

Supplementary Material

Diverse Modification of the 4-Methylphenyl Moiety of TAK-779 by Late-Stage Suzuki-Miyaura Cross-Coupling

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¹ H spectrum	48
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HPLC chromatogram	50
Exact MS spectra	51

2-[4-(Dimethylamino)phenyl]-N-[4-[N-methyl-N-(tetrahydro-2H-pyran-4-yl)aminomethyl]phenyl]-6,7-dihydro-5H-benzo[7]annulene-8-carboxamide (2f)

¹ H spectrum	53
¹³ C spectrum	53
gHSQC spectrum	54
HPLC chromatogram	55
Exact MS spectra	56

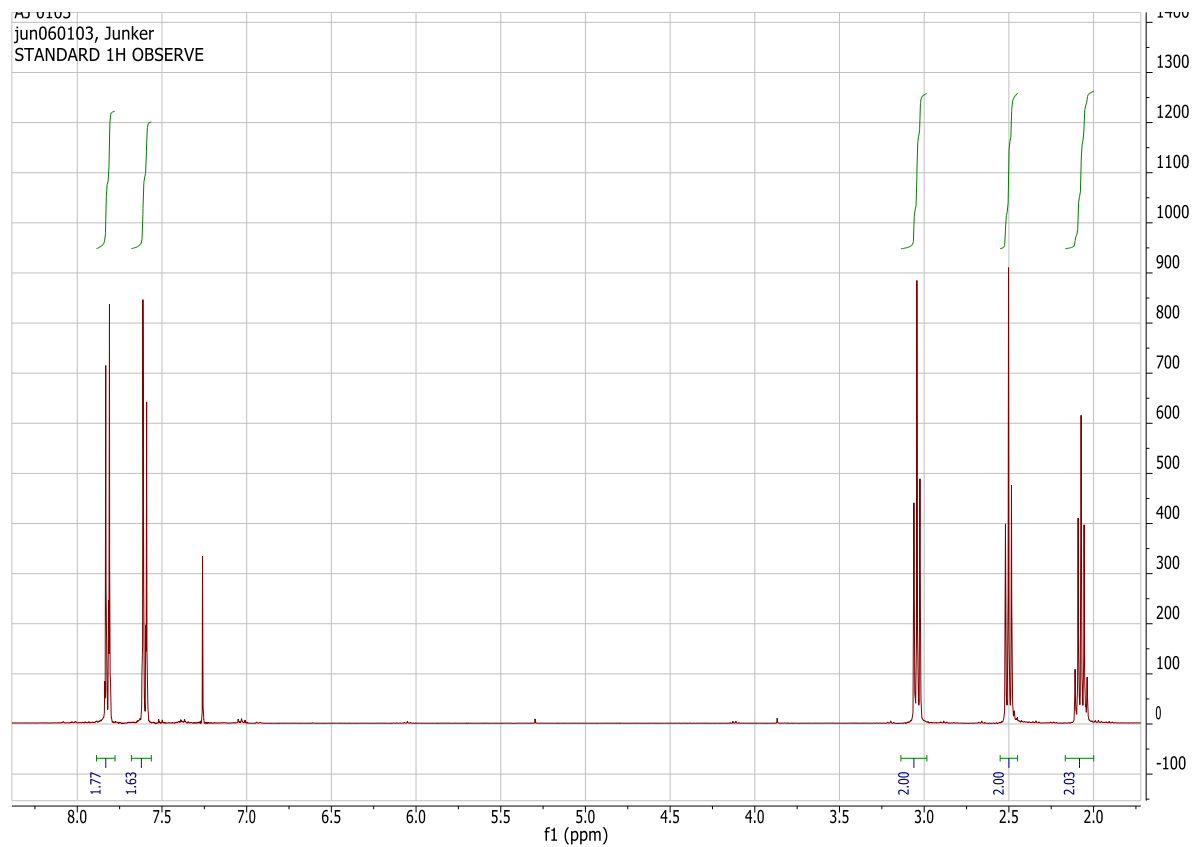
N-[4-[N-Methyl-N-(tetrahydro-2H-pyran-4-yl)aminomethyl]phenyl]-2-(pyridin-3-yl)-6,7-dihydro-5H-benzo[7]annulene-8-carboxamide (2g)

¹ H spectrum	58
¹³ C spectrum	58
gHSQC spectrum	59
HPLC chromatogram	60
Exact MS spectra	61

N-[4-[Methyl(tetrahydro-2H-pyran-4-yl)aminomethyl]phenyl]-2-(5-methylthiophen-2-yl)-6,7-dihydro-5H-benzo[7]annulene-8-carboxamide (2h)

¹ H spectrum	63
¹³ C spectrum	63
gHSQC spectrum	64
HPLC chromatogram	65
Exact MS spectra	66

5-(4-Bromophenyl)-5-oxo-pentanoic acid (4)



HPLC

Analyzed: 11.02.10 08:46

Reported: 11.02.10 15:15
Processed: 11.02.10 15:15

Data Path: D:\WIN32APP\HSM\Chromni\DATA\1176\

Application: Chromni

Sample Name: AJ0113

Injection from this vial: 1 of 1

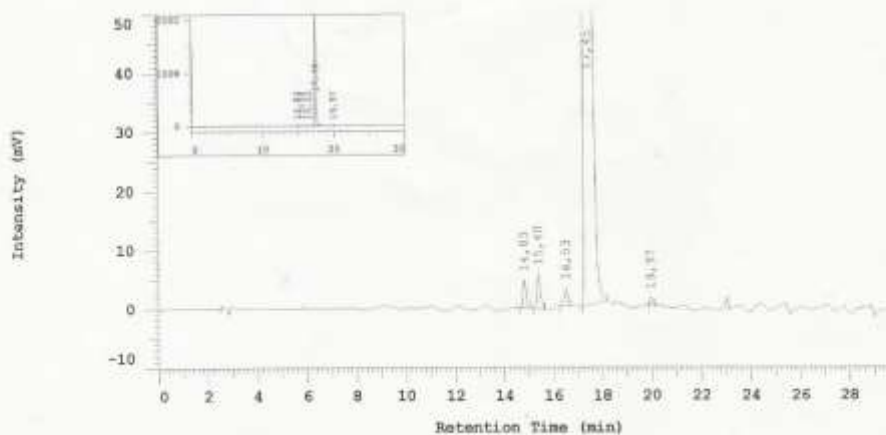
Series:1176

Vial Number: 19

Vial Type: UNK

Volume: 5,0 ul

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

Solvent B: ACN + 0,05%TFA

No.	RT	Area	Conc 1	BC
1	14,83	40788	0,196	MC
2	15,40	52660	0,253	MC
3	16,53	29956	0,144	MC
4	17,45	20711131	99,360	MC
5	19,97	10102	0,048	MC
		20844637	100,000	

Peak rejection level: 0

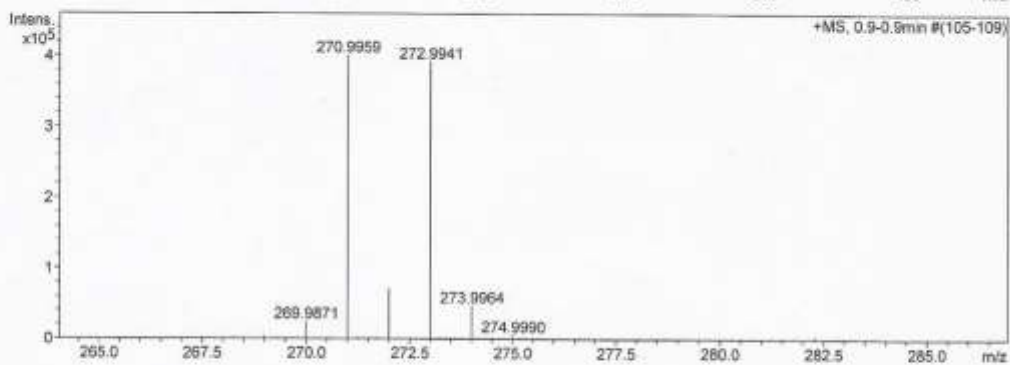
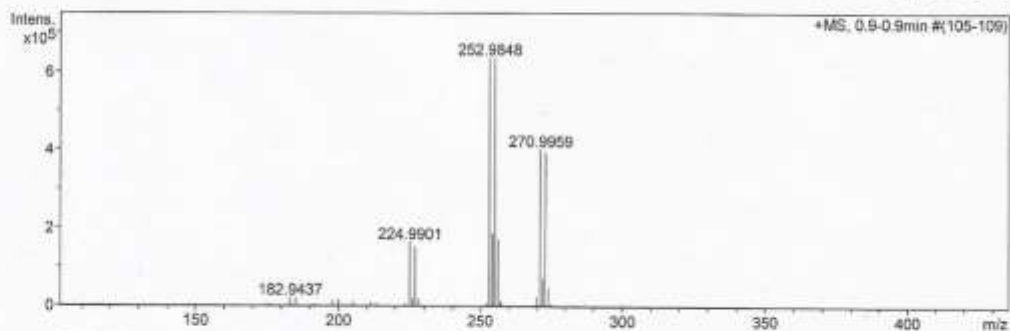
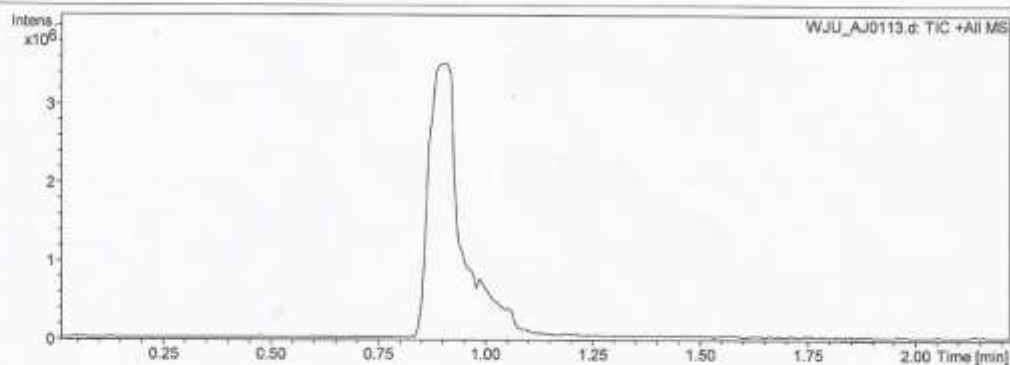
Generic Display Report

Analysis Info

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Method APCI_directprobe_positiv.m
Sample Name AJ0113
Comment Junker
APCI-Direkt
Kalibration mit Fettsaeureestern

Acquisition Date 9/4/2012 8:39:04 AM

Operator Sendker
Instrument micrOTOF-Q II



Mass Spectrum SmartFormula Report

Analysis Info

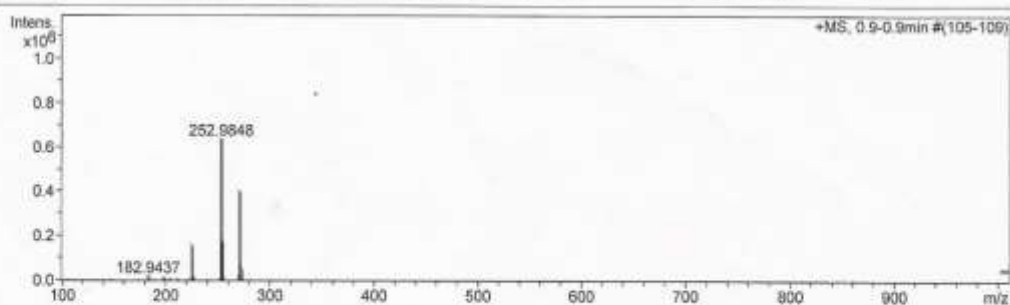
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Method APCI_directprobe_positiv.m
Sample Name AJ0113
Comment Junker
APCI-Direkt
Kalibration mit Fettsaeureestern

Acquisition Date 9/4/2012 8:39:04 AM

Operator Sender
Instrument / Ser# micrOTOF-Q II 10252

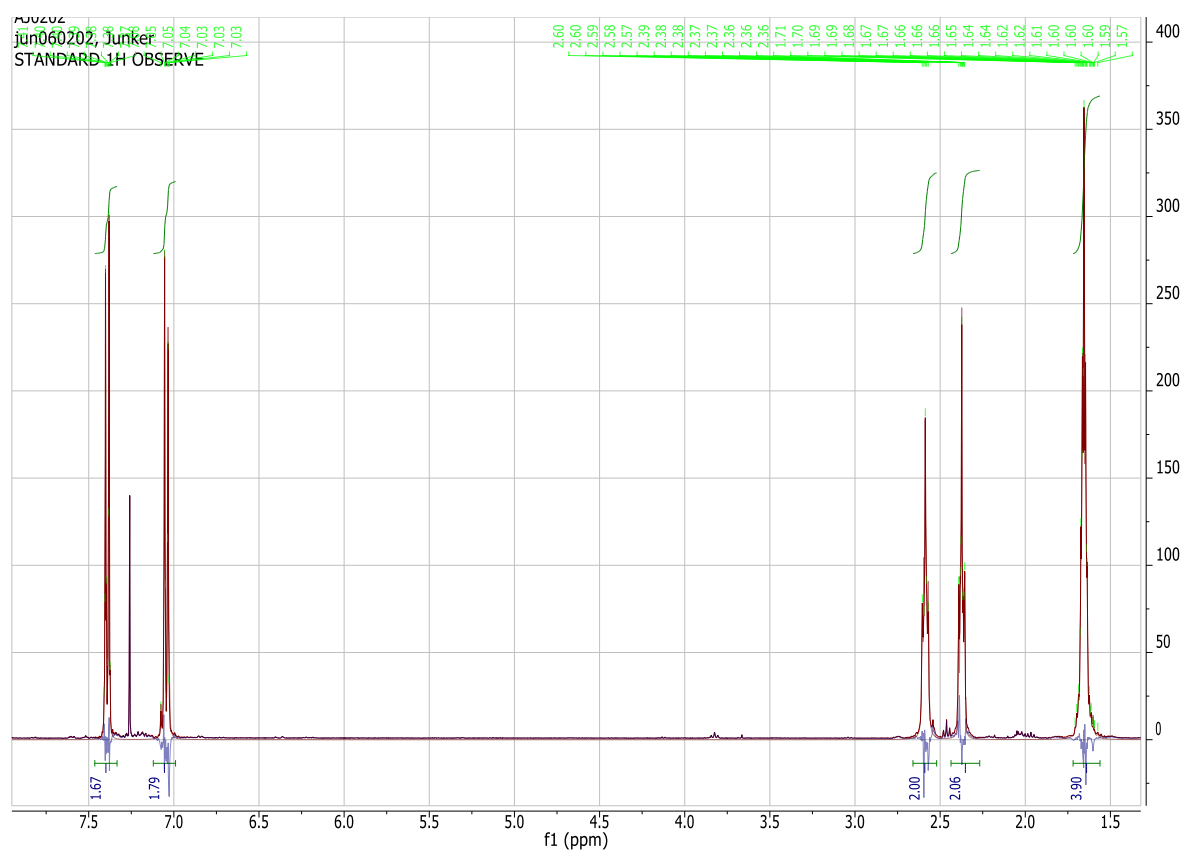
Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
270.9959	1	C 13 H 8 Br N 2	0.00	270.9885	-9.4	-34.6	17.7	10.5	even	ok
	2	C 11 H 12 Br O 3	100.00	270.9954	0.5	1.9	25.0	5.5	even	ok

5-(4-Bromophenyl) pentanoic acid (**5**)



HPLC

Analyzed: 18.02.10 11:49

Reported: 19.02.10 10:39

Processed: 19.02.10 10:39

Data Path: D:\WIN32APP\HSM\Chromni\DATA\1210\

Application: Chromni

Series:1210

Sample Name: AJ 0208

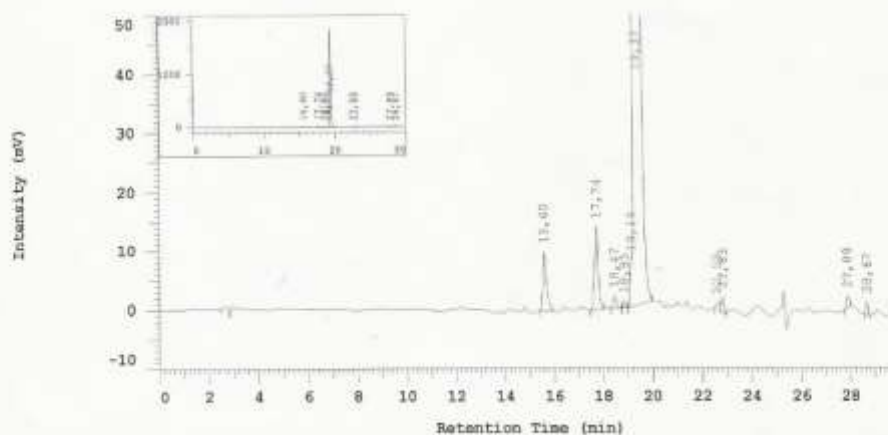
Vial Number: 22

Injection from this vial: 1 of 1

Vial Type: UNK

Volume: 5,0 ul

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

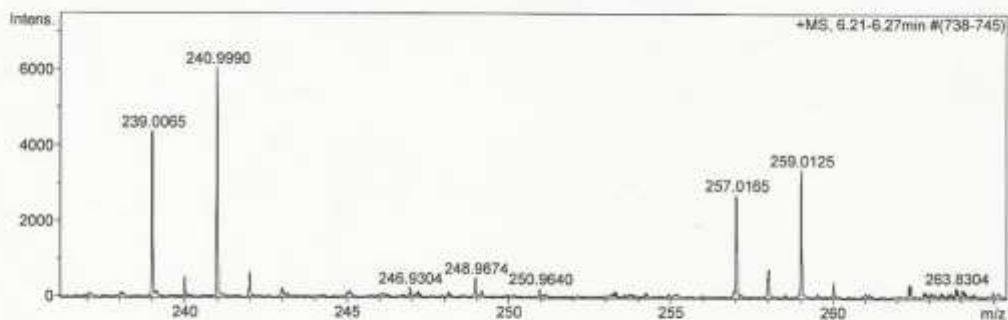
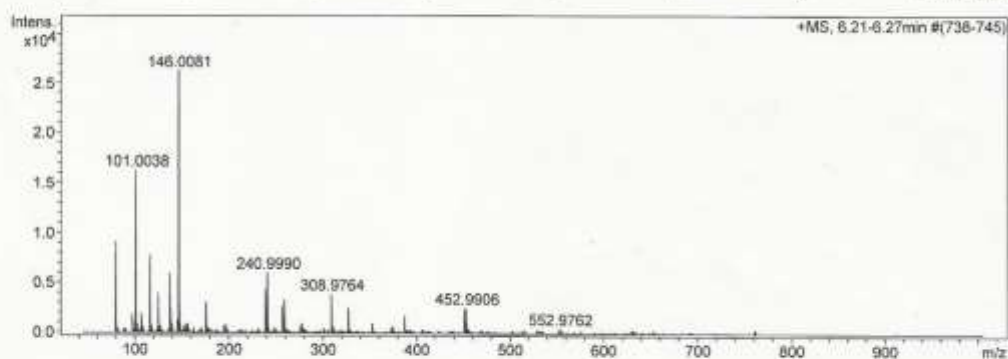
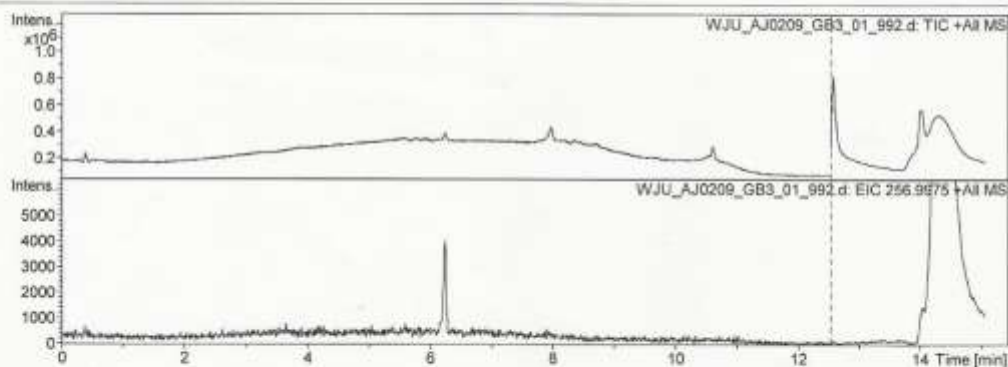
Solvent B: ACN + 0,05%TFA

No.	RT	Area	Conc 1	BC
1	15,60	99963	0,597	MC
2	17,74	145693	0,869	BB
3	18,47	20954	0,125	BB
4	18,85	7400	0,044	BB
5	19,14	205966	1,229	MC
6	19,37	16215217	96,764	VB
7	22,59	13259	0,079	MC
8	22,83	19830	0,118	BB
9	27,89	14126	0,084	MC
10	28,67	15029	0,090	MC
		16757437	100,000	

Peak rejection level: 0

Generic Display Report

Analysis Info		Acquisition Date	8/18/2010 2:34:55 PM
Analysis Name	D:\Data\IPMC\PharmChemie\Routine\2010_08_16\WJU_AJ0209_GB3_01_992.d	Operator	Meiners
Method	kurz_pos_ms_low.m	Instrument	micrOTOF-Q II
Sample Name	WJU_AJ0209		
Comment	Junker AJ0209		



257,0142 27ppm

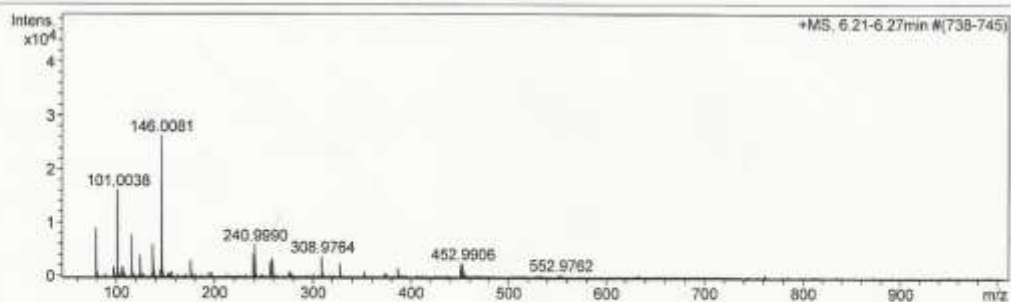
Mass Spectrum SmartFormula Report

Analysis Info

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Method kurz_pos_ms_low.m Operator Meiners
Sample Name WJU_AJ0209 Instrument / Ser# micrOTOF-Q II 10252
Comment Junker
AJ0209

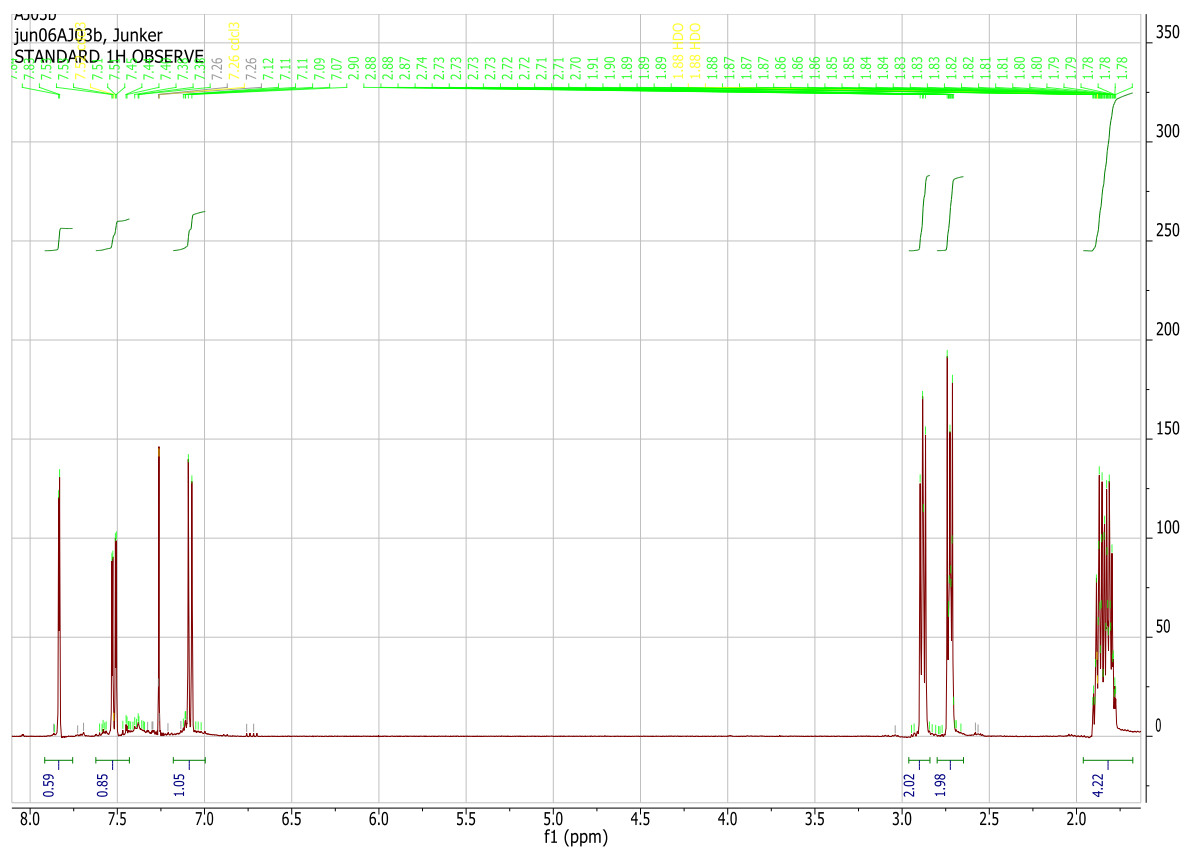
Acquisition Parameter

Source Type ESI Ion Polarity Positive Set Nebulizer 4.5 Bar
Focus Not active Set Capillary 4500 V Set Dry Heater 220 °C
Scan Begin 50 m/z Set End Plate Offset -500 V Set Dry Gas 9.0 l/min
Scan End 1000 m/z Set Collision Cell RF 130.0 Vpp Set Divert Valve Waste



Meas. m/z	#	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
257.0165	1	C 11 H 14 Br O 2	257.0172	-0.7	2.7	97.9	4.5	even	ok ✓
	2	C 6 H 14 Br N 2 O 4	257.0131	-3.3	-12.9	110.7	0.5	even	ok
	3	C 7 H 10 Br N 6	257.0145	-2.0	-7.7	115.3	5.5	even	ok

3-Bromo-6,7,8,9-tetrahydrobenzo[7]annulen-5-one (6)



