

Electronic Supplementary Information (ESI)

A Conjugated Small Organic molecules: Synthesis and Characterization of 4-Arylpyrazole Decorated Dibenzothiophene

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UV-Vis absorption and emission spectra

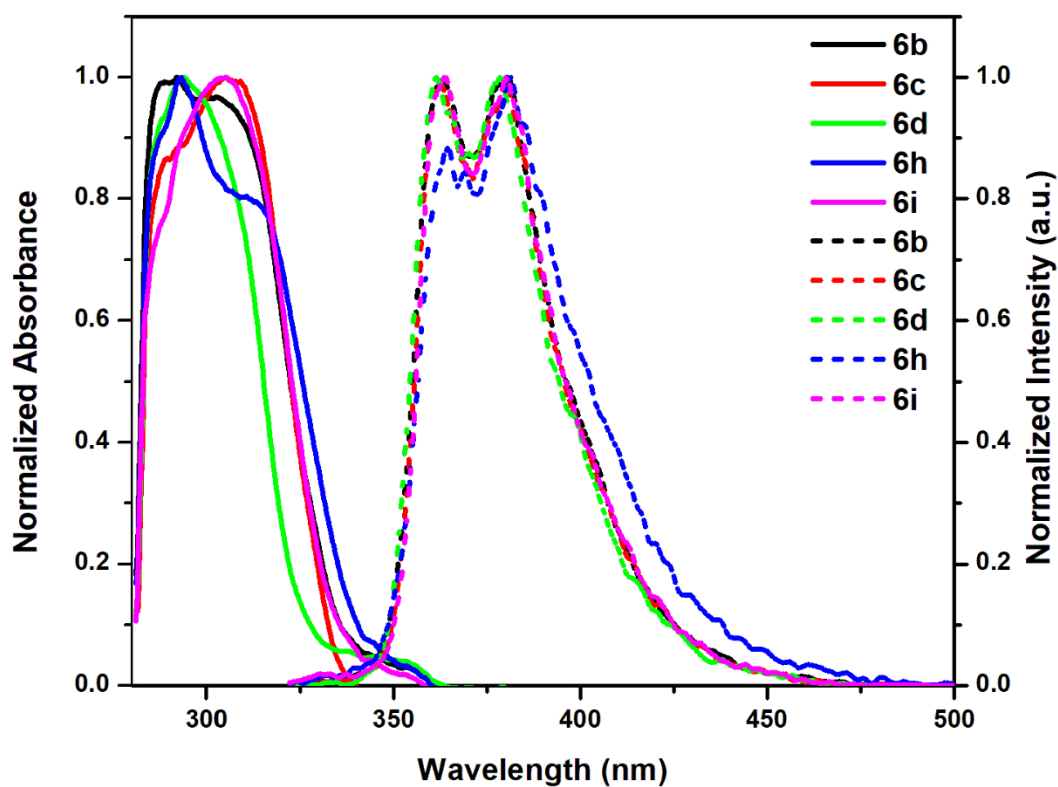
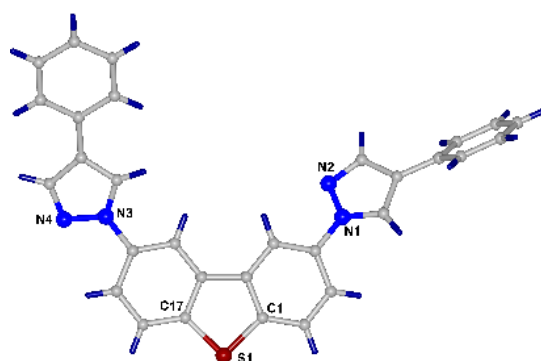


Figure S1. UV/Vis absorption (solid lines) and emission (dotted lines) spectra of **6b-d** and **6h**, **6i** in toluene (concentration 5×10^{-6} M; for **6g**, 1×10^{-5} M). The excitation wavelength was fixed at 290 nm.

	λ_{abs} (nm)	λ_{em} (nm)	Molar extension coefficient ($\text{M}^{-1}\text{cm}^{-1}$)
6a	309	361, 378	40,000
6b	292, 303	381, 362	49,298
6c	305	380, 362	46,838
6d	293	378, 361	65,828
6f	307	362, 378	41,020
6g	301	351, 376	51,800
6h	293, 310	381, 364	42,960
6i	304	380, 364	49,406

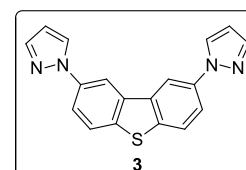
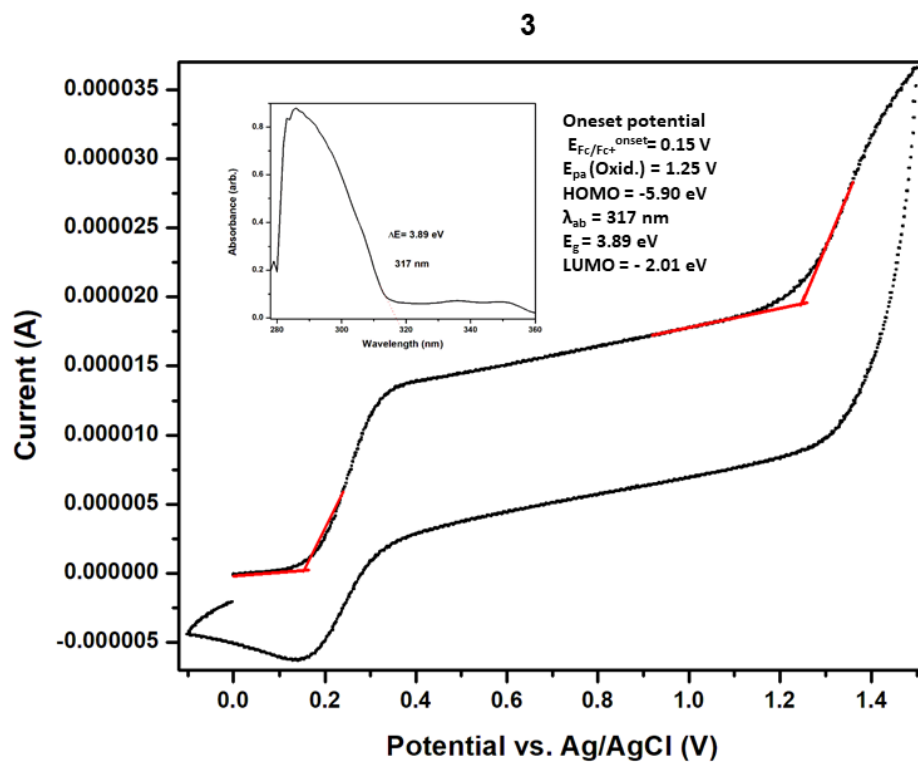
X-ray Crystallographic Analysis



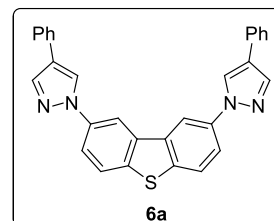
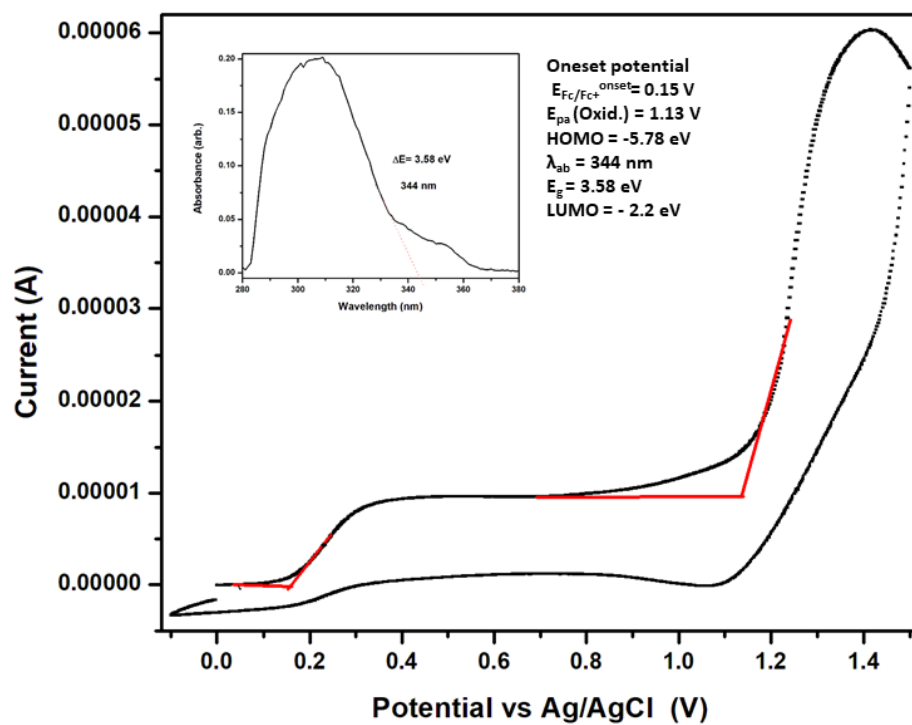
Parameters	6a
Empirical formula	C ₃₀ H ₂₀ N ₄ S ₁
Formula Weight	468.56
Temperature (K)	296(2)
Wavelength (Mo _K α)	0.71073 Å
Crystal system	Monoclinic
Space group	P21/c
Unit cell dimensions	
a =	23.0048(4) Å
b =	5.5362(1) Å
c =	18.3917(3) Å
α =	90.00°
β =	106.522(1)°
γ =	90.00°
Volume	2245.64(7) Å ³
Z, Density (Calculated)	4, 1.386 g/cm ³
Absorption coefficient	0.172 mm ⁻¹
F (000)	976
Crystal size (mm ³)	0.12 x 0.11 x 0.09
θ range for data collection	1.847 to 26.72°
Limiting indices	-29 ≤ h ≤ 28, -6 ≤ k ≤ 7, -23 ≤ l ≤ 23
Reflections collected	28252
Independent reflections	4713 [R(int) = 0.0321]
Completeness to θ (%)	99.5
Data / restraints / parameters	4713 / 0 / 316
Goodness - of - fit on F ²	1.029
Final R indices [I>2σ (I)]	R1 = 0.0354, wR2 = 0.0853
R indices (all data)	R1 = 0.0453, wR2 = 0.0905

Cyclic voltammograms

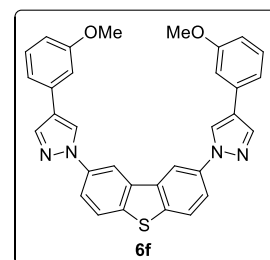
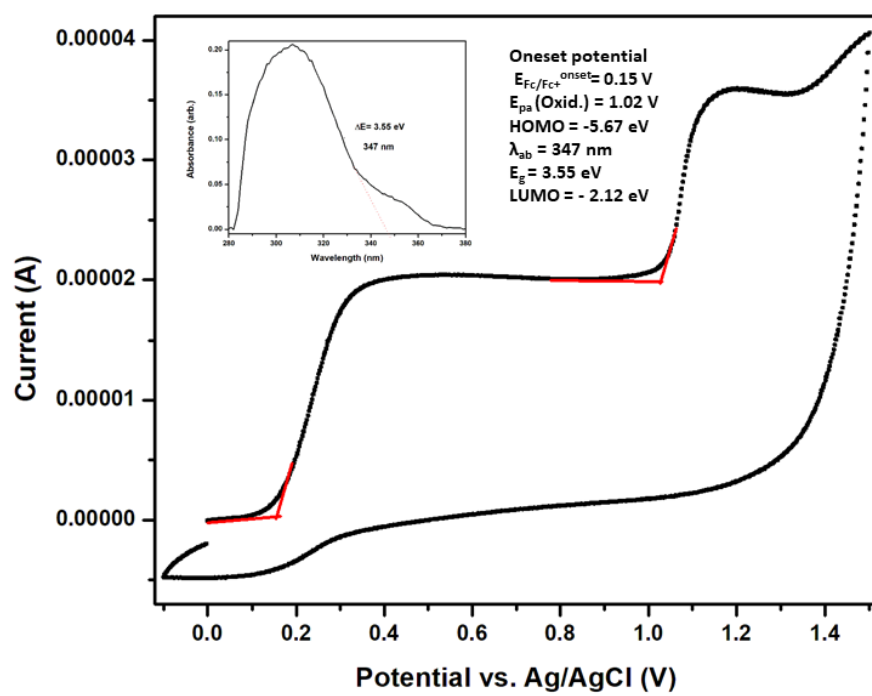
Highest occupied molecular orbital energy level (E_{HOMO}) of the compounds was calculated following E_{HOMO} (eV) = - (E_{pa} (Oxid.) - $E_{\text{Fc/Fc}^+}^{\text{onset}}$) - 4.80 eV, where E_{pa} (Oxid.) and $E_{\text{Fc/Fc}^+}^{\text{onset}}$ are onset oxidation potential of the compound and internal standard, respectively. Lowest unoccupied molecular orbital energy was obtained from $E(\text{LUMO}) = E_{\text{g}} + E(\text{HOMO})$; E_{g} is the band gap energy calculated from UV-visible spectra.

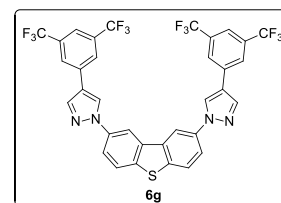
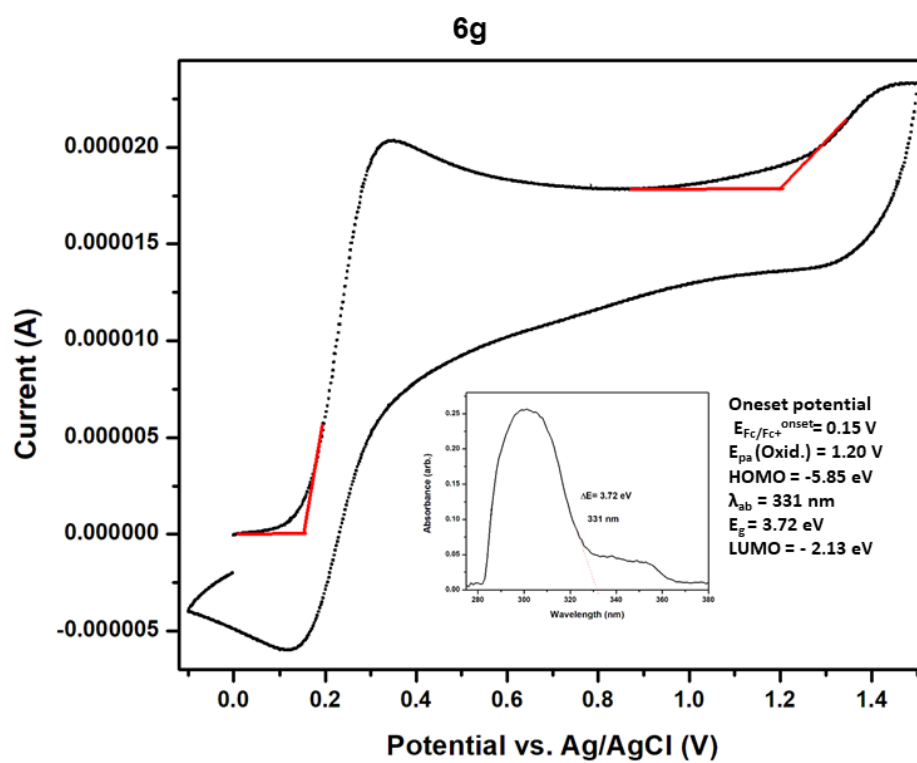


