

Chemical Synthesis and Structure-Activity Relationship Study Yield Desotamide A Analogues with Improved Antibacterial Activity

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Figures S1. The HRESIMS spectrum of 7

Mass Spectrum SmartFormula Report

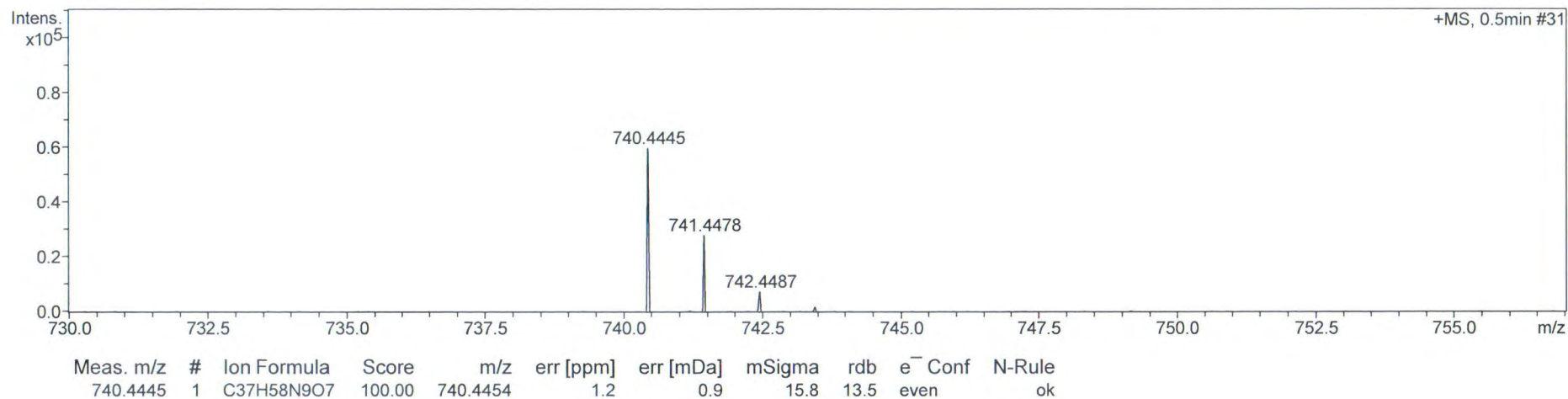
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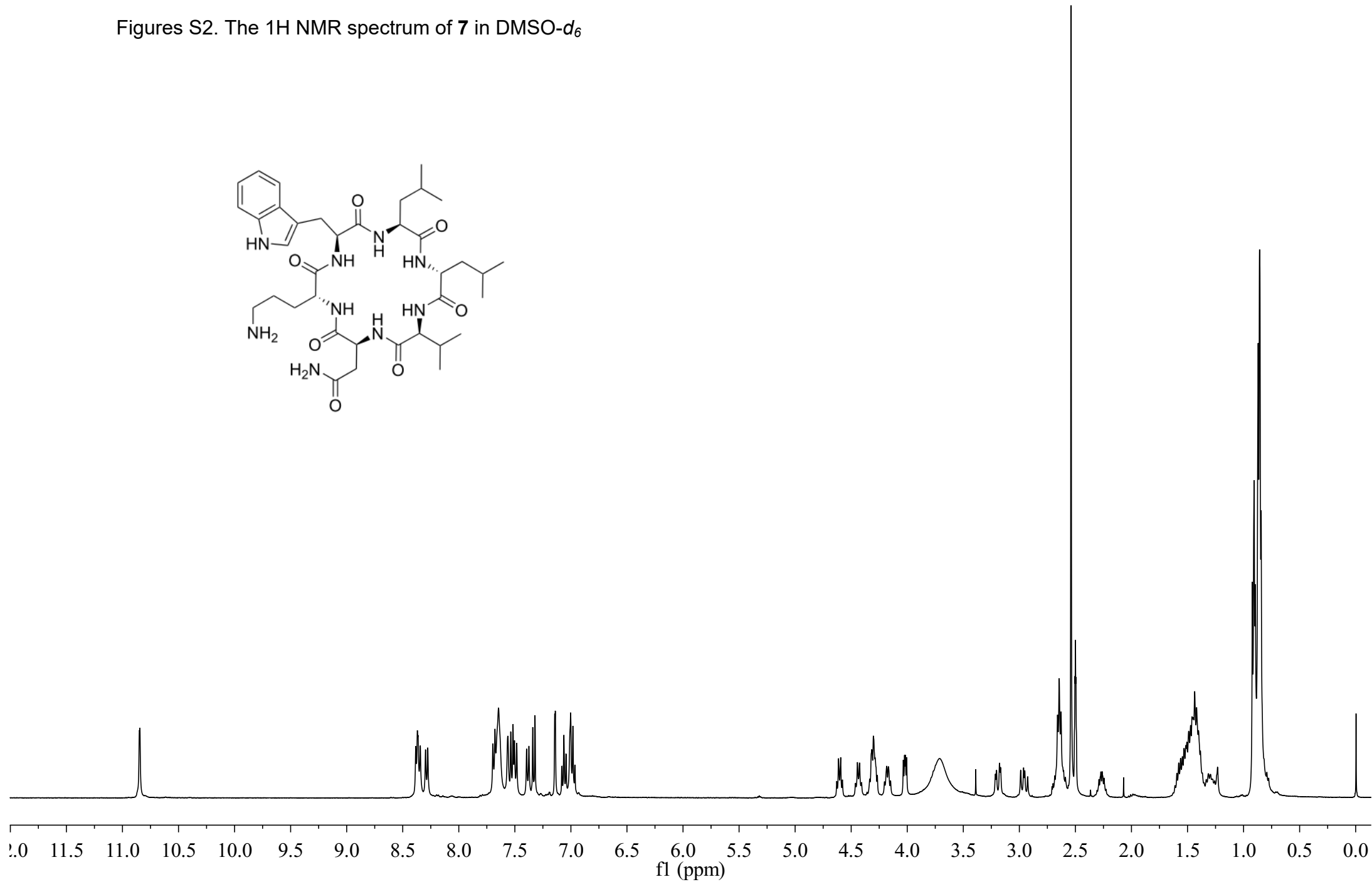
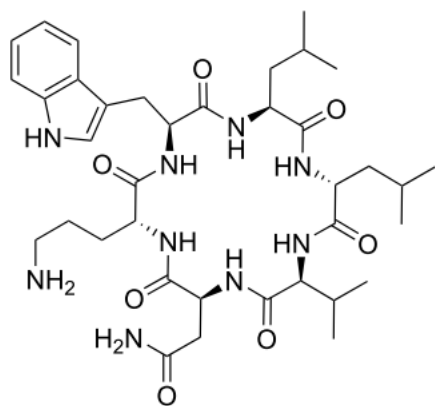
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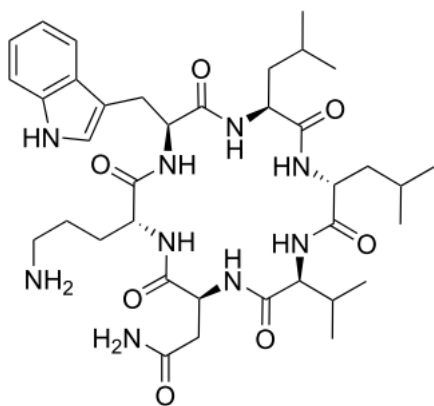
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		Set Corona	0 nA	Set APCI Heater	0 °C



Figures S2. The ^1H NMR spectrum of **7** in $\text{DMSO-}d_6$



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Figures S4. The HRESIMS spectrum of **8**

Mass Spectrum SmartFormula Report

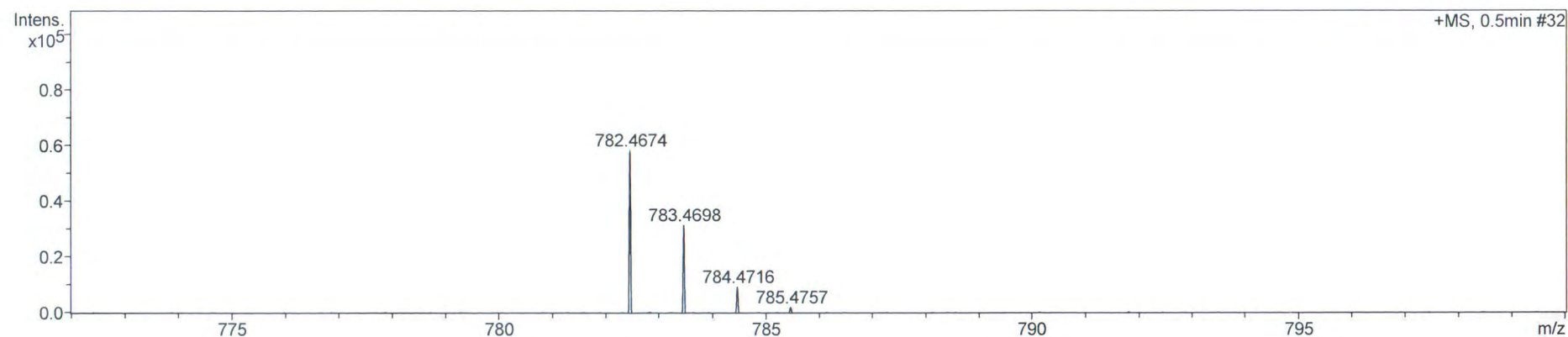
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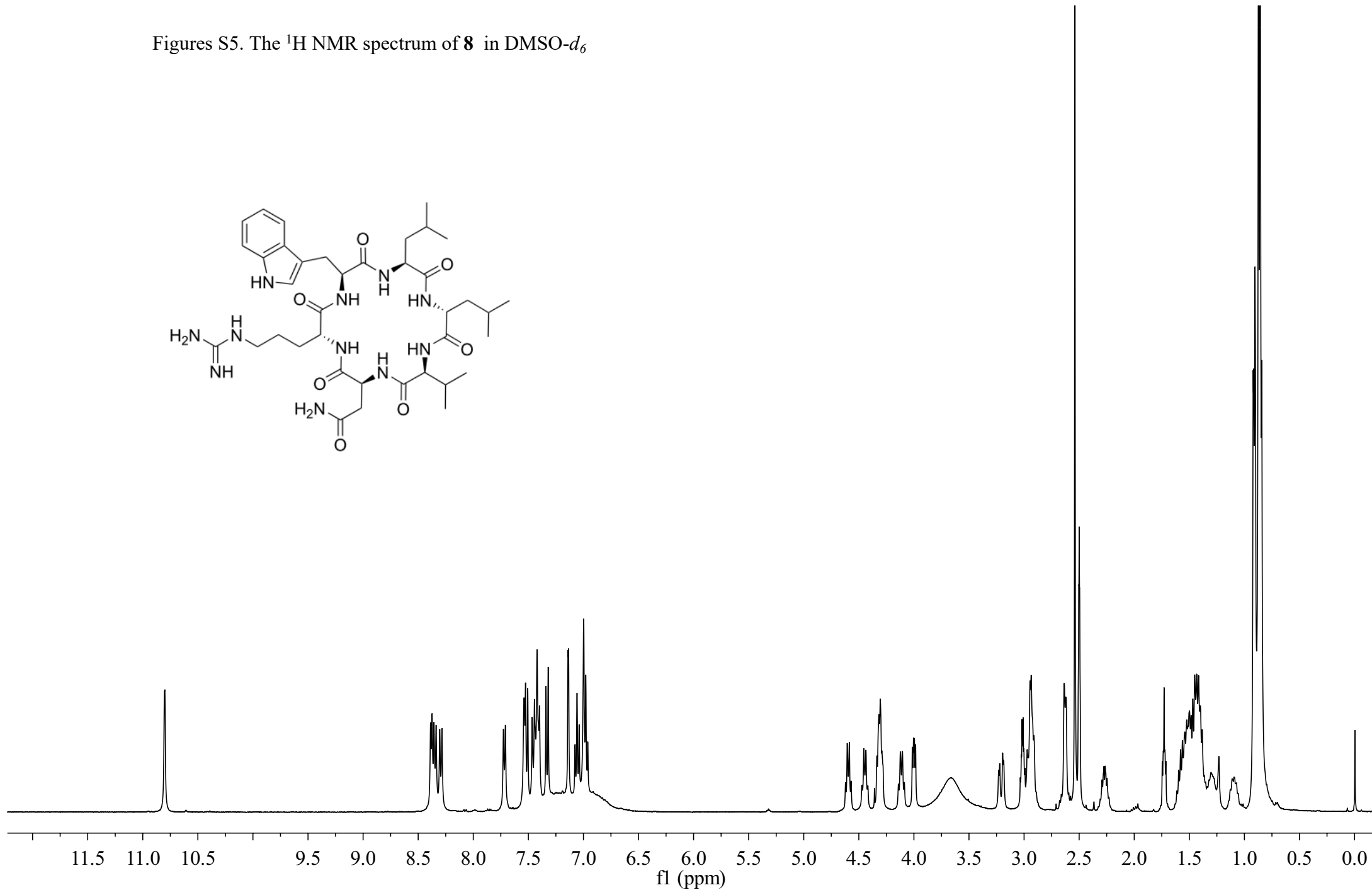
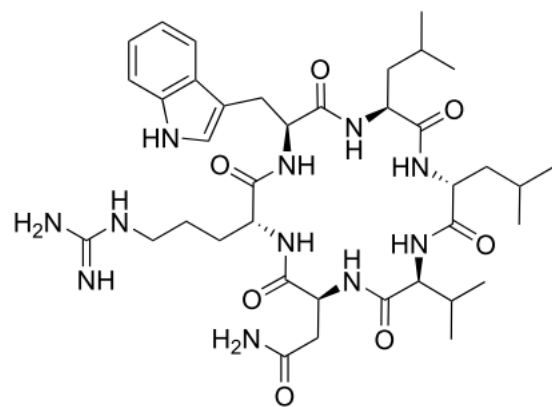
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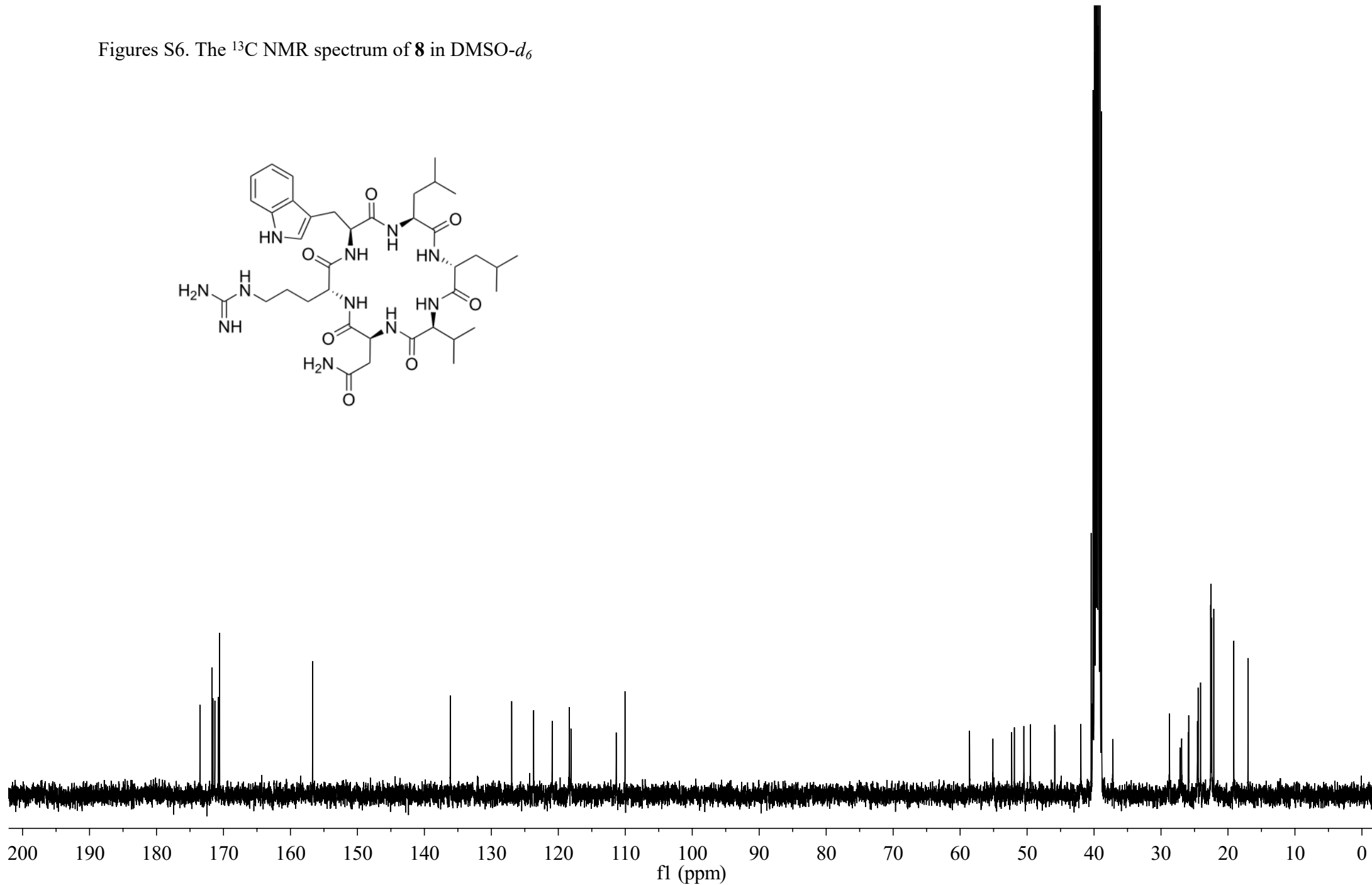
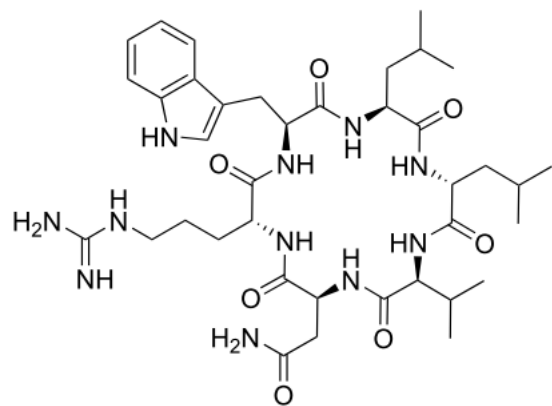