HPLC

Analyzed: 24.02.10 21:42

Reported: 25.02.10 16:24
 Processed: 25.02.10 16:24

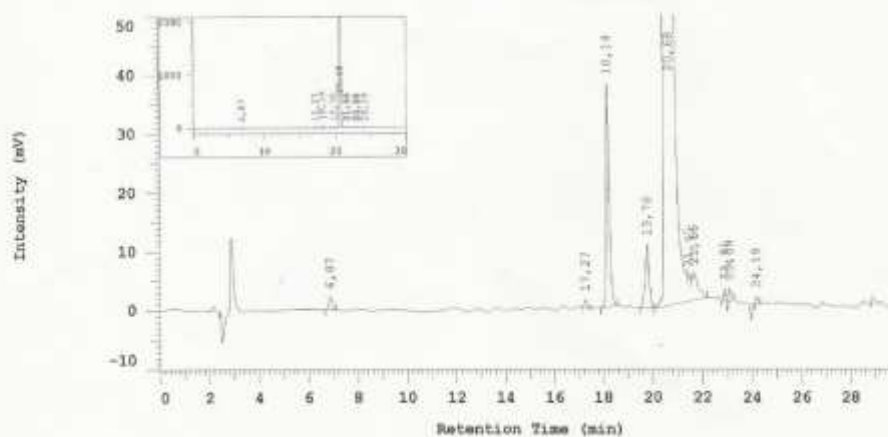
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 Application: Chromni

Series:1226
 Vial Number: 5
 Vial Type: UNK
 Volume: 5,0 ul

Sample Name: AJ 0323

Injection from this vial: 1 of 1

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

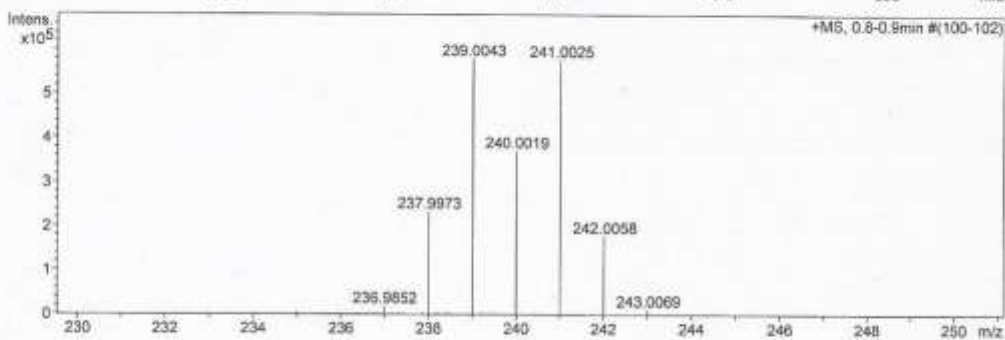
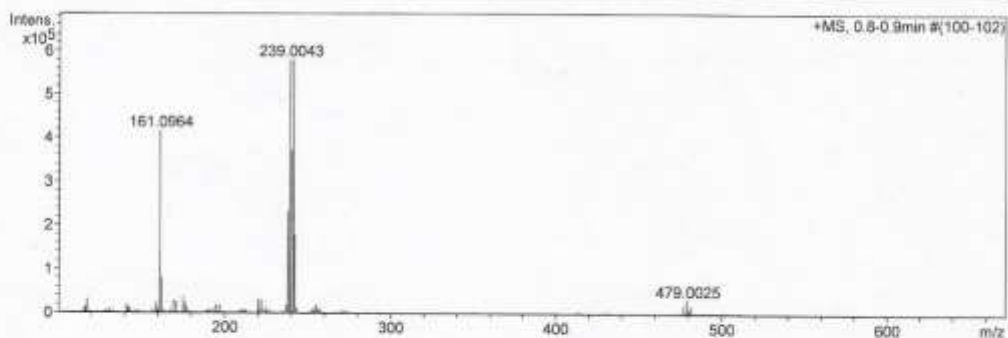
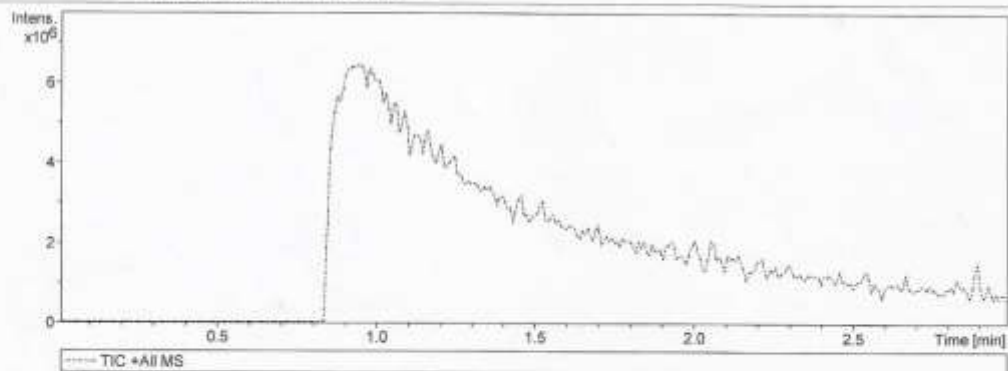
Solvent B: ACN + 0,05%TFA

No.	RT	Area	Conc 1	BC
1	6,87	22760	0,080	MC
2	17,27	10524	0,037	MC
3	18,19	327164	1,147	MC
4	19,78	116383	0,408	BB
5	20,68	27900563	97,792	MC
6	21,45	36189	0,127	MC
7	21,66	80167	0,281	MC
8	22,91	10454	0,037	MC
9	23,09	16657	0,058	MC
10	24,19	9664	0,034	MC
		28530525	100,000	

Peak rejection level: 0

Generic Display Report

Analysis Info		Acquisition Date	9/7/2012 8:20:42 AM
Analysis Name	D:\Data\PMc\Pharm\Chemie\Routine\APC\12_09\WJU_AJ03.d	Operator	Sendker
Method	APCI_directprobe_positiv.m	Instrument	micrOTOF-Q II
Sample Name	AJ03		
Comment	Junker APCI-Direkt Kalibration mit Fettsaeureestern		



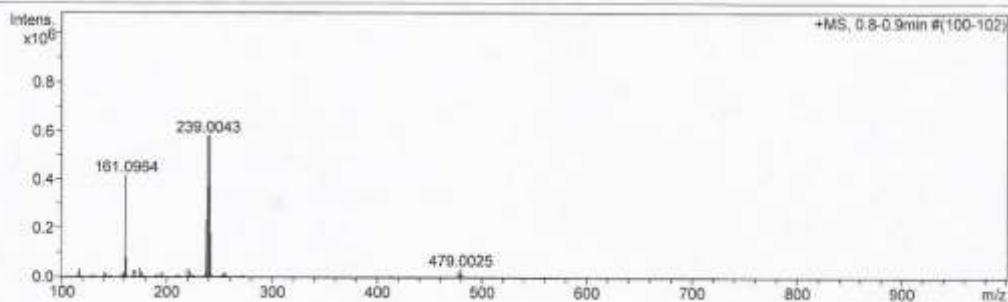
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: D:\Data\PMCI\PharmChemie\Routine\APCI\12_09WJU_AJ03.d
Method: APCI_directprobe_positiv.m
Sample Name: AJ03
Comment: Junker
APCI-Direkt
Kalibration mit Fettsaeureestern

Acquisition Date: 9/7/2012 8:20:42 AM
Operator: Sender
Instrument / Ser#: micrOTOF-Q II 10252

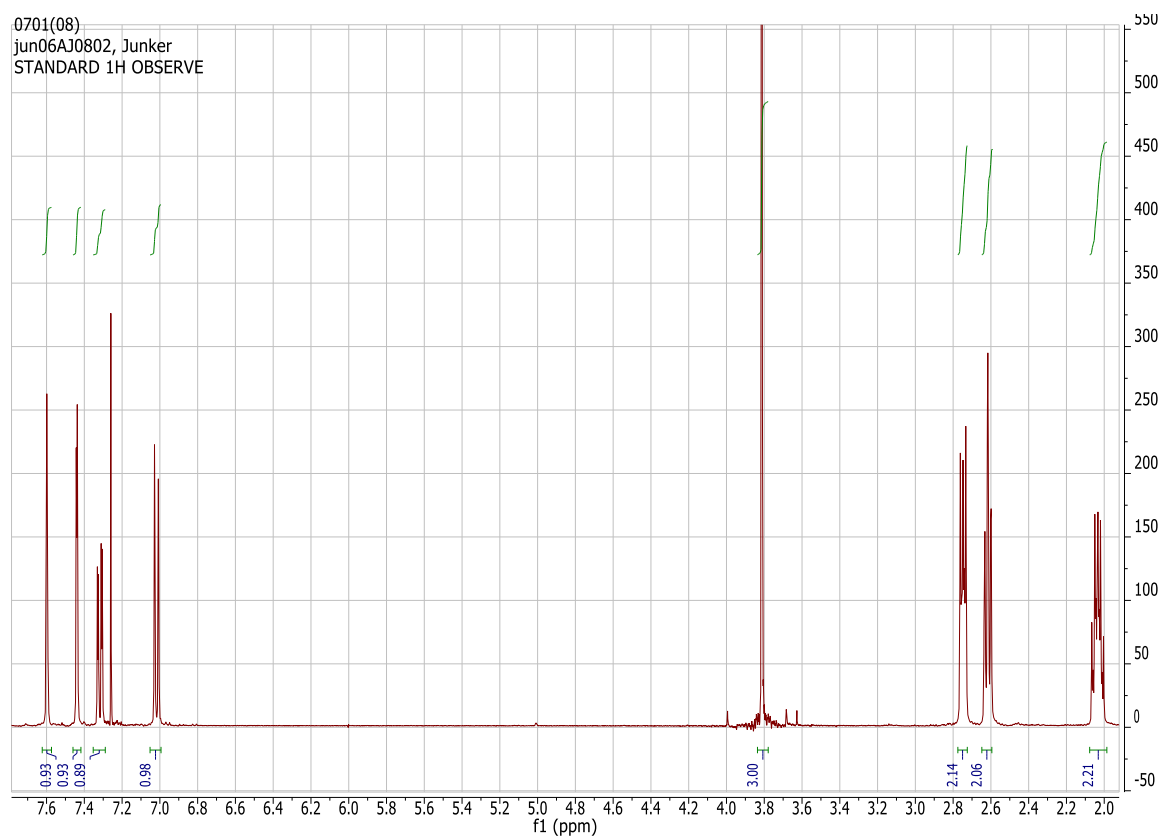
Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
239.0043	1	C 11 H 12 Br O	100.00	239.0066	-2.3	9.8	247.6	5.5	even	ok
	2	C 6 H 12 Br N 2 O 3	9.28	239.0026	-1.7	-7.0	274.3	1.5	even	ok

Methyl 2-bromo-6,7-dihydro-5H-benzo[7]annulene-8-carboxylate (9)



HPLC

Analyzed: 20.06.11 17:18

Reported: 21.06.11 09:38

Processed: 21.06.11 09:38

Data Path: D:\WIN32APP\HSM\Chromni\DATA\3186\

Application: Chromni

Series:3186

Sample Name: AJ0804

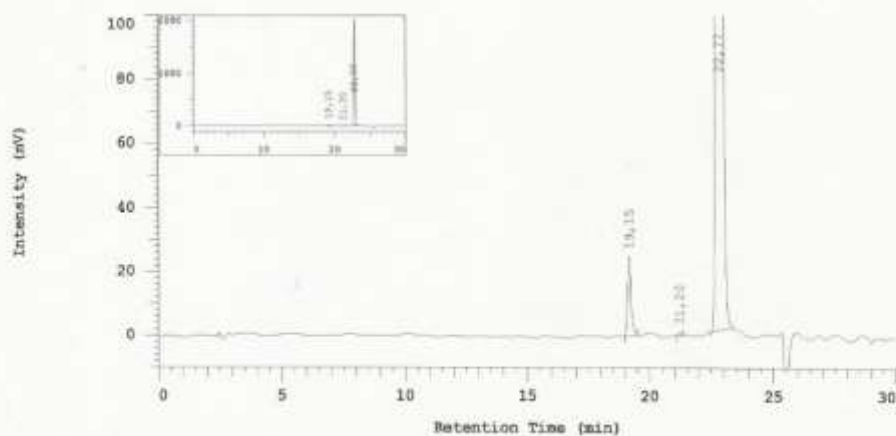
Vial Number: 5

Injection from this vial: 1 of 1

Vial Type: UNK

Volume: 5,0 ul

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

Solvent B: ACN + 0,05%TFA

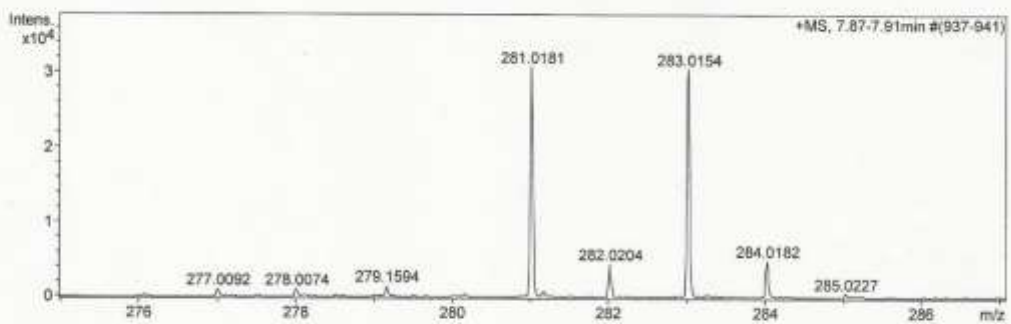
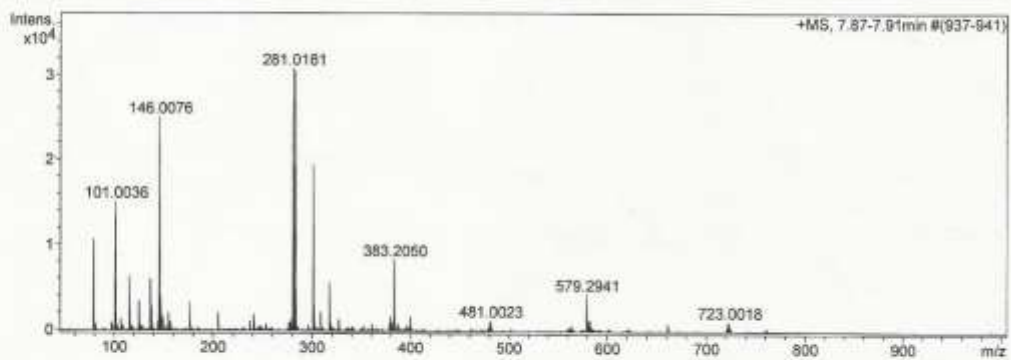
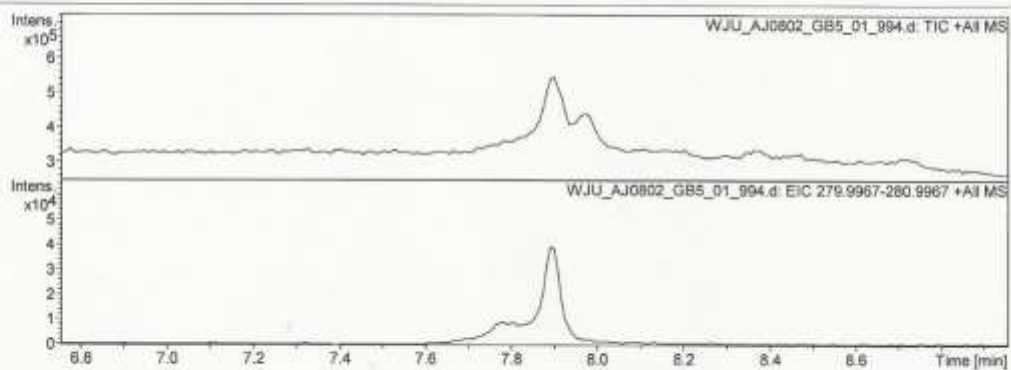
No.	RT	Area	Conc 1	BC
1	19,15	240471	1,228	MC
2	21,20	5846	0,030	BB
3	22,77	19338883	98,742	MC
		19585200	100,000	

Peak rejection level: 0

Generic Display Report

Analysis Info

Analysis Name	D:\Data\PMCI\PharmChemie\Routine\2010_08_16\WJU_AJ0802_GB5_01_994.d	Acquisition Date	8/16/2010 3:07:32 PM
Method	kurz_pos_ms_low.m	Operator	Meiners
Sample Name	WJU_AJ0802	Instrument	micrOTOF-Q II
Comment	Junker AJ0802		



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\PMC\PharmChemie\Routine\2010_08_16\WJU_AJ0802_GB5_01_994.d
Method kurz_pos_ms_low.m
Sample Name WJU_AJ0802
Comment Junker
AJ0802

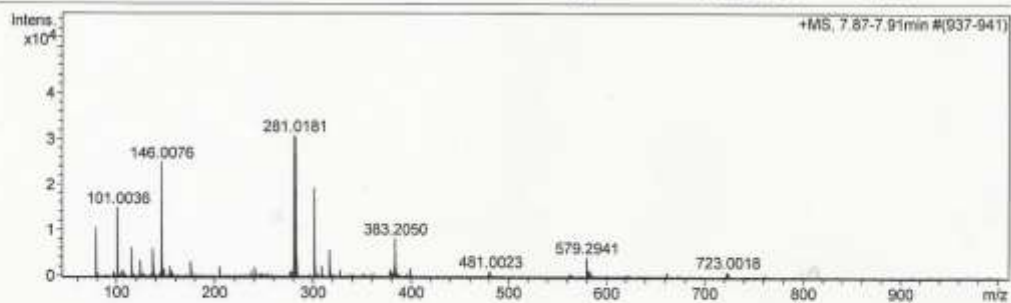
Acquisition Date 8/16/2010 3:07:32 PM

Operator Meiners

Instrument / Ser# micrOTOF-Q II 10252

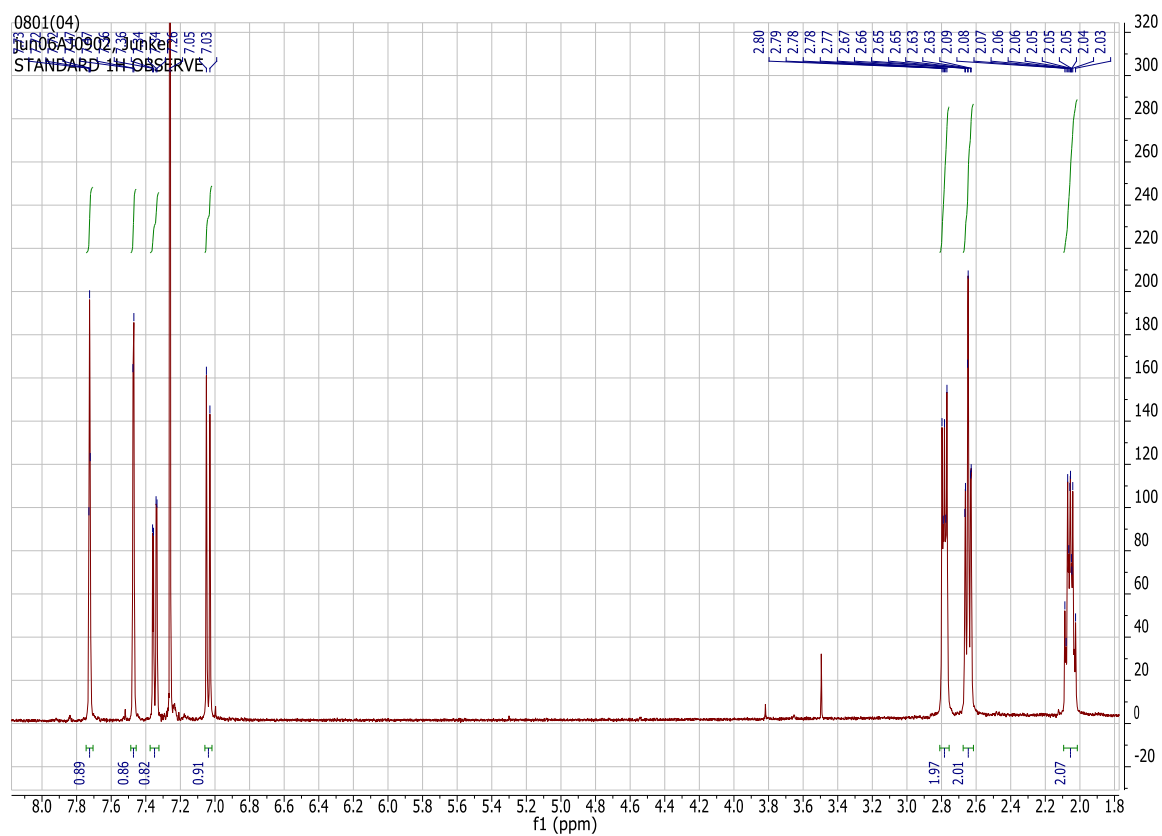
Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 1000 m/z
Ion Polarity Positive
Set Capillary 4500 V
Set End Plate Offset -500 V
Set Collision Cell RF 130.0 Vpp
Set Nebulizer 4.5 Bar
Set Dry Heater 220 °C
Set Dry Gas 9.0 l/min
Set Divert Valve Waste



Meas. m/z	#	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
281.0181	1	C 13 H 14 Br O 2	281.0172	-0.9	-3.4	10.3	6.5	even		ok ✓
	2	C 9 H 10 Br N 6	281.0145	-3.6	-12.9	23.3	7.5	even		ok ✓

2-Bromo-6,7-dihydro-5H-benzo[7]annulene-8-carboxylic acid (**10**)



HPLC

Analyzed: 20.06.11 17:59

Reported: 21.06.11 09:39
Processed: 21.06.11 09:39

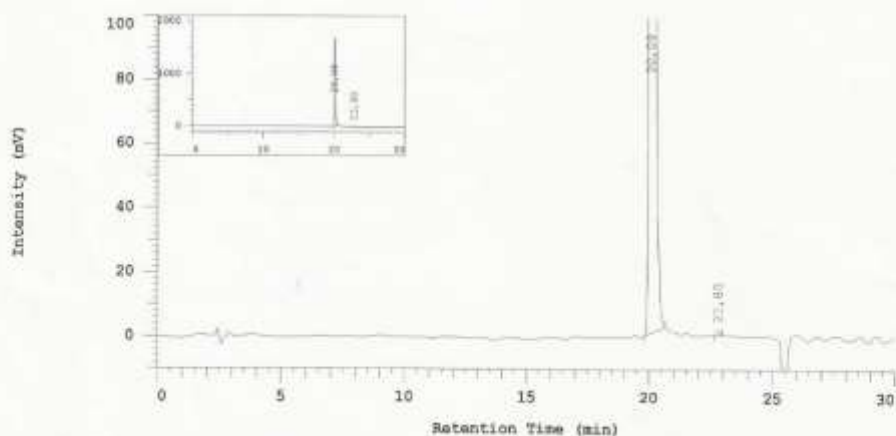
Data Path: D:\WIN32APP\HSM\Chromni\DATA\3187\
Application: Chromni

Sample Name: AJ0904

Series: 3187
Vial Number: 6
Vial Type: UNK
Volume: 5,0 ul

Injection from this vial: 1 of 1

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

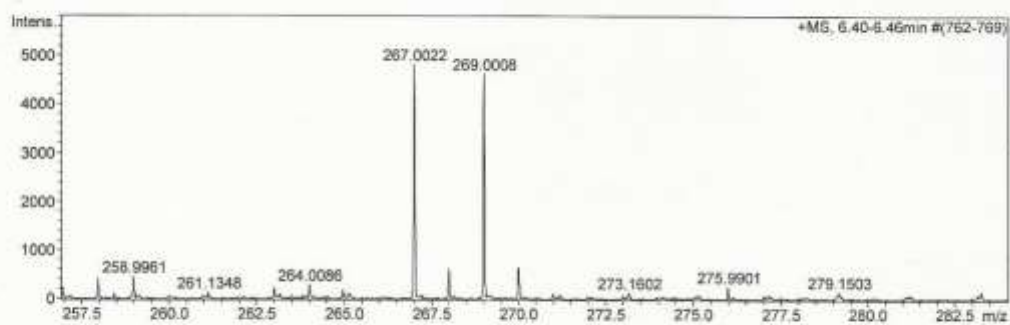
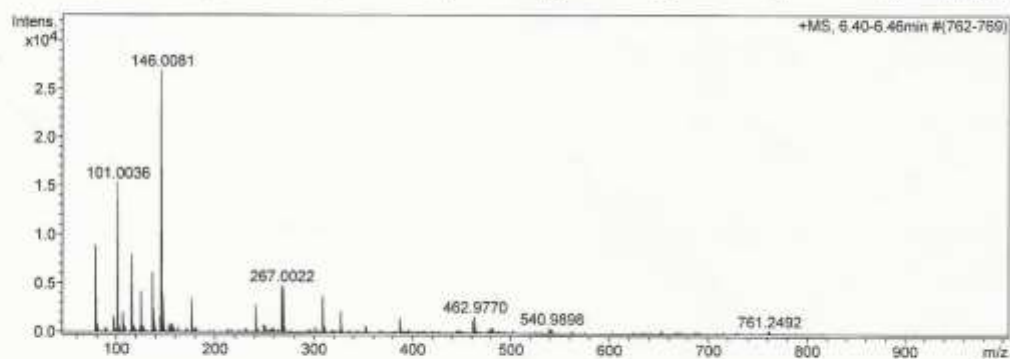
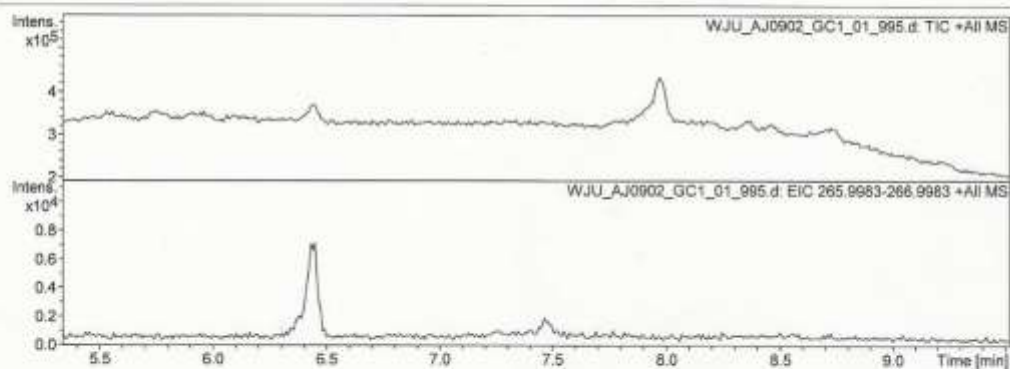
Solvent B: ACN + 0,05%TFA

No.	RT	Area	Conc 1	BC
1	20,09	16077145	99,936	MC
2	22,80	10224	0,064	BB
		16087369	100,000	

