

Curcumin inspired synthesis of unsymmetrical diarylpentanoids with highly potent anti-parasitic activities. *In silico* studies and DFT based stereochemical calculation

Zia Ud Din^{1*}, Alef dos Santos¹, Marilia Almeida Trapp¹, Danielle Lazarin-Bidóia², Francielle Pelegrin Garcia², Francieli Peron², Celso Vataru Nakamura², Edson Rodrigues-Filho¹

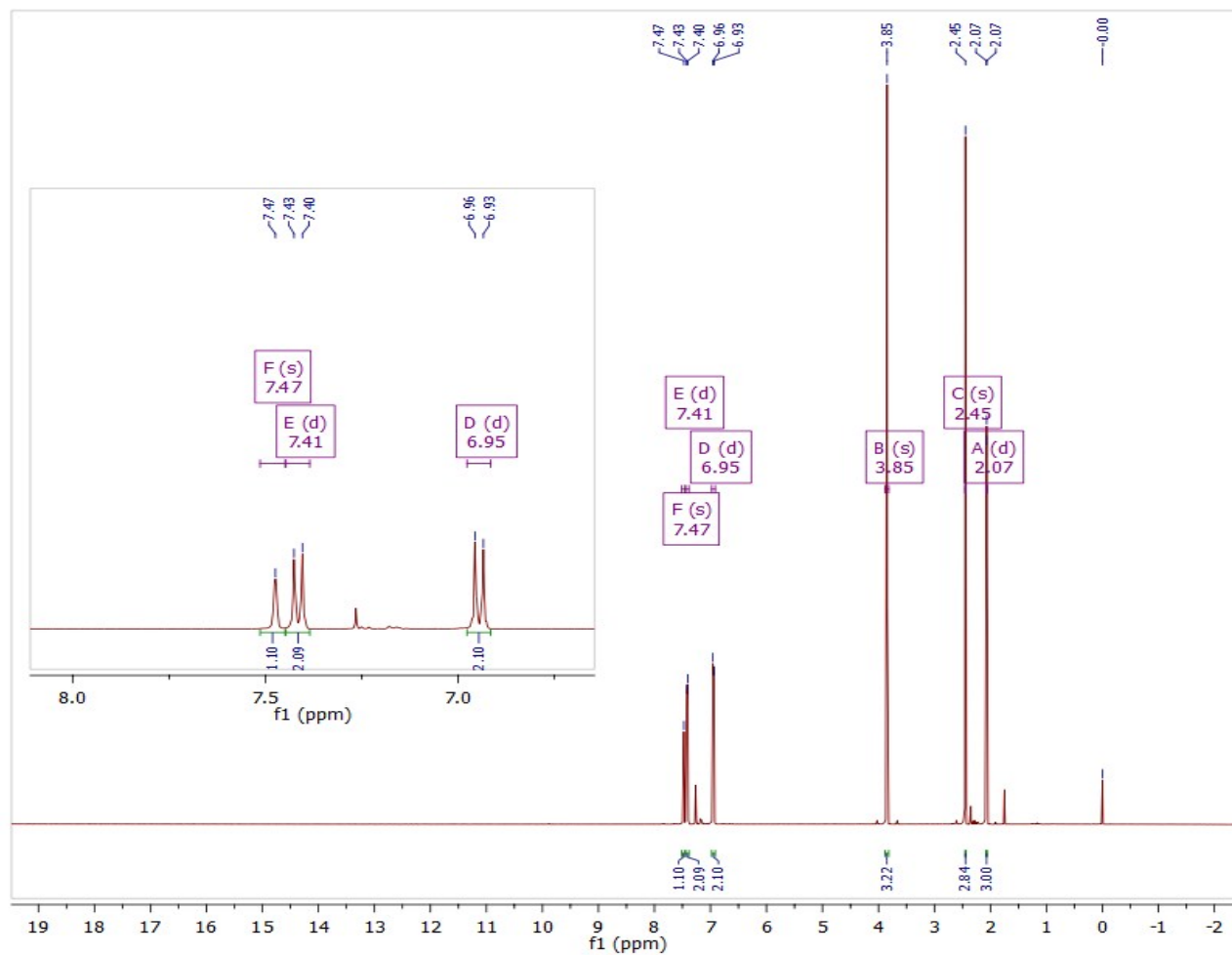
¹Departamento de Química, Universidade Federal de São Carlos CP 676, 13.565-905, São Carlos, SP, Brazil.

²Laboratório de Inovação Tecnológica no Desenvolvimento de Fármacos e Cosméticos, Universidade Estadual de Maringá, Av.Colombo 5790,87020-900, Bloco B-08,Sala 06, Maringá, PR,Brazil.

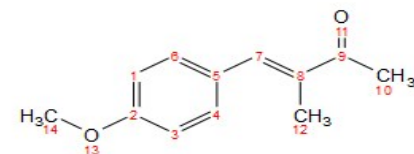
Supporting Information

NMR spectra of compounds 1-20	3-44
Mass spectra of compounds 1-20	45-64

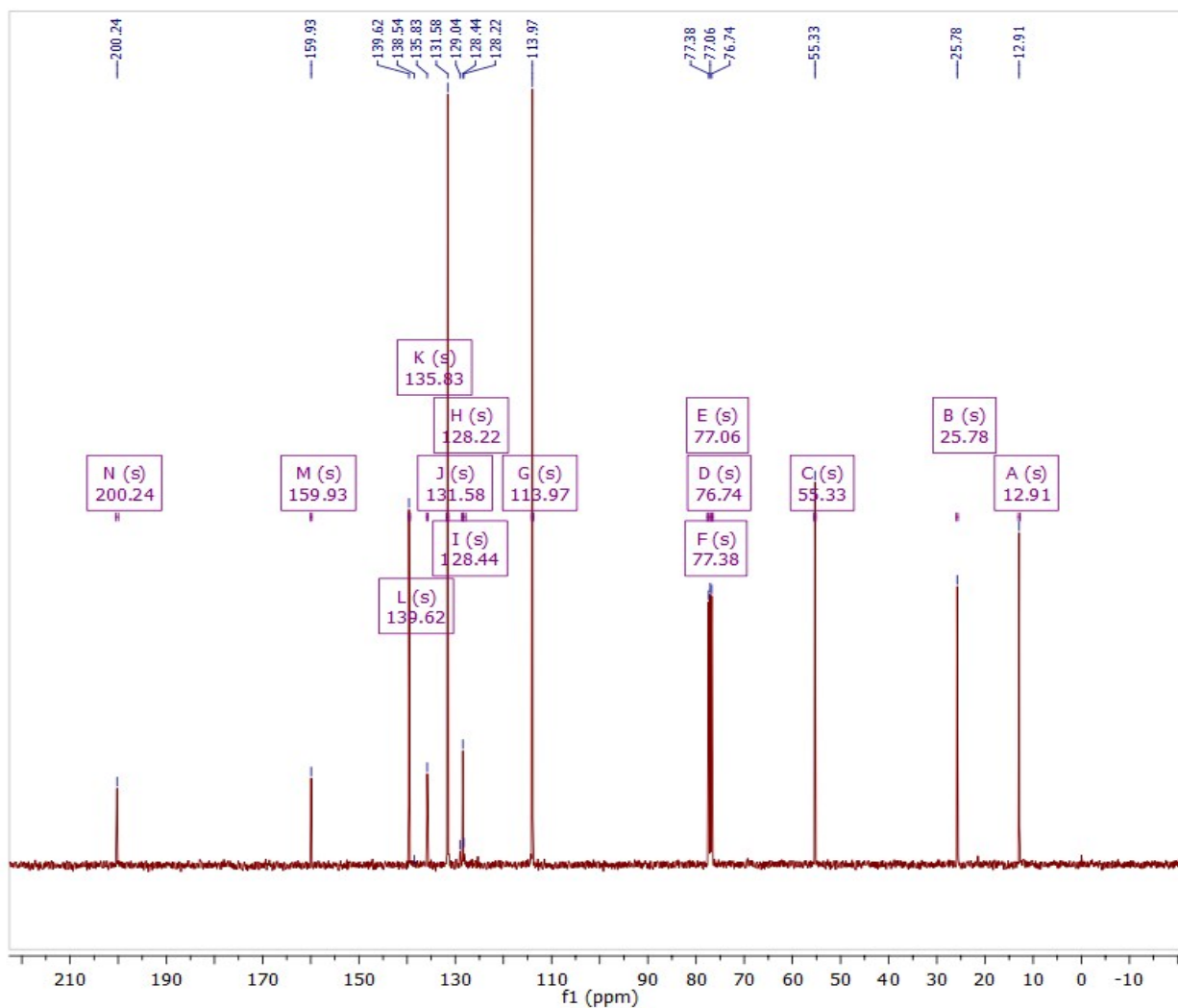
Compound (01) - ^1H NMR



Parameter	Value
1 Title	1A238_A2K2_04
2 Solvent	CDCl_3
3 Temperature	296.6
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	72
7 Relaxation Delay	1.0000
8 Pulse Width	8.7600
9 Acquisition Time	3.7225
10 Acquisition Date	2012-09-19T10:51:00
11 Modification Date	2012-09-19T10:51:14
12 Spectrometer Frequency	400.15
13 Spectral Width	8802.8
14 Lowest Frequency	-1007.1
15 Nucleus	^1H
16 Acquired Size	32768
17 Spectral Size	65536

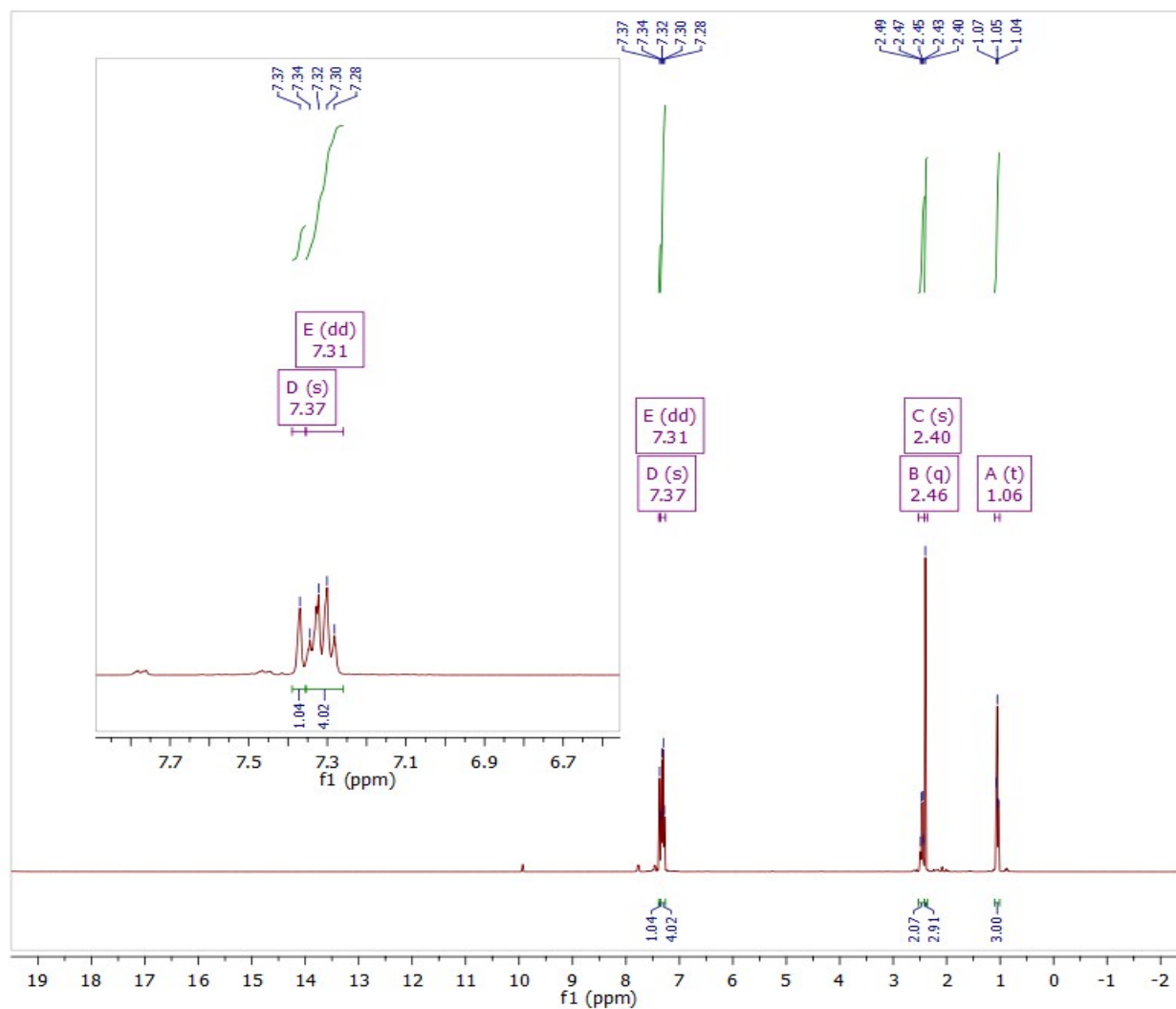


Compound (01) - ^{13}C NMR

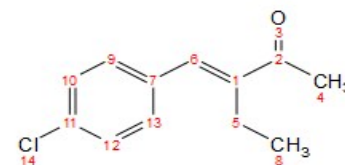


Parameter	Value
1 Title	1A238_A2K2_04_C
2 Solvent	CDCl3
3 Temperature	297.3
4 Pulse Sequence	zgpg30
5 Number of Scans	1024
6 Receiver Gain	2050
7 Relaxation Delay	0.1100
8 Pulse Width	8.7500
9 Acquisition Time	0.6641
10 Acquisition Date	2012-09-21T18:37:00
11 Modification Date	2012-09-21T21:38:00
12 Spectrometer Frequency	100.62
13 Spectral Width	24671.1
14 Lowest Frequency	-2274.2
15 Nucleus	13C
16 Acquired Size	16384
17 Spectral Size	32768

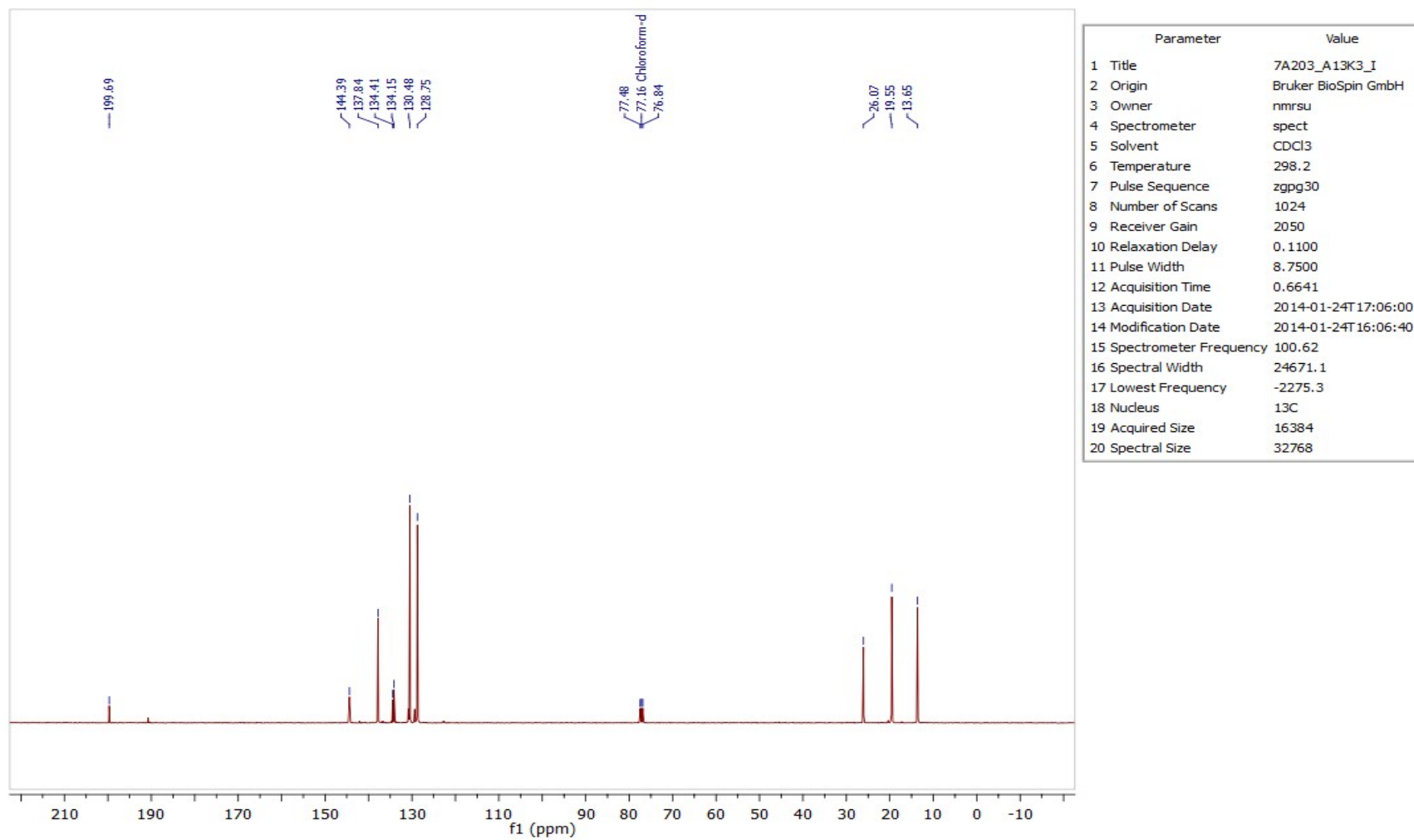
Compound (02) - ¹H NMR



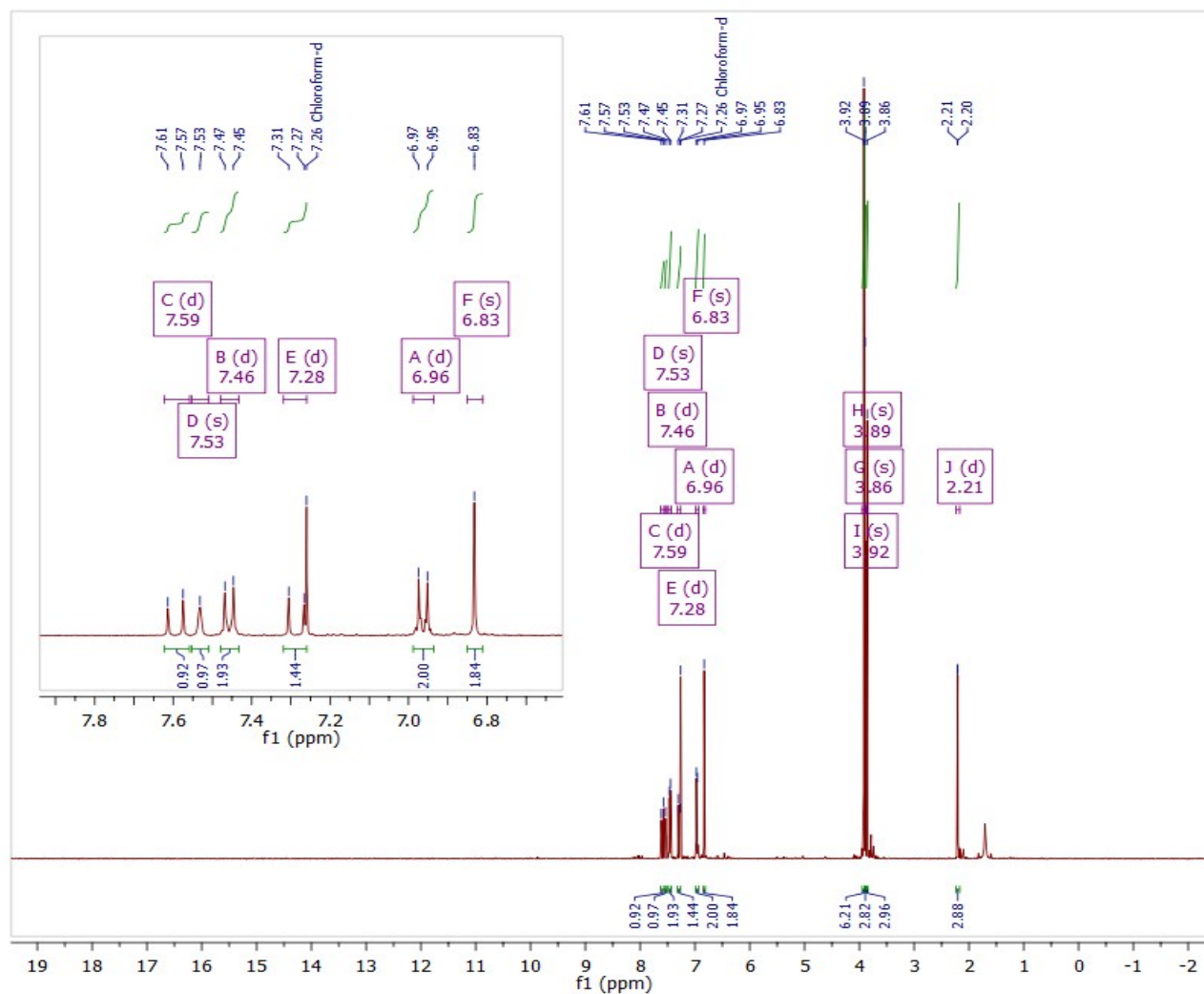
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1 Title	7A203_A13K3_I
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl ₃
6 Temperature	297.6
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	13
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	3.7225
13 Acquisition Date	2014-01-24T16:51:00
14 Modification Date	2014-01-24T15:51:20
15 Spectrometer Frequency	400.15
16 Spectral Width	8802.8
17 Lowest Frequency	-1000.1
18 Nucleus	¹ H
19 Acquired Size	32768
20 Spectral Size	65536



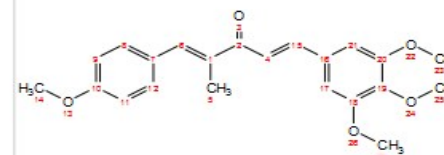
Compound (02) - ^{13}C NMR



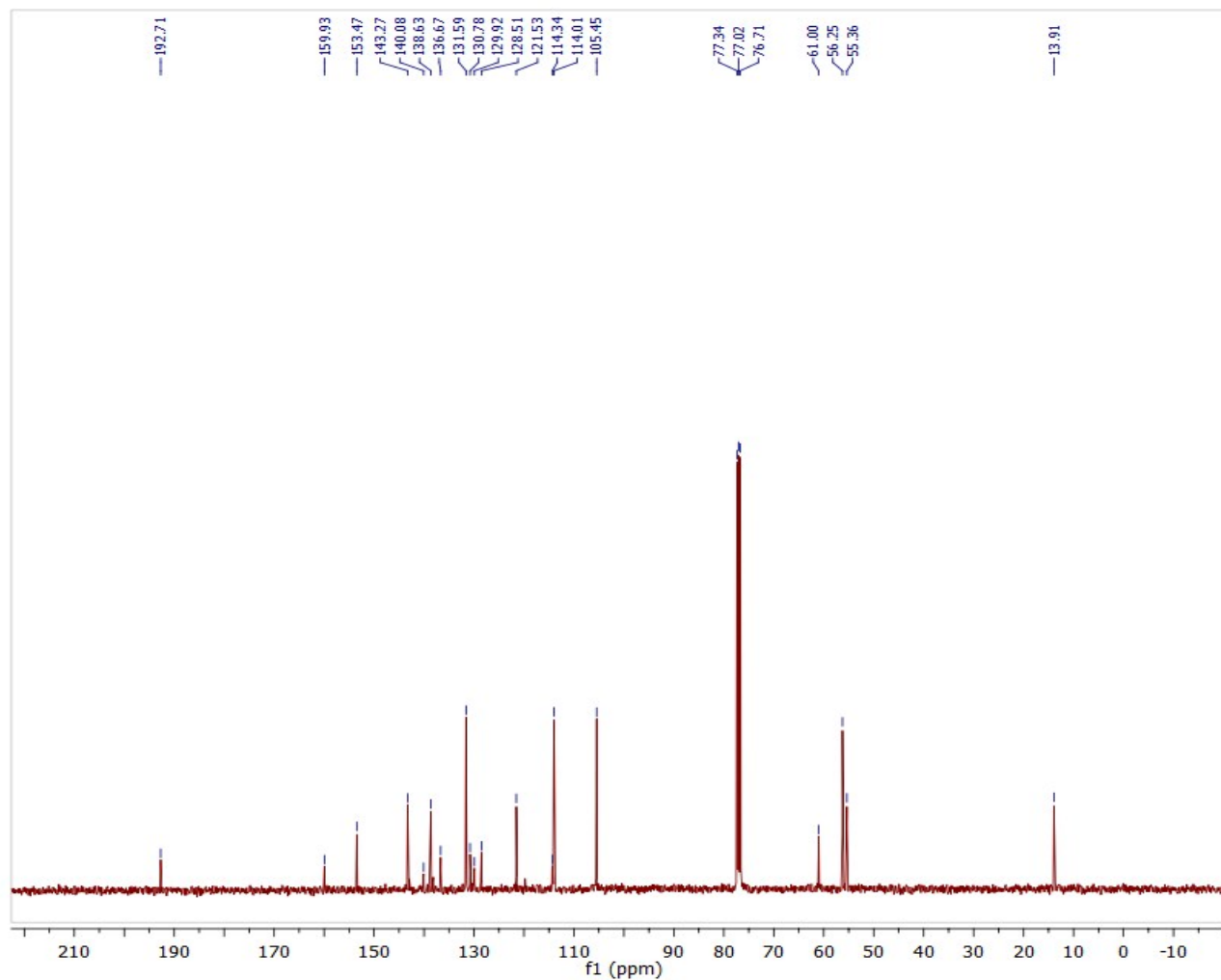
Compound (03) - ^1H NMR



Parameter	Value
1 Title	2A728_A2K2A6_57
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	299.8
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	2050
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	3.7225
13 Acquisition Date	2013-07-20T20:31:00
14 Modification Date	2013-07-20T23:29:00
15 Spectrometer Frequency	400.15
16 Spectral Width	8802.8
17 Lowest Frequency	-1009.3
18 Nucleus	^1H
19 Acquired Size	32768
20 Spectral Size	65536

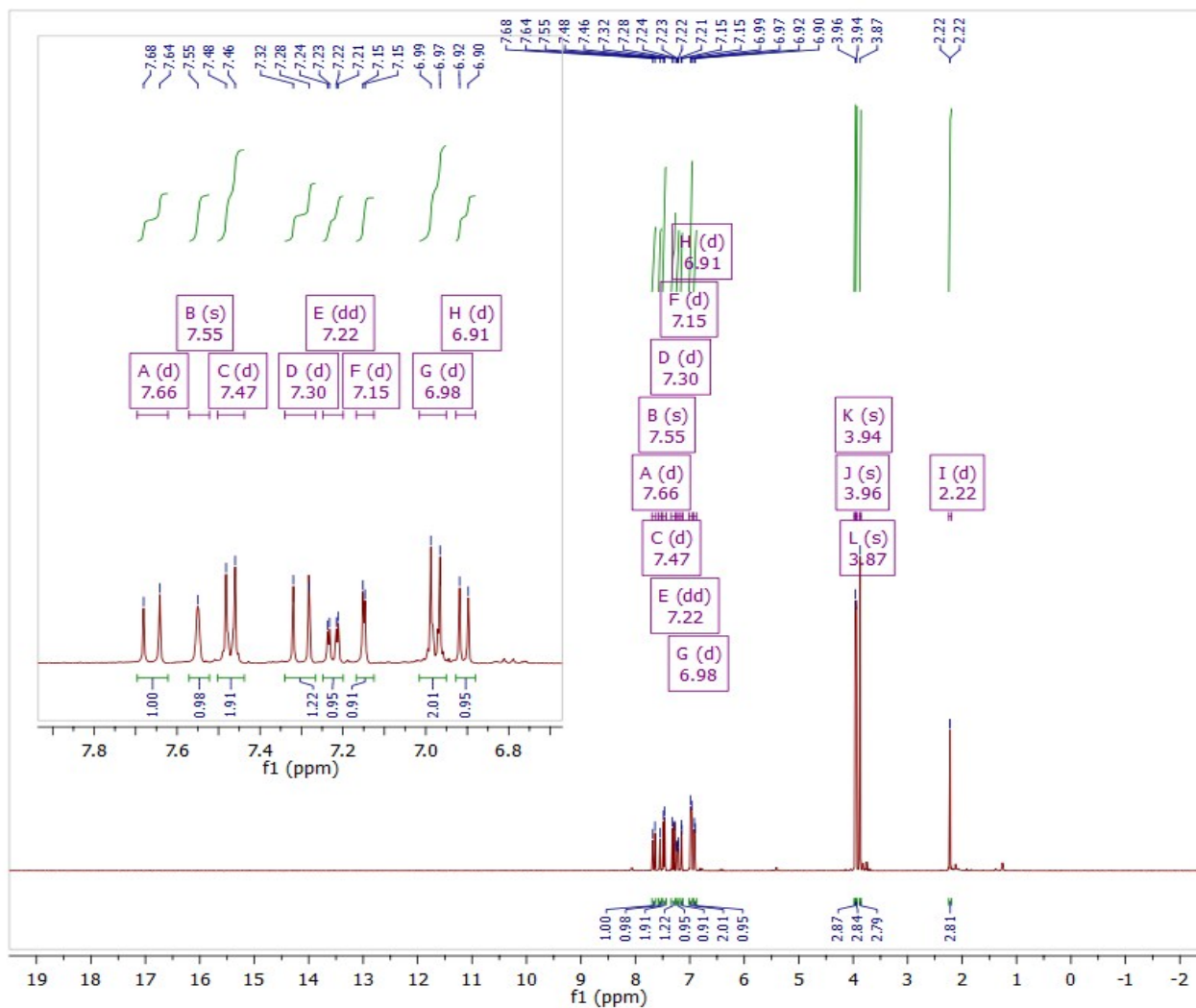


Compound (03)- ¹³C NMR

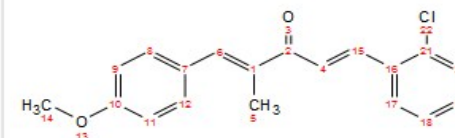


Parameter	Value
1 Title	7A907_A2K2A6
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl ₃
6 Temperature	297.8
7 Pulse Sequence	zgpg30
8 Number of Scans	2048
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2015-02-18T08:12:00
14 Modification Date	2015-02-20T09:24:35
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2274.2
18 Nucleus	¹³ C
19 Acquired Size	16384
20 Spectral Size	32768

