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Supplementary Information

for

Influence of Alkyl Chain Length on the Solid-State Properties and Transistor Performance of BN-Substituted Tetrathienonaphthalenes

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1. DSC Measurement

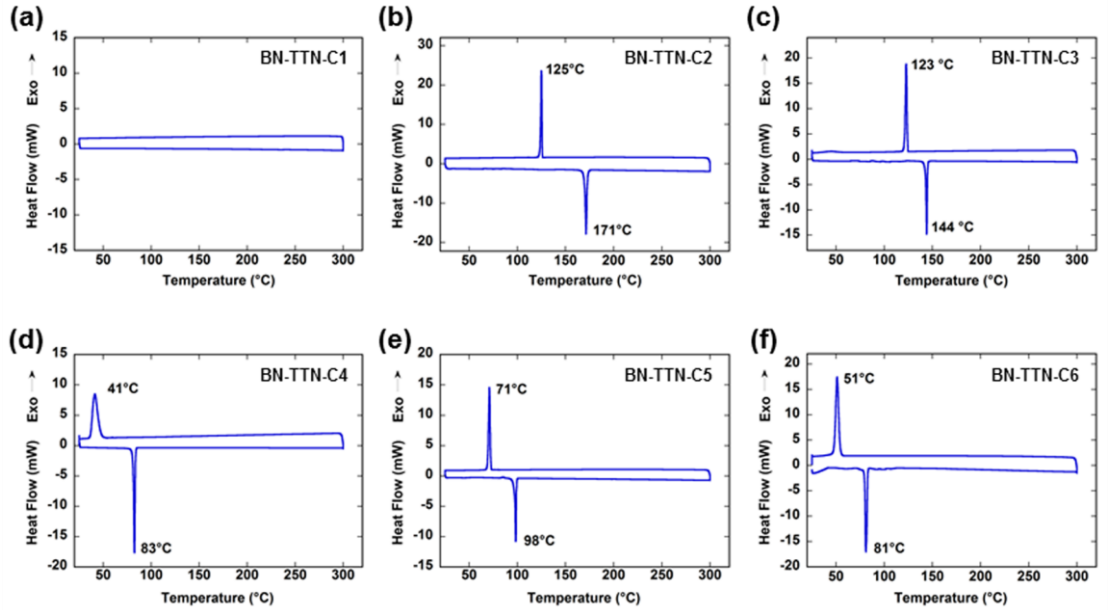


Fig. S1 DSC traces of BN-TTNs.

2. CV Measurement

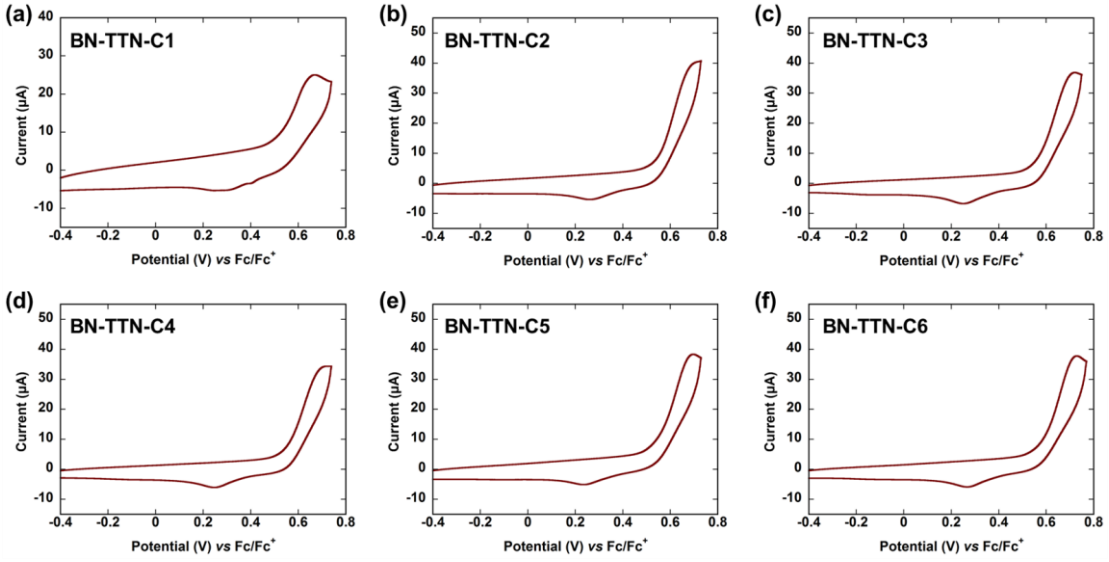


Fig. S2 Cyclic voltammograms of BN-TTNs in CH_2Cl_2 with 0.1 M *n*-Bu_4PF_6 as supporting electrolyte (scan rate: 100 mV s^{-1}). The HOMO energy levels are estimated from the oxidation onset values based on the equation HOMO = −4.80 − E_{ox}.

3. PES Measurement

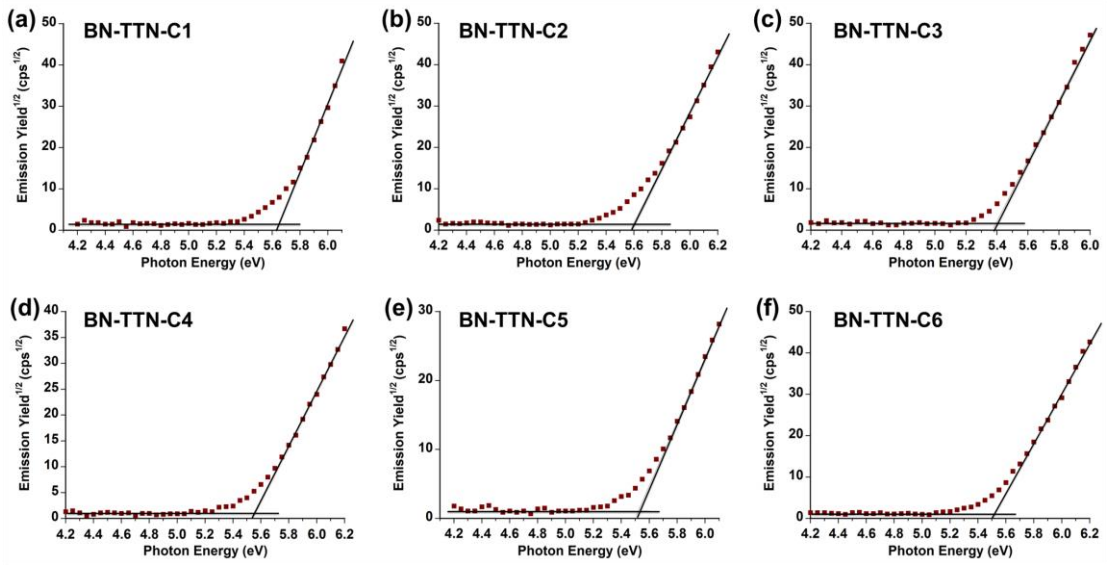


Fig. S3 Photoelectron spectra (PES) of BN-TTNs in film state.

4. XRD Patterns

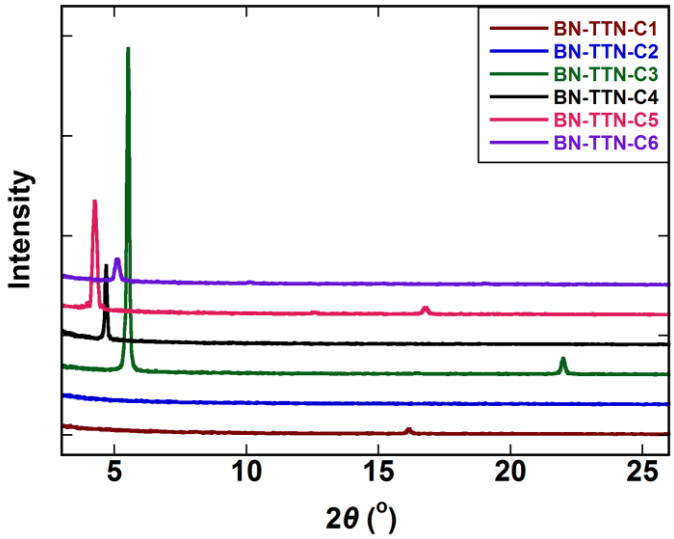


Fig. S4 XRD patterns of the thin films of BN-TTNs deposited on CYTOP-treated Si/SiO_2 substrates.

5. Emission Spectra

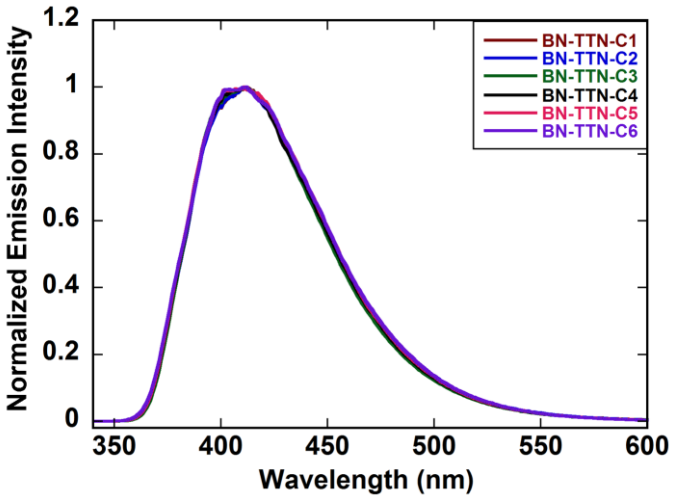


Fig. S5 Normalized emission spectra of BN-TTNs in CH_2Cl_2 solutions. The films of BN-TTNs are non-emissive due to the strong fluorescence quenching in aggregated state.

6. Single Crystal Data

Table S1. Summary of the single crystal data of BN-TTNs.

Compound	Crystal system	Space group	a (Å)	b (Å)	c (Å)	α (deg)	β (deg)	γ (deg)	ρ (mg/m^3)
BN-TTN-C1	Monoclinic	P2(1)/n	14.530(5)	7.119(2)	17.336(6)	90	92.113(5)	90	1.517
BN-TTN-C2	Triclinic	P-1	9.989(2)	11.179(2)	11.299(2)	74.02(3)	81.77(3)	72.90(3)	1.337
BN-TTN-C3	Triclinic	P-1	10.925(3)	15.116(3)	16.752(4)	80.320(11)	83.220(12)	75.300(9)	1.318
BN-TTN-C4	Triclinic	P-1	7.5956(3)	10.7442(5)	18.2411(8)	86.994(4)	83.691(4)	82.603(4)	1.309
BN-TTN-C5	Triclinic	P-1	8.4695(17)	13.030(3)	16.200(3)	99.16(3)	96.39(3)	104.33(3)	1.246
BN-TTN-C6	Triclinic	P-1	9.2070(12)	9.6380(13)	11.6280(19)	77.180(11)	85.610(12)	71.030(10)	1.204

Table S2. Crystal data and structure refinement for BN-TTN-C1 (CCDC 1007263).

Empirical formula	$C_{20}H_{16}BNS_4$	
Formula weight	409.39	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, $P2_1/n$	
Unit cell dimensions	a = 14.530(5) Å	alpha = 90 deg.
	b = 7.119(2) Å	beta = 92.113(5) deg.
	c = 17.336(6) Å	gamma = 90 deg.
Volume	1792.0(10) $Å^3$	
Z, Calculated density	4, 1.517 mg/m^3	
Absorption coefficient	0.534 mm^{-1}	

F(000)	848
Crystal size	0.33 × 0.27 × 0.05 mm
Theta range for data collection	2.35 to 27.48 deg.
Limiting indices	−18<=h<=18, −9<=k<=9, −22<=l<=22
Reflections collected / unique	13097 / 4094 [R(int) = 0.0572]
Completeness to theta = 27.48	99.7 %
Absorption correction	Multi-scan
Max. and min. transmission	0.9738 and 0.8434
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4094 / 0 / 239
Goodness-of-fit on F^2	1.160
Final R indices [I > 2sigma(I)]	R1 = 0.0524, wR2 = 0.1106
R indices (all data)	R1 = 0.0597, wR2 = 0.1146
Largest diff. peak and hole	0.401 and −0.297 e. $Å^{-3}$

Table S3. Crystal data and structure refinement for BN-TTN-C2 (CCDC 1007264).

Empirical formula	$C_{24}H_{24}BNS_4$	
Formula weight	465.49	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, *P*−1	
Unit cell dimensions	a = 9.989(2) Å	alpha = 74.02(3) deg.
	b = 11.179(2) Å	beta = 81.77(3) deg.
	c = 11.299(2) Å	gamma = 72.90(3) deg.
Volume	1156.7(4) $Å^3$	
Z, Calculated density	2, 1.337 mg/m^3	
Absorption coefficient	0.423 mm^{-1}	
F(000)	488	
Crystal size	0.29 × 0.17 × 0.17 mm	
Theta range for data collection	1.97 to 25.00 deg.	
Limiting indices	−11<=h<=11, −13<=k<=13, −13<=l<=13	
Reflections collected / unique	12860 / 4060 [R(int) = 0.0554]	
Completeness to theta = 25.00	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.6158	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4060 / 388 / 283	
Goodness-of-fit on F^2	1.106	

Final R indices [I > 2sigma(I)]	R1 = 0.0757, wR2 = 0.1986
R indices (all data)	R1 = 0.0936, wR2 = 0.2149
Largest diff. peak and hole	0.330 and −0.336 e. $Å^{-3}$

Table S4. Crystal data and structure refinement for BN-TTN-C3 (CCDC 913513).[1]

Empirical formula	$C_{28}H_{32}BNS_4$	
Formula weight	521.60	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, *P*−1	
Unit cell dimensions	a = 10.925(3) Å	alpha = 80.320(11) deg.
	b = 15.116(3) Å	beta = 83.220(12) deg.
	c = 16.752(4) Å	gamma = 75.300(9) deg.
Volume	2629.6(10) $Å^3$	
Z, Calculated density	4, 1.318 mg/m^3	
Absorption coefficient	0.380 mm^{-1}	
F(000)	1104	
Crystal size	0.38 × 0.23 × 0.04 mm	
Theta range for data collection	1.73 to 24.99 deg.	
Limiting indices	−12<=h<=12, −17<=k<=17, −19<=l<=19	
Reflections collected/unique	28928/9238 [R(int) = 0.0738]	
Completeness to theta = 24.99	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9850 and 0.8691	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9238 / 0 / 621	
Goodness-of-fit on F^2	1.288	
Final R indices [I > 2sigma(I)]	R1 = 0.0887, wR2 = 0.1458	
R indices (all data)	R1 = 0.1036, wR2 = 0.1517	
Largest diff. peak and hole	0.343 and −0.331 e. $Å^{-3}$	

Table S5. Crystal data and structure refinement for BN-TTN-C4 (CCDC 1007265).

Empirical formula	$C_{32}H_{40}BNS_4$	
Formula weight	577.70	
Temperature	100.00(10) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, *P*−1	
Unit cell dimensions	a = 7.5956(3) Å	alpha = 86.994(4) deg.
	b = 10.7442(5) Å	beta = 83.691(4) deg.

	c = 18.2411(8) Å gamma = 82.603(4) deg.
Volume	1466.19(12) $Å^3$
Z, Calculated density	2, 1.309 mg/m^3
Absorption coefficient	0.347 mm^{-1}
F(000)	616.0
Crystal size	0.20 × 0.10 × 0.10 mm
Theta range for data collection	5.66 to 52.04 deg.
Limiting indices	−9<=h<=9, −12<=k<=13, −22<=l<=22
Reflections collected / unique	12662 / 5625[R(int) = 0.0323]
Completeness to theta = 25.00	99.9 %
Absorption correction	spherical harmonics
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5625 / 0 / 347
Goodness-of-fit on F^2	1.049
Final R indices [I > 2sigma(I)]	R1 = 0.0342, wR2 = 0.0820
R indices (all data)	R1 = 0.0416, wR2 = 0.0872
Largest diff. peak and hole	0.37 and −0.34 e. $Å^{-3}$

Table S6. Crystal data and structure refinement for BN-TTN-C5 (CCDC 1007266).

Empirical formula	$C_{36}H_{48}BNS_4$
Formula weight	633.80
Temperature	133(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, *P*−1
Unit cell dimensions	a = 8.4695(17) Å alpha = 99.16(3) deg.
	b = 13.030(3) Å beta = 96.39(3) deg.
	c = 16.200(3) Å gamma = 104.33(3) deg.
Volume	1688.7(6) $Å^3$
Z, Calculated density	2, 1.246 mg/m^3
Absorption coefficient	0.308 mm^{-1}
F(000)	680
Crystal size	0.26 × 0.18 × 0.12 mm
Theta range for data collection	1.88 to 27.87 deg.
Limiting indices	−11<=h<=10, −17<=k<=17, −14<=l<=21
Reflections collected / unique	16894 / 7903 [R(int) = 0.0299]
Completeness to theta = 27.87	98.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9640 and 0.9243

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7903 / 0 / 383
Goodness-of-fit on F^2	1.062
Final R indices [I > 2sigma(I)]	R1 = 0.0363, wR2 = 0.0914
R indices (all data)	R1 = 0.0461, wR2 = 0.0964
Largest diff. peak and hole	0.380 and −0.484 e. $Å^{-3}$

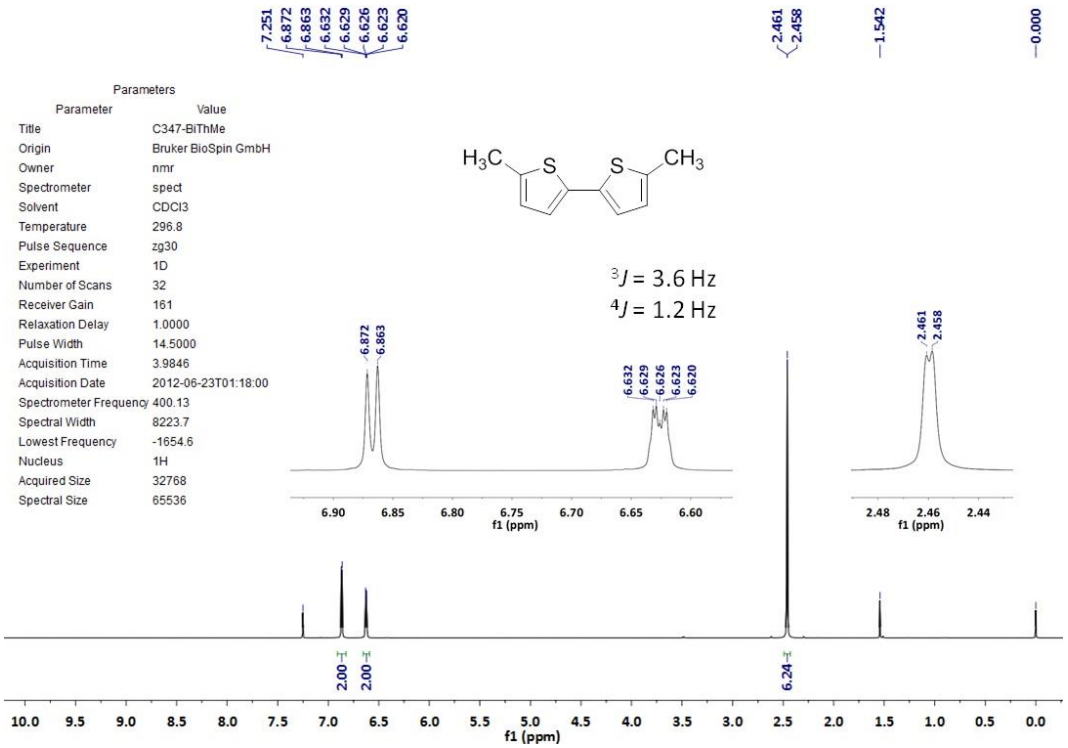
Table S7. Crystal data and structure refinement for BN-TTN-C6 (CCDC 913514).[1]

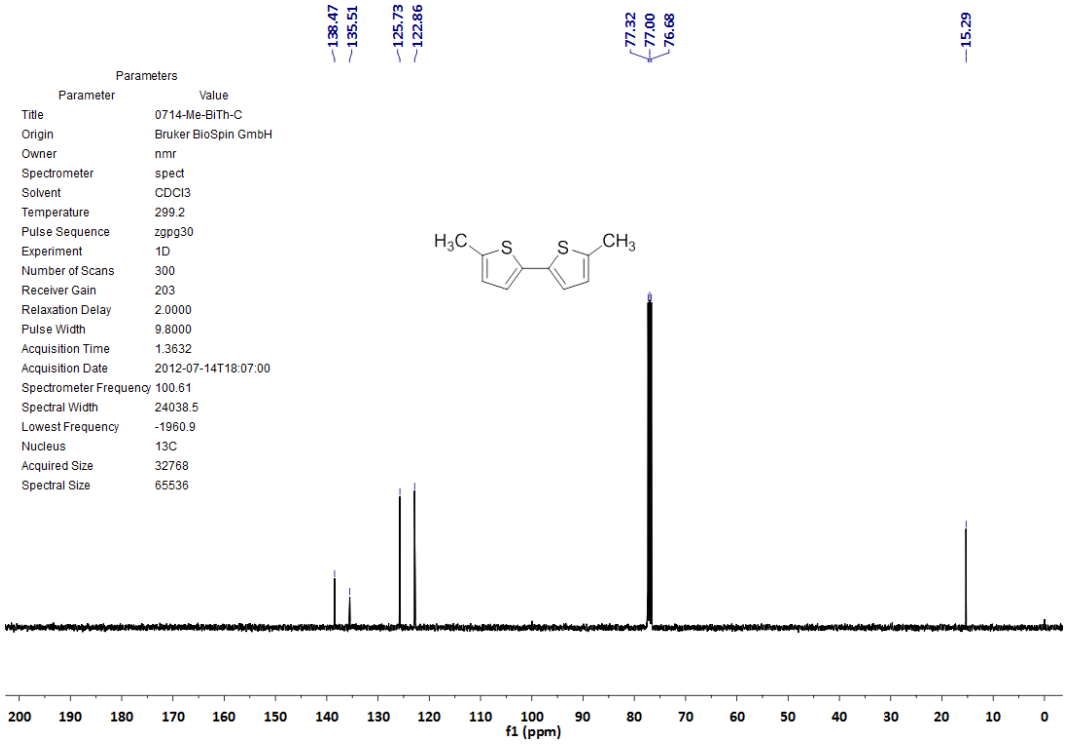
Empirical formula	$C_{40}H_{56}BNS_4$
Formula weight	689.91
Temperature	113(2) K
Wavelength	0.71075 Å
Crystal system, space group	Triclinic, *P*−1
Unit cell dimensions	a = 9.2070(12) Å alpha = 77.180(11) deg.
	b = 9.6380(13) Å beta = 85.610(12) deg.
	c = 11.6280(19) Å gamma = 71.030(10) deg.
Volume	951.5(2) $Å^3$
Z, Calculated density	1, 1.204 mg/m^3
Absorption coefficient	0.278 mm^{-1}
F(000)	372
Crystal size	0.32 × 0.24 × 0.22 mm
Theta range for data collection	1.80 to 27.95 deg.
Limiting indices	−12<=h<=12, −12<=k<=12, −15<=l<=15
Reflections collected/unique	12199/4541 [R(int) = 0.0455]
Completeness to theta = 27.95	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9413 and 0.9162
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4541 / 0 / 211
Goodness-of-fit on F^2	0.928
Final R indices [I > 2sigma(I)]	R1 = 0.0319, wR2 = 0.0709
R indices (all data)	R1 = 0.0478, wR2 = 0.0743
Extinction coefficient	0.0077(15)
Largest diff. peak and hole	0.255 and −0.232 e. $Å^{-3}$

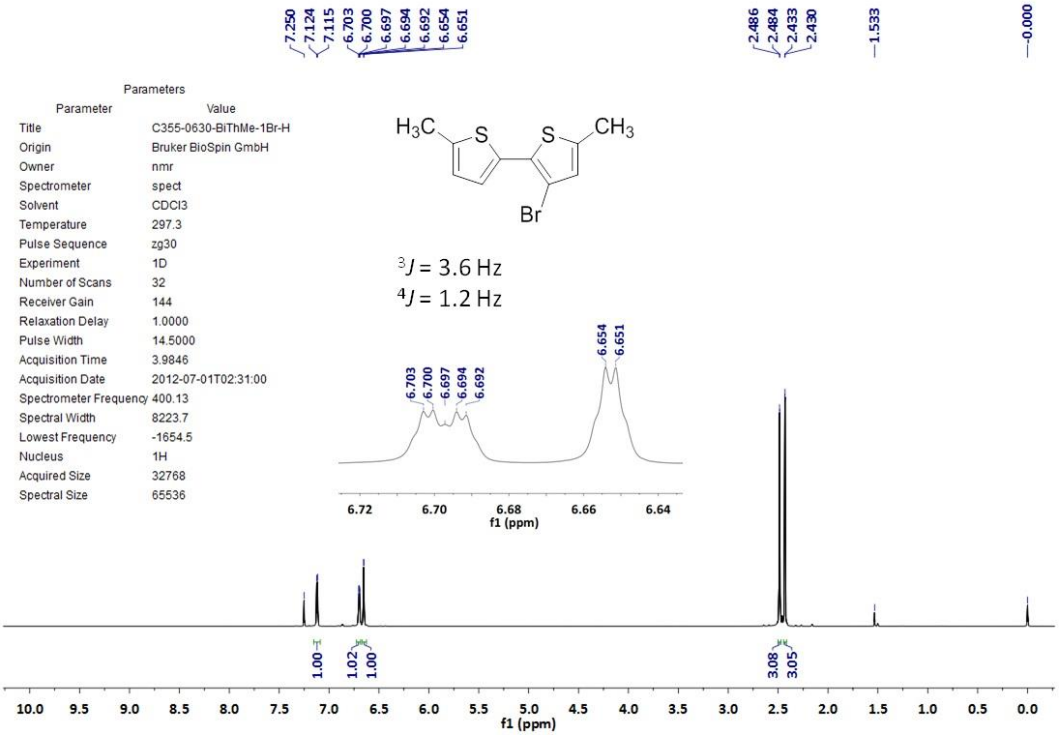
7. Reference

1. X.-Y. Wang, H.-R. Lin, T. Lei, D.-C. Yang, F.-D. Zhuang, J.-Y. Wang, S.-C. Yuan, J. Pei, *Angew. Chem. Int. Ed.* **2013**, *52*, 3117-3120.