Peak rejection level: 0

Generic Display Report

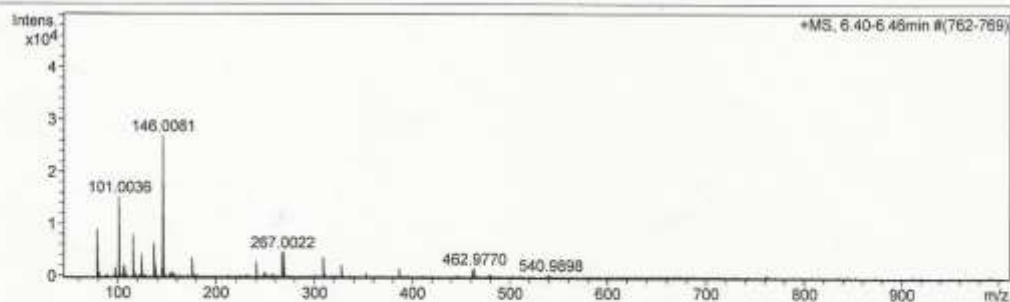
Analysis Info		Acquisition Date	8/16/2010 3:23:51 PM
Analysis Name	D:\Data\PMCI\Pharm\Chemie\Routine\2010_08_16\WJU_AJ0902_GC1_01_995.d	Operator	Meiners
Method	kurz_pos_ms_low.m	Instrument	micrOTOF-Q II
Sample Name	WJU_AJ0902		
Comment	Junker AJ0902		



Mass Spectrum SmartFormula Report

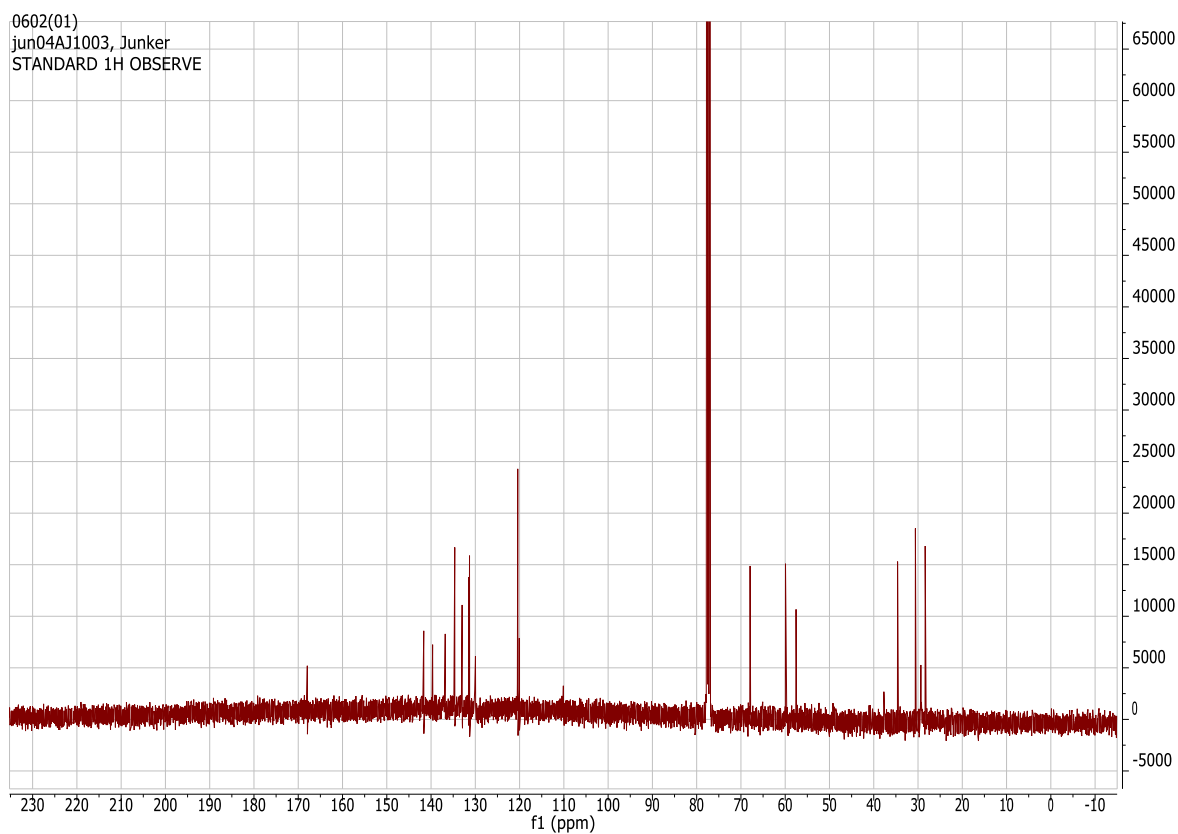
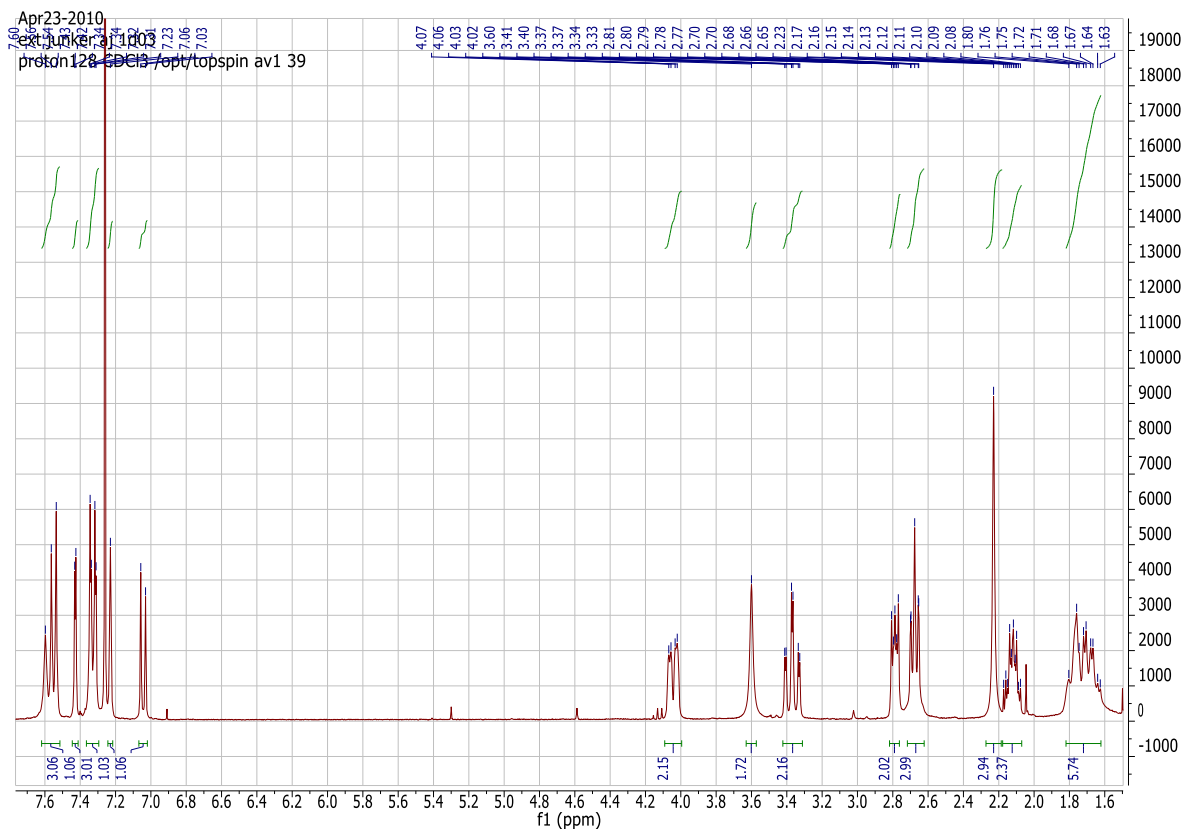
Analysis Info
Analysis Name: D:\Data\IPMC\PharmChemie\Routine\2010_08_16\WJU_AJ0902_GC1_01_995.d
Method: kurz_pos_ms_low.m
Sample Name: WJU_AJ0902
Comment: Junker
AJ0902
Acquisition Date: 8/16/2010 3:23:51 PM
Operator: Meiners
Instrument / Ser#: micrOTOF-Q II 10252

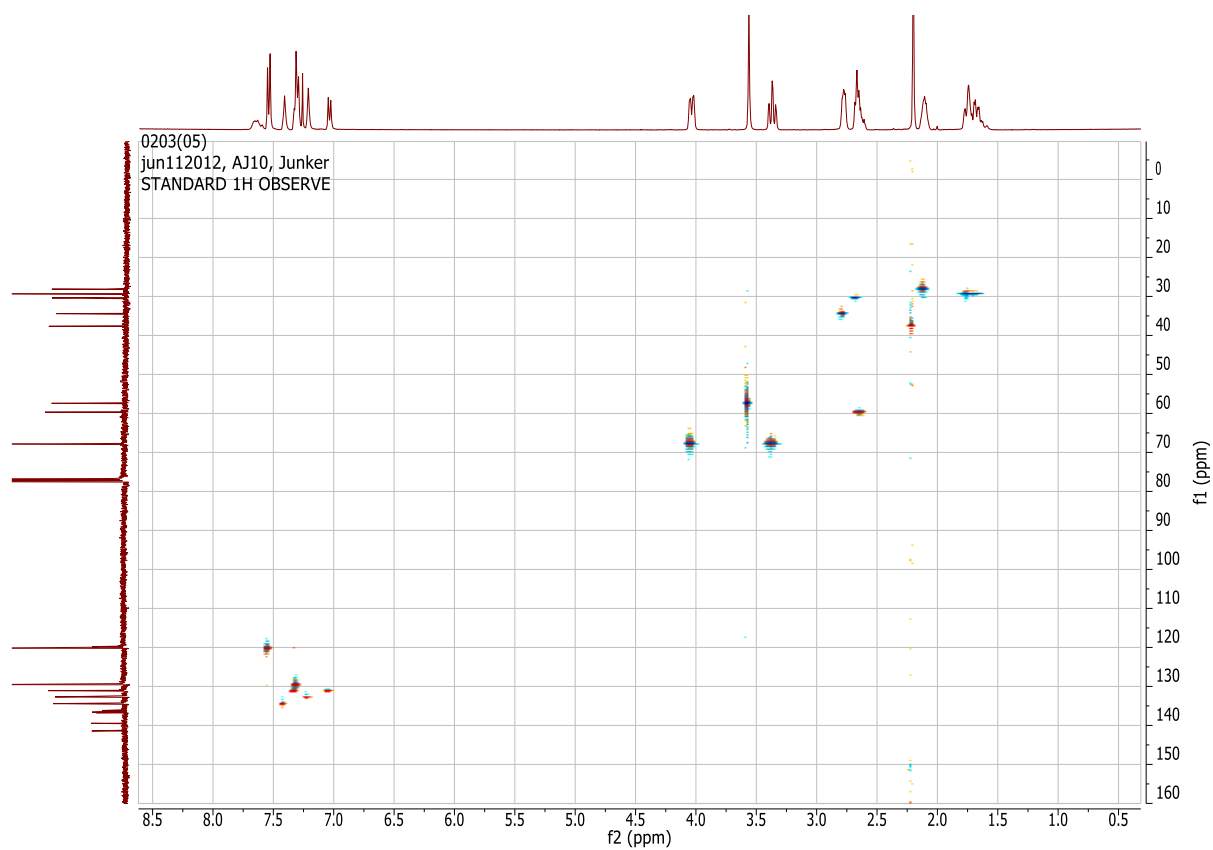
Acquisition Parameter
Source Type: ESI
Focus: Not active
Scan Begin: 50 m/z
Scan End: 1000 m/z
Ion Polarity: Positive
Set Capillary: 4500 V
Set End Plate Offset: -500 V
Set Collision Cell RF: 130.0 Vpp
Set Nebulizer: 4.5 Bar
Set Dry Heater: 220 °C
Set Dry Gas: 8.0 l/min
Set Divert Valve: Waste



Meas. m/z	#	Formula	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
267.0022	1	C ₁₂ H ₁₂ BrO ₂	267.0015	-0.7	-2.7	13.8	6.5	even	ok
	2	C ₈ H ₈ BrN ₆	266.9988	-3.4	-12.8	19.3	7.5	even	ok

2-Bromo-N-{4-[N-methyl-N-(tetrahydro-2H-pyran-4-yl)aminomethyl]phenyl}-6,7-dihydro-5H-benzo[7]annulene-8-carboxamide (**3**)





HPLC

Analyzed: 31.03.11 09:45

Reported: 31.03.11 15:23
Processed: 31.03.11 15:23

Data Path: D:\WIN32APP\HSM\Chromni\DATA\2898\
Application: Chromni

Sample Name: AJ1008

Series: 2898

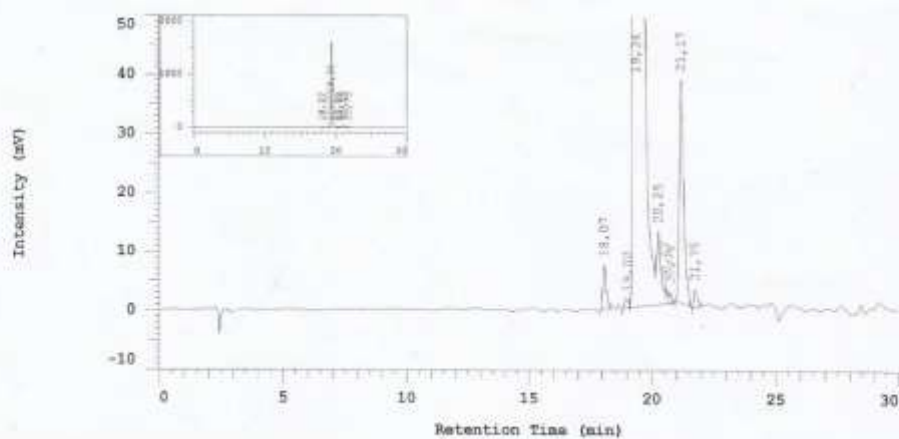
Vial Number: 20

Injection from this vial: 1 of 1

Vial Type: UNK

Volume: 5,0 ul

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

Solvent B: ACN + 0,05%TFA

No.	RT	Area	Conc 1	BC
1	18,07	68144	0,278	MC
2	19,00	15774	0,064	MC
3	19,34	23790344	96,903	MC
4	20,25	156101	0,636	MC
5	20,57	18924	0,077	MC
6	20,74	11031	0,045	MC
7	21,17	461853	1,881	MC
8	21,75	28486	0,116	BB
		24550657	100,000	

Peak rejection level: 0

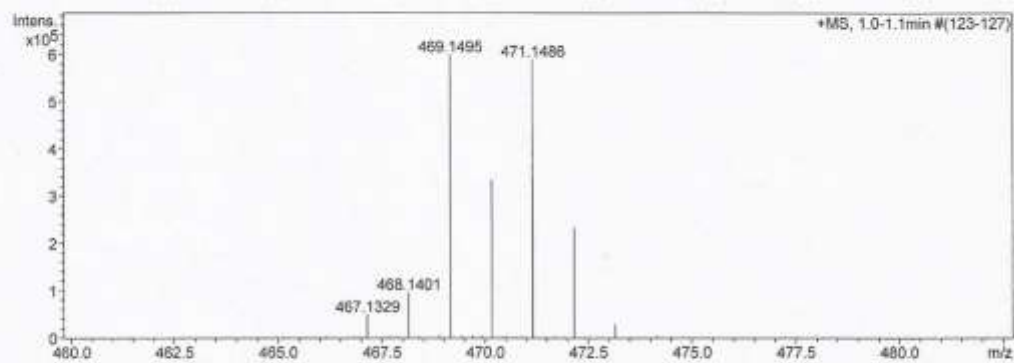
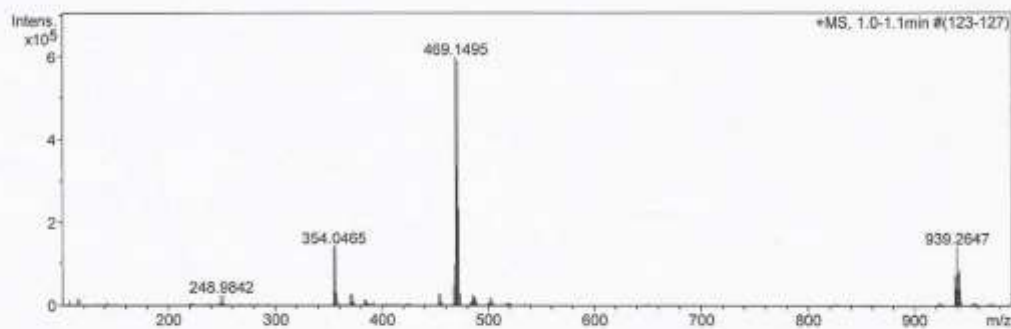
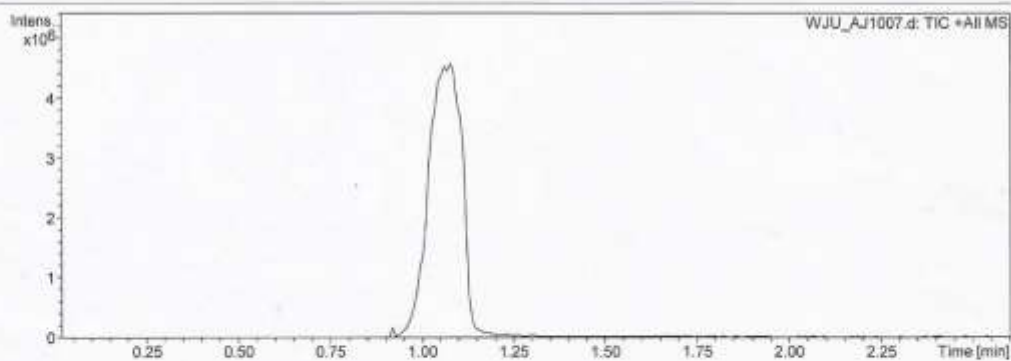
Generic Display Report

Analysis Info

Analysis Name E:\Meiners\12_09\WJU_AJ1007.d
Method APCI_directprobe_positiv.m
Sample Name AJ1007
Comment Junker
APCI-Direkt
Kalibration mit Fettsaeureestern

Acquisition Date 9/5/2012 8:52:07 AM

Operator Sendker
Instrument micrOTOF-Q II



Mass Spectrum SmartFormula Report

Analysis Info

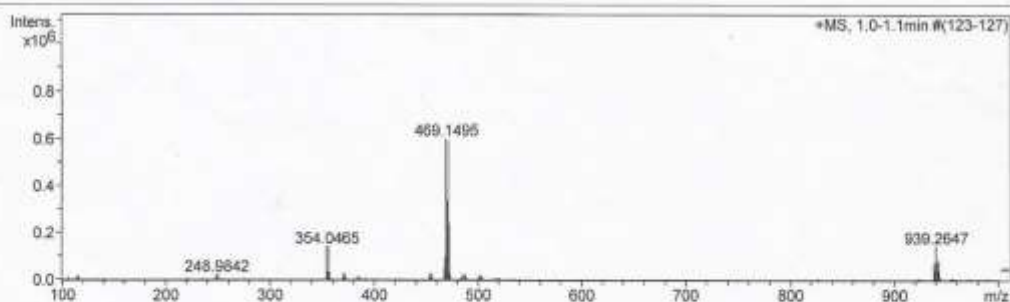
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Method APCI_directprobe_positiv.m
Sample Name AJ1007
Comment Junker
APCI-Direkt
Kalibration mit Fettsaeureestern

Acquisition Date 9/5/2012 8:52:07 AM

Operator Sender
Instrument / Ser# micrOTOF-Q II 10252

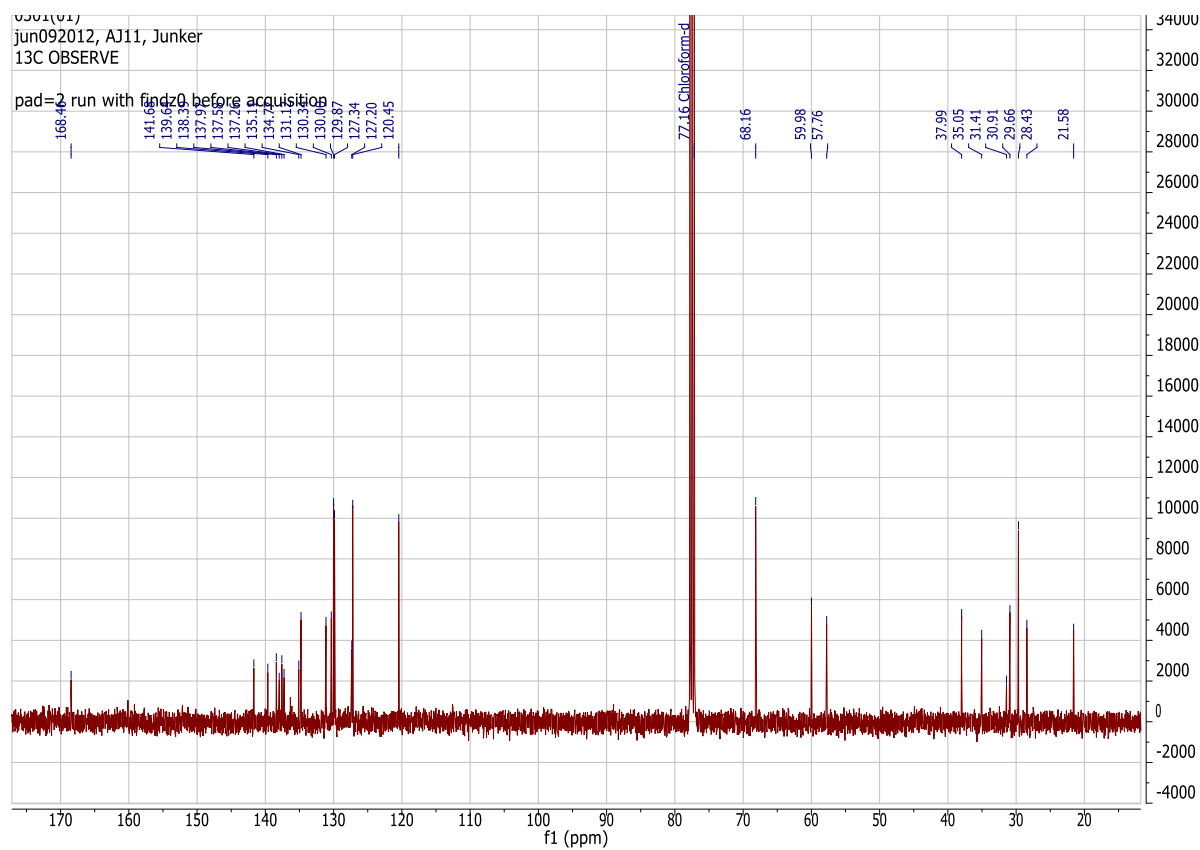
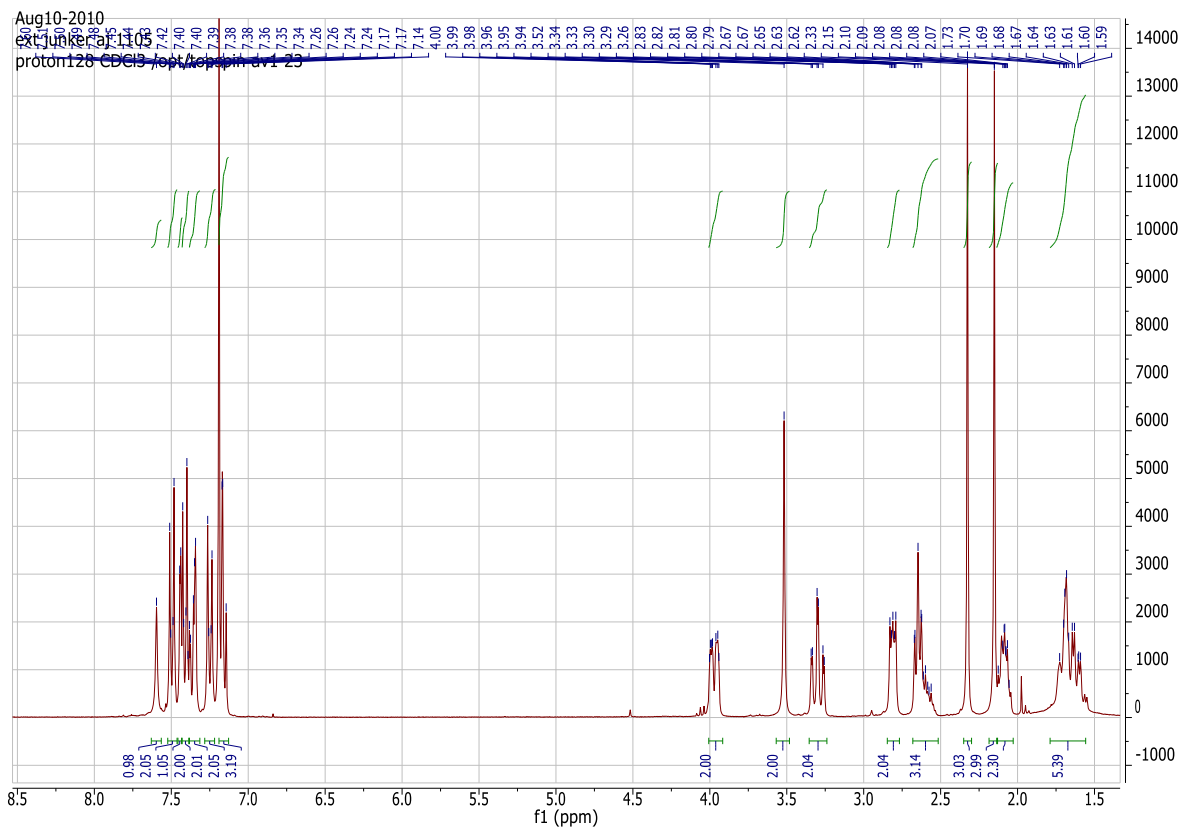
Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Mass. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
469.1495	1	C 30 H 30 Br	100.00	469.1525	3.1	6.5	103.6	15.5	even	ok
	2	C 25 H 30 Br N 2 O 2	75.81	469.1485	-1.0	-2.0	138.3	11.5	even	ok
	3	C 21 H 26 Br N 8	4.14	469.1458	-3.6	-7.8	149.1	12.5	even	ok
	4	C 15 H 26 Br N 12 O	0.56	469.1530	3.6	7.8	178.5	8.5	even	ok
	5	C 14 H 30 Br N 8 O 5	0.61	469.1517	2.2	4.8	193.4	3.5	even	ok
	6	C 10 H 26 Br N 14 O 3	0.63	469.1490	-0.4	-1.0	206.4	4.5	even	ok

2-(4-Methylphenyl)-N-{4-[N-methyl-N-(tetrahydro-2H-pyran-4-yl)aminomethyl]phenyl}-6,7-dihydro-5H-benzo[7]annulene-8-carboxamide (**2a**)