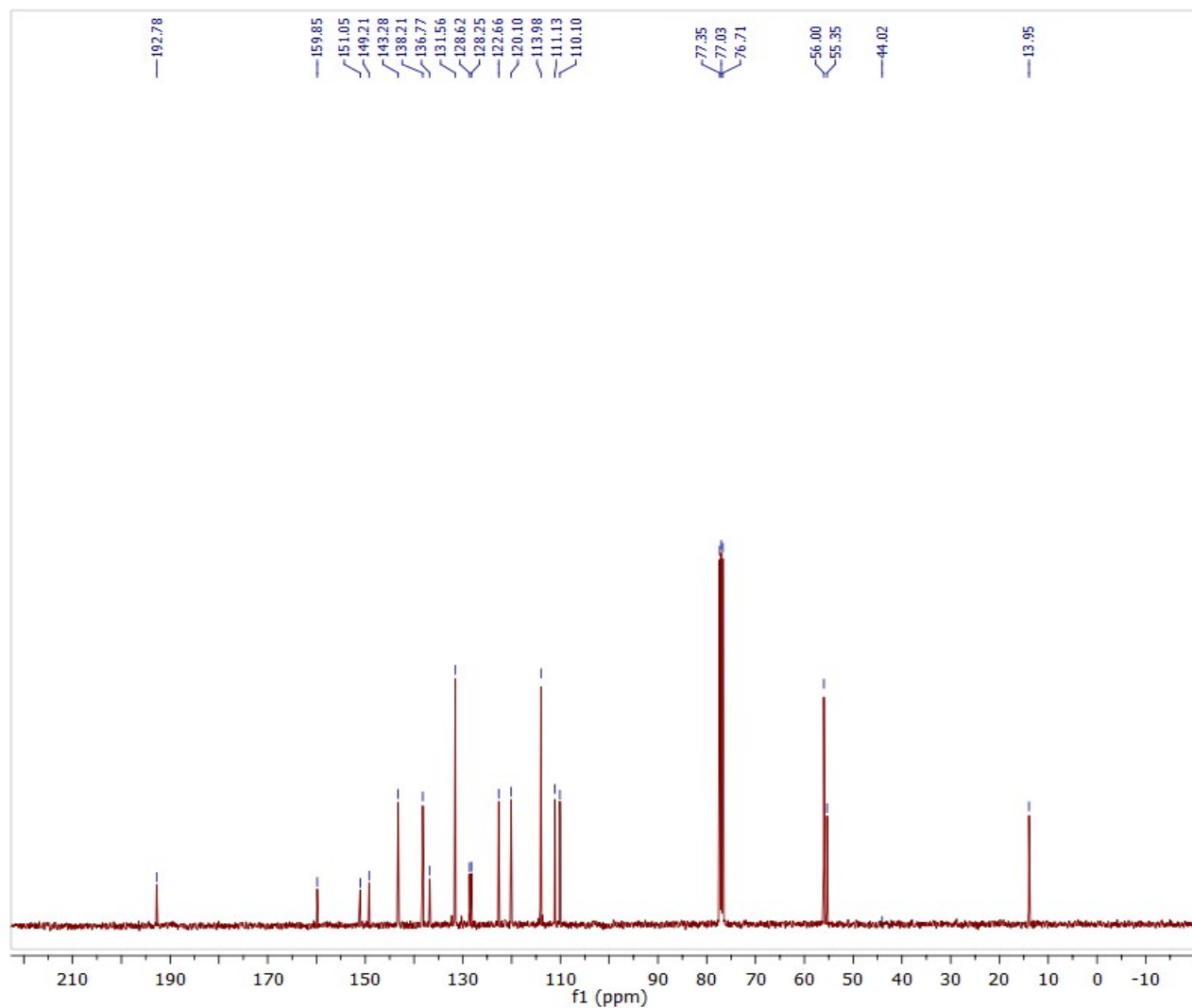
Compound (04) - ¹H NMR



Parameter	Value
1 Title	7A928_A2K2A9-54_Pure
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	299.9
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	2050
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	3.7224
13 Acquisition Date	2013-07-19T17:43:52
14 Modification Date	2013-07-19T20:41:00
15 Spectrometer Frequency	400.15
16 Spectral Width	8802.8
17 Lowest Frequency	-1000.1
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536

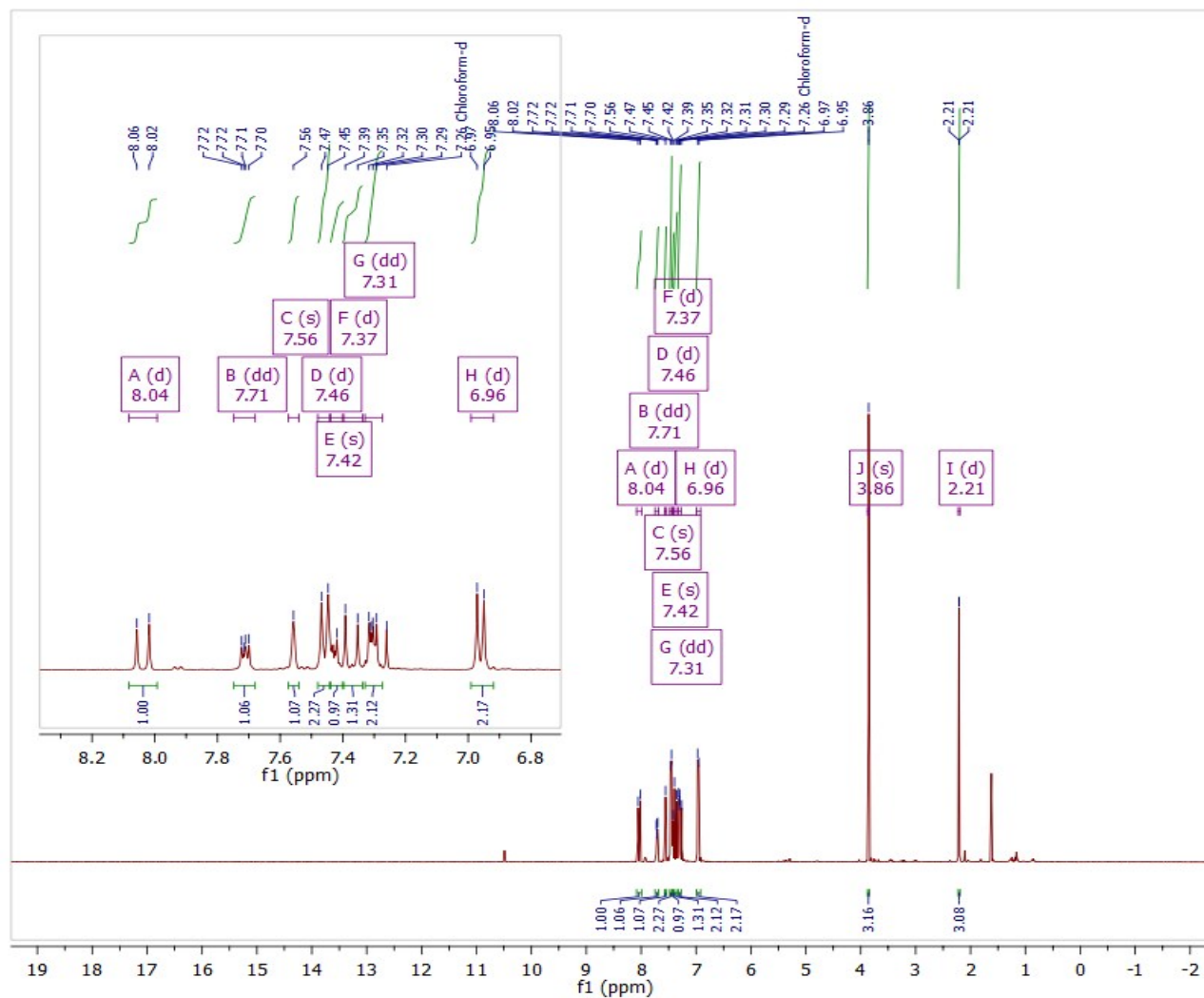


Compound (04)- ^{13}C NMR

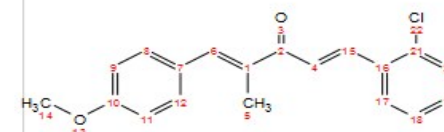


Parameter	Value
1 Title	7A907_A2K2A9
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl ₃
6 Temperature	297.8
7 Pulse Sequence	zgpg30
8 Number of Scans	2048
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2015-02-18T08:44:00
14 Modification Date	2015-02-20T09:24:29
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2274.2
18 Nucleus	^{13}C
19 Acquired Size	16384
20 Spectral Size	32768

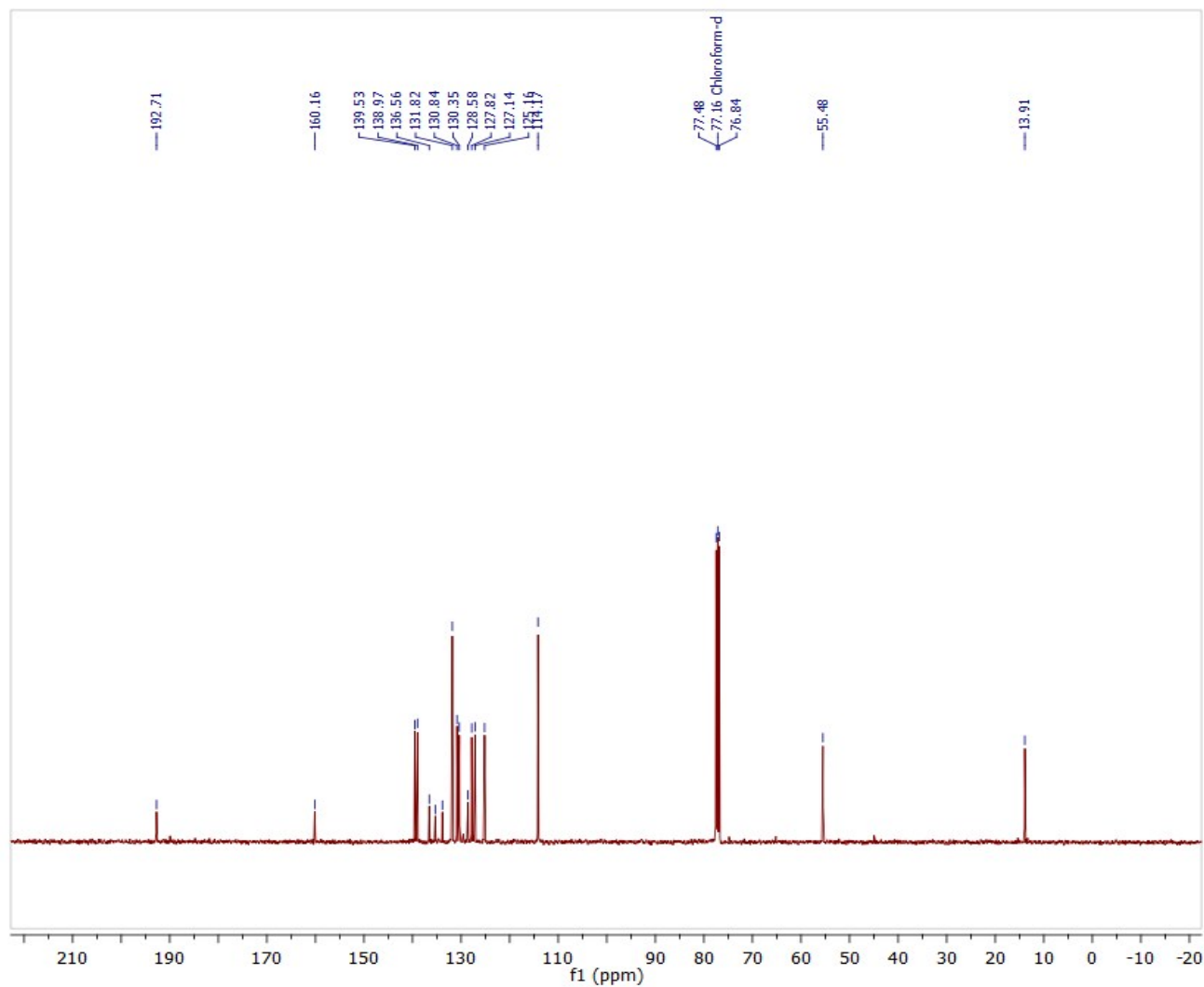
Compound (05) - ¹H NMR



Parameter	Value
1 Title	7A921_A2K2A12_51
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl ₃
6 Temperature	299.8
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	3.7225
13 Acquisition Date	2013-05-28T13:53:00
14 Modification Date	2013-05-28T13:53:58
15 Spectrometer Frequency	400.15
16 Spectral Width	8802.8
17 Lowest Frequency	-1009.3
18 Nucleus	¹ H
19 Acquired Size	32768
20 Spectral Size	65536

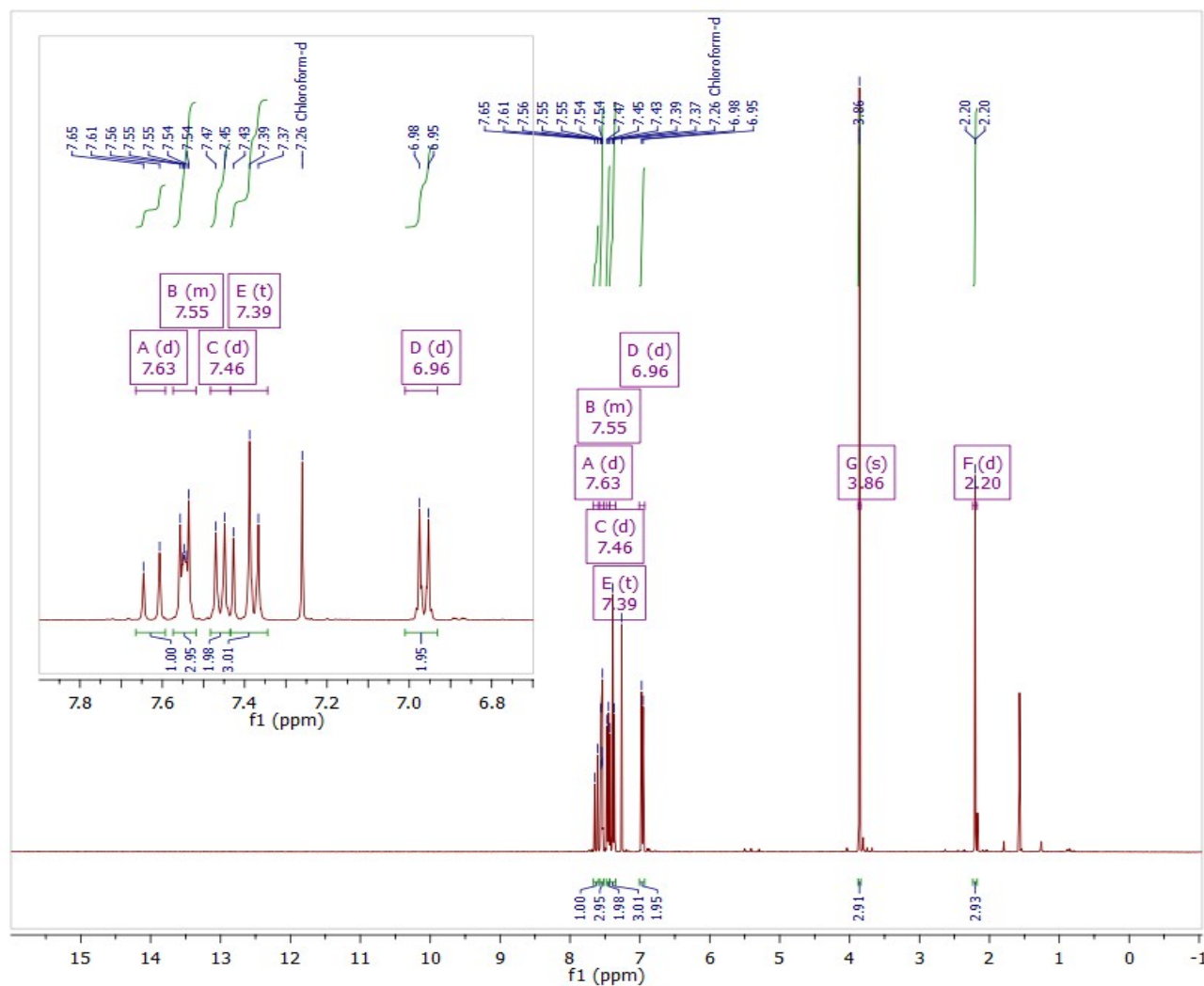


Compound (05)- ^{13}C NMR

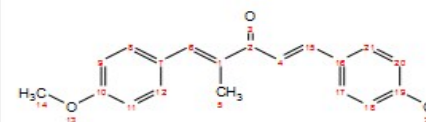


Parameter	Value
1 Title	7A921_A2K2A12_51
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	299.8
7 Pulse Sequence	zgpg30
8 Number of Scans	2048
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2013-05-28T14:23:00
14 Modification Date	2013-05-28T14:23:36
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2260.8
18 Nucleus	^{13}C
19 Acquired Size	16384
20 Spectral Size	32768

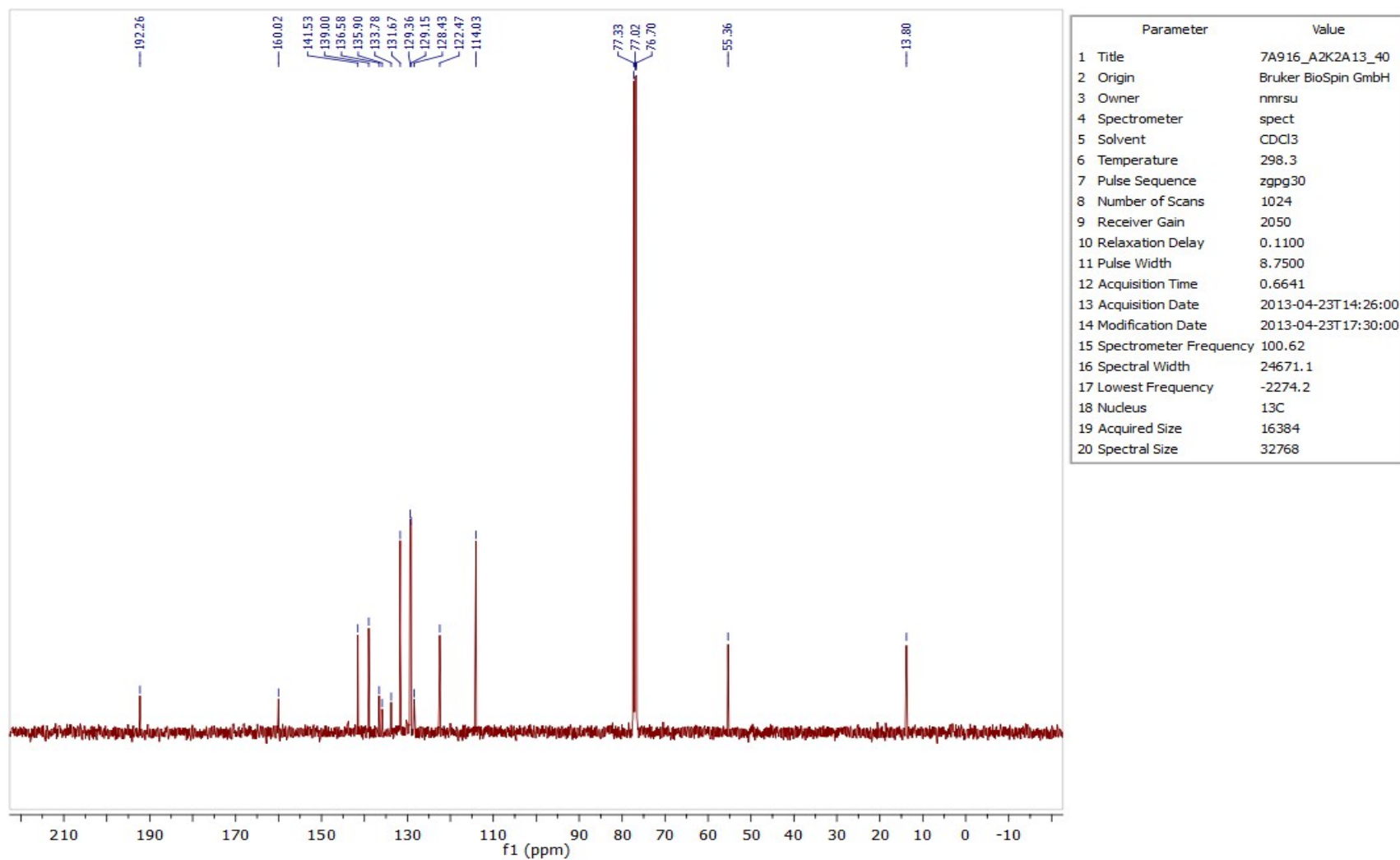
Compound (06) - ¹H NMR



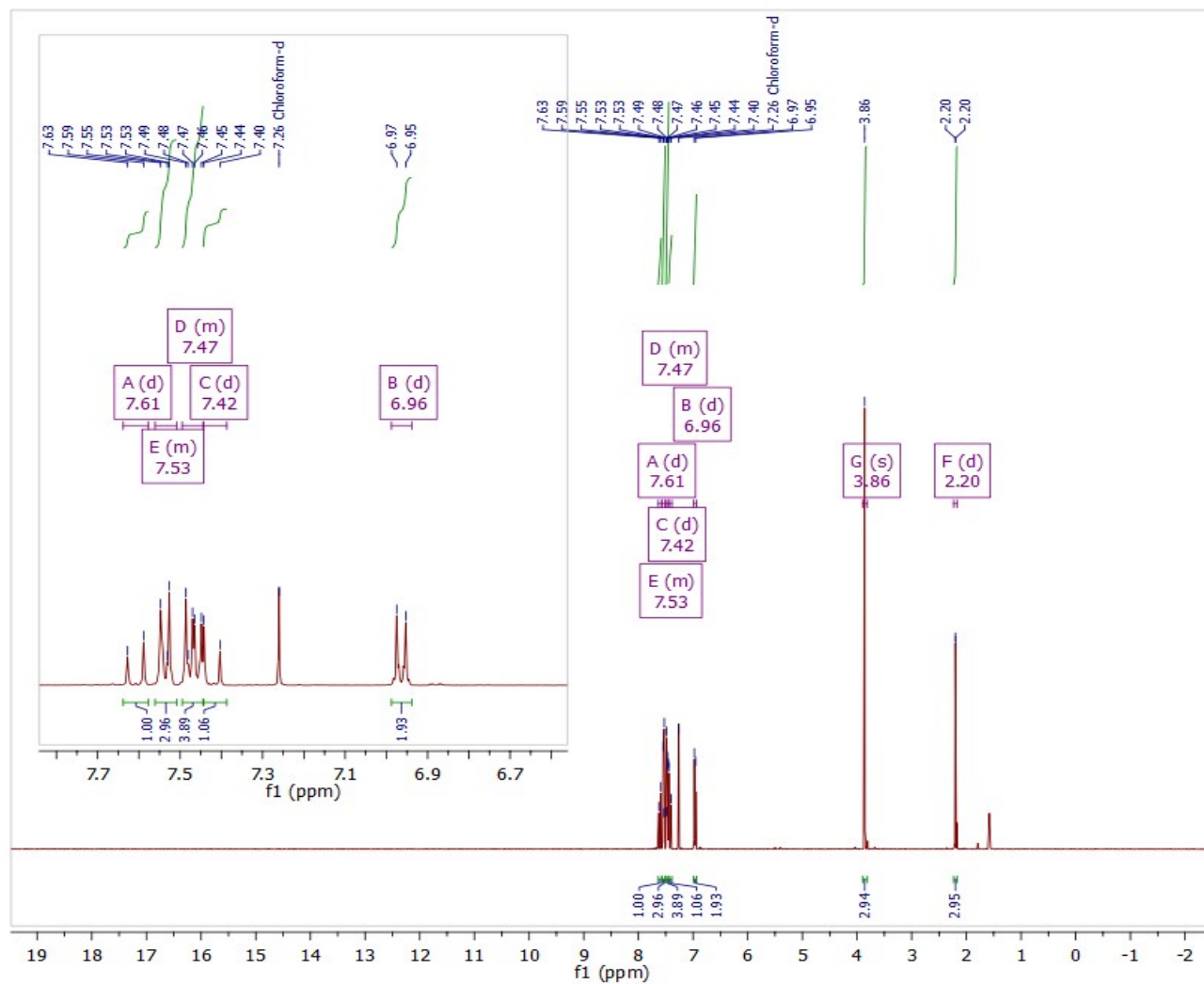
Parameter	Value
1 Title	7A916_A2K2A13_40
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.5
7 Pulse Sequence	zg30
8 Number of Scans	128
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	4.8060
13 Acquisition Date	2013-04-23T14:10:00
14 Modification Date	2013-04-23T17:15:00
15 Spectrometer Frequency	400.15
16 Spectral Width	6818.2
17 Lowest Frequency	-417.2
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



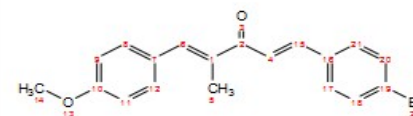
Compound (06)- ^{13}C NMR



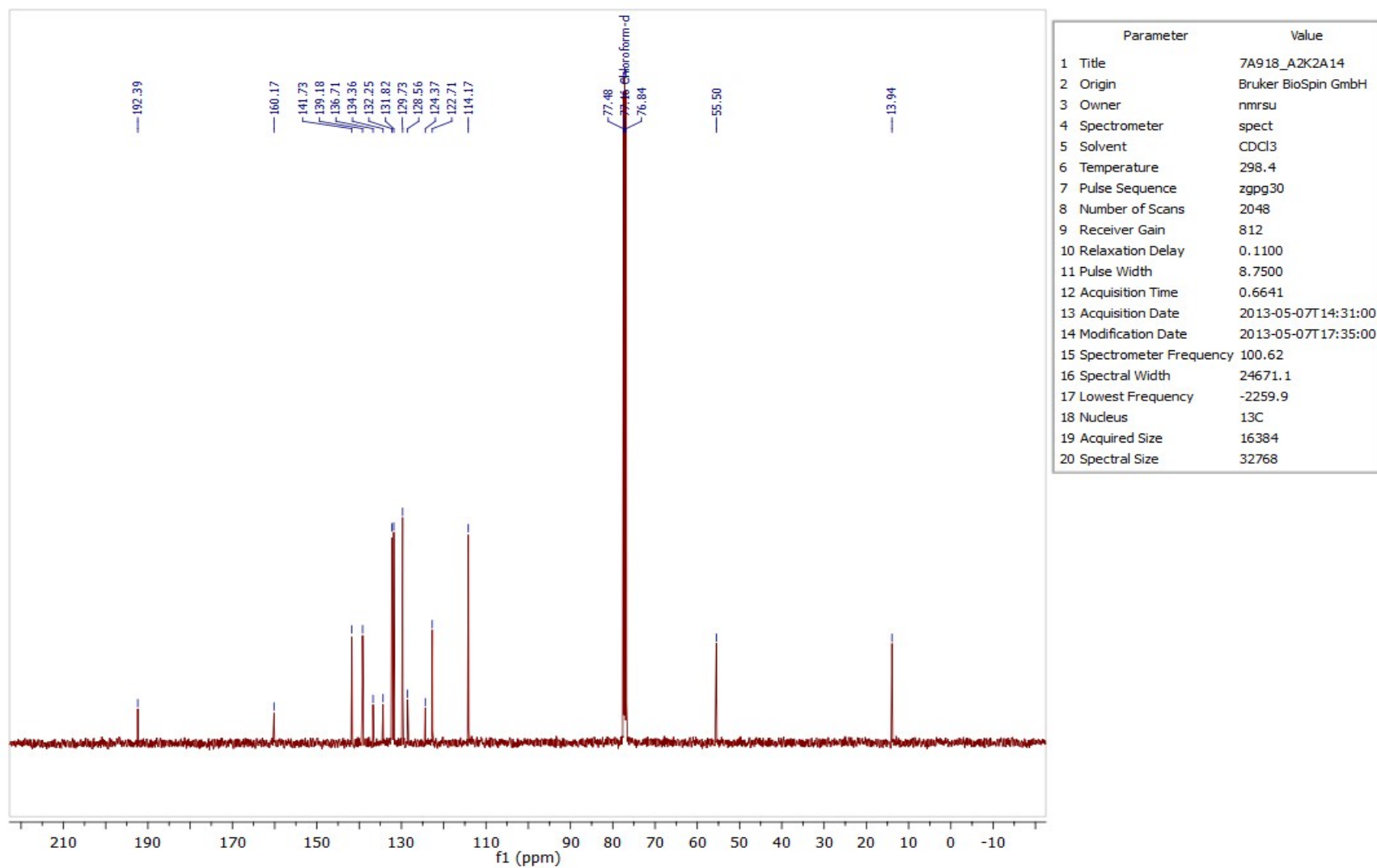
Compound (07) - ¹H NMR



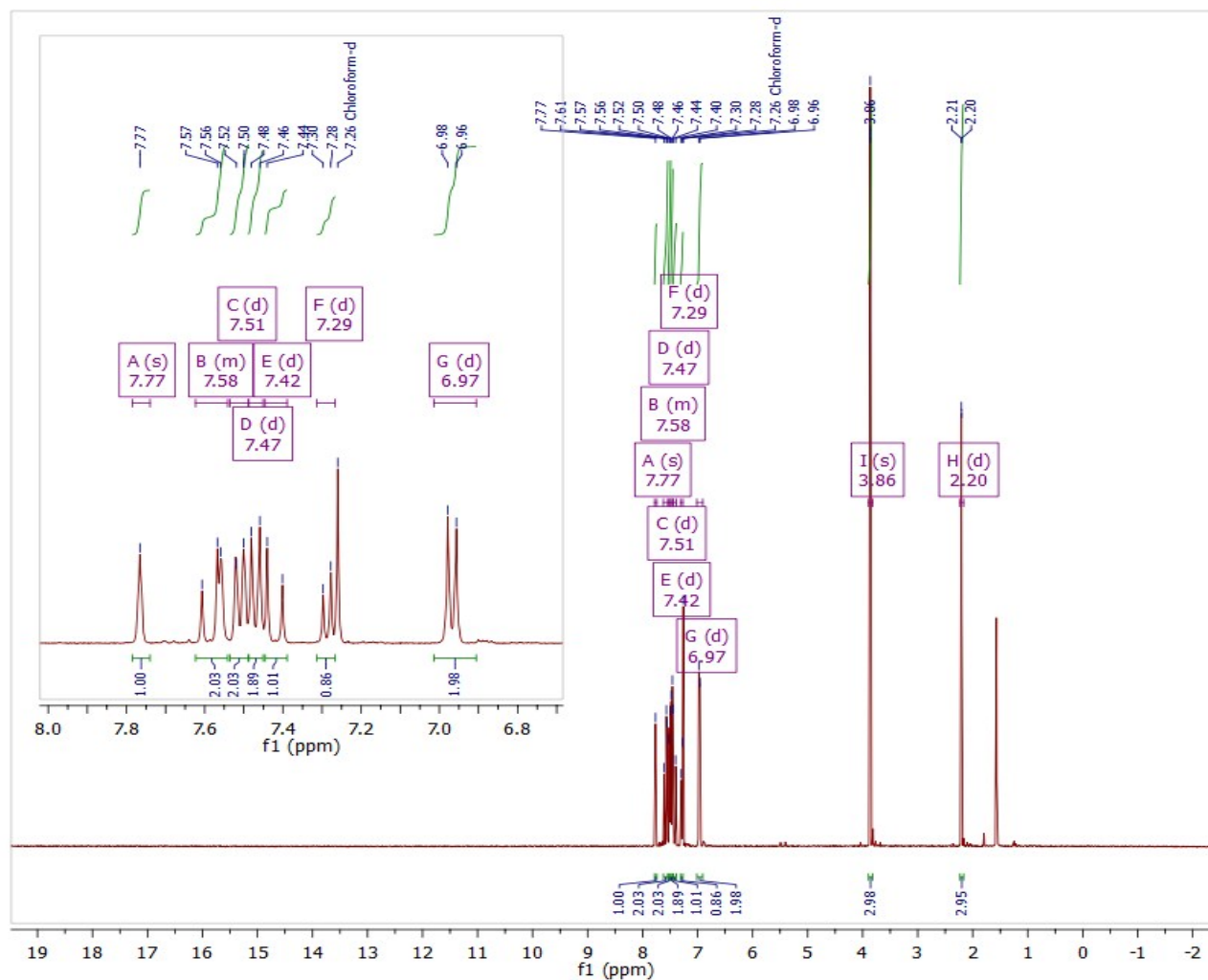
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1 Title	7A918_A2K2A14
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.2
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	3.7225
13 Acquisition Date	2013-05-07T14:01:00
14 Modification Date	2013-05-07T17:05:00
15 Spectrometer Frequency	400.15
16 Spectral Width	8802.8
17 Lowest Frequency	-1009.3
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



