

Supporting Information 2

Modulating β -Arrestin-2 Recruitment at the δ and μ Opioid Receptors Using Peptidomimetic Ligands

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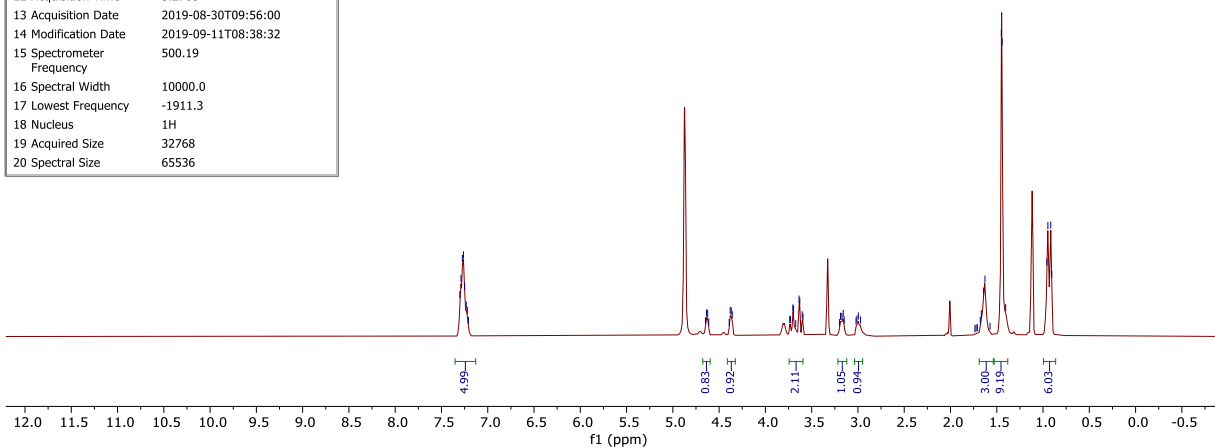
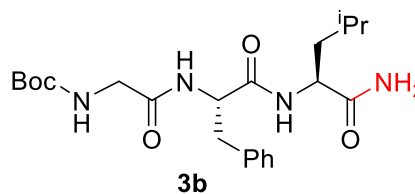
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1. NMR Spectra of Synthesized Compounds

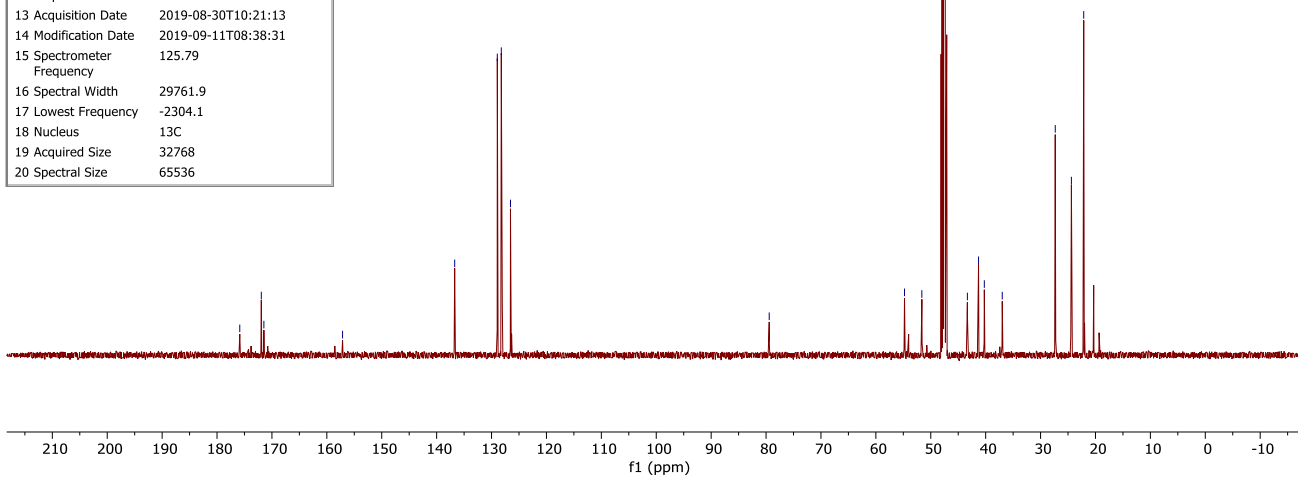
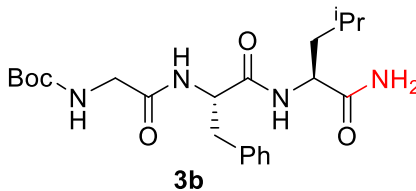
KKS-1-40.1.fid

Parameter	Value
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3 Solvent	MeOD
4 Temperature	298.2
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans	16
9 Receiver Gain	7.1
10 Relaxation Delay	1.0000
11 Pulse Width	12.0000
12 Acquisition Time	3.2768
13 Acquisition Date	2019-08-30T09:56:00
14 Modification Date	2019-09-11T08:38:32
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16 Spectral Width	10000.0
17 Lowest Frequency	-1911.3
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



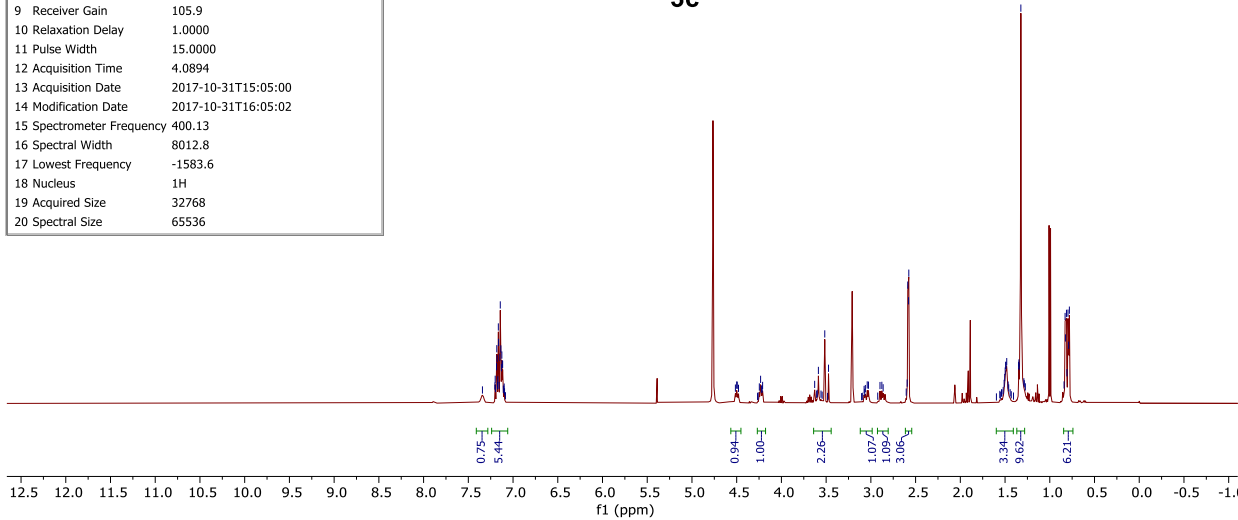
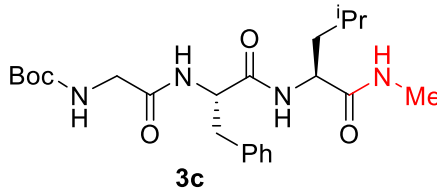
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3 Solvent	MeOD
4 Temperature	298.2
5 Pulse Sequence	zgpg30
6 Experiment	1D
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8 Number of Scans	1024
9 Receiver Gain	11.3
10 Relaxation Delay	0.1500
11 Pulse Width	10.0000
12 Acquisition Time	1.1010
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14 Modification Date	2019-09-11T08:38:31
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17 Lowest Frequency	-2304.1
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536



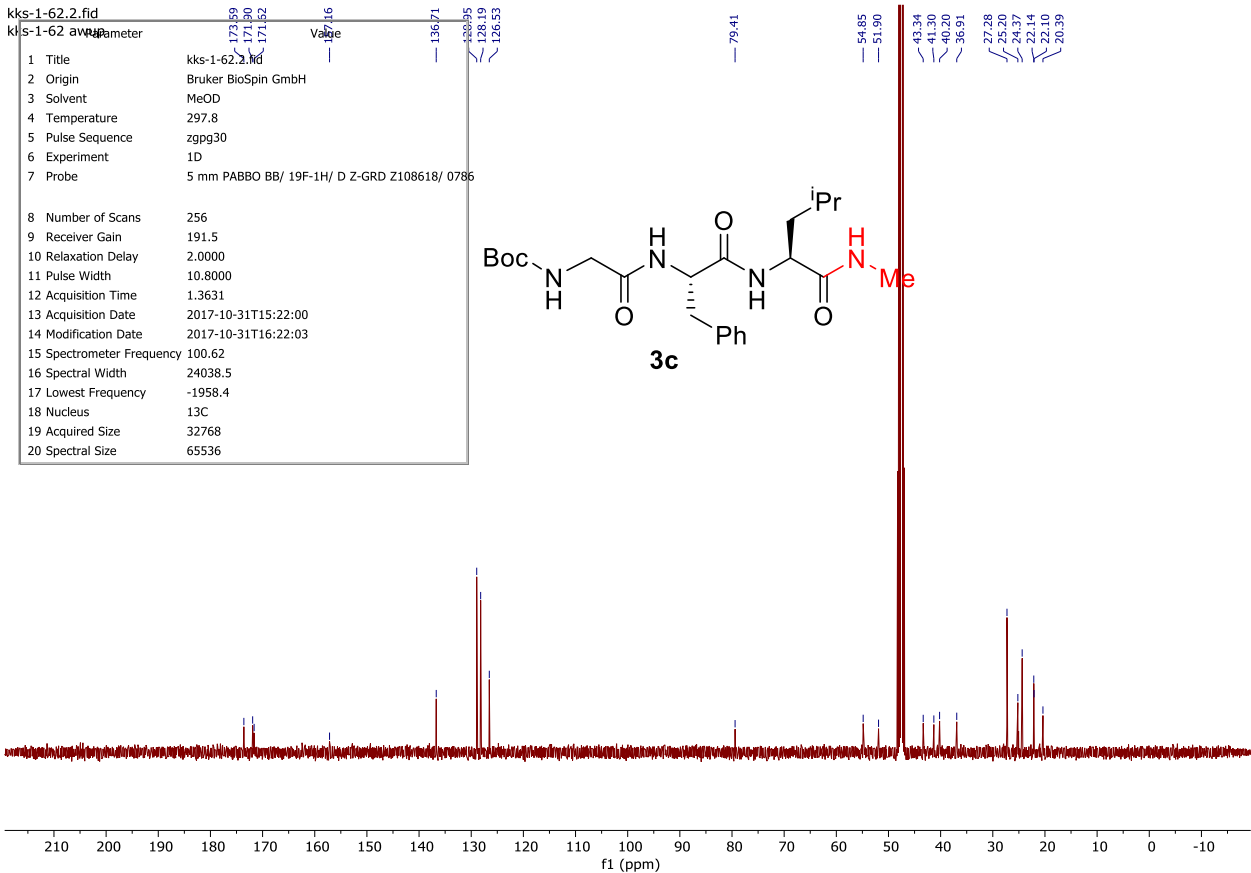
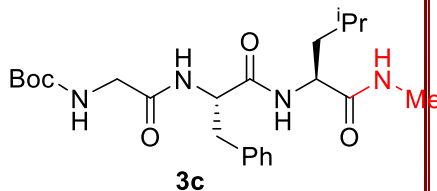
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Parameter	Value
1 Title	kks-1-62.1.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	297.4
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
8 Number of Scans	16
9 Receiver Gain	105.9
10 Relaxation Delay	1.0000
11 Pulse Width	15.0000
12 Acquisition Time	4.0894
13 Acquisition Date	2017-10-31T15:05:00
14 Modification Date	2017-10-31T16:05:02
15 Spectrometer Frequency	400.13
16 Spectral Width	8012.8
17 Lowest Frequency	-1583.6
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20 Spectral Size	65536



kks-1-62.2.fid
 kks-1-62.2.fid

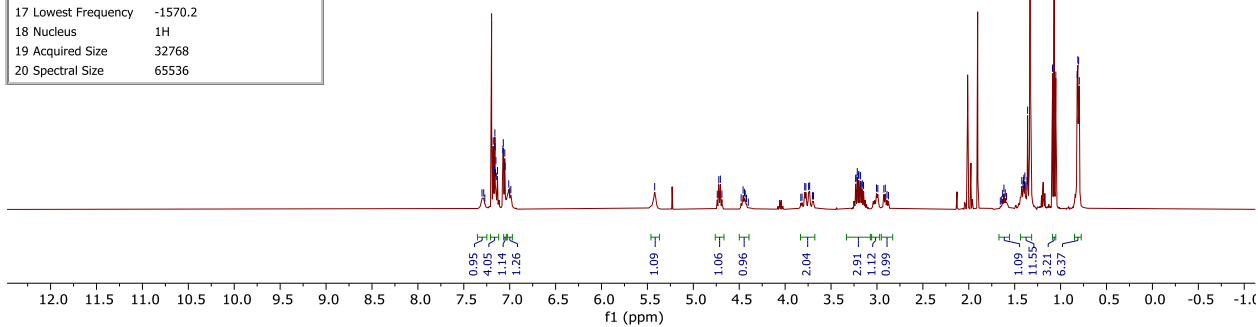
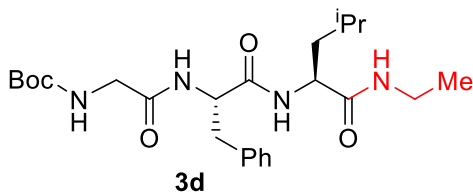
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2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	297.8
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
8 Number of Scans	256
9 Receiver Gain	191.5
10 Relaxation Delay	2.0000
11 Pulse Width	10.8000
12 Acquisition Time	1.3631
13 Acquisition Date	2017-10-31T15:22:00
14 Modification Date	2017-10-31T16:22:03
15 Spectrometer Frequency	100.62
16 Spectral Width	24038.5
17 Lowest Frequency	-1958.4
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536



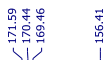
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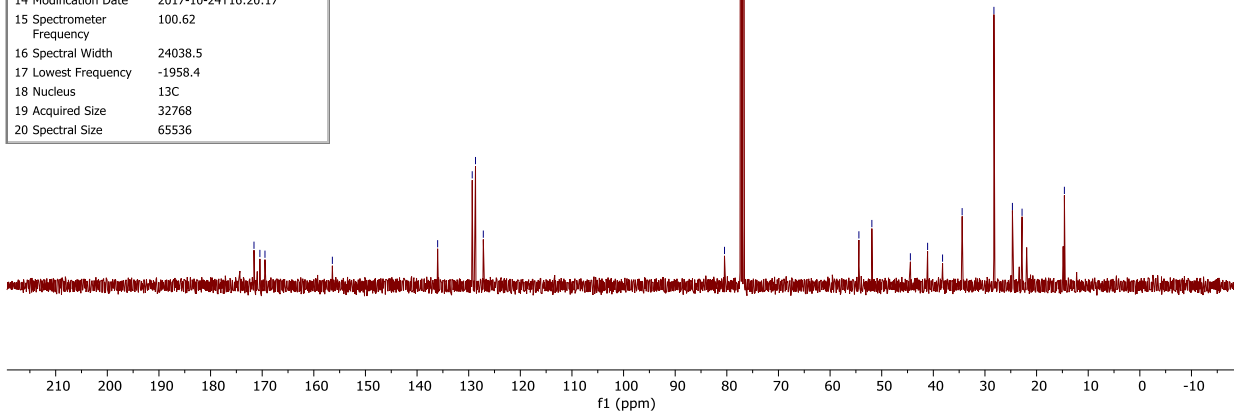
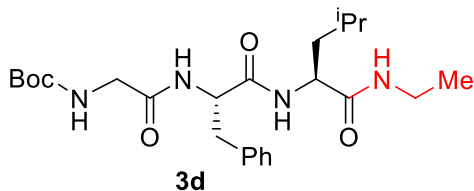
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2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.4
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
8 Number of Scans	16
9 Receiver Gain	120.9
10 Relaxation Delay	1.0000
11 Pulse Width	15.0000
12 Acquisition Time	4.0894
13 Acquisition Date	2017-10-24T13:34:00
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15 Spectrometer Frequency	400.13
16 Spectral Width	8012.8
17 Lowest Frequency	-1570.2
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



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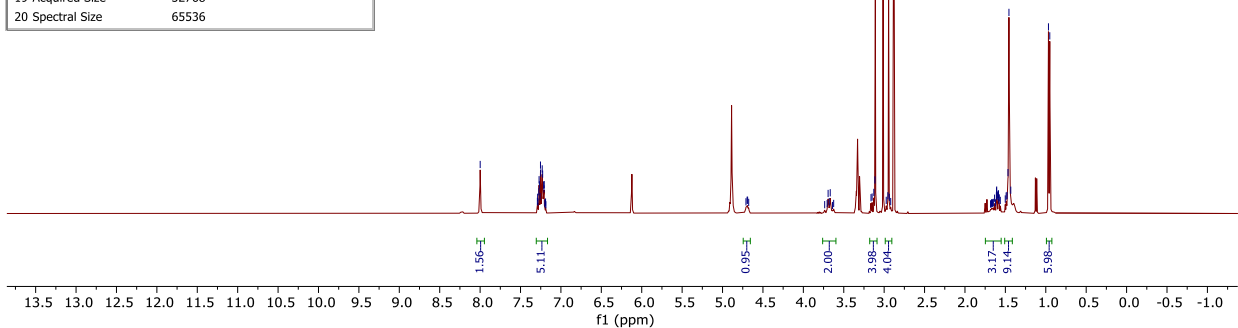
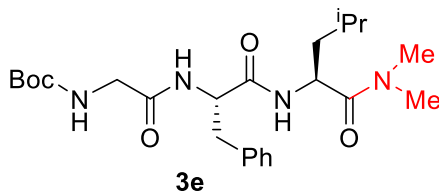
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2 Origin	Bruker BioSpin GmbH
3 Solvent	CDCl3
4 Temperature	296.7
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
8 Number of Scans	256
9 Receiver Gain	191.5
10 Relaxation Delay	2.0000
11 Pulse Width	10.8000
12 Acquisition Time	1.3631
13 Acquisition Date	2017-10-24T15:20:00
14 Modification Date	2017-10-24T16:20:17
15 Spectrometer Frequency	100.62
16 Spectral Width	24038.5
17 Lowest Frequency	-1958.4
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536



