

Supporting Information

Bile Acid Oligomers and their Combination with Antibiotics to Combat Microbial Infections

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²Department of Microbial Biotechnology, Panjab University, Chandigarh, 160014, India.

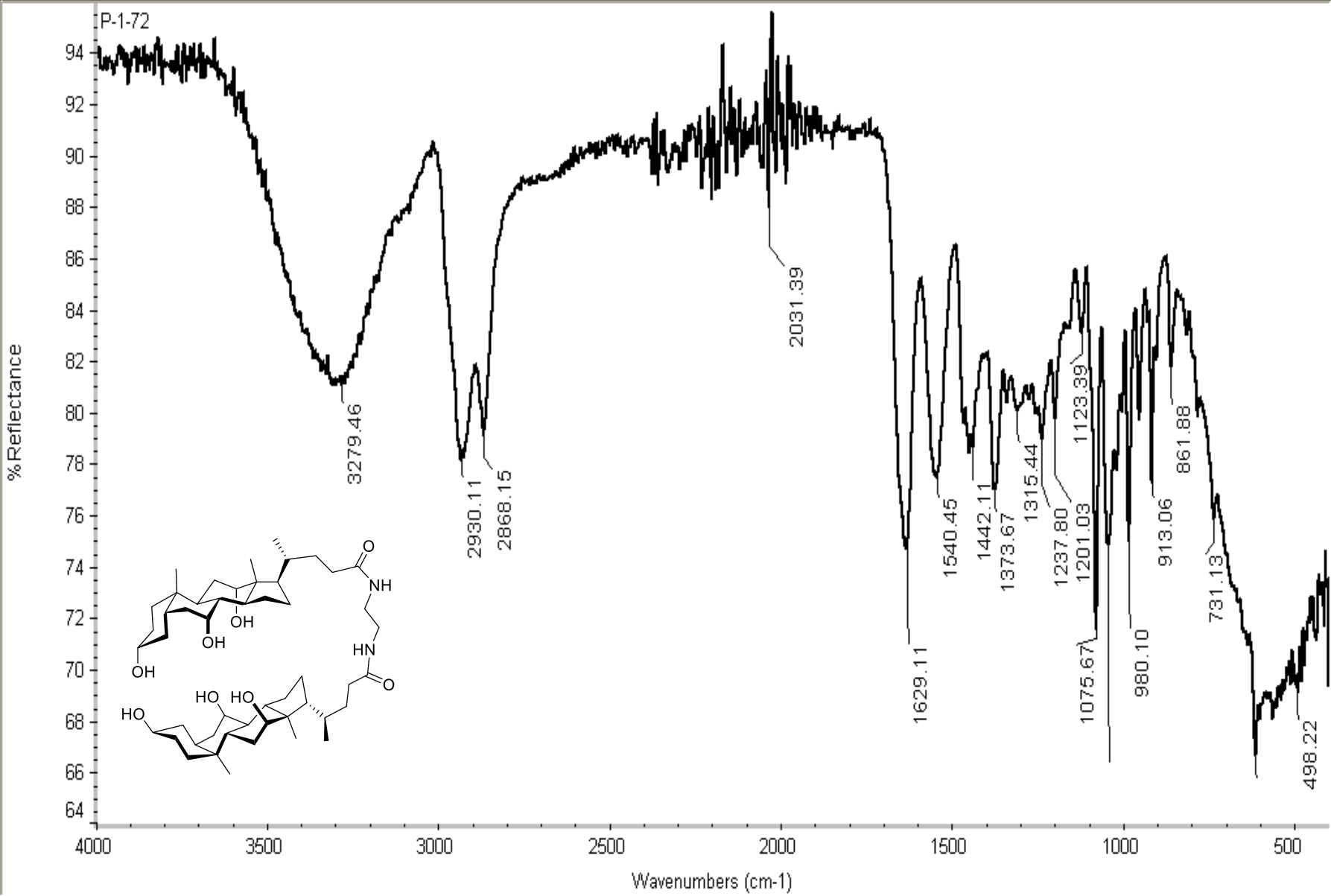
³Department of Biotechnology, Central University of Rajasthan, Ajmer, 305817, India.

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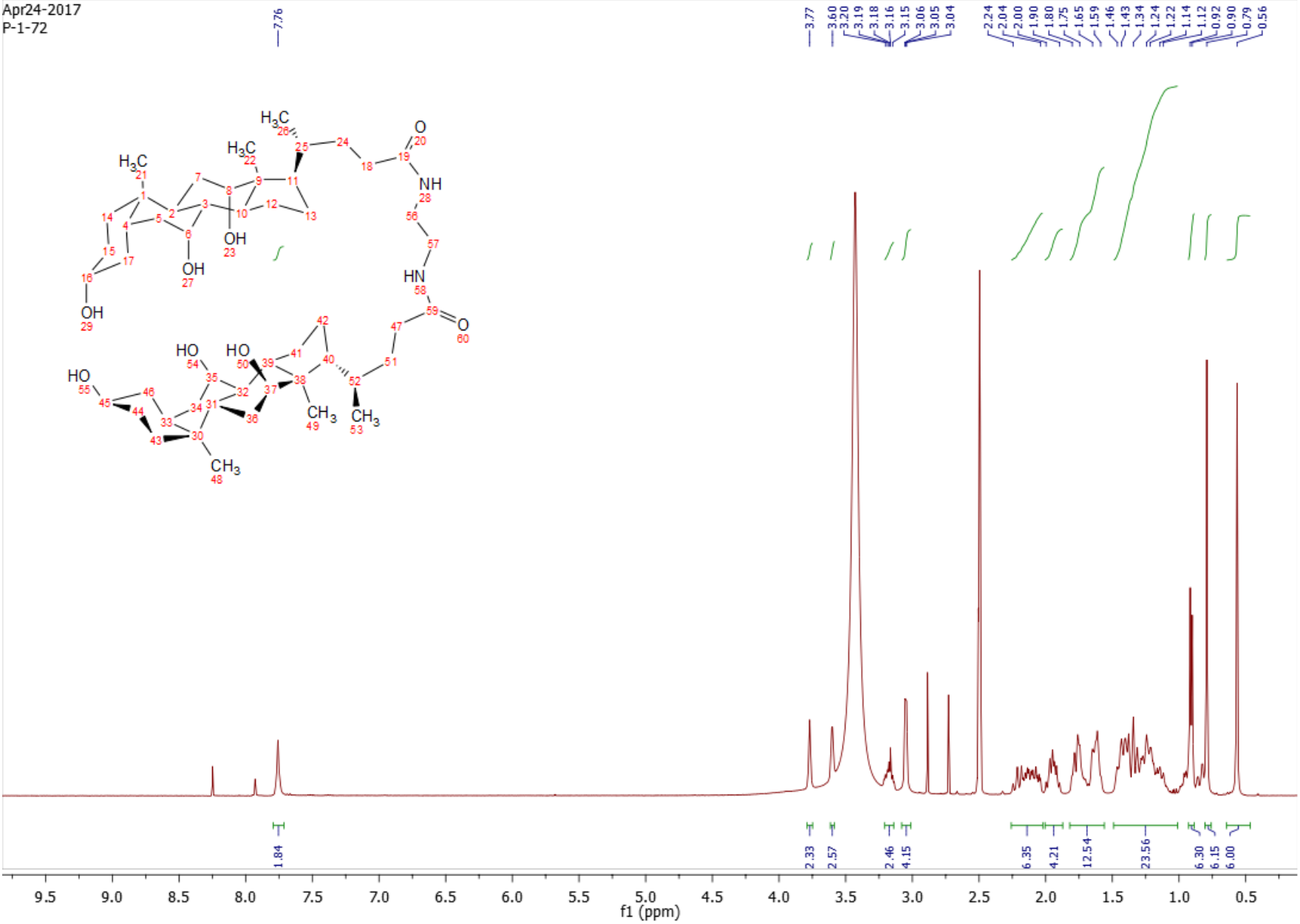
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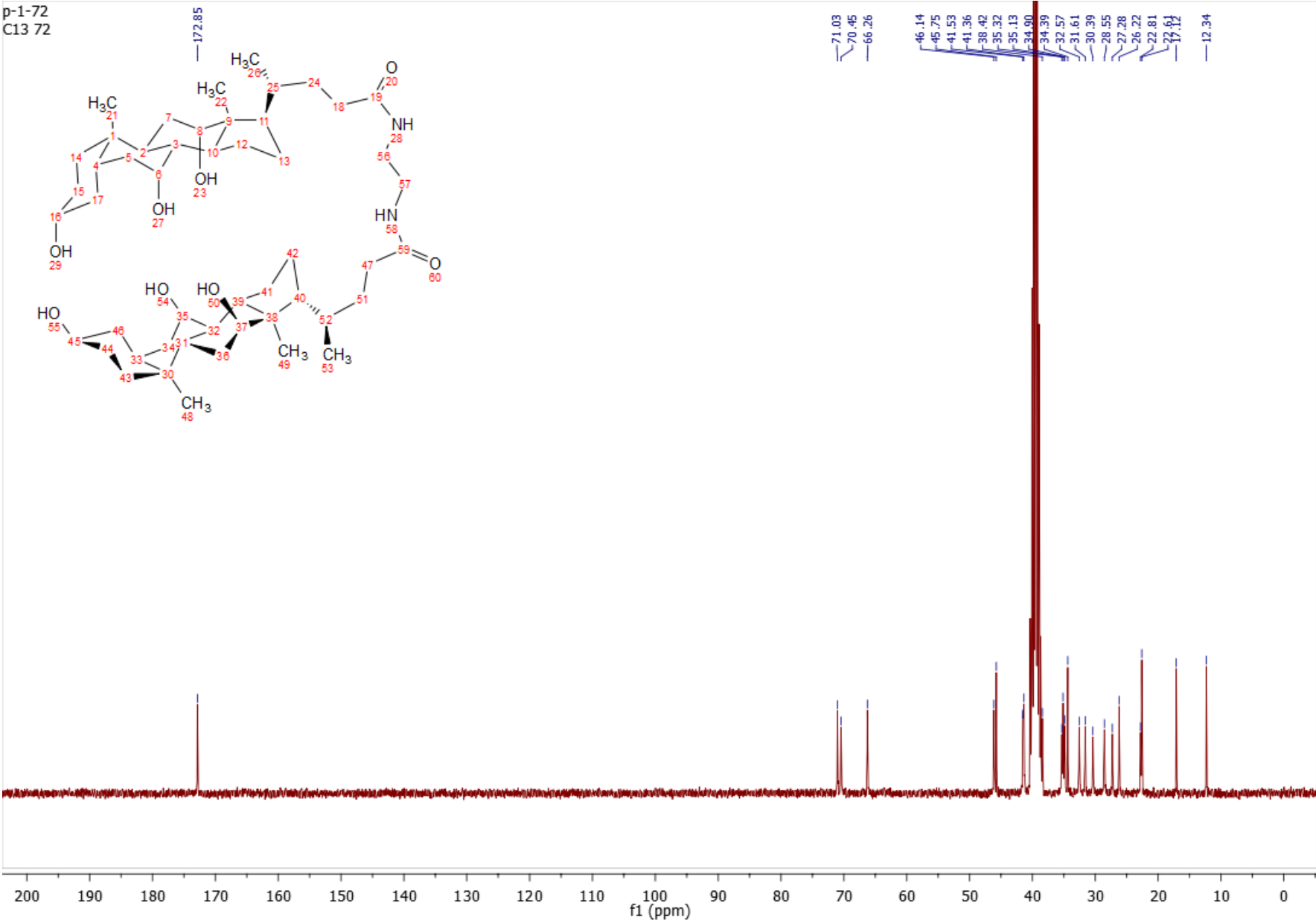
IR of Compound 7a



¹H NMR of Compound 7a (400 MHz, DMSO-d₆)



¹³C NMR of Compound 7a (75 MHz, DMSO-*d*₆)



HRMS of Compound 7a

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 45-50 H: 82-90 N: 0-2 O: 0-8

Sample Name : 10-02-P-172

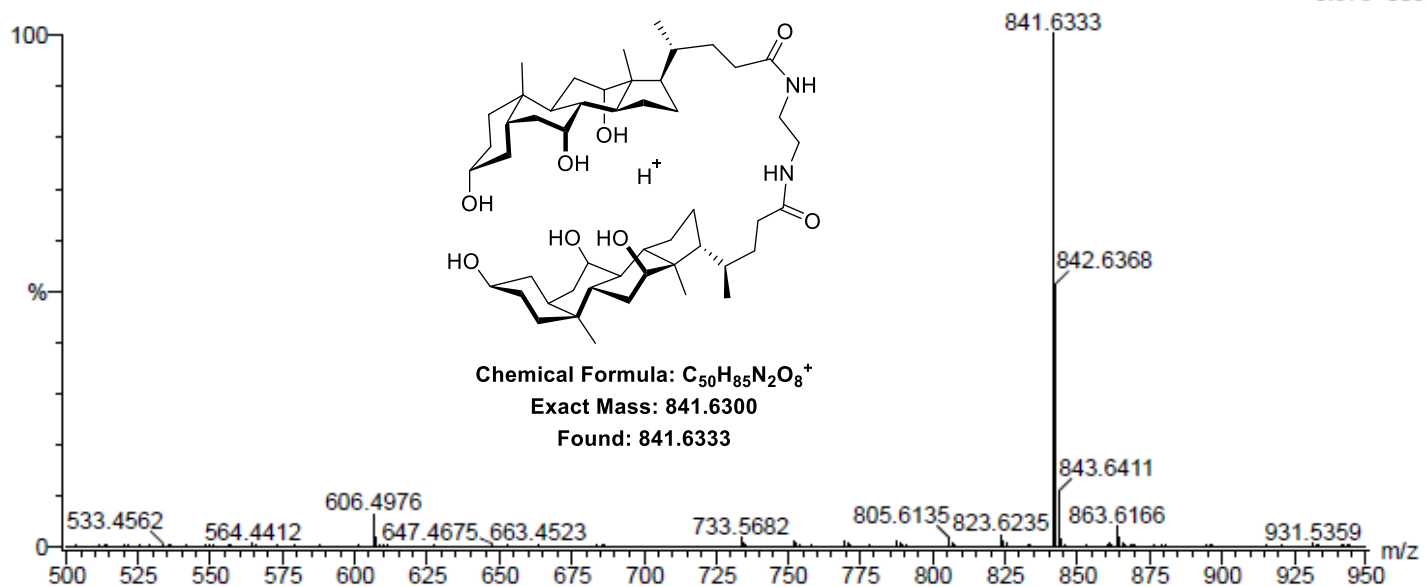
I.I.TROPAR

XEVO G2-XS QTOF

Test Name : HRMS-1

200818-10-02-P-172 19 (0.203) AM2 (Ar,19000.0,0.00,0.00); Cm (19:20)

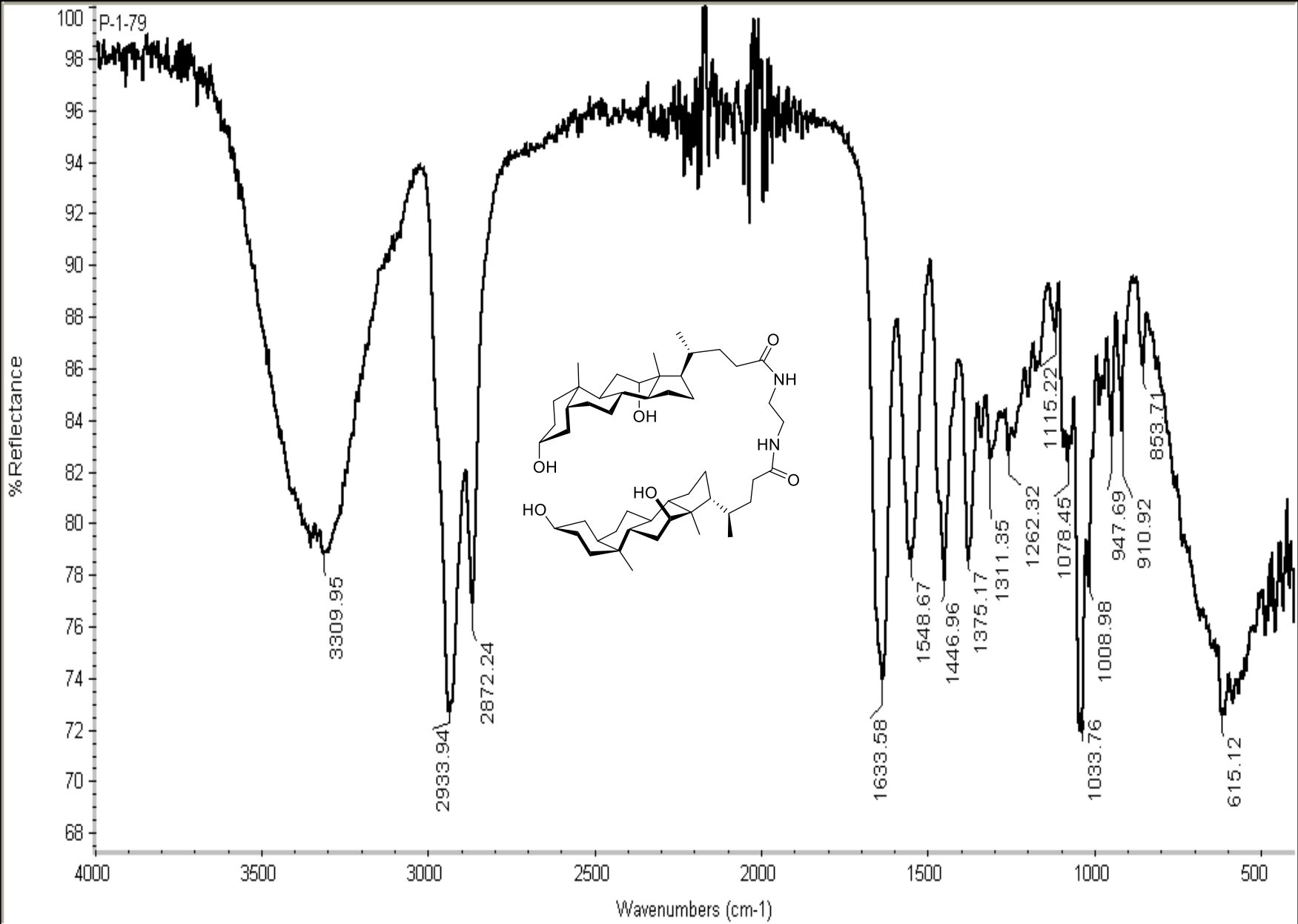
1: TOF MS ES+
8.97e+005



Minimum: -1.5
Maximum: 5.0 10.0 50.0

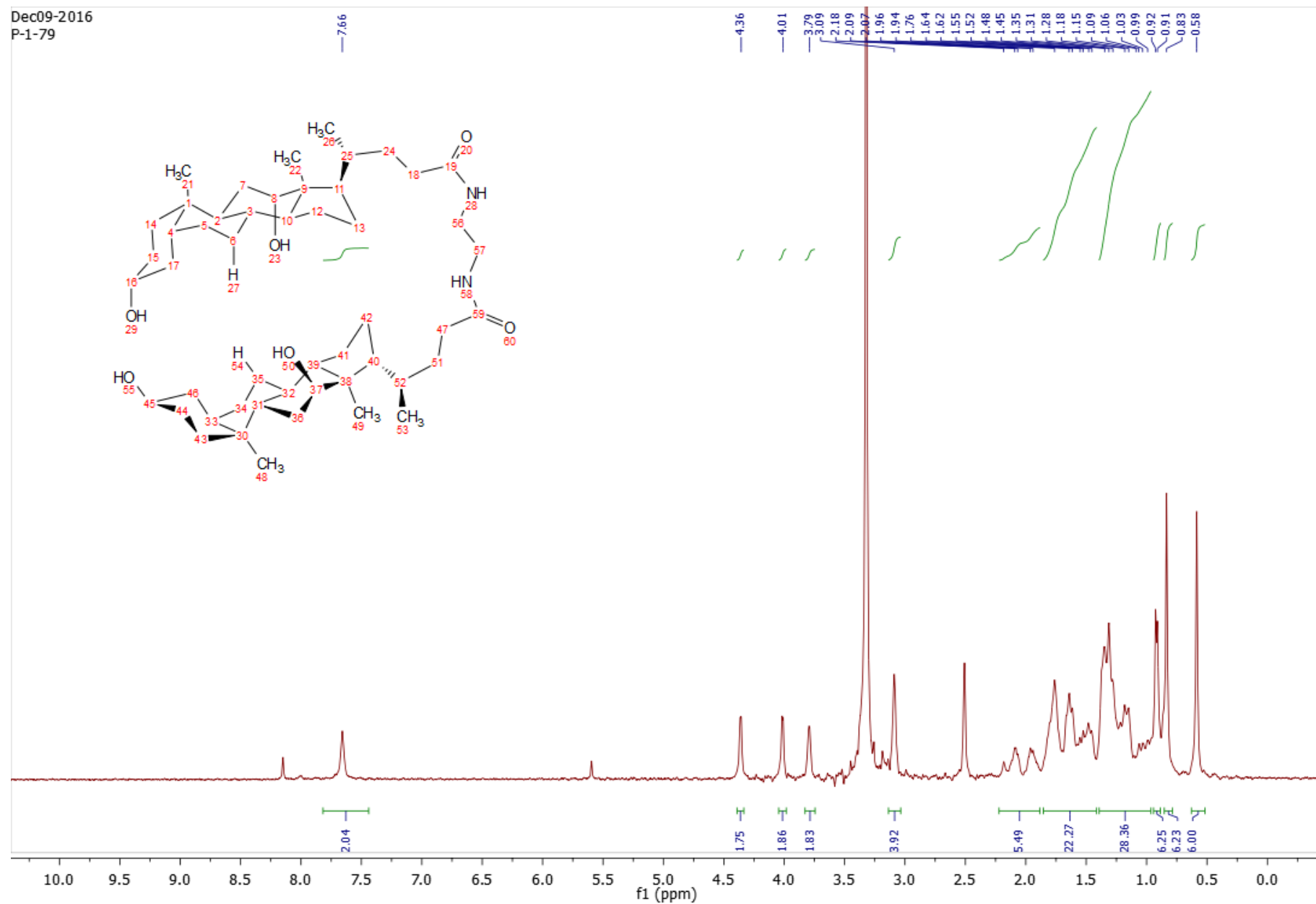
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
841.6333	841.6306	2.7	3.2	9.5	224.8	n/a	n/a	C50 H85 N2 O8

IR of Compound 7b

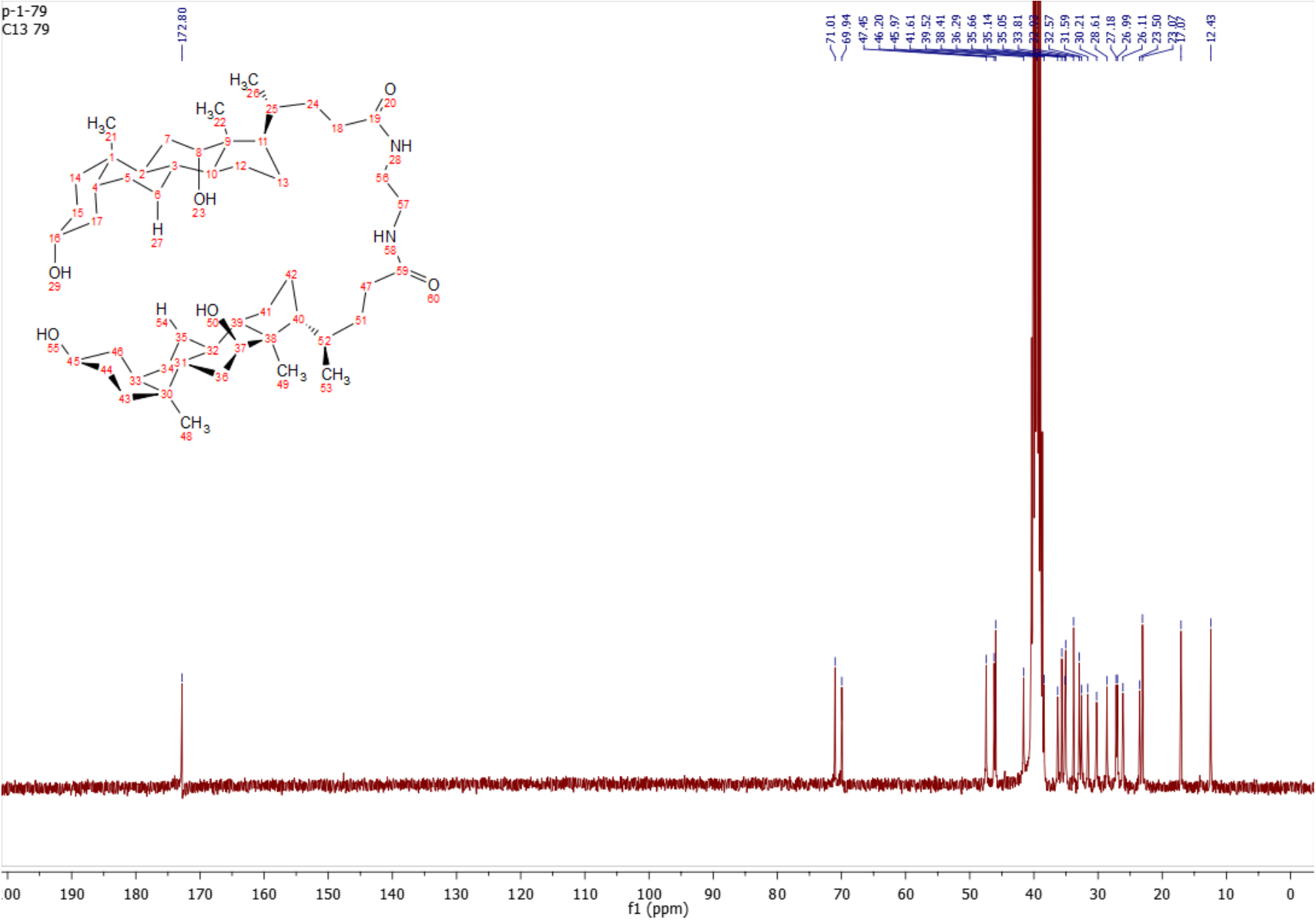


¹H NMR of Compound 7b (400 MHz, DMSO-d₆)

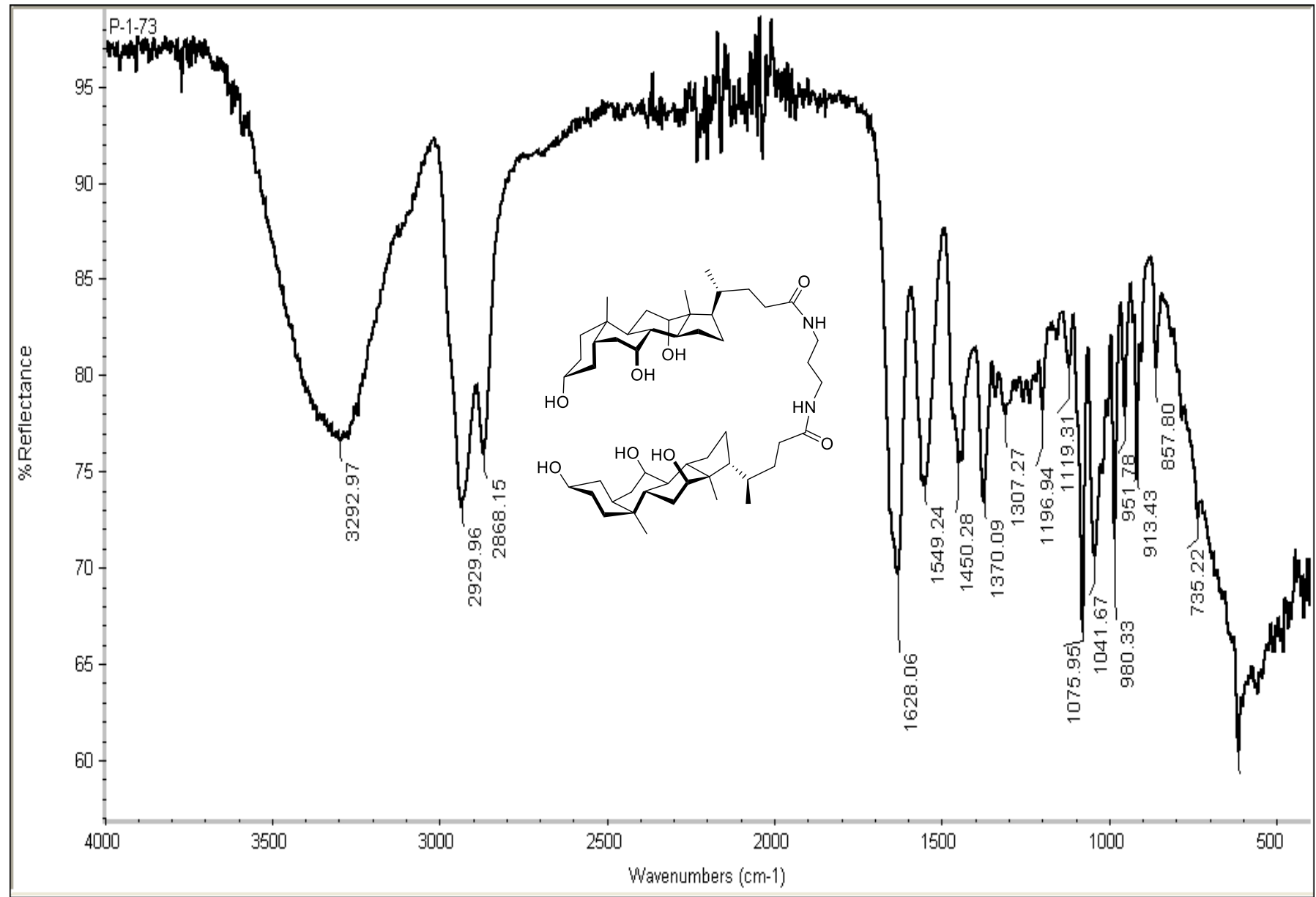
Dec09-2016
P-1-79



¹³C NMR of Compound 7b (75 MHz, DMSO-*d*₆)

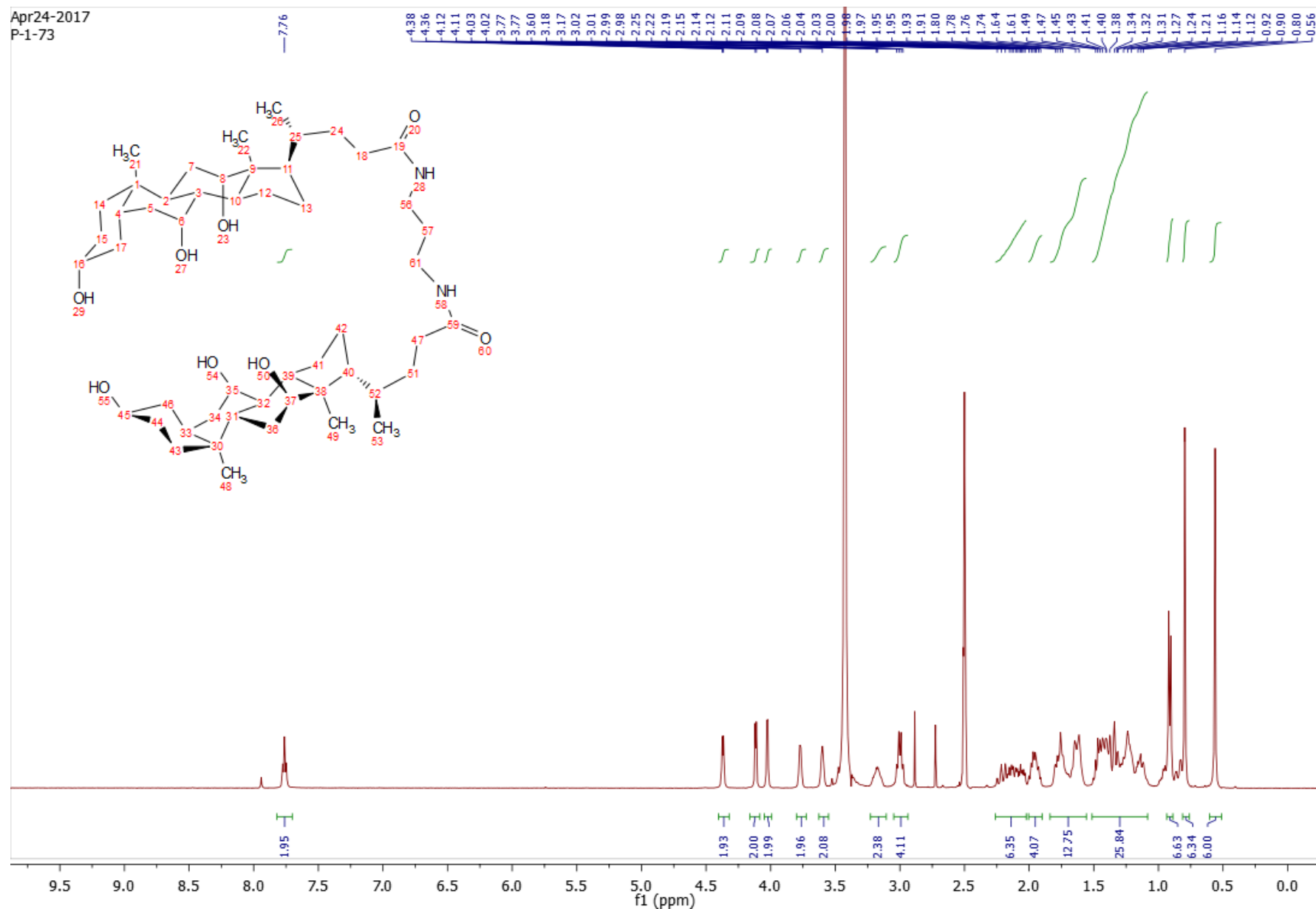


IR of Compound 8a

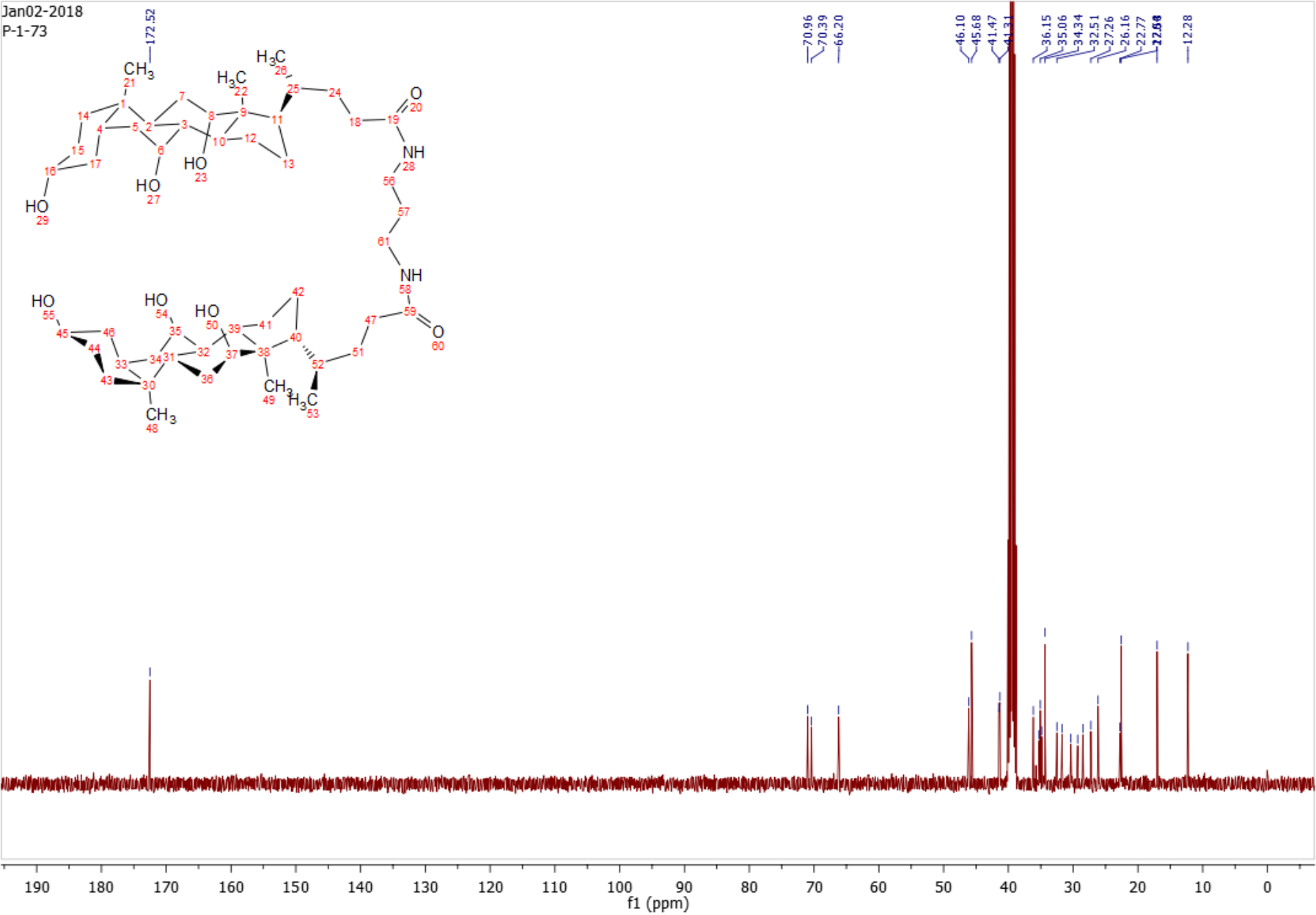


¹H NMR of Compound **8a** (400 MHz, DMSO-d₆)

Apr24-2017
P-1-73



¹³C NMR of Compound 8a (100 MHz, DMSO-d₆)



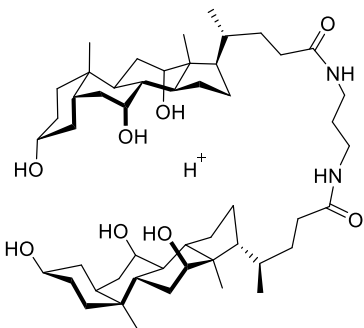
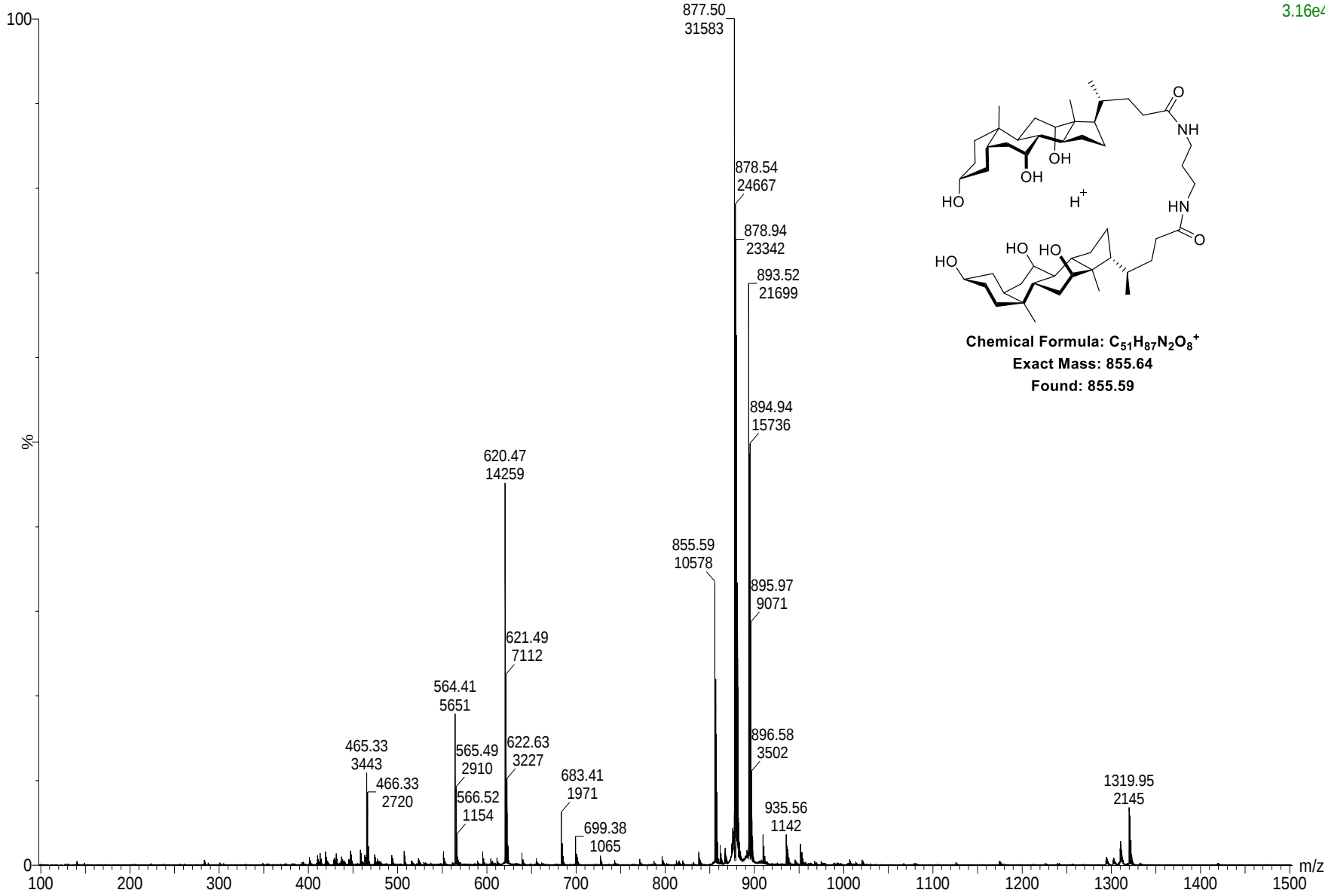
MS of Compound 8a

WATERS, Q-TOF MICROMASS (ESI-MS)

POONAM P-1-73 190418 17 (0.316) Cm (2:17)

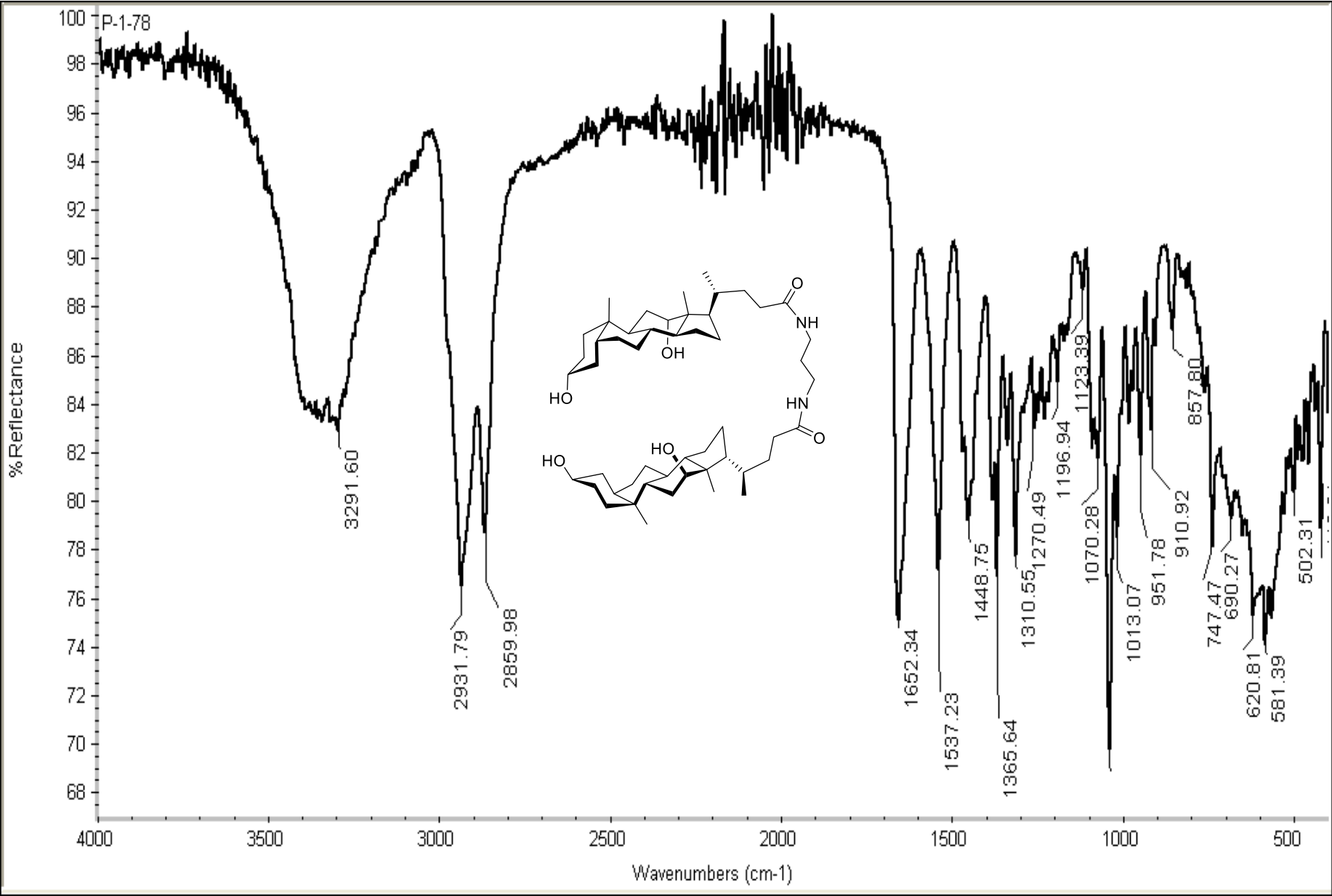
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH

TOF MS ES+
3.16e4



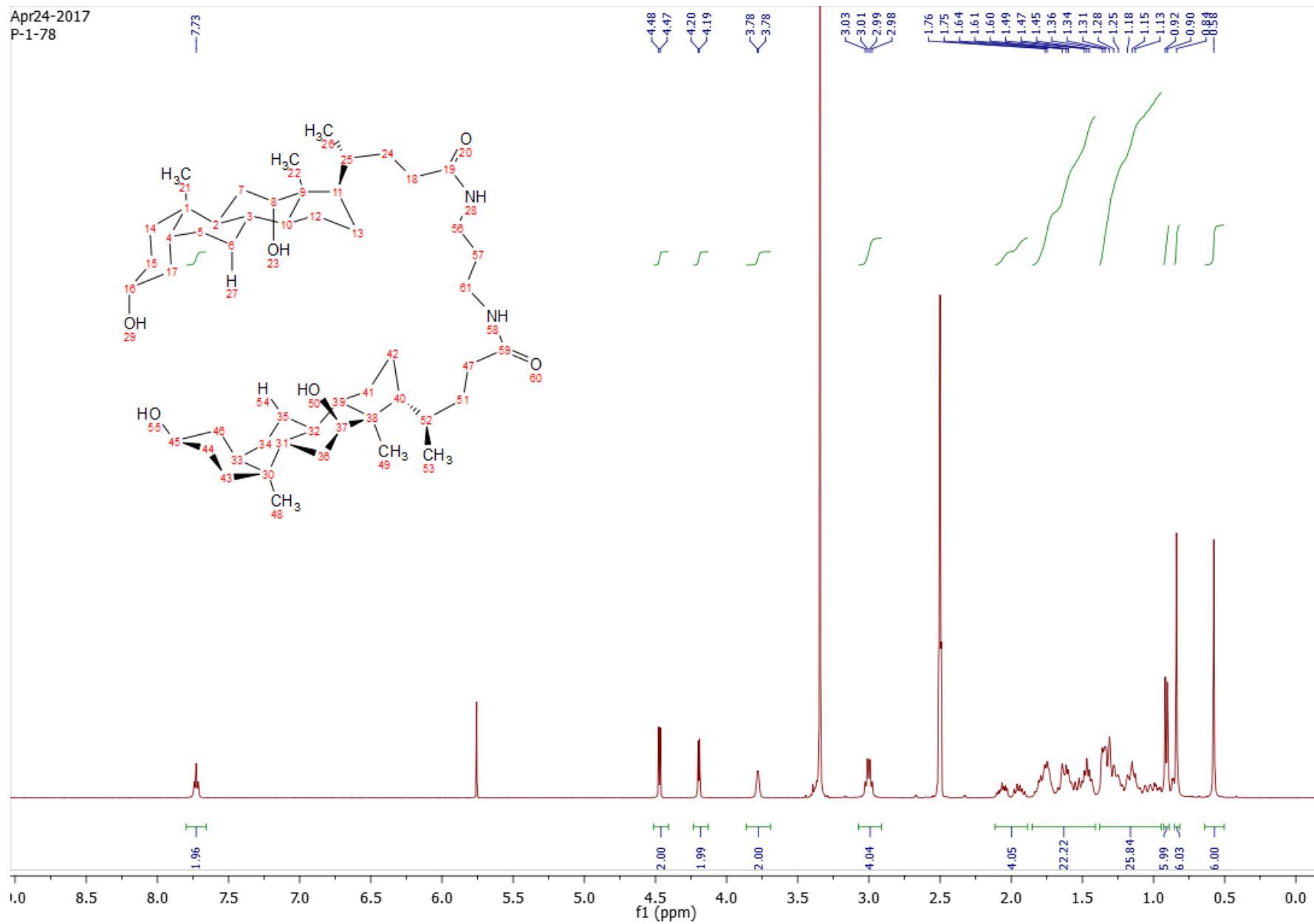
Chemical Formula: $C_{51}H_{87}N_2O_8^+$
Exact Mass: 855.64
Found: 855.59

IR of Compound 8b

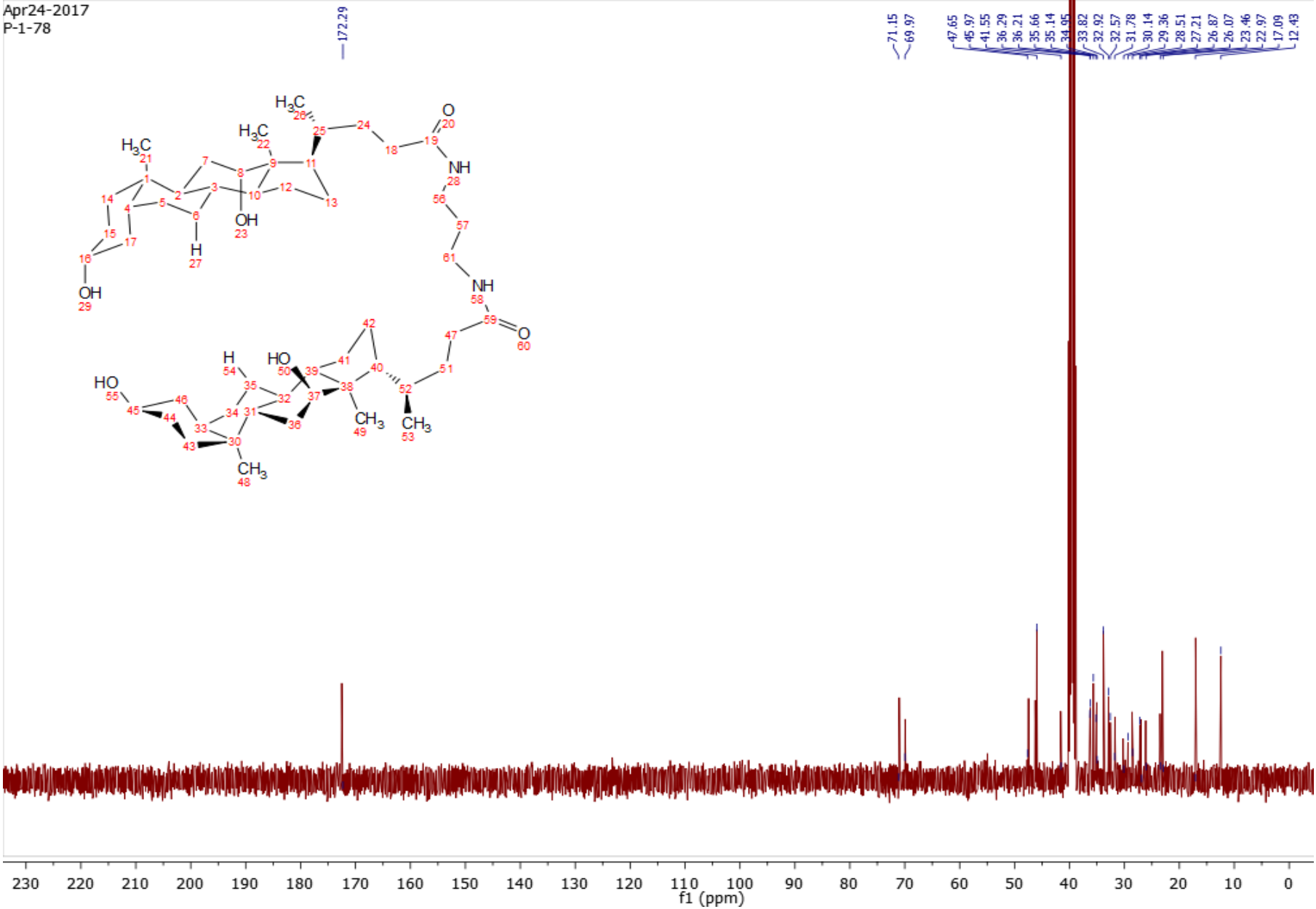


^1H NMR of Compound **8b** (400 MHz, DMSO- d_6)

Apr24-2017
P-1-78



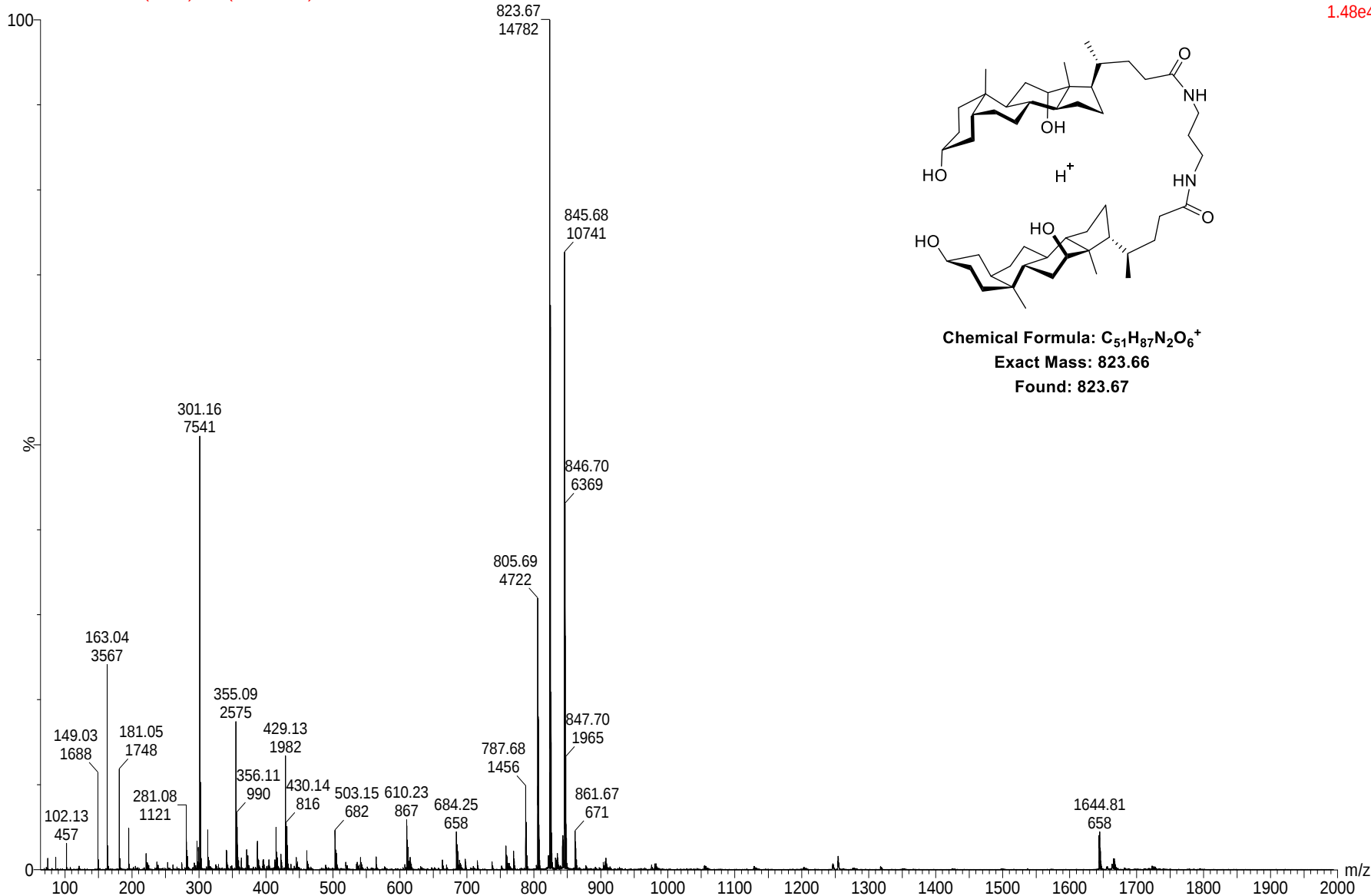
¹³C NMR of Compound 8b (100 MHz, DMSO-*d*₆)



MS of Compound 8b

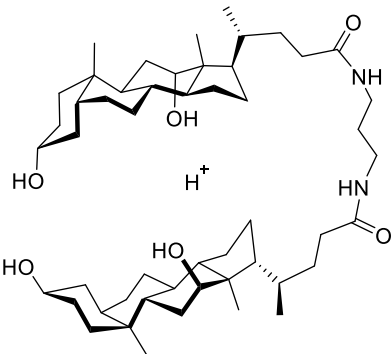
WATERS, Q-TOF MICROMASS (ESI-MS)

POONAM P-1-78 6 (0.212) Cm (3:10-13:23)



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TOF MS ES+
1.48e4

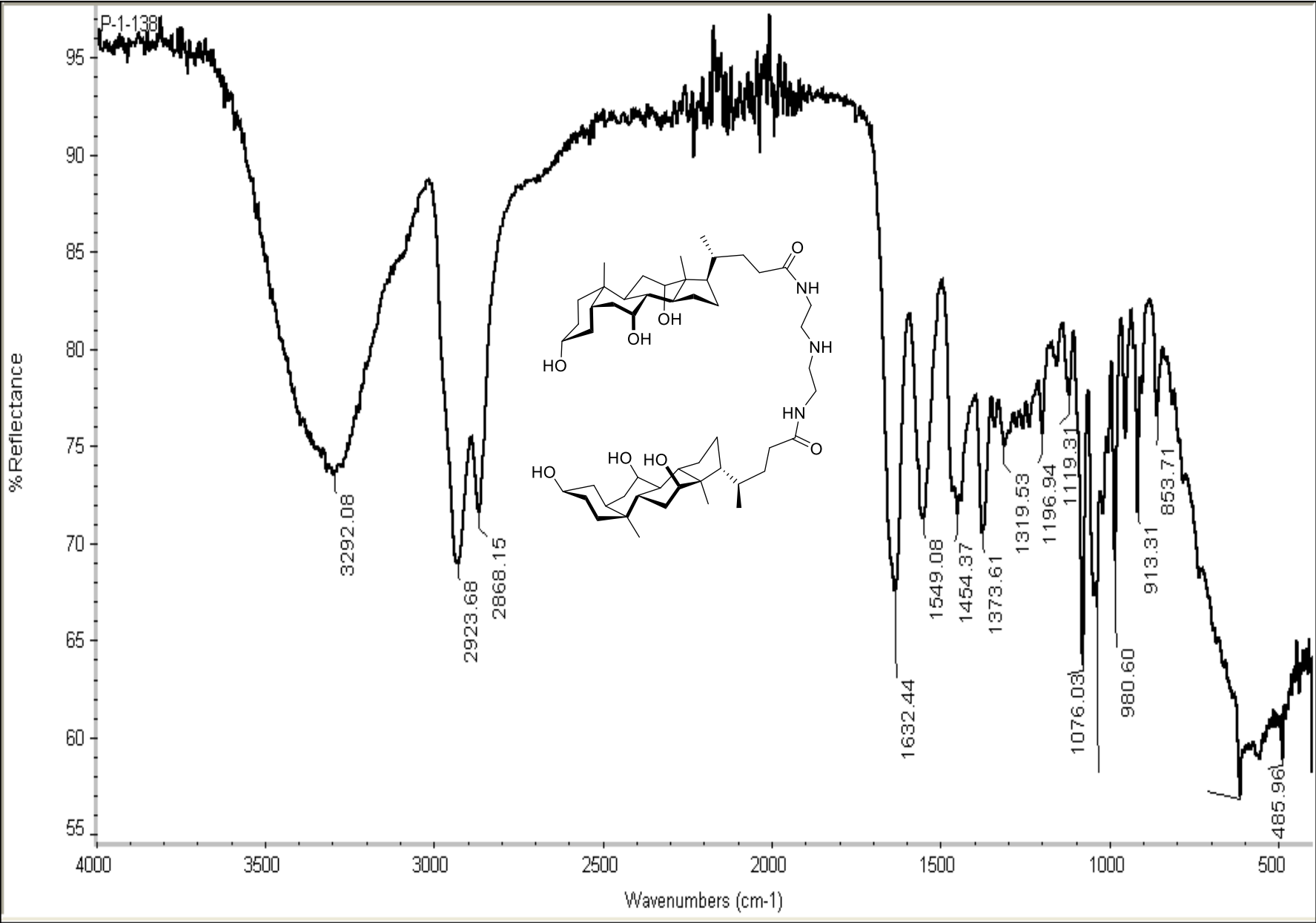


Chemical Formula: $C_{51}H_{87}N_2O_6^+$

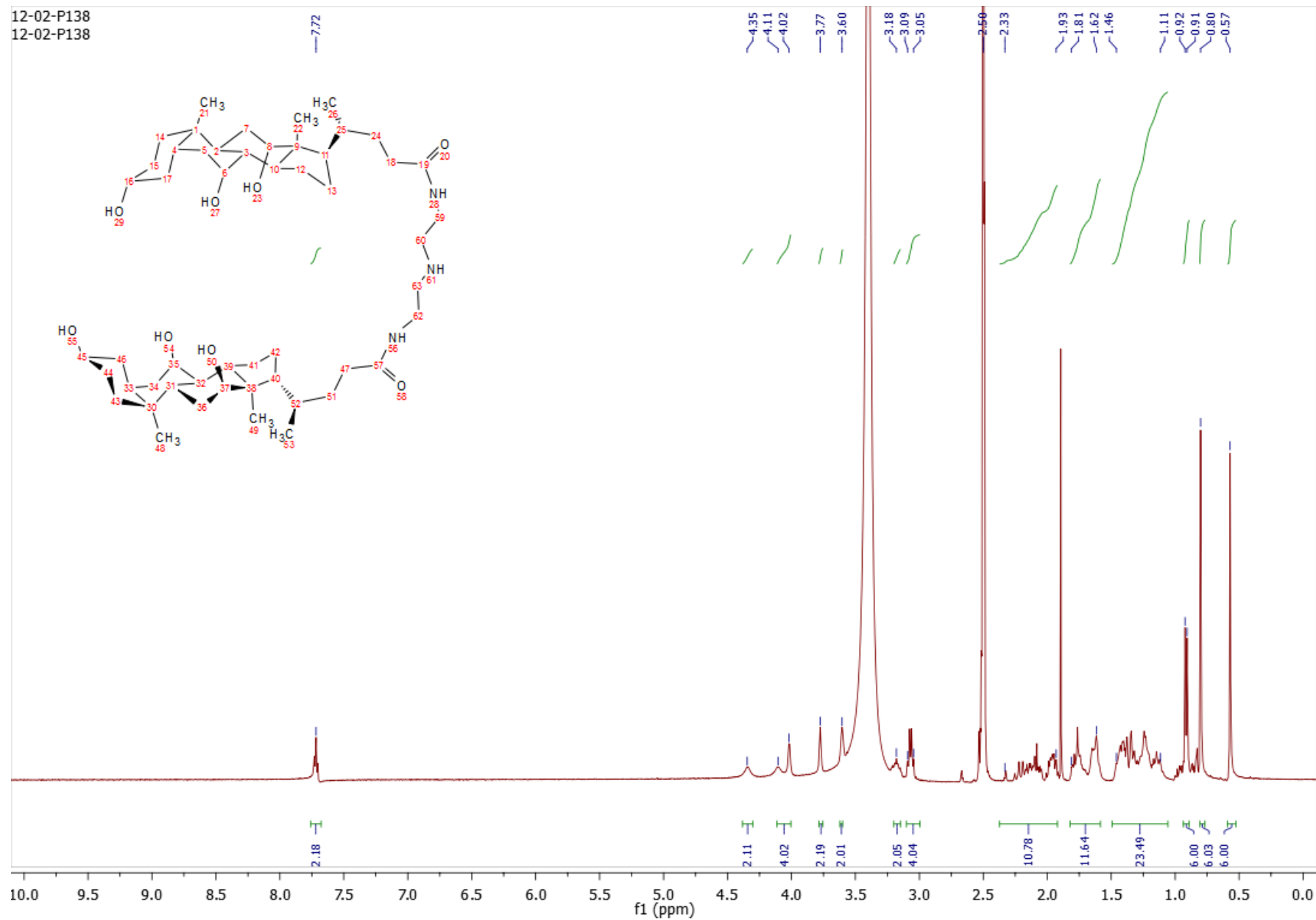
Exact Mass: 823.66

Found: 823.67

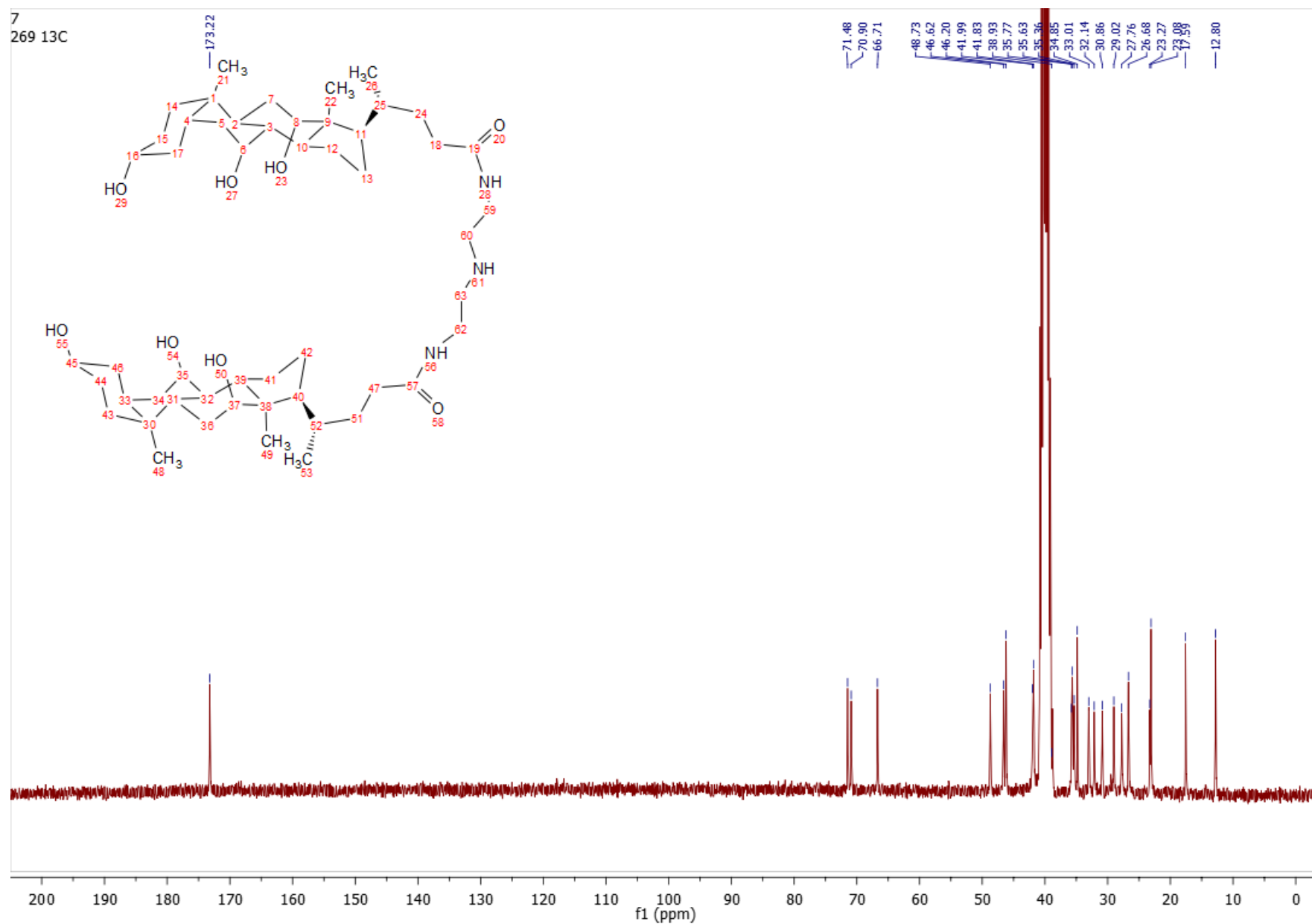
IR of Compound 9a



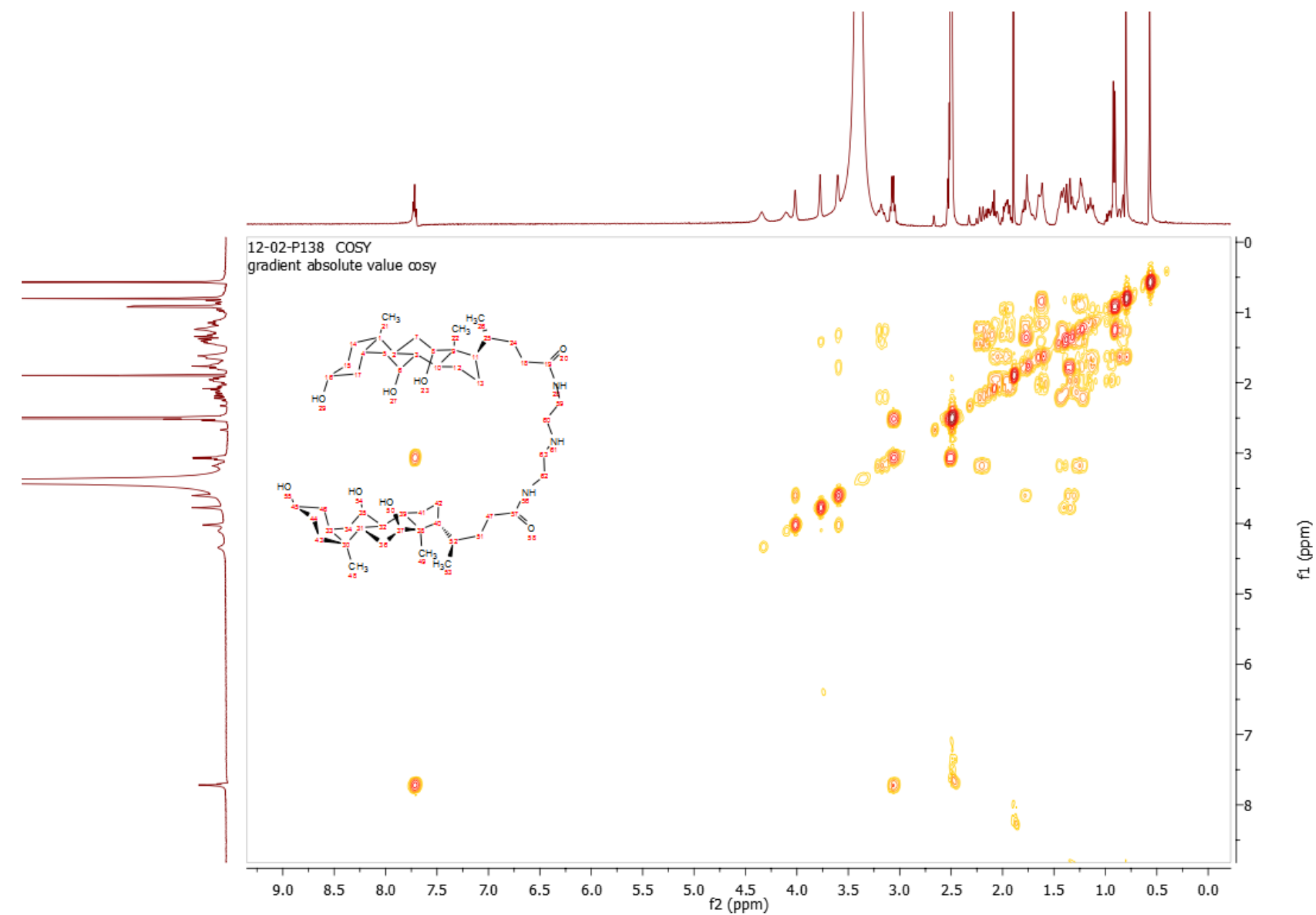
¹H NMR of Compound 9a (400 MHz, JEOL JNM ECS400, DMSO-d₆)



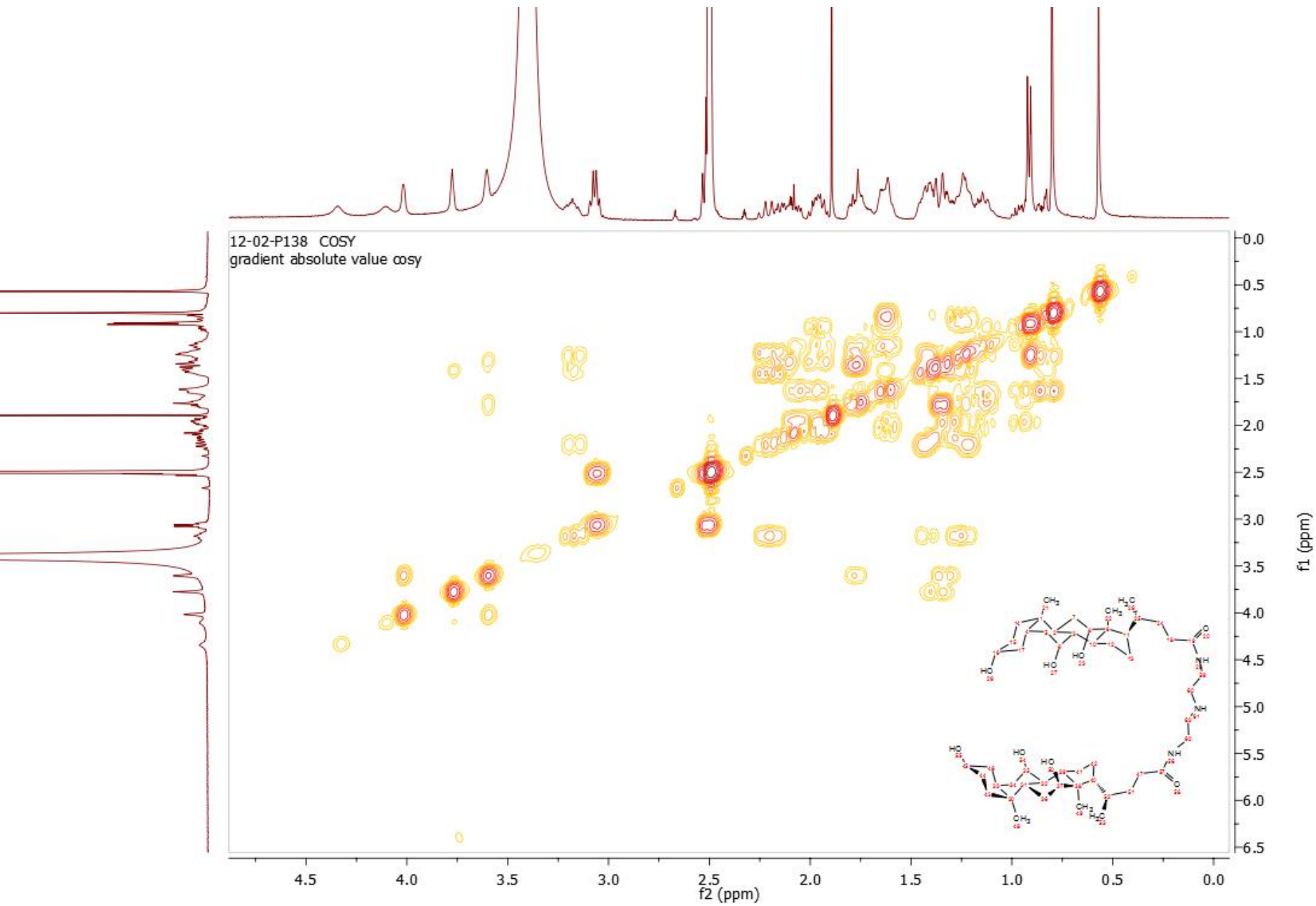
^{13}C NMR of Compound 9a (75 MHz, DMSO- d_6)



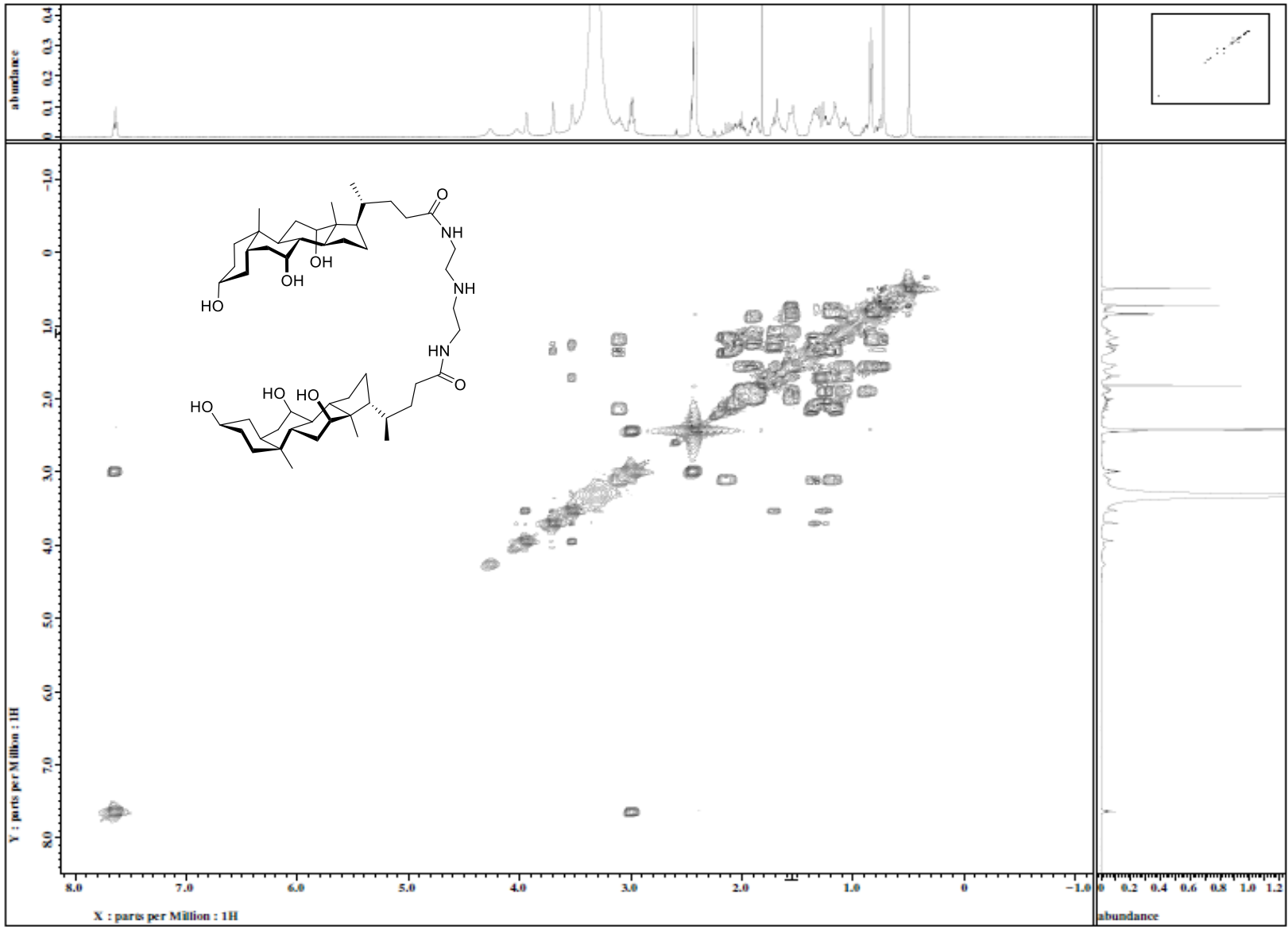
2D COSY NMR of Compound 9a (400 MHz, JEOL JNM ECS400, DMSO-d₆)



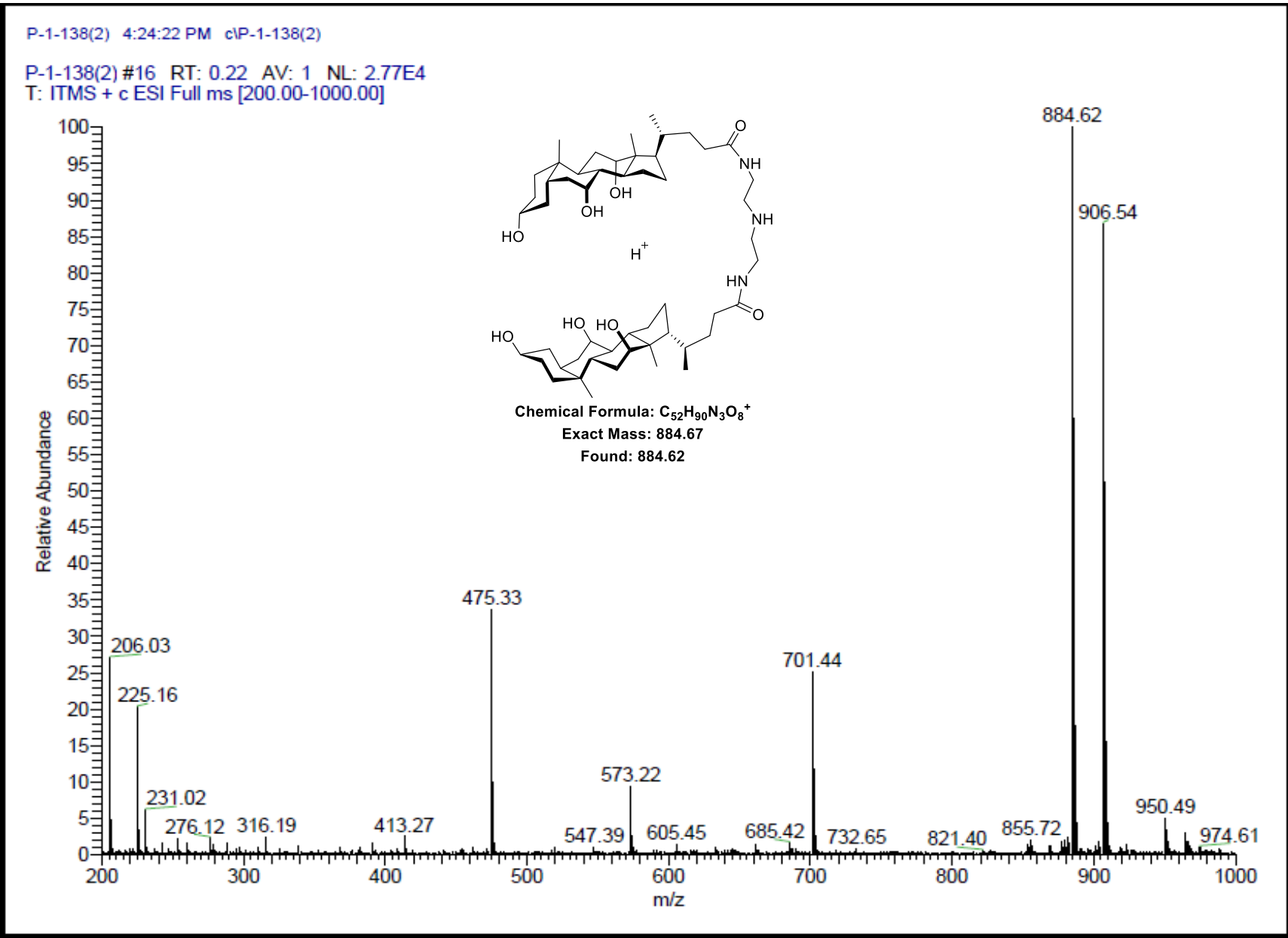
2D COSY NMR of Compound 9a (400 MHz, JEOL JNM ECS400, DMSO-d₆)



2D NOESY NMR of Compound **9a** (400 MHz, JEOL JNM ECS400, DMSO-*d*₆)



MS of Compound 9a



HRMS of Compound 9a

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 50-55 H: 85-91 N: 0-3 O: 0-8

Sample Name : P-1-138

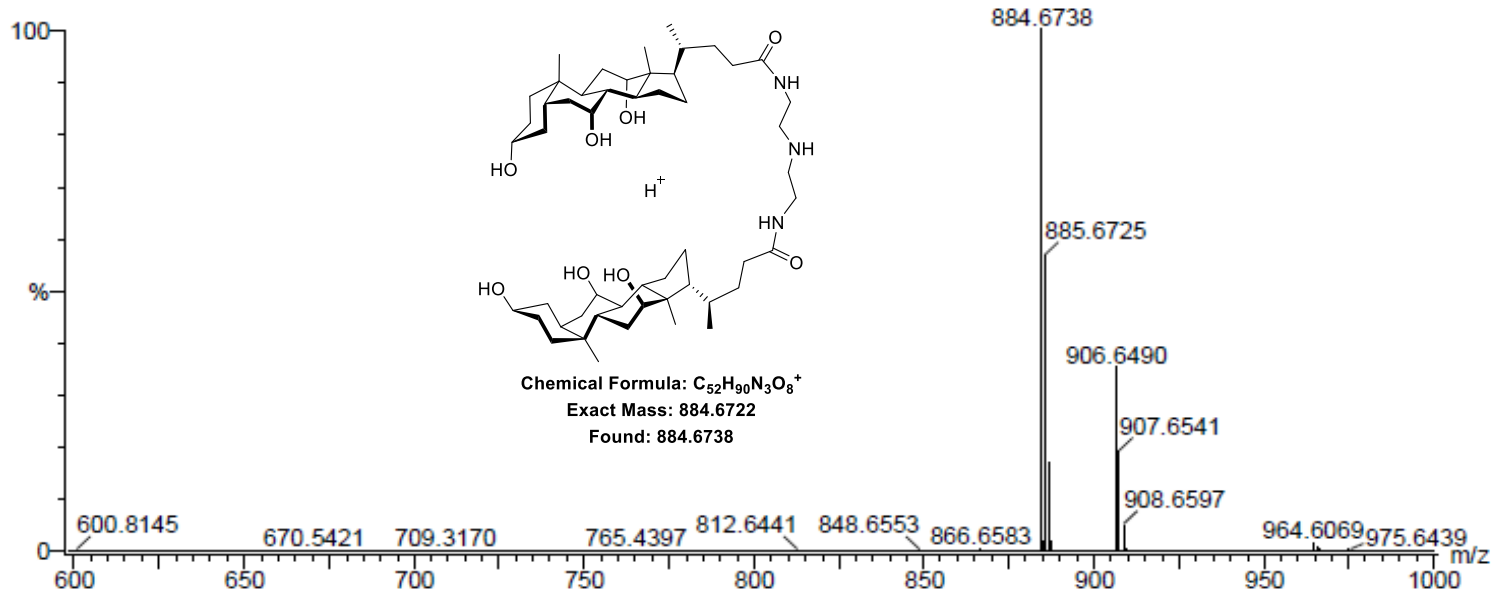
Test Name : HRMS-1

220218-P-1-138 18 (0.183) AM (Top,4, Ar,10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (18:20)

