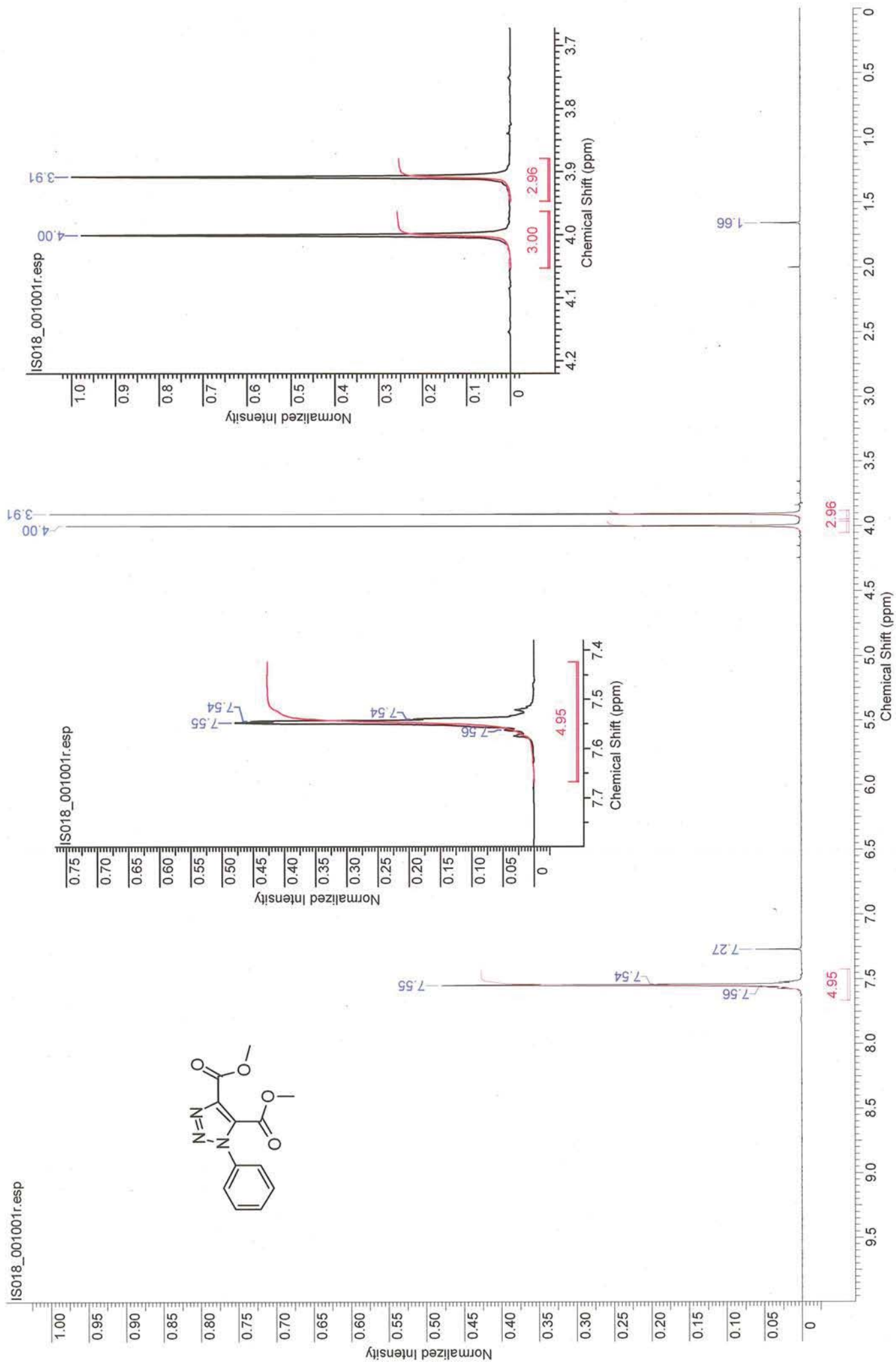
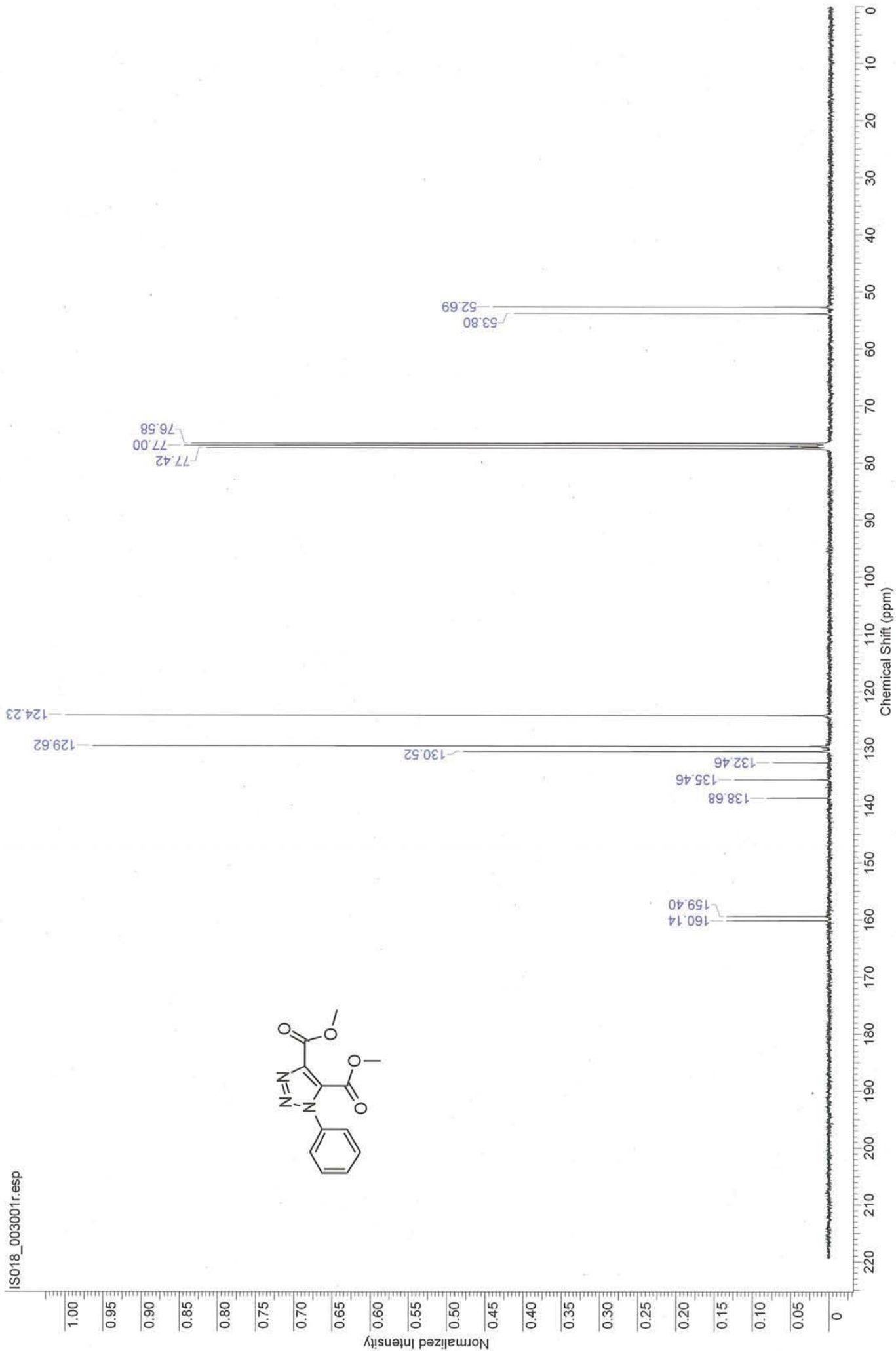


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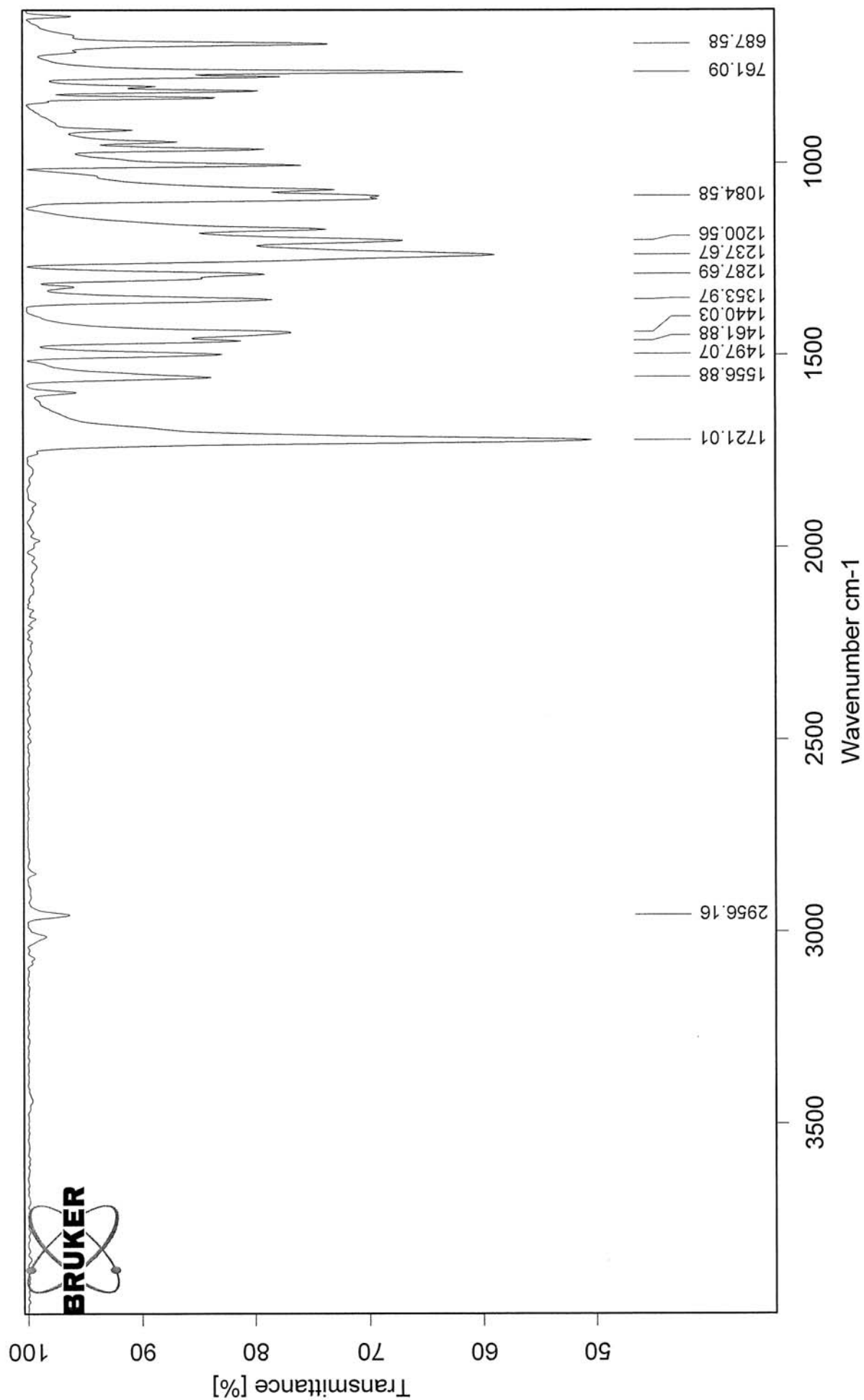
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ESI-MS: is-018

XMASS Mass Analysis for /Data/UNI\_FR/ALIM4569\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

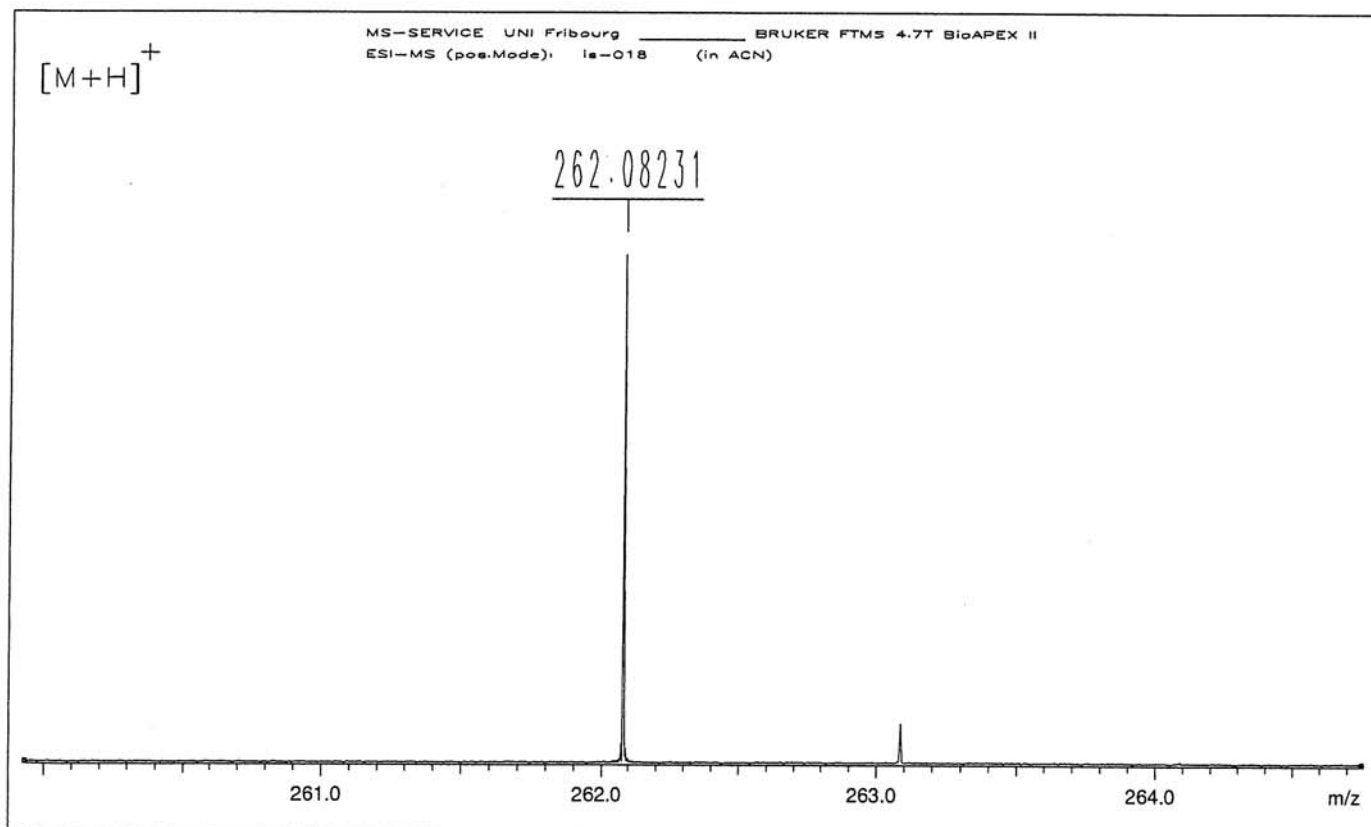
Ion mass = 262.0823110

Charge = +1

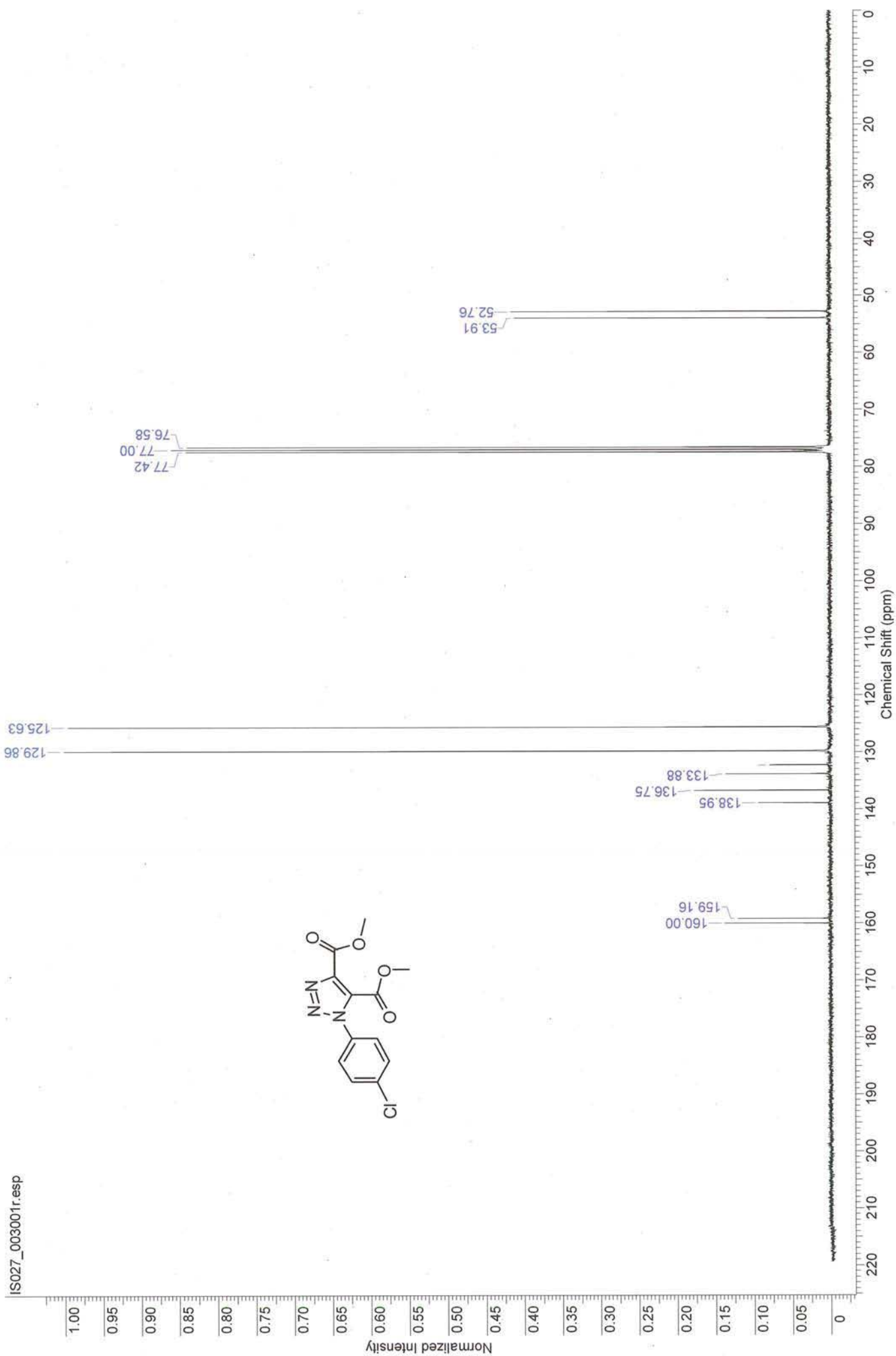
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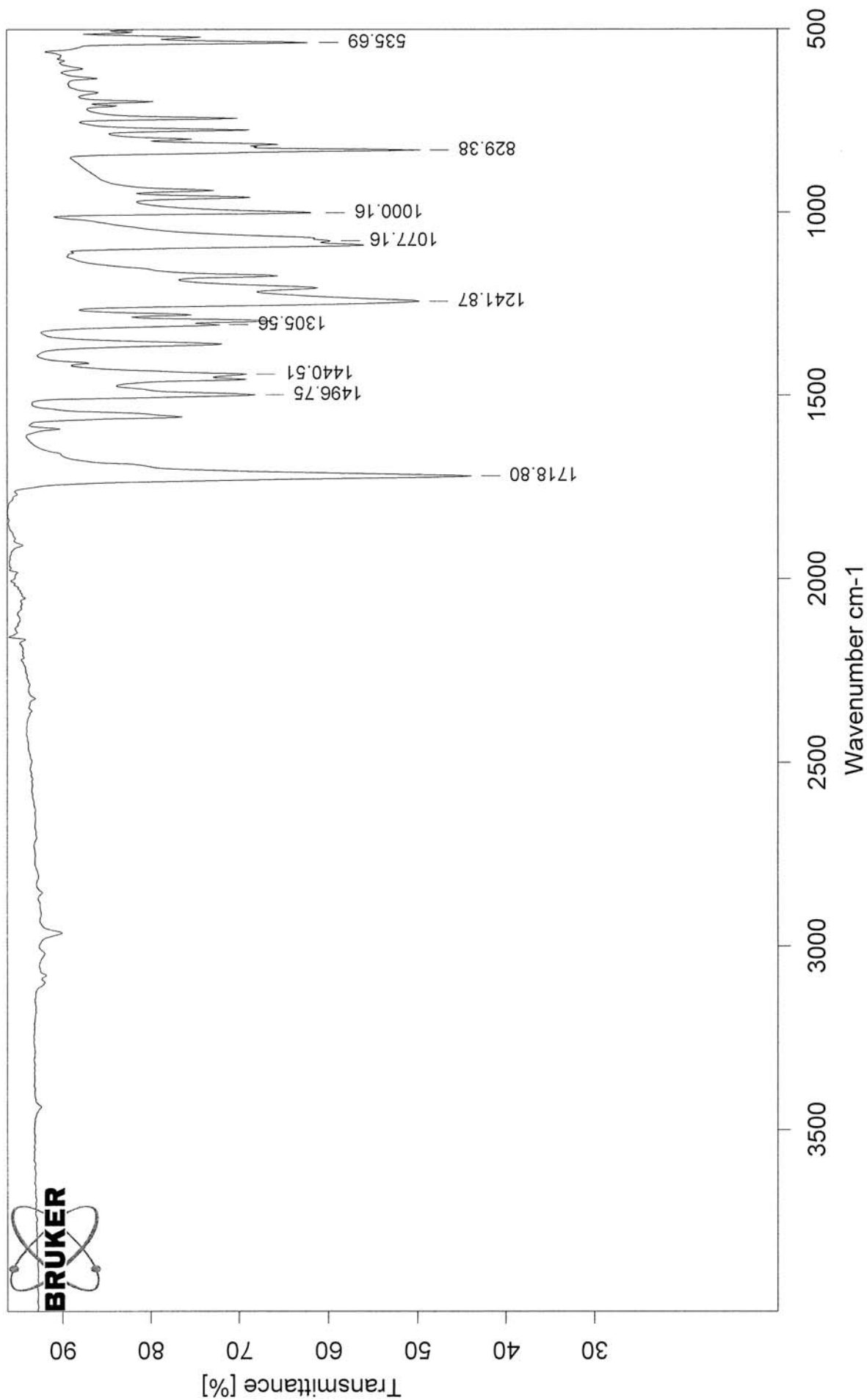
\*\*\* Mass Analysis for mass 262.0823110

1	12	12	3	4	0	262.0822323	8.5	7.869e-05
2	13	11	4	1	1	262.0825071	10.0	1.961e-04
3	10	10	6	3	0	262.0808896	9.0	1.421e-03
4	15	13	1	2	1	262.0838498	9.5	1.539e-03
5	10	13	3	4	1	262.0798270	5.5	2.484e-03
6	15	10	4	1	0	262.0849124	13.0	2.601e-03
7	9	14	2	7	0	262.0795522	4.0	2.759e-03
8	8	8	9	2	0	262.0795470	9.5	2.764e-03
9	8	11	6	3	1	262.0784843	6.0	3.827e-03
10	17	12	1	2	0	262.0862551	12.5	3.944e-03









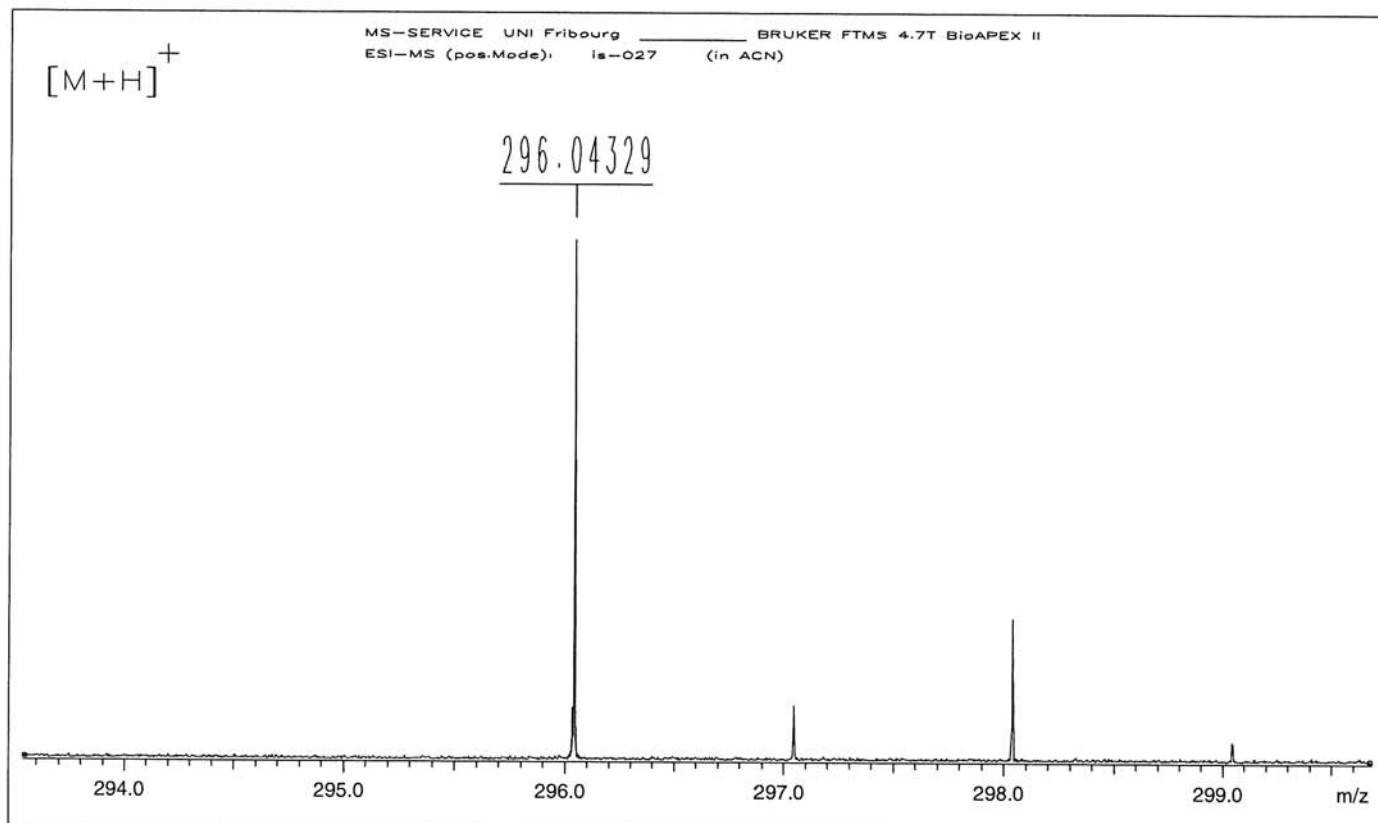
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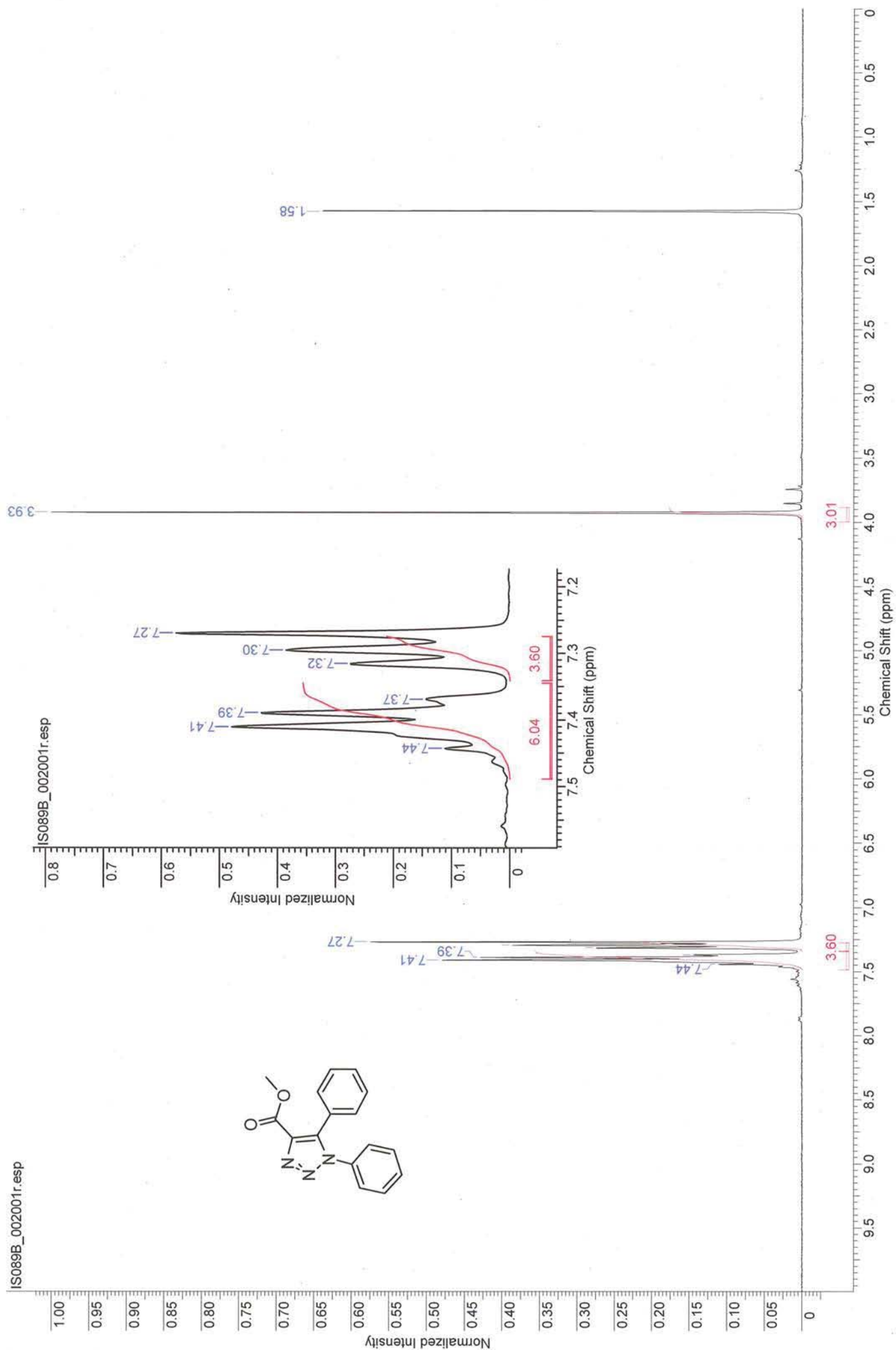
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XMASS Mass Analysis Constraints

