Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supplementary Information

Synthesis and Evaluation of Analogues of the Glycinocin Family of Calcium-Dependent Antibiotics

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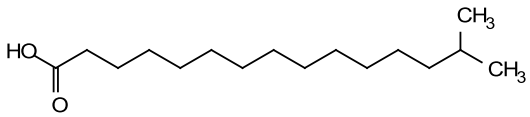
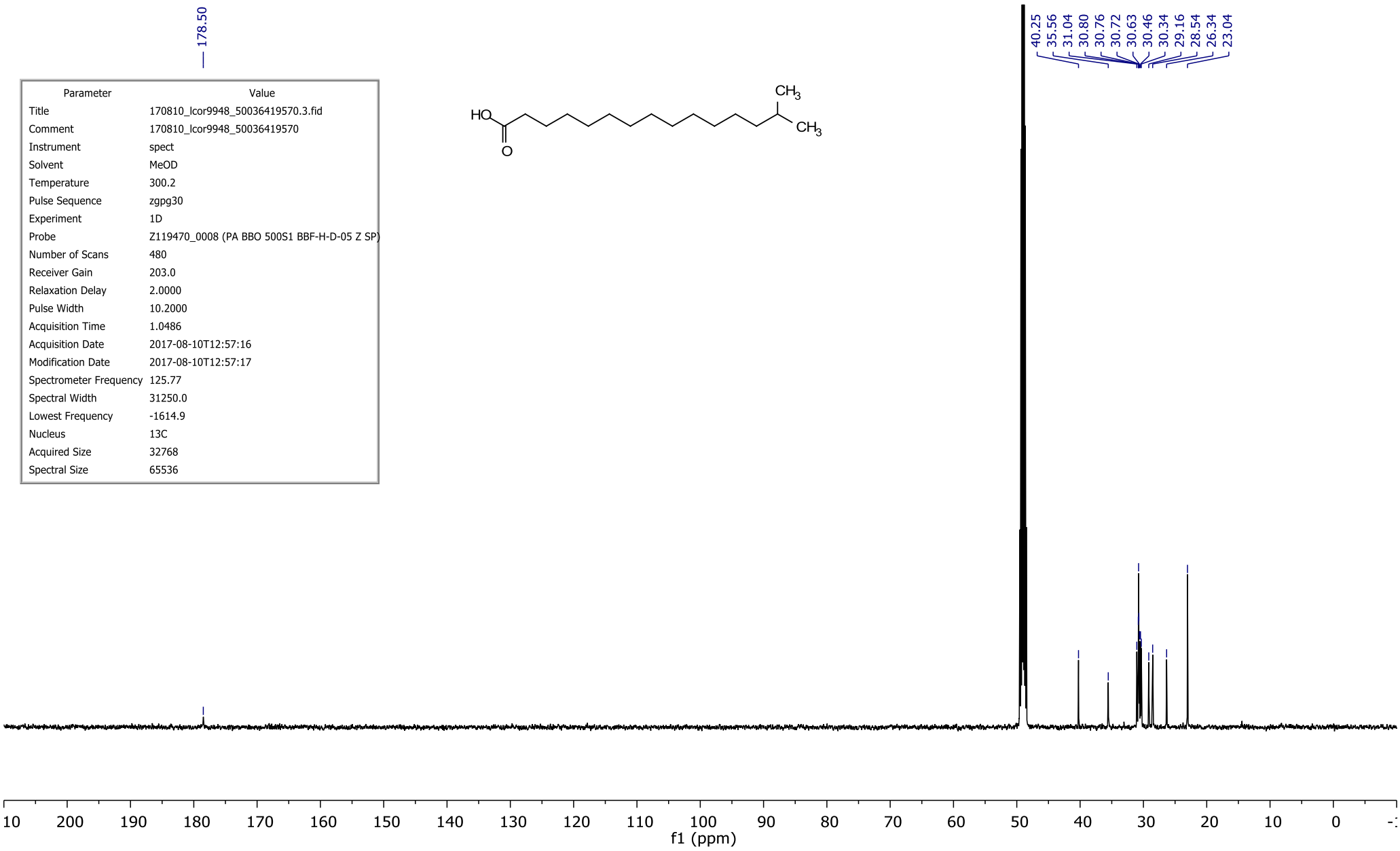
NMR Spectra for Novel Compounds

14-methylpentadecanoic acid (**6**) ^{1}H NMR (500 MHz, methanol-d_4)

Parameter	Value
Title	170810_lcor9948_50036 419570.1.fid
Comment	170810_lcor9948_50036 419570
Instrument	spect
Solvent	MeOD
Temperature	300.0
Pulse Sequence	zg
Experiment	1D
Probe	Z119470_0008 (PA BBO 500S1 BBF-H-D-05 Z SP)
Number of Scans	8
Receiver Gain	45.2
Relaxation Delay	2.0000
Pulse Width	14.0000
Acquisition Time	3.2769
Acquisition Date	2017-08-10T12:07:15
Modification Date	2017-08-10T12:07:15
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-2008.7
Nucleus	1H
Acquired Size	32768
Spectral Size	65536



14-methylpentadecanoic acid (**6**) ^{13}C NMR (126 MHz, methanol-d_4)



Parameter	Value
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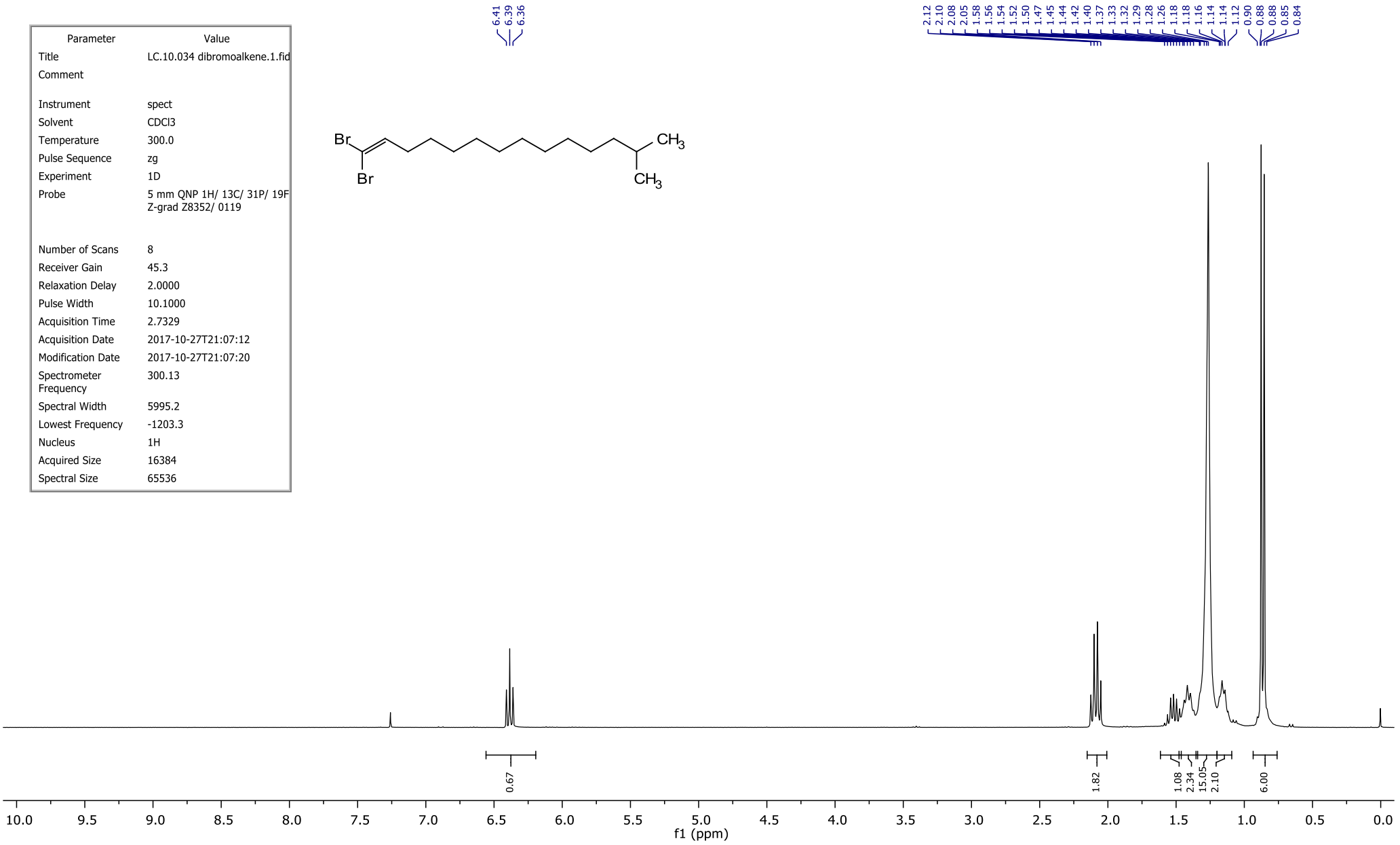
Comment	170810_lcor9948_50036419570
Instrument	spect
Solvent	MeOD
Temperature	300.2
Pulse Sequence	zgpg30
Experiment	1D
Probe	Z119470_0008 (PA BBO 500S1 BBF-H-D-05 Z SP)
Number of Scans	480
Receiver Gain	203.0
Relaxation Delay	2.0000
Pulse Width	10.2000
Acquisition Time	1.0486
Acquisition Date	2017-08-10T12:57:16
Modification Date	2017-08-10T12:57:17
Spectrometer Frequency	125.77
Spectral Width	31250.0
Lowest Frequency	-1614.9
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

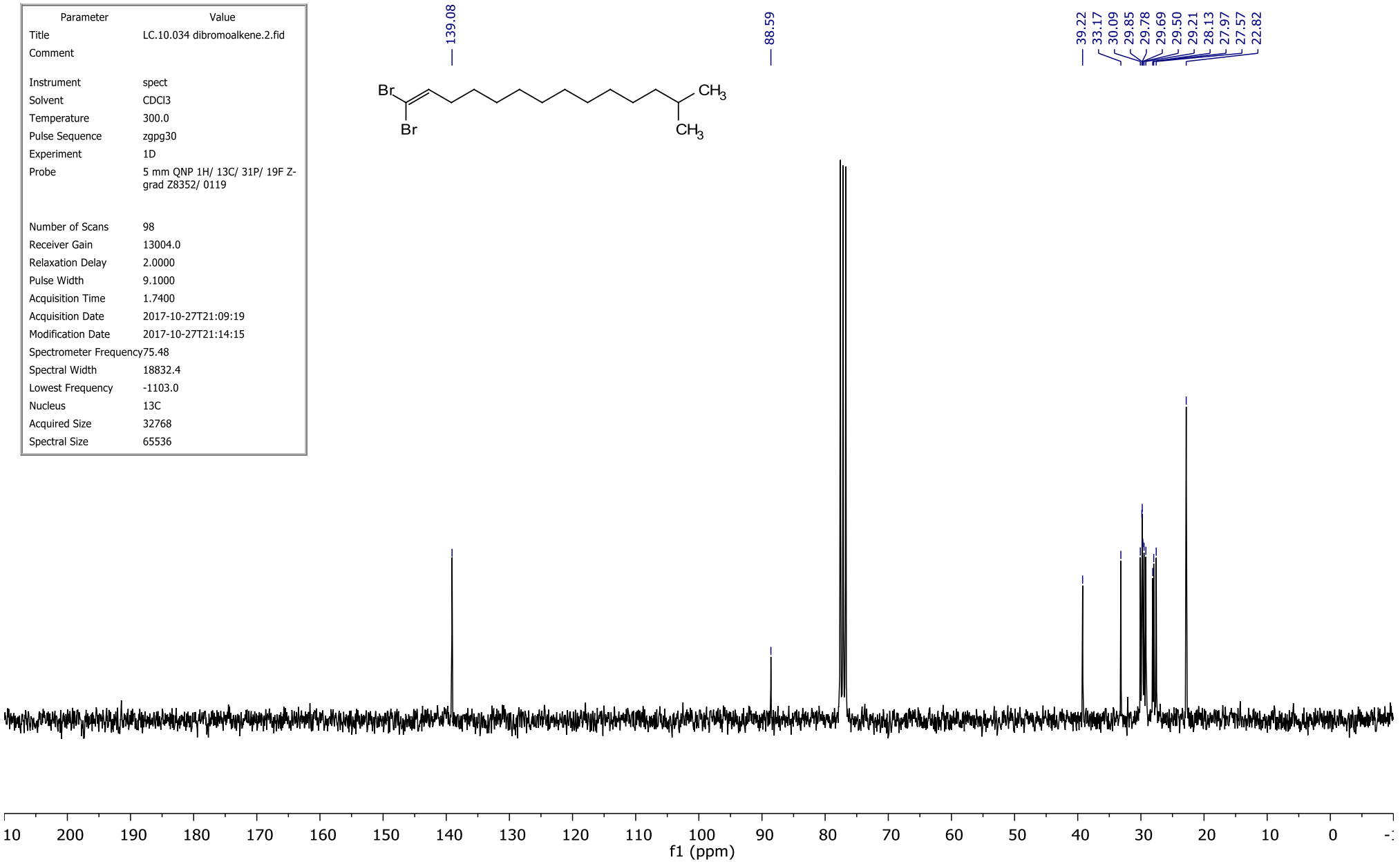
1,1-dibromo-13-methyltetradec-1-ene (**11**) ^{1}H NMR (300 MHz, chloroform-*d*)

Parameter	Value
Title	LC.10.034 dibromoalkene.1.fid
Comment	
Instrument	spect
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zg
Experiment	1D
Probe	5 mm QNP 1H/ 13C/ 31P/ 19F Z-grad Z8352/ 0119
Number of Scans	8
Receiver Gain	45.3
Relaxation Delay	2.0000
Pulse Width	10.1000
Acquisition Time	2.7329
Acquisition Date	2017-10-27T21:07:12
Modification Date	2017-10-27T21:07:20
Spectrometer Frequency	300.13
Spectral Width	5995.2
Lowest Frequency	-1203.3
Nucleus	1H
Acquired Size	16384
Spectral Size	65536



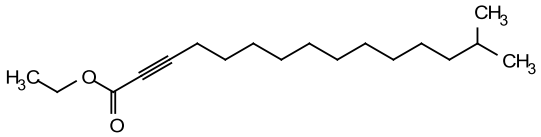
1,1-dibromo-13-methyltetradec-1-ene (**11**) ^{13}C NMR (75 MHz, chloroform-*d*)

Parameter	Value
Title	LC.10.034 dibromoalkene.2.fid
Comment	
Instrument	spect
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgpg30
Experiment	1D
Probe	5 mm QNP 1H/ 13C/ 31P/ 19F Z-grad Z8352/ 0119
Number of Scans	98
Receiver Gain	13004.0
Relaxation Delay	2.0000
Pulse Width	9.1000
Acquisition Time	1.7400
Acquisition Date	2017-10-27T21:09:19
Modification Date	2017-10-27T21:14:15
Spectrometer Frequency	75.48
Spectral Width	18832.4
Lowest Frequency	-1103.0
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



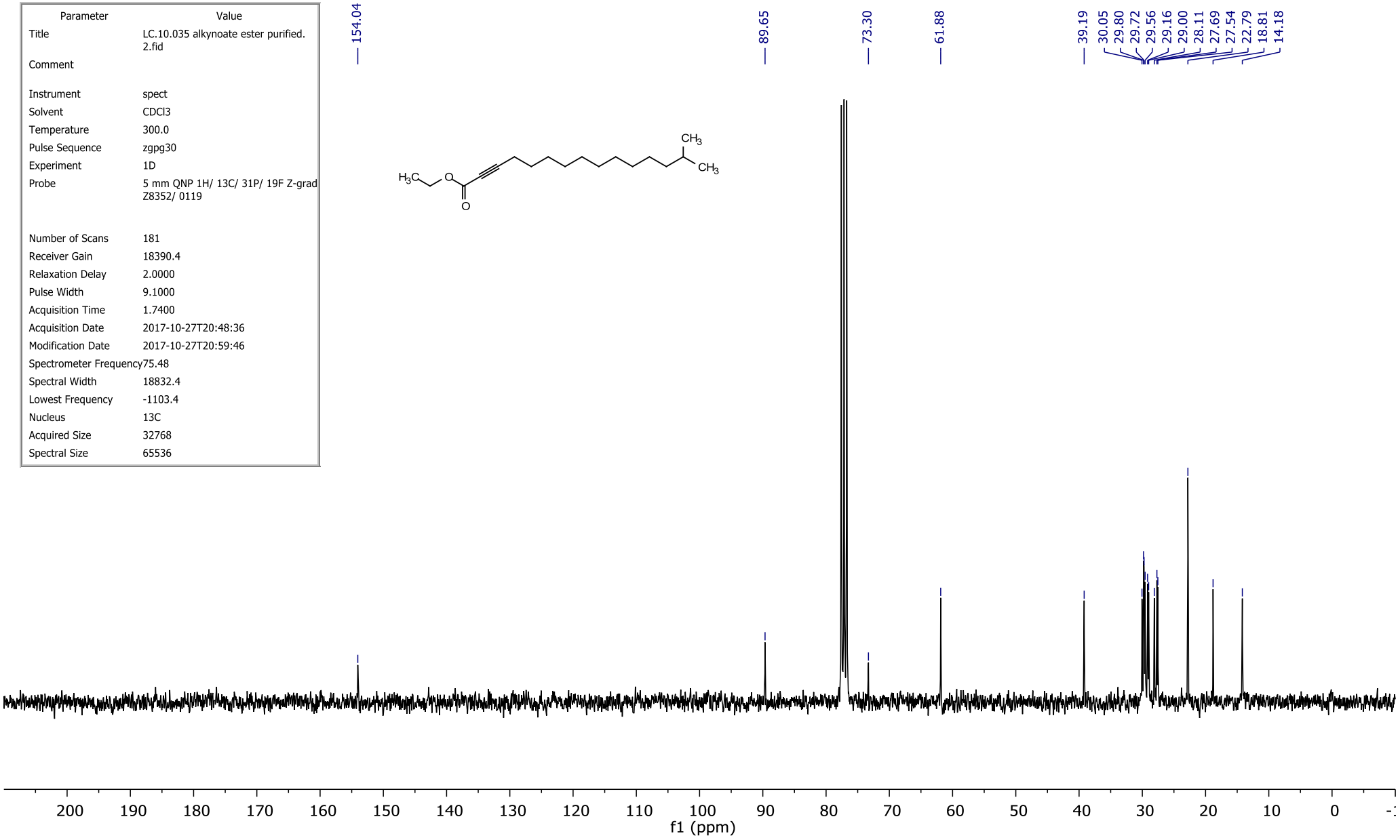
Ethyl 14-methylpentadec-2-ynoate (**12**) ^{1}H NMR (300 MHz, chloroform-*d*)

Parameter	Value
Title	LC.10.035 alkynoate ester purified.1.fid
Comment	
Instrument	spect
Solvent	CDCl3
Temperature	300.1
Pulse Sequence	zg
Experiment	1D
Probe	5 mm QNP 1H/ 13C/ 31P/ 19F Z-grad Z8352/ 0119
Number of Scans	8
Receiver Gain	181.0
Relaxation Delay	2.0000
Pulse Width	10.1000
Acquisition Time	2.7329
Acquisition Date	2017-10-27T15:35:36
Modification Date	2017-10-27T15:35:43
Spectrometer Frequency	300.13
Spectral Width	5995.2
Lowest Frequency	-1203.2
Nucleus	1H
Acquired Size	16384
Spectral Size	65536



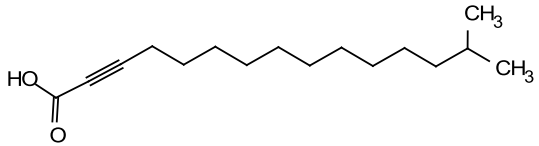
Ethyl 14-methylpentadec-2-ynoate (**12**) ^{13}C NMR (75 MHz, chloroform-*d*)

Parameter	Value
Title	LC.10.035 alkynoate ester purified. 2.fid
Comment	
Instrument	spect
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgpg30
Experiment	1D
Probe	5 mm QNP 1H/ 13C/ 31P/ 19F Z-grad Z8352/ 0119
Number of Scans	181
Receiver Gain	18390.4
Relaxation Delay	2.0000
Pulse Width	9.1000
Acquisition Time	1.7400
Acquisition Date	2017-10-27T20:48:36
Modification Date	2017-10-27T20:59:46
Spectrometer Frequency	75.48
Spectral Width	18832.4
Lowest Frequency	-1103.4
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



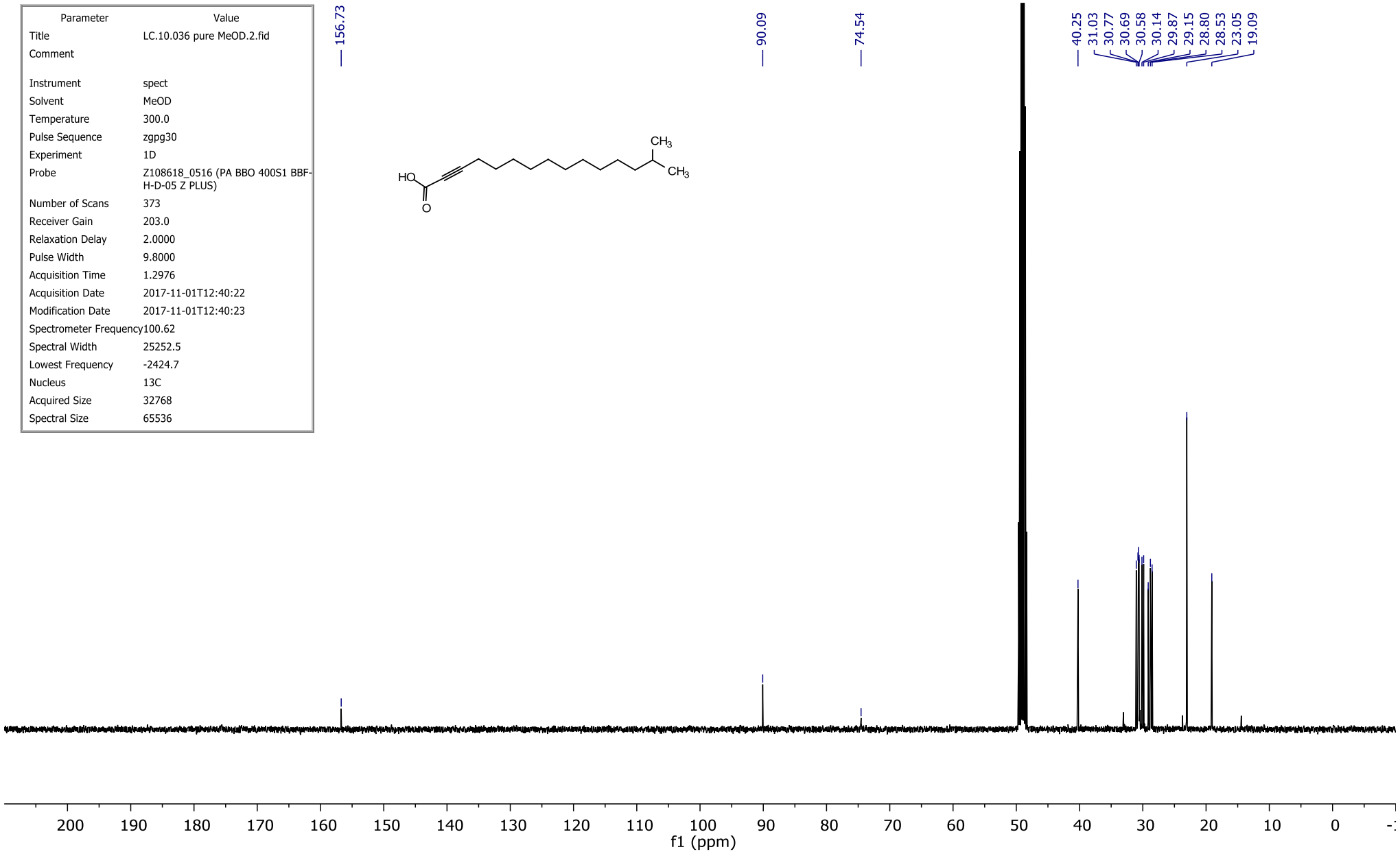
14-methylpentadec-2-ynoic acid (**7**) ^{1}H NMR (400 MHz, methanol-d_4)

Parameter	Value
Title	LC.10.036 pure MeOD.1.fid
Comment	
Instrument	spect
Solvent	MeOD
Temperature	300.0
Pulse Sequence	zg
Experiment	1D
Probe	Z108618_0516 (PA BBO 400S1 BBF-H-D-05 Z PLUS)
Number of Scans	1
Receiver Gain	57.0
Relaxation Delay	5.0000
Pulse Width	14.9000
Acquisition Time	3.0048
Acquisition Date	2017-11-01T12:16:57
Modification Date	2017-11-01T12:16:57
Spectrometer Frequency	400.13
Spectral Width	8000.0
Lowest Frequency	-1607.0
Nucleus	1H
Acquired Size	24038
Spectral Size	65536

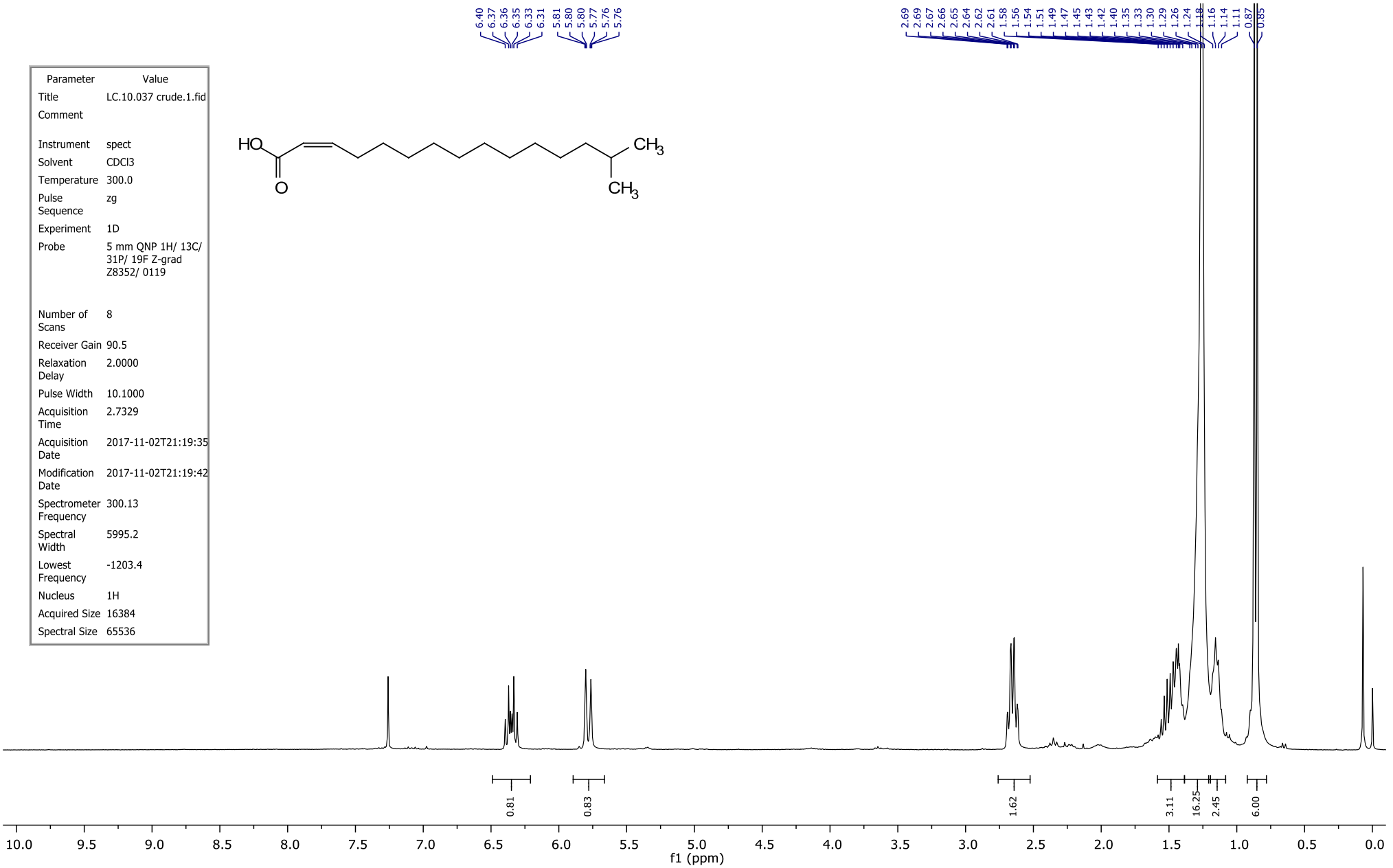


14-methylpentadec-2-ynoic acid (**7**) ^{13}C NMR (101 MHz, methanol-d_4)

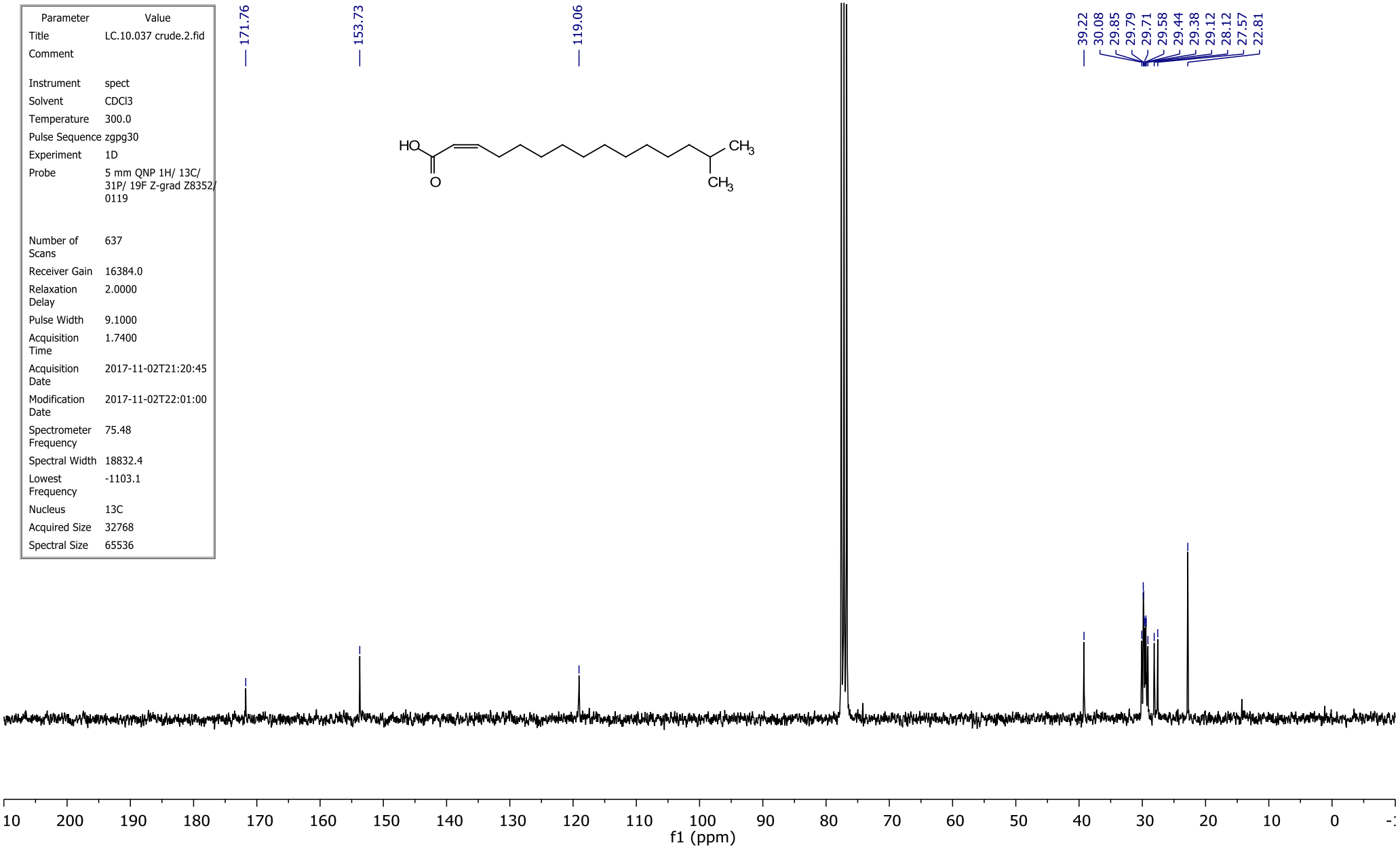
Parameter	Value
Title	LC.10.036 pure MeOD.2.fid
Comment	
Instrument	spect
Solvent	MeOD
Temperature	300.0
Pulse Sequence	zgpg30
Experiment	1D
Probe	Z108618_0516 (PA BBO 400S1 BBF-H-D-05 Z PLUS)
Number of Scans	373
Receiver Gain	203.0
Relaxation Delay	2.0000
Pulse Width	9.8000
Acquisition Time	1.2976
Acquisition Date	2017-11-01T12:40:22
Modification Date	2017-11-01T12:40:23
Spectrometer Frequency	100.62
Spectral Width	25252.5
Lowest Frequency	-2424.7
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



(*Z*)-14-methylpentadec-2-enoic acid (**8**) ^{1}H NMR (300 MHz, chloroform-*d*)

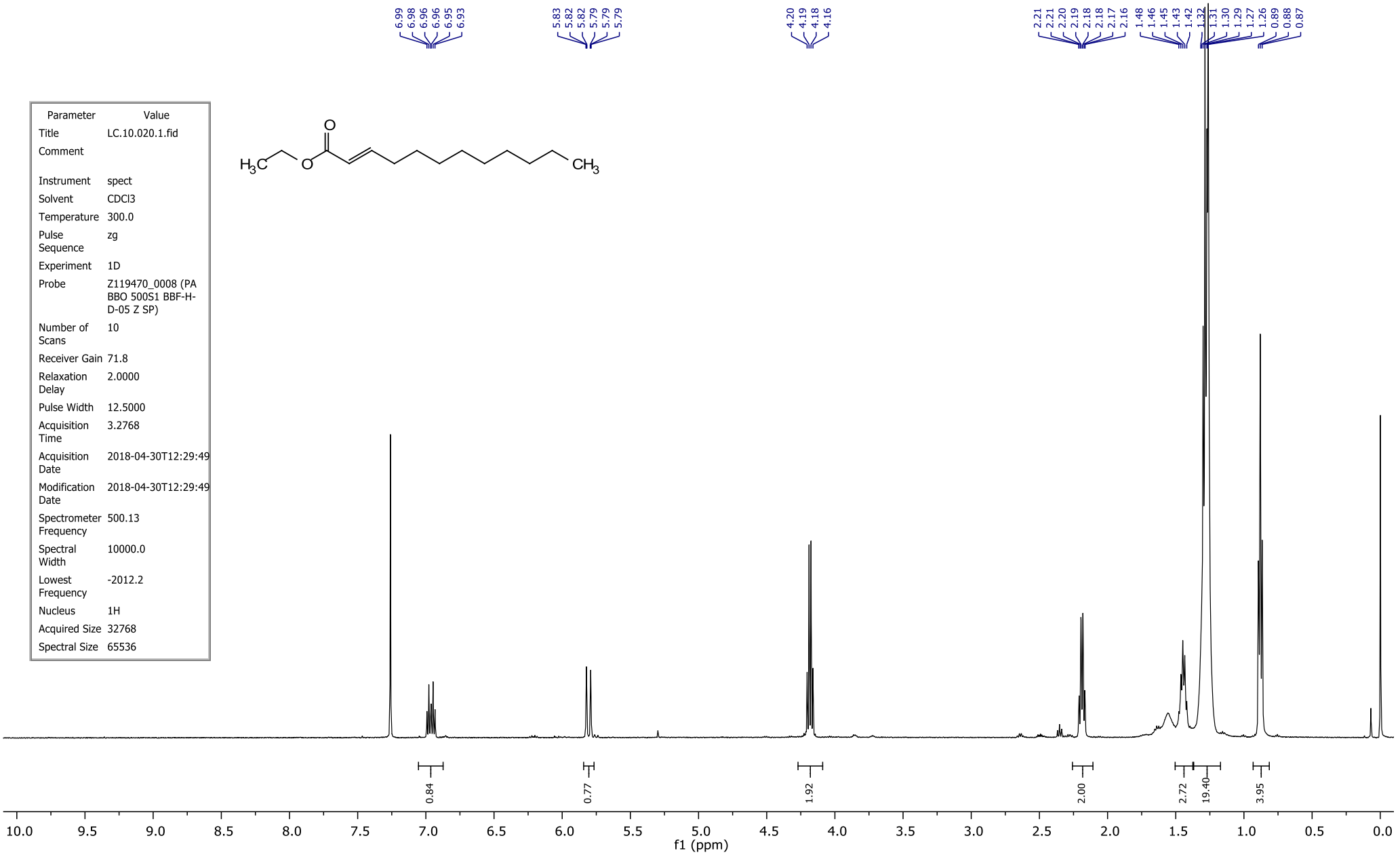


(*Z*)-14-methylpentadec-2-enoic acid (**8**) ^{13}C NMR (75 MHz, chloroform-*d*)



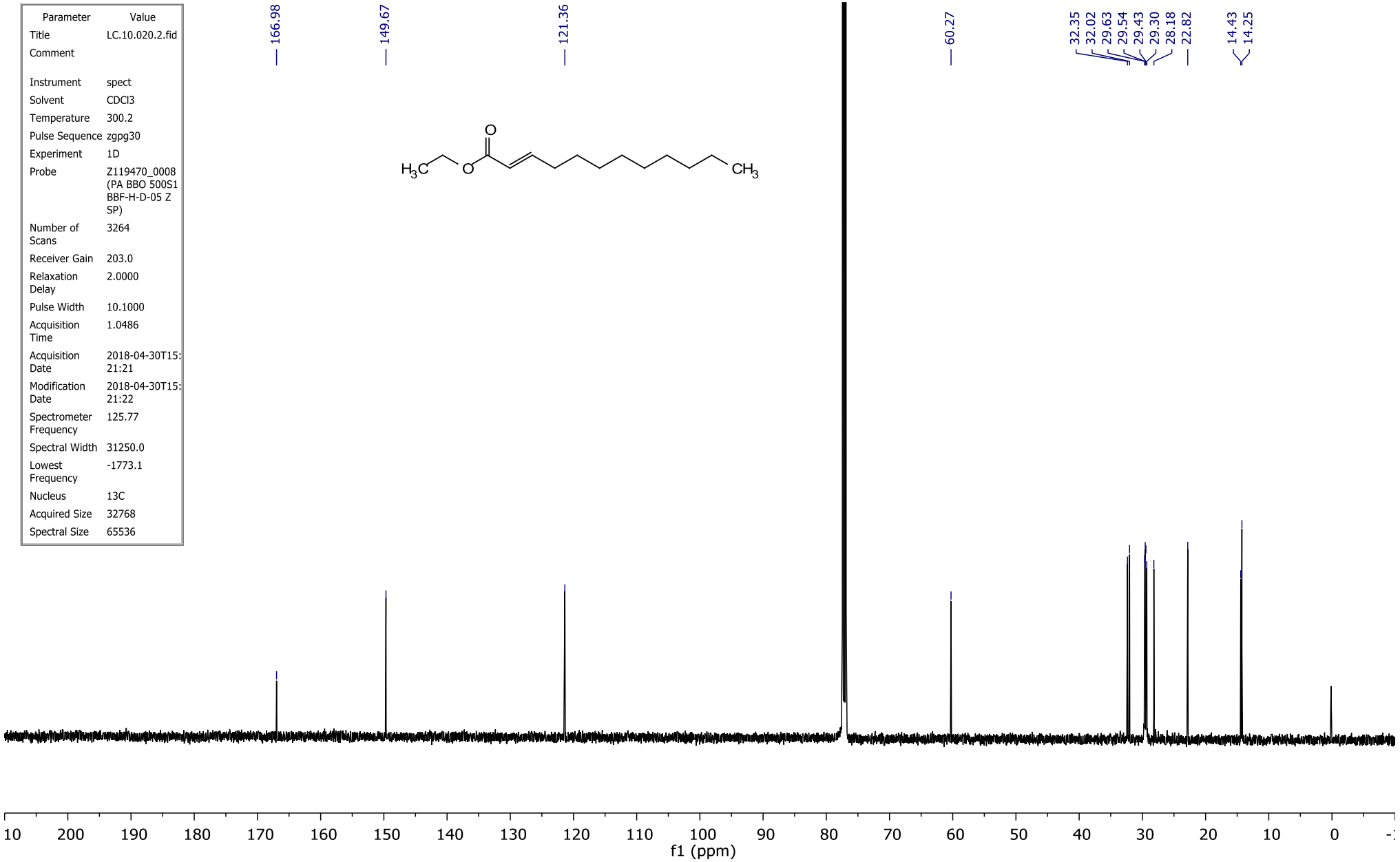
Parameter	Value
Title	LC.10.037 crude.2.fid
Comment	
Instrument	spect
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgpg30
Experiment	1D
Probe	5 mm QNP 1H/ 13C/ 31P/ 19F Z-grad Z8352/ 0119
Number of Scans	637
Receiver Gain	16384.0
Relaxation Delay	2.0000
Pulse Width	9.1000
Acquisition Time	1.7400
Acquisition Date	2017-11-02T21:20:45
Modification Date	2017-11-02T22:01:00
Spectrometer Frequency	75.48
Spectral Width	18832.4
Lowest Frequency	-1103.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

Ethyl (*E*)-dodec-2-enoate (**15**) ^{1}H NMR (500 MHz, chloroform-*d*)



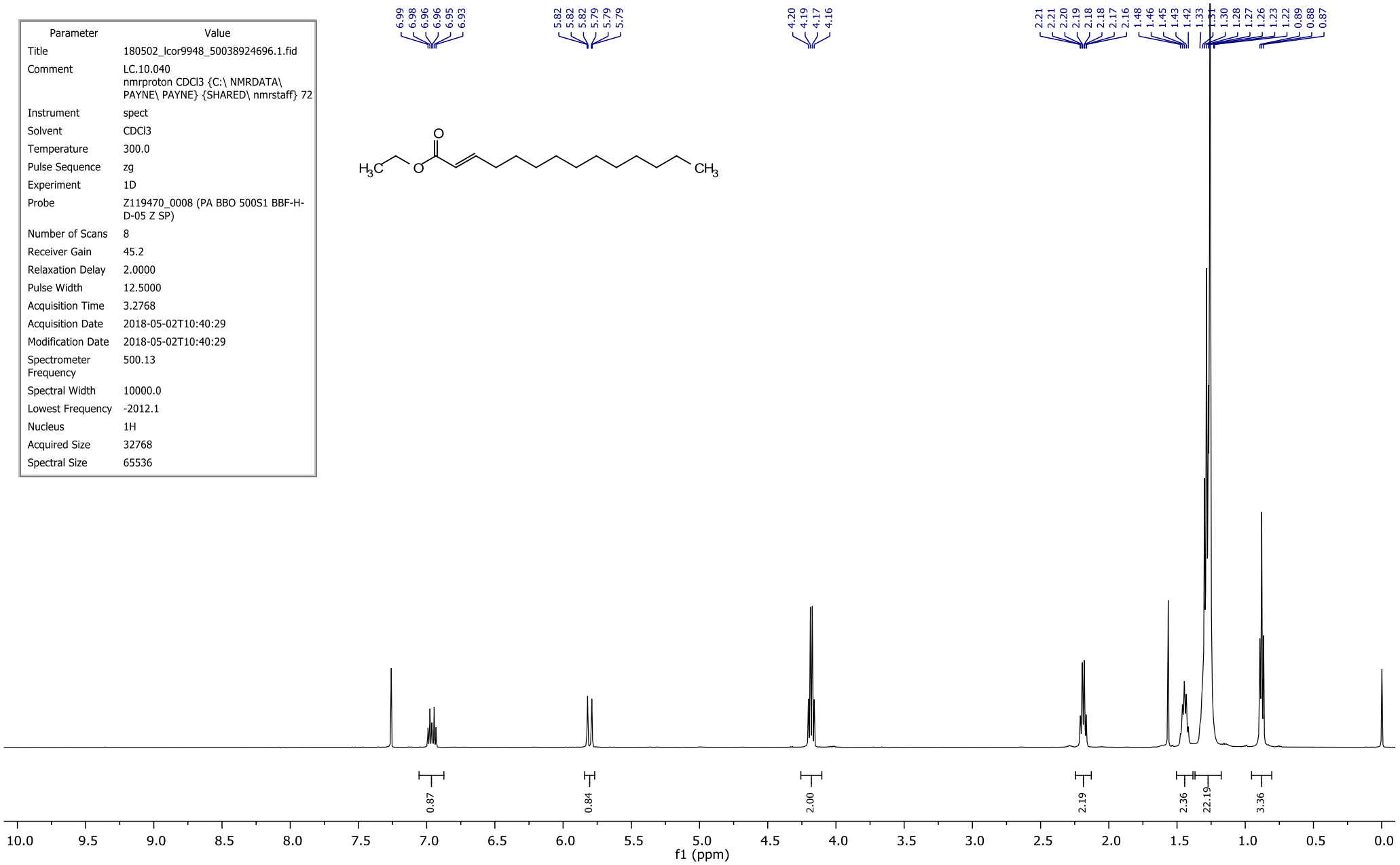
Ethyl (*E*)-dodec-2-enoate (**15**) ^{13}C NMR (126 MHz, chloroform-*d*)

Parameter	Value
Title	LC.10.020.2.fid
Comment	
Instrument	spect
Solvent	CDCl3
Temperature	300.2
Pulse Sequence	zgpg30
Experiment	1D
Probe	Z119470_0008 (PA BBO 500S1 BBF-H-D-05 Z SP)
Number of Scans	3264
Receiver Gain	203.0
Relaxation Delay	2.0000
Pulse Width	10.1000
Acquisition Time	1.0486
Acquisition Date	2018-04-30T15:21:21
Modification Date	2018-04-30T15:21:22
Spectrometer Frequency	125.77
Spectral Width	31250.0
Lowest Frequency	-1773.1
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



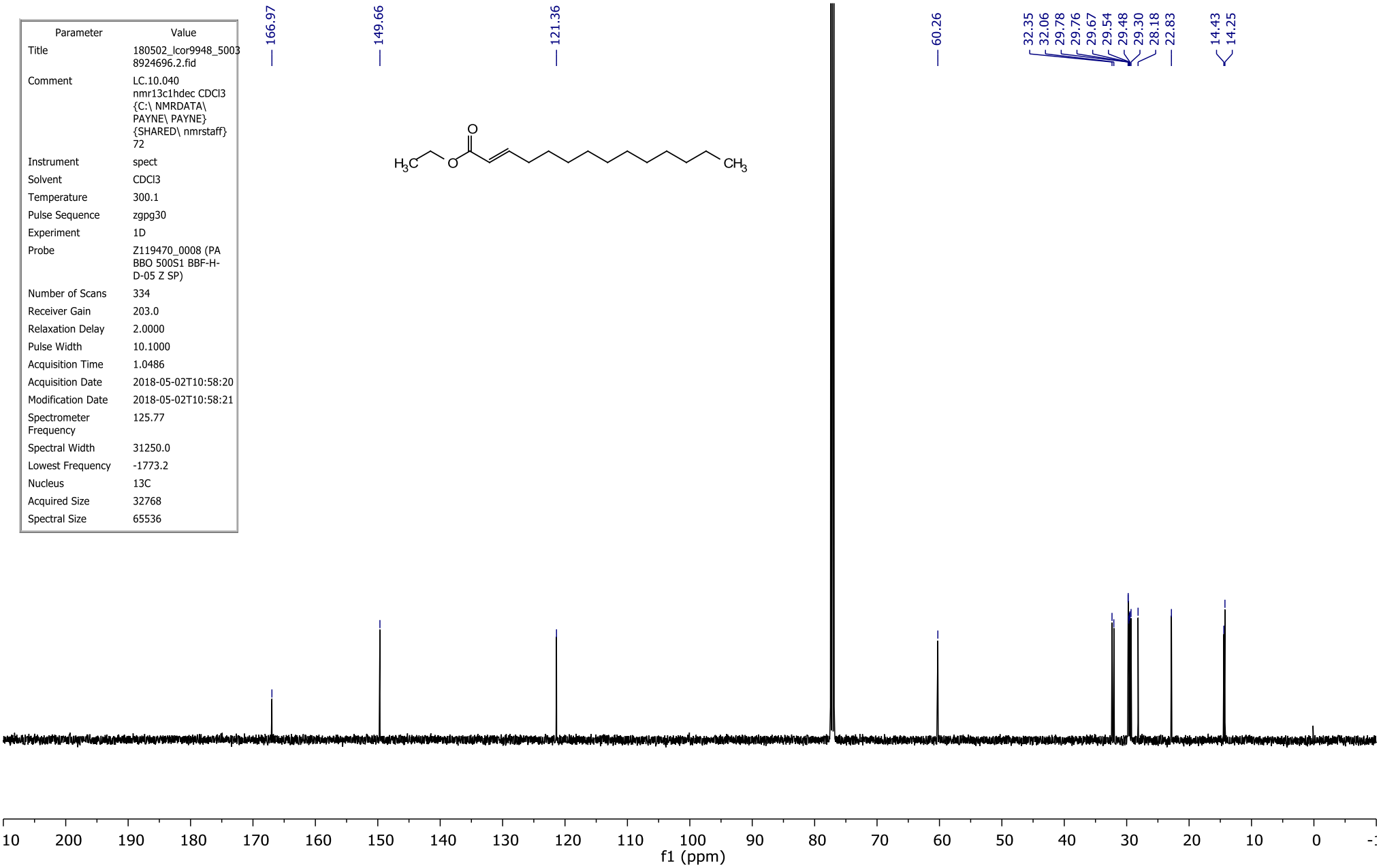
Ethyl (*E*)-tetradec-2-enoate (**16**) ^{1}H NMR (500 MHz, chloroform-*d*)

Parameter	Value
Title	180502_lcor9948_50038924696.1.fid
Comment	LC.10.040 nmrproton CDCl3 {C:\ NMRDATA\ PAYNE\ PAYNE} {SHARED\ nmrstaff} 72
Instrument	spect
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zg
Experiment	1D
Probe	Z119470_0008 (PA BBO 500S1 BBF-H-D-05 Z SP)
Number of Scans	8
Receiver Gain	45.2
Relaxation Delay	2.0000
Pulse Width	12.5000
Acquisition Time	3.2768
Acquisition Date	2018-05-02T10:40:29
Modification Date	2018-05-02T10:40:29
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-2012.1
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

