Zinc(II)-Mediated Generation of 5-Amino Substituted 2,3-Dihydro-1,2,4-oxadiazoles and Their Further Zn^{II}-Catalyzed and O_2-Involving Transformations

Andrey S. Smirnov,[a] Ekaterina S. Yandanova,[a] Nadezhda A. Bokach,[a]* Galina. L. Starova,[a] Vladislav V. Gurzhiy,[a] Margarita S. Avdontceva,[a] Andrey A. Zolotarev,[a] Vadim Yu. Kukushkin[a,b]*

(a) Saint Petersburg State University, 7/9 Universitetskaya Nab., 199034 Saint Petersburg, Russia

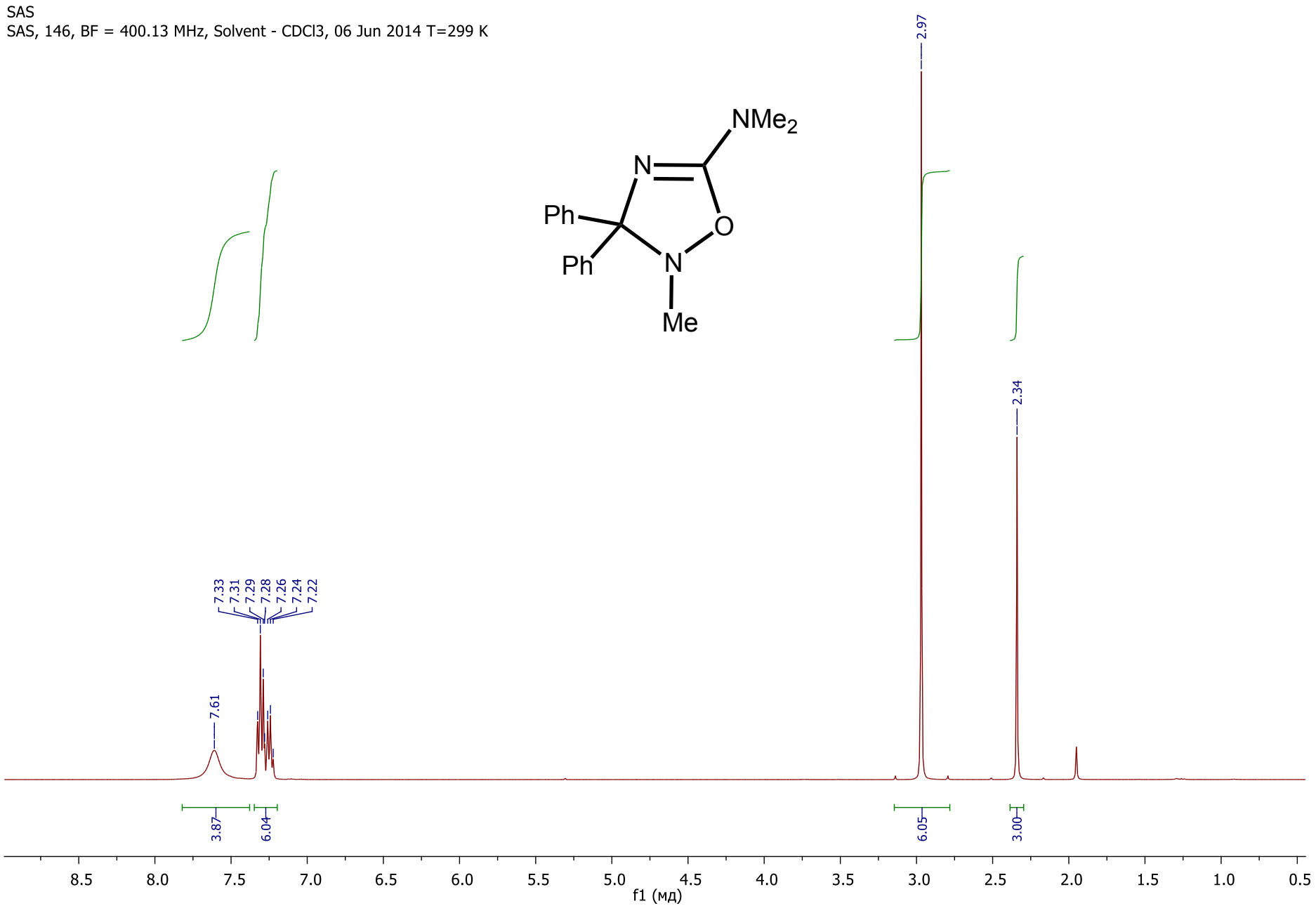
(b) Institute of Macromolecular Compounds of Russian Academy of Sciences, V.O. Bolshoii Pr. 31, 199004 Saint Petersburg, Russian Federation

New Journal of Chemistry

Electronic Supporting Information, File 2

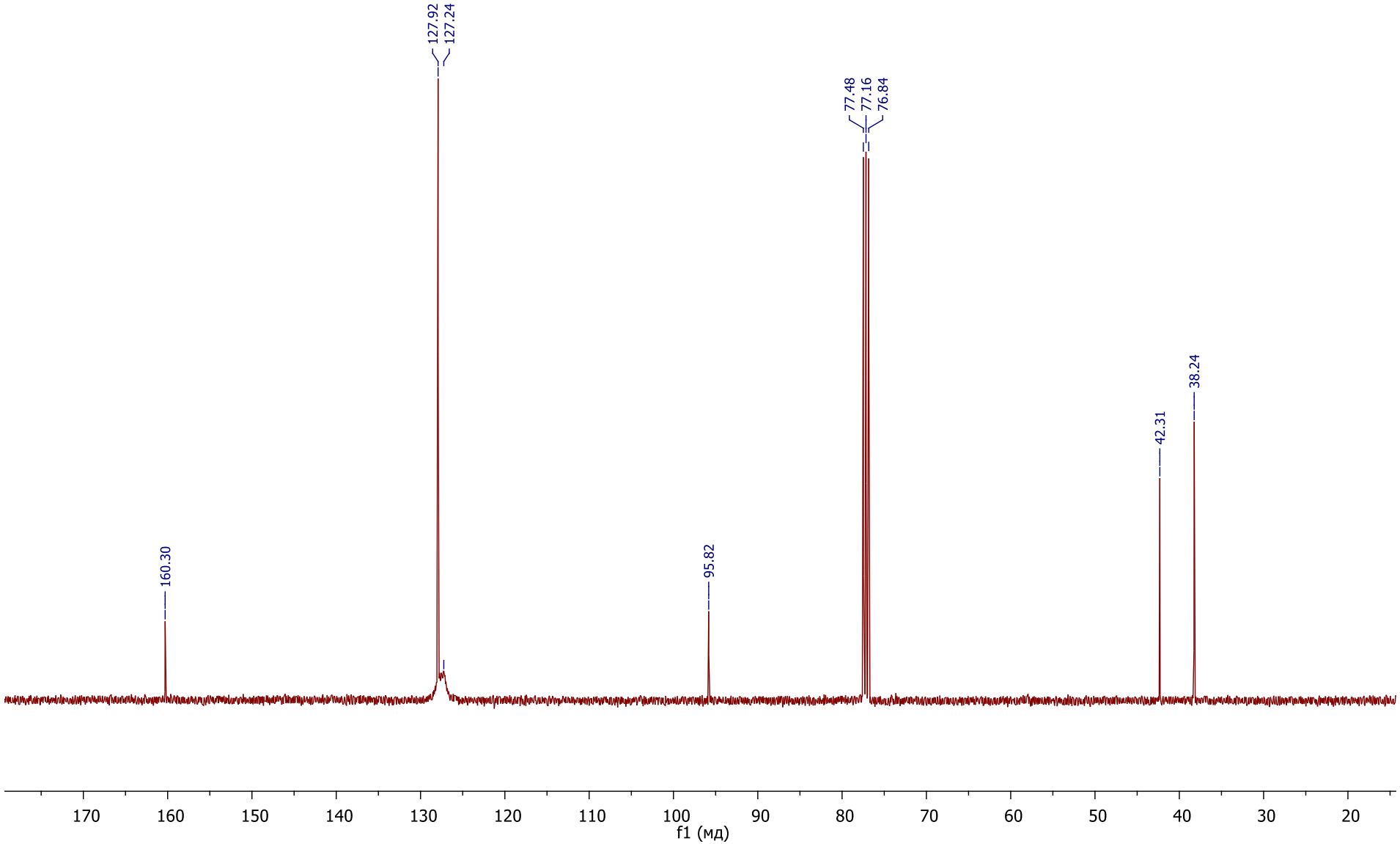
Table of Contents

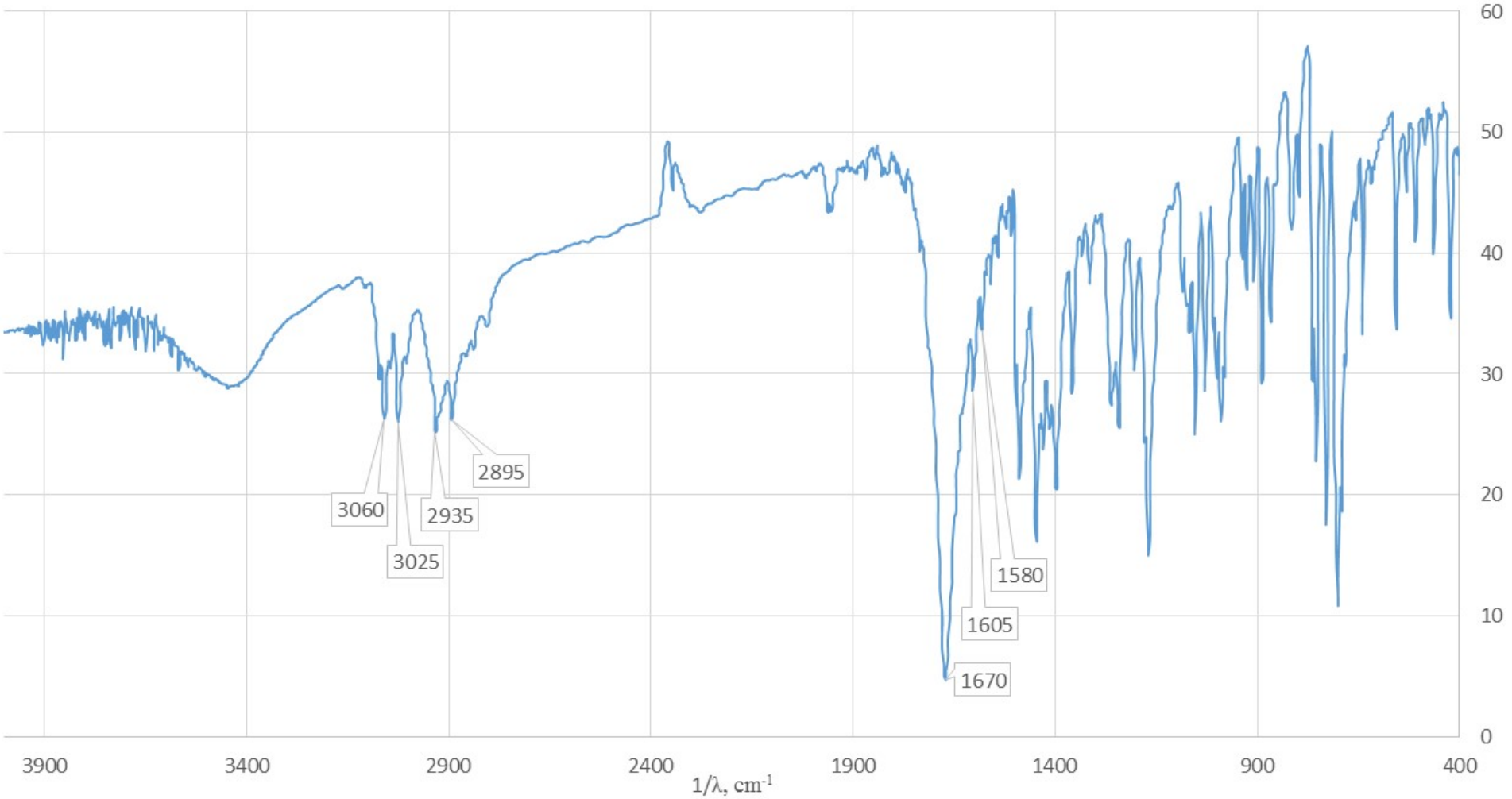
^{1}H *N,N*,2-trimethyl-3,3-diphenyl-2,3-dihydro-1,2,4-oxadiazol-5-amine (3aa).



^{13}C *N,N*,2-trimethyl-3,3-diphenyl-2,3-dihydro-1,2,4-oxadiazol-5-amine (3aa).

SASc
SASc, 147, BF = 100.612769 MHz, Solvent - CDCl3, 06 Jun 2014 T=300 K




60
50
40
30
20
10
0
3900
3400
2900
2400
1900
1400
900
400
1/λ, cm-1
3060
3025
2935
2895
1670
1605
1580

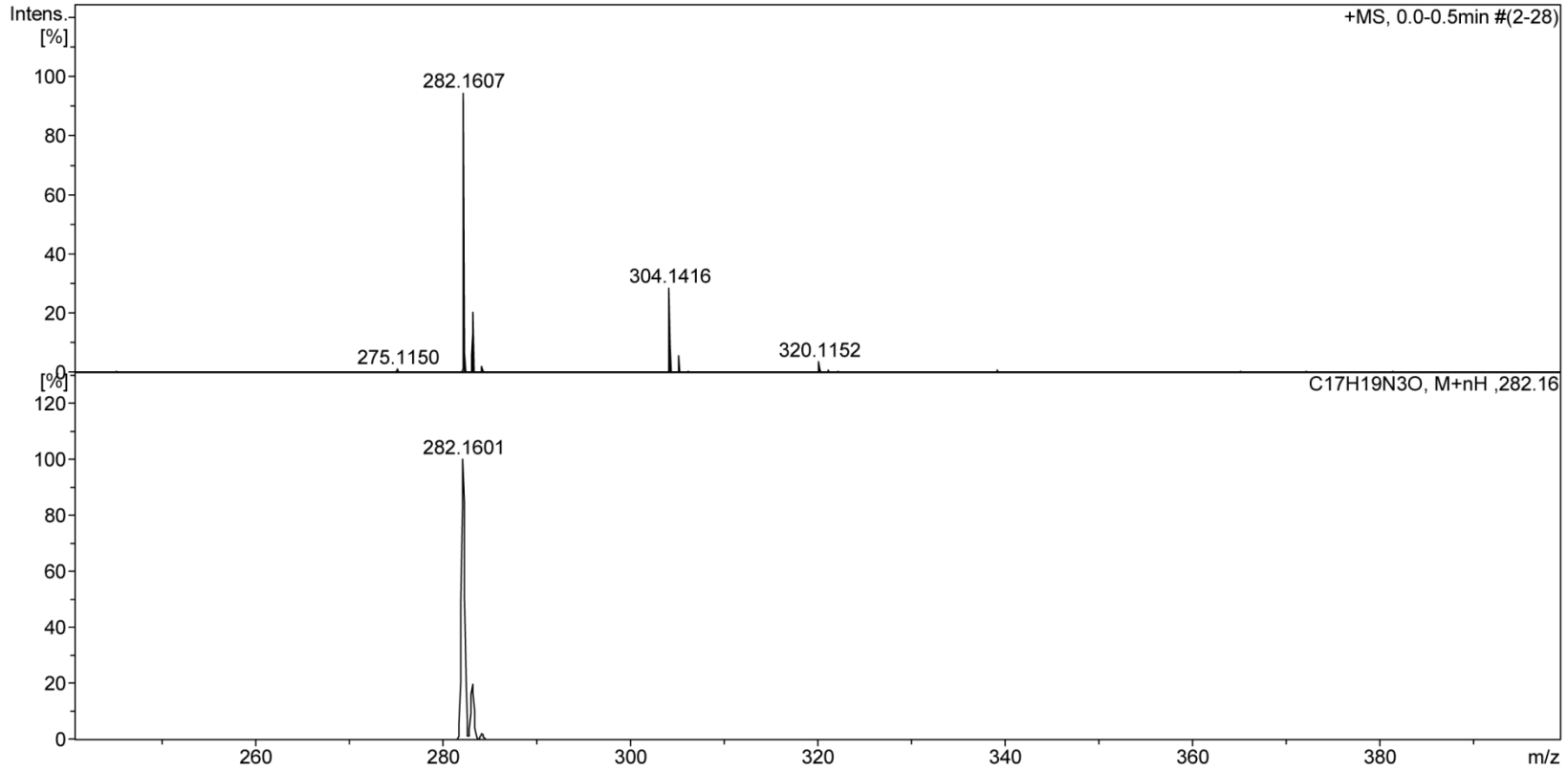
Mass Spectrum Report

Analysis Info

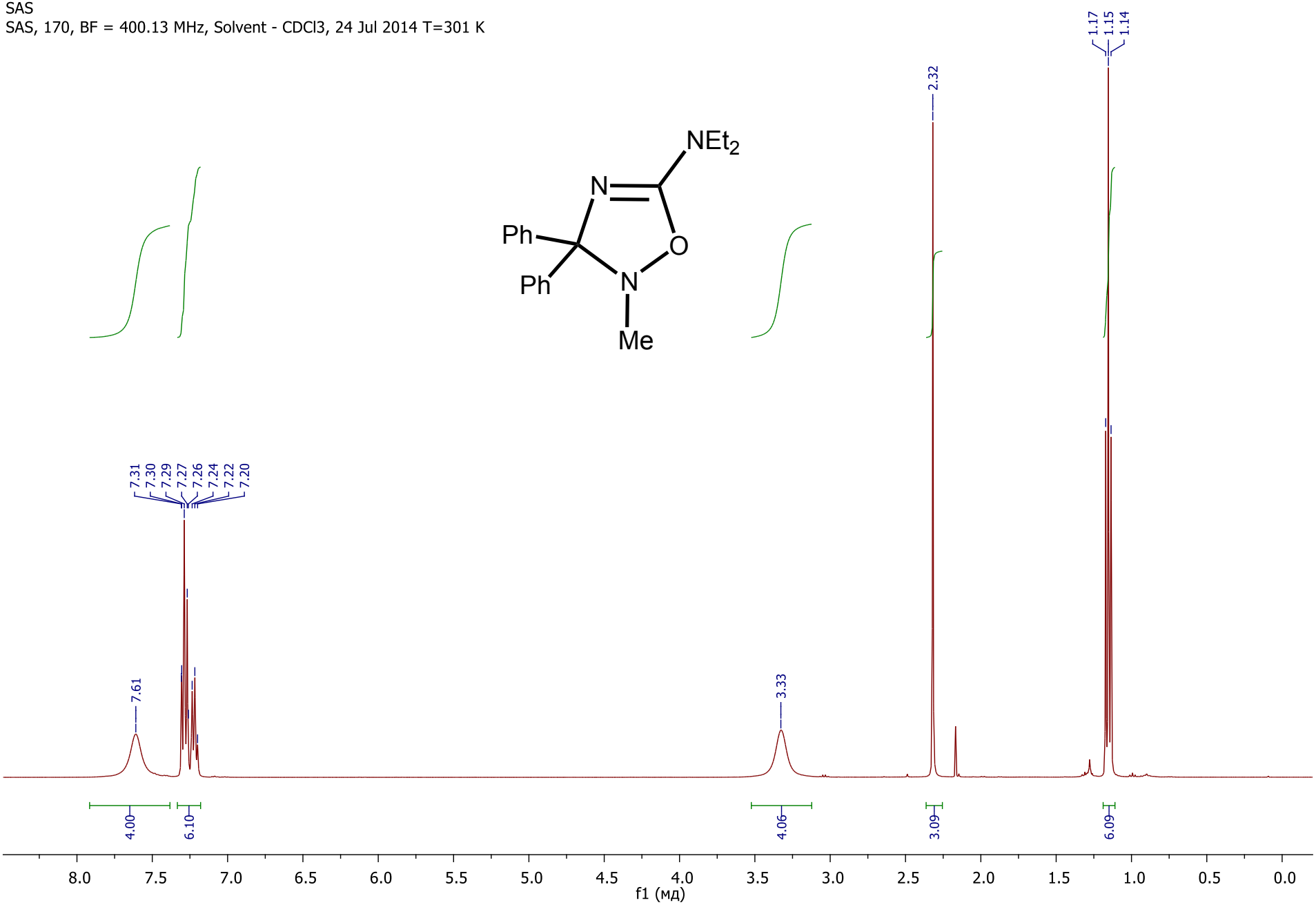
Analysis Name	D:\Data\June 2015\BUT6a.d	Acquisition Date	03.06.2015 16:38:40
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT6a	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

Acquisition Parameter

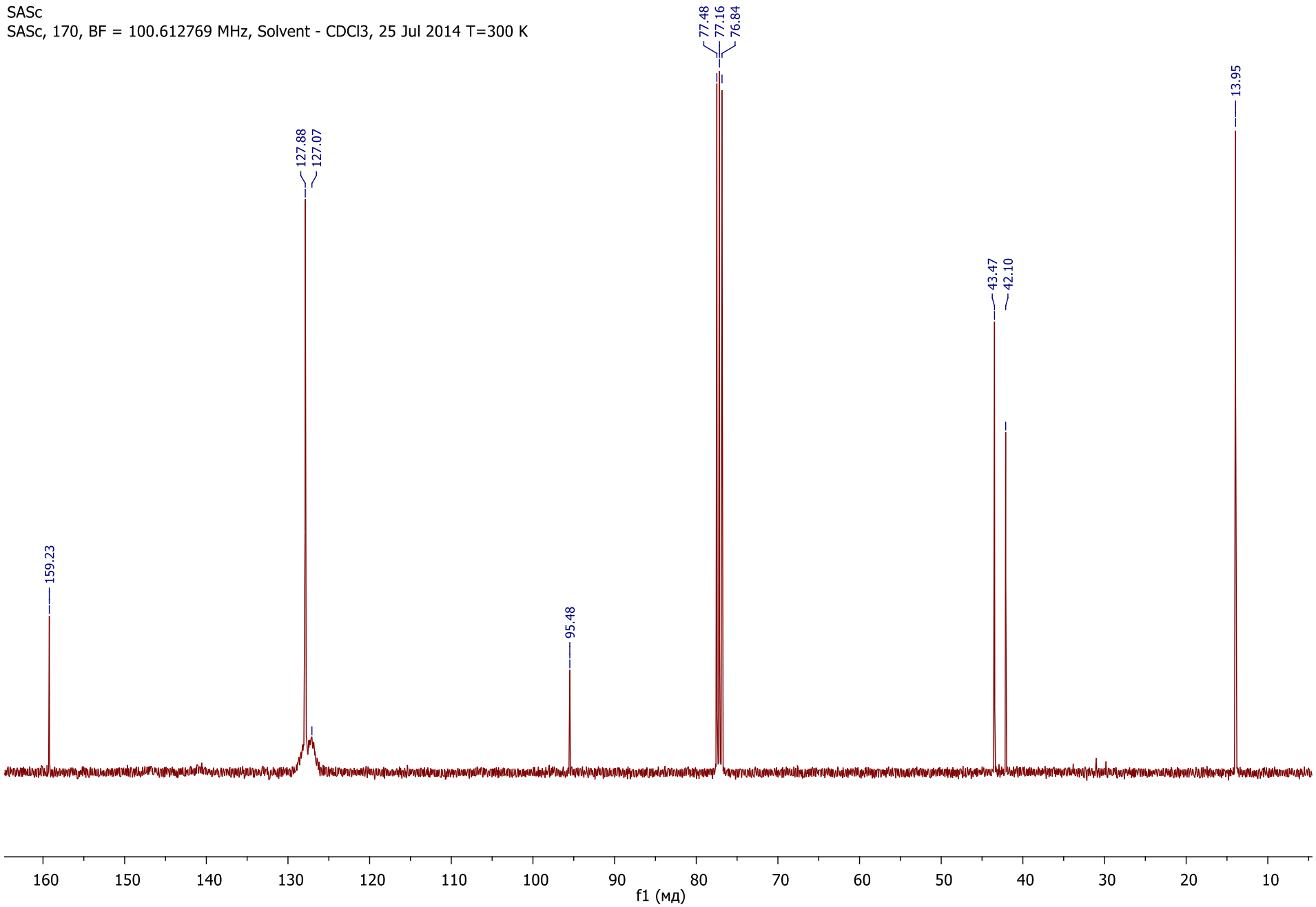
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



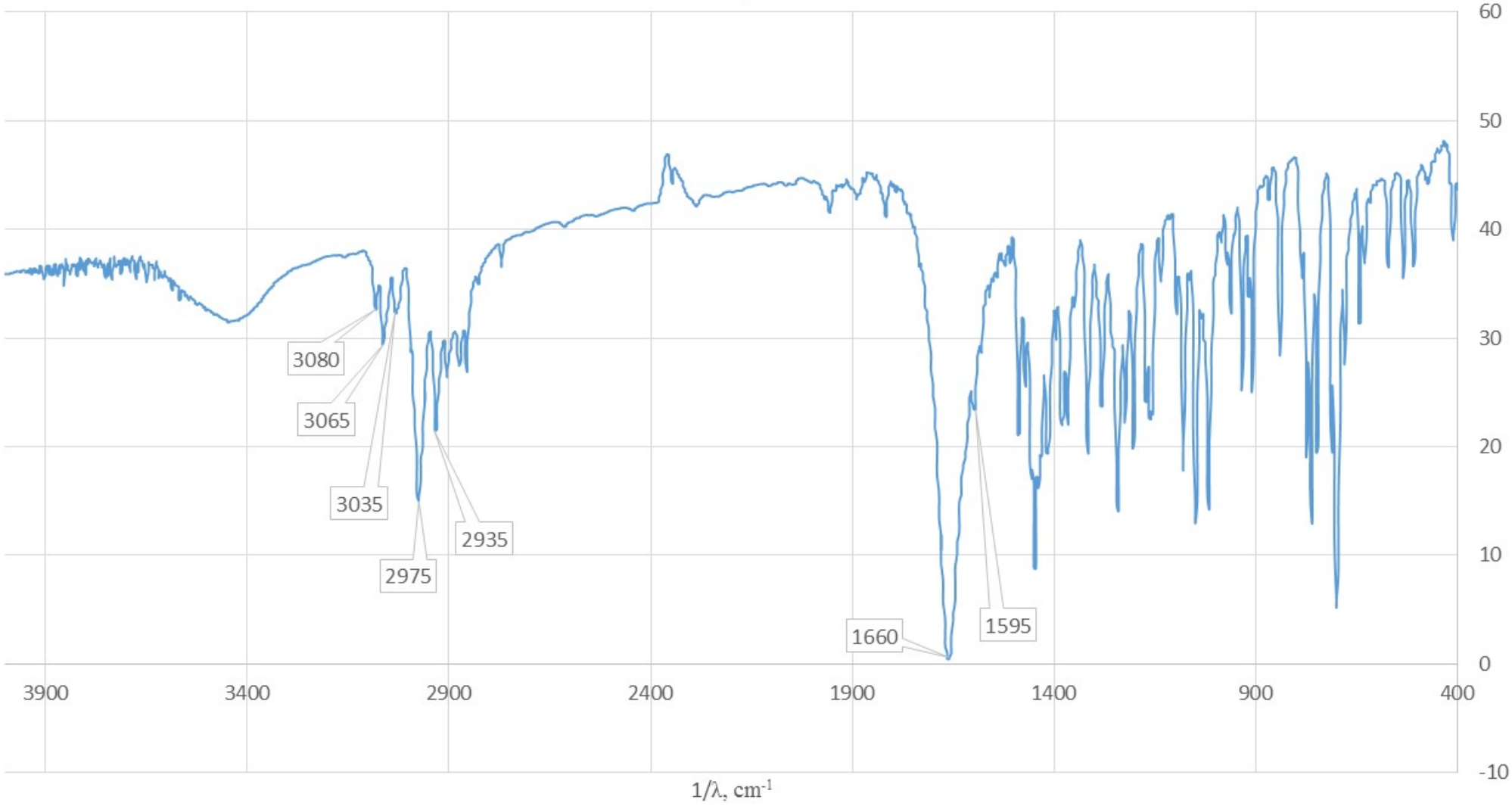
^{1}H *N,N*-diethyl-2-methyl-3,3-diphenyl-2,3-dihydro-1,2,4-oxadiazol-5-amine (3ba)



^{13}C *N,N*-diethyl-2-methyl-3,3-diphenyl-2,3-dihydro-1,2,4-oxadiazol-5-amine (3ba)



7


3080
3065
3035
2975
2935
1660
1595
3900
3400
2900
2400
1900
1400
900
400
60
50
40
30
20
10
0
-10
1/λ, cm-1

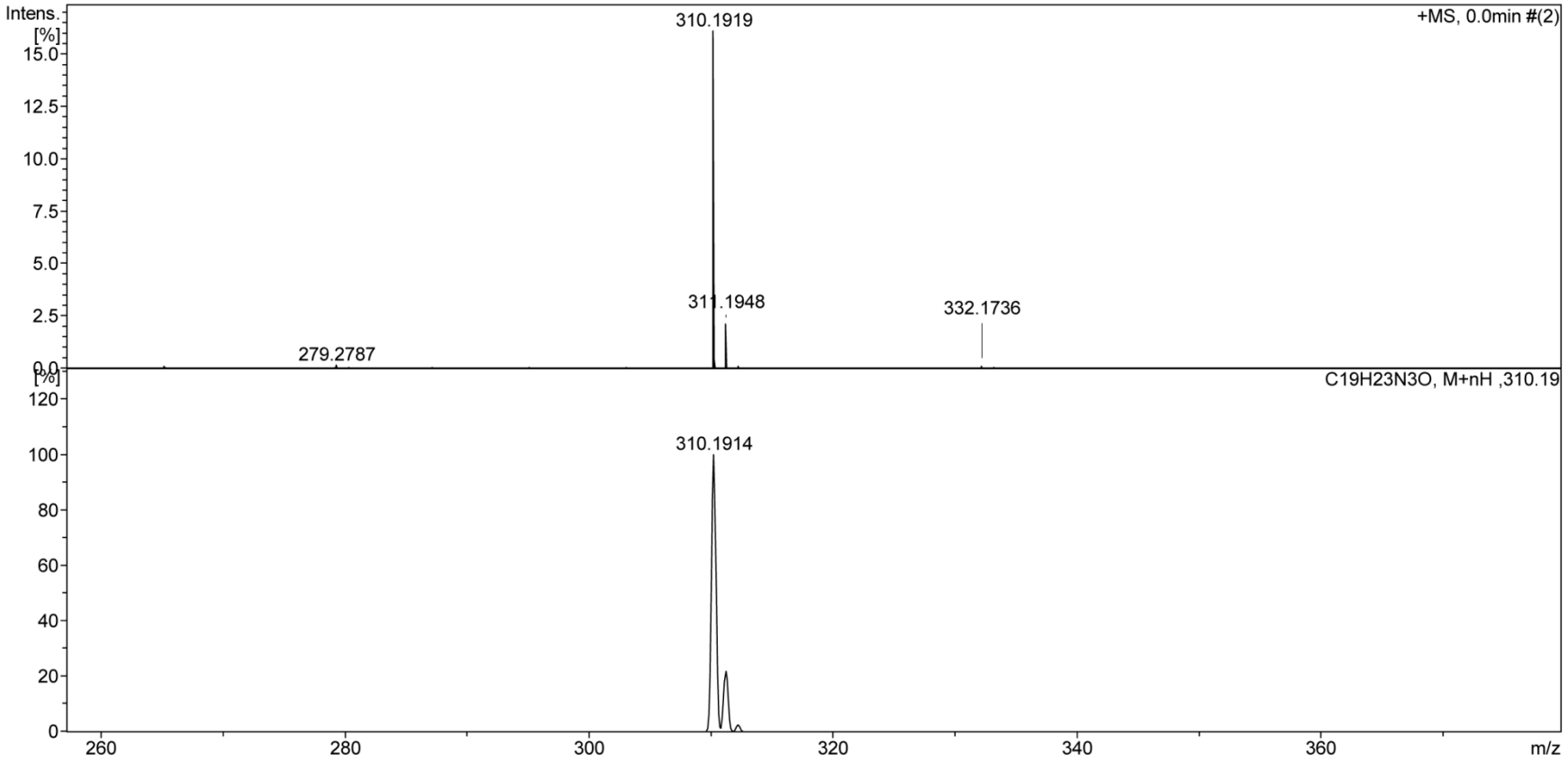
Display Report

Analysis Info

Analysis Name	D:\Data	Acquisition Date	29.07.2014 16:26:31
Method	tune_low_pos.m	Operator	BDAL@DE
Sample Name	SAS 183_F3_	Instrument	maXis 62
Comment			

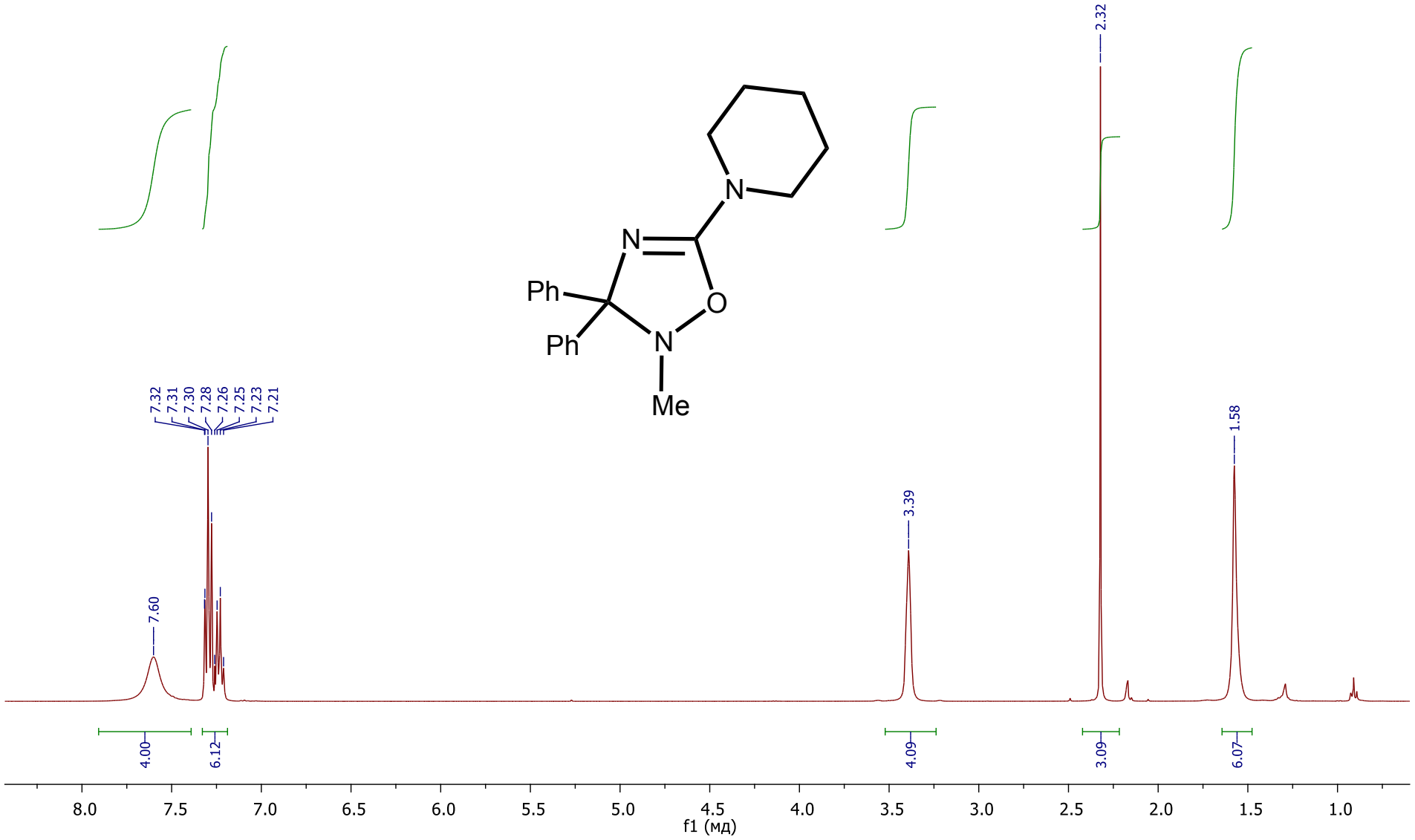
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	900 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



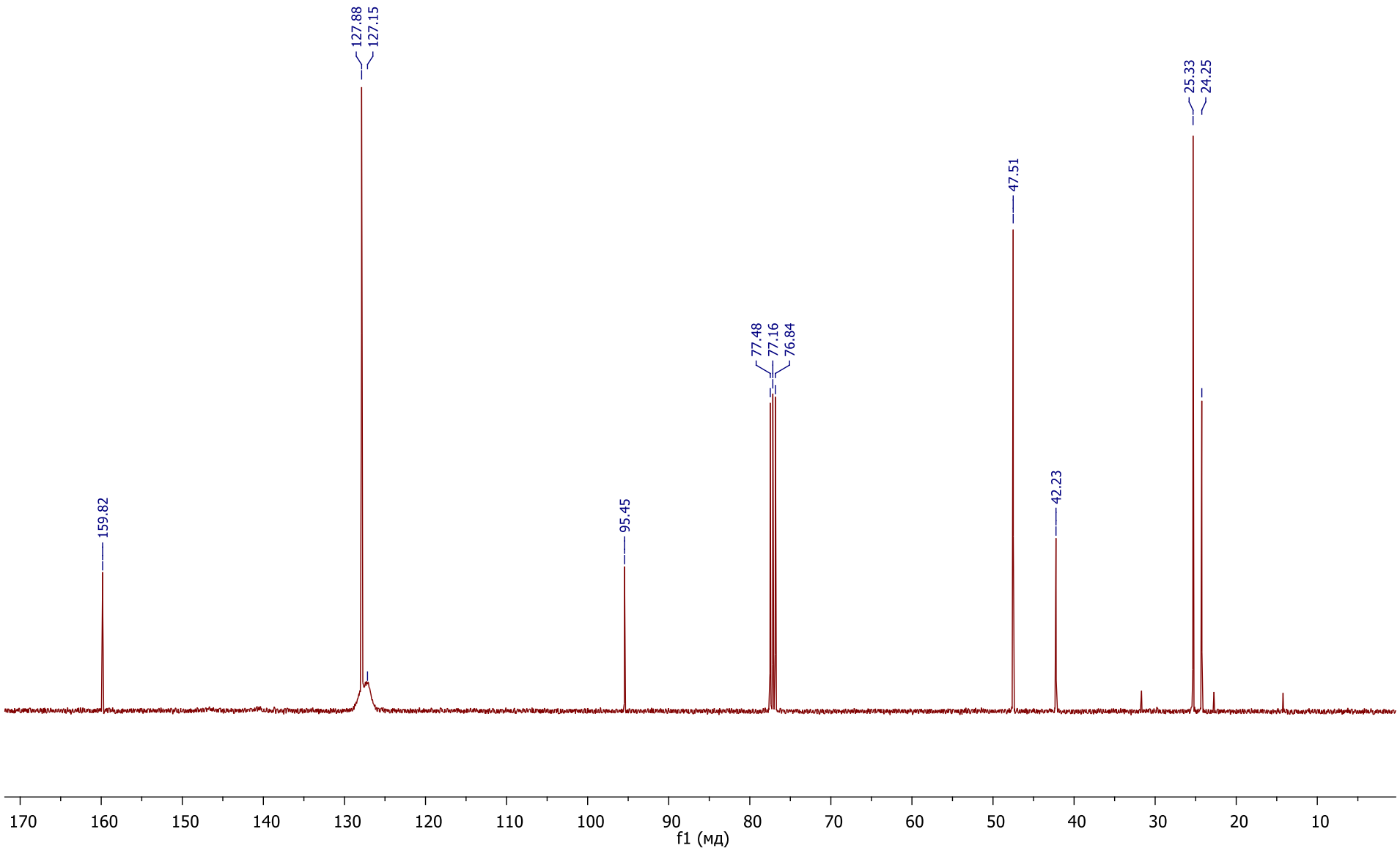
^{1}H 2-methyl-3,3-diphenyl-5-(piperidin-1-yl)-2,3-dihydro-1,2,4-oxadiazole (3ca).

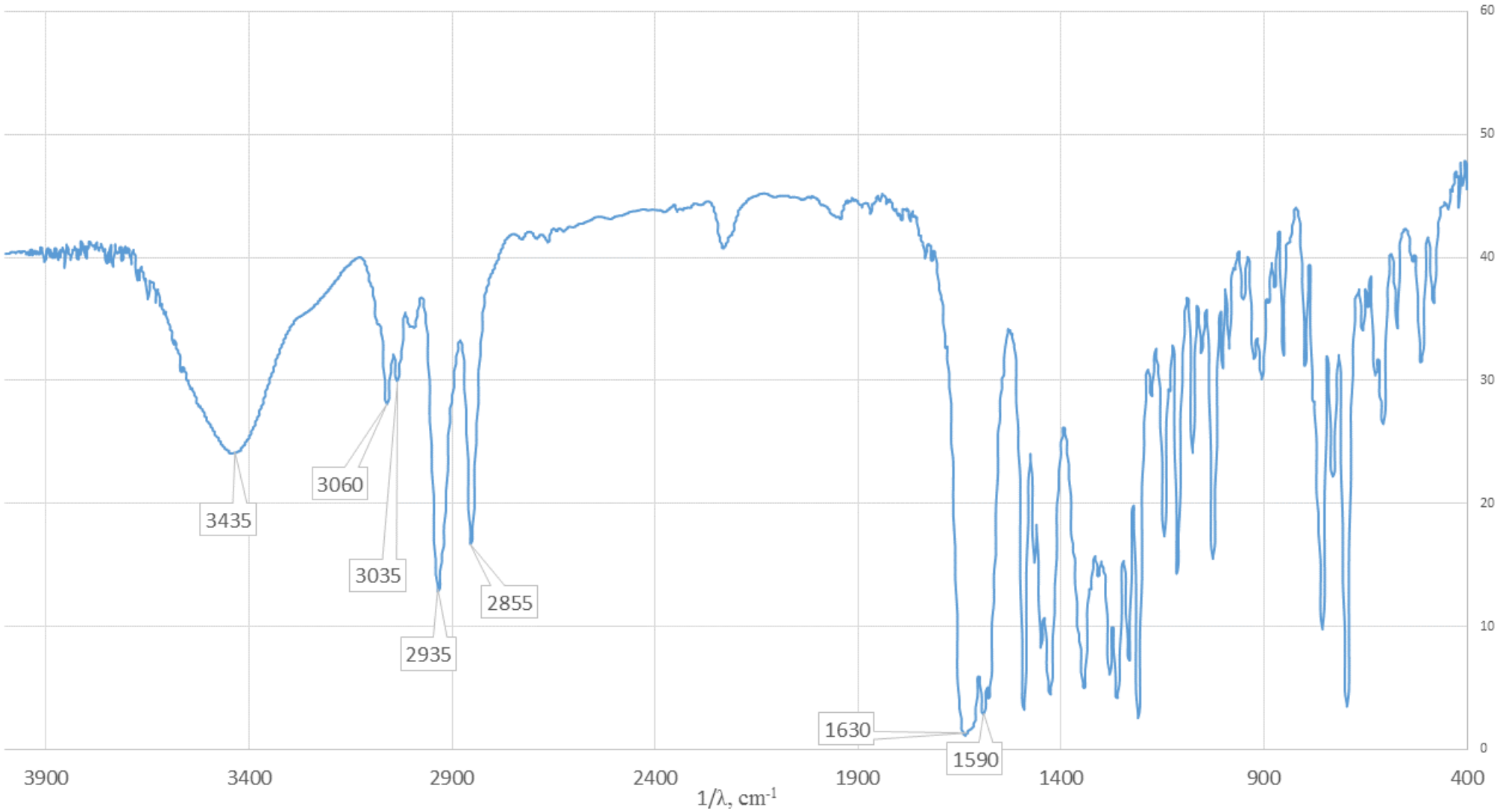
Compound8
SAS, 149, BF = 400.13 MHz, Solvent - CDCl3, 19 Jun 2014 T=298 K



^{13}C 2-methyl-3,3-diphenyl-5-(piperidin-1-yl)-2,3-dihydro-1,2,4-oxadiazole (3ca).

13C
SASc, 149, BF = 100.612769 MHz, Solvent - CDCl3, 19 Jun 2014 T=298 K




3435
3060
3035
2935
2855
1630
1590
3900
3400
2900
2400
1900
1400
900
400
1/λ, cm-1
60
50
40
30
20
10
0

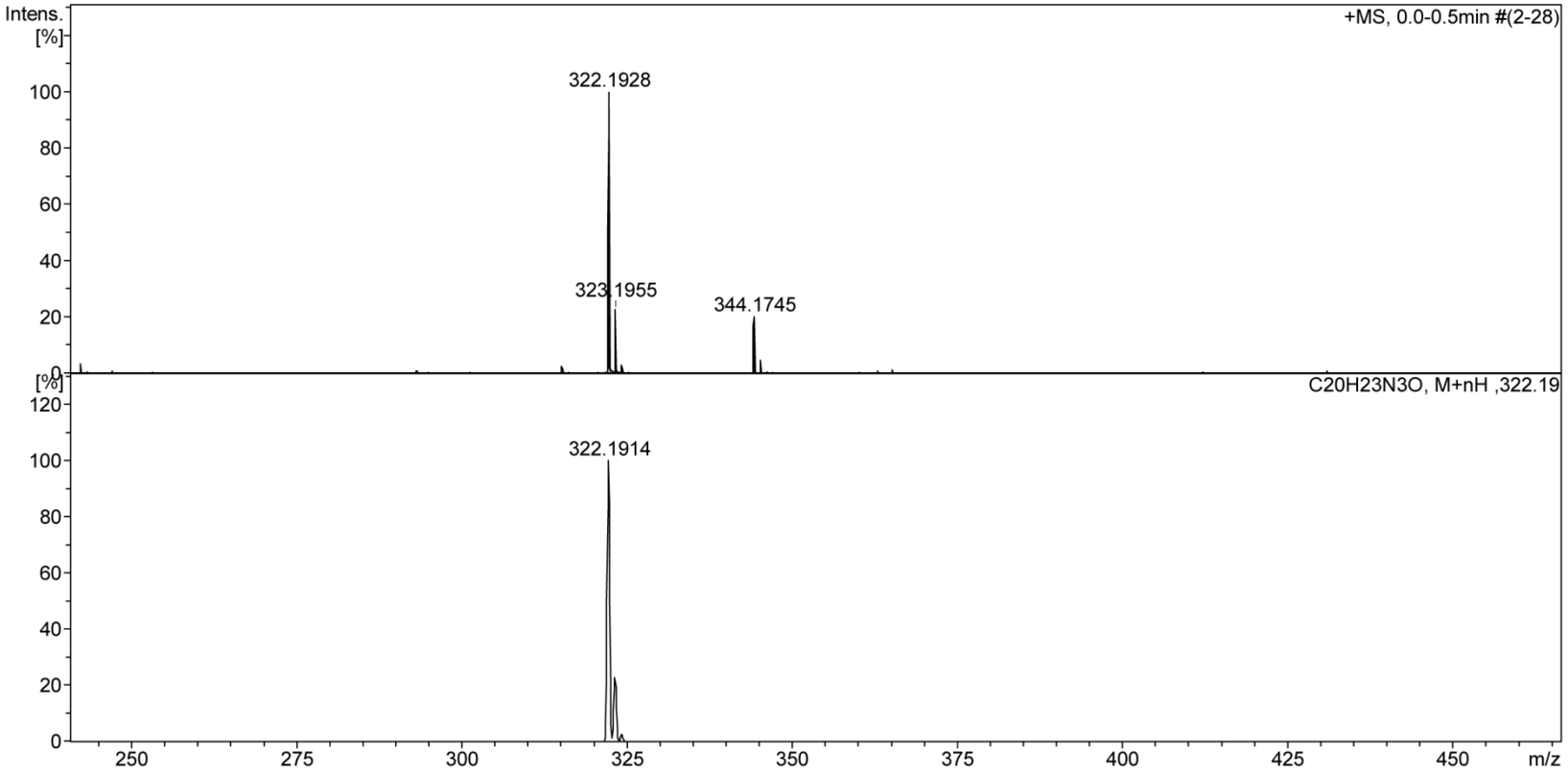
Mass Spectrum Report

Analysis Info

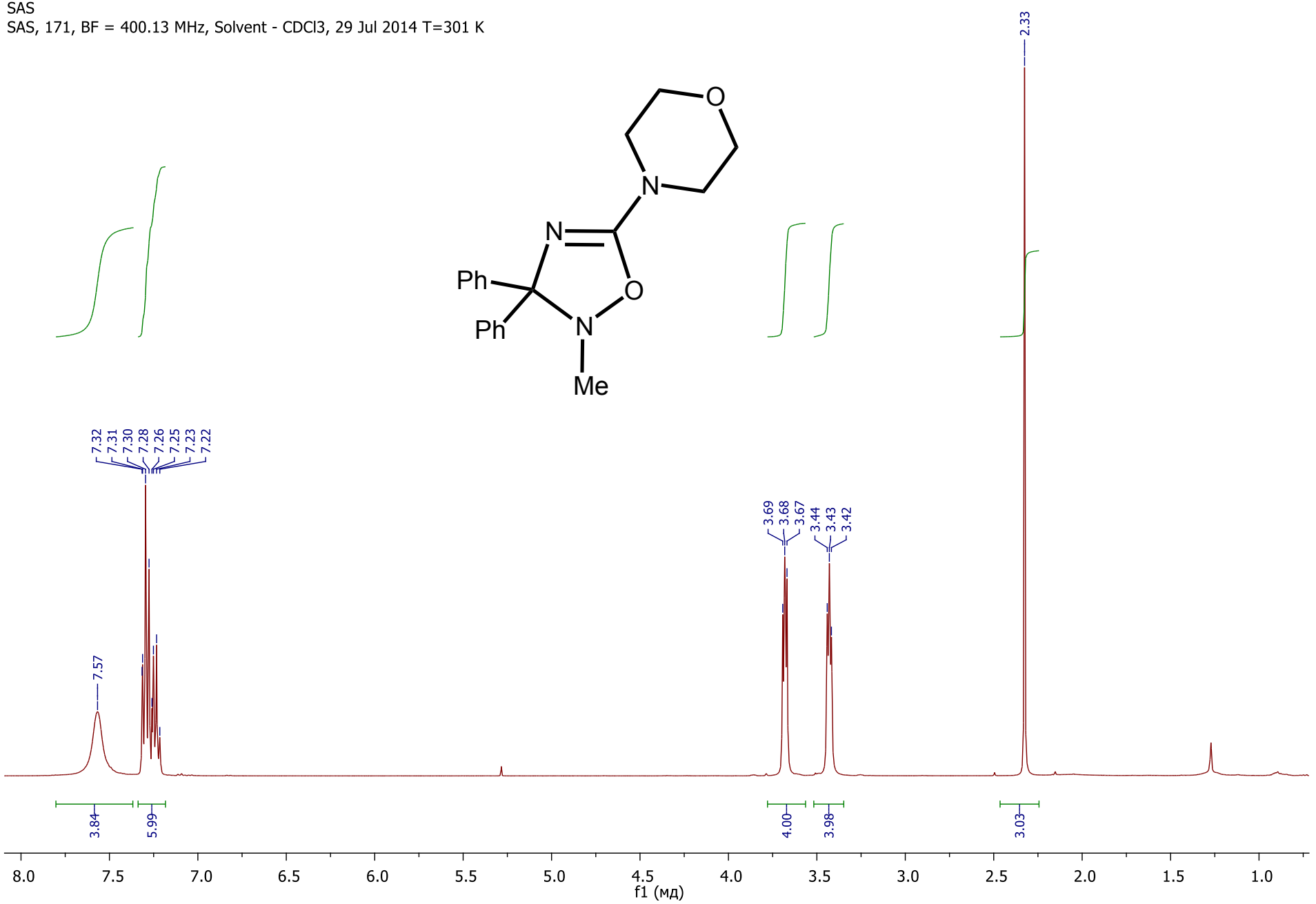
Analysis Name	D:\Data\mish2\SAS164_1.d	Acquisition Date	19.06.2014 18:04:12
Method	tune_low.m	Operator	Bruker Customer
Sample Name	SAS164_1	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

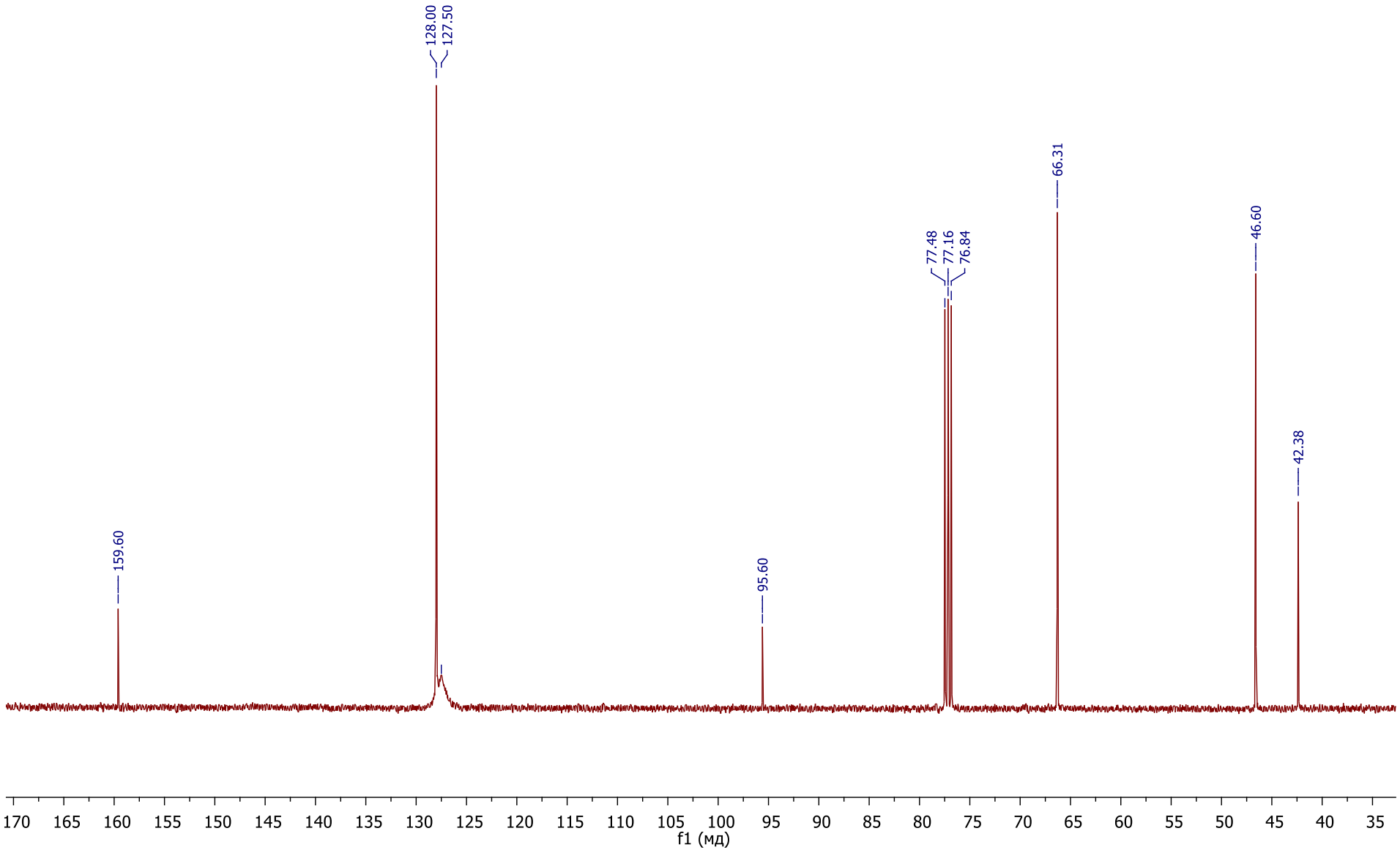


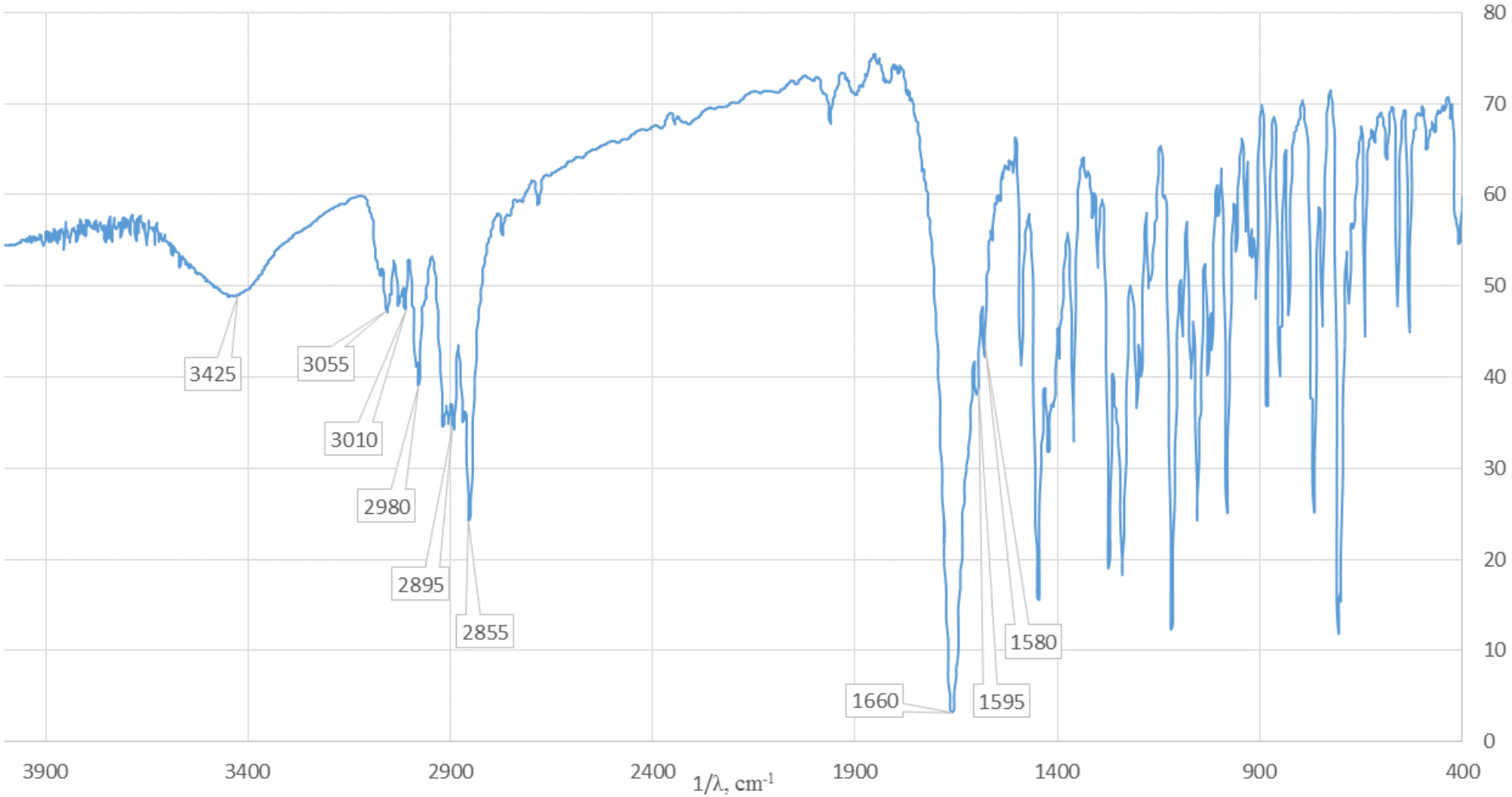
^{1}H 4-(2-methyl-3,3-diphenyl-2,3-dihydro-1,2,4-oxadiazol-5-yl)morpholine (3da).



