Supporting Information for

Quantifying Macrocyclization-induced Strain Utilizing N-phenylimides as Conformational Reporters

Bright U. Emenike,[a] David W. Shinn,[b] Ronald A. Spinelle,[a] Barney Yoo,[c] and Ambar M. Rosario[a]

[a] Department of Chemistry and Physics, State University of New York, 223 Store Hill Road, Old Westbury, NY 11568, USA

[b] United States Merchant Marine Academy, 300 Steamboat Road Kings Point, NY 11024, United States

[c] Department of Chemistry, Hunter College, City University of New York, New York, NY 10065, USA

emenikeb@oldwestbury.edu

Table of Contents

General Experimental

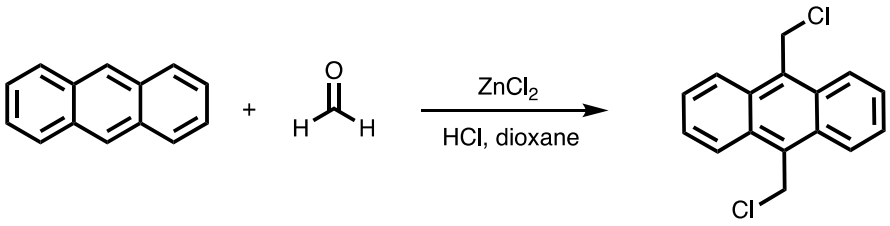
All reactions were carried out under an atmosphere of nitrogen in oven-dried glassware with magnetic stirring unless otherwise indicated. Reagents were purchased from commercial sources and used without further purification. Solvents for chemical reaction were dried. Purification of the reaction products was carried out by flash chromatography using silica gel 40-63 μm (230-400 mesh) unless otherwise stated. Reactions were monitored by proton NMR and/or thin layer chromatography. Visualization was accomplished with UV light, staining with 5% $KMnO_4$ or with panisaldehyde in EtOH solution. NMR was recorded using a 400 MHz Bruker spectrometer. Data are reported as (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet; integration; coupling constant(s) in Hz). Melting points were measured with a Gallenkamp melting point apparatus.

Measurement of interaction energies (ΔG)

The folded/unfolded ratios were measured by proton NMR spectra at room temperature (~ 25°C). The peak areas corresponding to the ortho proton in the folded and unfolded states were integrated. The CH-π interaction energies were estimated from the equation: $\Delta G = -RTlnK = -RTln[folded]/[unfolded]$.

Synthesis

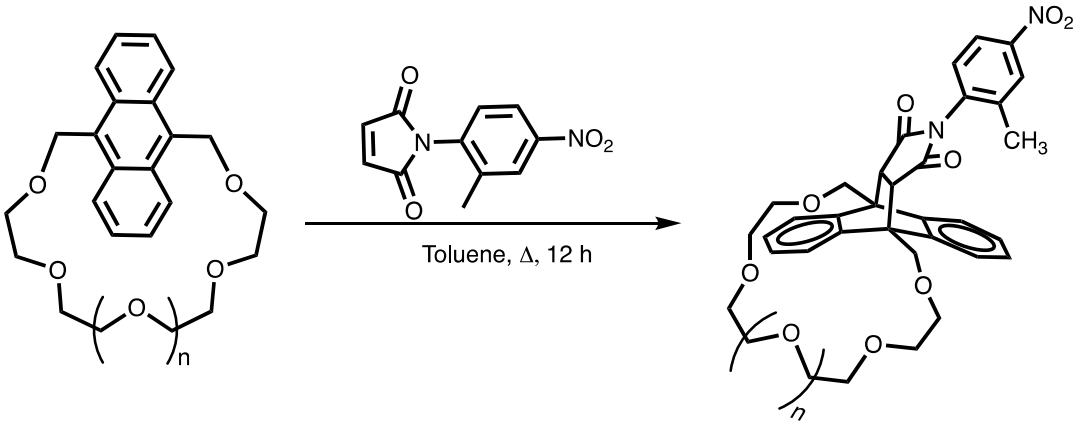
Preparation of 9,10-dichloromethylanthracene



To a stirred solution of anthracene (1.78 g, 10 mmol), anhydrous $ZnCl_2$ (1.64 g, 12 mmol), and paraformaldehyde (1.50 g, 50 mmol) in dioxane (20 mL) was slowly added concentrated aqueous hydrochloric acid (1N, 40 mL) at room temperature. After addition,

the mixture was refluxed gently for 3 h and allowed to stand for 16 h at room temperature. The resulting one granular solid was separated by filtration and washed with H_2O and dioxane to afford the crude product. The crude product was recrystallized from toluene to give 5 as yellowish solid. Yield: 65%. The NMR spectrum are consistent with previous synthesis.[1]

Diels-Alder: Preparation and characterization of Balances



General Procedure 2:[2] A mixture of the appropriate anthracenyl crown ether (0.9 mmol) and 1-(2-methyl-4-nitrophenyl)-1*H*-pyrrole-2,5-dione (1.0 mmol) in 1 ml xylene was heated in a sealed reaction tube overnight. The cooled reaction was then purified by column chromatography to yield the balance.

Balance 1. Melting point = 232-233°C

^{1}H-NMR (400 MHz; $CDCl_3$): δ 8.09-7.93 (m, 2H), 7.77-7.72 (m, 2H), 7.62-7.58 (m, 2H), 7.47 (dd, *J* = 5.7, 3.3 Hz, 1H), 7.38-7.32 (m, 3H), 7.05-7.03 (m, 1H), 5.75 (d, *J* = 8.6 Hz, 1H), 5.08 (dd, *J* = 10.4, 4.8 Hz, 2H), 4.77-4.74 (m, 2H), 3.99 (q, *J* = 3.2 Hz, 4H), 3.73-3.57 (m, 4H), 3.15-3.14 (m, 2H), 3.03-2.95 (m, 4H), 2.47-2.34 (m, 2H), 2.13-2.06 (m, 4H), 1.25 (s, 1H).

13-C NMR (101 MHz; $CDCl_3$): δ 173.6, 173.5, 148.1, 148.1, 147.9, 141.8, 141.2, 138.8, 138.7, 138.7, 138.7, 138.51, 137.8, 136.2, 136.2, 129.0, 128.9, 127.2, 127.1, 127.0, 126.9, 126.7, 126.7, 126.6, 126.6, 126.5, 125.8, 125.7, 125.1, 124.8, 124.8, 124.7, 124.4,

124.3, 124.2, 122.0, 121.5, 72.2, 72.0, 71.1, 71.1, 70.6, 70.5, 68.7, 68.6, 67.5, 67.3, 51.4, 50.7, 50.4, 17.9, 17.2

HRMS calculated for $C_{35}H_{36}N_2O_9$ $[M+H]^+$ 629.2499, found 629.2489

Balance 2. Melting point = 189-190°C

^{1}H-NMR (400 MHz; $CDCl_3$): δ 8.10-7.87 (m, 2H), 7.67 (ddd, *J* = 10.4, 5.7, 3.3 Hz, 2H), 7.27-7.10 (m, 6H), 5.65 (d, *J* = 8.6 Hz, 1H), 4.98-4.82 (m, 4H), 4.21-4.14 (m, 4H), 4.03-3.99 (m, 2H), 3.80-3.53 (m, 12H), 3.36-3.35 (m, 4H), 2.23 (s, 1H), 1.18 (s, 2H).

13-C NMR (101 MHz; $CDCl_3$): δ 175.6, 175.5, 147.9, 147.8, 143.2, 142.5, 140.7, 140.4, 138.4, 138.3, 137.2, 137.1, 129.1, 128.9, 126.8, 126.6, 126.1, 126.0, 125.6, 124.2, 124.0, 122.1, 121.9, 121.8, 121.6, 71.1, 71.0, 70.9, 70.9, 70.8, 70.7, 70.5, 70.4, 70.1, 67.1, 66.9, 49.2, 48.9, 46.1, 45.9, 16.8

HRMS calculated for $C_{37}H_{40}N_2O_{10}$ $[M+H]^+$ 673.2761, found 673.2755

Balance 3. Melting point = 104-109°C

^{1}H-NMR (400 MHz; $CDCl_3$): δ 8.12-7.88 (m, 2H), 7.69-7.62 (m, 2H), 7.27-7.19 (m, 6H), 5.66 (d, *J* = 8.5 Hz, 1H), 4.98-4.76 (m, 4H), 4.04-3.80 (m, 10H), 3.71-3.61 (m, 8H), 3.48-3.28 (m, 7H), 2.23 (s, 1H), 1.17 (s, 2H).

13-C NMR (101 MHz; $CDCl_3$): δ 16.7, 17.9, 46.5, 48.3, 48.6, 67.7, 70.3, 70.4, 70.5, 71.0, 71.0, 71.3, 121.6, 121.8, 122.4, 123.8, 123.1, 125.6, 125.6, 126.1, 126.3, 126.8, 126.9, 128.8, 129.3, 137.0, 138.3, 138.3, 140.4, 142.4, 143.0, 147.8, 148.0, 174.7

HRMS calculated for $C_{39}H_{44}N_2O_{11}$ $[M+H]^+$ 717.3023, found 717.3017

Balance 1$_N$. Melting point = 135-136°C

^{1}H-NMR (400 MHz; $CDCl_3$): δ 8.09-7.93 (m, 2H), 7.80 (ddd, *J* = 9.6, 5.9, 3.5 Hz, 2H), 7.60 (ddd, *J* = 7.0, 5.8, 3.3 Hz, 2H), 7.49 (dd, *J* = 5.7, 3.3 Hz, 1H), 7.42-7.38 (m, 3H), 7.17 (d, *J* =

6.9 Hz, 3H), 7.04 (dd, *J* = 8.2, 0.4 Hz,), 6.80-6.79 (m, 2H), 5.76 (d, *J* = 8.6 Hz, 1H), 5.06 (dd, *J* = 10.6, 5.1 Hz, 2H), 4.77 (dd, *J* = 10.6, 2.5 Hz, 2H), 4.00-3.97 (m, 4H), 3.64-3.45 (m, 4H), 3.13 (dd, *J* = 5.5, 2.8 Hz, 4H), 2.83-2.70 (m, 4H), 2.11 (s, 2H), 1.75-1.64 (m, 2H), 1.46-1.37 (m, 2H), 1.26 (s, 2H).

13-C NMR (101 MHz; $CDCl_3$): δ 173.6, 173.6, 148.1, 148.0, 142.0, 141.4, 140.9, 138.8, 138.8, 138.5, 137.8, 136.2, 136.2, 129.0, 128.9, 127.8, 127.1, 126.9, 126.4, 126.3, 125.8, 125.7, 125.0, 124.6, 124.4, 124.2, 122.0, 121.5, 72.9, 72.7, 72.3, 72.3, 69.9, 67.9, 67.7, 60.0, 59.9, 56.2, 56.1, 51.4, 50.8, 50.5, 30.9, 29.7, 17.9, 17.2

HRMS calculated for $C_{42}H_{43}N_3O_8$ $[M+H]^+$ 718.3128, found 718.3119

Balance 1$_S$. Melting point = 247-250°C

^{1}H-NMR (400 MHz; $CDCl_3$): δ 8.09-7.92 (m, 2H), 7.74-7.70 (m, 2H), 7.61-7.57 (m, 2H), 7.45-7.44 (m, 1H), 7.33 (ddd, *J* = 7.7, 5.7, 3.3 Hz, 3H), 7.04 (d, *J* = 8.4 Hz,), 5.74 (d, *J* = 8.6 Hz, 1H), 5.09 (dd, *J* = 10.4, 2.3 Hz, 2H), 4.72 (d, *J* = 10.4 Hz, 2H), 3.96 (q, *J* = 4.0 Hz, 4H), 3.73-3.58 (m, 4H), 3.19-3.09 (m, 2H), 3.03-2.96 (m, 4H), 2.10 (s, 2H), 2.10 (s, 2H), 1.52-1.30 (m, 4H), 1.24 (s, 1H).

13-C NMR (101 MHz; $CDCl_3$): δ 173.6, 173.5, 148.1, 148.0, 141.9, 141.3, 138.7, 138.7, 138.5, 137.8, 136.2, 129.0, 128.88, 127.0, 126.8, 126.5, 126.4, 125.8, 125.7, 125.2, 124.8, 124.3, 124.2, 122.0, 121.5, 72.8, 72.8, 72.0, 71.8, 70.6, 67.9, 67.7, 51.2, 50.5, 50.2, 31.5, 31.5, 17.9, 17.1

HRMS calculated for $C_{35}H_{36}N_2O_8S$ $[M+H]^+$ 645.2271, found 645.2260

Control balance C1. Melting point = 104-106°C.

^{1}H-NMR (400 MHz; $CDCl_3$): δ 8.11-7.88 (m, 2H), 7.67 (ddd, *J* = 12.4, 5.7, 3.3 Hz, 2H), 7.27-7.14 (m, 6H), 5.67 (d, *J* = 8.7 Hz, 1H), 4.93-4.85 (m, 4H), 4.05-4.01 (m, 4H), 3.75 (dt, *J* = 3.8, 1.8 Hz, 6H), 3.46 (s, 6H), 2.19 (d, *J* = 0.1 Hz, 1H), 1.17 (s, 2H).

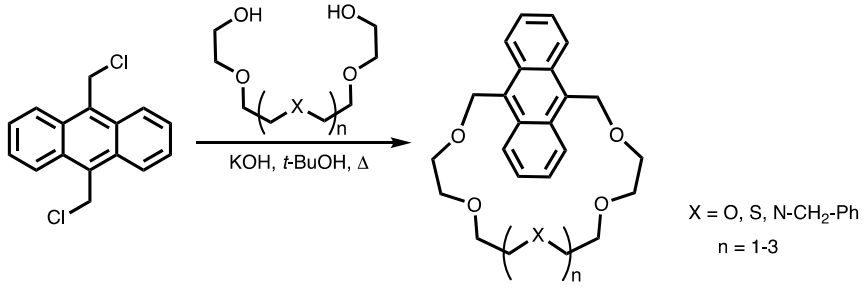
13-C NMR (101 MHz; $CDCl_3$): δ 174.4, 174.3, 148.0, 148.0, 142.7, 142.1, 140.1, 140.0, 139.6, 138.3, 138.1, 136.7, 136.6, 129.2, 128.8, 127.0, 126.9, 126.4, 126.3, 126.3, 125.7, 125.6, 125.5, 123.9, 123.7, 122.8, 122.7, 122.7, 122.6, 122.5, 122.5, 122.5, 122.5, 122.4, 122.4, 121.9, 121.6, 121.5, 71.9, 71.9, 71.0, 71.0, 68.2, 68.0, 68.0, 59.1, 59.0, 48.5, 48.2, 47.0, 47.0, 46.9, 18.0, 16.7

Control balance C2. Melting point = 176-178°C.

^{1}H-NMR (400 MHz; $CDCl_3$): δ 8.11-7.89 (m, 2H), 7.62 (ddd, *J* = 11.1, 5.7, 3.3 Hz, 2H), 7.25 (dt, *J* = 5.4, 2.6 Hz, 7H), 7.16 (d, *J* = 8.6 Hz, 1H), 5.66 (d, *J* = 8.6 Hz,), 4.87-4.76 (m, 4H), 3.95-3.89 (m, 4H), 3.80-3.70 (m, 2H), 2.20 (s, 1H), 1.42-1.38 (m, 6H), 1.17 (s, 2H).

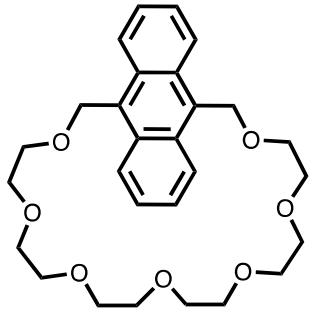
13-C NMR (101 MHz; $CDCl_3$): δ 174.37, 174.33, 147.98, 147.88, 143.0, 142.3, 140.2, 139.8, 138.4, 138.1, 136.74, 136.66, 129.2, 128.9, 127.02, 126.86, 126.38, 126.28, 125.69, 125.62, 123.81, 123.62, 122.72, 122.71, 121.9, 121.6, 77.4, 77.0, 76.7, 67.39, 67.20, 67.14, 67.13, 48.4, 48.2, 47.13, 47.11, 18.0, 16.7, 15.31, 15.29

Syntheses of the anthracenyl crown ethers



General procedure 1:
In a 250 ml round-bottom flask, a mixture of 4 mmol of the appropriate polyethylene glycol, 5 mmol of KOH, and 10 ml of tert-butanol was refluxed with stirring for 30 minutes. The reaction was then removed from heating and diluted with 60 ml of tert-butanol and followed by the addition of 2 mmol (0.55g) of 9,10-bis(chloromethyl)anthracene. The mixture was refluxed overnight, concentrated to a minimal volume, and then diluted with 40 ml of diethyl ether. The resulting organic mixture was washed with water. The organic

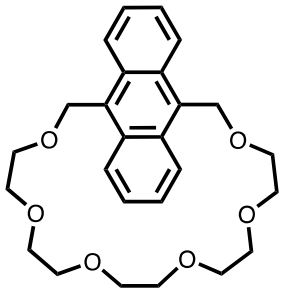
phase was concentrated and subjected to flash column chromatography purification using mixtures of ethyl acetate and hexane.