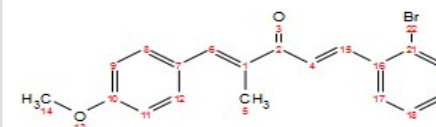
Compound (07)- ¹³C NMR



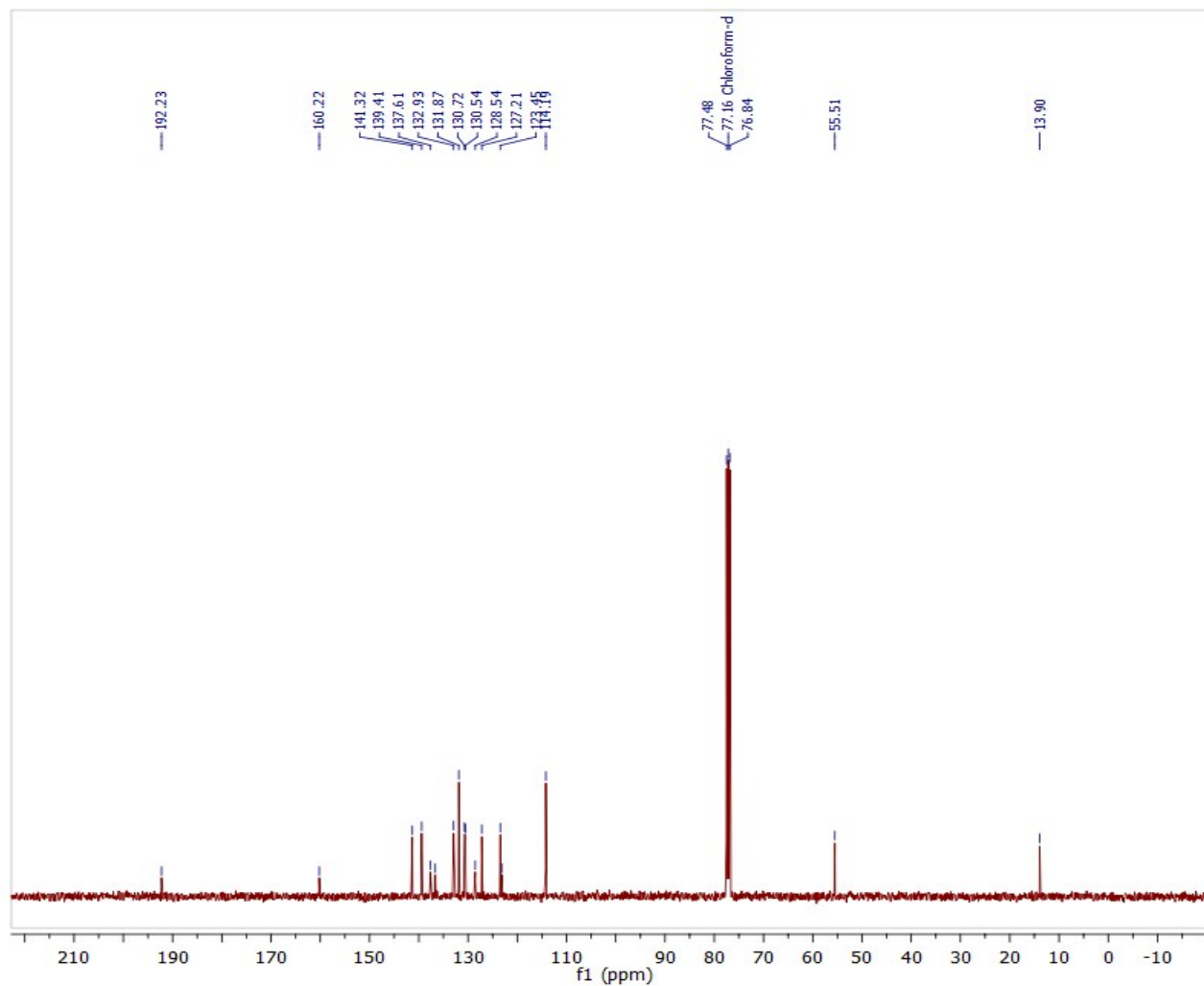
Compound (08) - ¹H NMR



Parameter	Value
1 Title	7C220_A2K2A21_49
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	299.9
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	3.7225
13 Acquisition Date	2013-05-24T17:56:00
14 Modification Date	2013-05-24T17:56:04
15 Spectrometer Frequency	400.15
16 Spectral Width	8802.8
17 Lowest Frequency	-1009.3
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536

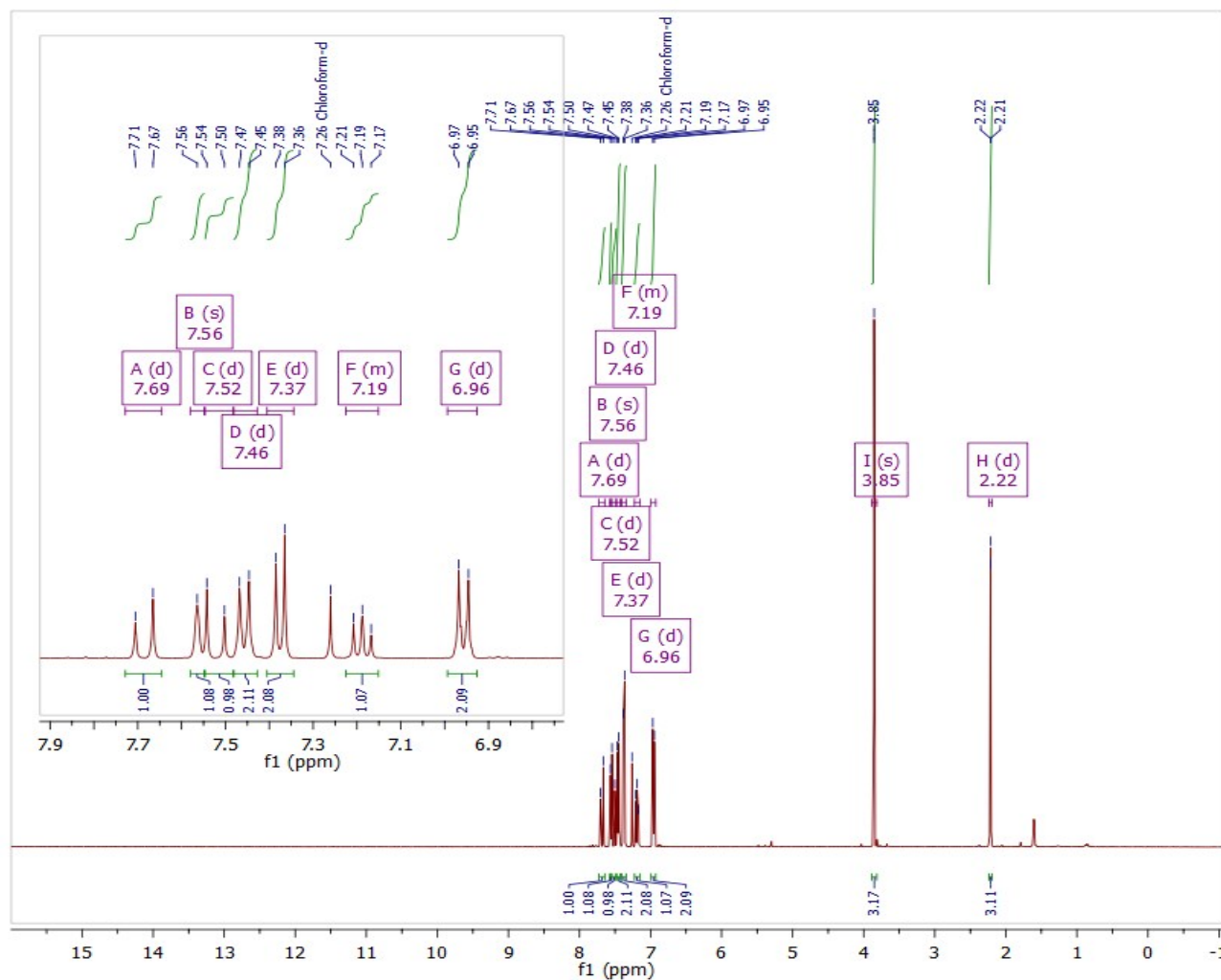


Compound (08)- ¹³C NMR

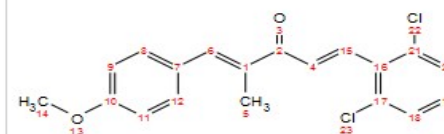


Parameter	Value
1 Title	7C220_A2K2A21_49
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsl
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	299.8
7 Pulse Sequence	zgpg30
8 Number of Scans	1024
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2013-05-24T18:12:00
14 Modification Date	2013-05-24T18:12:02
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2259.1
18 Nucleus	13C
19 Acquired Size	16384
20 Spectral Size	32768

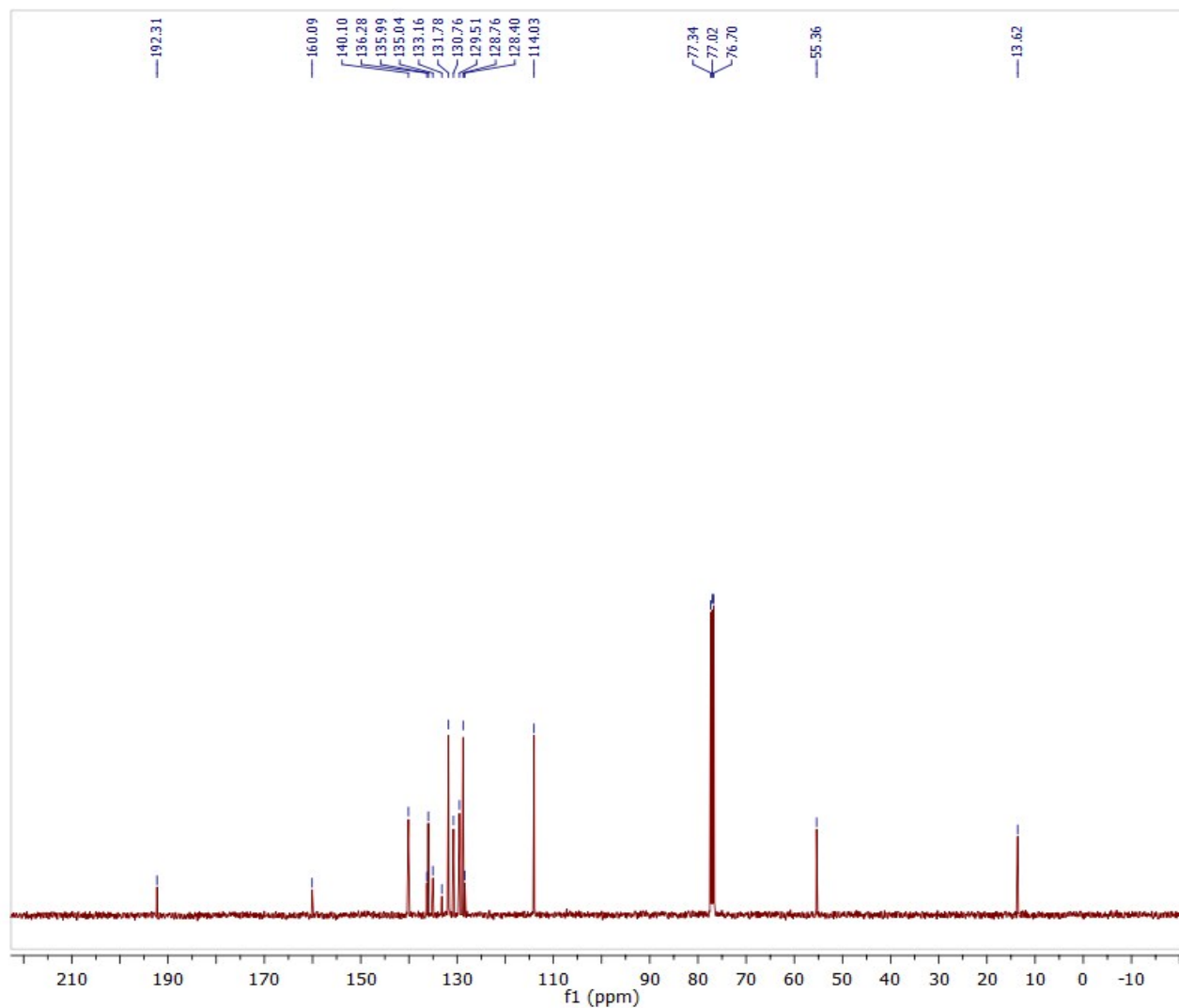
Compound (09) - ¹H NMR



Parameter	Value
1 Title	7A919_A2K2A16_43
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.7
7 Pulse Sequence	zg30
8 Number of Scans	64
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	4.8060
13 Acquisition Date	2013-05-13T14:01:00
14 Modification Date	2013-05-13T17:05:00
15 Spectrometer Frequency	400.15
16 Spectral Width	6818.2
17 Lowest Frequency	-417.2
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536

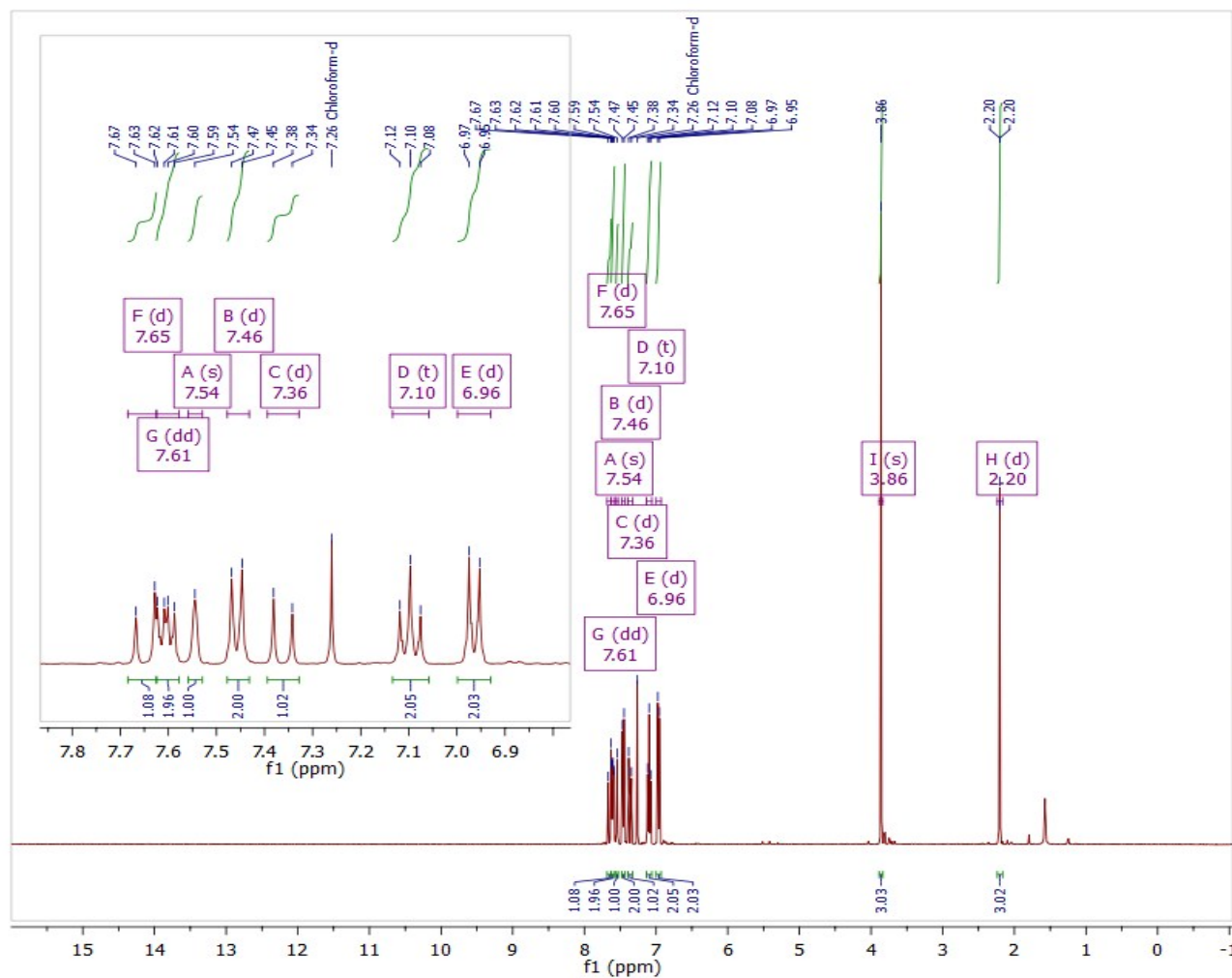


Compound (09)- ^{13}C NMR

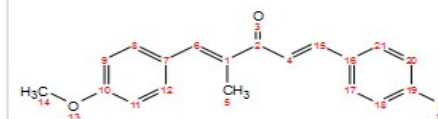


Parameter	Value
1 Title	7A919_A2K2A16_43
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl_3
6 Temperature	298.6
7 Pulse Sequence	zgpg30
8 Number of Scans	1024
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2013-05-13T14:16:00
14 Modification Date	2013-05-13T17:20:00
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2274.2
18 Nucleus	^{13}C
19 Acquired Size	16384
20 Spectral Size	32768

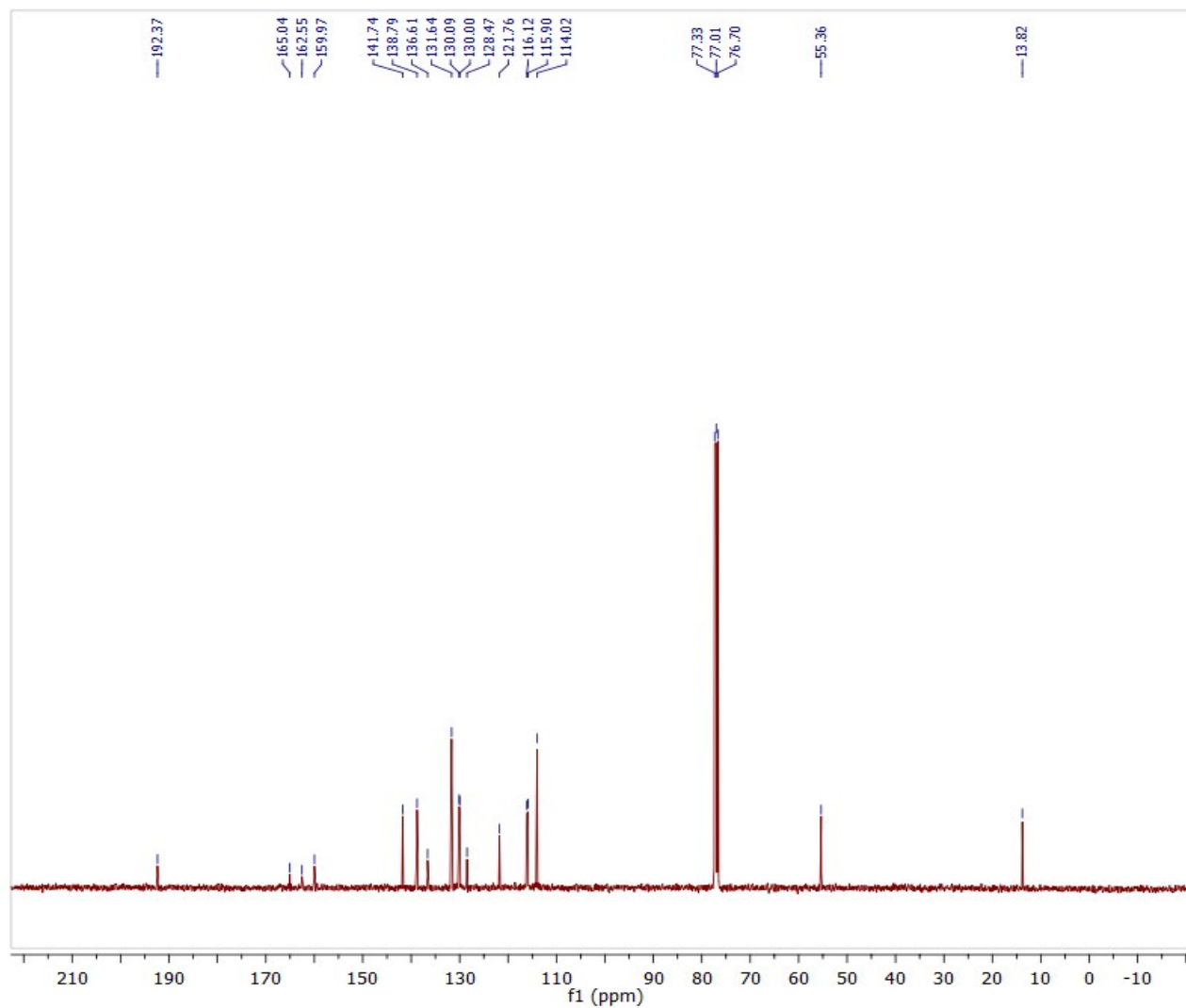
Compound (10) - ^1H NMR



Parameter	Value
1 Title	7A919_A2K2A17_44
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.7
7 Pulse Sequence	zg30
8 Number of Scans	64
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	4.8060
13 Acquisition Date	2013-05-13T14:26:00
14 Modification Date	2013-05-13T17:30:00
15 Spectrometer Frequency	400.15
16 Spectral Width	6818.2
17 Lowest Frequency	-417.2
18 Nucleus	^1H
19 Acquired Size	32768
20 Spectral Size	65536

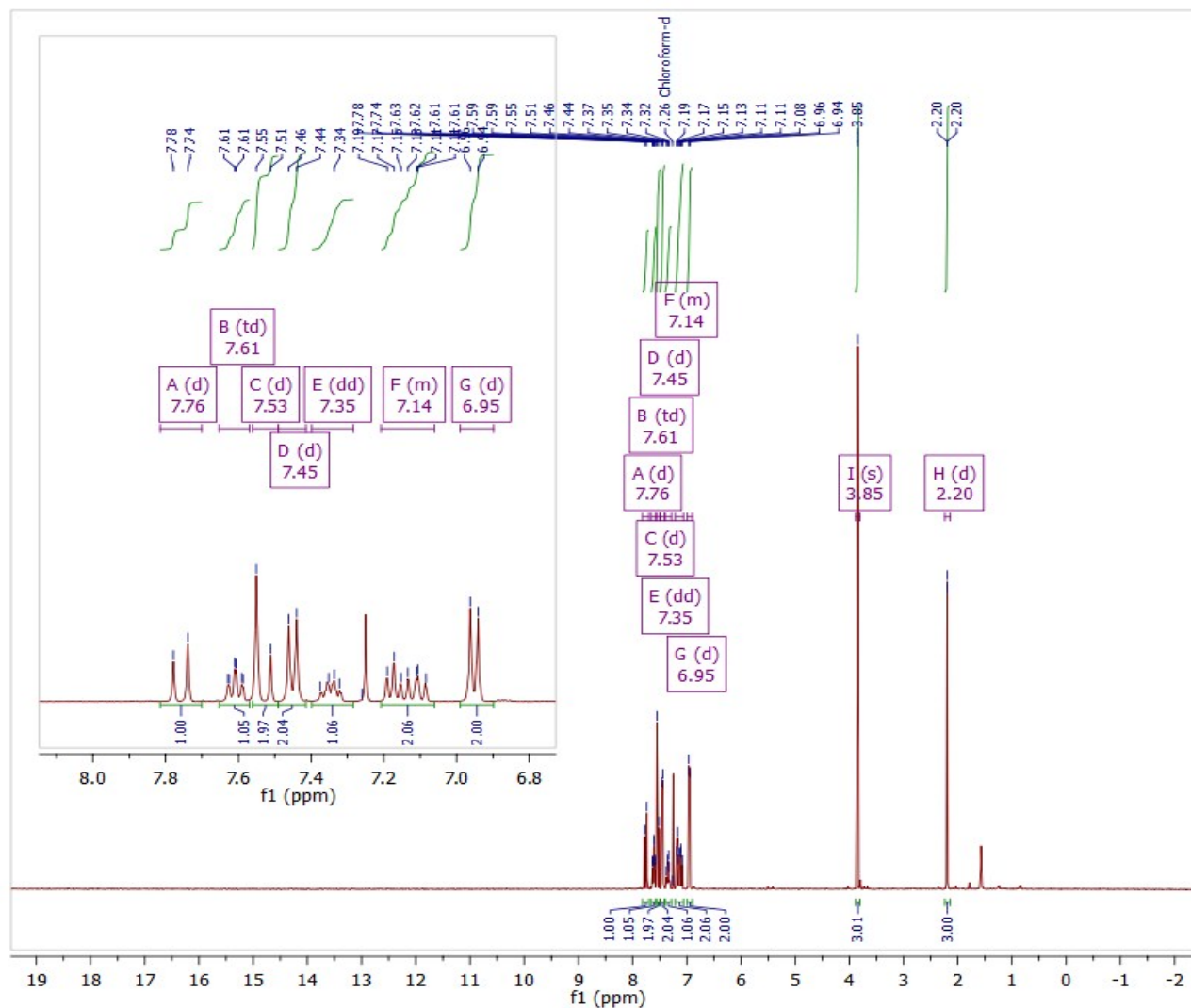


Compound (10)- ¹³C NMR

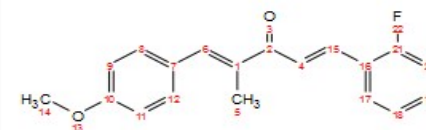


Parameter	Value
1 Title	7A919_A2K2A17_44
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	298.6
7 Pulse Sequence	zgpg30
8 Number of Scans	2048
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2013-05-13T14:56:00
14 Modification Date	2013-05-13T18:00:00
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2274.2
18 Nucleus	13C
19 Acquired Size	16384
20 Spectral Size	32768

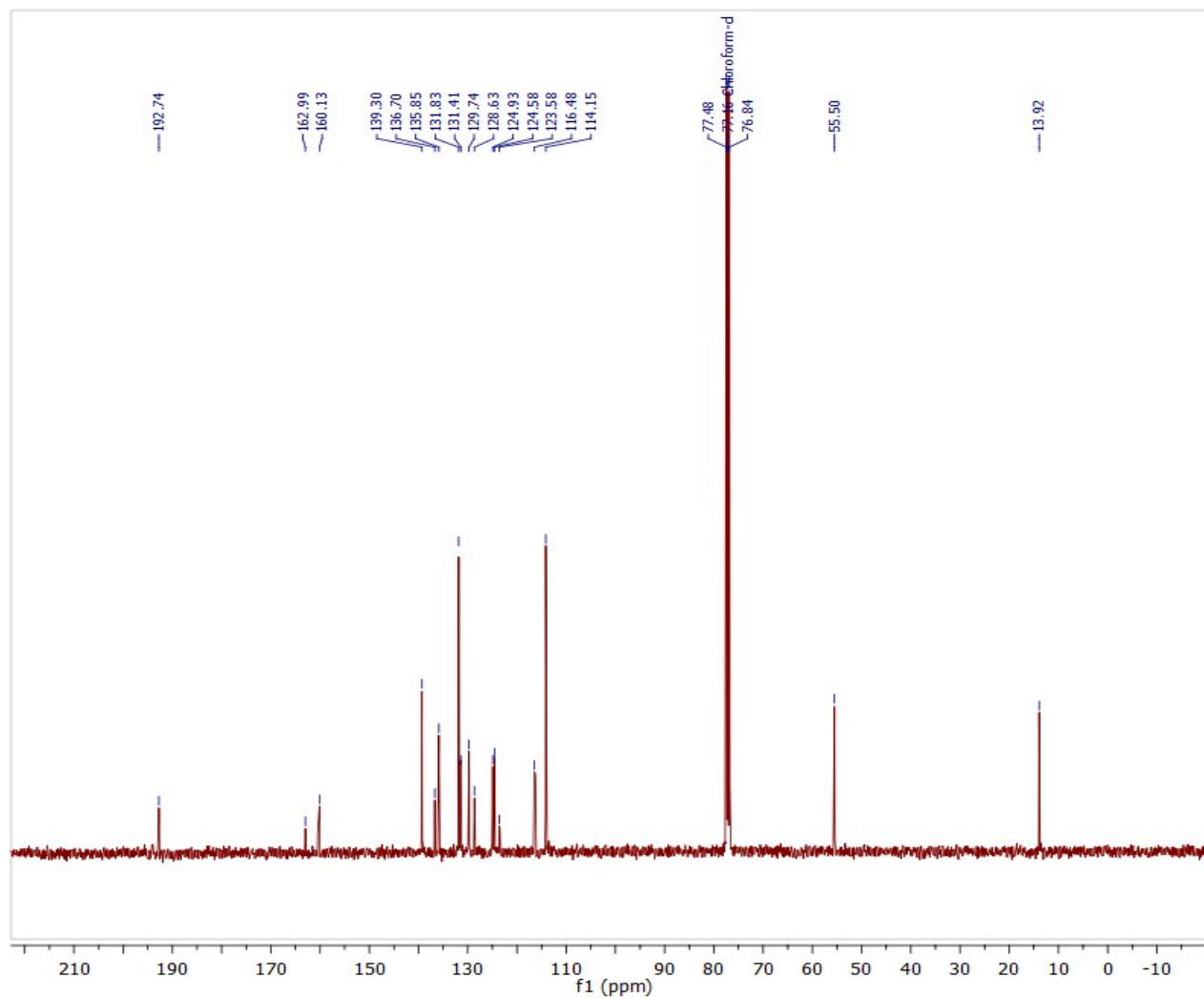
Compound (11) - ^1H NMR



Parameter	Value
1 Title	7A919_A2K2A19_46
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.7
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	3.7225
13 Acquisition Date	2013-05-15T15:54:00
14 Modification Date	2013-05-15T15:54:22
15 Spectrometer Frequency	400.15
16 Spectral Width	8802.8
17 Lowest Frequency	-1013.7
18 Nucleus	^1H
19 Acquired Size	32768
20 Spectral Size	65536