8. NMR Spectra



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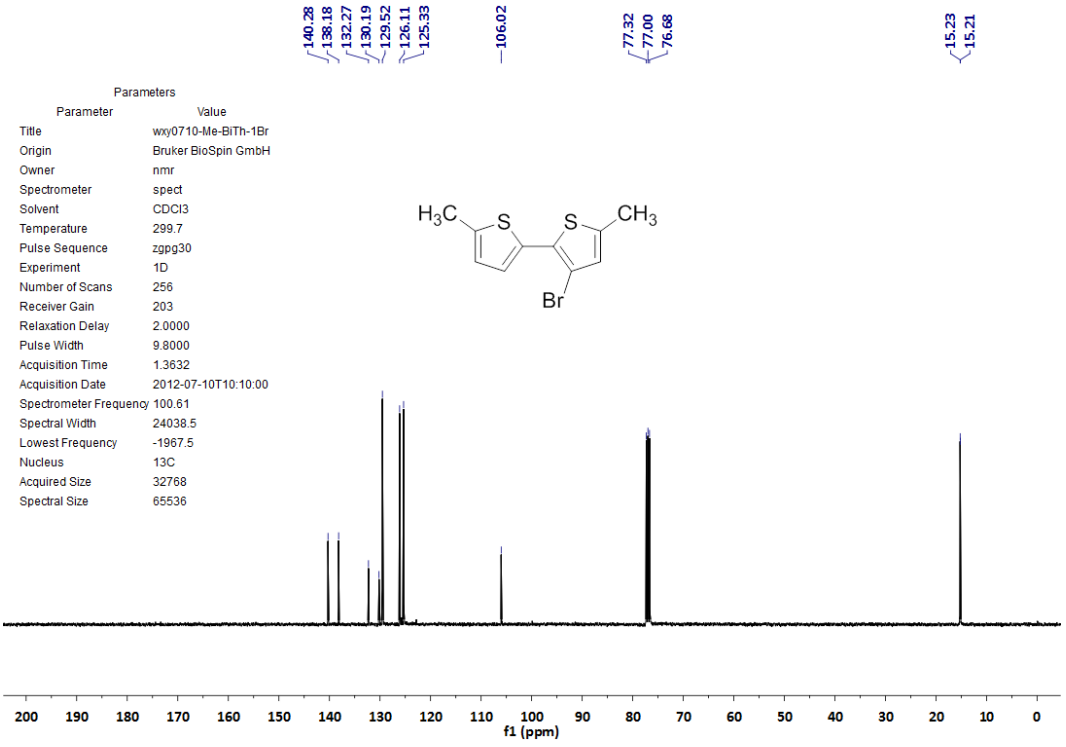
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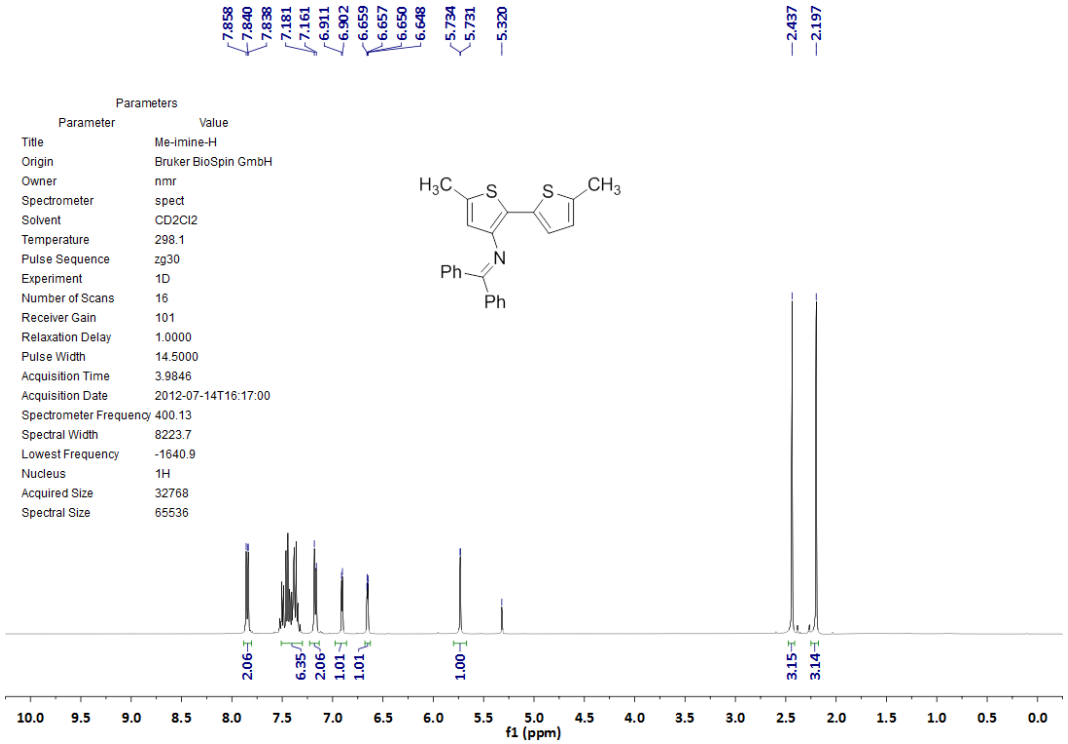
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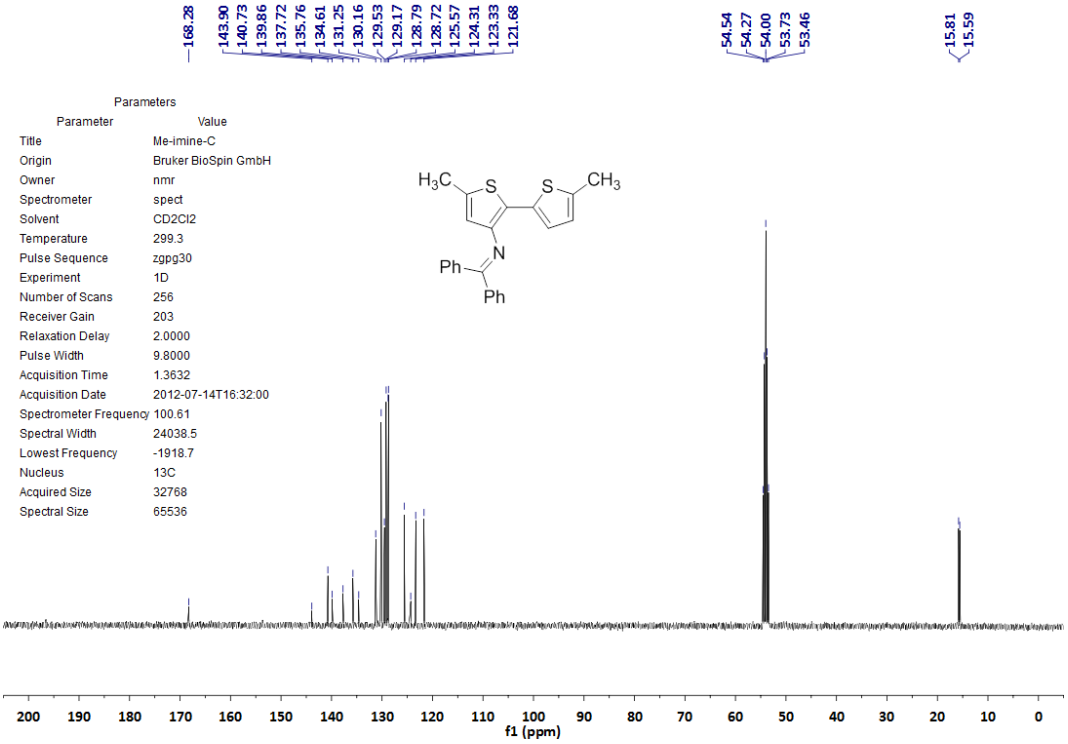
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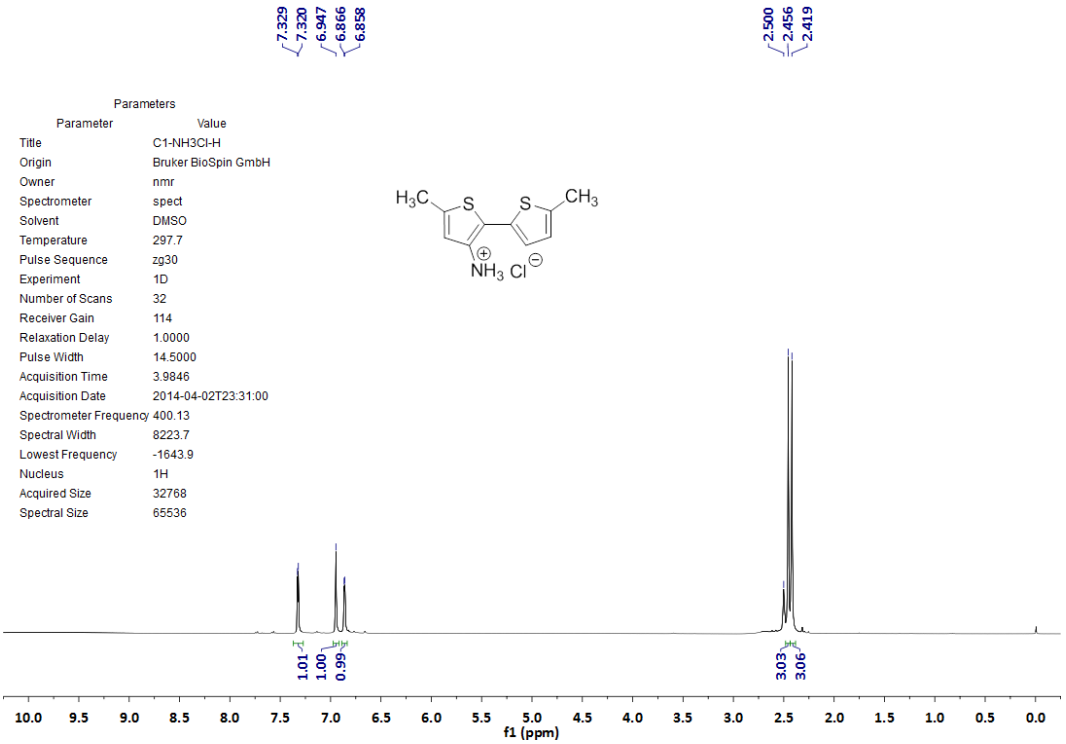
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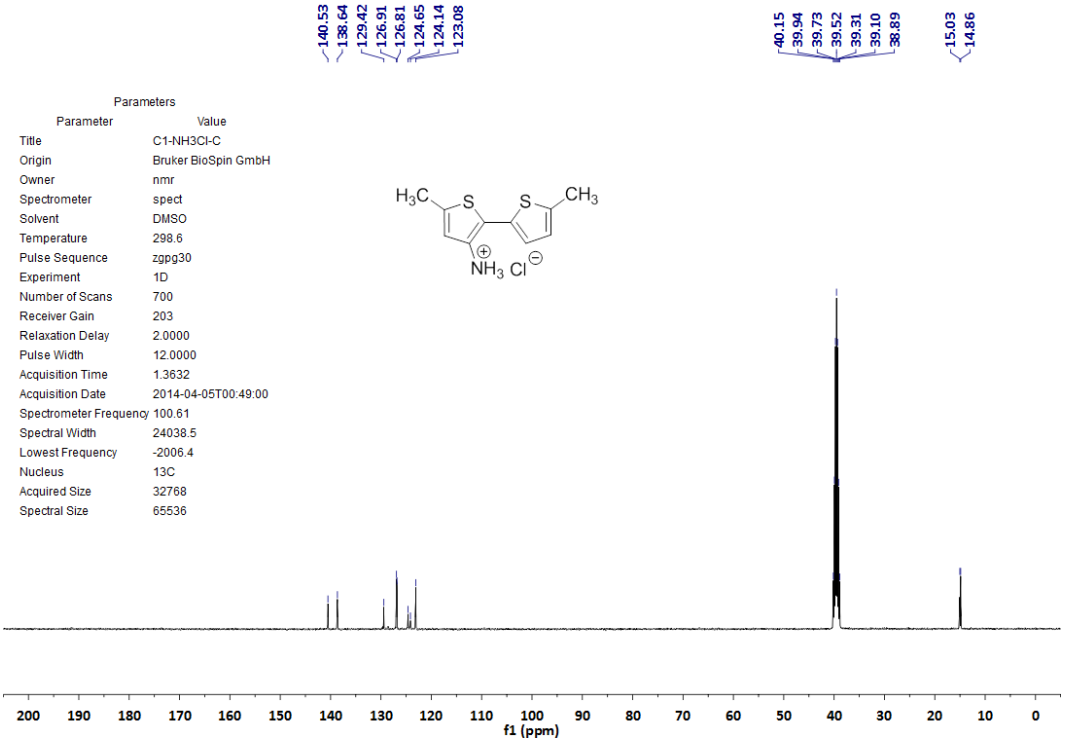
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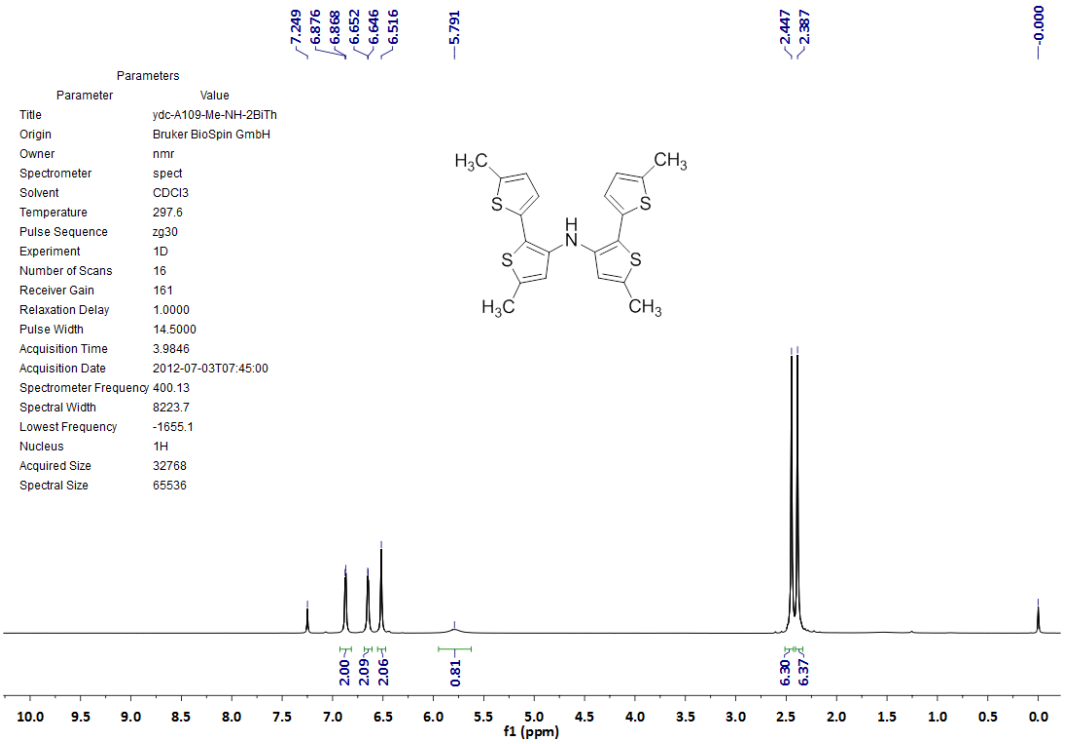
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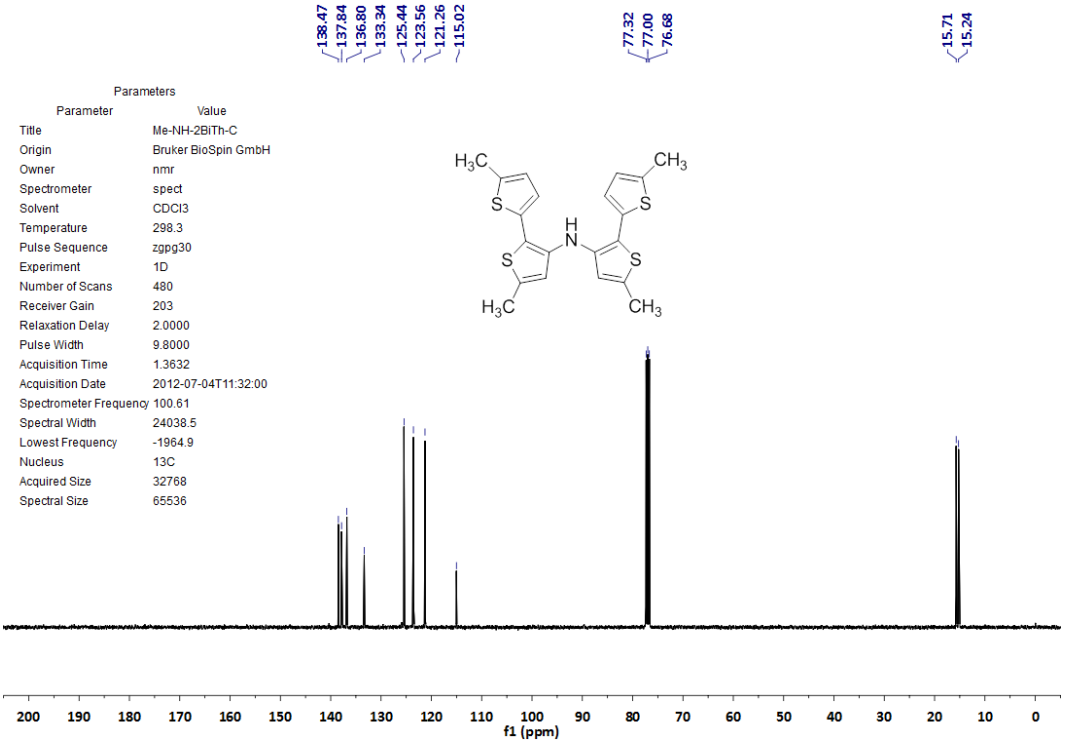
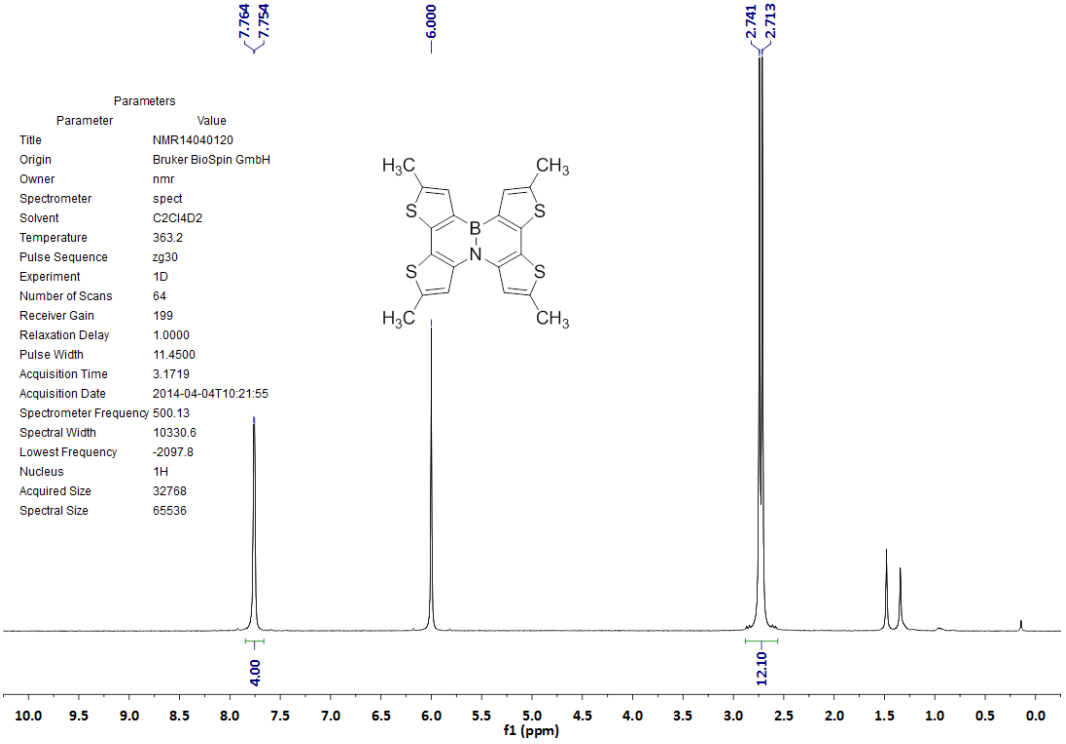
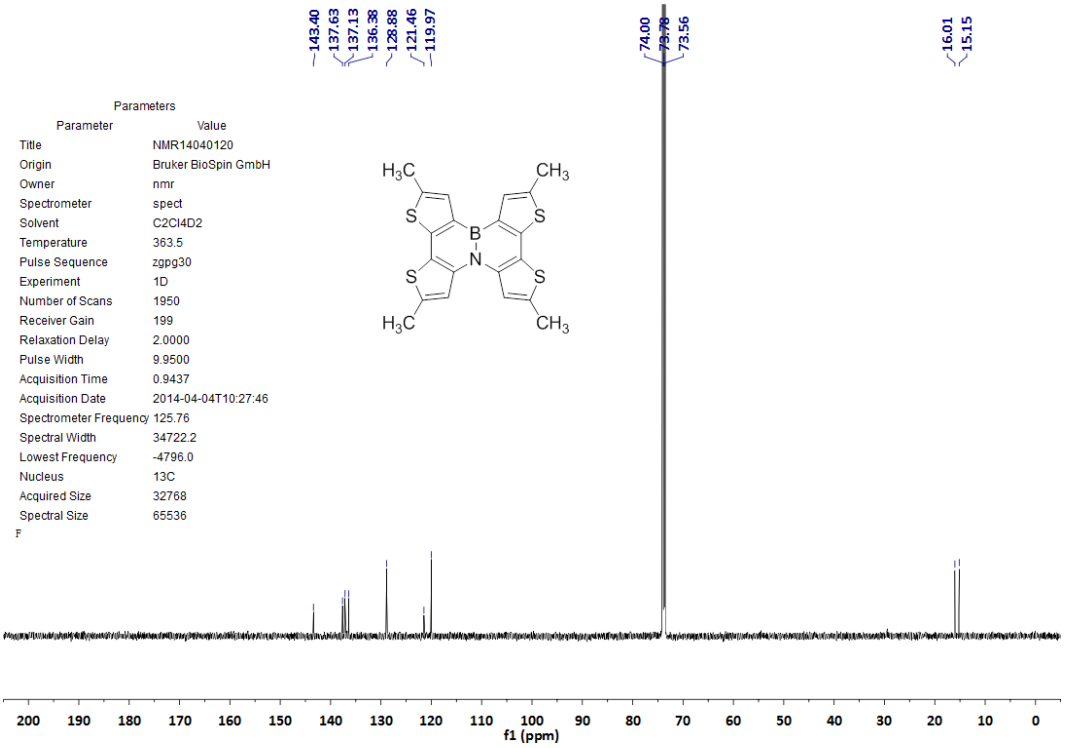
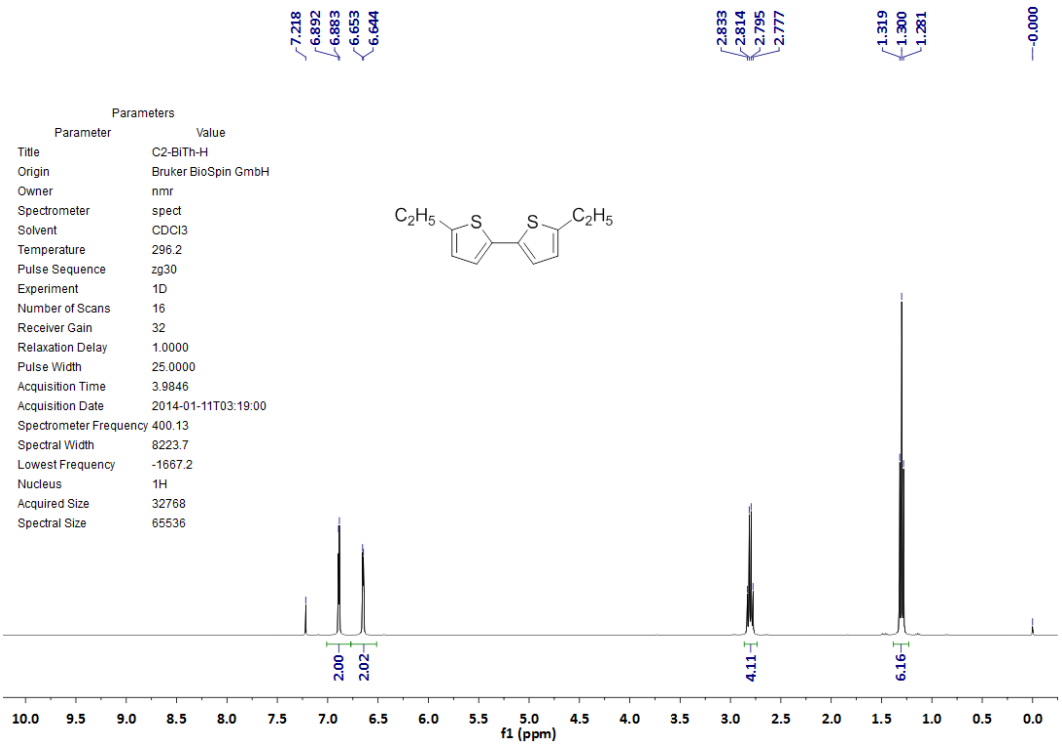
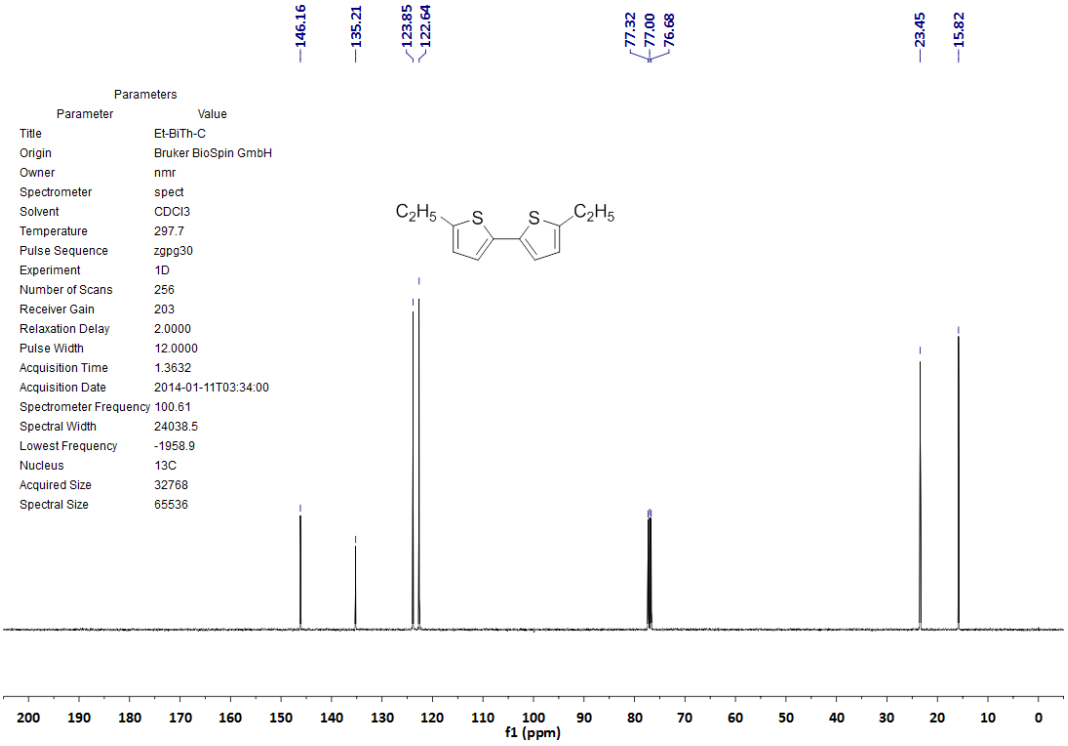
6.30
6.37
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

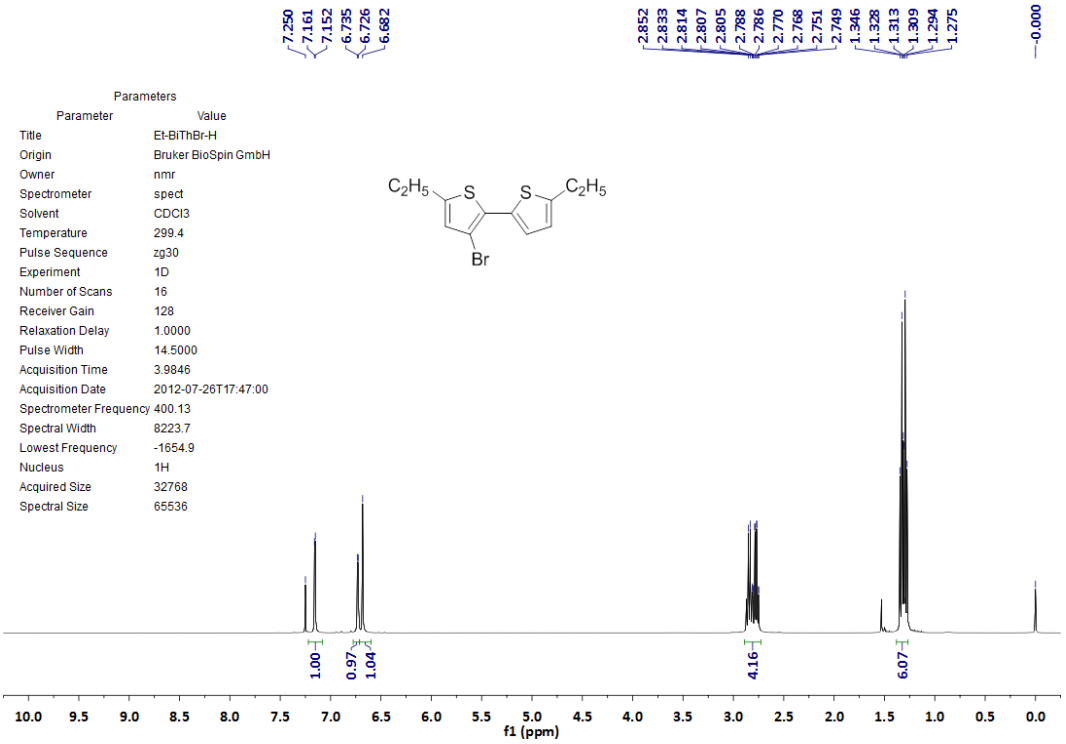

138.47
137.84
136.80
133.34
125.44
123.56
121.26
115.02
77.32
77.00
76.68
15.71
15.24
Parameters
Parameter Value
Title Me-NH-2BiTh-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.3
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 480
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-07-04T11:32:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1964.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
H3C
CH3
S
H
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