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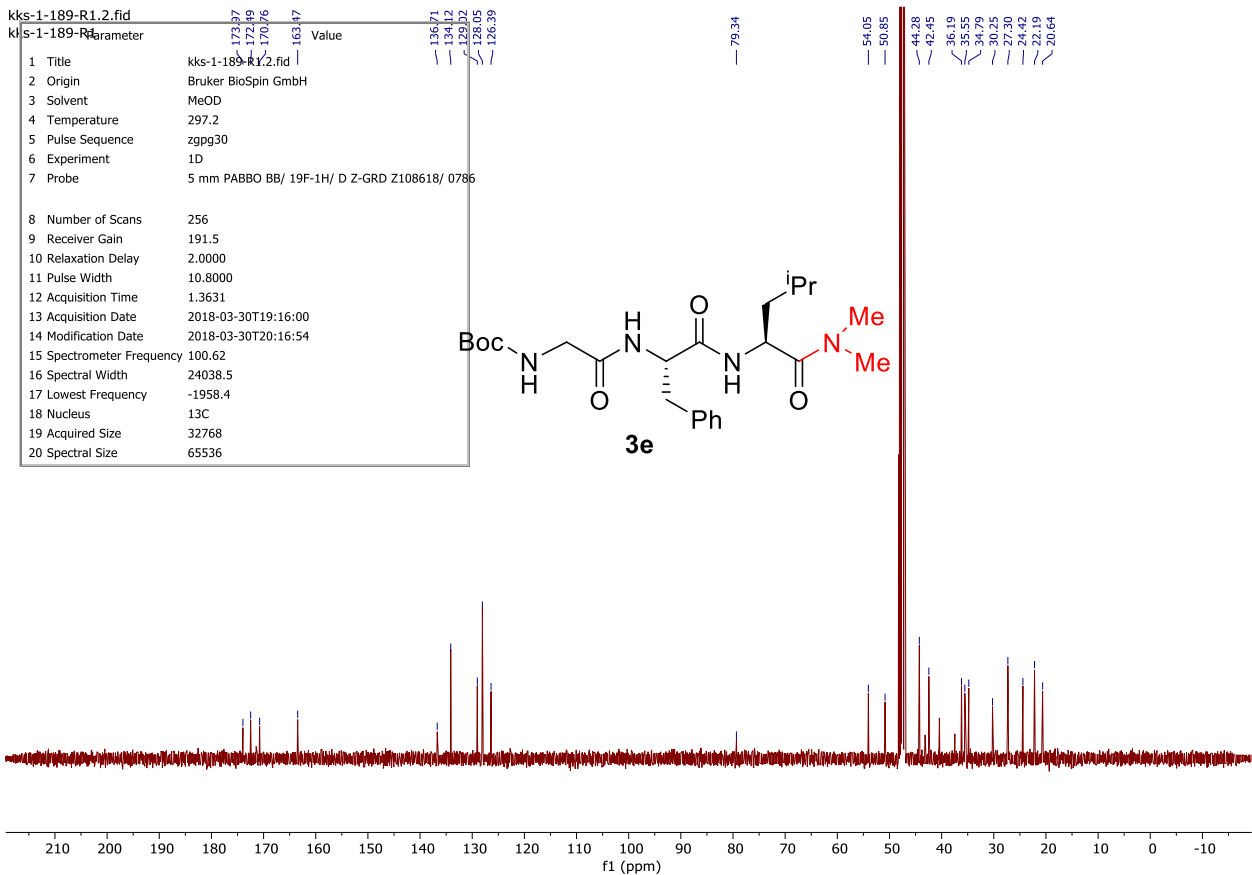
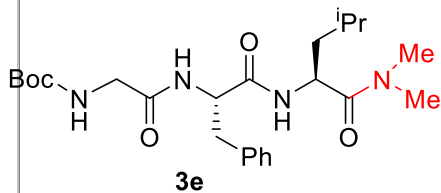
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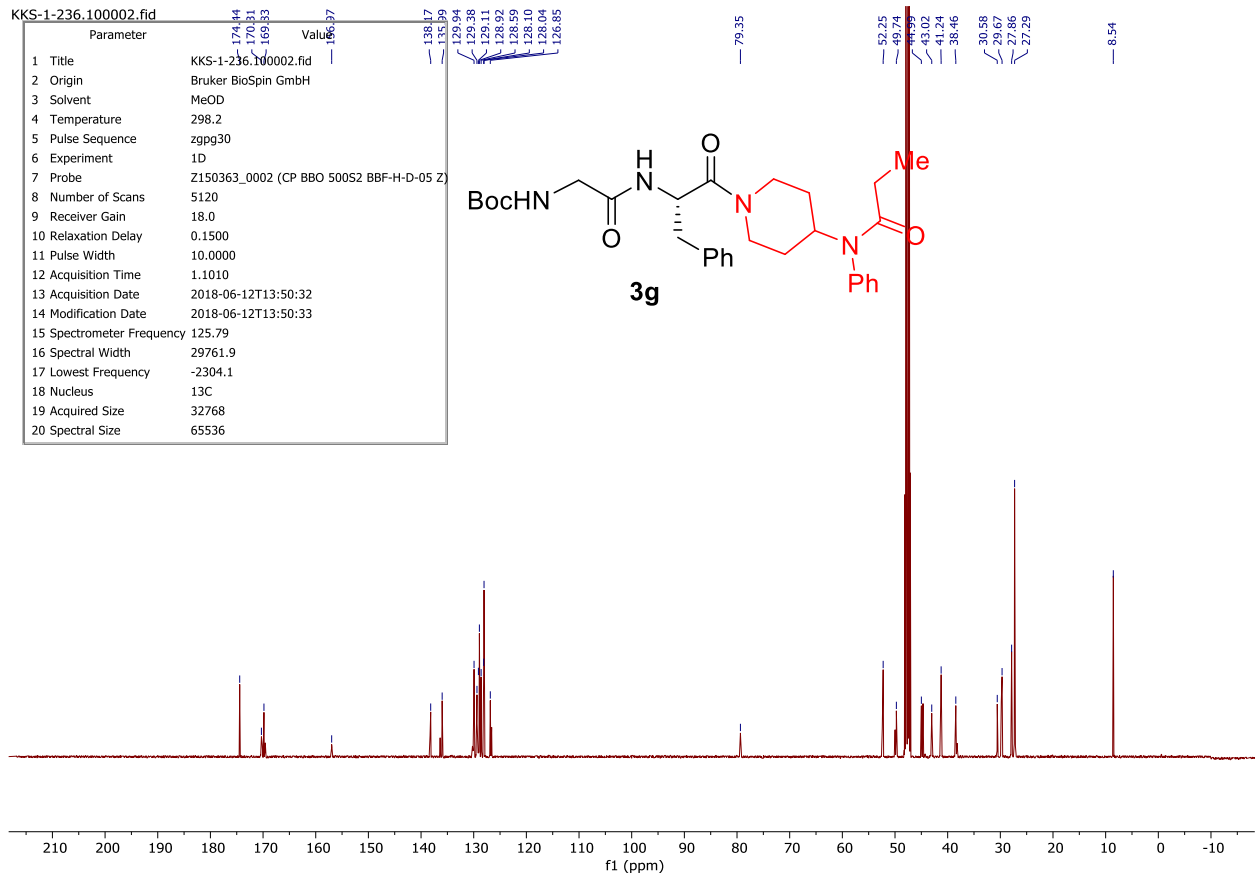
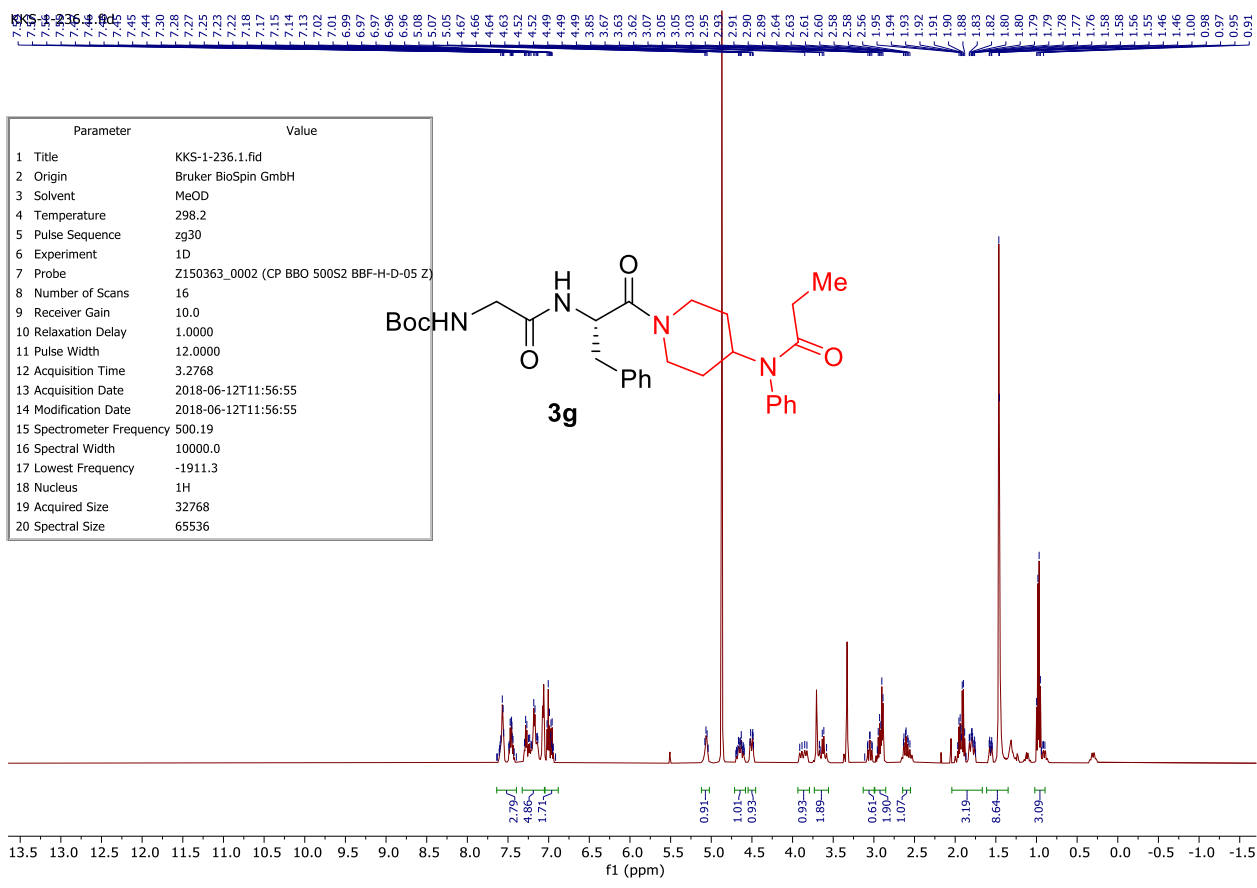
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2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	296.7
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
8 Number of Scans	16
9 Receiver Gain	100.7
10 Relaxation Delay	1.0000
11 Pulse Width	15.0000
12 Acquisition Time	4.0894
13 Acquisition Date	2018-03-30T18:59:00
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15 Spectrometer Frequency	400.13
16 Spectral Width	8012.8
17 Lowest Frequency	-1535.4
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



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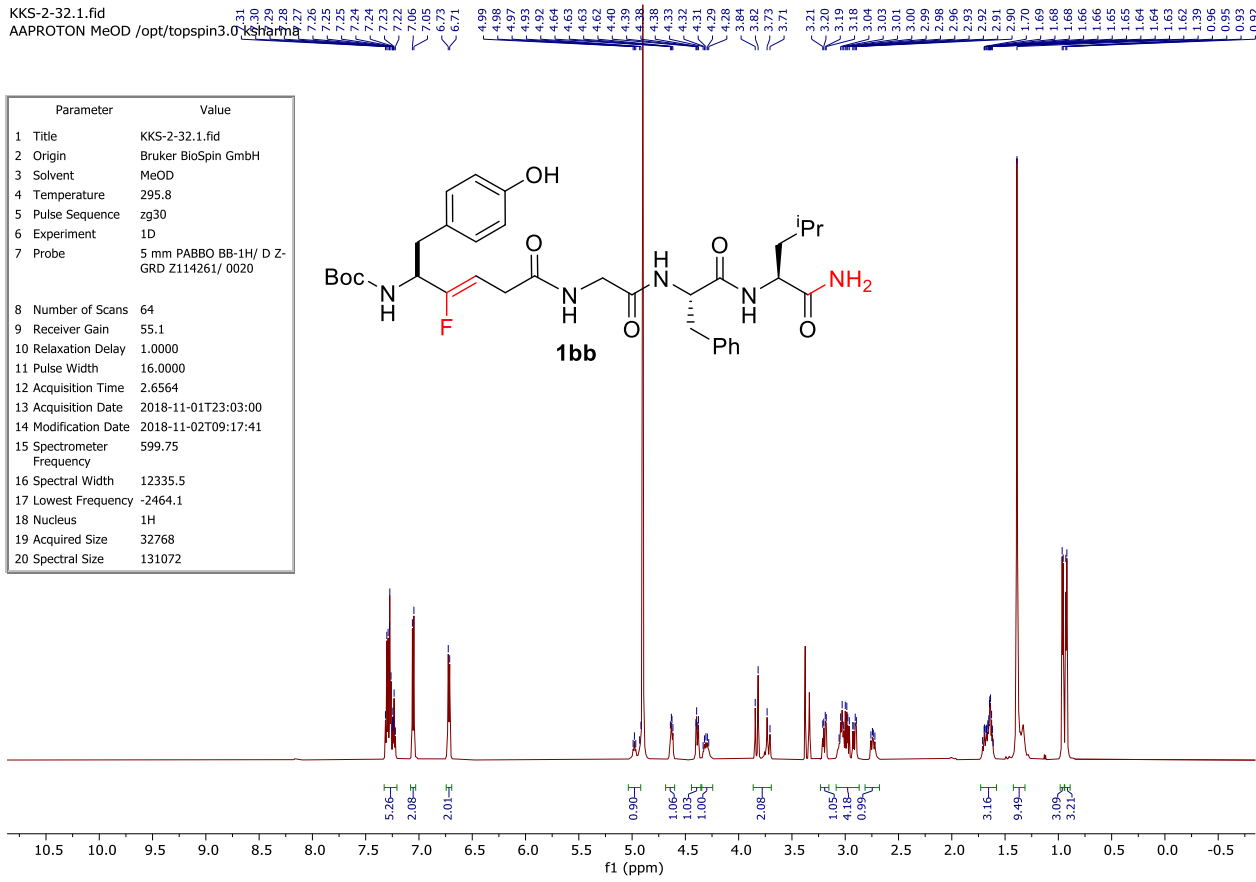
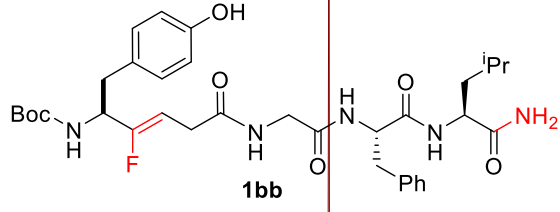
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2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	297.2
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0786
8 Number of Scans	256
9 Receiver Gain	191.5
10 Relaxation Delay	2.0000
11 Pulse Width	10.8000
12 Acquisition Time	1.3631
13 Acquisition Date	2018-03-30T19:16:00
14 Modification Date	2018-03-30T20:16:54
15 Spectrometer Frequency	100.62
16 Spectral Width	24038.5
17 Lowest Frequency	-1958.4
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536





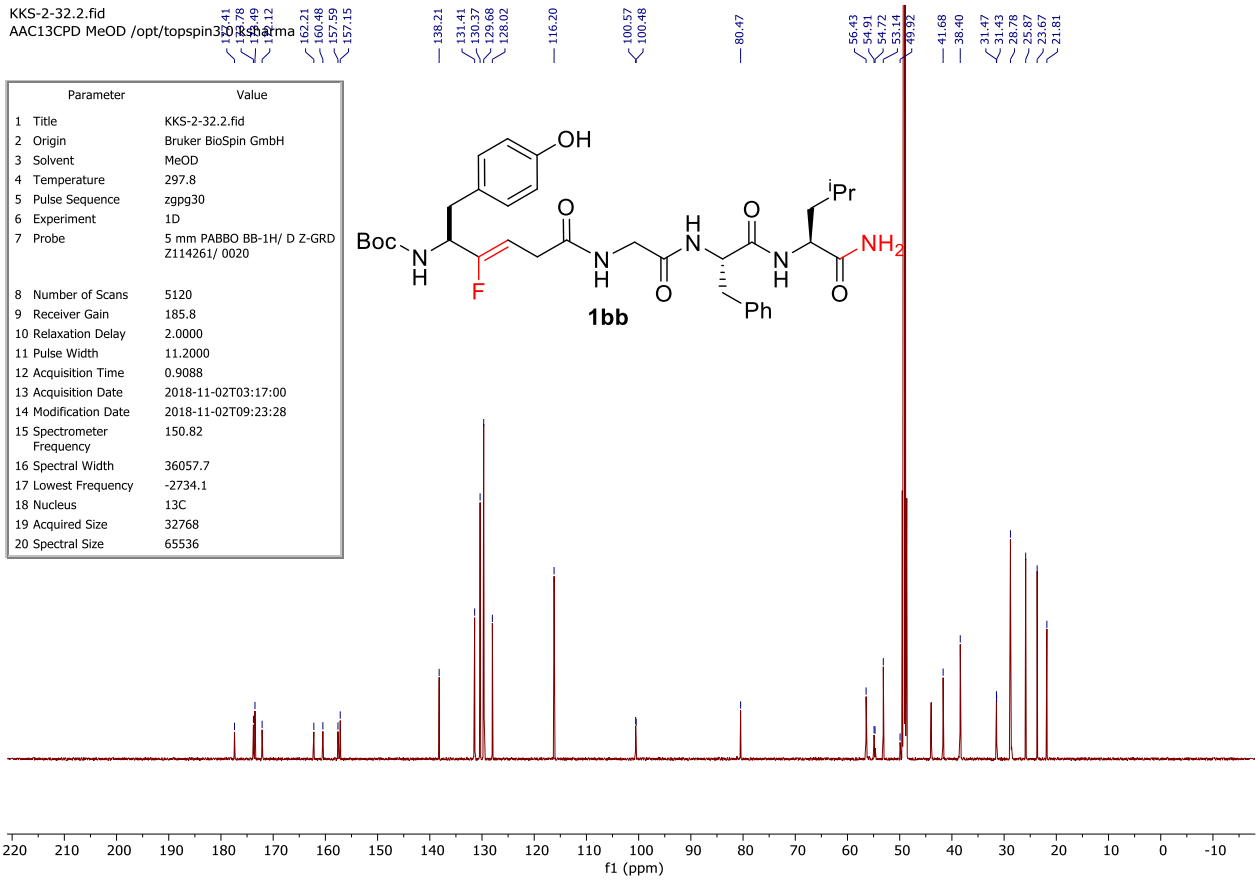
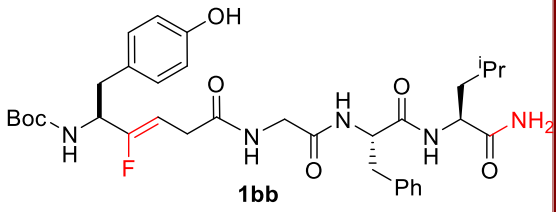
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3 Solvent	MeOD
4 Temperature	295.8
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	5 mm PABBO BB-1H/ D Z-GRD Z114261/ 0020
8 Number of Scans	64
9 Receiver Gain	55.1
10 Relaxation Delay	1.0000
11 Pulse Width	16.0000
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15 Spectrometer	599.75
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16 Spectral Width	12335.5
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18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	131072



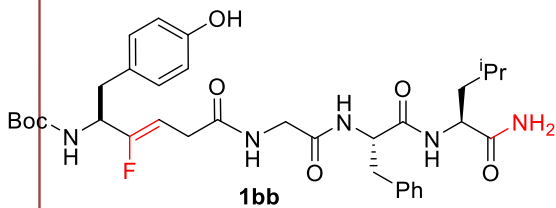
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Parameter	Value
1 Title	KKS-2-32.2.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	297.8
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Probe	5 mm PABBO BB-1H/ D Z-GRD Z114261/ 0020
8 Number of Scans	5120
9 Receiver Gain	185.8
10 Relaxation Delay	2.0000
11 Pulse Width	11.2000
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18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536

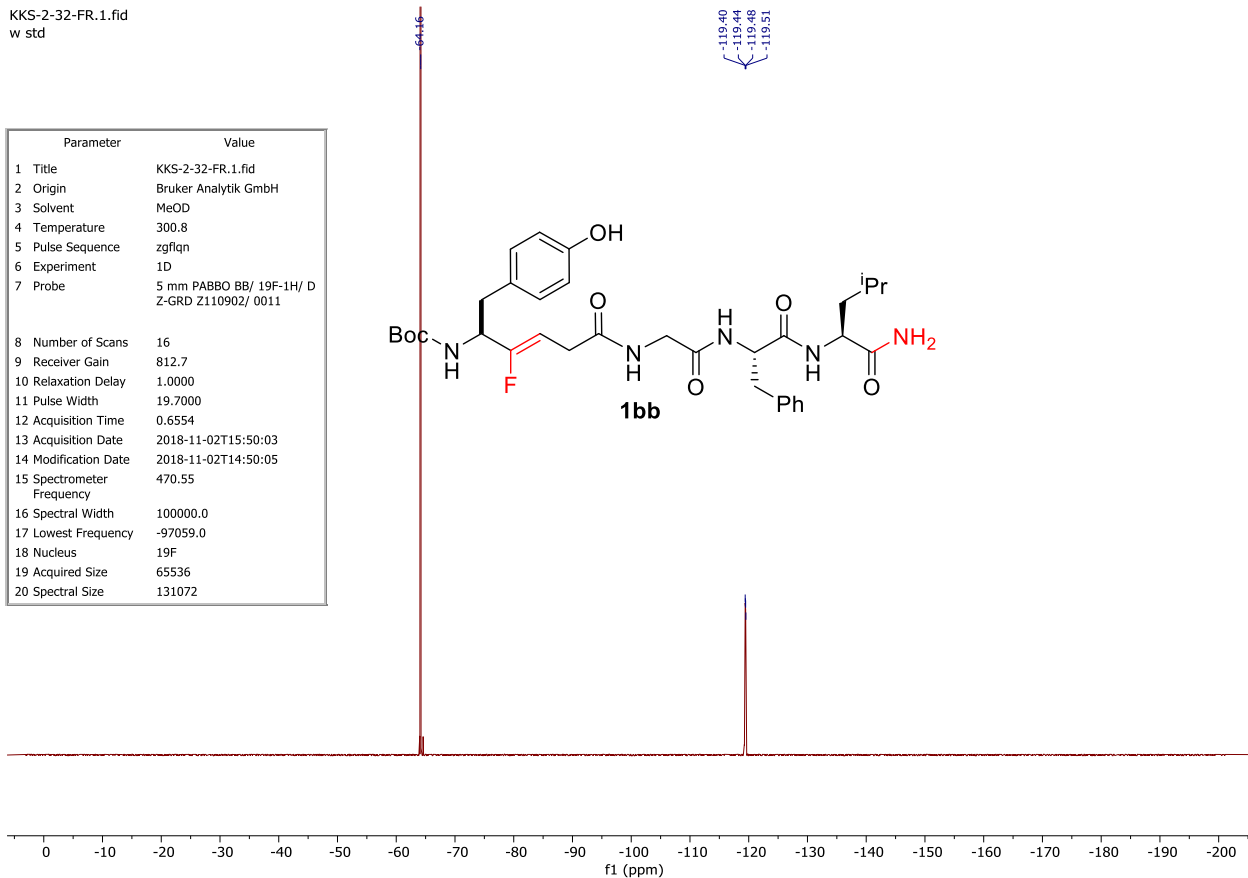


KKS-2-32-FR.1.fid
w std

Parameter	Value
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3 Solvent	MeOD
4 Temperature	300.8
5 Pulse Sequence	zgfgn
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z110902/ 0011
8 Number of Scans	16
9 Receiver Gain	812.7
10 Relaxation Delay	1.0000
11 Pulse Width	19.7000
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13 Acquisition Date	2018-11-02T15:50:03
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18 Nucleus	19F
19 Acquired Size	65536
20 Spectral Size	131072

