

## SUPPORTING INFORMATION

# Synthesis of FMRFaNV, a photoreleasable caged transmitter designed to study neurons-glia interactions in the central nervous system

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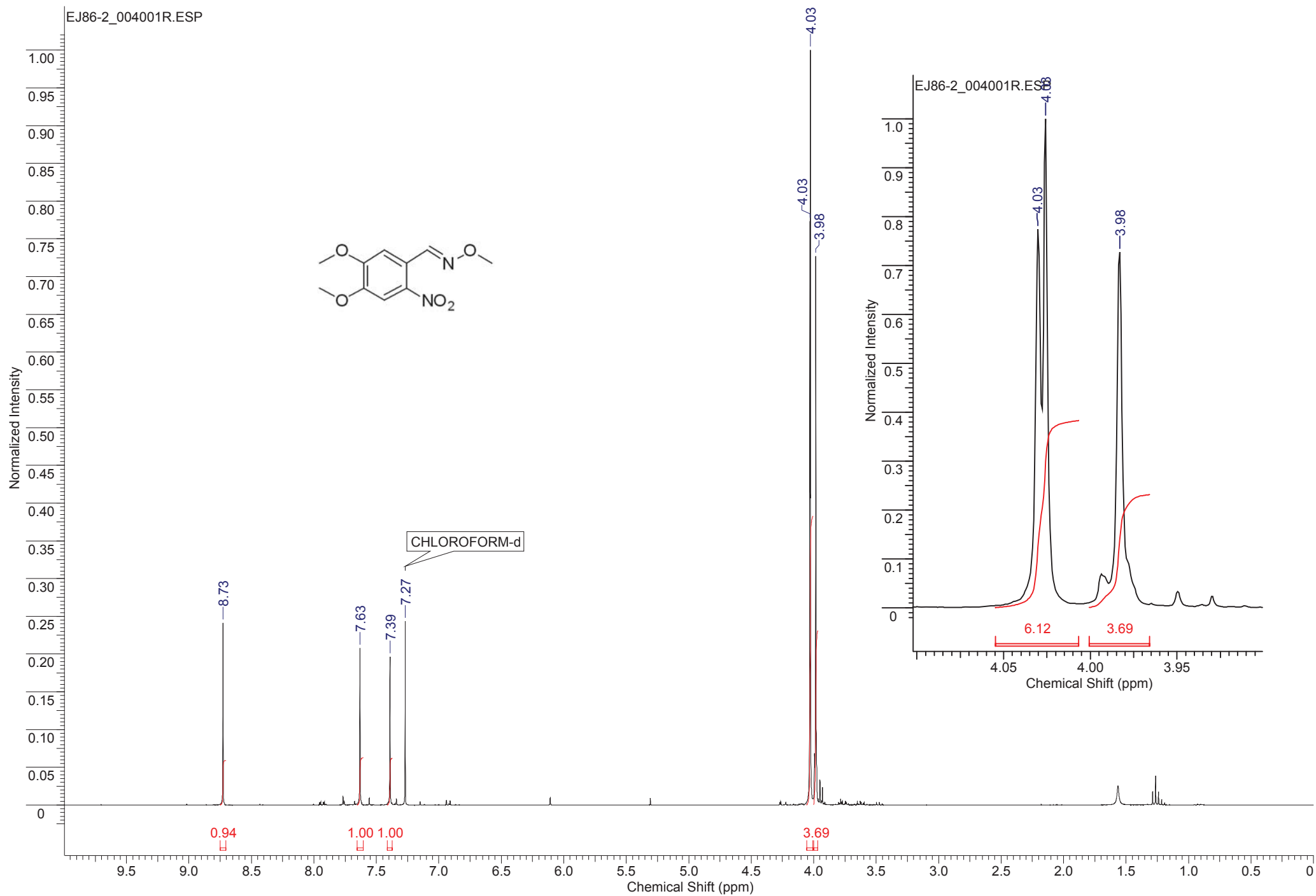
<sup>1</sup>*Department of Chemistry, University of Fribourg, Chemin du Musée 9, CH-1700 Fribourg, Switzerland*

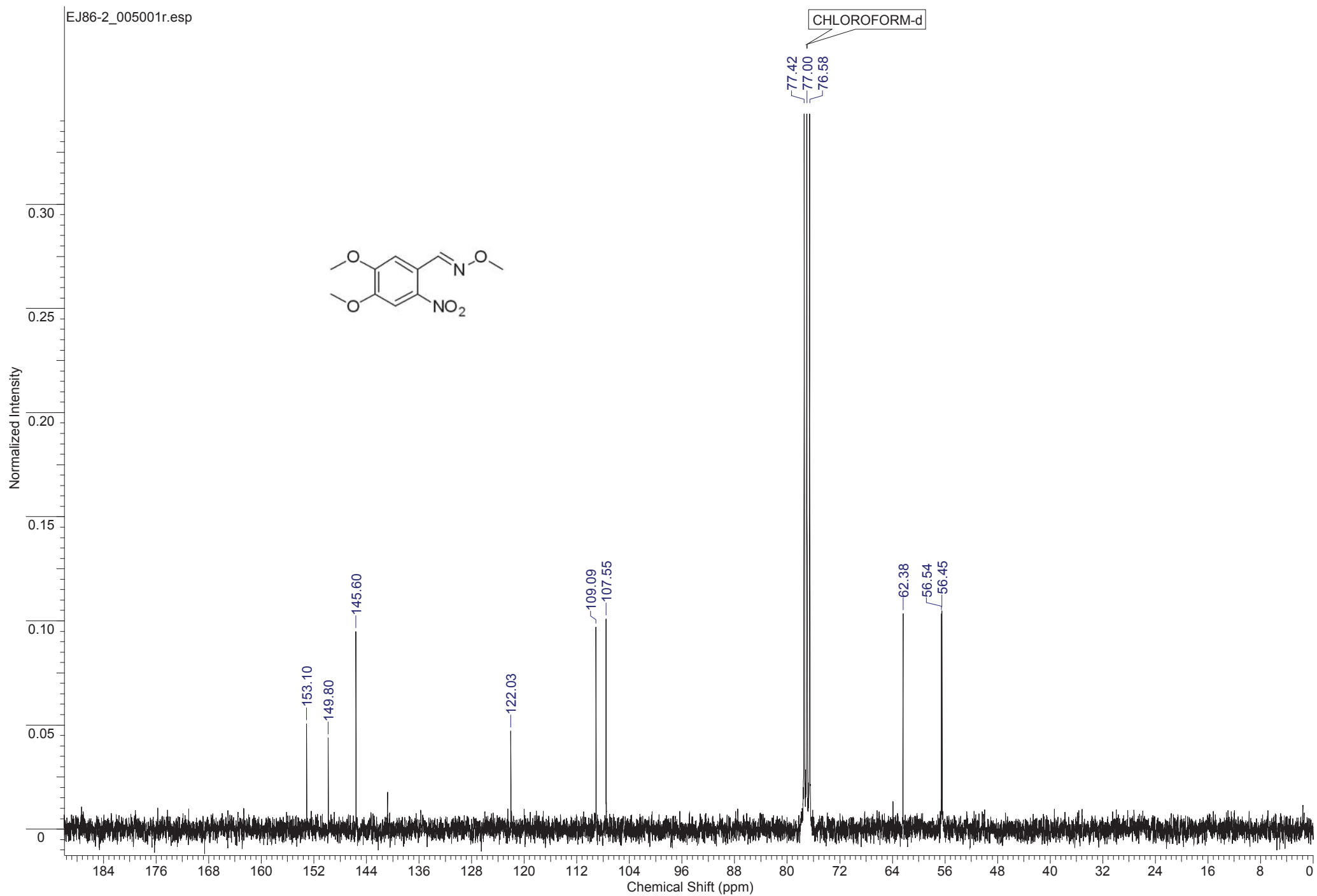
<sup>2</sup>*Department of Basic Neurosciences, School of Medicine, University of Geneva, rue Michel-Servet 1, CH-1211 Geneva 4, Switzerland*

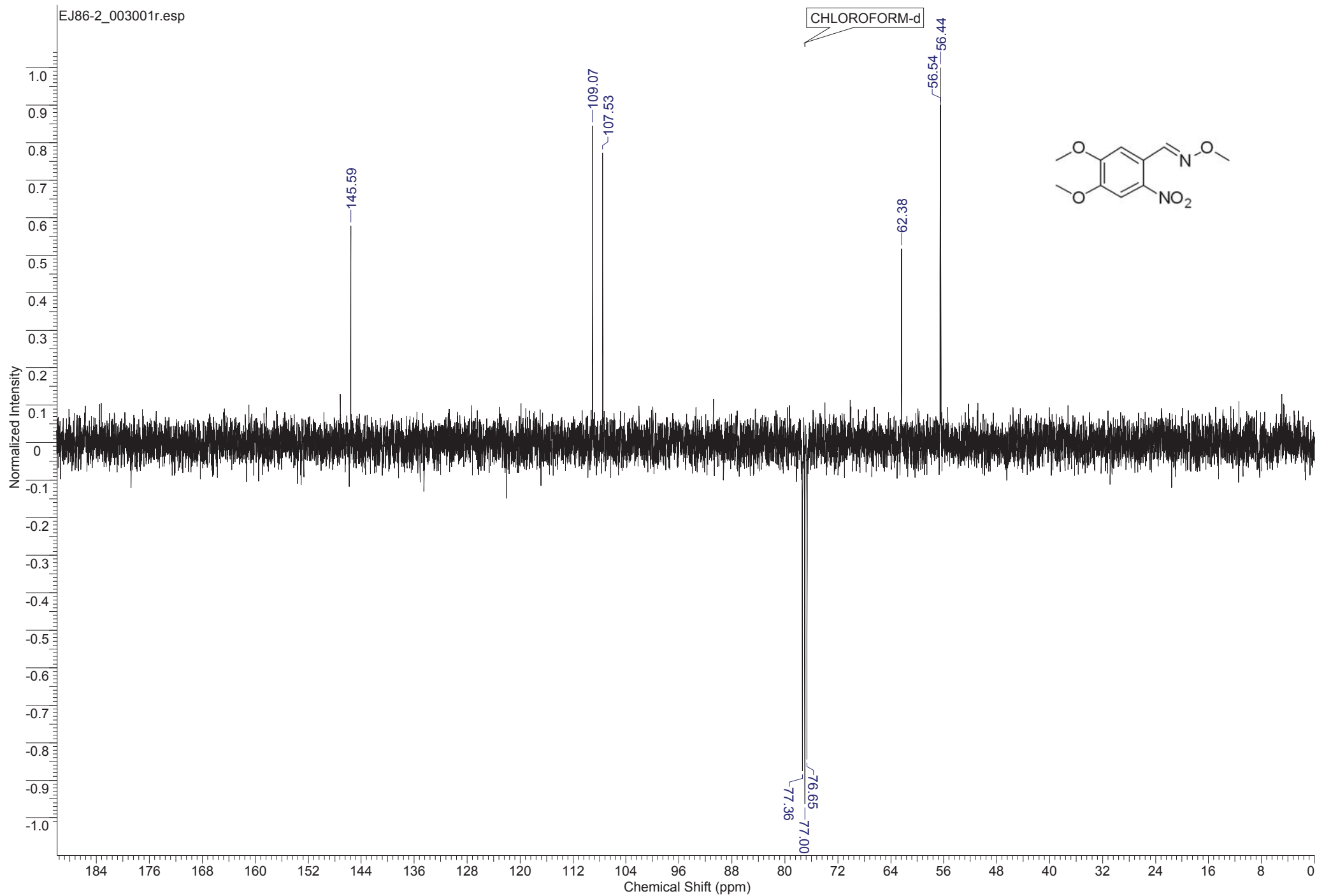
christian.bochet@unifr.ch

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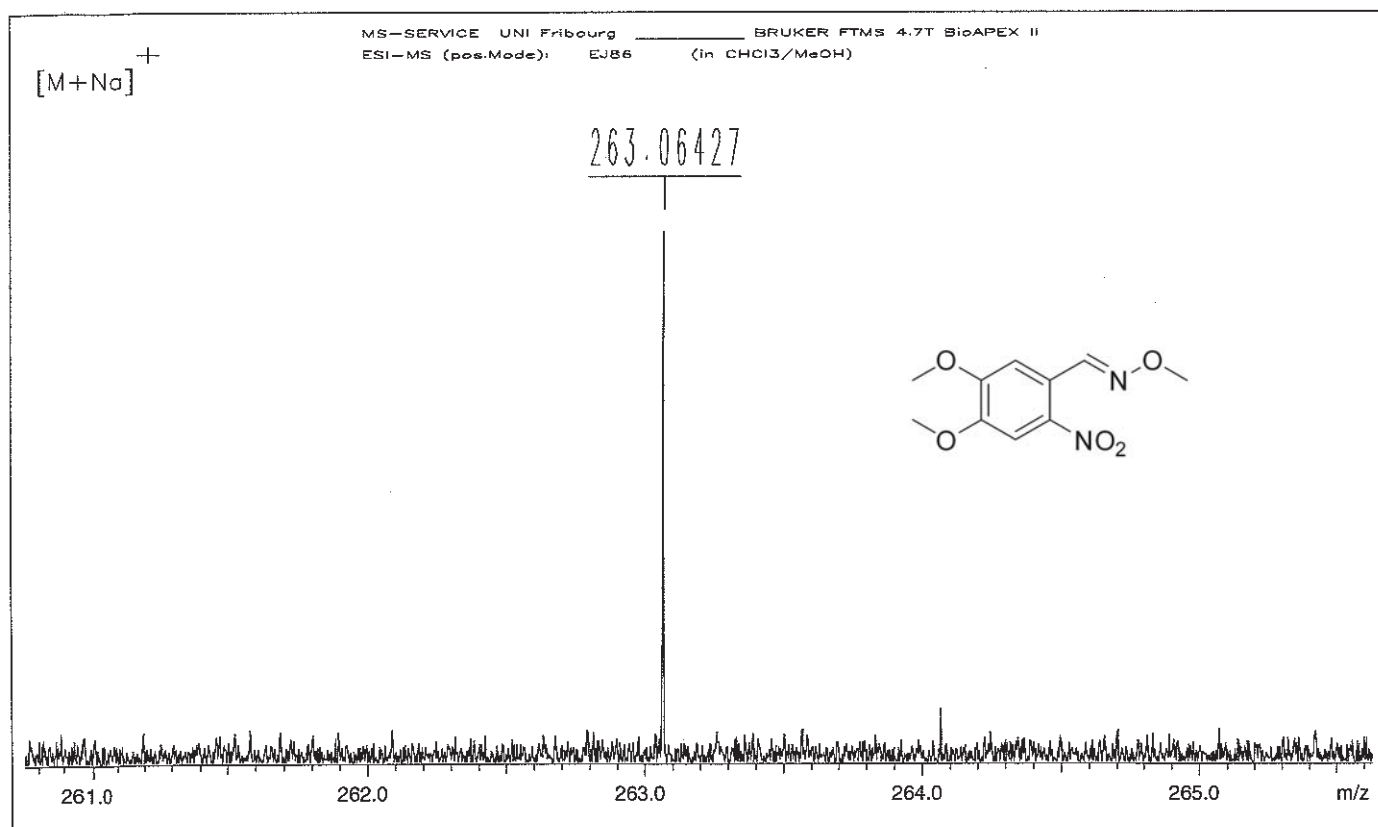
ESI-MS: EJ86

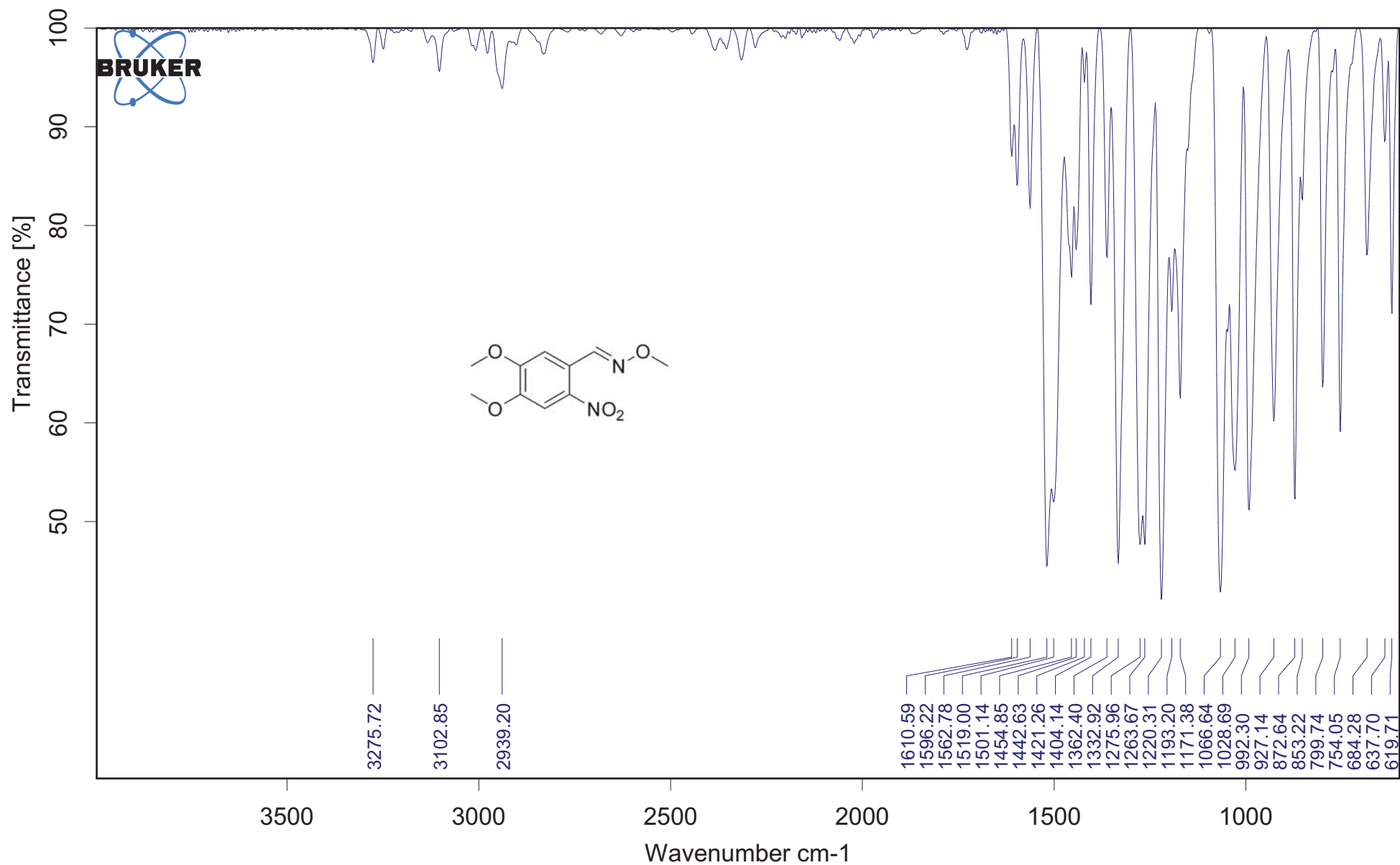
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XMASS Mass Analysis Constraints

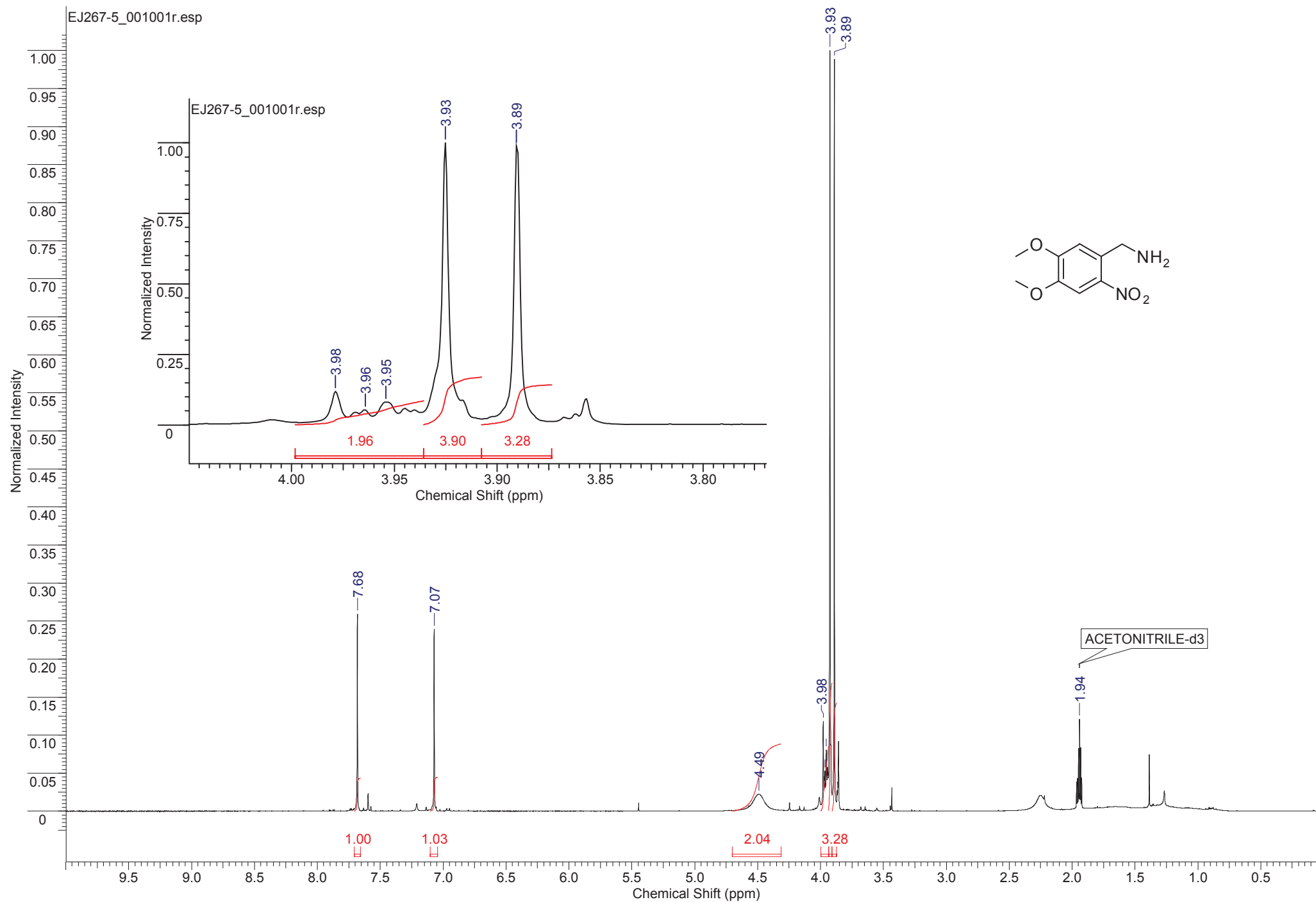
Ion mass = 263.0642670

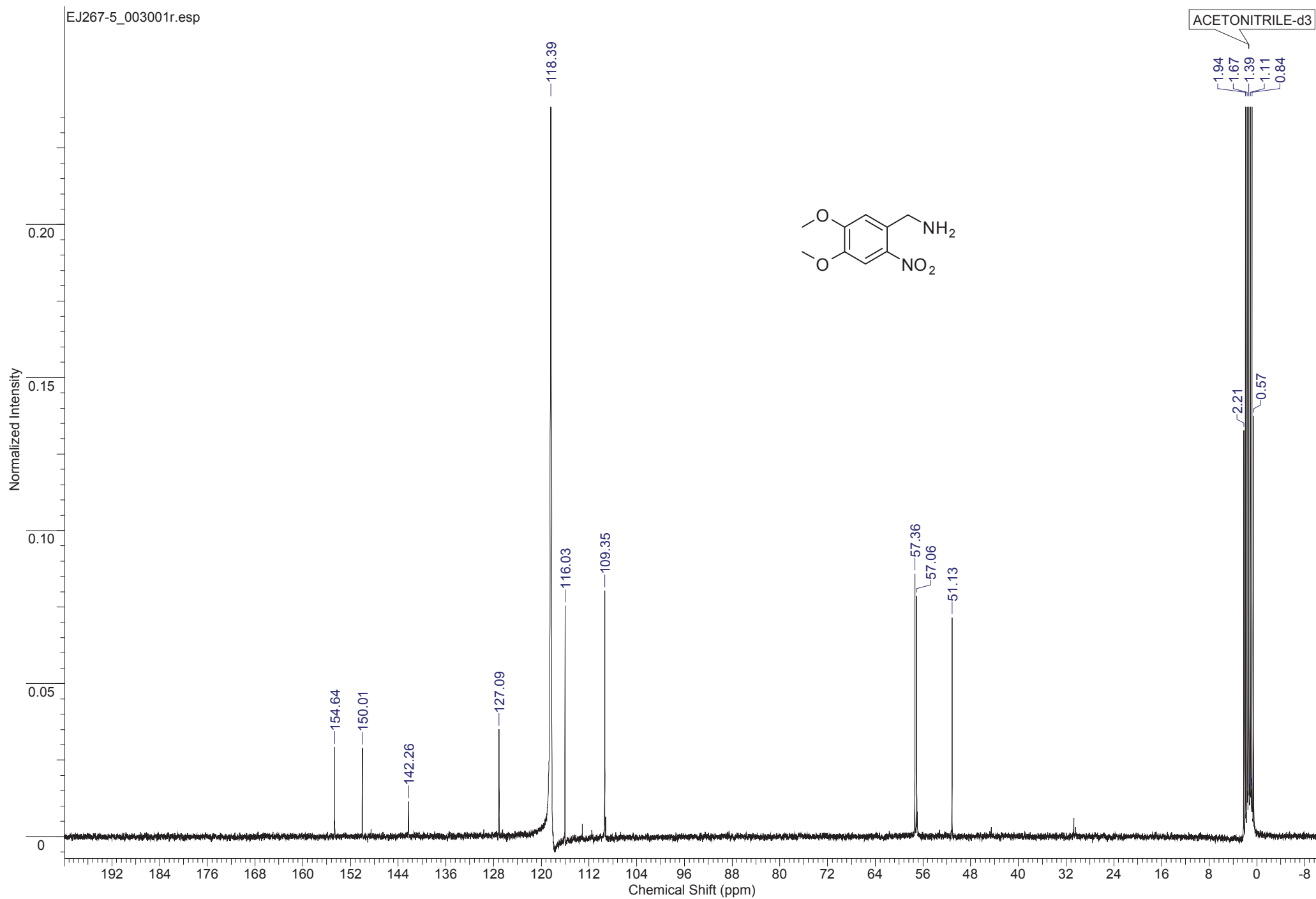
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 263.0642670								
1	10	12	2	5	1	263.0638426	5.5	4.244e-04
2	10	9	5	4	0	263.0649052	9.0	6.382e-04
3	9	13	1	8	0	263.0635678	4.0	6.992e-04
4	8	7	8	3	0	263.0635626	9.5	7.044e-04
5	11	8	6	1	1	263.0651800	10.5	9.130e-04
6	8	10	5	4	1	263.0624999	6.0	1.767e-03
7	12	11	2	5	0	263.0662479	8.5	1.981e-03
8	7	11	4	7	0	263.0622251	4.5	2.042e-03
9	13	10	3	2	1	263.0665227	10.0	2.256e-03
10	7	14	1	8	1	263.0611625	1.0	3.104e-03