Ion mass = 296.0432860

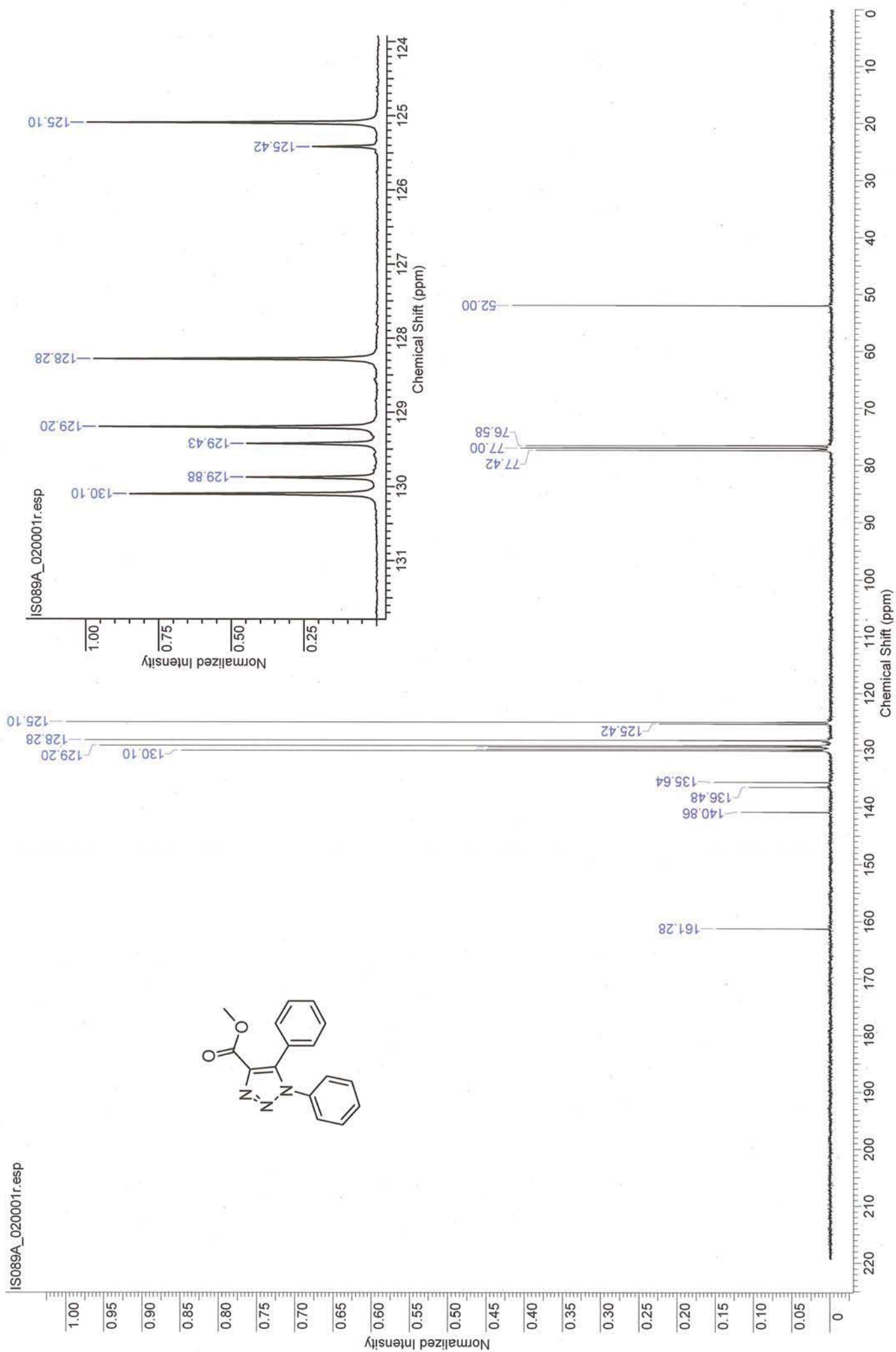
Charge = +1

#	C	H	35Cl	N	O	mass	DBE	error
*** Mass Analysis for mass 296.0432860								
1	12	11	1	3	4	296.0432600	8.5	2.601e-05
2	9	14	2	4	3	296.0437472	4.0	4.612e-04
3	11	16	2	1	4	296.0450898	3.5	1.804e-03
4	6	16	2	3	6	296.0410671	-0.5	2.219e-03
5	15	9	1	4	1	296.0459401	13.0	2.654e-03
6	9	13	1	2	7	296.0405799	4.0	2.706e-03
7	17	11	1	1	2	296.0472827	12.5	3.997e-03
8	7	11	1	5	6	296.0392372	4.5	4.049e-03
9	14	14	2	2	1	296.0477699	8.0	4.484e-03
10	6	15	1	1	10	296.0378998	-0.5	5.386e-03

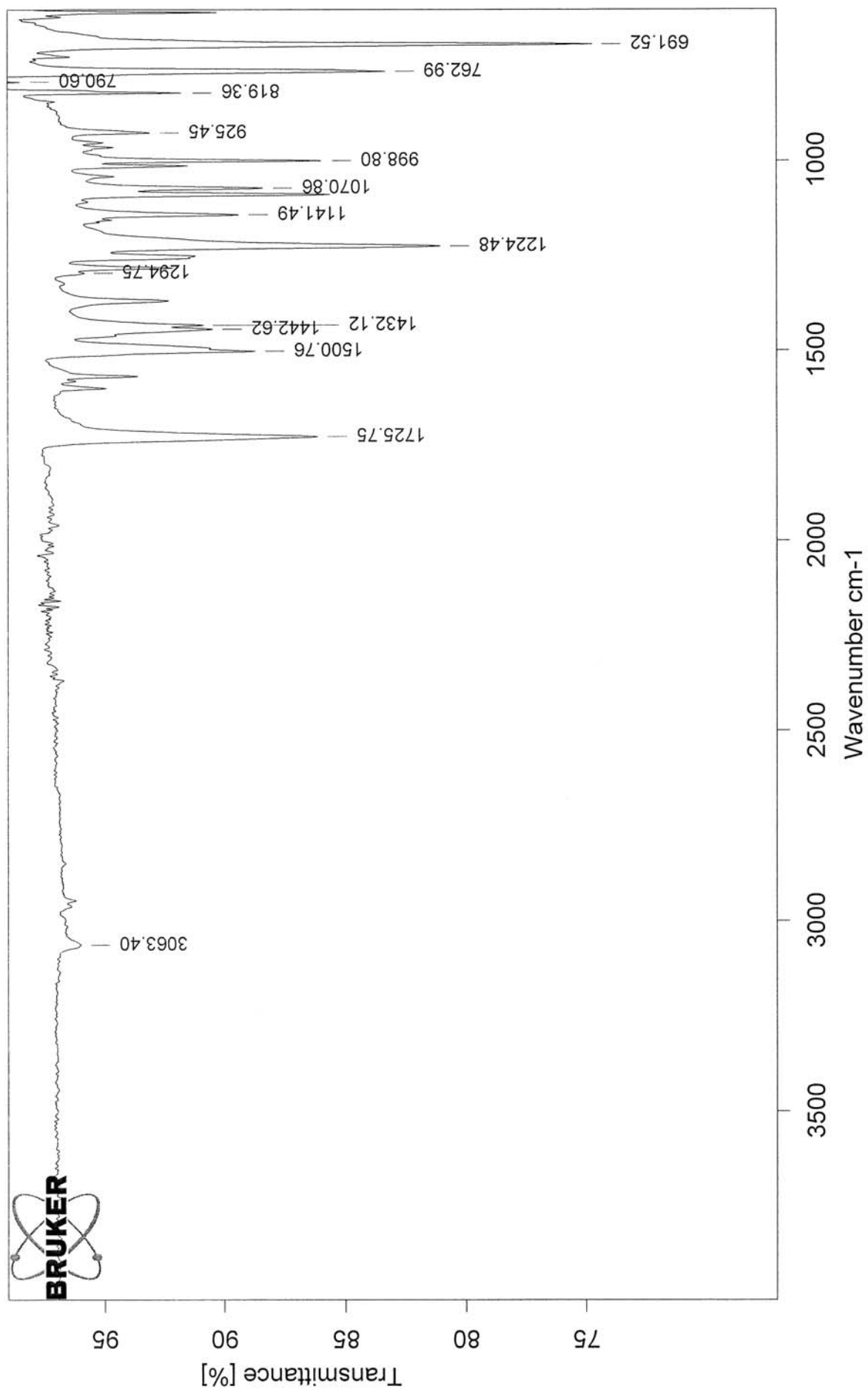












ESI-MS: IS089

XMASS Mass Analysis for /Data/UNI\_FR/ALIM4950\_ESI/5/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

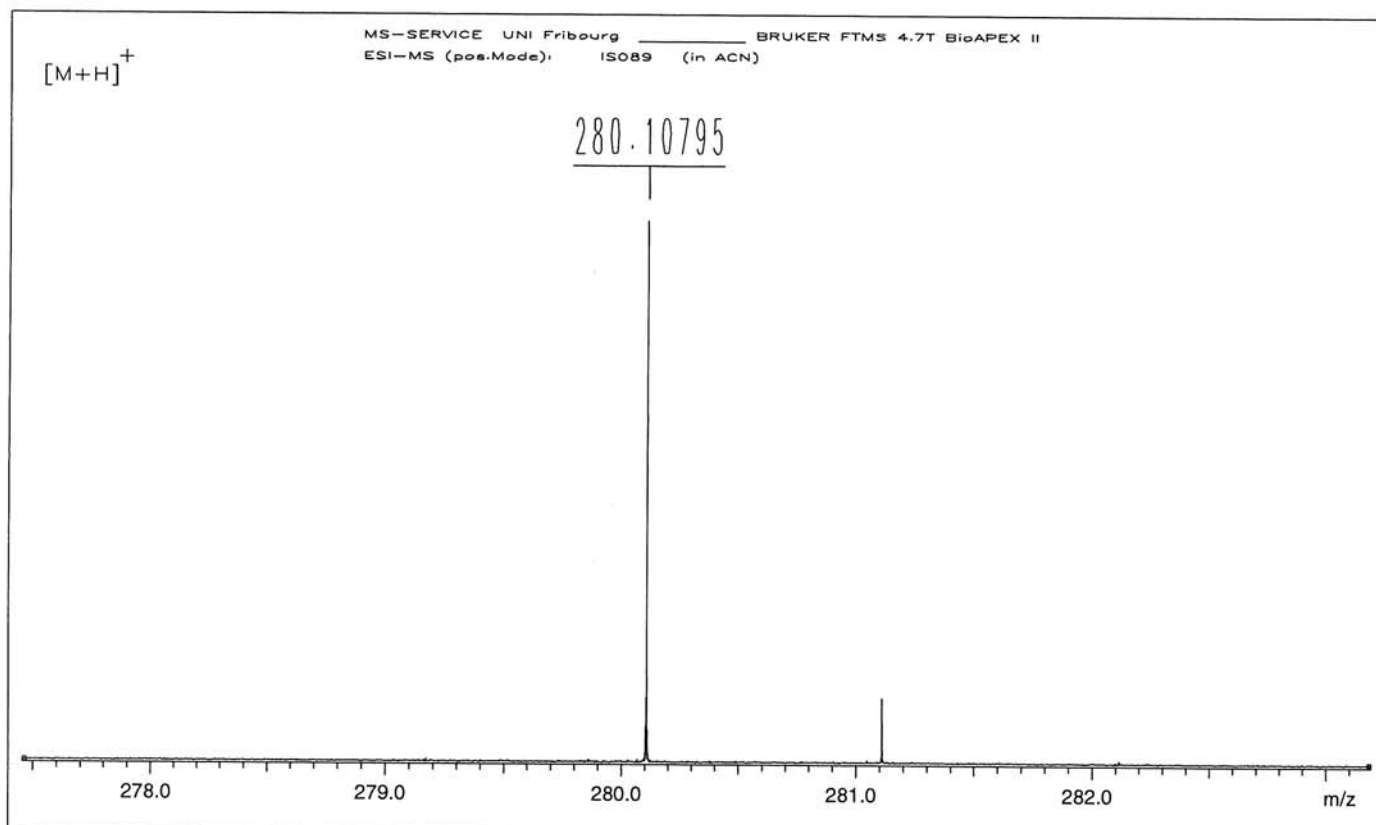
Ion mass = 280.1079540

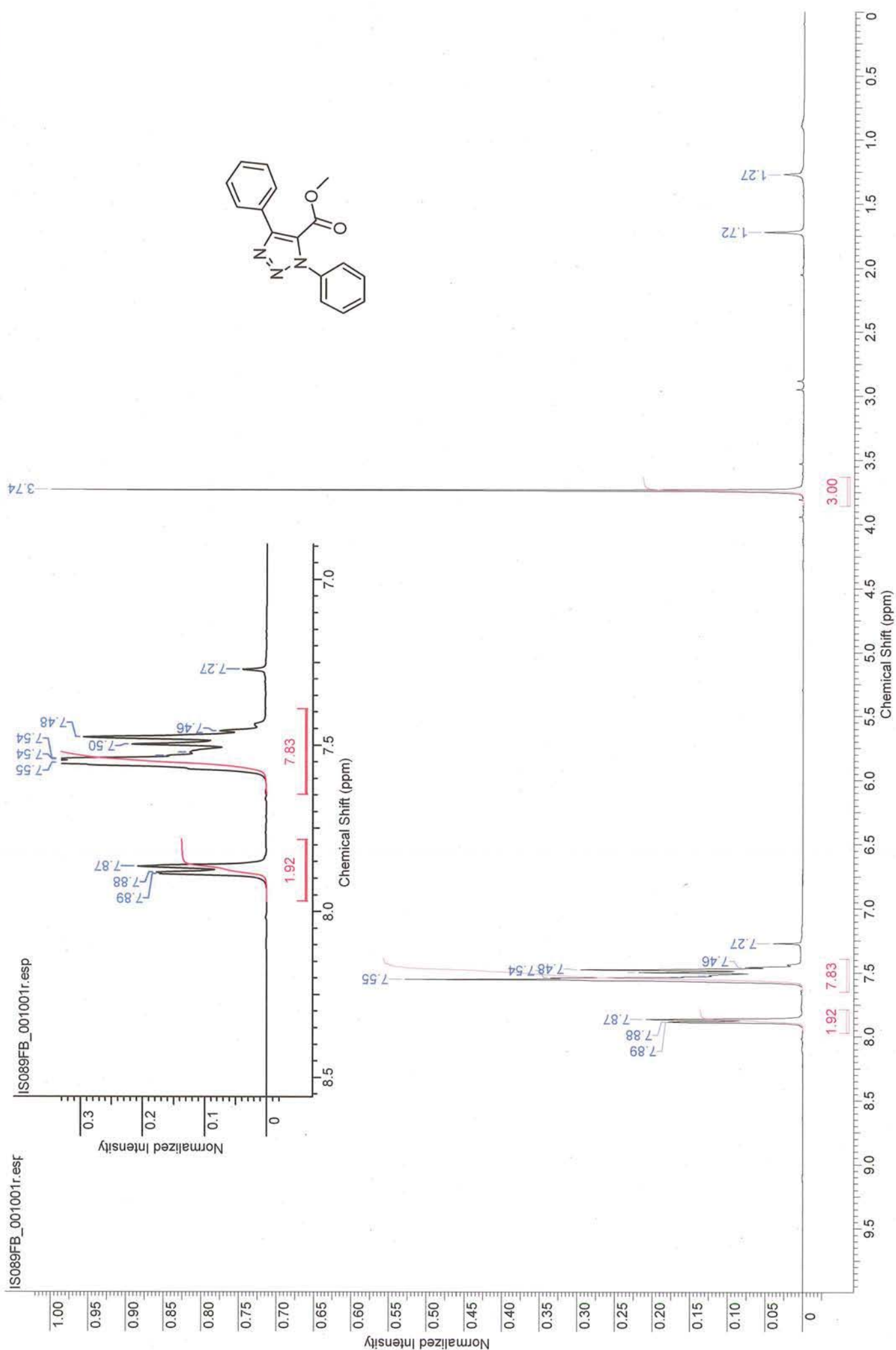
Charge = +1

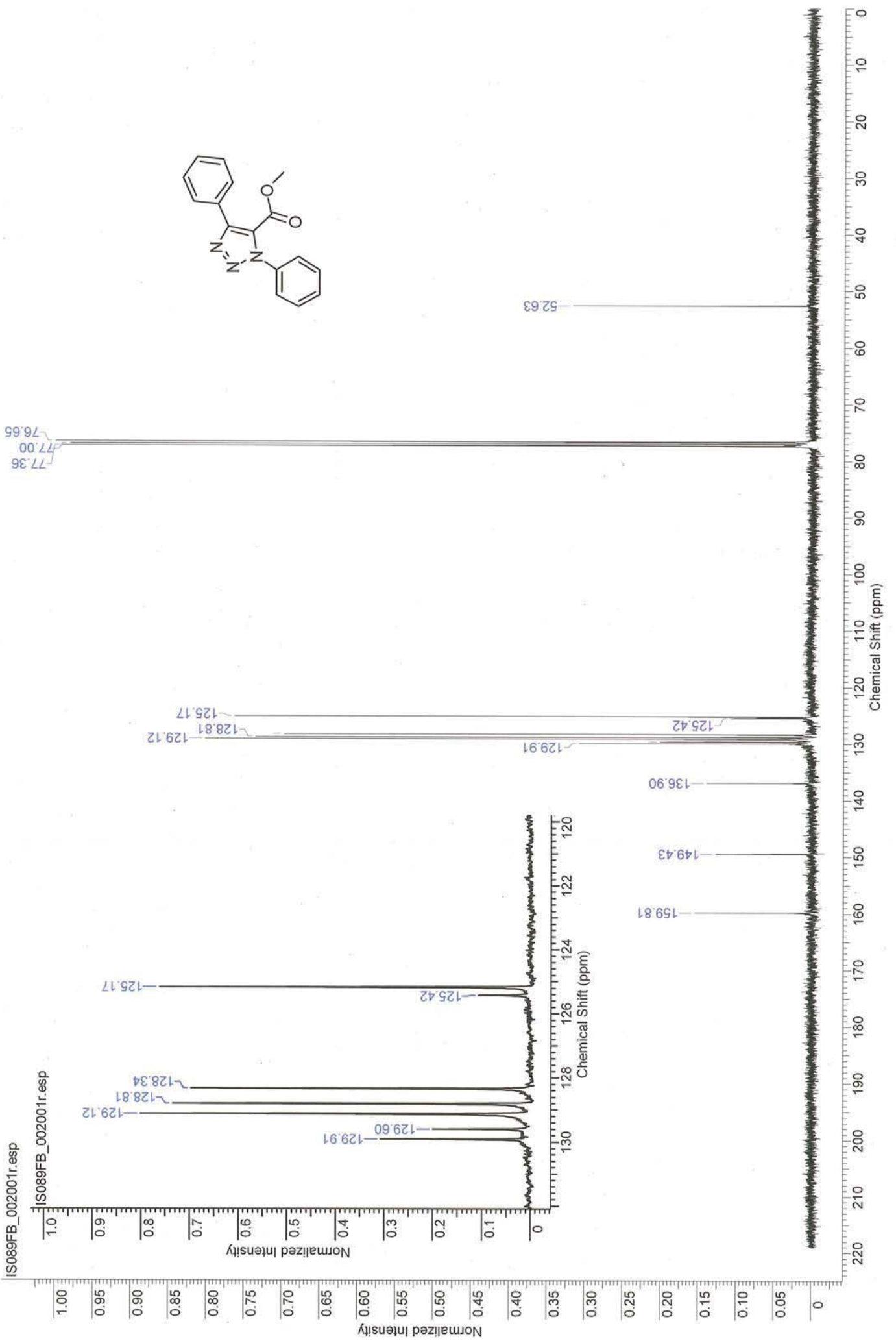
#	C	H	N	O	mass	DBE	error
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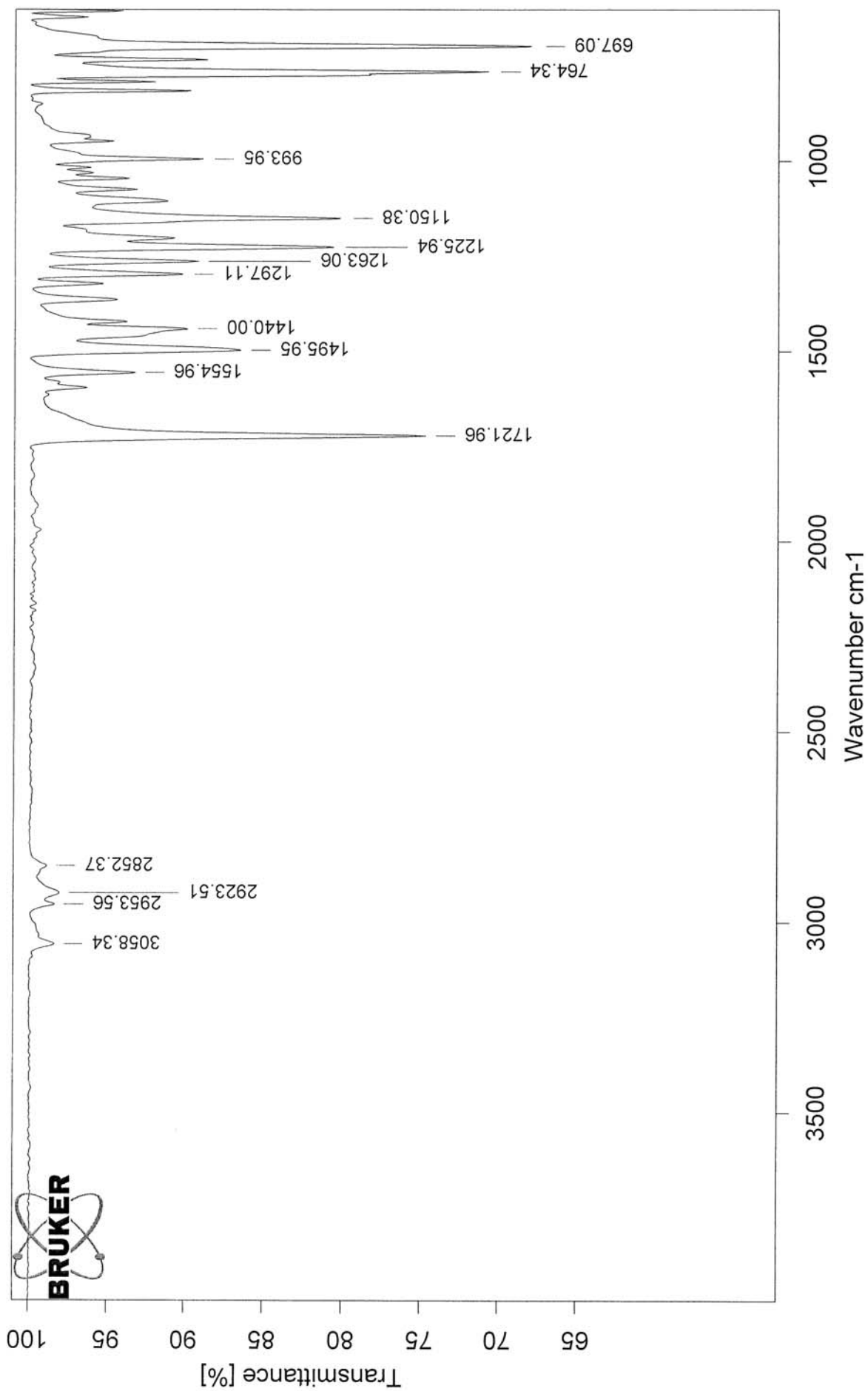
\*\*\* Mass Analysis for mass 280.1079540