^{13}C 4-(2-methyl-3,3-diphenyl-2,3-dihydro-1,2,4-oxadiazol-5-yl)morpholine (3da).

SASc
SASc, 171, BF = 100.612769 MHz, Solvent - CDCl3, 30 Jul 2014 T=300 K




3425
3055
3010
2980
2895
2855
1660
1595
1580
80
70
60
50
40
30
20
10
0
3900
3400
2900
2400
1900
1400
900
400
1/λ, cm-1

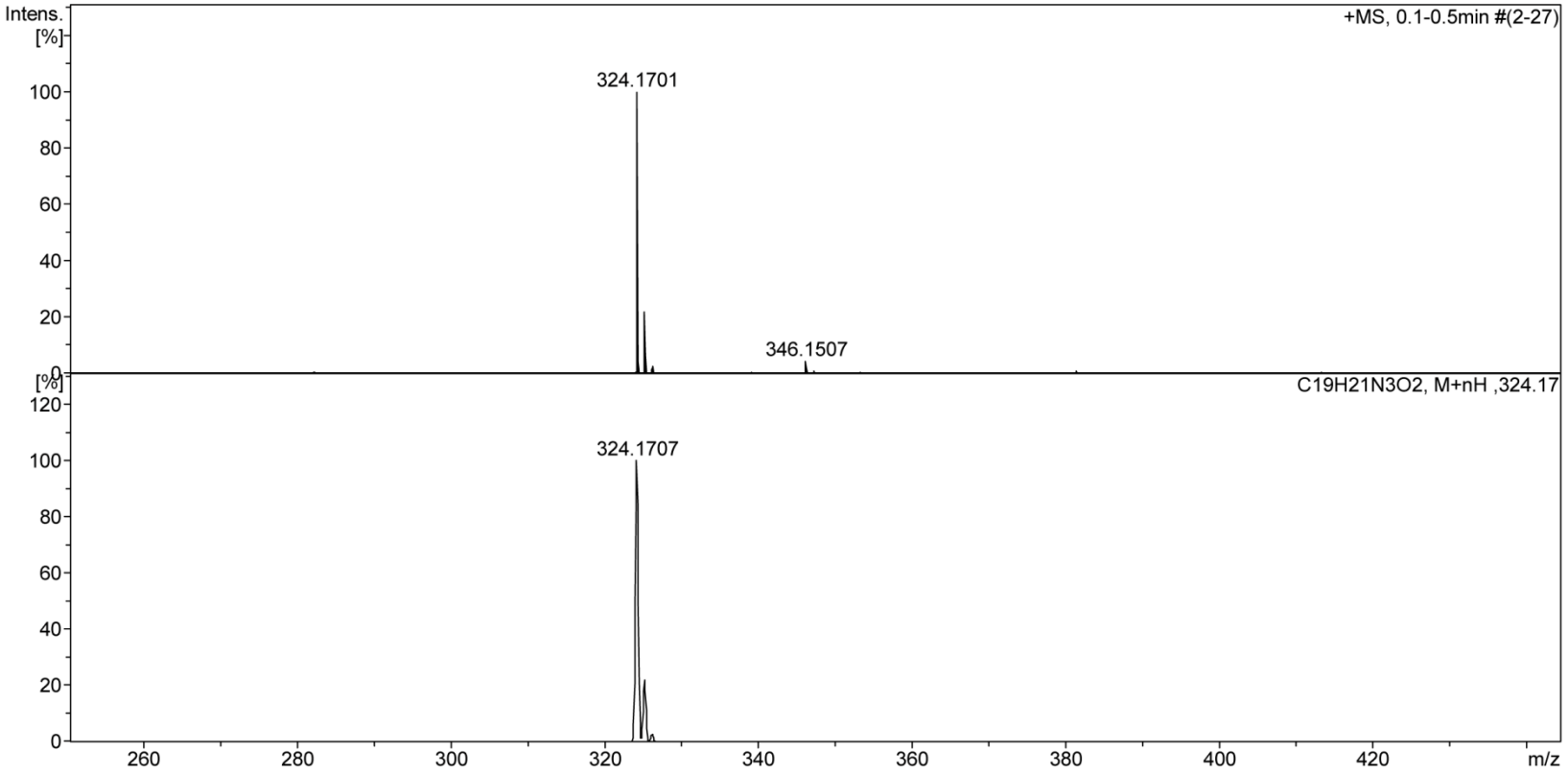
Mass Spectrum Report

Analysis Info

Analysis Name	D:\Data\June 2015\BUT9.d	Acquisition Date	03.06.2015 16:29:57
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT9	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

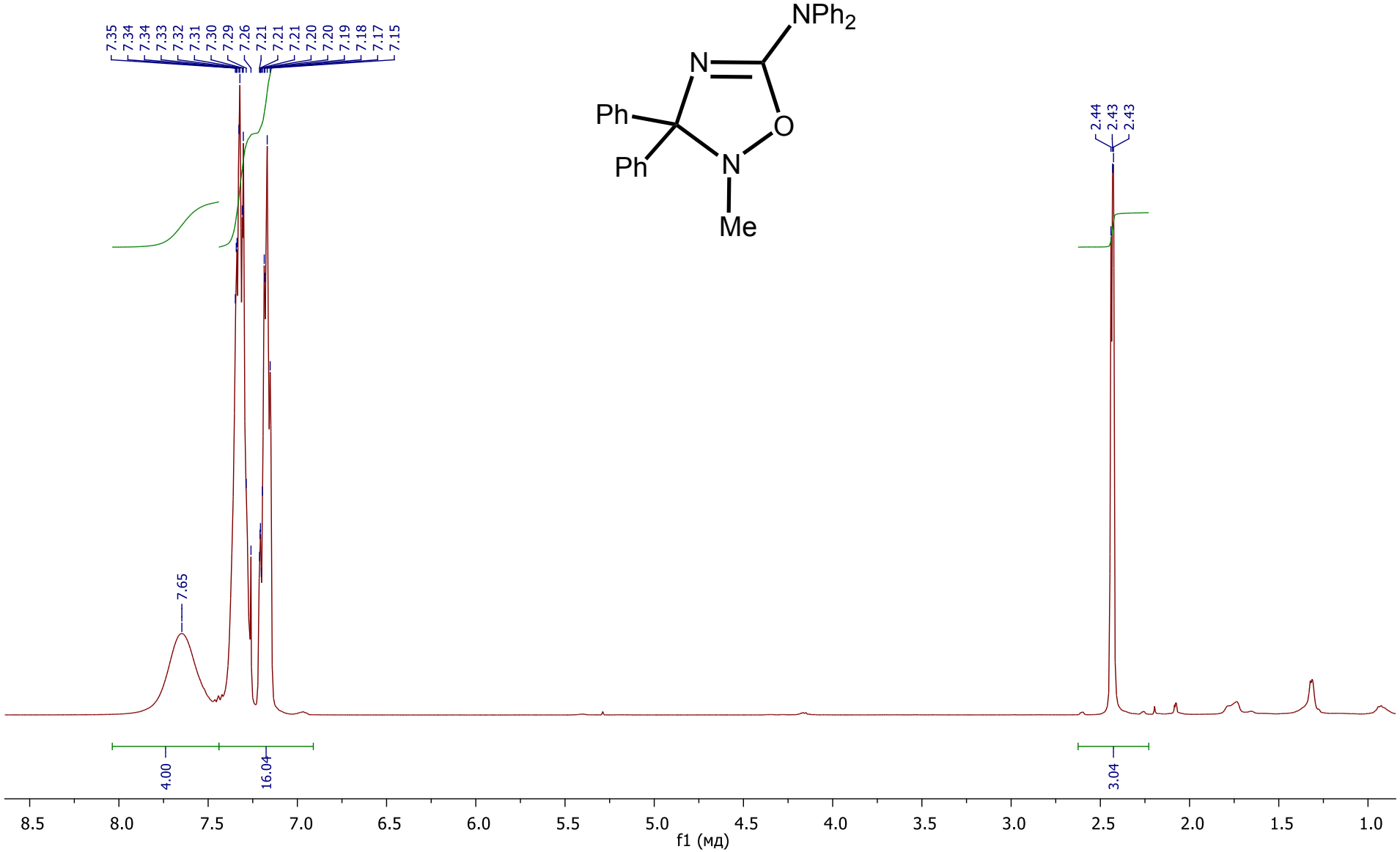
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



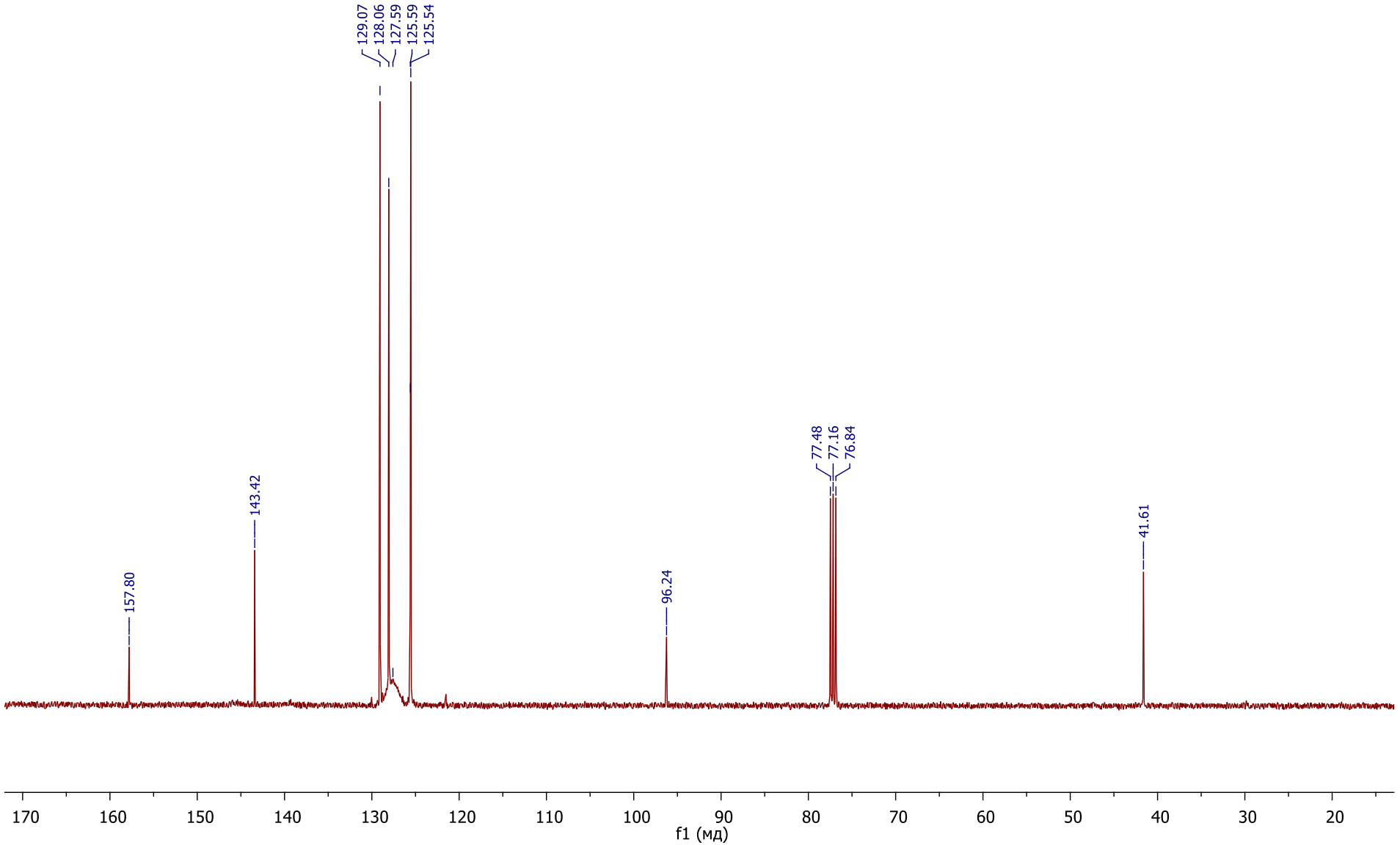
^{1}H 2-methyl-*N*,*N*,3,3-tetraphenyl-2,3-dihydro-1,2,4-oxadiazol-5-amine (3ea).

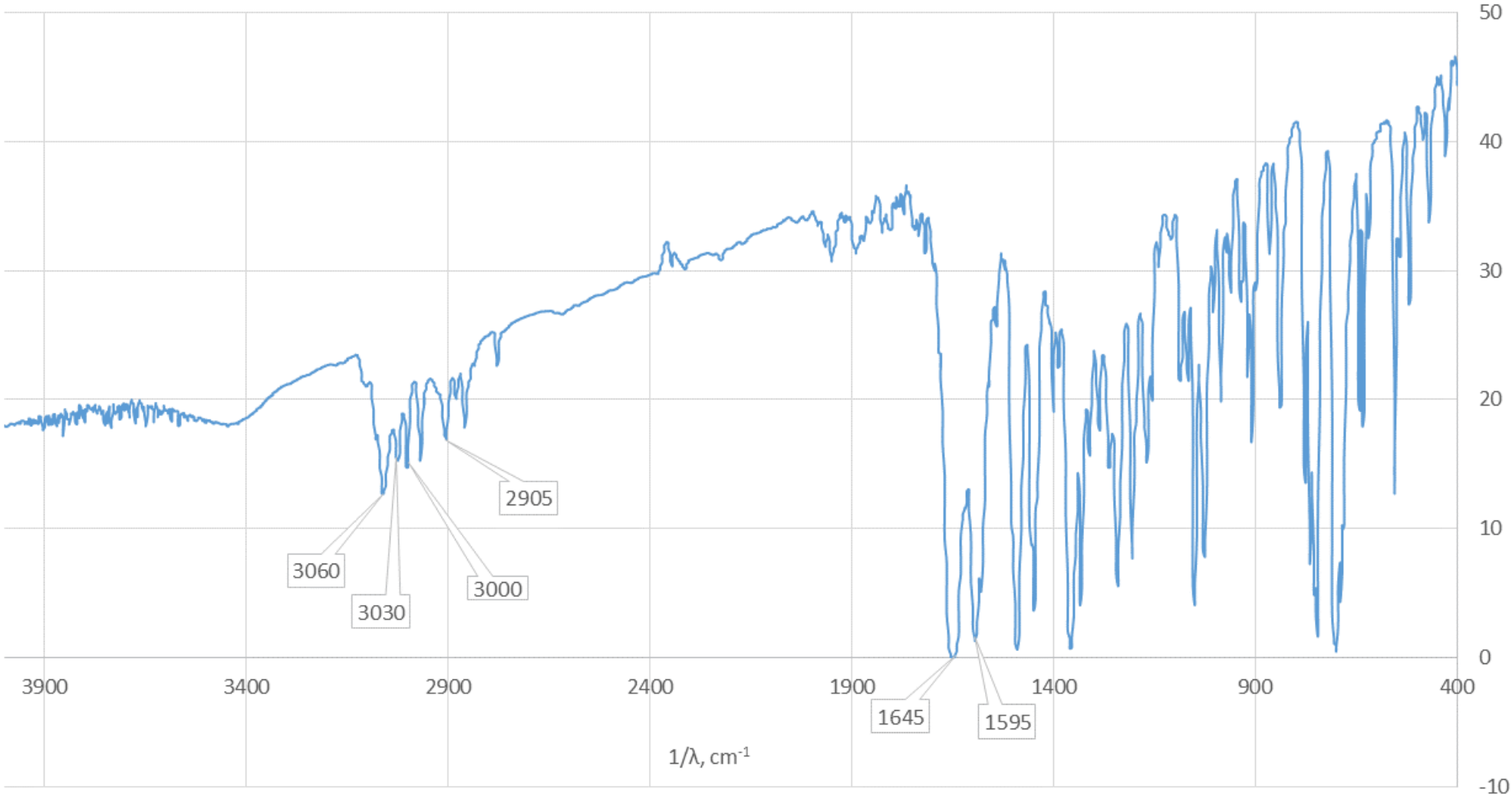
SAS
SAS, 156, BF = 400.13 MHz, Solvent - CDCl3, 30 Jun 2014 T=298 K



^{13}C 2-methyl-*N*,*N*,3,3-tetraphenyl-2,3-dihydro-1,2,4-oxadiazol-5-amine (3ea).

SASc
SASc, 156, BF = 100.612769 MHz, Solvent - CDCl3, 30 Jun 2014 T=299 K




50
40
30
20
10
0
-10
3900
3400
2900
2400
1900
1400
900
400
1/λ, cm-1
3060
3030
3000
2905
1645
1595

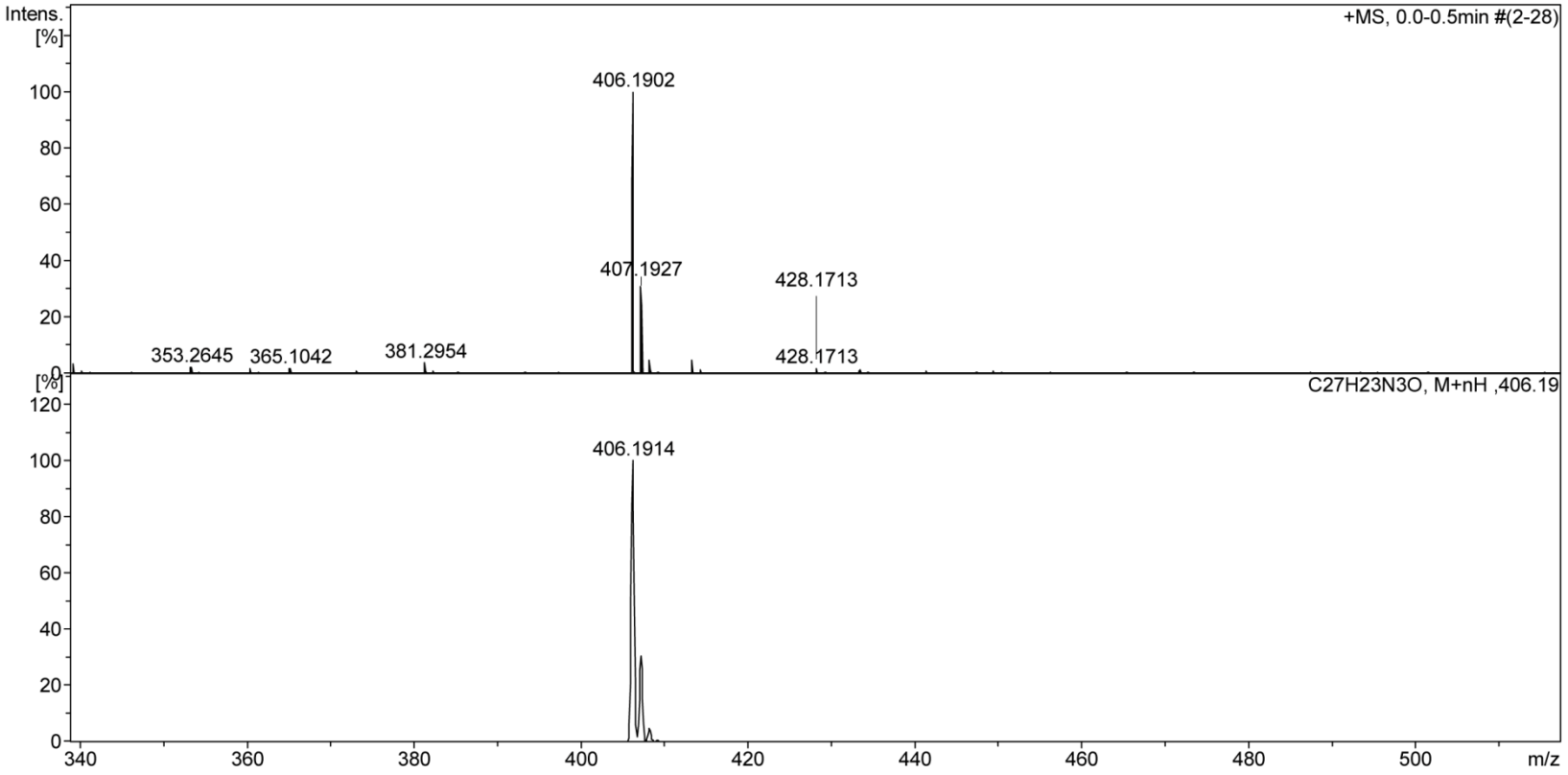
Mass Spectrum Report

Analysis Info

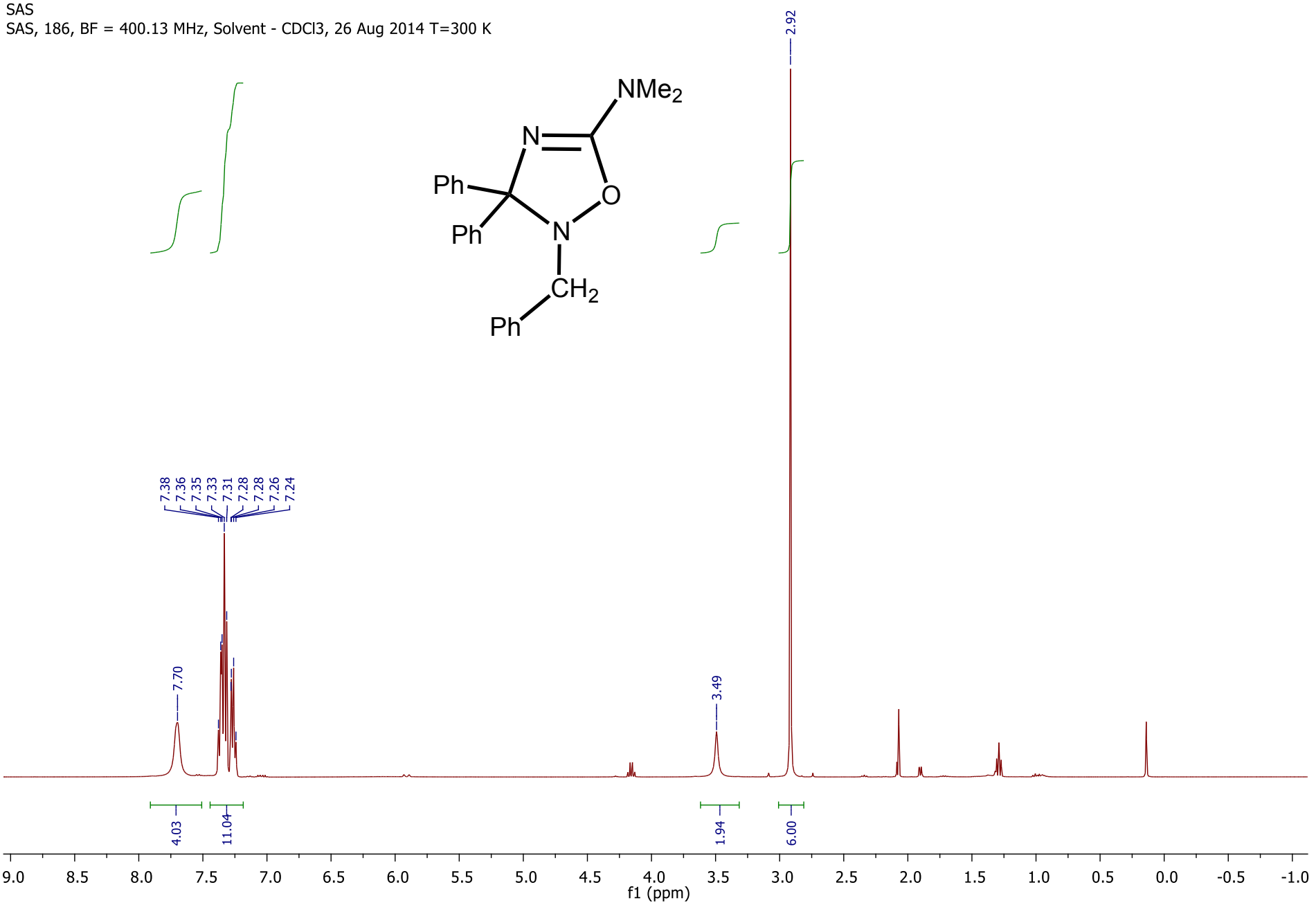
Analysis Name	D:\Data\June 2015\BUT10.d	Acquisition Date	03.06.2015 16:31:52
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT10	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

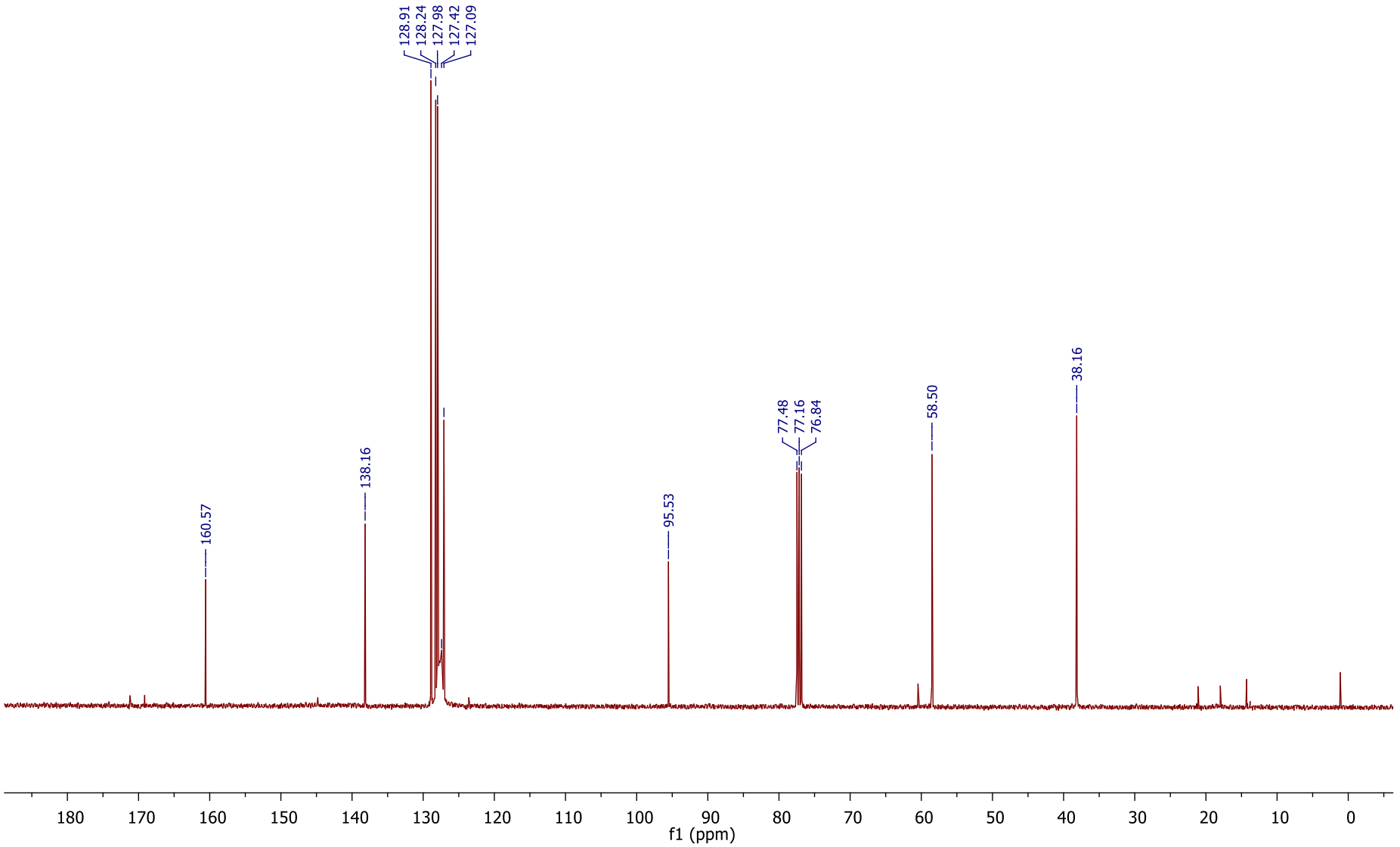


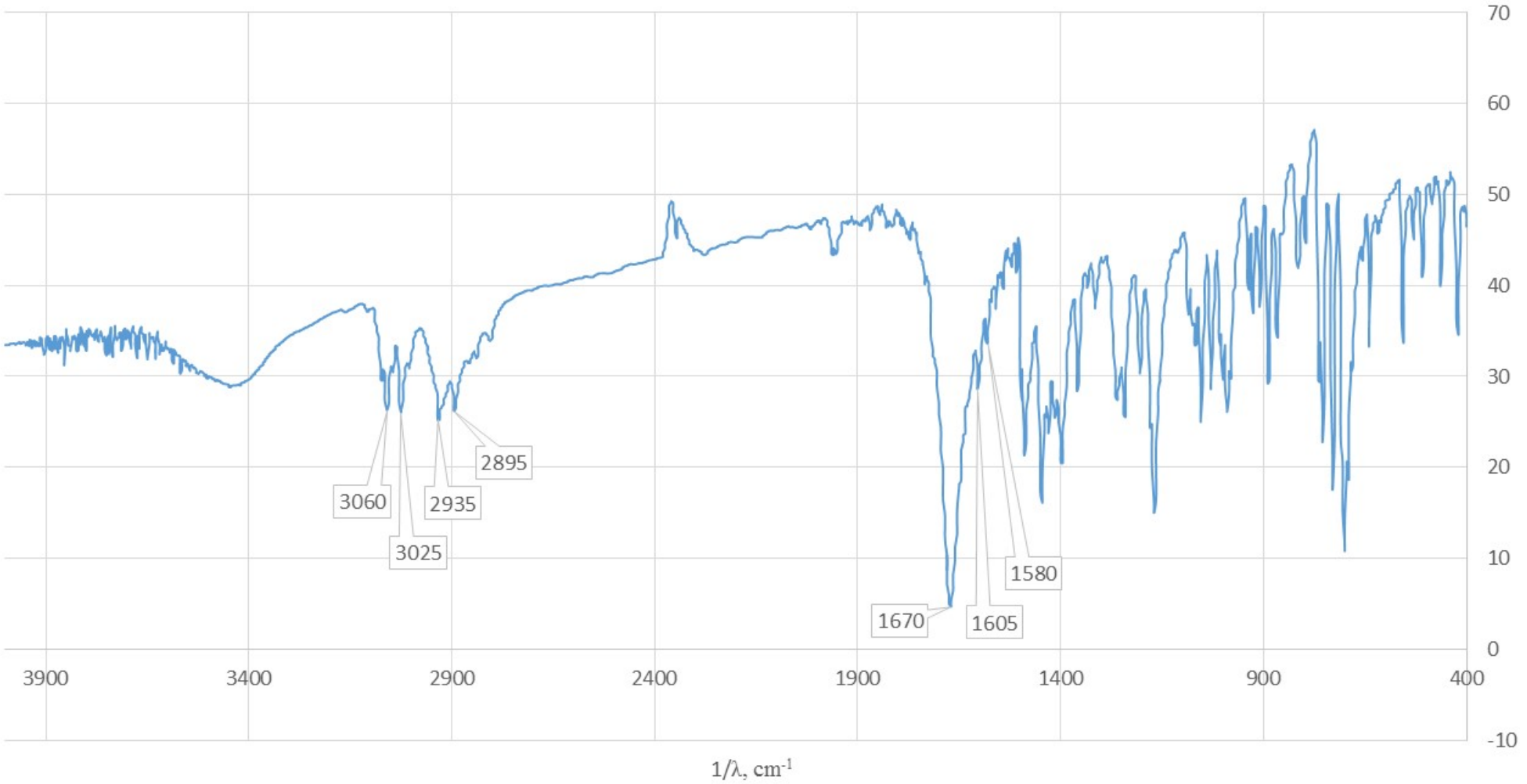
^{1}H 2-benzyl-N,N-dimethyl-3,3-diphenyl-2,3-dihydro-1,2,4-oxadiazol-5-amine (3ab)



^{13}C 2-benzyl-N,N-dimethyl-3,3-diphenyl-2,3-dihydro-1,2,4-oxadiazol-5-amine (3ab)

SASc
SASc, 186, BF = 100.612769 MHz, Solvent - CDCl3, 26 Aug 2014 T=300 K




70
60
50
40
30
20
10
0
-10
3900
3400
2900
2400
1900
1400
900
400
3060
3025
2935
2895
1670
1605
1580
1/λ, cm-1

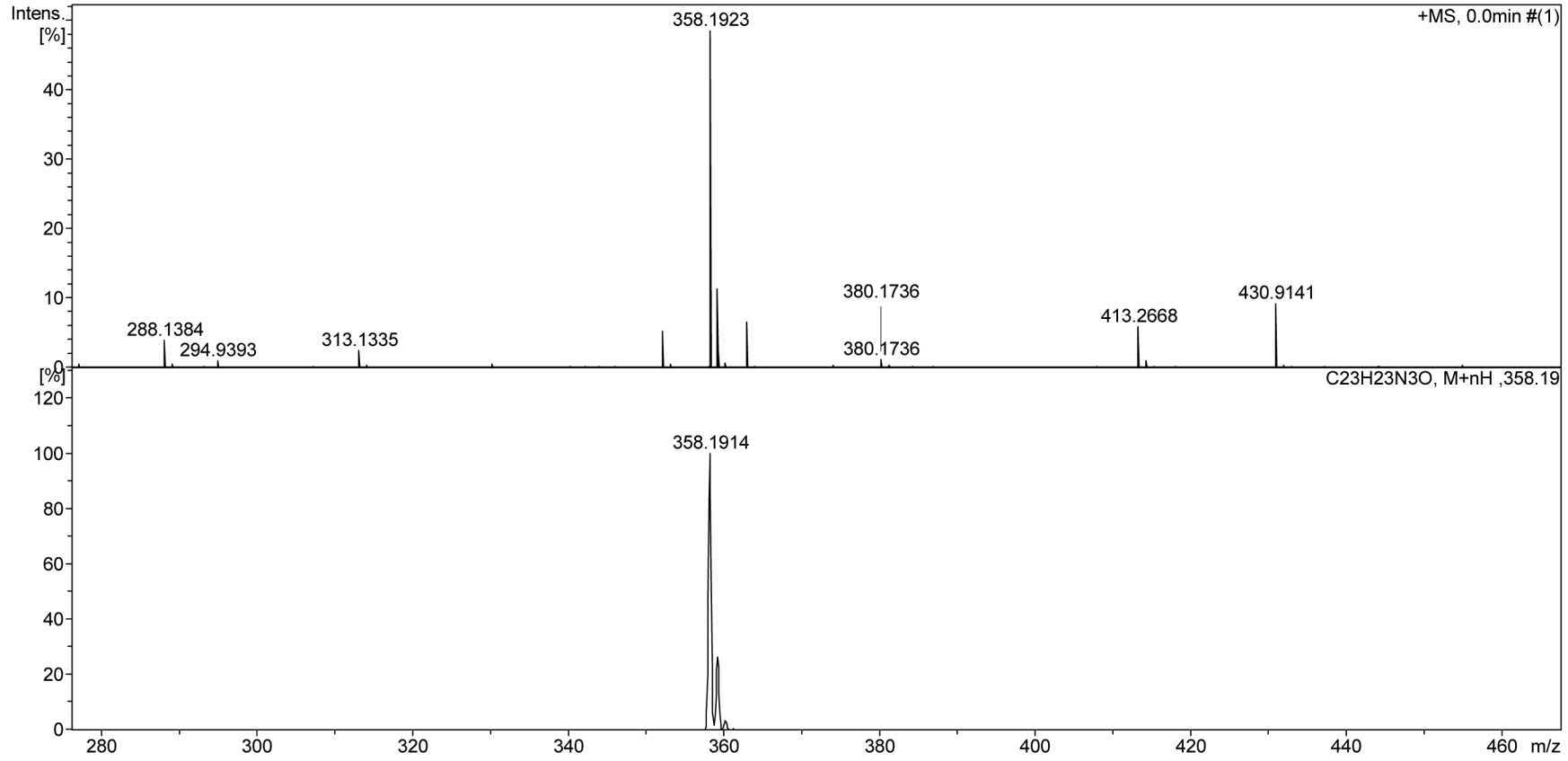
Display Report

Analysis Info

Analysis Name	C:\TEMP	Acquisition Date	28.08.2014 11:06:02
Method	tune_low_pos.m	Operator	BDAL@DE
Sample Name	SAS_210_F8_10_	Instrument	maXis 62
Comment			

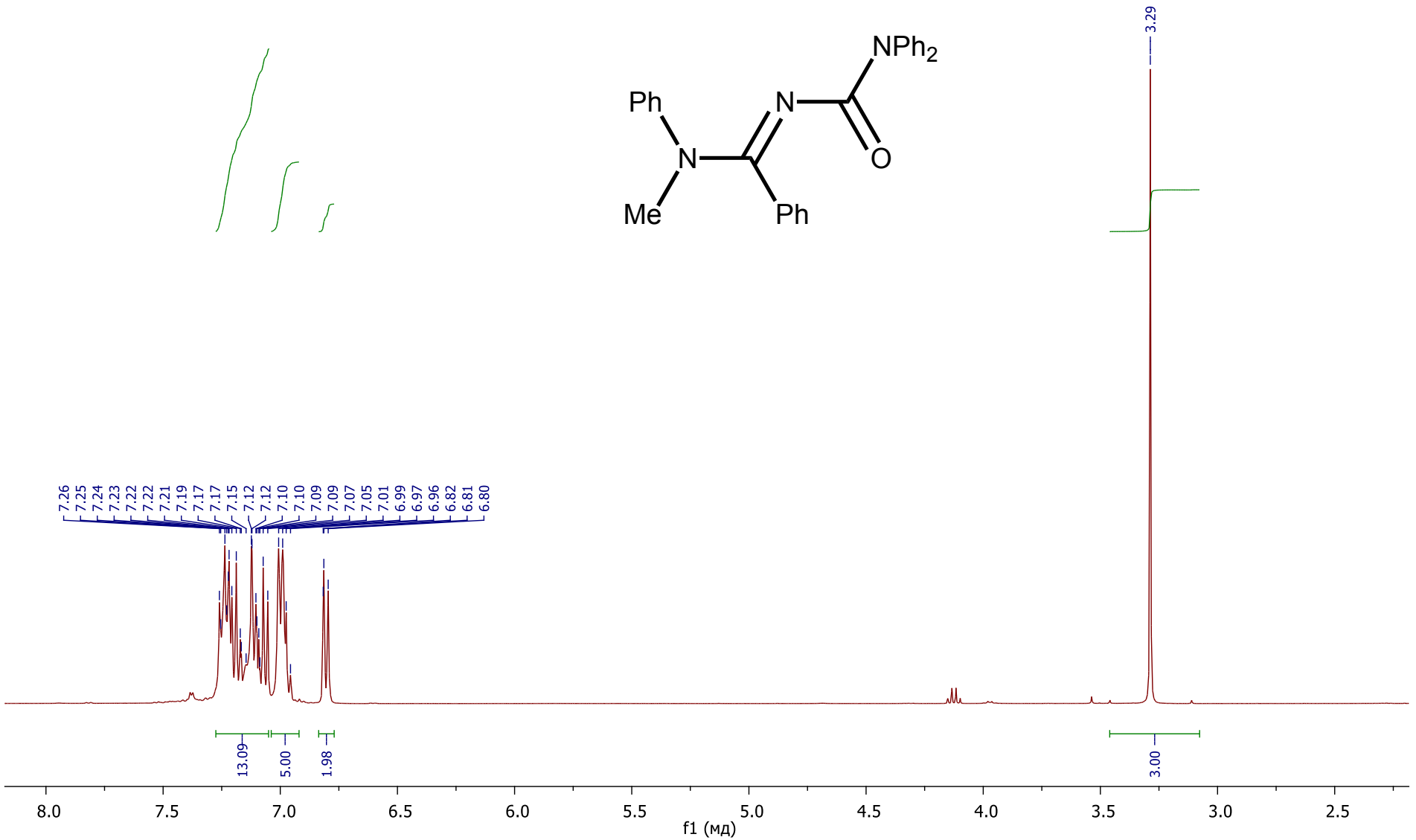
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1100 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



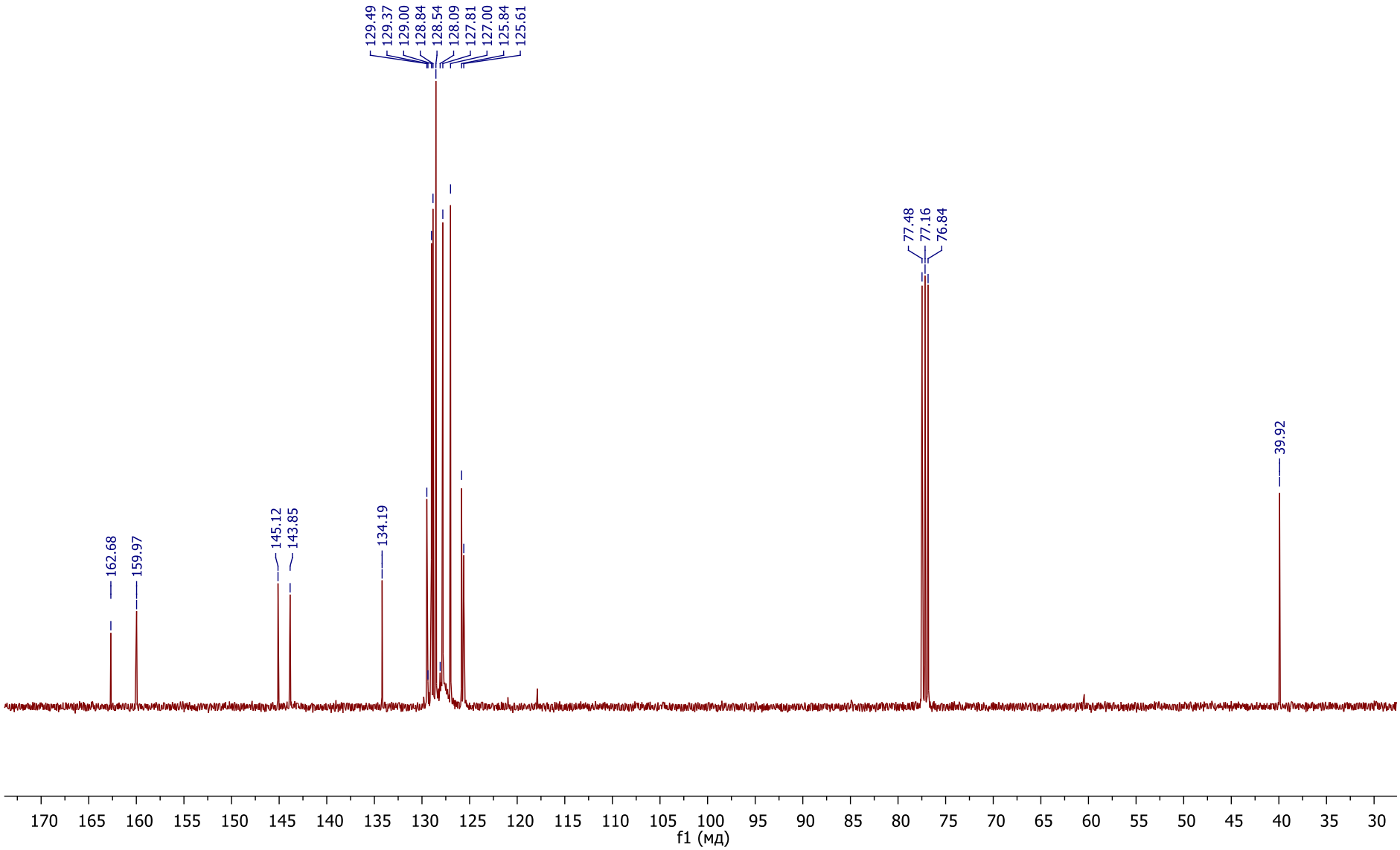
^{1}H *N′*-(diphenylcarbamoyl)-*N*-methyl-*N*-phenylbenzimidamide (4ea).

BUT
BUT, 208, BF = 400.13 MHz, Solvent - CDCl3, 29 Jan 2015 T=296 K

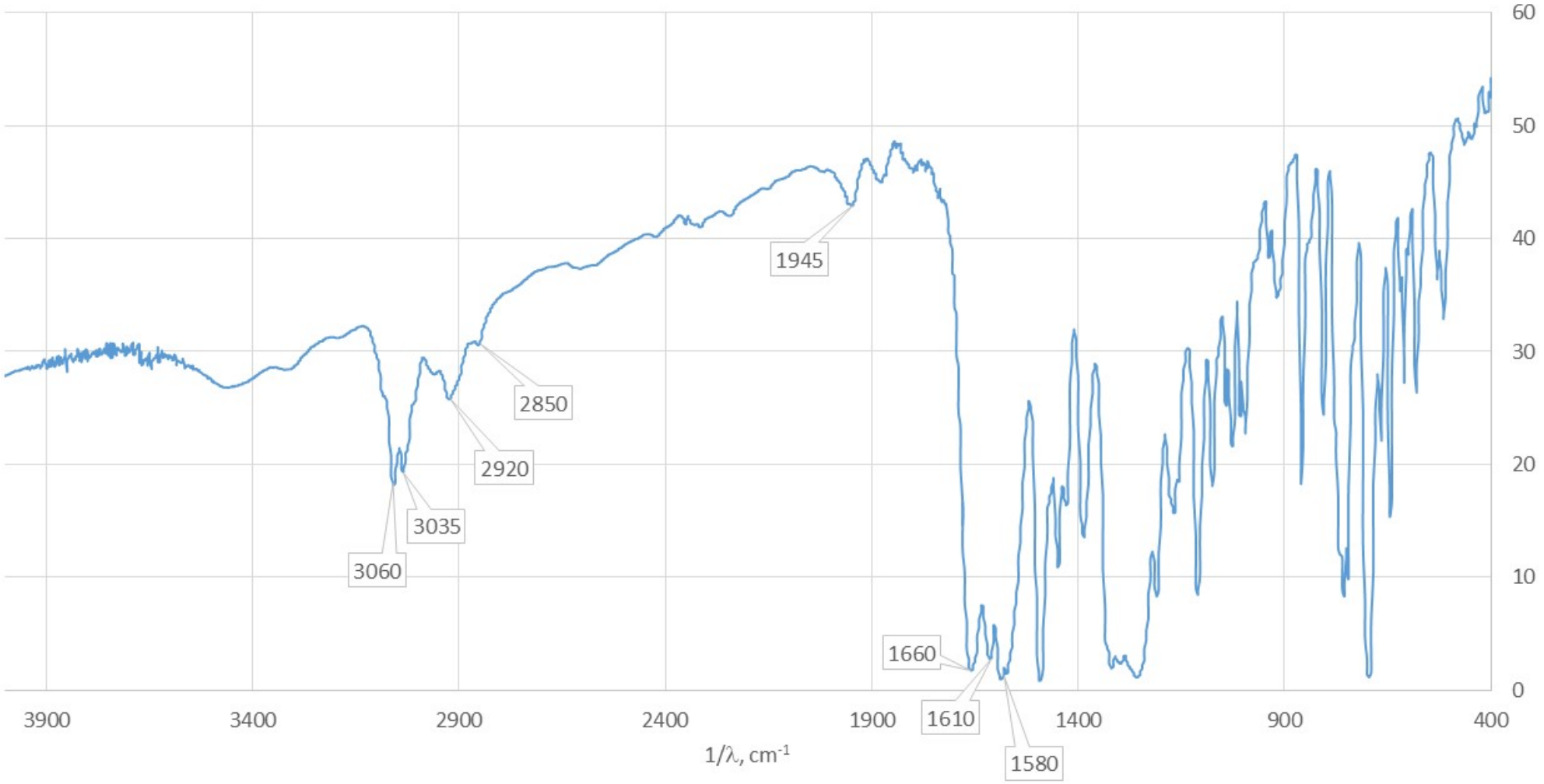


^{13}C *N′*-(diphenylcarbamoyl)-*N*-methyl-*N*-phenylbenzimidamide (4ea).