HPLC

Analyzed: 27.10.10 21:41

Reported: 28.10.10 16:22
 Processed: 28.10.10 16:22

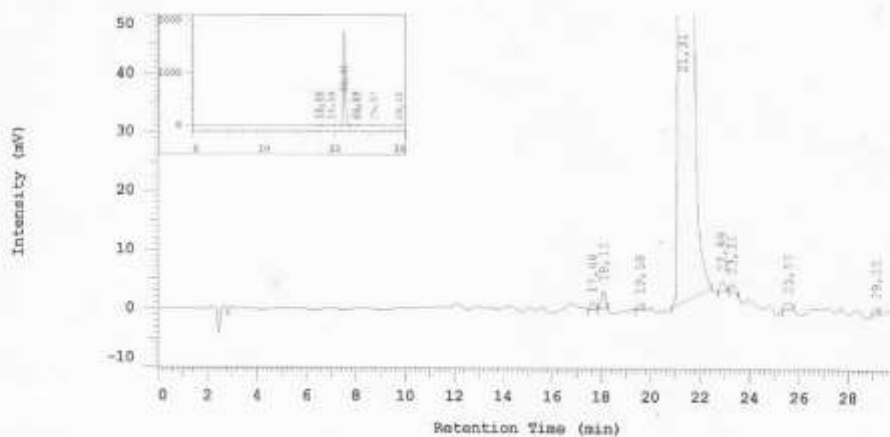
Data Path: D:\WIN32APP\HSM\Chromni\DATA\2304\
 Application: Chromni

Series: 2304
 Vial Number: 6
 Vial Type: UNK
 Volume: 5,0 ul

Sample Name: AJ1106

Injection from this vial: 1 of 1

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

Solvent B: ACN + 0,05%TFA

No.	RT	Area	Conc 1	BC
1	17,66	13404	0,039	BB
2	18,11	36545	0,108	BB
3	19,58	11382	0,033	BB
4	21,31	33844163	99,601	MC
5	22,89	19358	0,057	MC
6	23,31	20396	0,060	MC
7	25,57	22792	0,067	BB
8	29,15	11760	0,035	BB
		33979800	100,000	

Peak rejection level: 0

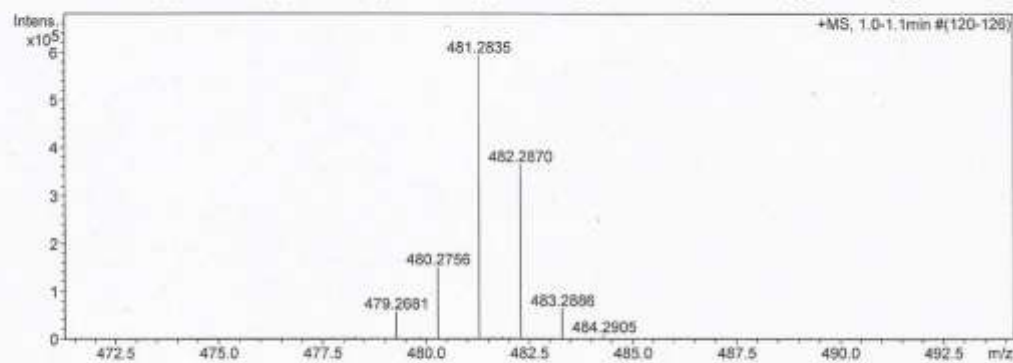
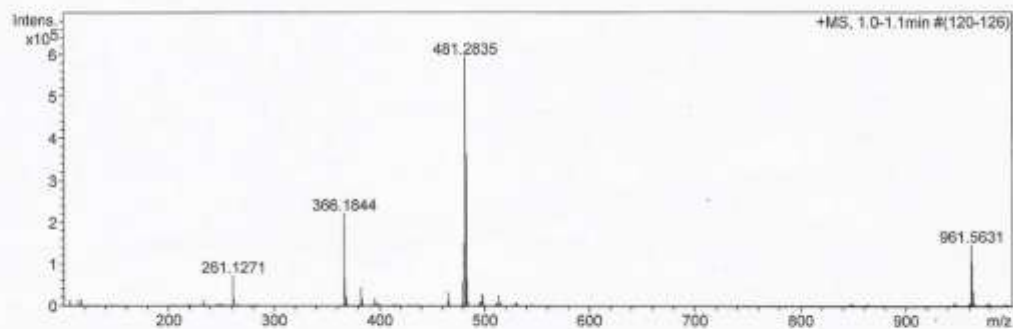
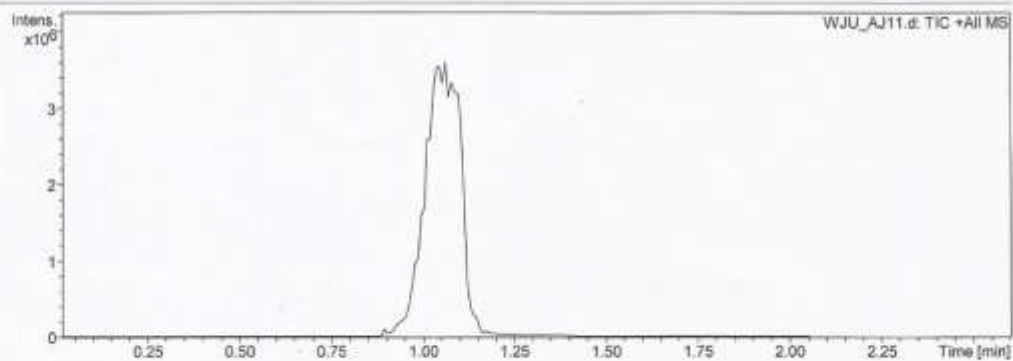
Generic Display Report

Analysis Info

Analysis Name E:\Weiners\12_09\WJU_AJ11.d
Method APCI_directprobe_positiv.m
Sample Name AJ11
Comment Junker
APCI-Direkt
Kalibration mit Fettsaeureestern

Acquisition Date 9/4/2012 11:44:15 AM

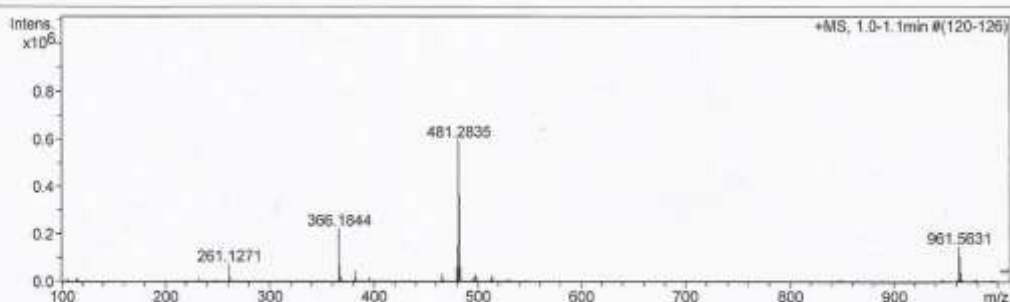
Operator Sendker
Instrument micrOTOF-Q II



Mass Spectrum SmartFormula Report

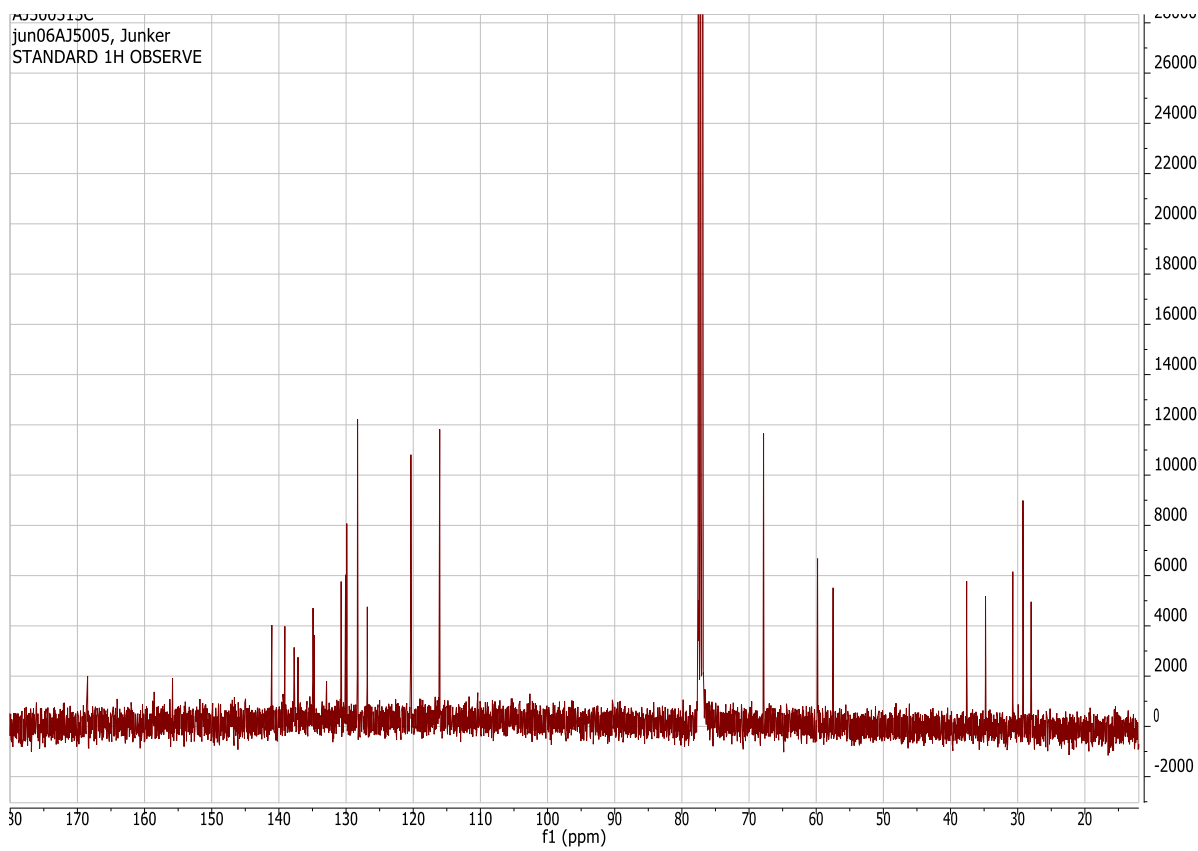
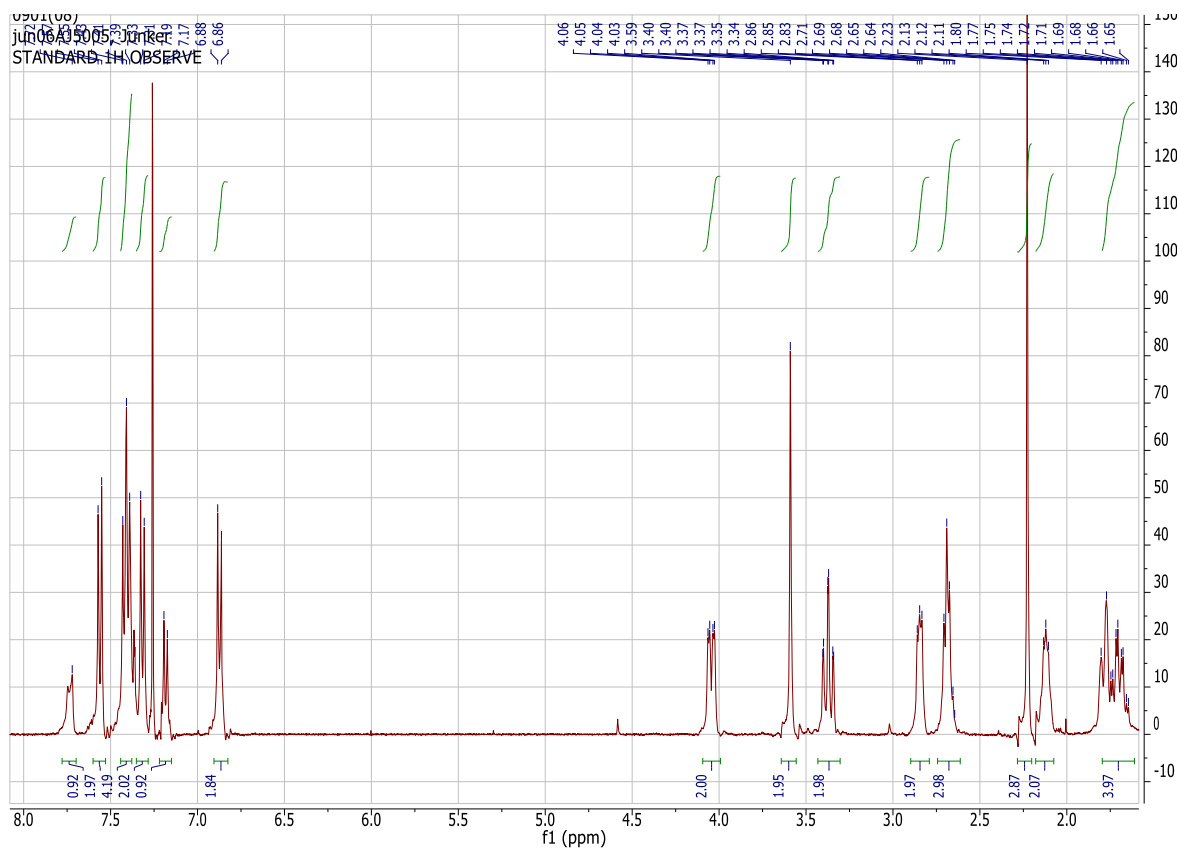
Analysis Info		Acquisition Date	9/4/2012 11:44:15 AM
Analysis Name	E:\Meiners\12_09WJU_AJ11.d	Operator	Sender
Method	APCI_directprobe_positiv.m	Instrument / Ser#	micrOTOF-Q II 10252
Sample Name	AJ11		
Comment	Junker APCI-Direkt Kalibration mit Fettsaeureestern		

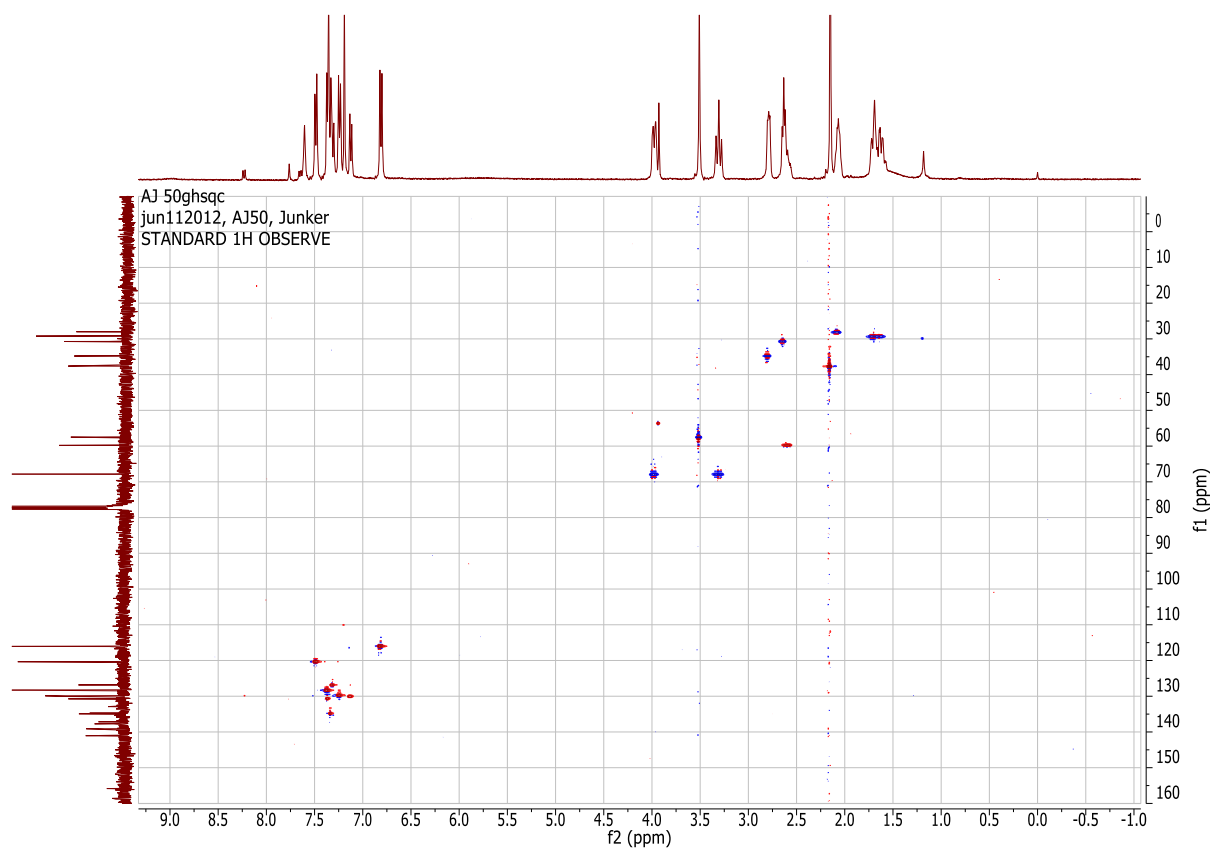
Acquisition Parameter					
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
481.2835	1	C ₃₂ H ₃₇ N ₂ O ₂	100.00	481.2850	1.5	3.1	128.7	15.5	even		ok
	2	C ₂₈ H ₃₃ N ₈	59.81	481.2823	-1.2	-2.5	140.4	16.5	even		ok
	3	C ₂₇ H ₃₇ N ₄ O ₄	10.10	481.2809	-2.5	-5.3	152.7	11.5	even		ok
	4	C ₂₆ H ₄₁ O ₈	1.11	481.2796	-3.9	-8.0	165.0	6.5	even		ok
	5	C ₂₀ H ₄₁ N ₄ O ₉	0.29	481.2868	3.3	6.9	190.6	2.5	even		ok
	6	C ₂₁ H ₃₇ N ₈ O ₅	0.02	481.2881	4.7	9.7	206.0	7.5	even		ok
	7	C ₁₇ H ₃₃ N ₁₄ O ₃	0.08	481.2855	2.0	4.1	219.3	8.5	even		ok
	8	C ₁₆ H ₃₇ N ₁₀ O ₇	0.05	481.2841	0.7	1.4	233.3	3.5	even		ok
	9	C ₁₃ H ₂₉ N ₂₀ O	0.04	481.2828	-0.7	-1.4	234.9	9.5	even		ok
	10	C ₁₂ H ₃₃ N ₁₆ O ₅	0.01	481.2814	-2.0	-4.2	246.5	4.5	even		ok

2-(4-Hydroxyphenyl)-N-{4-[N-methyl-N-(tetrahydro-2H-pyran-4-yl)aminomethyl]phenyl}-6,7-dihydro-5H-benzo[7]annulene-8-carboxamide (**2b**)





HPLC

Analyzed: 22.06.11 01:18

Reported: 22.06.11 11:32

Processed: 22.06.11 11:32

Data Path: D:\WIN32APP\HSM\Chromni\DATA\3219\

Application: Chromni

Series:3219

Sample Name: AJ5005

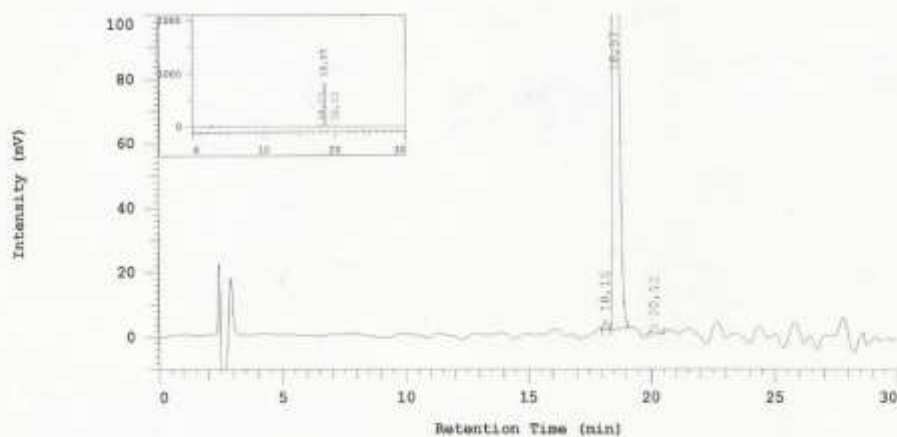
Vial Number: 17

Injection from this vial: 1 of 1

Vial Type: UNK

Volume: 5,0 ul

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

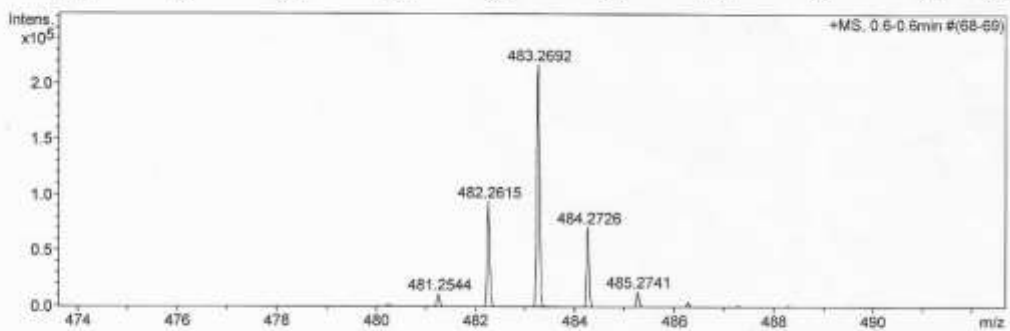
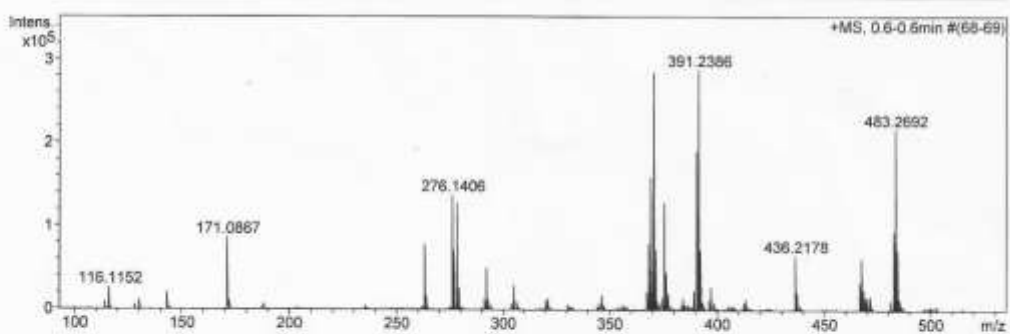
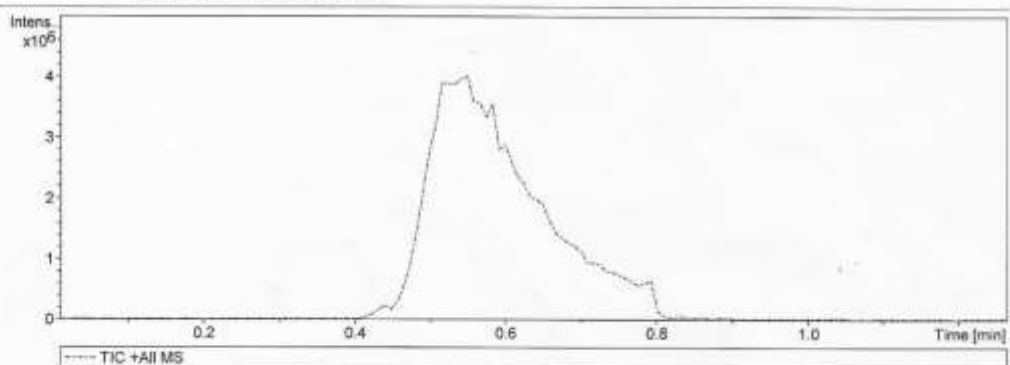
Solvent B: ACN + 0,05%TFA

No.	RT	Area	Conc 1	BC
1	18,15	23336	0,268	BB
2	18,57	8652428	99,290	MC
3	20,12	38556	0,442	BB
		8714320	100,000	

Peak rejection level: 0

Generic Display Report

Analysis Info		Acquisition Date	9/9/2010 2:34:18 PM
Analysis Name	D:\Data\PMCI\PharmChemie\Routine\2010_09\WJU_AJ5001.d	Operator	Meiners
Method	directprobe_default.m	Instrument	micrOTOF-Q II
Sample Name	AJ5001		
Comment	Junker AJ5001 APCI-Direkt Kalibration mit Fettsäureester		

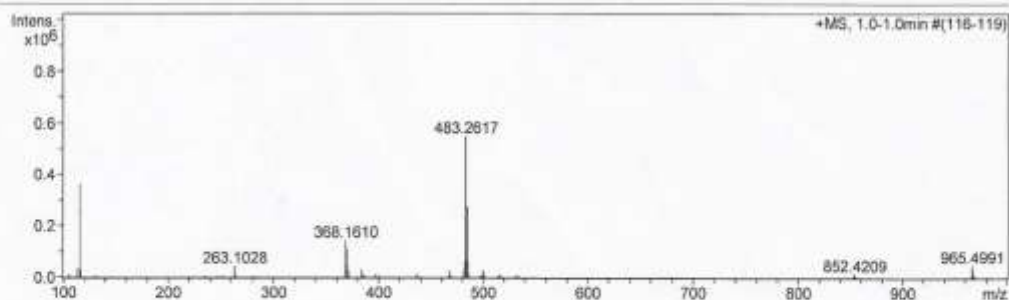


Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	9/11/2012 9:50:15 AM
Analysis Name	D:\Data\PMc\PharmChemie\Routine\APCI\12_09\WJU_AJ50.d	Operator	Sendker
Method	APCI_directprobe_positiv.m	Instrument / Ser#	micrOTOF-Q II 10252
Sample Name	AJ50		
Comment	Junker APCI-Direkt Kalibratinn mit Fettsaeureestern		