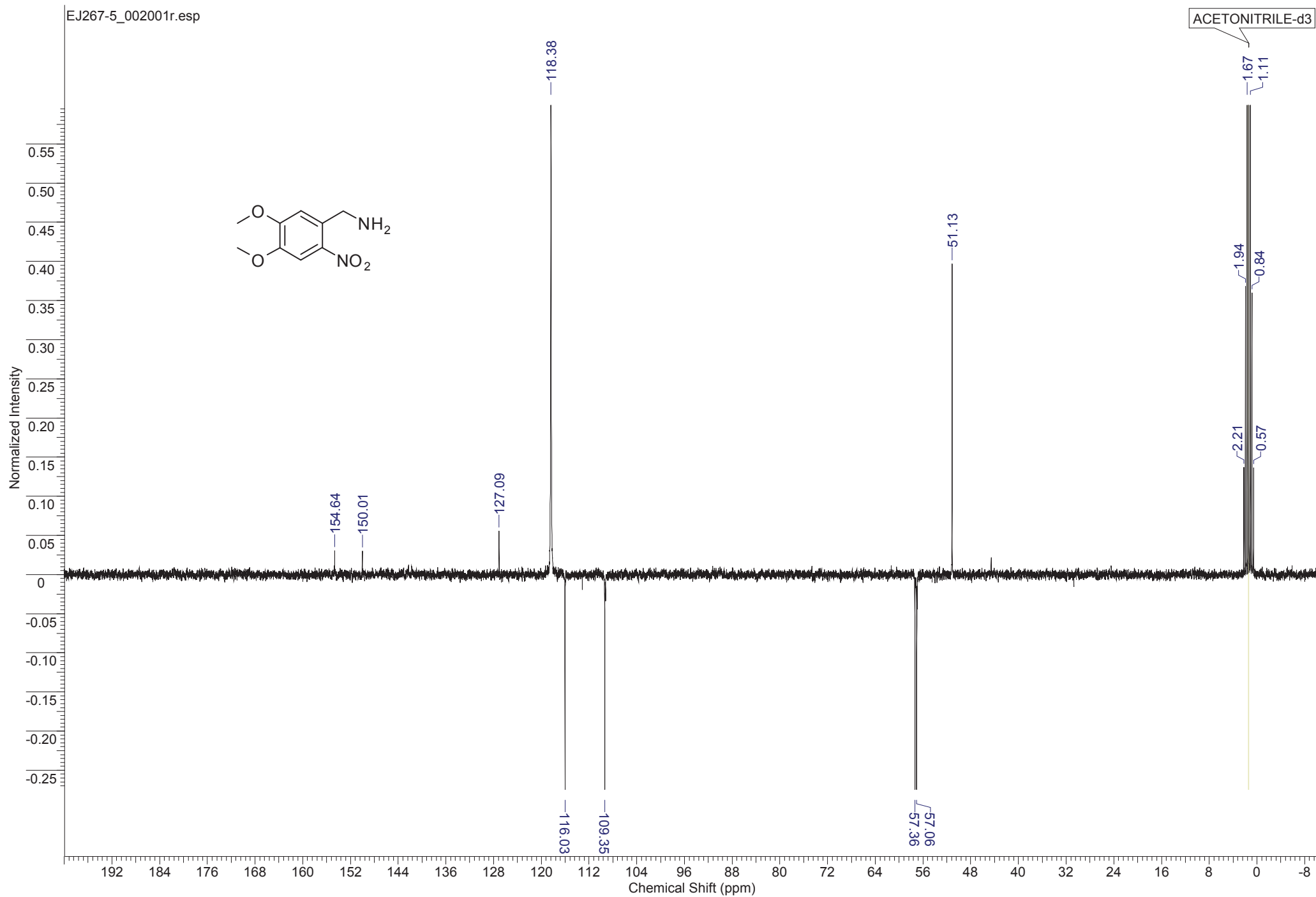












ESI-MS: EJ98

XMASS Mass Analysis for /Data/UNI\_FR/JANE5604\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

Ion mass = 213.0873300

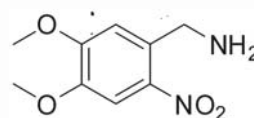
Charge = +1

#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 213.0873300							
1	9	13	2	4	213.0869833	4.5	3.467e-04
2	7	11	5	3	213.0856407	5.0	1.689e-03
3	12	11	3	1	213.0896634	9.0	2.333e-03
4	6	15	1	7	213.0843033	0.0	3.027e-03
5	5	9	8	2	213.0842980	5.5	3.032e-03
6	5	15	3	6	213.0955366	0.0	8.207e-03
7	13	11	1	2	213.0784300	9.0	8.900e-03
8	6	11	7	2	213.0968741	5.0	9.544e-03
9	11	9	4	1	213.0770874	9.5	1.024e-02
10	8	13	4	3	213.0982167	4.5	1.089e-02

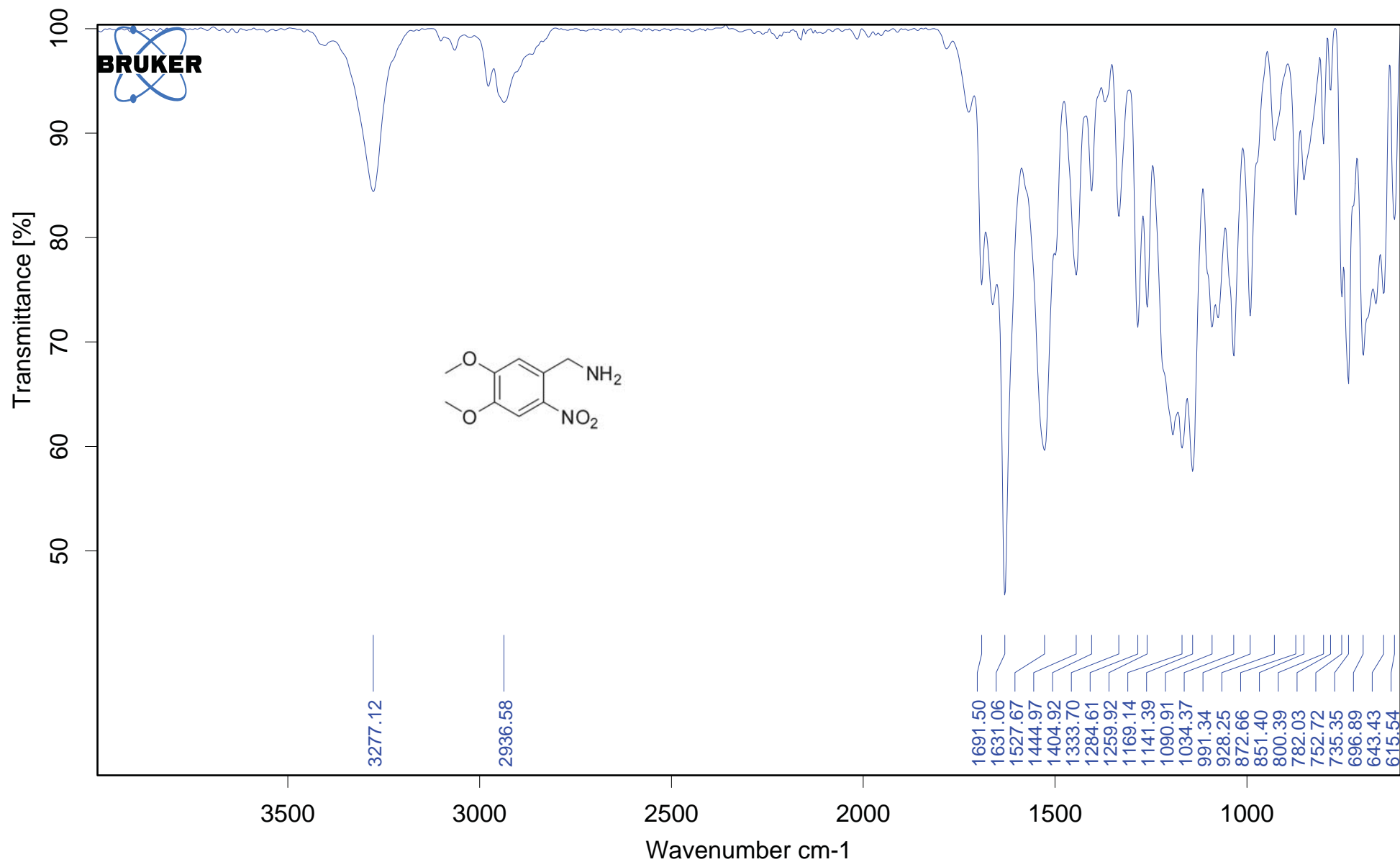
[M+H]<sup>+</sup>

MS-SERVICE UNI Fribourg BRUKER FTMS 4.7T BioAPEX II  
ESI-MS (pos.Mode): EJ98 (in ACN)

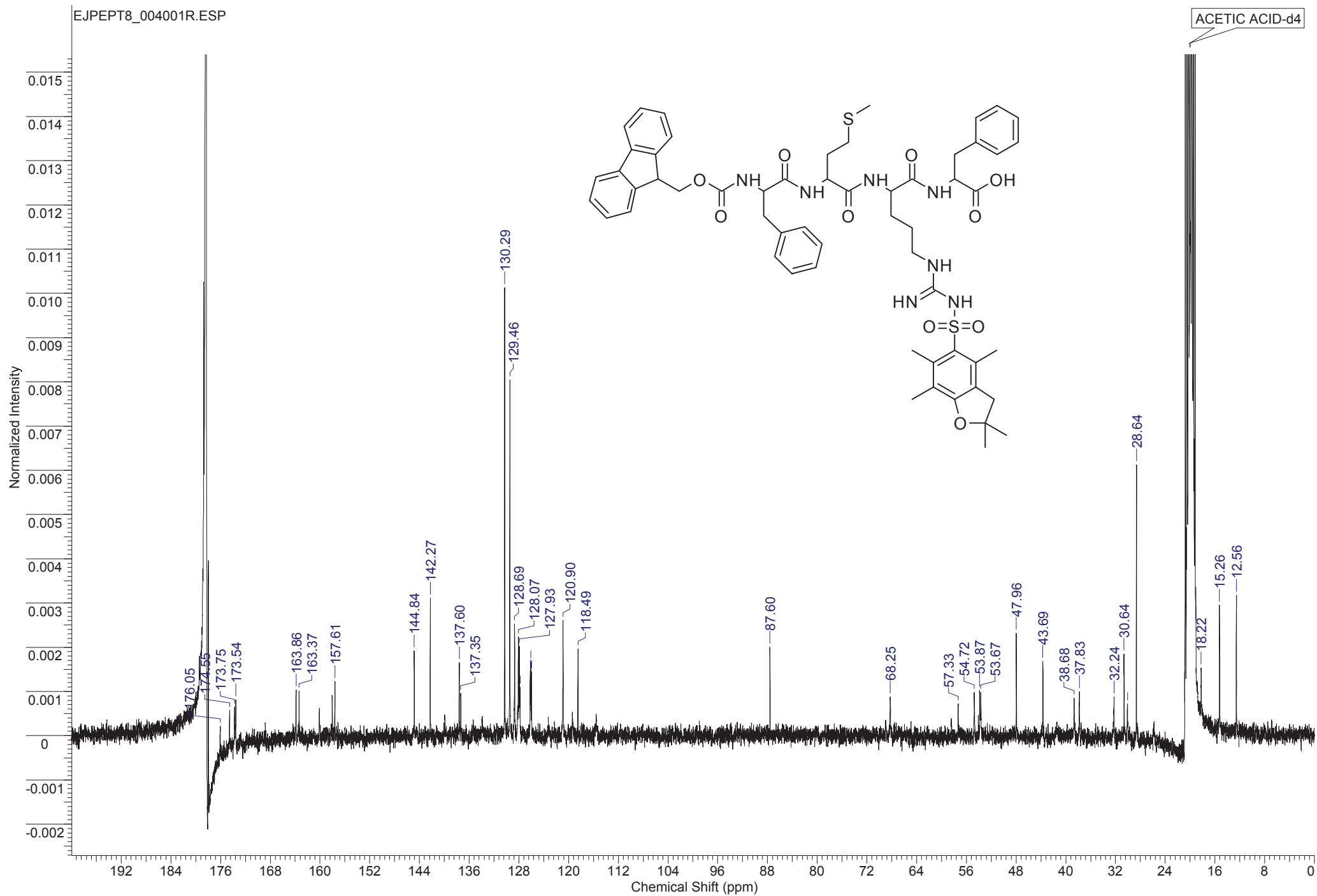
213.08733

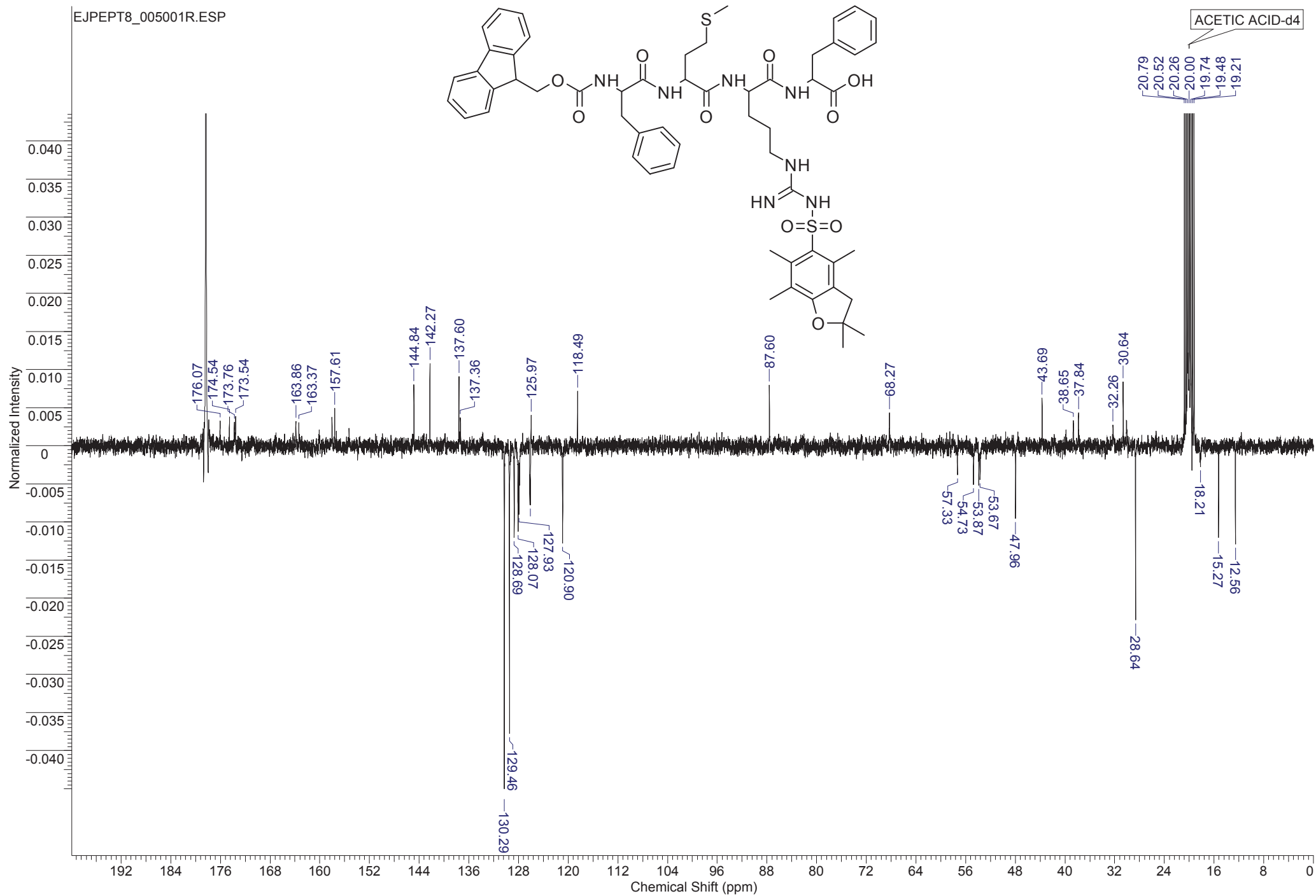


211.0 212.0 213.0 214.0 215.0 m/z









ESI-MS: PEPTS

XMASS Mass Analysis for /Data/UNI\_FR/JANE5621\_ESI/10/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

Ion mass = 1074.4465340

Charge = +1

#	C	H	N	O	S	mass	DBE	error
---	---	---	---	---	---	------	-----	-------

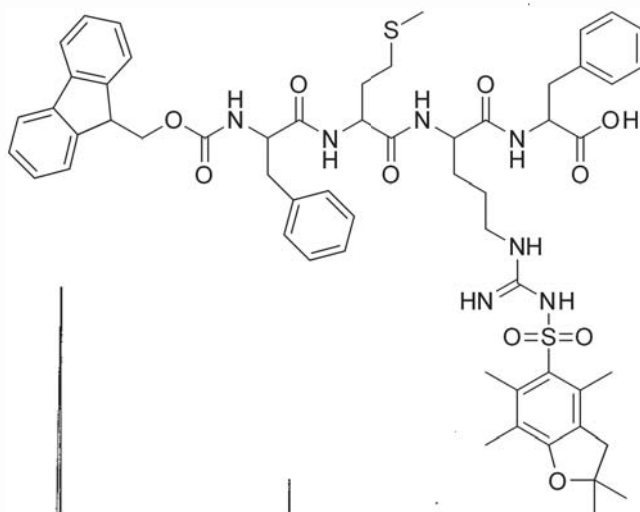
\*\*\* Mass Analysis for mass 1074.4465340

1	57	68	7	10	2	1074.4463592	27.5	1.748e-04
2	54	70	6	13	2	1074.4436792	23.0	2.855e-03
3	60	64	7	10	1	1074.4429884	32.5	3.546e-03
4	52	68	9	12	2	1074.4423365	23.5	4.198e-03
5	56	66	8	12	1	1074.4515417	28.0	5.008e-03
6	57	66	6	13	1	1074.4403083	28.0	6.226e-03
7	55	64	9	12	1	1074.4389657	28.5	7.568e-03
8	59	64	9	9	1	1074.4542218	32.5	7.688e-03
9	53	70	8	12	2	1074.4549126	23.0	8.379e-03
10	56	68	9	9	2	1074.4575926	27.5	1.106e-02

[M+H]<sup>+</sup>

MS-SERVICE UNI Fribourg BRUKER FTMS 4.7T BioAPEX II  
ESI-MS (pos-Mode): PEPTS (in ACN)