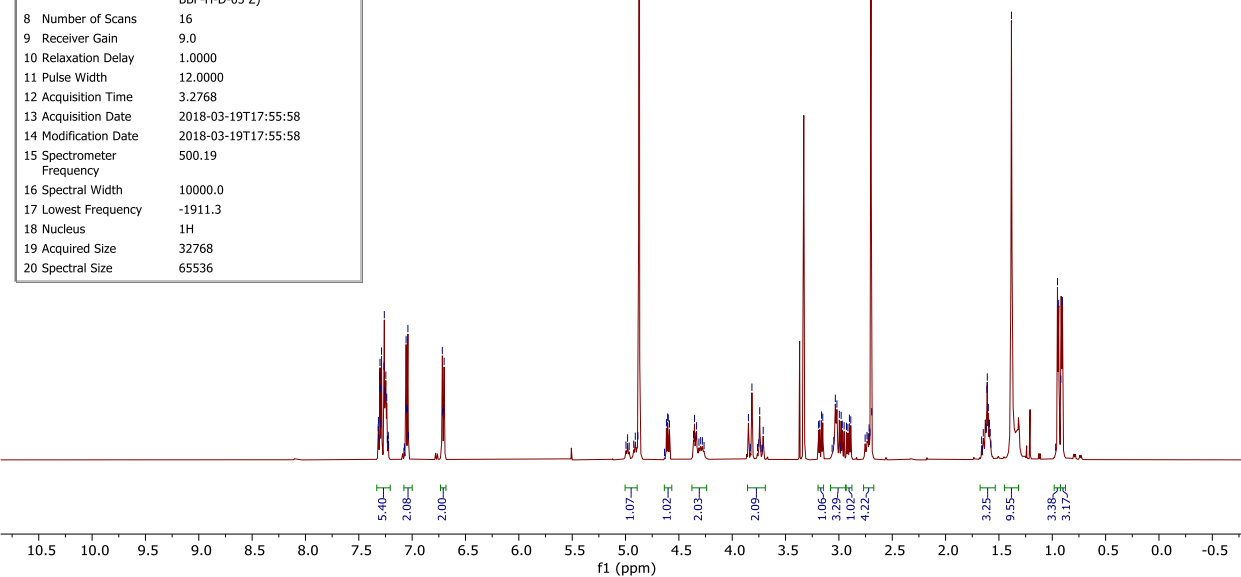
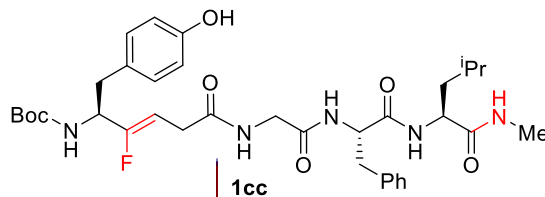


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-119.44
-119.48
-119.51



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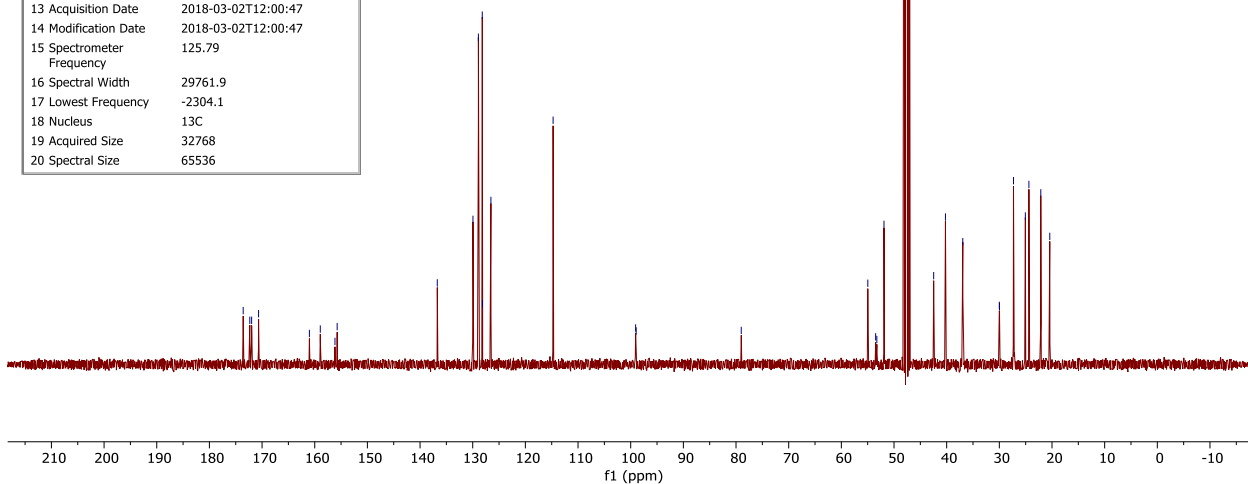
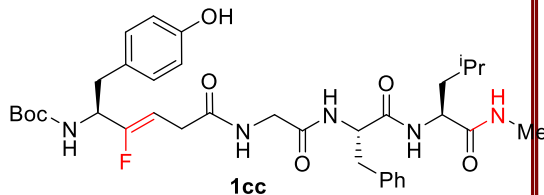
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3 Solvent	MeOD
4 Temperature	298.2
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans	16
9 Receiver Gain	9.0
10 Relaxation Delay	1.0000
11 Pulse Width	12.0000
12 Acquisition Time	3.2768
13 Acquisition Date	2018-03-19T17:55:58
14 Modification Date	2018-03-19T17:55:58
15 Spectrometer	500.19
Frequency	
16 Spectral Width	10000.0
17 Lowest Frequency	-1911.3
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



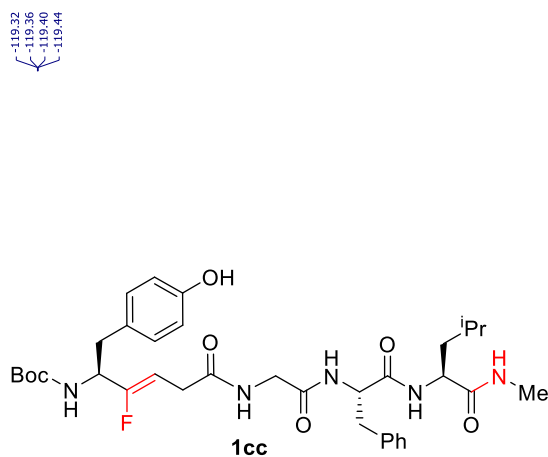
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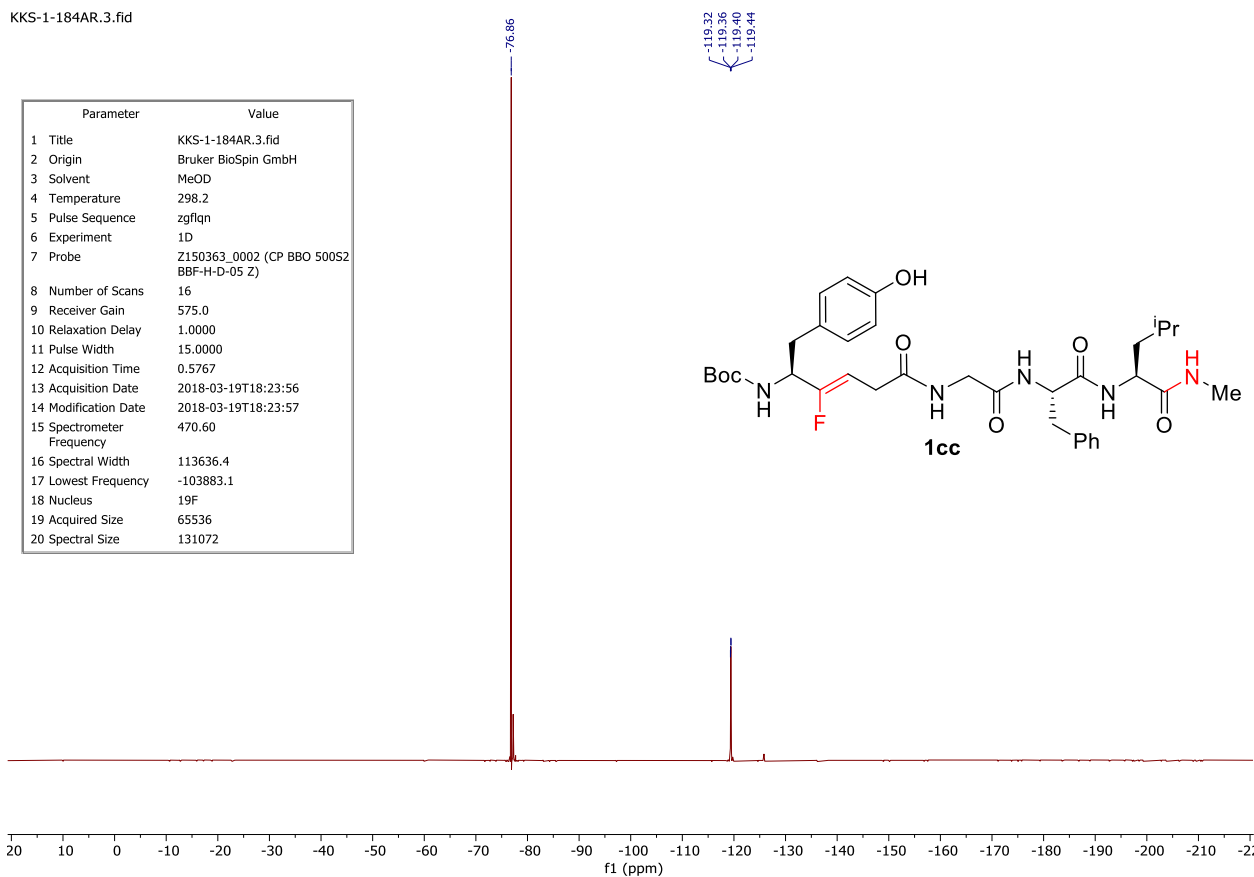
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2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	298.2
5 Pulse Sequence	zgpgg30
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 50052 BBF-H-D-05 Z)
8 Number of Scans	1024
9 Receiver Gain	18.0
10 Relaxation Delay	0.1500
11 Pulse Width	10.0000
12 Acquisition Time	1.1010
13 Acquisition Date	2018-03-02T12:00:47
14 Modification Date	2018-03-02T12:00:47
15 Spectrometer	125.79
Frequency	
16 Spectral Width	29761.9
17 Lowest Frequency	-2304.1
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536

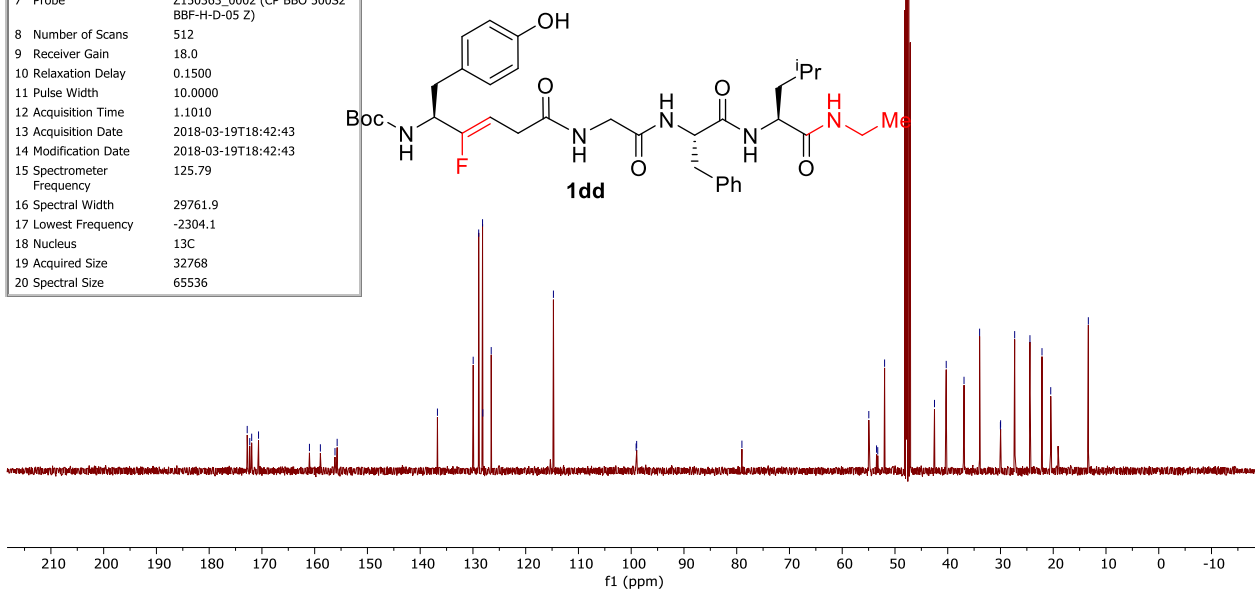
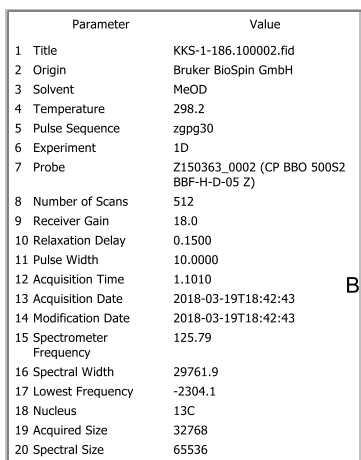
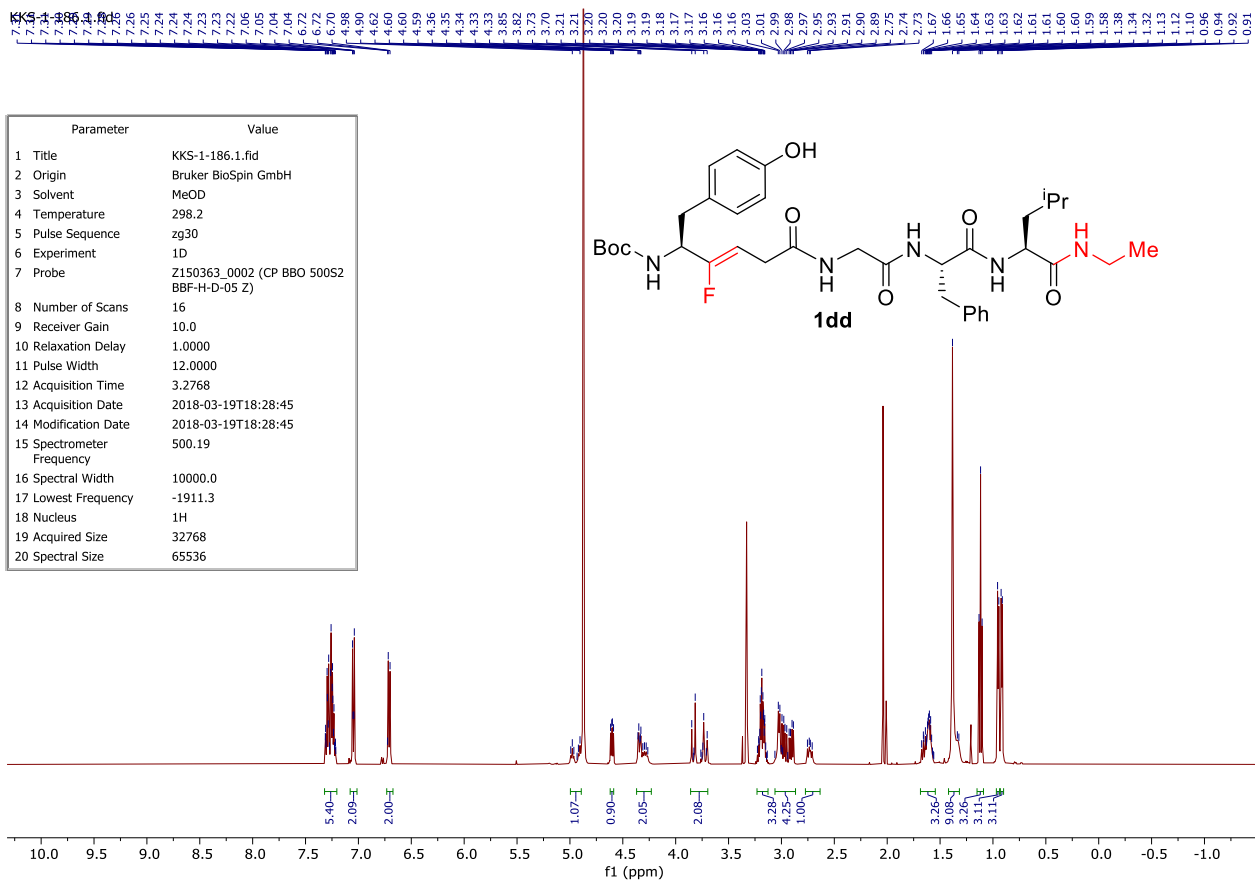


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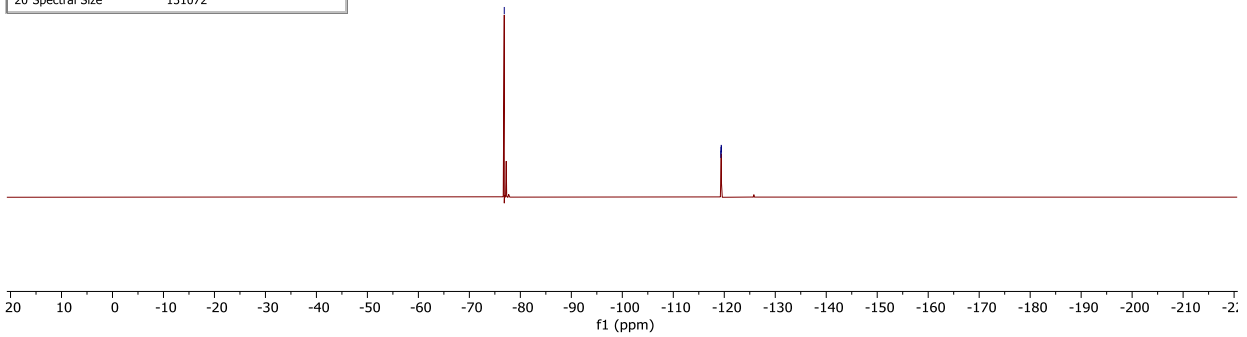
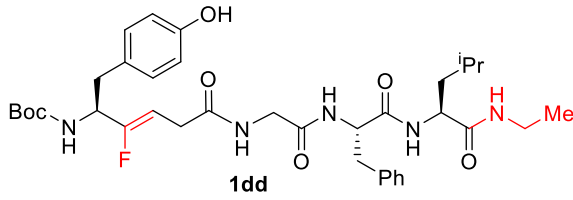


Parameter	Value
1 Title	KKS-1-184AR.3.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	298.2
5 Pulse Sequence	zgfgqn
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 50052 BBF-H-D-05 Z)
8 Number of Scans	16
9 Receiver Gain	575.0
10 Relaxation Delay	1.0000
11 Pulse Width	15.0000
12 Acquisition Time	0.5767
13 Acquisition Date	2018-03-19T18:23:56
14 Modification Date	2018-03-19T18:23:57
15 Spectrometer	470.60
Frequency	
16 Spectral Width	113636.4
17 Lowest Frequency	-103883.1
18 Nucleus	19F
19 Acquired Size	65536
20 Spectral Size	131072