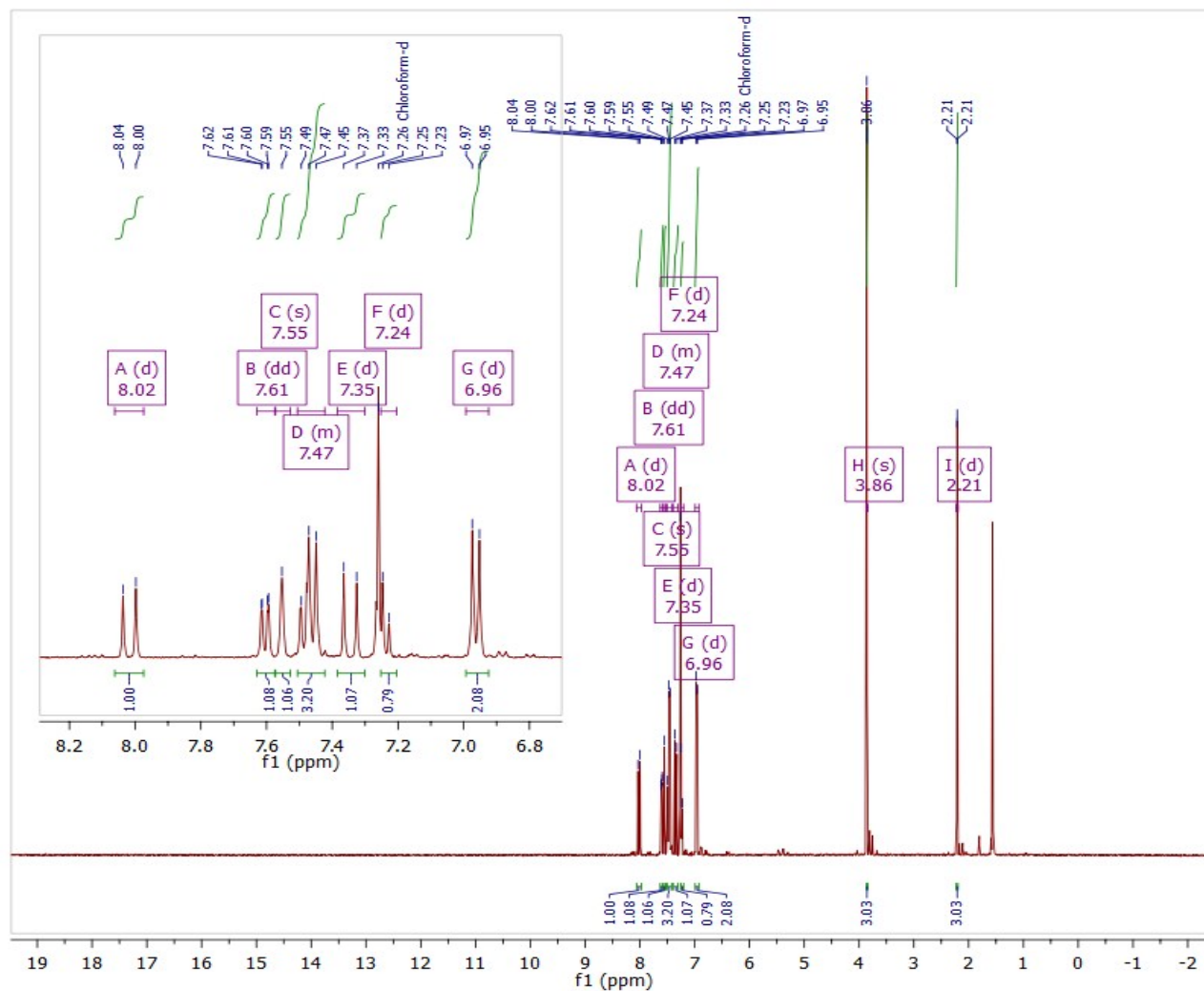


Compound (11)- ^{13}C NMR

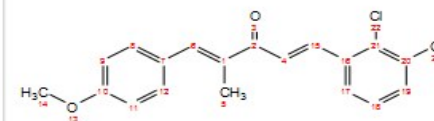


Parameter	Value
1 Title	7A919_A2K2A19_46
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl ₃
6 Temperature	298.8
7 Pulse Sequence	zgpg30
8 Number of Scans	2048
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2013-05-15T16:24:00
14 Modification Date	2013-05-15T16:24:14
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2259.7
18 Nucleus	^{13}C
19 Acquired Size	16384
20 Spectral Size	32768

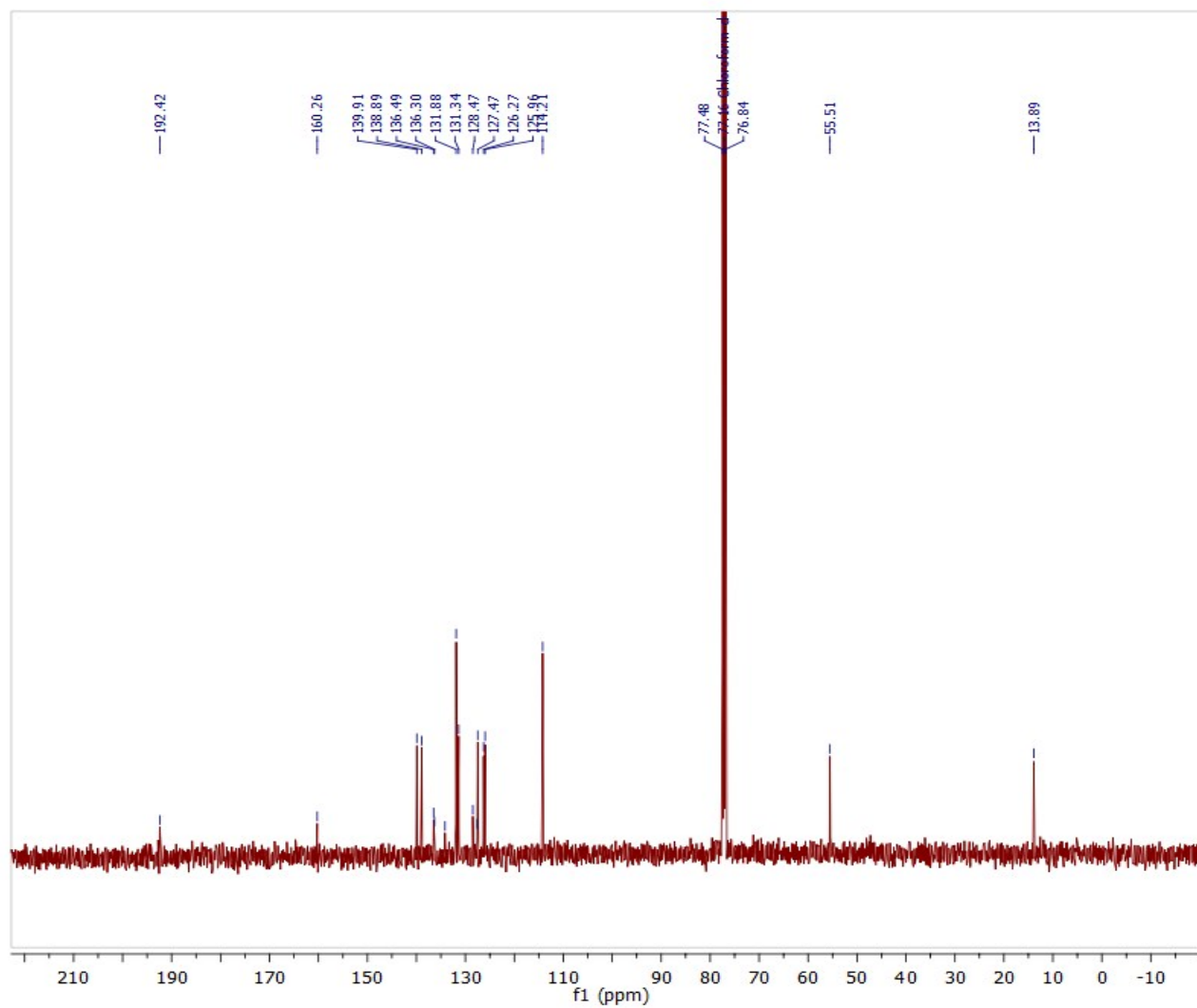
Compound (12) - ¹H NMR



Parameter	Value
1 Title	7A920_A2K2A20_47
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl ₃
6 Temperature	297.9
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	3.7225
13 Acquisition Date	2013-05-20T13:43:00
14 Modification Date	2013-05-20T13:43:38
15 Spectrometer Frequency	400.15
16 Spectral Width	8802.8
17 Lowest Frequency	-1009.7
18 Nucleus	¹ H
19 Acquired Size	32768
20 Spectral Size	65536

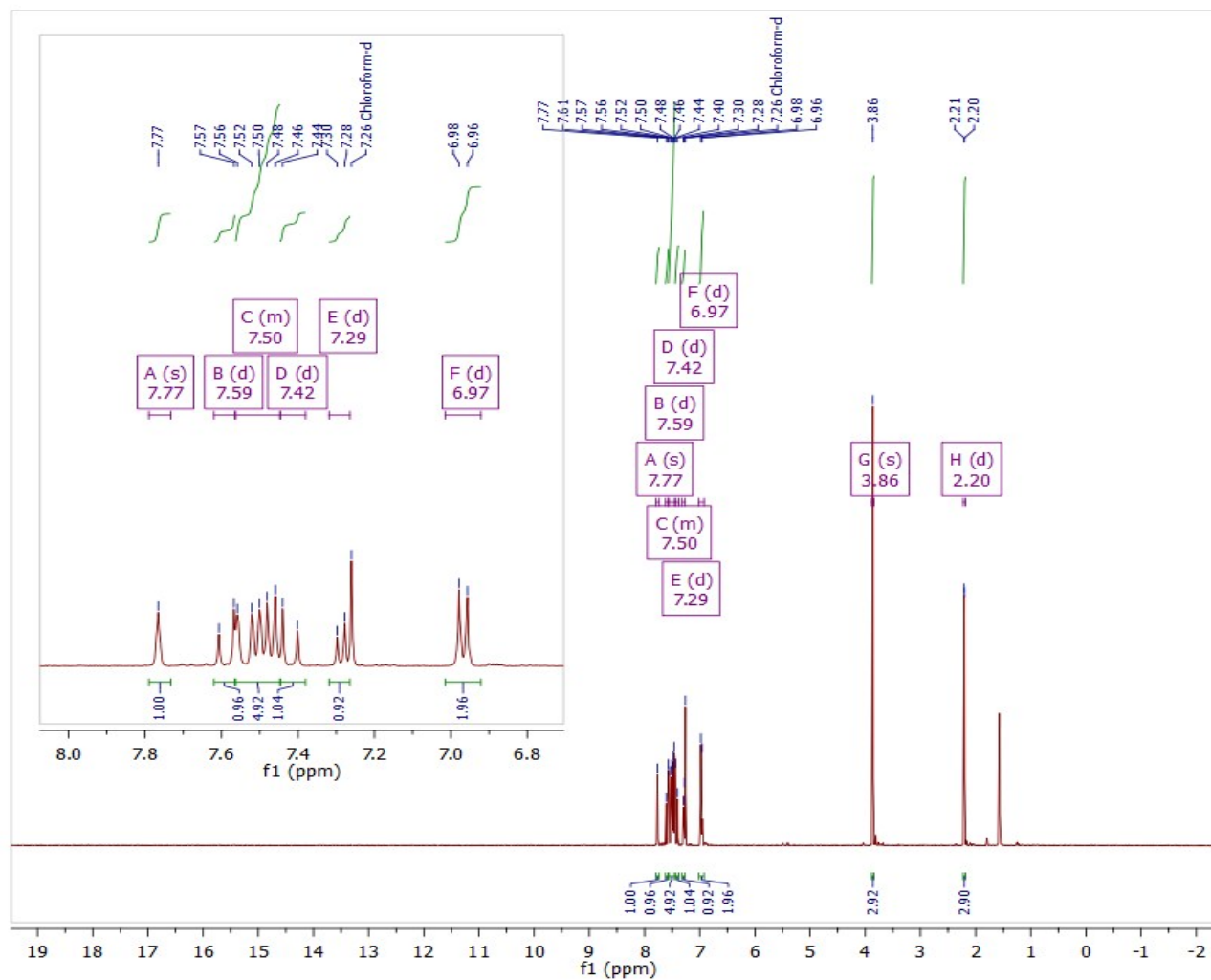


Compound (12)- ¹³C NMR

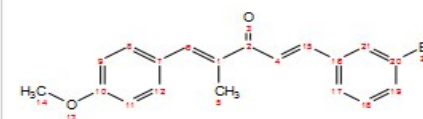


Parameter	Value
1 Title	7A920_A2K2A20_47
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrslu
4 Spectrometer	spect
5 Solvent	CDCl ₃
6 Temperature	298.7
7 Pulse Sequence	zgpg30
8 Number of Scans	1024
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2013-05-20T13:58:00
14 Modification Date	2013-05-20T13:59:02
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2259.3
18 Nucleus	¹³ C
19 Acquired Size	16384
20 Spectral Size	32768

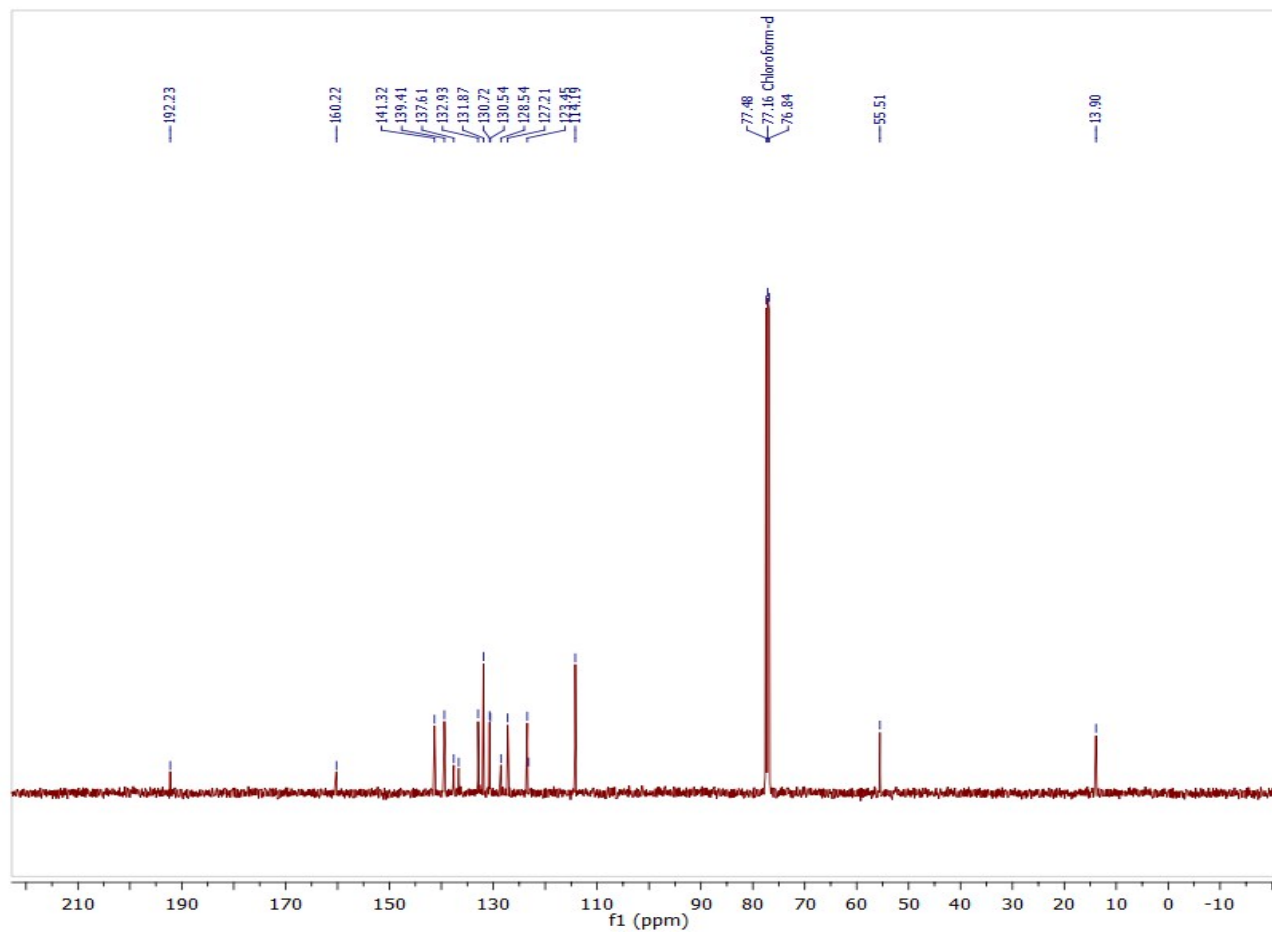
Compound (13) - ^1H NMR



Parameter	Value
1 Title	7C220_A2K2A21_49
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl ₃
6 Temperature	299.9
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	3.7225
13 Acquisition Date	2013-05-24T17:56:00
14 Modification Date	2013-05-24T17:56:04
15 Spectrometer Frequency	400.15
16 Spectral Width	8802.8
17 Lowest Frequency	-1009.3
18 Nucleus	^1H
19 Acquired Size	32768
20 Spectral Size	65536

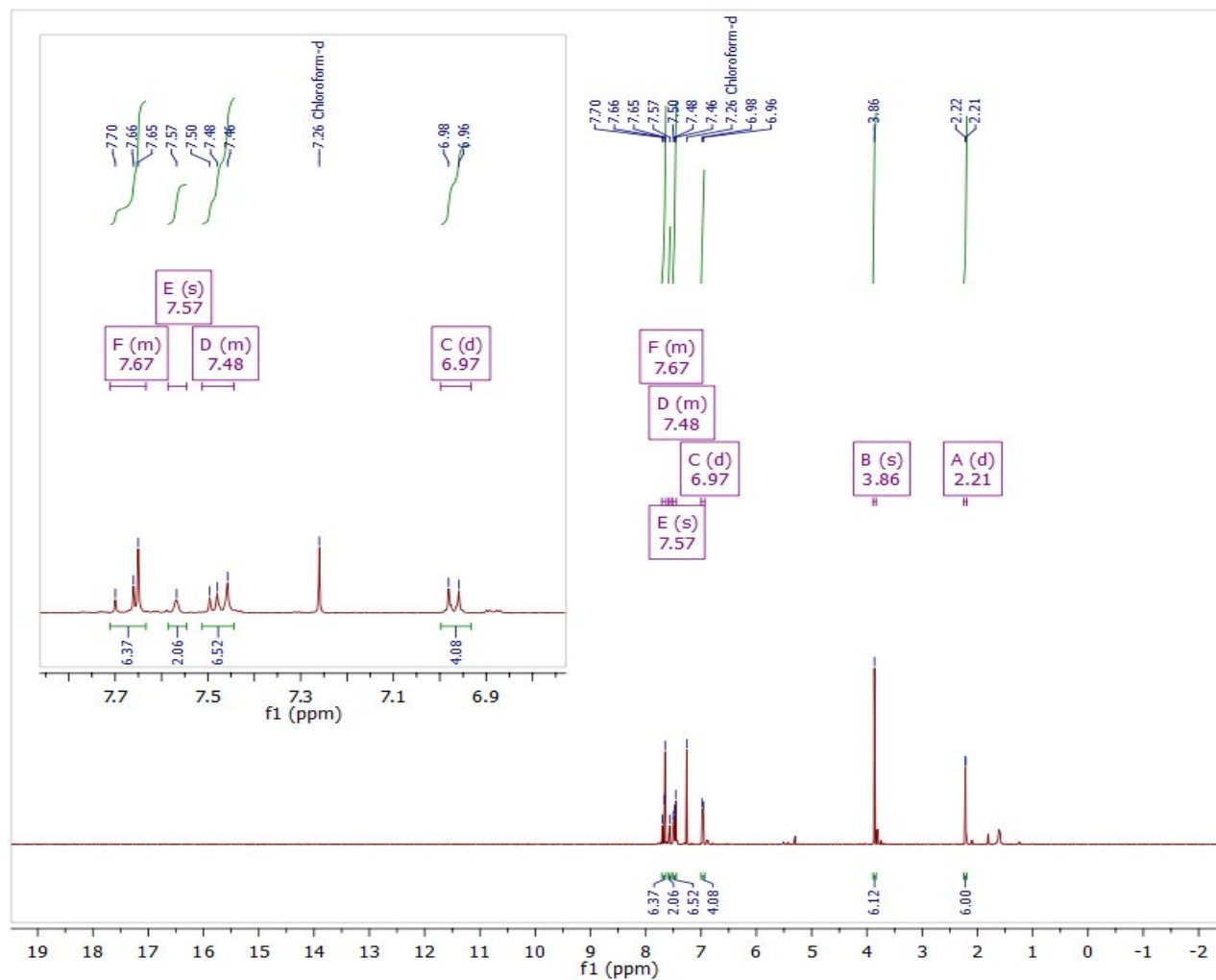


Compound (13)- ^{13}C NMR

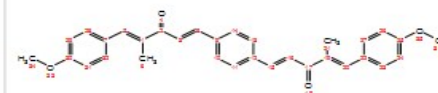


Parameter	Value
1 Title	7C220_A2K2A21_49
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl ₃
6 Temperature	299.8
7 Pulse Sequence	zgpg30
8 Number of Scans	1024
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2013-05-24T18:12:00
14 Modification Date	2013-05-24T18:12:02
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2259.1
18 Nucleus	^{13}C
19 Acquired Size	16384
20 Spectral Size	32768

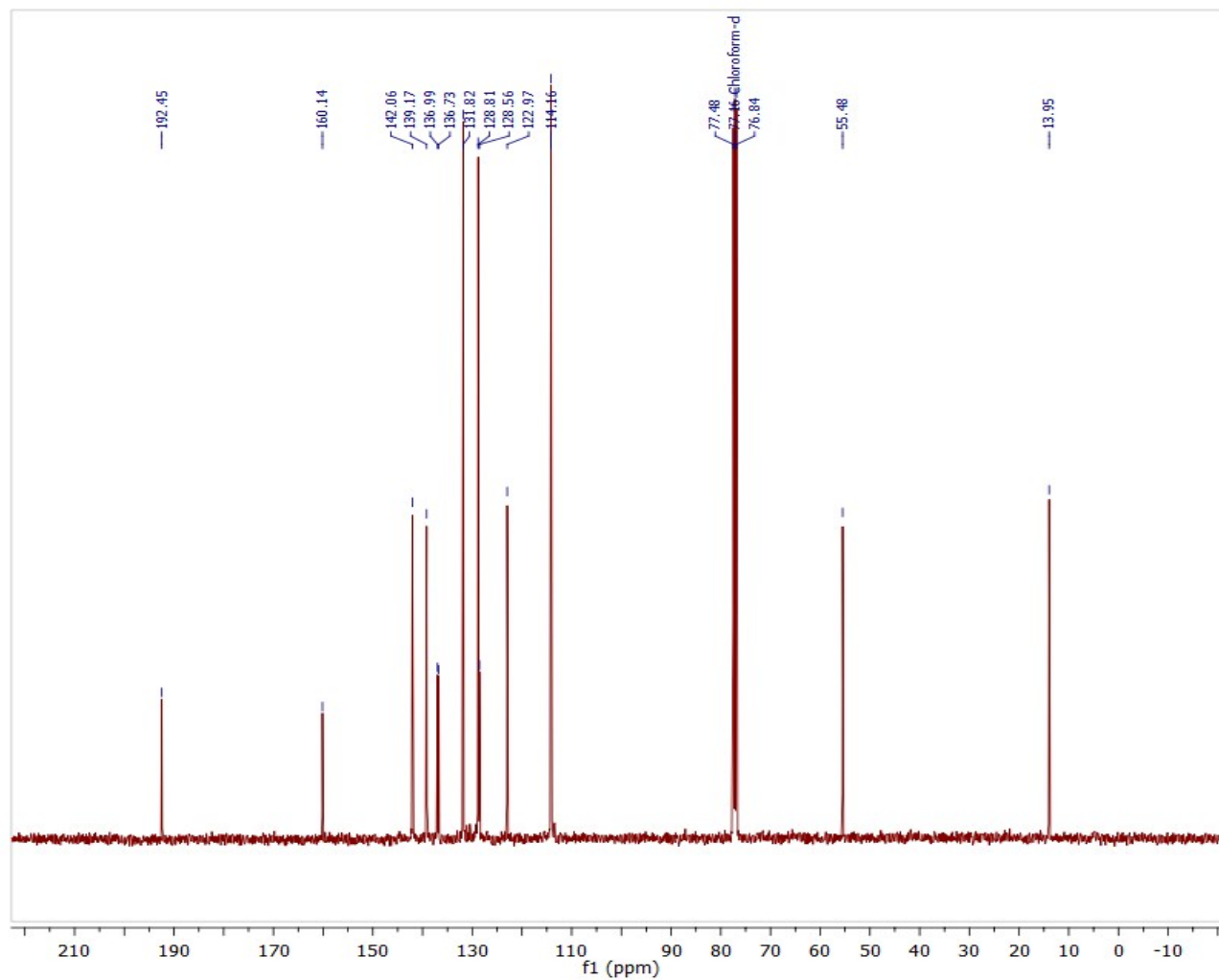
Compound (14) - ^1H NMR



Parameter	Value
1 Title	7A930_Af_11
2 Origin	Bruker BioSpin GmbH
3 Owner	nmsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	299.7
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	2050
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	3.7225
13 Acquisition Date	2013-08-02T18:17:00
14 Modification Date	2013-08-02T21:14:00
15 Spectrometer Frequency	400.15
16 Spectral Width	8802.8
17 Lowest Frequency	-1009.3
18 Nucleus	^1H
19 Acquired Size	32768
20 Spectral Size	65536

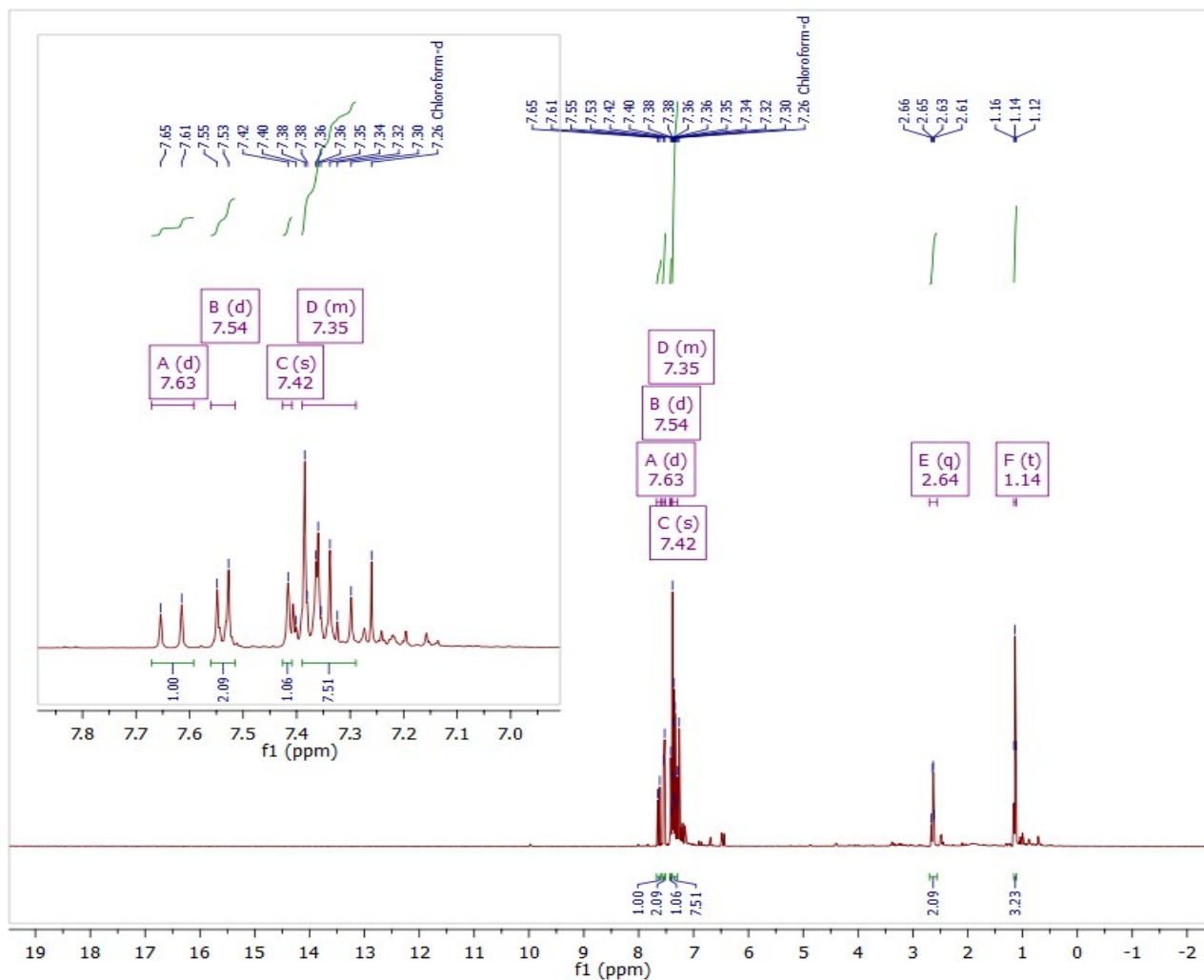


Compound (14)- ^{13}C NMR

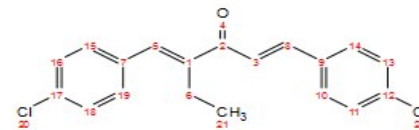


Parameter	Value
1 Title	7A934_Af-60-C
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl ₃
6 Temperature	297.7
7 Pulse Sequence	zgpg30
8 Number of Scans	2048
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2013-08-27T18:03:00
14 Modification Date	2013-08-27T20:59:00
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2262.3
18 Nucleus	^{13}C
19 Acquired Size	16384
20 Spectral Size	32768