BUTc
BUTc, 208, BF = 100.612769 MHz, Solvent - CDCl3, 29 Jan 2015 T=296 K



10a

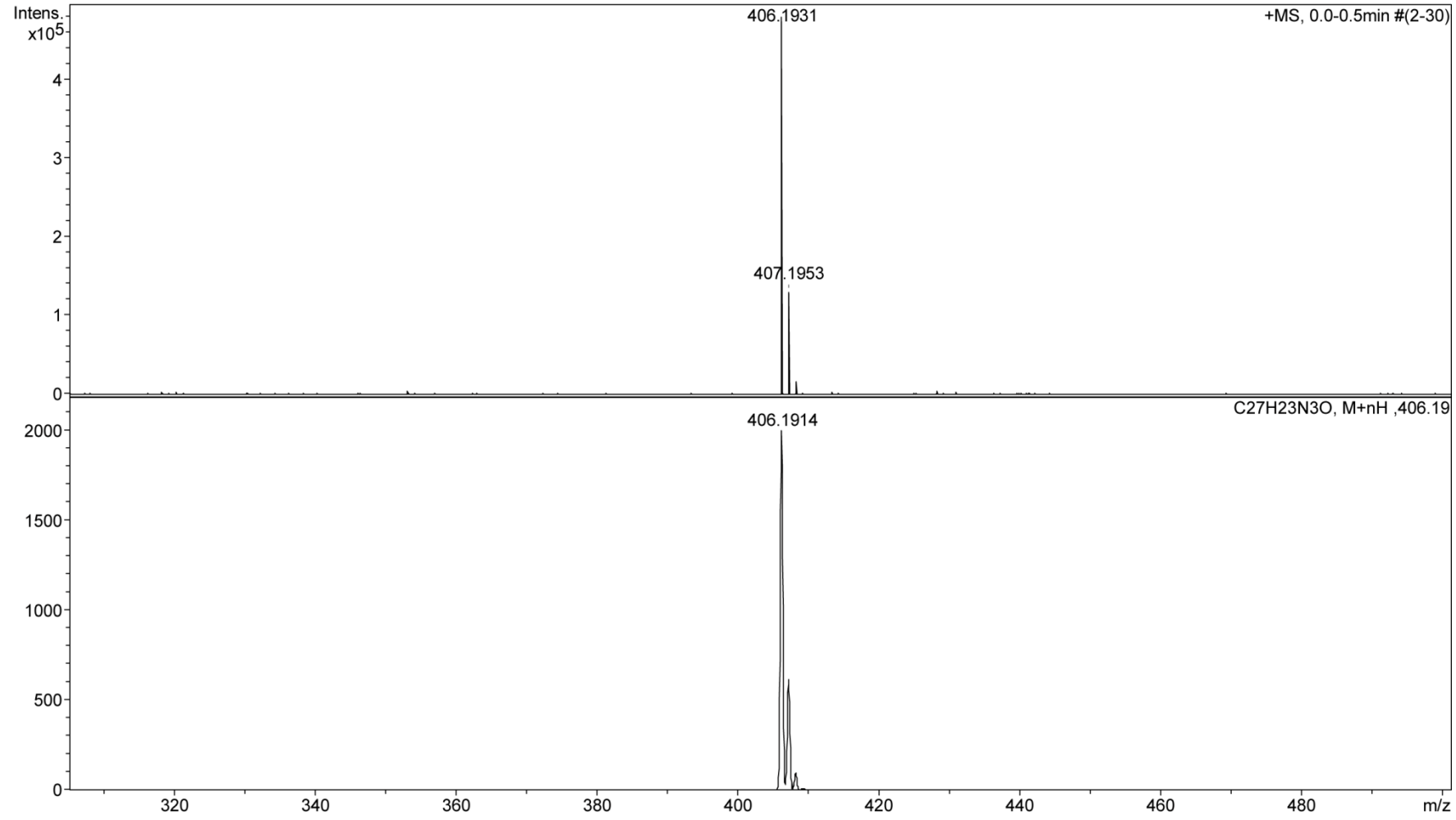

60
50
40
30
20
10
0
3900
3400
2900
2400
1900
1400
900
400
1/λ, cm-1
1945
2850
2920
3035
3060
1660
1610
1580

Analysis Info

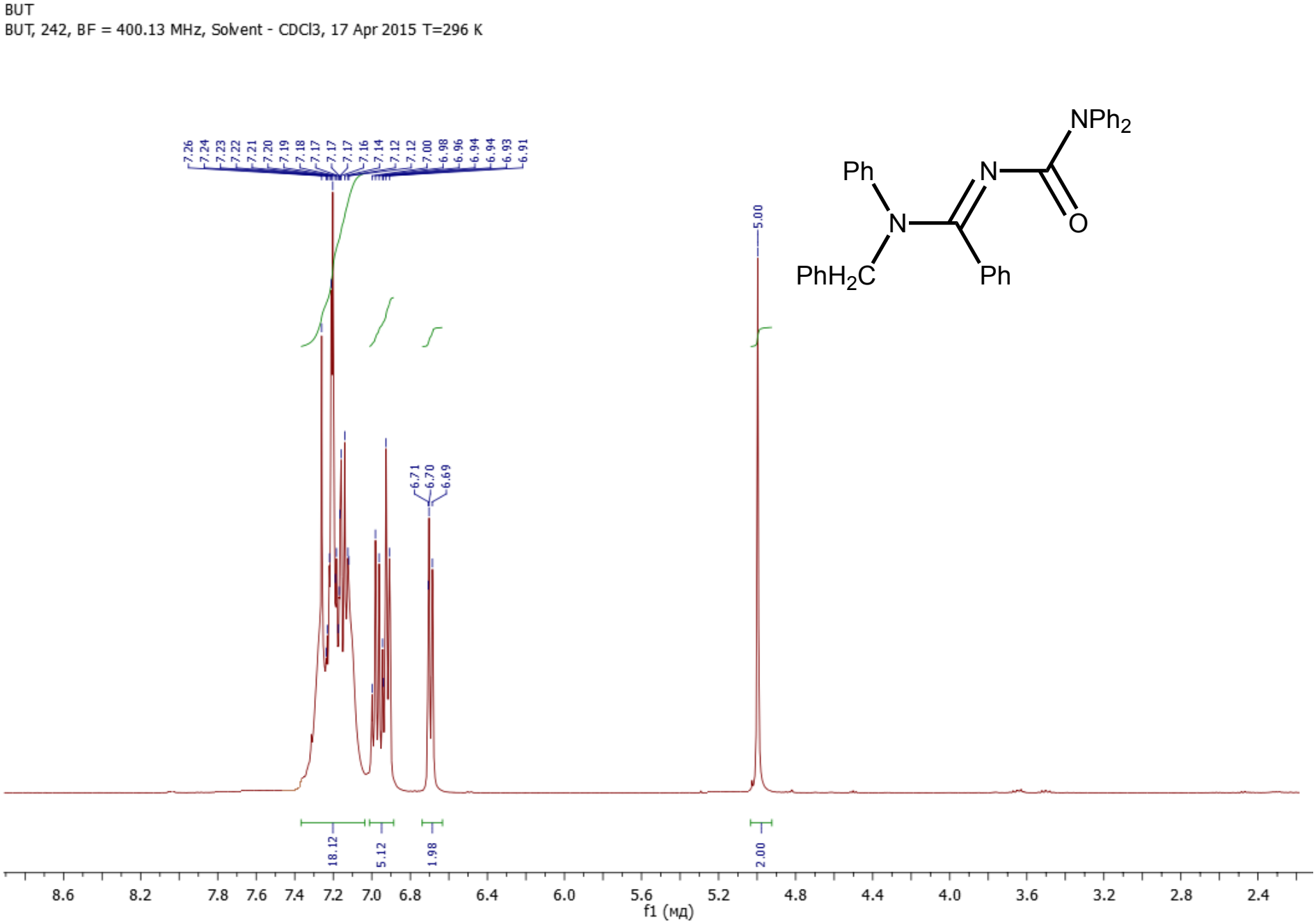
Analysis Name	D:\Data\Work\2015\january\29\BUT226_10000001.d	Acquisition Date	1/29/2015 12:17:01 PM
Method	tune_low_pos.m	Operator	BDAL@DE
Sample Name	BUT226_10	Instrument	maXis 62
Comment	MeOH		

Acquisition Parameter

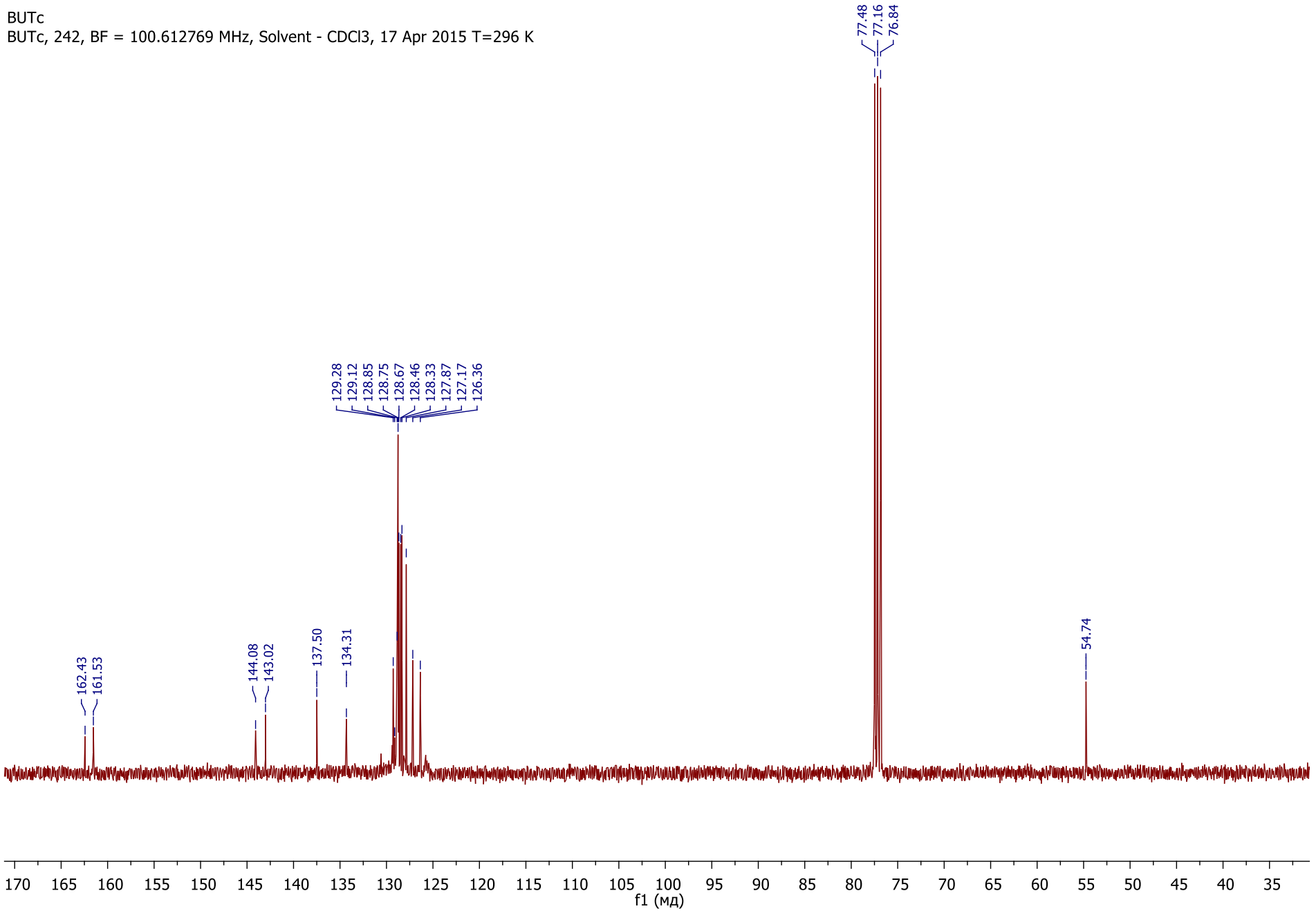
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1100 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

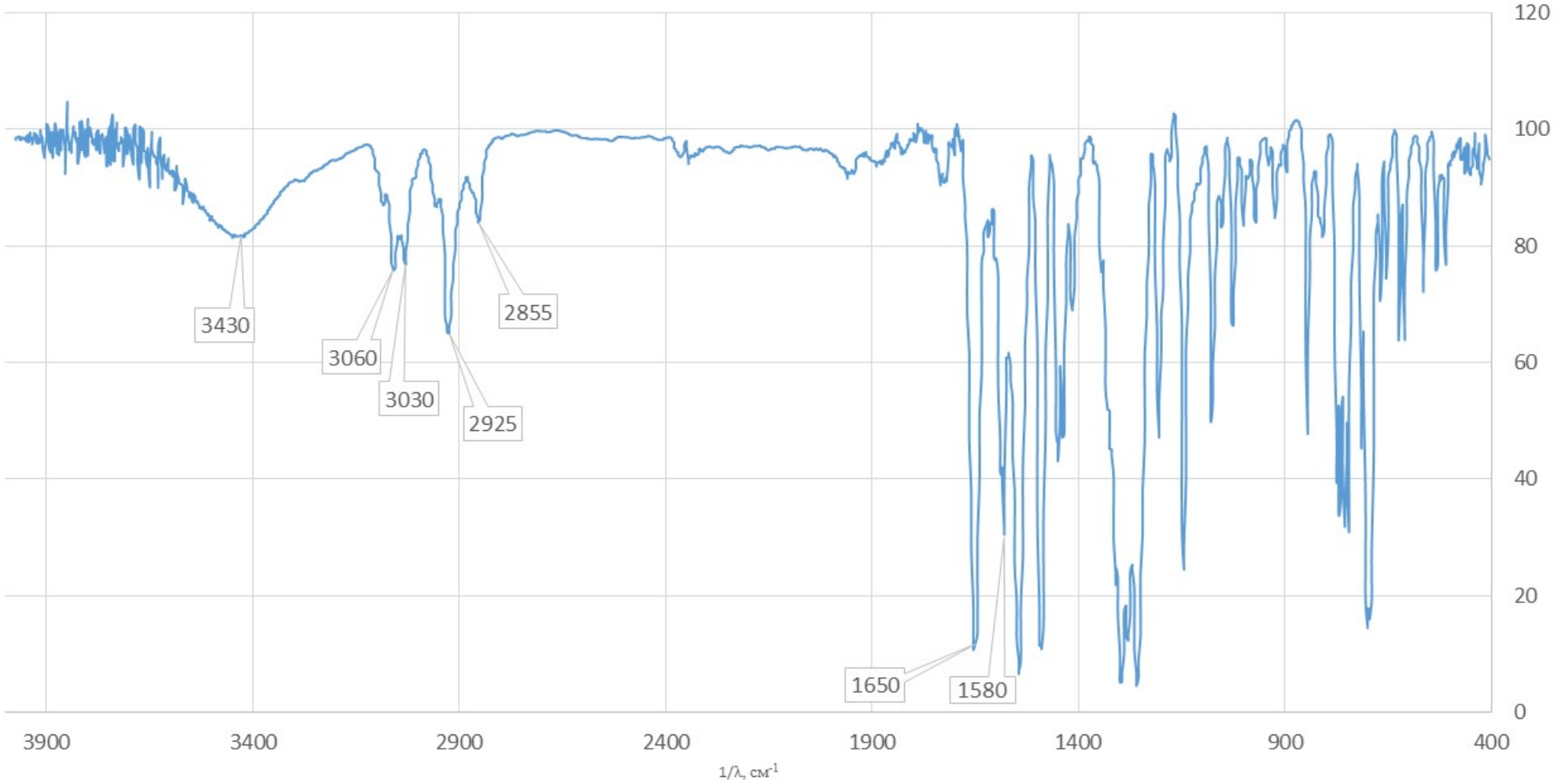


^{1}H *N*-benzyl-*N′*-(diphenylcarbamoyl)-*N*-phenylbenzimidamide (4eb).



^{13}C *N*-benzyl-*N′*-(diphenylcarbamoyl)-*N*-phenylbenzimidamide (4eb).




120
100
80
60
40
20
0
3900
3400
2900
2400
1900
1400
900
400
1/λ, см-1
3430
3060
3030
2925
2855
1650
1580

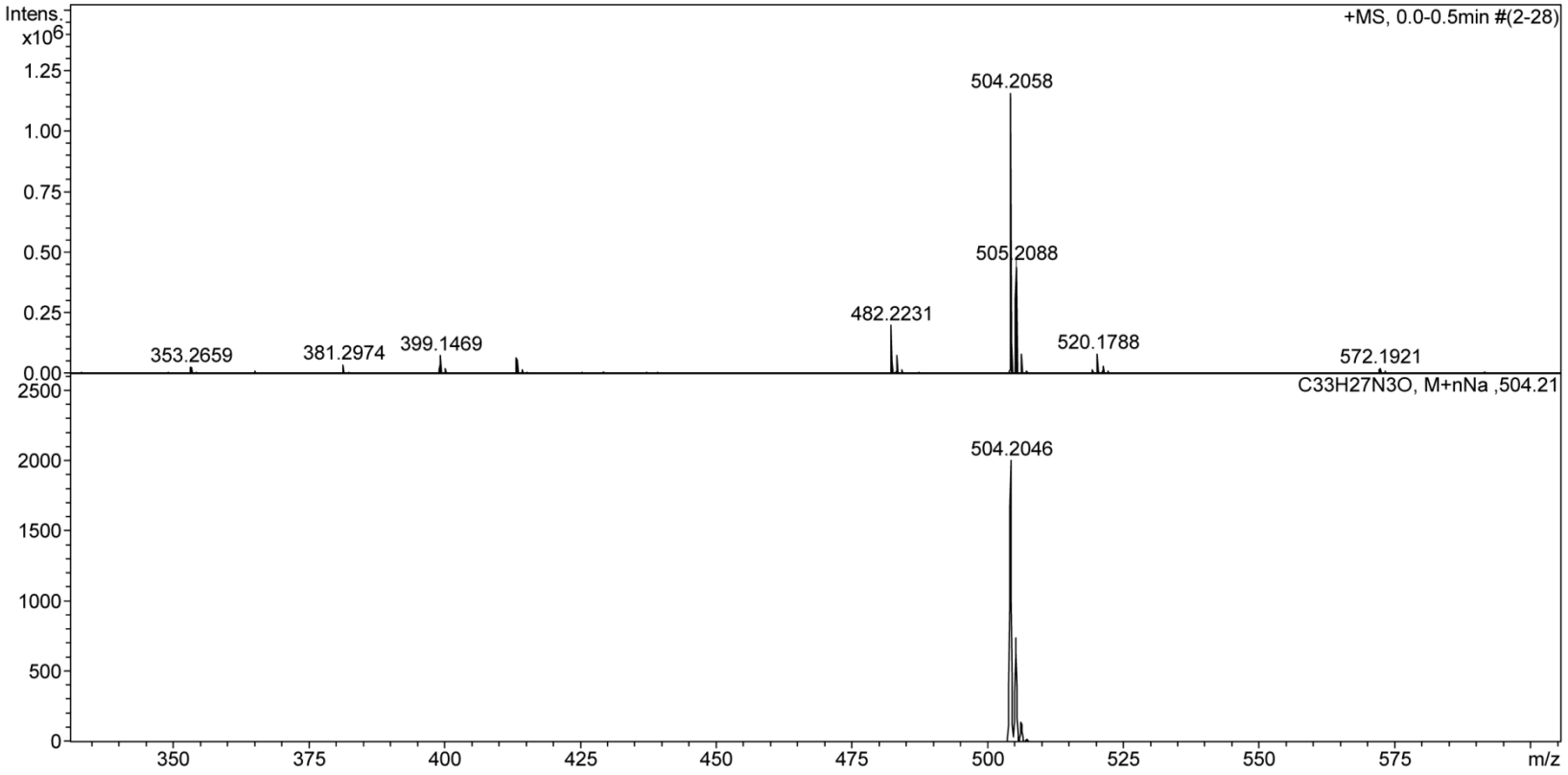
Mass Spectrum Report

Analysis Info

Analysis Name	D:\Data\april2015\BUT253_10.d	Acquisition Date	17.04.2015 17:27:39
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT253_10	Instrument / Ser#	micrOTOF 10223
Comment	MeOH		

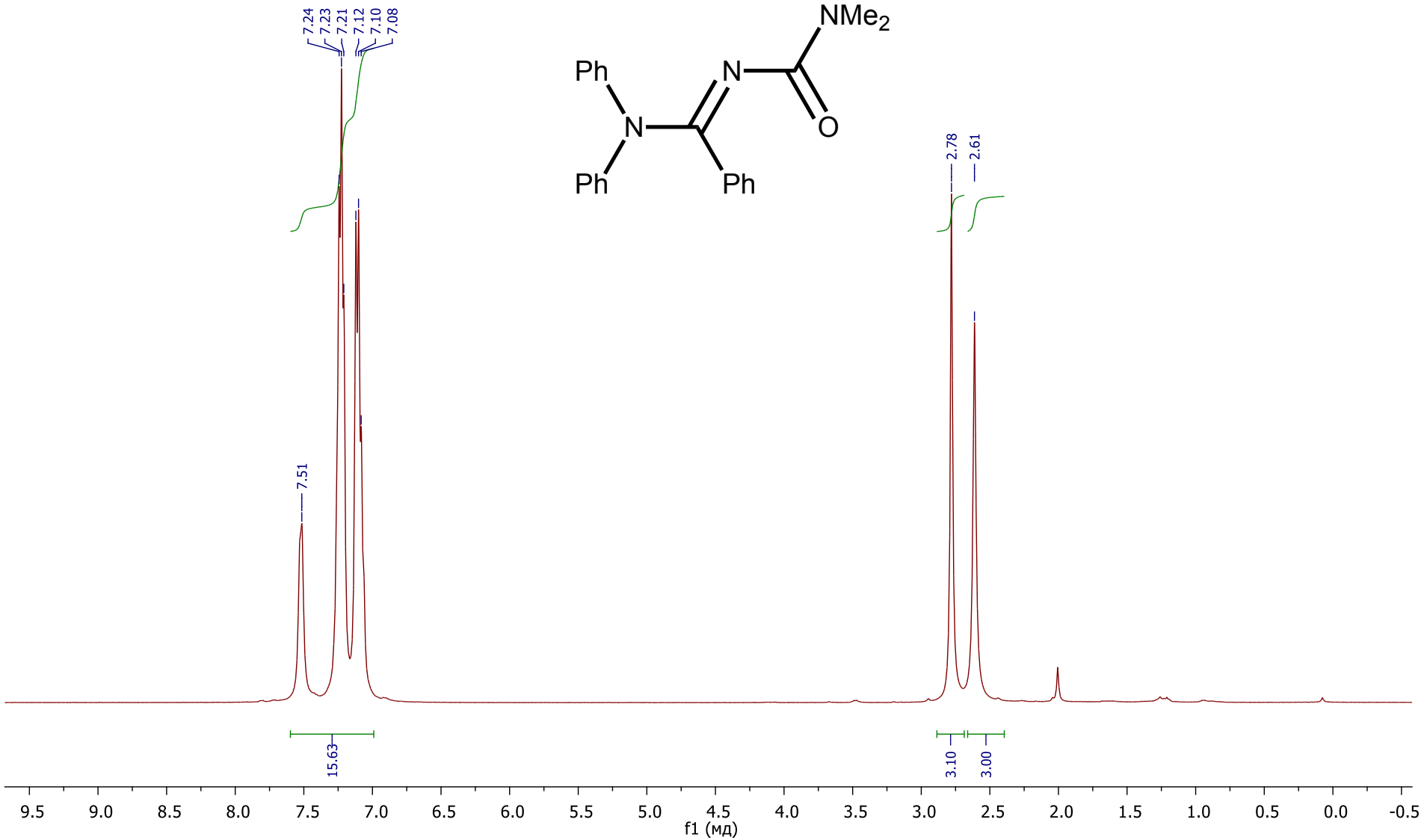
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



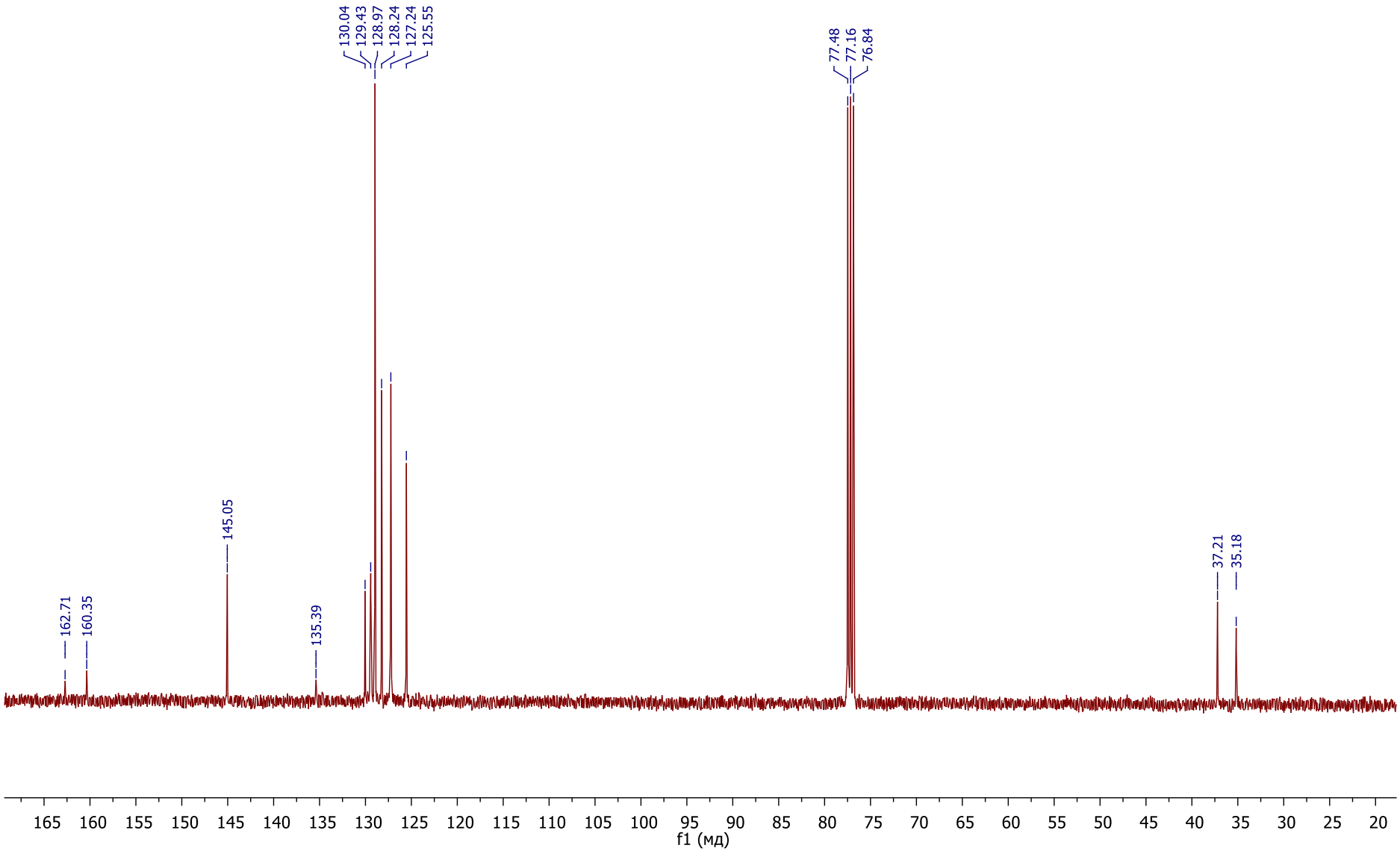
^{1}H *N*'-(dimethylcarbamoyl)-*N*,*N*-diphenylbenzimidamide (4ac).

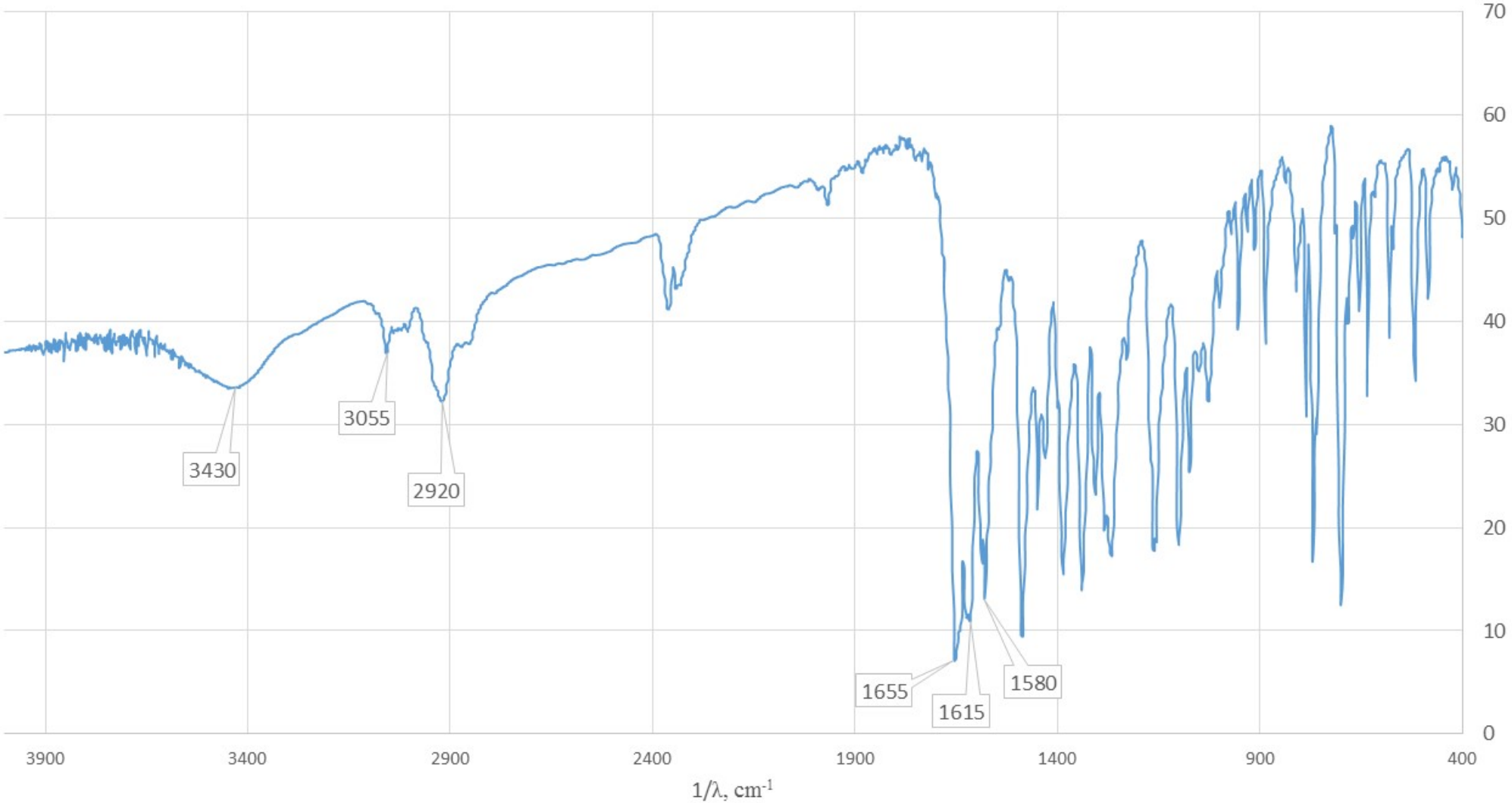
SAS
SAS, 87, BF = 400.13 MHz, Solvent - CDCl3, 17 Jan 2014 T=298 K



^{13}C *N*'-(dimethylcarbamoyl)-*N*,*N*-diphenylbenzimidamide (4ac).

SASc
SASc, 87, BF = 100.612769 MHz, Solvent - CDCl3, 17 Jan 2014 T=299 K




70
60
50
40
30
20
10
0
3900
3400
2900
2400
1900
1400
900
400
1/λ, cm-1
3430
3055
2920
1655
1615
1580

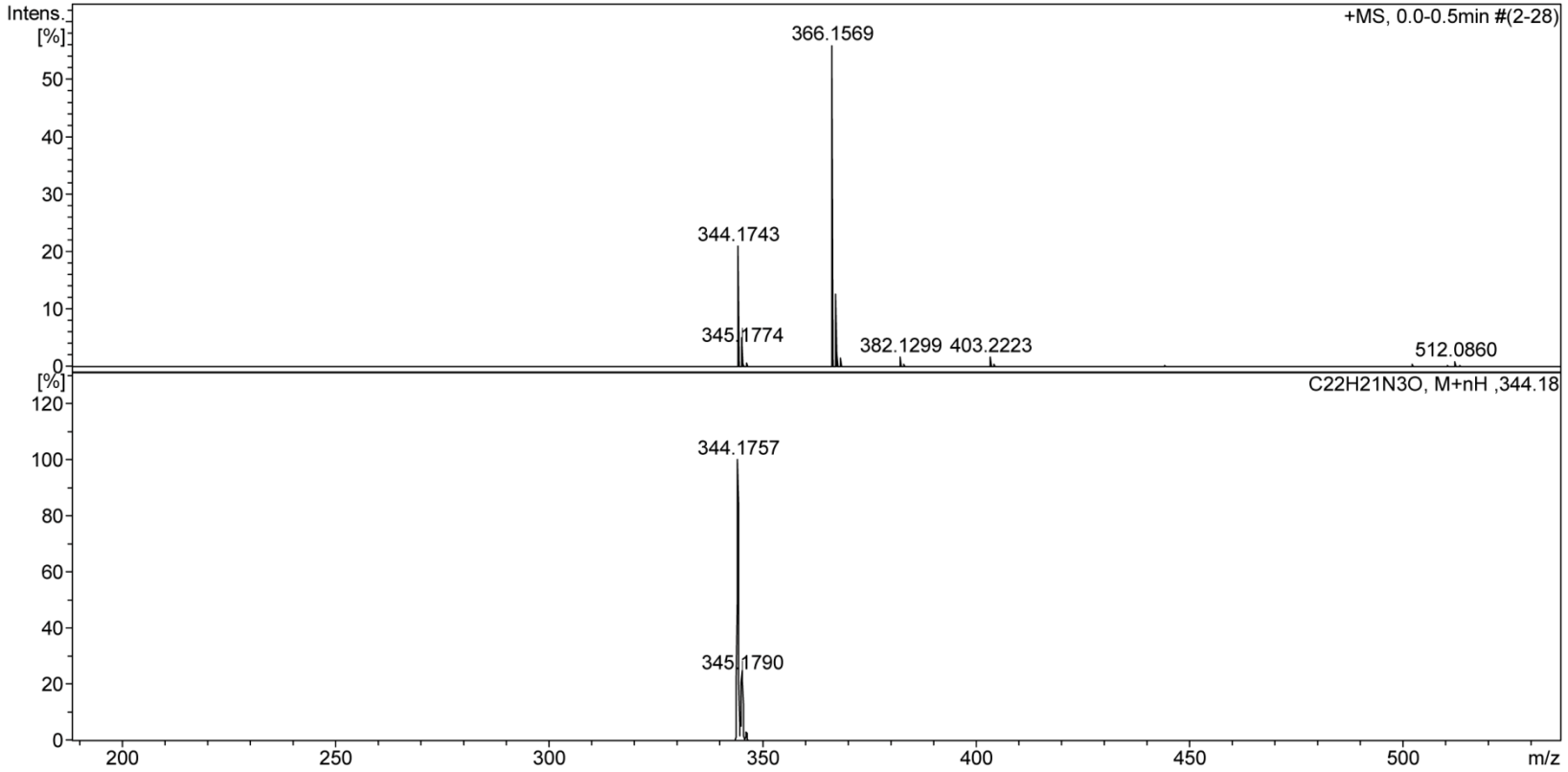
Mass Spectrum Report

Analysis Info

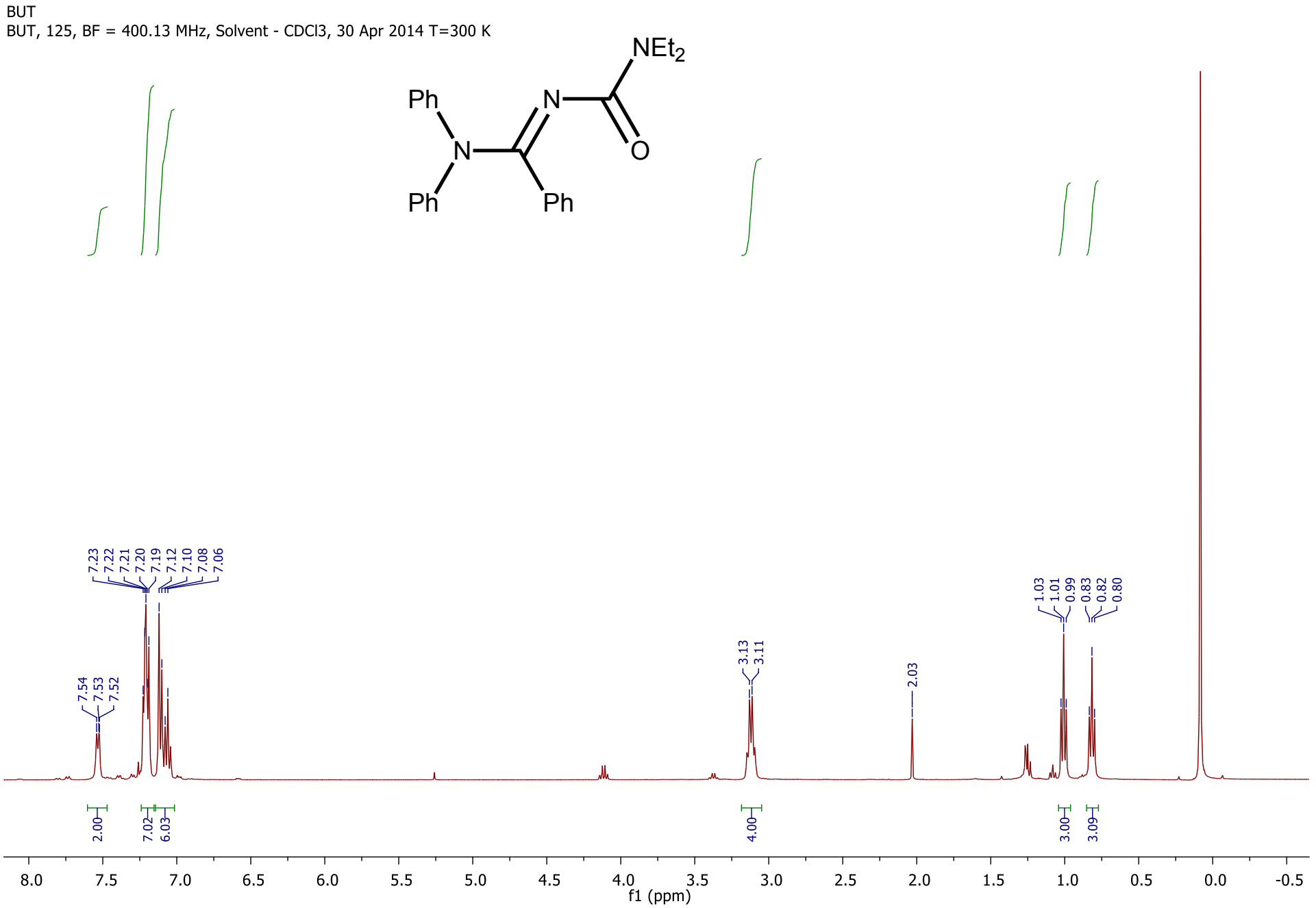
Analysis Name	D:\Data\mish\SAS98_2.d	Acquisition Date	07.02.2014 12:54:00
Method	tune_wide.m	Operator	Bruker Customer
Sample Name	SAS98_2	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

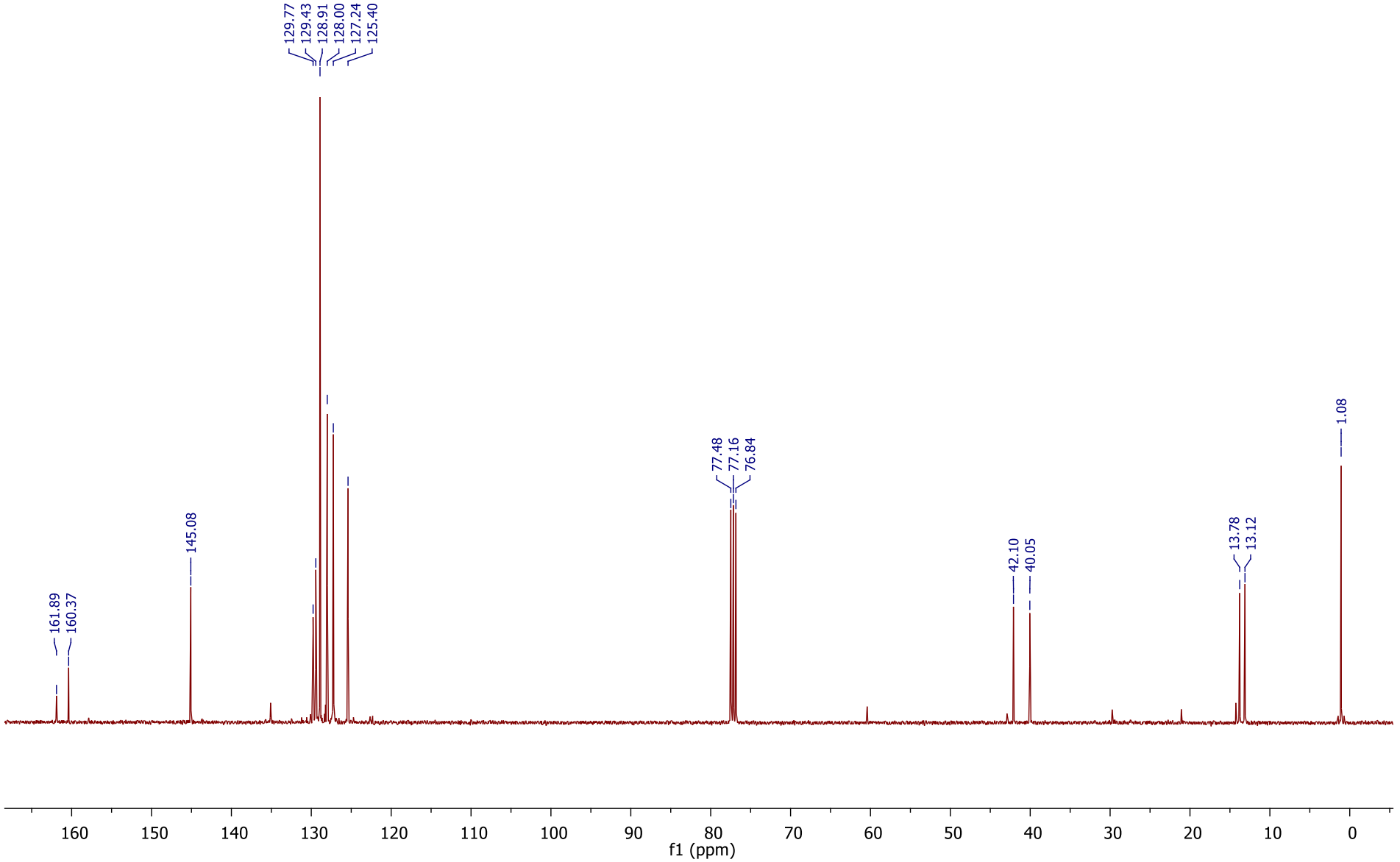


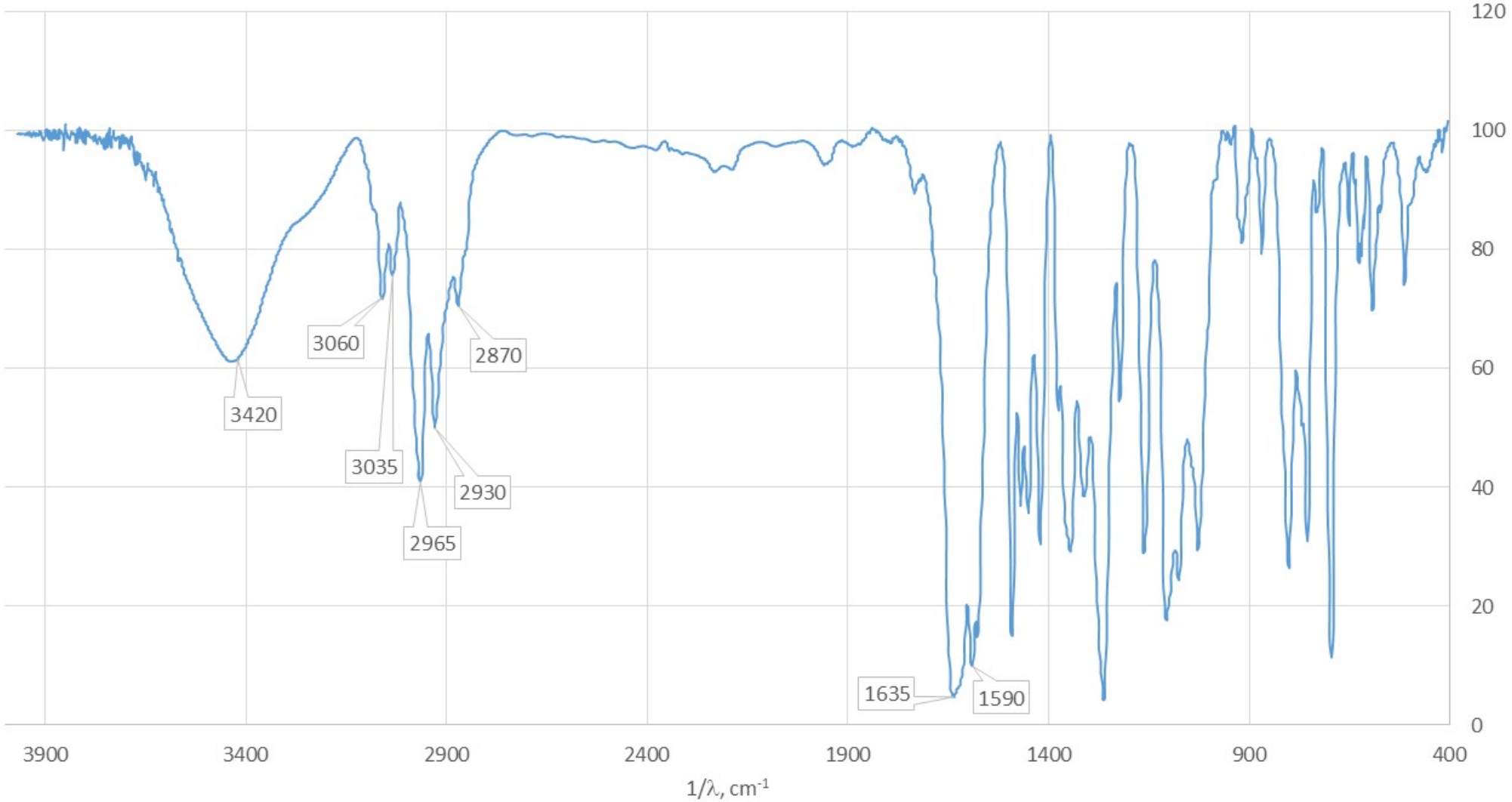
^{1}H *N'*-(diethylcarbamoyl)-*N,N*-diphenylbenzimidamide (4bc).



^{13}C *N'*-(diethylcarbamoyl)-*N,N*-diphenylbenzimidamide (4bc).

BUTc
BUTc, 125, BF = 100.612769 MHz, Solvent - CDCl3, 30 Apr 2014 T=300 K




120
100
80
60
40
20
0
3420
3060
3035
2965
2930
2870
1635
1590
3900
3400
2900
2400
1900
1400
900
400
1/λ, cm-1

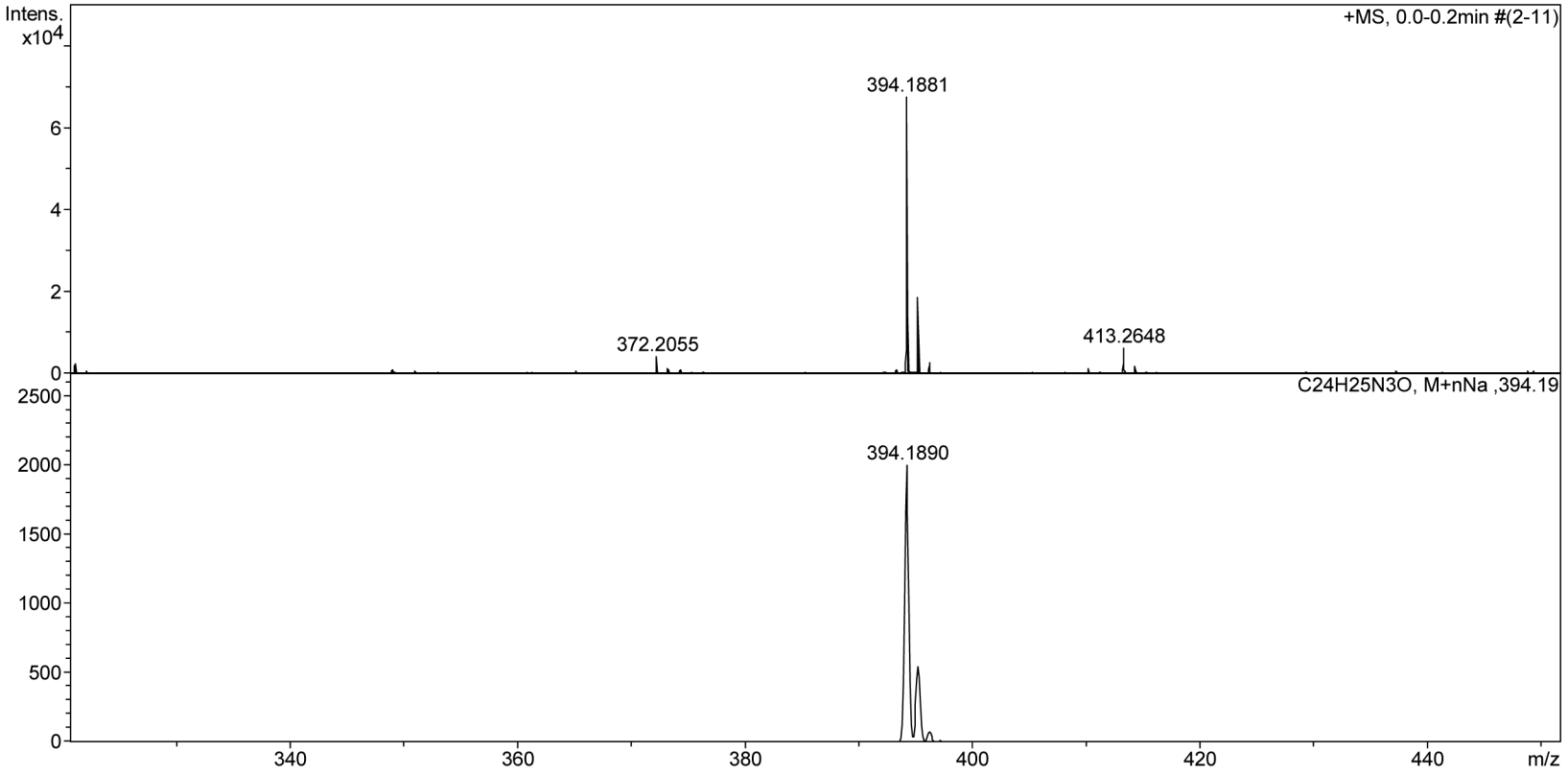
Mass Spectrum Report

Analysis Info

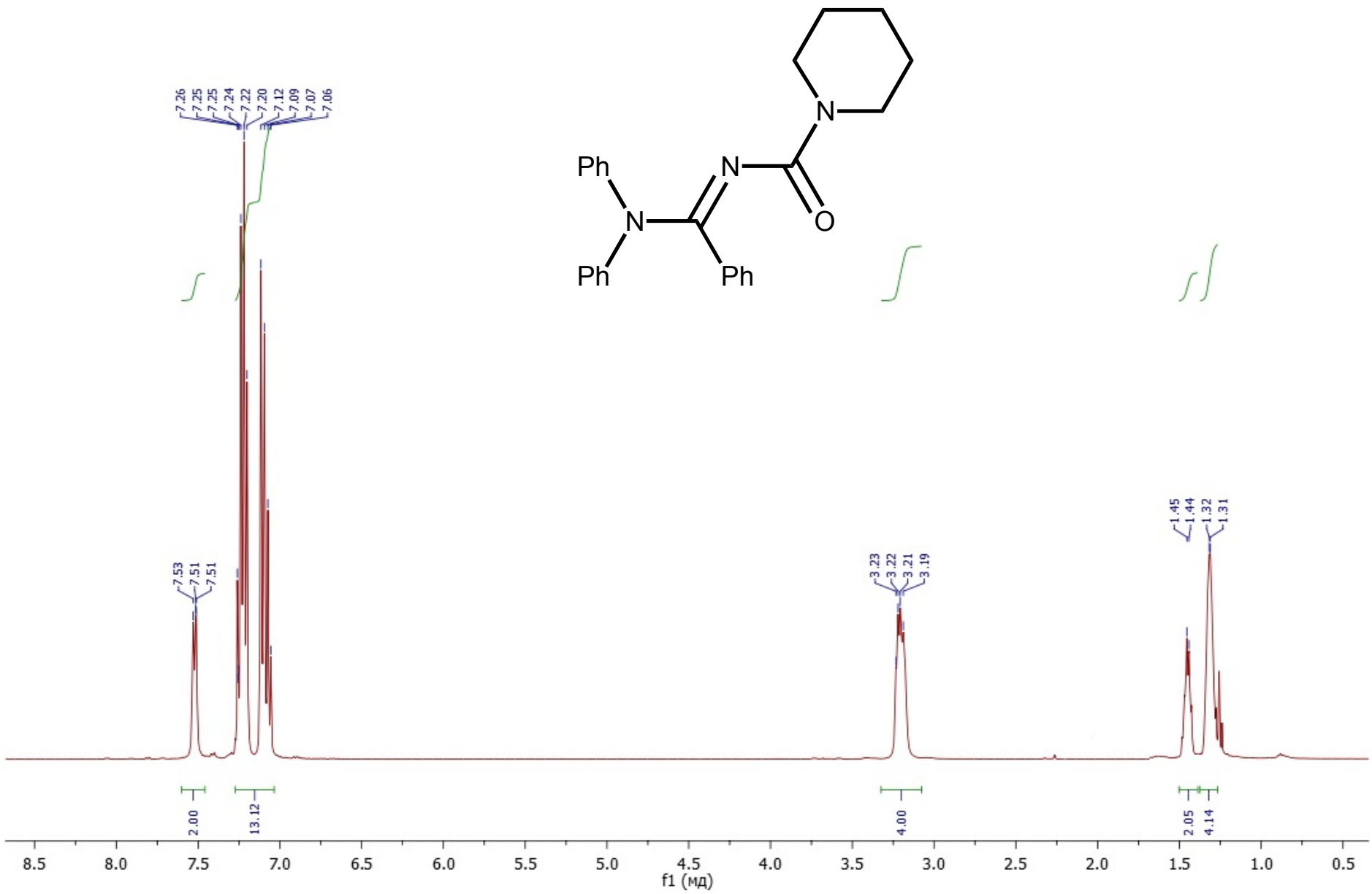
Analysis Name	D:\Data\mish2\BUT177_6.d	Acquisition Date	28.04.2014 16:38:01
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT177_6	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

Acquisition Parameter

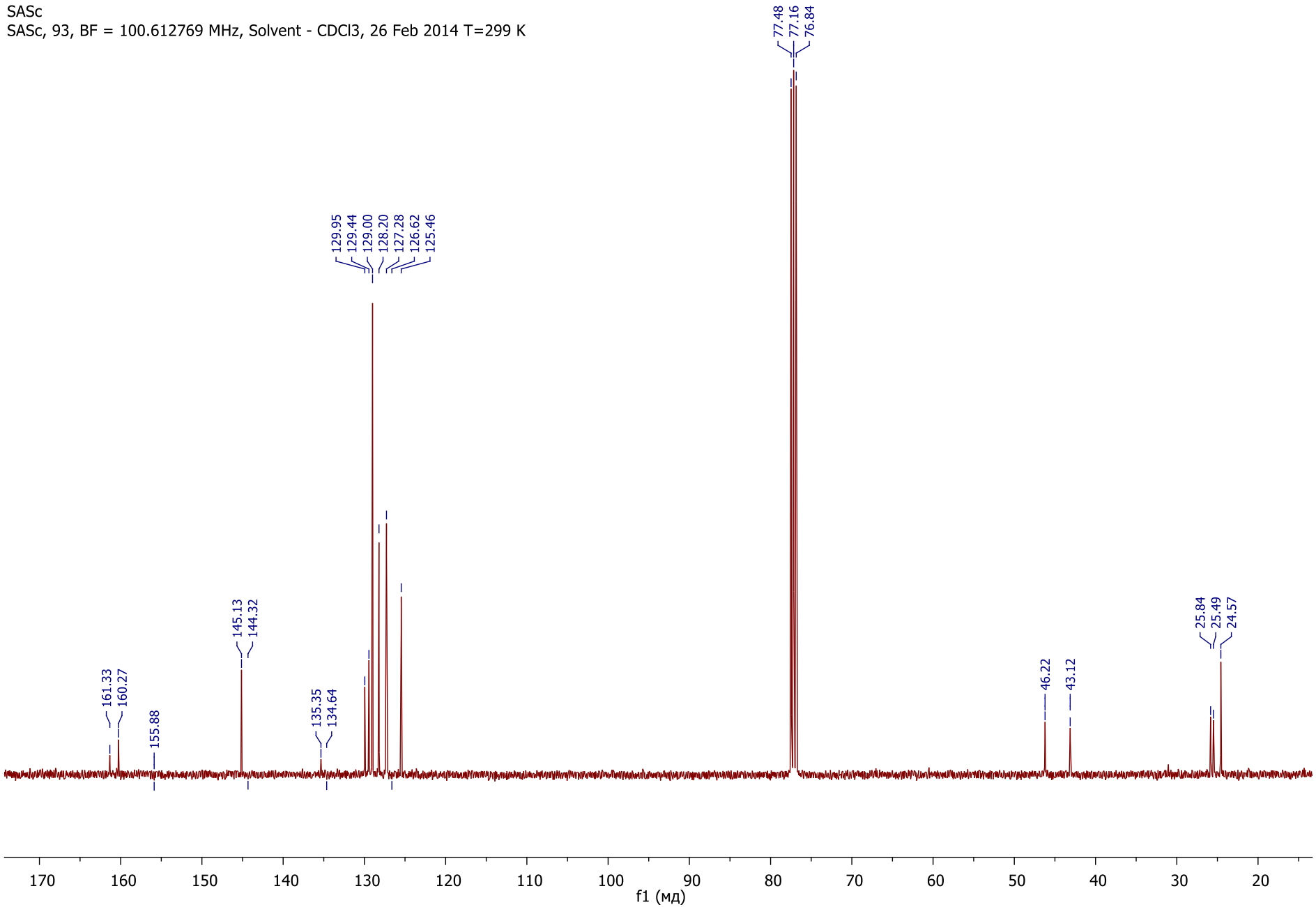
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

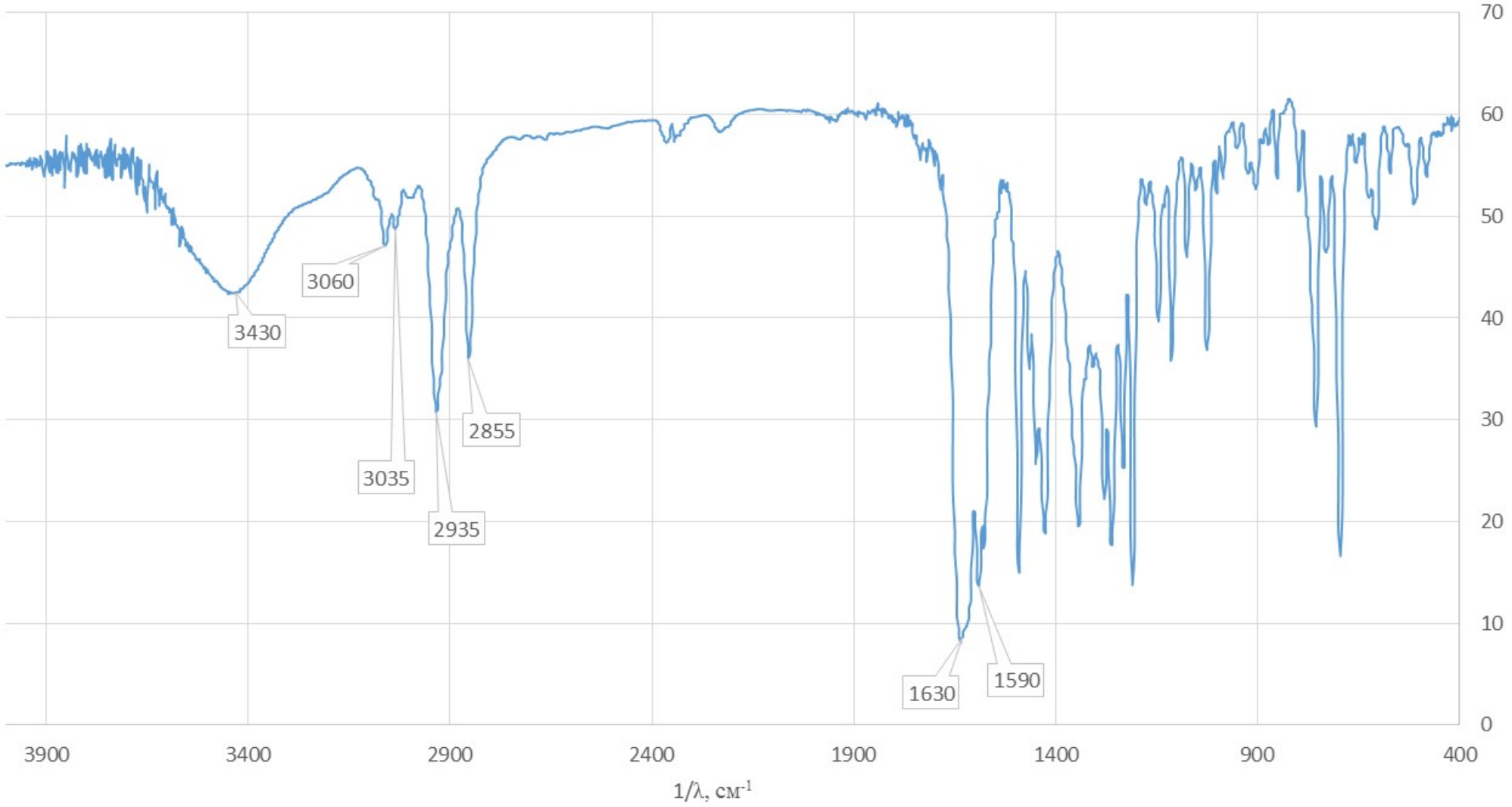


^{1}H *N*-((diphenylamino)(phenyl)methylene)piperidine-1-carboxamide (4cc).