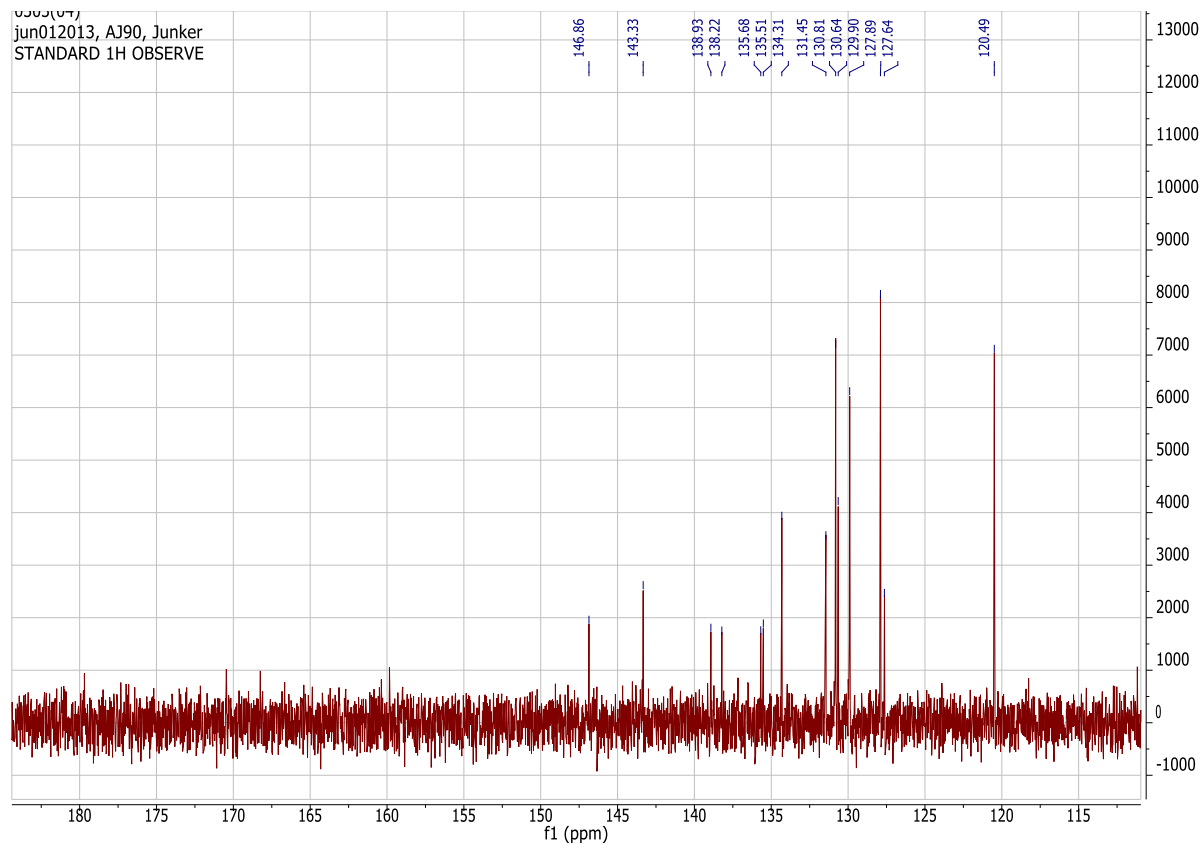
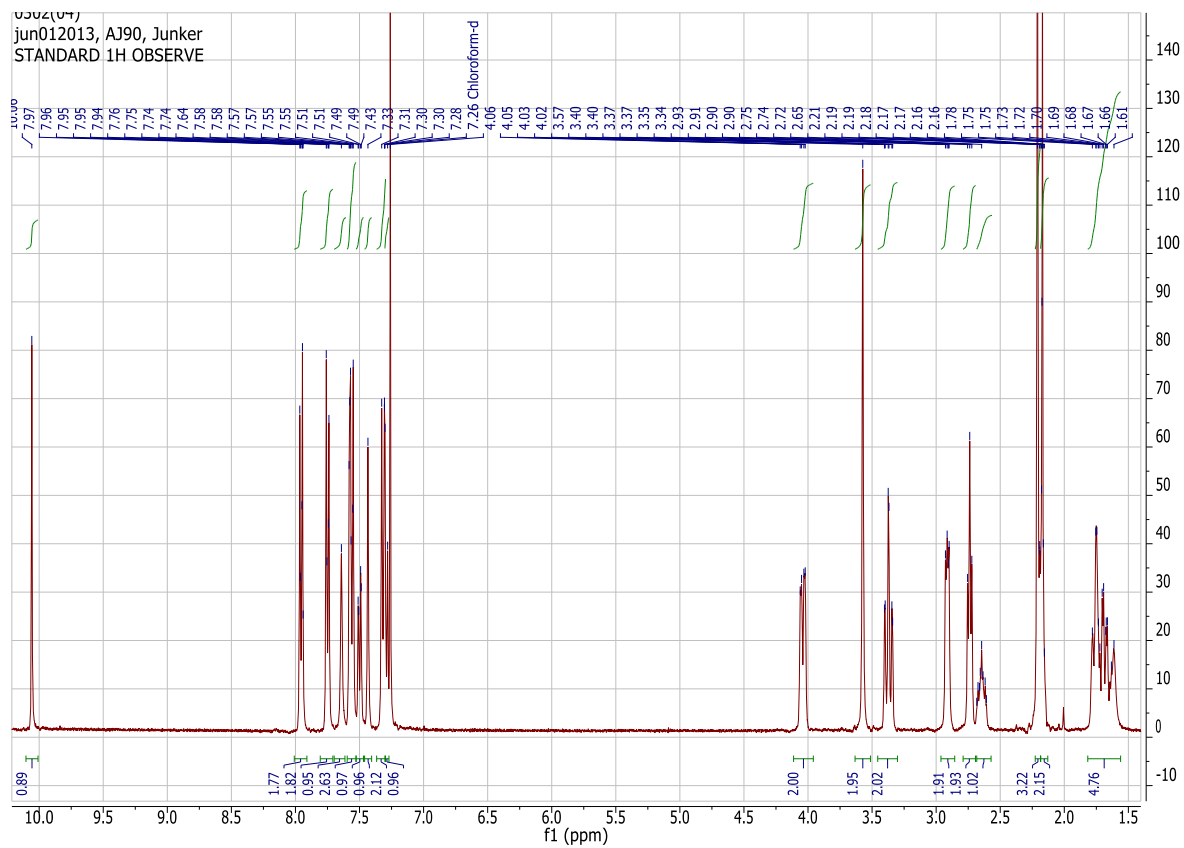
Acquisition Parameter

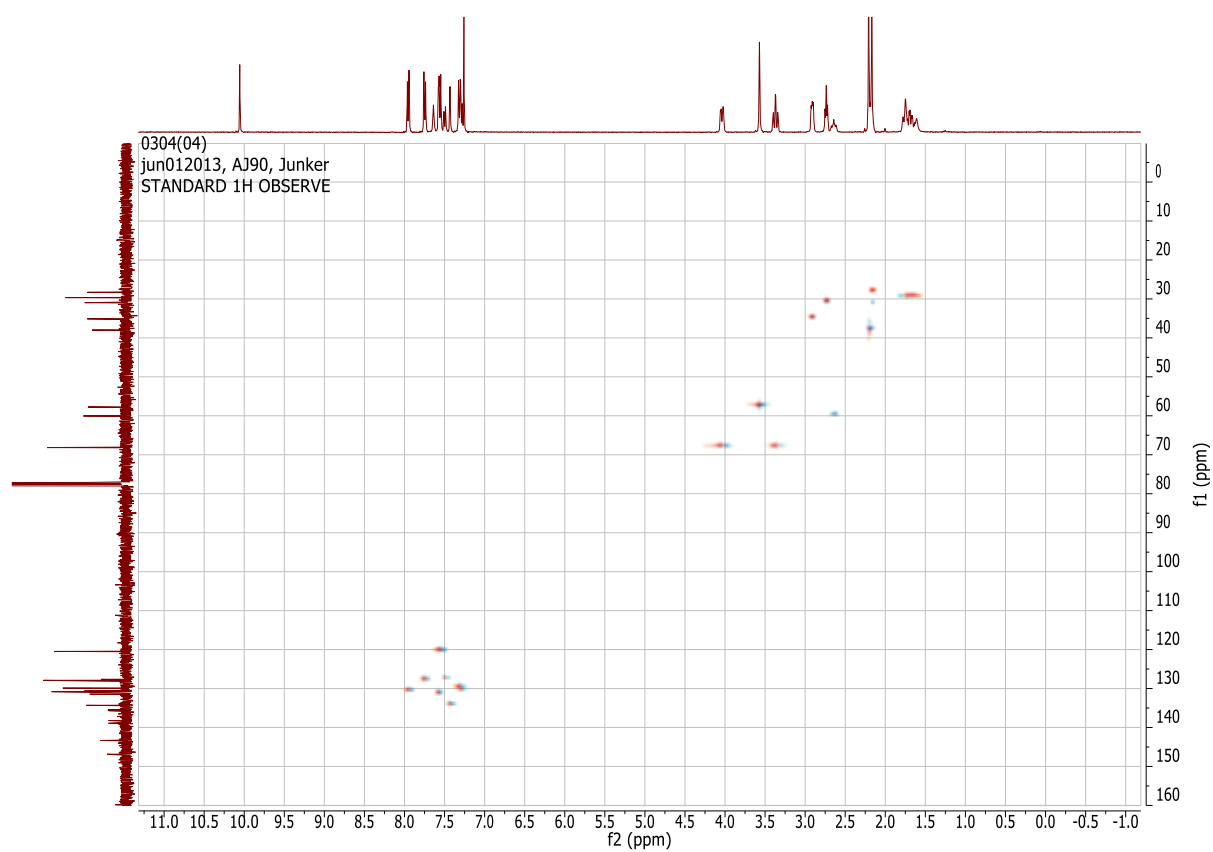
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
483.2617	1	C 31 H 35 N 2 O 3	37.33	483.2642	2.5	5.2	81.3	15.5	even	ok
	2	C 27 H 31 N 8 O	100.00	483.2615	-0.2	-0.3	93.7	16.5	even	ok
	3	C 25 H 39 O 9	5.26	483.2580	-2.8	-5.8	117.2	6.5	even	ok
	4	C 26 H 35 N 4 O 5	12.23	483.2602	-1.5	-3.1	121.2	11.5	even	ok
	5	C 16 H 31 N 14 O 4	0.23	483.2647	3.0	6.3	164.5	8.5	even	ok
	6	C 15 H 35 N 10 O 8	0.26	483.2634	1.7	3.5	177.9	3.5	even	ok
	7	C 12 H 27 N 20 O 2	0.48	483.2620	0.4	0.7	179.9	9.5	even	ok
	8	C 11 H 31 N 16 O 6	0.14	483.2607	-1.0	-2.0	191.3	4.5	even	ok
	9	C 8 H 23 N 26	0.05	483.2594	-2.3	-4.8	193.0	10.5	even	ok

2-(4-Formylphenyl)-N-{4-[N-methyl-N-(tetrahydro-2H-pyran-4-yl)aminomethyl]phenyl}-6,7-dihydro-5H-benzo[7]annulene-8-carboxamide (**2c**)





HPLC

Analyzed: 24.01.13 05:12

Reported: 25.01.13 10:17

Processed: 25.01.13 10:17

Data Path: D:\WIN32APP\HSM\Chromni\DATA\5855\

Application: Chromni

Series: 5855

Sample Name: AJ90

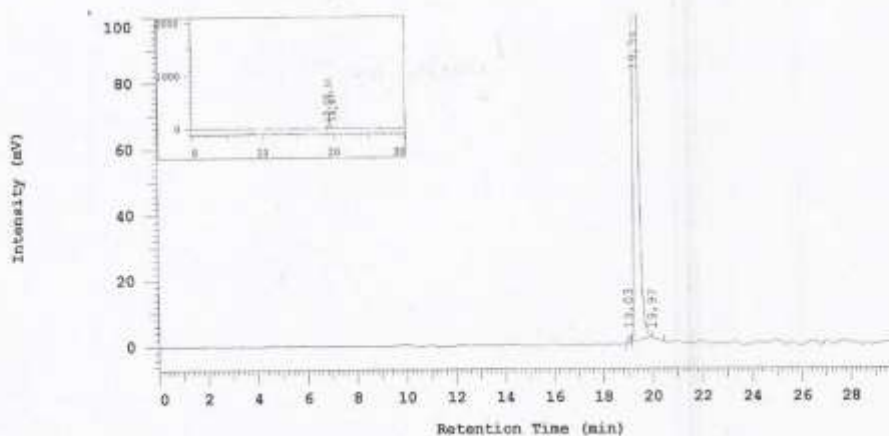
Vial Number: 14

Injection from this vial: 1 of 1

Vial Type: UNK

Volume: 5,0 uI

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

Solvent B: ACN + 0,05%TPA

No.	RT	Area	Conc 1	BC
1	19,03	13347	0,423	MC
2	19,34	3140548	99,577	MC
3	19,97	0	0,000	
		3153895	100,000	

Peak rejection level: 0

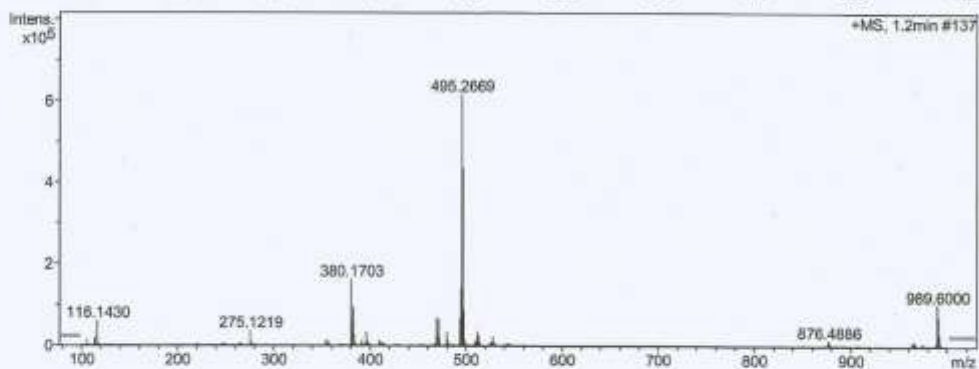
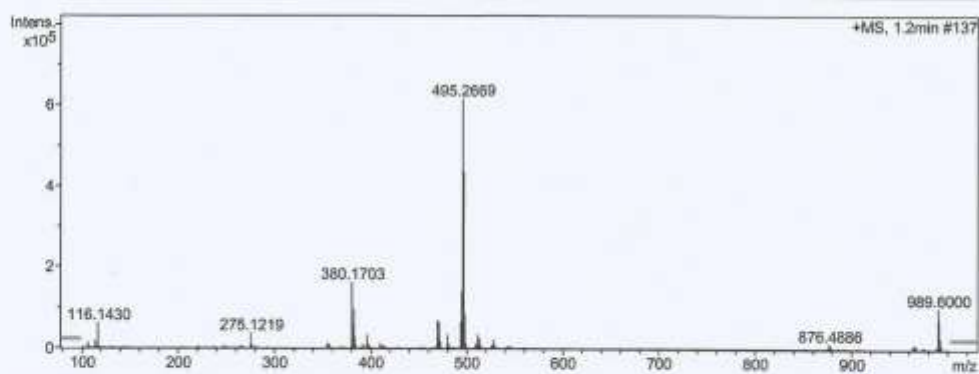
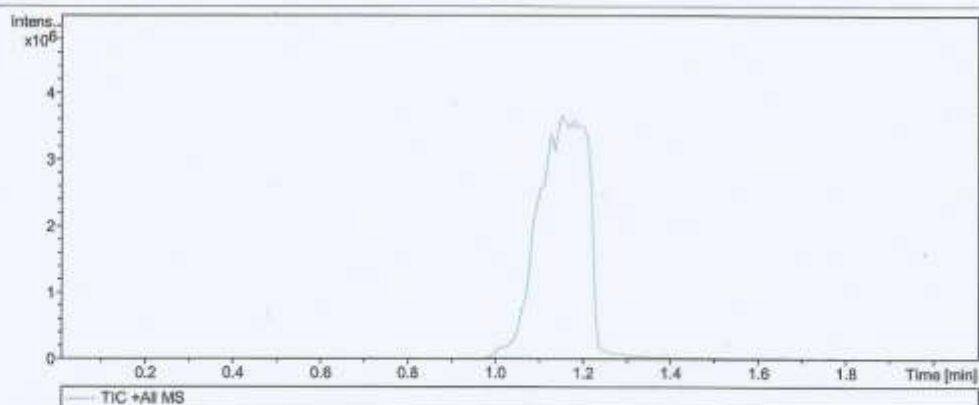
Generic Display Report

Analysis Info

Analysis Name \\p2-ms\PI\Pharm\Chemie\Routine\APCI\12_08\WJU_AJ9001.d
Method APCI_directprobe_positiv.m
Sample Name AJ9001
Comment Junker
APCI-Direkt
Kalibration mit Fettsaeureestern

Acquisition Date 02.08.2012 11:45:51

Operator Meiners
Instrument micrOTOF-Q II



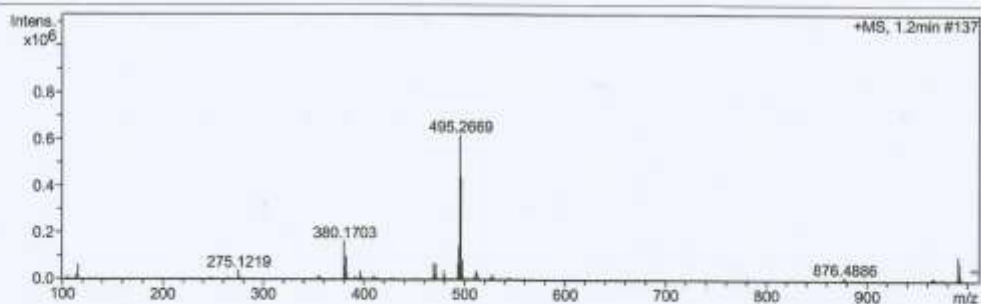
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	\p2-ms\PZ\PharmChemie\Routine\APCI\12_08\WJU_AJ9001.d	Acquisition Date	02.08.2012 11:45:51
Method	APCI_directprobe_positiv.m	Operator	Meiners
Sample Name	AJ9001	Instrument / Ser#	micrOTOF-Q II 10252
Comment	Junker APCI-Direkt Kalibration mit Fettsaeureestern		

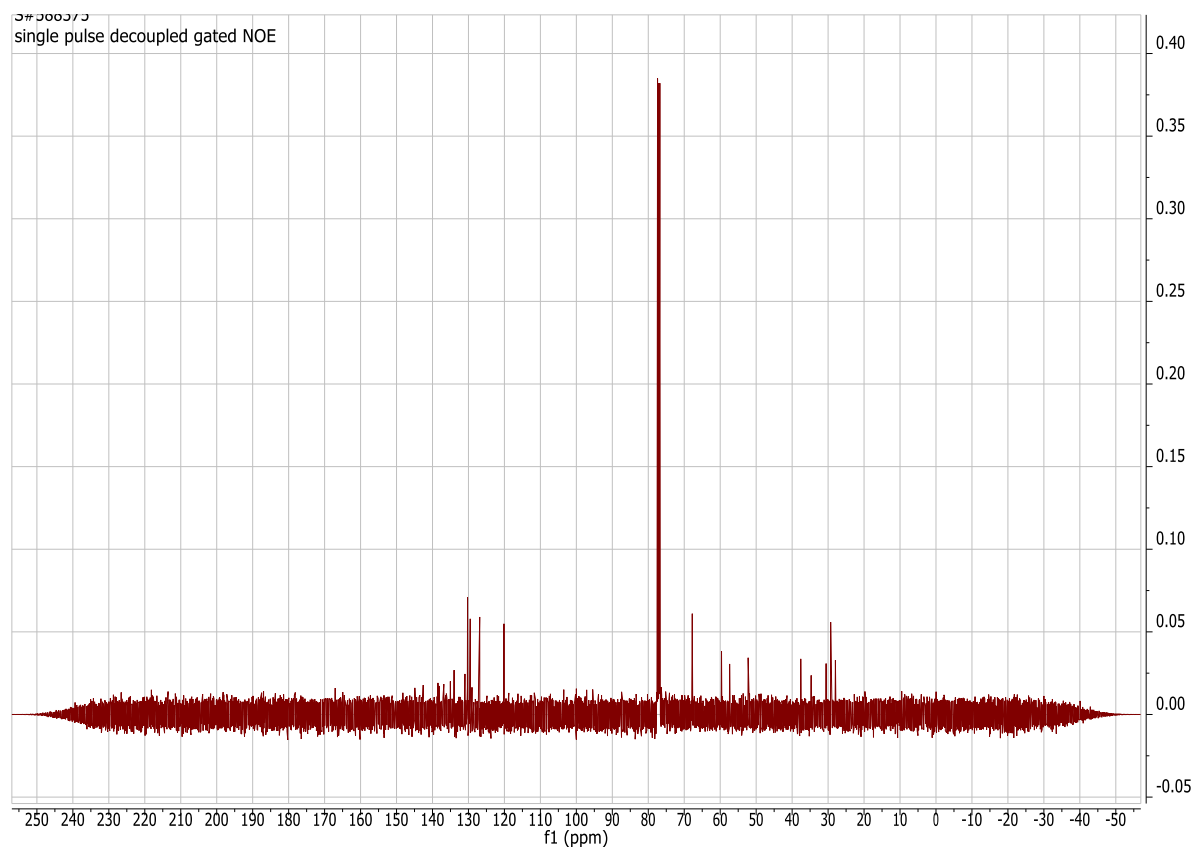
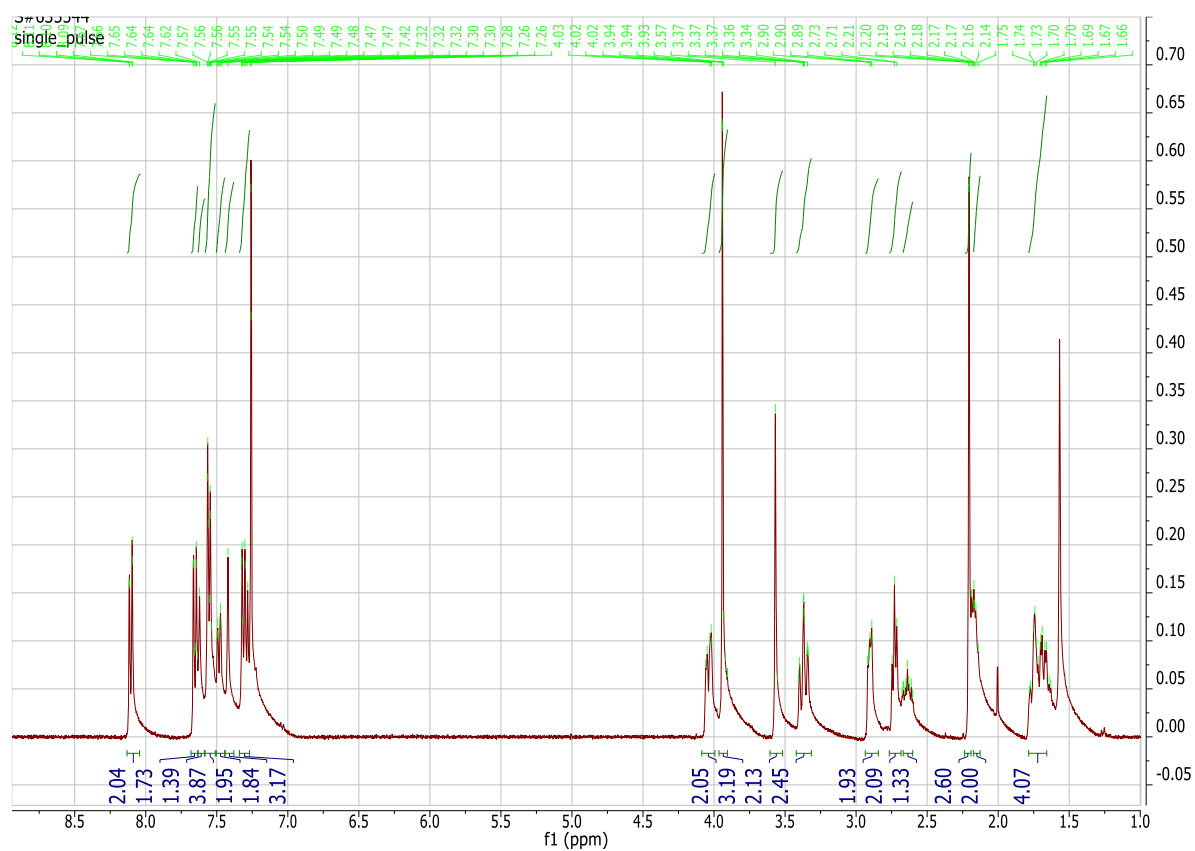
Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err (mDa)	err (ppm)	mSigma	rdb	e ⁻ Conf	N-Rule
471.1490	1	C ₁₉ H ₁₅ N ₁₄ O ₂	100.00	471.1497	0.7	1.4	5.3	19.5	even	ok
	2	C ₂₁ H ₂₇ O ₁₂	86.12	471.1497	0.7	1.4	13.2	8.5	even	ok
	3	C ₁₈ H ₁₉ N ₁₀ O ₆	82.63	471.1484	-0.7	-1.4	15.3	14.5	even	ok
495.2669	1	C ₃₇ H ₃₅ O	100.00	495.2682	1.3	2.6	153.3	20.5	even	ok
	2	C ₃₂ H ₃₅ N ₂ O ₃	6.02	495.2642	-2.7	-5.5	177.3	16.5	even	ok
	3	C ₂₀ H ₃₉ N ₄ O ₁₀	0.12	495.2661	-0.9	-1.8	237.3	3.5	even	ok
	4	C ₂₂ H ₃₁ N ₁₂ O ₂	0.02	495.2687	1.8	3.6	248.2	13.5	even	ok
	5	C ₂₁ H ₃₅ N ₈ O ₆	0.01	495.2674	0.5	0.9	262.1	8.5	even	ok
	6	C ₁₈ H ₂₇ N ₁₈	0.01	495.2661	-0.9	-1.8	263.6	14.5	even	ok
	7	C ₁₇ H ₃₁ N ₁₄ O ₄	0.00	495.2647	-2.2	-4.5	275.5	9.5	even	ok
496.2720	1	C ₁₈ H ₃₈ N ₇ O ₉	100.00	496.2726	0.5	1.1	17.9	3.5	even	ok
	2	C ₁₅ H ₃₀ N ₁₇ O ₃	84.94	496.2712	-0.8	-1.6	19.0	9.5	even	ok
512.2656	1	C ₂₉ H ₃₈ N ₇ O	49.77	512.2643	-1.5	-3.0	12.9	11.5	even	ok
	2	C ₃₀ H ₃₄ N ₅ O ₃	100.00	512.2656	-0.2	-0.4	14.7	16.5	even	ok
877.4908	1	C ₂₈ H ₆₅ N ₁₈ O ₁₄	54.43	877.4922	1.4	1.6	13.0	5.5	even	ok
	2	C ₂₆ H ₅₃ N ₃₂ O ₄	54.48	877.4922	1.4	1.6	13.3	16.5	even	ok
	3	C ₂₅ H ₅₇ N ₂₈ O ₈	100.00	877.4909	0.1	0.1	17.9	11.5	even	ok
965.4775	1	C ₃₉ H ₆₉ N ₁₀ O ₁₈	75.63	965.4786	1.1	1.1	16.1	10.5	even	ok
	2	C ₃₇ H ₅₇ N ₂₄ O ₈	73.37	965.4786	1.0	1.1	17.9	21.5	even	ok
989.6000	1	C ₆₀ H ₇₇ N ₈ O ₅	74.67	989.6011	1.2	1.2	13.7	28.5	even	ok

Methyl 4-[8-(N-{4-[N-methyl-N-(tetrahydro-2H-pyran-4-yl)aminomethyl]phenyl}carbamoyl)-6,7-dihydro-5H-benzo[7]annulen-2-yl]benzoate (**2d**)