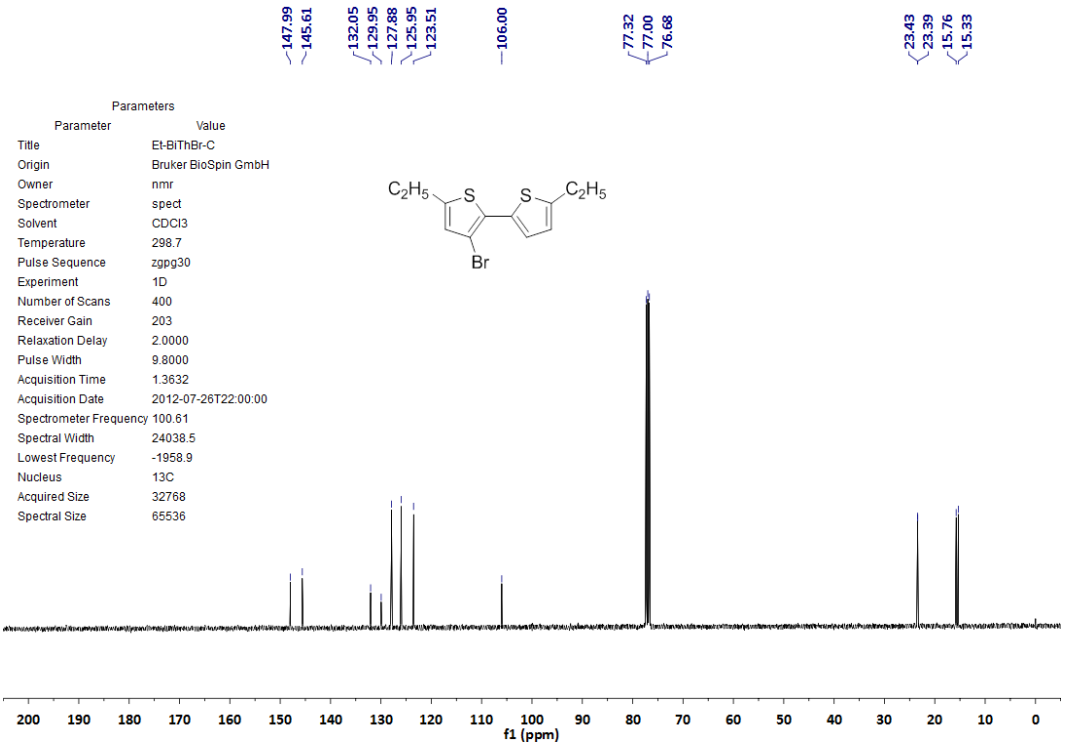

7.764
7.754
6.000
2.741
2.713
Parameters
Parameter Value
Title NMR14040120
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent C2Cl4D2
Temperature 363.2
Pulse Sequence zg30
Experiment 1D
Number of Scans 64
Receiver Gain 199
Relaxation Delay 1.0000
Pulse Width 11.4500
Acquisition Time 3.1719
Acquisition Date 2014-04-04T10:21:55
Spectrometer Frequency 500.13
Spectral Width 10330.6
Lowest Frequency -2097.8
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
4.00
12.10
10.0 9.5 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 0.0
f1 (ppm)

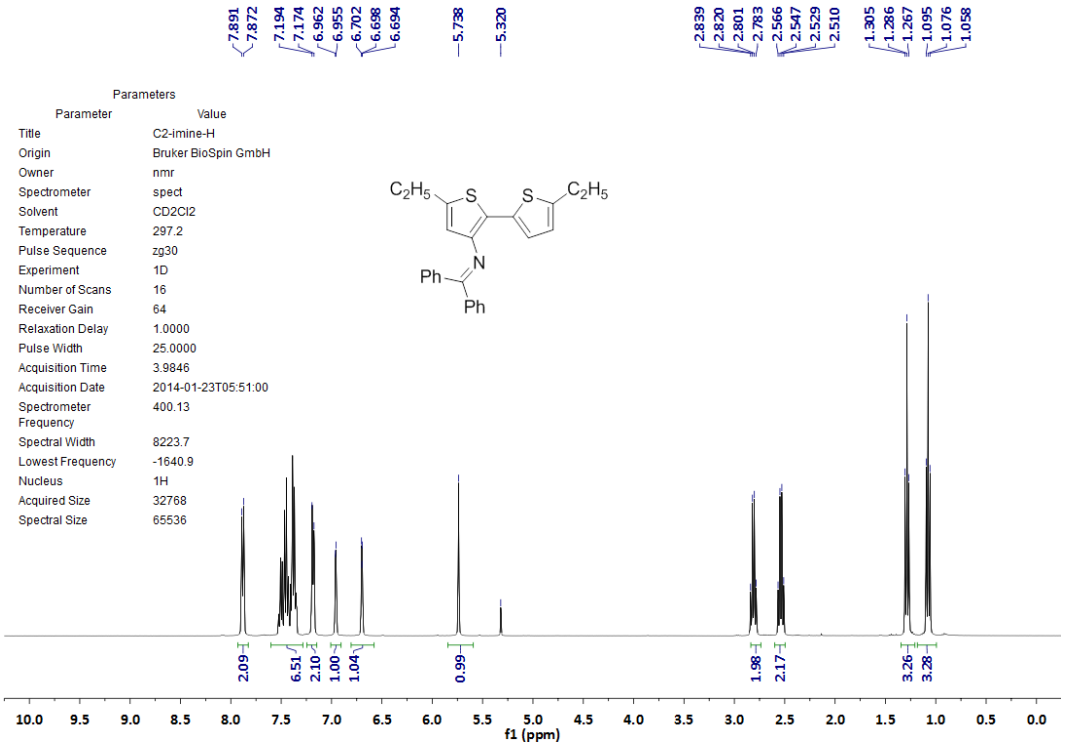

143.40
137.63
137.13
136.38
128.88
121.46
119.97
74.00
73.78
73.56
16.01
15.15
Parameters
Parameter Value
Title NMR14040120
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent C2Cl4D2
Temperature 363.5
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 1950
Receiver Gain 199
Relaxation Delay 2.0000
Pulse Width 9.9500
Acquisition Time 0.9437
Acquisition Date 2014-04-04T10:27:46
Spectrometer Frequency 125.76
Spectral Width 34722.2
Lowest Frequency -4796.0
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

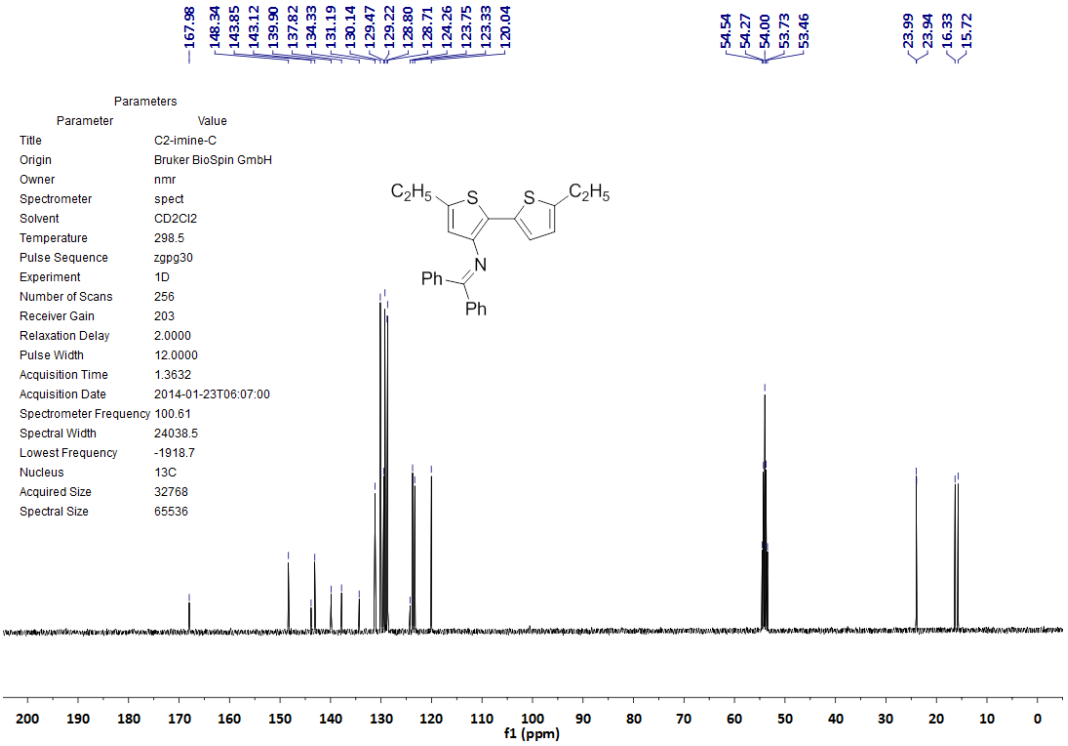

7.218
6.892
6.883
6.653
6.644
2.833
2.814
2.795
2.777
1.319
1.300
1.281
0.000
Parameters
Parameter Value
Title C2-BiTh-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 296.2
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 32
Relaxation Delay 1.0000
Pulse Width 25.0000
Acquisition Time 3.9846
Acquisition Date 2014-01-11T03:19:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1667.2
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C2H5
S
S
C2H5
2.00
2.02
4.11
6.16
10.0 9.5 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 0.0
f1 (ppm)

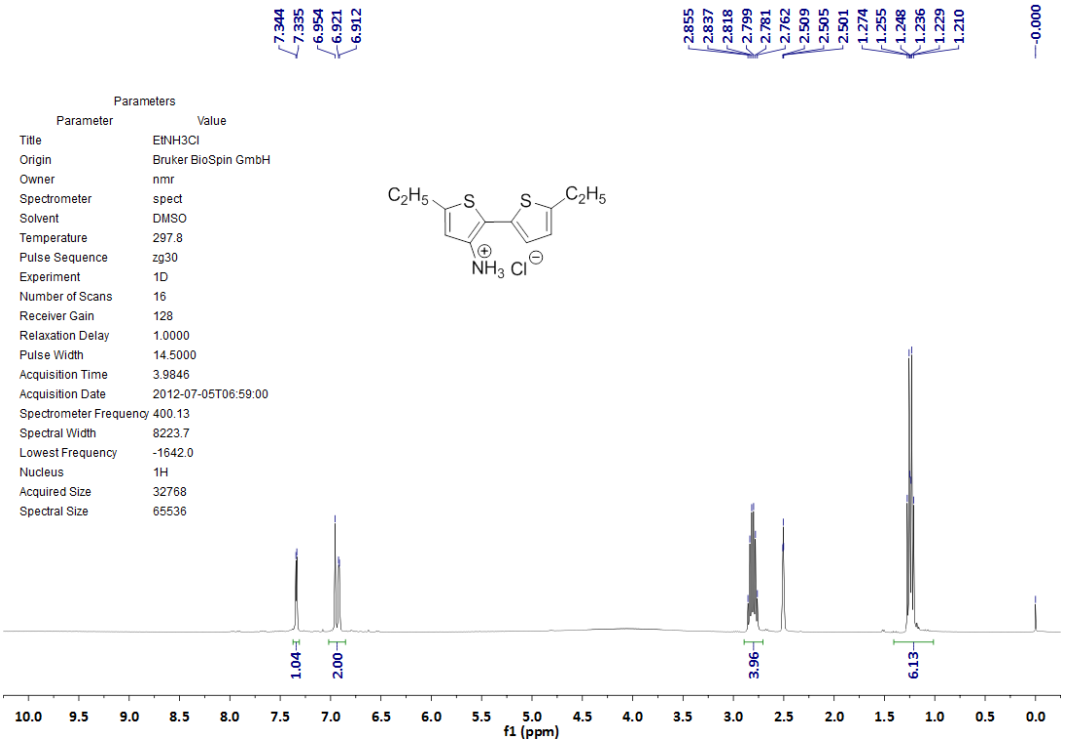

146.16
135.21
123.85
122.64
77.32
77.00
76.68
23.45
15.82
Parameters
Parameter Value
Title Et-BiTh-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 297.7
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 256
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 12.0000
Acquisition Time 1.3632
Acquisition Date 2014-01-11T03:34:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C2H5
S
S
C2H5
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

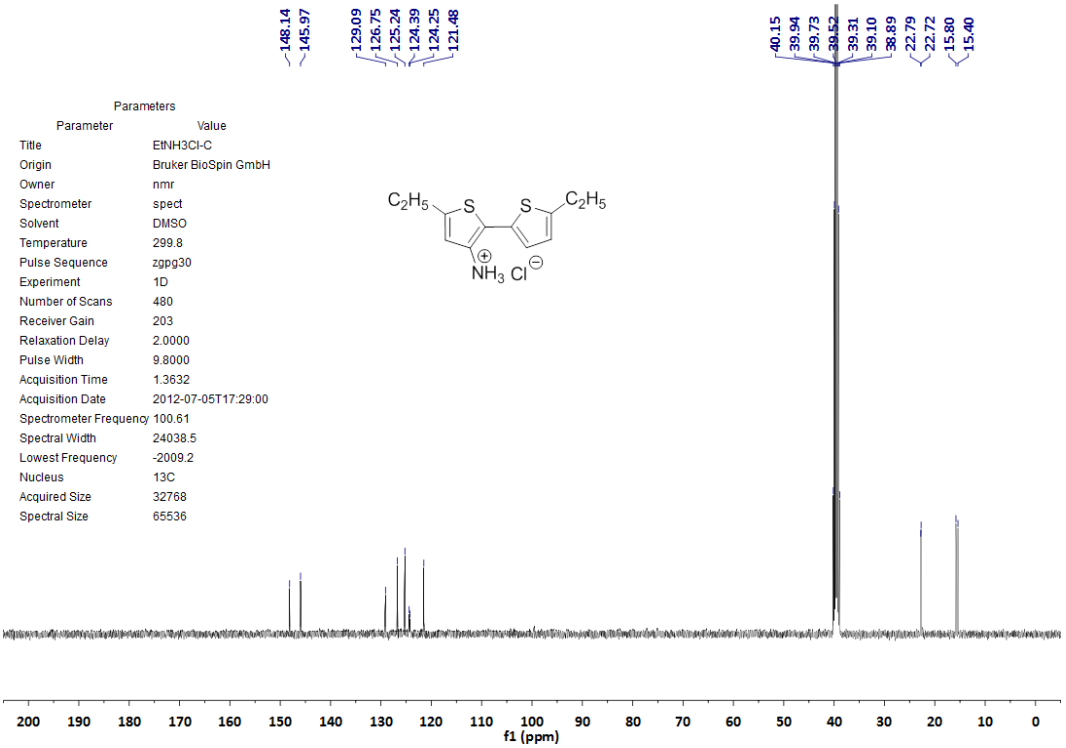

7.250
7.161
7.152
6.735
6.726
6.682
2.852
2.833
2.814
2.807
2.805
2.788
2.786
2.770
2.768
2.751
2.749
1.346
1.328
1.313
1.309
1.294
1.275
0.000
Parameters
Parameter Value
Title Et-BiThBr-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 299.4
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 128
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-07-26T17:47:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1654.9
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C2H5
S
S
C2H5
Br
1.00
0.97
1.04
4.16
6.07
10.0 9.5 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 0.0
f1 (ppm)

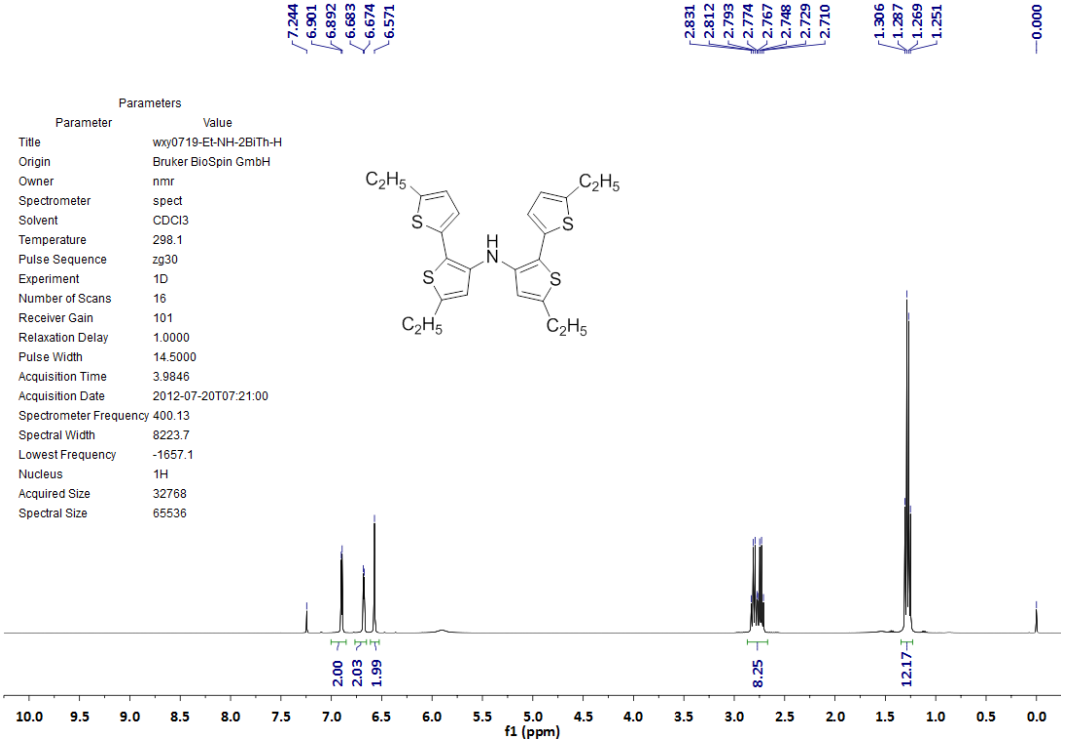

147.99
145.61
132.05
129.95
127.88
125.95
123.51
106.00
77.32
77.00
76.68
23.43
23.39
15.76
15.33
Parameters
Parameter Value
Title Et-BiThBr-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.7
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 400
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-07-26T22:00:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C2H5
S
S
C2H5
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

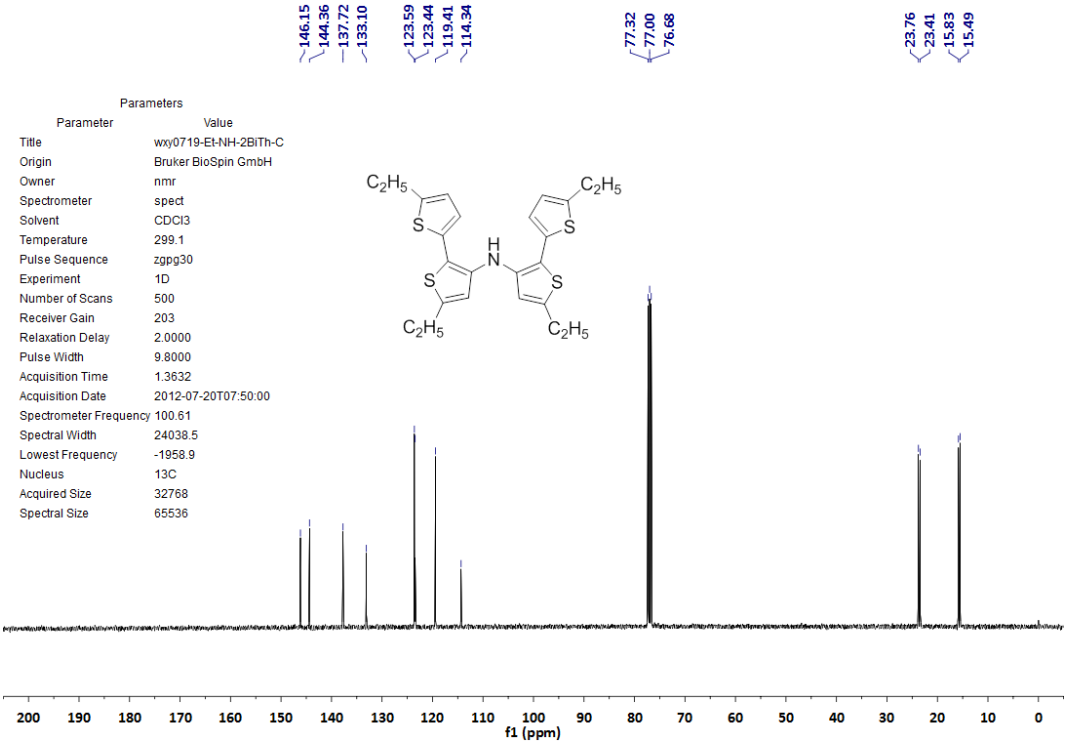

7.891
7.872
7.194
7.174
6.962
6.955
6.702
6.698
6.694
5.738
5.320
2.839
2.820
2.801
2.783
2.566
2.547
2.529
2.510
1.305
1.286
1.267
1.095
1.076
1.058
Parameters
Parameter Value
Title C2-imine-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CD2Cl2
Temperature 297.2
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 64
Relaxation Delay 1.0000
Pulse Width 25.0000
Acquisition Time 3.9846
Acquisition Date 2014-01-23T05:51:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1640.9
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C2H5
S
S
C2H5
N
Ph
Ph
2.09
6.51
2.10
1.00
1.04
0.99
1.98
2.17
3.26
3.28
10.0 9.5 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 0.0
f1 (ppm)

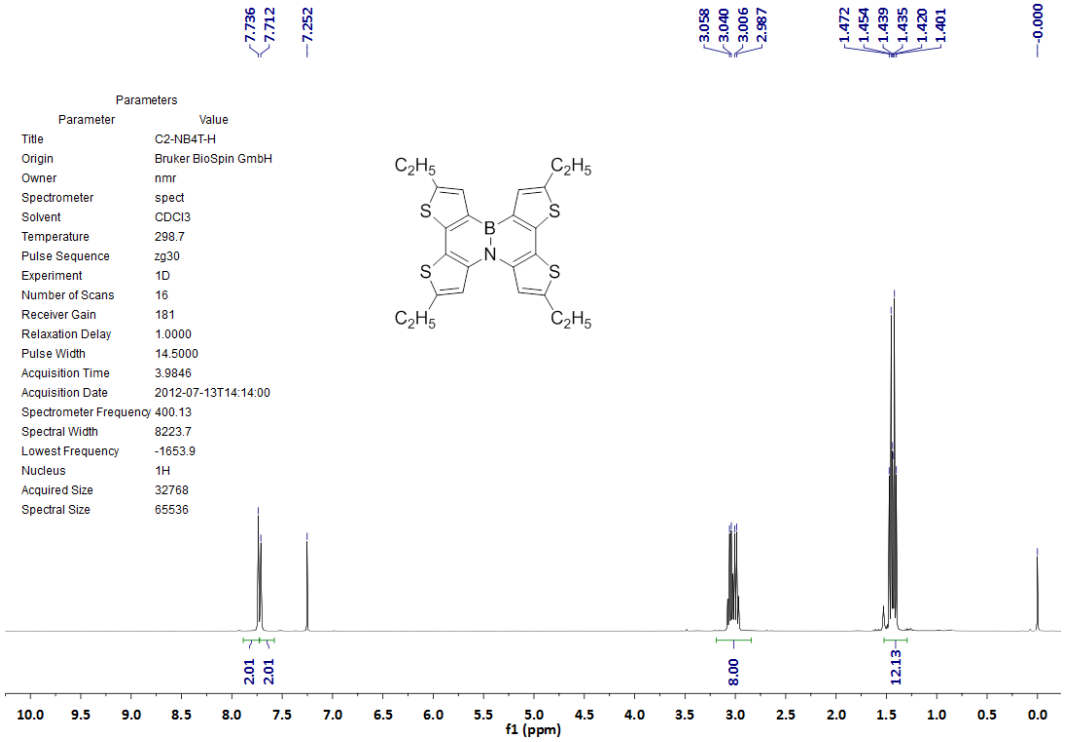

167.98
148.34
143.85
143.12
139.90
137.82
134.33
131.19
130.14
129.47
129.22
128.80
128.71
124.26
123.75
123.33
120.04
54.54
54.27
54.00
53.73
53.46
23.99
23.94
16.33
15.72
Parameters
Parameter Value
Title C2-imine-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CD2Cl2
Temperature 298.5
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 256
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 12.0000
Acquisition Time 1.3632
Acquisition Date 2014-01-23T06:07:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1918.7
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C2H5
S
S
C2H5
N
Ph
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

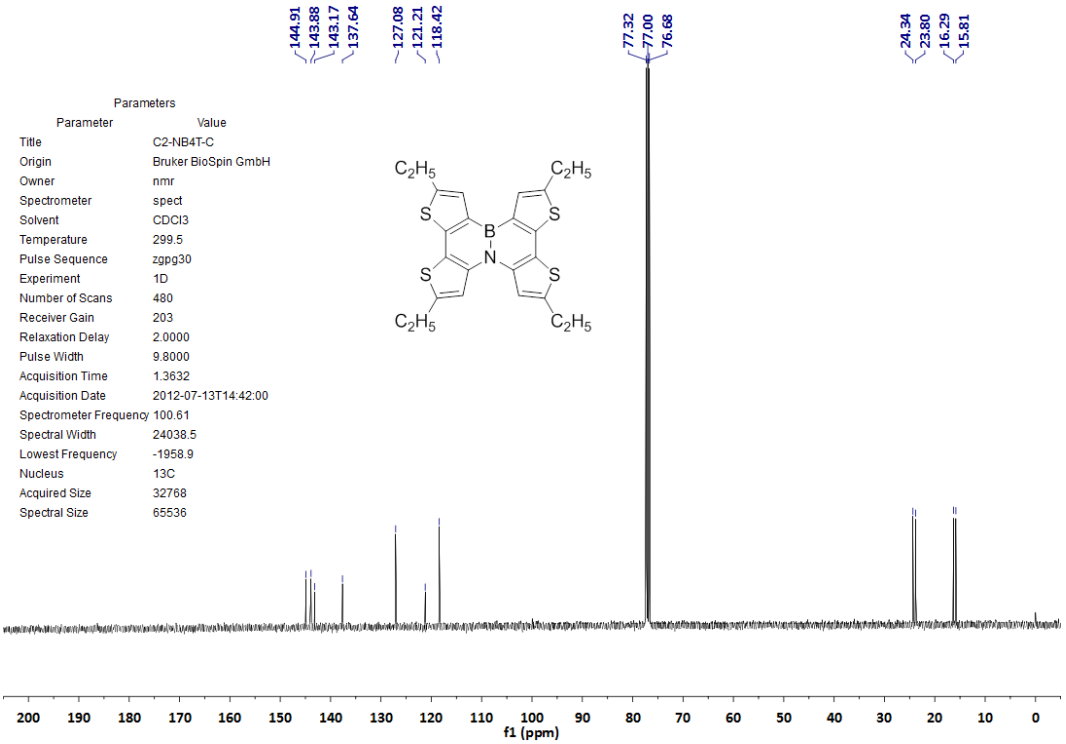

7.344
7.335
6.954
6.921
6.912
2.855
2.837
2.818
2.799
2.781
2.762
2.509
2.505
2.501
1.274
1.255
1.248
1.236
1.229
1.210
0.000
Parameters
Parameter Value
Title EtNH3Cl
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent DMSO
Temperature 297.8
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 128
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-07-05T06:59:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1642.0
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C2H5
S
S
C2H5
NH3 Cl
1.04
2.00
3.96
6.13
10.0 9.5 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 0.0
f1 (ppm)

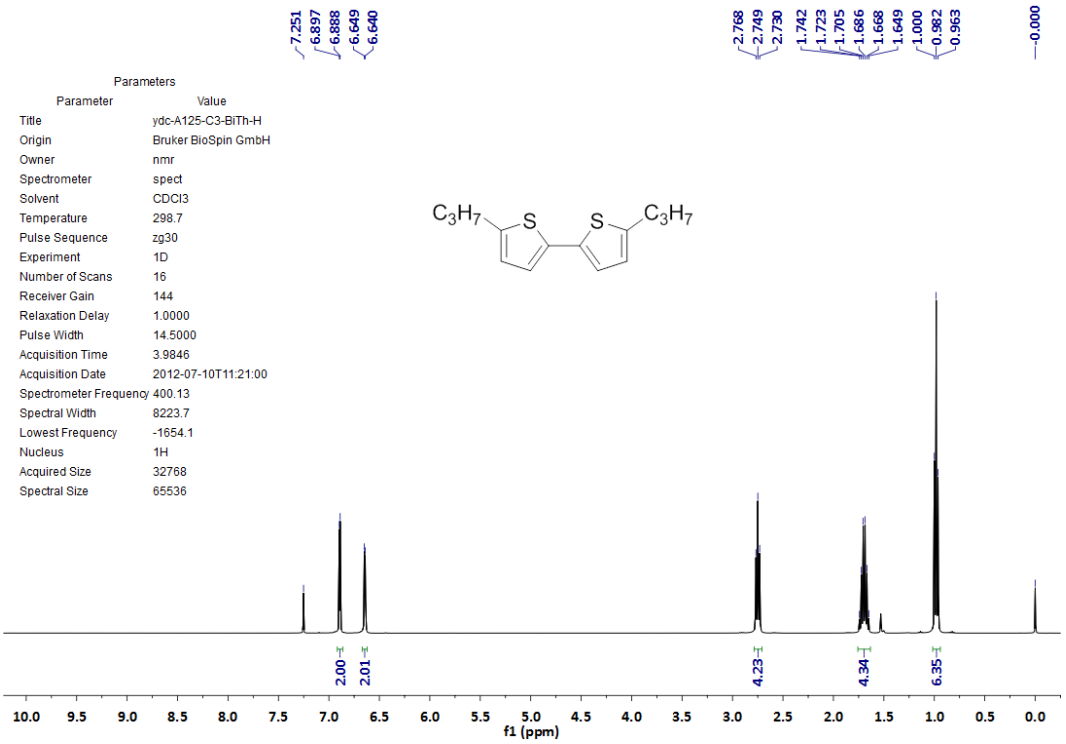

148.14
145.97
129.09
126.75
125.24
124.39
124.25
121.48
40.15
39.94
39.73
39.52
39.31
39.10
38.89
22.79
22.72
15.80
15.40
Parameters
Parameter Value
Title EtNH3Cl-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent DMSO
Temperature 299.8
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 480
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-07-05T17:29:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -2009.2
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C2H5
S
S
C2H5
NH3 Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

