq5-39
EXPNO	2
PROCNO	1
Date_	20190326
Time	21.28
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	100
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	296.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



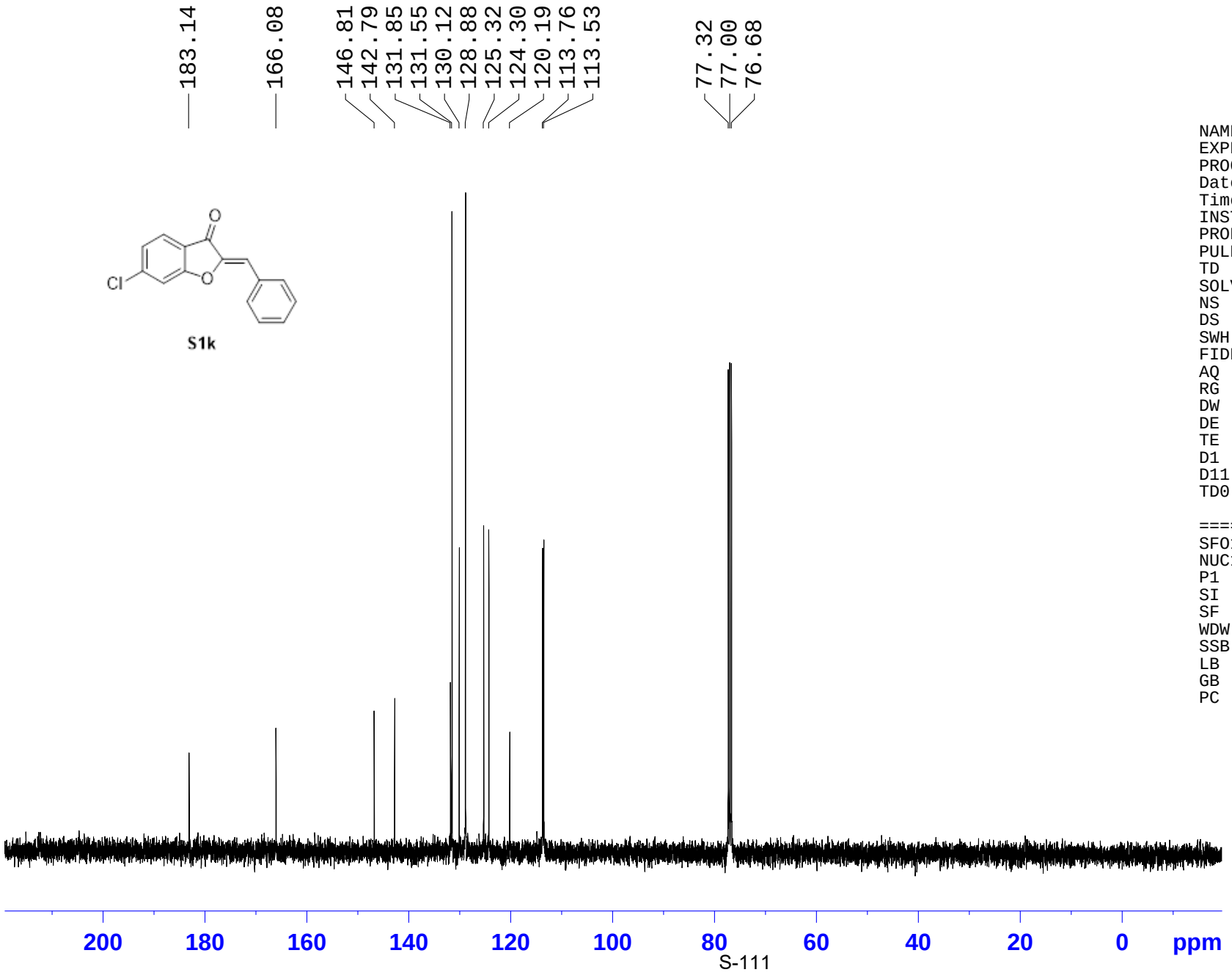

```
NAME                fq5-74
EXPNO                    1
PROCNO                   1
Date_             20190409
Time                 21.47
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       4
DS                       0
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ               4.0894966 sec
RG                   82.92
DW                   62.400 usec
DE                    6.50 usec
TE                   298.0 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                   14.50 usec
SI                   65536
SF            400.1300100 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



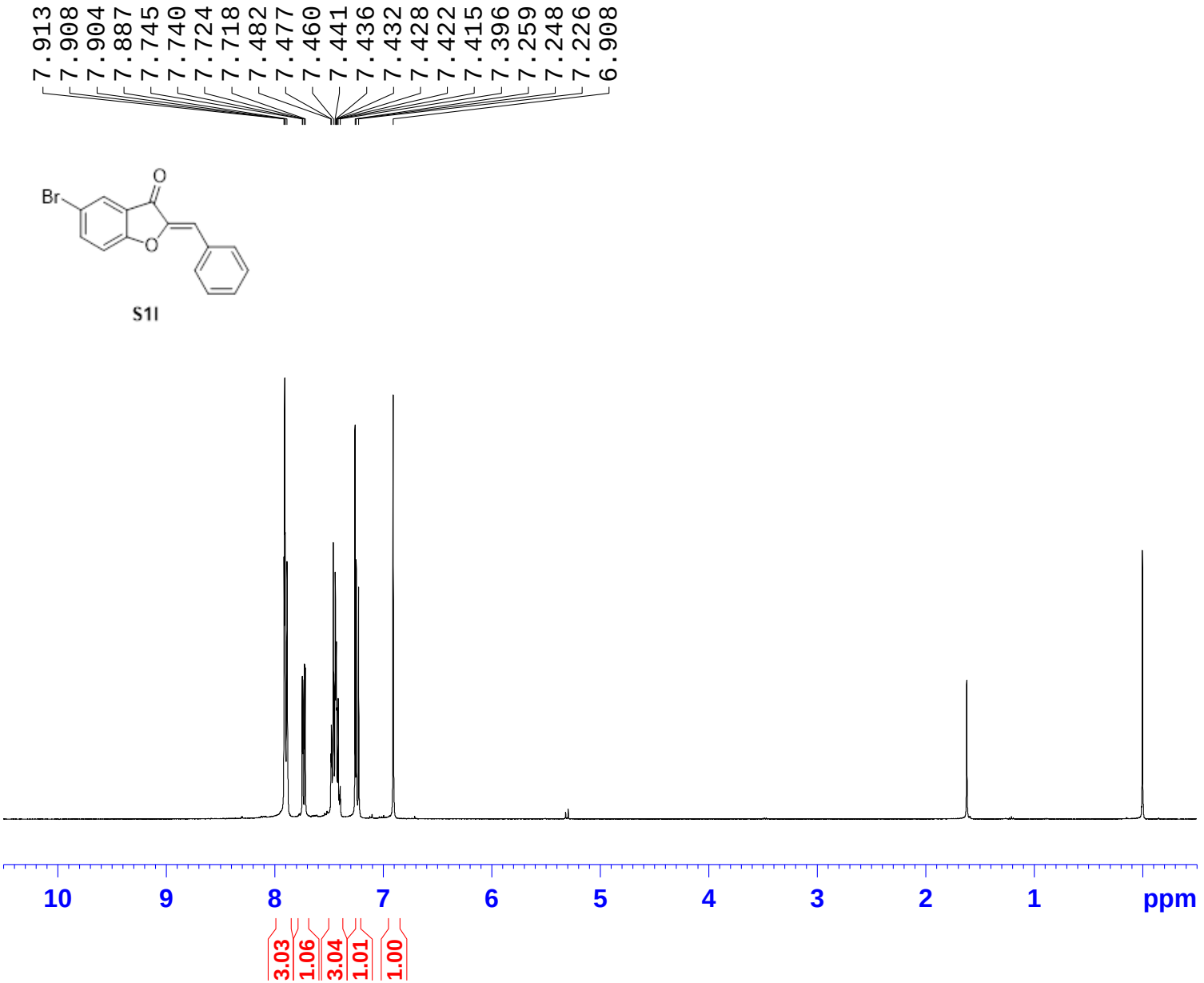
NAME	fq5-74
EXPNO	2
PROCNO	1
Date_	20190409
Time	22.07
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	298.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127767 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



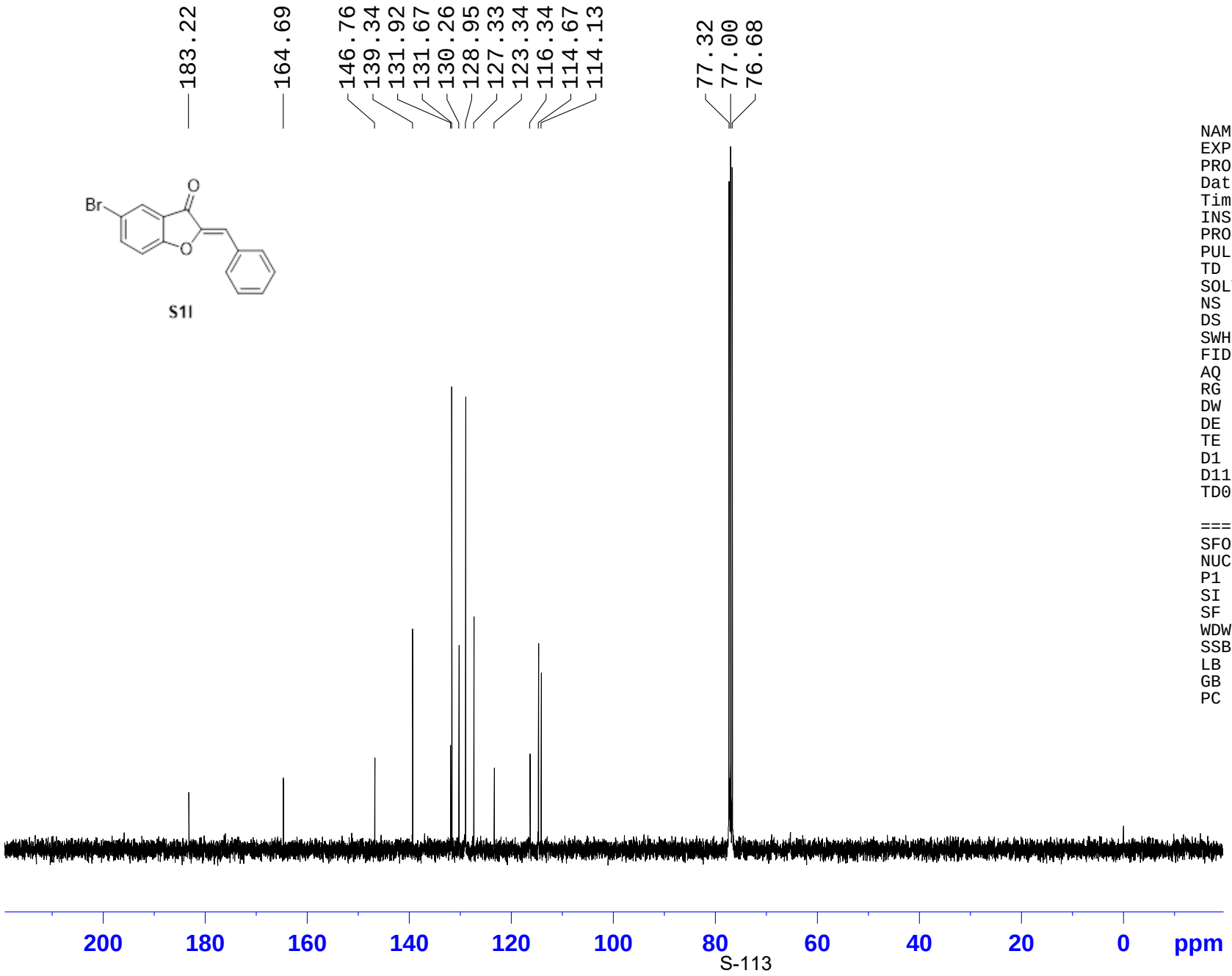

```
NAME            fq5-28-1
EXPNO                  1
PROCNO                 1
Date_           20190320
Time               13.52
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     9
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894966 sec
RG                 70.97
DW                62.400 usec
DE                 6.50 usec
TE                296.4 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
SI                 65536
SF           400.1300106 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



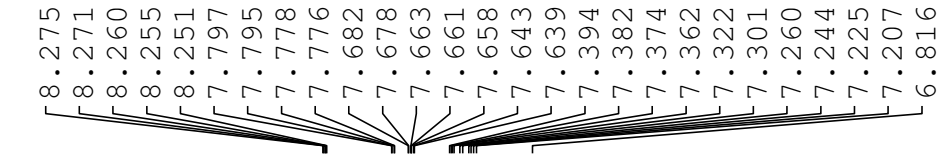
NAME	fq5-28-1
EXPNO	2
PROCNO	1
Date_	20190320
Time	13.54
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	40
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	297.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127779 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

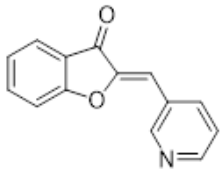



```
NAME                fq5-64
EXPNO                    1
PROCNO                   1
Date_             20190408
Time                 11.00
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       4
DS                       0
SWH               8012.820 Hz
FIDRES             0.122266 Hz
AQ                4.0894966 sec
RG                   142.88
DW                   62.400 usec
DE                    6.50 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                    1H
P1                   14.50 usec
SI                   65536
SF             400.1300106 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



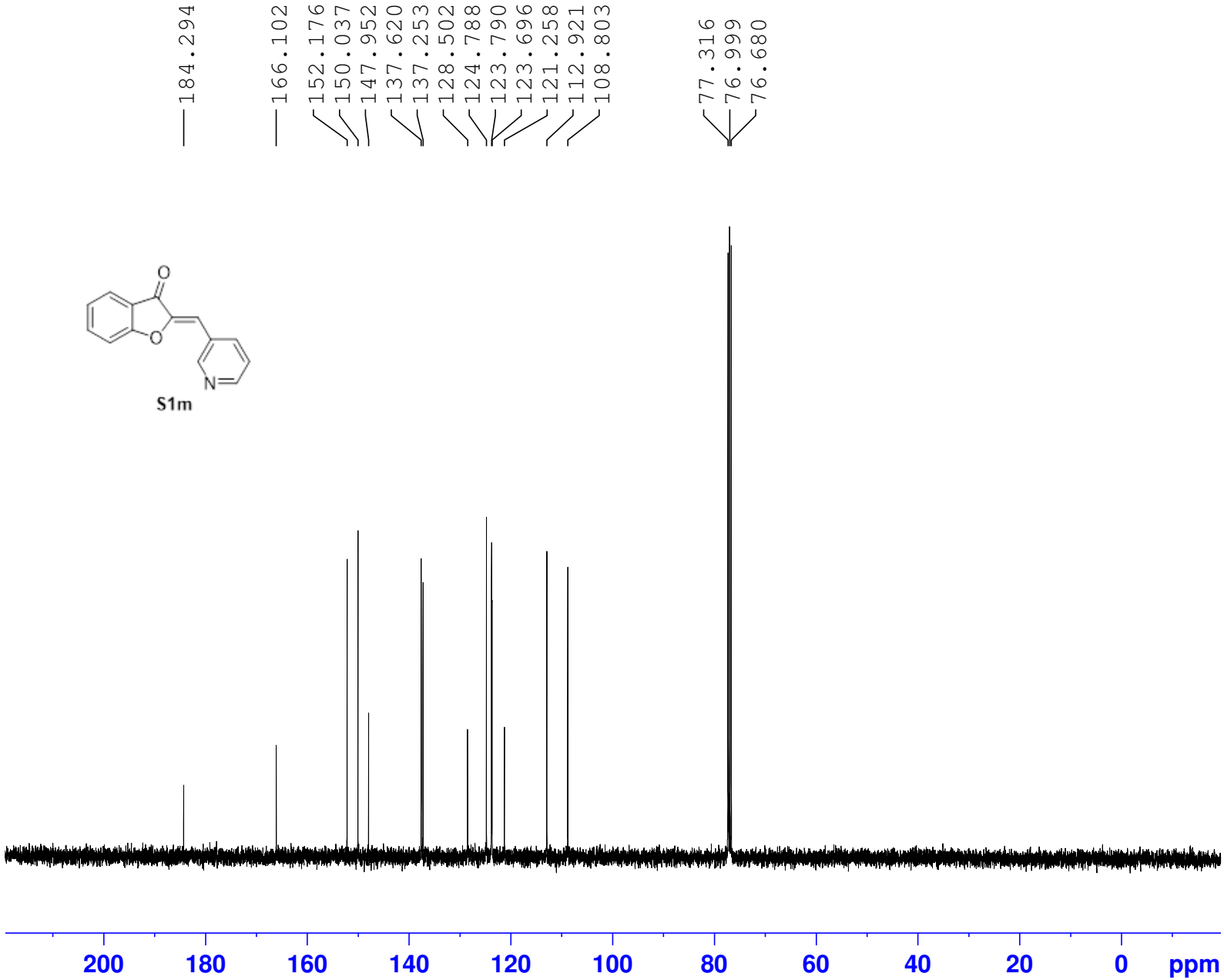

```
NAME              fq5-64
EXPNO                  2
PROCNO                 1
Date_           20190408
Time               11.02
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   80
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG               196.92
DW                20.800 usec
DE                 6.50 usec
TE                298.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF          100.6127728 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



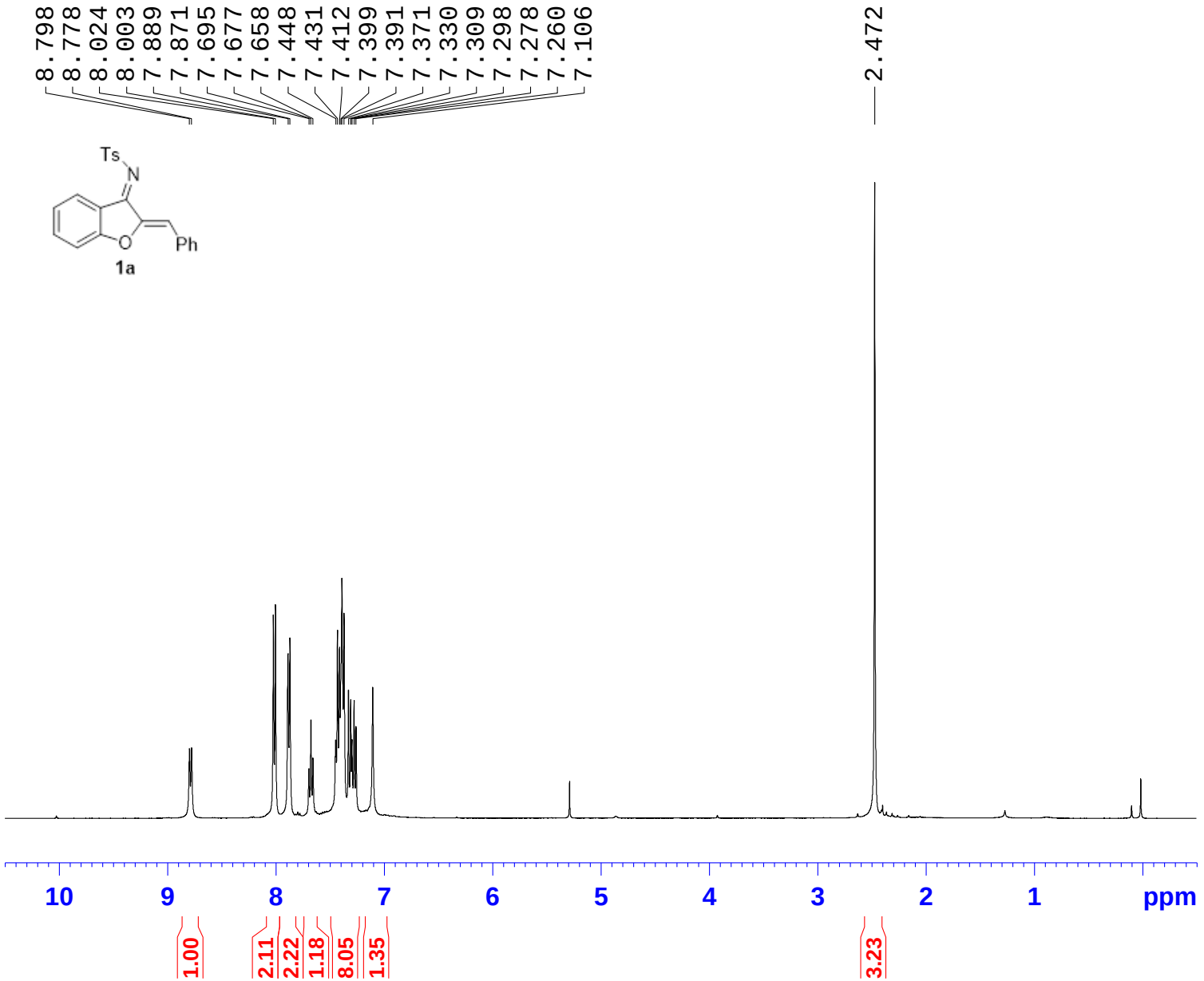


S1m

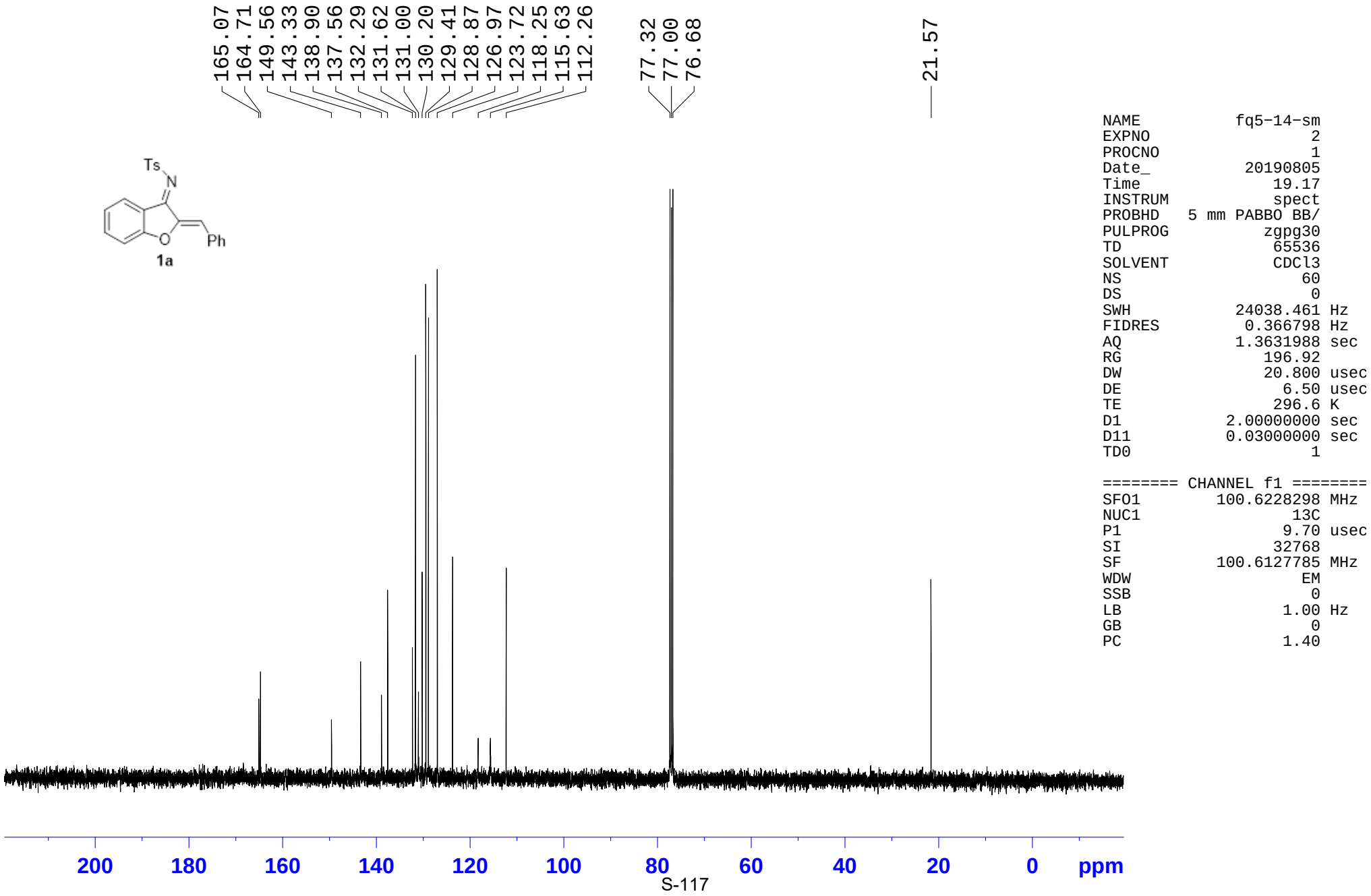

```
Current Data Parameters
NAME                  fq5-30
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190323
Time                  15.15
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                   112.31
DW                   62.400 usec
DE                    6.50 usec
TE                   295.5 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                    14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                    65536
SF             400.1300102 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```



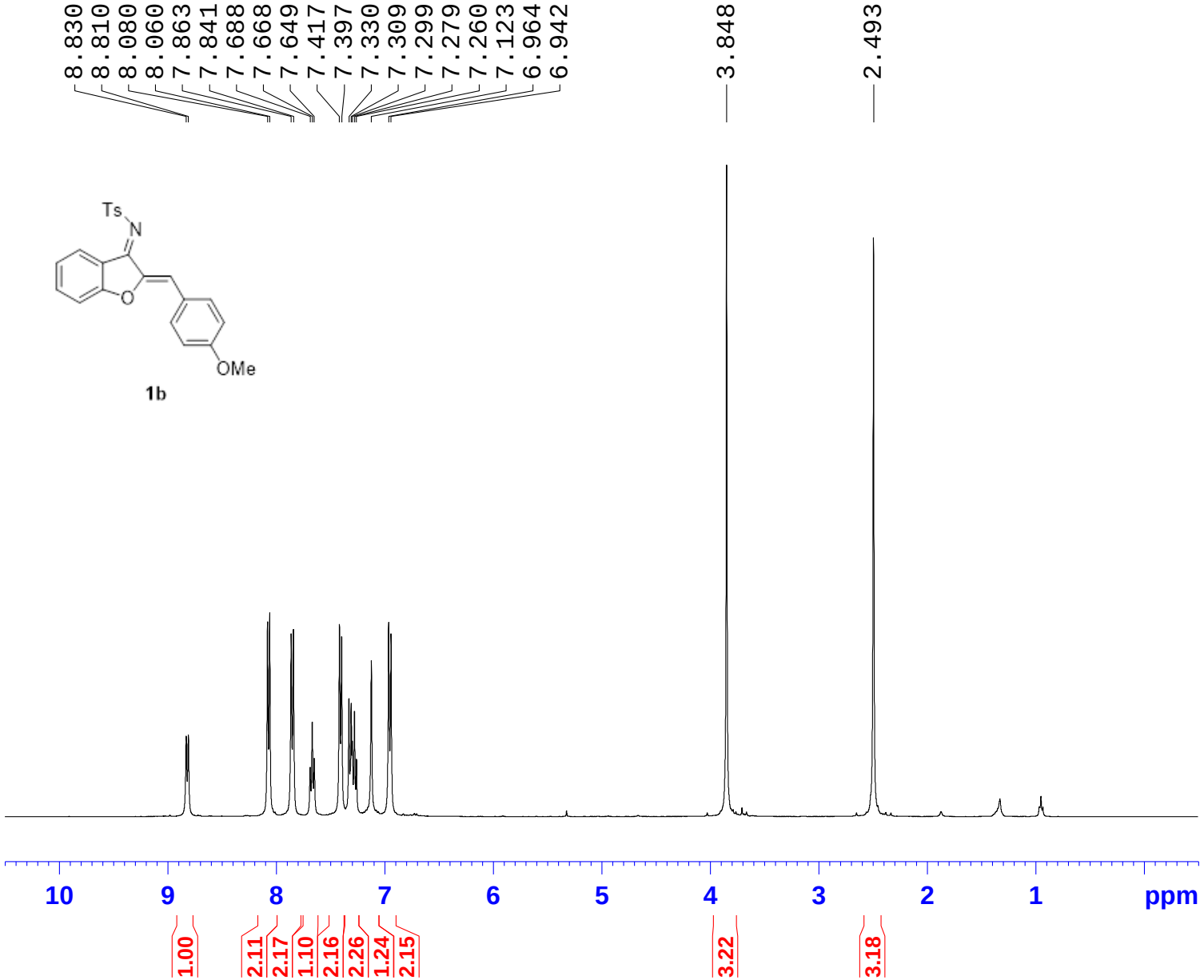

```
Current Data Parameters
NAME                  fq5-30
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190323
Time                  15.16
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        80
DS                         0
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631488 sec
RG                   196.92
DW                   20.800 usec
DE                    6.50 usec
TE                   296.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            100.6228298 MHz
NUC1                    13C
P1                     9.70 usec
PLW1            46.98899841 W

======== CHANNEL f2 ========
SFO2            400.1316005 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                 90.00 usec
PLW2            11.99499989 W
PLW12            0.34213999 W
PLW13            0.27713001 W

F2 - Processing parameters
SI                     32768
SF              100.6127759 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                     1.40
```



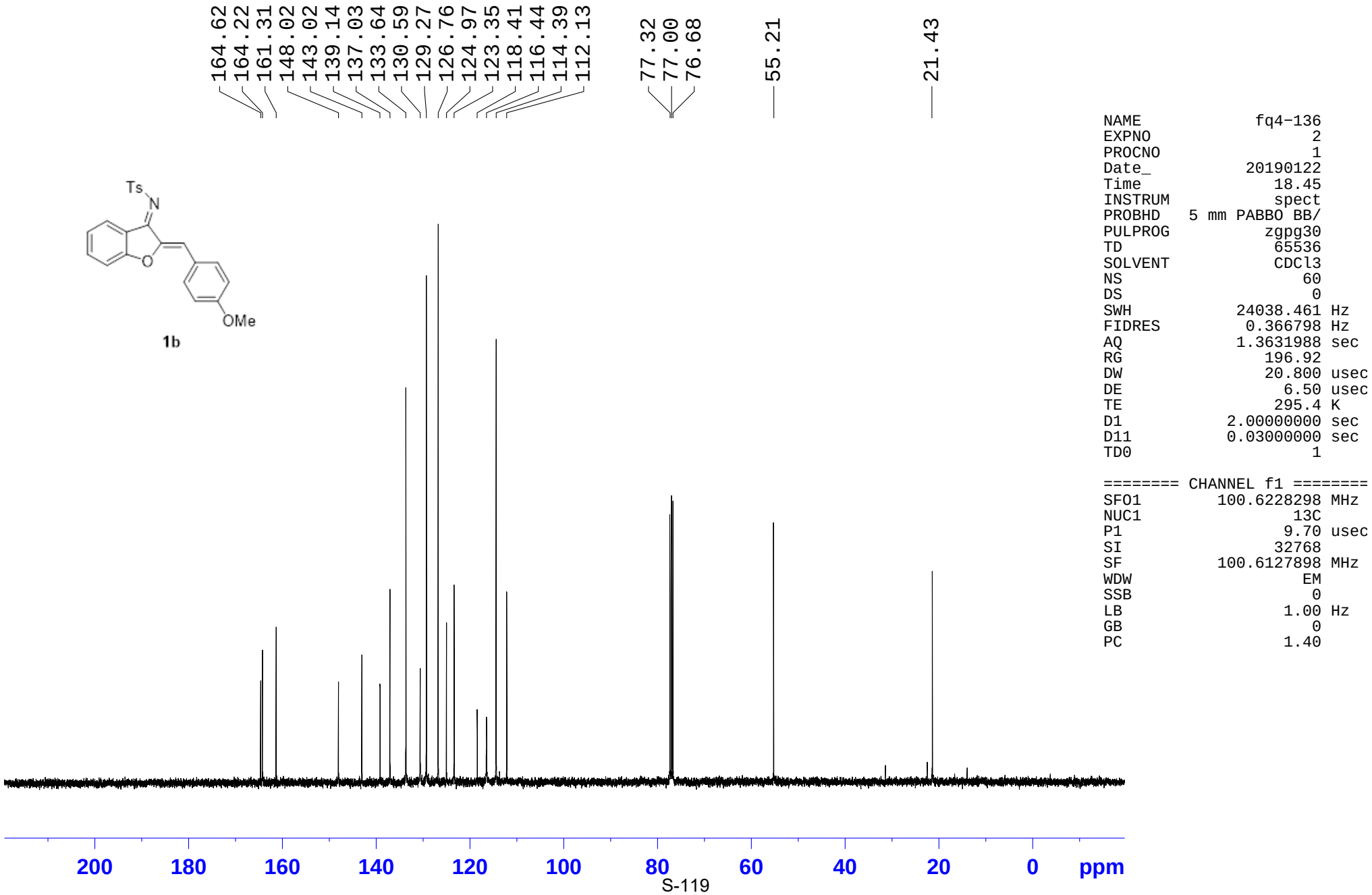

```
NAME           fq5-14-sm
EXPNO                  1
PROCNO                 1
Date_           20190805
Time               19.16
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894966 sec
RG                 70.97
DW                 62.400 usec
DE                  6.50 usec
TE                 296.1 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
SI                 65536
SF           400.1300101 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



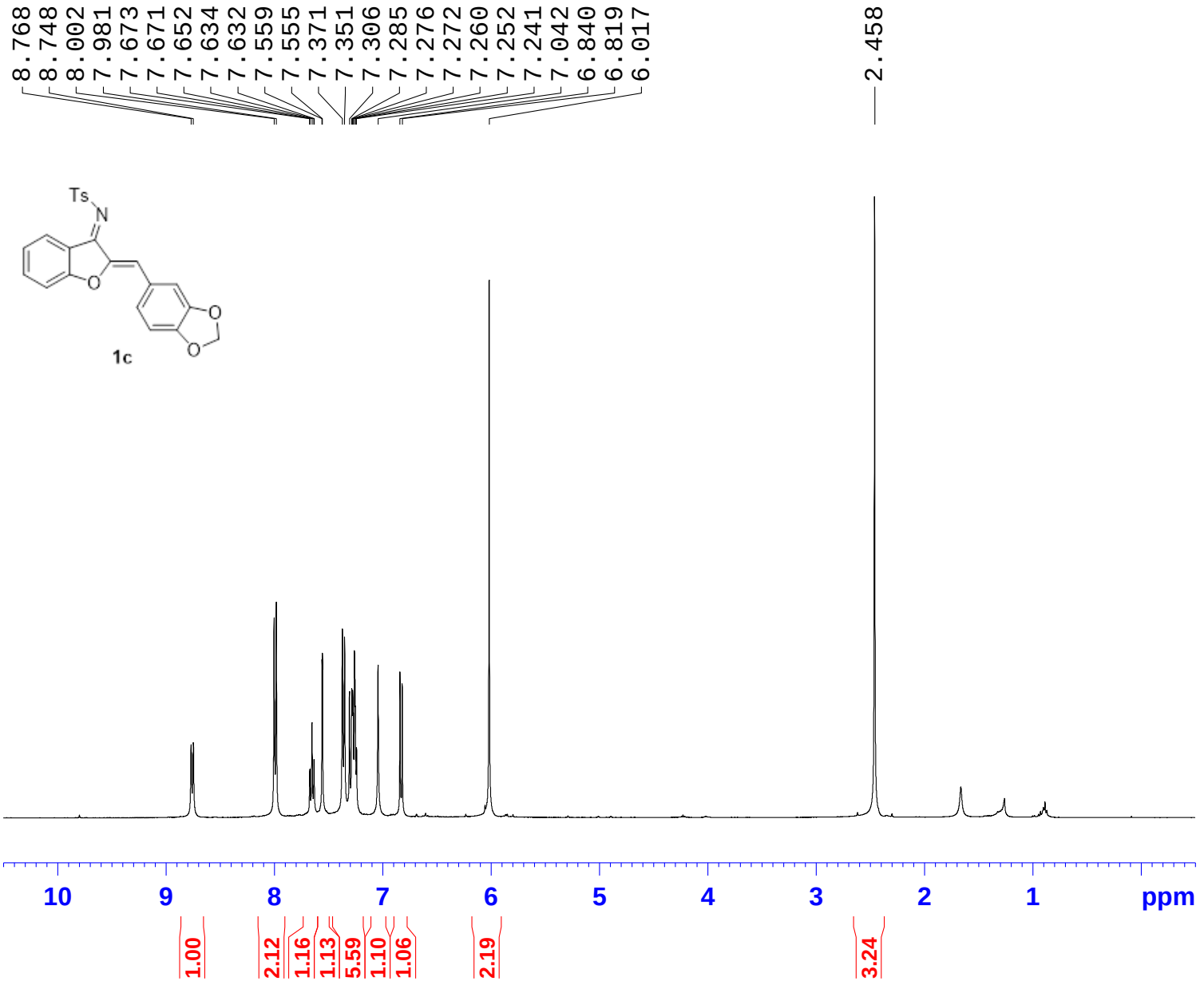
NAME	fq5-14-sm
EXPNO	2
PROCNO	1
Date_	20190805
Time	19.17
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	60
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	296.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127785 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