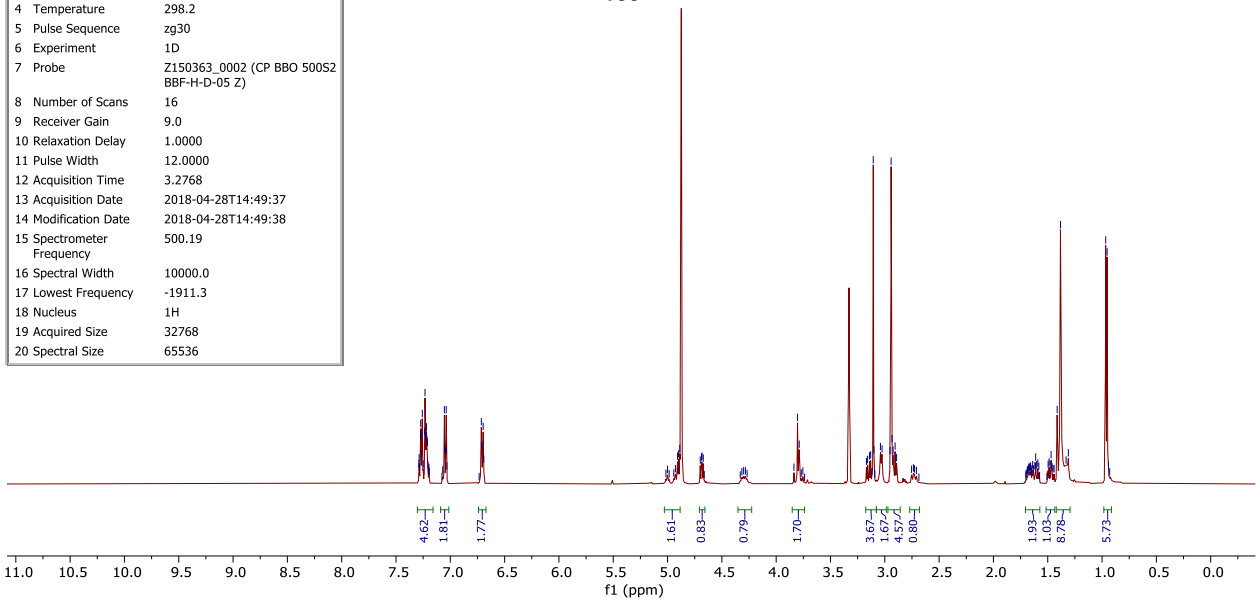
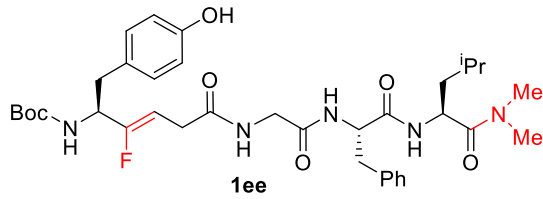


Parameter	Value
1 Title	KKS-1-186.4.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	298.2
5 Pulse Sequence	zgfgq
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans	16
9 Receiver Gain	645.0
10 Relaxation Delay	1.0000
11 Pulse Width	15.0000
12 Acquisition Time	0.5767
13 Acquisition Date	2018-03-19T19:11:21
14 Modification Date	2018-03-19T19:11:22
15 Spectrometer	470.60
Frequency	
16 Spectral Width	113636.4
17 Lowest Frequency	-103883.1
18 Nucleus	19F
19 Acquired Size	65536
20 Spectral Size	131072



7.175, 7.144, 7.114, 7.084, 7.054, 7.024, 7.25, 7.24, 7.23, 7.22, 7.21, 7.20, 7.19, 7.18, 7.17, 7.16, 7.15, 7.14, 7.13, 7.12, 7.11, 7.10, 7.09, 7.08, 7.07, 7.06, 7.05, 7.04, 7.03, 7.02, 7.01, 7.00, 6.99, 6.98, 6.97, 6.96, 6.95, 6.94, 6.93, 6.92, 6.91, 6.90, 6.89, 6.88, 6.87, 6.86, 6.85, 6.84, 6.83, 6.82, 6.81, 6.80, 6.79, 6.78, 6.77, 6.76, 6.75, 6.74, 6.73, 6.72, 6.71, 6.70, 6.69, 6.68, 6.67, 6.66, 6.65, 6.64, 6.63, 6.62, 6.61, 6.60, 6.59, 6.58, 6.57, 6.56, 6.55, 6.54, 6.53, 6.52, 6.51, 6.50, 6.49, 6.48, 6.47, 6.46, 6.45, 6.44, 6.43, 6.42, 6.41, 6.40, 6.39, 6.38, 6.37, 6.36, 6.35, 6.34, 6.33, 6.32, 6.31, 6.30, 6.29, 6.28, 6.27, 6.26, 6.25, 6.24, 6.23, 6.22, 6.21, 6.20, 6.19, 6.18, 6.17, 6.16, 6.15, 6.14, 6.13, 6.12, 6.11, 6.10, 6.09, 6.08, 6.07, 6.06, 6.05, 6.04, 6.03, 6.02, 6.01, 6.00, 5.99, 5.98, 5.97, 5.96, 5.95, 5.94, 5.93, 5.92, 5.91, 5.90, 5.89, 5.88, 5.87, 5.86, 5.85, 5.84, 5.83, 5.82, 5.81, 5.80, 5.79, 5.78, 5.77, 5.76, 5.75, 5.74, 5.73, 5.72, 5.71, 5.70, 5.69, 5.68, 5.67, 5.66, 5.65, 5.64, 5.63, 5.62, 5.61, 5.60, 5.59, 5.58, 5.57, 5.56, 5.55, 5.54, 5.53, 5.52, 5.51, 5.50, 5.49, 5.48, 5.47, 5.46, 5.45, 5.44, 5.43, 5.42, 5.41, 5.40, 5.39, 5.38, 5.37, 5.36, 5.35, 5.34, 5.33, 5.32, 5.31, 5.30, 5.29, 5.28, 5.27, 5.26, 5.25, 5.24, 5.23, 5.22, 5.21, 5.20, 5.19, 5.18, 5.17, 5.16, 5.15, 5.14, 5.13, 5.12, 5.11, 5.10, 5.09, 5.08, 5.07, 5.06, 5.05, 5.04, 5.03, 5.02, 5.01, 5.00, 4.99, 4.98, 4.97, 4.96, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67, 4.66, 4.65, 4.64, 4.63, 4.62, 4.61, 4.60, 4.59, 4.58, 4.57, 4.56, 4.55, 4.54, 4.53, 4.52, 4.51, 4.50, 4.49, 4.48, 4.47, 4.46, 4.45, 4.44, 4.43, 4.42, 4.41, 4.40, 4.39, 4.38, 4.37, 4.36, 4.35, 4.34, 4.33, 4.32, 4.31, 4.30, 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.23, 4.22, 4.21, 4.20, 4.19, 4.18, 4.17, 4.16, 4.15, 4.14, 4.13, 4.12, 4.11, 4.10, 4.09, 4.08, 4.07, 4.06, 4.05, 4.04, 4.03, 4.02, 4.01, 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.91, 3.90, 3.89, 3.88, 3.87, 3.86, 3.85, 3.84, 3.83, 3.82, 3.81, 3.80, 3.79, 3.78, 3.77, 3.76, 3.75, 3.74, 3.73, 3.72, 3.71, 3.70, 3.69, 3.68, 3.67, 3.66, 3.65, 3.64, 3.63, 3.62, 3.61, 3.60, 3.59, 3.58, 3.57, 3.56, 3.55, 3.54, 3.53, 3.52, 3.51, 3.50, 3.49, 3.48, 3.47, 3.46, 3.45, 3.44, 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.31, 1.30, 1.29, 1.28, 1.27, 1.26, 1.25, 1.24, 1.23, 1.22, 1.21, 1.20, 1.19, 1.18, 1.17, 1.16, 1.15, 1.14, 1.13, 1.12, 1.11, 1.10, 1.09, 1.08, 1.07, 1.06, 1.05, 1.04, 1.03, 1.02, 1.01, 1.00, 0.99, 0.98, 0.97, 0.96, 0.95, 0.94

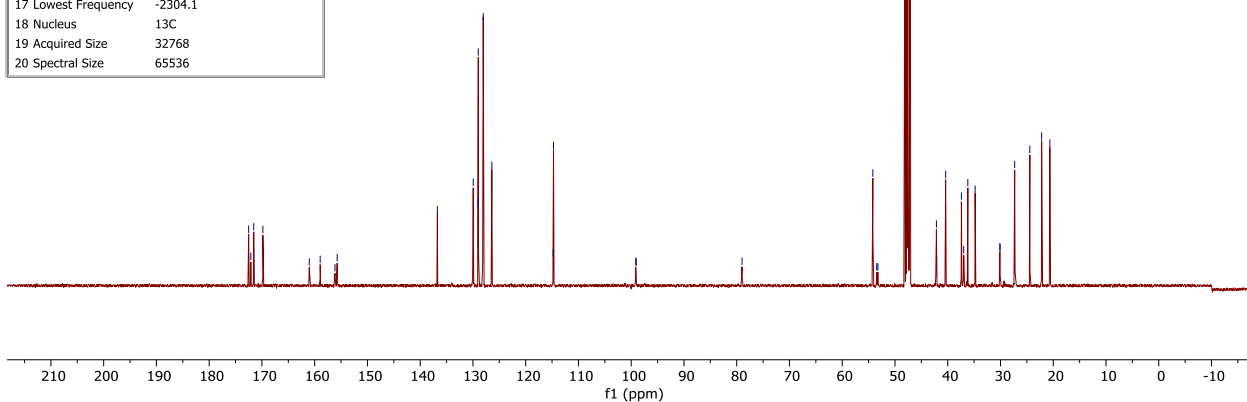
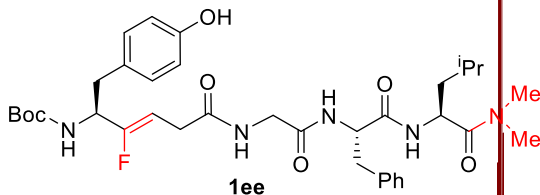
Parameter	Value
1 Title	KKS-1-204.1.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	298.2
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans	16
9 Receiver Gain	9.0
10 Relaxation Delay	1.0000
11 Pulse Width	12.0000
12 Acquisition Time	3.2768
13 Acquisition Date	2018-04-28T14:49:37
14 Modification Date	2018-04-28T14:49:38
15 Spectrometer	500.19
Frequency	
16 Spectral Width	10000.0
17 Lowest Frequency	-1911.3
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



KKS-1-204.100004.fid
5000 scans

172.52
172.11
171.82
169.82
161.03
158.96
156.15
155.74
136.74
129.95
128.99
128.98
128.05
126.41
114.78
114.73
98.14
98.04
78.99
54.20
53.47
53.23
42.18
40.40
37.41
36.97
36.19
34.81
30.12
29.96
27.31
24.43
22.20
20.64

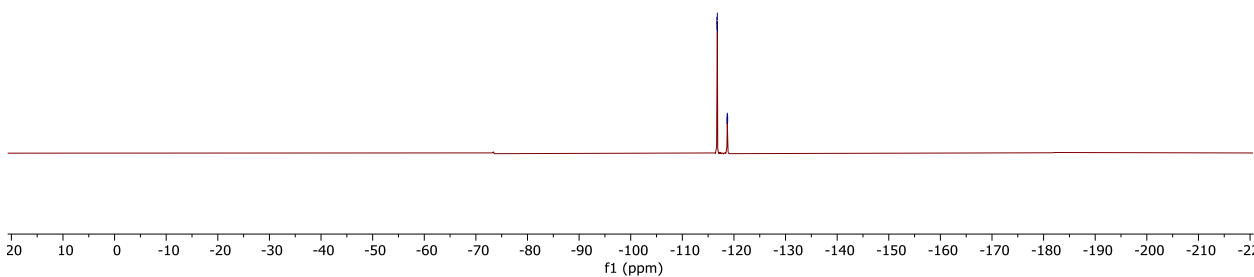
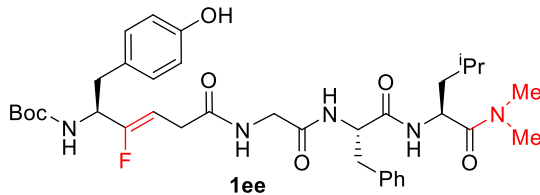
Parameter	Value
1 Title	KKS-1-204.100004.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	298.2
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans	5000
9 Receiver Gain	20.2
10 Relaxation Delay	0.1500
11 Pulse Width	10.0000
12 Acquisition Time	1.1010
13 Acquisition Date	2018-04-28T16:45:37
14 Modification Date	2018-04-28T16:45:37
15 Spectrometer Frequency	125.79
16 Spectral Width	29761.9
17 Lowest Frequency	-2304.1
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536



KKS-1-204-R.3.fid

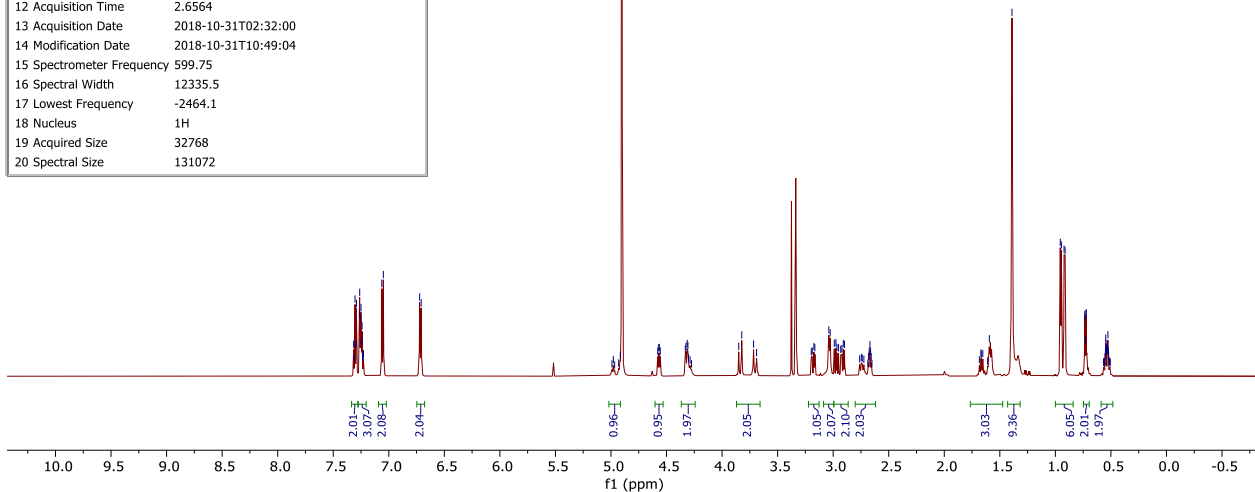
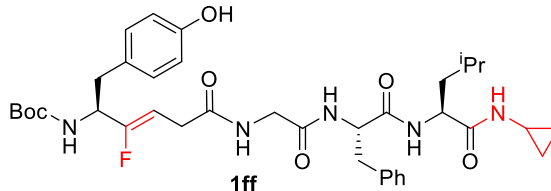
-116.70
-116.73
-116.78
-116.81
-118.67
-118.72
-118.73
-118.78

Parameter	Value
1 Title	KKS-1-204-R.3.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	DMSO
4 Temperature	298.2
5 Pulse Sequence	zgfgn
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans	16
9 Receiver Gain	575.0
10 Relaxation Delay	1.0000
11 Pulse Width	15.0000
12 Acquisition Time	0.5767
13 Acquisition Date	2018-06-05T10:18:13
14 Modification Date	2018-06-05T10:18:14
15 Spectrometer Frequency	470.60
16 Spectral Width	113636.4
17 Lowest Frequency	-103883.1
18 Nucleus	19F
19 Acquired Size	65536
20 Spectral Size	131072



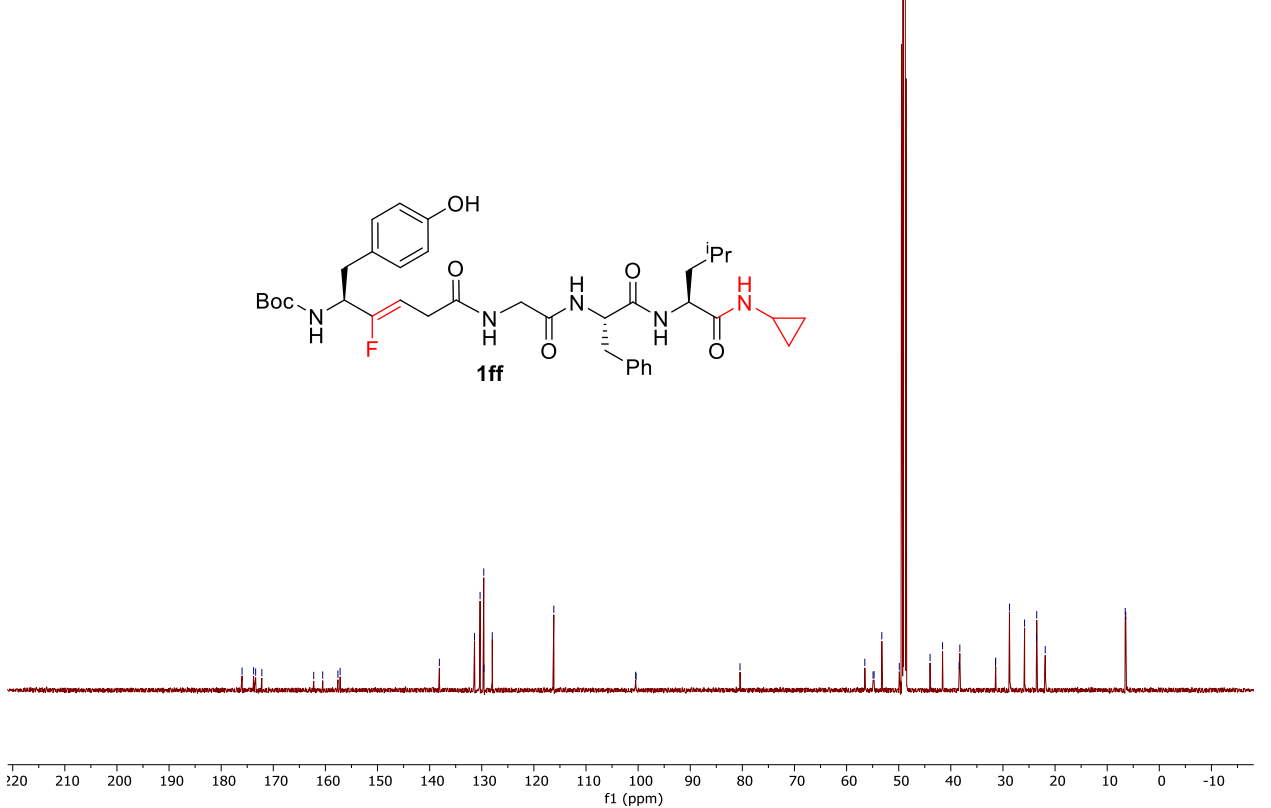
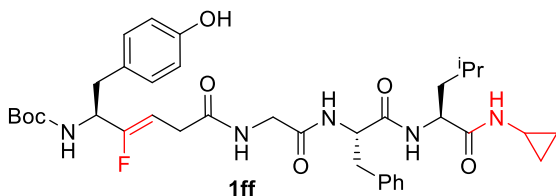
KKS-2-30.1.fid
 APROTON MeOD /opt/topspin3.0/ksatma

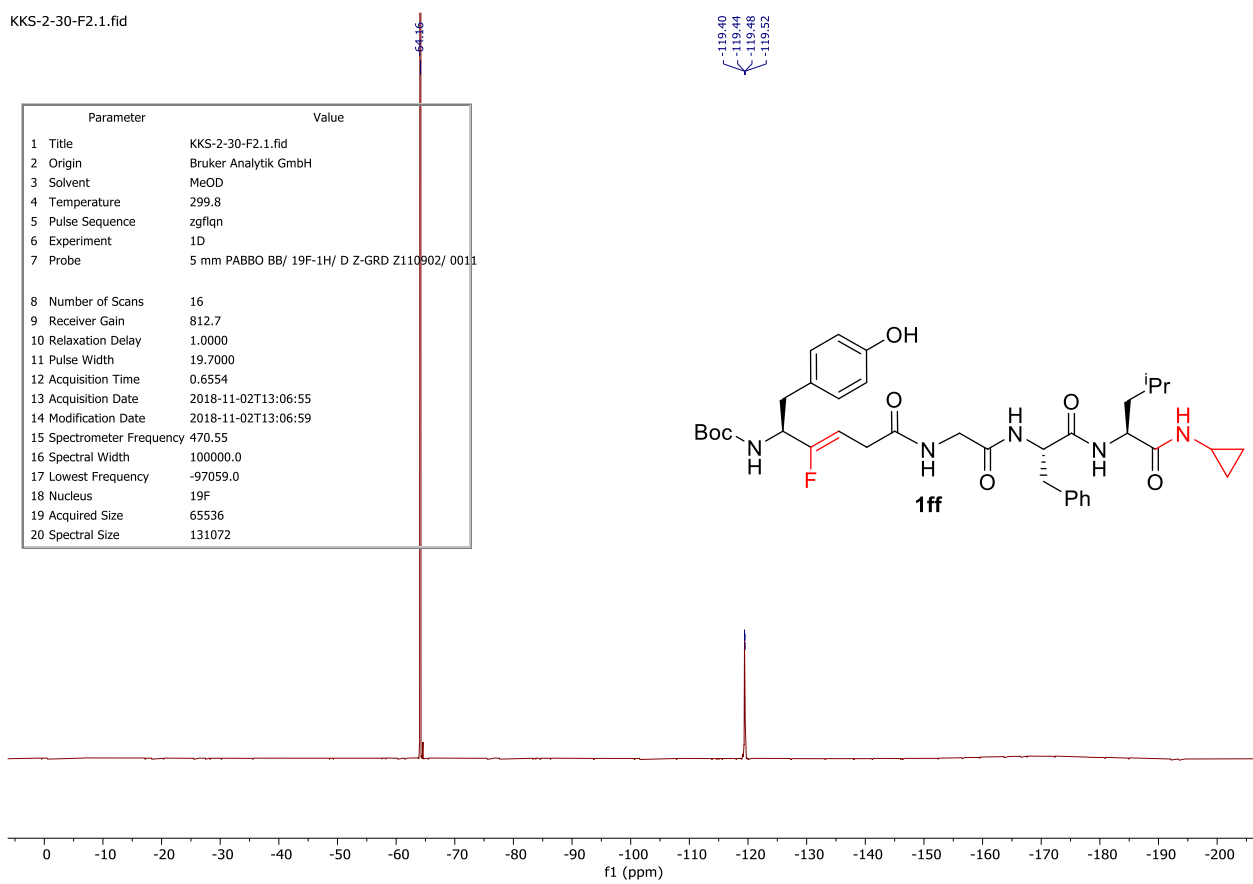
Parameter	Value
1 Title	KKS-2-30.1.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	296.2
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	5 mm PABBO BB-1H/ D Z-GRD Z114261/ 0020
8 Number of Scans	64
9 Receiver Gain	165.6
10 Relaxation Delay	1.0000
11 Pulse Width	16.0000
12 Acquisition Time	2.6564
13 Acquisition Date	2018-10-31T02:32:00
14 Modification Date	2018-10-31T10:49:04
15 Spectrometer Frequency	599.75
16 Spectral Width	12335.5
17 Lowest Frequency	-2464.1
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	131072