6a

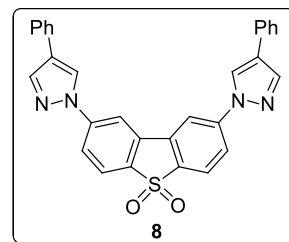
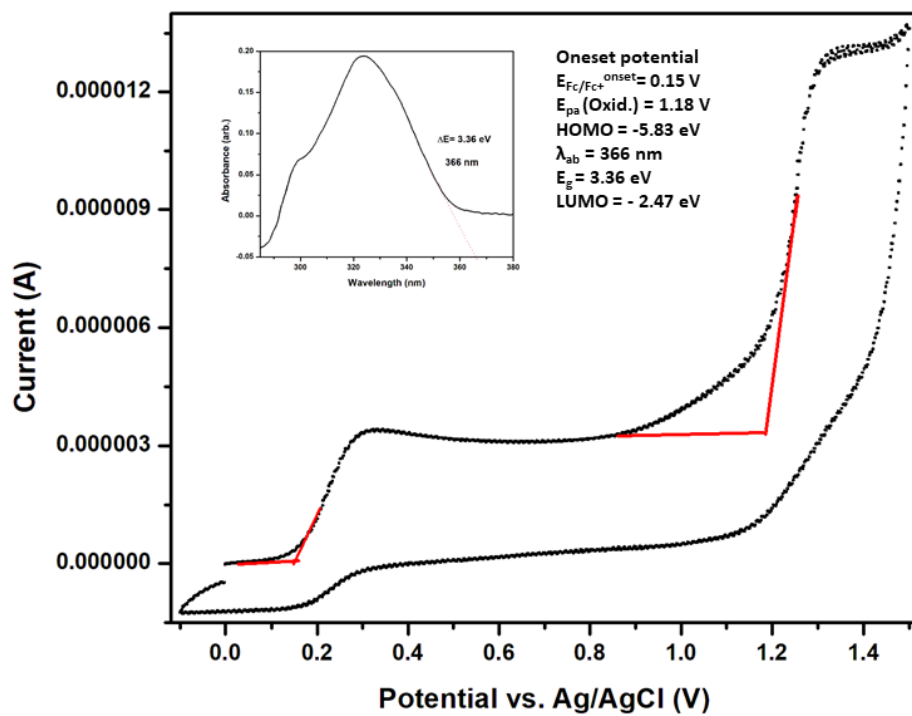


6f

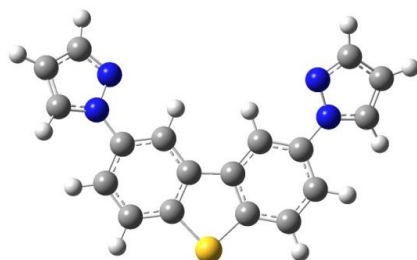




8



Cartesian coordinates of optimized structures with electronic energy (no imaginary frequencies were present)



E(RB3LYP) = -1310.563720 Hartree

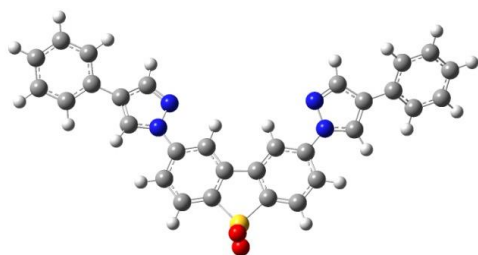
C	-2.96947700	0.01817800	0.03333800
C	-3.48614700	1.32393400	0.06021000
C	-2.63214400	2.41799200	0.04217700
C	-1.25576600	2.19949900	0.01703500
C	-0.72702700	0.89167500	0.01024000
C	-1.59705700	-0.20252500	0.01229400
H	-4.55495400	1.48523400	0.11785900
H	-3.03806900	3.42214600	0.06474700
H	-1.22713000	-1.21875600	0.00290900
C	1.25576600	2.19949900	-0.01703500
C	2.63214400	2.41799200	-0.04217700
C	3.48614700	1.32393400	-0.06021000
C	2.96947700	0.01817800	-0.03333800
C	1.59705700	-0.20252500	-0.01229400
C	0.72702700	0.89167500	-0.01024000
H	3.03806900	3.42214600	-0.06474700
H	4.55495400	1.48523400	-0.11785900
H	1.22713000	-1.21875600	-0.00290900
S	0.00000000	3.43908000	0.00000000
N	-3.43974600	-2.29792100	0.49909600
N	3.85432200	-1.09343600	-0.03358700
N	3.43974600	-2.29792100	-0.49909600
N	-3.85432200	-1.09343600	0.03358700
C	4.48085800	-3.10529200	-0.34297700
H	4.40445100	-4.13737900	-0.65095600
C	5.58428500	-2.43384000	0.22983600
C	5.14289200	-1.14366600	0.41833800
H	5.62708700	-0.28673700	0.85511300
C	-5.14289300	-1.14366600	-0.41833800
H	-5.62708800	-0.28673700	-0.85511300
C	-5.58428500	-2.43384000	-0.22983500
C	-4.48085800	-3.10529200	0.34297700
H	-4.40445100	-4.13737900	0.65095600
H	-6.55356500	-2.83337800	-0.47877300
H	6.55356500	-2.83337800	0.47877300



E(RB3LYP)= -3121.382314 Hartree

C	2.92457500	2.18270800	-0.62113500
C	3.42750300	3.47025200	-0.86773100
C	2.57366400	4.56411200	-0.88625600
C	1.21088700	4.35982000	-0.67509900
C	0.69523000	3.06660800	-0.44622200
C	1.56639700	1.97403800	-0.41432100
H	4.48106100	3.61584400	-1.06924300
H	2.96702400	5.55470700	-1.07938900
H	1.20689100	0.96947000	-0.23735900
C	-1.27863900	4.38385500	-0.35138000
C	-2.64421200	4.61641900	-0.19371600
C	-3.48376200	3.54047700	0.05779000
C	-2.96413900	2.23816500	0.13191800
C	-1.60321800	2.00235000	-0.02052800
C	-0.74607100	3.08060500	-0.25790800
H	-3.05027300	5.61916900	-0.24765700
H	-4.53943100	3.71666700	0.22030300
H	-1.23067600	0.98960800	0.05253700
S	-0.04187600	5.60094500	-0.66575900
N	3.35557000	-0.17562200	-0.86868300
N	-3.83695300	1.14098300	0.37293300
N	-3.36794500	0.00845300	0.95312300
N	3.81111100	1.07025500	-0.58643700
C	-4.40692900	-0.80890900	1.00673100
H	-4.29149600	-1.78357000	1.45735500
C	-5.57947100	-0.21883900	0.46286200
C	-5.15849700	1.03927100	0.06318800
H	-5.68094400	1.82584800	-0.45469100
C	5.13687400	1.06473200	-0.27878600
H	5.66101200	1.96729100	-0.01376200
C	5.57700100	-0.24528100	-0.37547900
C	4.41022300	-0.96524900	-0.74888100
H	4.29938100	-2.02625800	-0.91711300
C	6.92661600	-0.76536000	-0.13601700
C	7.35423000	-1.95322500	-0.74558000
C	7.82503000	-0.09663000	0.70711000
C	8.63431600	-2.44995200	-0.51740700
H	6.69172100	-2.48228200	-1.41858600
C	9.10677800	-0.59463400	0.92142700

H	7.51567500	0.80650800	1.21781200
C	9.52534400	-1.77636900	0.31455100
H	10.52024200	-2.16314300	0.48670600
C	-6.91729800	-0.80469800	0.33848800
C	-8.06160100	0.00303800	0.28128000
C	-7.08776000	-2.19481700	0.27474200
C	-9.32718600	-0.56159600	0.15365400
H	-7.96667500	1.07865000	0.35949700
C	-8.35799600	-2.75177400	0.15823900
H	-6.22269000	-2.84521300	0.29485800
C	-9.49047500	-1.94348500	0.09335700
H	-10.47543300	-2.37952100	-0.00064800
C	-8.51067600	-4.25151300	0.15171000
C	-10.52891600	0.33989800	0.03355500
C	9.04168400	-3.75990100	-1.14238000
C	10.06555800	0.18381600	1.78523000
F	-7.46172800	-4.86633800	-0.43796500
F	-8.59343900	-4.74792000	1.41141900
F	-9.62567100	-4.64823000	-0.49705700
F	-10.38508100	1.47630000	0.75233800
F	-10.73868200	0.72018000	-1.25207400
F	-11.66260300	-0.25927200	0.45240700
F	8.46714600	-3.94621100	-2.35129900
F	10.37730100	-3.85005400	-1.31407000
F	8.67419200	-4.81385900	-0.37161100
F	10.71087800	1.14186000	1.07266500
F	11.01622700	-0.60163500	2.33183200
F	9.43499000	0.81796100	2.79929400

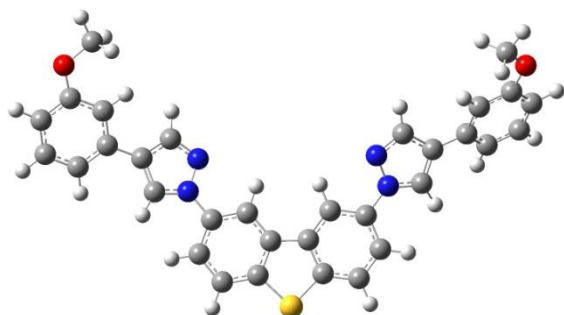


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E(RB3LYP)= -1923.195741 Hartree

C	2.96227700	0.87870700	-0.19986300
C	3.48984700	2.17407800	-0.28344400
C	2.64084800	3.27794800	-0.25105200
C	1.27965700	3.05678600	-0.15131600
C	0.73317700	1.77146500	-0.08209700
C	1.58134800	0.67039500	-0.10279200
H	4.55477400	2.32910700	-0.39210900
H	3.04247600	4.28183500	-0.31592100

H	1.20759400	-0.34229300	-0.04890000
C	-1.29296800	3.05689300	0.02144000
C	-2.65484600	3.27858800	0.11101300
C	-3.50004200	2.17499100	0.20025800
C	-2.96826200	0.87881400	0.18138700
C	-1.58684500	0.67010600	0.09325100
C	-0.74223800	1.77150900	0.01691600
H	-3.05952400	4.28324100	0.12535400
H	-4.56550400	2.33083900	0.30293400
H	-1.20986900	-0.34285600	0.09011400
S	-0.00865800	4.31397000	-0.09650500
N	3.32219200	-1.48232000	-0.46392100
N	-3.82596500	-0.24373400	0.25513100
N	-3.32318200	-1.46526500	0.57260700
N	3.82303000	-0.24419300	-0.21460800
C	-4.36011800	-2.28364900	0.53883400
H	-4.22130000	-3.32667900	0.78197400
C	-5.56825900	-1.61253300	0.19750000
C	-5.17281300	-0.30099400	0.02143300
H	-5.73486100	0.56121600	-0.29360300
C	5.17308900	-0.28415200	0.00290900
H	5.74320200	0.60159600	0.22352200
C	5.57348300	-1.60031400	-0.11698800
C	4.36487400	-2.29228500	-0.41227000
H	4.22272000	-3.35119300	-0.56972500
C	6.92437100	-2.15763600	0.03624600
C	7.30439900	-3.31150600	-0.66582300
C	7.86651800	-1.55639400	0.88507600
C	8.58264400	-3.84441200	-0.52491300
H	6.60027200	-3.78370600	-1.34160900
C	9.14699700	-2.08460300	1.01866000
H	7.58718900	-0.68133600	1.46150900
C	9.51103600	-3.23232500	0.31550800
H	8.85626700	-4.73509500	-1.07942000
H	9.85842100	-1.60558200	1.68209700
H	10.50699700	-3.64622700	0.42336100
C	-6.91469500	-2.18267400	0.05473800
C	-8.05984300	-1.41399500	0.31432700
C	-7.08718800	-3.51639200	-0.34574000
C	-9.33279900	-1.95684500	0.16778300
H	-7.95163300	-0.38996400	0.65445400
C	-8.36059300	-4.06151100	-0.48302000
H	-6.21842200	-4.12508200	-0.56978800
C	-9.48952900	-3.28399000	-0.22996300
H	-10.20399000	-1.34575500	0.37596300
H	-8.47104900	-5.09356600	-0.79657900
H	-10.48102100	-3.70810600	-0.33929400
O	-0.09438600	5.03165900	-1.37193300
O	0.07464900	5.09462200	1.14159600

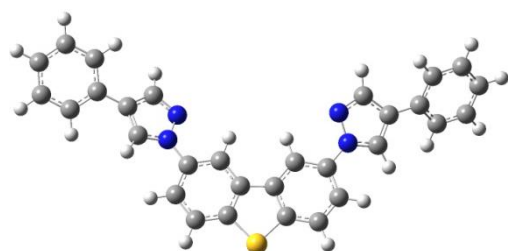


6f

E(RB3LYP)= -2001.902142 Hartree

C	2.91738000	1.76148100	-0.24505800
C	3.43606400	3.04914700	-0.45971300
C	2.58840400	4.14646500	-0.52184700
C	1.21548000	3.94786300	-0.38636200
C	0.68378700	2.65613600	-0.18919100
C	1.54797100	1.56012100	-0.11304000
H	4.49958900	3.19200100	-0.60109000
H	2.99588000	5.13609300	-0.68974600
H	1.17541900	0.55671100	0.04163000
C	-1.28882200	3.97943000	-0.19864600
C	-2.66027600	4.21432700	-0.11559600
C	-3.51534400	3.13998400	0.08662900
C	-3.00582700	1.83478800	0.18703400
C	-1.63794700	1.59813700	0.10825000
C	-0.76615300	2.67453700	-0.07941500
H	-3.06064000	5.21818400	-0.19022400
H	-4.57786800	3.31916300	0.18909500
H	-1.27242700	0.58437400	0.19921500
S	-0.03238600	5.19407600	-0.44211600
N	3.34237800	-0.60118800	-0.43749200
N	-3.89225600	0.74161700	0.37743000
N	-3.44747800	-0.41042900	0.93718900
N	3.79554000	0.64758900	-0.16594300
C	-4.49729400	-1.21763100	0.94343800
H	-4.40395400	-2.20482700	1.37138300
C	-5.65237500	-0.60468500	0.38730300
C	-5.21035500	0.65776200	0.03298200
H	-5.71734900	1.46025500	-0.47514200
C	5.11621500	0.63976900	0.17781600
H	5.64162700	1.54225200	0.43948000
C	5.55299400	-0.67173300	0.11933300
C	4.39215500	-1.39145200	-0.27280600
H	4.28276400	-2.45554300	-0.42164700
C	6.89611200	-1.19330100	0.40952600
C	7.35365700	-2.34927600	-0.24758000
C	7.73479500	-0.56013100	1.33323800
C	8.62602200	-2.85601700	0.01814600

H	6.71421300	-2.82447600	-0.97869200
C	9.00846000	-1.06981400	1.58560500
H	7.38598400	0.31276100	1.87207900
C	9.46077000	-2.21076700	0.93881400
H	9.65169400	-0.57520300	2.30497800
H	10.44556000	-2.61990000	1.12780400
C	-6.99614600	-1.17443300	0.21673800
C	-8.13510400	-0.36232700	0.24438300
C	-7.14936500	-2.55879400	0.02276000
C	-9.39982600	-0.92483700	0.07162200
H	-8.03690000	0.70155100	0.42462600
C	-8.41921000	-3.11295700	-0.13999800
H	-6.26720700	-3.18246900	-0.02242500
C	-9.55246700	-2.29056700	-0.11821800
H	-10.27811800	-0.28931700	0.09678000
H	-10.52825900	-2.74165700	-0.24961600
O	-8.65740800	-4.44292200	-0.33649700
O	9.14926900	-3.96833900	-0.57625400
C	8.35778500	-4.67578800	-1.52083900
H	8.10711000	-4.04888500	-2.38348100
H	8.96873000	-5.51429400	-1.85115100
H	7.43653100	-5.05619900	-1.06622500
C	-7.55392000	-5.33753000	-0.37269500
H	-6.87135000	-5.09889900	-1.19555500
H	-7.00160300	-5.33050200	0.57333700
H	-7.97914600	-6.32685200	-0.53350600



6a

E(RB3LYP)= -1772.789294 Hartree

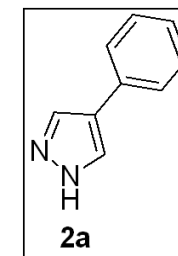
C	2.95256100	1.18439900	-0.28684200
C	3.46331800	2.48863800	-0.39314300
C	2.61121000	3.58307900	-0.34210800
C	1.24142000	3.36654200	-0.20255200
C	0.71731500	2.05977200	-0.11426600
C	1.58615800	0.96544600	-0.15146000
H	4.52380600	2.64873900	-0.53889500
H	3.01256600	4.58573200	-0.42694000
H	1.21952100	-0.04960800	-0.08216600