INDIAN INSTITUTE OF TECHNOLOGY
ROPAR

XEVO G2-XS QTOF

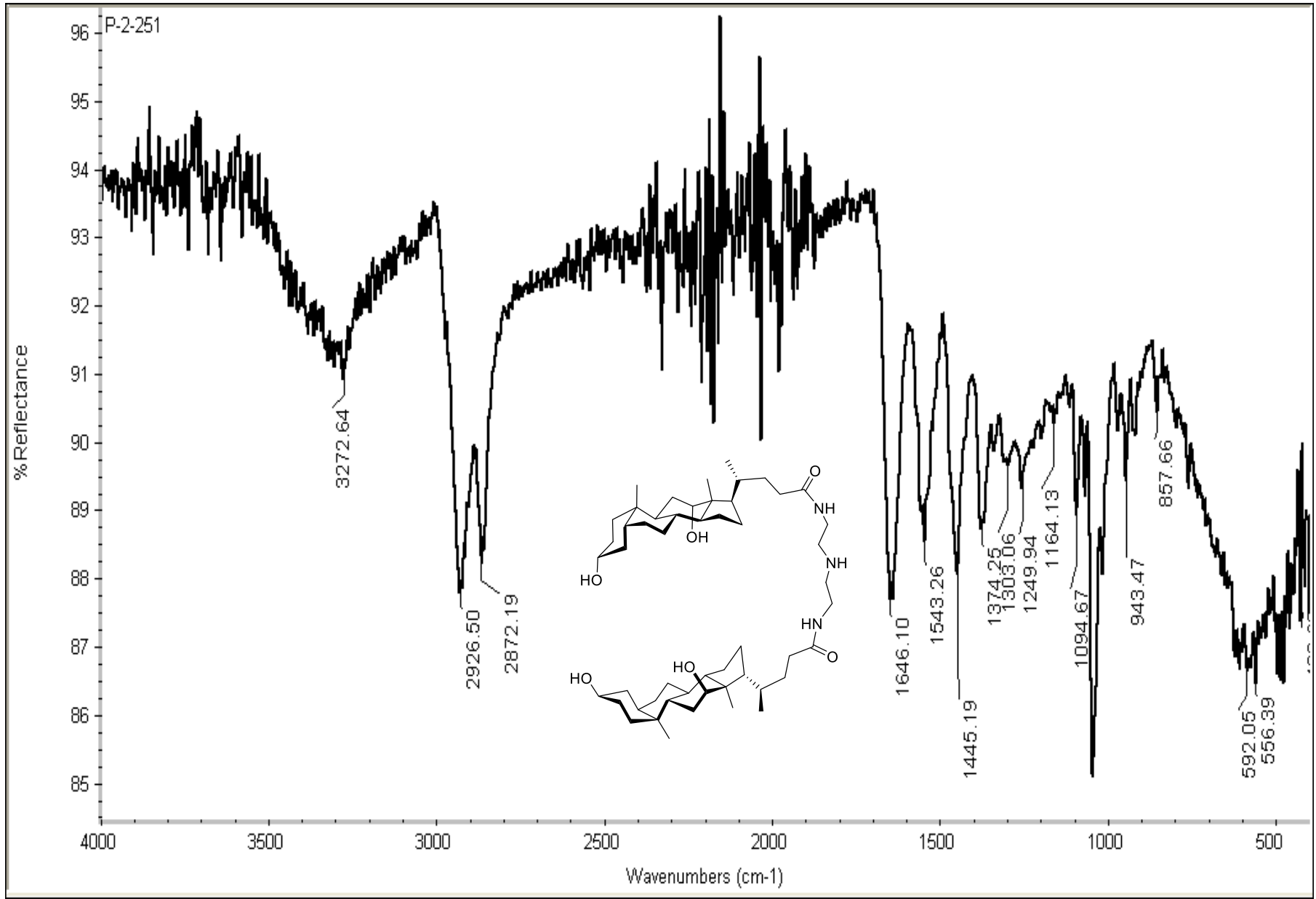
1: TOF MS ES+
7.11e+006



Minimum: -1.5
Maximum: 5.0 5.0 50.0

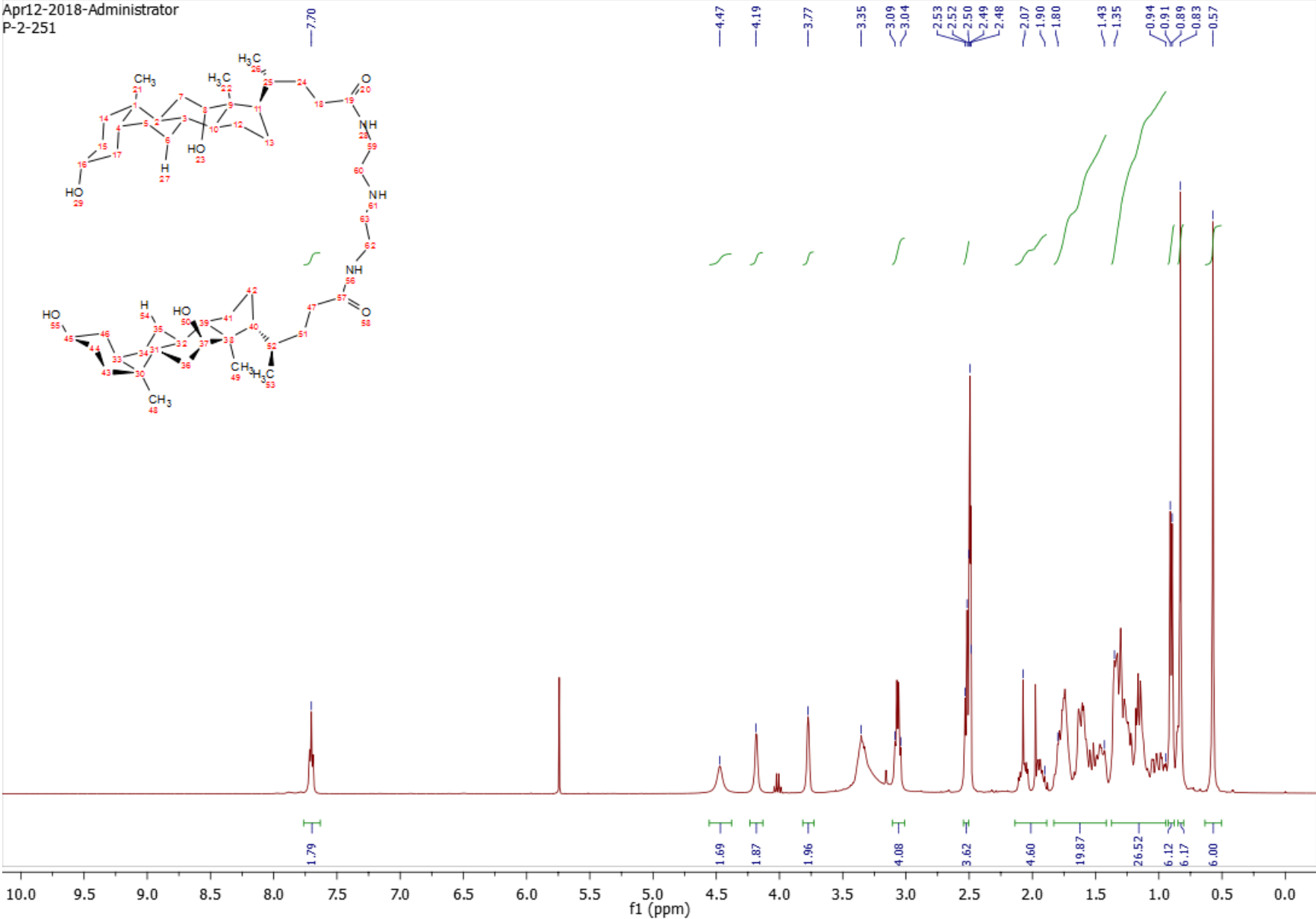
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
884.6738	884.6728	1.0	1.1	9.5	245.5	n/a	n/a	C52 H90 N3 O8

IR of Compound 9b



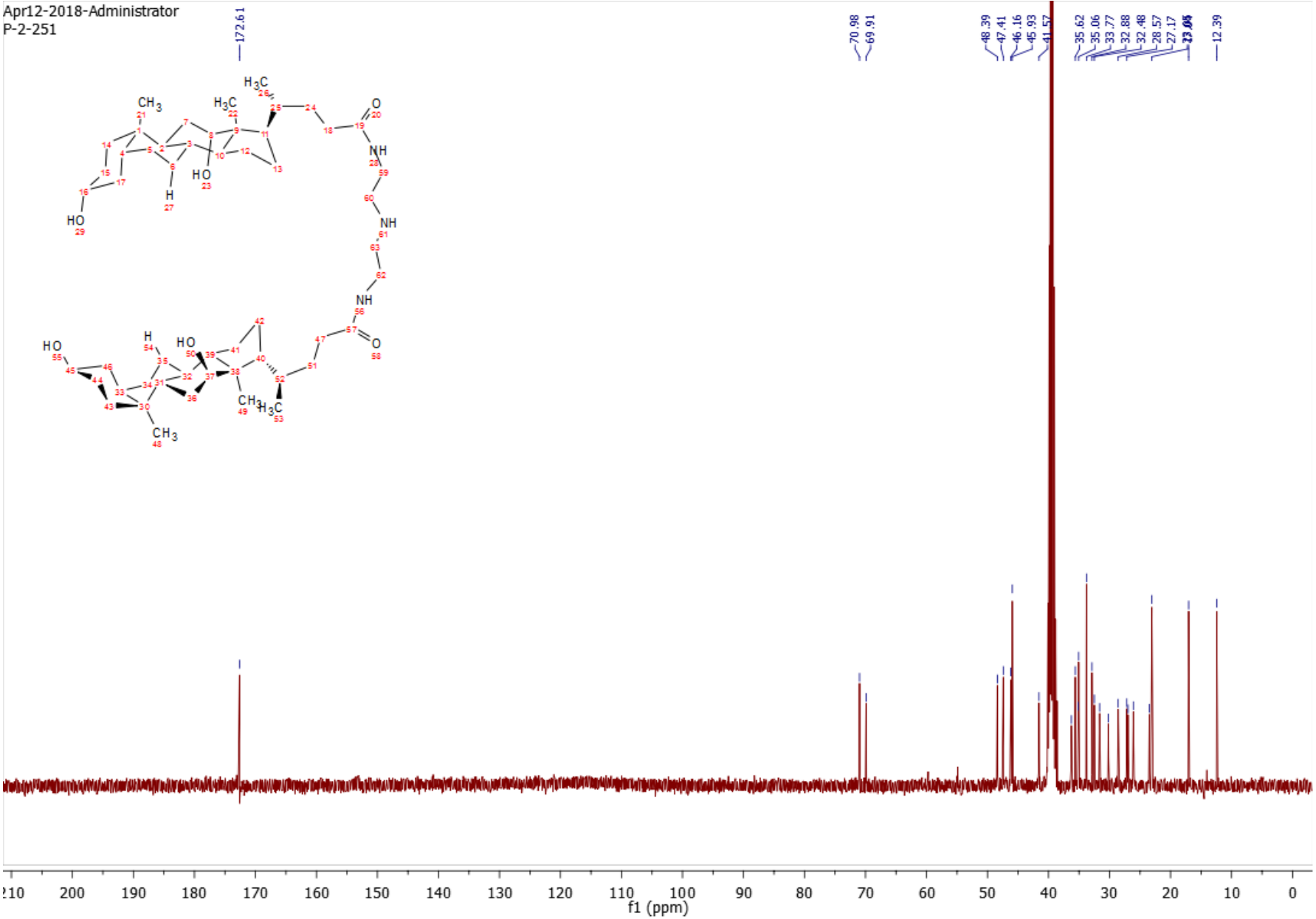
¹H NMR of Compound 9b (400 MHz, DMSO-d₆)

Apr12-2018-Administrator
P-2-251



¹³C NMR of Compound 9b (100 MHz, DMSO-*d*₆)

Apr12-2018-Administrator
P-2-251



HRMS of Compound 9b

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

6 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 45-55 H: 80-90 N: 0-3 O: 0-6

Sample Name : 10-02-251

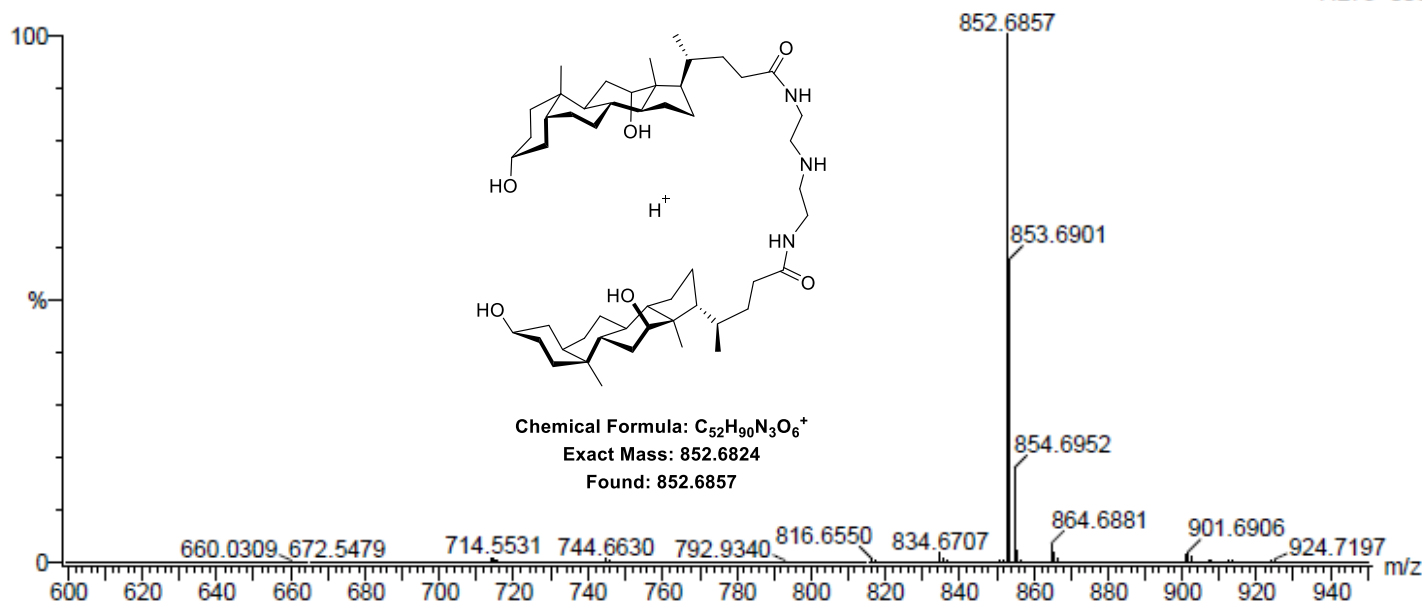
I.I.TROPAR

XEVO G2-XS QTOF

Test Name : HRMS-1

200818-10-02-251 19 (0.203) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (19:21)

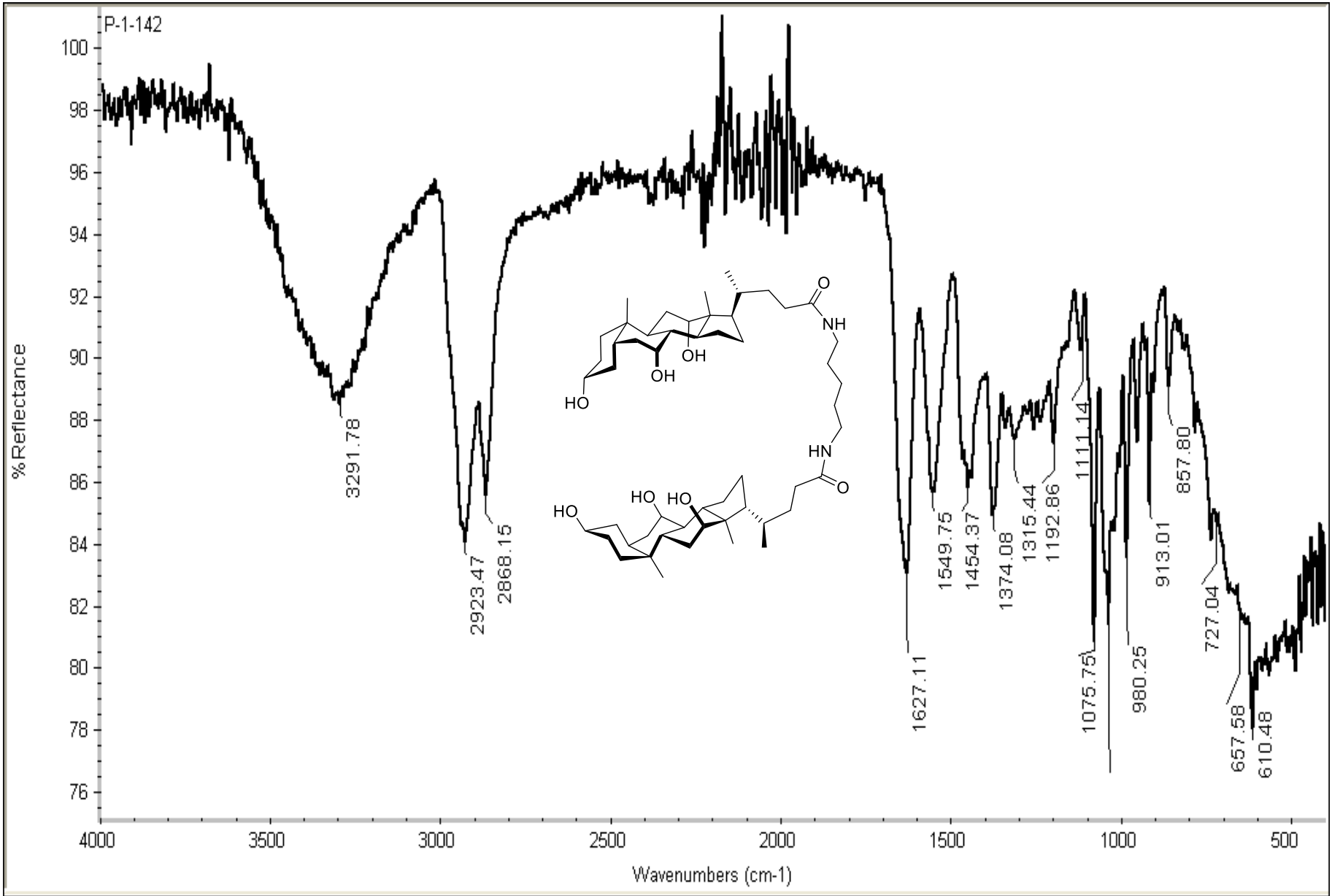
1: TOF MS ES+
7.27e+006



Minimum: -1.5
Maximum: 5.0 10.0 50.0

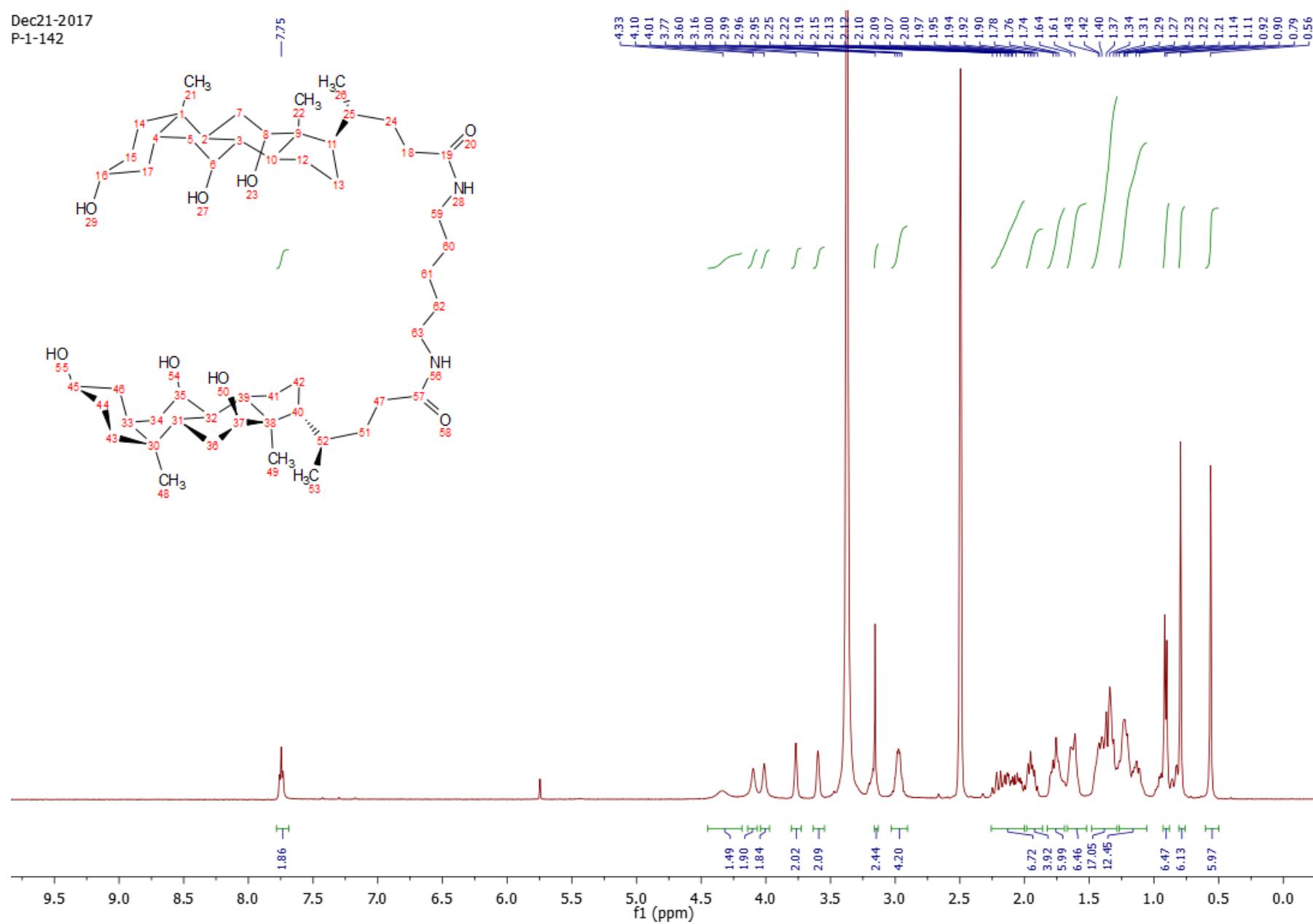
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
852.6857	852.6830	2.7	3.2	9.5	292.0	n/a	n/a	C52 H90 N3 O6

IR of Compound 10

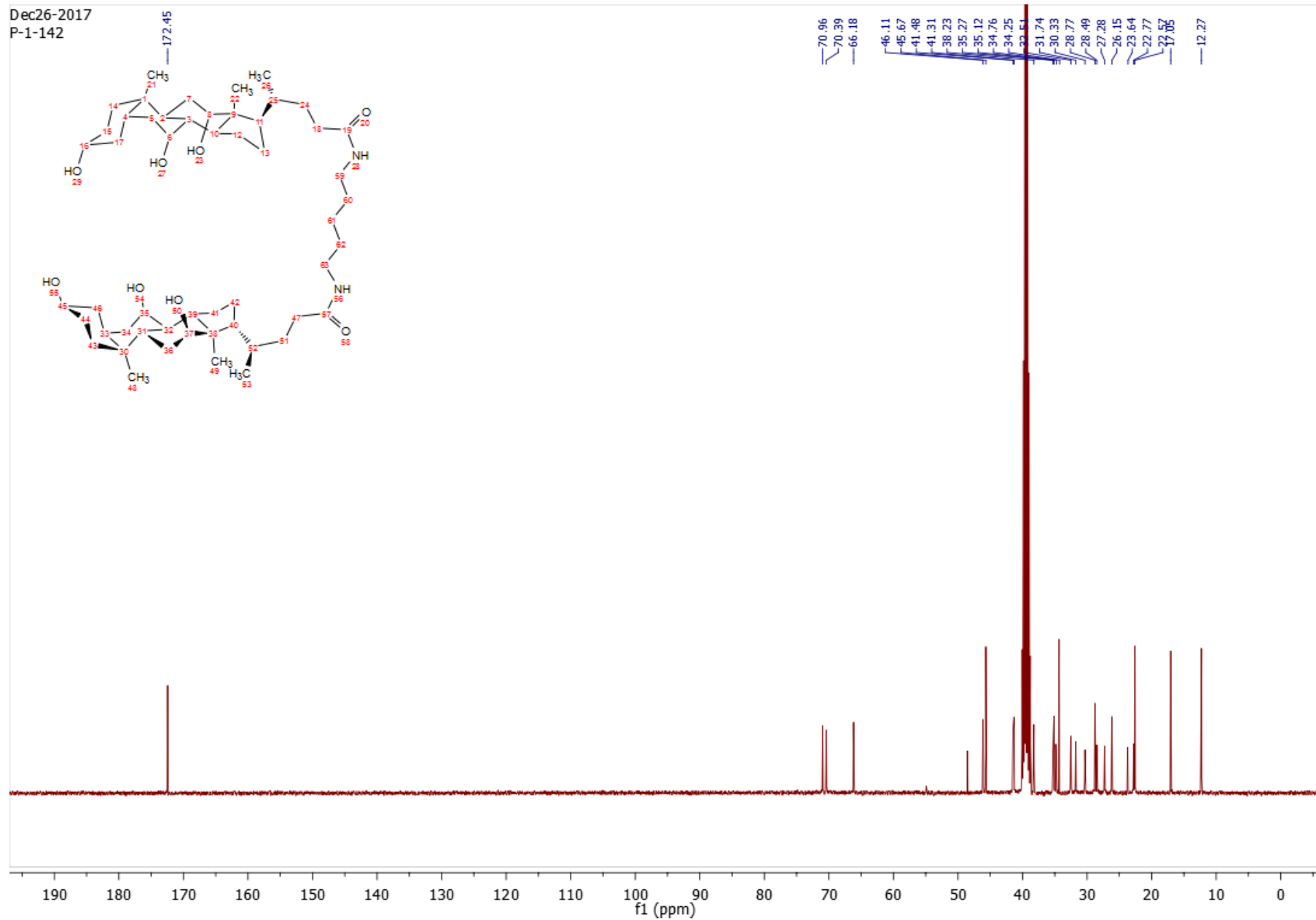


^1H NMR of Compound **10** (400 MHz, $\text{DMSO}-d_6$)

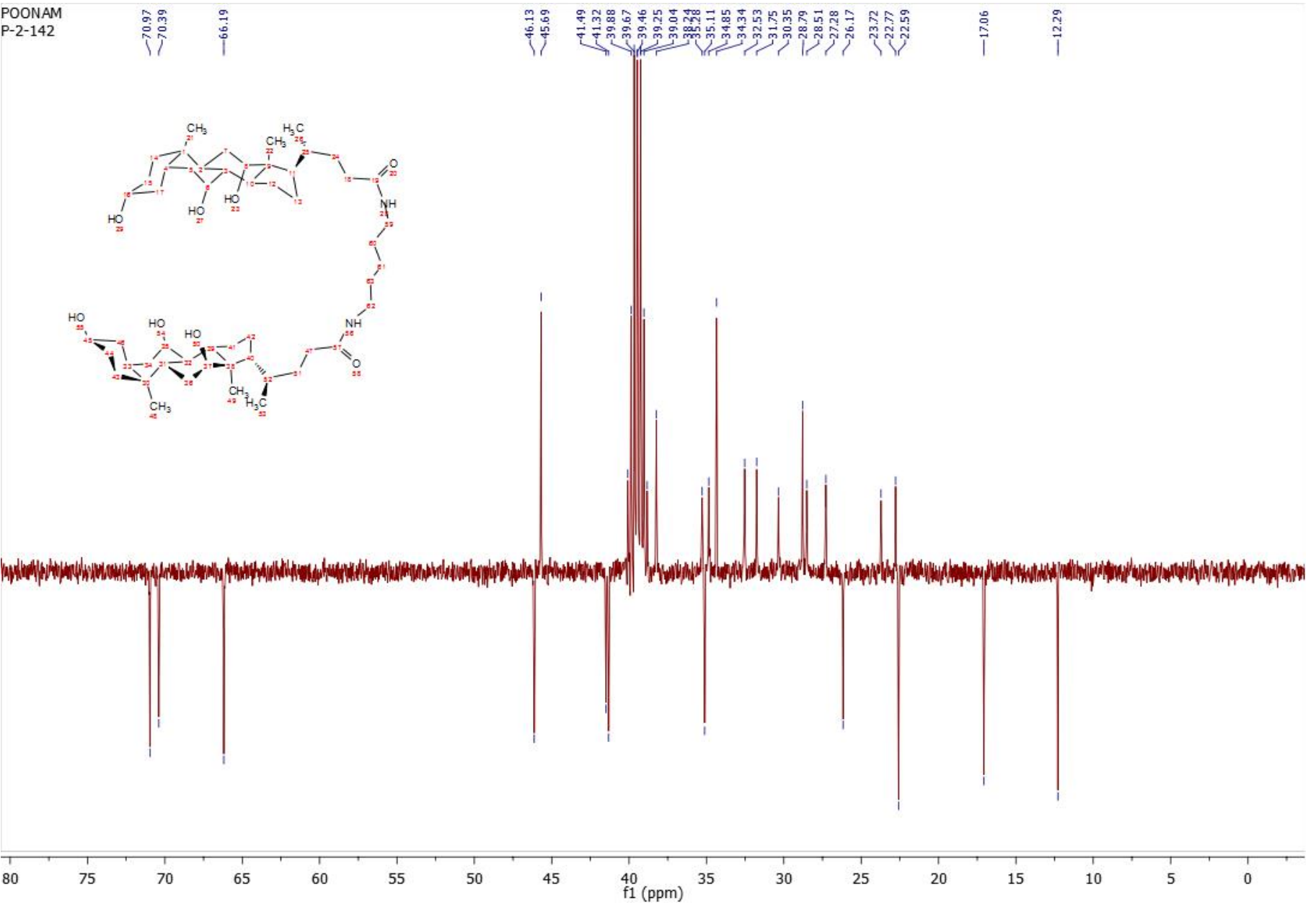
Dec21-2017
P-1-142



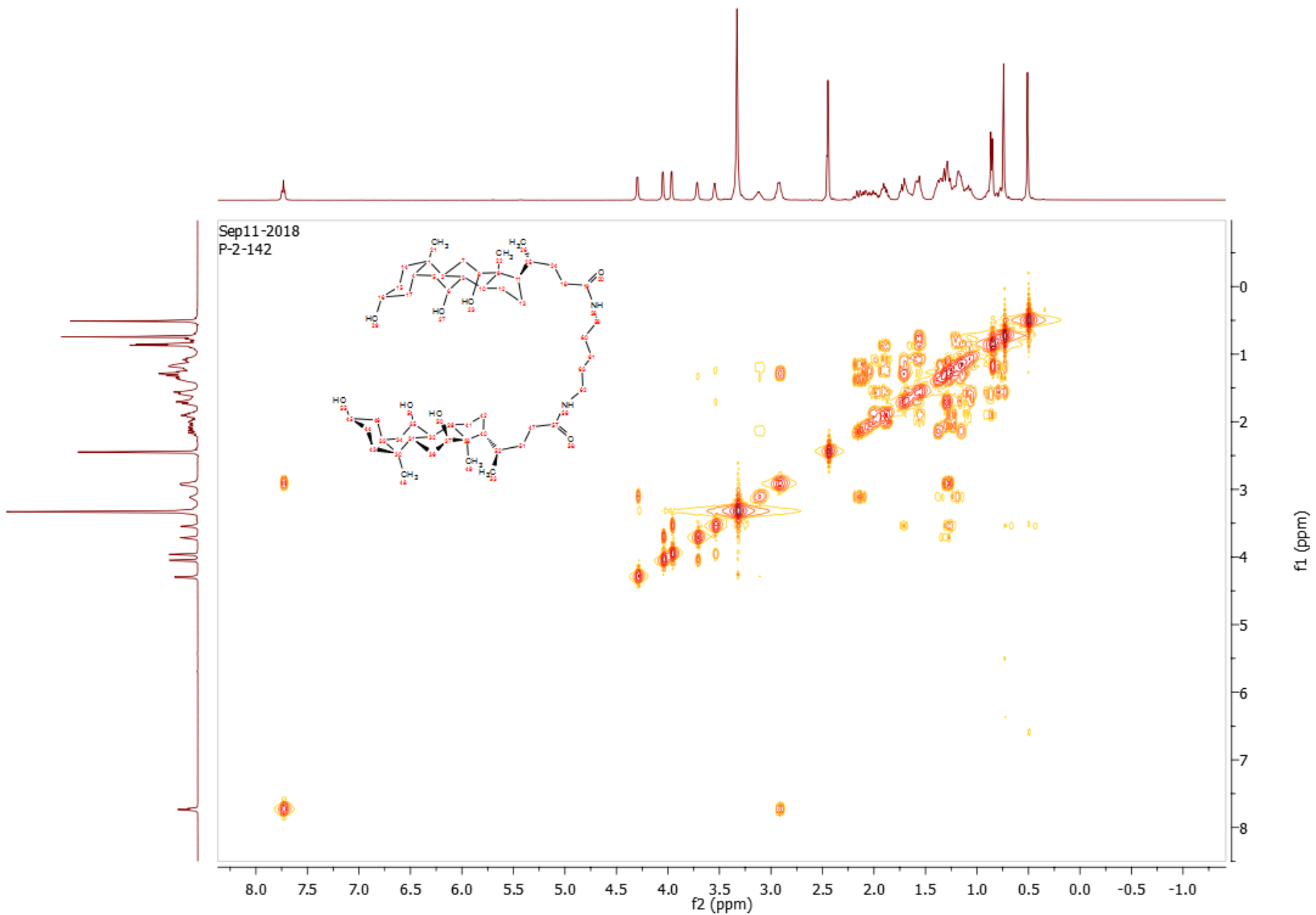
^{13}C NMR of Compound **10** (100 MHz, DMSO- d_6)



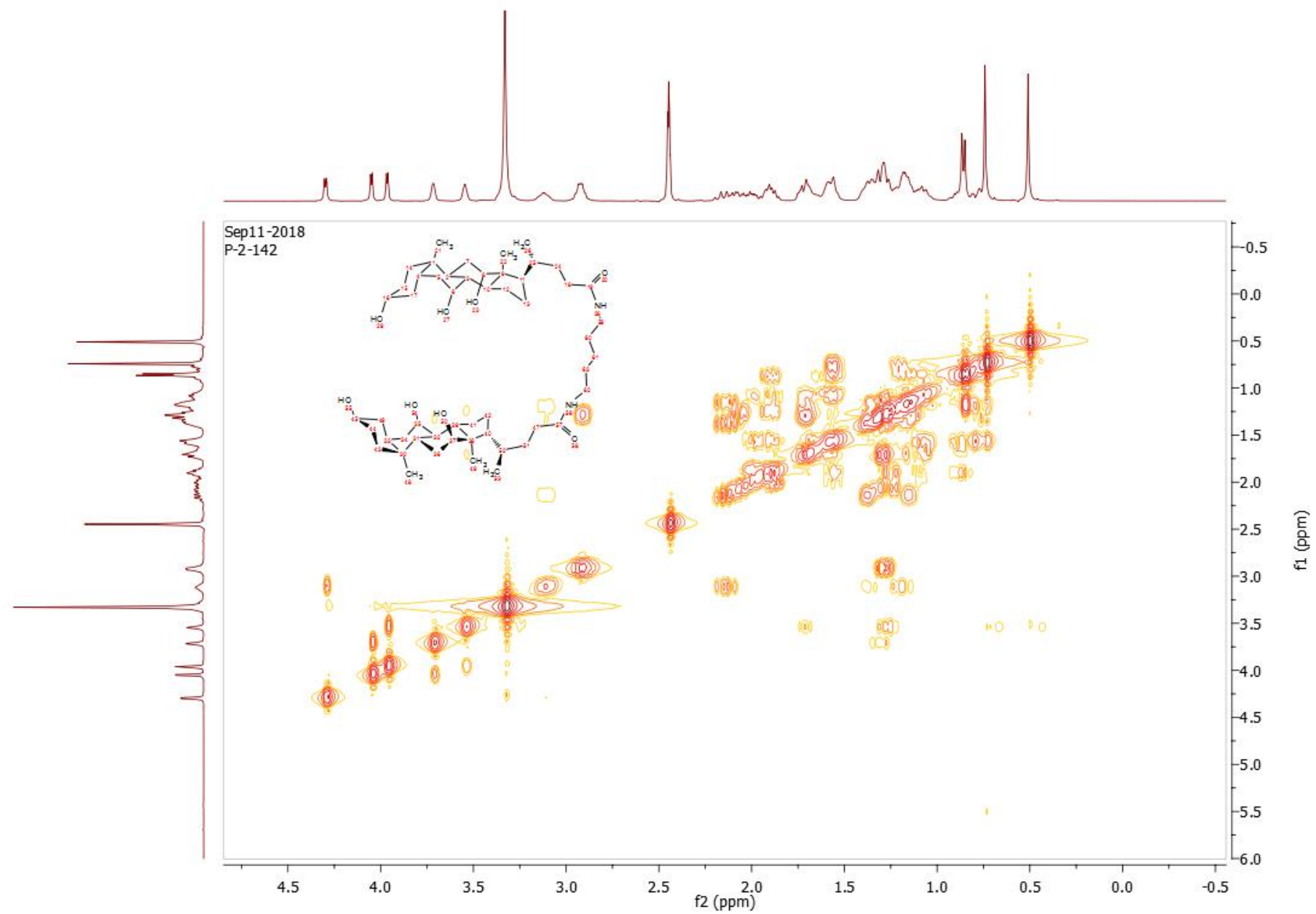
DEPT NMR of Compound 10 (100 MHz, DMSO-d₆)



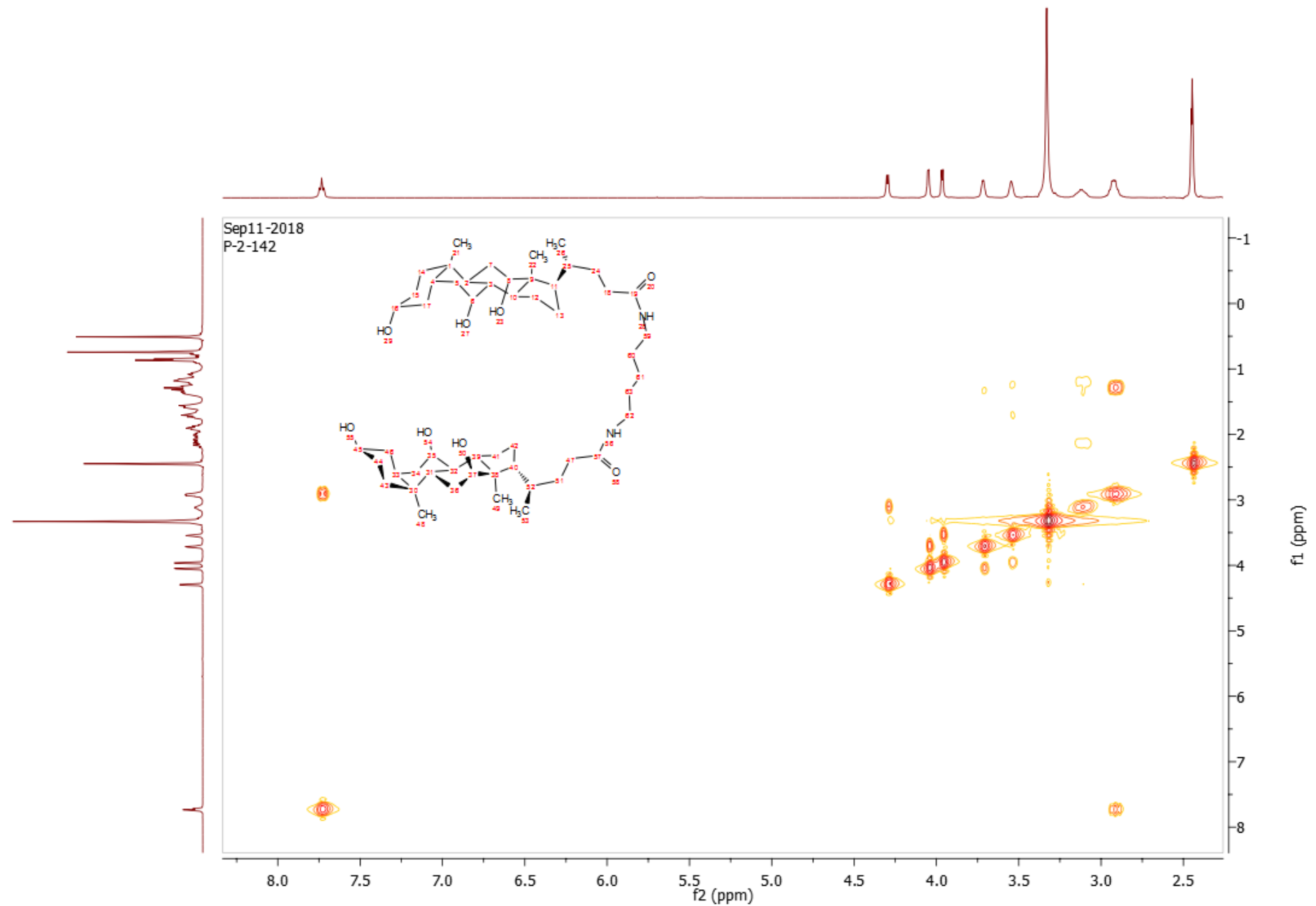
2D COSY NMR of Compound 10 (400 MHz, DMSO-d₆)



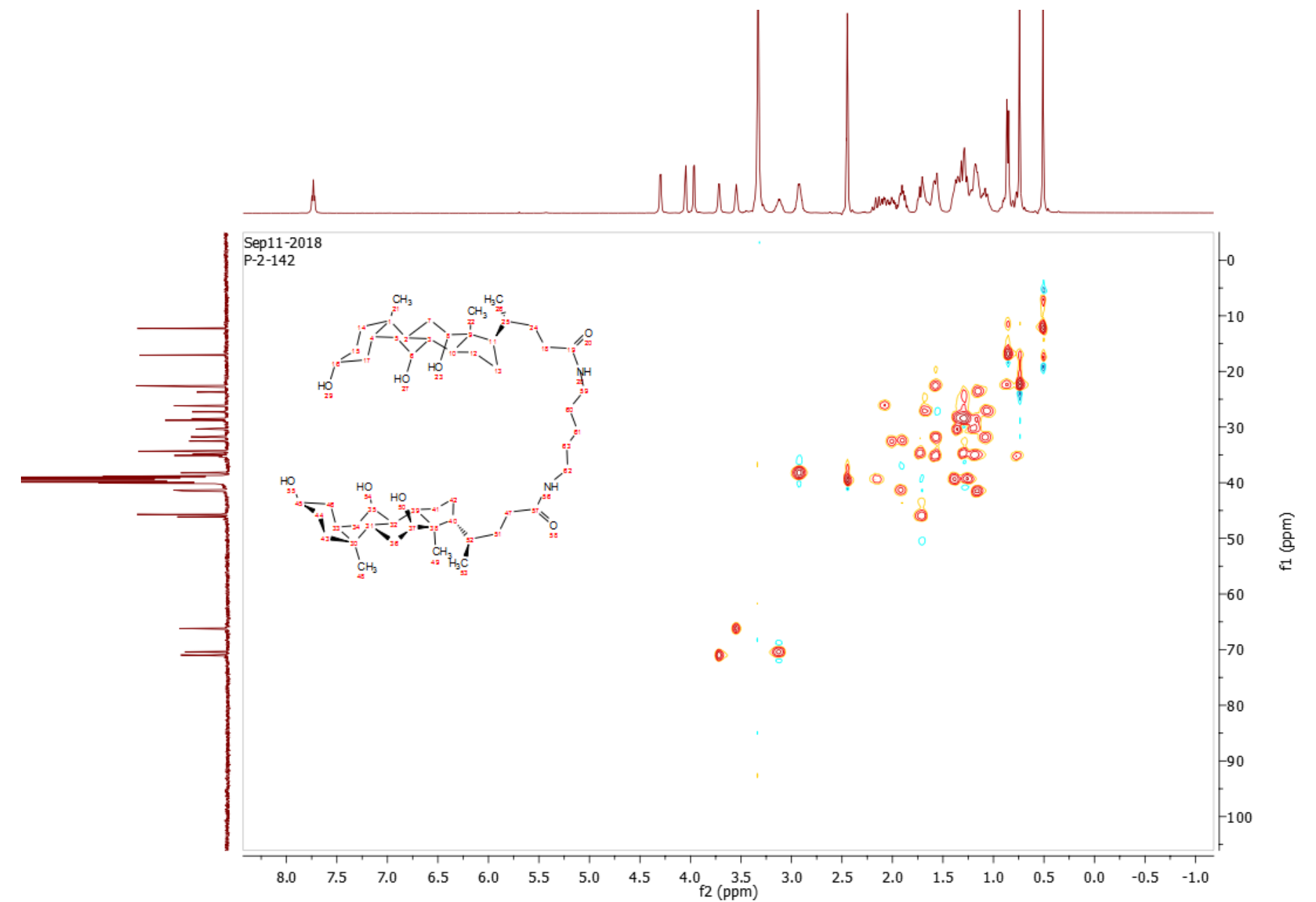
2D COSY NMR of Compound 10 (400 MHz, DMSO-d₆)



