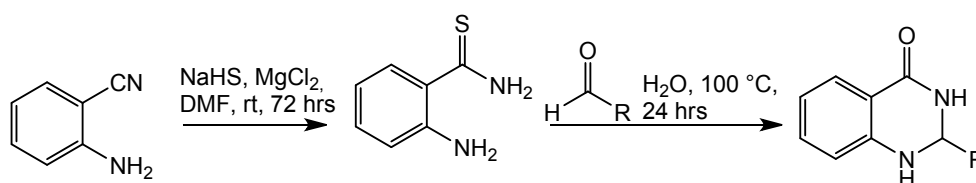


## Supporting Information

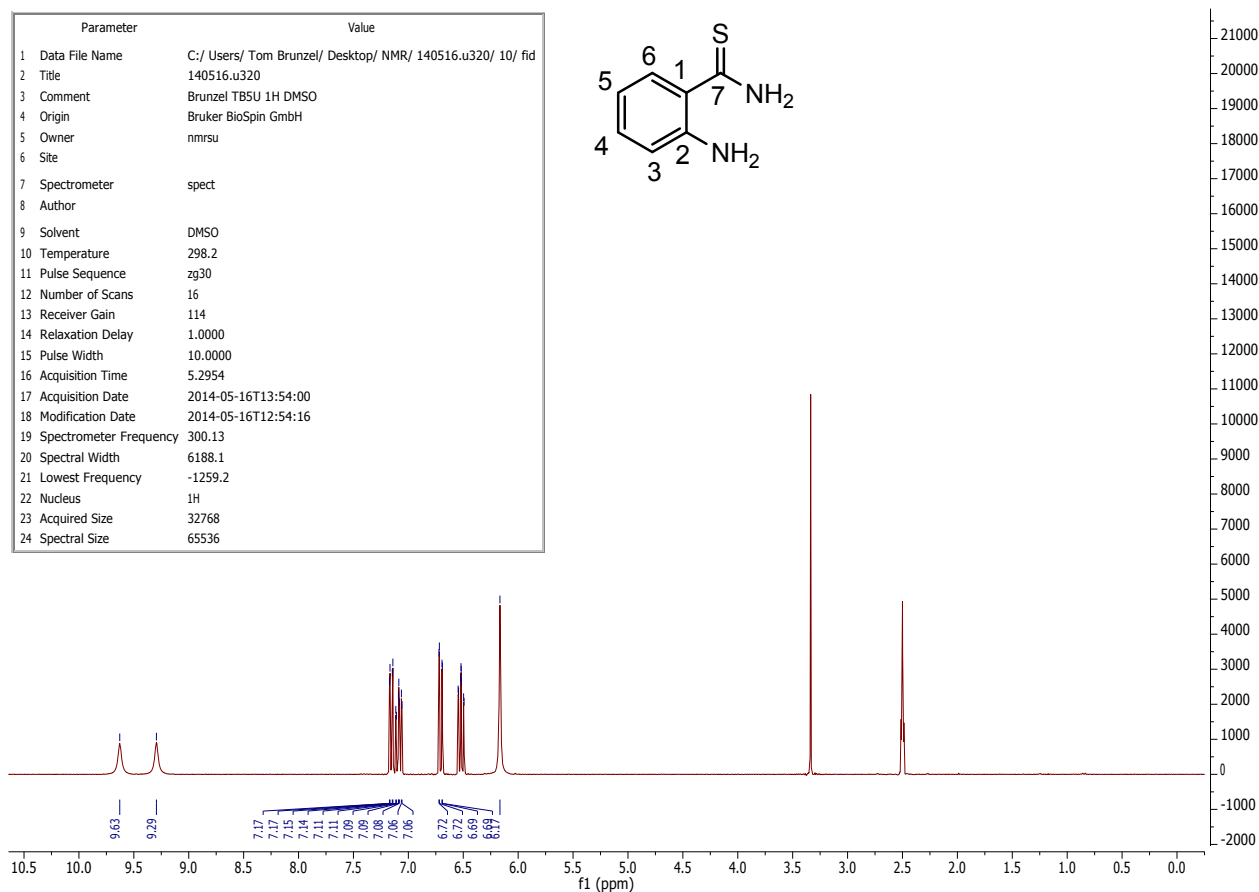
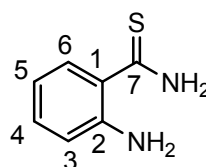
**General remarks:** All Chemicals were commercial available and were used without further purification. Dry DMF over molecular sieve and distilled water were used as solvents. NMR-data was recorded by Bruker AVANCE 300 III, Bruker AVANCE 250 III, Bruker ARX 300 and Bruker ARX 400 spectrometers.  $^{13}\text{C}$ - and  $^1\text{H}$ -spectra were referenced to residue solvent signals. Peaks were characterized as singlet (*s*), doublet (*d*), doublet of doublet (*dd*), triplet (*t*), doublet of triplets (*dt*), quartet (*q*) and multiplet (*m*). Gas-chromatographie-mass-analysis was measured by an Agilent HP-5890 with Agilent HP-5973 Mass Selective Detector (EI) and HP-5-capillary column using helium as carrier gas. Elemental analysis was performed on a Flash EA 112 and IR-spectra were recorded on a Nicolet 380 FT-IR spectrometer. IR-bands are classified as strong (*s*), medium (*m*) and weak (*w*). Column-chromatographie was carried out using Merck 60 Silica-Gel (0.043 - 0.06 mm) and distilled solvents were used.

### General experimental procedure:

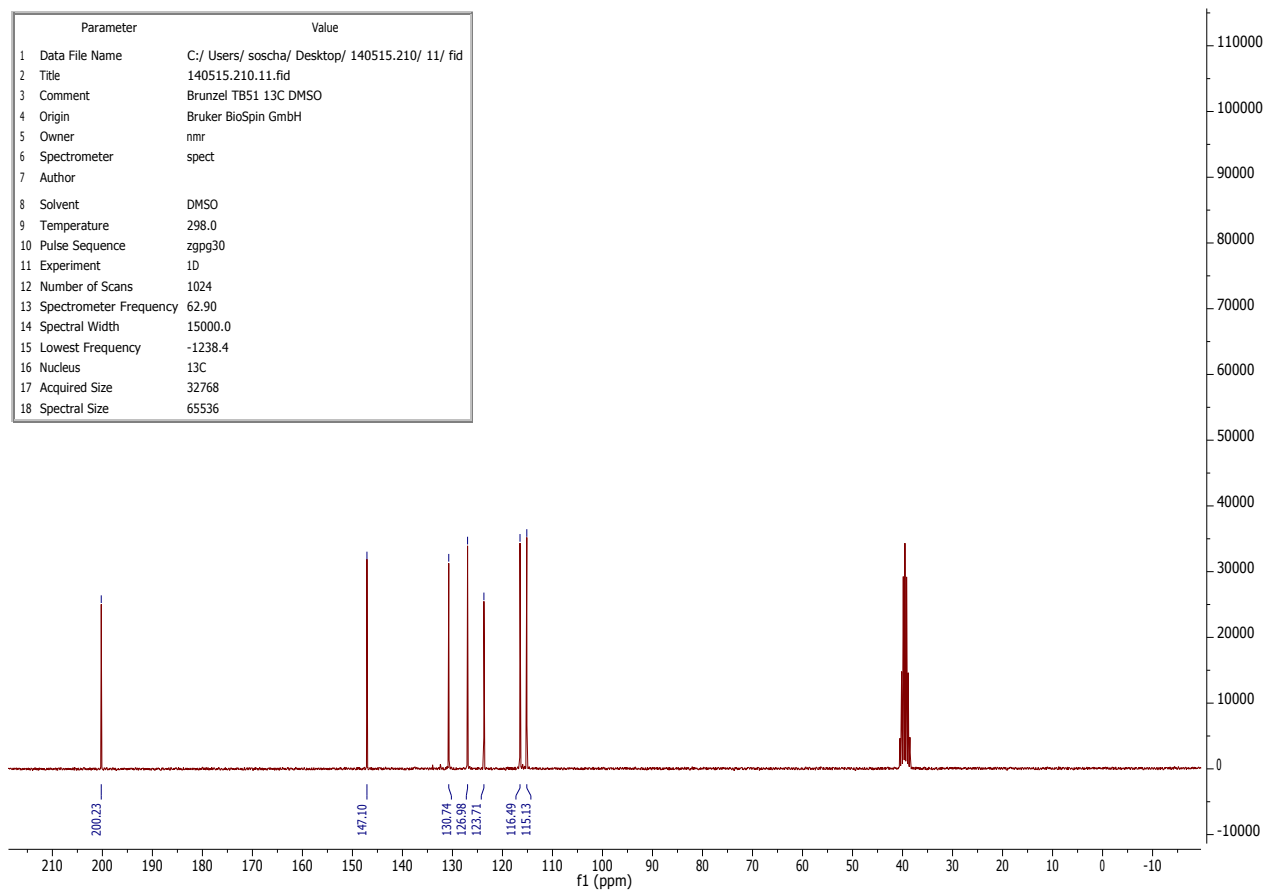


### 2-Aminobenzothioamide (1a):

Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140516.u320/10/fid
2 Title	140516.u320
3 Comment	Brunzel TB5U 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsru
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	114
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	5.2954
17 Acquisition Date	2014-05-16T13:54:00
18 Modification Date	2014-05-16T12:54:16
19 Spectrometer Frequency	300.13
20 Spectral Width	6188.1
21 Lowest Frequency	-1259.2
22 Nucleus	$^1\text{H}$
23 Acquired Size	32768
24 Spectral Size	65536

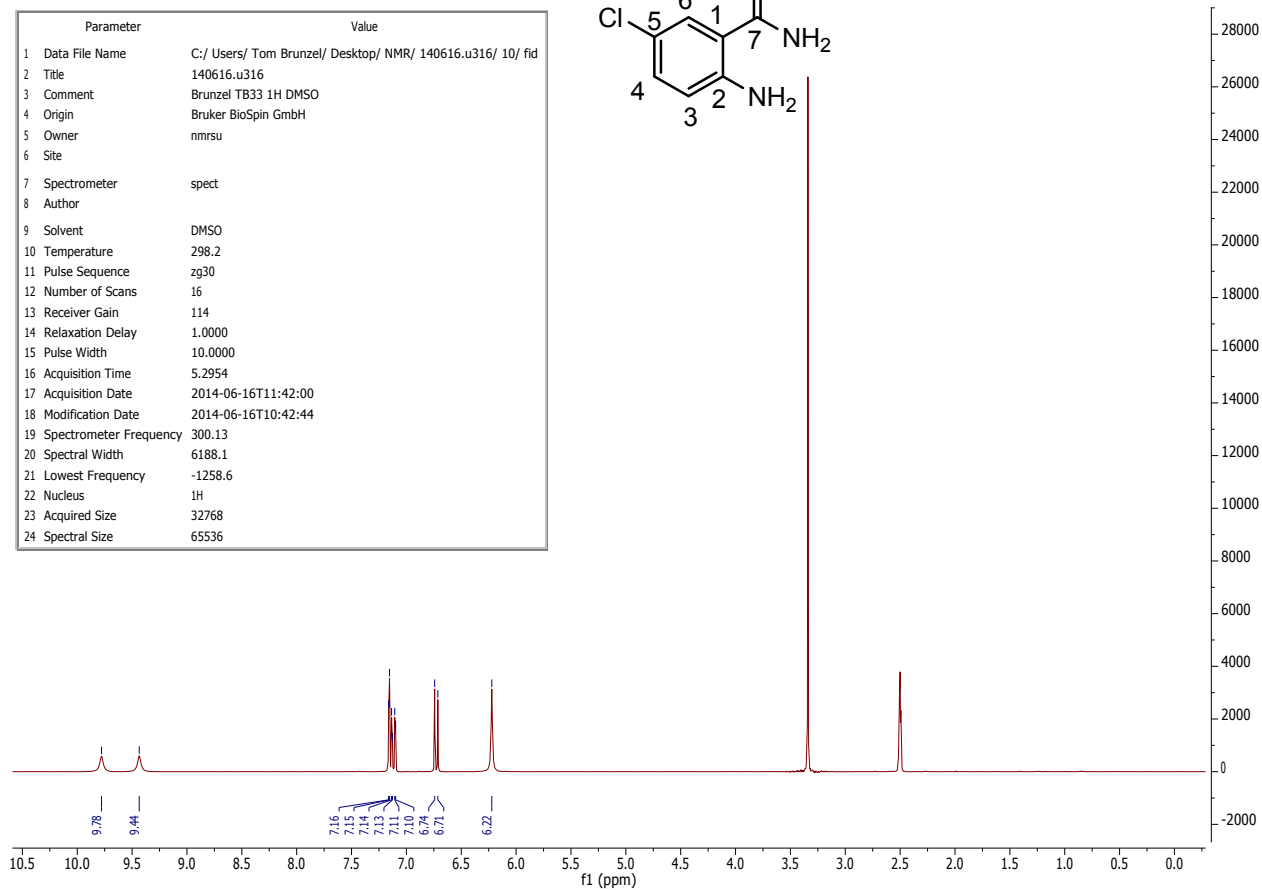
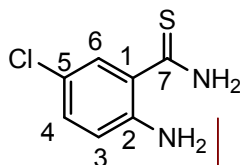


Parameter	Value
1 Data File Name	C:/ Users/ soscha/ Desktop/ 140515.210/ 11/ fid
2 Title	140515.210.11.fid
3 Comment	Brunzel TB51 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	298.0
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	1024
13 Spectrometer Frequency	62.90
14 Spectral Width	15000.0
15 Lowest Frequency	-1238.4
16 Nucleus	13C
17 Acquired Size	32768
18 Spectral Size	65536

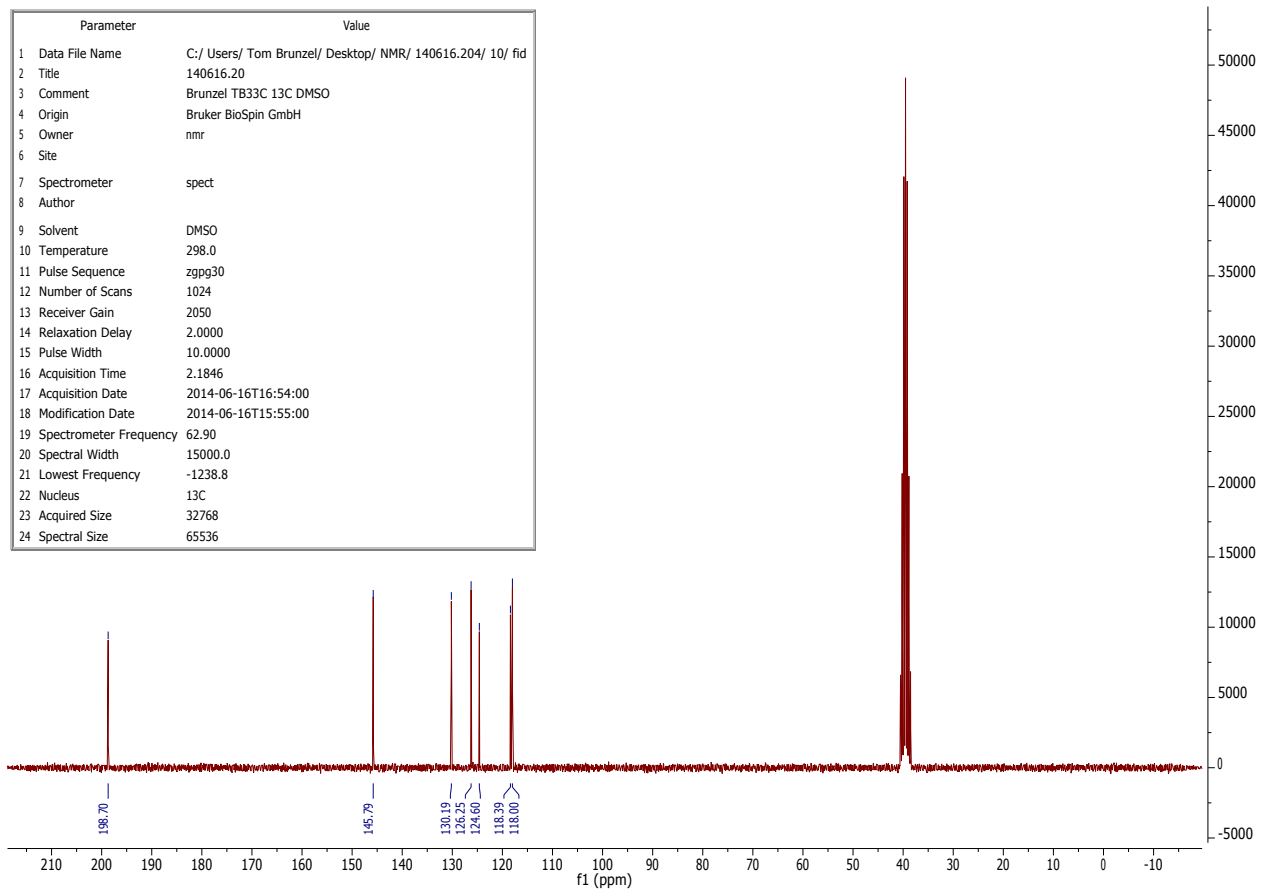


## 2-Amino-5-chlorobenzothioamide (1b):

Parameter	Value
1 Data File Name	C:/ Users/ Tom Brunzel/ Desktop/ NMR/ 140616.u316/ 10/ fid
2 Title	140616.u316
3 Comment	Brunzel TB33 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	114
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	5.2954
17 Acquisition Date	2014-06-16T11:42:00
18 Modification Date	2014-06-16T10:42:44
19 Spectrometer Frequency	300.13
20 Spectral Width	6188.1
21 Lowest Frequency	-1258.6
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

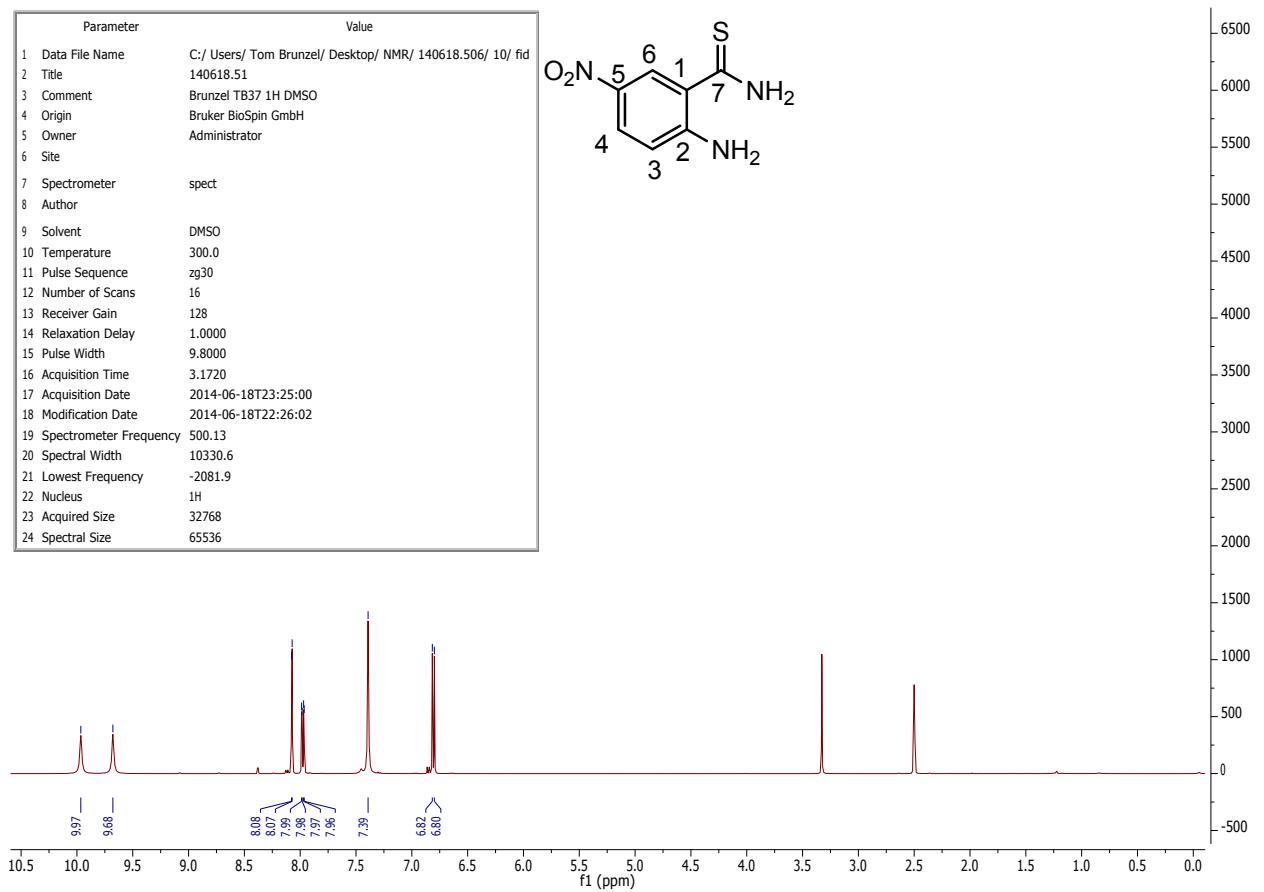
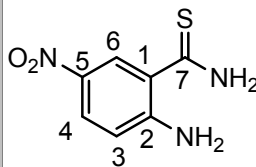


Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140616.204/10/fid
2 Title	140616.20
3 Comment	Brunzel TB33C 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Number of Scans	1024
13 Receiver Gain	2050
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	2.1846
17 Acquisition Date	2014-06-16T16:54:00
18 Modification Date	2014-06-16T15:55:00
19 Spectrometer Frequency	62.90
20 Spectral Width	15000.0
21 Lowest Frequency	-1238.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

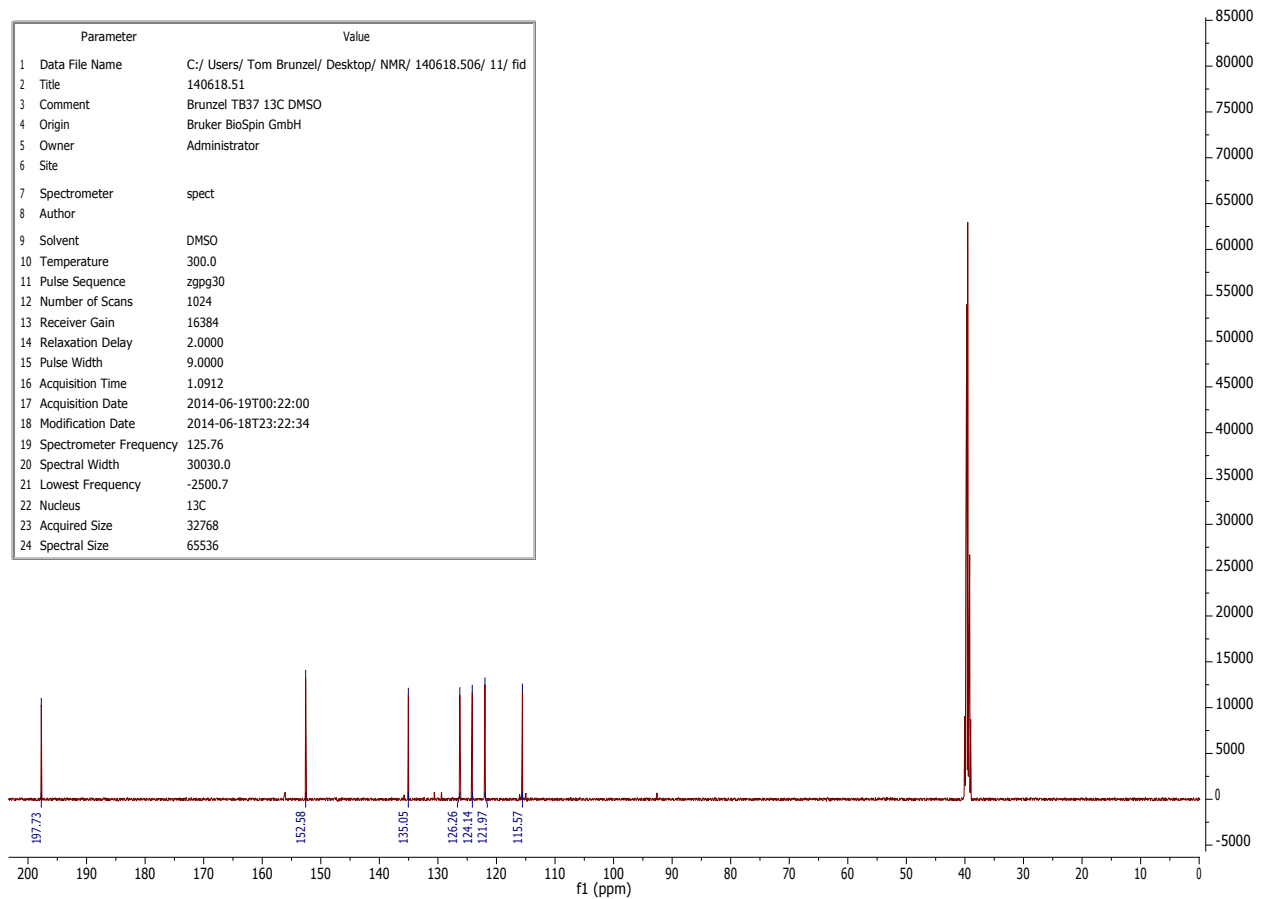


## 2-Amino-5-nitrobenzothioamide (1c):

Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140618.506/10/fid
2 Title	140618.51
3 Comment	Brunzel TB37 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	128
14 Relaxation Delay	1.0000
15 Pulse Width	9.8000
16 Acquisition Time	3.1720
17 Acquisition Date	2014-06-18T23:25:00
18 Modification Date	2014-06-18T22:26:02
19 Spectrometer Frequency	500.13
20 Spectral Width	10330.6
21 Lowest Frequency	-2081.9
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

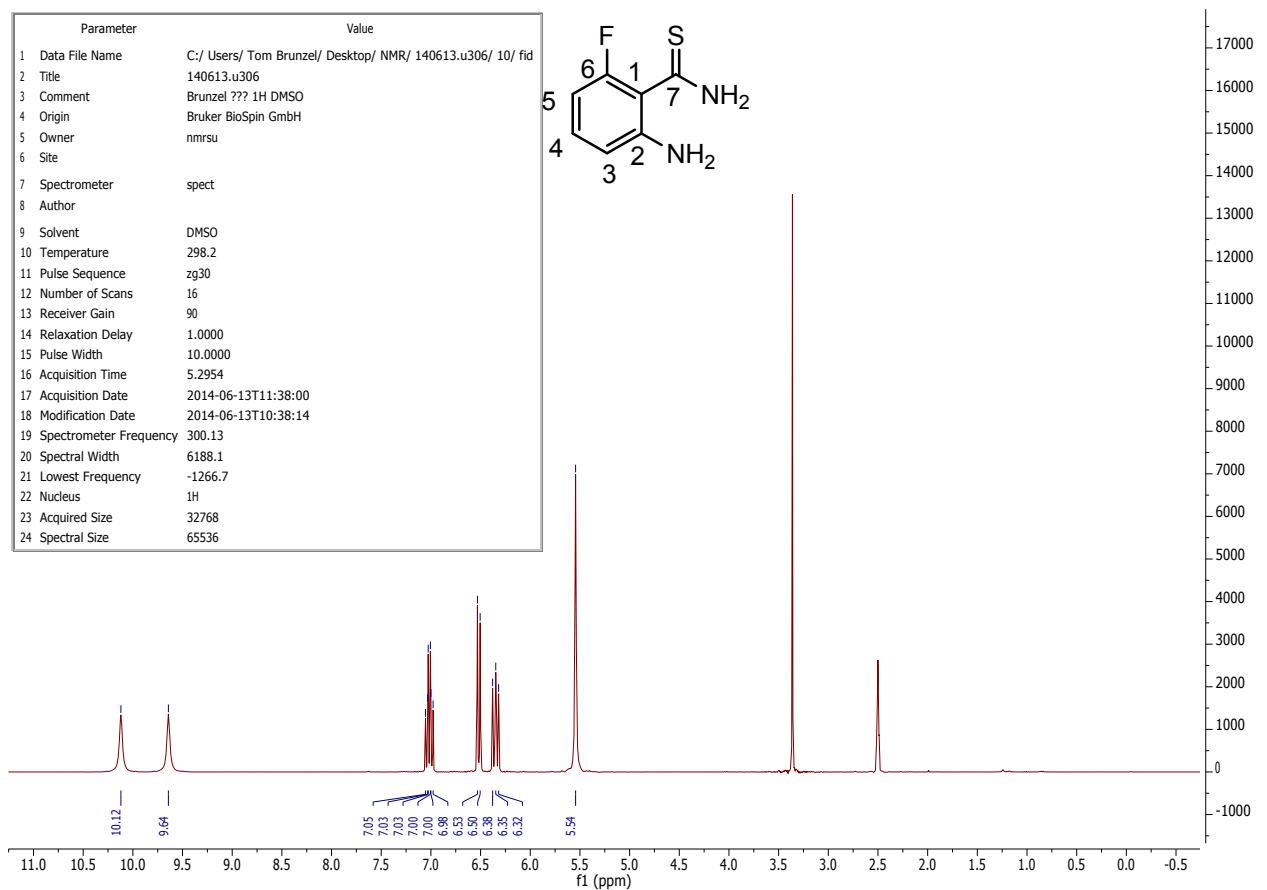
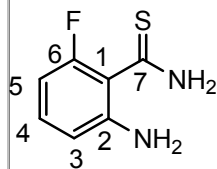


Parameter	Value
1 Data File Name	C:/ Users/ Tom Brunzel/ Desktop/ NMR/ 140618.506/ 11/ fid
2 Title	140618.51
3 Comment	Brunzel TB37 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Number of Scans	1024
13 Receiver Gain	16384
14 Relaxation Delay	2.0000
15 Pulse Width	9.0000
16 Acquisition Time	1.0912
17 Acquisition Date	2014-06-19T00:22:00
18 Modification Date	2014-06-18T23:22:34
19 Spectrometer Frequency	125.76
20 Spectral Width	30030.0
21 Lowest Frequency	-2500.7
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

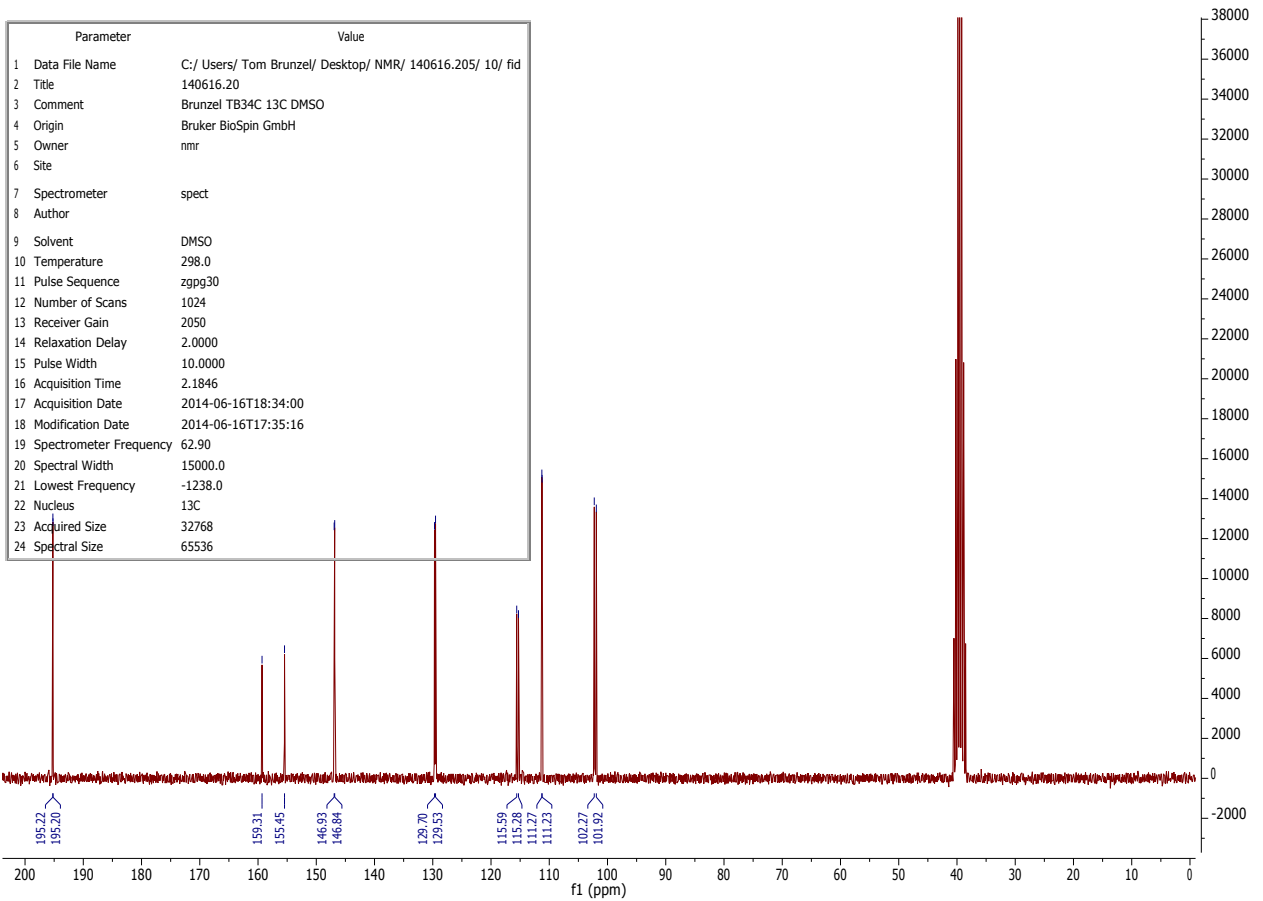


## 2-Amino-6-fluorobenzothioamide (1d):

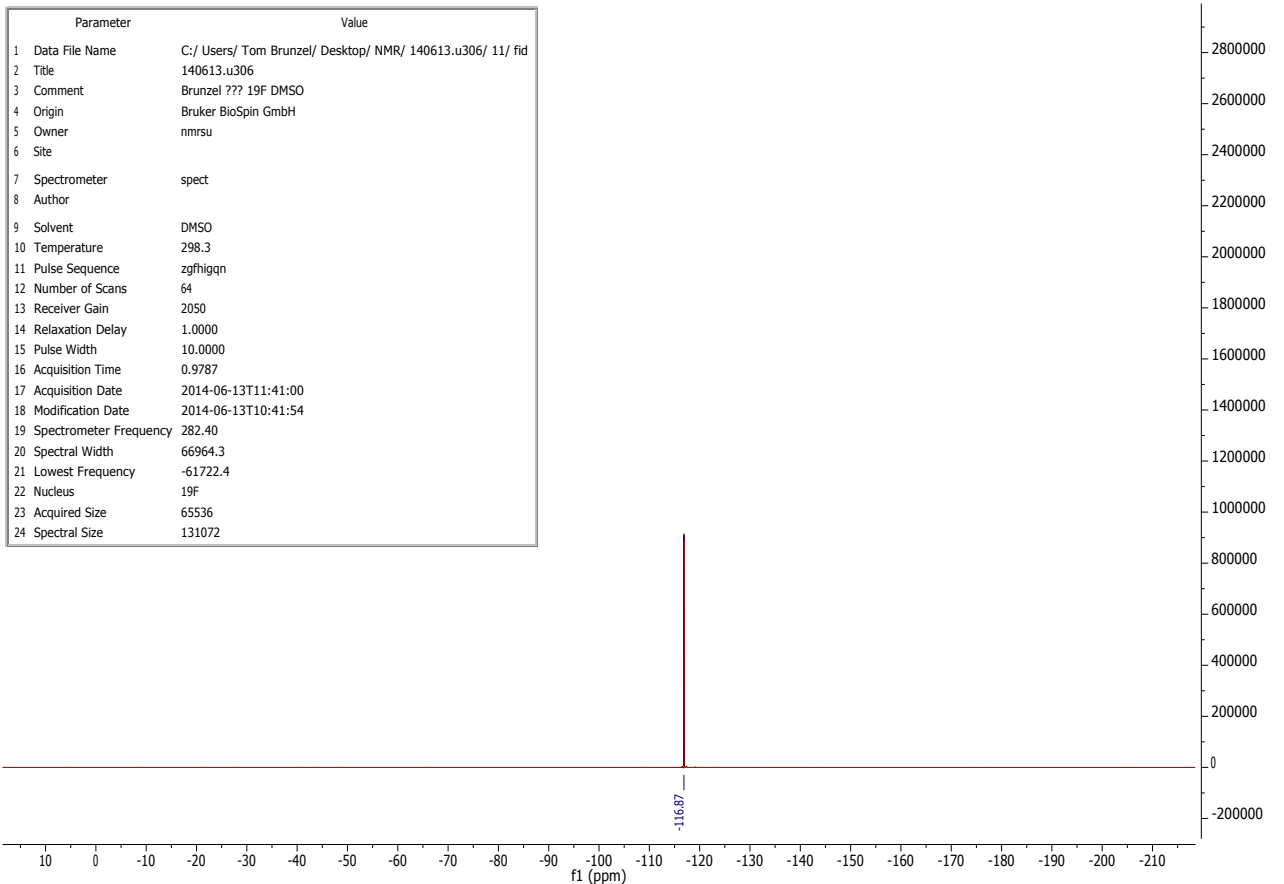
Parameter	Value
1 Data File Name	C:/ Users/ Tom Brunzel/ Desktop/ NMR/ 140613.u306/ 10/ fid
2 Title	140613.u306
3 Comment	Brunzel ??? 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	90
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	5.2954
17 Acquisition Date	2014-06-13T11:38:00
18 Modification Date	2014-06-13T10:38:14
19 Spectrometer Frequency	300.13
20 Spectral Width	6188.1
21 Lowest Frequency	-1266.7
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140616.205/10/fid
2 Title	140616.20
3 Comment	Brunzel TB34C 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Number of Scans	1024
13 Receiver Gain	2050
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	2.1846
17 Acquisition Date	2014-06-16T18:34:00
18 Modification Date	2014-06-16T17:35:16
19 Spectrometer Frequency	62.90
20 Spectral Width	15000.0
21 Lowest Frequency	-1238.0
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

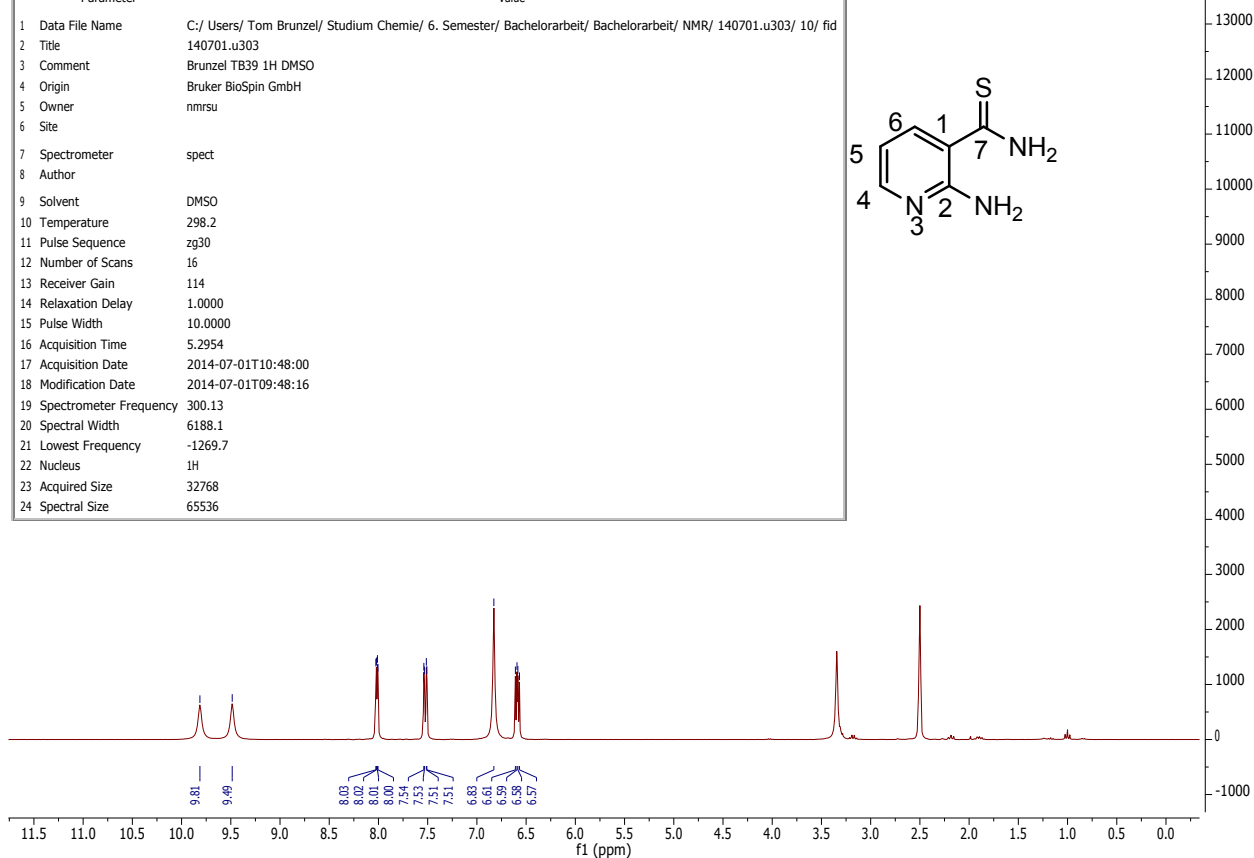
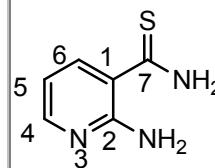


Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140613.u306/11/fid
2 Title	140613.u306
3 Comment	Brunzel ??? 19F DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.3
11 Pulse Sequence	zgfhgq
12 Number of Scans	64
13 Receiver Gain	2050
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	0.9787
17 Acquisition Date	2014-06-13T11:41:00
18 Modification Date	2014-06-13T10:41:54
19 Spectrometer Frequency	282.40
20 Spectral Width	66964.3
21 Lowest Frequency	-61722.4
22 Nucleus	19F
23 Acquired Size	65536
24 Spectral Size	131072

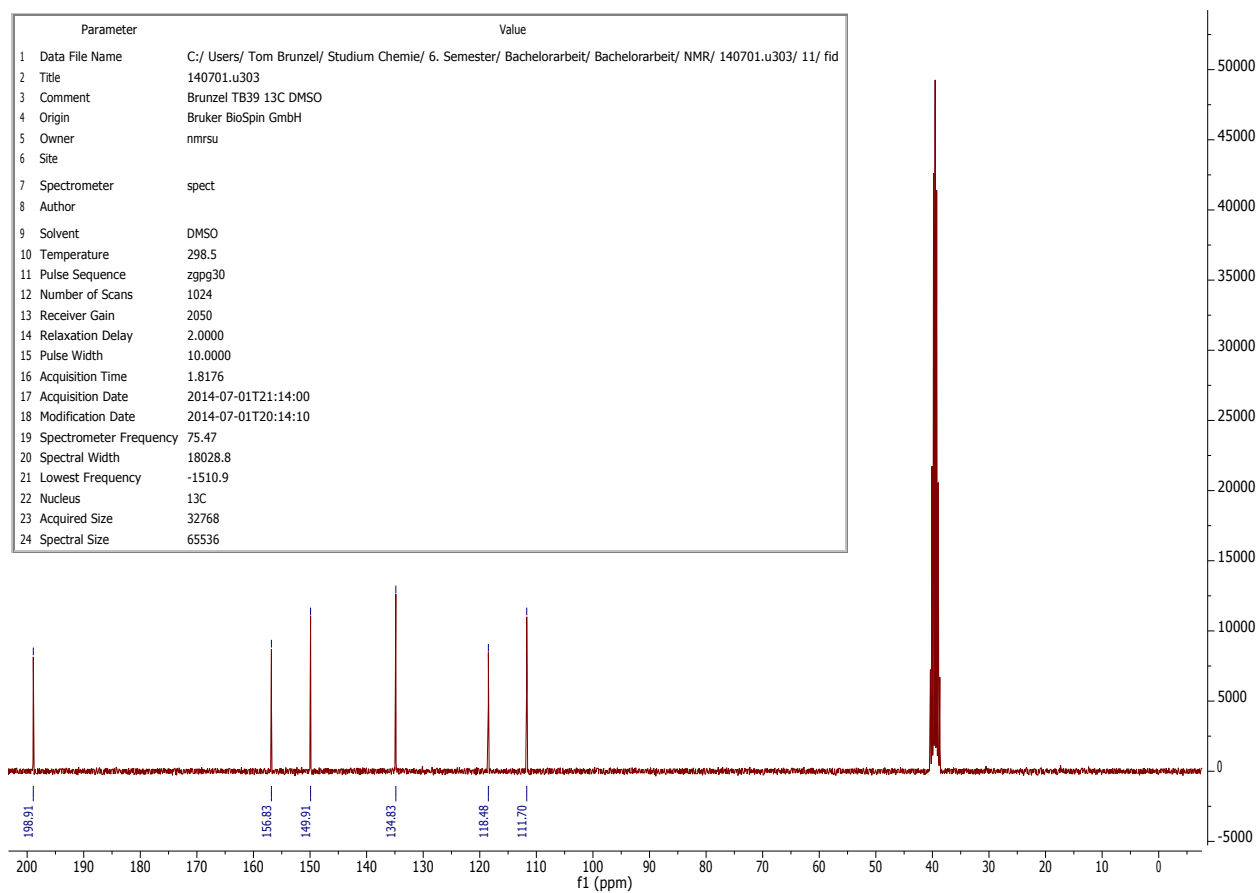


## 2-Aminopyridine-3-carbothioamide (1e):

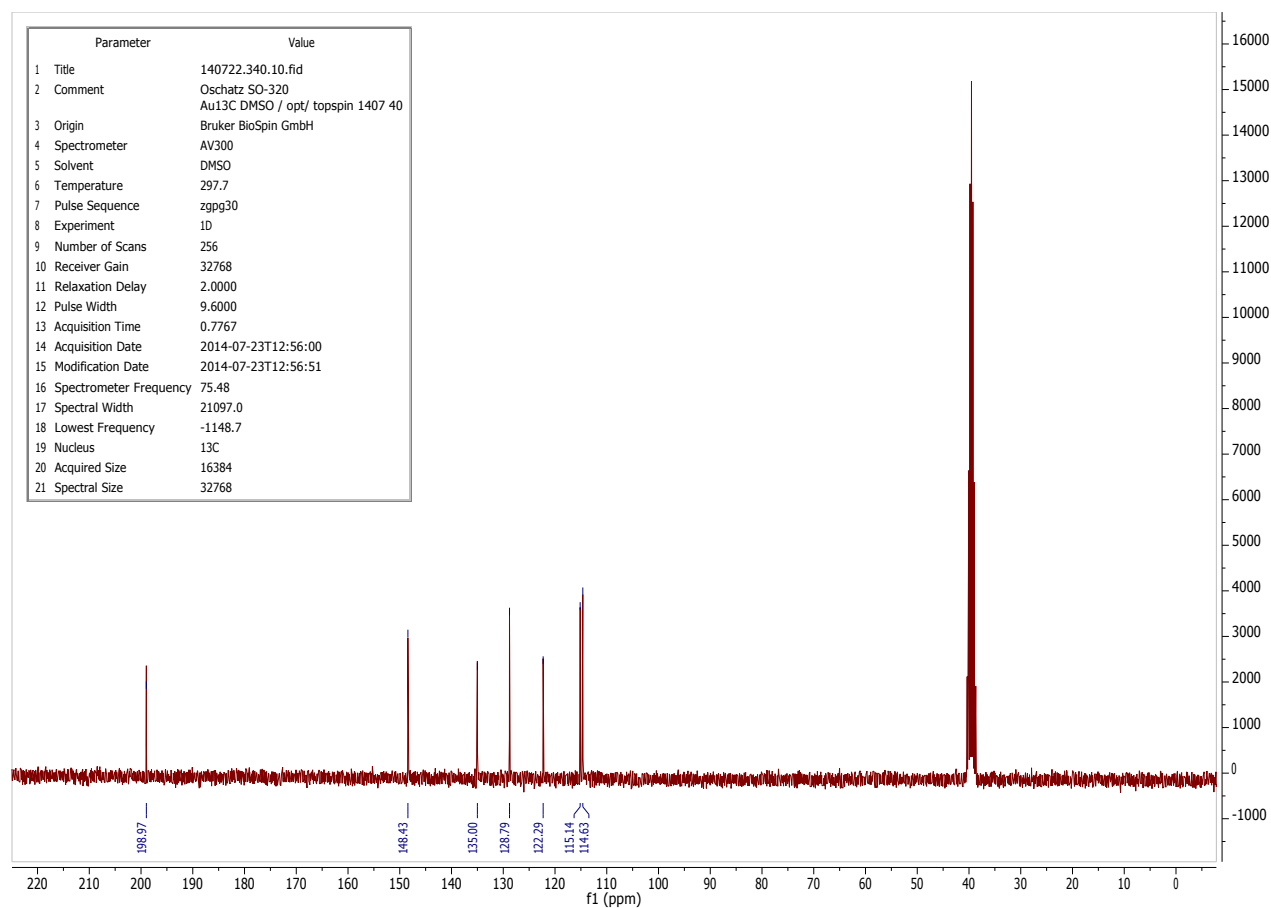
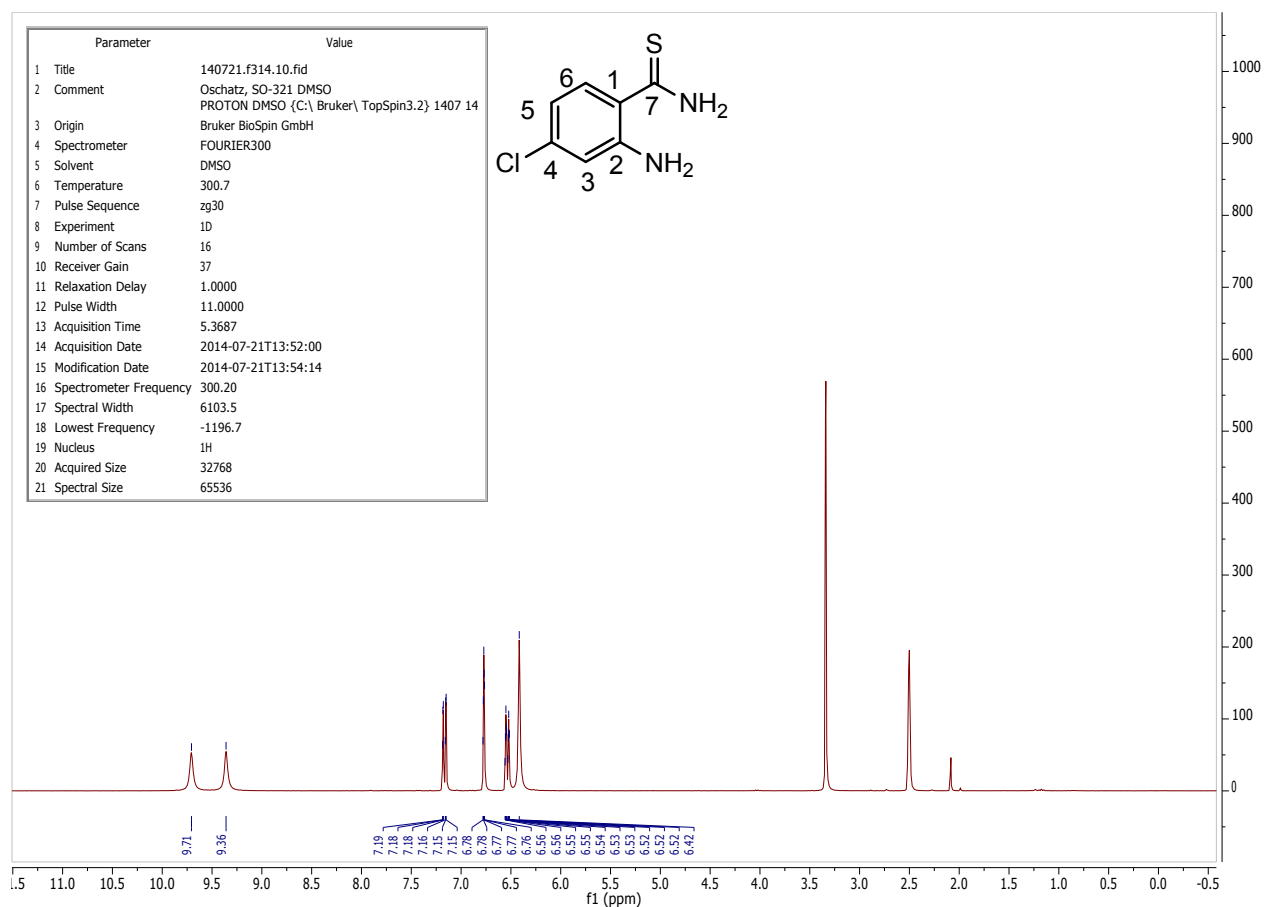
Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Studium Chemie/6. Semester/Bachelorarbeit/Bachelorarbeit/NMR/140701.u303/10/ fid
2 Title	140701.u303
3 Comment	Brunzel TB39 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	114
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	5.2954
17 Acquisition Date	2014-07-01T10:48:00
18 Modification Date	2014-07-01T09:48:16
19 Spectrometer Frequency	300.13
20 Spectral Width	6188.1
21 Lowest Frequency	-1269.7
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



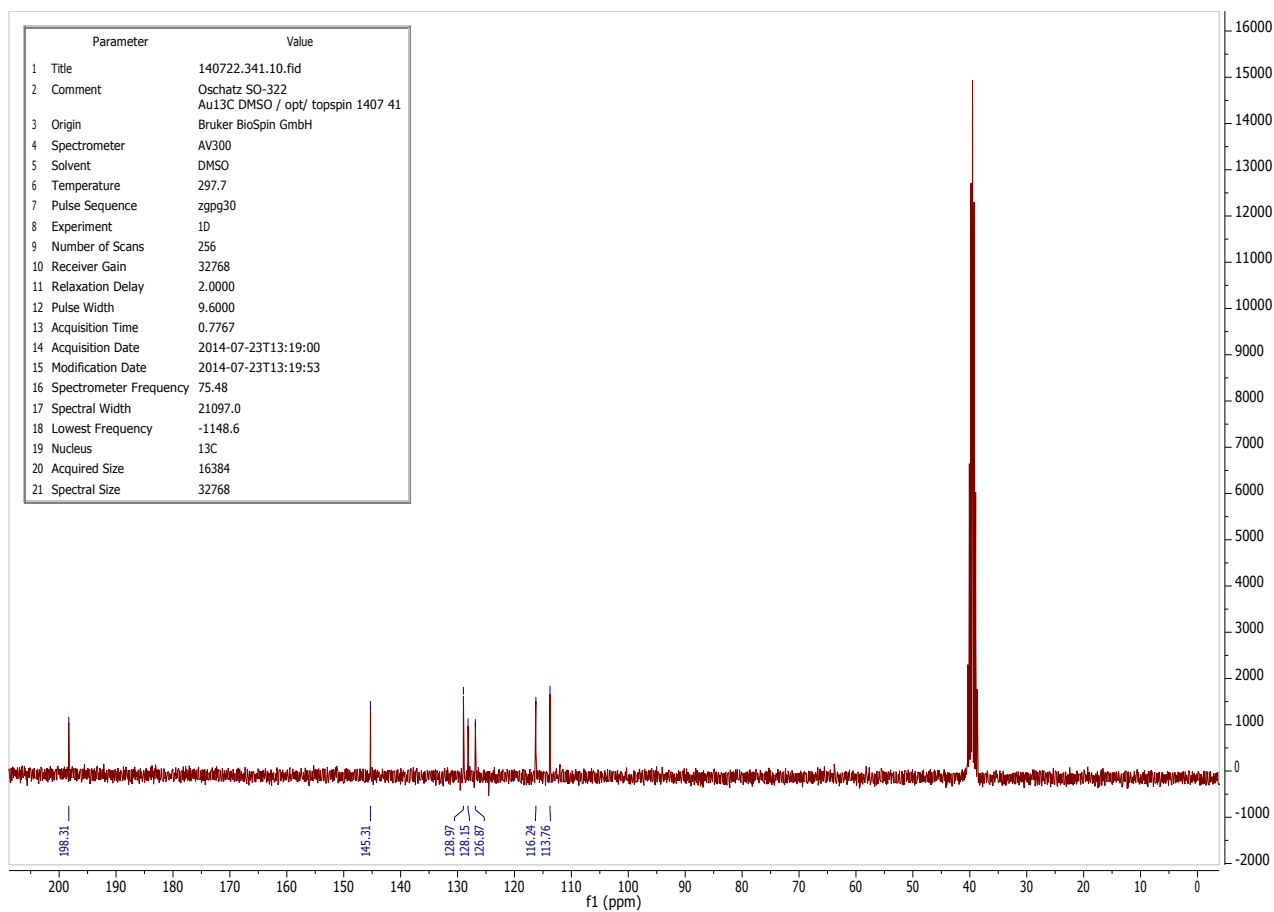
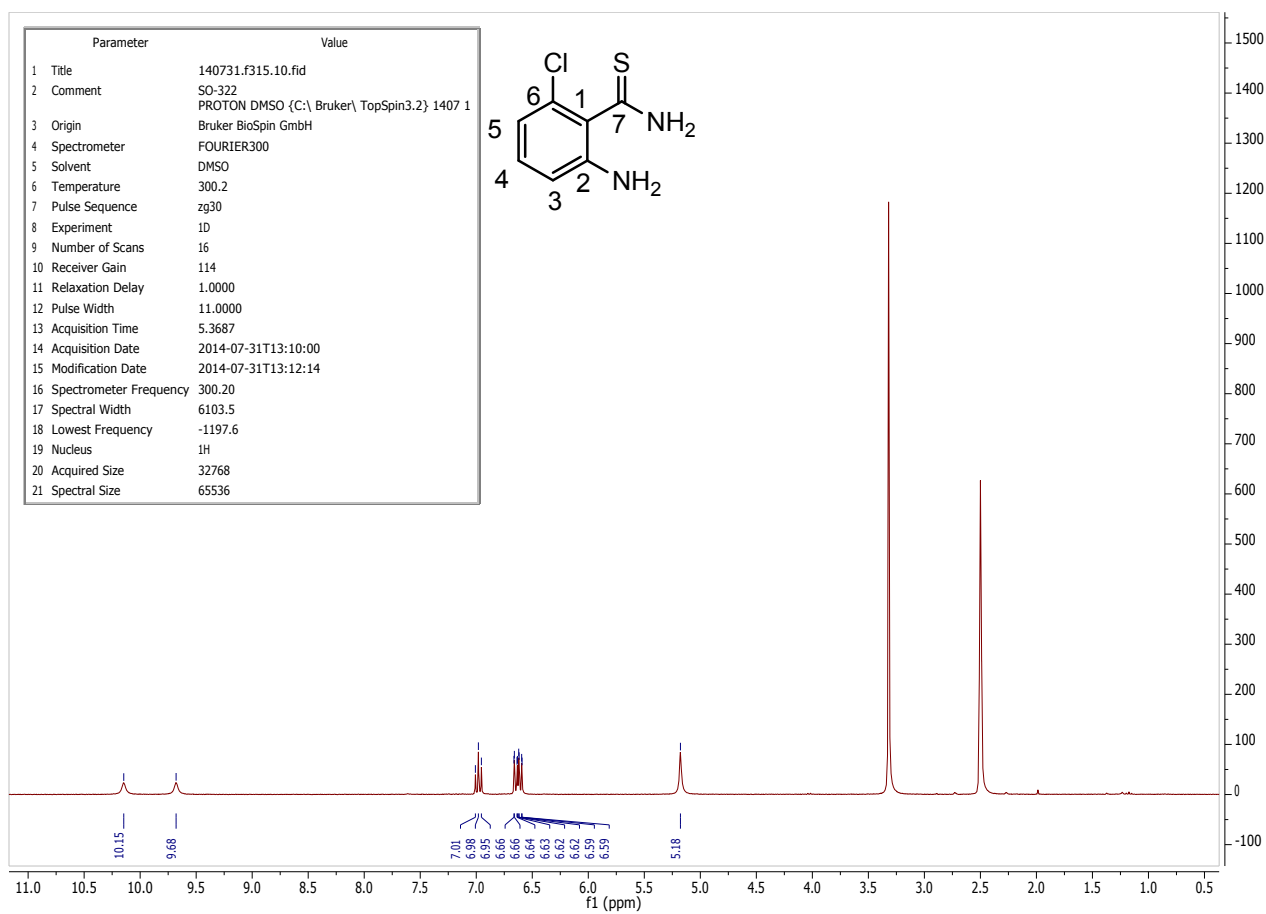
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1 Data File Name	C:/Users/Tom Brunzel/Studium Chemie/6. Semester/Bachelorarbeit/Bachelorarbeit/NMR/140701.u303/11/ fid
2 Title	140701.u303
3 Comment	Brunzel TB39 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.5
11 Pulse Sequence	zgpg30
12 Number of Scans	1024
13 Receiver Gain	2050
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	1.8176
17 Acquisition Date	2014-07-01T21:14:00
18 Modification Date	2014-07-01T20:14:10
19 Spectrometer Frequency	75.47
20 Spectral Width	18028.8
21 Lowest Frequency	-1510.9
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536



## 2-Amino-4-chlorobenzothioamide (1f):

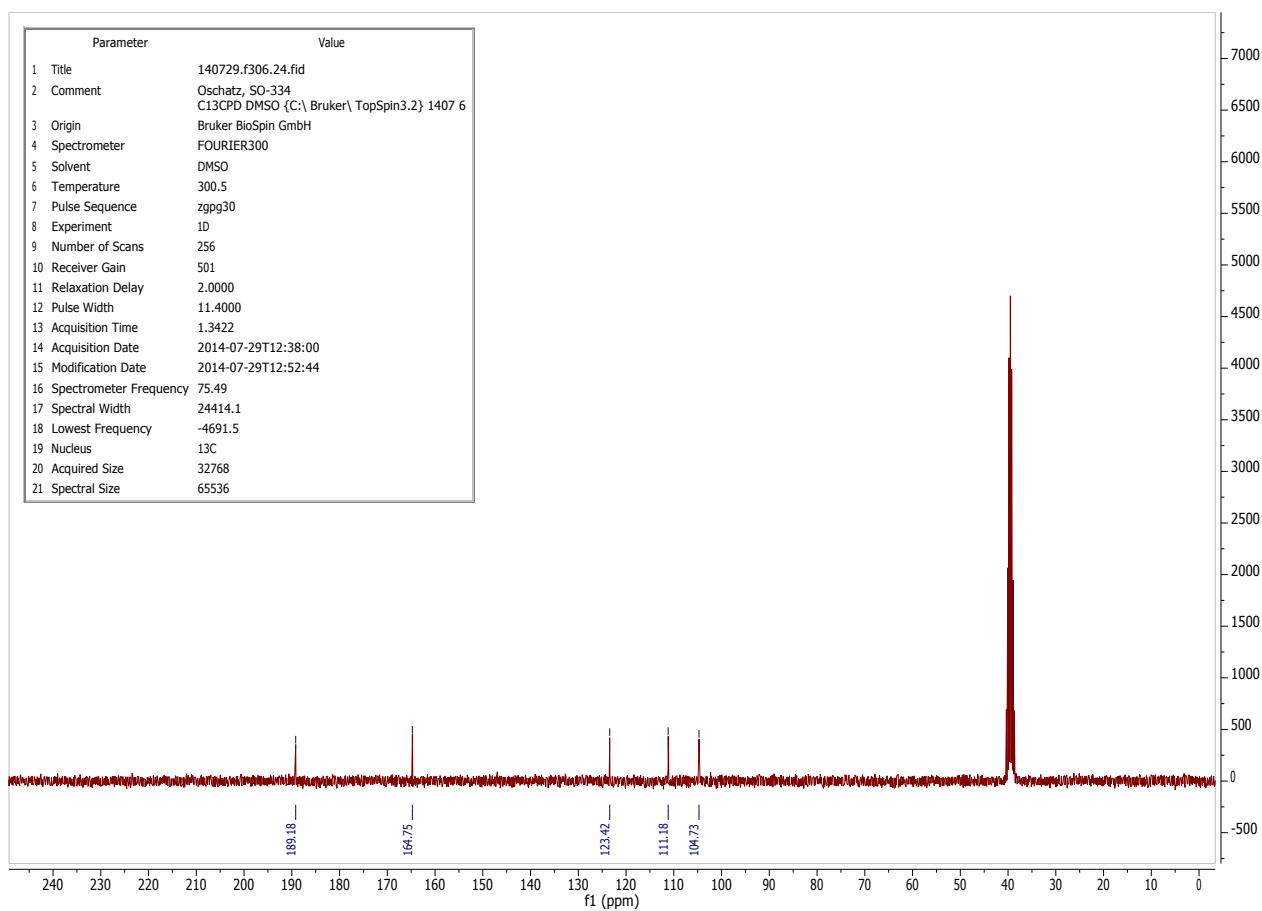
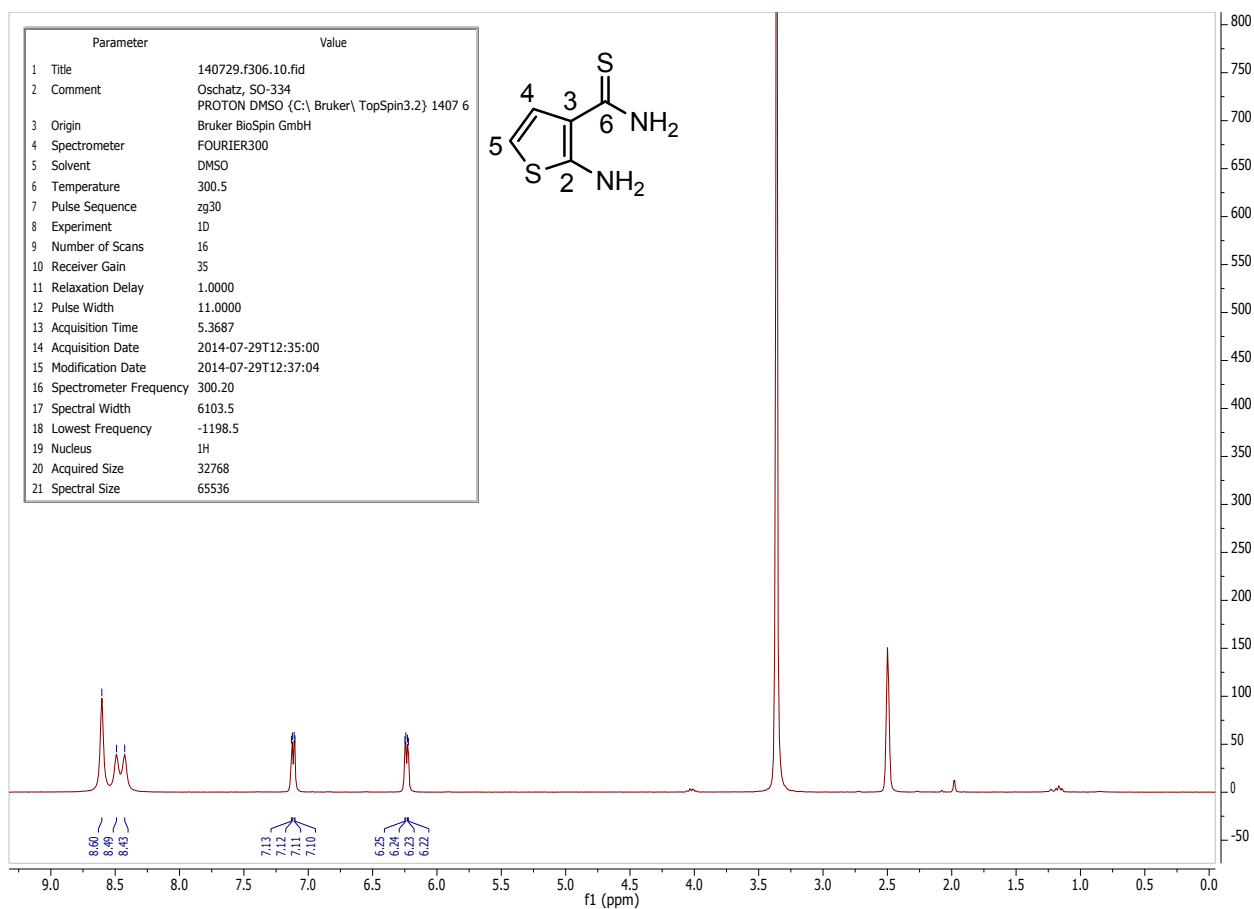


## 2-Amino-6-chlorobenzothioamide (1g):

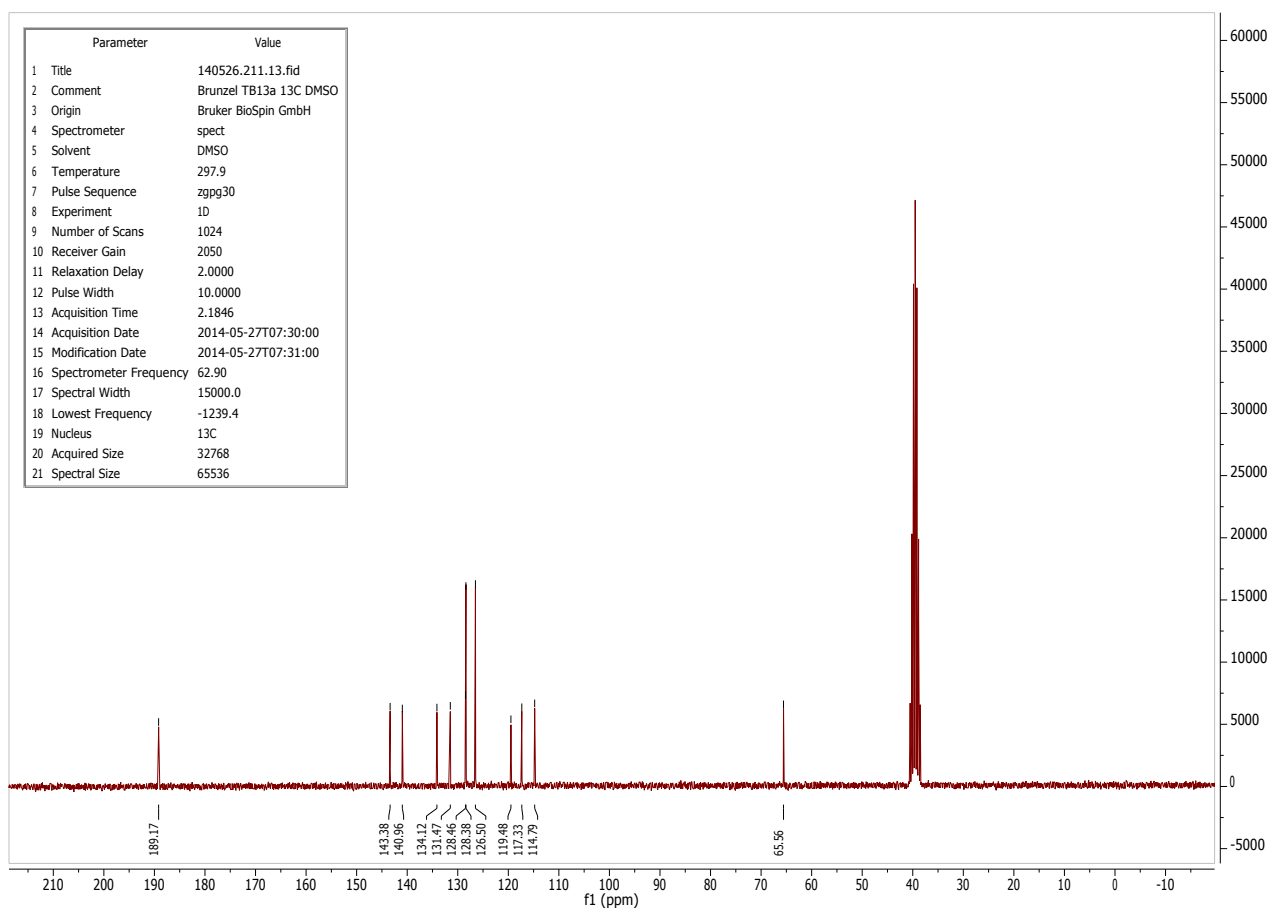
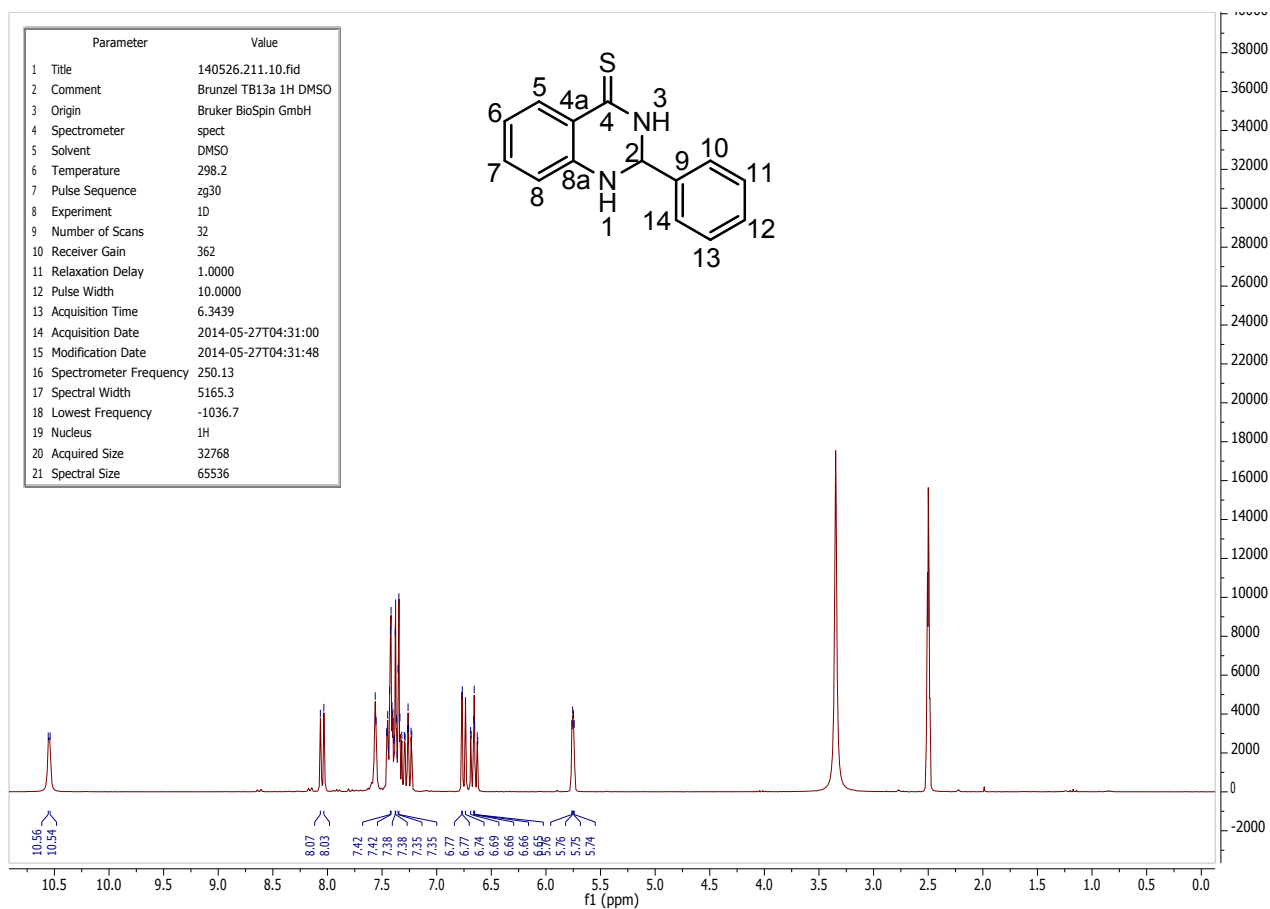




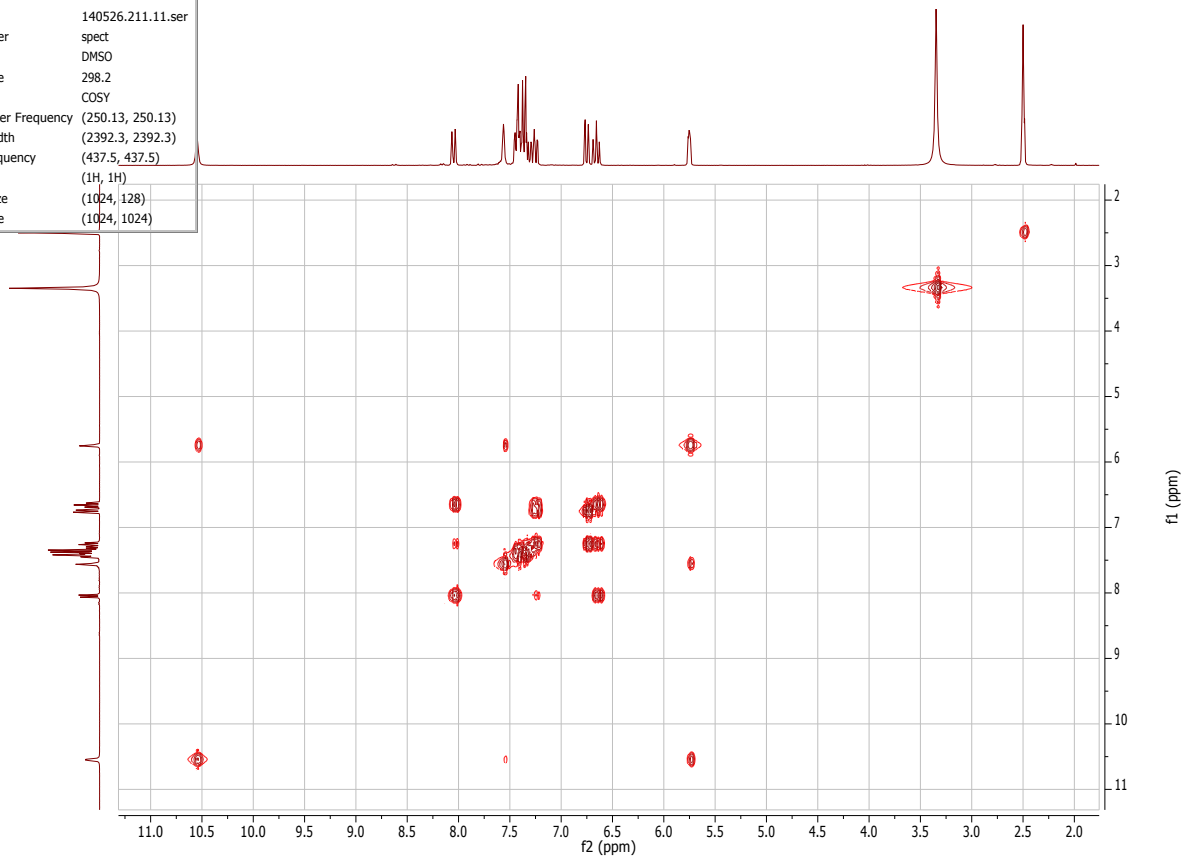
## 2-Aminothiophene-3-carbothioamide (1h):



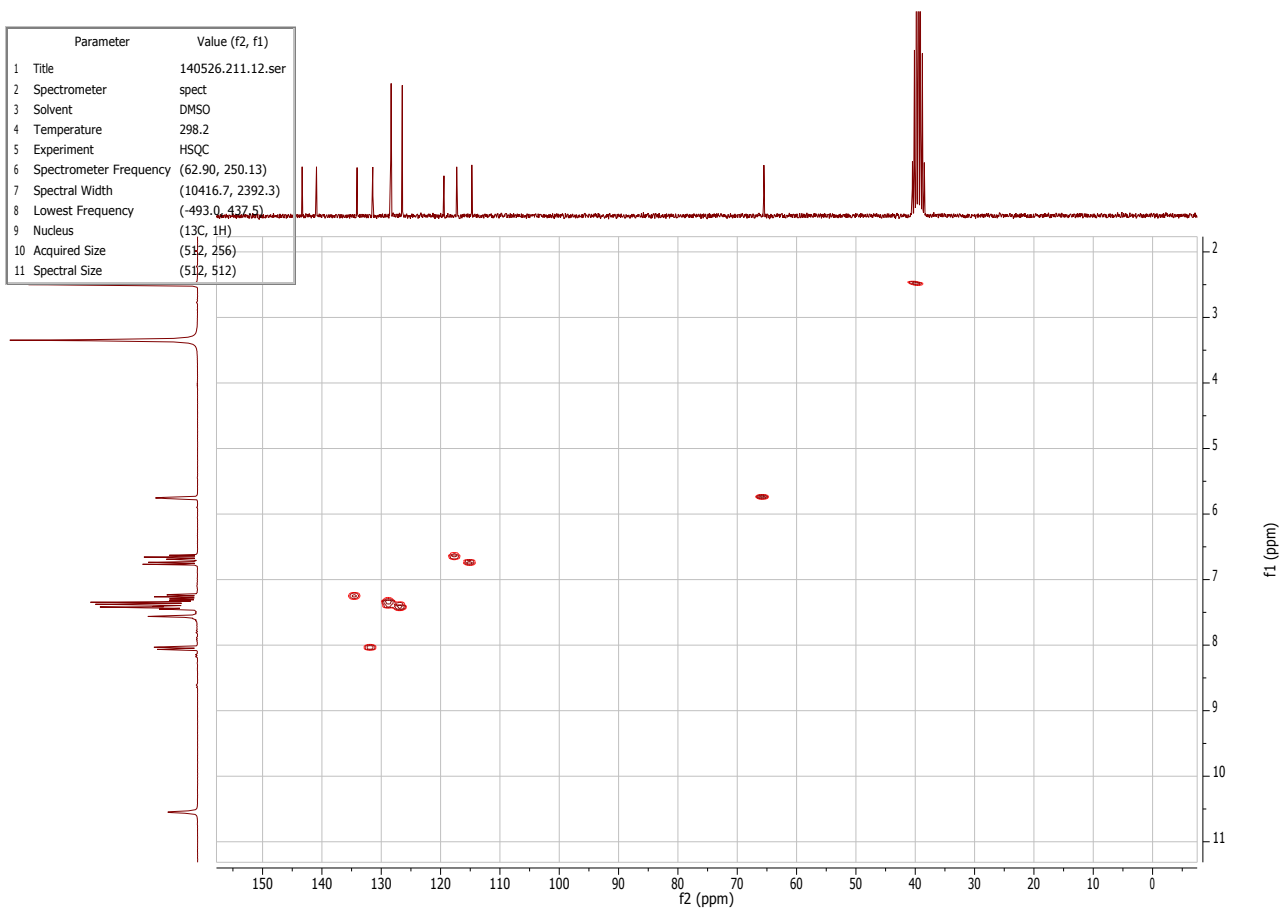
## 2-Phenyl-2,3-dihydroquinazoline-4(1H)-thione (2a):



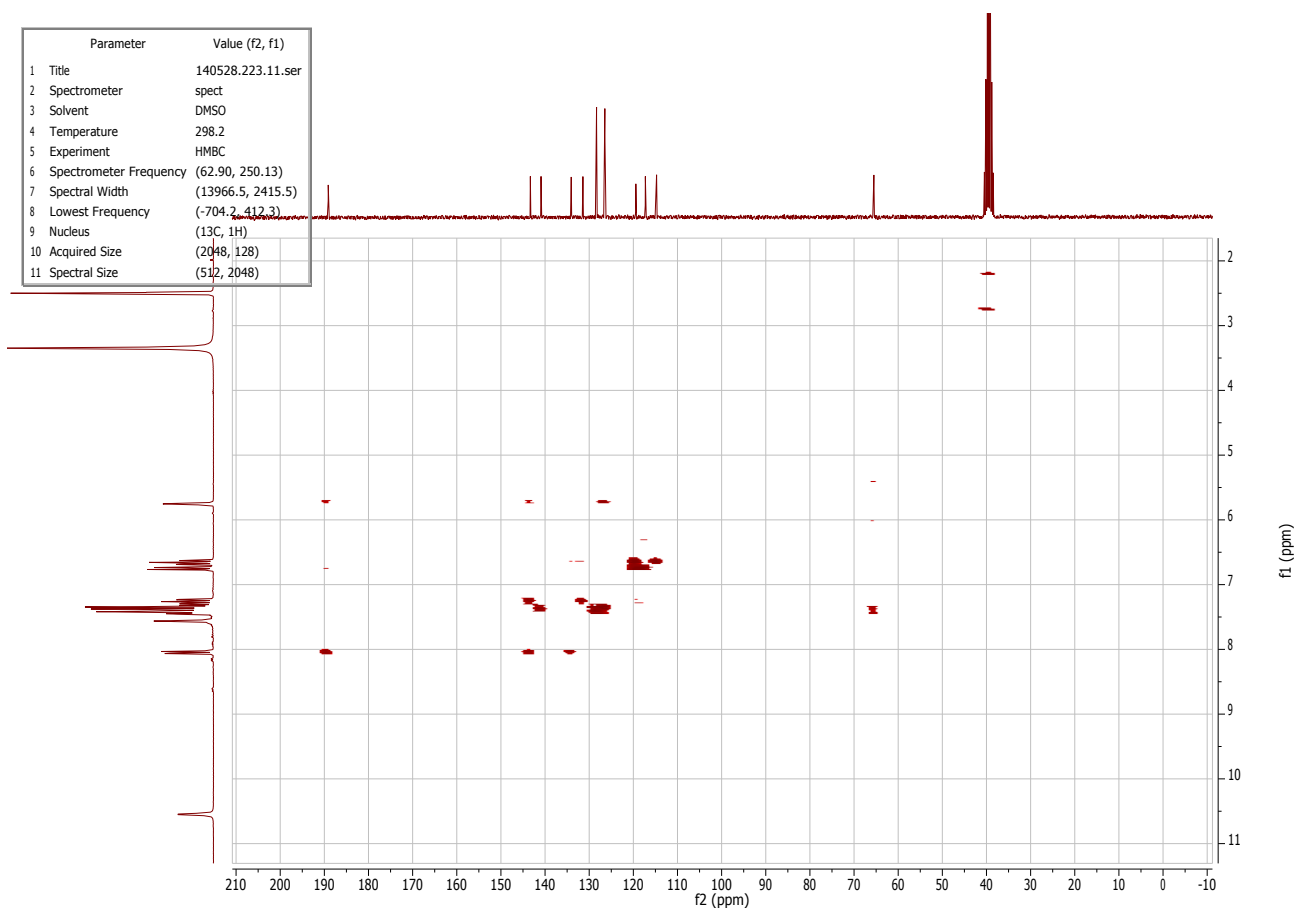
Parameter	Value (f2, f1)
1 Title	140526.211.11.ser
2 Spectrometer	spect
3 Solvent	DMSO
4 Temperature	298.2
5 Experiment	COSY
6 Spectrometer Frequency	(250.13, 250.13)
7 Spectral Width	(2392.3, 2392.3)
8 Lowest Frequency	(437.5, 437.5)
9 Nucleus	(1H, 1H)
10 Acquired Size	(1024, 128)
11 Spectral Size	(1024, 1024)



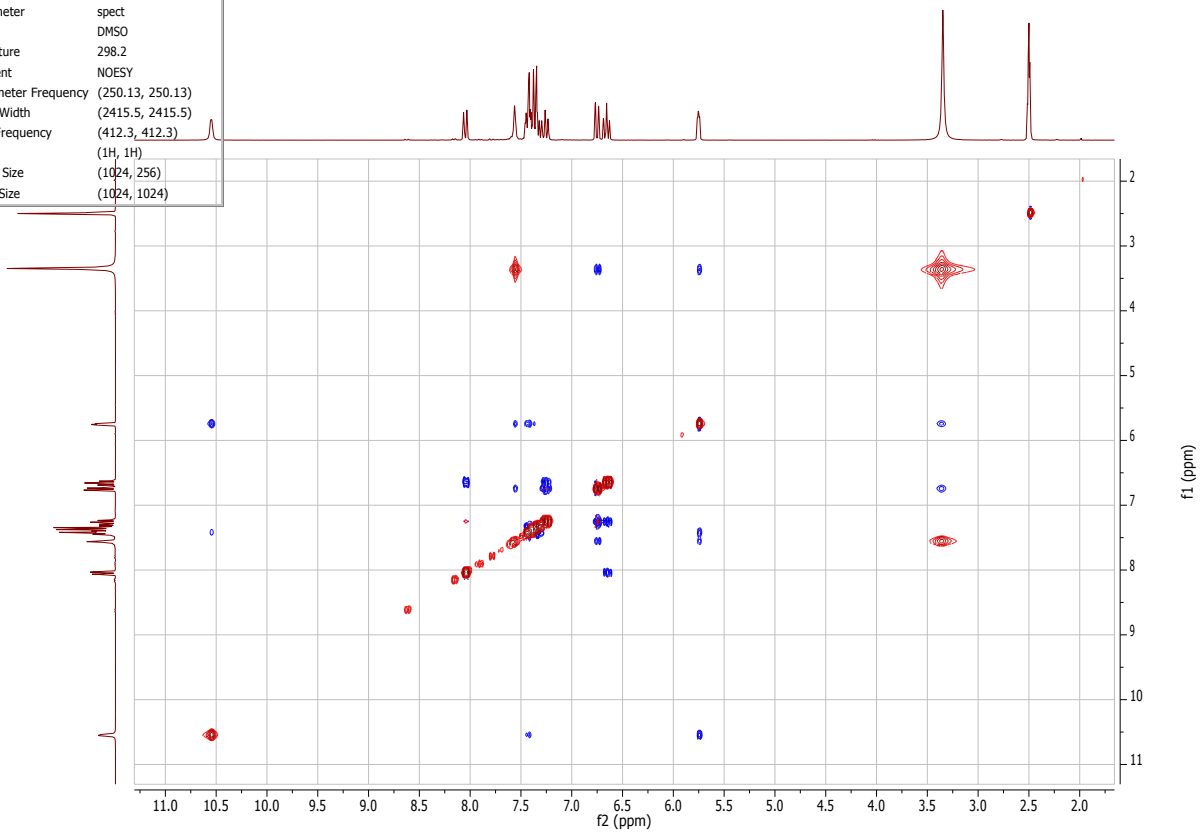
Parameter	Value (f2, f1)
1 Title	140526.211.12.ser
2 Spectrometer	spect
3 Solvent	DMSO
4 Temperature	298.2
5 Experiment	HSQC
6 Spectrometer Frequency	(62.90, 250.13)
7 Spectral Width	(10416.7, 2392.3)
8 Lowest Frequency	(-493.0, 437.5)
9 Nucleus	(13C, 1H)
10 Acquired Size	(512, 256)
11 Spectral Size	(512, 512)



Parameter	Value (f2, f1)
1 Title	140528.223.11.ser
2 Spectrometer	spect
3 Solvent	DMSO
4 Temperature	298.2
5 Experiment	HMBC
6 Spectrometer Frequency	(62.90, 250.13)
7 Spectral Width	(13966.5, 2415.5)
8 Lowest Frequency	(-704.2, 412.3)
9 Nucleus	(13C, 1H)
10 Acquired Size	(2048, 128)
11 Spectral Size	(512, 2048)

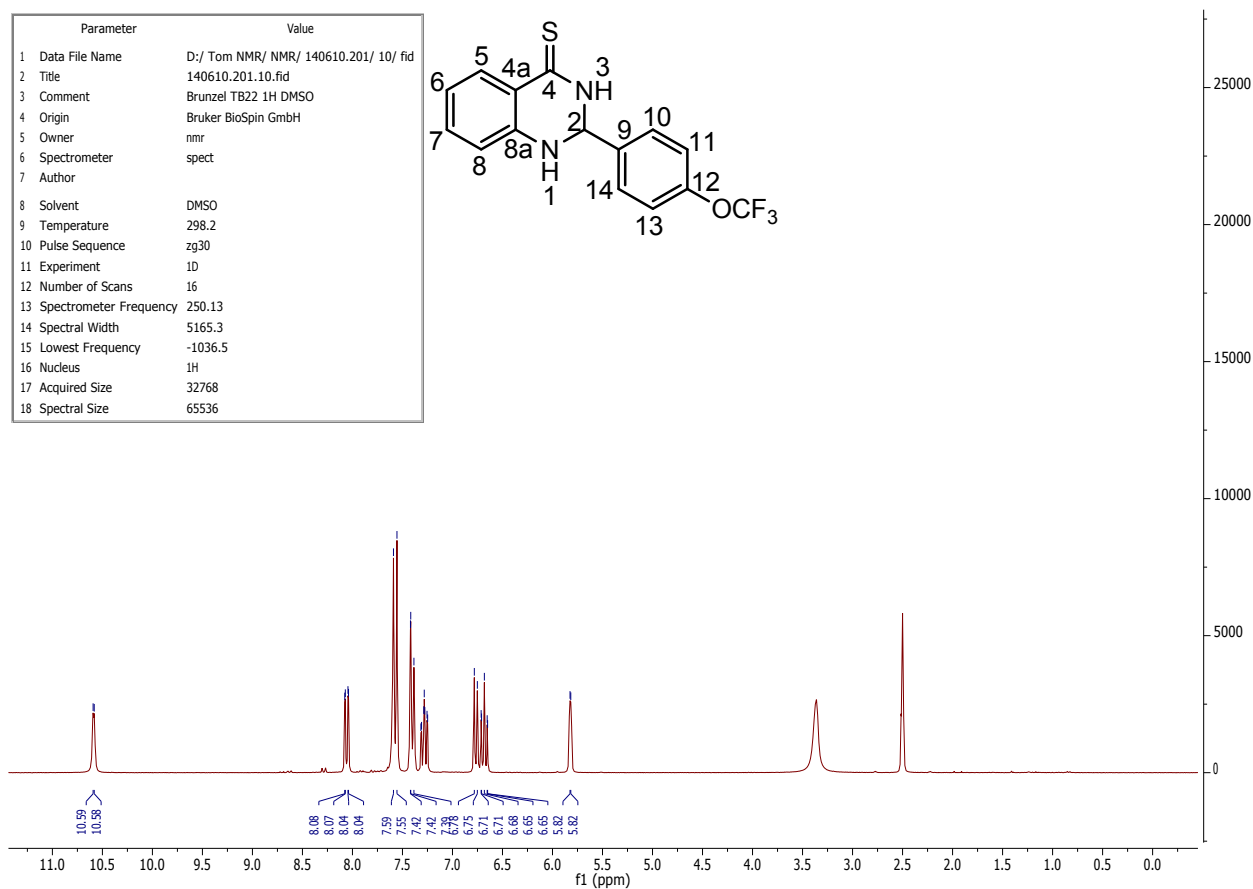
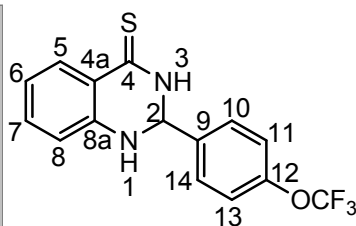


Parameter	Value (f2, f1)
1 Title	140528.223.12.1.2rr
2 Spectrometer	spect
3 Solvent	DMSO
4 Temperature	298.2
5 Experiment	NOESY
6 Spectrometer Frequency	(250.13, 250.13)
7 Spectral Width	(2415.5, 2415.5)
8 Lowest Frequency	(412.3, 412.3)
9 Nucleus	(1H, 1H)
10 Acquired Size	(1024, 256)
11 Spectral Size	(1024, 1024)

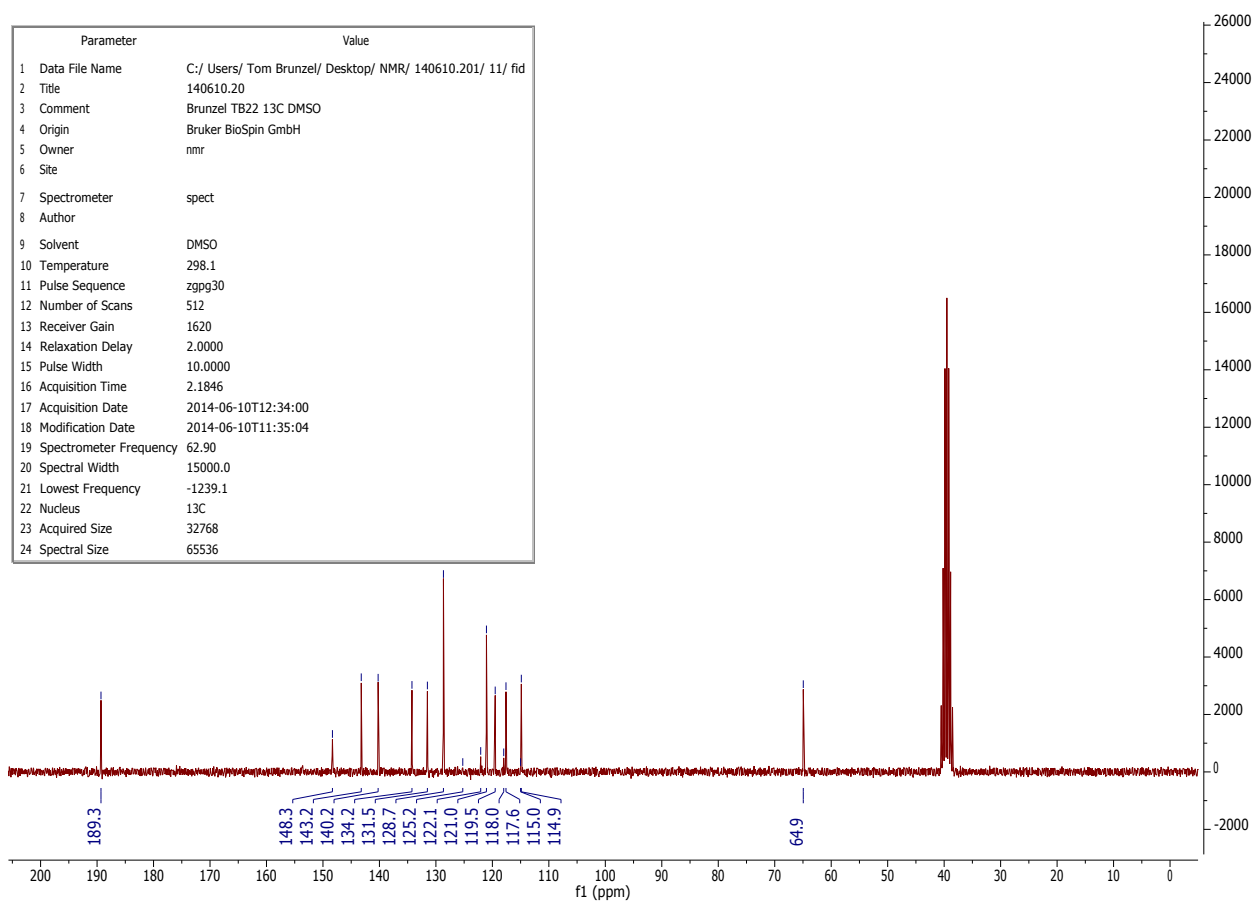


## 2-(4-Trifluoromethoxy)phenyl-2,3-dihydroquinazoline-4(1H)-thione (2b):

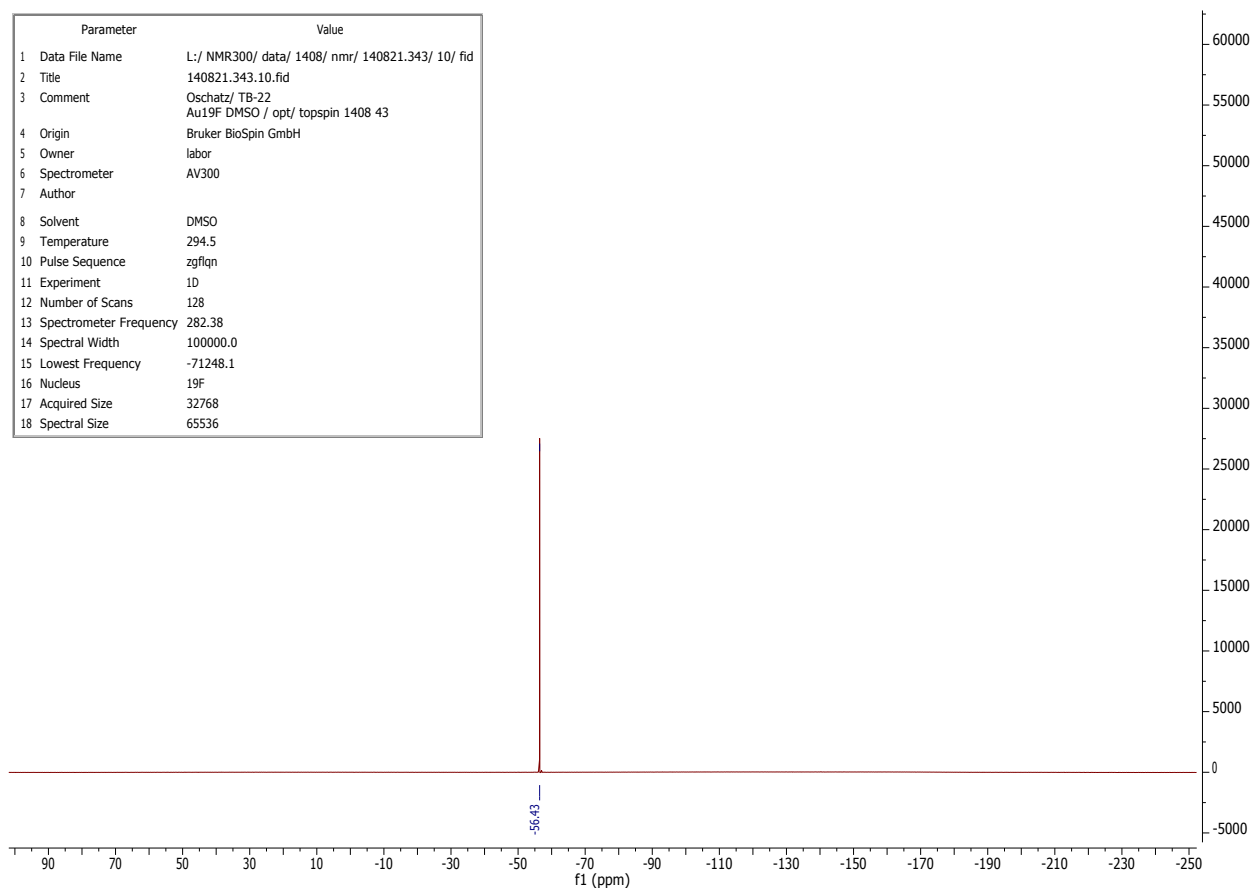
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1 Data File Name	D:/ Tom NMR/ NMR/ 140610.201/ 10/ fid
2 Title	140610.201.10.fid
3 Comment	Brunzel TB22 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	298.2
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	16
13 Spectrometer Frequency	250.13
14 Spectral Width	5165.3
15 Lowest Frequency	-1036.5
16 Nucleus	1H
17 Acquired Size	32768
18 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/ Users/ Tom Brunzel/ Desktop/ NMR/ 140610.201/ 11/ fid
2 Title	140610.20
3 Comment	Brunzel TB22 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Number of Scans	512
13 Receiver Gain	1620
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	2.1846
17 Acquisition Date	2014-06-10T12:34:00
18 Modification Date	2014-06-10T11:35:04
19 Spectrometer Frequency	62.90
20 Spectral Width	15000.0
21 Lowest Frequency	-1239.1
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

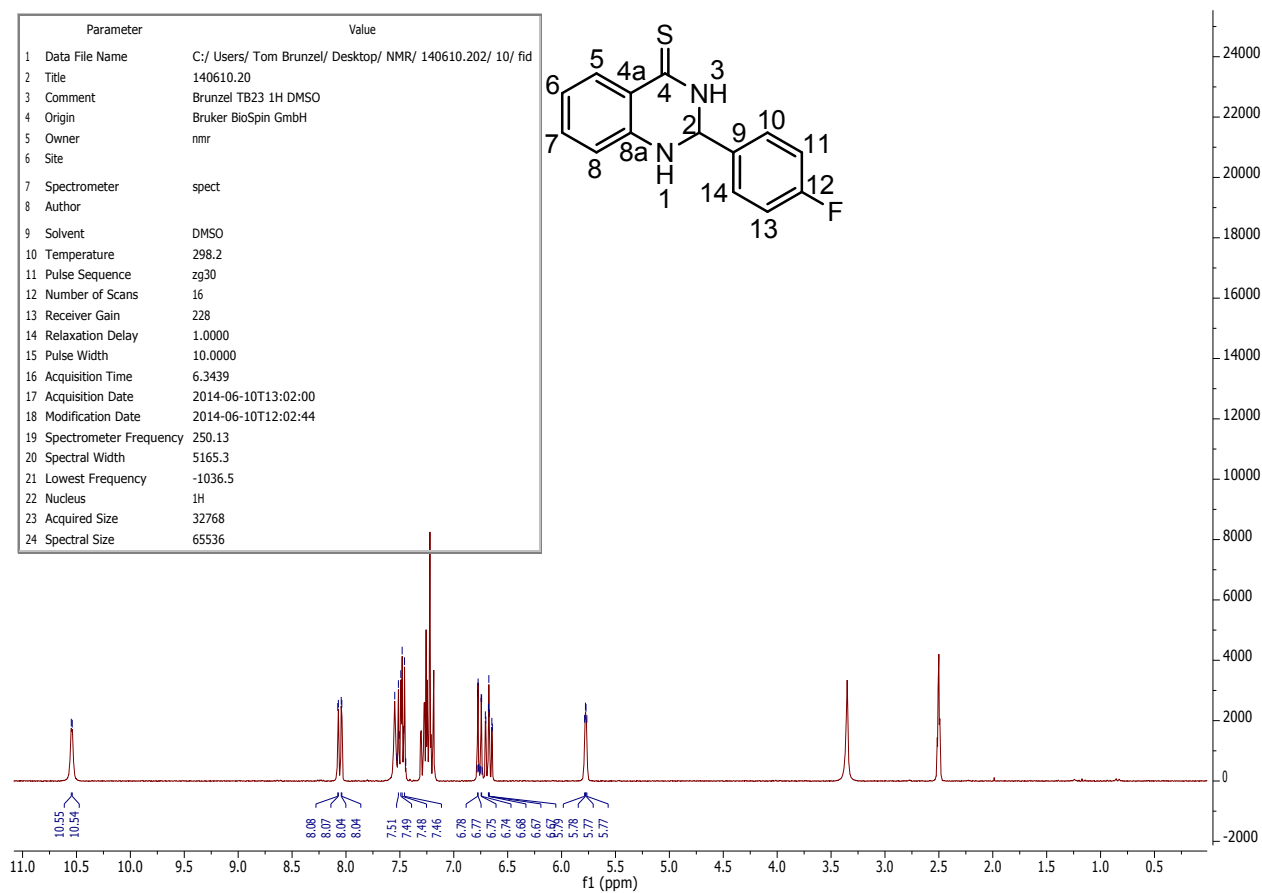
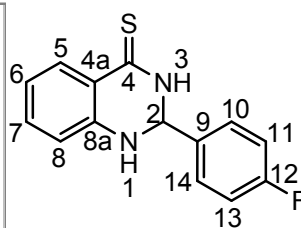


Parameter	Value
1 Data File Name	L:/ NMR300/ data/ 1408/ nmr/ 140821.343/ 10/ fid
2 Title	140821.343.10.fid
3 Comment	Oschatz/ TB-22 Au19F DMSO / opt/ topspin 1408 43
4 Origin	Bruker BioSpin GmbH
5 Owner	labor
6 Spectrometer	AV300
7 Author	
8 Solvent	DMSO
9 Temperature	294.5
10 Pulse Sequence	zgfgq
11 Experiment	1D
12 Number of Scans	128
13 Spectrometer Frequency	282.38
14 Spectral Width	100000.0
15 Lowest Frequency	-71248.1
16 Nucleus	19F
17 Acquired Size	32768
18 Spectral Size	65536

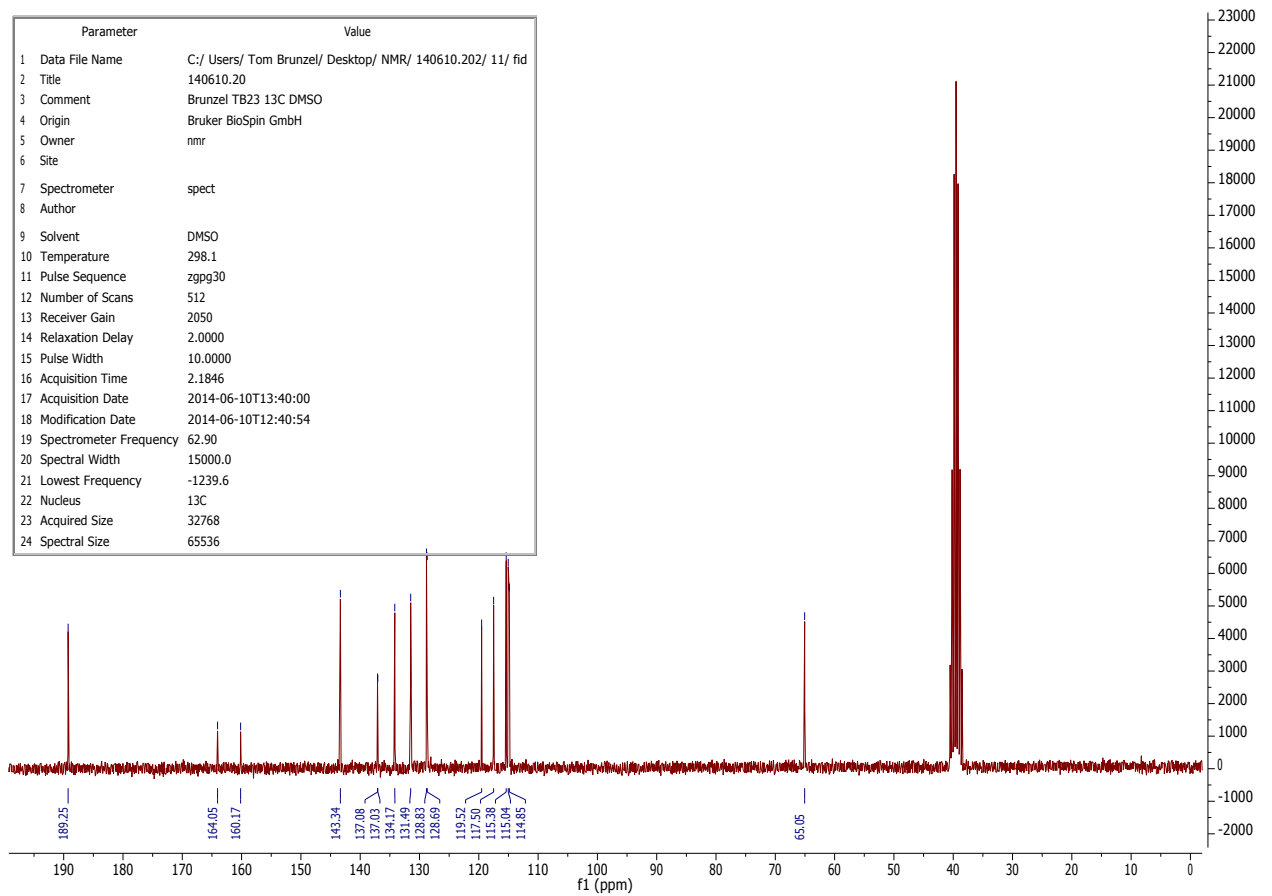


## 2-(4-Fluorophenyl)-2,3-dihydroquinazoline-4(1H)-thione (2c):

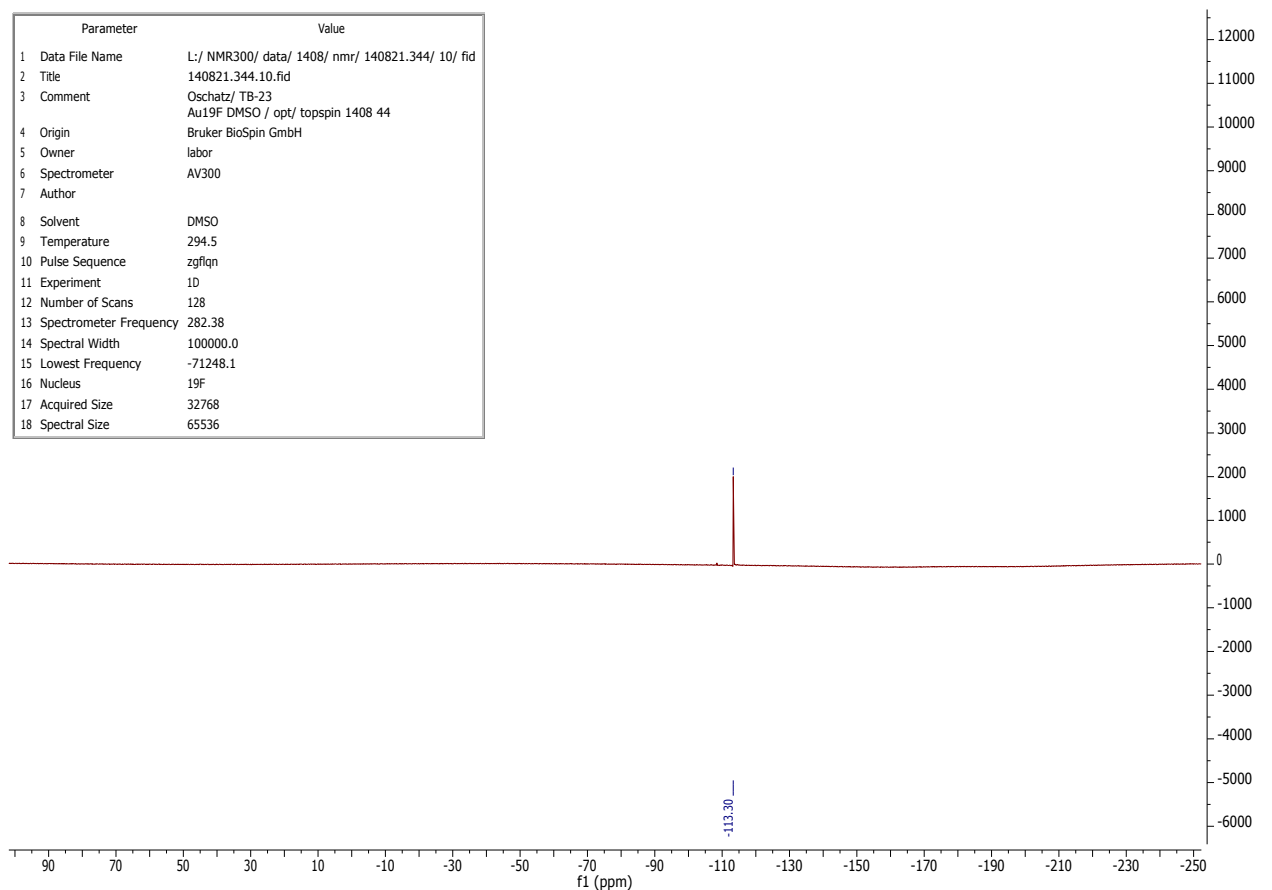
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1 Data File Name	C:/ Users/ Tom Brunzel/ Desktop/ NMR/ 140610.202/ 10/ fid
2 Title	140610.20
3 Comment	Brunzel TB23 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	228
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	6.3439
17 Acquisition Date	2014-06-10T13:02:00
18 Modification Date	2014-06-10T12:02:44
19 Spectrometer Frequency	250.13
20 Spectral Width	5165.3
21 Lowest Frequency	-1036.5
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



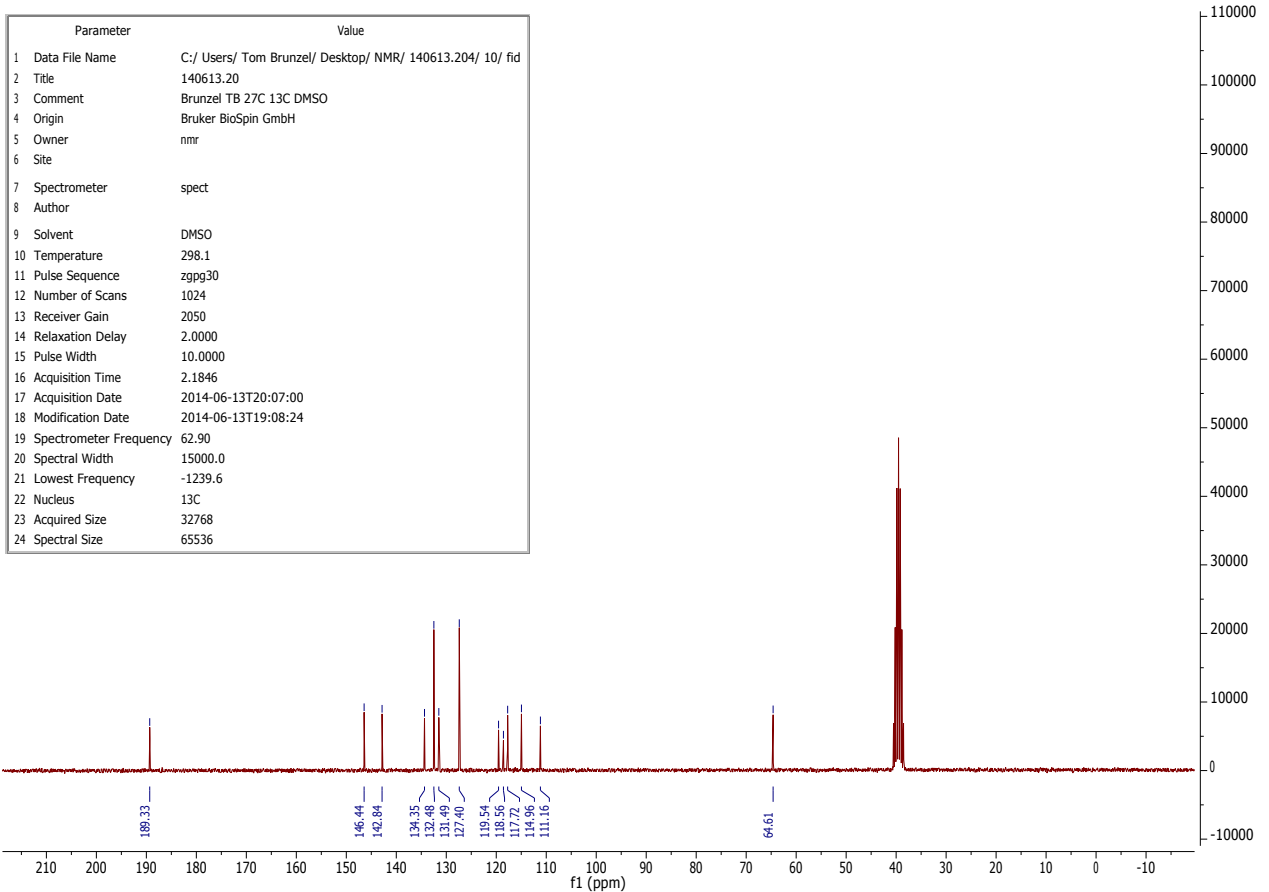
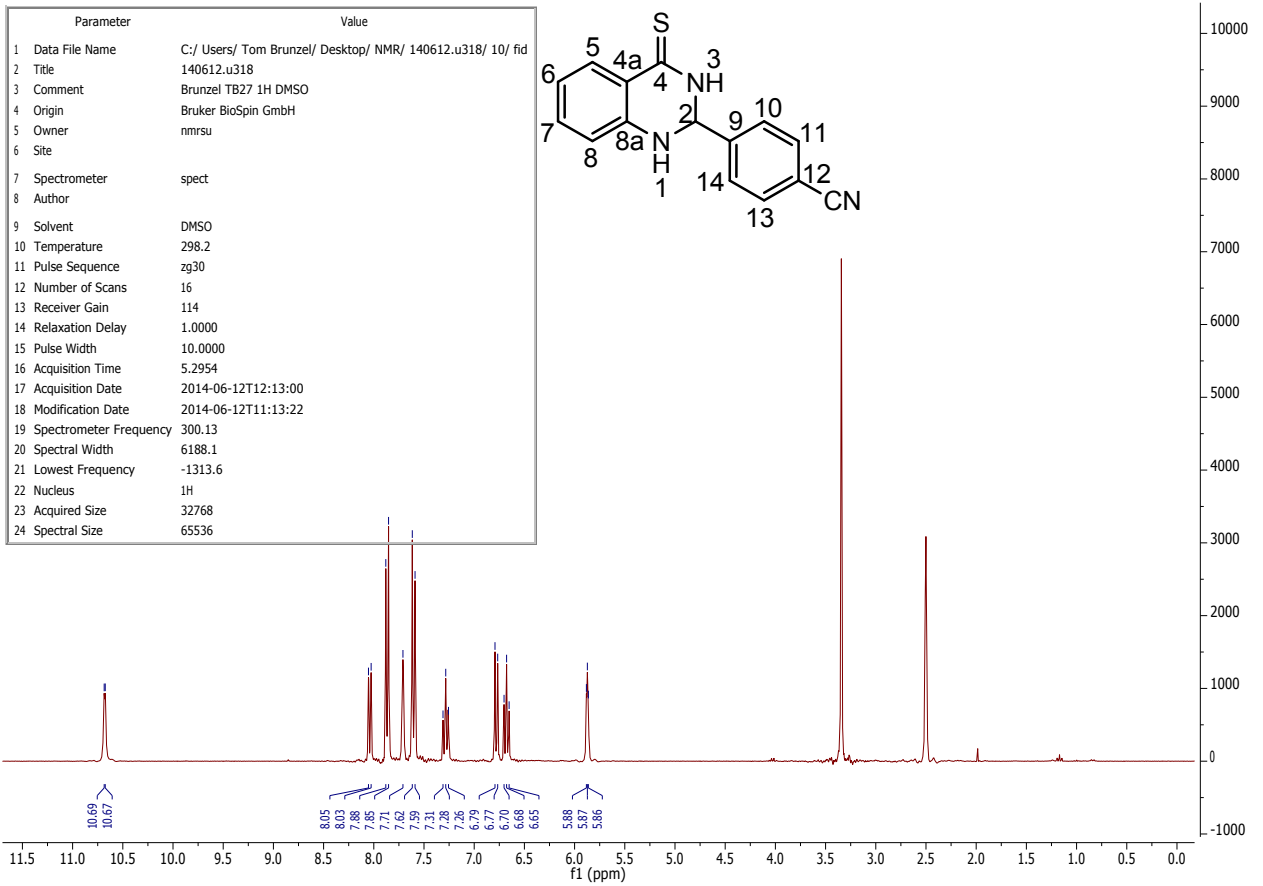
Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140610.202/11/fid
2 Title	140610.20
3 Comment	Brunzel TB23 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Number of Scans	512
13 Receiver Gain	2050
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	2.1846
17 Acquisition Date	2014-06-10T13:40:00
18 Modification Date	2014-06-10T12:40:54
19 Spectrometer Frequency	62.90
20 Spectral Width	15000.0
21 Lowest Frequency	-1239.6
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536



Parameter	Value
1 Data File Name	L:/NMR300/data/1408/nmr/140821.344/10/fid
2 Title	140821.344.10.fid
3 Comment	Oschatz/ TB-23 Au19F DMSO / opt/ topspin 1408 44
4 Origin	Bruker BioSpin GmbH
5 Owner	labor
6 Spectrometer	AV300
7 Author	
8 Solvent	DMSO
9 Temperature	294.5
10 Pulse Sequence	zgfgq
11 Experiment	1D
12 Number of Scans	128
13 Spectrometer Frequency	282.38
14 Spectral Width	100000.0
15 Lowest Frequency	-71248.1
16 Nucleus	19F
17 Acquired Size	32768
18 Spectral Size	65536



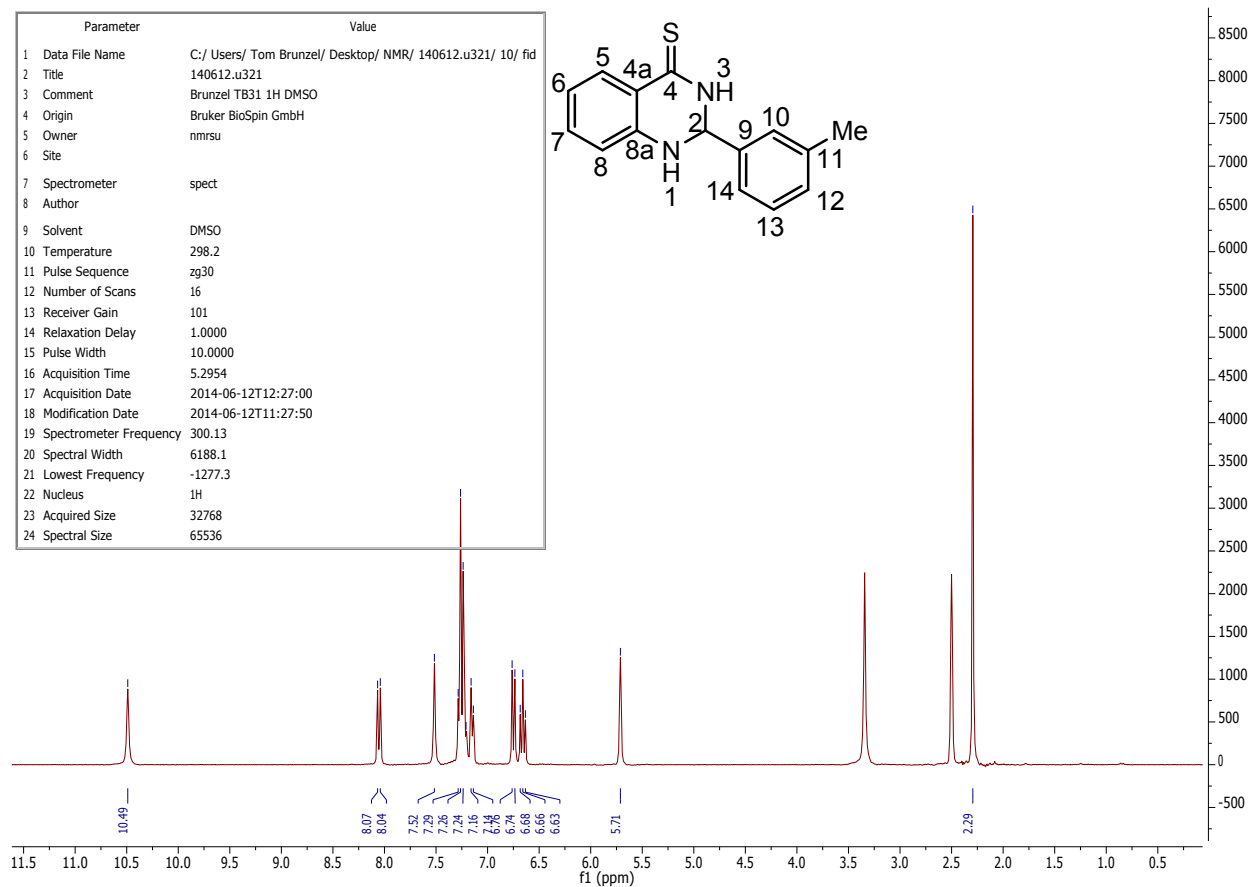
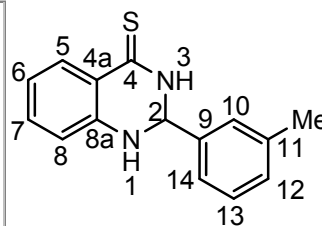
## 2-(4-Cyanophenyl)-2,3-dihydroquinazoline-4(1H)-thione (2d):



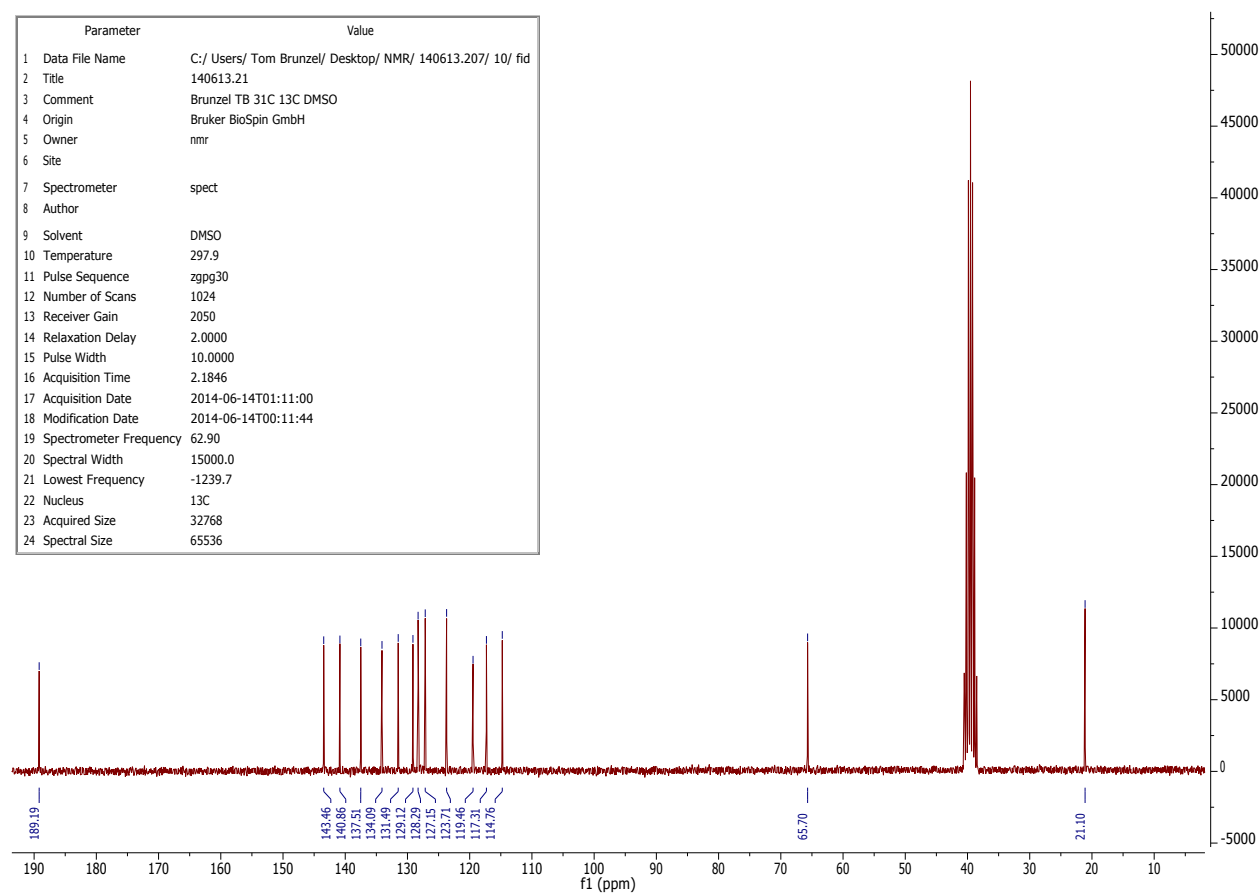


## 2-(3-Methylphenyl)-2,3-dihydroquinazoline-4(1H)-thione (2e):

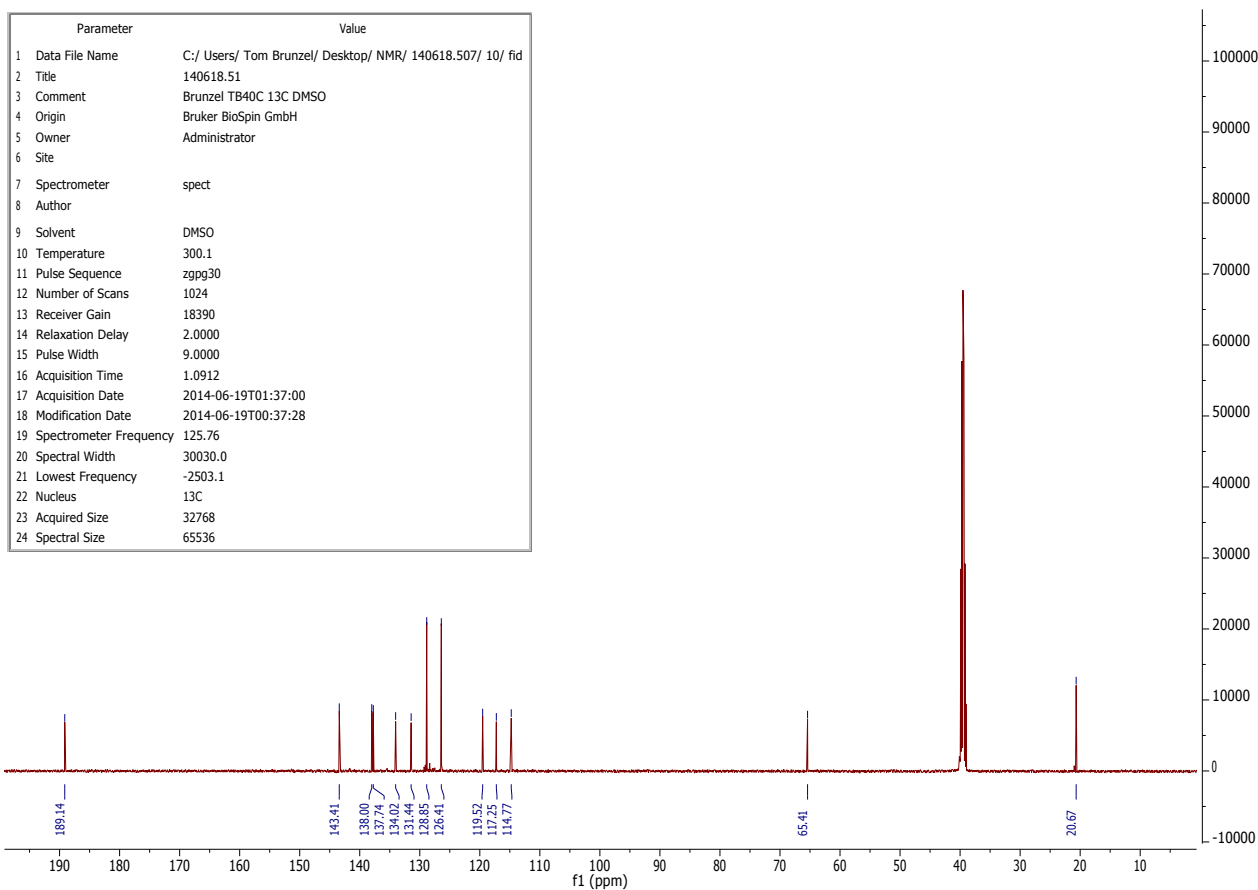
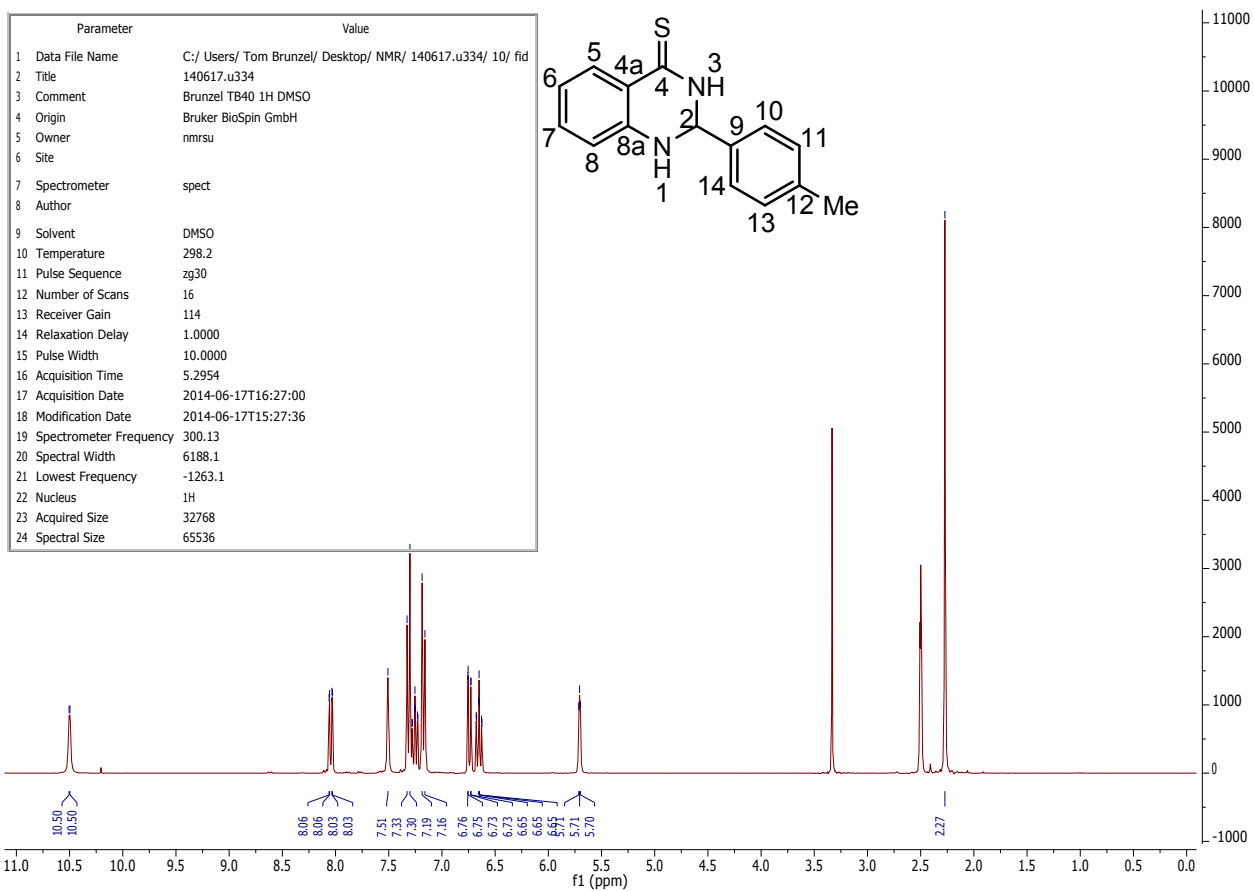
Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140612.u321/10/fid
2 Title	140612.u321
3 Comment	Brunzel TB31 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsru
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	101
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	5.2954
17 Acquisition Date	2014-06-12T12:27:00
18 Modification Date	2014-06-12T11:27:50
19 Spectrometer Frequency	300.13
20 Spectral Width	6188.1
21 Lowest Frequency	-1277.3
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140613.207/10/fid
2 Title	140613.21
3 Comment	Brunzel TB 31C 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	297.9
11 Pulse Sequence	zpgg30
12 Number of Scans	1024
13 Receiver Gain	2050
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	2.1846
17 Acquisition Date	2014-06-14T01:11:00
18 Modification Date	2014-06-14T00:11:44
19 Spectrometer Frequency	62.90
20 Spectral Width	15000.0
21 Lowest Frequency	-1239.7
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

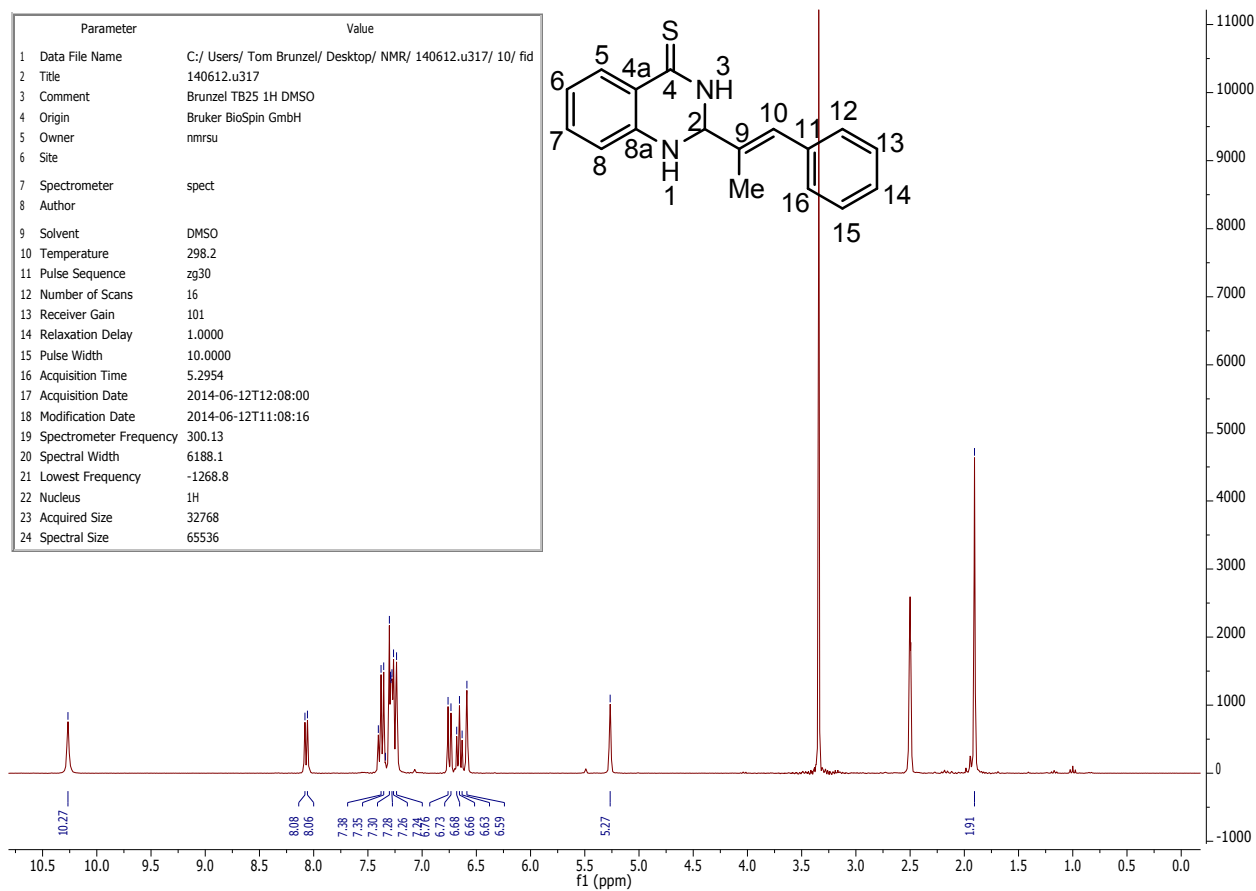
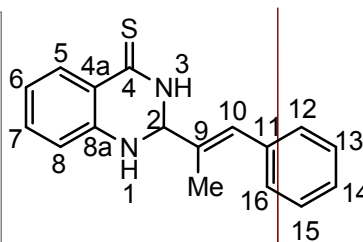


## 2-(4-Methylphenyl)-2,3-dihydroquinazoline-4(1H)-thione (2f):

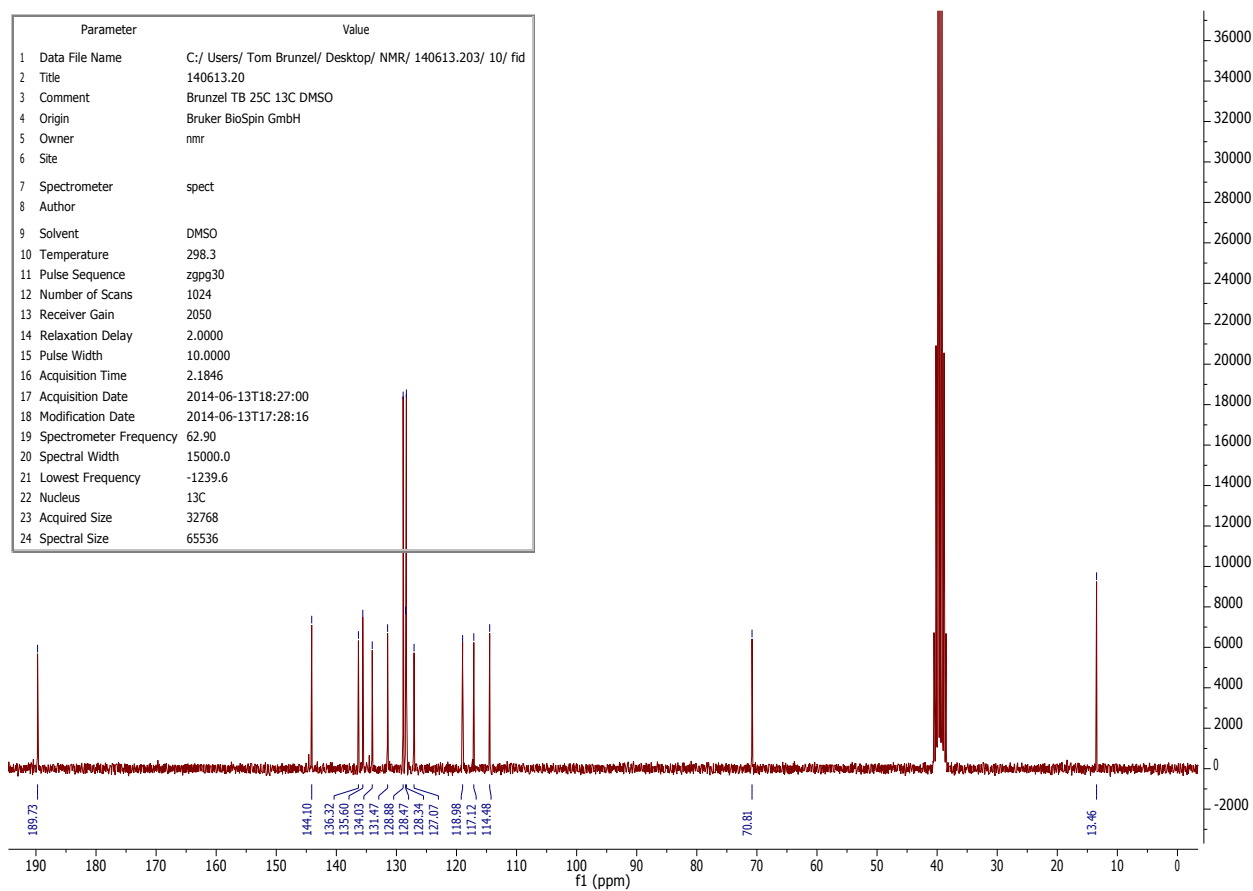


**(E)-2-(1-Phenylprop-1-en-2-yl)-2,3-dihydroquinazoline-4(1H)-thione (2g):**

Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140612.u317/10/ fid
2 Title	140612.u317
3 Comment	Brunzel TB25 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	101
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	5.2954
17 Acquisition Date	2014-06-12T12:08:00
18 Modification Date	2014-06-12T11:08:16
19 Spectrometer Frequency	300.13
20 Spectral Width	6188.1
21 Lowest Frequency	-1268.8
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

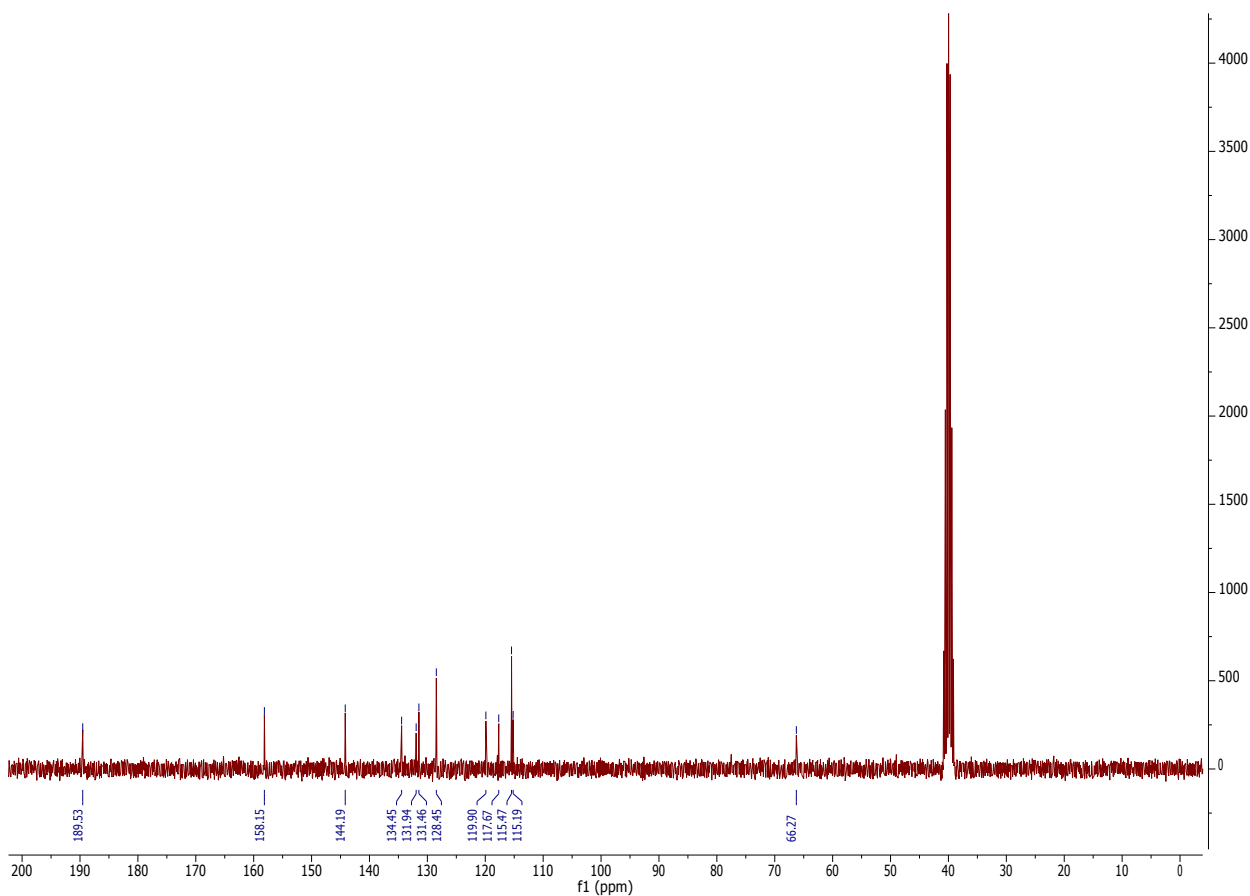
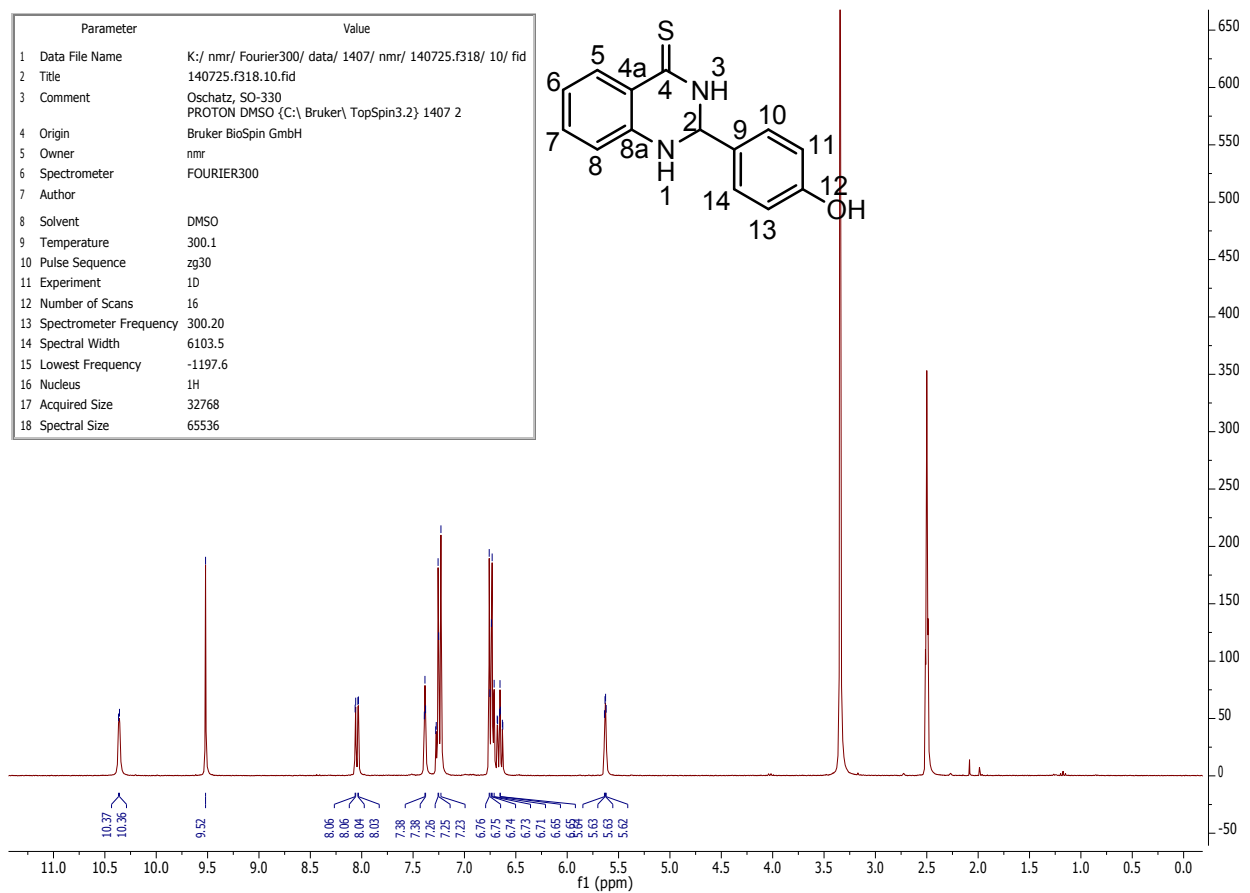
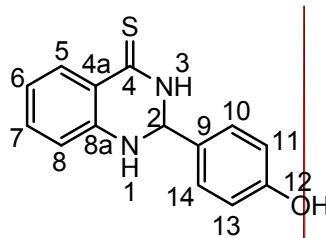


Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140613.203/10/ fid
2 Title	140613.20
3 Comment	Brunzel TB 25C 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.3
11 Pulse Sequence	zgpg30
12 Number of Scans	1024
13 Receiver Gain	2050
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	2.1846
17 Acquisition Date	2014-06-13T18:27:00
18 Modification Date	2014-06-13T17:28:16
19 Spectrometer Frequency	62.90
20 Spectral Width	15000.0
21 Lowest Frequency	-1239.6
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536



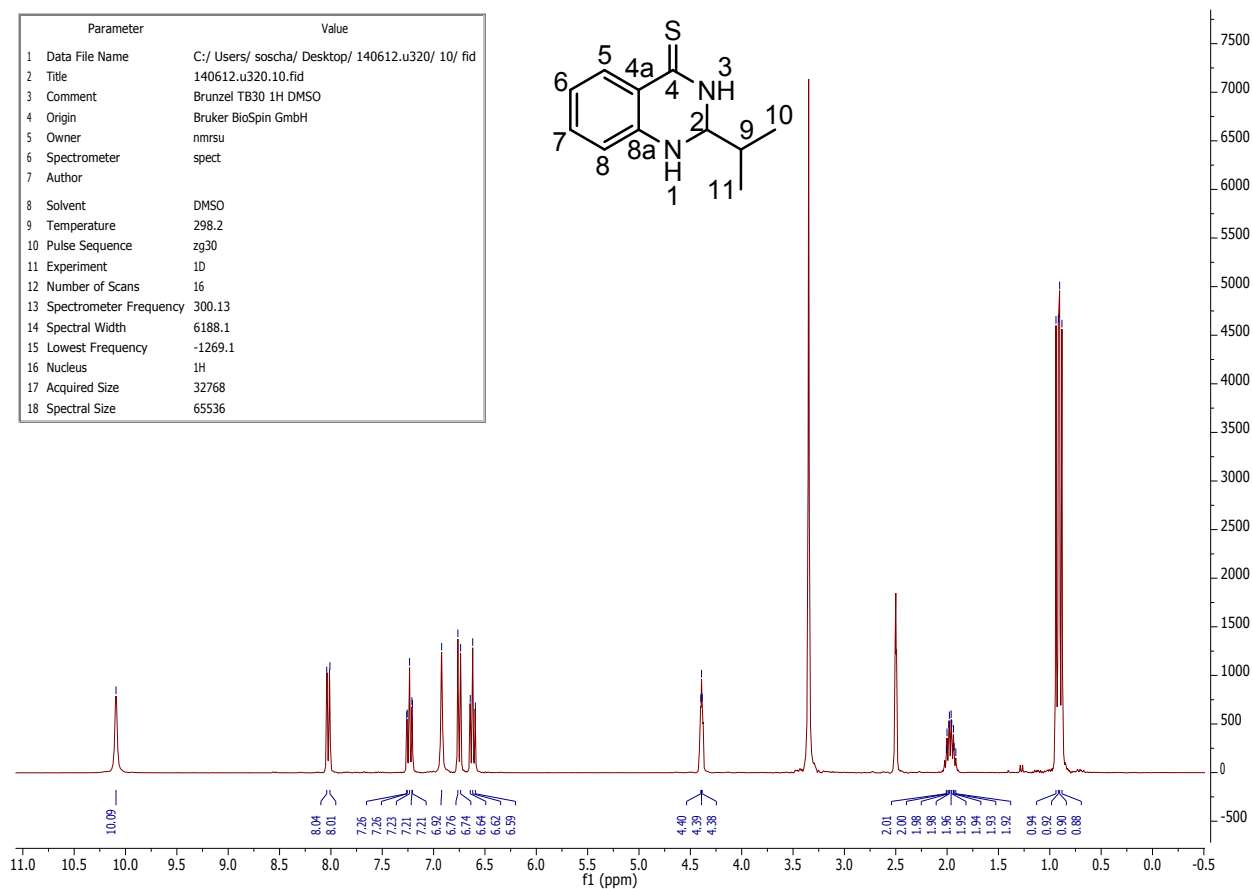
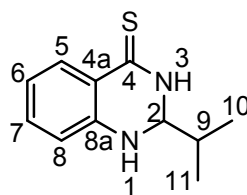
## 2-(4-Hydroxyphenyl)-2,3-dihydroquinazoline-4(1H)-thione (2h):

Parameter	Value
1 Data File Name	K:\ nmr\ Fourier300\ data\ 1407\ nmr\ 140725.f318\ 10\ fid
2 Title	140725.f318.10.fid
3 Comment	Oschatz, SO-330 PROTON DMSO (C:\ Bruker\ TopSpin3.2) 1407 2
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Spectrometer	FOURIER300
7 Author	
8 Solvent	DMSO
9 Temperature	300.1
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	16
13 Spectrometer Frequency	300.20
14 Spectral Width	6103.5
15 Lowest Frequency	-1197.6
16 Nucleus	<sup>1</sup> H
17 Acquired Size	32768
18 Spectral Size	65536

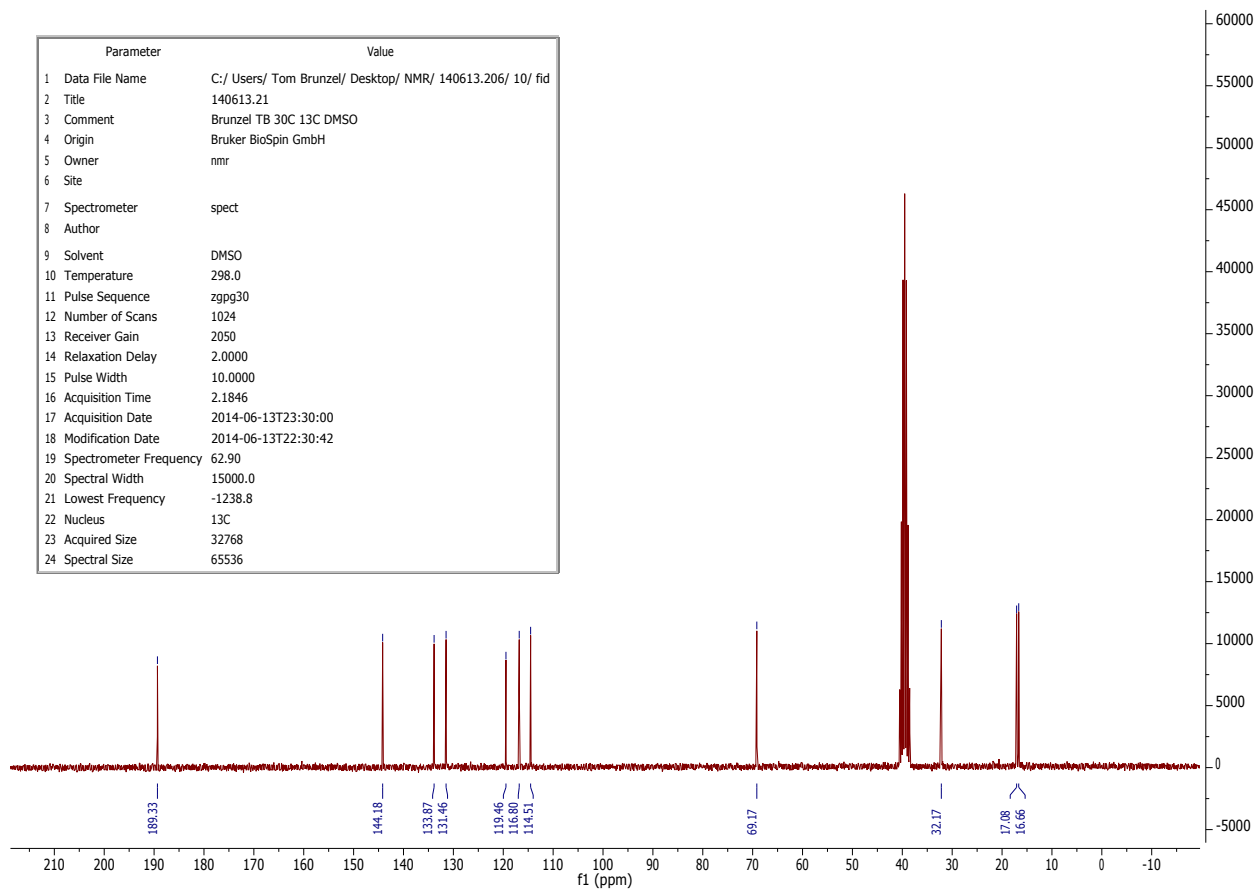


## 2-(Isopropyl)-2,3-dihydroquinazoline-4(1H)-thione (2i):

Parameter	Value
1 Data File Name	C:/ Users/ soscha/ Desktop/ 140612.u320/ 10/ fid
2 Title	140612.u320.10.fid
3 Comment	Brunzel TB30 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsru
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	298.2
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	16
13 Spectrometer Frequency	300.13
14 Spectral Width	6188.1
15 Lowest Frequency	-1269.1
16 Nucleus	1H
17 Acquired Size	32768
18 Spectral Size	65536

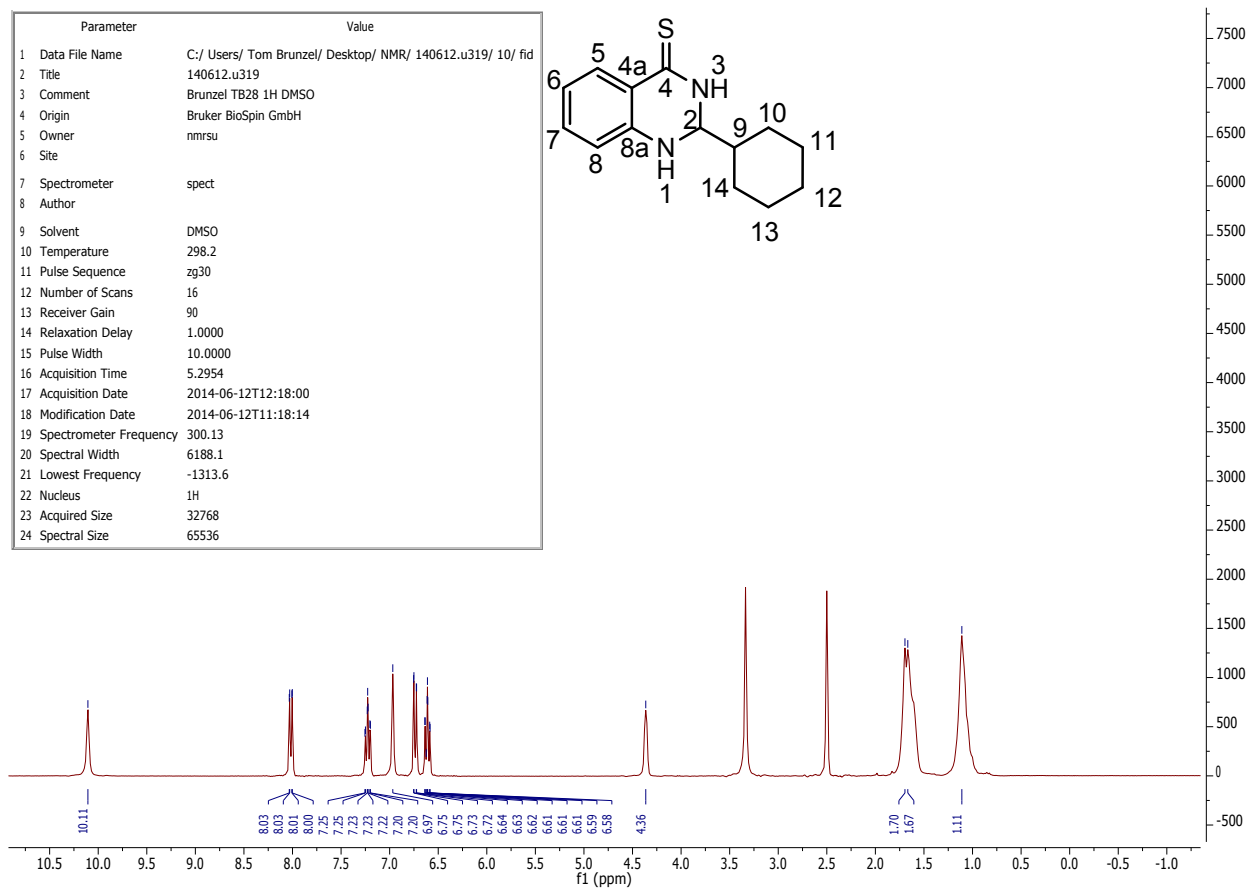
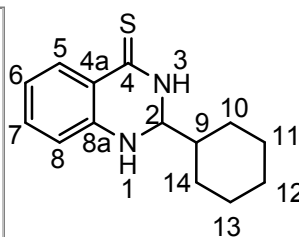


Parameter	Value
1 Data File Name	C:/ Users/ Tom Brunzel/ Desktop/ NMR/ 140613.206/ 10/ fid
2 Title	140613.21
3 Comment	Brunzel TB 30C 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Number of Scans	1024
13 Receiver Gain	2050
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	2.1846
17 Acquisition Date	2014-06-13T23:30:00
18 Modification Date	2014-06-13T22:30:42
19 Spectrometer Frequency	62.90
20 Spectral Width	15000.0
21 Lowest Frequency	-1238.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

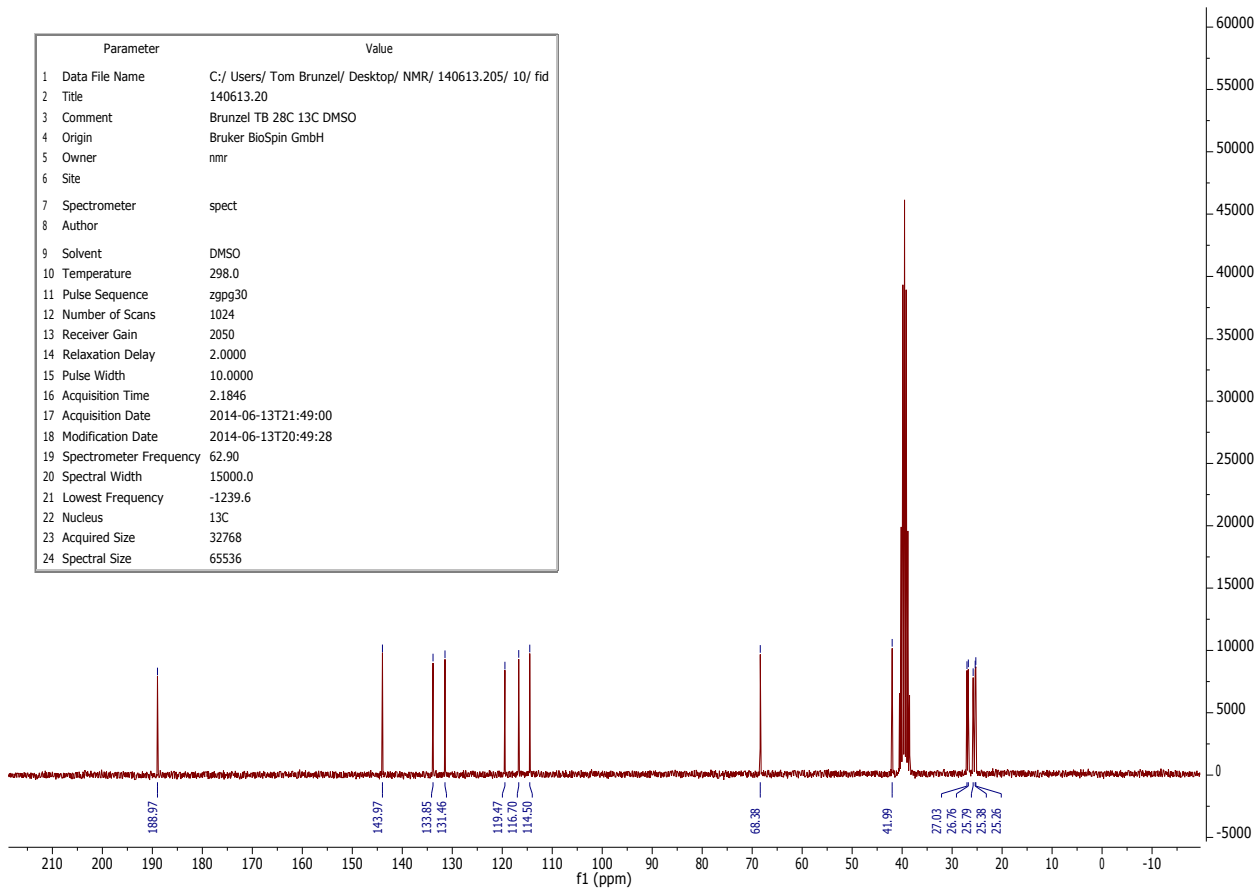


## 2-(Cyclohexyl)-2,3-dihydroquinazoline-4(1H)-thione (2j):

Parameter	Value
1 Data File Name	C:/ Users/ Tom Brunzel/ Desktop/ NMR/ 140612.u319/ 10/ fid
2 Title	140612.u319
3 Comment	Brunzel TB28 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	90
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	5.2954
17 Acquisition Date	2014-06-12T12:18:00
18 Modification Date	2014-06-12T11:18:14
19 Spectrometer Frequency	300.13
20 Spectral Width	6188.1
21 Lowest Frequency	-1313.6
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

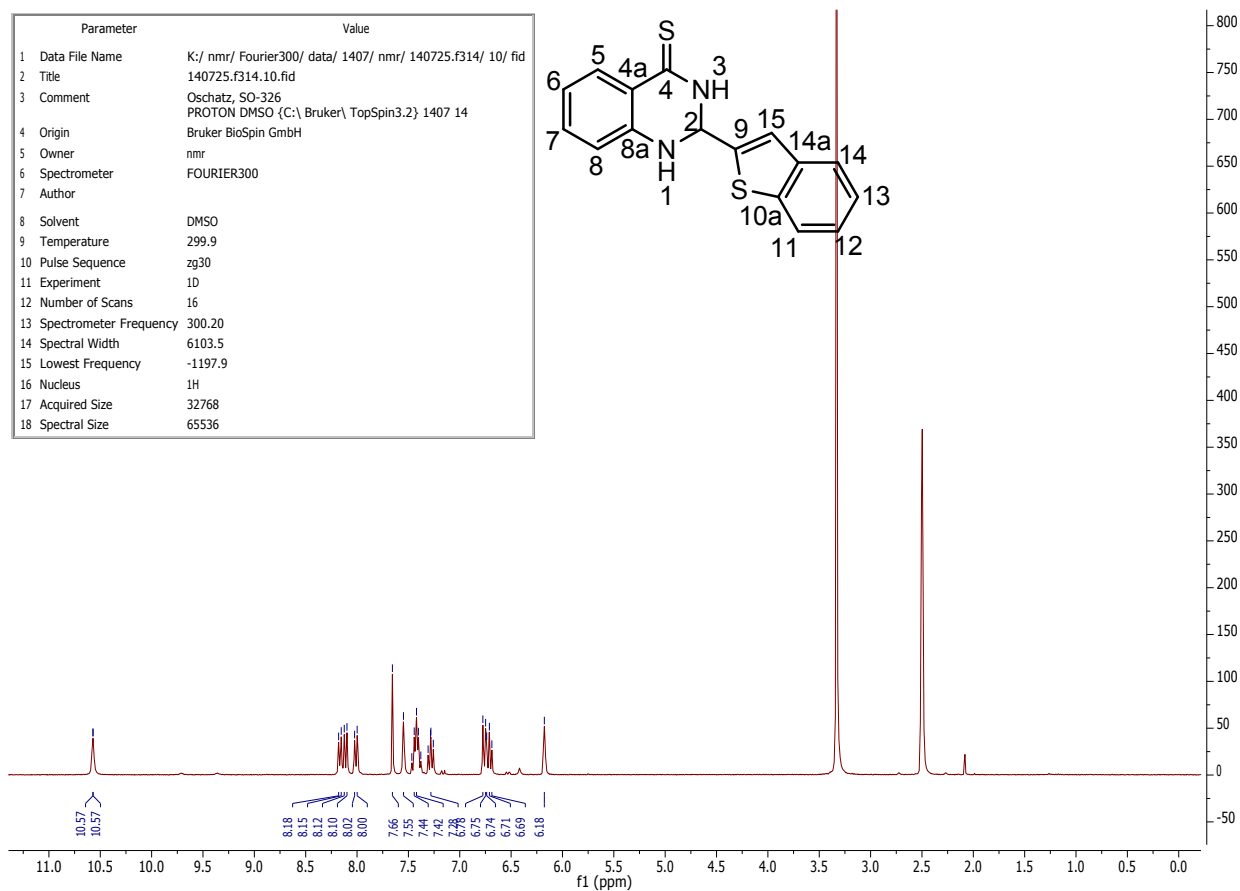
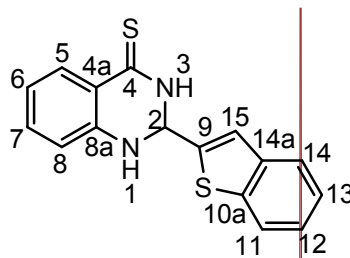


Parameter	Value
1 Data File Name	C:/ Users/ Tom Brunzel/ Desktop/ NMR/ 140613.205/ 10/ fid
2 Title	140613.20
3 Comment	Brunzel TB 28C 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Number of Scans	1024
13 Receiver Gain	2050
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	2.1846
17 Acquisition Date	2014-06-13T21:49:00
18 Modification Date	2014-06-13T20:49:28
19 Spectrometer Frequency	62.90
20 Spectral Width	15000.0
21 Lowest Frequency	-1239.6
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

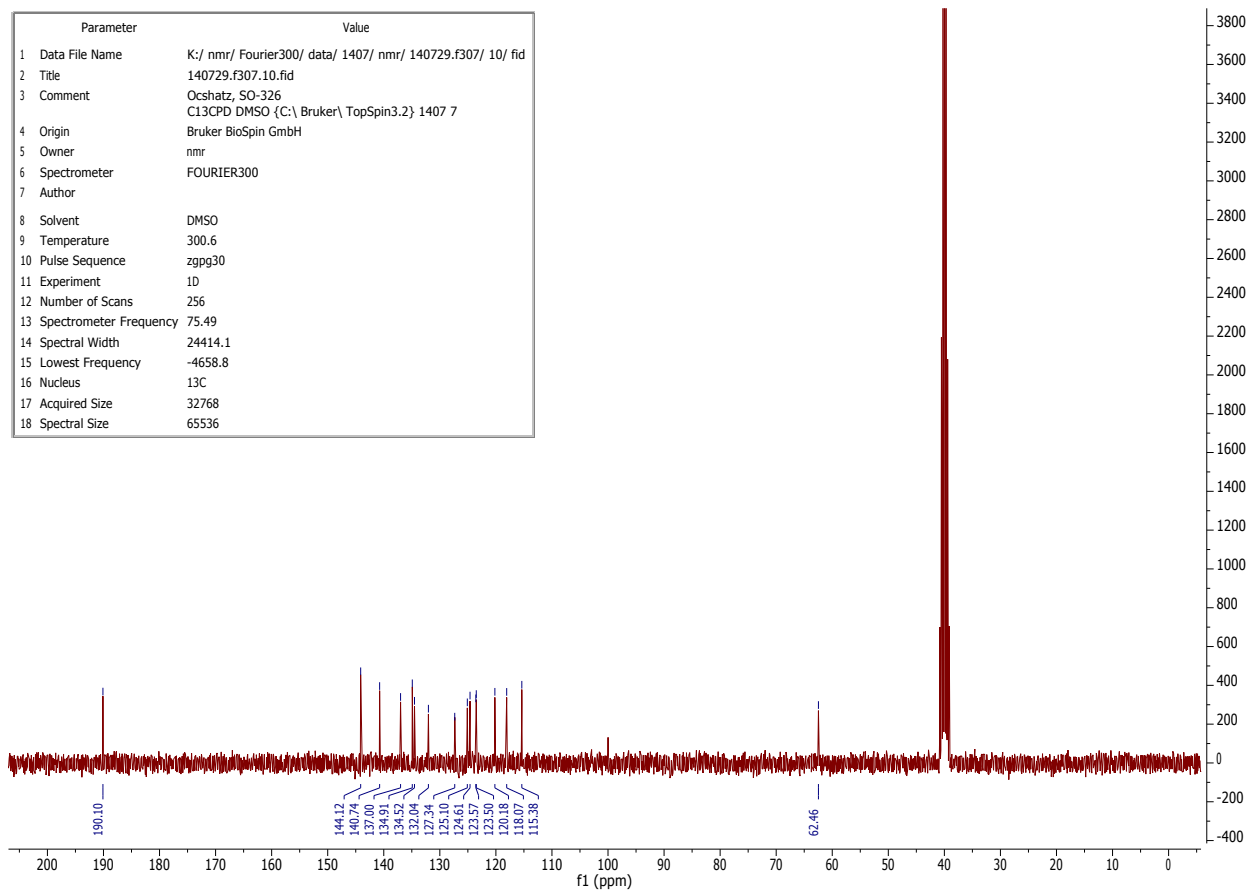


## 2-(Benzo[*b*]thiophen-2-yl)-2,3-dihydroquinazoline-4(1*H*)-thione (2k):

Parameter	Value
1 Data File Name	K:/ nmr/ Fourier300/ data/ 1407/ nmr/ 140725.f314/ 10/ fid
2 Title	140725.f314.10.fid
3 Comment	Oschatz, SO-326 PROTON DMSO {C:\ Bruker\ TopSpin3.2} 1407 14
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Spectrometer	FOURIER300
7 Author	
8 Solvent	DMSO
9 Temperature	299.9
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	16
13 Spectrometer Frequency	300.20
14 Spectral Width	6103.5
15 Lowest Frequency	-1197.9
16 Nucleus	<sup>1</sup> H
17 Acquired Size	32768
18 Spectral Size	65536

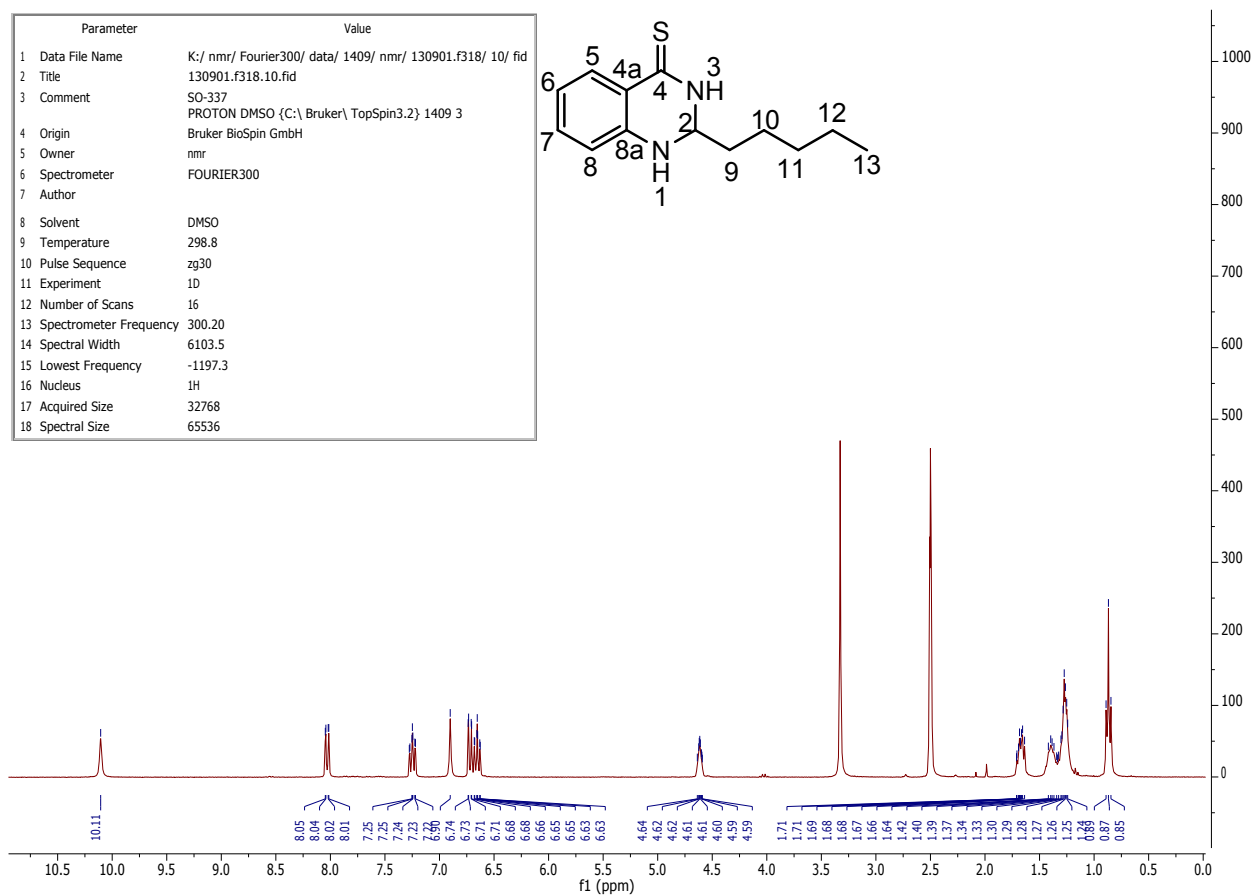
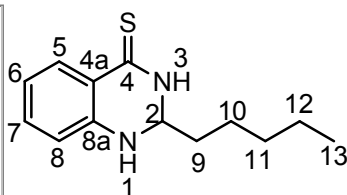


Parameter	Value
1 Data File Name	K:/ nmr/ Fourier300/ data/ 1407/ nmr/ 140729.f307/ 10/ fid
2 Title	140729.f307.10.fid
3 Comment	Oschatz, SO-326 C13CPD DMSO {C:\ Bruker\ TopSpin3.2} 1407 7
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Spectrometer	FOURIER300
7 Author	
8 Solvent	DMSO
9 Temperature	300.6
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	256
13 Spectrometer Frequency	75.49
14 Spectral Width	24414.1
15 Lowest Frequency	-4658.8
16 Nucleus	<sup>13</sup> C
17 Acquired Size	32768
18 Spectral Size	65536

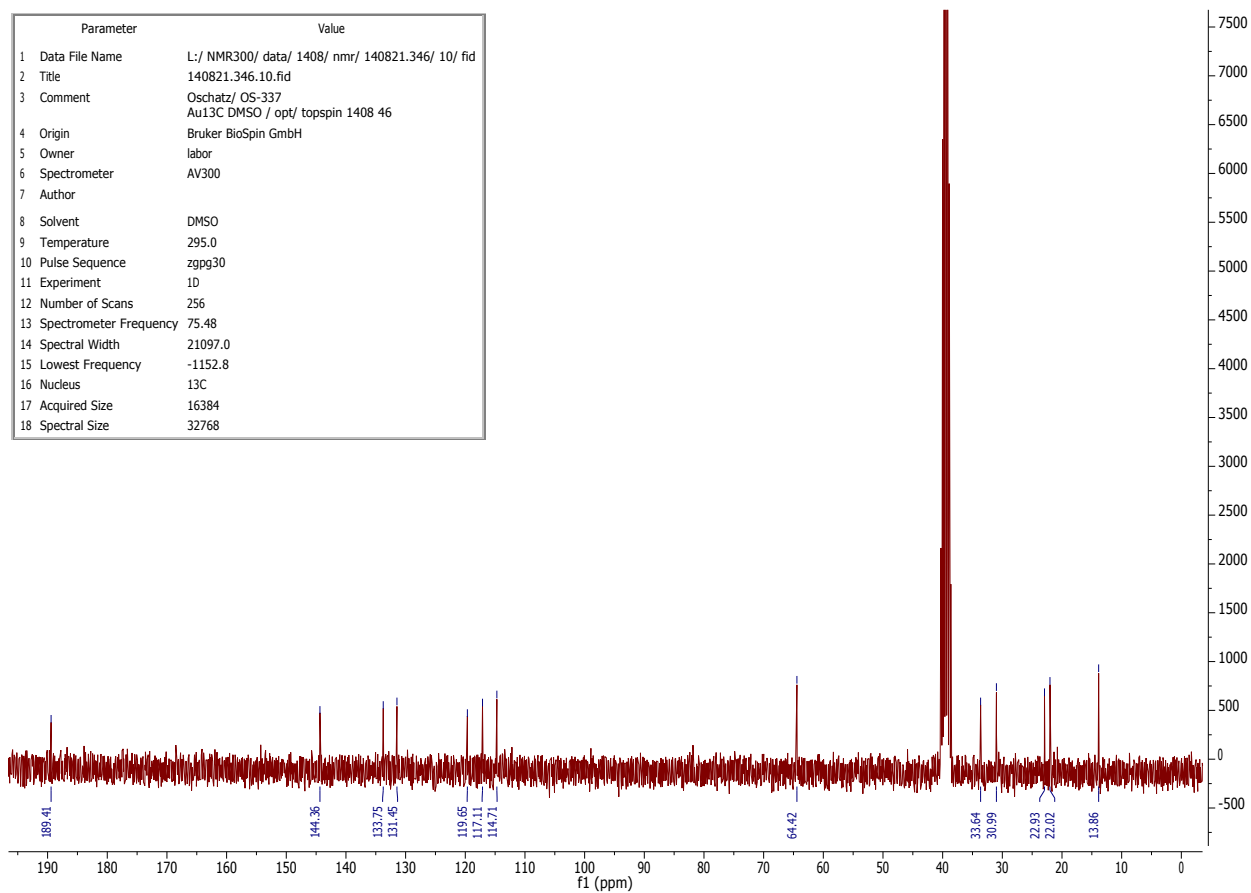


## 2-Pentyl-2,3-dihydroquinazoline-4(1H)-thione (2l):

Parameter	Value
1 Data File Name	K:/ nmr/ Fourier300/ data/ 1409/ nmr/ 130901.f318/ 10/ fid
2 Title	130901.f318.10.fid
3 Comment	SO-337 PROTON DMSO {C:\ Bruker\ TopSpin3.2} 1409 3
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Spectrometer	FOURIER300
7 Author	
8 Solvent	DMSO
9 Temperature	298.8
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	16
13 Spectrometer Frequency	300.20
14 Spectral Width	6103.5
15 Lowest Frequency	-1197.3
16 Nucleus	<sup>1</sup> H
17 Acquired Size	32768
18 Spectral Size	65536



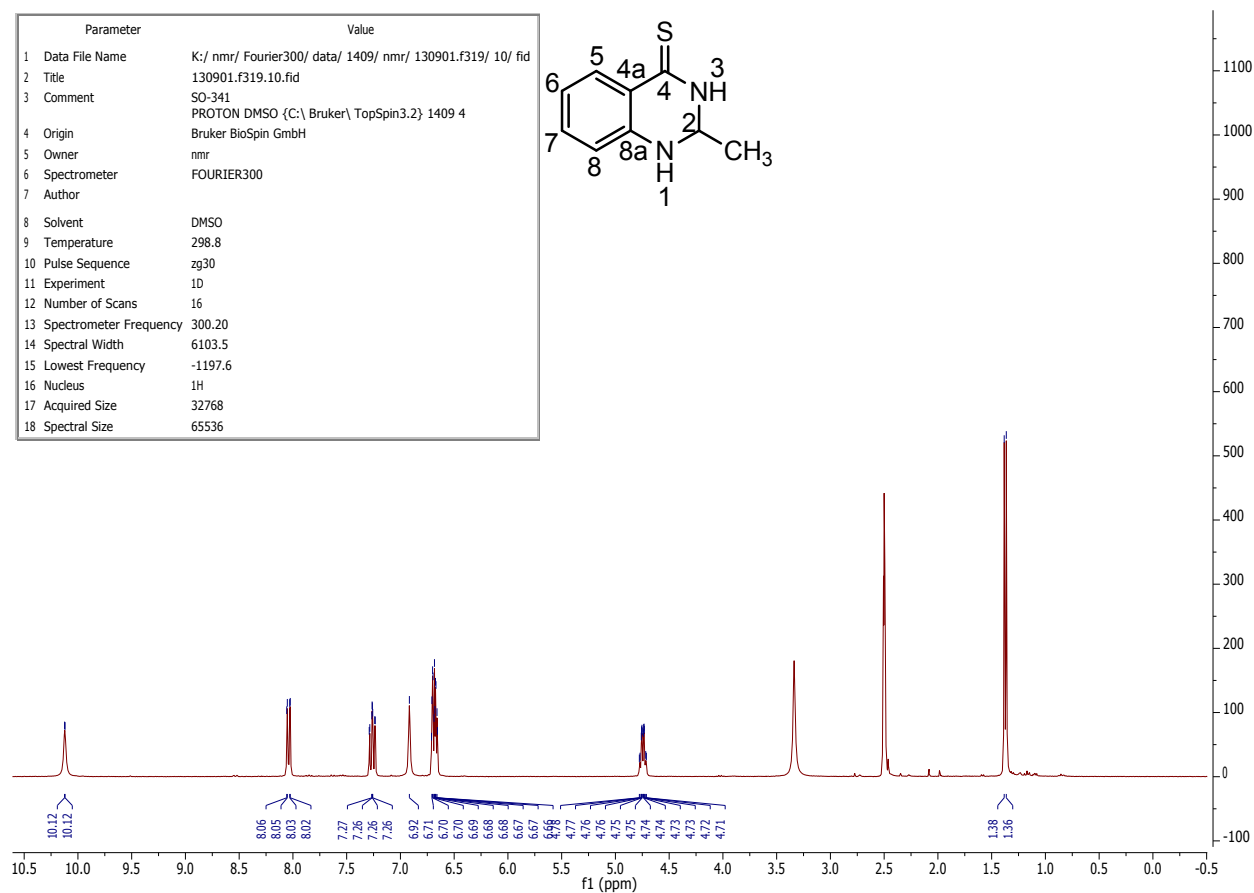
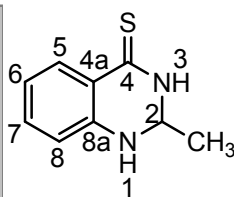
Parameter	Value
1 Data File Name	L:/ NMR300/ data/ 1408/ nmr/ 140821.346/ 10/ fid
2 Title	140821.346.10.fid
3 Comment	Oschatz/ OS-337 Au13C DMSO / opt/ topspin 1408 46
4 Origin	Bruker BioSpin GmbH
5 Owner	labor
6 Spectrometer	AV300
7 Author	
8 Solvent	DMSO
9 Temperature	295.0
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	256
13 Spectrometer Frequency	75.48
14 Spectral Width	21097.0
15 Lowest Frequency	-1152.8
16 Nucleus	<sup>13</sup> C
17 Acquired Size	16384
18 Spectral Size	32768



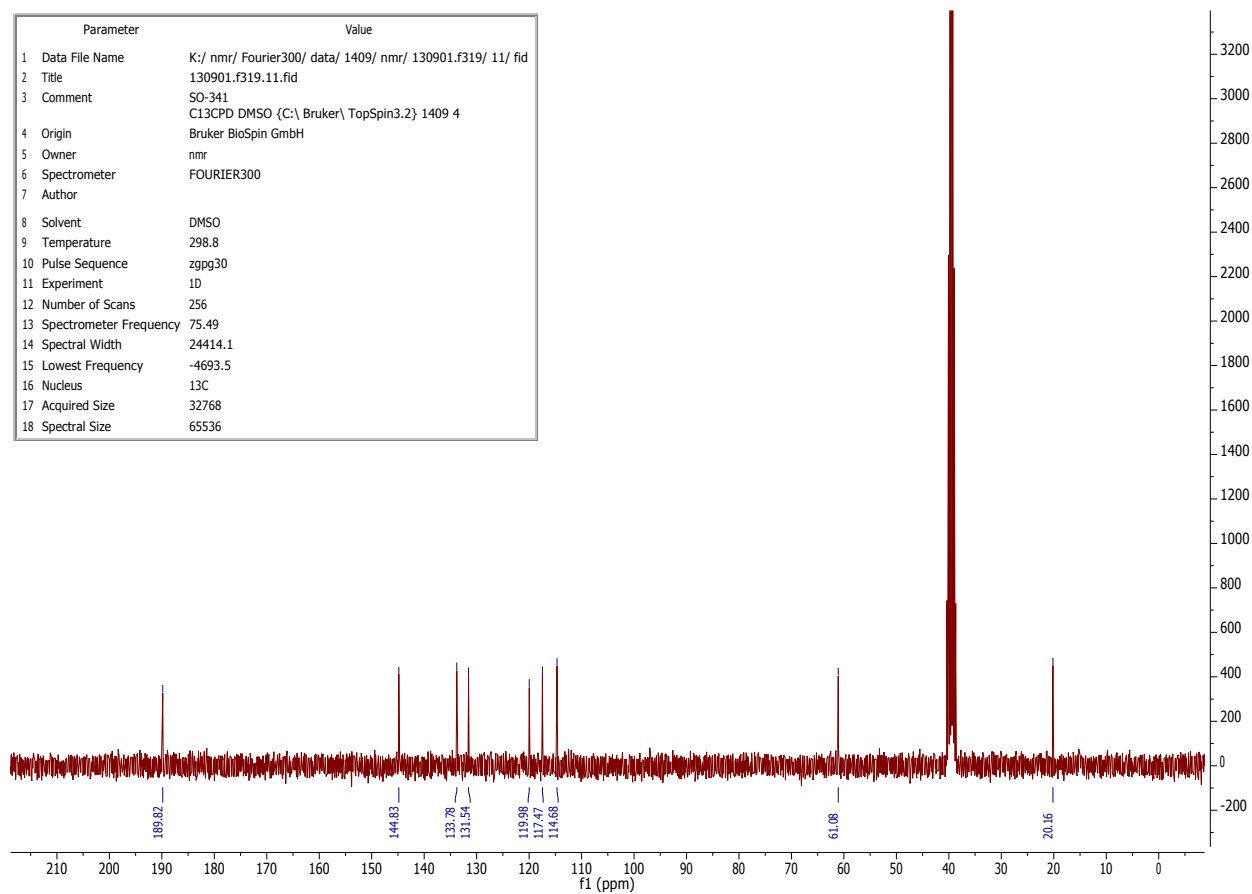


## 2-Methyl-2,3-dihydroquinazoline-4(1H)-thione (2m)

Parameter	Value
1 Data File Name	K:/ nmr/ Fourier300/ data/ 1409/ nmr/ 130901.f319/ 10/ fid
2 Title	130901.f319.10.fid
3 Comment	SO-341 PROTON DMSO {C:\ Bruker\ TopSpin3.2} 1409 4
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Spectrometer	FOURIER300
7 Author	
8 Solvent	DMSO
9 Temperature	298.8
10 Pulse Sequence	zg30
11 Experiment	1D
12 Number of Scans	16
13 Spectrometer Frequency	300.20
14 Spectral Width	6103.5
15 Lowest Frequency	-1197.6
16 Nucleus	<sup>1</sup> H
17 Acquired Size	32768
18 Spectral Size	65536

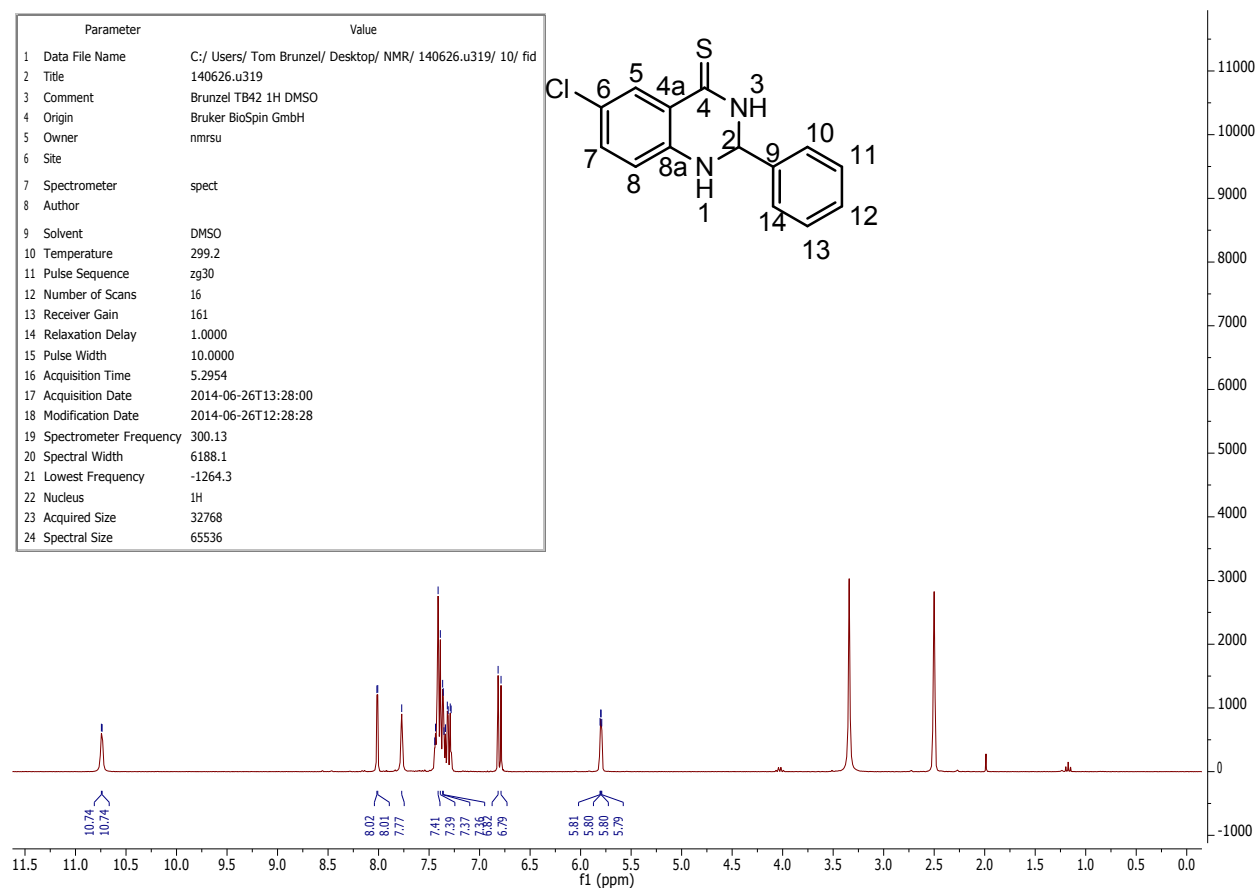
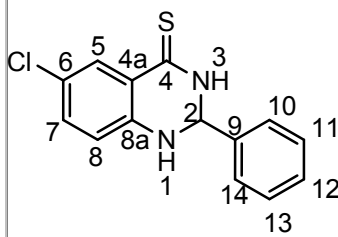


Parameter	Value
1 Data File Name	K:/ nmr/ Fourier300/ data/ 1409/ nmr/ 130901.f319/ 11/ fid
2 Title	130901.f319.11.fid
3 Comment	SO-341 C13CPD DMSO {C:\ Bruker\ TopSpin3.2} 1409 4
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Spectrometer	FOURIER300
7 Author	
8 Solvent	DMSO
9 Temperature	298.8
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	256
13 Spectrometer Frequency	75.49
14 Spectral Width	24414.1
15 Lowest Frequency	-4693.5
16 Nucleus	<sup>13</sup> C
17 Acquired Size	32768
18 Spectral Size	65536

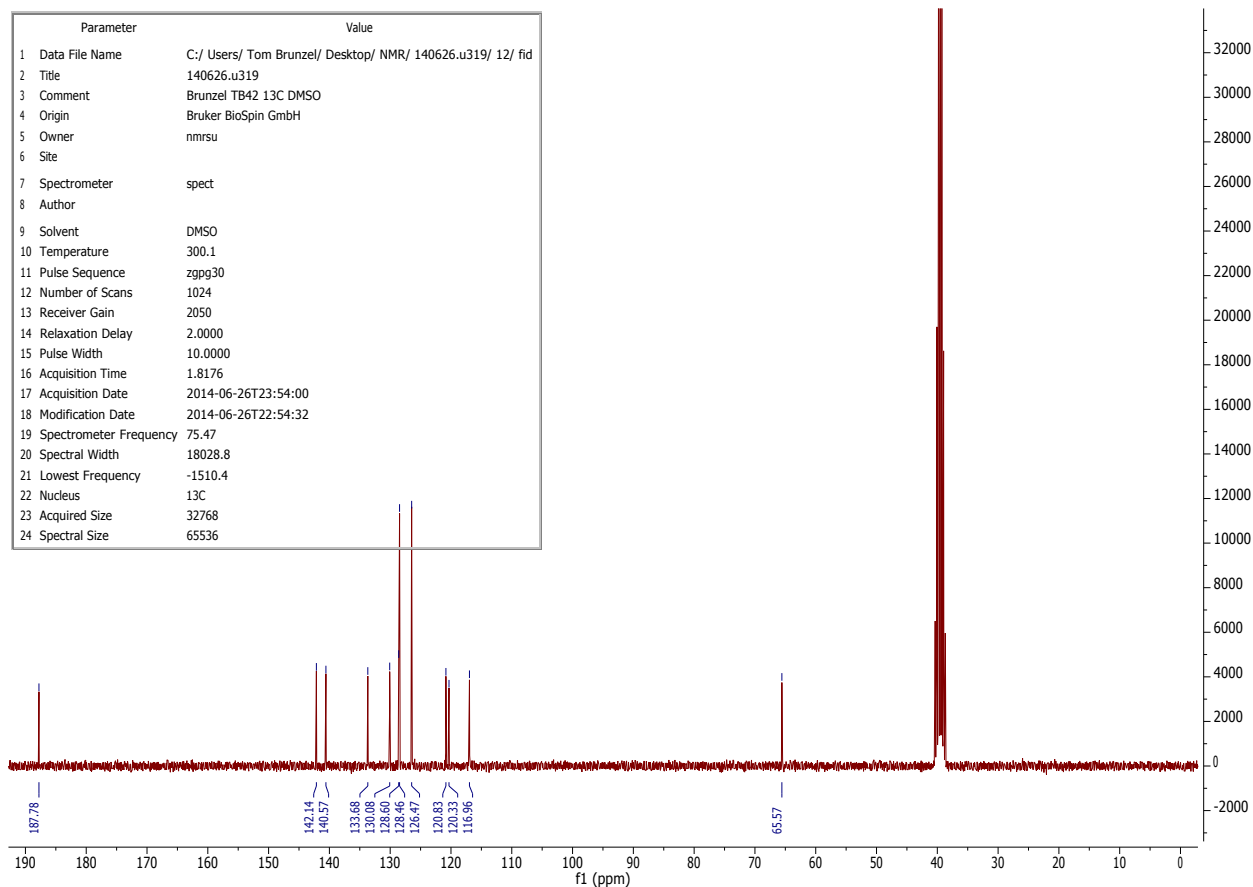


## 6-Chloro-2-phenyl-2,3-dihydroquinazoline-4(1H)-thione (2n):

Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140626.u319/10/ fid
2 Title	140626.u319
3 Comment	Brunzel TB42 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	299.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	161
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	5.2954
17 Acquisition Date	2014-06-26T13:28:00
18 Modification Date	2014-06-26T12:28:28
19 Spectrometer Frequency	300.13
20 Spectral Width	6188.1
21 Lowest Frequency	-1264.3
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

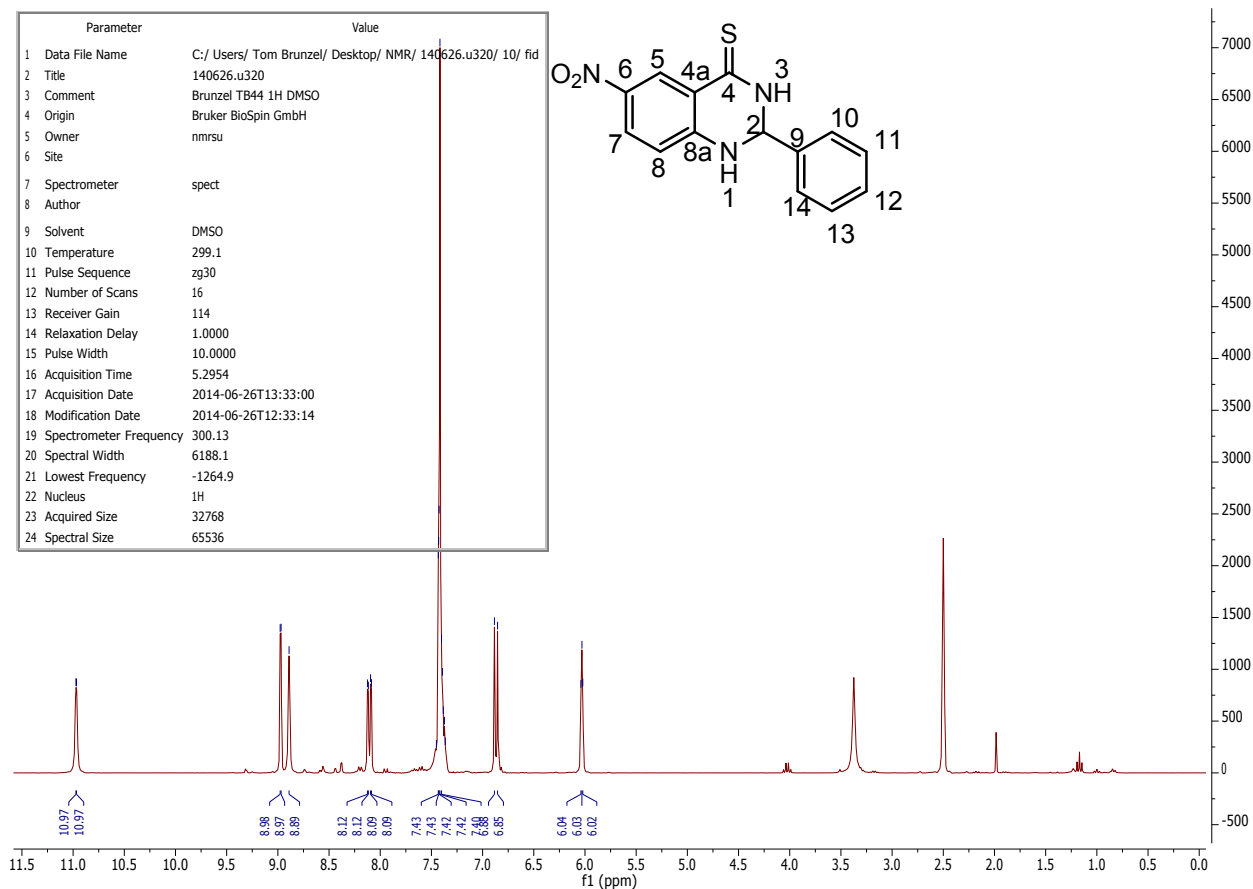
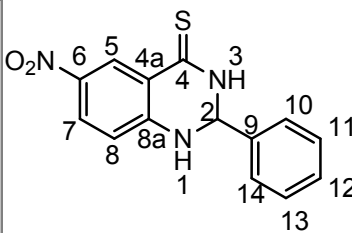


Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140626.u319/12/ fid
2 Title	140626.u319
3 Comment	Brunzel TB42 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	300.1
11 Pulse Sequence	zgpg30
12 Number of Scans	1024
13 Receiver Gain	2050
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	1.8176
17 Acquisition Date	2014-06-26T23:54:00
18 Modification Date	2014-06-26T22:54:32
19 Spectrometer Frequency	75.47
20 Spectral Width	18028.8
21 Lowest Frequency	-1510.4
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

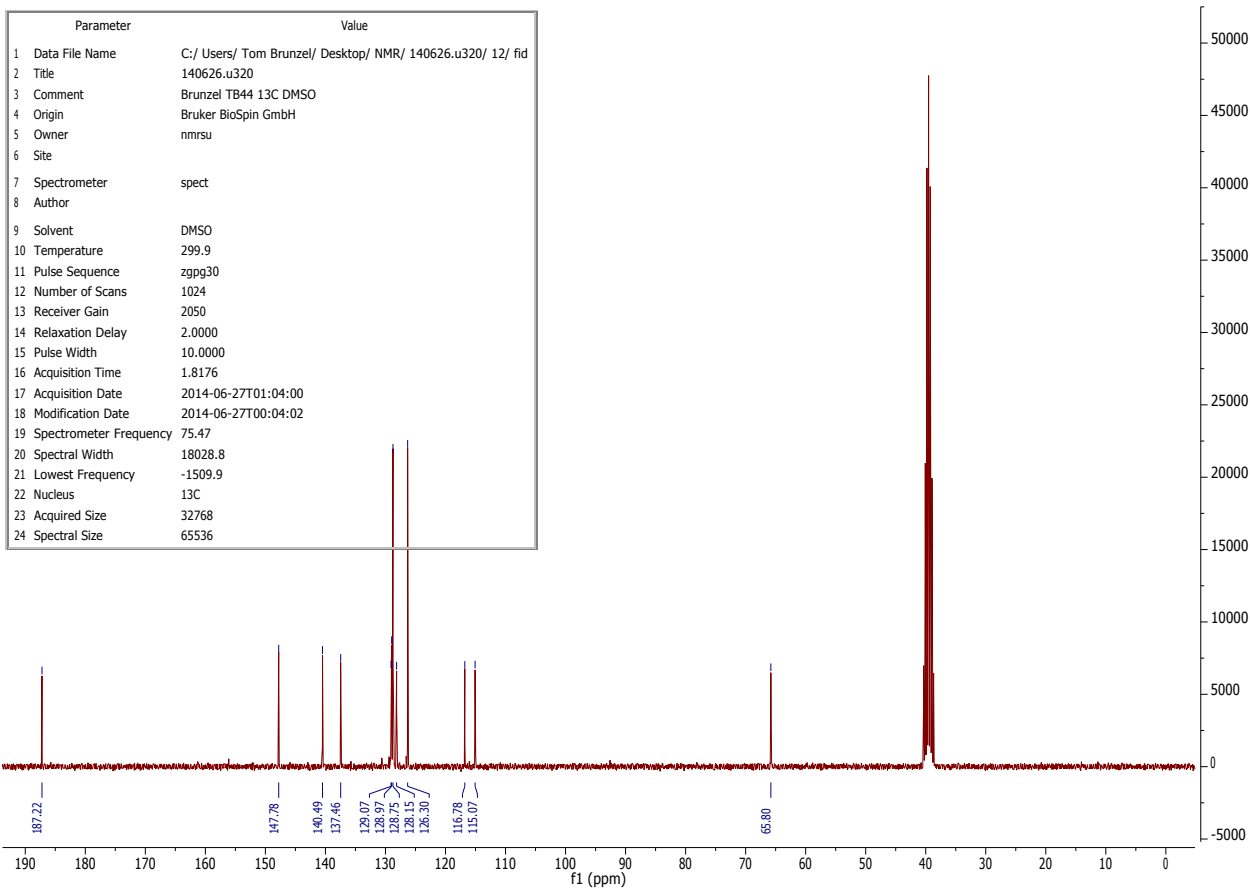


# 6-Nitro-2-phenyl-2,3-dihydroquinazoline-4(1H)-thione (2o)

Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140626.u320/10/fid
2 Title	140626.u320
3 Comment	Brunzel TB44 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	299.1
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	114
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	5.2954
17 Acquisition Date	2014-06-26T13:33:00
18 Modification Date	2014-06-26T12:33:14
19 Spectrometer Frequency	300.13
20 Spectral Width	6188.1
21 Lowest Frequency	-1264.9
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

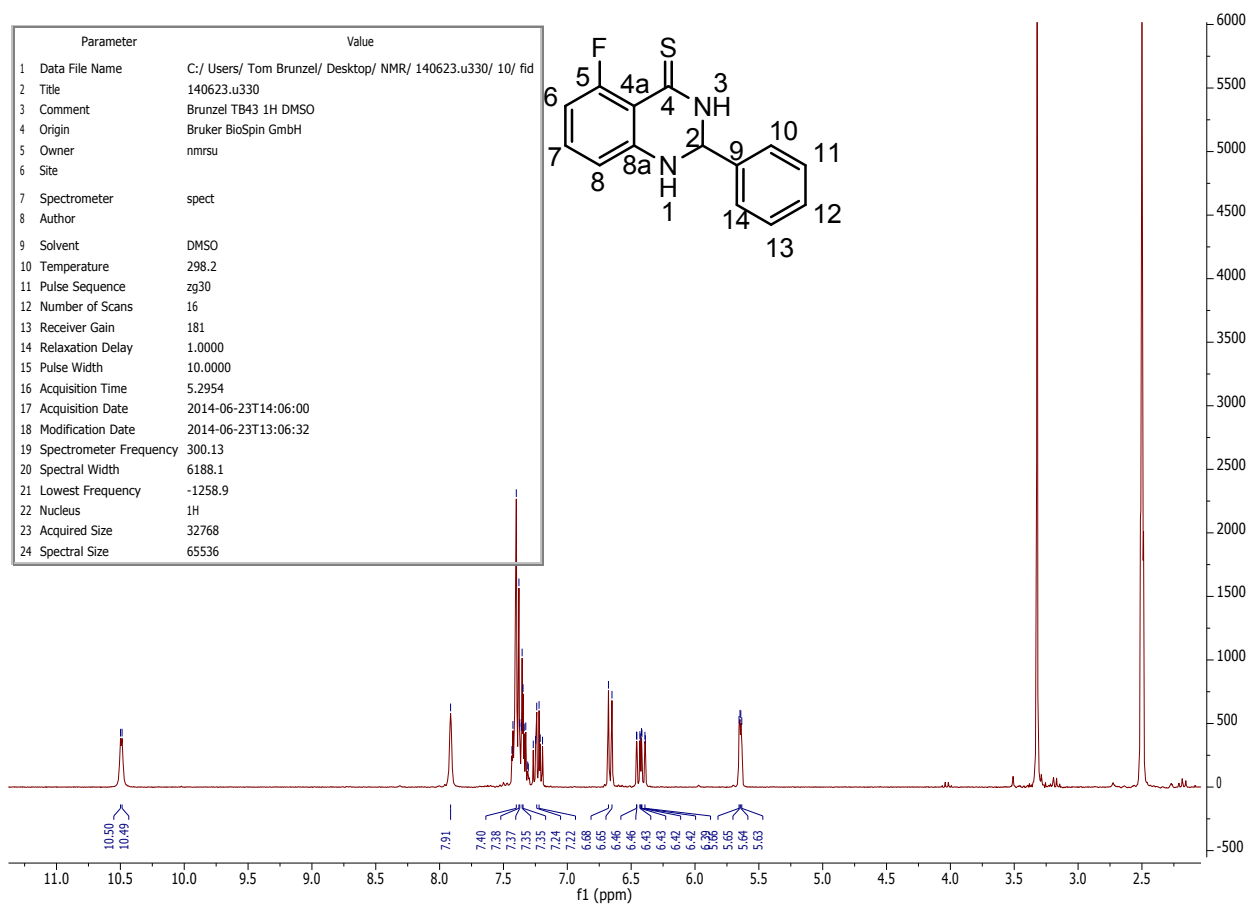
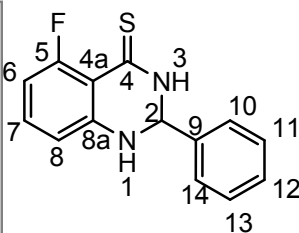


Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140626.u320/12/fid
2 Title	140626.u320
3 Comment	Brunzel TB44 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	299.9
11 Pulse Sequence	zpgg30
12 Number of Scans	1024
13 Receiver Gain	2050
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	1.8176
17 Acquisition Date	2014-06-27T01:04:00
18 Modification Date	2014-06-27T00:04:02
19 Spectrometer Frequency	75.47
20 Spectral Width	18028.8
21 Lowest Frequency	-1509.9
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

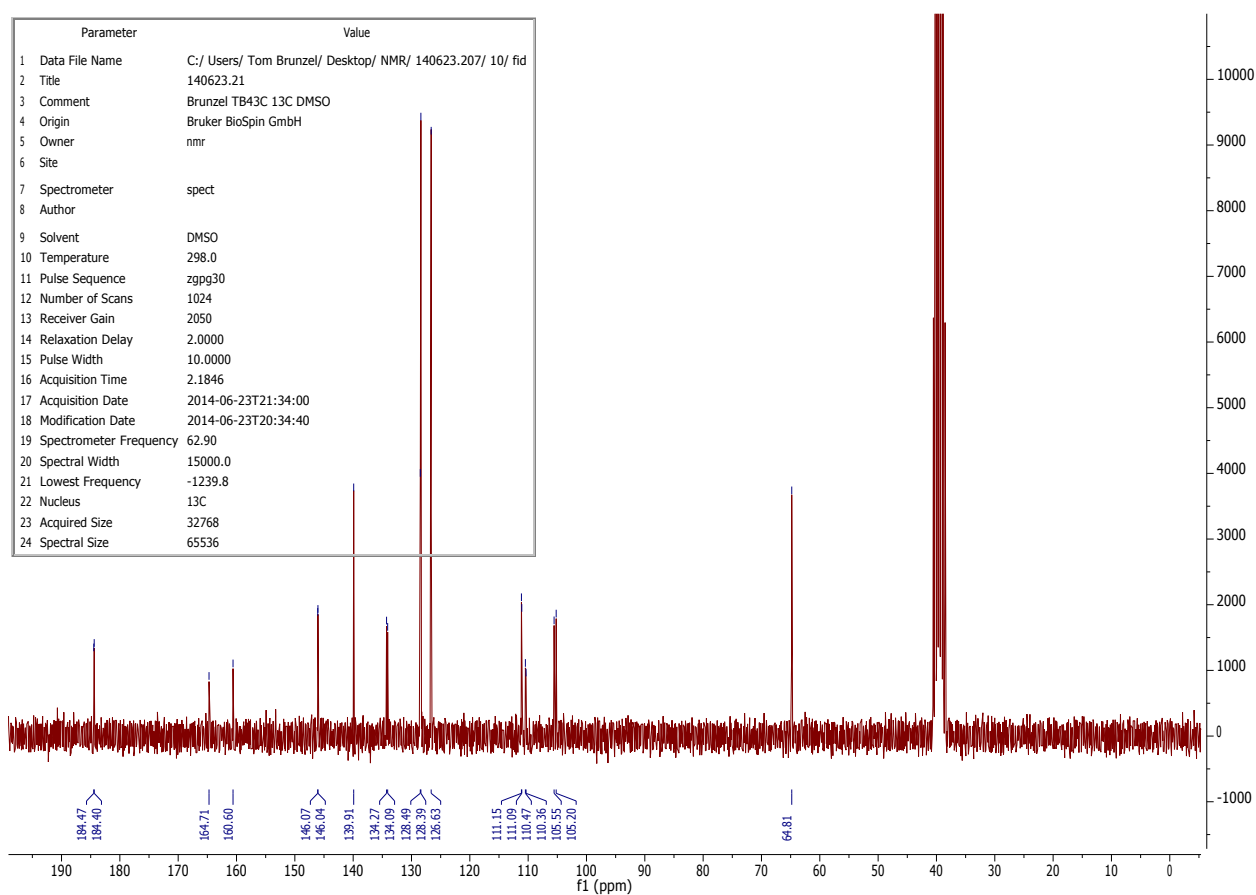


### 5-Fluoro-2-phenyl-2,3-dihydroquinazoline-4(1H)-thione (2p):

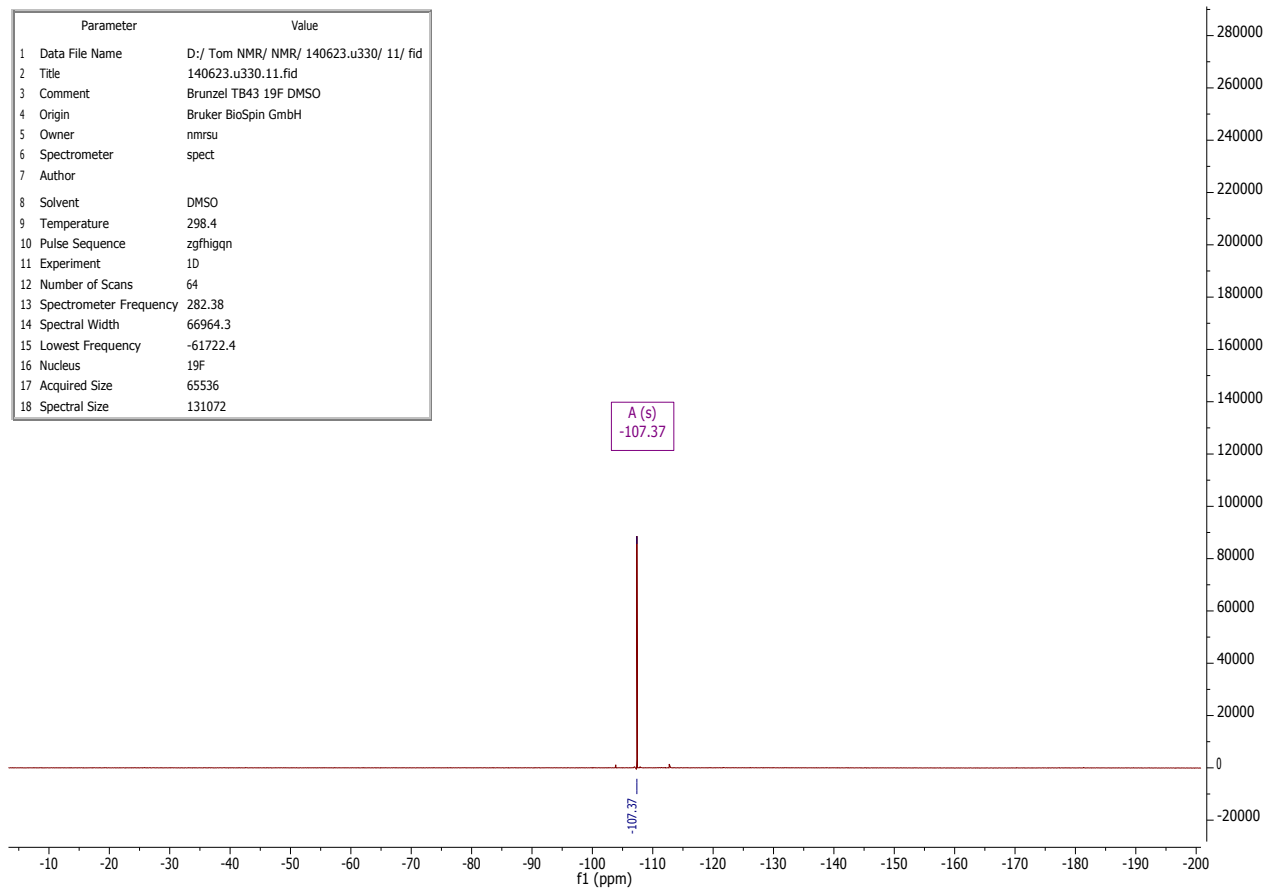
Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140623.u330/10/fid
2 Title	140623.u330
3 Comment	Brunzel TB43 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	181
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	5.2954
17 Acquisition Date	2014-06-23T14:06:00
18 Modification Date	2014-06-23T13:06:32
19 Spectrometer Frequency	300.13
20 Spectral Width	6188.1
21 Lowest Frequency	-1258.9
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/Users/Tom Brunzel/Desktop/NMR/140623.207/10/fid
2 Title	140623.21
3 Comment	Brunzel TB43C 13C DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Number of Scans	1024
13 Receiver Gain	2050
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	2.1846
17 Acquisition Date	2014-06-23T21:34:00
18 Modification Date	2014-06-23T20:34:40
19 Spectrometer Frequency	62.90
20 Spectral Width	15000.0
21 Lowest Frequency	-1239.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

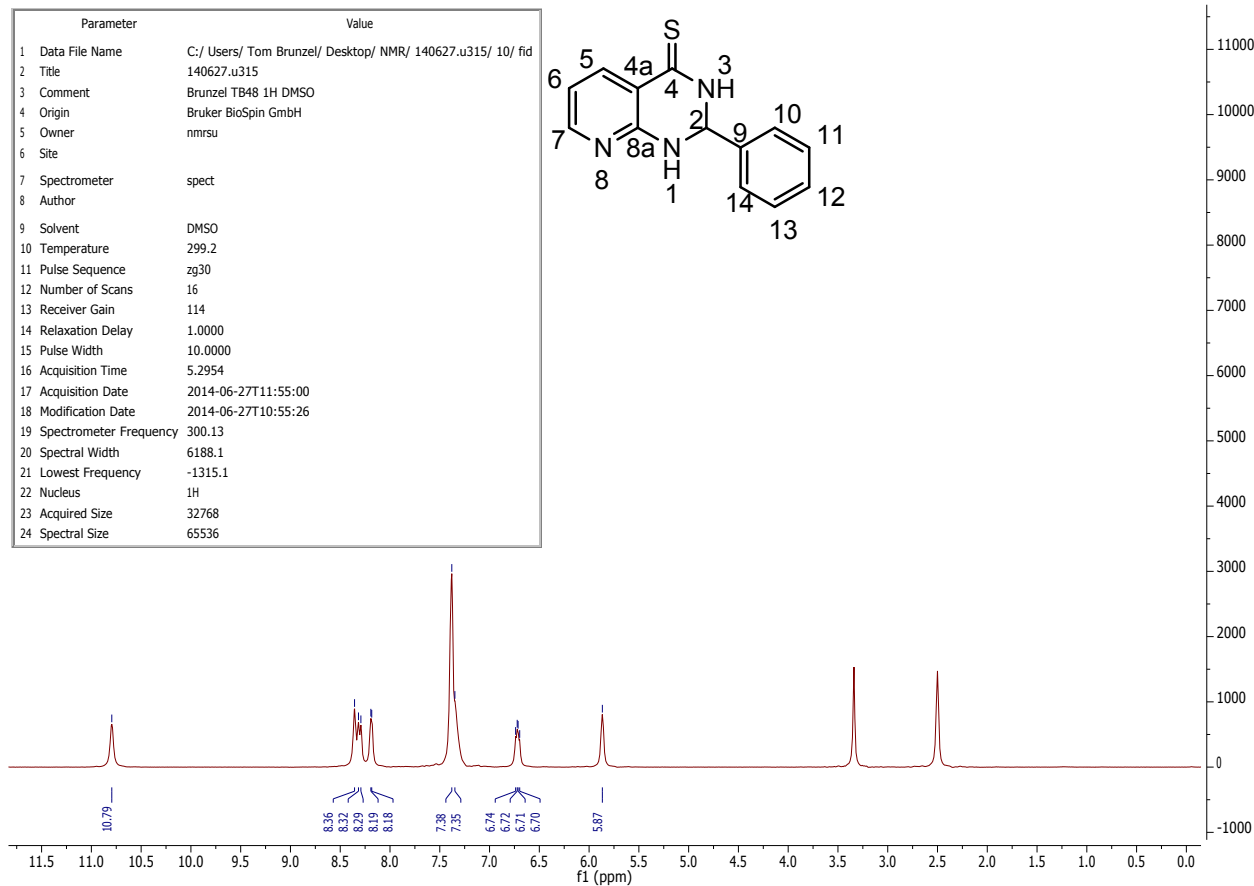
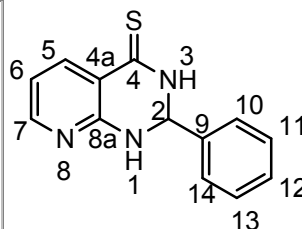


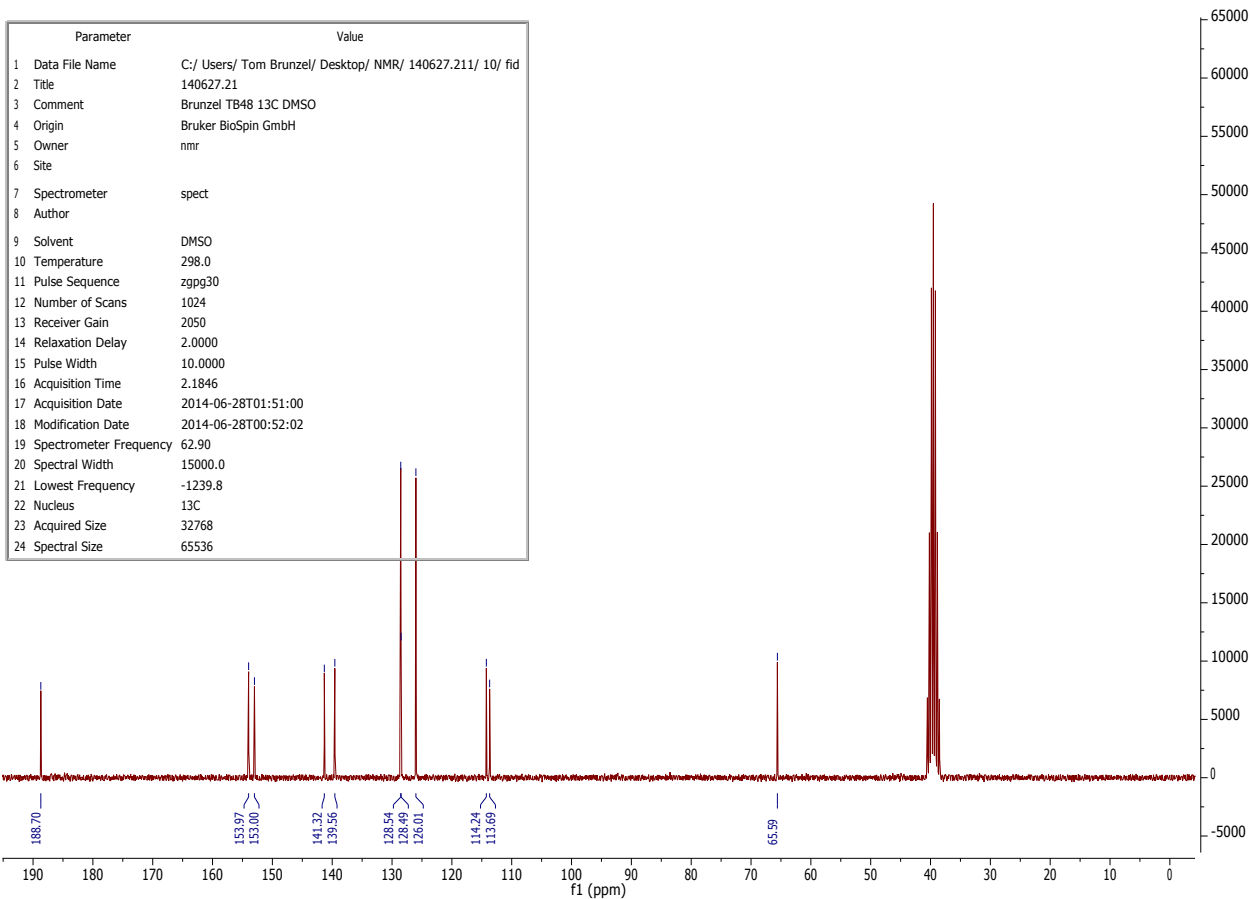
Parameter	Value
1 Data File Name	D:/ Tom NMR/ NMR/ 140623.u330/ 11/ fid
2 Title	140623.u330.11.fid
3 Comment	Brunzel TB43 19F DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	298.4
10 Pulse Sequence	zgfhgqn
11 Experiment	1D
12 Number of Scans	64
13 Spectrometer Frequency	282.38
14 Spectral Width	66964.3
15 Lowest Frequency	-61722.4
16 Nucleus	19F
17 Acquired Size	65536
18 Spectral Size	131072



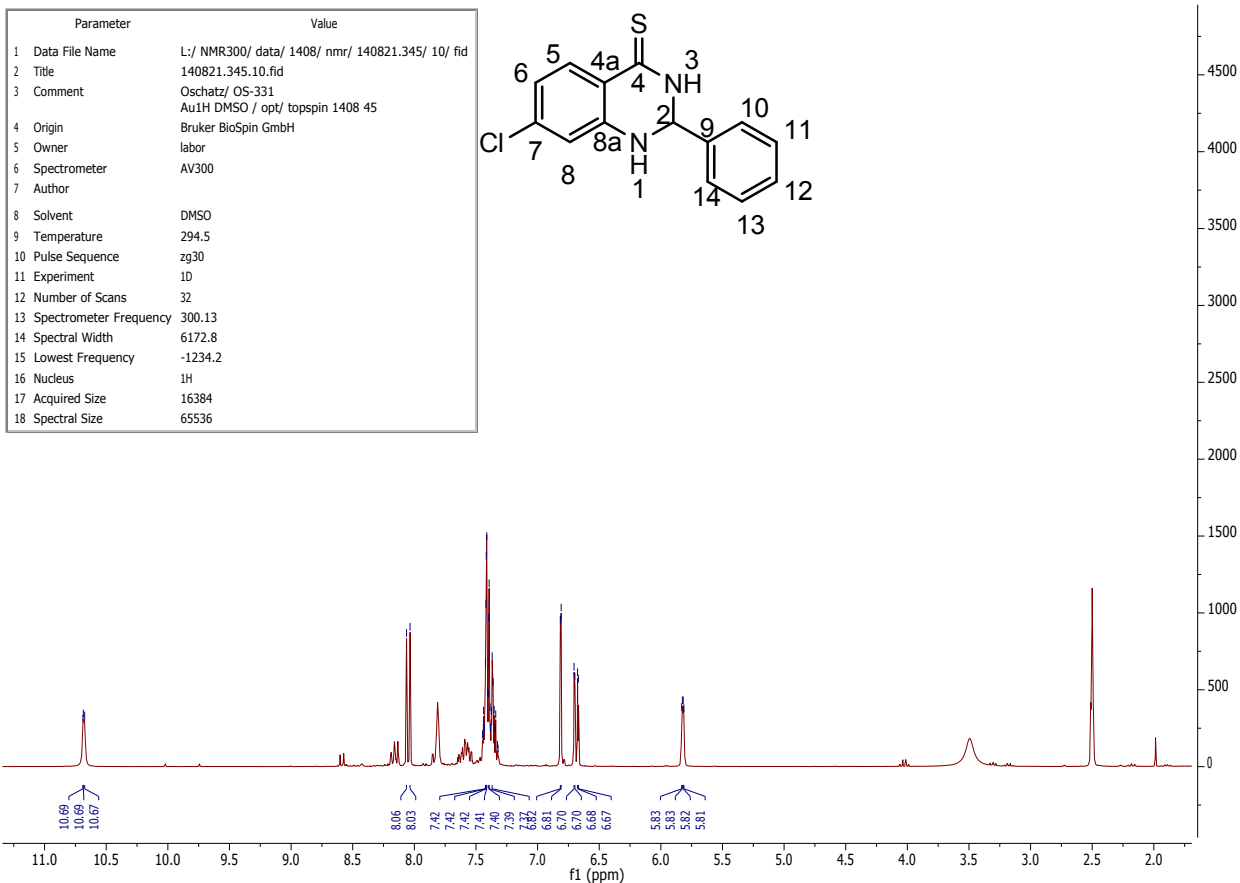
## 2-Phenyl-2,3-dihydropyrido[2,3-d]pyrimidine-4(1H)-thione (2q):

Parameter	Value
1 Data File Name	C:/ Users/ Tom Brunzel/ Desktop/ NMR/ 140627.u315/ 10/ fid
2 Title	140627.u315
3 Comment	Brunzel TB48 1H DMSO
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	299.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	114
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	5.2954
17 Acquisition Date	2014-06-27T11:55:00
18 Modification Date	2014-06-27T10:55:26
19 Spectrometer Frequency	300.13
20 Spectral Width	6188.1
21 Lowest Frequency	-1315.1
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

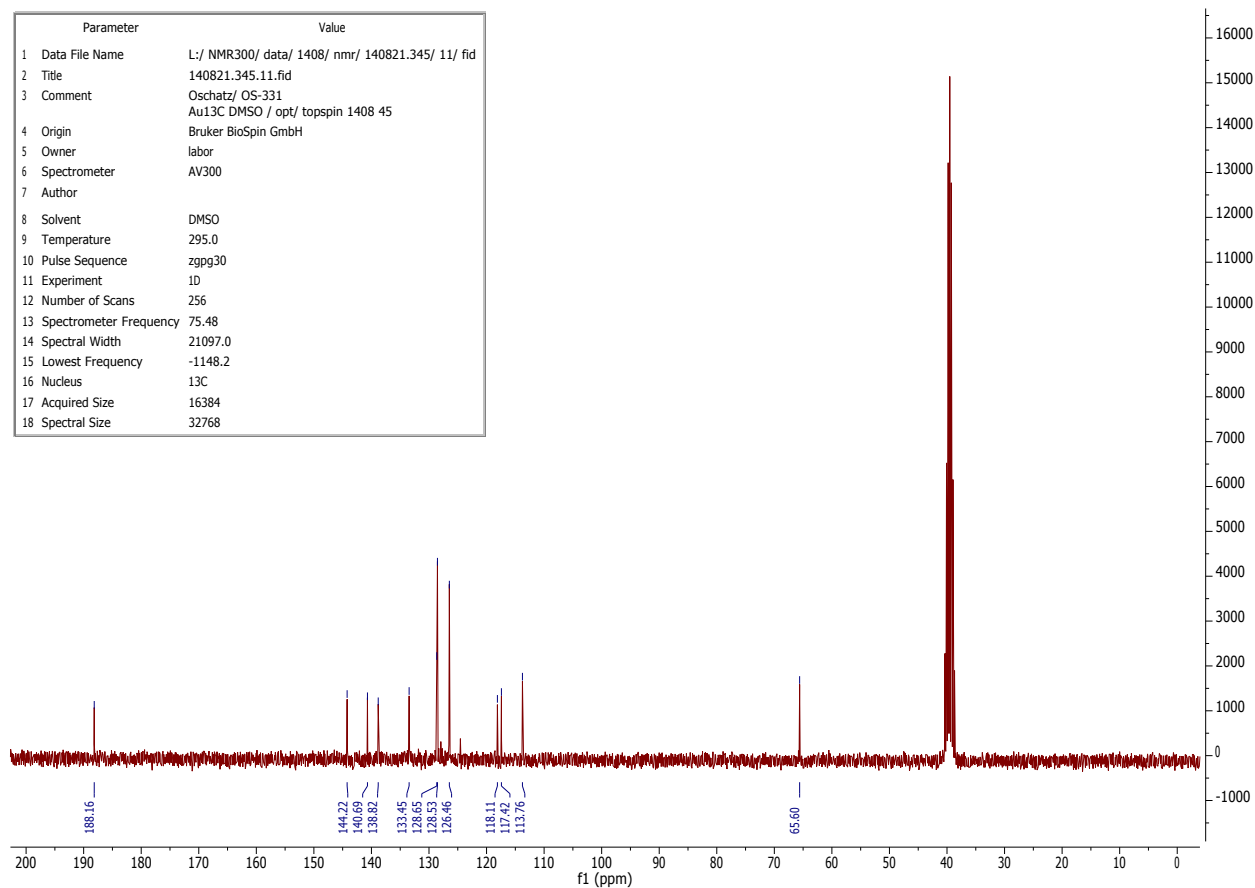




**7-Chloro-2-phenyl-2,3-dihydroquinazoline-4(1H)-thione (2r):**



Parameter	Value
1 Data File Name	L:/ NMR300/ data/ 1408/ nmr/ 140821.345/ 11/ fid
2 Title	140821.345.11.fid
3 Comment	Oschatz/ OS-331 Au13C DMSO / opt/ topspin 1408 45
4 Origin	Bruker BioSpin GmbH
5 Owner	labor
6 Spectrometer	AV300
7 Author	
8 Solvent	DMSO
9 Temperature	295.0
10 Pulse Sequence	zgpg30
11 Experiment	1D
12 Number of Scans	256
13 Spectrometer Frequency	75.48
14 Spectral Width	21097.0
15 Lowest Frequency	-1148.2
16 Nucleus	13C
17 Acquired Size	16384
18 Spectral Size	32768



## 2D-coupling pattern of 2a

The H-H-COSY-experiment shows the coupling of both of the nitrogen-attached protons with the hydrogen atom at position 2. Additionally, the NOESY-experiment shows the interaction of the thiolactam-proton with the phenyl ring as well as the interaction of the amine-proton with the hydrogen atoms in position 8 and 10/14 (Fig. 2). These analytical data indicated that the ring closure involves an exocyclic sulfur atom.