HPLC

Analyzed: 20.09.12 07:40

Reported: 21.09.12 08:58

Processed: 21.09.12 08:58

Data Path: D:\WIN32APP\HSM\Chromni\DATA\5281\

Application: Chromni

Series:5281

Sample Name: AJ91A

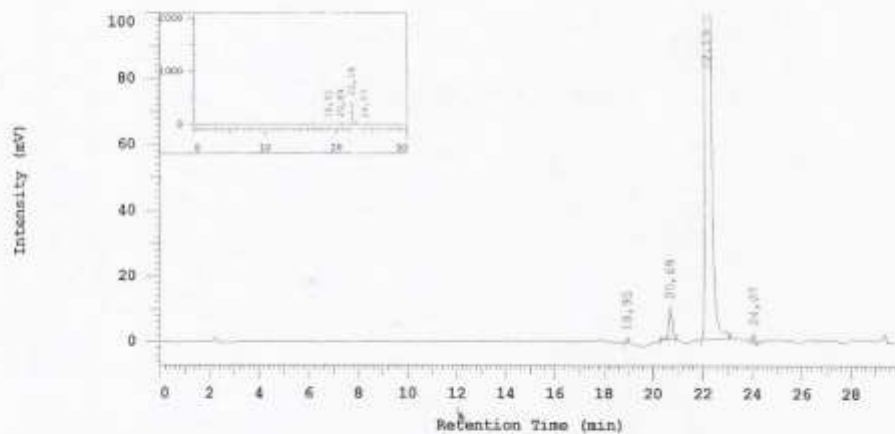
Vial Number: 20

Injection from this vial: 1 of 1

Vial Type: UNK

Volume: 5,0 ul

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

Solvent B: ACN + 0,05%TFA

No.	RT	Area	Conc 1	BC
1	18,95	7714	0,160	BB
2	20,69	89493	1,861	BB
3	22,19	4697648	97,695	BB
4	24,07	13635	0,284	BB
		4808490	100,000	

Peak rejection level: 0

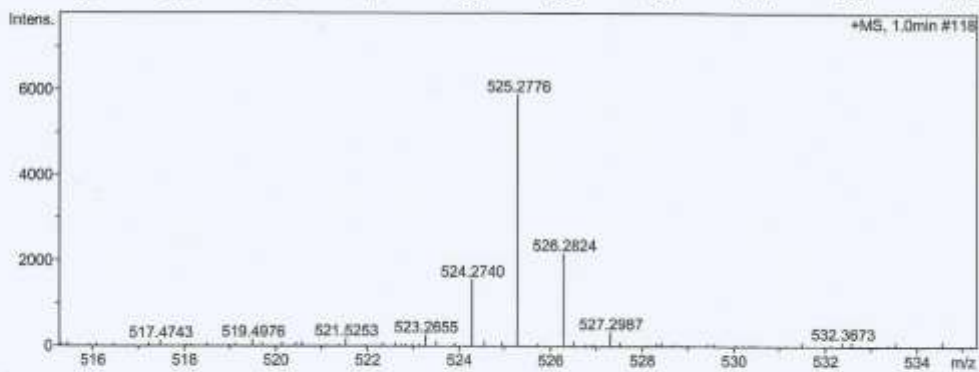
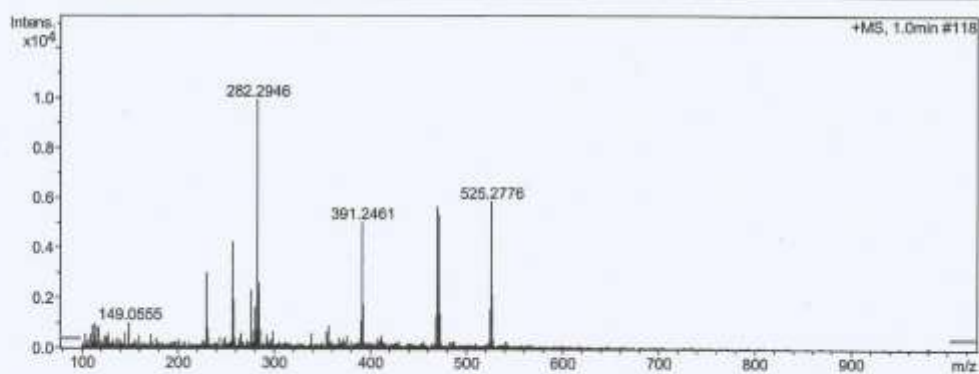
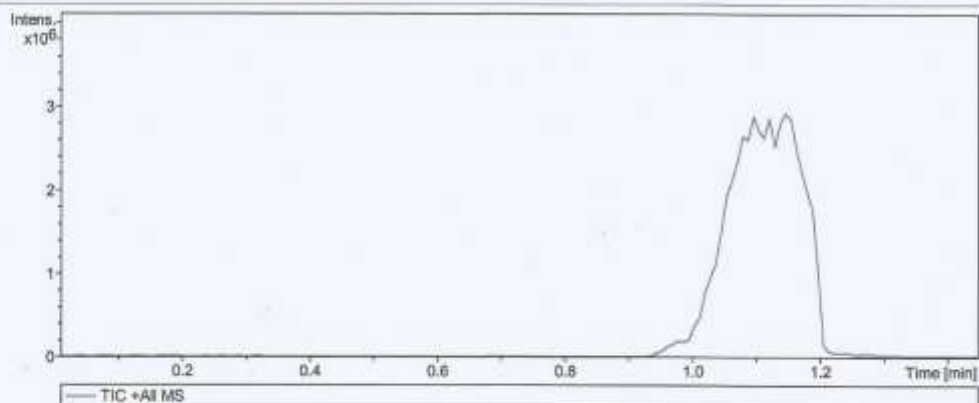
Generic Display Report

Analysis Info

Analysis Name: \\p2-ms\PI\PharmChemie\Routine\APCI\12_08\WJU_AJ9101.d
Method: APCI_directprobe_positiv.m
Sample Name: AJ9101
Comment: Junker
APCI-Direkt
Kalibration mit Fettsaeureestern

Acquisition Date: 02.08.2012 11:48:14

Operator: Meiners
Instrument: micrOTOF-Q II



Mass Spectrum SmartFormula Report

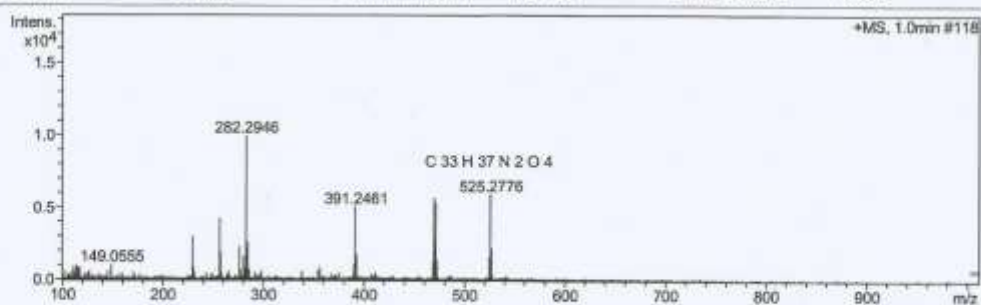
Analysis Info

Analysis Name: \\p2-ms\PIZ\PharmChemie\Routine\APCI\12_08\WJU_AJ9101.d
 Method: APCI_directprobe_positiv.m
 Sample Name: AJ9101
 Comment: Junker
 APCI-Direkt
 Kalibration mit Fettsaureestern

Acquisition Date: 02.08.2012 11:48:14
 Operator: Meiners
 Instrument / Ser#: micrOTOF-Q II 10252

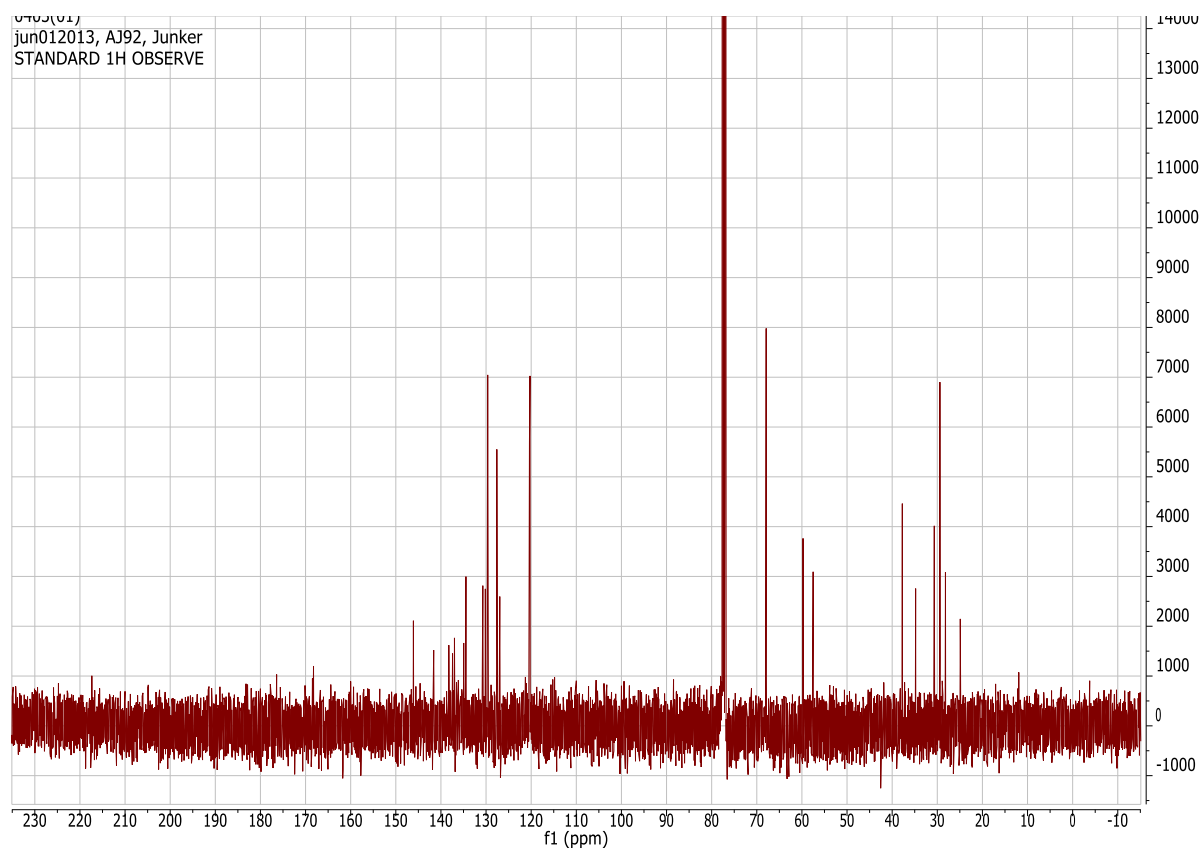
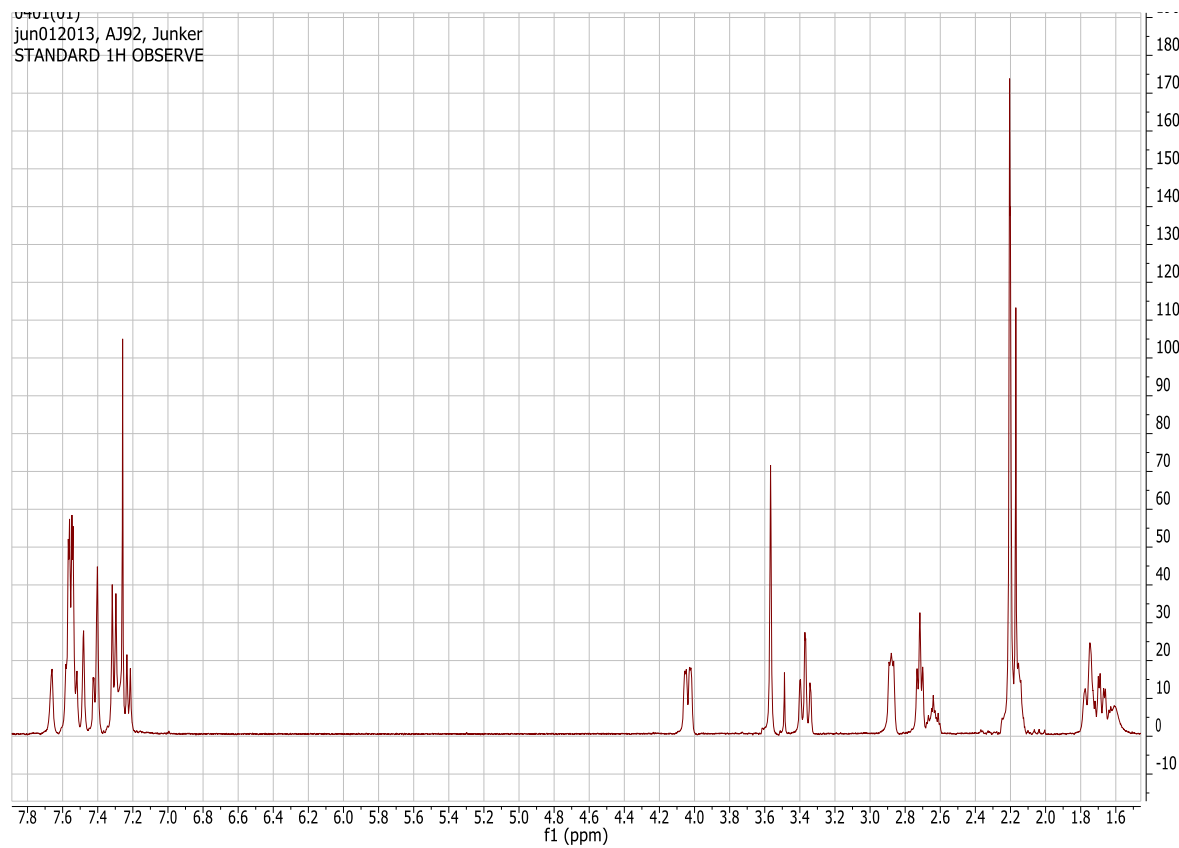
Acquisition Parameter

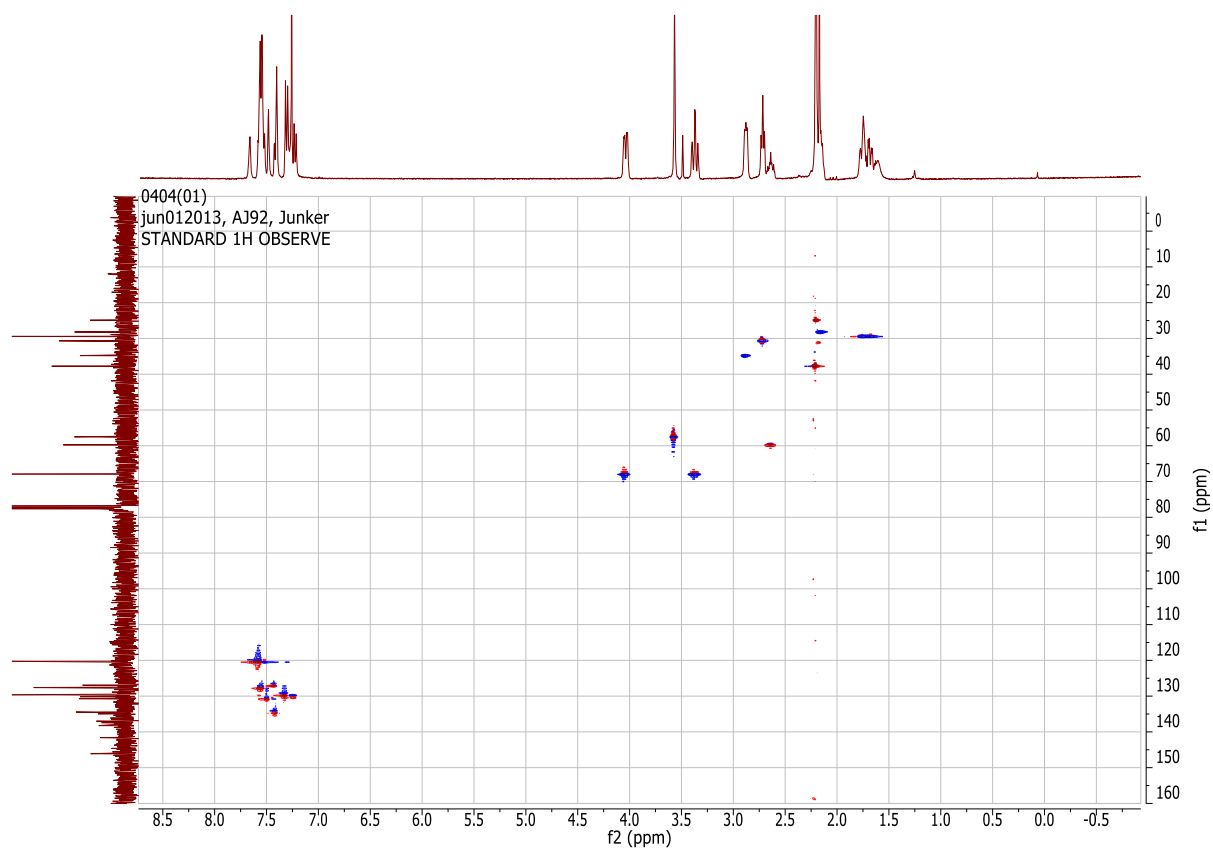
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
338.3535	1	C 21 H 44 N 3	100.00	338.3530	-0.5	-1.5	16.3	1.5	even	ok	
471.1496	1	C 19 H 15 N 14 O 2	100.00	471.1497	0.1	0.2	4.3	19.5	even	ok	
	2	C 22 H 23 N 4 O 8	48.81	471.1510	1.4	3.0	4.8	13.5	even	ok	
	3	C 21 H 27 O 12	82.54	471.1497	0.1	0.2	14.5	8.5	even	ok	
	4	C 18 H 19 N 10 O 8	44.25	471.1484	-1.3	-2.7	15.9	14.5	even	ok	
525.2776	1	C 33 H 37 N 2 O 4	100.00	525.2748	-2.8	-5.3	11.0	16.5	even	ok	

2-[4-(Acetamido)phenyl]-N-{4-[N-methyl-N-(tetrahydro-2H-pyran-4-yl)aminomethyl]phenyl}-6,7-dihydro-5H-benzo[7]annulene-8-carboxamide (**2e**)





HPLC

Analyzed: 05.07.12 08:11

Reported: 05.07.12 15:55

Processed: 05.07.12 15:55

Data Path: D:\WIN32APP\HSM\Chromni\DATA\4978\

Application: Chromni

Series:4978

Sample Name: AJ9201

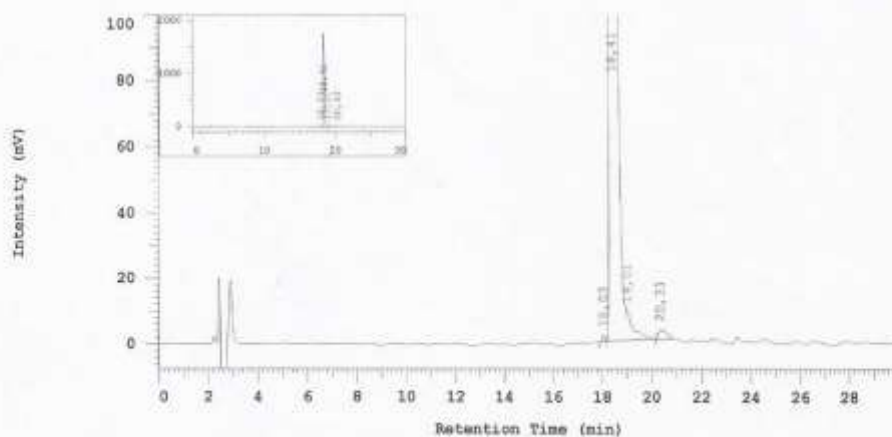
Vial Number: 19

Injection from this vial: 1 of 1

Vial Type: UNK

Volume: 5,0 ul

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

Solvent B: ACN + 0,05%TFA

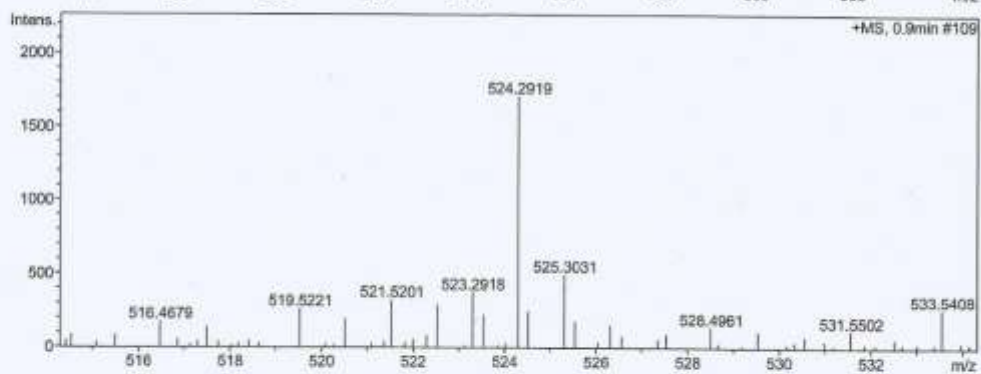
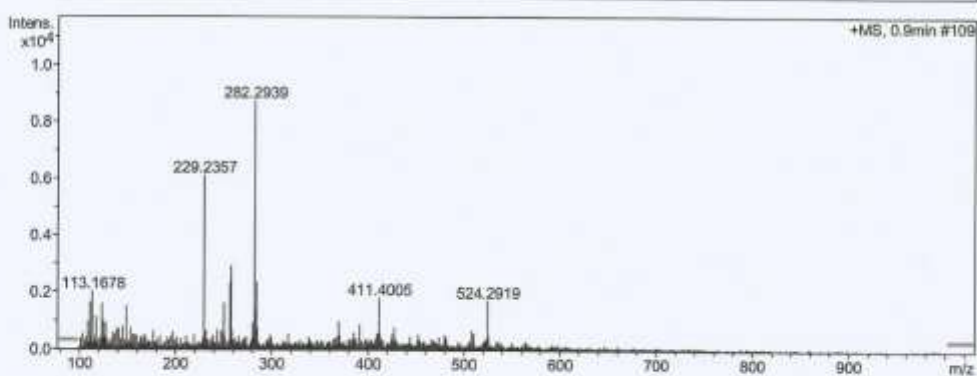
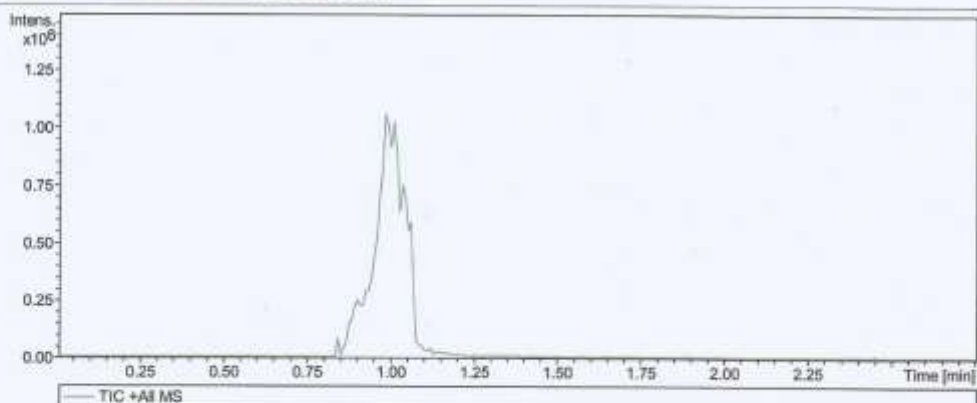
No.	RT	Area	Conc 1	BC
1	18,03	14581	0,067	BB
2	18,41	21532304	98,900	MC
3	19,01	170567	0,783	MC
4	20,33	54233	0,249	MC
		21771685	100,000	

Peak rejection level: 0

Generic Display Report

Analysis Info

Analysis Name	\\pz-ms\PIZ\PharmChemie\Routine\APCI\12_08\WJU_AJ9201.d	Acquisition Date	02.08.2012 11:29:03
Method	APCI_directprobe_positiv.m	Operator	Meiners
Sample Name	AJ9201	Instrument	micrOTOF-Q II
Comment	Junker APCI-Direkt Kalibration mit Fettsaureestern		



Mass Spectrum SmartFormula Report

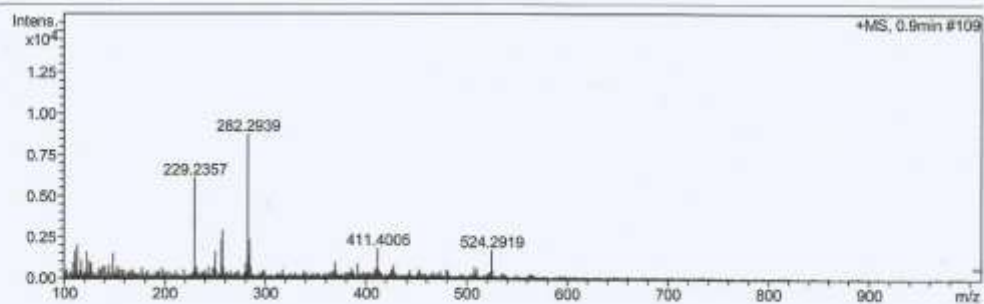
Analysis Info

Analysis Name: \\p2-ms\PZ\PharmChemie\Routine\APCI\12_08\WJU_AJ8201.d
Method: APCI_directprobe_positiv.m
Sample Name: AJ8201
Comment: Junker
APCI-Direkt
Kalibration mit Fettsaeureestern

Acquisition Date: 02.08.2012 11:29:03
Operator: Meiners
Instrument / Ser#: micrOTOF-Q II 10252