C	-1.25944800	3.36916000	0.02868000
C	-2.63007500	3.58910400	0.15490300
C	-3.47814500	2.49676800	0.27266500
C	-2.96282400	1.19029400	0.24561100
C	-1.59567700	0.96816600	0.12367500
C	-0.73064100	2.06128800	0.02044500
H	-3.03482800	4.59370300	0.17830500
H	-4.53941300	2.66073700	0.40846200
H	-1.22552100	-0.04797700	0.11597900
S	-0.01122300	4.60678800	-0.12463600
N	3.38173800	-1.14931300	-0.69815800
N	-3.84244700	0.08019500	0.34948900
N	-3.38620200	-1.11466400	0.79976600
N	3.83541700	0.07211400	-0.32251000
C	-4.43211100	-1.92483800	0.74703400
H	-4.32936900	-2.94617300	1.08260500
C	-5.59660800	-1.27093100	0.26109200
C	-5.16426800	0.02042400	0.01472400
H	-5.67944800	0.86274900	-0.41475400
C	5.16132900	0.03912200	-0.00125600
H	5.68696700	0.91746100	0.33239500
C	5.60083500	-1.26011400	-0.18441700
C	4.43581800	-1.94678600	-0.62173400
H	4.32794000	-2.99323900	-0.86579300
C	6.94840500	-1.80277600	0.03434800
C	7.40309800	-2.90755000	-0.70212600
C	7.81591500	-1.23734700	0.98211500
C	8.67831900	-3.42728800	-0.49843300
H	6.75917400	-3.35123300	-1.45307800
C	9.09427300	-1.75109800	1.17844400
H	7.47844700	-0.40147400	1.58500700
C	9.53189400	-2.85029600	0.44050300
H	9.00881200	-4.28007200	-1.08106100
H	9.74615000	-1.29926600	1.91798600
H	10.52583700	-3.25349100	0.59706400
C	-6.93767500	-1.83381300	0.05565400
C	-8.08533000	-1.03073500	0.14746100
C	-7.10544000	-3.19600100	-0.23785200
C	-9.35285500	-1.56761300	-0.05741200
H	-7.98449200	0.01860700	0.40201700
C	-8.37409800	-3.73475700	-0.43235900
H	-6.23381800	-3.83370800	-0.33280200
C	-9.50431900	-2.92325300	-0.34631200
H	-10.22533300	-0.92828500	0.02053600
H	-8.47916300	-4.78965600	-0.66052400
H	-10.49192900	-3.34250400	-0.50077700

8.049
7.605
7.590
7.352
7.338
7.324
7.185
7.172

3.398

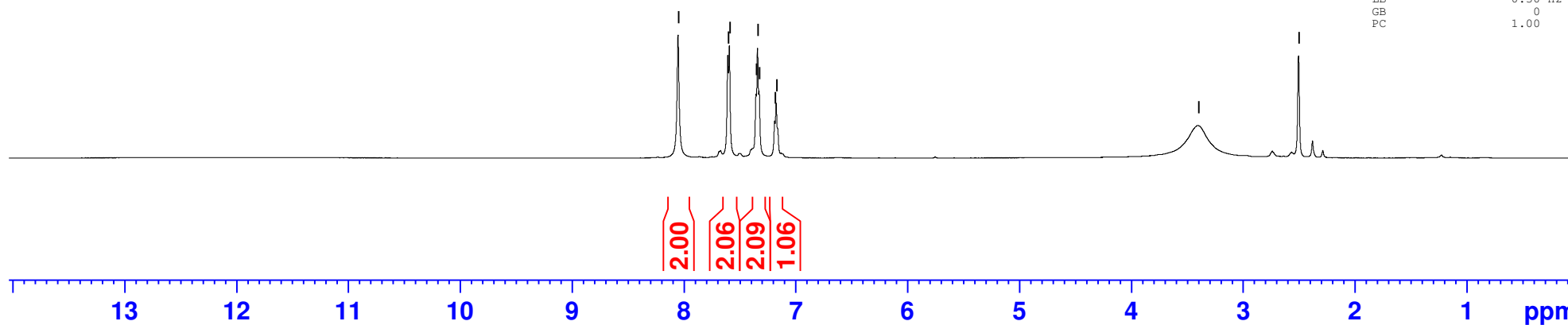
2.500



Current Data Parameters
NAME 4-PHENYL PY
EXPNO 12
PROCNO 1

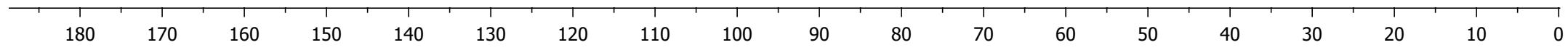
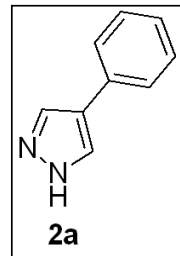
F2 - Acquisition Parameters
Date_ 20200109
Time_ 19.44 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 144
DW 50.000 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.3030894 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

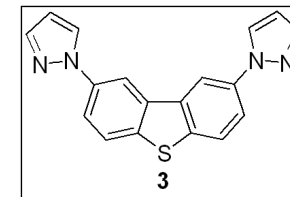


133.42
130.17
129.28
127.05
126.35
125.61
121.66

40.60
40.39
40.18
39.98
39.77
39.56
39.35



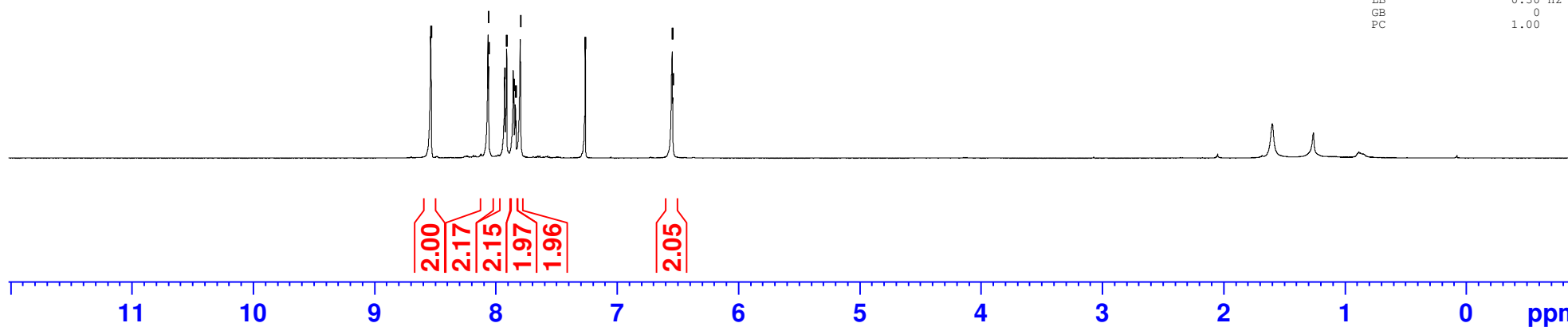
8.535
8.531
8.062
8.057
7.925
7.913
7.908
7.854
7.850
7.837
7.832
7.796
7.266
7.260
6.547
6.543
6.539

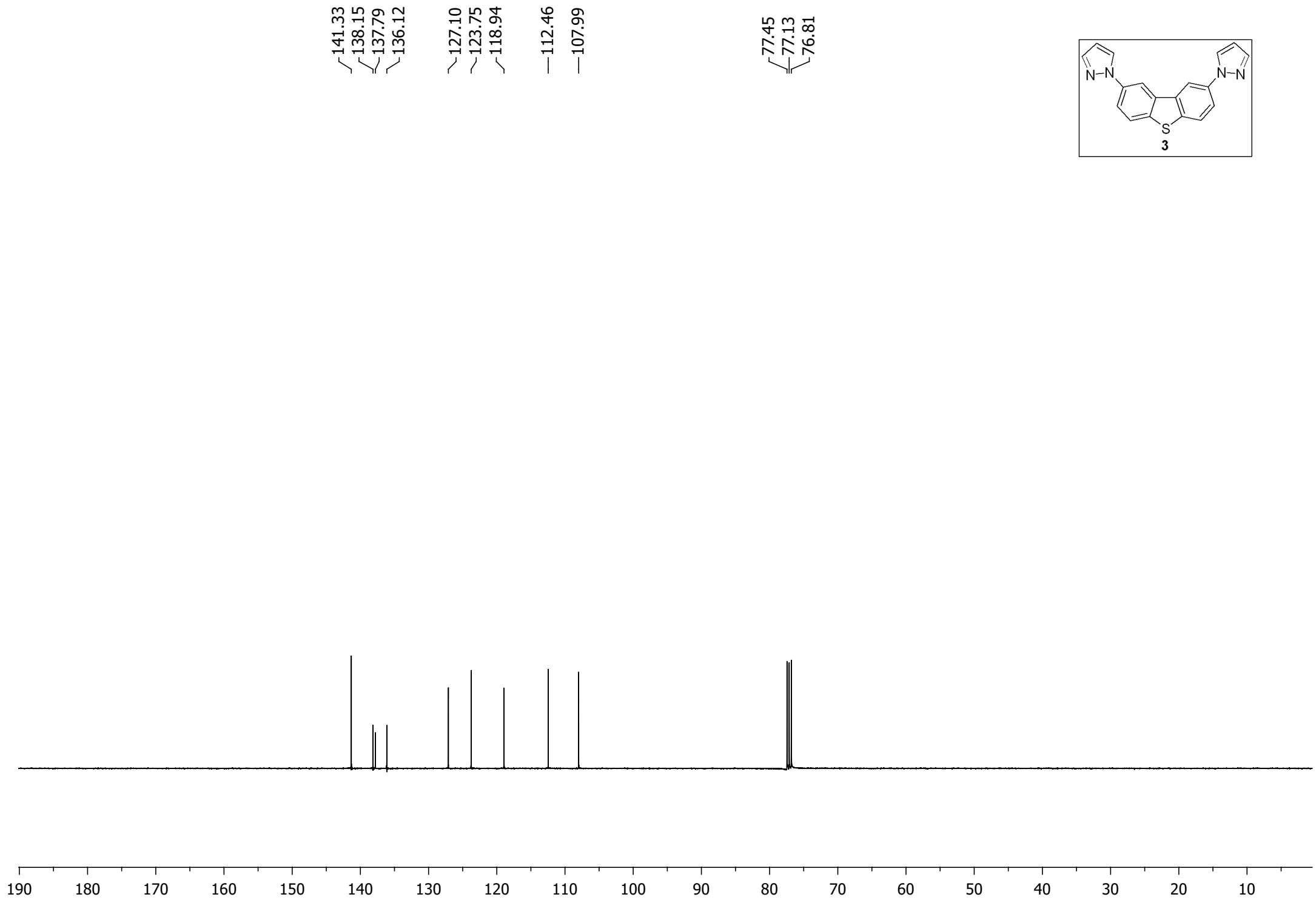


Current Data Parameters
NAME PYDBT
EXPNO 3
PROCNO 1

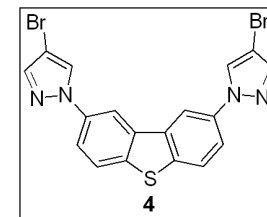
F2 - Acquisition Parameters
Date_ 20200107
Time_ 17.30 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 362
DW 50.000 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
SFO1 500.3030894 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





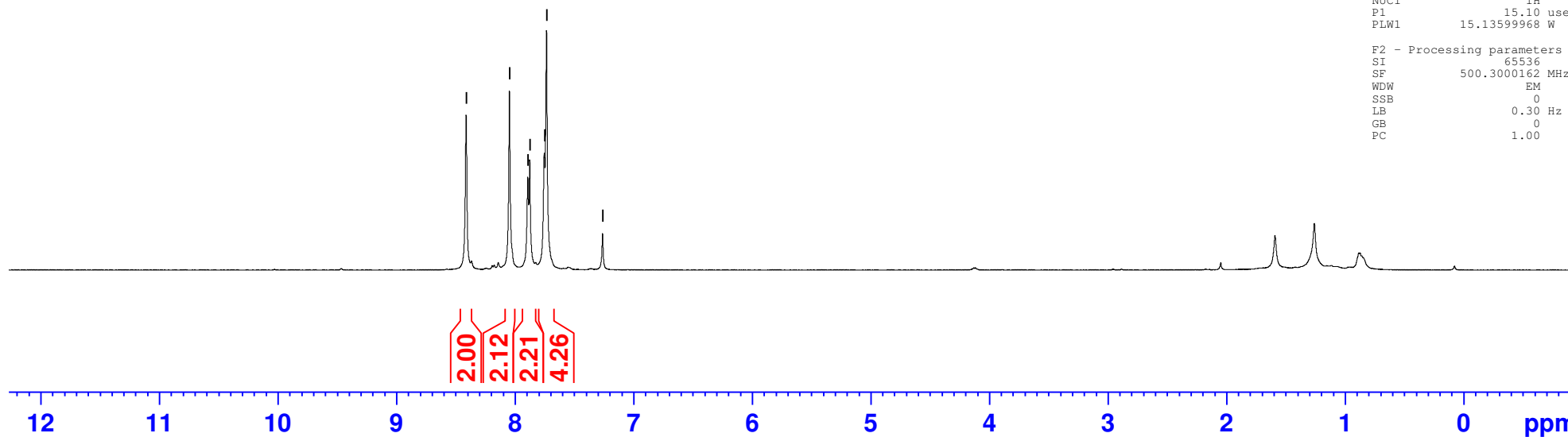
8.411
8.046
7.891
7.875
7.752
7.733
7.260

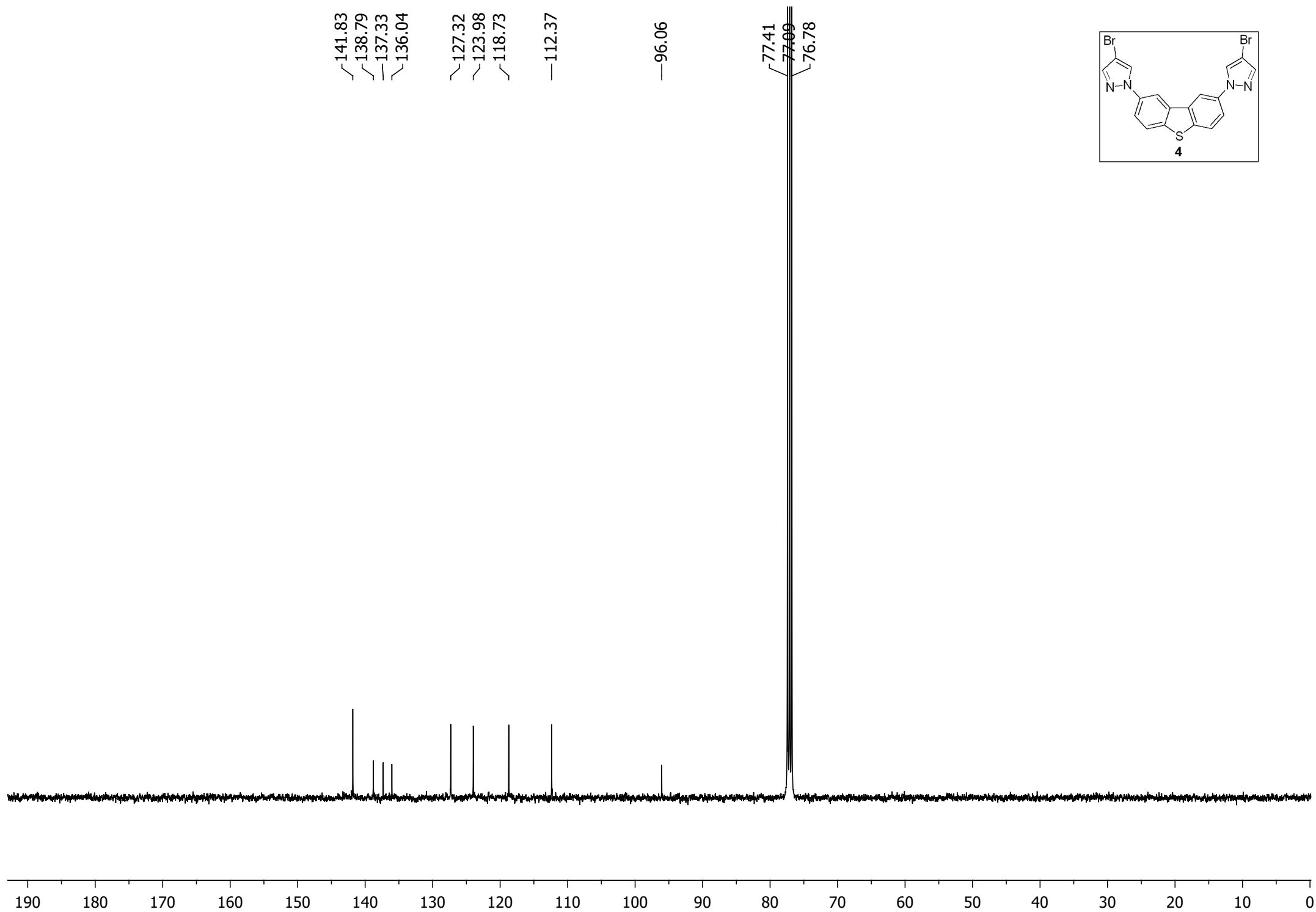


Current Data Parameters
NAME Br-PYDBT
EXPNO 10
PROCNO 1

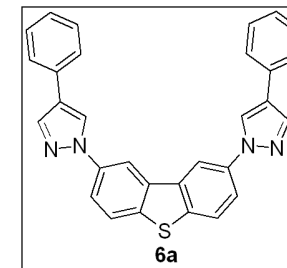
F2 - Acquisition Parameters
Date_ 20200109
Time_ 19.35 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 322
DW 50.000 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.3030894 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000162 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