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Figures S5. The ^1H NMR spectrum of **8** in $\text{DMSO-}d_6$



Figures S6. The ^{13}C NMR spectrum of **8** in $\text{DMSO-}d_6$



Figures S7. The HRESIMS spectrum of **9**

Mass Spectrum SmartFormula Report

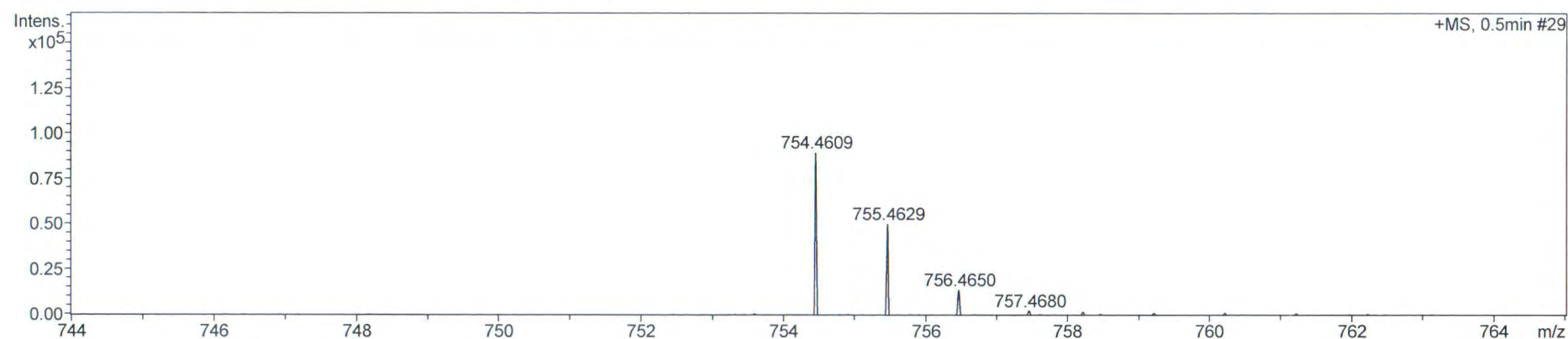
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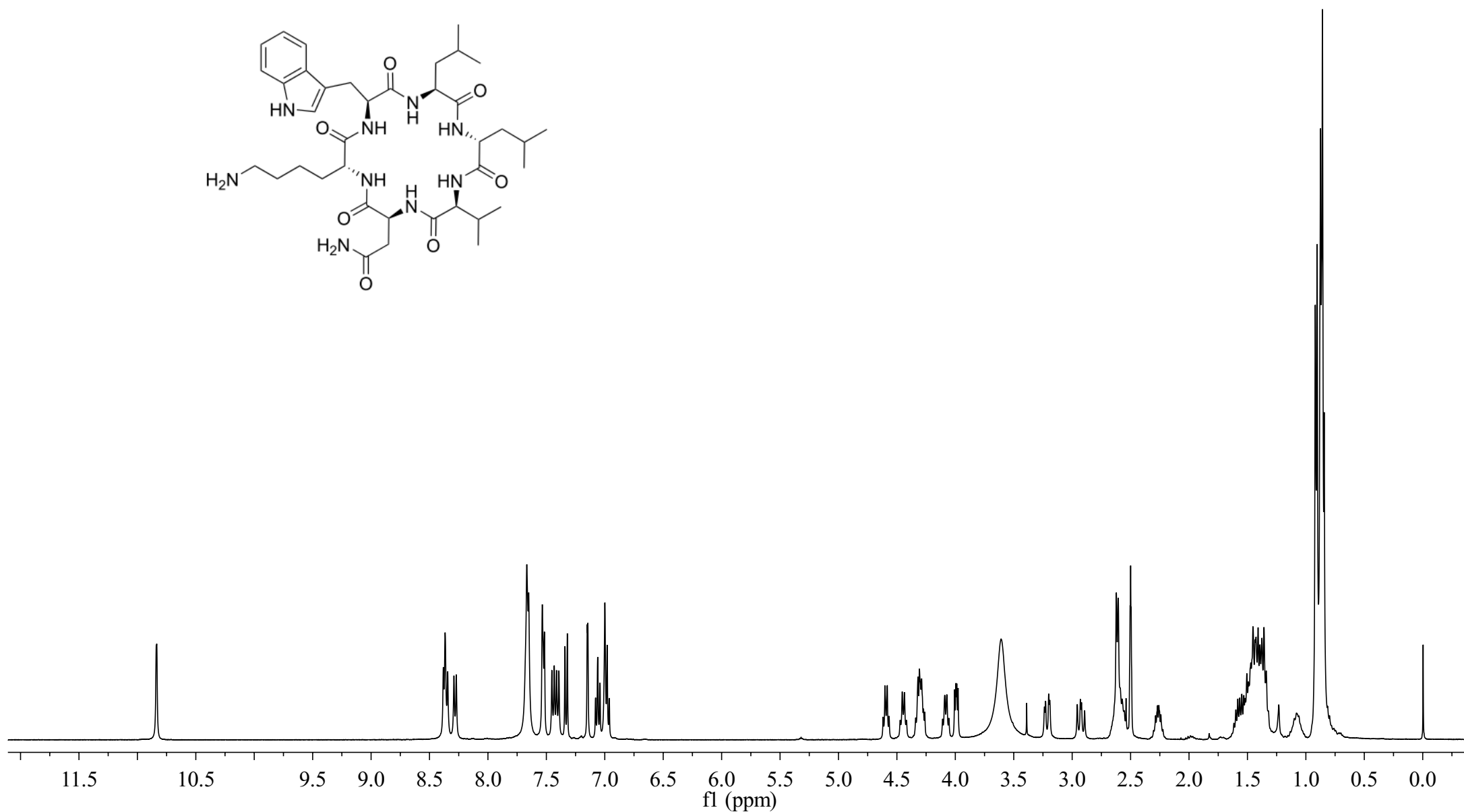
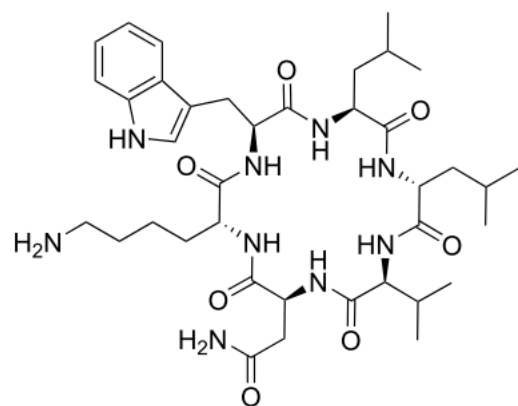
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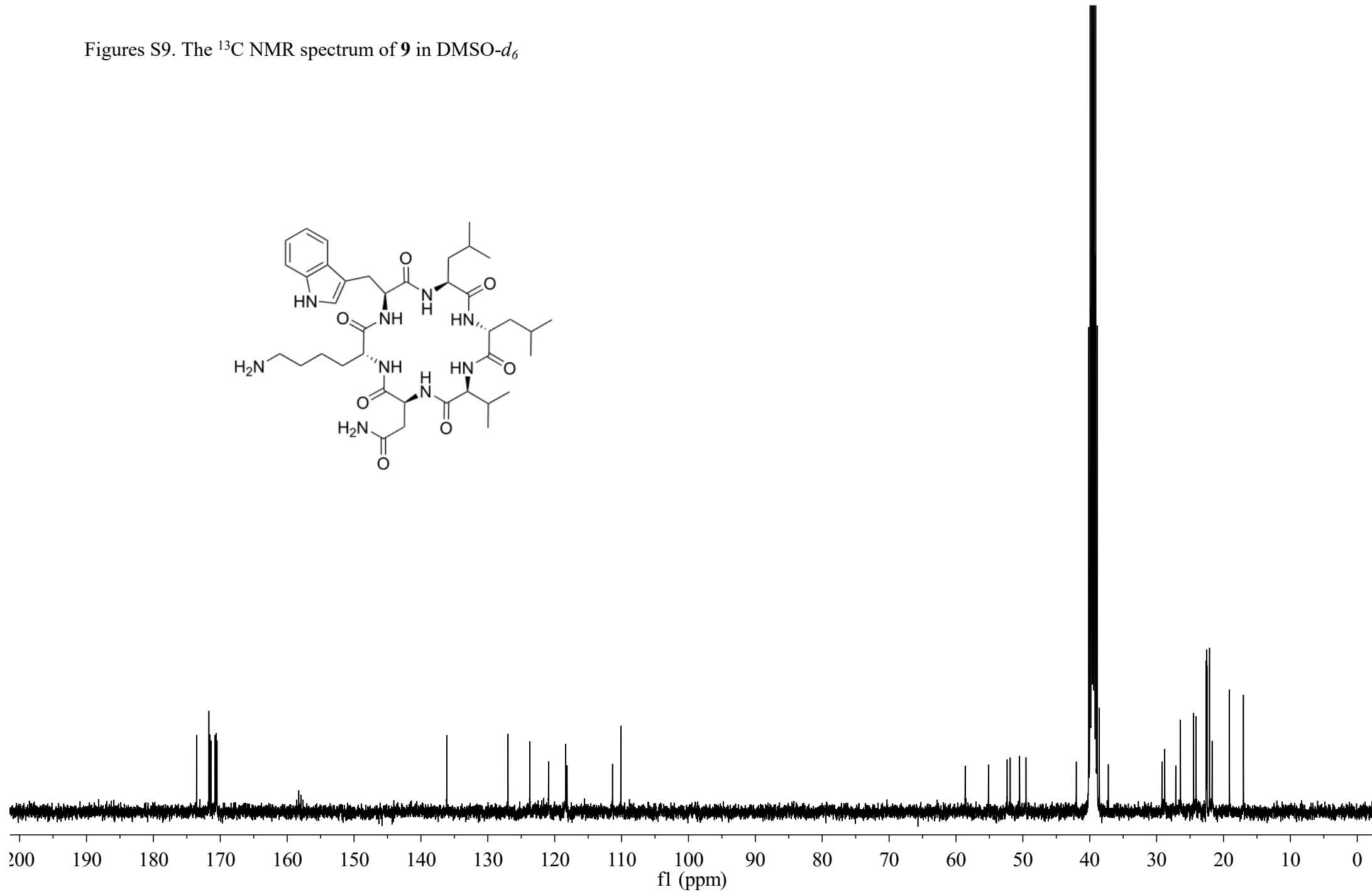
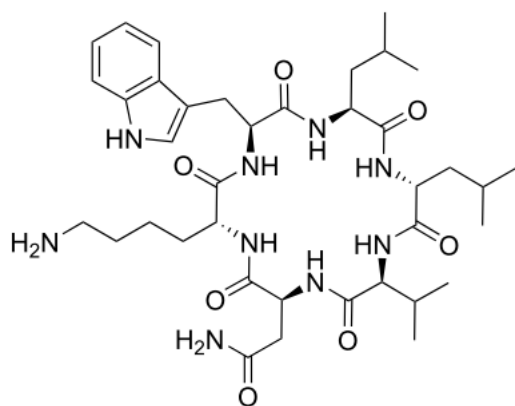