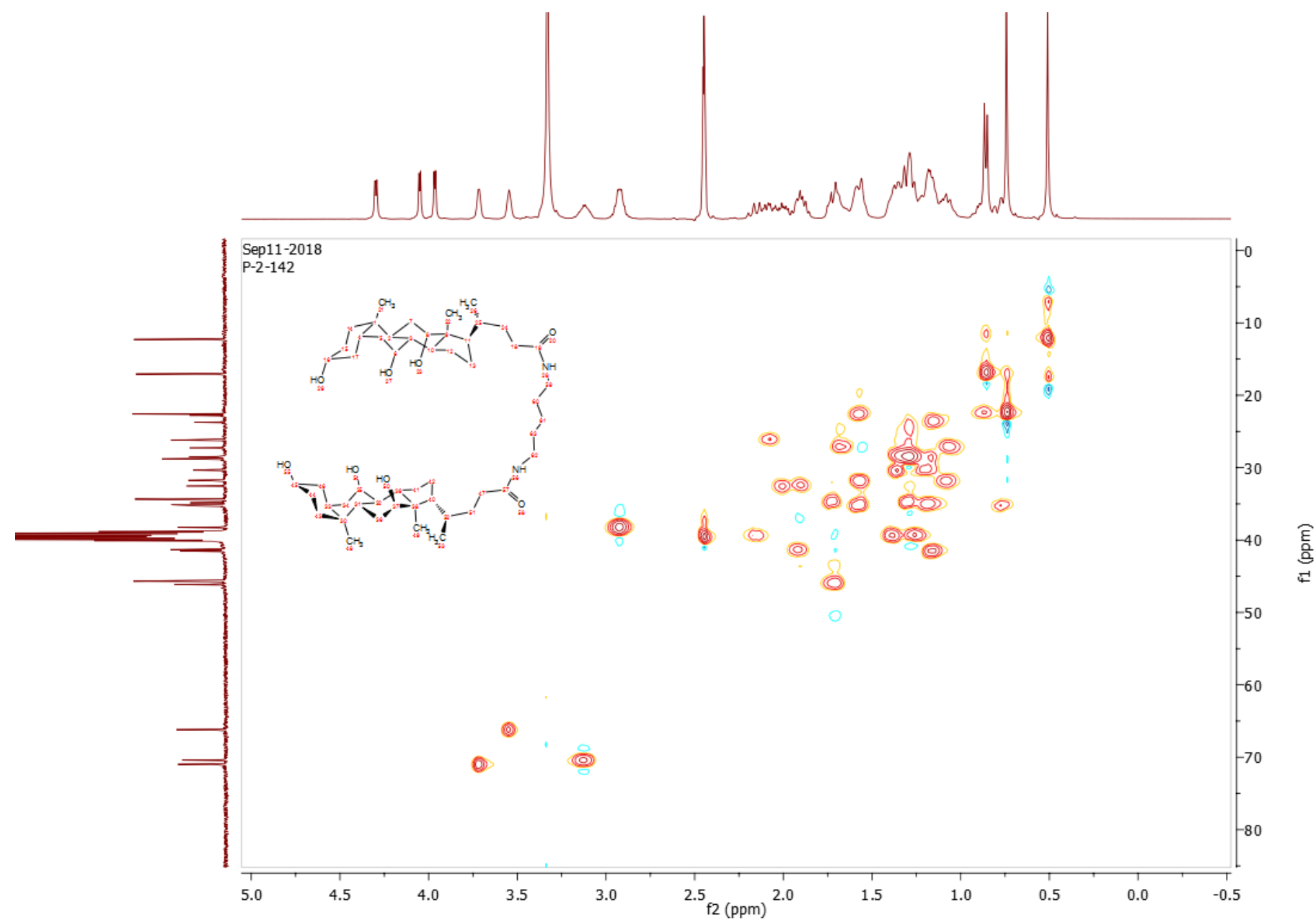
2D COSY NMR of Compound 10 (400 MHz, DMSO-d₆)



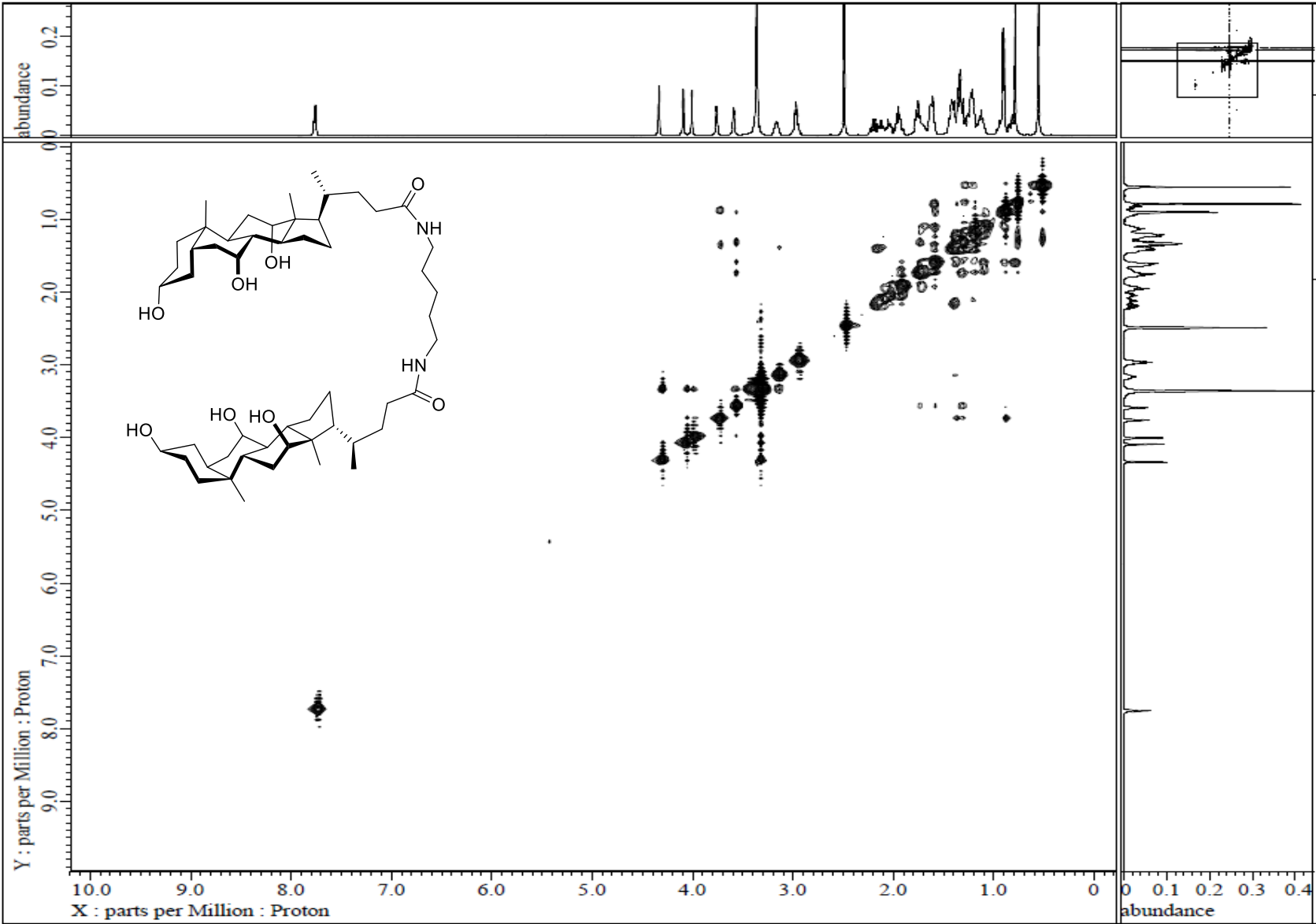
2D HSQC NMR of Compound 10 (400 MHz, DMSO-d₆)



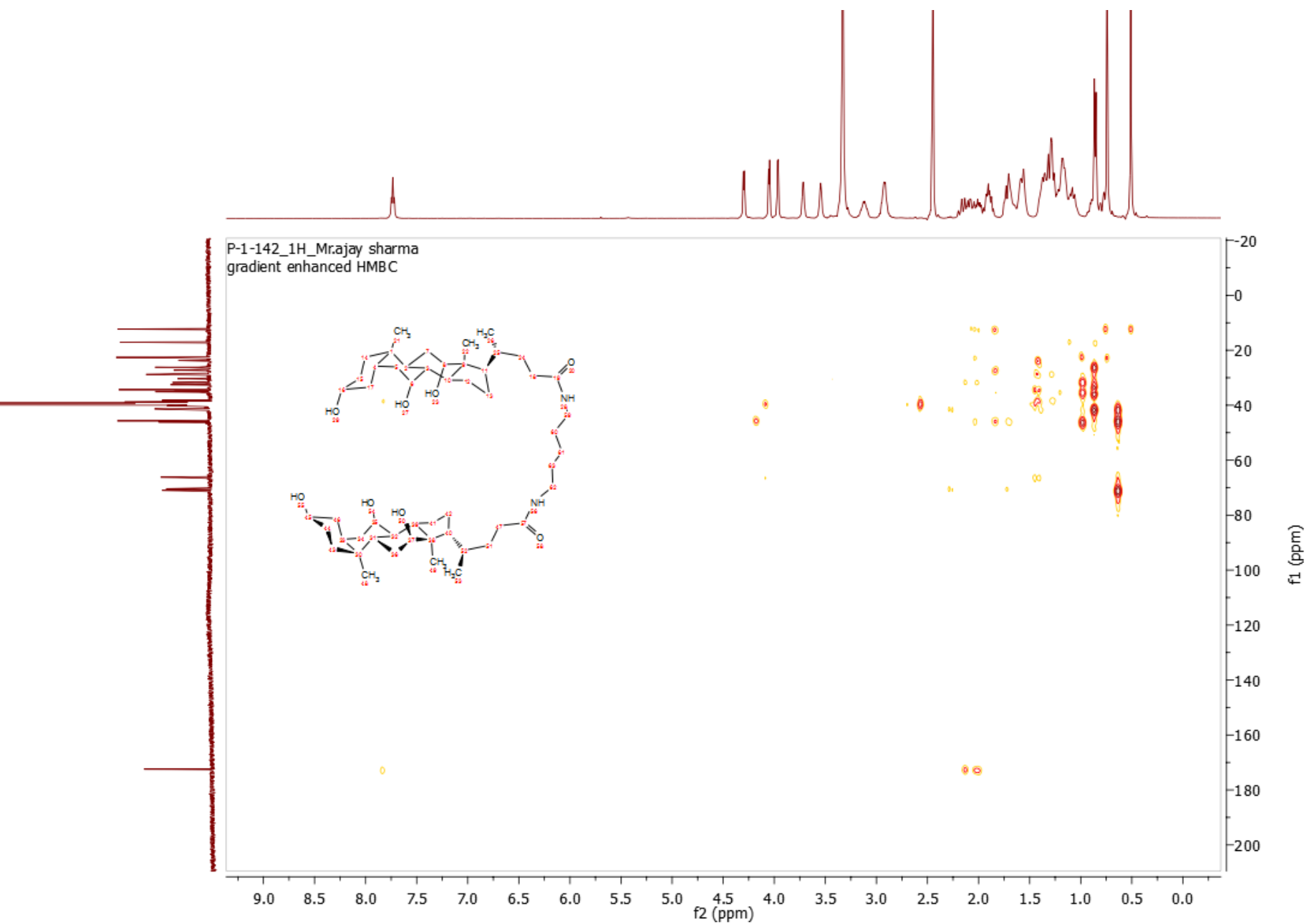
2D HSQC NMR of Compound 10 (400 MHz, DMSO-d₆)



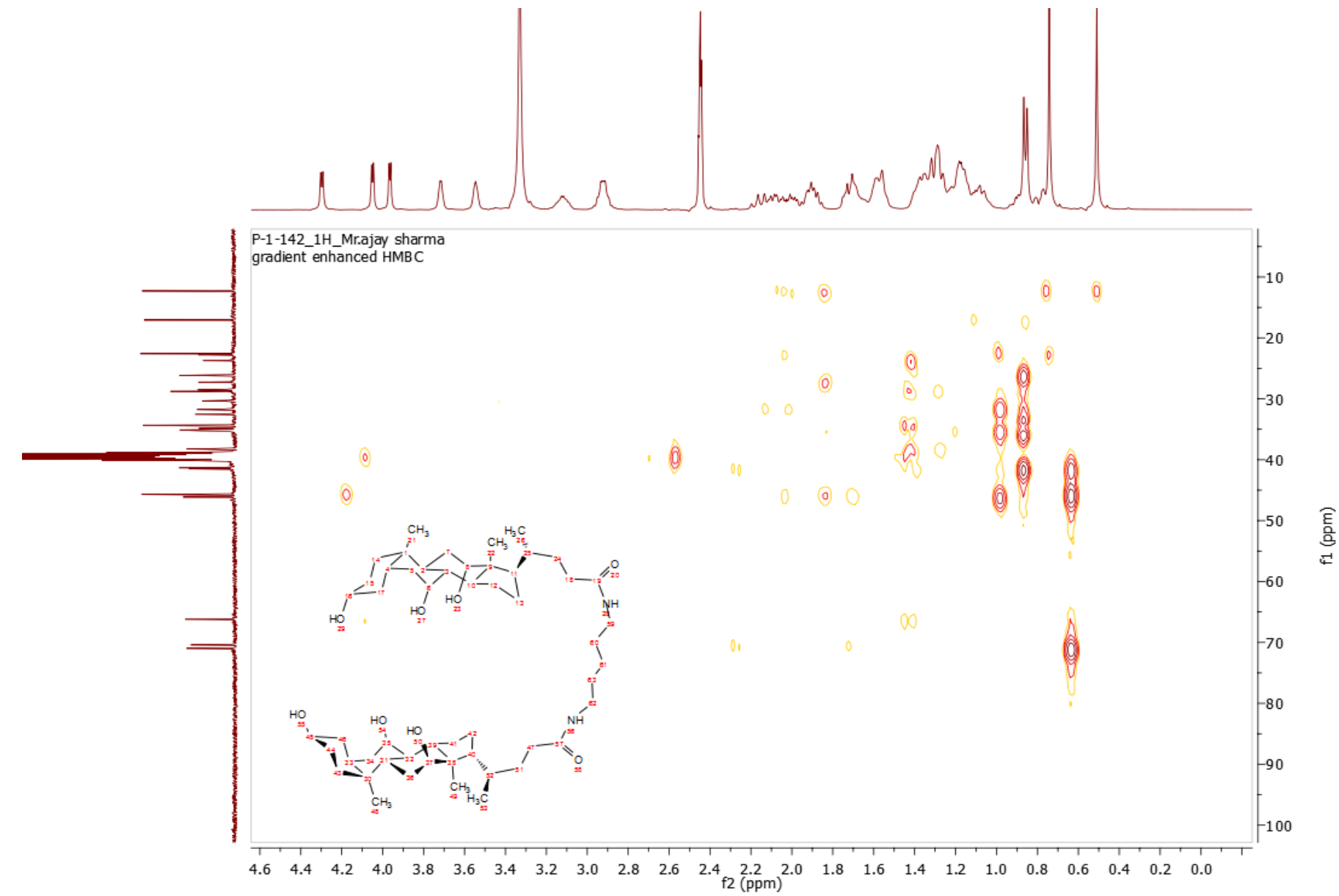
2D NOESY NMR of Compound 10 (500 MHz, DMSO-d₆)



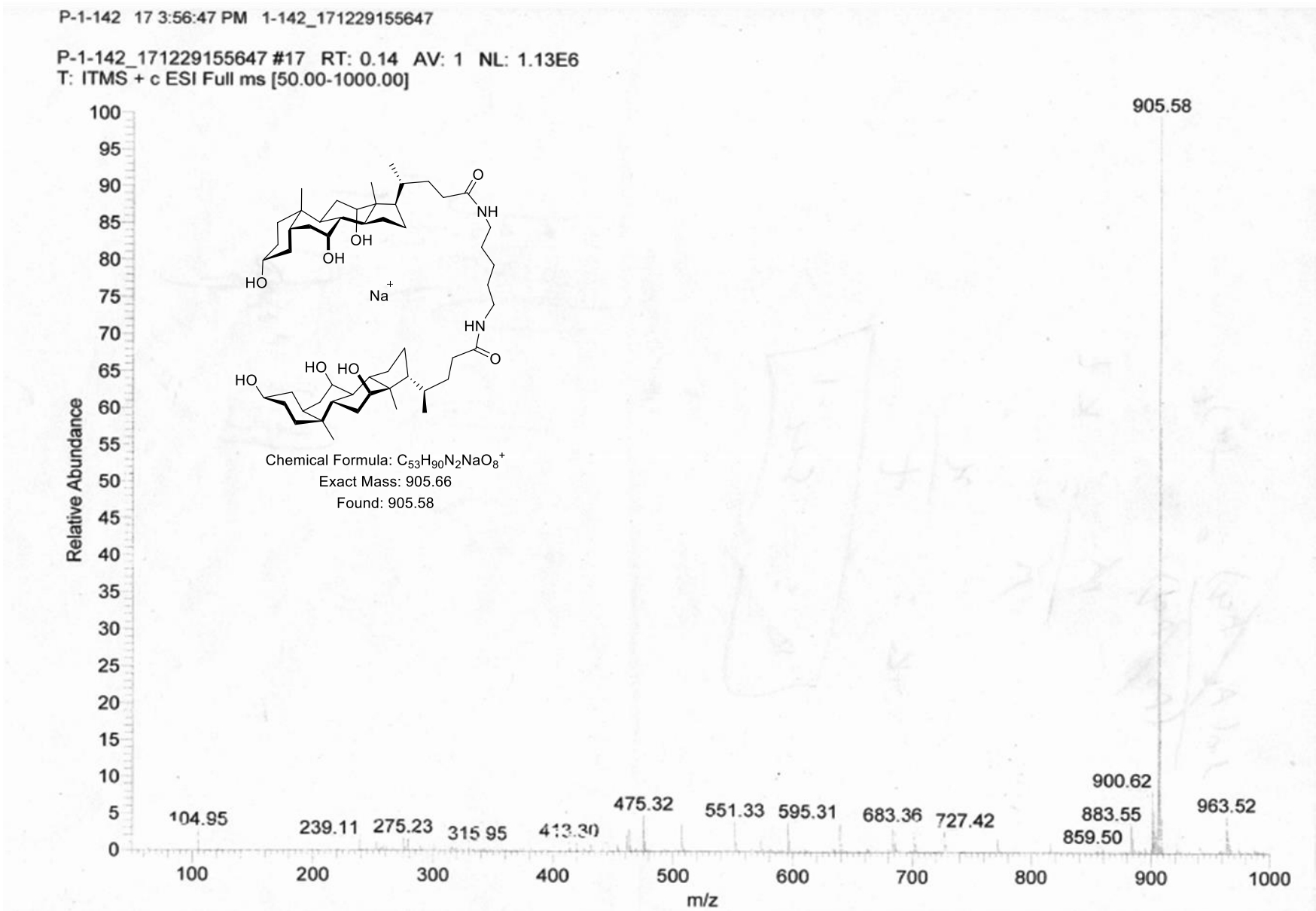
2D HMBC NMR of Compound 10 (500 MHz, DMSO-d₆)



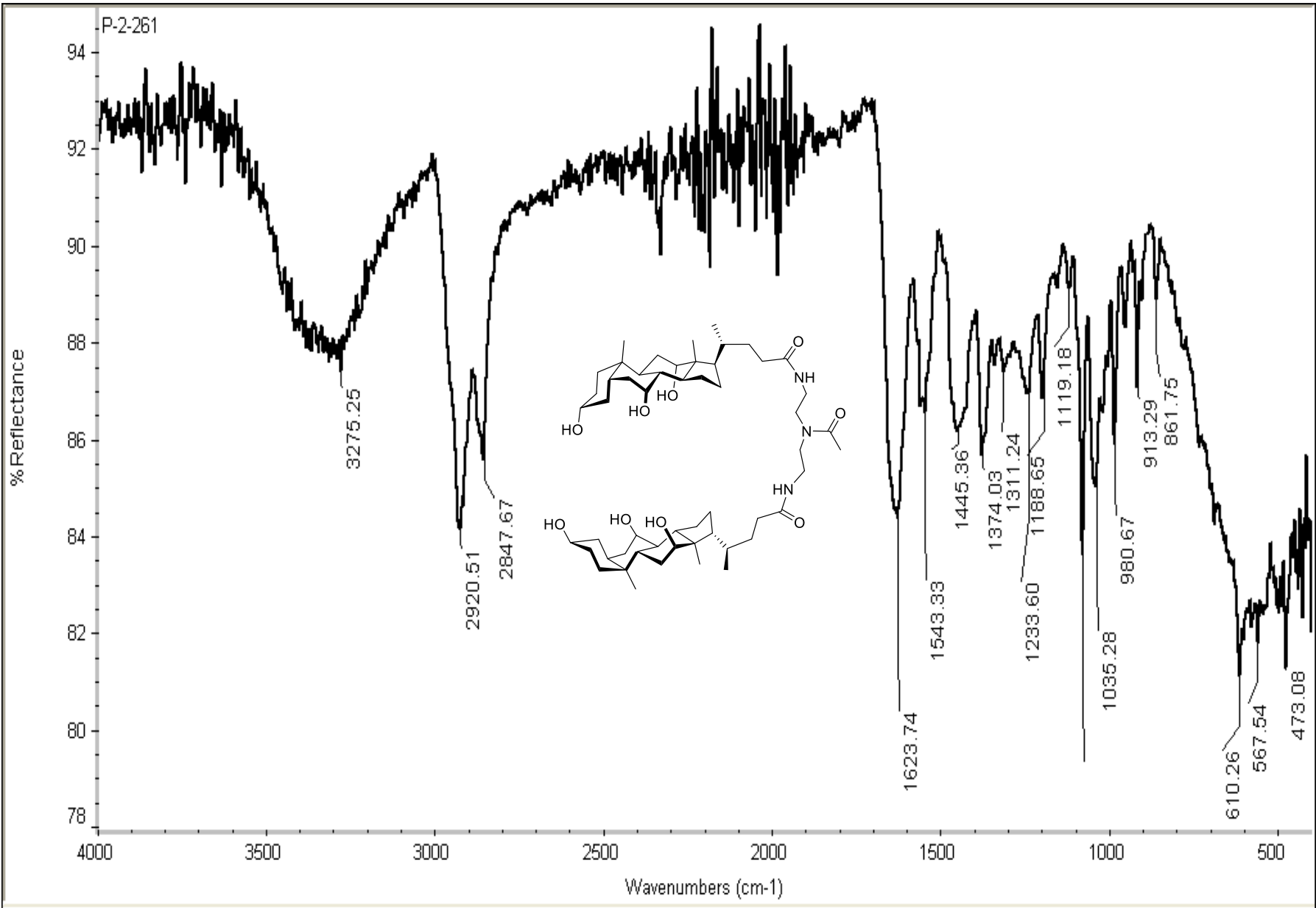
2D HMBC NMR of Compound 10 (500 MHz, DMSO-d₆)



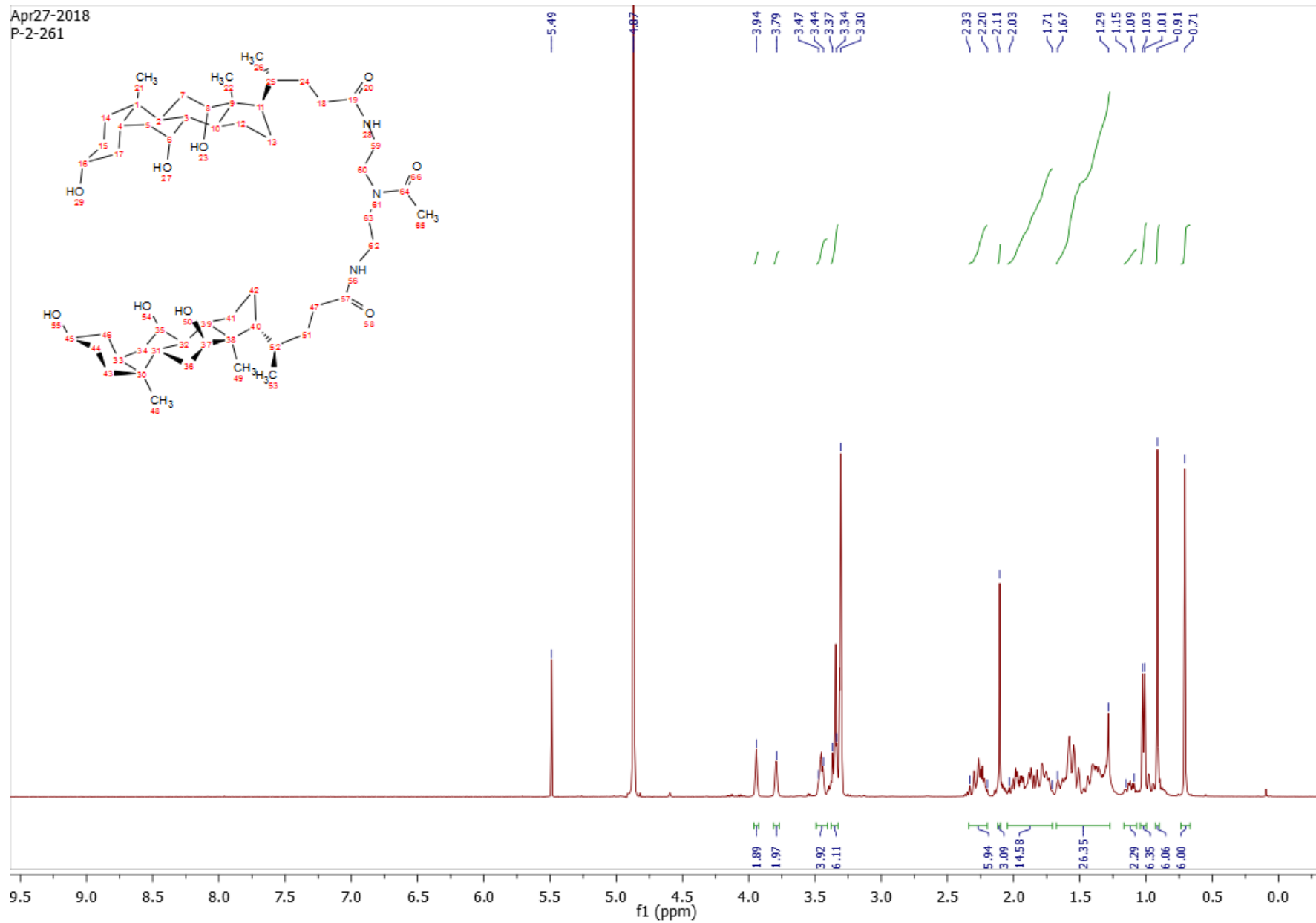
MS of Compound 10



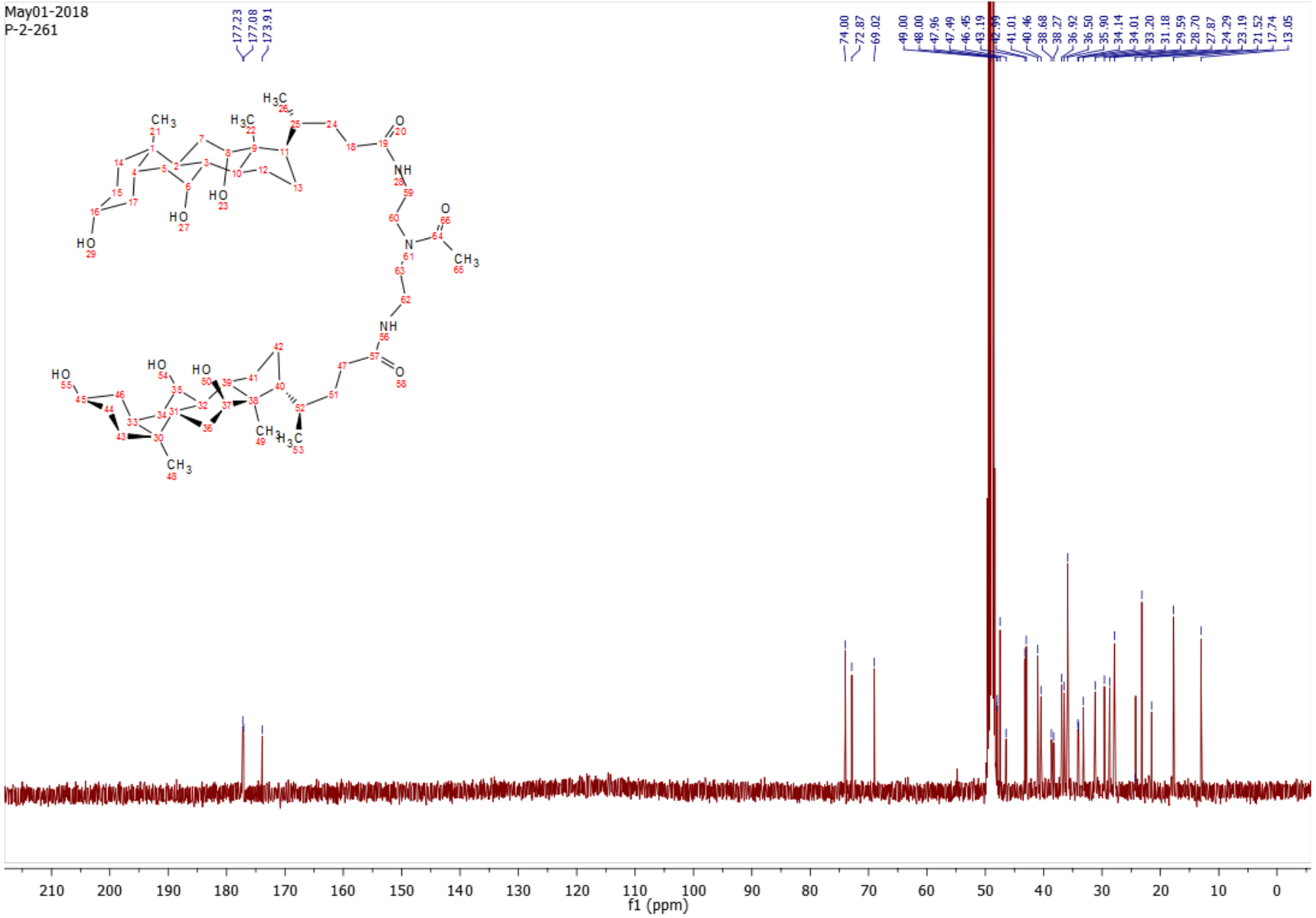
IR of Compound 11



¹H NMR of Compound 11 (400 MHz, CD₃OD)



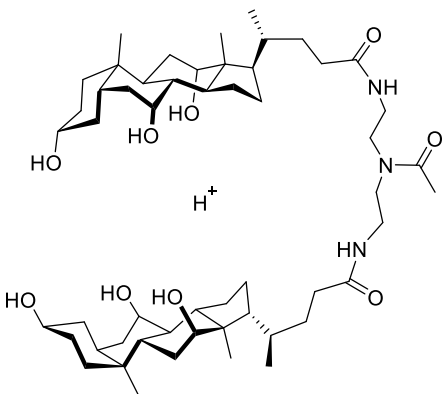
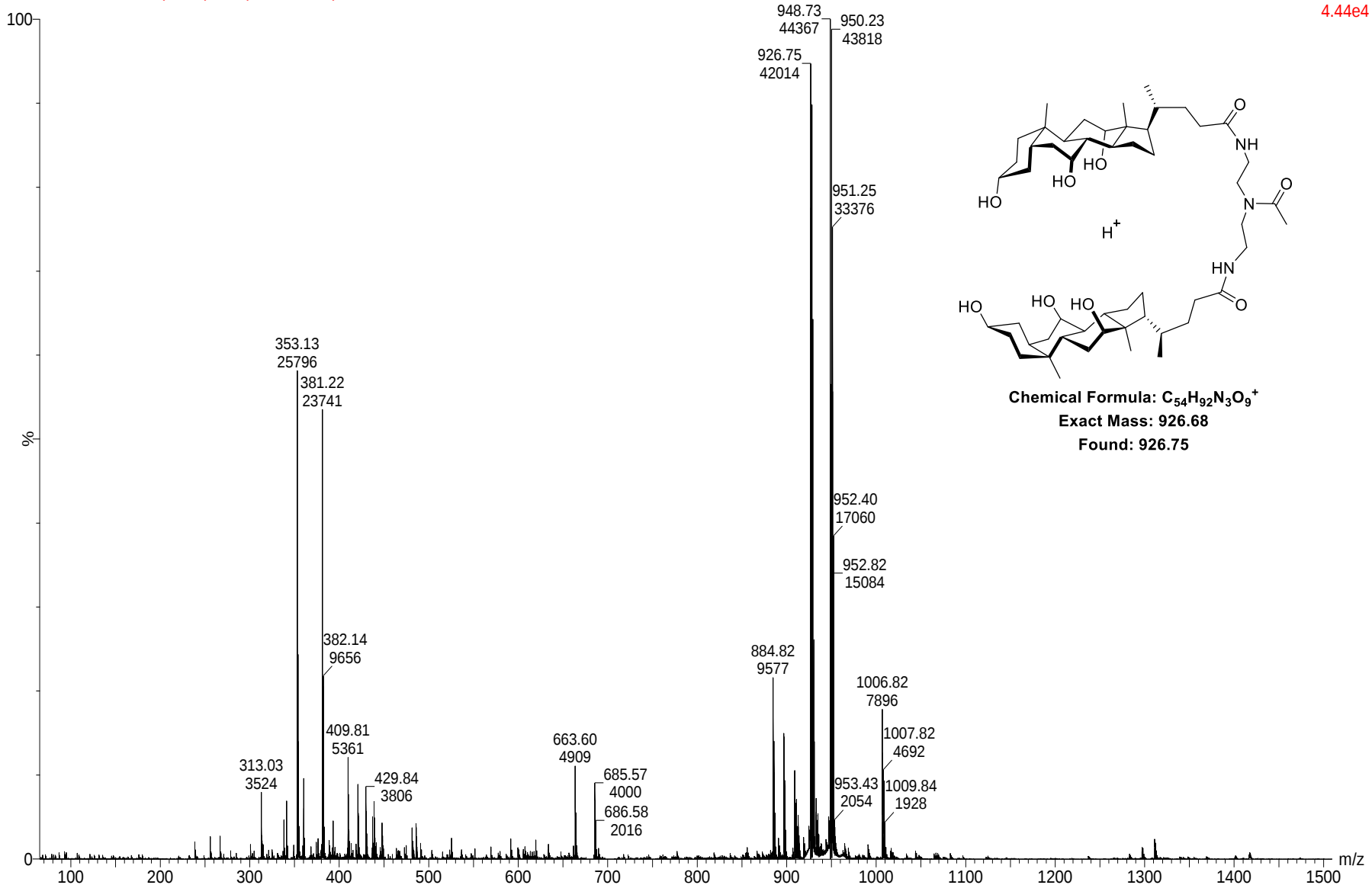
¹³C NMR of Compound 11 (100 MHz, CD₃OD)



MS of Compound 11

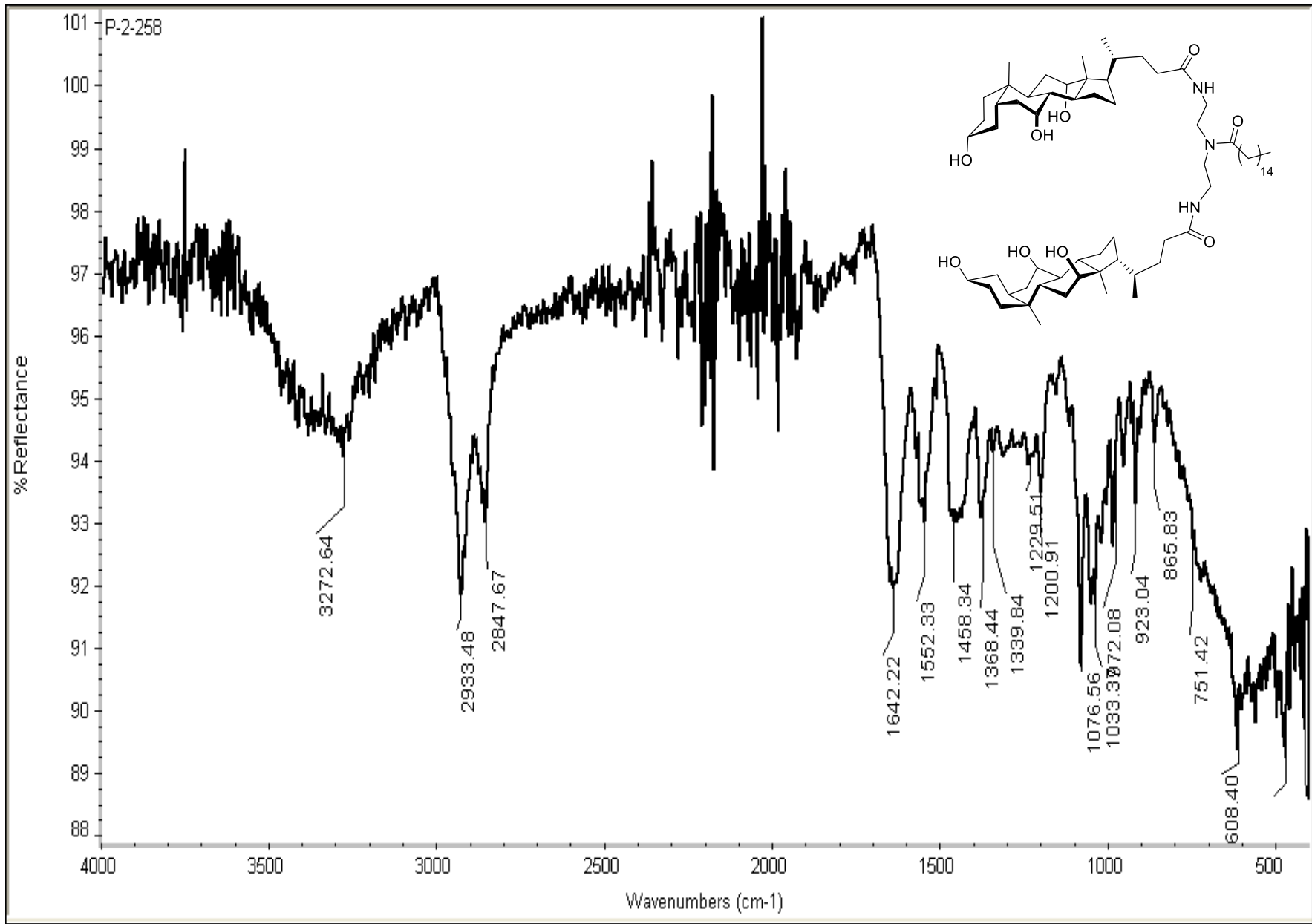
WATERS, Q-TOF MICROMASS (ESI-MS)
POONAM P-2-255 18 (0.334) Cm (12:36-49:87)

SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
4.44e4

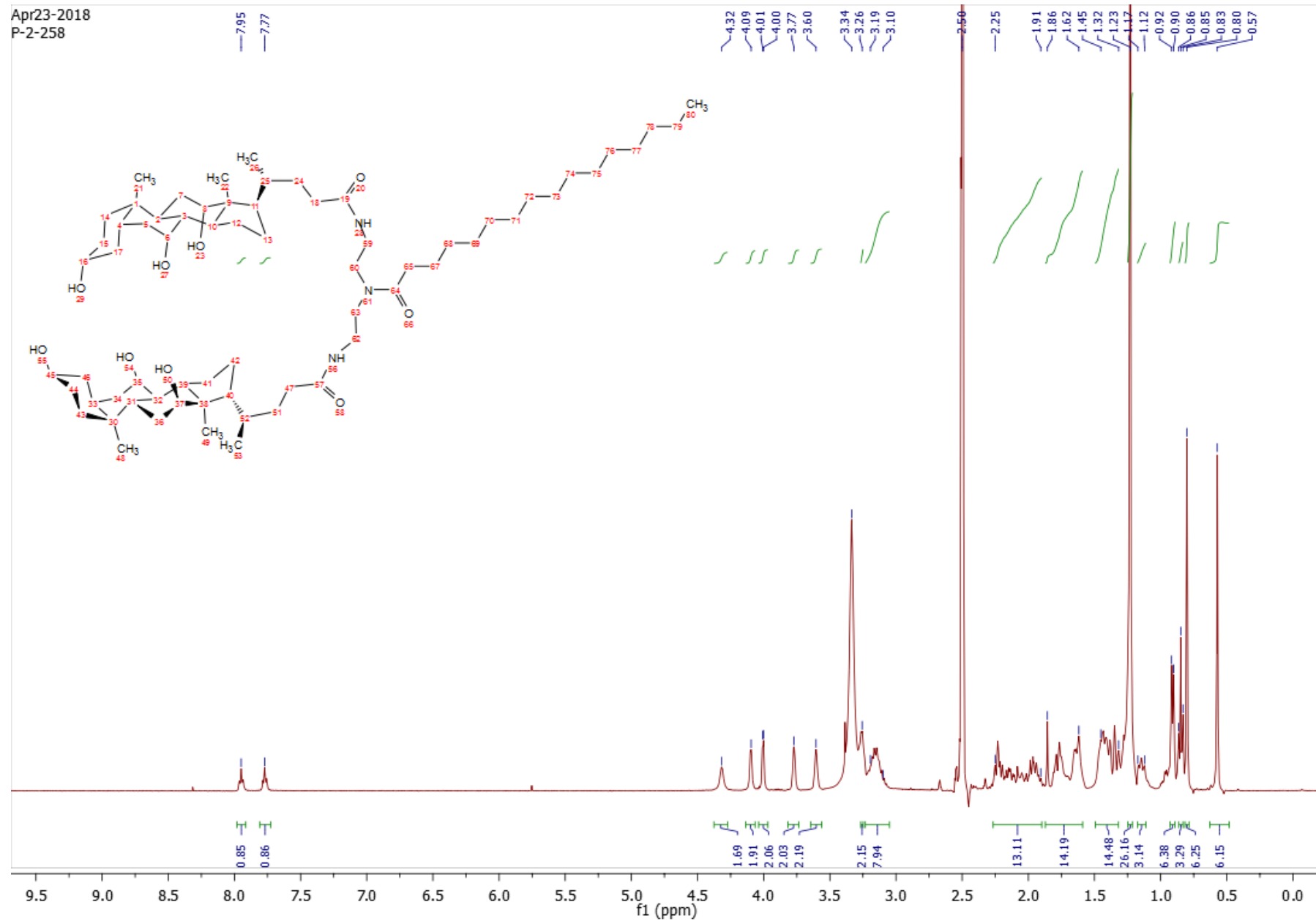


Chemical Formula: $C_{54}H_{92}N_3O_9^+$
Exact Mass: 926.68
Found: 926.75

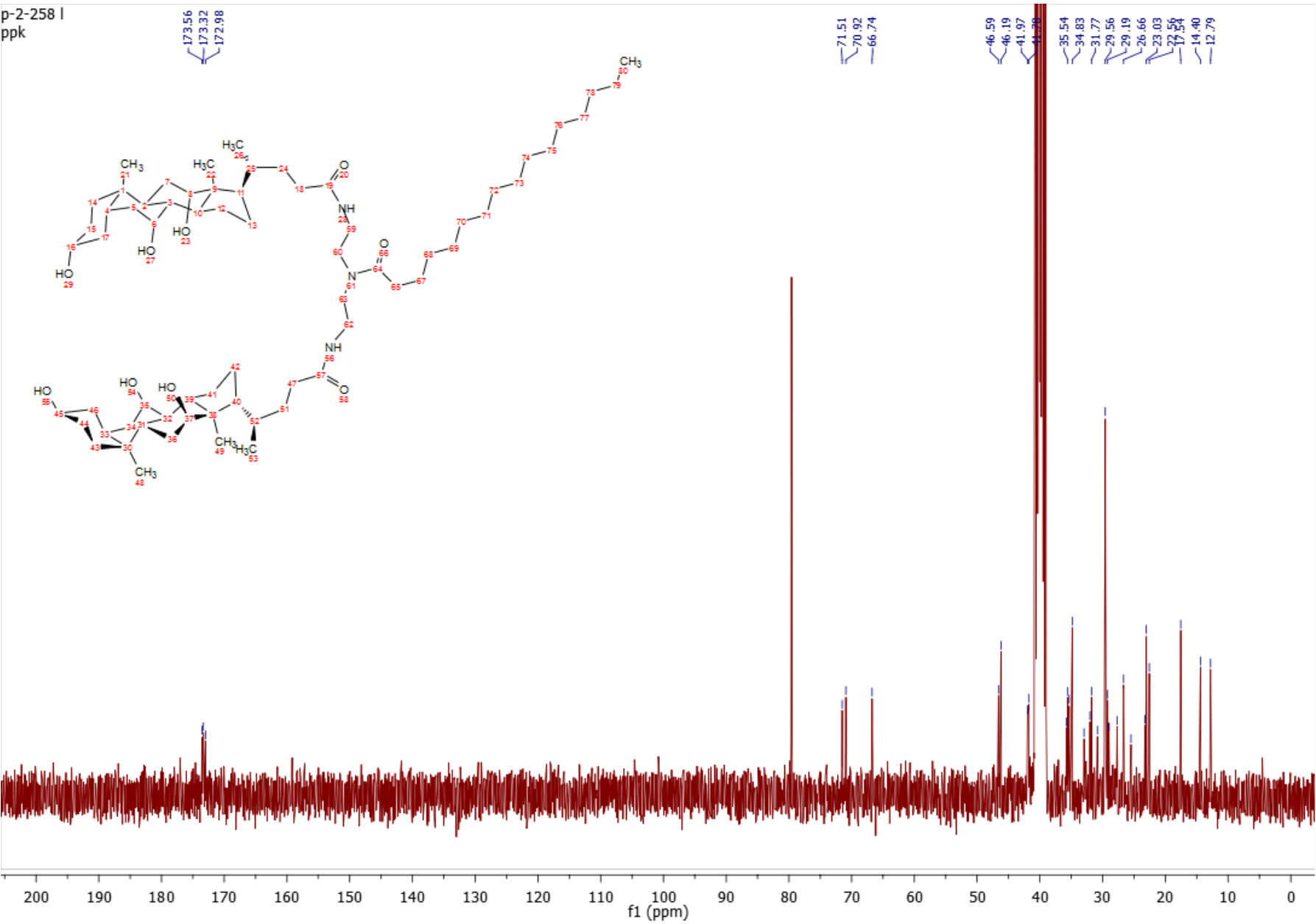
IR of Compound 12



^1H NMR of Compound 12 (400 MHz, DMSO- d_6)