1074.44653



1073.0

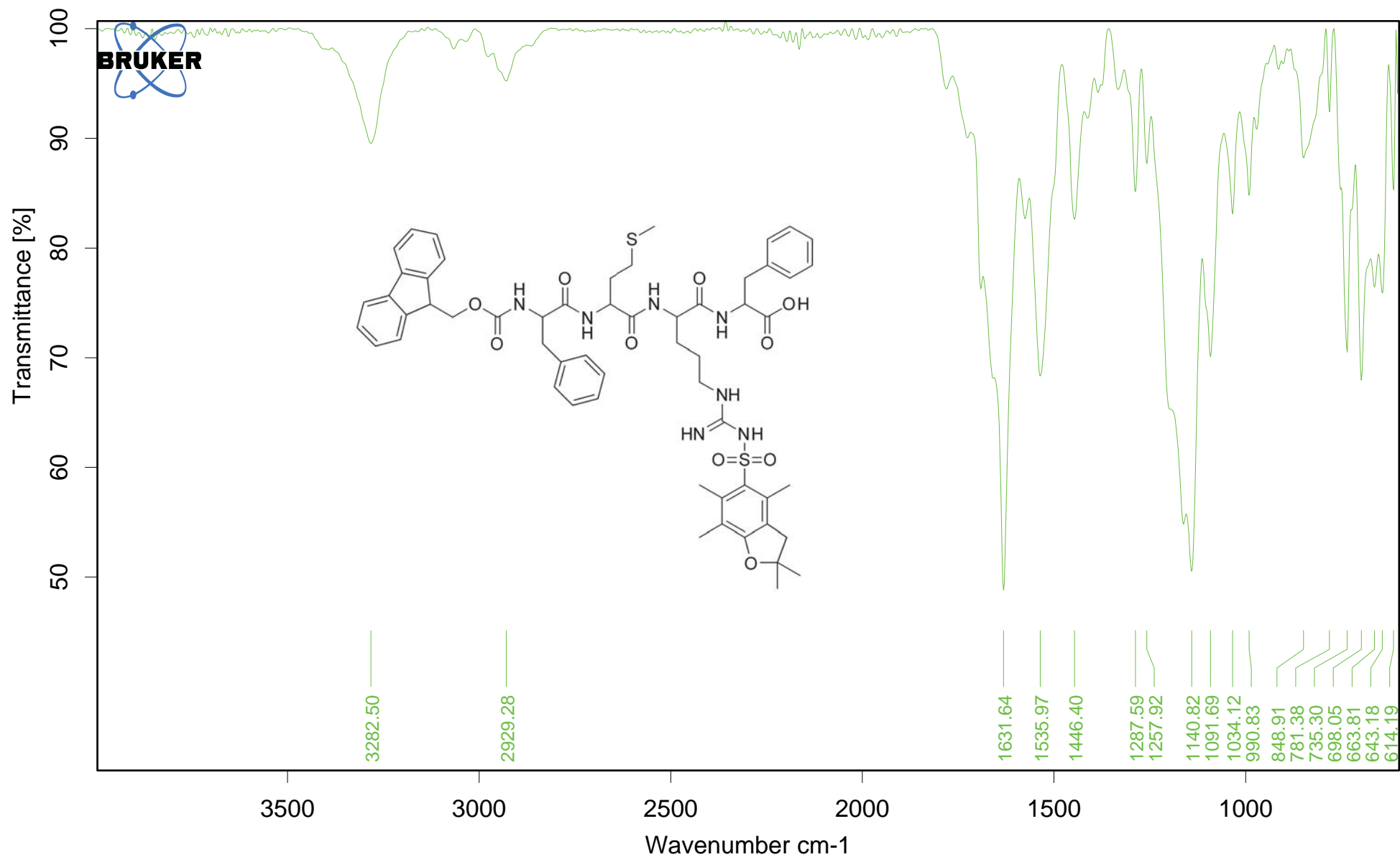
1074.0

1075.0

1076.0

1077.0

m/z



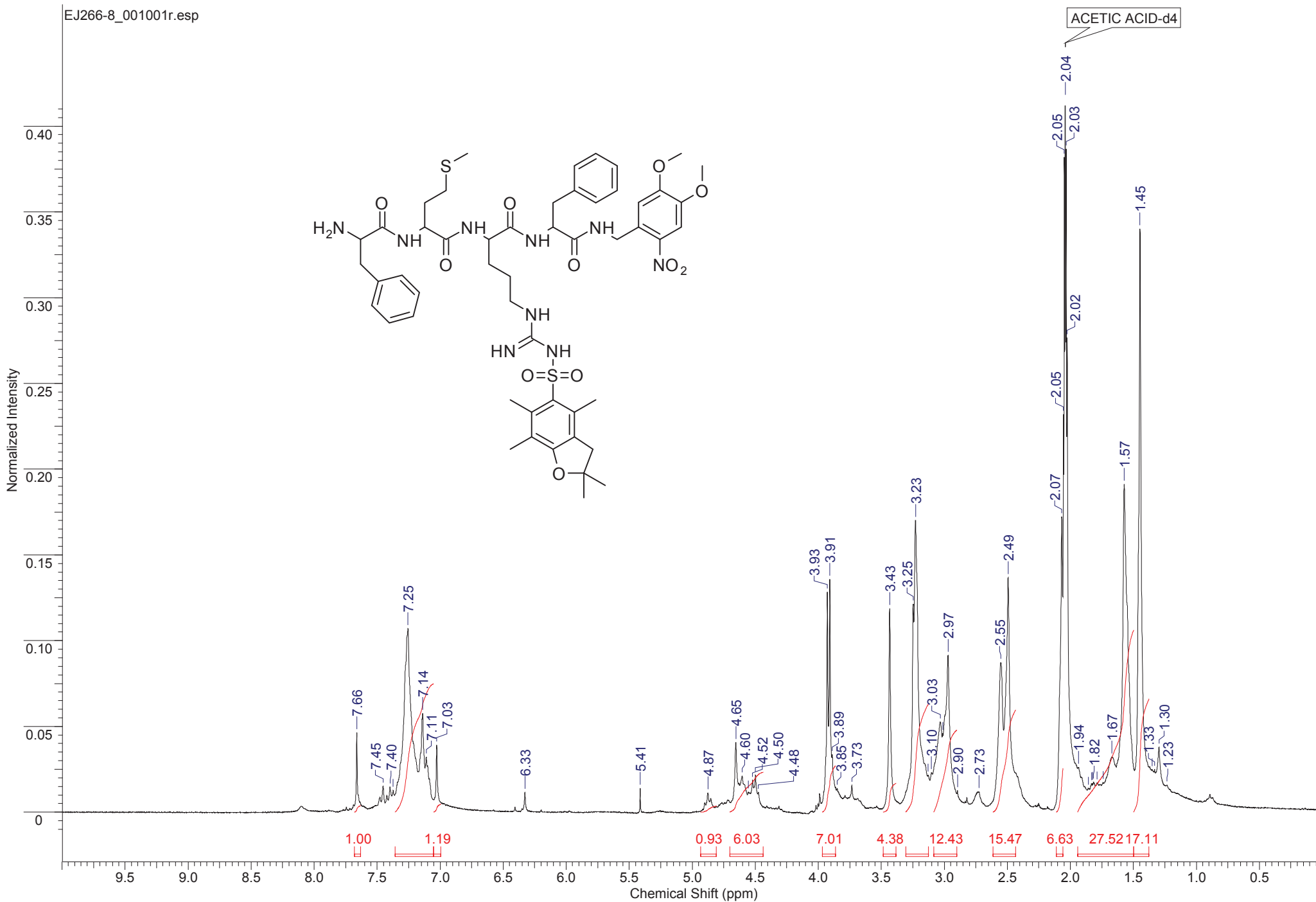
U:\Master\Sem2\TP OC\EJPept5.0

EJPept5

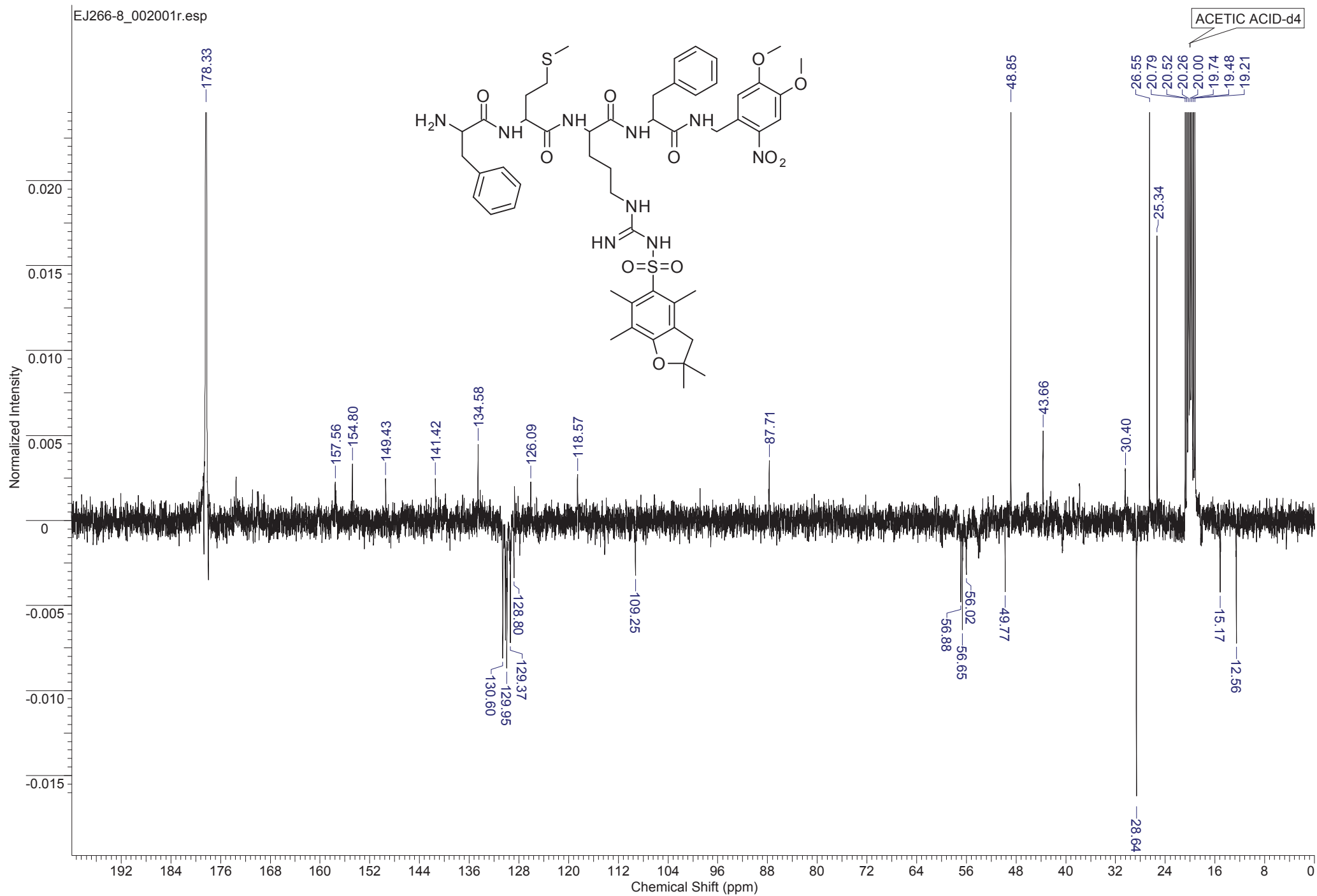
white powder

21/03/2011









ACETIC ACID-d4

ESI-MS: EJ102

XMASS Mass Analysis for /Data/UNI\_FR/JANE5620\_ESI/10/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

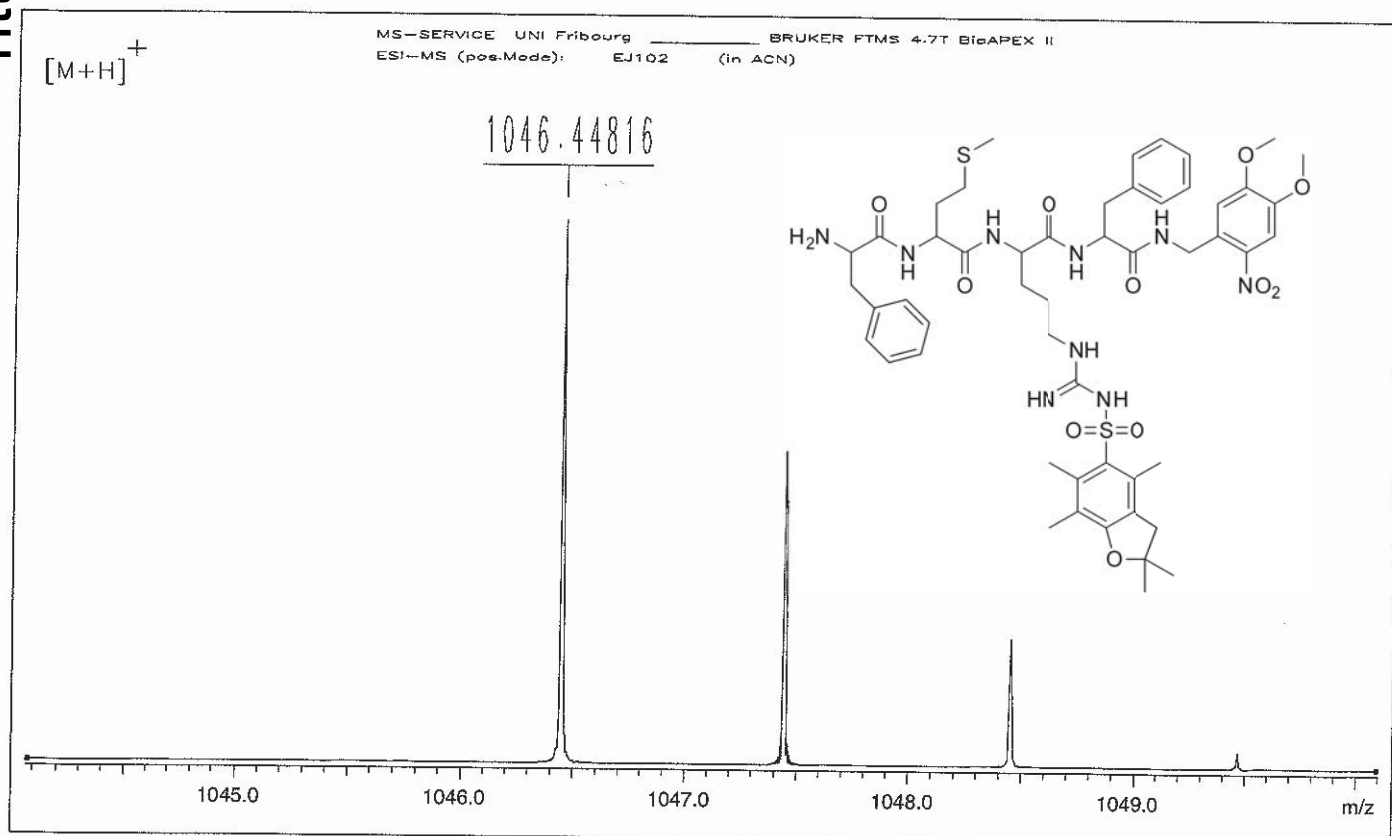
Ion mass = 1046.4481610

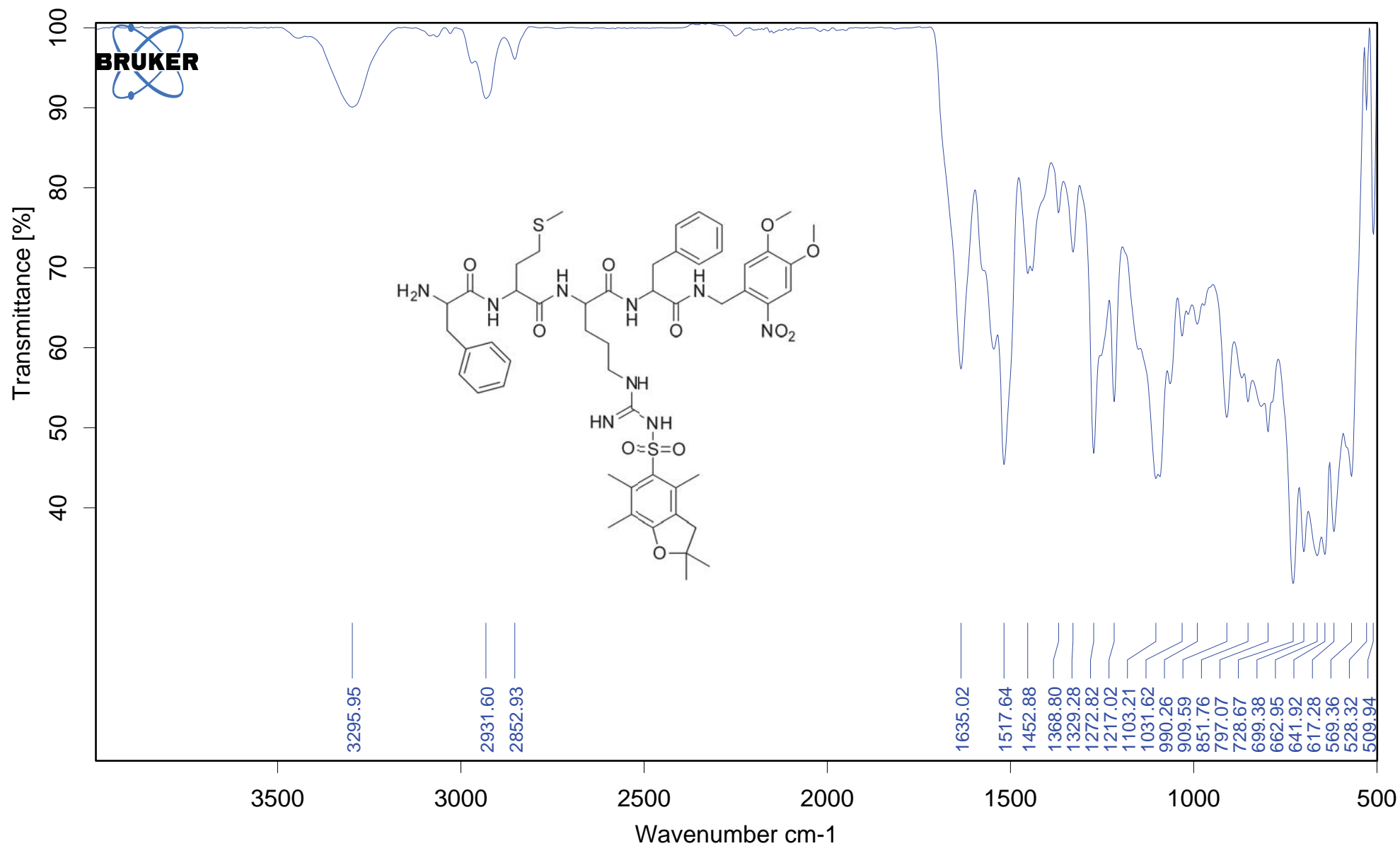
Charge = +1

#	C	H	N	O	S	mass	DBE	error
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\*\*\* Mass Analysis for mass 1046.4481610

1	51	68	9	11	2	1046.4474219	22.5	7.391e-04
2	57	62	10	8	1	1046.4467311	32.0	1.430e-03
3	54	66	10	8	2	1046.4501019	27.0	1.941e-03
4	49	66	12	10	2	1046.4460792	23.0	2.082e-03
5	48	64	13	12	1	1046.4512617	23.5	3.101e-03
6	54	64	9	11	1	1046.4440511	27.5	4.110e-03
7	50	66	10	13	1	1046.4526044	23.0	4.443e-03
8	46	68	11	13	2	1046.4433991	18.5	4.762e-03
9	52	62	12	10	1	1046.4427084	28.0	5.453e-03
10	45	68	13	12	2	1046.4546325	18.5	6.472e-03



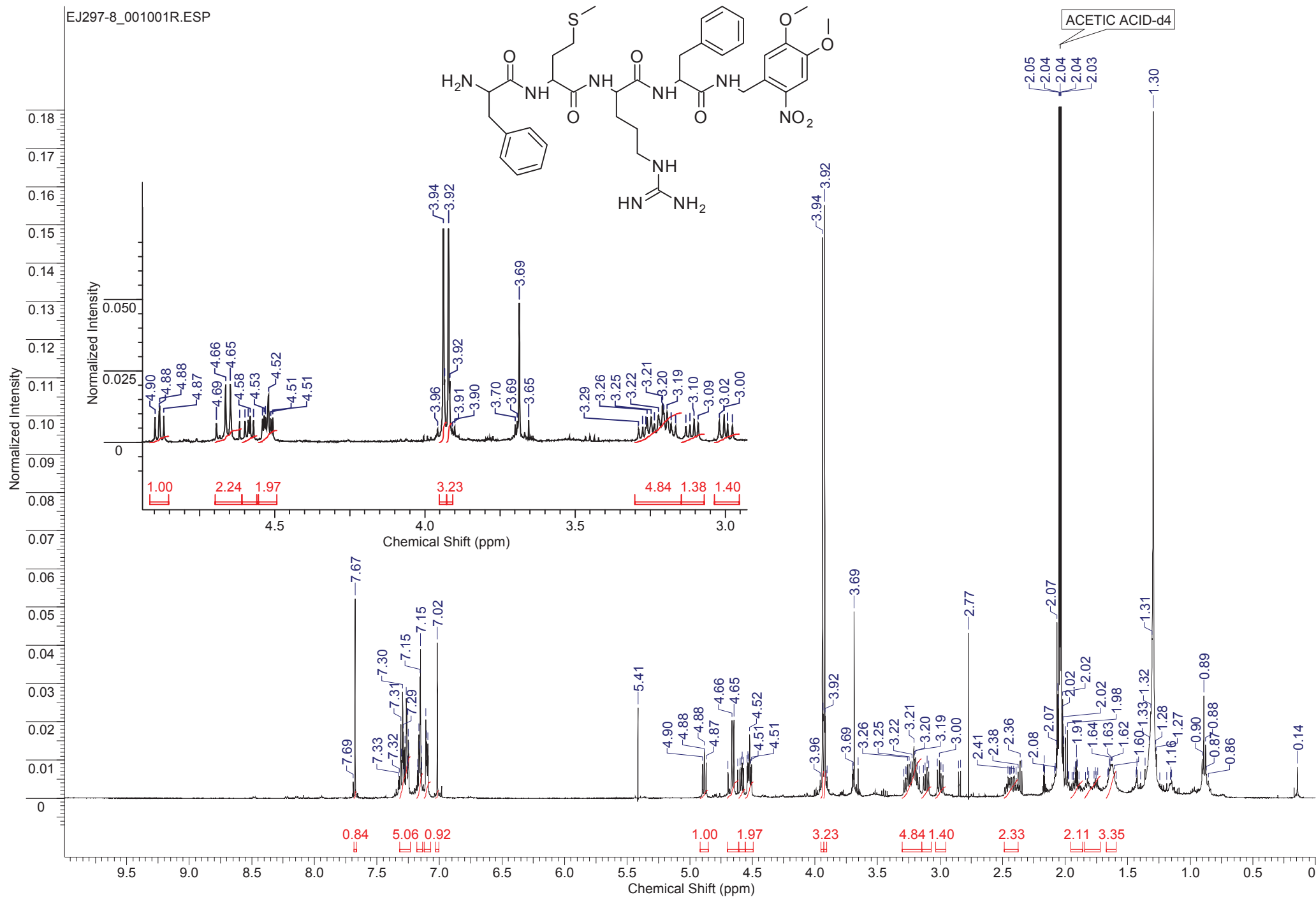


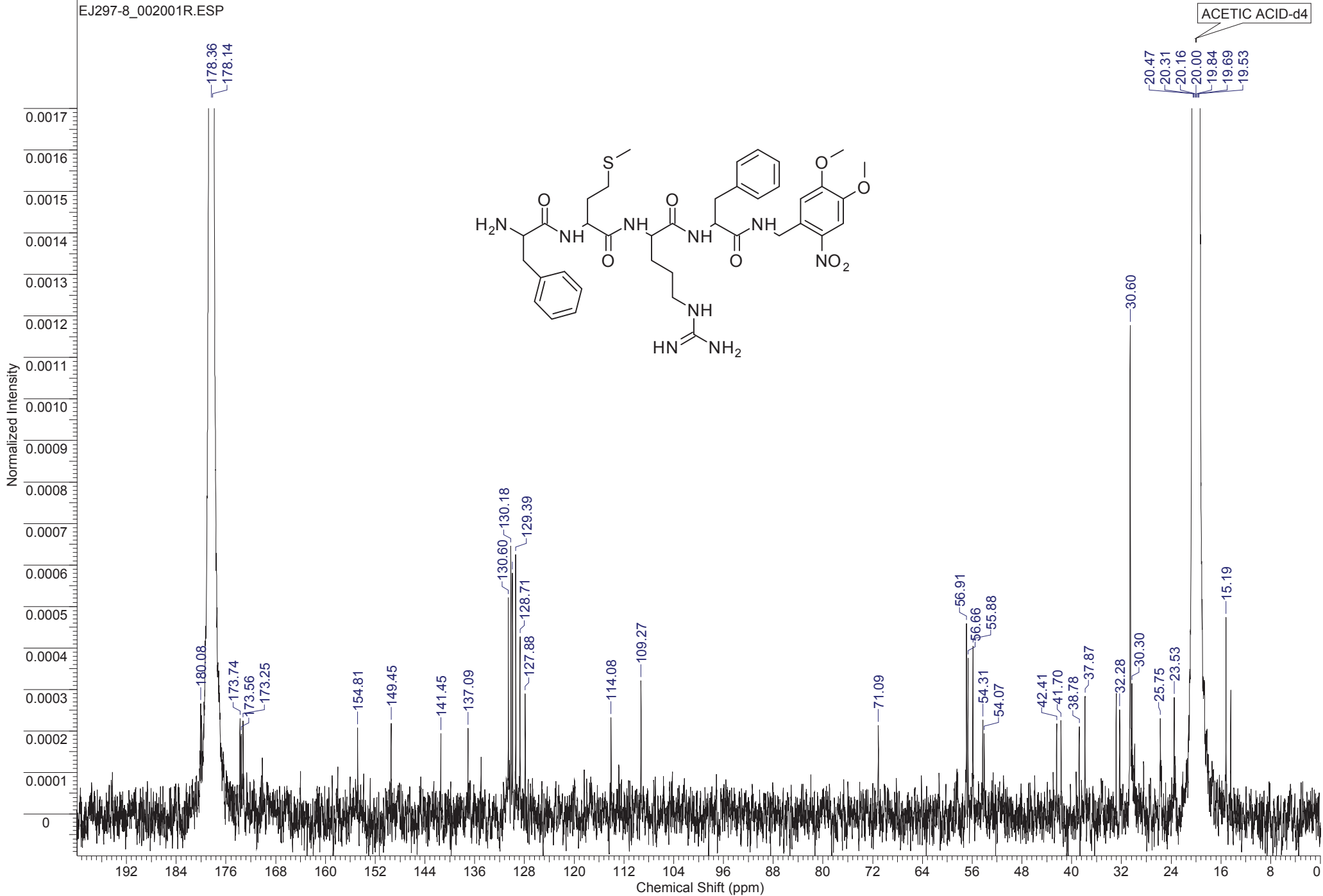
U:\Master\Sem2\TP OC\IR\IR non trattati\EJ102.0