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754.4609	1	C ₃₈ H ₆₀ N ₉ O ₇	100.00	754.4610	-0.1	-0.1	57.0	13.5	even	ok

Figures S8. The ^1H NMR spectrum of **9** in $\text{DMSO}-d_6$



Figures S9. The ^{13}C NMR spectrum of **9** in $\text{DMSO-}d_6$



Figures S10. The HRESIMS spectrum of **10**

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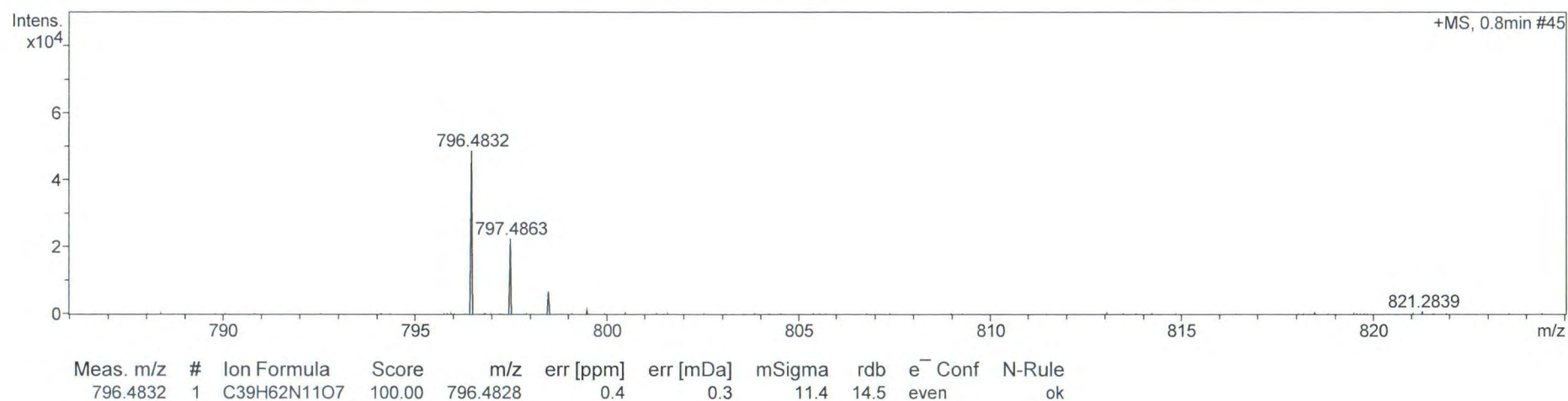
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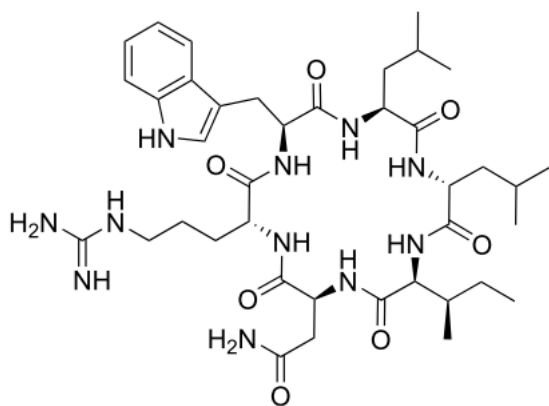
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CC(C)C[C@H](C(=O)N[C@@H](C(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)N[C@@H](CCCCNC(=N)N)C(=O)N[C@@H](CC(=O)N)C(=O)N[C@@H](C)C)C(=O)N

C[C@H](C)[C@@H](NC(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)NCC[C@H](N)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)NCCC(N)=N

Figures S13. The HRESIMS spectrum of **11**

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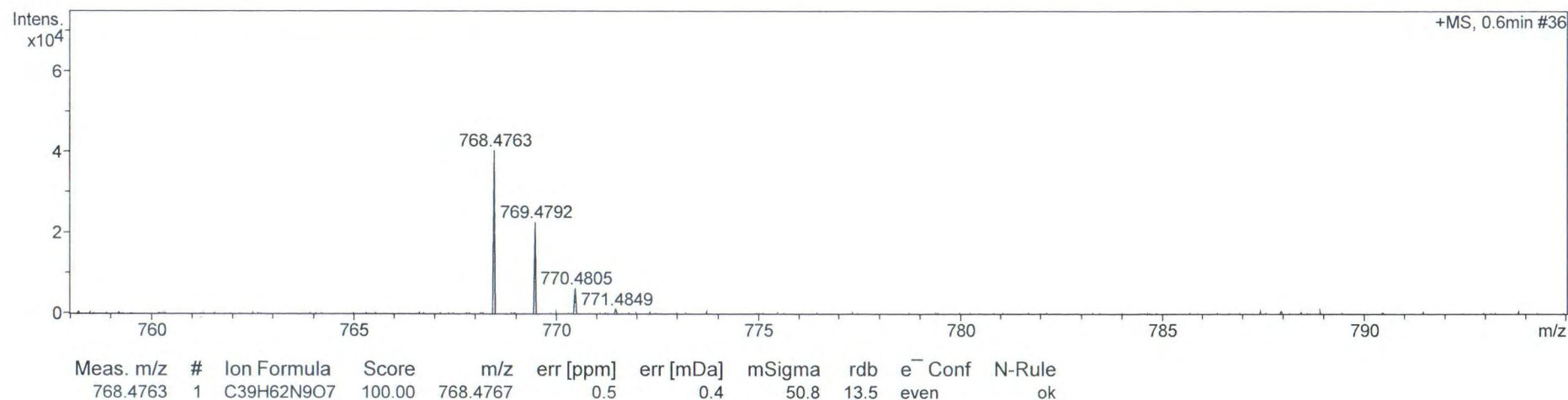
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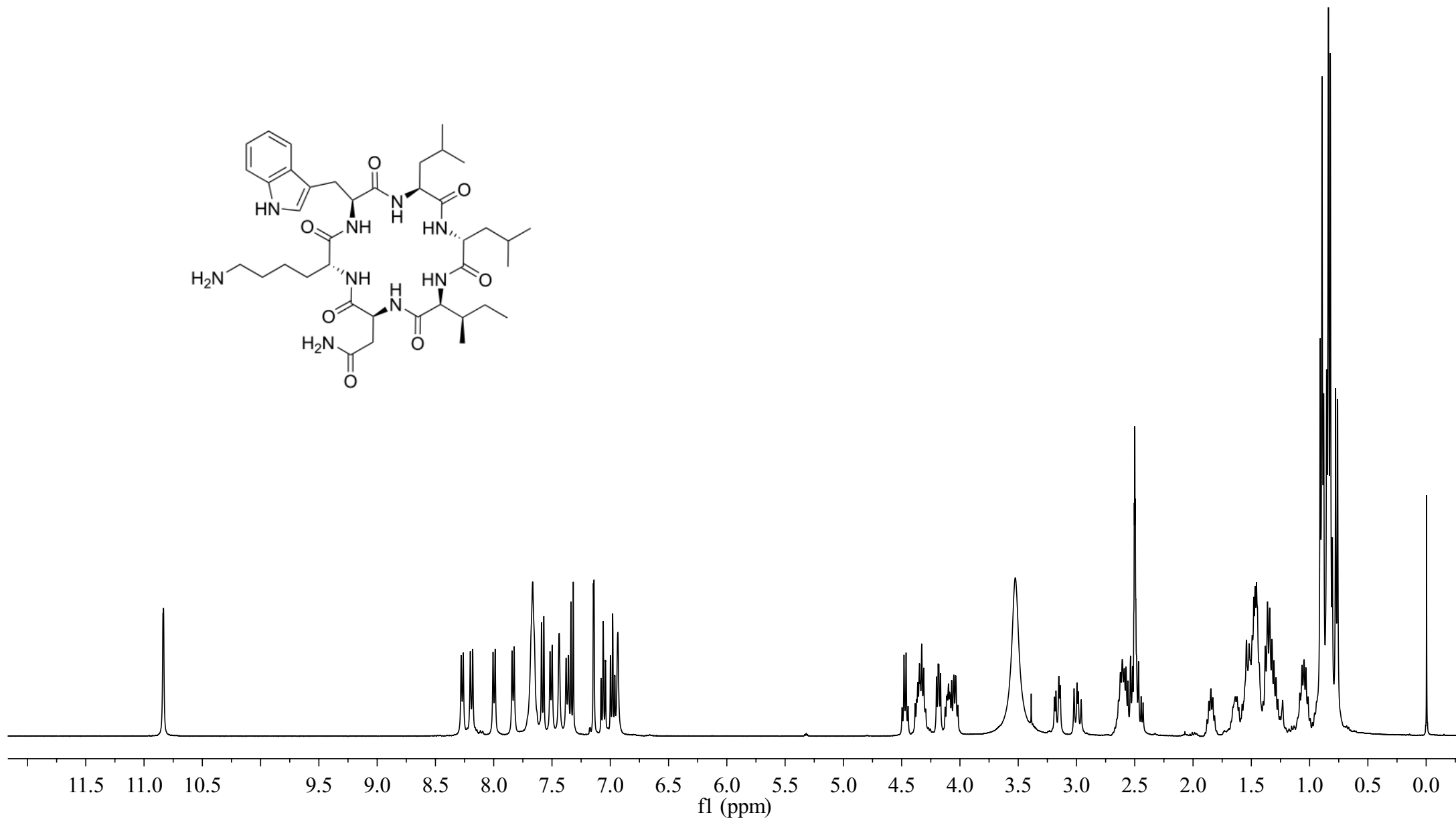
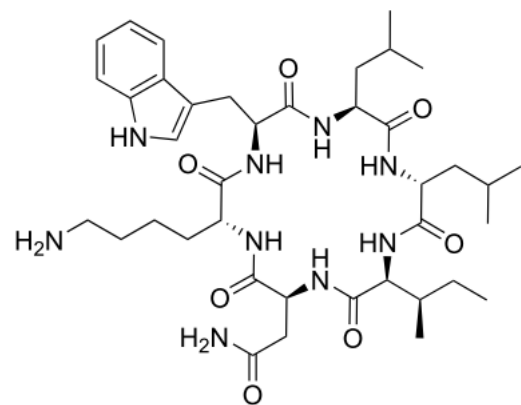
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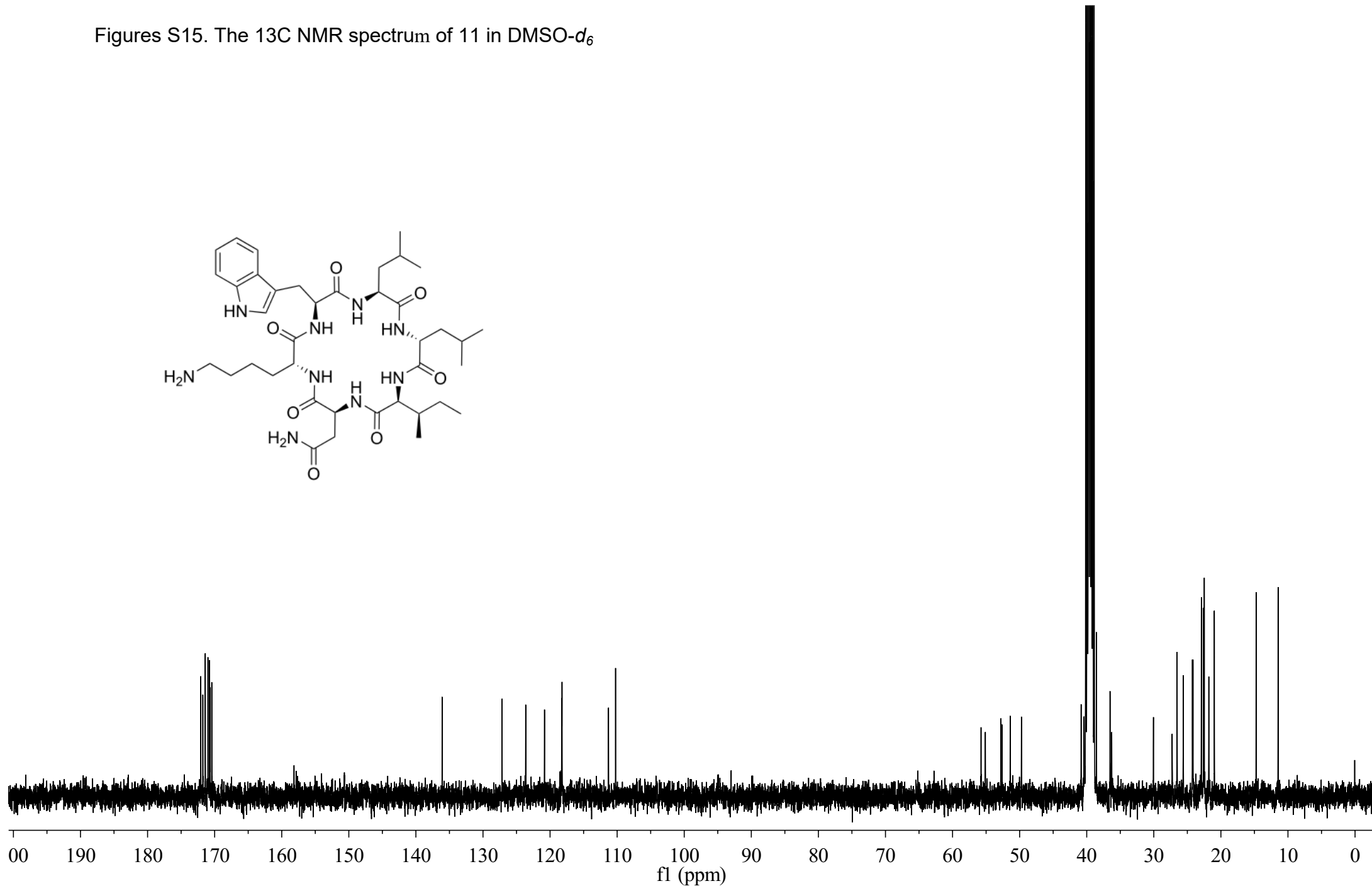
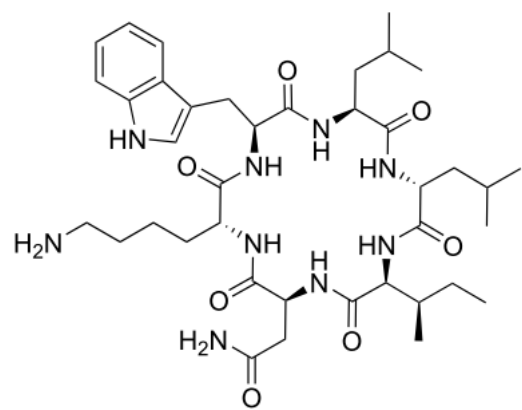
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Figures S14. The ^1H NMR spectrum of **11** in $\text{DMSO-}d_6$