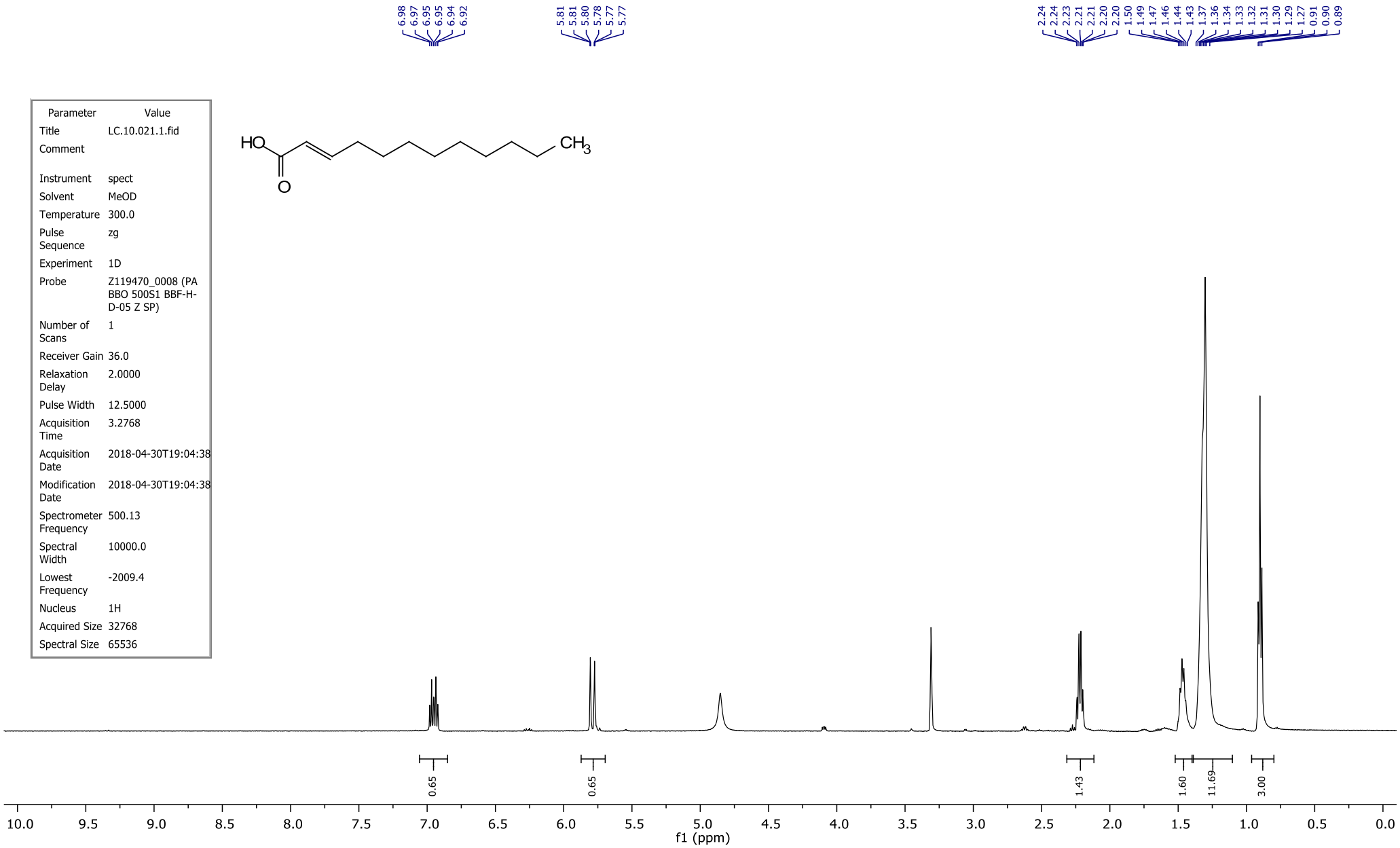


Ethyl (*E*)-tetradec-2-enoate (**16**) ^{13}C NMR (126 MHz, chloroform-*d*)

Parameter	Value
Title	180502_lcor9948_5003 8924696.2.fid
Comment	LC.10.040 nmr13c1hdec CDCl3 {C:\ NMRDATA\ PAYNE\ PAYNE} {SHARED\ nmrstaff} 72
Instrument	spect
Solvent	CDCl3
Temperature	300.1
Pulse Sequence	zgpg30
Experiment	1D
Probe	Z119470_0008 (PA BBO 500S1 BBF-H-D-05 Z SP)
Number of Scans	334
Receiver Gain	203.0
Relaxation Delay	2.0000
Pulse Width	10.1000
Acquisition Time	1.0486
Acquisition Date	2018-05-02T10:58:20
Modification Date	2018-05-02T10:58:21
Spectrometer Frequency	125.77
Spectral Width	31250.0
Lowest Frequency	-1773.2
Nucleus	13C
Acquired Size	32768
Spectral Size	65536



(*E*)-dodec-2-enoic acid (**13**) ^{1}H NMR (500 MHz, methanol-d_4)



Parameter	Value
Title	LC.10.021.1.fid
Comment	
Instrument	spect
Solvent	MeOD
Temperature	300.0
Pulse Sequence	zg
Experiment	1D
Probe	Z119470_0008 (PABBO 500S1 BBF-H-D-05 Z SP)
Number of Scans	1
Receiver Gain	36.0
Relaxation Delay	2.0000
Pulse Width	12.5000
Acquisition Time	3.2768
Acquisition Date	2018-04-30T19:04:38
Modification Date	2018-04-30T19:04:38
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-2009.4
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

(*E*)-dodec-2-enoic acid (**13**) ^{13}C NMR (126 MHz, methanol-d_4)

Parameter	Value
Title	LC.10.021.2.fid
Comment	
Instrument	spect
Solvent	MeOD
Temperature	300.1
Pulse Sequence	zgpg30
Experiment	1D
Probe	Z119470_0008 (PA BBO 500S1 BBF-H-D-05 Z SP)
Number of Scans	27
Receiver Gain	203.0
Relaxation Delay	2.0000
Pulse Width	10.1000
Acquisition Time	1.0486
Acquisition Date	2018-04-30T19:09:16
Modification Date	2018-04-30T19:09:17
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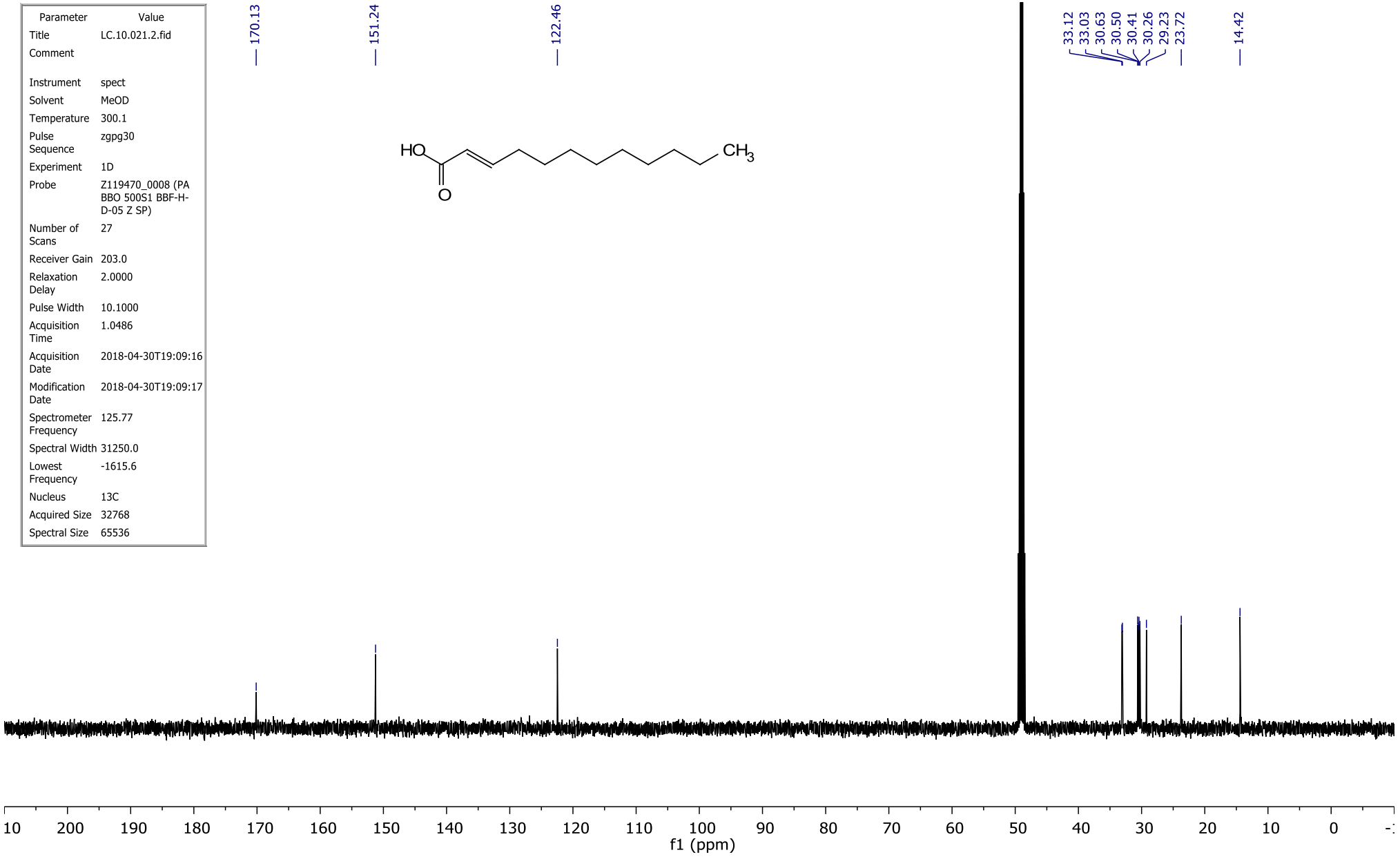
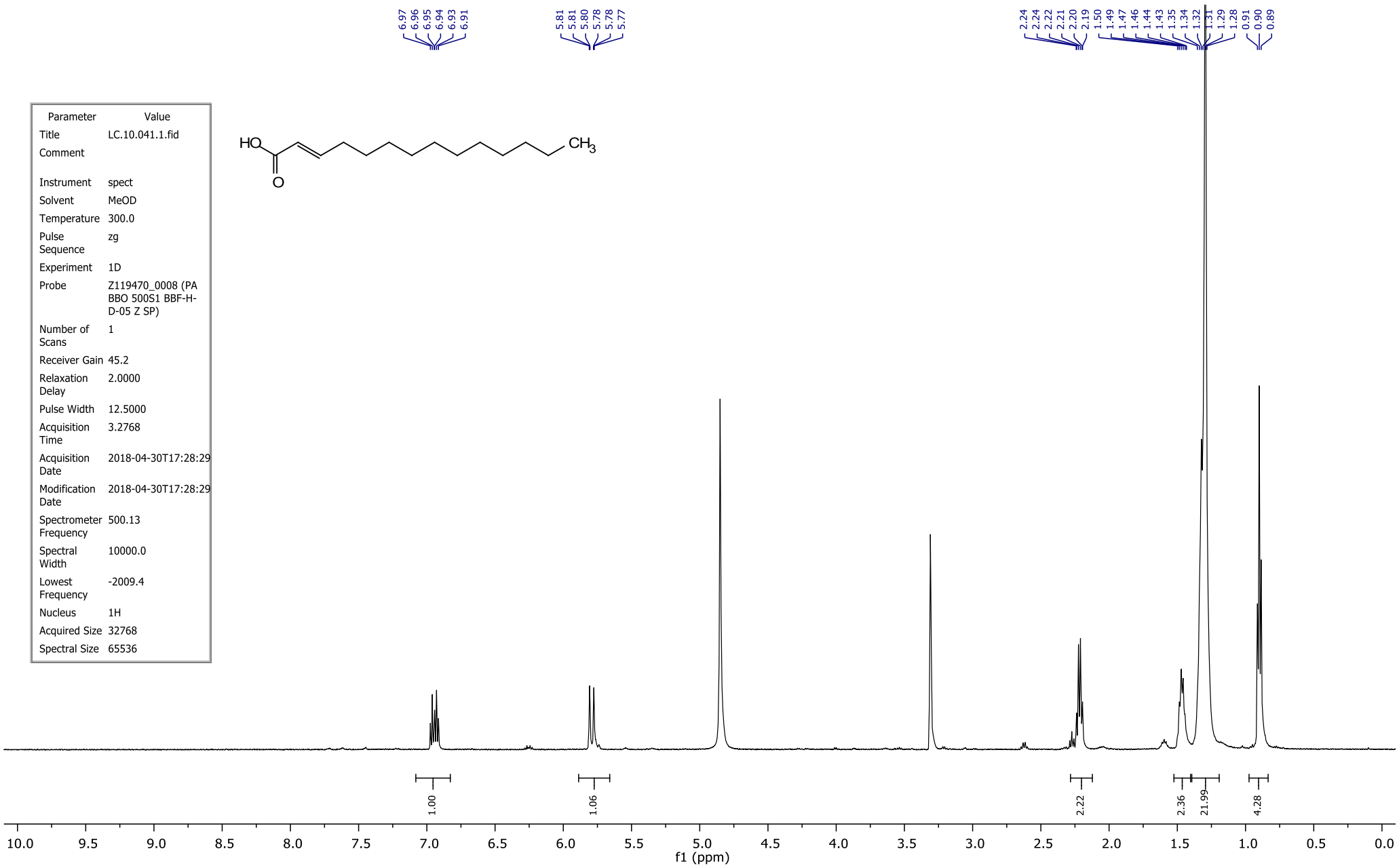
Spectral Width	31250.0
Lowest Frequency	-1615.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

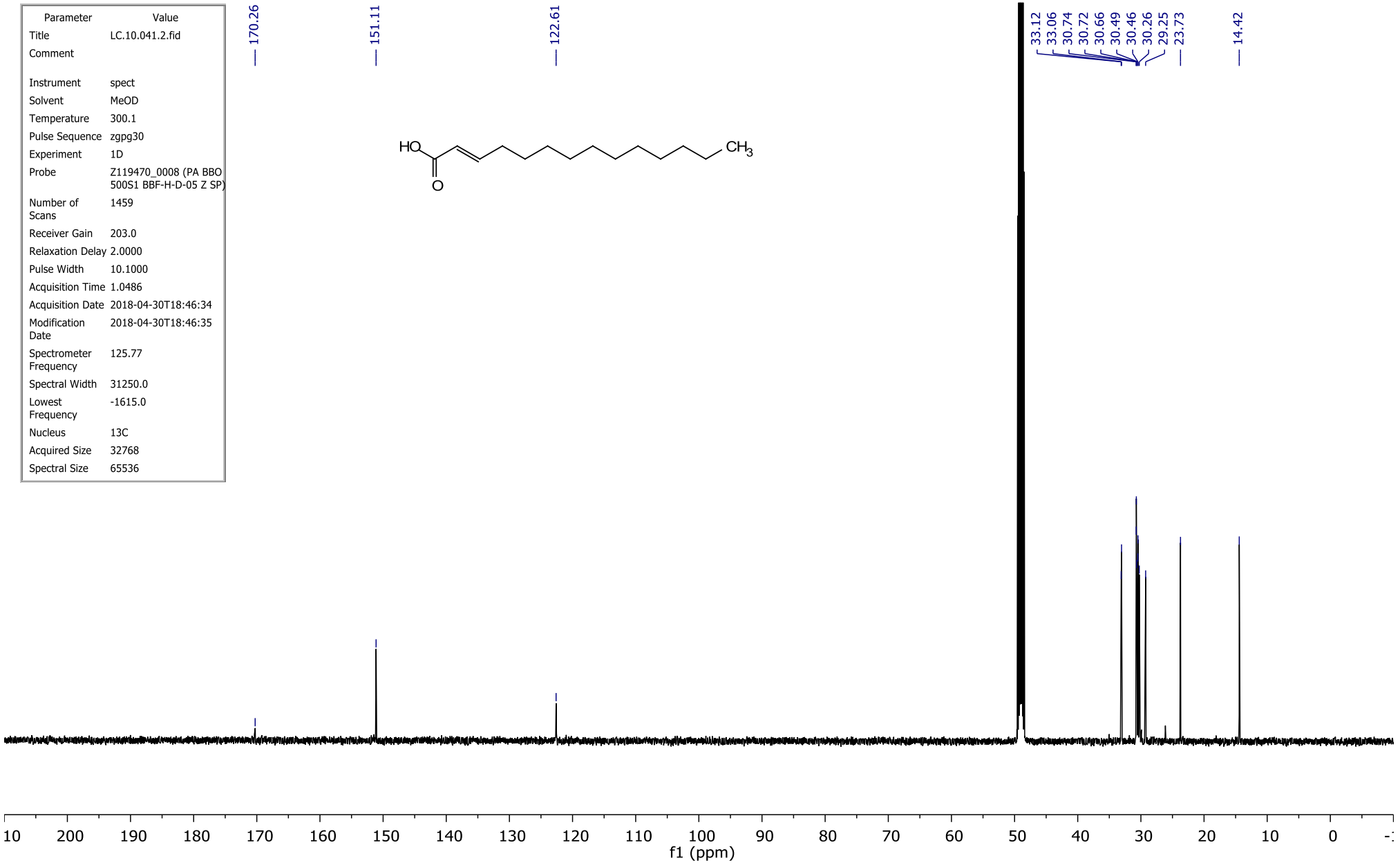


(*E*)-tetradec-2-enoic acid (**14**) ^{1}H NMR (500 MHz, methanol-d_4)

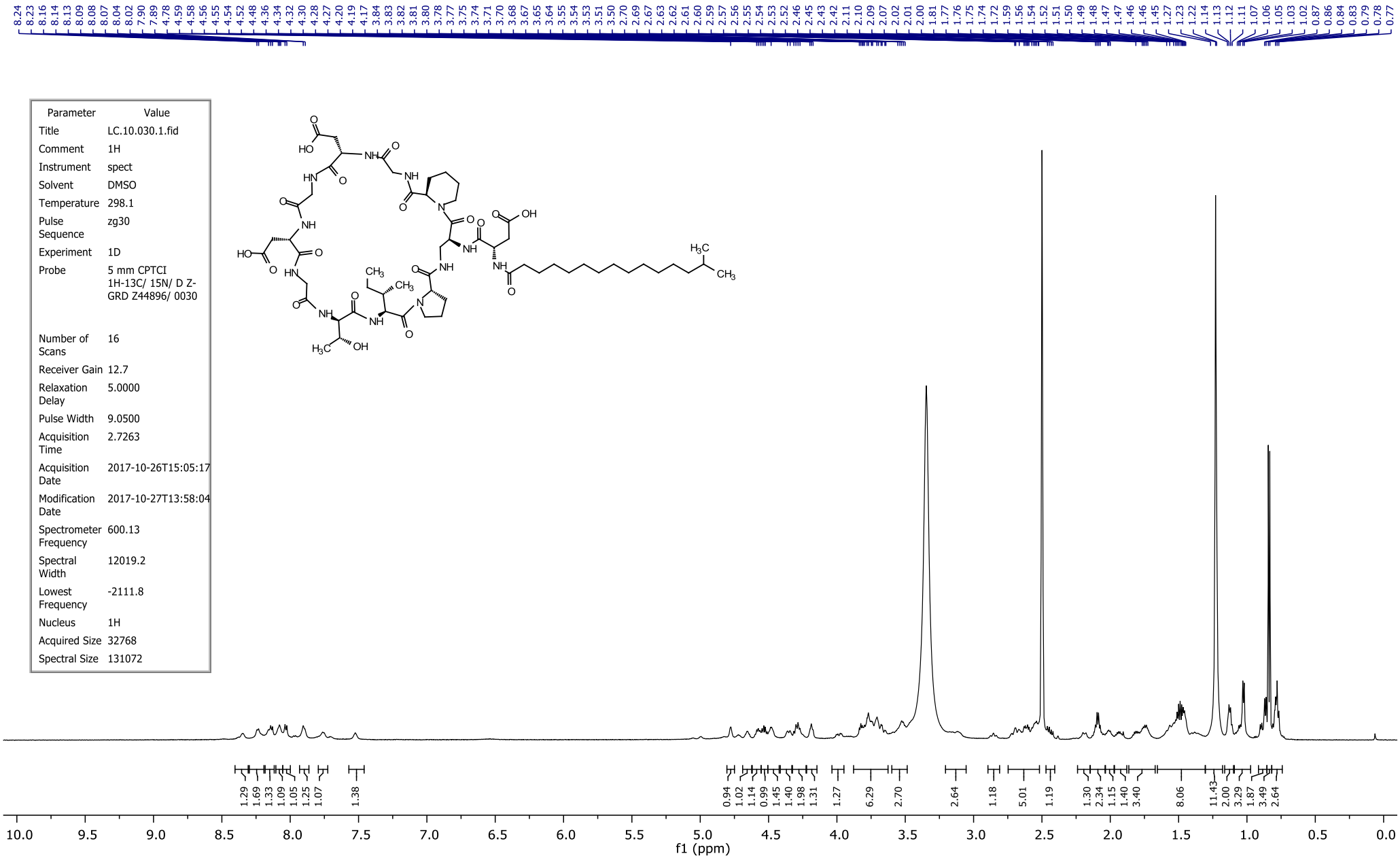


(*E*)-tetradec-2-enoic acid (**14**) ^{13}C NMR (126 MHz, methanol-d_4)

Parameter	Value
Title	LC.10.041.2.fid
Comment	
Instrument	spect
Solvent	MeOD
Temperature	300.1
Pulse Sequence	zgpg30
Experiment	1D
Probe	Z119470_0008 (PA BBO 500S1 BBF-H-D-05 Z SP)
Number of Scans	1459
Receiver Gain	203.0
Relaxation Delay	2.0000
Pulse Width	10.1000
Acquisition Time	1.0486
Acquisition Date	2018-04-30T18:46:34
Modification Date	2018-04-30T18:46:35
Spectrometer Frequency	125.77
Spectral Width	31250.0
Lowest Frequency	-1615.0
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

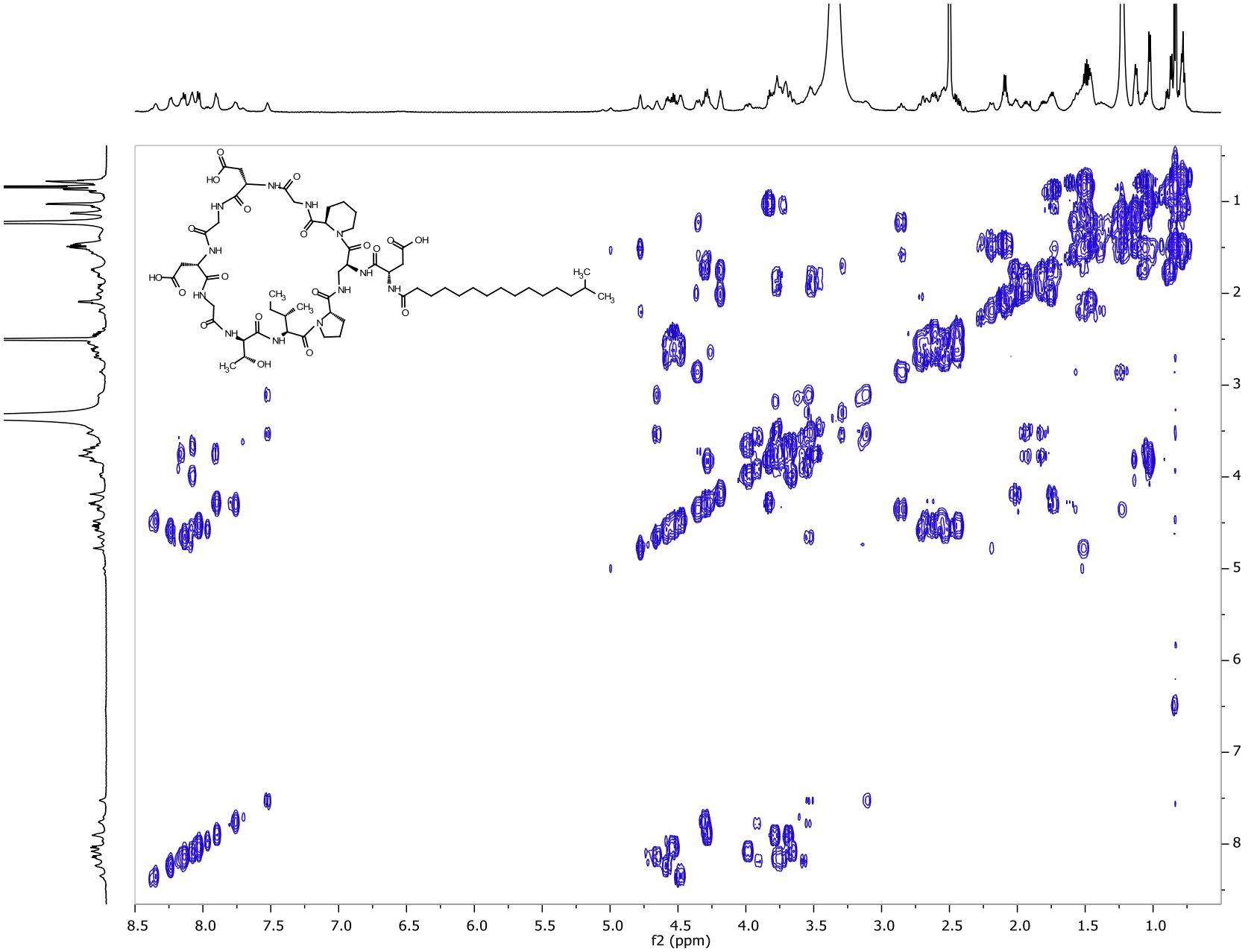


14-methylpentadecanoyl analogue (**18**) ^{1}H NMR (600 MHz, DMSO-d_6)



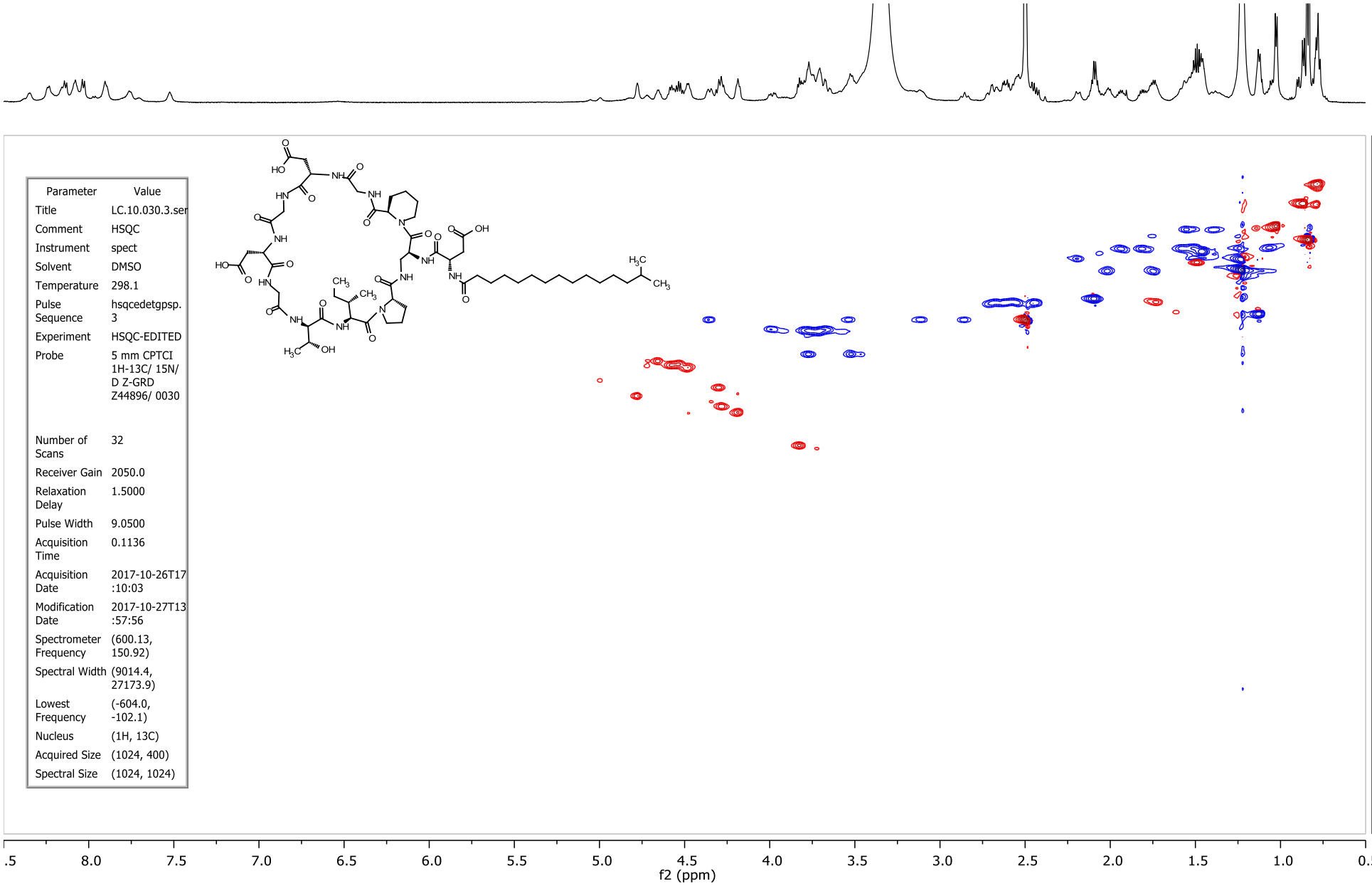
Parameter	Value
Title	LC.10.030.1.fid
Comment	1H
Instrument	spect
Solvent	DMSO
Temperature	298.1
Pulse Sequence	zg30
Experiment	1D
Probe	5 mm CPTCI 1H-13C/ 15N/ D Z-GRD Z44896/ 0030
Number of Scans	16
Receiver Gain	12.7
Relaxation Delay	5.0000
Pulse Width	9.0500
Acquisition Time	2.7263
Acquisition Date	2017-10-26T15:05:17
Modification Date	2017-10-27T13:58:04
Spectrometer Frequency	600.13
Spectral Width	12019.2
Lowest Frequency	-2111.8
Nucleus	1H
Acquired Size	32768
Spectral Size	131072

14-methylpentadecanoyl analogue (**18**) COSY (600 MHz, DMSO-d_6)

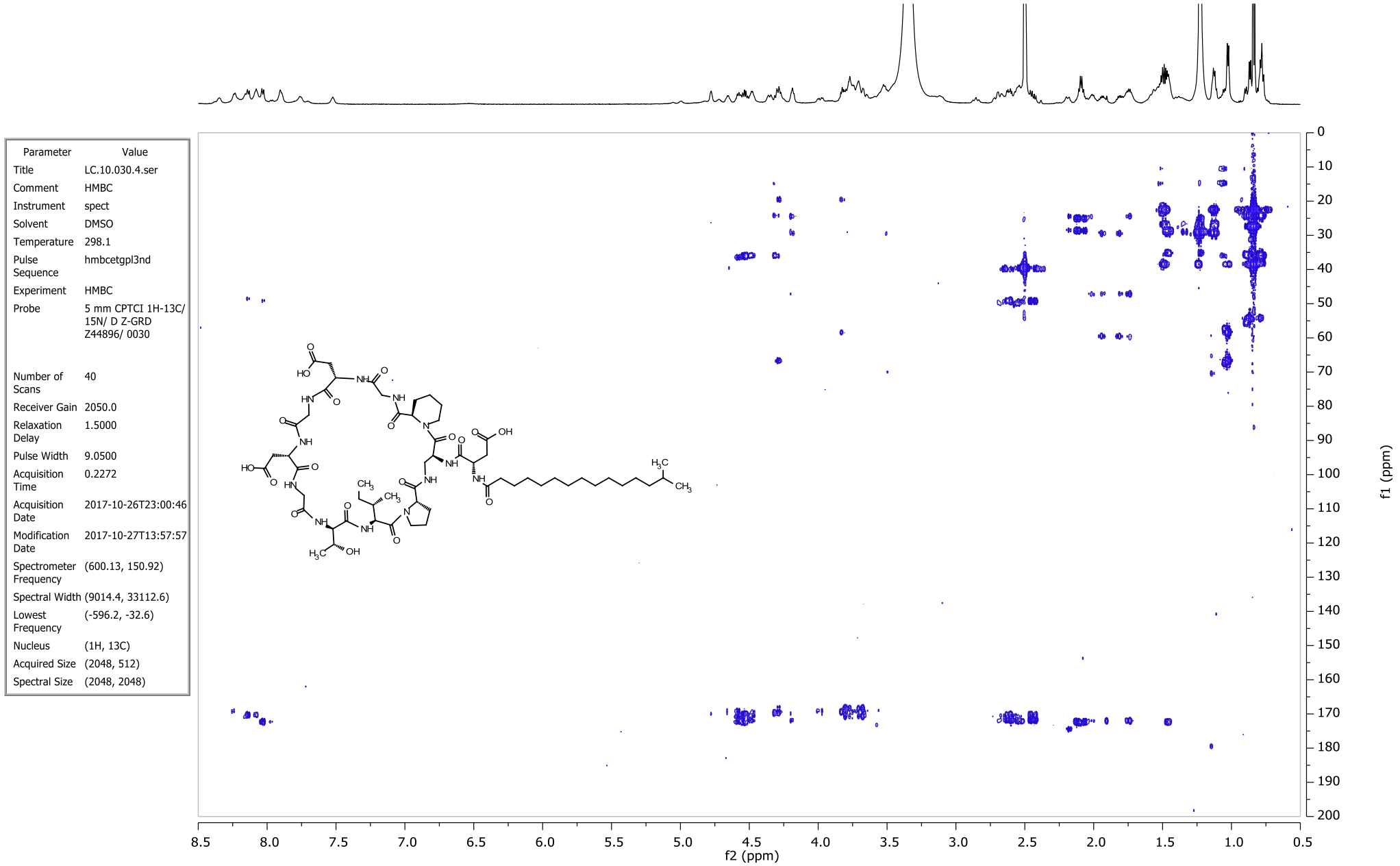


Parameter	Value
Title	LC.10.030.2.ser
Comment	COSY
Instrument	spect
Solvent	DMSO
Temperature	298.1
Pulse Sequence	cosygpmfppqf
Experiment	COSY
Probe	5 mm CPTCI 1H-13C/ 15N/ D Z-GRD Z44896/ 0030
Number of Scans	16
Receiver Gain	2050.0
Relaxation Delay	1.5000
Pulse Width	9.0500
Acquisition Time	0.2272
Acquisition Date	2017-10-26T15:06:37
Modification Date	2017-10-27T13:58:05
Spectrometer Frequency	(600.13, 600.13)
Spectral Width	(9014.4, 9009.0)
Lowest Frequency	(-598.6, -606.1)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

14-methylpentadecanoyl analogue (**18**) HSQC (600/150 MHz, DMSO-d_6)

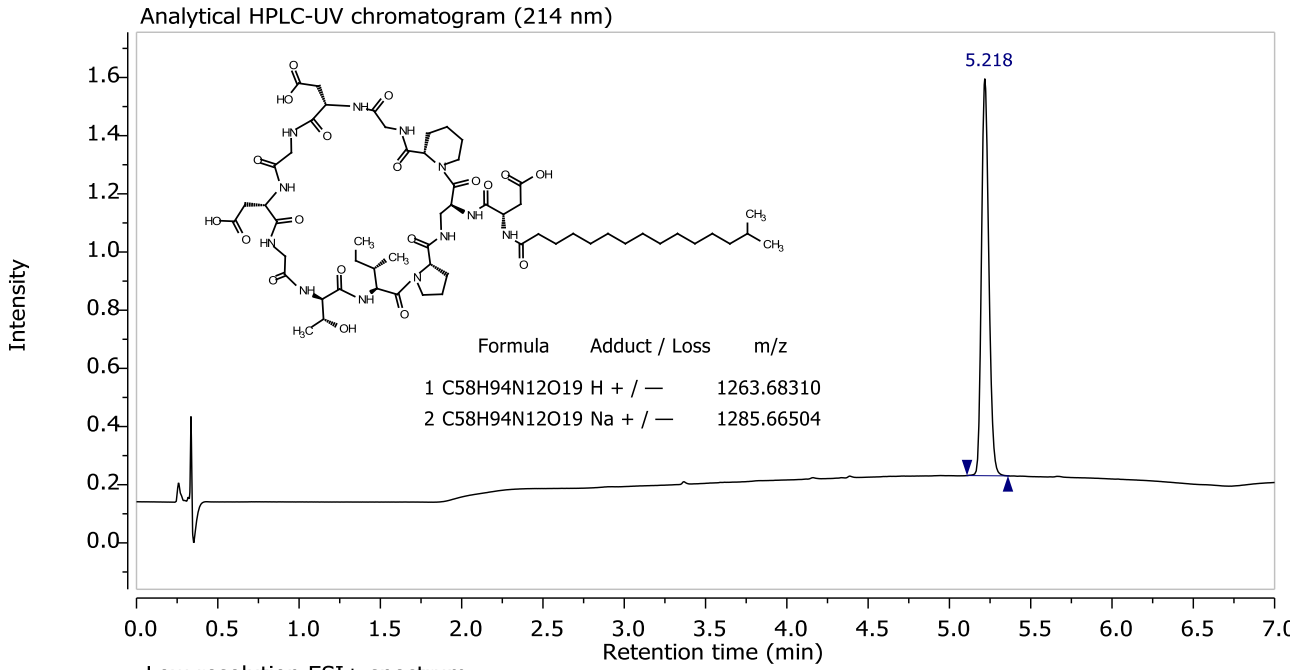


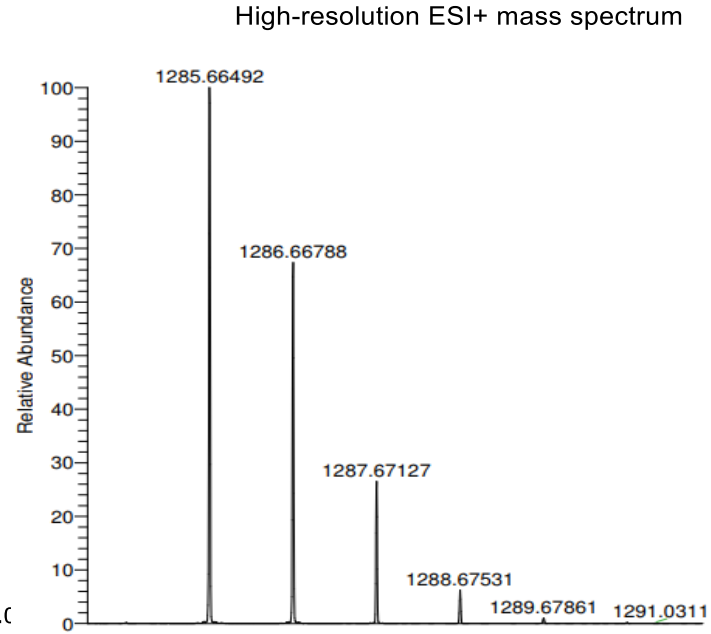
14-methylpentadecanoyl analogue (**18**) HMBC (600/150 MHz, DMSO-d_6)

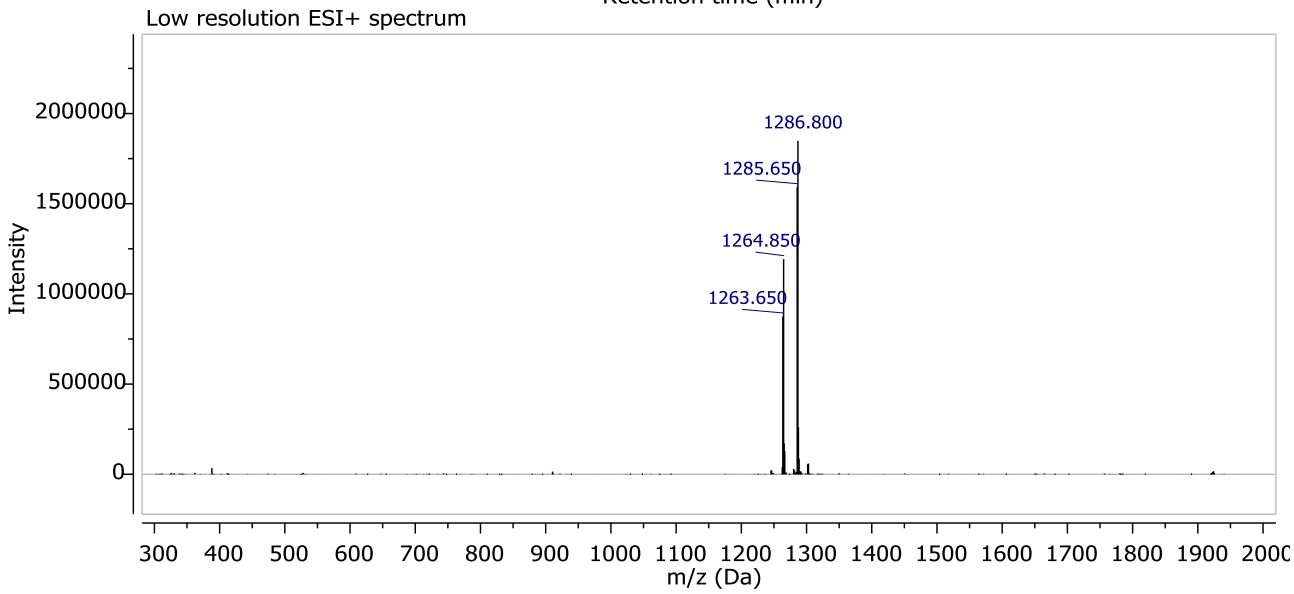


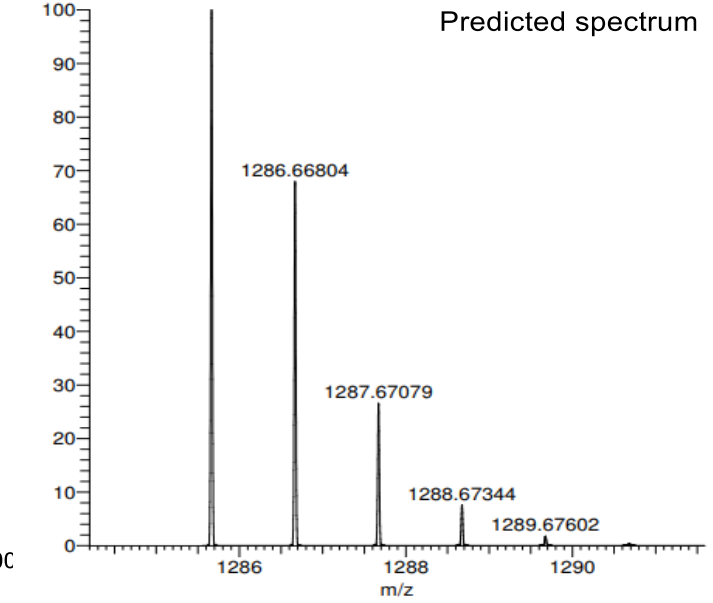
Parameter	Value
Title	LC.10.030.4.ser
Comment	HMBC
Instrument	spect
Solvent	DMSO
Temperature	298.1
Pulse Sequence	hmbcetgpl3nd
Experiment	HMBC
Probe	5 mm CPTCI 1H-13C/ 15N/ D Z-GRD Z44896/ 0030
Number of Scans	40
Receiver Gain	2050.0
Relaxation Delay	1.5000
Pulse Width	9.0500
Acquisition Time	0.2272
Acquisition Date	2017-10-26T23:00:46
Modification Date	2017-10-27T13:57:57
Spectrometer Frequency	(600.13, 150.92)
Spectral Width	(9014.4, 33112.6)
Lowest Frequency	(-596.2, -32.6)
Nucleus	(1H, 13C)
Acquired Size	(2048, 512)
Spectral Size	(2048, 2048)

14-methylpentadecanoyl analogue (**18**) Analytical HPLC, low and high-resolution ESI+ MS



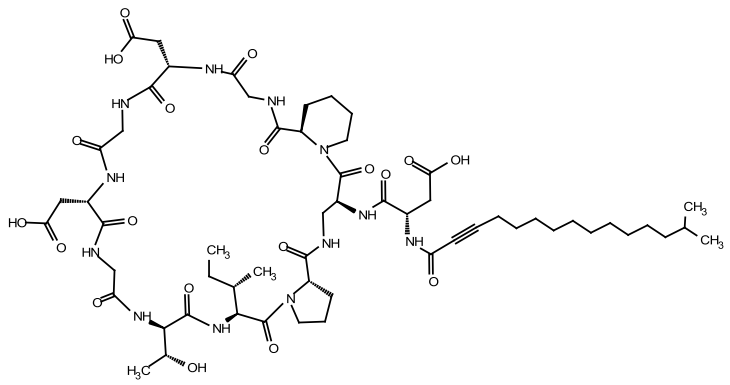




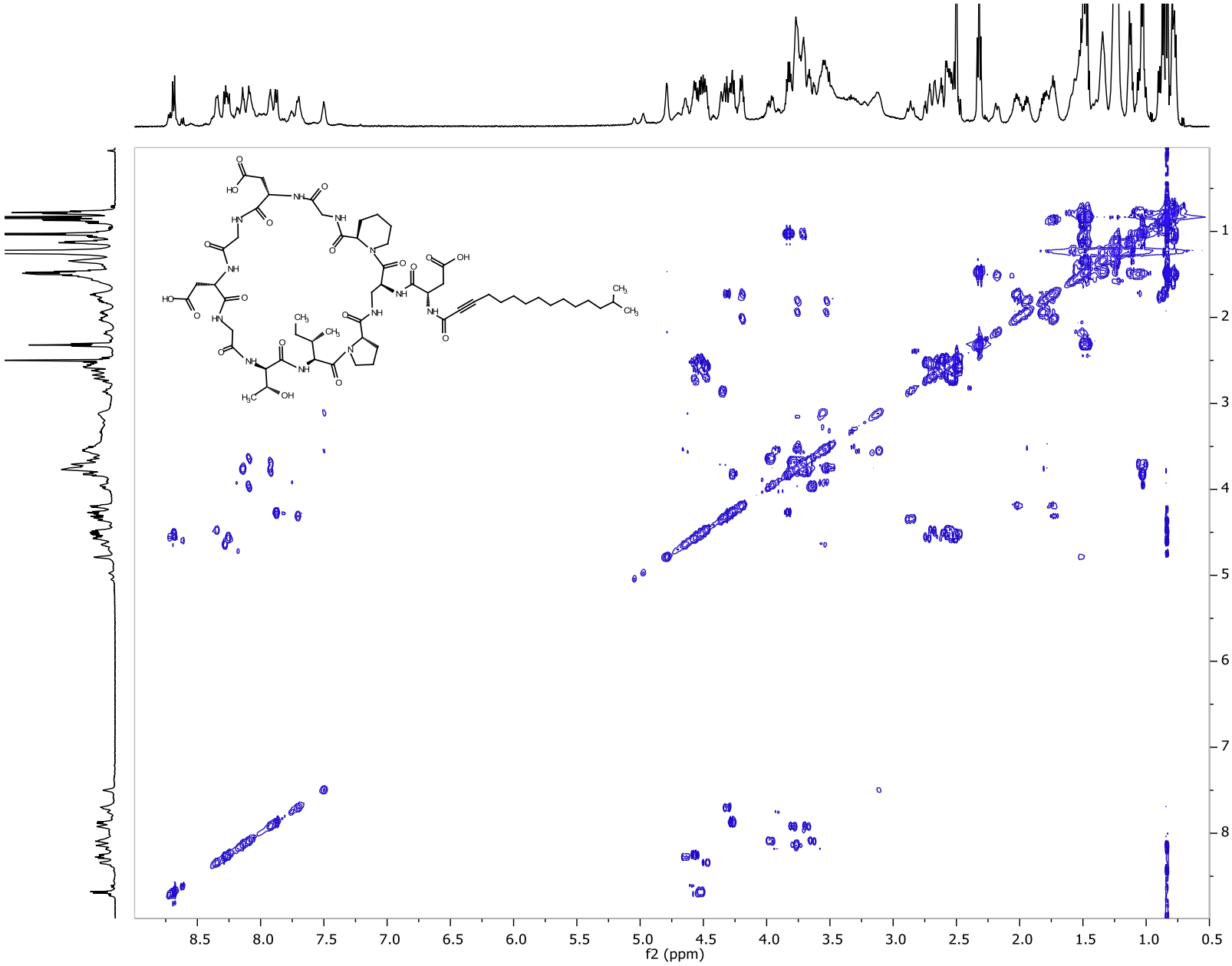


14-methylpentadec-2-ynoyl analogue (**19**) ^{1}H NMR (500 MHz, DMSO-d_6)

Parameter	Value
Title	LC.10.038.1.fid
Comment	1H
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	zg
Experiment	1D
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	14
Receiver Gain	101.0
Relaxation Delay	2.0000
Pulse Width	4.9000
Acquisition Time	3.2768
Acquisition Date	2017-12-18T15:44:32
Modification Date	2017-12-18T15:44:33
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-2002.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