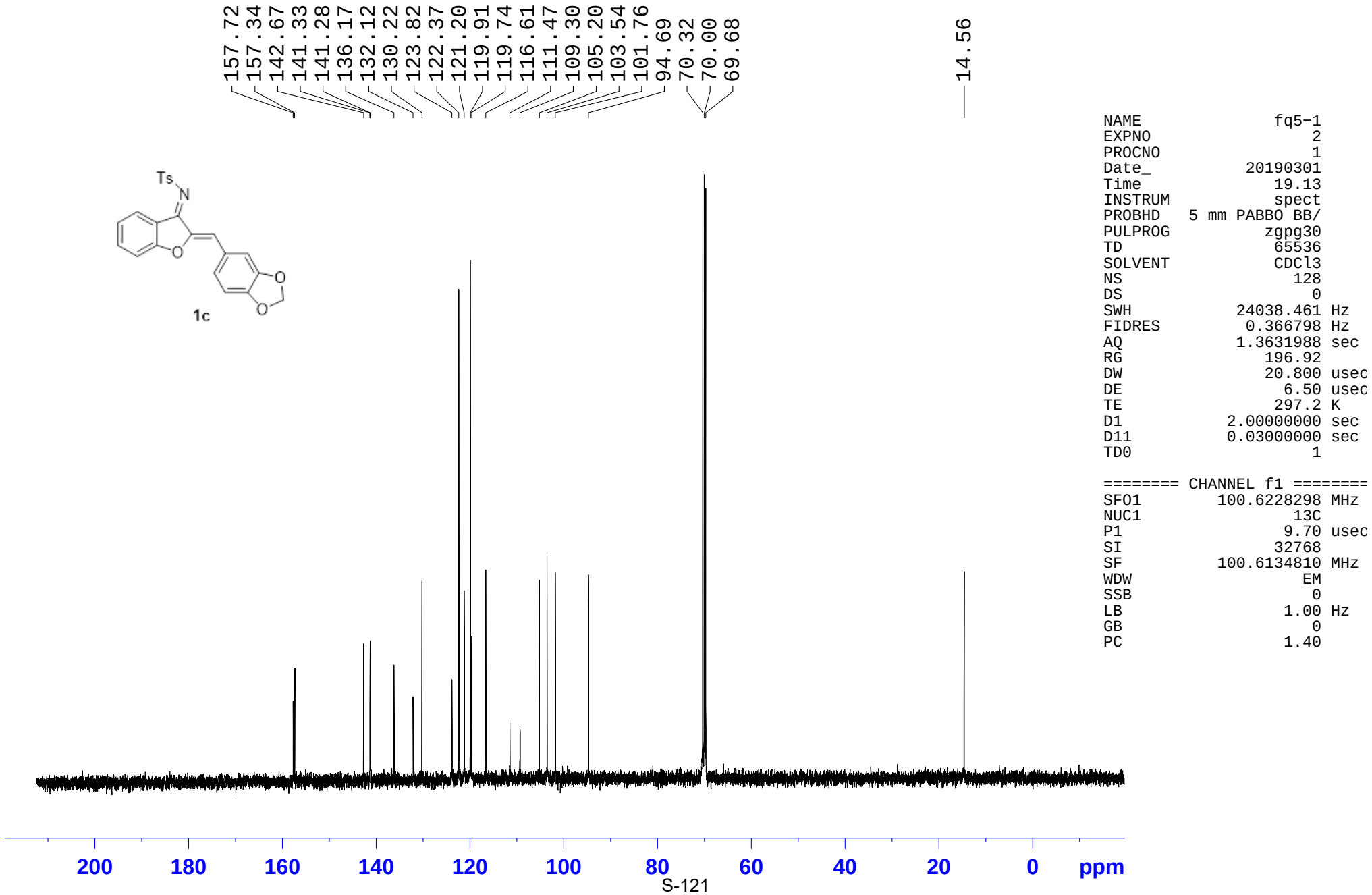

```
NAME            fq4-136
EXPNO                 1
PROCNO                1
Date_          20190122
Time              18.43
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ            4.0894966 sec
RG                 19.7
DW                62.400 usec
DE                 6.50 usec
TE                294.8 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                14.50 usec
SI                65536
SF          400.1299863 MHz
WDW                 EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



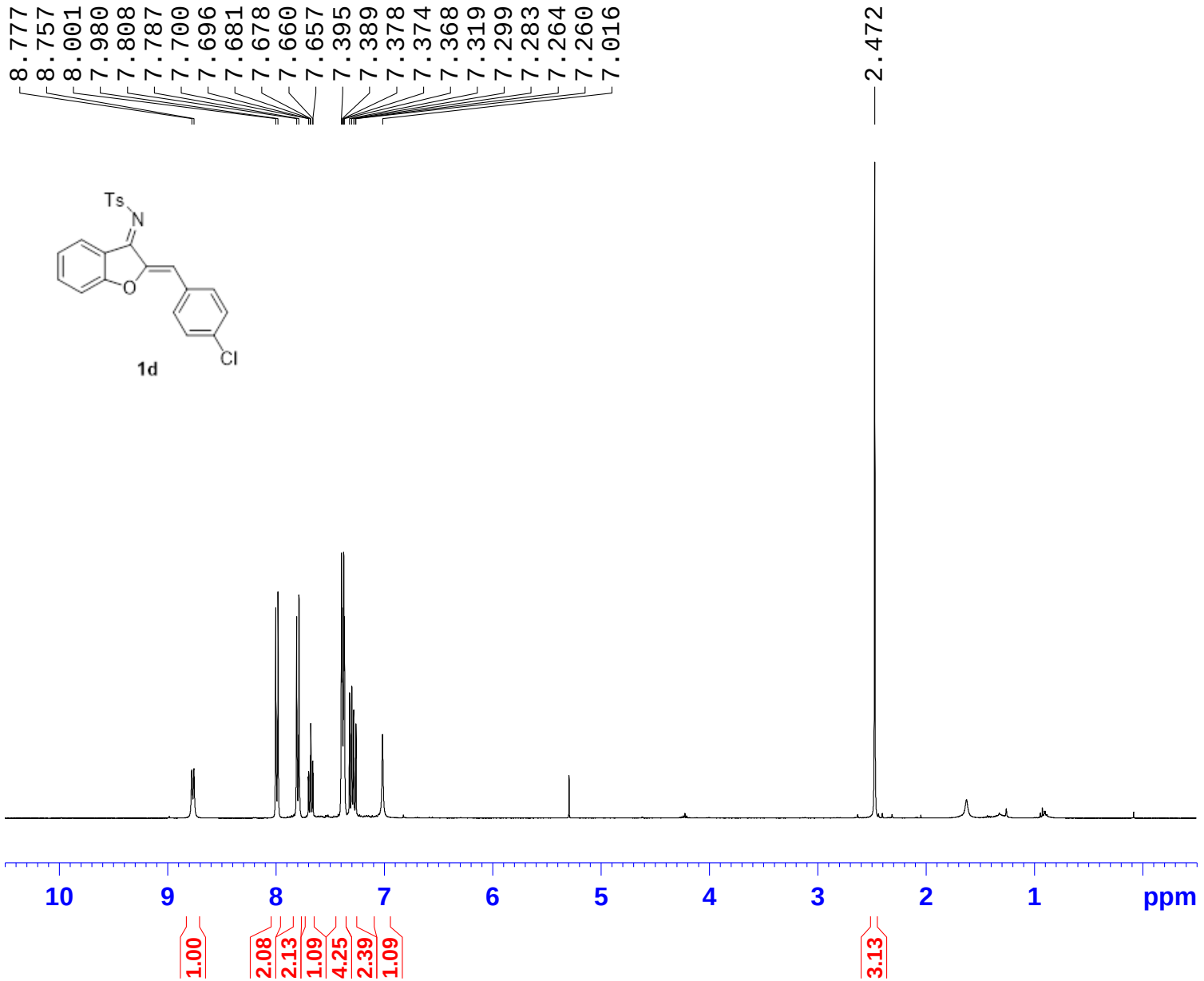
NAME	fq4-136
EXPNO	2
PROCNO	1
Date_	20190122
Time	18.45
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	60
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	295.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127898 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



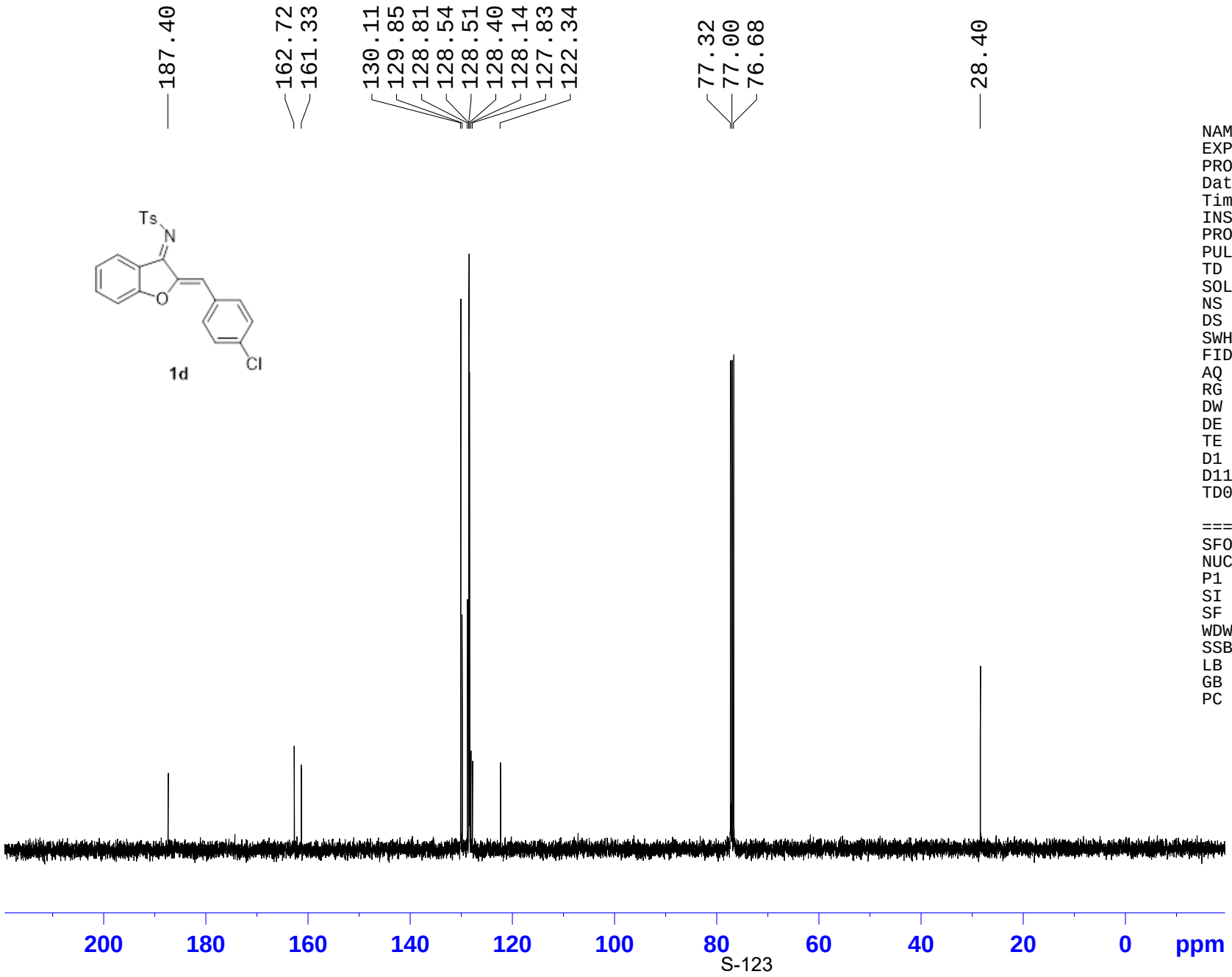
NAME	fq5-1
EXPNO	1
PROCNO	1
Date_	20190301
Time	19.11
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	82.92
DW	62.400 usec
DE	6.50 usec
TE	296.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	14.50 usec
SI	65536
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

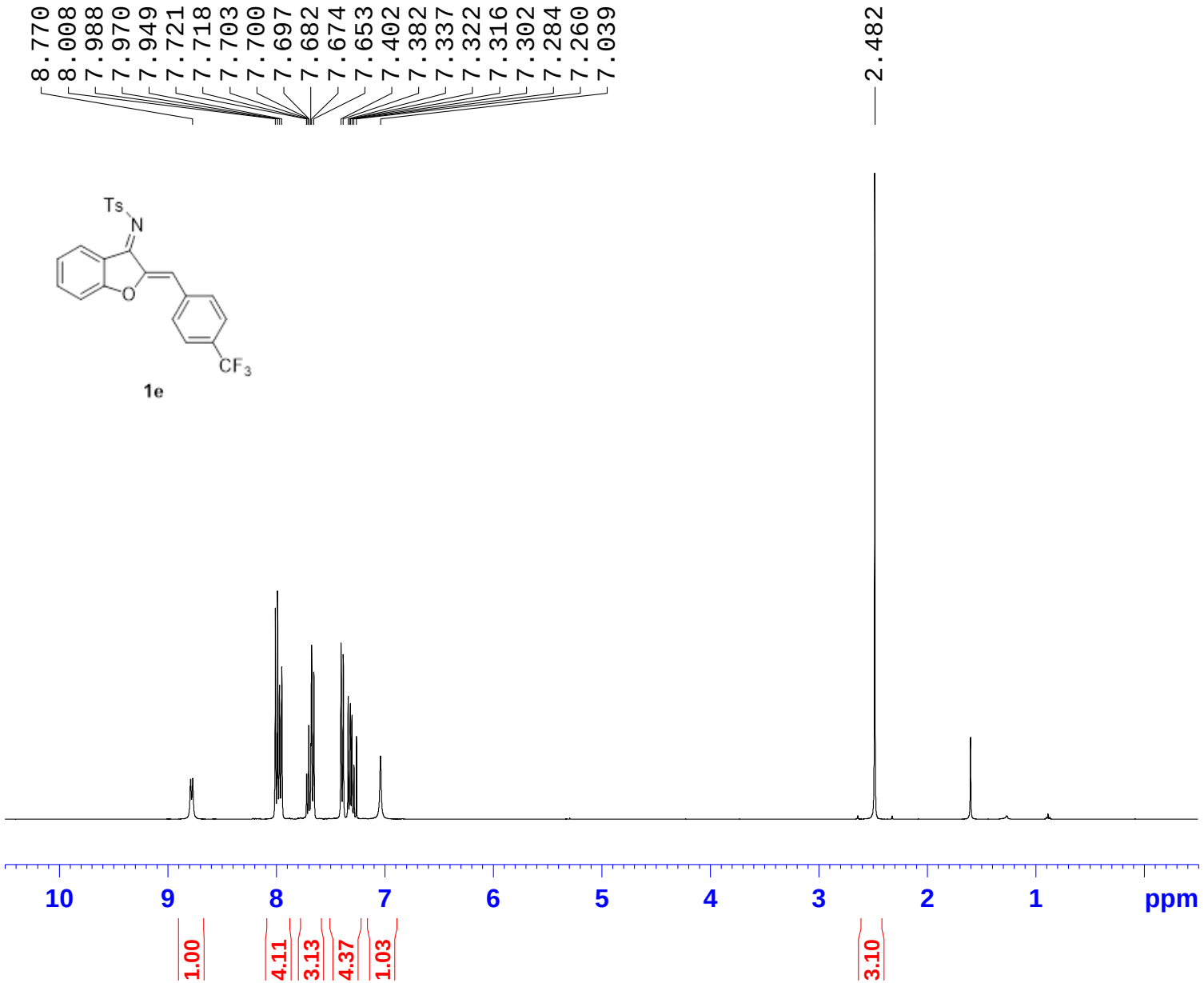


NAME	fq5-1
EXPNO	2
PROCNO	1
Date_	20190301
Time	19.13
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	128
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	297.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6134810 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

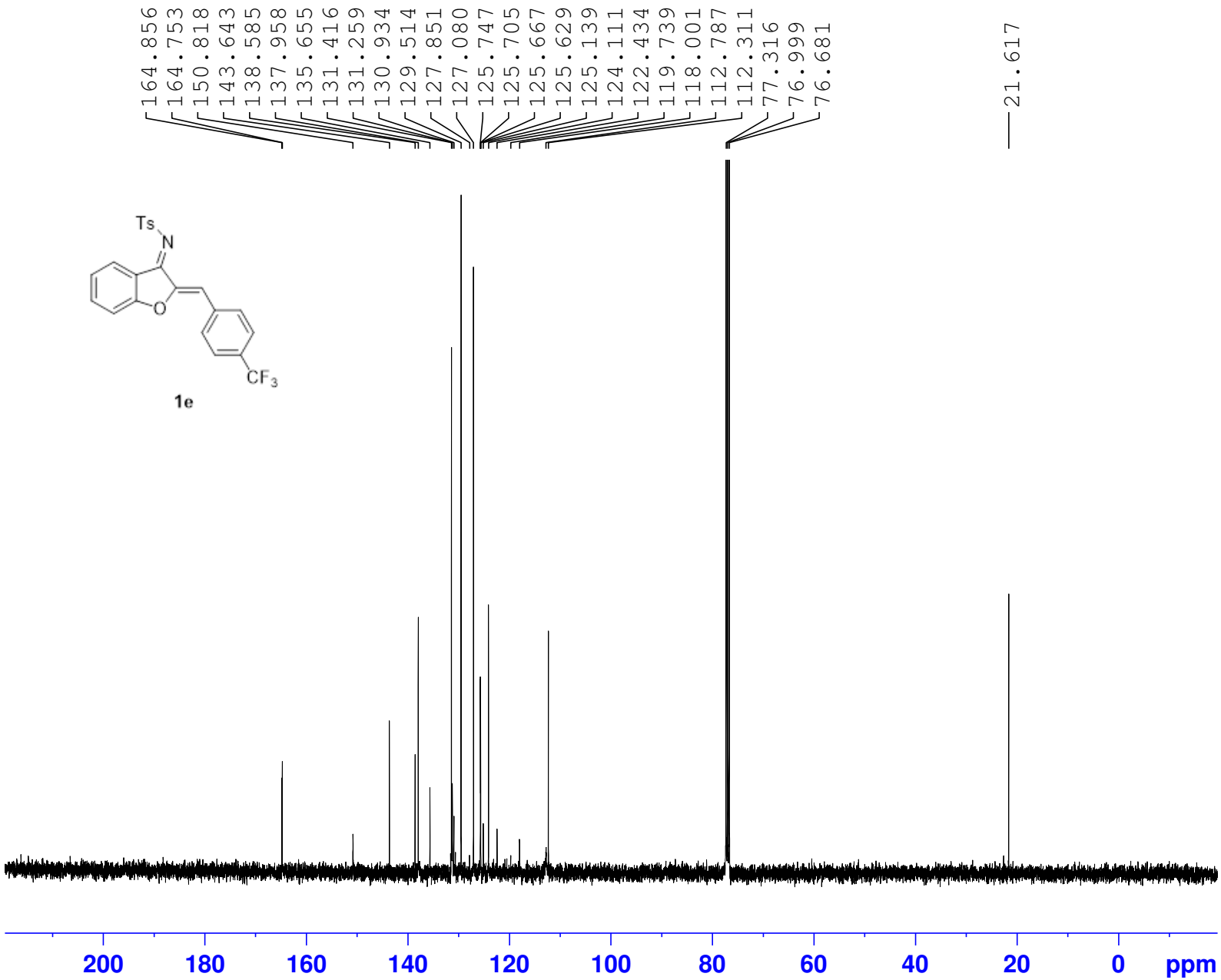


NAME	fq4-164
EXPNO	1
PROCNO	1
Date_	20190213
Time	14.29
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	4
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	82.92
DW	62.400 usec
DE	6.50 usec
TE	295.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	14.50 usec
SI	65536
SF	400.1300102 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

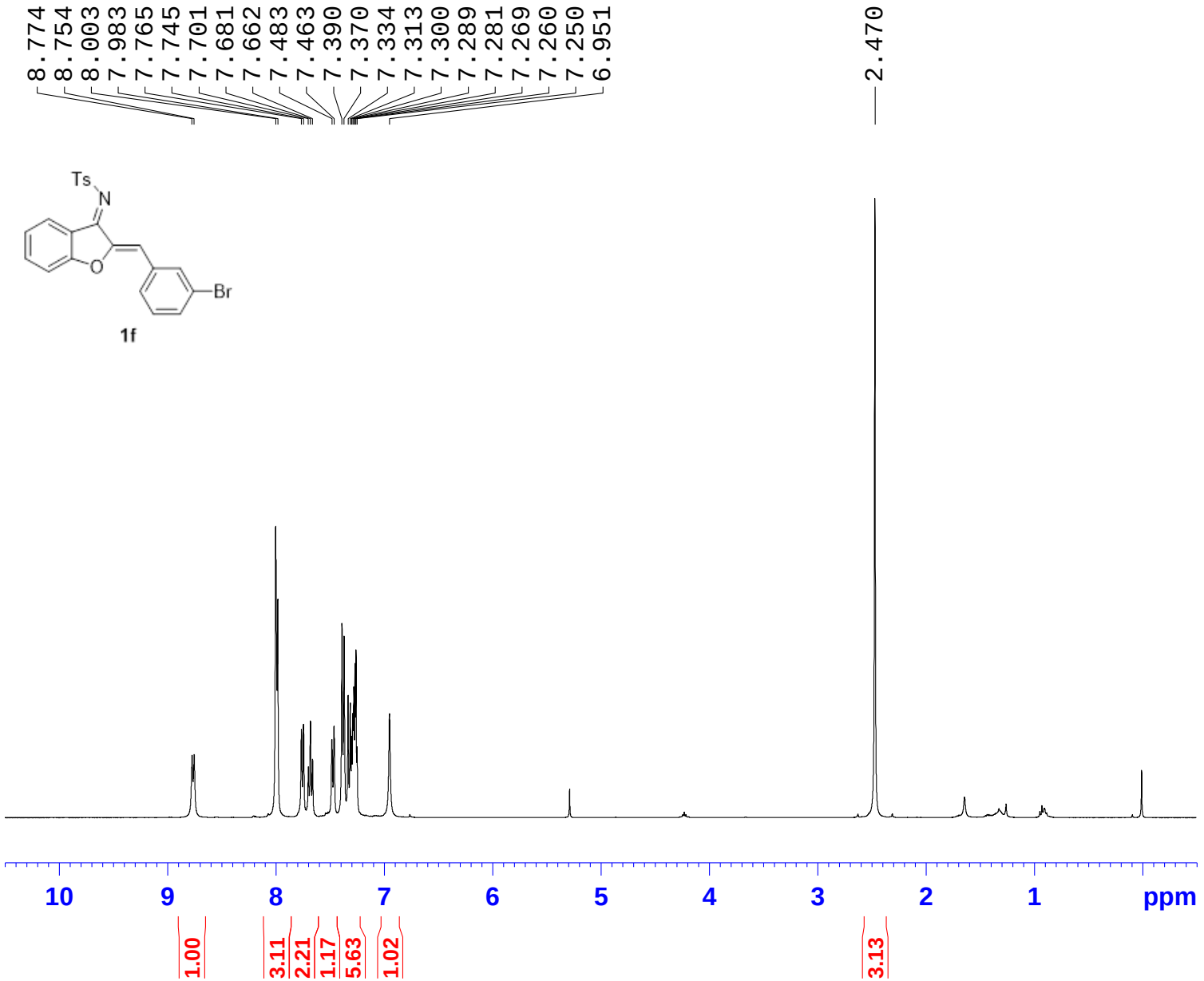

187.40
162.72
161.33
130.11
129.85
128.81
128.54
128.51
128.40
128.14
127.83
122.34
77.32
77.00
76.68
28.40
Ts
N
O
Cl
1d
NAME fq5-164-1-1
EXPNO 2
PROCNO 1
Date_ 20190603
Time 21.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 48
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
SI 32768
SF 100.6127776 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm



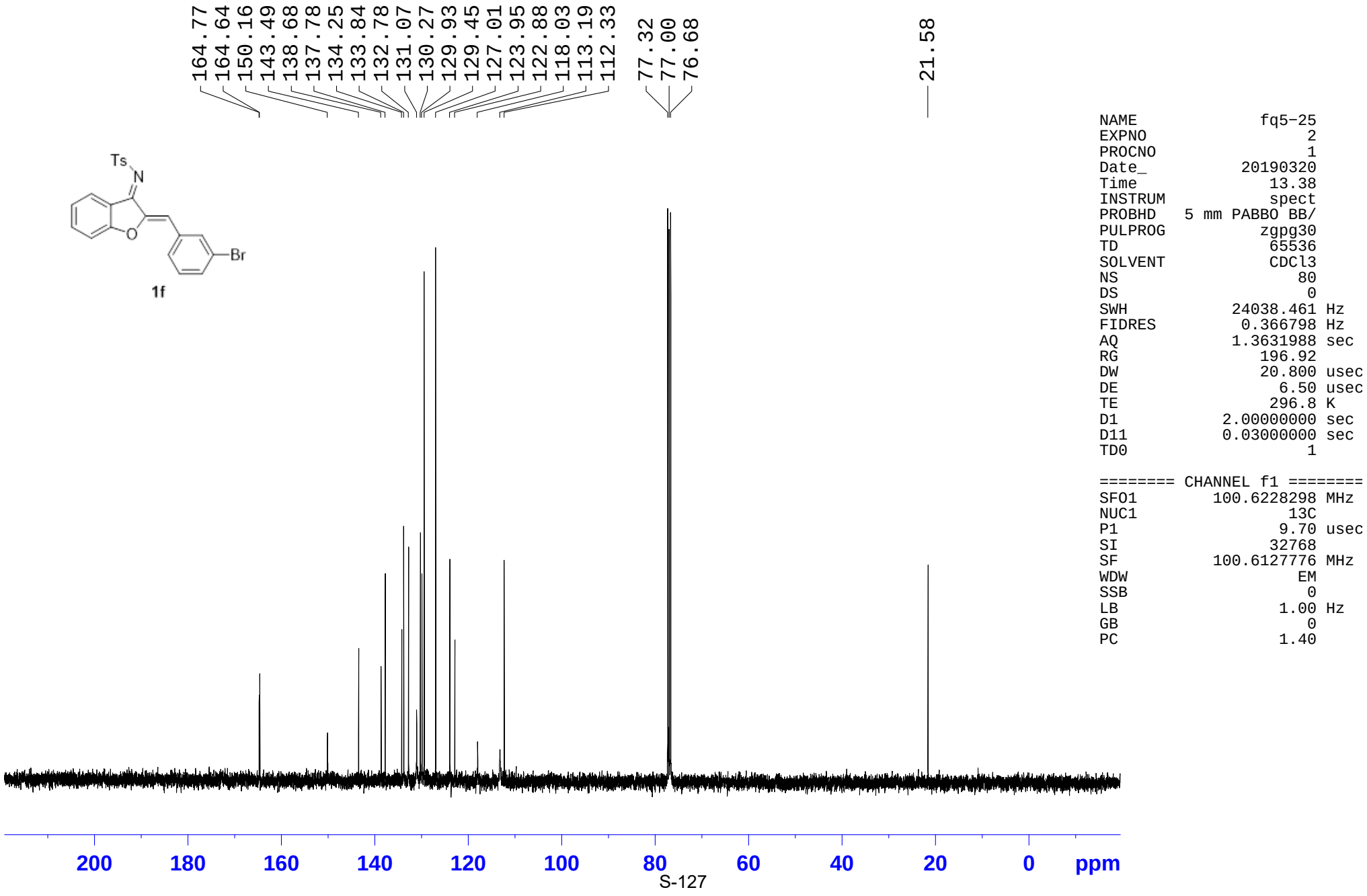

```
NAME            fq4-180
EXPNO                 1
PROCNO                1
Date_          20190222
Time              20.35
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    4
DS                    0
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ           4.0894966 sec
RG               112.31
DW               62.400 usec
DE                6.50 usec
TE               295.9 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                  1H
P1                14.50 usec
SI                65536
SF          400.1300102 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

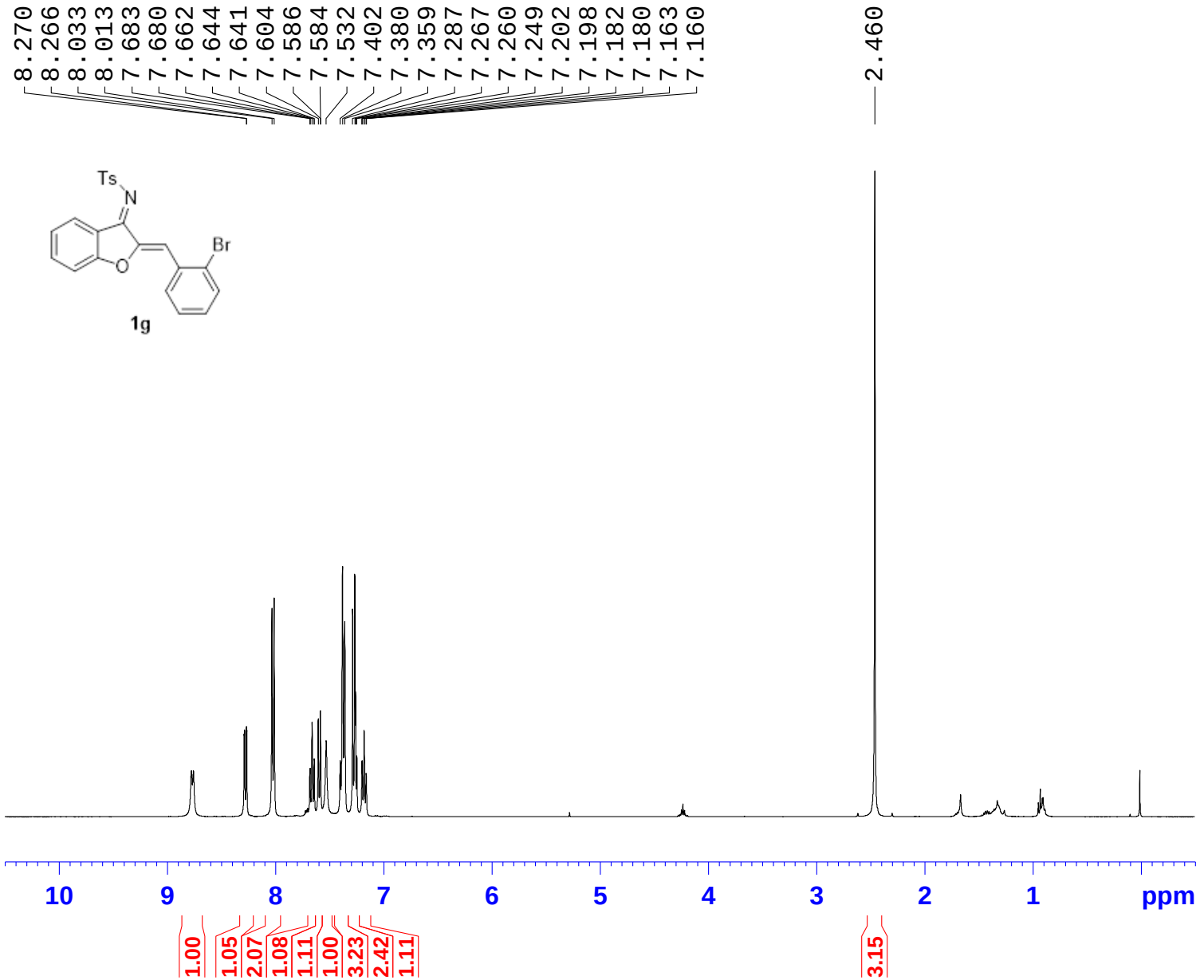



```
Current Data Parameters
NAME                 fq4-180
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20190222
Time                   20.38
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       200
DS                         0
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     196.92
DW                     20.800 usec
DE                      6.50 usec
TE                     296.6 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             100.6228298 MHz
NUC1                     13C
P1                     9.70 usec
PLW1             46.98899841 W

======== CHANNEL f2 ========
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2             11.99499989 W
PLW12             0.34213999 W
PLW13             0.27713001 W

F2 - Processing parameters
SI                       32768
SF               100.6127735 MHz
WDW                         EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

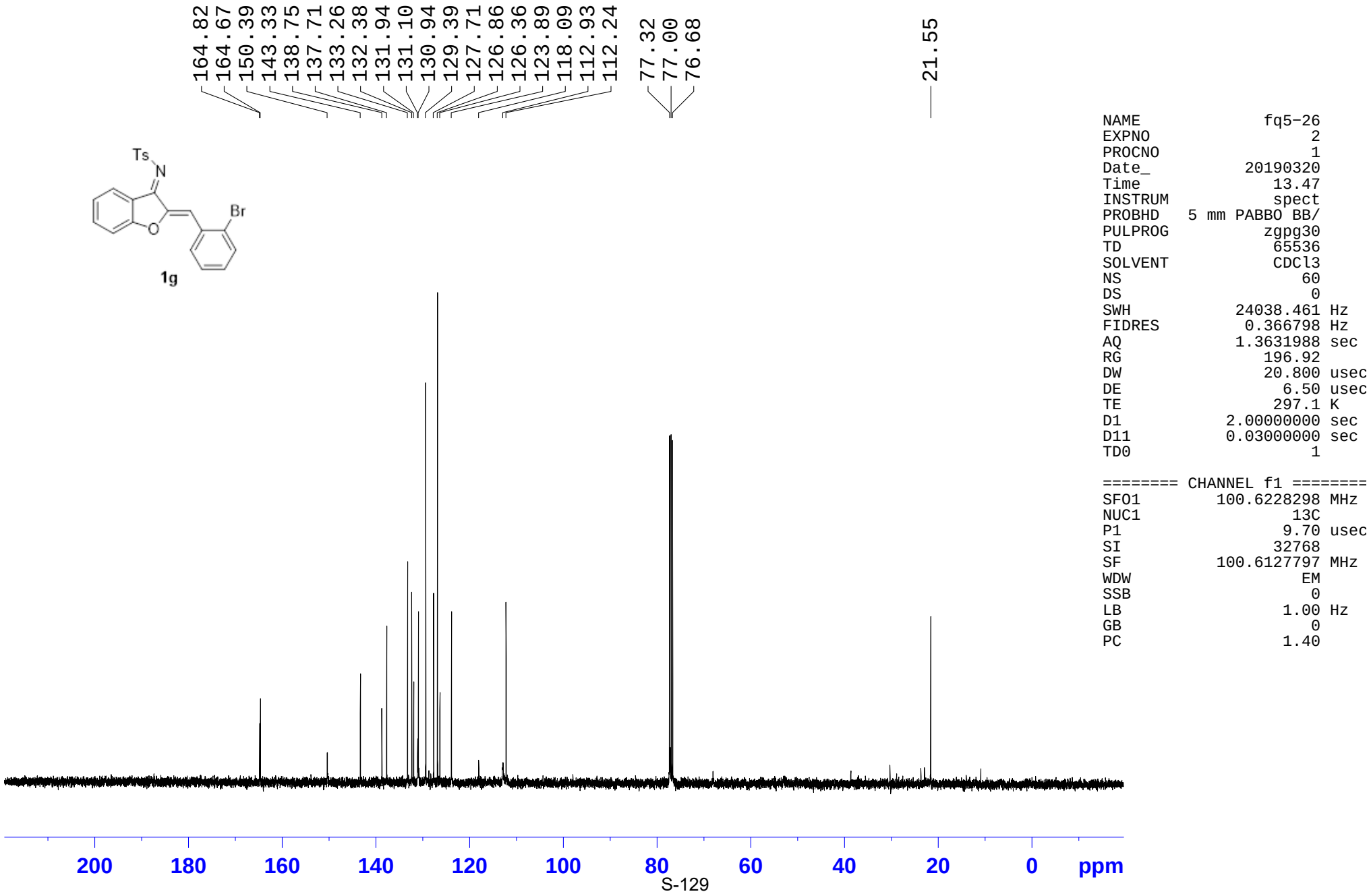


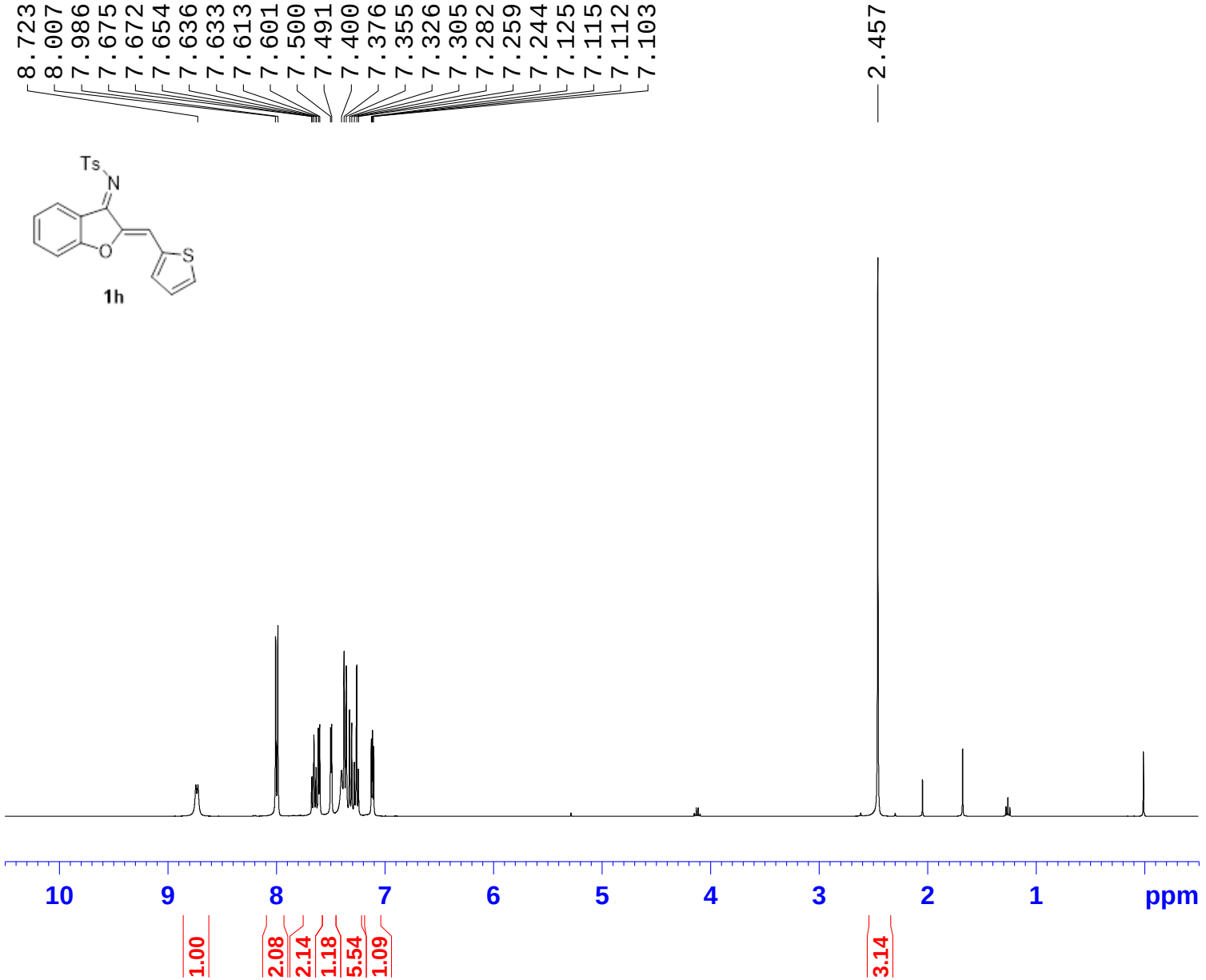

```
NAME                fq5-25
EXPNO                    1
PROCNO                   1
Date_             20190320
Time                 13.37
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ               4.0894966 sec
RG                   62.93
DW                   62.400 usec
DE                    6.50 usec
TE                   296.3 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                   14.50 usec
SI                   65536
SF            400.1300105 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```


164.77
164.64
150.16
143.49
138.68
137.78
134.25
133.84
132.78
131.07
130.27
129.93
129.45
127.01
123.95
122.88
118.03
113.19
112.33
77.32
77.00
76.68
21.58
Ts
N
O
Br
1f
NAME fq5-25
EXPNO 2
PROCNO 1
Date_ 20190320
Time 13.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 80
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
SI 32768
SF 100.6127776 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

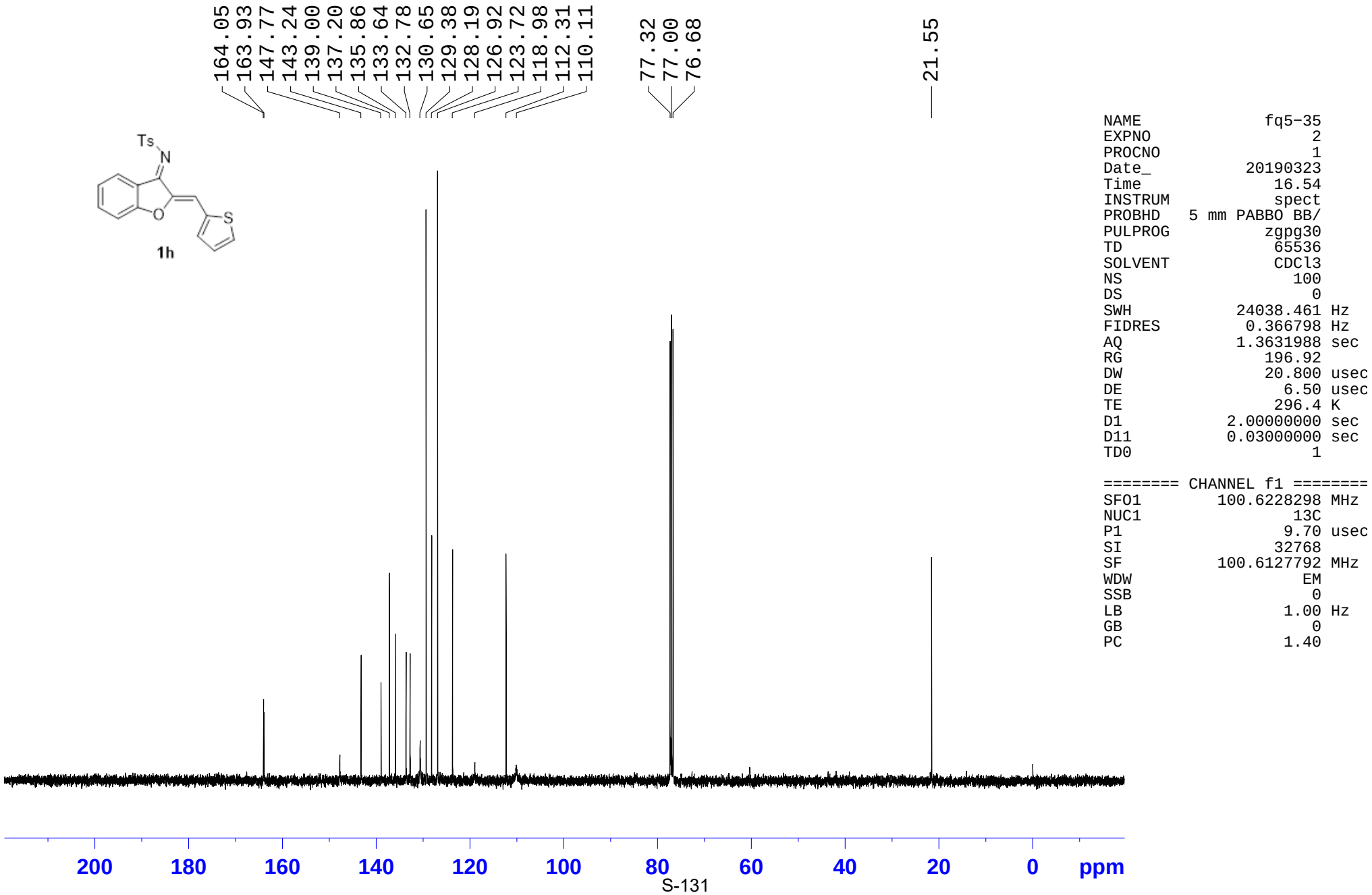


NAME	fq5-26
EXPNO	1
PROCNO	1
Date_	20190320
Time	13.45
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	34.77
DW	62.400 usec
DE	6.50 usec
TE	296.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	14.50 usec
SI	65536
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