3,6,9,12,15,18,21-heptaoxa-1(9,10)-anthracenacyclodocosaphane

Prepared according to General Procedure 1. Yield = 32%. ^{1}H-NMR (400 MHz; $CDCl_3$): δ 8.51 (dd, *J* = 6.9, 3.3 Hz, 4H), 7.58 (dd, *J* = 6.9, 3.3 Hz, 4H), 5.59 (s, 4H), 3.79-3.77 (m, 4H), 3.67-3.64 (m, 4H), 3.45-3.43 (m, 4H), 3.39-3.36 (m, 4H), 3.21-3.18 (m, 5H), 3.16-3.14 (m, 4H).

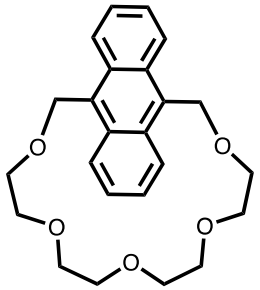
13-C NMR (101 MHz; $CDCl_3$): δ 130.7, 130.5, 125.7, 125.1, 70.8, 70.6, 70.4, 70.3, 69.7, 65.2



3,6,9,12,15,18-hexaoxa-1(9,10)-anthracenacyclononadecaphane

Prepared according to General Procedure 1. Yield = 33%. ^{1}H-NMR (400 MHz; $CDCl_3$): δ 8.52 (dd, *J* = 6.9, 3.3 Hz, 4H), 7.58 (dd, *J* = 6.8, 3.1 Hz, 4H), 5.61 (s, 4H), 3.71 (dd, *J* = 5.5, 3.5 Hz, 6H), 3.56 (dd, *J* = 5.3, 3.6 Hz, 4H), 3.27-3.20 (m, 8H), 2.95 (s, 4H).

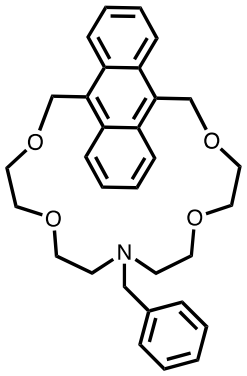
13-C NMR (101 MHz; $CDCl_3$): δ 130.7, 130.5, 125.6, 125.2, 70.5, 70.3, 70.1, 69.7, 69.1, 64.8



3,6,9,12,15-pentaoxa-1(9,10)-anthracenacyclohexadecaphane

Prepared using General Procedure 1: Yield = 28%. ^{1}H-NMR (400 MHz; aceton-d_6): δ 8.63 (dd, *J* = 7.0, 3.3 Hz, 4H), 7.61-7.59 (m, 4H), 5.66 (s, 4H), 3.61-3.59 (m, 5H), 3.30-3.28 (m, 4H), 2.91 (dd, *J* = 5.7, 5.2 Hz, 4H), 2.67 (t, *J* = 5.6 Hz, 4H).

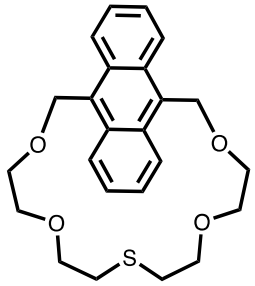
13-C NMR (101 MHz; $CDCl_3$): δ 130.7, 130.6, 125.6, 125.2, 77.5, 77.2, 76.8, 70.1, 70.0, 69.9, 69.0, 64.2



9-benzyl-3,6,12,15-tetraoxa-9-aza-1(9,10)-anthracenacyclohexadecaphane

Prepared using General Procedure 1: Yield = 29%. ^{1}H-NMR (400 MHz; $CDCl_3$): δ 8.55 (dd, *J* = 7.0, 3.3 Hz, 4H), 7.59 (dd, *J* = 6.9, 3.2 Hz, 4H), 7.26-7.12 (m, 5H), 5.63 (s, 4H), 3.61 (t, *J* = 4.5 Hz, 4H), 3.31 (dd, *J* = 8.1, 3.5 Hz, 6H), 2.81 (t, *J* = 6.7 Hz, 4H), 1.89 (t, *J* = 6.7 Hz, 4H).

13-C NMR (101 MHz; $CDCl_3$): δ 139.5, 130.8, 130.7, 128.7, 128.0, 126.7, 125.6, 125.2, 69.8, 68.8, 68.8, 64.5, 59.5, 53.5

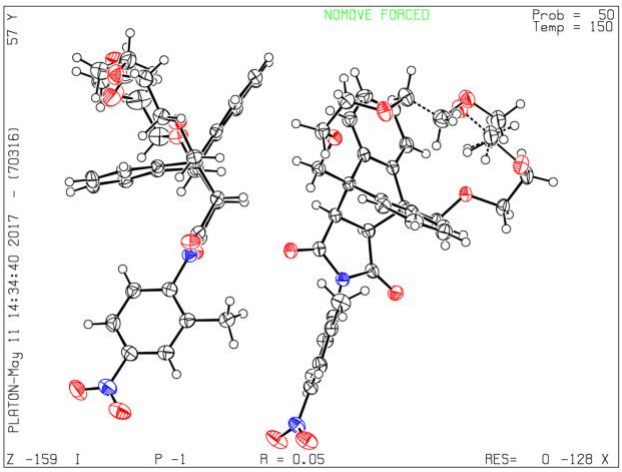


3,6,12,15-tetraoxa-9-thia-1(9,10)-anthracenacyclohexadecaphane

Prepared using General Procedure 1: Yield = 25%. ^{1}H-NMR (400 MHz; $CDCl_3$): δ 8.54 (dd, *J* = 6.9, 3.3 Hz, 4H), 7.62-7.59 (m, 4H), 5.64 (s, 4H), 3.70-3.68 (m, 4H), 3.35-3.33 (m, 4H), 2.98 (t, *J* = 7.2 Hz, 4H), 1.89 (t, *J* = 7.2 Hz, 4H).

13-C NMR (101 MHz; $CDCl_3$): δ 130.8, 130.6, 125.7, 125.2, 70.7, 69.8, 69.7, 64.7, 31.5

X-ray crystal structure of Balance 1 (CCDC number 1858930)



Bond precision: C-C = 0.0024 A Wavelength=1.54178

Cell: a=10.6256(6) b=14.6830(8) c=20.9217(10)
alpha=110.478(3) beta=90.035(2) gamma=90.542(2)

Temperature: 150 K

	Calculated	Reported
Volume	3057.7(3)	3057.7(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C35 H36 N2 O9	C35 H36 N2 O9
Sum formula	C35 H36 N2 O9	C35 H36 N2 O9
Mr	628.66	628.66
Dx,g cm-3	1.366	1.366
Z	4	4
Mu (mm-1)	0.818	0.818
F000	1328.0	1328.0
F000'	1332.37	
h,k,lmax	13,18,26	13,17,26
Nref	13347	12348
Tmin,Tmax	0.872,0.921	0.609,0.754
Tmin'	0.870	

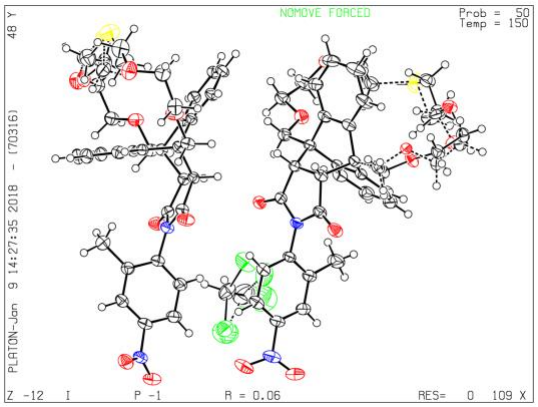
Correction method= # Reported T Limits: Tmin=0.609 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.925 Theta(max)= 80.121

R(reflections)= 0.0497(9787) wR2(reflections)= 0.1311(12348)

S = 1.047 Npar= 838

X-ray crystal structure of Balance 1_S (CCDC number 2321755)



Bond precision: C-C = 0.0036 A Wavelength=0.71073

Cell: a=10.0840(6) b=15.1221(8) c=22.3730(13)
alpha=100.593(2) beta=94.039(2) gamma=95.970(2)

Temperature: 150 K

	Calculated	Reported
Volume	3321.3(3)	3321.3(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C35 H36 N2 O8 S), C H Cl3	2(C35 H36 N2 O8 S), C H Cl3
Sum formula	C71 H73 Cl3 N4 O16 S2	C71 H73 Cl3 N4 O16 S2
Mr	1408.80	1408.80
Dx,g cm-3	1.409	1.409
Z	2	2
Mu (mm-1)	0.274	0.274
F000	1476.0	1476.0
F000'	1478.07	
h,k,lmax	14,21,32	14,21,31
Nref	20450	29270
Tmin,Tmax	0.936,0.970	0.635,0.746
Tmin'	0.884	

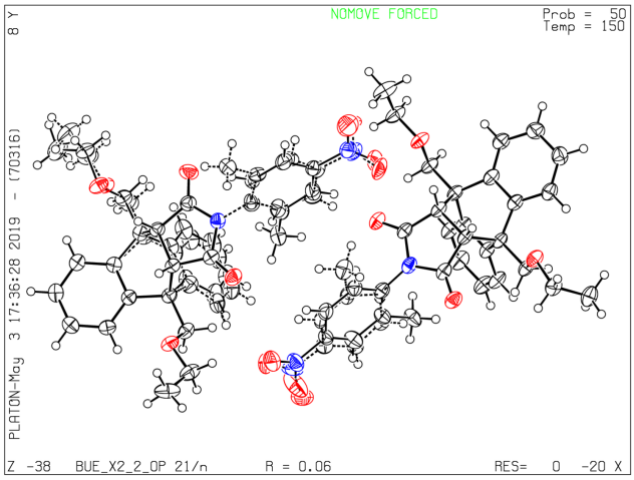
Correction method= # Reported T Limits: Tmin=0.635 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.431 Theta(max)= 30.594

R(reflections)= 0.0552(20258) wR2(reflections)= 0.1584(29270)

S = 1.043 Npar= 1004

X-ray crystal structure of Balance C1 (CCDC number 2321756)



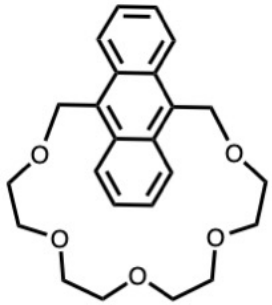

```
Bond precision:      C-C = 0.0022 A                Wavelength=0.71073
Cell:        a=17.0682(11)    b=11.8271(7)     c=27.346(3)
             alpha=90         beta=106.721(4)  gamma=90
Temperature: 150 K
                    Calculated                       Reported
Volume              5286.9(8)                        5286.9(7)
Space group         P 21/n                           P 21/n
Hall group          -P 2yn                           -P 2yn
Moiety formula      C31 H30 N2 O6                    ?
Sum formula         C31 H30 N2 O6                    C124 H120 N8 O24
Mr                  526.57                           2106.27
Dx,g cm-3           1.323                            1.323
Z                   8                                2
Mu (mm-1)           0.092                            0.092
F000                2224.0                           2224.0
F000'               2225.10
h,k,lmax            24,16,39                         24,16,39
Nref                16186                            15010
Tmin,Tmax           0.951,0.961                      0.665,0.746
Tmin'               0.951
Correction method= # Reported T Limits: Tmin=0.665
Tmax=0.746 AbsCorr = MULTI-SCAN
Data completeness= 0.927        Theta(max)= 30.542
R(reflections)= 0.0566( 10258)     wR2(reflections)= 0.1732( 15010)
S = 1.106              Npar= 995
```

References

(1) Kannan, A.; Rajakumar, P. *RSC Advances* **2015**, *5*, 73951.

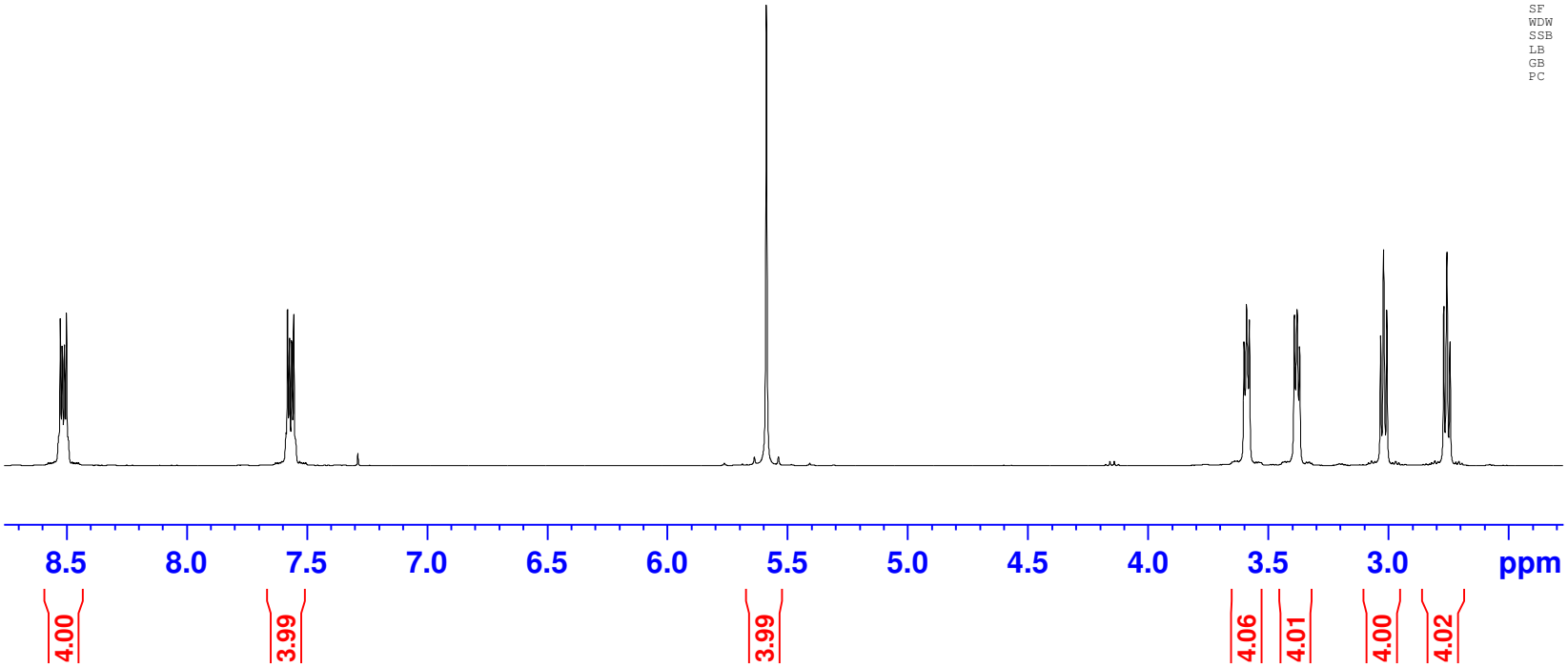
(2) Emenike, B. U.; Sevimler, A.; Farshadmand, A.; Roman, A. J. *Physical Chemistry Chemical Physics* **2023**, *25*, 17808.