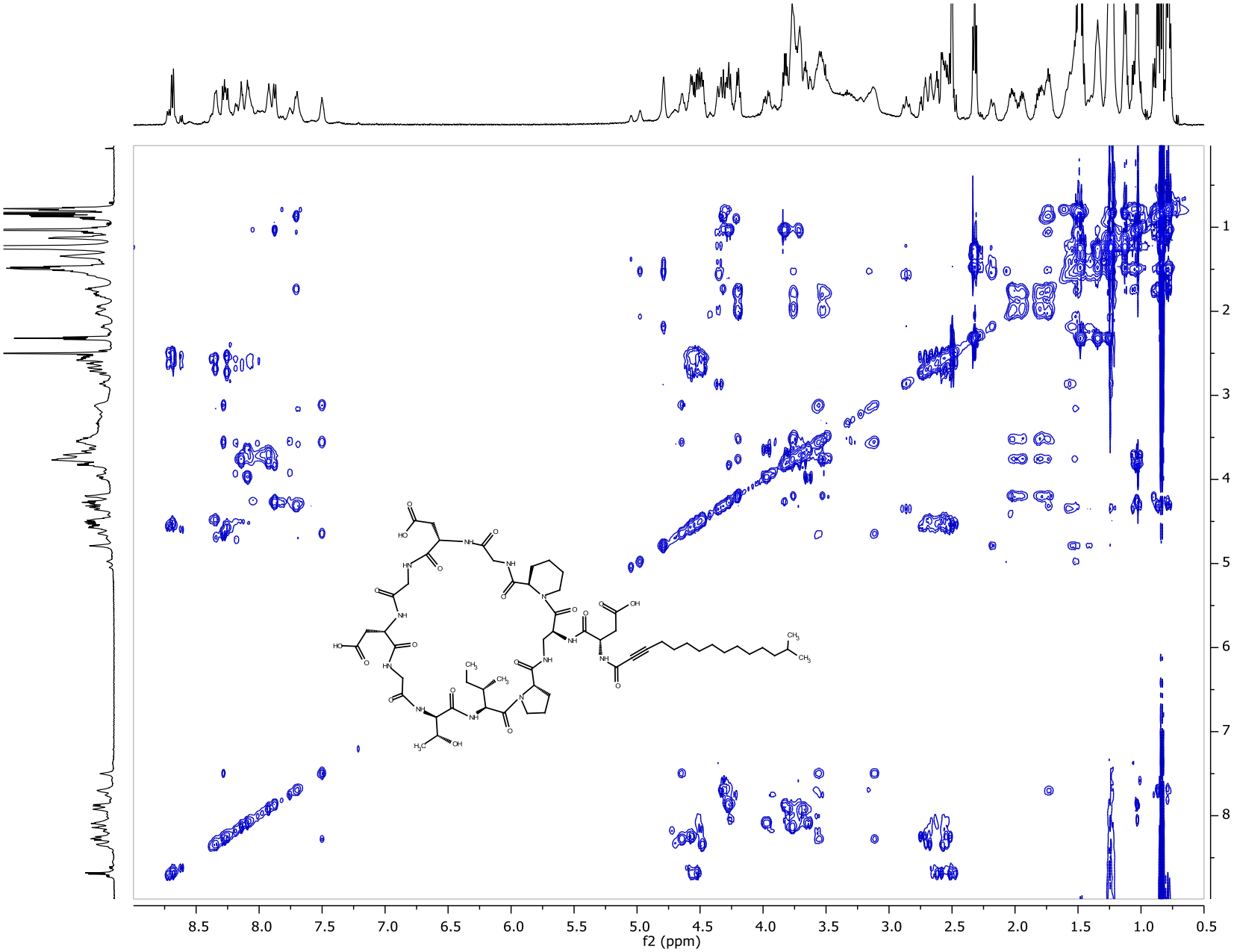


14-methylpentadec-2-ynoyl analogue (**19**) COSY (500 MHz, DMSO-d_6)



Parameter	Value
Title	LC.10.038.3.ser
Comment	COSY
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	cosygpqf
Experiment	COSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	20
Receiver Gain	203.0
Relaxation Delay	1.3000
Pulse Width	5.2500
Acquisition Time	0.4547
Acquisition Date	2017-12-18T18:06:29
Modification Date	2017-12-18T20:38:32
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(4504.5, 4500.5)
Lowest Frequency	(-5.2, -5.1)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

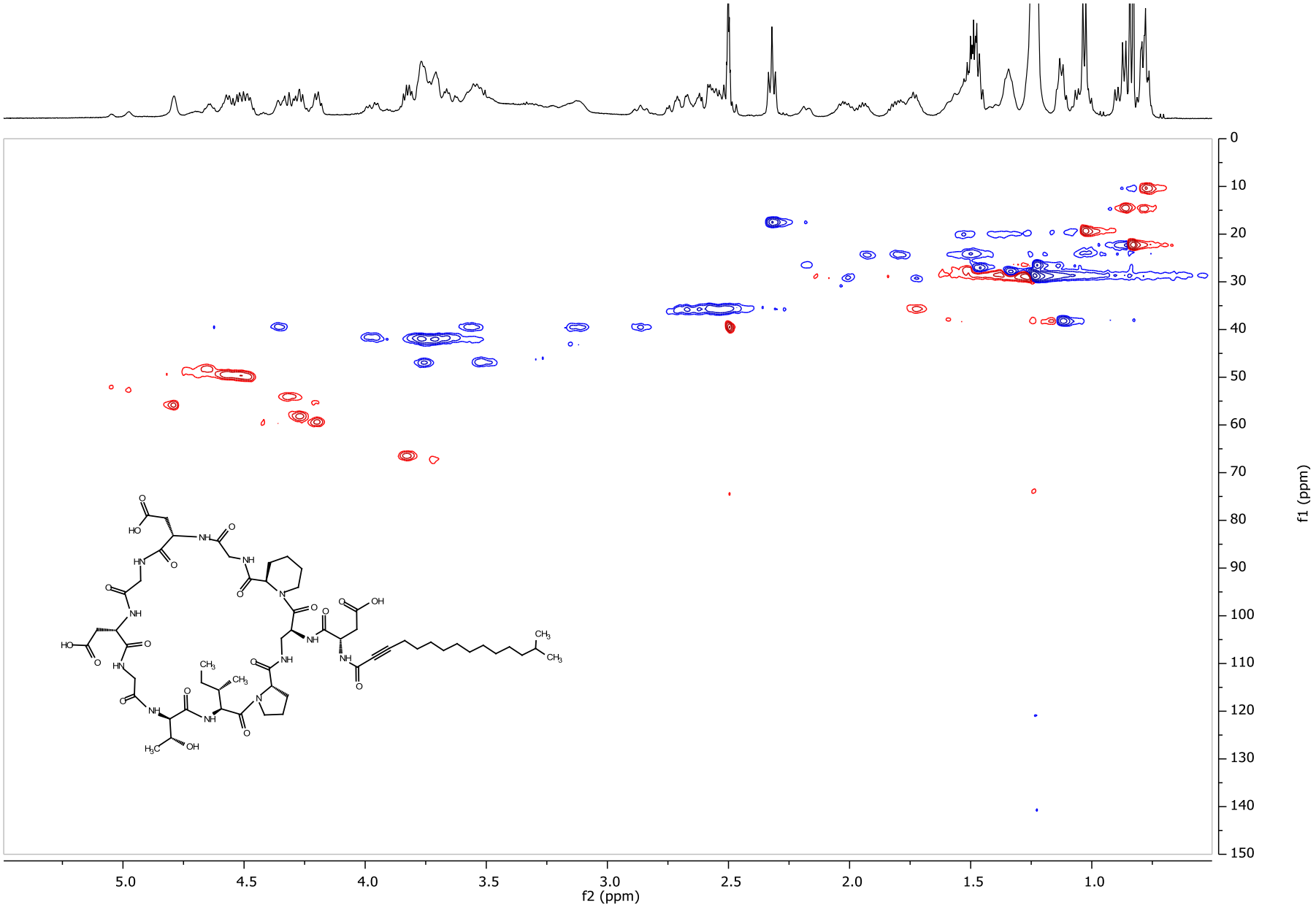
14-methylpentadec-2-ynoyl analogue (**19**) TOCSY (500 MHz, DMSO-d_6)



Parameter	Value
Title	LC.10.038.4.ser
Comment	TOCSY
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	dipsi2etgpsi
Experiment	2D-TOCSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	20
Receiver Gain	203.0
Relaxation Delay	1.3000
Pulse Width	5.2500
Acquisition Time	0.4547
Acquisition Date	2017-12-18T20:39:36
Modification Date	2017-12-18T23:18:26
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(4504.5, 4500.5)
Lowest Frequency	(-4.7, -3.6)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

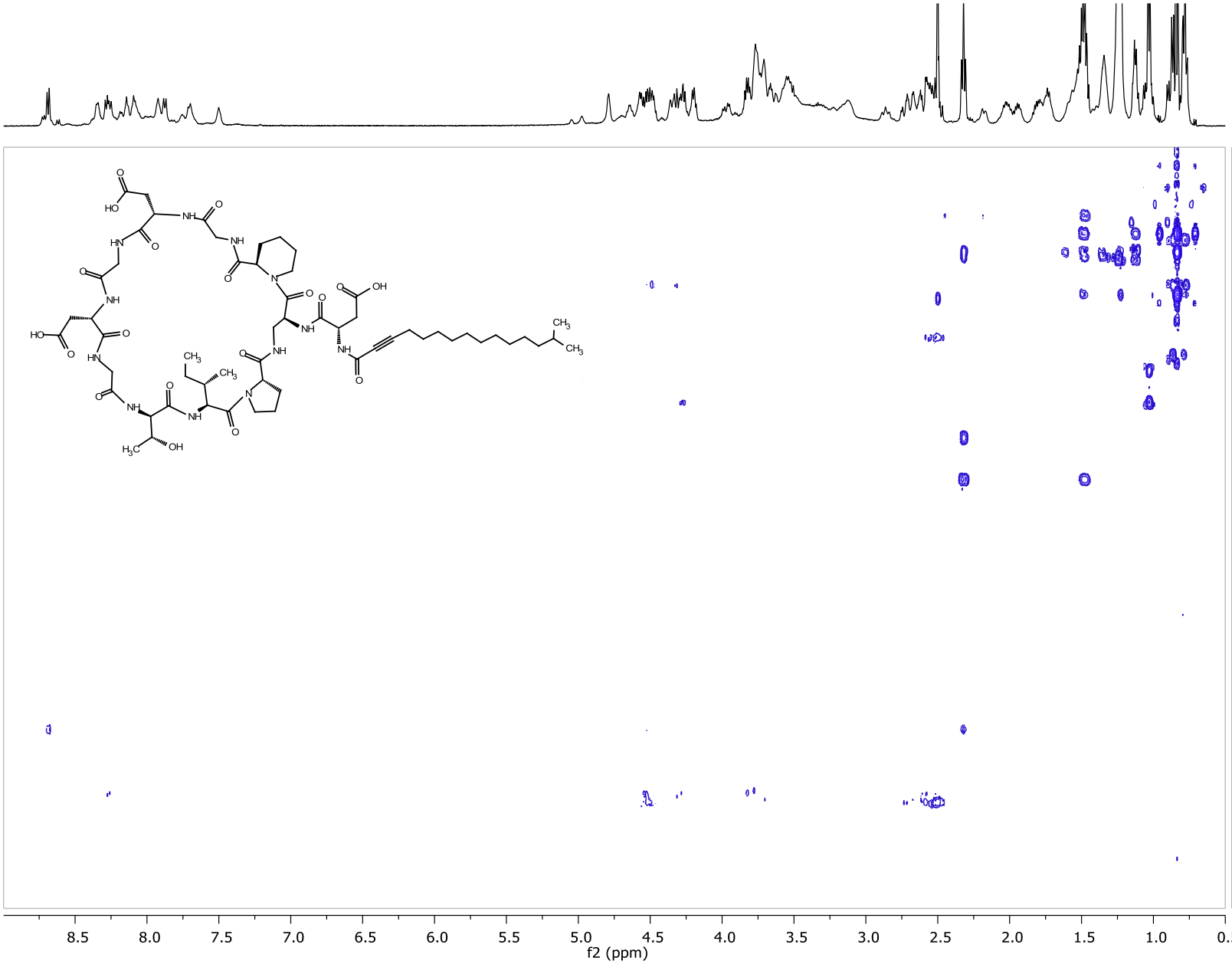
14-methylpentadec-2-ynoyl analogue (**19**) HSQC (500/126 MHz, DMSO-d_6)

Parameter	Value
Title	LC. 10.038.2.ser
Comment	HSQC
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hsqcedgpph
Experiment	HSQC-EDITED
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	20
Receiver Gain	203.0
Relaxation Delay	1.3000
Pulse Width	5.2500
Acquisition Time	0.2048
Acquisition Date	2017-12-18T15 :55:27
Modification Date	2017-12-18T18 :05:11
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(2500.0, 20833.3)
Lowest Frequency	(246.9, -1078.9)
Nucleus	(1H, 13C)
Acquired Size	(512, 256)
Spectral Size	(512, 512)

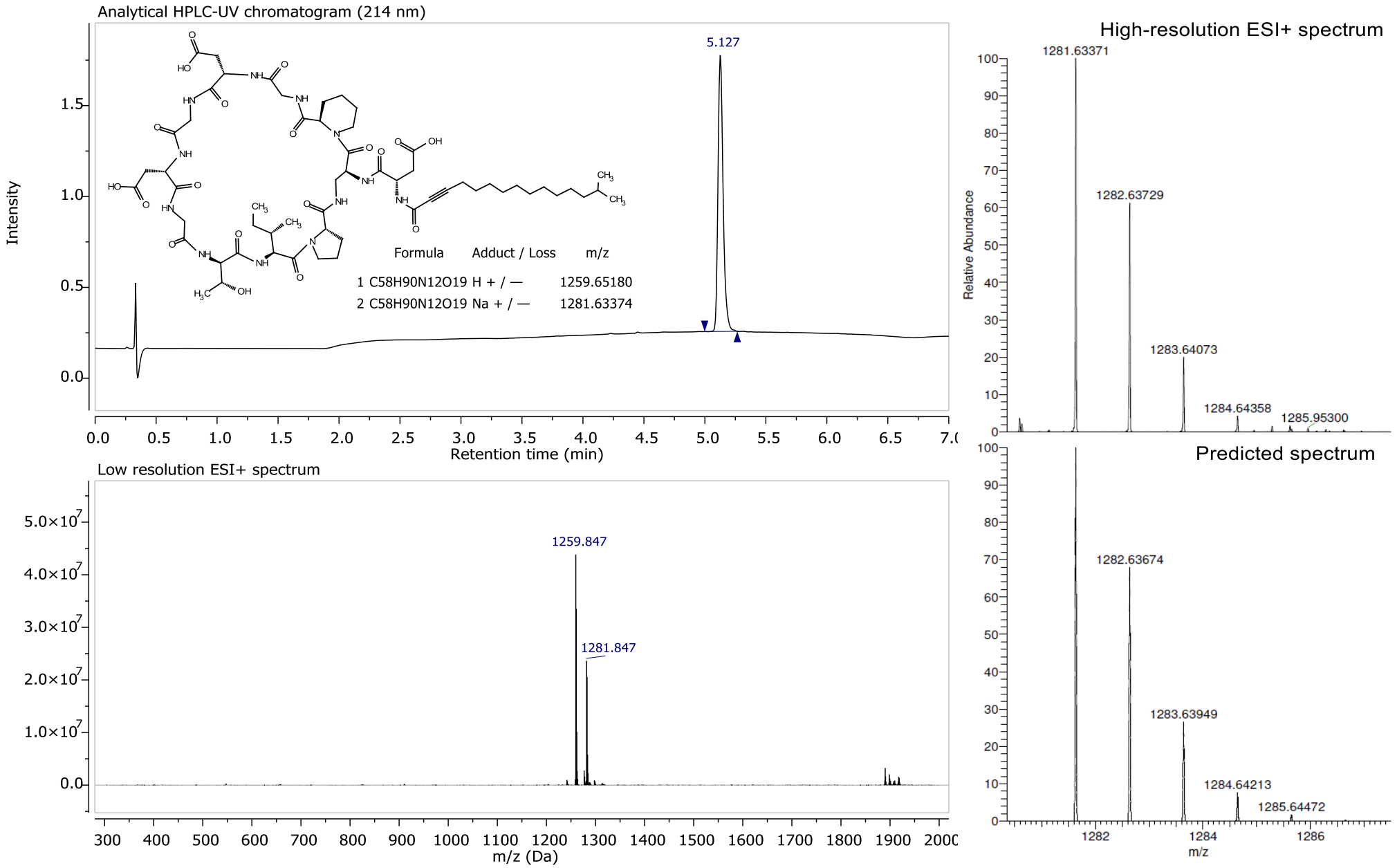


14-methylpentadec-2-ynoyl analogue (**19**) HMBC (500/126 MHz, DMSO-d_6)

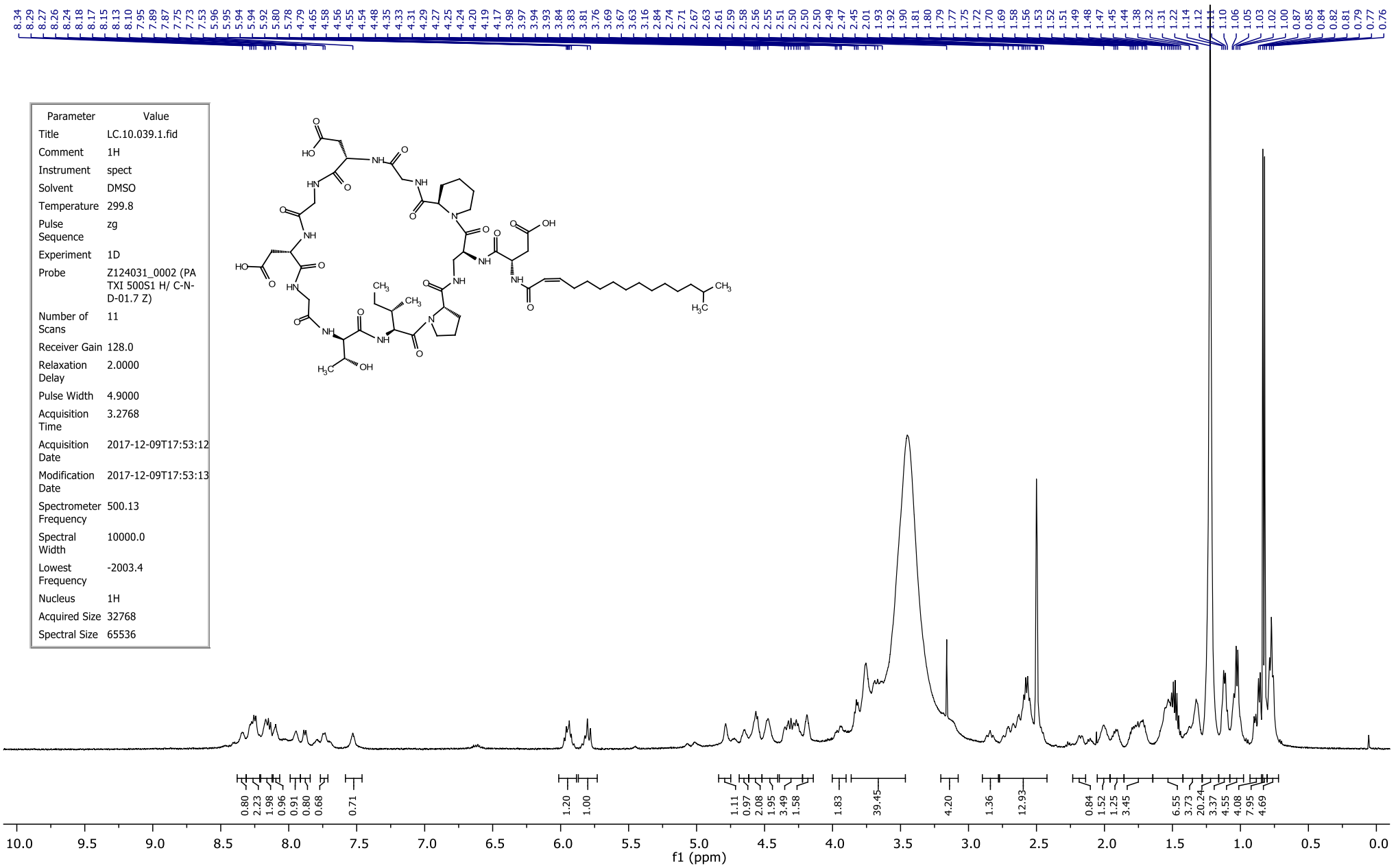
Parameter	Value
Title	LC.10.038.5.ser
Comment	HMBC
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hmbcgplpndqf
Experiment	HMBC
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	128
Receiver Gain	203.0
Relaxation Delay	1.3000
Pulse Width	5.2500
Acquisition Time	0.4547
Acquisition Date	2017-12-18T23:23:02
Modification Date	2017-12-19T09:08:42
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(4504.5, 25125.6)
Lowest Frequency	(-4.7, -41.4)
Nucleus	(1H, 13C)
Acquired Size	(2048, 152)
Spectral Size	(2048, 1024)



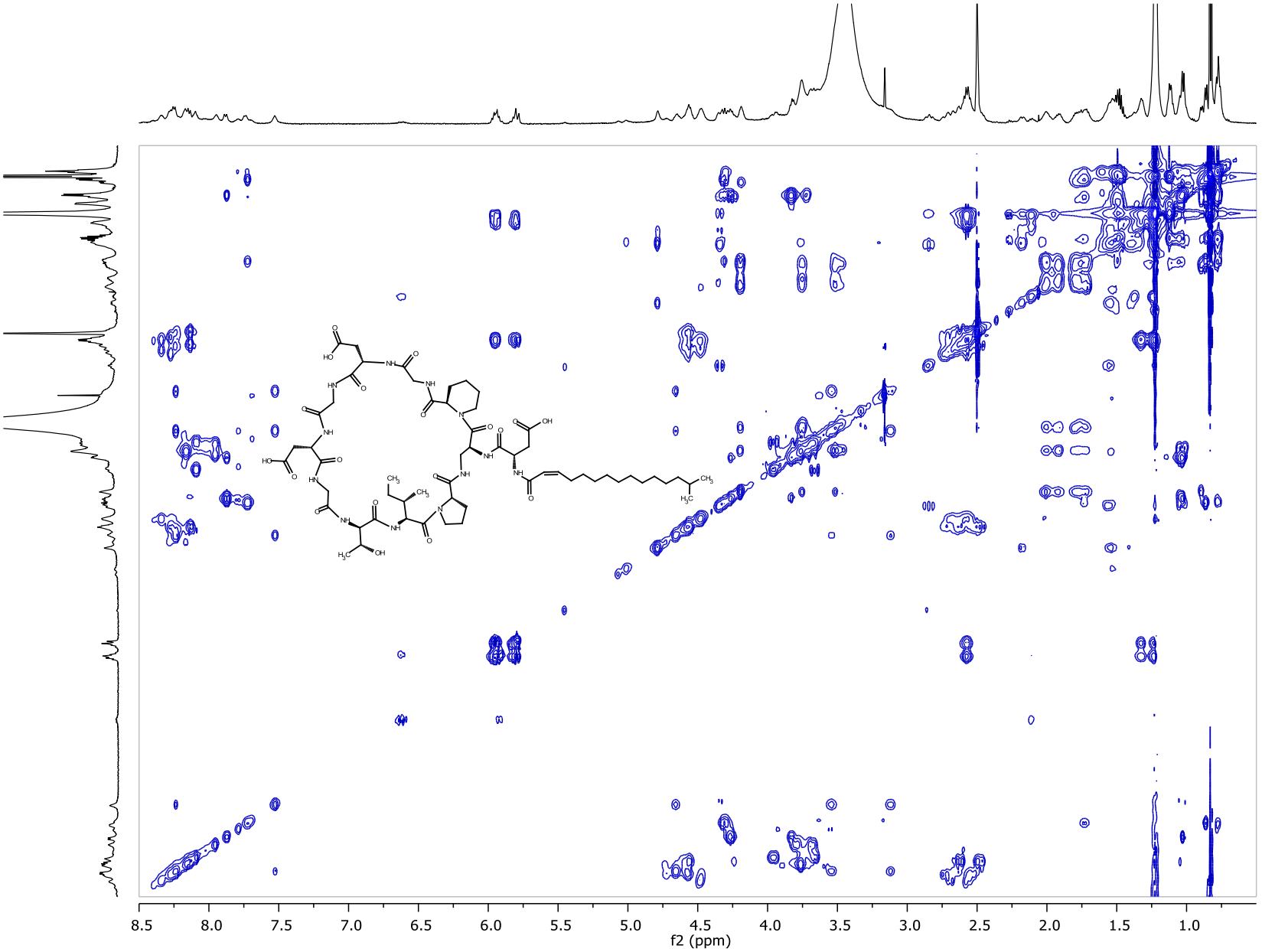
14-methylpentadec-2-ynoyl analogue (**19**) Analytical HPLC, low and high-resolution ESI+ MS



(*Z*)-14-methylpentadec-2-enoyl analogue (**20**) ^{1}H NMR (500 MHz, DMSO-d_6)

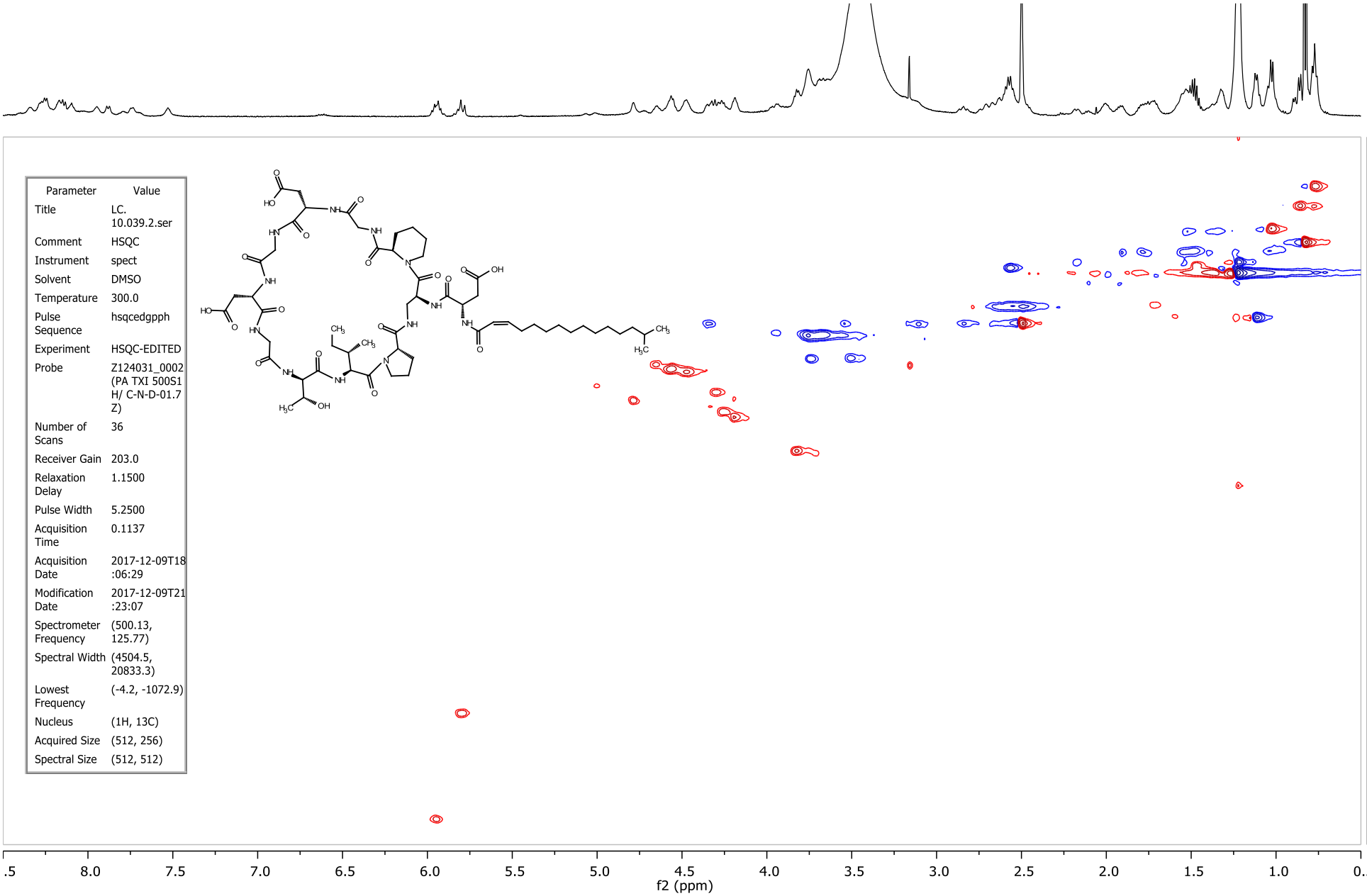


(*Z*)-14-methylpentadec-2-enoyl analogue (**20**) TOCSY (500 MHz, DMSO-d_6)



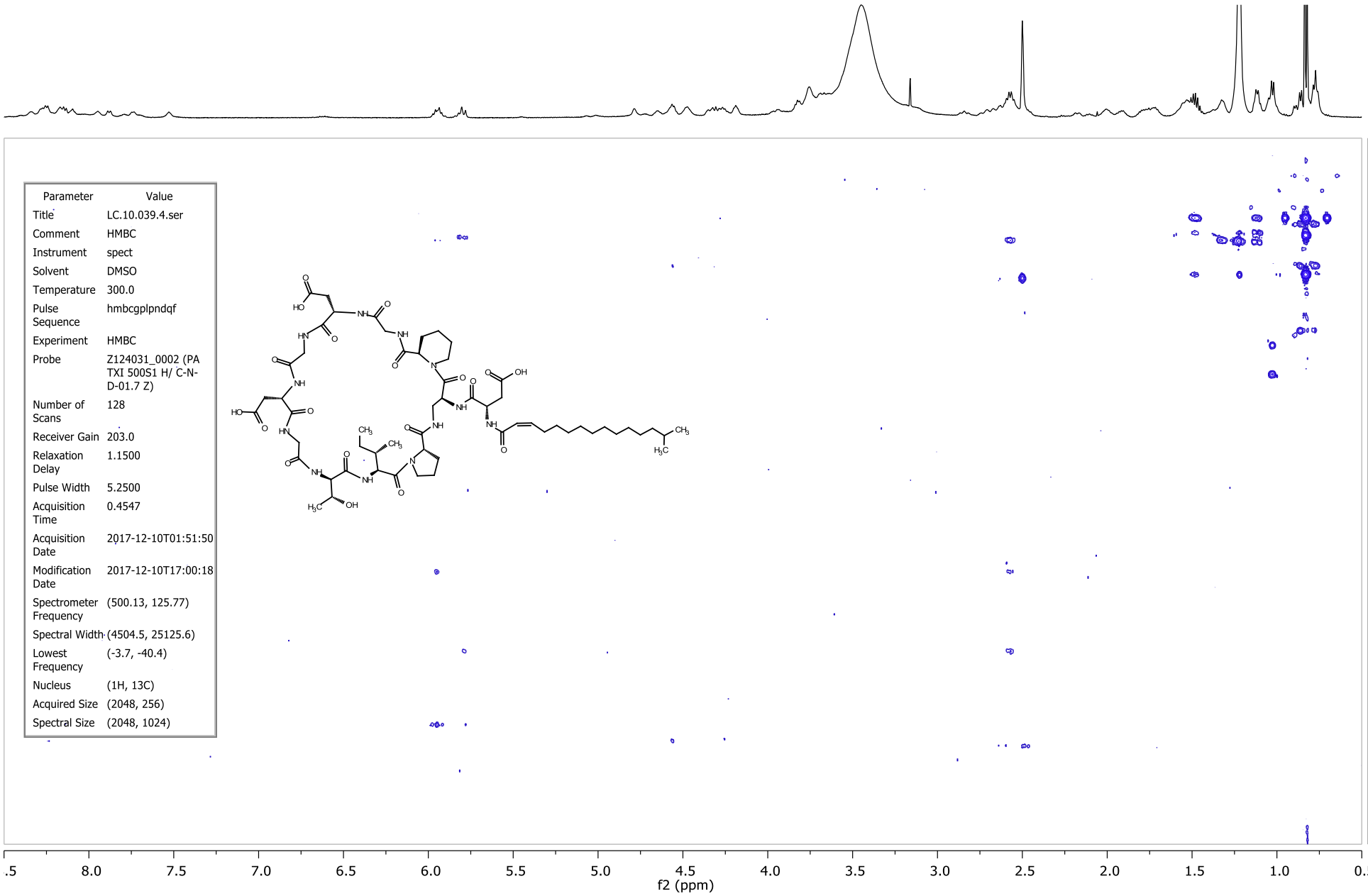
Parameter	Value
Title	LC.10.039.3.ser
Comment	TOCSY
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	dipsi2etgpsi
Experiment	2D-TOCSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	36
Receiver Gain	203.0
Relaxation Delay	1.1500
Pulse Width	5.2500
Acquisition Time	0.4547
Acquisition Date	2017-12-09T21:24:36
Modification Date	2017-12-10T01:47:36
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(4504.5, 4500.5)
Lowest Frequency	(-4.7, -4.6)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

(*Z*)-14-methylpentadec-2-enoyl analogue (**20**) HSQC (500/126 MHz, DMSO-d_6)

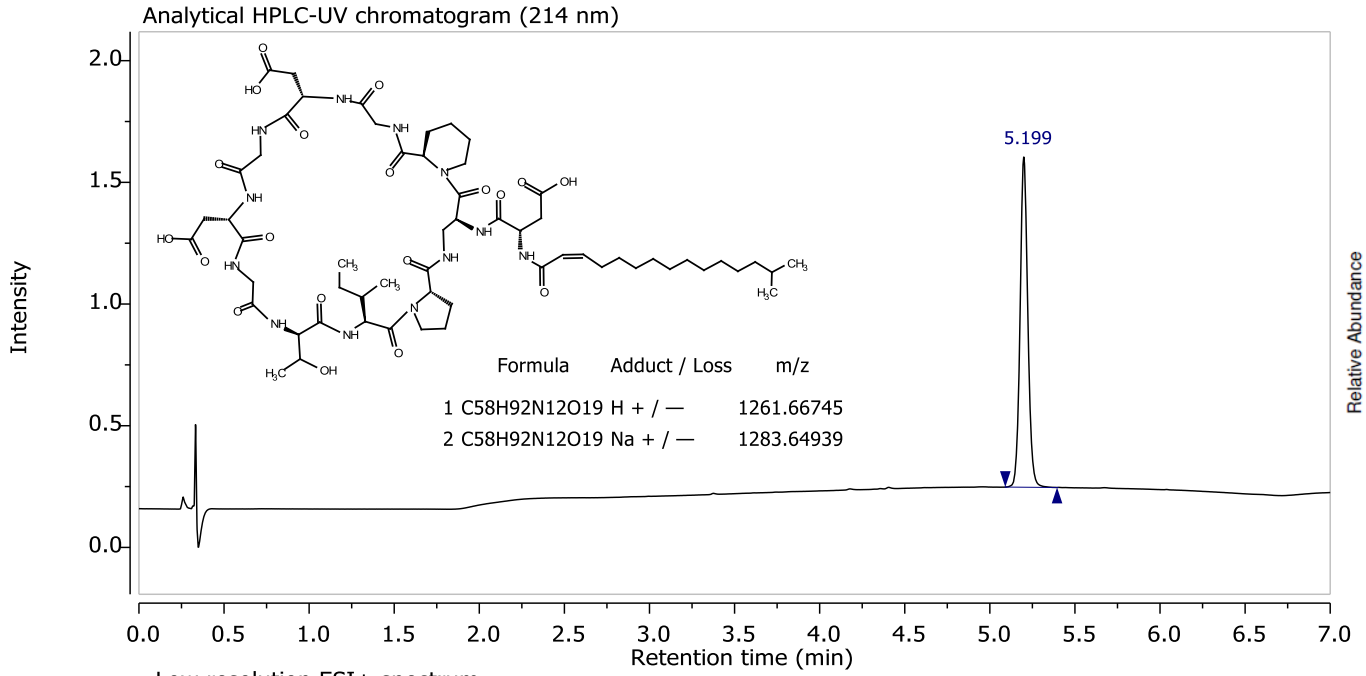


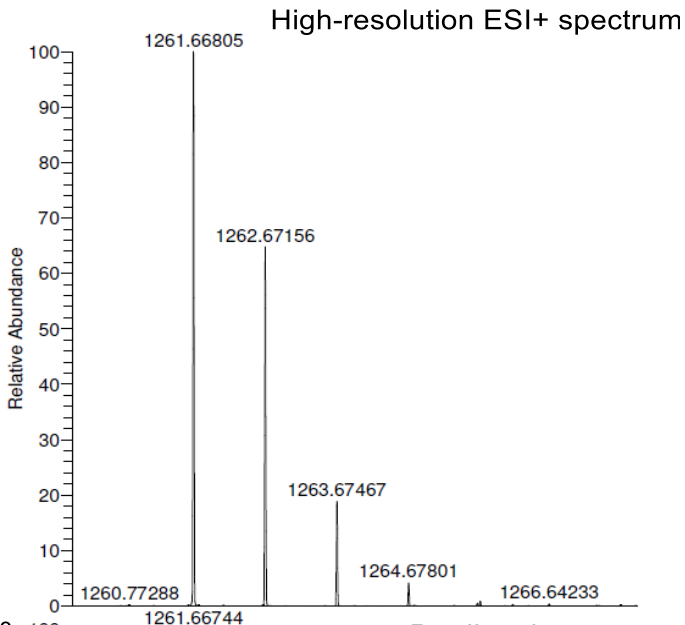
Parameter	Value
Title	LC. 10.039.2.ser
Comment	HSQC
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hsqcedgpph
Experiment	HSQC-EDITED
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	36
Receiver Gain	203.0
Relaxation Delay	1.1500
Pulse Width	5.2500
Acquisition Time	0.1137
Acquisition Date	2017-12-09T18 :06:29
Modification Date	2017-12-09T21 :23:07
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(4504.5, 20833.3)
Lowest Frequency	(-4.2, -1072.9)
Nucleus	(1H, 13C)
Acquired Size	(512, 256)
Spectral Size	(512, 512)

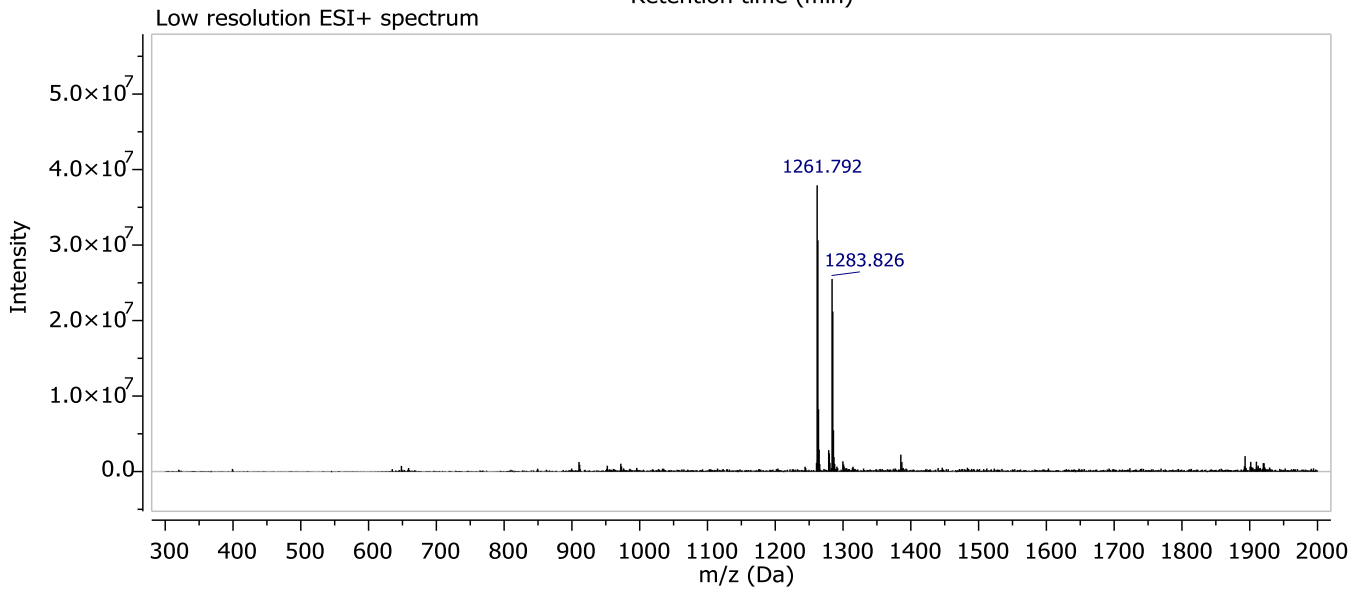
(*Z*)-14-methylpentadec-2-enoyl analogue (**20**) HMBC (500/126 MHz, DMSO-d_6)

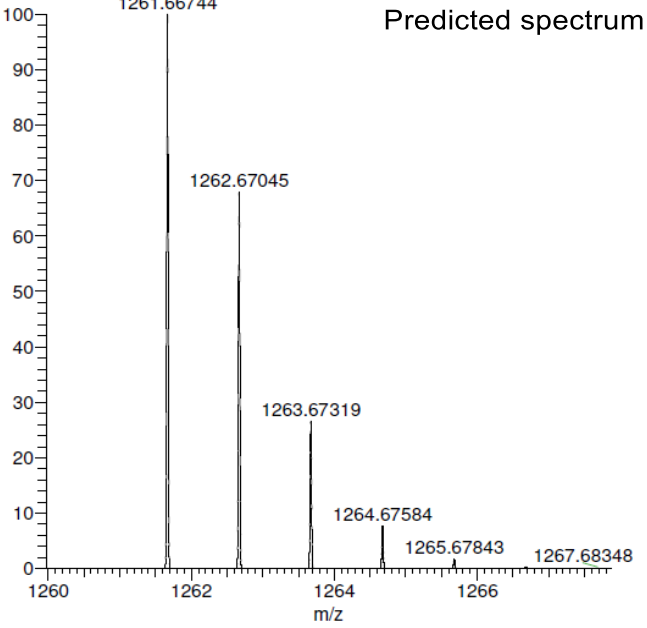


(*Z*)-14-methylpentadec-2-enoyl analogue (**20**) Analytical HPLC, low and high-resolution ESI+ MS



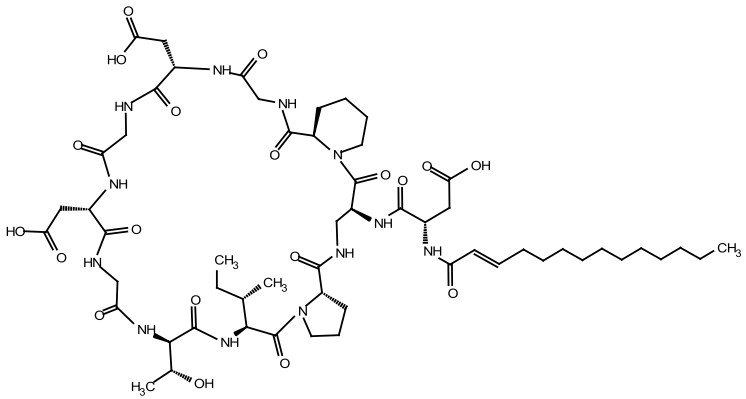




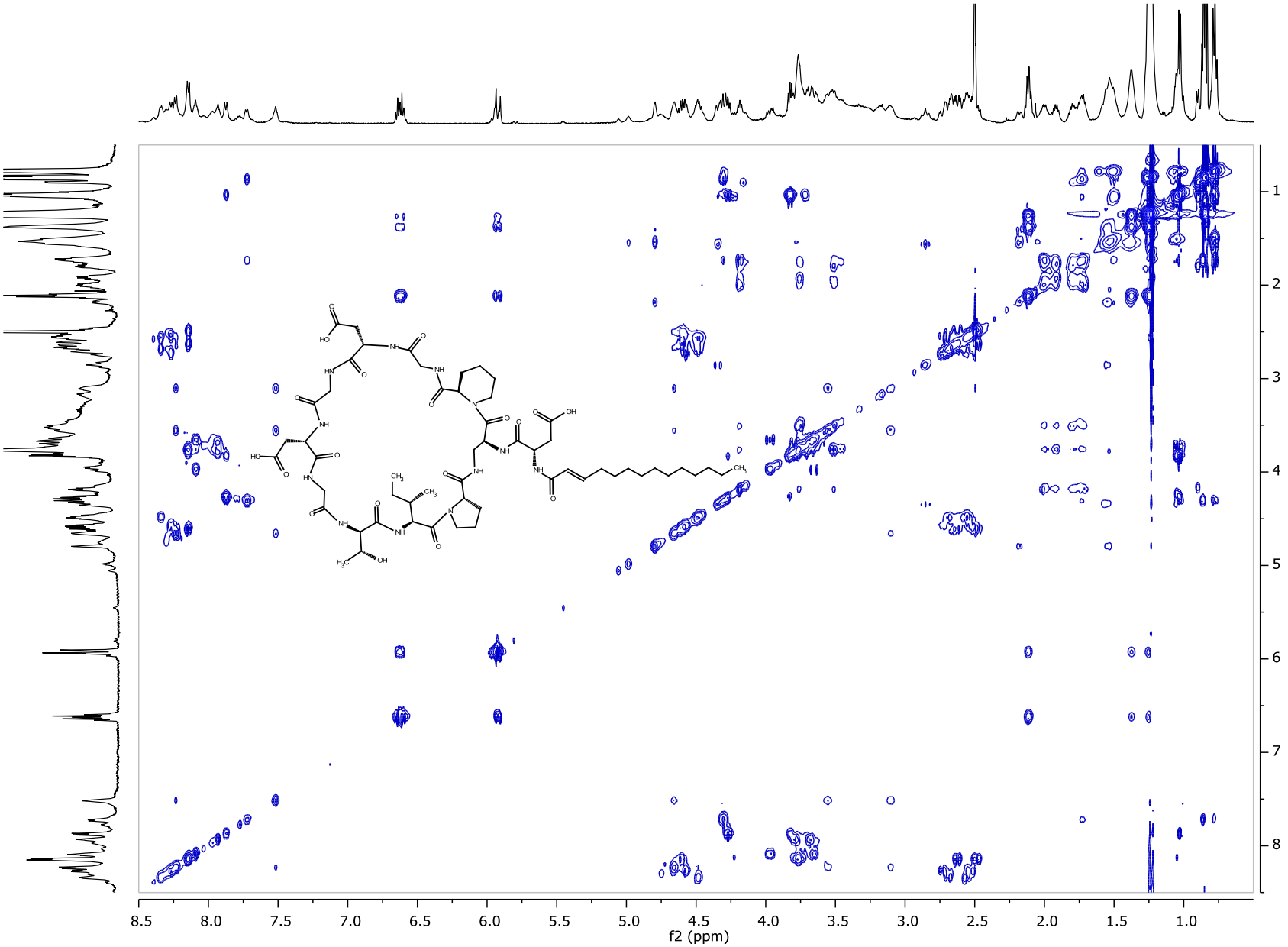


(*E*)-Tetradec-2-enoyl analogue (**21**) ^{1}H NMR (500 MHz, DMSO-d_6)

Parameter	Value
Title	LC.10.042.1.fid
Comment	1H
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	zg
Experiment	1D
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	10
Receiver Gain	114.0
Relaxation Delay	2.0000
Pulse Width	4.9000
Acquisition Time	3.2768
Acquisition Date	2017-12-14T15:10:16
Modification Date	2017-12-14T15:10:16
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-2002.9
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

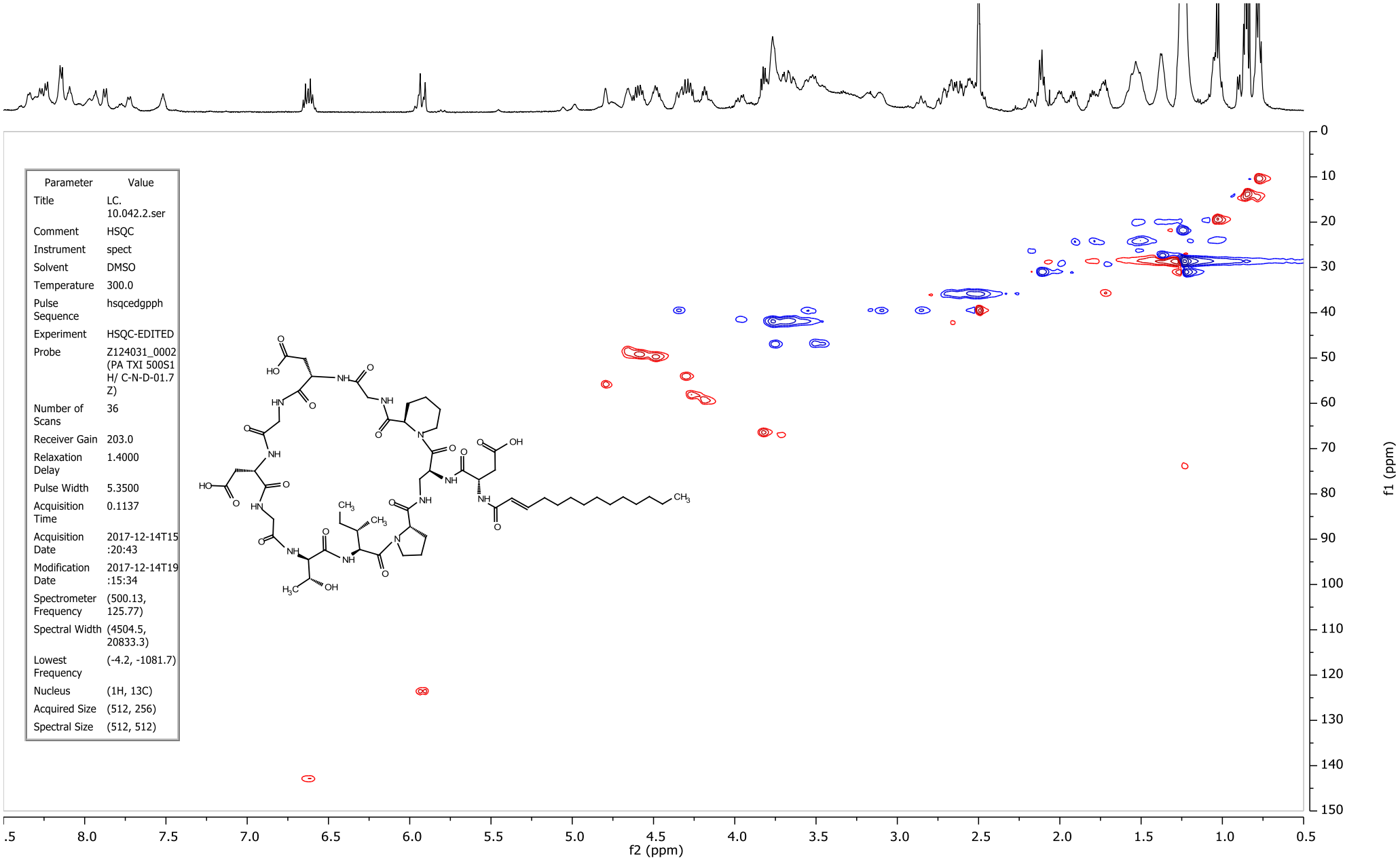


(*E*)-Tetradec-2-enoyl analogue (**21**) TOCSY (500 MHz, DMSO-d_6)