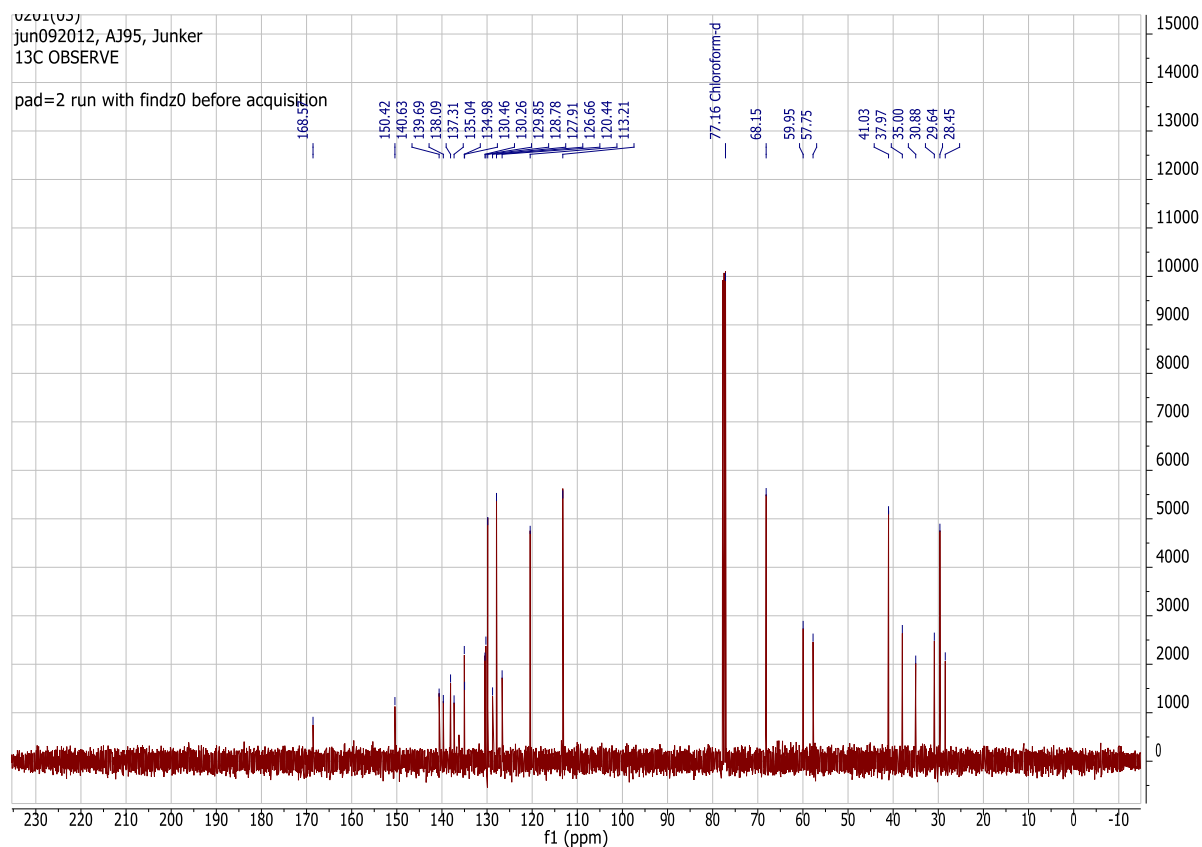
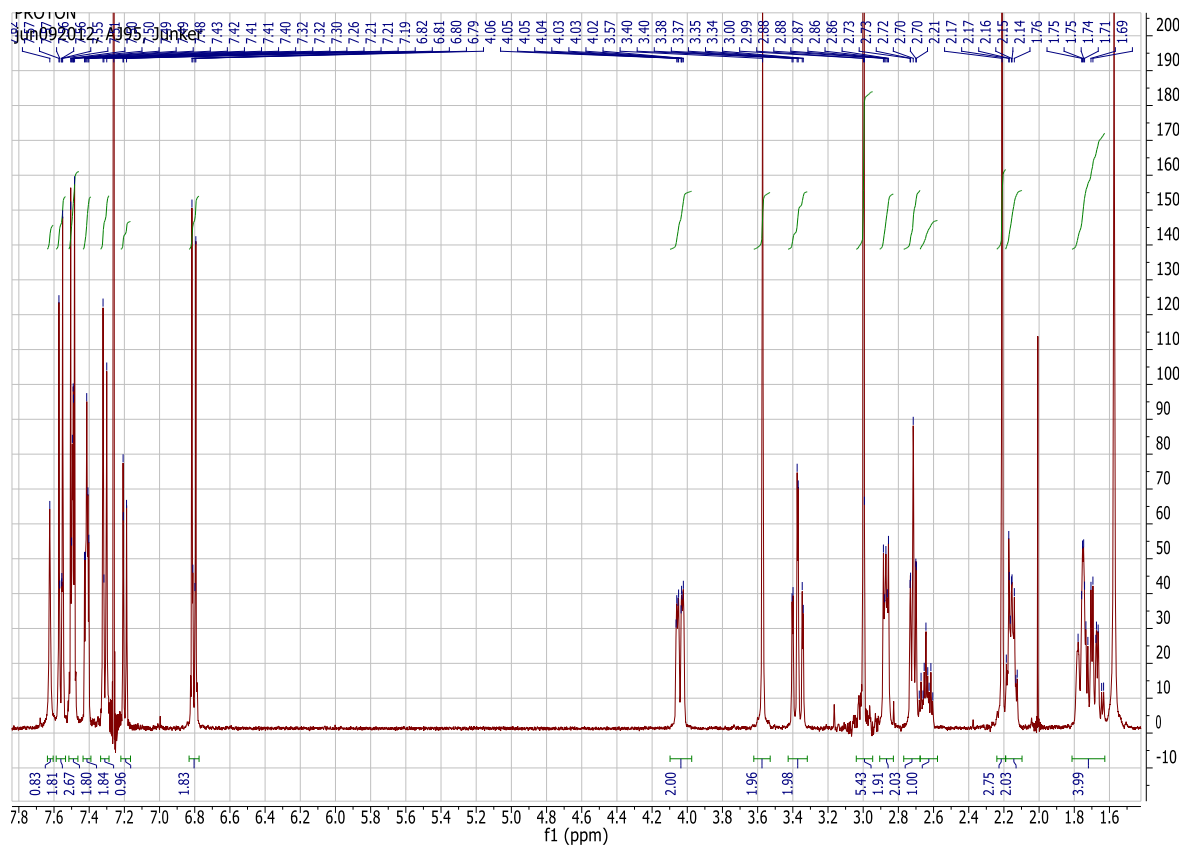
Acquisition Parameter

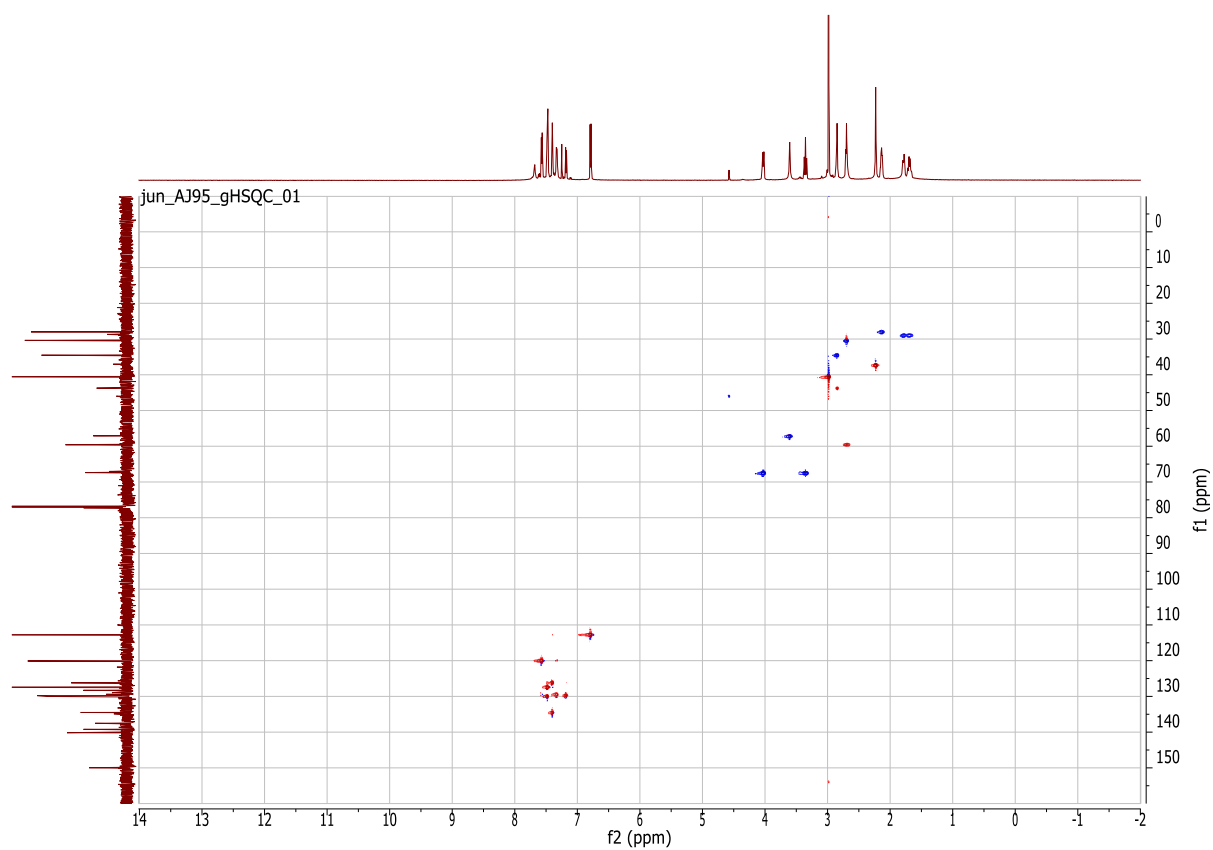
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
149.0578	1	C ₉ H ₉ O ₂	59.69	149.0597	2.0	13.1	17.3	5.5	even		ok
250.1090	1	C ₁₃ H ₁₆ N ₄ O ₄	56.41	250.1074	-1.6	-6.4	18.5	6.5	even		ok
524.2919	1	C ₂₂ H ₃₈ N ₈ O ₆	48.23	524.2940	2.1	4.0	23.2	8.5	even		ok
	2	C ₂₁ H ₄₂ N ₅ O ₁₀	100.00	524.2926	0.8	1.4	27.5	3.5	even		ok
	3	C ₃₃ H ₃₈ N ₃ O ₃	54.69	524.2908	-1.1	-2.1	43.4	16.5	even		ok

2-[4-(Dimethylamino)phenyl]-N-{4-[N-methyl-N-(tetrahydro-2H-pyran-4-yl)aminomethyl]phenyl}-6,7-dihydro-5H-benzo[7]annulene-8-carboxamide (**2f**)





HPLC

Analyzed: 20.09.12 02:50

Reported: 21.09.12 08:55

Processed: 21.09.12 08:55

Data Path: D:\WIN32APP\HSM\Chromni\DATA\5274\

Application: Chromni

Series: 5274

Sample Name: AJ95

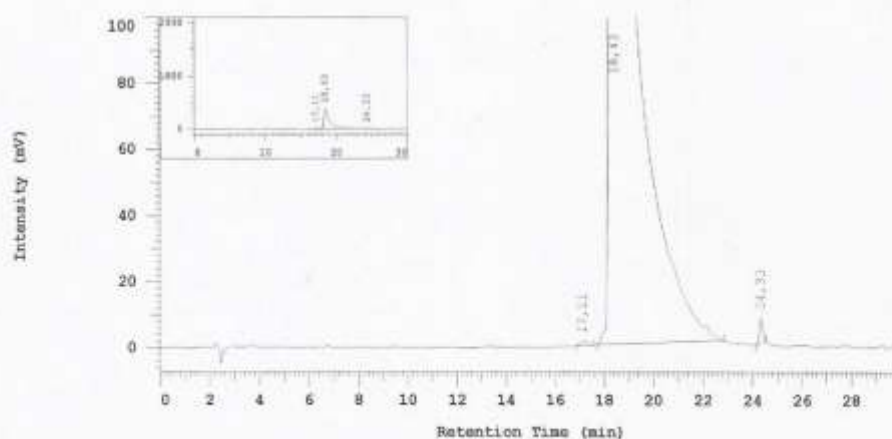
Vial Number: 14

Injection from this vial: 1 of 1

Vial Type: UNK

Volume: 5,0 ul

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

Solvent B: ACN + 0,05%TFA

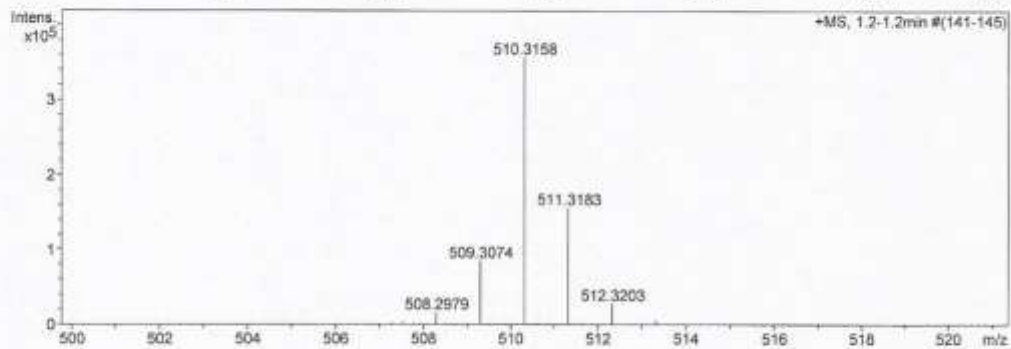
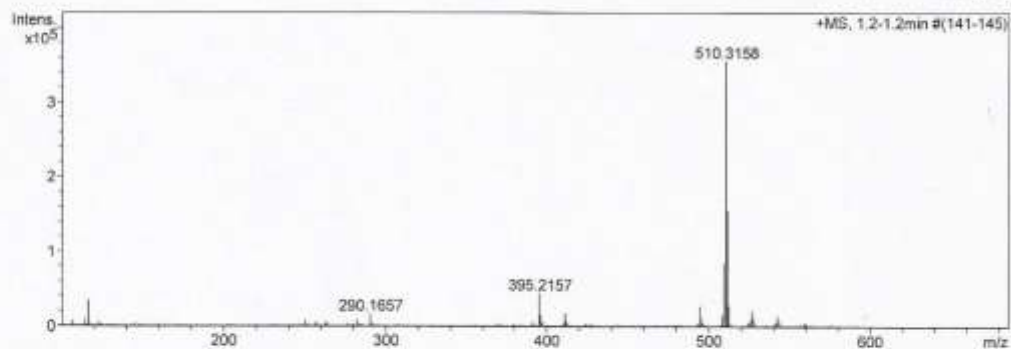
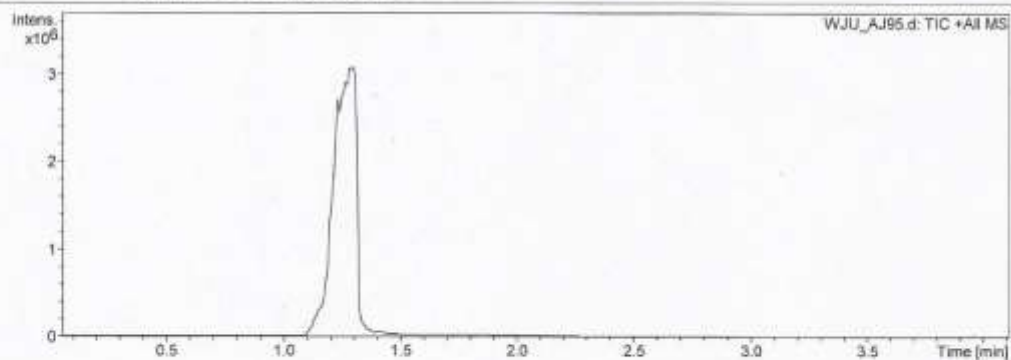
No.	RT	Area	Conc 1	BC
1	17,11	27263	0,129	BB
2	18,43	21104094	99,540	MC
3	24,33	70181	0,331	BB
		21201538	100,000	

Peak rejection level: 0

Generic Display Report

Analysis Info

Analysis Name	D:\Data\IPMC\PharmChemie\Routine\APCI\12_09\WJU_AJ95.d	Acquisition Date	9/20/2012 11:22:46 AM
Method	APCI_directprobe_positiv.m	Operator	Sendker
Sample Name	AJ95	Instrument	micrOTOF-Q II
Comment	Junker APCI-Direkt Kalibration mit Fettsaureestern		



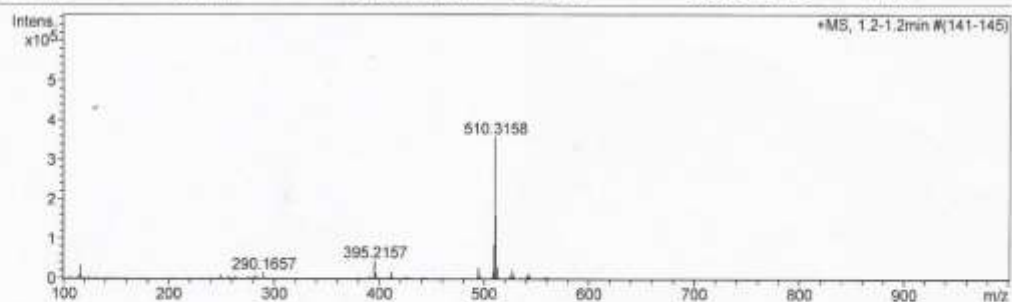
Mass Spectrum SmartFormula Report

Analysis Info
Analysis Name: D:\Data\PMC\PharmChemie\Routine\APC\12_09\WJU_AJ95.d
Method: APCI_directprobe_positiv.m
Sample Name: AJ95
Comment: Junker
APCI-Direkt
Kalibration mit Fettsaureestern

Acquisition Date: 9/20/2012 11:22:46 AM
Operator: Sendker
Instrument / Ser#: micrOTOF-Q II 10252

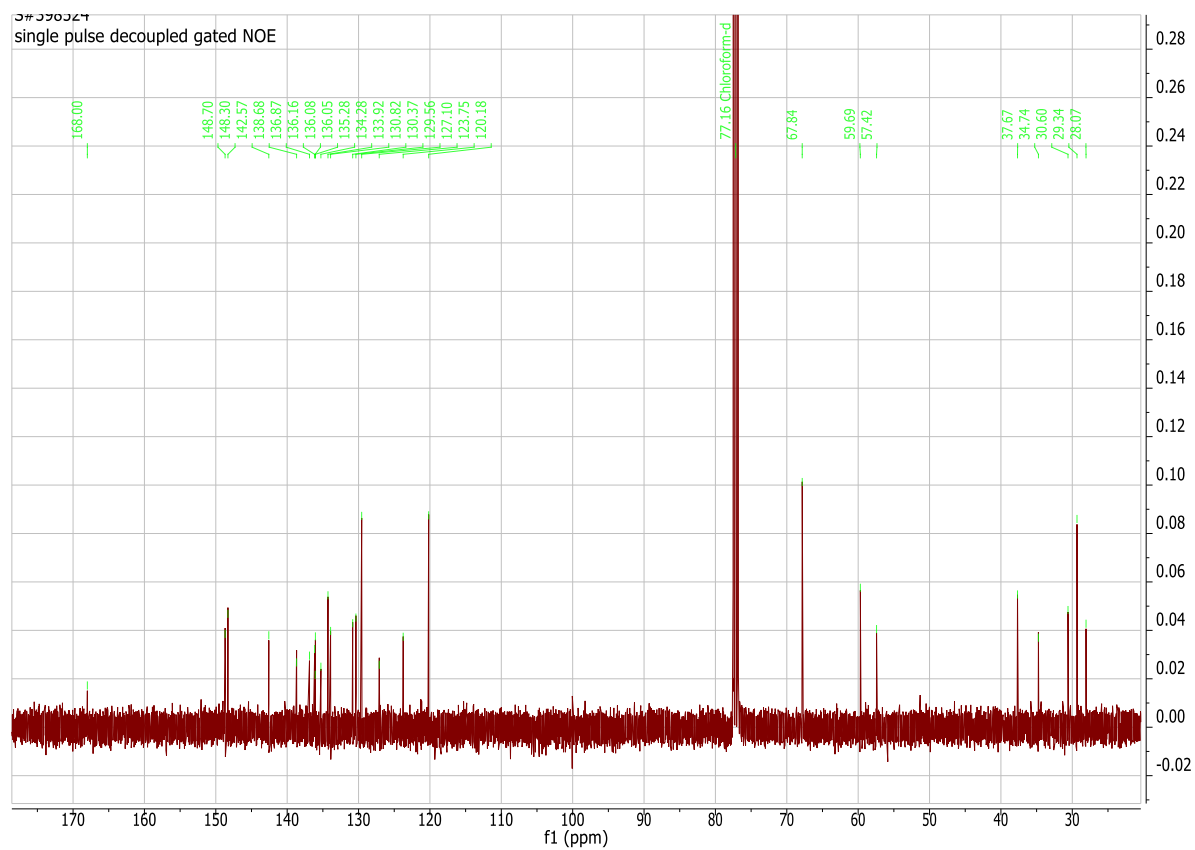
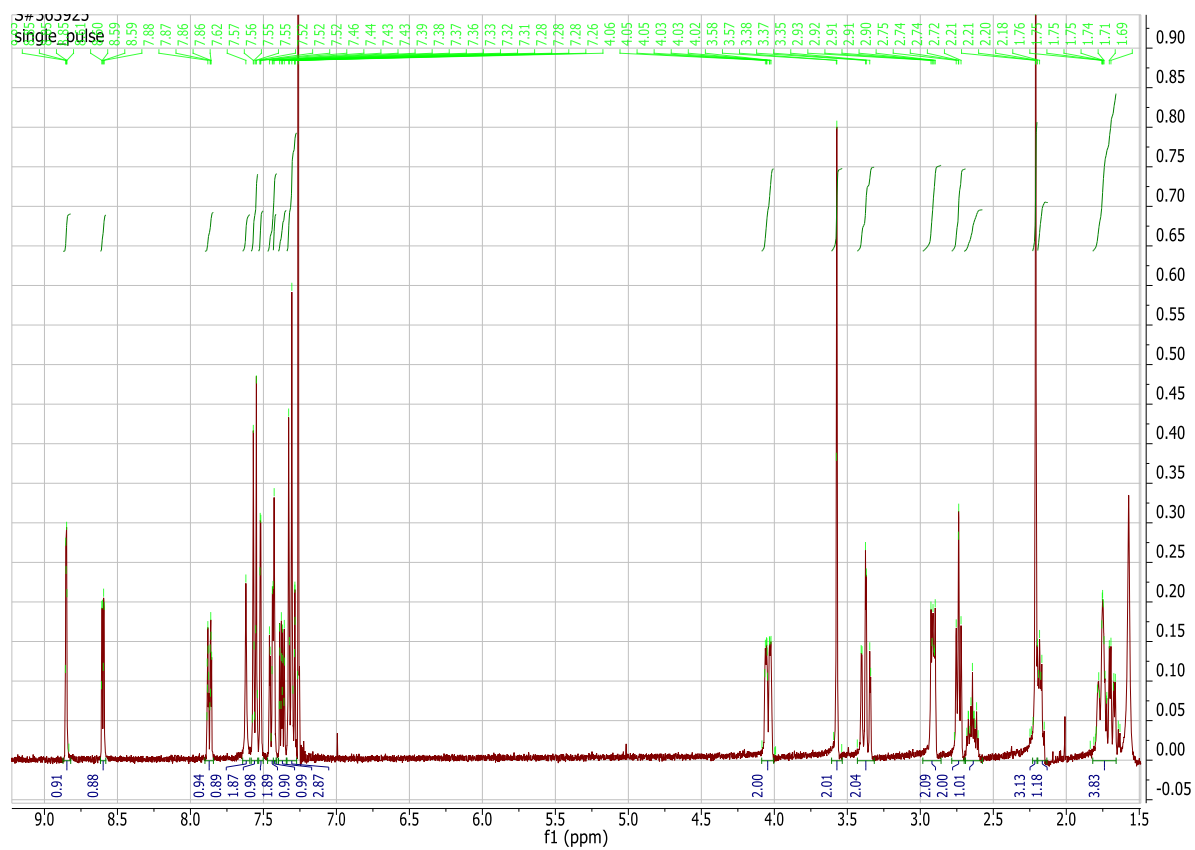
Acquisition Parameter

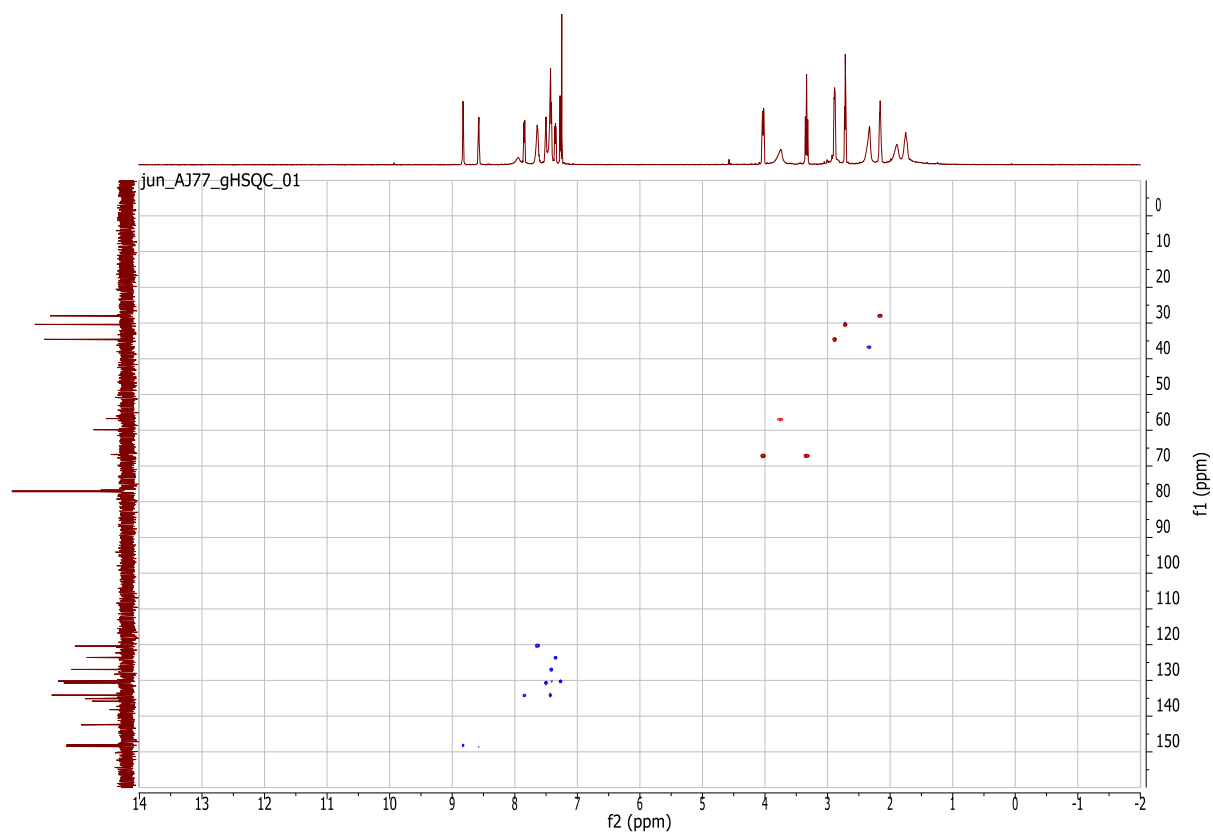
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
510.3158	1	C 38 H 40 N	100.00	510.3155	-0.3	-0.6	9.8	19.5	even	ok
	2	C 33 H 40 N 3 O 2	2.13	510.3115	-4.3	-8.5	32.3	15.5	even	ok

N-{4-[*N*-Methyl-*N*-(tetrahydro-2*H*-pyran-4-yl)aminomethyl]phenyl}-2-(pyridin-3-yl)-6,7-dihydro-5*H*-benzo[7]annulene-8-carboxamide (**2g**)