^{13}C *N*-((diphenylamino)(phenyl)methylene)piperidine-1-carboxamide (4cc).




3430
3060
3035
2935
2855
1630
1590
70
60
50
40
30
20
10
0
3900
3400
2900
2400
1900
1400
900
400
1/λ, см-1

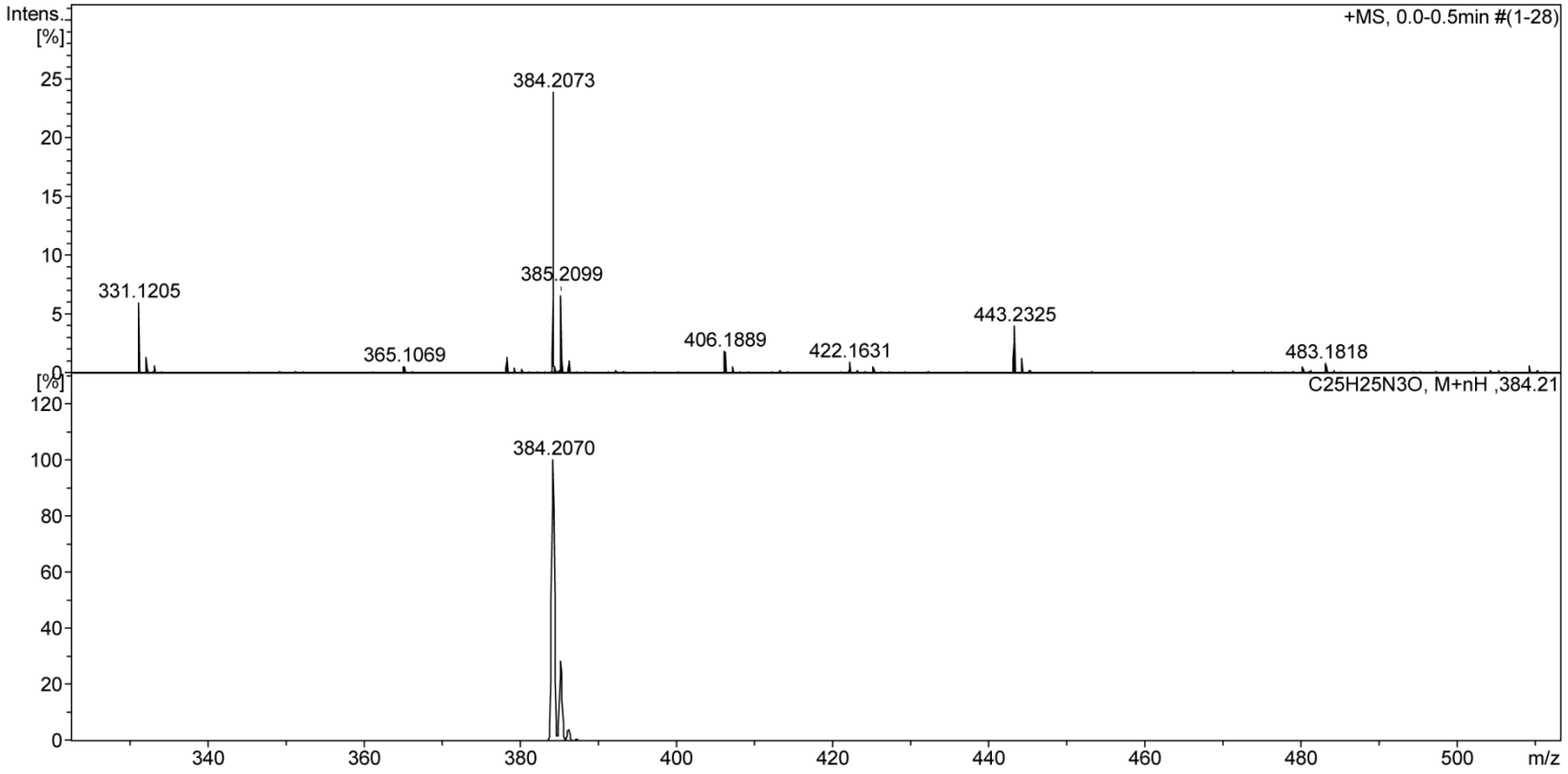
Mass Spectrum Report

Analysis Info

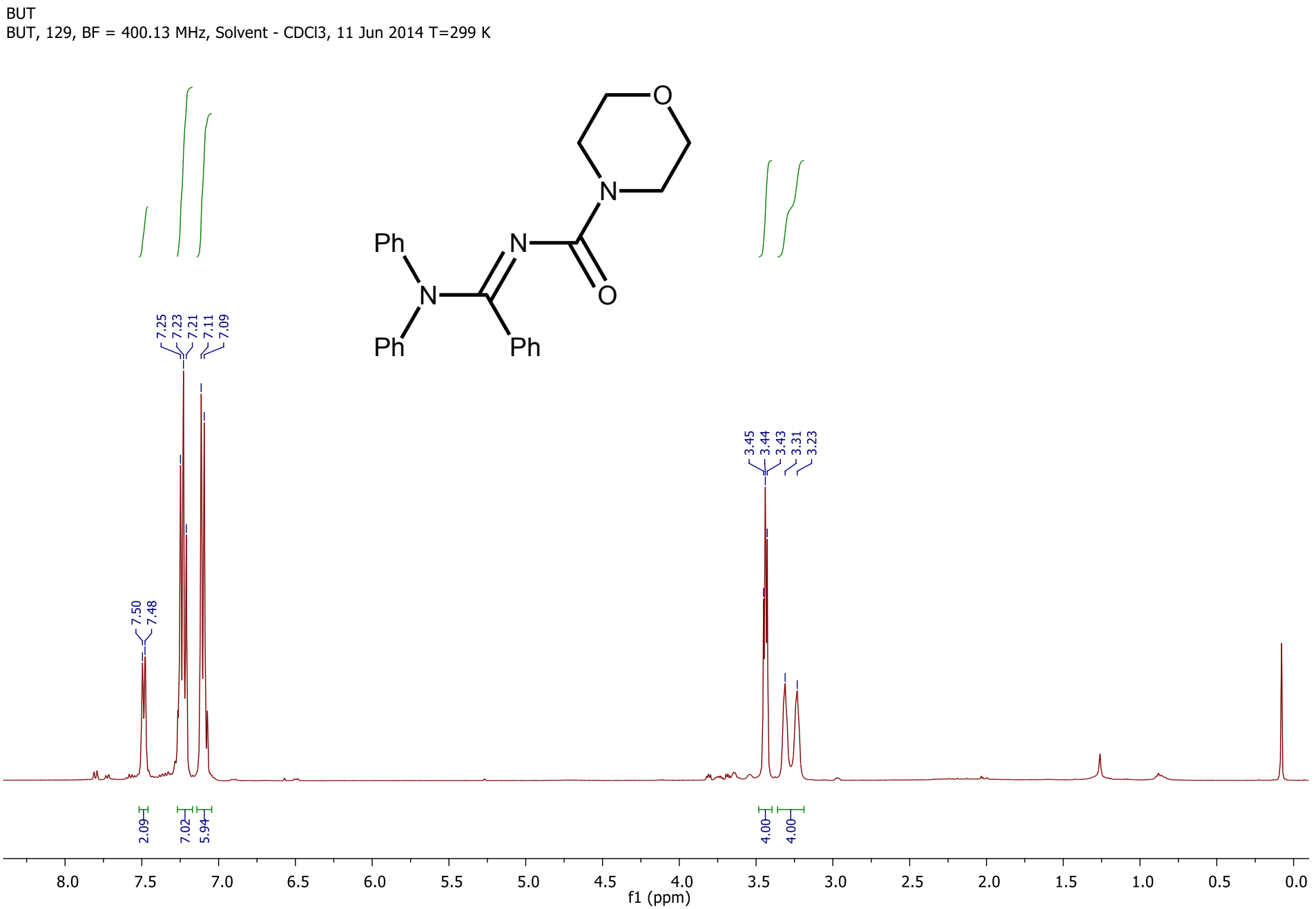
Analysis Name	D:\Data\mish\SAS113_F5_7.d	Acquisition Date	25.02.2014 11:50:54
Method	tune_low.m	Operator	Bruker Customer
Sample Name	SAS113_F5_7	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

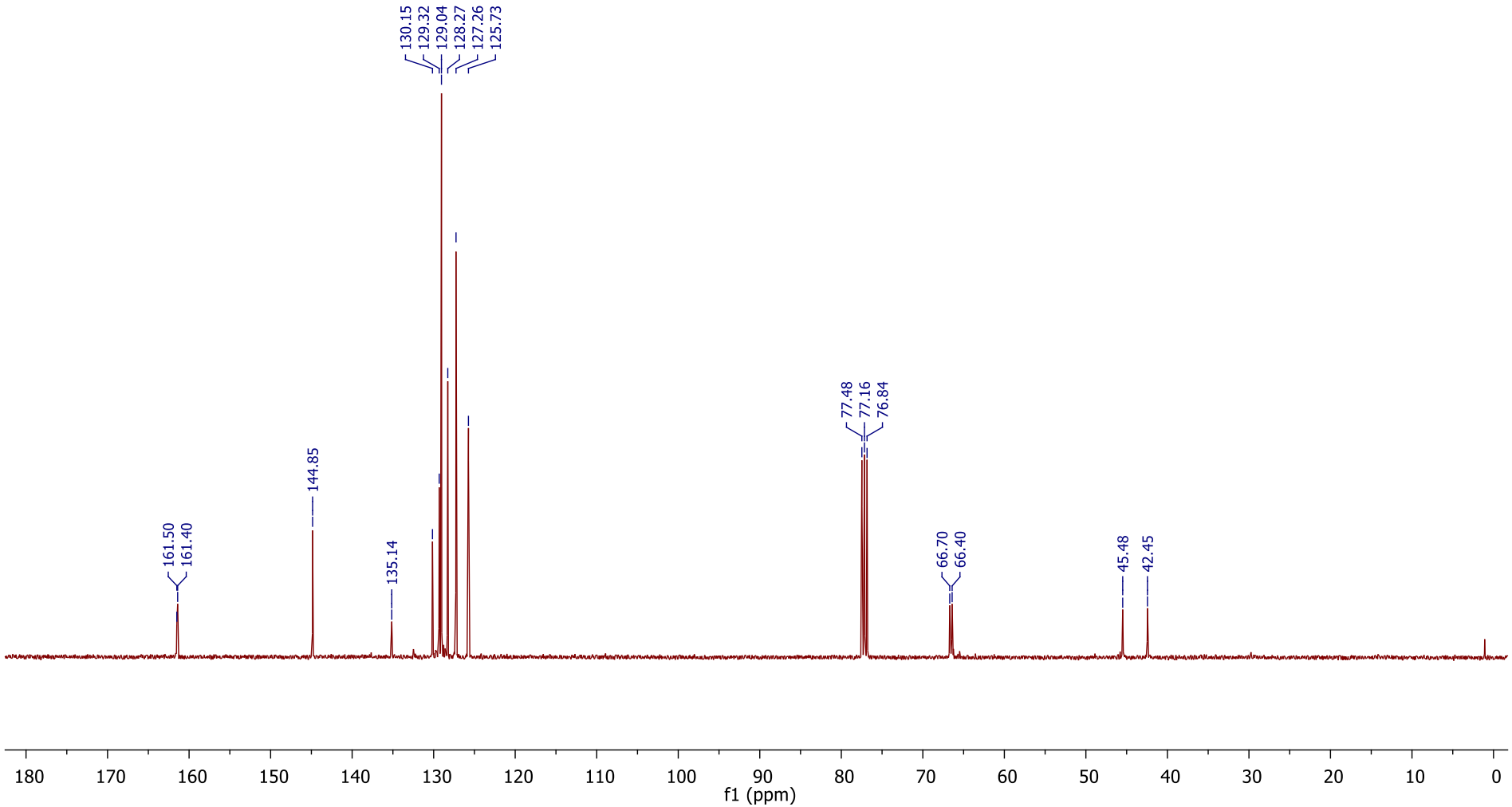


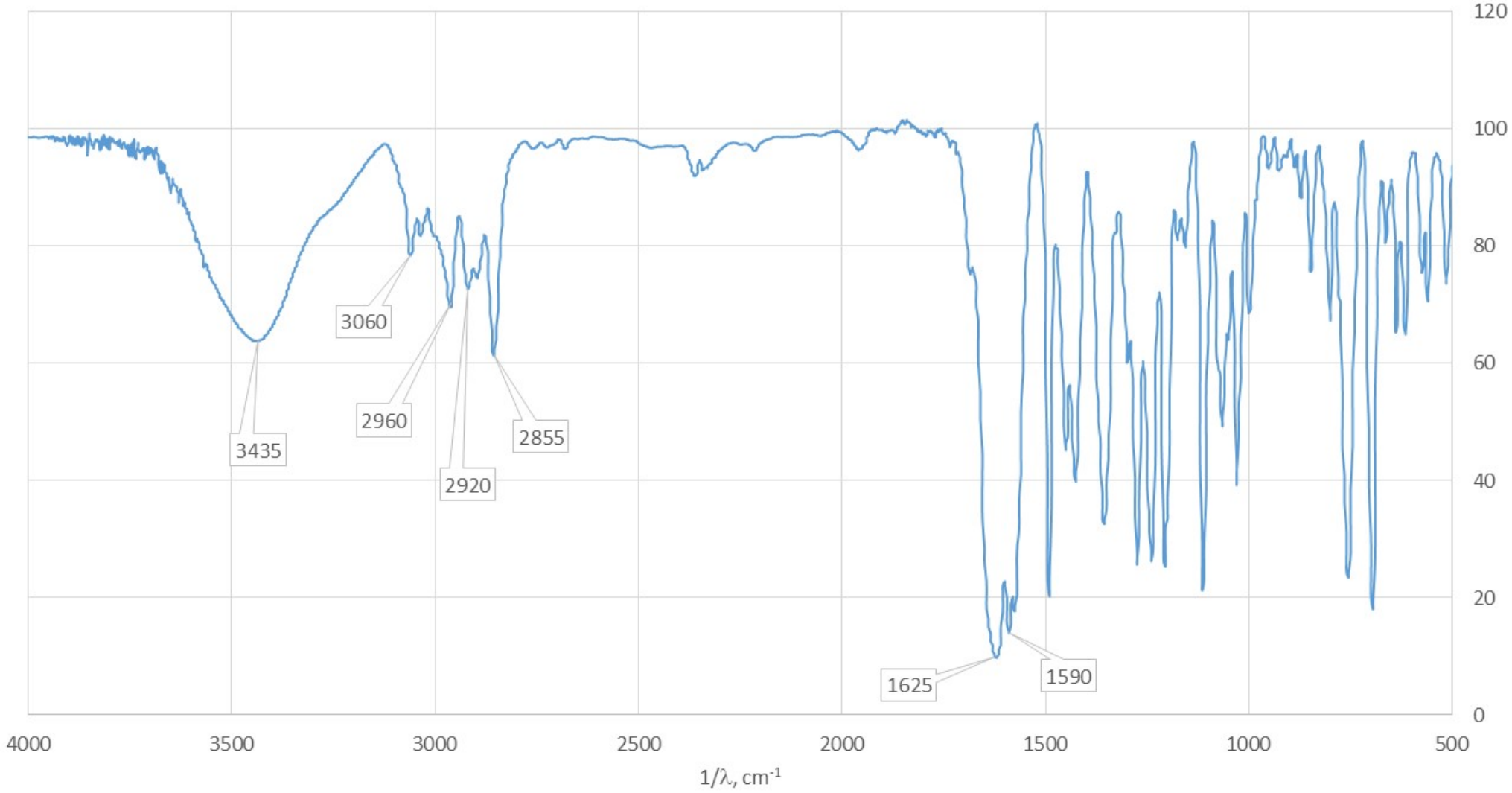
^{1}H *N*-((diphenylamino)(phenyl)methylene)morpholine-4-carboxamidemethyleneamide (4dc).



^{13}C *N*-((diphenylamino)(phenyl)methylene)morpholine-4-carboxamidemethyleneamide (4dc).

BUTc
BUTc, 129, BF = 100.612769 MHz, Solvent - CDCl3, 11 Jun 2014 T=299 K




120
100
80
60
40
20
0
4000
3500
3000
2500
2000
1500
1000
500
1/λ, cm-1
3435
3060
2960
2920
2855
1625
1590

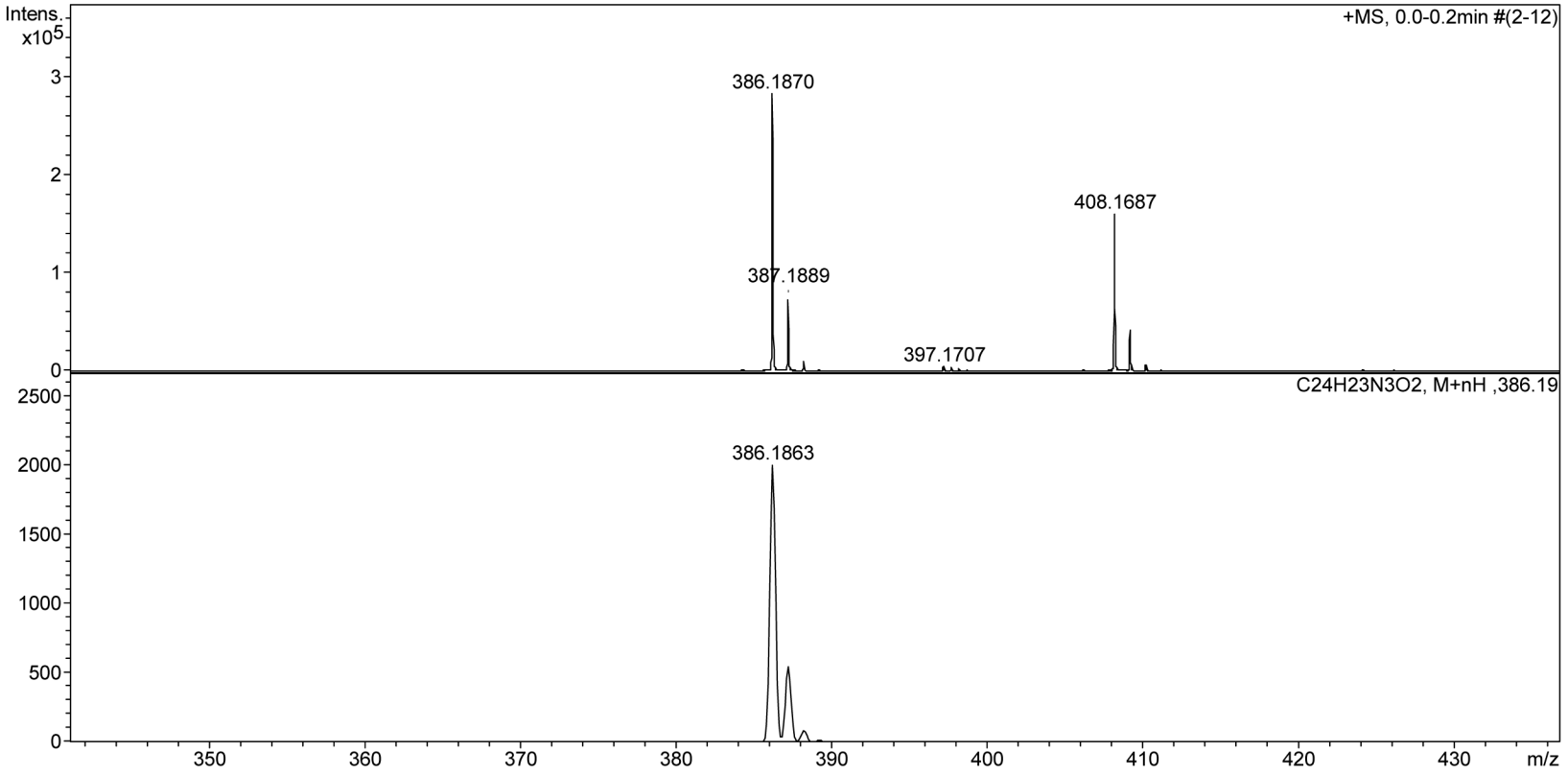
Mass Spectrum Report

Analysis Info

Analysis Name	D:\Data\mish2\BUT178_fr10-13.d	Acquisition Date	16.05.2014 12:22:31
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT178_fr10-13	Instrument / Ser#	micrOTOF 10223
Comment	MeOH100v		

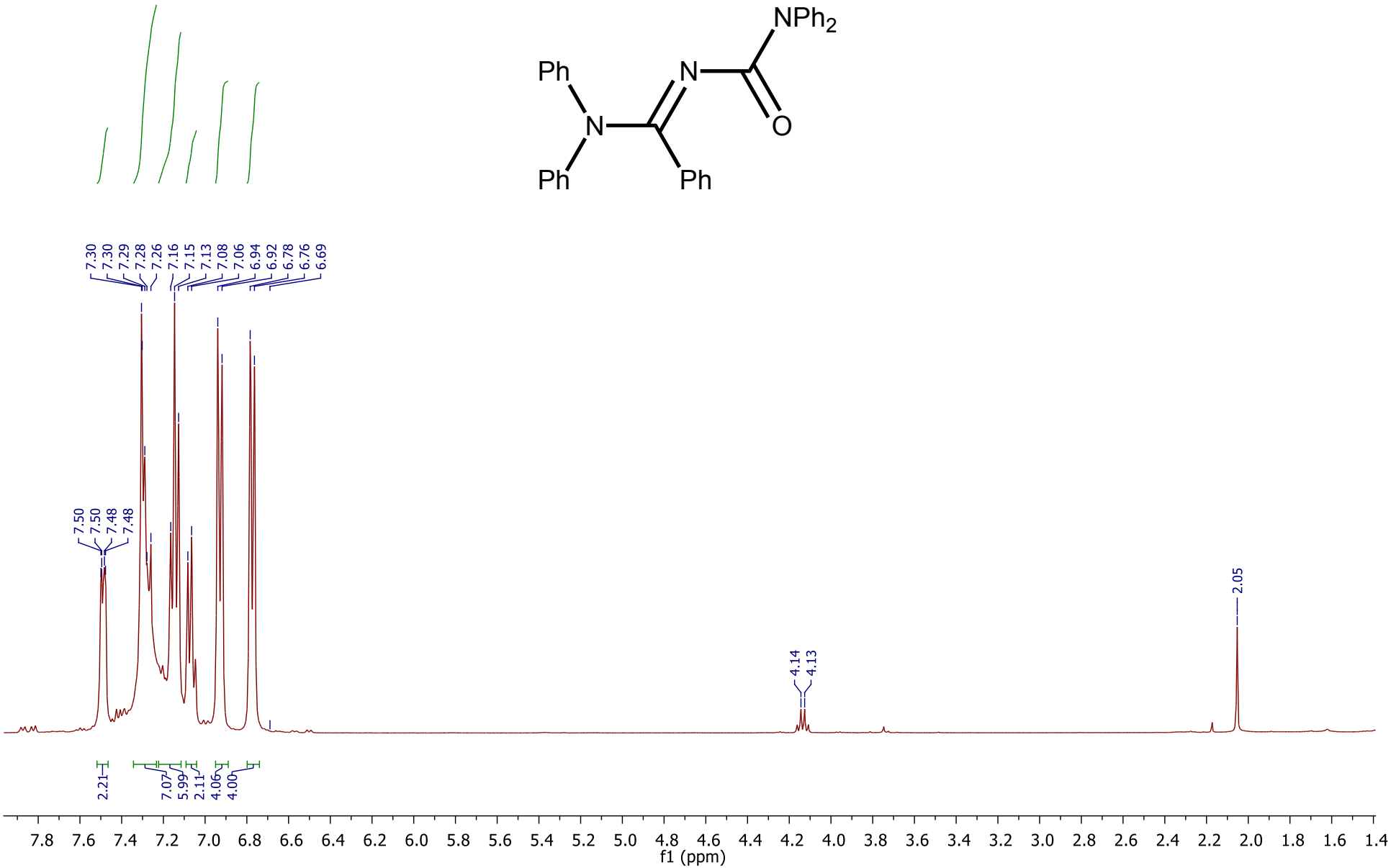
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



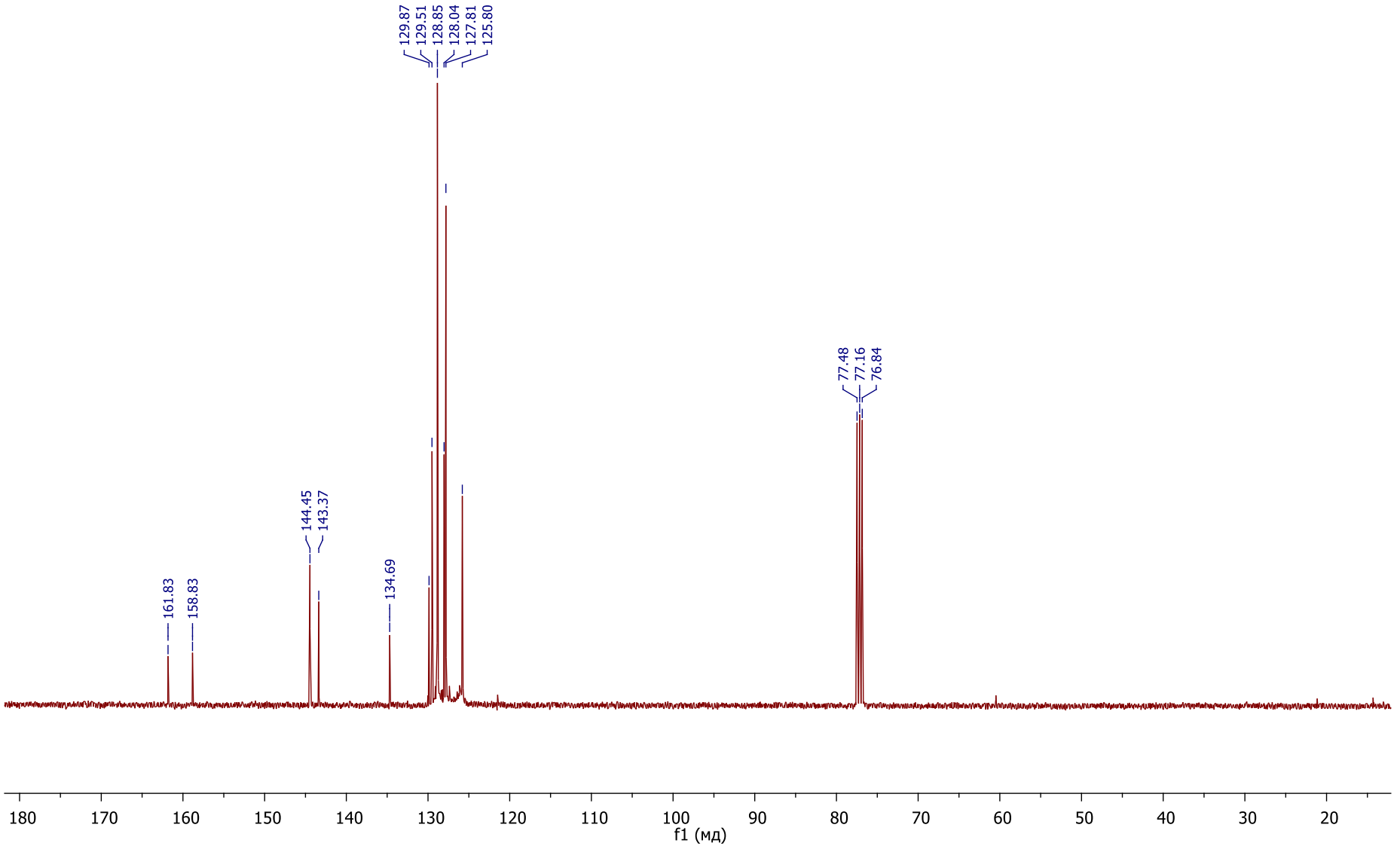
^{1}H *N′*-(diphenylcarbamoyl)-*N*,*N*-diphenylbenzimidamide (4ec).

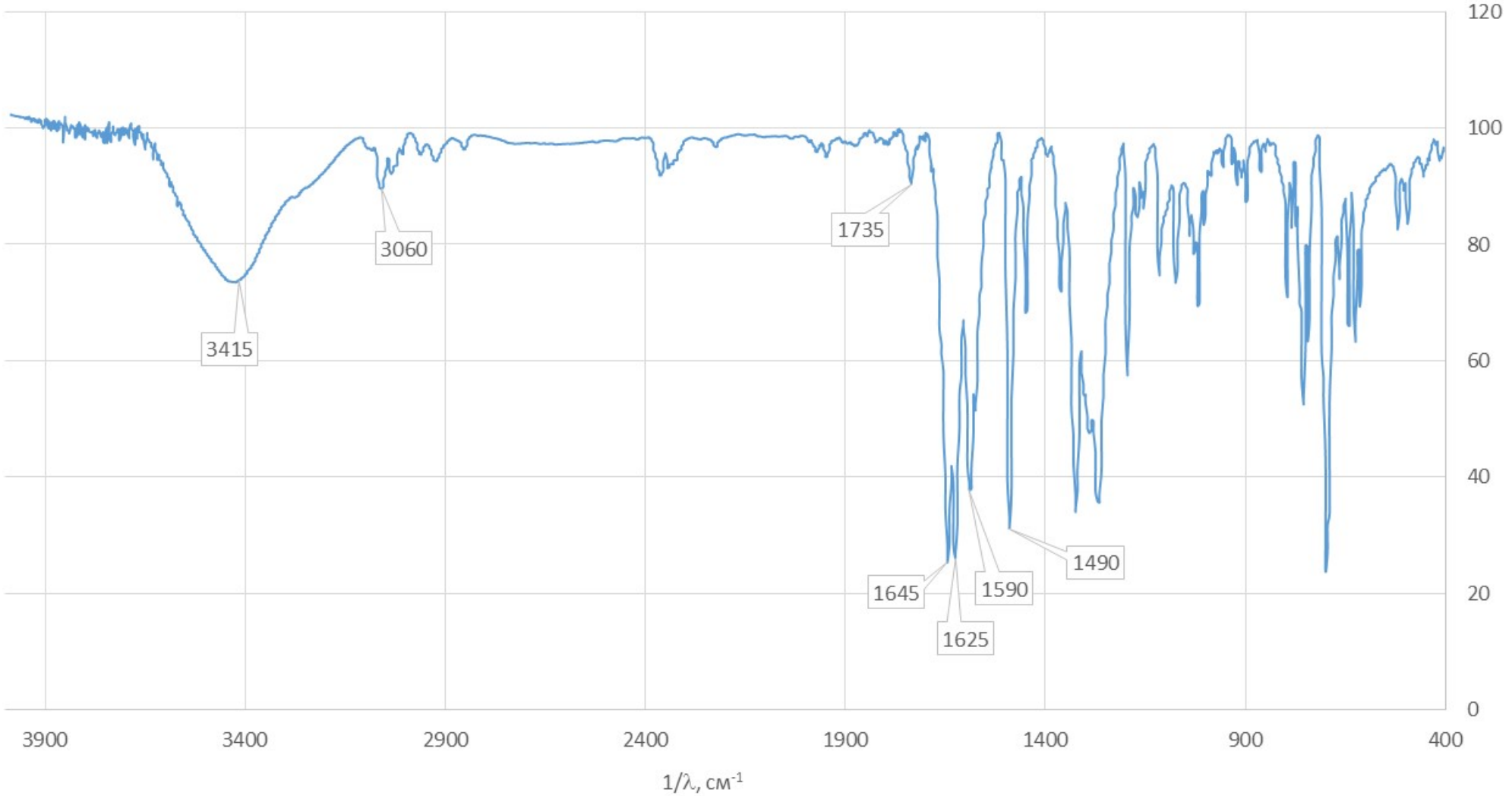
BUT
BUT, 121, BF = 400.13 MHz, Solvent - CDCl3, 22 Apr 2014 T=299 K



^{13}C *N′*-(diphenylcarbamoyl)-*N,N*-diphenylbenzimidamide (4ec).

BUTc
BUTc, 121, BF = 100.612769 MHz, Solvent - CDCl3, 22 Apr 2014 T=300 K




120
100
80
60
40
20
0
3900
3400
2900
2400
1900
1400
900
400
1/λ, см-1
3415
3060
1735
1645
1625
1590
1490

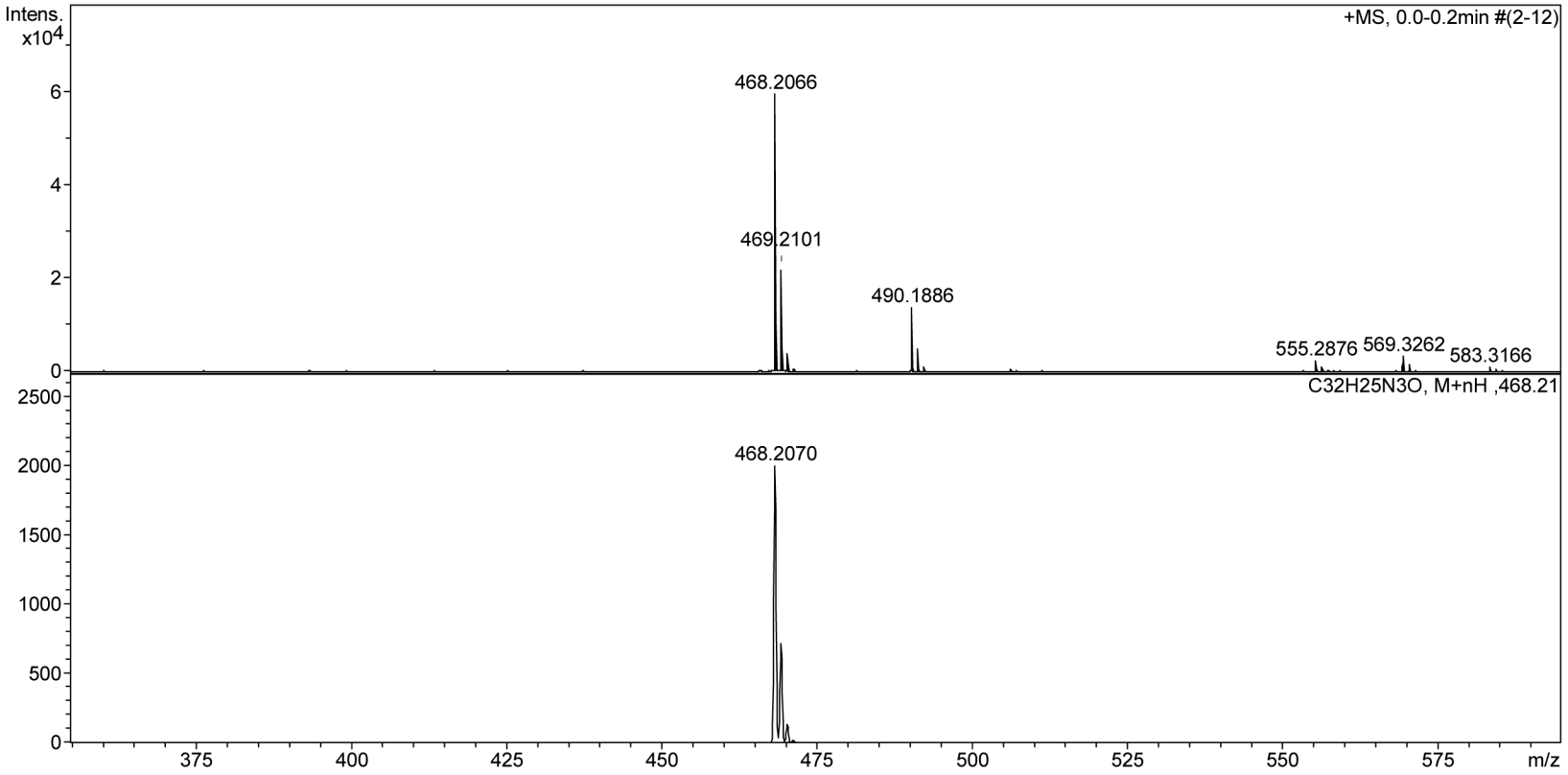
Mass Spectrum Report

Analysis Info

Analysis Name	D:\Data\mish2\BUT174_fr9-13.d	Acquisition Date	22.04.2014 15:40:44
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT174_fr9-13	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

Acquisition Parameter

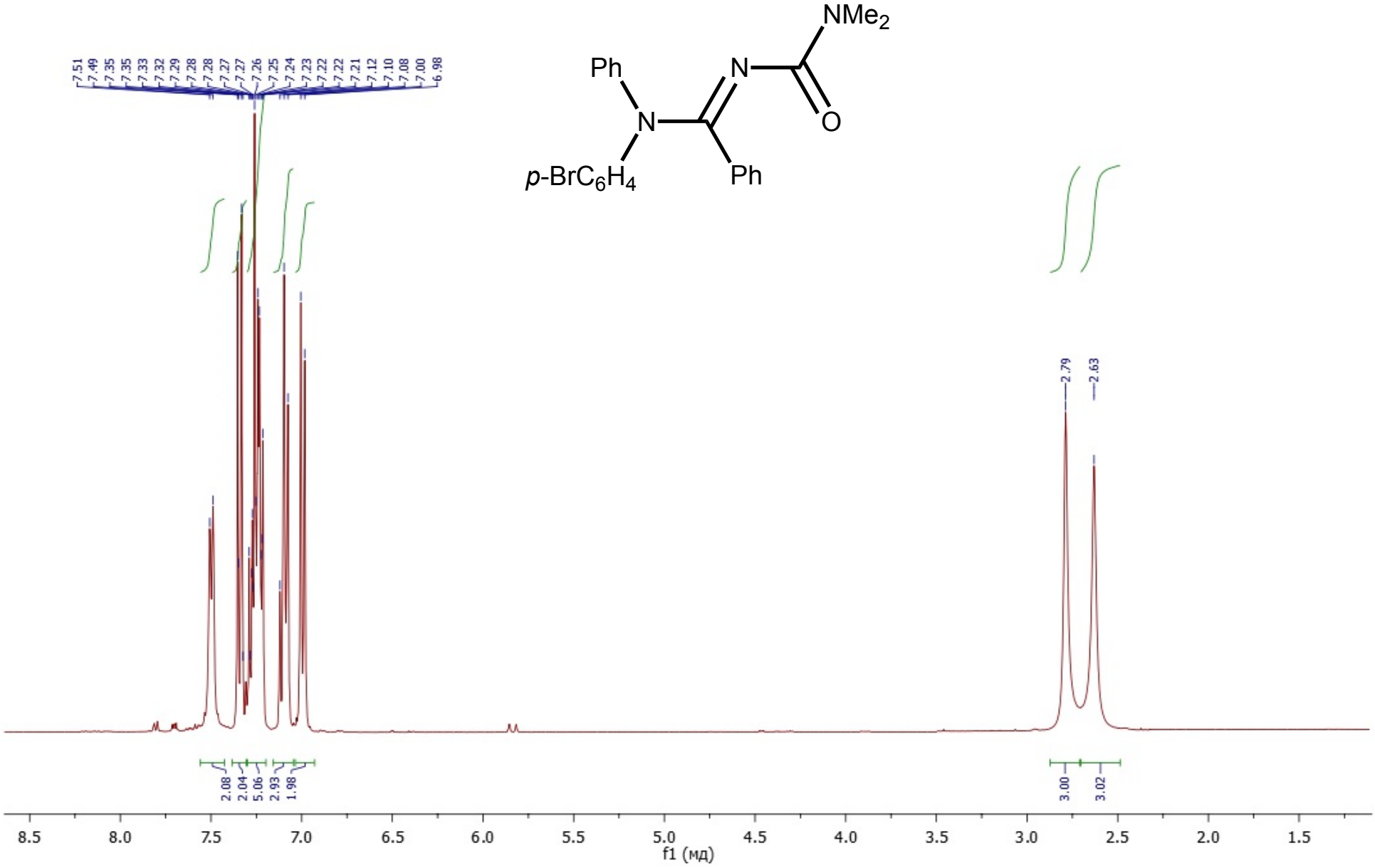
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



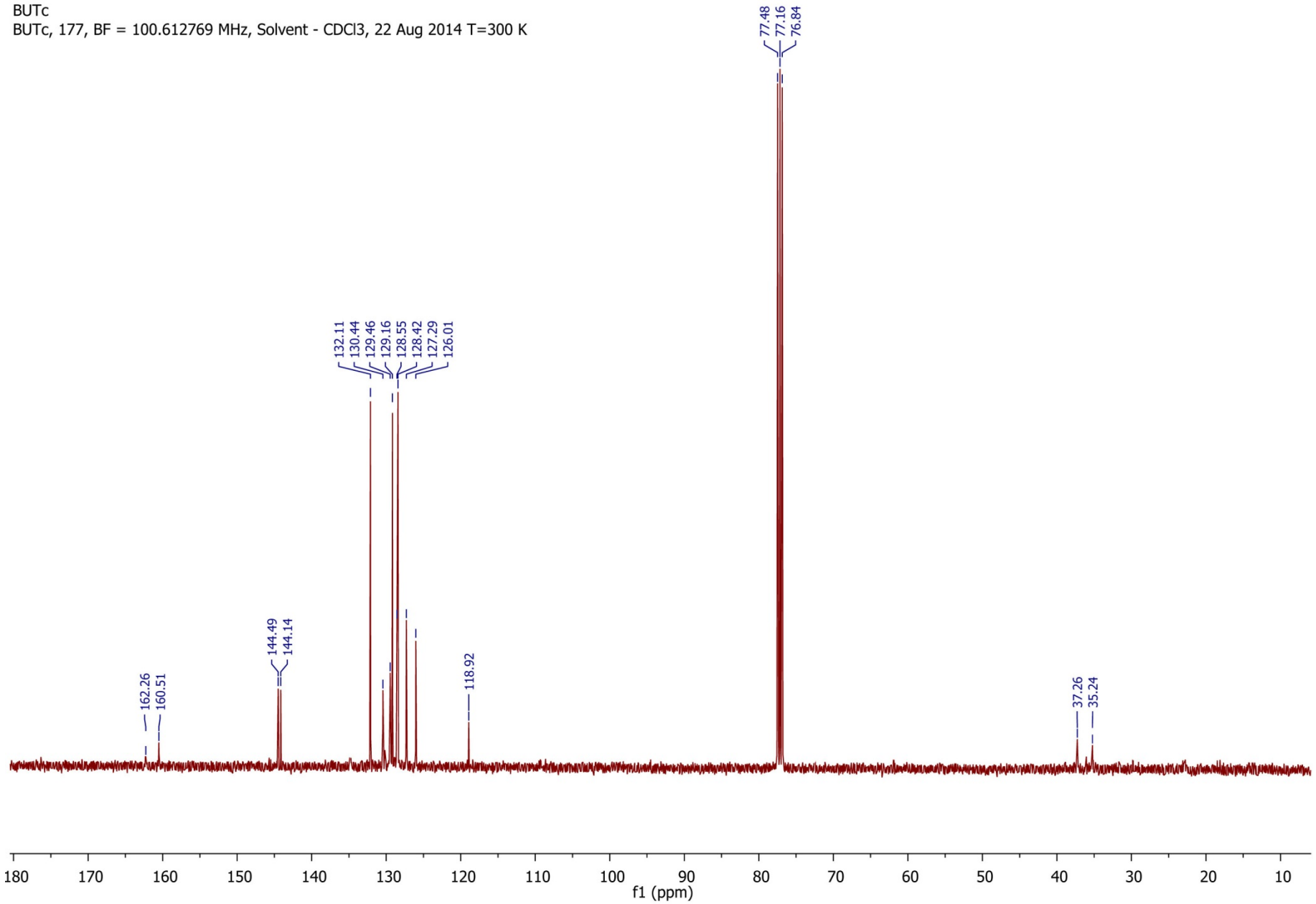
^{1}H 4-bromo-*N*′-(dimethylcarbamoyl)-*N*,*N*-diphenylbenzimidamide (4ad)

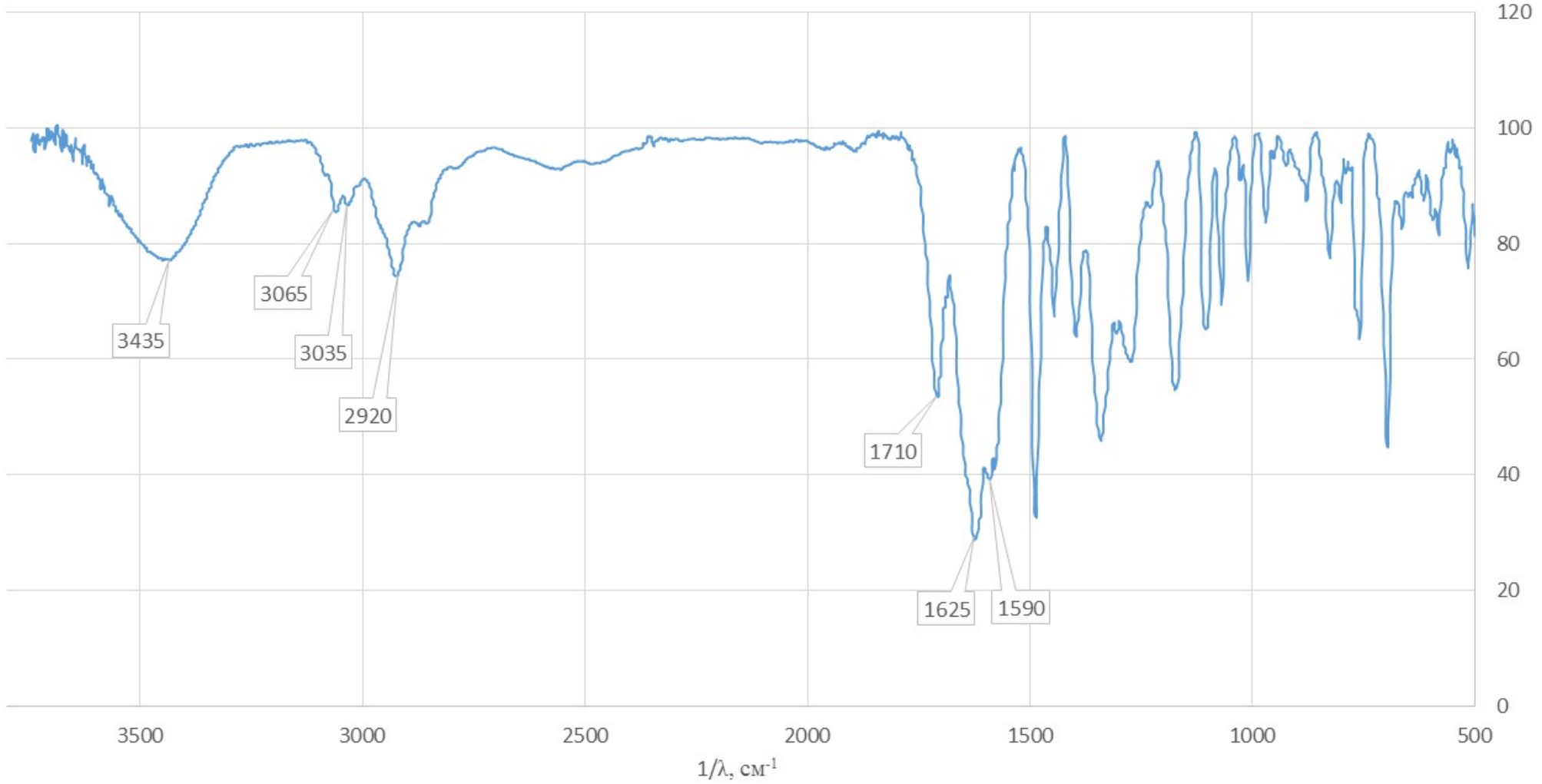
BUT

BUT, 177, BF = 400.13 MHz, Solvent - CDCl3, 21 Aug 2014 T=300 K



^{1}H 4-bromo-*N*′-(dimethylcarbamoyl)-*N*,*N*-diphenylbenzimidamide (4ad).