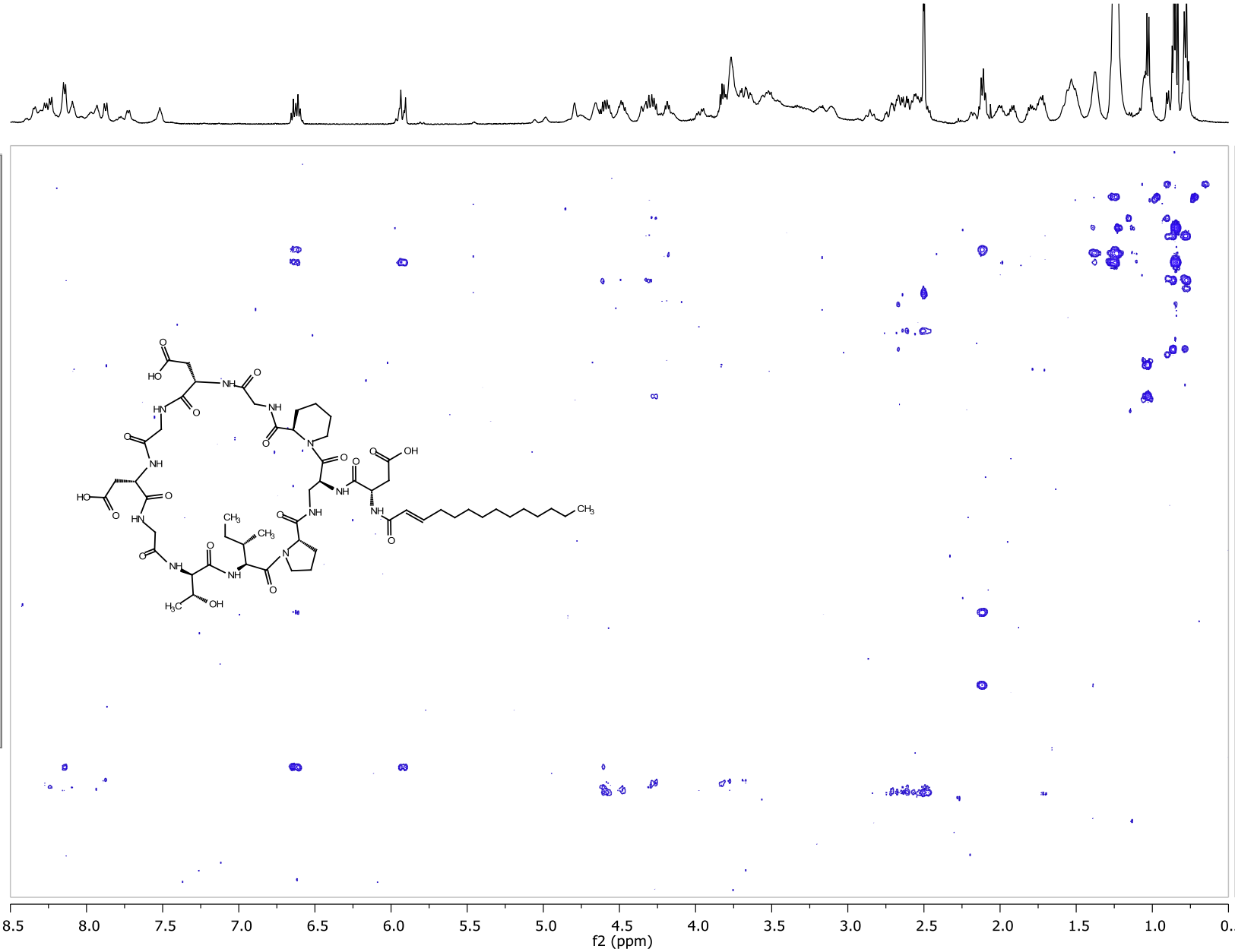


Parameter	Value
Title	LC.10.042.3.ser
Comment	TOCSY
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	dipsi2etgpsi
Experiment	2D-TOCSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	25
Receiver Gain	203.0
Relaxation Delay	1.4000
Pulse Width	5.3500
Acquisition Time	0.4547
Acquisition Date	2017-12-14T19:17:09
Modification Date	2017-12-14T22:46:19
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(4504.5, 4500.5)
Lowest Frequency	(-5.2, -3.1)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

(*E*)-Tetradec-2-enoyl analogue (**21**) HSQC (500/126 MHz, DMSO-d_6)

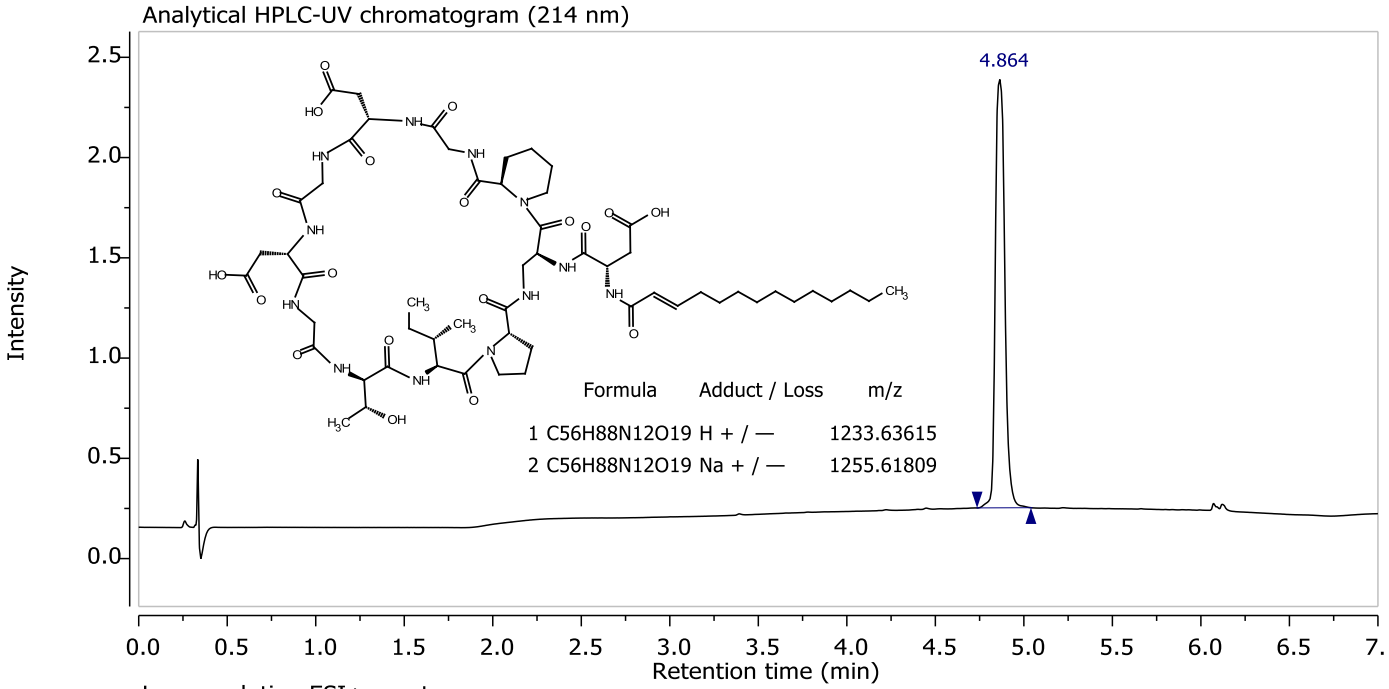


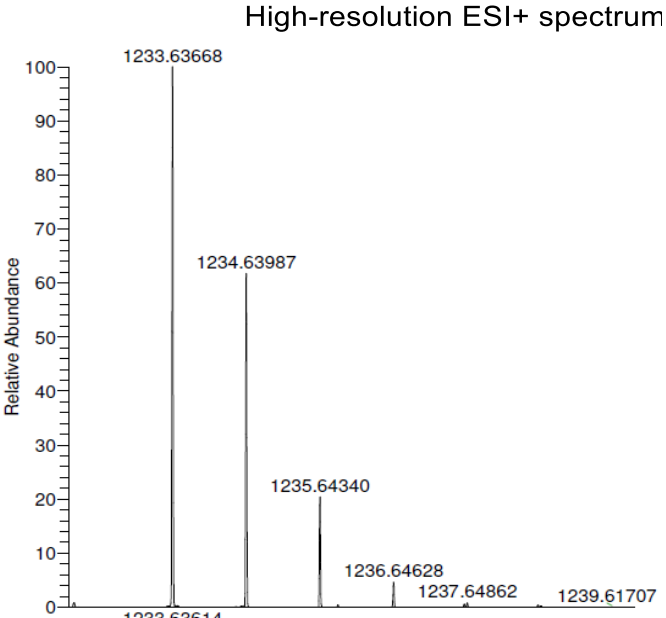
(*E*)-Tetradec-2-enoyl analogue (**21**) HMBC (500/126 MHz, DMSO-d_6)

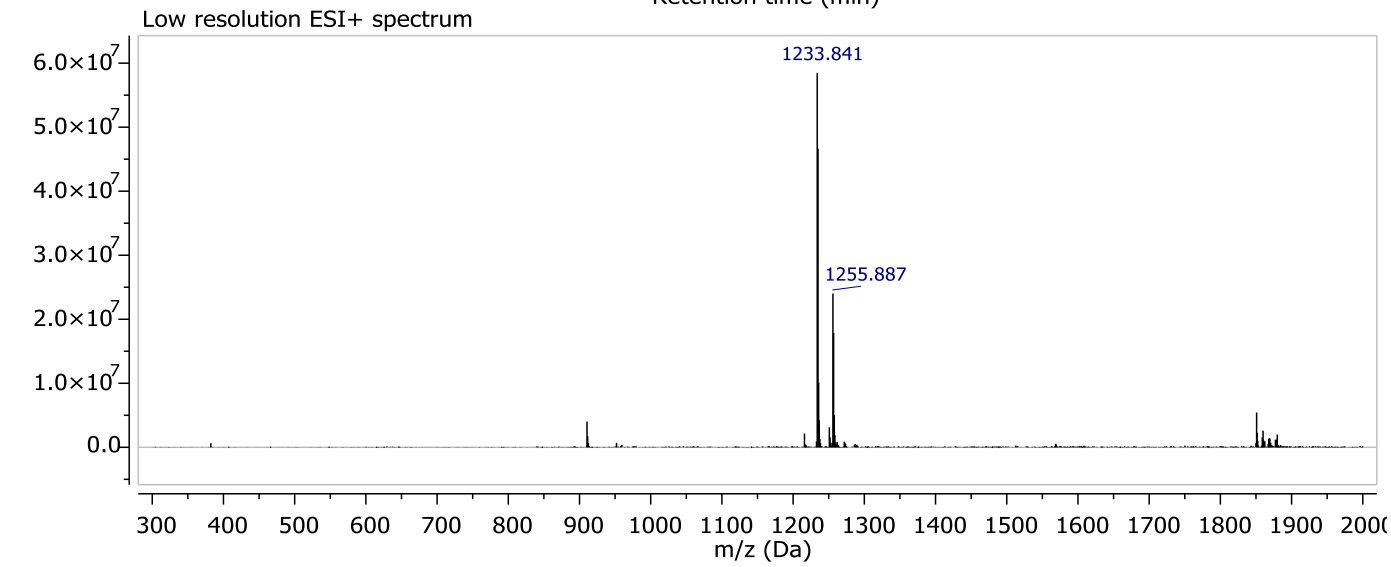


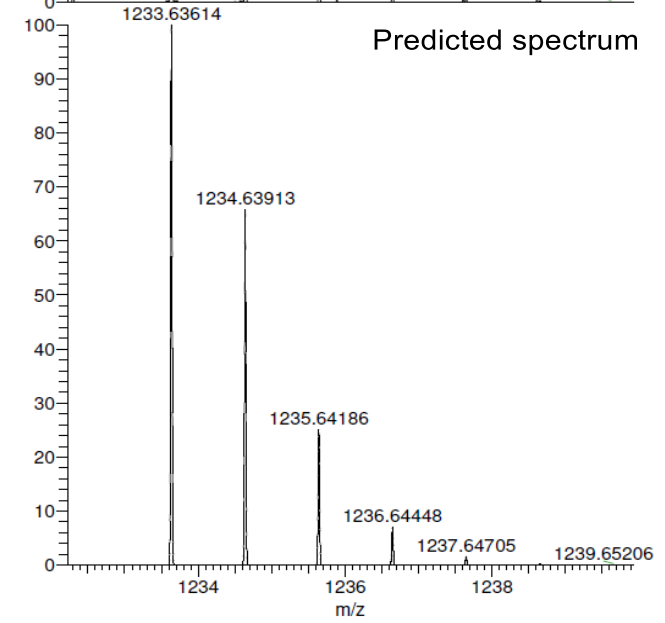
Parameter	Value
Title	LC.10.042.4.ser
Comment	HMBC
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hmbcgplpndqf
Experiment	HMBC
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	128
Receiver Gain	203.0
Relaxation Delay	1.4000
Pulse Width	5.3500
Acquisition Time	0.4547
Acquisition Date	2017-12-14T22:51:10
Modification Date	2017-12-15T15:51:02
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(4504.5, 25125.6)
Lowest Frequency	(-3.2, -89.4)
Nucleus	(1H, 13C)
Acquired Size	(2048, 250)
Spectral Size	(2048, 1024)

(E)-Tetradec-2-enoyl analogue (**21**) Analytical HPLC, low and high-resolution ESI+ MS

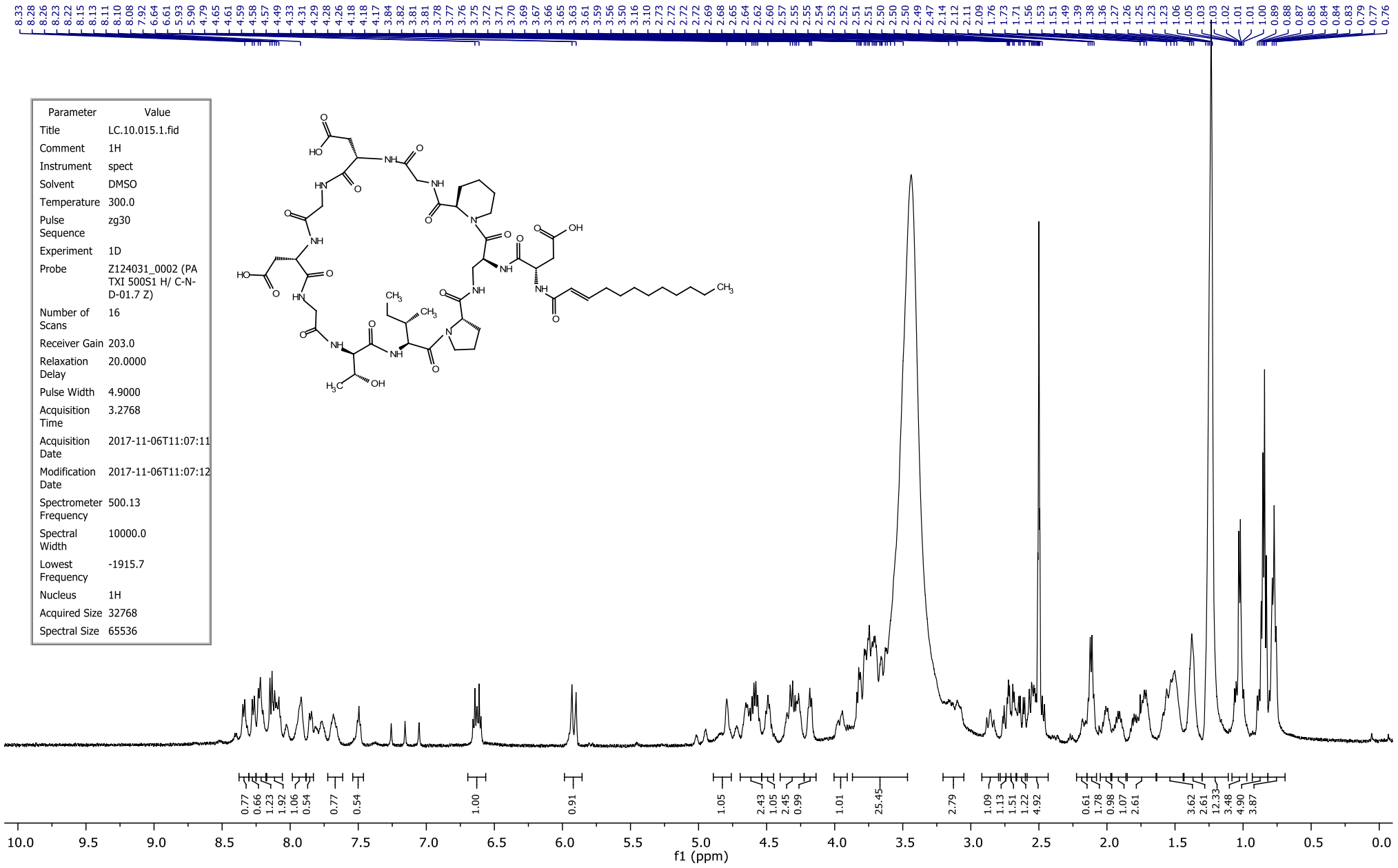




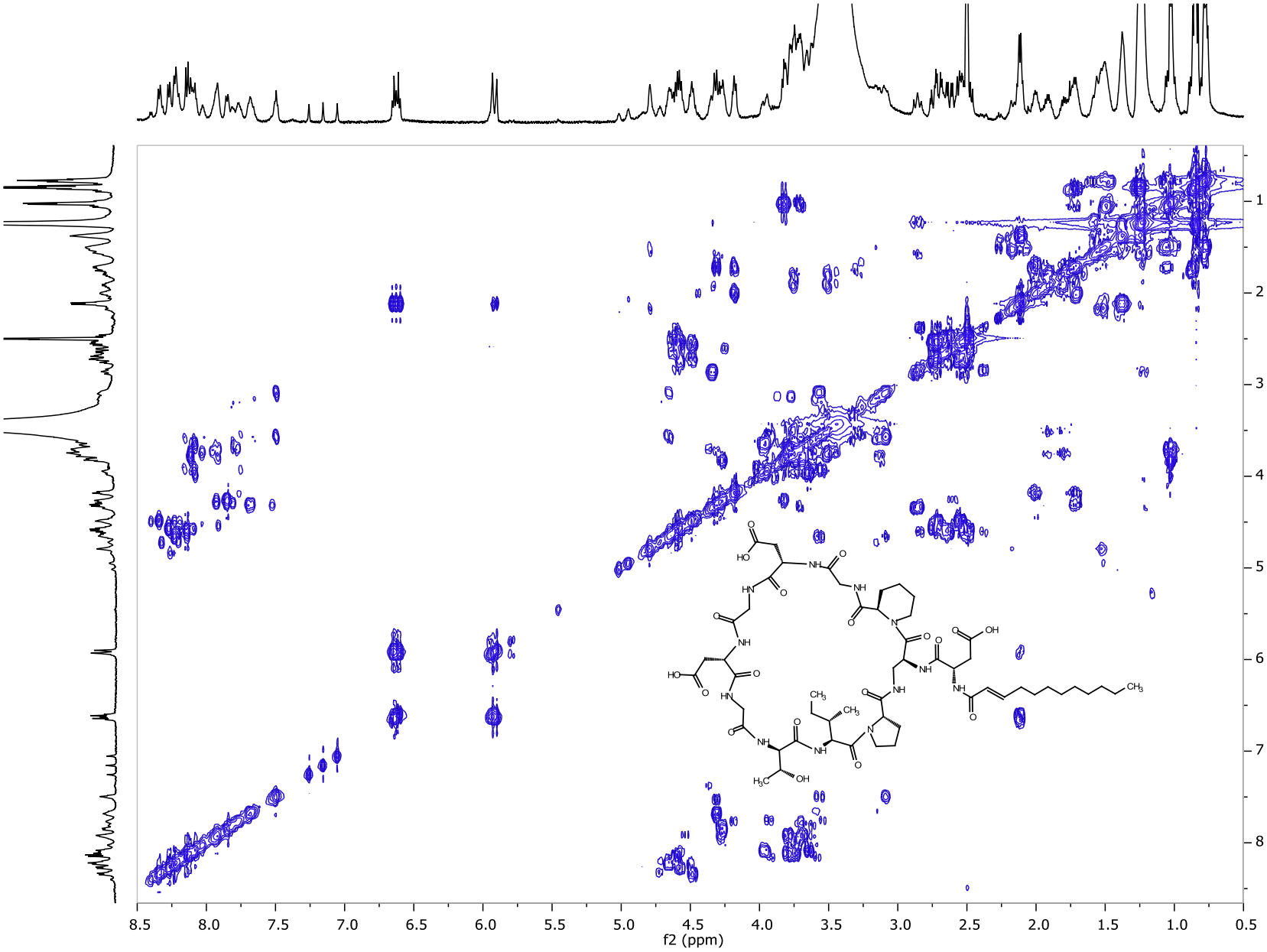




(*E*)-Dodec-2-enoyl analogue (**22**) ^{1}H NMR (500 MHz, DMSO-d_6)

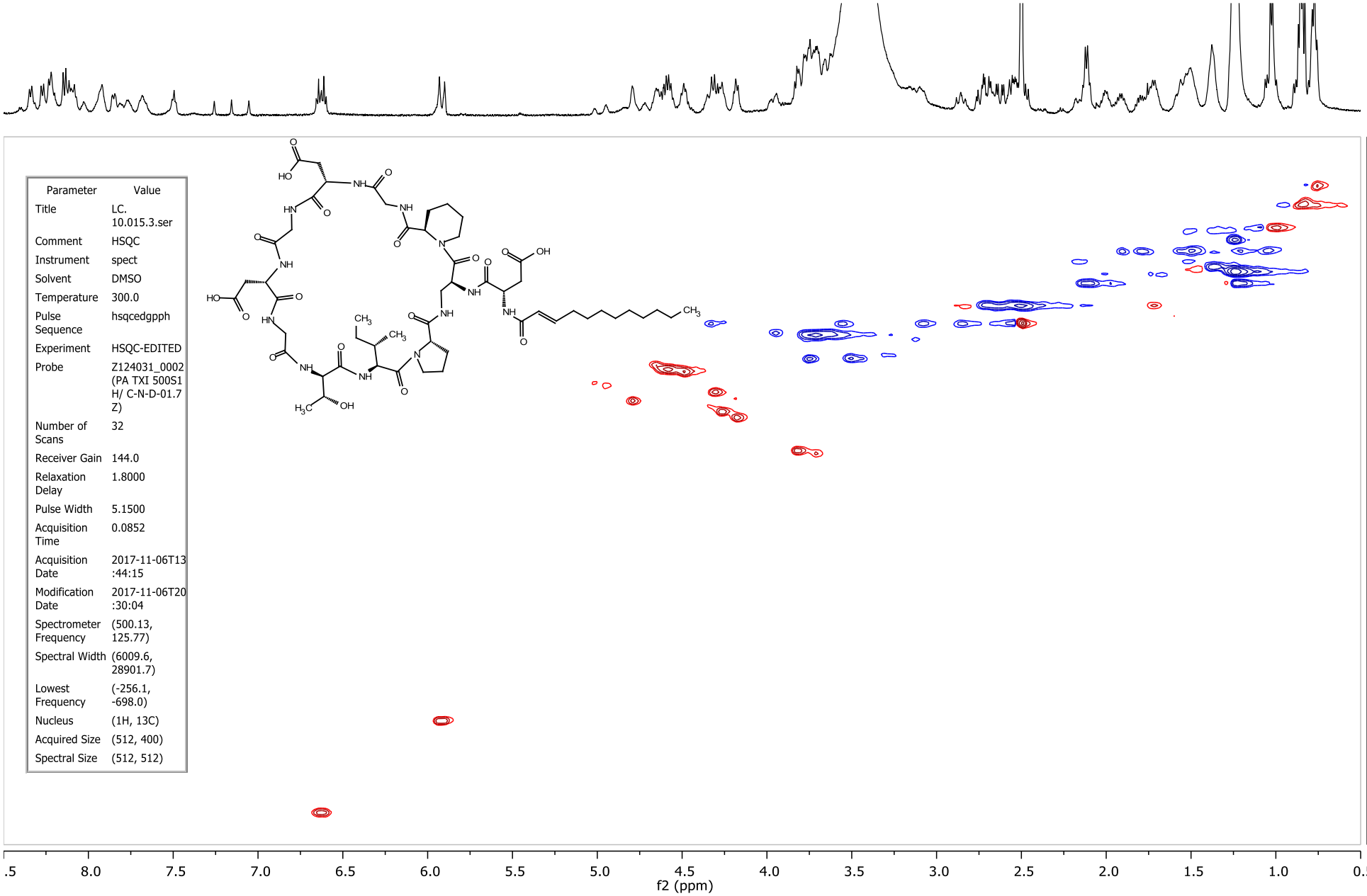


(*E*)-Dodec-2-enoyl analogue (**22**) COSY (500 MHz, DMSO-d_6)



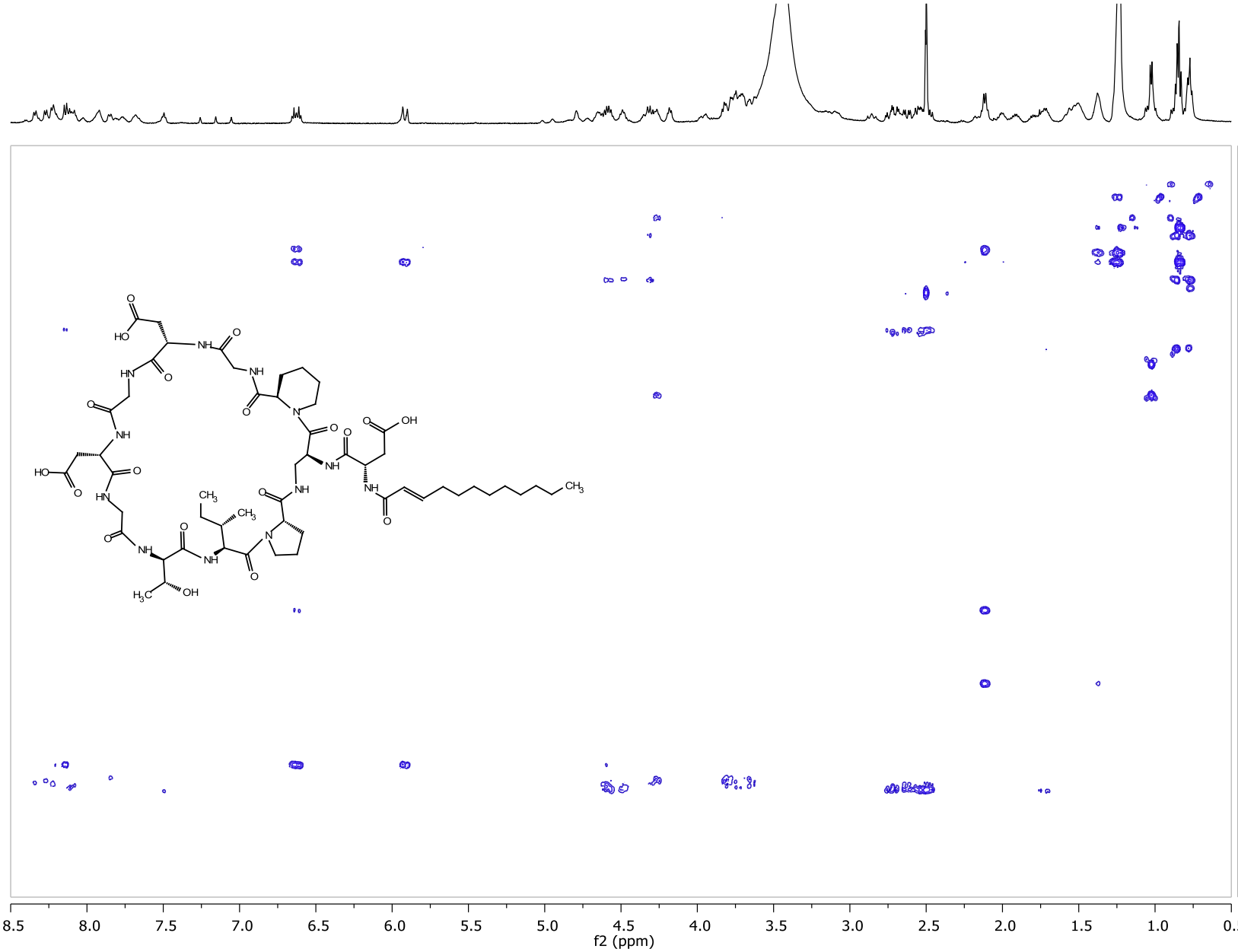
Parameter	Value
Title	LC.10.015.2.ser
Comment	COSY
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	cosygpqf
Experiment	COSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	16
Receiver Gain	203.0
Relaxation Delay	1.8000
Pulse Width	5.1500
Acquisition Time	0.3408
Acquisition Date	2017-11-06T11:15:07
Modification Date	2017-11-06T13:42:34
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(6009.6, 6002.4)
Lowest Frequency	(-259.6, -254.0)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

(*E*)-Dodec-2-enoyl analogue (**22**) HSQC (500/126 MHz, DMSO-d_6)



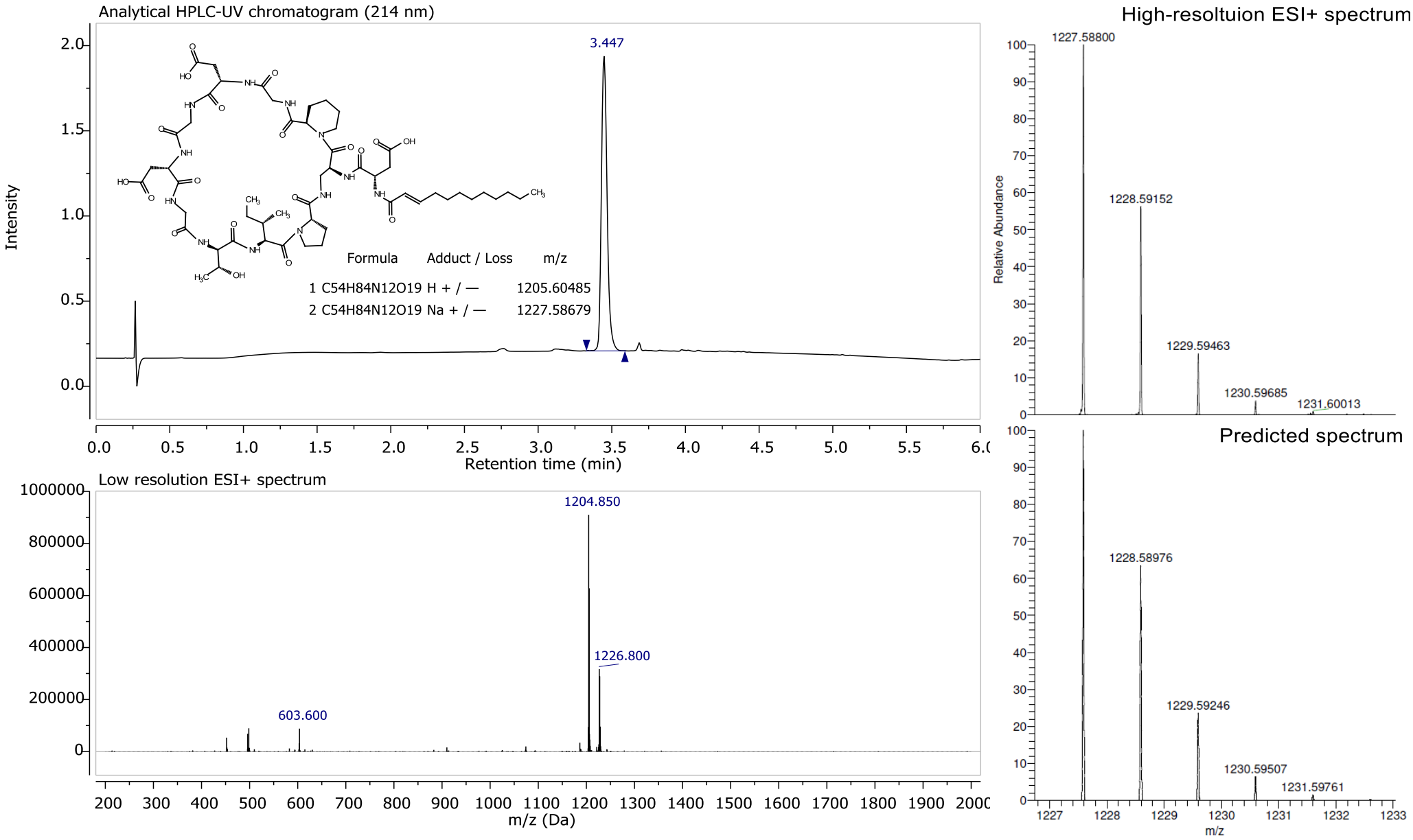
Parameter	Value
Title	LC. 10.015.3.ser
Comment	HSQC
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hsqcedgpph
Experiment	HSQC-EDITED
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	32
Receiver Gain	144.0
Relaxation Delay	1.8000
Pulse Width	5.1500
Acquisition Time	0.0852
Acquisition Date	2017-11-06T13 :44:15
Modification Date	2017-11-06T20 :30:04
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(6009.6, 28901.7)
Lowest Frequency	(-256.1, -698.0)
Nucleus	(1H, 13C)
Acquired Size	(512, 400)
Spectral Size	(512, 512)

(*E*)-Dodec-2-enoyl analogue (**22**) HMBC (500/126 MHz, DMSO-d_6)

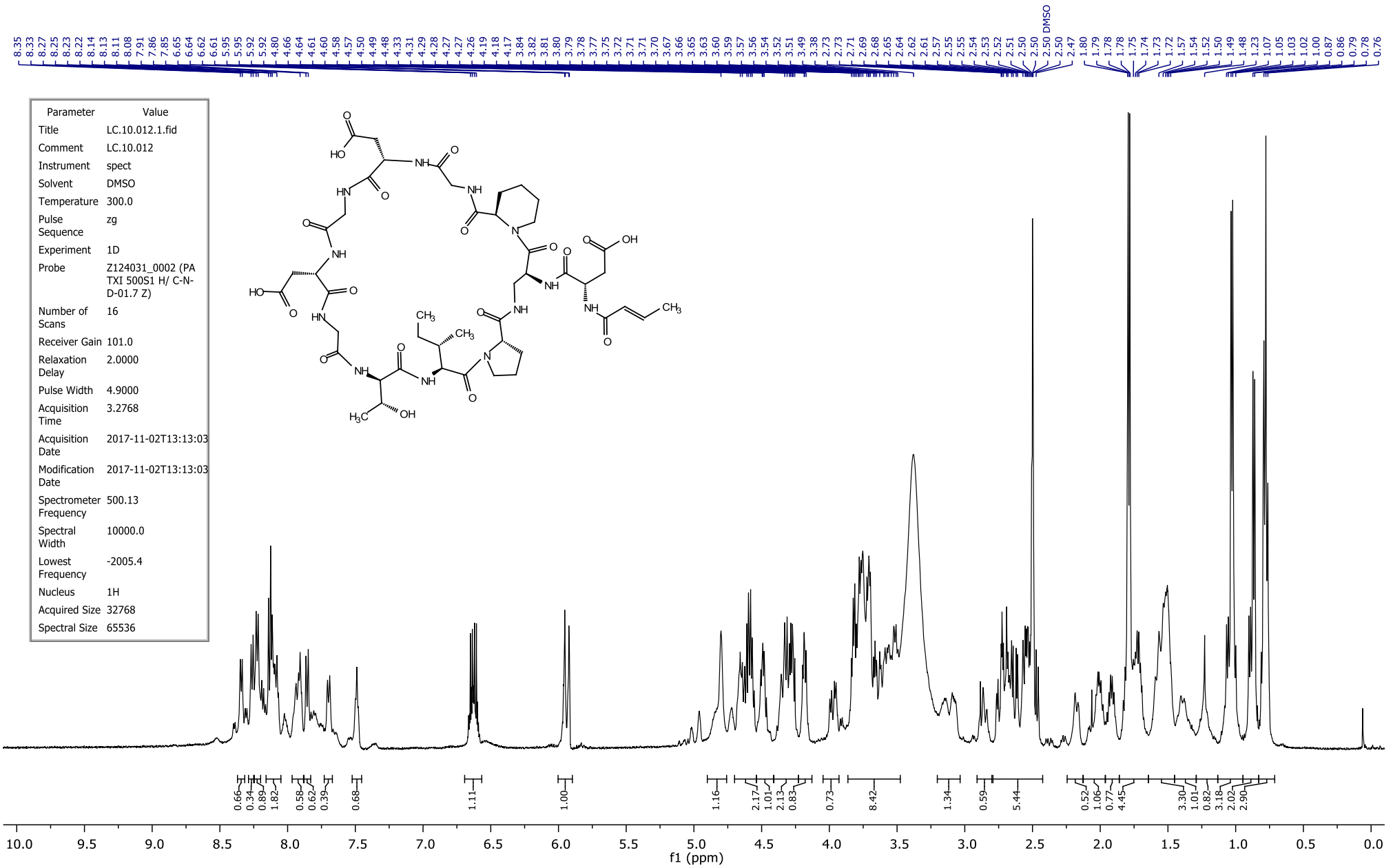


Parameter	Value
Title	LC.10.015.4.ser
Comment	HMBC
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hmbcgplpndqf
Experiment	HMBC
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	72
Receiver Gain	203.0
Relaxation Delay	1.8000
Pulse Width	5.1500
Acquisition Time	0.3408
Acquisition Date	2017-11-06T20:33:23
Modification Date	2017-11-07T10:03:36
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(6009.6, 28901.7)
Lowest Frequency	(-258.1, -707.5)
Nucleus	(1H, 13C)
Acquired Size	(2048, 307)
Spectral Size	(2048, 2048)

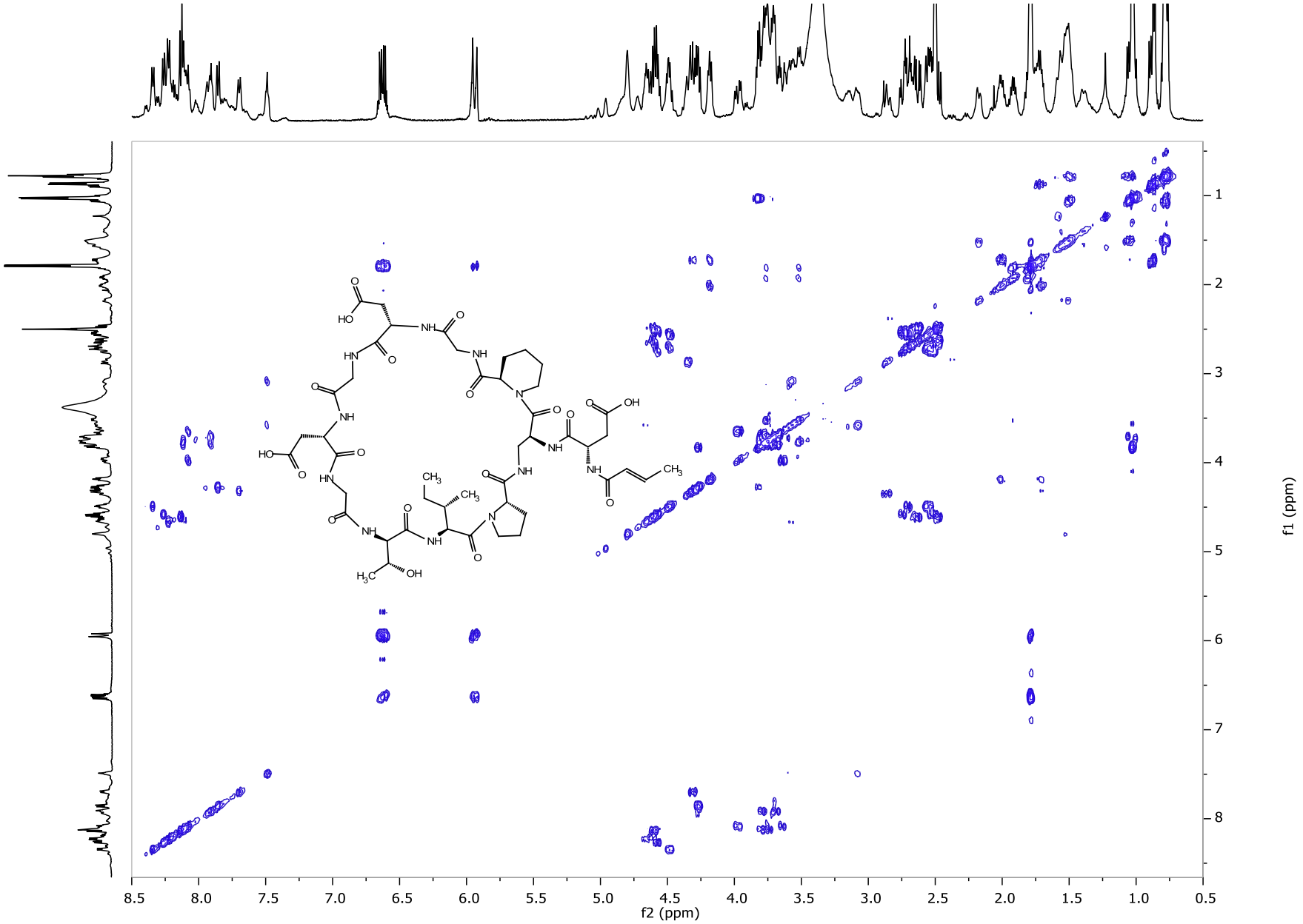
(*E*)-Dodec-2-enoyl analogue (**22**) Analytical HPLC, low and high-resolution ESI+ MS



(*E*)-But-2-enoyl analogue (**23**) ^{1}H NMR (500 MHz, DMSO-d_6)

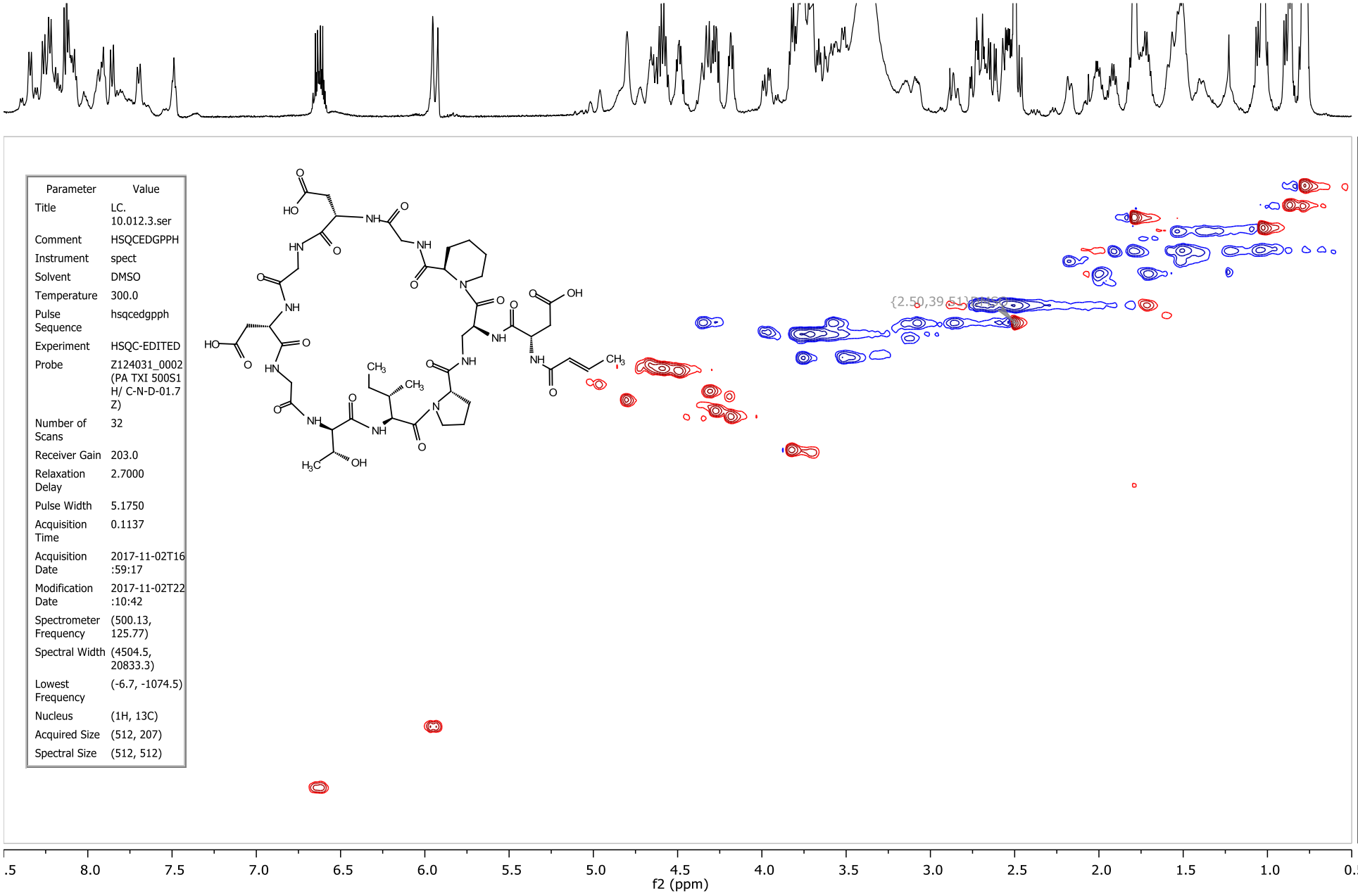


(*E*)-But-2-enoyl analogue (**23**) COSY (500 MHz, DMSO-d_6)



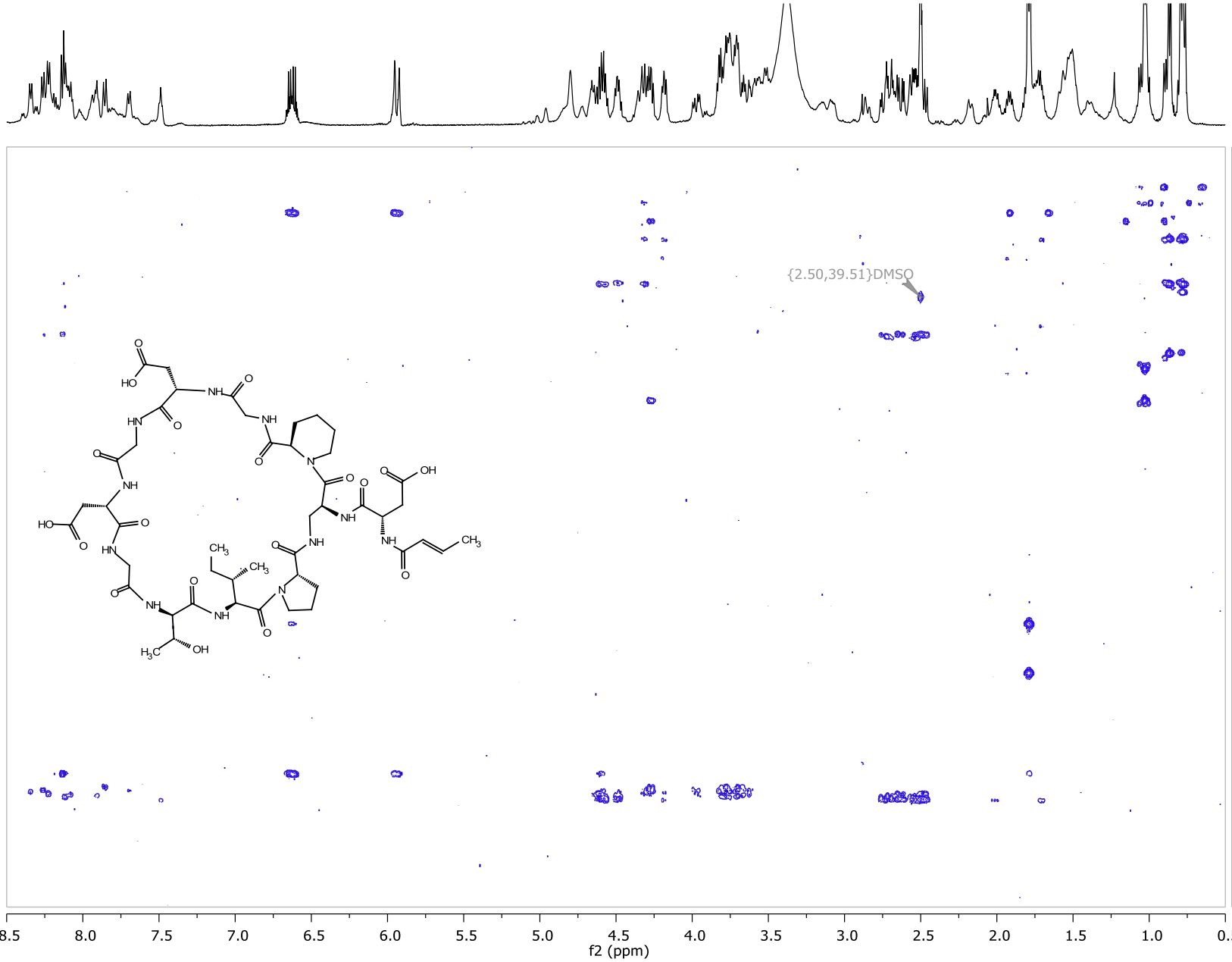
Parameter	Value
Title	LC.10.012.2.ser
Comment	LC.10.012
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	cosygpqf
Experiment	COSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	16
Receiver Gain	203.0
Relaxation Delay	2.7000
Pulse Width	5.1750
Acquisition Time	0.4547
Acquisition Date	2017-11-02T13:19:56
Modification Date	2017-11-02T16:56:48
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(4504.5, 4500.5)
Lowest Frequency	(-13.7, -3.1)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

(*E*)-But-2-enoyl analogue (**23**) HSQC (500/126 MHz, DMSO-d_6)



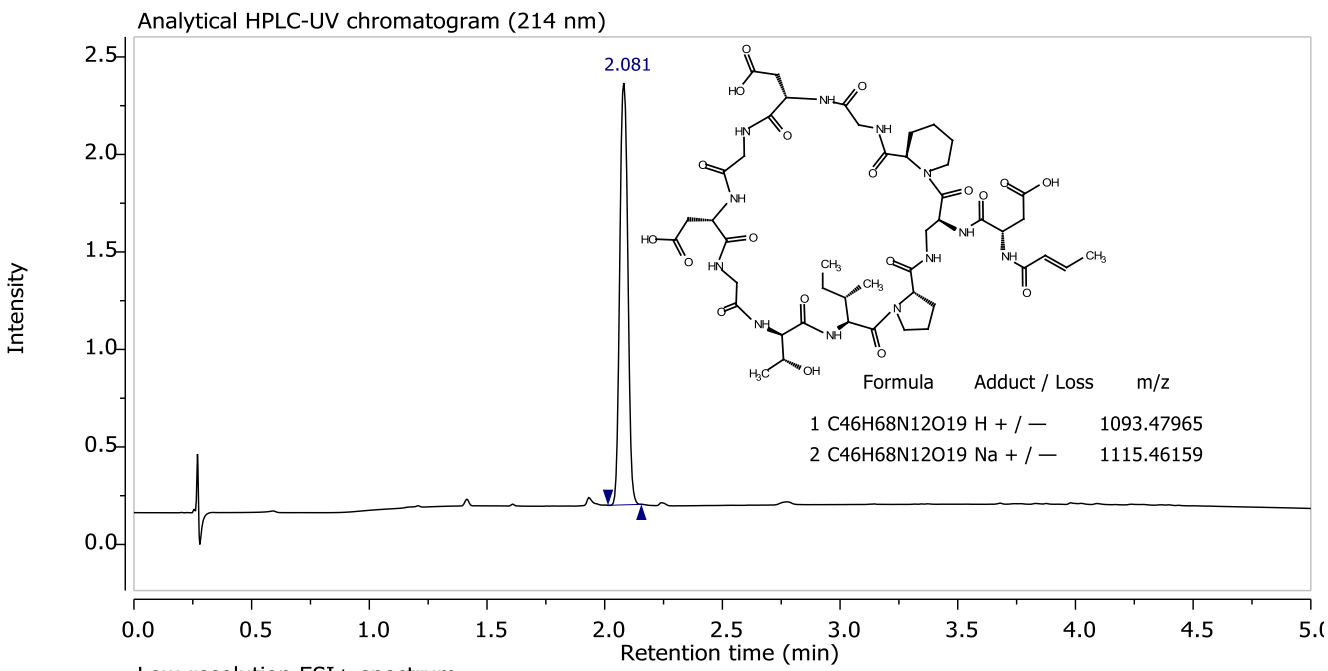
Parameter	Value
Title	LC. 10.012.3.ser
Comment	HSQCEDGPPH
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hsqcedgpph
Experiment	HSQC-EDITED
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	32
Receiver Gain	203.0
Relaxation Delay	2.7000
Pulse Width	5.1750
Acquisition Time	0.1137
Acquisition Date	2017-11-02T16 :59:17
Modification Date	2017-11-02T22 :10:42
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(4504.5, 20833.3)
Lowest Frequency	(-6.7, -1074.5)
Nucleus	(1H, 13C)
Acquired Size	(512, 207)
Spectral Size	(512, 512)