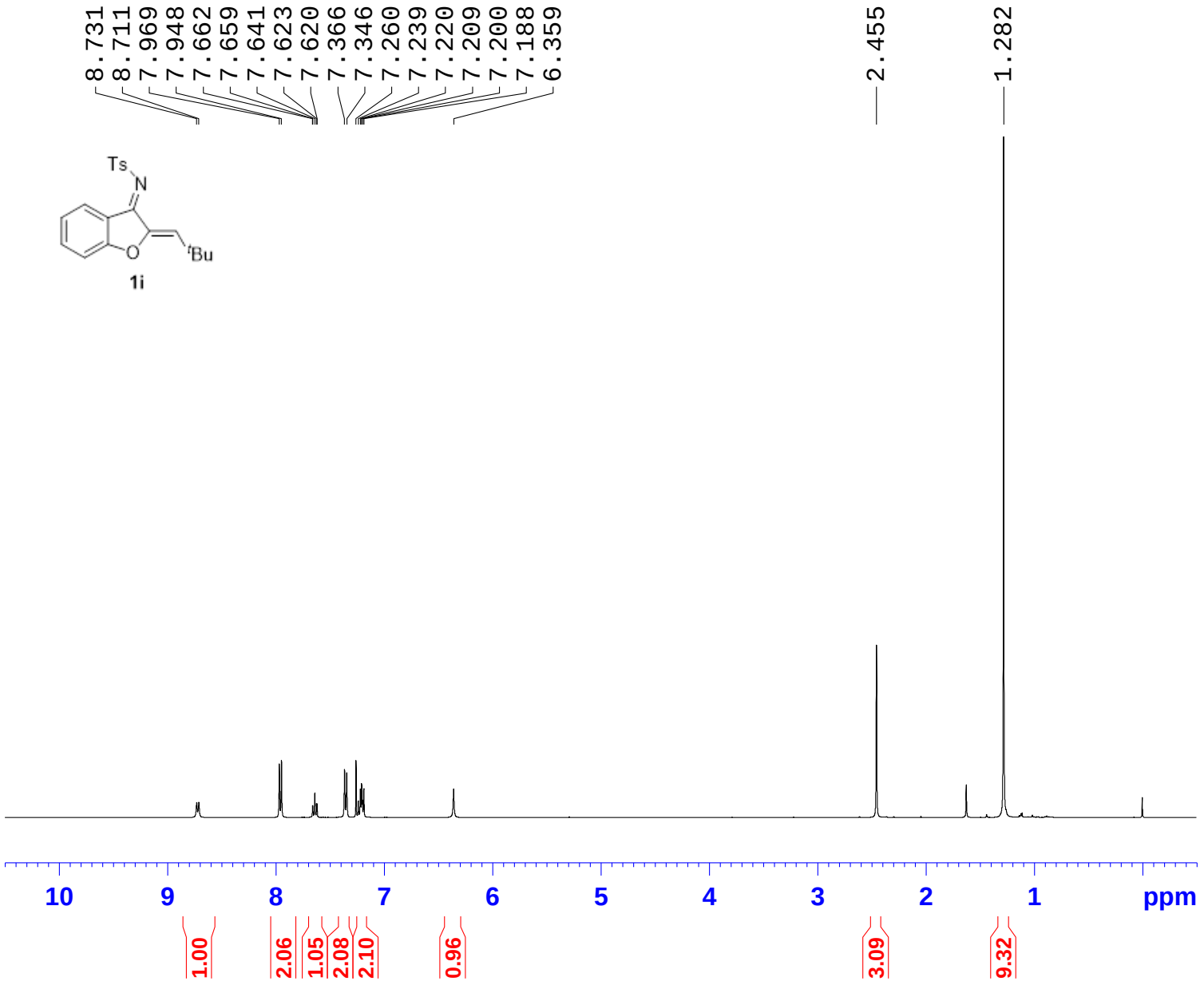

164.82
164.67
150.39
143.33
138.75
137.71
133.26
132.38
131.94
131.10
130.94
129.39
127.71
126.86
126.36
123.89
118.09
112.93
112.24
77.32
77.00
76.68
21.55
Ts
N
O
Br
1g
NAME fq5-26
EXPNO 2
PROCNO 1
Date_ 20190320
Time 13.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 60
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
SI 32768
SF 100.6127797 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm



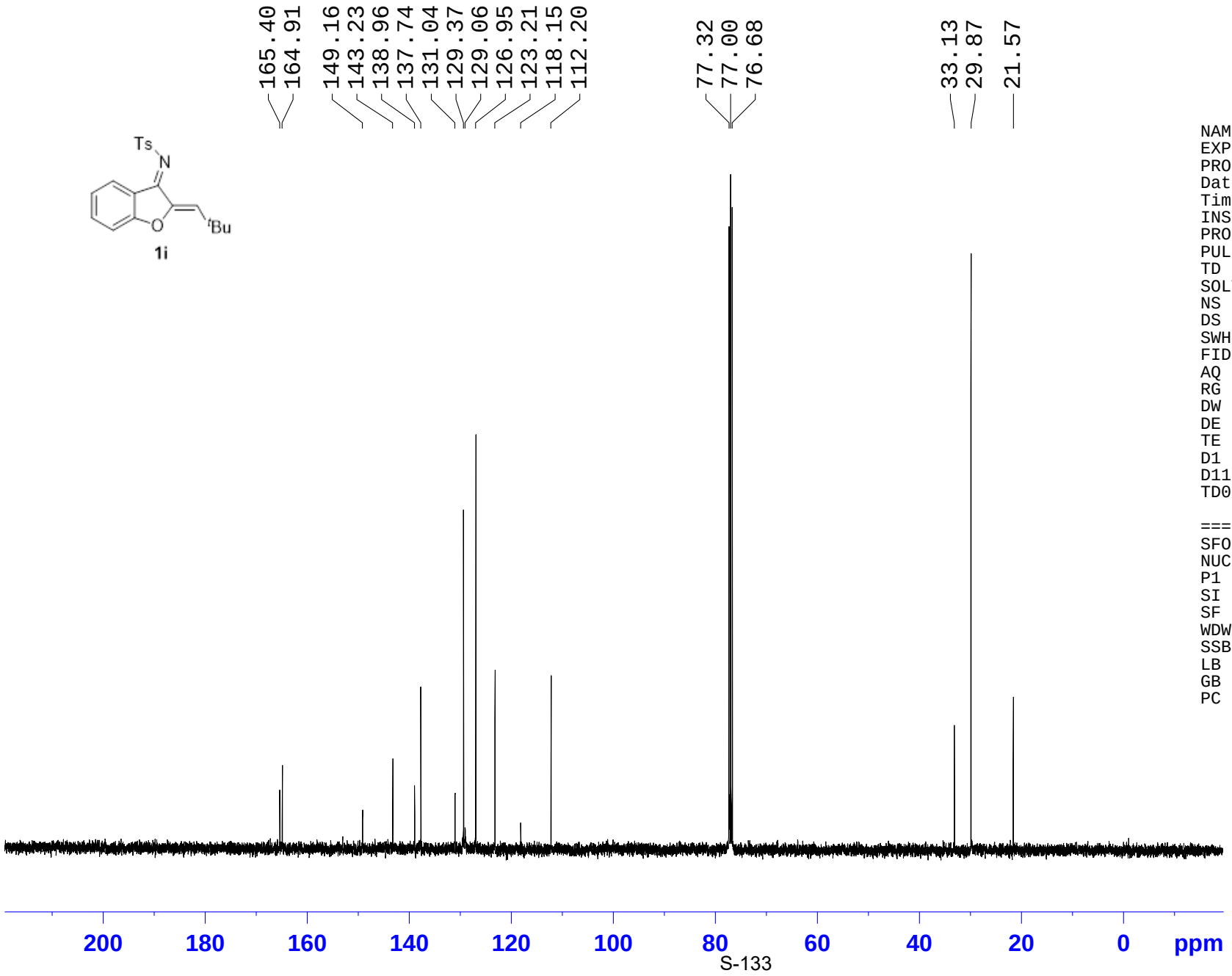

```
NAME              fq5-35
EXPNO                  1
PROCNO                 1
Date_           20190323
Time               16.52
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894966 sec
RG                 39.46
DW                 62.400 usec
DE                  6.50 usec
TE                 295.8 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
SI                 65536
SF           400.1300105 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



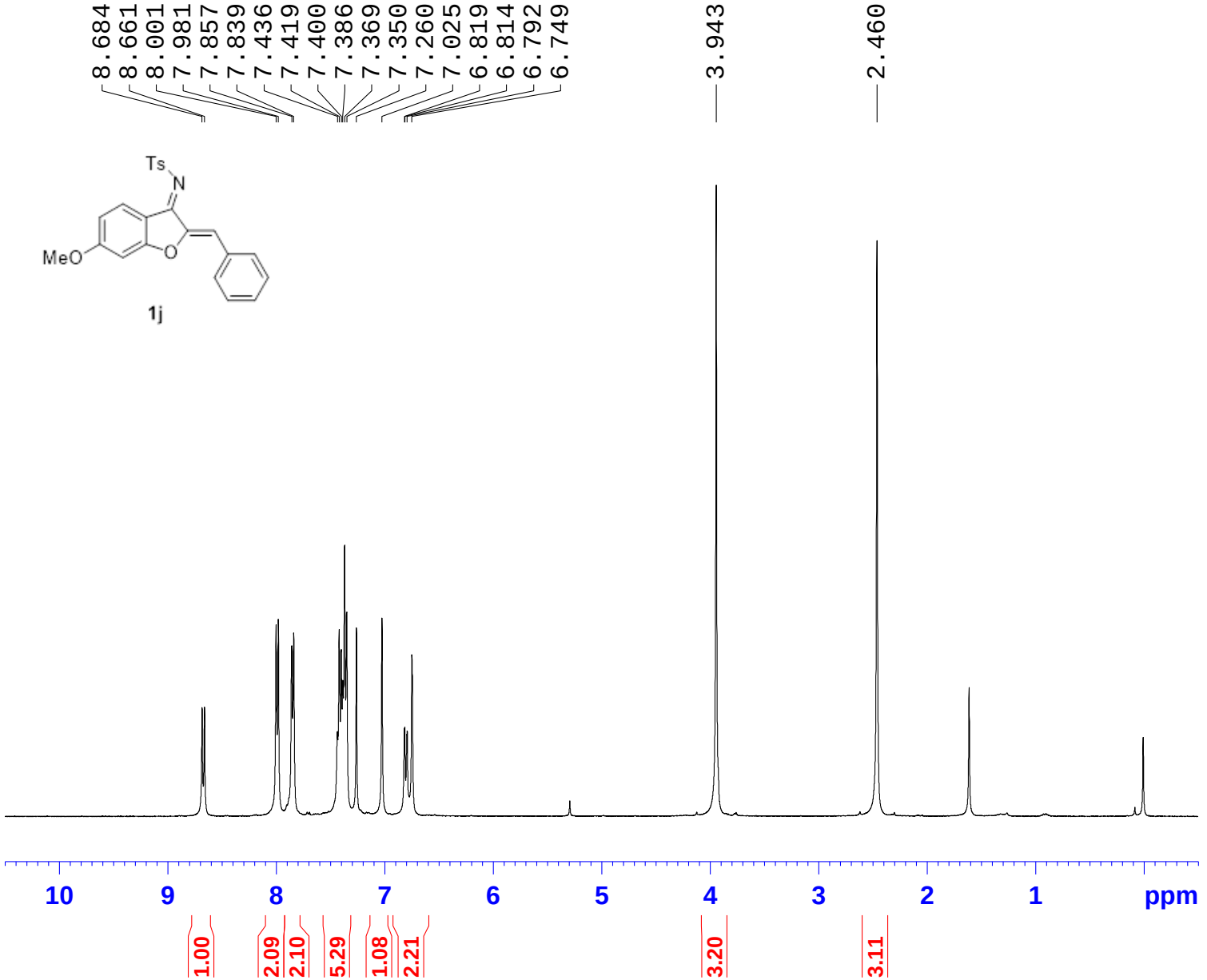
NAME	fq5-35
EXPNO	2
PROCNO	1
Date_	20190323
Time	16.54
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	100
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	296.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127792 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



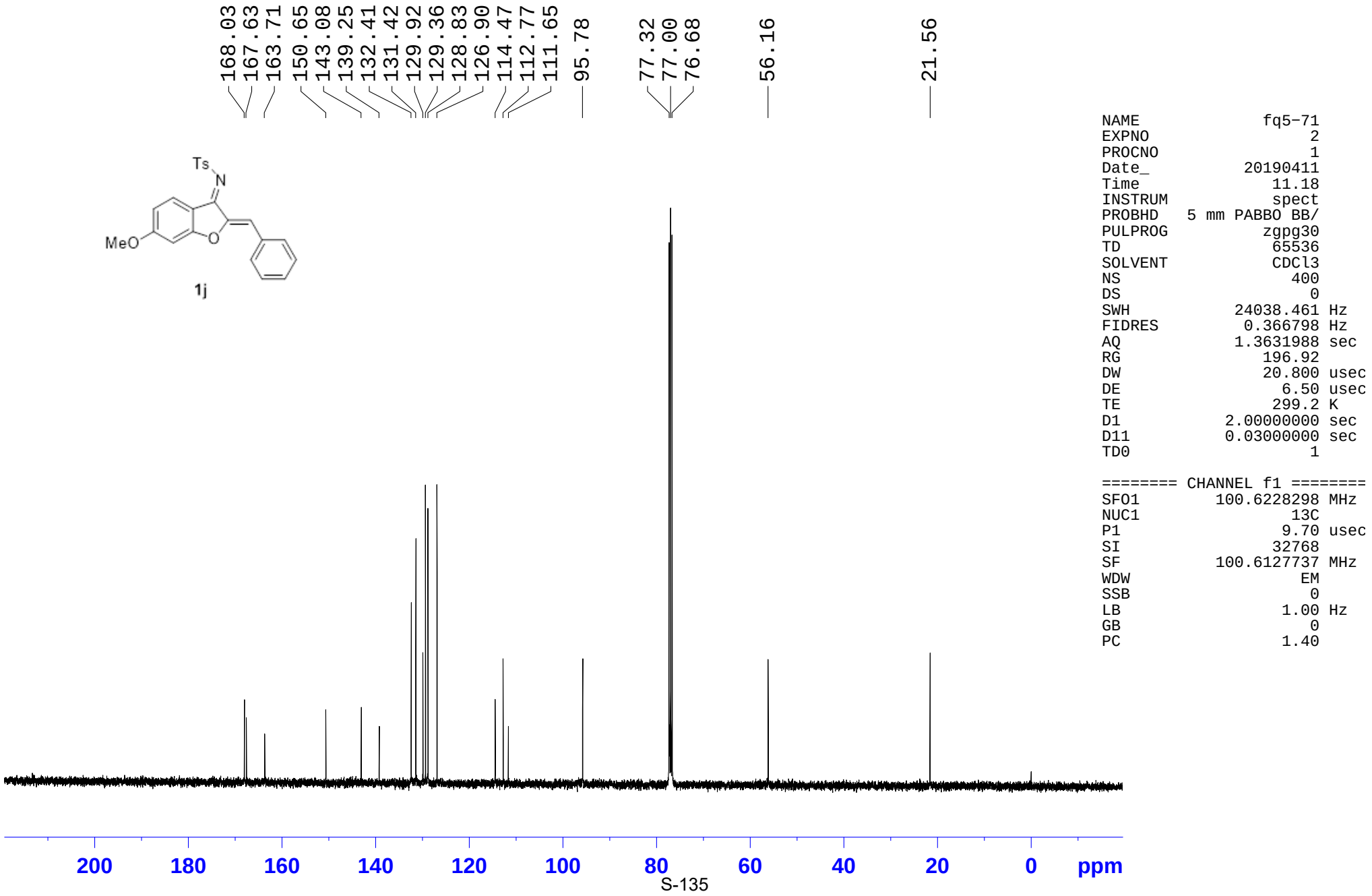

```
NAME                fq5-45
EXPNO                    1
PROCNO                   1
Date_             20190327
Time                 20.39
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       0
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ               4.0894966 sec
RG                   82.92
DW                 62.400 usec
DE                  6.50 usec
TE                 295.8 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                  14.50 usec
SI                   65536
SF            400.1300102 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

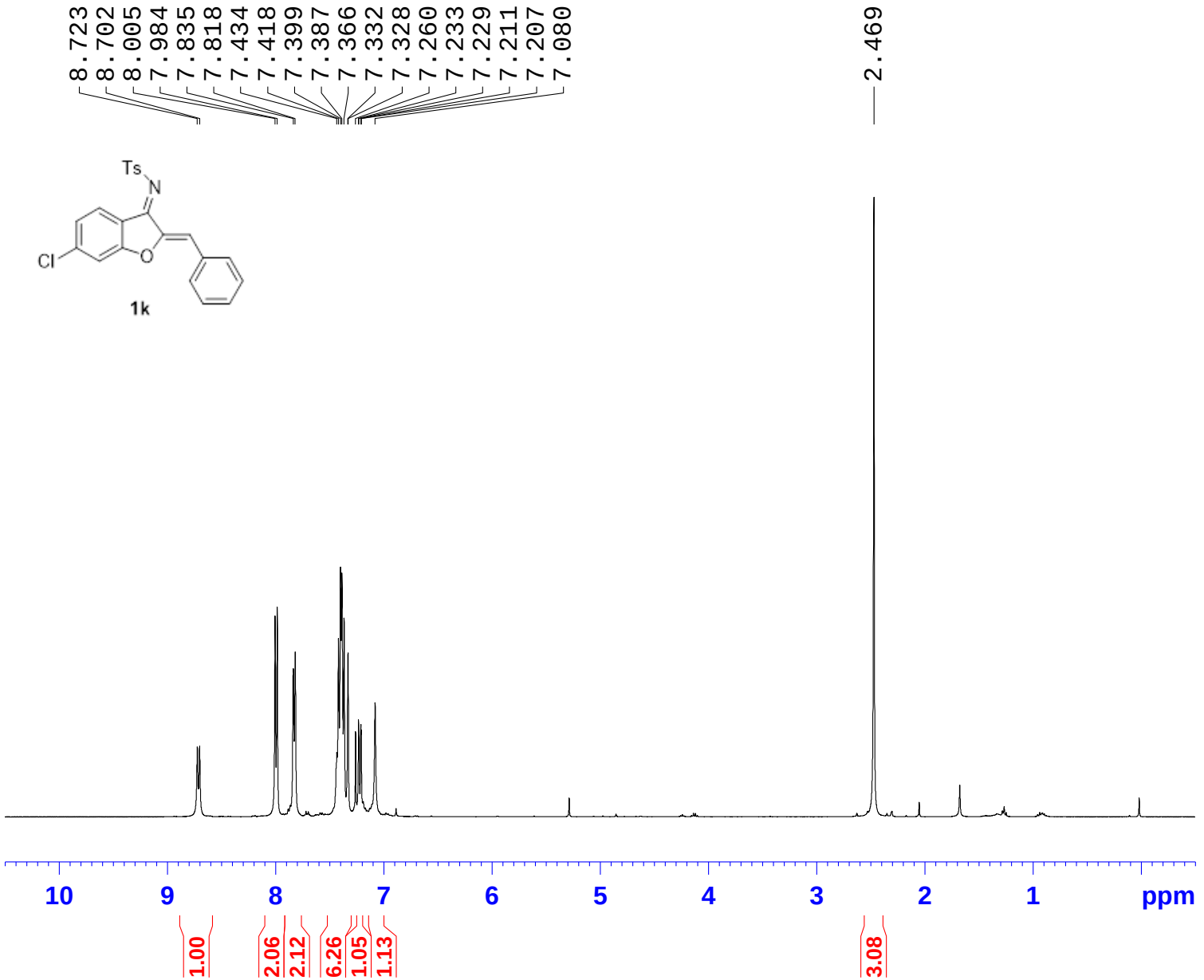


NAME	fq5-45
EXPNO	2
PROCNO	1
Date_	20190327
Time	20.42
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	120
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	296.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127744 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

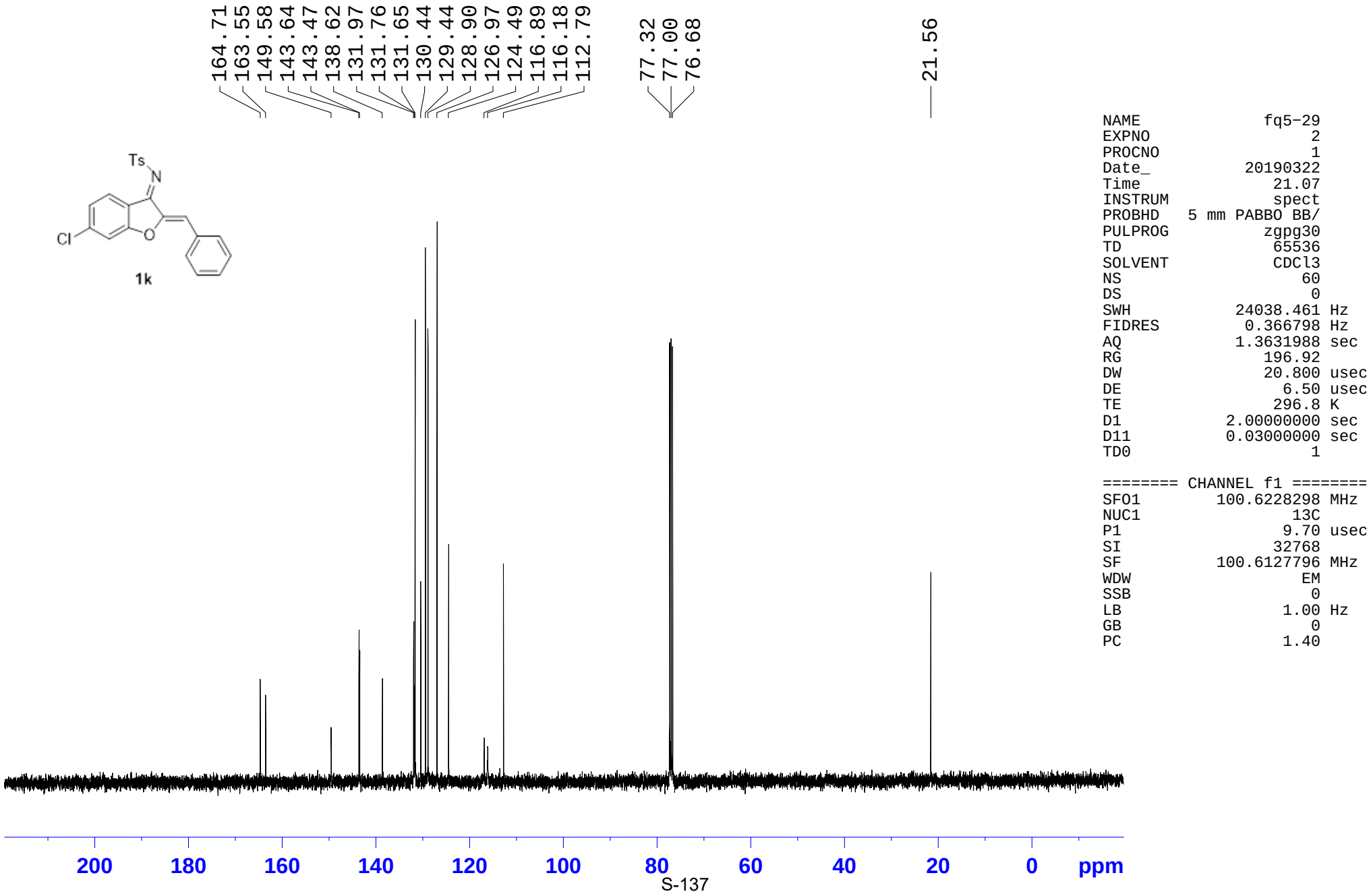



```
NAME                fq5-71
EXPNO                    1
PROCNO                   1
Date_             20190411
Time                 11.14
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       4
DS                       0
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894966 sec
RG                   103.52
DW                   62.400 usec
DE                    6.50 usec
TE                   298.4 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                    1H
P1                   14.50 usec
SI                   65536
SF              400.1300104 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

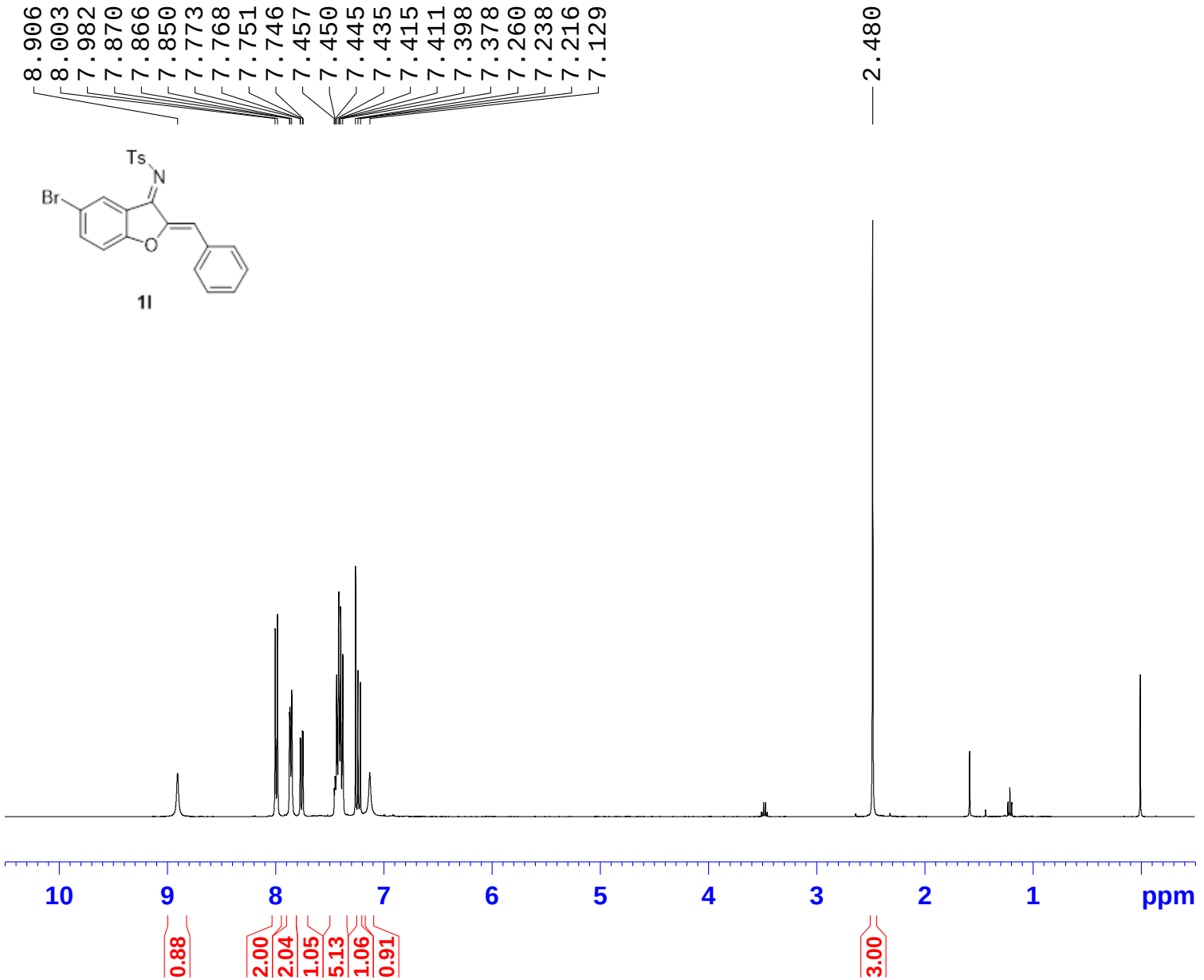

168.03
167.63
163.71
150.65
143.08
139.25
132.41
131.42
129.92
129.36
128.83
126.90
114.47
112.77
111.65
95.78
77.32
77.00
76.68
56.16
21.56
Ts
N
MeO
O
1j
NAME fq5-71
EXPNO 2
PROCNO 1
Date_ 20190411
Time 11.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
SI 32768
SF 100.6127737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm



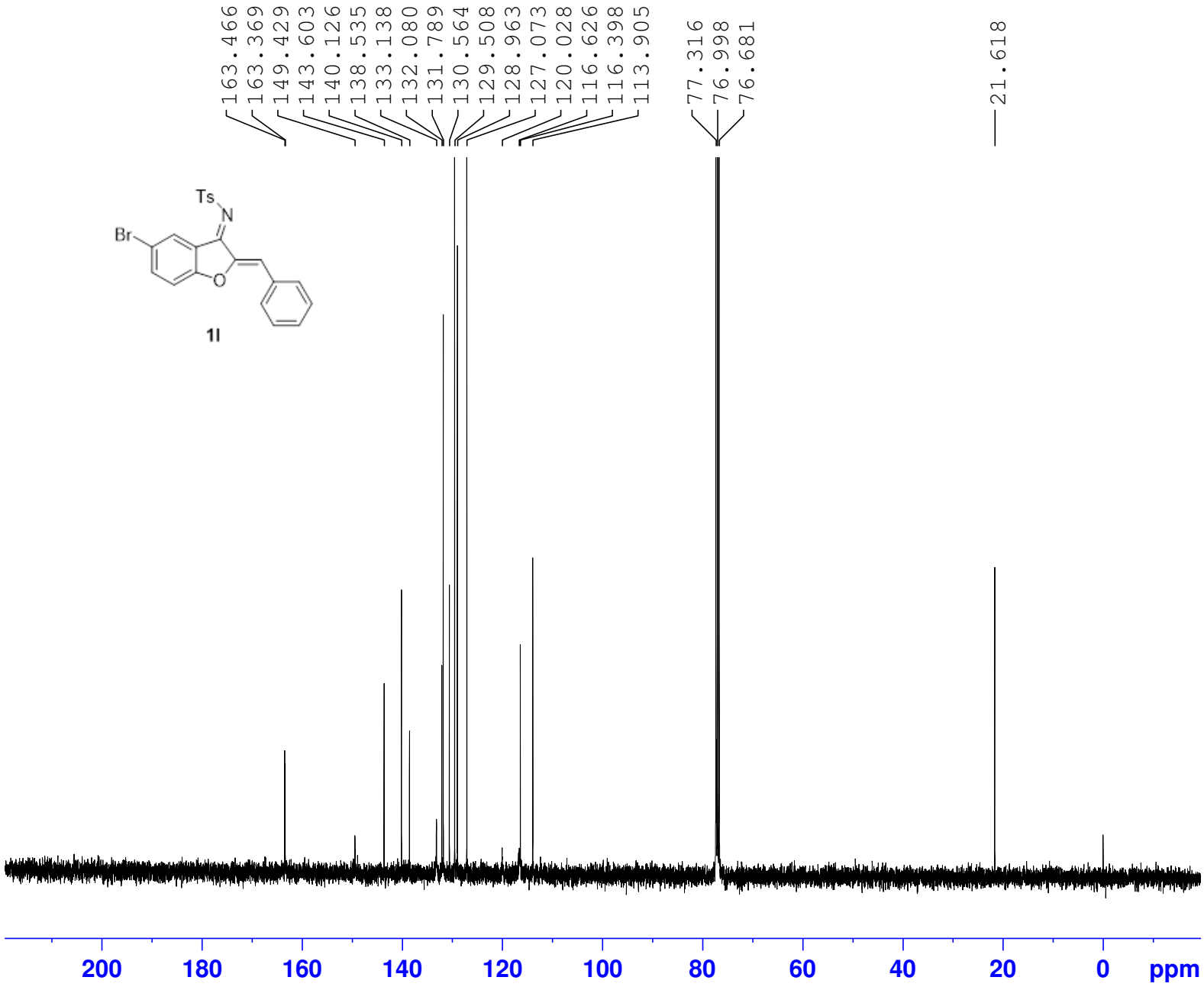
NAME	fq5-29
EXPNO	1
PROCNO	1
Date_	20190322
Time	21.06
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	4
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	4.51
DW	62.400 usec
DE	6.50 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	14.50 usec
SI	65536
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



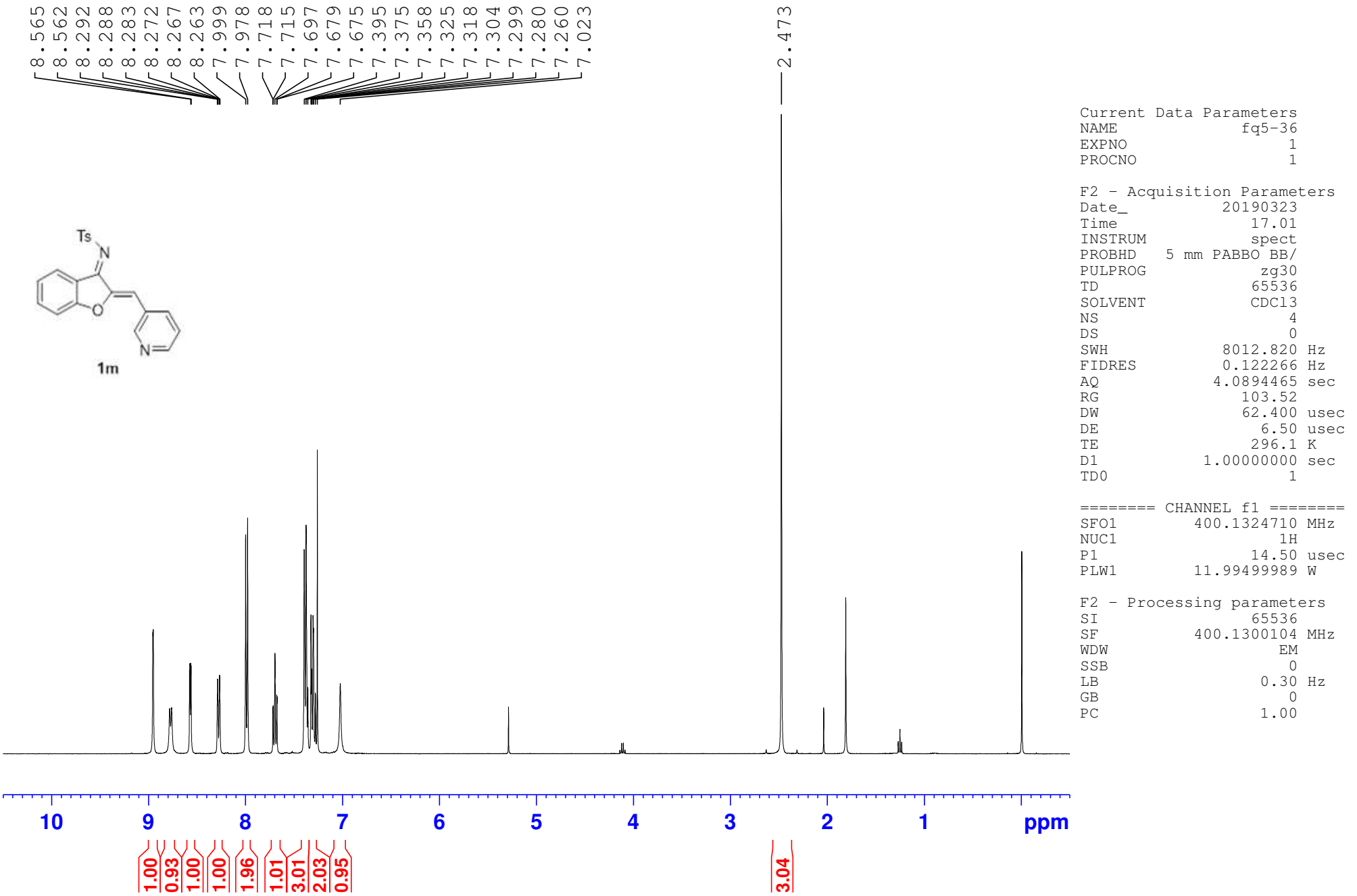
NAME	fq5-29
EXPNO	2
PROCNO	1
Date_	20190322
Time	21.07
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	60
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	296.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127796 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



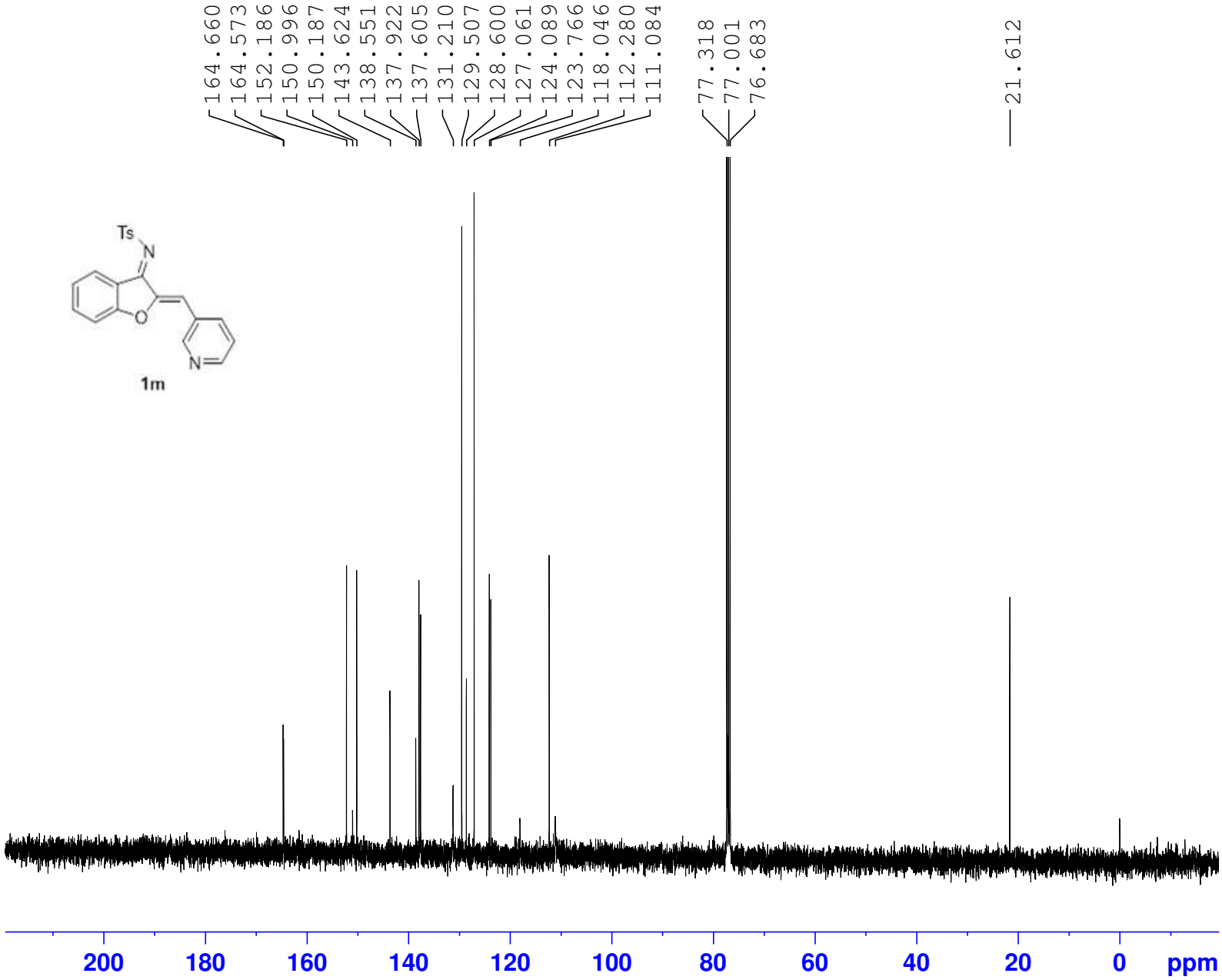
NAME	fq5-70
EXPNO	1
PROCNO	1
Date_	20190411
Time	10.57
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	4
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	88.84
DW	62.400 usec
DE	6.50 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	14.50 usec
SI	65536
SF	400.1300103 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



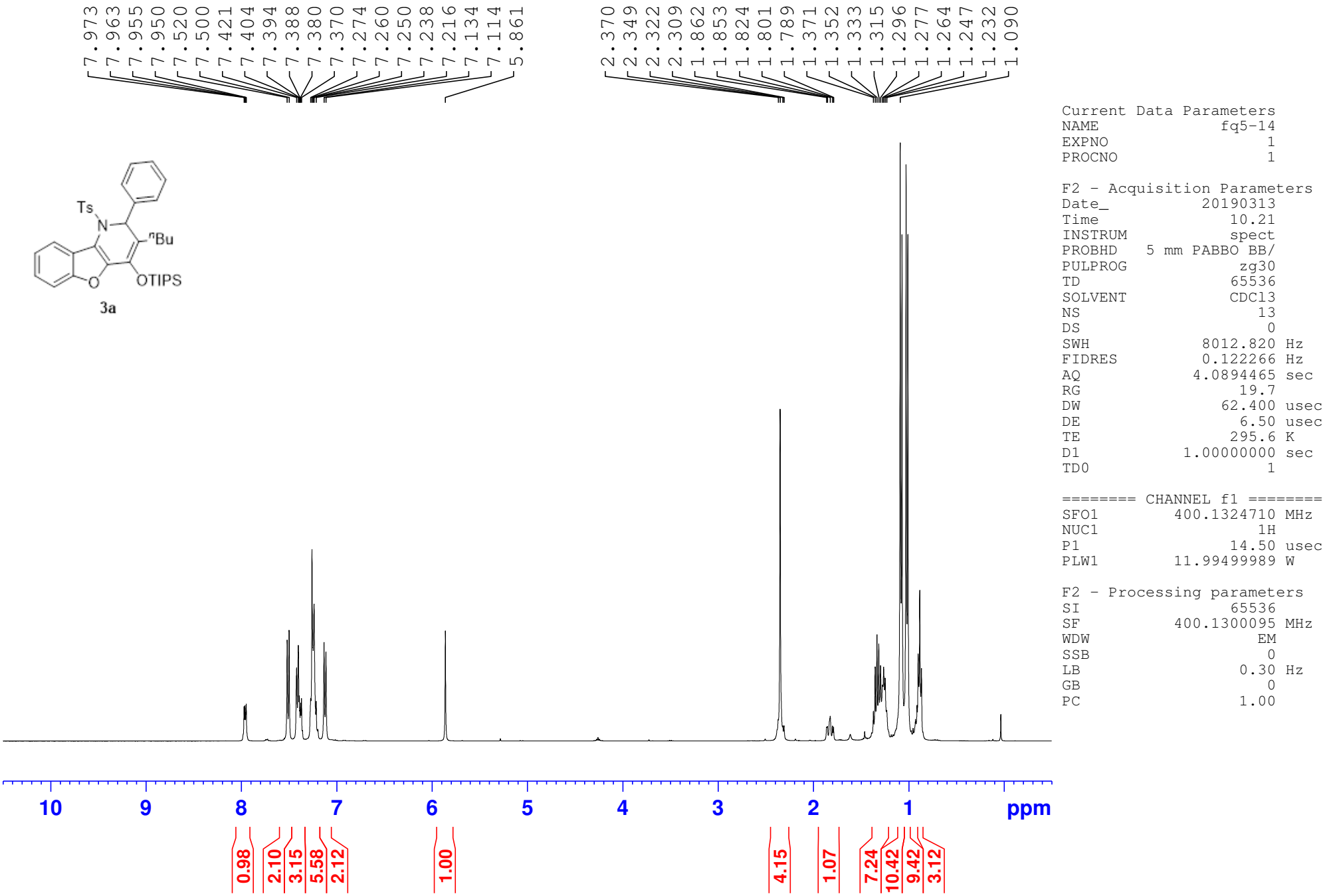