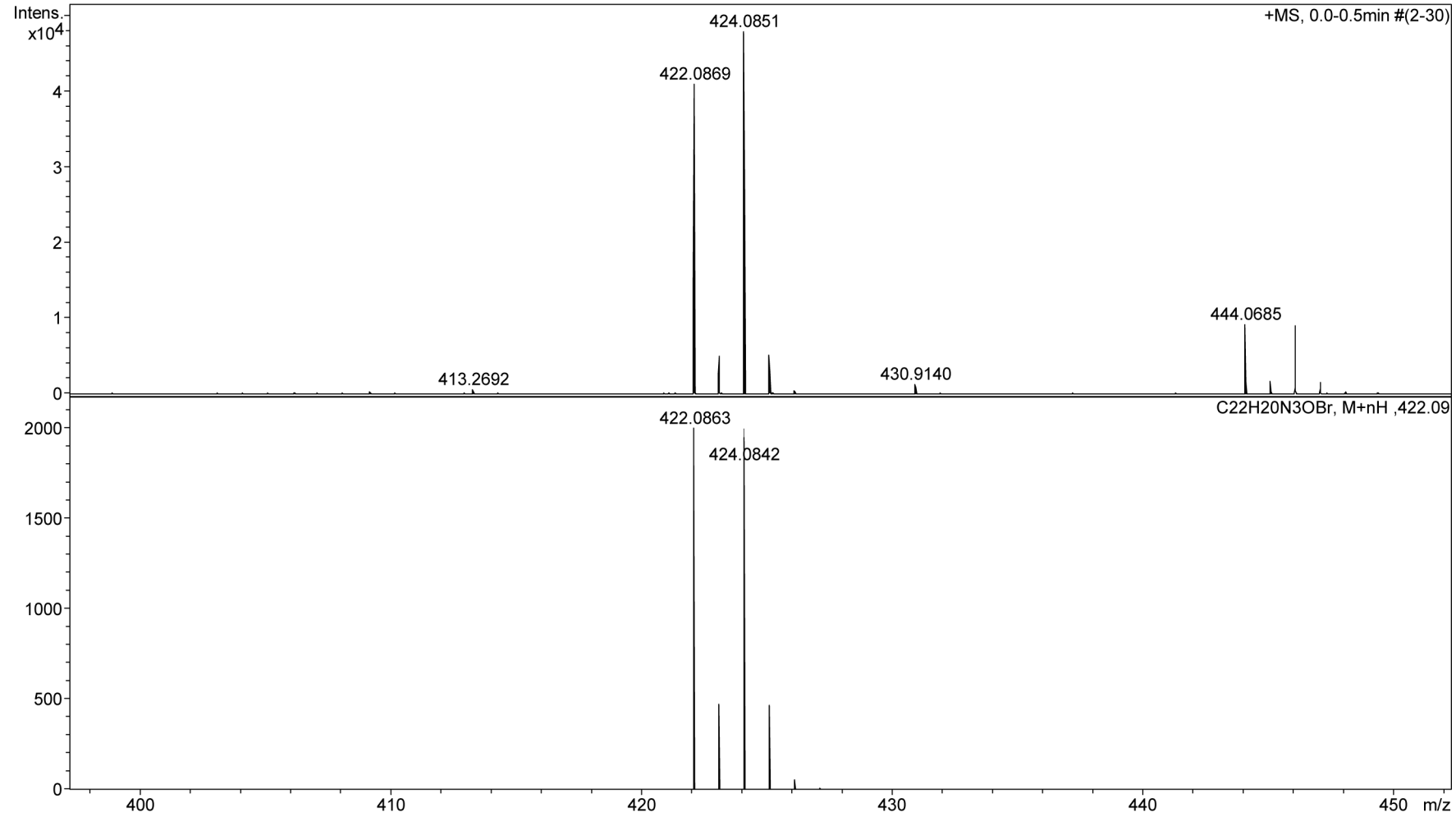

120
100
80
60
40
20
0
3500
3000
2500
2000
1500
1000
500
1/λ, см-1
3435
3065
3035
2920
1710
1625
1590

Analysis Info

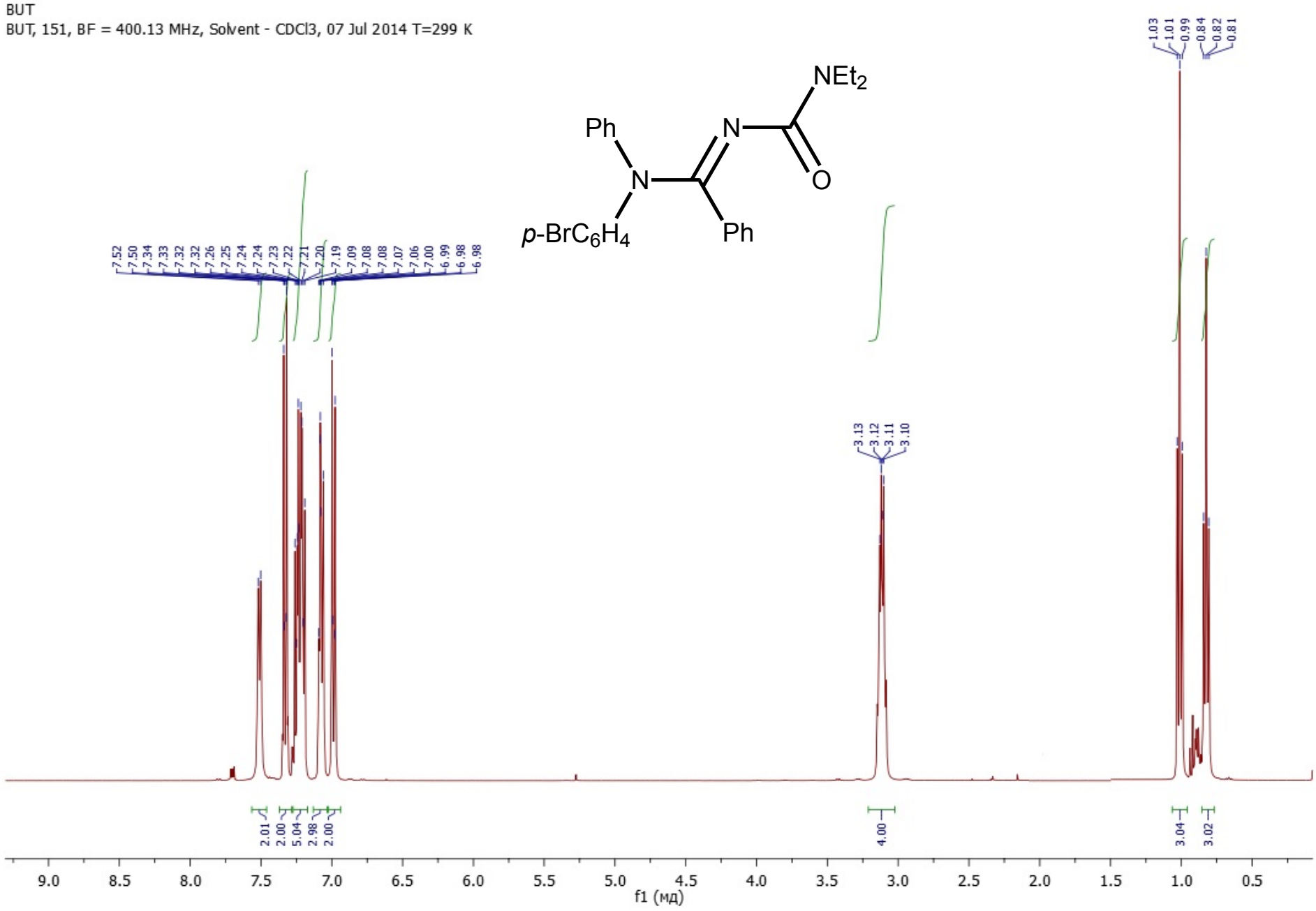
Analysis Name	D:\Data\Work\2014\november\18\BUT224_1000001.d	Acquisition Date	11/19/2014 2:09:37 PM
Method	tune_low_pos_50_1500_200ulmin.m	Operator	BDAL@DE
Sample Name	BUT224_1	Instrument	maXis 62
Comment	MeOH		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



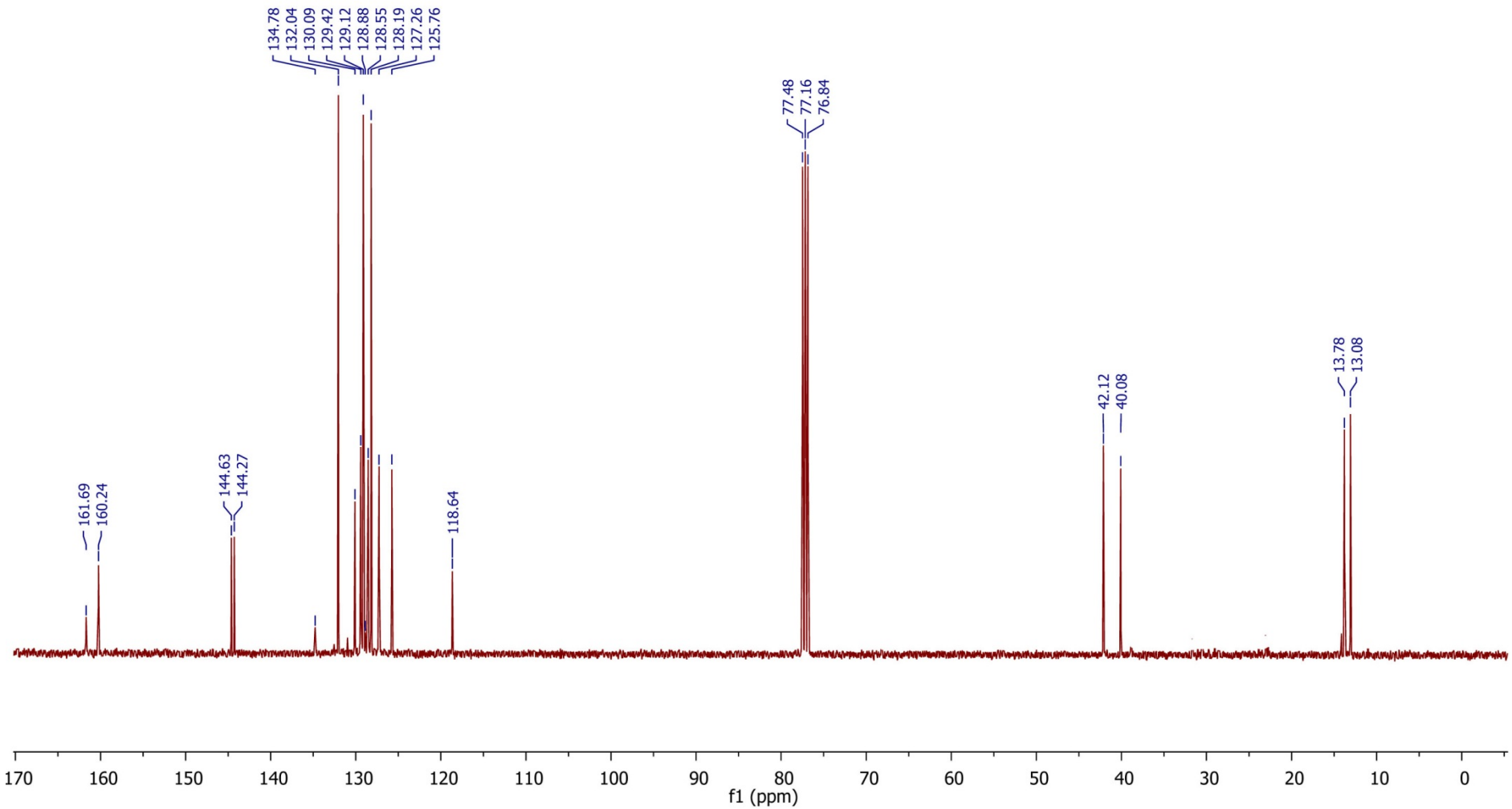
^{1}H *N*-(4-bromophenyl)-*N*'-(diethylcarbamoyl)-*N*-phenylbenzimidamide (4bd).

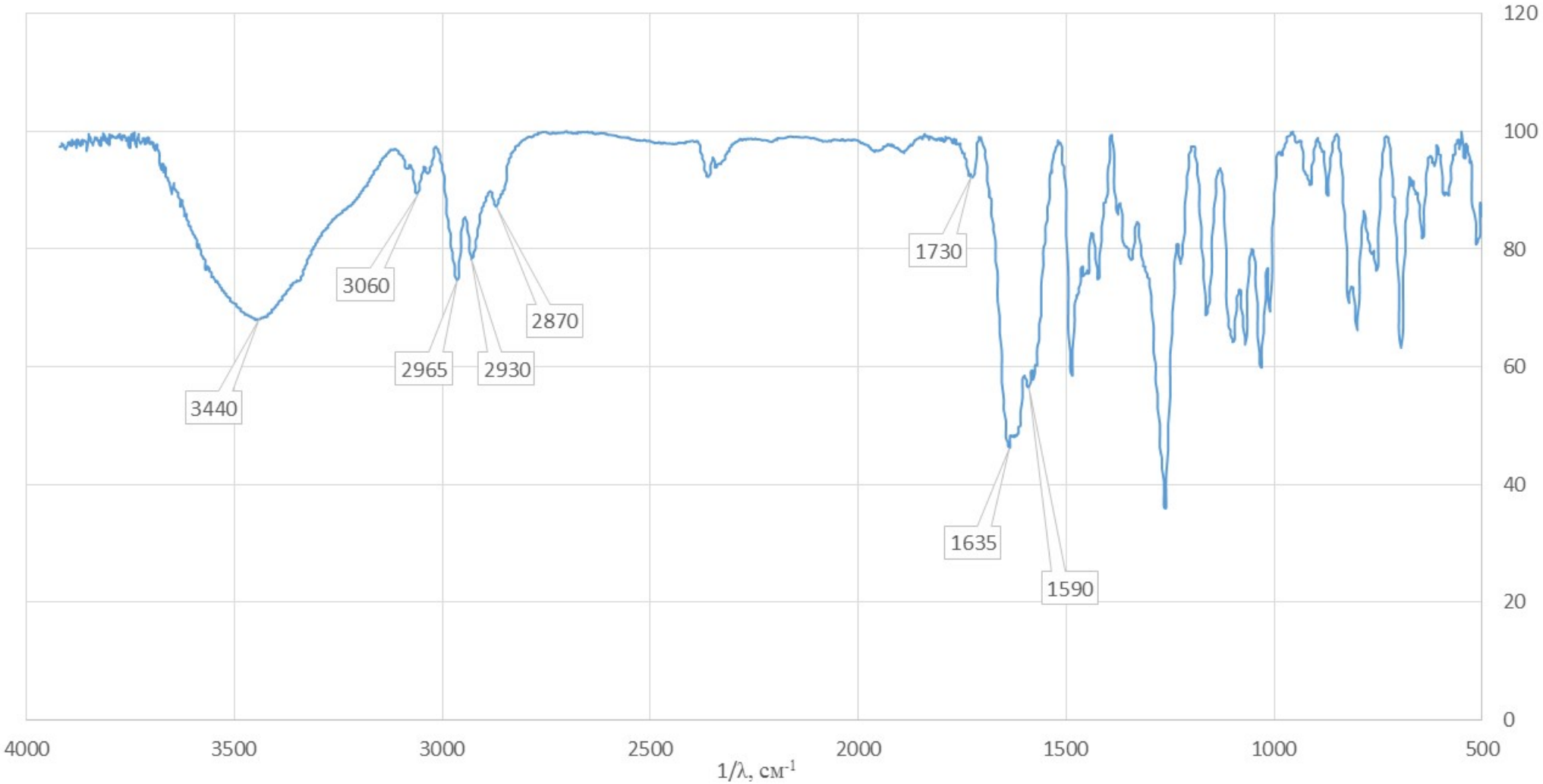


^{13}C *N*-(4-bromophenyl)-*N*'-(diethylcarbamoyl)-*N*-phenylbenzimidamide (4bd).

BUTc

BUTc, 151, BF = 100.612769 MHz, Solvent - CDCl3, 08 Jul 2014 T=299 K




120
100
80
60
40
20
0
4000
3500
3000
2500
2000
1500
1000
500
1/λ, см-1
3440
3060
2965
2930
2870
1730
1635
1590

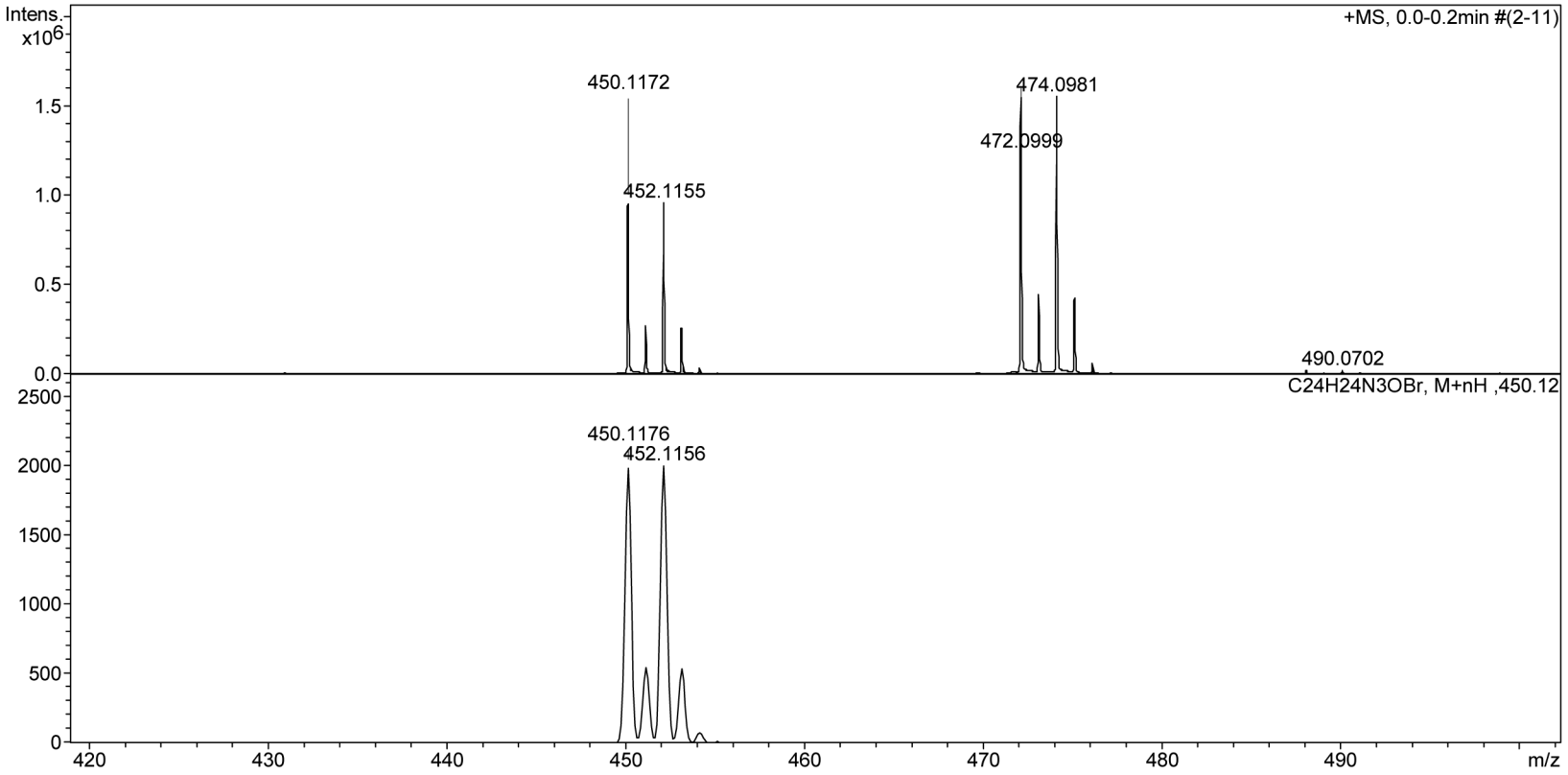
Mass Spectrum Report

Analysis Info

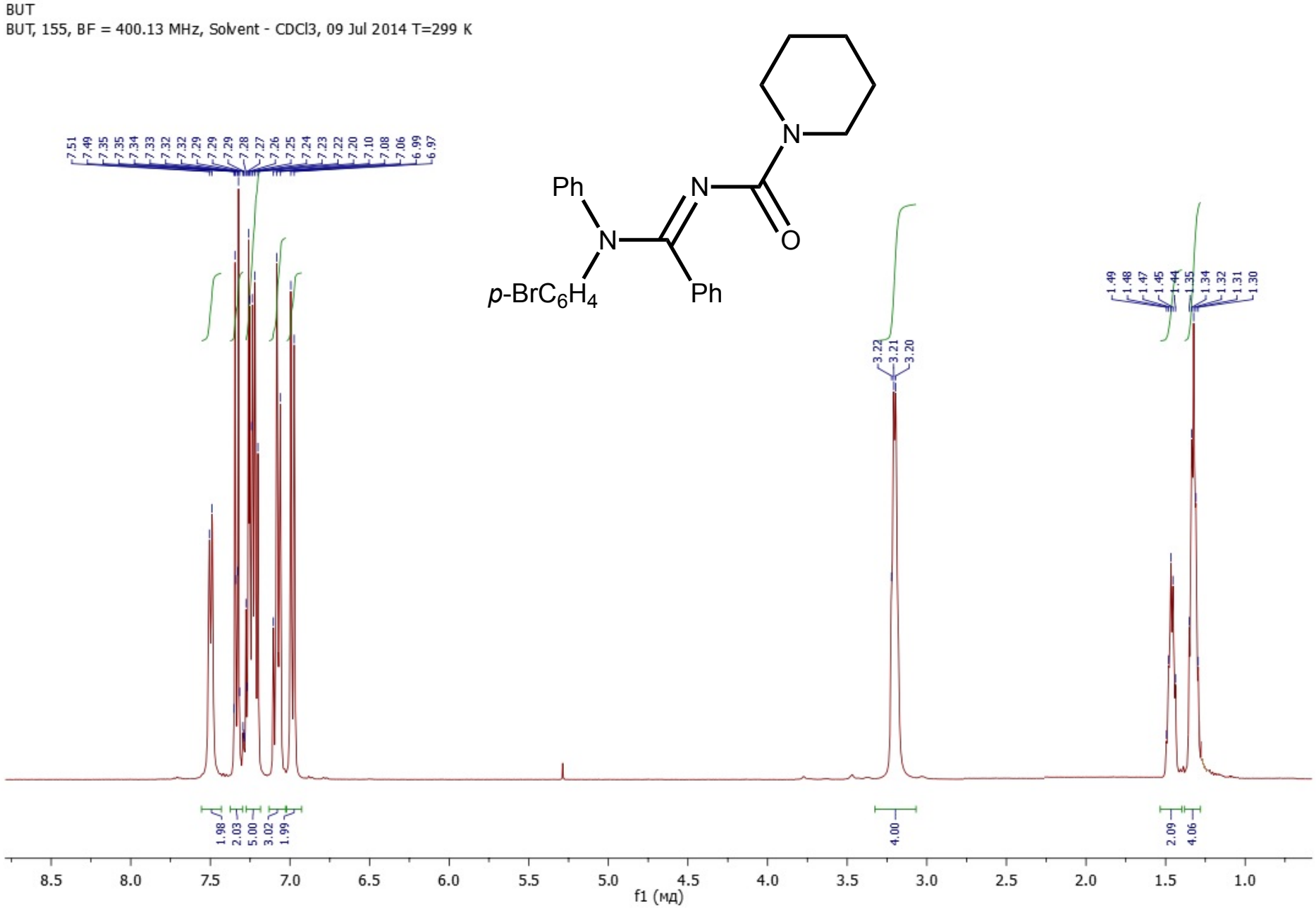
Analysis Name	D:\Data\mish2\BUT198fr6-7.d	Acquisition Date	09.07.2014 14:24:37
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT198fr6-7	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

Acquisition Parameter

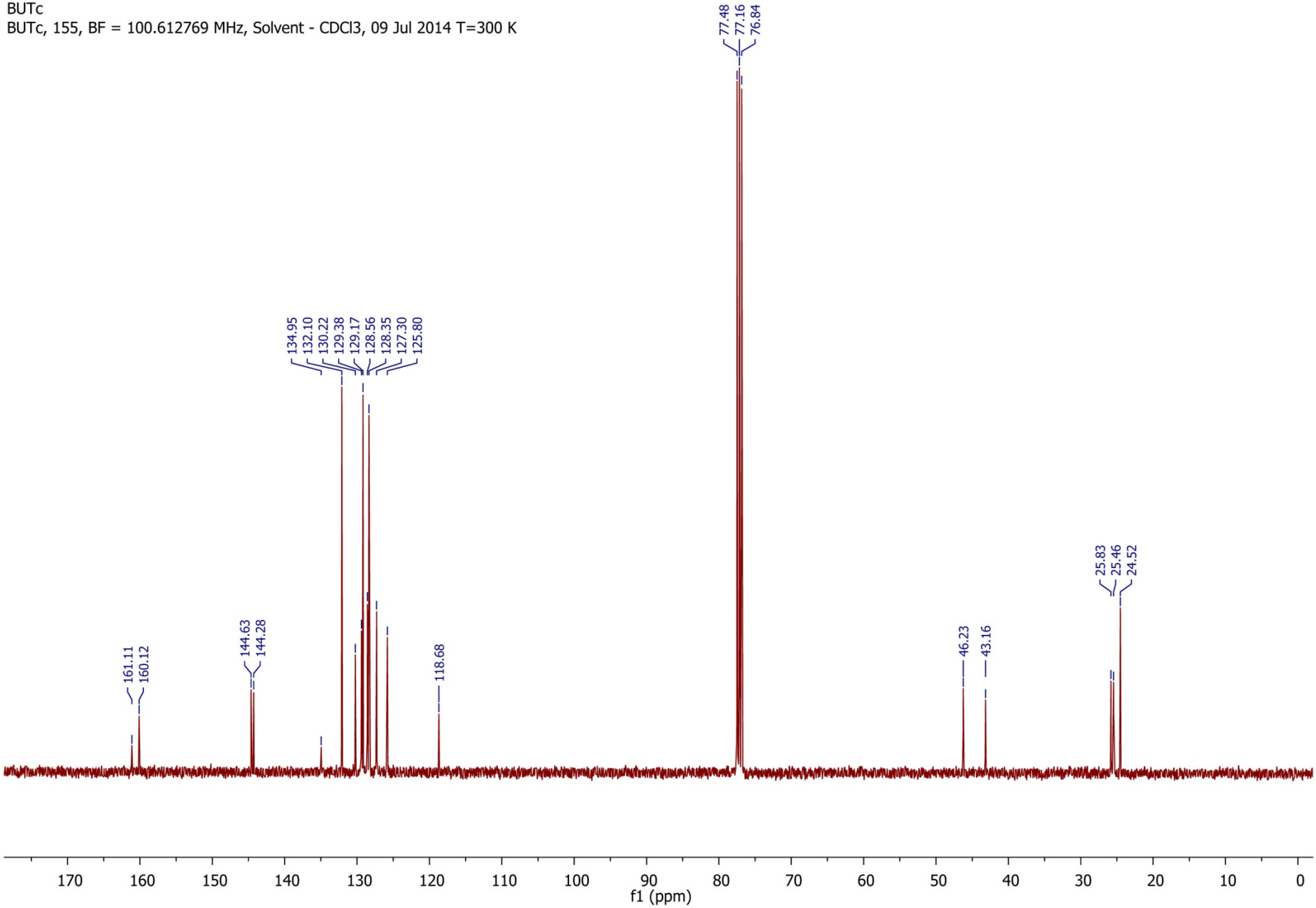
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

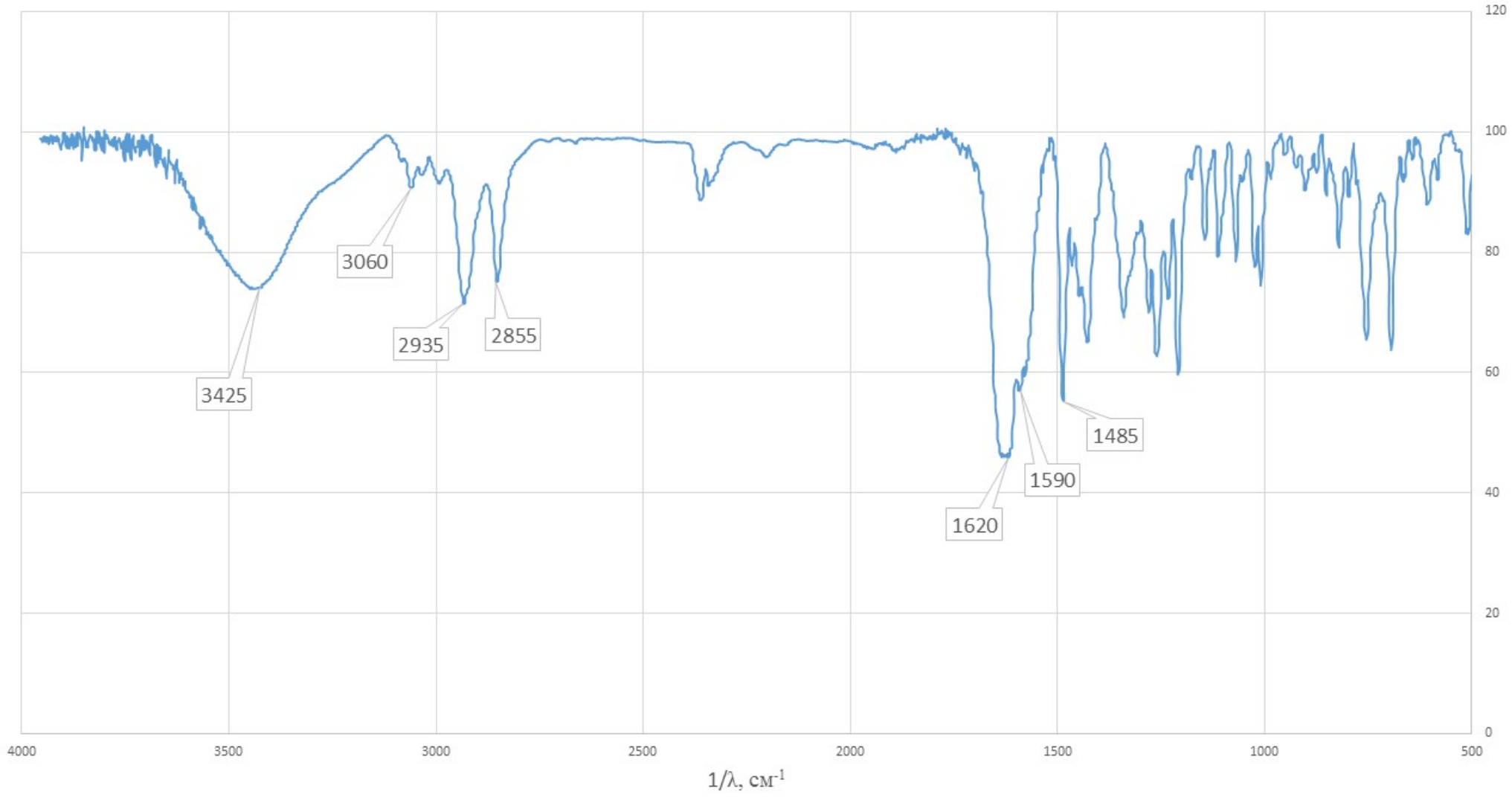


[1]H Piperidine-1-carboxylic acid [(4-bromo-phenyl)-phenyl-amino]-phenyl-methyleneamide (4cd).



^{13}C Piperidine-1-carboxylic acid [(4-bromo-phenyl)-phenyl-amino]-phenyl-methyleneamide (4cd).




3425
3060
2935
2855
1620
1590
1485
120
100
80
60
40
20
0
4000
3500
3000
2500
2000
1500
1000
500
1/λ, см-1

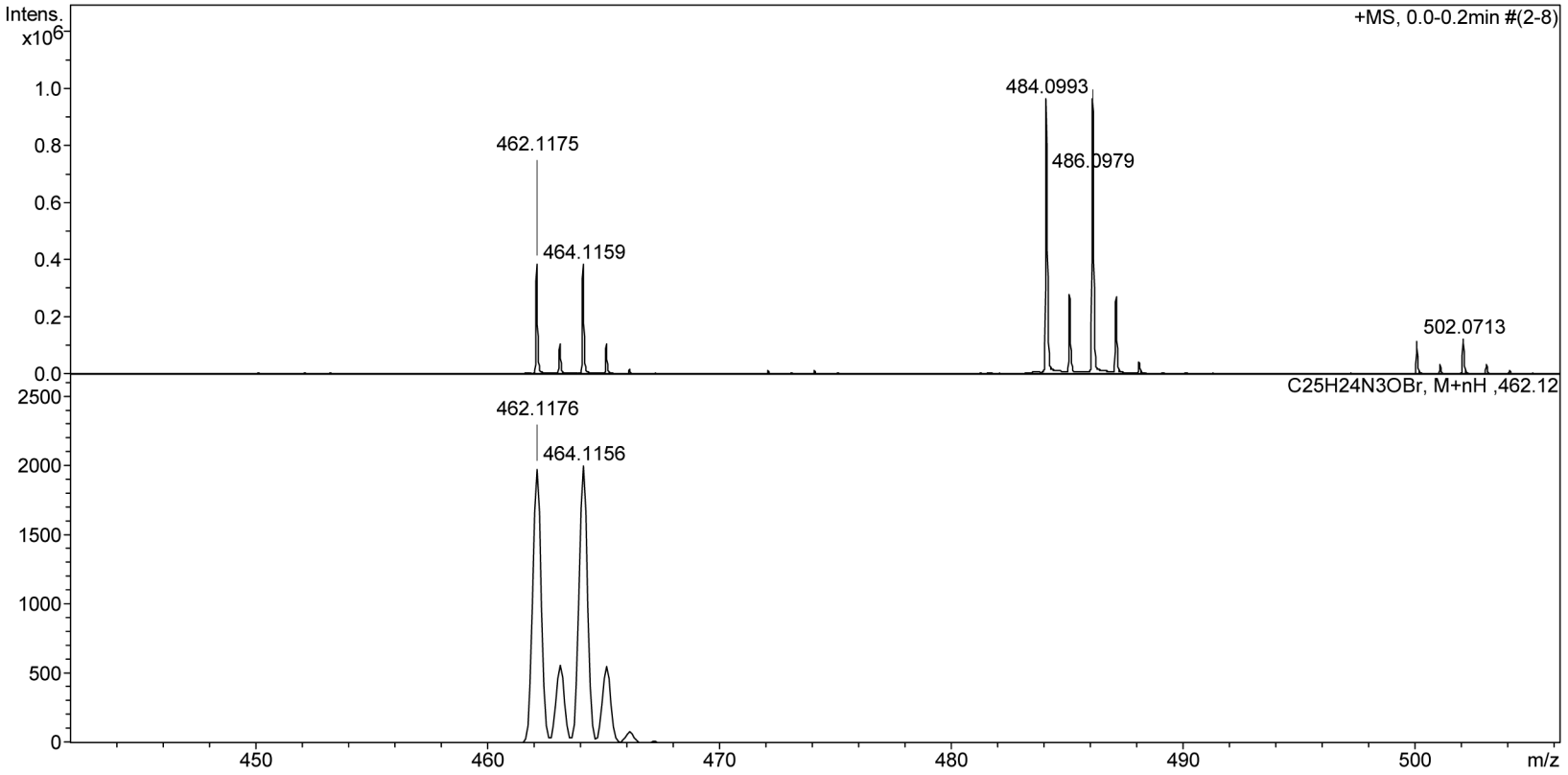
Mass Spectrum Report

Analysis Info

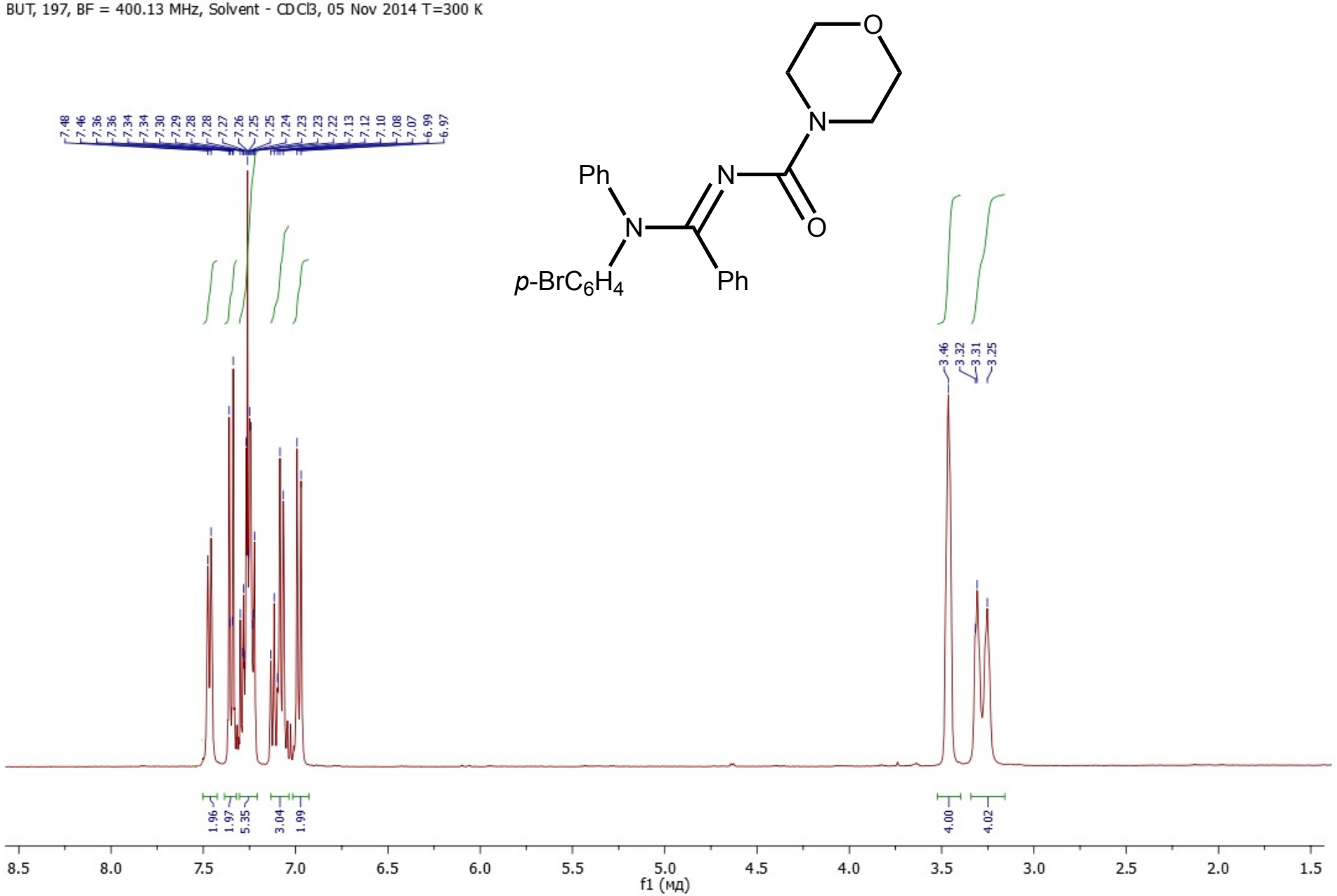
Analysis Name	D:\Data\mish2\BUT199fr10-11.d	Acquisition Date	09.07.2014 14:42:45
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT199fr10-11	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

Acquisition Parameter

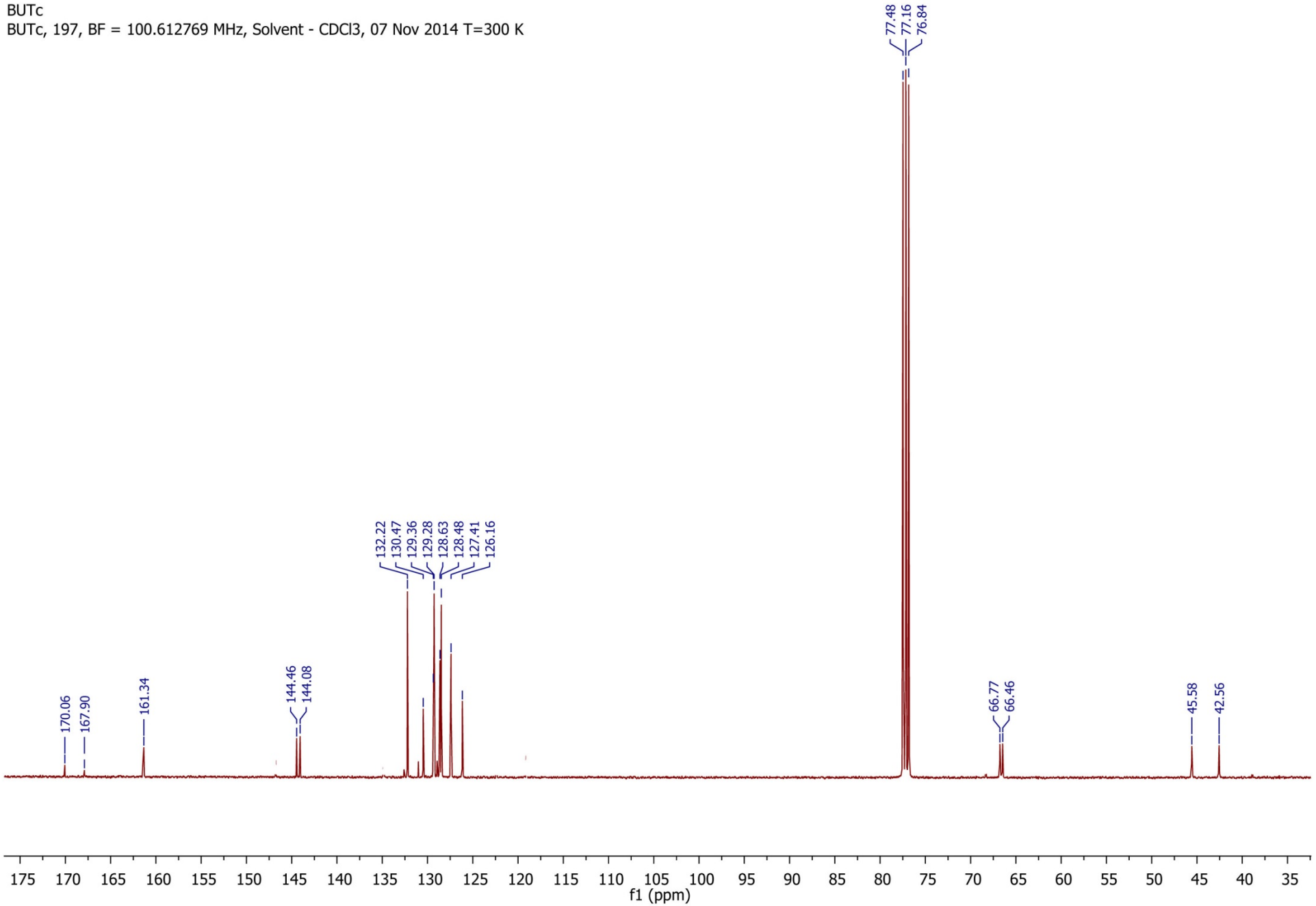
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

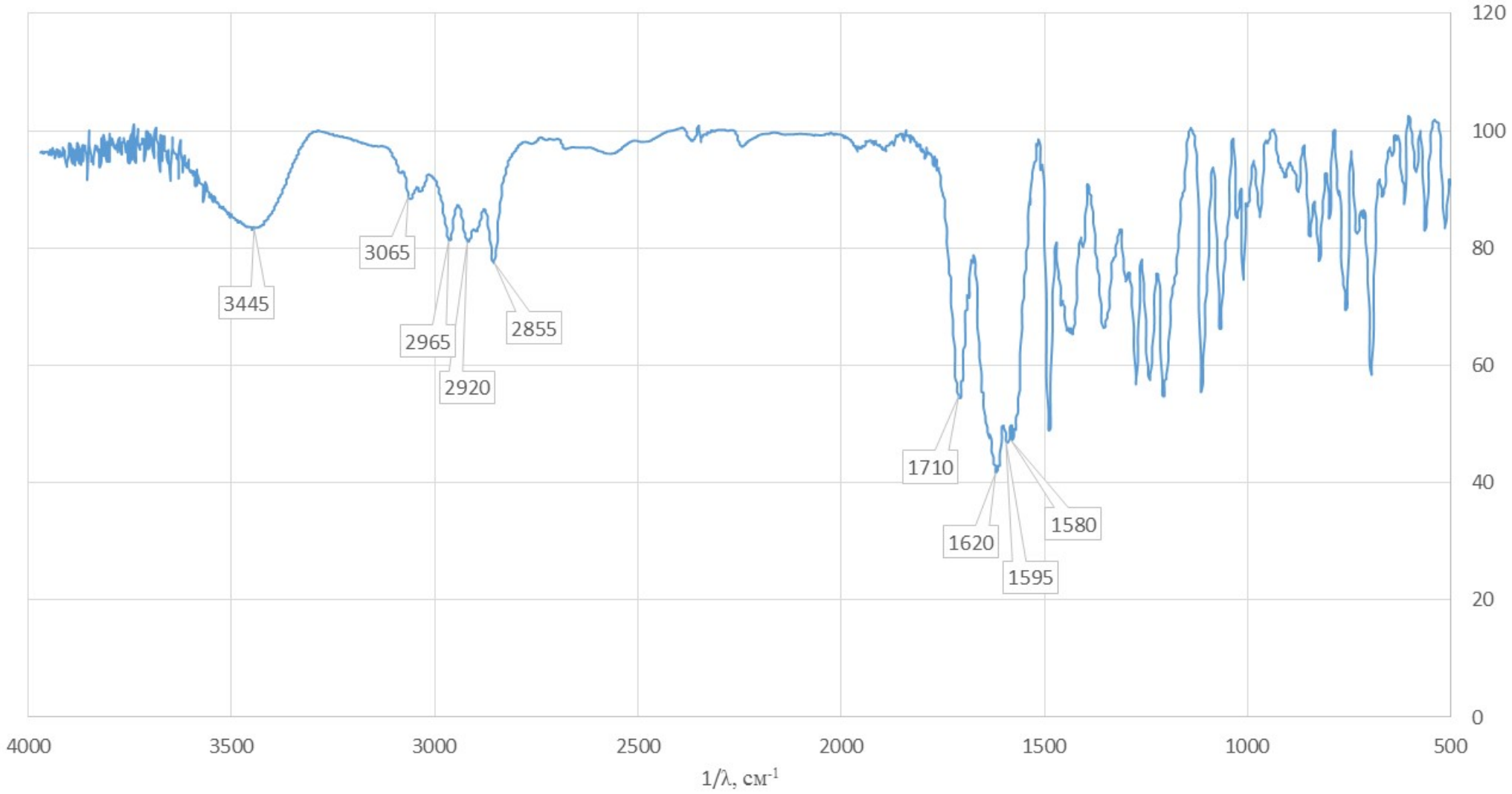


^{1}H *N*-((4-bromophenyl)(diphenylamino)methylene)morpholine-4-carboxamide (4dd).



^{13}C *N*-((4-bromophenyl)(diphenylamino)methylene)morpholine-4-carboxamide (4dd).



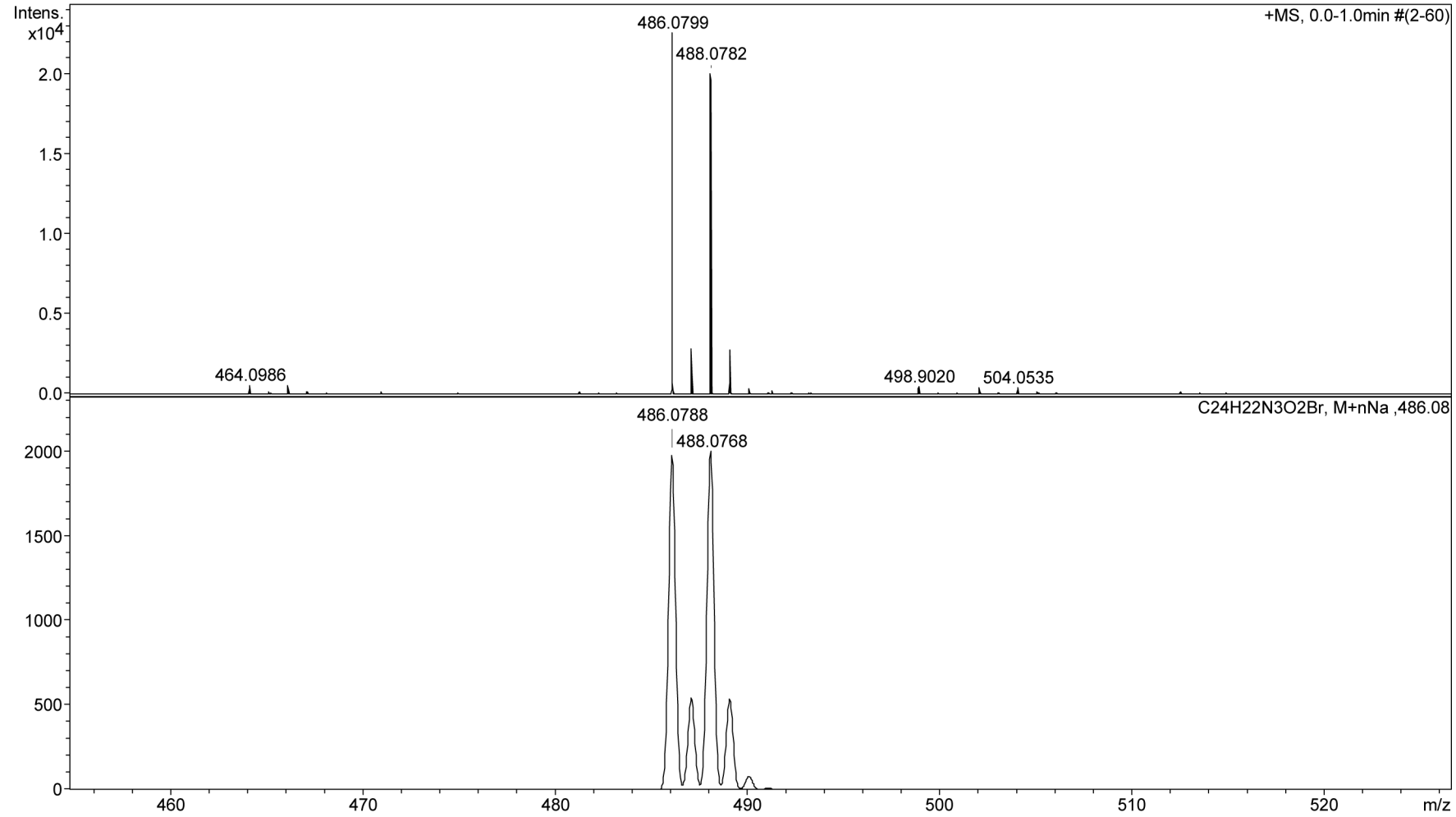

120
100
80
60
40
20
0
4000
3500
3000
2500
2000
1500
1000
500
1/λ, см-1
3445
3065
2965
2920
2855
1710
1620
1595
1580

Analysis Info

Analysis Name	D:\Data\Work\2014\november\05\BUT224_11000001.d	Acquisition Date	11/5/2014 4:54:43 PM
Method	tune_low_pos.m	Operator	BDAL@DE
Sample Name	BUT224_11	Instrument	maXis 62
Comment	MeOH		

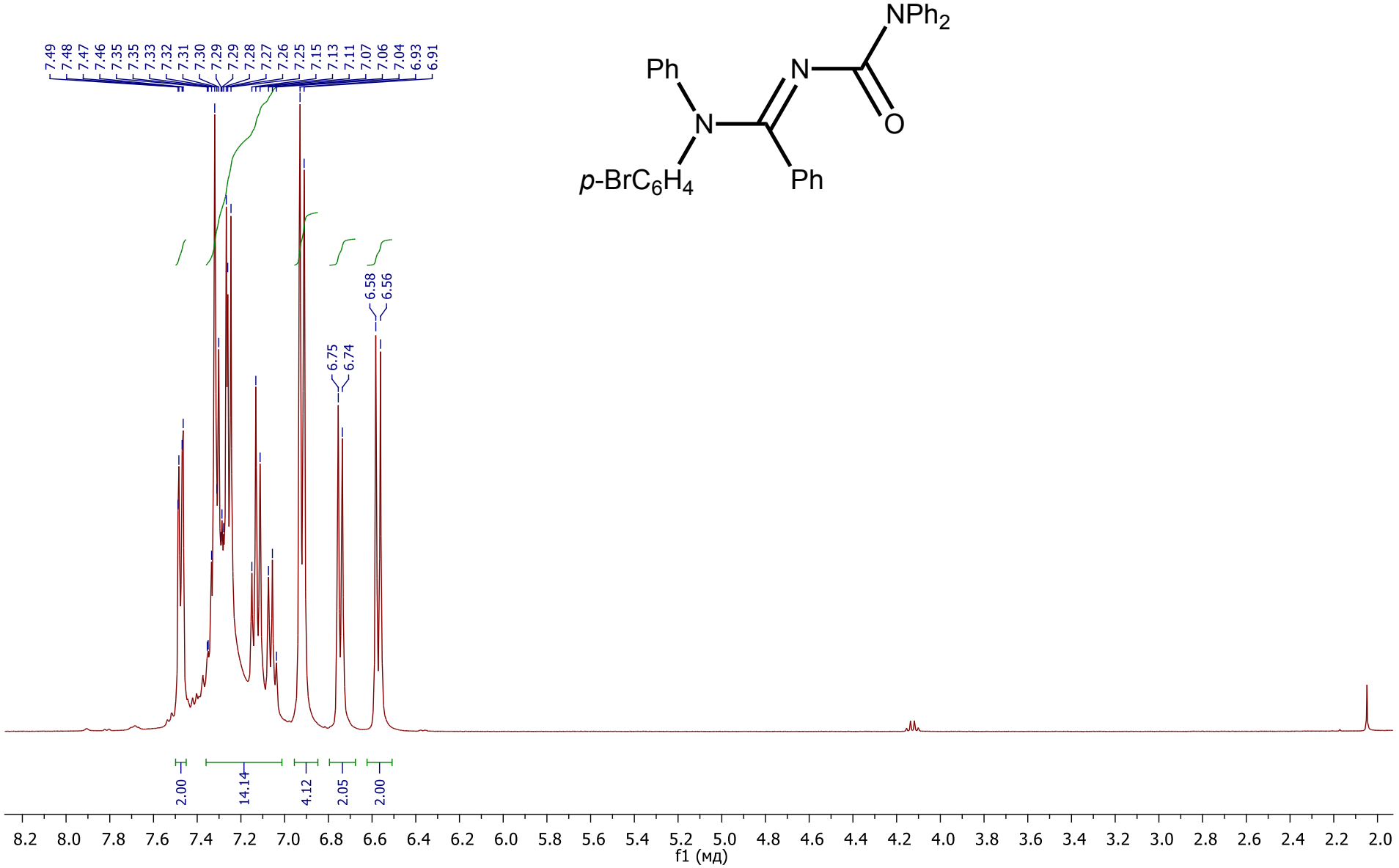
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1100 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

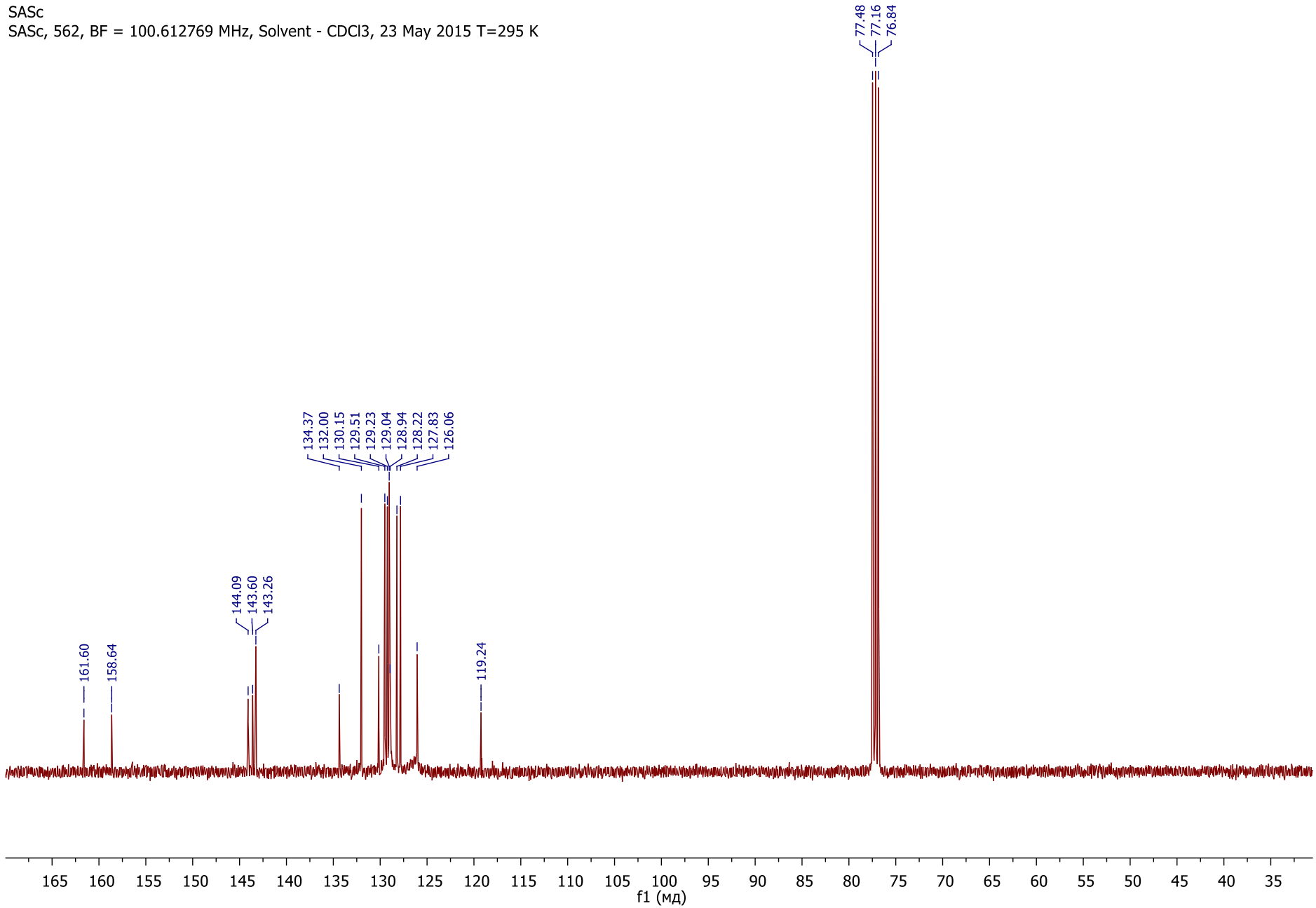


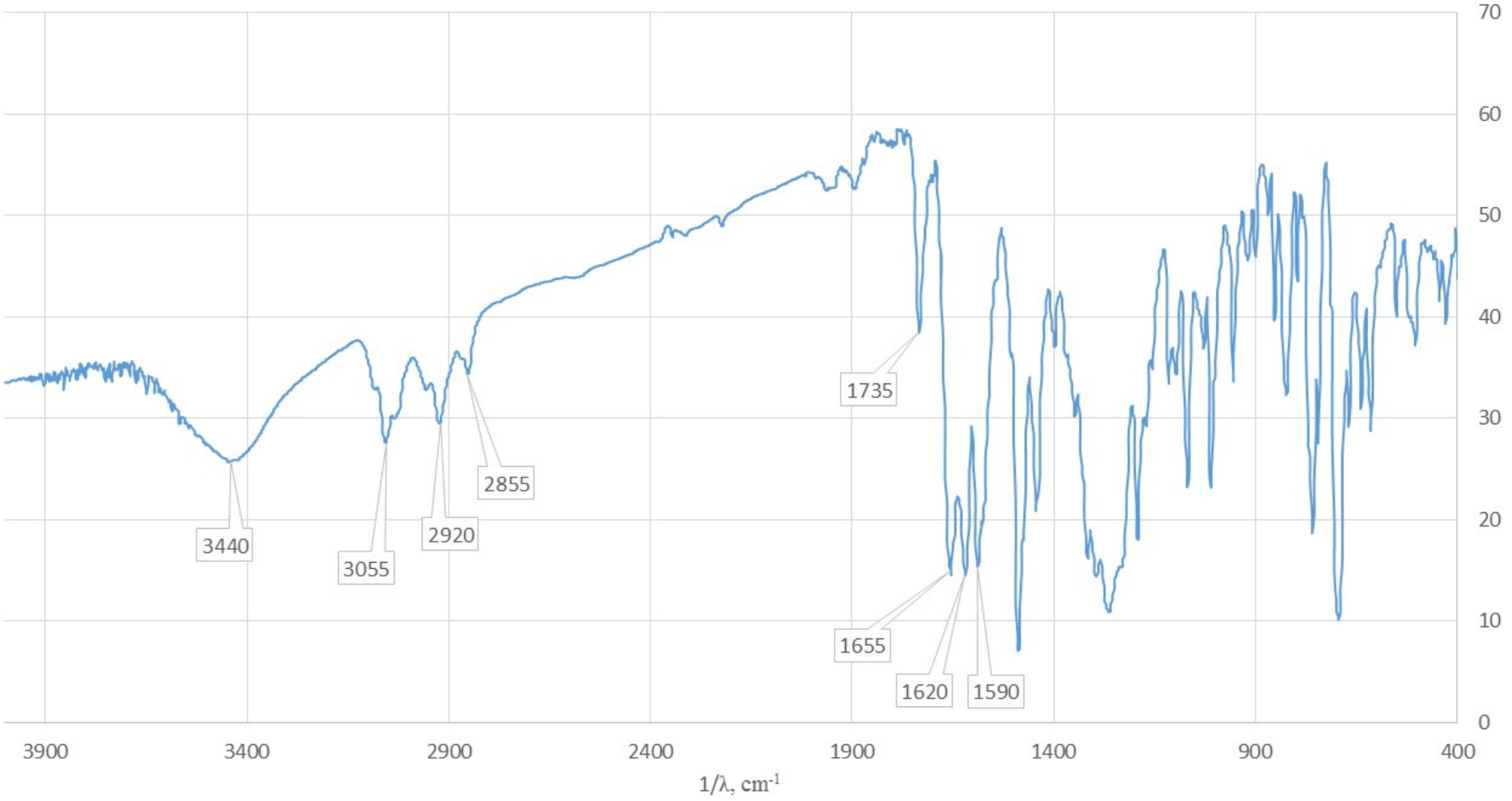
^{1}H 4-bromo-*N′*-(diphenylcarbamoyl)-*N*,*N*-diphenylbenzimidamide (4ed).