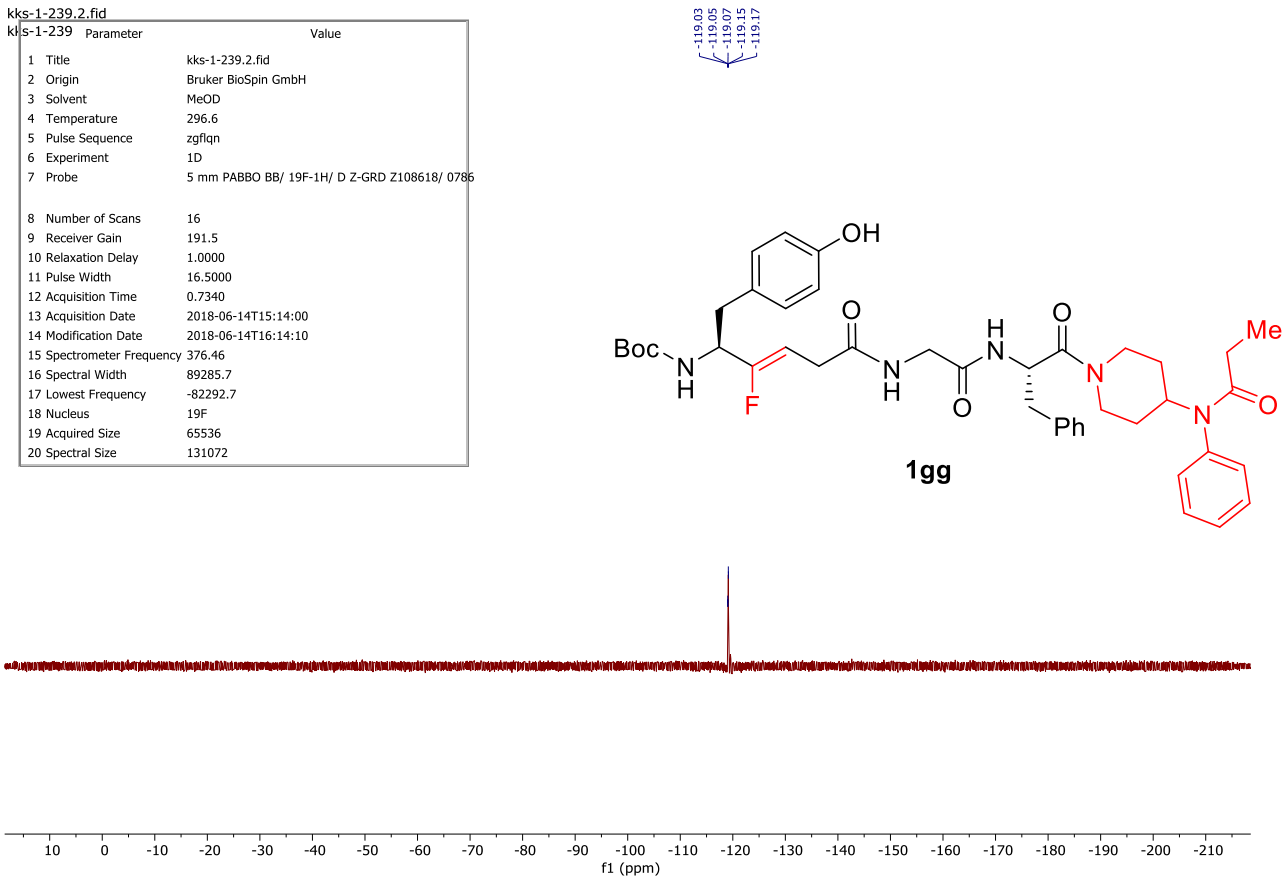
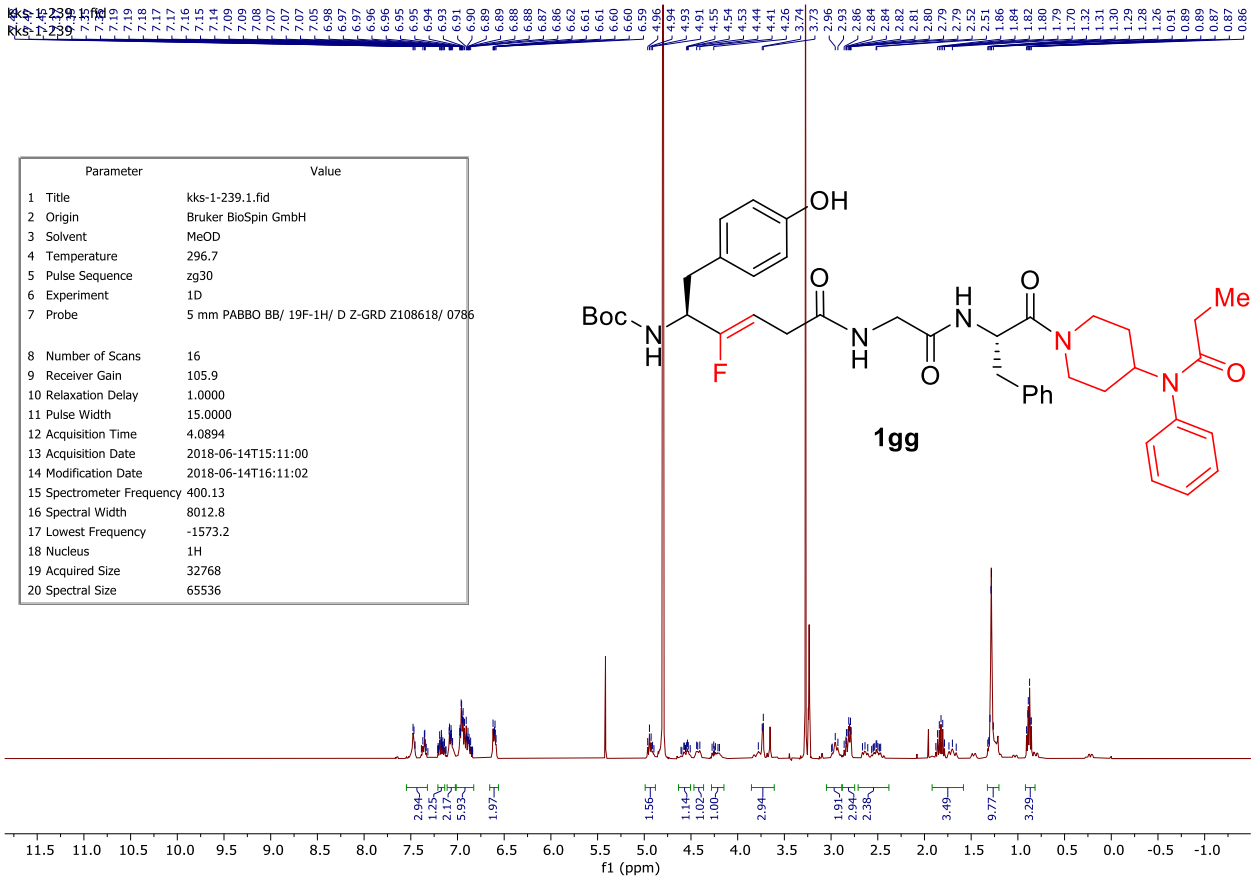


KKS-2-30.2.fid
 AAC13CPD MeOD /opt/topspin3.0/ksatma

138.13
 130.32
 129.62
 129.58
 127.99
 116.17
 100.48
 100.39
 80.45
 56.50
 54.92
 54.73
 53.24
 49.88
 43.98
 41.59
 38.49
 37.43
 31.43
 31.40
 28.75
 25.85
 23.56
 23.52
 21.89
 6.54
 6.43

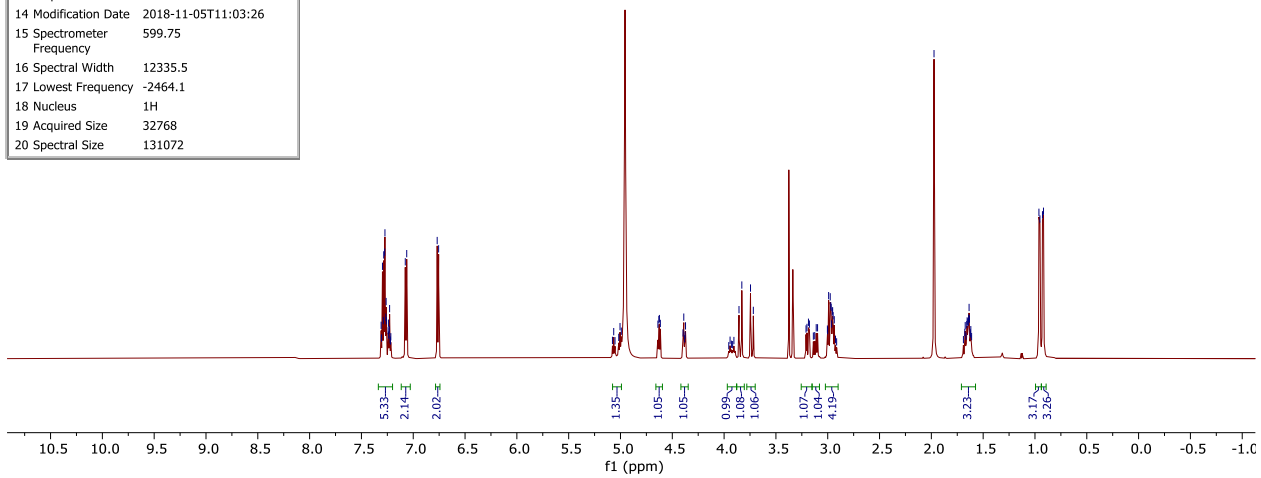
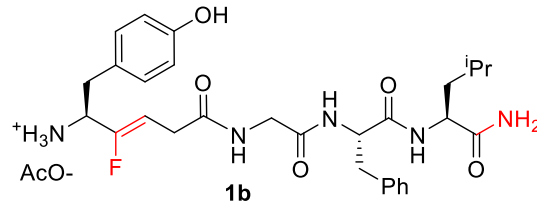






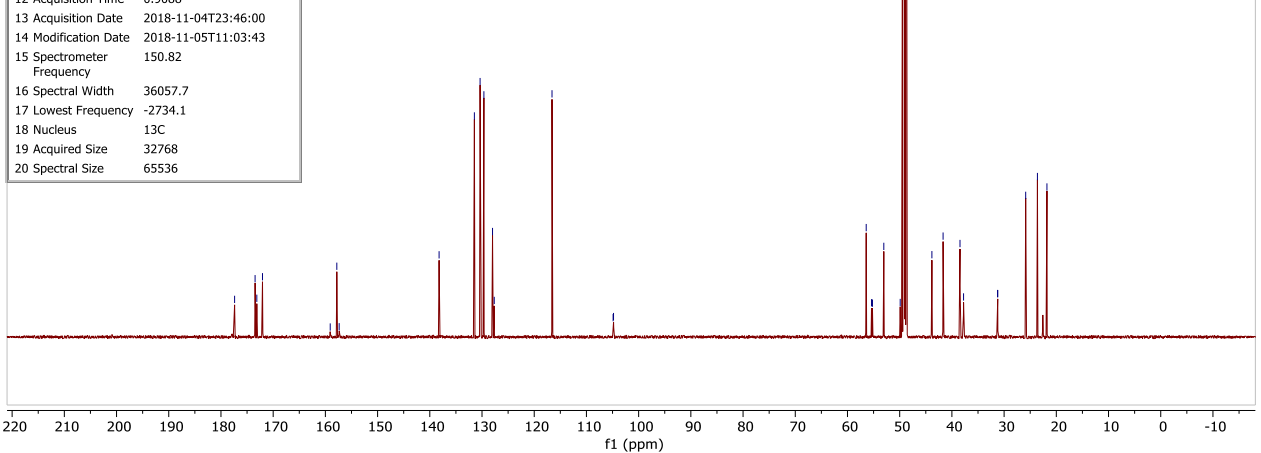
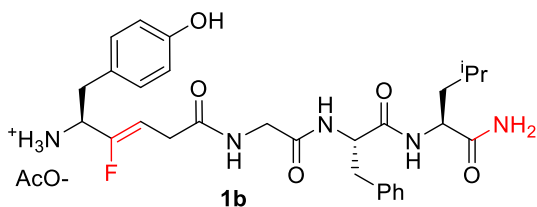
KKS-2-36.1.fid
 AAPROTIN MeOD /opt/topspin3.0/ksharma

Parameter	Value
1 Title	KKS-2-36.1.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	296.1
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	5 mm PABBO BB-1H/ D Z-GRD Z114261/ 0020
8 Number of Scans	64
9 Receiver Gain	87.1
10 Relaxation Delay	1.0000
11 Pulse Width	16.0000
12 Acquisition Time	2.6564
13 Acquisition Date	2018-11-04T19:32:00
14 Modification Date	2018-11-05T11:03:26
15 Spectrometer	599.75
Frequency	
16 Spectral Width	12335.5
17 Lowest Frequency	-2464.1
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	131072



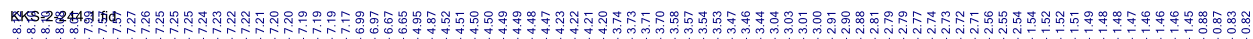
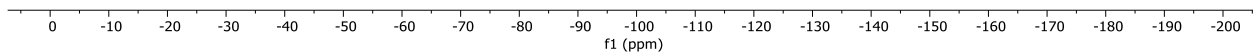
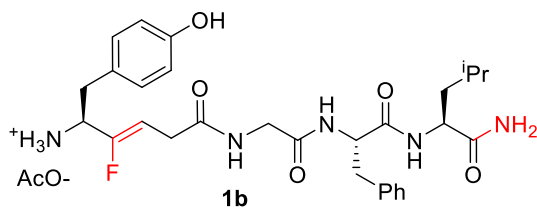
KKS-2-36.2.fid
 AAC13CPD MeOD /opt/topspin3.0/ksharma

Parameter	Value
1 Title	KKS-2-36.2.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	297.4
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Probe	5 mm PABBO BB-1H/ D Z-GRD Z114261/ 0020
8 Number of Scans	5120
9 Receiver Gain	185.8
10 Relaxation Delay	2.0000
11 Pulse Width	11.2000
12 Acquisition Time	0.9088
13 Acquisition Date	2018-11-04T23:46:00
14 Modification Date	2018-11-05T11:03:43
15 Spectrometer	150.82
Frequency	
16 Spectral Width	36057.7
17 Lowest Frequency	-2734.1
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536

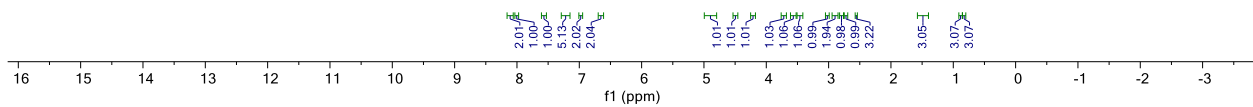
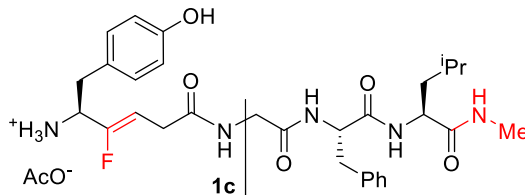


KKS-2-36-F.1.fid

Parameter	Value
1 Title	KKS-2-36-F.1.fid
2 Origin	Bruker Analytik GmbH
3 Solvent	MeOD
4 Temperature	299.8
5 Pulse Sequence	zgfgn
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z110902/ 0011
8 Number of Scans	16
9 Receiver Gain	912.3
10 Relaxation Delay	1.0000
11 Pulse Width	19.7000
12 Acquisition Time	0.6554
13 Acquisition Date	2018-11-06T13:23:48
14 Modification Date	2018-11-06T13:23:51
15 Spectrometer Frequency	470.55
16 Spectral Width	100000.0
17 Lowest Frequency	-96588.4
18 Nucleus	19F
19 Acquired Size	65536
20 Spectral Size	131072

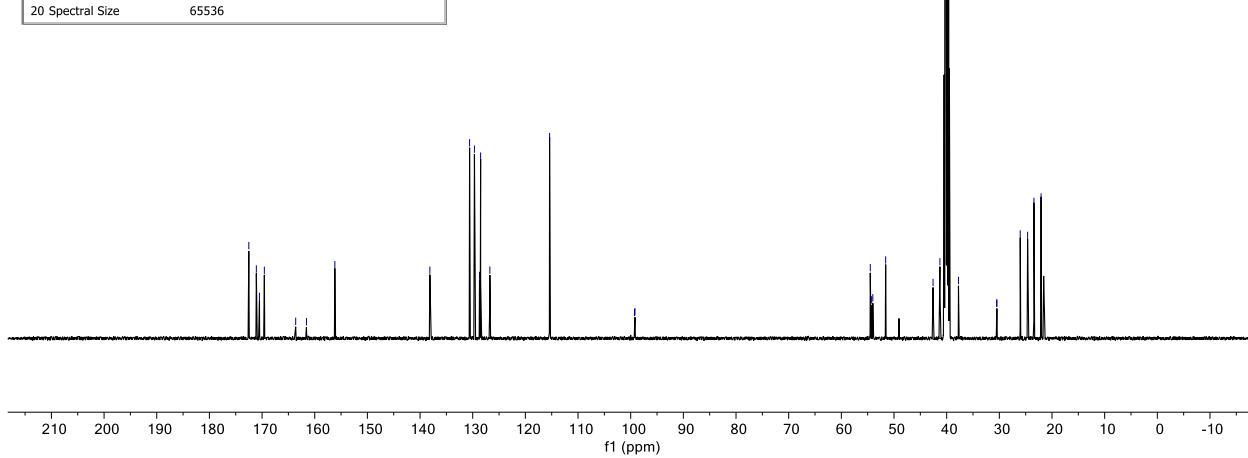
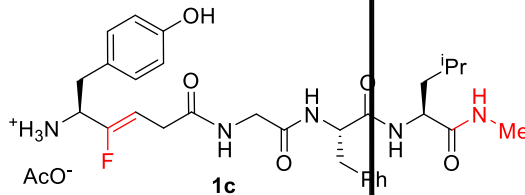


Parameter	Value
1 Title	KKS-2-244.1.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	DMSO
4 Temperature	298.2
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans	16
9 Receiver Gain	7.1
10 Relaxation Delay	1.0000
11 Pulse Width	12.0000
12 Acquisition Time	3.2768
13 Acquisition Date	2019-08-27T16:38:17
14 Modification Date	2019-08-27T15:38:17
15 Spectrometer Frequency	500.19
16 Spectral Width	10000.0
17 Lowest Frequency	-1911.3
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