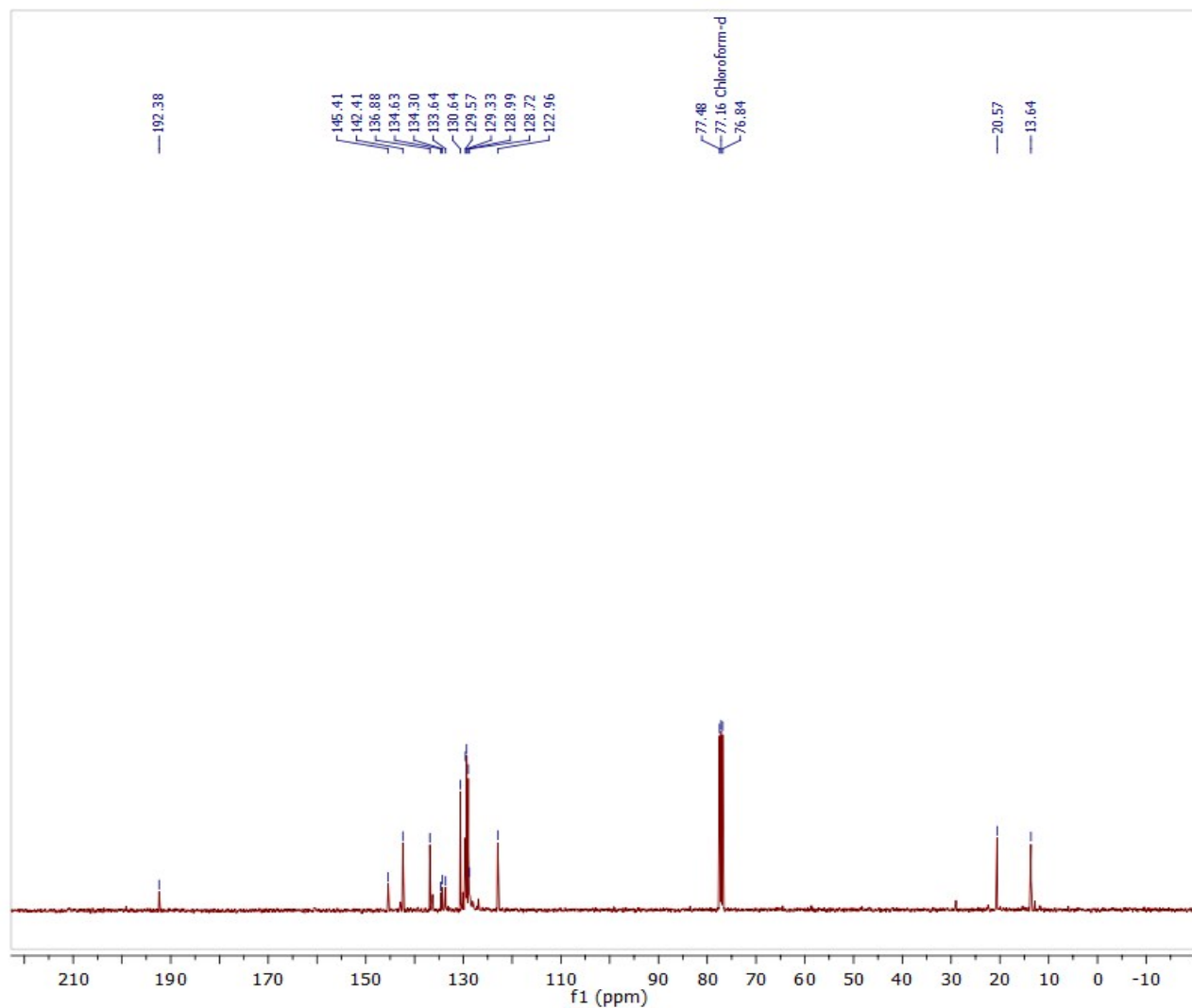
Compound (15) - ^1H NMR



Parameter	Value
1 Title	7A203_A13K3A13
2 Origin	Bruker BioSpin GmbH
3 Owner	nmsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.7
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	3.7225
13 Acquisition Date	2014-01-24T16:31:00
14 Modification Date	2014-01-24T15:31:36
15 Spectrometer Frequency	400.15
16 Spectral Width	8802.8
17 Lowest Frequency	-1009.3
18 Nucleus	^1H
19 Acquired Size	32768
20 Spectral Size	65536

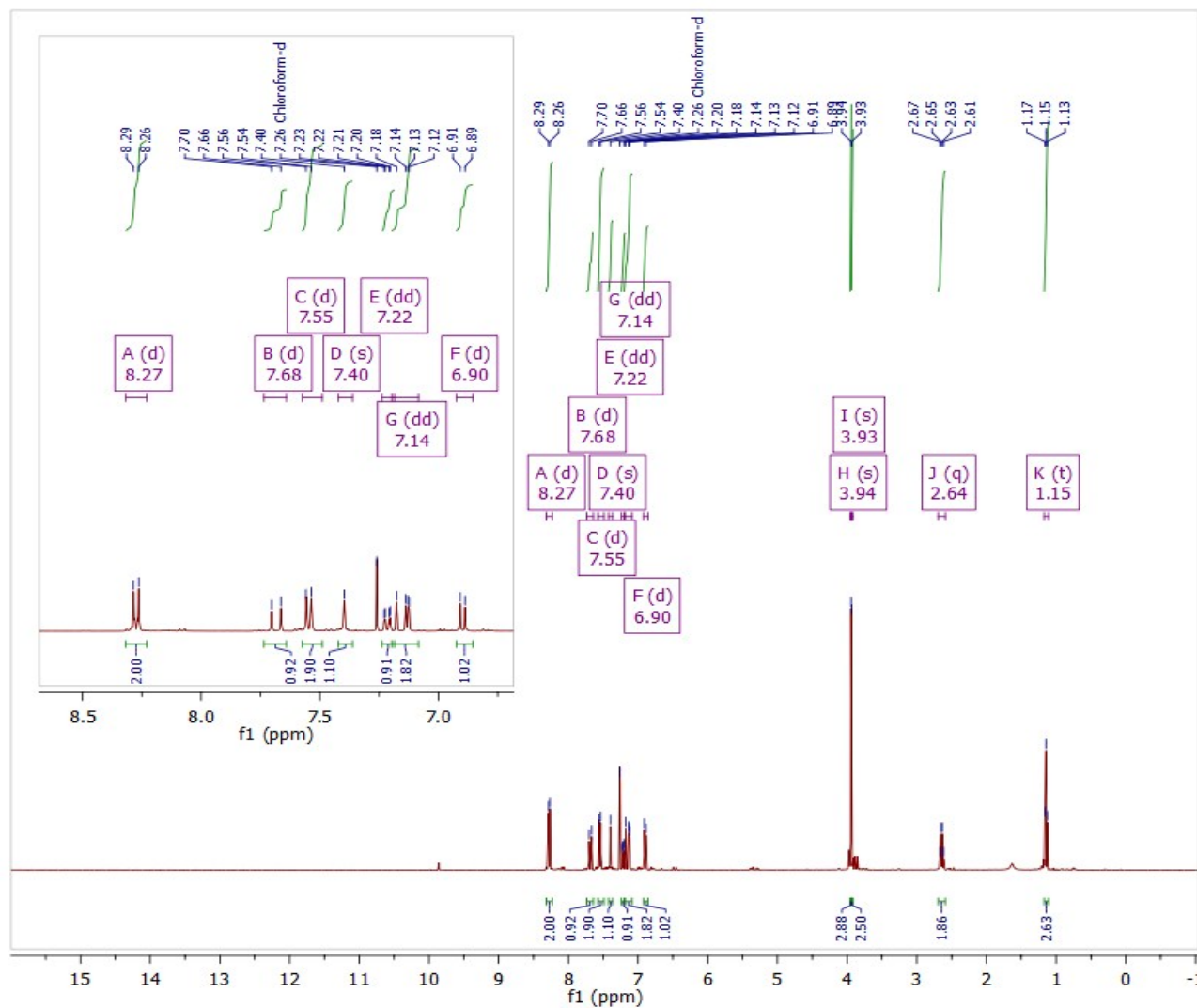


Compound (15)- ^{13}C NMR

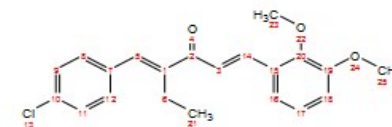


Parameter	Value
1 Title	7A203_A13K3A13
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	298.2
7 Pulse Sequence	zgpg30
8 Number of Scans	1024
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2014-01-24T16:46:00
14 Modification Date	2014-01-24T15:46:58
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2261.3
18 Nucleus	^{13}C
19 Acquired Size	16384
20 Spectral Size	32768

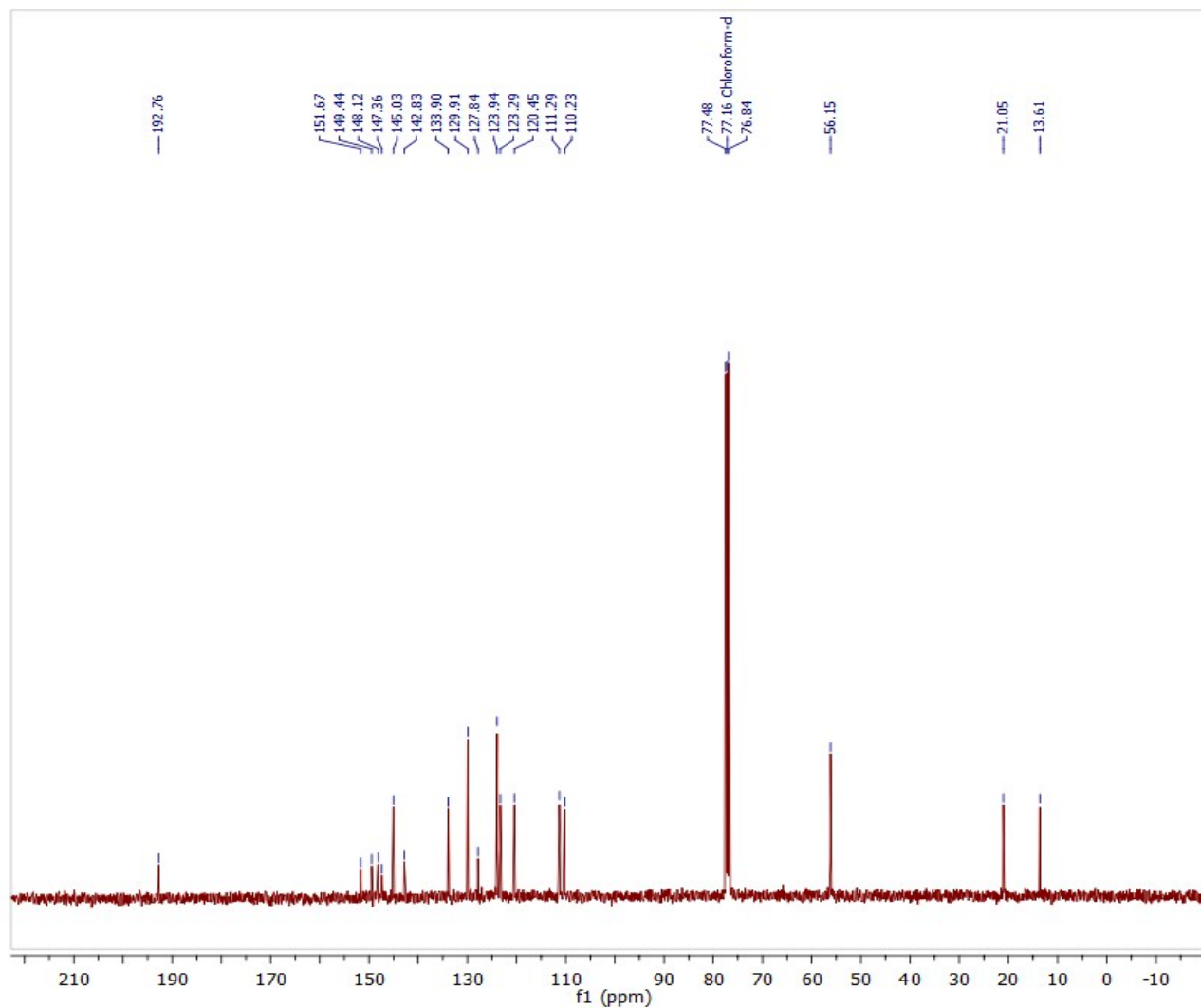
Compound (16) - ¹H NMR



Parameter	Value
1 Title	7A908_A13K3A10_HC
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.8
7 Pulse Sequence	zg30
8 Number of Scans	64
9 Receiver Gain	181
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	4.8060
13 Acquisition Date	2015-02-23T15:54:00
14 Modification Date	2015-02-23T17:32:41
15 Spectrometer Frequency	400.15
16 Spectral Width	6818.2
17 Lowest Frequency	-417.2
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536

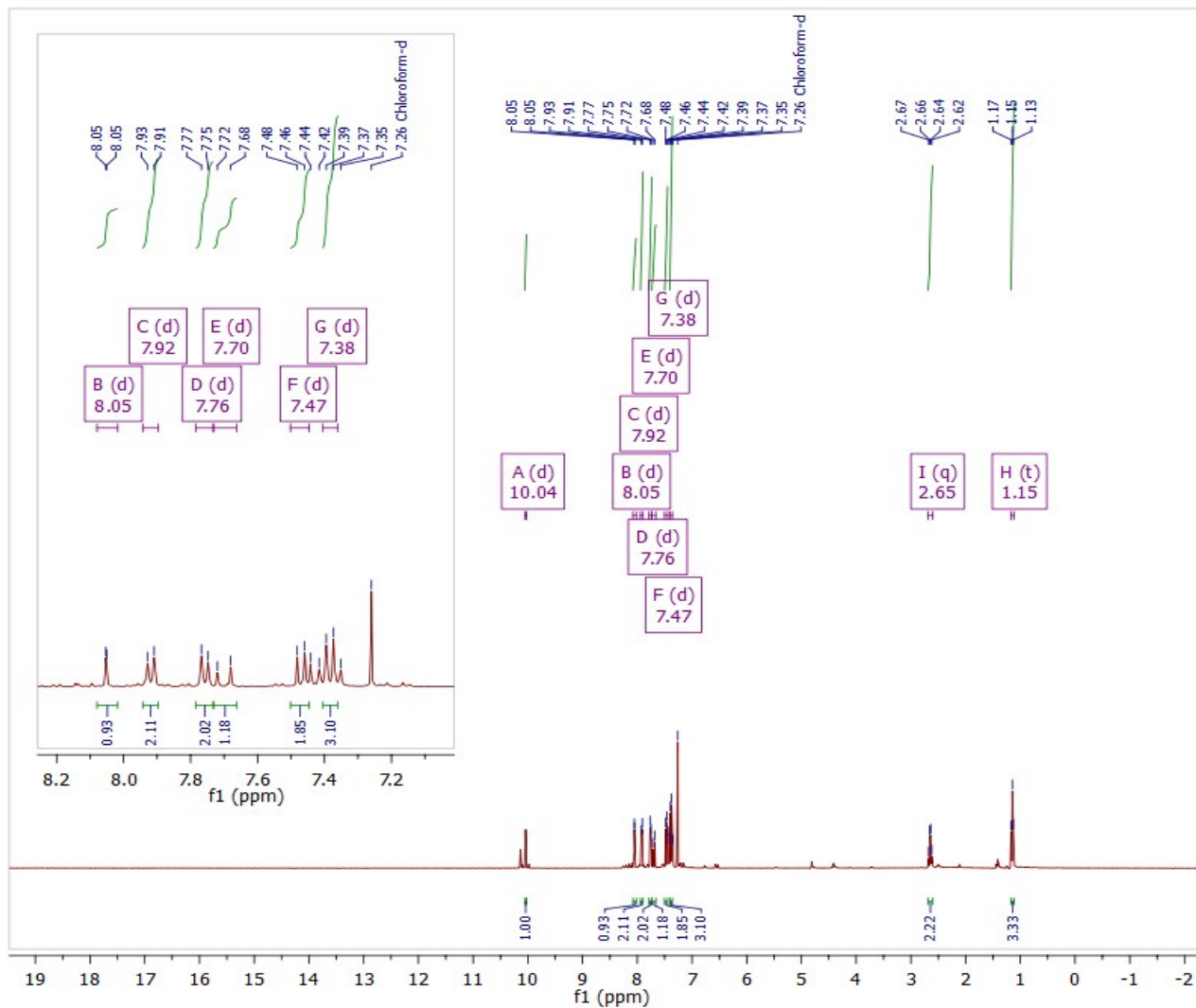


Compound (16)- ^{13}C NMR

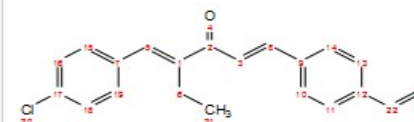


Parameter	Value
1 Title	7A908_A13K3A10_HC
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.8
7 Pulse Sequence	zgpg30
8 Number of Scans	1024
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2015-02-23T16:09:00
14 Modification Date	2015-02-23T17:32:39
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2260.4
18 Nucleus	^{13}C
19 Acquired Size	16384
20 Spectral Size	32768

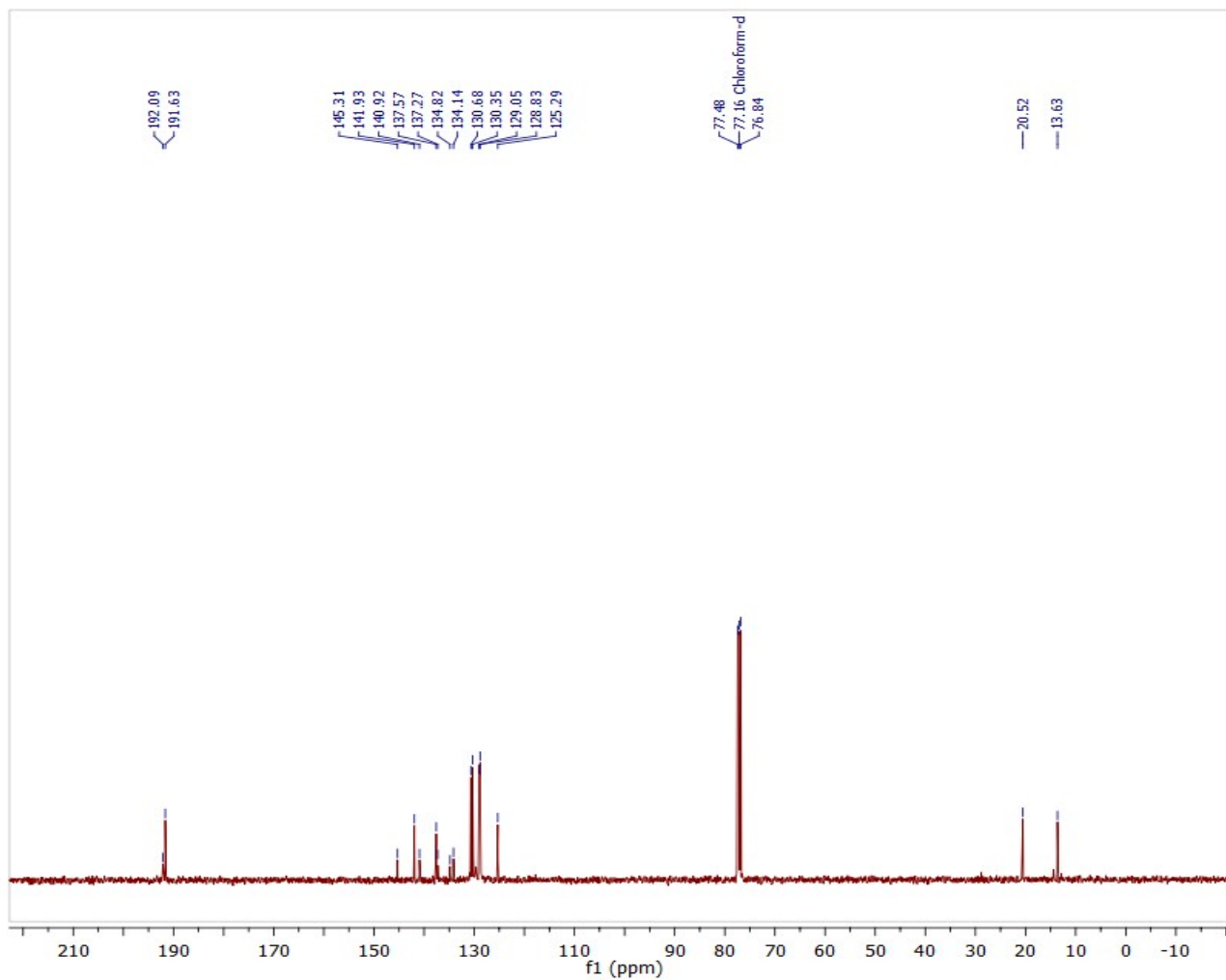
Compound (17) - ¹H NMR



Parameter	Value
1 Title	7A203_A13K3A22
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.6
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	3.7225
13 Acquisition Date	2014-01-24T17:11:00
14 Modification Date	2014-01-24T16:11:08
15 Spectrometer Frequency	400.15
16 Spectral Width	8802.8
17 Lowest Frequency	-1009.3
18 Nucleus	¹ H
19 Acquired Size	32768
20 Spectral Size	65536

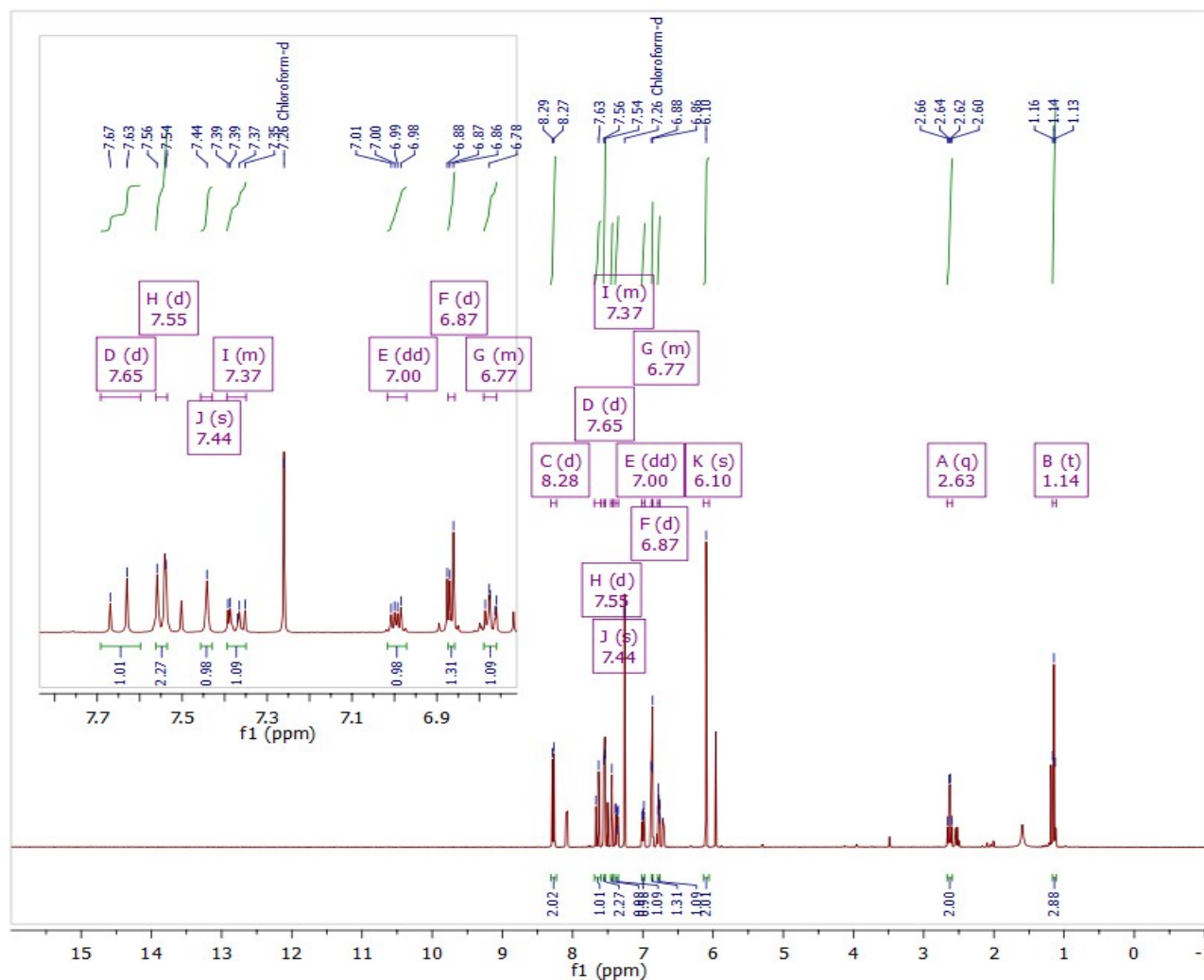


Compound (17)- ^{13}C NMR

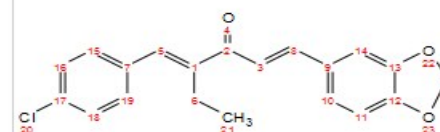


Parameter	Value
1 Title	7A203_A13K3A22
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	298.3
7 Pulse Sequence	zgpg30
8 Number of Scans	1024
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2014-01-24T17:26:00
14 Modification Date	2014-01-24T16:26:46
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2260.6
18 Nucleus	^{13}C
19 Acquired Size	16384
20 Spectral Size	32768

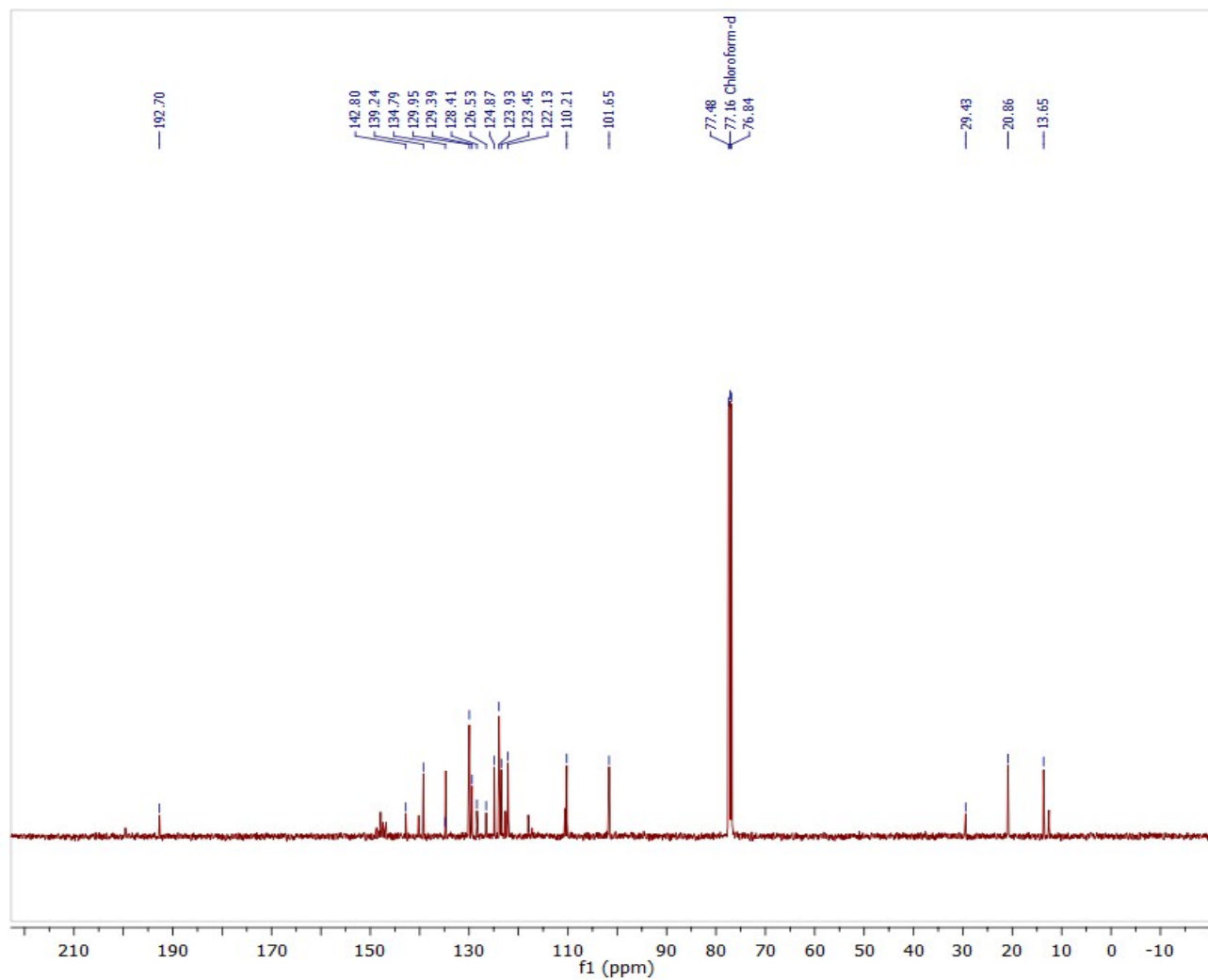
Compound (18) - ¹H NMR



Parameter	Value
1 Title	7A942_A11K3A5_21
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.3
7 Pulse Sequence	zg30
8 Number of Scans	64
9 Receiver Gain	114
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	4.8060
13 Acquisition Date	2013-10-28T04:43:00
14 Modification Date	2013-10-28T05:37:00
15 Spectrometer Frequency	400.15
16 Spectral Width	6818.2
17 Lowest Frequency	-417.2
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536