SAS
SAS, 562, BF = 400.13 MHz, Solvent - CDCl3, 23 May 2015 T=295 K



^{13}C 4-bromo-*N′*-(diphenylcarbamoyl)-*N*,*N*-diphenylbenzimidamide (4ed).




3440
3055
2920
2855
1735
1655
1620
1590
3900
3400
2900
2400
1900
1400
900
400
1/λ, cm-1
70
60
50
40
30
20
10
0

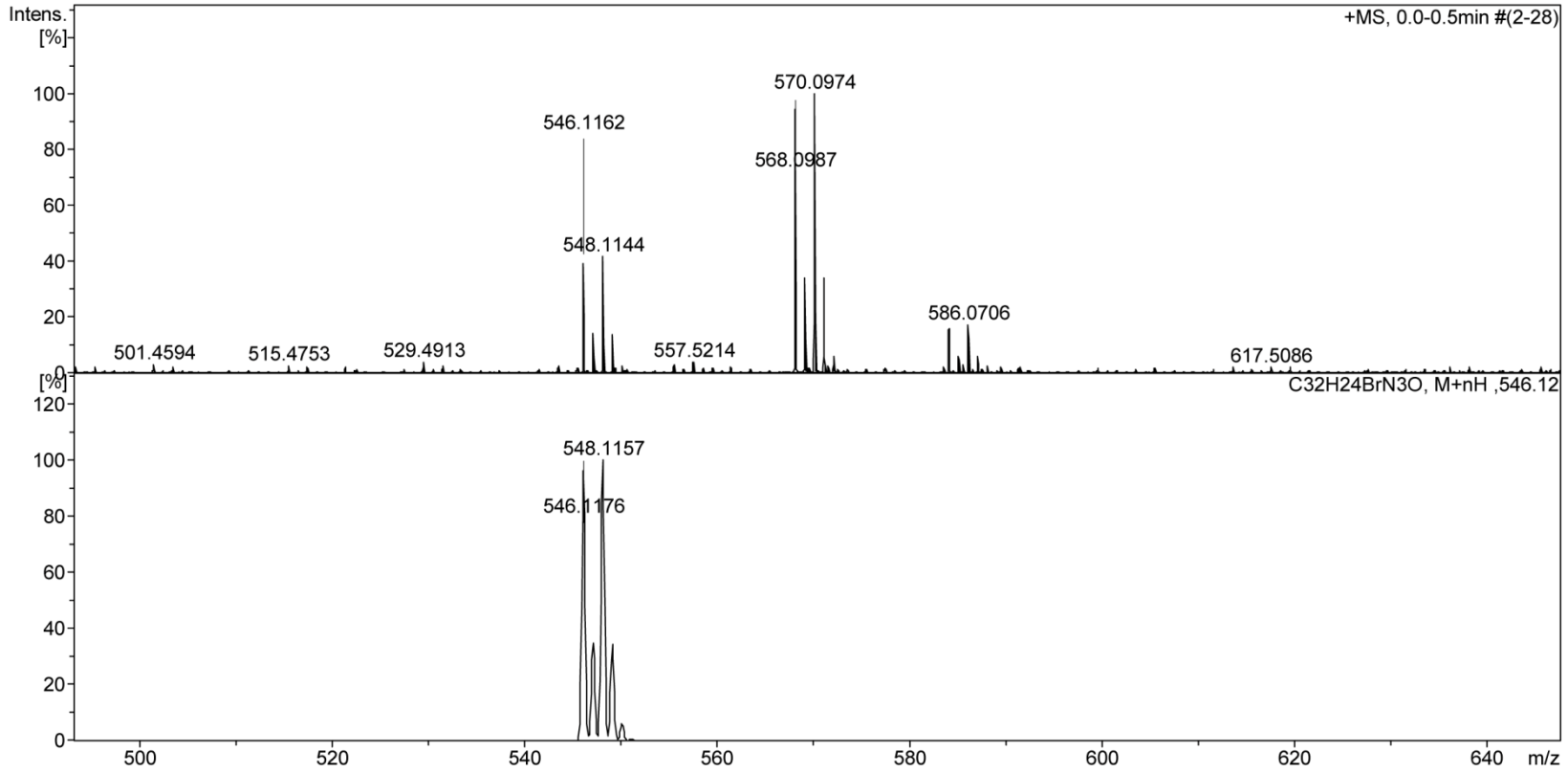
Mass Spectrum Report

Analysis Info

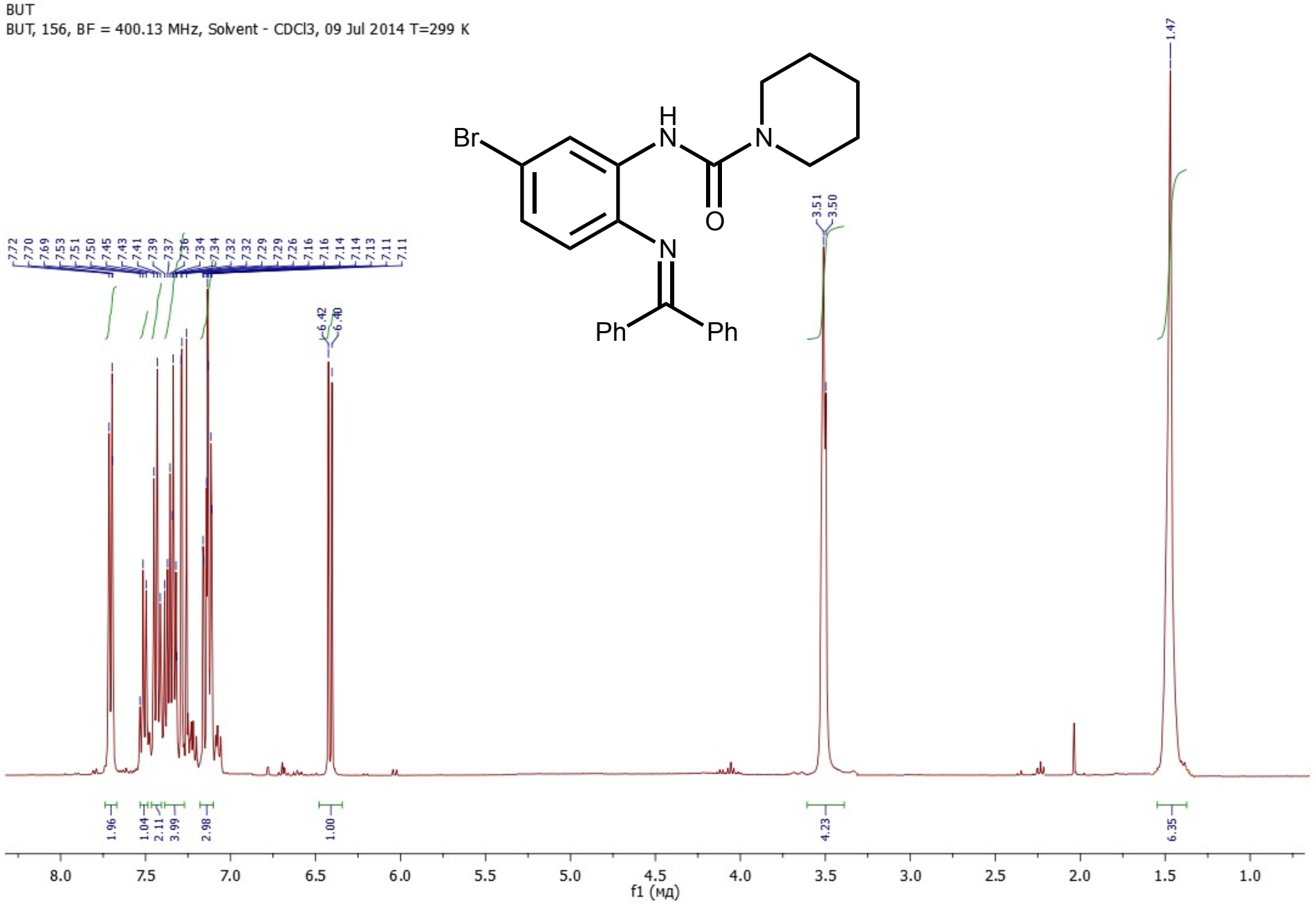
Analysis Name	D:\Data\June 2015\BUT22.d	Acquisition Date	03.06.2015 16:34:03
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT22	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

Acquisition Parameter

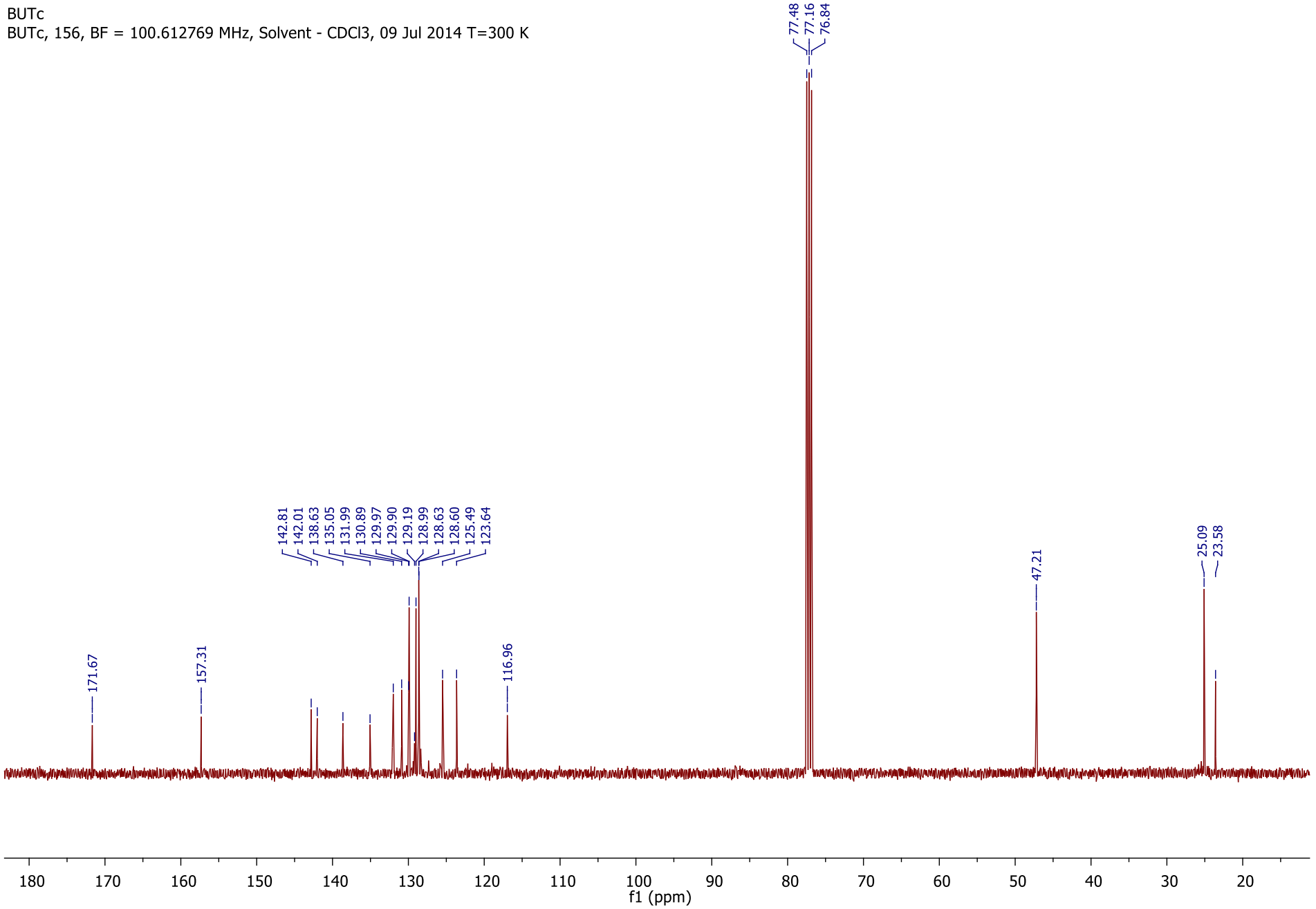
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



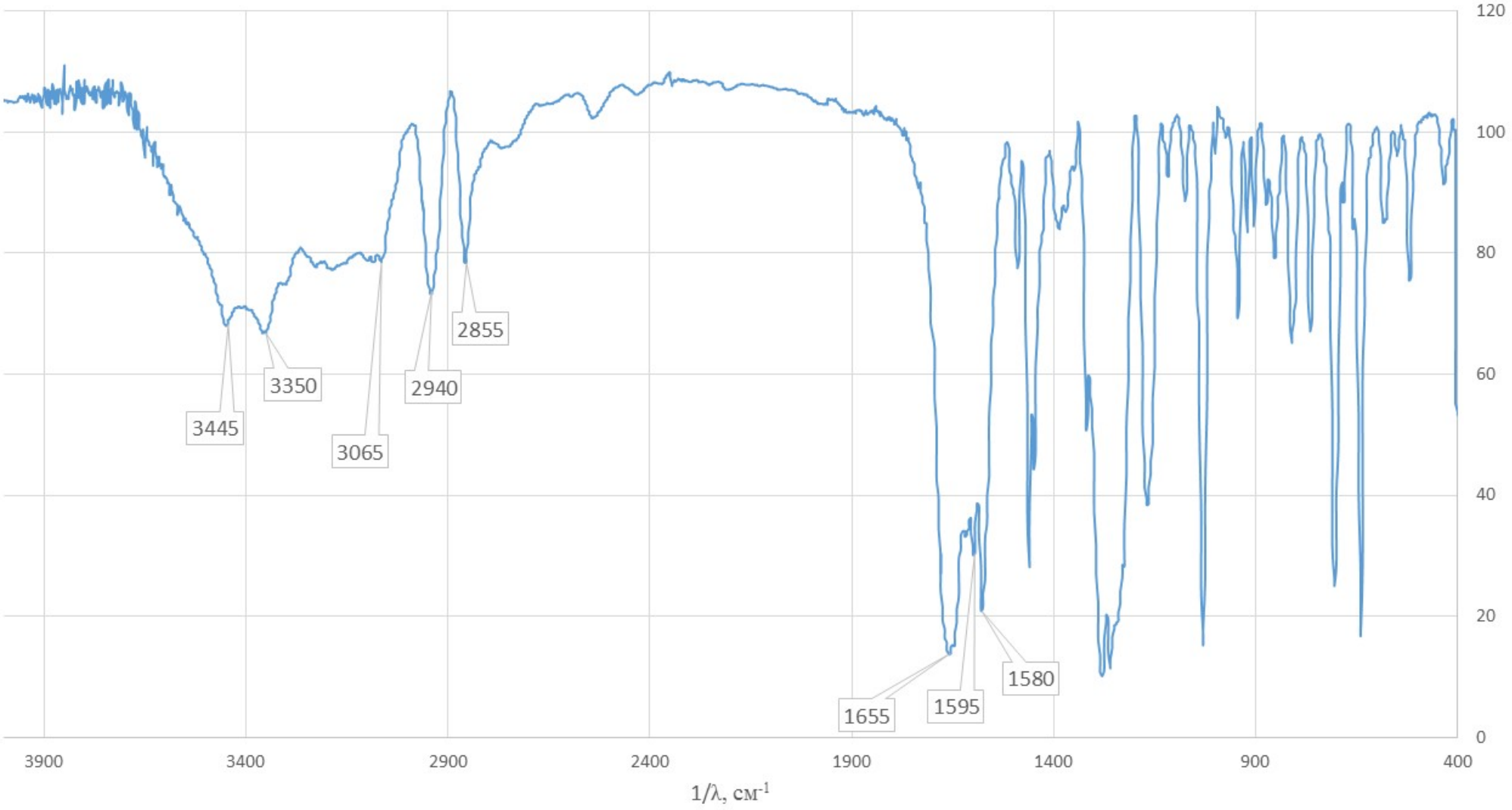
^{1}H *N*-(5-bromo-2-((diphenylmethylene)amino)phenyl)piperidine-1-carboxamide (6cd).



^{13}C *N*-(5-bromo-2-((diphenylmethylene)amino)phenyl)piperidine-1-carboxamide (6cd).



20b


120
100
80
60
40
20
0
3445
3350
3065
2940
2855
1655
1595
1580
3900
3400
2900
2400
1900
1400
900
400
1/λ, см-1

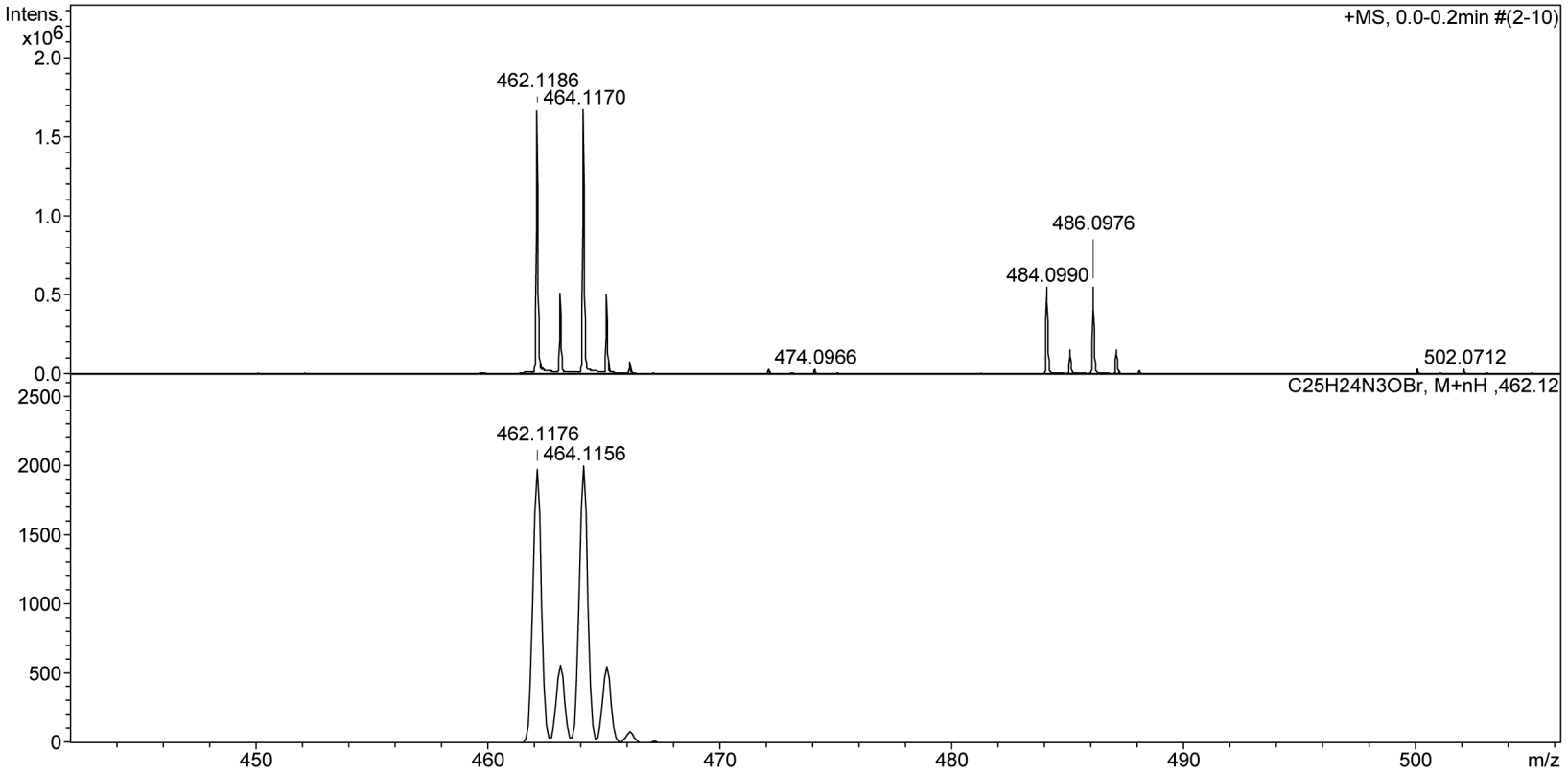
Mass Spectrum Report

Analysis Info

Analysis Name	D:\Data\mish2\BUT199fr12.d	Acquisition Date	09.07.2014 14:44:57
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT199fr12	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

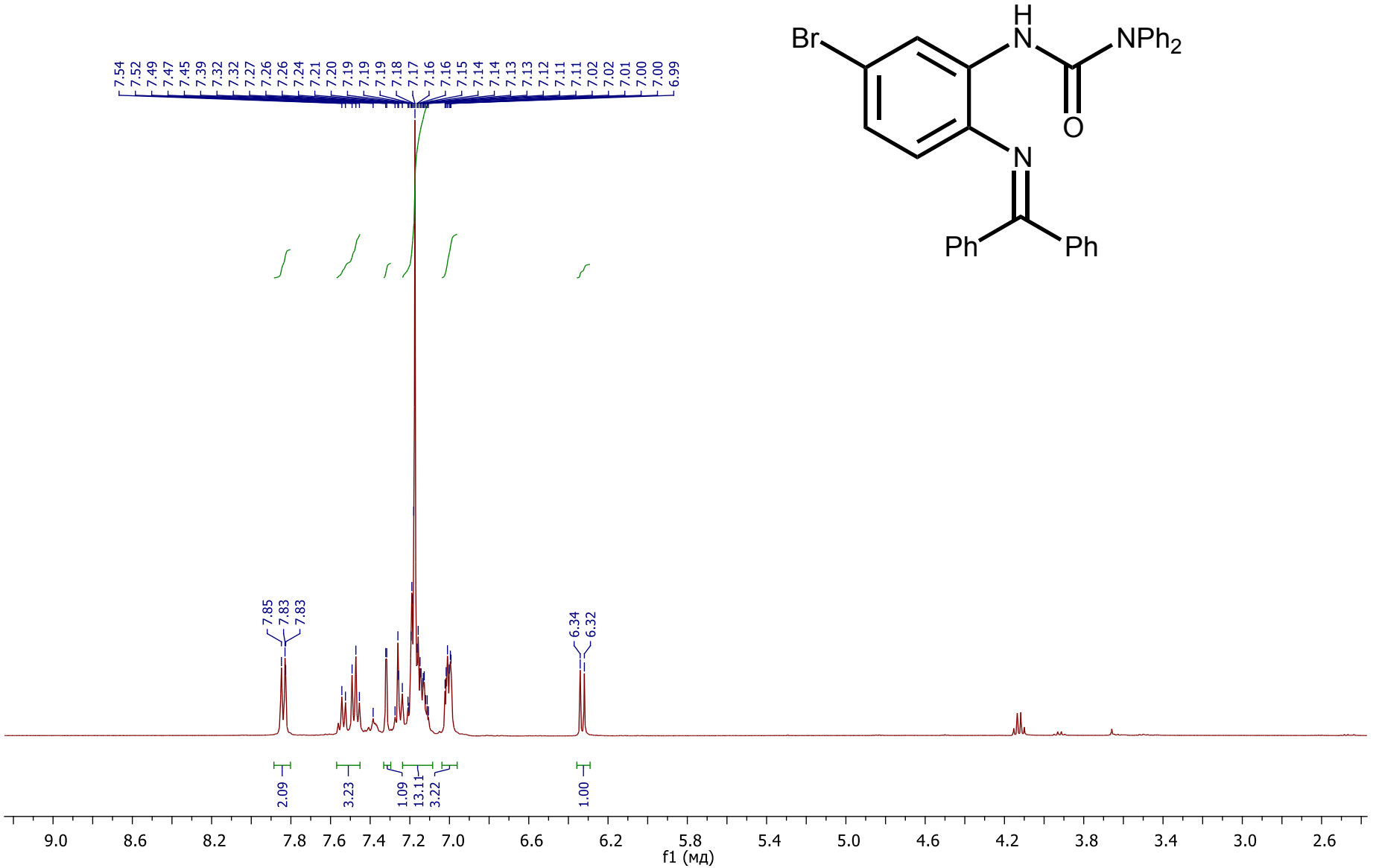
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



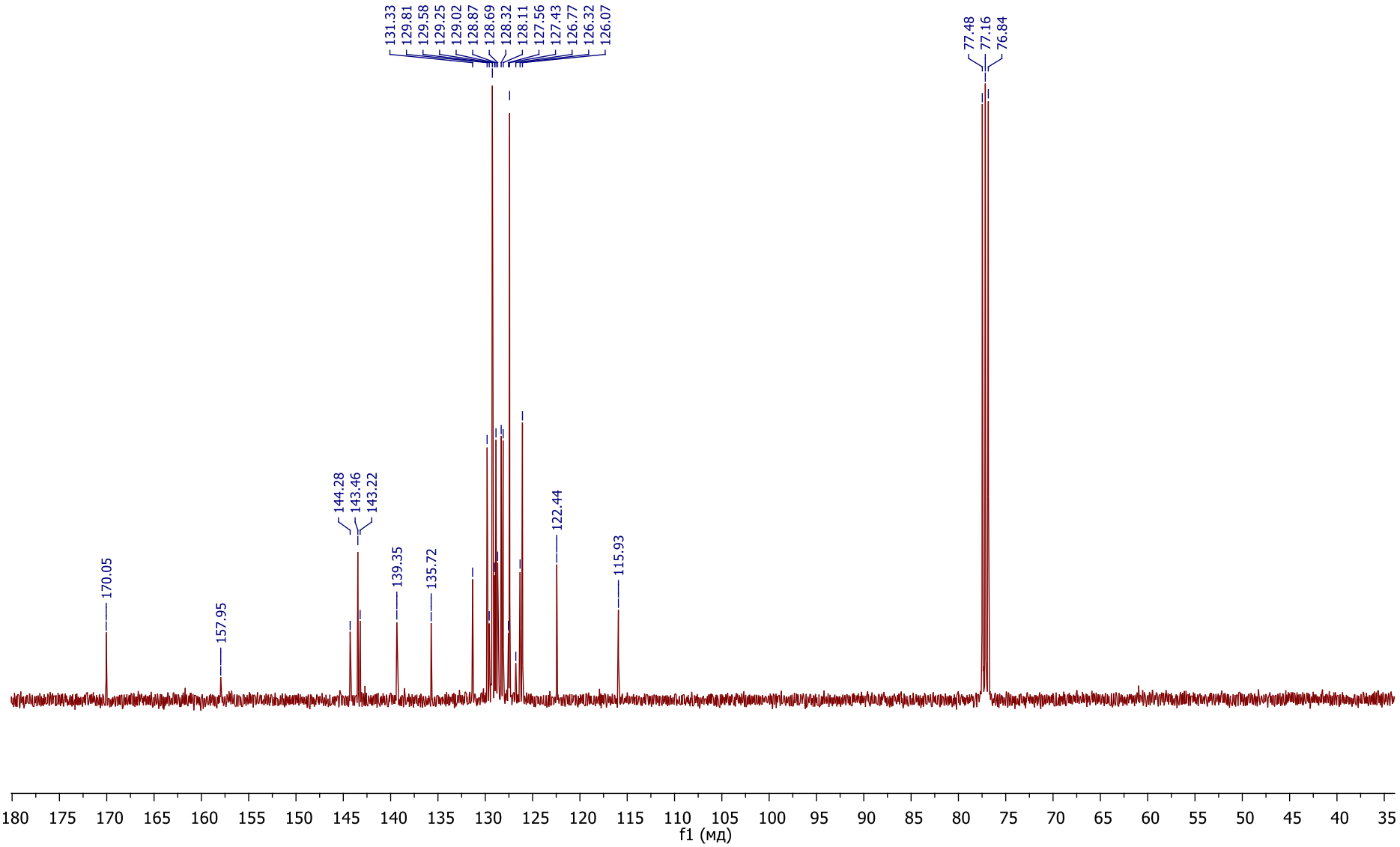
^{1}H *N′*-(4-bromo-2-(diphenylmethyleneamino)phenyl)-*N,N*-diphenylcarbamimidic acid (6ed).

AMJ
AMJ, 247, BF = 400.13 MHz, Solvent - CDCl3, 21 May 2015 T=295 K

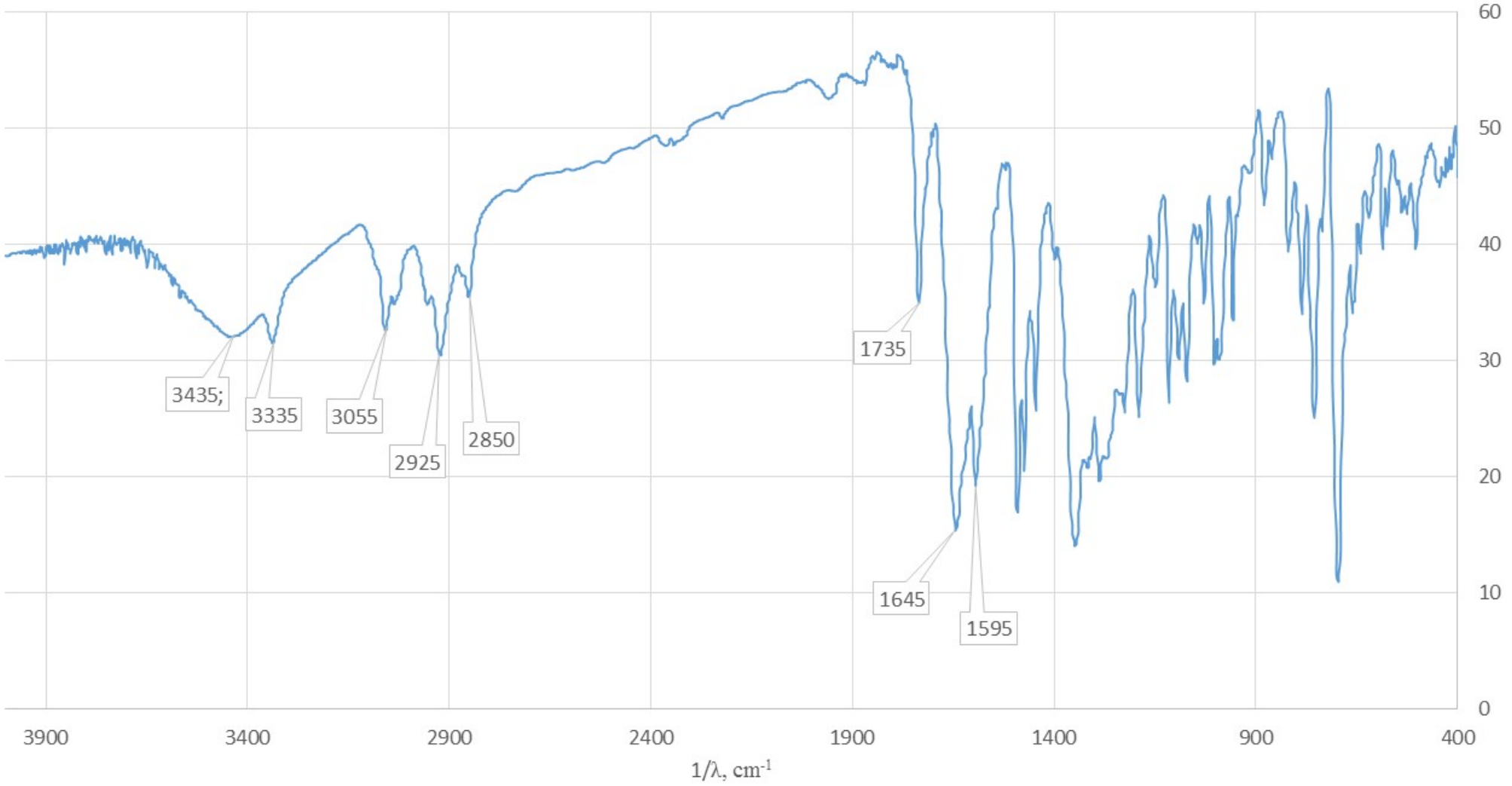


^{13}C *N′*-(4-bromo-2-(diphenylmethyleneamino)phenyl)-*N,N*-diphenylcarbamimidic acid (6ed).

SASc
SASc, 255, BF = 100.612769 MHz, Solvent - CDCl3, 19 Jun 2015 T=296 K



22b


3435;
3335
3055
2925
2850
1735
1645
1595
60
50
40
30
20
10
0
3900
3400
2900
2400
1900
1400
900
400
1/λ, cm-1

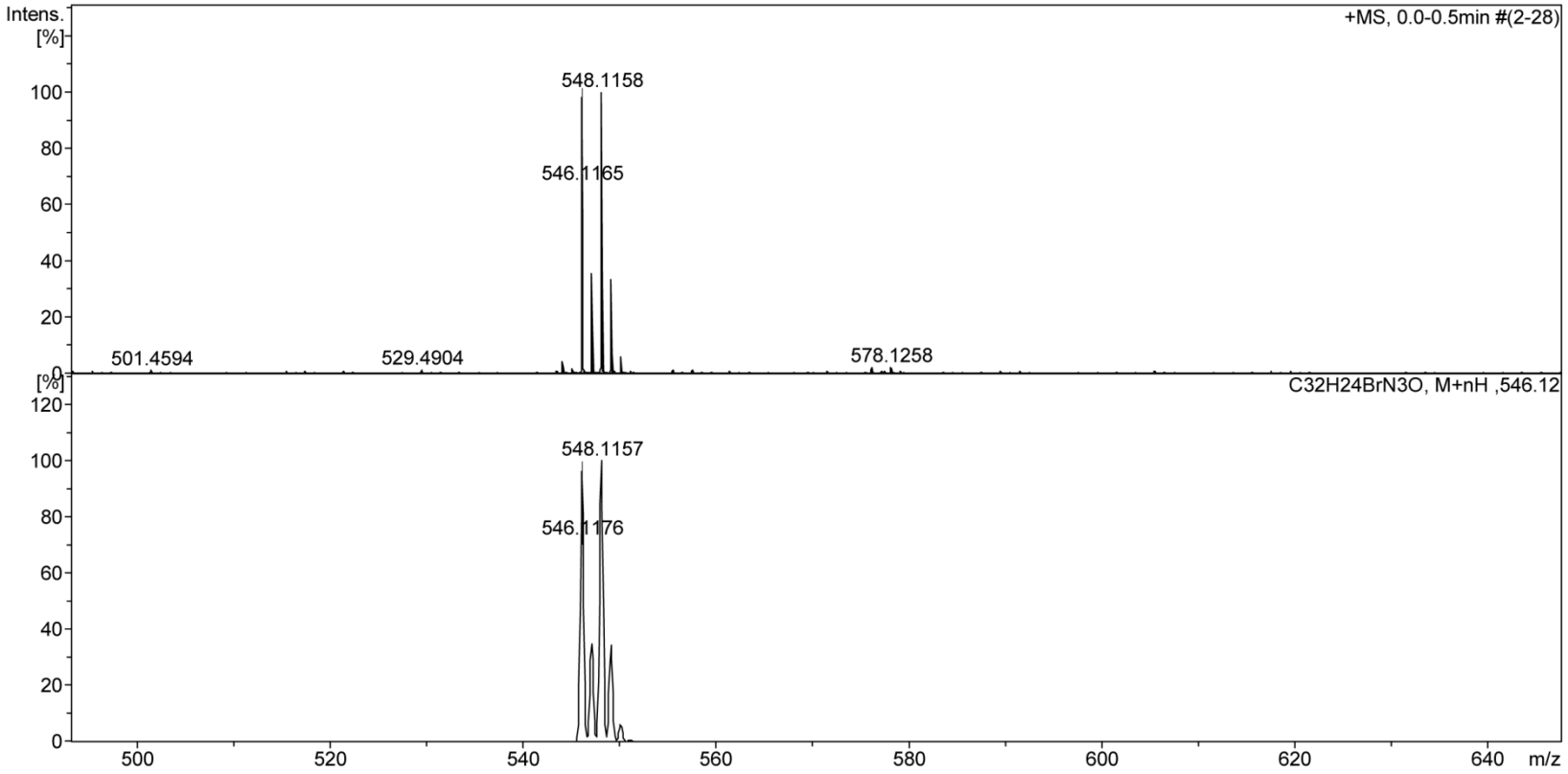
Mass Spectrum Report

Analysis Info

Analysis Name	D:\Data\June 2015\BUT22b.d	Acquisition Date	03.06.2015 16:36:14
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT22b	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

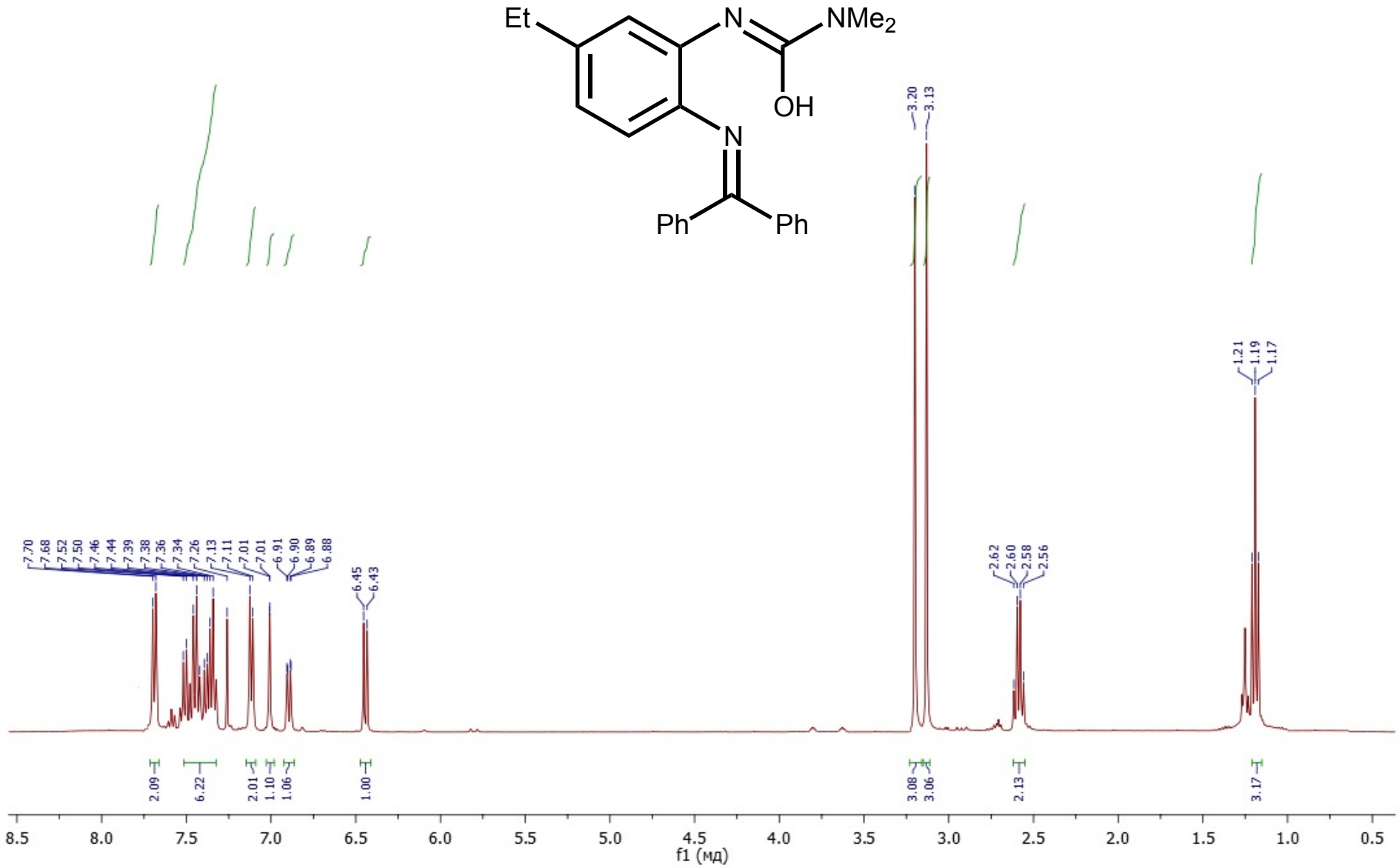
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

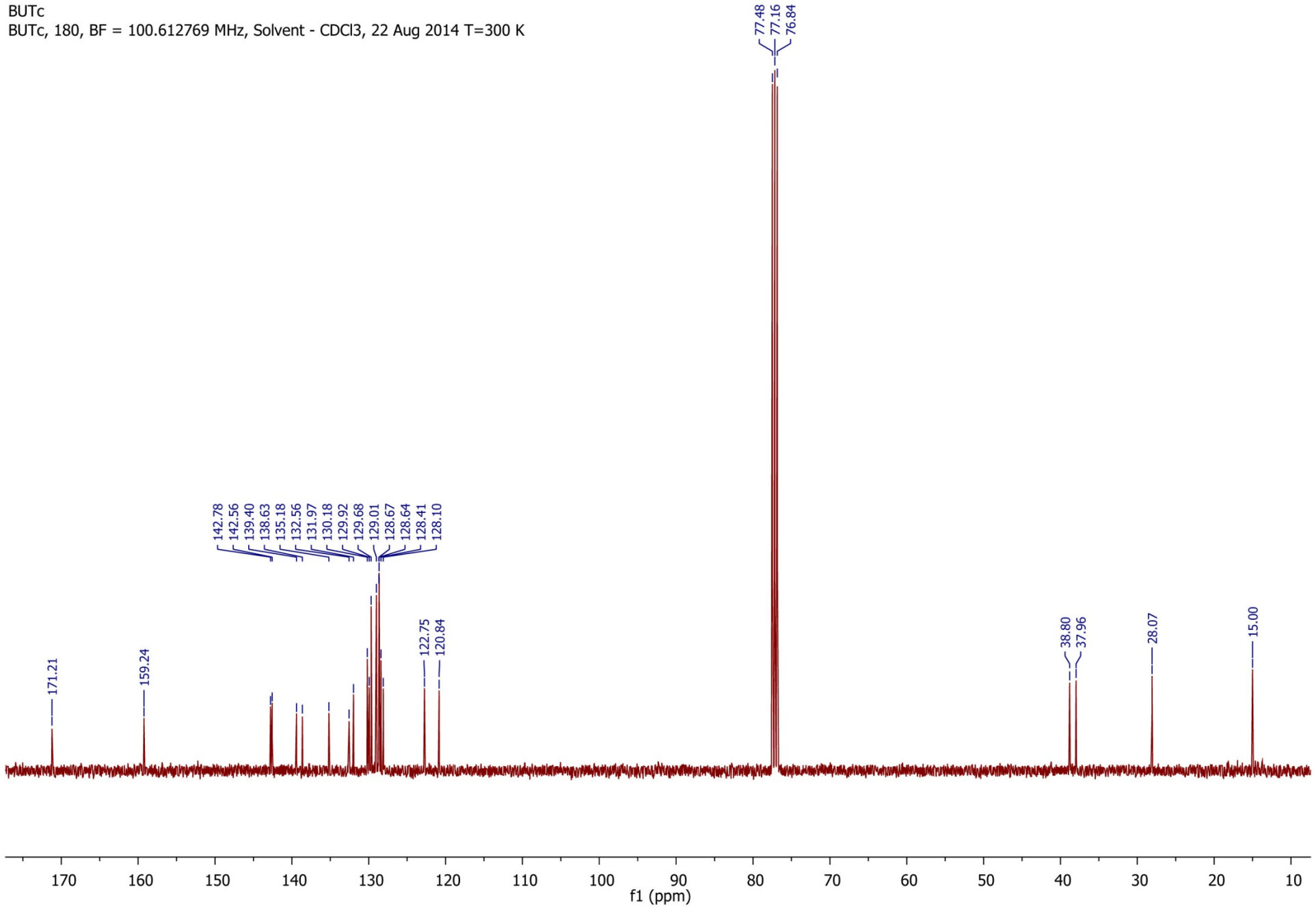


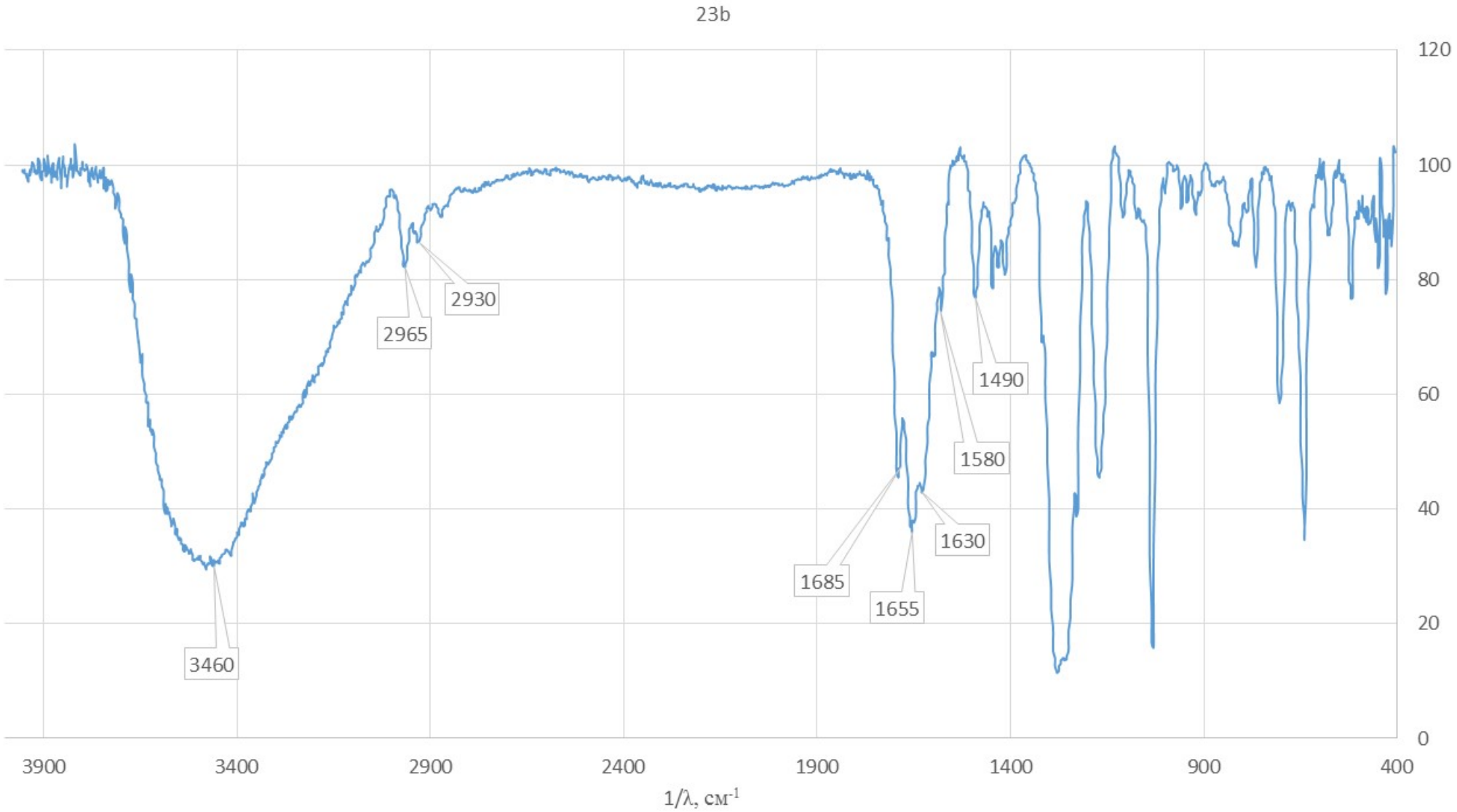
^{1}H 3-(2-((diphenylmethylene)amino)-5-ethylphenyl)-1,1-dimethylurea (6ae).

BUT
BUT, 180, BF = 400.13 MHz, Solvent - CDCl3, 22 Aug 2014 T=300 K



^{13}C 3-(2-((diphenylmethylene)amino)-5-ethylphenyl)-1,1-dimethylurea (6ae).