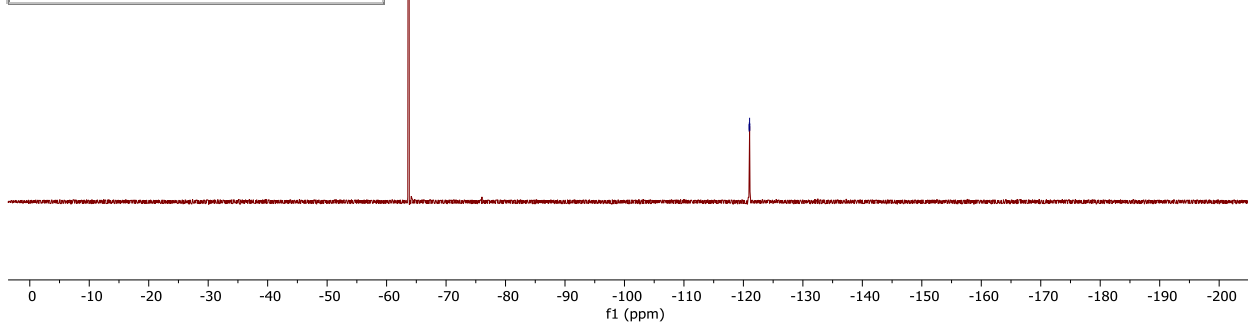
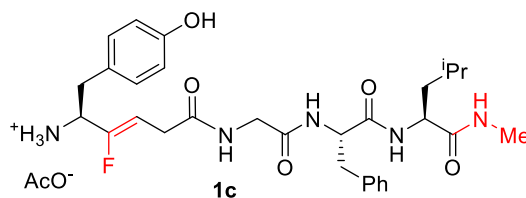
KKS-2-244_100002.fid

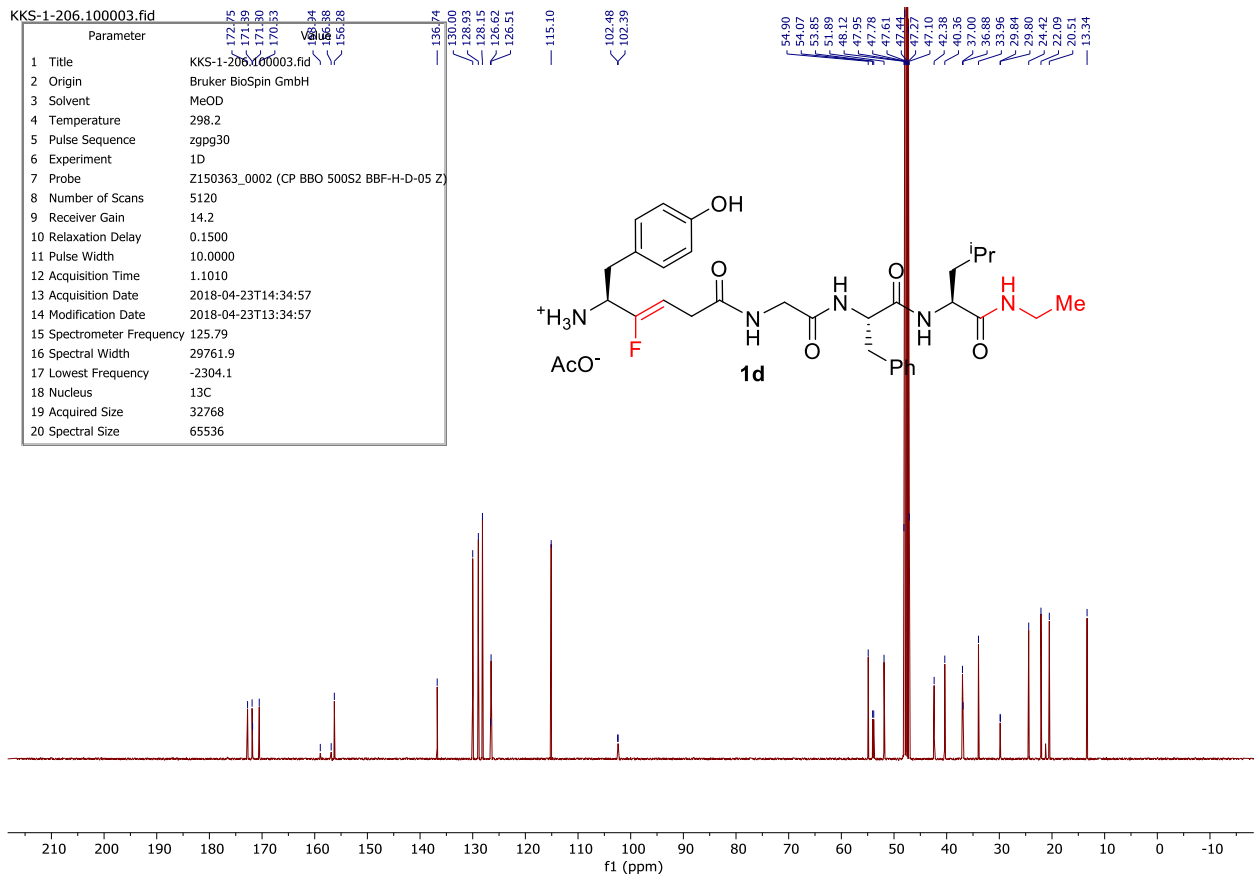
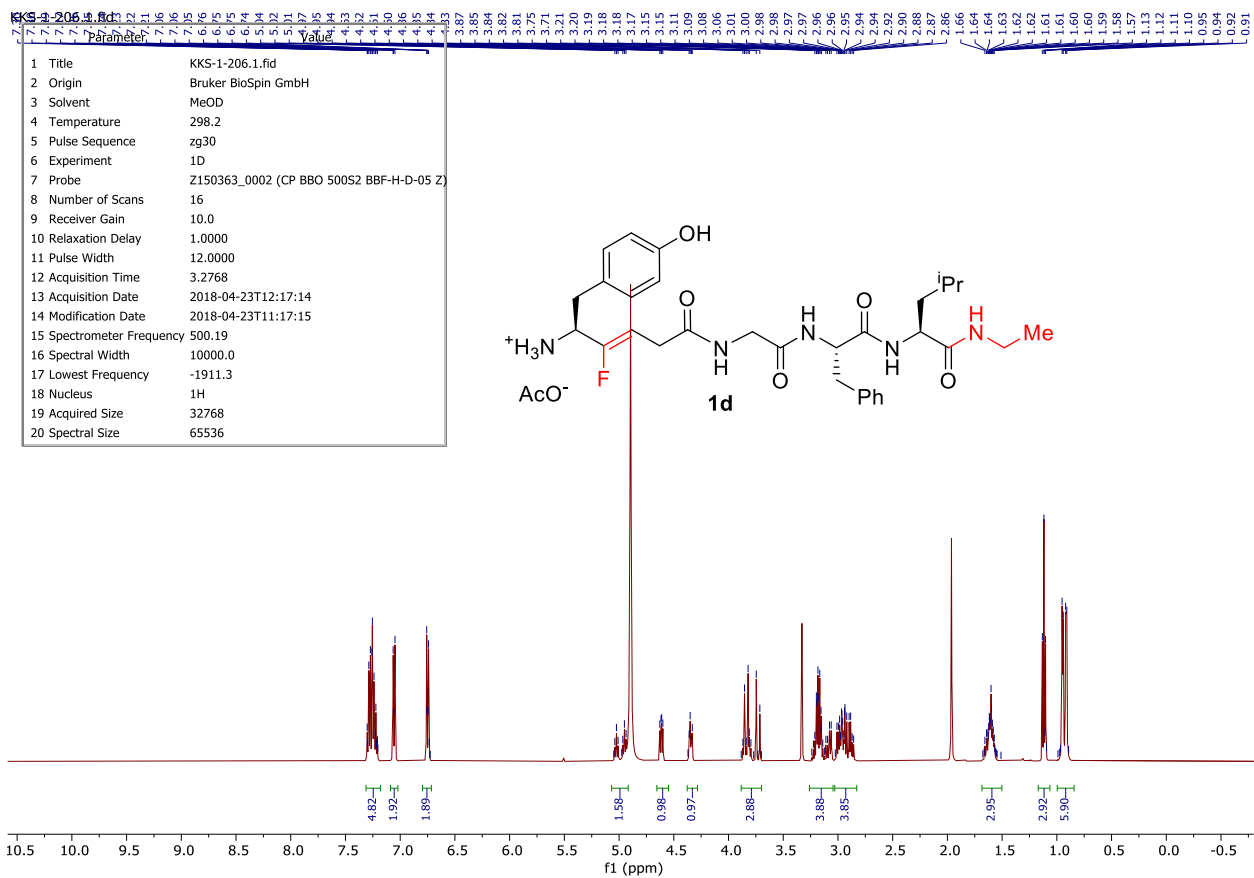
Parameter	Value
1 Title	KKS-2-244_100002.fid
2 Origin	Bruker Biospin GmbH
3 Solvent	DMSO
4 Temperature	298.2
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans	5120
9 Receiver Gain	12.7
10 Relaxation Delay	0.1500
11 Pulse Width	10.0000
12 Acquisition Time	1.1010
13 Acquisition Date	2019-08-27T18:34:02
14 Modification Date	2019-08-27T17:34:02
15 Spectrometer Frequency	125.79
16 Spectral Width	29761.9
17 Lowest Frequency	-2304.1
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536



kks-2-244-F with std.1.fid

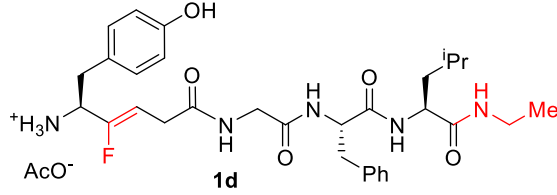
Parameter	Value
1 Title	kks-2-244-F with std.1.fid
2 Origin	Bruker Analytik GmbH
3 Solvent	DMSO
4 Temperature	298.2
5 Pulse Sequence	zgfgqn
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z110902/ 0011
8 Number of Scans	16
9 Receiver Gain	724.1
10 Relaxation Delay	1.0000
11 Pulse Width	19.7000
12 Acquisition Time	0.6554
13 Acquisition Date	2019-08-29T10:10:15
14 Modification Date	2019-08-29T10:10:17
15 Spectrometer Frequency	470.50
16 Spectral Width	100000.0
17 Lowest Frequency	-97054.3
18 Nucleus	19F
19 Acquired Size	65536
20 Spectral Size	131072



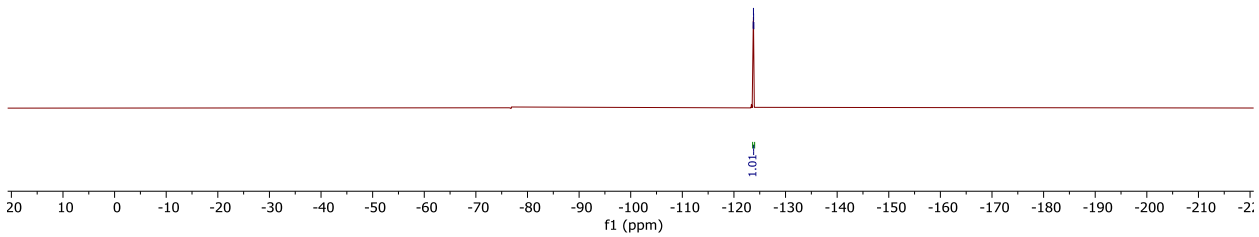


KKS-1-206.4.fid

Parameter	Value
1 Title	KKS-1-206.4.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	298.2
5 Pulse Sequence	zgfgqn
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans	16
9 Receiver Gain	406.0
10 Relaxation Delay	1.0000
11 Pulse Width	15.0000
12 Acquisition Time	0.5767
13 Acquisition Date	2018-04-23T14:40:18
14 Modification Date	2018-04-23T13:40:18
15 Spectrometer Frequency	470.60
16 Spectral Width	113636.4
17 Lowest Frequency	-103883.1
18 Nucleus	19F
19 Acquired Size	65536
20 Spectral Size	131072

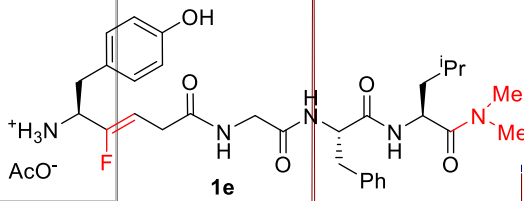


-123.73
-123.78
-123.81
-123.85

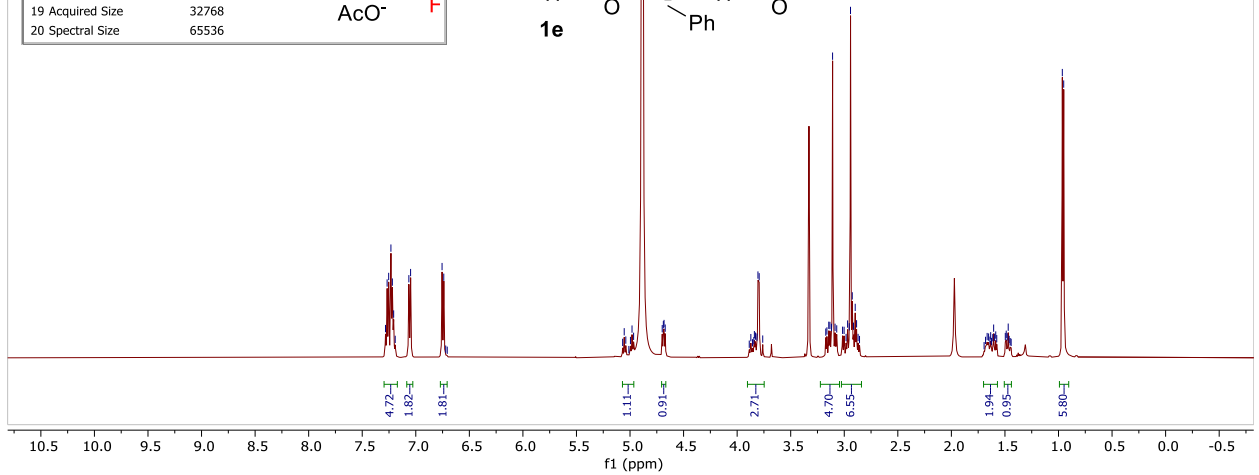


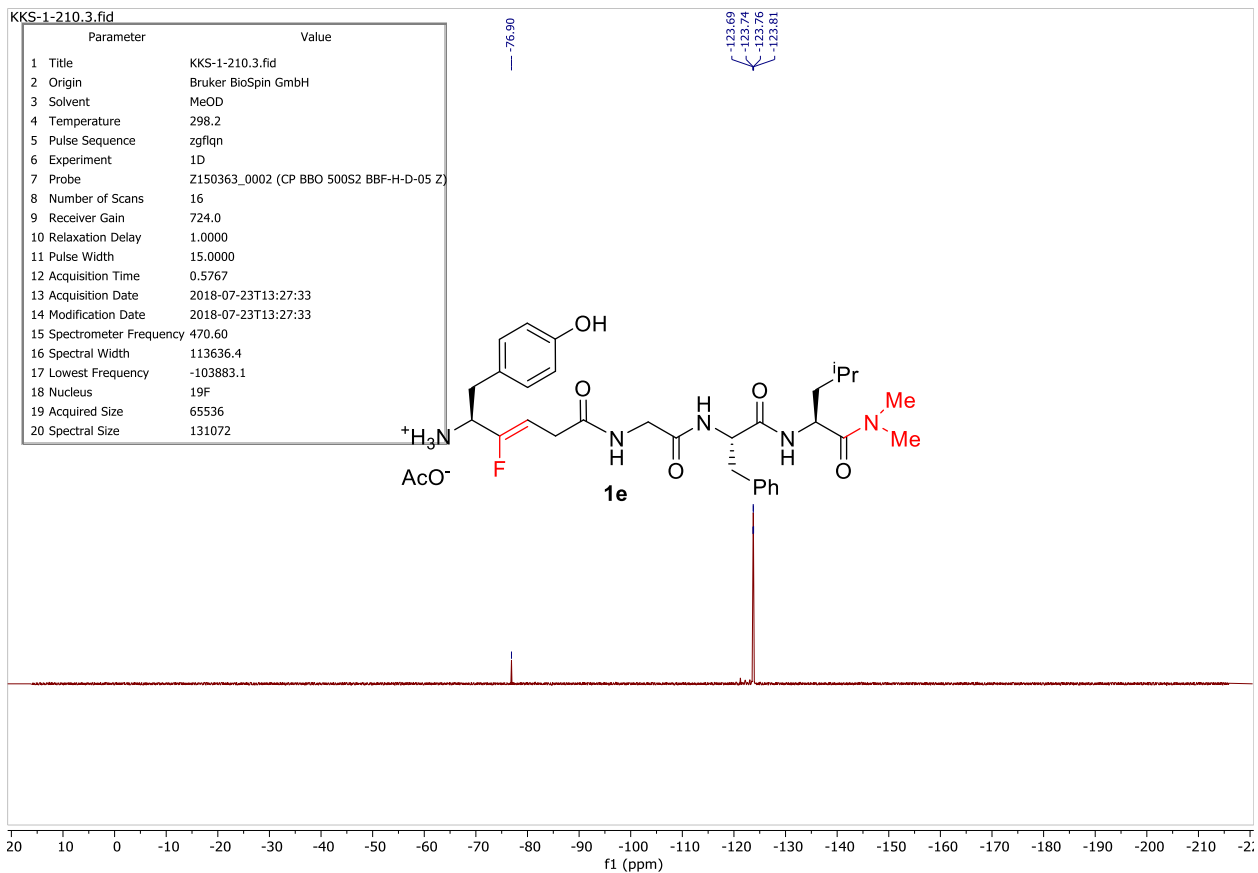
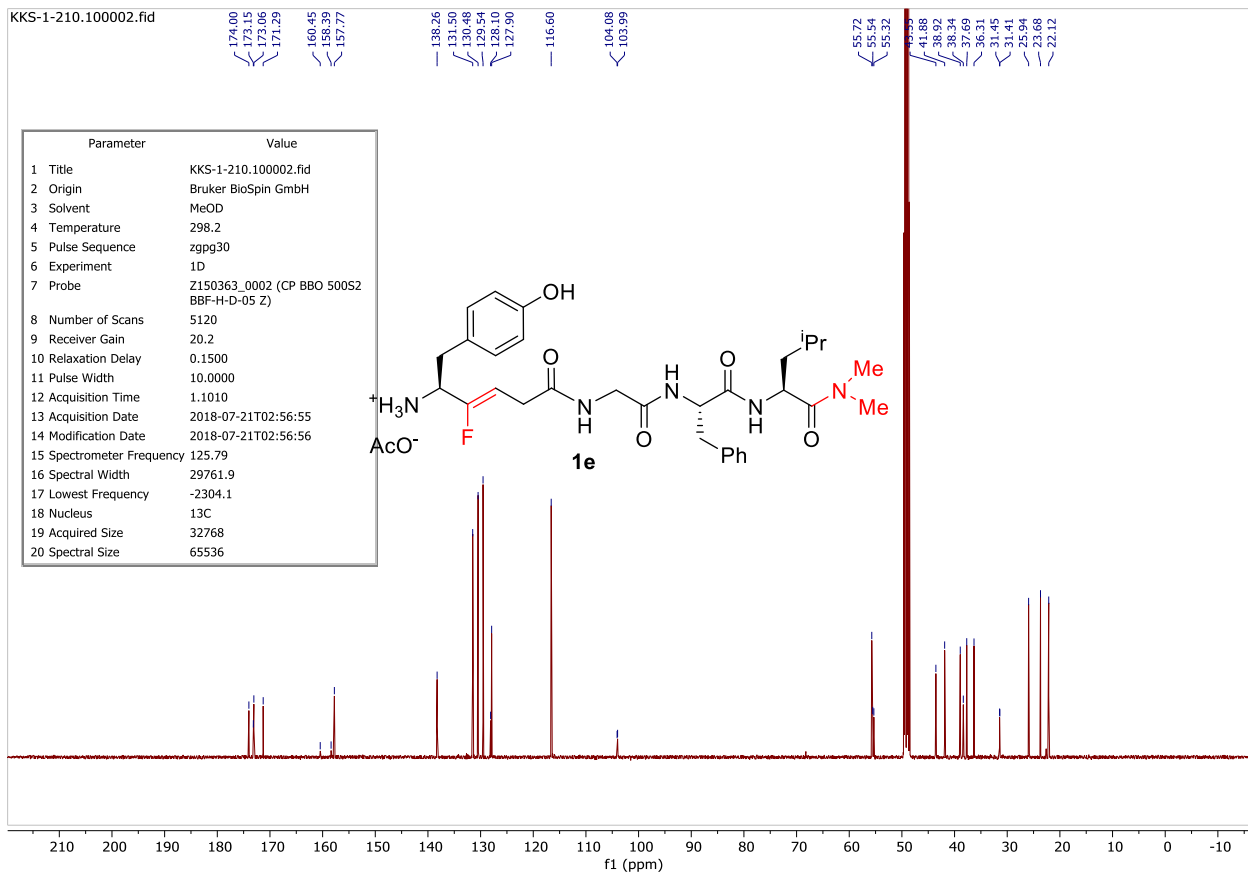
KKS-1-210.1.fid

Parameter	Value
1 Title	KKS-1-210.1.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	298.2
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans	16
9 Receiver Gain	9.0
10 Relaxation Delay	1.0000
11 Pulse Width	12.0000
12 Acquisition Time	3.2768
13 Acquisition Date	2018-07-21T00:09:10
14 Modification Date	2018-07-21T00:09:10
15 Spectrometer Frequency	500.19
16 Spectral Width	10000.0
17 Lowest Frequency	-1911.3
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