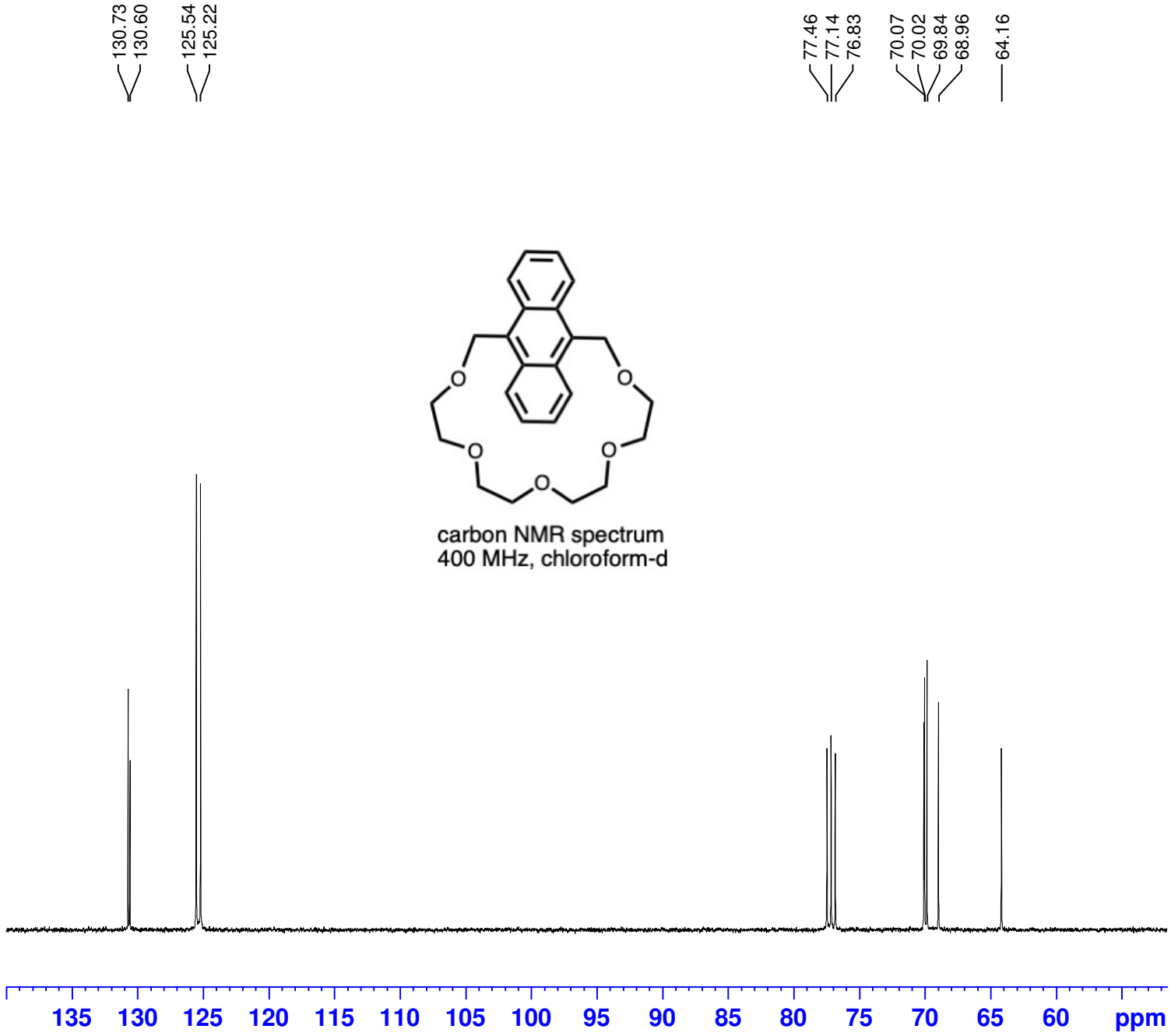
8.551 8.534 8.527 8.519 8.510 8.502 8.478 7.605 7.588 7.581 7.573 7.564 7.556 7.550 7.531 7.289 5.638 5.588 5.539 4.159 4.141 3.640 3.628 3.601 3.590 3.579 3.551 3.540 3.429 3.419 3.391 3.380 3.370 3.341 3.330 3.070 3.056 3.033 3.020 3.007 2.970 2.806 2.793 2.770 2.756 2.744 2.720 2.706



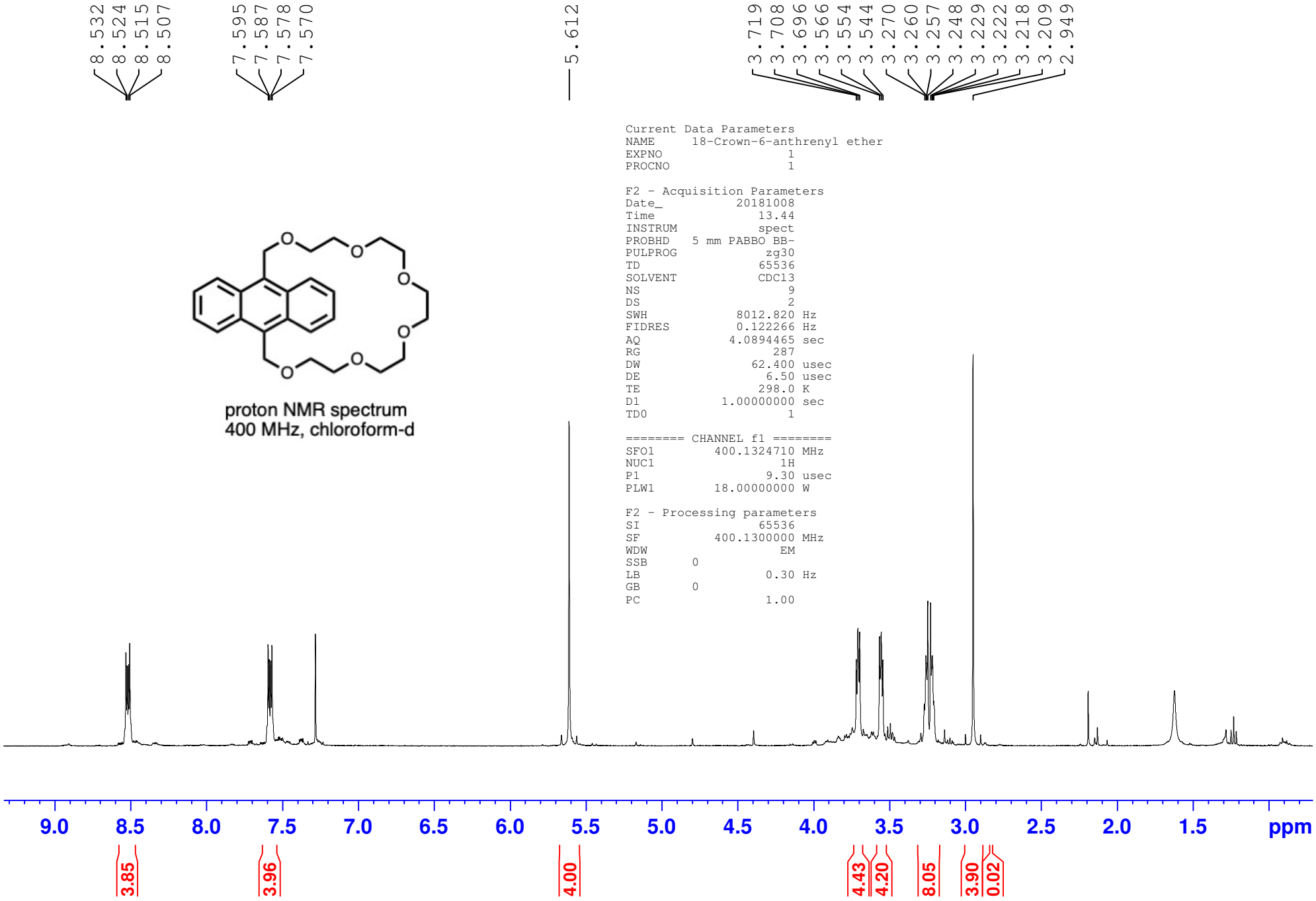
proton NMR spectrum
400 MHz, chloroform-d

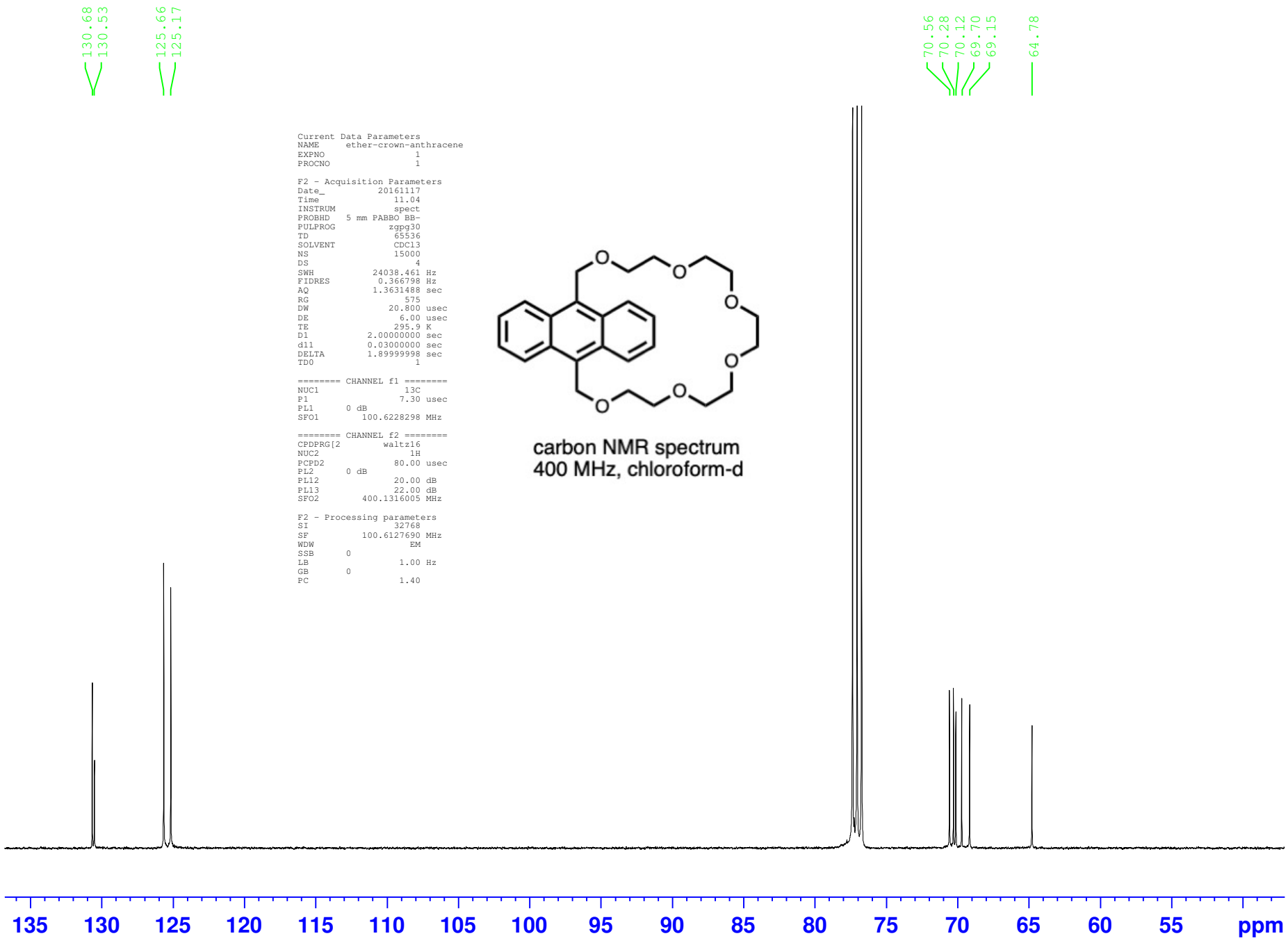
```
Current Data Parameters
NAME      anthracenyl-tetraethylene-crown-ether
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170103
Time              10.48
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9845889 sec
RG                50.8
DW               60.800 usec
DE                6.00 usec
TE               295.2 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                9.30 usec
PL1       0 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

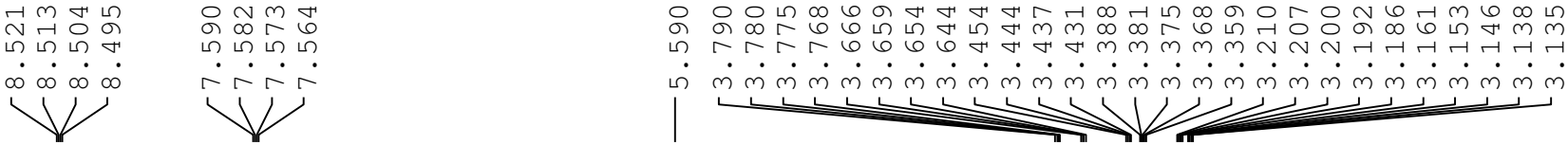


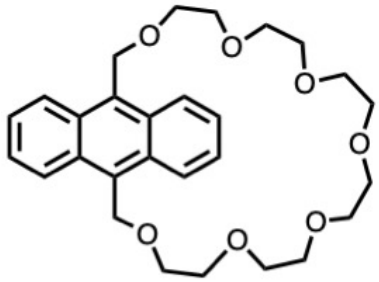



```
Current Data Parameters
NAME      anthracenyl-tetraethylene-crown-ether-carbon
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_             20170103
Time                11.01
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   150
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                 32768
DW                20.800 usec
DE                 6.00 usec
TE                 295.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   7.30 usec
PL1       0 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2                80.00 usec
PL2       0 dB
PL12                 20.00 dB
PL13                 22.00 dB
SFO2          400.1316005 MHz

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


8.532
8.524
8.515
8.507
7.595
7.587
7.578
7.570
5.612
3.719
3.708
3.696
3.566
3.554
3.544
3.270
3.260
3.257
3.248
3.229
3.222
3.218
3.209
2.949
Current Data Parameters
NAME 18-Crown-6-anthrenyl ether
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181008
Time 13.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 287
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 9.30 usec
PLW1 18.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
proton NMR spectrum
400 MHz, chloroform-d
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
3.85
3.96
4.00
4.43
4.20
8.05
3.90
0.02

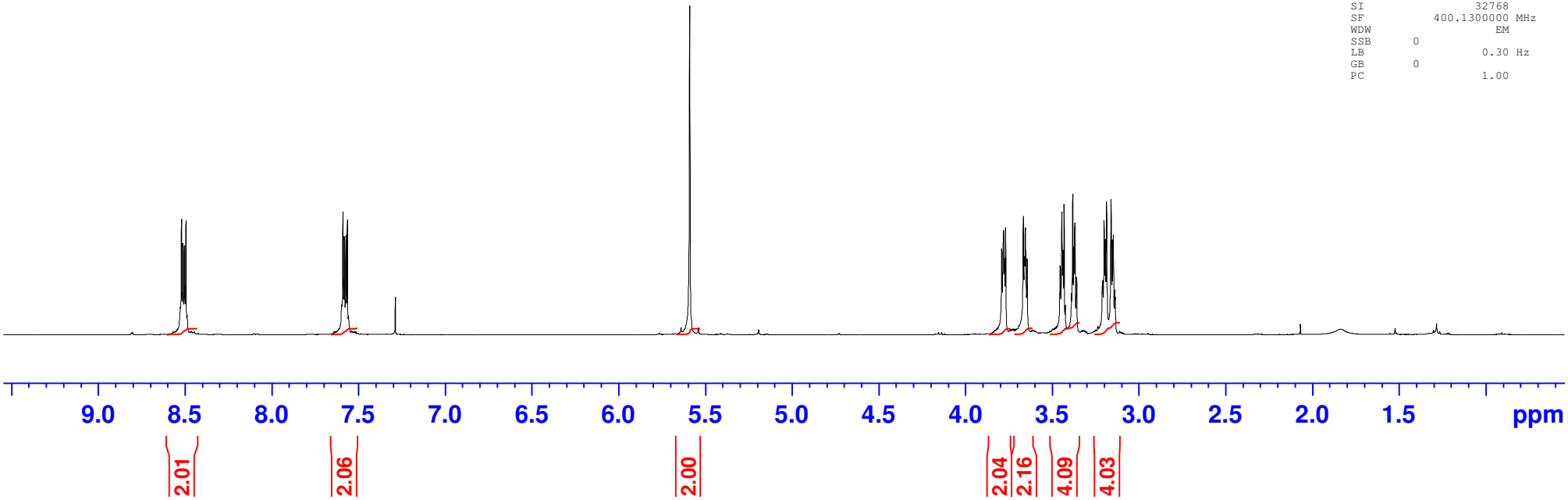

130.68
130.53
125.66
125.17
70.56
70.28
70.12
69.70
69.15
64.78
Current Data Parameters
NAME ether-crown-anthracene
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161117
Time 11.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 15000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 575
DW 20.800 usec
DE 6.00 usec
TE 295.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.30 usec
PL1 0 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 20.00 dB
PL13 22.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
carbon NMR spectrum
400 MHz, chloroform-d
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
ppm

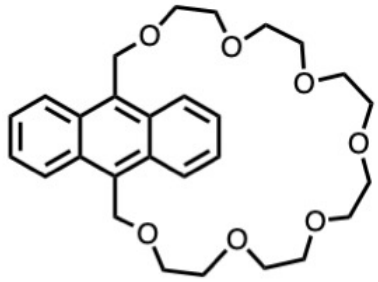




proton NMR spectrum
400 MHz, chloroform-d

```
Current Data Parameters
NAME      7-membered-anthracene
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20170718
Time                   17.58
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                      128
DW                   60.800 usec
DE                    6.00 usec
TE                   296.5 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     9.30 usec
PL1         0 dB
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                    32768
SF              400.1300000 MHz
WDW                      EM
SSB         0
LB                     0.30 Hz
GB          0
PC                     1.00
```