1	16	14	3	2	280.1080531	11.5	9.913e-05
2	14	12	6	1	280.1067105	12.0	1.244e-03
3	13	16	2	5	280.1053731	7.0	2.581e-03
4	5	14	9	5	280.1112410	3.5	3.287e-03
5	6	20	2	10	280.1112463	-2.0	3.292e-03
6	11	14	5	4	280.1040304	7.5	3.924e-03
7	7	16	6	6	280.1125837	3.0	4.630e-03
8	10	18	1	8	280.1026930	2.5	5.261e-03
9	9	12	8	3	280.1026877	8.0	5.266e-03
10	8	12	10	2	280.1139211	8.0	5.967e-03









U:\IR\_spectra\IS089.2 IS089B white yellow solid

09/07/2010



ESI-MS: IS089B

XMASS Mass Analysis for /Data/UNI\_FR/ALIM5004\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

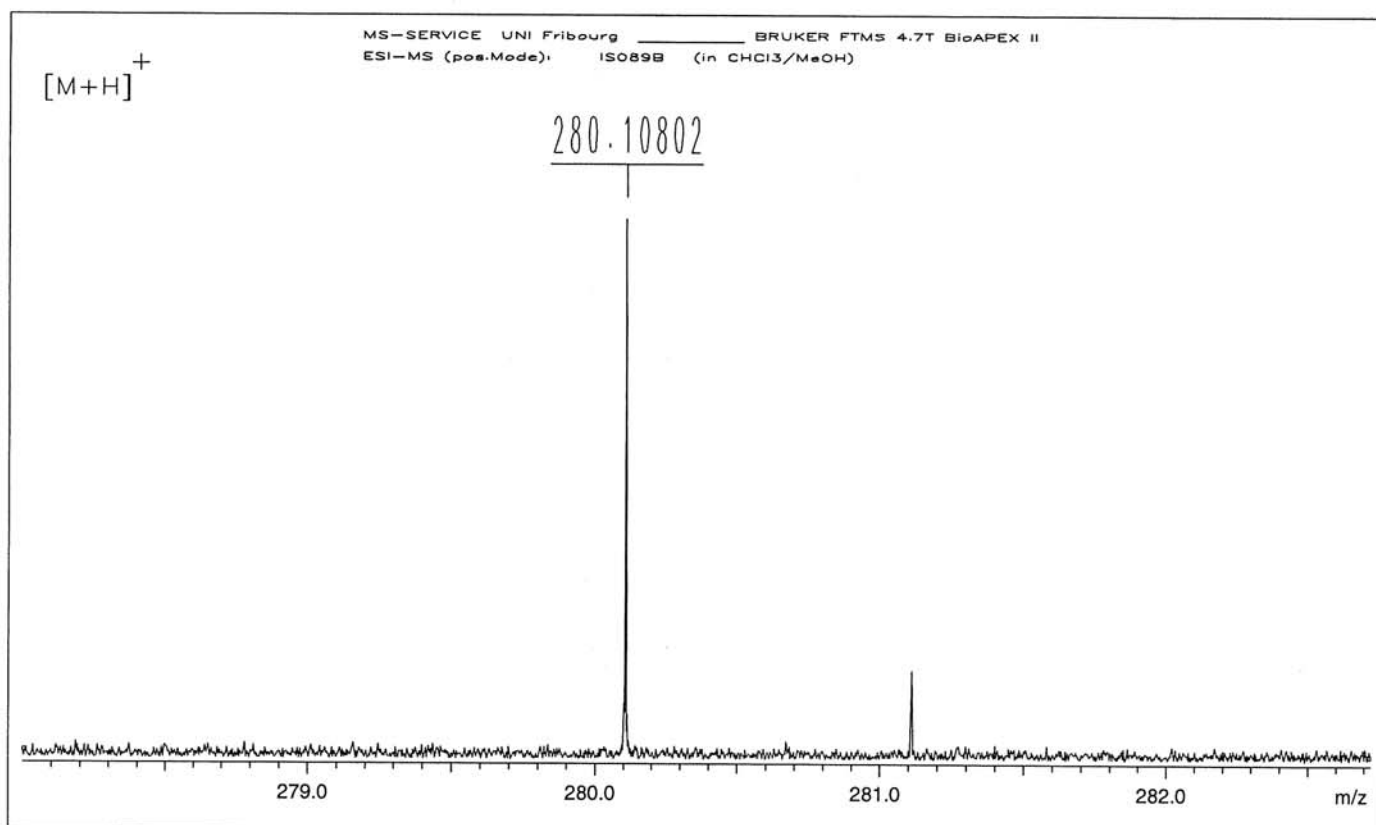
Ion mass = 280.1080220

Charge = +1

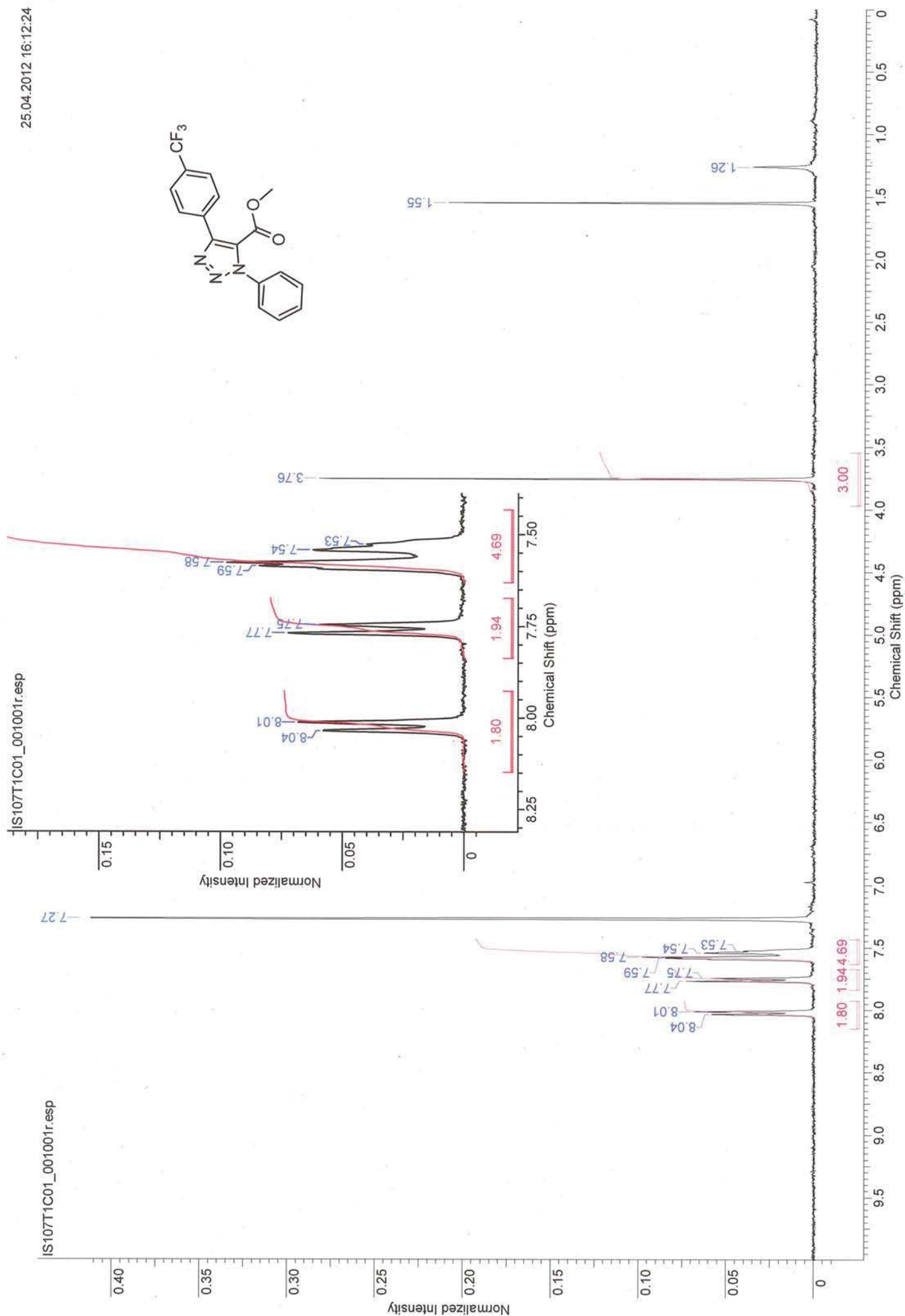
#	C	H	N	O	mass	DBE	error
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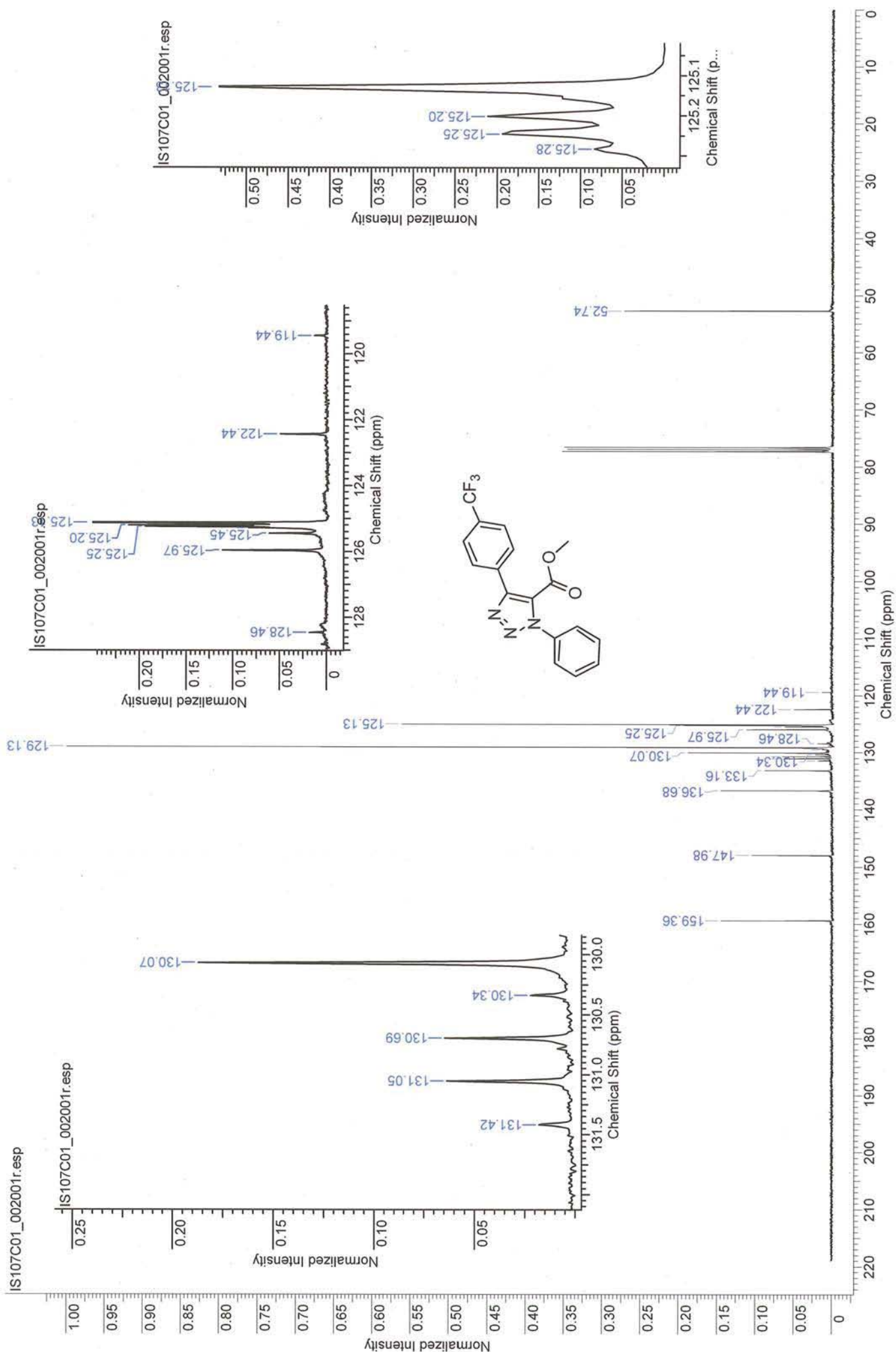
\*\*\* Mass Analysis for mass 280.1080220

1	16	14	3	2	280.1080531	11.5	3.113e-05
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3	13	16	2	5	280.1053731	7.0	2.649e-03
4	5	14	9	5	280.1112410	3.5	3.219e-03
5	6	20	2	10	280.1112463	-2.0	3.224e-03
6	11	14	5	4	280.1040304	7.5	3.992e-03
7	7	16	6	6	280.1125837	3.0	4.562e-03
8	10	18	1	8	280.1026930	2.5	5.329e-03
9	9	12	8	3	280.1026877	8.0	5.334e-03
10	8	12	10	2	280.1139211	8.0	5.899e-03

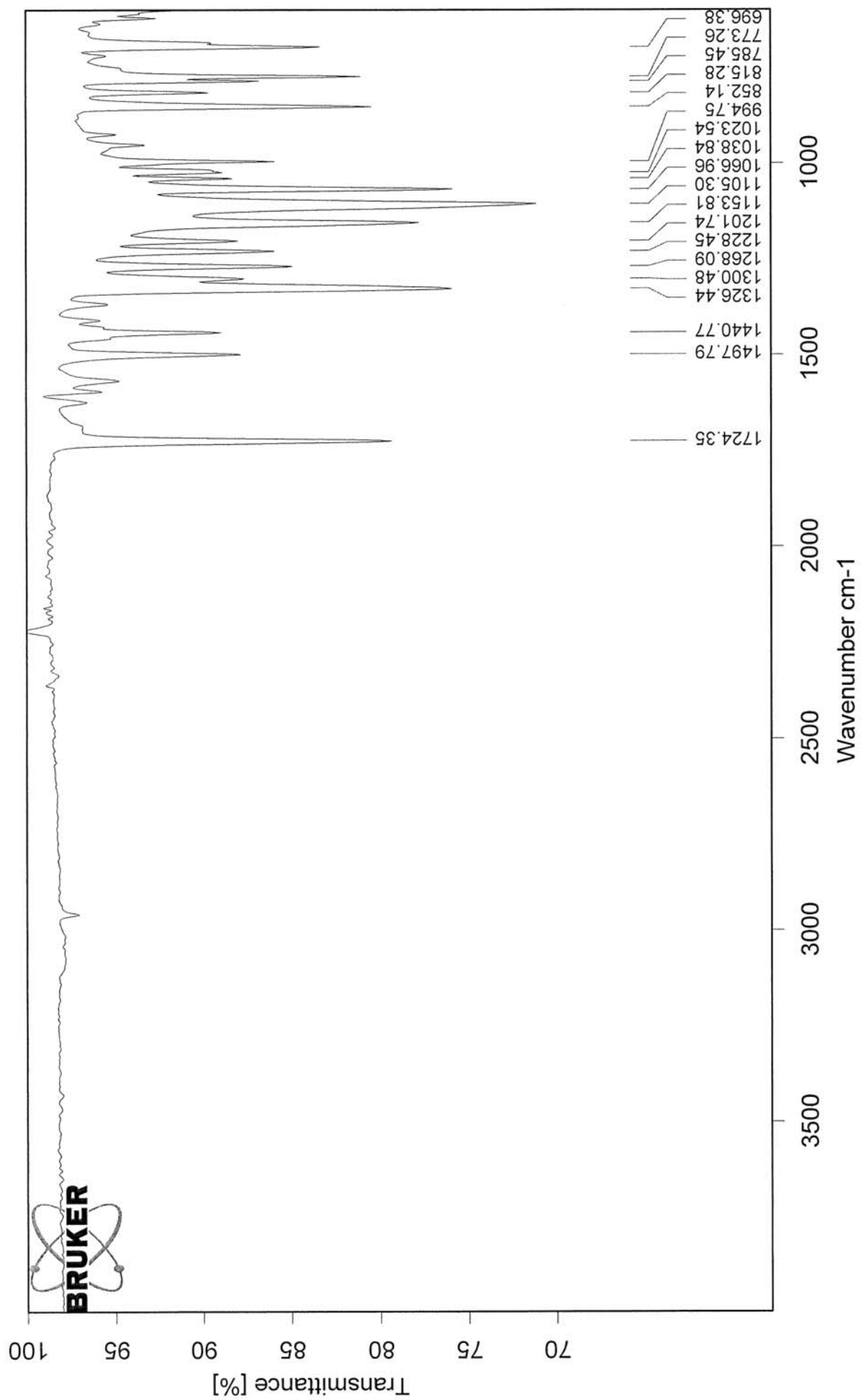














ESI-MS: IS107C01

XMASS Mass Analysis for /Data/UNI\_FR/ALIM5062\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

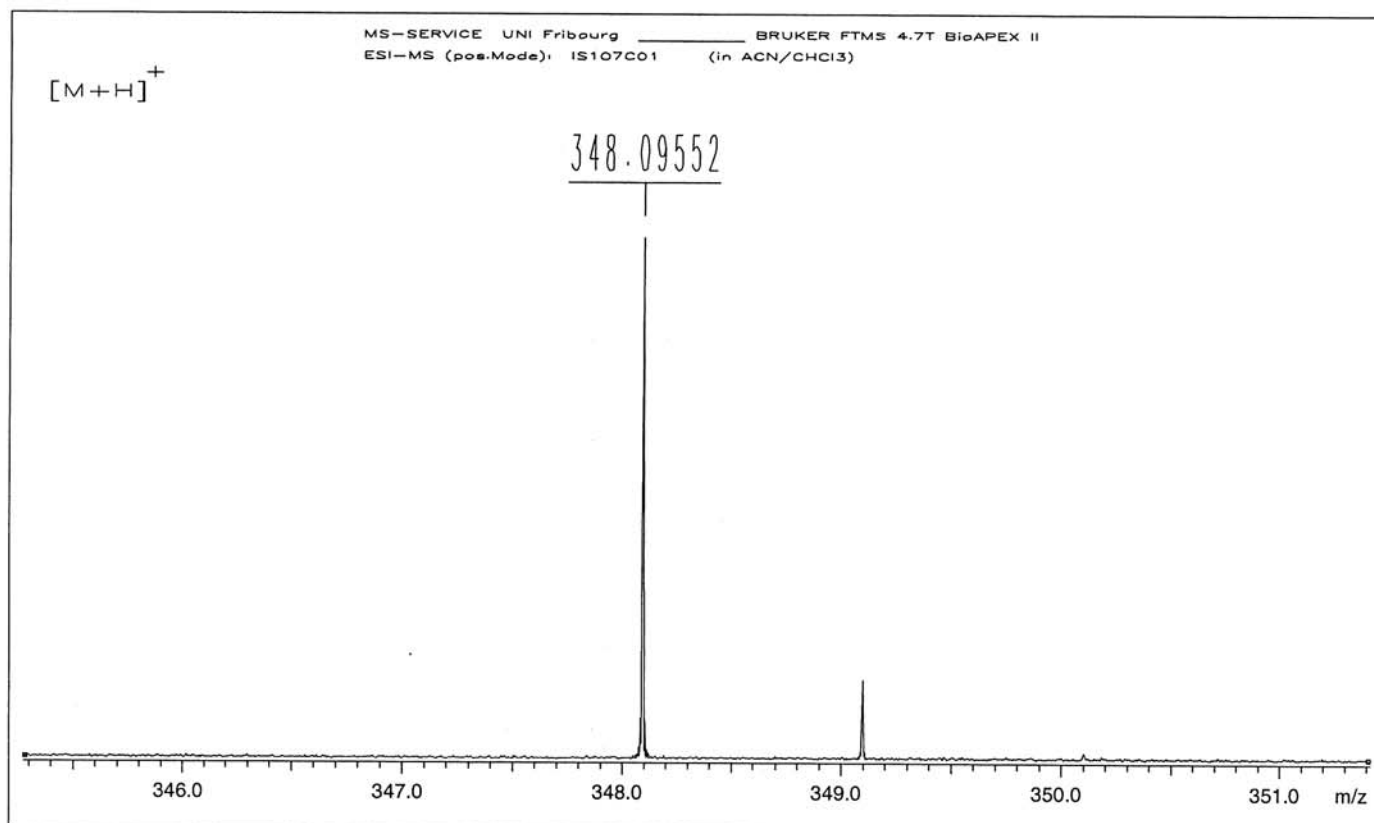
Ion mass = 348.0955240

Charge = +1

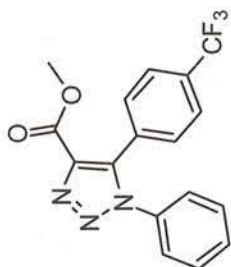
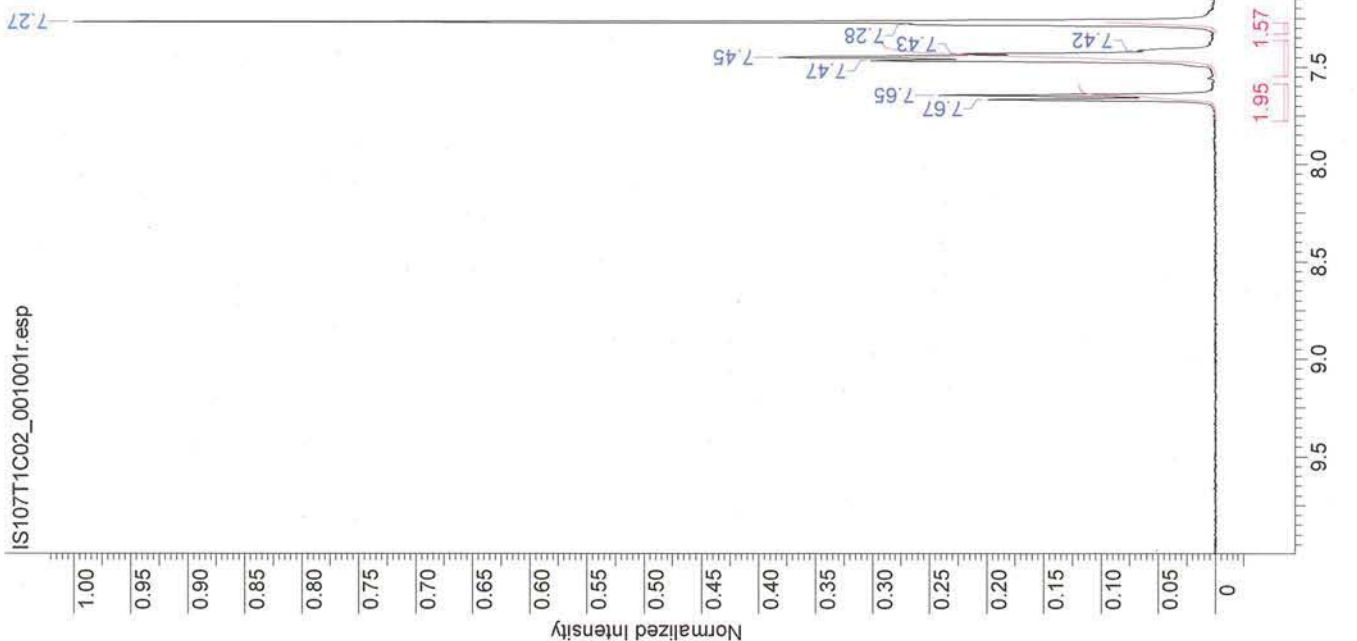
#	C	H	F	N	O	mass	DBE	error
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\*\*\* Mass Analysis for mass 348.0955240

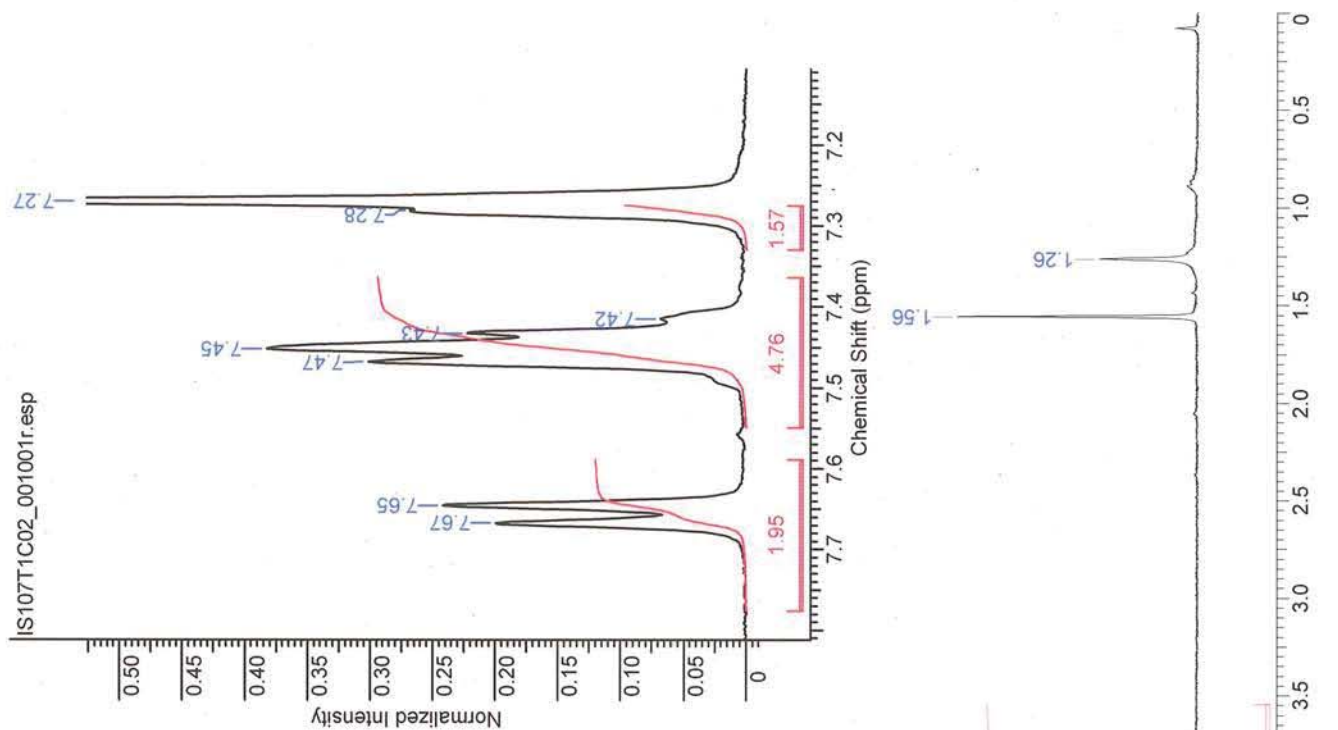
1	17	13	3	3	2	348.0954377	11.5	8.630e-05
2	14	14	4	3	3	348.0965806	7.5	1.057e-03
3	20	12	2	3	1	348.0942948	15.5	1.229e-03
4	11	15	5	3	4	348.0977234	3.5	2.199e-03
5	14	15	3	2	5	348.0927576	7.0	2.766e-03
6	16	15	1	3	5	348.0990252	10.5	3.501e-03
7	17	14	2	2	4	348.0916148	11.0	3.909e-03
8	12	13	3	5	4	348.0914150	7.5	4.109e-03
9	14	13	5	4	1	348.1004035	8.0	4.879e-03
10	20	13	1	2	3	348.0904719	15.0	5.052e-03