Figures S15. The ^{13}C NMR spectrum of 11 in $\text{DMSO}-d_6$



Figures S16. The HRESIMS spectrum of **12**

Mass Spectrum SmartFormula Report

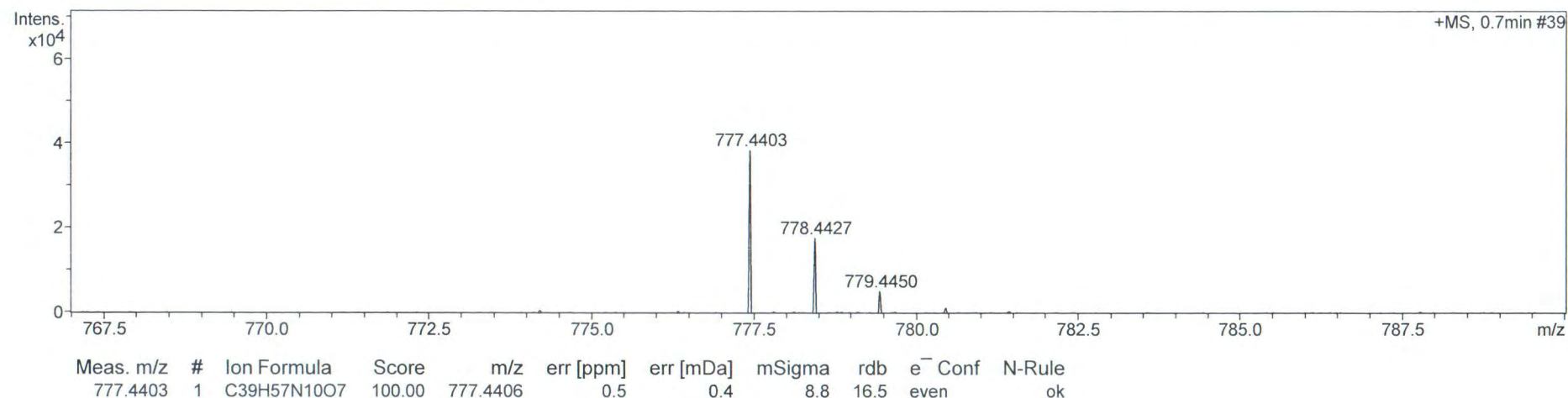
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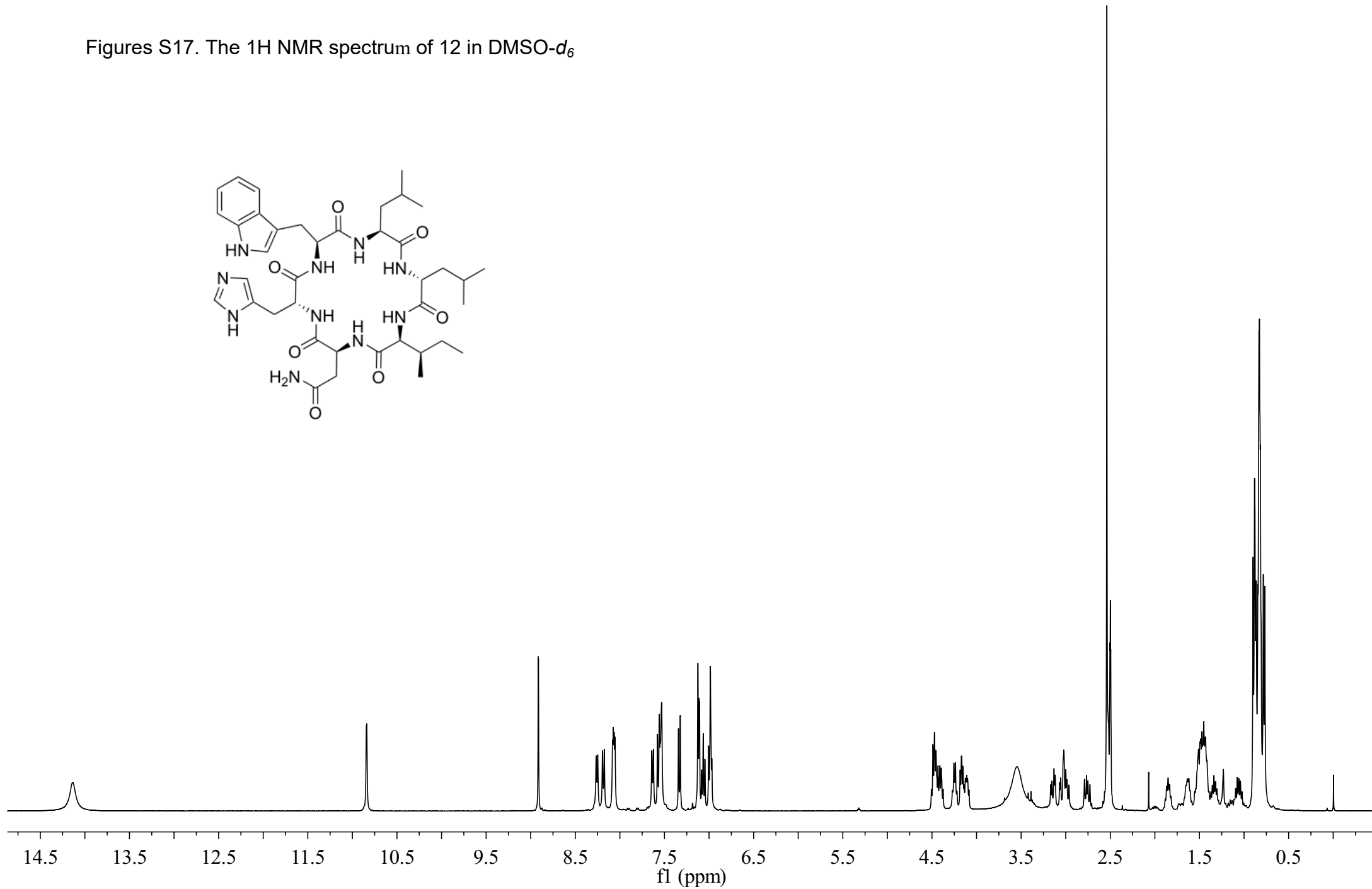
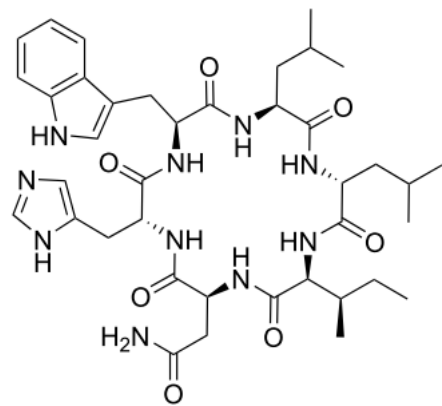
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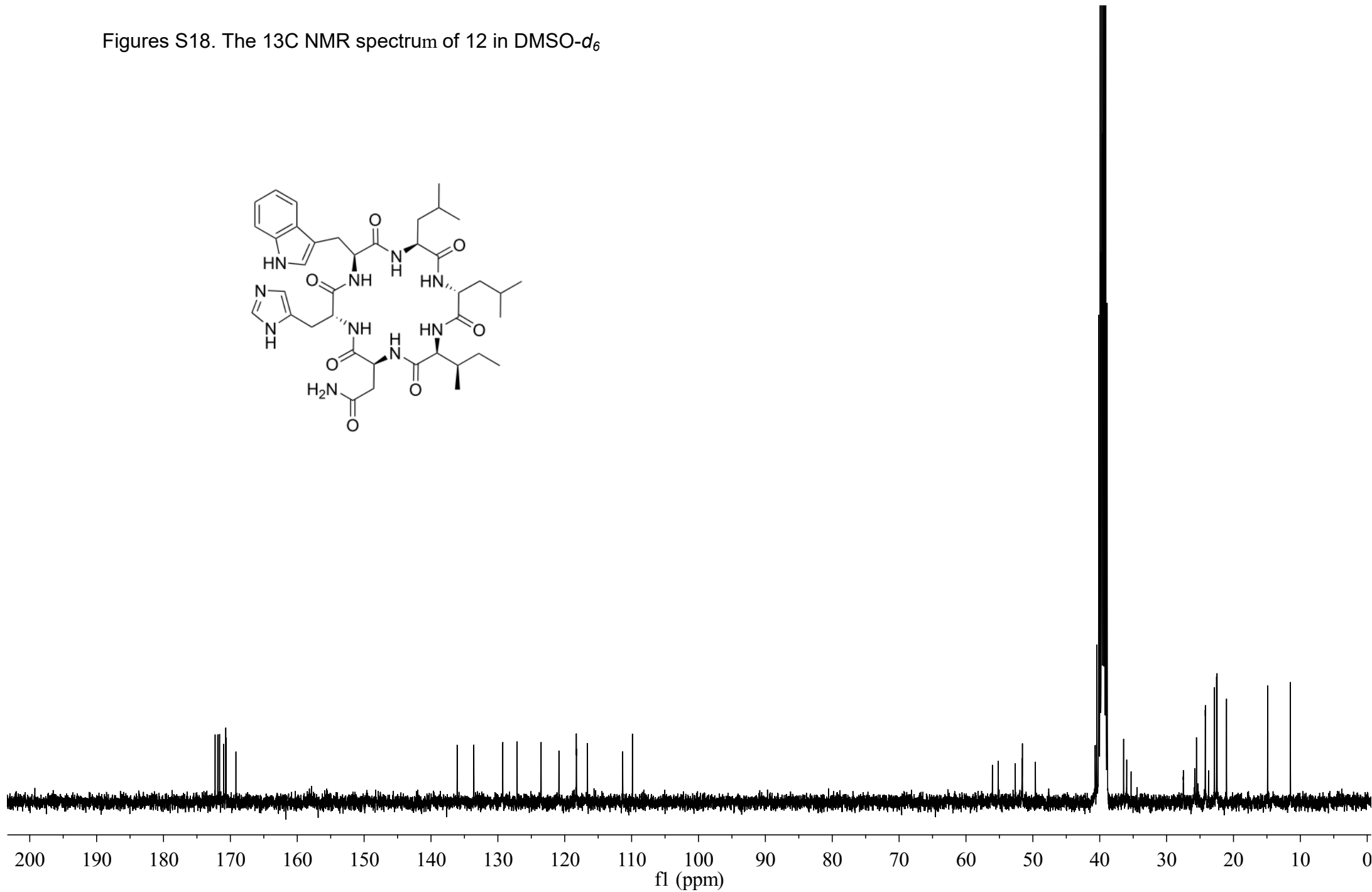
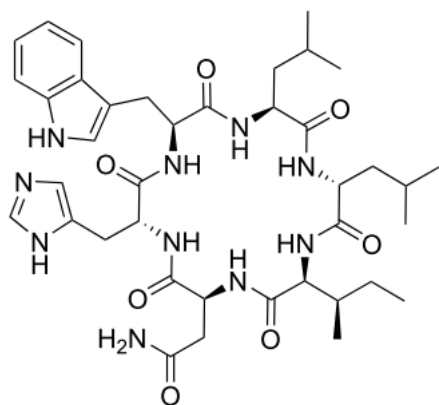
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		Set Corona	0 nA	Set APCI Heater	0 °C