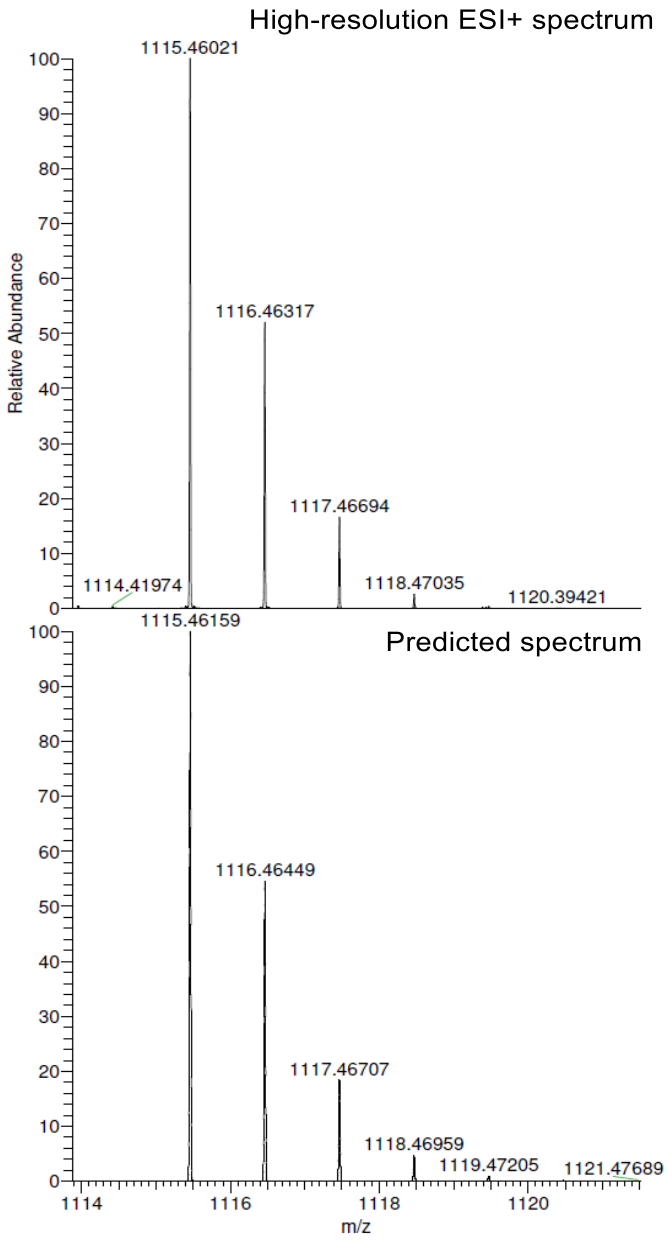
(*E*)-But-2-enoyl analogue (**23**) HMBC (500/126 MHz, DMSO-d_6)

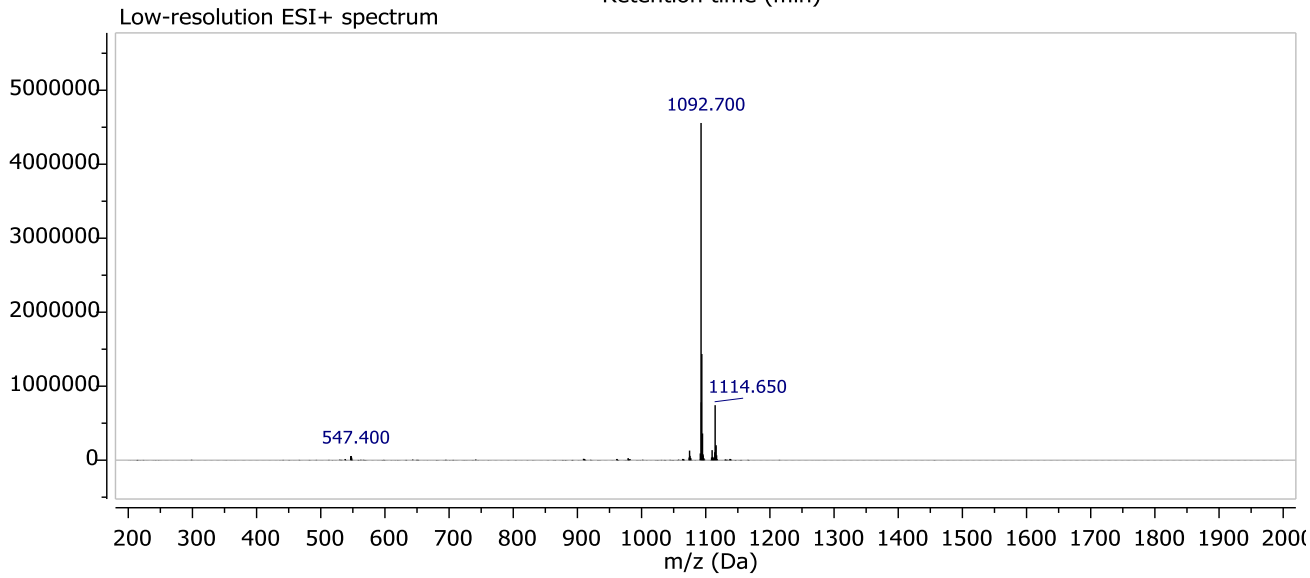


Parameter	Value
Title	LC.10.012.4.ser
Comment	LC.10.012
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hmbcgplpndqf
Experiment	HMBC
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	64
Receiver Gain	203.0
Relaxation Delay	2.7000
Pulse Width	5.1750
Acquisition Time	0.4547
Acquisition Date	2017-11-02T22:15:07
Modification Date	2017-11-03T17:26:05
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(4504.5, 27933.0)
Lowest Frequency	(-14.7, -1451.8)
Nucleus	(1H, 13C)
Acquired Size	(2048, 336)
Spectral Size	(2048, 2048)

(E)-But-2-enoyl analogue (**23**) Analytical HPLC, low and high-resolution ESI+ MS

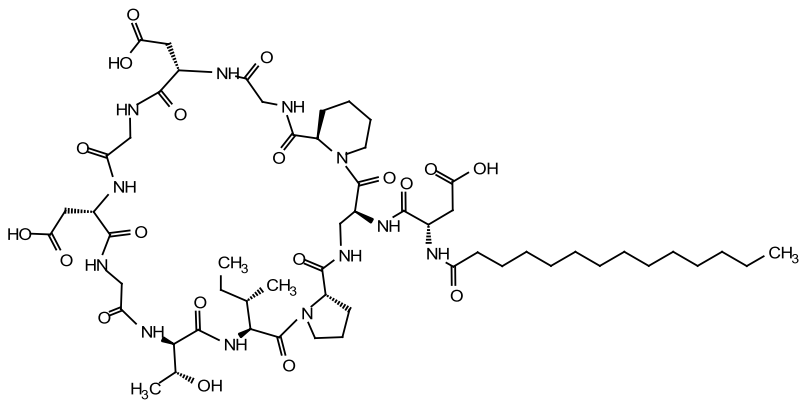




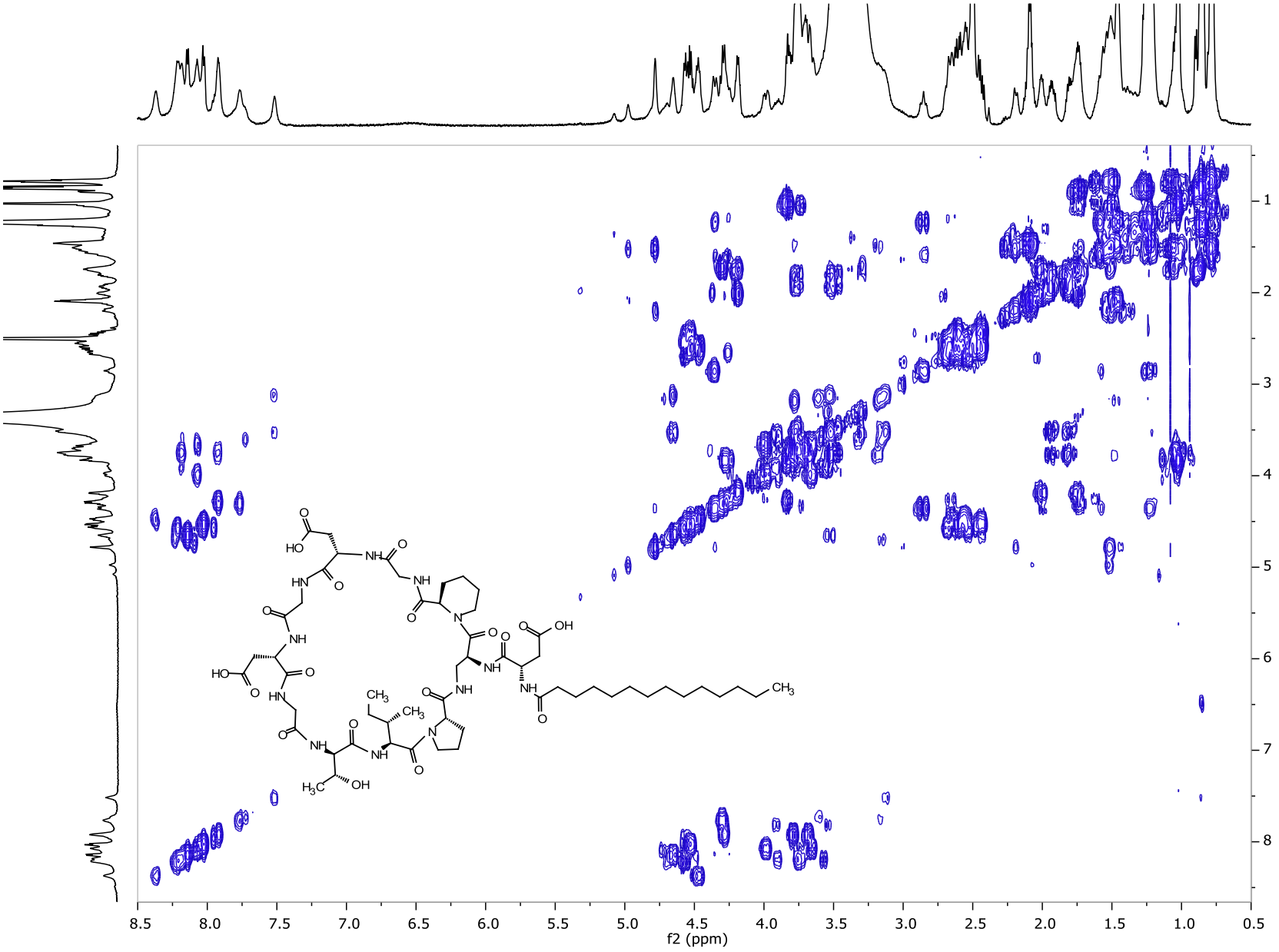


Tetradecanoyl analogue (**24**) ^{1}H NMR (600 MHz, DMSO-d_6)

Parameter	Value
Title	LC.10.017.1.fid
Comment	1H
Instrument	spect
Solvent	DMSO
Temperature	298.1
Pulse Sequence	zg30
Experiment	1D
Probe	5 mm CPTCI 1H-13C/ 15N/ D Z-GRD Z44896/ 0030
Number of Scans	16
Receiver Gain	18.0
Relaxation Delay	2.0000
Pulse Width	8.5000
Acquisition Time	2.7263
Acquisition Date	2017-10-23T13:20:53
Modification Date	2017-10-25T11:05:48
Spectrometer Frequency	600.13
Spectral Width	12019.2
Lowest Frequency	-2111.2
Nucleus	1H
Acquired Size	32768
Spectral Size	131072

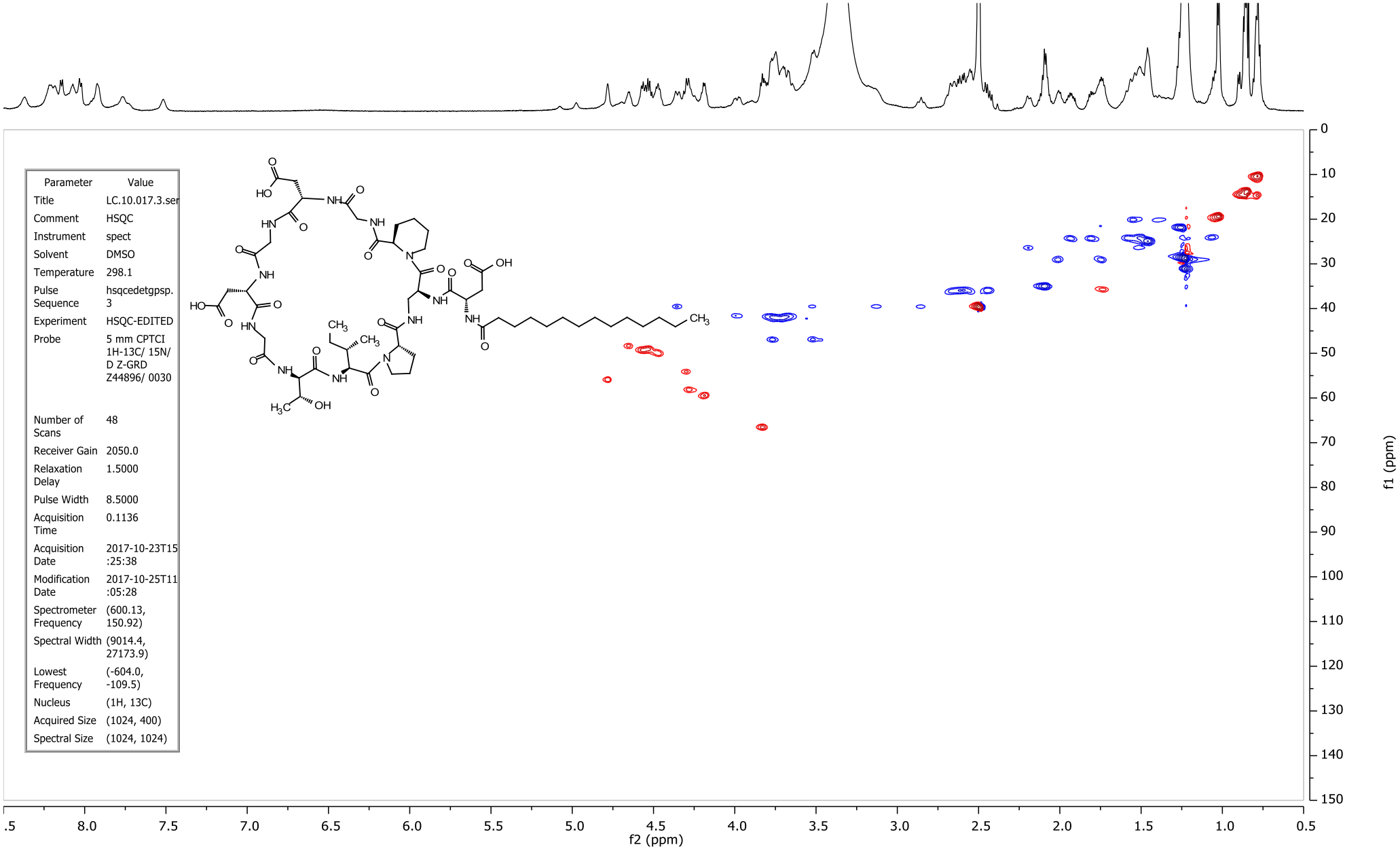


Tetradecanoyl analogue (**24**) COSY (600 MHz, DMSO-d_6)



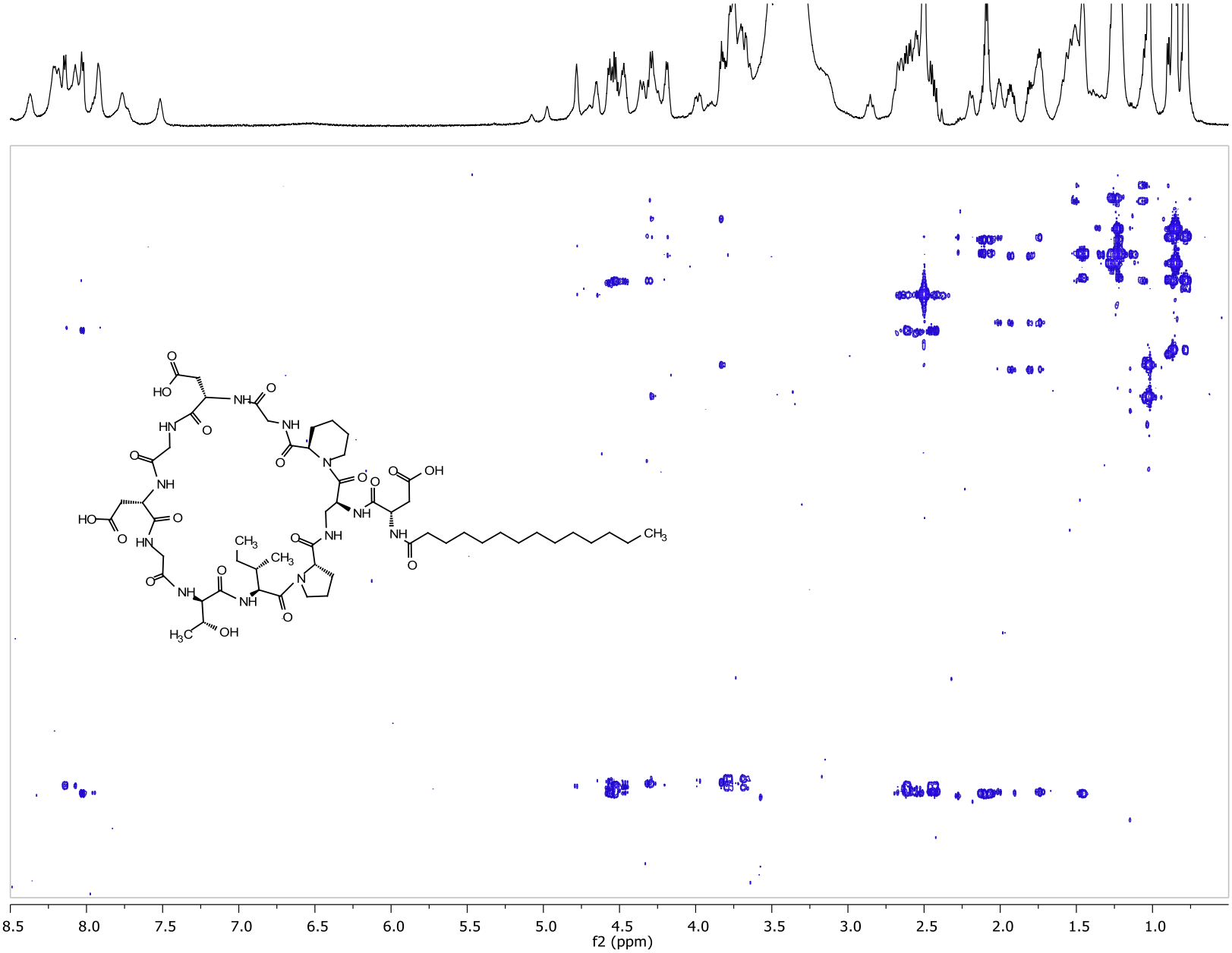
Parameter	Value
Title	LC.10.017.2.ser
Comment	COSY
Instrument	spect
Solvent	DMSO
Temperature	298.1
Pulse Sequence	cosygpmfppqf
Experiment	COSY
Probe	5 mm CPTCI 1H-13C/ 15N/ D Z-GRD Z44896/ 0030
Number of Scans	16
Receiver Gain	2050.0
Relaxation Delay	1.5000
Pulse Width	8.5000
Acquisition Time	0.2272
Acquisition Date	2017-10-23T13:22:04
Modification Date	2017-10-25T11:05:49
Spectrometer Frequency	(600.13, 600.13)
Spectral Width	(9014.4, 9009.0)
Lowest Frequency	(-597.4, -603.7)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

Tetradecanoyl analogue (**24**) HSQC (600/151 MHz, DMSO-d_6)

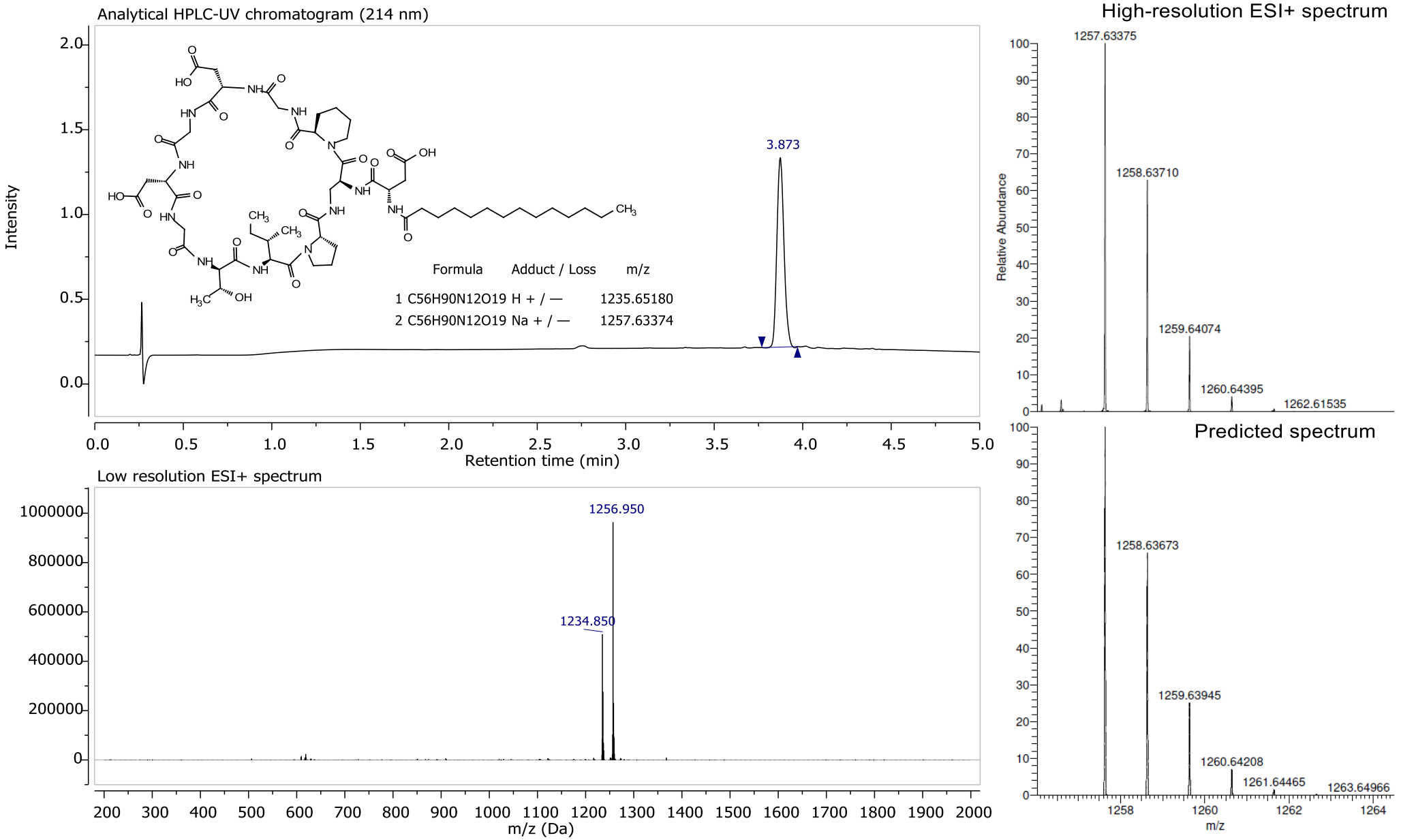


Tetradecanoyl analogue (**24**) HMBC (600/151 MHz, DMSO-d_6)

Parameter	Value
Title	LC.10.017.4.ser
Comment	HMBC
Instrument	spect
Solvent	DMSO
Temperature	298.1
Pulse Sequence	hmbcetgpl3nd
Experiment	HMBC
Probe	5 mm CPTCI 1H-13C/ 15N/ D Z-GRD Z44896/ 0030
Number of Scans	40
Receiver Gain	2050.0
Relaxation Delay	1.5000
Pulse Width	8.5000
Acquisition Time	0.2272
Acquisition Date	2017-10-24T00:10:25
Modification Date	2017-10-25T11:05:39
Spectrometer Frequency	(600.13, 150.92)
Spectral Width	(9014.4, 33112.6)
Lowest Frequency	(-596.8, -32.9)
Nucleus	(1H, 13C)
Acquired Size	(2048, 491)
Spectral Size	(2048, 2048)

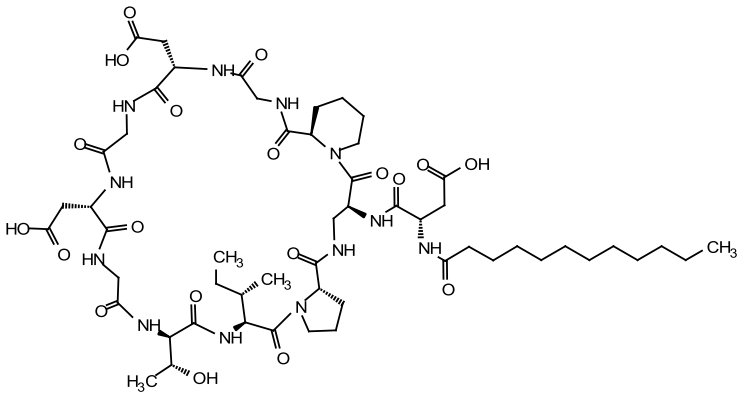


Tetradecanoyl analogue (**24**) Analytical HPLC, low and high-resolution ESI+ MS

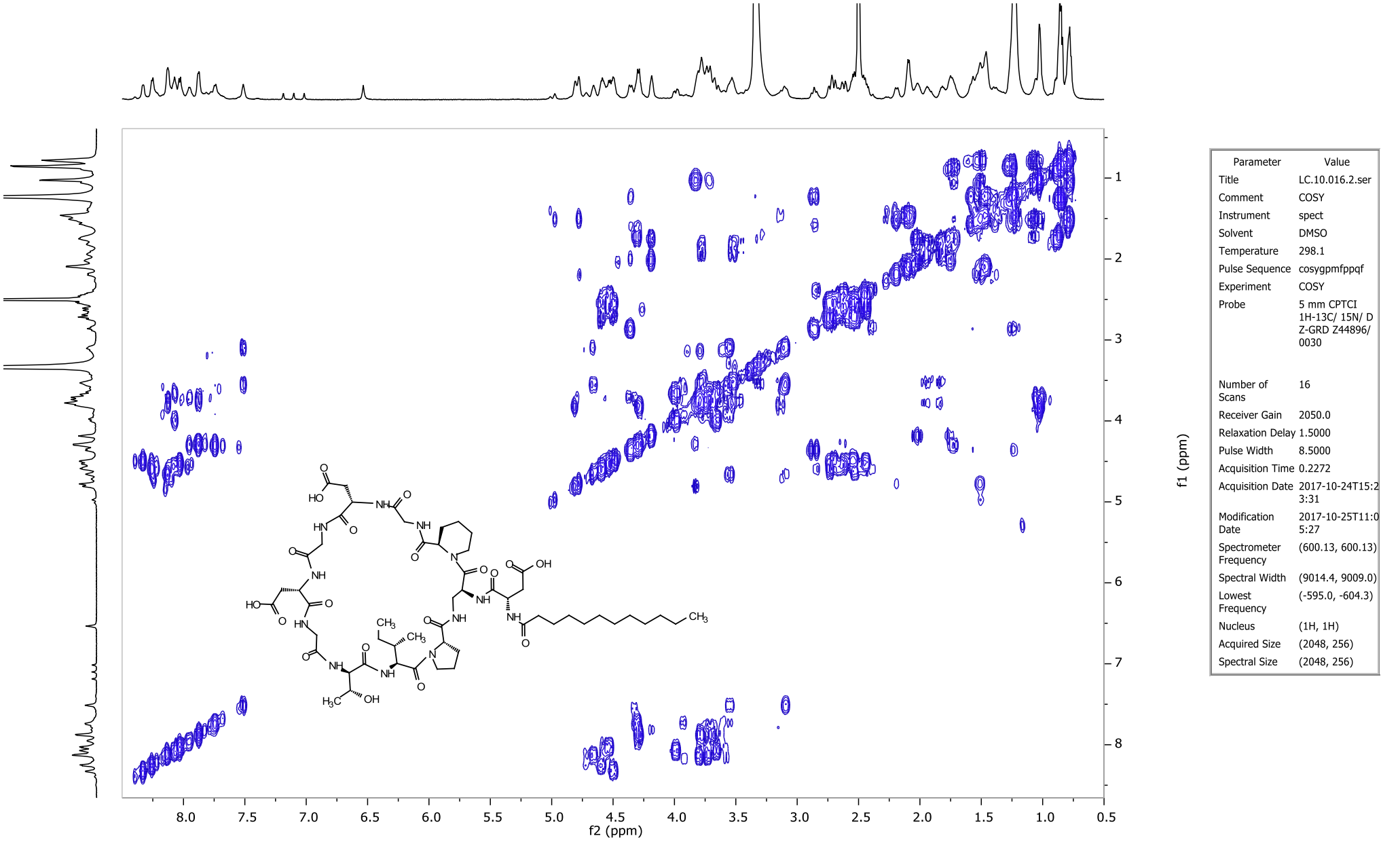


Dodecanoyl analogue (**25**) ^{1}H NMR (600 MHz, DMSO-d_6)

Parameter	Value
Title	LC.10.016.1.fid
Comment	1H
Instrument	spect
Solvent	DMSO
Temperature	298.1
Pulse Sequence	zg30
Experiment	1D
Probe	5 mm CPTCI 1H-13C/ 15N/ D Z-GRD Z44896/ 0030
Number of Scans	16
Receiver Gain	12.7
Relaxation Delay	2.0000
Pulse Width	8.5000
Acquisition Time	2.7263
Acquisition Date	2017-10-24T15:22:09
Modification Date	2017-10-25T11:05:26
Spectrometer Frequency	600.13
Spectral Width	12019.2
Lowest Frequency	-2110.0
Nucleus	1H
Acquired Size	32768
Spectral Size	131072

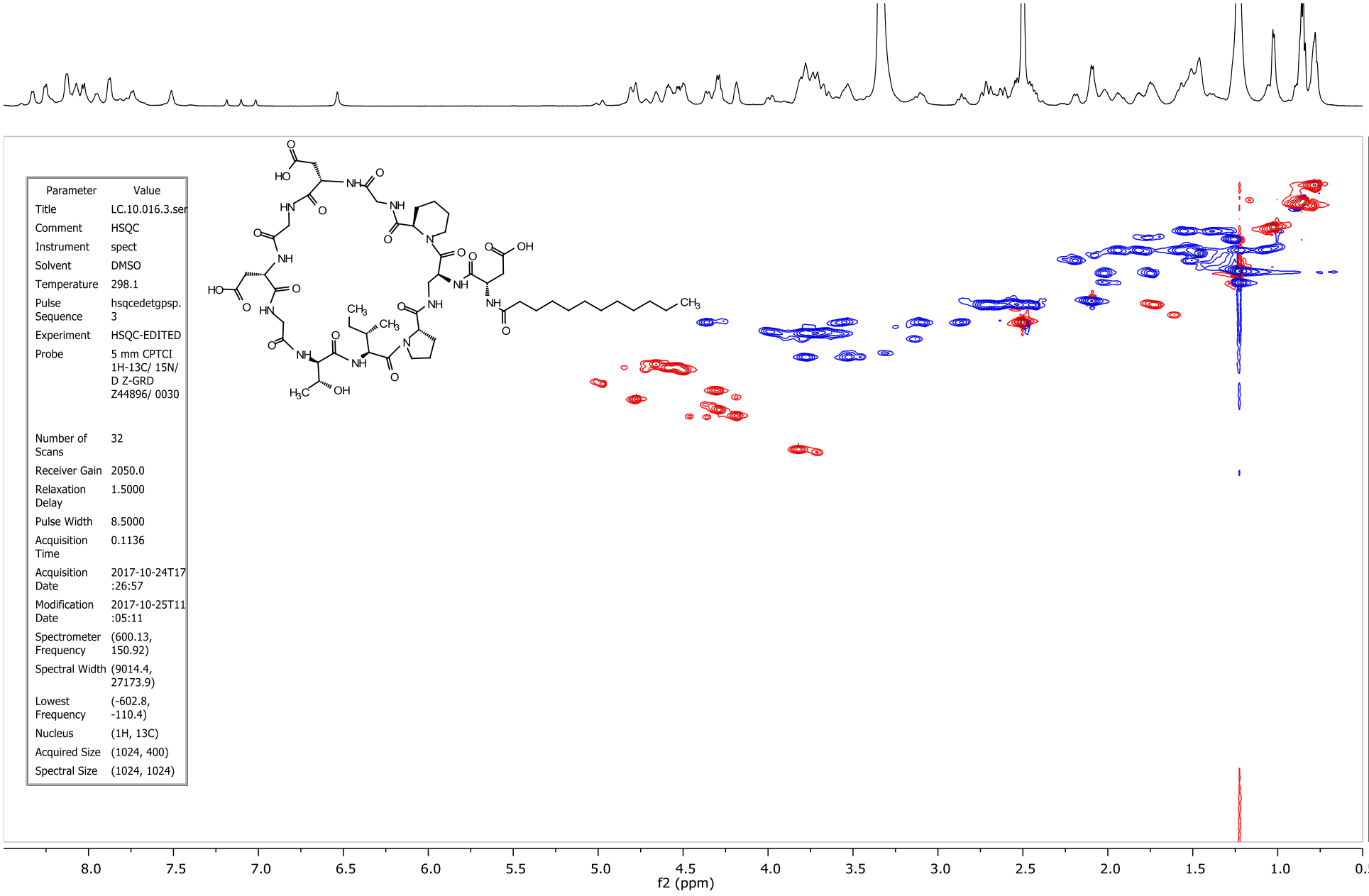


Dodecanoyl analogue (**25**) COSY (600 MHz, DMSO-d_6)



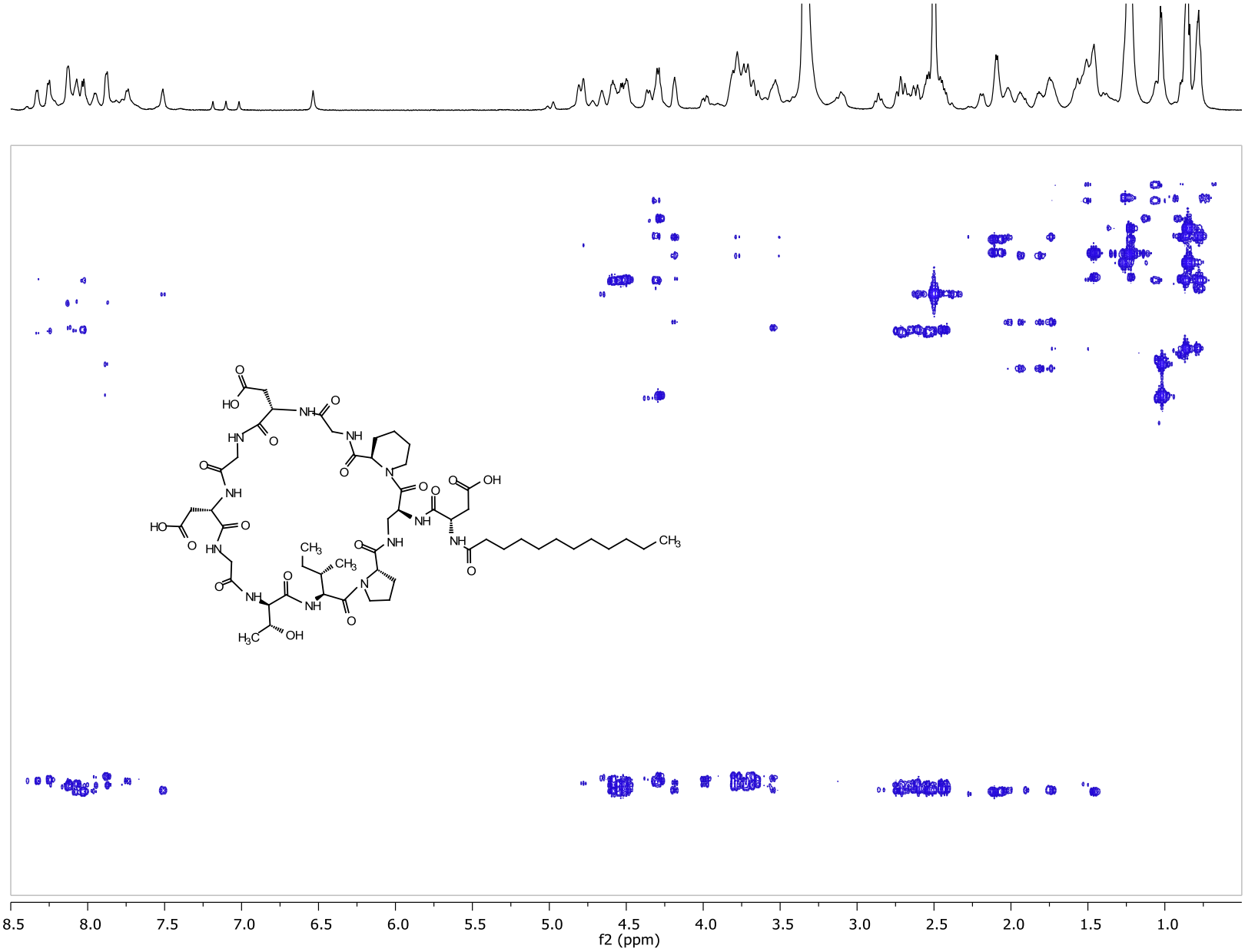
Parameter	Value
Title	LC.10.016.2.ser
Comment	COSY
Instrument	spect
Solvent	DMSO
Temperature	298.1
Pulse Sequence	cosygpmfppqf
Experiment	COSY
Probe	5 mm CPTCI 1H-13C/ 15N/ D Z-GRD Z44896/ 0030
Number of Scans	16
Receiver Gain	2050.0
Relaxation Delay	1.5000
Pulse Width	8.5000
Acquisition Time	0.2272
Acquisition Date	2017-10-24T15:23:31
Modification Date	2017-10-25T11:05:27
Spectrometer Frequency	(600.13, 600.13)
Spectral Width	(9014.4, 9009.0)
Lowest Frequency	(-595.0, -604.3)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

Dodecanoyl analogue (**25**) HSQC (600/151 MHz, DMSO-d_6)

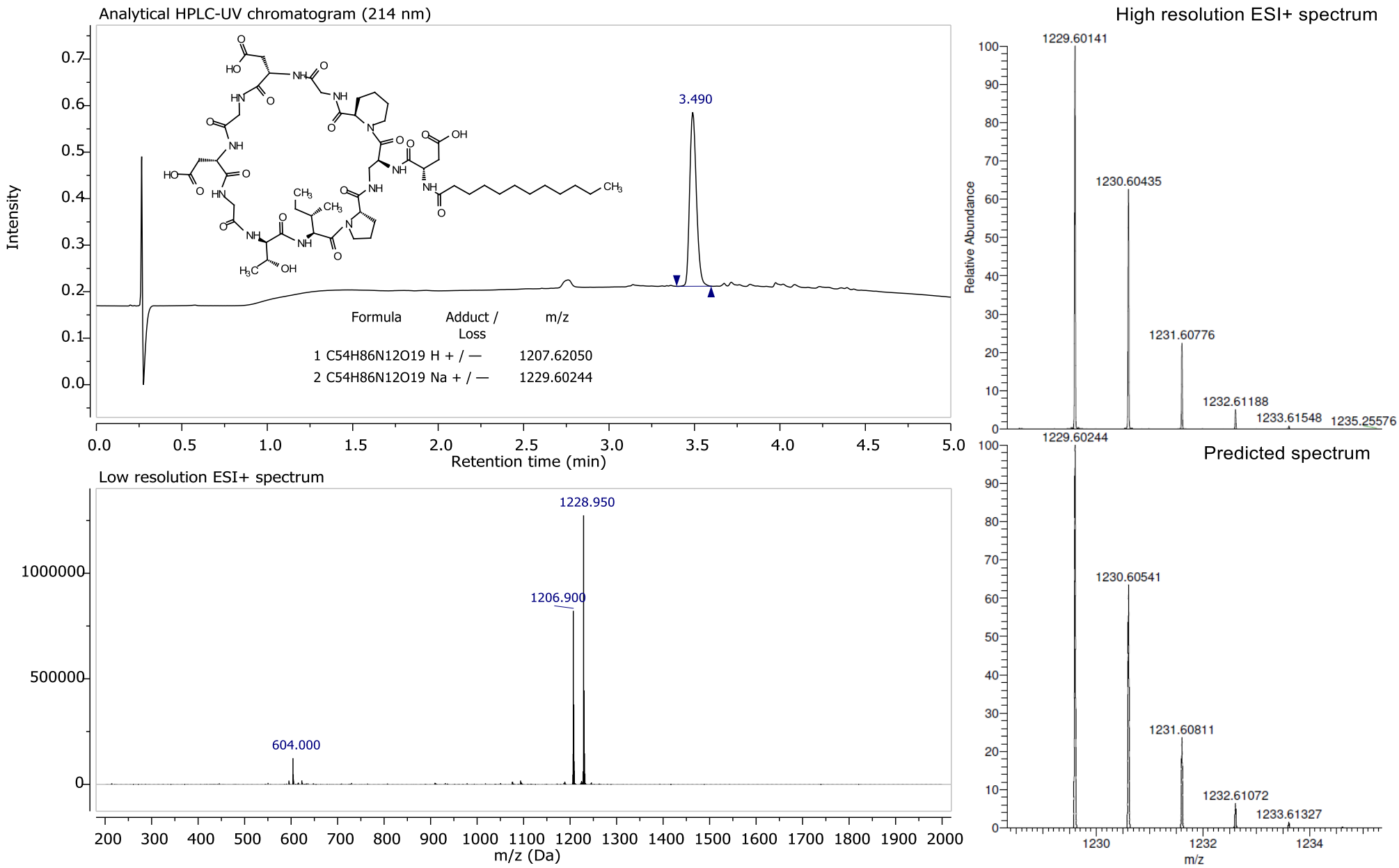


Dodecanoyl analogue (**25**) HMBC (600/151 MHz, DMSO-d_6)

Parameter	Value
Title	LC.10.016.4.ser
Comment	HMBC
Instrument	spect
Solvent	DMSO
Temperature	298.1
Pulse Sequence	hmbcetgpl3nd
Experiment	HMBC
Probe	5 mm CPTCI 1H-13C/ 15N/ D Z-GRD Z44896/ 0030
Number of Scans	40
Receiver Gain	2050.0
Relaxation Delay	1.5000
Pulse Width	8.5000
Acquisition Time	0.2272
Acquisition Date	2017-10-24T23:17:40
Modification Date	2017-10-25T11:05:20
Spectrometer Frequency	(600.13, 150.92)
Spectral Width	(9014.4, 33112.6)
Lowest Frequency	(-596.8, -32.2)
Nucleus	(1H, 13C)
Acquired Size	(2048, 502)
Spectral Size	(2048, 2048)

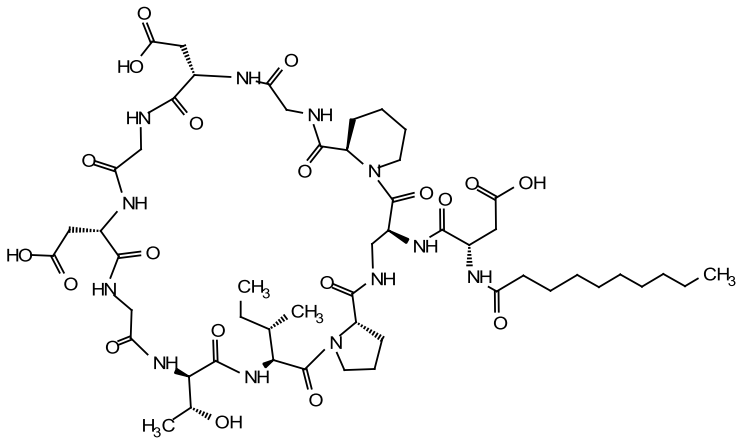


Dodecanoyl analogue (**25**) Analytical HPLC, low and high-resolution ESI+ MS

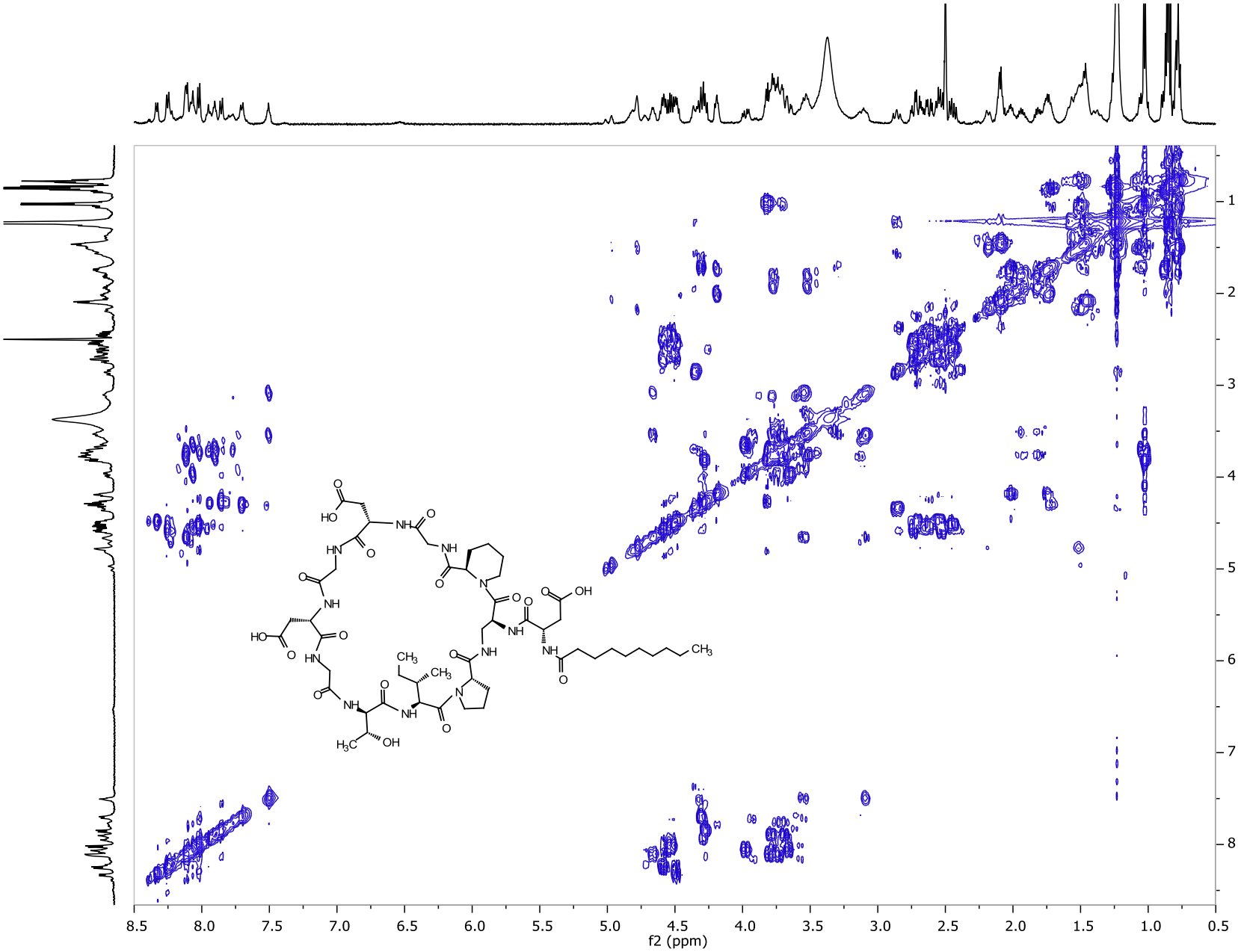


Decanoyl analogue (**26**) ^{1}H NMR (500 MHz, DMSO-d_6)

Parameter	Value
Title	LC.10.014.1.fid
Comment	1H NMR
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	zg
Experiment	1D
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	1
Receiver Gain	90.5
Relaxation Delay	2.0000
Pulse Width	4.9000
Acquisition Time	3.2768
Acquisition Date	2017-10-23T14:46:41
Modification Date	2017-10-23T14:46:41
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-2005.4
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