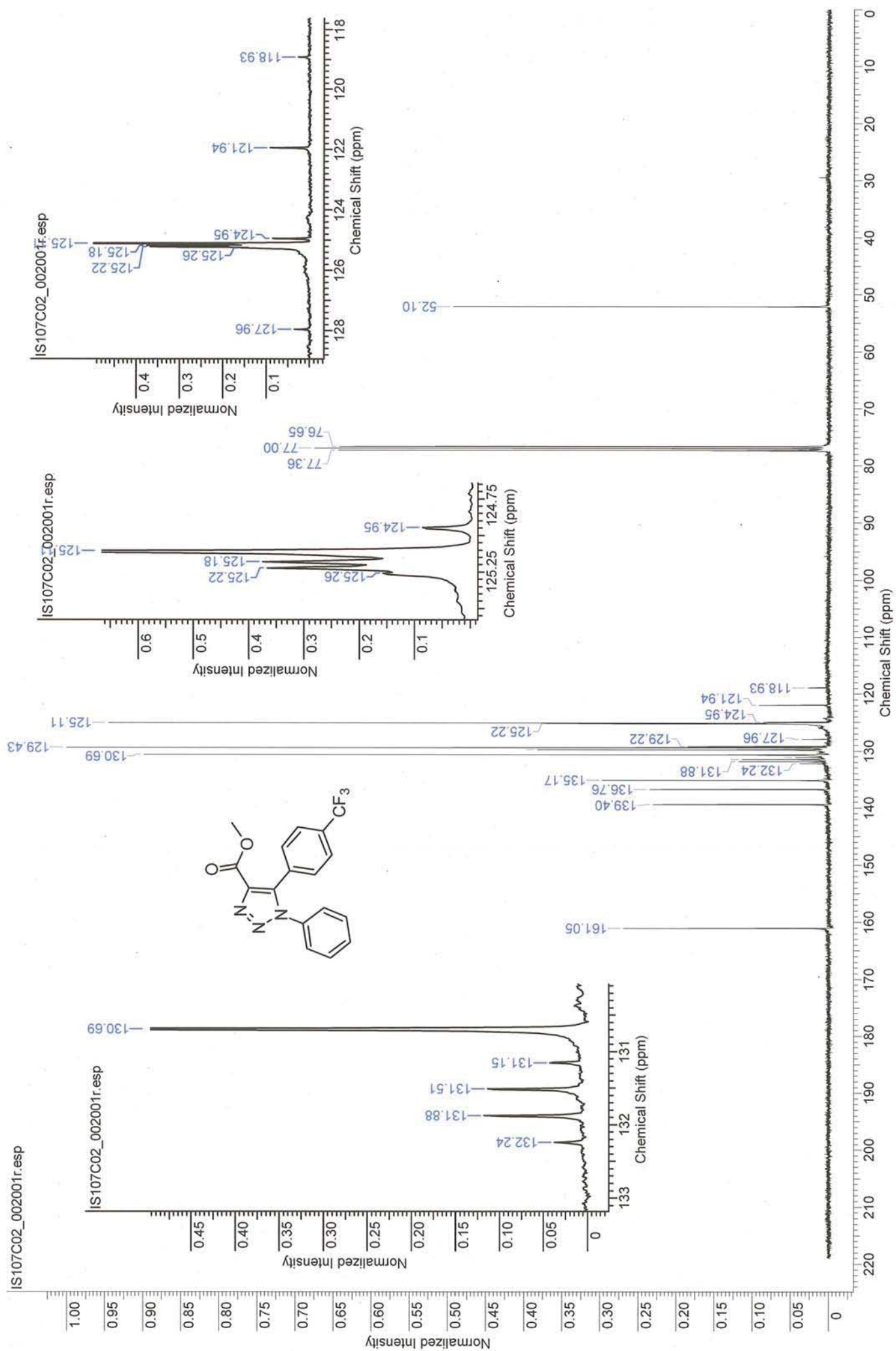


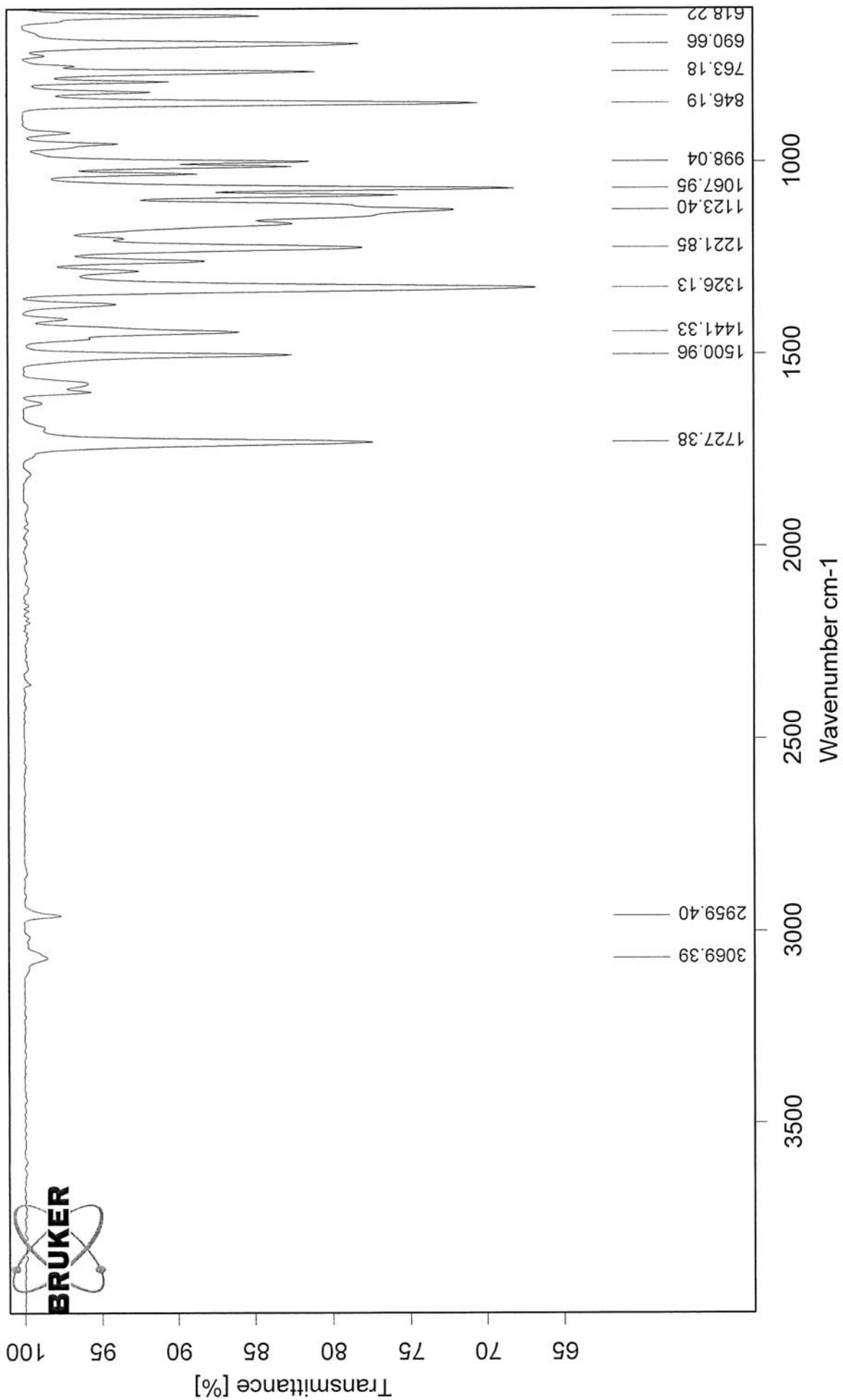
IS107T1C02\_001001r.esp



3.94







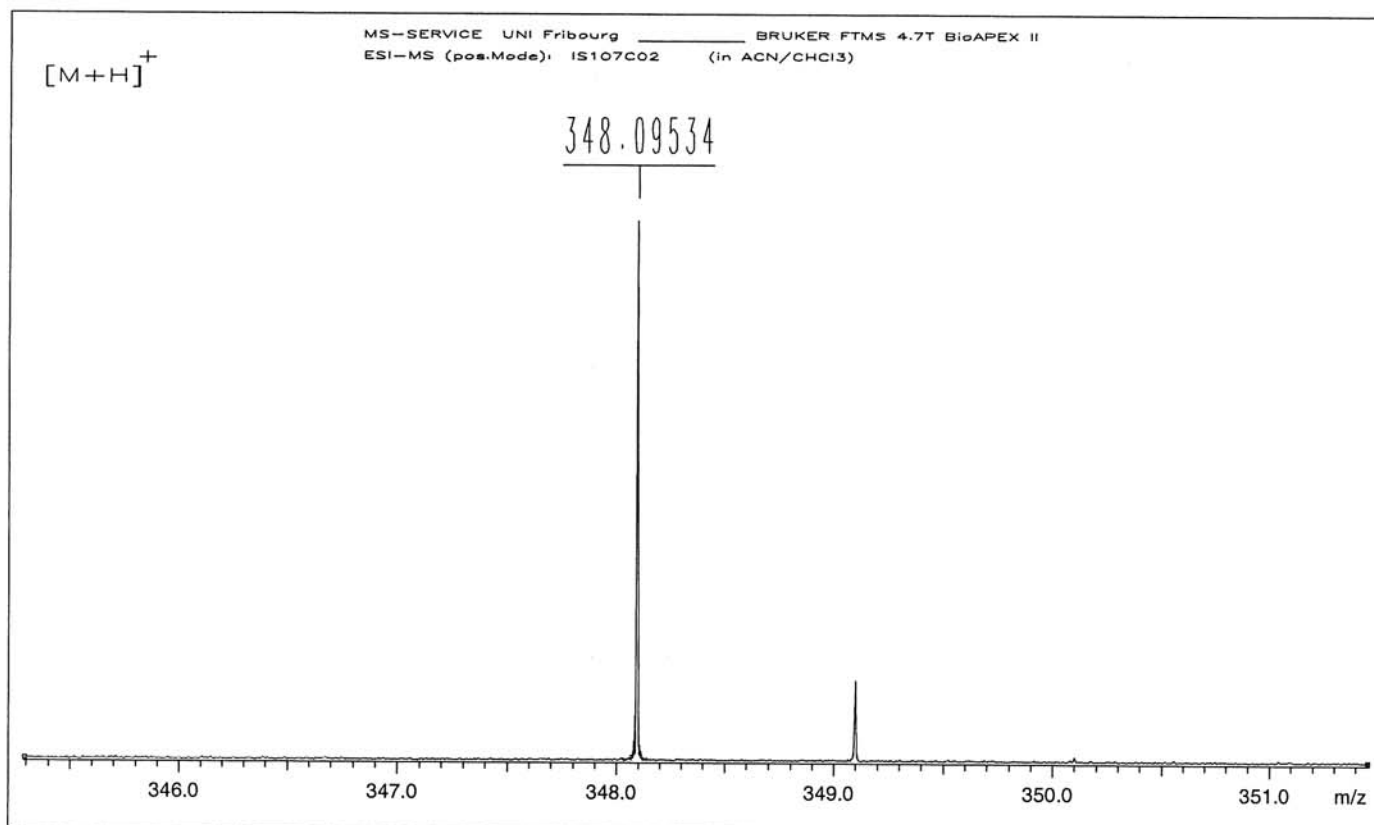
ESI-MS: IS107C02

XMASS Mass Analysis for /Data/UNI\_FR/ALIM5063\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

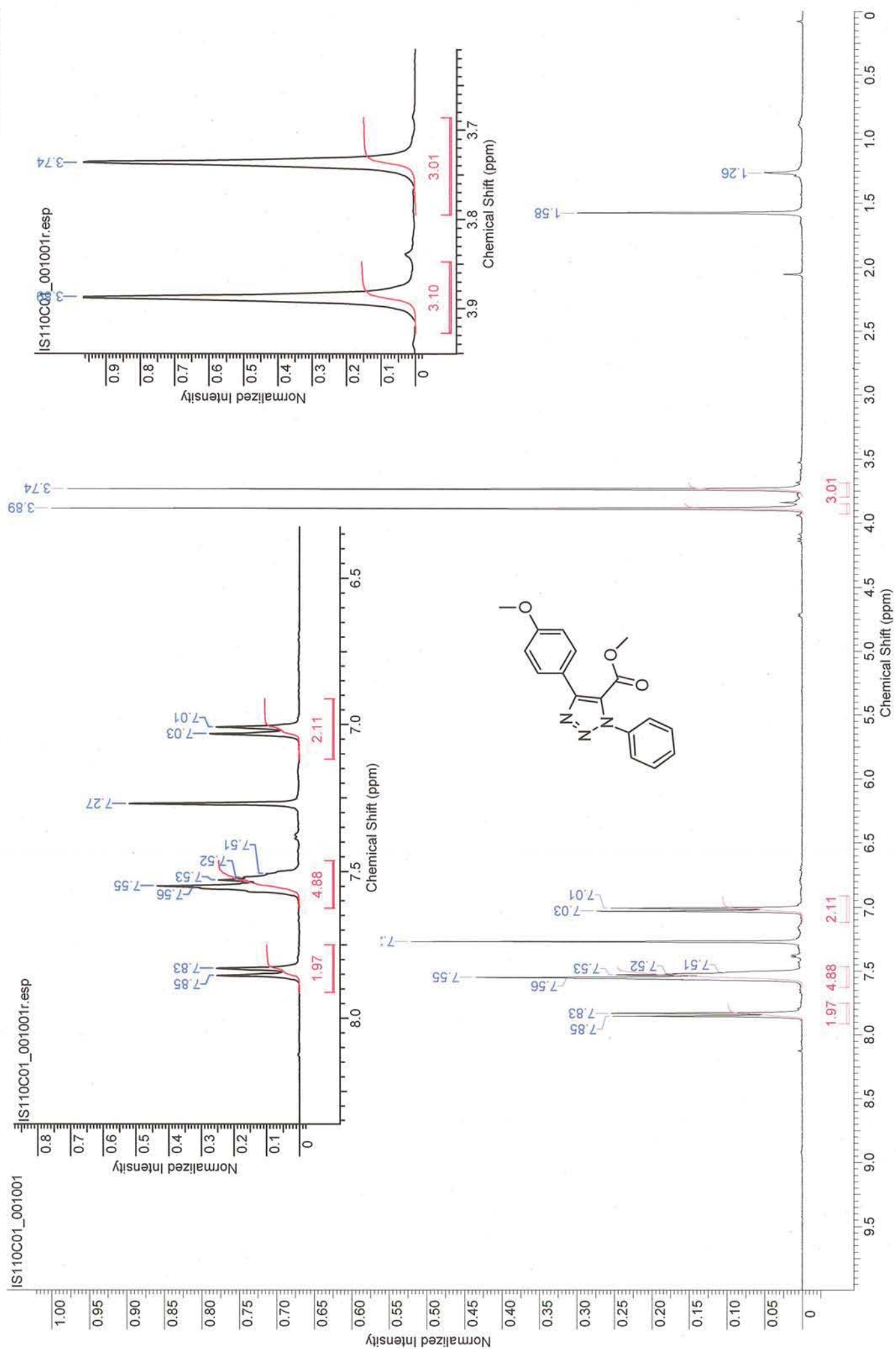
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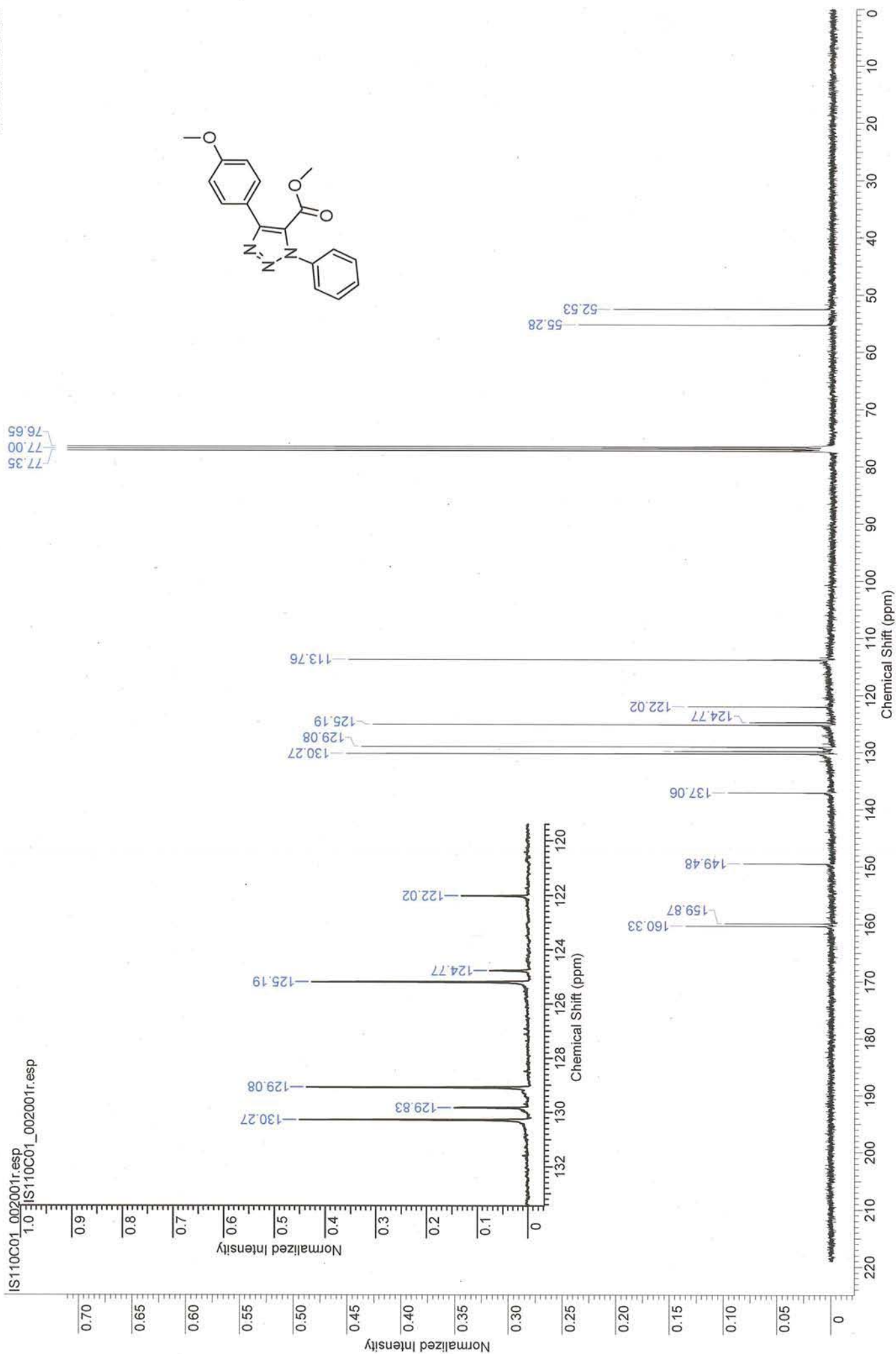
Charge = +1

#	C	H	F	N	O	mass	DBE	error
*** Mass Analysis for mass 348.0953440								
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2	20	12	2	3	1	348.0942948	15.5	1.049e-03
3	14	14	4	3	3	348.0965806	7.5	1.237e-03
4	11	15	5	3	4	348.0977234	3.5	2.379e-03
5	14	15	3	2	5	348.0927576	7.0	2.586e-03
6	16	15	1	3	5	348.0990252	10.5	3.681e-03
7	17	14	2	2	4	348.0916148	11.0	3.729e-03
8	12	13	3	5	4	348.0914150	7.5	3.929e-03
9	20	13	1	2	3	348.0904719	15.0	4.872e-03
10	14	13	5	4	1	348.1004035	8.0	5.059e-03

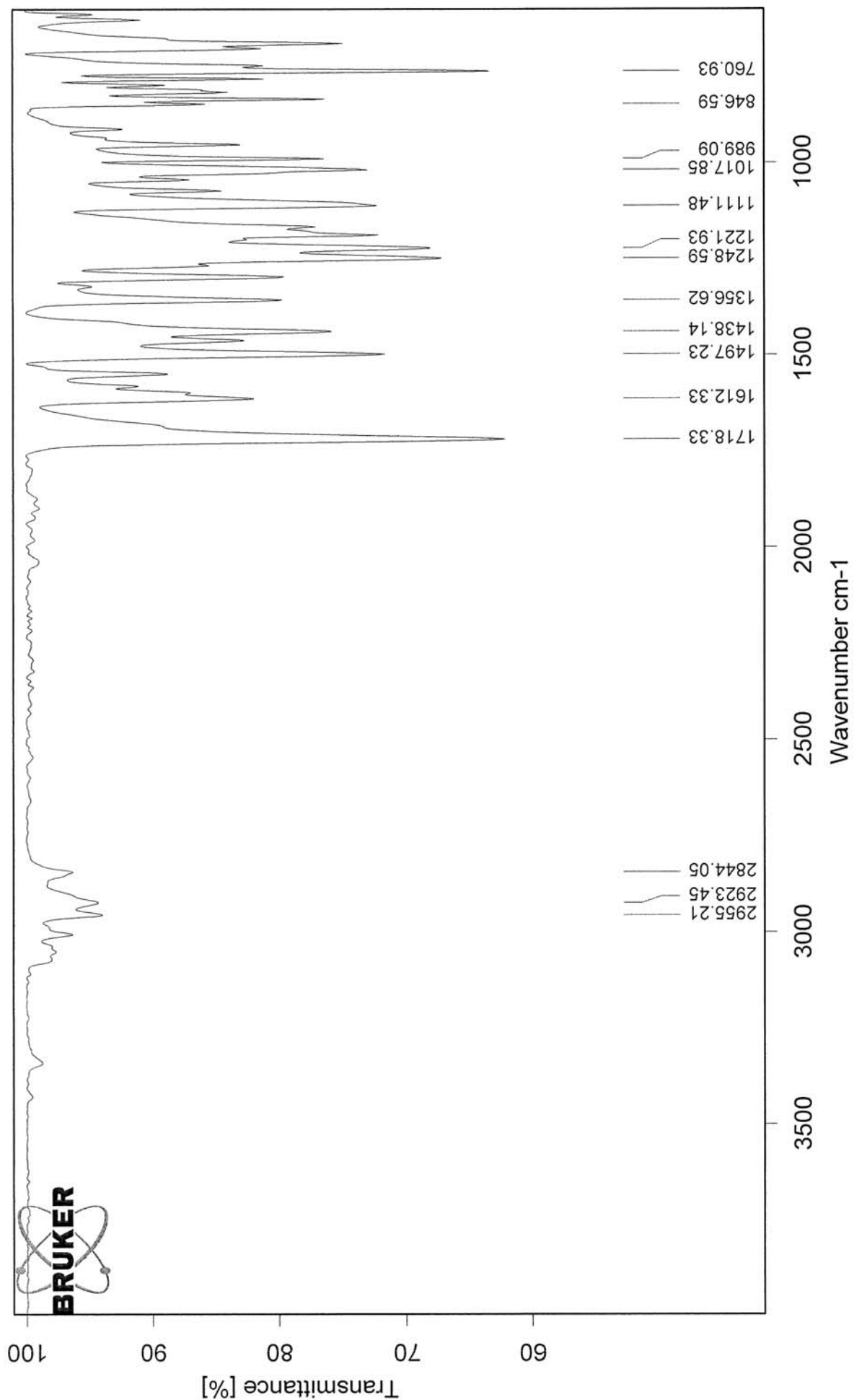












ESI-MS: IS0C01

XMASS Mass Analysis for /Data/UNI\_FR/ALIM50778\_ESI/5/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