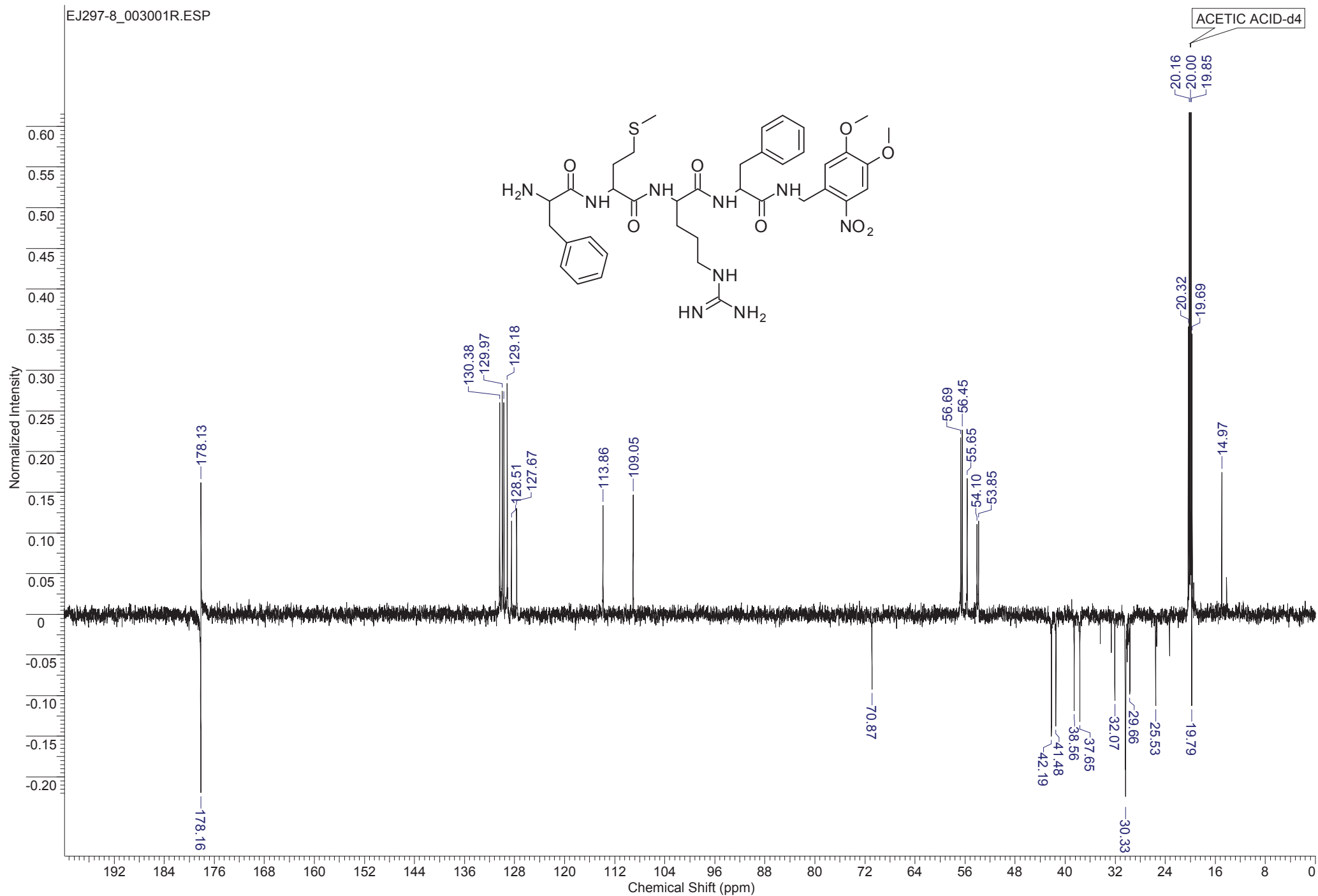
EJ102

yellow powder

30/03/2011









ESI-MS: EJ103

XMASS Mass Analysis for /Data/UNI\_FR/JANE5619\_ESI/10/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

Ion mass = 794.3650100

Charge = +1

#	C	H	N	O	S	mass	DBE	error
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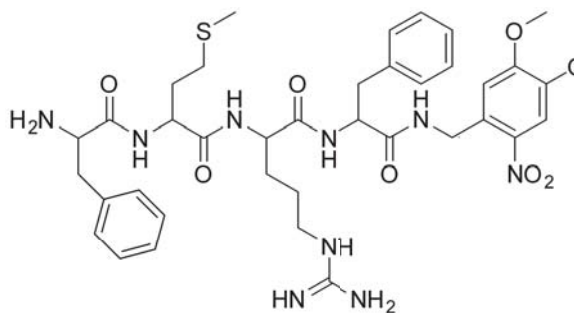
\*\*\* Mass Analysis for mass 794.3650100

1	38	52	9	8	1	794.3654068	17.5	3.968e-04
2	46	56	3	5	2	794.3655897	20.5	5.797e-04
3	44	54	6	4	2	794.3642471	21.0	7.629e-04
4	40	54	6	9	1	794.3667495	17.0	1.739e-03
5	43	58	2	8	2	794.3629096	16.0	2.100e-03
6	42	52	9	3	2	794.3629044	21.5	2.106e-03
7	49	52	3	5	1	794.3622189	25.5	2.791e-03
8	41	50	10	5	1	794.3680869	22.0	3.077e-03
9	42	56	3	10	1	794.3680921	16.5	3.082e-03
10	49	54	4	2	2	794.3682698	25.0	3.260e-03

[M+H]<sup>+</sup>

MS-SERVICE UNI Fribourg BRUKER FTMS 4.7T BioAPEX II  
ESI-MS (pos.Mode): EJ103 (in ACN)

794.36501



793.0

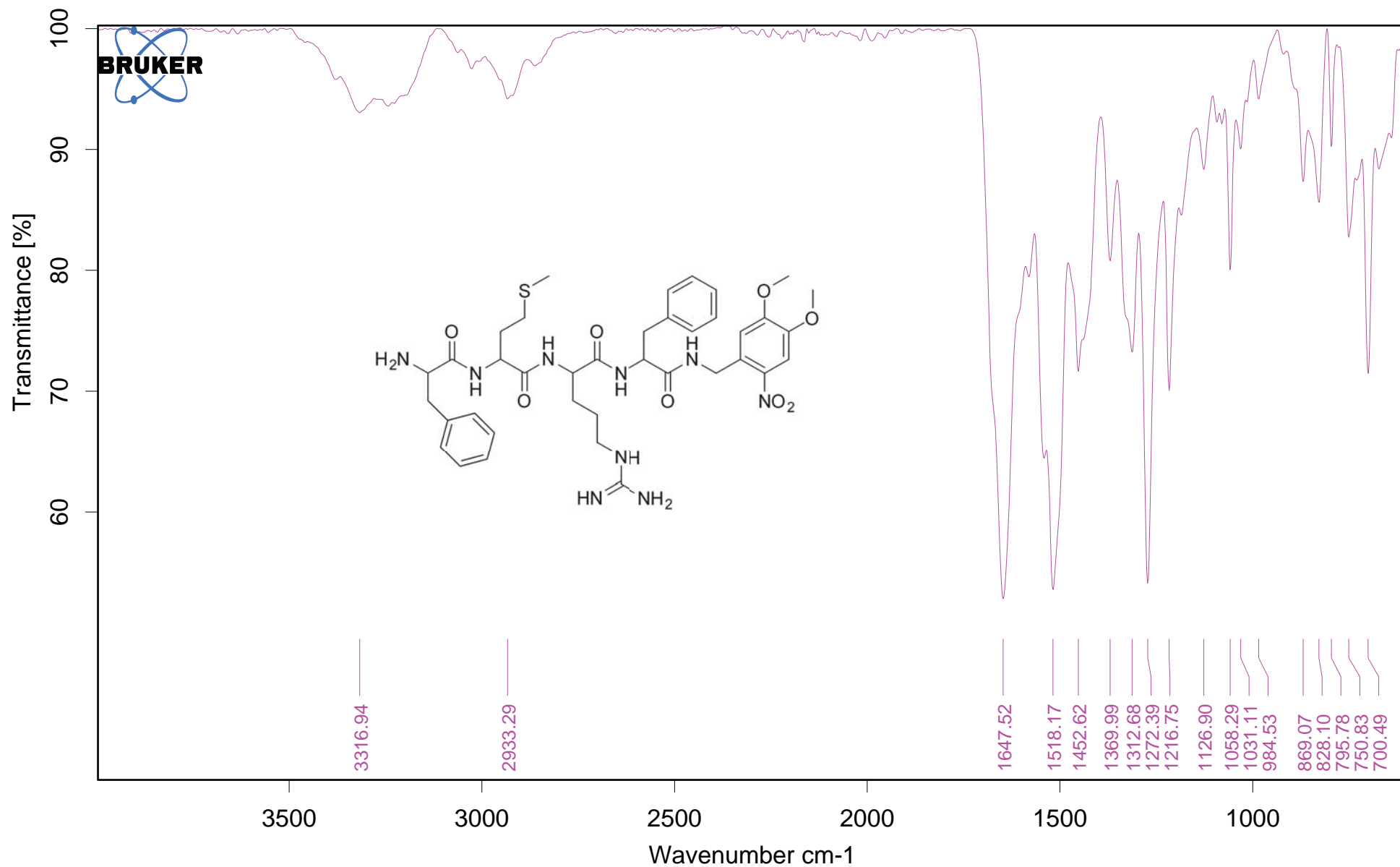
794.0

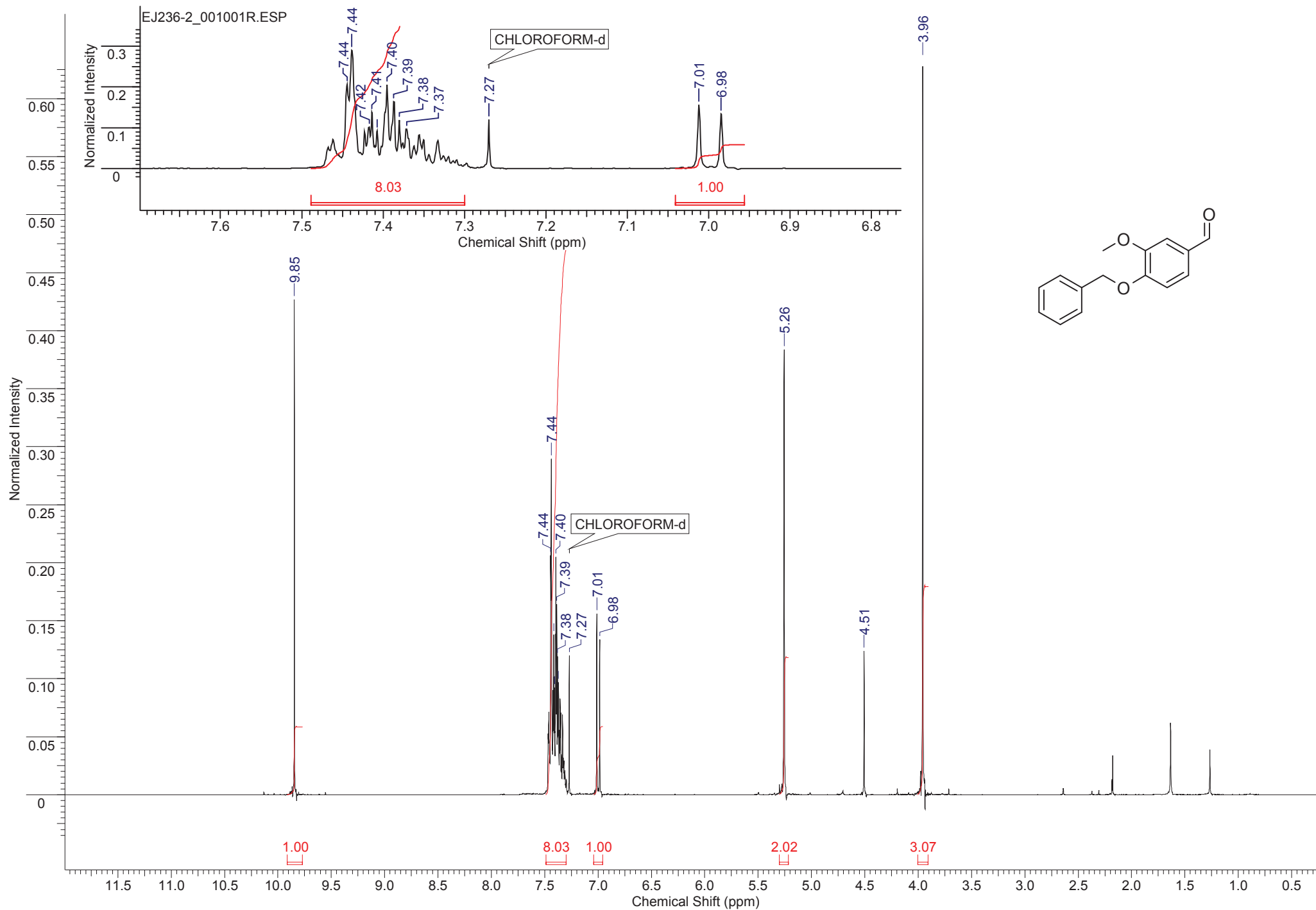
795.0

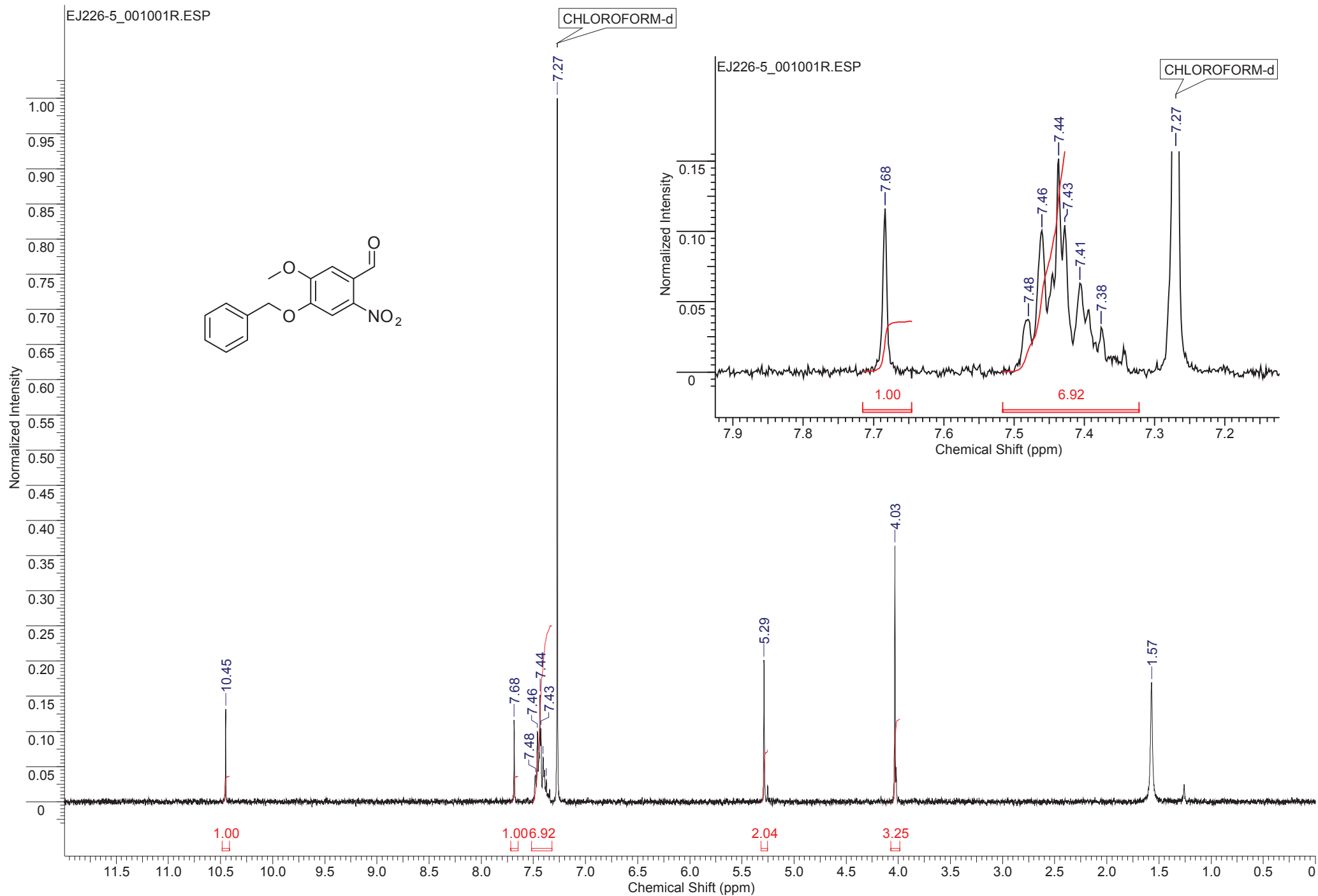
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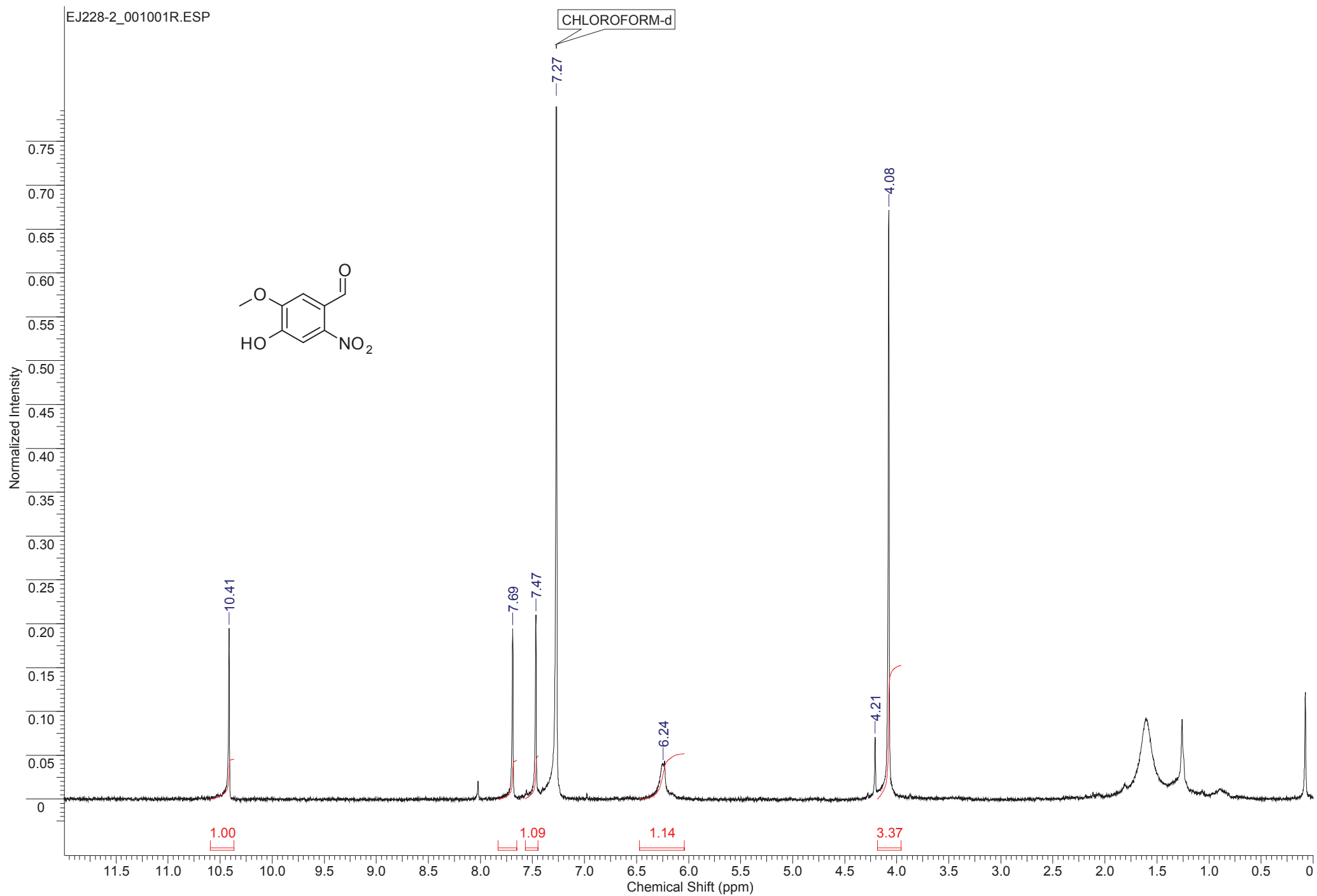
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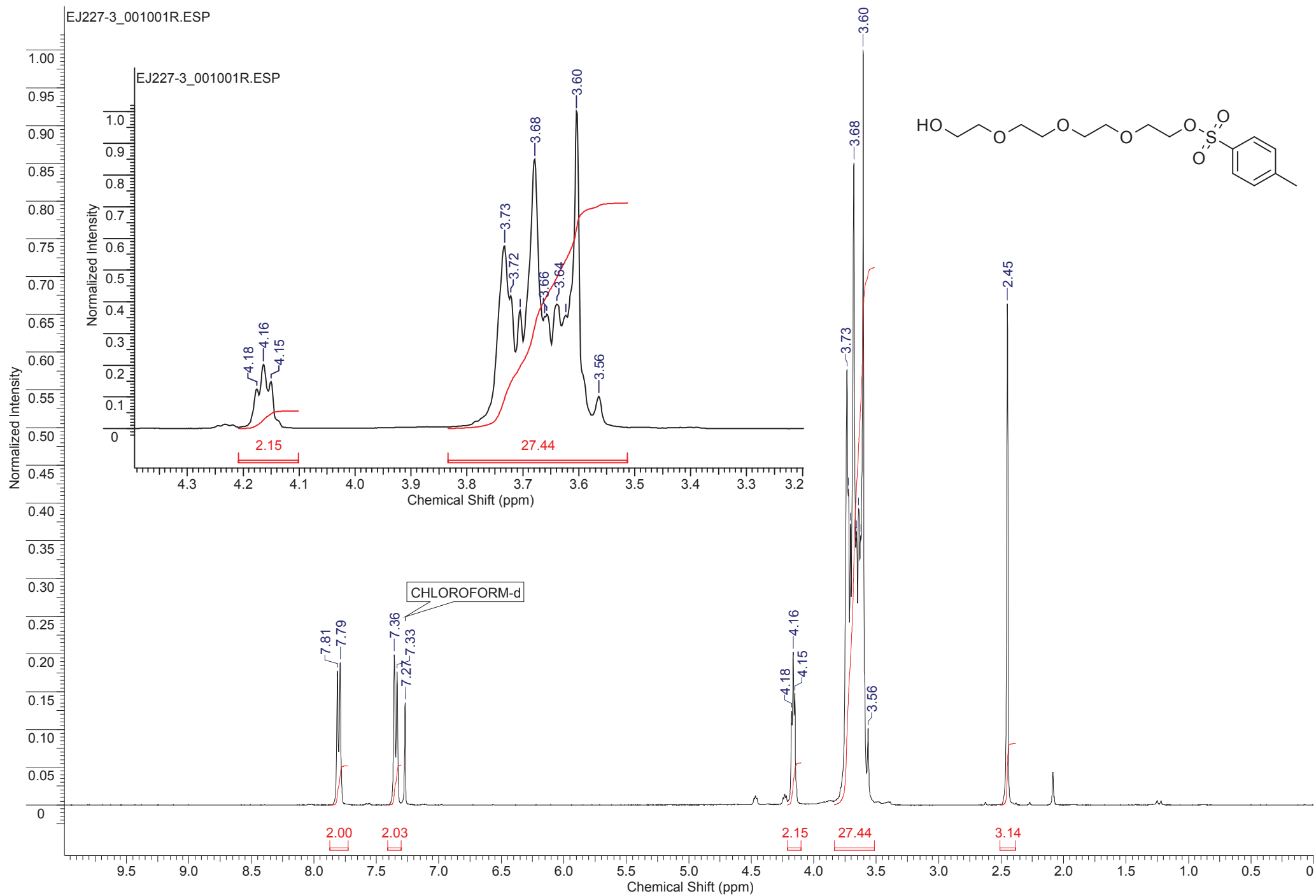
m/z