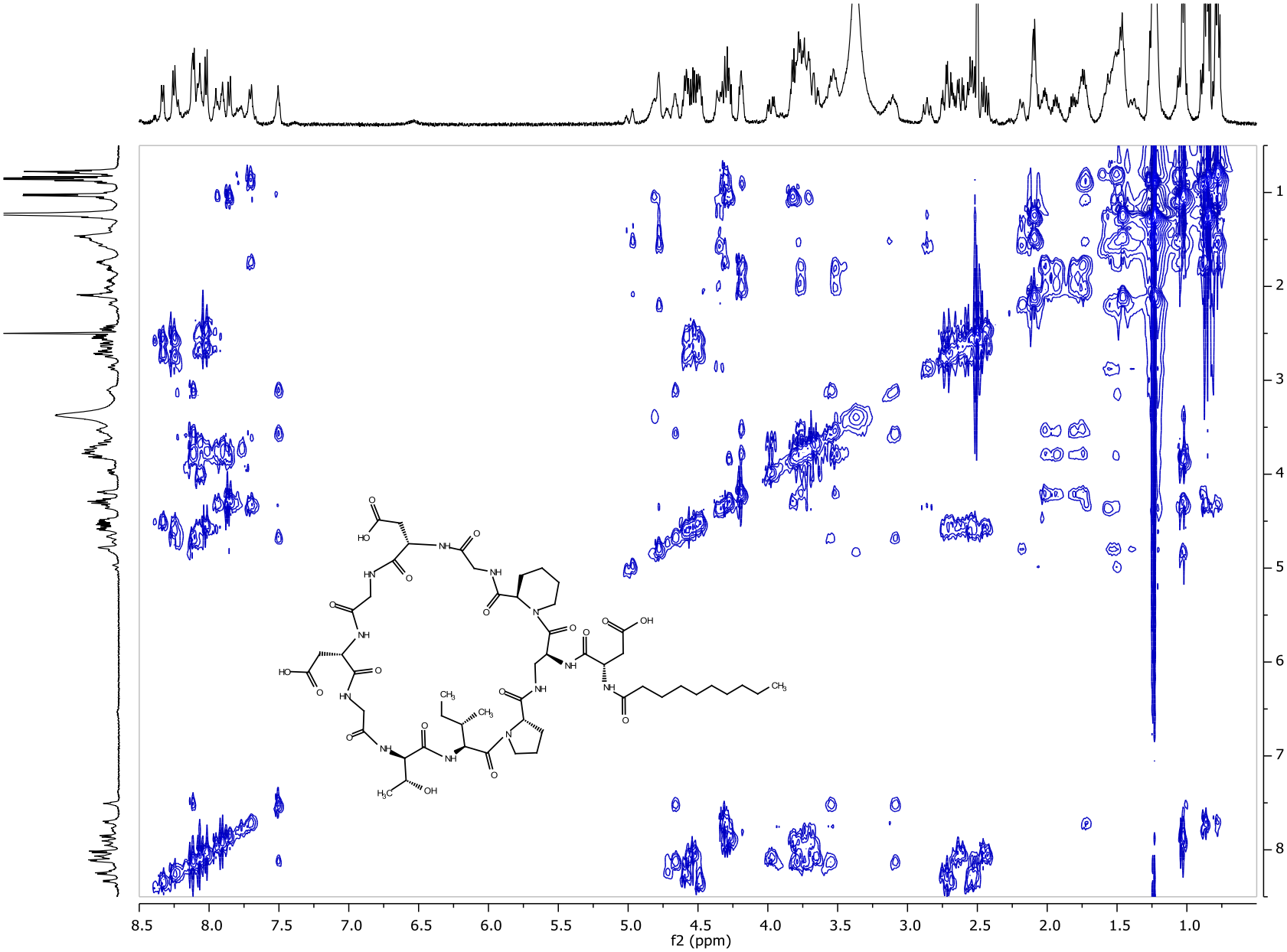


Decanoyl analogue (**26**) COSY (500 MHz, DMSO-d_6)



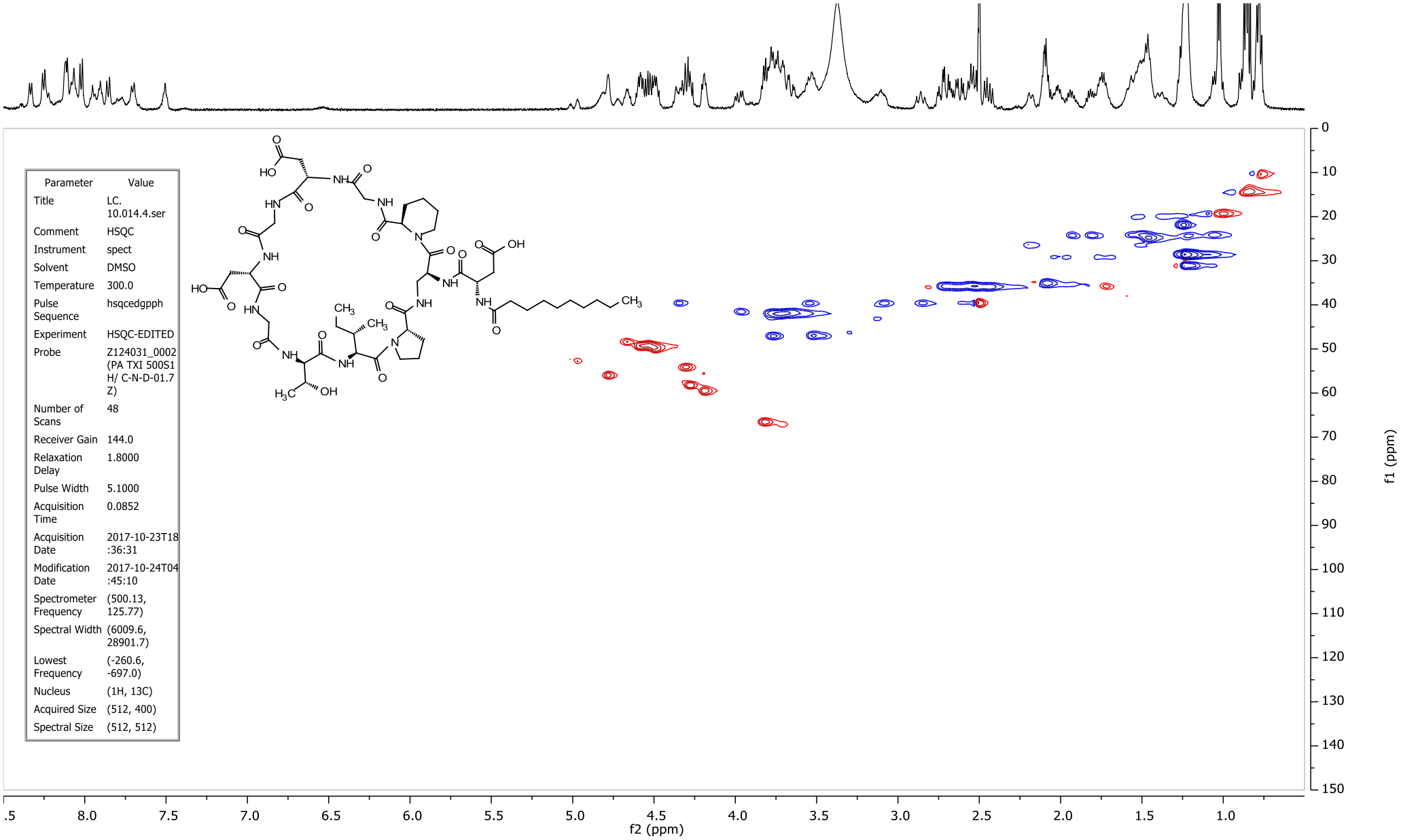
Parameter	Value
Title	LC.10.014.2.ser
Comment	COSY
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	cosygpqf
Experiment	COSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	24
Receiver Gain	203.0
Relaxation Delay	1.8000
Pulse Width	5.1000
Acquisition Time	0.3408
Acquisition Date	2017-10-23T14:53:11
Modification Date	2017-10-23T18:34:19
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(6009.6, 6002.4)
Lowest Frequency	(-267.1, -262.0)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

Decanoyl analogue (**26**) TOCSY (500 MHz, DMSO-d_6)



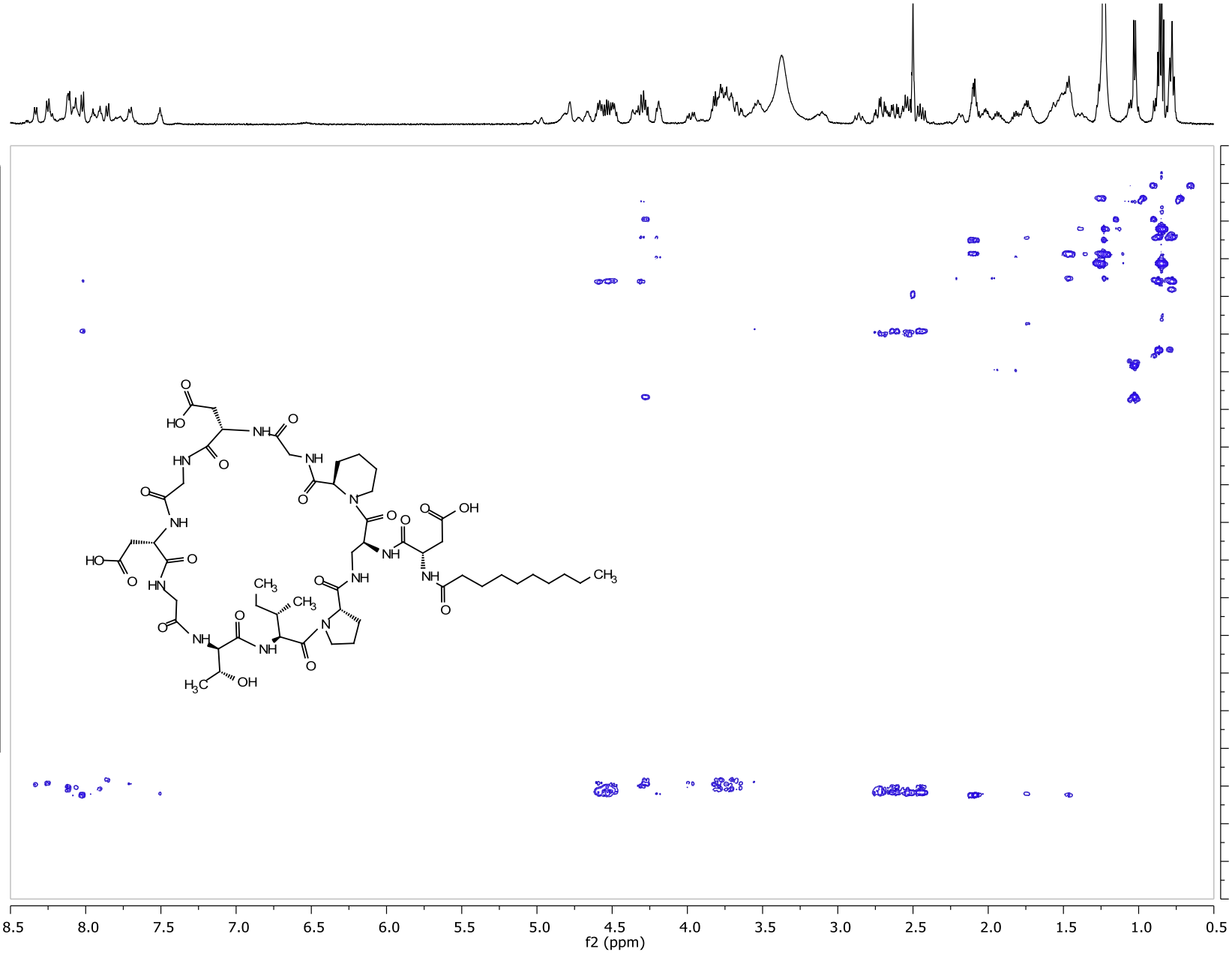
Parameter	Value
Title	LC.10.014.3.ser
Comment	TOCSY
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	dipsi2etgpsi
Experiment	2D-TOCSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	24
Receiver Gain	101.0
Relaxation Delay	1.8000
Pulse Width	5.1000
Acquisition Time	0.3408
Acquisition Date	2017-10-24T04:46:29
Modification Date	2017-10-24T08:36:52
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(6009.6, 6002.4)
Lowest Frequency	(-261.1, -248.5)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

Decanoyl analogue (**26**) HSQC (500/126 MHz, DMSO-d_6)

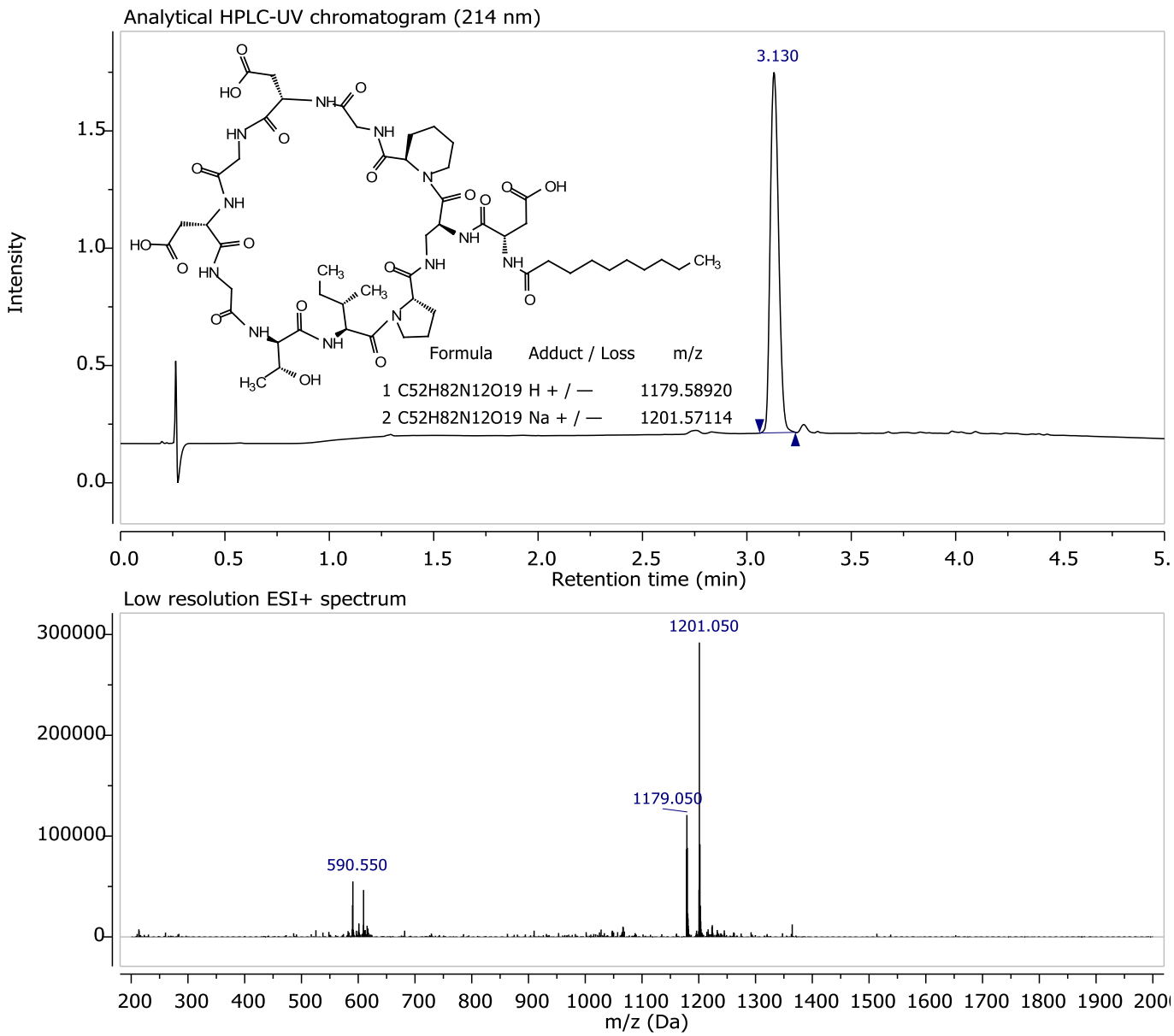


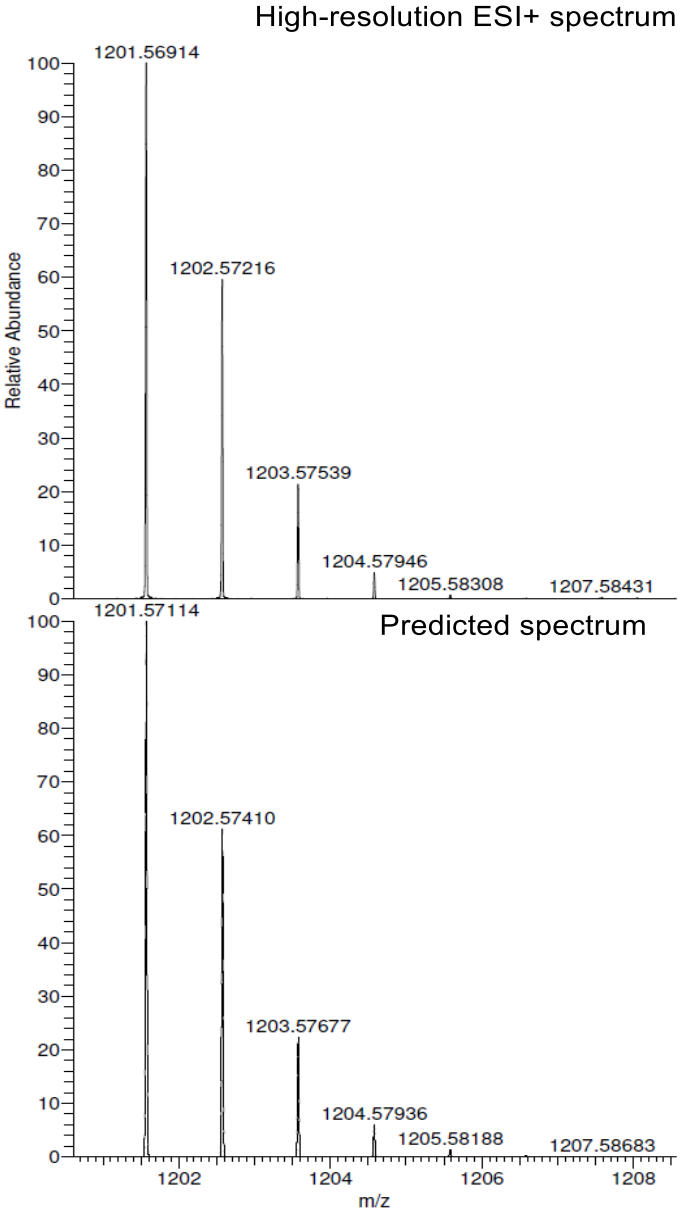
Decanoyl analogue (**26**) HMBC (500/126 MHz, DMSO-d_6)

Parameter	Value
Title	LC.10.014.5.ser
Comment	HMBC
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hmbcgplpndqf
Experiment	HMBC
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	54
Receiver Gain	203.0
Relaxation Delay	1.8000
Pulse Width	5.1000
Acquisition Time	0.3408
Acquisition Date	2017-10-24T11:48:00
Modification Date	2017-10-25T01:00:52
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(6009.6, 28901.7)
Lowest Frequency	(-267.1, -678.1)
Nucleus	(1H, 13C)
Acquired Size	(2048, 400)
Spectral Size	(2048, 2048)



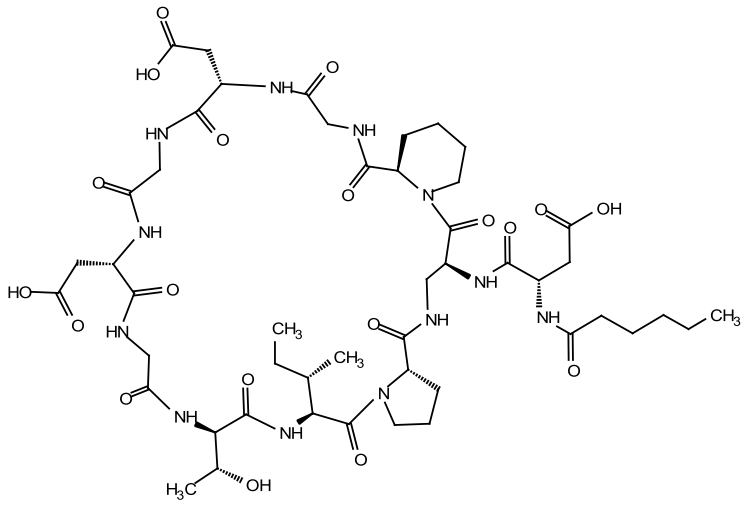
Decanoyl analogue (**26**) Analytical HPLC, low and high-resolution ESI+ MS



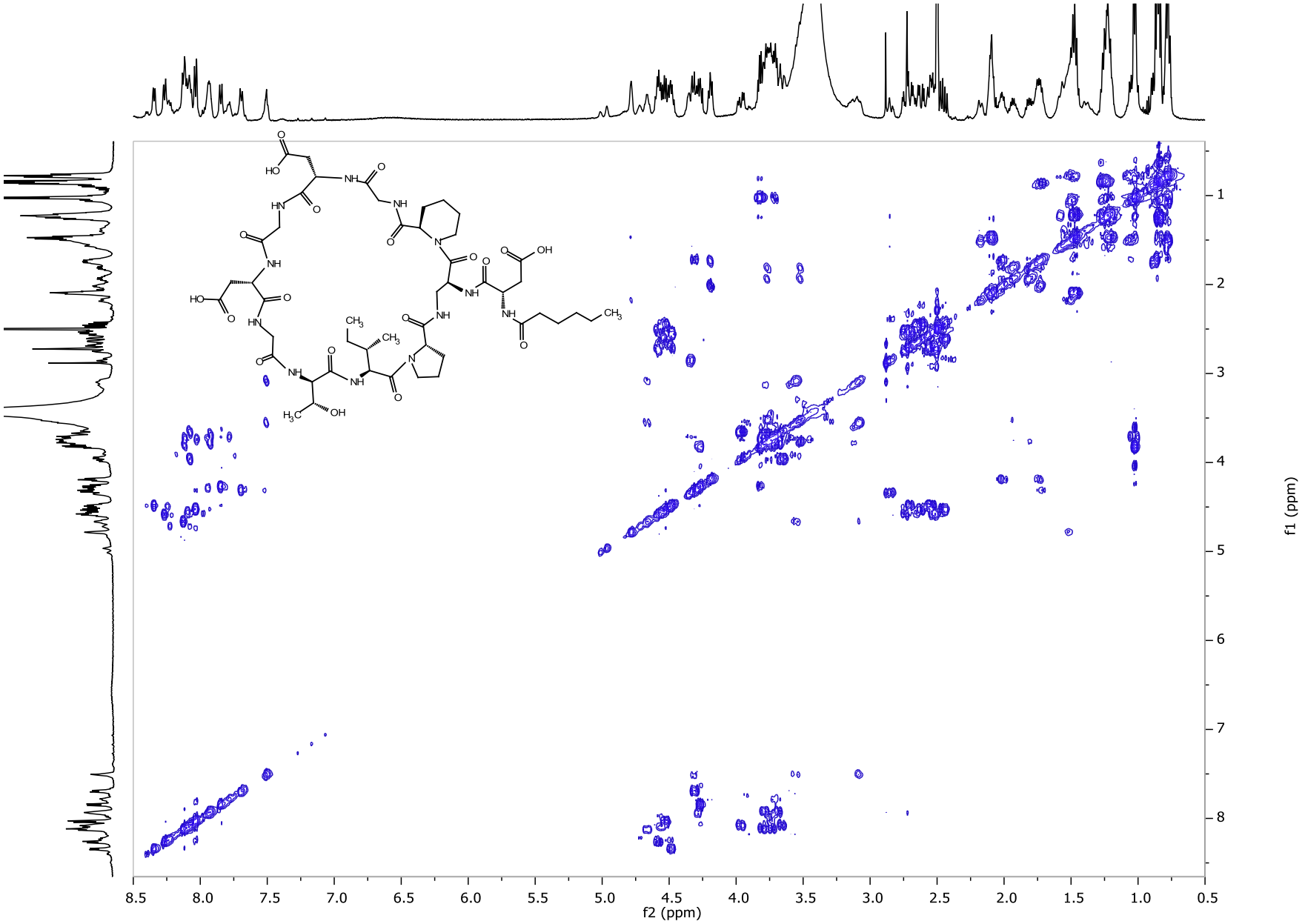


Hexanoyl analogue (**27**) ^{1}H NMR (500 MHz, DMSO-d_6)

Parameter	Value
Title	LC.10.013.1.fid
Comment	1H NMR
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	zg
Experiment	1D
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	16
Receiver Gain	101.0
Relaxation Delay	2.0000
Pulse Width	4.9000
Acquisition Time	3.2768
Acquisition Date	2017-11-01T11:11:45
Modification Date	2017-11-01T11:11:45
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-2005.4
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

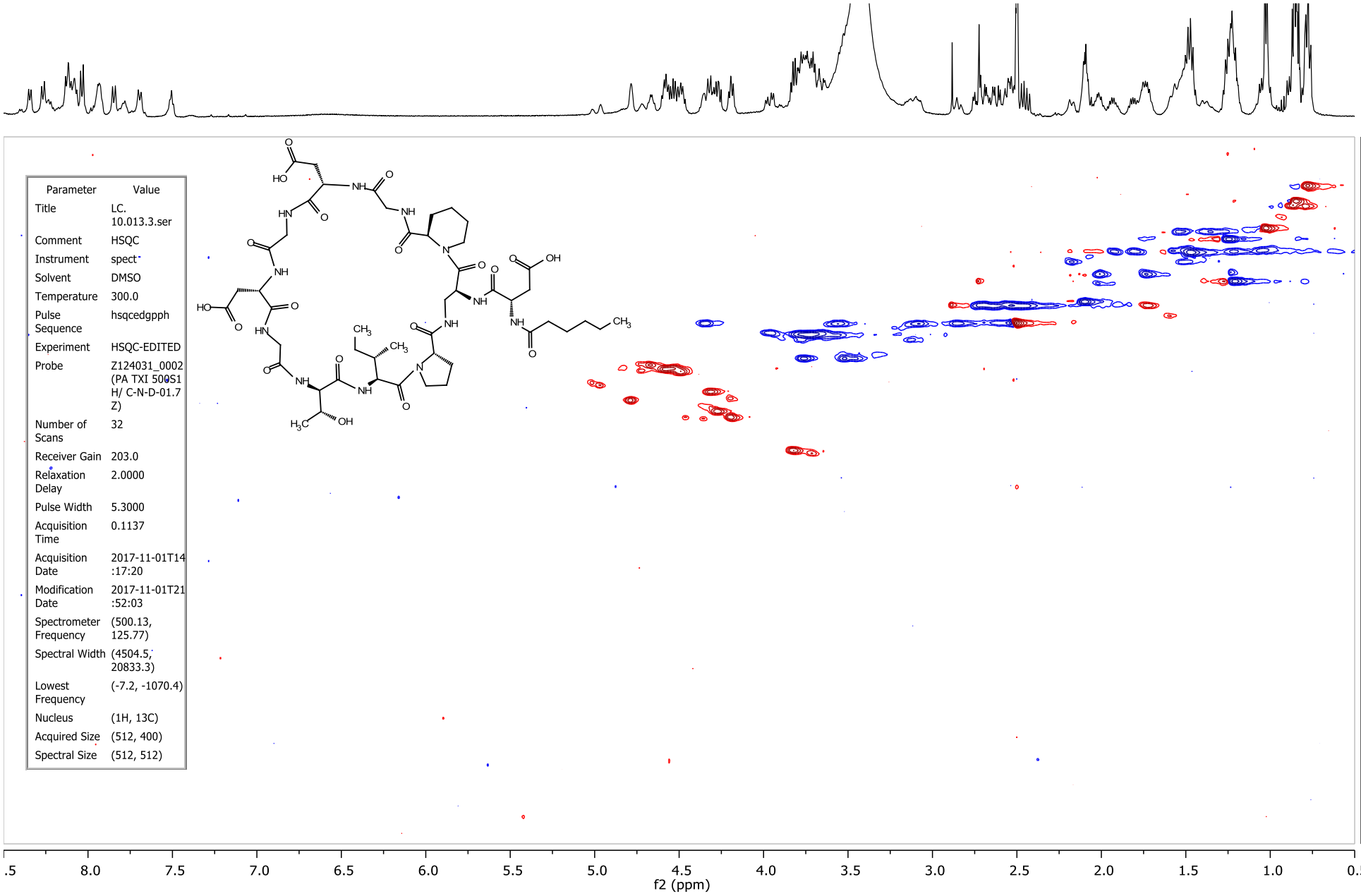


Hexanoyl analogue (**27**) COSY (500 MHz, DMSO-d_6)



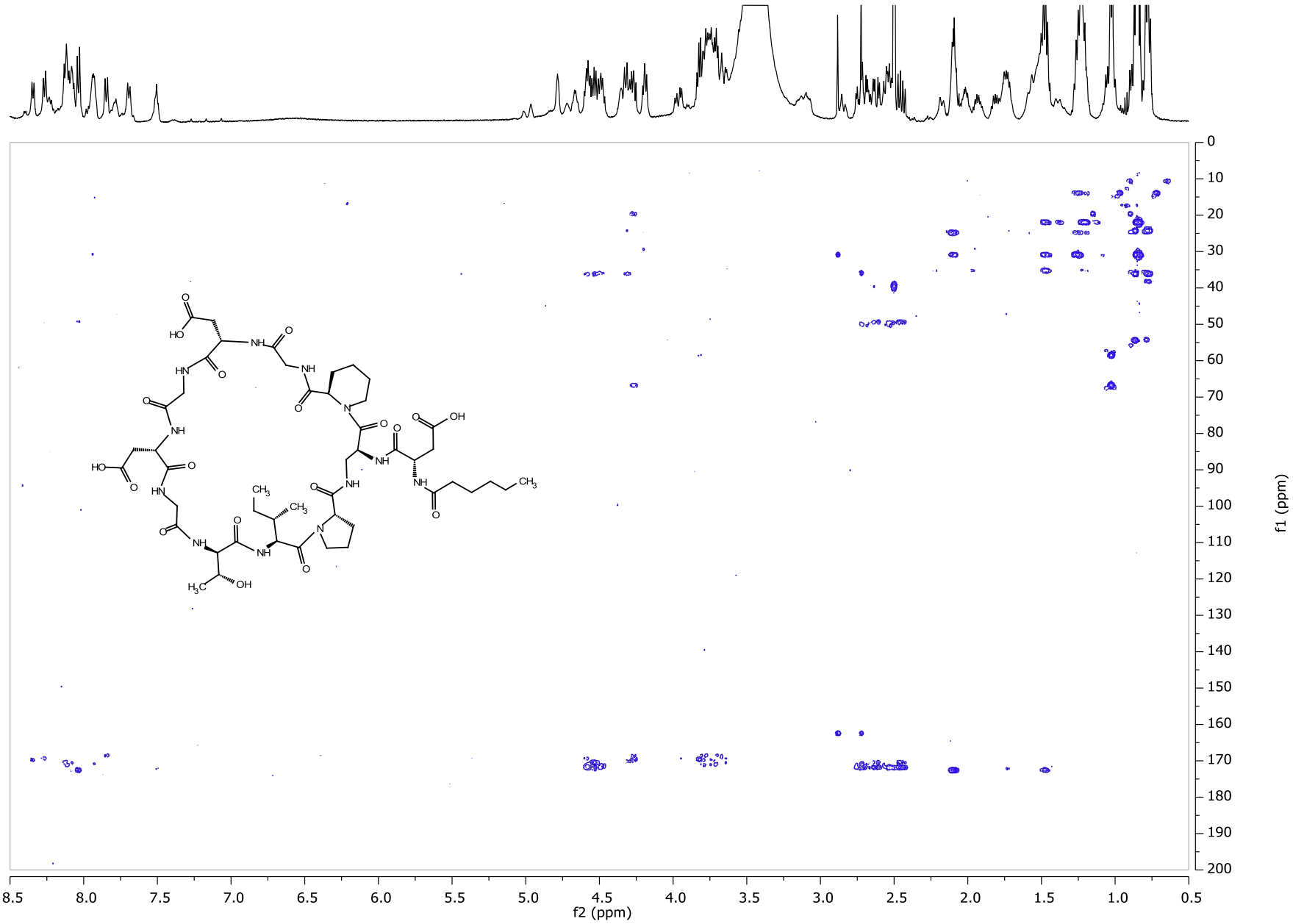
Parameter	Value
Title	LC.10.013.2.ser
Comment	COSY
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	cosygpqf
Experiment	COSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	16
Receiver Gain	203.0
Relaxation Delay	2.0000
Pulse Width	5.3000
Acquisition Time	0.4547
Acquisition Date	2017-11-01T11:26:13
Modification Date	2017-11-01T14:15:29
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(4504.5, 4500.5)
Lowest Frequency	(-13.7, -6.1)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

Hexanoyl analogue (**27**) HSQC (500/126 MHz, DMSO-d_6)

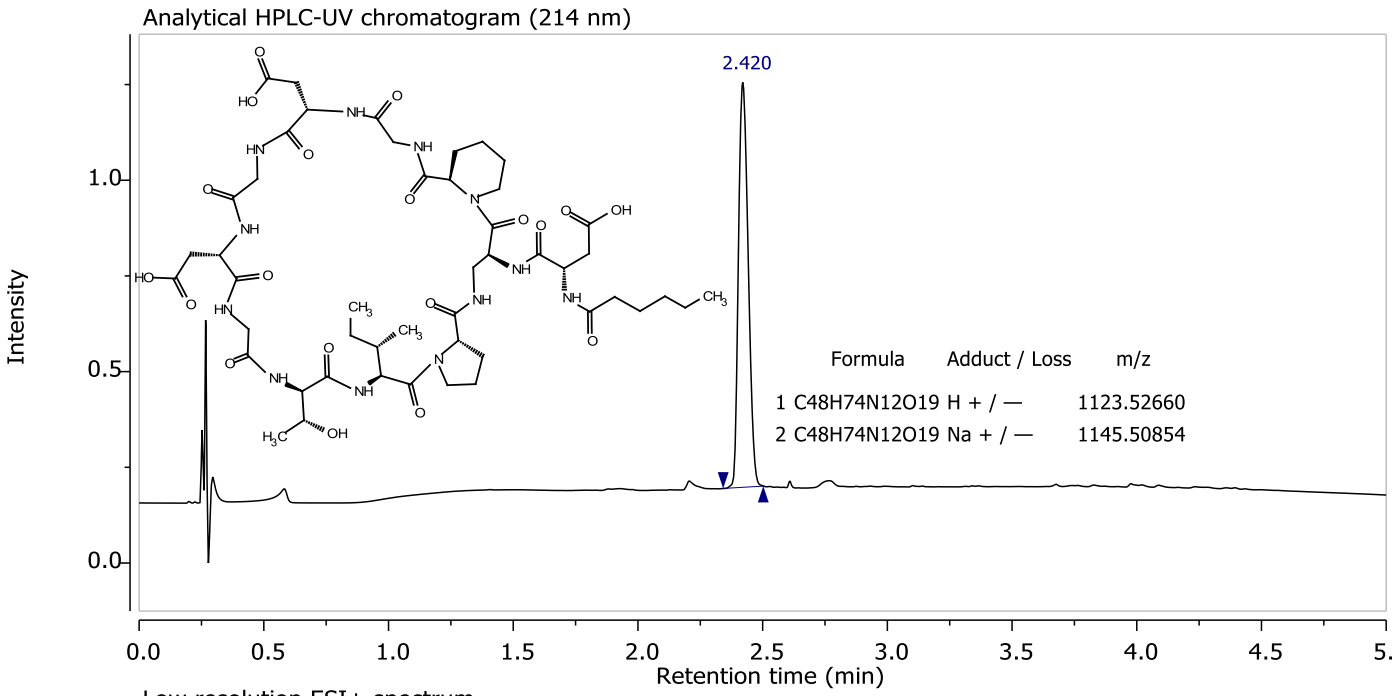


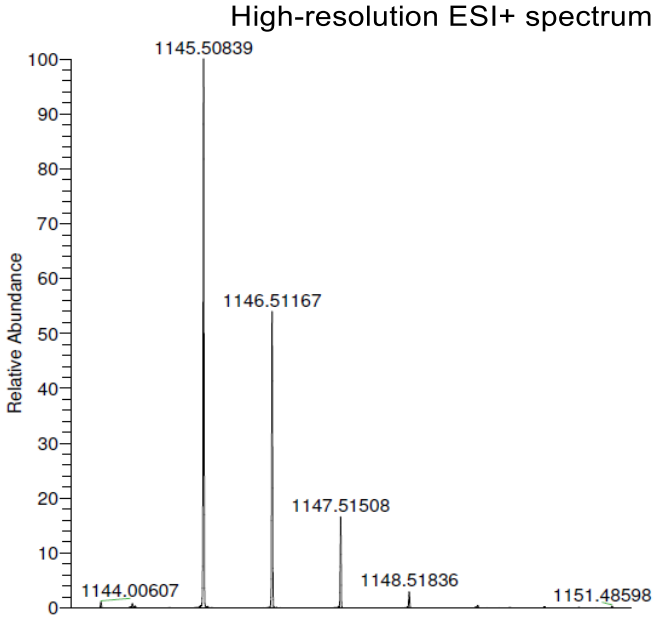
Hexanoyl analogue (**27**) HMBC (500/126 MHz, DMSO-d_6)

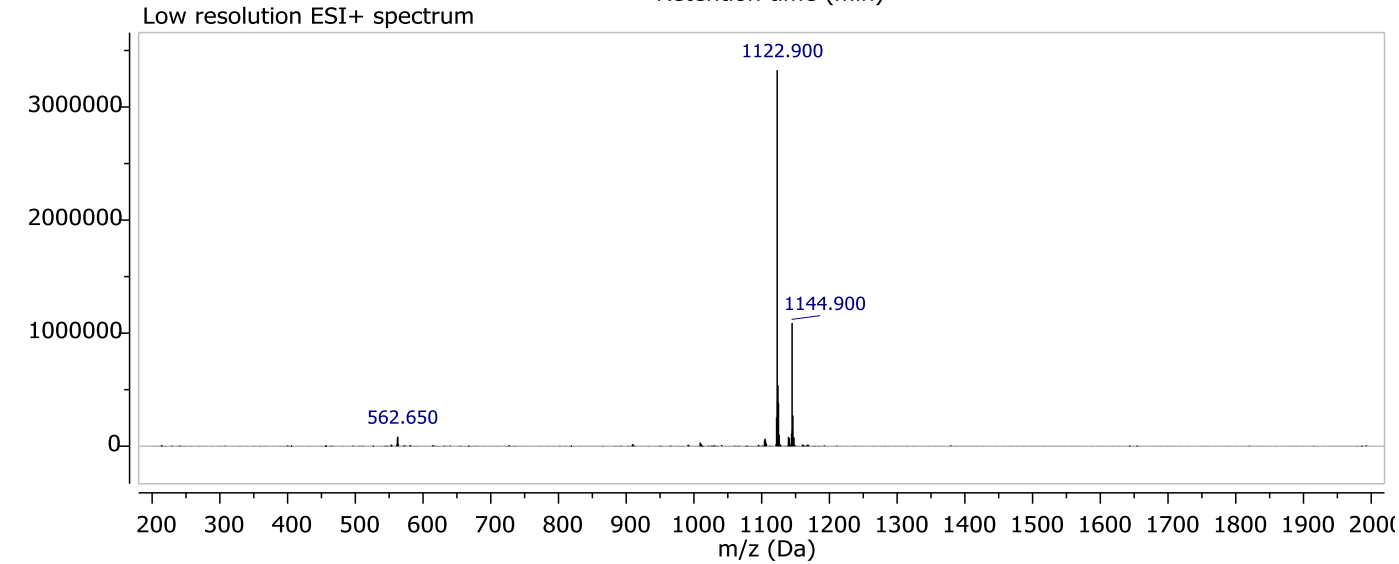
Parameter	Value
Title	LC.10.013.4.ser
Comment	HMBC
Instrument	spect
Solvent	DMSO
Temperature	299.9
Pulse Sequence	hmbcgplpndqf
Experiment	HMBC
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	54
Receiver Gain	203.0
Relaxation Delay	2.0000
Pulse Width	5.3000
Acquisition Time	0.4547
Acquisition Date	2017-11-01T21:55:06
Modification Date	2017-11-02T12:35:45
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(4504.5, 27933.0)
Lowest Frequency	(-14.7, -1444.1)
Nucleus	(1H, 13C)
Acquired Size	(2048, 389)
Spectral Size	(2048, 2048)

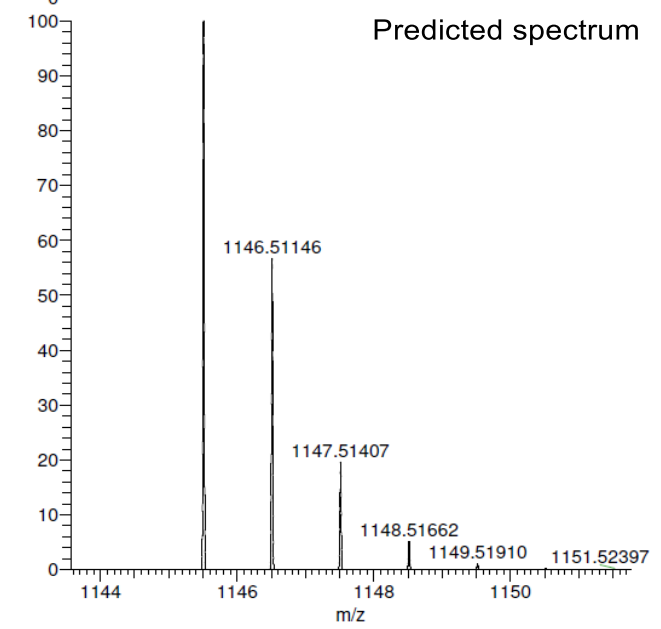


Hexanoyl analogue (**27**) Analytical HPLC, low and high-resolution ESI+ MS

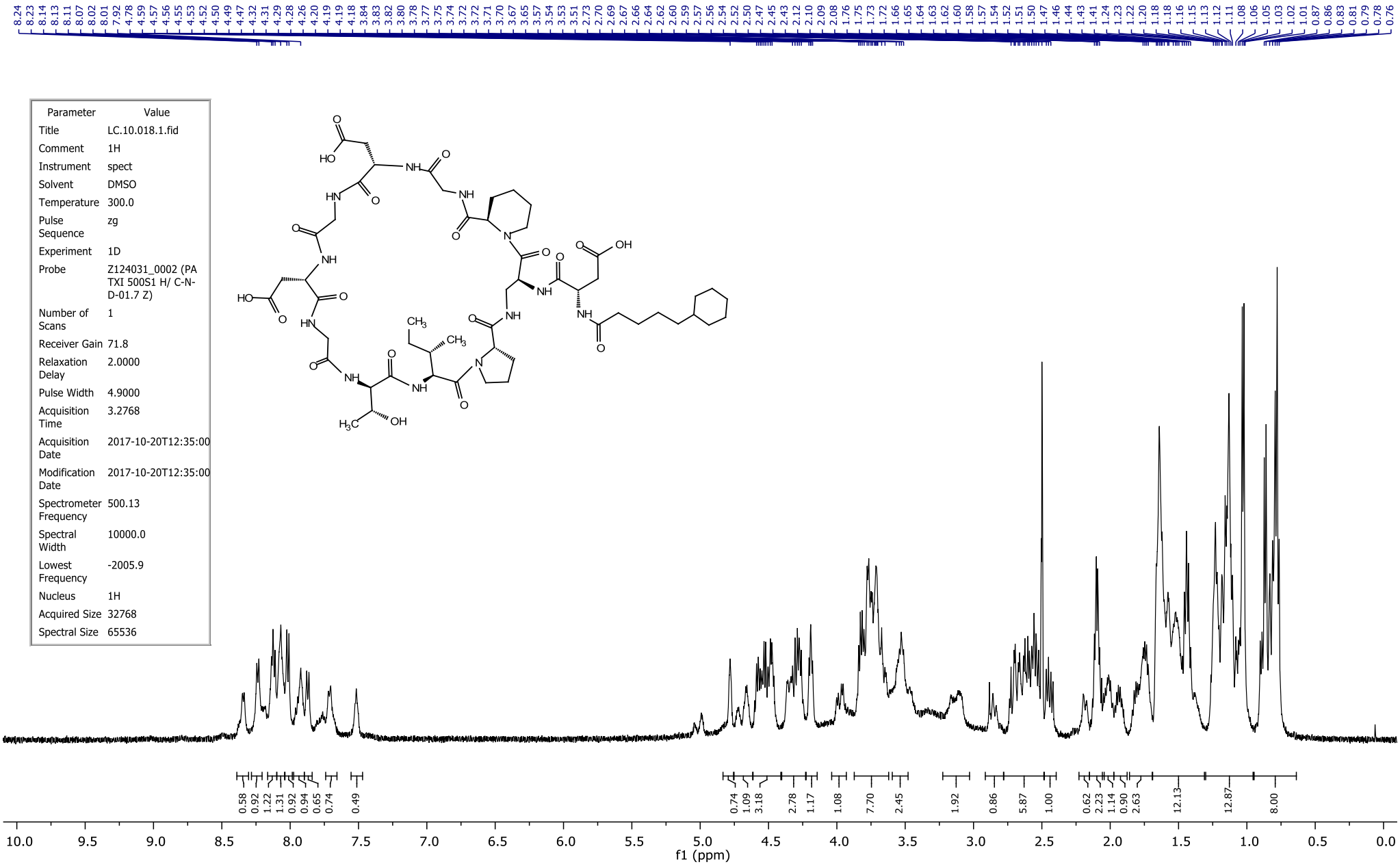




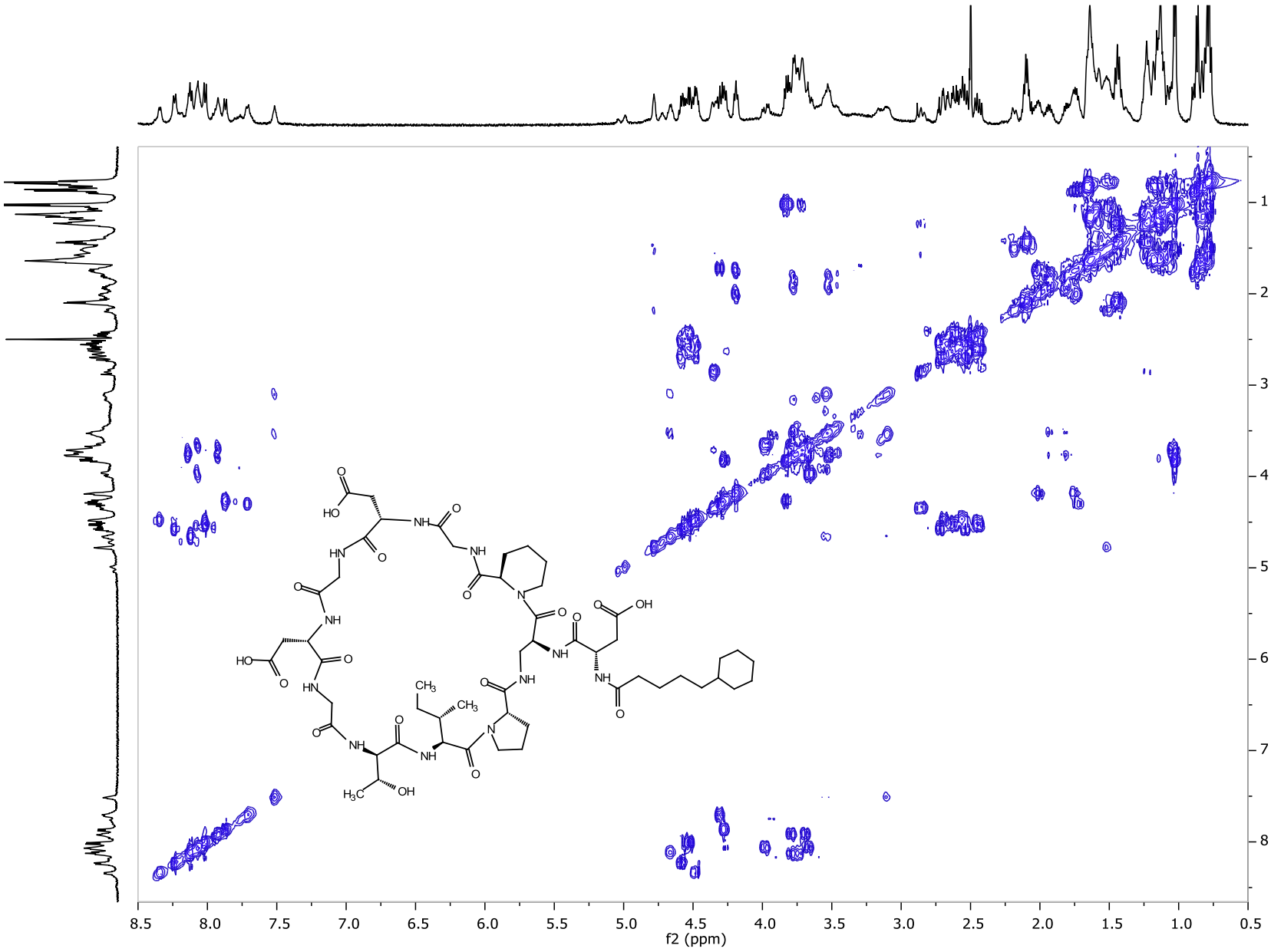




5-Cyclohexanepentanoyl analogue (**28**) ^{1}H NMR (500 MHz, DMSO-d_6)

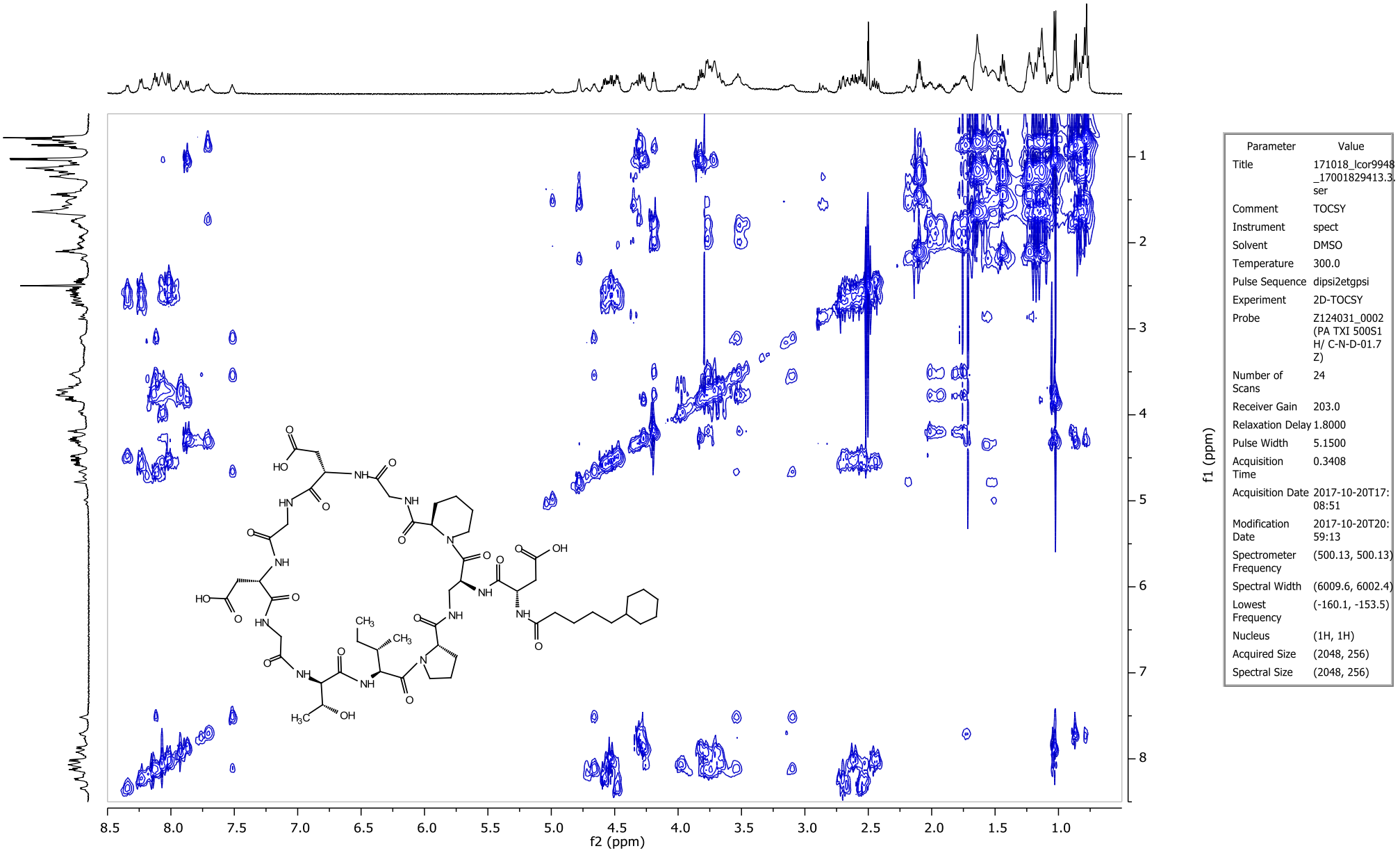


5-Cyclohexanepentanoyl analogue (**28**) COSY (500 MHz, DMSO-d_6)