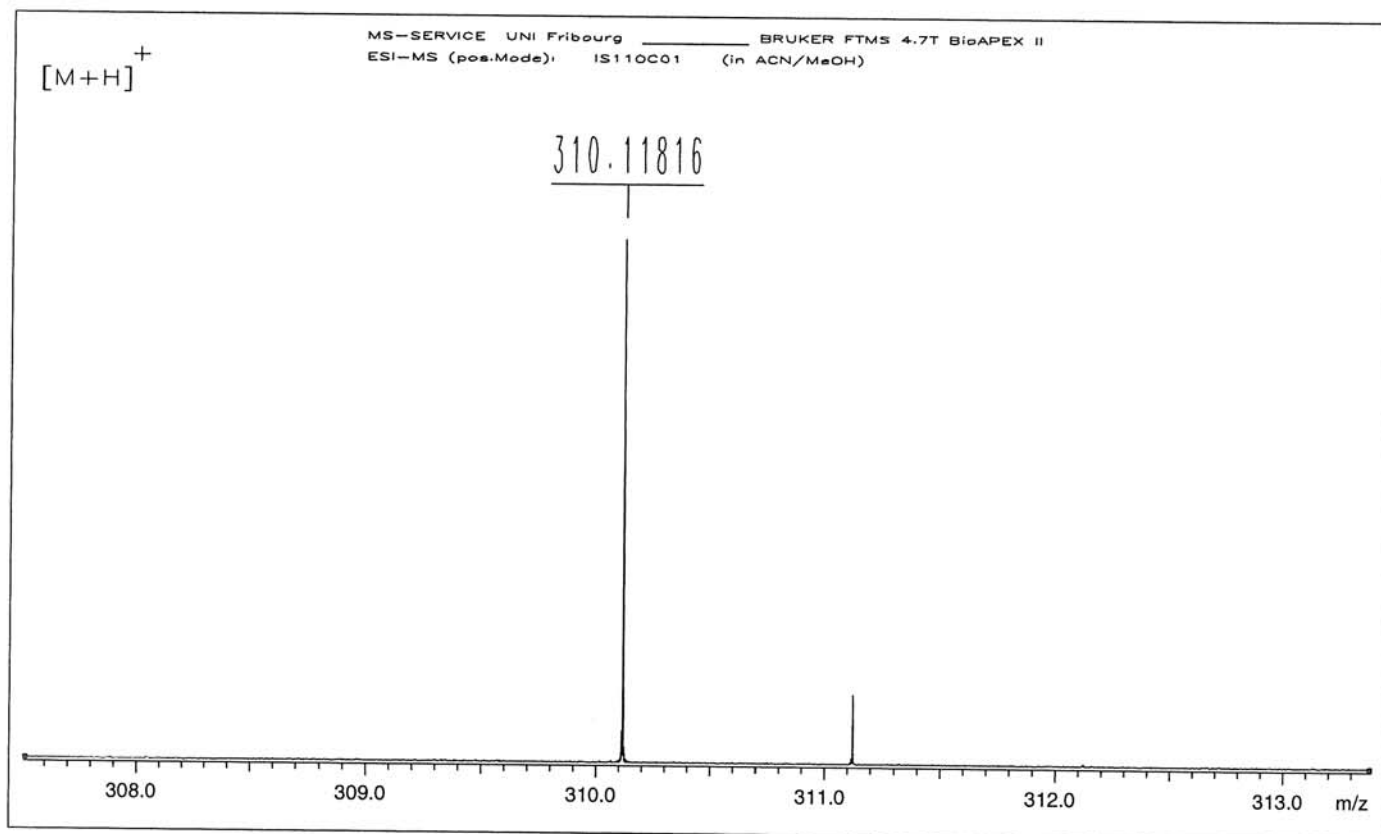
Ion mass = 310.1181560

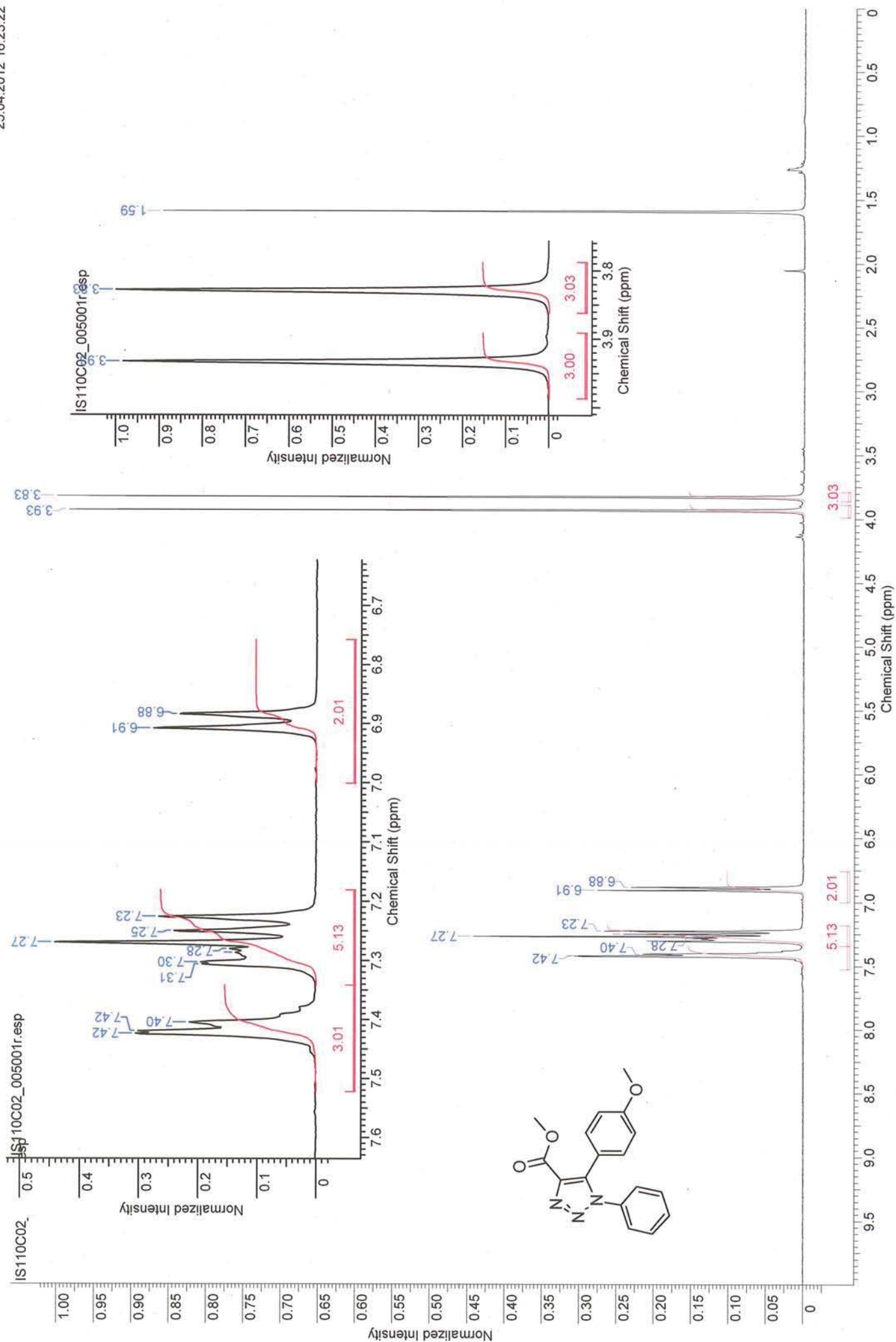
Charge = +1

#	C	H	N	O	mass	DBE	error
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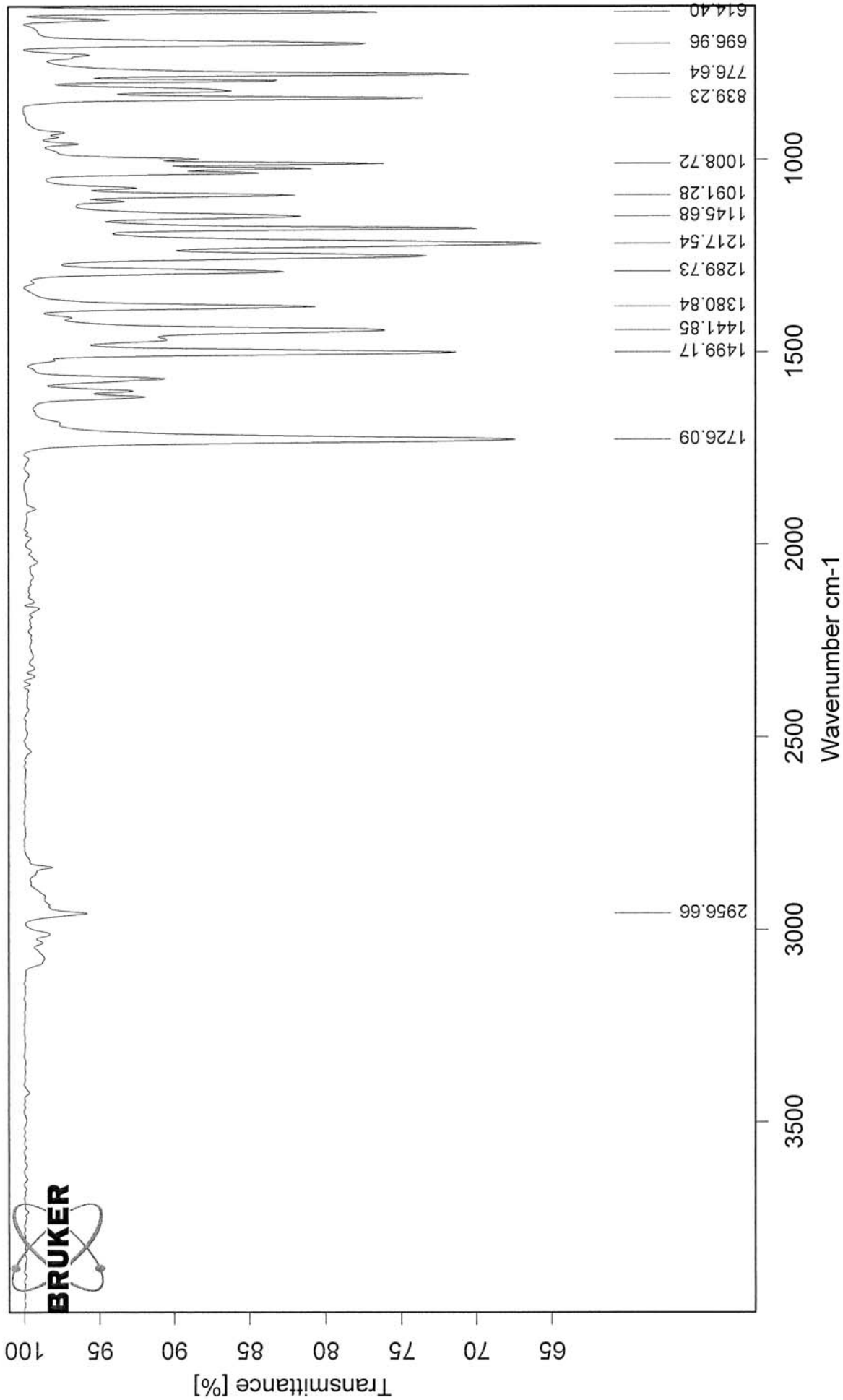
\*\*\* Mass Analysis for mass 310.1181560

1	17	16	3	3	310.1186178	11.5	4.618e-04
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3	12	16	5	5	310.1145951	7.5	3.561e-03
4	22	16	1	1	310.1226406	15.5	4.485e-03
5	11	16	7	4	310.1258285	7.5	7.672e-03
6	21	14	2	1	310.1100645	16.0	8.091e-03
7	13	18	4	5	310.1271711	7.0	9.015e-03
8	18	16	1	4	310.1073844	11.5	1.077e-02
9	16	16	5	2	310.1298512	11.5	1.170e-02
10	16	14	4	3	310.1060418	12.0	1.211e-02











ESI-MS: IS0C02

XMASS Mass Analysis for /Data/UNI\_FR/ALIM5077\_ESI/5/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

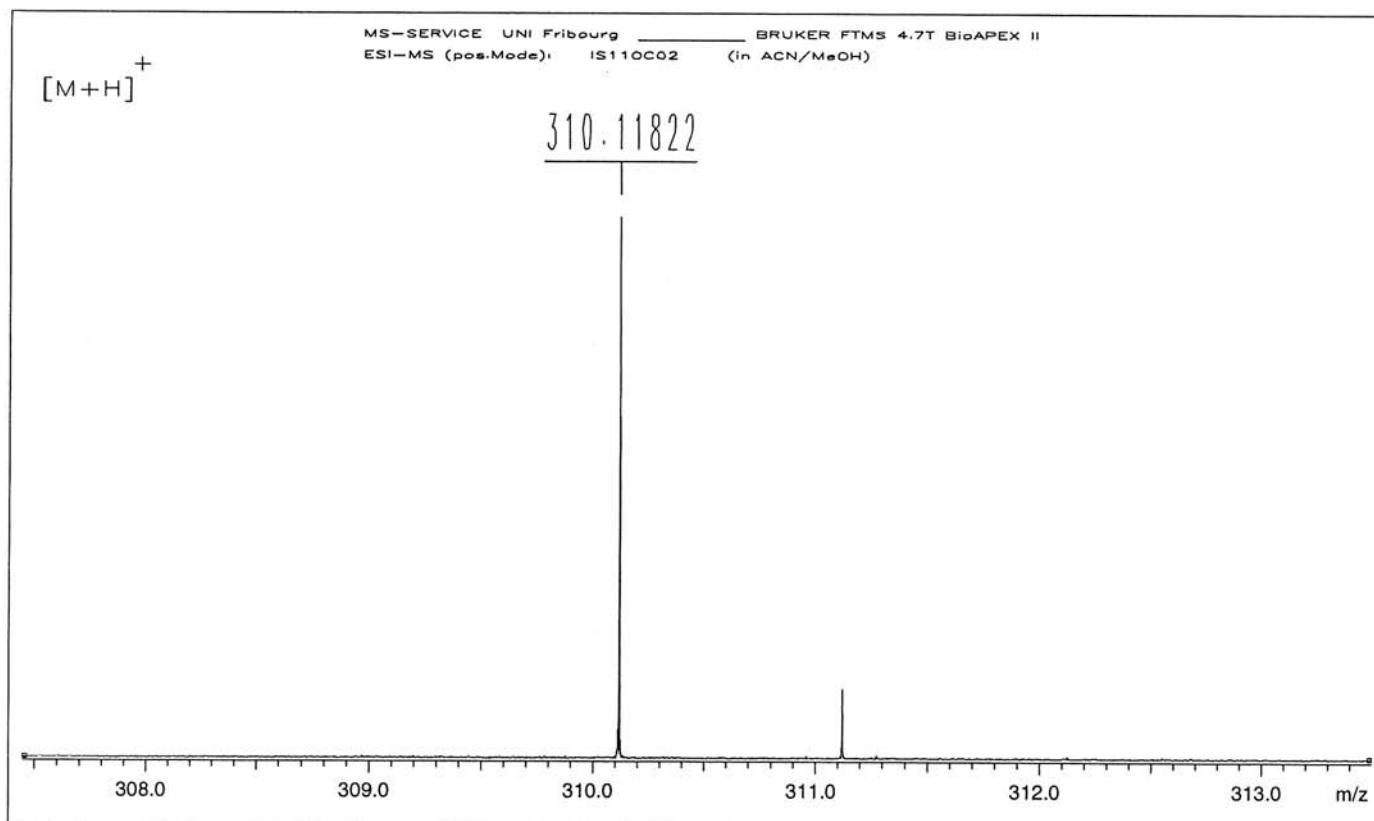
**Ion mass = 310.1182180**

Charge = +1

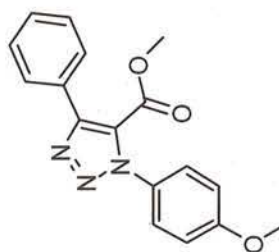
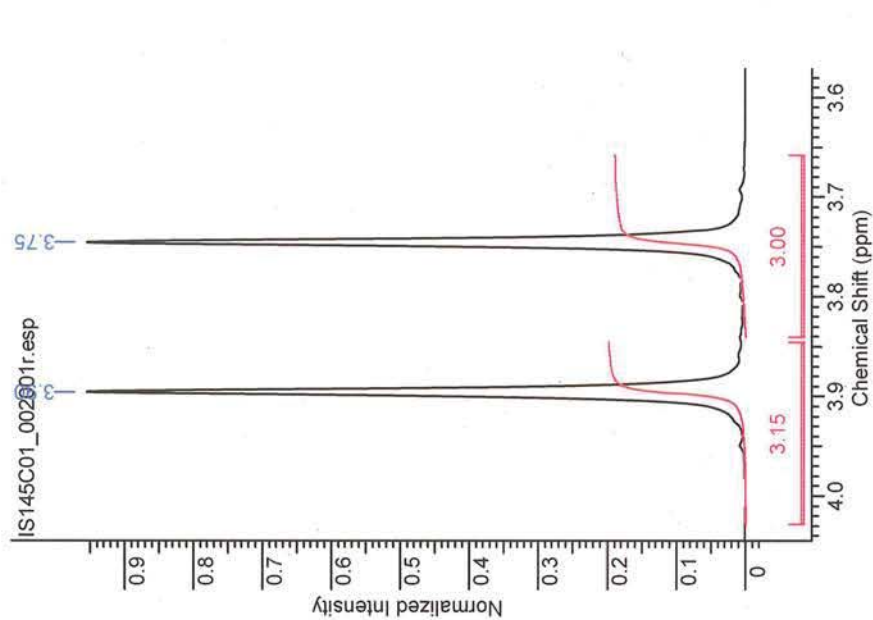
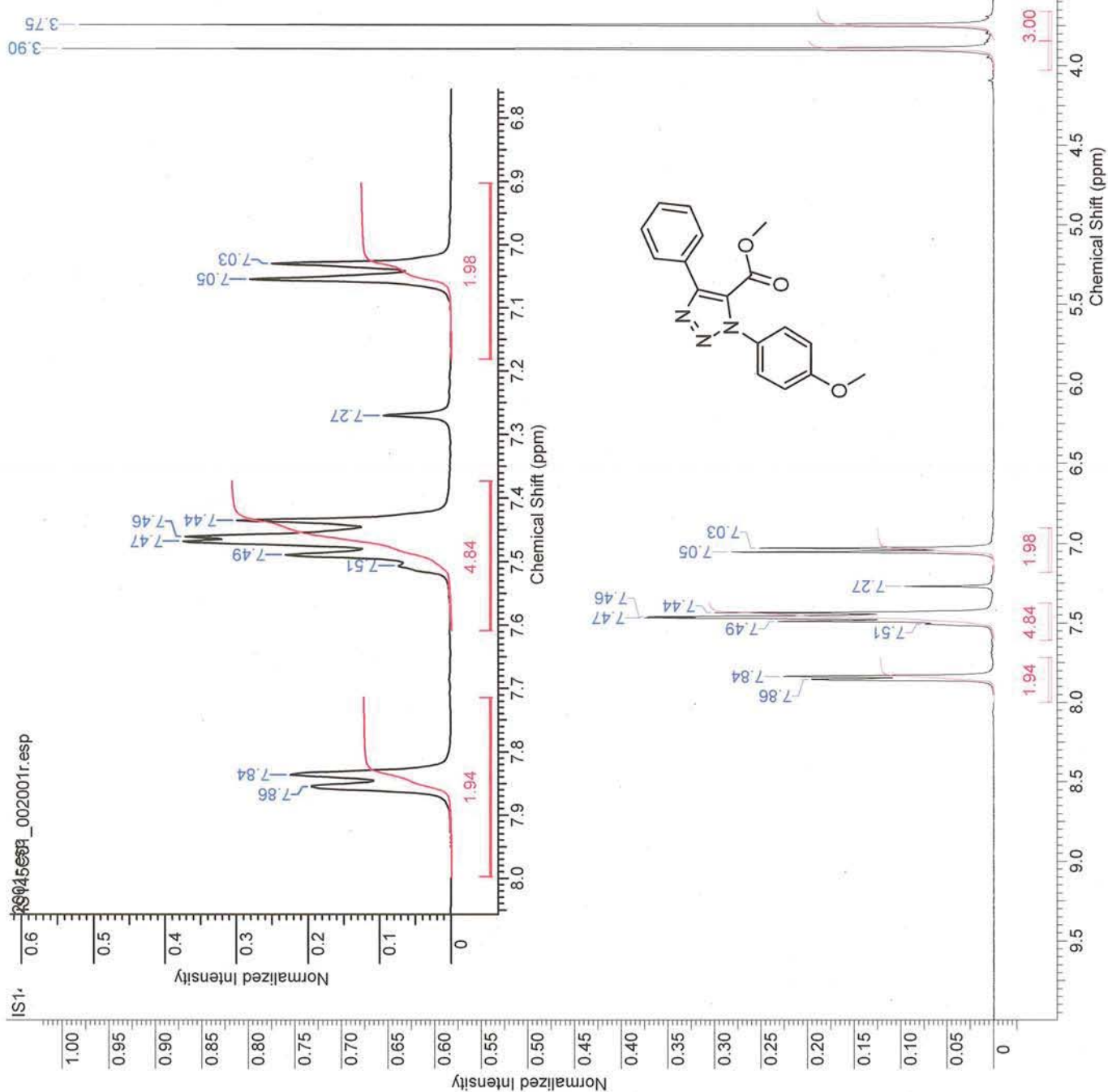
#	C	H	N	O	mass	DBE	error
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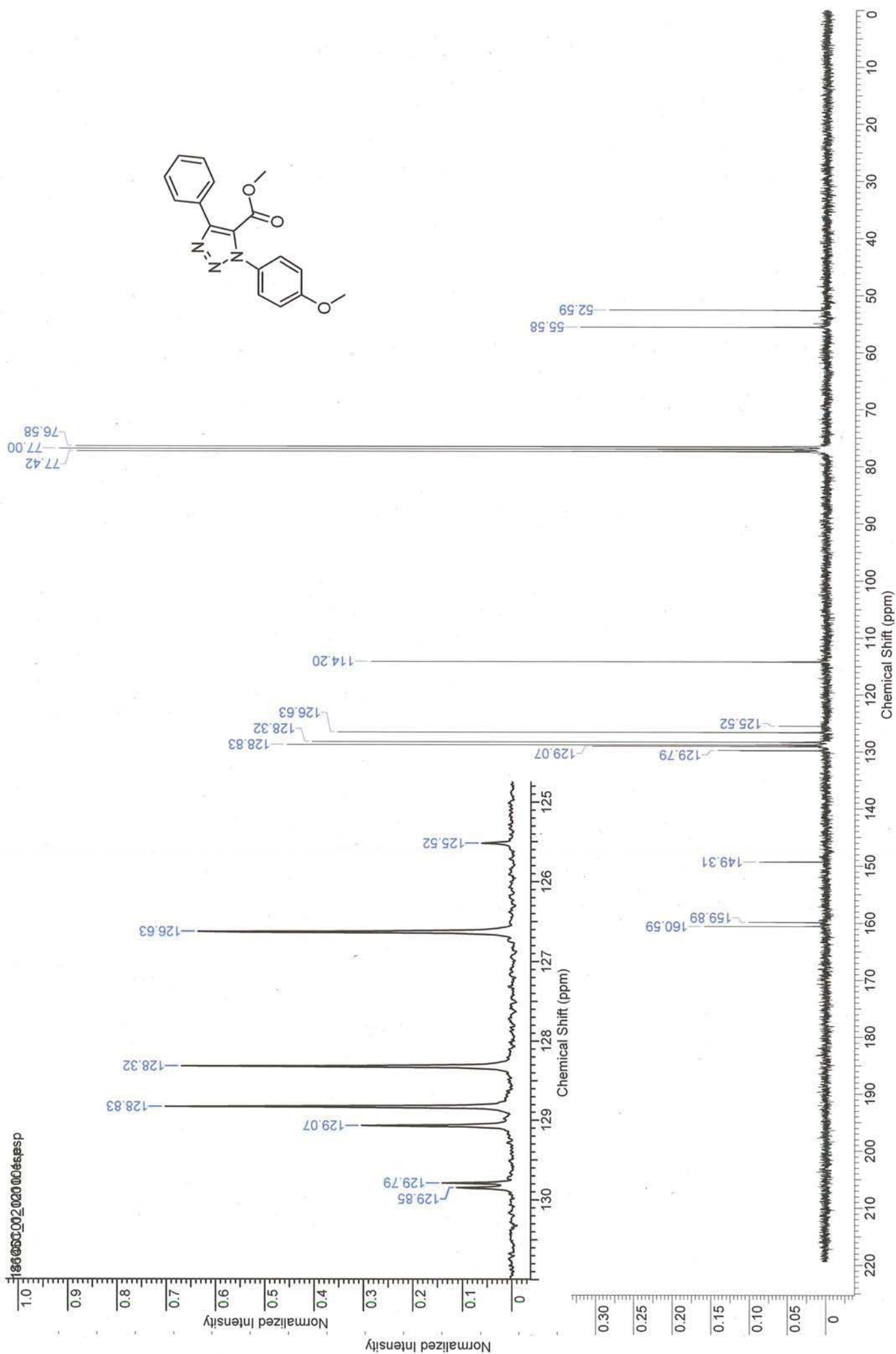
\*\*\* Mass Analysis for mass 310.1182180

1	17	16	3	3	310.1186178	11.5	3.998e-04
2	15	14	6	2	310.1172751	12.0	9.429e-04
3	12	16	5	5	310.1145951	7.5	3.623e-03
4	22	16	1	1	310.1226406	15.5	4.423e-03
5	11	16	7	4	310.1258285	7.5	7.610e-03
6	21	14	2	1	310.1100645	16.0	8.153e-03
7	13	18	4	5	310.1271711	7.0	8.953e-03
8	18	16	1	4	310.1073844	11.5	1.083e-02
9	16	16	5	2	310.1298512	11.5	1.163e-02
10	16	14	4	3	310.1060418	12.0	1.218e-02