8.557
8.553
8.297
8.064
7.927
7.910
7.885
7.880
7.867
7.863
7.623
7.620
7.617
7.606
7.604
7.450
7.447
7.435
7.422
7.419
7.321
7.318
7.316
7.304
7.291
7.289
7.286
7.260

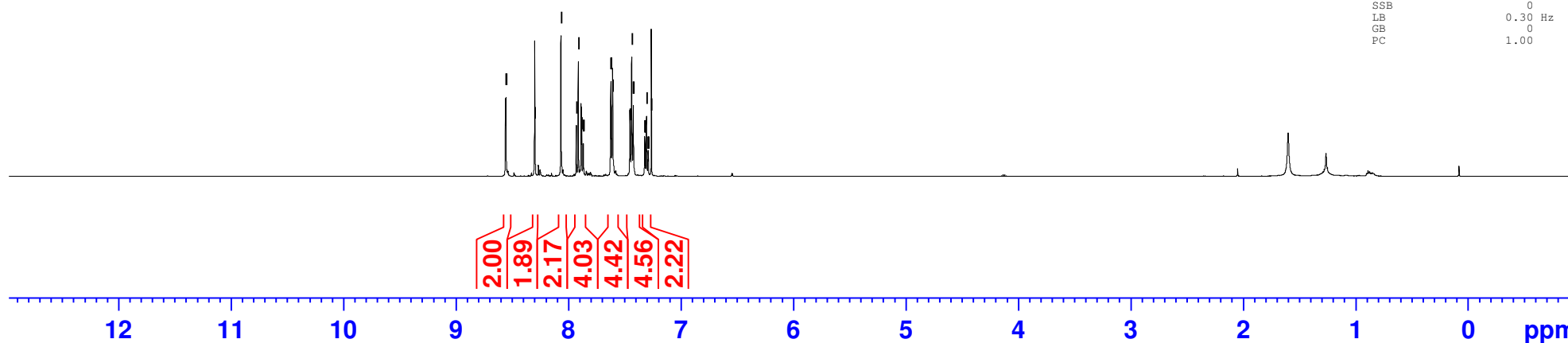


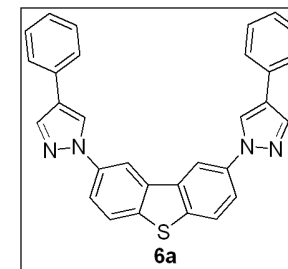
Current Data Parameters
NAME Ph
EXPNO 140
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190704
Time 20.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 32
DW 50.000 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 500.3030896 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





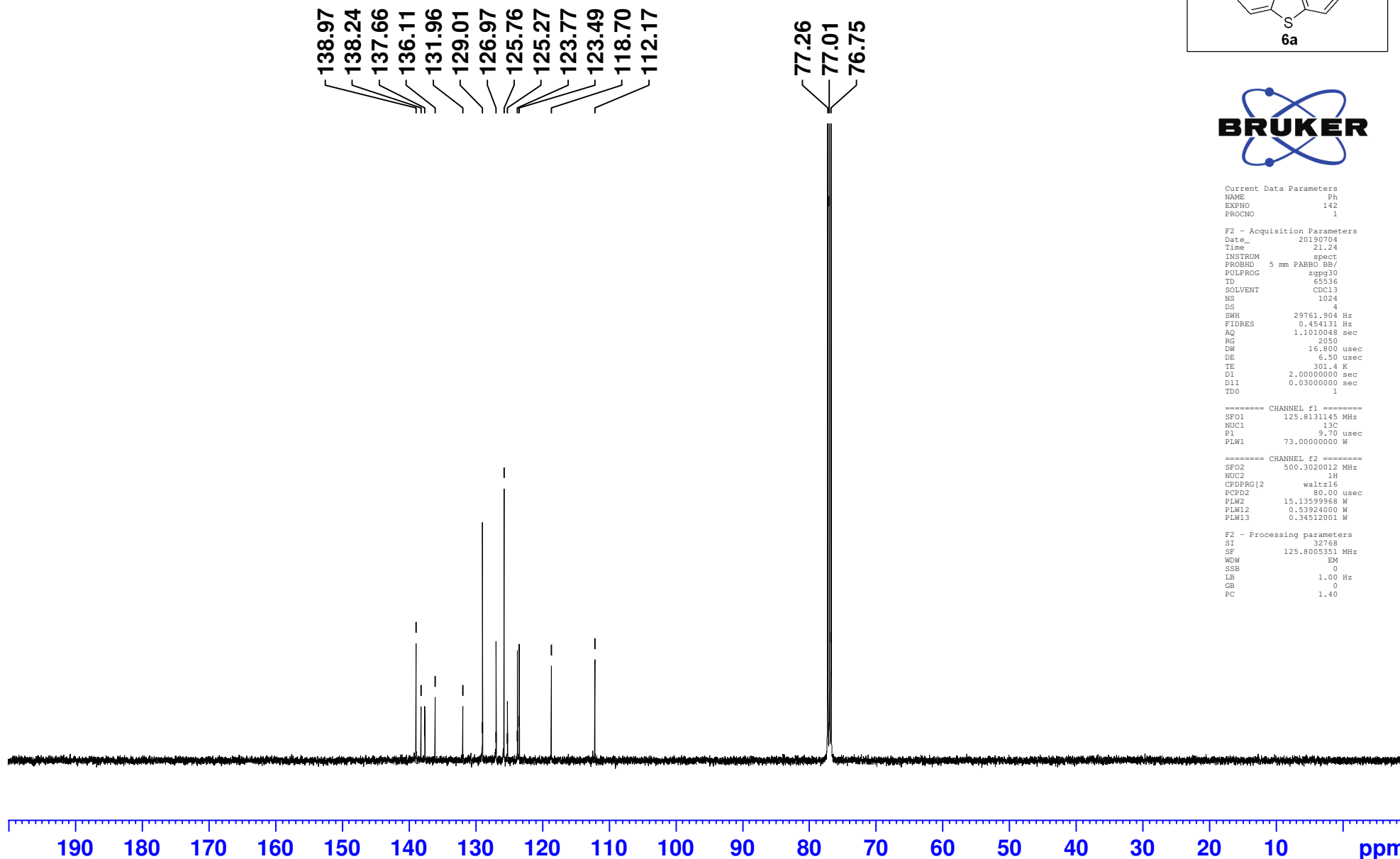
Current Data Parameters
NAME Ph
EXPNO 142
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190704
Time 21.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 301.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.8131145 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W

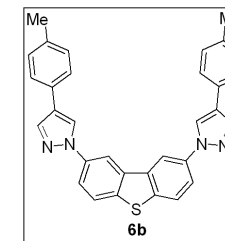
===== CHANNEL f2 =====
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.34512001 W

F2 - Processing parameters
SI 32768
SF 125.8005351 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



8.556
8.552
8.271
8.039
7.927
7.910
7.887
7.883
7.869
7.865
7.516
7.500
7.260
7.251
7.236

— 2.397

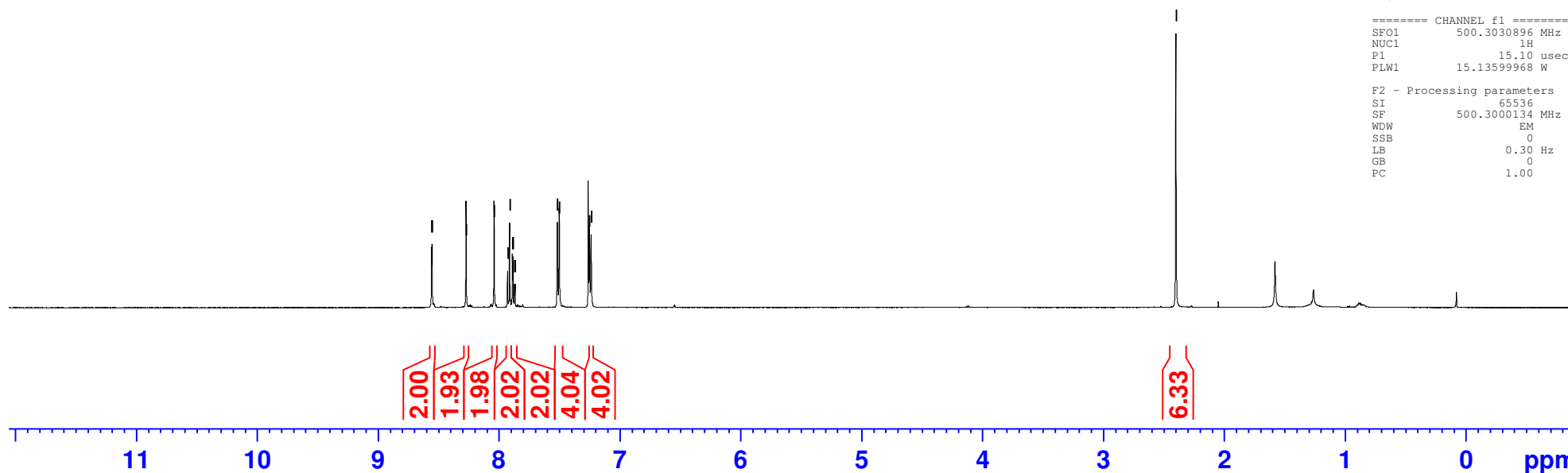


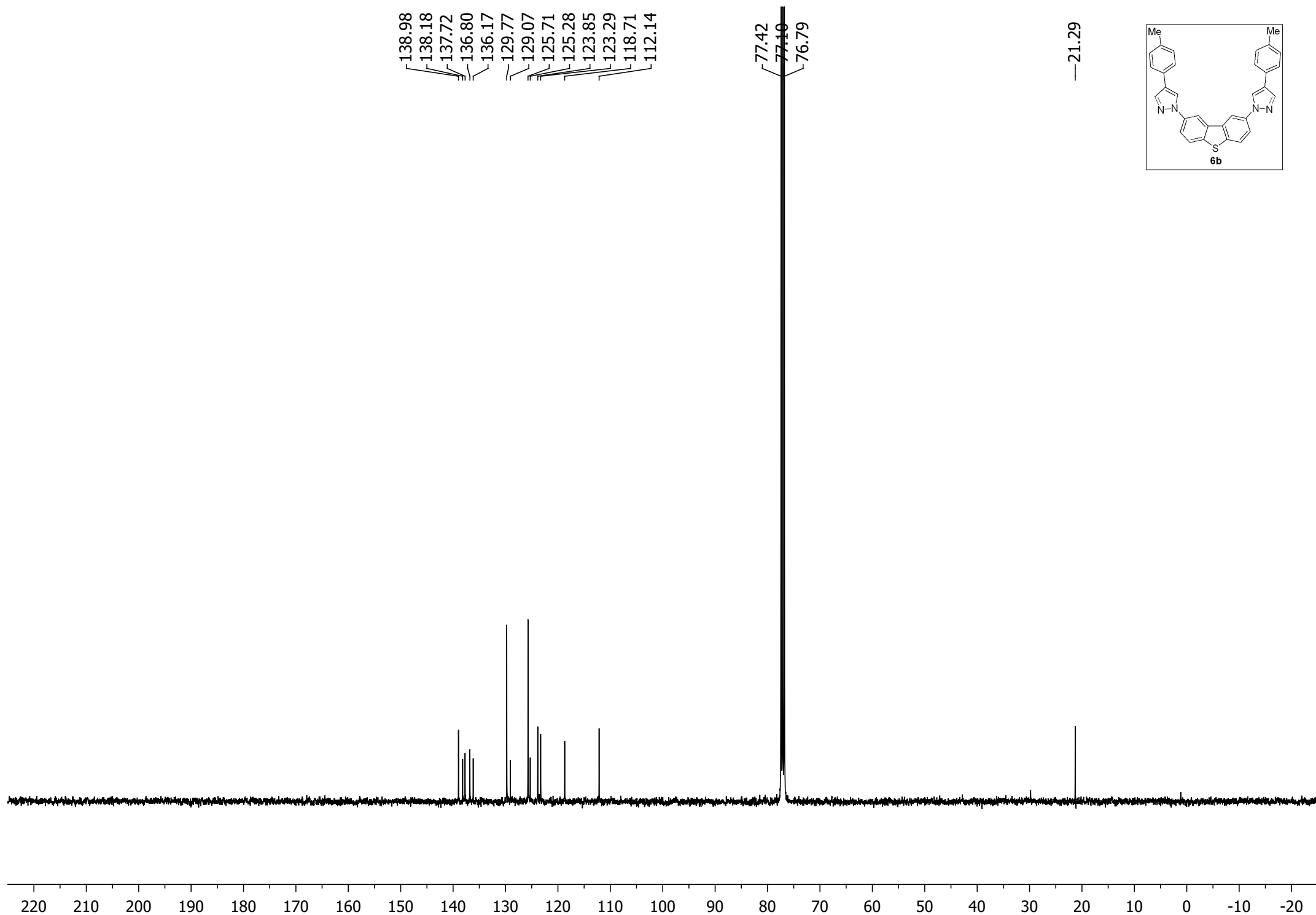
Current Data Parameters
NAME 4-Me
EXPNO 100
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190710
Time 18.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 228
DW 50.000 usec
DE 6.50 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1

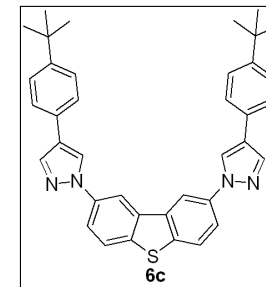
===== CHANNEL f1 =====
SF01 500.3030896 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





8.509
8.261
8.046
7.882
7.865
7.852
7.834
7.557
7.540
7.469
7.453
7.260



Current Data Parameters
NAME 4-tBu
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190716
Time 0.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 128
DW 50.000 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 500.3030896 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000135 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1.380