```
Current Data Parameters
NAME                 fq5-70
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_             20190411
Time                 10.58
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      240
DS                        0
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                   196.92
DW                  20.800 usec
DE                   6.50 usec
TE                  298.6 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           100.6228298 MHz
NUC1                    13C
P1                    9.70 usec
PLW1           46.98899841 W

======== CHANNEL f2 ========
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           11.99499989 W
PLW12           0.34213999 W
PLW13           0.27713001 W

F2 - Processing parameters
SI                    32768
SF             100.6127733 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```



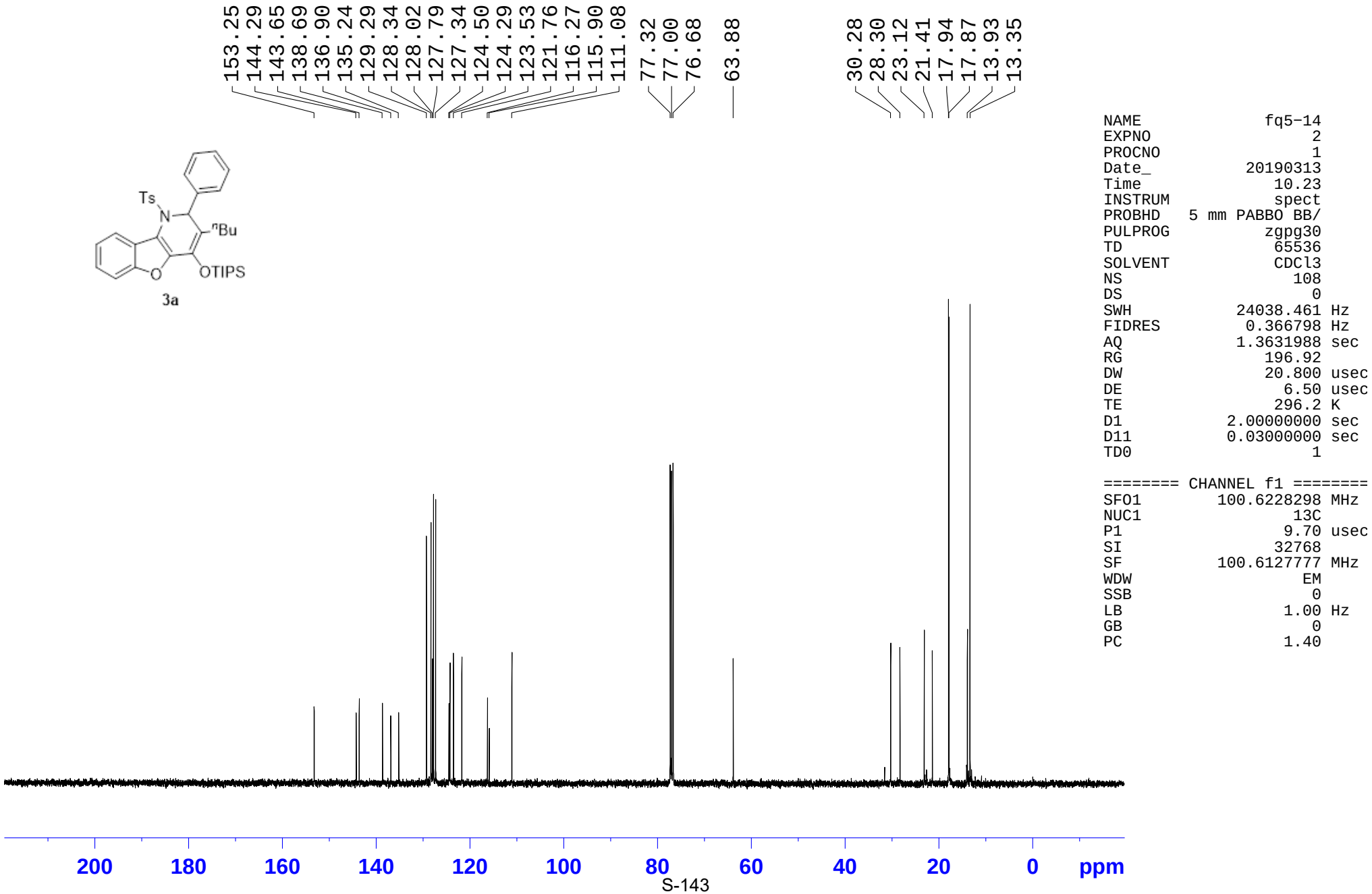

```
Current Data Parameters
NAME                  fq5-36
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190323
Time                  17.01
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        4
DS                        0
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894465 sec
RG                   103.52
DW                   62.400 usec
DE                    6.50 usec
TE                   296.1 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                      1H
P1                    14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                    65536
SF             400.1300104 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```

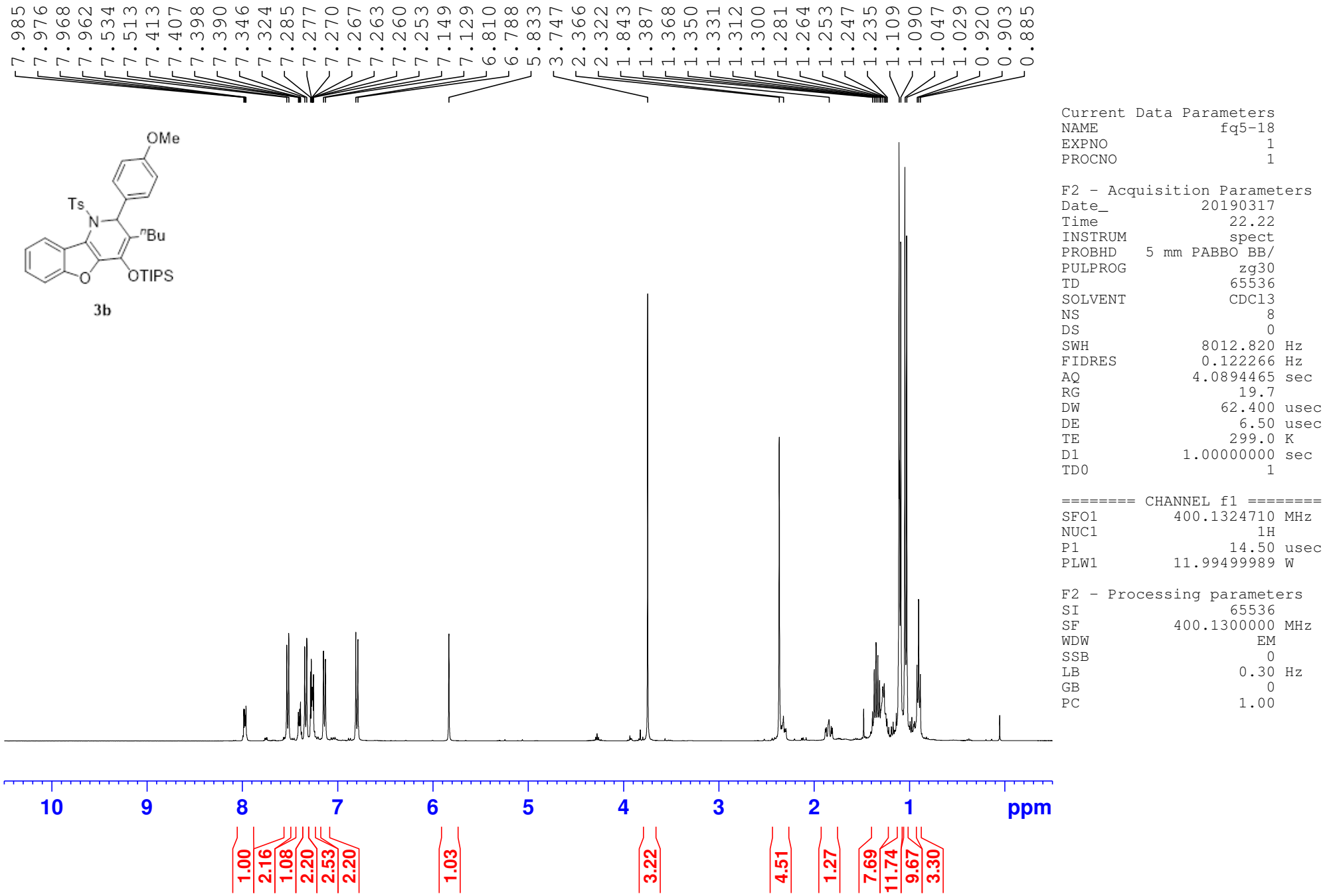


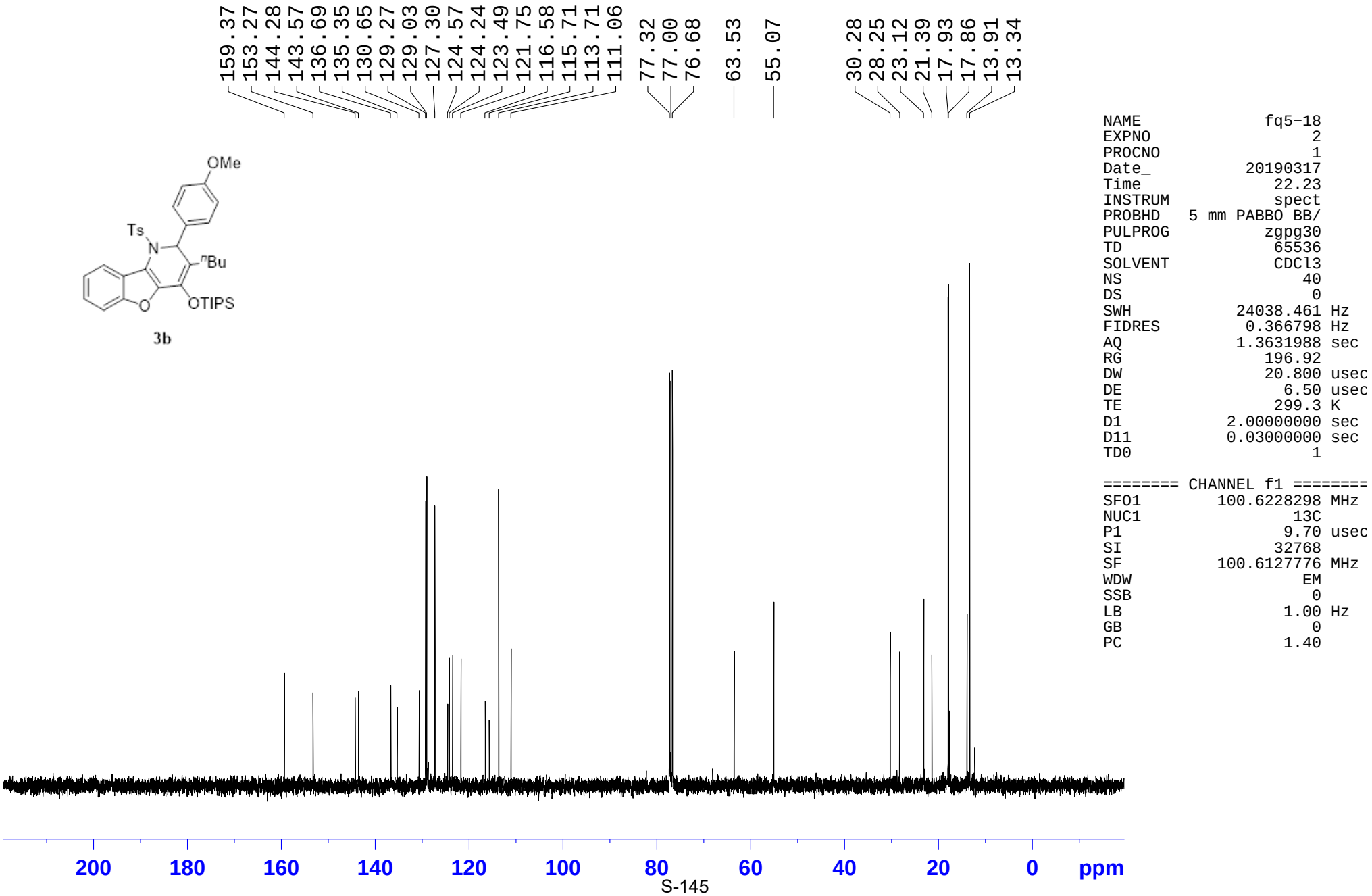

```
Current Data Parameters
NAME                  fq5-36
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190323
Time                  17.04
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       120
DS                         0
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631488 sec
RG                    196.92
DW                    20.800 usec
DE                     6.50 usec
TE                    296.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            100.6228298 MHz
NUC1                    13C
P1                     9.70 usec
PLW1           46.98899841 W

======== CHANNEL f2 ========
SFO2            400.1316005 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                 90.00 usec
PLW2           11.99499989 W
PLW12           0.34213999 W
PLW13           0.27713001 W

F2 - Processing parameters
SI                     32768
SF              100.6127746 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                     1.40
```

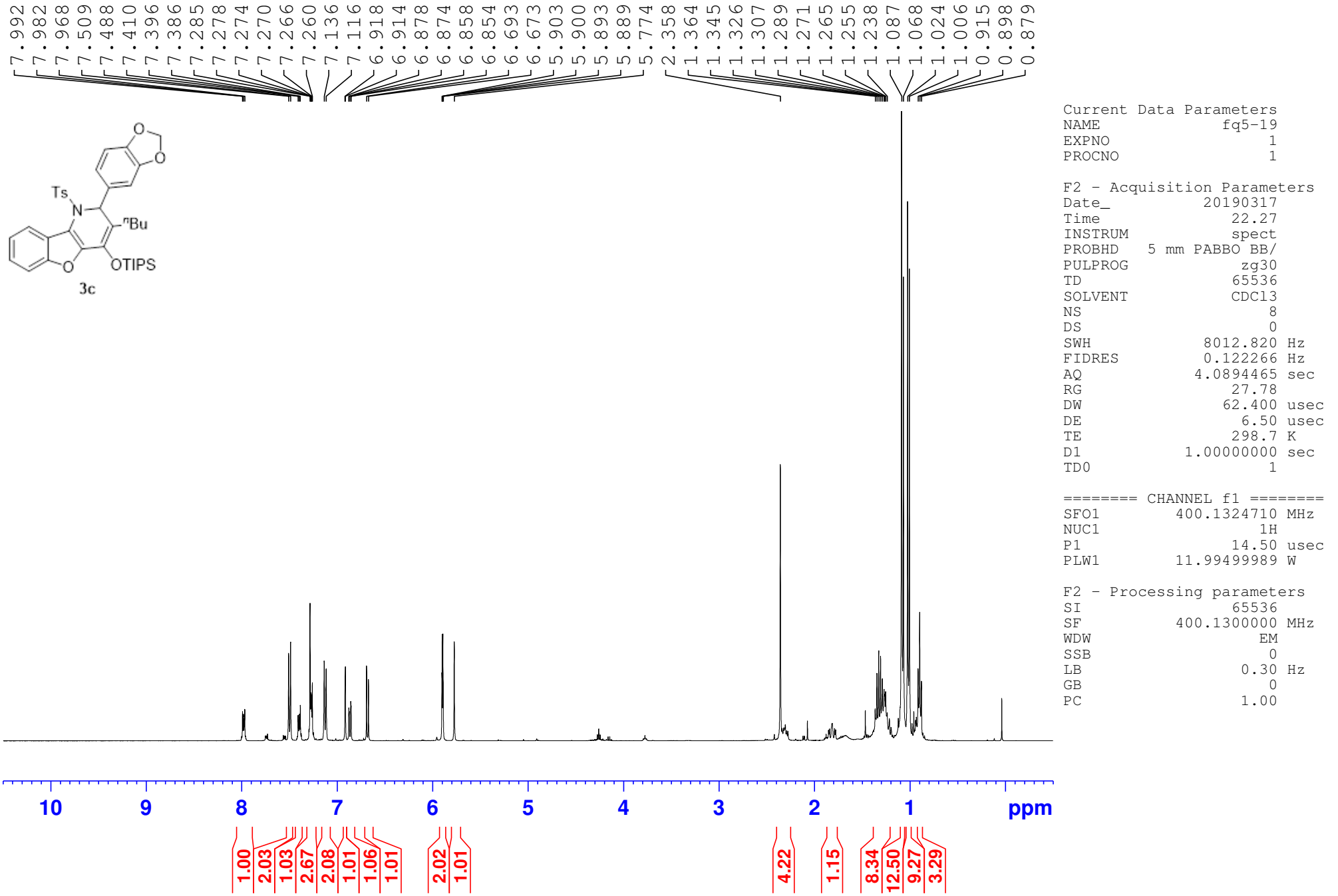



```
Current Data Parameters
NAME                  fq5-14
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190313
Time                  10.21
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       13
DS                        0
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                      19.7
DW                   62.400 usec
DE                    6.50 usec
TE                   295.6 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                   14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                    65536
SF             400.1300095 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```


153.25
144.29
143.65
138.69
136.90
135.24
129.29
128.34
128.02
127.79
127.34
124.50
124.29
123.53
121.76
116.27
115.90
111.08
77.32
77.00
76.68
63.88
30.28
28.30
23.12
21.41
17.94
17.87
13.93
13.35
Ts
N
nBu
OTIPS
O
3a
NAME fq5-14
EXPNO 2
PROCNO 1
Date_ 20190313
Time 10.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 108
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
SI 32768
SF 100.6127777 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm


7.985
7.976
7.968
7.962
7.534
7.513
7.413
7.407
7.398
7.390
7.346
7.324
7.285
7.277
7.270
7.267
7.263
7.260
7.253
7.149
7.129
6.810
6.788
5.833
3.747
2.366
2.322
1.843
1.387
1.368
1.350
1.331
1.312
1.300
1.281
1.264
1.253
1.247
1.235
1.109
1.090
1.047
1.029
0.920
0.903
0.885
OMe
Ts
N
nBu
O
OTIPS
3b
Current Data Parameters
NAME fq5-18
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190317
Time 22.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 19.7
DW 62.400 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.16
1.08
2.20
2.53
2.20
1.03
3.22
4.51
1.27
7.69
11.74
9.67
3.30


159.37
153.27
144.28
143.57
136.69
135.35
130.65
129.27
129.03
127.30
124.57
124.24
123.49
121.75
116.58
115.71
113.71
111.06
77.32
77.00
76.68
63.53
55.07
30.28
28.25
23.12
21.39
17.93
17.86
13.91
13.34
OMe
Ts
N
nBu
OTIPS
O
3b
NAME fq5-18
EXPNO 2
PROCNO 1
Date_ 20190317
Time 22.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 40
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
SI 32768
SF 100.6127776 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

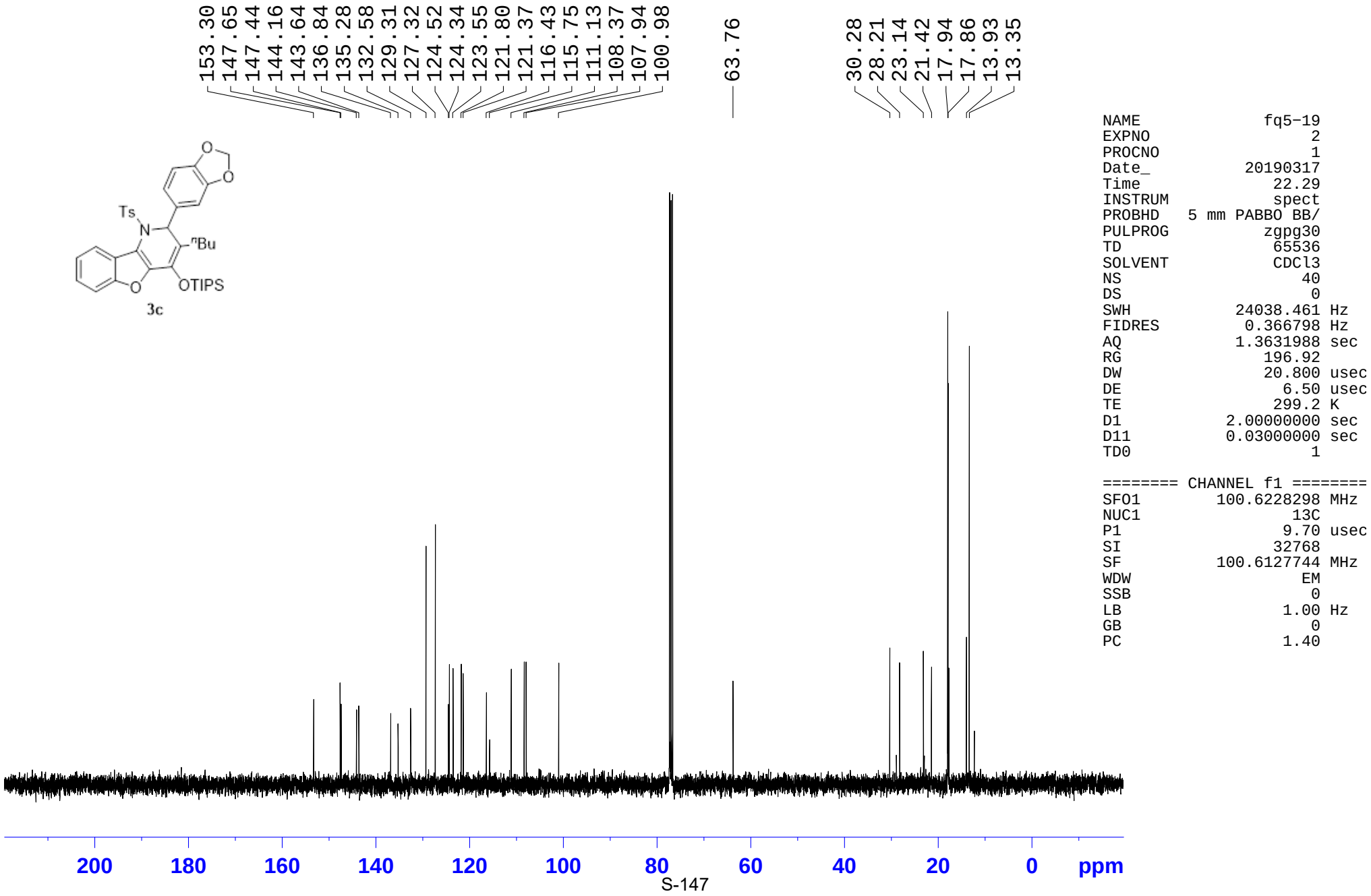


Current Data Parameters
NAME fq5-19
EXPNO 1
PROCNO 1

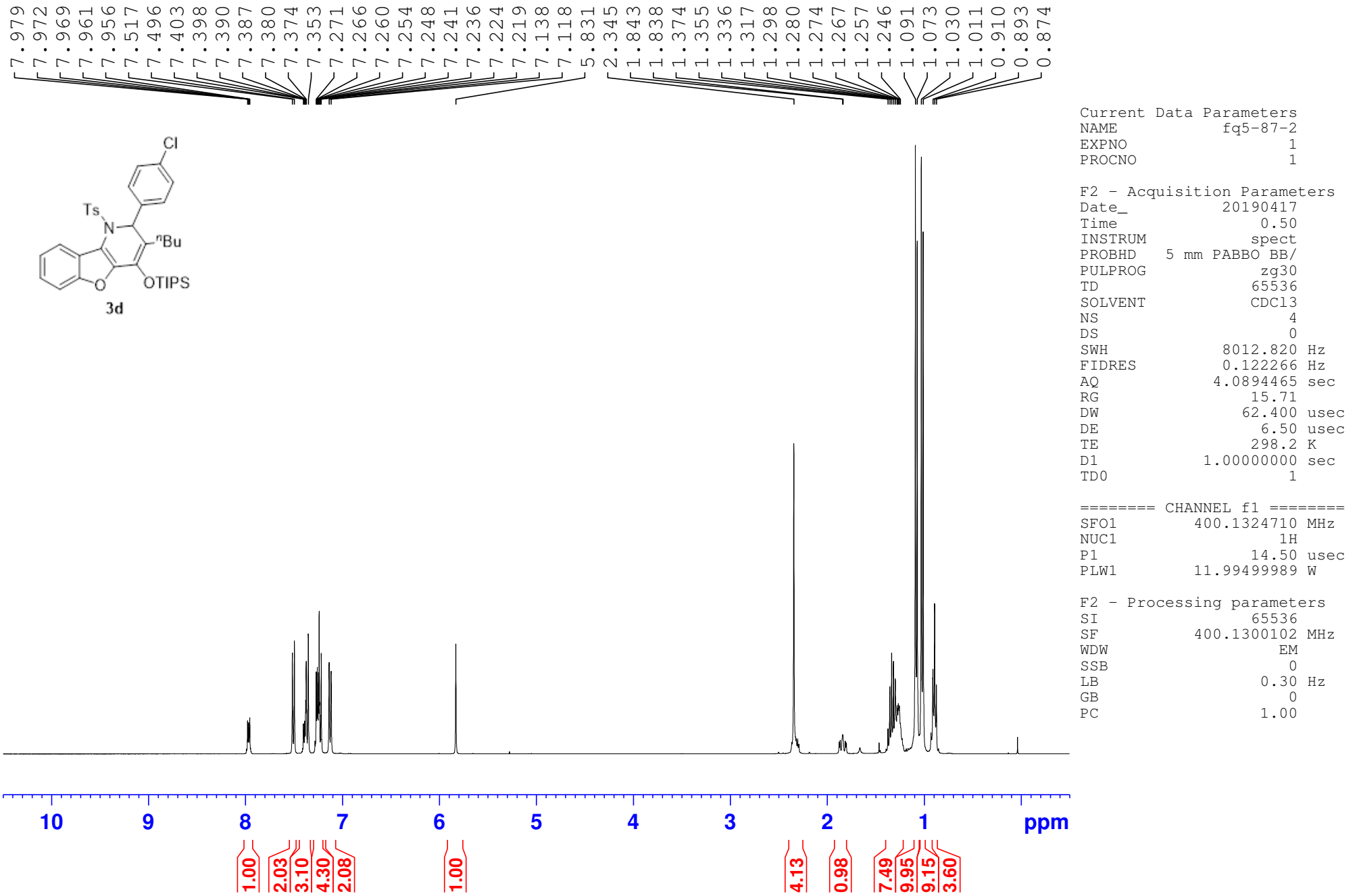
F2 - Acquisition Parameters
Date_ 20190317
Time 22.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 27.78
DW 62.400 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

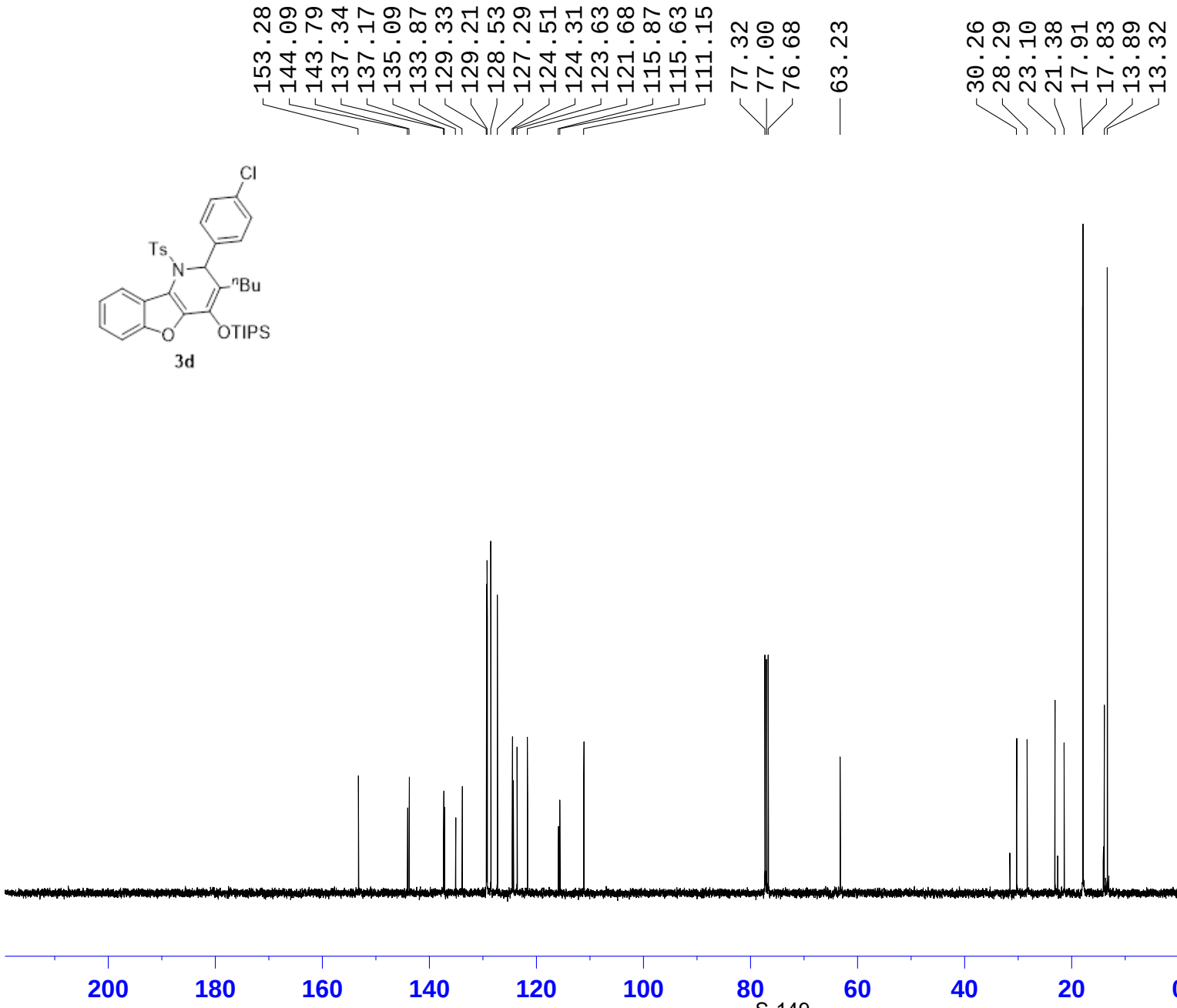
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



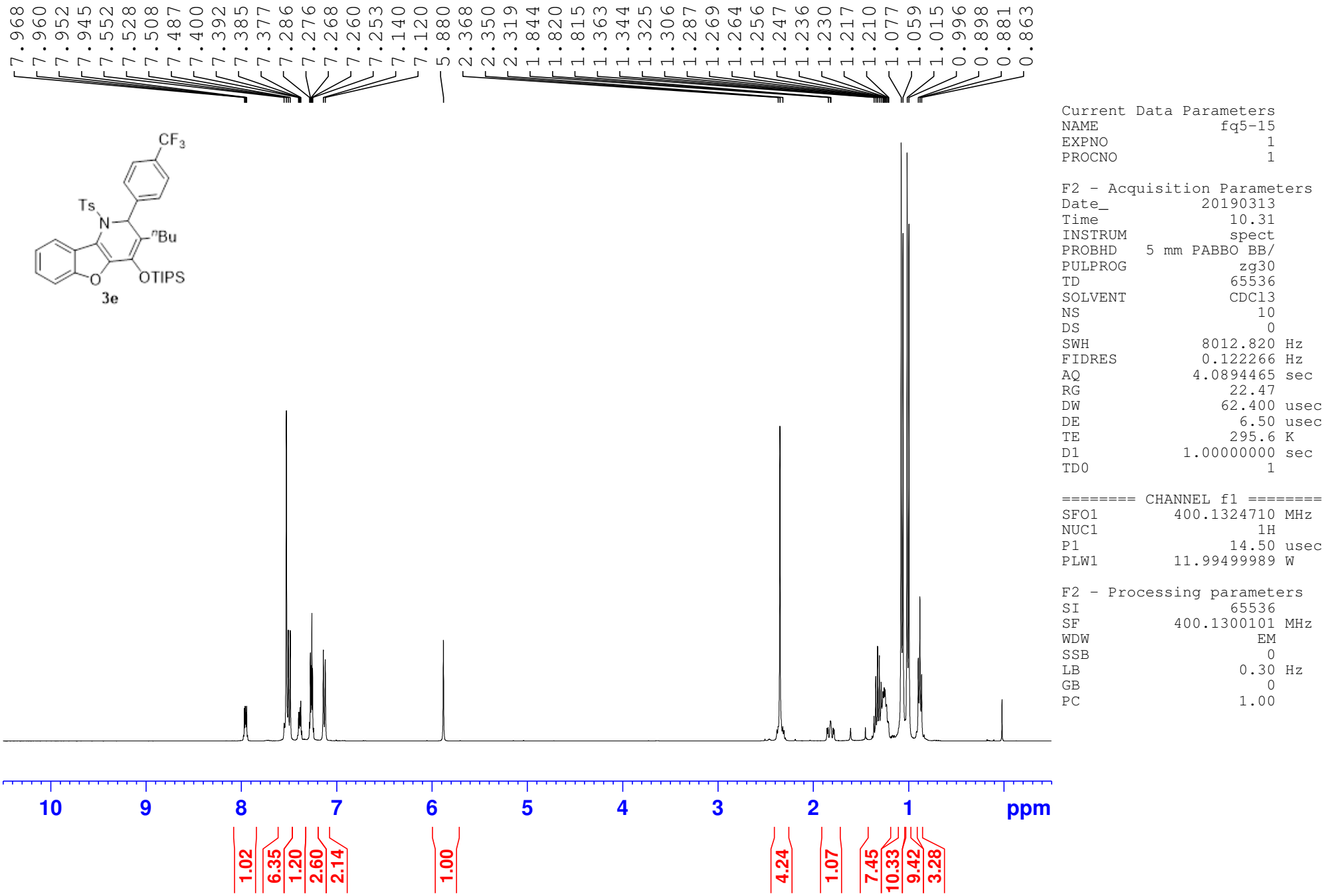
NAME	fq5-19
EXPNO	2
PROCNO	1
Date_	20190317
Time	22.29
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	40
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	299.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127744 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