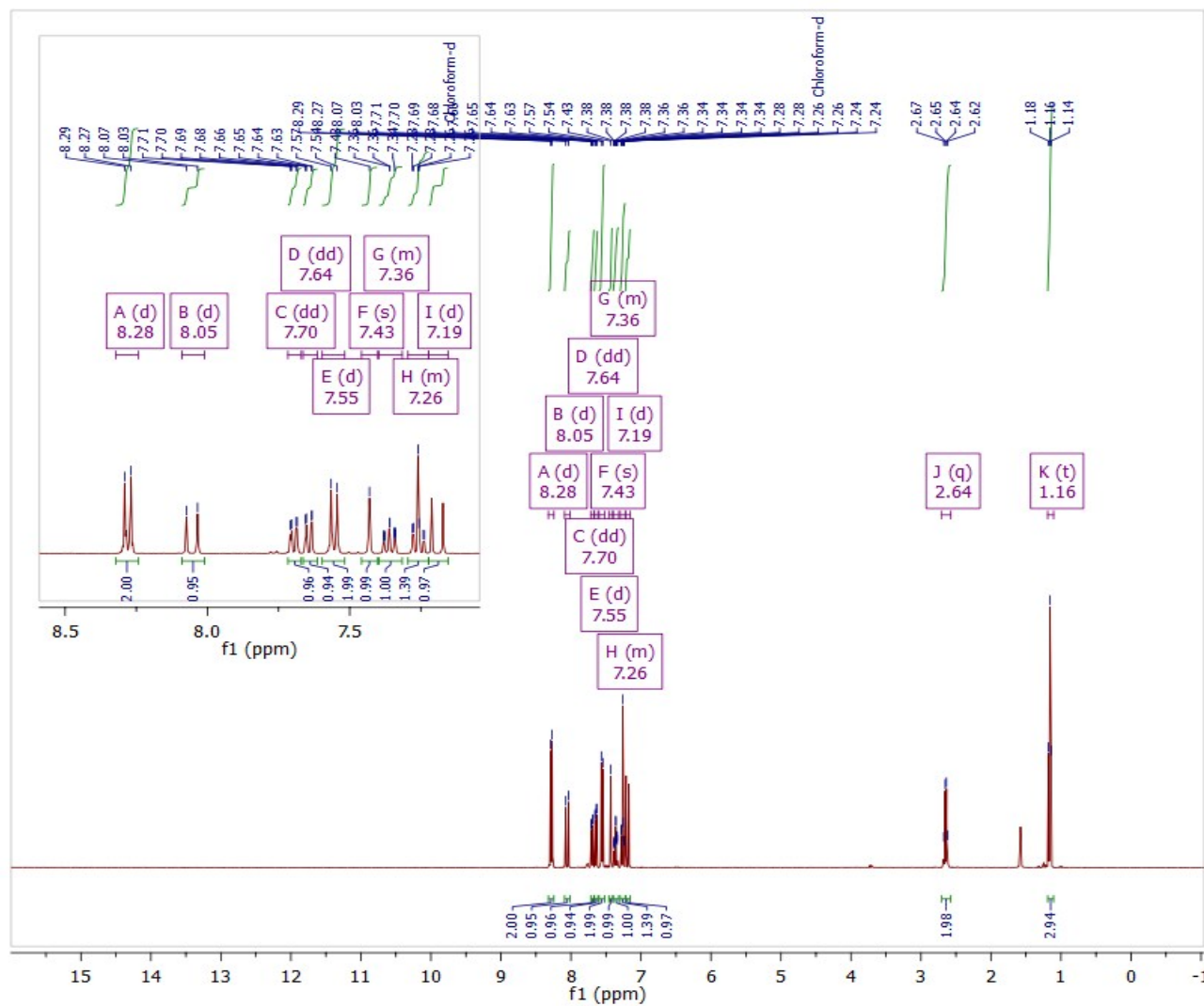


Compound (18)- ¹³C NMR

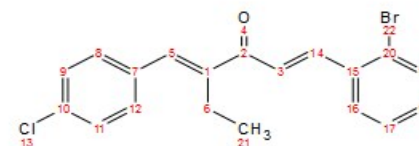


Parameter	Value
1 Title	7A942_A11K3A5_21
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	298.0
7 Pulse Sequence	zgpg30
8 Number of Scans	2048
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2013-10-28T05:13:00
14 Modification Date	2013-10-28T06:06:00
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2260.2
18 Nucleus	13C
19 Acquired Size	16384
20 Spectral Size	32768

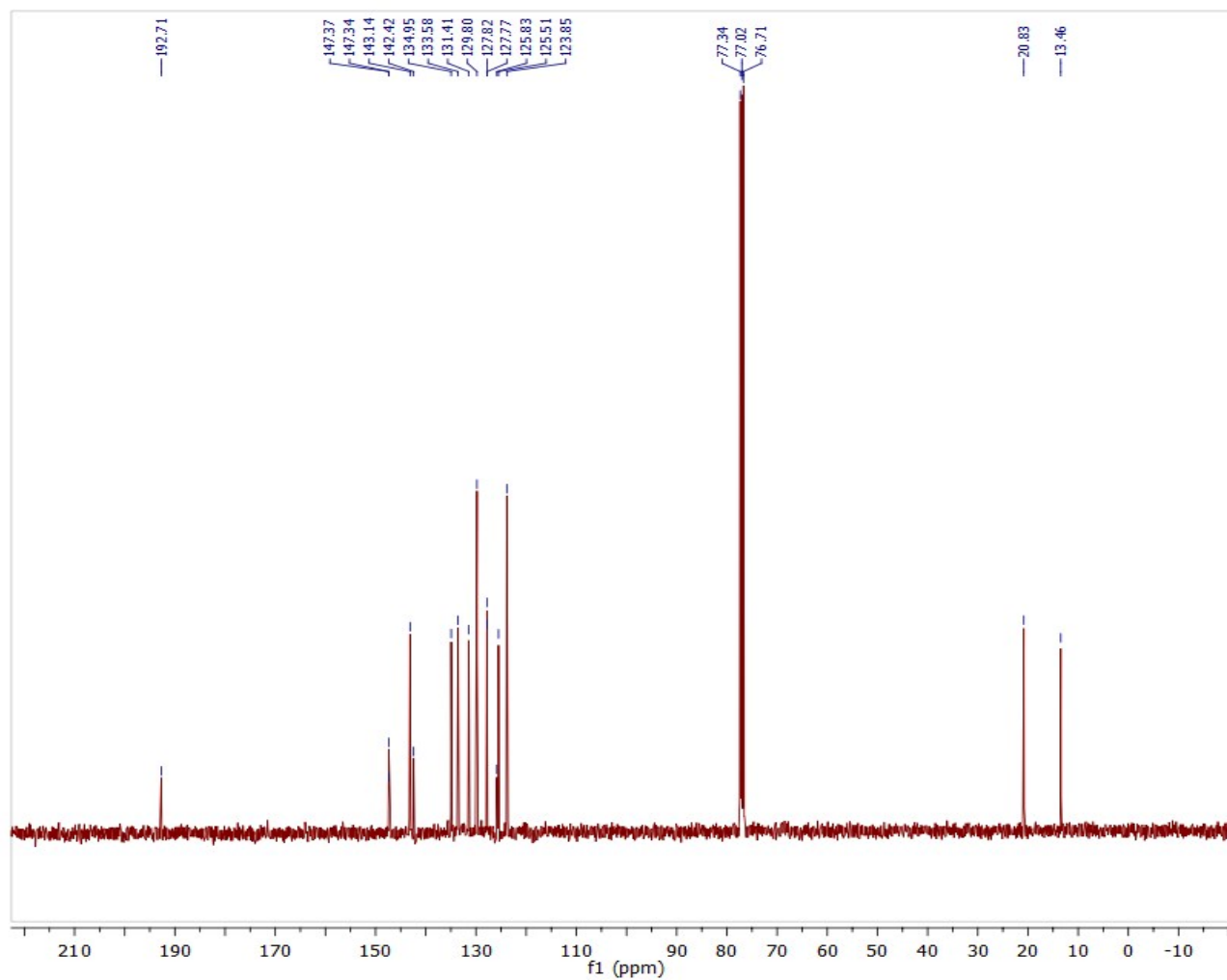
Compound (19) - ^1H NMR



Parameter	Value
1 Title	7A908_A13K3A23_HC
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.8
7 Pulse Sequence	zg30
8 Number of Scans	64
9 Receiver Gain	181
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	4.8060
13 Acquisition Date	2015-02-23T16:19:00
14 Modification Date	2015-02-23T17:32:38
15 Spectrometer Frequency	400.15
16 Spectral Width	6818.2
17 Lowest Frequency	-417.2
18 Nucleus	^1H
19 Acquired Size	32768
20 Spectral Size	65536

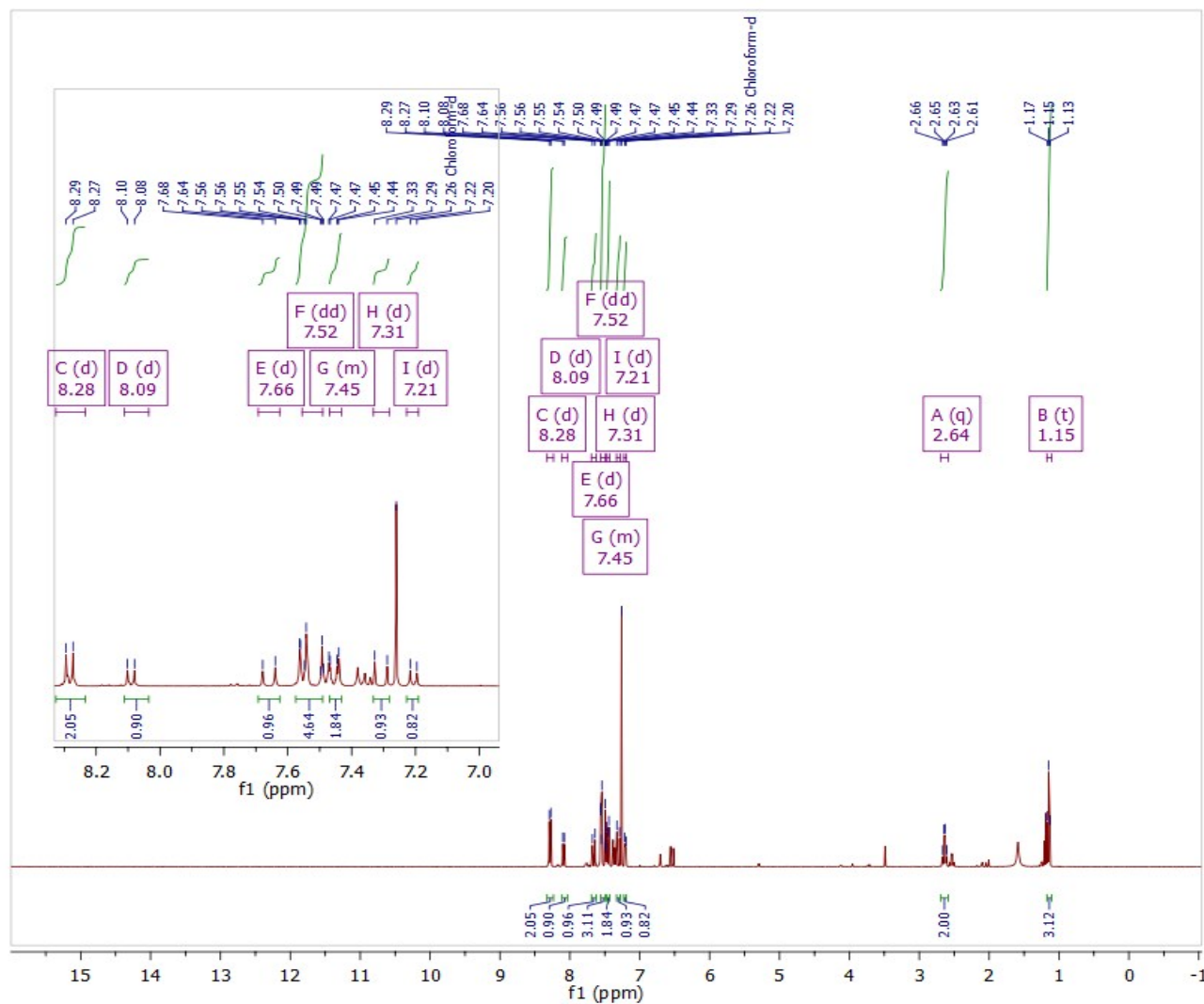


Compound (19)- ¹³C NMR

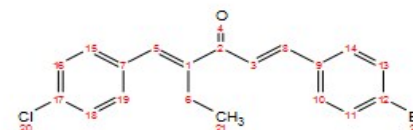


Parameter	Value
1 Title	7A908_A13K3A23_HC
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl ₃
6 Temperature	297.8
7 Pulse Sequence	zgpg30
8 Number of Scans	1024
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2015-02-23T16:35:00
14 Modification Date	2015-02-23T17:32:36
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2274.2
18 Nucleus	¹³ C
19 Acquired Size	16384
20 Spectral Size	32768

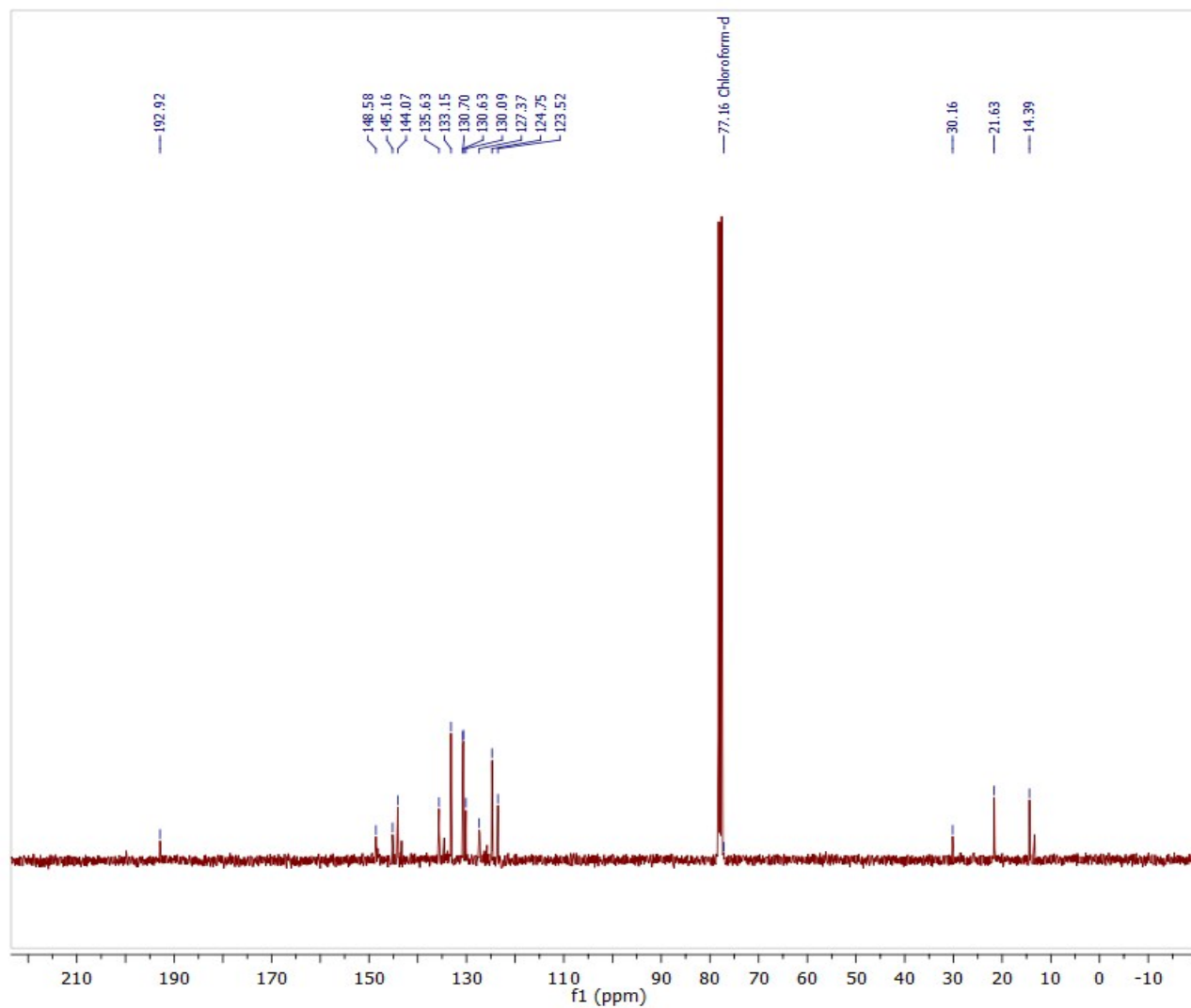
Compound (20) - ¹H NMR



Parameter	Value
1 Title	7A942_A11K3A14_22
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.4
7 Pulse Sequence	zg30
8 Number of Scans	64
9 Receiver Gain	203
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	4.8060
13 Acquisition Date	2013-10-28T03:25:00
14 Modification Date	2013-10-28T04:18:00
15 Spectrometer Frequency	400.15
16 Spectral Width	6818.2
17 Lowest Frequency	-417.2
18 Nucleus	¹ H
19 Acquired Size	32768
20 Spectral Size	65536

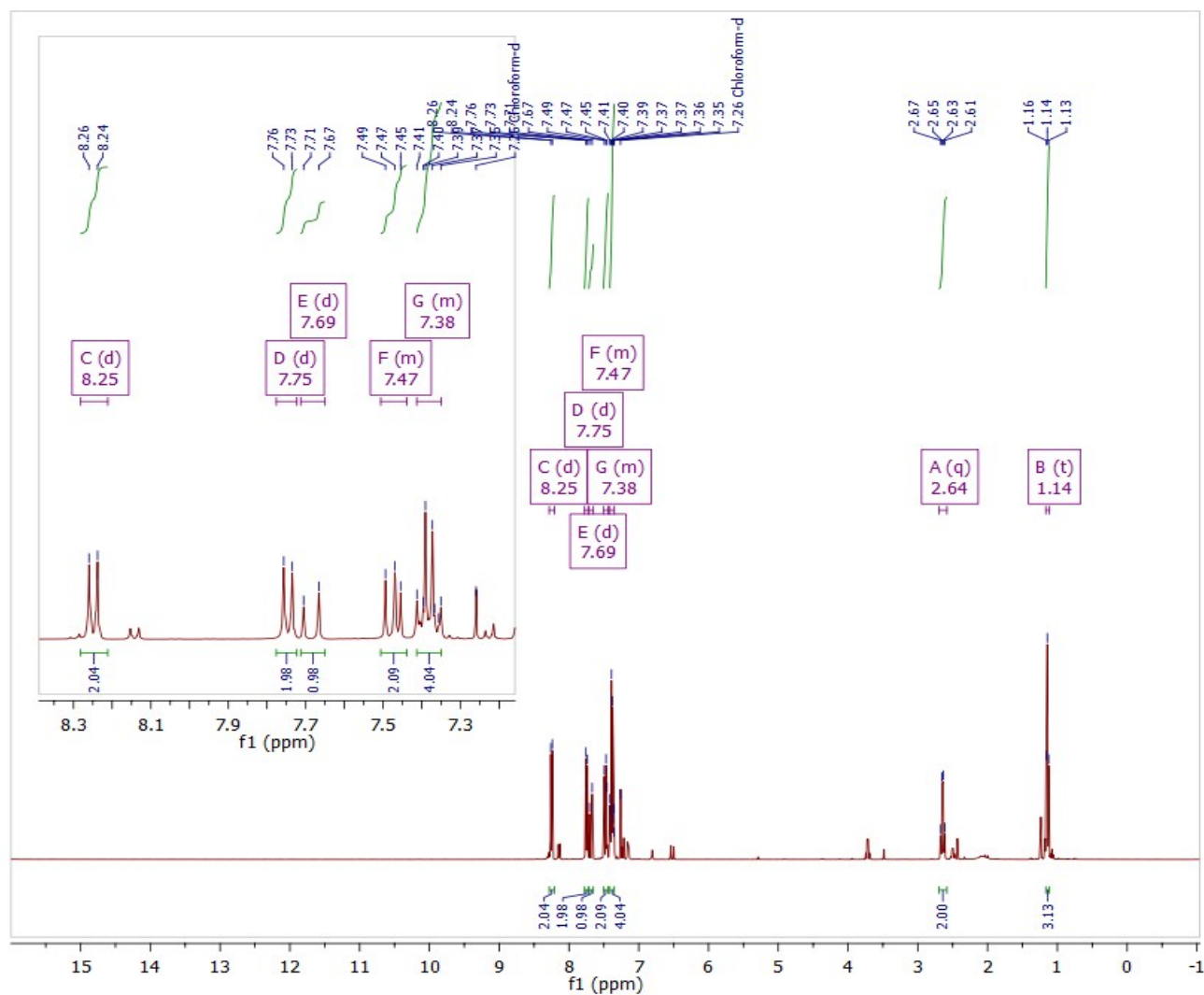


Compound (20)- ¹³C NMR

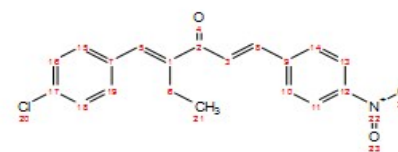


Parameter	Value
1 Title	7A942_A11K3A14_22
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsl
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	298.2
7 Pulse Sequence	zgpg30
8 Number of Scans	2048
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2013-10-28T03:54:00
14 Modification Date	2013-10-28T04:48:00
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2184.0
18 Nucleus	13C
19 Acquired Size	16384
20 Spectral Size	32768

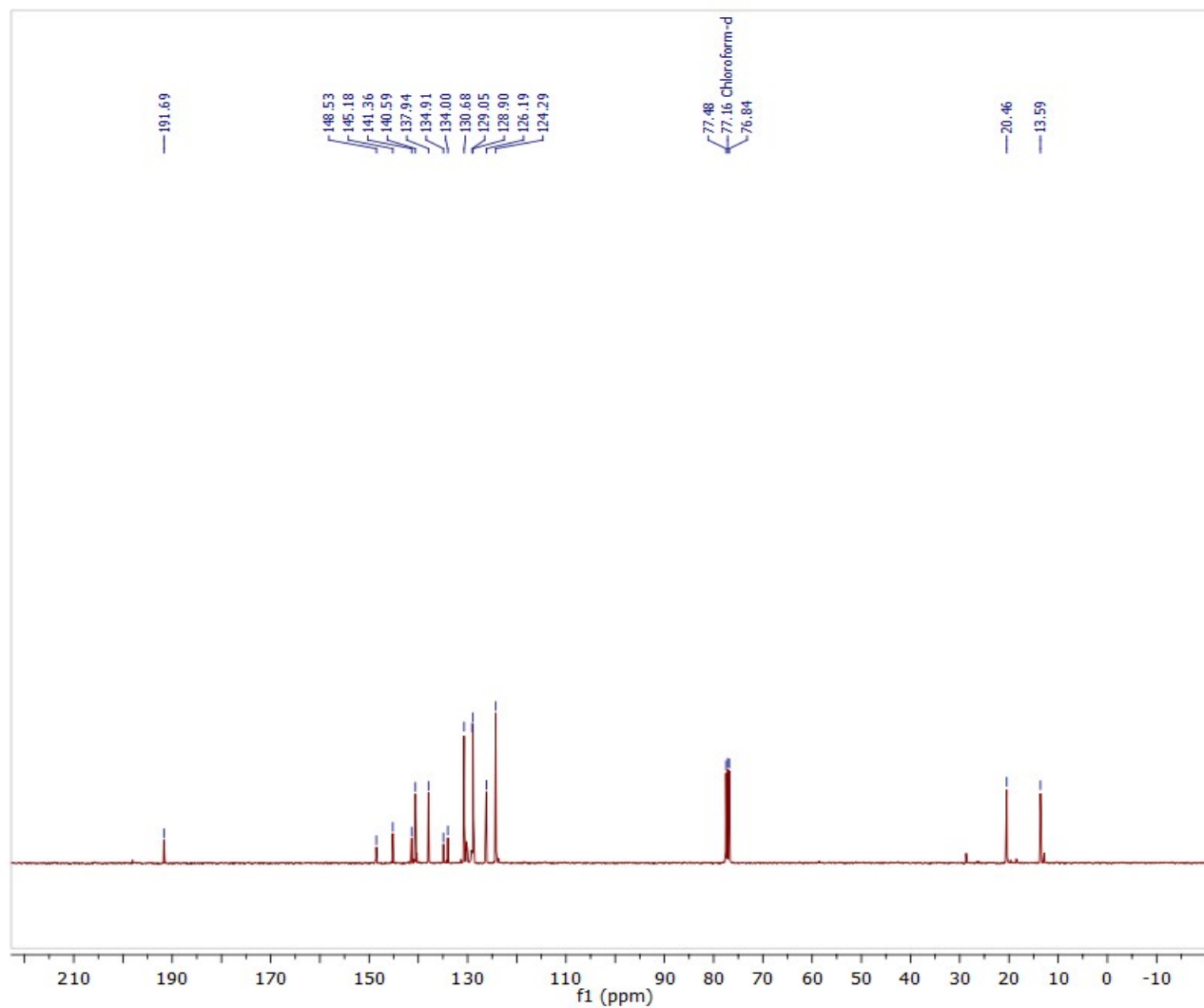
Compound (21) - ¹H NMR



Parameter	Value
1 Title	7A942_A13K3A11_18
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	297.2
7 Pulse Sequence	zg30
8 Number of Scans	64
9 Receiver Gain	57
10 Relaxation Delay	1.0000
11 Pulse Width	8.7600
12 Acquisition Time	4.8060
13 Acquisition Date	2013-10-28T02:44:00
14 Modification Date	2013-10-28T03:38:00
15 Spectrometer Frequency	400.15
16 Spectral Width	6818.2
17 Lowest Frequency	-417.2
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



Compound (21)- ^{13}C NMR

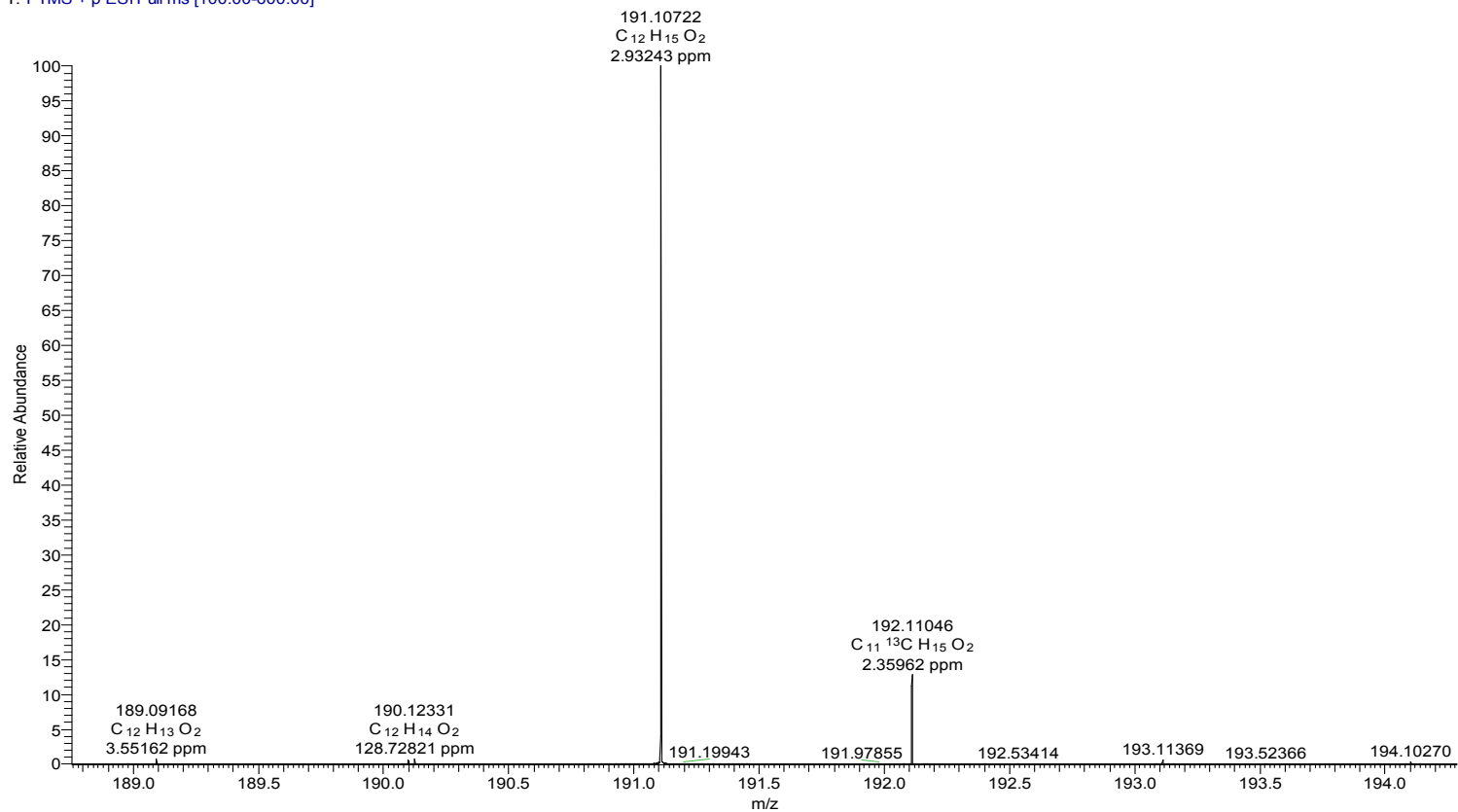


Parameter	Value
1 Title	7A942_A13K3A11_18
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Spectrometer	spect
5 Solvent	CDCl3
6 Temperature	298.2
7 Pulse Sequence	zgpg30
8 Number of Scans	2048
9 Receiver Gain	2050
10 Relaxation Delay	0.1100
11 Pulse Width	8.7500
12 Acquisition Time	0.6641
13 Acquisition Date	2013-10-28T03:14:00
14 Modification Date	2013-10-28T04:08:00
15 Spectrometer Frequency	100.62
16 Spectral Width	24671.1
17 Lowest Frequency	-2263.1
18 Nucleus	^{13}C
19 Acquired Size	16384
20 Spectral Size	32768

Mass Spectrum- HRMS ESI (+)(-)

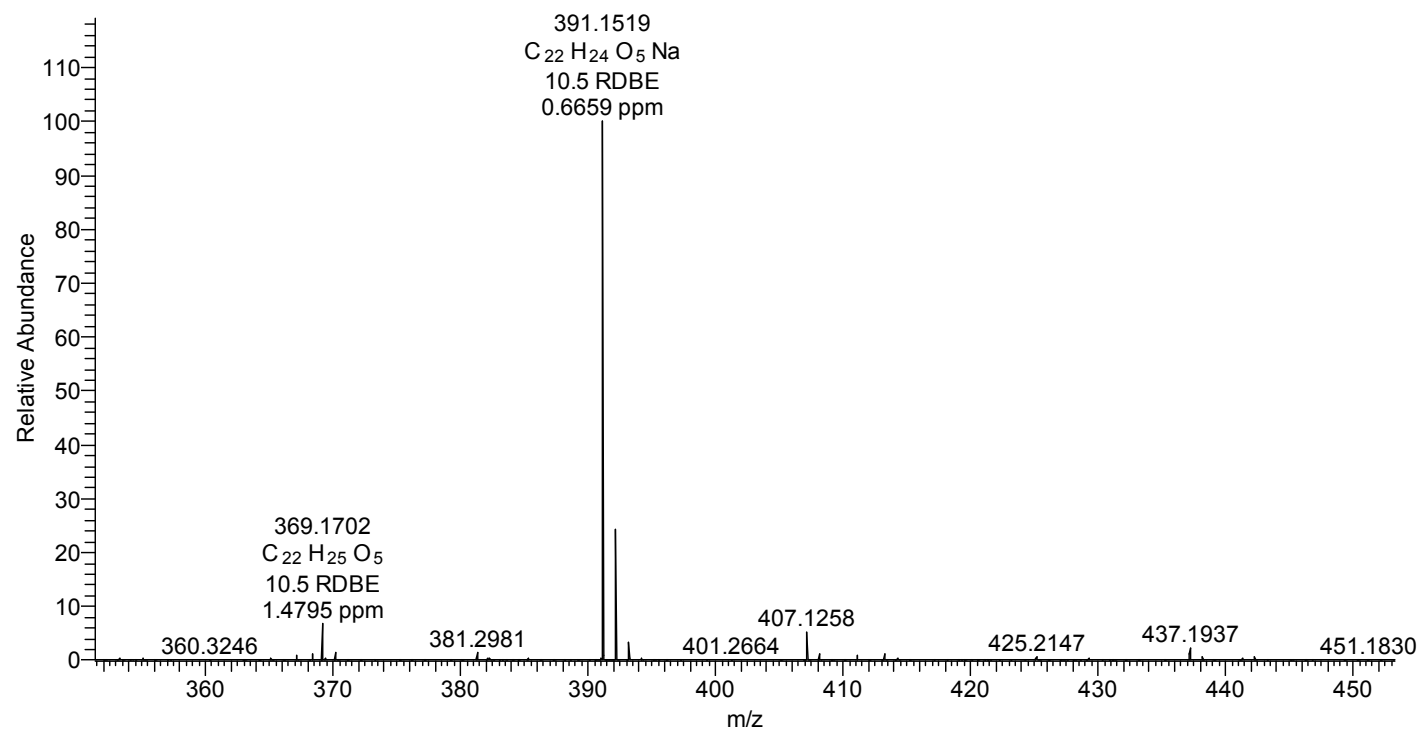
Compound_1

a2k2 #5-8 RT: 0.16-0.29 AV: 4 NL: 2.42E7
T: FTMS + p ESI Full ms [100.00-600.00]