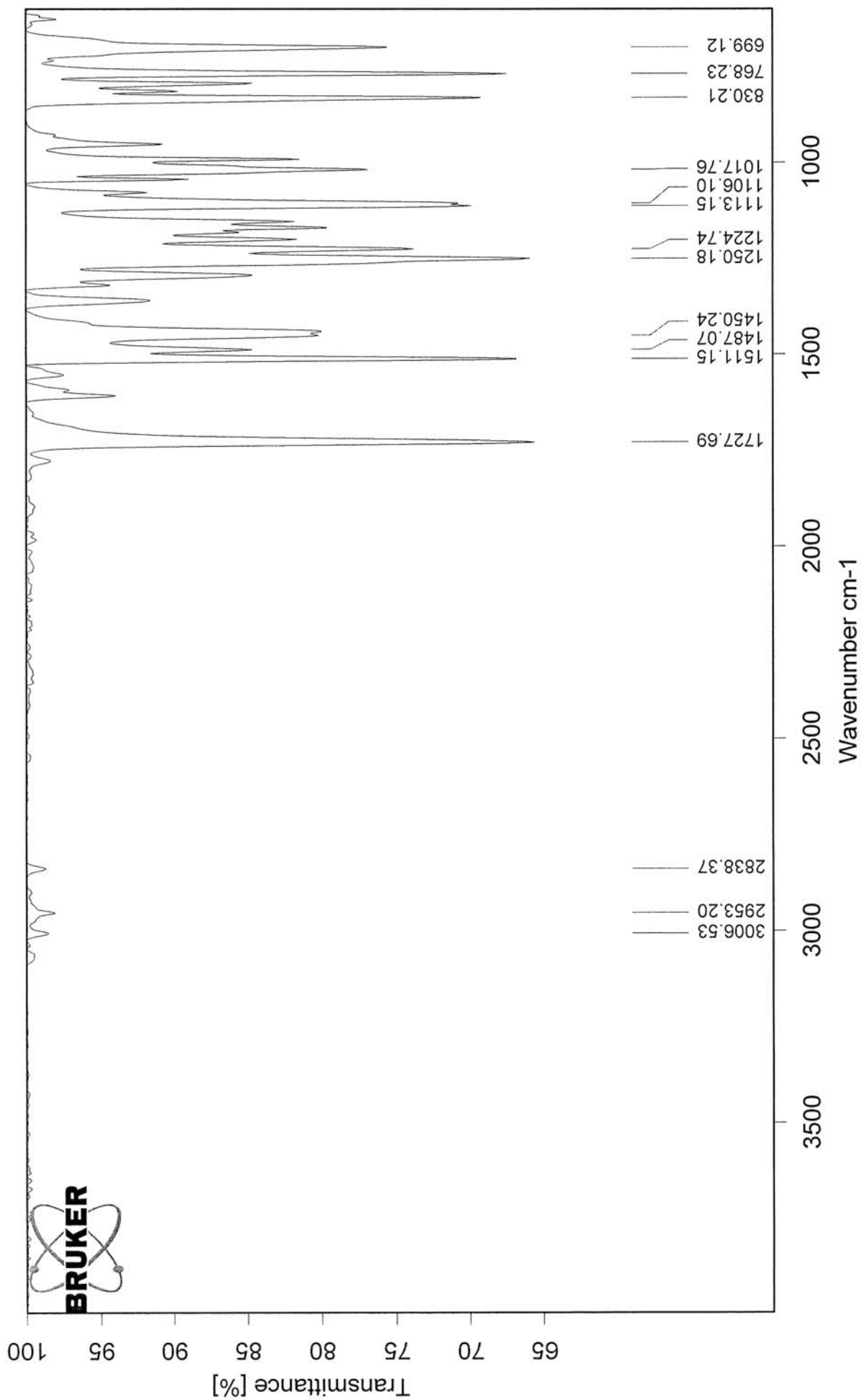












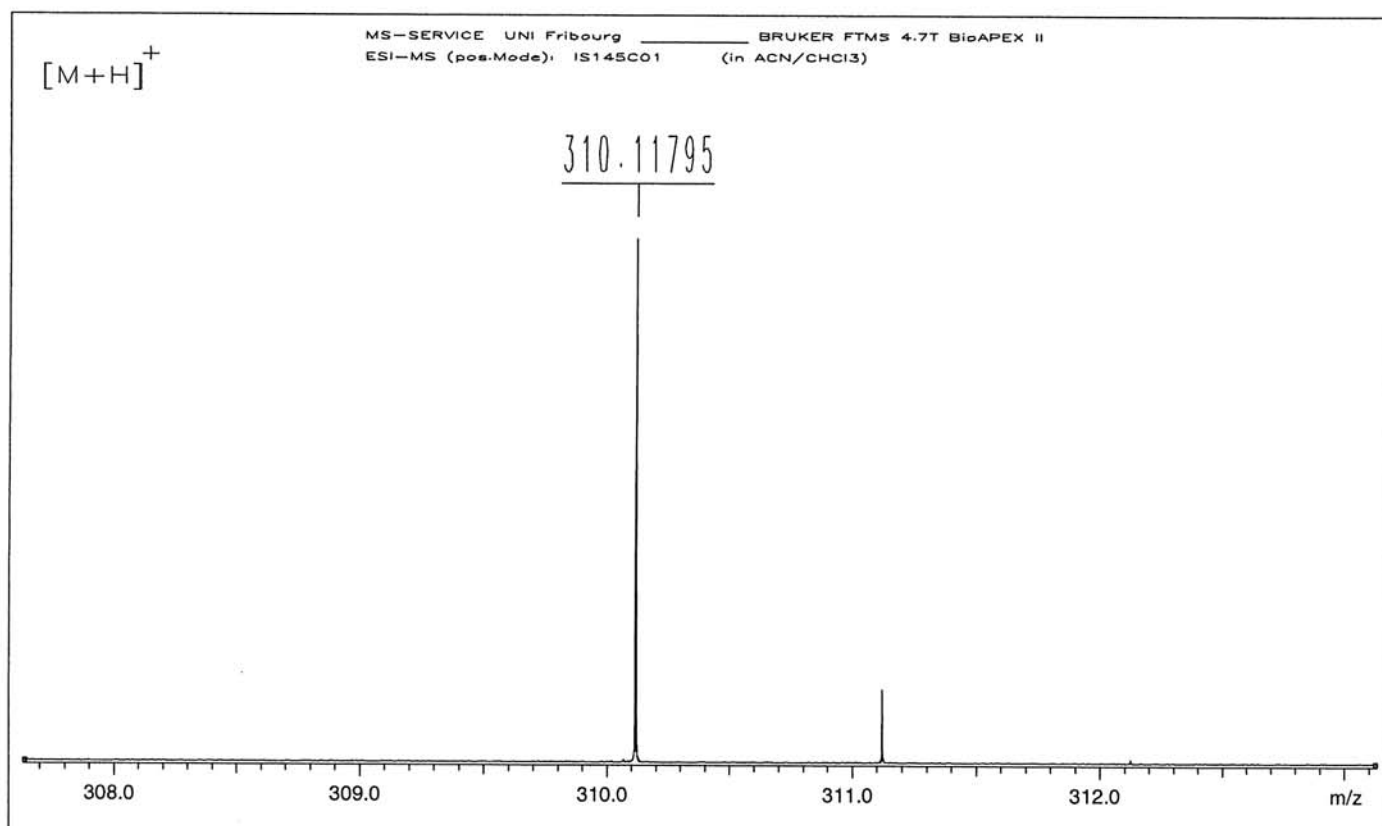
ESI-MS: IS145C01

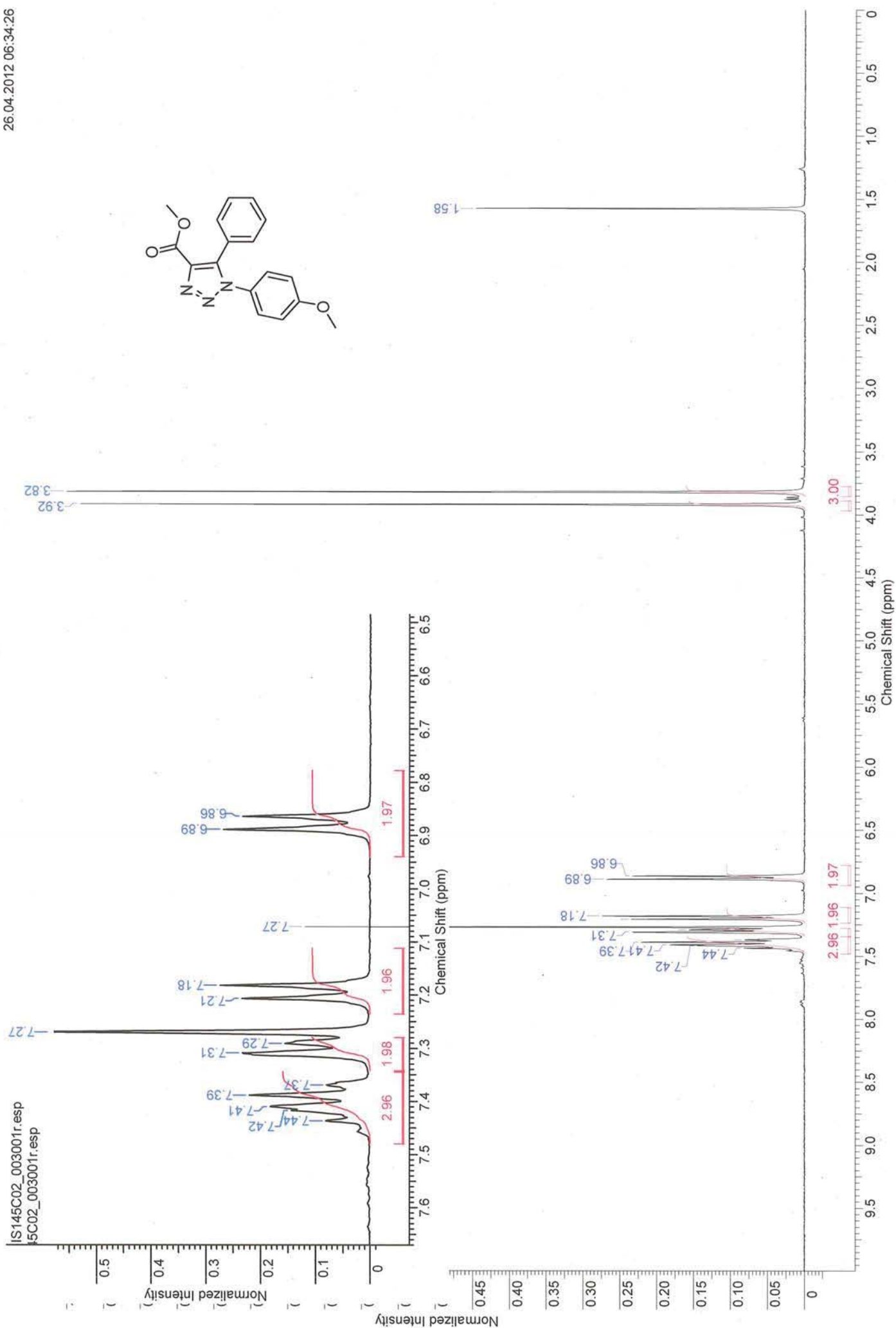
XMASS Mass Analysis for /Data/UNI\_FR/ALIM5267\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

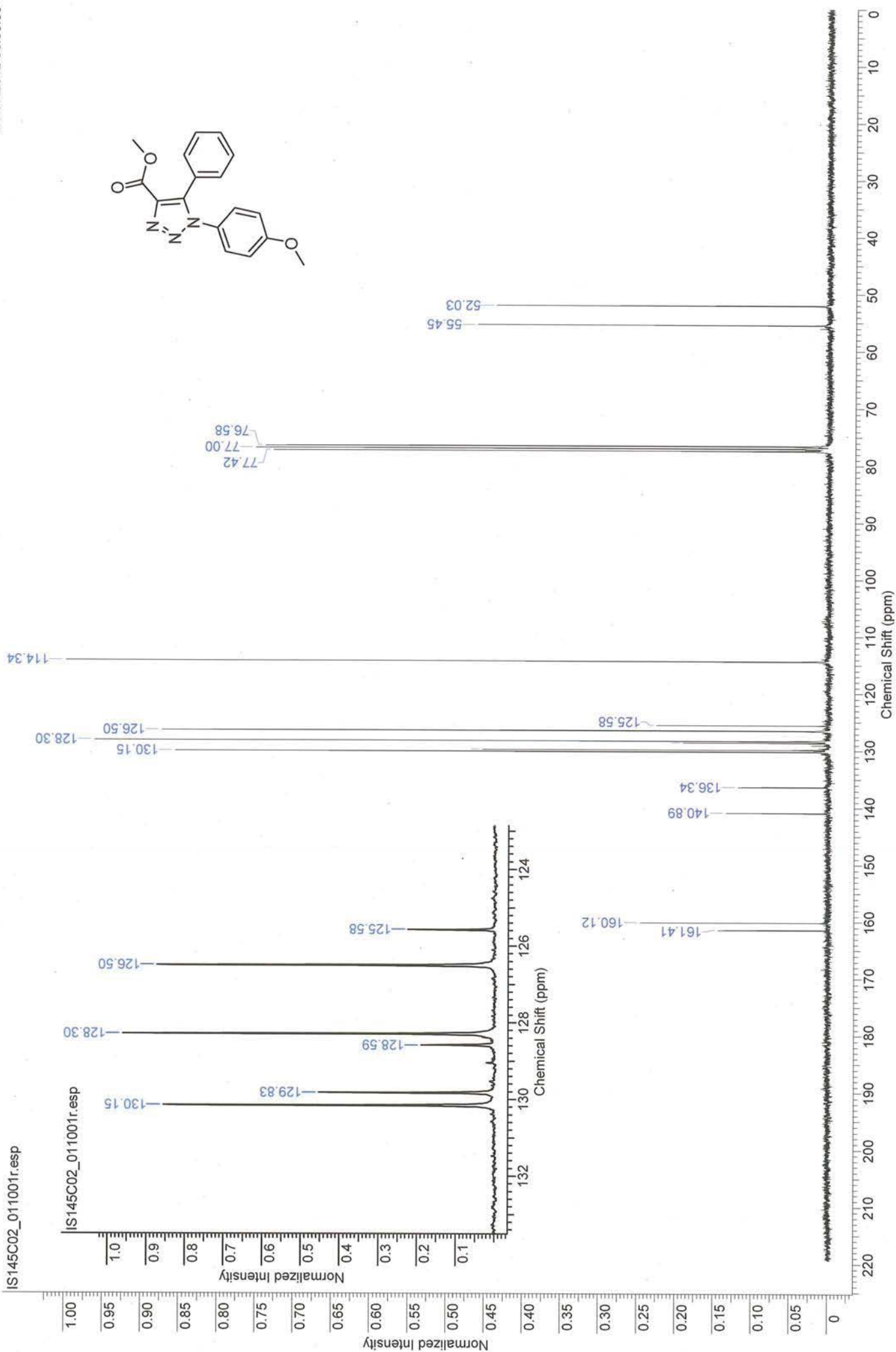
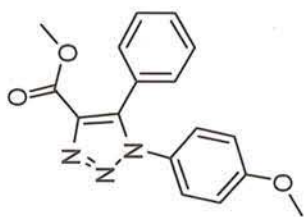
Ion mass = 310.1179500

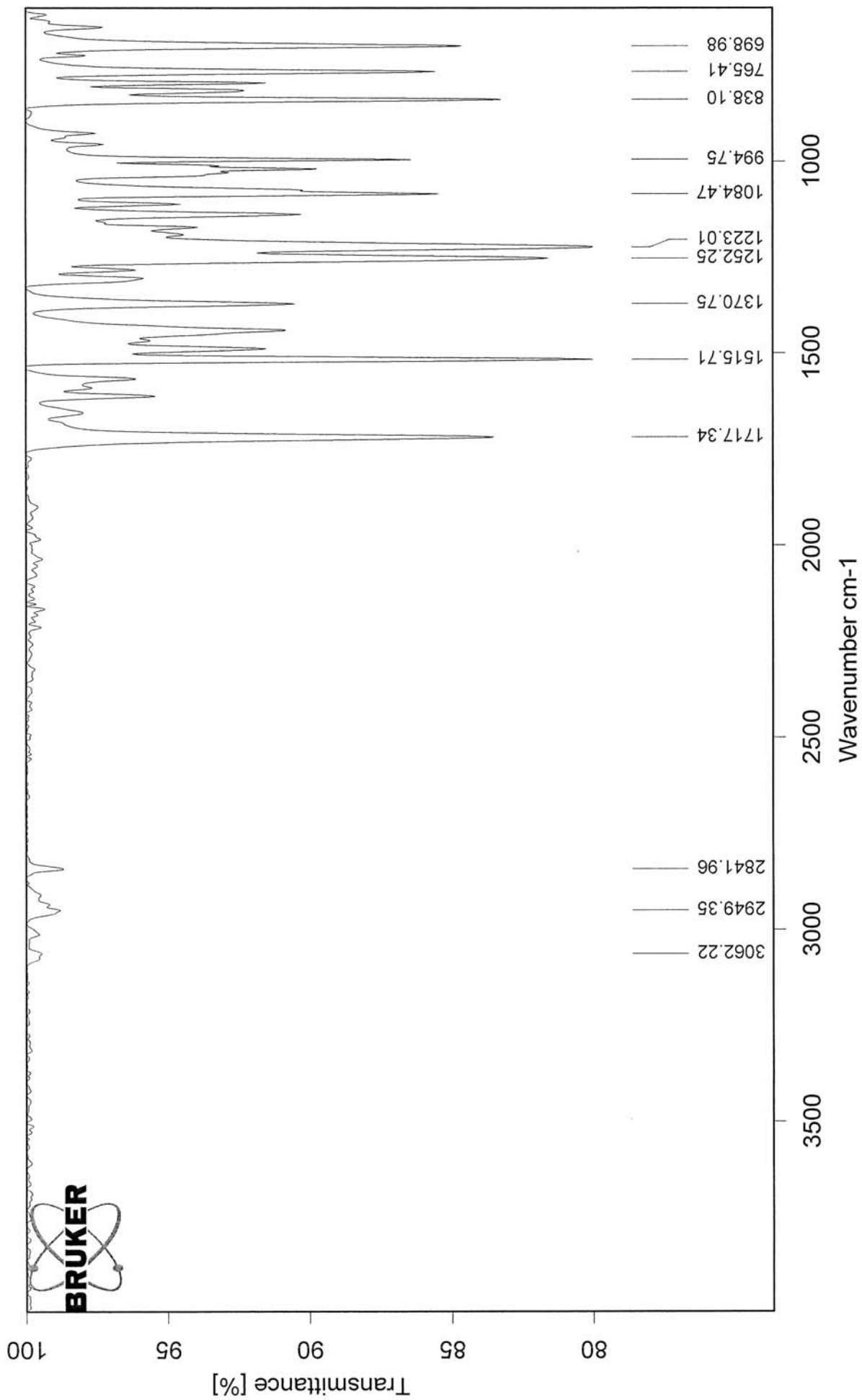
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 310.1179500								
1	17	16	3	3	0	310.1186178	11.5	6.678e-04
2	15	17	3	3	1	310.1162125	8.5	1.737e-03
3	14	18	2	6	0	310.1159377	7.0	2.012e-03
4	20	17	1	1	1	310.1202353	12.5	2.285e-03
5	8	21	3	8	1	310.1220858	-0.5	4.136e-03
6	12	19	2	6	1	310.1135324	4.0	4.418e-03
7	22	16	1	1	0	310.1226406	15.5	4.691e-03
8	11	20	1	9	0	310.1132577	2.5	4.692e-03
9	9	18	4	8	0	310.1119150	3.0	6.035e-03
10	10	20	3	8	0	310.1244911	2.5	6.541e-03











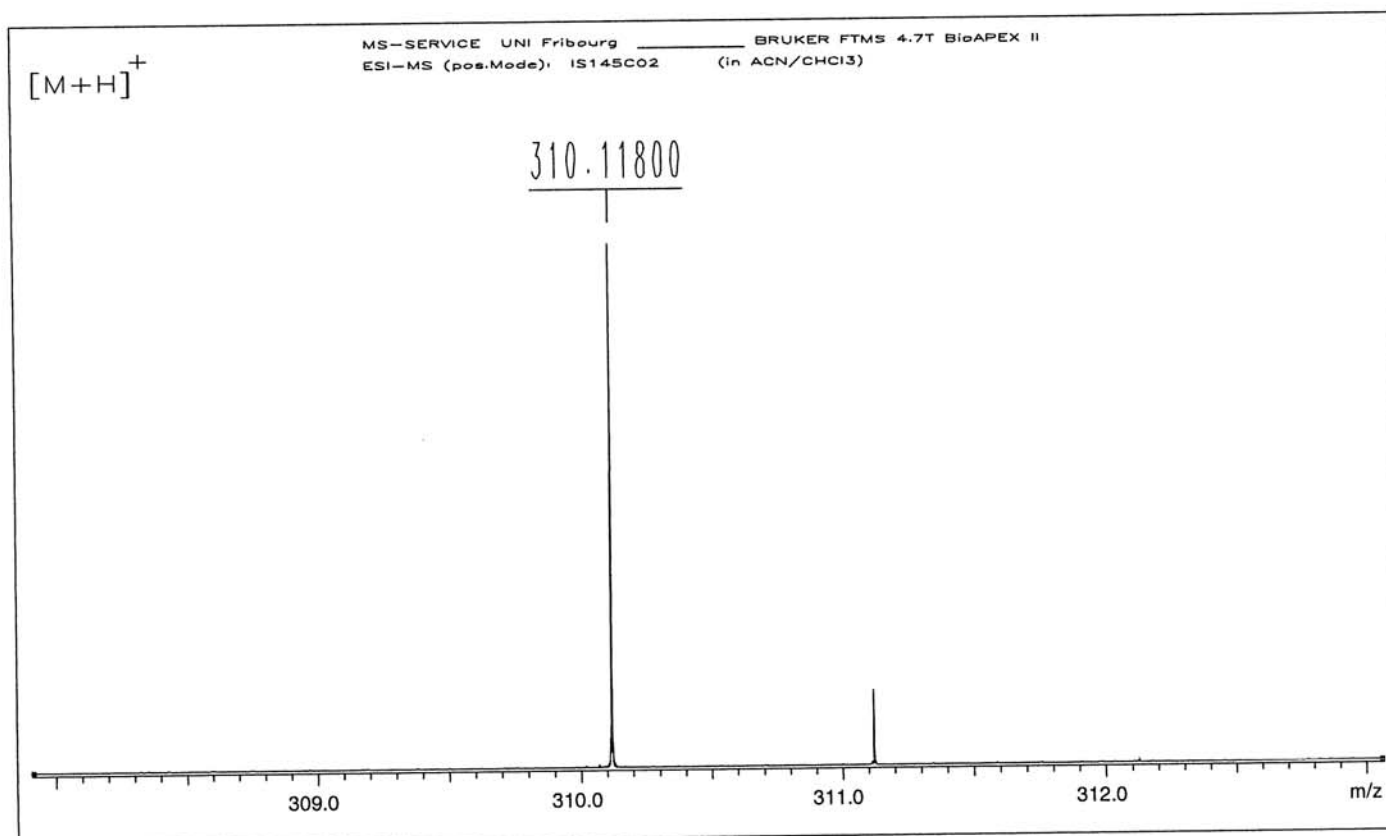
ESI-MS: IS145C02

XMASS Mass Analysis for /Data/UNI\_FR/ALIM5265\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

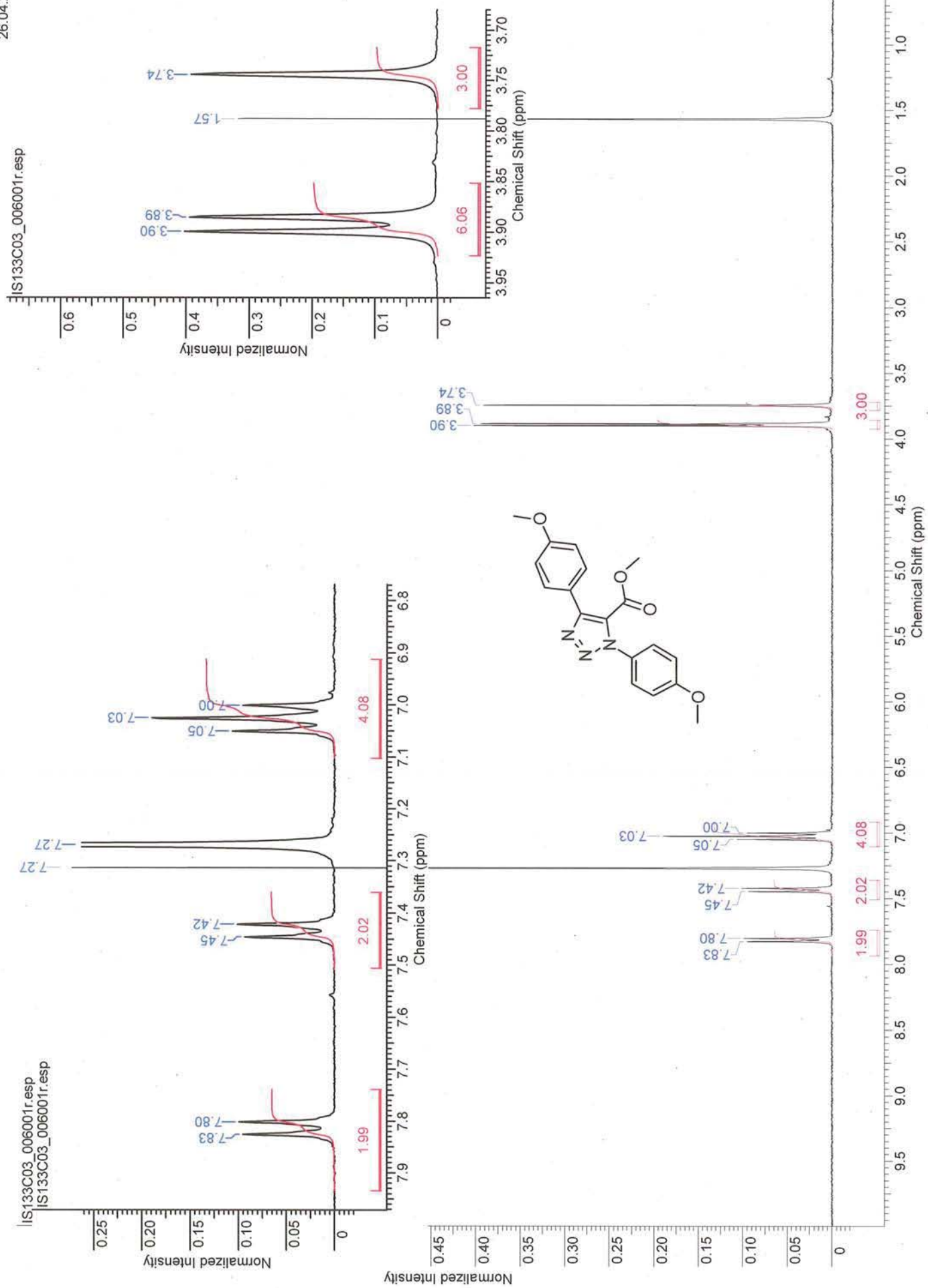
Ion mass = 310.1179980

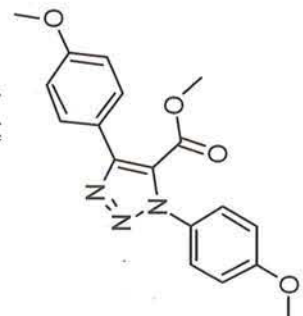
Charge = +1

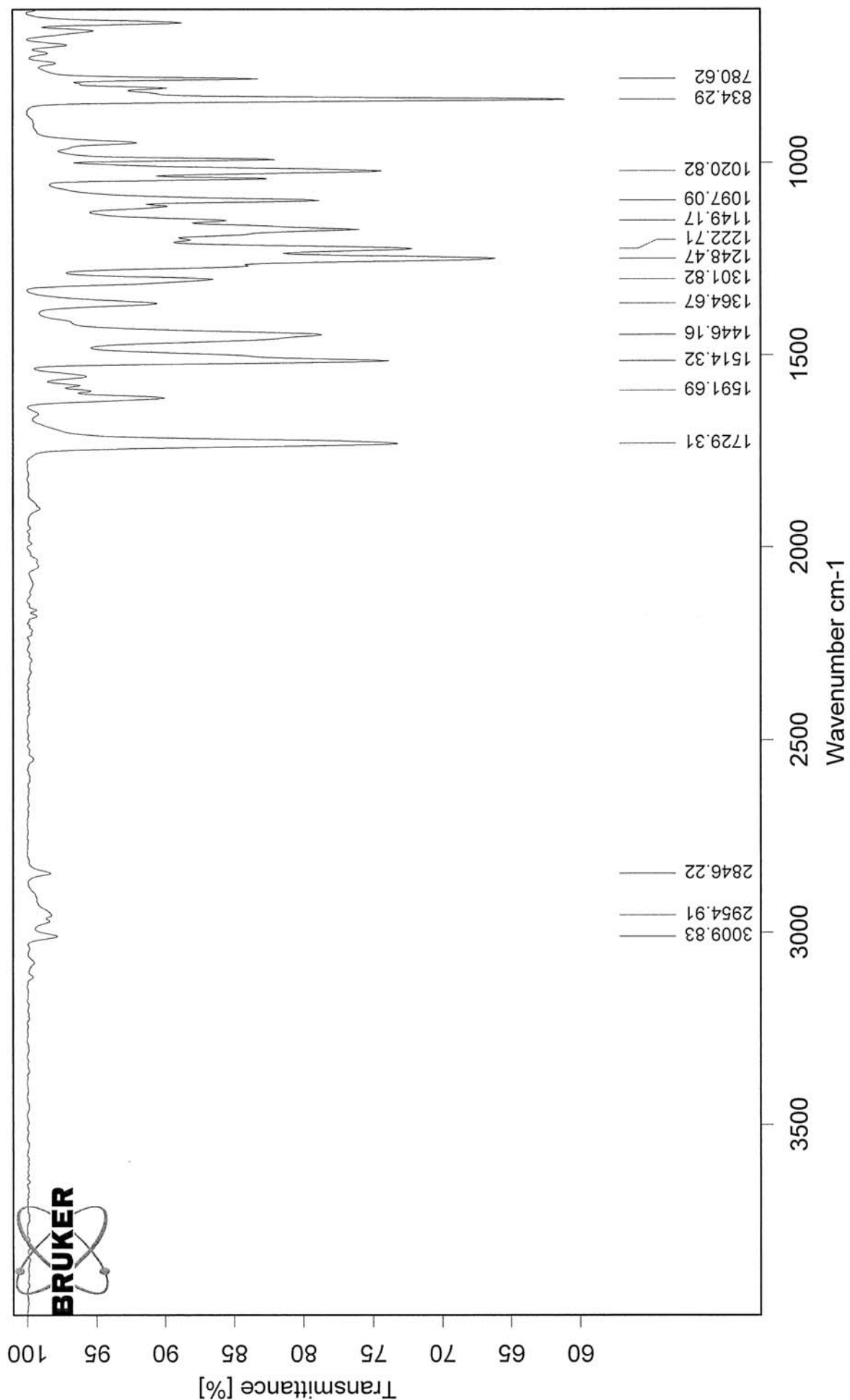
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 310.1179980								
1	17	16	3	3	0	310.1186178	11.5	6.198e-04
2	15	14	6	2	0	310.1172751	12.0	7.229e-04
3	15	17	3	3	1	310.1162125	8.5	1.785e-03
4	14	18	2	6	0	310.1159377	7.0	2.060e-03
5	13	12	9	1	0	310.1159325	12.5	2.066e-03
6	20	17	1	1	1	310.1202353	12.5	2.237e-03
7	5	20	5	10	0	310.1204683	-1.5	2.470e-03
8	6	19	6	7	1	310.1207431	0.0	2.745e-03
9	13	15	6	2	1	310.1148698	9.0	3.128e-03
10	12	16	5	5	0	310.1145951	7.5	3.403e-03