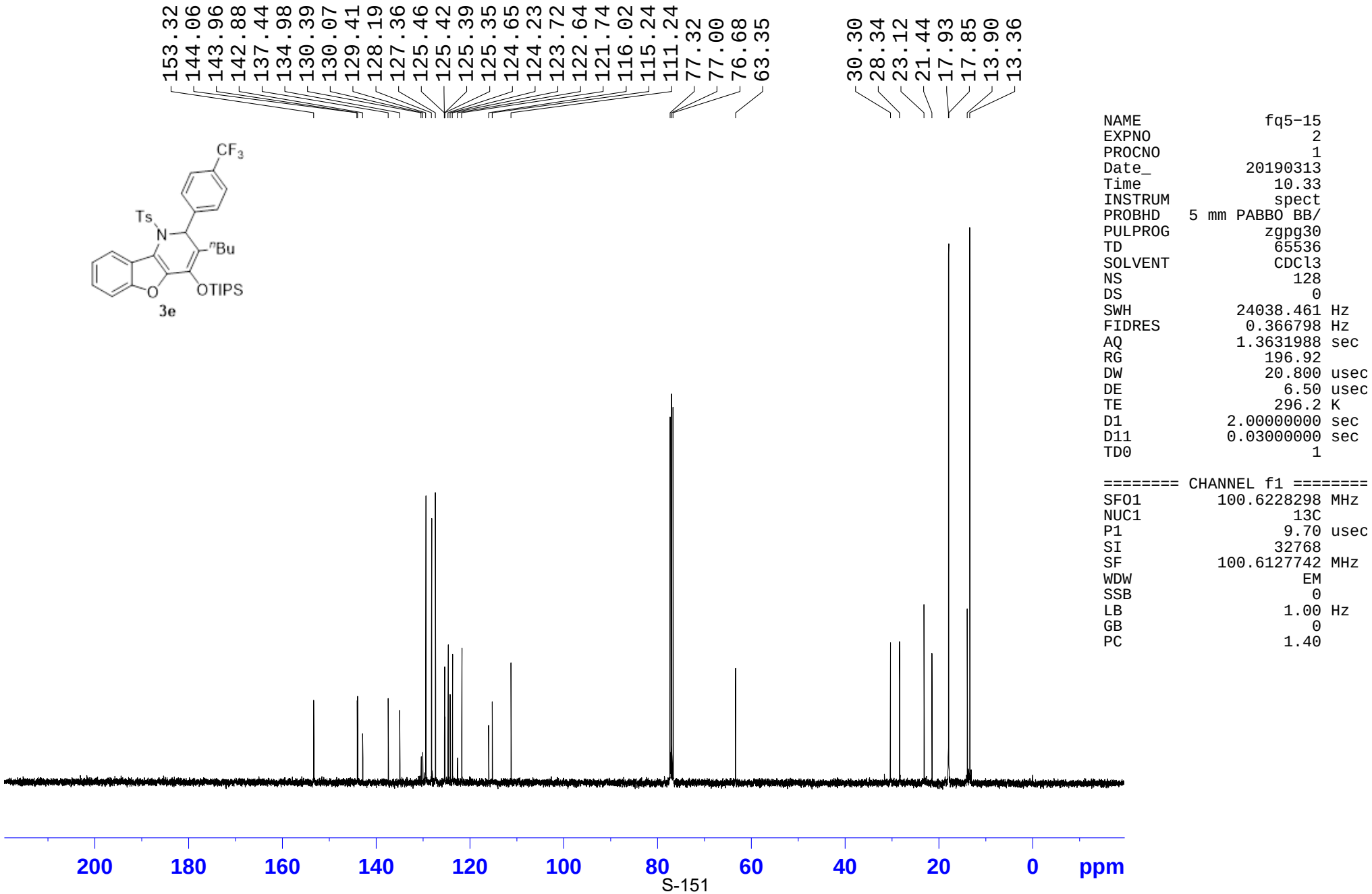

```
Current Data Parameters
NAME                  fq5-87-2
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20190417
Time                      0.50
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           4
DS                           0
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894465 sec
RG                       15.71
DW                     62.400 usec
DE                      6.50 usec
TE                     298.2 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                        1H
P1                      14.50 usec
PLW1            11.99499989 W

F2 - Processing parameters
SI                       65536
SF              400.1300102 MHz
WDW                         EM
SSB                          0
LB                      0.30 Hz
GB                           0
PC                       1.00
```

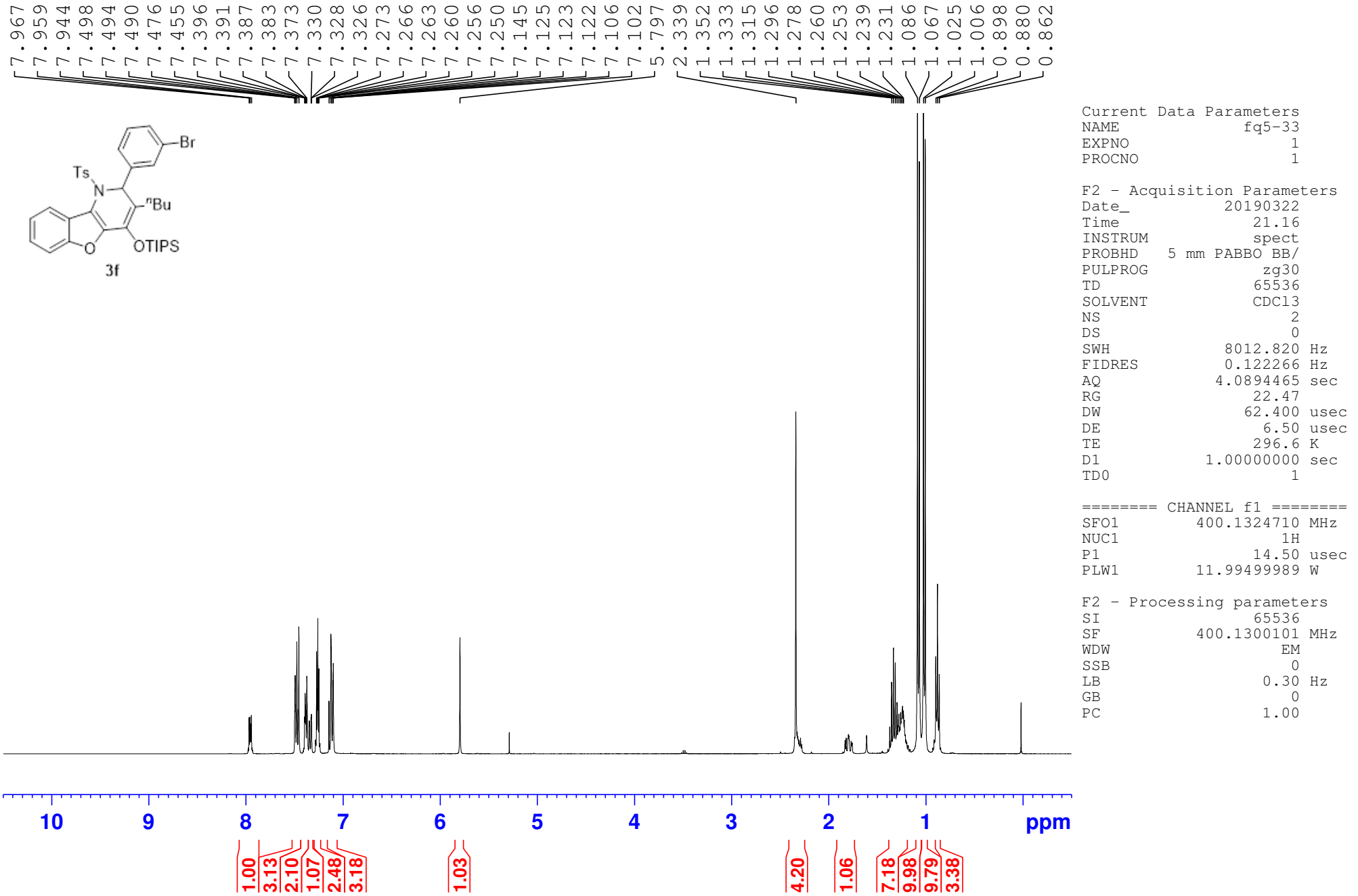


NAME	fq5-87-2
EXPNO	2
PROCNO	1
Date_	20190417
Time	0.52
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	40
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	298.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127799 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

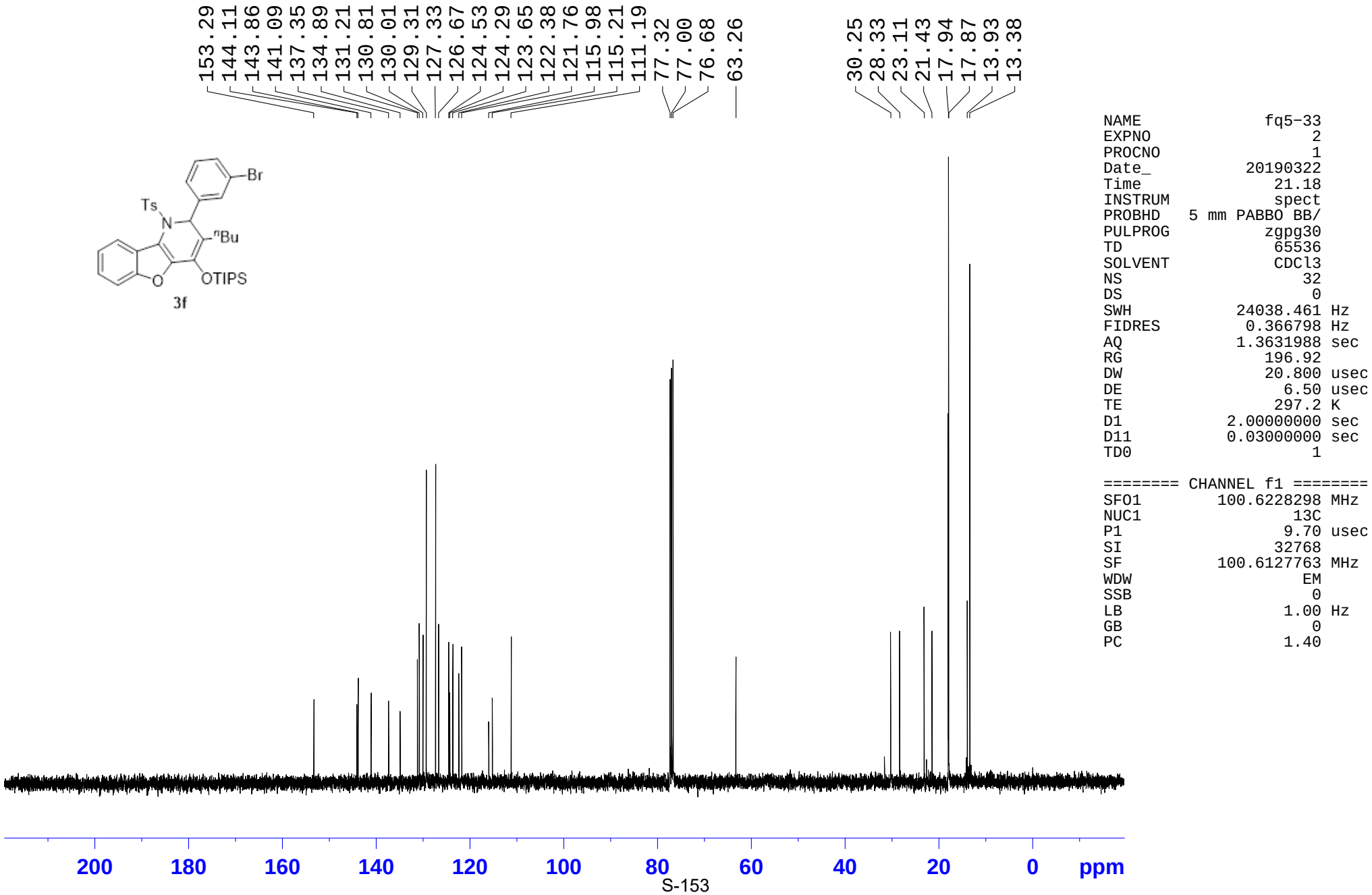



```
Current Data Parameters
NAME                  fq5-15
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20190313
Time                   10.31
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       10
DS                        0
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                     22.47
DW                  62.400 usec
DE                   6.50 usec
TE                   295.6 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                   14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                    65536
SF             400.1300101 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     1.00
```

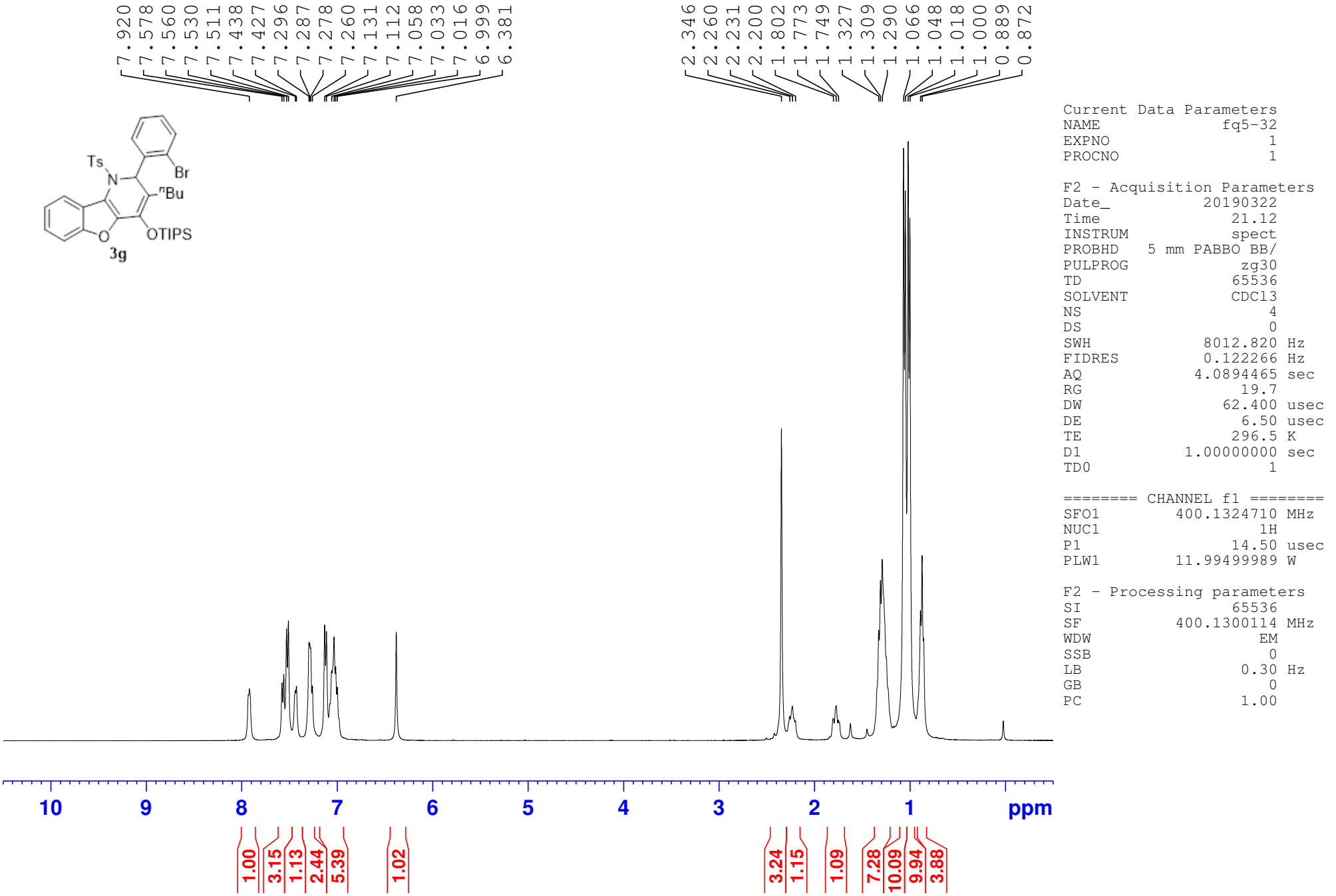

153.32
144.06
143.96
142.88
137.44
134.98
130.39
130.07
129.41
128.19
127.36
125.46
125.42
125.39
125.35
124.65
124.23
123.72
122.64
121.74
116.02
115.24
111.24
77.32
77.00
76.68
63.35
30.30
28.34
23.12
21.44
17.93
17.85
13.90
13.36
CF3
Ts
N
nBu
O
OTIPS
3e
NAME fq5-15
EXPNO 2
PROCNO 1
Date_ 20190313
Time 10.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
SI 32768
SF 100.6127742 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm



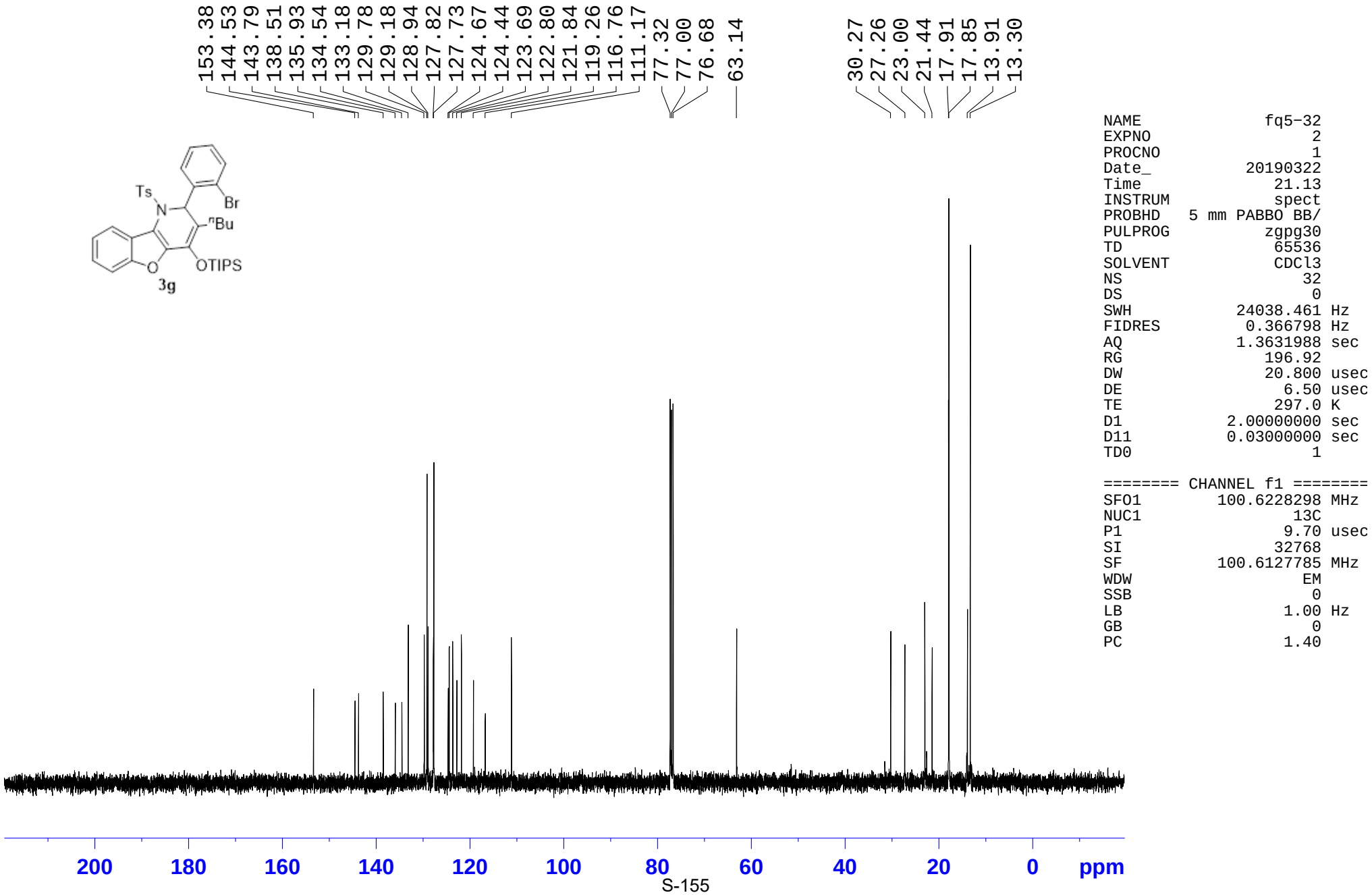

```
Current Data Parameters
NAME                  fq5-33
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190322
Time                  21.16
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                         2
DS                         0
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                    22.47
DW                  62.400 usec
DE                   6.50 usec
TE                  296.6 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                   14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                    65536
SF             400.1300101 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                    1.00
```



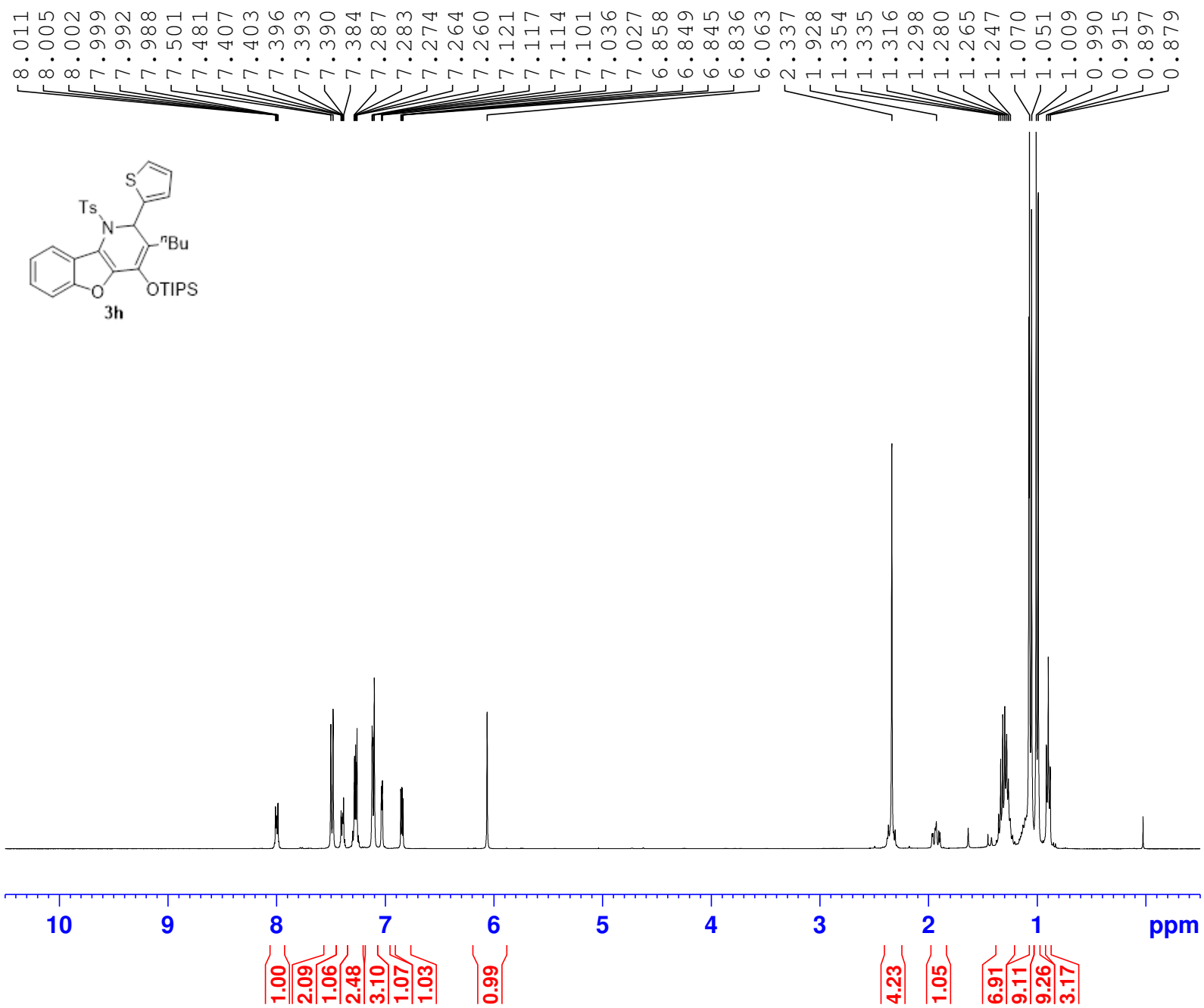
NAME	fq5-33
EXPNO	2
PROCNO	1
Date_	20190322
Time	21.18
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	297.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127763 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



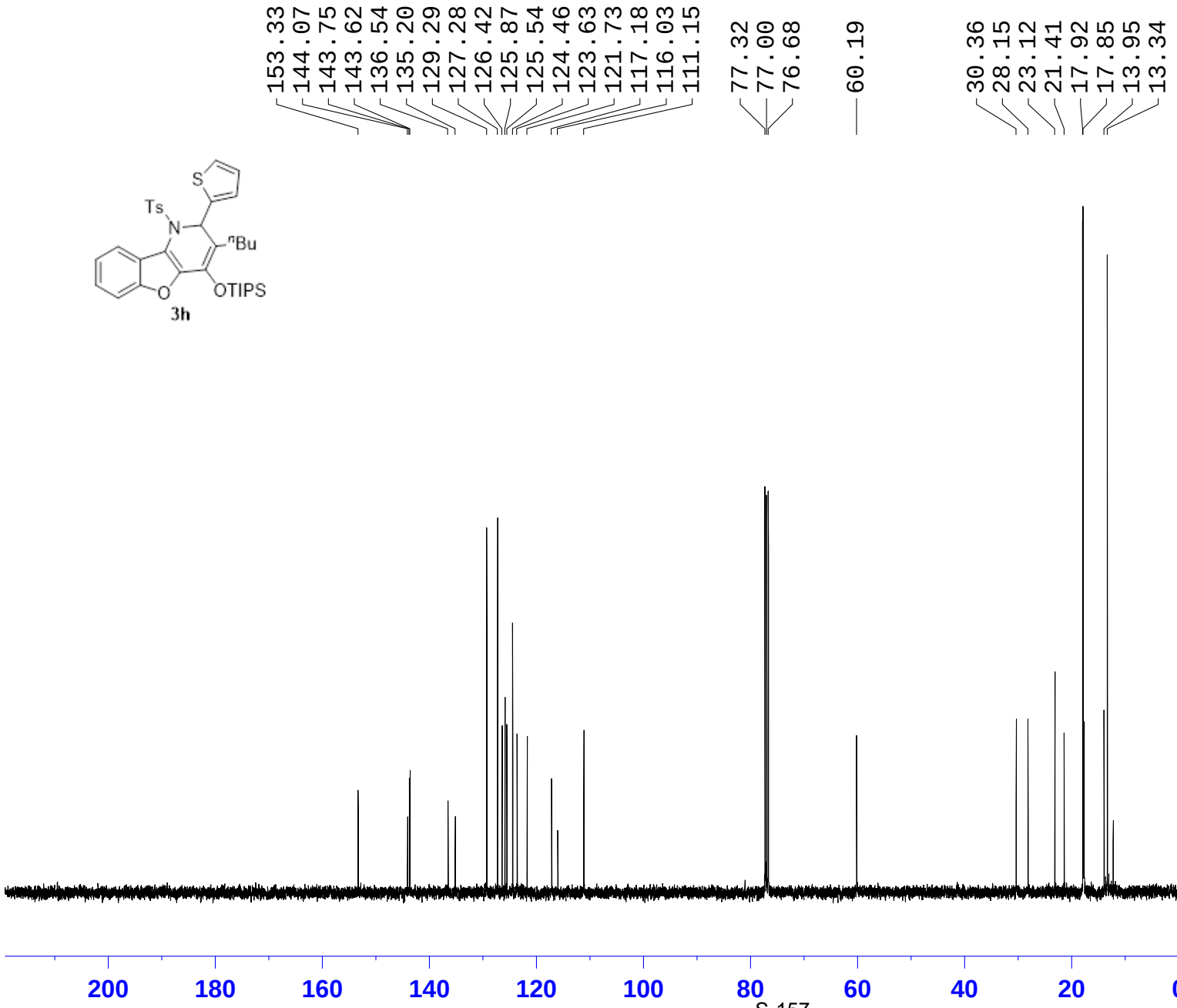

```
Current Data Parameters
NAME                  fq5-32
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190322
Time                  21.12
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        4
DS                        0
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894465 sec
RG                       19.7
DW                  62.400 usec
DE                   6.50 usec
TE                   296.5 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                  14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                    65536
SF             400.1300114 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     1.00
```



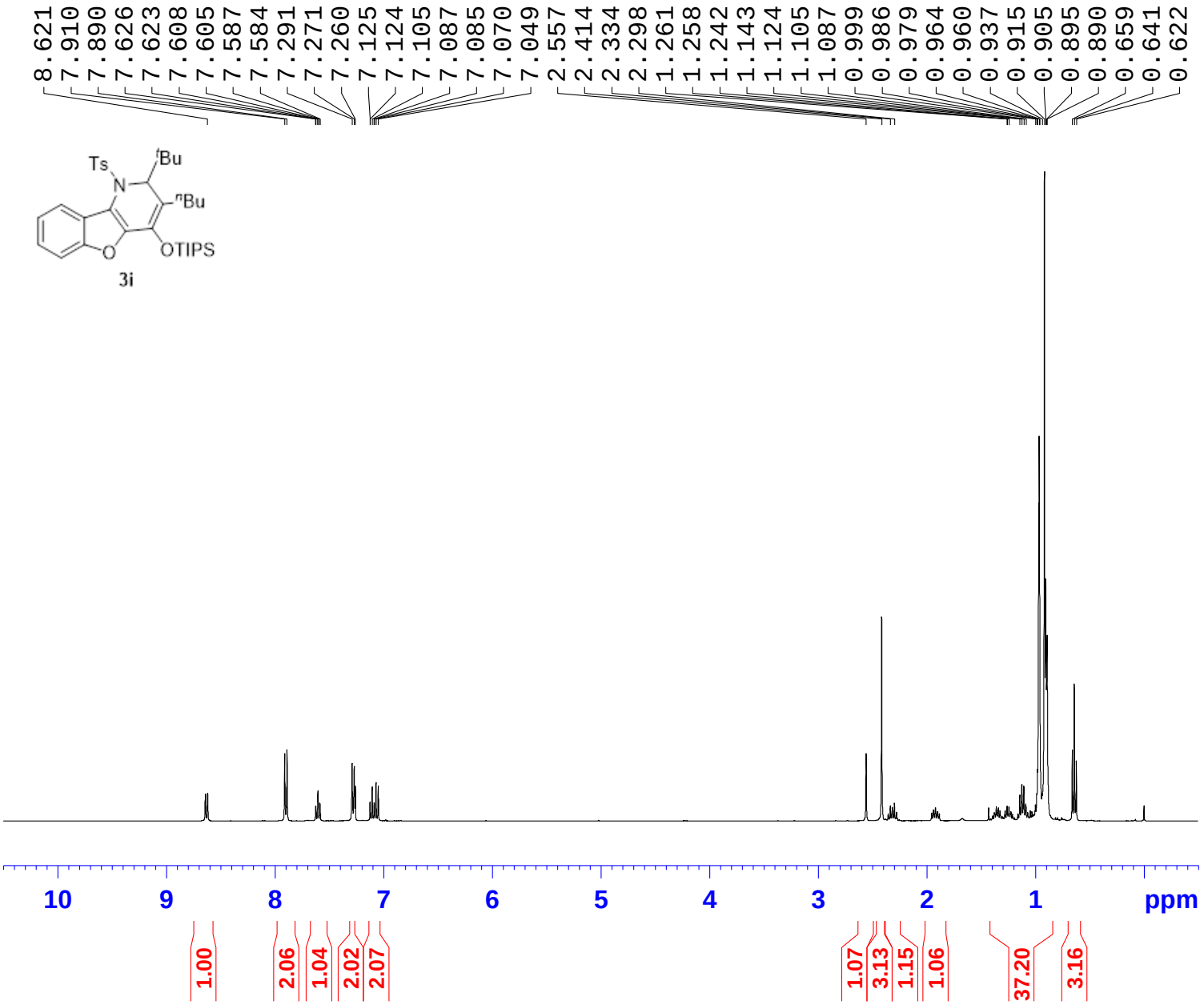
NAME	fq5-32
EXPNO	2
PROCNO	1
Date_	20190322
Time	21.13
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	297.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127785 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



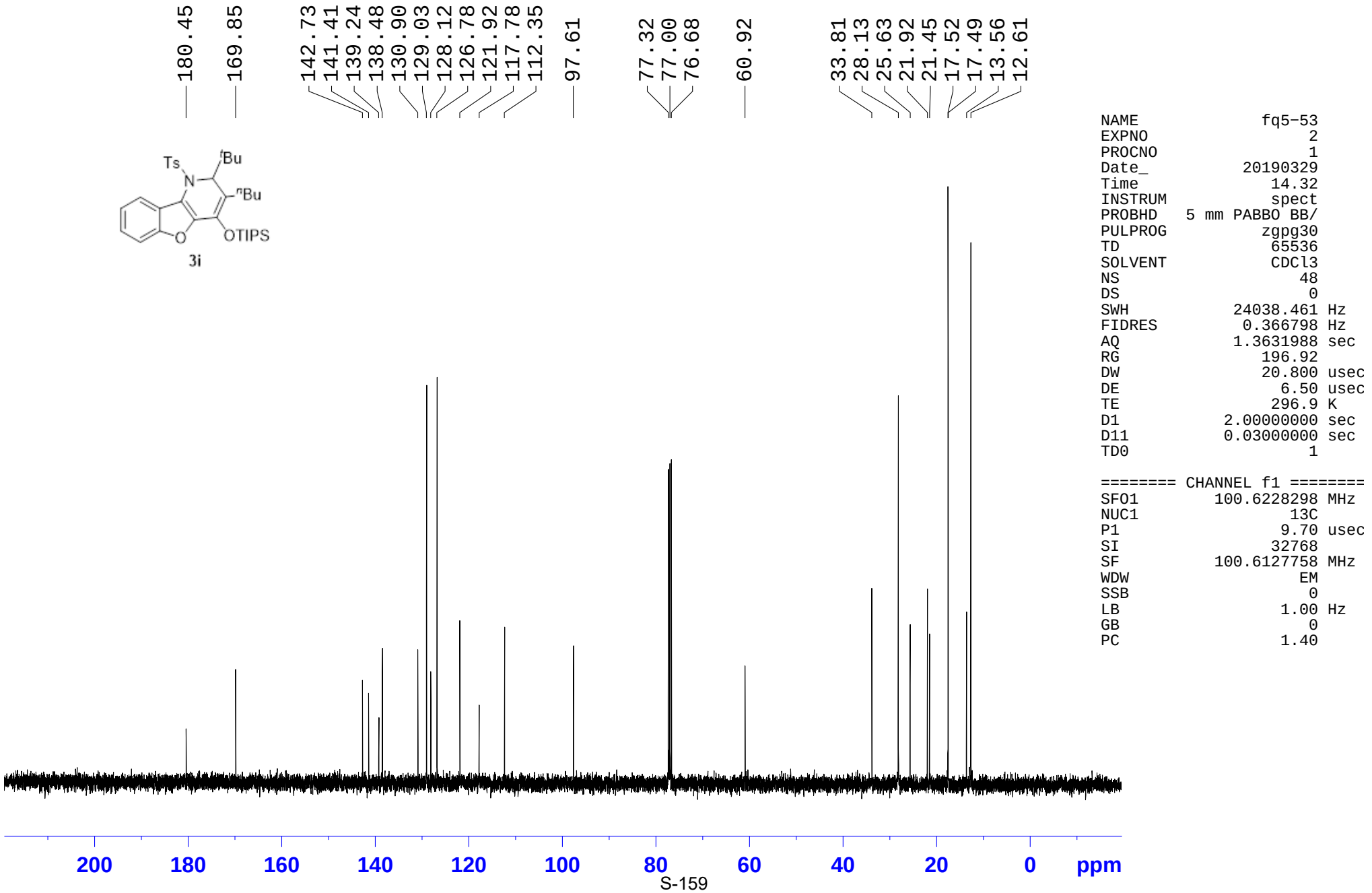

```
Current Data Parameters
NAME                  fq5-37
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20190325
Time                   22.18
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                         4
DS                         0
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                      19.7
DW                   62.400 usec
DE                    6.50 usec
TE                   296.5 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                   14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                    65536
SF             400.1300102 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     1.00
```

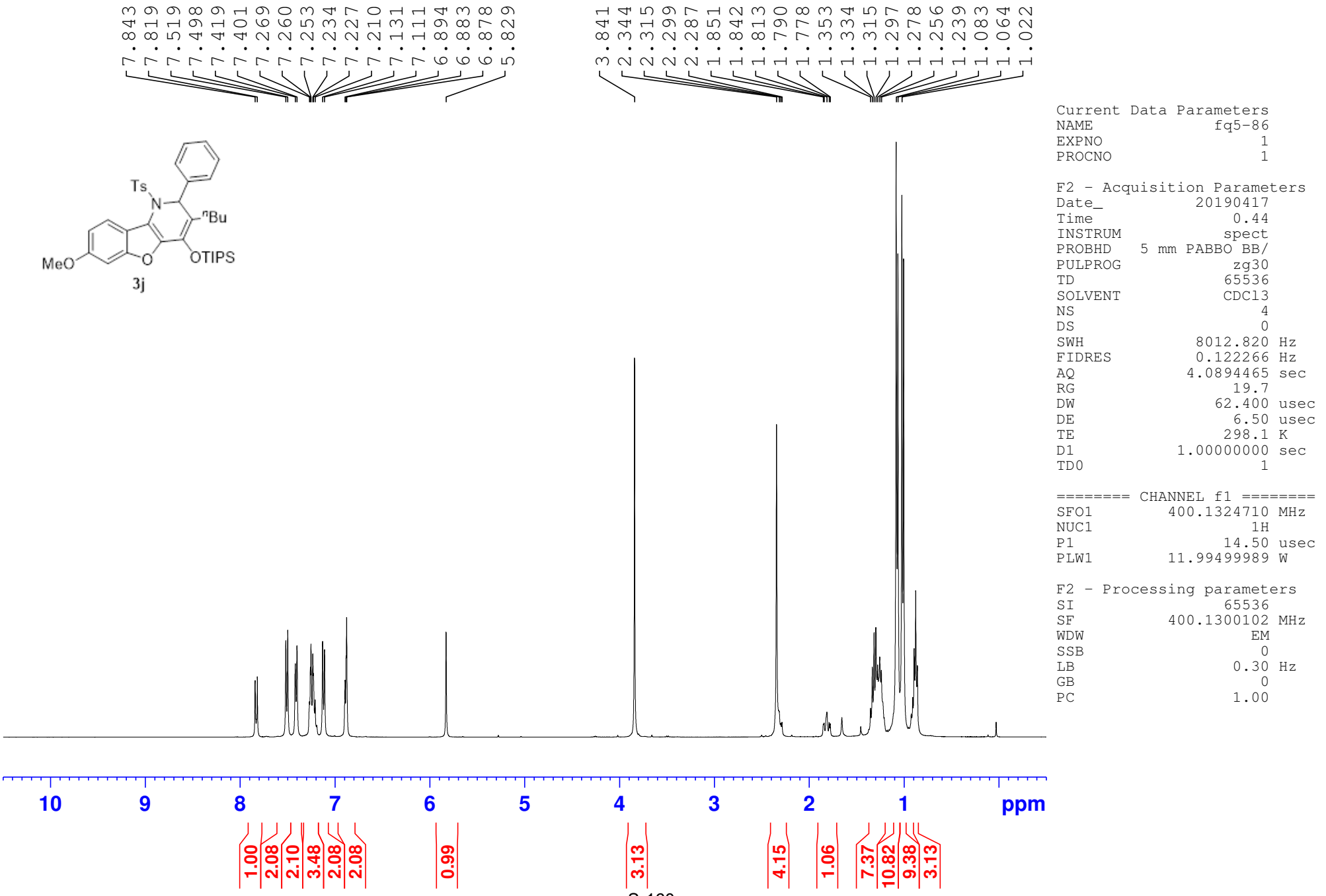


NAME	fq5-37
EXPNO	2
PROCNO	1
Date_	20190325
Time	22.19
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	40
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	297.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127775 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