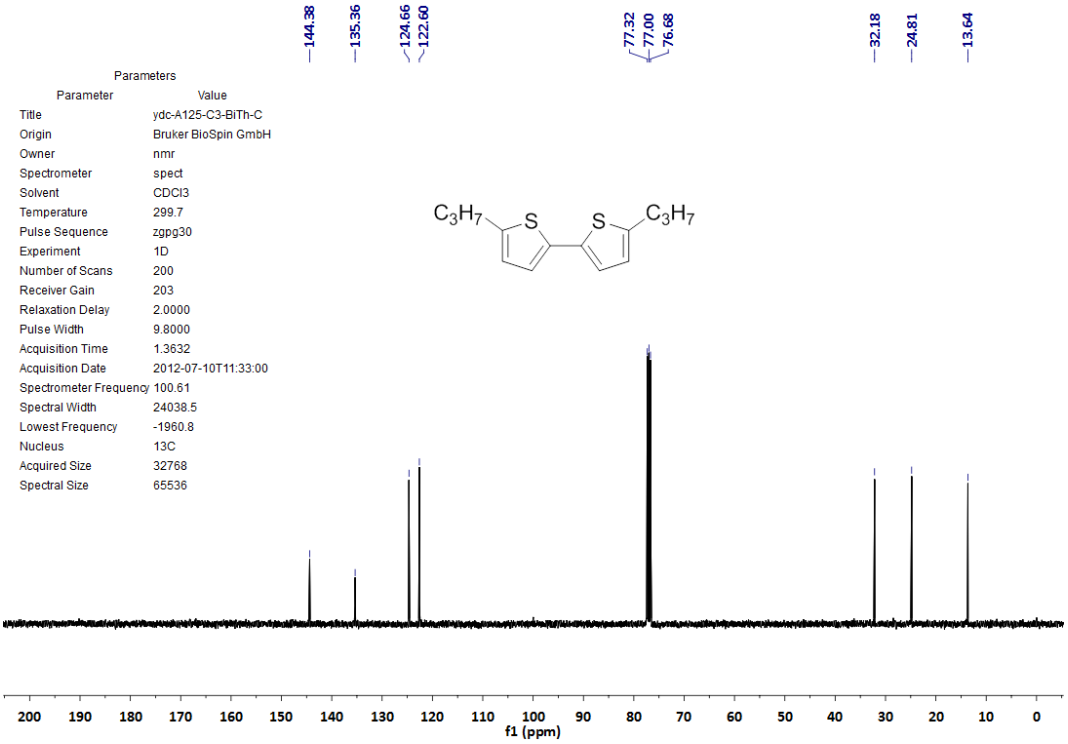

7.244
6.901
6.892
6.683
6.674
6.571
2.831
2.812
2.793
2.774
2.767
2.748
2.729
2.710
1.306
1.287
1.269
1.251
0.000
Parameters
Parameter Value
Title wxy0719-Et-NH-2BiTh-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.1
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 101
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-07-20T07:21:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1657.1
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
2.00
2.03
1.99
8.25
12.17
10.0 9.5 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 0.0
f1 (ppm)

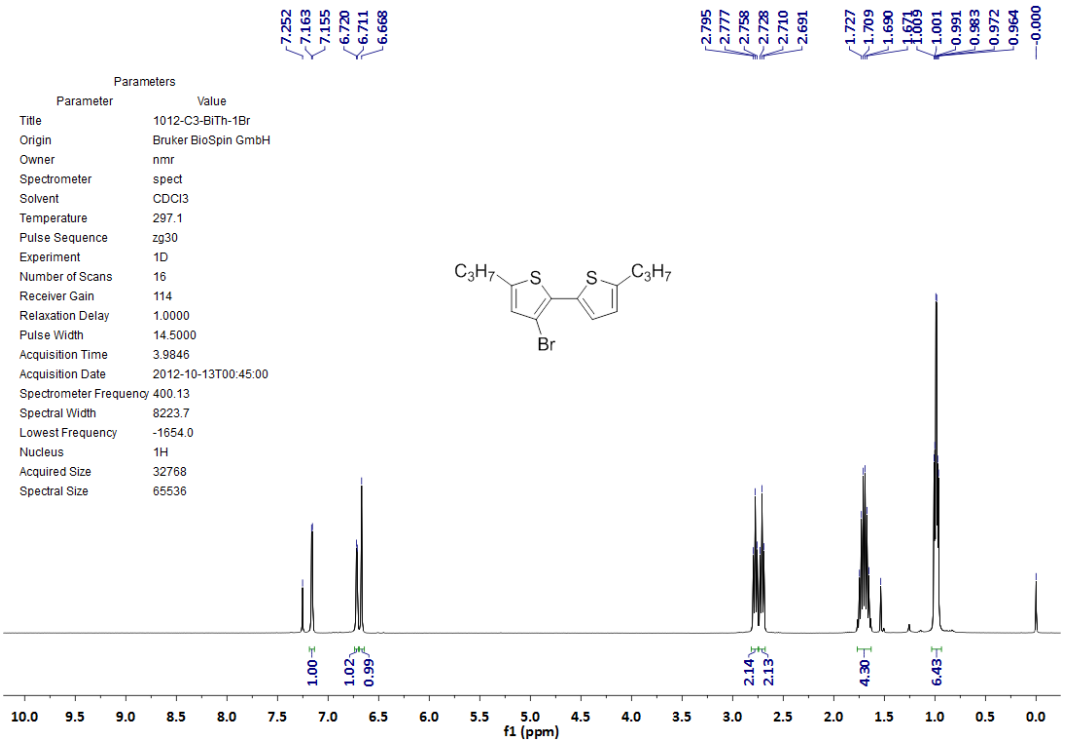

146.15
144.36
137.72
133.10
123.59
123.44
119.41
114.34
77.32
77.00
76.68
23.76
23.41
15.83
15.49
Parameters
Parameter Value
Title wxy0719-Et-NH-2BiTh-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 299.1
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 500
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-07-20T07:50:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

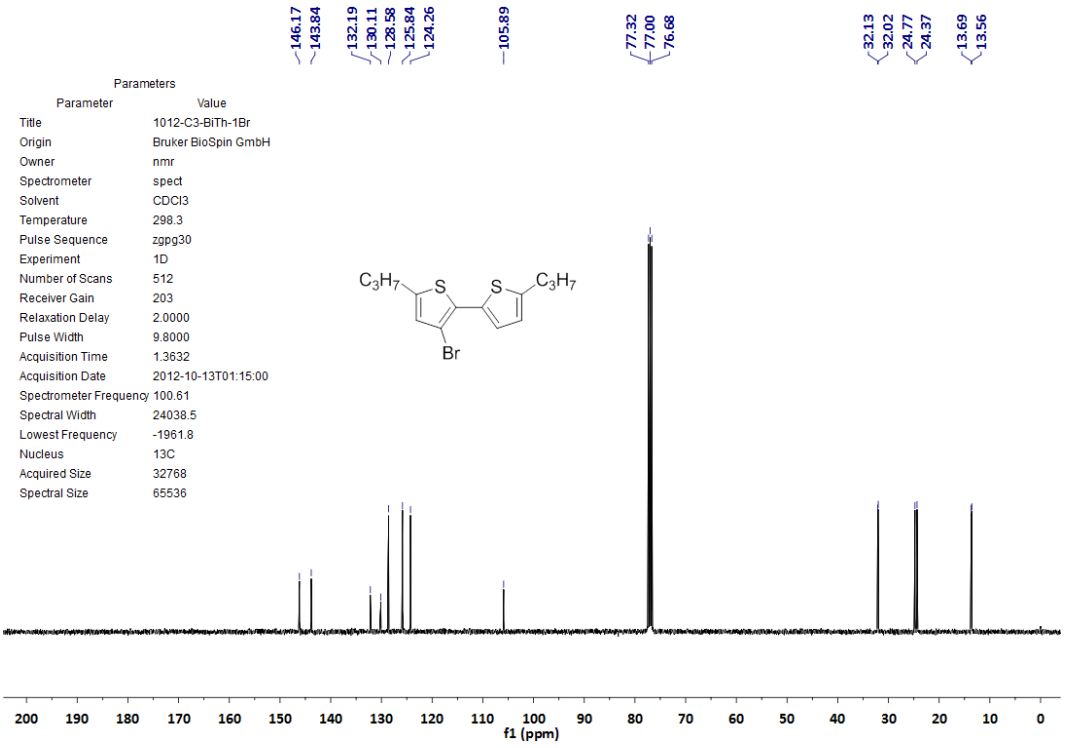

7.736
7.712
7.252
3.058
3.040
3.006
2.987
1.472
1.454
1.439
1.435
1.420
1.401
-0.000
Parameters
Parameter Value
Title C2-NB4T-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.7
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 181
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-07-13T14:14:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1653.9
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
2.01
2.01
8.00
12.13
10.0 9.5 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 0.0
f1 (ppm)

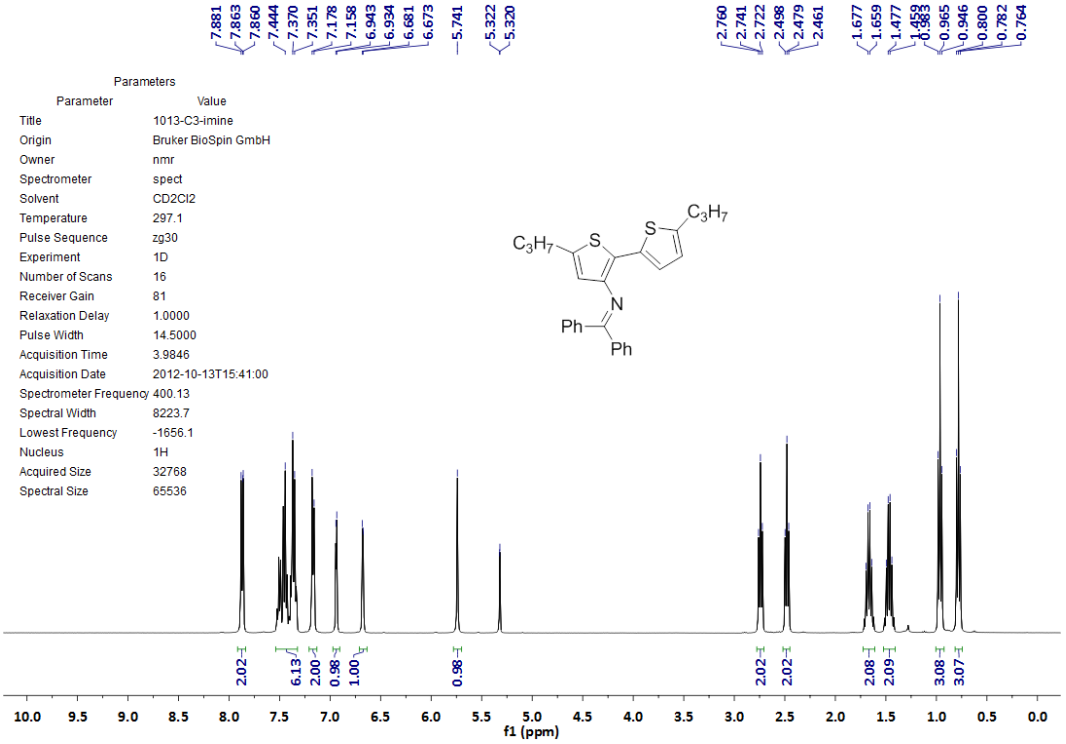

144.91
143.88
143.17
137.64
127.08
121.21
118.42
77.32
77.00
76.68
24.34
23.80
16.29
15.81
Parameters
Parameter Value
Title C2-NB4T-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 299.5
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 480
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-07-13T14:42:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

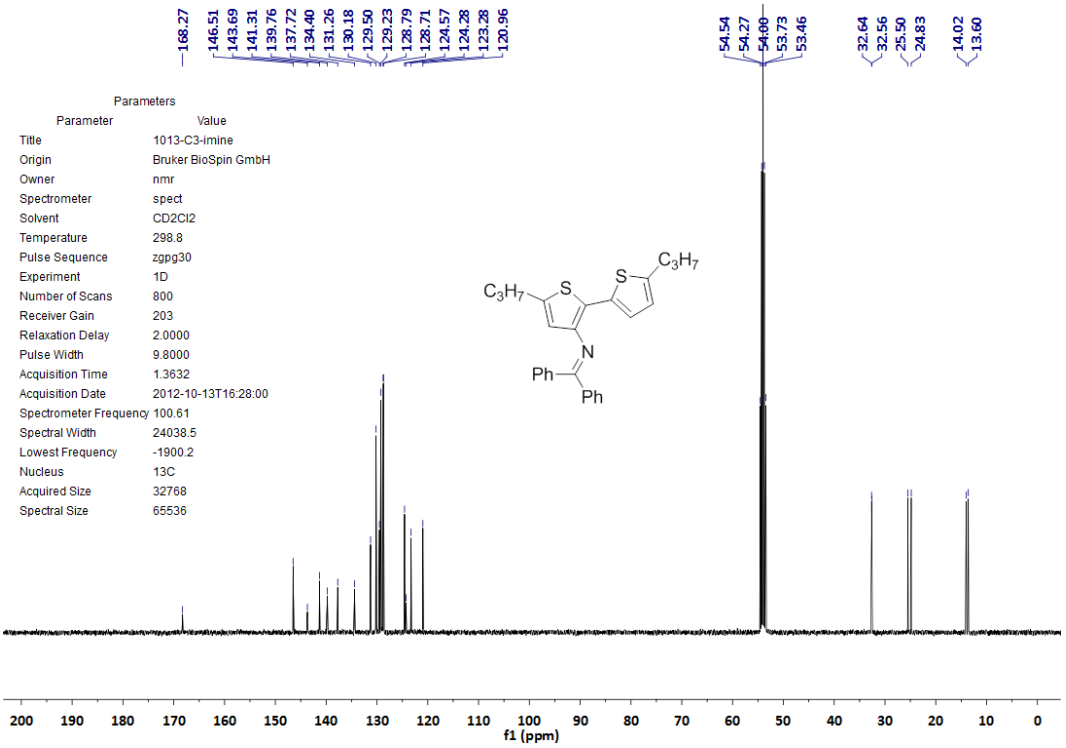

7.251
6.897
6.888
6.649
6.640
2.768
2.749
2.730
1.742
1.723
1.705
1.686
1.668
1.649
1.000
0.982
0.963
-0.000
Parameters
Parameter Value
Title ydc-A125-C3-BiTh-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.7
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 144
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-07-10T11:21:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1654.1
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C3H7
S
S
C3H7
2.00
2.01
4.23
4.34
6.35
10.0 9.5 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 0.0
f1 (ppm)

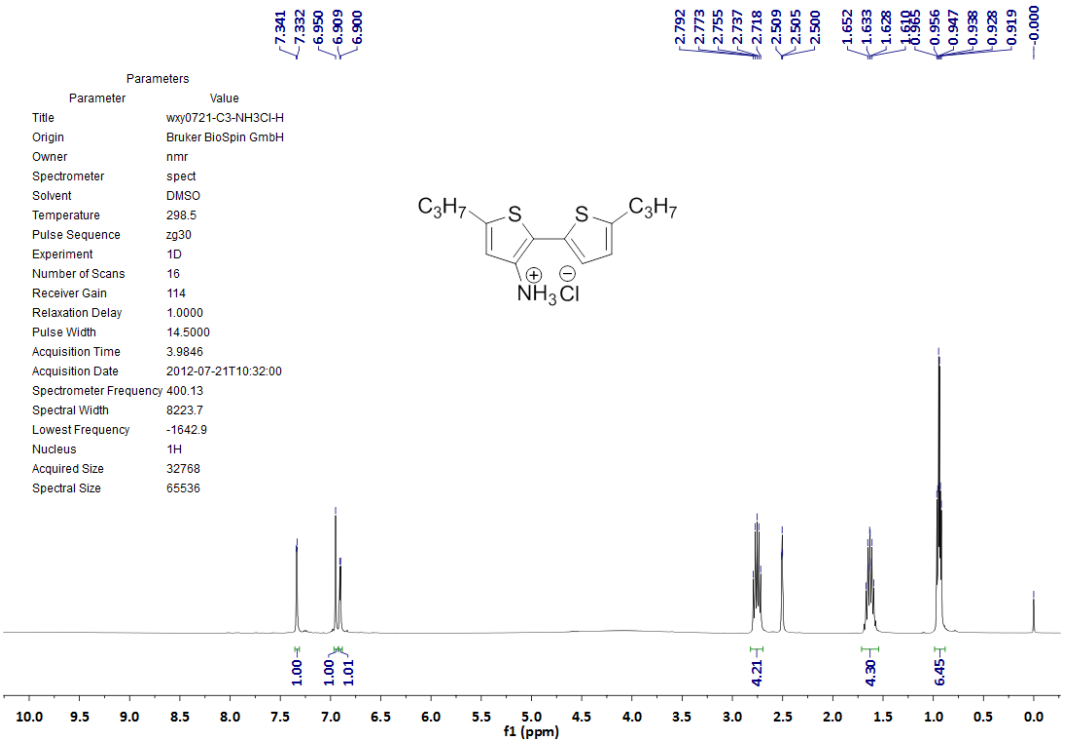

144.38
135.36
124.66
122.60
77.32
77.00
76.68
32.18
24.81
13.64
Parameters
Parameter Value
Title ydc-A125-C3-BiTh-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 299.7
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 200
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-07-10T11:33:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1960.8
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C3H7
S
S
C3H7
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

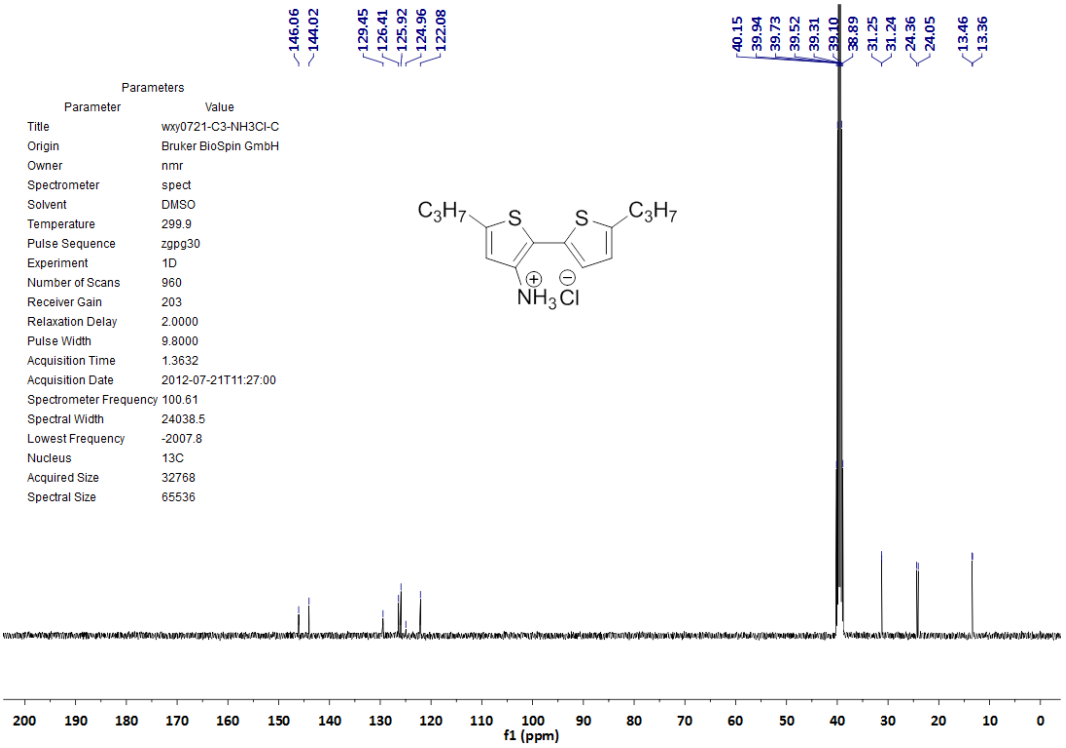

7.252
7.163
7.155
6.720
6.711
6.668
2.795
2.777
2.758
2.728
2.710
2.691
1.727
1.709
1.690
1.671
1.003
1.001
0.991
0.983
0.972
0.964
0.000
Parameters
Parameter Value
Title 1012-C3-BiTh-1Br
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 297.1
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 114
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-10-13T00:45:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1654.0
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C3H7
S
S
C3H7
Br
1.00
1.02
0.99
2.14
2.13
4.30
6.43
10.0 9.5 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 0.0
f1 (ppm)

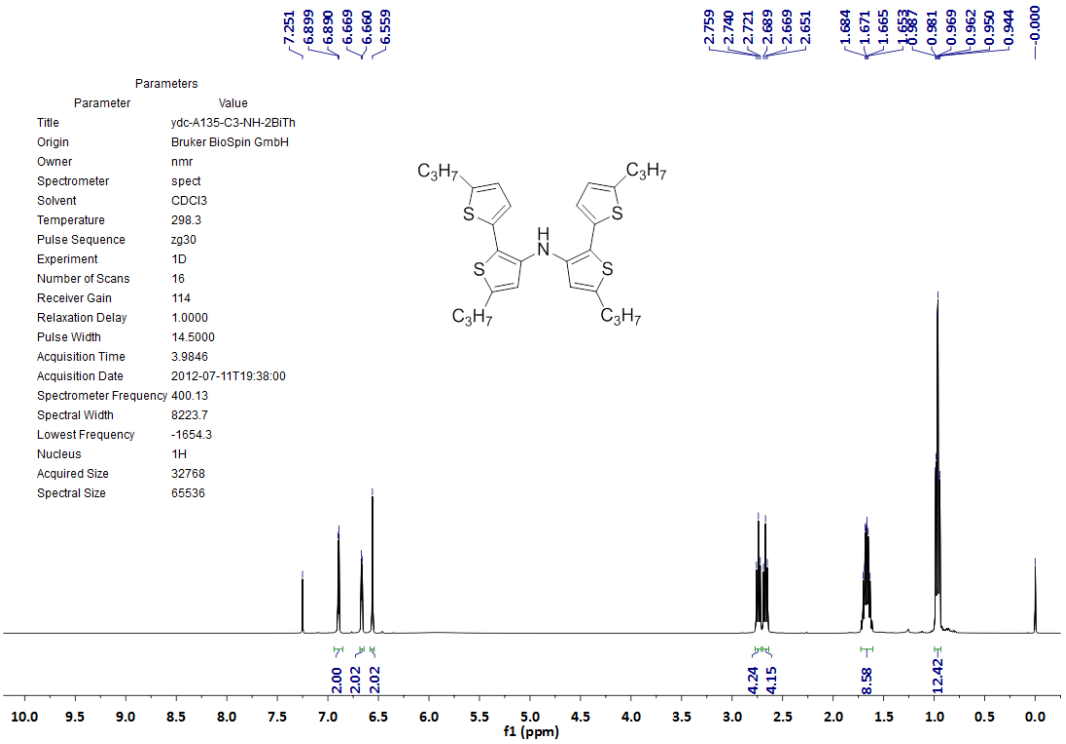

146.17
143.84
132.19
130.11
128.58
125.84
124.26
105.89
77.32
77.00
76.68
32.13
32.02
24.77
24.37
13.69
13.56
Parameters
Parameter Value
Title 1012-C3-BiTh-1Br
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.3
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 512
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-10-13T01:15:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1961.8
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C3H7
S
S
C3H7
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

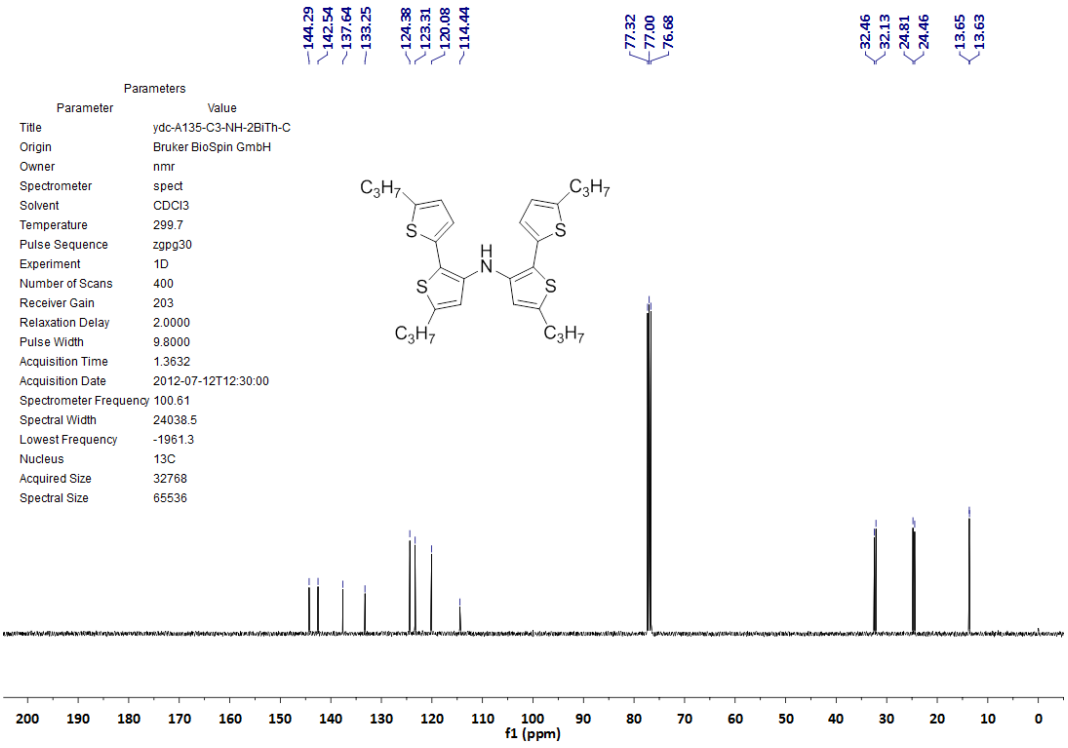

7.881
7.863
7.860
7.444
7.370
7.351
7.178
7.158
6.943
6.934
6.681
6.673
5.741
5.322
5.320
2.760
2.741
2.722
2.498
2.479
2.461
1.677
1.659
1.477
0.965
0.946
0.800
0.782
0.764
Parameters
Parameter Value
Title 1013-C3-imine
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CD2Cl2
Temperature 297.1
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 81
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-10-13T15:41:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1656.1
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C3H7
S
S
C3H7
N
Ph
Ph
2.02
6.13
2.00
0.98
1.00
0.98
2.02
2.02
2.08
2.09
3.08
3.07
10.0 9.5 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 0.0
f1 (ppm)