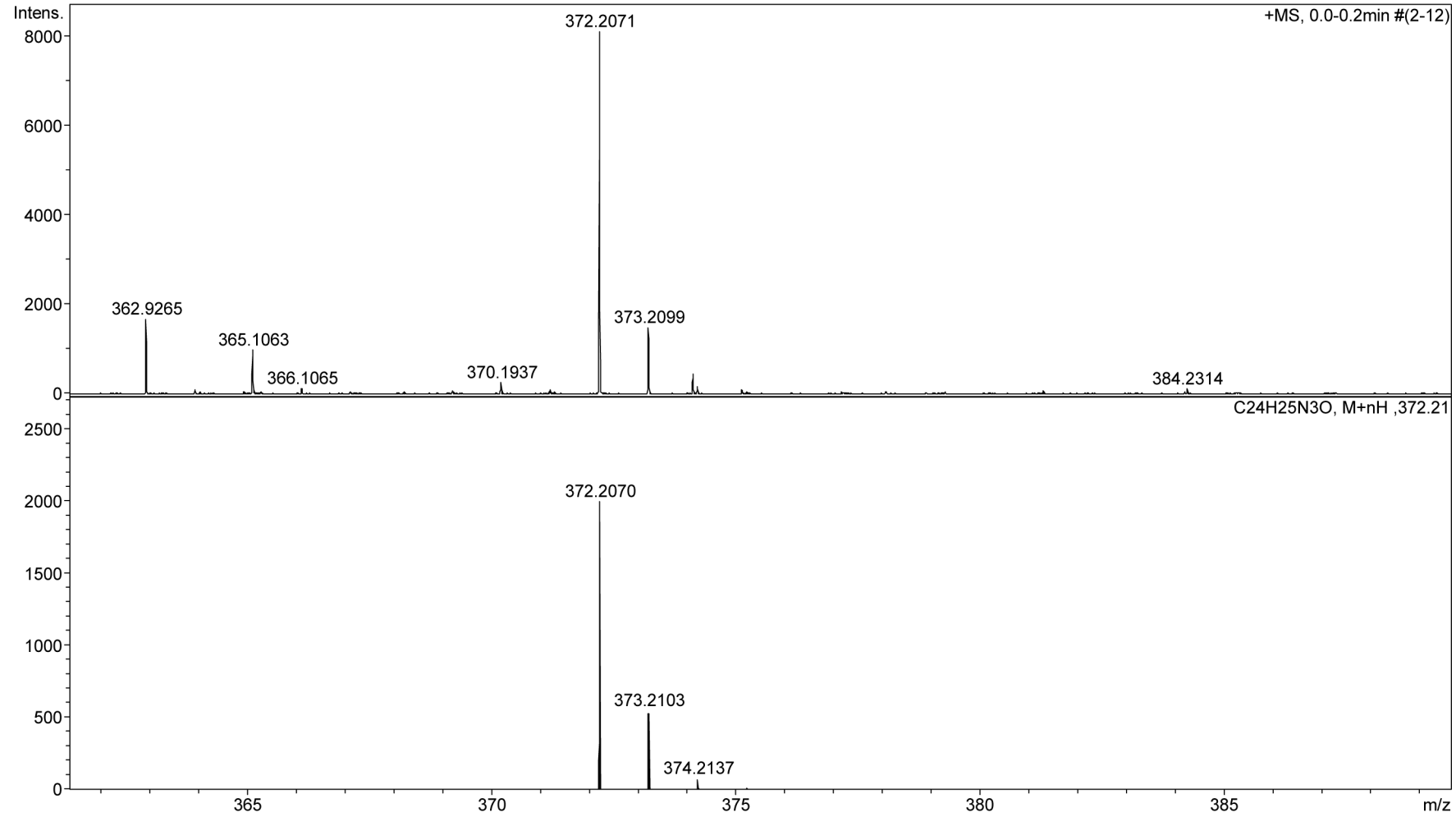

23b
120
100
80
60
40
20
0
3900
3400
2900
2400
1900
1400
900
400
1/λ, см-1
3460
2965
2930
1685
1655
1630
1580
1490

Analysis Info

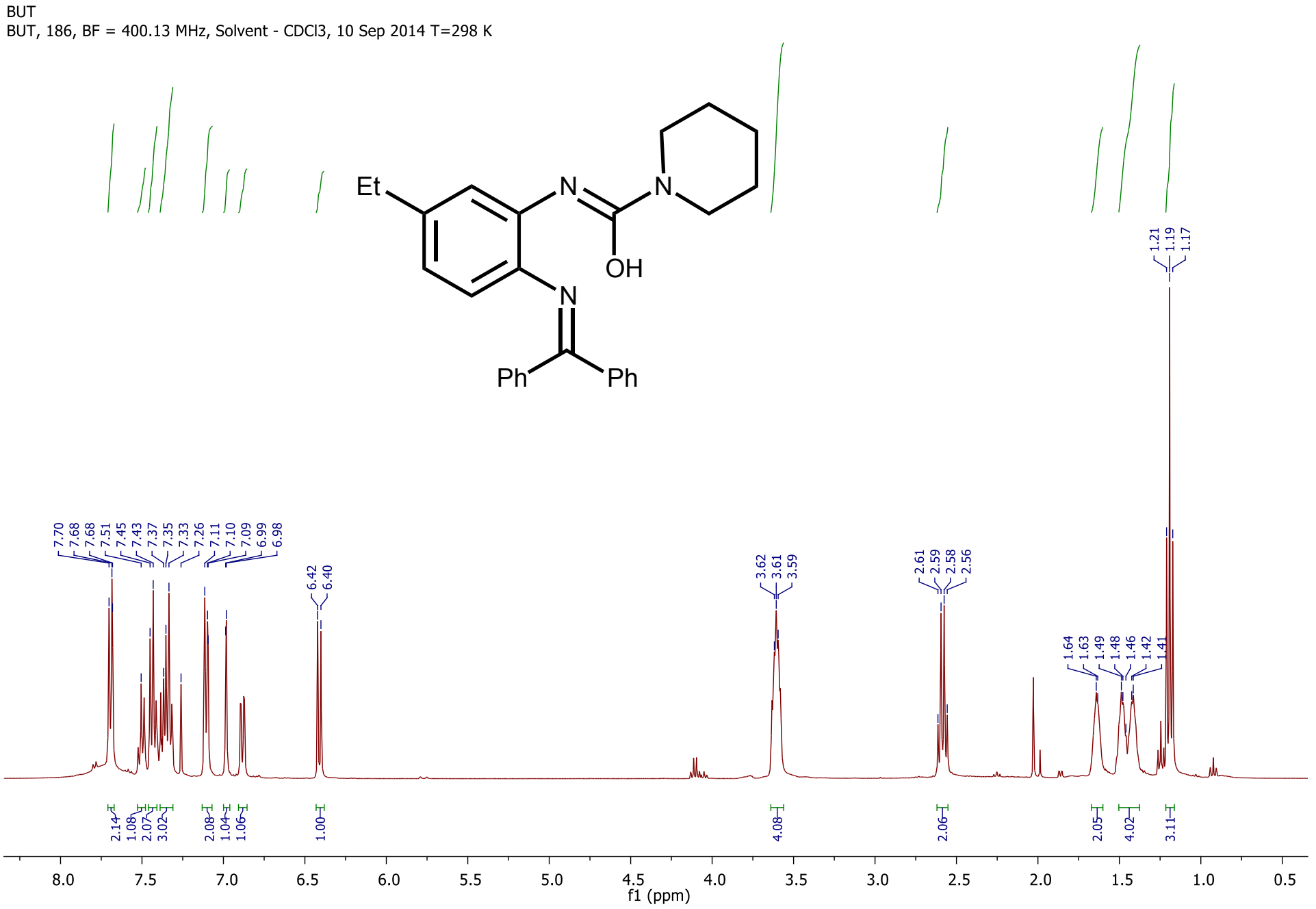
Analysis Name	D:\Data\Work\2014\October\29\BUT219_3000001.d	Acquisition Date	10/30/2014 5:19:10 PM
Method	tune_low_pos.m	Operator	BDAL@DE
Sample Name	BUT219_3	Instrument	maXis 62
Comment	MeOH		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1100 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

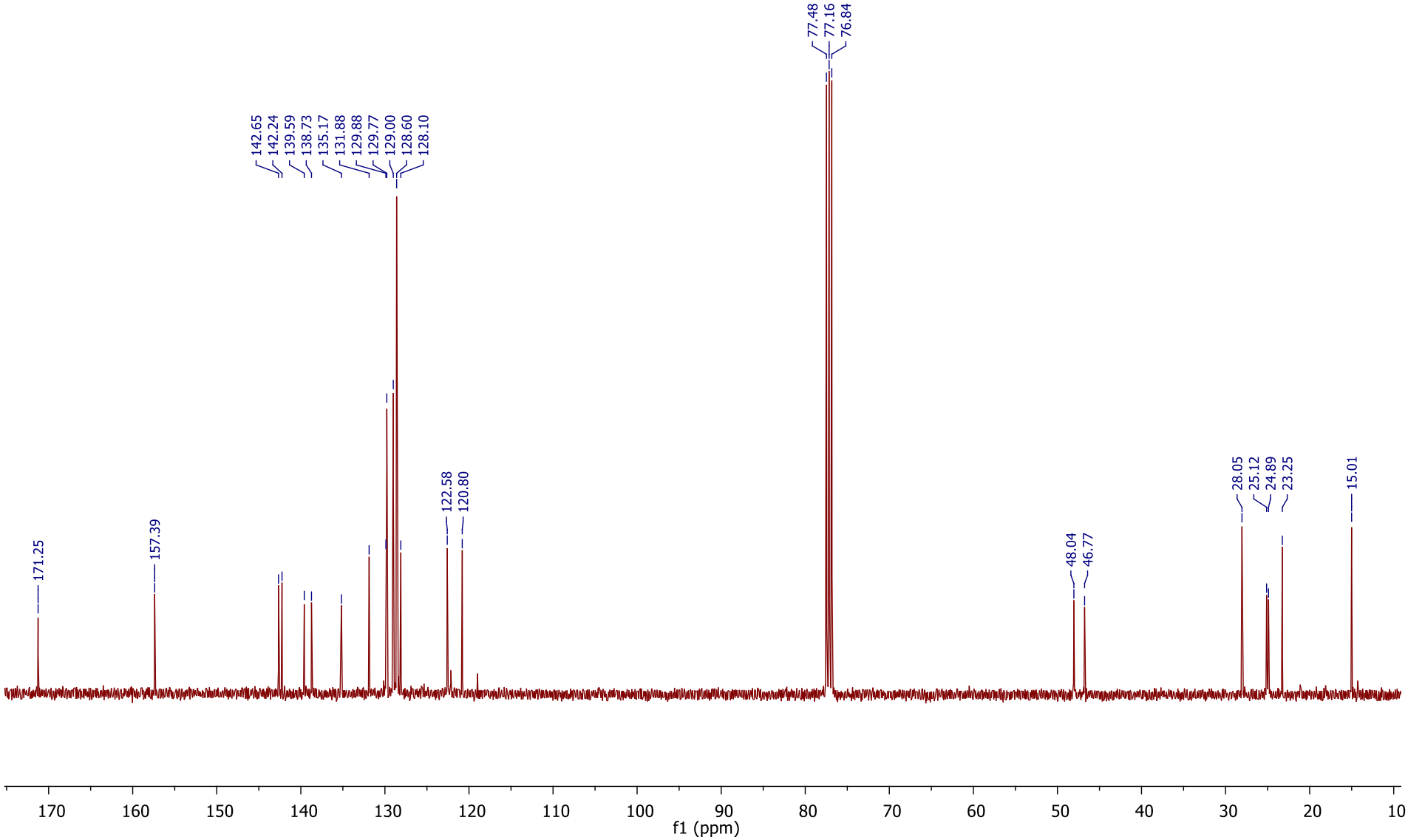


^{1}H *N′*-(dimethylcarbamoyl)-*N*-(4-ethylphenyl)-*N*-phenylbenzimidamide (6ce).

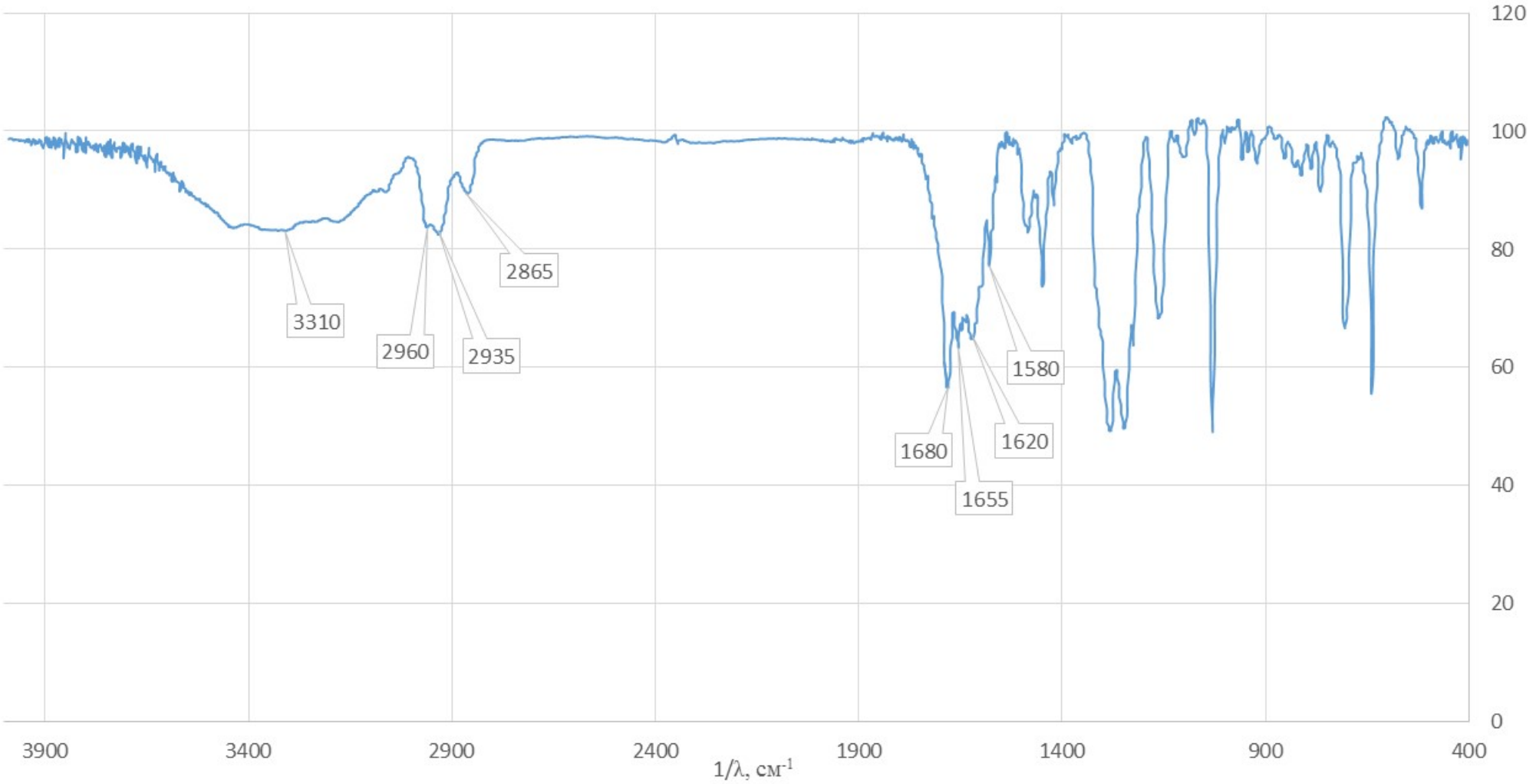


^{13}C *N′*-(dimethylcarbamoyl)-*N*-(4-ethylphenyl)-*N*-phenylbenzimidamide (6ce).

BUTc
BUTc, 186, BF = 100.612769 MHz, Solvent - CDCl3, 10 Sep 2014 T=299 K



24b

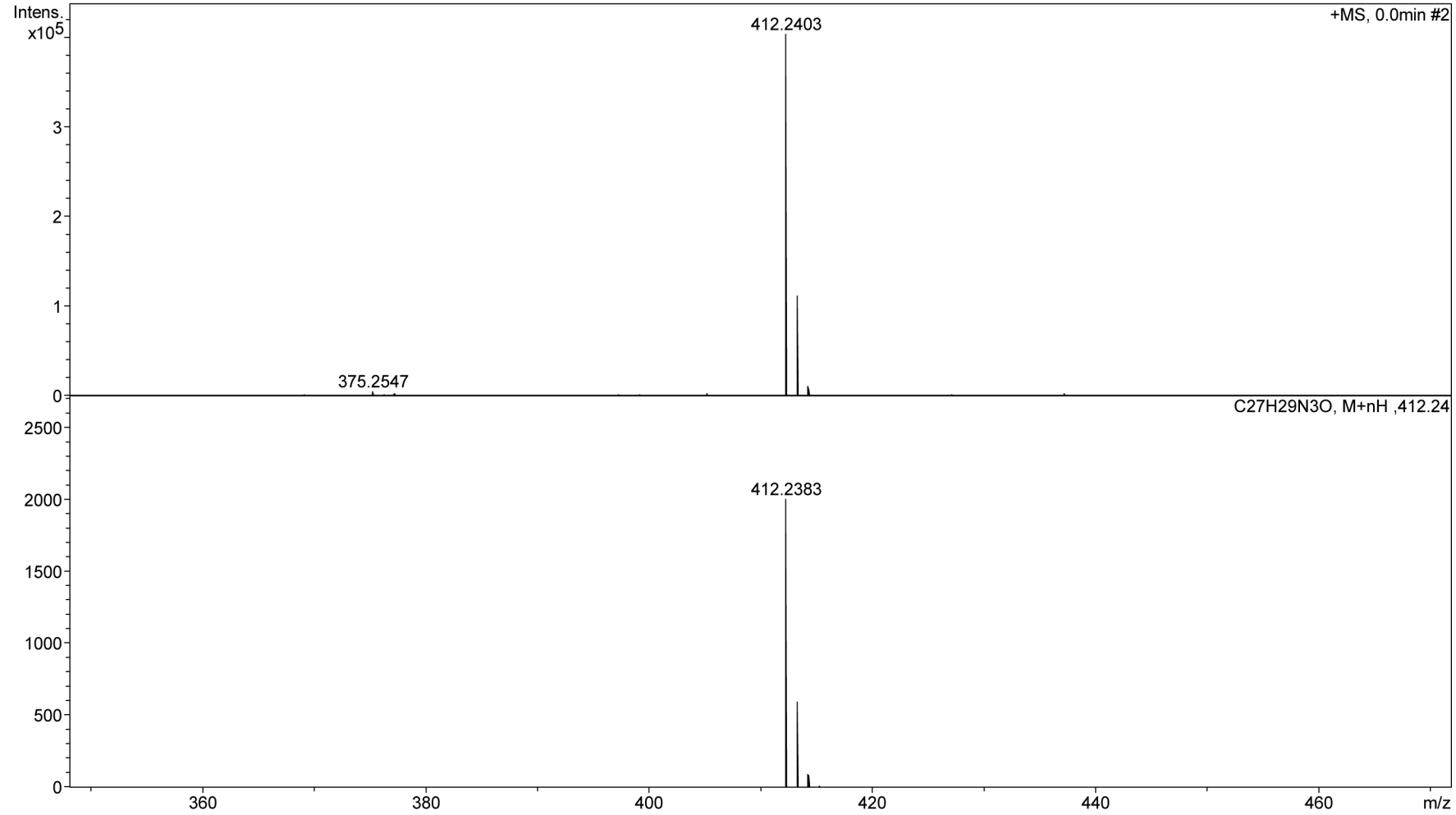

120
100
80
60
40
20
0
3900
3400
2900
2400
1900
1400
900
400
1/λ, см-1
3310
2960
2935
2865
1680
1655
1620
1580

Analysis Info

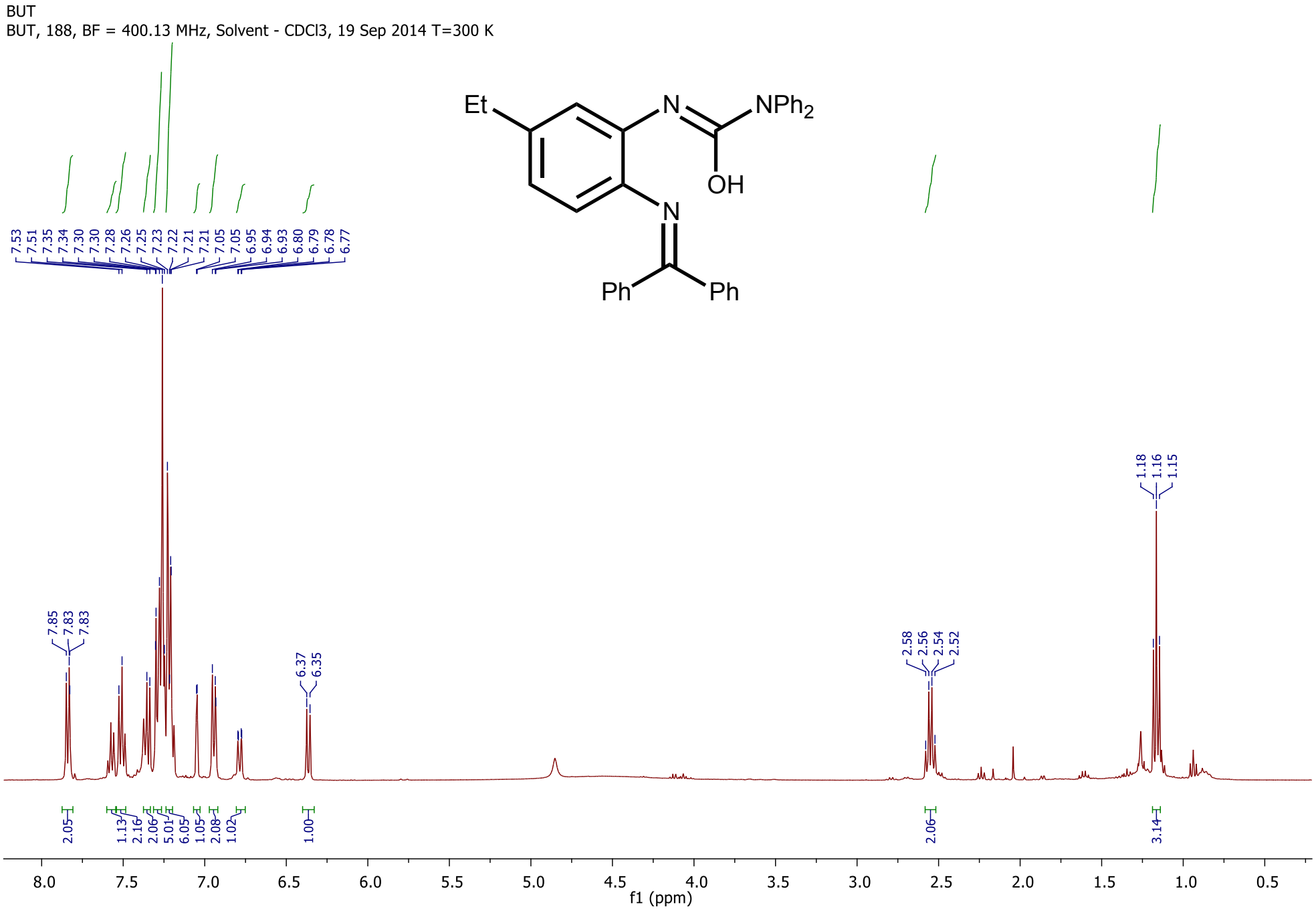
Analysis Name	D:\Data\Work\2014\Saptermber\09\BUT_221_25_000004.d	Acquisition Date	9/10/2014 12:15:19 PM
Method	tune_low_pos.m	Operator	BDAL@DE
Sample Name	BUT_221_25_	Instrument	maXis 62
Comment			

Acquisition Parameter

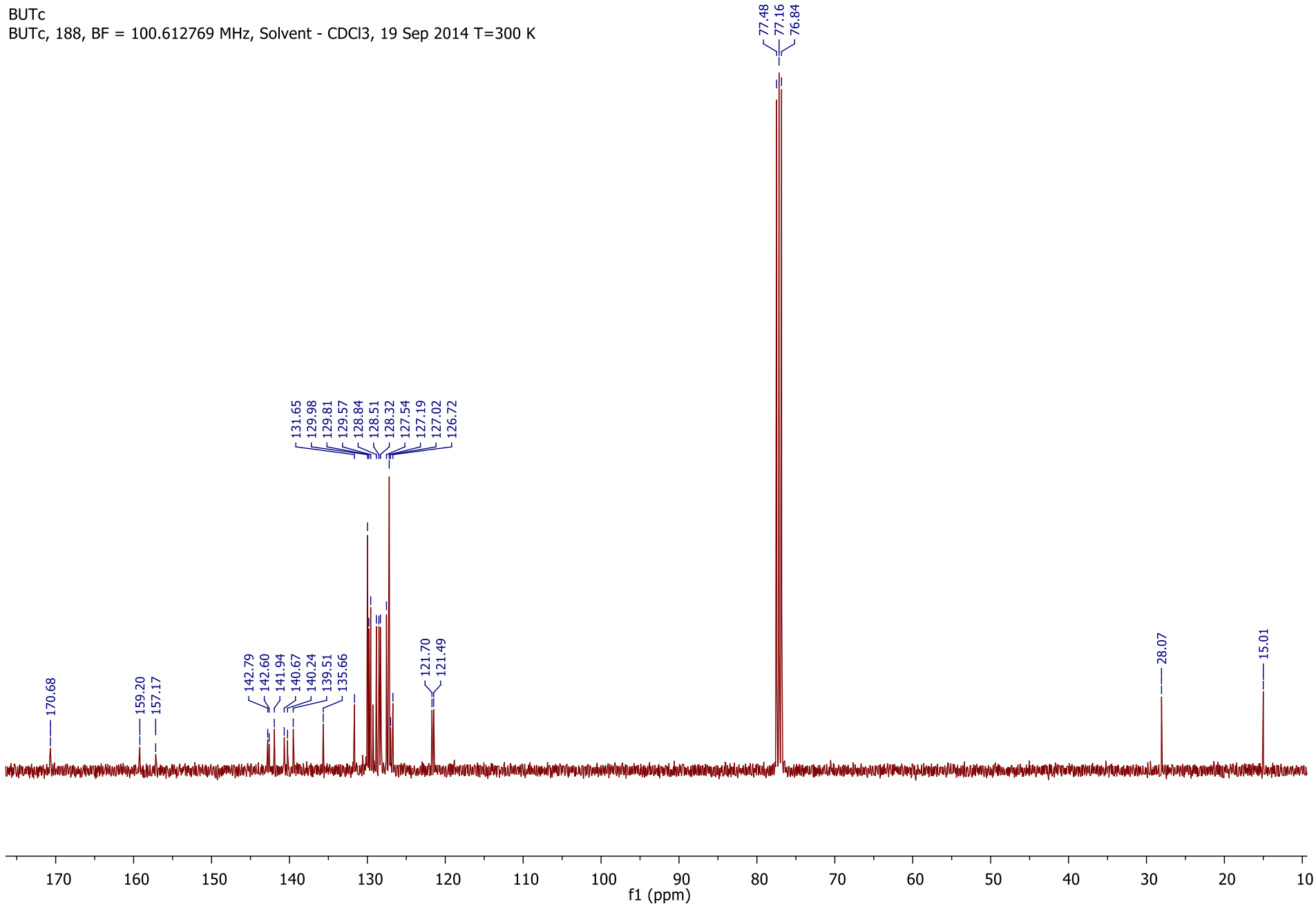
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1100 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



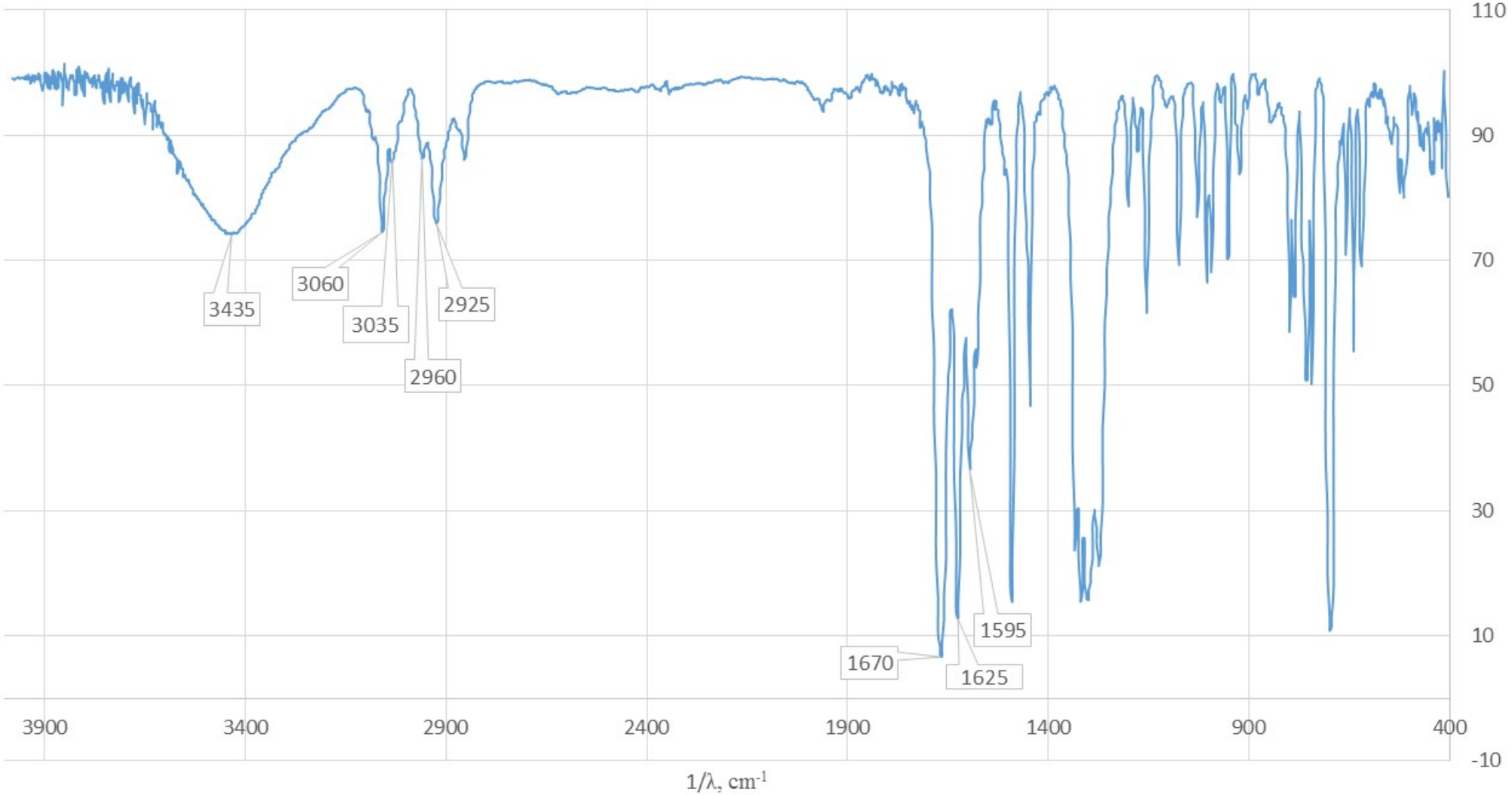
^{1}H 3-(2-((diphenylmethylene)amino)-5-ethylphenyl)-1,1-diphenylurea (6ee).



^{13}C 3-(2-((diphenylmethylene)amino)-5-ethylphenyl)-1,1-diphenylurea (6ee).



25b


110
90
70
50
30
10
-10
3435
3060
3035
2960
2925
1670
1625
1595
3900
3400
2900
2400
1900
1400
900
400
1/λ, cm-1

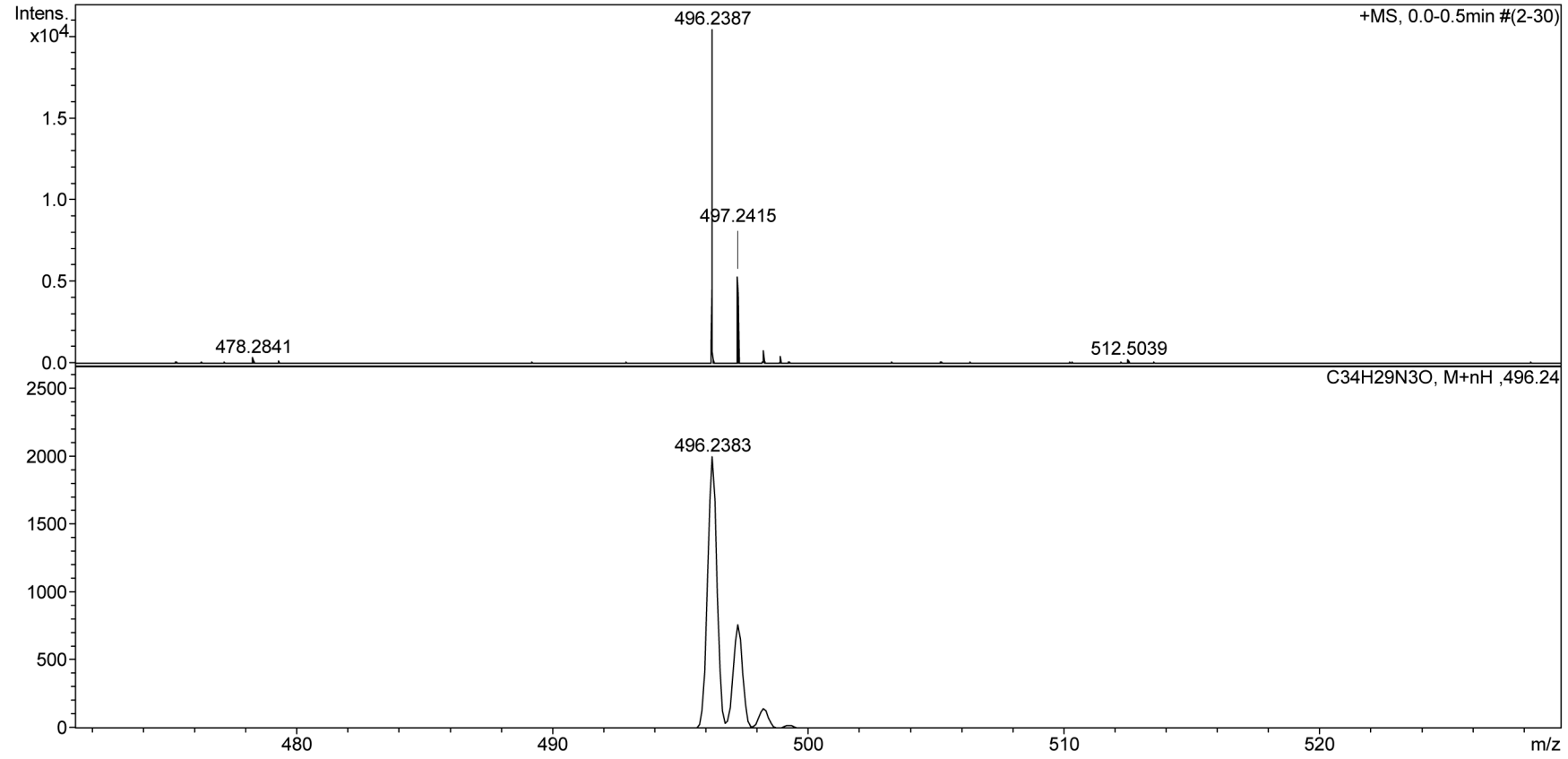
Display Report

Analysis Info

Analysis Name	G:\BUT\BUT_220_15_000001.d	Acquisition Date	09.09.2014 10:36:09
Method	tune_low_pos.m	Operator	BDAL@DE
Sample Name	BUT_220_15_	Instrument	maXis 62
Comment			

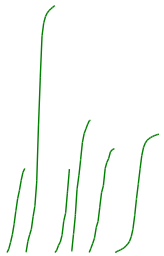
Acquisition Parameter

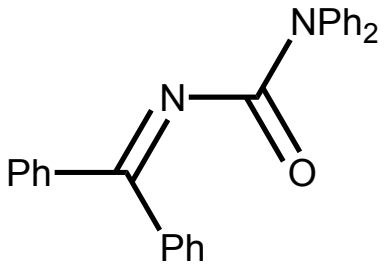
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1100 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source

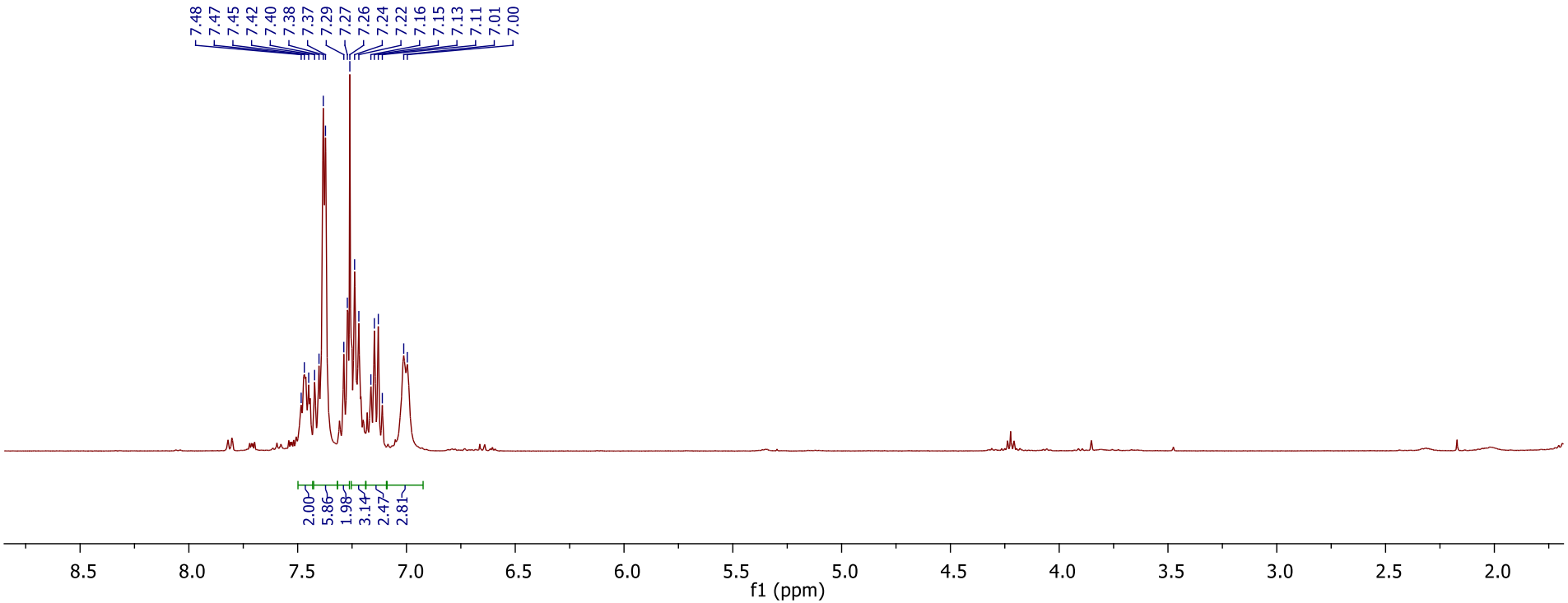


^{1}H 3-(diphenylmethylene)-1,1-diphenylurea (5e)

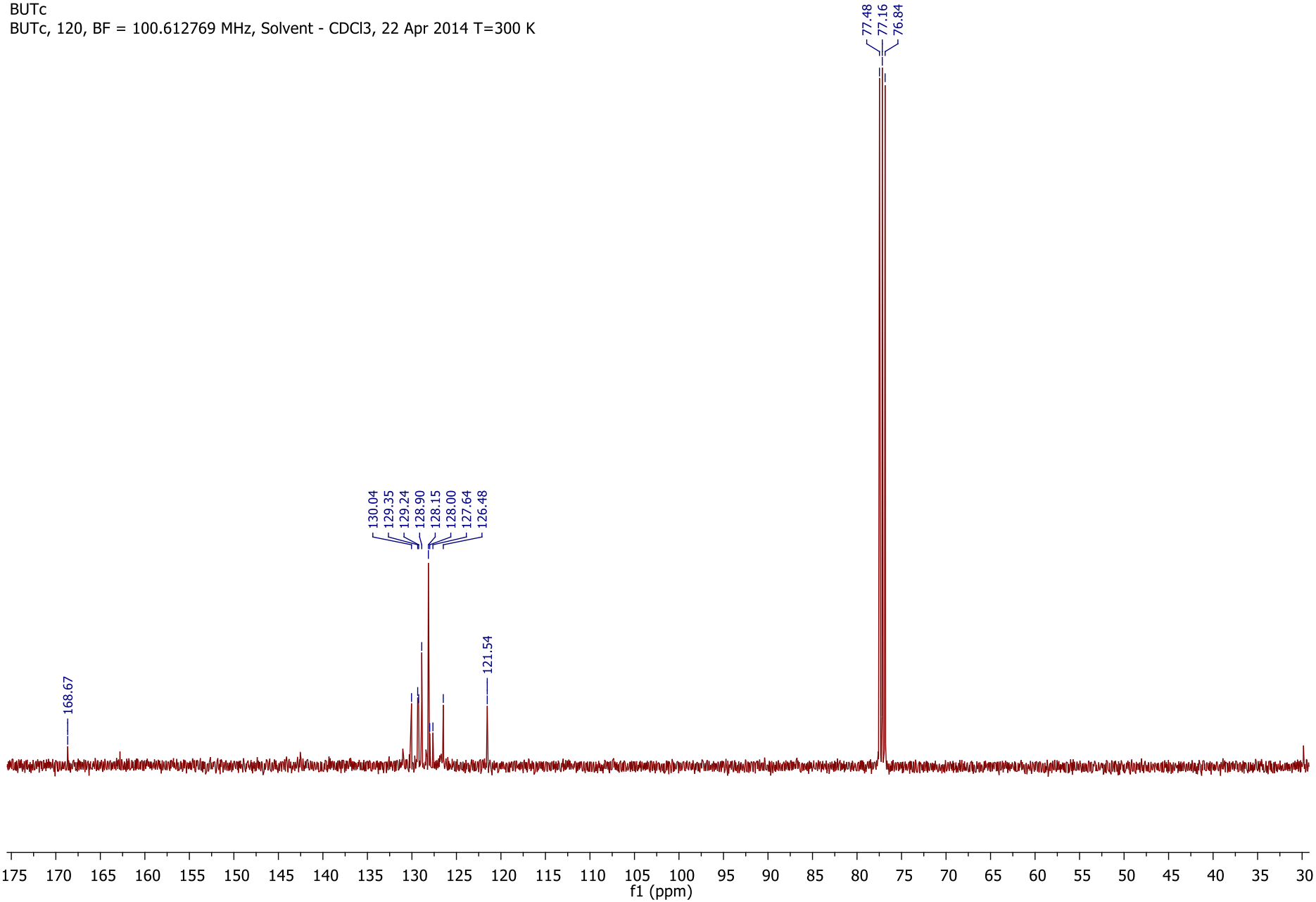
BUT
BUT, 120, BF = 400.13 MHz, Solvent - CDCl3, 22 Apr 2014 T=299 K



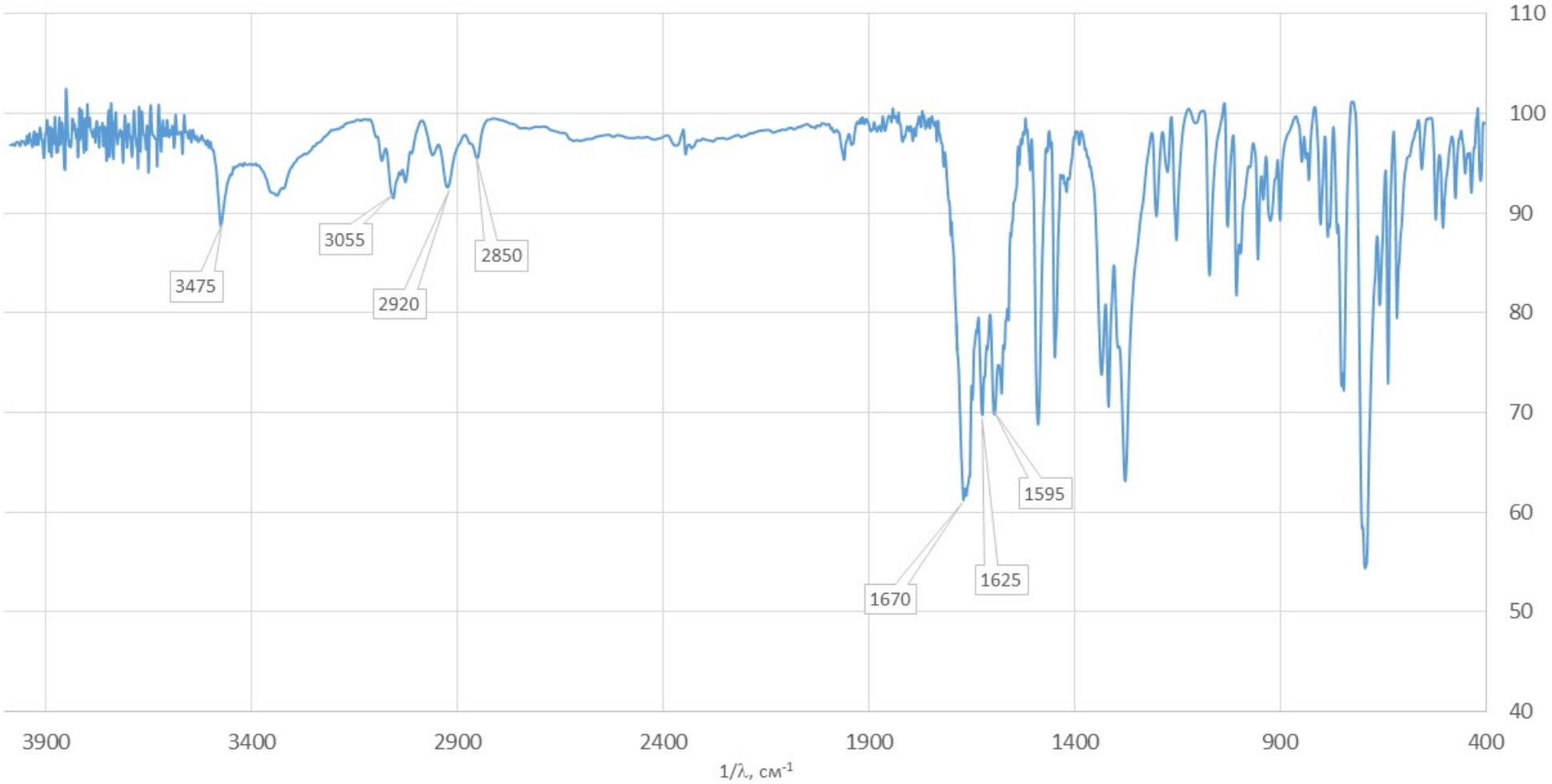




^{13}C 3-(diphenylmethylene)-1,1-diphenylurea (5e)



12a


3475
3055
2920
2850
1670
1625
1595
110
100
90
80
70
60
50
40
3900
3400
2900
2400
1900
1400
900
400
1/λ, см-1

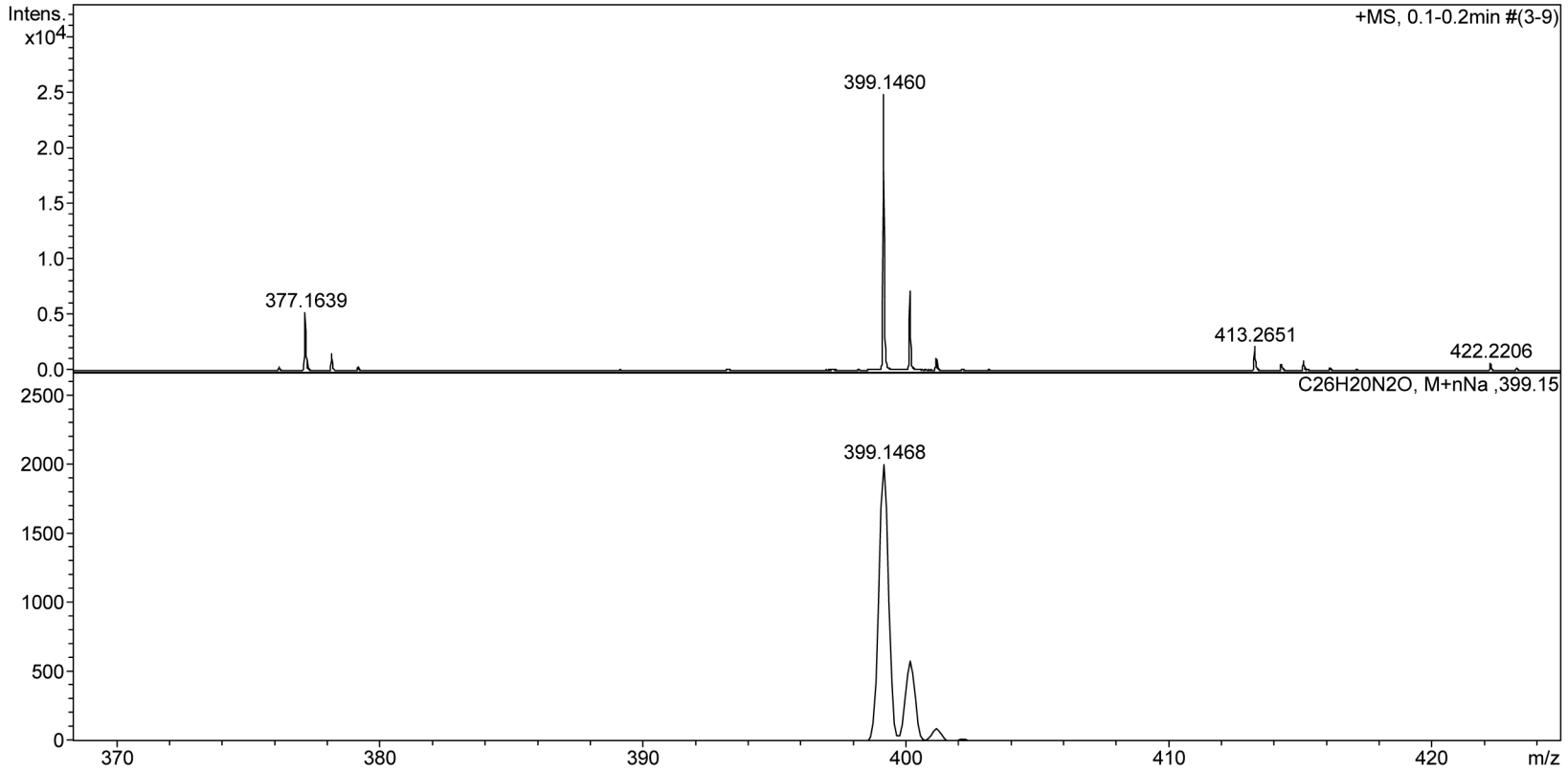
Mass Spectrum Report

Analysis Info

Analysis Name	D:\Data\mish2\BUT174_fr4-6.d	Acquisition Date	22.04.2014 15:38:38
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT174_fr4-6	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

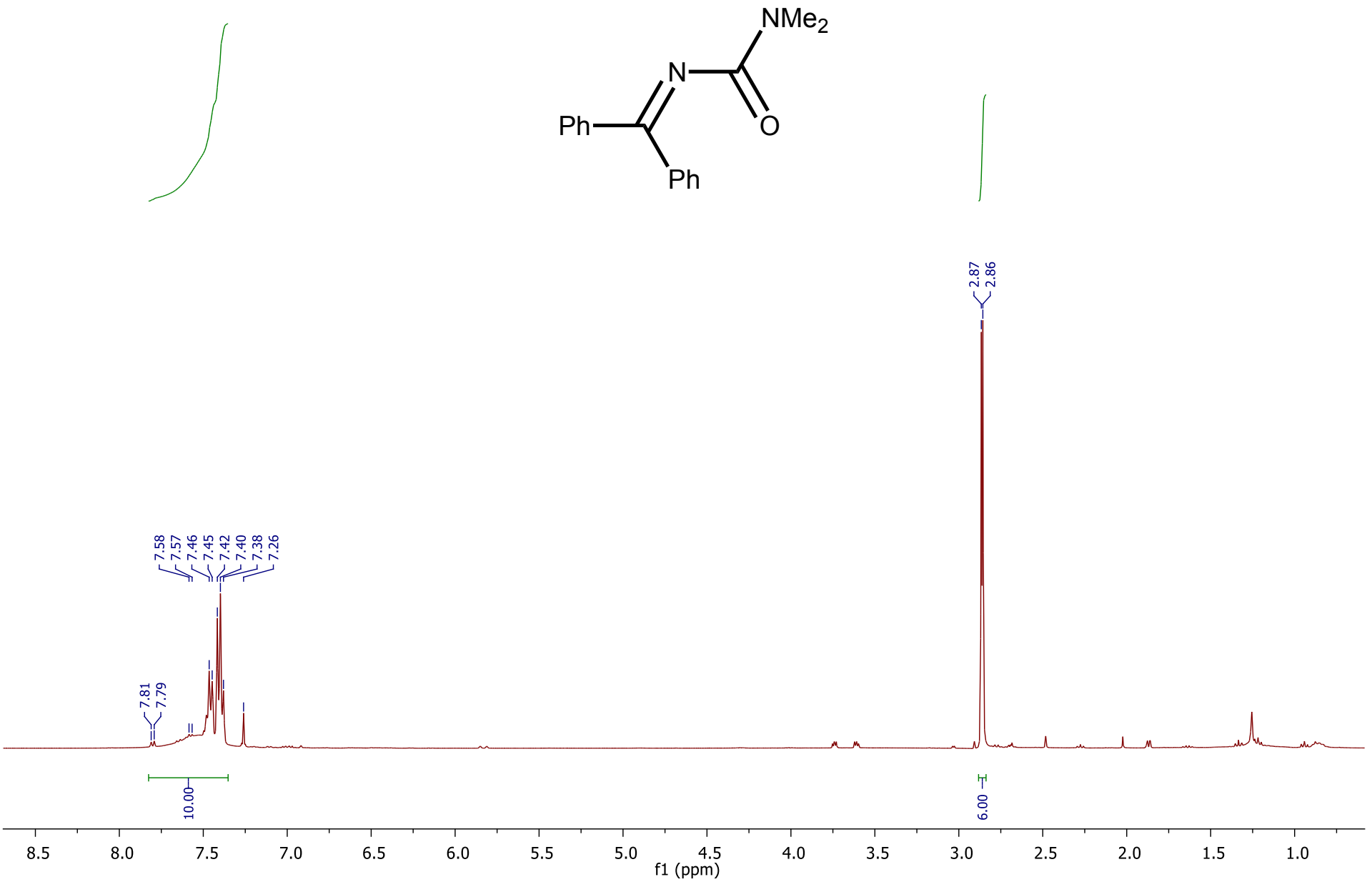
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