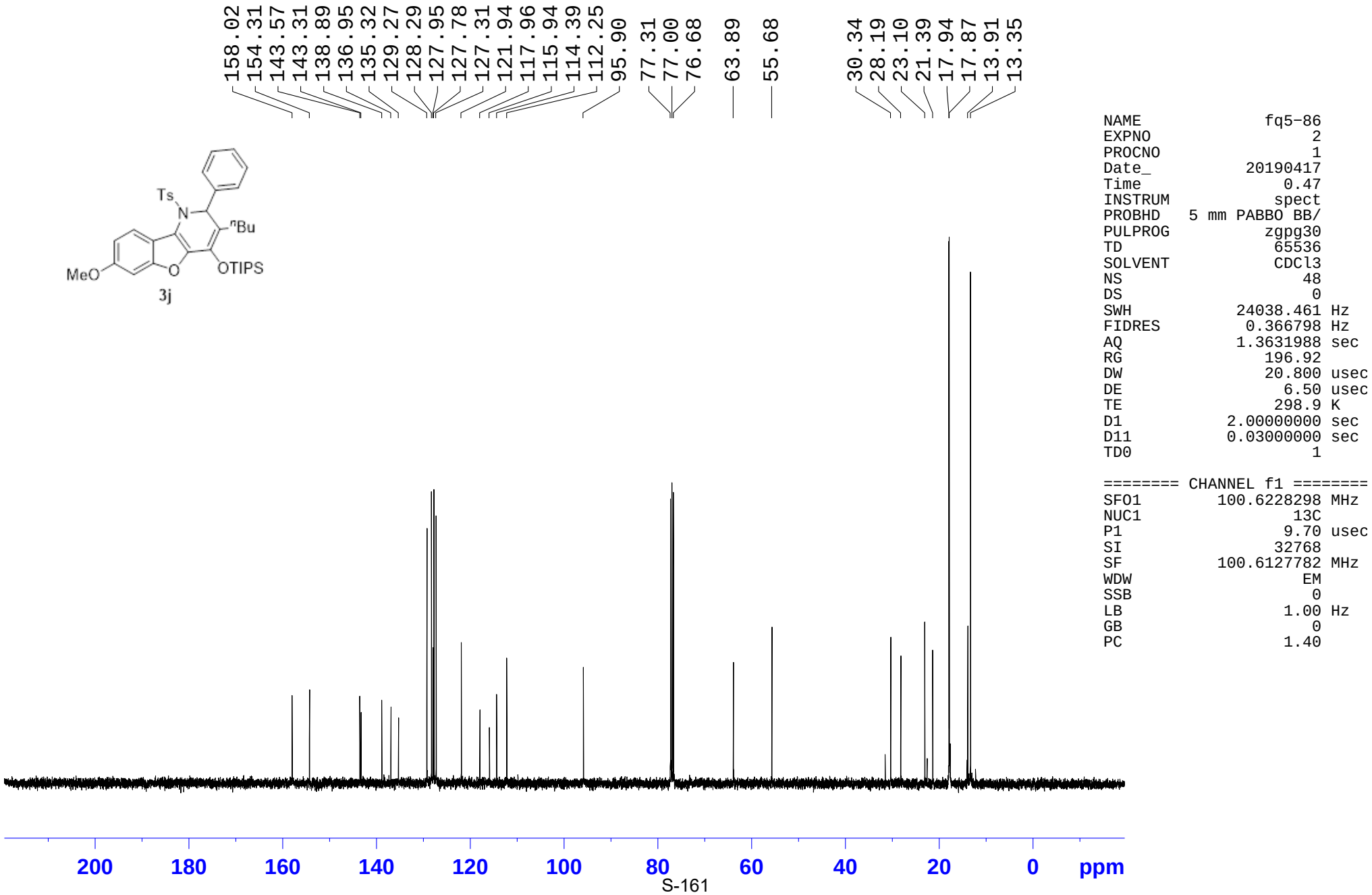


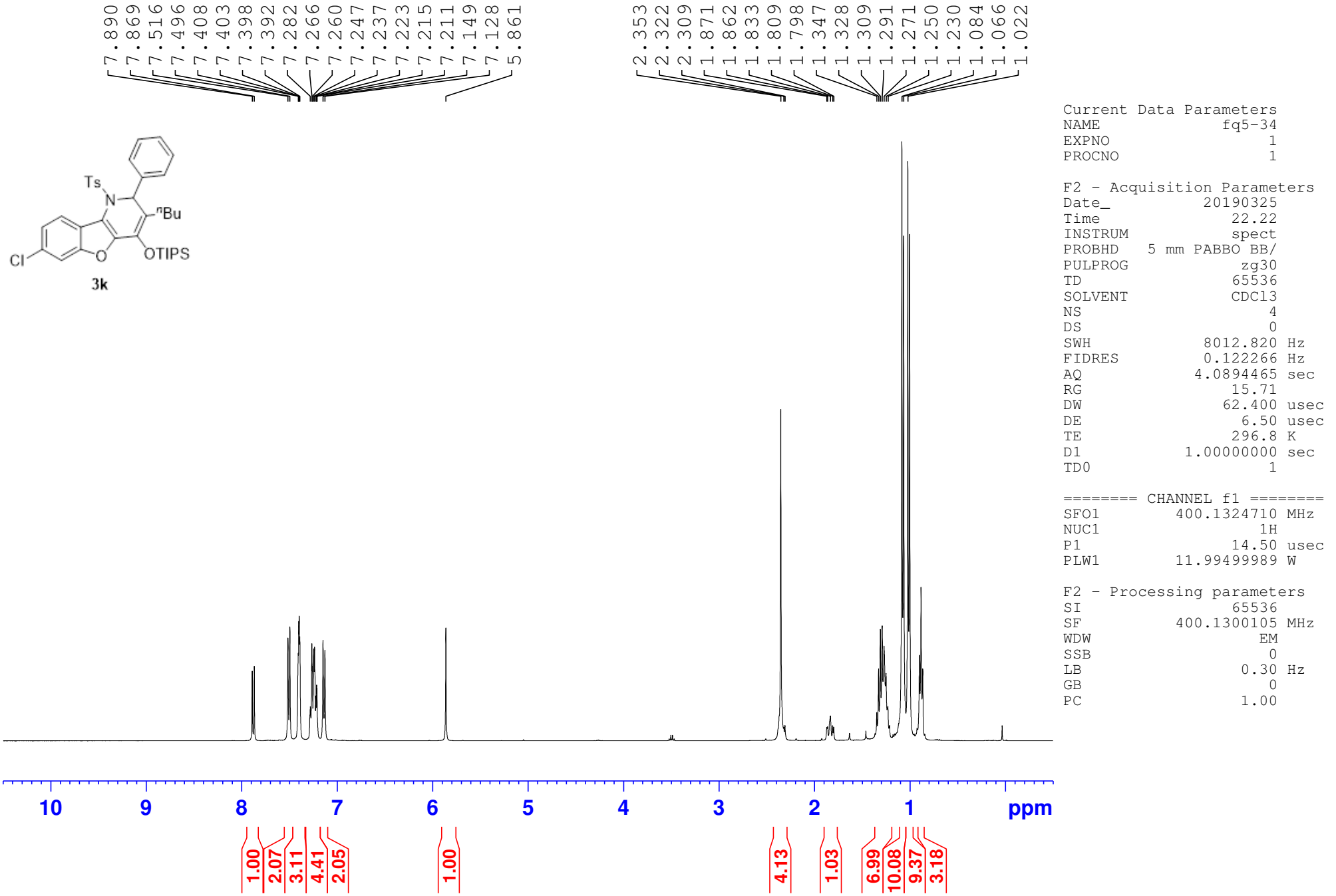

```
NAME                fq5-53
EXPNO                    1
PROCNO                   1
Date_             20190329
Time                 14.29
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       4
DS                       0
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ               4.0894966 sec
RG                    19.7
DW                  62.400 usec
DE                   6.50 usec
TE                  296.1 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                    1H
P1                   14.50 usec
SI                   65536
SF              400.1300100 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```


180.45
169.85
142.73
141.41
139.24
138.48
130.90
129.03
128.12
126.78
121.92
117.78
112.35
97.61
77.32
77.00
76.68
60.92
33.81
28.13
25.63
21.92
21.45
17.52
17.49
13.56
12.61
Ts
N
tBu
nBu
O
OTIPS
3i
NAME fq5-53
EXPNO 2
PROCNO 1
Date_ 20190329
Time 14.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 48
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
SI 32768
SF 100.6127758 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

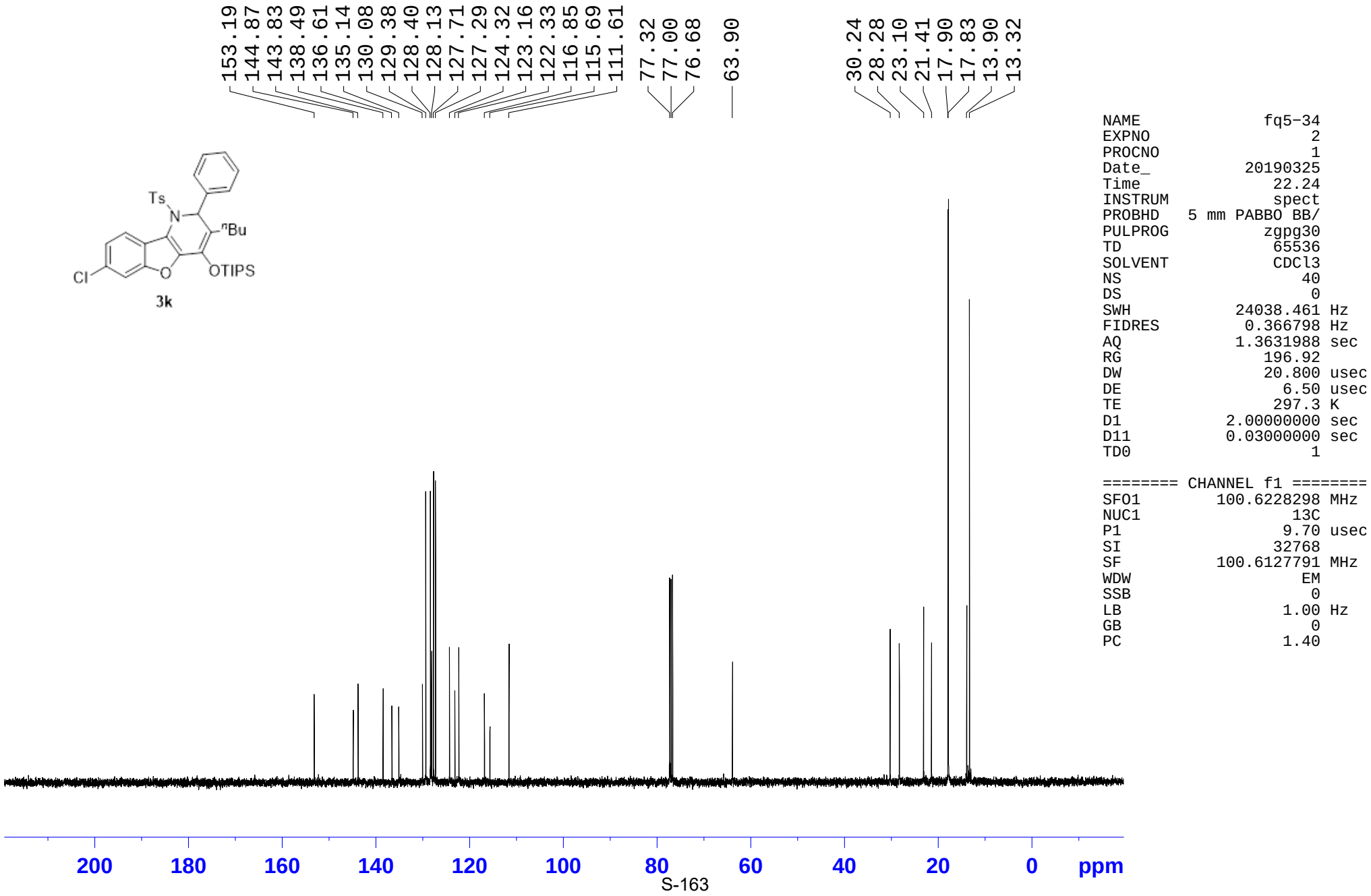


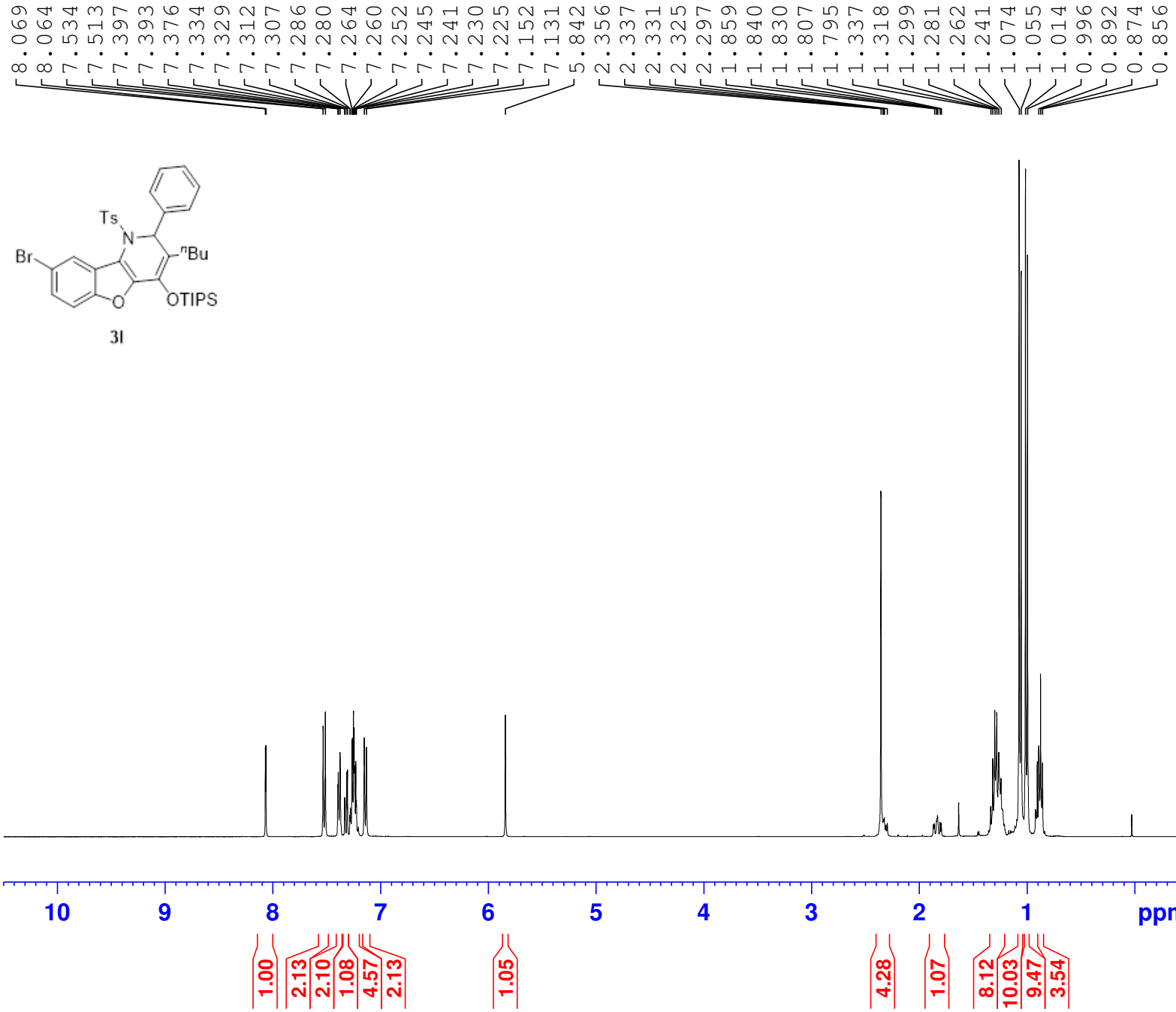

```
Current Data Parameters
NAME                  fq5-86
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190417
Time                   0.44
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        4
DS                        0
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                      19.7
DW                   62.400 usec
DE                    6.50 usec
TE                   298.1 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                      1H
P1                   14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                    65536
SF             400.1300102 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```


158.02
154.31
143.57
143.31
138.89
136.95
135.32
129.27
128.29
127.95
127.78
127.31
121.94
117.96
115.94
114.39
112.25
95.90
77.31
77.00
76.68
63.89
55.68
30.34
28.19
23.10
21.39
17.94
17.87
13.91
13.35
Ts
N
nBu
MeO
O
OTIPS
3j
NAME fq5-86
EXPNO 2
PROCNO 1
Date_ 20190417
Time 0.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 48
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
SI 32768
SF 100.6127782 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

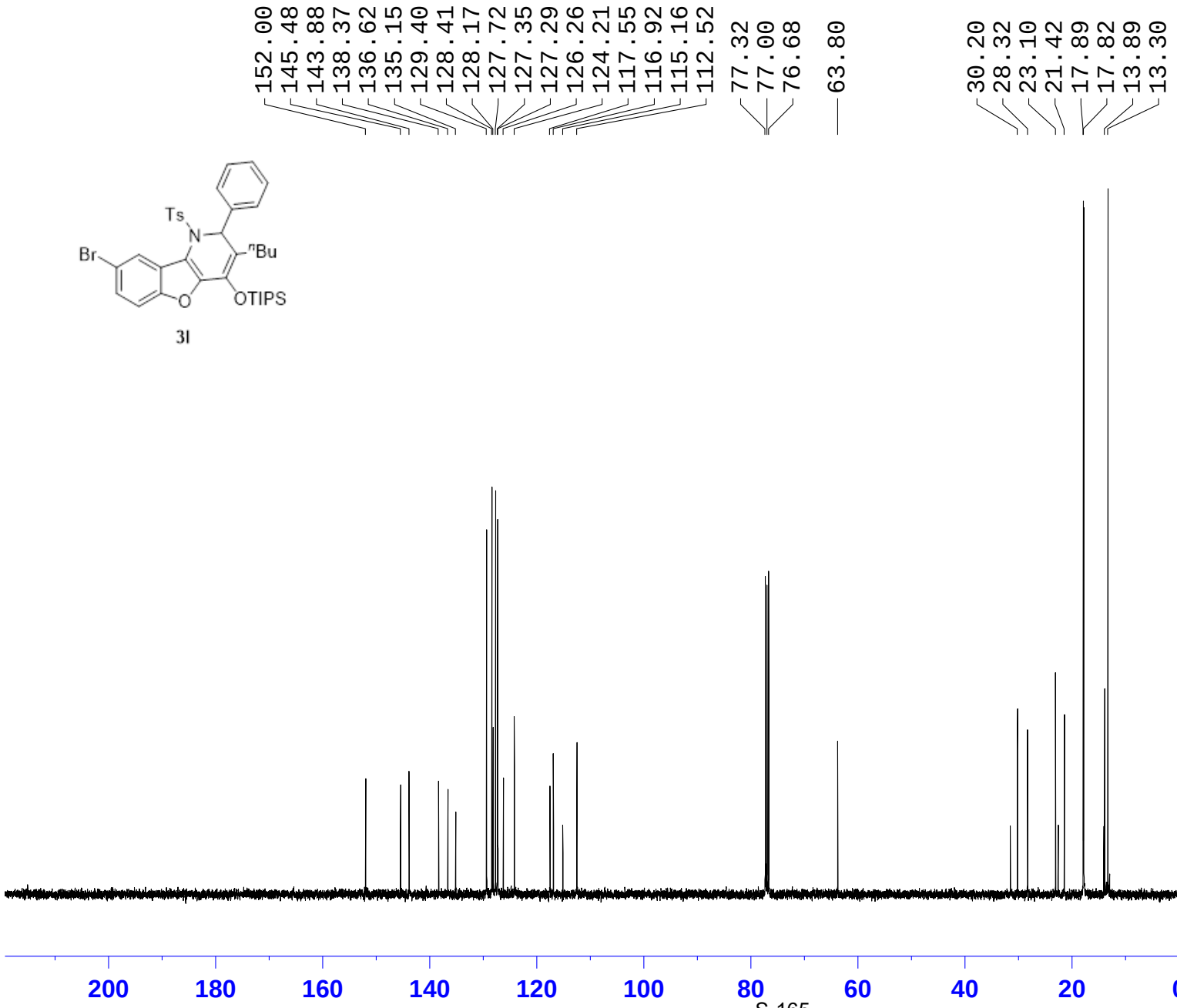



```
Current Data Parameters
NAME                  fq5-34
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190325
Time                  22.22
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                         4
DS                         0
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                     15.71
DW                   62.400 usec
DE                    6.50 usec
TE                   296.8 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                    14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                    65536
SF             400.1300105 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```


153.19
144.87
143.83
138.49
136.61
135.14
130.08
129.38
128.40
128.13
127.71
127.29
124.32
123.16
122.33
116.85
115.69
111.61
77.32
77.00
76.68
63.90
30.24
28.28
23.10
21.41
17.90
17.83
13.90
13.32
Ts
N
nBu
Cl
O
OTIPS
3k
NAME fq5-34
EXPNO 2
PROCNO 1
Date_ 20190325
Time 22.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 40
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
SI 32768
SF 100.6127791 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

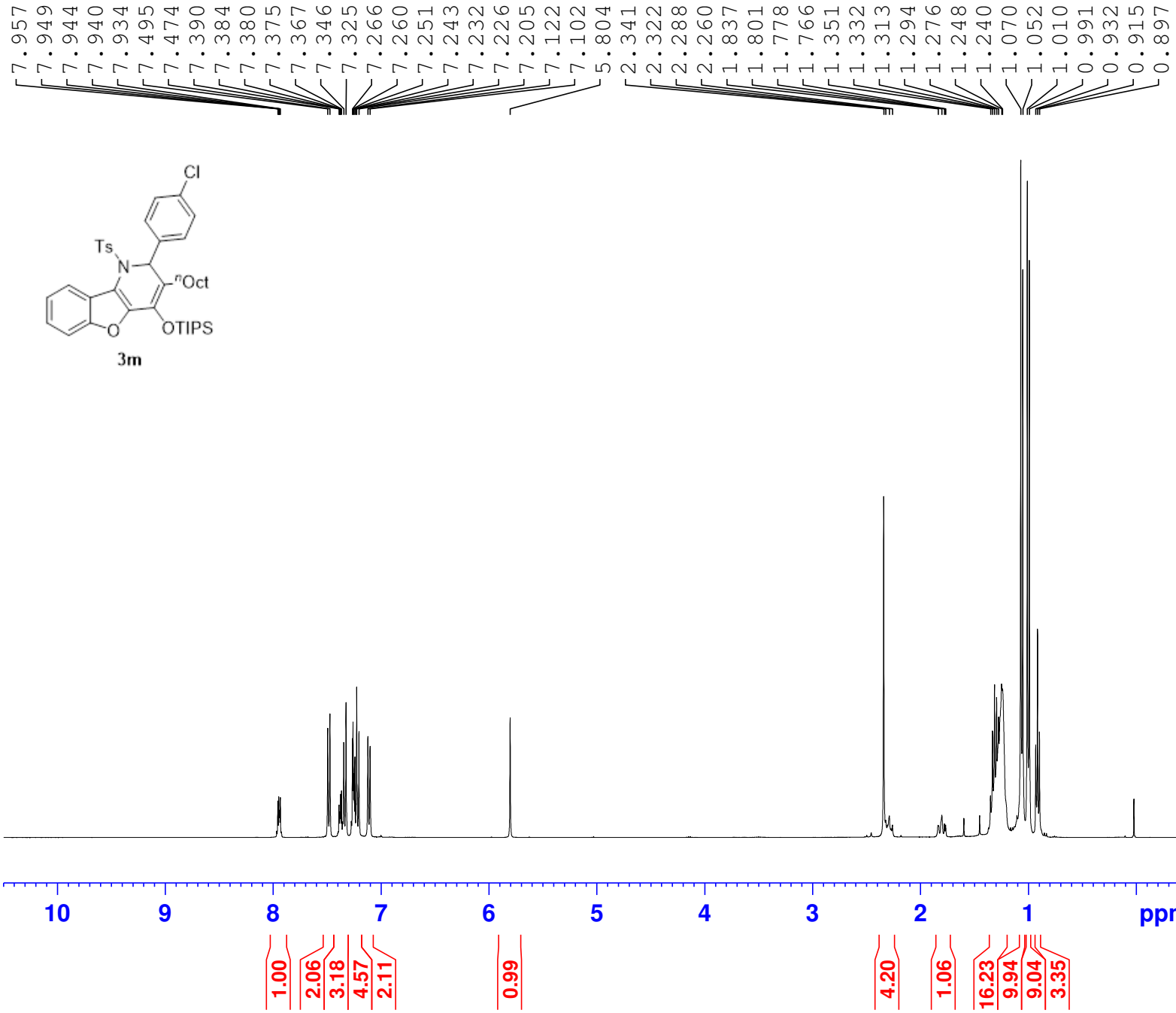



```
Current Data Parameters
NAME                  fq5-85
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190417
Time                   0.38
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                         4
DS                         0
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                     17.38
DW                   62.400 usec
DE                    6.50 usec
TE                   298.1 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                      1H
P1                    14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                    65536
SF             400.1300102 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

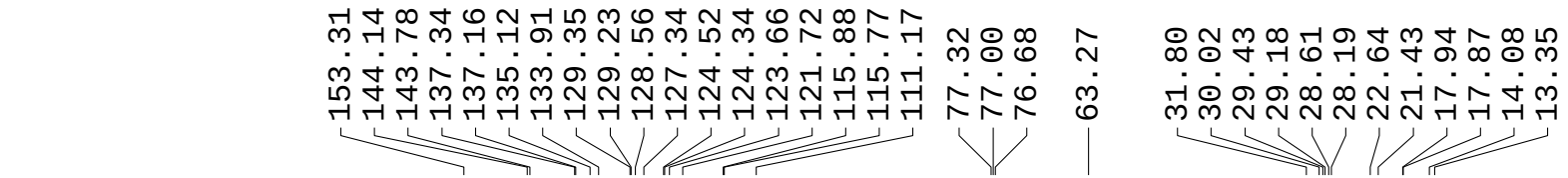


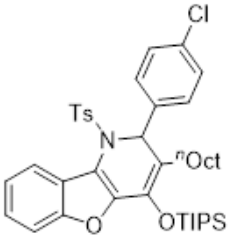
3l

NAME	fq5-85
EXPNO	2
PROCNO	1
Date_	20190417
Time	0.41
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	56
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	298.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127783 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



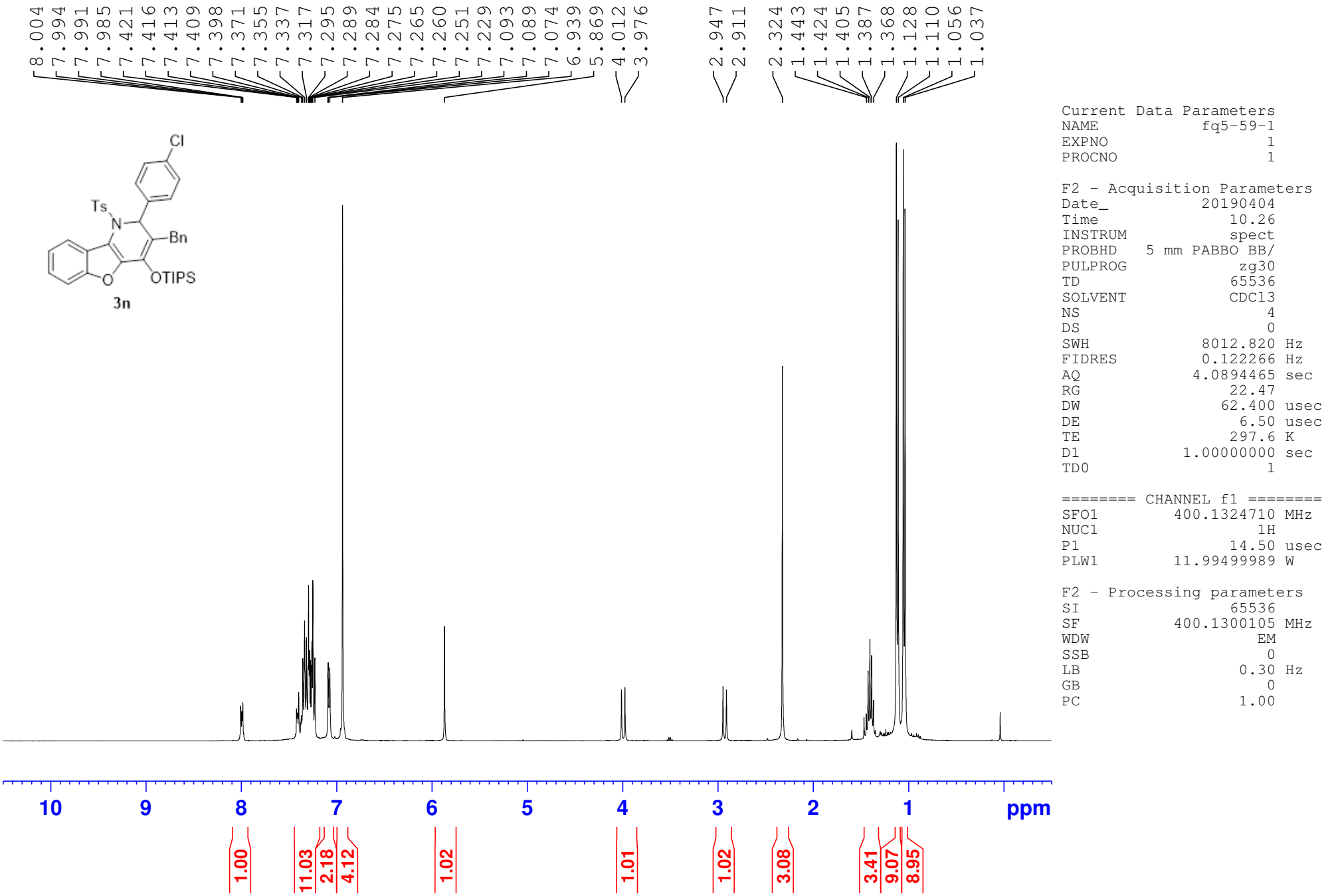

```
Current Data Parameters
NAME                  fq5-60
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20190404
Time                   1.06
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                         4
DS                         0
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                      19.7
DW                   62.400 usec
DE                    6.50 usec
TE                   298.1 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                      1H
P1                   14.50 usec
PLW1           11.99499989 W

F2 - Processing parameters
SI                    65536
SF             400.1300101 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     1.00
```



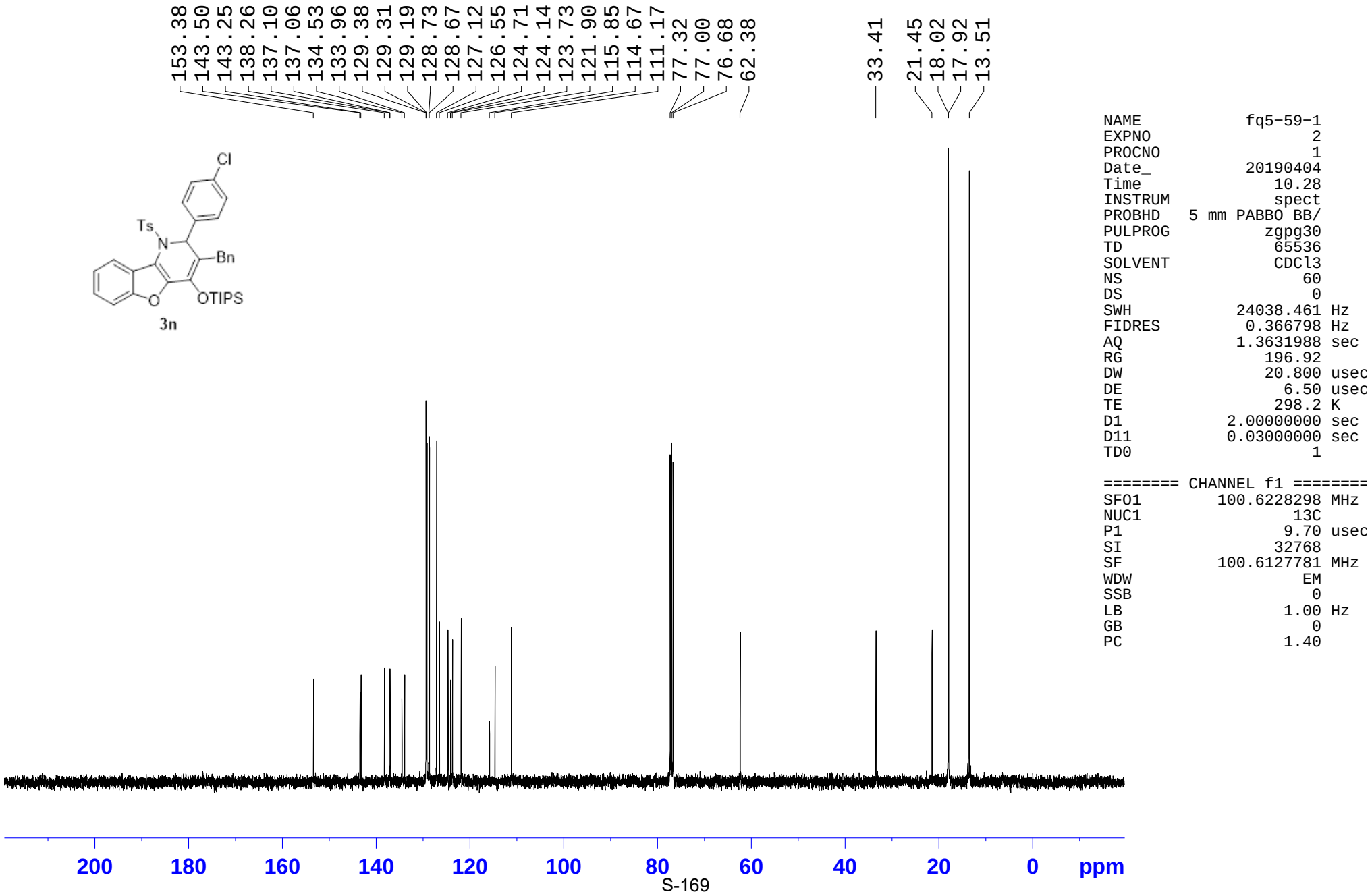


3m

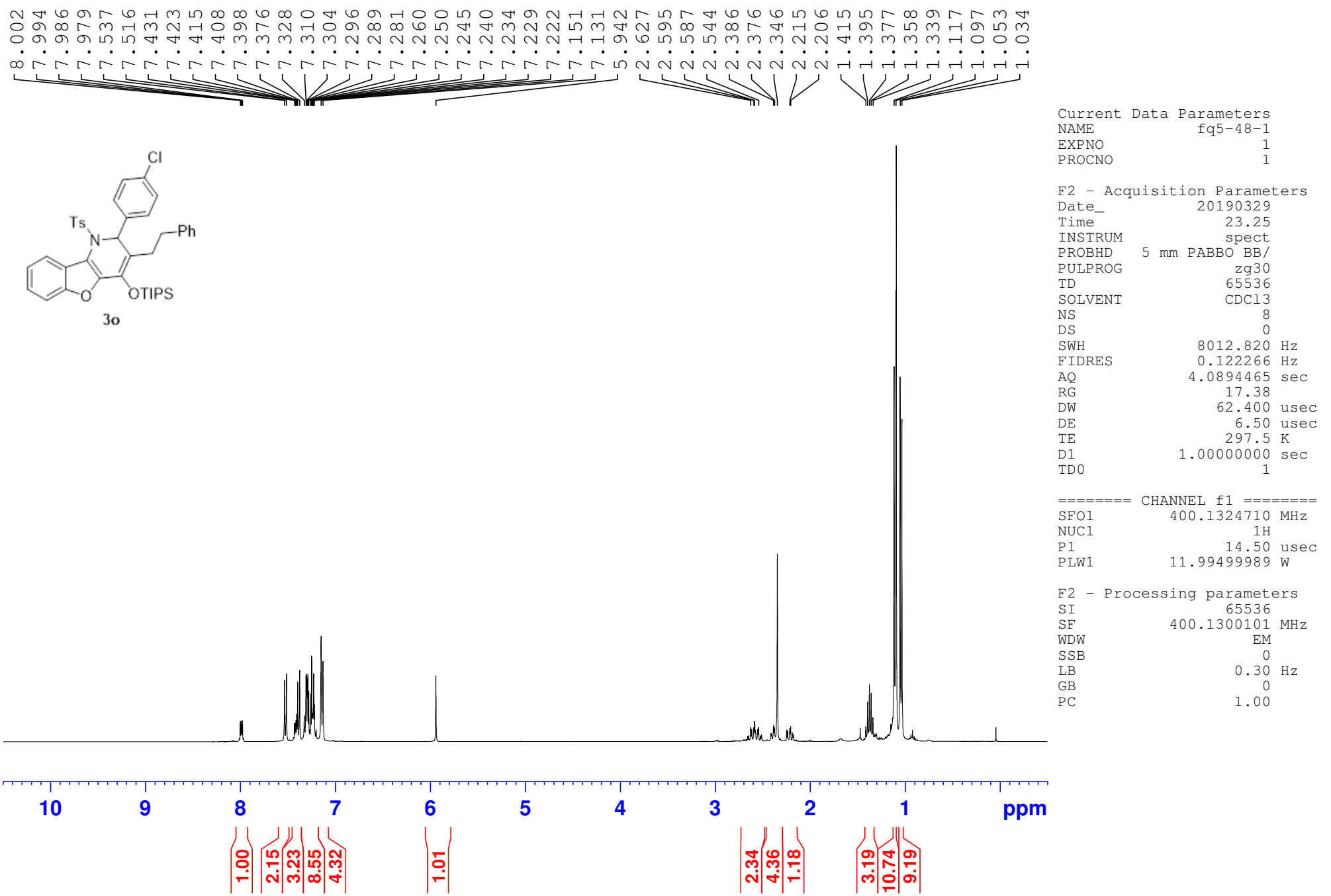
NAME	fq5-60
EXPNO	2
PROCNO	1
Date_	20190404
Time	1.08
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	48
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	298.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127747 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