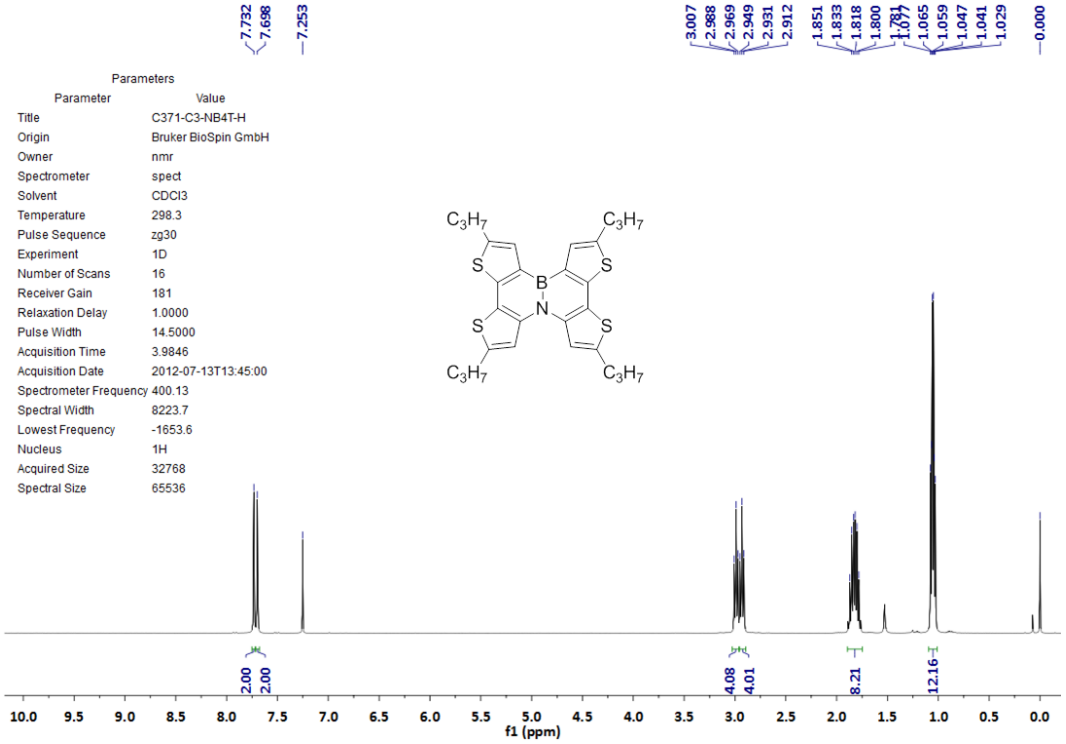

168.27
146.51
143.69
141.31
139.76
137.72
134.40
131.26
130.18
129.50
129.23
128.79
128.71
124.57
124.28
123.28
120.96
54.54
54.27
54.00
53.73
53.46
32.64
32.56
25.50
24.83
14.02
13.60
Parameters
Parameter Value
Title 1013-C3-imine
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CD2Cl2
Temperature 298.8
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 800
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-10-13T16:28:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1900.2
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C3H7
S
S
C3H7
N
Ph
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

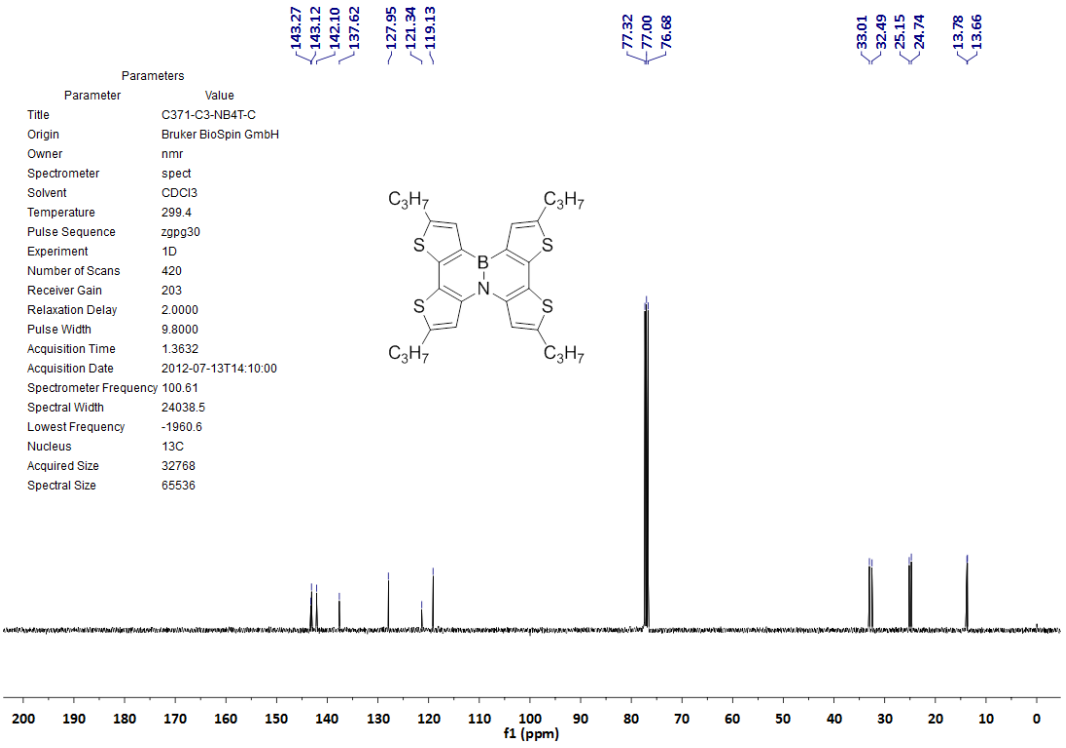

7.341
7.332
6.950
6.909
6.900
2.792
2.773
2.755
2.737
2.718
2.509
2.505
2.500
1.652
1.633
1.628
1.610
0.965
0.956
0.947
0.938
0.928
0.919
-0.000
Parameters
Parameter Value
Title wxy0721-C3-NH3Cl-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent DMSO
Temperature 298.5
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 114
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-07-21T10:32:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1642.9
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C3H7
S
S
C3H7
NH3Cl
1.00
1.00
1.01
4.21
4.30
6.45
10.0 9.5 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 0.0
f1 (ppm)

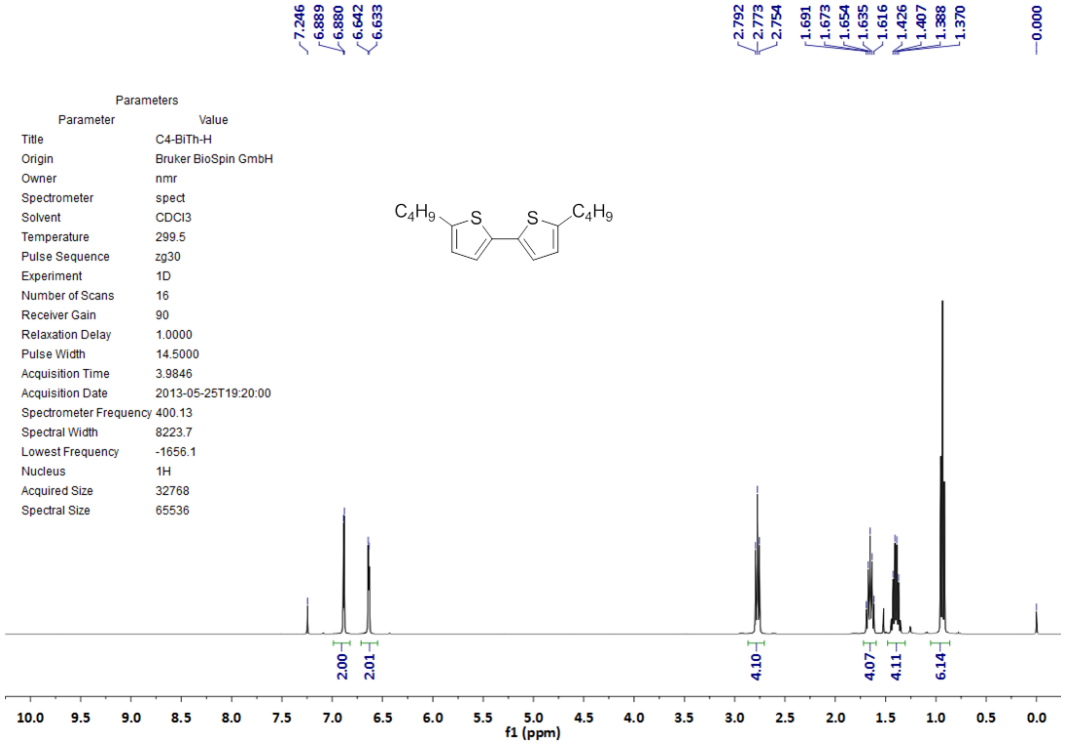

146.06
144.02
129.45
126.41
125.92
124.96
122.08
40.15
39.94
39.73
39.52
39.31
39.10
38.89
31.25
31.24
24.36
24.05
13.46
13.36
Parameters
Parameter Value
Title wxy0721-C3-NH3Cl-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent DMSO
Temperature 299.9
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 960
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-07-21T11:27:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -2007.8
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C3H7
S
S
C3H7
NH3Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

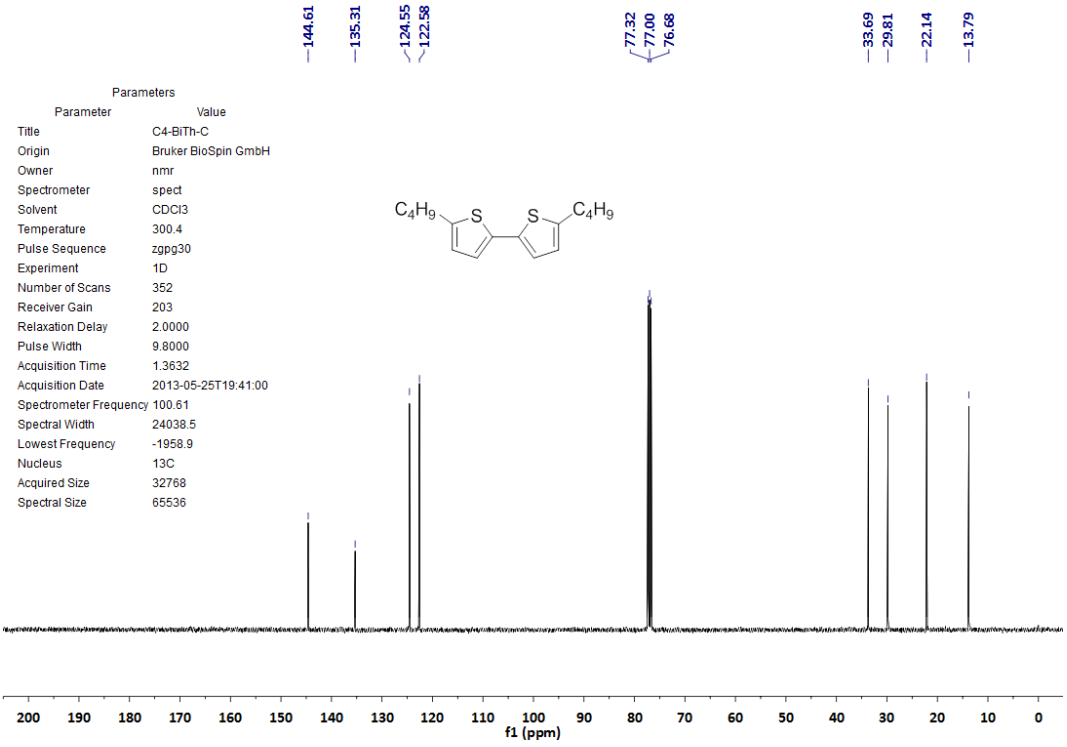

7.251
6.899
6.890
6.669
6.660
6.559
2.759
2.740
2.721
2.689
2.669
2.651
1.684
1.671
1.665
0.981
0.969
0.962
0.950
0.944
-0.000
Parameters
Parameter Value
Title ydc-A135-C3-NH-2BiTh
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.3
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 114
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-07-11T19:38:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1654.3
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
2.00
2.02
2.02
4.24
4.15
8.58
12.42
f1 (ppm)

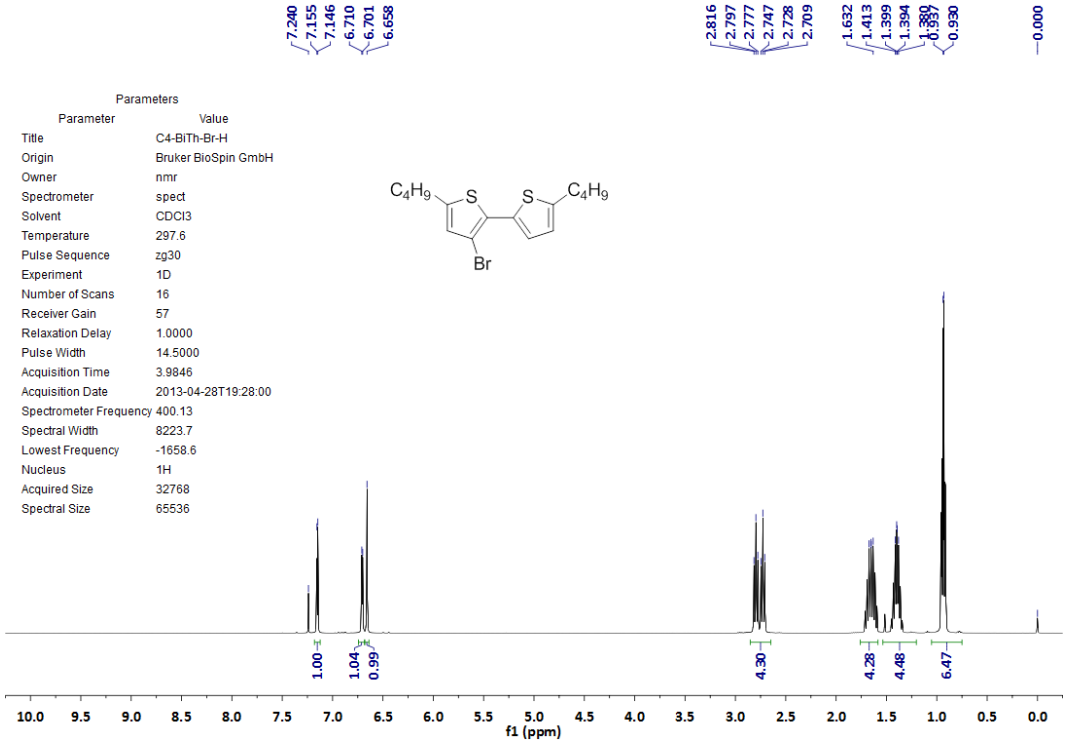

144.29
142.54
137.64
133.25
124.38
123.31
120.08
114.44
77.32
77.00
76.68
32.46
32.13
24.81
24.46
13.65
13.63
Parameters
Parameter Value
Title ydc-A135-C3-NH-2BiTh-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 299.7
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 400
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-07-12T12:30:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1961.3
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
f1 (ppm)

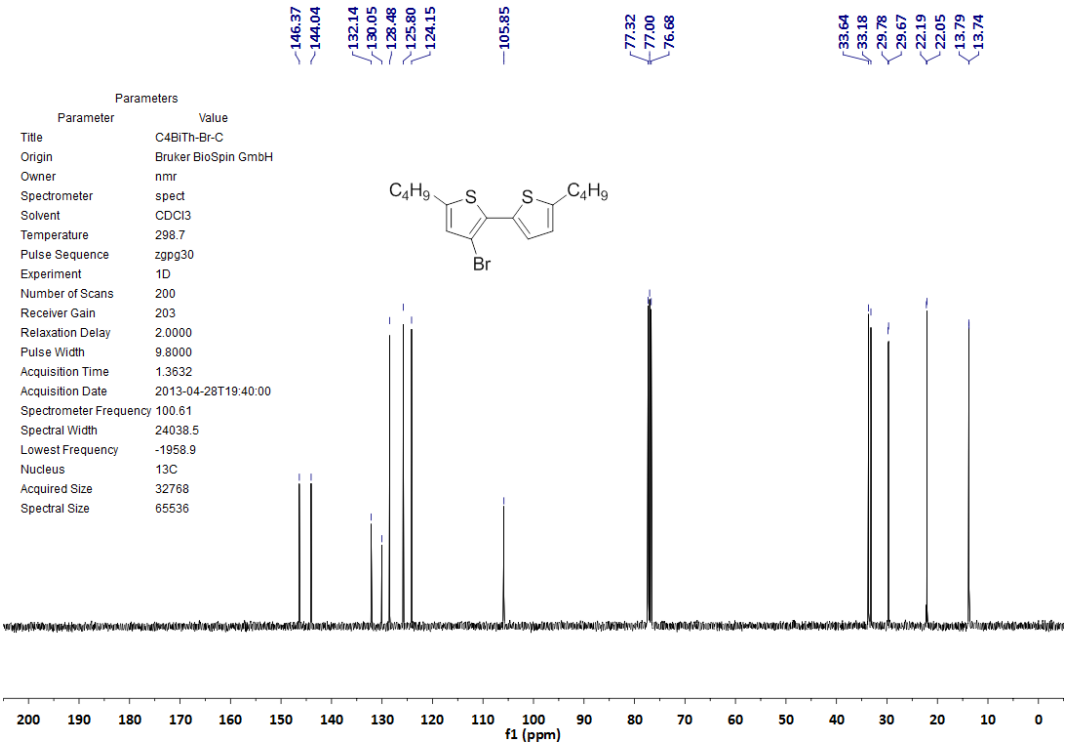

7.732
7.698
7.253
3.007
2.988
2.969
2.949
2.931
2.912
1.851
1.833
1.818
1.800
1.781
1.077
1.065
1.059
1.047
1.041
1.029
0.000
Parameters
Parameter Value
Title C371-C3-NB4T-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.3
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 181
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-07-13T13:45:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1653.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C3H7
S
B
N
2.00
2.00
4.08
4.01
8.21
12.16
10.0 9.5 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 0.0
f1 (ppm)

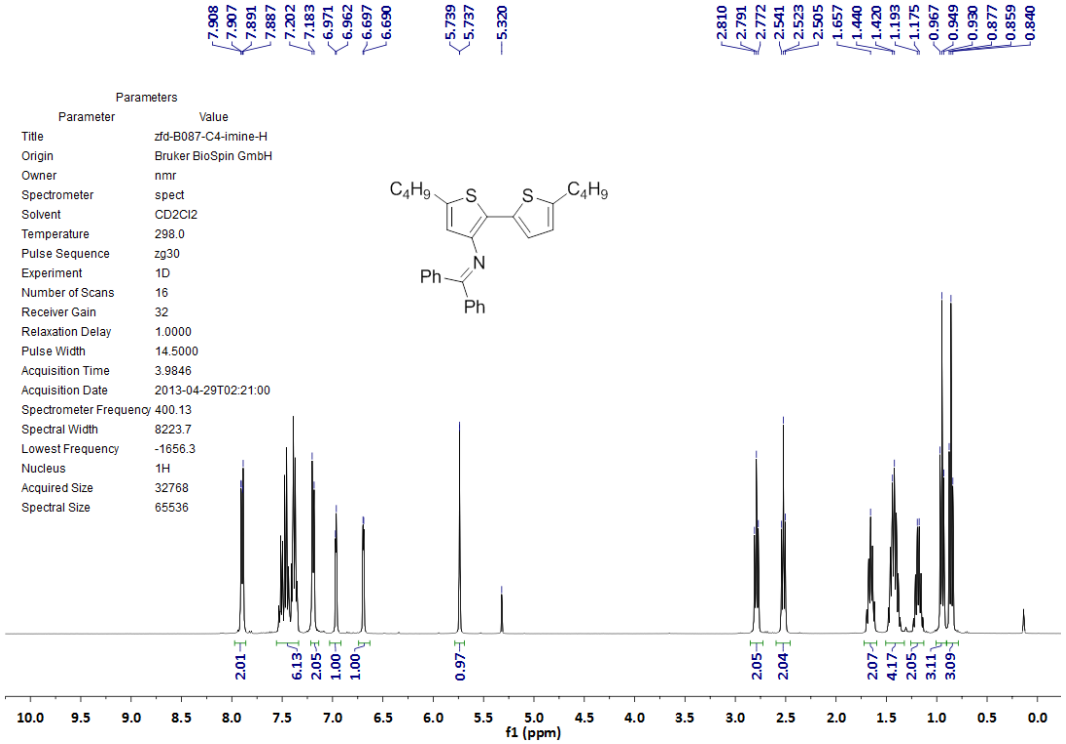

143.27
143.12
142.10
137.62
127.95
121.34
119.13
77.32
77.00
76.68
33.01
32.49
25.15
24.74
13.78
13.66
Parameters
Parameter Value
Title C371-C3-NB4T-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 299.4
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 420
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-07-13T14:10:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1960.6
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C3H7
S
B
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

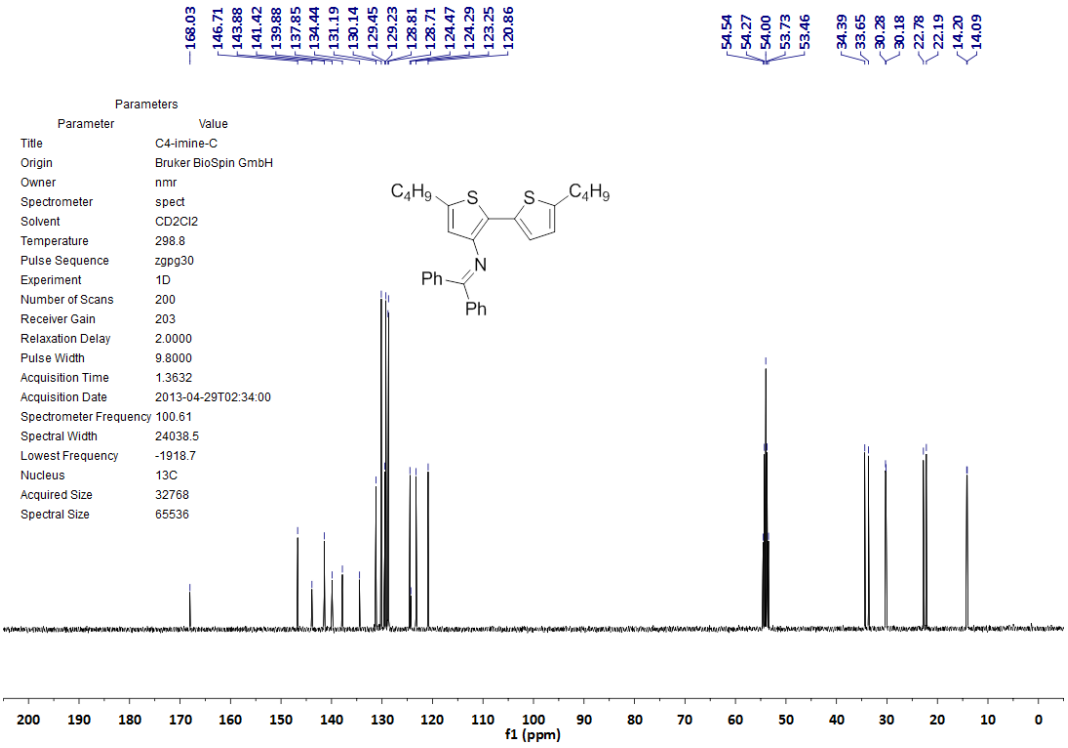

7.246
6.889
6.880
6.642
6.633
2.792
2.773
2.754
1.691
1.673
1.654
1.635
1.616
1.426
1.407
1.388
1.370
0.000
Parameters
Parameter Value
Title C4-BiTh-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 299.5
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 90
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2013-05-25T19:20:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1656.1
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C4H9 S S C4H9
2.00
2.01
4.10
4.07
4.11
6.14
10.0 9.5 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 0.0
f1 (ppm)

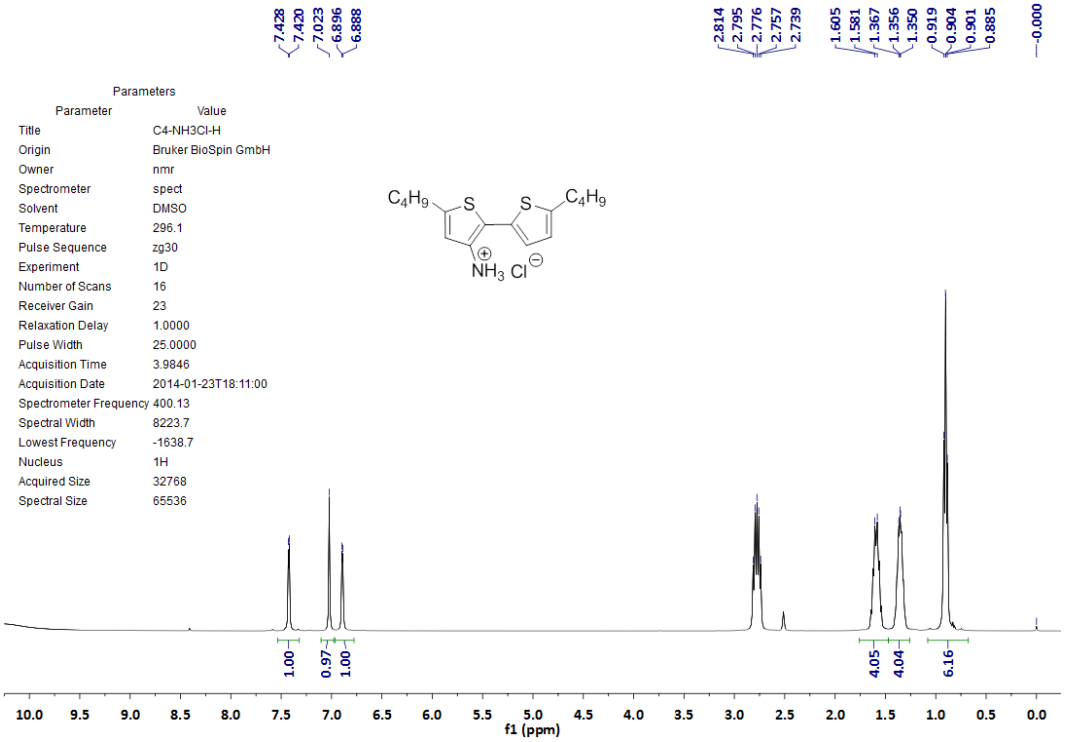

144.61
135.31
124.55
122.58
77.32
77.00
76.68
33.69
29.81
22.14
13.79
Parameters
Parameter Value
Title C4-BiTh-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 300.4
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 352
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2013-05-25T19:41:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C4H9 S S C4H9
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.240
7.155
7.146
6.710
6.701
6.658
2.816
2.797
2.777
2.747
2.728
2.709
1.632
1.413
1.399
1.394
1.380
0.937
0.930
0.000
Parameters
Parameter Value
Title C4-BiTh-Br-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 297.6
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 57
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2013-04-28T19:28:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1658.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C4H9
S
S
C4H9
Br
1.00
1.04
0.99
4.30
4.28
4.48
6.47
10.0 9.5 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 0.0
f1 (ppm)


146.37
144.04
132.14
130.05
128.48
125.80
124.15
105.85
77.32
77.00
76.68
33.64
33.18
29.78
29.67
22.19
22.05
13.79
13.74
Parameters
Parameter Value
Title C4BiTh-Br-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.7
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 200
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2013-04-28T19:40:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C4H9
S
S
C4H9
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

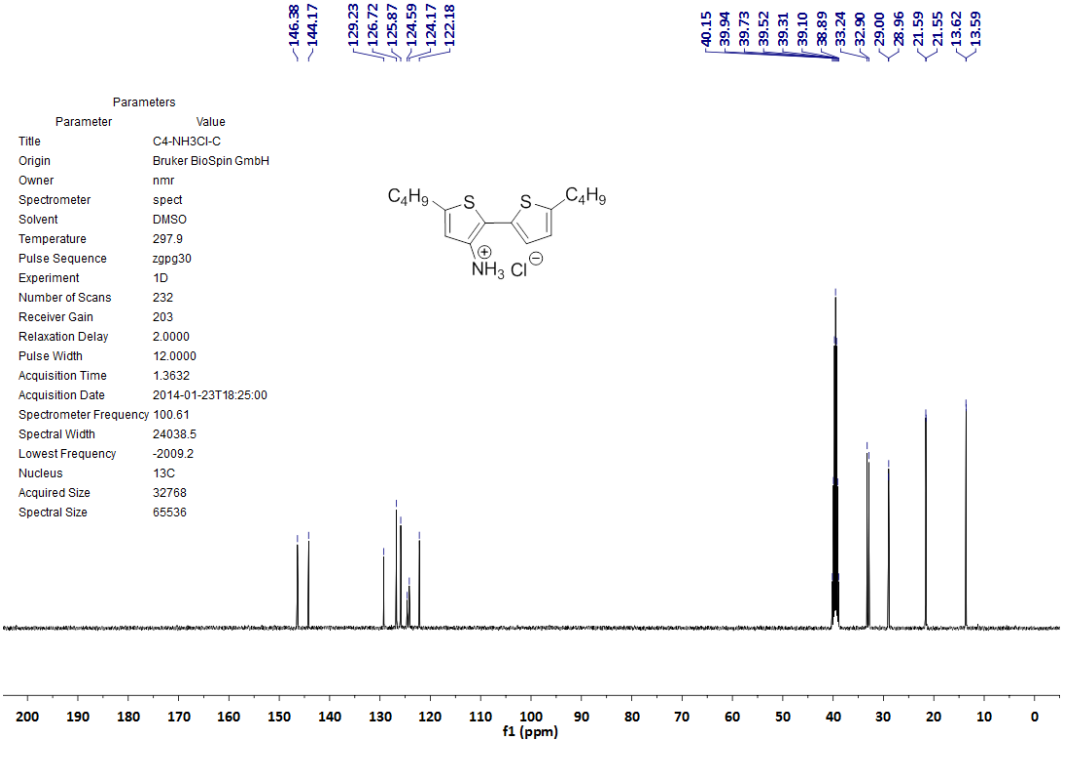

7.908
7.907
7.891
7.887
7.202
7.183
6.971
6.962
6.697
6.690
5.739
5.737
5.320
2.810
2.791
2.772
2.541
2.523
2.505
1.657
1.440
1.420
1.193
1.175
0.967
0.949
0.930
0.877
0.859
0.840
Parameters
Parameter Value
Title zfd-B087-C4-imine-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CD2Cl2
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 32
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2013-04-29T02:21:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1656.3
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C4H9
S
S
C4H9
N
Ph
Ph
2.01
6.13
2.05
1.00
1.00
0.97
2.05
2.04
2.07
4.17
2.05
3.11
3.09
10.0 9.5 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 0.0
f1 (ppm)