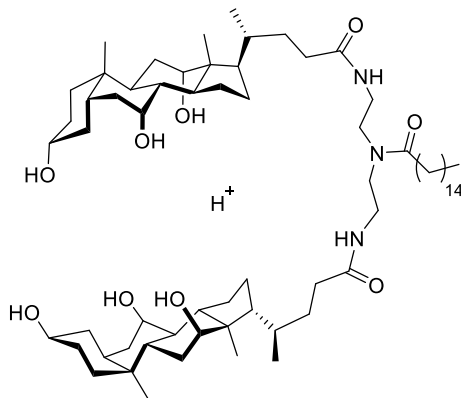
¹³C NMR of Compound 12 (75 MHz, DMSO-*d*₆)



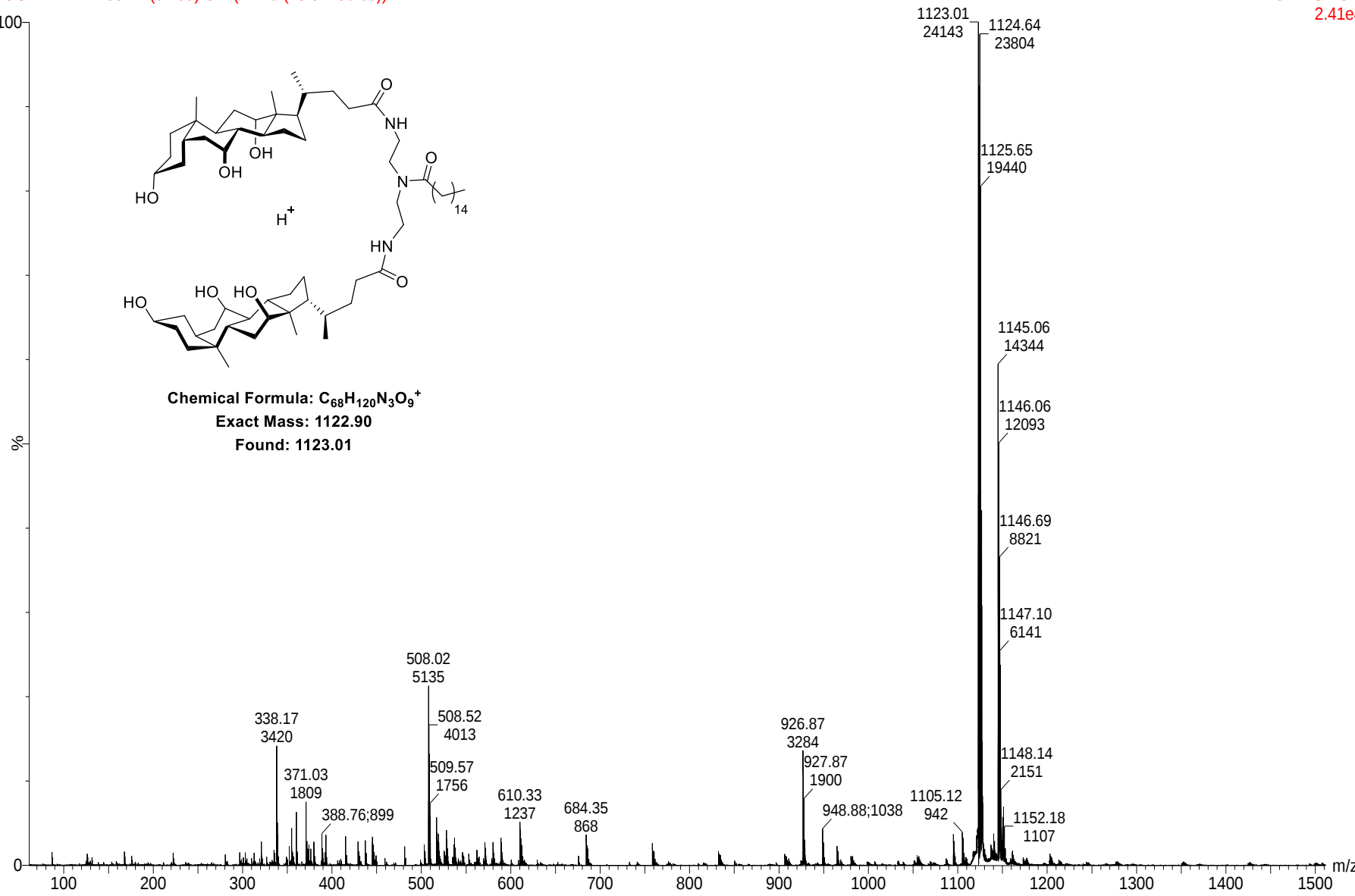
MS of Compound 12

WATERS, Q-TOF MICROMASS (ESI-MS)
POONAM P-2-258 22 (0.409) Cm (11:26-(73:84+50:66))

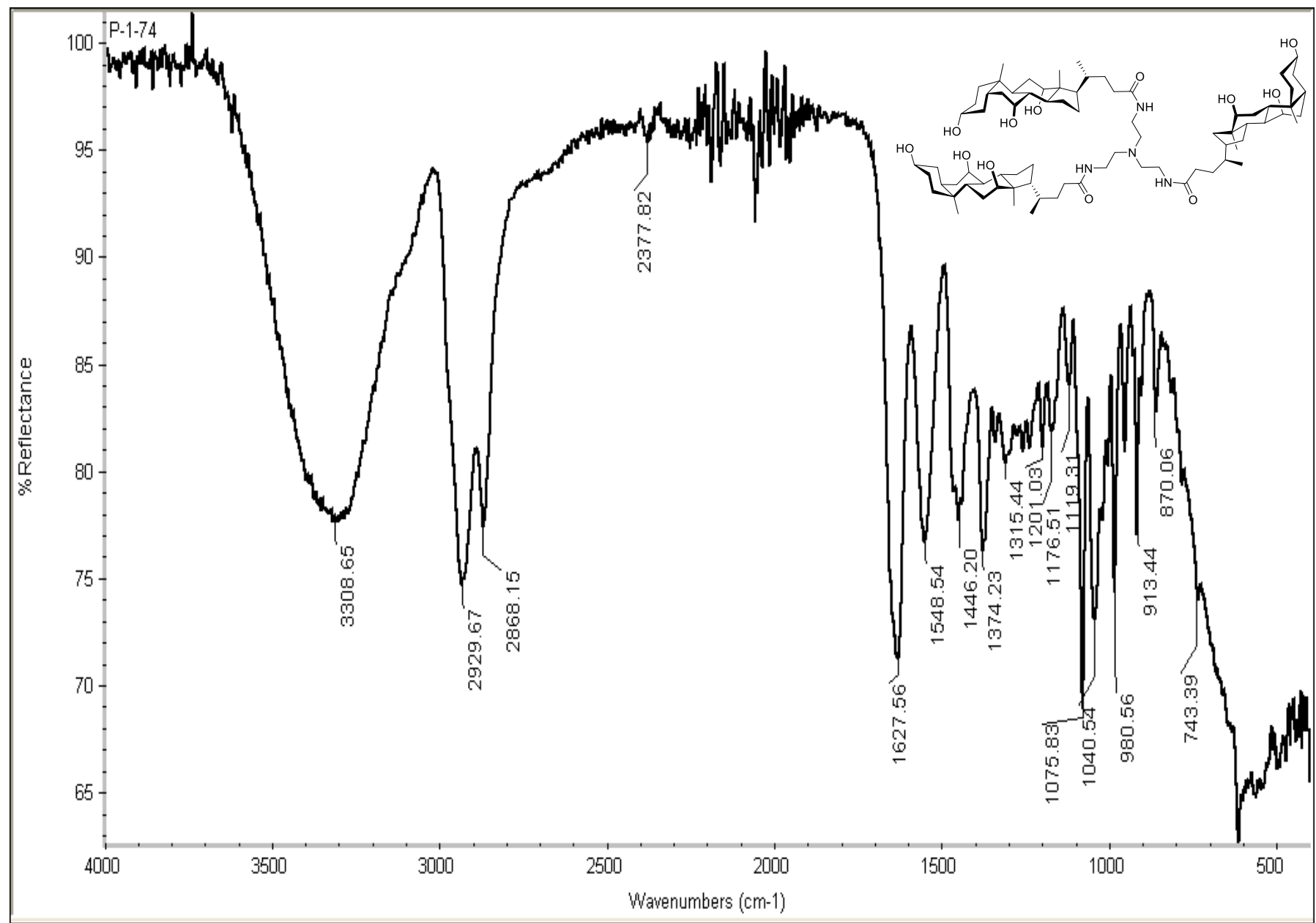
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
2.41e4



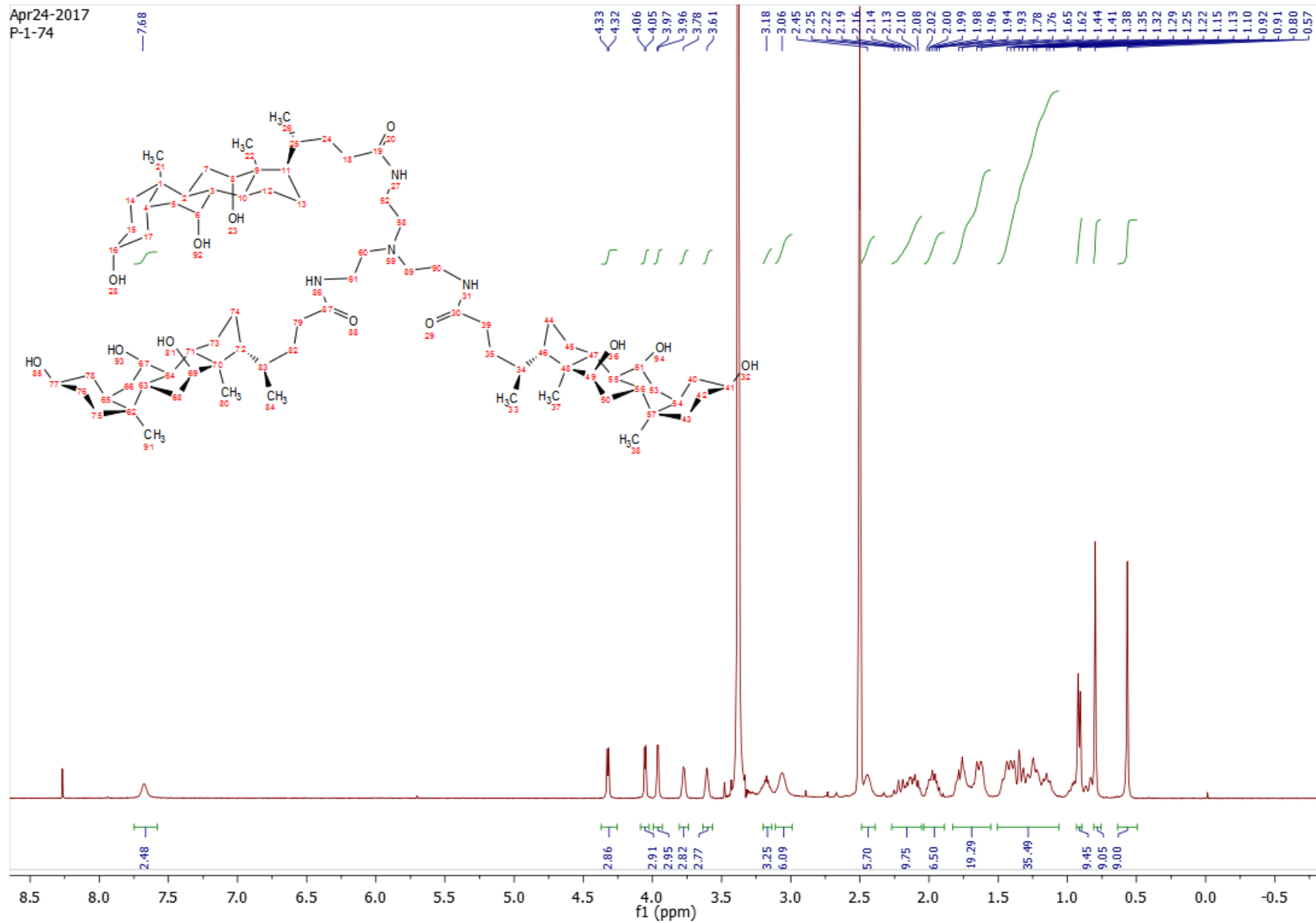
Chemical Formula: $C_{68}H_{120}N_3O_9^+$
Exact Mass: 1122.90
Found: 1123.01



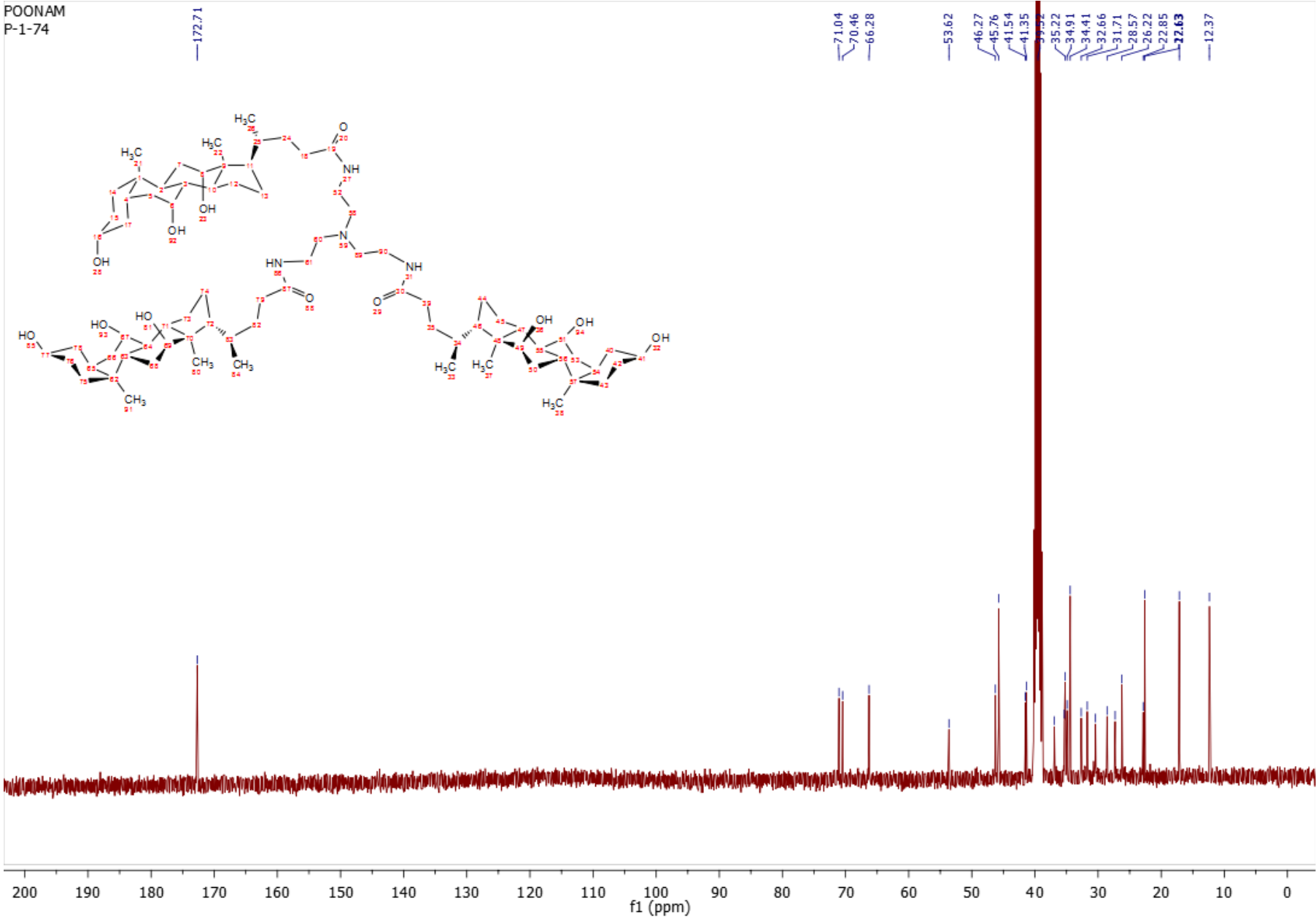
IR of Compound 13a



¹H NMR of Compound 13a (400 MHz, DMSO-d₆)

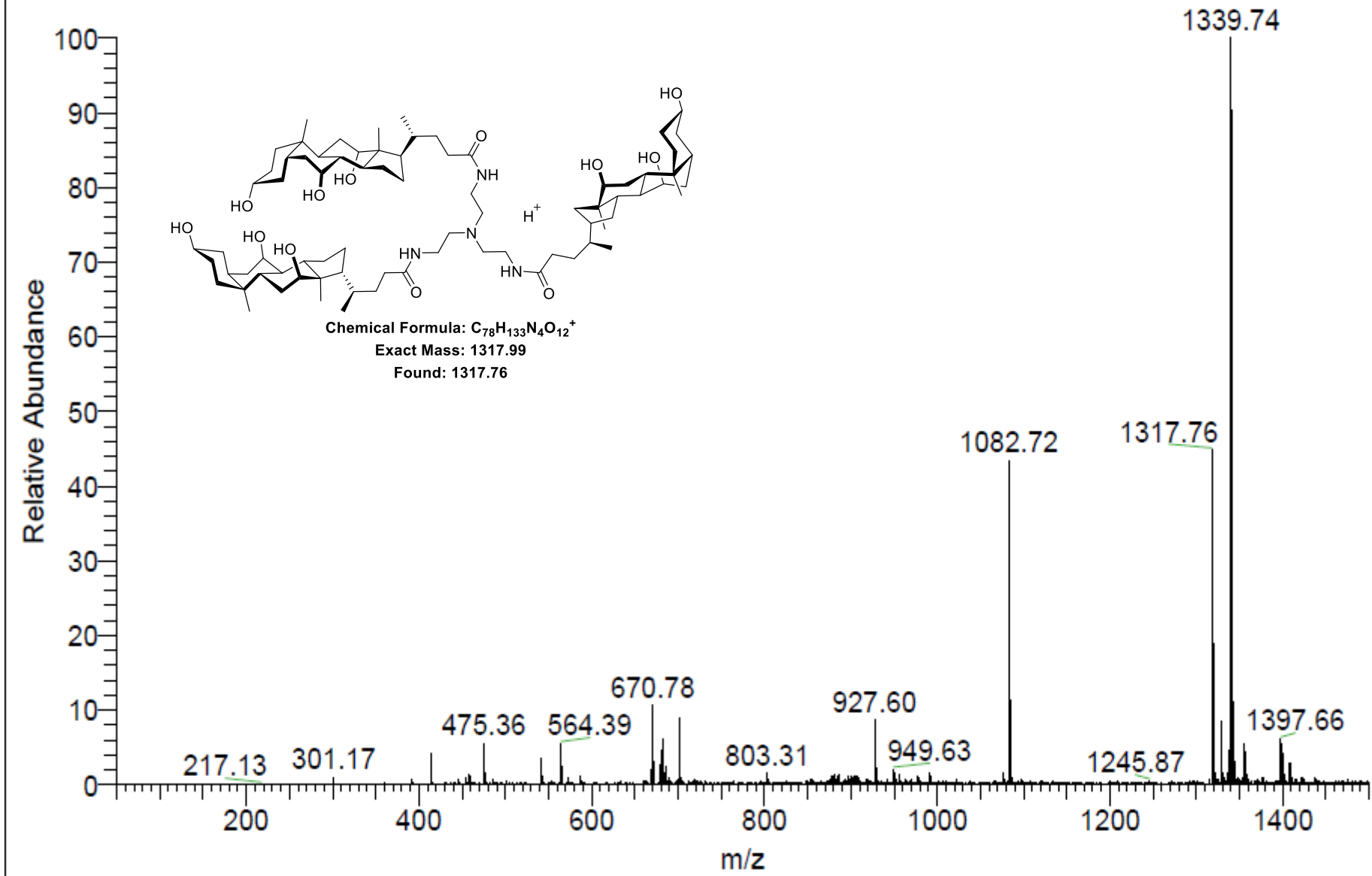


¹³C NMR of Compound 13a (100 MHz, DMSO-d₆)

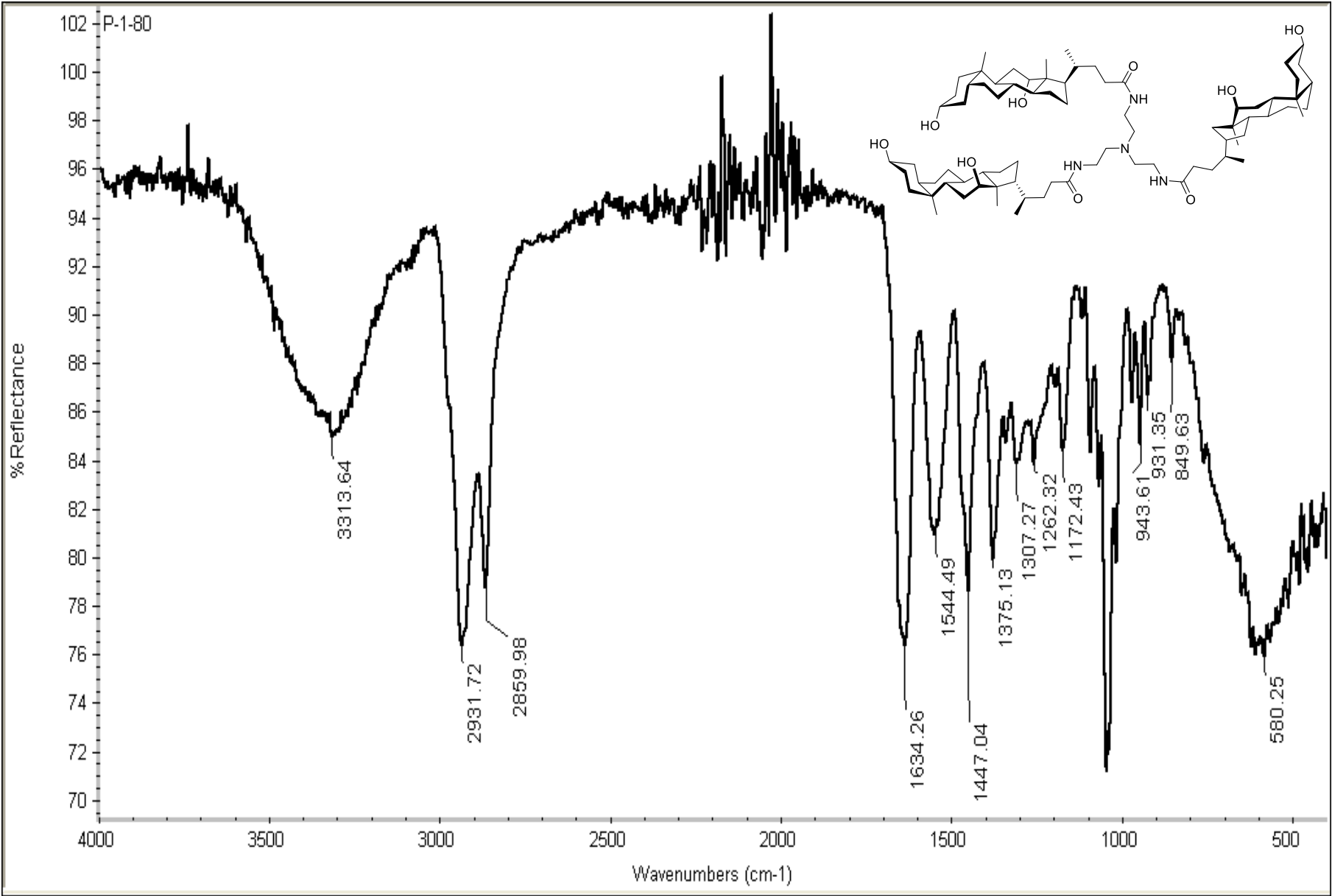


MS of Compound 13a

P-1-74_180105110401 #17 RT: 0.17 AV: 1 NL: 7.38E5
T: ITMS + c ESI Full ms [50.00-1500.00]

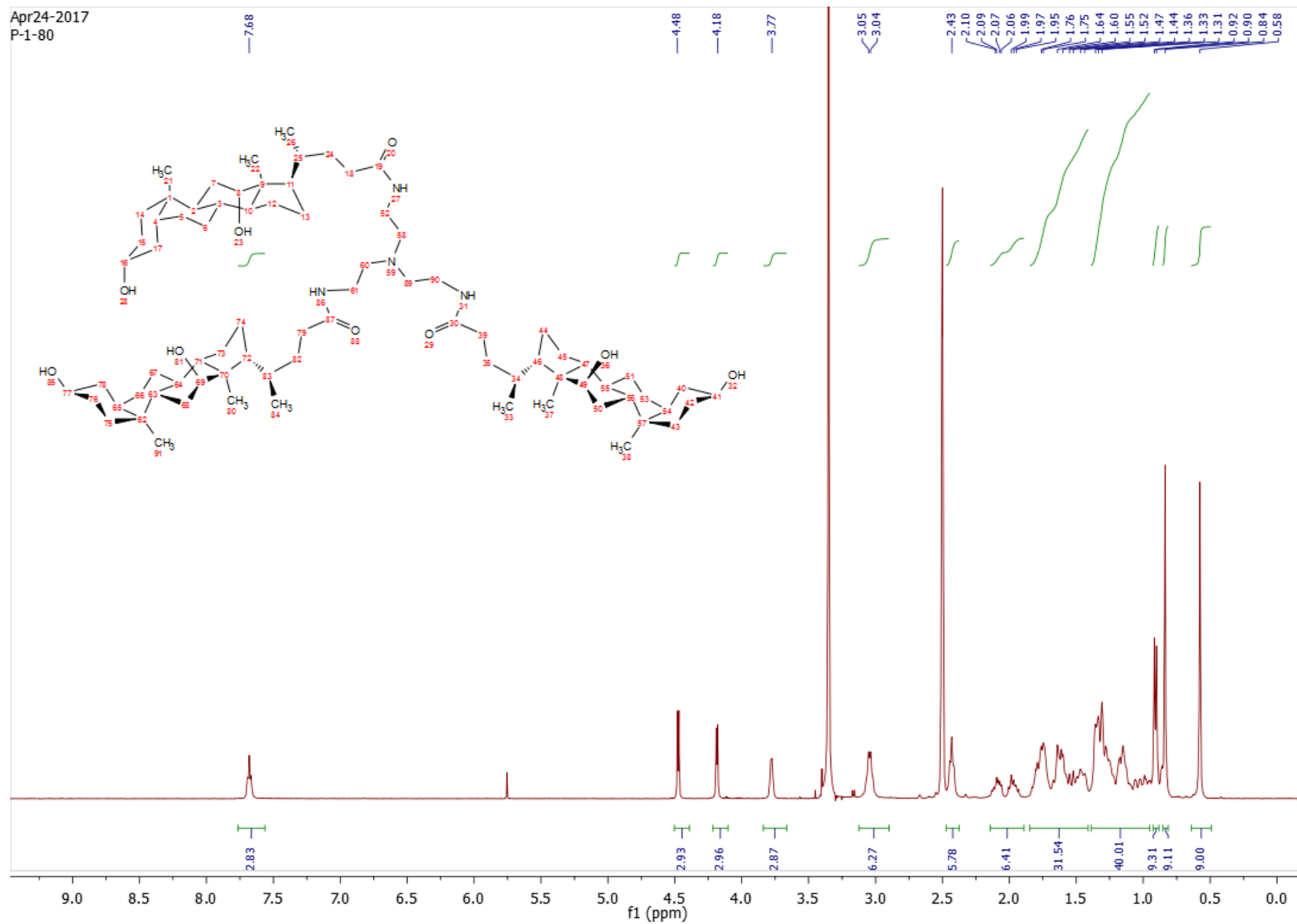


IR of Compound **13b**

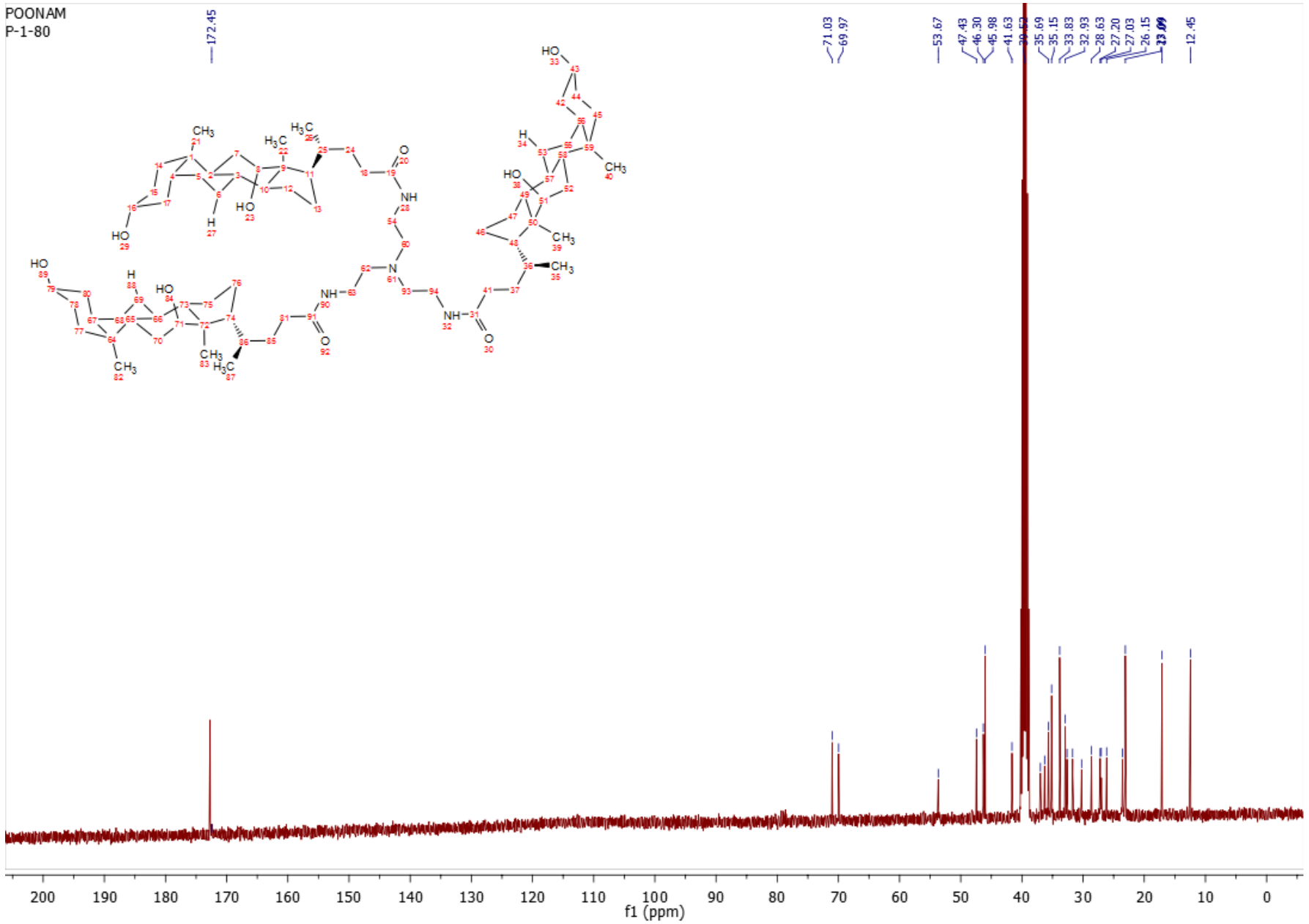


¹H NMR of Compound **13b** (400 MHz, DMSO-*d*₆)

Apr24-2017
P-1-80



¹³C NMR of Compound 13b (100 MHz, DMSO-d₆)



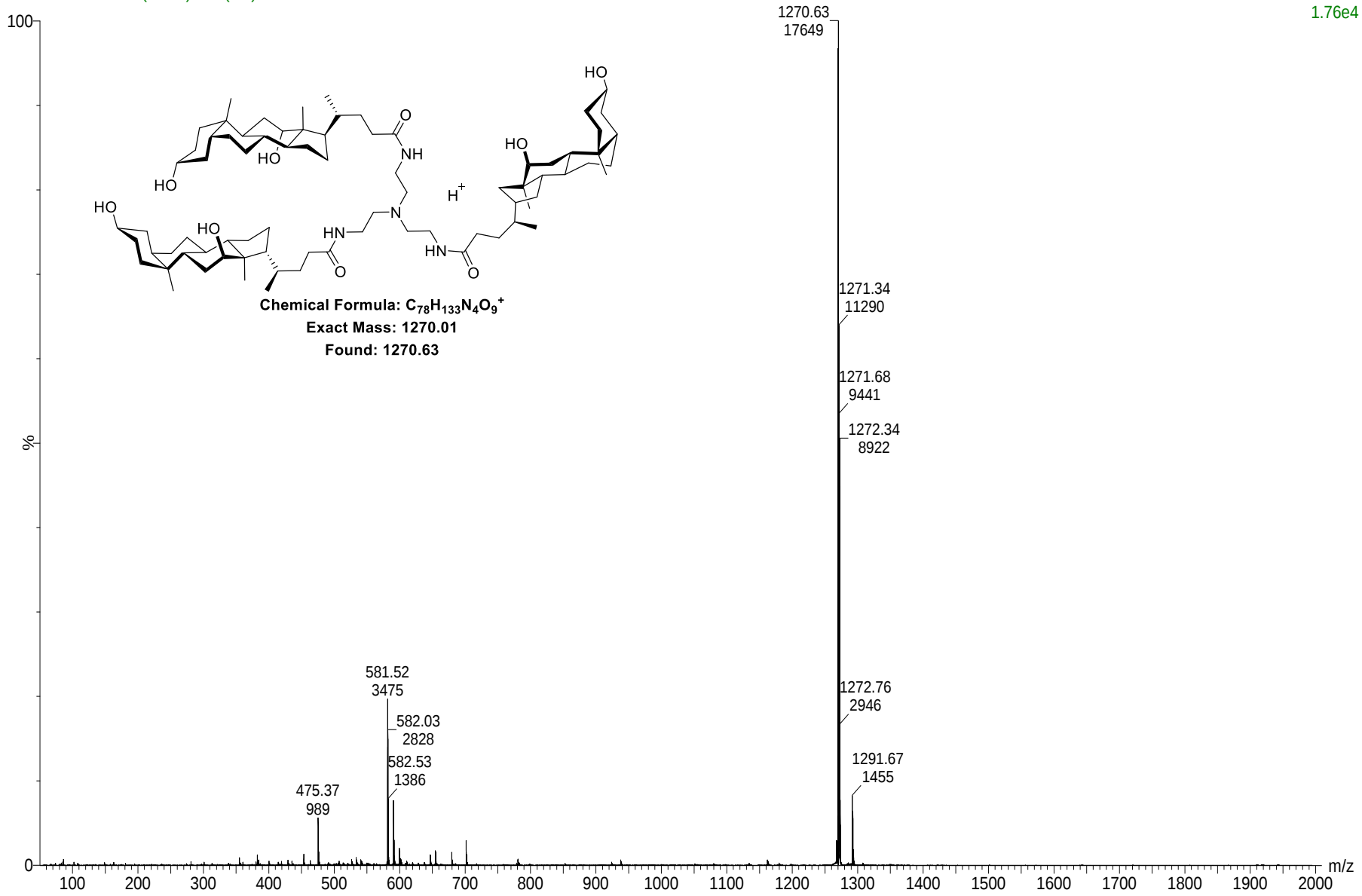
MS of Compound 13b

WATERS, Q-TOF MICROMASS (ESI-MS)

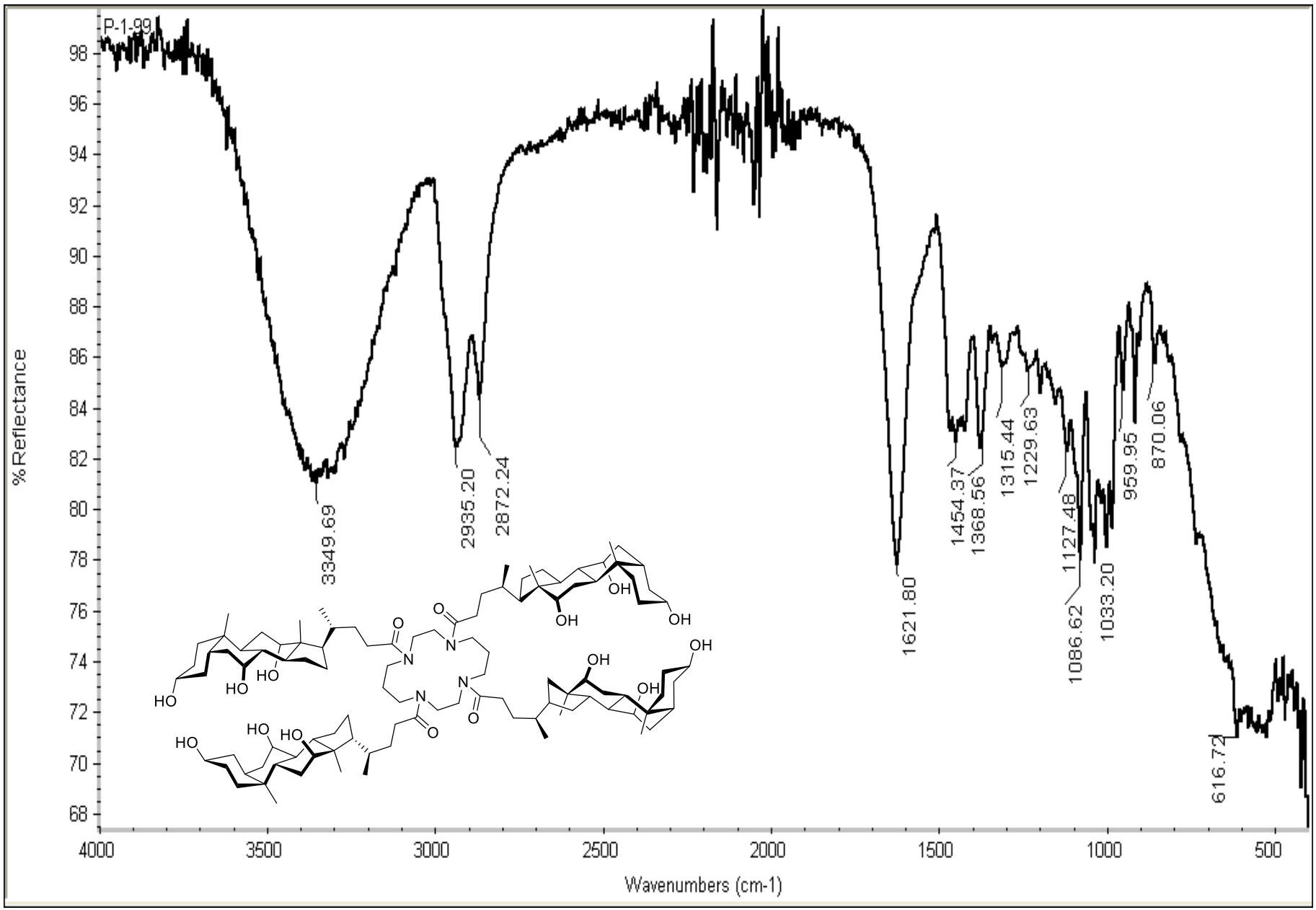
POONAM P-1-80 8 (0.282) Cm (4:8)

SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH

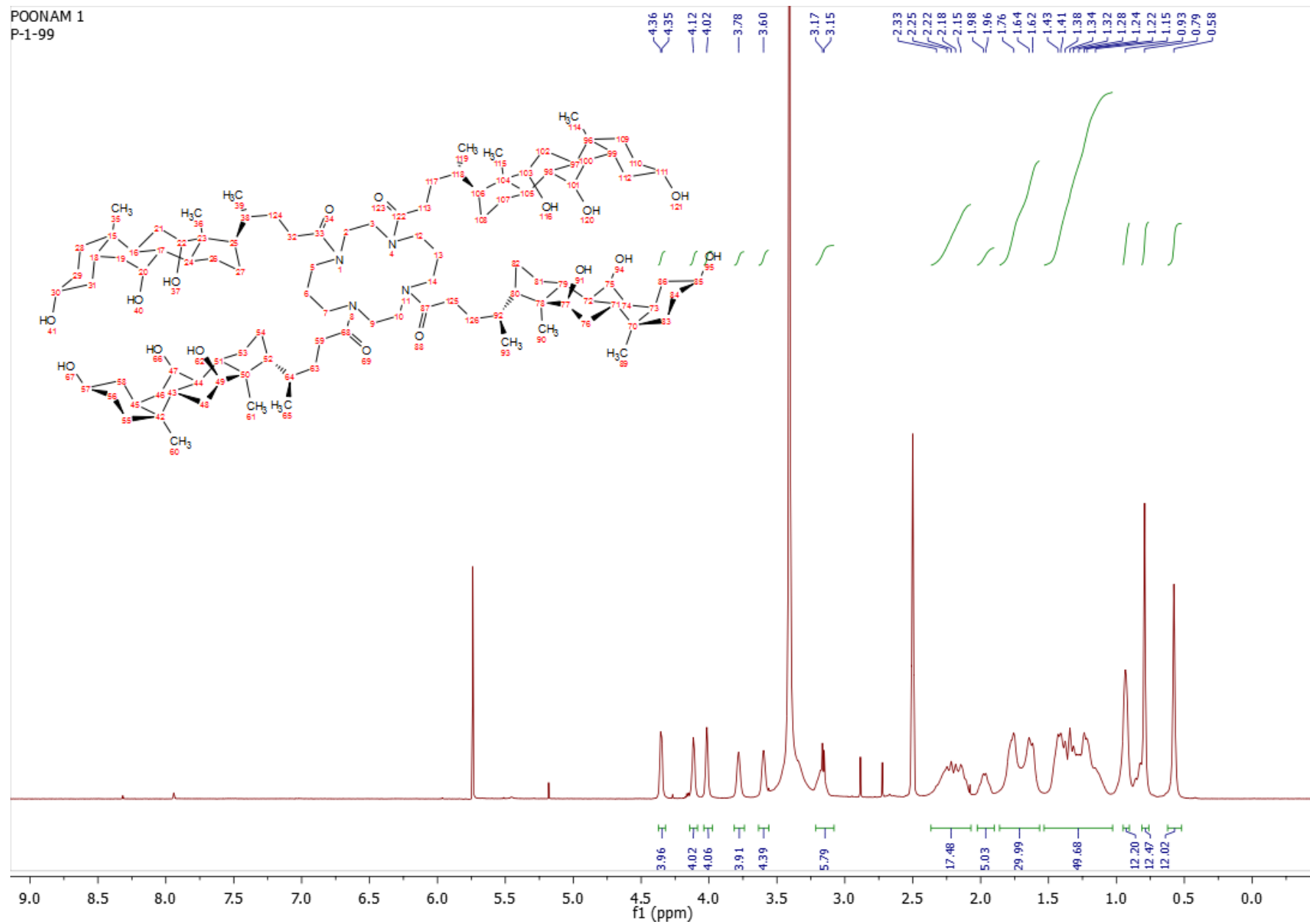
TOF MS ES+
1.76e4



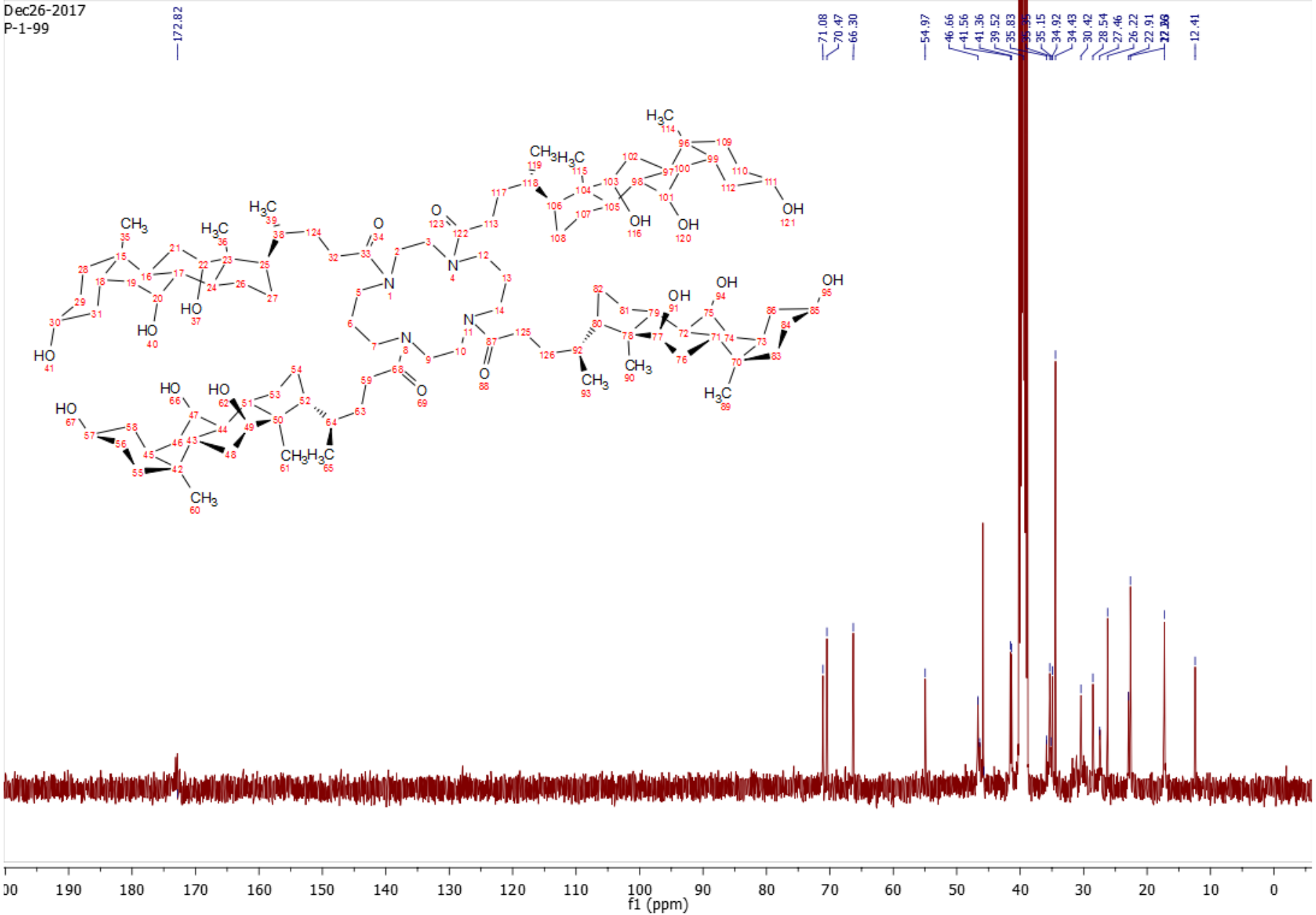
IR of Compound 14



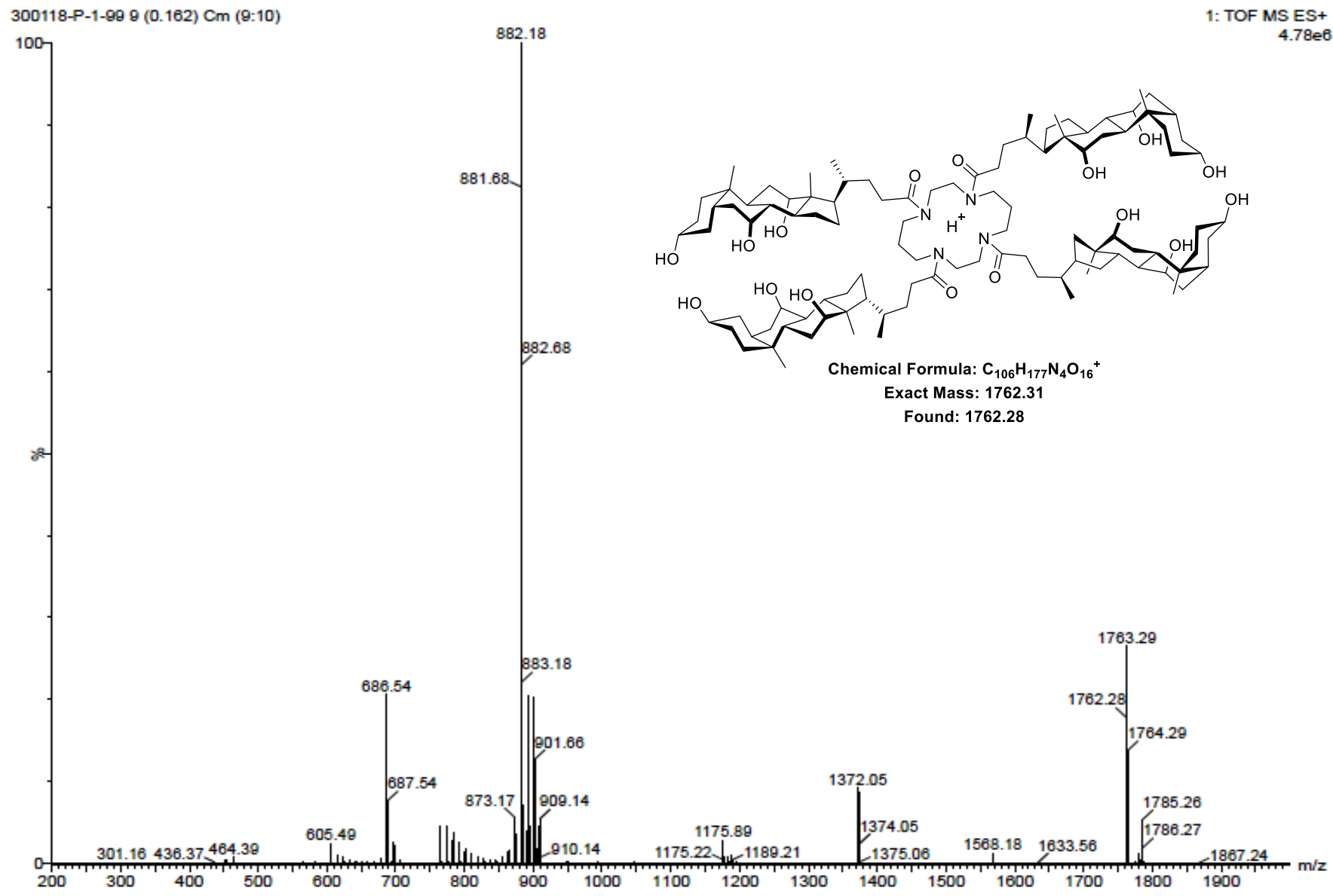
^1H NMR of Compound 14 (400 MHz, DMSO- d_6)



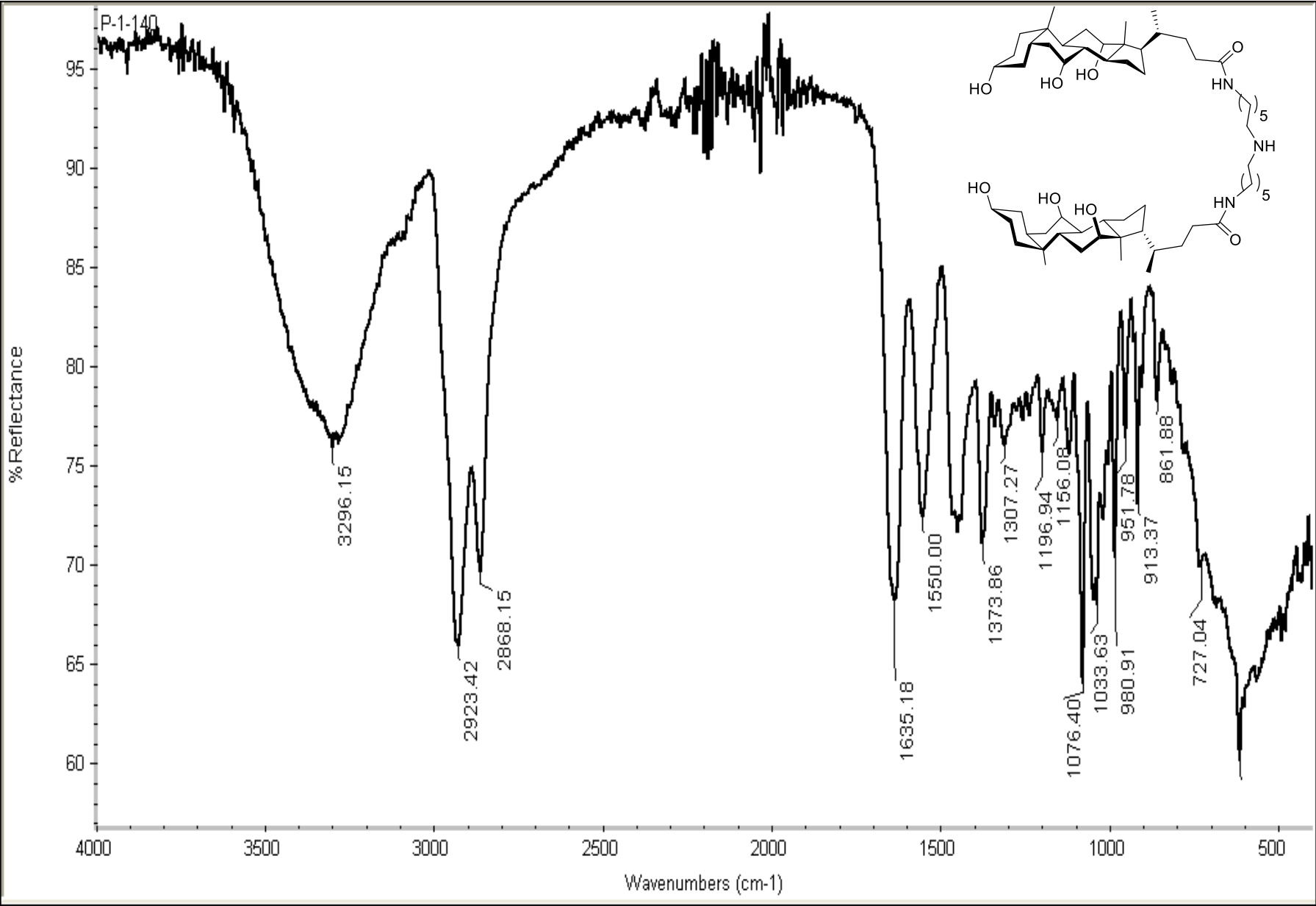
¹³C NMR of Compound 14 (100 MHz, DMSO-*d*₆)



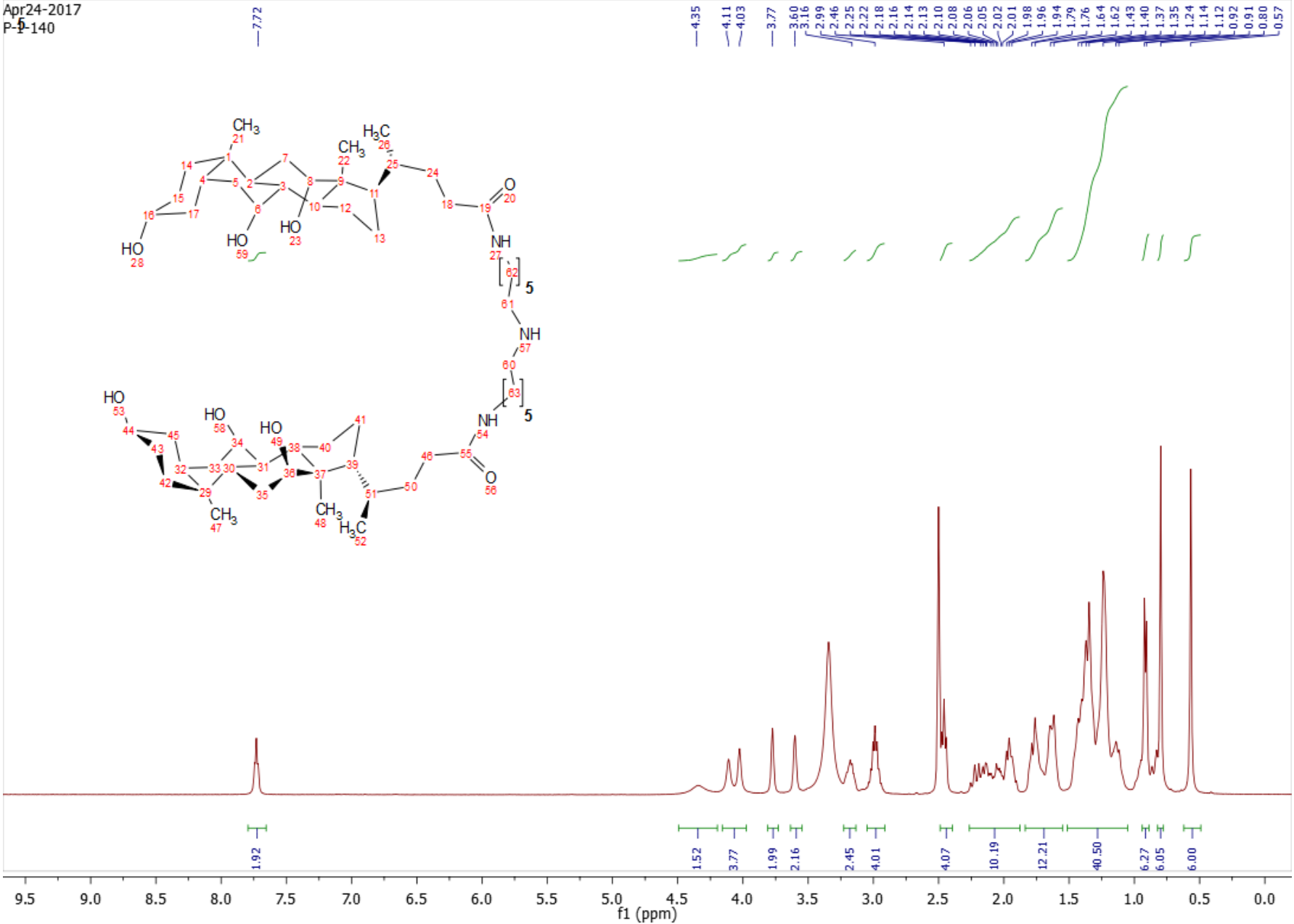
MS of Compound 14



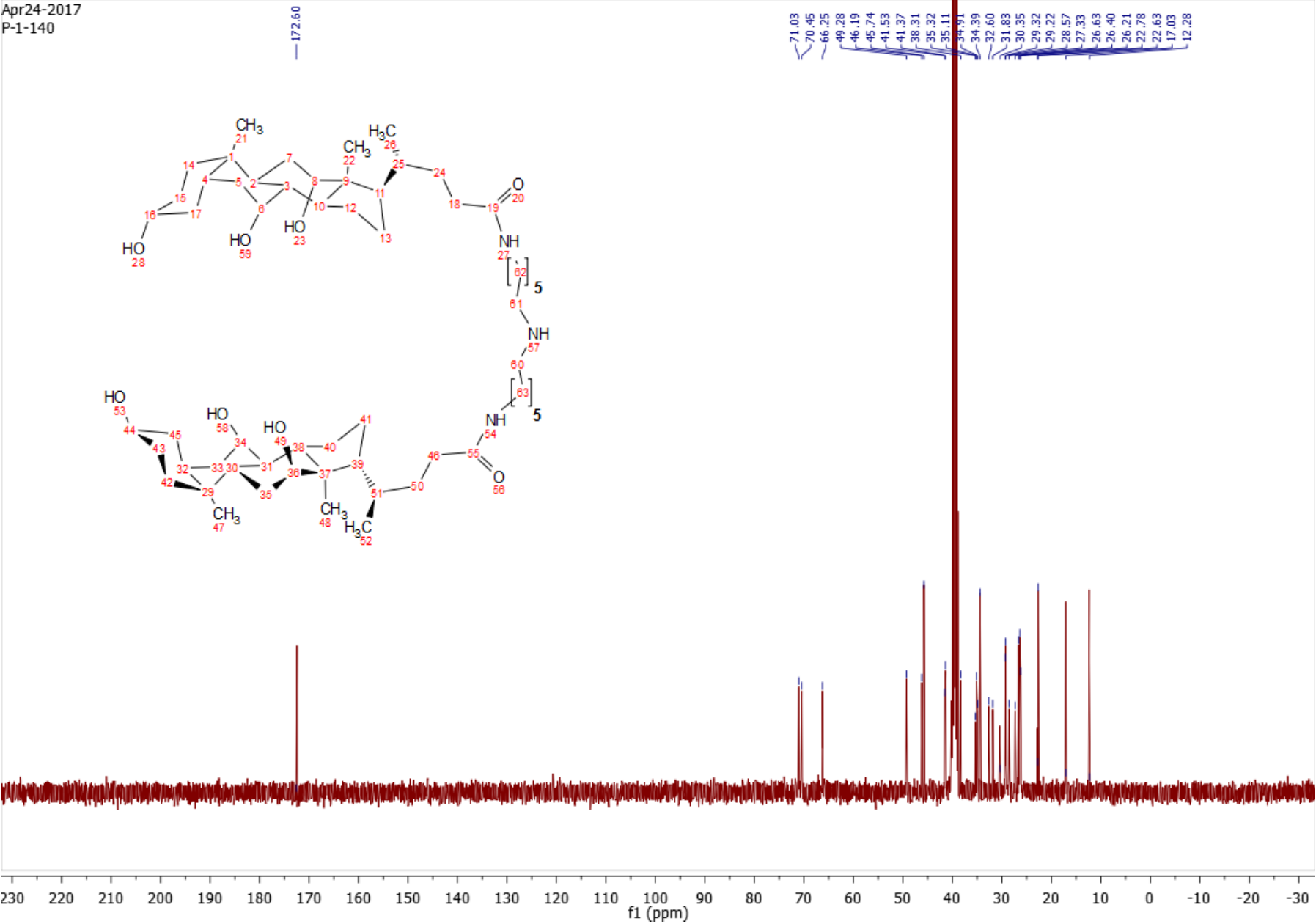
IR of Compound 15a



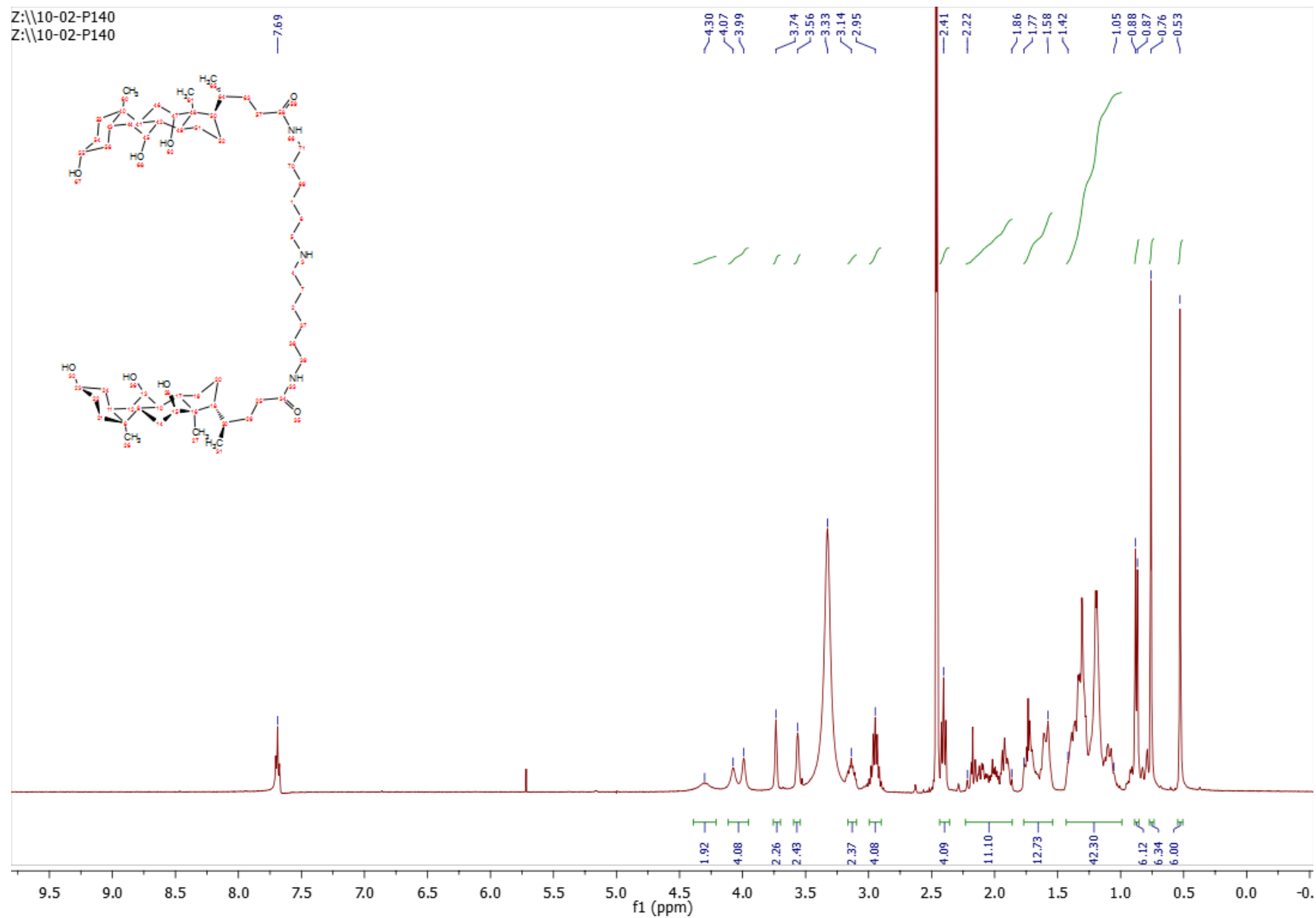
¹H NMR of Compound 15a (400 MHz, DMSO-d₆)



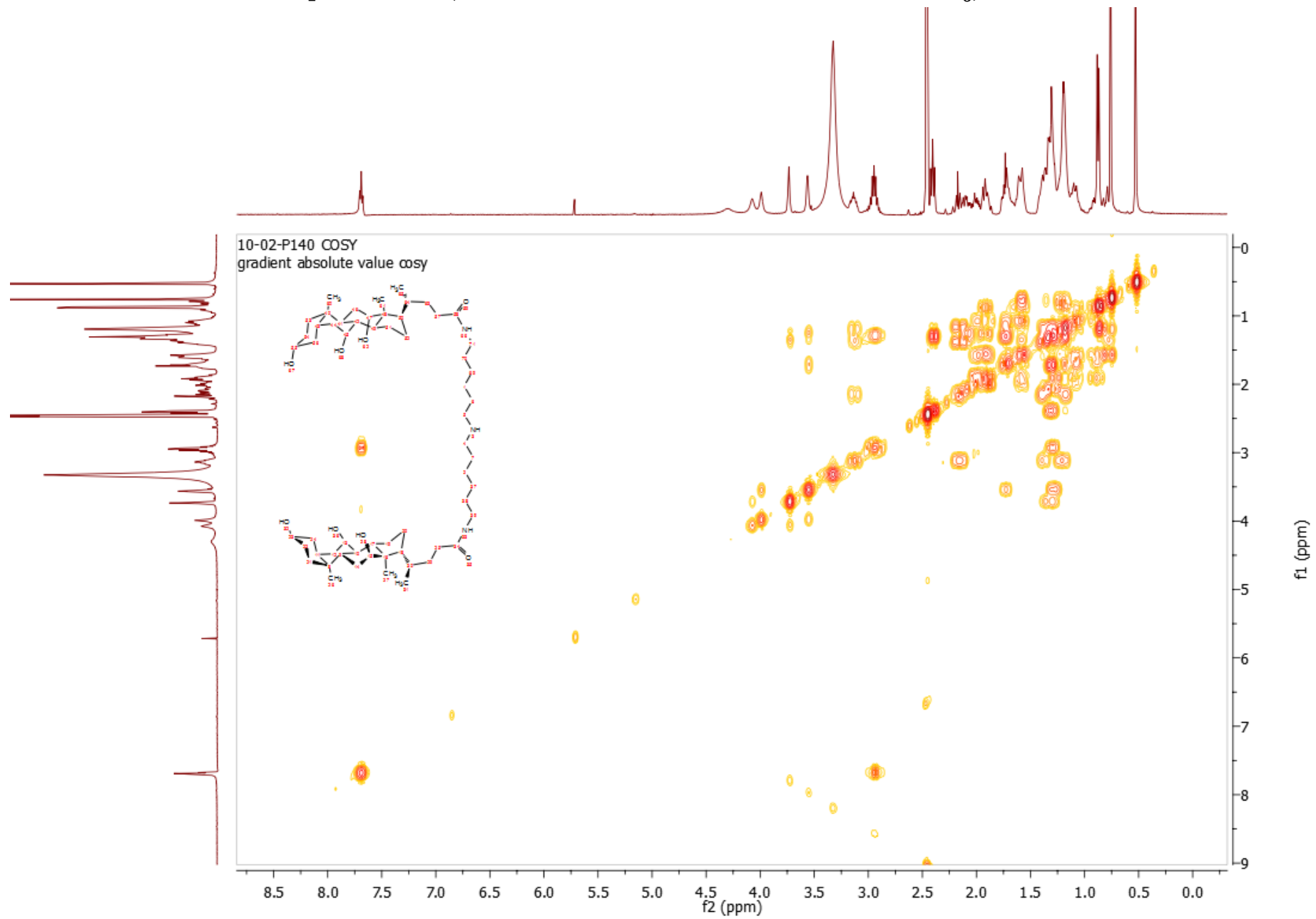
¹³C NMR of Compound 15a (100 MHz, DMSO-d₆)



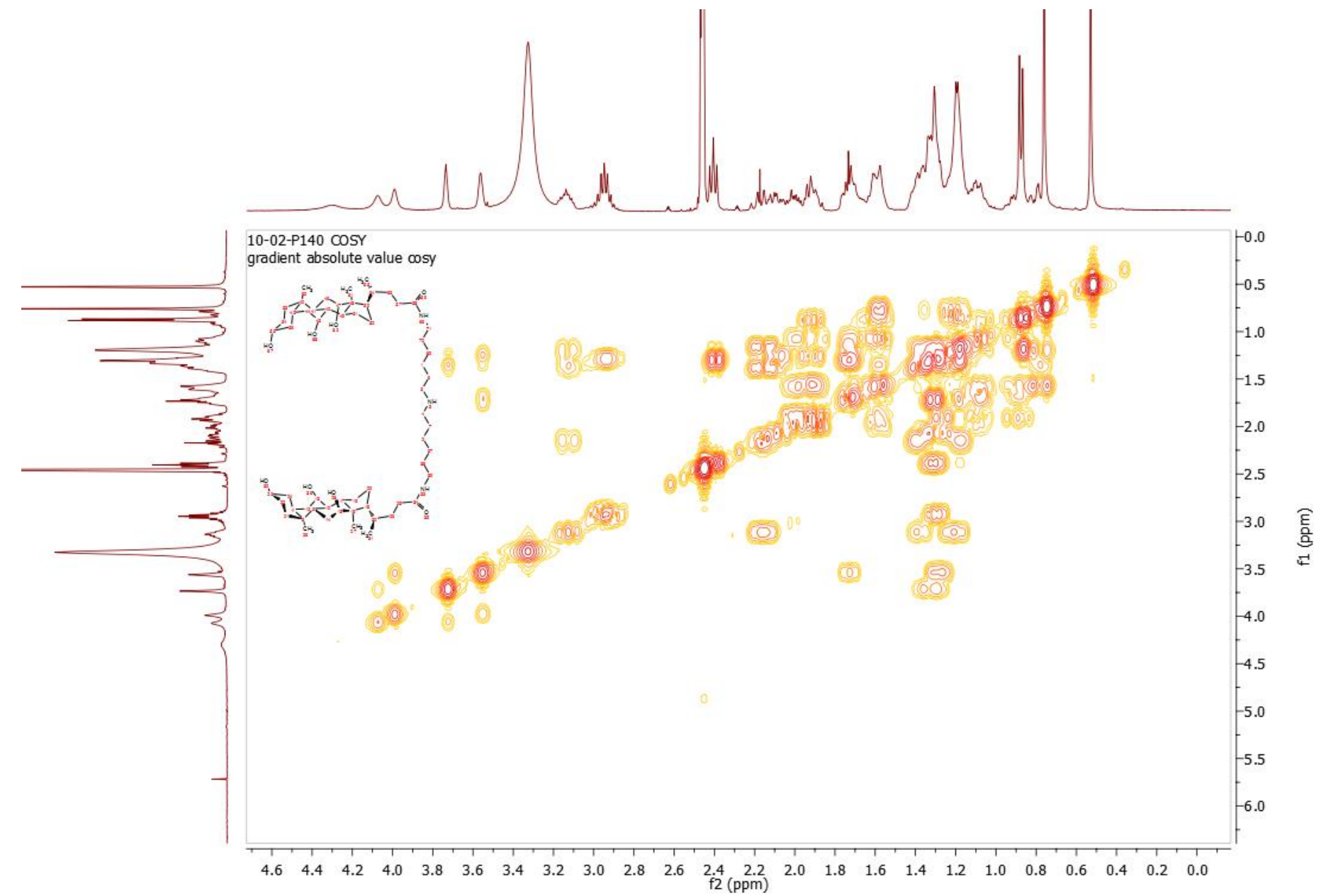
^1H NMR of Compound 15a (400 MHz, JEOL JNM ECS400, DMSO- d_6)



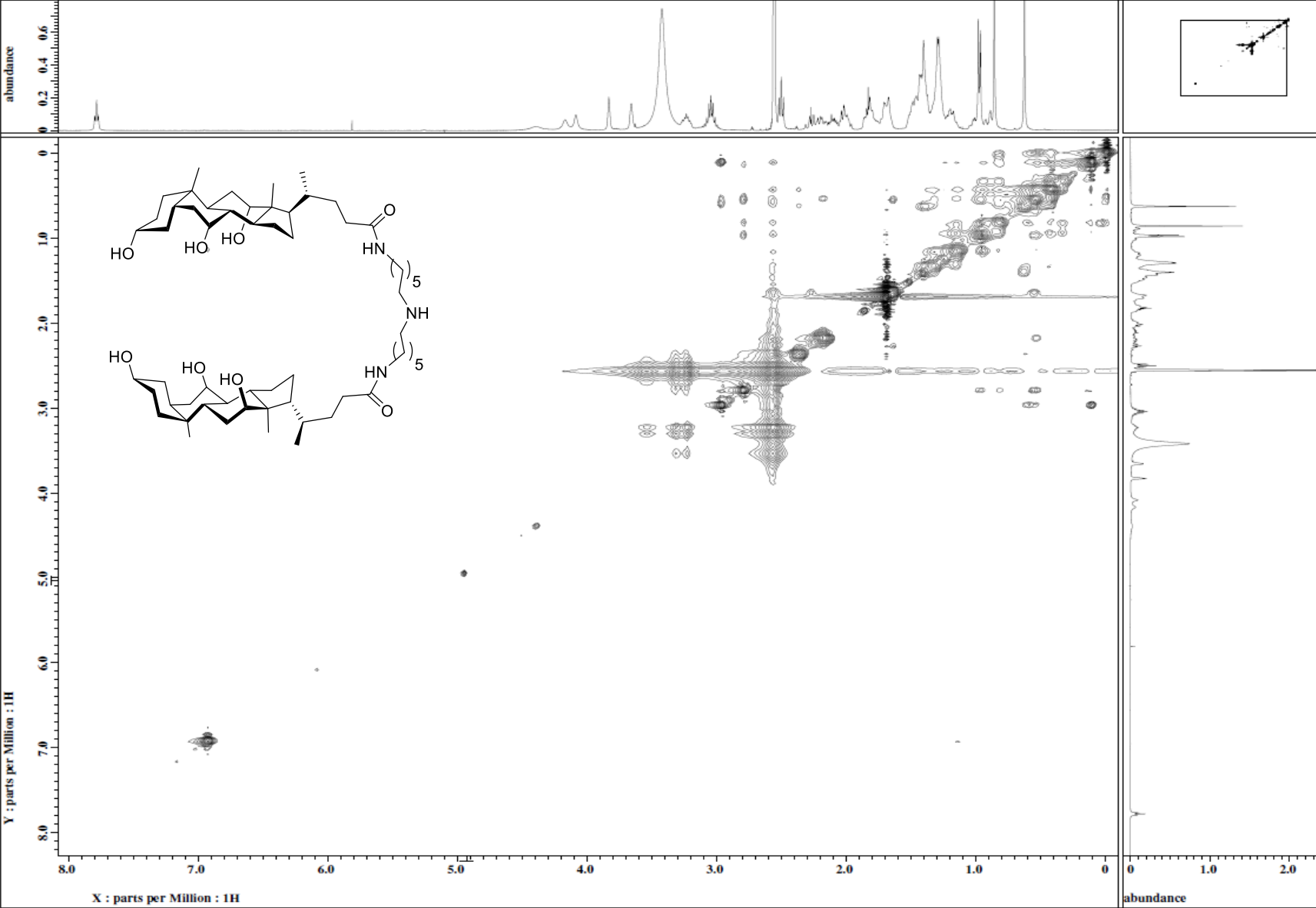
2D COSY NMR of Compound 15a (400 MHz, JEOL JNM ECS400, DMSO-d₆)



2D COSY NMR of Compound 15a (400 MHz, JEOL JNM ECS400, DMSO-*d*₆)



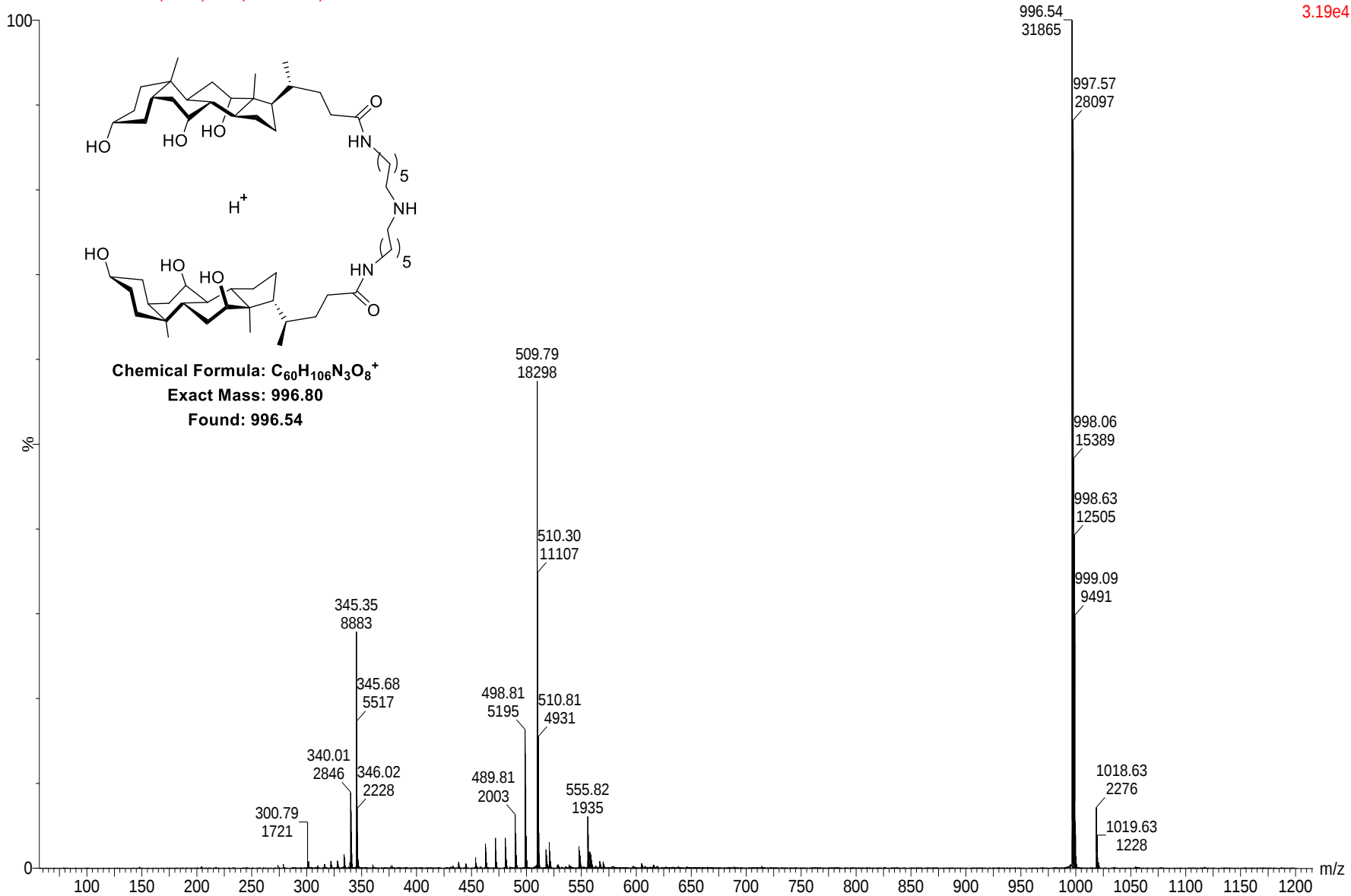
2D NOESY NMR of Compound 15a (400 MHz, JEOL JNM ECS400, DMSO-d₆)



MS of Compound 15a

WATERS, Q-TOF MICROMASS (ESI-MS)
POONAM P-1-140 18 (0.334) Cm (5:29-36:57)

SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
3.19e4



HRMS of Compound 15a

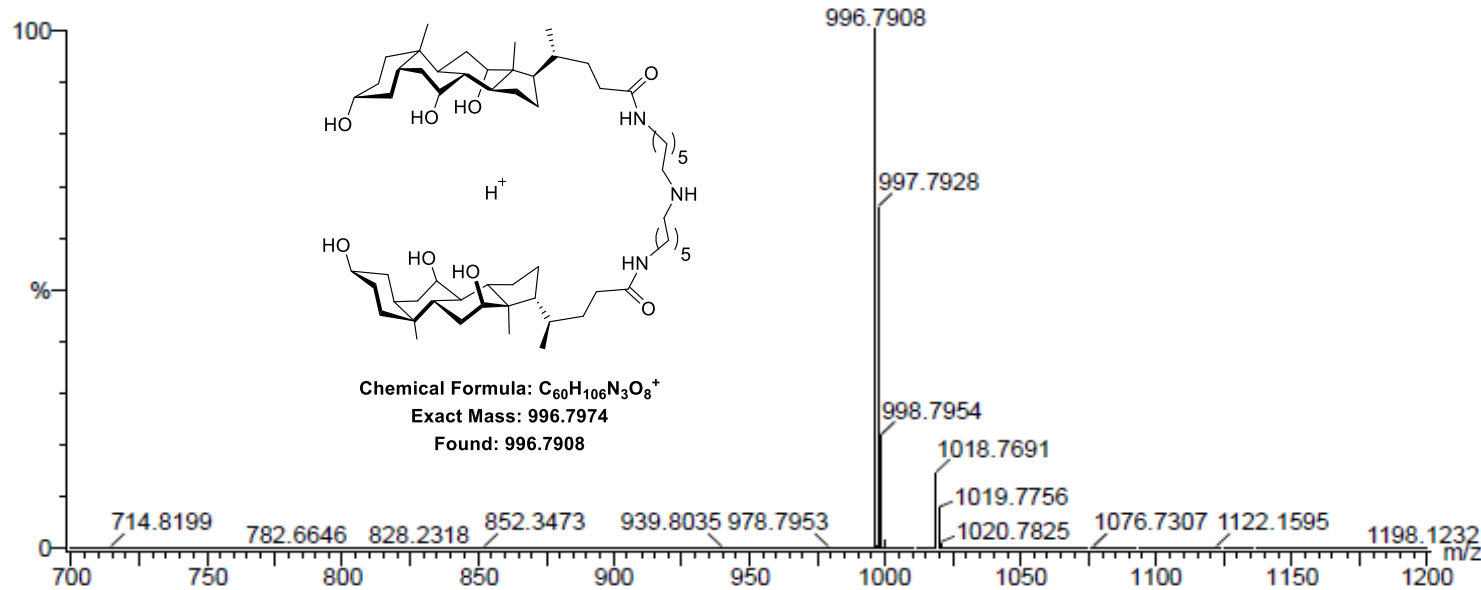
Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
14 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 50-60 H: 85-110 N: 0-3 O: 0-8
Sample Name : P-1-140
Test Name : HRMS-1
220218-P-1-140- 18 (0.183) AM (Top,4, Ar,10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (18)