18.24

2.00

1.99

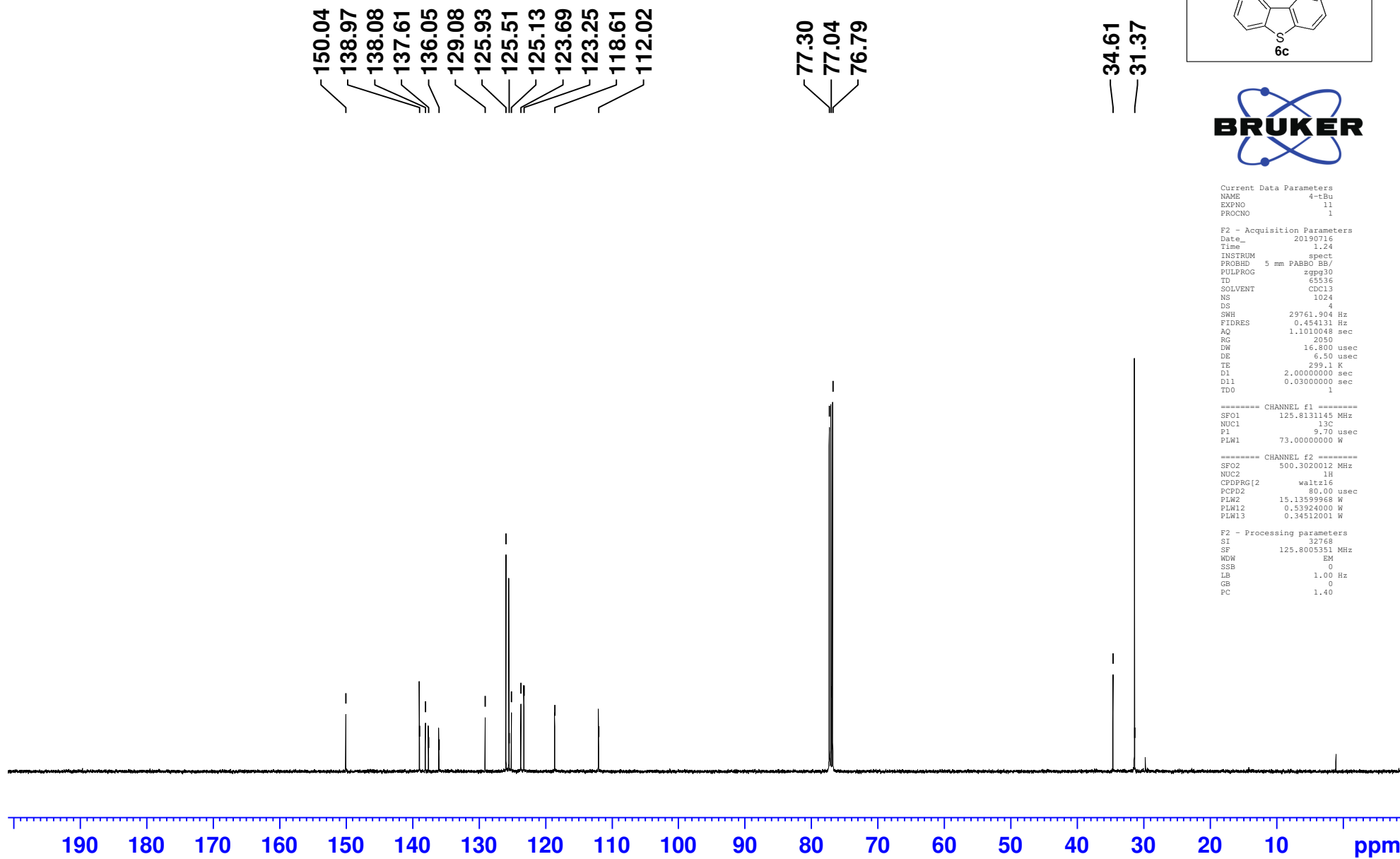
2.02

4.10

4.14

4.14

12 11 10 9 8 7 6 5 4 3 2 1 0 ppm



Current Data Parameters
NAME 4-tBu
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190716
Time 1.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

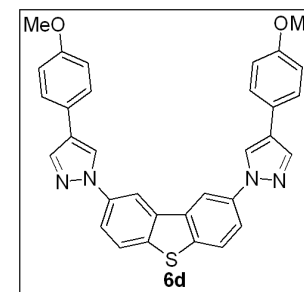
===== CHANNEL f1 =====
SF01 125.8131145 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W

===== CHANNEL f2 =====
SF02 500.3020012 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.34512001 W

F2 - Processing parameters
SI 32768
SF 125.8005351 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

8.556
8.552
8.227
8.001
7.928
7.911
7.884
7.880
7.867
7.863
7.541
7.524
7.260
6.984
6.967

3.860

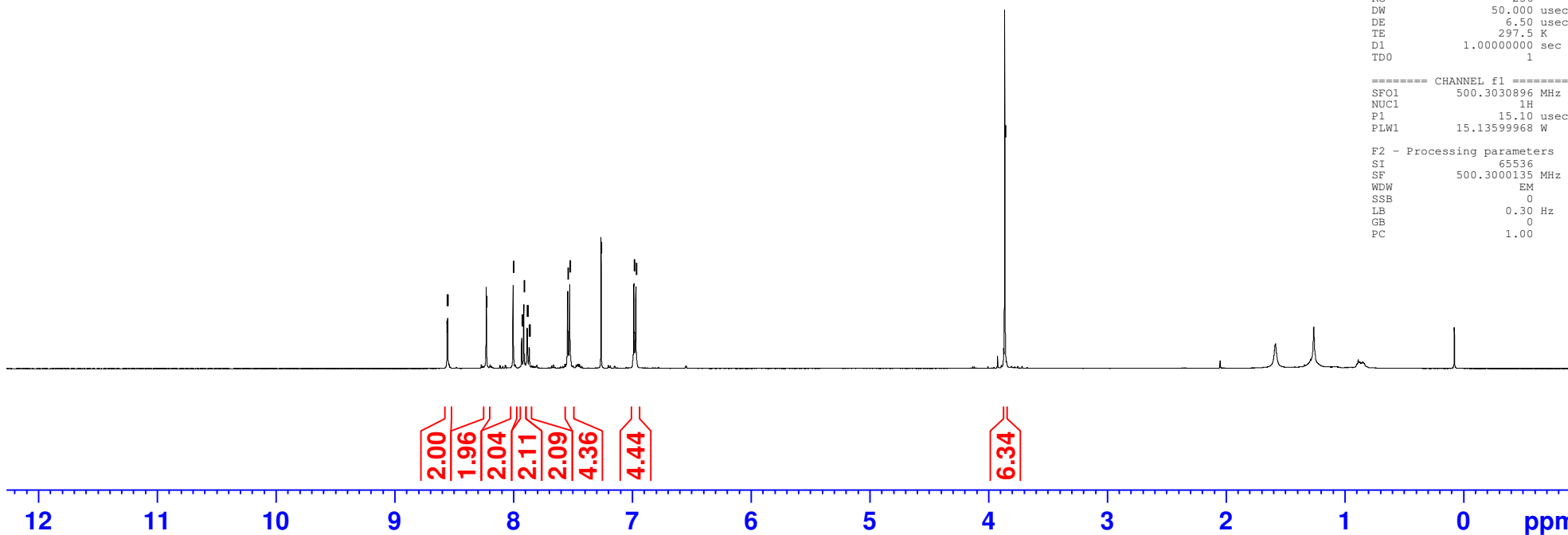


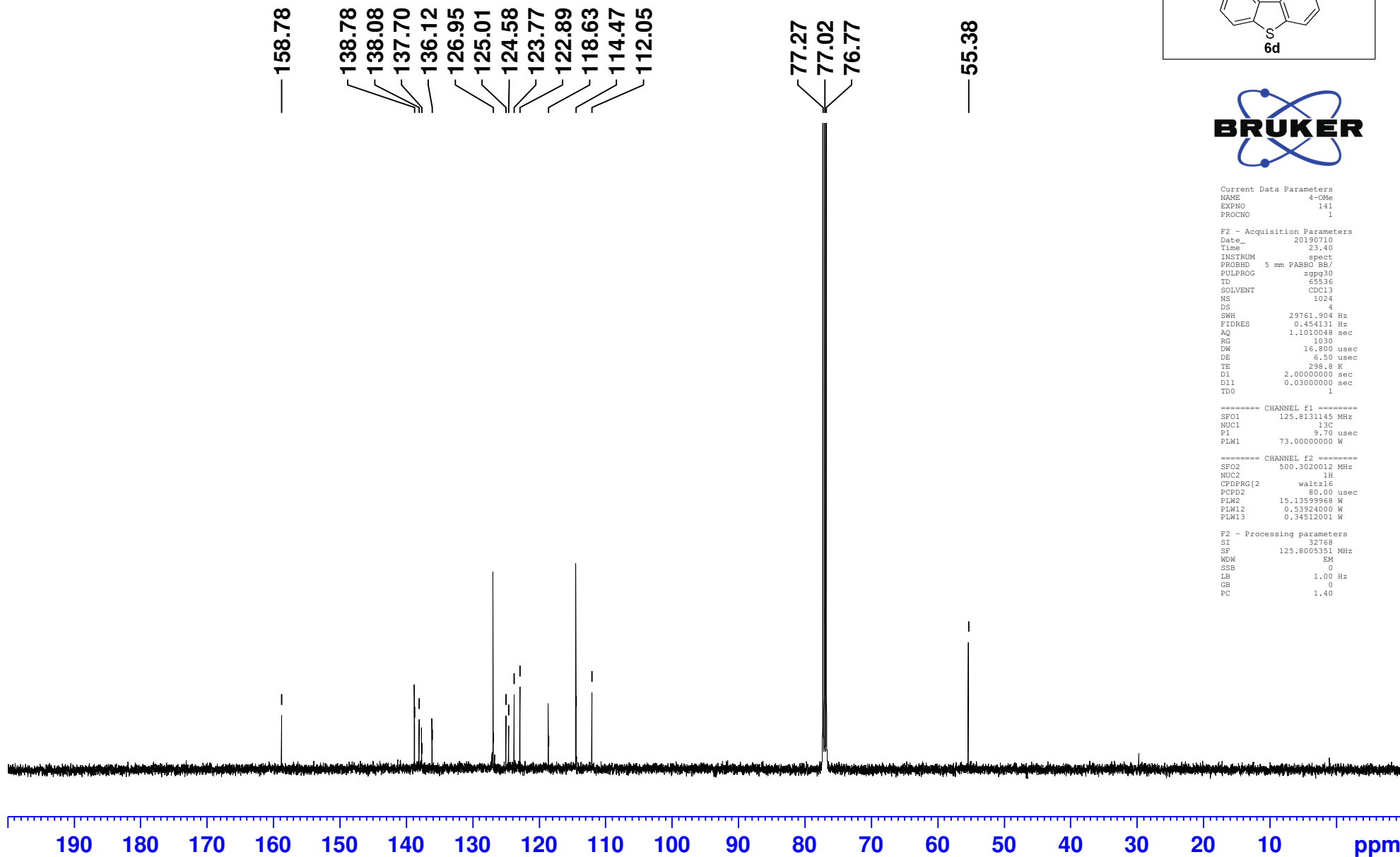
Current Data Parameters
NAME 4-OMe
EXPNO 140
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190710
Time 22.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 12
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 256
DW 50.000 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 500.3030896 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000135 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME 4-OMe
EXPNO 141
PROCNO 1

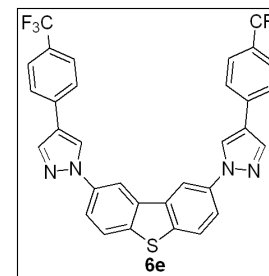
F2 - Acquisition Parameters
Date_ 20190710
Time 23.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 1030
DW 16.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.8131145 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W

===== CHANNEL f2 =====
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.34512001 W

F2 - Processing parameters
SI 32768
SF 125.8005351 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

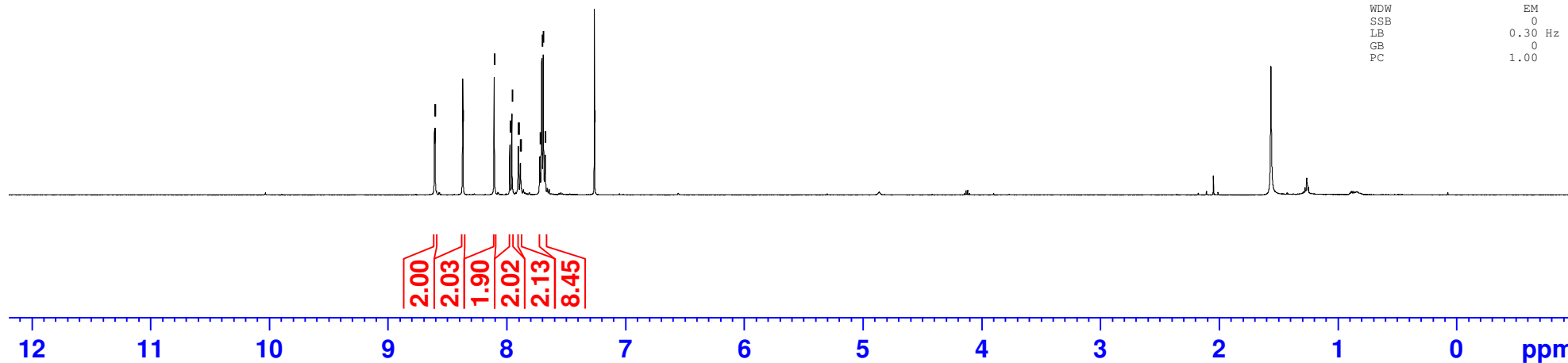
8.606
8.602
8.369
8.104
7.972
7.955
7.902
7.898
7.885
7.881
7.720
7.703
7.690
7.673
7.260

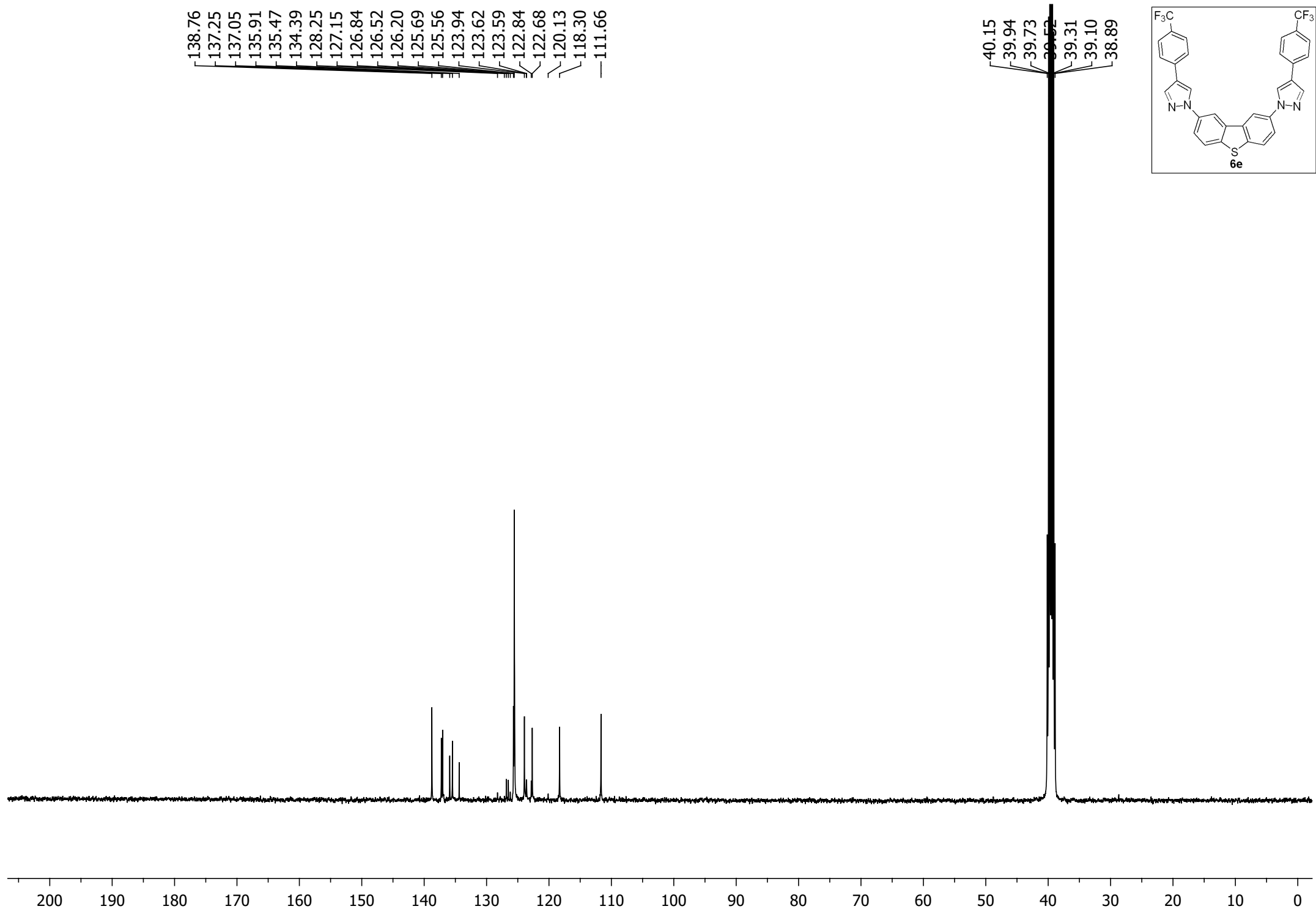


Current Data Parameters
NAME 4-CF3
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200122
Time_ 17.42 h
INSTRUM spect
PROBHD Z115265_0004 (zg30)
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 456
DW 50.000 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
SFO1 500.3030894 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