ESI-MS: IS133C03

XMASS Mass Analysis for /Data/UNI\_FR/ALIM5246\_ESI/5/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

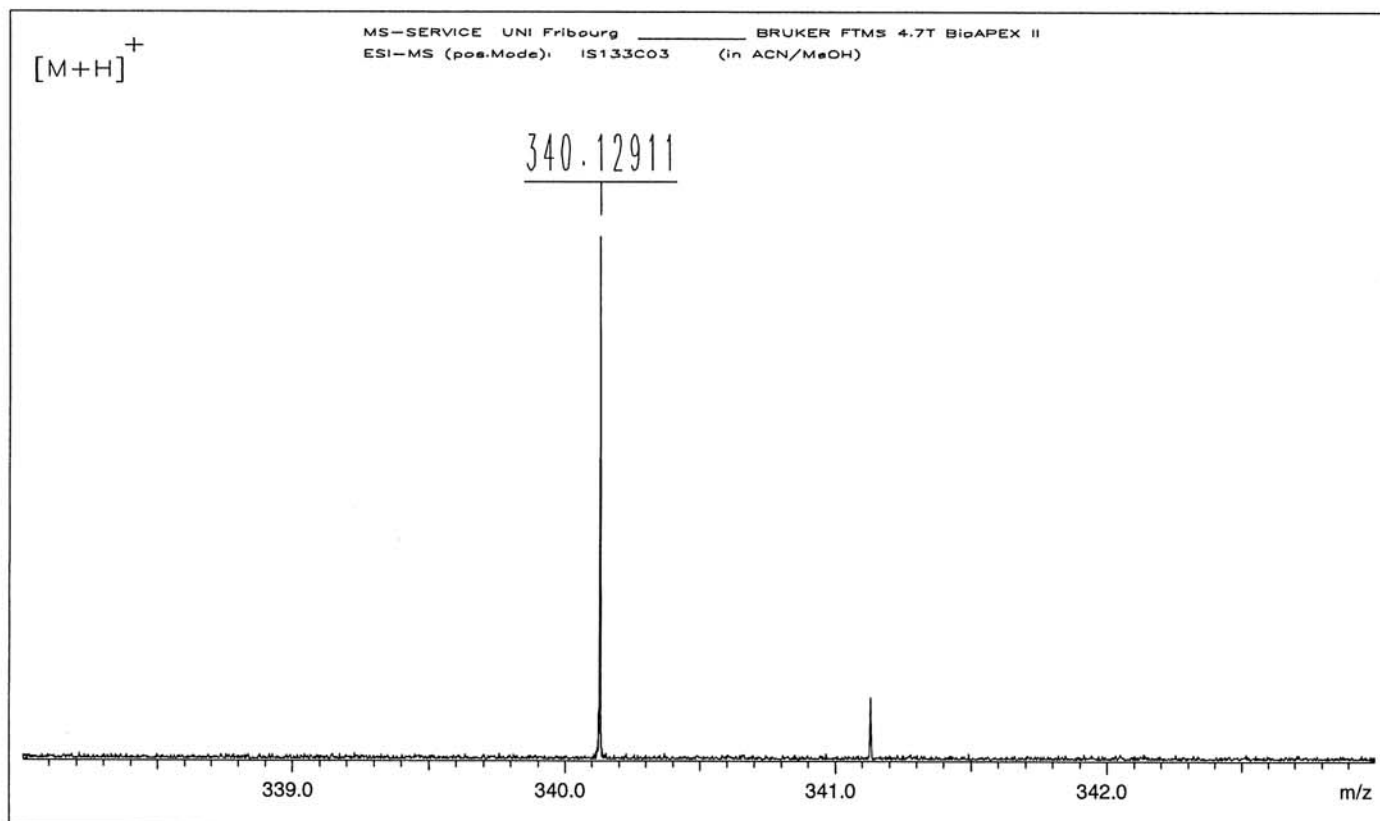
Ion mass = 340.1291080

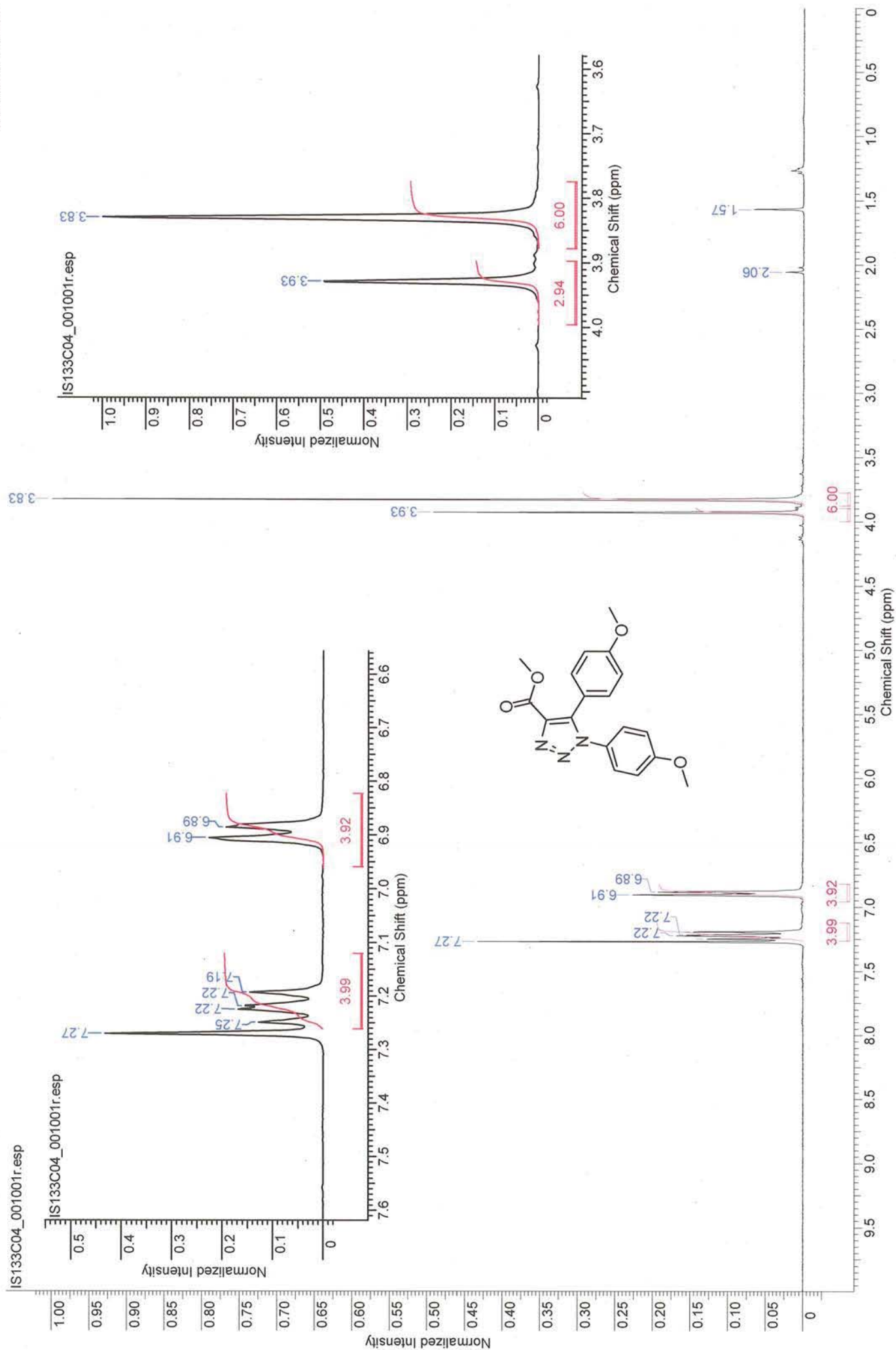
Charge = +1

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

\*\*\* Mass Analysis for mass 340.1291080

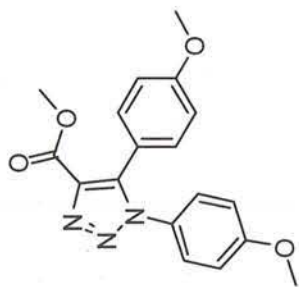
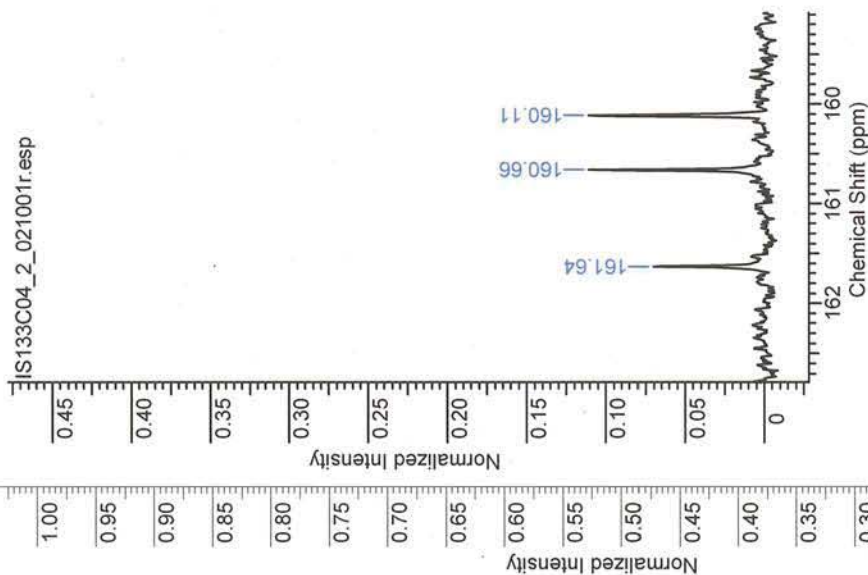
1	18	18	3	4	340.1291825	11.5	7.450e-05
2	16	16	6	3	340.1278398	12.0	1.268e-03
3	15	20	2	7	340.1265024	7.0	2.606e-03
4	14	14	9	2	340.1264972	12.5	2.611e-03
5	21	16	4	1	340.1318626	16.0	2.755e-03
6	7	18	9	7	340.1323704	3.5	3.262e-03
7	13	18	5	6	340.1251598	7.5	3.948e-03
8	23	18	1	2	340.1332052	15.5	4.097e-03
9	9	20	6	8	340.1337131	3.0	4.605e-03
10	12	22	1	10	340.1238224	2.5	5.286e-03



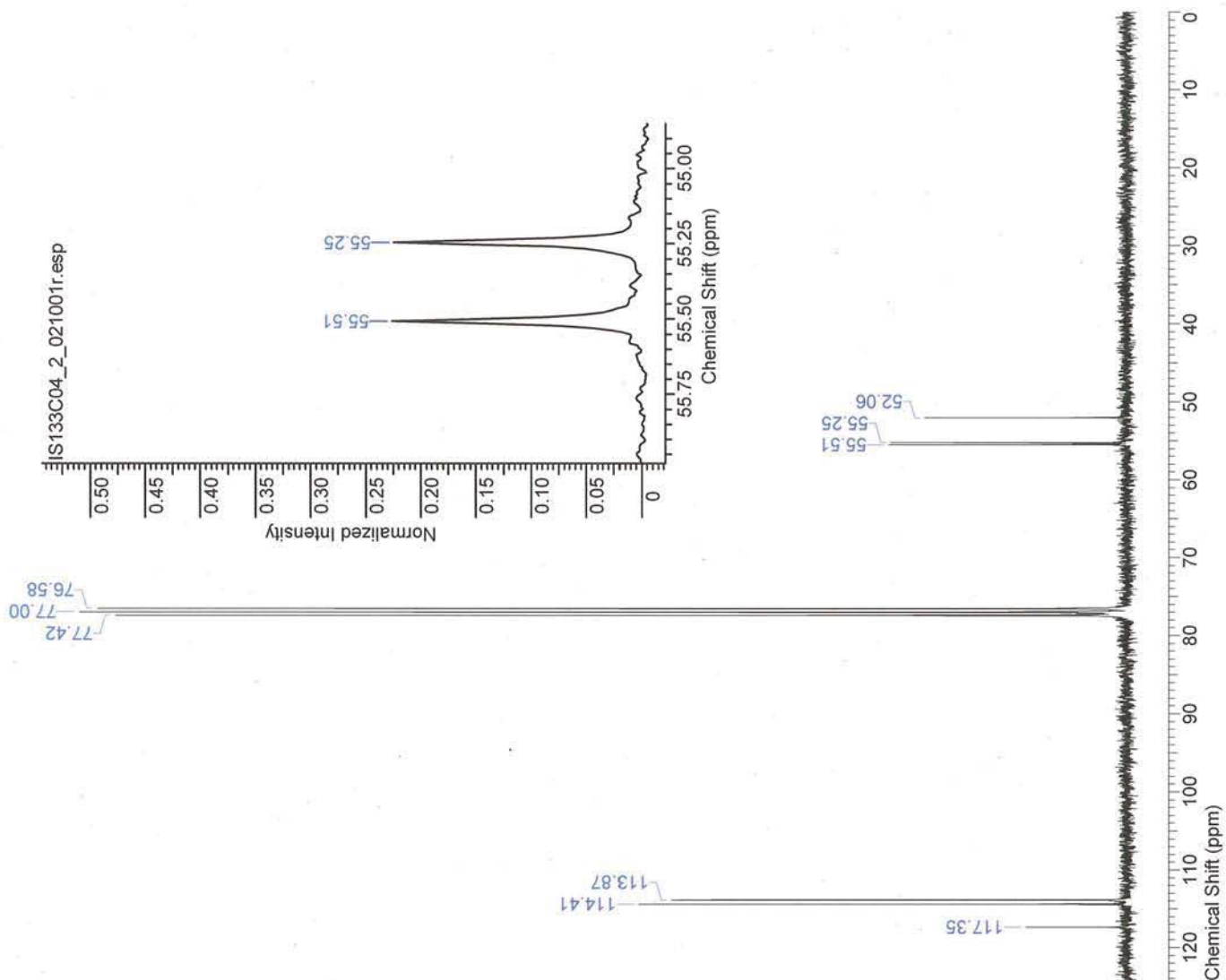




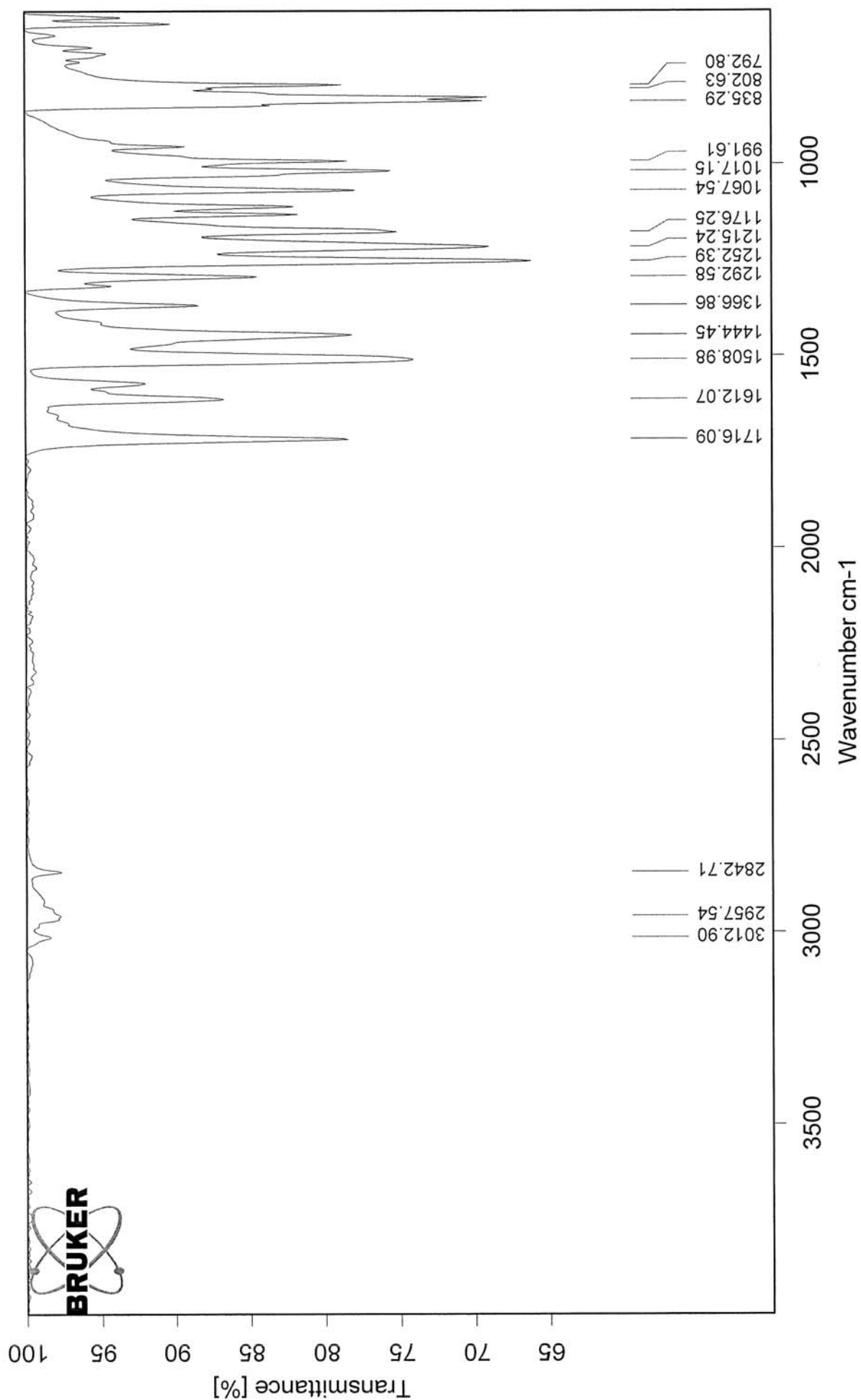
S133C04 2 021001r.esp



77.42  
—77.00  
76.58







ESI-MS: IS133C04

XMASS Mass Analysis for /Data/UNI\_FR/ALIM5244\_ESI/5/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