INDIAN INSTITUTE OF TECHNOLOGY
ROPAR

XEVO G2-XS QTOF
1: TOF MS ES+
1.70e+006



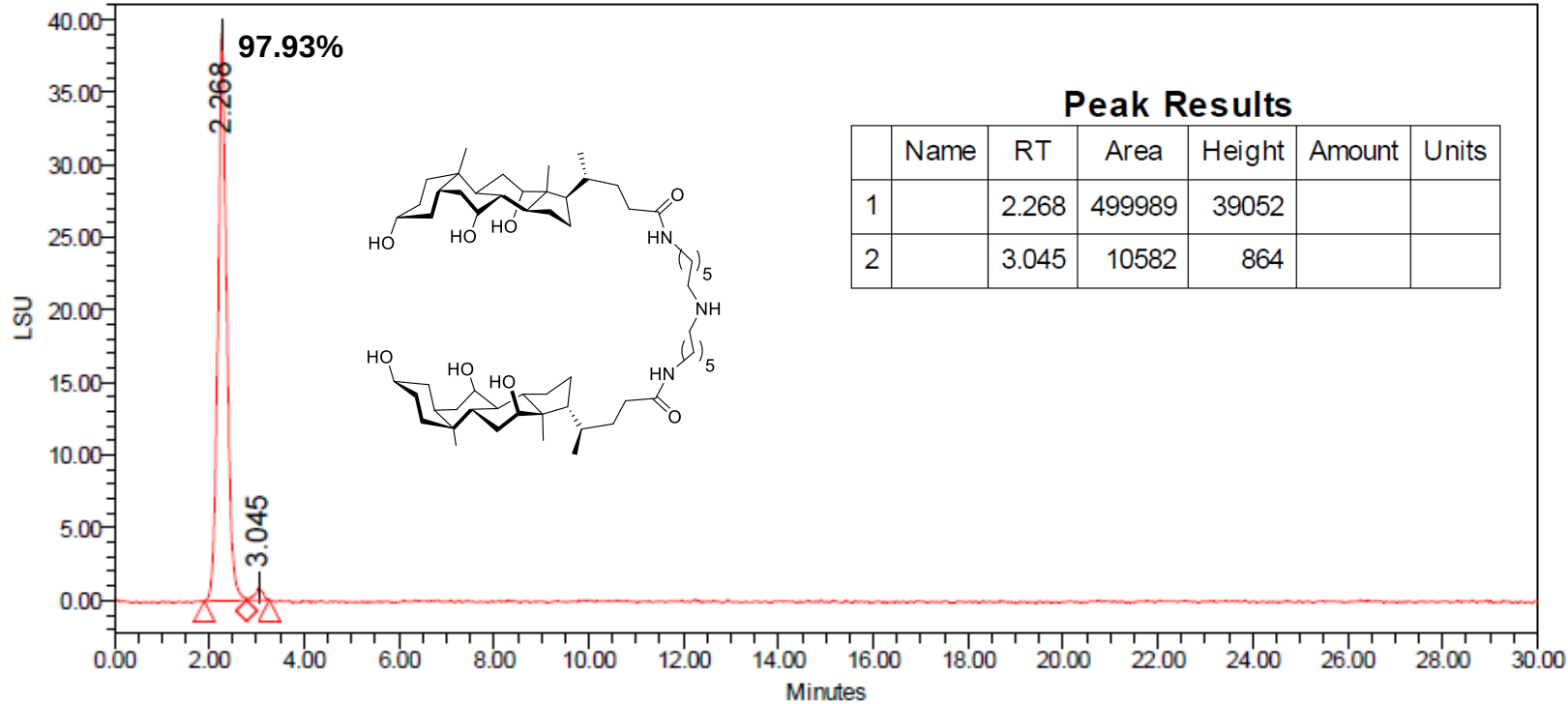
Minimum: -1.5
Maximum: 5.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
996.7908	996.7980	-7.2	-7.2	9.5	122.2	n/a	n/a	C60 H106 N3 O8

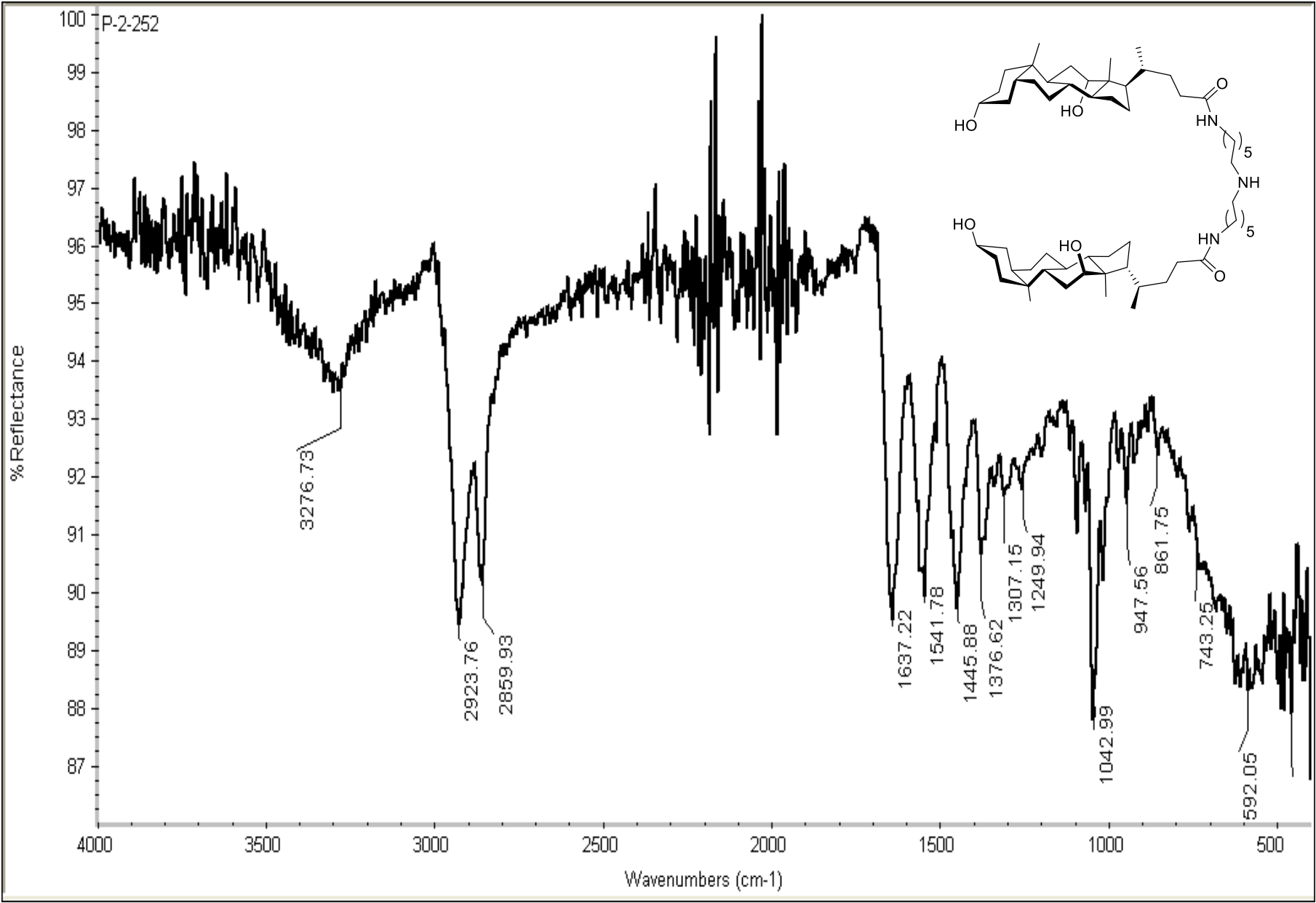
HPLC Data of Compound 15a

SAMPLE INFORMATION			
Sample Name:	P-1-140 50ug (1)	Acquired By:	Shivanshi
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	Mohini
Injection #:	1	Processing Method:	P1 140 50ug
Injection Volume:	20.00 ul	Channel Name:	ELSD Signal
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	ELSD Signal
Date Acquired:	6/25/2018 2:57:48 PM IST		
Date Processed:	6/25/2018 3:41:24 PM IST		

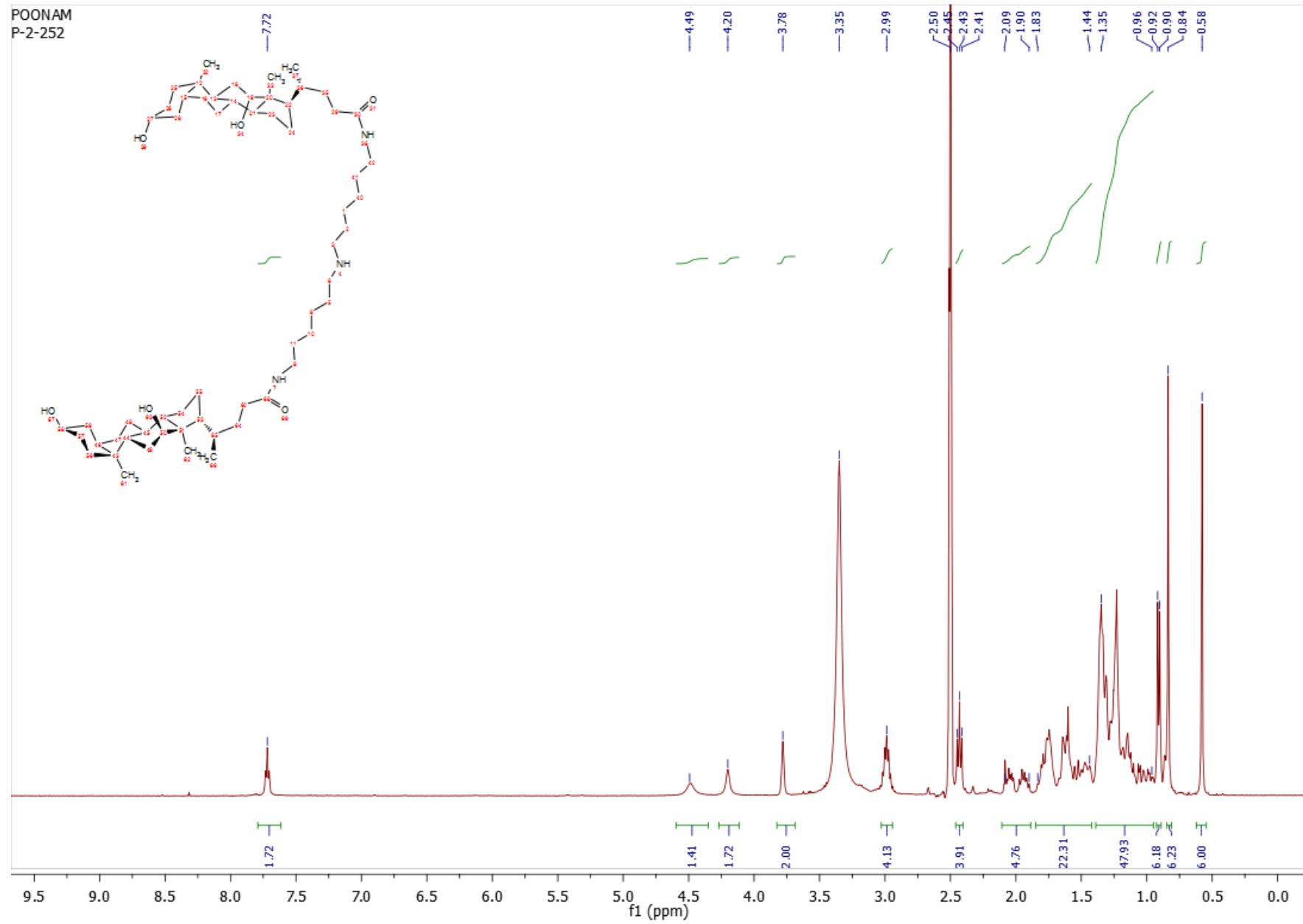
Auto-Scaled Chromatogram



IR of Compound 15b

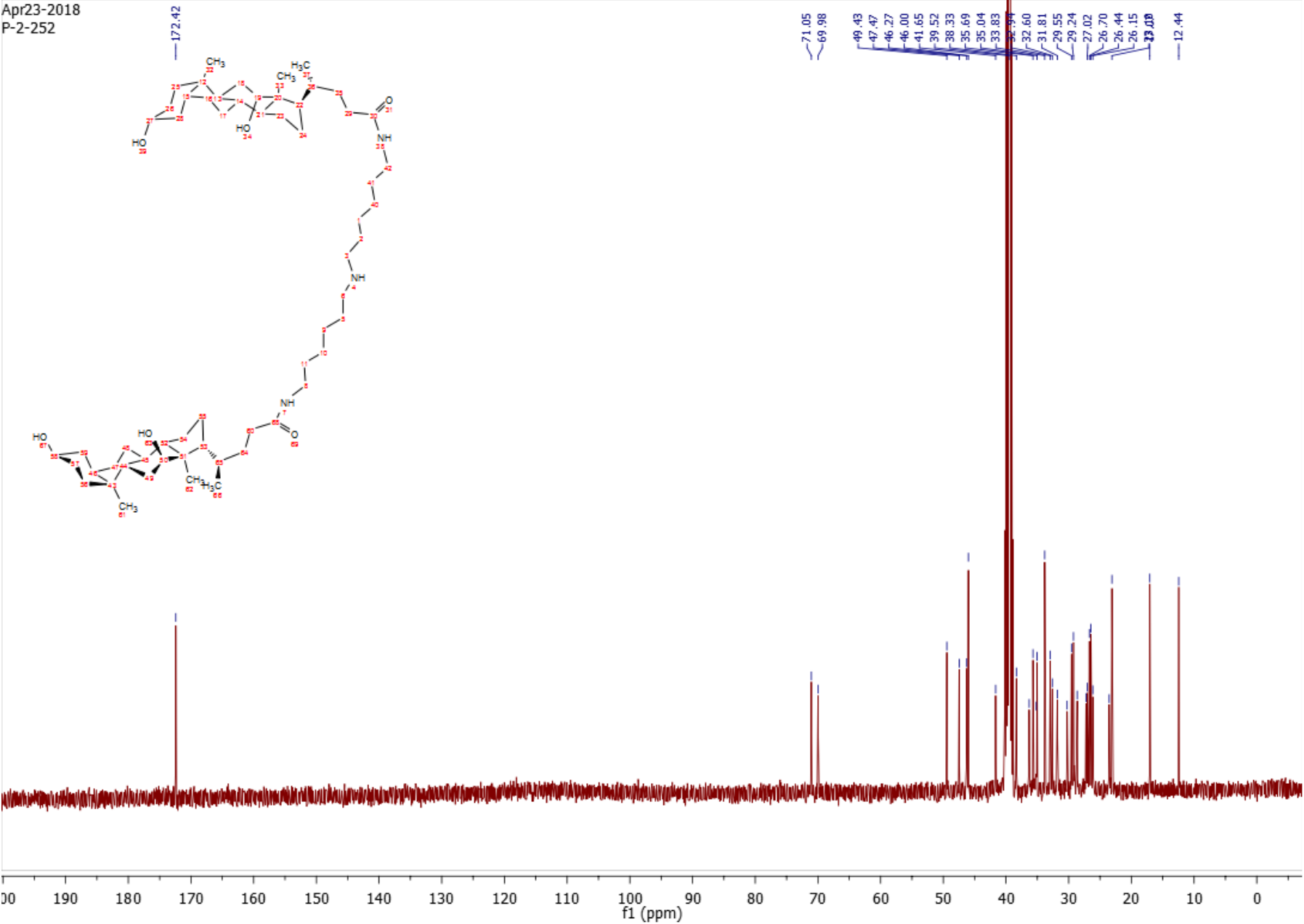


¹H NMR of Compound **15b** (400 MHz, DMSO-*d*₆)



¹³C NMR of Compound 15b (100 MHz, DMSO-d₆)

Apr23-2018
P-2-252

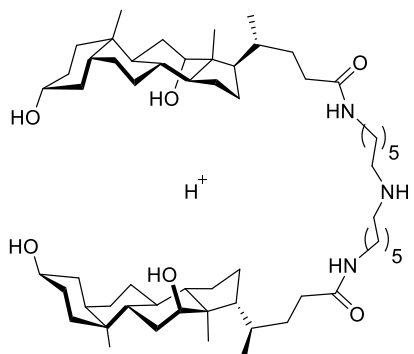
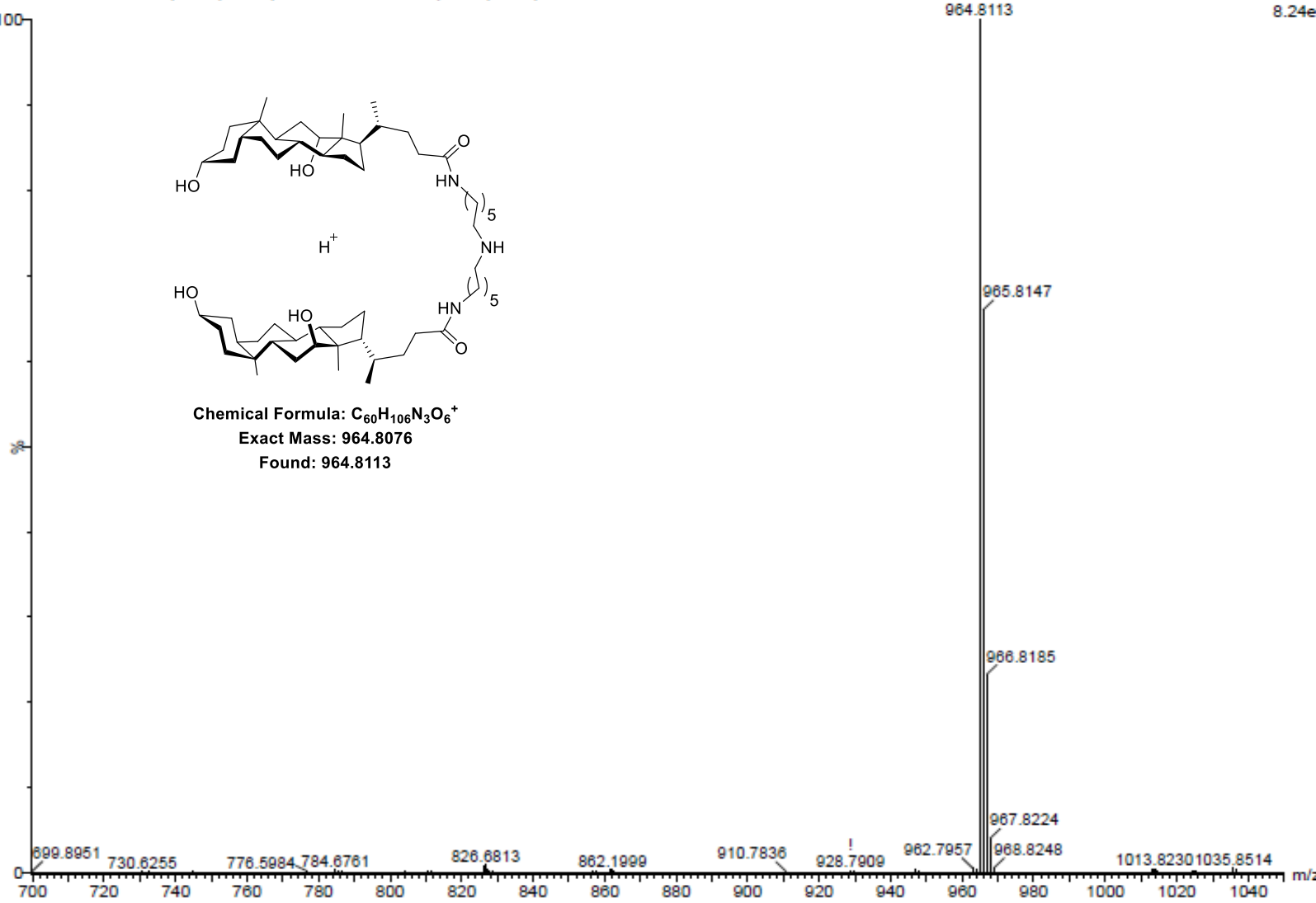


HRMS of Compound 15b

Sample Name : 10-02-252
Test Name : HRMS-1
200818-10-02-252- 19 (0.203) AM2 (Ar,19000.0,0.00,0.00); Cm (19:20)

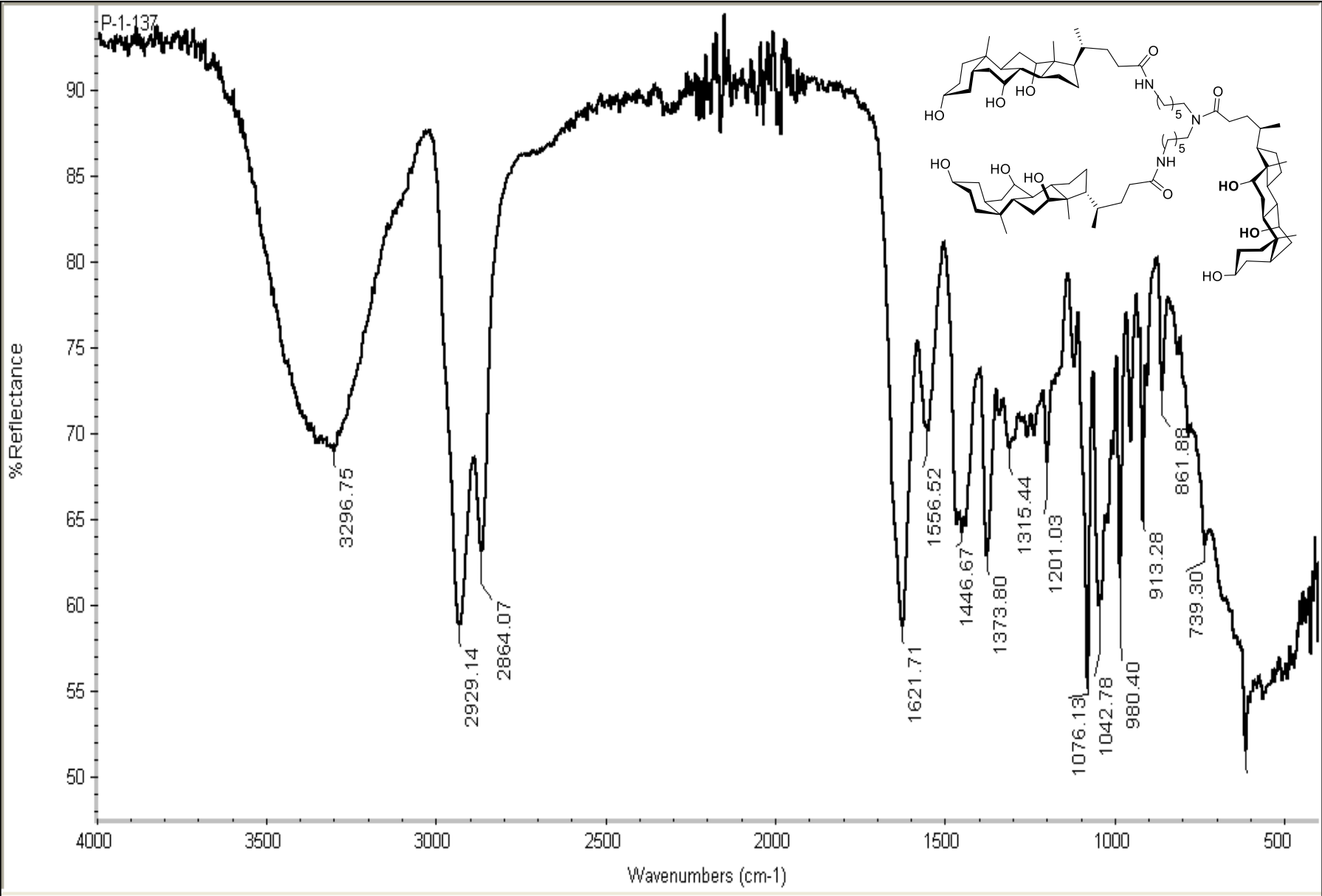
XEVO G2-XS QTOF

1: TOF MS ES+
8.24e6

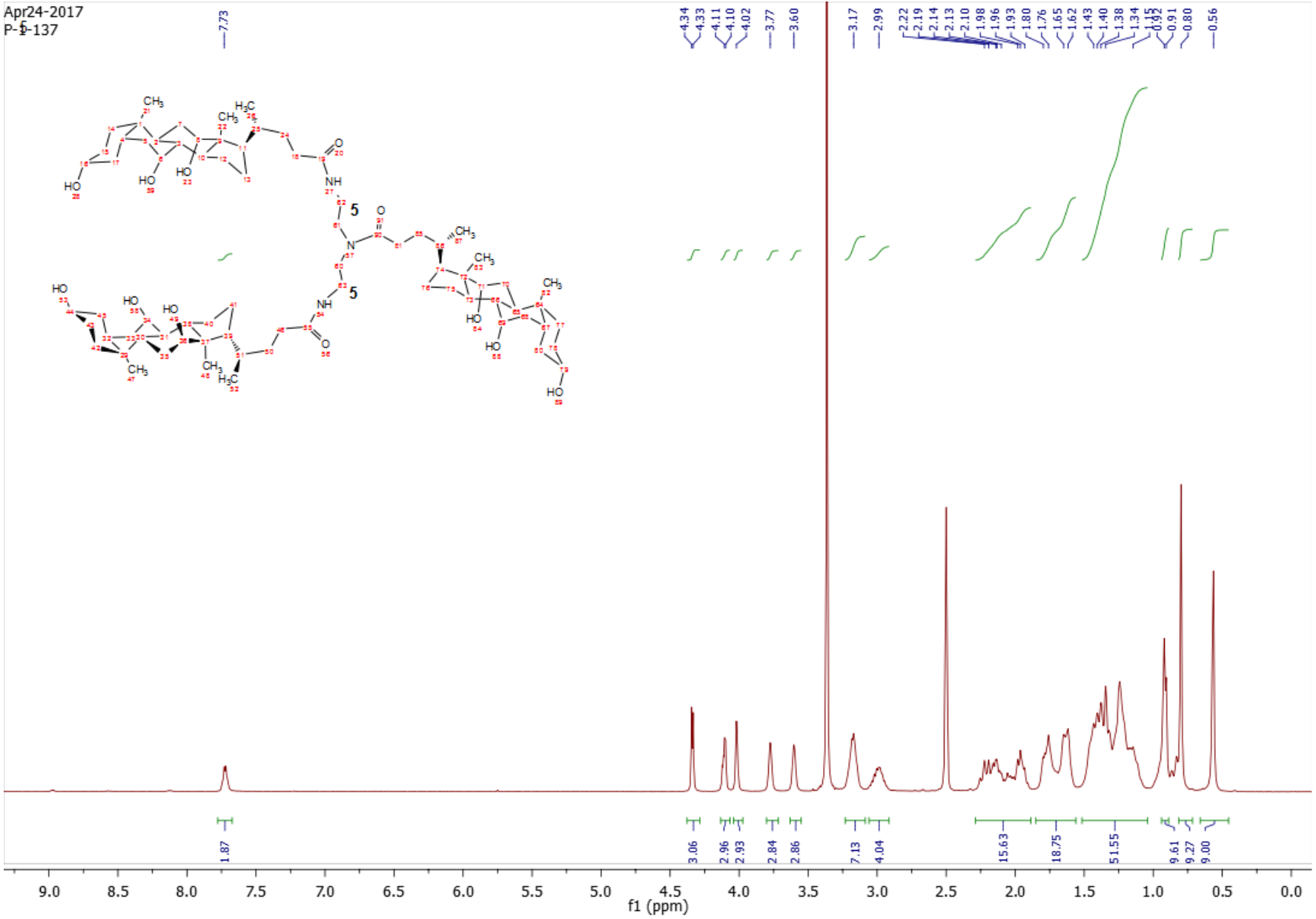


Chemical Formula: $C_{60}H_{106}N_3O_6^+$
Exact Mass: 964.8076
Found: 964.8113

IR of Compound 16

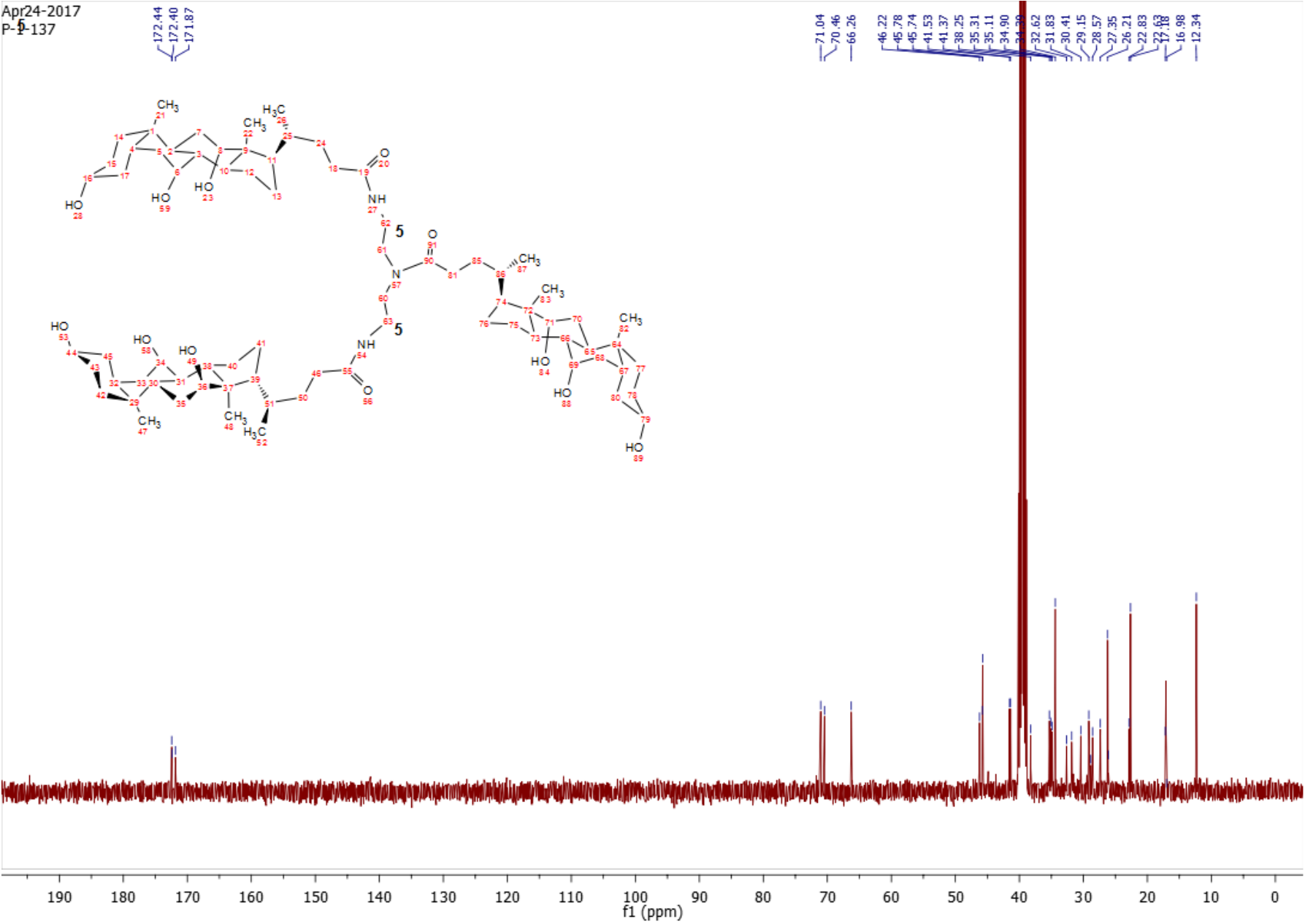


¹H NMR of Compound 16 (400 MHz, DMSO-d₆)



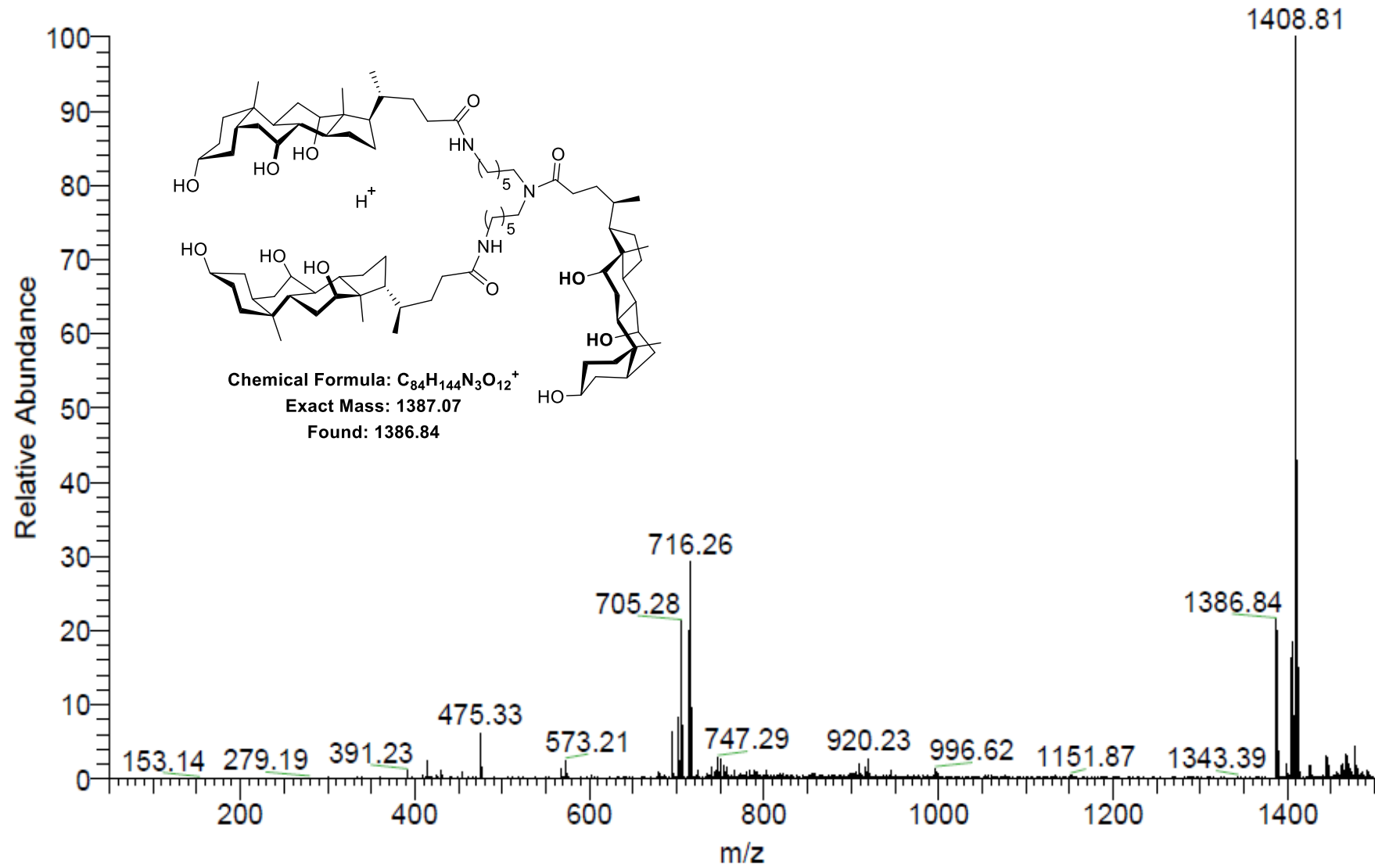
¹³C NMR of Compound 16 (100 MHz, DMSO-*d*₆)

Apr24-2017
P-137

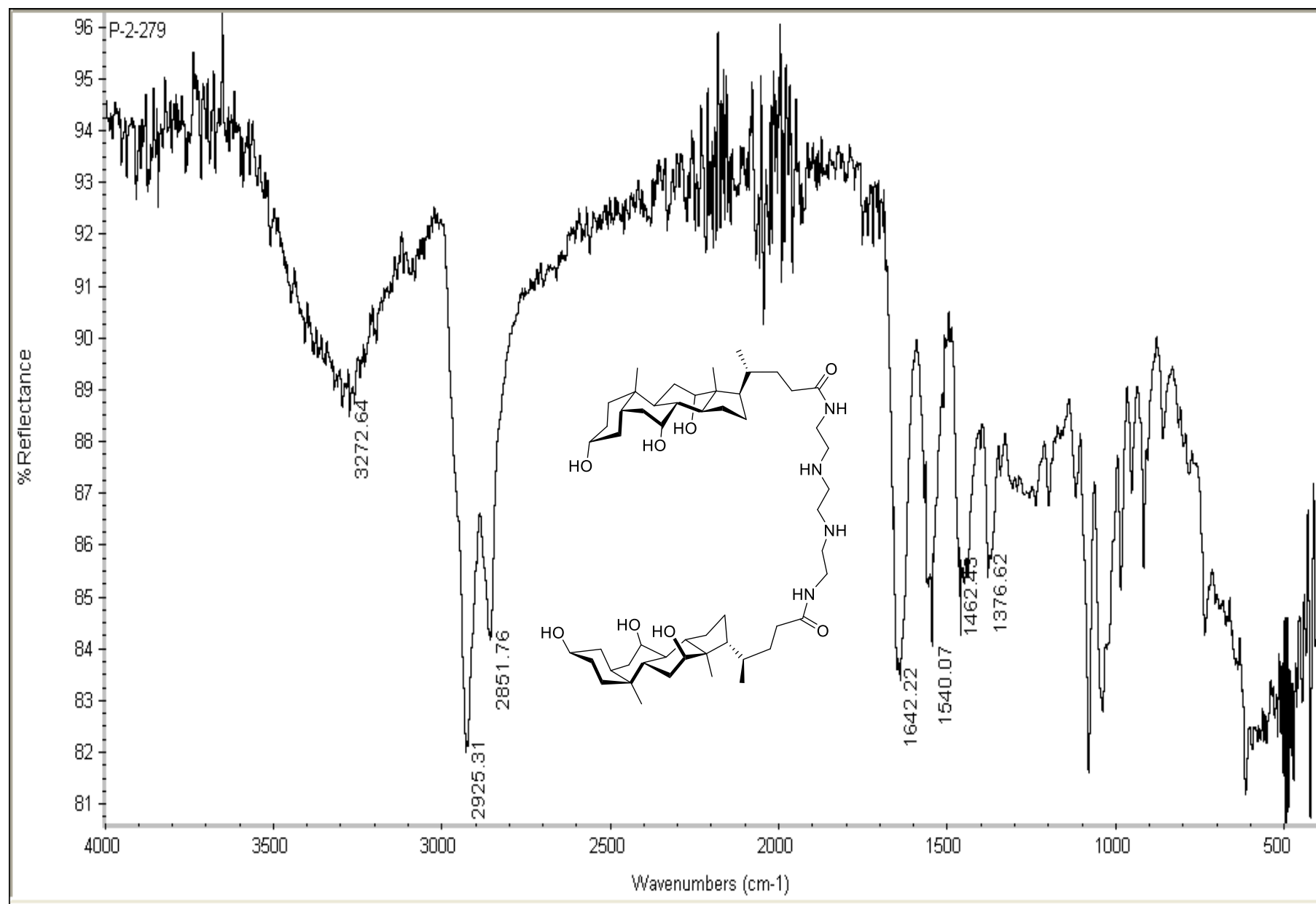


MS of Compound 16

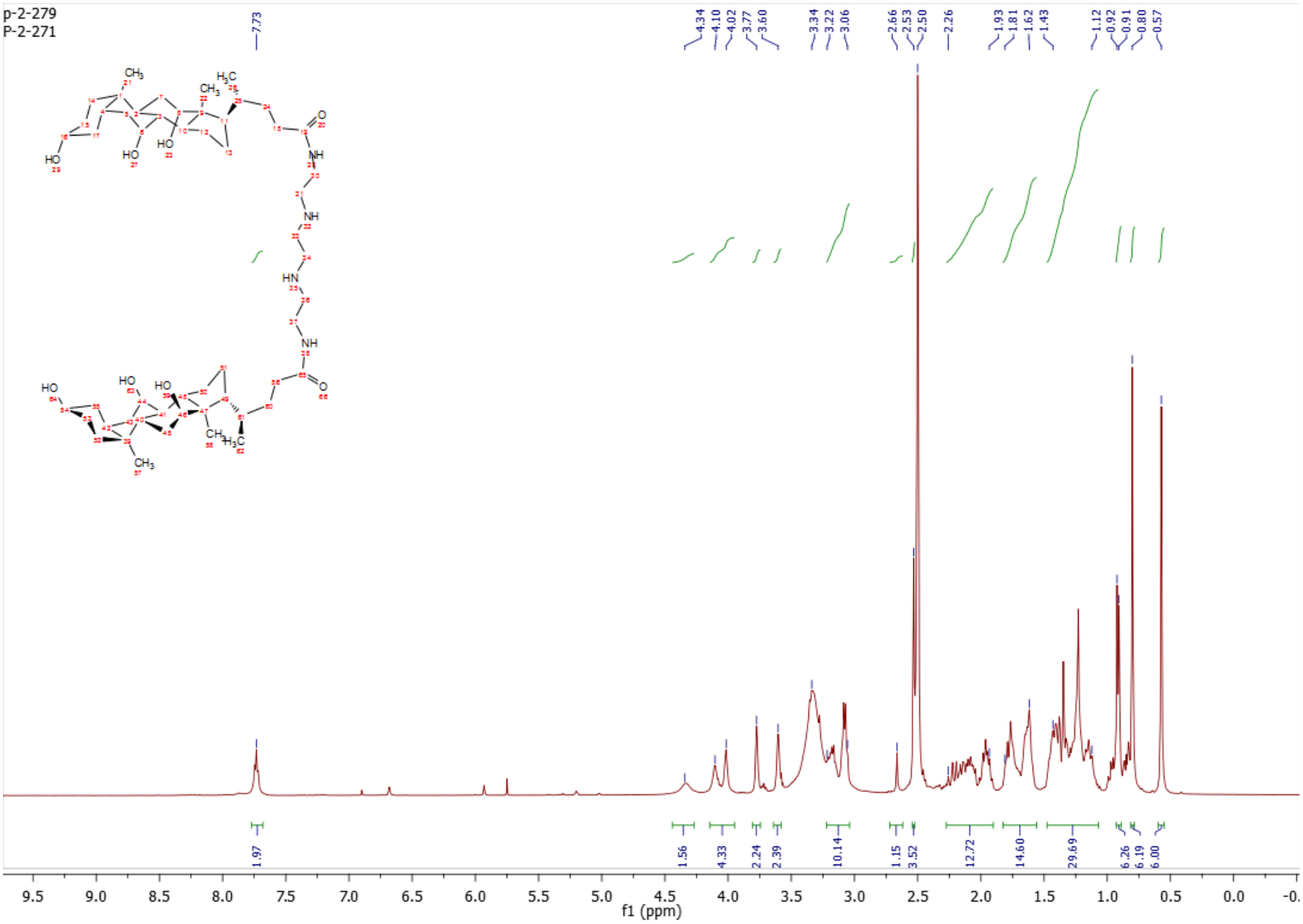
P-1-137_180105110401 #18 RT: 0.19 AV: 1 NL: 6.94E5
T: ITMS + c ESI Full ms [50.00-1500.00]



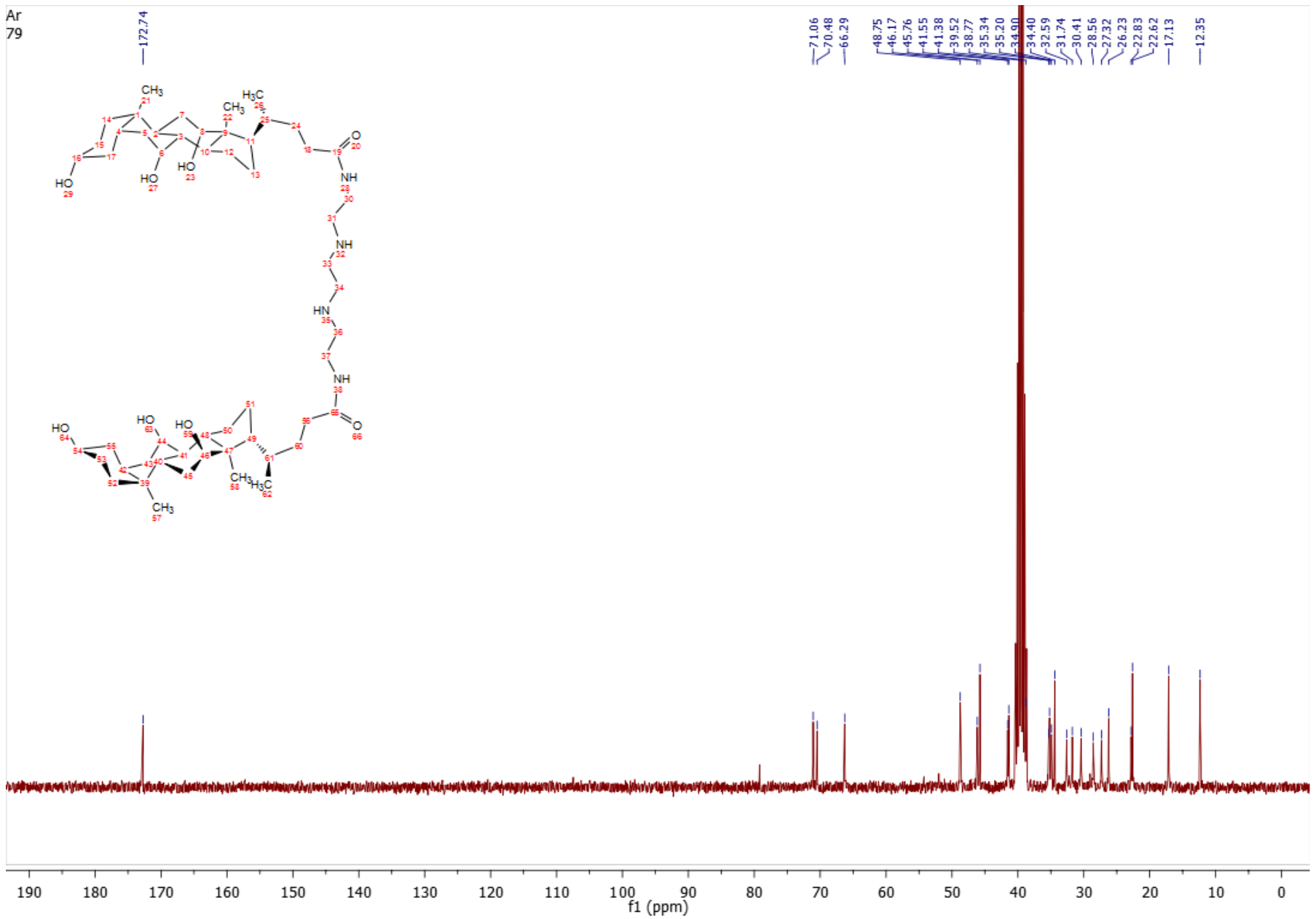
IR of Compound 17



¹H NMR of Compound 17 (400 MHz, DMSO-d₆)