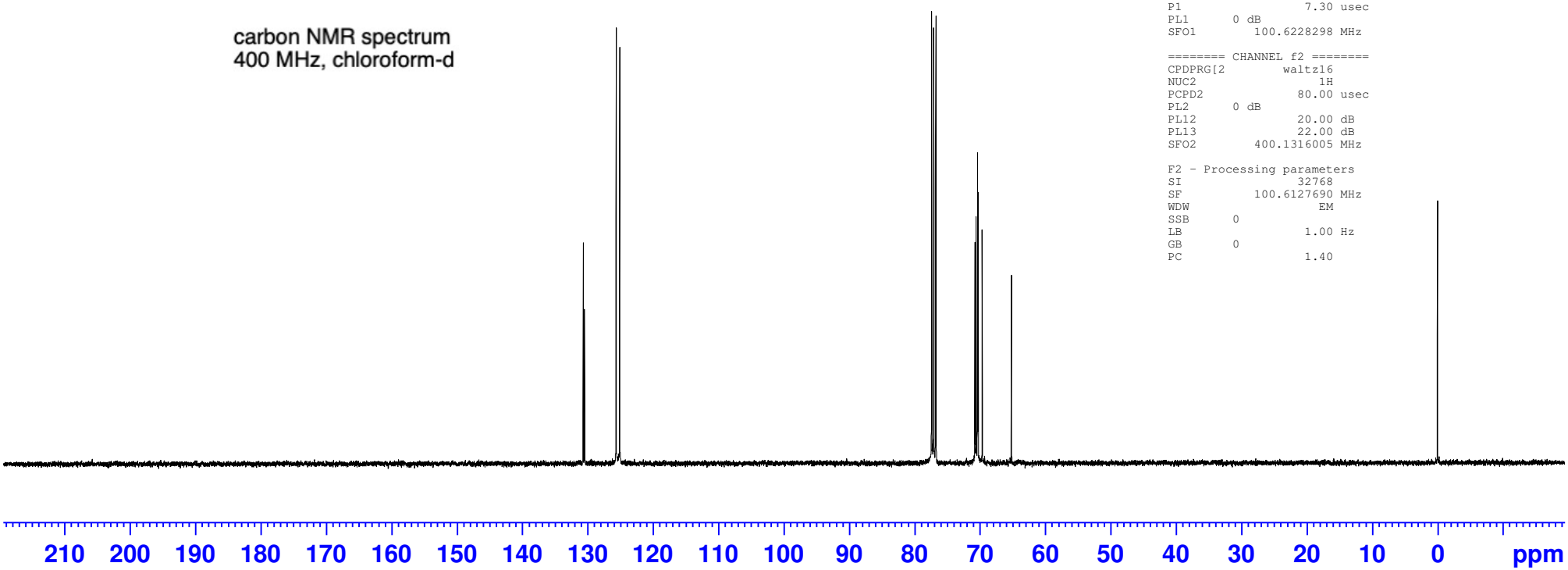


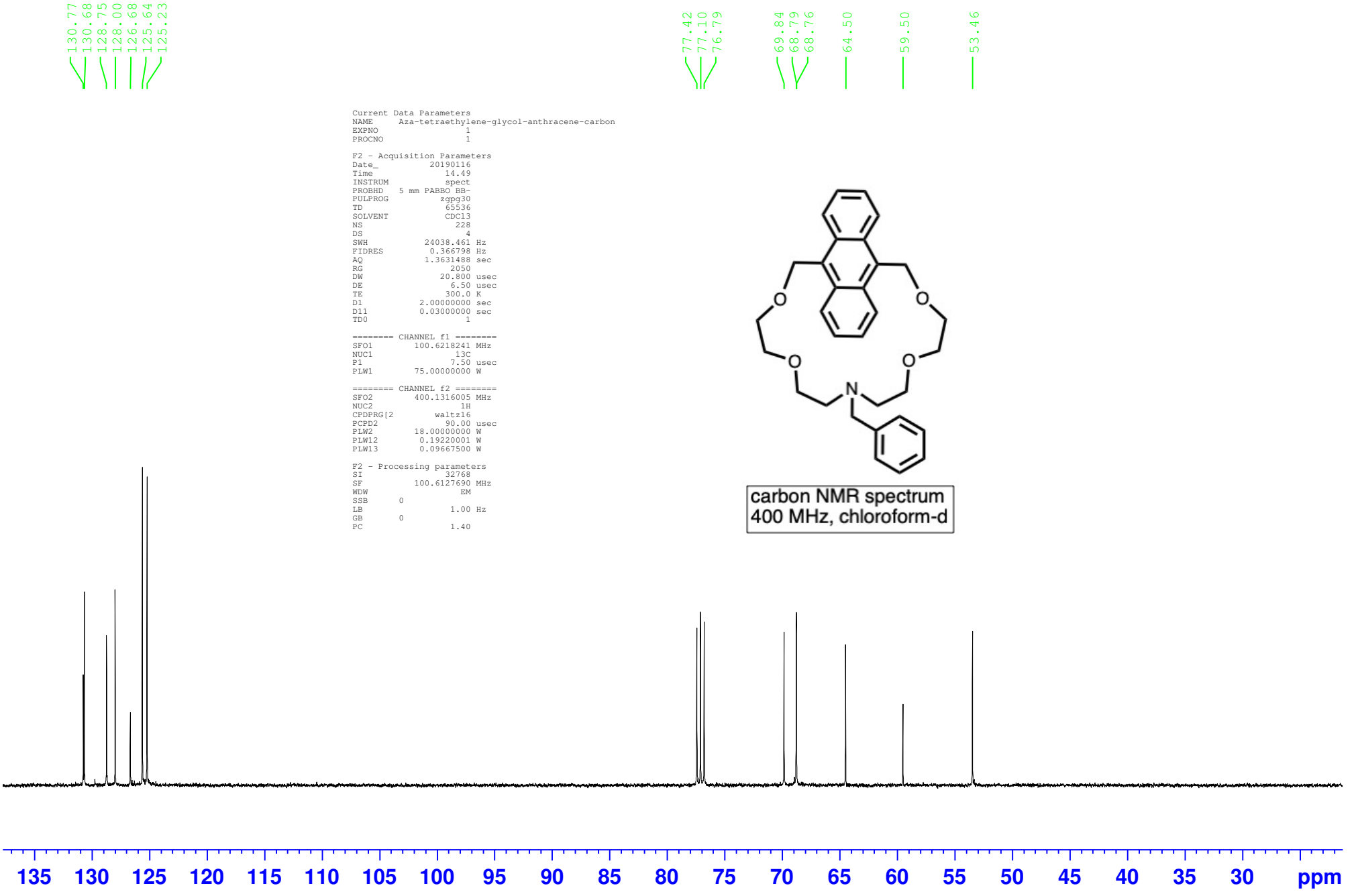
carbon NMR spectrum
400 MHz, chloroform-d

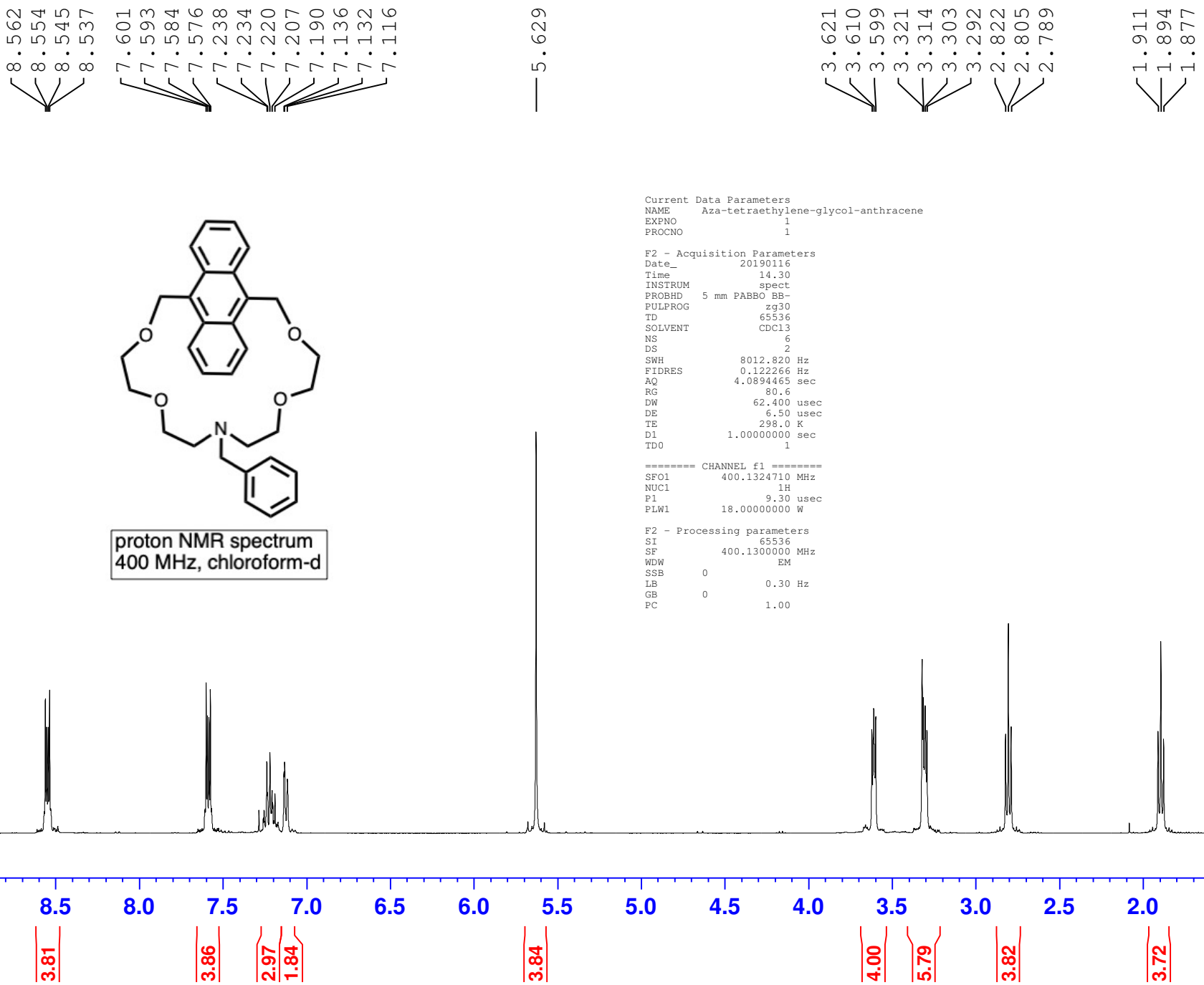
130.71
130.50
125.67
125.14

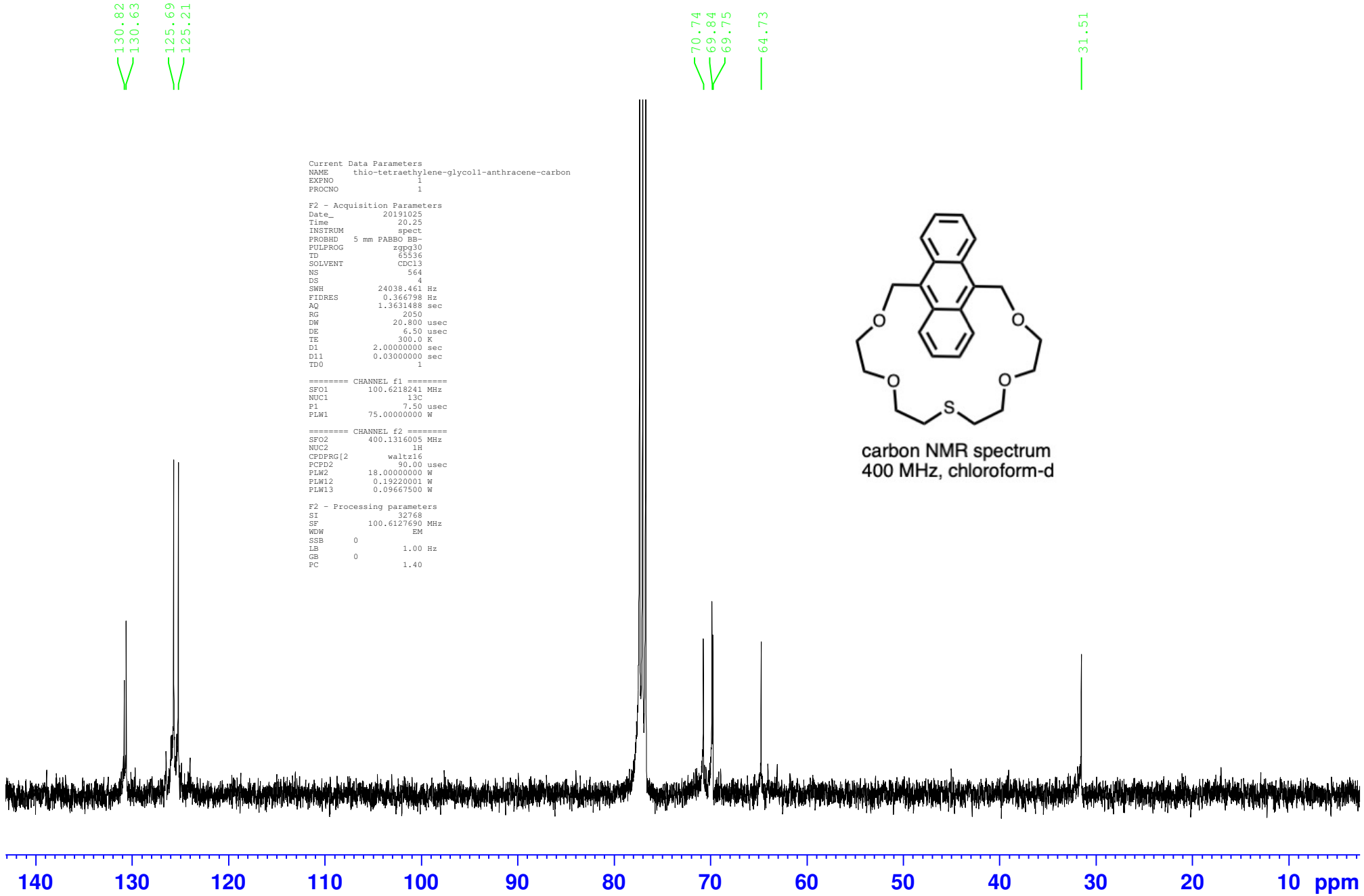
70.77
70.61
70.38
70.36
70.28
69.66
65.20