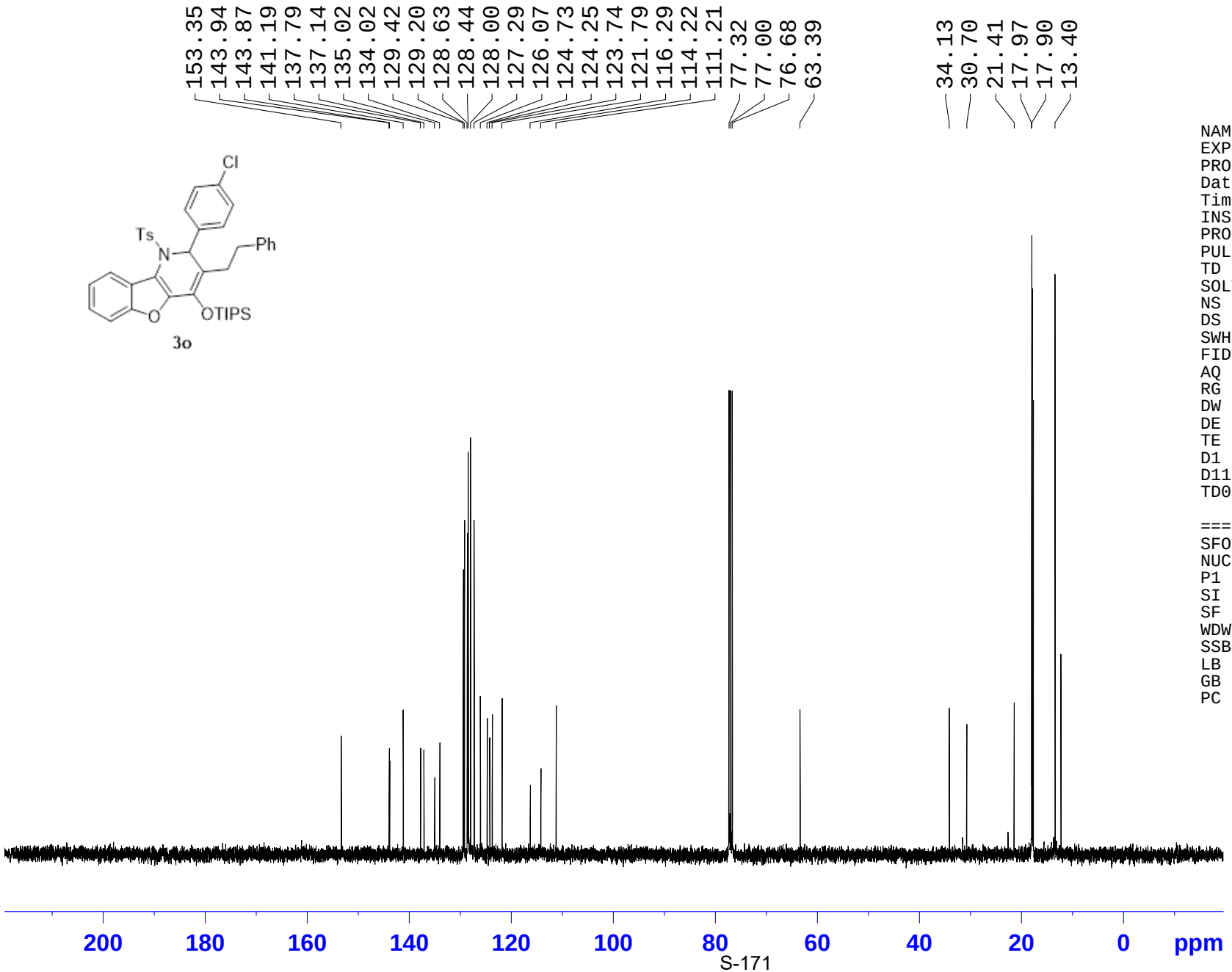

```
Current Data Parameters
NAME                  fq5-59-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20190404
Time                     10.26
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           4
DS                           0
SWH                  8012.820 Hz
FIDRES               0.122266 Hz
AQ                   4.0894465 sec
RG                       22.47
DW                     62.400 usec
DE                      6.50 usec
TE                     297.6 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                        1H
P1                      14.50 usec
PLW1            11.99499989 W

F2 - Processing parameters
SI                       65536
SF              400.1300105 MHz
WDW                         EM
SSB                          0
LB                      0.30 Hz
GB                           0
PC                      1.00
```



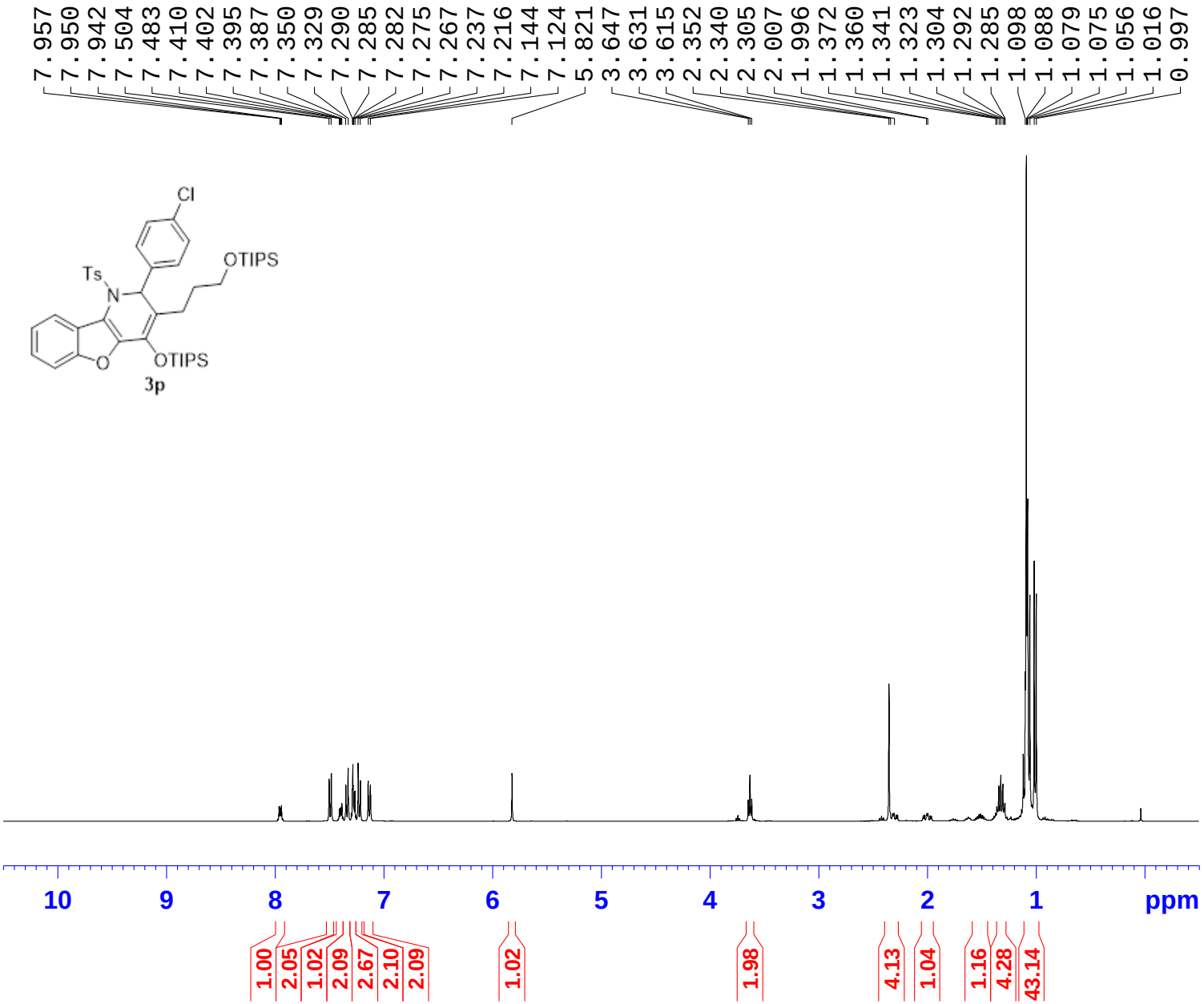
NAME	fq5-59-1
EXPNO	2
PROCNO	1
Date_	20190404
Time	10.28
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	60
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127781 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



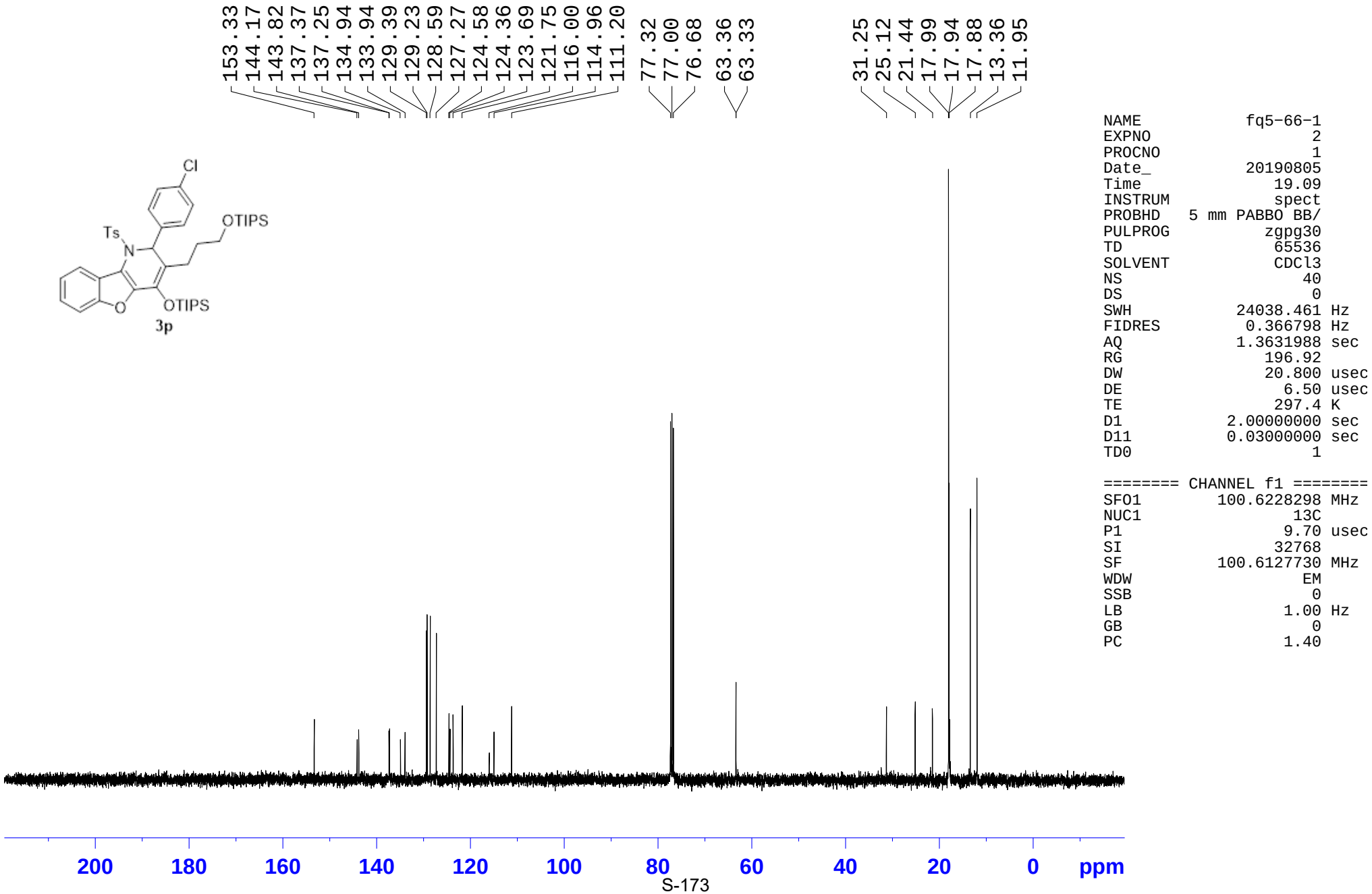

```
Current Data Parameters
NAME                  fq5-48-1
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20190329
Time                     23.25
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           8
DS                           0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                       17.38
DW                     62.400 usec
DE                      6.50 usec
TE                      297.5 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1             11.99499989 W

F2 - Processing parameters
SI                       65536
SF               400.1300101 MHz
WDW                         EM
SSB                          0
LB                      0.30 Hz
GB                           0
PC                        1.00
```



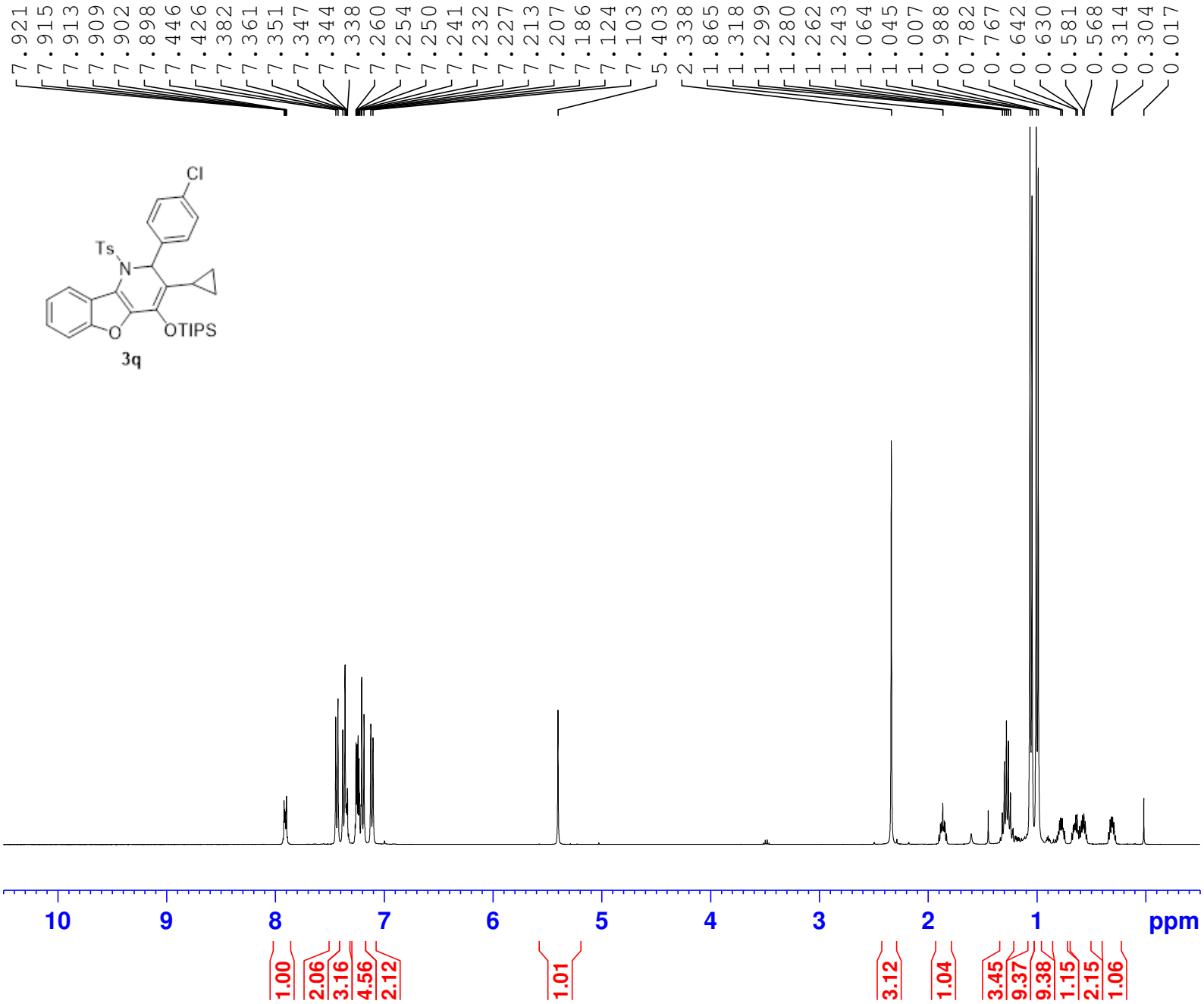
NAME	fq5-48-1
EXPNO	2
PROCNO	1
Date_	20190329
Time	23.28
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	52
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	298.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127798 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40




```
NAME            fq5-66-1
EXPNO                  1
PROCNO                 1
Date_           20190805
Time               19.06
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     4
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894966 sec
RG                 25.32
DW                62.400 usec
DE                 6.50 usec
TE                296.7 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                  1H
P1                 14.50 usec
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



NAME	fq5-66-1
EXPNO	2
PROCNO	1
Date_	20190805
Time	19.09
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	40
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	297.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127730 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

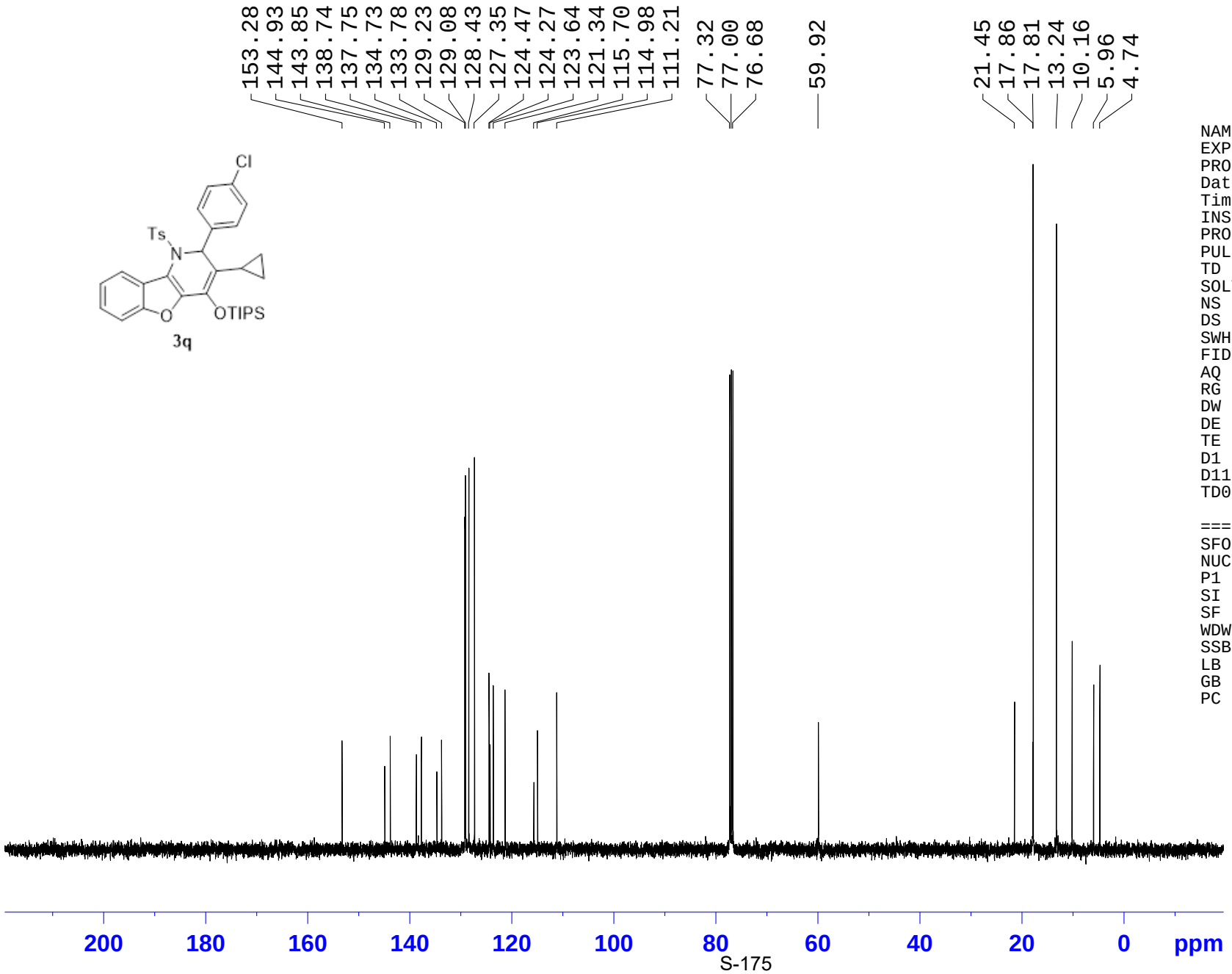


Current Data Parameters
NAME fq5-68
EXPNO 1
PROCNO 1

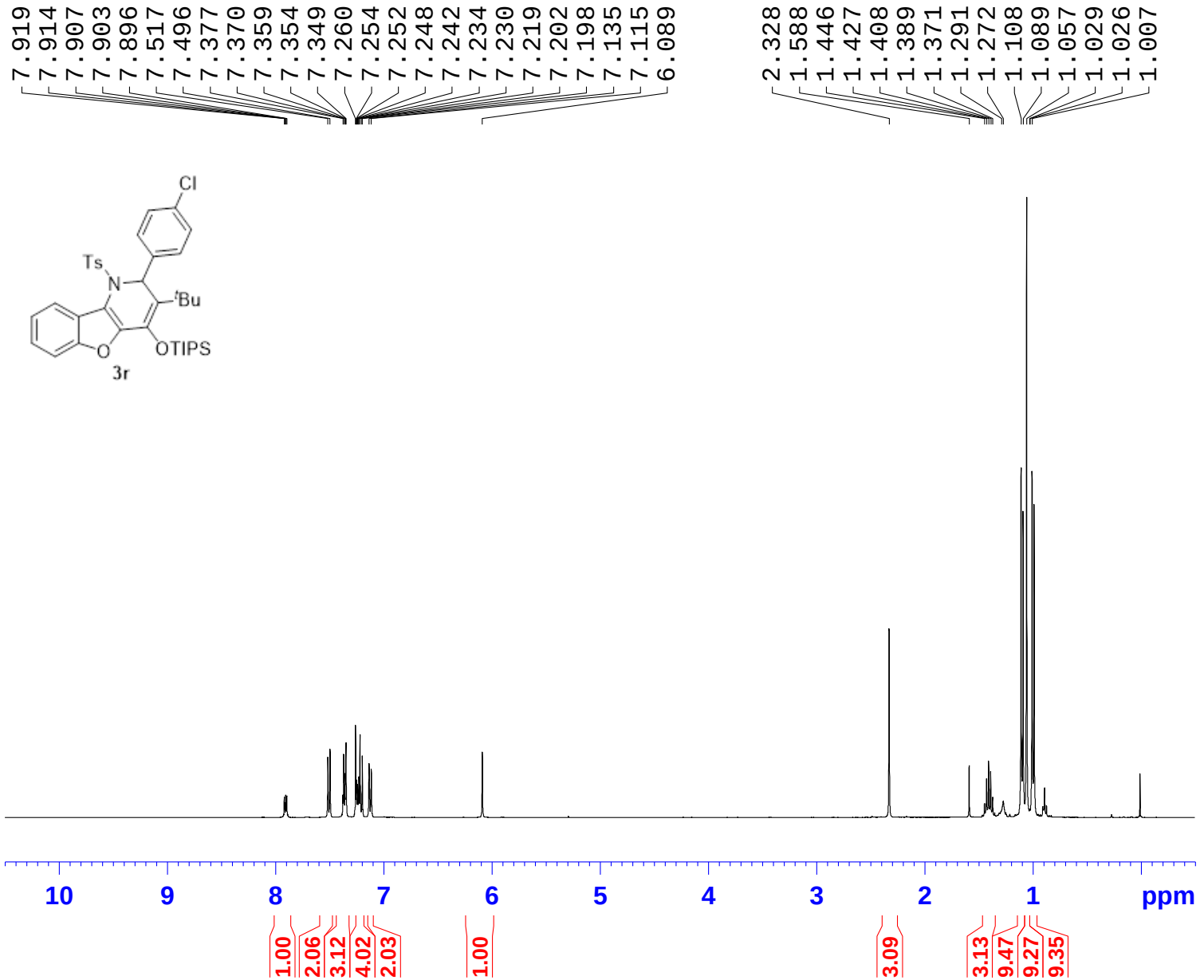
F2 - Acquisition Parameters
Date_ 20190405
Time 22.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 25.32
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

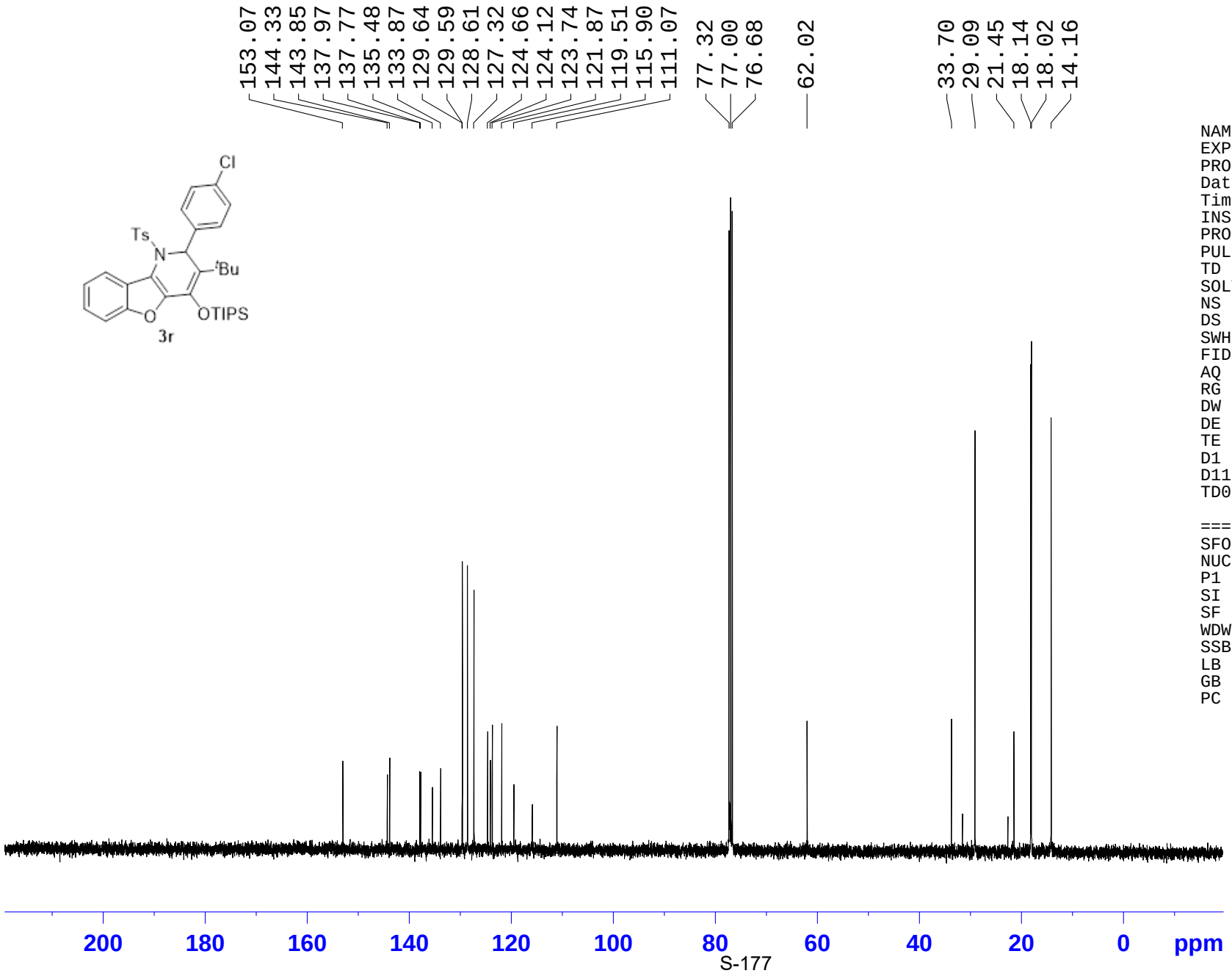
F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



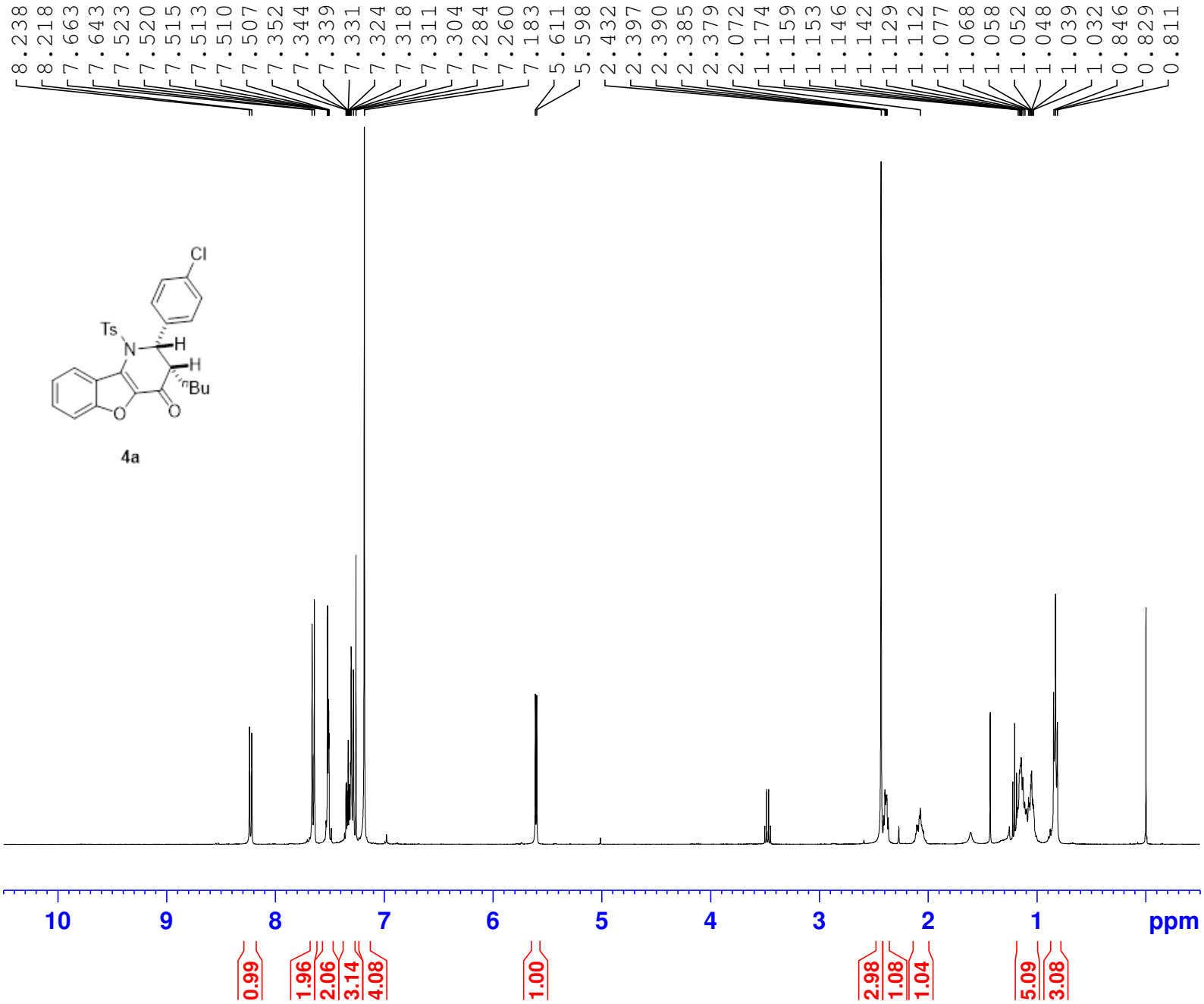
NAME	fq5-68
EXPNO	2
PROCNO	1
Date_	20190405
Time	22.58
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	52
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	298.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127749 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



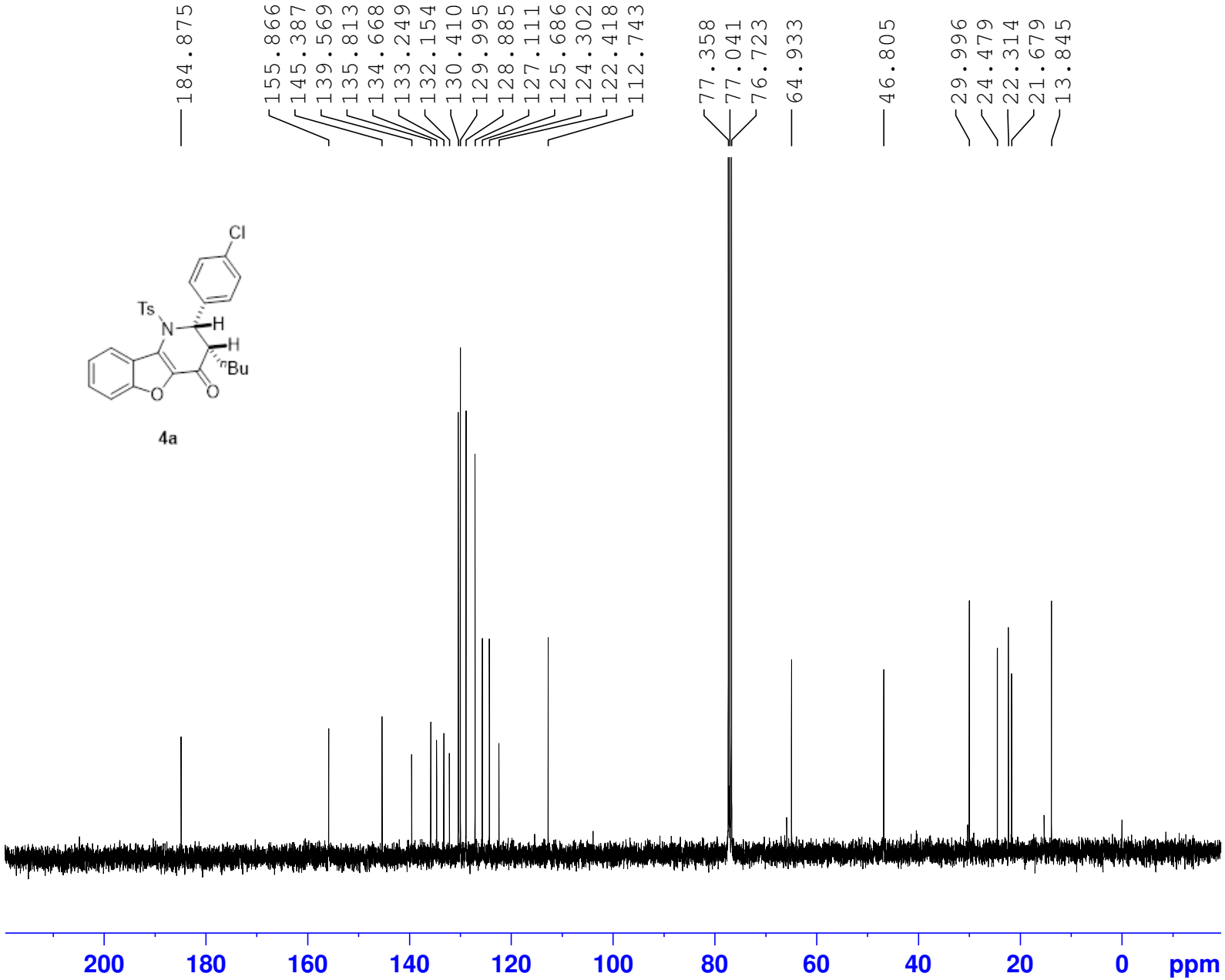

```
NAME                fq5-84
EXPNO                    1
PROCNO                   1
Date_             20190417
Time                 0.29
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       4
DS                       0
SWH               8012.820 Hz
FIDRES             0.122266 Hz
AQ               4.0894966 sec
RG                   31.55
DW                   62.400 usec
DE                    6.50 usec
TE                   297.8 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                   14.50 usec
SI                   65536
SF            400.1300102 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



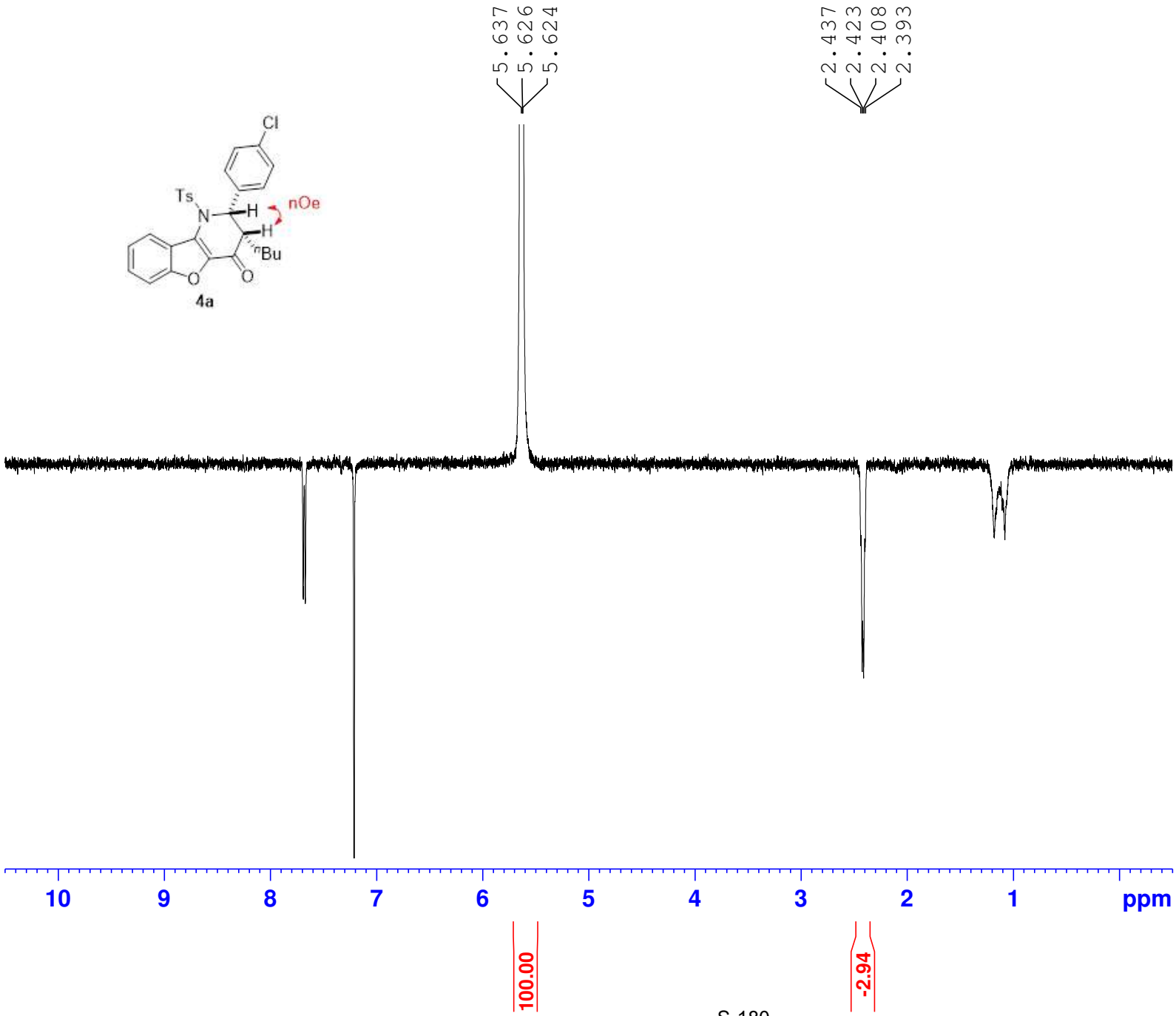
NAME	fq5-84
EXPNO	2
PROCNO	1
Date_	20190417
Time	0.34
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	80
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	298.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127730 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