Figures S17. The ^1H NMR spectrum of 12 in $\text{DMSO-}d_6$



Figures S18. The ^{13}C NMR spectrum of 12 in $\text{DMSO}-d_6$



Figures S19. The HRESIMS spectrum of **13**

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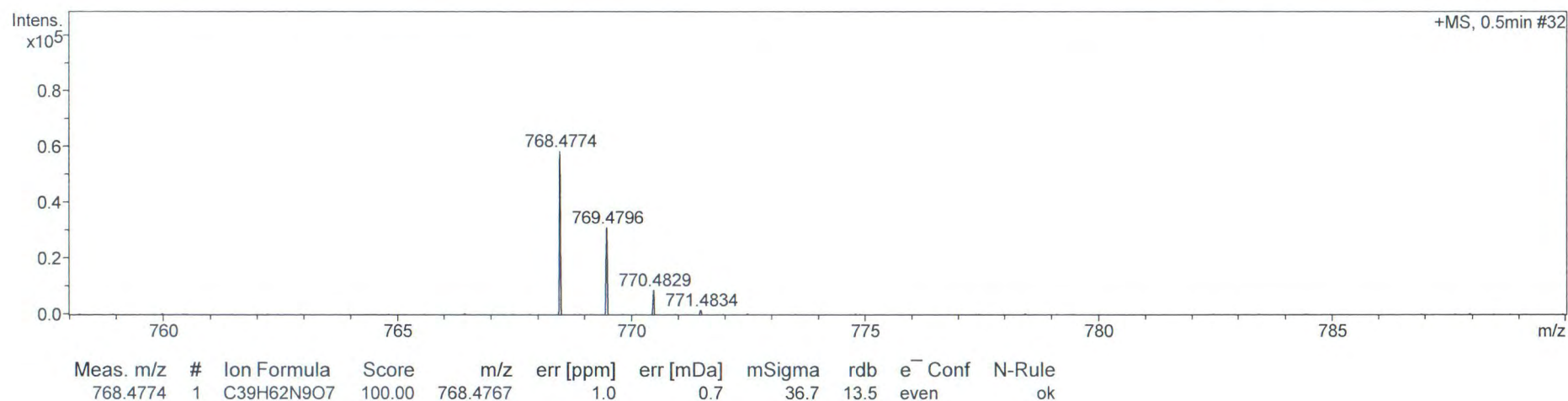
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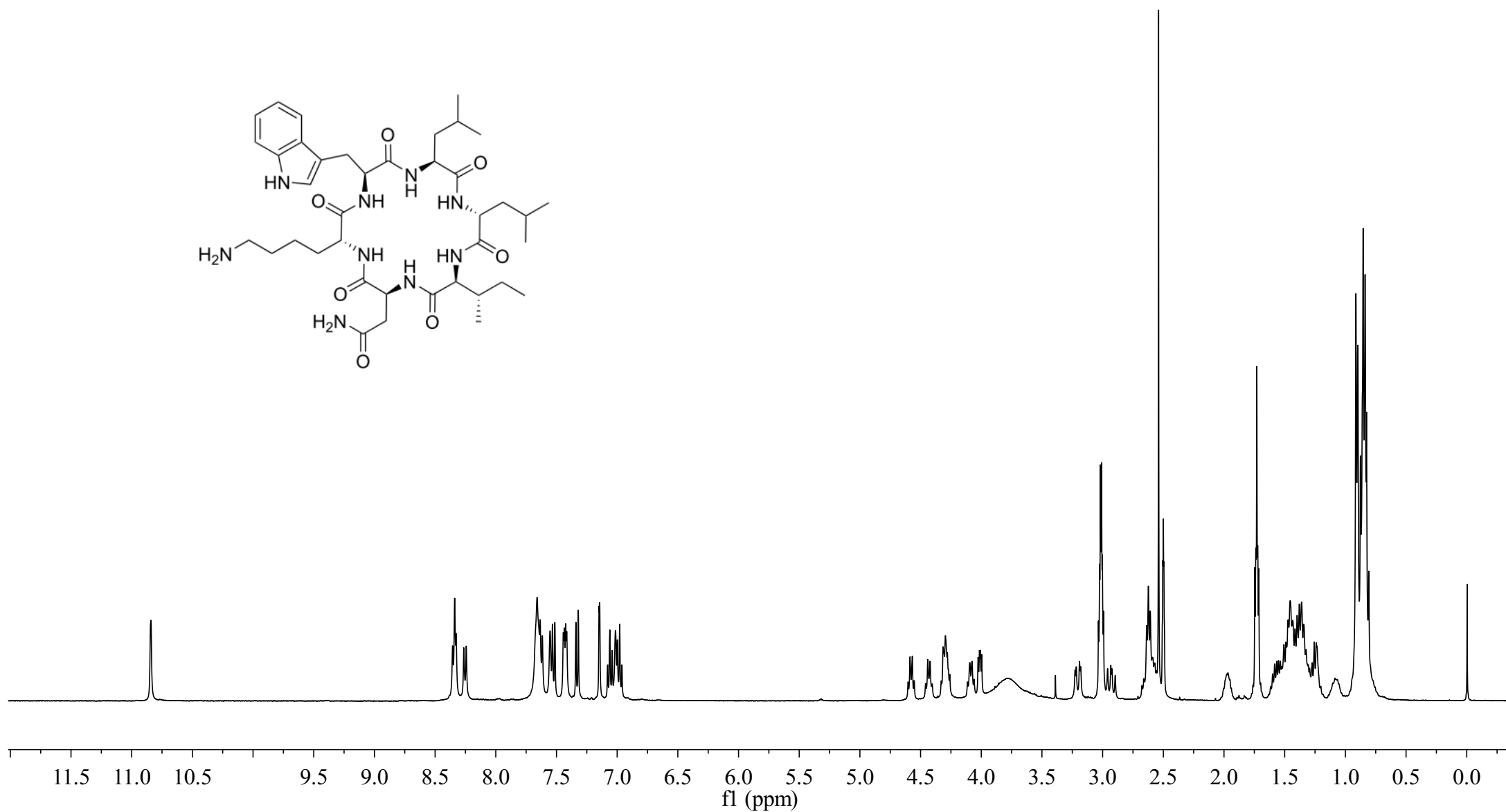
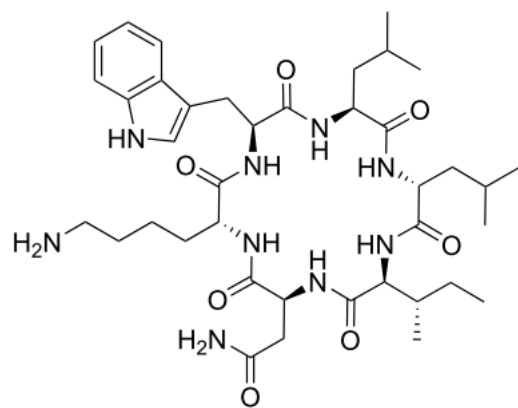
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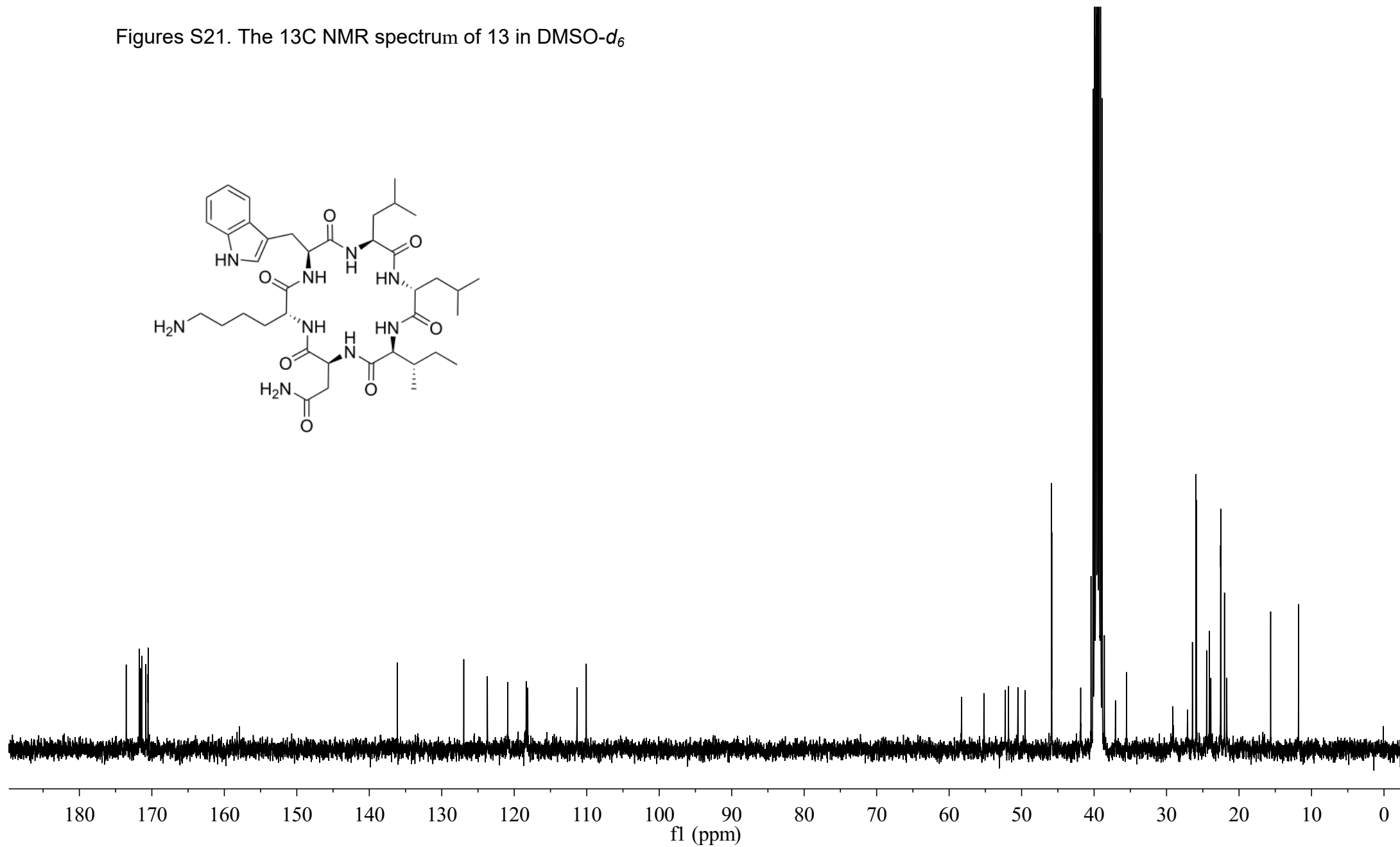
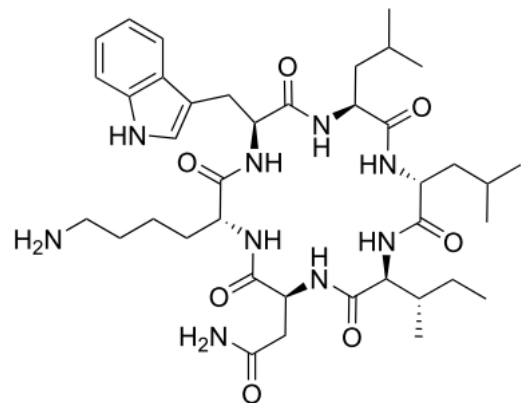
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Page 1 of 1