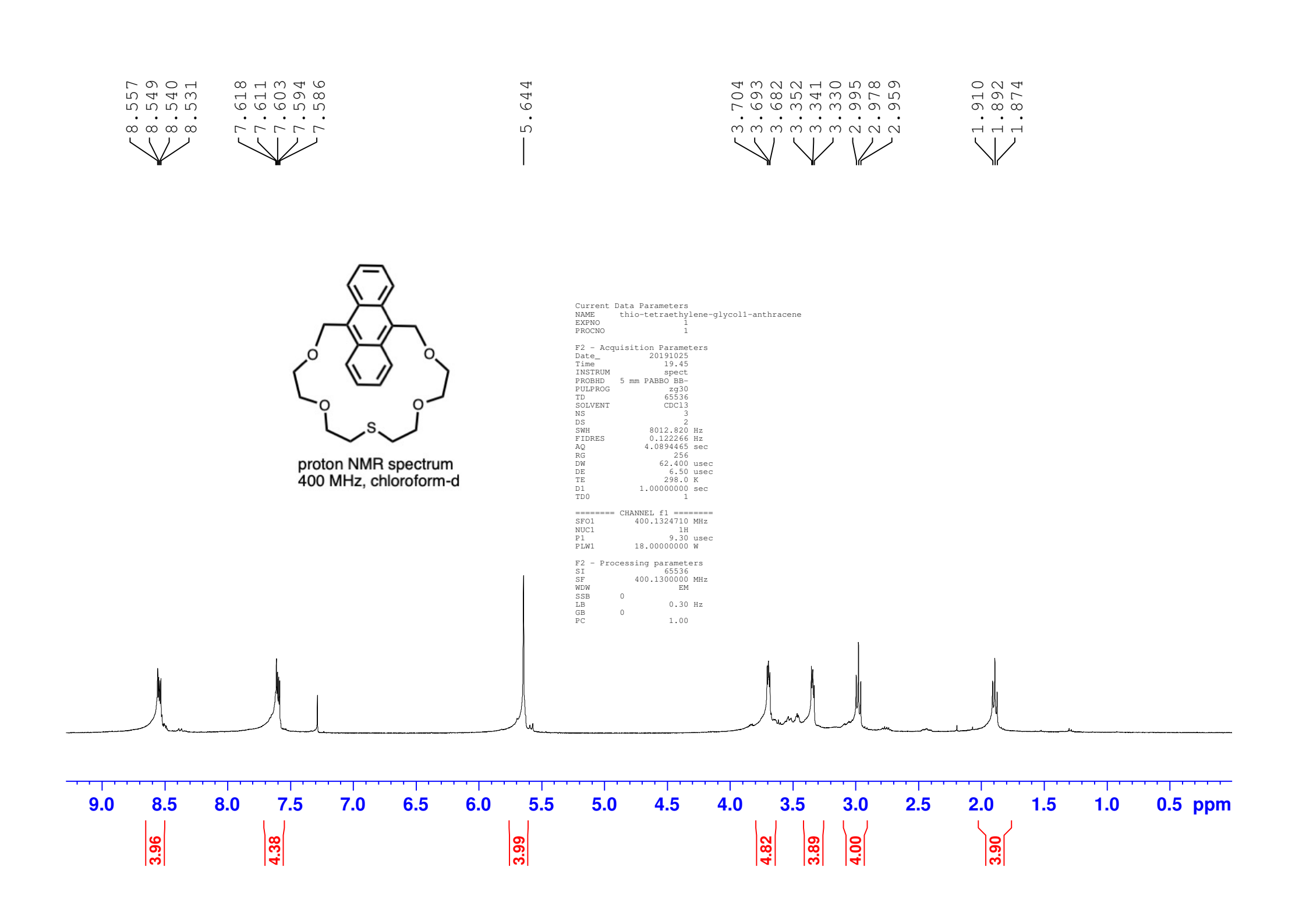
```
Current Data Parameters
NAME      7-membered-anthracene-carbon
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170718
Time              19.01
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                1024
DS                   4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG                 575
DW              20.800 usec
DE               6.00 usec
TE               297.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                 7.30 usec
PL1       0 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2              80.00 usec
PL2       0 dB
PL12               20.00 dB
PL13               22.00 dB
SFO2         400.1316005 MHz

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

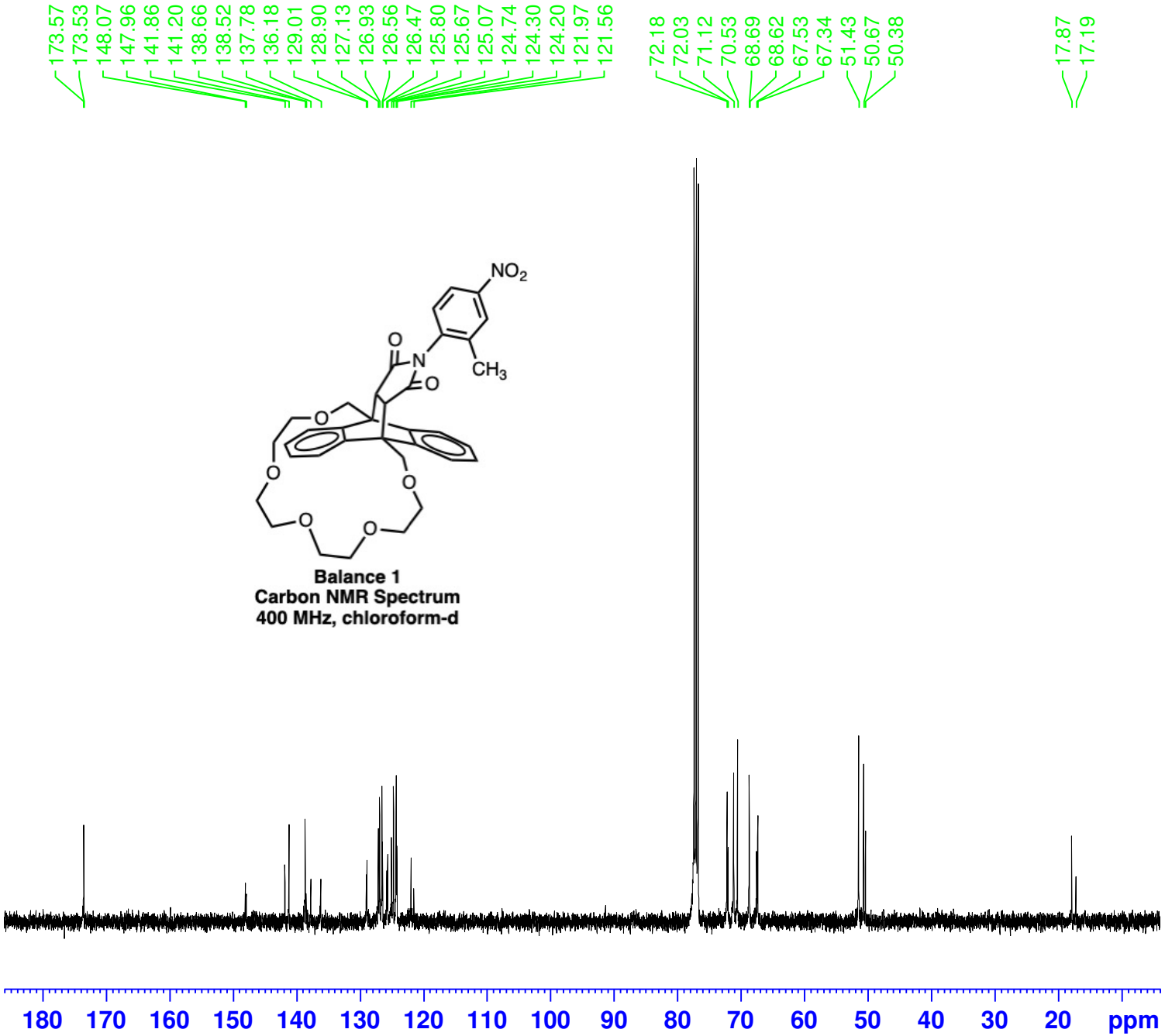



130.77
130.68
128.75
128.00
126.68
125.64
125.23
77.42
77.10
76.79
69.84
68.79
68.76
64.50
59.50
53.46
Current Data Parameters
NAME Aza-tetraethylene-glycol-anthracene-carbon
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190116
Time 14.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 228
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6218241 MHz
NUC1 13C
P1 7.50 usec
PLW1 75.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.19220001 W
PLW13 0.09667500 W
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
O
O
N
carbon NMR spectrum
400 MHz, chloroform-d
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
ppm

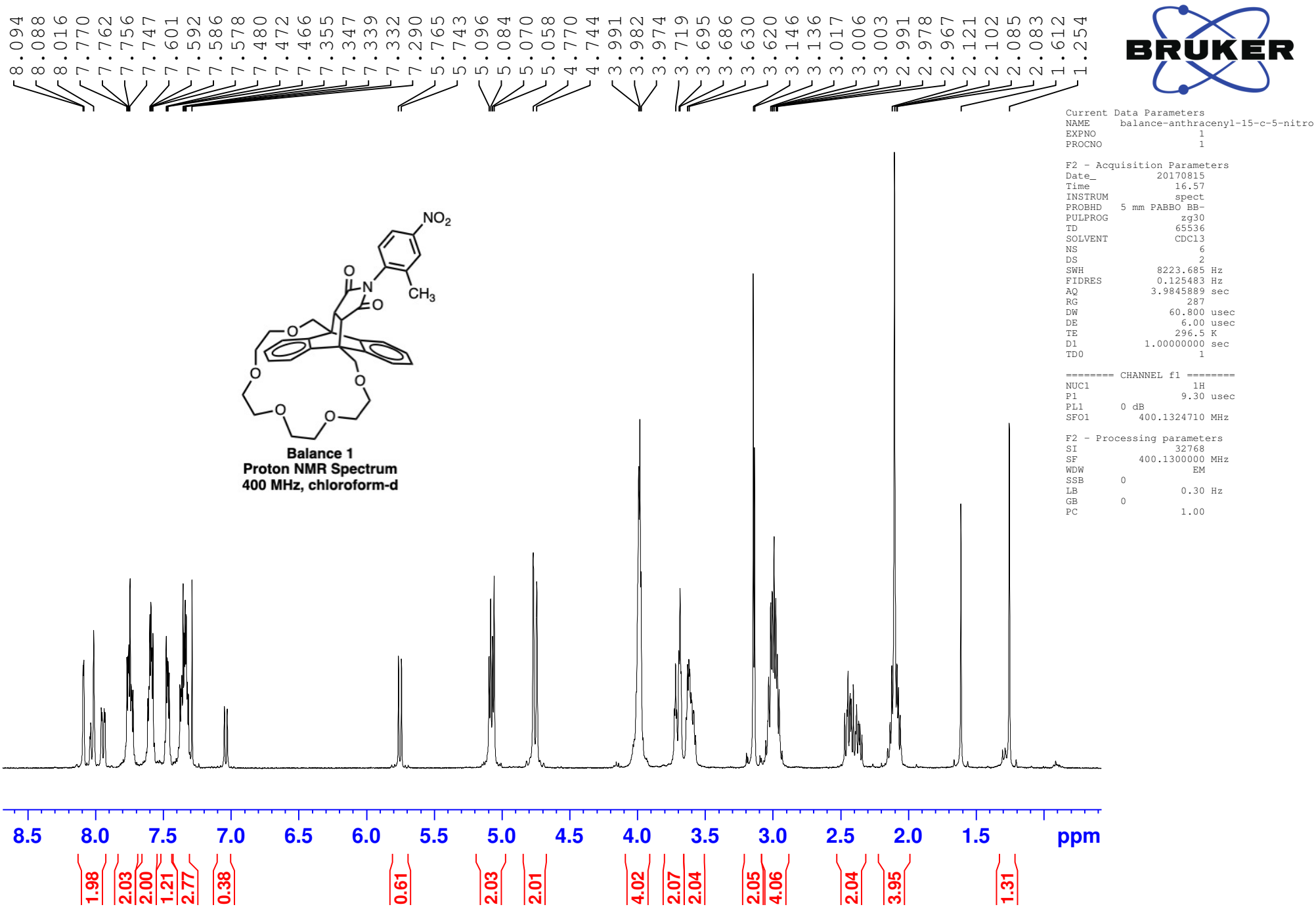

8.562
8.554
8.545
8.537
7.601
7.593
7.584
7.576
7.238
7.234
7.220
7.207
7.190
7.136
7.132
7.116
5.629
3.621
3.610
3.599
3.321
3.314
3.303
3.292
2.822
2.805
2.789
1.911
1.894
1.877
O
O
O
O
N
proton NMR spectrum
400 MHz, chloroform-d
Current Data Parameters
NAME Aza-tetraethylene-glycol-anthracene
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190116
Time 14.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 80.6
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 9.30 usec
PLW1 18.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
3.81
3.86
2.97
1.84
3.84
4.00
5.79
3.82
3.72

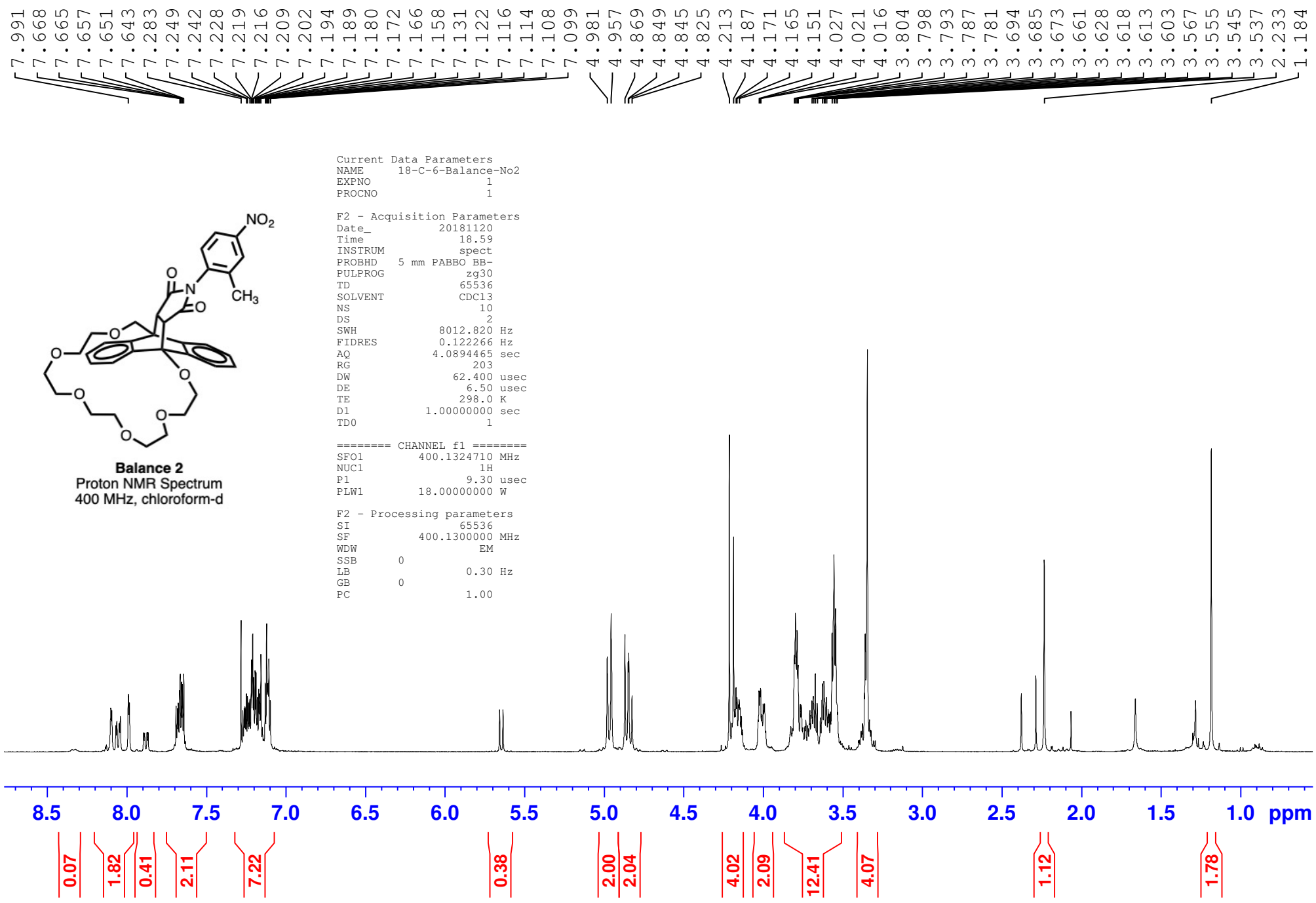

130.82
130.63
125.69
125.21
70.74
69.84
69.75
64.73
31.51
Current Data Parameters
NAME thio-tetraethylene-glycol1-anthracene-carbon
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191025
Time 20.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 564
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6218241 MHz
NUC1 13C
P1 7.50 usec
PLW1 75.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.19220001 W
PLW13 0.09667500 W
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O
O
O
O
S
carbon NMR spectrum
400 MHz, chloroform-d
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

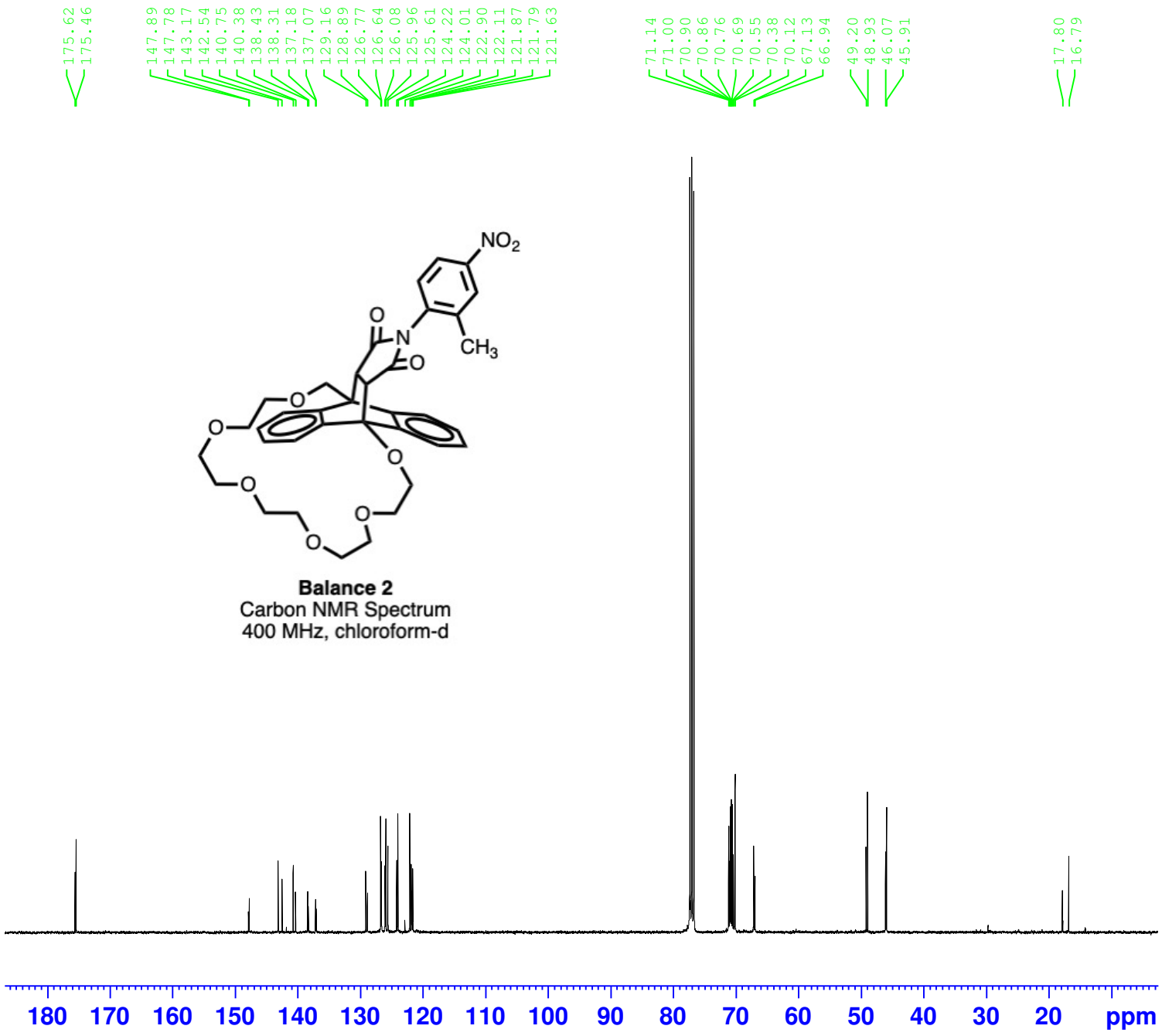

8.557
8.549
8.540
8.531
7.618
7.611
7.603
7.594
7.586
5.644
3.704
3.693
3.682
3.352
3.341
3.330
2.995
2.978
2.959
1.910
1.892
1.874
O
O
O
O
S
proton NMR spectrum
400 MHz, chloroform-d
Current Data Parameters
NAME thio-tetraethylene-glycol1-anthracene
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191025
Time 19.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 3
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 256
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 9.30 usec
PLW1 18.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
3.96
4.38
3.99
4.82
3.89
4.00
3.90



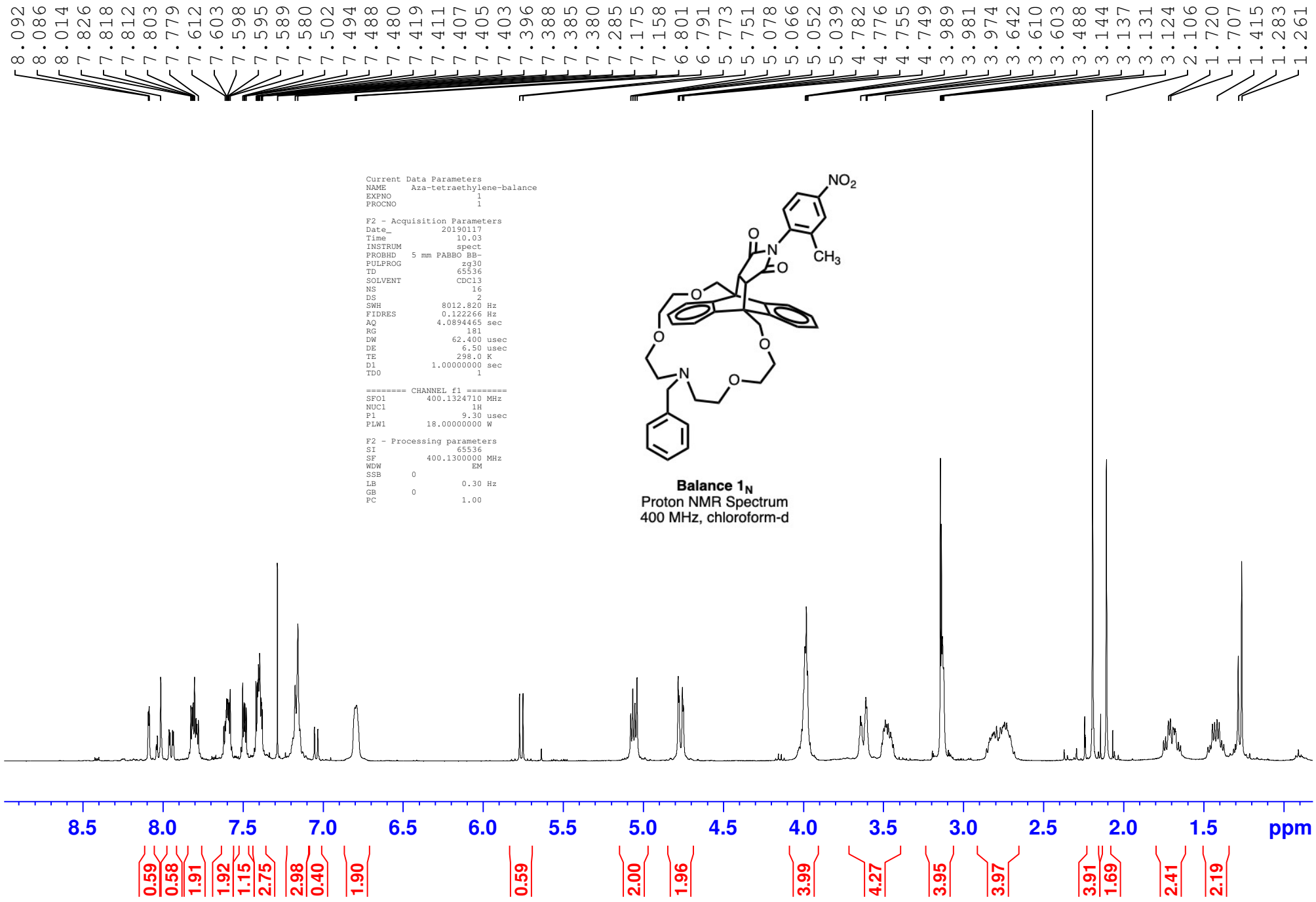