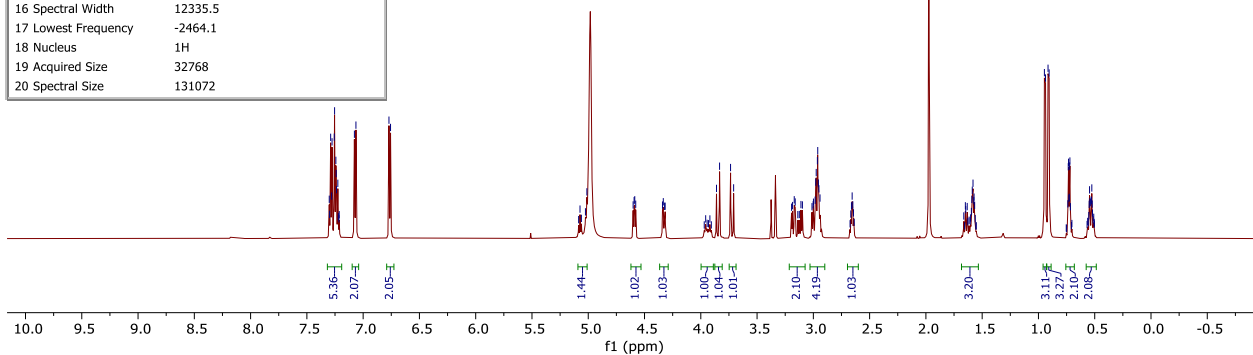
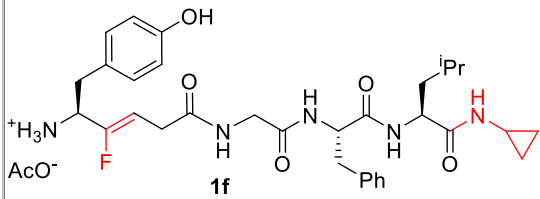
7.88
7.77
7.75
7.73
7.72
7.71
7.68
7.66
7.65
6.75
6.74
5.05
5.04
5.00
4.98
4.97
4.70
4.69
4.68
4.67
3.87
3.84
3.83
3.81
3.81
3.79
3.79
3.17
3.16
3.14
3.13
3.12
3.11
3.09
3.07
3.07
3.00
2.98
2.97
2.95
2.94
2.93
2.91
2.90
2.88
2.86
2.86
1.68
1.67
1.65
1.64
1.63
1.62
1.61
1.61
1.60
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1.49
1.48
1.47
1.46
1.46
1.06
1.06





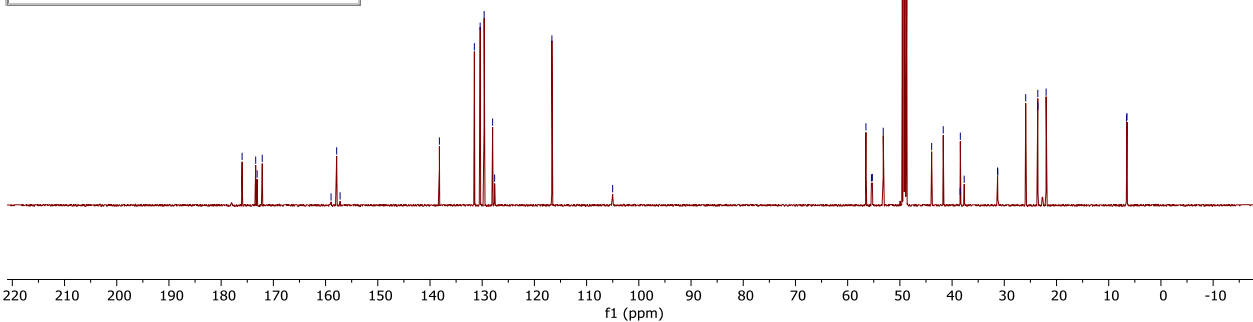
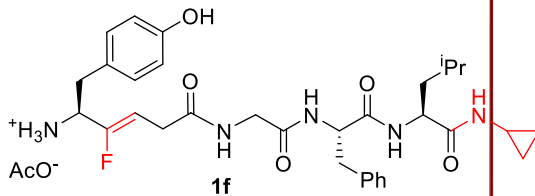
KKS-2-35.1.fid
 AAC13CPD MeOD /opt/topspin3.0/rsarma

Parameter	Value
1 Title	KKS-2-35.1.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	296.2
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	5 mm PABBO BB-1H/ D Z-GRD Z114261/ 0020
8 Number of Scans	64
9 Receiver Gain	62.4
10 Relaxation Delay	1.0000
11 Pulse Width	16.0000
12 Acquisition Time	2.6564
13 Acquisition Date	2018-11-07T03:29:00
14 Modification Date	2018-11-07T08:57:04
15 Spectrometer Frequency	599.75
16 Spectral Width	12335.5
17 Lowest Frequency	-2464.1
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	131072



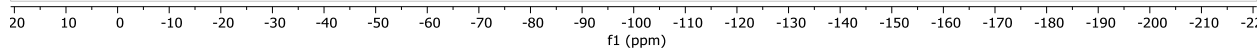
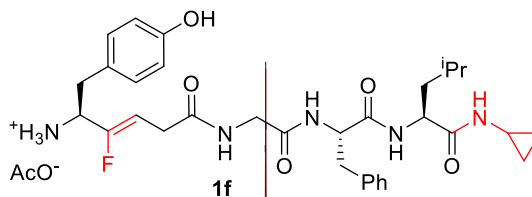
KKS-2-35.2.fid
 AAC13CPD MeOD /opt/topspin3.0/rsarma

Parameter	Value
1 Title	KKS-2-35.2.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	MeOD
4 Temperature	297.5
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Probe	5 mm PABBO BB-1H/ D Z-GRD Z114261/ 0020
8 Number of Scans	4096
9 Receiver Gain	185.8
10 Relaxation Delay	2.0000
11 Pulse Width	11.2000
12 Acquisition Time	0.9088
13 Acquisition Date	2018-11-07T06:52:00
14 Modification Date	2018-11-07T08:57:49
15 Spectrometer Frequency	150.82
16 Spectral Width	36057.7
17 Lowest Frequency	-2734.1
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536



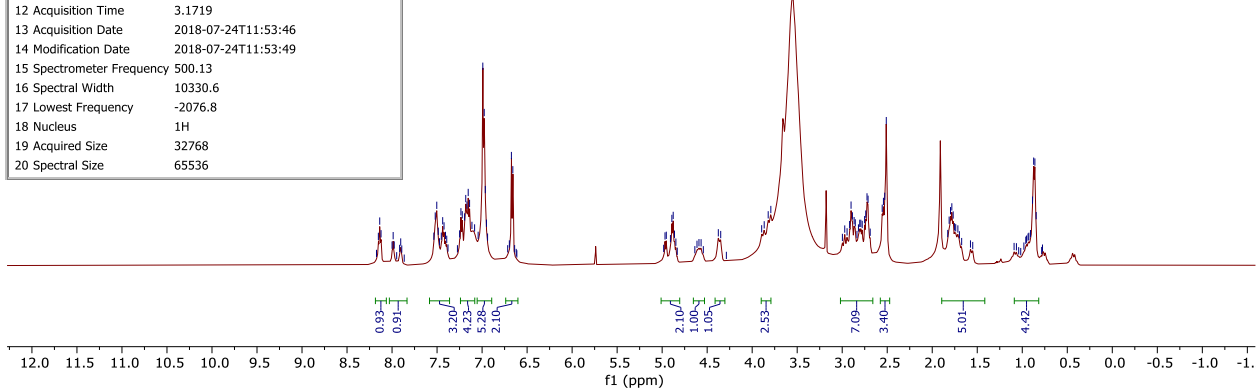
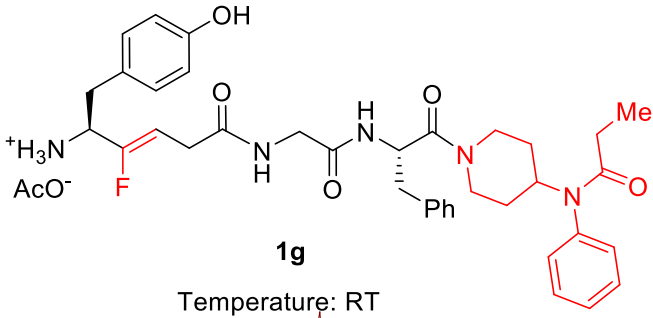
KKS-2-35-R_3.fid

Parameter	Value
1 Title	KKS-2-35-R_3.fid
2 Origin	Bruker BioSpin GmbH
3 Solvent	DMSO
4 Temperature	298.1
5 Pulse Sequence	zgfgq
6 Experiment	1D
7 Probe	Z150363_0002 (CP BBO 500S2 BBF-H-D-05 Z)
8 Number of Scans	16
9 Receiver Gain	812.0
10 Relaxation Delay	1.0000
11 Pulse Width	15.0000
12 Acquisition Time	0.5767
13 Acquisition Date	2018-12-27T16:15:02
14 Modification Date	2018-12-27T16:15:02
15 Spectrometer Frequency	470.60
16 Spectral Width	113636.4
17 Lowest Frequency	-103883.1
18 Nucleus	¹⁹ F
19 Acquired Size	65536
20 Spectral Size	131072



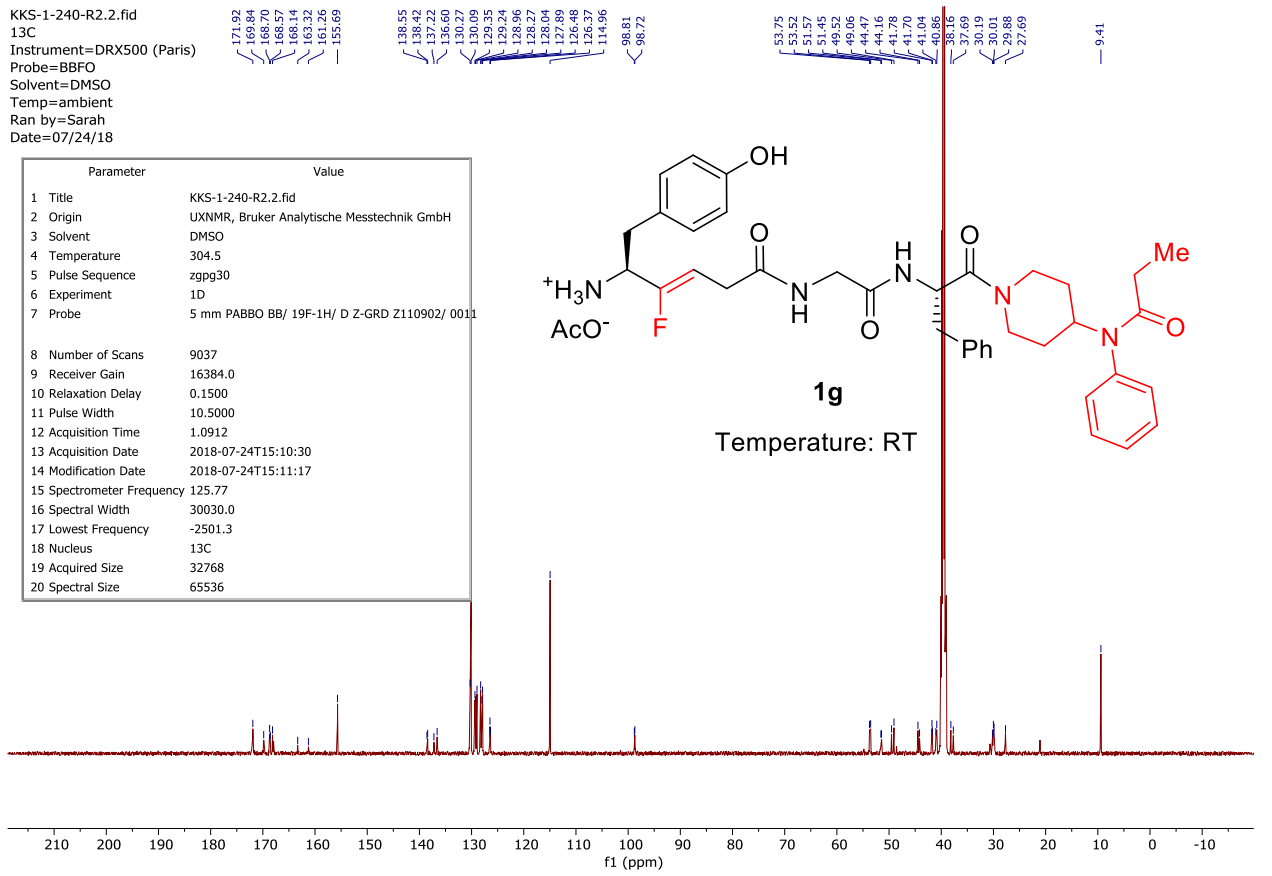
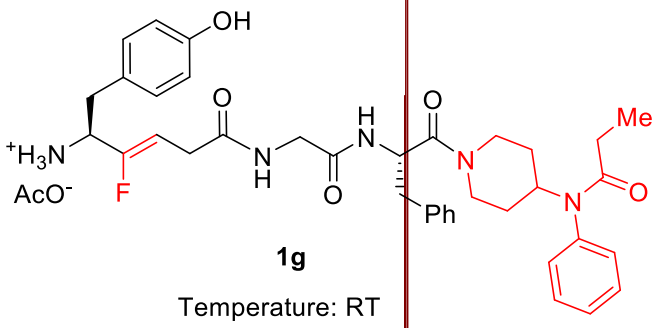
KKS-1-240-R2.1.fid
 Instrument=DRX500 (Paris)
 Probe=BBFO
 Solvent=DMSO
 Temp=ambient
 Ran by=Sarah
 Date=07/24/18

Parameter	Value
1 Title	KKS-1-240-R2.1.fid
2 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
3 Solvent	DMSO
4 Temperature	301.7
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z110902/ 0011
8 Number of Scans	16
9 Receiver Gain	71.8
10 Relaxation Delay	1.0000
11 Pulse Width	15.2000
12 Acquisition Time	3.1719
13 Acquisition Date	2018-07-24T11:53:46
14 Modification Date	2018-07-24T11:53:49
15 Spectrometer Frequency	500.13
16 Spectral Width	10330.6
17 Lowest Frequency	-2076.8
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



KKS-1-240-R2.2.fid
 13C
 Instrument=DRX500 (Paris)
 Probe=BBFO
 Solvent=DMSO
 Temp=ambient
 Ran by=Sarah
 Date=07/24/18

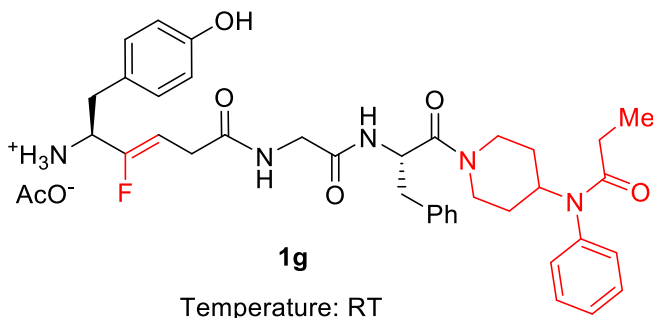
Parameter	Value
1 Title	KKS-1-240-R2.2.fid
2 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
3 Solvent	DMSO
4 Temperature	304.5
5 Pulse Sequence	zgpg30
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z110902/ 0011
8 Number of Scans	9037
9 Receiver Gain	16384.0
10 Relaxation Delay	0.1500
11 Pulse Width	10.5000
12 Acquisition Time	1.0912
13 Acquisition Date	2018-07-24T15:10:30
14 Modification Date	2018-07-24T15:11:17
15 Spectrometer Frequency	125.77
16 Spectral Width	30030.0
17 Lowest Frequency	-2501.3
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536



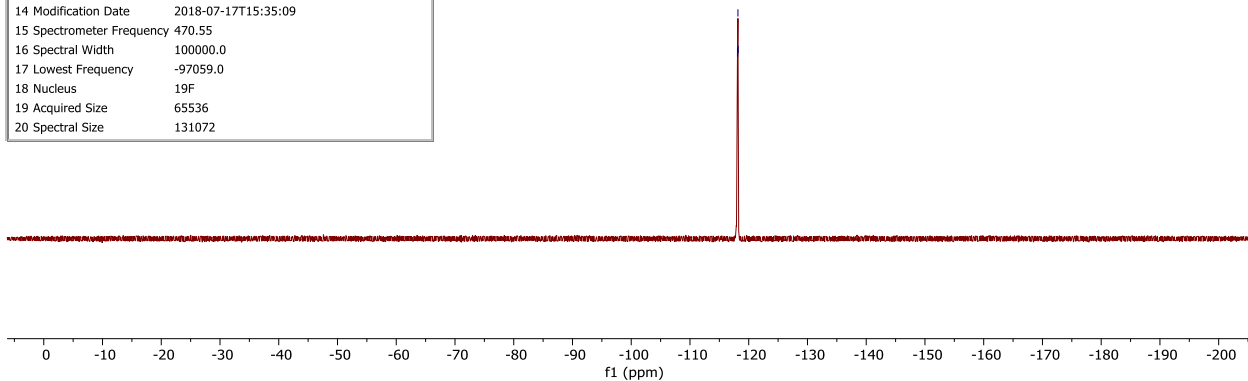
KKS-1-240-R.12.fid
 KKS-1-240-R
 19F (run at 30 C; after heating to 100 C)

Instrument=DRX500 (Paris)
 Probe=BBFO
 Solvent=DMSO
 Temp=ambient
 Ran by=Sarah
 Date=07/17/18

Parameter	Value
1 Title	KKS-1-240-R.12.fid
2 Origin	Bruker Analytik GmbH
3 Solvent	DMSO
4 Temperature	305.4
5 Pulse Sequence	zgflq
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z110902/0011
8 Number of Scans	16
9 Receiver Gain	912.3
10 Relaxation Delay	1.0000
11 Pulse Width	19.7000
12 Acquisition Time	0.6554
13 Acquisition Date	2018-07-17T15:35:05
14 Modification Date	2018-07-17T15:35:09
15 Spectrometer Frequency	470.55
16 Spectral Width	100000.0
17 Lowest Frequency	-97059.0
18 Nucleus	19F
19 Acquired Size	65536
20 Spectral Size	131072

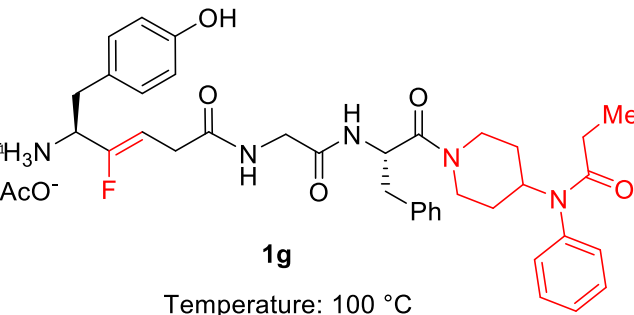


Temperature: RT

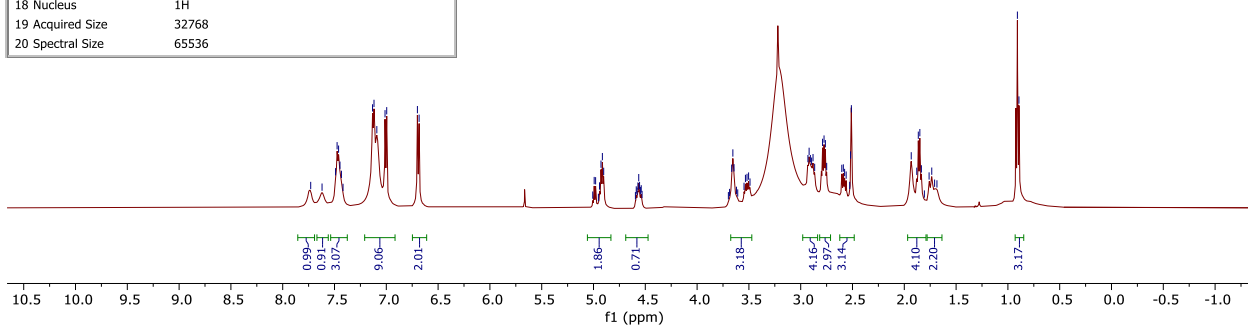


KKS-1-240-R2.101.fid
 1H at 100 C
 Instrument=DRX500 (Paris)
 Probe=BBFO
 Solvent=DMSO
 Temp=100 C
 Ran by=Sarah
 Date=07/26/18

Parameter	Value
1 Title	KKS-1-240-R2.101.fid
2 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
3 Solvent	DMSO
4 Temperature	372.4
5 Pulse Sequence	zg30
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z110902/0011
8 Number of Scans	16
9 Receiver Gain	90.5
10 Relaxation Delay	1.0000
11 Pulse Width	15.2000
12 Acquisition Time	3.1719
13 Acquisition Date	2018-07-26T11:16:03
14 Modification Date	2018-07-26T11:16:06
15 Spectrometer Frequency	500.13
16 Spectral Width	10330.6
17 Lowest Frequency	-2076.8
18 Nucleus	1H
19 Acquired Size	32768
20 Spectral Size	65536