Figures S20. The ^1H NMR spectrum of 13 in $\text{DMSO}-d_6$



Figures S21. The ^{13}C NMR spectrum of 13 in $\text{DMSO}-d_6$



Figures S22. The HRESIMS spectrum of **14**

Mass Spectrum SmartFormula Report

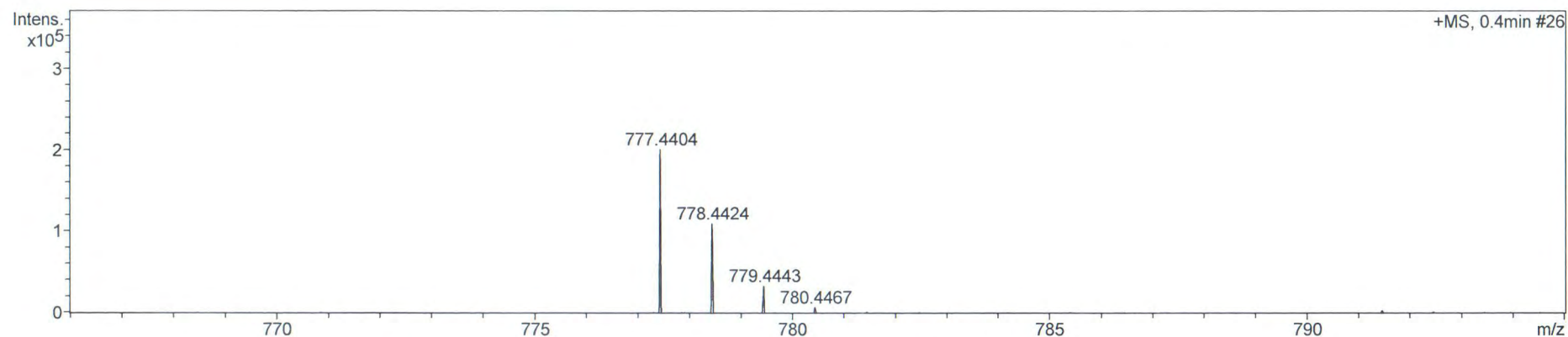
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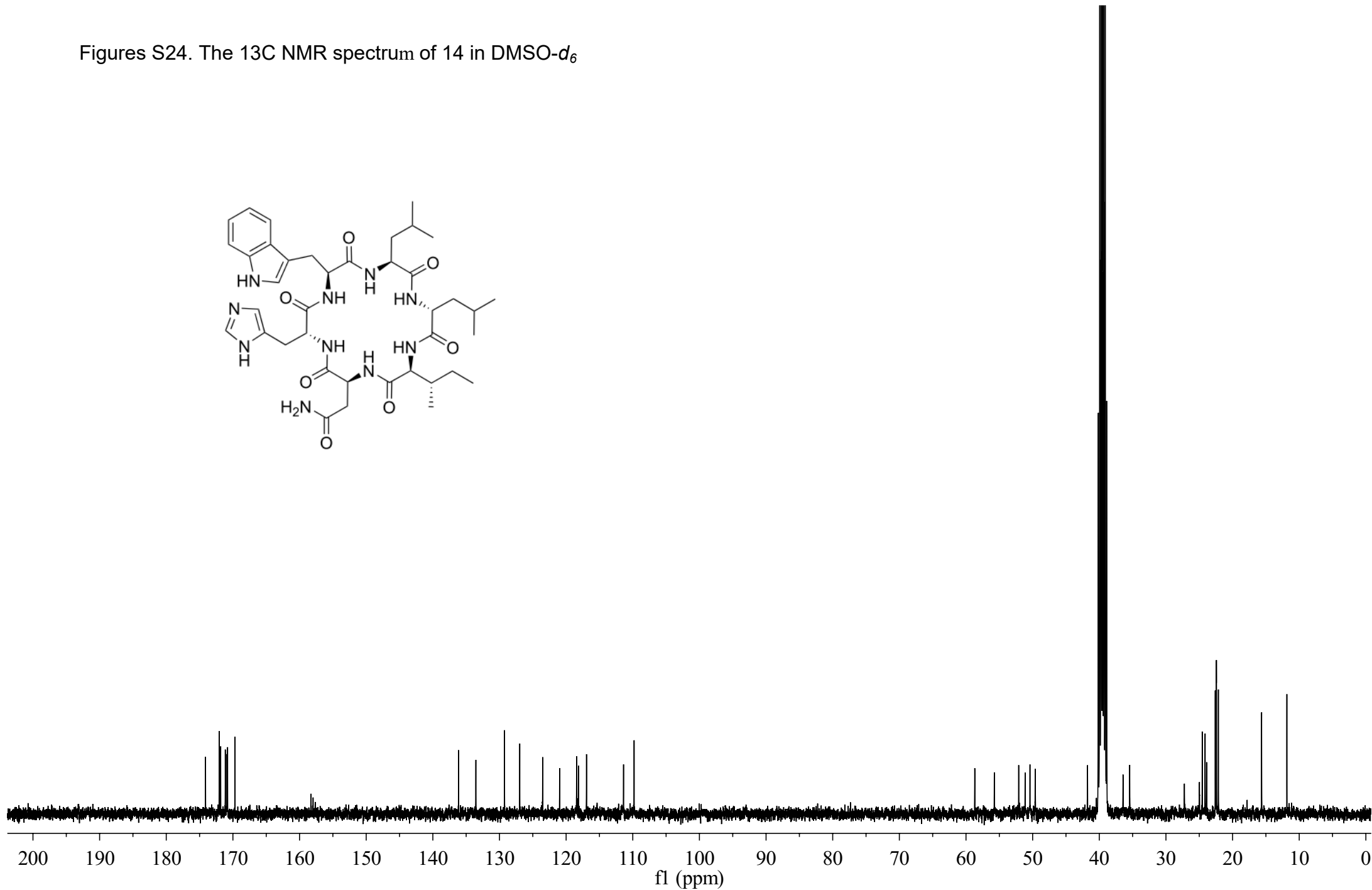
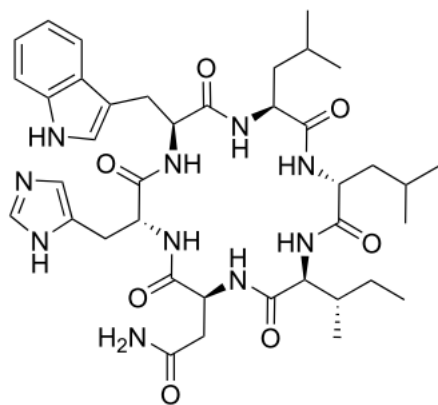
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777.4404	1	C39H57N10O7	100.00	777.4406	0.3	0.2	45.5	16.5	even	ok

[illegible]

Figures S24. The ^{13}C NMR spectrum of 14 in $\text{DMSO-}d_6$



Figures S25. The HRESIMS spectrum of **15**

Mass Spectrum SmartFormula Report

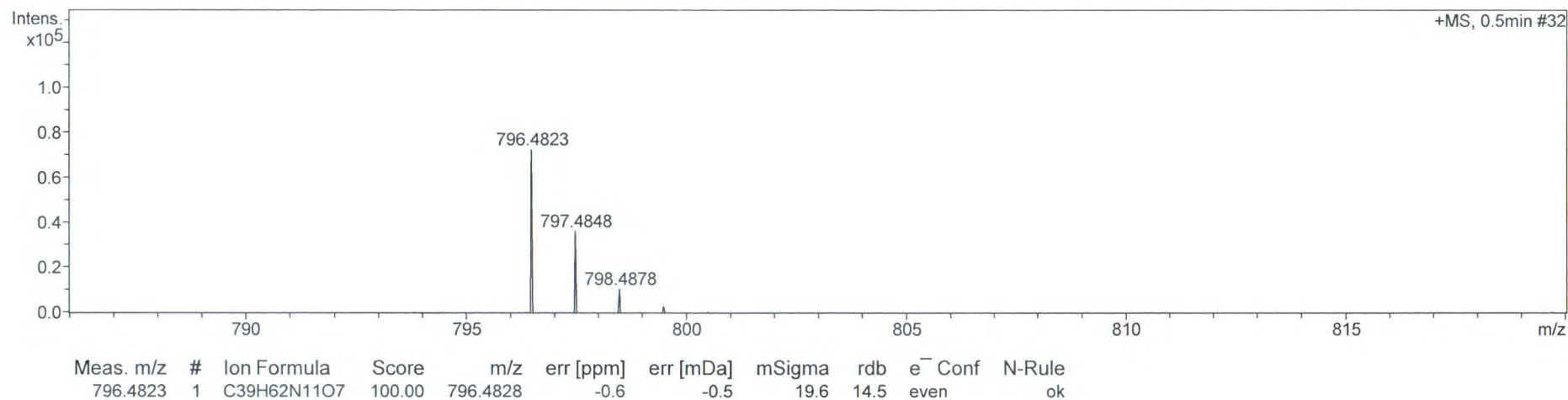
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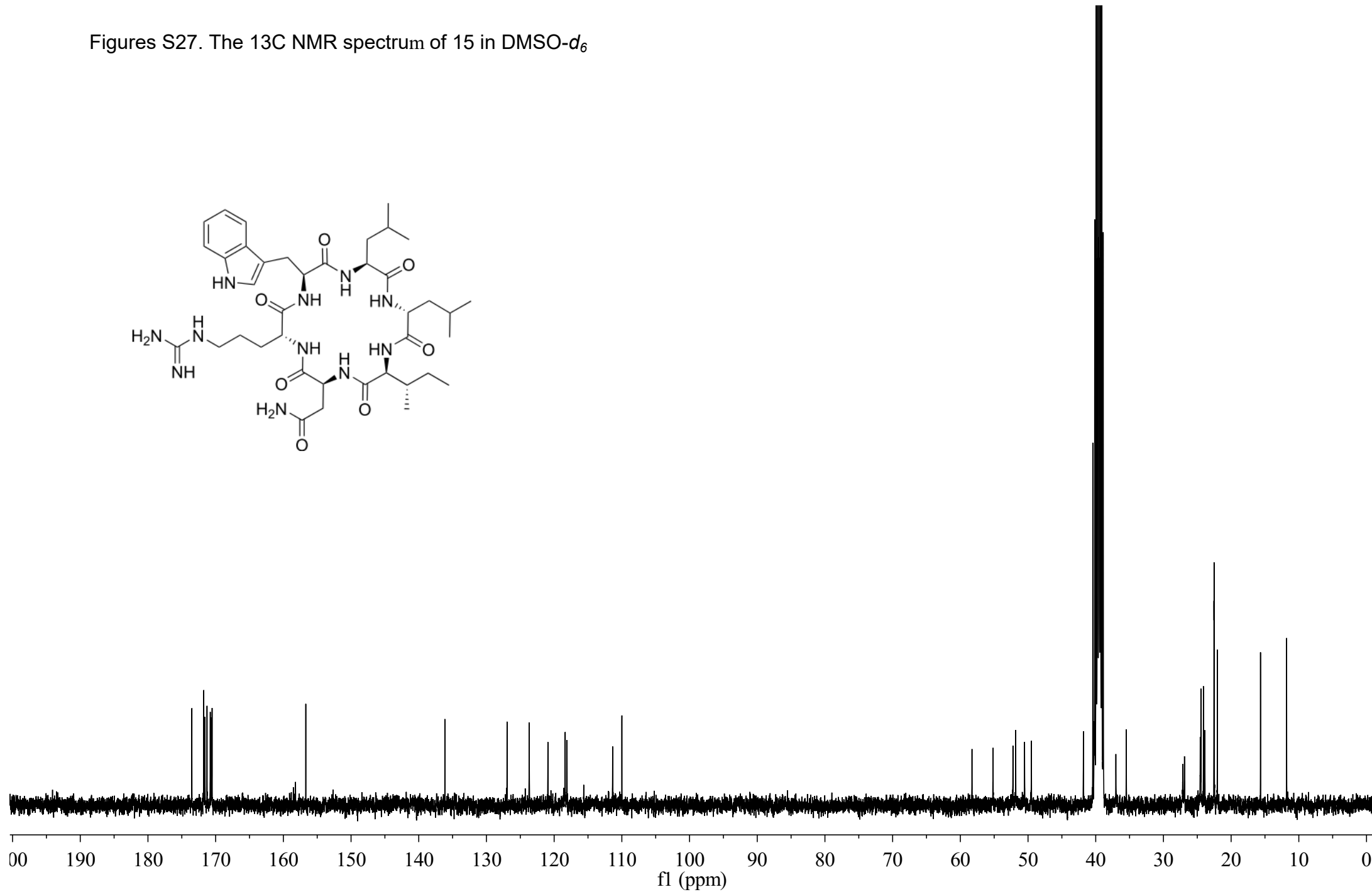
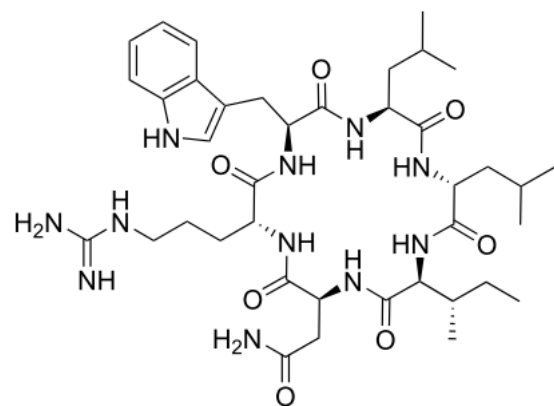
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[illegible]