```
Current Data Parameters
NAME      15-C-5-No2-balance-carbon
EXPNO                             1
PROCNO                            1

F2 - Acquisition Parameters
Date_                      20180718
Time                          21.08
INSTRUM                       spect
PROBHD    5 mm PABBO BB-
PULPROG                     zgpg30
TD                           65536
SOLVENT                      CDCl3
NS                             640
DS                               4
SWH                      24038.461 Hz
FIDRES                    0.366798 Hz
AQ                        1.3631488 sec
RG                            2050
DW                          20.800 usec
DE                           6.50 usec
TE                          300.0 K
D1                     2.00000000 sec
D11                    0.03000000 sec
TD0                              1

======== CHANNEL f1 ========
SFO1                 100.6218241 MHz
NUC1                         13C
P1                          7.50 usec
PLW1                 75.00000000 W

======== CHANNEL f2 ========
SFO2                 400.1316005 MHz
NUC2                         1H
CPDPRG[2                 waltz16
PCPD2                       90.00 usec
PLW2                 18.00000000 W
PLW12                 0.19220001 W
PLW13                 0.09667500 W

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

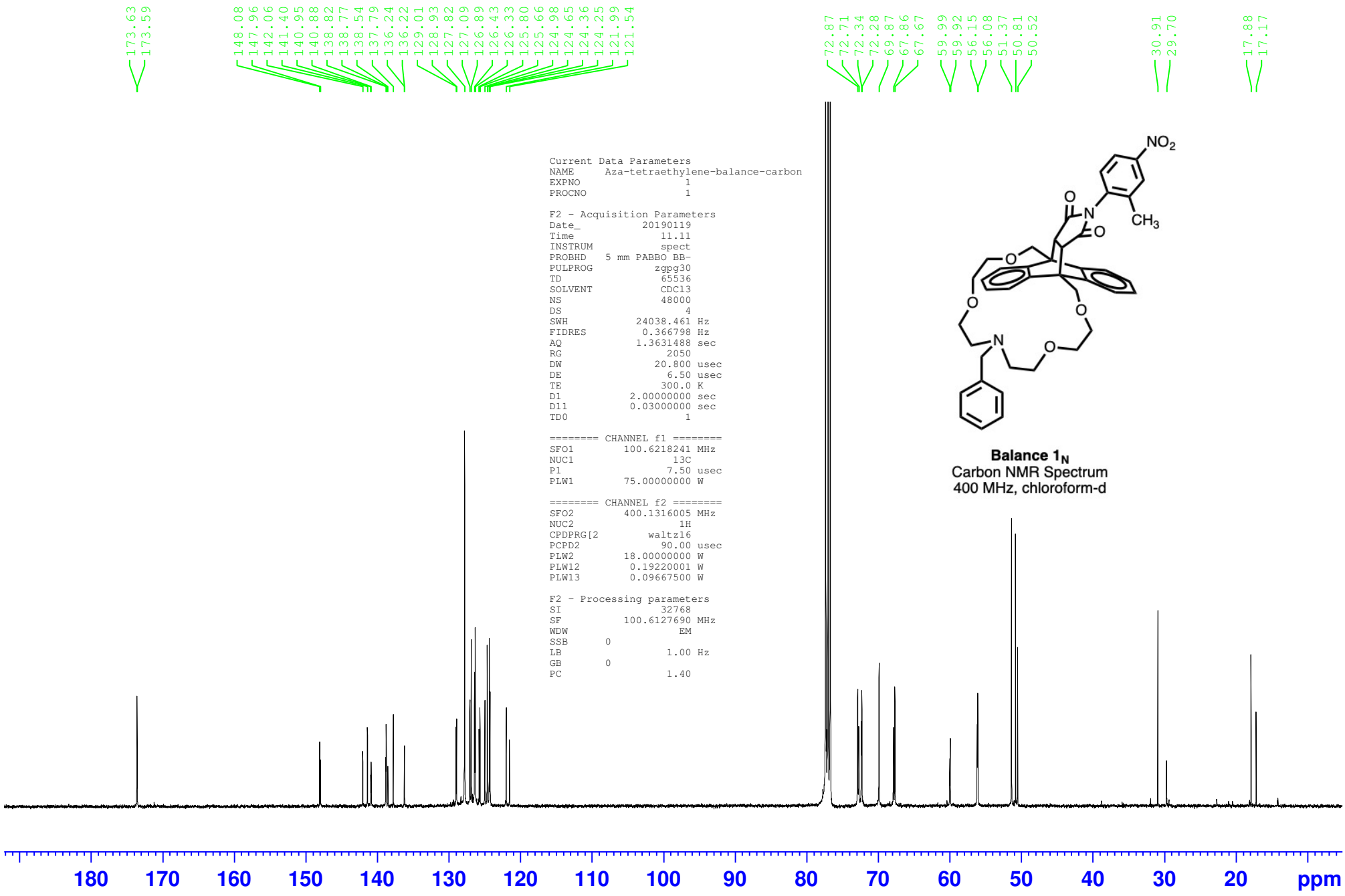

8.094
8.088
8.016
7.770
7.762
7.756
7.747
7.601
7.592
7.586
7.578
7.480
7.472
7.466
7.355
7.347
7.339
7.332
7.290
5.765
5.743
5.096
5.084
5.070
5.058
4.770
4.744
3.991
3.982
3.974
3.719
3.695
3.686
3.630
3.620
3.146
3.136
3.017
3.006
3.003
2.991
2.978
2.967
2.121
2.102
2.085
2.083
1.612
1.254
BRUKER
Current Data Parameters
NAME balance-anthracenyl-15-c-5-nitro
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170815
Time 16.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 287
DW 60.800 usec
DE 6.00 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.30 usec
PL1 0 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
NO2
CH3
Balance 1
Proton NMR Spectrum
400 MHz, chloroform-d
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.98
2.03
2.00
1.21
2.77
0.38
0.61
2.03
2.01
4.02
2.07
2.04
2.05
4.06
2.04
3.95
1.31

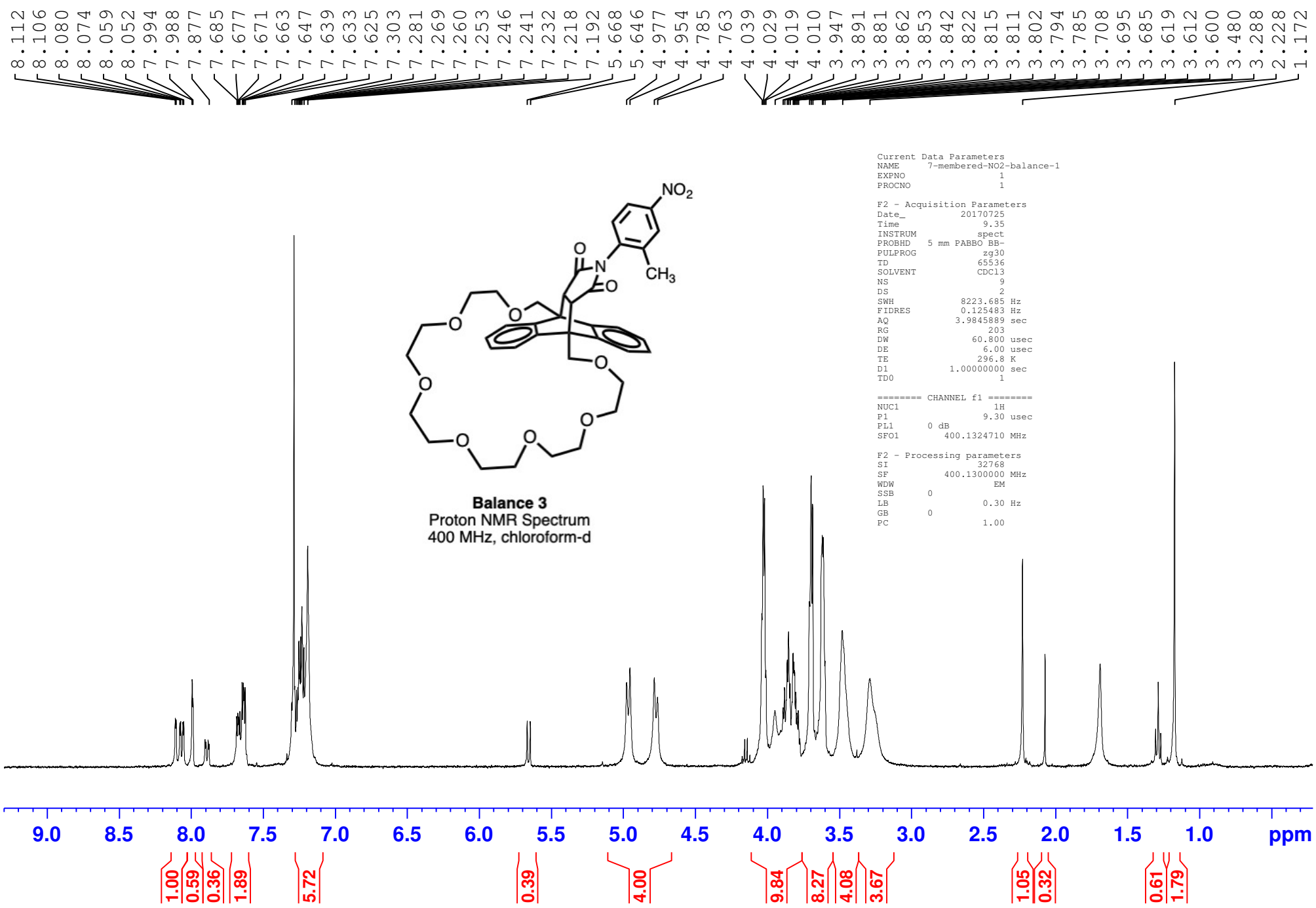

7.991
7.668
7.665
7.657
7.651
7.643
7.283
7.249
7.242
7.228
7.219
7.216
7.209
7.202
7.194
7.189
7.180
7.172
7.166
7.158
7.131
7.122
7.116
7.114
7.108
7.099
4.981
4.957
4.869
4.849
4.845
4.825
4.213
4.187
4.171
4.165
4.151
4.027
4.021
4.016
3.804
3.798
3.793
3.787
3.781
3.694
3.685
3.673
3.661
3.628
3.618
3.613
3.603
3.567
3.555
3.545
3.537
2.233
1.184
NO2
O
N
O
CH3
O
O
O
O
O
O
O
Balance 2
Proton NMR Spectrum
400 MHz, chloroform-d
Current Data Parameters
NAME 18-C-6-Balance-No2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181120
Time 18.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 10
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
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 9.30 usec
PLW1 18.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.07
1.82
0.41
2.11
7.22
0.38
2.00
2.04
4.02
2.09
12.41
4.07
1.12
1.78