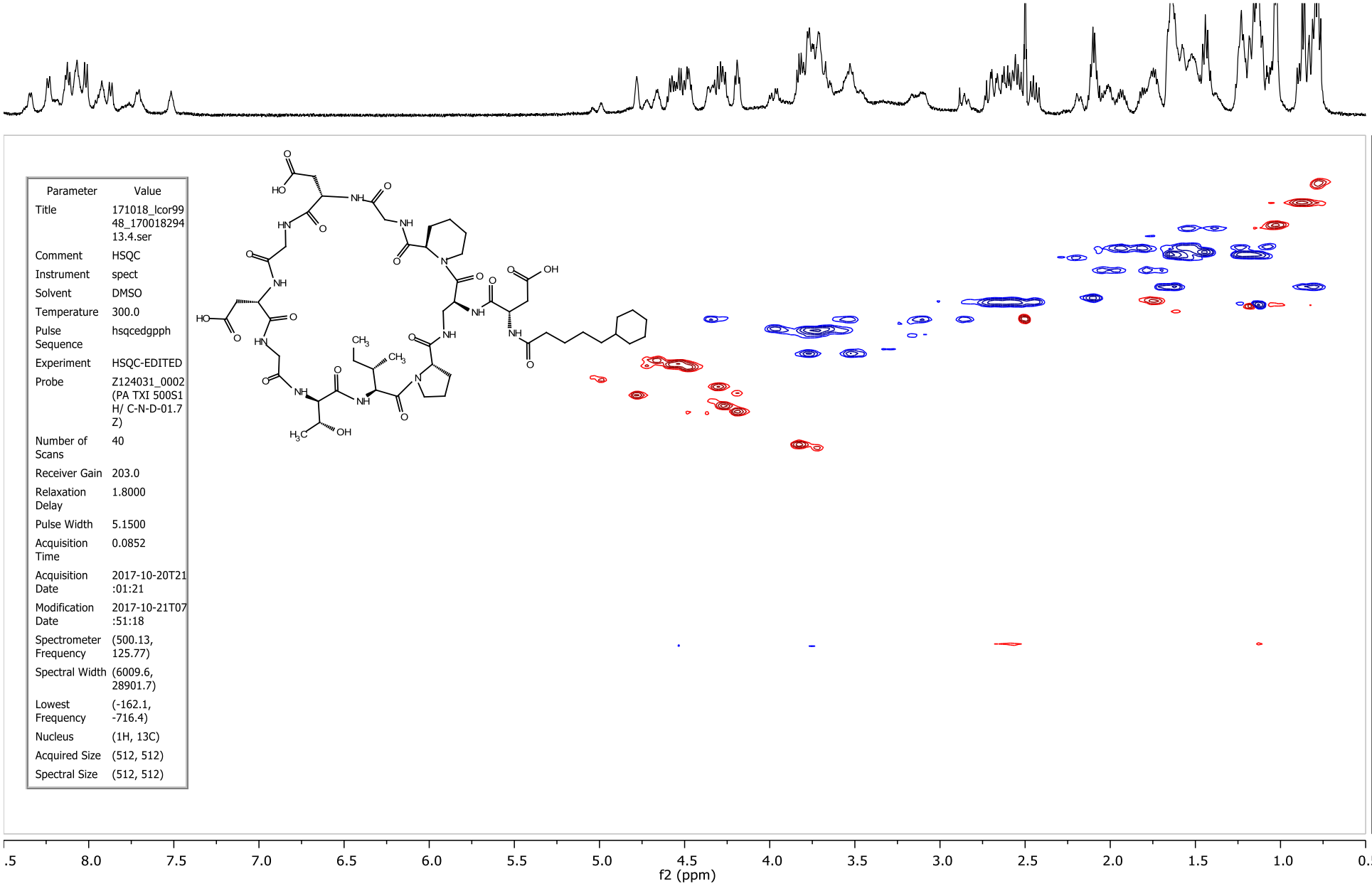
Parameter	Value
Title	171018_lcor9948_17001829413.2.ser
Comment	COSY
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	cosygpqf
Experiment	COSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	24
Receiver Gain	203.0
Relaxation Delay	1.8000
Pulse Width	5.1500
Acquisition Time	0.3408
Acquisition Date	2017-10-20T13:26:17
Modification Date	2017-10-20T17:07:24
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(6009.6, 6002.4)
Lowest Frequency	(-166.1, -159.0)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

5-Cyclohexanepentanoyl analogue (**28**) TOCSY (500 MHz, DMSO-d_6)



Parameter	Value
Title	171018_lcor9948_17001829413.3.ser
Comment	TOCSY
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	dipsi2etgpsi
Experiment	2D-TOCSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	24
Receiver Gain	203.0
Relaxation Delay	1.8000
Pulse Width	5.1500
Acquisition Time	0.3408
Acquisition Date	2017-10-20T17:08:51
Modification Date	2017-10-20T20:59:13
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(6009.6, 6002.4)
Lowest Frequency	(-160.1, -153.5)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

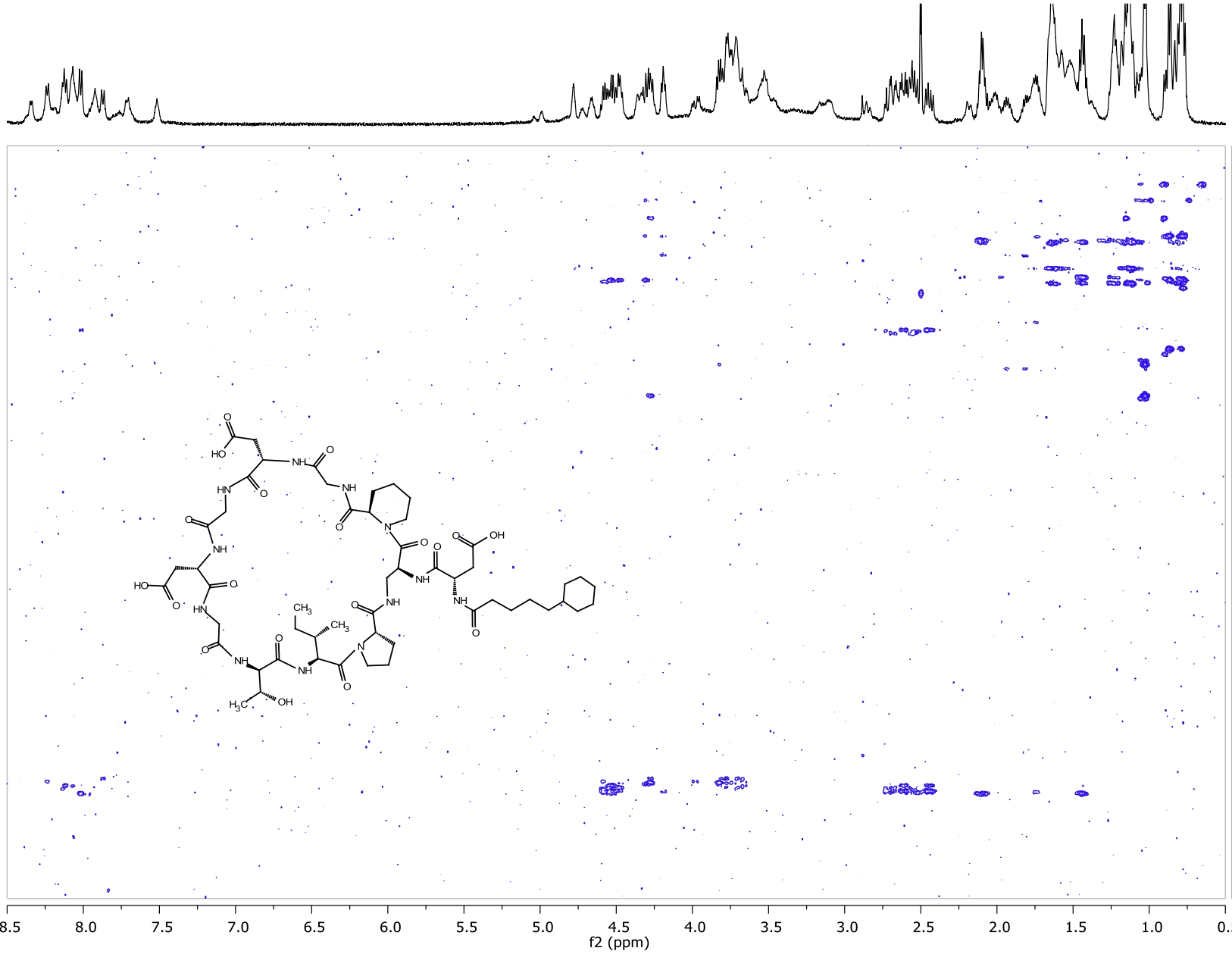
5-Cyclohexanepentanoyl analogue (**28**) HSQC (500/126 MHz, DMSO-d_6)



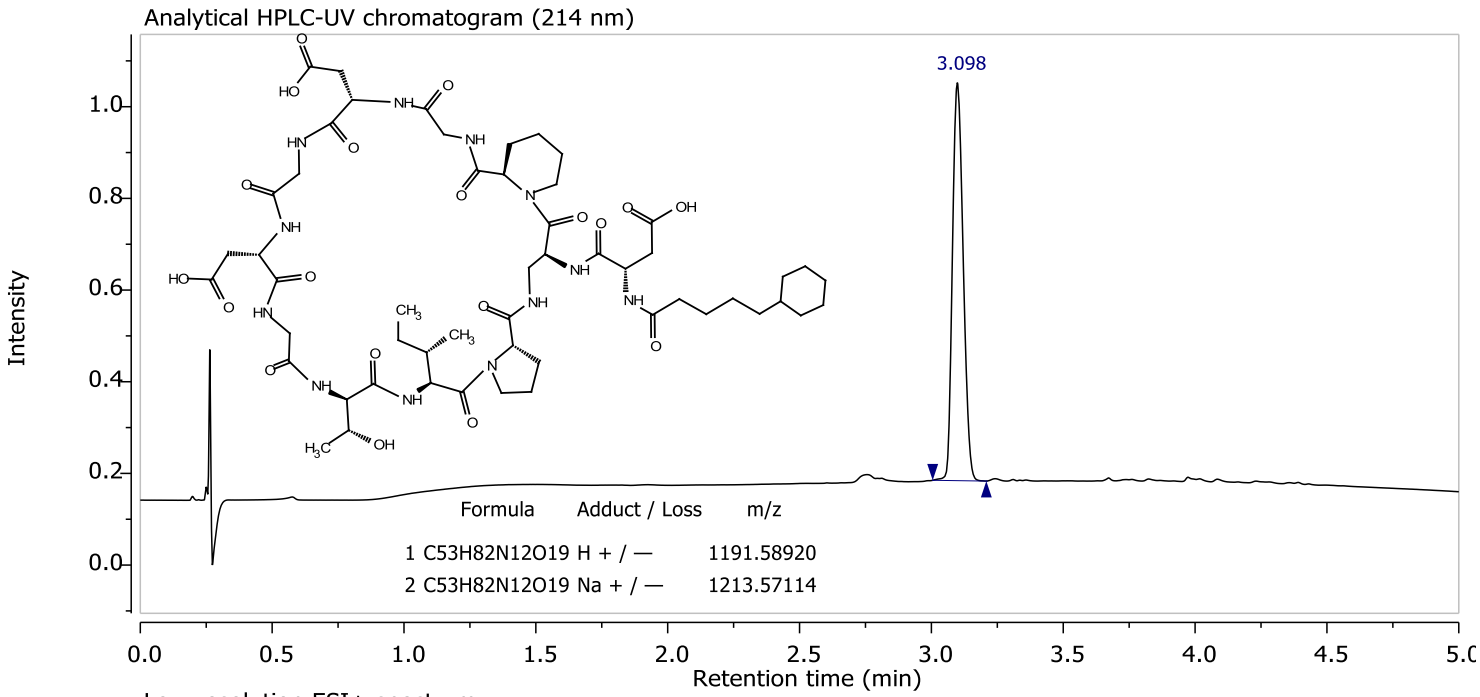
Parameter	Value
Title	171018_lcor9948_17001829413.4.ser
Comment	HSQC
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hsqcedgpph
Experiment	HSQC-EDITED
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	40
Receiver Gain	203.0
Relaxation Delay	1.8000
Pulse Width	5.1500
Acquisition Time	0.0852
Acquisition Date	2017-10-20T21:01:21
Modification Date	2017-10-21T07:51:18
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(6009.6, 28901.7)
Lowest Frequency	(-162.1, -716.4)
Nucleus	(1H, 13C)
Acquired Size	(512, 512)
Spectral Size	(512, 512)

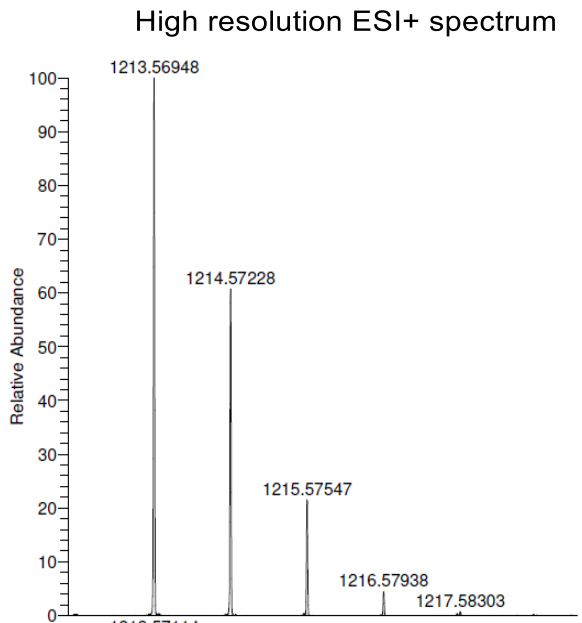
5-Cyclohexanepentanoyl analogue (**28**) HMBC (500/126 MHz, DMSO-d_6)

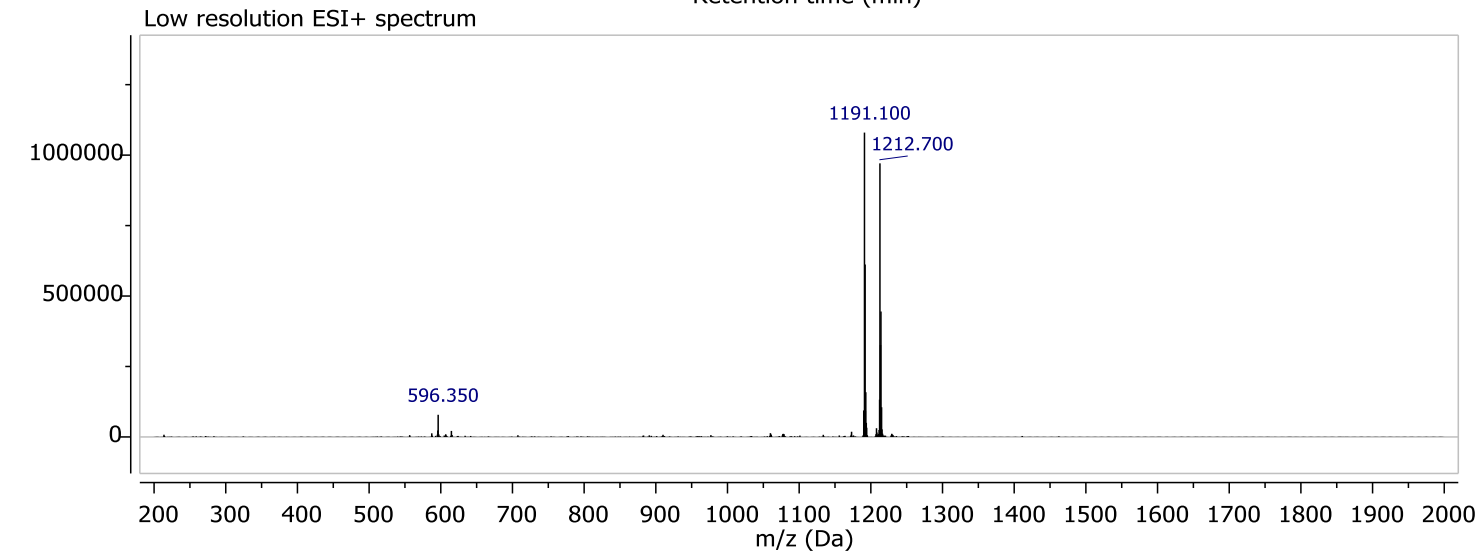
Parameter	Value
Title	LC.10.018.5.ser
Comment	HMBC
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hmbcgplpndqf
Experiment	HMBC
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	48
Receiver Gain	203.0
Relaxation Delay	1.8000
Pulse Width	5.1500
Acquisition Time	0.3408
Acquisition Date	2017-10-21T07:53:55
Modification Date	2017-10-21T22:57:26
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(6009.6, 28248.6)
Lowest Frequency	(-168.6, -386.0)
Nucleus	(1H, 13C)
Acquired Size	(2048, 512)
Spectral Size	(2048, 2048)

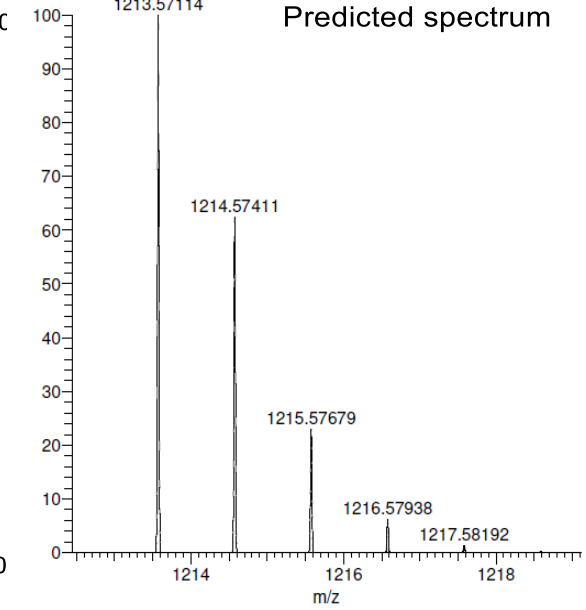


5-Cyclohexanepentanoyl analogue (**28**) Analytical HPLC, low and high-resolution ESI+ MS

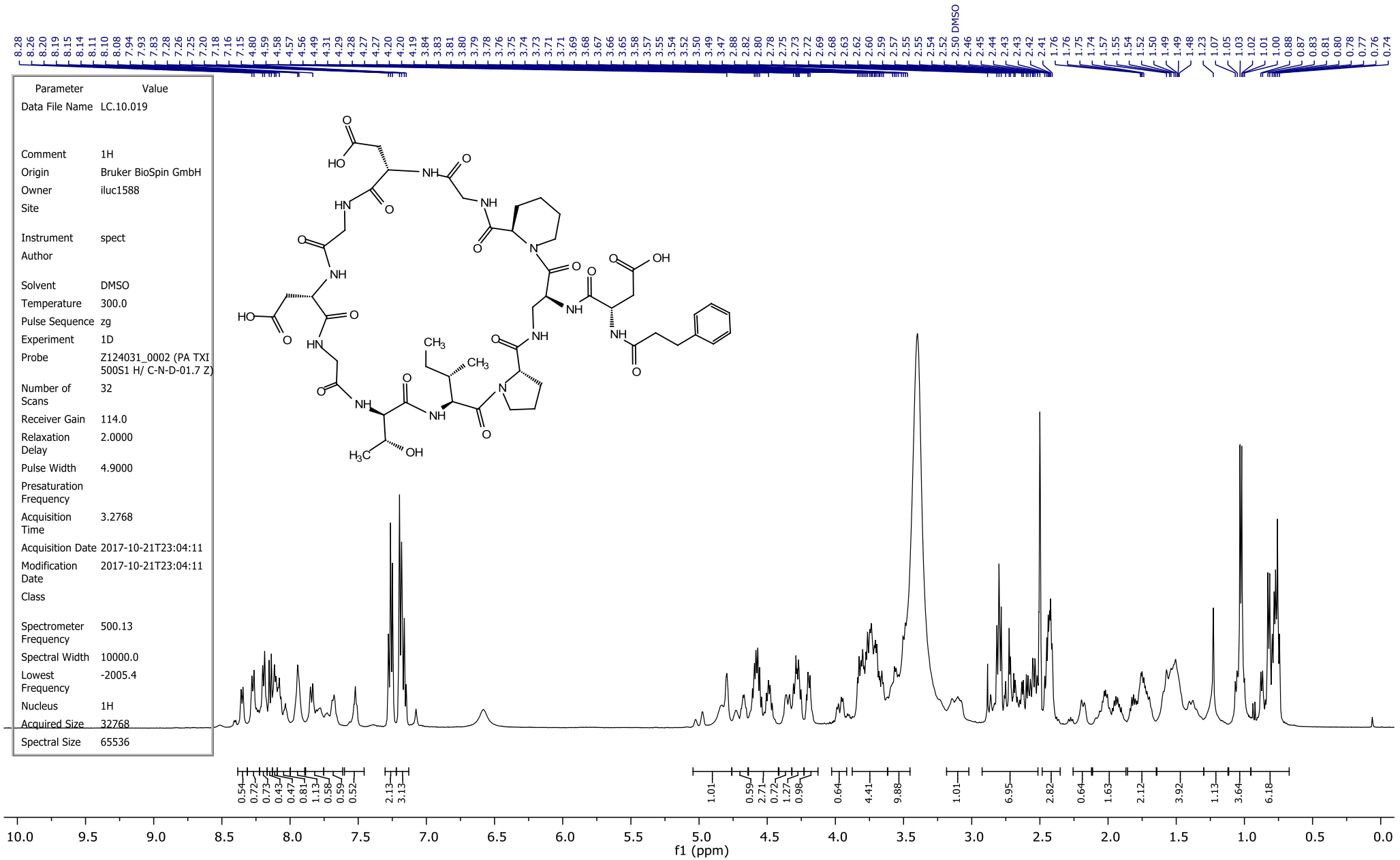




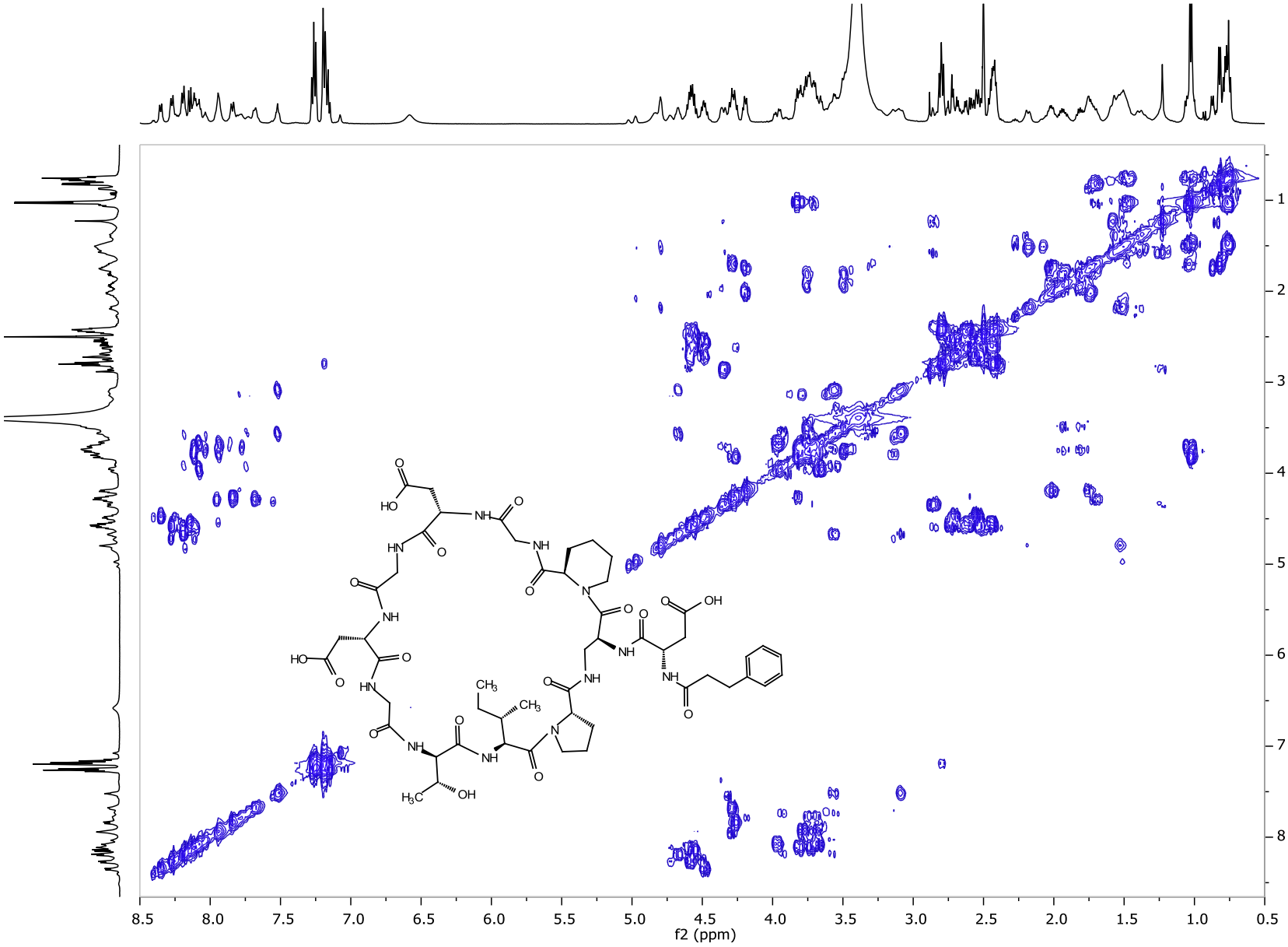




3-Phenylpropanoyl analogue (**29**) ^{1}H NMR (500 MHz, DMSO-d_6)

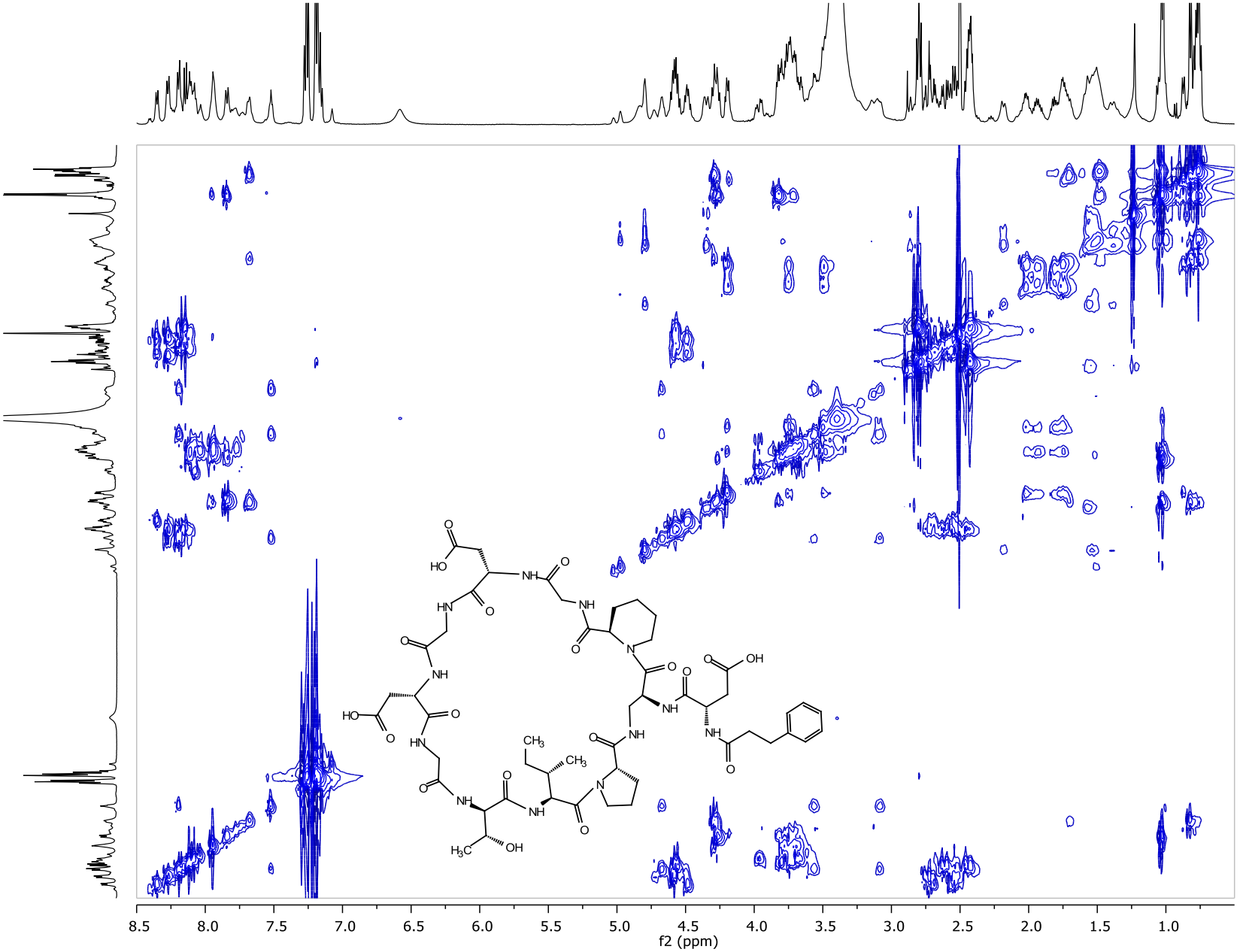


3-Phenylpropanoyl analogue (**29**) COSY (500 MHz, DMSO-d_6)



Parameter	Value
Data File Name	171020_lcor9948_17001832068/2/ ser
Title	171020_lcor9948_17001832068.2.ser
Comment	COSY
Origin	Bruker BioSpin GmbH
Owner	iluc1588
Site	
Instrument	spect
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	cosygpqf
Experiment	COSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	24
Receiver Gain	203.0
Relaxation Delay	2.1000
Pulse Width	5.2250
Presaturation Frequency	
Acquisition Time	0.3408
Acquisition Date	2017-10-21T23:06:07
Modification Date	2017-10-22T03:17:52
Class	
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(6009.6, 6002.4)
Lowest Frequency	(-168.1, -158.5)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

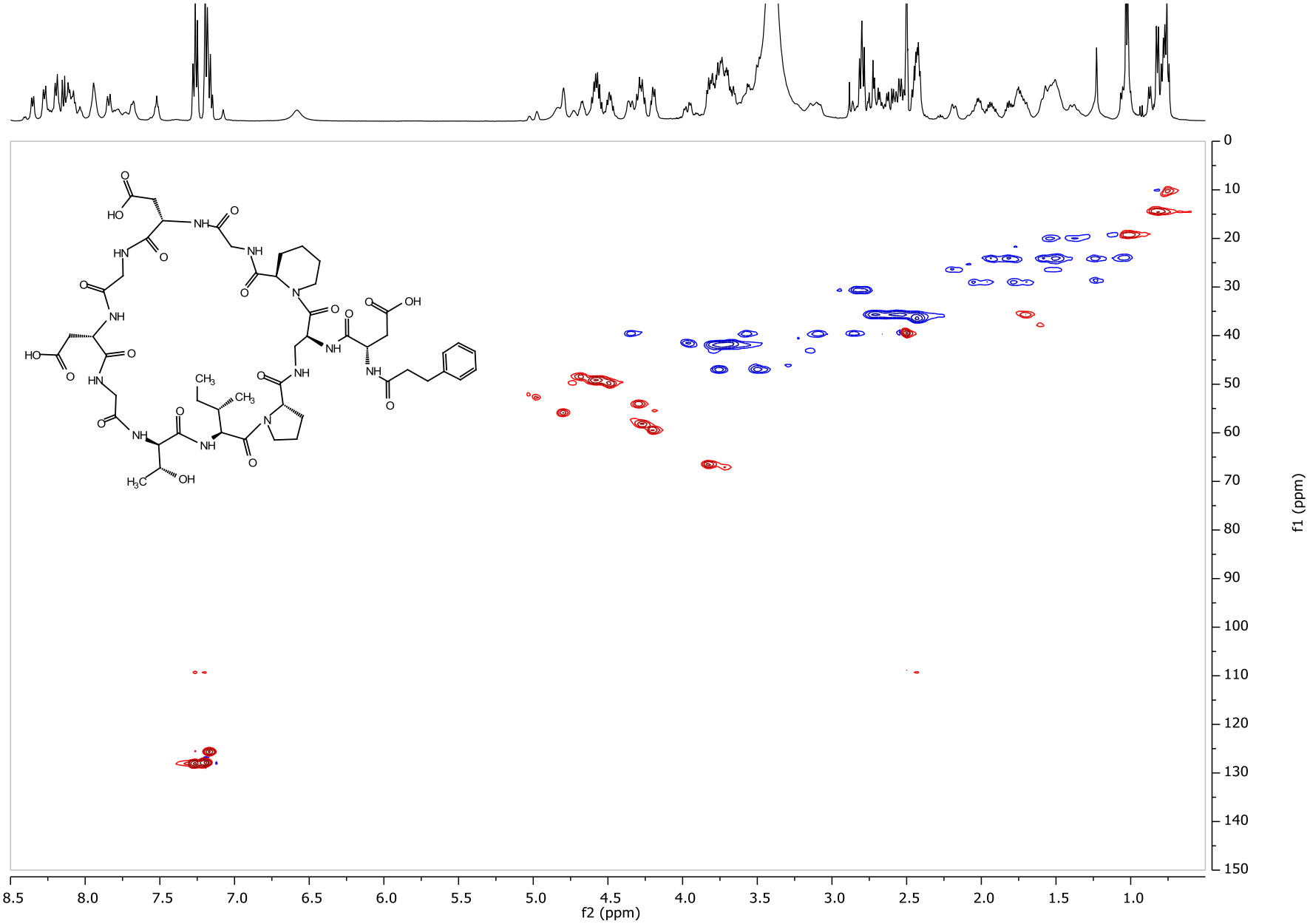
3-Phenylpropanoyl analogue (**29**) TOCSY (500 MHz, DMSO-d_6)



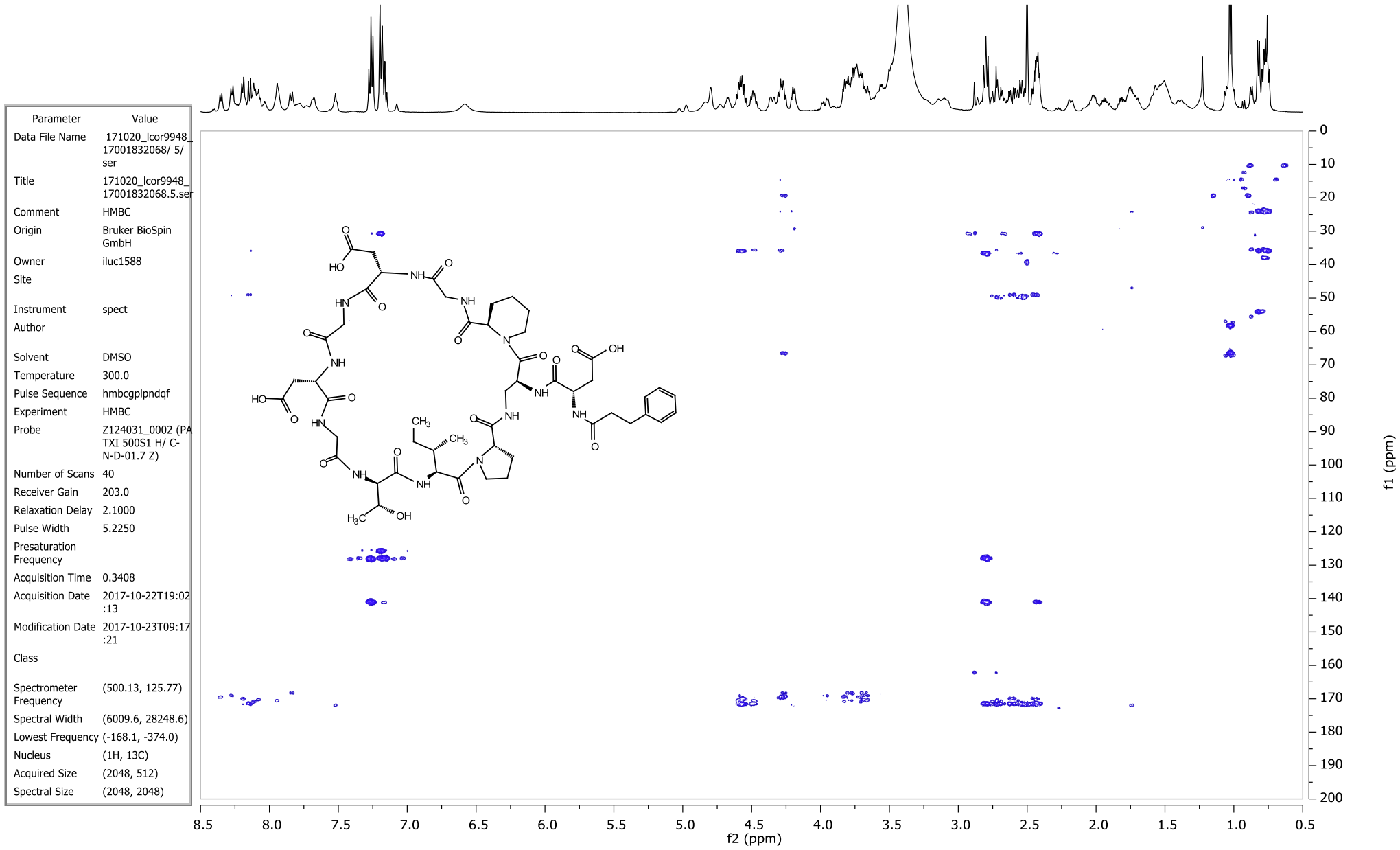
Parameter	Value
Data File Name	171020_lcor9948_17001832068/3/ ser
Title	171020_lcor9948_17001832068.3.ser
Comment	TOCSY
Origin	Bruker BioSpin GmbH
Owner	iluc1588
Site	
Instrument	spect
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	dipsi2etgpsi
Experiment	2D-TOCSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	24
Receiver Gain	203.0
Relaxation Delay	2.1000
Pulse Width	5.2250
Presaturation Frequency	
Acquisition Time	0.3408
Acquisition Date	2017-10-22T03:19:29
Modification Date	2017-10-22T07:40:25
Class	
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(6009.6, 6002.4)
Lowest Frequency	(-158.1, -150.0)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

3-Phenylpropanoyl analogue (**29**) HSQC (500/126 MHz, DMSO-d_6)

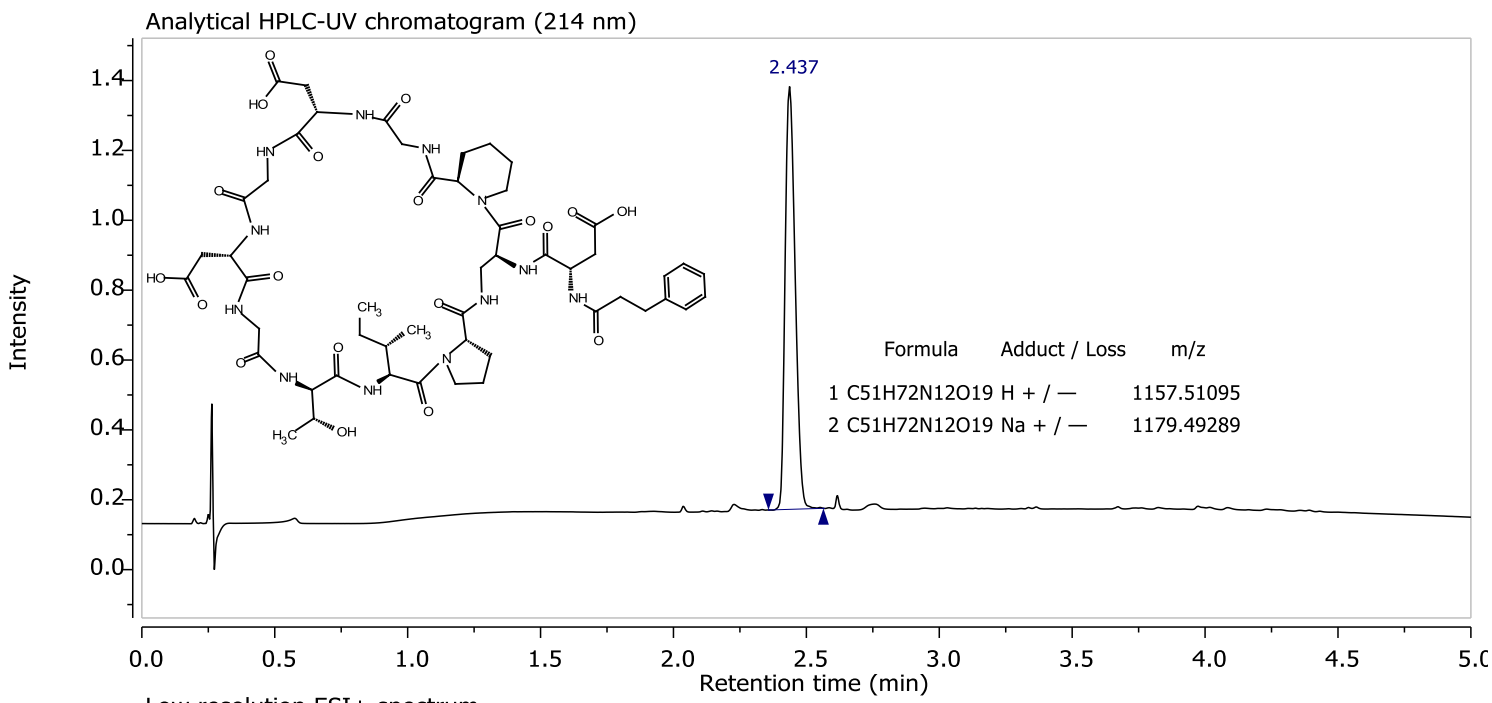
Parameter	Value
Data File Name	171020_lcor9948_17001832068/4/ ser
Comment	HSQC
Origin	Bruker BioSpin GmbH
Owner	iluc1588
Site	
Instrument	spect
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hsqcedgpph
Experiment	HSQC-EDITED
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	36
Receiver Gain	203.0
Relaxation Delay	2.1000
Pulse Width	5.2250
Presaturation Frequency	
Acquisition Time	0.0852
Acquisition Date	2017-10-22T07:42:40
Modification Date	2017-10-22T18:59:37
Class	
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(6009.6, 28901.7)
Lowest Frequency	(-158.6, -706.2)
Nucleus	(1H, 13C)
Acquired Size	(512, 512)
Spectral Size	(512, 512)

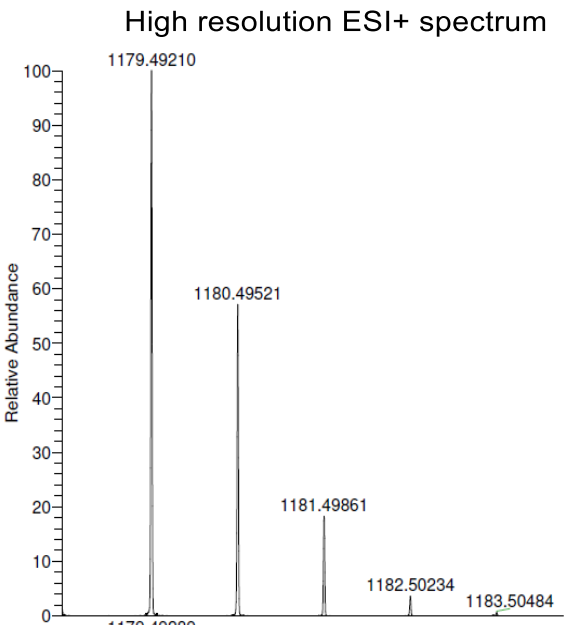


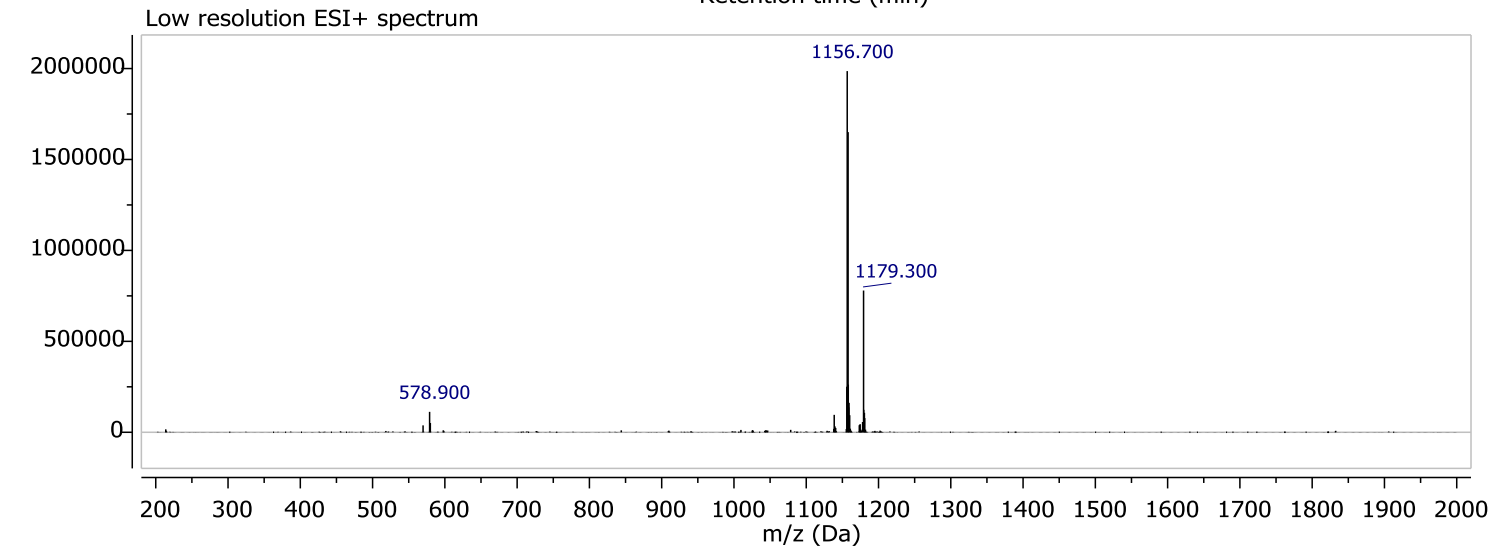
3-Phenylpropanoyl analogue (**29**) HMBC (500/126 MHz, DMSO-d_6)

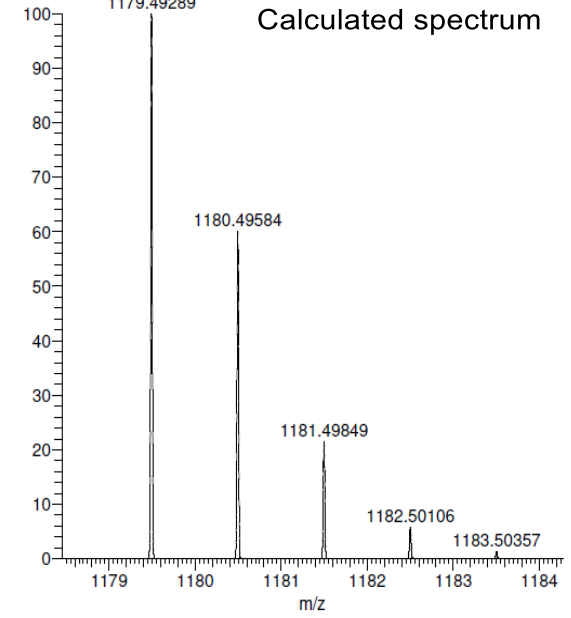


3-Phenylpropanoyl analogue (**29**) Analytical HPLC, low and high-resolution ESI+ MS