168.03
146.71
143.88
141.42
139.88
137.85
134.44
131.19
130.14
129.45
129.23
128.81
128.71
124.47
124.29
123.25
120.86
54.54
54.27
54.00
53.73
53.46
34.39
33.65
30.28
30.18
22.78
22.19
14.20
14.09
Parameters
Parameter Value
Title C4-imine-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CD2Cl2
Temperature 298.8
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 200
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2013-04-29T02:34:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1918.7
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C4H9
S
S
C4H9
N
Ph
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



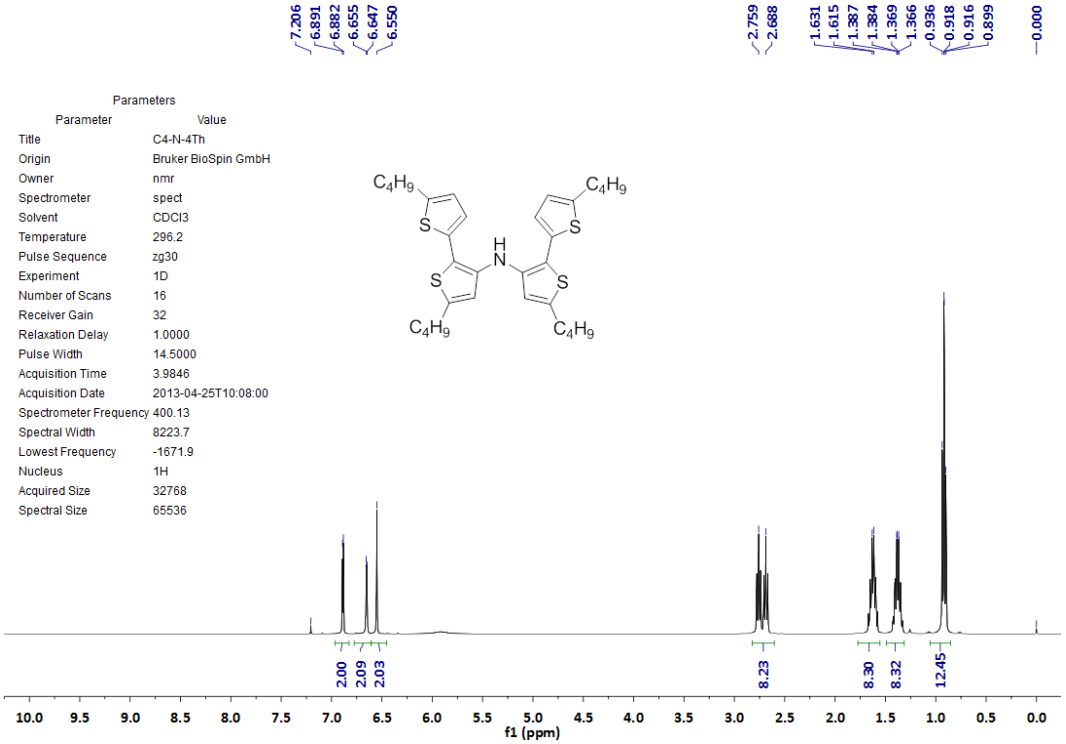
Parameters

Parameter	Value
Title	C4-NH3Cl-H
Origin	Bruker BioSpin GmbH
Owner	nmr
Spectrometer	spect
Solvent	DMSO
Temperature	296.1
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	23
Relaxation Delay	1.0000
Pulse Width	25.0000
Acquisition Time	3.9846
Acquisition Date	2014-01-23T18:11:00
Spectrometer Frequency	400.13
Spectral Width	8223.7
Lowest Frequency	-1638.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



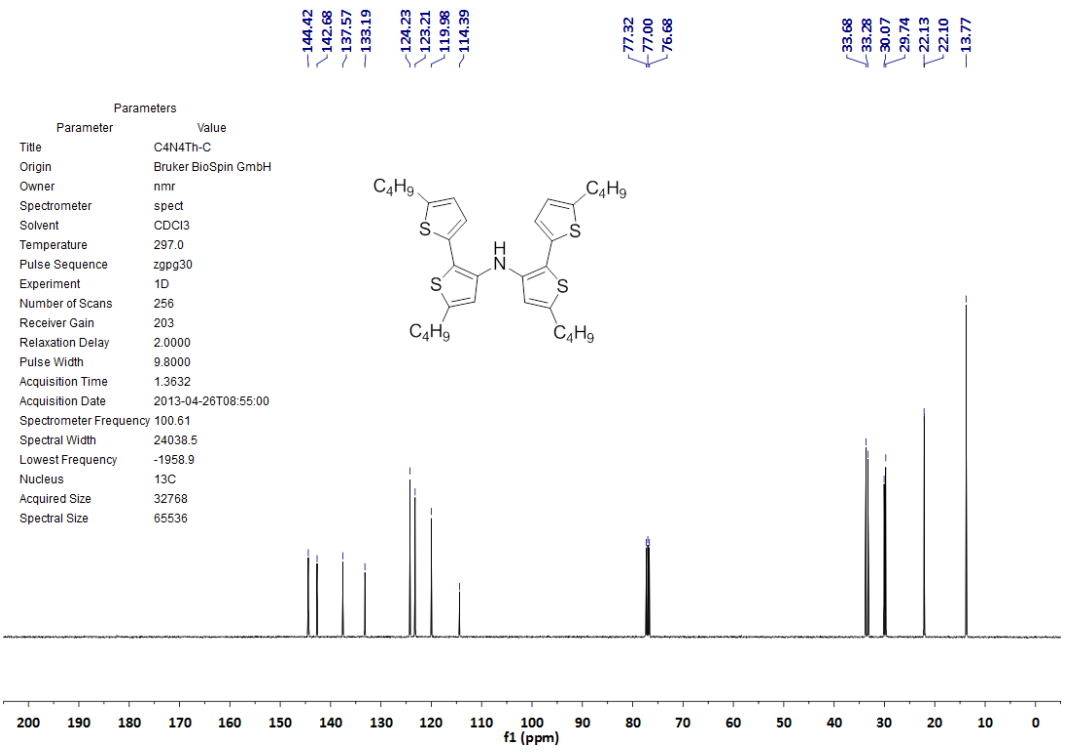
Parameters

Parameter	Value
Title	C4-NH3Cl-C
Origin	Bruker BioSpin GmbH
Owner	nmr
Spectrometer	spect
Solvent	DMSO
Temperature	297.9
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	232
Receiver Gain	203
Relaxation Delay	2.0000
Pulse Width	12.0000
Acquisition Time	1.3632
Acquisition Date	2014-01-23T18:25:00
Spectrometer Frequency	100.61
Spectral Width	24038.5
Lowest Frequency	-2009.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



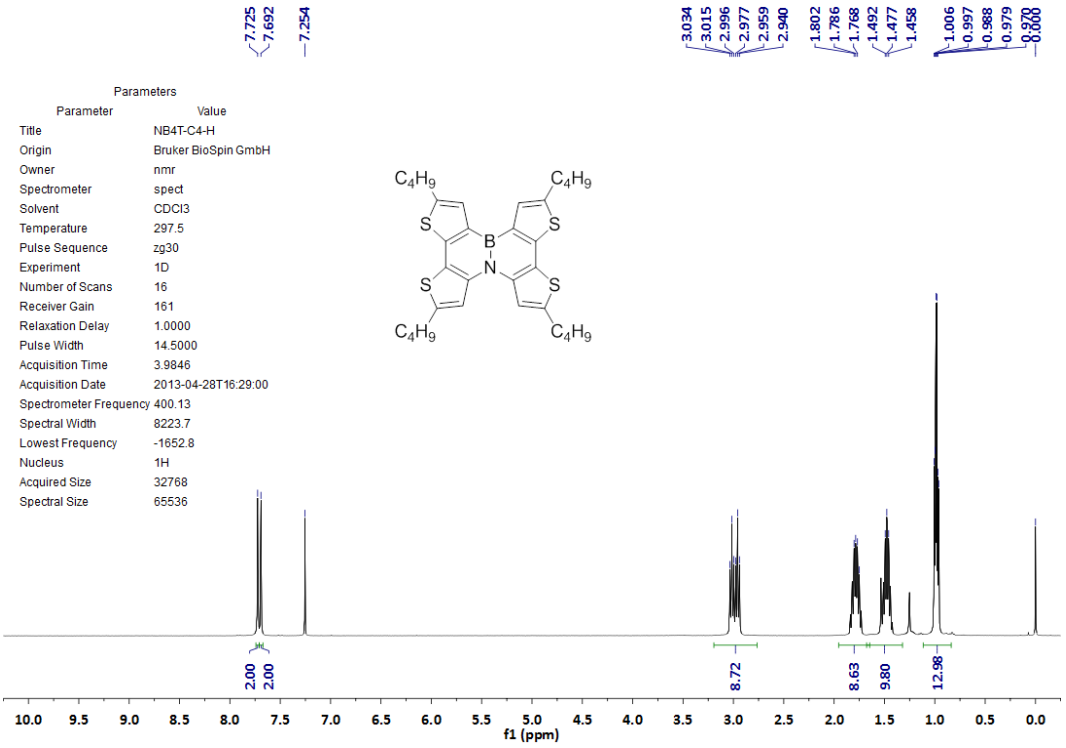
Parameters

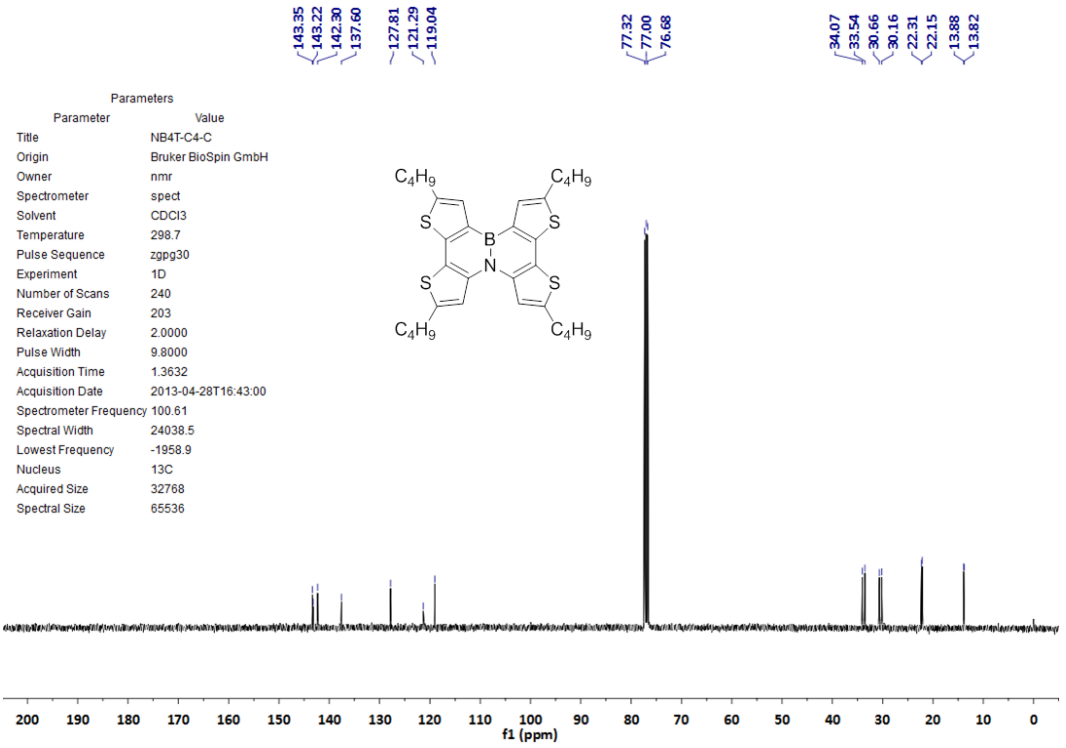
Parameter	Value
Title	C4-N-4Th
Origin	Bruker BioSpin GmbH
Owner	nmr
Spectrometer	spect
Solvent	CDCl3
Temperature	296.2
Pulse Sequence	zg30
Experiment	1D
Number of Scans	16
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	14.5000
Acquisition Time	3.9846
Acquisition Date	2013-04-25T10:08:00
Spectrometer Frequency	400.13
Spectral Width	8223.7
Lowest Frequency	-1671.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

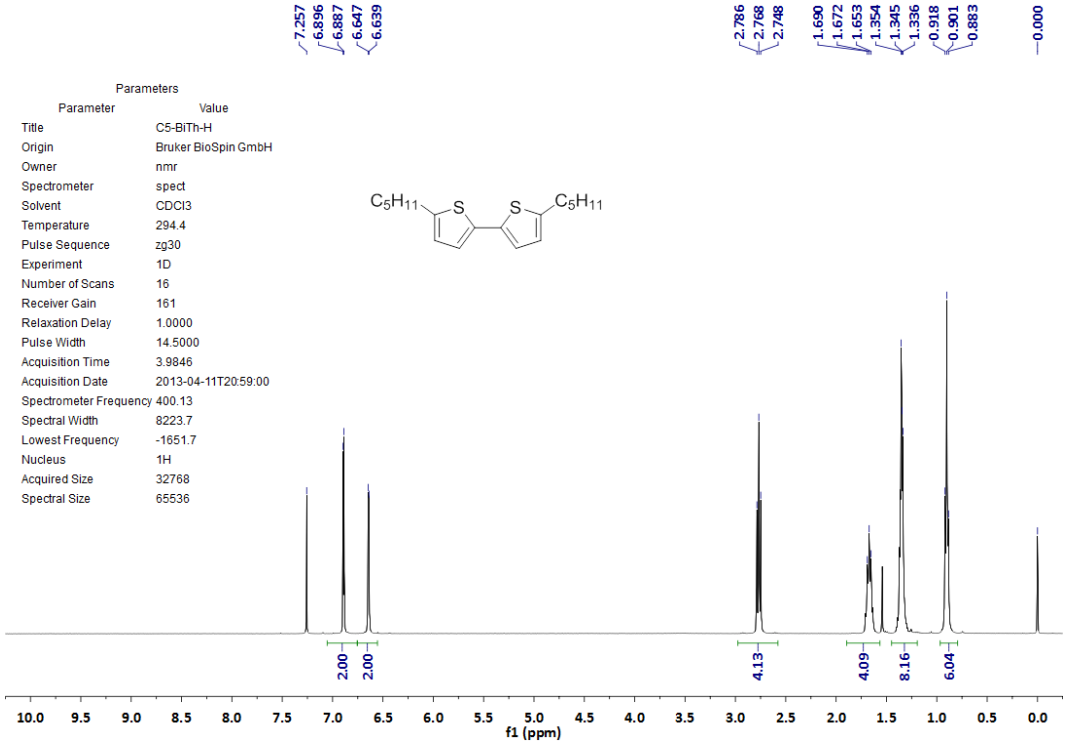


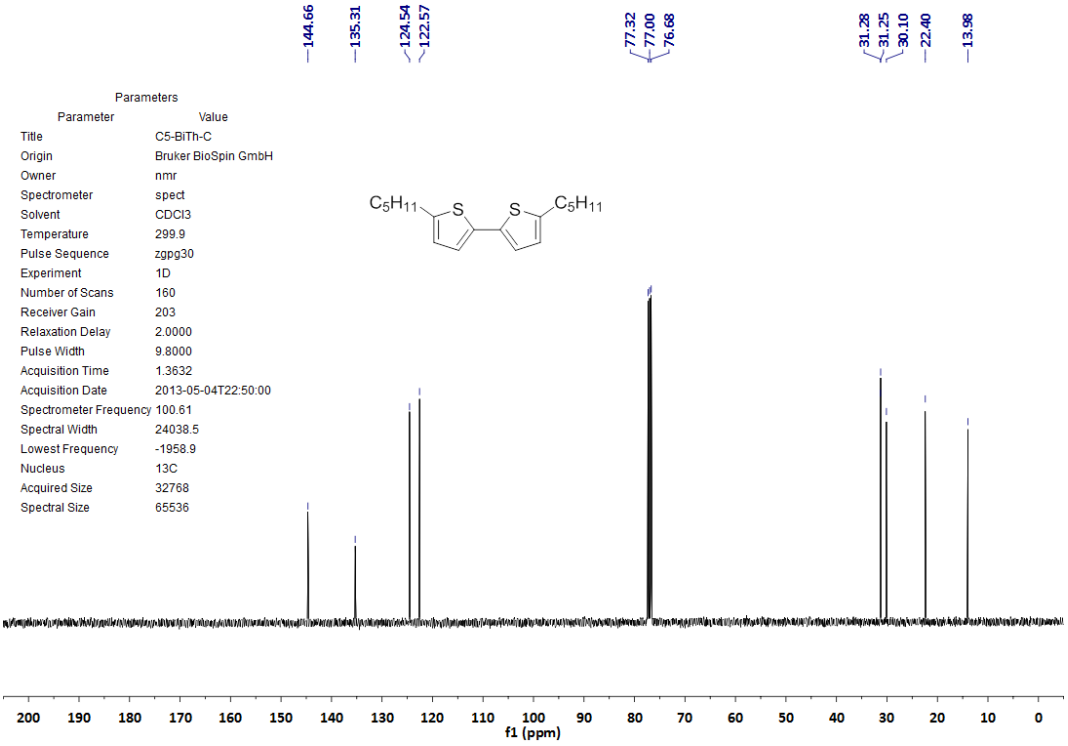
Parameters

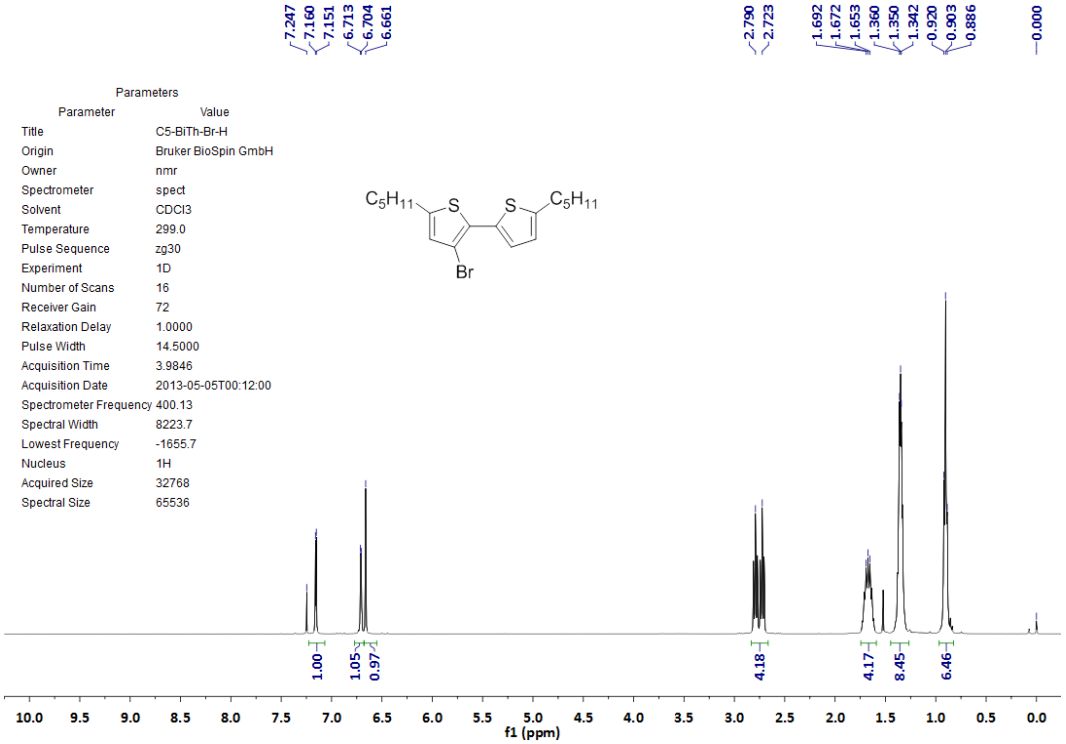
Parameter	Value
Title	C4N4Th-C
Origin	Bruker BioSpin GmbH
Owner	nmr
Spectrometer	spect
Solvent	CDCl3
Temperature	297.0
Pulse Sequence	zgpg30
Experiment	1D
Number of Scans	256
Receiver Gain	203
Relaxation Delay	2.0000
Pulse Width	9.8000
Acquisition Time	1.3632
Acquisition Date	2013-04-26T08:55:00
Spectrometer Frequency	100.61
Spectral Width	24038.5
Lowest Frequency	-1958.9
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

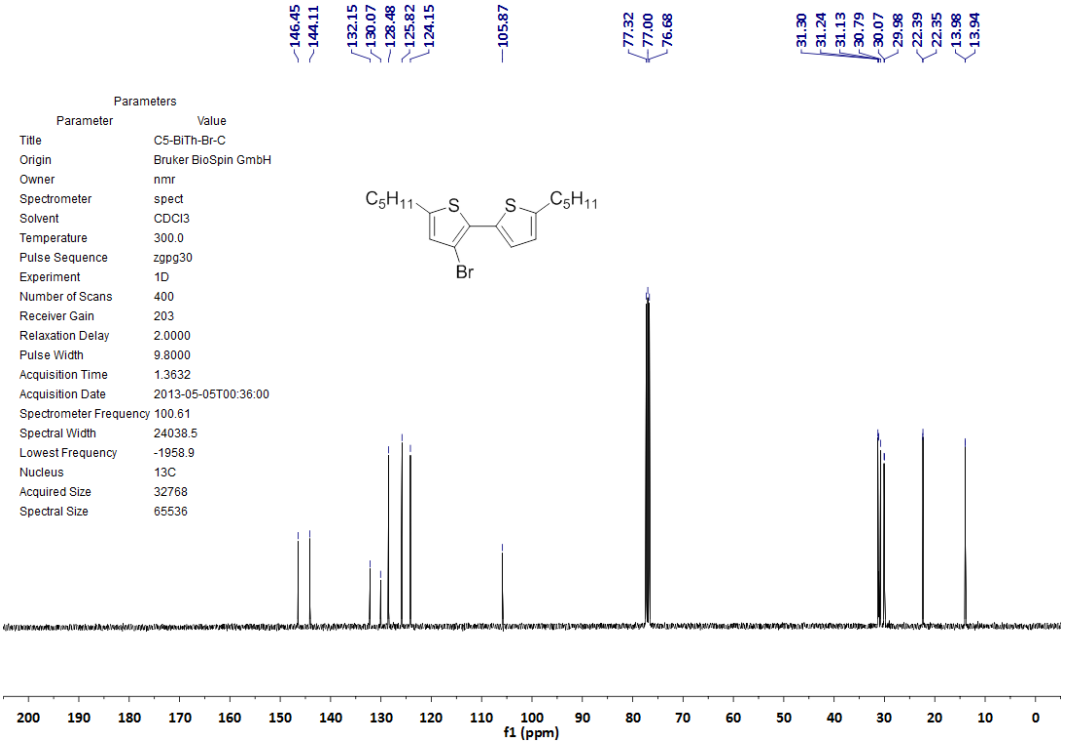

7.725
7.692
7.254
3.034
3.015
2.996
2.977
2.959
2.940
1.802
1.786
1.768
1.492
1.477
1.458
1.006
0.997
0.988
0.979
0.970
0.000
Parameters
Parameter Value
Title NB4T-C4-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 297.5
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 161
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2013-04-28T16:29:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1652.8
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C4H9
S
B
N
2.00
2.00
8.72
8.63
9.80
12.98
10.0 9.5 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 0.0
f1 (ppm)

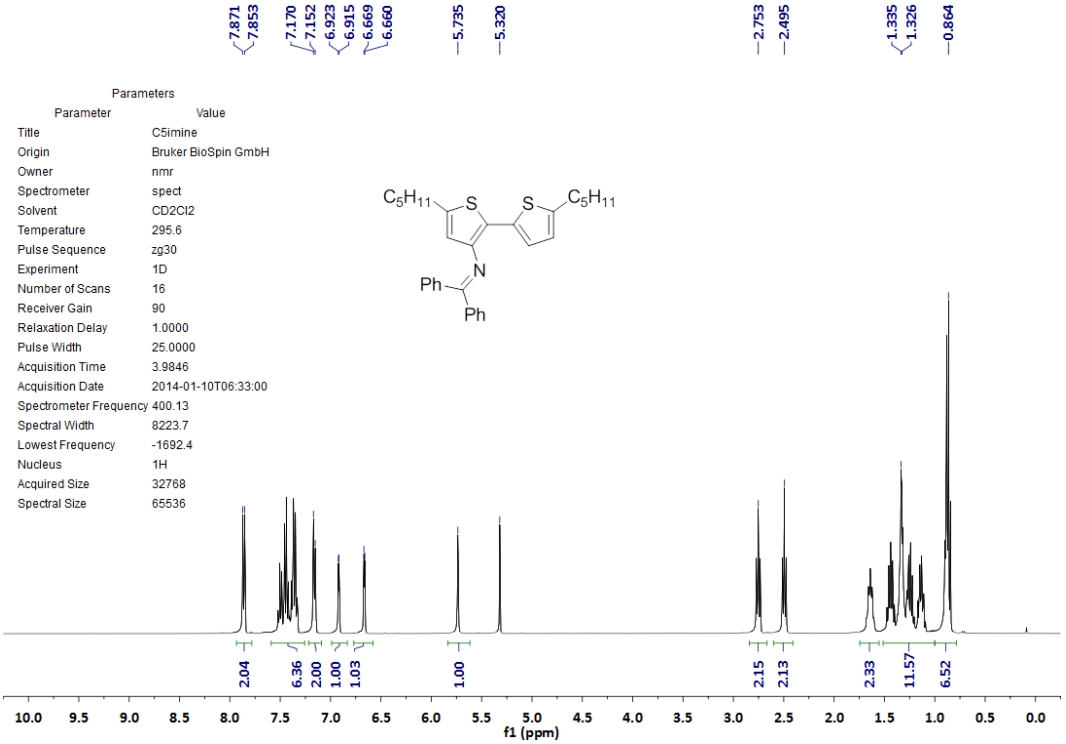

143.35
143.22
142.30
137.60
127.81
121.29
119.04
77.32
77.00
76.68
34.07
33.54
30.66
30.16
22.31
22.15
13.88
13.82
Parameters
Parameter Value
Title NB4T-C4-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.7
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 240
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2013-04-28T16:43:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C4H9
S
B
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

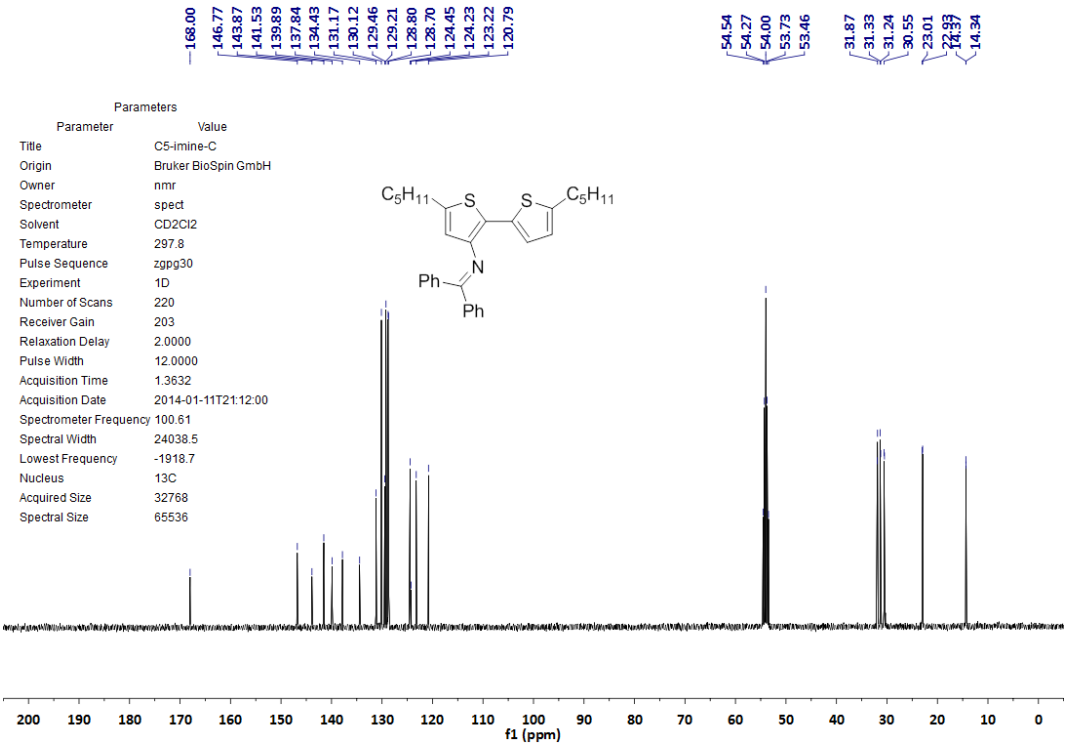

7.257
6.896
6.887
6.647
6.639
2.786
2.768
2.748
1.690
1.672
1.653
1.354
1.345
1.336
0.918
0.901
0.883
0.000
Parameters
Parameter Value
Title C5-BiTh-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 294.4
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 161
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2013-04-11T20:59:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1651.7
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C5H11
S
S
C5H11
2.00
2.00
4.13
4.09
8.16
6.04
10.0 9.5 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 0.0
f1 (ppm)