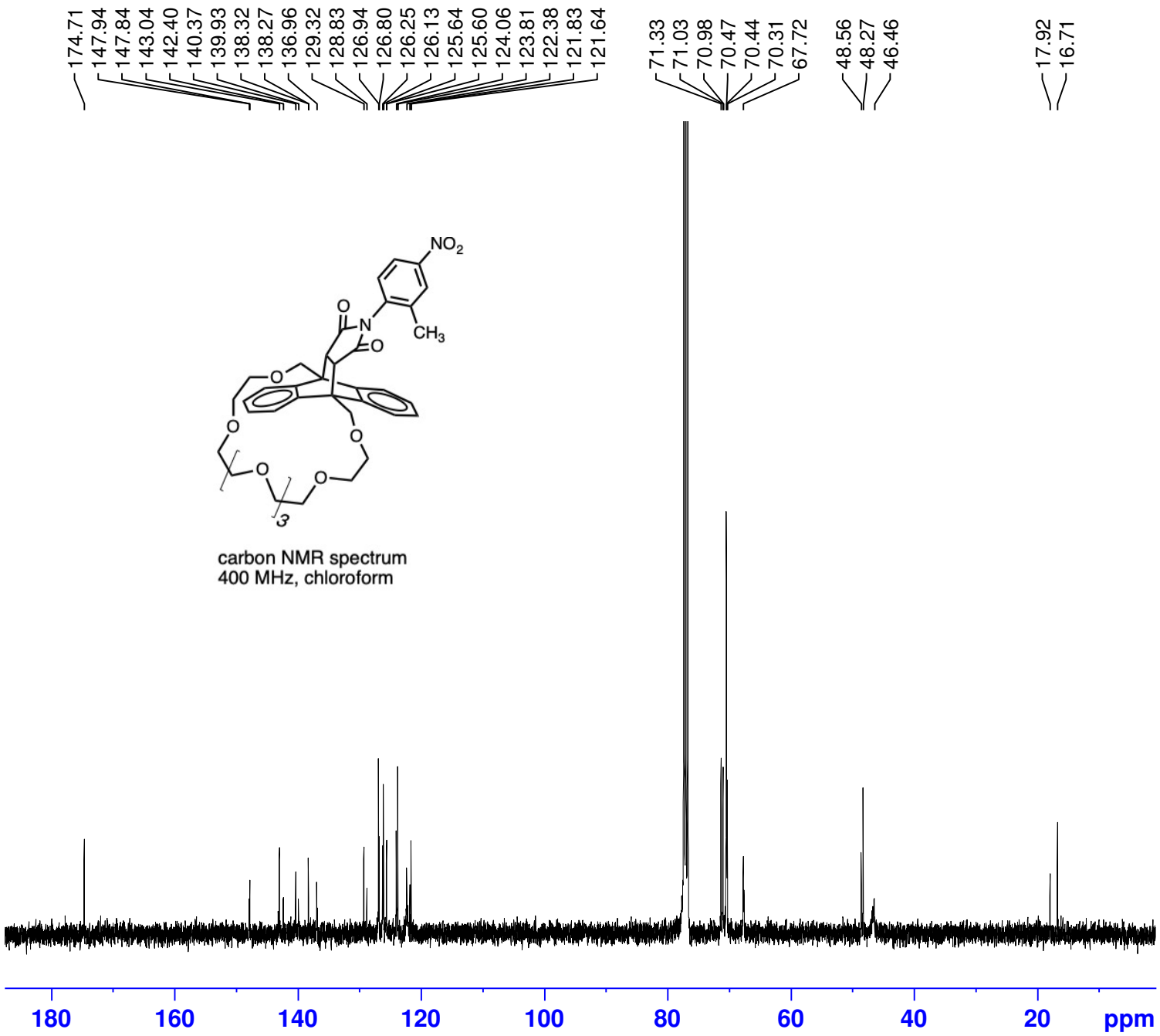



```
Current Data Parameters
NAME      18-C-6-Balance-No2-carbon
EXPNO                             1
PROCNO                            1

F2 - Acquisition Parameters
Date_                      20181121
Time                           8.17
INSTRUM                       spect
PROBHD   5 mm PABBO BB-
PULPROG                     zgpg30
TD                           65536
SOLVENT                      CDCl3
NS                           13796
DS                               4
SWH                      24038.461 Hz
FIDRES                    0.366798 Hz
AQ                       1.3631488 sec
RG                            2050
DW                          20.800 usec
DE                           6.50 usec
TE                          300.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                              1

======== CHANNEL f1 ========
SFO1                 100.6218241 MHz
NUC1                         13C
P1                          7.50 usec
PLW1                 75.00000000 W

======== CHANNEL f2 ========
SFO2                 400.1316005 MHz
NUC2                         1H
CPDPRG[2                 waltz16
PCPD2                       90.00 usec
PLW2                 18.00000000 W
PLW12                 0.19220001 W
PLW13                 0.09667500 W

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

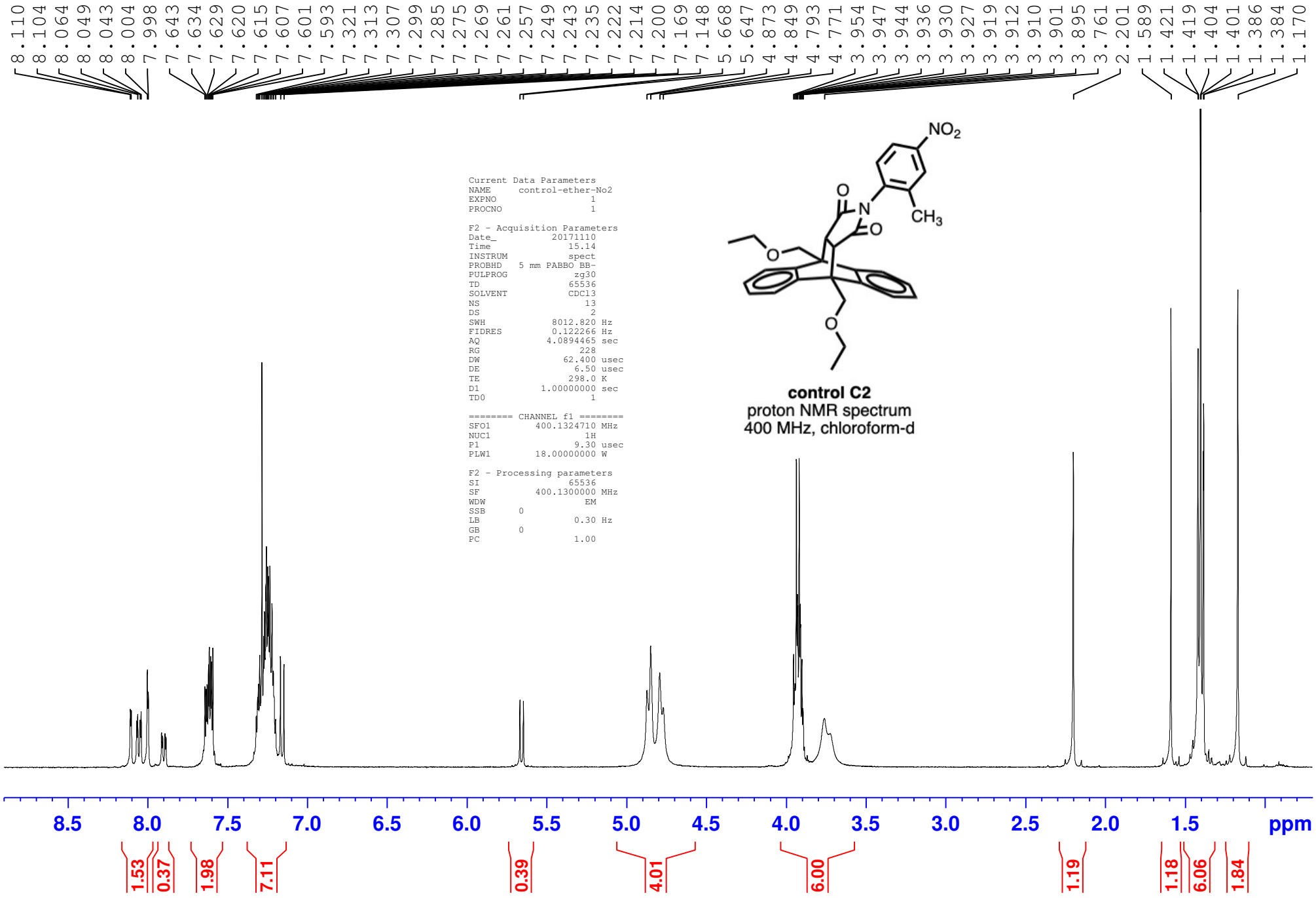

8.092
8.086
8.014
7.826
7.818
7.812
7.803
7.779
7.612
7.603
7.598
7.595
7.589
7.580
7.502
7.494
7.488
7.480
7.419
7.411
7.407
7.405
7.403
7.396
7.388
7.385
7.380
7.285
7.175
7.158
6.801
6.791
5.773
5.751
5.078
5.066
5.052
5.039
4.782
4.776
4.755
4.749
3.989
3.981
3.974
3.642
3.610
3.603
3.488
3.144
3.137
3.131
3.124
2.106
1.720
1.707
1.415
1.283
1.261
Current Data Parameters
NAME Aza-tetraethylene-balance
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190117
Time 10.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 181
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 9.30 usec
PLW1 18.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
NO2
CH3
Balance 1N
Proton NMR Spectrum
400 MHz, chloroform-d
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
0.59
0.58
1.91
1.92
1.15
2.75
2.98
0.40
1.90
0.59
2.00
1.96
3.99
4.27
3.95
3.97
3.91
1.69
2.41
2.19

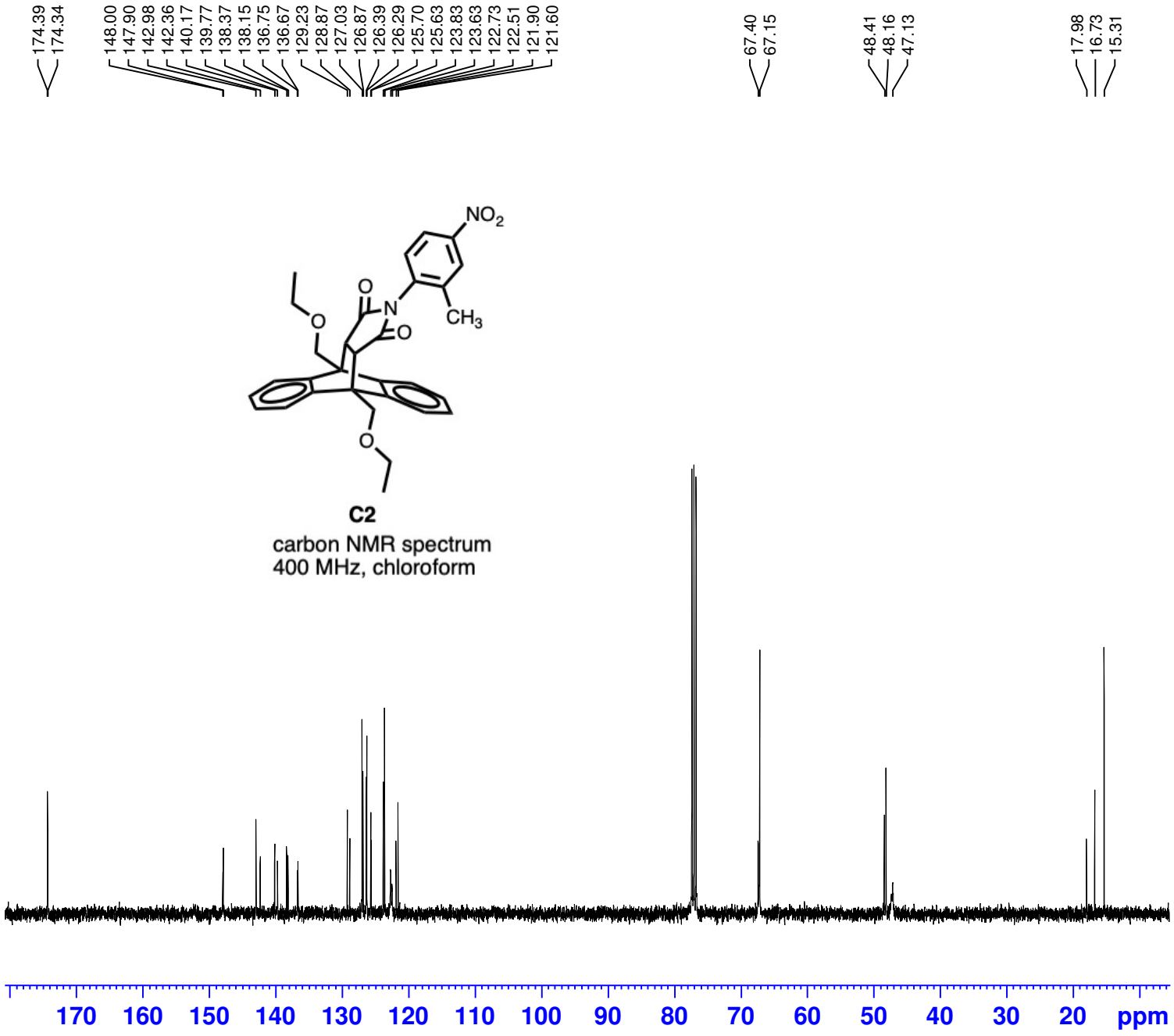

173.63
173.59
148.08
147.96
142.06
141.40
140.95
140.88
138.82
138.77
138.54
137.79
136.24
136.22
129.01
128.93
127.82
127.09
126.89
126.43
126.33
125.80
125.66
124.98
124.65
124.36
124.25
121.99
121.54
72.87
72.71
72.34
72.28
69.87
67.86
67.67
59.99
59.92
56.15
56.08
51.37
50.81
50.52
30.91
29.70
17.88
17.17
Current Data Parameters
NAME Aza-tetraethylene-balance-carbon
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190119
Time 11.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 48000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6218241 MHz
NUC1 13C
P1 7.50 usec
PLW1 75.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.19220001 W
PLW13 0.09667500 W
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
NO2
CH3
Balance 1N
Carbon NMR Spectrum
400 MHz, chloroform-d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.112
8.106
8.080
8.074
8.059
8.052
7.994
7.988
7.877
7.685
7.677
7.671
7.663
7.647
7.639
7.633
7.625
7.303
7.281
7.269
7.260
7.253
7.246
7.241
7.232
7.218
7.192
5.668
5.646
4.977
4.954
4.785
4.763
4.039
4.029
4.019
4.010
3.947
3.891
3.881
3.862
3.853
3.842
3.822
3.815
3.811
3.802
3.794
3.785
3.708
3.695
3.685
3.619
3.612
3.600
3.480
3.288
2.228
1.172
NO2
N
O
CH3
Balance 3
Proton NMR Spectrum
400 MHz, chloroform-d
Current Data Parameters
NAME 7-membered-NO2-balance-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170725
Time 9.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.30 usec
PL1 0 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
0.59
0.36
1.89
5.72
0.39
4.00
9.84
8.27
4.08
3.67
1.05
0.32
0.61
1.79

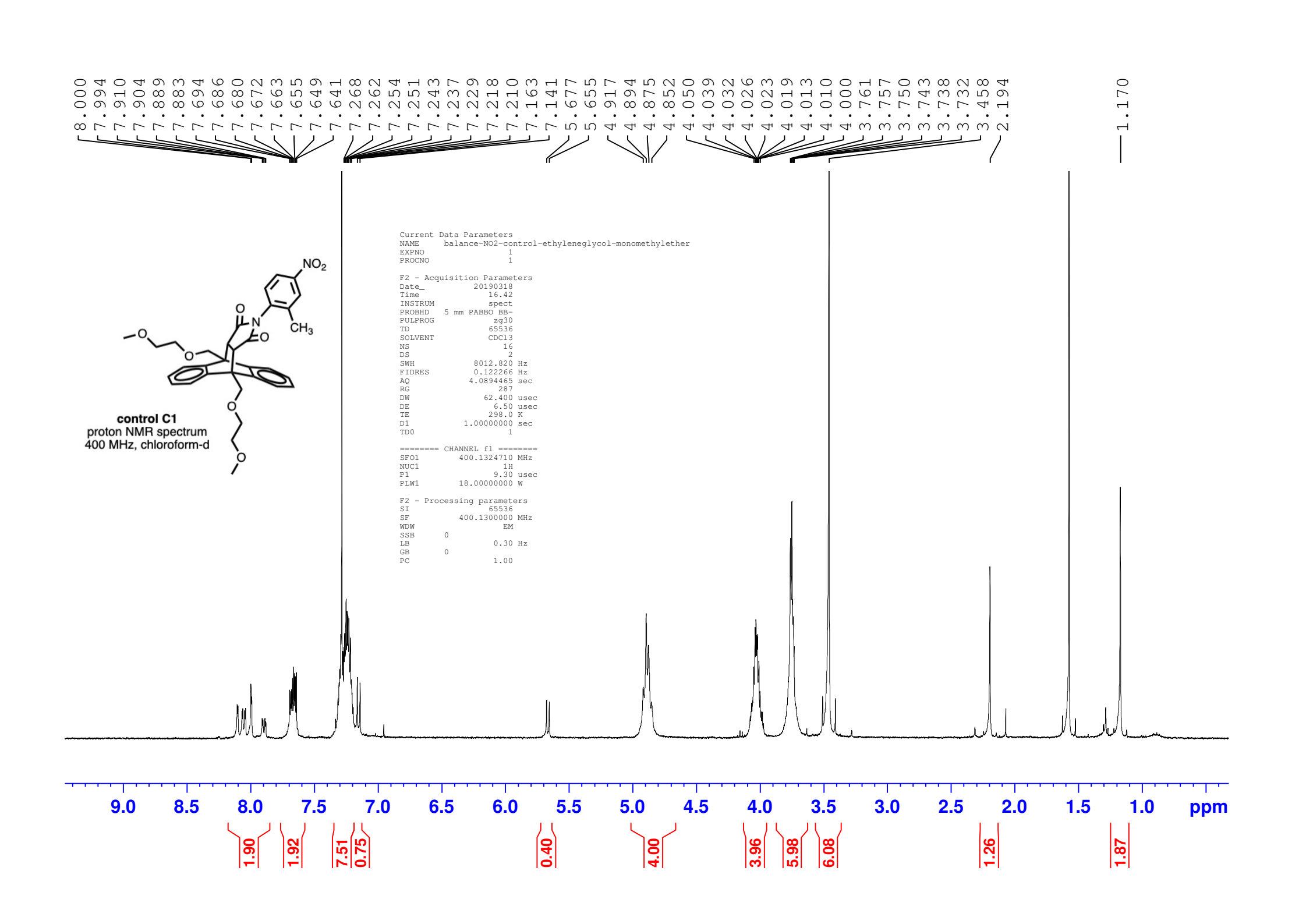


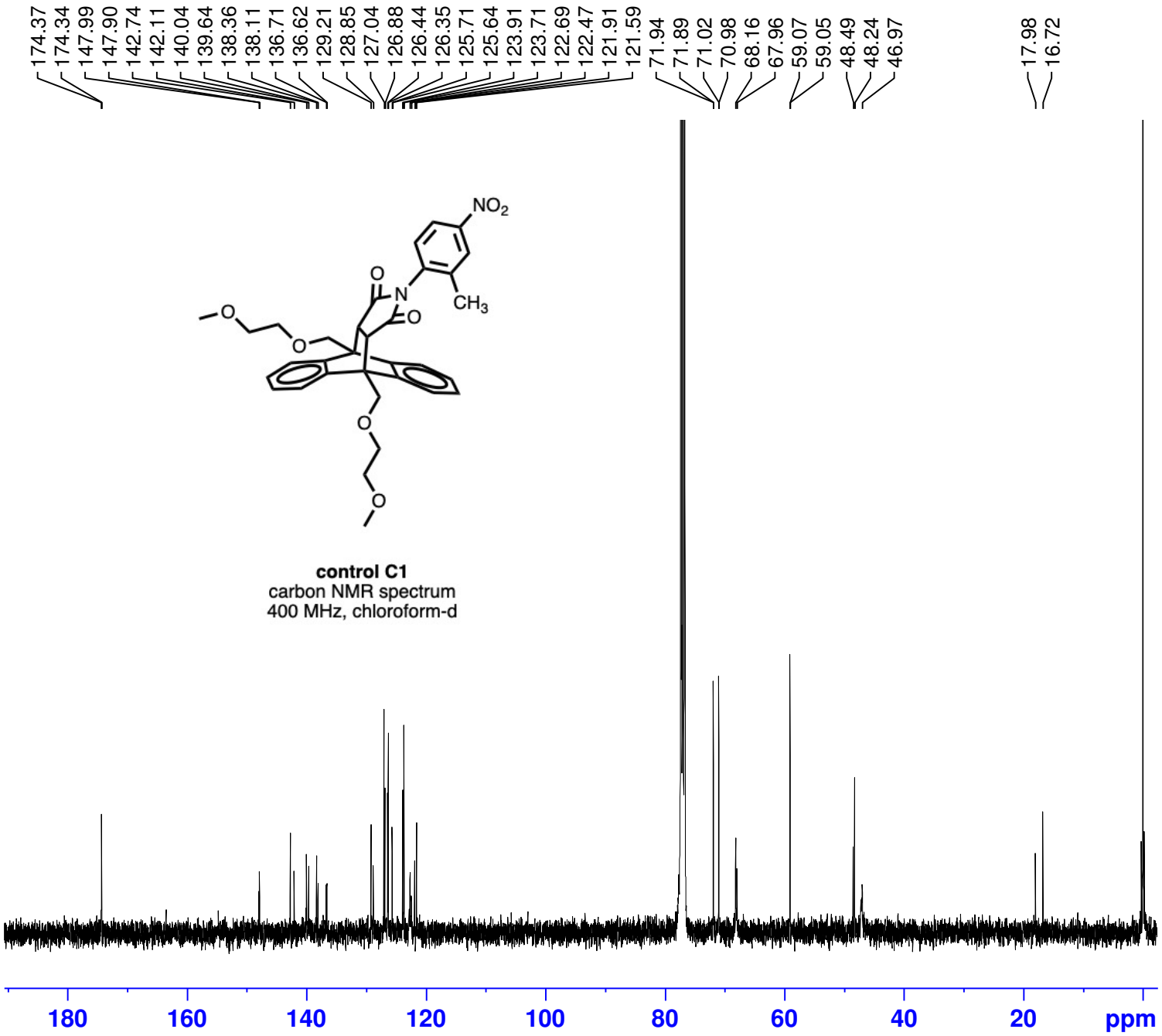