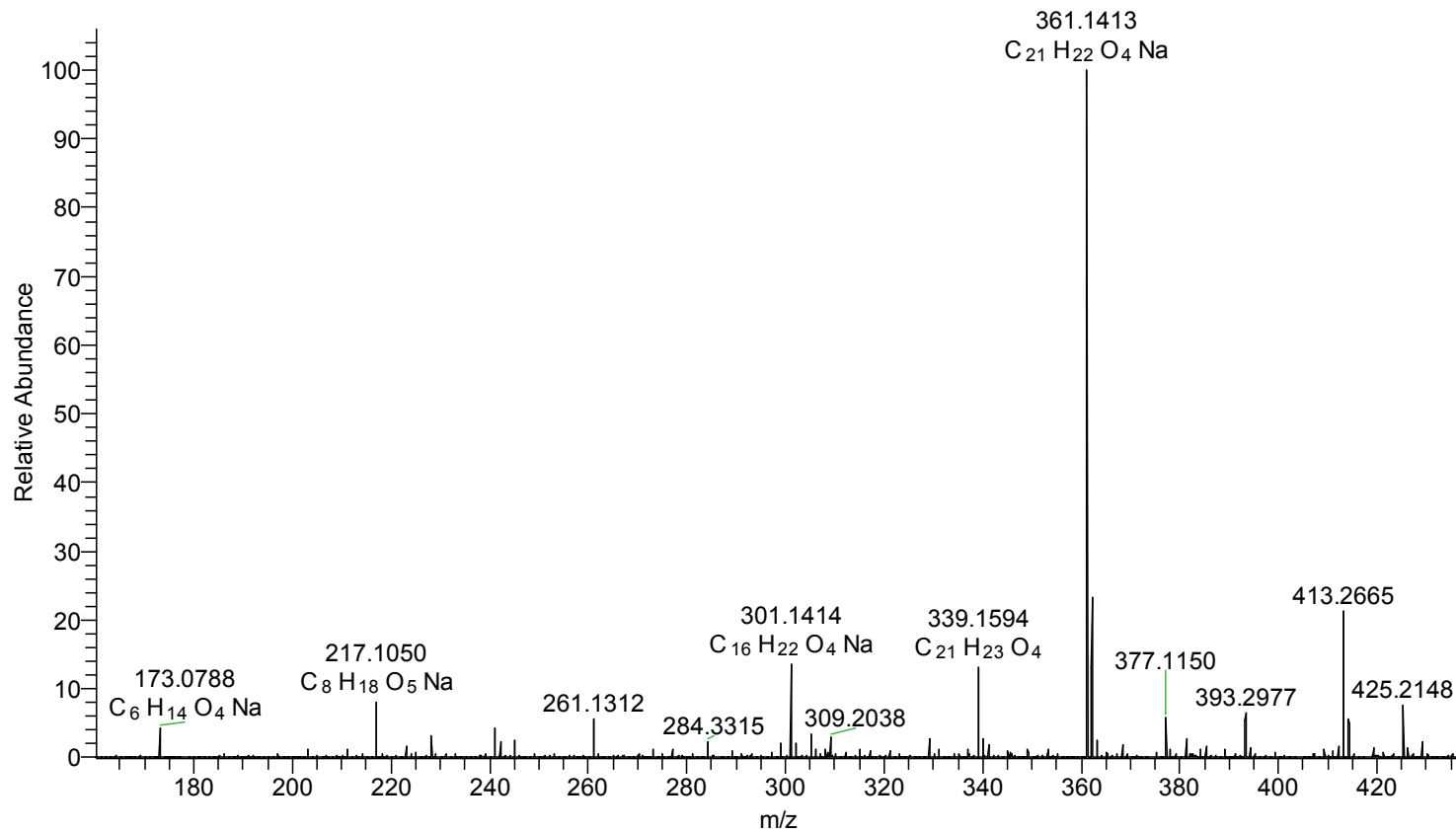
Compound_3

A2K2A6_151022094719 #1 RT: 896.31 AV: 1 NL: 1.93E8
T: FTMS + p ESI Full ms [150.00-2000.00]



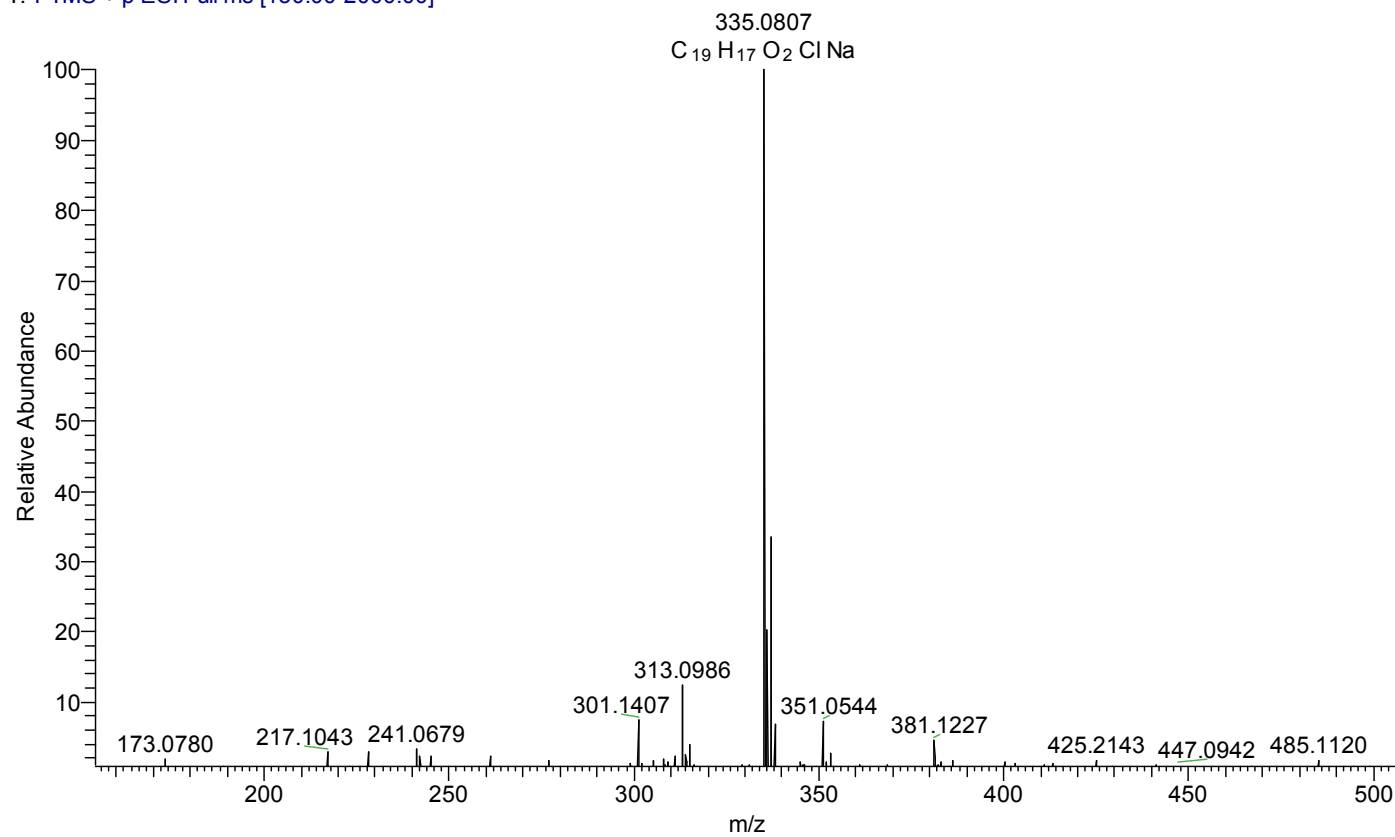
Compound_4

A2K2A9_151022094719 #1 RT: 900.34 AV: 1 NL: 4.54E7
T: FTMS + p ESI Full ms [150.00-2000.00]



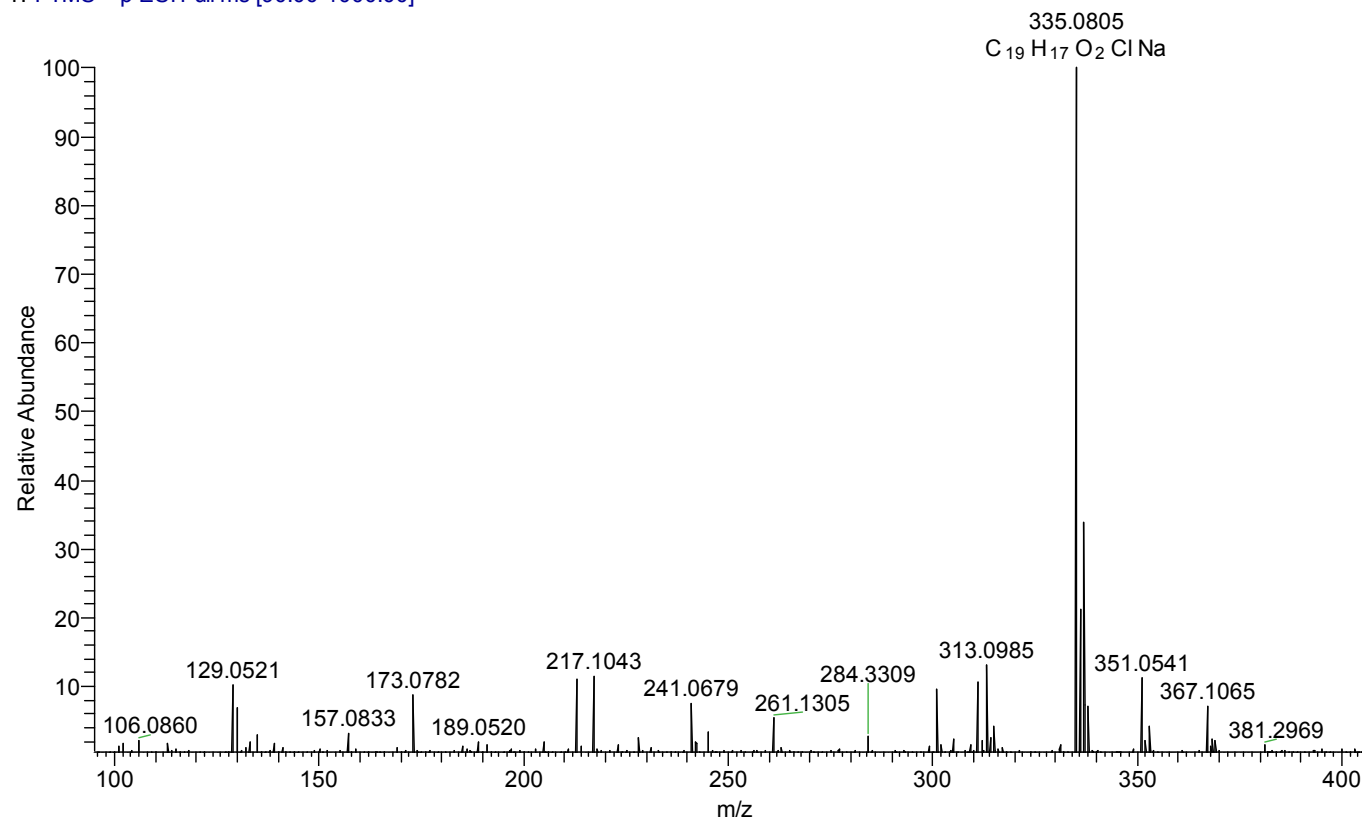
Compound_5

A2K2A12_151022095538 #1 RT: 904.55 AV: 1 NL: 5.21E7
T: FTMS + p ESI Full ms [150.00-2000.00]



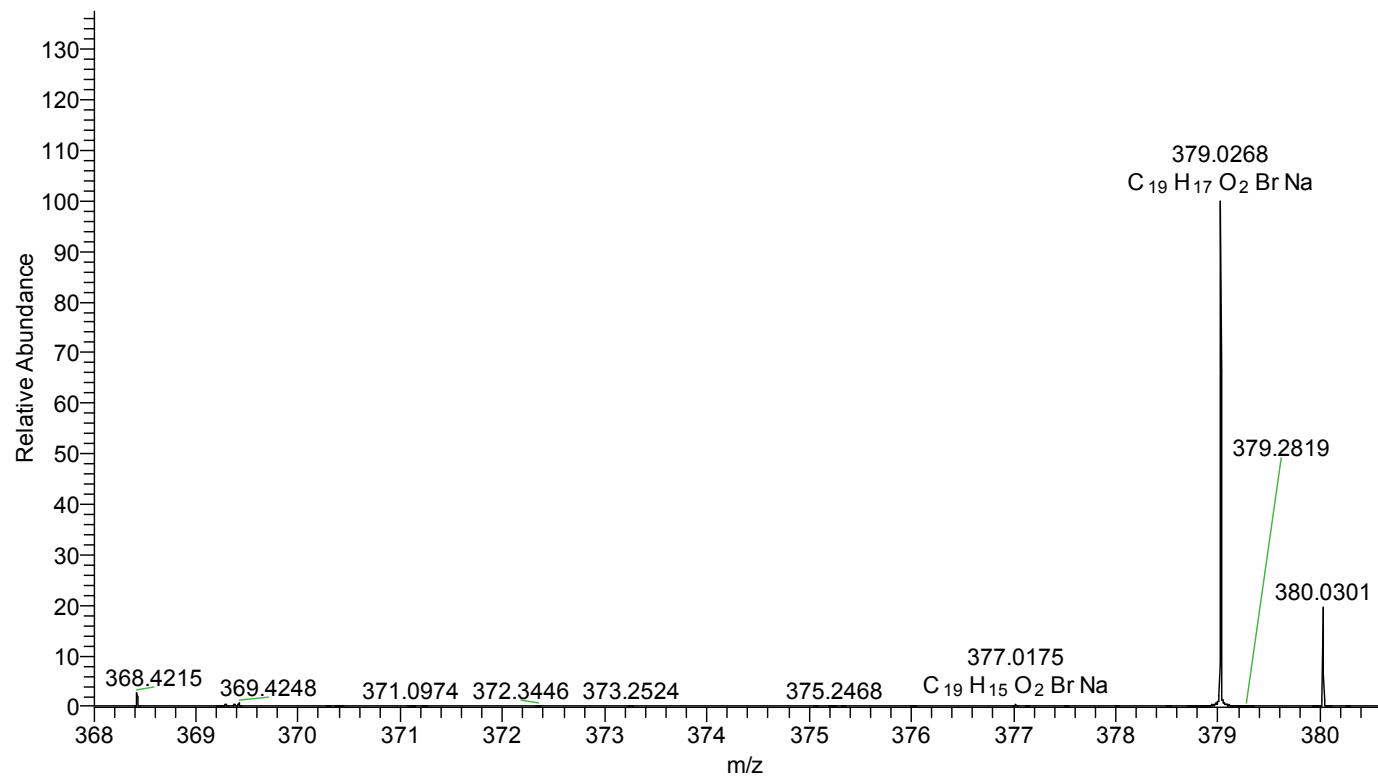
Compound_6

A2K2A13_151022095538 #1 RT: 911.37 AV: 1 NL: 2.28E8
T: FTMS +p ESI Full ms [90.00-1000.00]



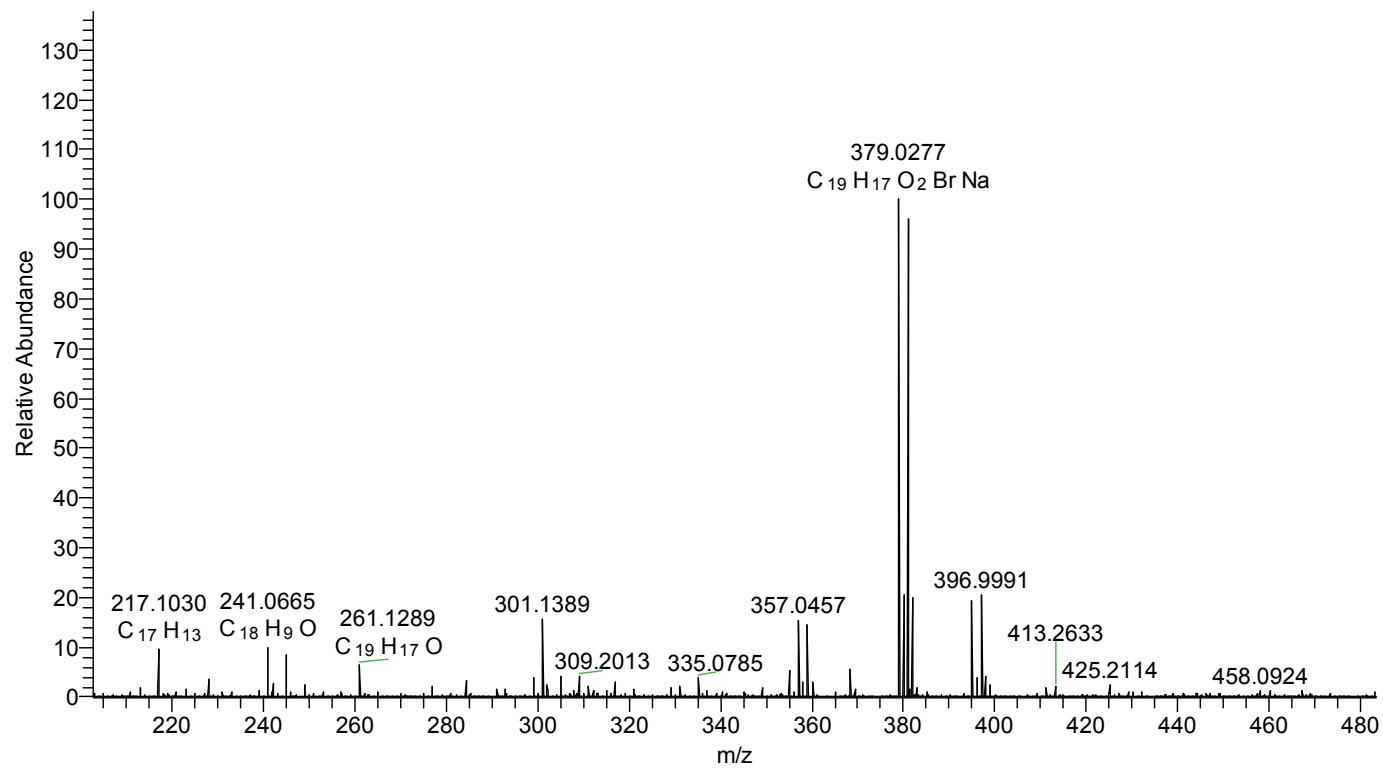
Compound_7

A2K2A14_151022095538 #1 RT: 918.73 AV: 1 NL: 2.73E7
T: FTMS +p ESI Full ms [200.00-1000.00]



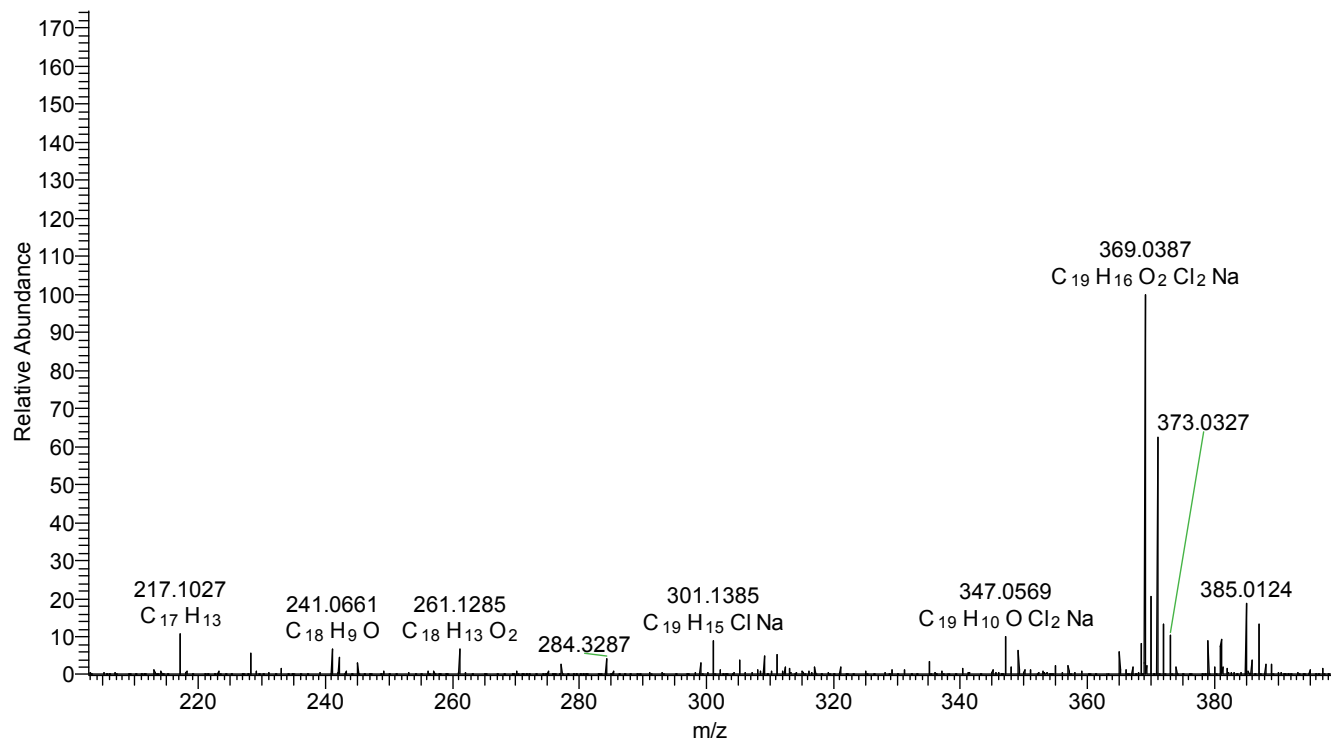
Compound_8

A2K2A15_151022095538 #1 RT: 920.22 AV: 1 NL: 6.97E7
T: FTMS + p ESI Full ms [200.00-1000.00]



Compound_9

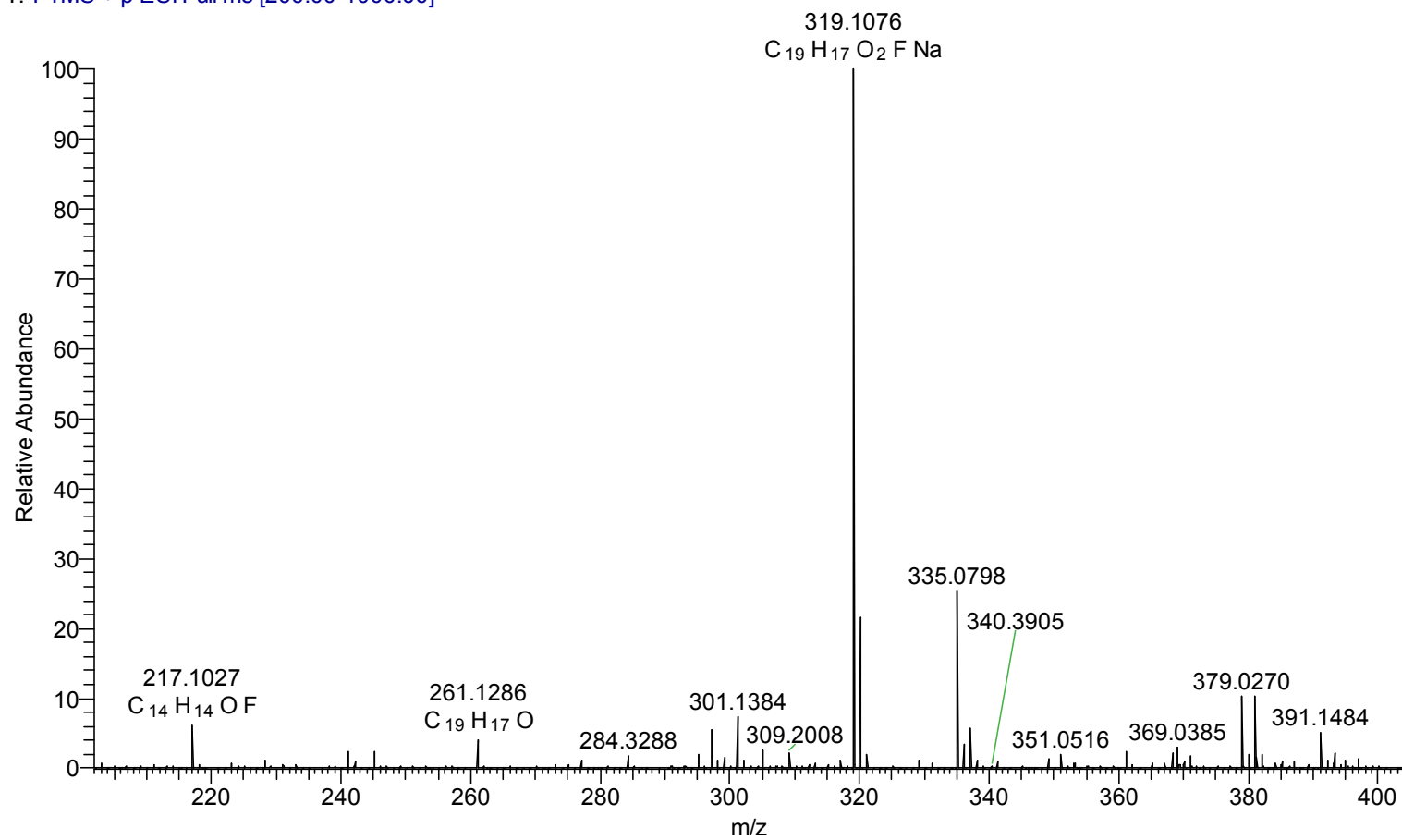
A2K2A16_151022095538 #1 RT: 923.80 AV: 1 NL: 1.01E8
T: FTMS + p ESI Full ms [200.00-1000.00]



Compound_10

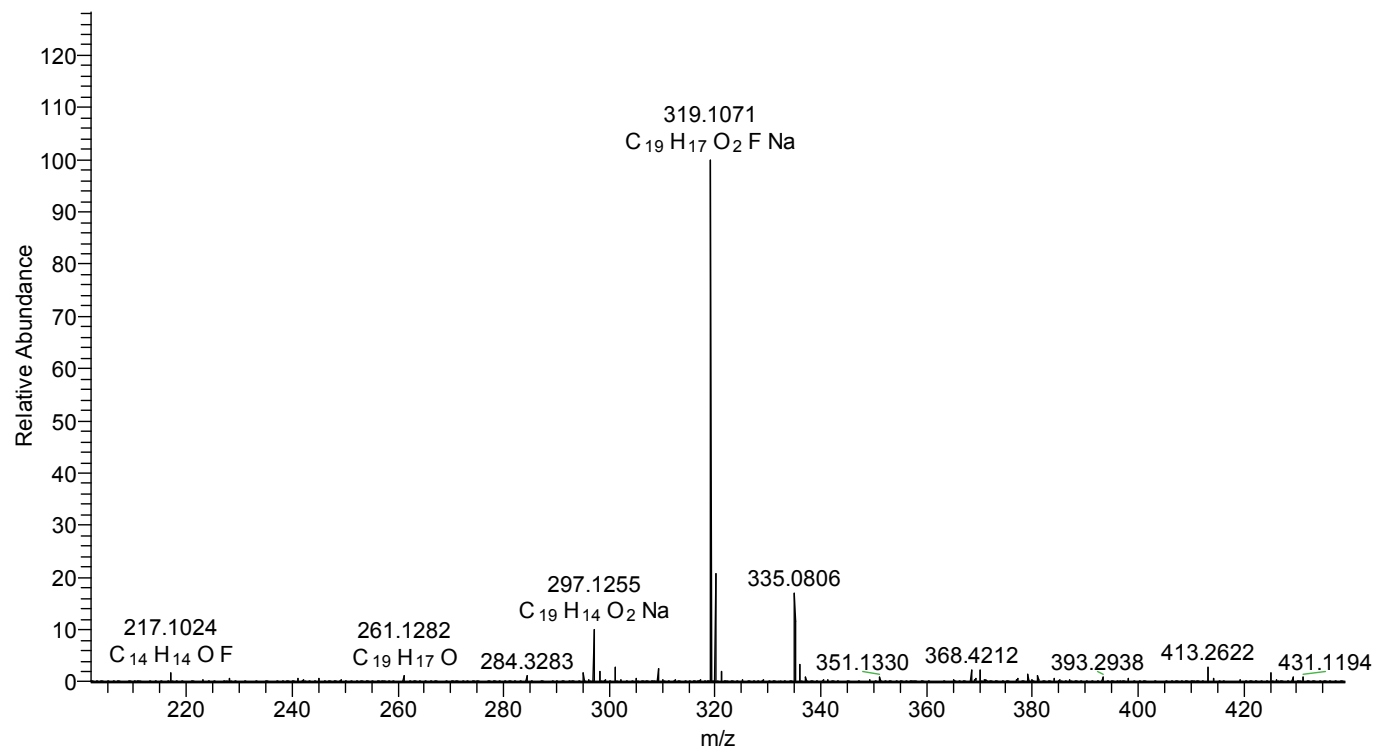
A2K2A17_151022095538 #1 RT: 926.15 AV: 1 NL: 3.73E8

T: FTMS + p ESI Full ms [200.00-1000.00]