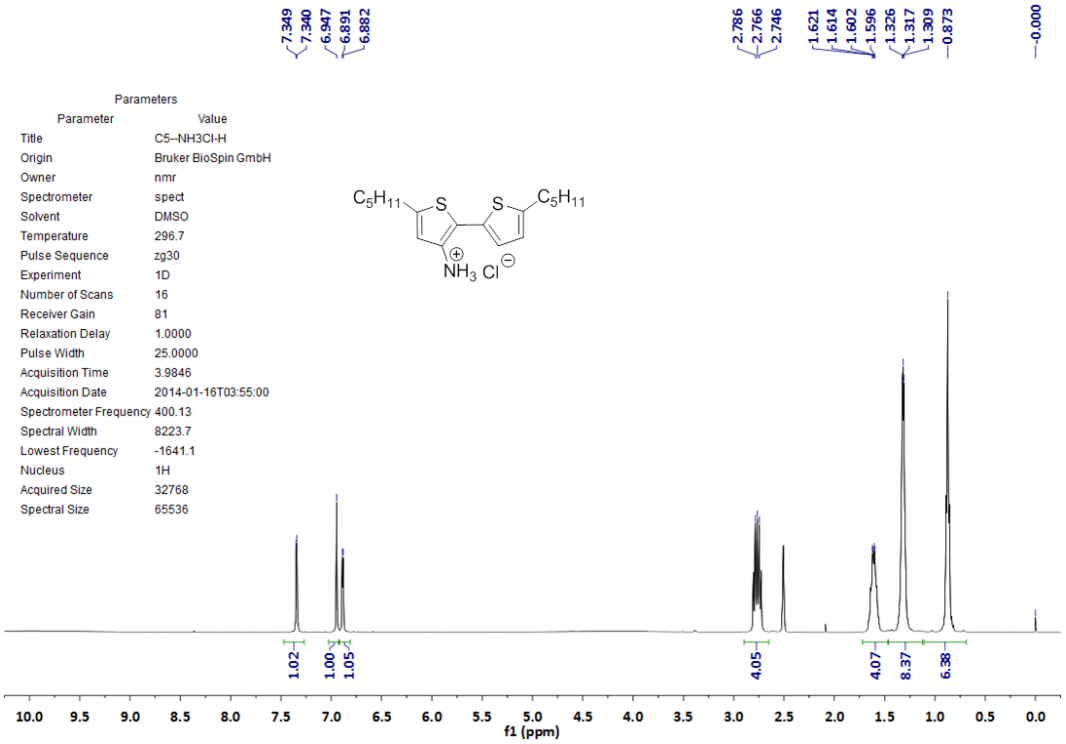

144.66
135.31
124.54
122.57
77.32
77.00
76.68
31.28
31.25
30.10
22.40
13.98
Parameters
Parameter Value
Title C5-BiTh-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 299.9
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 160
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2013-05-04T22:50:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C5H11
S
S
C5H11
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

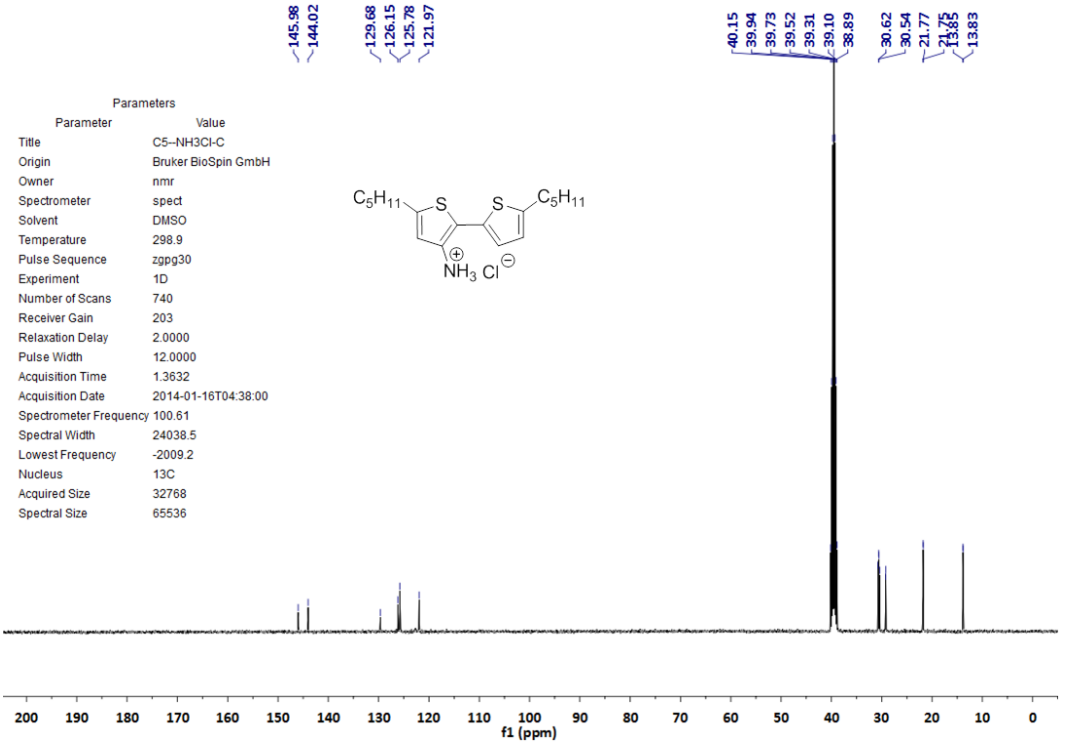

7.247
7.160
7.151
6.713
6.704
6.661
2.790
2.723
1.692
1.672
1.653
1.360
1.350
1.342
0.920
0.903
0.886
0.000
Parameters
Parameter Value
Title C5-BiTh-Br-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 299.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 72
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2013-05-05T00:12:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1655.7
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C5H11
S
S
C5H11
Br
1.00
1.05
0.97
4.18
4.17
8.45
6.46
10.0 9.5 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 0.0
f1 (ppm)

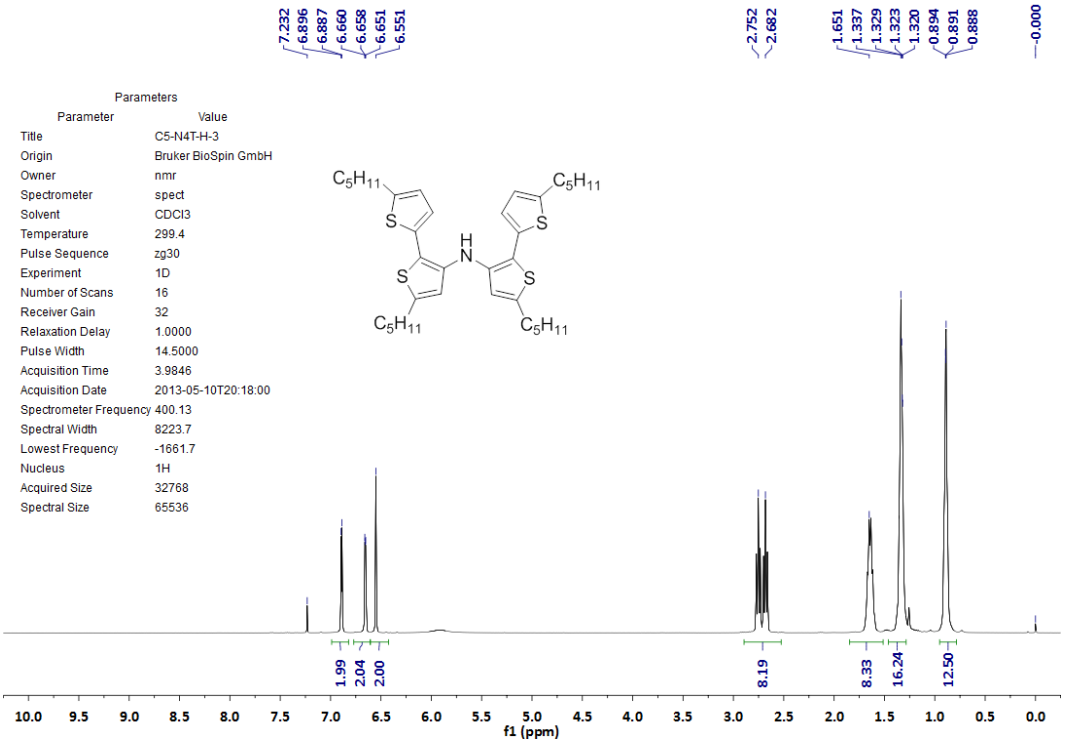

146.45
144.11
132.15
130.07
128.48
125.82
124.15
105.87
77.32
77.00
76.68
31.30
31.24
31.13
30.79
30.07
29.98
22.39
22.35
13.98
13.94
Parameters
Parameter Value
Title C5-BiTh-Br-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 300.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 400
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2013-05-05T00:36:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C5H11
S
S
C5H11
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

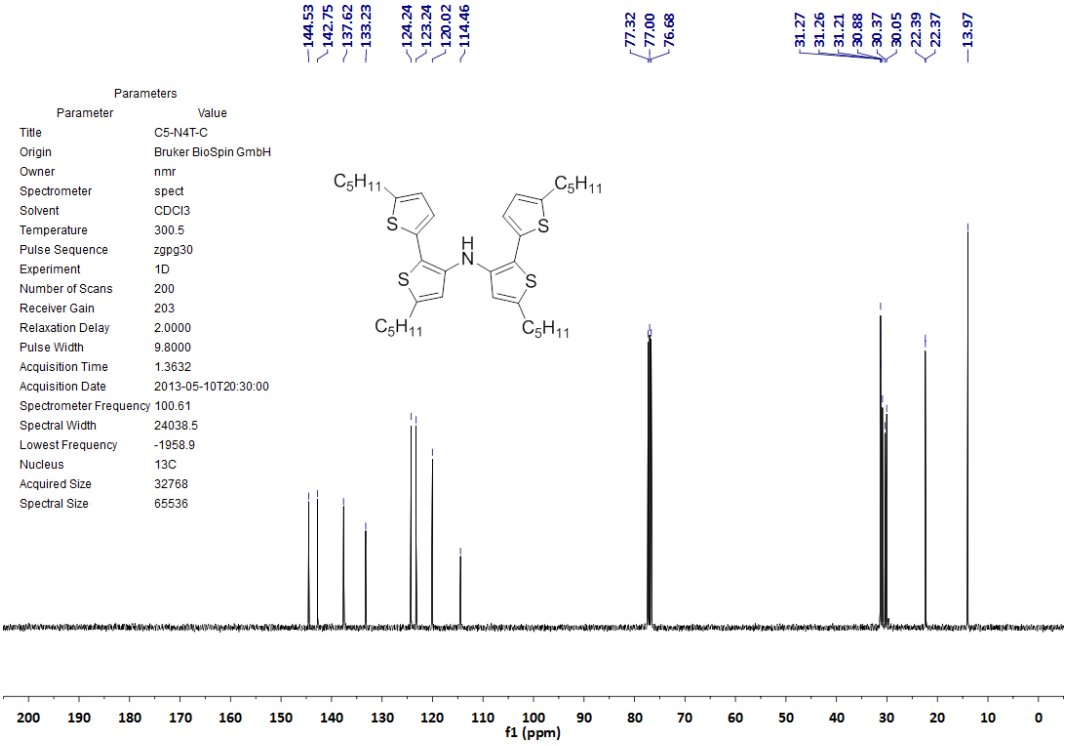

7.871
7.853
7.170
7.152
6.923
6.915
6.669
6.660
5.735
5.320
2.753
2.495
1.335
1.326
0.864
Parameters
Parameter Value
Title C5imine
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CD2Cl2
Temperature 295.6
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 90
Relaxation Delay 1.0000
Pulse Width 25.0000
Acquisition Time 3.9846
Acquisition Date 2014-01-10T06:33:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1692.4
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C5H11
S
S
C5H11
N
Ph
Ph
2.04
6.36
2.00
1.00
1.03
1.00
2.15
2.13
2.33
11.57
6.52
10.0 9.5 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 0.0
f1 (ppm)

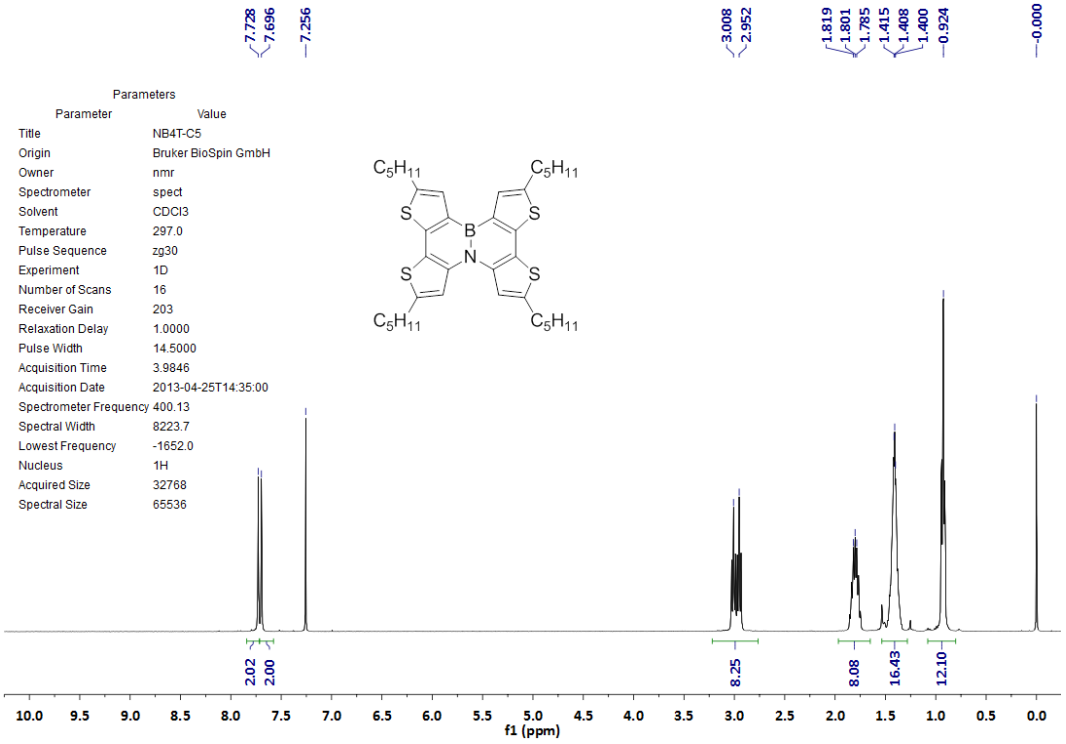

168.00
146.77
143.87
141.53
139.89
137.84
134.43
131.17
130.12
129.46
129.21
128.80
128.70
124.45
124.23
123.22
120.79
54.54
54.27
54.00
53.73
53.46
31.87
31.33
31.24
30.55
23.01
22.33
22.17
14.34
Parameters
Parameter Value
Title C5-imine-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CD2Cl2
Temperature 297.8
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 220
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 12.0000
Acquisition Time 1.3632
Acquisition Date 2014-01-11T21:12:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1918.7
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C5H11
S
S
C5H11
N
Ph
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

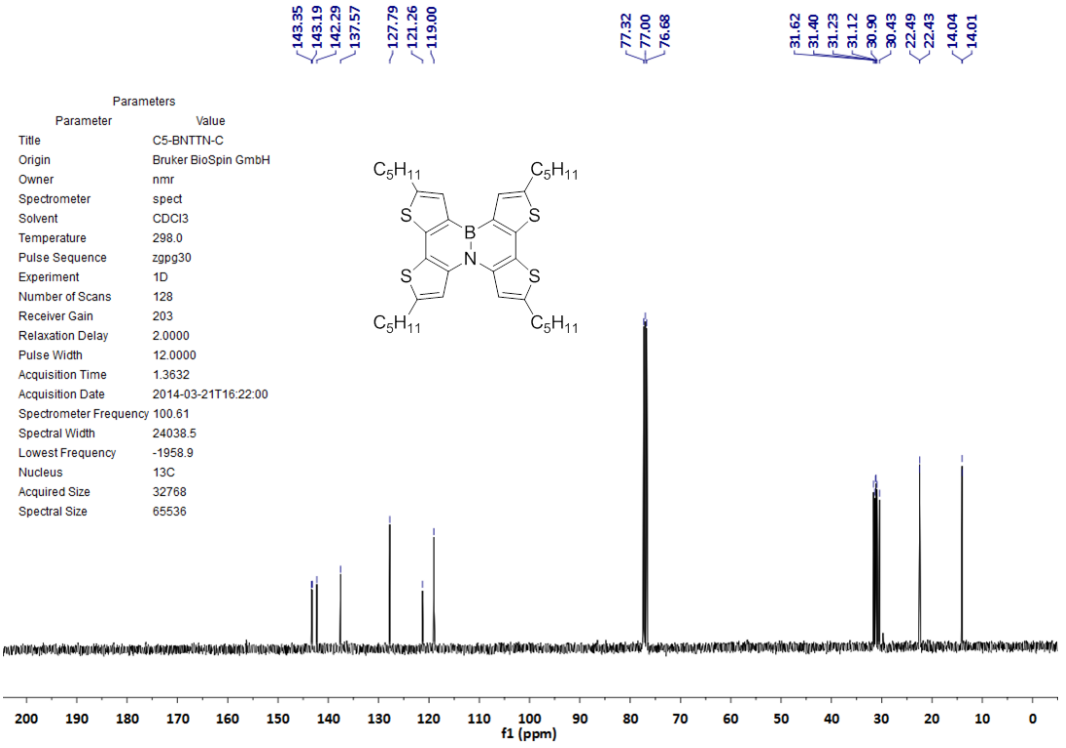

7.349
7.340
6.947
6.891
6.882
2.786
2.766
2.746
1.621
1.614
1.602
1.596
1.326
1.317
1.309
0.873
0.000
Parameters
Parameter Value
Title C5--NH3Cl-H
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent DMSO
Temperature 296.7
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 81
Relaxation Delay 1.0000
Pulse Width 25.0000
Acquisition Time 3.9846
Acquisition Date 2014-01-16T03:55:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1641.1
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C5H11
S
S
C5H11
NH3 Cl
1.02
1.00
1.05
4.05
4.07
8.37
6.38
10.0 9.5 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 0.0
f1 (ppm)

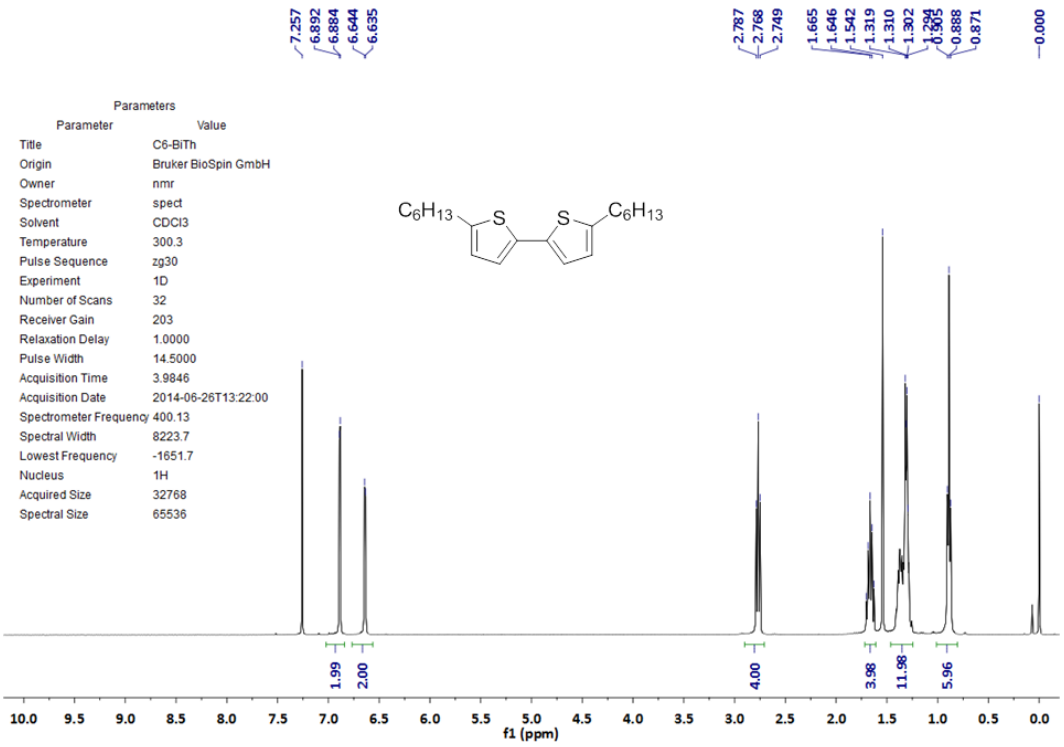

145.98
144.02
129.68
126.15
125.78
121.97
40.15
39.94
39.73
39.52
39.31
39.10
38.89
30.62
30.54
21.77
21.75
13.85
13.83
Parameters
Parameter Value
Title C5--NH3Cl-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent DMSO
Temperature 298.9
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 740
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 12.0000
Acquisition Time 1.3632
Acquisition Date 2014-01-16T04:38:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -2009.2
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C5H11
S
S
C5H11
NH3 Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

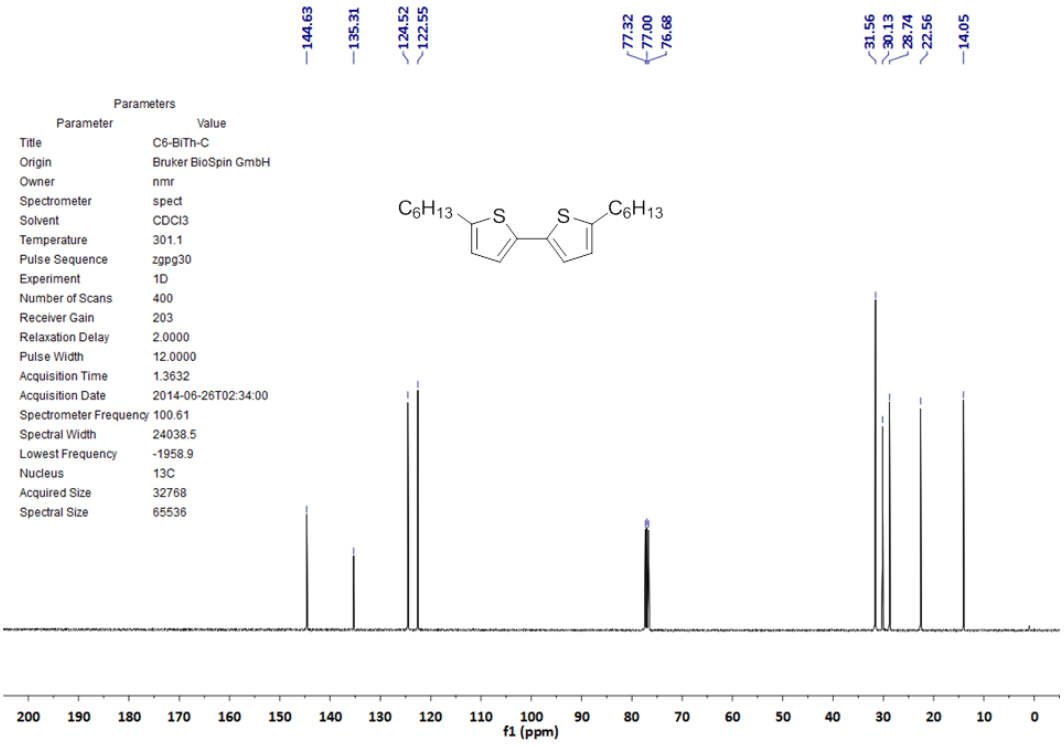

7.232
6.896
6.887
6.660
6.658
6.651
6.551
2.752
2.682
1.651
1.337
1.329
1.323
1.320
0.894
0.891
0.888
-0.000
Parameters
Parameter Value
Title C5-N4T-H-3
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 299.4
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 32
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2013-05-10T20:18:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1661.7
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
1.99
2.04
2.00
8.19
8.33
16.24
12.50
f1 (ppm)

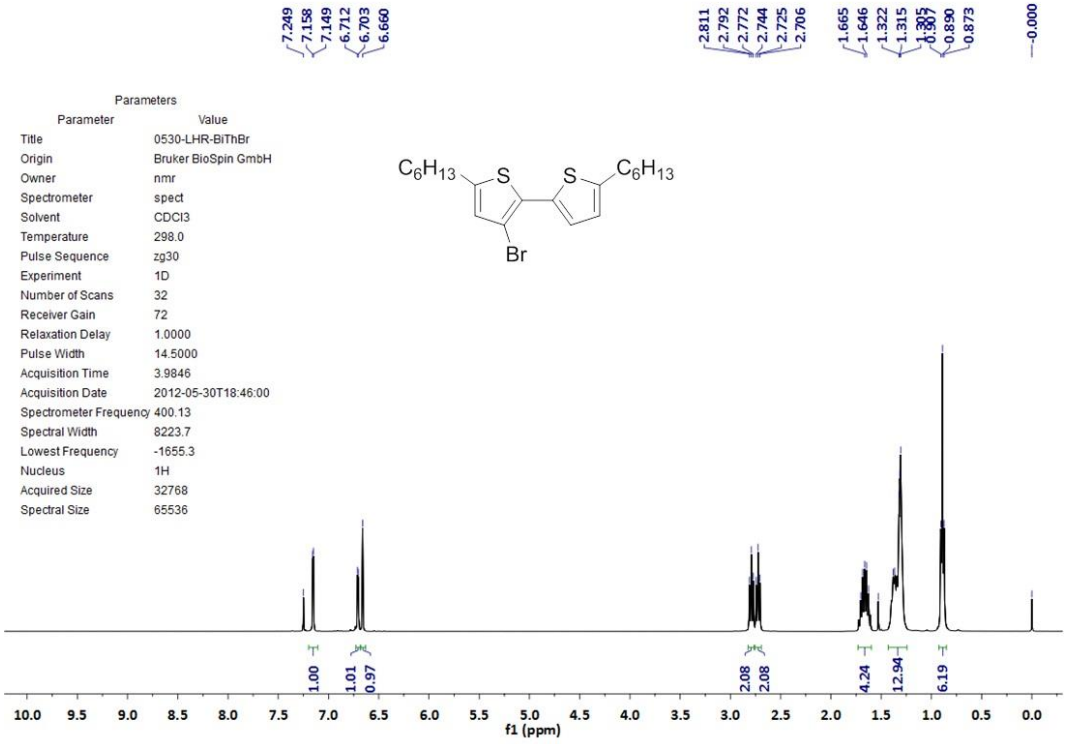

144.53
142.75
137.62
133.23
124.24
123.24
120.02
114.46
77.32
77.00
76.68
31.27
31.26
31.21
30.88
30.37
30.05
22.39
22.37
13.97
Parameters
Parameter Value
Title C5-N4T-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 300.5
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 200
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2013-05-10T20:30:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
f1 (ppm)