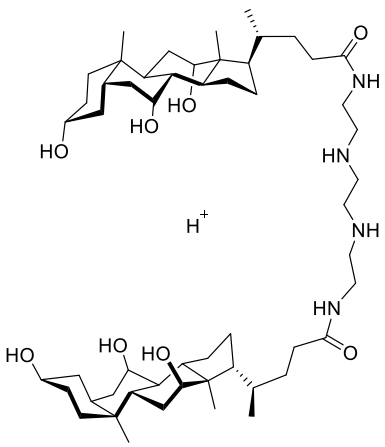
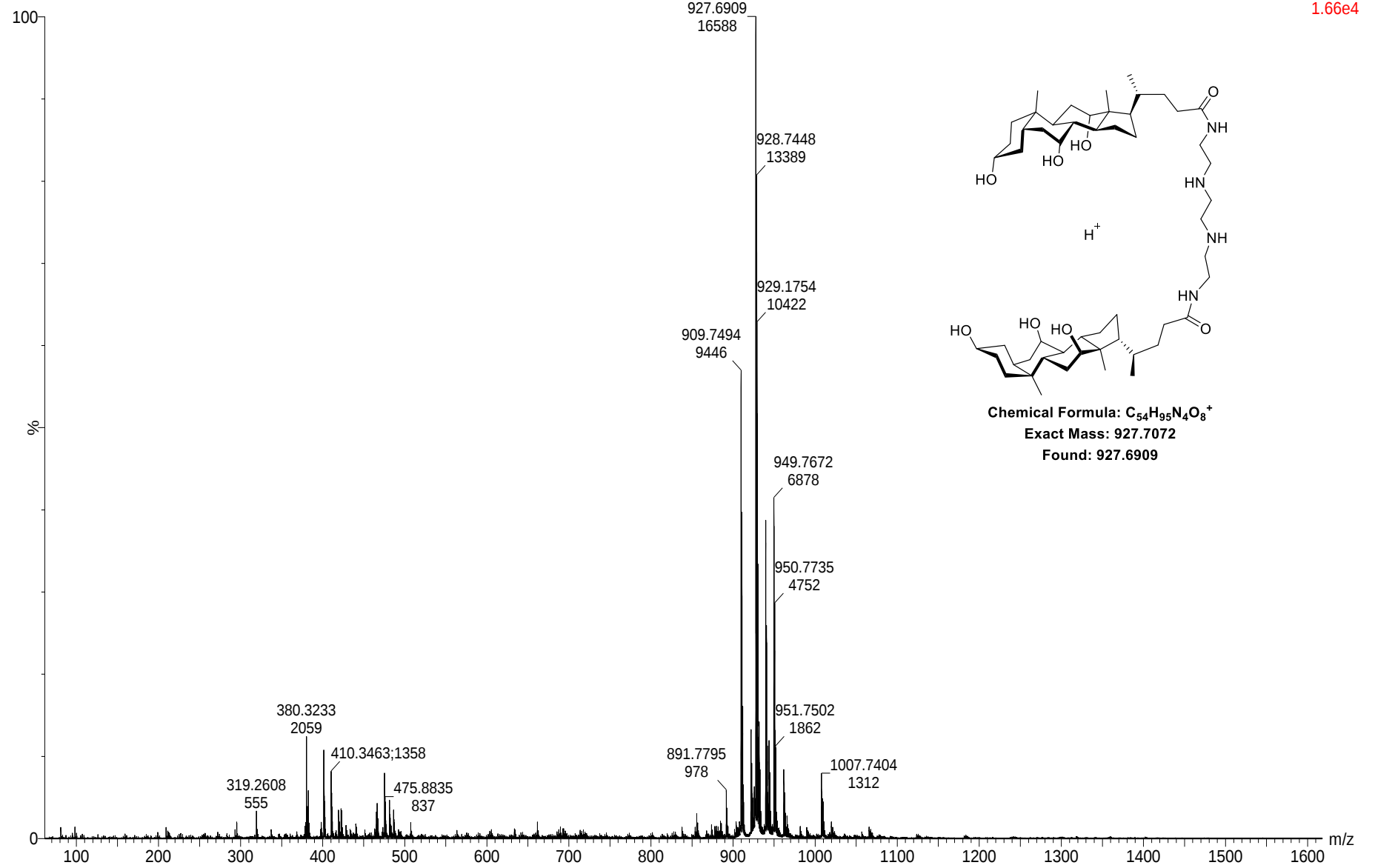
¹³C NMR of Compound 17 (75 MHz, DMSO-d₆)



MS of Compound 17

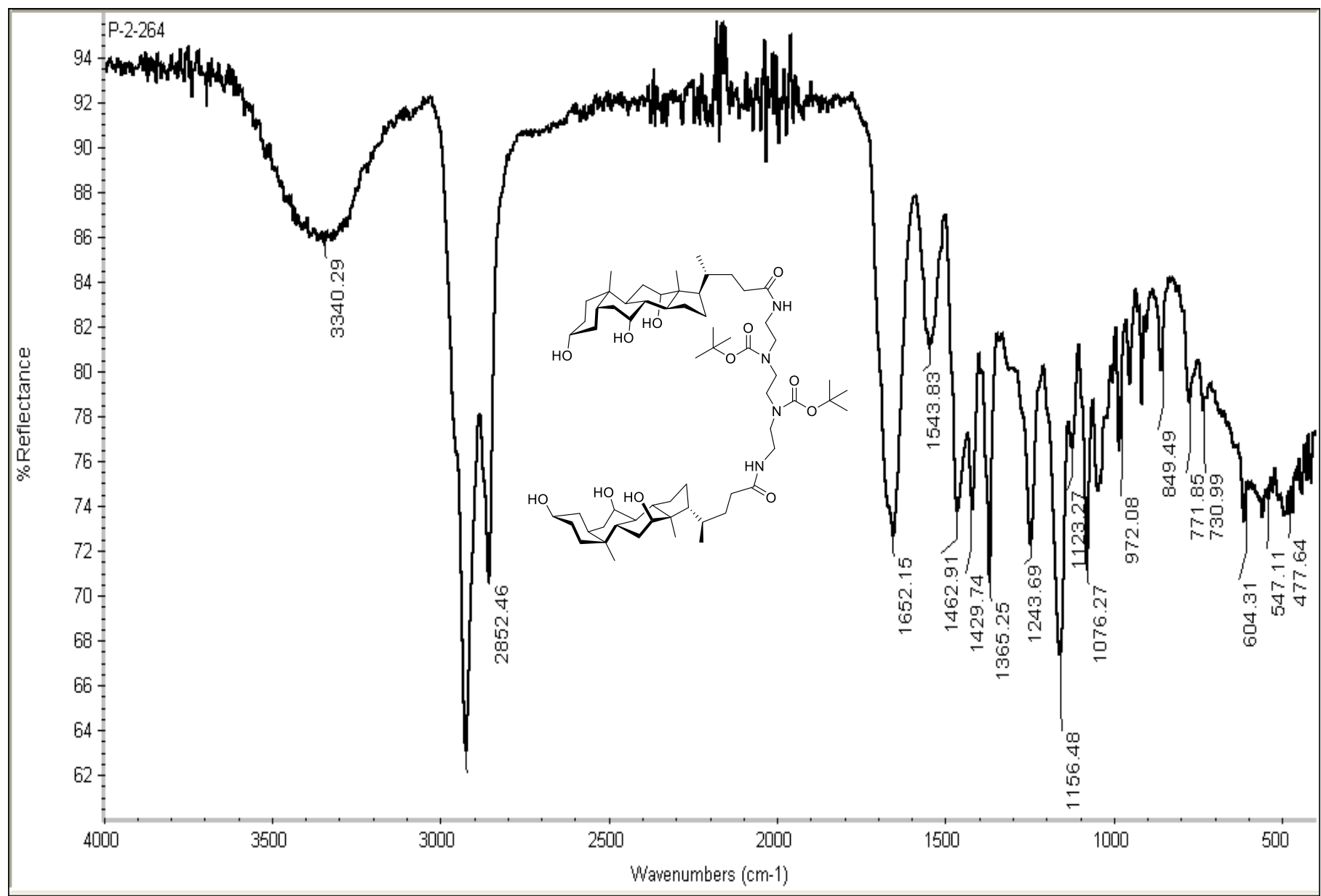
WATERS, Q-TOF MICROMASS (ESI-MS)
POONAM P-2-279 R 56 (1.040) Cm (32:59)

SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
1: TOF MS ES+
1.66e4

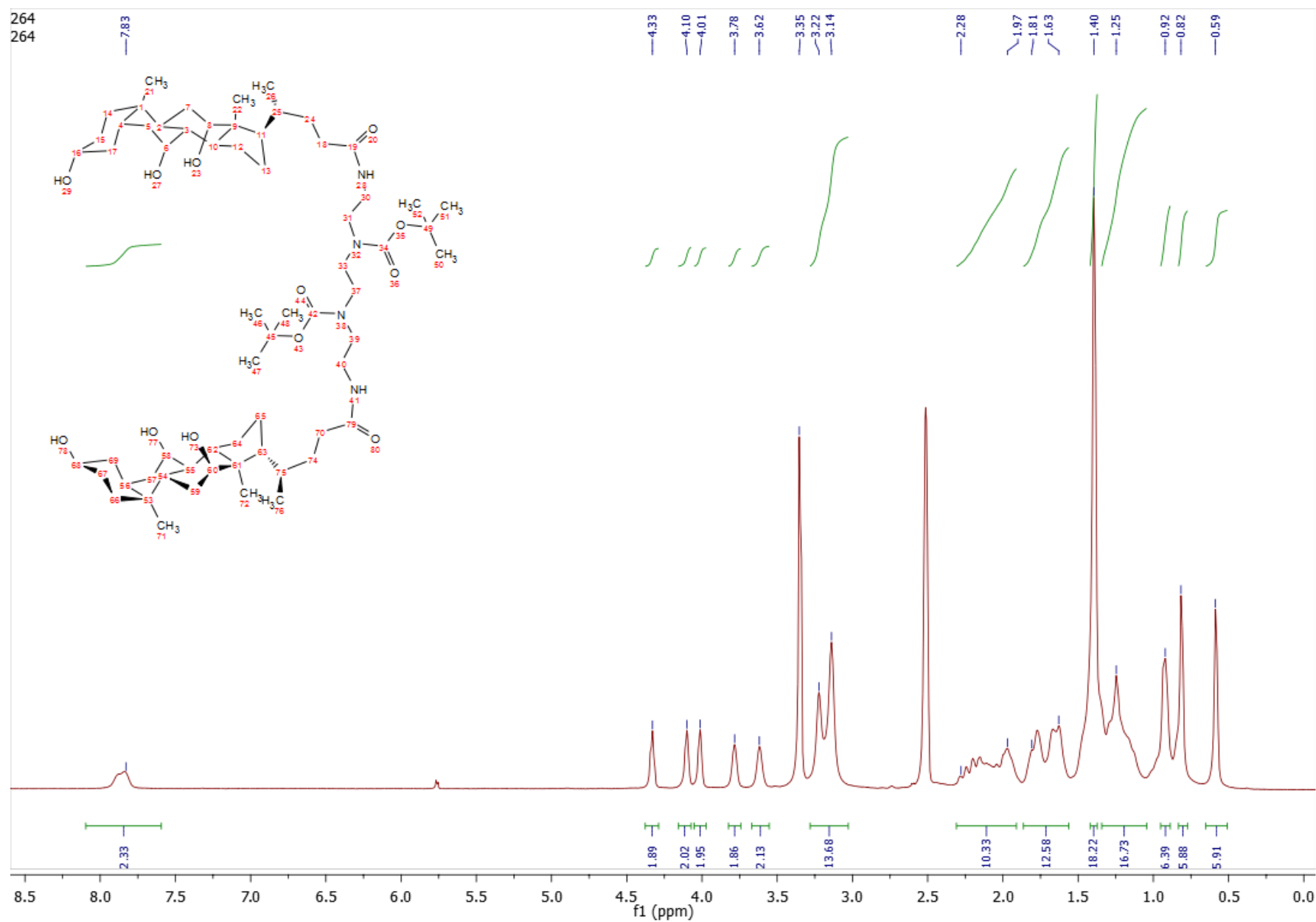


Chemical Formula: $C_{54}H_{95}N_4O_8^+$
Exact Mass: 927.7072
Found: 927.6909

IR of Compound 18

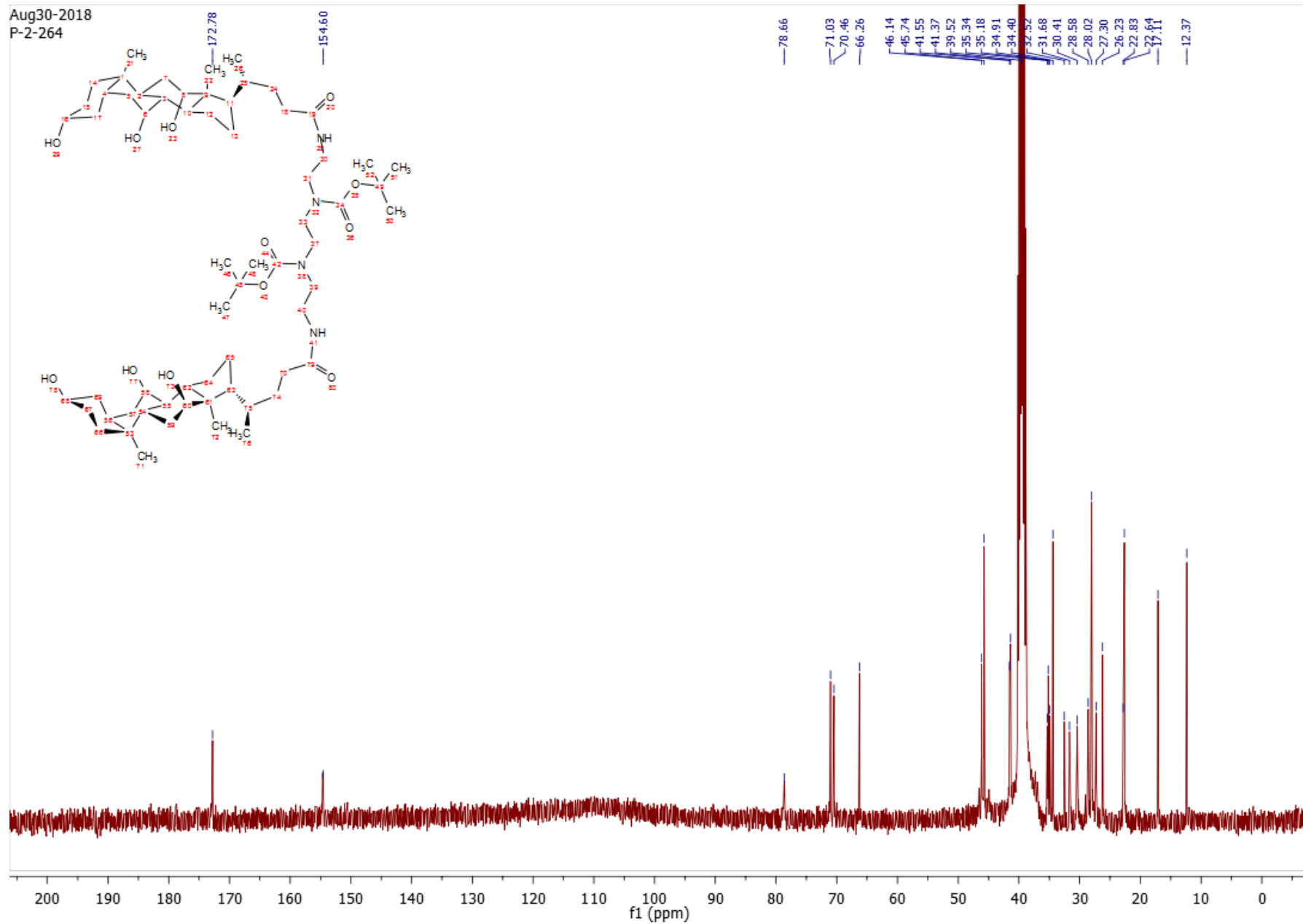


^1H NMR of Compound **18** (400 MHz, $\text{DMSO-}d_6$)



^{13}C NMR of Compound **18** (100 MHz, DMSO- d_6)

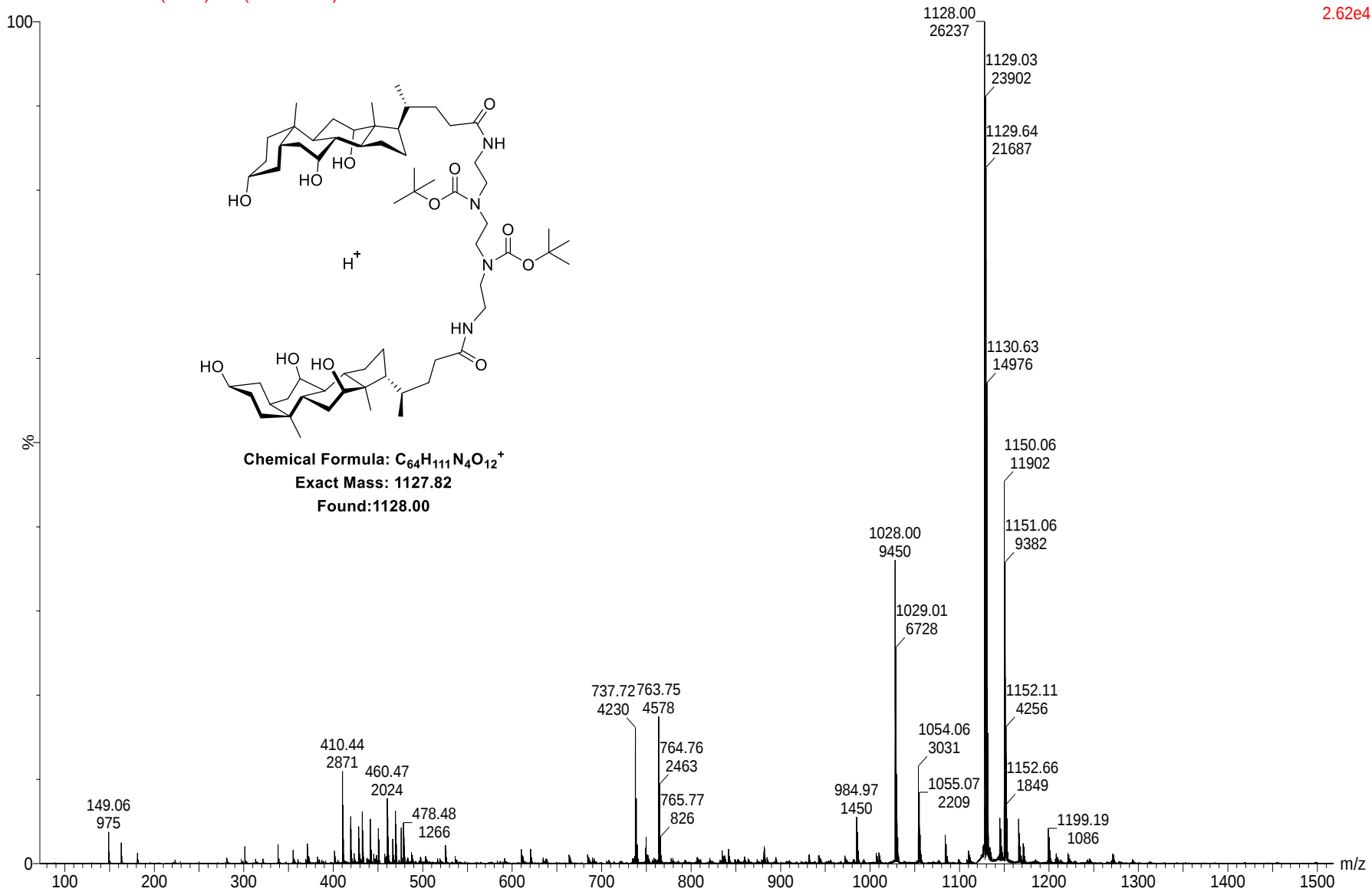
Aug30-2018
P-2-264



MS of Compound 18

WATERS, Q-TOF MICROMASS (ESI-MS)
POONAM P-2-264 18 (0.334) Cm (10:31-48:82)

SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
2.62e4



HRMS of Compound 19

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 12-15 H: 25-30 N: 0-3 O: 0-4

Sample Name : 10-02-267

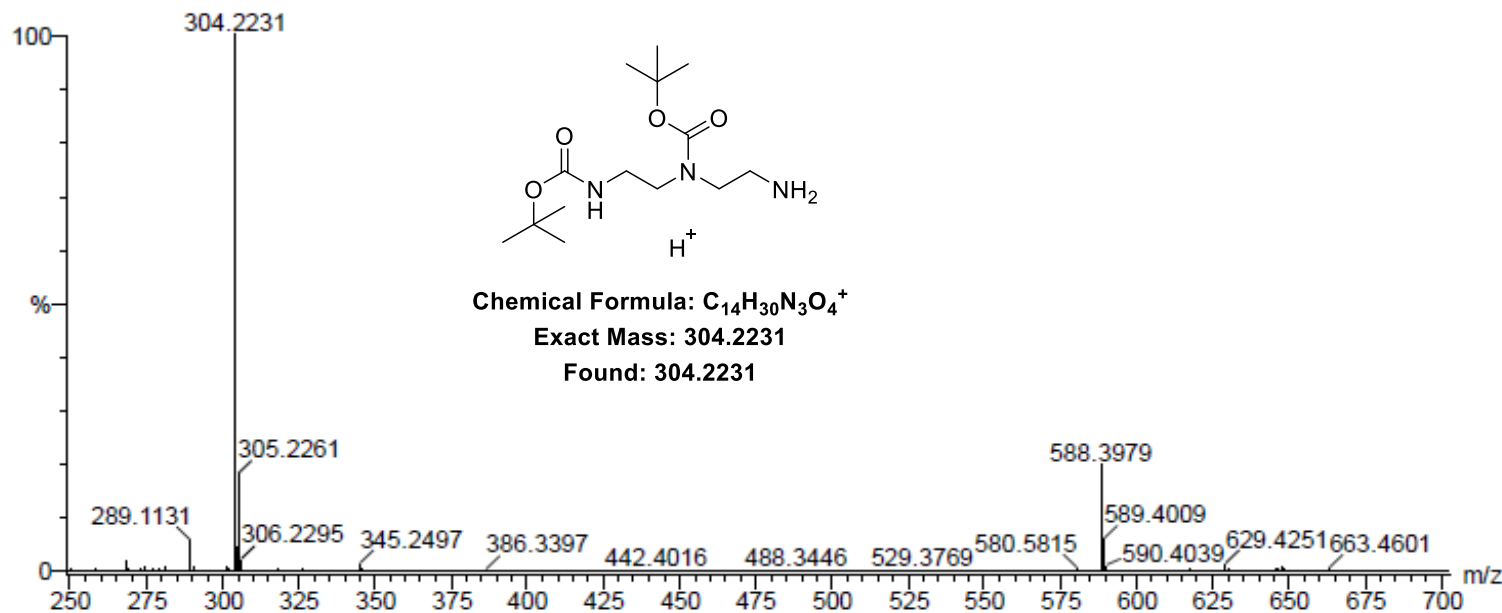
I.I.T.ROPAR

XEVO G2-XS QTOF

Test Name : HRMS-1

200818-10-02-267 18 (0.183) AM2 (Ar,19000.0,0.00,0.00); Cm (18:20)

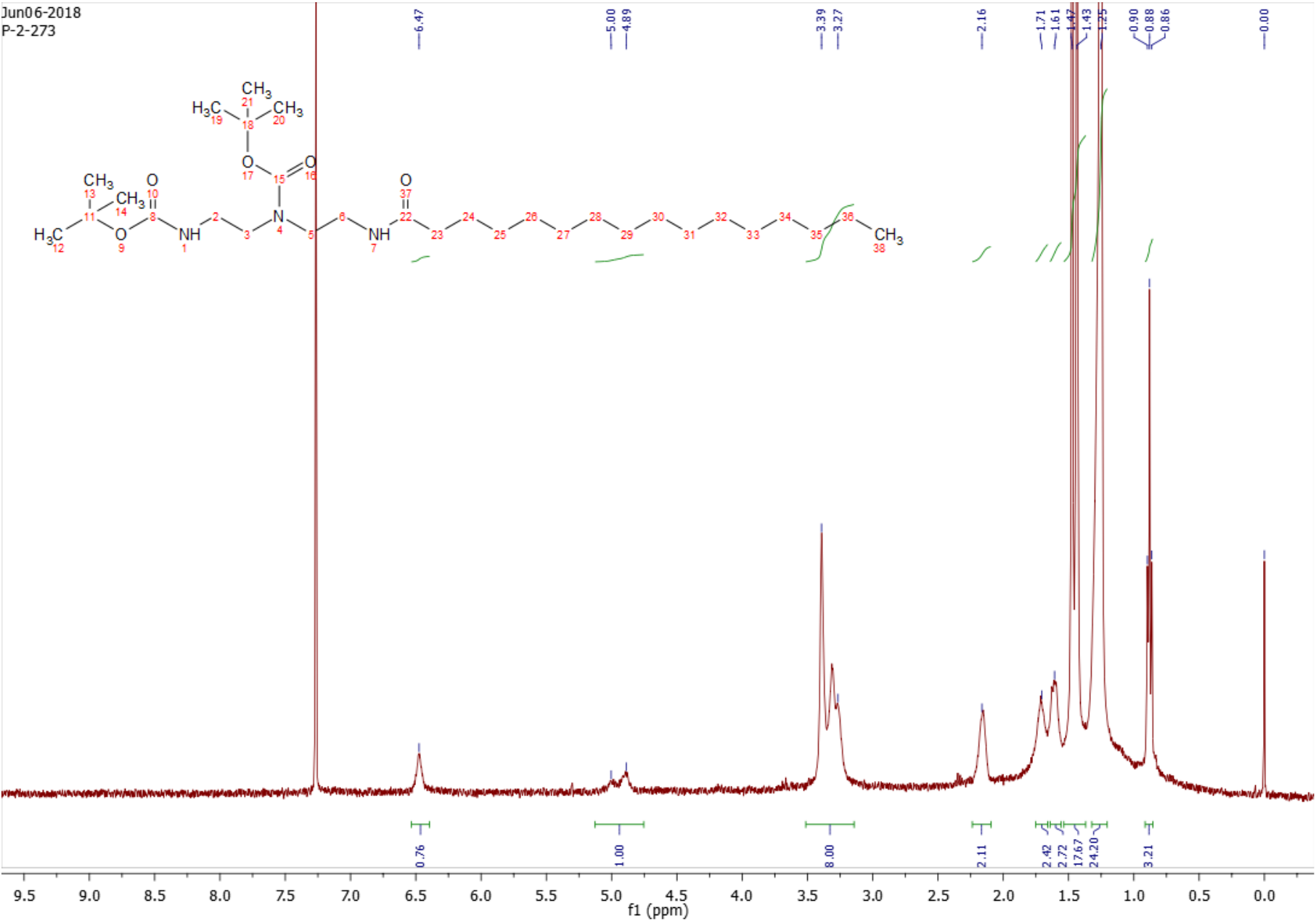
1: TOF MS ES+
6.32e+006



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
304.2231	304.2236	-0.5	-1.6	1.5	640.8	n/a	n/a	C14 H30 N3 O4

¹H NMR of Compound 20 (400 MHz, CDCl₃)



HRMS of Compound 20

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 29-34 H: 55-60 N: 0-3 O: 0-8

Sample Name : 10-02-275

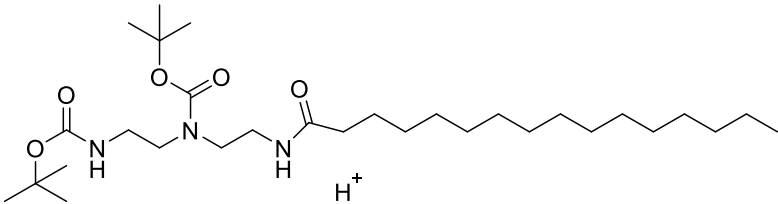
Test Name : HRMS-1

200818-10-02-275 20 (0.211) AM2 (Ar,19000.0,0.00,0.00); Cm (20:22)

I.I.TROPAR

XEVO G2-XS QTOF

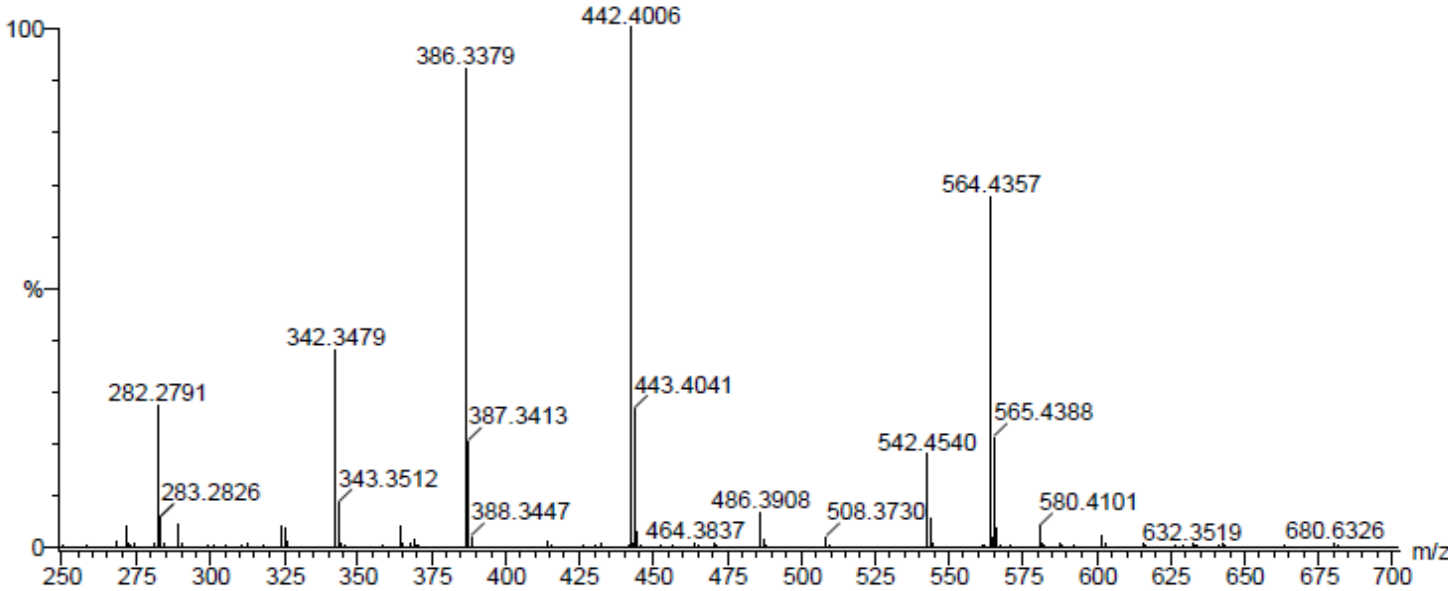
1: TOF MS ES+
8.80e+006



Chemical Formula: C₃₀H₆₀N₃O₅⁺

Exact Mass: 542.4527

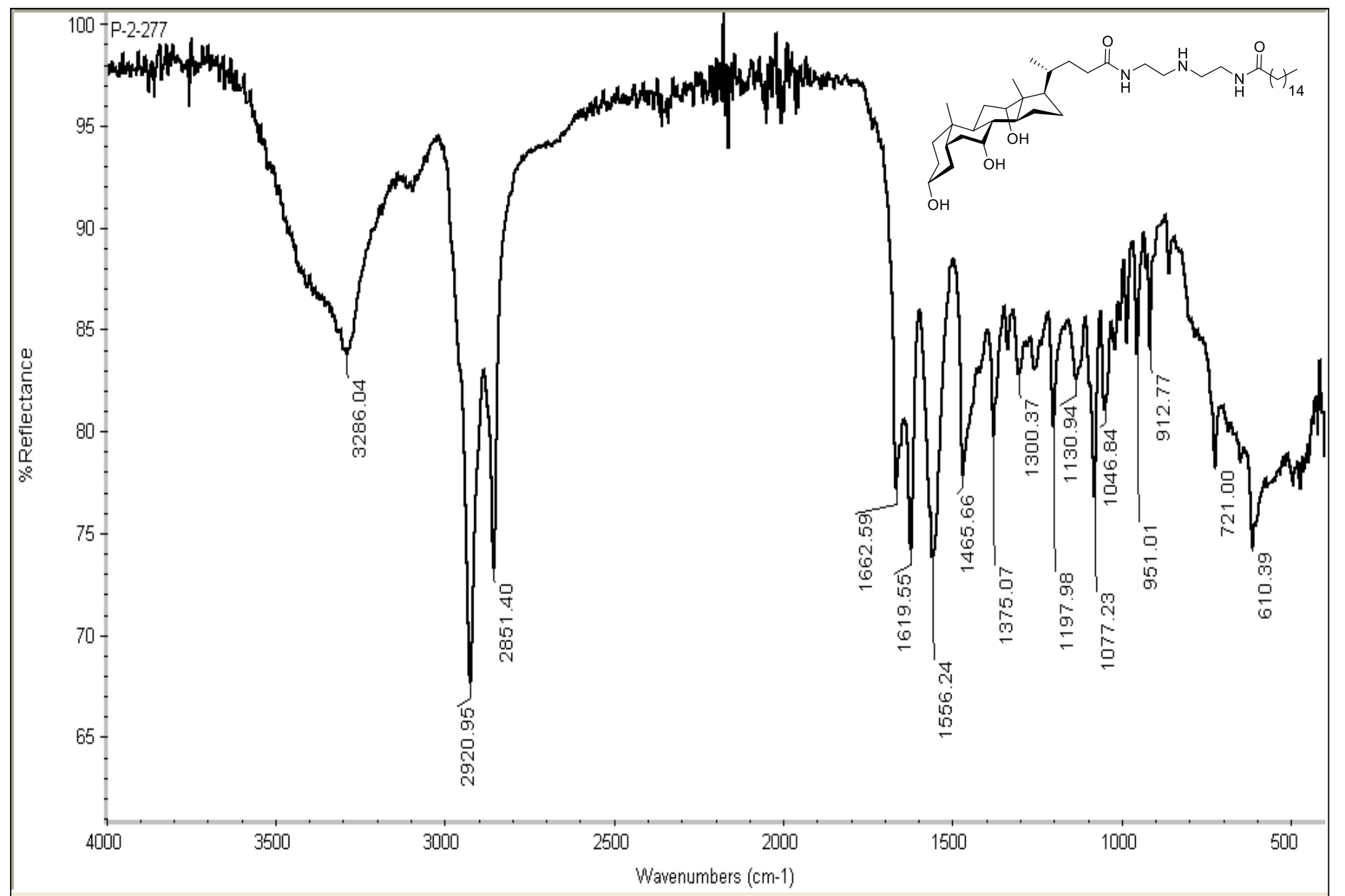
Found: 542.4540



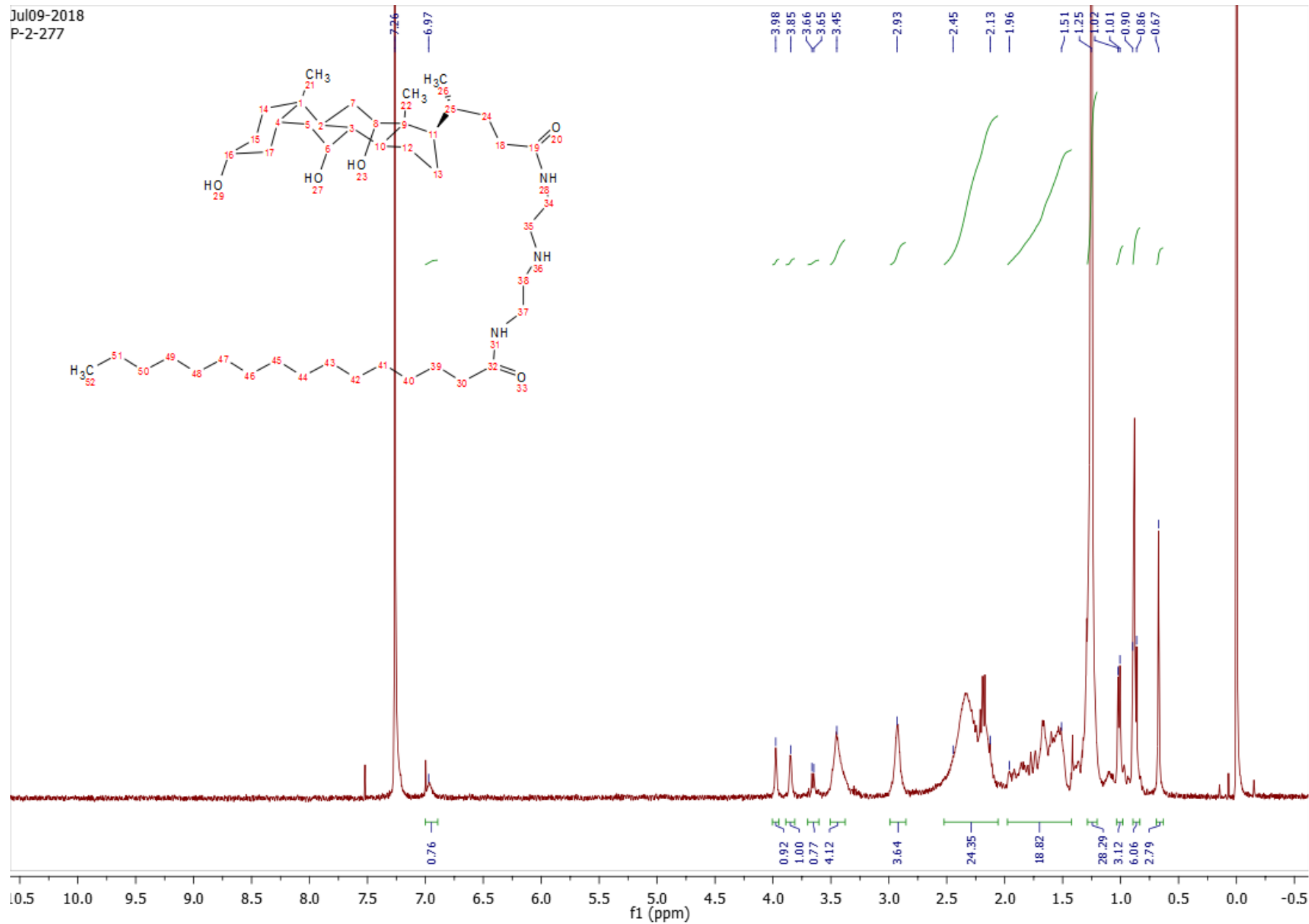
Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
542.4540	542.4533	0.7	1.3	2.5	364.3	n/a	n/a	C30 H60 N3 O5

IR of Compound 22



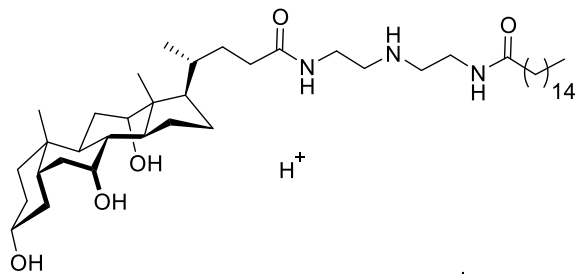
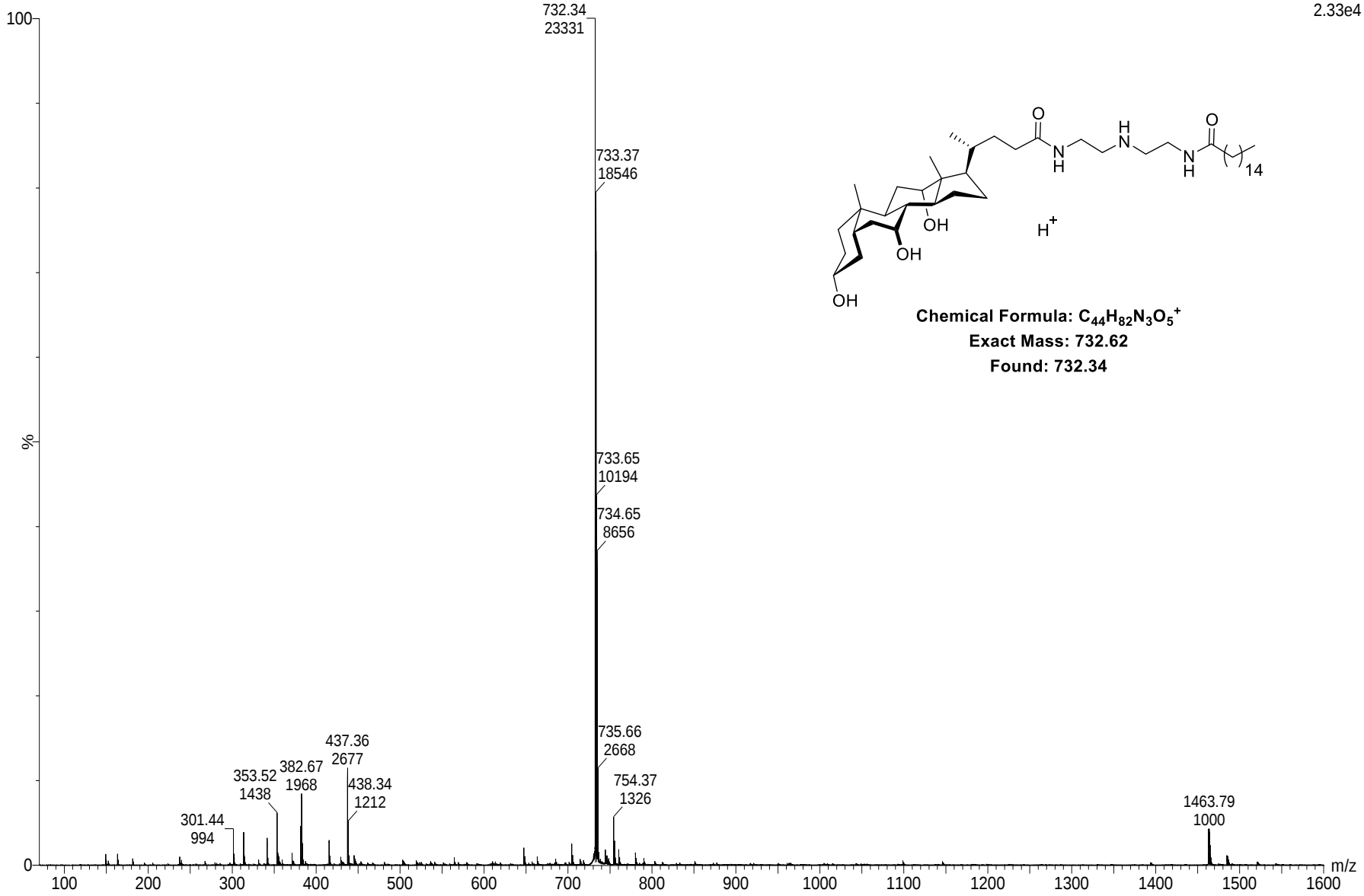
^1H NMR of Compound 22 (400 MHz, CDCl_3)



MS of Compound 22

WATERS, Q-TOF MICROMASS (ESI-MS)
MADHURI P-2-277 13 (0.242) Cm (12:29-52:66)

SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
2.33e4



Chemical Formula: $C_{44}H_{82}N_3O_5^+$
Exact Mass: 732.62
Found: 732.34