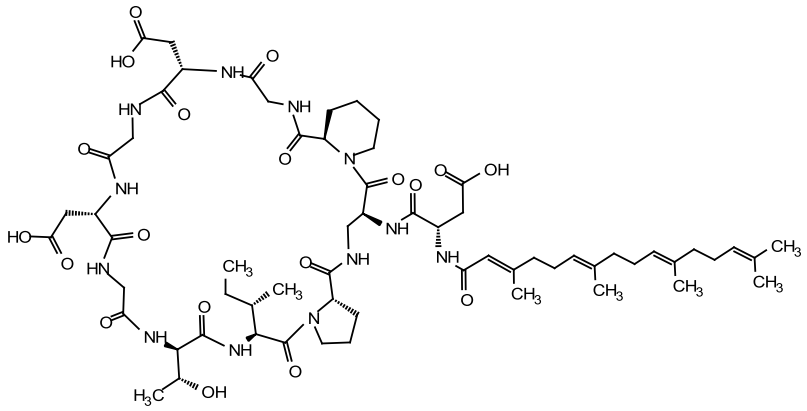




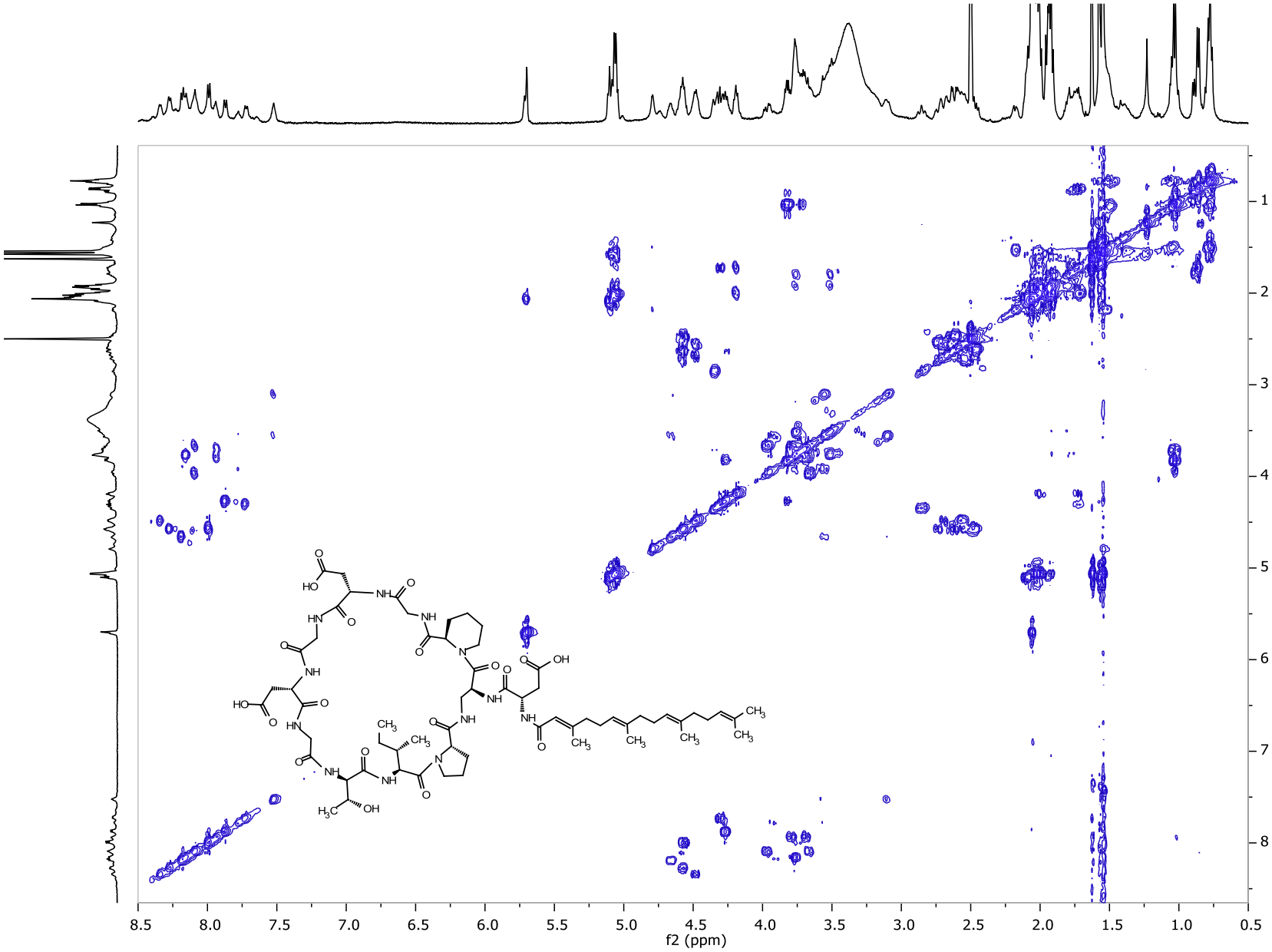


Geranylgeranoyl analogue (**30**) ^{1}H NMR (500 MHz, DMSO-d_6)

Parameter	Value
Title	LC.10.029.1.fid
Comment	1H
Instrument	spect
Solvent	DMSO
Temperature	300.1
Pulse Sequence	zg
Experiment	1D
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	32
Receiver Gain	203.0
Relaxation Delay	2.0000
Pulse Width	4.9000
Acquisition Time	3.2768
Acquisition Date	2017-10-18T11:54:56
Modification Date	2017-10-18T11:54:56
Spectrometer Frequency	500.13
Spectral Width	10000.0
Lowest Frequency	-2005.4
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

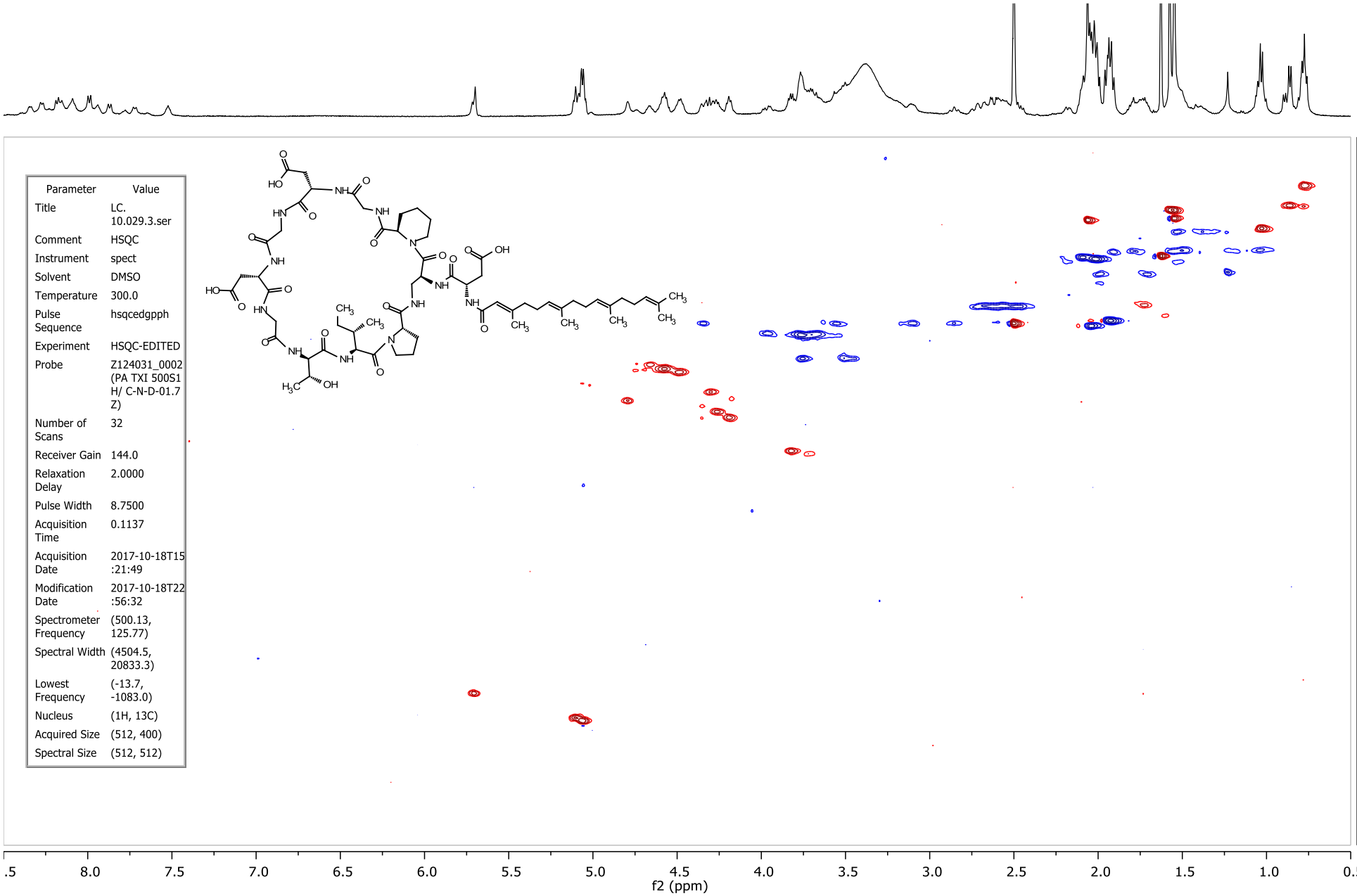


Geranylgeranoyl analogue (**30**) COSY (500 MHz, DMSO-d_6)



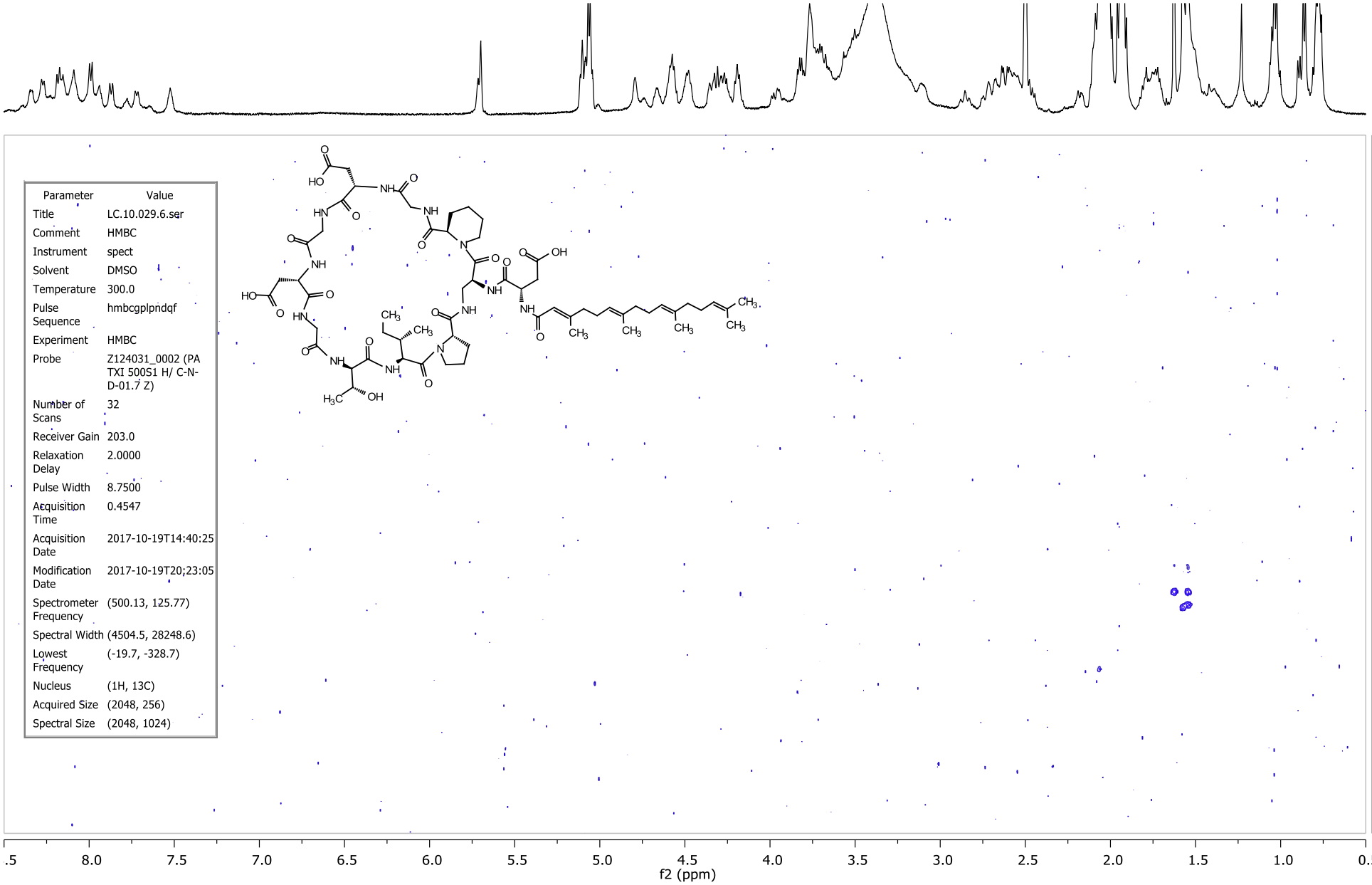
Parameter	Value
Title	LC.10.029.2.ser
Comment	COSY
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	cosygpqf
Experiment	COSY
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	16
Receiver Gain	203.0
Relaxation Delay	2.0000
Pulse Width	8.7500
Acquisition Time	0.4547
Acquisition Date	2017-10-18T12:07:19
Modification Date	2017-10-18T14:56:34
Spectrometer Frequency	(500.13, 500.13)
Spectral Width	(4504.5, 4500.5)
Lowest Frequency	(-18.2, -7.1)
Nucleus	(1H, 1H)
Acquired Size	(2048, 256)
Spectral Size	(2048, 256)

Geranylgeranoyl analogue (**30**) HSQC (500/126 MHz, DMSO-d_6)

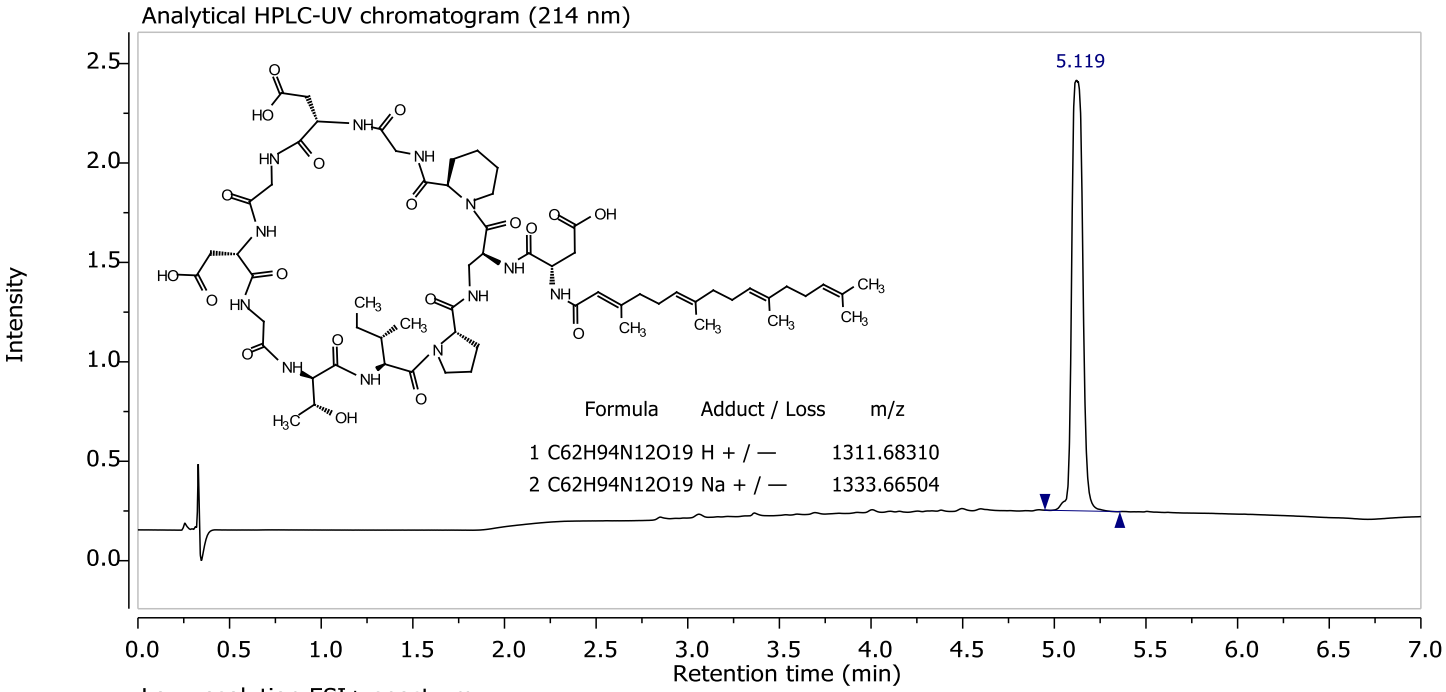


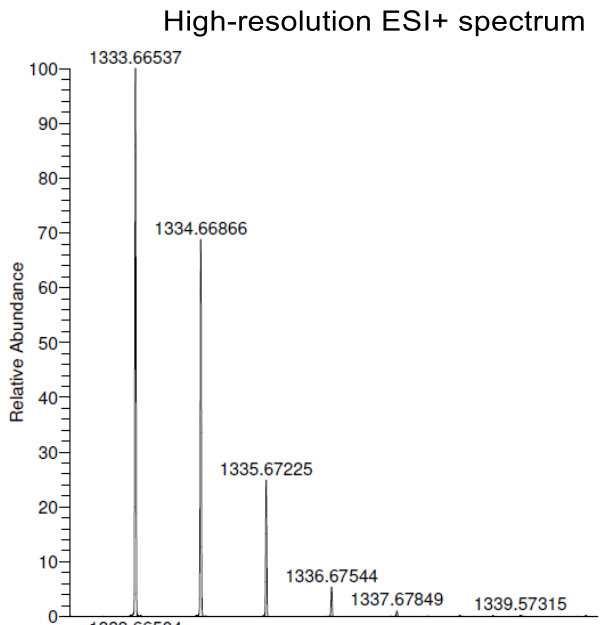
Parameter	Value
Title	LC. 10.029.3.ser
Comment	HSQC
Instrument	spect
Solvent	DMSO
Temperature	300.0
Pulse Sequence	hsqcedgpph
Experiment	HSQC-EDITED
Probe	Z124031_0002 (PA TXI 500S1 H/ C-N-D-01.7 Z)
Number of Scans	32
Receiver Gain	144.0
Relaxation Delay	2.0000
Pulse Width	8.7500
Acquisition Time	0.1137
Acquisition Date	2017-10-18T15 :21:49
Modification Date	2017-10-18T22 :56:32
Spectrometer Frequency	(500.13, 125.77)
Spectral Width	(4504.5, 20833.3)
Lowest Frequency	(-13.7, -1083.0)
Nucleus	(1H, 13C)
Acquired Size	(512, 400)
Spectral Size	(512, 512)

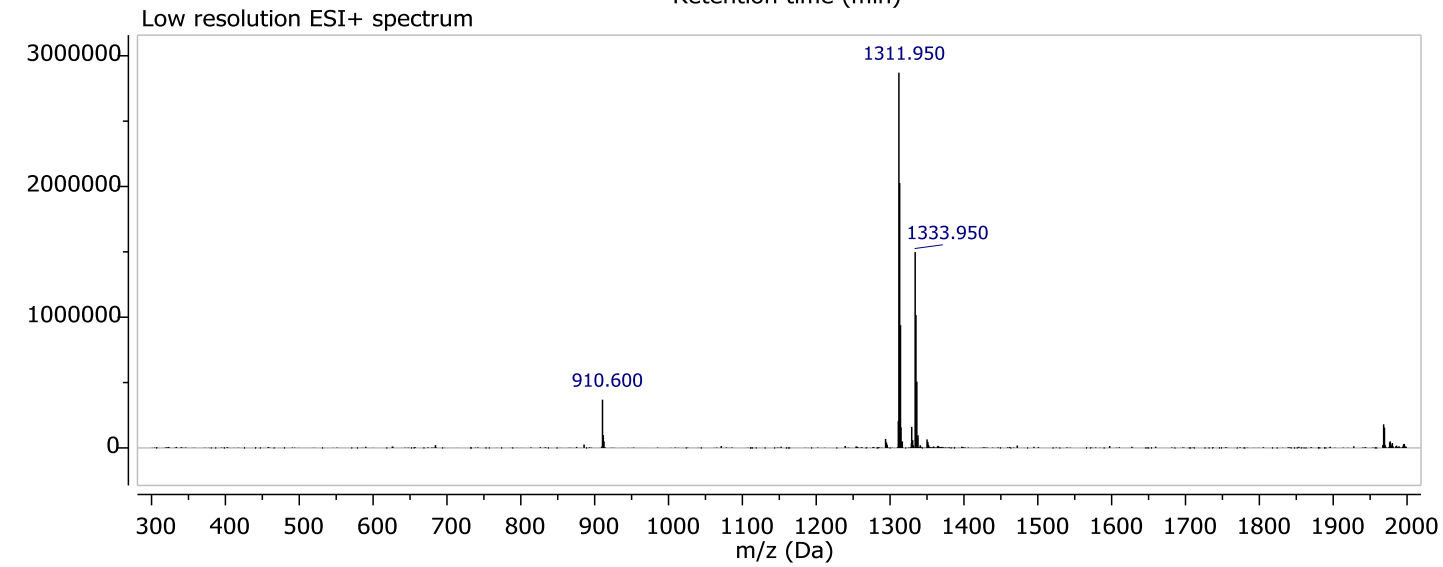
Geranylgeranoyl analogue (**30**) HMBC (500/126 MHz, DMSO-d_6)

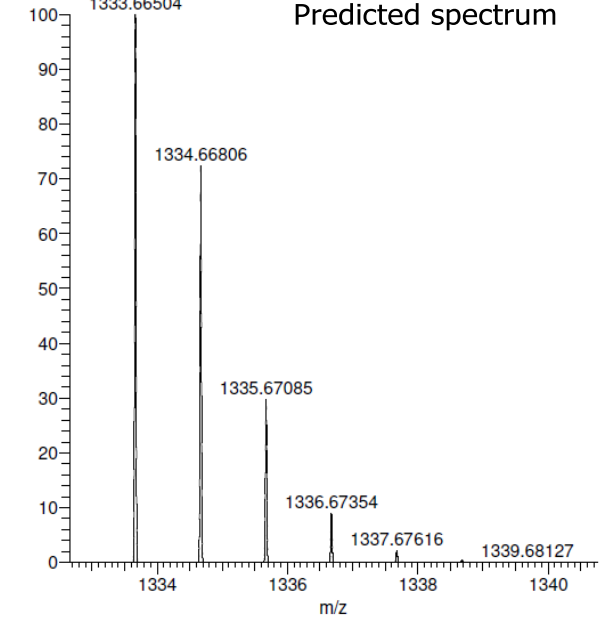


Geranylgeranoyl analogue (**30**) Analytical HPLC, low and high-resolution ESI+ MS









^{1}H AND ^{13}C CHEMICAL SHIFTS FOR GLYCINOCIN ANALOGUES AS DERIVED FROM HSQC AND HMBC

Assignment	14-methylpentadecanoyl analogue (**18**)		(Z)-14-methylpentadec-2-enoyl analogue (**20**)		14-methylpentadec-2-ynoyl analogue (**19**)		(E)-2-butenoyl analogue (**23**)		(E)-2-dodecanoyl analogue (**22**)		(E)-2-tetradecanoyl analogue (**21**)	
	δ H	**δ C**	**δ H**	**δ C**	**δ H**	**δ C**	**δ H**	**δ C**	**δ H**	**δ C**	**δ H**	**δ C**
1Asp1	-	170.2	-	170.3	-	169.4	-	170.1	-	169.9	-	169.8
1Asp2	4.53	49.1	4.56	49.1	4.52	49.6	4.59	49.1	4.60	49.2	4.61	49.1
1Asp2NH	8.03	-	8.14	-	8.69	-	8.13	-	8.14	-	8.14	-
1Asp3	2.62 2.44	35.9	2.62 2.48	35.9	2.61 2.50	35.6	2.63 2.48^	35.8^	2.63 2.49^	35.9^	2.63 2.49	35.9^
1Asp4	-	171.7	-	*	-	171.5	-	171.6	-	171.4	-	171.4
2Dap1	-	*	-	*	-	*	-	*	-	*	-	*
2Dap2	4.66	48.4	4.65	48.3	4.64	48.2	4.65	48.7	4.65	48.3	4.66	48.7
2Dap2NH	8.14	-	8.25	-	8.28	-	8.23	-	8.23	-	8.24	-
2Dap3	3.54 3.11	39.6	3.54 3.11	39.6	3.56 3.12	39.5	3.57 3.11	39.5	3.55 3.11	39.6	3.55 3.11	39.5
2Dap3NH	7.52	-	7.53	-	7.50	-	7.49	-	7.49	-	7.52	-
3Pip1	-	170.2	-	*	-	*	-	170.4	-	170.3	-	169.8
3Pip2	4.78	55.9	4.79	55.8	4.79	55.8	4.80	55.9	4.79	56.0	4.80	55.8
3Pip3	2.19 1.51	26.5	2.18 1.54	26.6	2.18 1.49	26.5	2.18 1.53	26.4	2.17 1.53	26.4	2.18 1.53	26.4
3Pip4	1.55 1.39	20.2	1.55 1.39	20.2	1.53 1.38	20.0	1.53 1.39	20.1	1.53 1.38	20.0	1.53 1.38	20.0
3Pip5	1.58 1.25	24.3	1.57 1.25	24.3	1.58 1.25	24.3	1.58 1.23	24.2	1.58 1.22	24.2	1.58 1.23	24.2
3Pip6	4.35 2.86	39.6	4.34 2.84	39.6	4.36 2.86	39.4	4.35 2.86	39.5	4.34 2.86	39.6	4.35 2.86	39.5
4Gly1	-	169.1	-	*	-	*	-	169.2	-	169.0	-	168.9
4Gly2	3.99 3.66	41.6	3.96 3.66	41.5	3.97 3.64	41.6	3.97 3.64	41.5	3.96 3.64	41.6	3.97 3.65	41.5
4Gly2NH	8.08	-	8.10	-	8.09	-	8.08	-	8.08	-	8.09	-
5Asp1	-	170.3	-	*	-	171.0	-	170.9	-	170.9	-	170.7
5Asp2	4.58	49.3	4.56	49.2	4.57	49.5	4.58	49.1	4.57	49.3	4.57	49.1
5Asp2NH	8.24	-	8.28	-	8.26	-	8.26	-	8.27	-	8.27	-
5Asp3	2.71 2.53	36.1^	2.72 2.54	35.9^	2.73 2.52	36.2^	2.74 2.52^	35.7^	2.74 2.53	35.7^	2.73 2.53	36.0^
5Asp4	-	172.0	-	*	-	171.8^	-	171.6	-	171.5	-	171.4
6Gly1	-	-	-	*	-	-	-	169.6	-	169.6	-	*
6Gly2	3.75	41.9^	3.75	41.9^	3.76	41.9^	3.77	41.8^	3.76	42.0^	3.76	41.8^
6Gly2NH	8.16	-	8.17	-	8.14	-	8.11	-	8.11	-	8.15	-
7Asp1	-	170.5	-	*	-	*	-	170.7	-	170.7	-	170.4
7Asp2	4.48	49.9	4.48	49.8	4.48	49.8	4.49	49.8	4.48	49.6	4.48	49.6
7Asp2NH	8.35	-	8.34	-	8.35	-	8.34	-	8.34	-	8.34	-
7Asp3	2.70 2.54	35.6^	2.68 2.56	35.9^	2.68 2.56	35.8^	2.70 2.55^	35.7^	2.70 2.56^	35.6^	2.68 2.56	35.4^
7Asp4	-	172.1	-	*	-	171.7^	-	171.5	-	171.5	-	170.9
8Gly1	-	*	-	*	-	168.3	-	168.4	-	168.3	-	168.0
8Gly2	3.75	42.1^	3.79 3.68	42.1	3.78 3.68	41.9^	3.78 3.71	41.9^	3.75	42.2^	3.79 3.69	41.9^
8Gly2NH	7.91	-	7.95	-	7.92	-	7.91	-	7.92	-	7.93	-
9Thr1	-	*	-	*	-	169.2	-	169.3	-	169.3	-	*
9Thr2	4.28	58.2	4.26	58.3	4.26	58.2	4.27	58.2	4.26	58.2	4.27	58.2
9Thr2NH	7.90	-	7.88	-	7.88	-	7.86	-	7.85	-	7.87	-
9Thr3	3.83	66.6	3.83	66.6	3.82	66.5	3.82	66.5	3.82	66.5	3.82	66.5
9Thr4	1.03	19.3	1.03	19.3	1.03	19.3	1.03	19.3	1.03	19.4	1.03	19.3
10Ile1	-	169.6	-	*	-	170.1	-	*	-	*	-	*
10Ile2	4.30	54.2	4.31	54.1	4.32	54.1	4.31	54.0	4.31	54.1	4.31	54.0
10Ile2NH	7.76	-	7.74	-	7.71	-	7.70	-	7.68	-	7.73	-
10Ile3	1.73	35.8	1.73	35.6	1.73	35.8	1.71	35.7	1.73	35.7	1.73	35.7
10Ile3Me	0.86	14.7	0.86	14.6	0.86	14.7	0.87	14.5	0.86	14.6	0.86	14.6
10Ile4	1.51 1.06	24.0	1.50 1.05	24.2	1.51 1.06	24.0	1.51 1.06	24.0	1.51 1.04	24.1	1.51 1.05	24.1
10Ile5	0.78	10.4	0.77	10.4	0.78	10.4	0.78	10.4	0.77	10.3	0.78	10.4
11Pro1	-	171.9	-	*	-	*	-	172.0	-	171.7	-	*
11Pro2	4.19	59.4	4.19	59.4	4.19	59.4	4.18	59.3	4.18	59.5	4.18	59.3
11Pro3	2.02 1.75	29.1	2.00 1.72	29.1	2.02 1.72	29.1	2.01 1.71	29.1	2.01 1.71	29.1	2.01 1.71	29.1
11Pro4	1.94 1.81	24.4	1.91 1.79	24.5	1.94 1.81	24.4	1.92 1.81	24.2	1.91 1.79	24.2	1.92 1.80	24.3
11Pro5	3.78 3.53	46.9	3.74 3.51	47.0	3.78 3.53	46.9	3.76 3.52	46.9	3.76 3.52	47.0	3.76 3.52	46.9
FA1	-	172.3	-	165.6	-	152.5	-	164.8	-	164.8	-	164.6
FA2	2.09	35.0	5.79	122.1	-	76.1	5.94	125.3	5.92	123.7	5.92	123.5
FA3	1.46	24.9	5.95	144.6	-	87.1	6.63	138.1	6.63	143.2	6.63	142.9
FA4	1.23	26.6	2.57	27.7	2.32	17.5	1.79	17.1	2.12	31.0	2.11	31.0
FA5	1.23	28.9	1.22^	28.8^	1.46	27.0	-	-	1.38	27.5	1.37	27.3
FA6	1.23	28.9	1.22^	28.8^	1.34	27.7	-	-	1.24^	28.6^	1.23^	28.6^
FA7	1.23	28.9	1.22^	28.8^	1.24^	28.7^	-	-	1.24^	28.6^	1.23^	28.6^
FA8	1.23	28.9	1.22^	28.8^	1.24^	28.7^	-	-	1.24^	28.6^	1.23^	28.6^
FA9	1.23	28.9	1.22^	28.8^	1.24^	28.7^	-	-	1.24^	28.6^	1.23^	28.6^
FA10	1.23	28.9	1.22^	28.8^	1.24^	28.7^	-	-	1.23	31.0	1.23^	28.6^
FA11	1.23	28.9	1.22^	28.8^	1.24^	28.7^	-	-	1.25	21.9	1.23^	28.6^
FA12	1.23	28.9	1.22	26.5	1.23	26.5	-	-	0.84	14.2	1.22	31
FA13	1.12	38.4	1.12	38.2	1.12	38.2	-	-	-	-	1.24	21.8
FA14	1.49	27.3	1.48	27.1	1.48	27.4	-	-	-	-	0.85	13.9
FA15	0.84	22.4	0.83	22.3	0.84	22.3	-	-	-	-	-	-

*No HMBC observed for this atom or assignment is ambiguous

^Value represents a best approximation from overlapping HSQC and/or HMBC signals

Assignment	Hexanoyl analogue (**27**)			Decanoyl analogue (**26**)			Dodecanoyl analogue (**25**)			Tetradecanoyl analogue (**24**)			5-Cyclohexanepentanoyl analogue (**28**)			3-Phenylpropanoyl analogue (**29**)			Geranylgeranoyl analogue (**30**)		
	δ H		**δ C**	**δ H**		**δ C**	**δ H**		**δ C**	**δ H**		**δ C**	**δ H**		**δ C**	**δ H**		**δ C**	**δ H**		**δ C**
1Asp1	-		170.3	-		170.1	-		170.7	-		170.2	-		169.9	-		170.0	-		*
1Asp2	4.53		49.4	4.53		49.0	4.53		49.1	4.53		49.1	4.53		49.1	4.57		49.2	4.56		49.2
1Asp2NH	8.04		-	8.02		-	8.02		-	8.02		-	8.02		-	8.14		-	7.99		-
1Asp3	2.62	2.45	35.8	2.62	2.46	35.8^	2.62	2.44	35.8	2.61	2.44	35.9	2.61	2.44	35.8	2.62	2.44	35.7	2.62	2.47	35.9
1Asp4	-		171.7	-		171.7	-		171.7	-		171.7	-		171.5	-		171.5	-		*
2Dap1	-		*	-		*	-		*	-		*	-		*	-		*	-		*
2Dap2	4.66		48.4	4.66		48.3	4.66		48.4	4.65		48.3	4.66		48.4	4.67		48.4	4.66		48.3
2Dap2NH	8.13		-	8.11		-	8.13		-	8.14		-	8.12		-	8.19		-	8.18		-
2Dap3	3.55	3.08	39.7	3.54	3.08	39.7	3.54	3.10	39.5	3.52	3.13	39.5	3.54	3.11	39.6	3.56	3.10	39.6	3.56	3.10	39.6
2Dap3NH	7.51		-	7.51		-	7.51		-	7.52		-	7.52		-	7.52		-	7.52		-
3Pip1	-		170.5	-		170.4	-		170.2	-		170.2	-		170.1	-		170.3	-		*
3Pip2	4.78		55.9	4.78		55.9	4.79		55.8	4.78		55.9	4.78		55.8	4.80		55.9	4.79		55.8
3Pip3	2.18	1.53	26.5	2.18	1.53	26.5	2.18	1.51	26.4	2.19	1.51	26.4	2.18	1.51	26.3	2.18	1.52	26.4	2.18	1.52	26.4
3Pip4	1.54	1.37	20.1	1.54	1.37	20.1	1.54	1.39	20.1	1.55	1.39	20.1	1.55	1.39	20.2	1.54	1.38	20.0	1.54	1.38	20.0
3Pip5	1.58	1.22	24.2	1.57	1.22	24.1	1.57	1.25	24.2	1.58	1.24	24.2	1.58	1.25	24.3	1.58	1.24	24.1	1.55	1.21	24.1
3Pip6	4.35	2.84	39.6	4.34	2.85	39.6	4.34	2.86	39.5	4.35	2.85	39.6	4.35	2.86	39.5	4.35	2.86	39.5	4.34	2.85	39.5
4Gly1	-		169.2	-		169.2	-		169.2	-		*	-		168.9	-		169.0	-		*
4Gly2	3.96	3.66	41.6	3.98	3.66	41.6	3.98	3.66	41.5	3.99	3.66	41.6	3.98	3.66	41.6	3.97	3.66	41.5	3.97	3.66	41.5
4Gly2NH	8.08		-	8.07		-	8.07		-	8.07		-	8.07		-	8.08		-	8.09		-
5Asp1	-		171.2	-		171.1	-		170.6	-		*	-		170.9	-		170.9	-		*
5Asp2	4.58		49.4	4.58		49.4	4.59		49.2	4.57		49.3	4.58		49.2	4.58		49.2	4.57		49.2
5Asp2NH	8.27		-	8.25		-	8.25		-	8.21		-	8.24		-	8.27		-	8.27		-
5Asp3	2.74	2.52^	35.8	2.74	2.55	35.7^	2.74^	2.53^	35.8^	2.69^	2.53^	36.4^	2.71	2.53	35.8^	2.74	2.54	35.7^	2.73^	2.55^	36.0^
5Asp4	-		171.8^	-		171.7^	-		171.9^	-		172.2^	-		171.7	-		171.6^	-		*
6Gly1	-		169.7	-		169.6	-		169.4	-		*	-		*	-		169.5	-		-
6Gly2	3.76		41.8^	3.77		42.0^	3.75		41.8^	3.75		42.1^	3.76		41.9	3.77		41.9^	3.77		41.9^
6Gly2NH	8.12		-	8.11		-	8.13		-	8.18		-	8.14		-	8.11		-	8.15		-
7Asp1	-		170.7	-		170.7	-		168.2	-		170.6	-		170.5	-		170.5	-		*
7Asp2	4.48		49.4	4.49		49.8	4.5		49.7	4.47		50.0	4.48		49.8	4.49		49.8	4.48		49.8
7Asp2NH	8.34		-	8.33		-	8.33		-	8.37		-	8.34		-	8.35		-	8.34		-
7Asp3	2.7	2.55^	35.7	2.71	2.56	35.8^	2.71^	2.54^	35.6^	2.66^	2.56^	36.0^	2.66	2.55	35.8^	2.70	2.54	35.7^	2.70^	2.57^	35.9^
7Asp4	-		171.8^	-		171.5^	-		171.8^	-		172.0^	-		171.3	-		171.5^	-		*
8Gly1	-		168.5	-		168.3	-		170.6	-		*	-		168.1	-		168.2	-		*
8Gly2	3.73		41.8^	3.76		42.0^	3.74		41.8^	3.75		42.1^	3.73		42.1	3.75		41.9	3.79	3.69	41.8^
8Gly2NH	7.93		-	7.90		-	7.88		-	7.92		-	7.92		-	8.03		-	7.94		-
9Thr1	-		169.4	-		169.4	-		169.4	-		*	-		169.2	-		169.3	-		*
9Thr2	4.27		58.2	4.28		58.2	4.29		58.1	4.28		58.2	4.27		58.1	4.27		58.1	4.26		58.2
9Thr2NH	7.85		-	7.86		-	7.88		-	7.92		-	7.87		-	7.84		-	7.87		-
9Thr3	3.82		66.5	3.82		66.5	3.82		66.5	3.83		66.5	3.82		66.5	3.83		66.5	3.82		66.5

9Thr4	1.02		19.4	1.03		19.3	1.03		19.3	1.03		19.3	1.03		19.3	1.03		19.3	1.03		19.3
10Ile1	-		170.1	-		170.1	-		169.8	-		169.6	-		169.7	-		169.7	-		*
10Ile2	4.31		54.1	4.30		54.1	4.30		54.0	4.30		54.1	4.30		54.0	4.30		54.0	4.30		54.0
10Ile2NH	7.69		-	7.70		-	7.74		-	7.77		-	7.71		-	7.68		-	7.72		-
10Ile3	1.72		35.8	1.72		35.8	1.73		35.8	1.74		35.7	1.74		35.6	1.70		35.7	1.72		35.6
10Ile3Me	0.87		14.5	0.86		14.3	0.85		13.8	0.86		14.5	0.86		14.7	0.82		14.6	0.86		14.5
10Ile4	1.47	1.05	24.5	1.50	1.05	24.1	1.50	1.06	24.0	1.51	1.06	24.0	1.51	1.06	24.0	1.51	1.05	24.0	1.50	1.04	24.0
10Ile5	0.78		10.4	0.78		10.4	0.78		10.4	0.78		10.4	0.78		10.4	0.76		10.2	0.77		10.3
11Pro1	-		172.1	-		172.0	-		172	-		*	-		*	-		171.9	-		*
11Pro2	4.19		59.5	4.19		59.5	4.19		59.4	4.19		59.4	4.19		59.3	4.20		59.4	4.19		59.4
11Pro3	2.01	1.73	29.2	2.02	1.74	29.1	2.02	1.75	29.0	2.01	1.75	28.9	2.02	1.75	29.1	2.02	1.74	29.0	1.99	1.71	29.0
11Pro4	1.92	1.81	24.3	1.93	1.81	24.3	1.93	1.82	24.2	1.93	1.81	24.3	1.94	1.81	24.4	1.94	1.81	24.2	1.91	1.81	24.2
11Pro5	3.76	3.52	47.0	3.77	3.52	47.0	3.77	3.53	46.9	3.77	3.52	46.9	3.78	3.53	46.9	3.76	3.50	46.9	3.76	3.50	46.9
FA1	-		172.5	-		172.4	-		172.3	-		172.3	-		172.1	-		171.5	-		*
FA2	2.09		35.0	2.09		35.0	2.09		35.0	2.09		35.0	2.10		35.0	2.80		30.7	5.70		117.8
FA3	1.47		24.4	1.46		24.7	1.46		24.9	1.46		24.9	1.44		25.2	2.42		36.4	-	(2.06) [2]	152.9 (17.6)[2]
FA4	1.21		30.6	1.23		31.1	1.23		31.1	1.22		31.1	1.23		25.7	-		141.0 [1]	2.04		40.0
FA5	1.25		21.6	1.24^		28.6^	1.23^		28.6^	1.23^		28.8^	1.13		36.4	7.19 [1]		128.0 [1]	2.09		25.5
FA6	0.85		13.6	1.24^		28.6^	1.23^		28.6^	1.23^		28.8^	1.18 [1]		36.8	7.26 [1]		128.1 [1]	5.10 [3]		123.0 [2]
FA7	-		-	1.24^		28.6^	1.23^		28.6^	1.23^		28.8^	1.64 [1]	0.81 [1]	32.5 [1]	7.17 [1]		125.7 [1]	-	(1.57) [2,3]	135.2 [3] (15.4)[2,3]
FA8	-		-	1.24^		28.6^	1.23^		28.6^	1.23^		28.8^	1.61 [1]^	1.16 [1]^	25.6 [1]	-		-	1.92		38.9
FA9	-		-	1.24^		21.8	1.23^		28.6^	1.23^		28.8^	1.61 [1]^	1.13 [1]^	25.5 [1]	-		-	2.02		25.8
FA10	-		-	0.85		14.2	1.23^		28.6^	1.23^		28.8^	-		-	-		-	5.07 [3]		123.2 [3]
FA11	-		-	-		-	1.26		21.9	1.23^		28.8^	-		-	-		-	-	(1.55) [2,3]	134.5 [3] (15.5)[2,3]
FA12	-		-	-		-	0.87		14.4	1.23^		28.8^	-		-	-		-	1.92		38.9
FA13	-		-	-		-	-		-	1.26		21.9	-		-	-		-	2.02		25.8
FA14	-		-	-		-	-		-	0.85		13.8	-		-	-		-	5.06		123.7
FA15	-		-	-		-	-		-	-		-	-		-	-		-	-		130.8
FA16																			1.63	(1.55) [2]	25.2 (17.3)[2]

*No HMBC observed for this atom or assignment is ambiguous

^Value represents a best approximation from overlapping HSQC and/or HMBC signals

[1]Signal corresponding to the FA Phenyl or cyclohexyl group

[2]Signal corresponding to a FA side chain methyl group

[3]Ambiguity exists between the following pairs of assignments (FA6/FA10, FA7/FA11, FA7Me/FA11Me)

ANTIMICROBIAL SCREENING DATA

Glycinocin Analogues Screening Average (μM)						
	S. aureus (ATCC 29213)		*B. subtilis* (ATCC 23857)		*P. aeruginosa* (ATCC 27853)	
	MHB	CAMHB (50)	MHB	CAMHB (50)	MHB	CAMHB (50)
Rifampin	0.0060	0.0080	0.15	0.11	>66	>66
Daptomycin	22	0.34	22	0.94	>66	>66
Vancomycin	0.94	0.51	0.097	0.11	>66	>66
Gentamicin	1.3	4.4	0.39	0.064	1.0	8.4
Glycinocin A (1)	>66	11	>66	17	>66	>66
Glycinocin B (2)	>66	5.5	>66	8.3	>66	>66
Glycinocin C (3)	>66	17	>66	11	>66	>66
(*E*)-But-2-enoyl analogue (23)	>66	>66	>66	>66	>66	>66
(*E*)-Dodec-2-enoyl analogue (22)	>66	>66	>66	55	>66	>66
Hexanoyl analogue (27)	>66	>66	>66	>66	>66	>66
Decanoyl analogue (26)	>66	>66	>66	>66	>66	>66
Dodecanoyl analogue (25)	>66	>66	>66	>66	>66	>66
Tetradecanoyl analogue (24)	>66	16.5	>66	17	>66	>66
5-cyclohexanepentanoyl analogue (28)	>66	>66	>66	>66	>66	>66
3-Phenylpropanoyl analogue (29)	>66	>66	>66	>66	>66	>66
Glycinocin Analogues Screening Average (μg/mL)						
	S. aureus (ATCC 29213)		*B. subtilis* (ATCC 23857)		*P. aeruginosa* (ATCC 27853)	
	MHB	CAMHB (50)	MHB	CAMHB (50)	MHB	CAMHB (50)
Rifampin	0.0049	0.0066	0.12	0.091	>54	>54
Daptomycin	36	0.55	36	1.5	>110	>110
Vancomycin	1.4	0.74	0.14	0.16	>96	>96
Gentamicin	0.62	2.1	0.19	0.031	0.48	4.0
Glycinocin A (1)	>82	14	>82	21	>82	>82
Glycinocin B (2)	>83	6.9	>83	10	>83	>83
Glycinocin C (3)	>81	21	>81	14	>81	>81
(*E*)-But-2-enoyl analogue (23)	>72	>72	>72	>72	>72	>72
(*E*)-Dodec-2-enoyl analogue (22)	>80	>80	>80	66	>80	>80
Hexanoyl analogue (27)	>74	>74	>74	>74	>74	>74
Decanoyl analogue (26)	>78	>78	>78	>78	>78	>78
Dodecanoyl analogue (25)	>80	>80	>80	>80	>80	>80
Tetradecanoyl analogue (24)	>82	20	>82	21	>82	>82
5-cyclohexanepentanoyl analogue (28)	>79	>79	>79	>79	>79	>79
3-Phenylpropanoyl analogue (29)	>76	>76	>76	>76	>76	>76

	Glycinocin Analogues Screening Average (μM)				Glycinocin Analogues Screening Average (μg/mL)			
	E. faecium (ATCC 6569)				*E. faecium* (ATCC 6569)			
	MHB	CAMHB (50)	CAMHB (100)	CAMHB (200)	MHB	CAMHB (50)	CAMHB (100)	CAMHB (200)
Rifampin	0.69	0.69	0.86	1.0	0.57	0.57	0.71	0.85
Daptomycin	8.3	0.17	0.03	0.04	13	0.28	0.04	0.06
Vancomycin	0.26	0.52	0.52	0.52	0.37	0.75	0.75	0.75
Glycinocin A (1)	33	4.1	4.1	2.1	41	5.2	5.2	2.6
Glycinocin B (2)	17	4.1	2.1	2.1	21	5.2	2.6	2.6
Glycinocin C (3)	44	14	4.1	4.1	54	17	5.1	5.1
Tetradecanoyl analogue (24)	55	8.3	4.1	4.1	68	10	5.1	5.1

Glycinocin Analogues Screening Average (μM)														
	S. aureus (ATCC 29213)				*B. subtilis* (ATCC 23857)				*E. faecium* (ATCC 6569)				*P. aeruginosa* (ATCC 27853)	
	MHB	CAMHB (50)	CAMHB (100)	CAMHB (200)	MHB	CAMHB (50)	CAMHB (100)	CAMHB (200)	MHB	CAMHB (50)	CAMHB (100)	CAMHB (200)	MHB	CAMHB (50)
Rifampin	0.0054	0.0054	0.004	0.004	0.35	0.35	0.52	0.34	0.52	0.52	1.0	1.0	33	33
Daptomycin	5.5	0.86	0.26	0.26	8.3	1.0	0.52	0.43	6.2	0.11	0.02	0.02	>66	>66
Vancomycin	0.69	1.4	1.6	2.1	0.13	0.26	0.43	0.43	0.26	0.34	0.52	0.52	>66	>66
Gentamicin	2.8	1.7	2.1	4.1	0.18	0.13	0.13	0.17	11	8.3	17	25	2.1	4.1
Glycinocin A (1)	>66	17	8.3	4.1	>66	17	4.1	4.1	28	5.5	2.1	2.1	>66	>66
Glycinocin B (2)	66.0	8.3	8.3	4.1	>66	17	8.3	4.1	14	2.1	2.1	2.1	>66	>66
Glycinocin C (3)	>66	17	17	8.3	>66	33	8.3	4.1	66	6.9	4.1	2.8	>66	>66
14-methylpentadecanoyl analogue (18)	66	17	8.3	4.1	66	29	17	8.3	28	4.1	2.1	2.1	>66	>66
(*Z*)-14-methylpentadec-2-enoyl analogue (20)	66	17	8.3	6.2	66	33	17	11	28	4.1	2.1	2.1	>66	>66
14-methylpentadec-2-ynoyl analogue (19)	>66	33	17	8.3	>66	66	17	11	66	8.3	4.1	4.1	>66	>66
(*E*)-Tetradec-2-enoyl analogue (21)	>66	22	8.3	4.1	>66	33	11	4.1	>66	6.9	2.1	3.1	>66	>66
Geranylgeranoyl analogue (30)	33	8.3	4.1	4.1	66	29	11	8.3	11	3.4	2.1	2.1	>66	>66
Glycinocin Analogues Screening Average (μg/mL)														
	S. aureus (ATCC 29213)				*B. subtilis* (ATCC 23857)				*E. faecium* (ATCC 6569)				*P. aeruginosa* (ATCC 27853)	
	MHB	CAMHB (50)	CAMHB (100)	CAMHB (200)	MHB	CAMHB (50)	CAMHB (100)	CAMHB (200)	MHB	CAMHB (50)	CAMHB (100)	CAMHB (200)	MHB	CAMHB (50)
Rifampin	0.0044	0.0044	0.0033	0.0033	0.29	0.29	0.42	0.28	0.42	0.42	0.85	0.85	27	27.16
Daptomycin	8.9	1.4	0.42	0.42	13	1.7	0.84	0.70	10	0.17	0.04	0.04	>110	>110
Vancomycin	1.0	2.0	2.2	3.0	0.19	0.37	0.62	0.62	0.37	0.50	0.75	0.75	>96	>96
Gentamicin	1.3	0.82	0.98	2.0	0.08	0.06	0.06	0.08	5.3	3.9	7.9	12	0.98	2.0
Glycinocin A (1)	>82	21	10	5.2	>82	21	5.2	5.2	34	6.9	2.6	2.6	>82	>82
Glycinocin B (2)	83	10	10	5.2	>83	21	10	5.2	17	2.6	2.6	2.6	>83	>83
Glycinocin C (3)	>81	20	20	10	>81	41	10	5.1	81	8.5	5.1	3.4	>81	>81
14-methylpentadecanoyl analogue (18)	83	21	10	5.2	83	36	21	10	35	5.2	2.6	2.6	>84	>84
(*Z*)-14-methylpentadec-2-enoyl analogue (20)	83	21	10	7.8	83	42	21	14	35	5.2	2.6	2.6	>84	>84
14-methylpentadec-2-ynoyl analogue (19)	>84	42	21	10	>84	83	21	14	83	10	5.2	5.2	>84	>84
(*E*)-Tetradec-2-enoyl analogue (21)	>82	27	10	5.1	>82	41	14	5.1	>82	8.5	2.5	3.8	>82	>82
Geranylgeranoyl analogue (30)	43	11	5.4	5.4	87	38	14	11	14	4.5	2.7	2.7	>87	>87