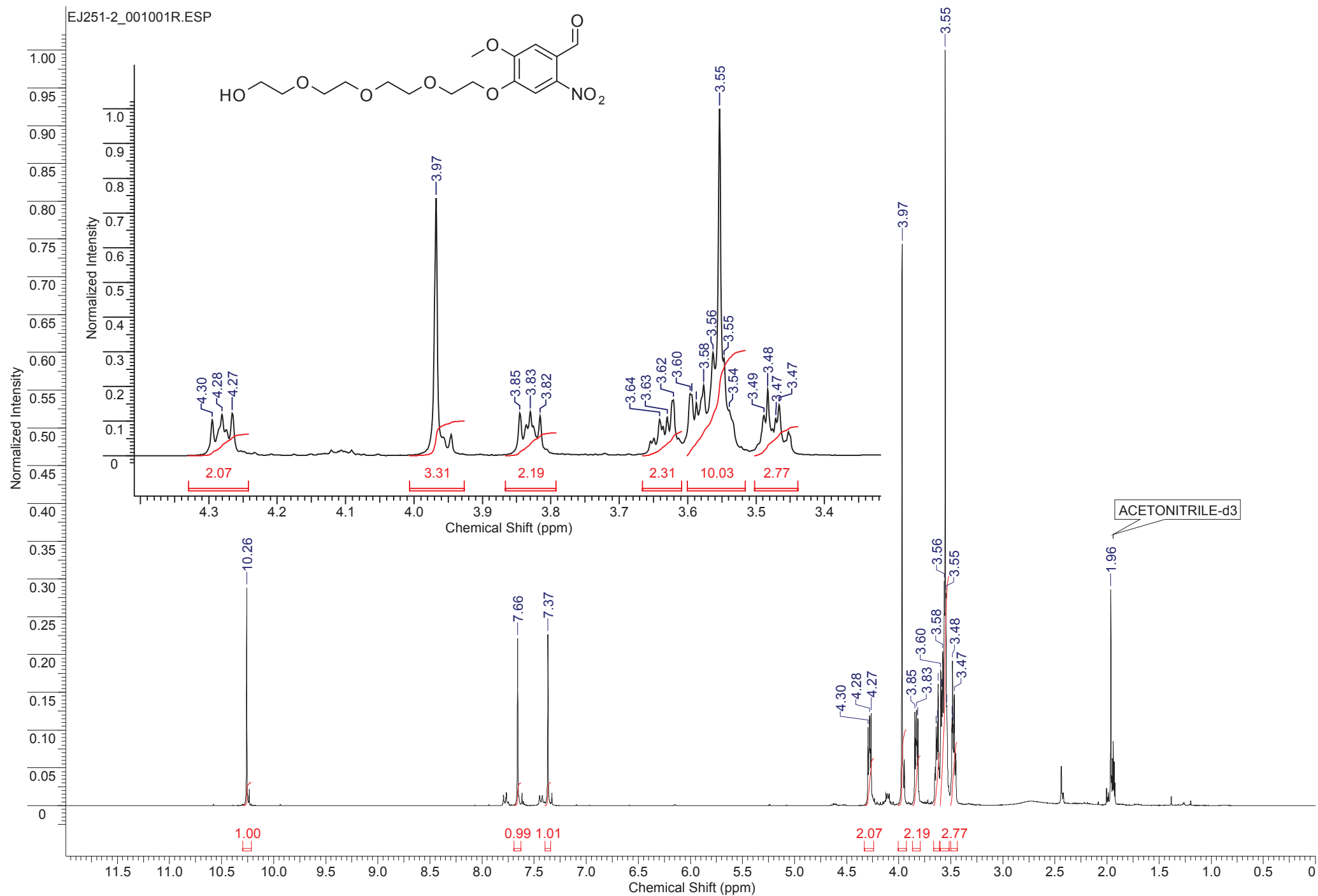


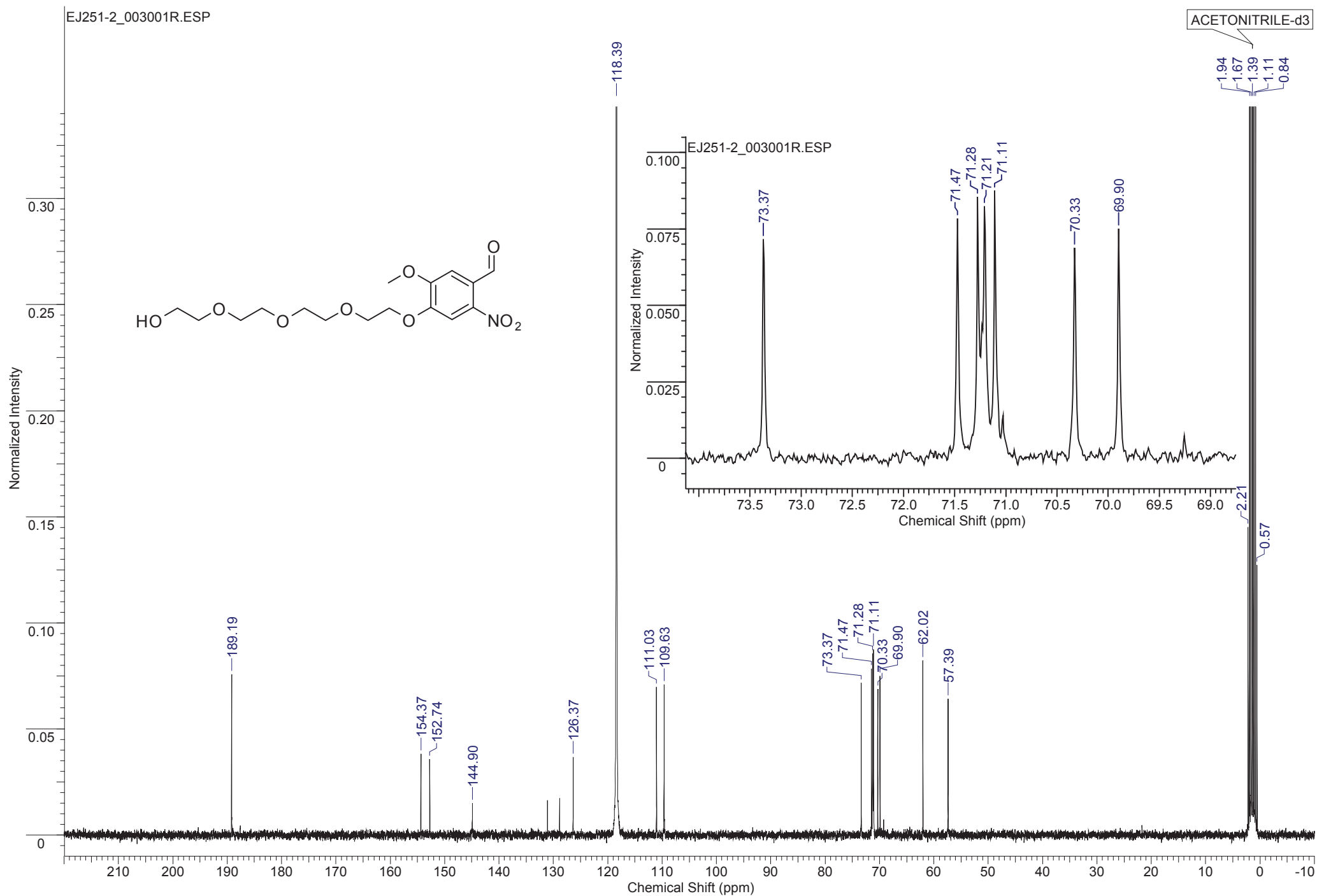




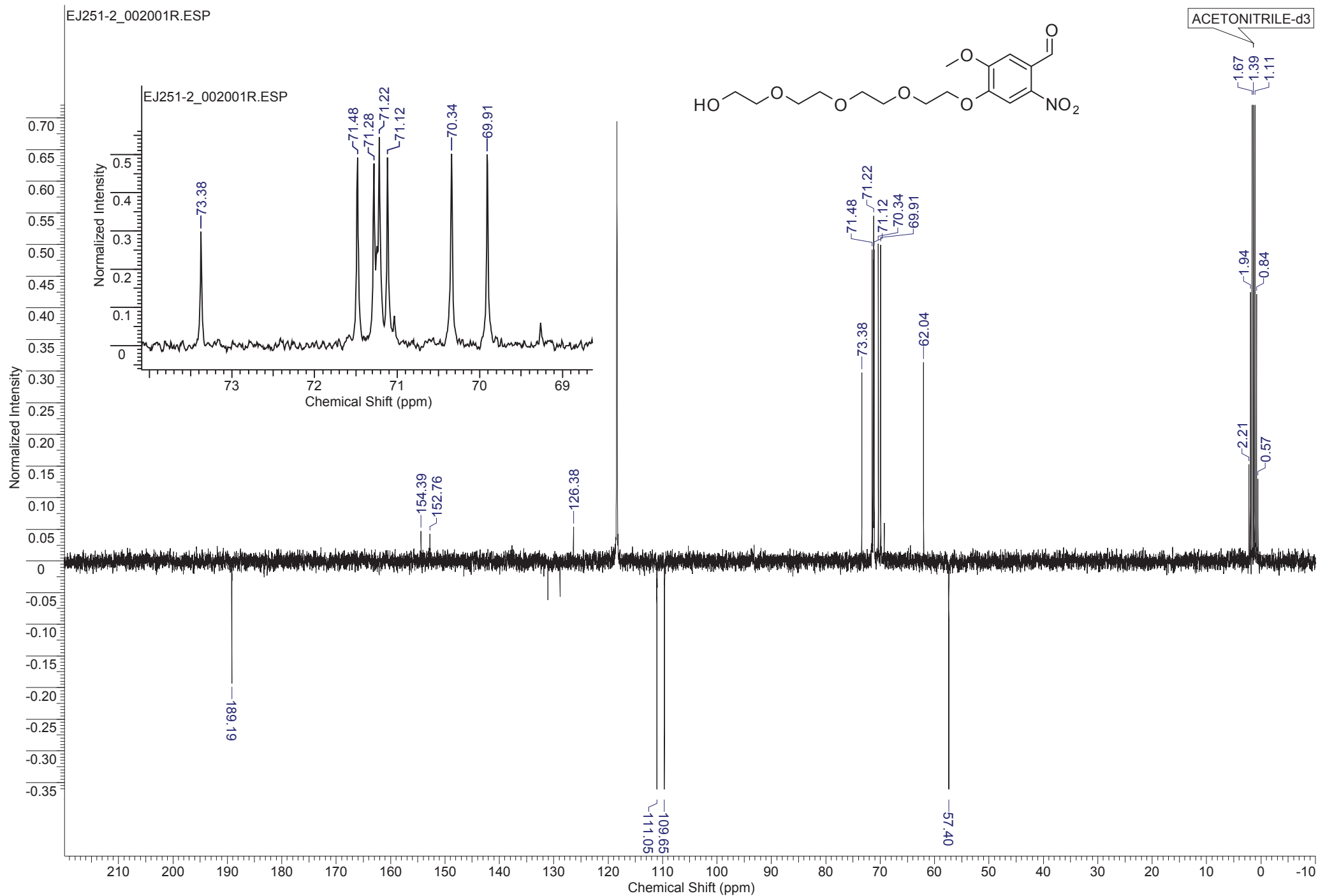












ESI-MS: EJ230-6

XMASS Mass Analysis for /Data/UNI\_FR/ELIA6492\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

Ion mass = 396.1269420

Charge = +1

#	C	H	N	O	Na	mass	DBE	error
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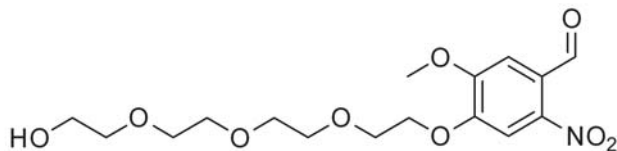
\*\*\* Mass Analysis for mass 396.1269420

1	16	23	1	9	1	396.1265024	5.5	4.396e-04
2	15	17	8	4	1	396.1264972	11.0	4.448e-04
3	16	20	4	8	0	396.1275651	9.0	6.231e-04
4	14	18	7	7	0	396.1262224	9.5	7.196e-04
5	17	19	5	5	1	396.1278398	10.5	8.978e-04
6	28	16	2	1	0	396.1257146	22.0	1.227e-03
7	14	21	4	8	1	396.1251598	6.0	1.782e-03
8	17	16	8	4	0	396.1289025	14.0	1.960e-03
9	18	22	1	9	0	396.1289077	8.5	1.966e-03
10	13	22	3	11	0	396.1248850	4.5	2.057e-03

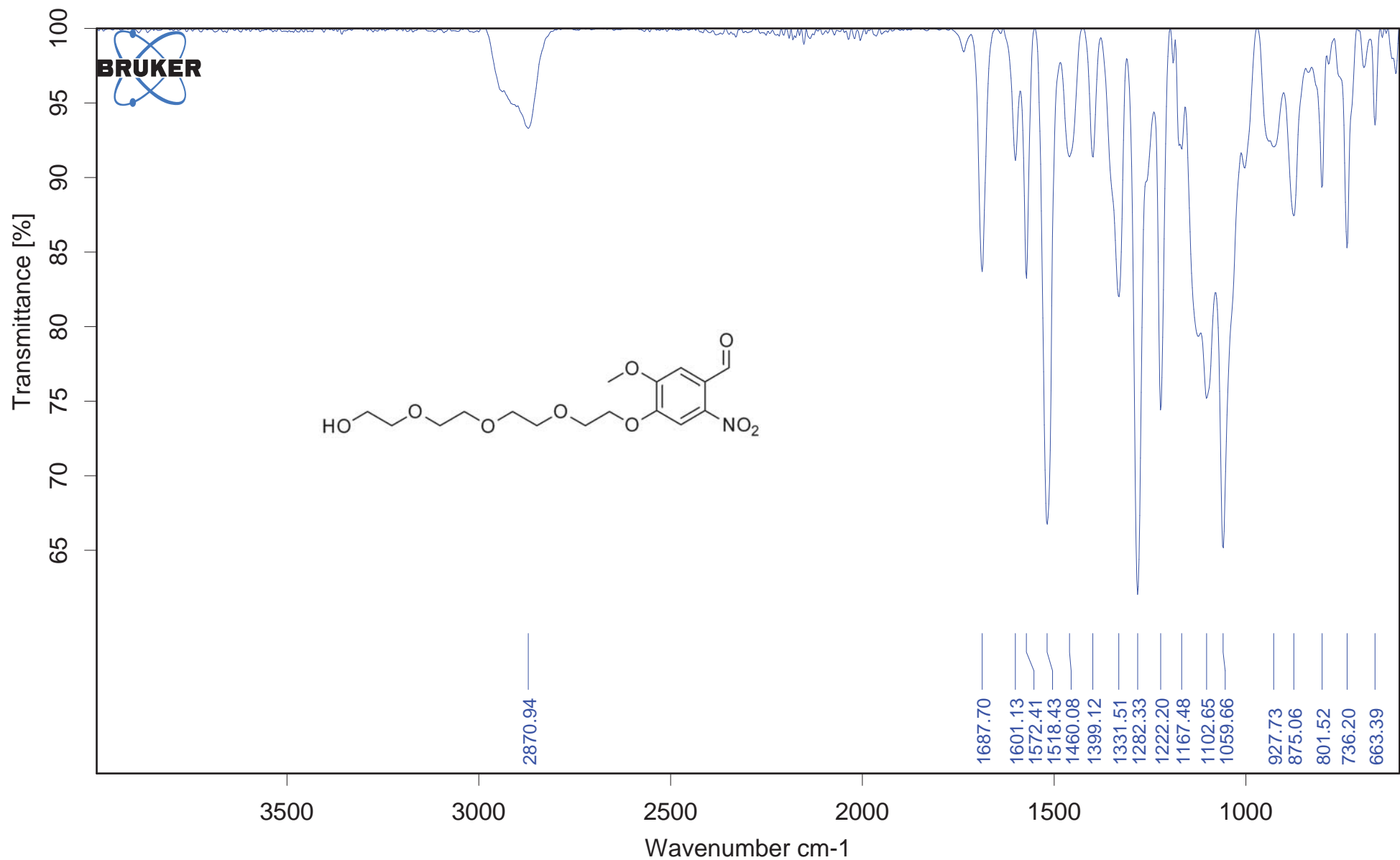
[M+Na]<sup>+</sup>

MS-SERVICE UNI Fribourg BRUKER FTMS 4.7T BioAPEX II  
ESI-MS (pos.Mode): EJ230-6 (in ACN)