HPLC

Analyzed: 05.07.12 05:25

Reported: 05.07.12 15:49
Processed: 05.07.12 15:48

Data Path: D:\WIN32APP\HSM\Chromni\DATA\4974\

Application: Chromni

Series:4974

Sample Name: AJ7701

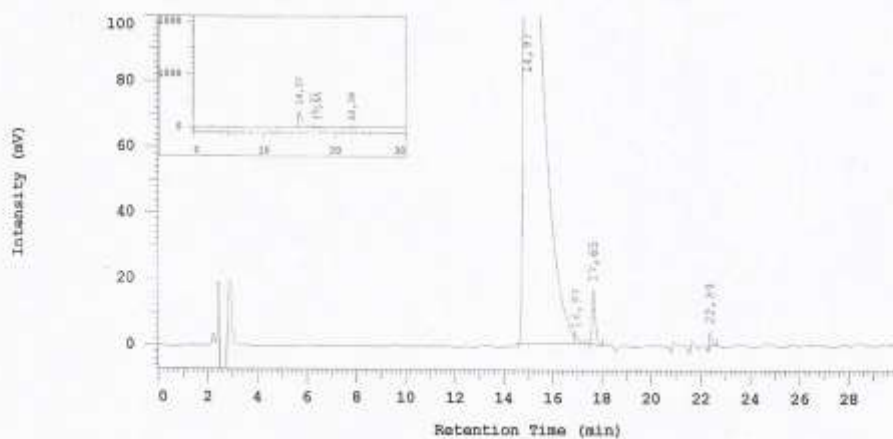
Vial Number: 15

Injection from this vial: 1 of 1

Vial Type: UNK

Volume: 5,0 ul

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

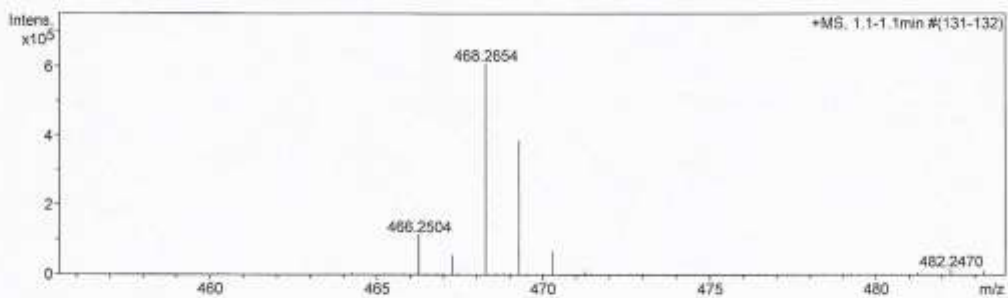
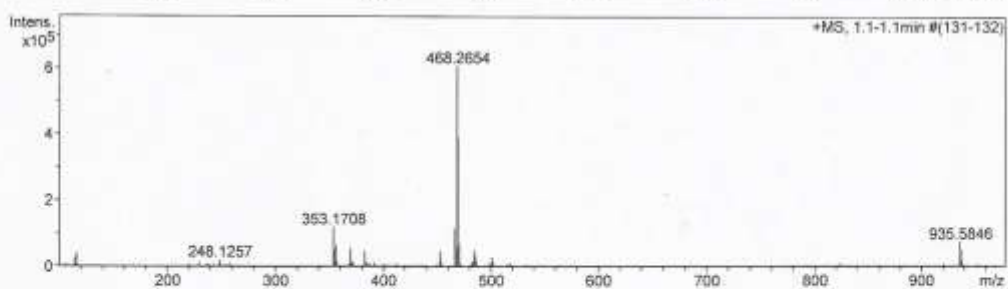
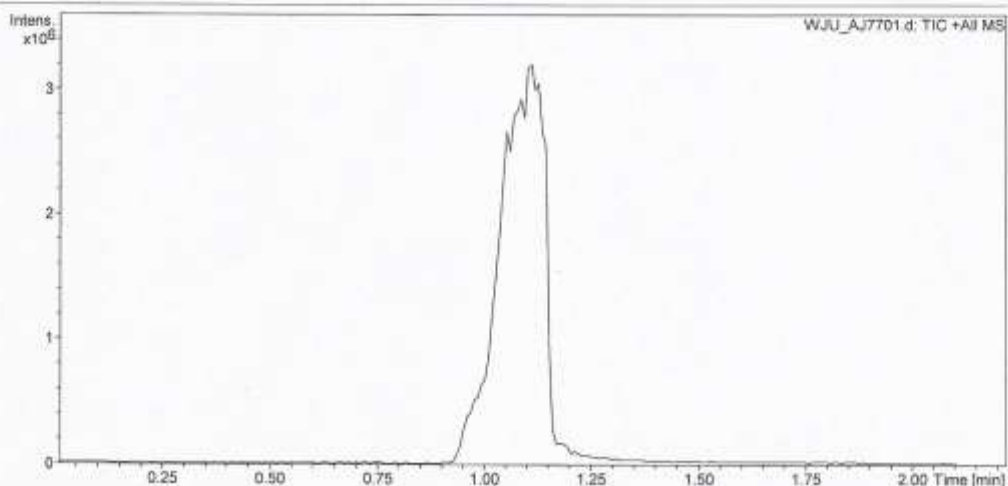
Solvent B: ACN + 0,05%TFA

No.	RT	Area	Conc 1	BC
1	14,97	11287230	98,134	MC
2	16,97	31255	0,272	MC
3	17,65	148383	1,290	MC
4	22,39	34939	0,304	MC
		11501807	100,000	

Peak rejection level: 0

Generic Display Report

Analysis Info		Acquisition Date	8/2/2012 10:50:34 AM
Analysis Name	D:\Data\PMCI\Pharm\Chemie\Routine\APCI\12_08\WJU_AJ7701.d	Operator	Meiners
Method	APCI_directprobe_positiv.m	Instrument	micrOTOF-Q II
Sample Name	AJ7701		
Comment	Junker APCI-Direkt Kalibration mit Fettsaureestern		

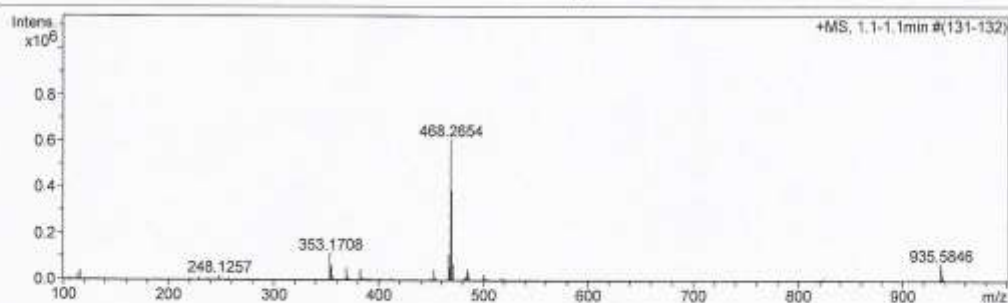


Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	8/2/2012 10:50:34 AM
Analysis Name	D:\Data\PMC\PharmChemie\Routine\APCI\12_08\WJU_AJ7701.d	Operator	Meiners
Method	APCI_directprobe_positiv.m	Instrument / Ser#	microTOF-Q II 10252
Sample Name	AJ7701		
Comment	Junker APCI-Direkt Kalibration mit Fettsaeureestern		

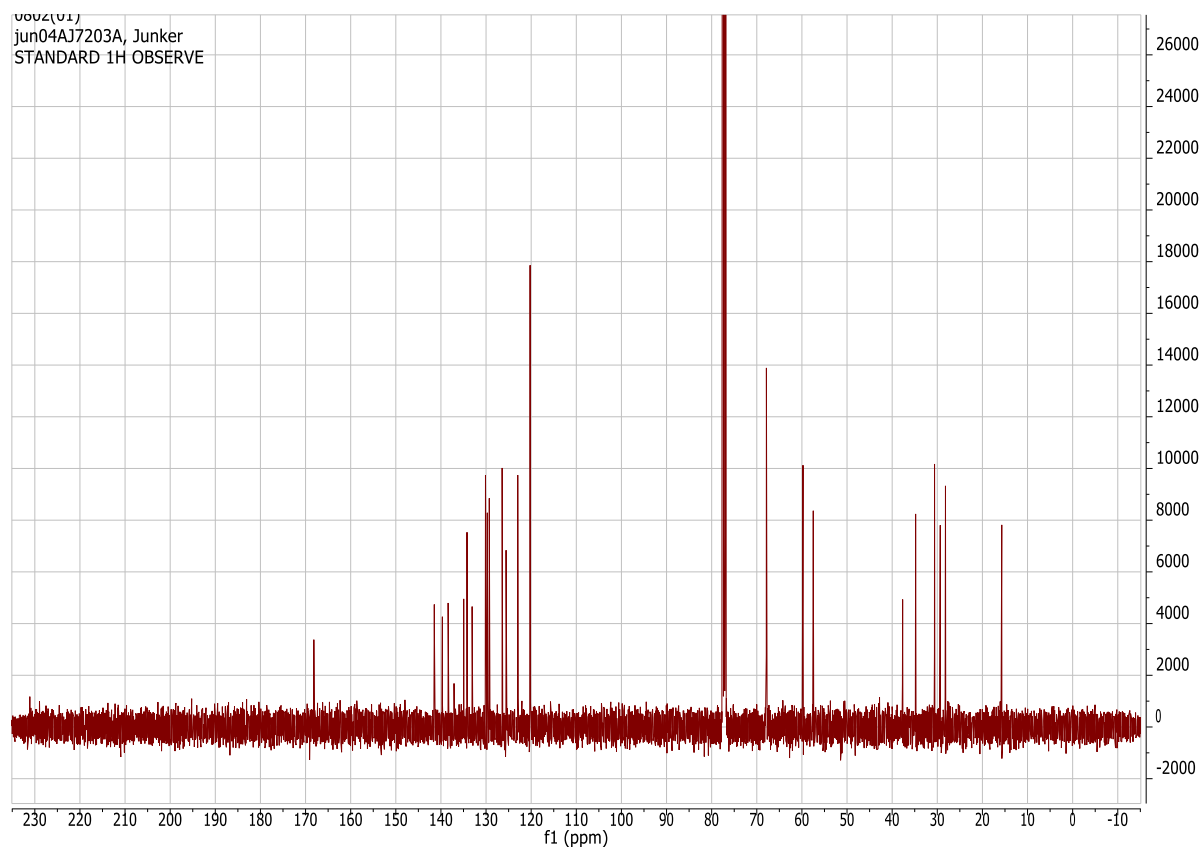
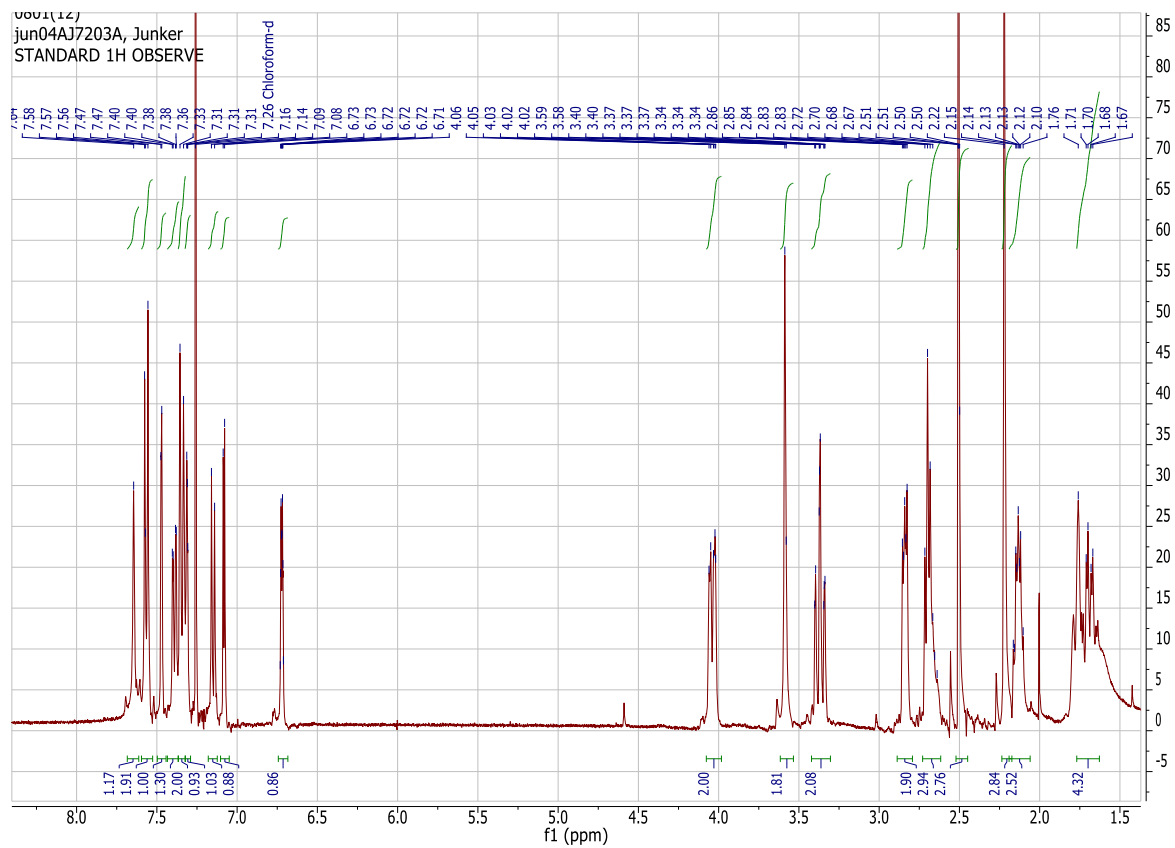
Acquisition Parameter

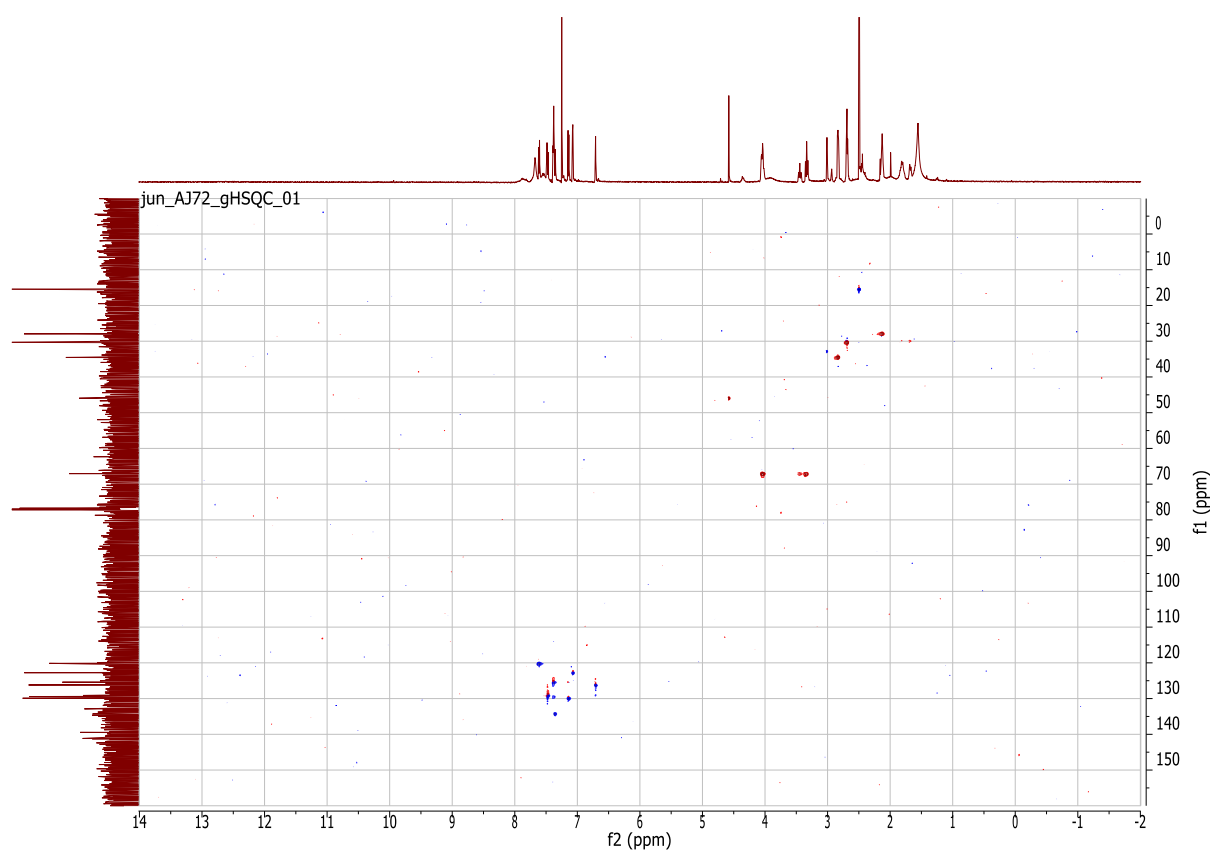
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
468.2654	1	C 35 H 34 N	67.67	468.2686	3.2	6.9	126.2	19.5	even	ok
	2	C 30 H 34 N 3 O 2	100.00	468.2846	-0.8	-1.7	150.3	15.5	even	ok
	3	C 26 H 30 N 9	0.70	468.2619	-3.5	-7.4	189.0	16.5	even	ok
	4	C 18 H 38 N 5 O 9	0.73	468.2864	1.1	2.2	212.0	2.5	even	ok
	5	C 20 H 30 N 13 O	0.04	468.2691	3.7	8.0	219.0	12.5	even	ok
	6	C 19 H 34 N 9 O 5	0.05	468.2677	2.4	5.1	230.7	7.5	even	ok
	7	C 15 H 30 N 15 O 3	0.04	468.2651	-0.3	-0.6	246.0	6.5	even	ok
	8	C 14 H 34 N 11 O 7	0.01	468.2637	-1.8	-3.5	257.9	3.5	even	ok
	9	C 11 H 26 N 21 O	0.00	468.2624	-3.0	-6.4	259.3	9.5	even	ok

N-{4-[Methyl(tetrahydro-2H-pyran-4-yl)aminomethyl]phenyl}-2-(5-methylthiophen-2-yl)-6,7-dihydro-5H-benzo[7]annulene-8-carboxamide (**2h**)





HPLC

Analyzed: 20.04.11 05:17

Reported: 20.04.11 14:17

Processed: 20.04.11 14:17

Data Path: D:\WIN32APP\HSM\Chromni\DATA\2995\

Application: Chromni

Series:2995

Sample Name: AJ7203B

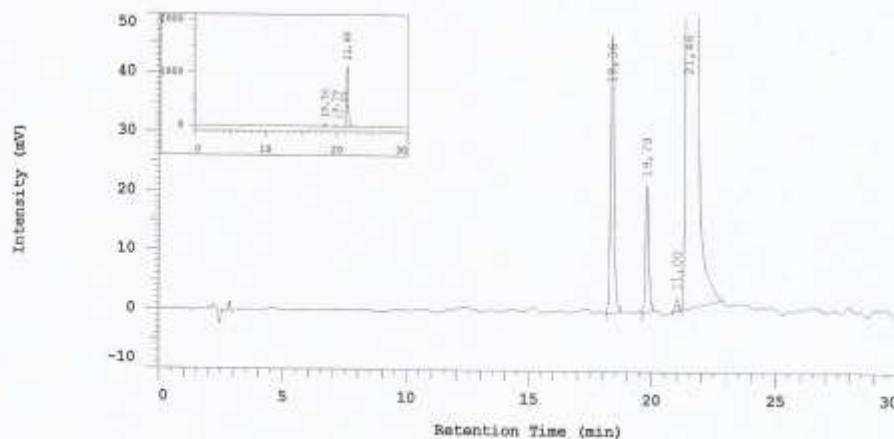
Vial Number: 14

Injection from this vial: 1 of 1

Vial Type: UNK

Volume: 5,0 ul

Chrom Type: HPLC Channel : 1



Acquisition Method: Chromni

Blank Subtr Sample Name: ACN

Column Type: 010

Solvent A: Wasser + 0,05%TFA

Developed by: Jens

Solvent B: ACN + 0,05%TFA

No.	RT	Area	Conc 1	BC
1	18,36	444850	2,625	MC
2	19,79	191792	1,132	BB
3	21,00	13310	0,079	BB
4	21,46	16294235	96,164	MC
		16944187	100,000	

Peak rejection level: 0

Generic Display Report

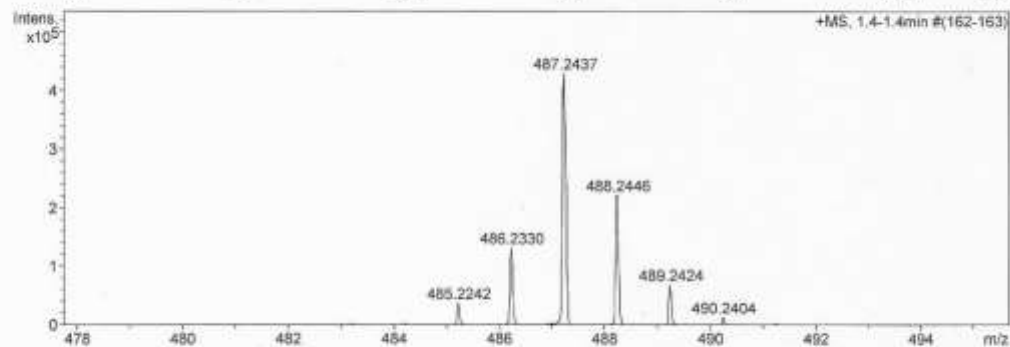
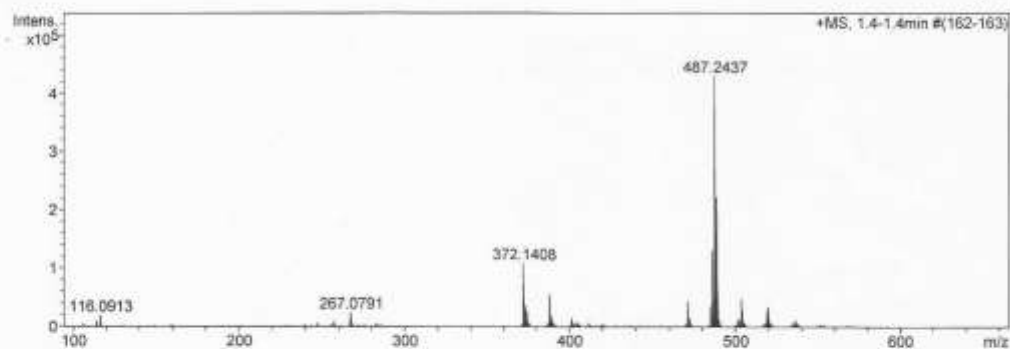
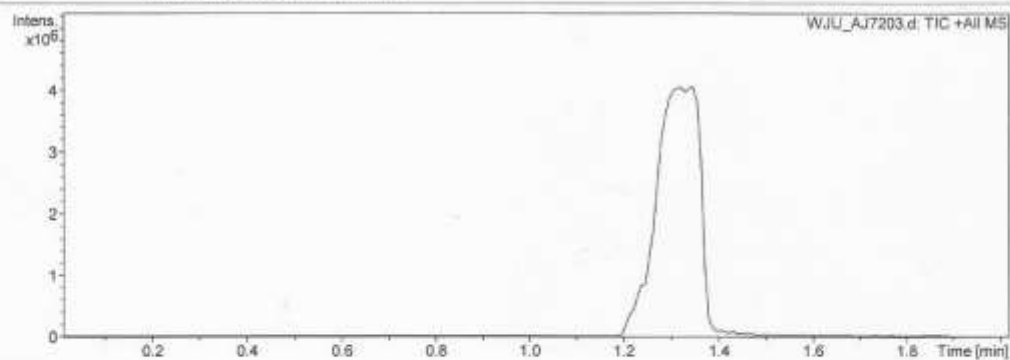
Analysis Info

Analysis Name D:\Data\IPMC\PharmChemie\Routine\2011_5\WJU_AJ7203.d
Method APCI_directprobe_default.m
Sample Name AJ7203
Comment Junker
APCI-Direkt
Kalibration mit Fettsaeureestern

Acquisition Date 5/2/2011 2:38:46 PM

Operator Meiners

Instrument micrOTOF-Q II



Mass Spectrum SmartFormula Report

Analysis Info

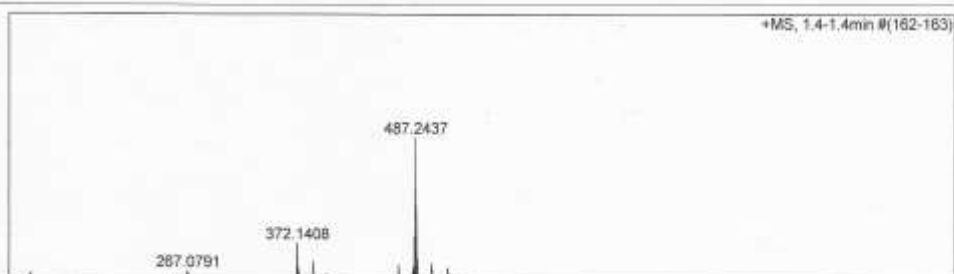
Analysis Name D:\Data\IPMC\PharmChemie\Routine\2011_5WJU_AJ7203.d
 Method APCI_directprobe_default.m
 Sample Name AJ7203
 Comment Junker
 APCI-Direkt
 Kalibration mit Fettsaeureestern

Acquisition Date 5/2/2011 2:38:46 PM

Operator Meiners
 Instrument / Ser# micrOTOF-Q II 10252

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	3.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
487.2437	1	C ₃₅ H ₃₅ S	100.00	487.2454	1.7	-3.6	65.6	18.5	even	ok
	2	C ₂₇ H ₃₉ N ₂ O ₂ S ₂	63.69	487.2447	1.1	2.2	88.0	9.5	even	ok
	3	C ₃₀ H ₃₅ N ₂ O ₂ S	25.11	487.2414	-2.3	-4.7	90.1	14.5	even	ok
	4	C ₂₀ H ₃₉ N ₈ S ₃	15.77	487.2454	1.8	3.6	108.3	5.5	even	ok
	5	C ₂₃ H ₃₅ N ₈ S ₂	16.62	487.2421	-1.6	-3.3	109.6	10.5	even	ok
	6	C ₂₂ H ₄₇ O ₃ S ₄	3.08	487.2403	-3.4	-7.0	112.0	-0.5	even	ok
	7	C ₁₉ H ₄₃ N ₄ O ₄ S ₃	19.26	487.2441	0.4	0.9	119.5	0.5	even	ok
	8	C ₂₂ H ₃₉ N ₄ O ₄ S ₂	2.88	487.2407	-2.9	-6.0	122.0	5.5	even	ok
	9	C ₂₃ H ₃₉ N ₂ O ₇ S	1.05	487.2472	3.6	7.4	128.1	5.5	even	ok
	10	C ₂₀ H ₃₁ N ₁₂ O ₅	3.70	487.2459	2.2	4.6	128.4	11.5	even	ok
	11	C ₁₅ H ₃₉ N ₁₀ O ₂ S ₃	3.56	487.2414	-2.3	-4.6	129.0	1.5	even	ok
	12	C ₁₉ H ₃₅ N ₈ O ₅ S	4.66	487.2446	0.9	1.9	139.8	6.5	even	ok
	13	C ₁₅ H ₃₁ N ₁₄ O ₃ S	1.26	487.2419	-1.8	-3.7	151.6	7.5	even	ok
	14	C ₁₈ H ₃₉ N ₄ O ₉ S	2.78	487.2432	-0.4	-0.9	151.6	1.5	even	ok
	15	C ₁₂ H ₃₅ N ₁₄ O ₃ S ₂	0.87	487.2452	1.6	3.3	158.9	2.5	even	ok
	16	C ₁₄ H ₃₅ N ₁₀ O ₇ S	0.18	487.2405	-3.1	-6.4	163.2	2.5	even	ok