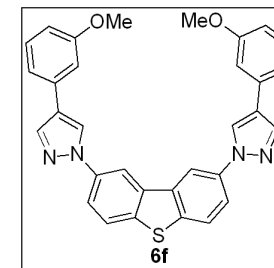
F2 - Processing parameters
SI 65536
SF 500.3000135 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





8.480
8.245
8.030
7.870
7.853
7.830
7.813
7.351
7.335
7.320
7.260
7.192
7.177
7.125
6.852
6.838

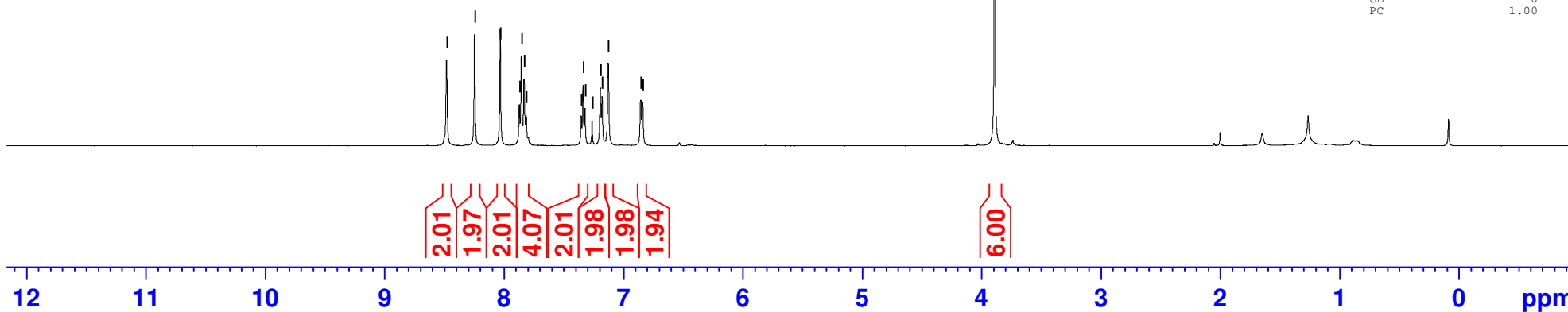
3.887

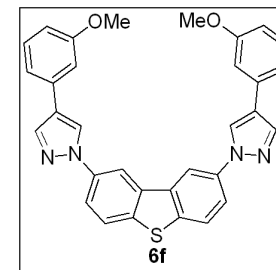


Current Data Parameters
NAME Feb07-2020
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200207
Time 19.02 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 203
DW 50.000 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
SFO1 500.3030894 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000145 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





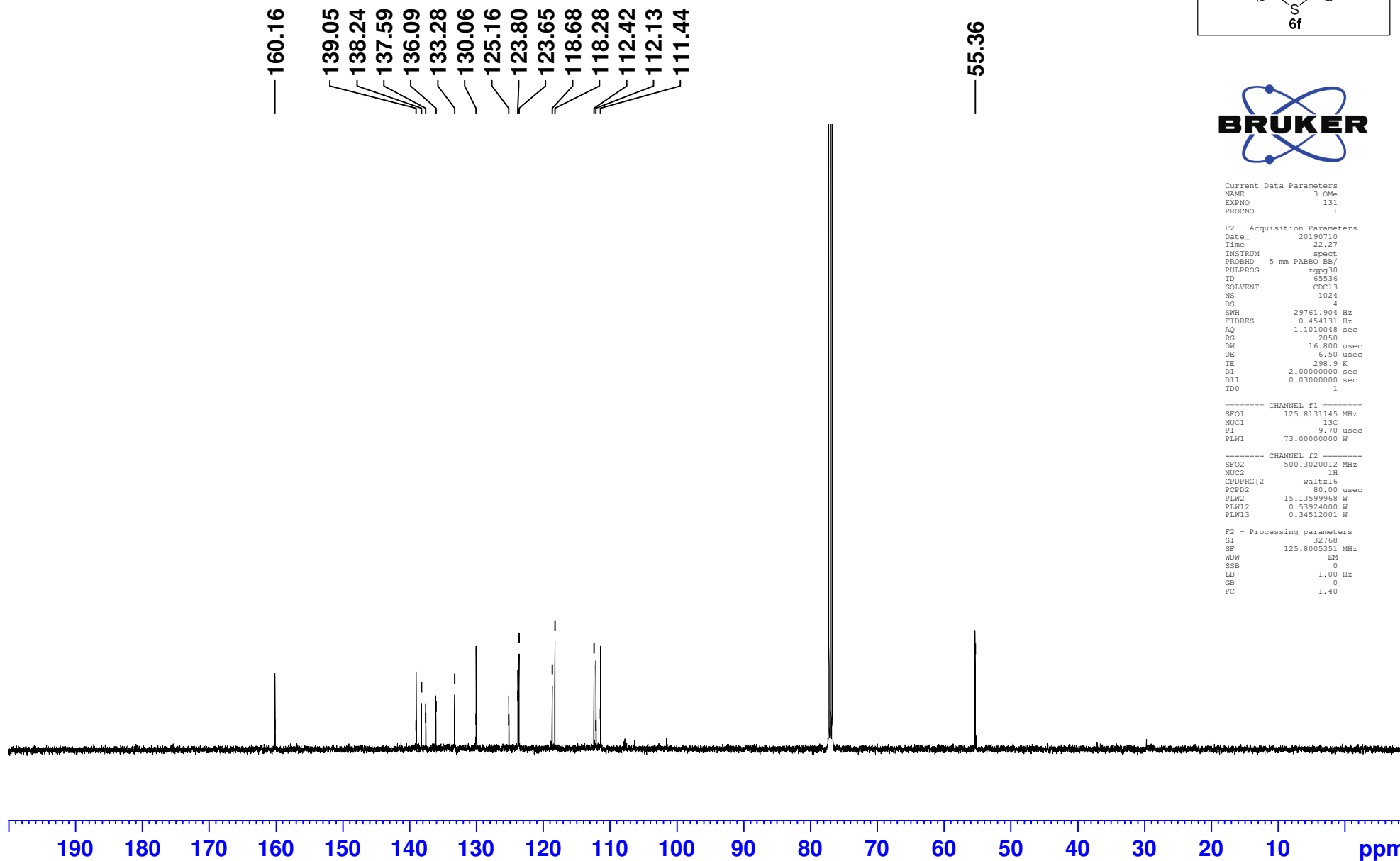
Current Data Parameters
 NAME 3-OMe
 EXPNO 131
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190710
 Time 22.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 2050
 DW 16.800 usec
 DE 6.50 usec
 TE 298.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

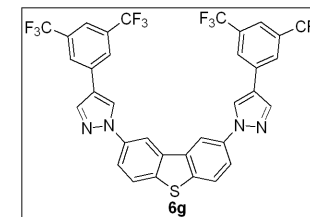
===== CHANNEL f1 =====
 SFO1 125.8131145 MHz
 NUC1 13C
 P1 9.70 usec
 PLW1 73.00000000 W

===== CHANNEL f2 =====
 SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 15.13599968 W
 PLW12 0.53924000 W
 PLW13 0.34512001 W

F2 - Processing parameters
 SI 32768
 SF 125.8005351 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



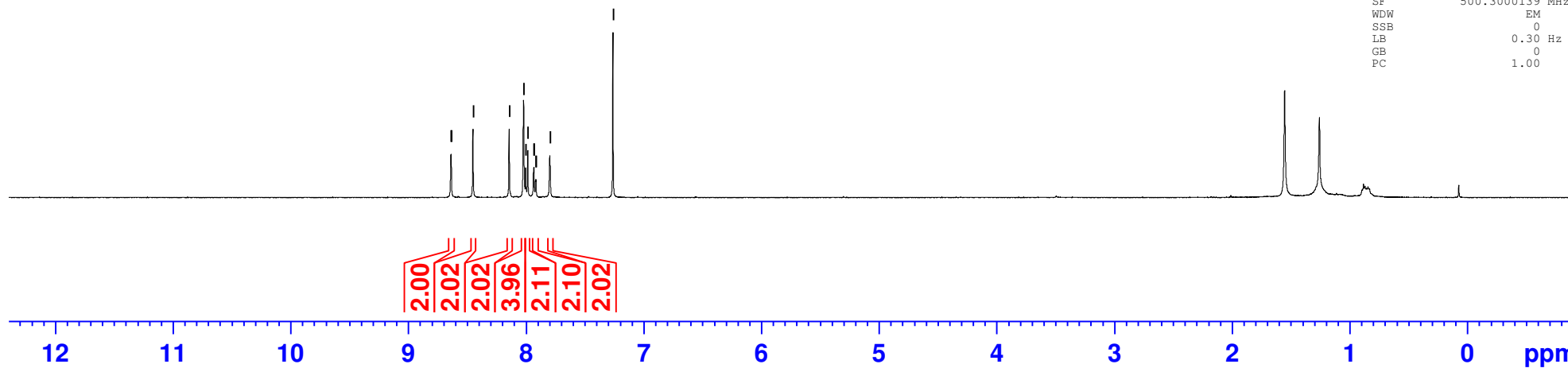
8.638
8.634
8.450
8.142
8.019
8.001
7.984
7.935
7.931
7.918
7.914
7.796
7.260

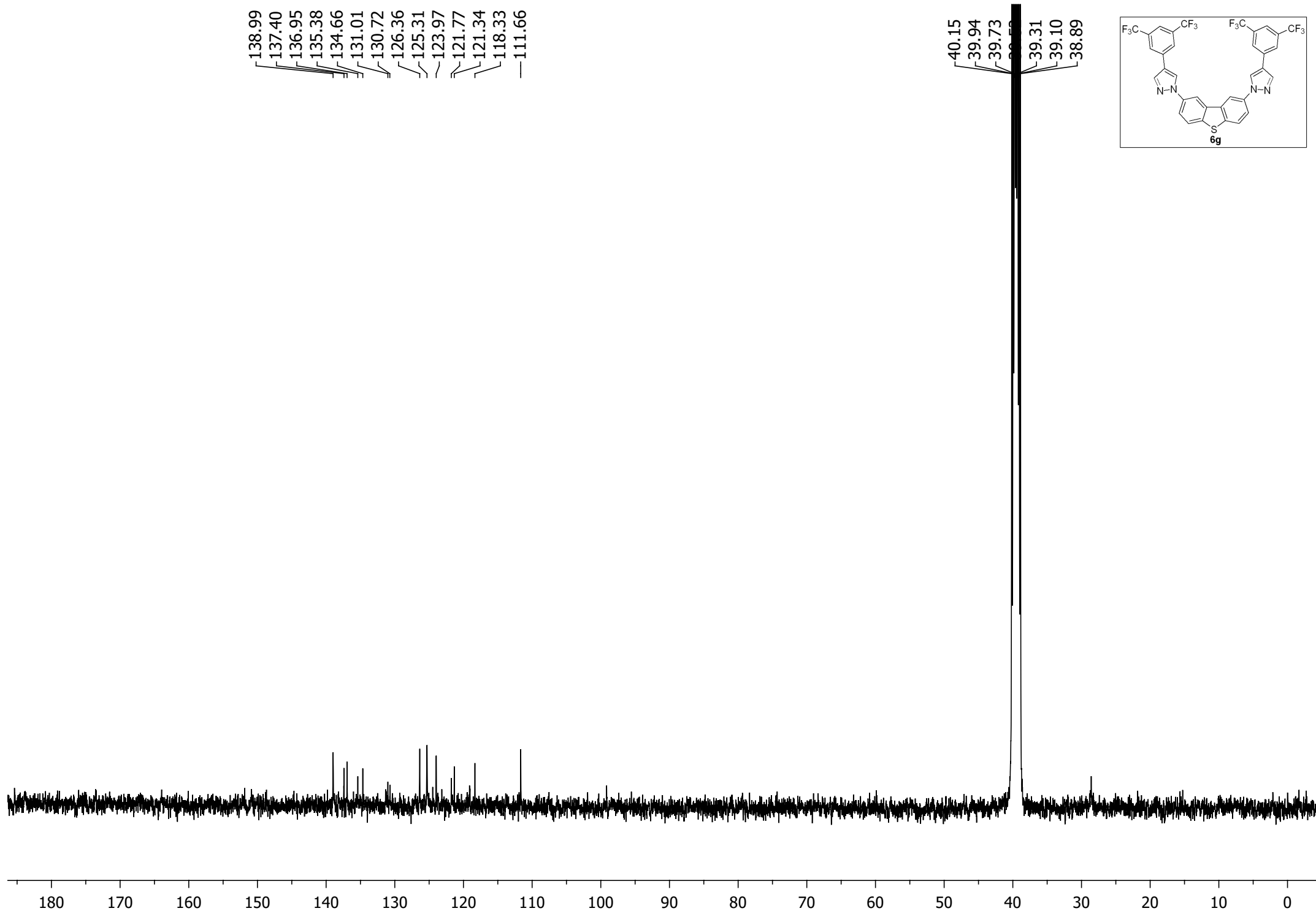


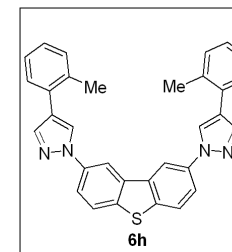
Current Data Parameters
NAME Feb06-2020
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200206
Time_ 10.06 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 406
DW 50.000 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
SFO1 500.3030894 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