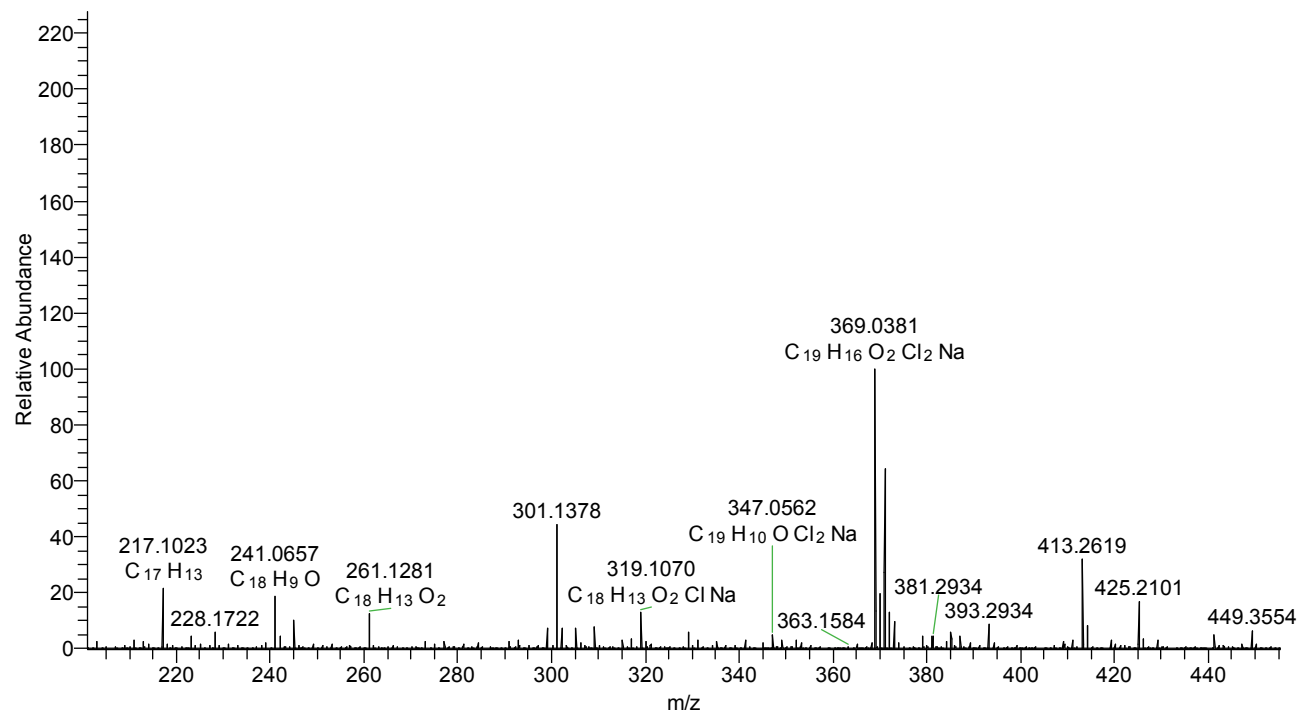
Compound_11

A2K2A19_151022101713 #1 RT: 928.52 AV: 1 NL: 7.60E8
T: FTMS + p ESI Full ms [200.00-1000.00]



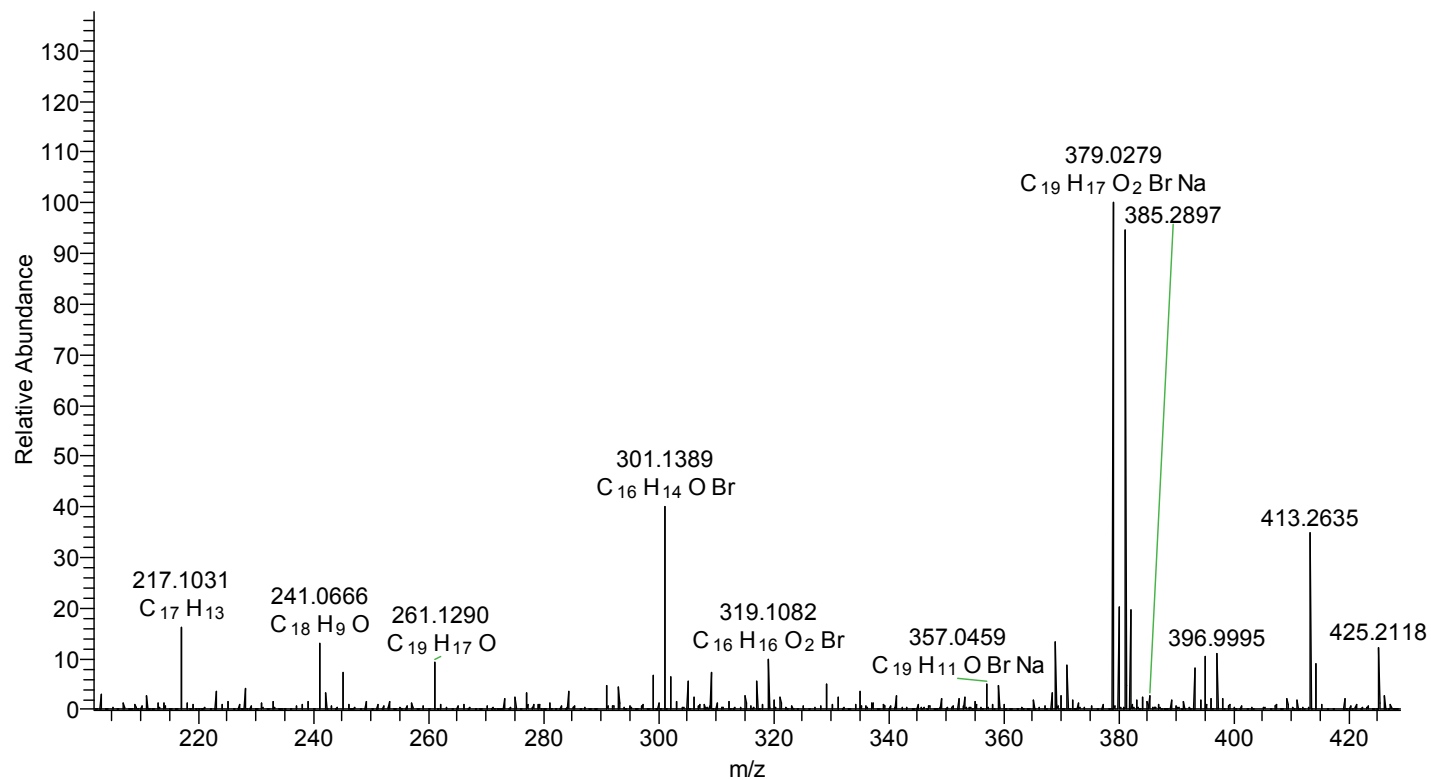
Compound_12

A2K2A20_151022101713 #1 RT: 931.96 AV: 1 NL: 4.49E7
T: FTMS + p ESI Full ms [200.00-1000.00]



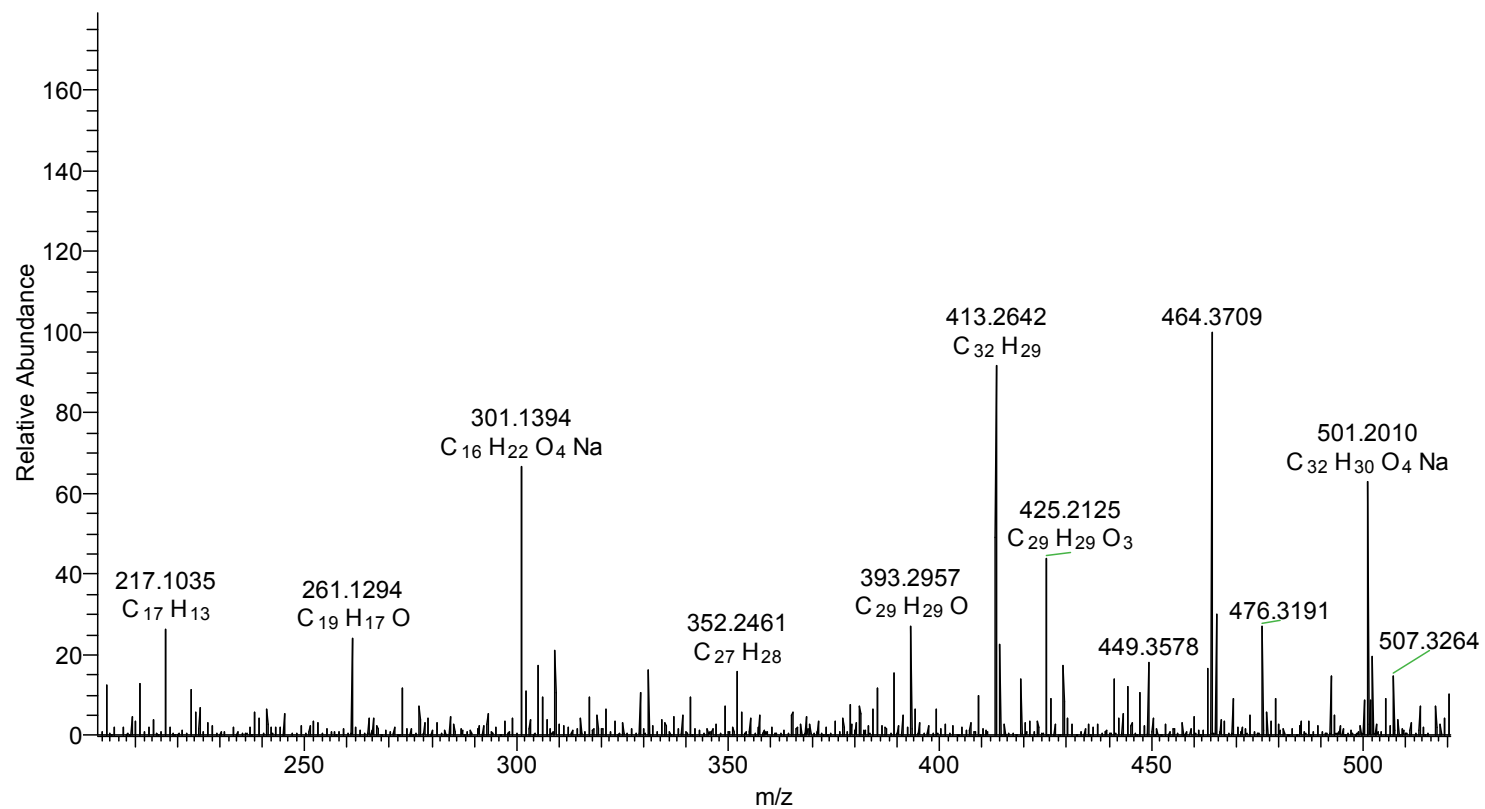
Compound_13

A2K2A21_151022102406 #1 RT: 934.58 AV: 1 NL: 5.66E7
T: FTMS +p ESI Full ms [200.00-1000.00]



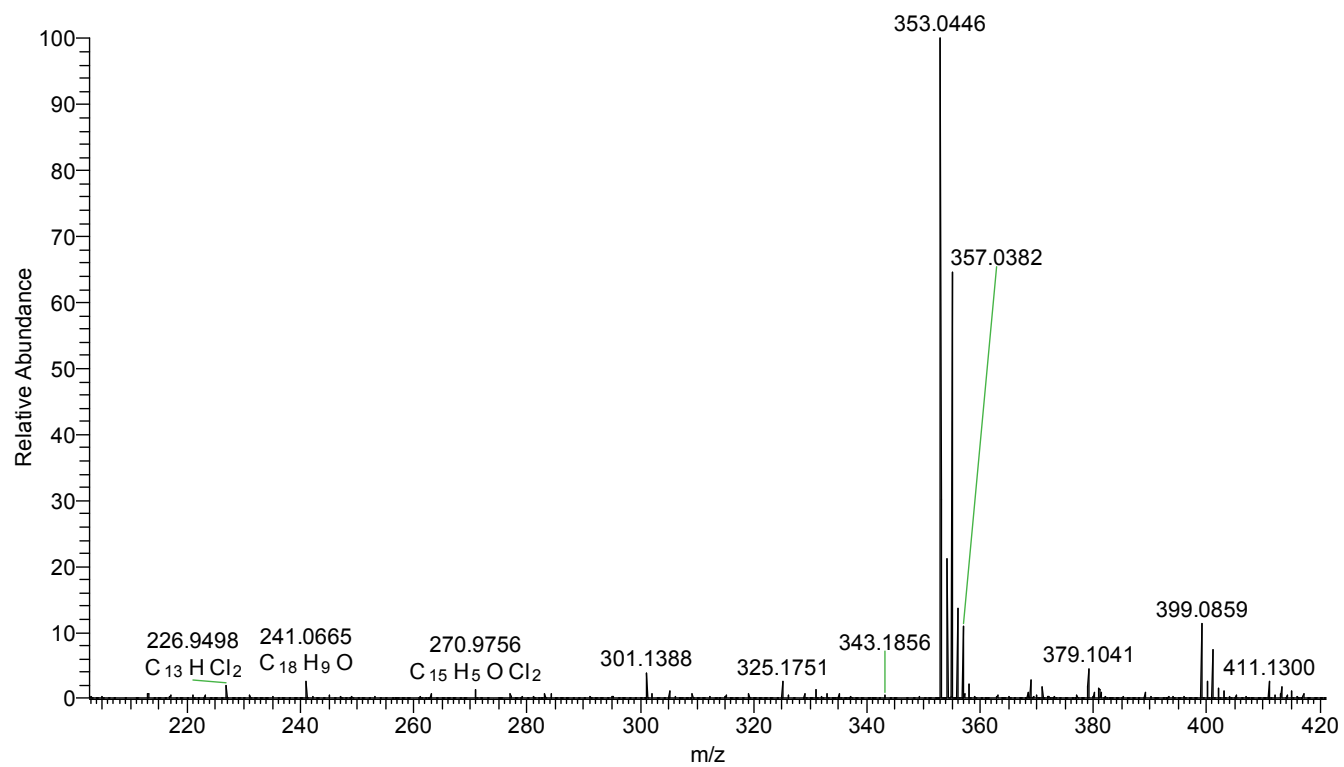
Compound_14

A2K2A22_151022102406 #1 RT: 936.84 AV: 1 NL: 4.17E7
T: FTMS + p ESI Full ms [200.00-1000.00]



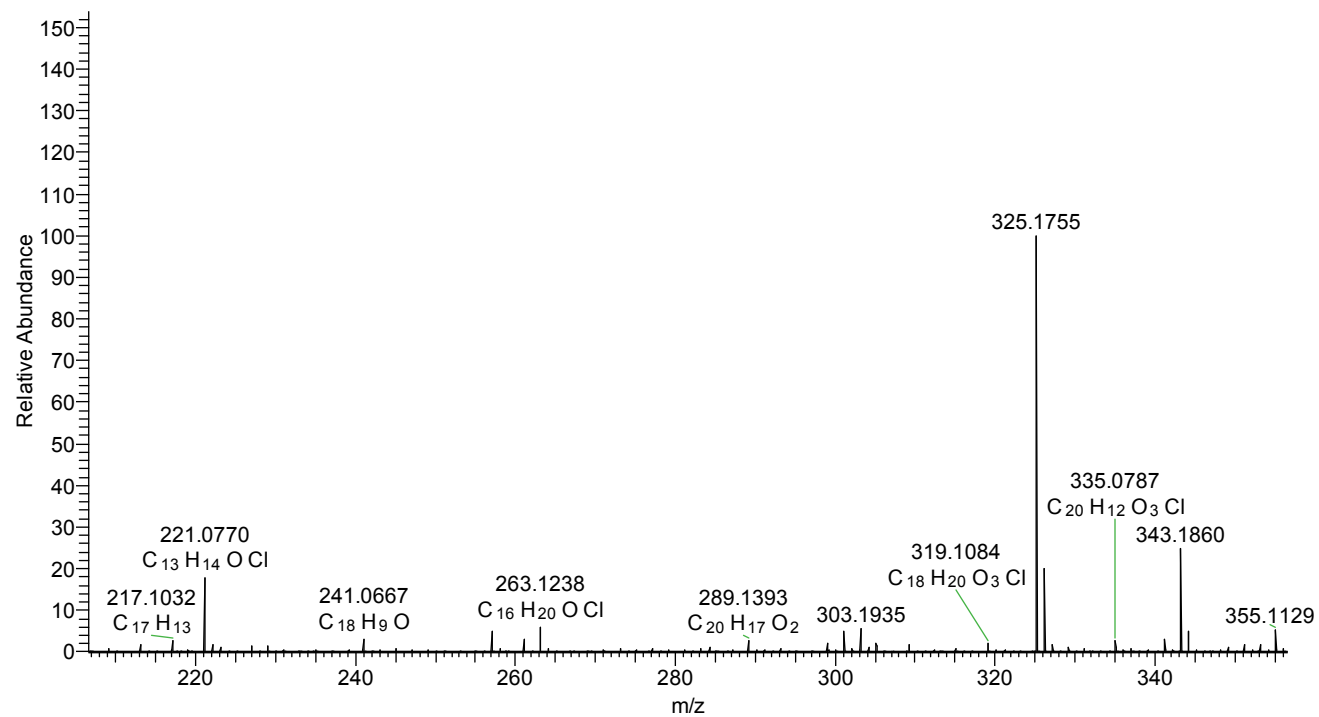
Compound_15

A13K3A13_151022104007 #1 RT: 962.21 AV: 1 NL: 9.92E8
T: FTMS + p ESI Full ms [200.00-1000.00]



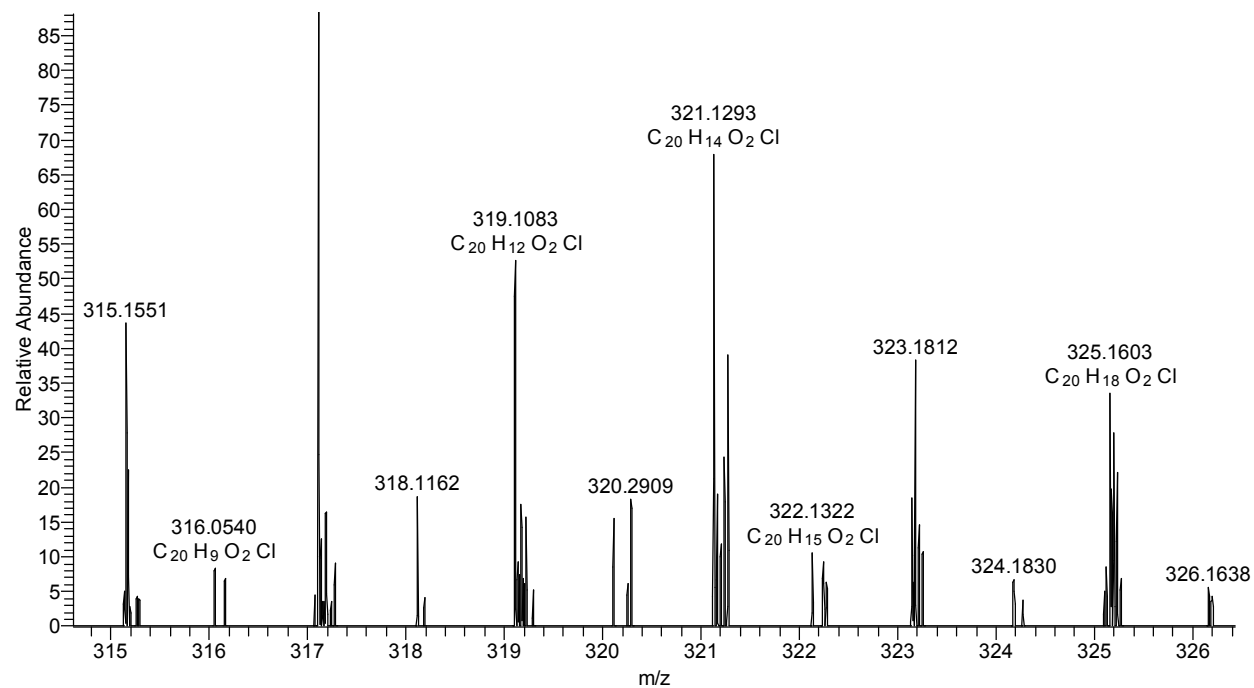
Compound_16

A13K3A10_151022104007 #1 RT: 955.42 AV: 1 NL: 3.88E8
T: FTMS + p ESI Full ms [200.00-1000.00]



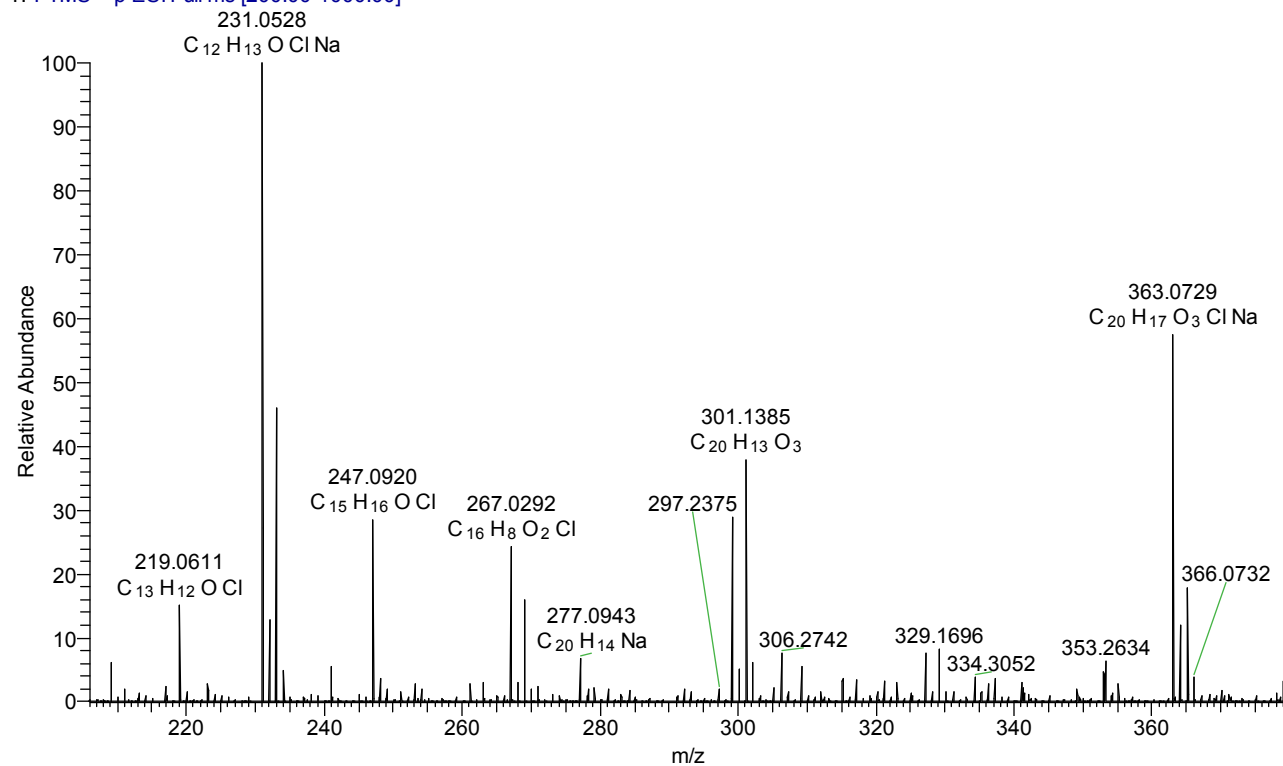
Compound_17

A2K2A22_151022102406 #1 RT: 936.84 AV: 1 NL: 4.03E6
T: FTMS + p ESI Full ms [200.00-1000.00]



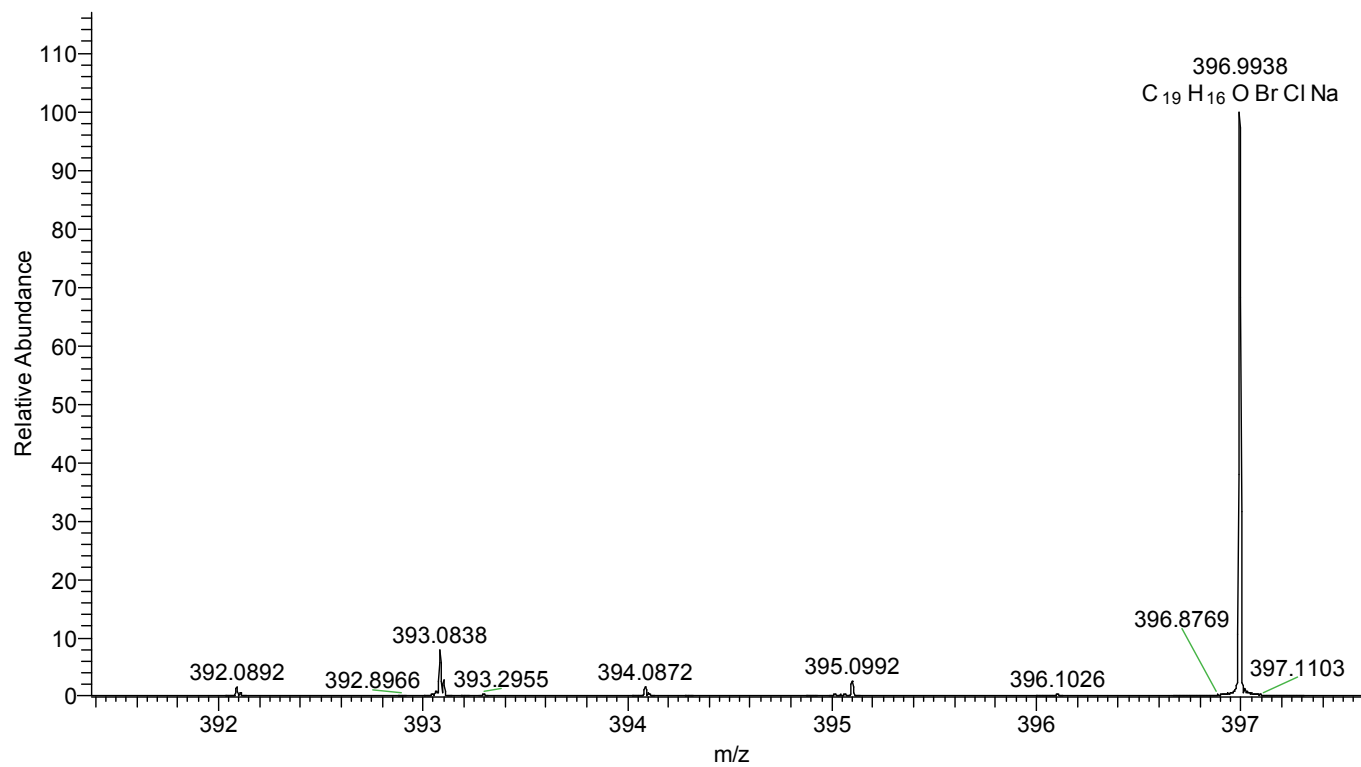
Compound_18

A13K3A5_151022104007 #1 RT: 972.82 AV: 1 NL: 1.39E8
T: FTMS +p ESI Full ms [200.00-1000.00]



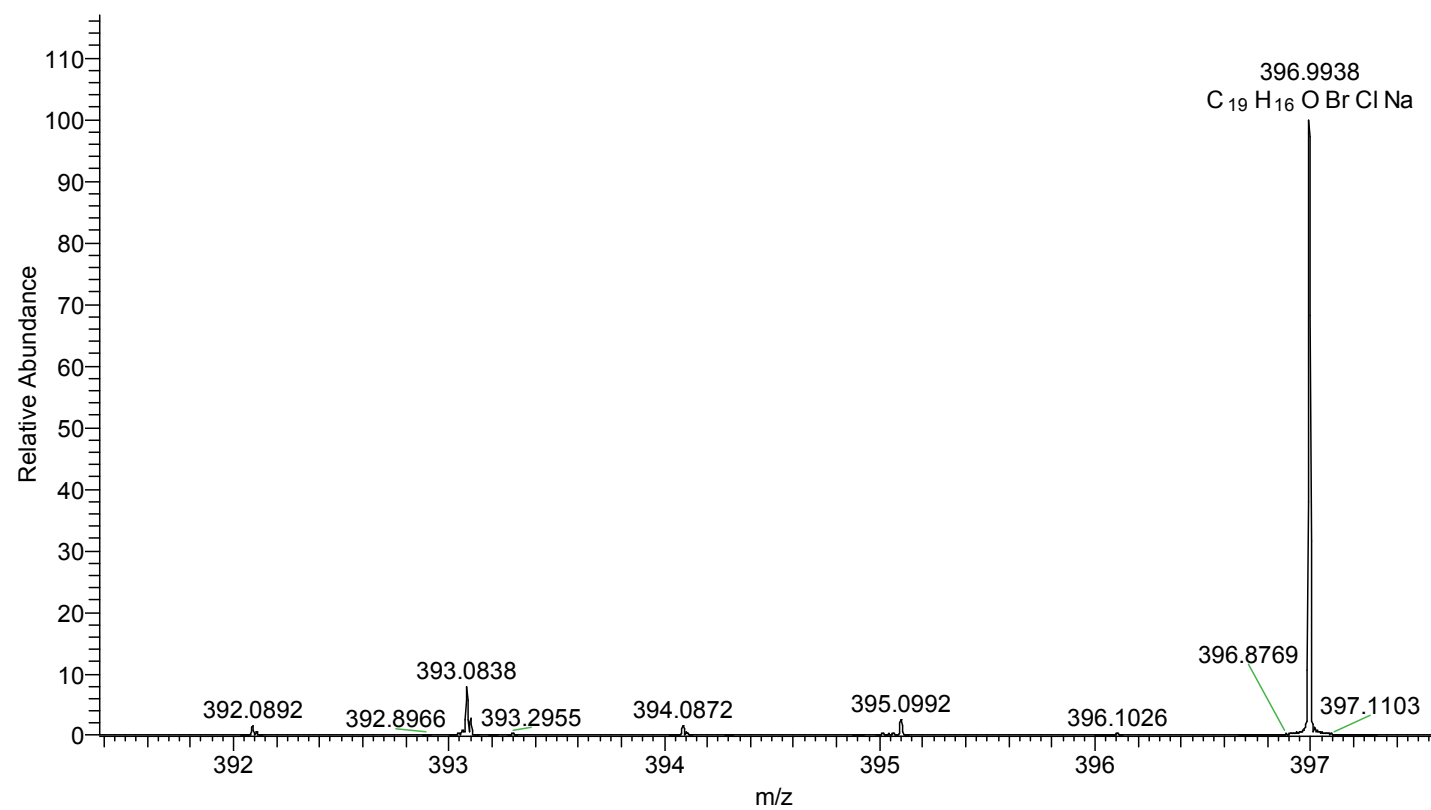
Compound_19

a13k3a23_151022104007 #1 RT: 979.04 AV: 1 NL: 1.79E8
T: FTMS + p ESI Full ms [200.00-1000.00]



Compound_20

a13k3a23_151022104007 #1 RT: 979.04 AV: 1 NL: 1.79E8
T: FTMS + p ESI Full ms [200.00-1000.00]



Compound_21

A13K3A11_151022111643 #1 RT: 987.96 AV: 1 NL: 3.53E8
T: FTMS + p ESI Full ms [200.00-1000.00]