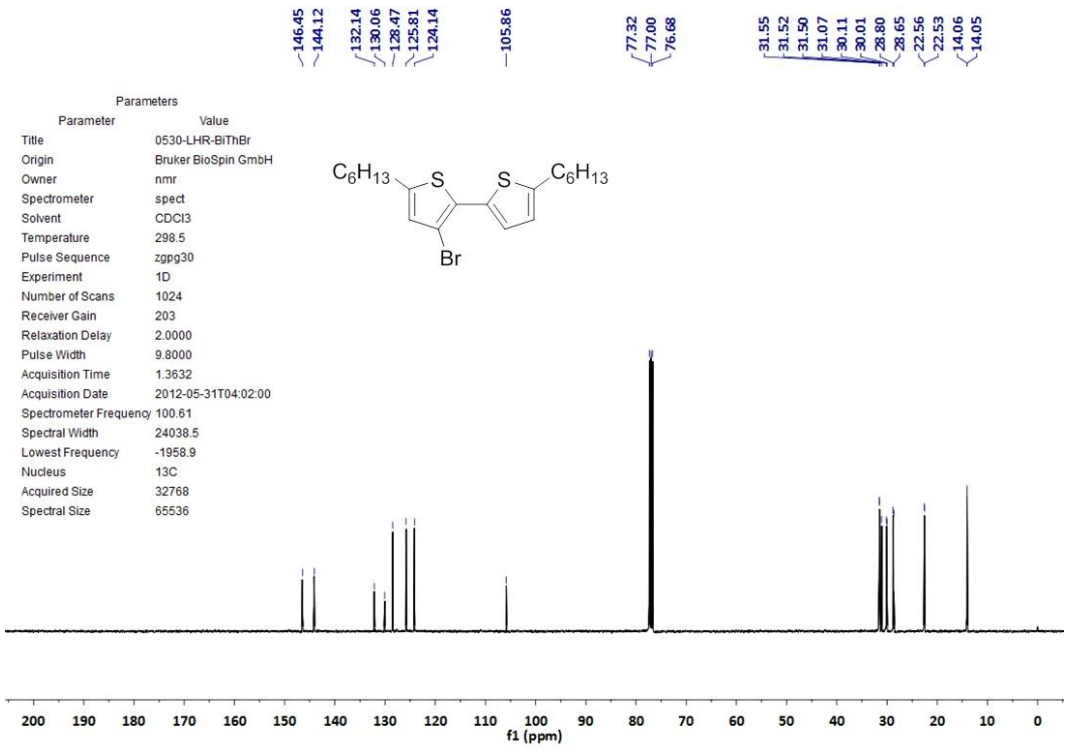

7.728
7.696
7.256
3.008
2.952
1.819
1.801
1.785
1.415
1.408
1.400
0.924
0.000
Parameters
Parameter Value
Title NB4T-C5
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 297.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 203
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2013-04-25T14:35:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1652.0
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C5H11
S
B
N
2.02
2.00
8.25
8.08
16.43
12.10
f1 (ppm)

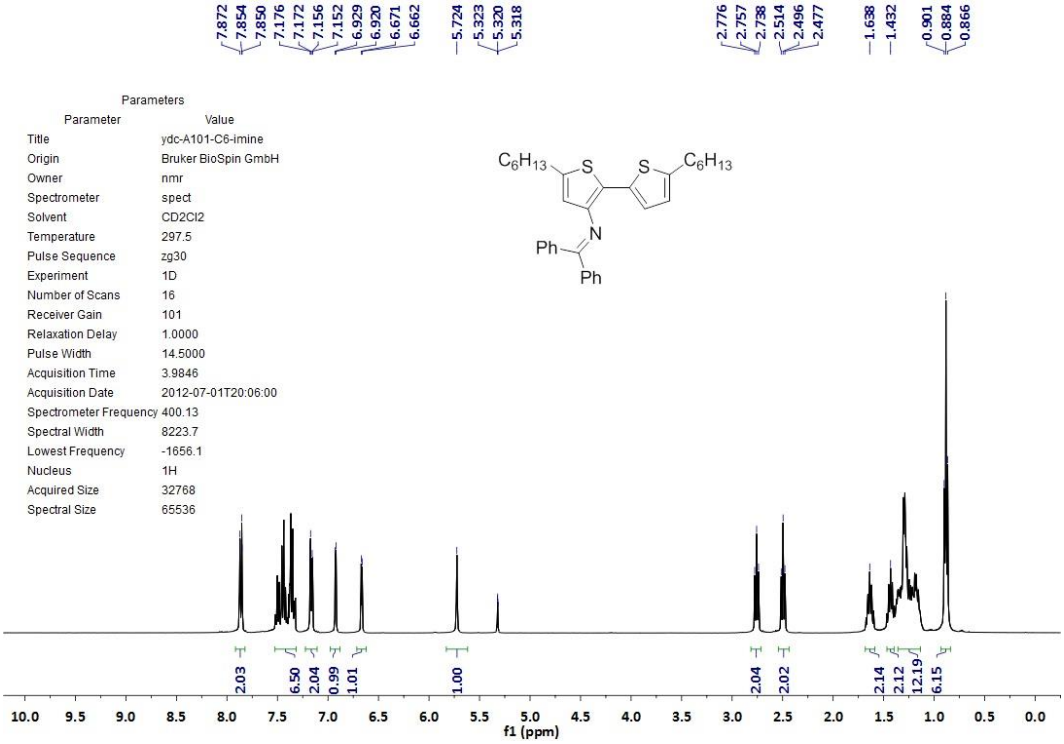

143.35
143.19
142.29
137.57
127.79
121.26
119.00
77.32
77.00
76.68
31.62
31.40
31.23
31.12
30.90
30.43
22.49
22.43
14.04
14.01
Parameters
Parameter Value
Title C5-BNTTN-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 128
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 12.0000
Acquisition Time 1.3632
Acquisition Date 2014-03-21T16:22:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C5H11
S
B
N
f1 (ppm)

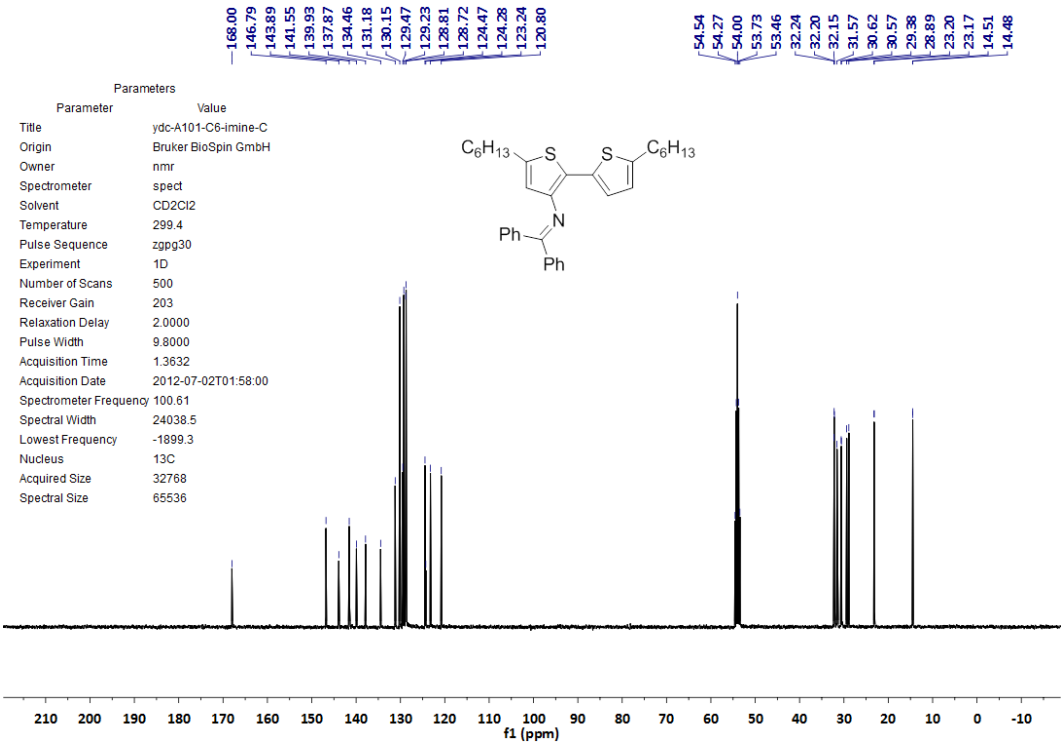

7.257
6.892
6.884
6.644
6.635
2.787
2.768
2.749
1.665
1.646
1.542
1.319
1.310
1.302
0.888
0.871
0.000
Parameters
Parameter Value
Title C6-BiTh
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 300.3
Pulse Sequence zg30
Experiment 1D
Number of Scans 32
Receiver Gain 203
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2014-06-26T13:22:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1651.7
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C6H13
S
S
C6H13
1.99
2.00
4.00
3.98
11.98
5.96
10.0 9.5 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 0.0
f1 (ppm)

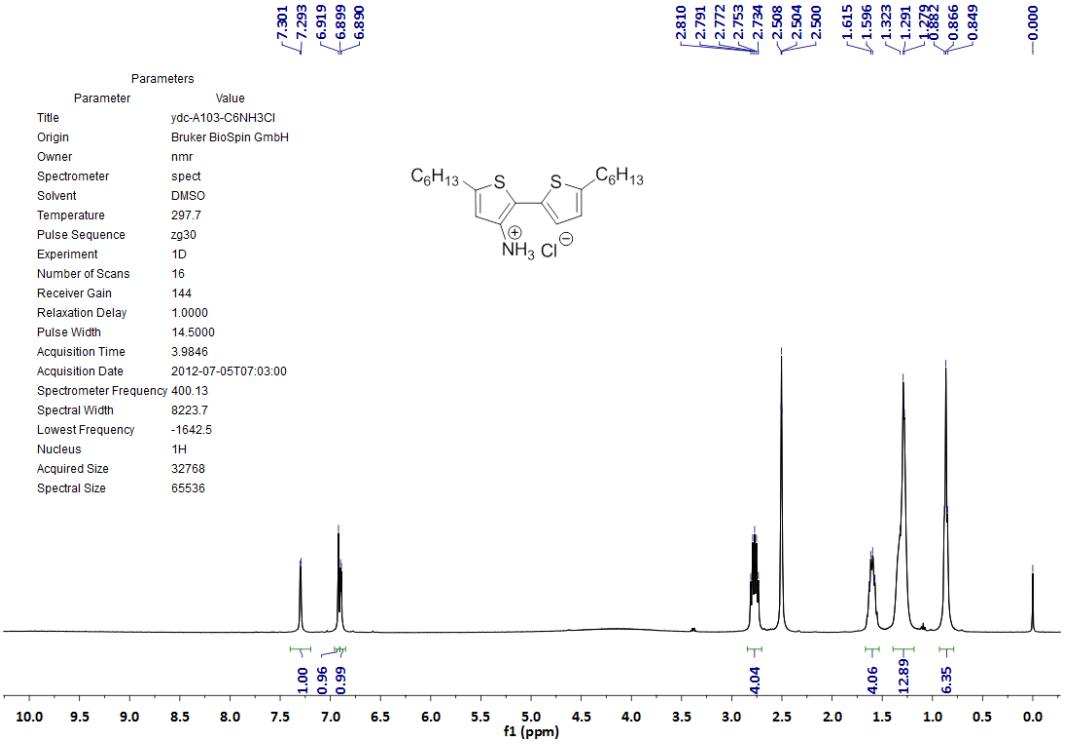

144.63
135.31
124.52
122.55
77.32
77.00
76.68
31.56
30.13
28.74
22.56
14.05
Parameters
Parameter Value
Title C6-BiTh-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 301.1
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 400
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 12.0000
Acquisition Time 1.3632
Acquisition Date 2014-06-26T02:34:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C6H13
S
S
C6H13
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

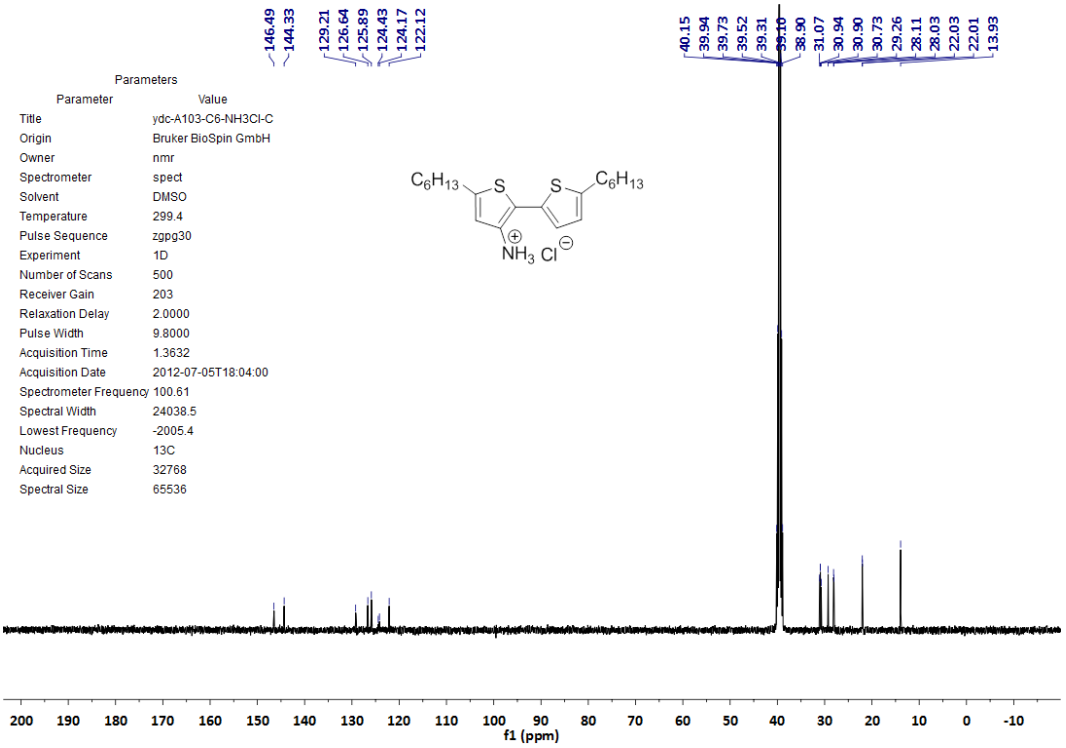

7.249
7.158
7.149
6.712
6.703
6.660
2.811
2.792
2.772
2.744
2.725
2.706
1.665
1.646
1.322
1.315
0.890
0.873
-0.000
Parameters
Parameter Value
Title 0530-LHR-BiThBr
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Number of Scans 32
Receiver Gain 72
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-05-30T18:46:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1655.3
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C6H13
S
S
C6H13
Br
1.00
1.01
0.97
2.08
2.08
4.24
12.94
6.19
10.0 9.5 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 0.0
f1 (ppm)

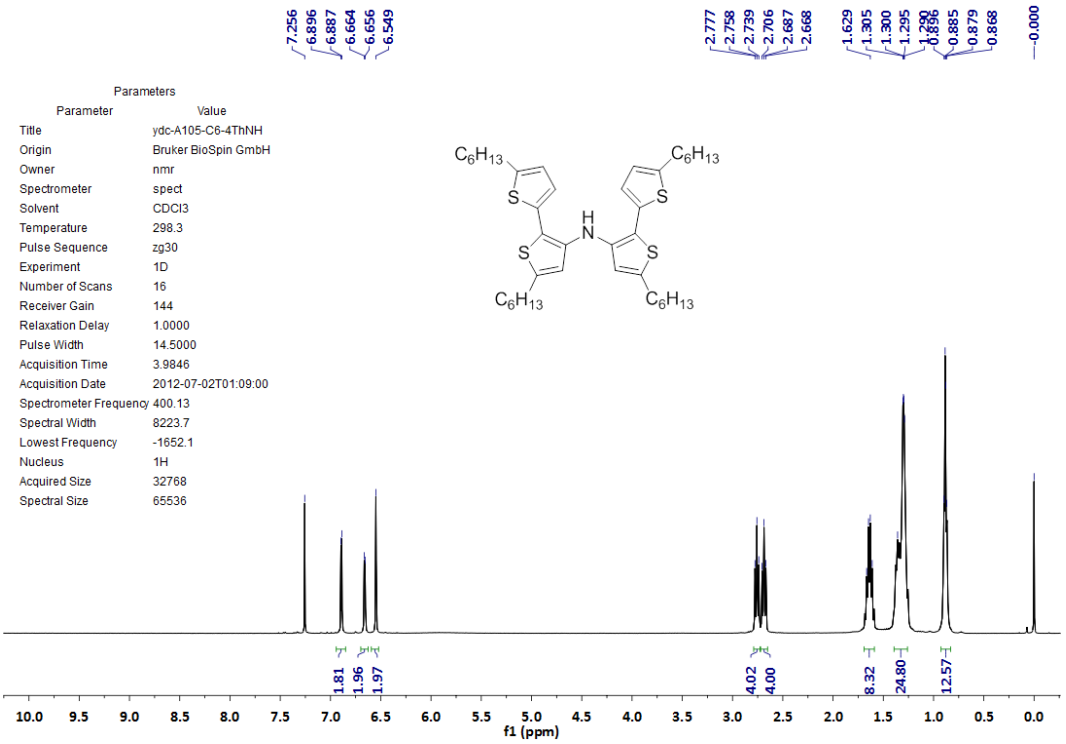

146.45
144.12
132.14
130.06
128.47
125.81
124.14
105.86
77.32
77.00
76.68
31.55
31.52
31.50
31.07
30.11
30.01
28.80
28.65
22.56
22.53
14.06
14.05
Parameters
Parameter Value
Title 0530-LHR-BiThBr
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.5
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 1024
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-05-31T04:02:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C6H13
S
S
C6H13
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

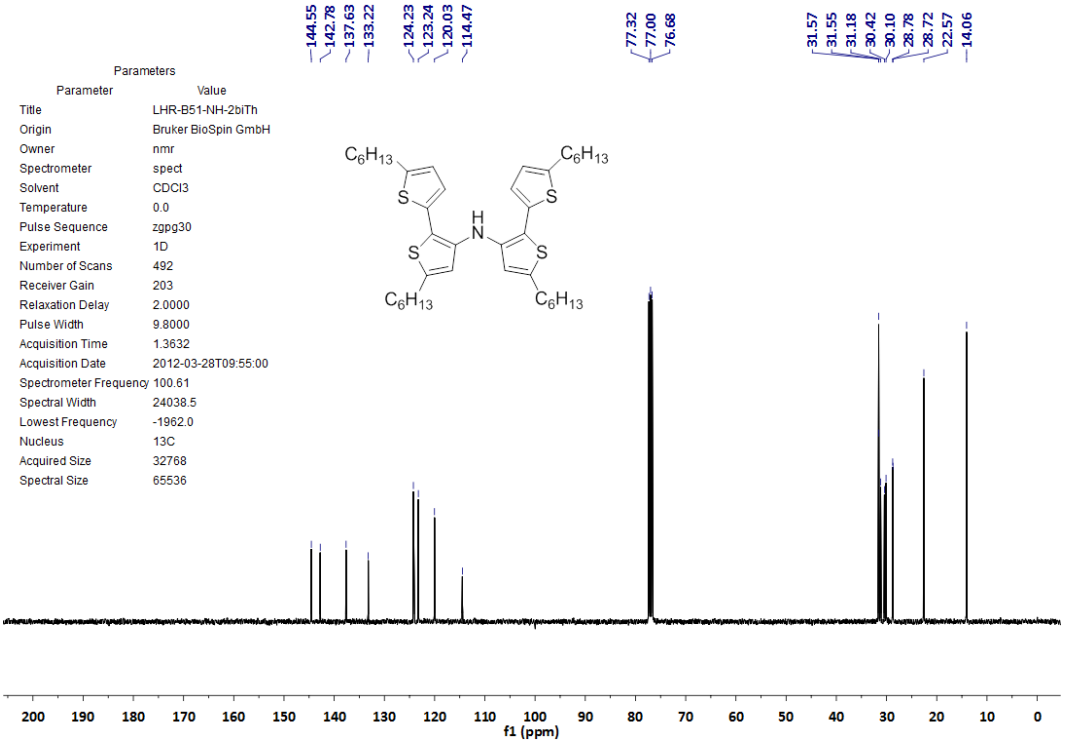

7.872
7.854
7.850
7.176
7.172
7.156
7.152
6.929
6.920
6.671
6.662
5.724
5.323
5.320
5.318
2.776
2.757
2.738
2.514
2.496
2.477
1.638
1.432
0.901
0.884
0.866
Parameters
Parameter Value
Title ydc-A101-C6-imine
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CD2Cl2
Temperature 297.5
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 101
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-07-01T20:06:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1656.1
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C6H13
S
S
C6H13
N
Ph
Ph
2.03
6.50
2.04
0.99
1.01
1.00
2.04
2.02
2.14
2.12
12.19
6.15
10.0 9.5 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 0.0
f1 (ppm)

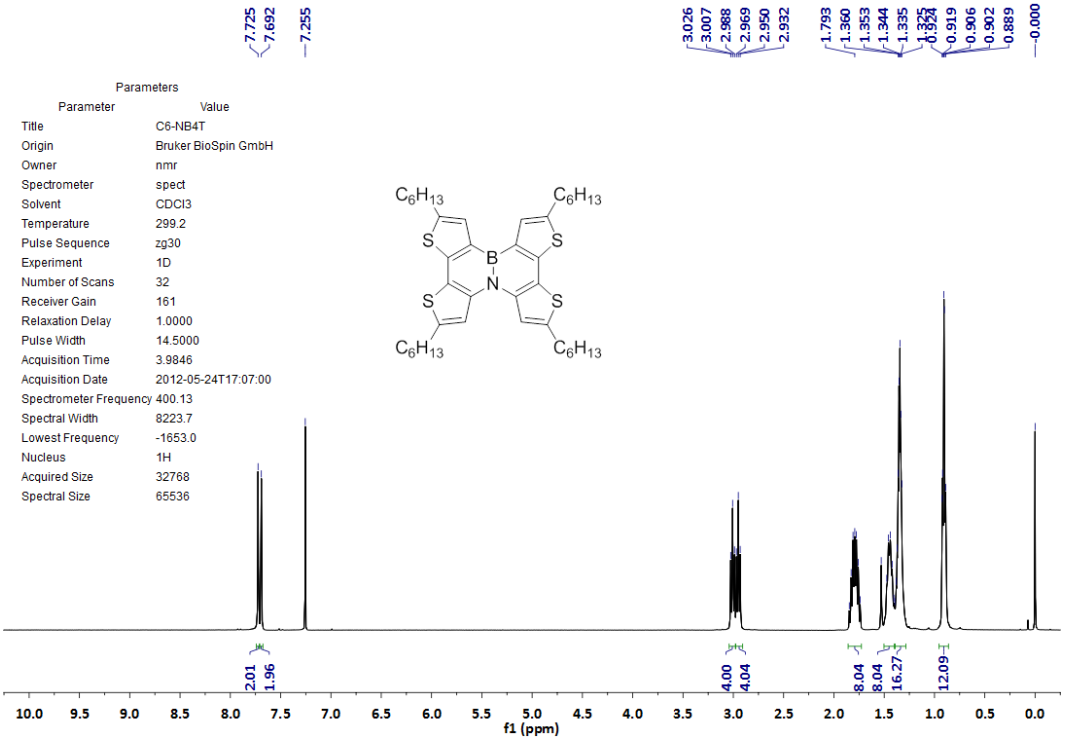

168.00
146.79
143.89
141.55
139.93
137.87
134.46
131.18
130.15
129.47
129.23
128.81
128.72
124.47
124.28
123.24
120.80
54.54
54.27
54.00
53.73
53.46
32.24
32.20
32.15
31.57
30.62
30.57
29.38
28.89
23.20
23.17
14.51
14.48
Parameters
Parameter Value
Title ydc-A101-C6-imine-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CD2Cl2
Temperature 299.4
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 500
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-07-02T01:58:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1899.3
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C6H13
S
S
C6H13
N
Ph
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

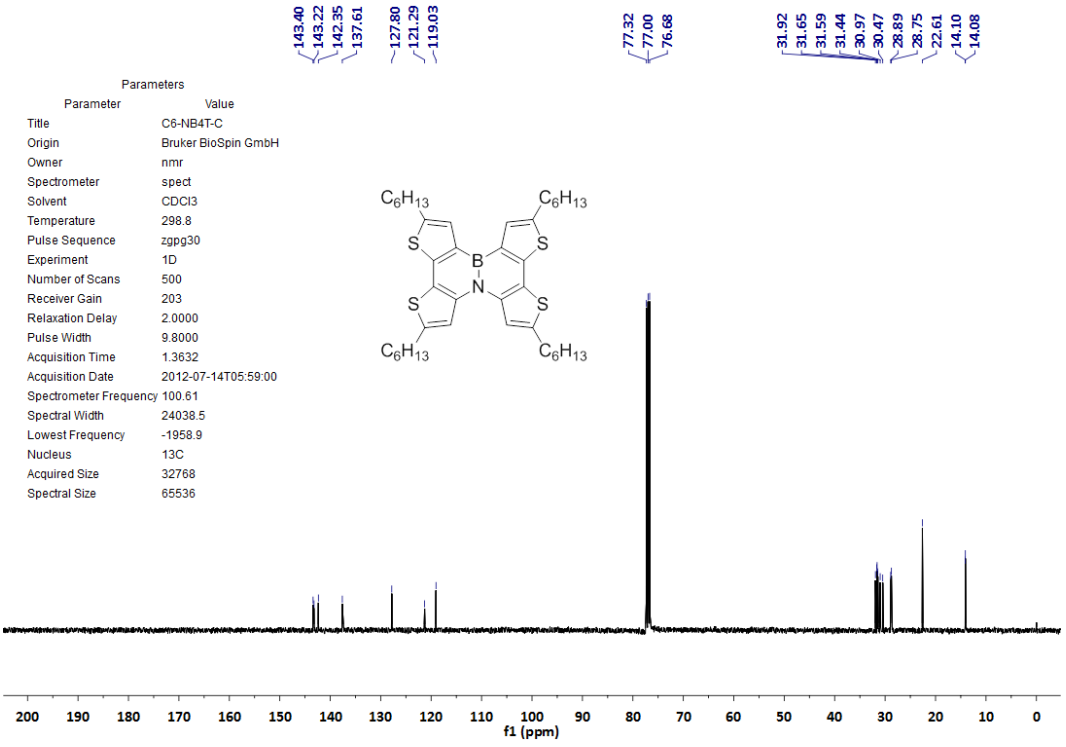

7.301
7.293
6.919
6.899
6.890
2.810
2.791
2.772
2.753
2.734
2.508
2.504
2.500
1.615
1.596
1.323
1.291
1.279
0.882
0.866
0.849
0.000
Parameters
Parameter Value
Title ydc-A103-C6NH3Cl
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent DMSO
Temperature 297.7
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 144
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-07-05T07:03:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1642.5
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C6H13
S
S
C6H13
NH3 Cl
1.00
0.96
0.99
4.04
4.06
12.89
6.35
10.0 9.5 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 0.0
f1 (ppm)


146.49
144.33
129.21
126.64
125.89
124.43
124.17
122.12
40.15
39.94
39.73
39.52
39.31
39.10
38.90
31.07
30.94
30.90
30.73
29.26
28.11
28.03
22.03
22.01
13.93
Parameters
Parameter Value
Title ydc-A103-C6-NH3Cl-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent DMSO
Temperature 299.4
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 500
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-07-05T18:04:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -2005.4
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C6H13
S
S
C6H13
NH3 Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.256
6.896
6.887
6.664
6.656
6.549
2.777
2.758
2.739
2.706
2.687
2.668
1.629
1.305
1.300
1.295
1.290
0.896
0.885
0.879
0.868
-0.000
Parameters
Parameter Value
Title ydc-A105-C6-4ThNH
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.3
Pulse Sequence zg30
Experiment 1D
Number of Scans 16
Receiver Gain 144
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-07-02T01:09:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1652.1
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C6H13
S
H
N
1.81
1.96
1.97
4.02
4.00
8.32
24.80
12.57
10.0 9.5 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 0.0
f1 (ppm)


144.55
142.78
137.63
133.22
124.23
123.24
120.03
114.47
77.32
77.00
76.68
31.57
31.55
31.18
30.42
30.10
28.78
28.72
22.57
14.06
Parameters
Parameter Value
Title LHR-B51-NH-2biTh
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 0.0
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 492
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-03-28T09:55:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1962.0
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C6H13
S
H
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.725
7.692
7.255
3.026
3.007
2.988
2.969
2.950
2.932
1.793
1.360
1.353
1.344
1.335
1.325
0.924
0.919
0.906
0.902
0.889
-0.000
Parameters
Parameter Value
Title C6-NB4T
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 299.2
Pulse Sequence zg30
Experiment 1D
Number of Scans 32
Receiver Gain 161
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 3.9846
Acquisition Date 2012-05-24T17:07:00
Spectrometer Frequency 400.13
Spectral Width 8223.7
Lowest Frequency -1653.0
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
C6H13
S
B
N
2.01
1.96
4.00
4.04
8.04
8.04
16.27
12.09
10.0 9.5 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 0.0
f1 (ppm)


143.40
143.22
142.35
137.61
127.80
121.29
119.03
77.32
77.00
76.68
31.92
31.65
31.59
31.44
30.97
30.47
28.89
28.75
22.61
14.10
14.08
Parameters
Parameter Value
Title C6-NB4T-C
Origin Bruker BioSpin GmbH
Owner nmr
Spectrometer spect
Solvent CDCl3
Temperature 298.8
Pulse Sequence zgpg30
Experiment 1D
Number of Scans 500
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 9.8000
Acquisition Time 1.3632
Acquisition Date 2012-07-14T05:59:00
Spectrometer Frequency 100.61
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
C6H13
S
B
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)