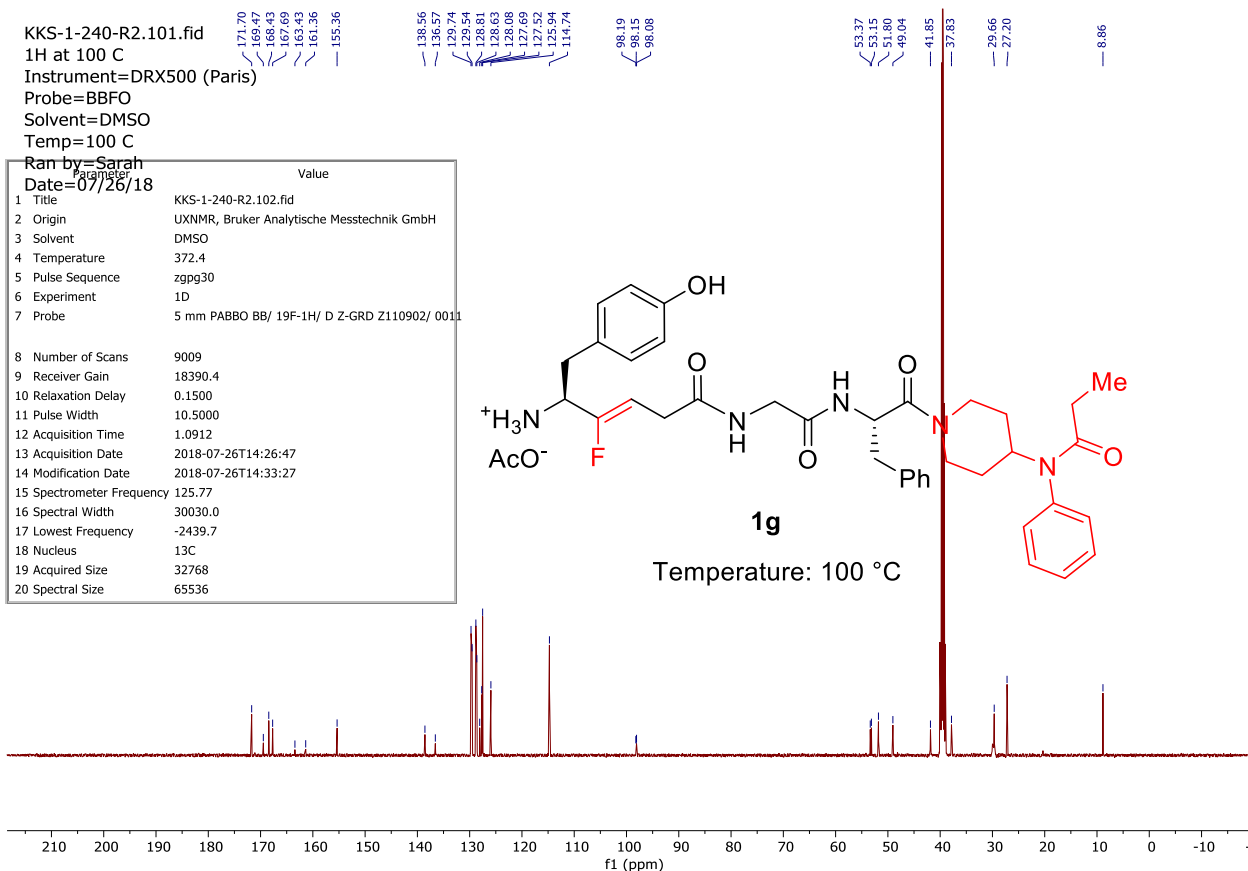
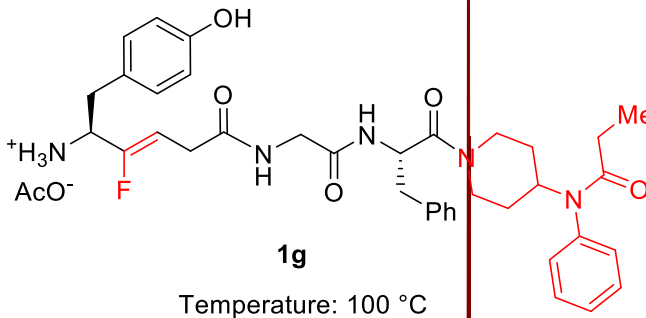
Temperature: 100 °C



KKS-1-240-R2.101.fid
 1H at 100 C
 Instrument=DRX500 (Paris)
 Probe=BBFO
 Solvent=DMSO
 Temp=100 C

Ran by=Sarah
 Date=07/26/18

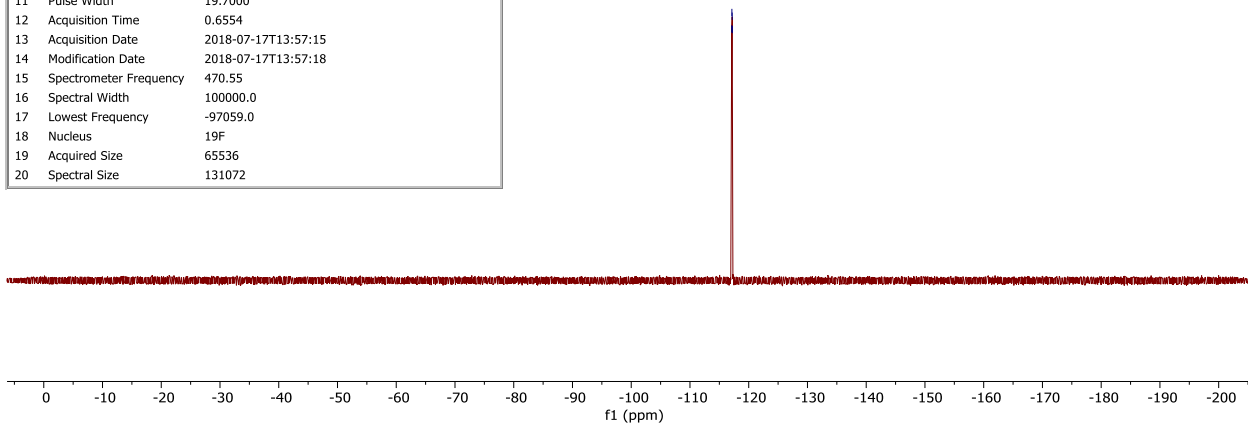
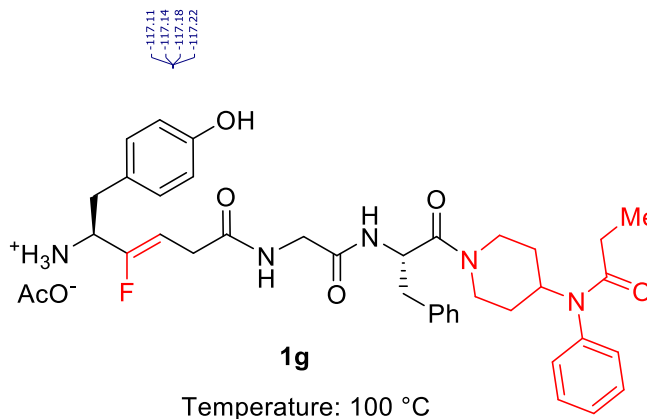
Parameter	Value
1 Title	KKS-1-240-R2.102.fid
2 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
3 Solvent	DMSO
4 Temperature	372.4
5 Pulse Sequence	zpgg30
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z110902/ 0011
8 Number of Scans	9009
9 Receiver Gain	18390.4
10 Relaxation Delay	0.1500
11 Pulse Width	10.5000
12 Acquisition Time	1.0912
13 Acquisition Date	2018-07-26T14:26:47
14 Modification Date	2018-07-26T14:33:27
15 Spectrometer Frequency	125.77
16 Spectral Width	30030.0
17 Lowest Frequency	-2439.7
18 Nucleus	13C
19 Acquired Size	32768
20 Spectral Size	65536



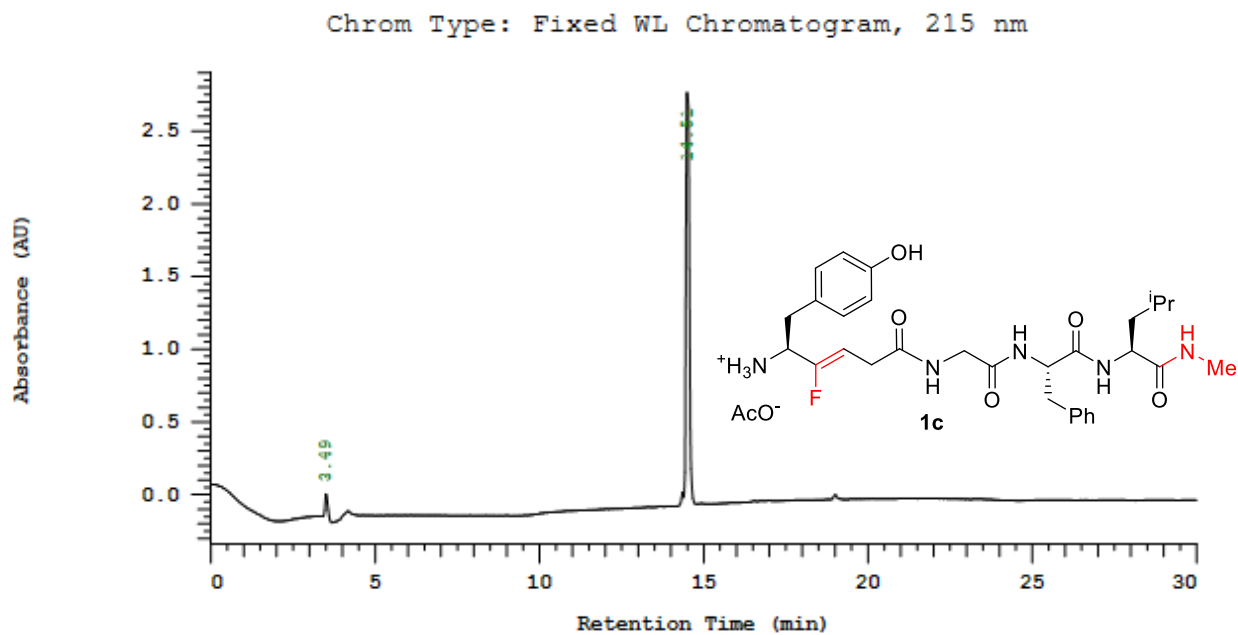
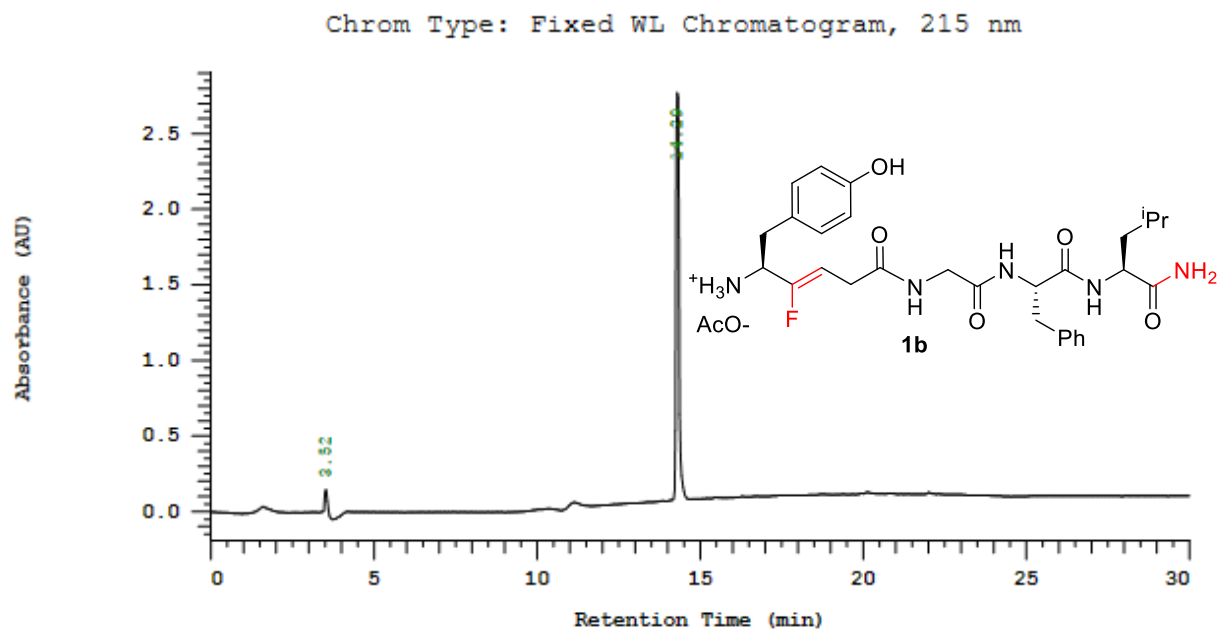
KKS-1-240-R.102.fid
 KKS-1-240-R
 19F

Instrument=DRX500 (Paris)
 Probe=BBFO
 Solvent=DMSO
 Temp=100
 Ran by=Sarah
 Date=07/17/18

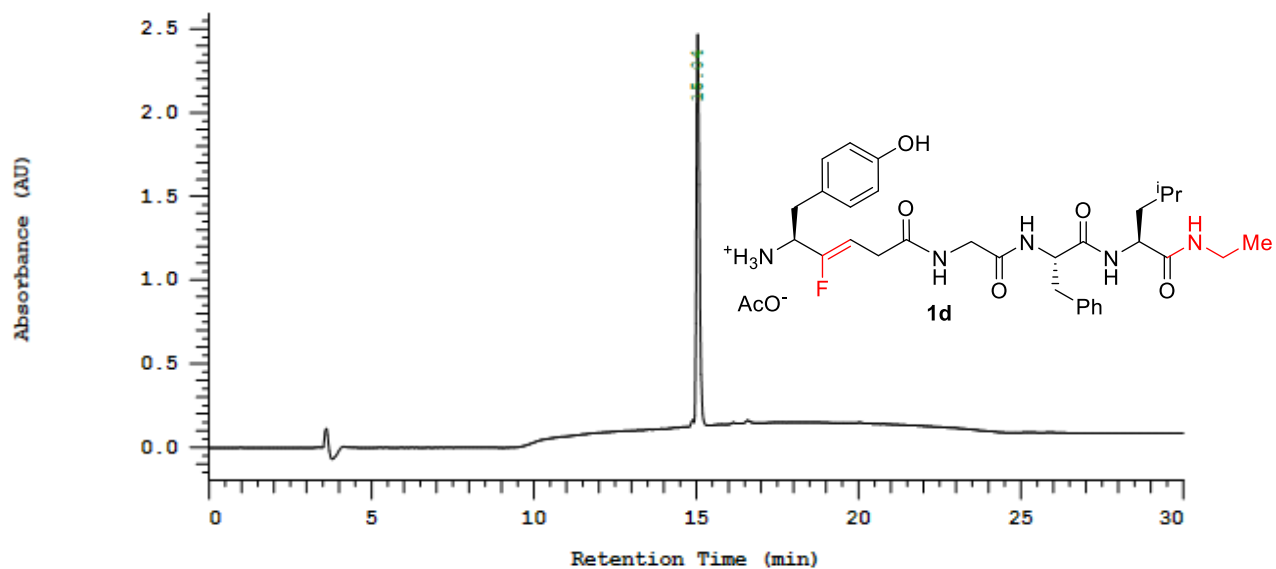
Parameter	Value
1 Title	KKS-1-240-R.102.fid
2 Origin	Bruker Analytik GmbH
3 Solvent	DMSO
4 Temperature	372.4
5 Pulse Sequence	zgfgn
6 Experiment	1D
7 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z110902/ 0011
8 Number of Scans	16
9 Receiver Gain	1024.0
10 Relaxation Delay	1.0000
11 Pulse Width	19.7000
12 Acquisition Time	0.6554
13 Acquisition Date	2018-07-17T13:57:15
14 Modification Date	2018-07-17T13:57:18
15 Spectrometer Frequency	470.55
16 Spectral Width	100000.0
17 Lowest Frequency	-97059.0
18 Nucleus	19F
19 Acquired Size	65536
20 Spectral Size	131072



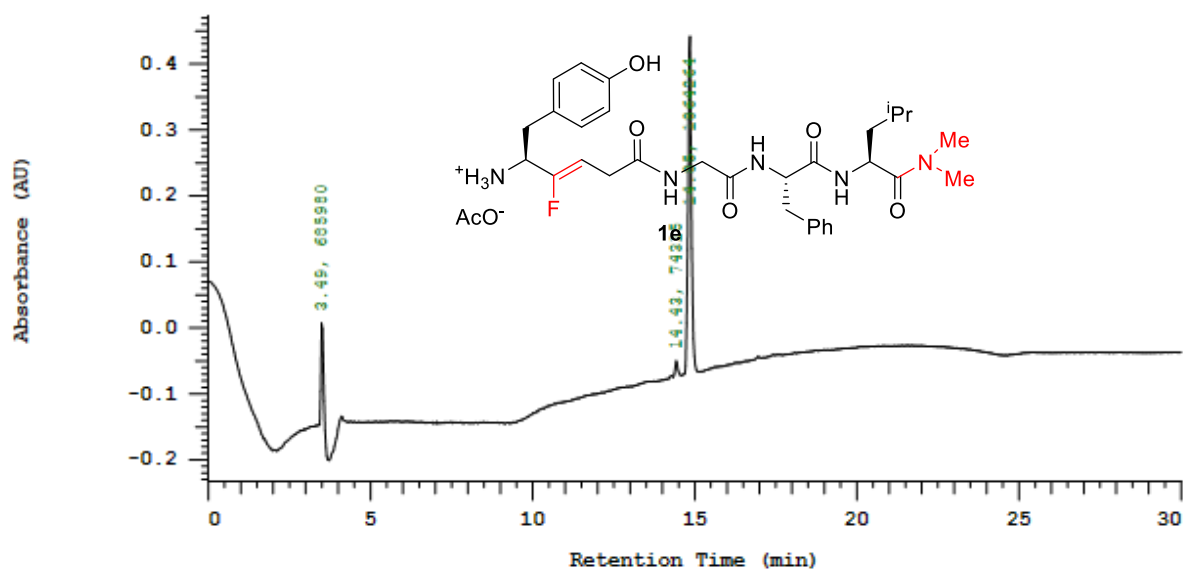
2. HPLC Chromatograms of Final Compounds



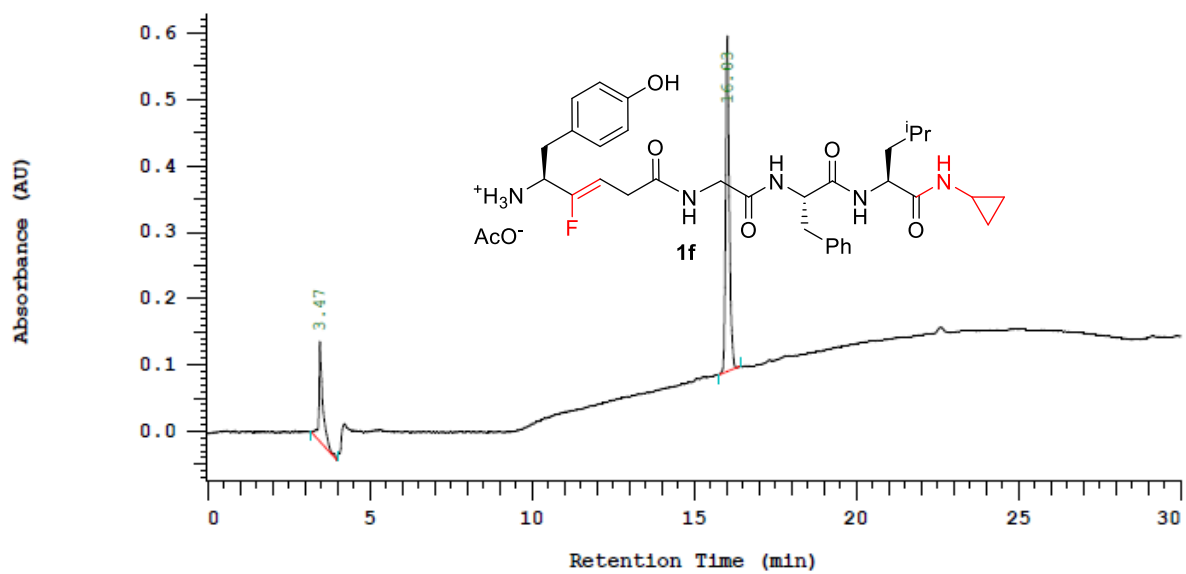
Chrom Type: Fixed WL Chromatogram, 215 nm



Chrom Type: Fixed WL Chromatogram, 215 nm



Chrom Type: Fixed WL Chromatogram, 215 nm



Chrom Type: Fixed WL Chromatogram, 215 nm