Figures S27. The ^{13}C NMR spectrum of 15 in $\text{DMSO}-d_6$



Figures S28. The HRESIMS spectrum of **16**

Mass Spectrum SmartFormula Report

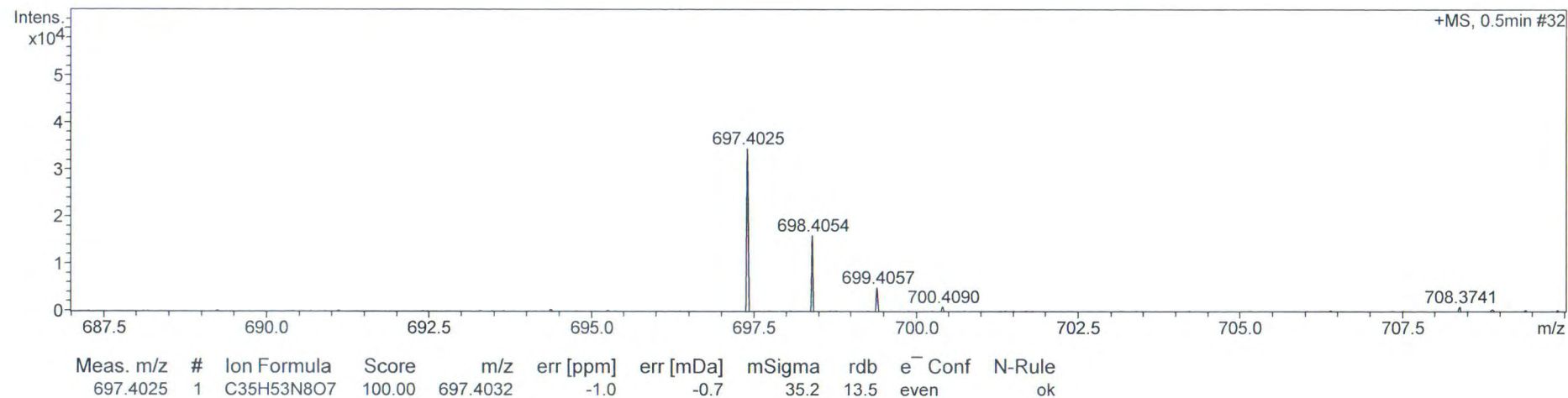
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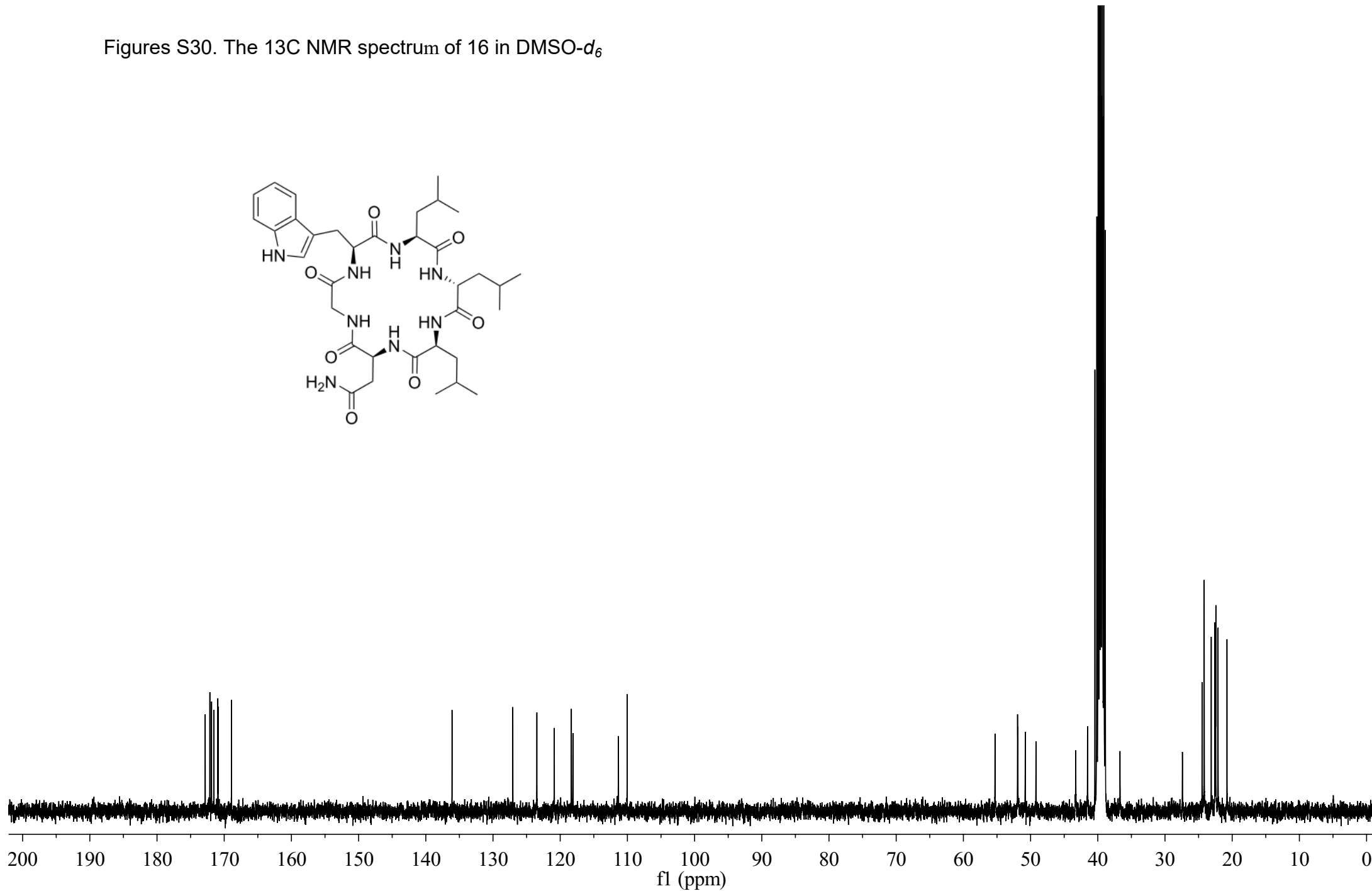
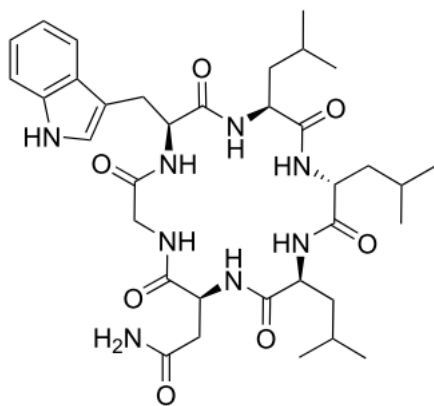
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		Set Corona	0 nA	Set APCI Heater	0 °C



C[C@H](C)CC(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)NC(=O)[C@H](C)CC(C)C

Figures S30. The ^{13}C NMR spectrum of 16 in $\text{DMSO-}d_6$



Figures S31. The HRESIMS spectrum of **17**

Mass Spectrum SmartFormula Report

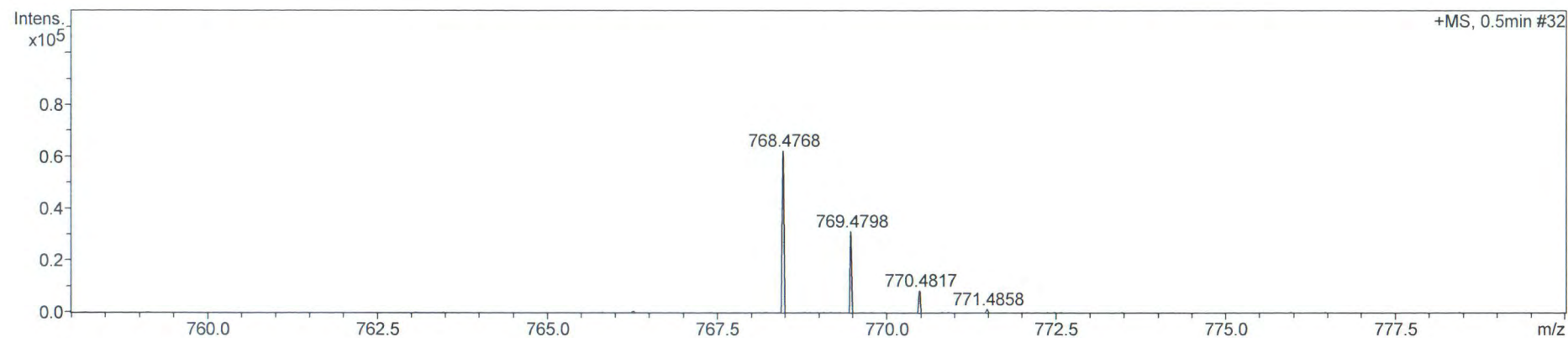
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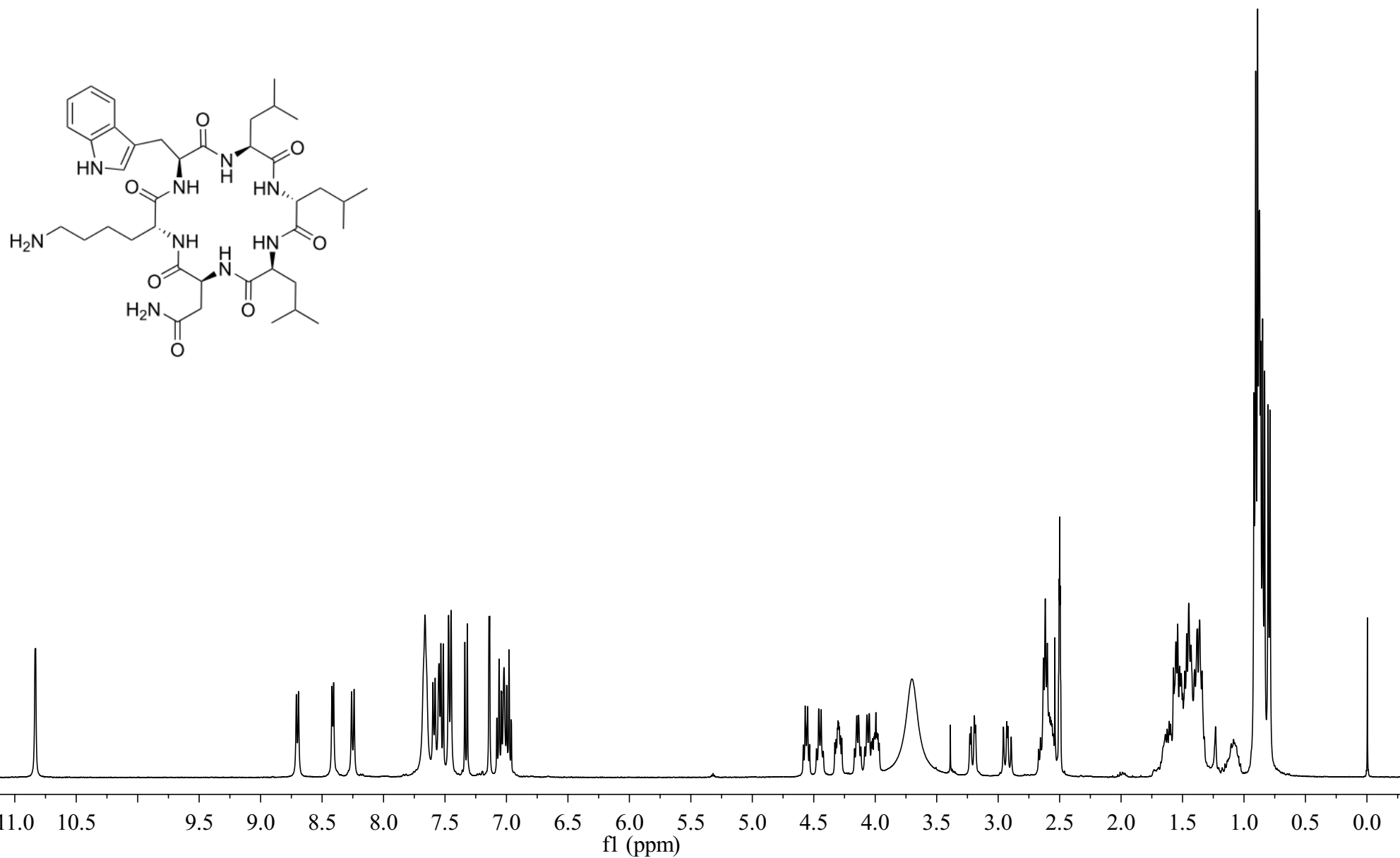
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		Set Corona	0 nA	Set APCI Heater	0 °C