```
Current Data Parameters
NAME      21-C-7-Balance-NO2-carbon
EXPNO                             1
PROCNO                            1

F2 - Acquisition Parameters
Date_                      20231223
Time                          16.51
INSTRUM                       spect
PROBHD    5 mm PABBO BB-
PULPROG                     zgpg30
TD                           65536
SOLVENT                      CDCl3
NS                            3105
DS                               4
SWH                      24038.461 Hz
FIDRES                    0.366798 Hz
AQ                        1.3631488 sec
RG                            2050
DW                          20.800 usec
DE                           6.50 usec
TE                          300.0 K
D1                     2.00000000 sec
D11                    0.03000000 sec
TD0                              1

======== CHANNEL f1 ========
SFO1                 100.6228293 MHz
NUC1                         13C
P1                          7.50 usec
PLW1                75.00000000 W

======== CHANNEL f2 ========
SFO2                 400.1316005 MHz
NUC2                         1H
CPDPRG[2                 waltz16
PCPD2                       90.00 usec
PLW2                18.00000000 W
PLW12                0.19220001 W
PLW13                0.09667500 W

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


8.110
8.104
8.064
8.049
8.043
8.004
7.998
7.643
7.634
7.629
7.620
7.615
7.607
7.601
7.593
7.321
7.313
7.307
7.299
7.285
7.275
7.269
7.261
7.257
7.249
7.243
7.235
7.222
7.214
7.200
7.169
7.148
5.668
5.647
4.873
4.849
4.793
4.771
3.954
3.947
3.944
3.936
3.930
3.927
3.919
3.912
3.910
3.901
3.895
3.761
2.201
1.589
1.421
1.419
1.404
1.401
1.386
1.384
1.170
Current Data Parameters
NAME control-ether-No2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171110
Time 15.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 13
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 228
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 9.30 usec
PLW1 18.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
NO2
O
N
O
CH3
O
O
control C2
proton NMR spectrum
400 MHz, chloroform-d
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1.53
0.37
1.98
7.11
0.39
4.01
6.00
1.19
1.18
6.06
1.84




```
Current Data Parameters
NAME      diethoxy-balance-No2-control-carbon
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231223
Time              13.39
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  218
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1                13C
P1                 7.50 usec
PLW1         75.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         18.00000000 W
PLW12         0.19220001 W
PLW13         0.09667500 W

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


8.000
7.994
7.910
7.904
7.889
7.883
7.694
7.686
7.680
7.672
7.663
7.655
7.649
7.641
7.268
7.262
7.254
7.251
7.243
7.237
7.229
7.218
7.210
7.163
7.141
5.677
5.655
4.917
4.894
4.875
4.852
4.050
4.039
4.032
4.026
4.023
4.019
4.013
4.010
4.000
3.761
3.757
3.750
3.743
3.738
3.732
3.458
2.194
1.170
Current Data Parameters
NAME balance-NO2-control-ethyleneglycol-monomethylether
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190318
Time 16.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 287
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 9.30 usec
PLW1 18.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
control C1
proton NMR spectrum
400 MHz, chloroform-d
NO2
CH3
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.90
1.92
7.51
0.75
0.40
4.00
3.96
5.98
6.08
1.26
1.87



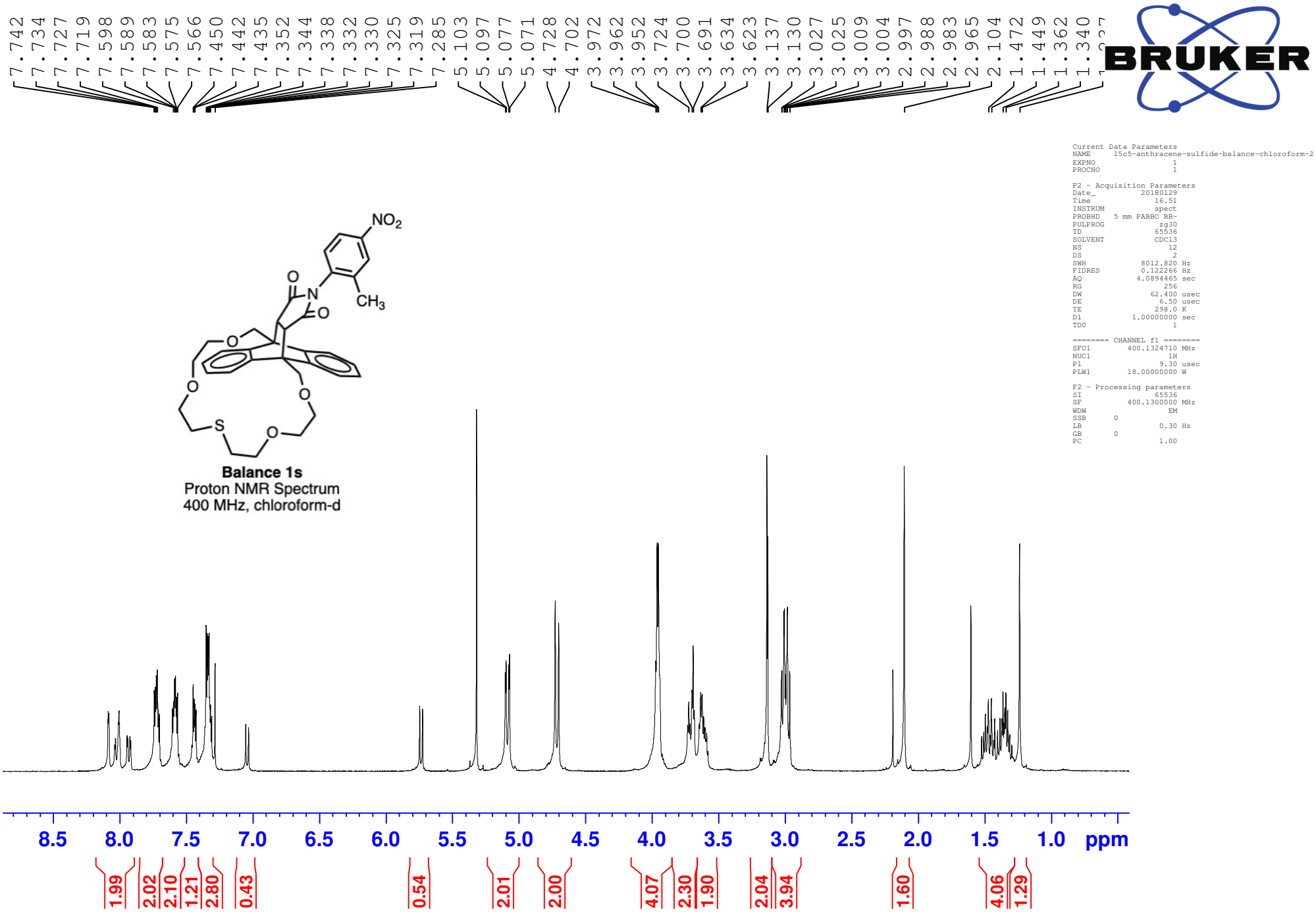
Current Data Parameters
NAME balance-NO2-control-ethyleneglycol-monomethylether-carbon
EXPNO 1
PROCNO 1

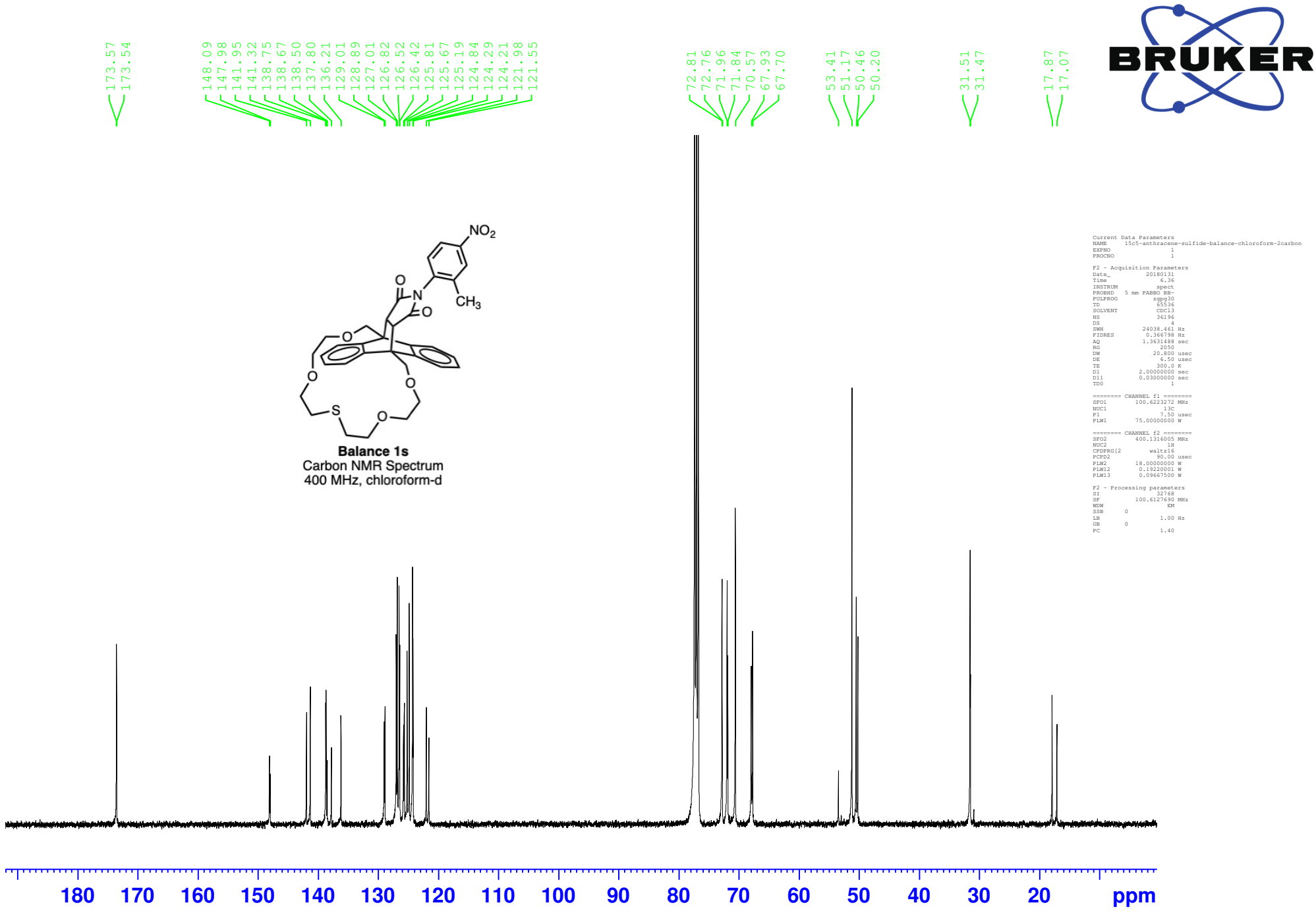
F2 - Acquisition Parameters
Date_ 20190319
Time 7.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 15000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228303 MHz
NUC1 13C
P1 7.50 usec
PLW1 75.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.19220001 W
PLW13 0.09667500 W

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


7.742
7.734
7.727
7.719
7.598
7.589
7.583
7.575
7.566
7.450
7.442
7.435
7.352
7.344
7.338
7.332
7.330
7.325
7.319
7.285
5.103
5.097
5.077
5.071
4.728
4.702
3.972
3.962
3.952
3.724
3.700
3.691
3.634
3.623
3.137
3.130
3.027
3.025
3.009
3.004
2.997
2.988
2.983
2.965
2.104
1.472
1.449
1.362
1.340
BRUKER
Current Data Parameters
NAME 15c5-anthracene-sulfide-balance-chloroform-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180129
Time 16.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 256
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 9.30 usec
PLW1 18.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
NO2
CH3
O
N
S
Balance 1s
Proton NMR Spectrum
400 MHz, chloroform-d
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.99
2.02
2.10
1.21
2.80
0.43
0.54
2.01
2.00
4.07
2.30
1.90
2.04
3.94
1.60
4.06
1.29


173.57
173.54
148.09
147.98
141.95
141.32
138.75
138.67
138.50
137.80
136.21
129.01
128.89
127.01
126.82
126.52
126.42
125.81
125.67
125.19
124.84
124.29
124.21
121.98
121.55
72.81
72.76
71.96
71.84
70.57
67.93
67.70
53.41
51.17
50.46
50.20
31.51
31.47
17.87
17.07
NO2
CH3
Balance 1s
Carbon NMR Spectrum
400 MHz, chloroform-d
Current Data Parameters
NAME 15c5-anthracene-sulfide-balance-chloroform-2carbon
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180131
Time 6.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 36196
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6223272 MHz
NUC1 13C
P1 7.50 usec
PLW1 75.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 18.00000000 W
PLW12 0.19220001 W
PLW13 0.09667500 W
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm