

Supporting Information

Palladium-catalyzed tandem reaction of 2-chloroquinoline-3-carbaldehydes and isocyanides

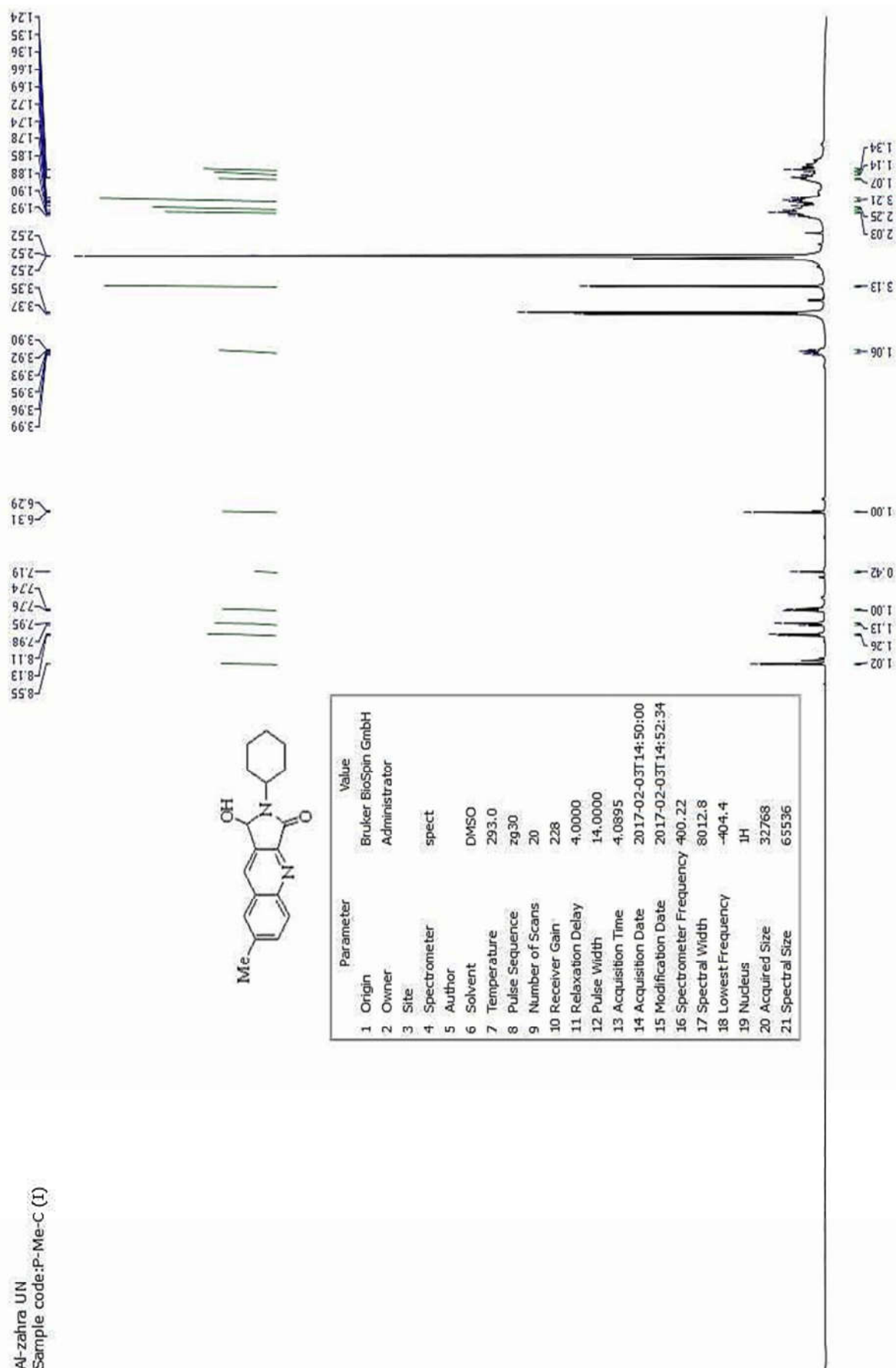
Morteza Shiri,^{a,*} Maryam Ranjbar,^a Zahra Yasaei,^a Fatemeh Zamanian,^a Behrouz Notash^b

^aDepartment of Chemistry, Faculty of Physics and Chemistry, Alzahra University, Vanak, Tehran 1993893973, Iran.

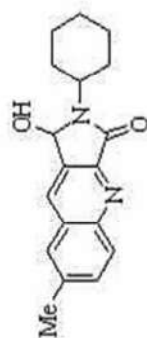
E-mail: mshiri@alzahra.ac.ir, Fax: +98 21 88041344

^bDepartment of Chemistry, Shahid Beheshti University, G. C., Evin, Tehran, 1983963113, Iran

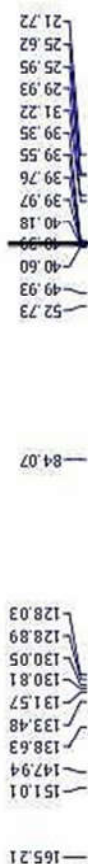
Al-zahra UN
Sample code: P-Me-C (I)



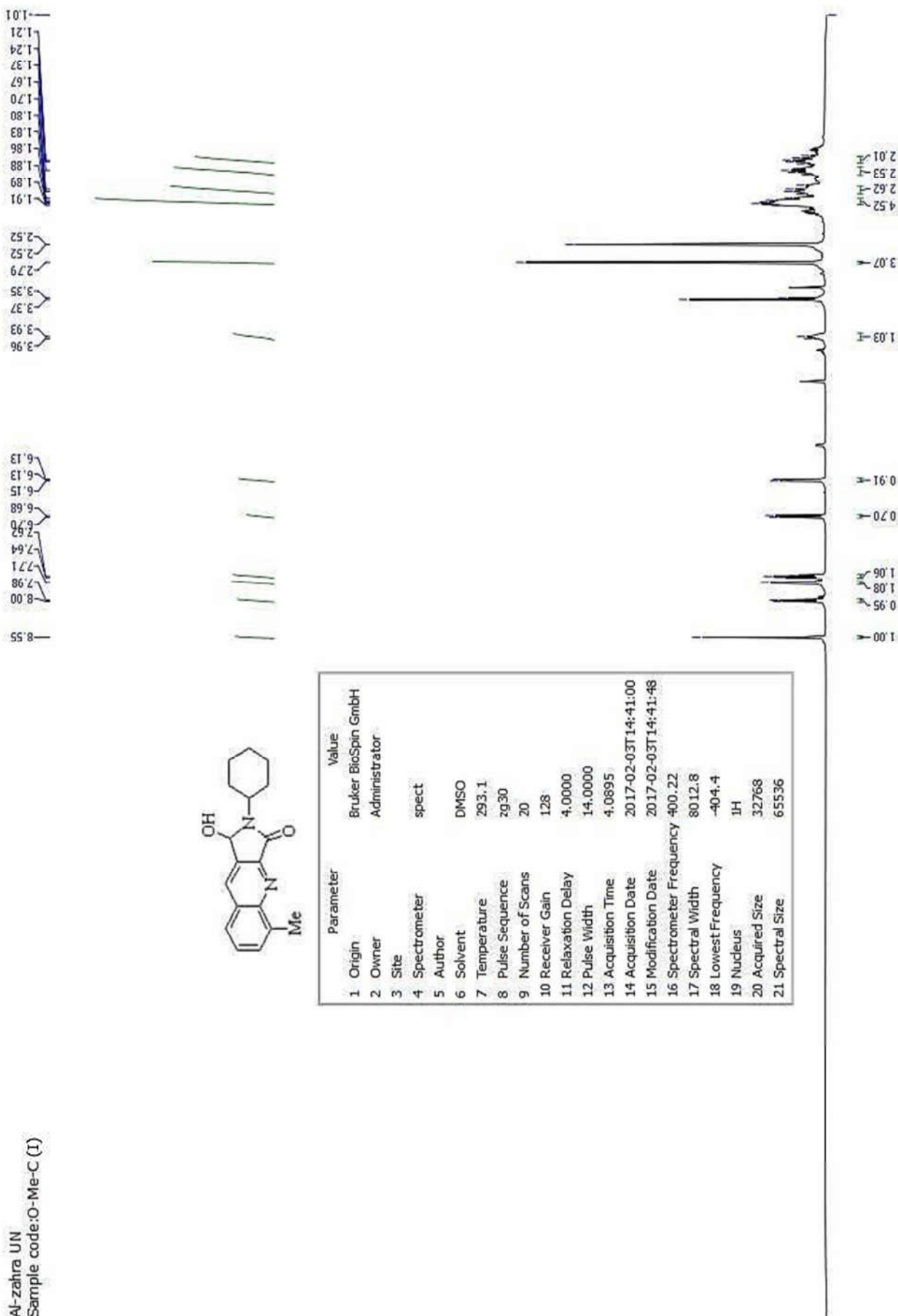
Al-zahra UN
Sample code:P-Me-C (I)



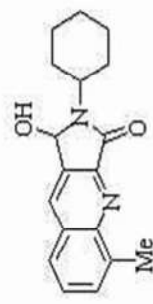
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1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	spect
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	294.5
8 Pulse Sequence	zgpg30
9 Number of Scans	3750
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-02-08T11:51:00
15 Modification Date	2017-02-08T13:48:16
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



Al-zahra UN
Sample code:O-Me-C (1)



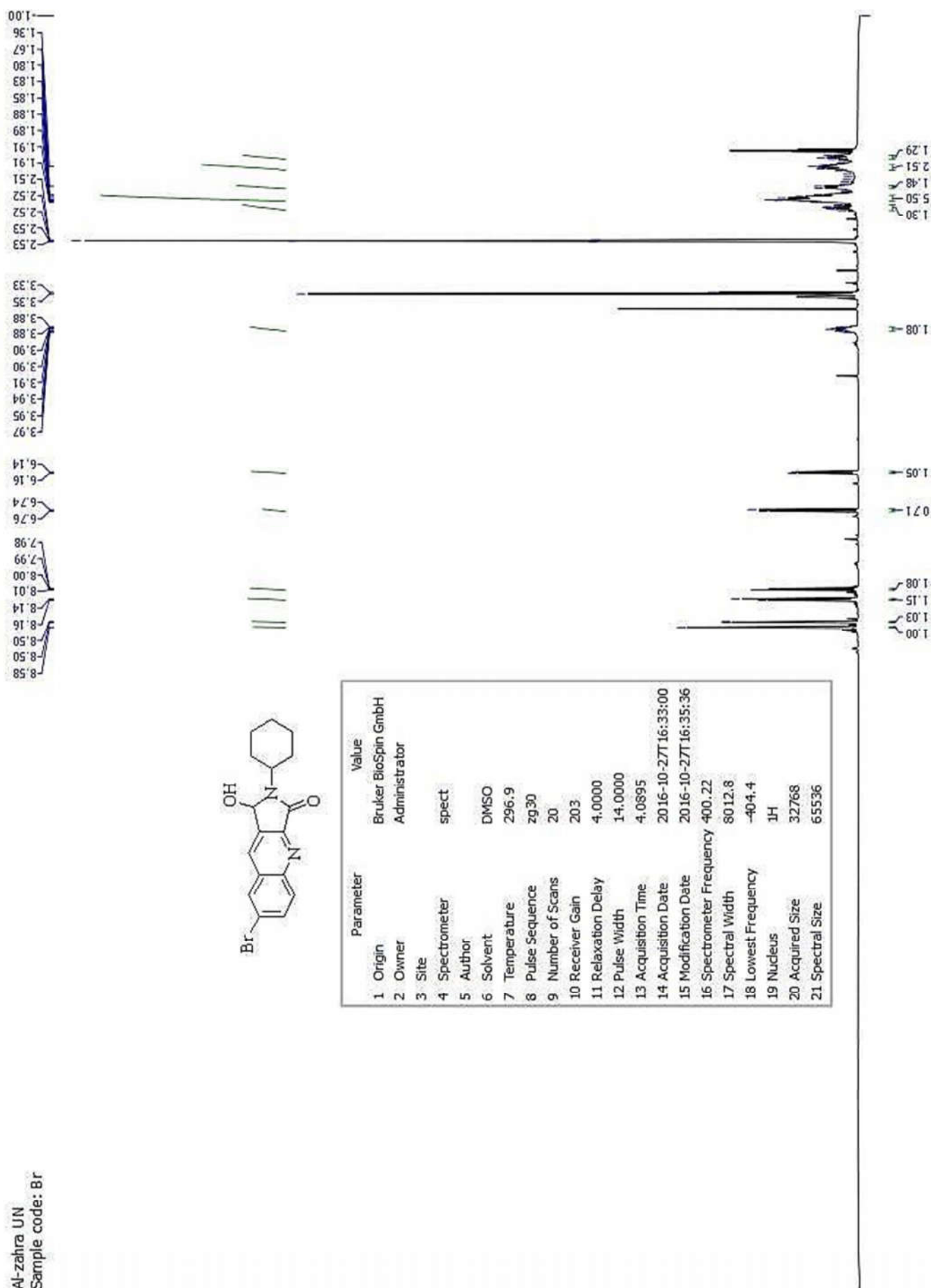
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Sample code:O-Me-C (I)



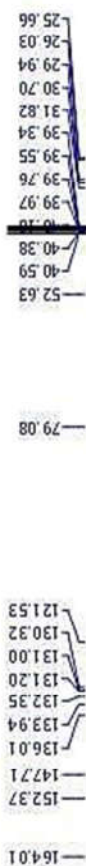
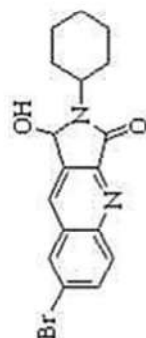
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1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	293.6
8 Pulse Sequence	zgpg30
9 Number of Scans	2000
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-02-08T08:49:00
15 Modification Date	2017-02-08T09:55:08
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



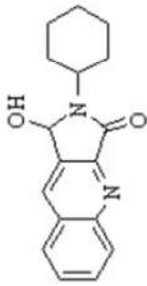
Al-zahra UN
Sample code: Br



Al-zahra UN
Sample code:Br-C

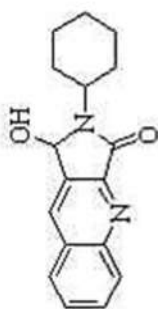


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	spect
4 Spectrometer	DMSO
5 Author	293.1
6 Solvent	zgpg30
7 Temperature	2050
8 Pulse Sequence	1.0000
9 Number of Scans	8192
10 Receiver Gain	9.0000
11 Relaxation Delay	0.9176
12 Pulse Width	2016-12-25T19:53:00
13 Acquisition Time	2016-12-26T00:19:34
14 Acquisition Date	100.64
15 Modification Date	35714.3
16 Spectrometer Frequency	-5277.7
17 Spectral Width	13C
18 Lowest Frequency	32768
19 Nucleus	65536
20 Acquired Size	
21 Spectral Size	



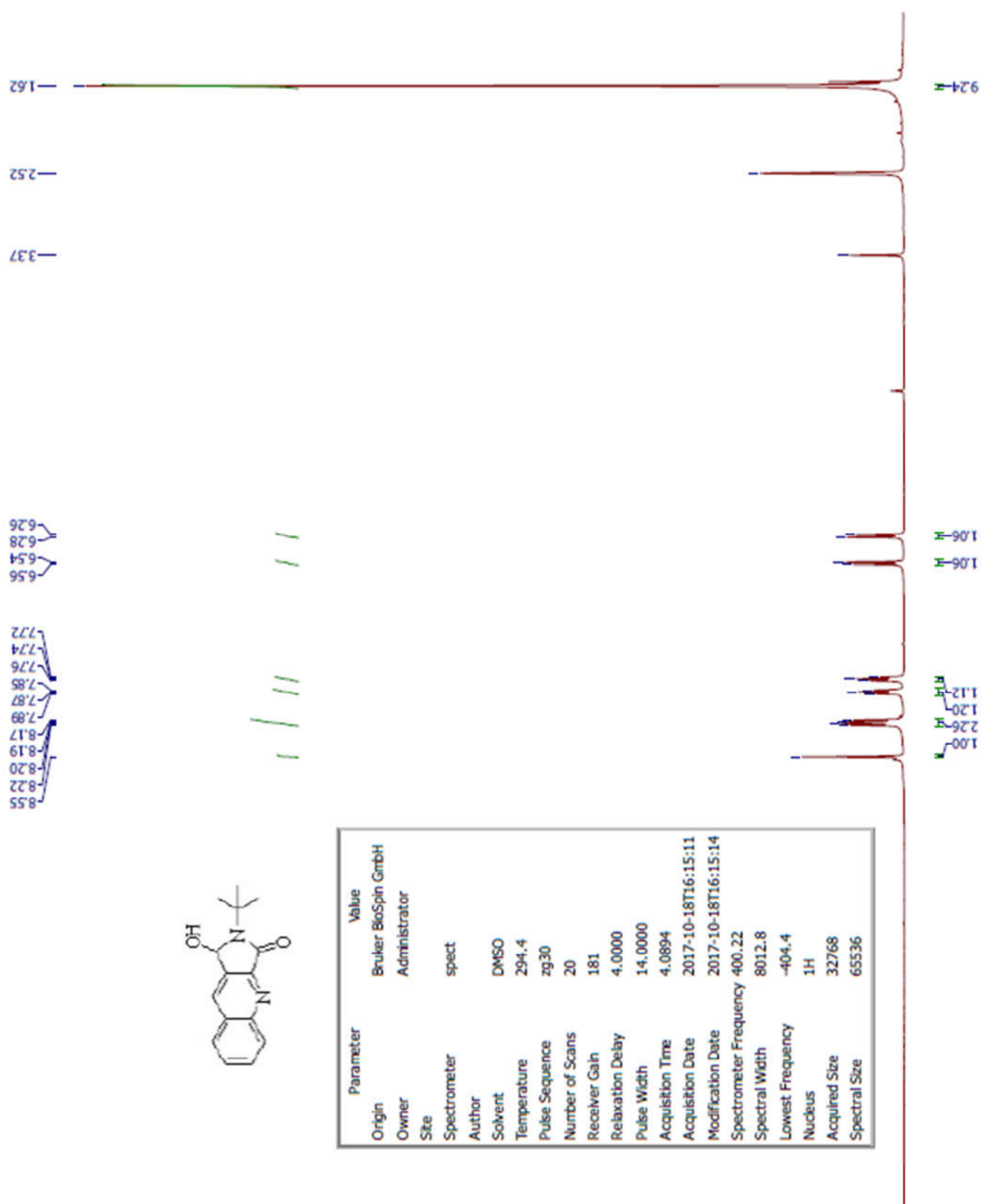
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2 Owner	root
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	380.0
8 Pulse Sequence	zg30
9 Number of Scans	32
10 Receiver Gain	40
11 Relaxation Delay	2.0000
12 Pulse Width	14.9000
13 Acquisition Time	2.0972
14 Acquisition Date	2017-10-23T15:02:00
15 Modification Date	2017-10-23T15:04:34
16 Spectrometer Frequency	300.13
17 Spectral Width	7812.5
18 Lowest Frequency	-1507.6
19 Nucleus	¹ H
20 Acquired Size	16384
21 Spectral Size	32768



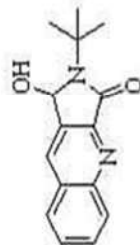


Parameter	Value
1. Origin	Bruker BioSpin GmbH
2. Owner	Administrator
3. Site	
4. Spectrometer	spect
5. Author	
6. Solvent	DMSO
7. Temperature	297.3
8. Pulse Sequence	zgpg30
9. Number of Scans	8002
10. Receiver Gain	2050
11. Relaxation Delay	1.0000
12. Pulse Width	9.0000
13. Acquisition Time	0.9176
14. Acquisition Date	2016-11-10T07:38:00
15. Modification Date	2016-11-10T12:01:58
16. Spectrometer Frequency	100.64
17. Spectral Width	35714.3
18. Lowest Frequency	-5277.7
19. Nucleus	¹³ C
20. Acquired Size	32768
21. Spectral Size	65536





Al-zahra UN
Sample code:H-t



Parameter	Value
1. Origin	Bruker BioSpin GmbH
2. Owner	Administrator
3. Site	
4. Spectrometer	spect
5. Author	
6. Solvent	DMSO
7. Temperature	294.6
8. Pulse Sequence	zgpg30
9. Number of Scans	8192
10. Receiver Gain	2050
11. Relaxation Delay	1.0000
12. Pulse Width	9.0000
13. Acquisition Time	0.9176
14. Acquisition Date	2017-01-15T18:49:00
15. Modification Date	2017-01-15T23:17:48
16. Spectrometer Frequency	100.64
17. Spectral Width	35714.3
18. Lowest Frequency	-5277.7
19. Nucleus	¹³ C
20. Acquired Size	32768
21. Spectral Size	65536





NAME Al-zahra UN

EXPNO 367

PROCNO 1

Date_ 20161122

Time 14.23

INSTRUM spect

PROBHD 5 mm PABBO BB-

PULPROG zg30

TD 65536

SOLVENT DMSO

NS 20

DS 0

SWH 8012.820 Hz

FIDRES 0.122266 Hz

AQ 4.0894966 sec

RG 144

DW 62.400 usec

DE 6.50 usec

TE 293.6 K

D1 4.00000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 1H

P1 14.00 usec

PL1 -2.00 dB

PL1W 11.86359406 W

SFO1 400.2236020 MHz

SI 32768

SF 400.2200000 MHz

WDW EM

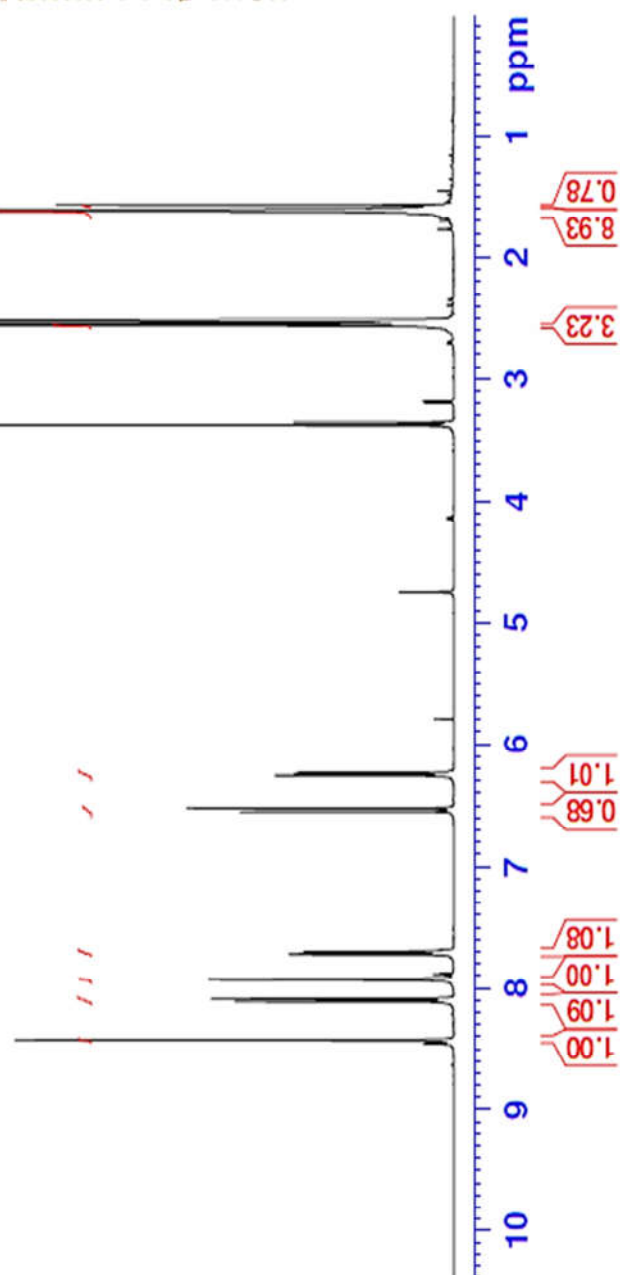
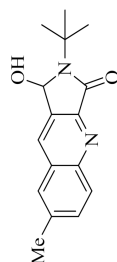
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LB 0.30 Hz

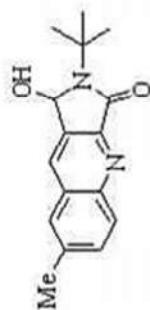
GB 0

PC 1.00

8.423
8.107
8.085
7.925
7.718
7.713
7.696
7.692
6.541
6.515
6.253
6.236
6.227
4.746
3.374
3.351
3.182
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2.540
2.531
2.527
2.522
2.518
2.513
1.611
1.570

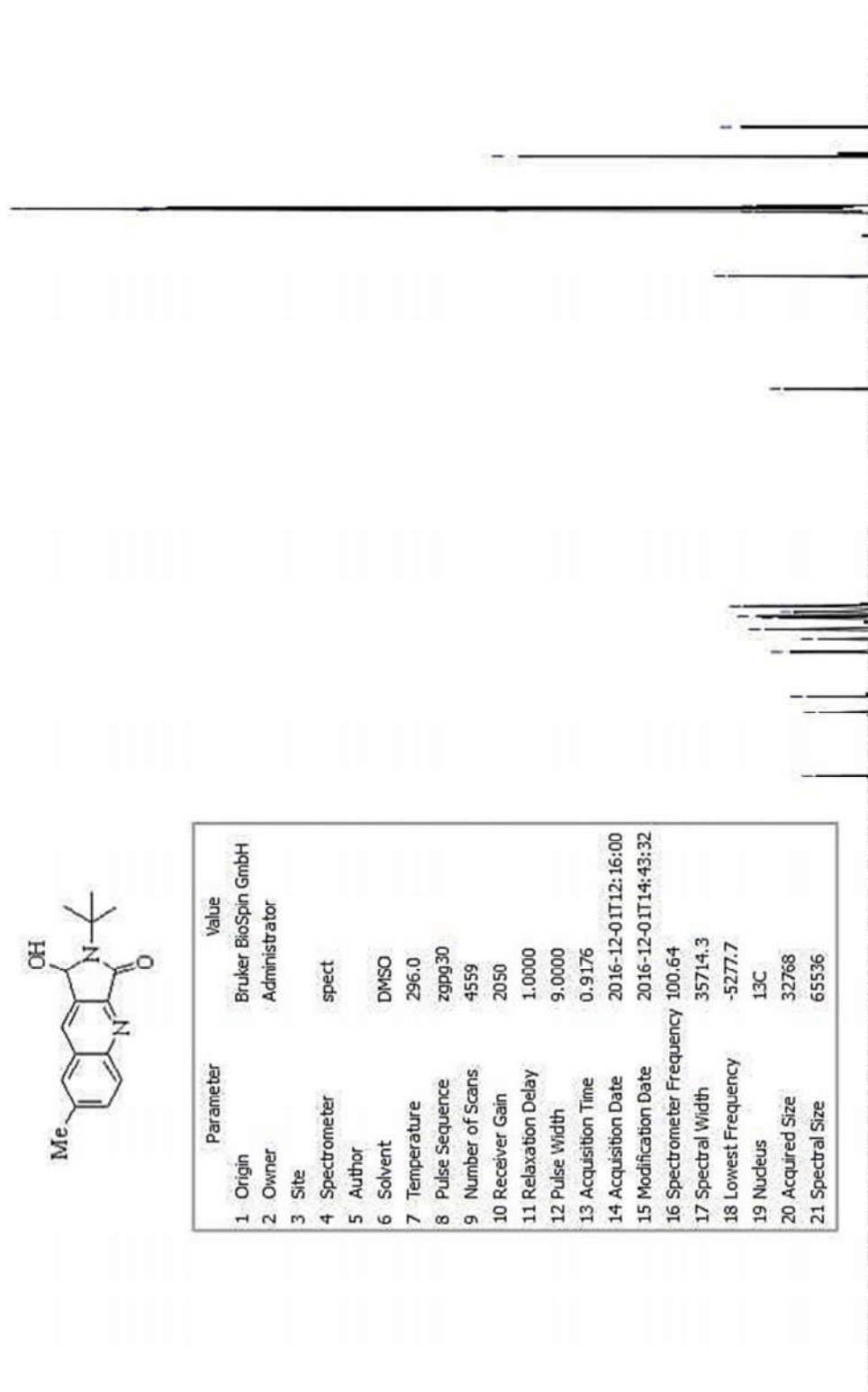


Al-zahra UN
Sample code:p-Me-T

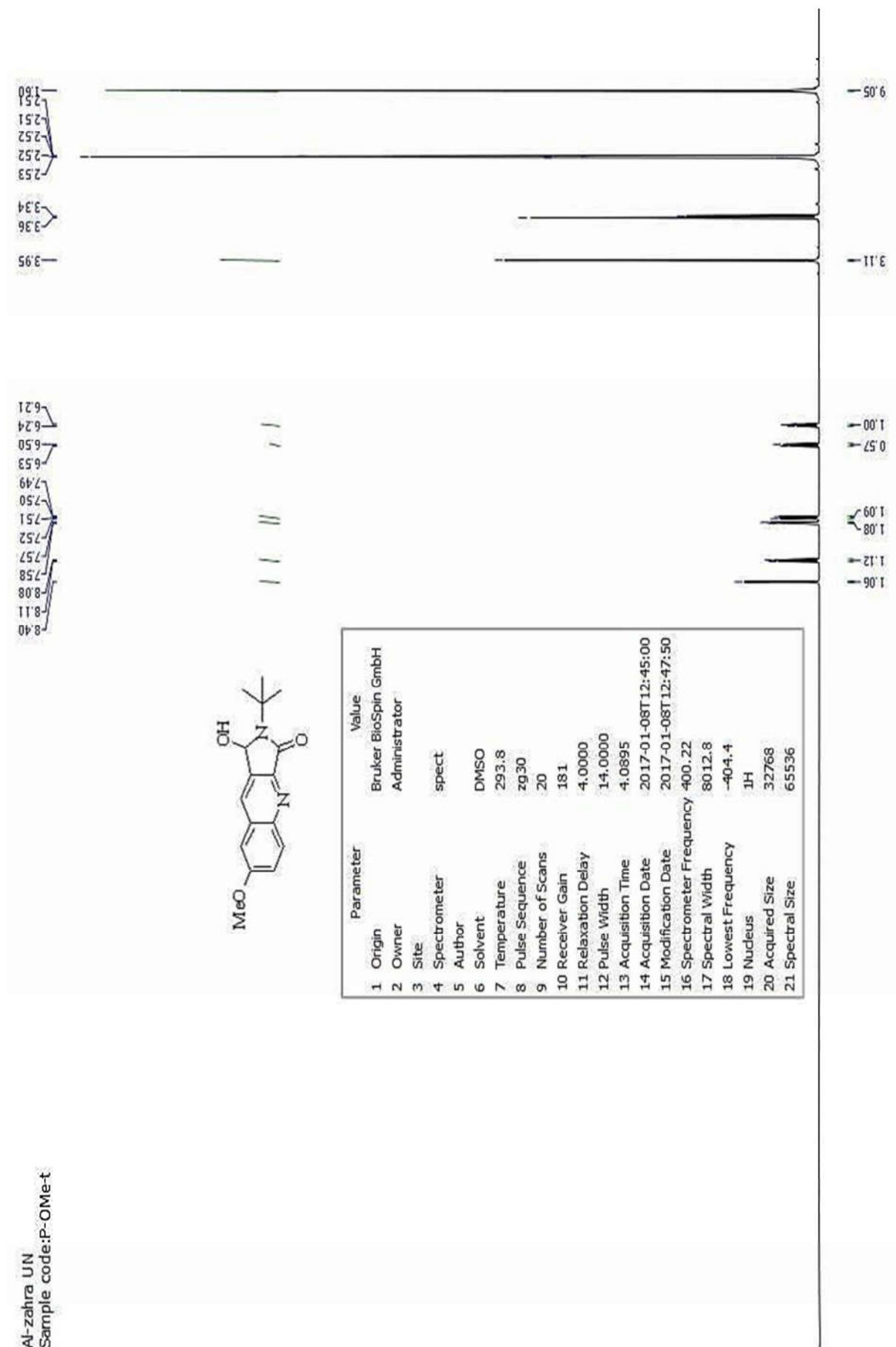


165.45
151.38
147.78
138.06
135.08
132.96
130.49
129.99
129.16
127.87
79.81
79.72
54.99
54.92
40.42
40.21
40.00
38.89
21.70

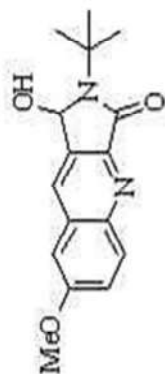
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1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	spect
4 Spectrometer	DMSO
5 Author	296.0
6 Solvent	zgpg30
7 Temperature	4559
8 Pulse Sequence	2050
9 Number of Scans	1.0000
10 Receiver Gain	9.0000
11 Relaxation Delay	0.9176
12 Pulse Width	2016-12-01T12:16:00
13 Acquisition Time	2016-12-01T14:43:32
14 Acquisition Date	100.64
15 Modification Date	35714.3
16 Spectrometer Frequency	-5277.7
17 Spectral Width	13C
18 Lowest Frequency	32768
19 Nucleus	65536
20 Acquired Size	
21 Spectral Size	



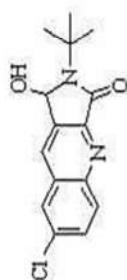
Al-zahra UN
Sample code:P-OMe-t



Al-zahra UN
Sample code:P-OMe-t

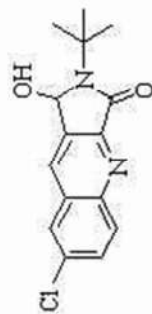


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	293.6
8 Pulse Sequence	zgpg30
9 Number of Scans	2500
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-01-16T08:40:00
15 Modification Date	2017-01-16T10:02:30
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	291.1
8 Pulse Sequence	zg30
9 Number of Scans	20
10 Receiver Gain	228
11 Relaxation Delay	4.0000
12 Pulse Width	14.0000
13 Acquisition Time	4.0895
14 Acquisition Date	2017-02-05T08:31:00
15 Modification Date	2017-02-05T08:31:04
16 Spectrometer Frequency	400.22
17 Spectral Width	8012.8
18 Lowest Frequency	-404.4
19 Nucleus	¹ H
20 Acquired Size	32768
21 Spectral Size	65536

Al-zahra UN
Sample code:2-Cl-t

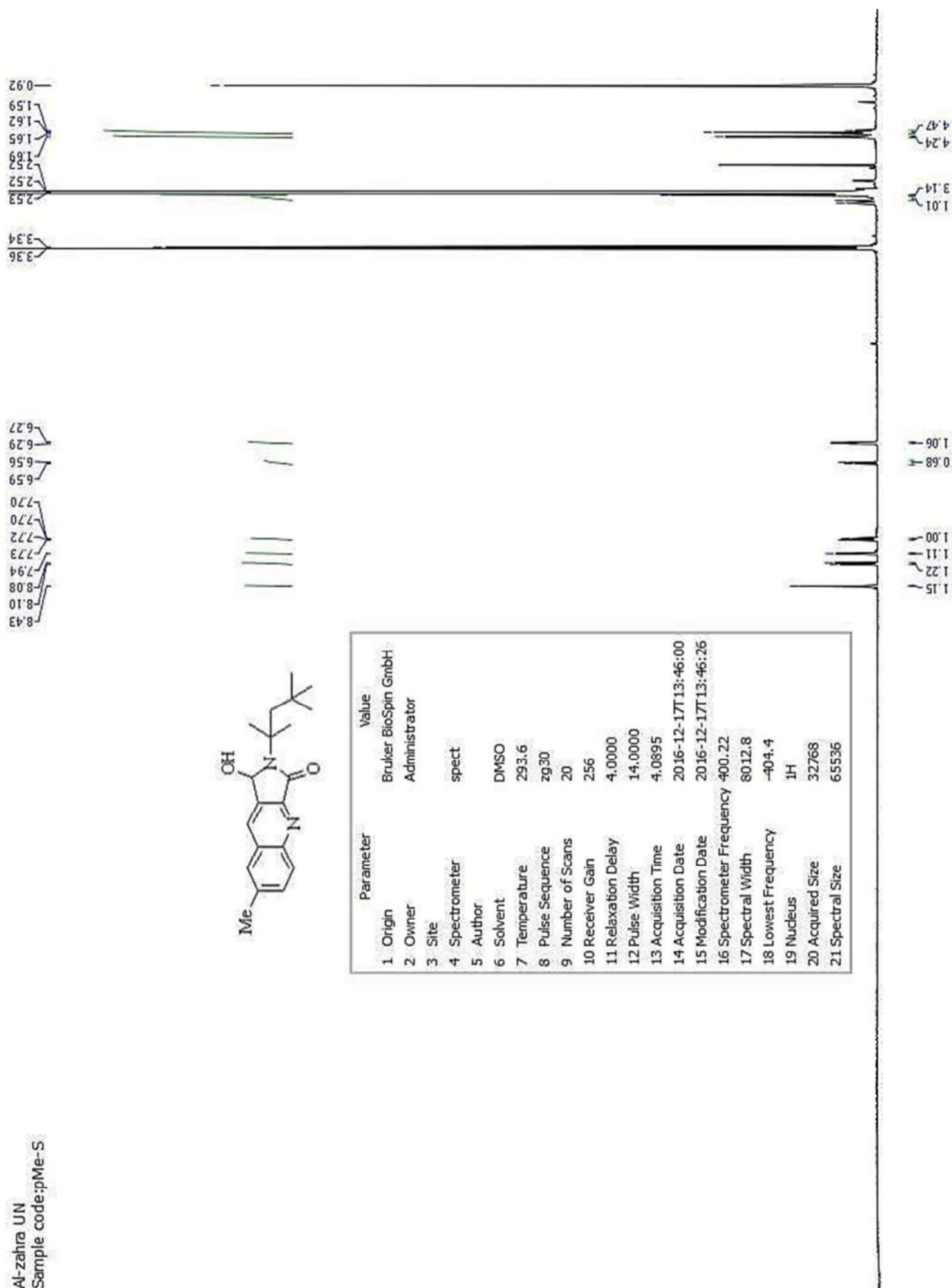


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	293.9
8 Pulse Sequence	zgpg30
9 Number of Scans	4811
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-02-13T09:13:00
15 Modification Date	2017-02-13T11:52:10
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536

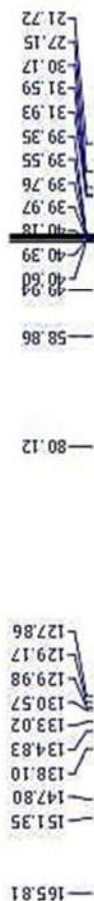
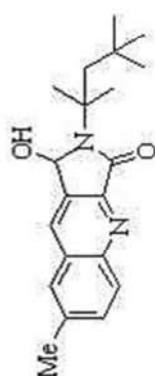
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39.96
39.76
28.28

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131.32
130.71
129.94
127.91

Al-zahra UN
Sample code:pMe-S

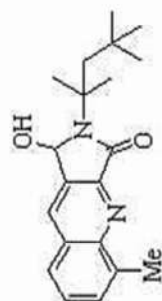


Al-zahra UN
Sample code:pMe-S

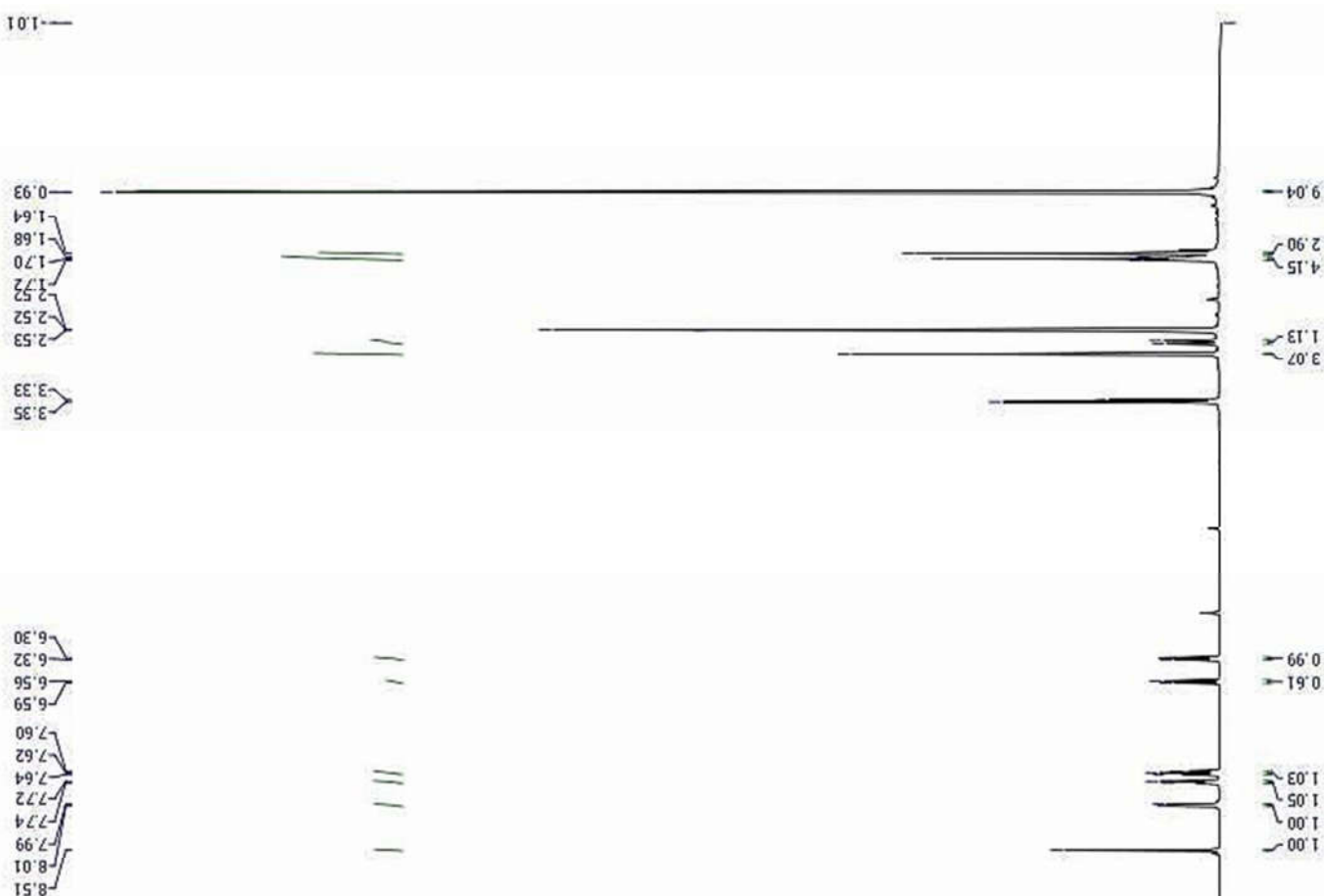


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	spect
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	293.3
8 Pulse Sequence	zgpg30
9 Number of Scans	8192
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2016-12-22T13:58:00
15 Modification Date	2016-12-22T18:28:38
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17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536

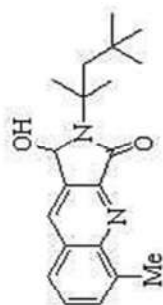
Al-zahra UN
Sample code: OMe-S



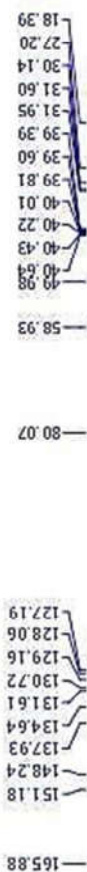
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1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	297.0
8 Pulse Sequence	zg30
9 Number of Scans	20
10 Receiver Gain	203
11 Relaxation Delay	4.0000
12 Pulse Width	14.0000
13 Acquisition Time	4.0895
14 Acquisition Date	2016-10-27T16:52:00
15 Modification Date	2016-10-27T16:54:44
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17 Spectral Width	8012.8
18 Lowest Frequency	-404.4
19 Nucleus	¹ H
20 Acquired Size	32768
21 Spectral Size	65536



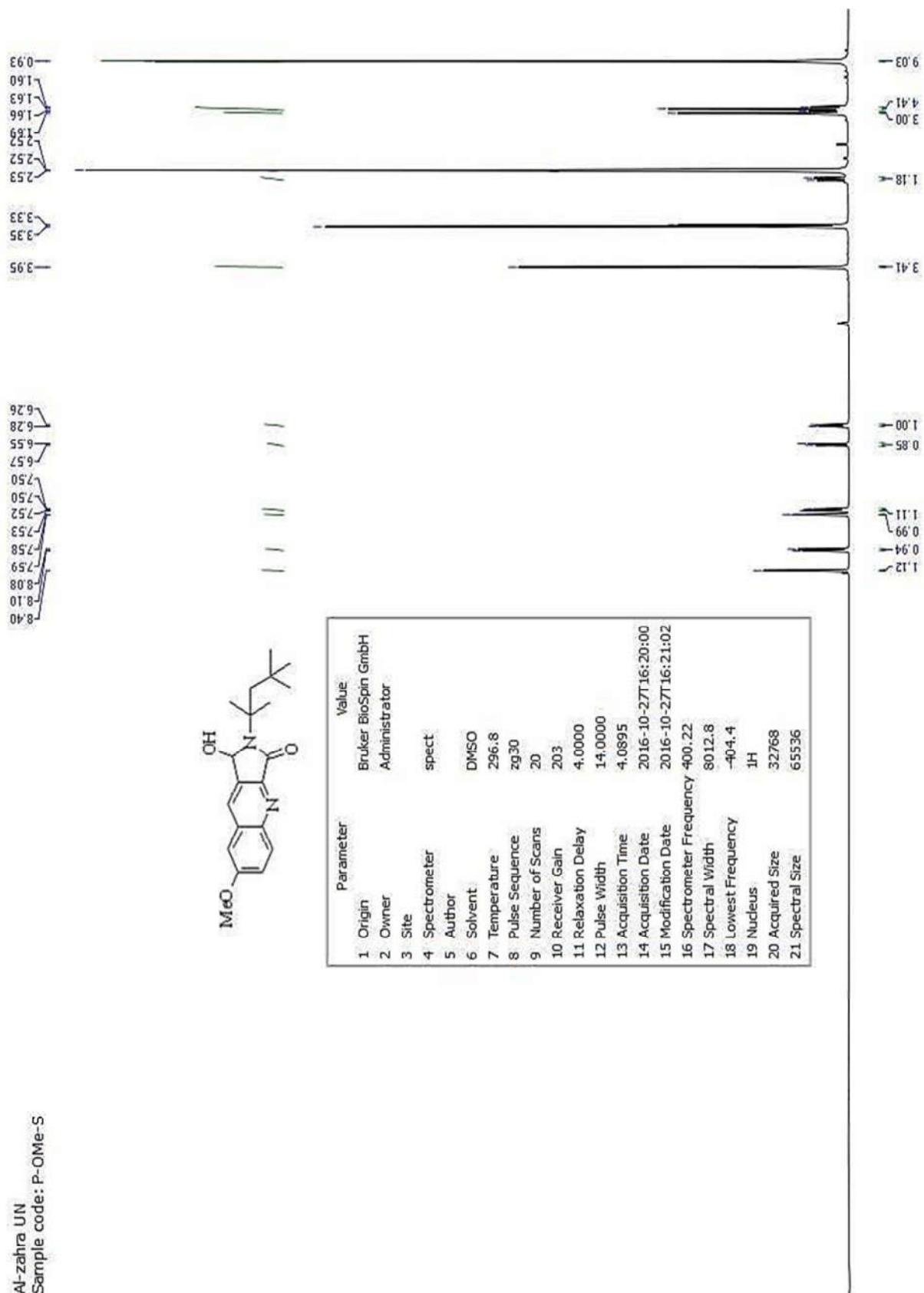
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Sample code:OMe-S



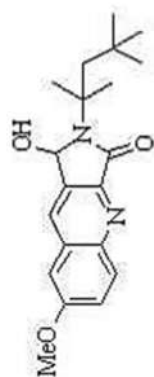
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2 Owner	Administrator
3 Site	spect
4 Spectrometer	DMSO
5 Author	297.9
6 Solvent	zgpg30
7 Temperature	8192
8 Pulse Sequence	2050
9 Number of Scans	1.0000
10 Receiver Gain	9.0000
11 Relaxation Delay	0.9176
12 Pulse Width	2016-11-10T12:07:00
13 Acquisition Time	2016-11-10T16:34:56
14 Acquisition Date	100.64
15 Modification Date	35714.3
16 Spectrometer Frequency	-5277.7
17 Spectral Width	13C
18 Lowest Frequency	32768
19 Nucleus	65536
20 Acquired Size	
21 Spectral Size	



Al-zahra UN
Sample code: P-OMe-S

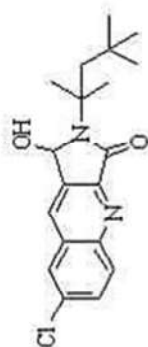


Al-zahra UN
Sample code:P-OMe-S

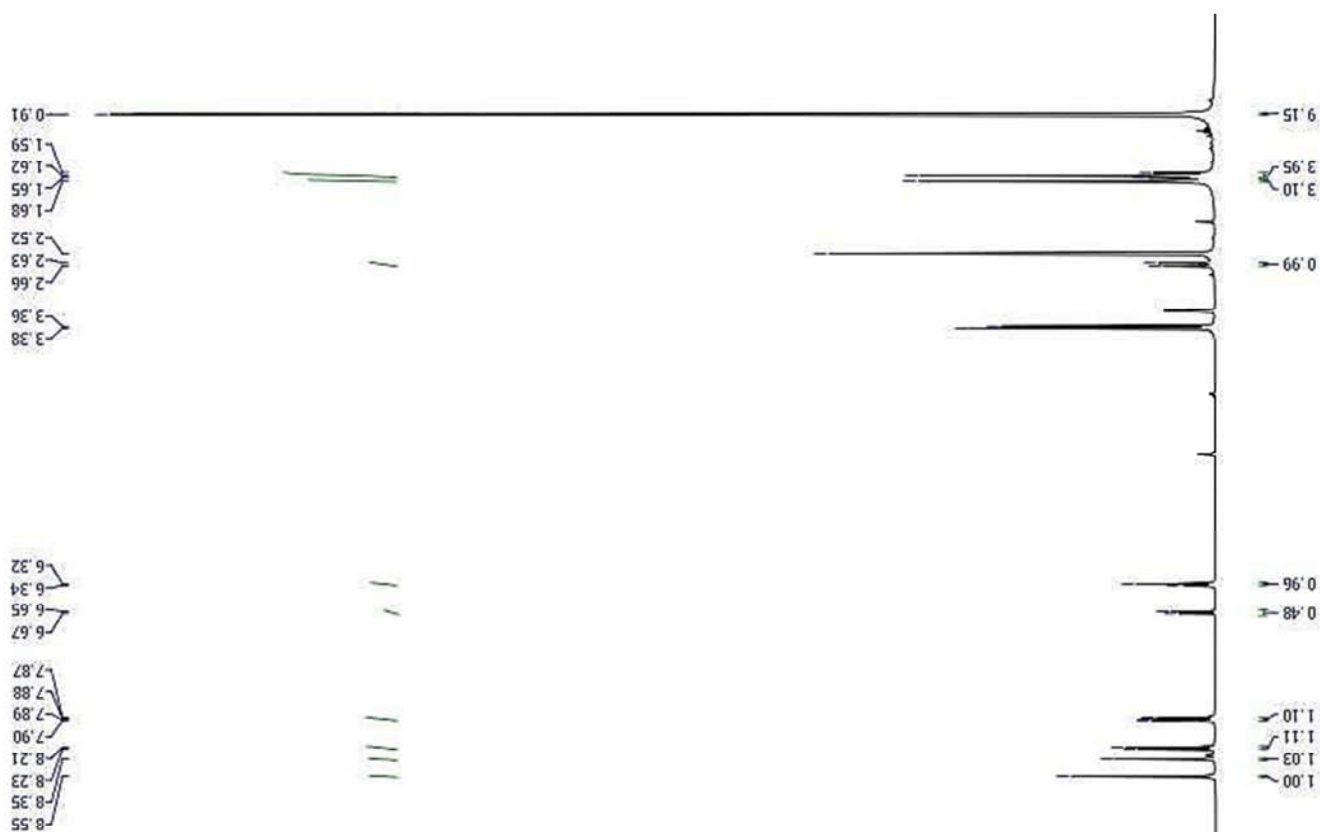


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	spect
4 Spectrometer	
5 Author	
6 Solvent	DMSO
7 Temperature	297.0
8 Pulse Sequence	zgpg30
9 Number of Scans	6200
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2016-11-09T16:25:00
15 Modification Date	2016-11-09T19:50:30
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-52777.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536

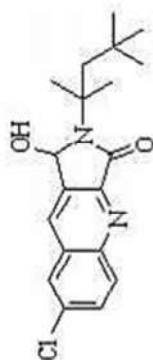
Al-zahra UN
Sample code: Cl-S (II)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	293.5
8 Pulse Sequence	zg30
9 Number of Scans	20
10 Receiver Gain	128
11 Relaxation Delay	4.0000
12 Pulse Width	14.0000
13 Acquisition Time	4.0895
14 Acquisition Date	2017-02-03T15:12:00
15 Modification Date	2017-02-03T15:14:16
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17 Spectral Width	8012.8
18 Lowest Frequency	-404.4
19 Nucleus	¹ H
20 Acquired Size	32768
21 Spectral Size	65536

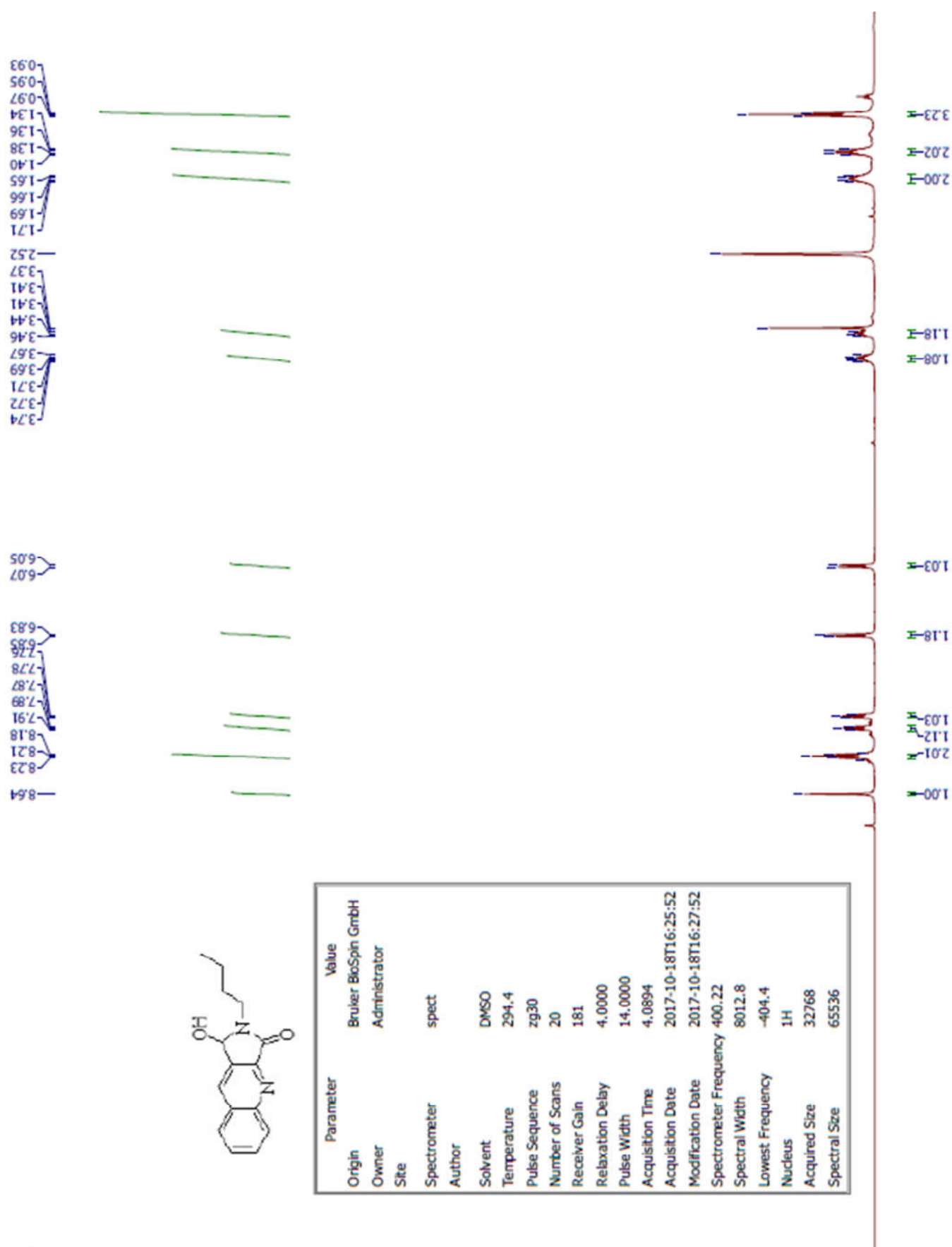


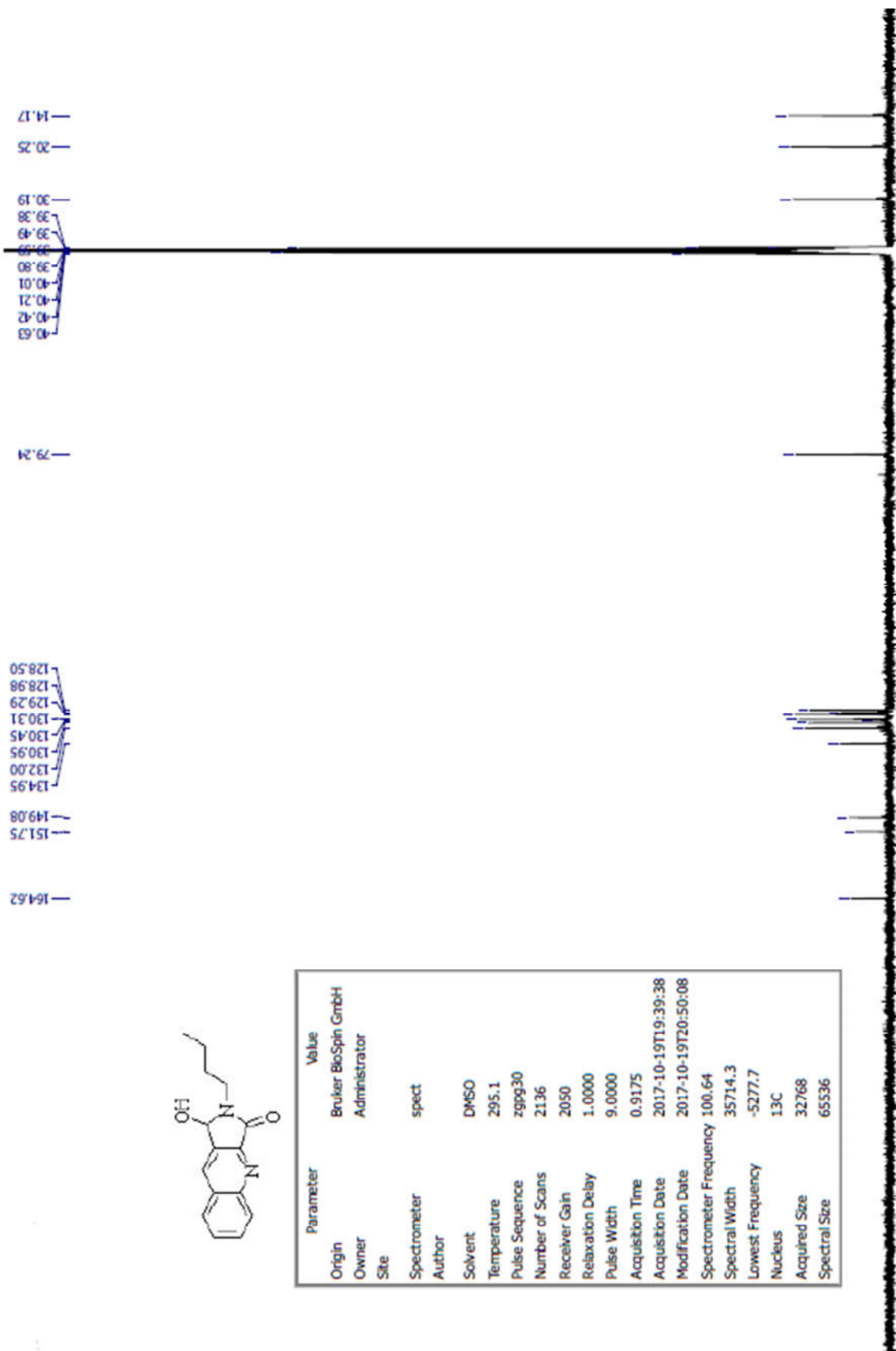
Al-zahra UN
Sample code:2-H-S

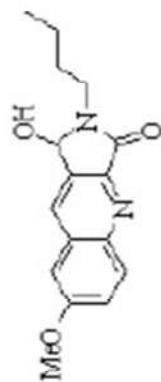


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	293.7
8 Pulse Sequence	zgpg30
9 Number of Scans	4800
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-02-12T13:28:00
15 Modification Date	2017-02-12T16:05:30
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536

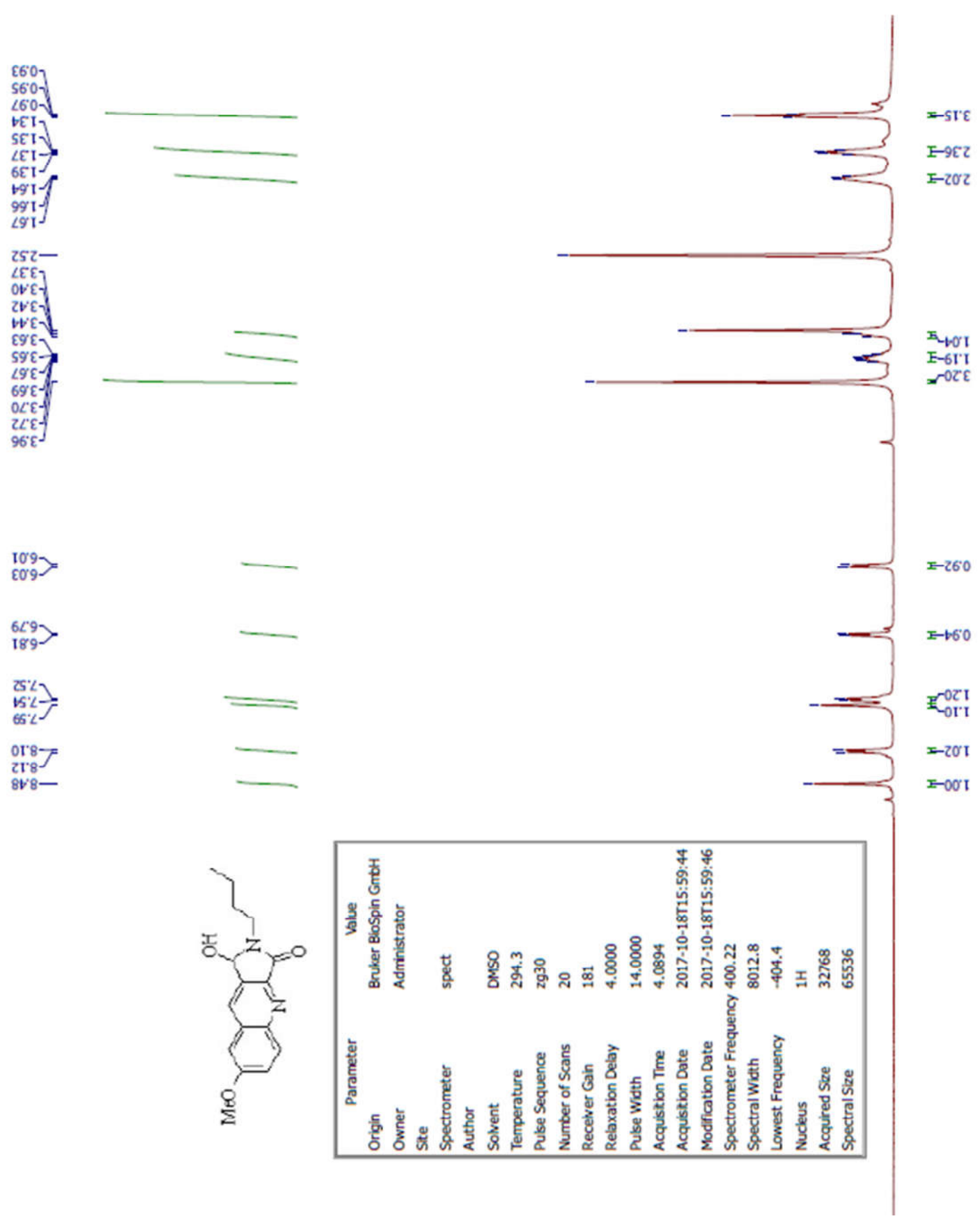


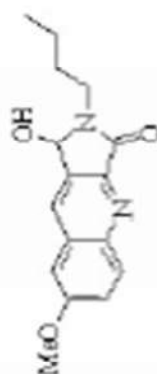




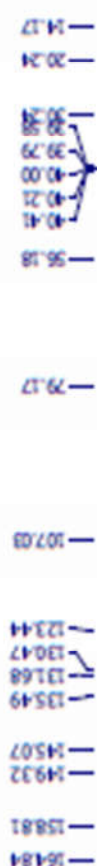


Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	Administrator
Site	spect
Spectrometer	
Author	
Solvent	DMSO
Temperature	294.3
Pulse Sequence	zg30
Number of Scans	20
Receiver Gain	181
Relaxation Delay	4.0000
Pulse Width	14.0000
Acquisition Time	4.0894
Acquisition Date	2017-10-18T15:59:44
Modification Date	2017-10-18T15:59:46
Spectrometer Frequency	400.22
Spectral Width	8012.8
Lowest Frequency	-404.4
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536

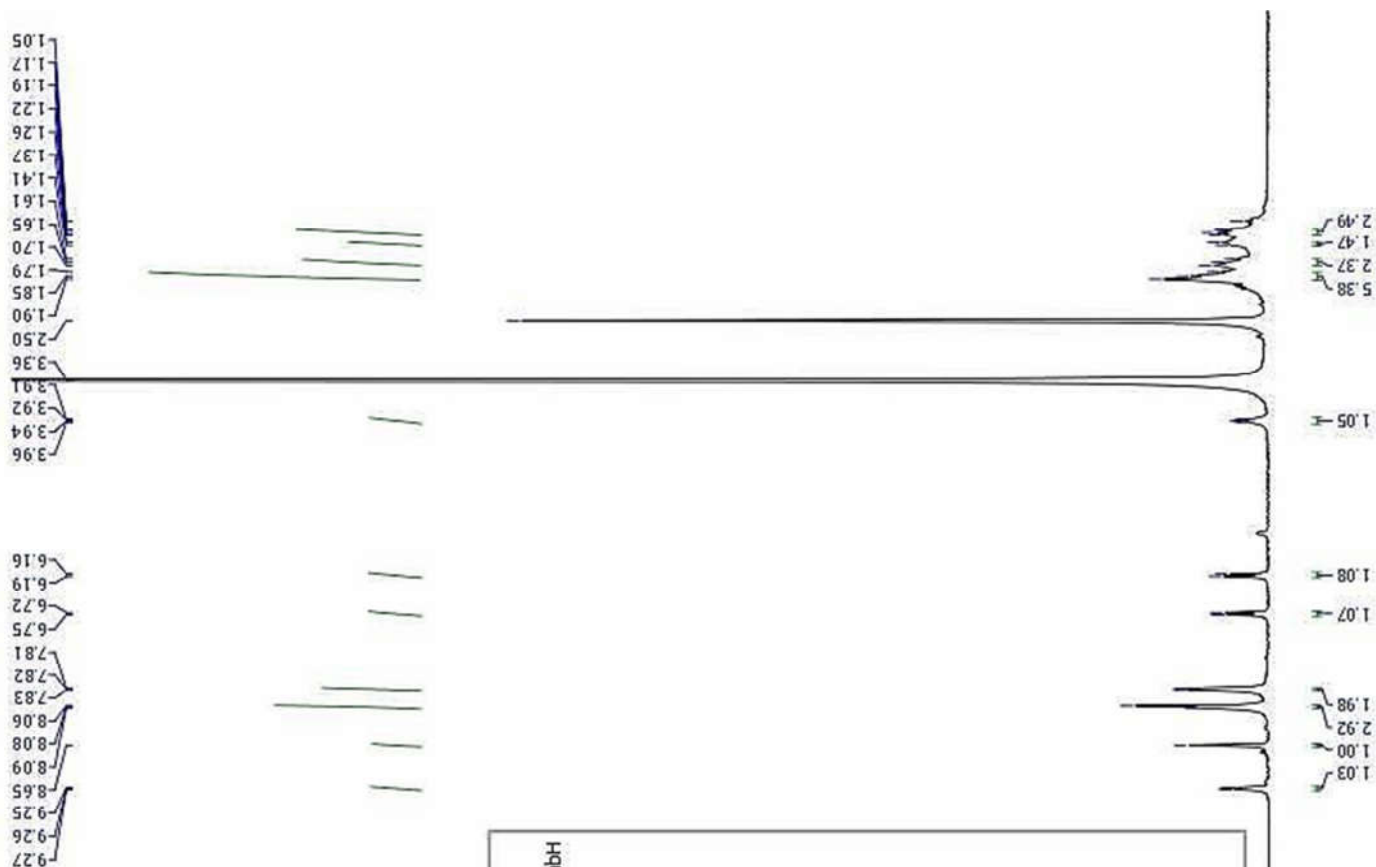
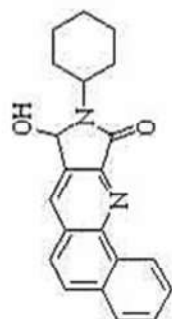




Parameter	Value
Origin	Bruker Biospin GmbH
Owner	Administrator
Site	spect
Spectrometer	author
Solvent	DMSO
Temperature	295.6
Pulse Sequence	zgpg30
Number of Scans	1000
Receiver Gain	2050
Relaxation Delay	1.0000
Pulse Width	9.0000
Acquisition Time	0.9175
Acquisition Date	2017-10-19T18:50:37
Modification Date	2017-10-19T19:23:36
Spectrometer Frequency	100.64
Spectral Width	35714.3
Lowest Frequency	-5277.7
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

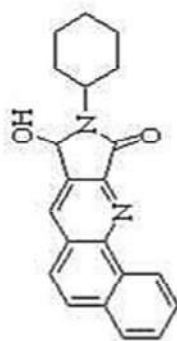


Dr.shiri
ISO
1H NMR

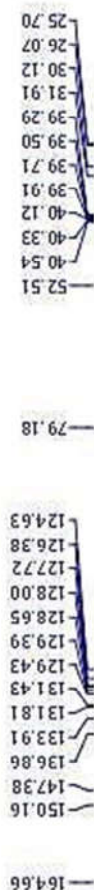


Parameter	Value
1 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
2 Owner	root
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	380.0
8 Pulse Sequence	zg30
9 Number of Scans	32
10 Receiver Gain	40
11 Relaxation Delay	2.0000
12 Pulse Width	14.9000
13 Acquisition Time	2.0972
14 Acquisition Date	2016-09-25T14:40:00
15 Modification Date	2016-09-25T13:42:22
16 Spectrometer Frequency	300.13
17 Spectral Width	7812.5
18 Lowest Frequency	-1507.6
19 Nucleus	¹ H
20 Acquired Size	16384
21 Spectral Size	32768

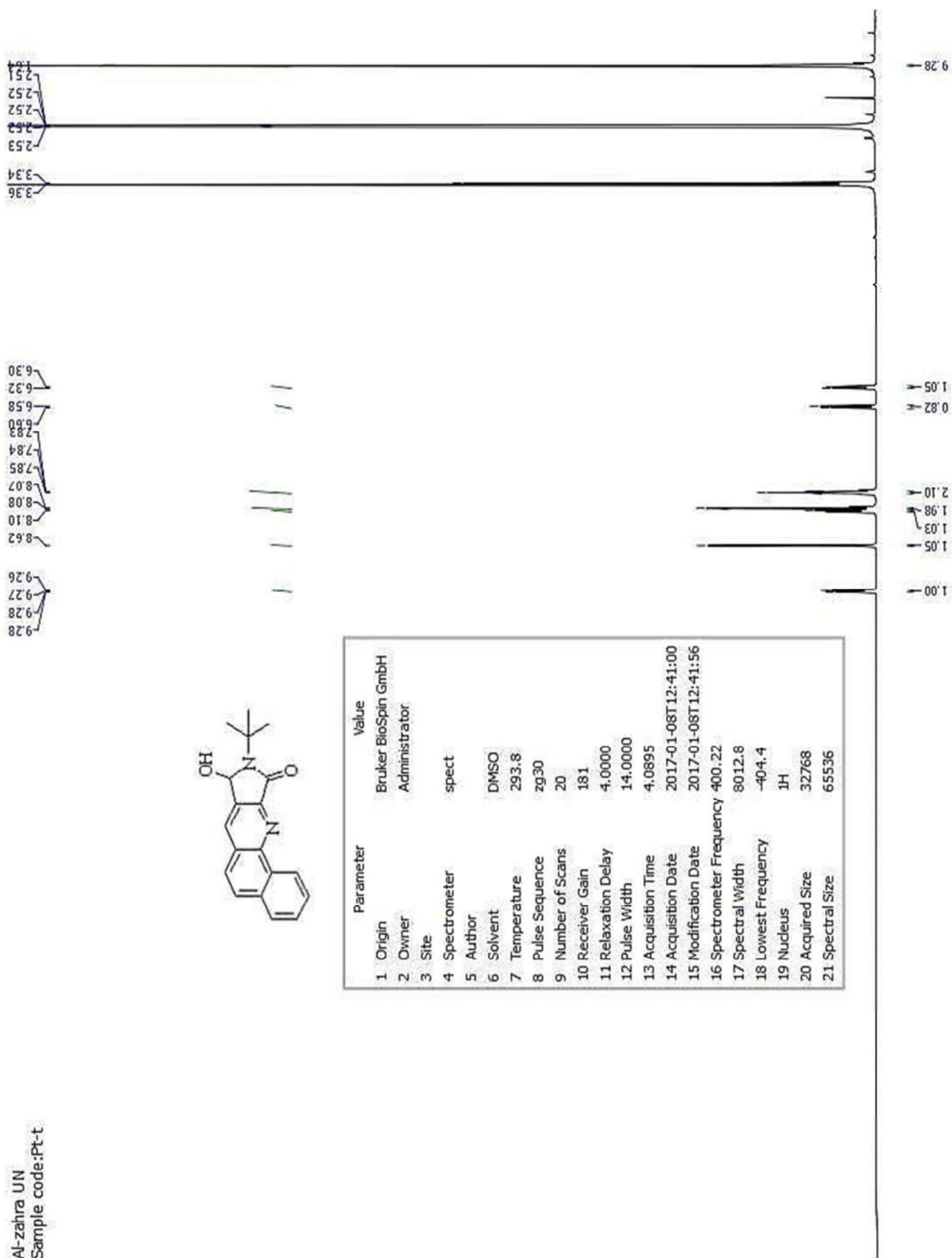
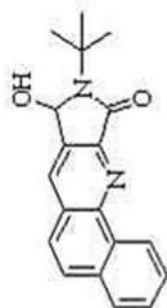
Al-zahra UN
Sample code:2Ph-C (I)



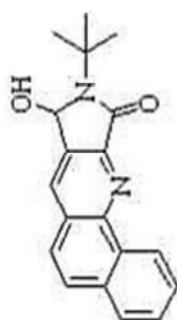
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	293.6
8 Pulse Sequence	zgpg30
9 Number of Scans	1420
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-02-12T07:31:00
15 Modification Date	2017-02-12T08:18:28
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



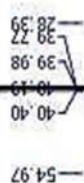
Al-zahra UN
Sample code:Pt-t



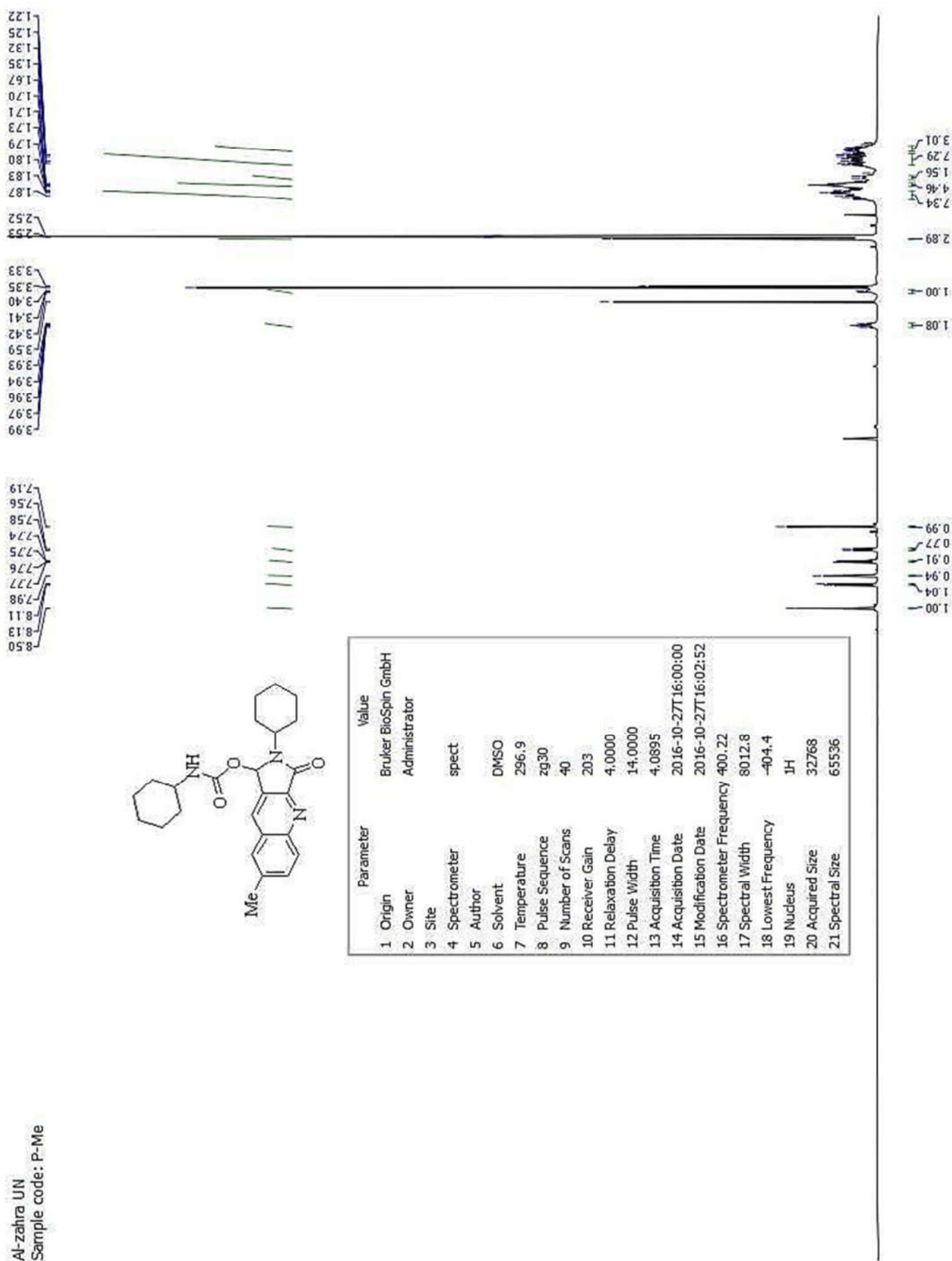
Al-zahra UN
Sample code:Pt-t



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	294.3
8 Pulse Sequence	zgpg30
9 Number of Scans	4000
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-01-15T16:32:00
15 Modification Date	2017-01-15T18:44:18
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-52777.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536

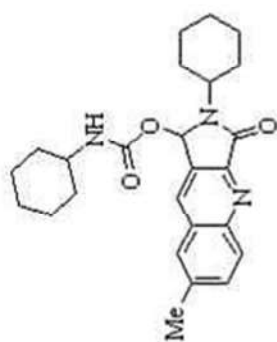


Al-zahra UN
Sample code: P-Me



Al-zahra UN

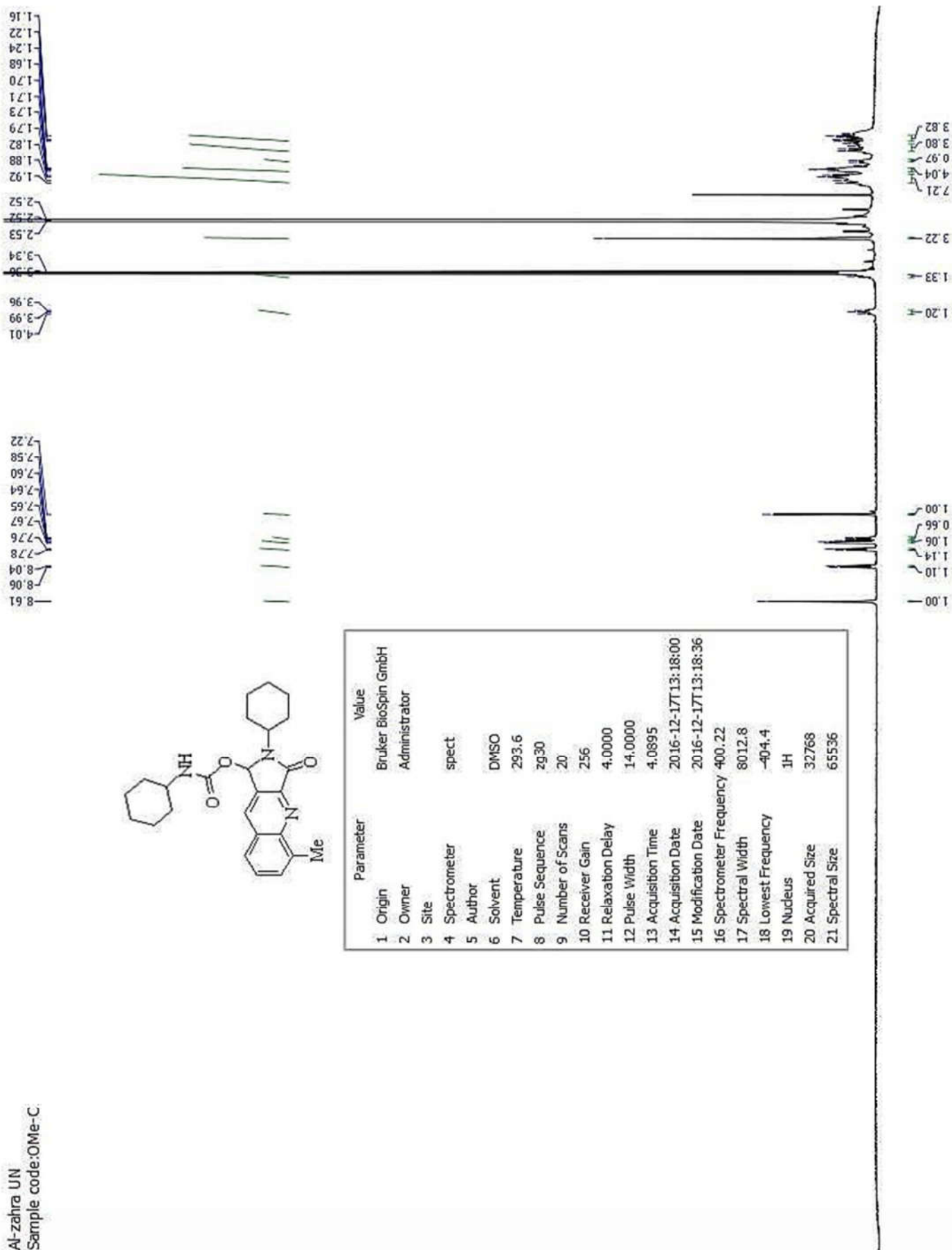
Sample code:P-Me-C (II)



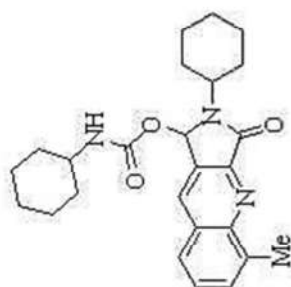
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	294.4
8 Pulse Sequence	zgpg30
9 Number of Scans	6618
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-02-09T07:44:00
15 Modification Date	2017-02-09T11:22:02
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



Al-zahra UN
Sample code:OMe-C



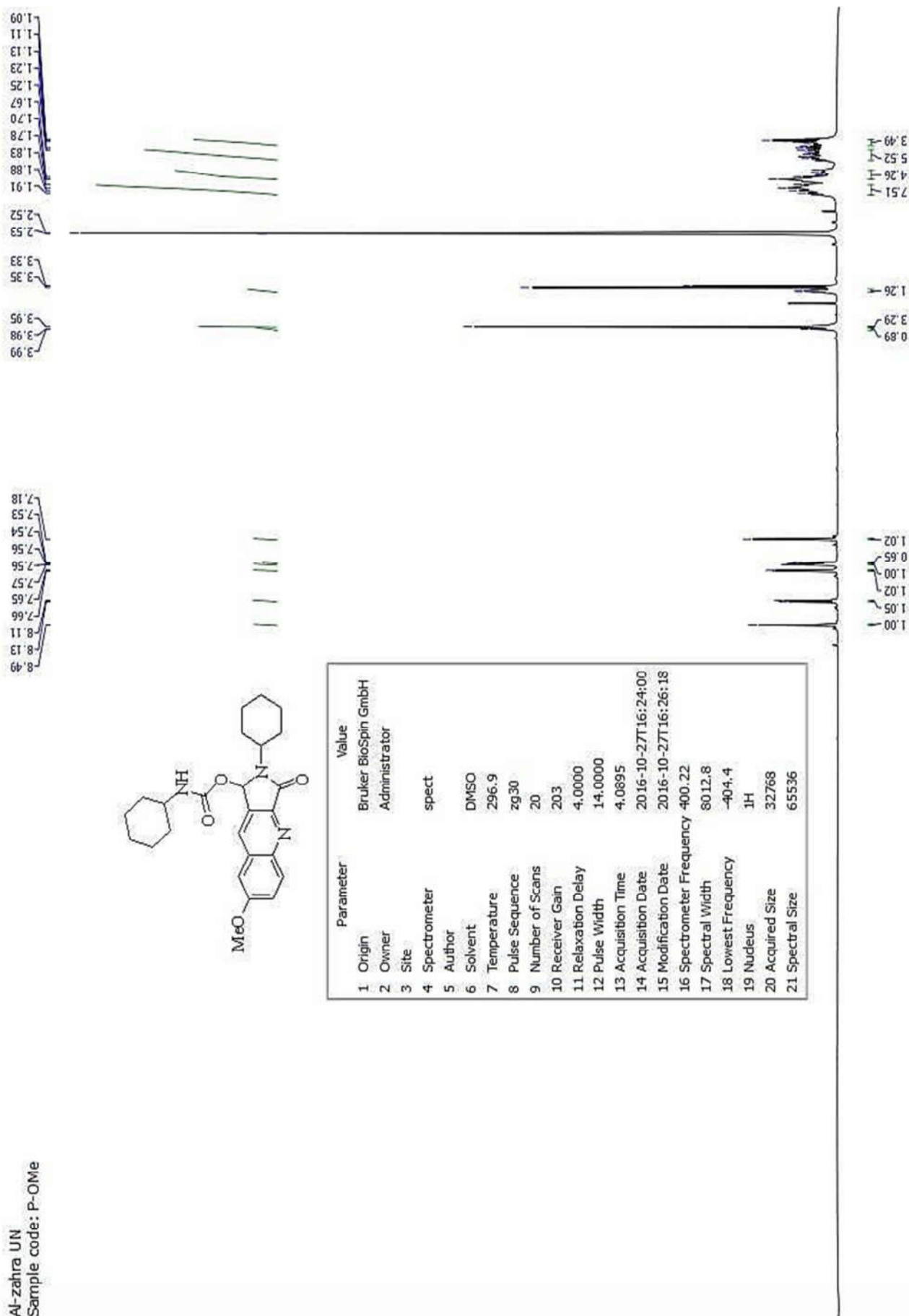
Al-zahra UN
Sample code:P-Me-C (I)



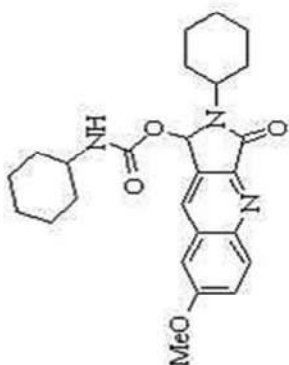
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	spect
4 Spectrometer	
5 Author	
6 Solvent	DMSO
7 Temperature	294.5
8 Pulse Sequence	zgpg30
9 Number of Scans	3750
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-02-08T11:51:00
15 Modification Date	2017-02-08T13:48:16
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



Al-zahra UN
Sample code: P-OMe



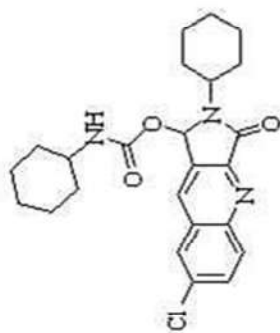
Al-zahra UN
Sample code:OMe-C



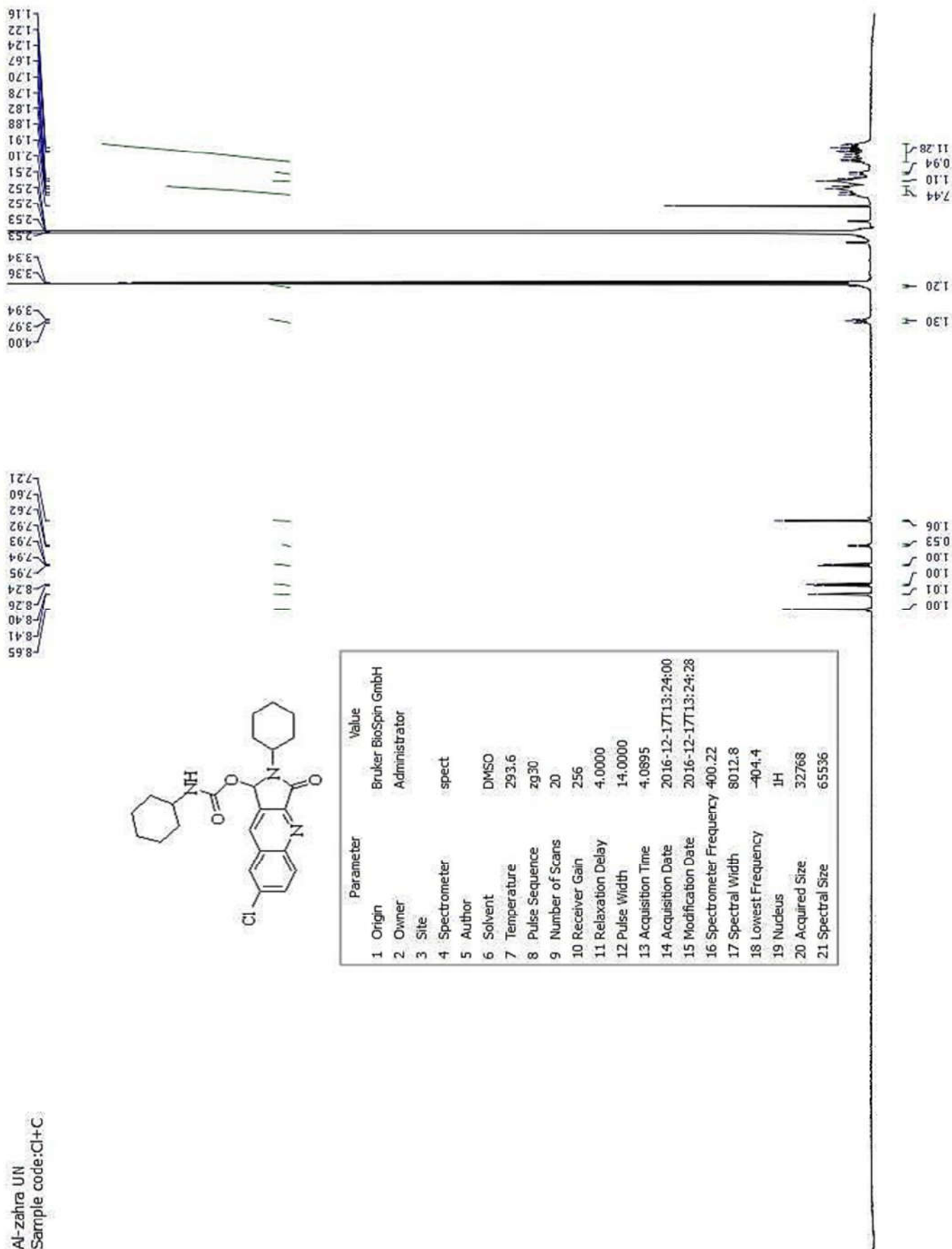
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	294.5
8 Pulse Sequence	zgpg30
9 Number of Scans	7550
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2016-12-31T16:29:00
15 Modification Date	2016-12-31T20:38:14
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



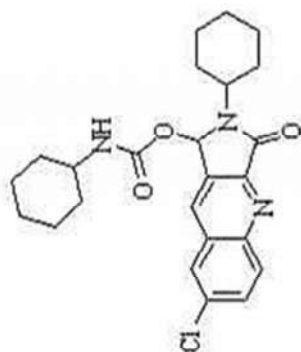
Al-zahra UN
Sample code:Cl+C



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	293.6
8 Pulse Sequence	zg30
9 Number of Scans	20
10 Receiver Gain	256
11 Relaxation Delay	4.0000
12 Pulse Width	14.0000
13 Acquisition Time	4.0895
14 Acquisition Date	2016-12-17T13:24:00
15 Modification Date	2016-12-17T13:24:28
16 Spectrometer Frequency	400.22
17 Spectral Width	8012.8
18 Lowest Frequency	-404.4
19 Nucleus	¹ H
20 Acquired Size	32768
21 Spectral Size	65536



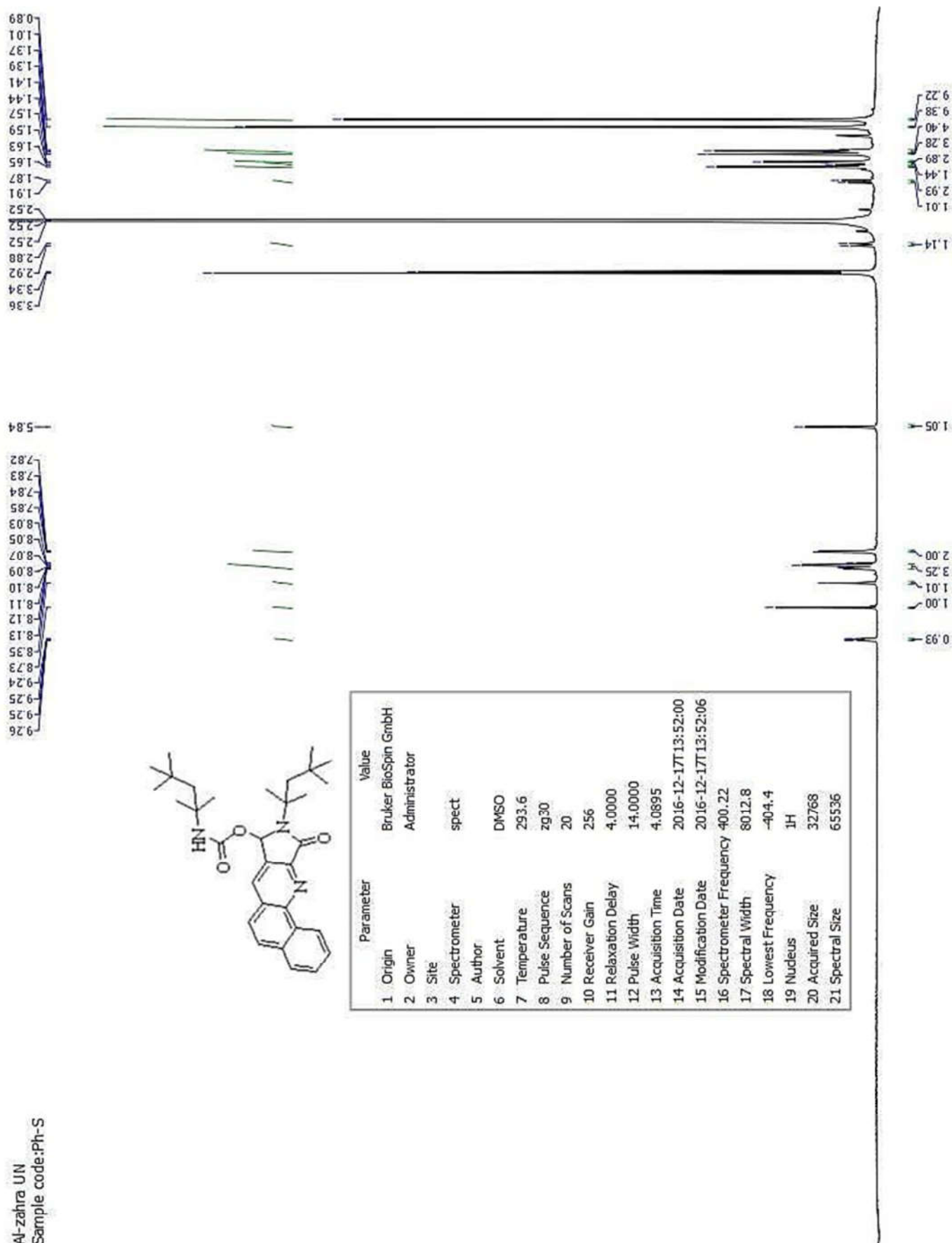
Al-zahra UN
Sample code: Cl+C



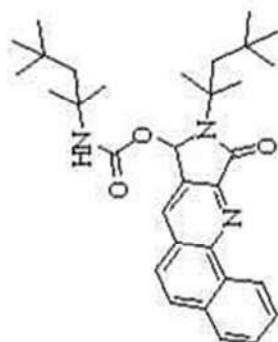
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	294,0
8 Pulse Sequence	zgpg30
9 Number of Scans	8192
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2016-12-31T20:40:00
15 Modification Date	2017-01-01T01:10:30
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



Al-zahra UN
Sample code:Ph-S



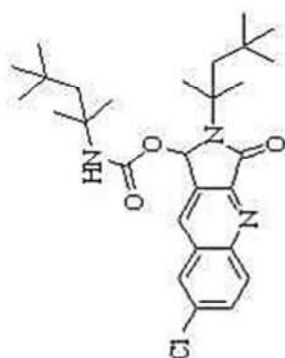
Al-zahra UN
Sample code: Ph-S (II)



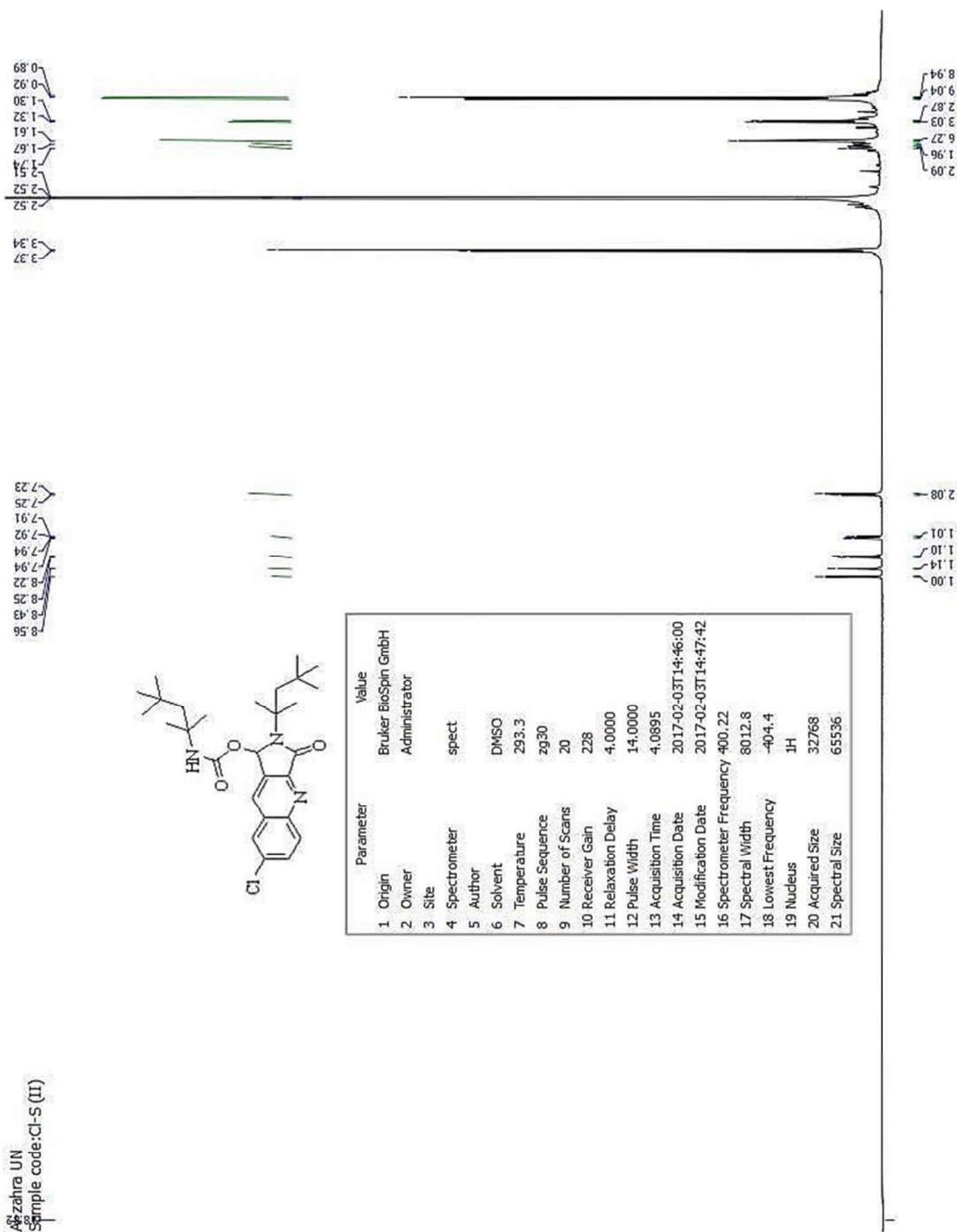
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	spect
4 Spectrometer	
5 Author	
6 Solvent	DMSO
7 Temperature	294.5
8 Pulse Sequence	zgpg30
9 Number of Scans	4100
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-02-08T14:27:00
15 Modification Date	2017-02-08T16:41:58
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



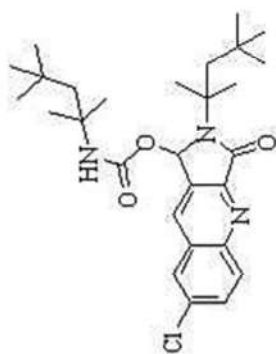
Al Zahra UN
Sample code: Cl-S (II)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	293.3
8 Pulse Sequence	zg30
9 Number of Scans	20
10 Receiver Gain	228
11 Relaxation Delay	4.0000
12 Pulse Width	14.0000
13 Acquisition Time	4.0895
14 Acquisition Date	2017-02-03T14:46:00
15 Modification Date	2017-02-03T14:47:42
16 Spectrometer Frequency	400.22
17 Spectral Width	8012.8
18 Lowest Frequency	-404.4
19 Nucleus	¹ H
20 Acquired Size	32768
21 Spectral Size	65536

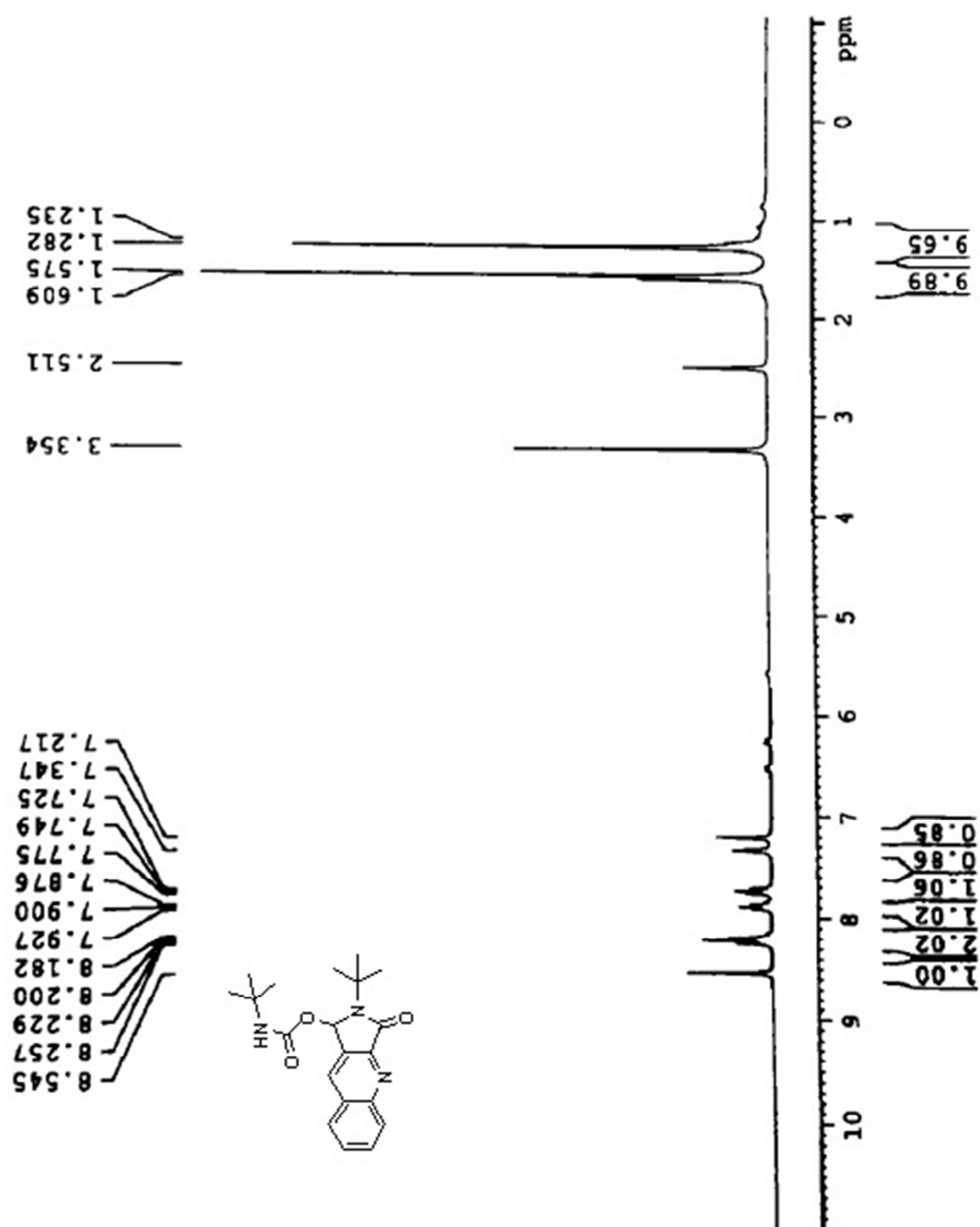


Al-zahra UN
Sample code: Cl-S (II)



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	294.6
8 Pulse Sequence	zgpg30
9 Number of Scans	1020
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-02-08T13:52:00
15 Modification Date	2017-02-08T14:24:40
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536





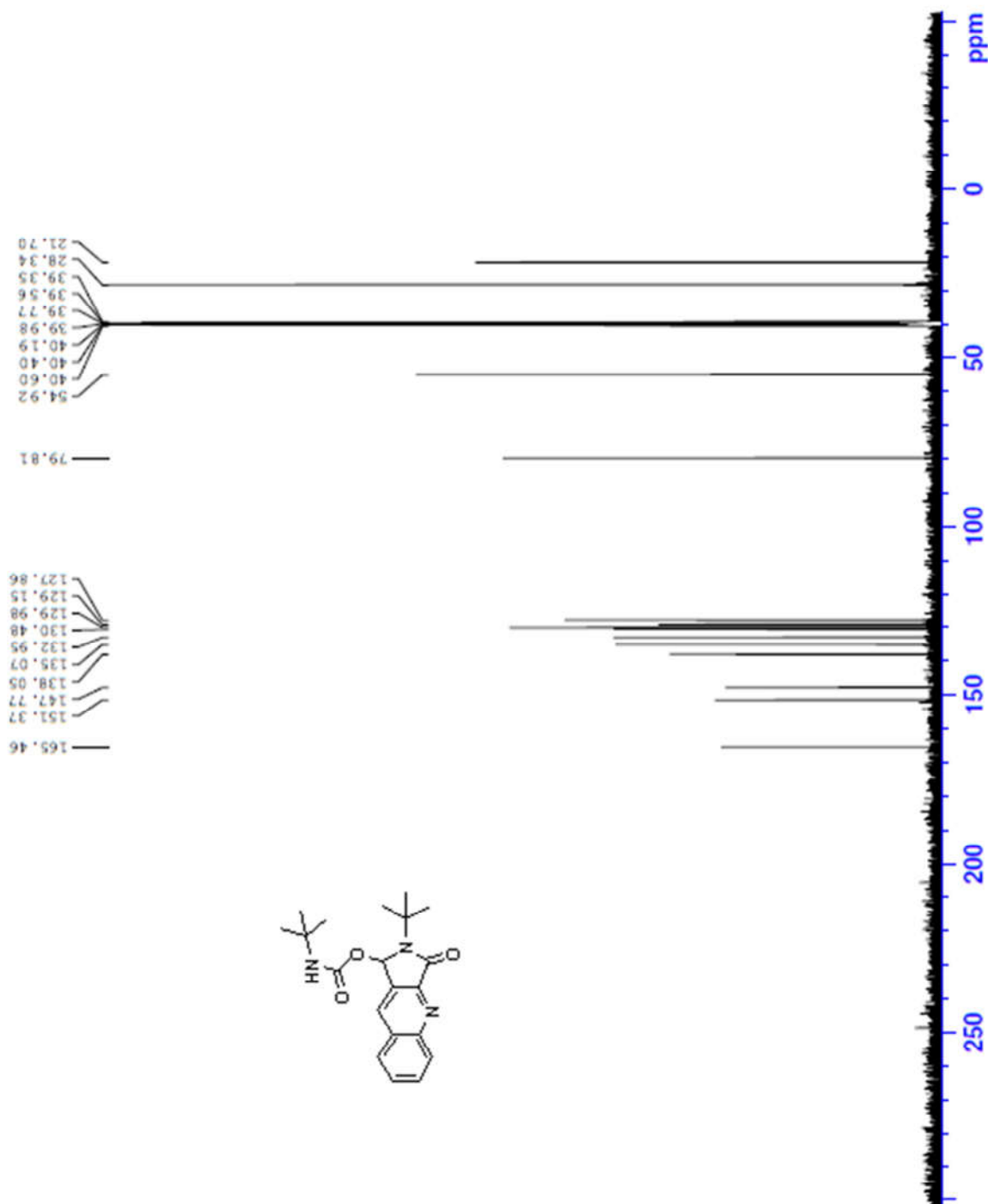
Sample code: 2-Me-t (Dr. Shiri)



NAME Al-zahra UN
EXPNO 505
PROCNO 1
Date_ 20170724
Time 21.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 232
DS 0
SWH 35714.285 Hz
FIDRES 0.544957 Hz
AQ 0.9175540 sec
RG 2050
DW 14.000 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

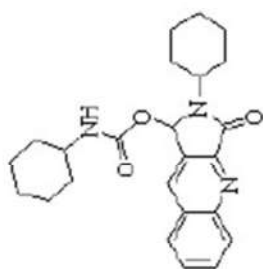
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



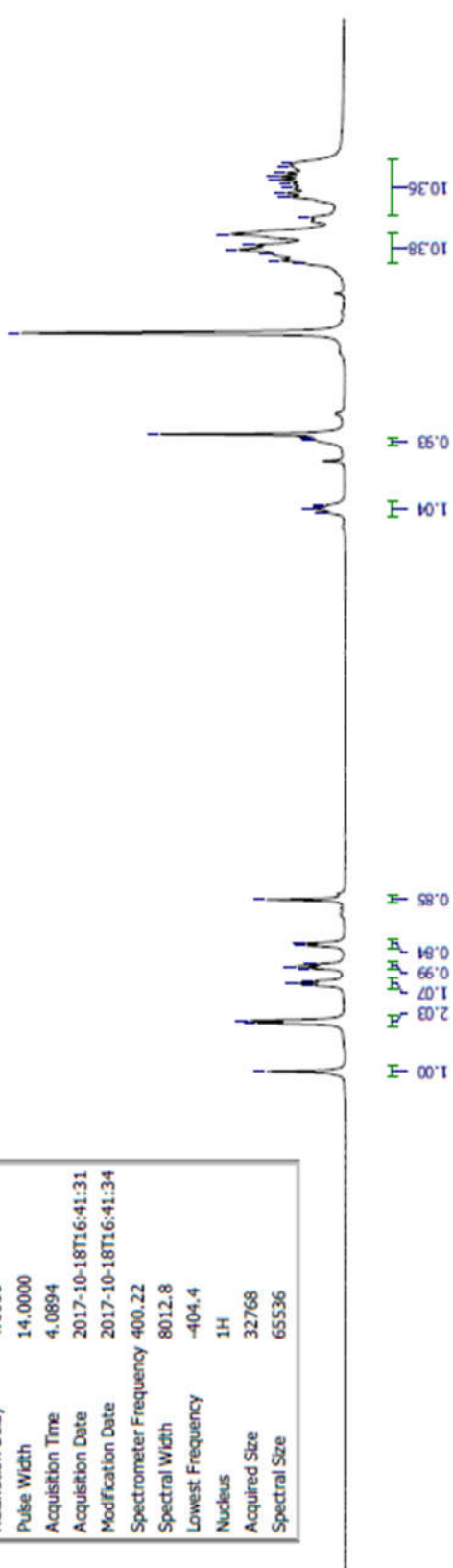
1.11
1.14
1.19
1.22
1.25
1.29
1.32
1.36
1.39
1.70
1.80
1.83
1.87
1.92
1.95
2.52

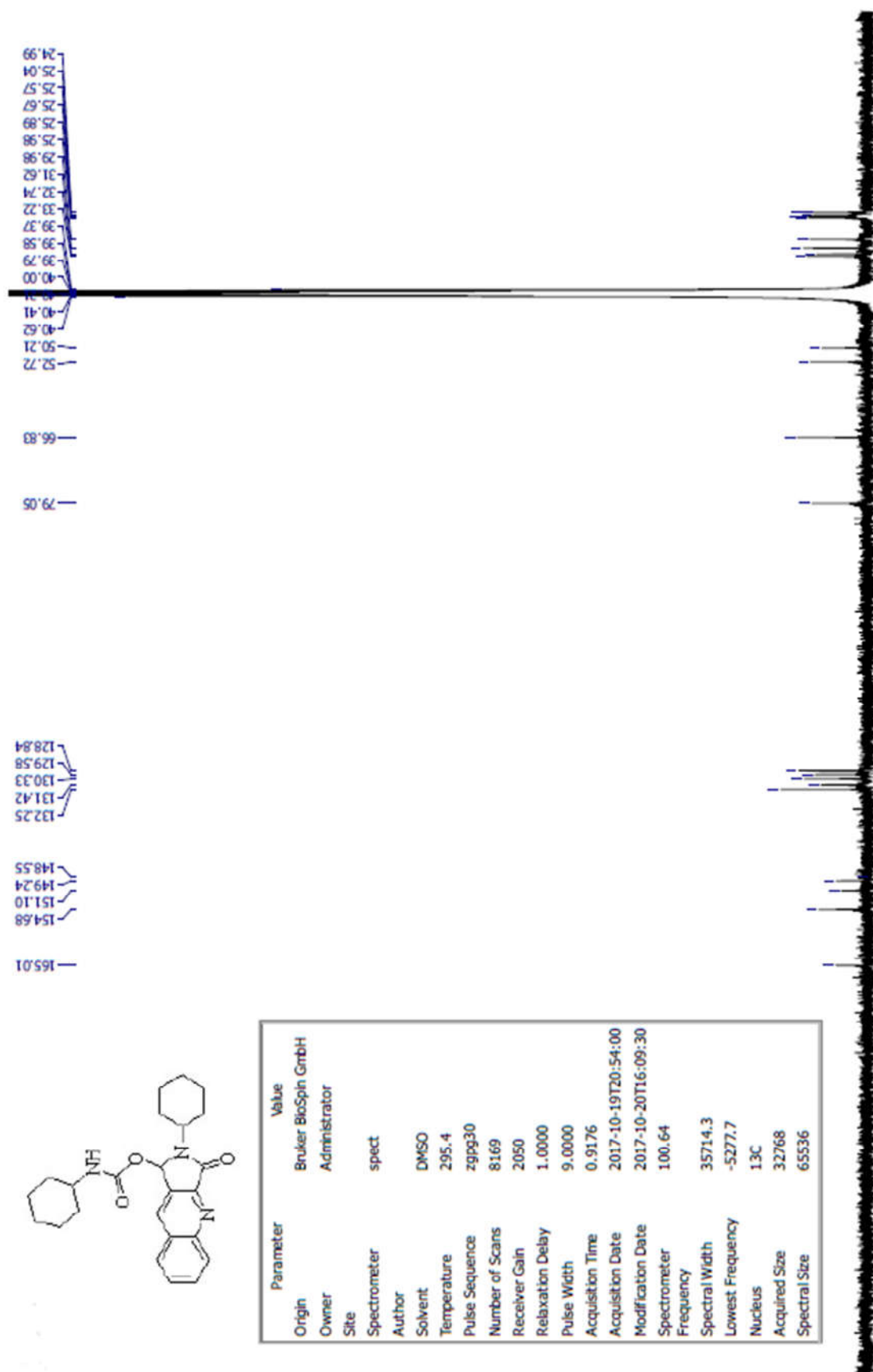
3.36
3.39
3.40
3.41
3.95
3.95
3.98
4.00

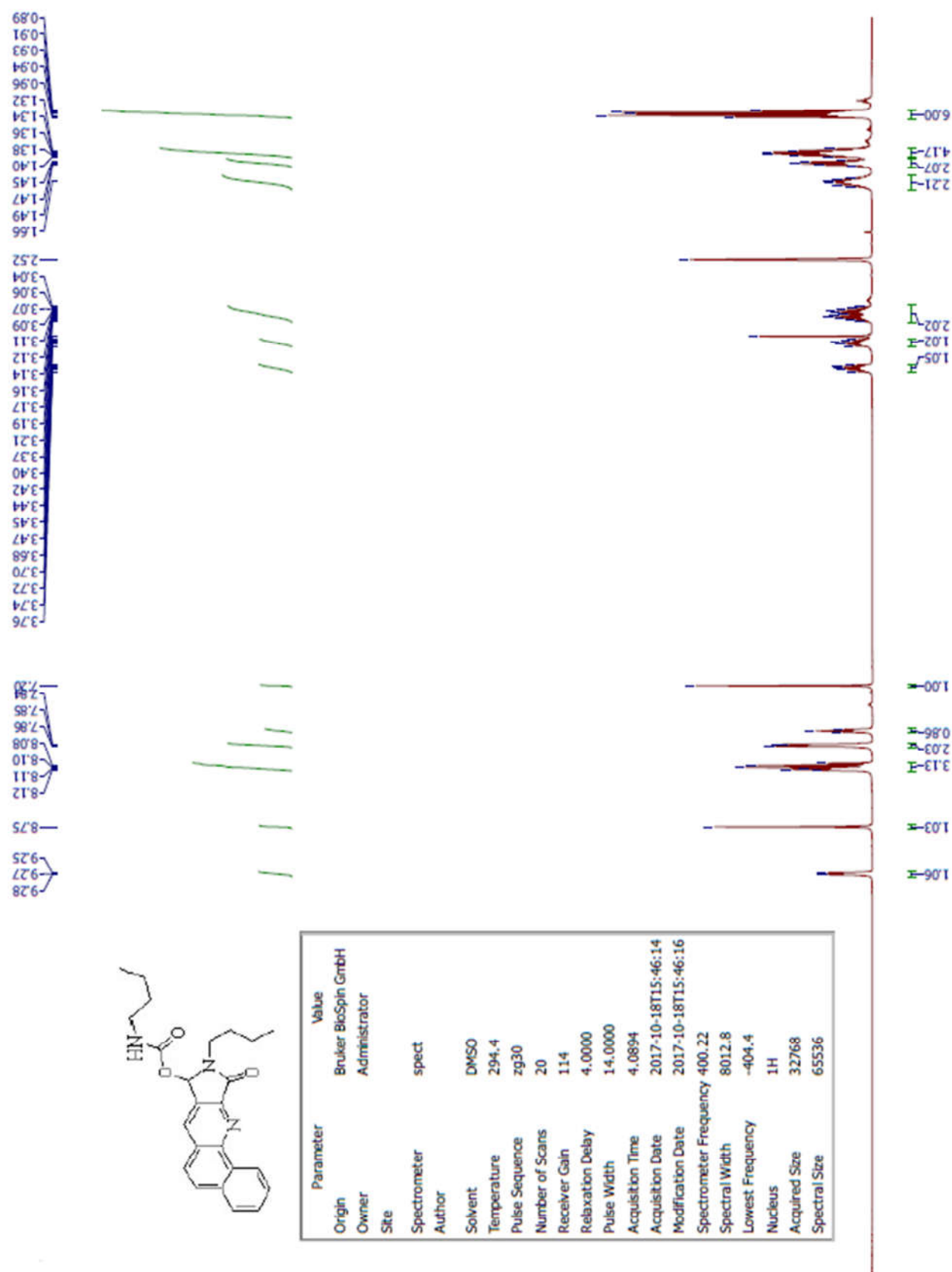
7.22
7.58
7.60
7.77
7.79
7.92
8.22
8.24
8.65



Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	Administrator
Site	spect
Spectrometer	
Author	
Solvent	DMSO
Temperature	294.6
Pulse Sequence	zg30
Number of Scans	20
Receiver Gain	181
Relaxation Delay	4.0000
Pulse Width	14.0000
Acquisition Time	4.0894
Acquisition Date	2017-10-18T16:41:31
Modification Date	2017-10-18T16:41:34
Spectrometer Frequency	400.22
Spectral Width	8012.8
Lowest Frequency	-404.4
Nucleus	¹ H
Acquired Size	32768
Spectral Size	65536





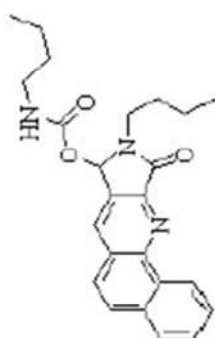


40.89
40.62
40.57
40.41
40.20
40.00
39.79
39.58
39.37
31.82
30.40
20.14
19.87
14.10
14.05

79.59

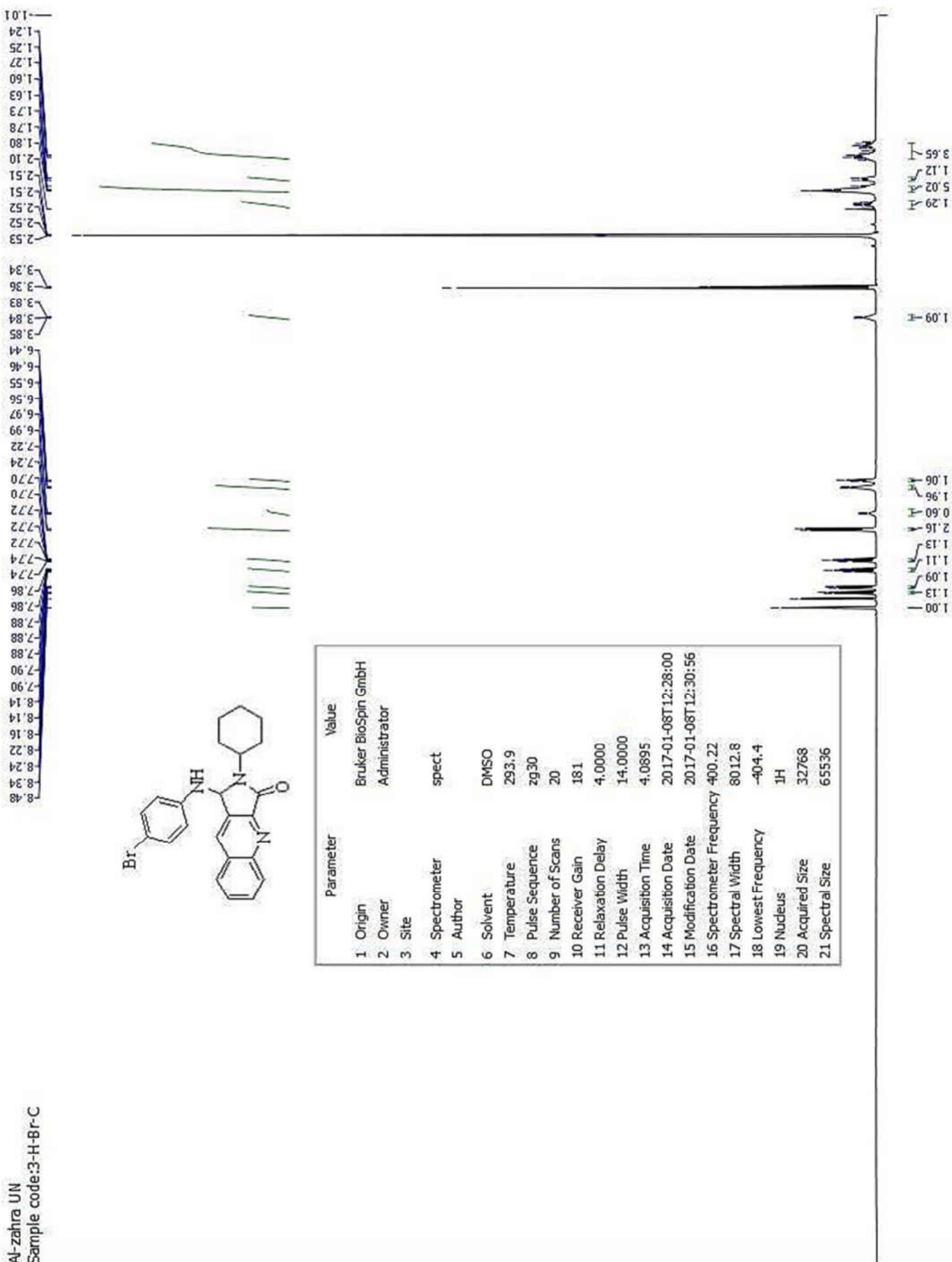
155.82
149.43
147.75
134.06
133.54
132.48
131.25
129.86
129.59
128.64
128.05
127.68
126.28
124.66

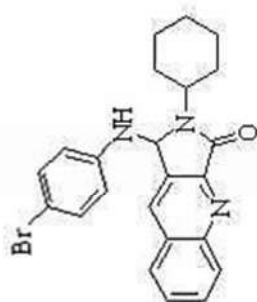
165.54



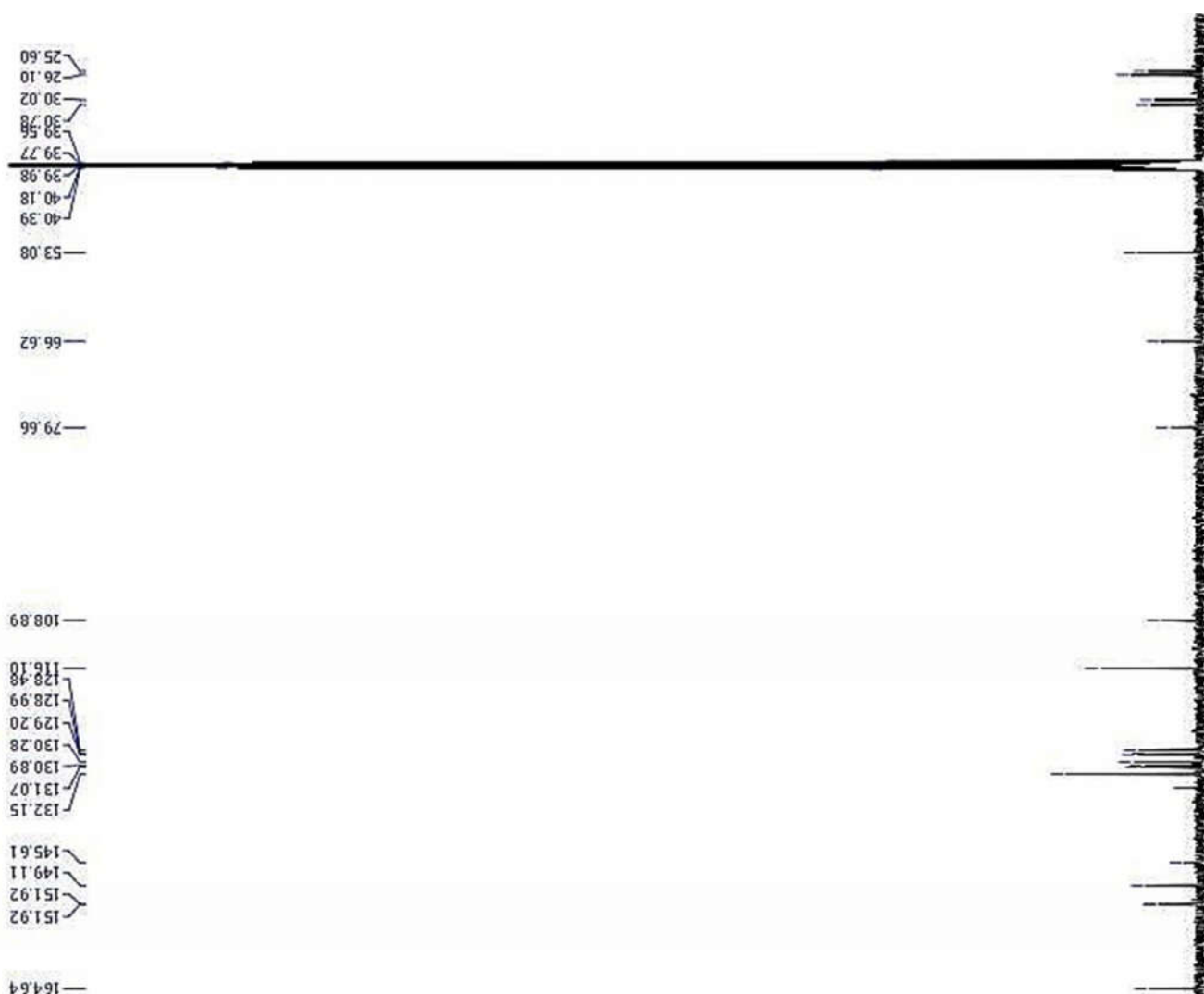
Parameter	Value
Origin	Bruker BioSpin GmbH
Owner	Administrator
Site	spect
Spectrometer	
Author	
Solvent	DMSO
Temperature	295.4
Pulse Sequence	zgpg30
Number of Scans	300
Receiver Gain	2050
Relaxation Delay	1.0000
Pulse Width	9.0000
Acquisition Time	0.9175
Acquisition Date	2017-10-19T19:26:12
Modification Date	2017-10-19T19:36:04
Spectrometer Frequency	100.64
Spectral Width	35714.3
Lowest Frequency	-5277.7
Nucleus	¹³ C
Acquired Size	32768
Spectral Size	65536

Al-zahra UN
Sample code:3-H-Br-C

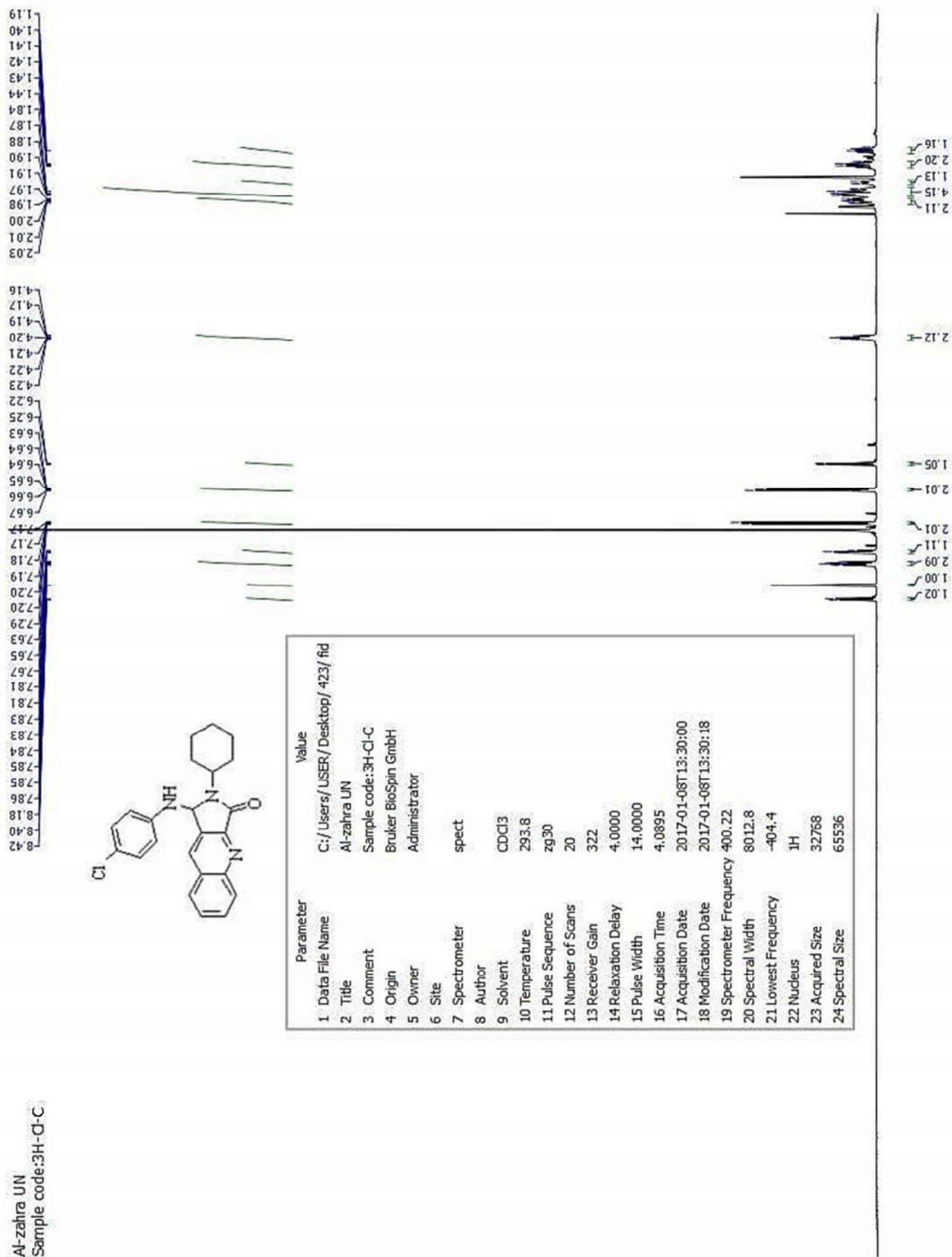




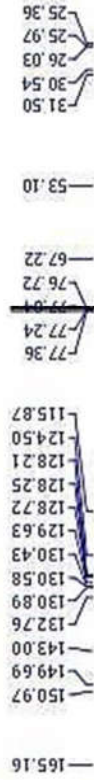
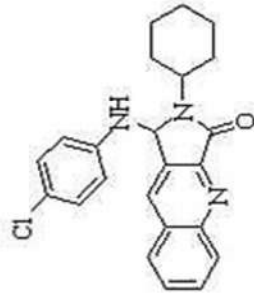
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	293.6
8 Pulse Sequence	zgpg30
9 Number of Scans	2001
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-01-16T07:35:00
15 Modification Date	2017-01-16T08:38:20
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



Al-zahra UN
Sample code:3H-D-C



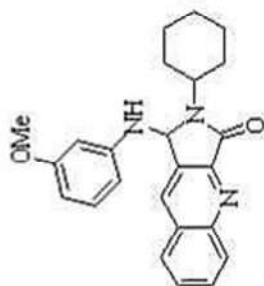
Al-zahra UN
Sample code:3H-Q-C



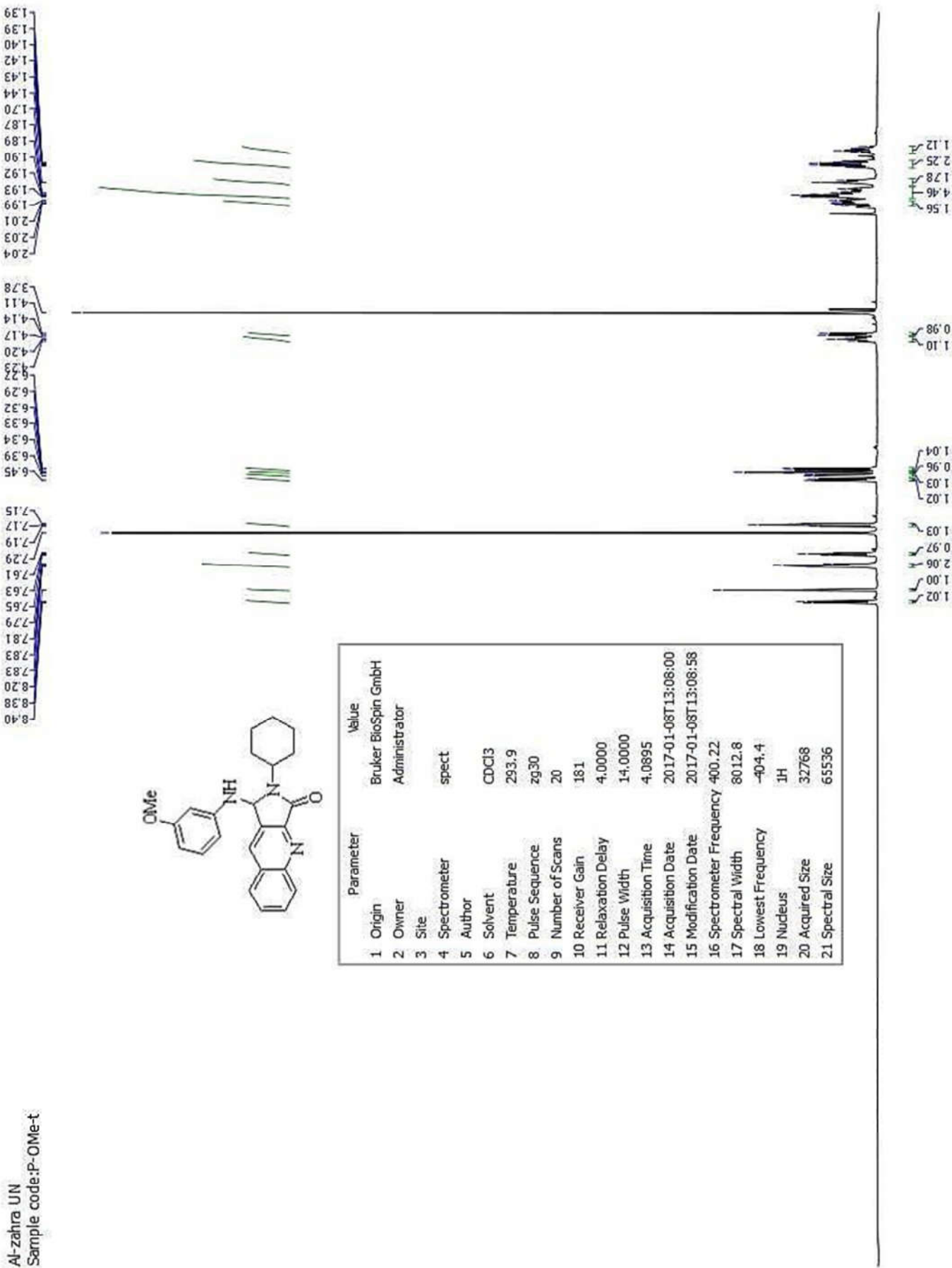
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	CDCl3
7 Temperature	294.5
8 Pulse Sequence	zgpg30
9 Number of Scans	4909
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-01-15T13:32:00
15 Modification Date	2017-01-15T16:13:02
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	13C
20 Acquired Size	32768
21 Spectral Size	65536



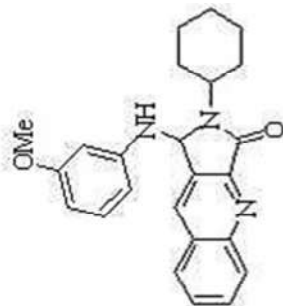
Year	Population (millions)
1995	100.0
1996	101.0
1997	102.0
1998	103.0
1999	104.0
2000	105.0
2001	106.0
2002	107.0
2003	108.0
2004	109.0
2005	110.0
2006	111.0
2007	112.0
2008	113.0
2009	114.0
2010	115.0
2011	116.0
2012	117.0
2013	118.0
2014	119.0
2015	120.0
2016	121.0
2017	122.0
2018	123.0
2019	124.0
2020	125.0



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	CDCl3
7 Temperature	293.9
8 Pulse Sequence	zg30
9 Number of Scans	20
10 Receiver Gain	181
11 Relaxation Delay	4.0000
12 Pulse Width	14.0000
13 Acquisition Time	4.0895
14 Acquisition Date	2017-01-08T13:08:00
15 Modification Date	2017-01-08T13:08:58
16 Spectrometer Frequency	400.22
17 Spectral Width	8012.8
18 Lowest Frequency	-404.4
19 Nucleus	1H
20 Acquired Size	32768
21 Spectral Size	65536



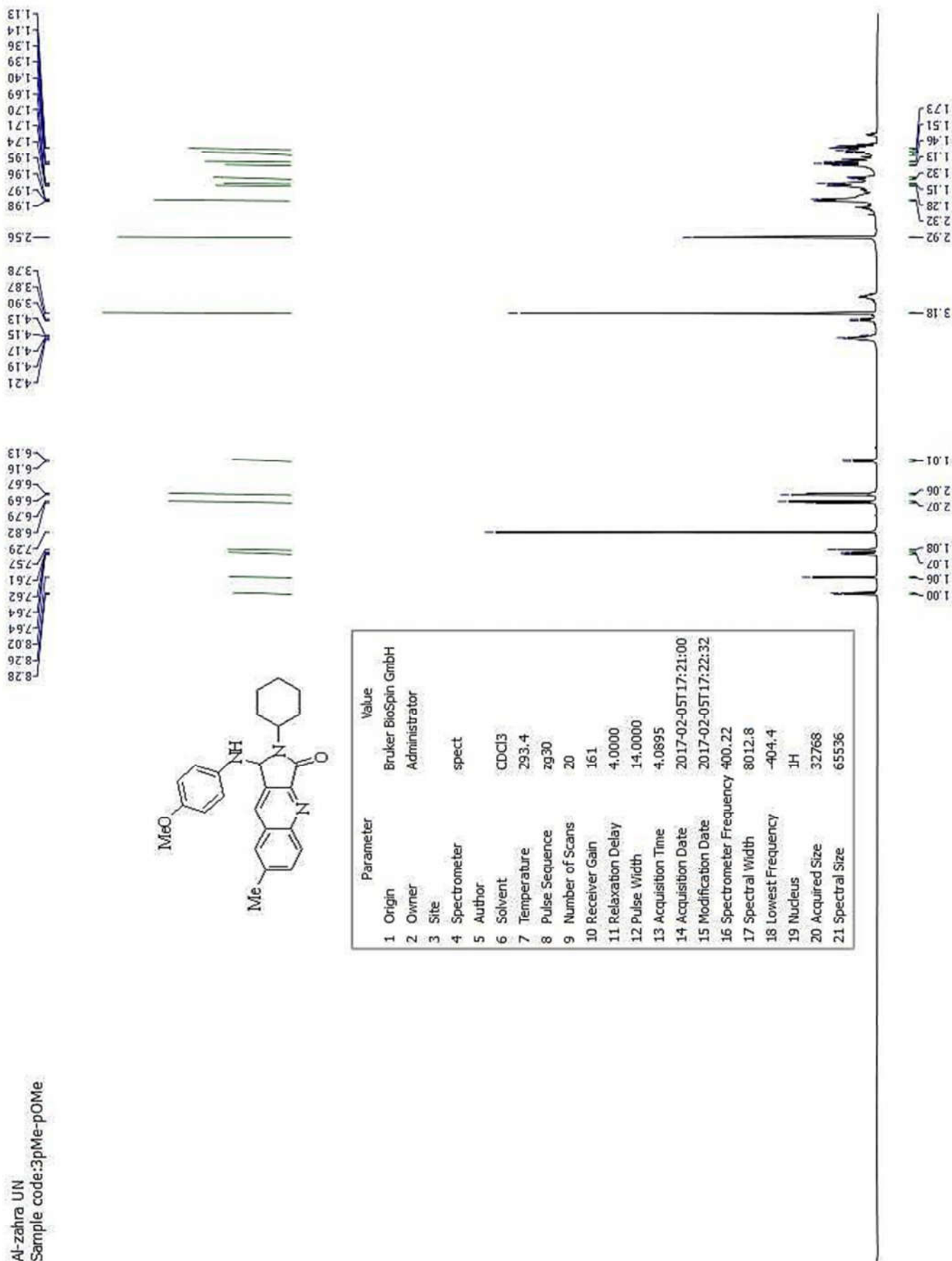
Al-zahra UN
Sample code:3H-mo-m-C



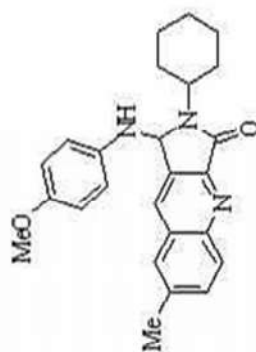
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	CDCl3
7 Temperature	294.0
8 Pulse Sequence	zgpg30
9 Number of Scans	2240
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-01-15T12:10:00
15 Modification Date	2017-01-15T13:24:06
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



Al-zahra UN
Sample code:3pMe-pOMe



Al-zahra UN
Sample code:3pMe-pOMe

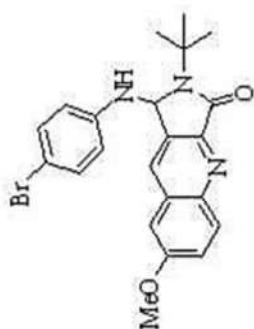


Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	spect
4 Spectrometer	
5 Author	
6 Solvent	CDCl3
7 Temperature	294.7
8 Pulse Sequence	zgpg30
9 Number of Scans	3370
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-02-08T17:36:00
15 Modification Date	2017-02-08T19:27:14
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536

77.37
77.25
77.05
76.73
68.56
55.63
53.12
33.98
31.44
24.97
21.73

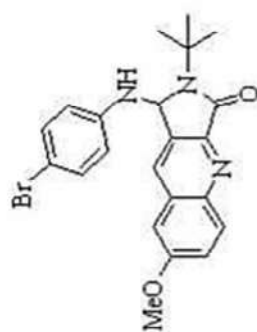
165.37
156.79
153.57
150.34
148.20
138.25
132.71
130.42
129.59
127.03
116.75
115.07

Al-zahra UN
Sample code:3POMe-Br-t

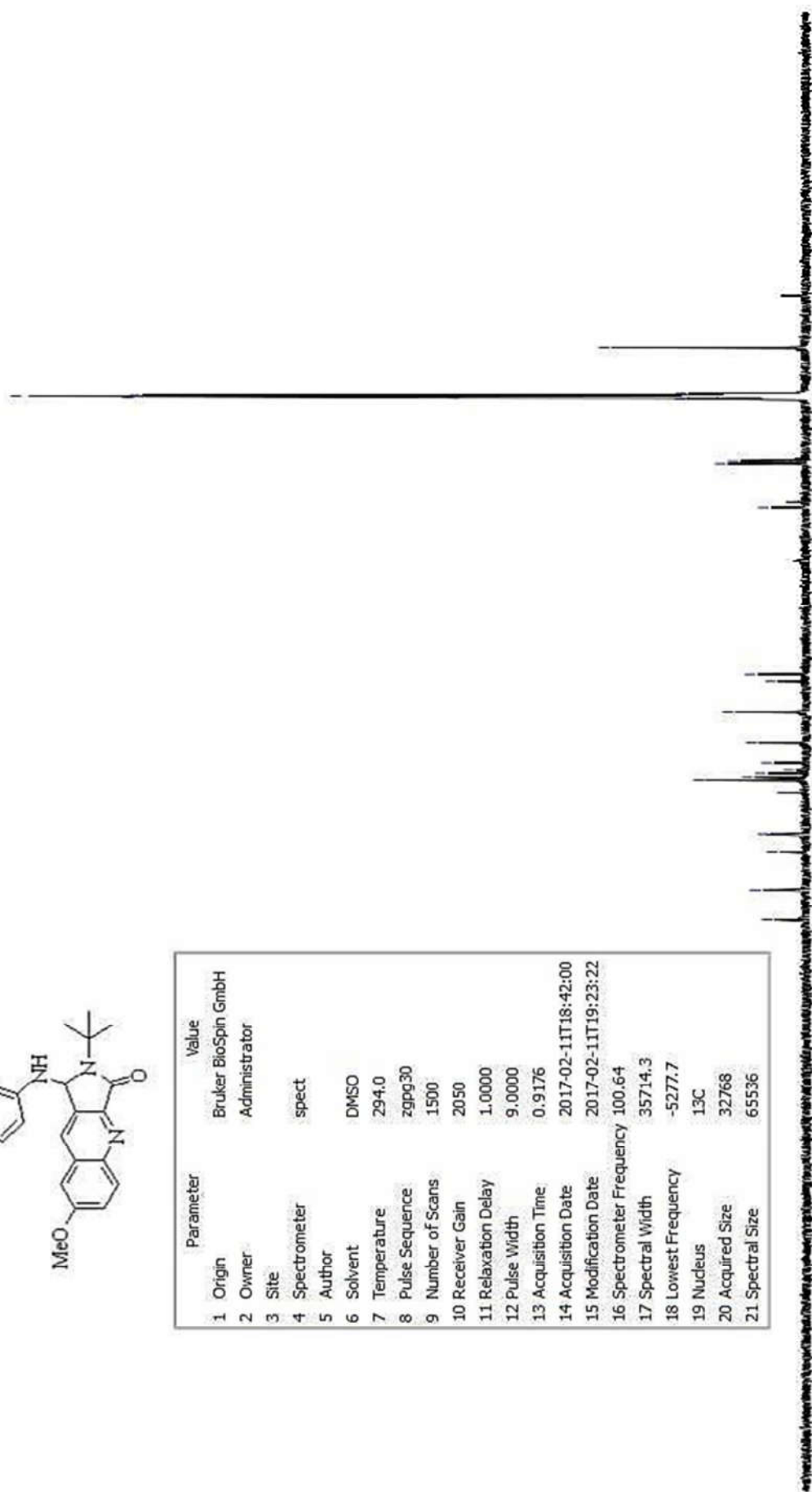


Parameter	Value
1 Data File Name	C:/Users/USER/Desktop/ 443/ fd
2 Title	Al-zahra UN
3 Comment	Sample code:3POMe-Br-t
4 Origin	Bruker BioSpin GmbH
5 Owner	Administrator
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	291.9
11 Pulse Sequence	zg30
12 Number of Scans	20
13 Receiver Gain	144
14 Relaxation Delay	4.0000
15 Pulse Width	14.0000
16 Acquisition Time	4.0895
17 Acquisition Date	2017-02-05T08:37:00
18 Modification Date	2017-02-05T08:37:44
19 Spectrometer Frequency	400.22
20 Spectral Width	8012.8
21 Lowest Frequency	-404.4
22 Nucleus	¹ H
23 Acquired Size	32768
24 Spectral Size	65536

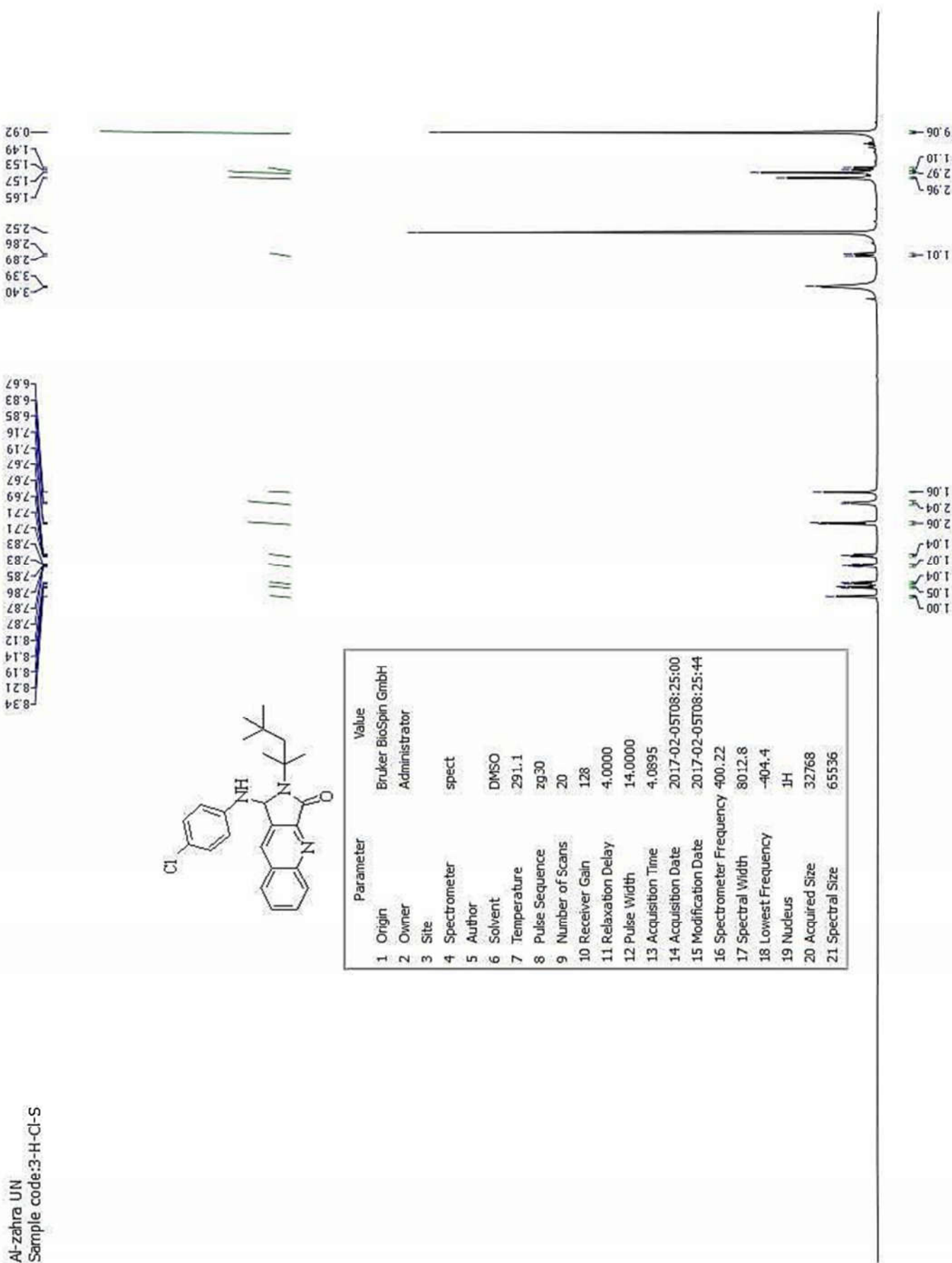
Al-zahra UN
Sample code:3POMe-Br-t



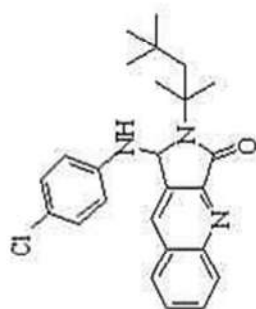
Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	
4 Spectrometer	spect
5 Author	
6 Solvent	DMSO
7 Temperature	294.0
8 Pulse Sequence	zgpg30
9 Number of Scans	1500
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-02-11T18:42:00
15 Modification Date	2017-02-11T19:23:22
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



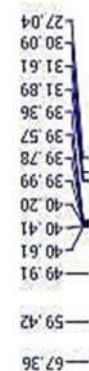
Al-zahra UN
Sample code:3-H-Cl-S



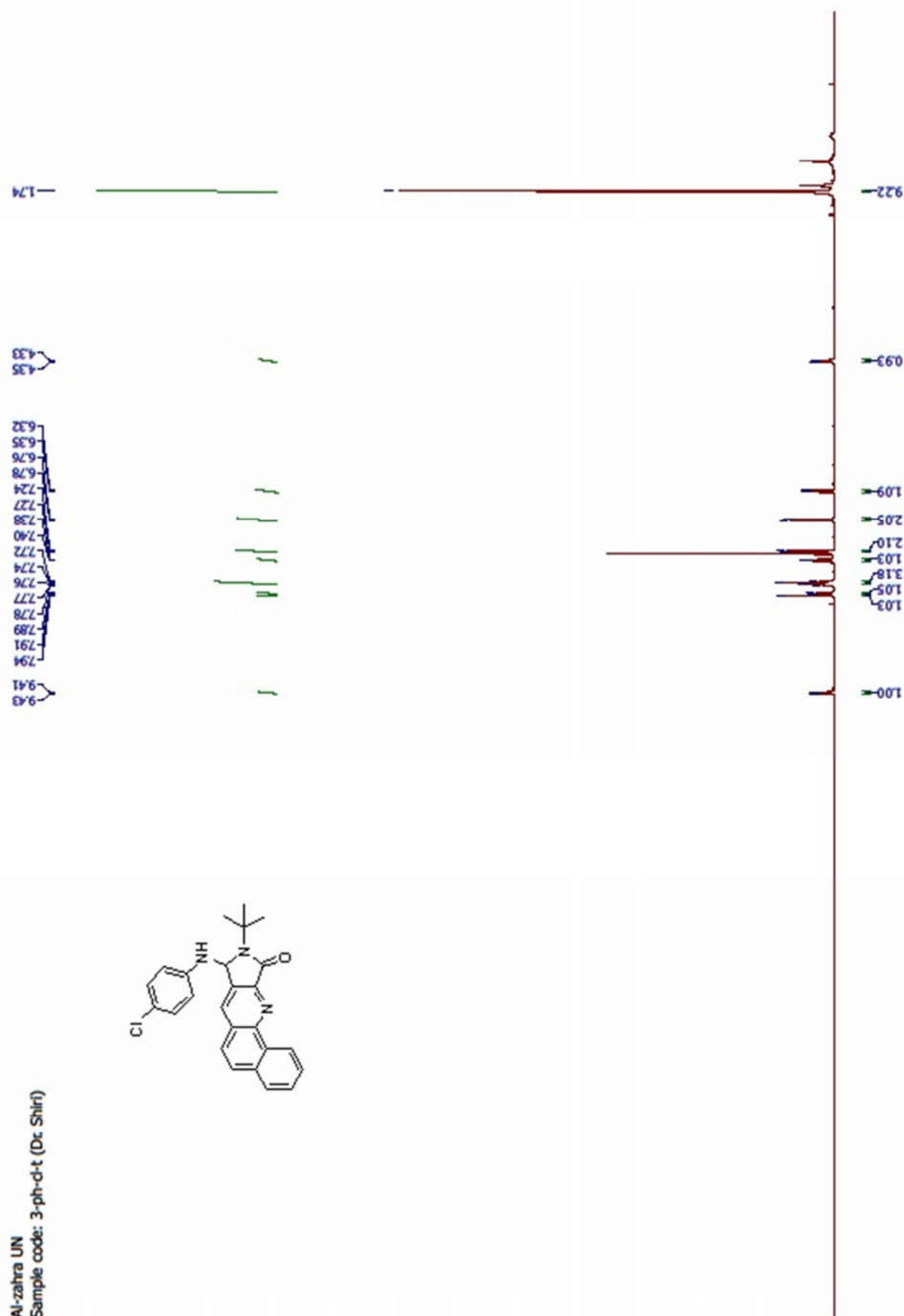
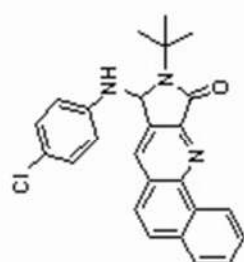
Al-zahra UN
Sample code:3-H-Cl-S



Parameter	Value
1 Origin	Bruker BioSpin GmbH
2 Owner	Administrator
3 Site	spect
4 Spectrometer	
5 Author	
6 Solvent	DMSO
7 Temperature	295.4
8 Pulse Sequence	zgpg30
9 Number of Scans	560
10 Receiver Gain	2050
11 Relaxation Delay	1.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.9176
14 Acquisition Date	2017-02-09T07:16:00
15 Modification Date	2017-02-09T07:28:36
16 Spectrometer Frequency	100.64
17 Spectral Width	35714.3
18 Lowest Frequency	-5277.7
19 Nucleus	¹³ C
20 Acquired Size	32768
21 Spectral Size	65536



Al-zahra UN
Sample code: 3-ph-d-t (Dc Shiri)

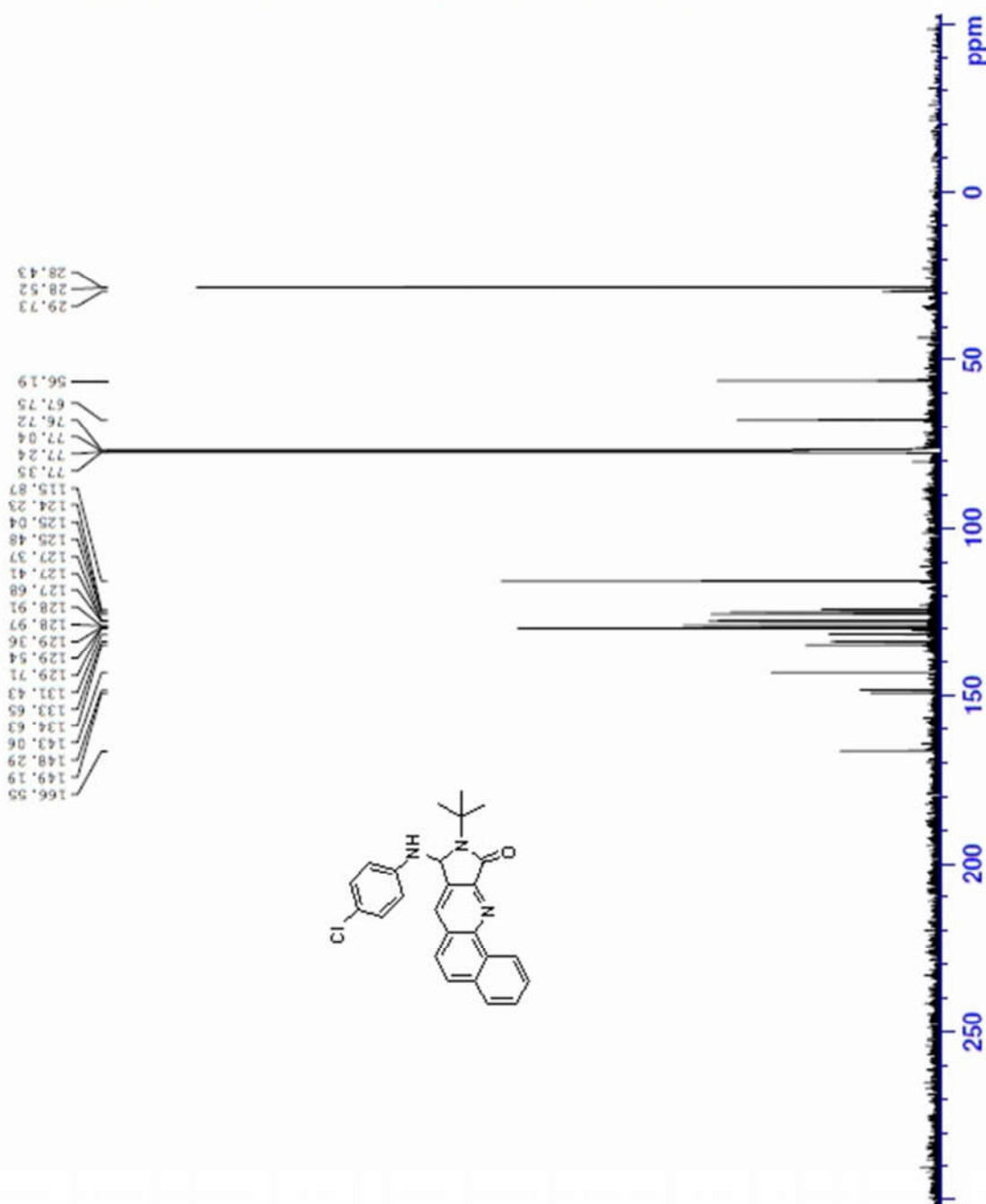




NAME Al-zahra UN
 EXPNO 487
 PROCNO 1
 Date_ 20170723
 Time 23.40
 INSTRUM spect
 PROHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8192
 DS 0
 SWH 35714.285 Hz
 FIDRES 0.544957 Hz
 AQ 0.9175540 sec
 RG 2050
 DW 14.000 usec
 DE 6.50 usec
 TE 295.7 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

CHANNEL f1
 NUC1 ¹³C
 P1 9.00 usec
 PL1 -0.90 dB
 PL1W 42.02801895 W
 SFO1 100.6479784 MHz

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 90.00 usec
 PL2 -2.00 dB
 PL12 14.16 dB
 PL13 17.90 dB
 PL2W 11.86359406 W
 PL12W 0.28722104 W
 PL13W 0.12139934 W
 SFO2 400.2216009 MHz
 SI 32768
 SF 100.6353990 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



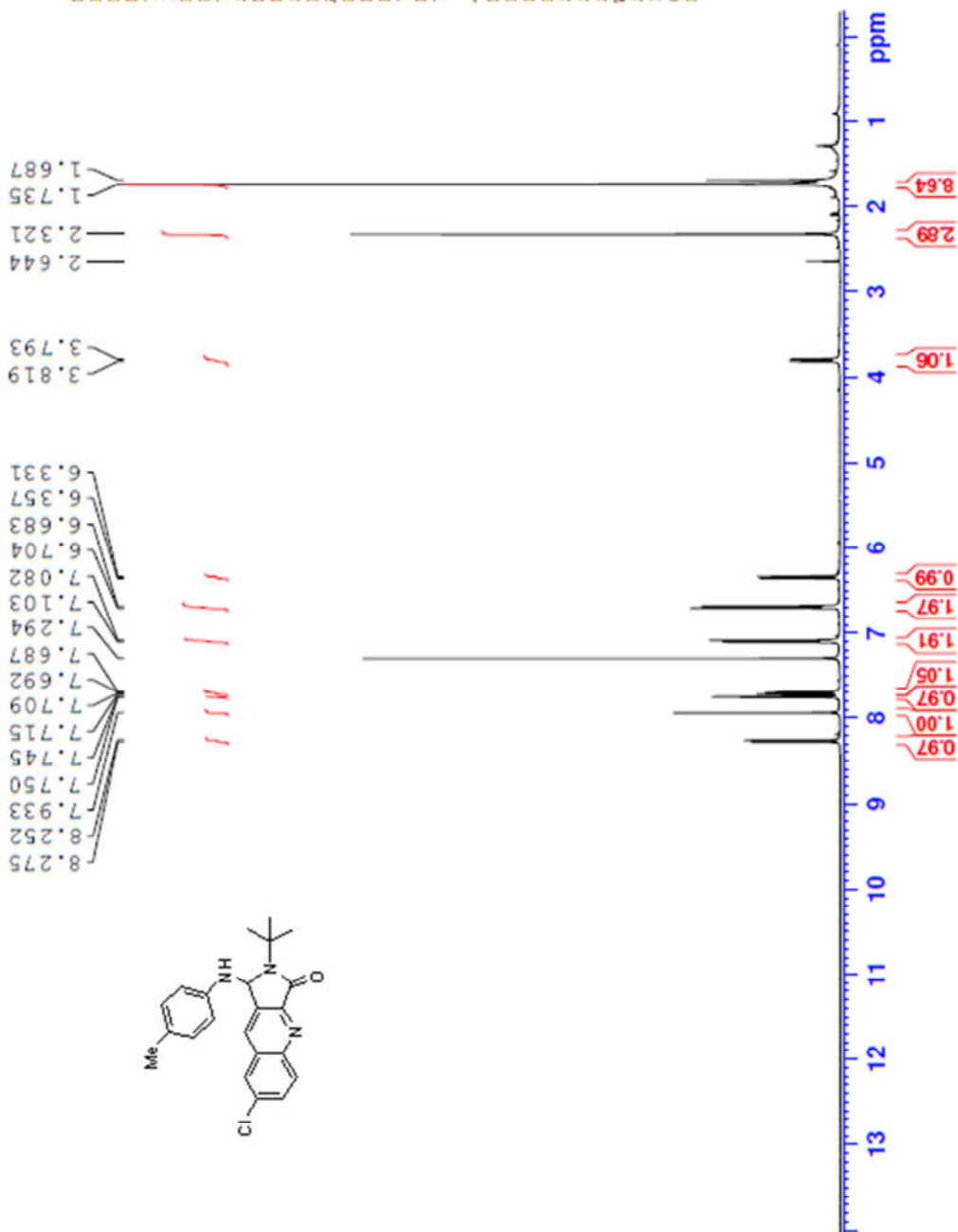
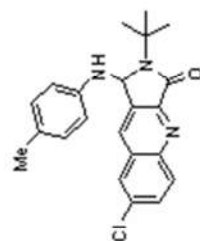
Sample code: 3-cl-me-t (Dr. Shiri)



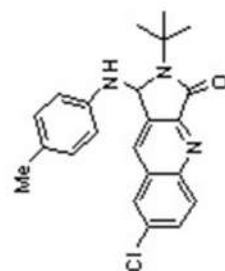
NAME Al-zahra UN
EXPNO 486
PROCNO 1
Date_ 20170721
Time 14.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
F1F2 1930
ID 65536
SOLVENT CDCl3
NS 20
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 256
DW 62.400 usec
DE 6.50 usec
TE 293.4 K
D1 4.0000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 14.00 usec
PL1 -2.00 dB
PLW 11.86359406 W
SFO1 400.2236020 MHz
SI 32768
SF 400.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.275
8.252
7.933
7.750
7.745
7.715
7.709
7.692
7.687
7.294
7.103
7.082
6.704
6.683
6.357
6.331



Sample code: 3-cl-me-t (Dr. Shiri)



NAME Al-zahra UN
EXPNO 488
PROCNO 1
Date_ 20170724
Time 8.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 900
DS 0
SWH 35714.285 Hz
FIDRES 0.544957 Hz
AQ 0.9175540 sec
RG 2050
DW 14.000 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL12W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