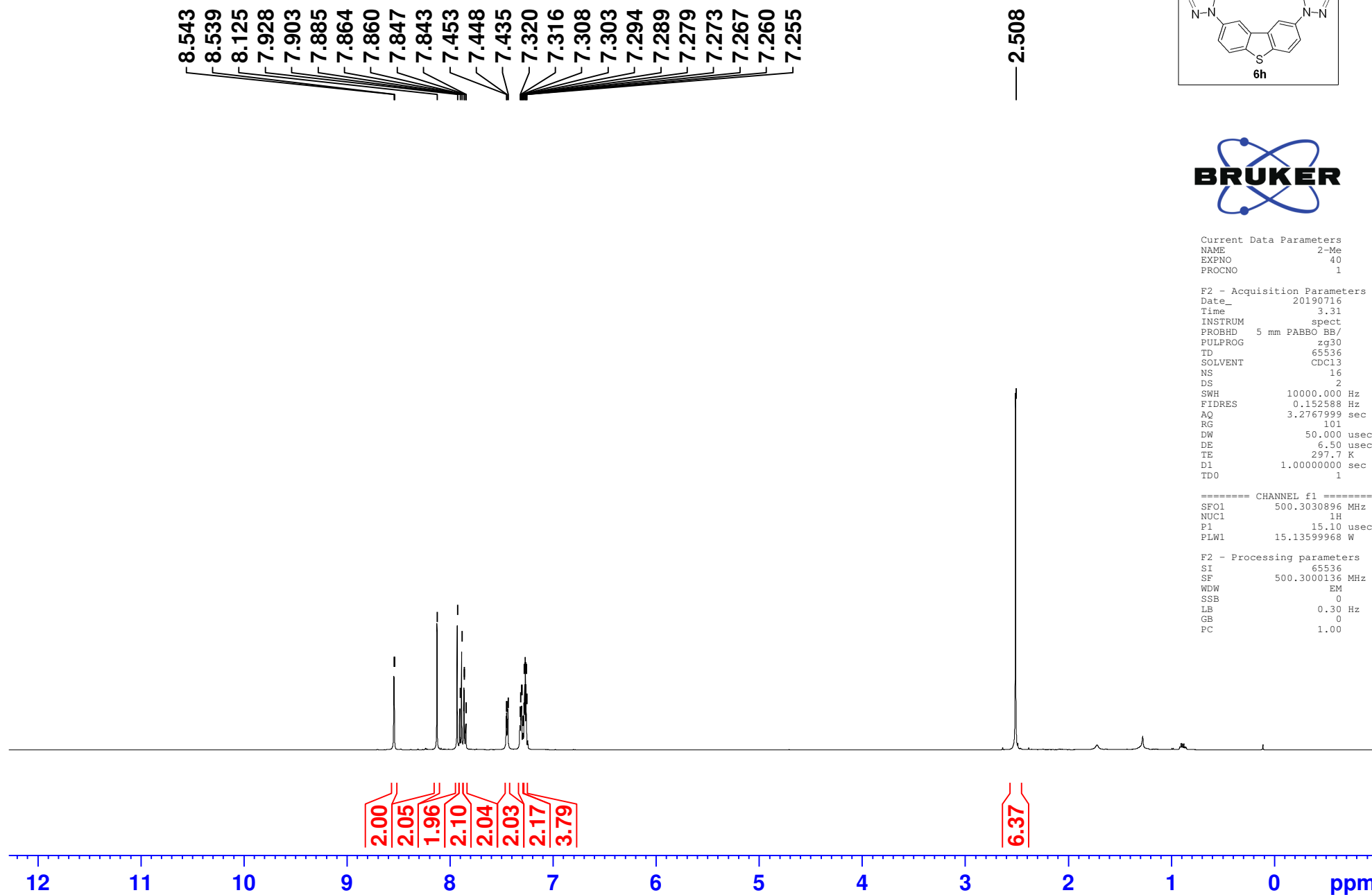


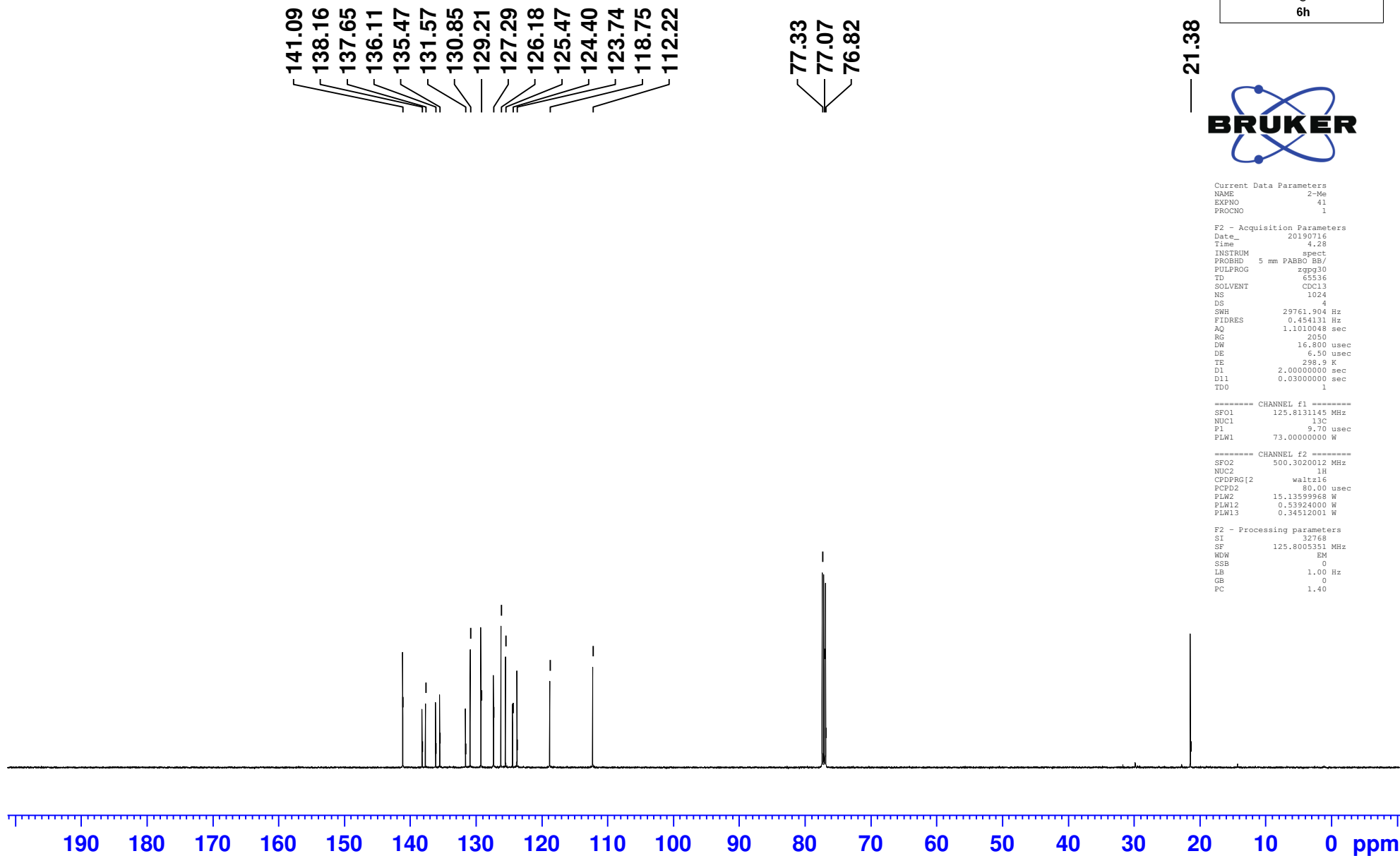
Current Data Parameters
 NAME 2-Me
 EXPNO 40
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190716
 Time 3.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 101
 DW 50.000 usec
 DE 6.50 usec
 TE 297.7 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 500.3030896 MHz
 NUC1 1H
 P1 15.10 usec
 PLW1 15.13599968 W

F2 - Processing parameters
 SI 65536
 SF 500.3000136 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





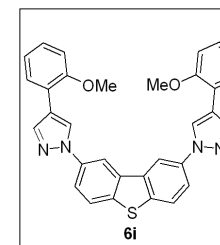
Current Data Parameters
 NAME 2-Me
 EXPNO 41
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190716
 Time 4.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 2050
 DW 16.800 usec
 DE 6.50 usec
 TE 298.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 125.8131145 MHz
 NUC1 13C
 P1 9.70 usec
 PLW1 73.00000000 W

===== CHANNEL f2 =====
 SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 15.13599968 W
 PLW12 0.53924000 W
 PLW13 0.34512001 W

F2 - Processing parameters
 SI 32768
 SF 125.8005351 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

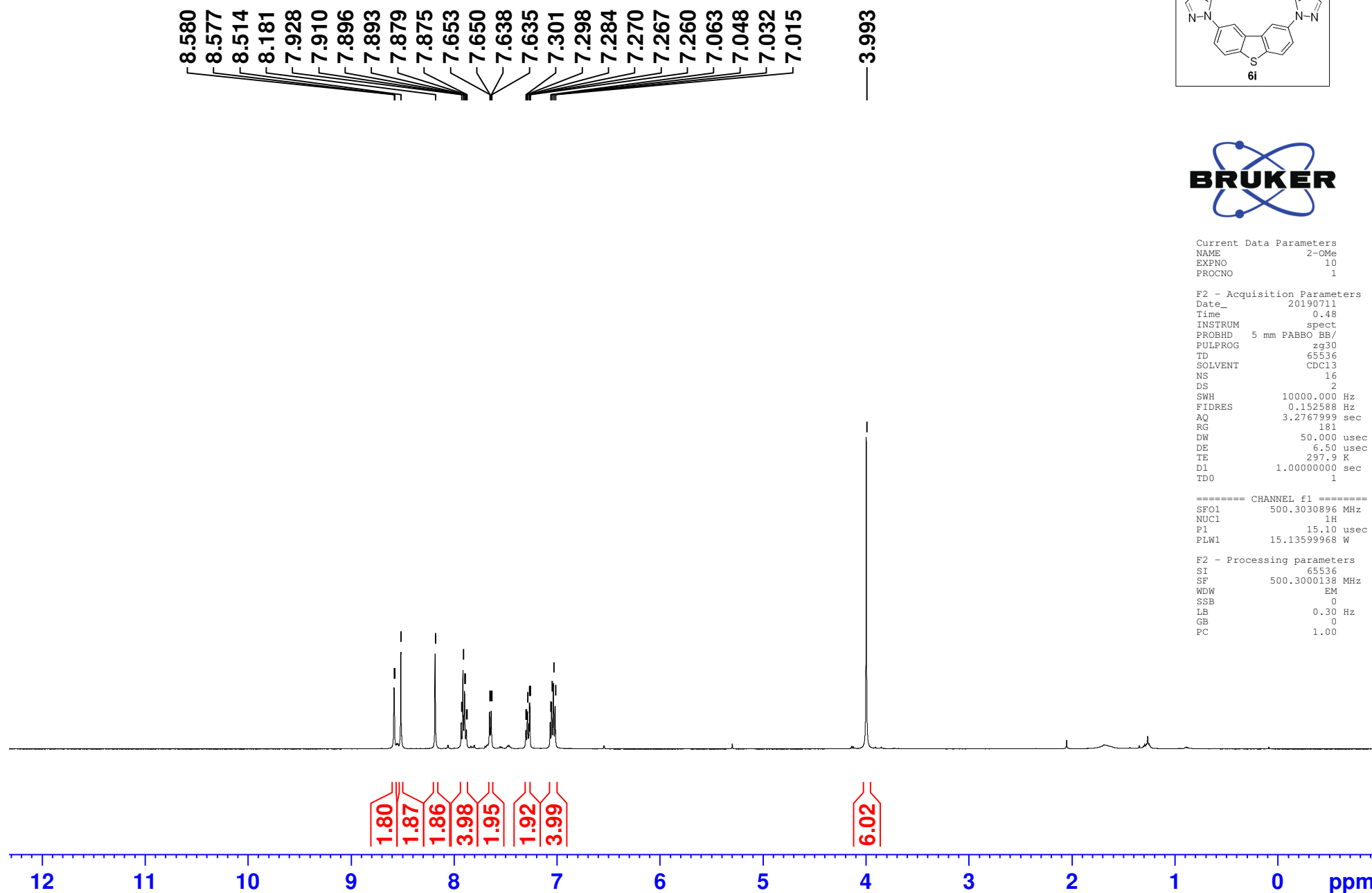


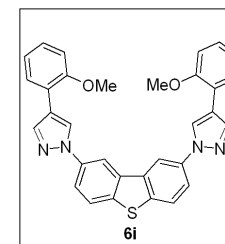
Current Data Parameters
NAME 2-OMe
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190711
Time 0.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 181
DW 50.000 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 500.3030896 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





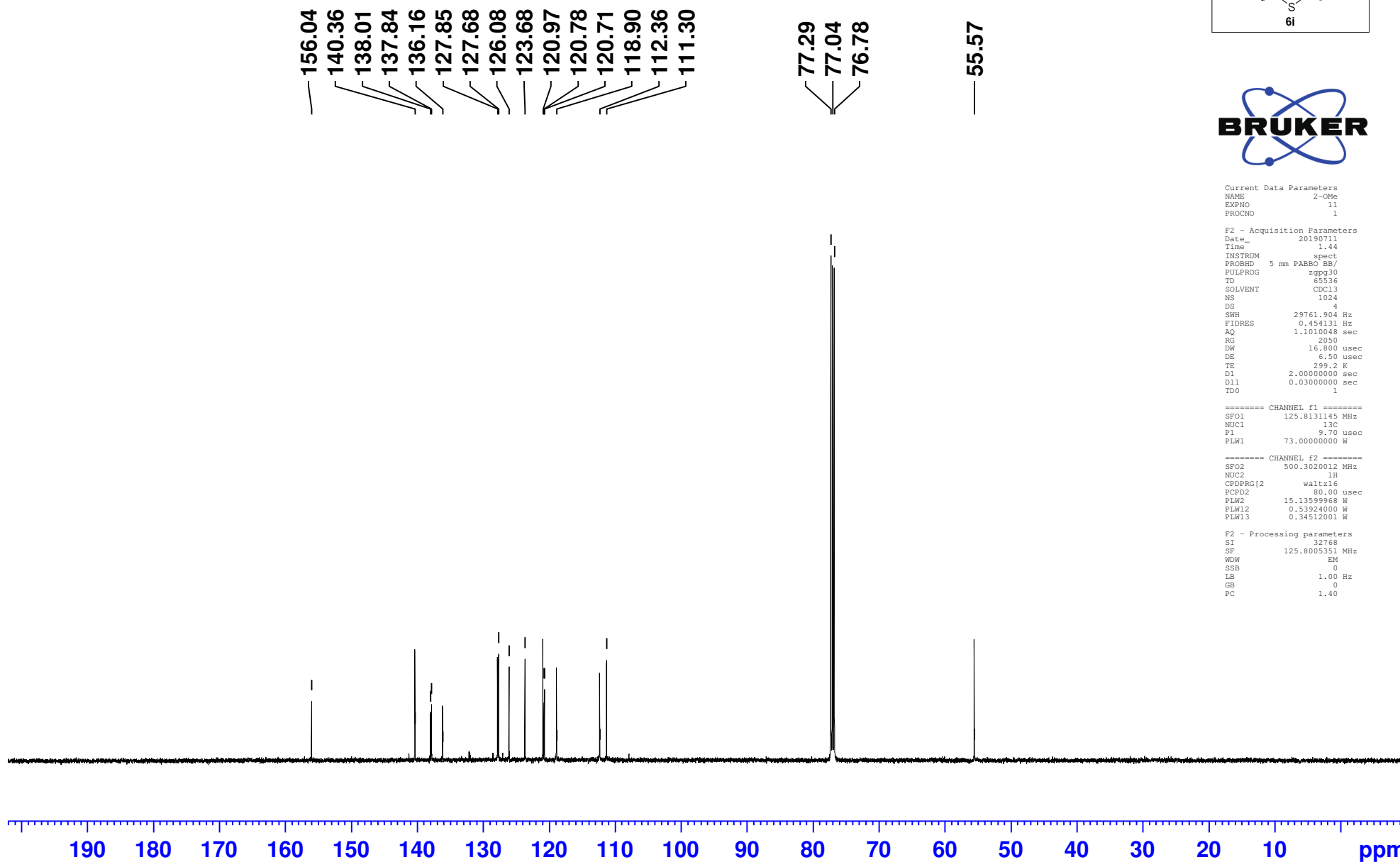
Current Data Parameters
NAME 2-OMe
EXPNO 11
PROCNO 1

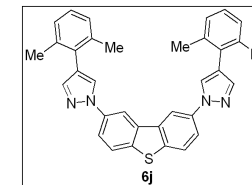
F2 - Acquisition Parameters
Date_ 20190711
Time 1.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 125.8131145 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W

===== CHANNEL f2 =====
SF02 500.3020012 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.34512001 W

F2 - Processing parameters
SI 32768
SF 125.8005351 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
 NAME 2,6-Me
 EXPNO 100
 PROCNO 1