396.12694



394.0 395.0 396.0 397.0 398.0 399.0 m/z

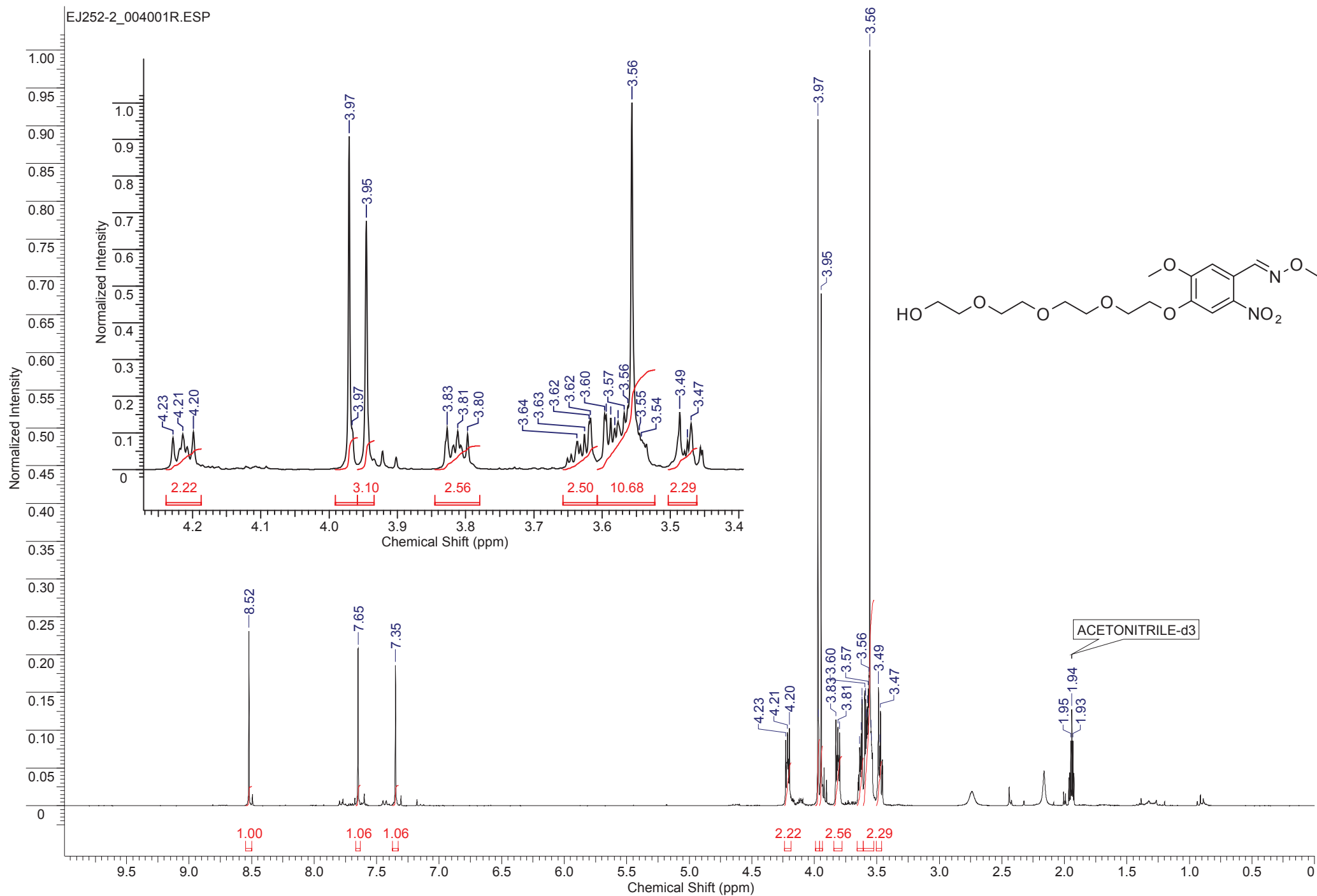


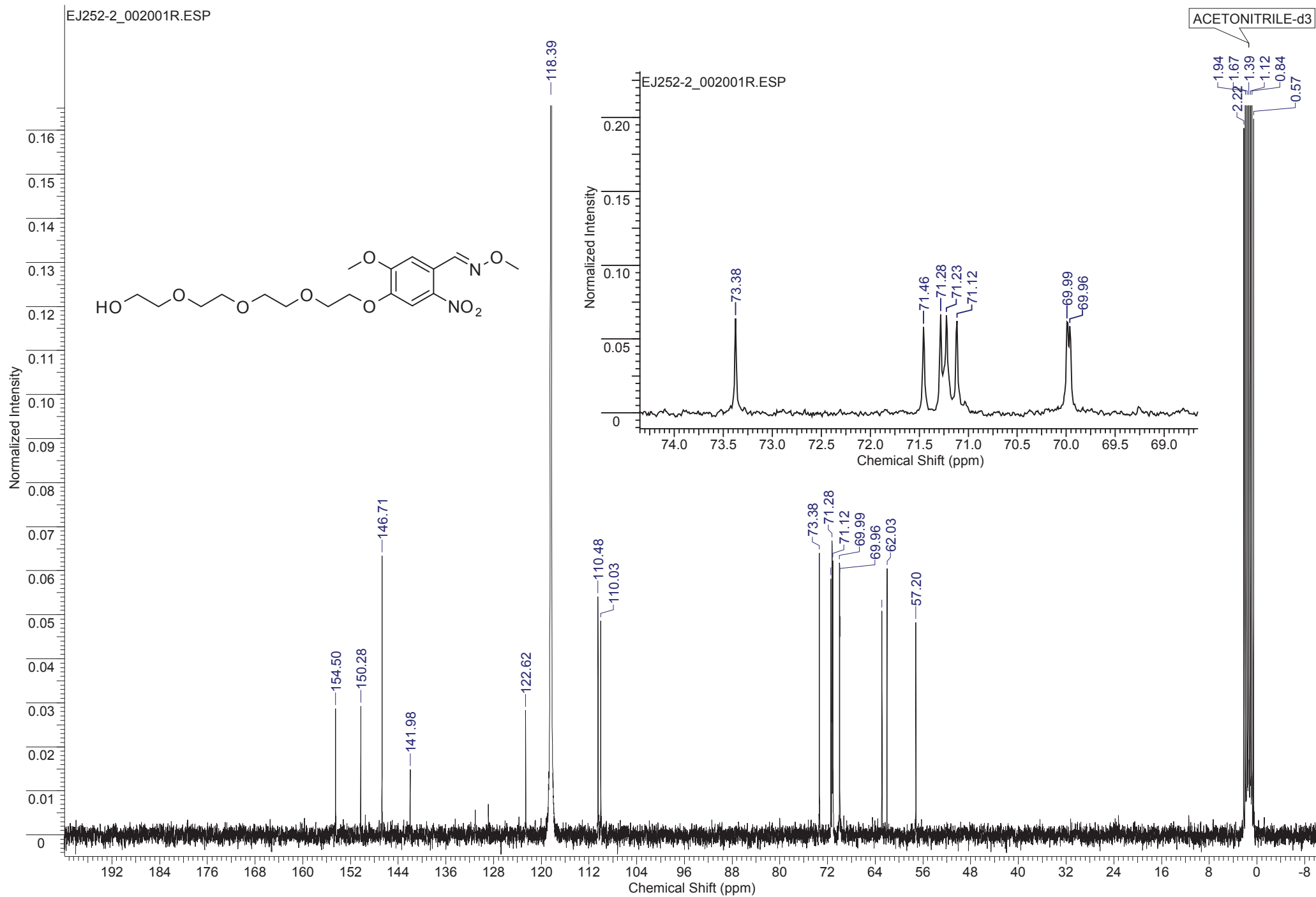
U:\IR\EJ251-2.0

EJ251-2

oil

25/04/2012







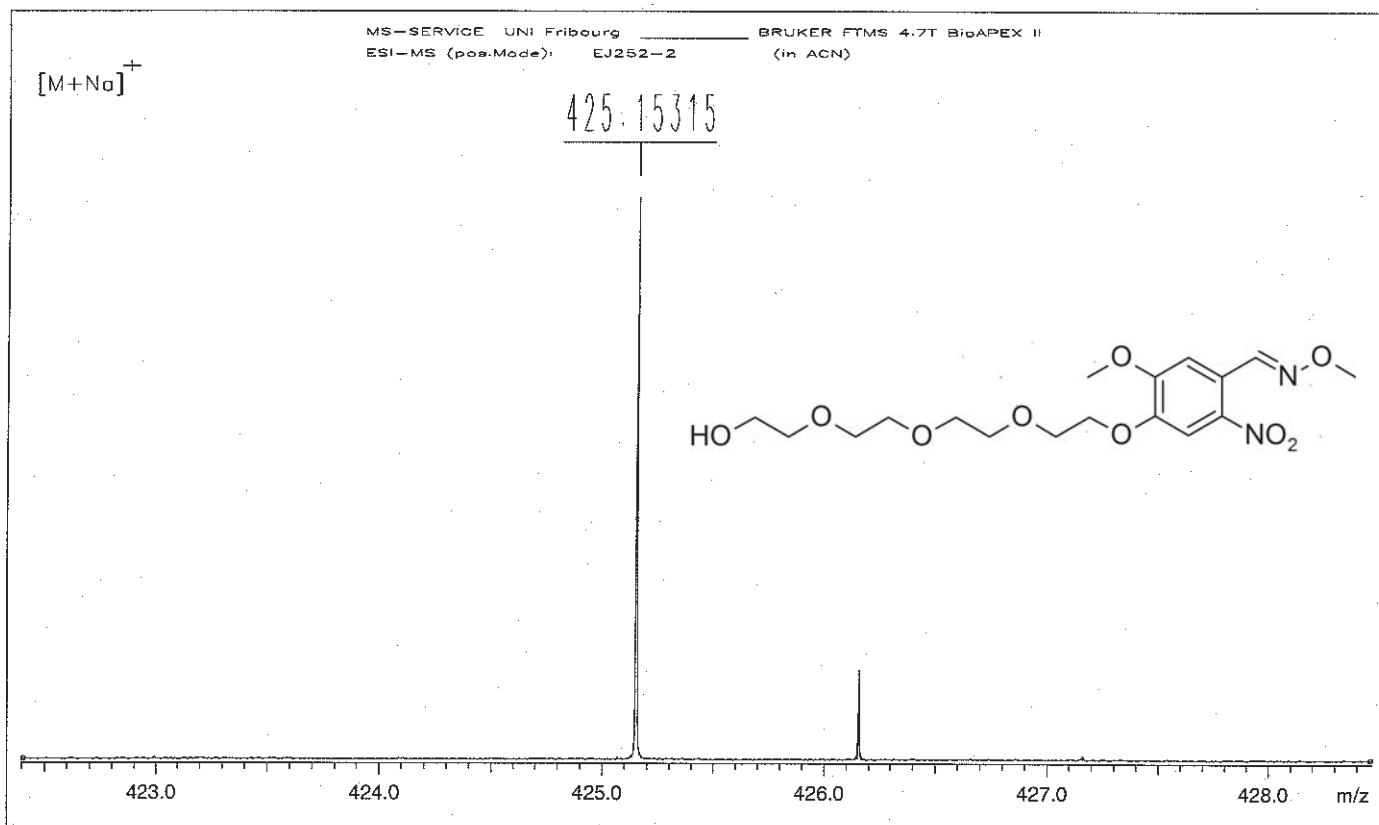
ESI-MS: EJ252-2

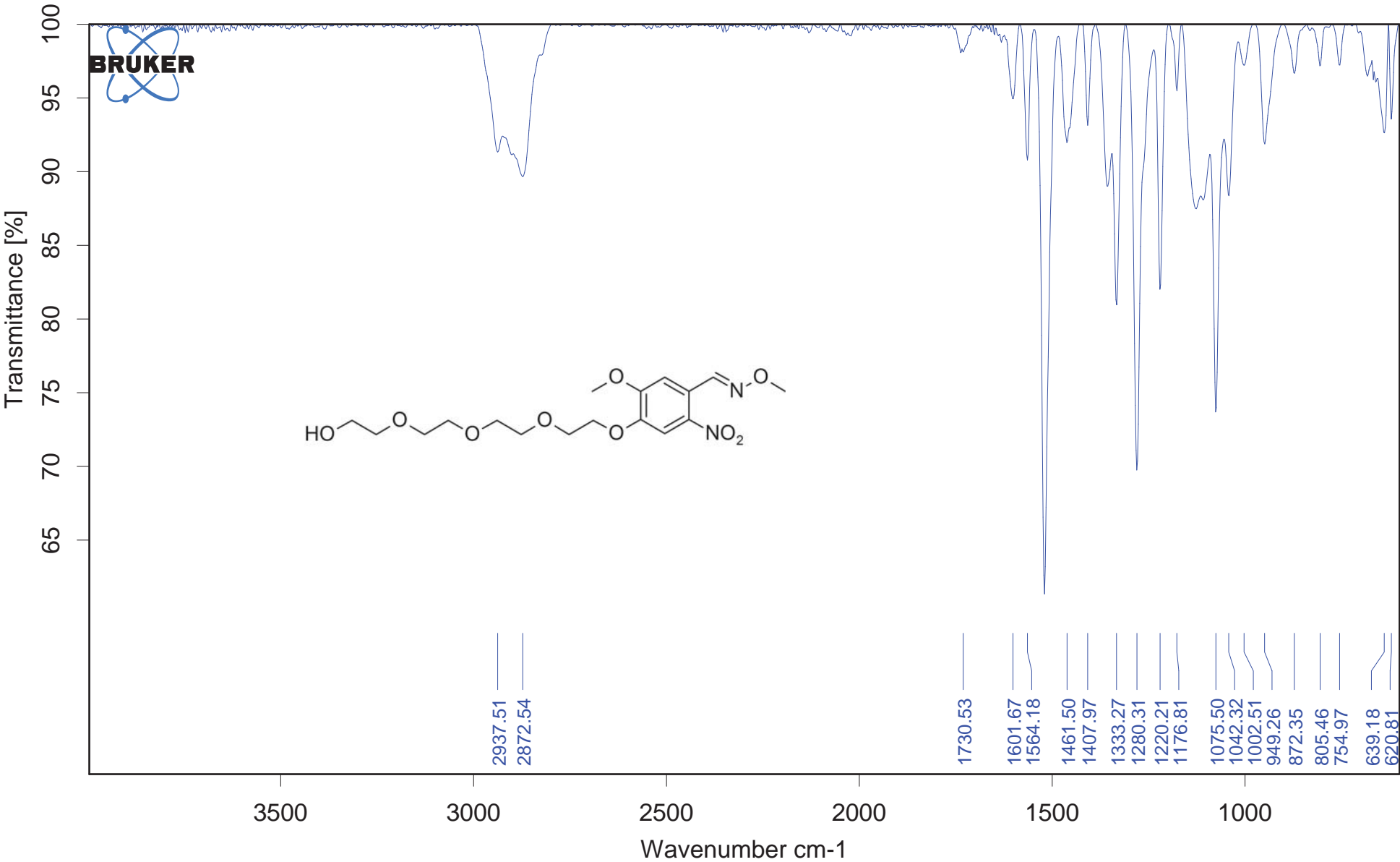
XMASS Mass Analysis for /Data/UNI\_FR/ELIA6589\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

Ion mass = 425.1531510

Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 425.1531510								
1	17	26	2	9	1	425.1530515	5.5	9.947e-05
2	16	20	9	4	1	425.1530463	11.0	1.047e-04
3	15	21	8	7	0	425.1527715	9.5	3.795e-04
4	17	23	5	8	0	425.1541142	9.0	9.632e-04
5	18	22	6	5	1	425.1543889	10.5	1.238e-03
6	15	24	5	8	1	425.1517089	6.0	1.442e-03
7	18	19	9	4	0	425.1554516	14.0	2.301e-03
8	19	25	2	9	0	425.1554568	8.5	2.306e-03
9	19	18	10	1	1	425.1557263	15.5	2.575e-03
10	20	24	3	6	1	425.1557316	10.0	2.581e-03



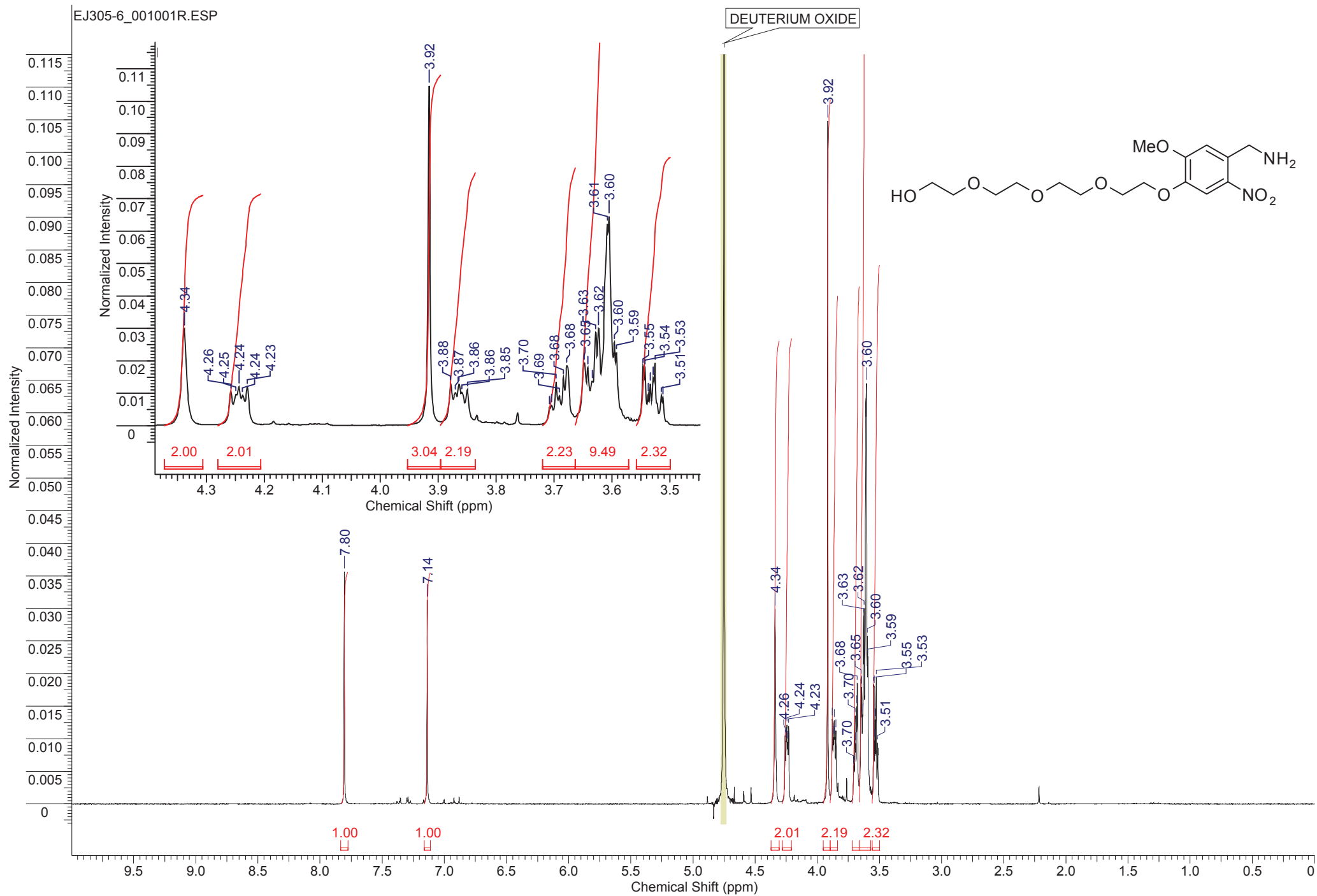


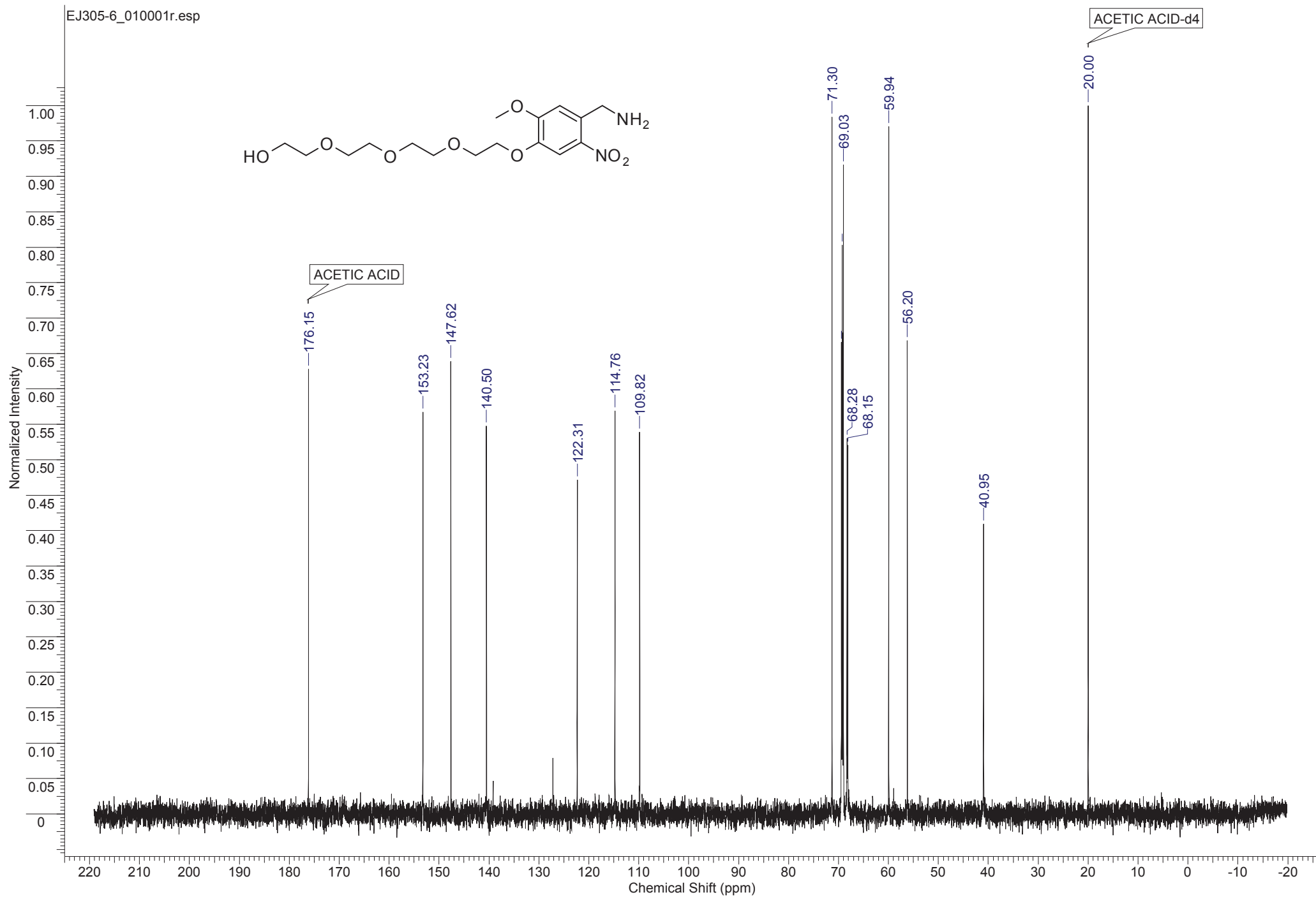
EJ252-2

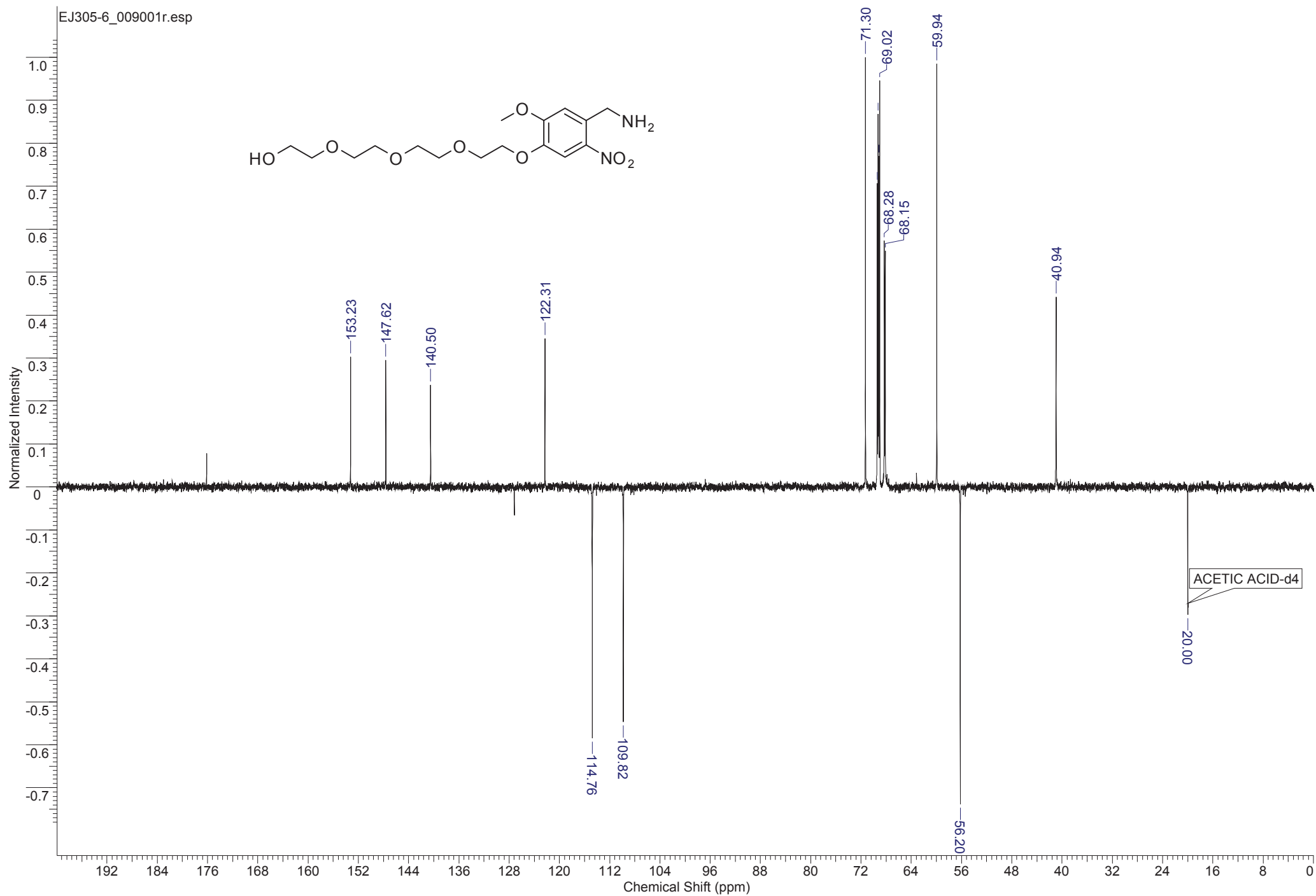
oil

25/04/2012









ESI-MS: EJ253-6

XMASS Mass Analysis for /Data/UNI\_FR/ELIA6586\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

Ion mass = 375.1754740

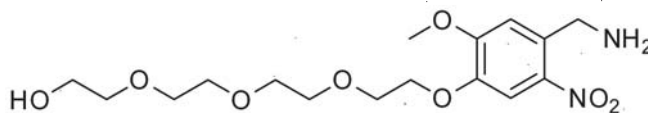
Charge = +1

#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 375.1754740							
1	16	27	2	8	375.1761923	4.5	7.183e-04
2	11	27	4	10	375.1721695	0.5	3.304e-03
3	19	25	3	5	375.1788723	9.0	3.398e-03
4	23	23	2	3	375.1703190	13.5	5.155e-03
5	22	23	4	2	375.1815524	13.5	6.078e-03
6	24	25	1	3	375.1828951	13.0	7.421e-03
7	20	25	1	6	375.1676390	9.0	7.835e-03
8	18	23	4	5	375.1662963	9.5	9.178e-03
9	12	29	3	10	375.1847456	0.0	9.272e-03
10	15	25	3	8	375.1636162	5.0	1.186e-02

[M+H]<sup>+</sup>

MS-SERVICE UNI Fribourg BRUKER FTMS 4.7T BioAPEX II  
ESI-MS (pos-Mode): EJ253-6 (in ACN)

375.17547



373.0

374.0

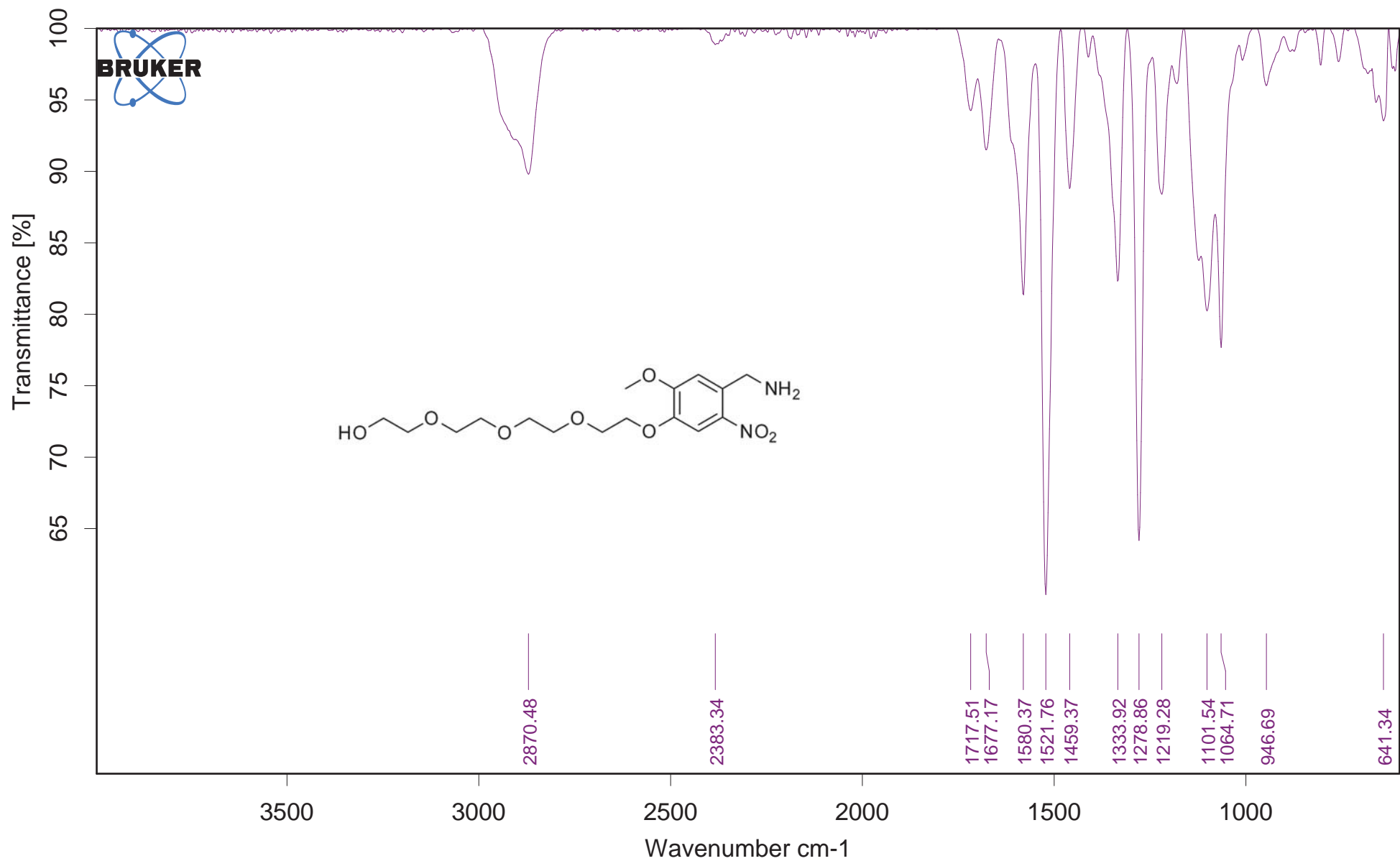
375.0

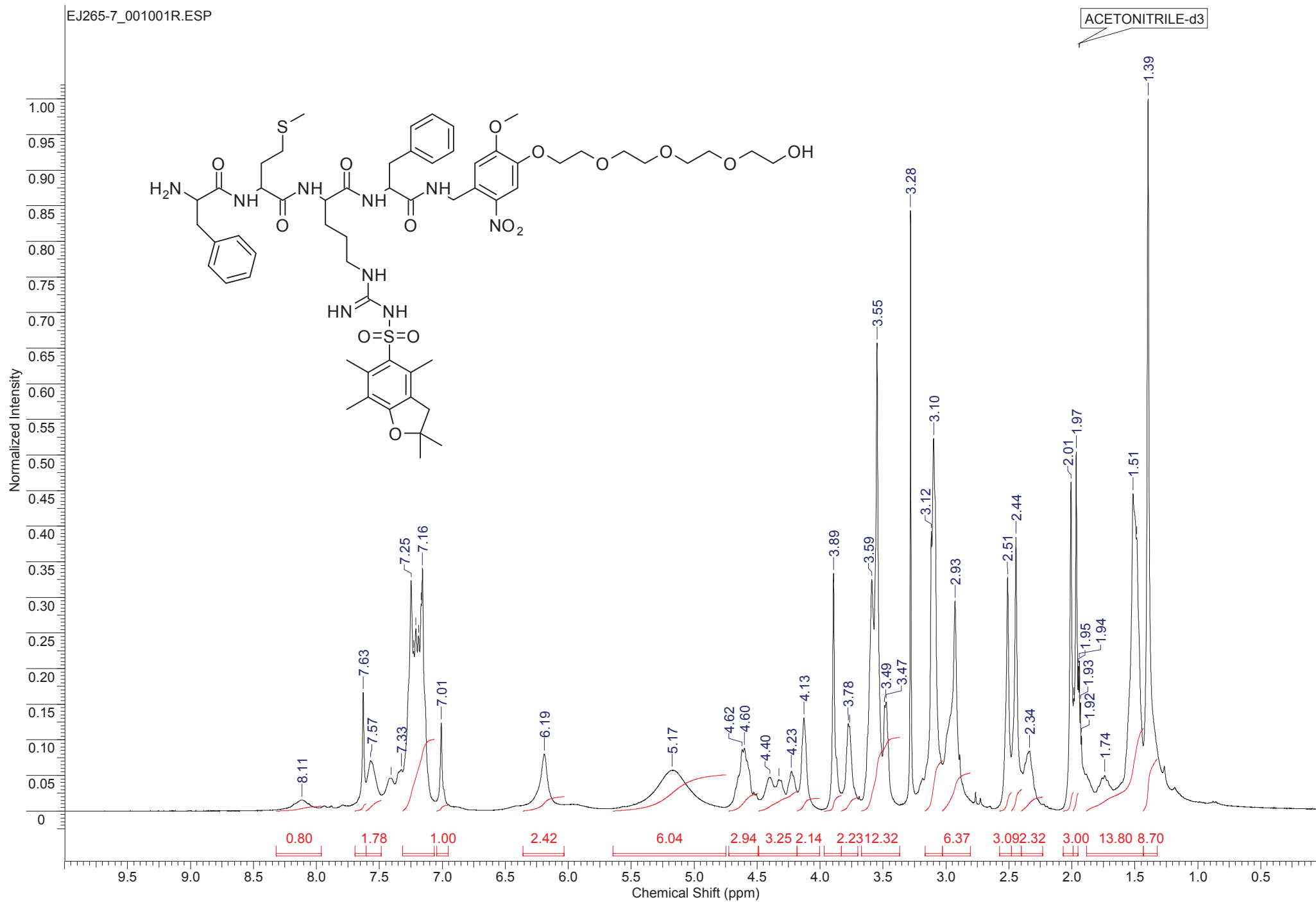
376.0

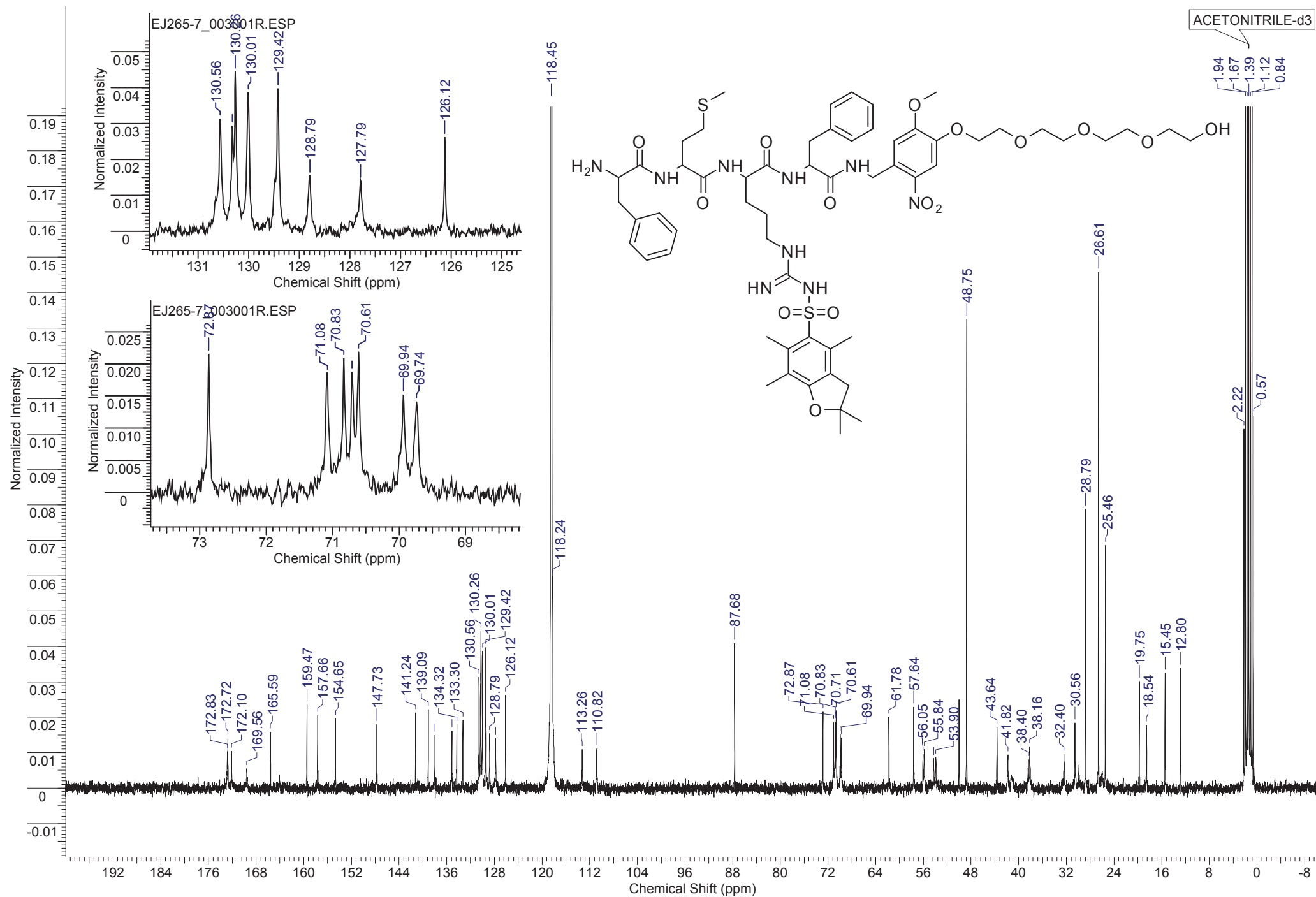
377.0

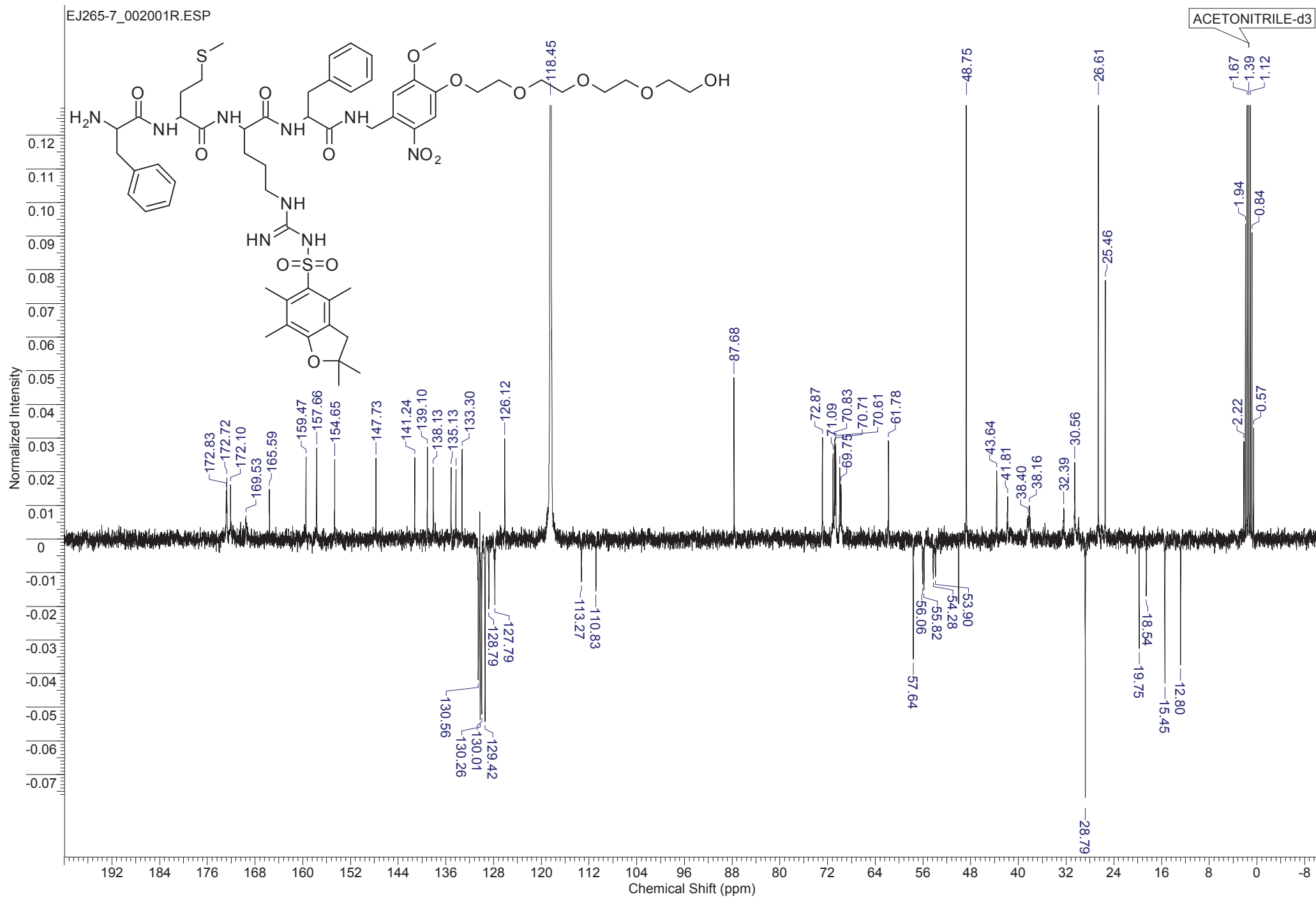
378.0

m/z











ESI-MS: EJ265-7

XMASS Mass Analysis for /Data/UNI\_FR/ELIA6666\_ESI/10/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

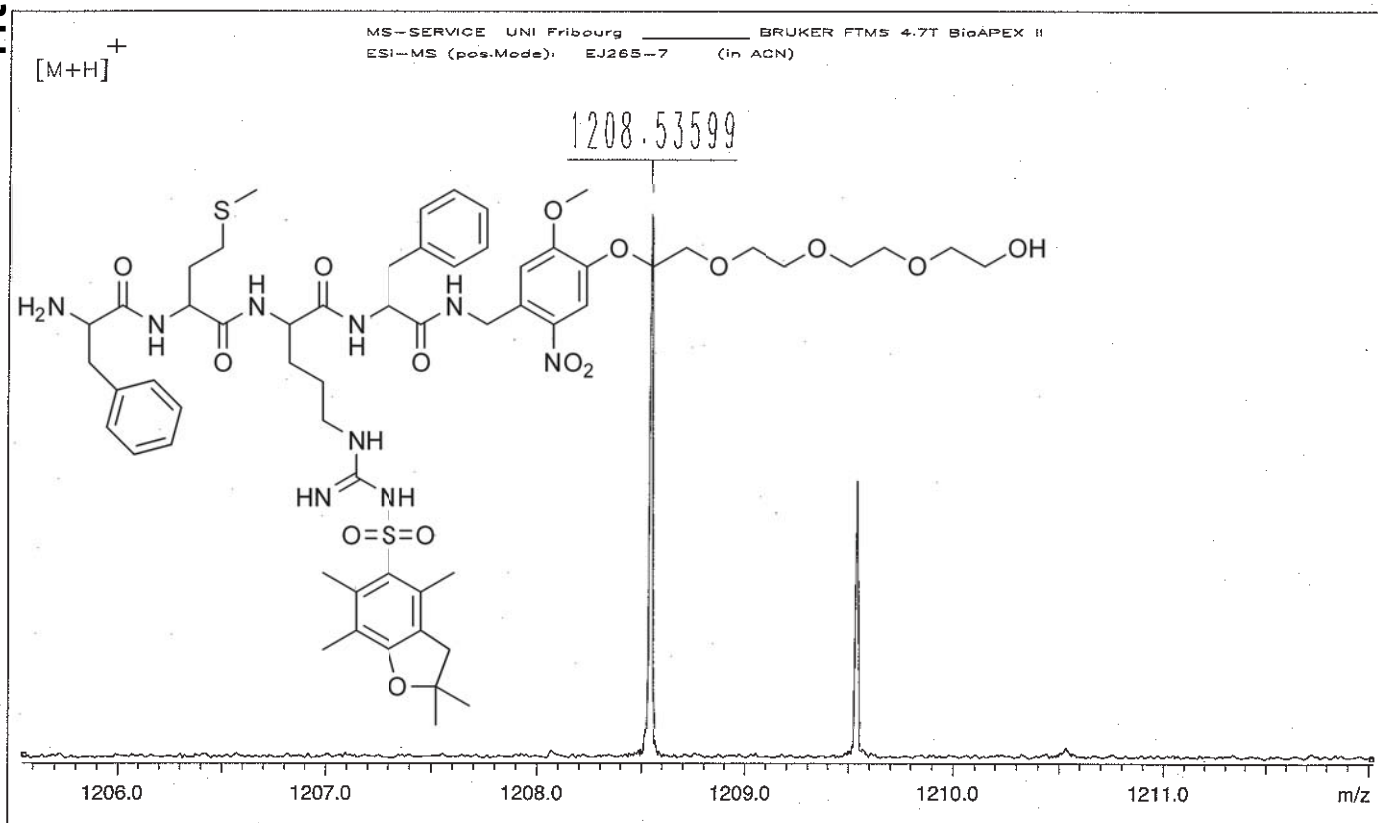
Ion mass = 1208.5359860

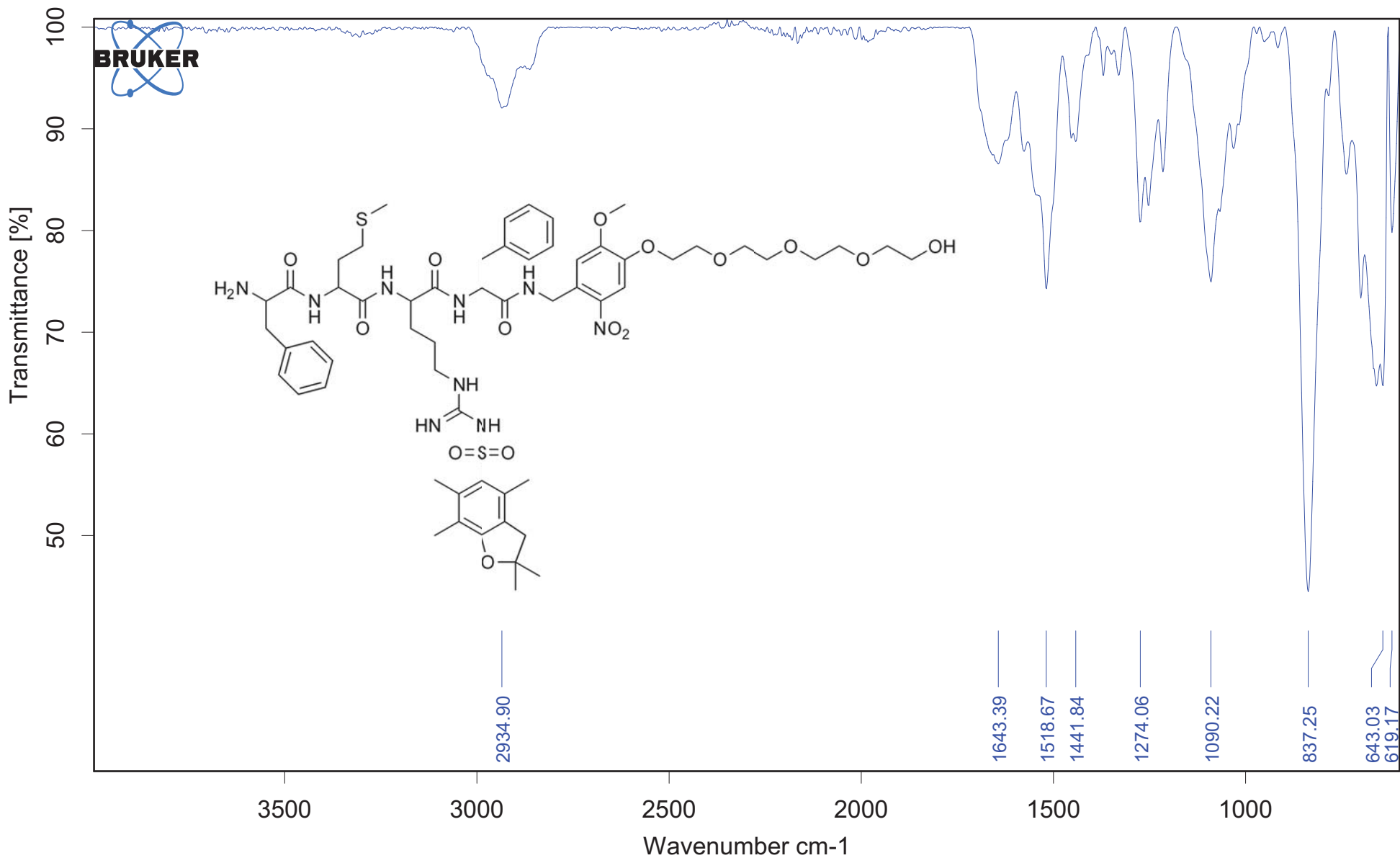
Charge = +1

#	C	H	N	O	S	mass	DBE	error
---	---	---	---	---	---	------	-----	-------

\*\*\* Mass Analysis for mass 1208.5359860

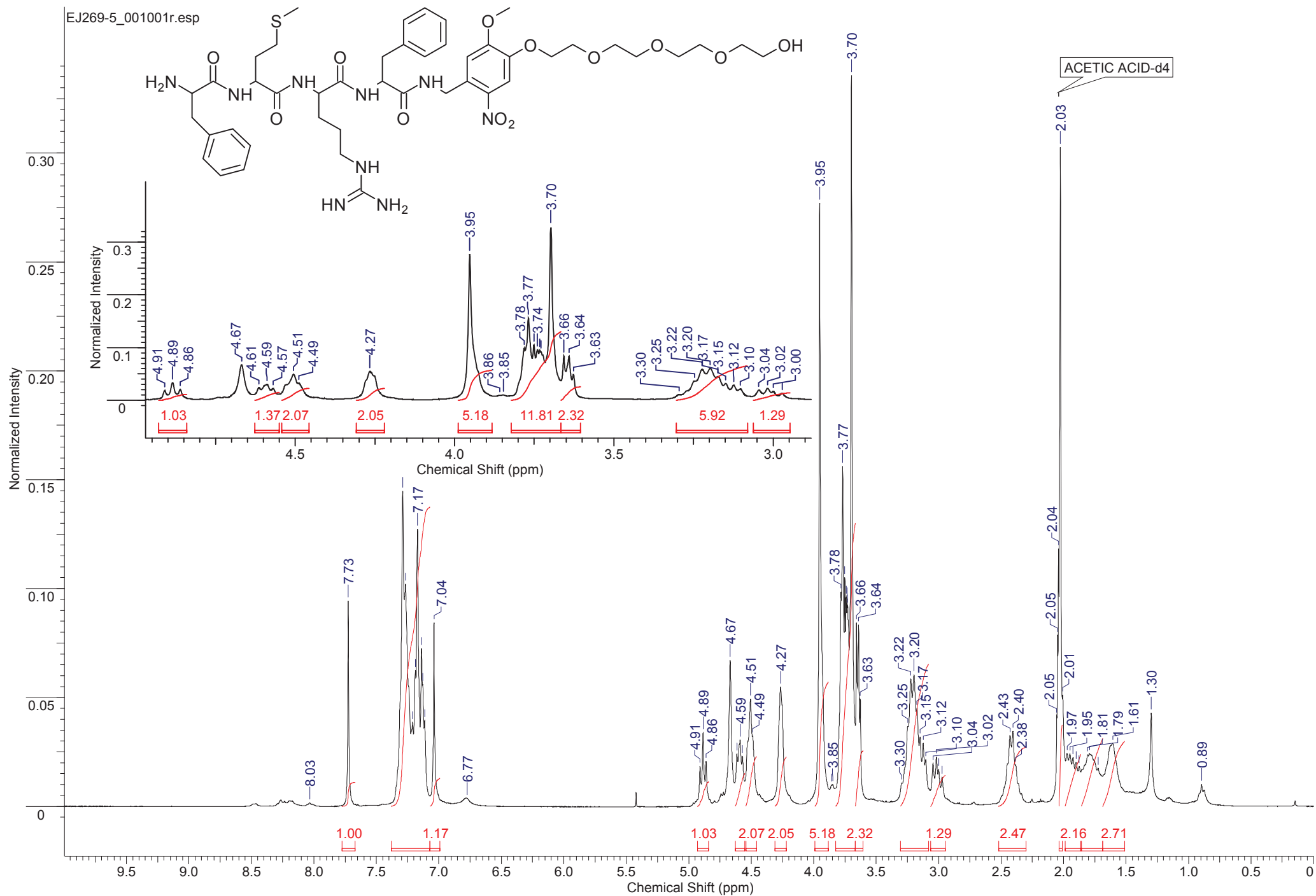
1	58	82	9	15	2	1208.5366308	22.5	6.448e-04
2	56	80	12	14	2	1208.5352881	23.0	6.979e-04
3	56	88	8	13	4	1208.5348191	17.0	1.167e-03
4	66	78	7	13	1	1208.5372827	31.5	1.297e-03
5	53	84	12	14	3	1208.5386590	18.0	2.673e-03
6	61	78	9	15	1	1208.5332600	27.5	2.726e-03
7	53	82	11	17	2	1208.5326081	18.5	3.378e-03
8	53	90	7	16	4	1208.5321391	12.5	3.847e-03
9	55	86	9	15	3	1208.5400016	17.5	4.016e-03
10	59	76	12	14	1	1208.5319173	28.0	4.069e-03

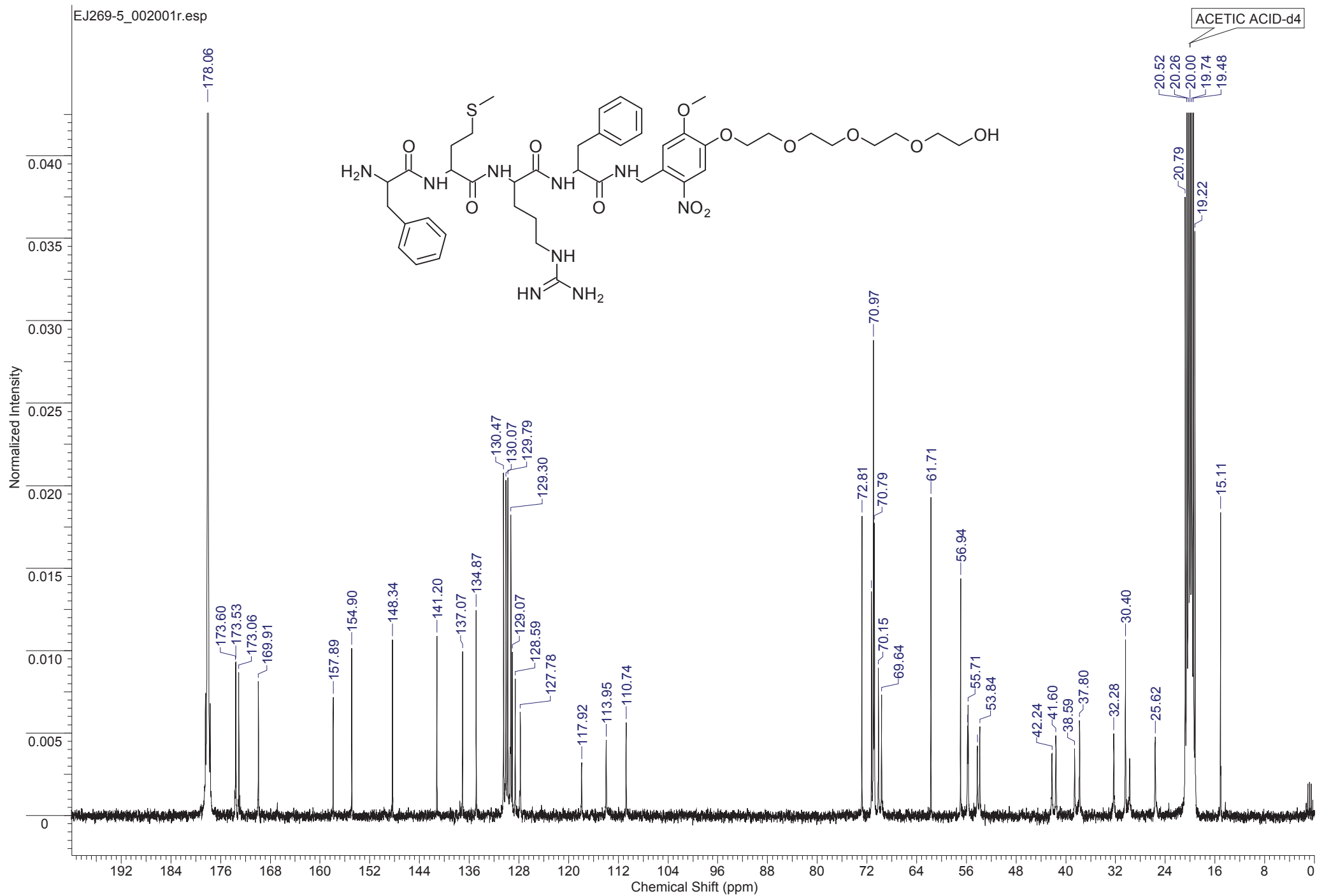


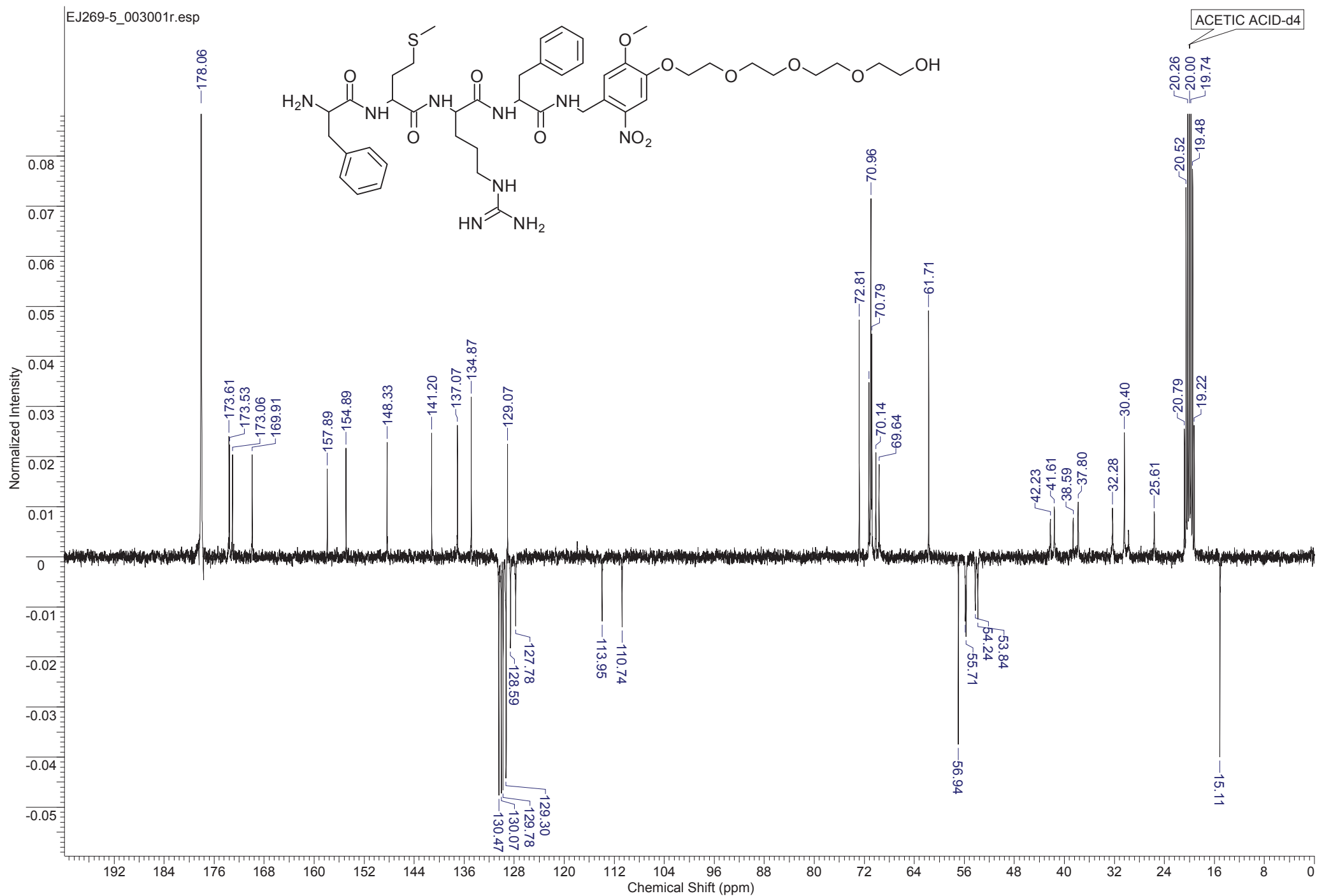


yellow oil

30/05/2012







ESI-MS: EJ269-4

XMASS Mass Analysis for /Data/UNI\_FR/ELIA6676\_ESI/10/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

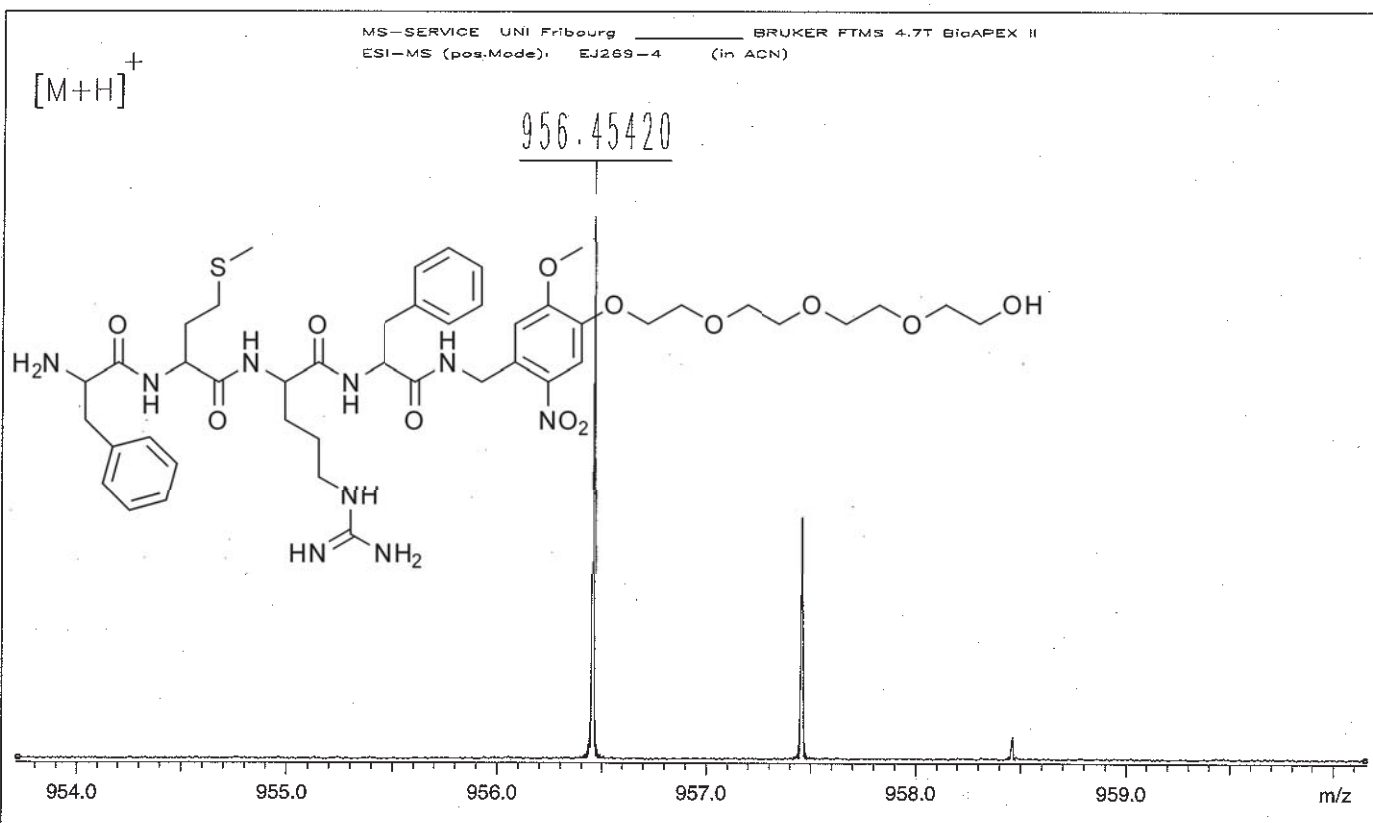
Ion mass = 956.4541990

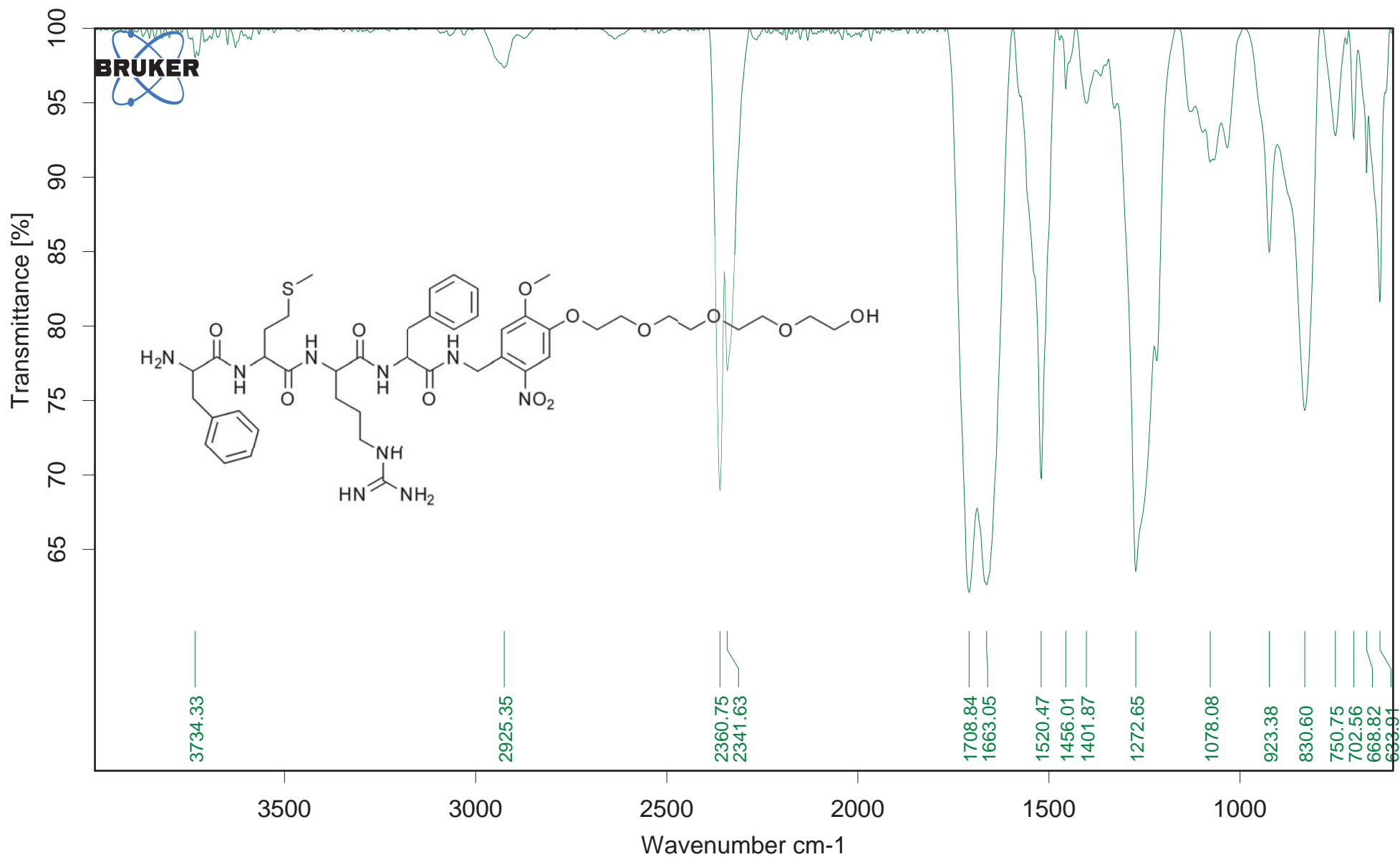
Charge = +1

#	C	H	N	O	S	mass	DBE	error
---	---	---	---	---	---	------	-----	-------

\*\*\* Mass Analysis for mass 956.4541990

1	45	66	9	12	1	956.4546157	17.5	4.167e-04
2	51	68	6	8	2	956.4534560	21.0	7.430e-04
3	43	64	12	11	1	956.4532731	18.0	9.259e-04
4	38	66	15	10	2	956.4553012	13.5	1.102e-03
5	57	62	7	5	1	956.4527652	30.5	1.434e-03
6	35	68	14	13	2	956.4526211	9.0	1.578e-03
7	46	62	13	8	1	956.4559531	22.5	1.754e-03
8	47	68	6	13	1	956.4559584	17.0	1.759e-03
9	54	66	7	5	2	956.4561361	25.5	1.937e-03
10	49	66	9	7	2	956.4521133	21.5	2.086e-03



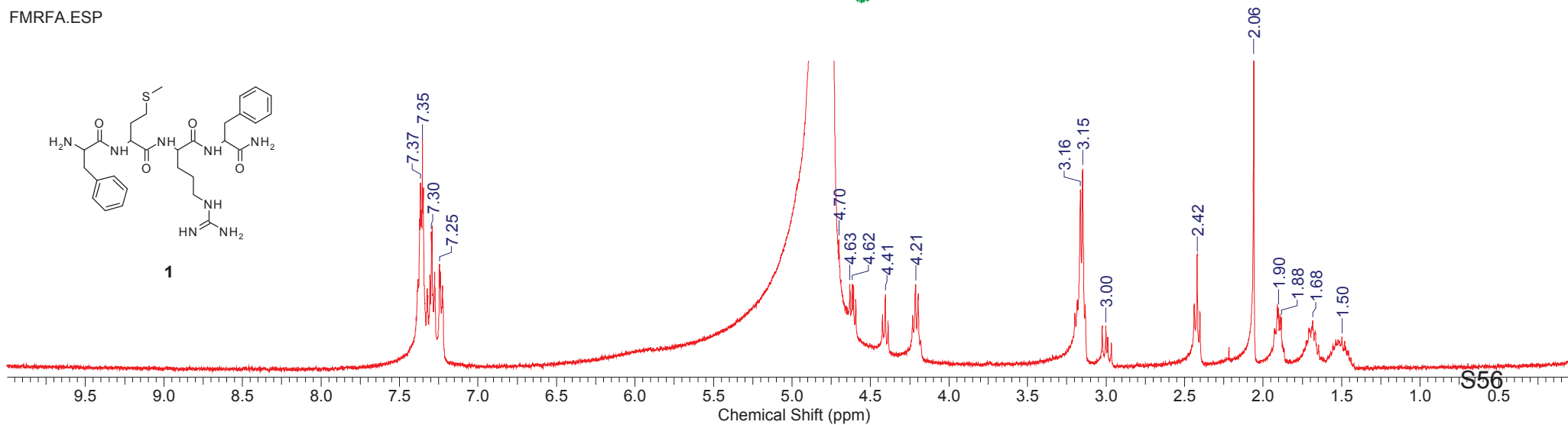
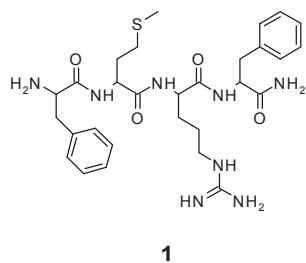
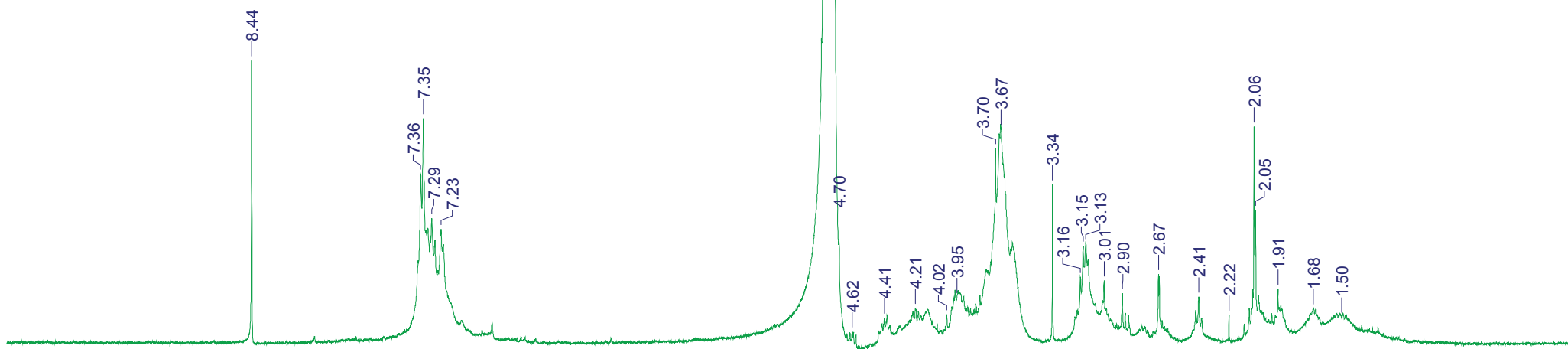
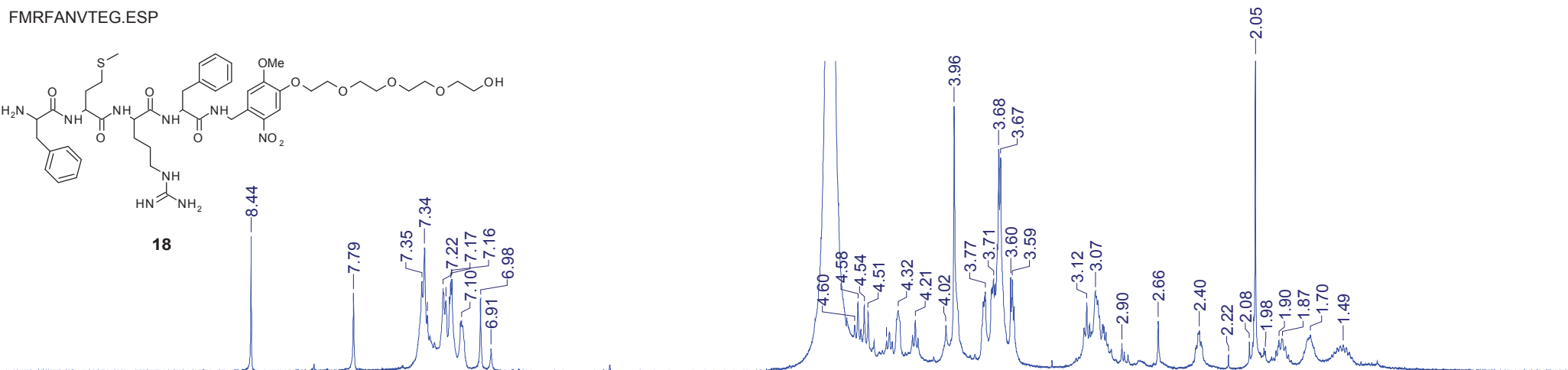
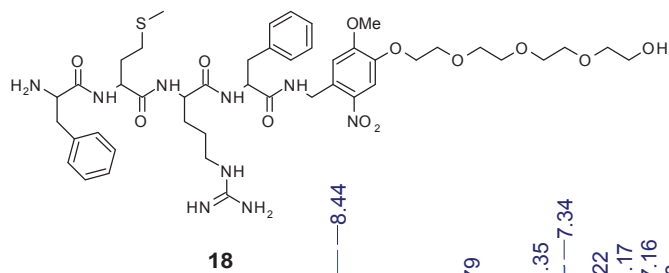


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EJ269-5

oil

06/06/2012







Comment 1

Comment 2

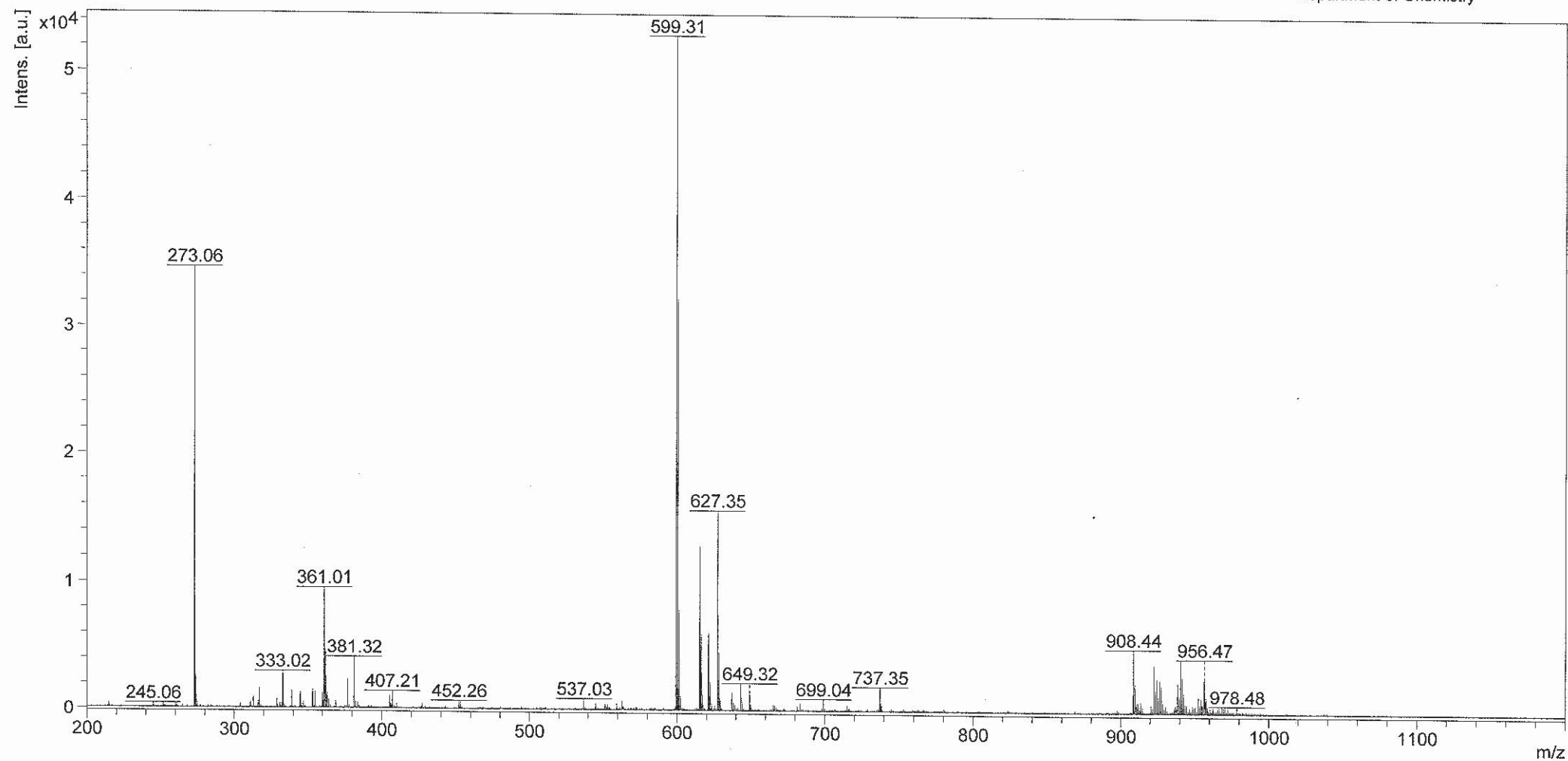
**MEJ-FMRFa in DHB**

Mass spectrometry service

University of Fribourg

Department of Chemistry

Instrument type: MALDI-TOF BRUKER ultrafleXtreme



Bruker Daltonics flexAnalysis

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