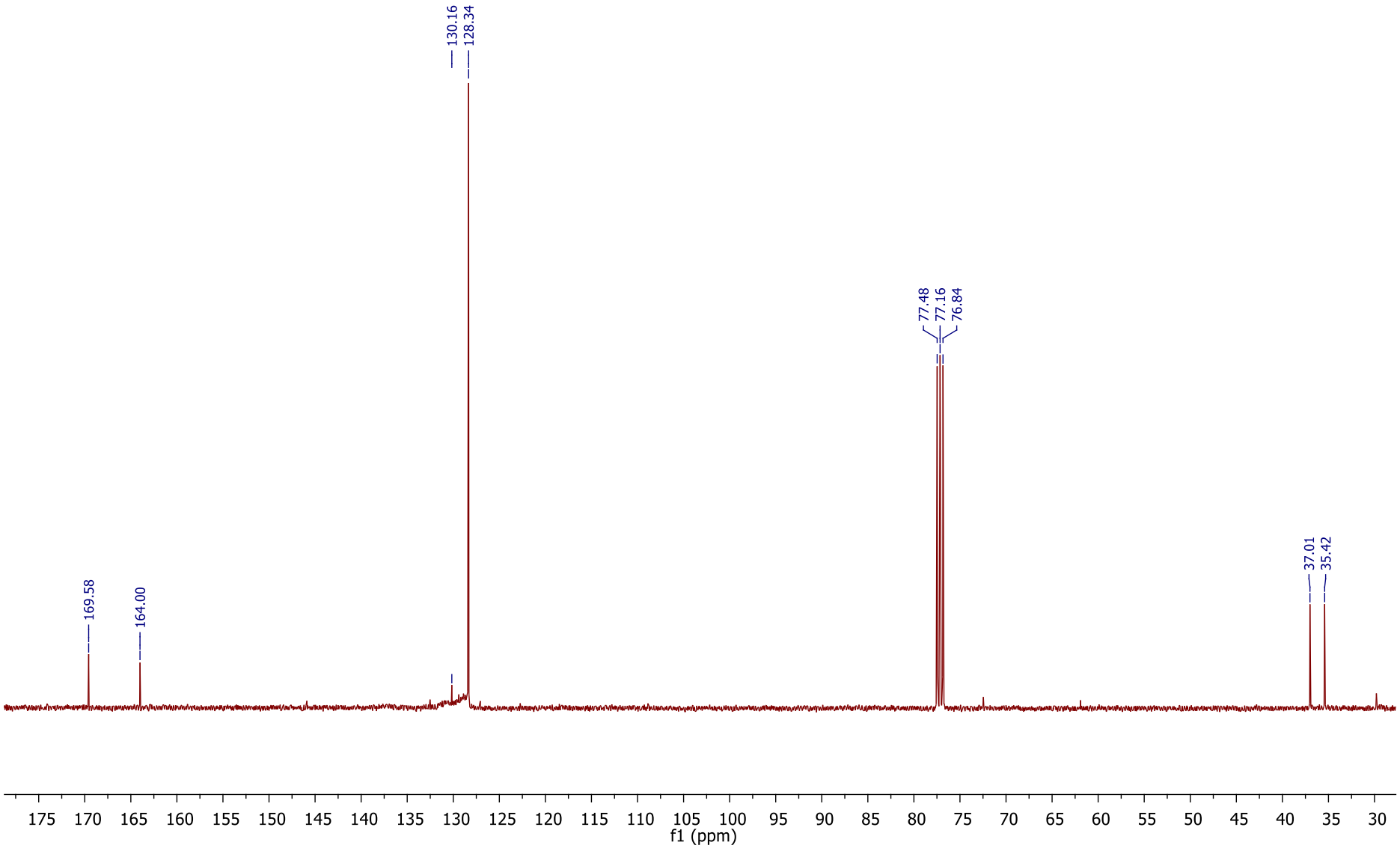
^{1}H 3-(diphenylmethylene)-1,1-dimethylurea (5a)

BUT
BUT, 190, BF = 400.13 MHz, Solvent - CDCl3, 30 Sep 2014 T=300 K

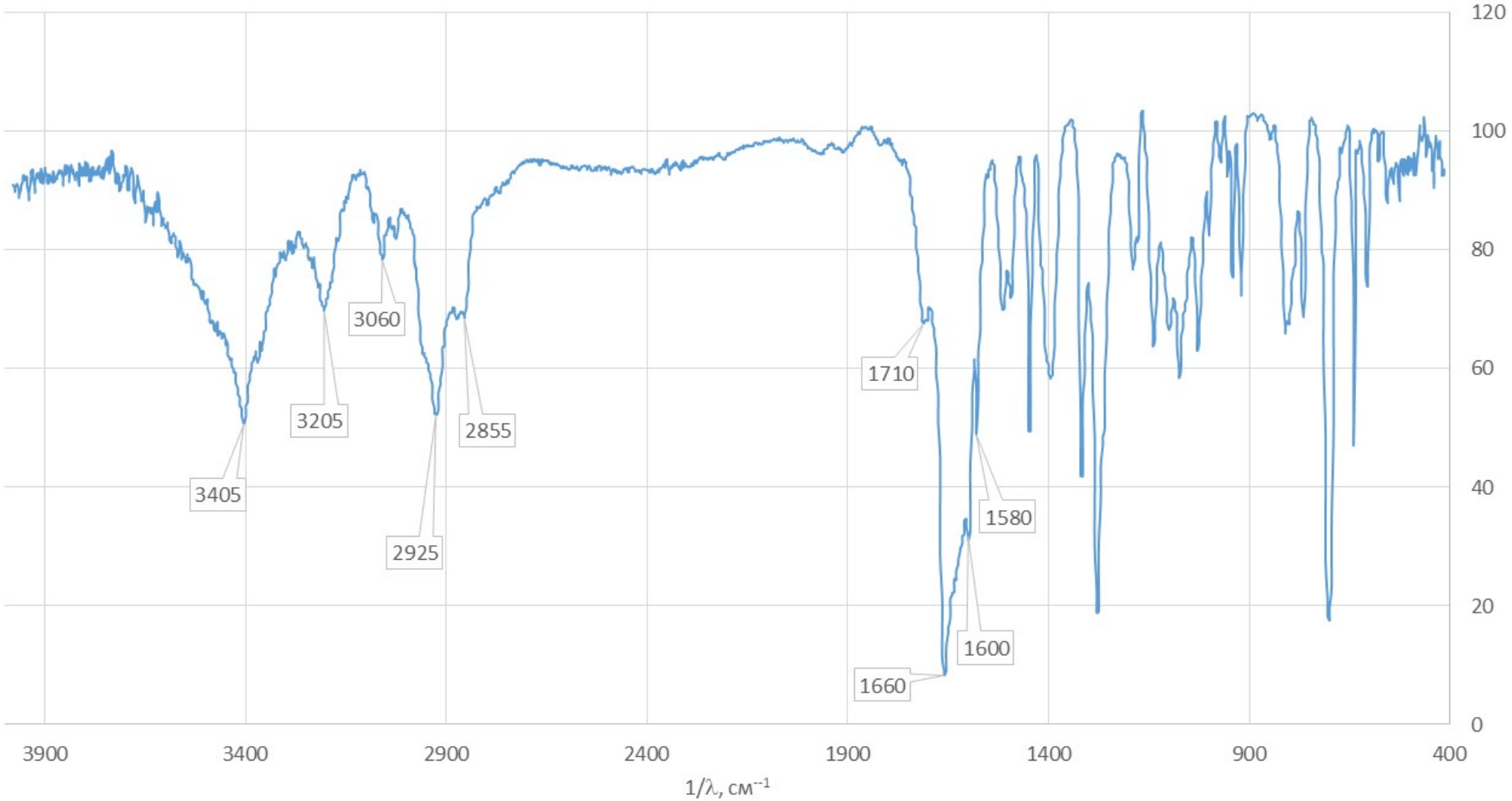


^{13}C 3-(diphenylmethylene)-1,1-dimethylurea (5a)

BUTc
BUTc, 190, BF = 100.612769 MHz, Solvent - CDCl3, 30 Sep 2014 T=300 K



13a


120
100
80
60
40
20
0
3900
3400
2900
2400
1900
1400
900
400
1/λ, см⁻¹
3405
3205
3060
2925
2855
1710
1660
1600
1580

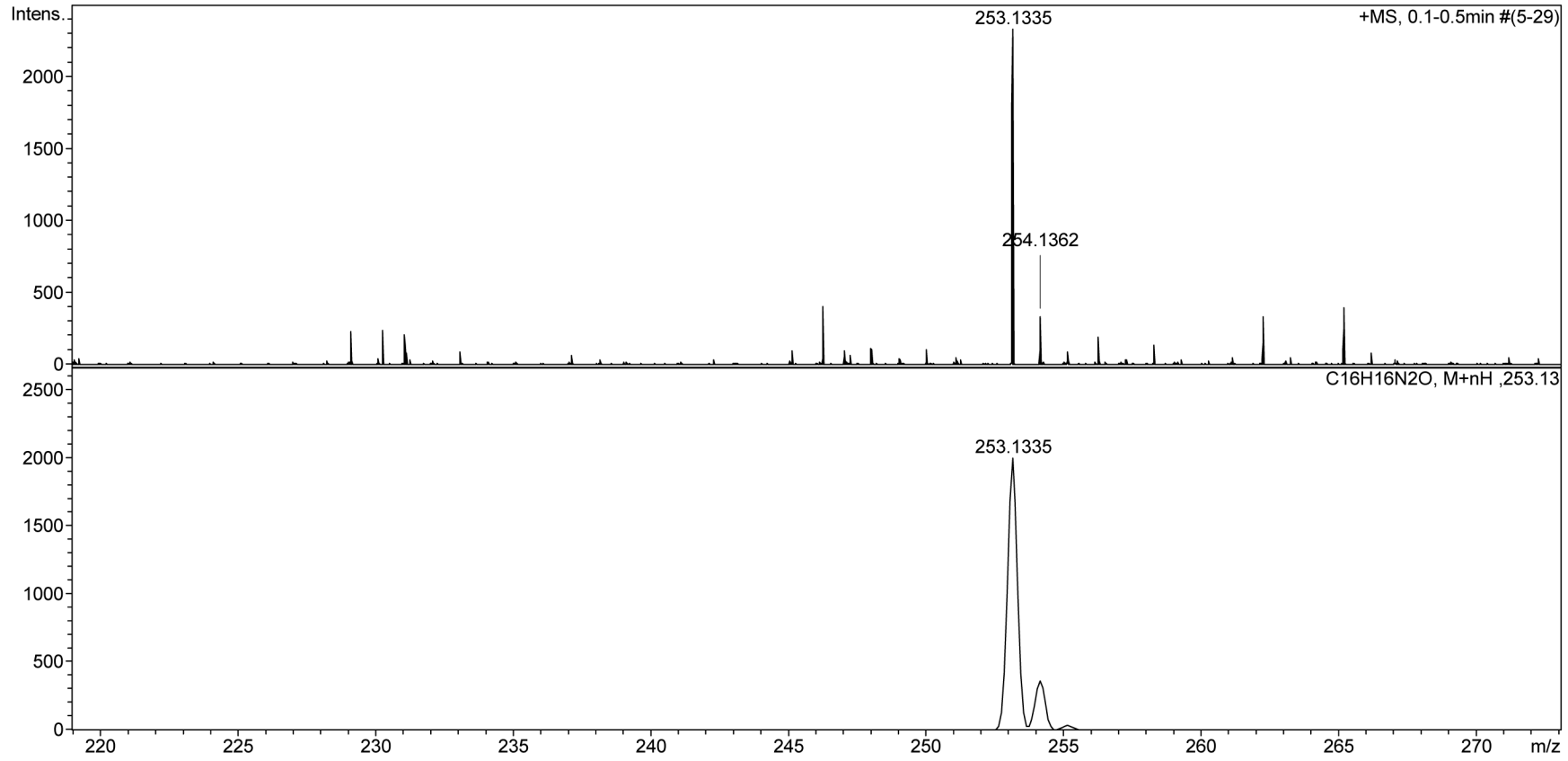
Display Report

Analysis Info

Analysis Name	G:\BUT\BUT_218_14_a000001.d	Acquisition Date	22.08.2014 12:58:46
Method	tune_low_pos.m	Operator	BDAL@DE
Sample Name	BUT_218_14_a	Instrument	maXis 62
Comment			

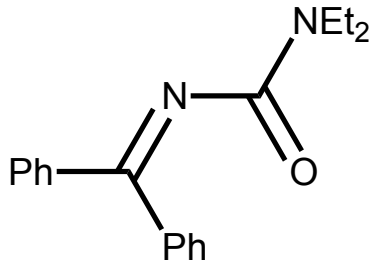
Acquisition Parameter

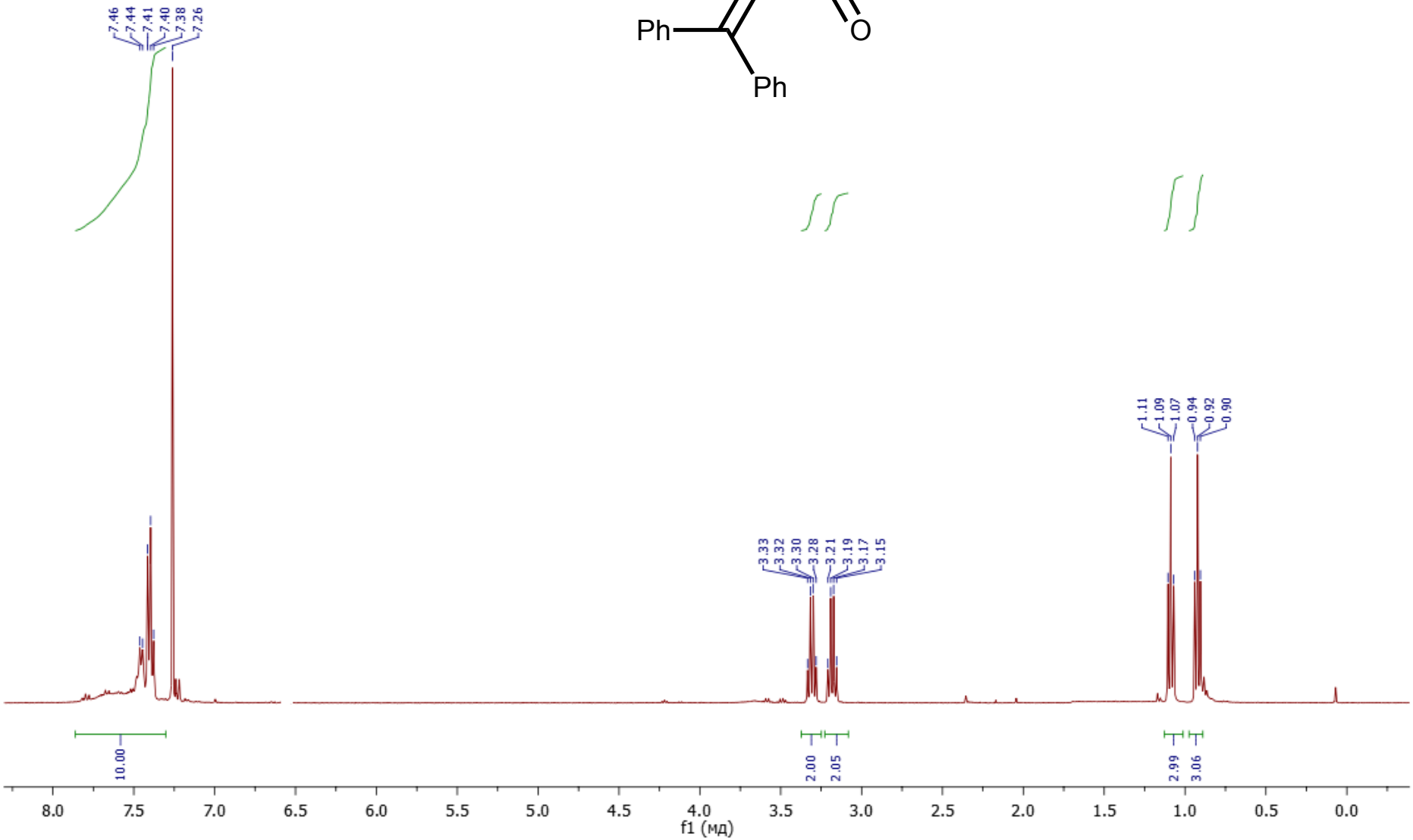
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1100 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Source



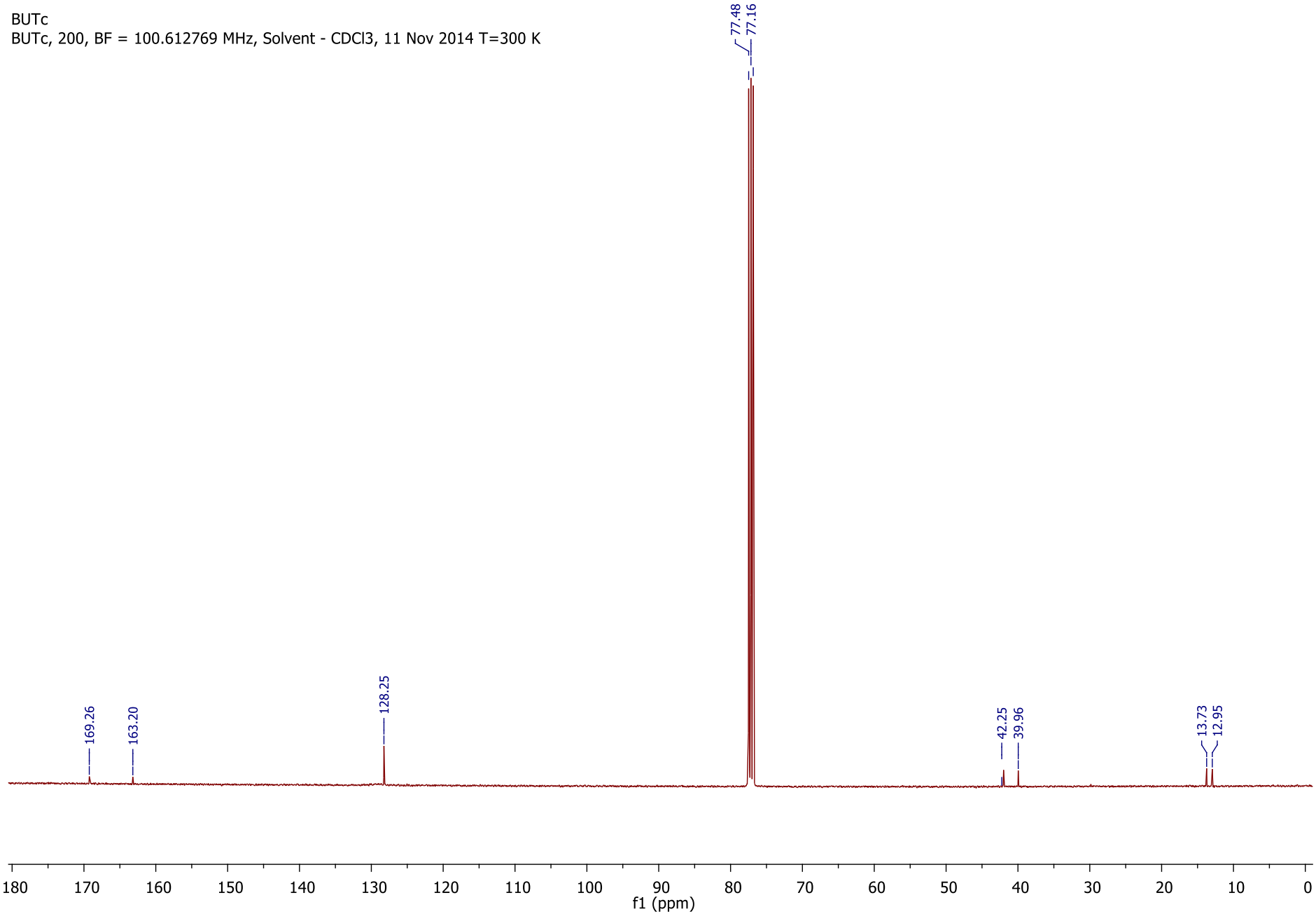
[1]H 3-(diphenylmethylene)-1,1-diethylurea (5b)

BUT
BUT, 150, BF = 400.13 MHz, Solvent - CDCl3, 07 Jul 2014 T=299 K

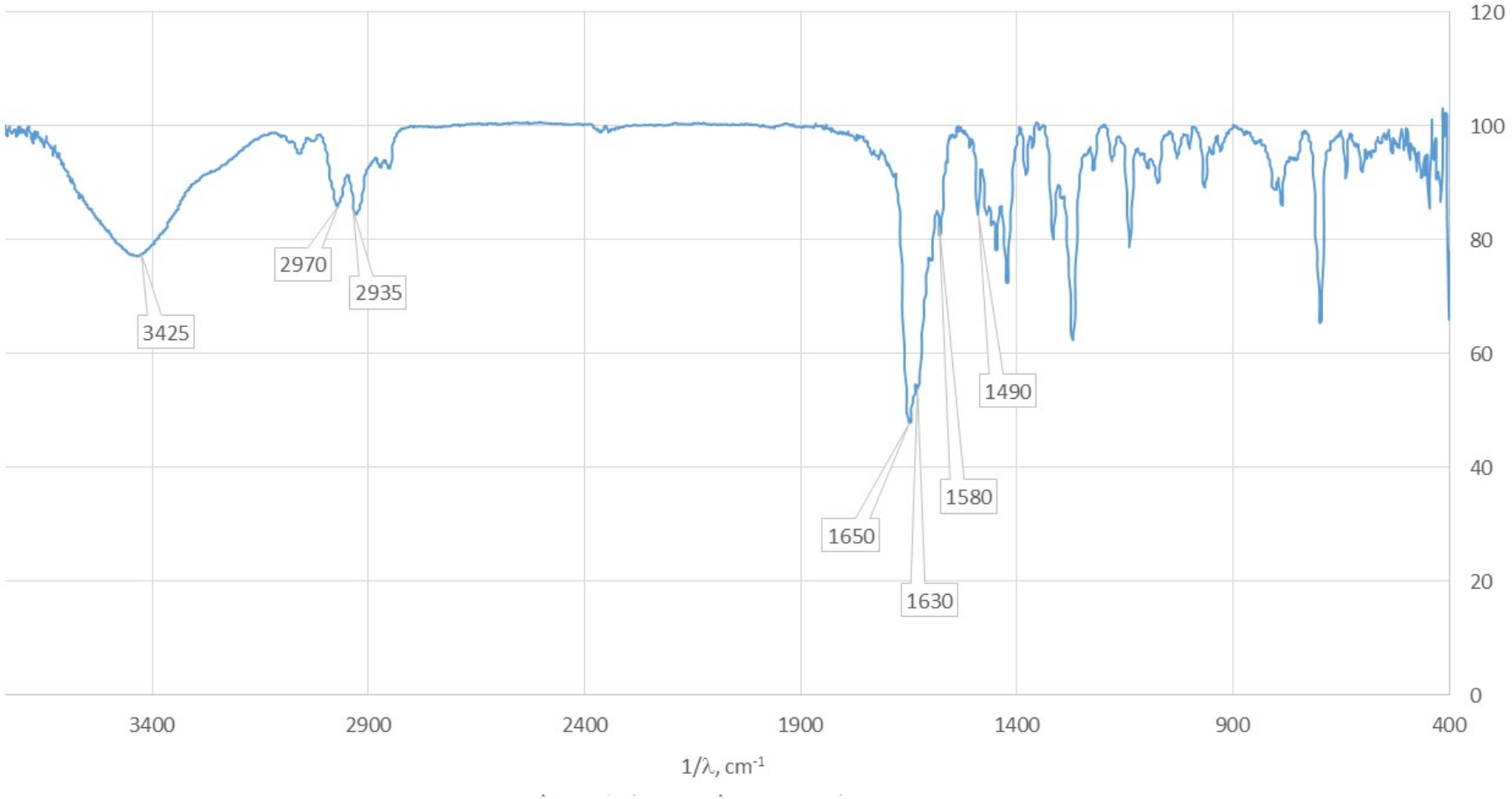




^{13}C 3-(diphenylmethylene)-1,1-diethylurea (5b)



14a


120
100
80
60
40
20
0
3400
2900
2400
1900
1400
900
400
1/λ, cm-1
3425
2970
2935
1650
1630
1580
1490

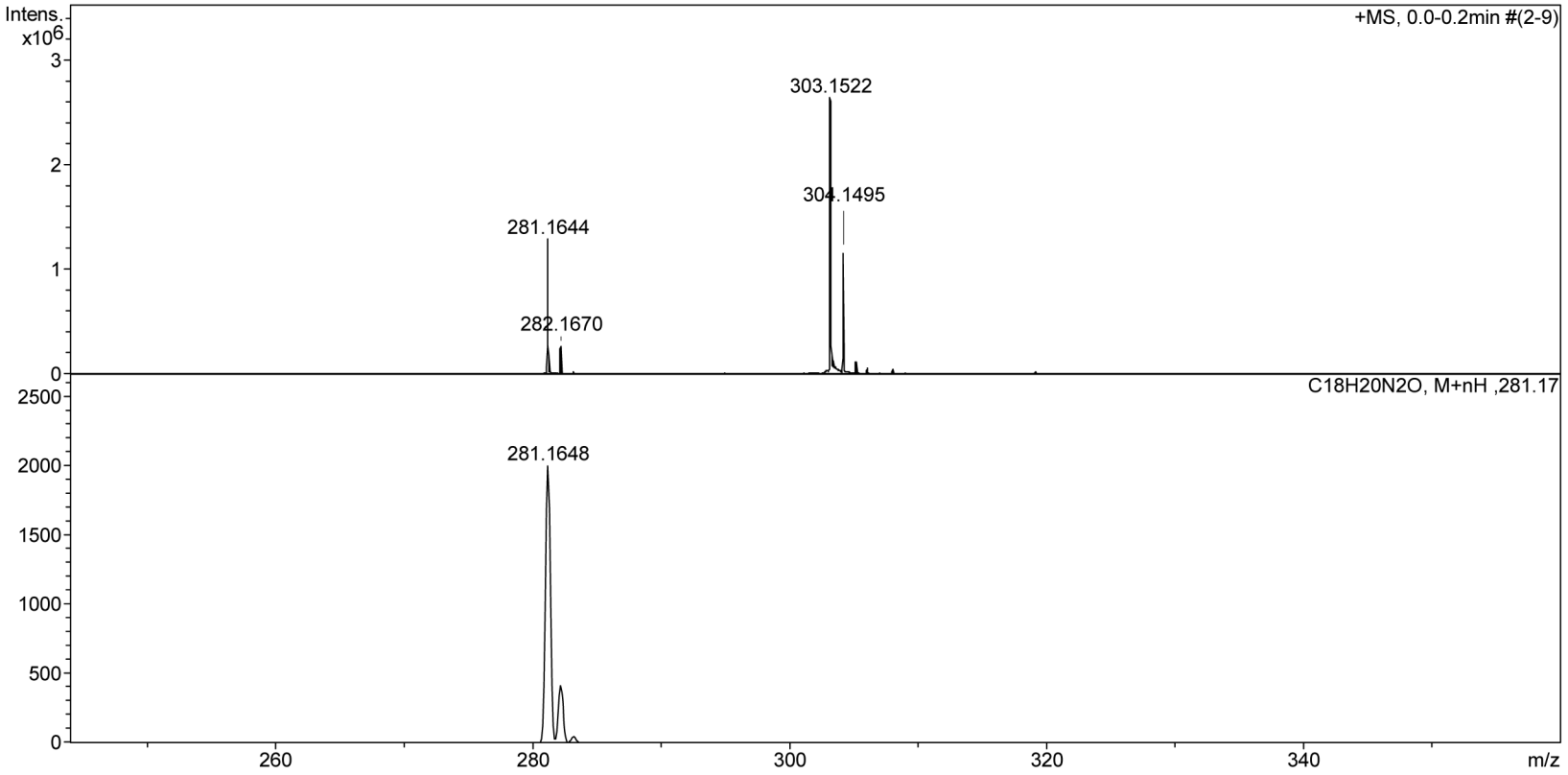
Mass Spectrum Report

Analysis Info

Analysis Name	D:\Data\mish2\BUT198fr4.d	Acquisition Date	09.07.2014 14:22:38
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT198fr4	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

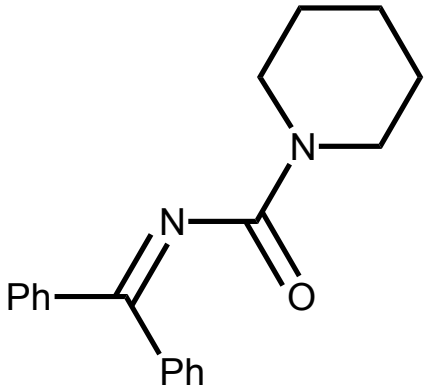
Acquisition Parameter

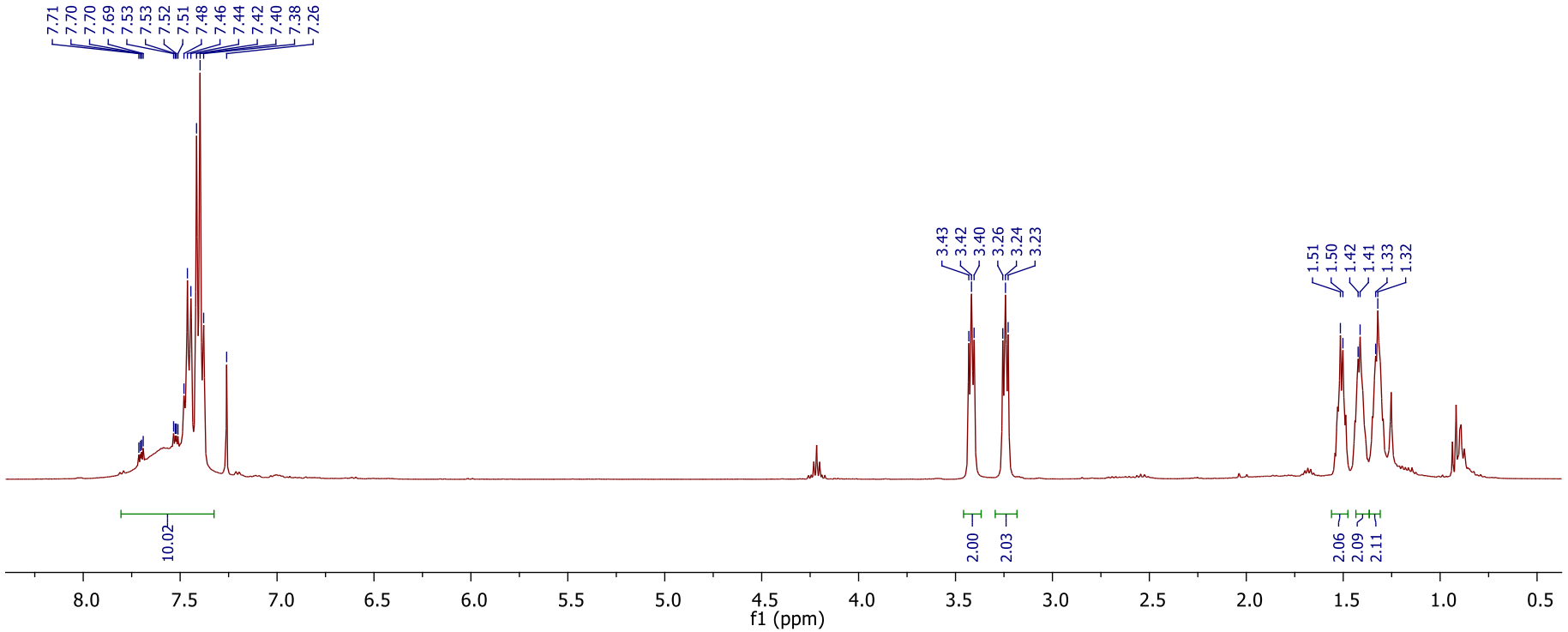
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



^{1}H N-(diphenylmethylene)piperidine-1-carboxamide (5c)

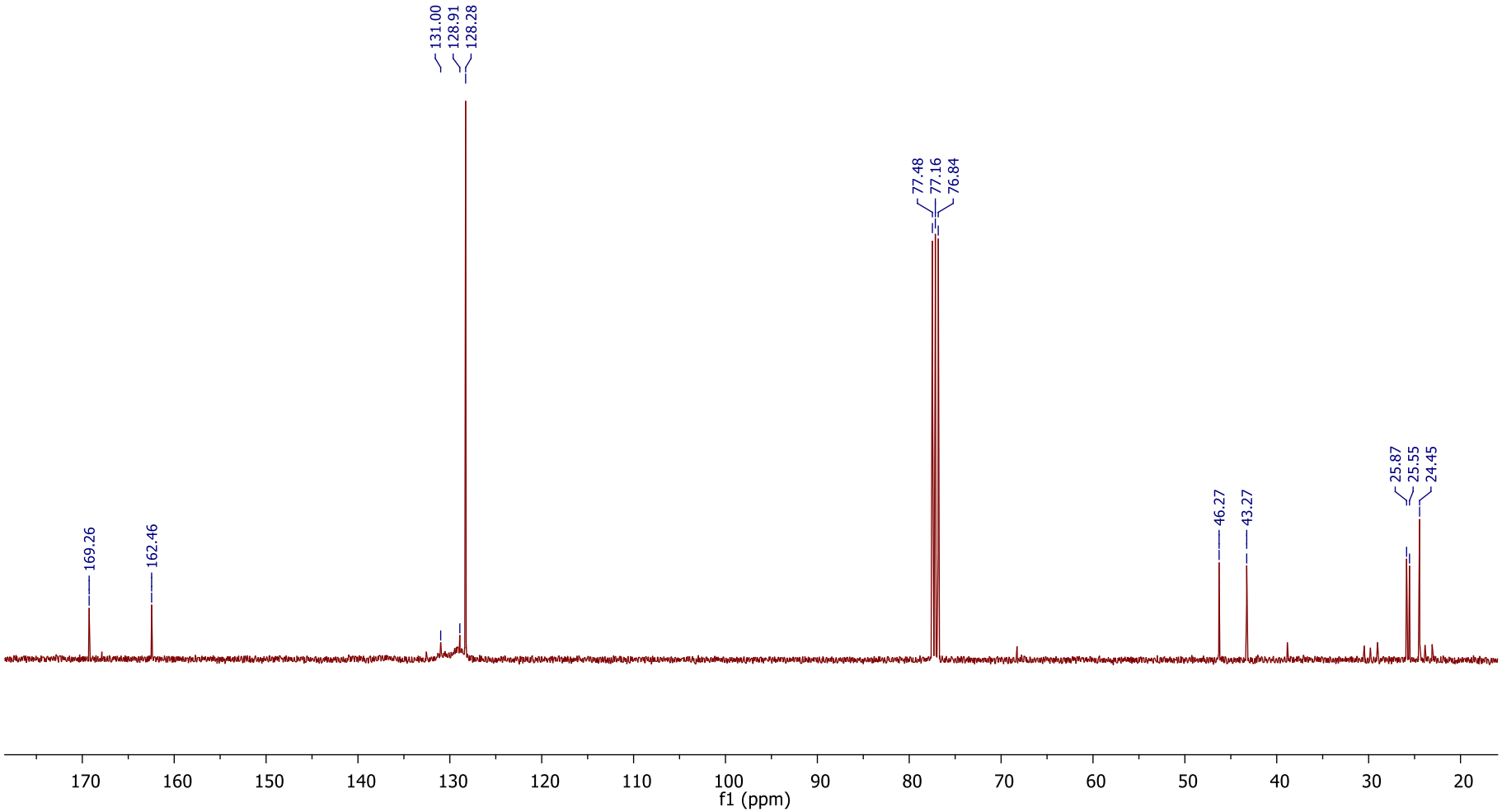
BUT
BUT, 185, BF = 400.13 MHz, Solvent - CDCl3, 10 Sep 2014 T=298 K



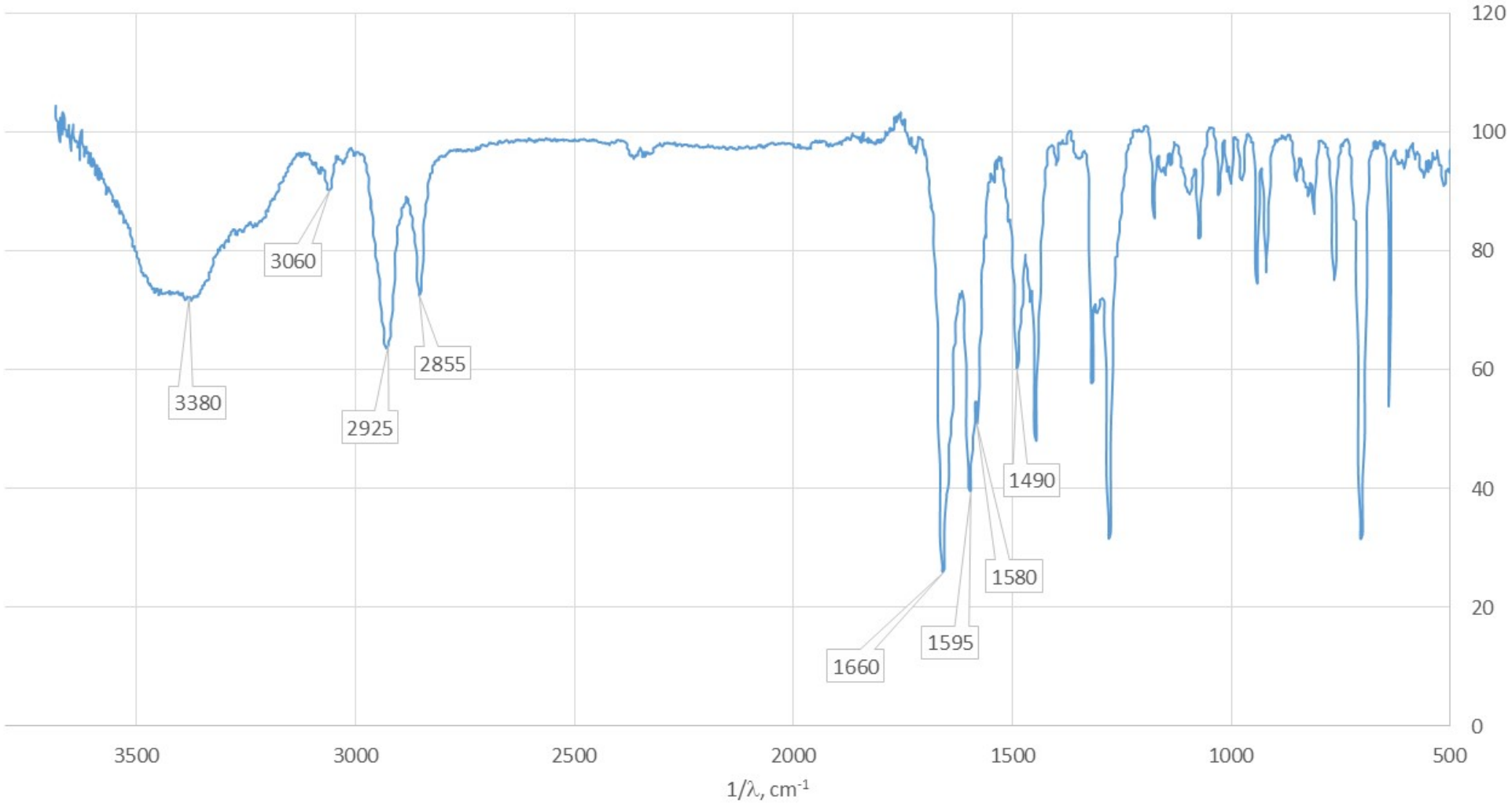


^{13}C N-(diphenylmethylene)piperidine-1-carboxamide (5c)

BUTc
BUTc, 185, BF = 100.612769 MHz, Solvent - CDCl3, 10 Sep 2014 T=299 K



15a


120
100
80
60
40
20
0
3500
3000
2500
2000
1500
1000
500
1/λ, cm-1
3380
3060
2925
2855
1660
1595
1580
1490

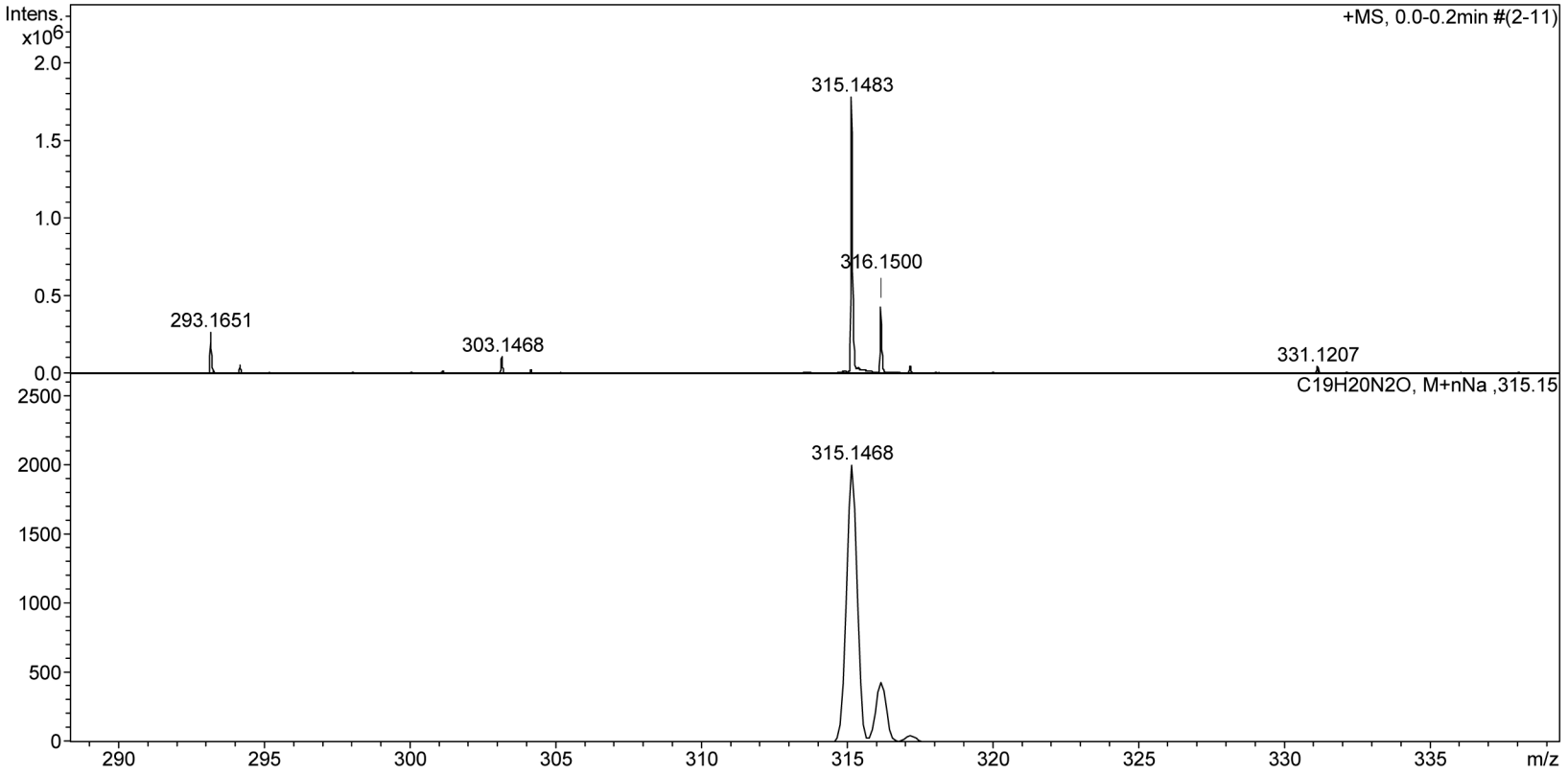
Mass Spectrum Report

Analysis Info

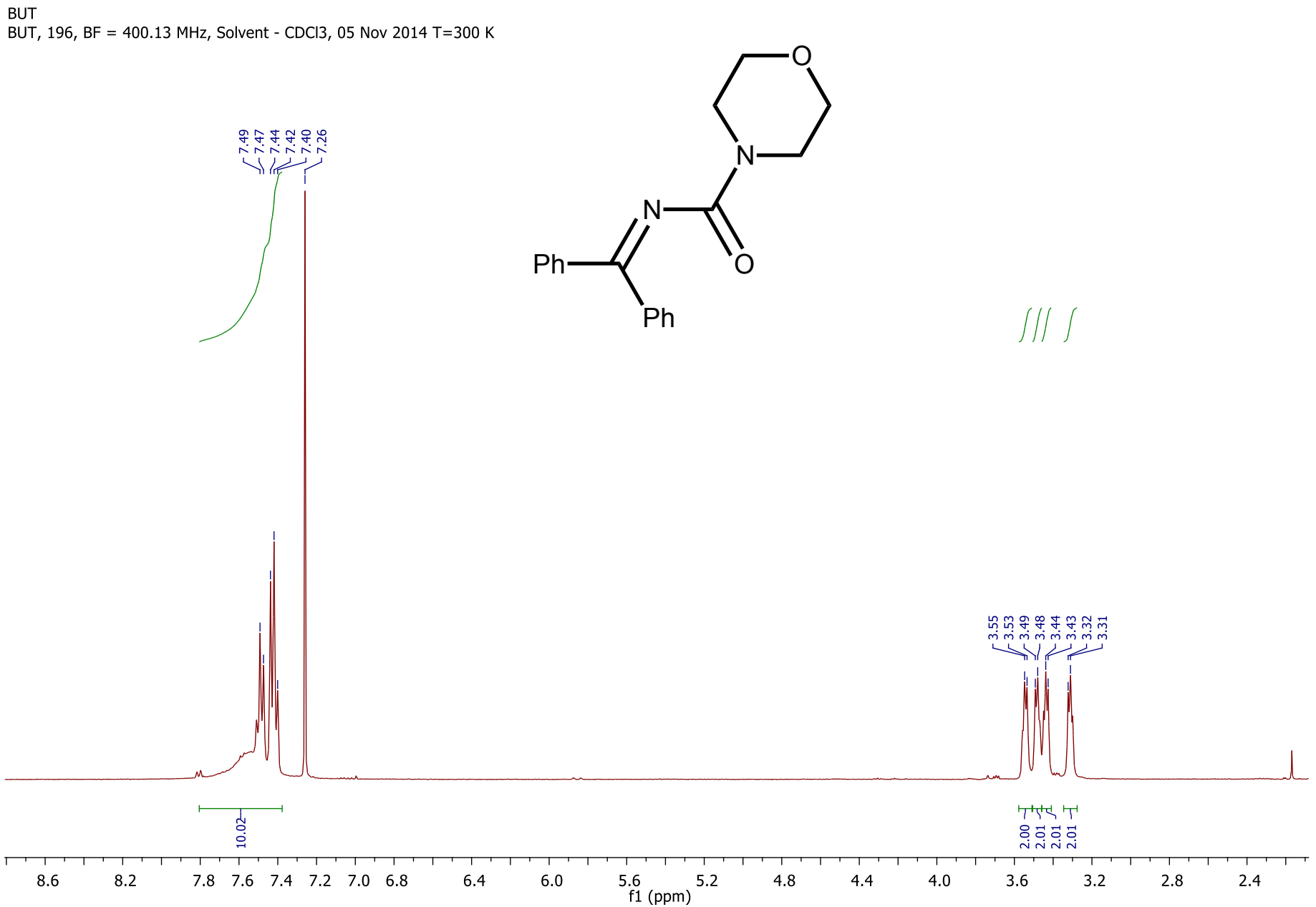
Analysis Name	D:\Data\mish2\BUT199fr4-7.d	Acquisition Date	09.07.2014 14:36:52
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT199fr4-7	Instrument / Ser#	micrOTOF 10223
Comment	MeOH 100v		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

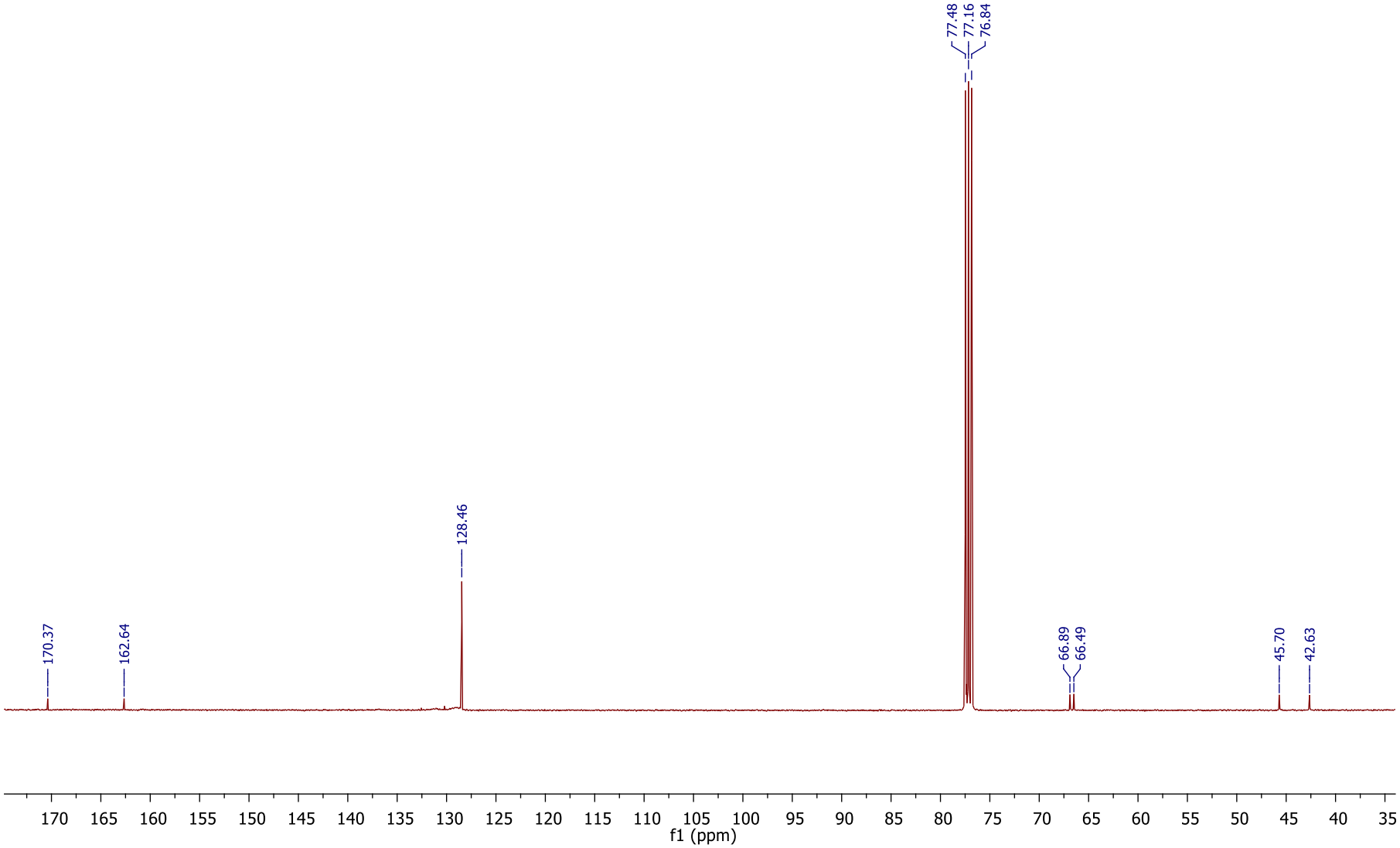


[1]H N-(diphenylmethylene)morpholine-4-carboxamide (5d)

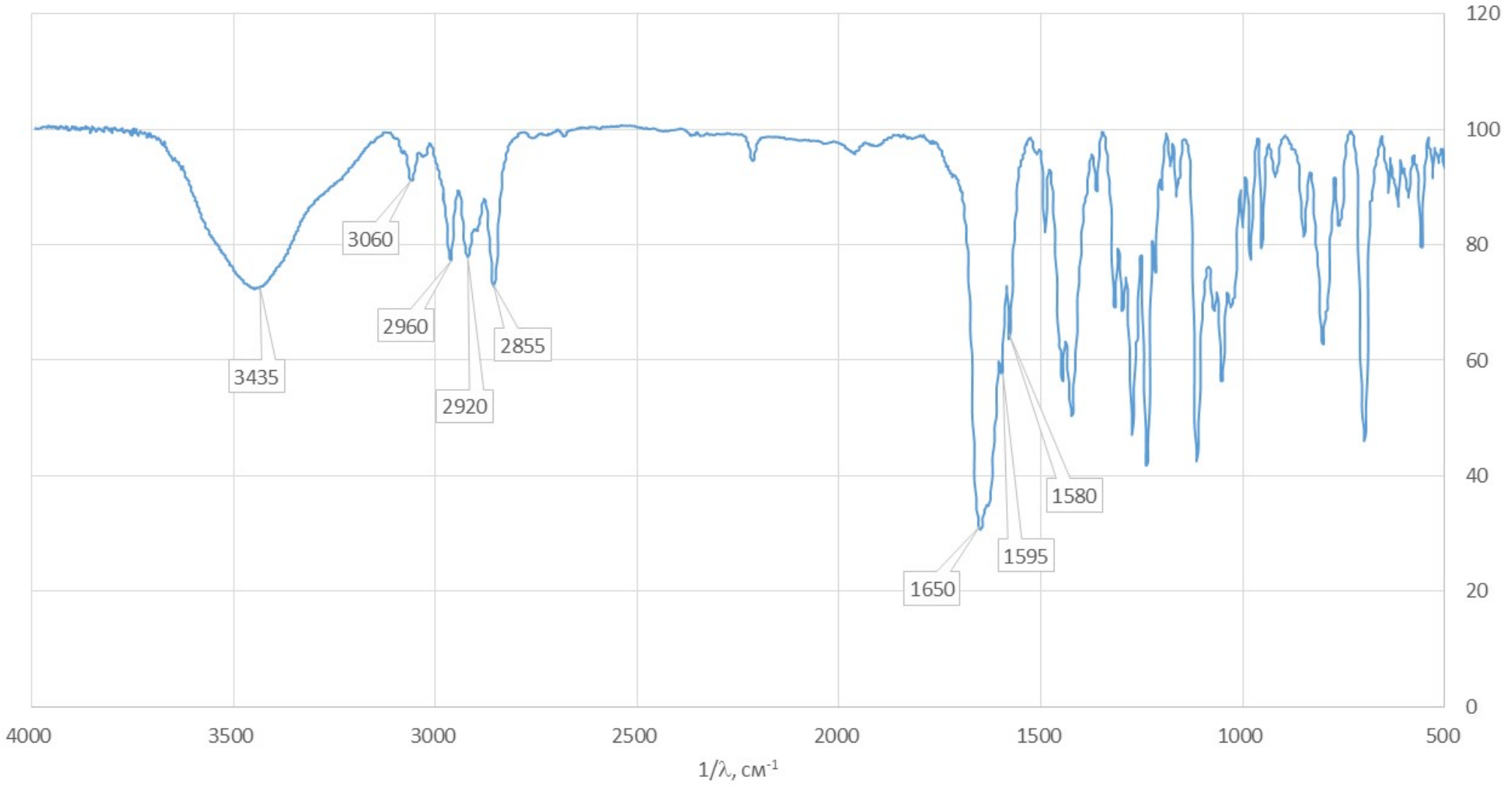


^{13}C N-(diphenylmethylene)morpholine-4-carboxamide (5d)

BUTc
BUTc, 196, BF = 100.612769 MHz, Solvent - CDCl3, 07 Nov 2014 T=300 K



16a


120
100
80
60
40
20
0
3435
3060
2960
2920
2855
1650
1595
1580
4000
3500
3000
2500
2000
1500
1000
500
1/λ, см-1

Mass Spectrum Report

Analysis Info

Analysis Name	D:\Data\mish2\BUT178_2.d	Acquisition Date	15.05.2014 12:51:15
Method	tune_low.m	Operator	Bruker Customer
Sample Name	BUT178_2	Instrument / Ser#	micrOTOF 10223
Comment	MeOH100v		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	8.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source