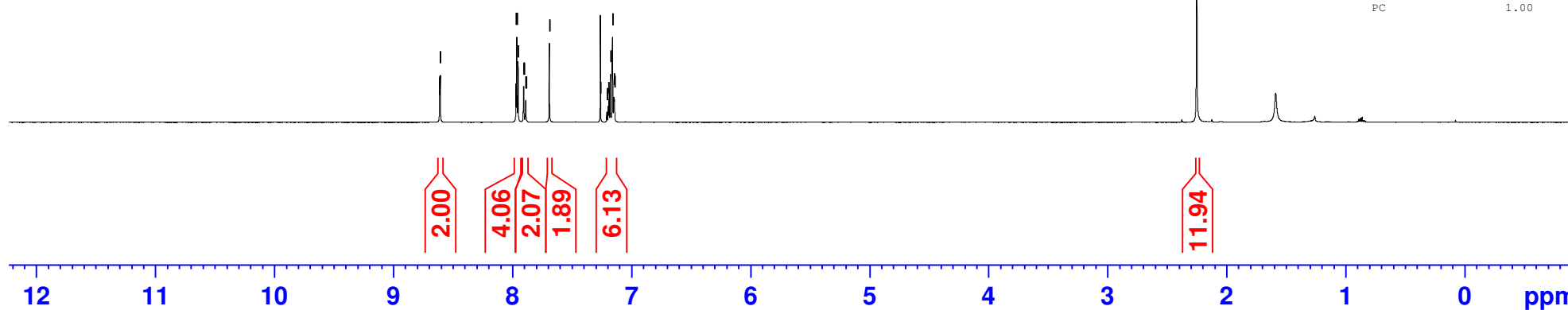
F2 - Acquisition Parameters
 Date_ 20190715
 Time 22.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 228
 DW 50.000 usec
 DE 6.50 usec
 TE 297.8 K
 D1 1.00000000 sec
 TD0 1

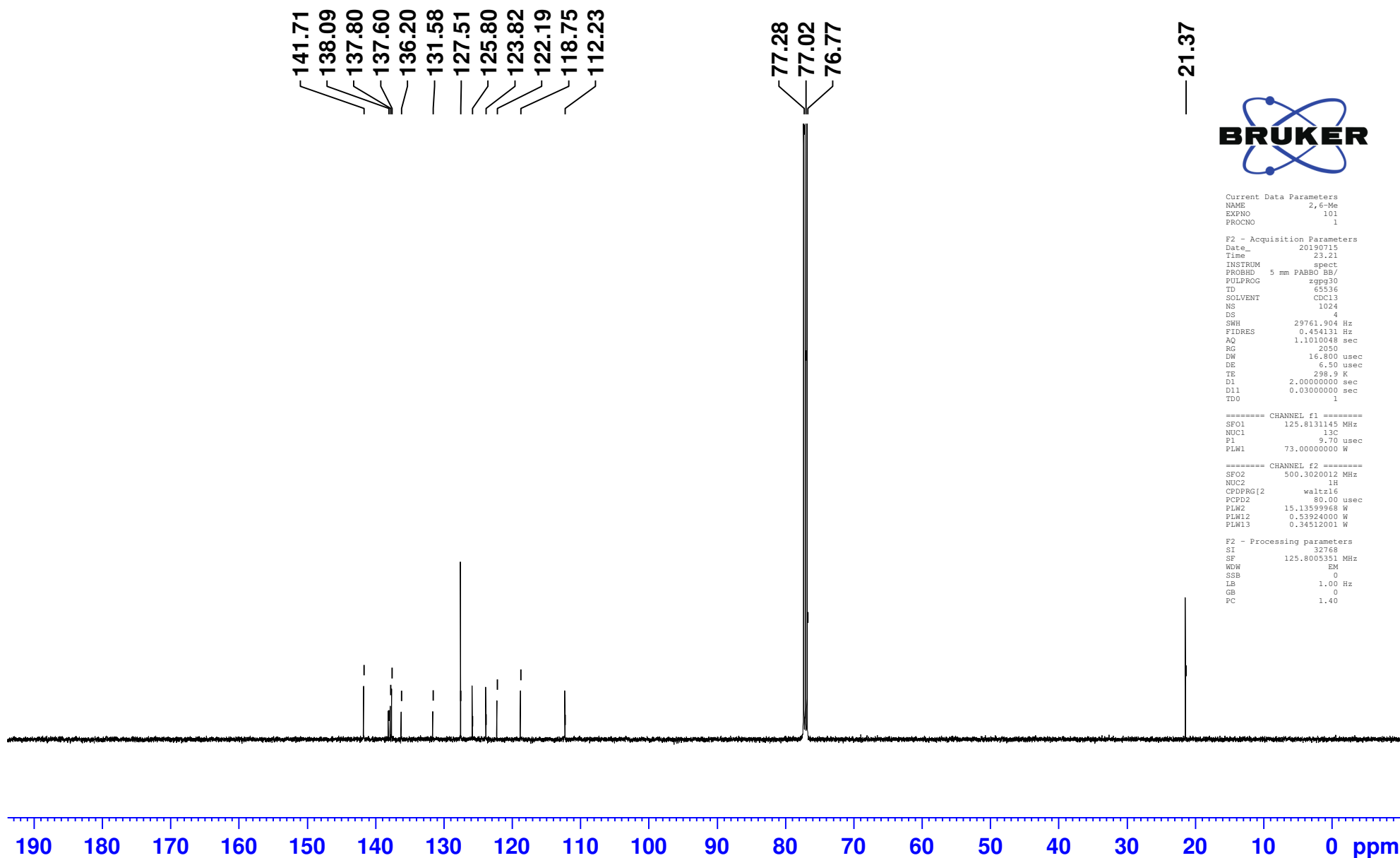
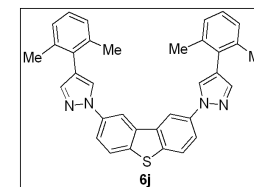
===== CHANNEL f1 =====
 SF01 500.3030896 MHz
 NUC1 1H
 P1 15.10 usec
 PLW1 15.13599968 W

F2 - Processing parameters
 SI 65536
 SF 500.3000134 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.609
8.605
7.968
7.961
7.951
7.906
7.902
7.889
7.884
7.688
7.260
7.205
7.193
7.187
7.175
7.158
7.145
7.141

— 2.248





Current Data Parameters
NAME 2,6-Me
EXPNO 101
PROCNO 1

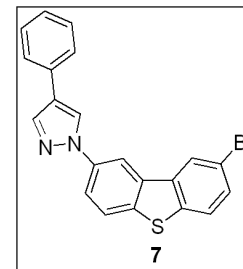
F2 - Acquisition Parameters
Date_ 20190715
Time 23.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.8131145 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W

===== CHANNEL f2 =====
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.34512001 W

F2 - Processing parameters
SI 32768
SF 125.8005351 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

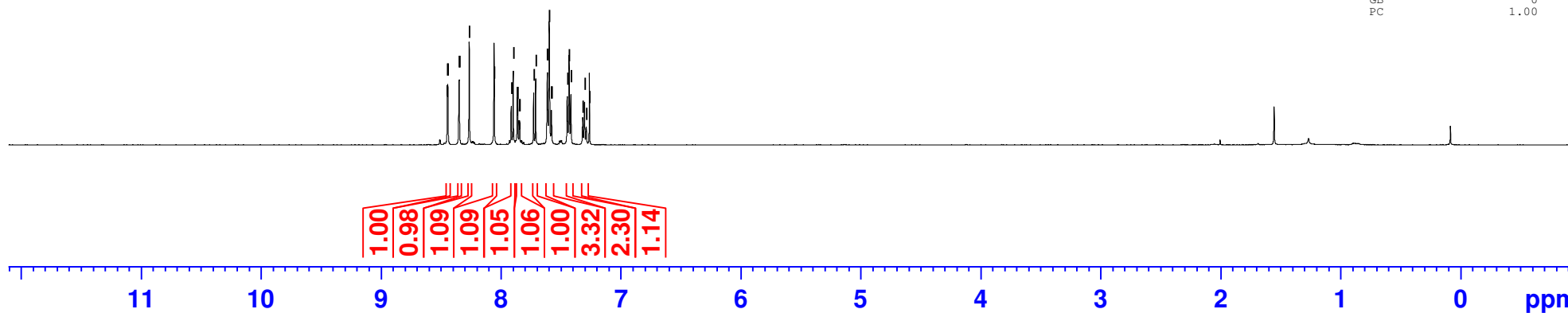
8.444
8.440
8.348
8.345
8.262
8.055
7.912
7.895
7.863
7.859
7.845
7.841
7.725
7.708
7.612
7.610
7.595
7.578
7.575
7.445
7.430
7.414
7.316
7.301
7.286
7.260

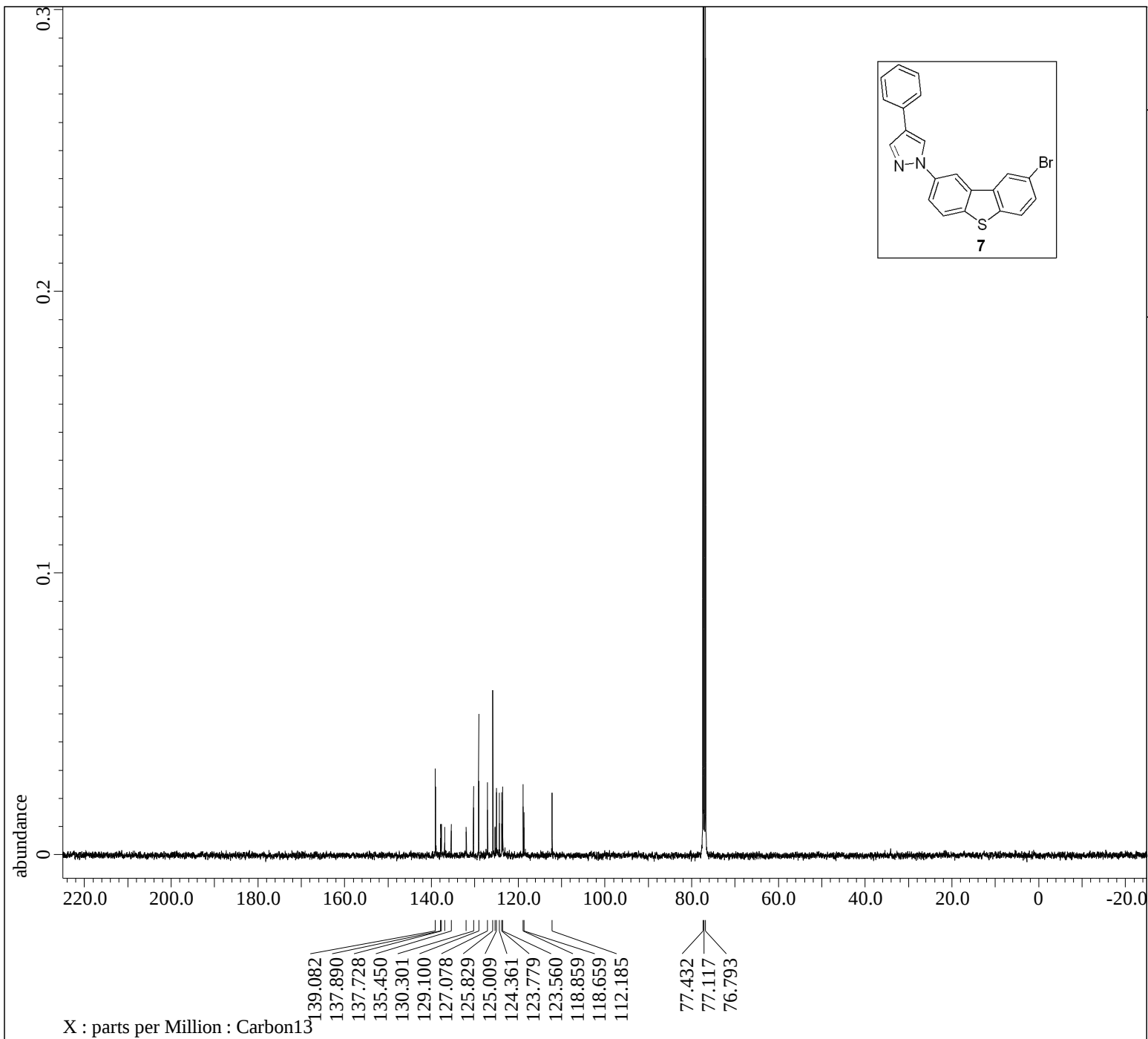


Current Data Parameters
NAME 7
EXPNO 17
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200217
Time 19.00 h
INSTRUM spect
PROBHD Z115265_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 406
DW 50.000 usec
DE 6.50 usec
TE 301.8 K
D1 1.00000000 sec
TD0 1
SFO1 500.3030894 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

F2 - Processing parameters
SI 65536
SF 500.3000134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





```

---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
  
```

```

Filename      = CURAJ-RSJ-7_Carbon-1-3.j
Author        = datum
Experiment     = carbon.jxp
Sample_Id      = CURAJ-RSJ-7
Solvent        = CHLOROFORM-D
Creation_Time  = 20-FEB-2020 12:34:44
Revision_Time  = 20-FEB-2020 13:37:08
Current_Time   = 20-FEB-2020 13:37:17
  
```

```

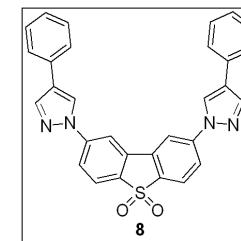
Comment       = single pulse decoupled g
Data_Format    = 1D COMPLEX
Dim_Size       = 26214
Dim_Title      = Carbon13
Dim_Units      = [ppm]
Dimensions     = X
Site           = JNM-ECS400
Spectrometer   = DELTA2_NMR
  
```

```

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.04333312[s]
X_Domain       = 13C
X_Freq         = 100.52530333[MHz]
X_Offset       = 100[ppm]
X_Points       = 32768
X_Prescans     = 4
X_Resolution   = 0.95846665[Hz]
X_Sweep        = 31.40703518[kHz]
X_Sweep_Clipped = 25.12562814[kHz]
Irr_Domain     = Proton
Irr_Freq       = 399.78219838[MHz]
Irr_Offset     = 5[ppm]
Clipped        = FALSE
Scans          = 1729
Total_Scans    = 1729
  
```

```

Relaxation_Delay = 2[s]
Recvr_Gain       = 50
Temp_Get         = 19.1[dC]
X_90_Width       = 8.83[us]
X_Acq_Time       = 1.04333312[s]
X_Angle          = 30[deg]
X_Atn            = 5[dB]
X_Pulse          = 2.94333333[us]
Irr_Atn_Dec      = 20.7[dB]
Irr_Atn_Noe      = 20.7[dB]
Irr_Noise        = WALTZ
Irr_Pwidth       = 0.115[ms]
Decoupling       = TRUE
  
```

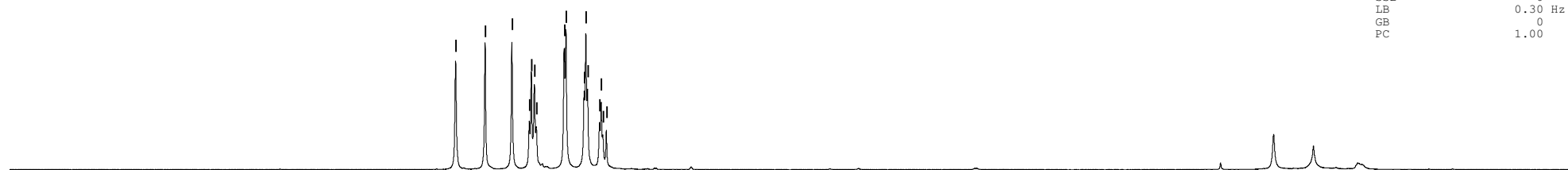


Current Data Parameters
 NAME DBT SUL
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200109
 Time_ 19.40 h
 INSTRUM spect
 PROBHD Z115265_0004 (
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 287
 DW 50.000 usec
 DE 6.50 usec
 TE 296.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.3030894 MHz
 NUC1 1H
 P1 15.10 usec
 PLW1 15.13599968 W

F2 - Processing parameters
 SI 65536
 SF 500.3000153 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.539
 8.288
 8.061
 7.913
 7.896
 7.871
 7.854
 7.617
 7.603
 7.448
 7.434
 7.419
 7.317
 7.303
 7.289
 7.259



2.00
 1.96
 2.00
 4.08
 4.05
 4.23
 2.15