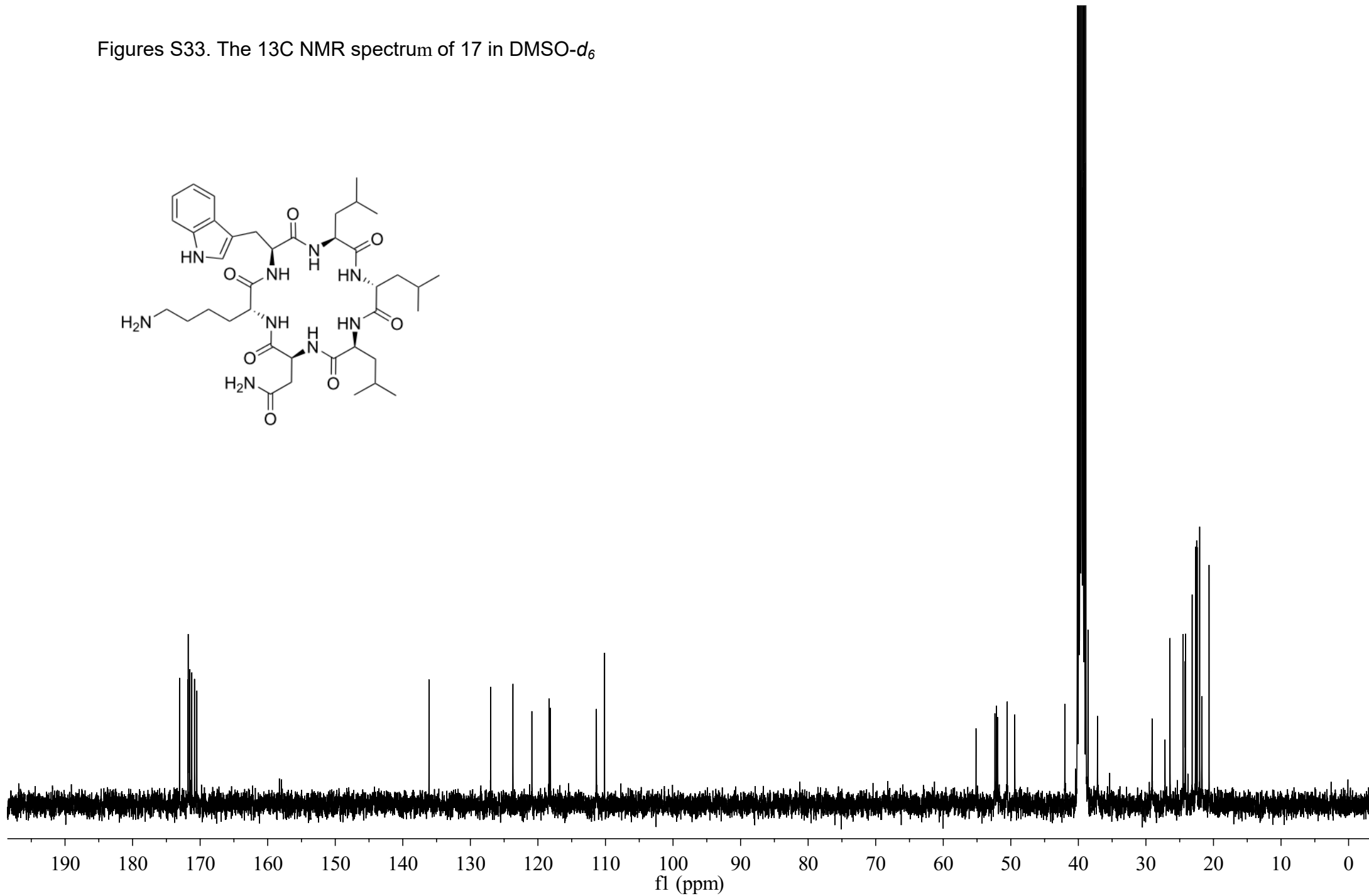
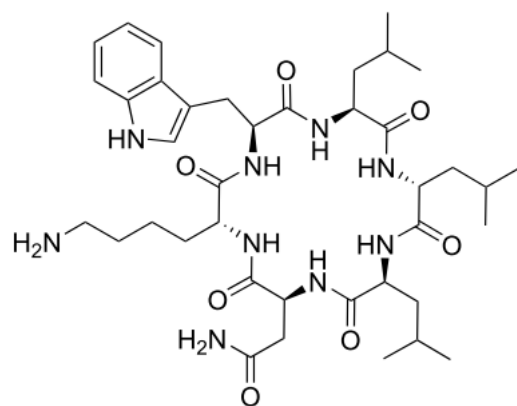


Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdB	e ⁻ Conf	N-Rule
768.4768	1	C39H62N9O7	100.00	768.4767	0.1	0.1	20.2	13.5	even	ok

Figures S32. The ^1H NMR spectrum of 17 in $\text{DMSO-}d_6$



Figures S33. The ^{13}C NMR spectrum of 17 in $\text{DMSO}-d_6$



Figures S34. The HRESIMS spectrum of **18**

Mass Spectrum SmartFormula Report

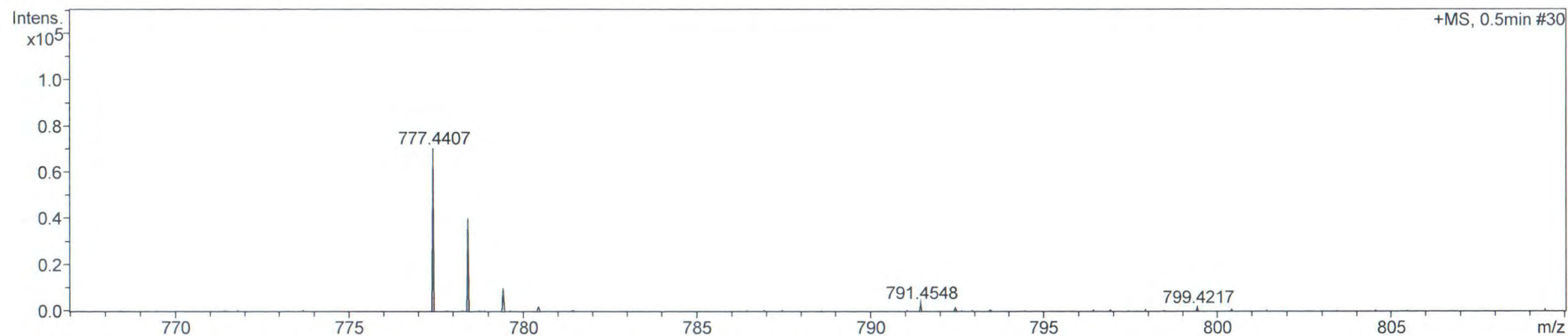
Analysis Info

Analysis Name D:\Data\MS\data\202102\liqinglian_A10_pos_60_01_10001.d
 Method LC_Direct Infusion_pos_100-1000mz.m
 Sample Name liqinglian_A10_pos
 Comment

Acquisition Date 2/8/2021 3:10:24 PM
 Operator SCSIO
 Instrument maXis 255552.00029

Acquisition Parameter

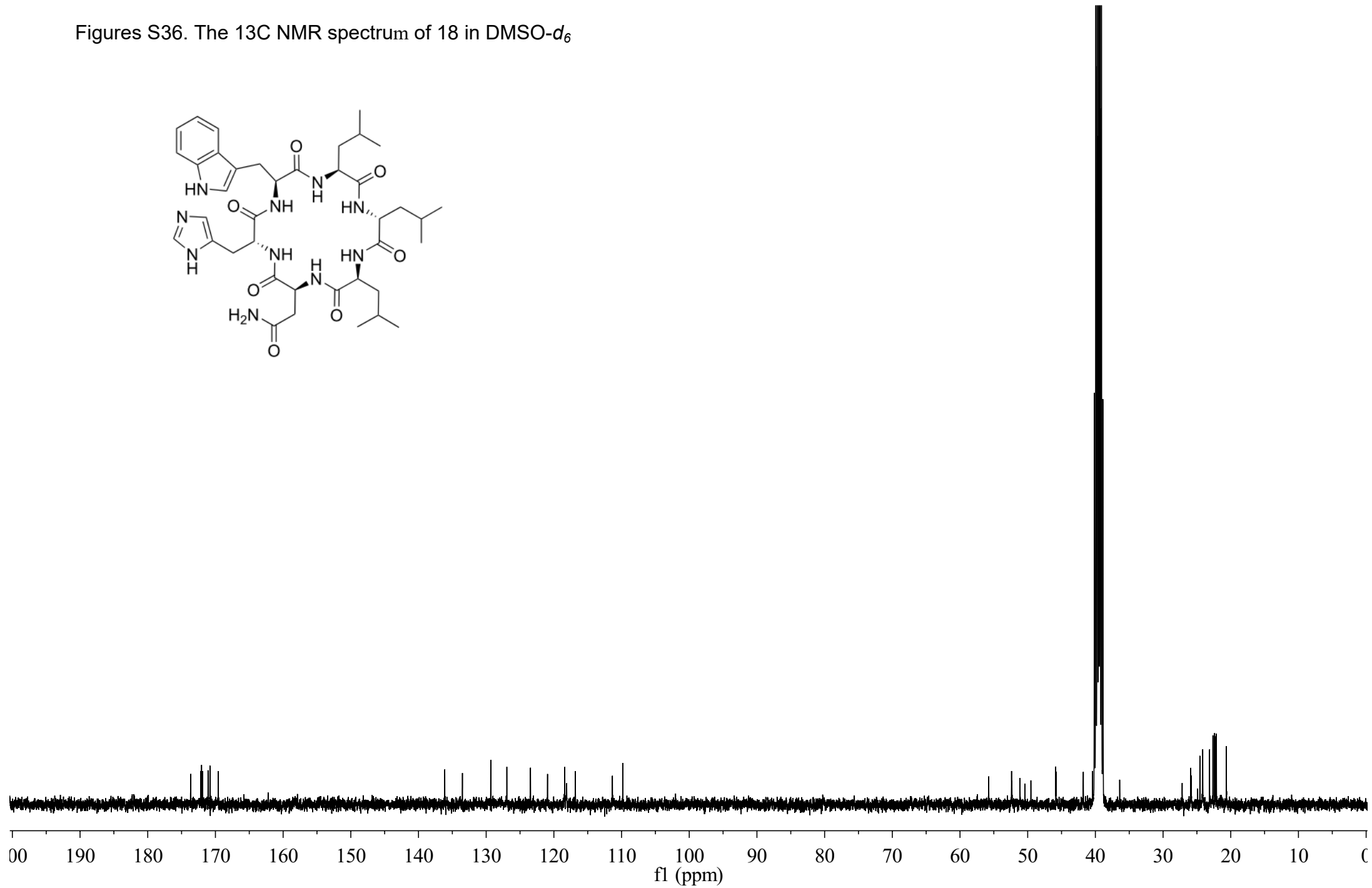
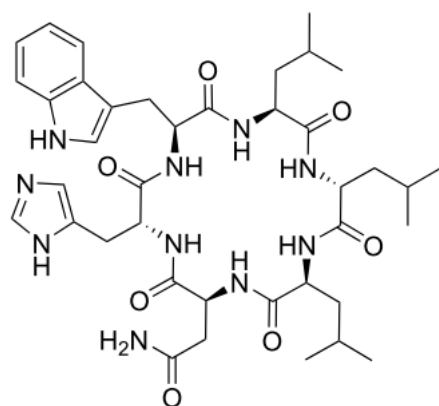
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
777.4407	1	C39H57N10O7	100.00	777.4406	-0.1	-0.1	53.4	16.5	even	ok
799.4217	1	C39H56N10NaO7	100.00	799.4226	1.1	0.8	40.7	16.5	even	ok

[illegible]

Figures S36. The ^{13}C NMR spectrum of 18 in $\text{DMSO-}d_6$



Figures S37. The HRESIMS spectrum of **19**

Mass Spectrum SmartFormula Report

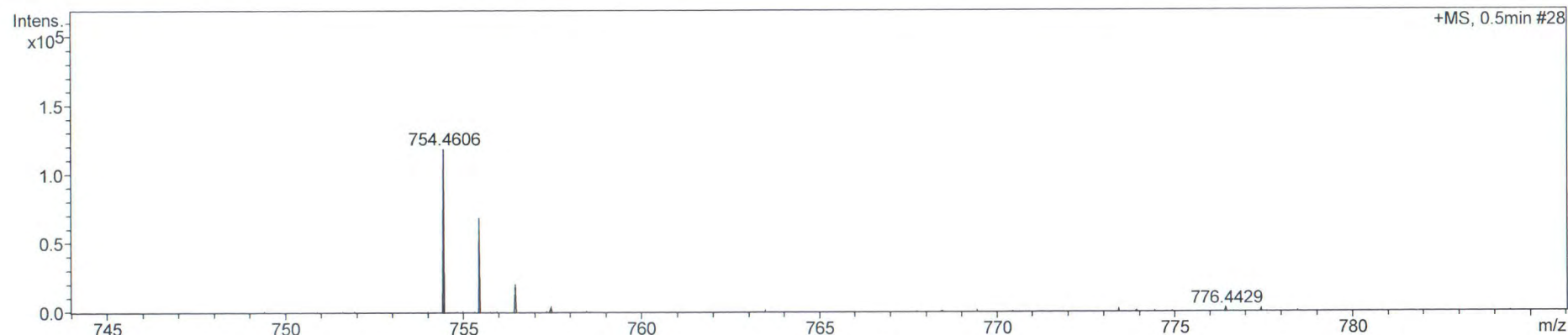
Analysis Info

Analysis Name D:\Data\MS\data\202102\liqinglian_A11_pos_45_01_10002.d
 Method LC_Direct Infusion_pos_100-1000mz.m
 Sample Name liqinglian_A11_pos
 Comment

Acquisition Date 2/8/2021 3:13:53 PM
 Operator SCSIO
 Instrument maXis 255552.00029

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
754.4606	1	C38H60N9O7	100.00	754.4610	-0.6	-0.4	69.8	13.5	even	ok
776.4429	1	C38H59N9NaO7	100.00	776.4430	0.0	0.0	156.2	13.5	even	ok

Chemical structure of the compound is shown above the spectrum. The spectrum displays peaks corresponding to the structure, with a major peak around 1.0 ppm and several smaller peaks in the aromatic and aliphatic regions.

Figures S39. The ^{13}C NMR spectrum of 19 in $\text{DMSO-}d_6$