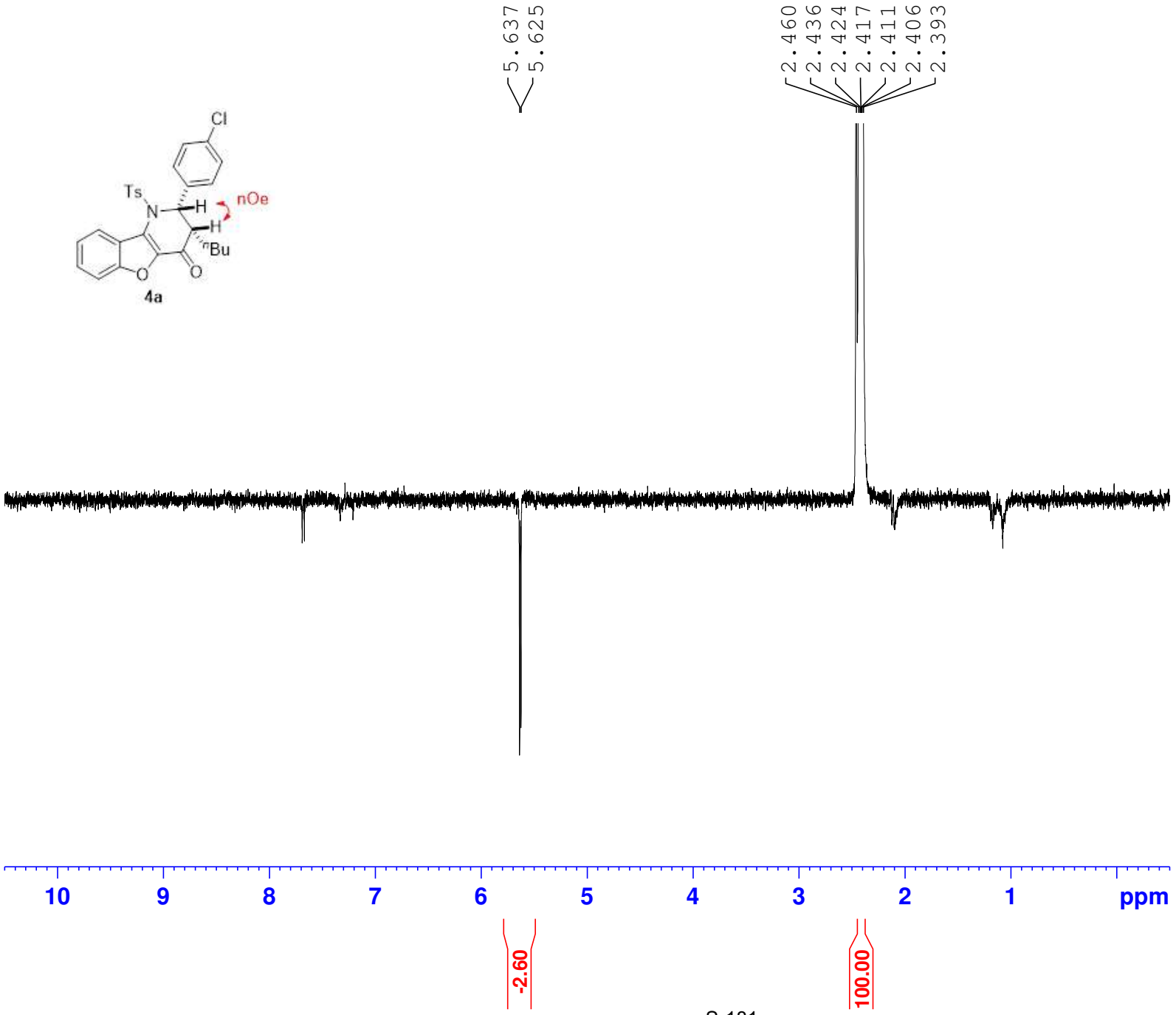

```
Current Data Parameters
NAME          fq10-146-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201225
Time               14.19
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 49.32
DW                62.400 usec
DE                 6.50 usec
TE                296.8 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300100 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```



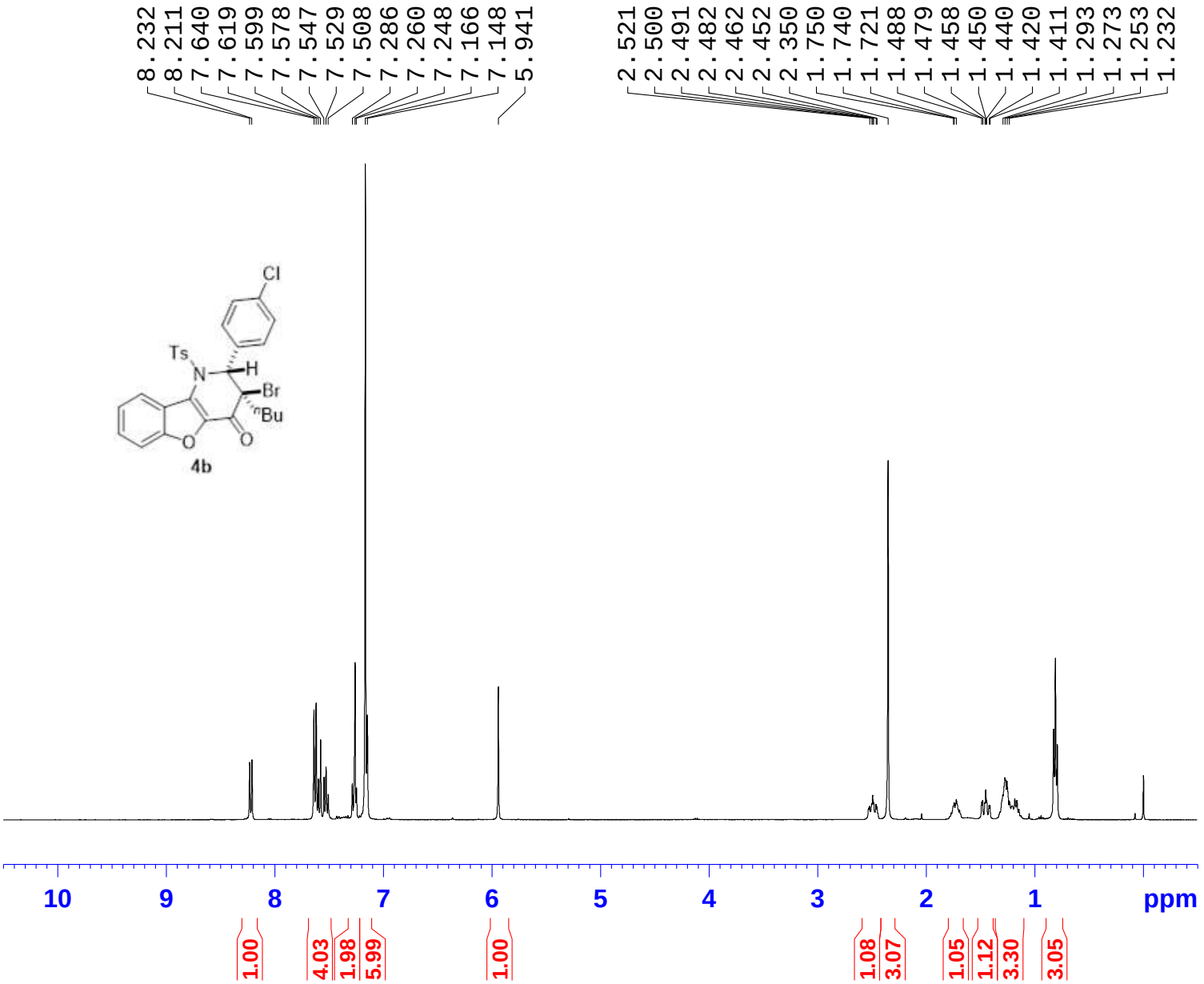

```
Current Data Parameters
NAME          fq10-146-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201225
Time               14.22
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               297.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```



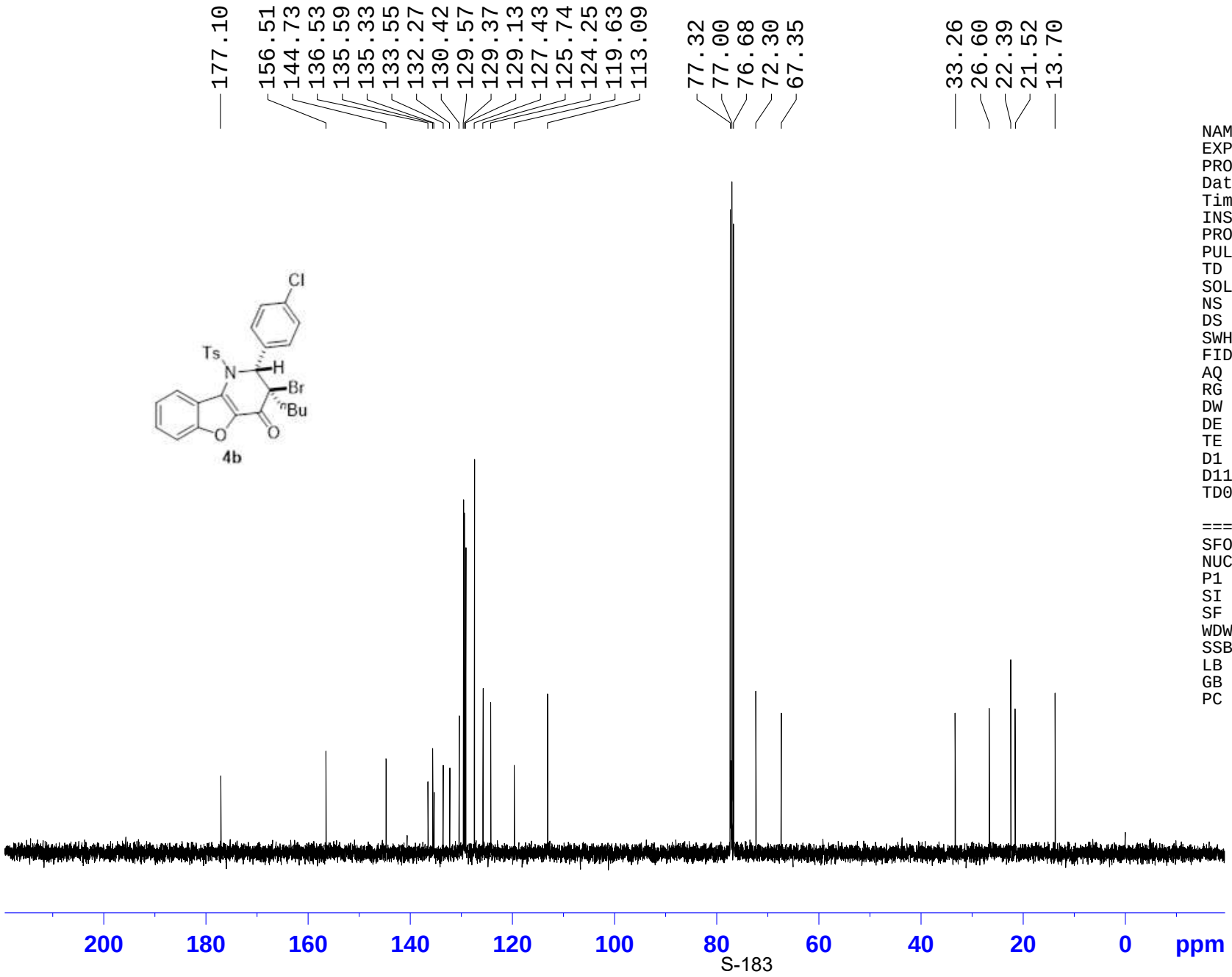

```
Current Data Parameters
NAME          fq10-146-1
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201225
Time               14.30
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          selnogp
TD                 65536
SOLVENT            CDCl3
NS                    40
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                196.92
DW                62.400 usec
DE                 6.50 usec
TE                296.8 K
D1             1.00000000 sec
D8             0.30000001 sec
D16            0.00020000 sec
D20            0.14880000 sec
TD0                    1
ZGOPTNS

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                14.50 usec
P2                29.00 usec
P12            80802.69 usec
PLW0                   0 W
PLW1         11.99499989 W
SPNAM[2] Gaus1_180r.1000
SPOAL2               0.500
SPOFFS2           -218.10 Hz
SPW2           0.00000912 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPZ1              15.00 %
GPZ2              40.00 %
P16             1000.00 usec

F2 - Processing parameters
SI                 65536
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                  1.00
```



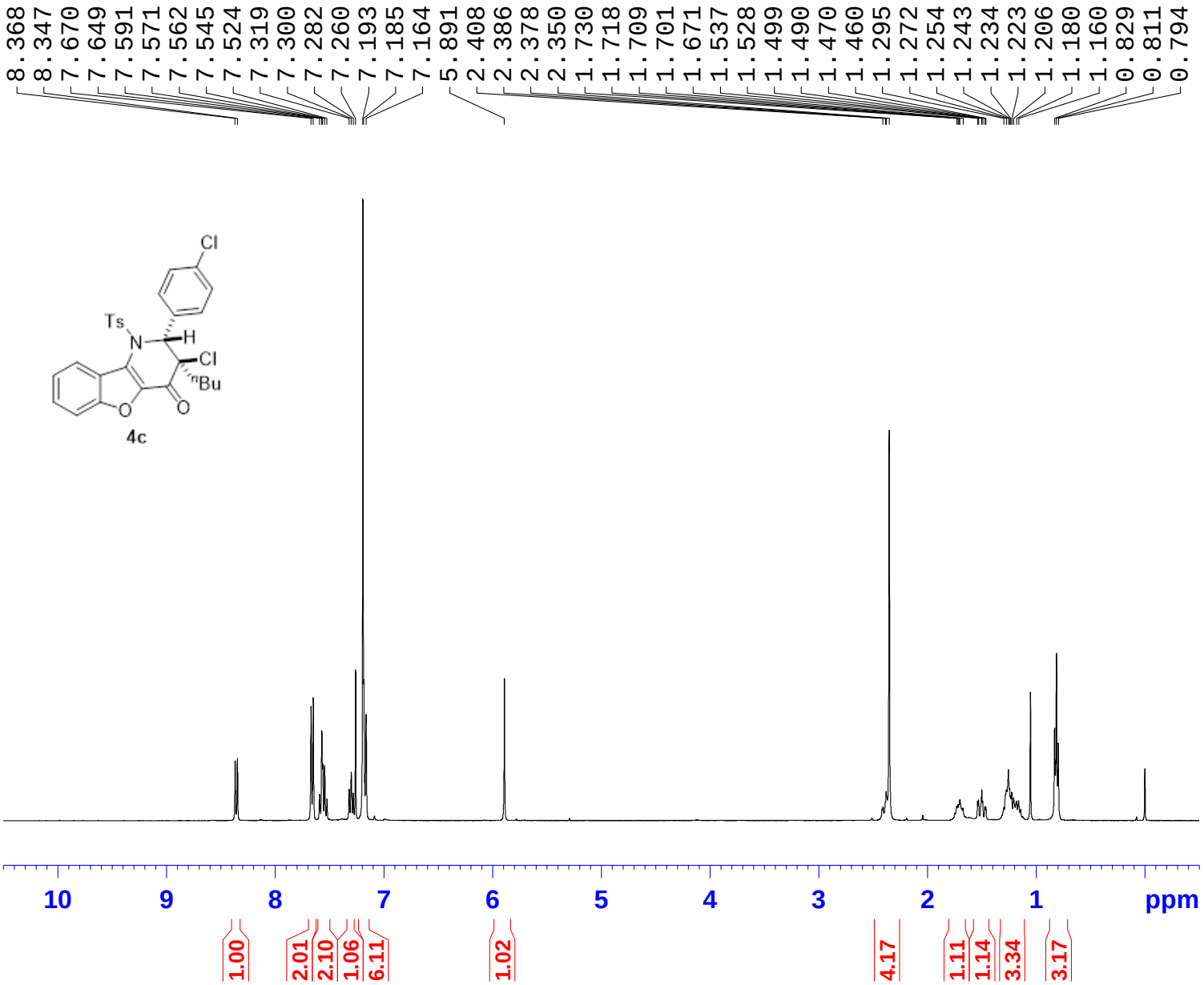

```
Current Data Parameters
NAME            fq10-146
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201228
Time               21.56
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          selnogp
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                196.92
DW                62.400 usec
DE                 6.50 usec
TE                297.2 K
D1             1.00000000 sec
D8             0.30000001 sec
D16            0.00020000 sec
D20            0.14880000 sec
TD0                    1
ZGOPTNS

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                14.50 usec
P2                29.00 usec
P12            85199.44 usec
PLW0                   0 W
PLW1         11.99499989 W
SPNAM[2] Gaus1_180r.1000
SPOAL2               0.500
SPOFFS2         -1505.72 Hz
SPW2          0.00000820 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPZ1              15.00 %
GPZ2              40.00 %
P16             1000.00 usec

F2 - Processing parameters
SI                 65536
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



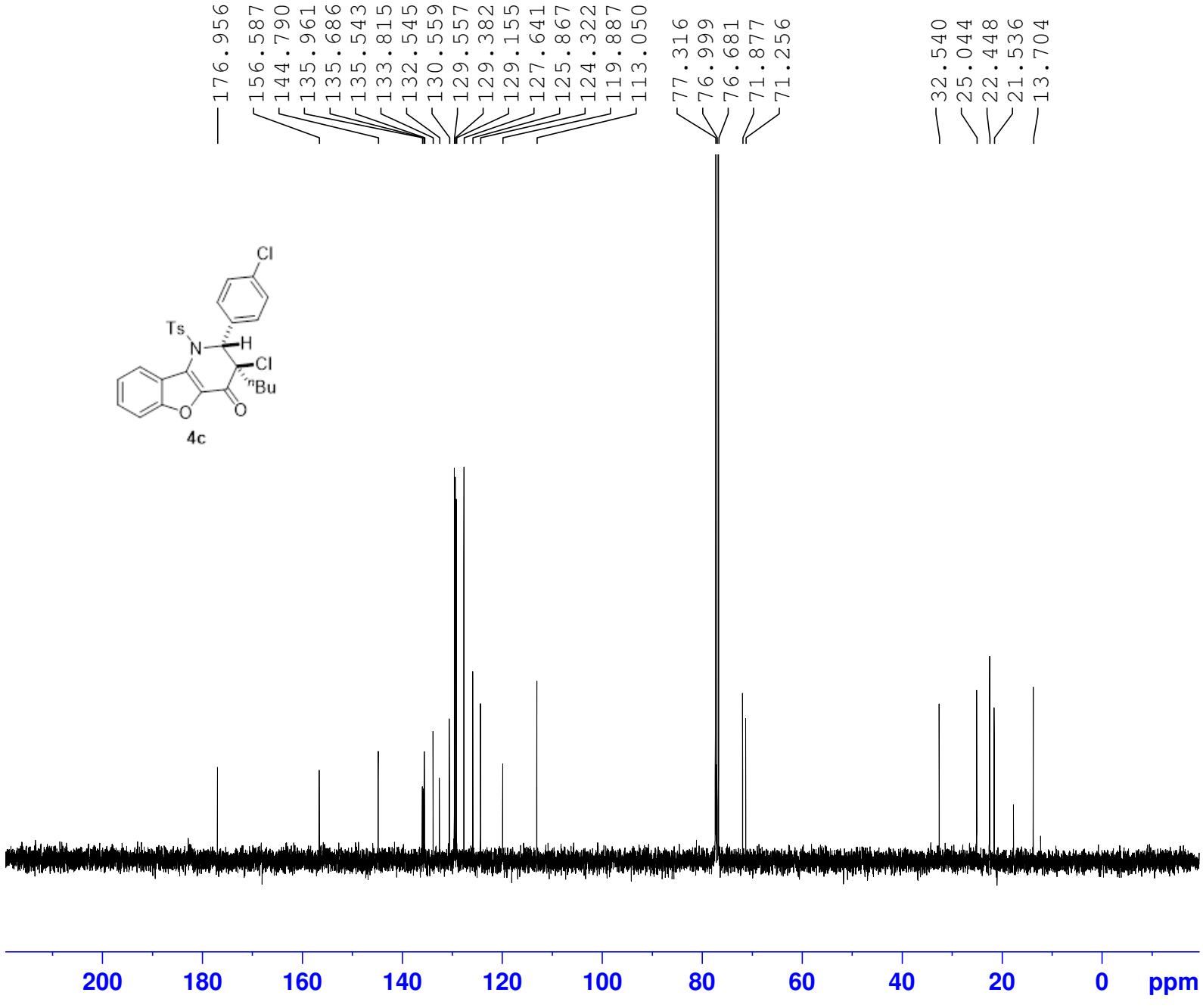

```
NAME           fq5-122-1
EXPNO                  1
PROCNO                 1
Date_           20190521
Time               14.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894966 sec
RG                 70.97
DW                 62.400 usec
DE                  6.50 usec
TE                 297.8 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
SI                 65536
SF           400.1300100 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



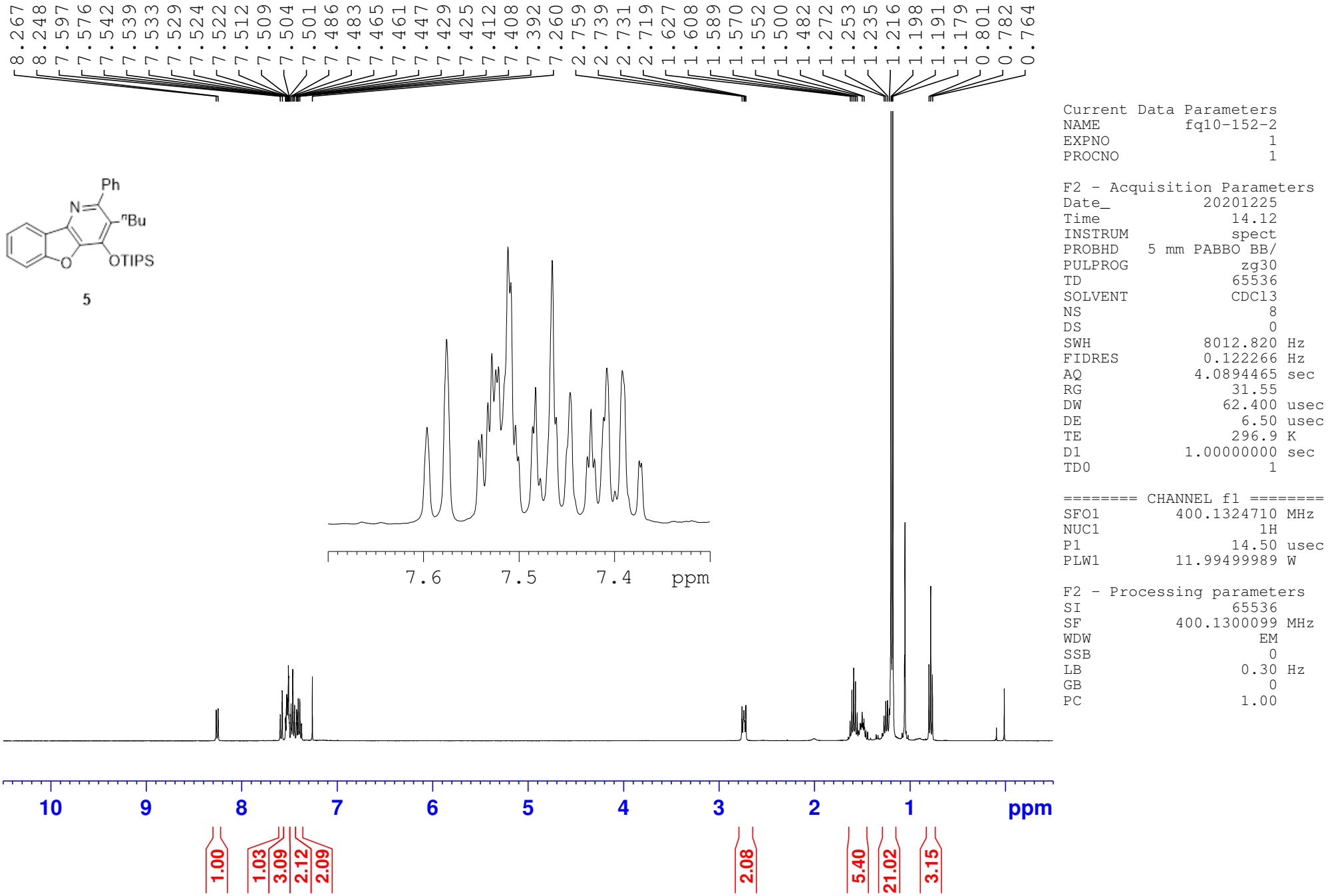
NAME	fq5-122-1
EXPNO	2
PROCNO	1
Date_	20190521
Time	14.47
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	60
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127738 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



NAME	fq5-122-2
EXPNO	1
PROCNO	1
Date_	20190521
Time	14.53
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	70.97
DW	62.400 usec
DE	6.50 usec
TE	297.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	14.50 usec
SI	65536
SF	400.1300103 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
Current Data Parameters
NAME          fq5-122-2
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20190521
Time              14.55
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                   40
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW                20.800 usec
DE                 6.50 usec
TE                298.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6127735 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

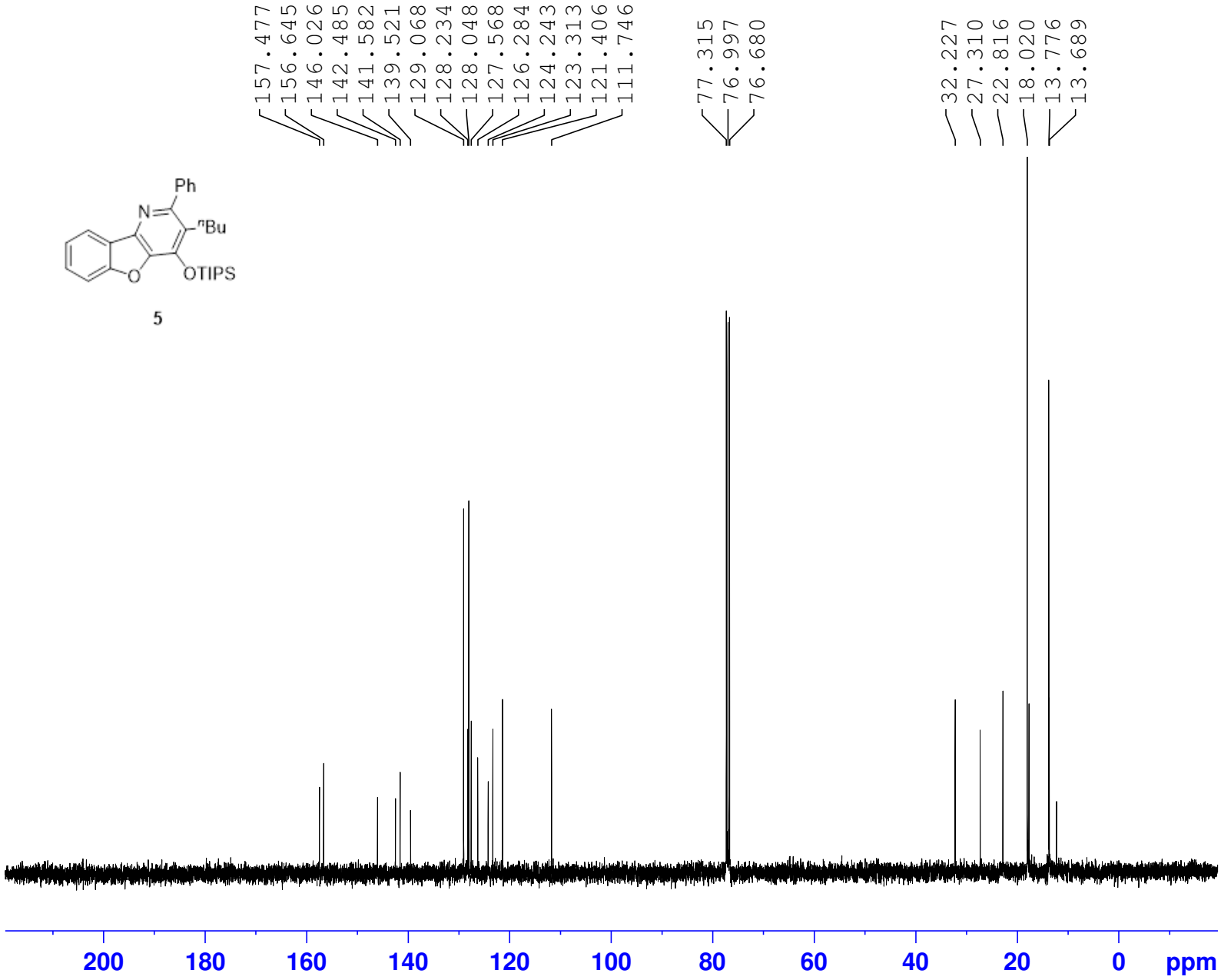


Current Data Parameters
NAME fq10-152-2
EXPNO 1
PROCNO 1

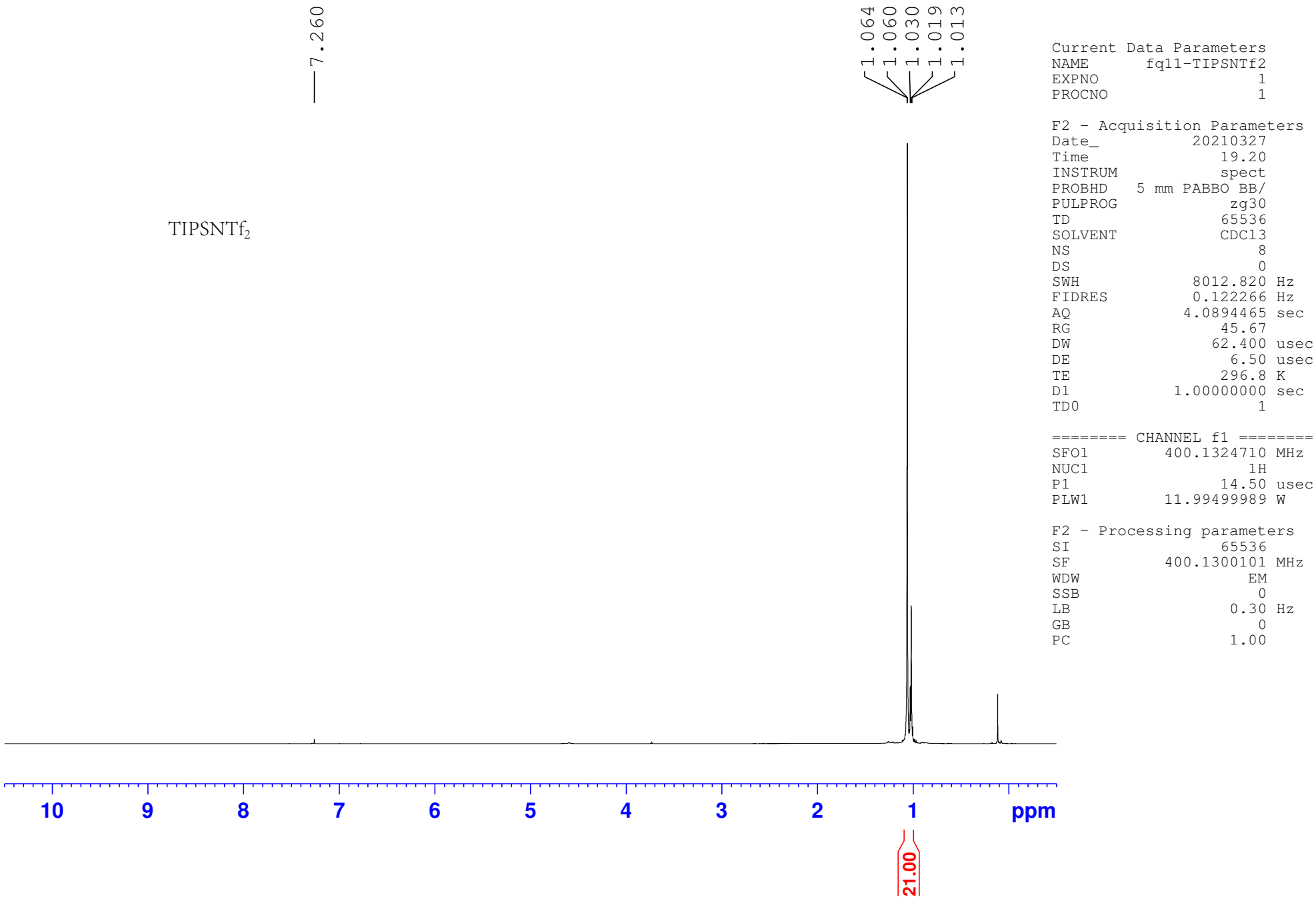
F2 - Acquisition Parameters
Date_ 20201225
Time 14.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 31.55
DW 62.400 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




```
Current Data Parameters
NAME          fq10-152-2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201225
Time               14.14
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   40
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127741 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

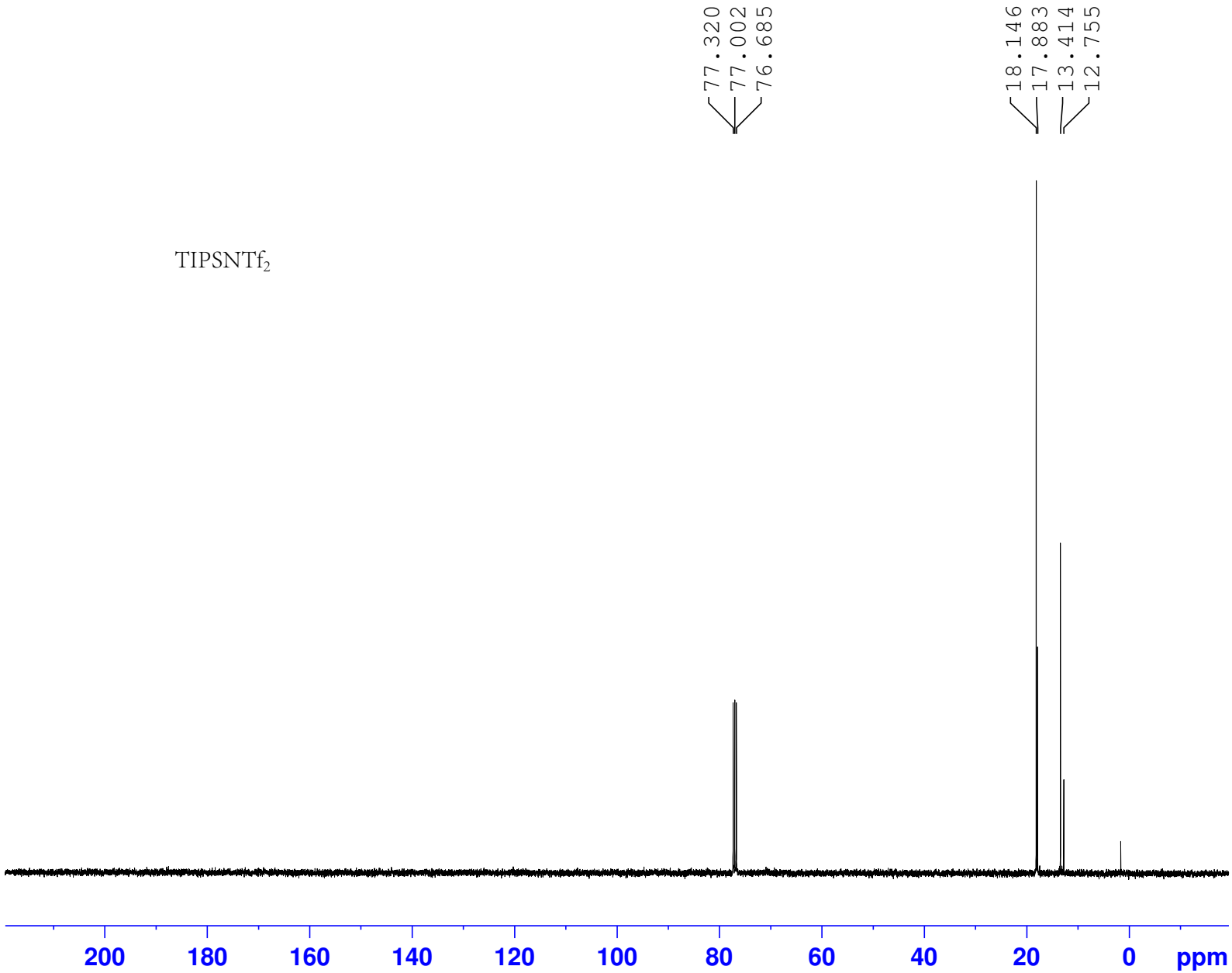


Current Data Parameters
NAME fq11-TIPSNTf2
EXPNO 1
PROCNO 1

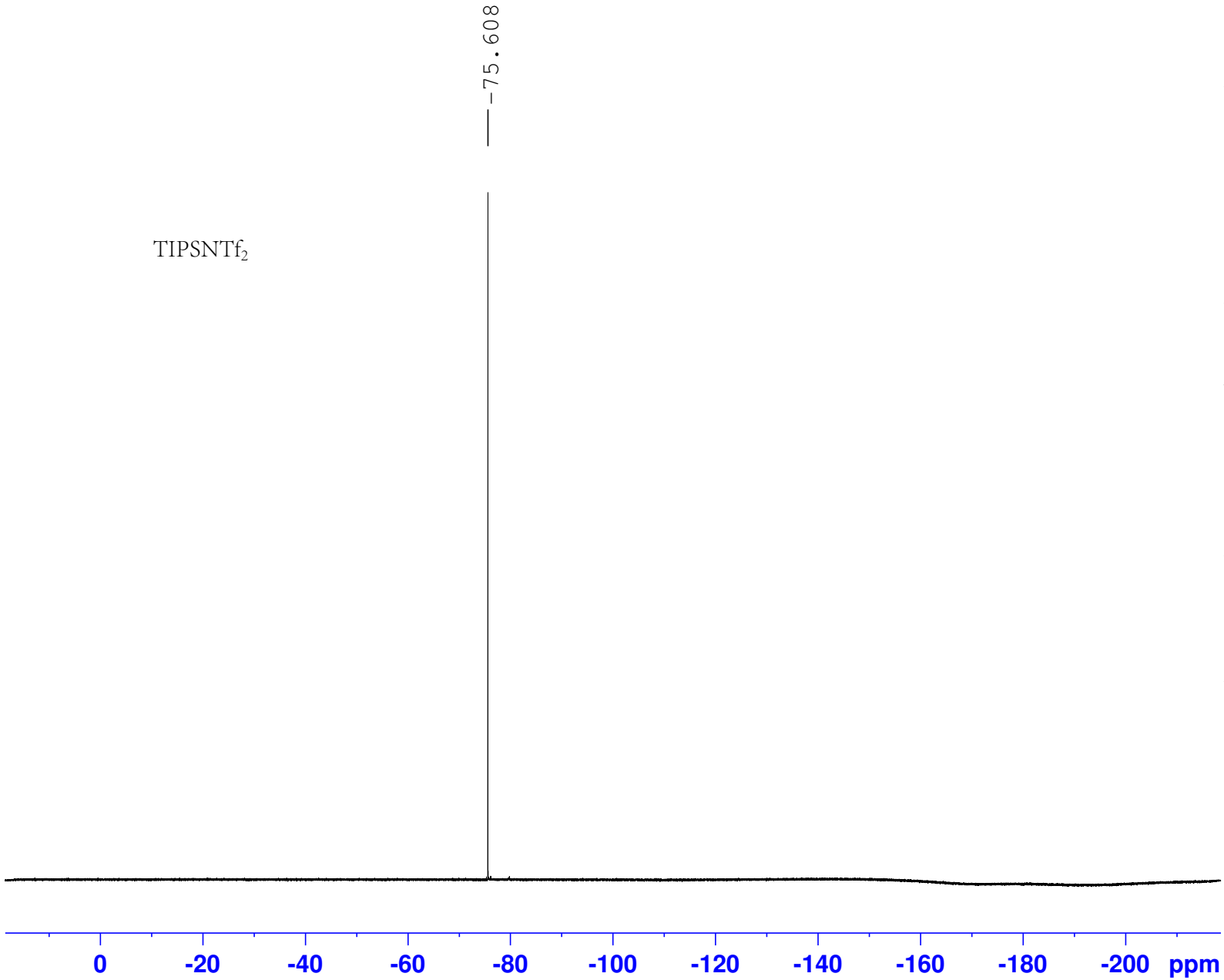
F2 - Acquisition Parameters
Date_ 20210327
Time 19.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 45.67
DW 62.400 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 14.50 usec
PLW1 11.99499989 W

F2 - Processing parameters
SI 65536
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




```
Current Data Parameters
NAME       fq11-TIPSNTf2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210327
Time               19.21
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   40
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127678 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME      fq11-TIPSNTf2
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20210327
Time              19.24
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgflqn
TD             131072
SOLVENT          CDCl3
NS                  16
DS                   0
SWH          89285.711 Hz
FIDRES        0.681196 Hz
AQ           0.7340032 sec
RG              196.92
DW               5.600 usec
DE                6.50 usec
TE               297.2 K
D1          1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1       376.4607164 MHz
NUC1               19F
P1               14.70 usec
PLW1       15.99600029 W

F2 - Processing parameters
SI                65536
SF         376.4983660 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```