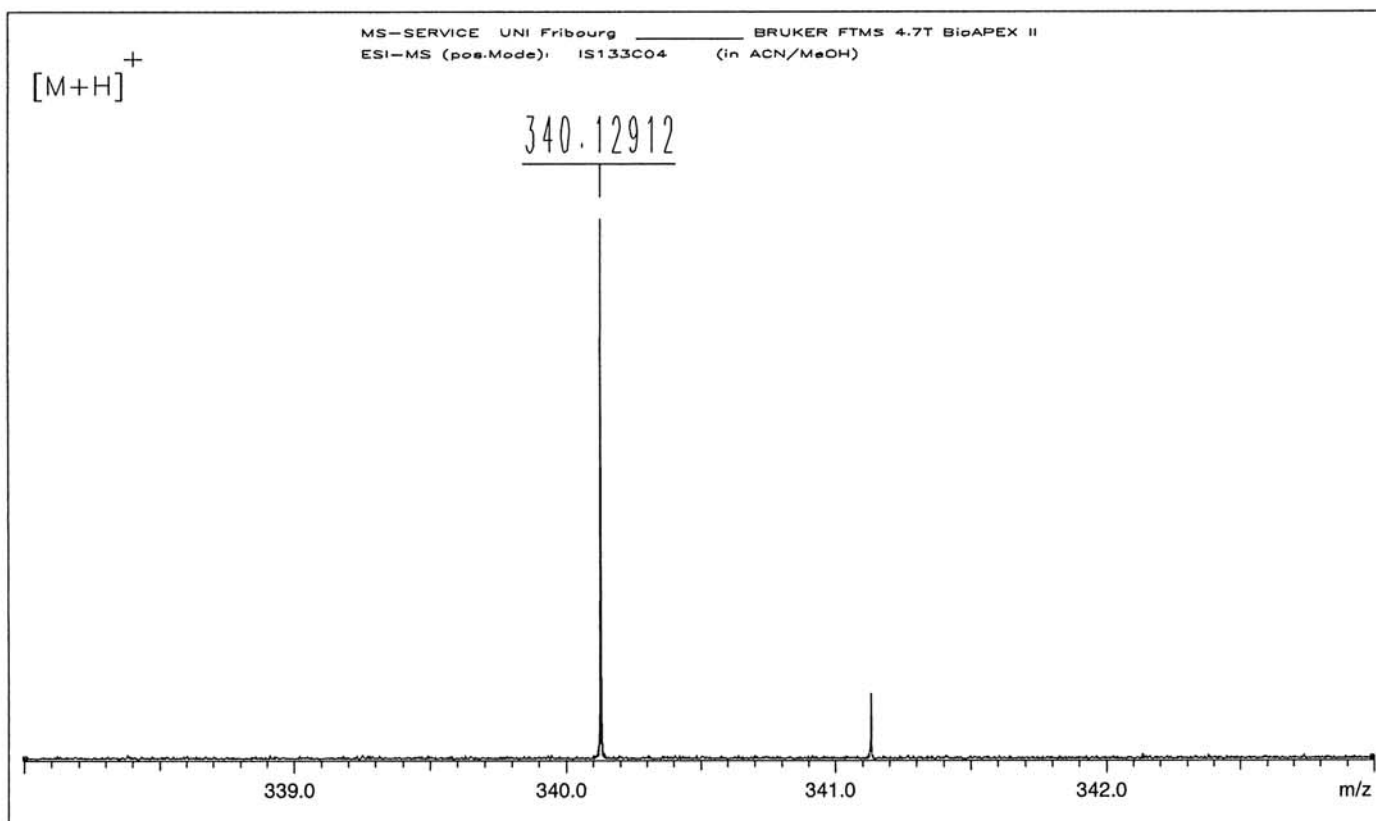
Ion mass = 340.1291160

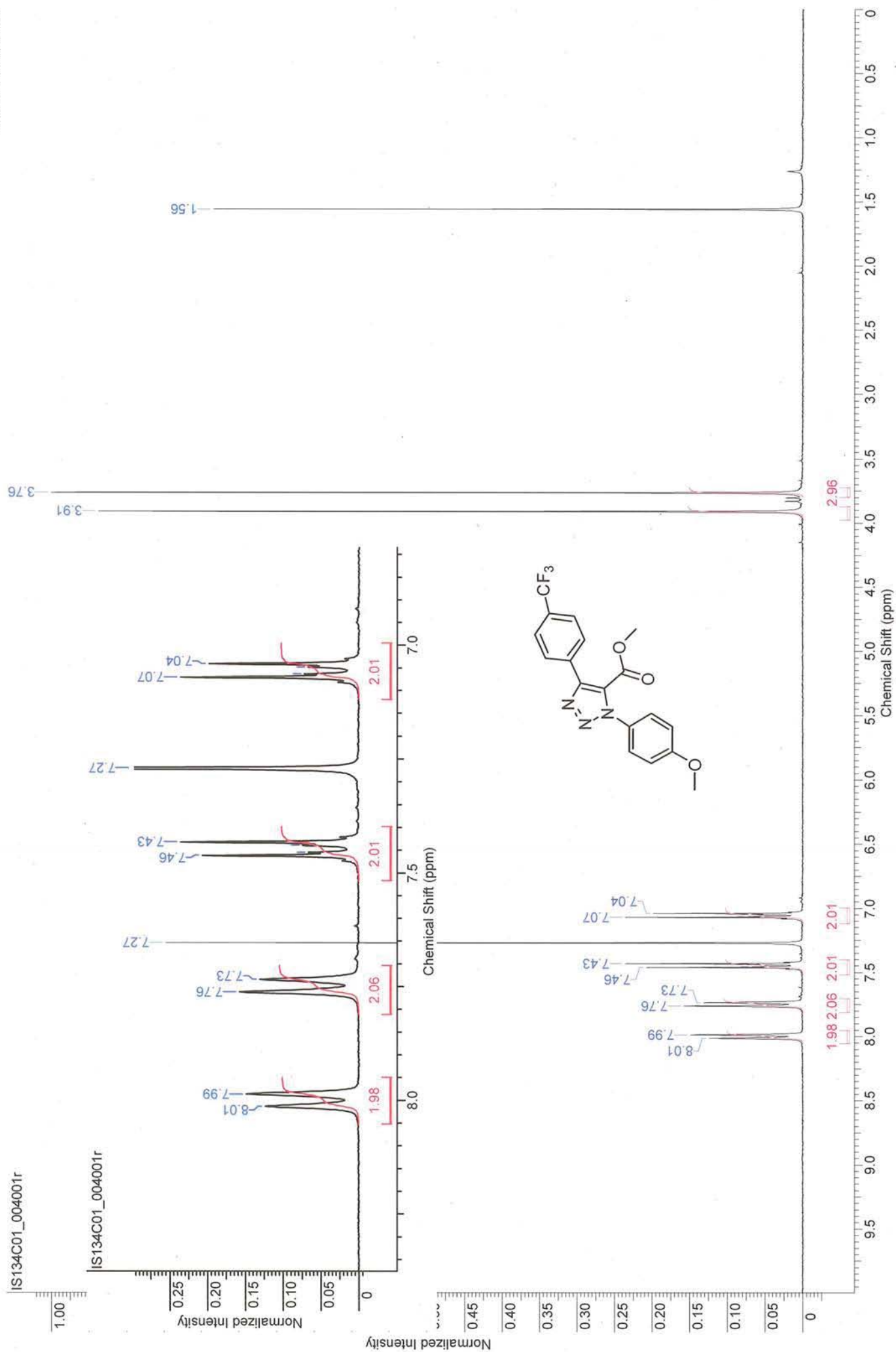
Charge = +1

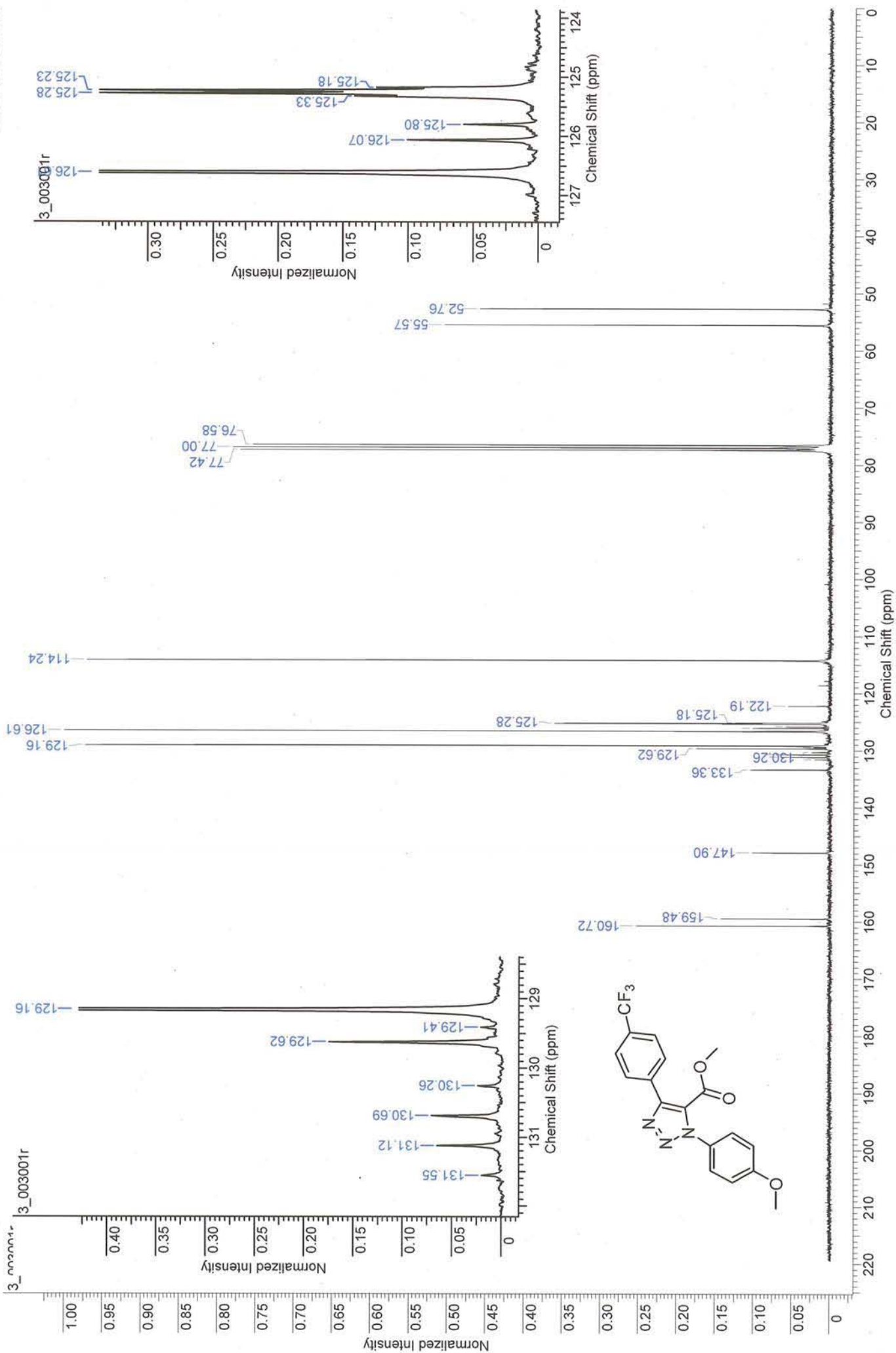
#	C	H	N	O	mass	DBE	error
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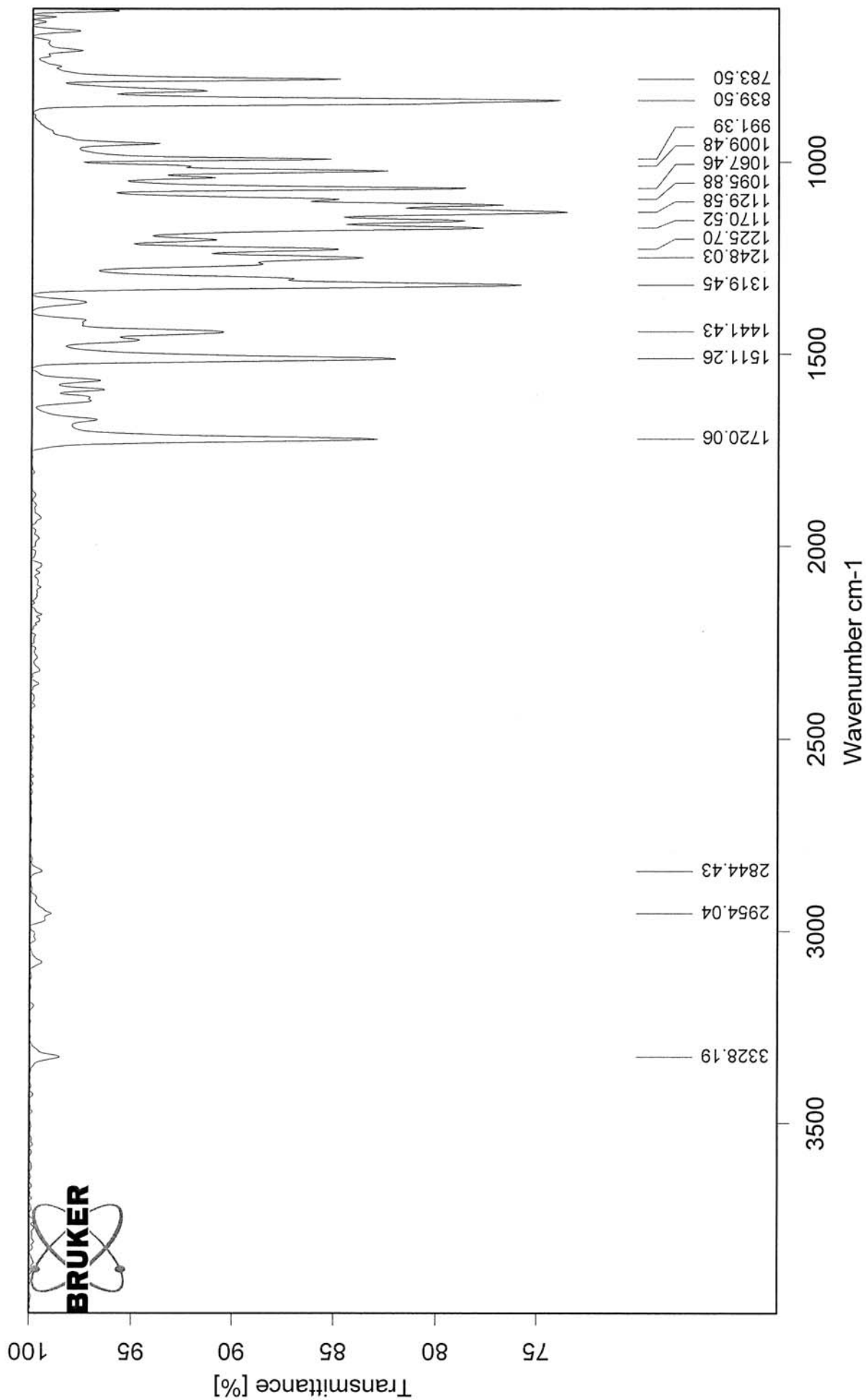
\*\*\* Mass Analysis for mass 340.1291160

1	18	18	3	4	340.1291825	11.5	6.650e-05
2	16	16	6	3	340.1278398	12.0	1.276e-03
3	15	20	2	7	340.1265024	7.0	2.614e-03
4	14	14	9	2	340.1264972	12.5	2.619e-03
5	21	16	4	1	340.1318626	16.0	2.747e-03
6	7	18	9	7	340.1323704	3.5	3.254e-03
7	13	18	5	6	340.1251598	7.5	3.956e-03
8	23	18	1	2	340.1332052	15.5	4.089e-03
9	9	20	6	8	340.1337131	3.0	4.597e-03
10	12	22	1	10	340.1238224	2.5	5.294e-03









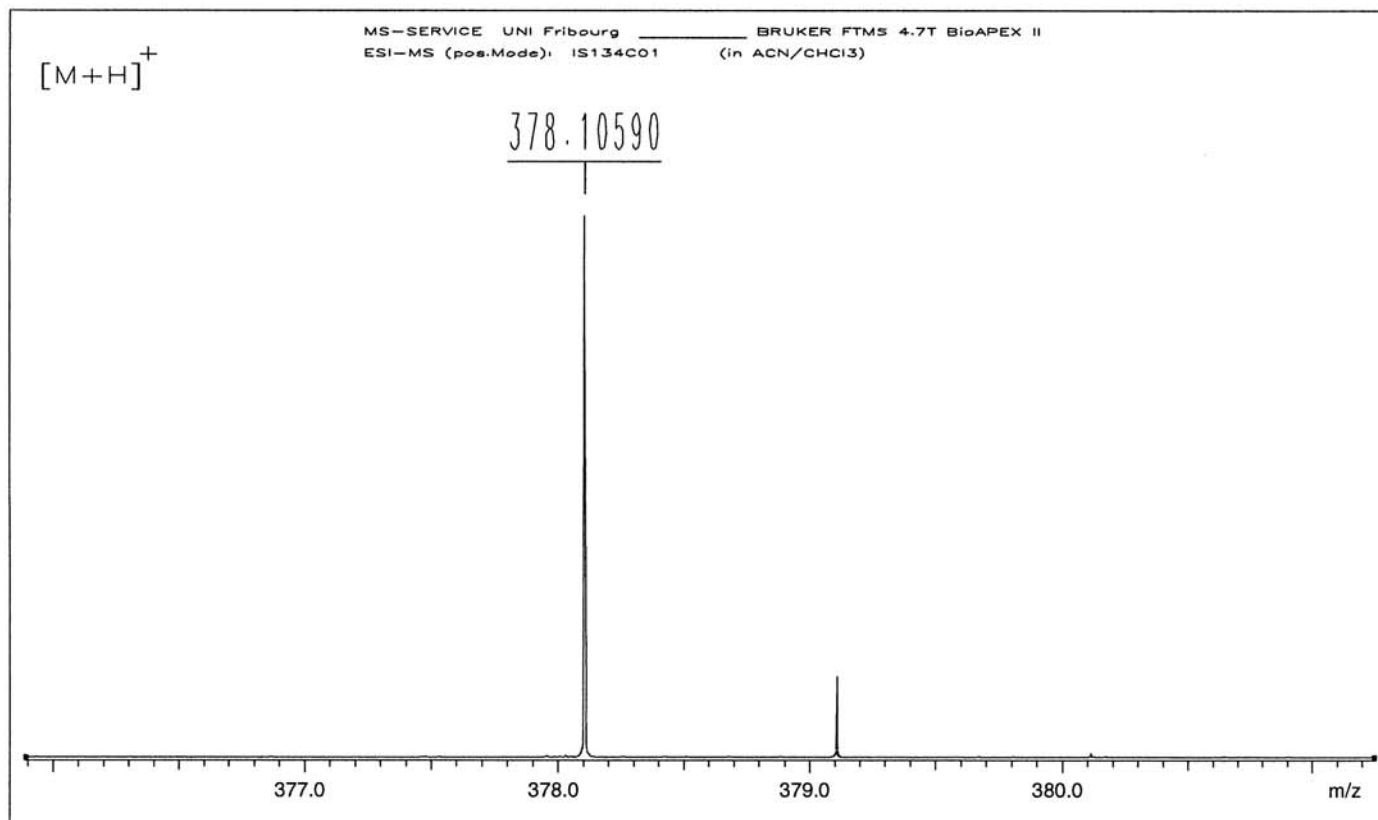
ESI-MS: IS134C01

XMASS Mass Analysis for /Data/UNI\_FR/ALIM5264\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

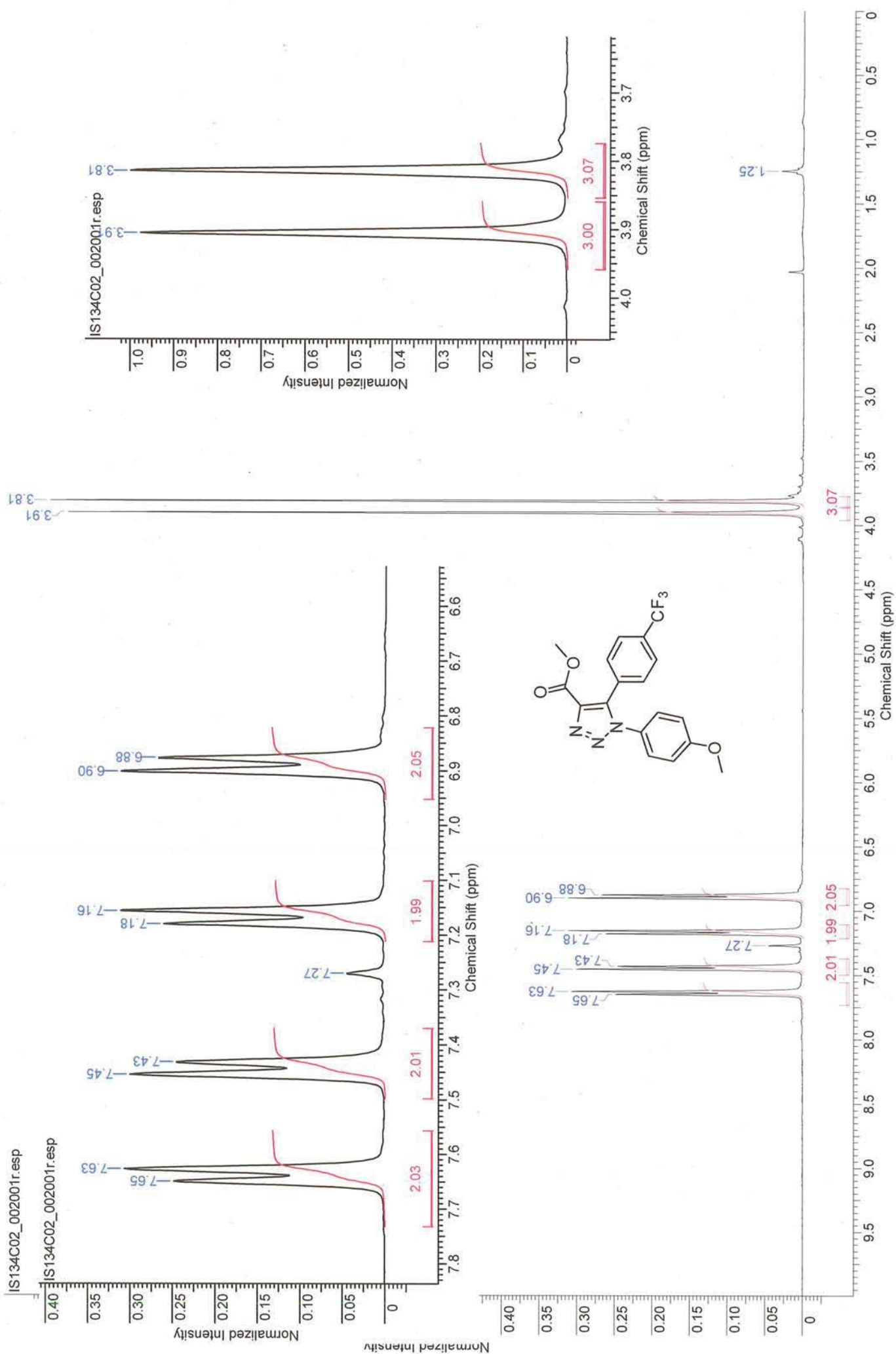
Ion mass = 378.1058990

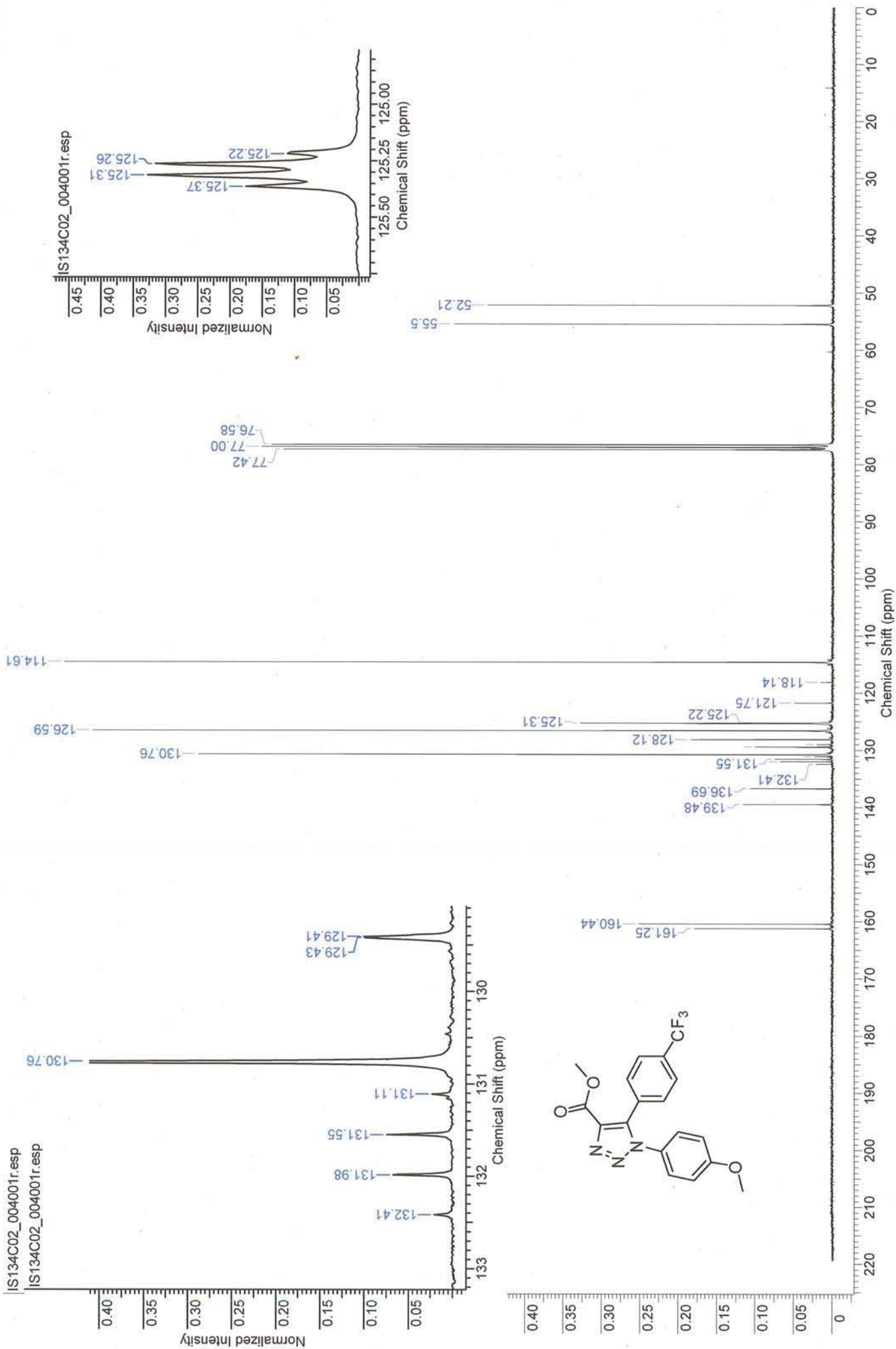
Charge = +1

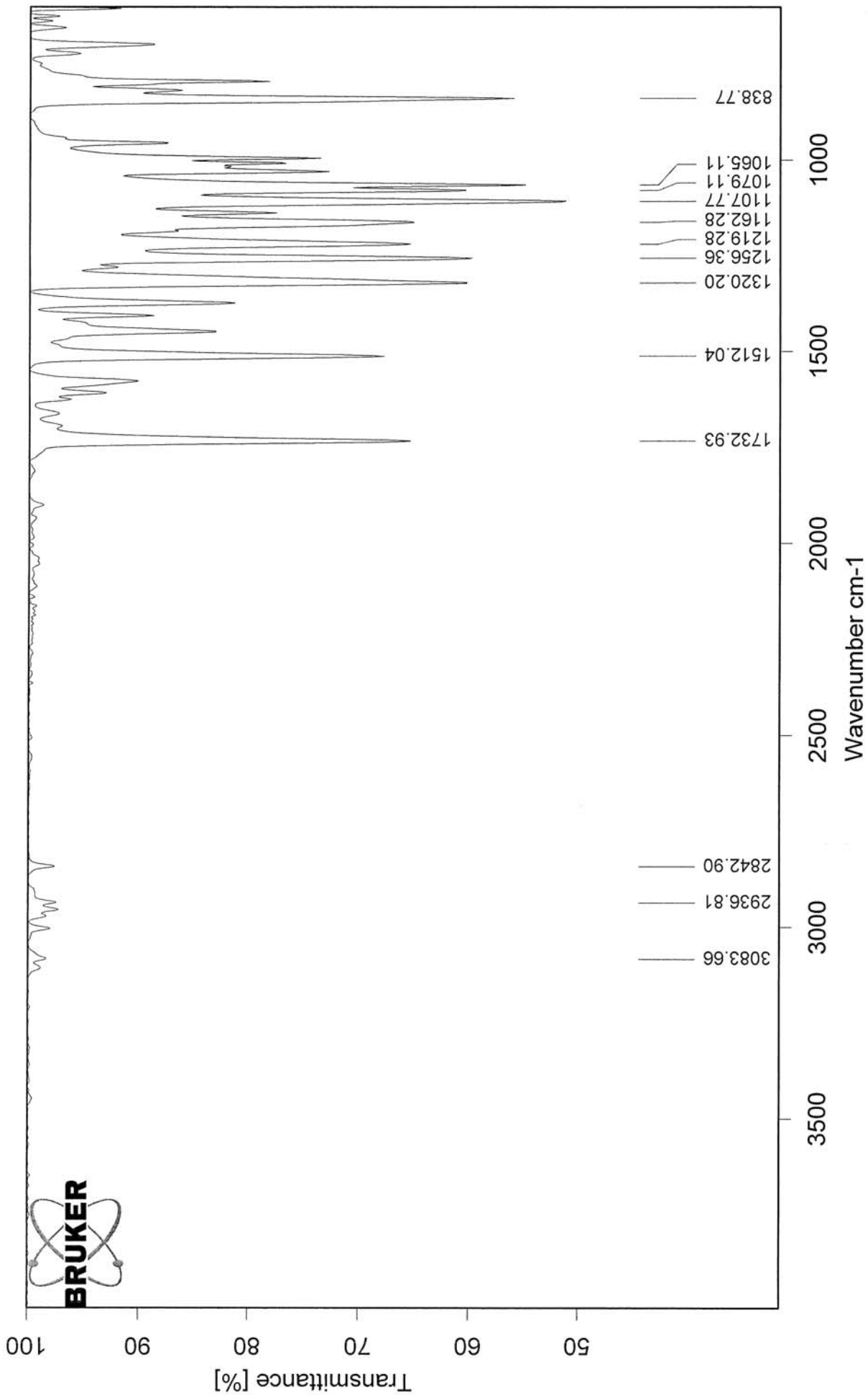
#	C	H	N	F	O	Na	mass	DBE	error
*** Mass Analysis for mass 378.1058990									
1	18	15	3	3	3	0	378.1060024	11.5	1.034e-04
2	21	14	3	2	2	0	378.1048595	15.5	1.039e-03
3	13	17	3	4	4	1	378.1047399	4.5	1.159e-03
4	15	16	3	4	4	0	378.1071452	7.5	1.246e-03
5	16	15	4	4	1	1	378.1074200	9.0	1.521e-03
6	21	16	1	3	1	1	378.1076198	12.5	1.721e-03
7	24	13	3	1	1	0	378.1037167	19.5	2.182e-03
8	16	16	3	3	3	1	378.1035971	8.5	2.302e-03
9	16	14	3	6	1	0	378.1035577	8.5	2.341e-03
10	13	16	4	5	2	1	378.1085629	5.0	2.664e-03













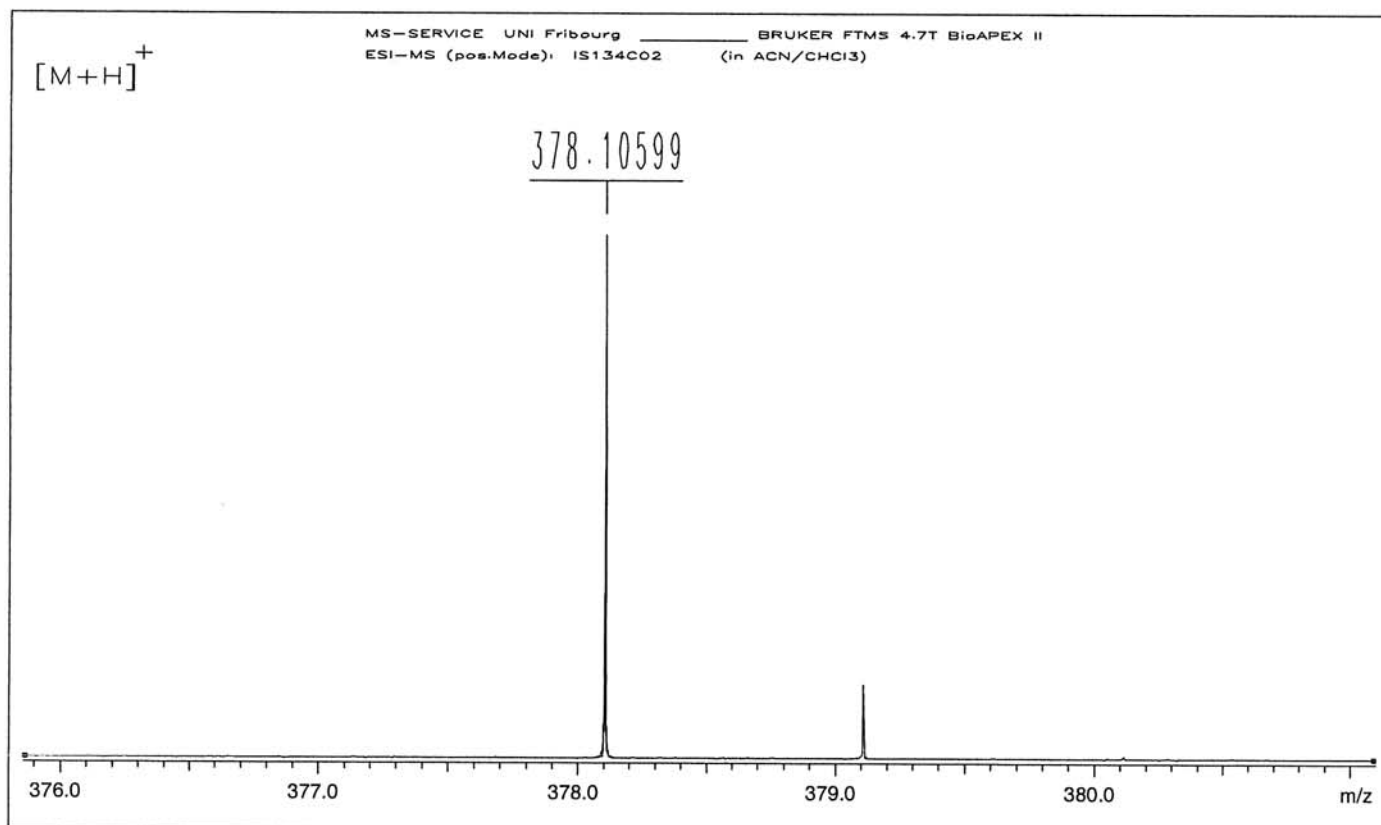
ESI-MS: IS134C02

XMASS Mass Analysis for /Data/UNI\_FR/ALIM5263\_ESI/5/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

Ion mass = 378.1059890

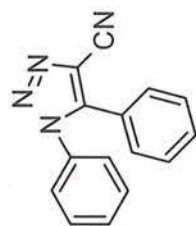
Charge = +1

#	C	H	N	F	O	Na	mass	DBE	error
*** Mass Analysis for mass 378.1059890									
1	18	15	3	3	3	0	378.1060024	11.5	1.338e-05
2	21	14	3	2	2	0	378.1048595	15.5	1.129e-03
3	15	16	3	4	4	0	378.1071452	7.5	1.156e-03
4	13	17	3	4	4	1	378.1047399	4.5	1.249e-03
5	16	15	4	4	1	1	378.1074200	9.0	1.431e-03
6	21	16	1	3	1	1	378.1076198	12.5	1.631e-03
7	24	13	3	1	1	0	378.1037167	19.5	2.272e-03
8	16	16	3	3	3	1	378.1035971	8.5	2.392e-03
9	16	14	3	6	1	0	378.1035577	8.5	2.431e-03
10	13	16	4	5	2	1	378.1085629	5.0	2.574e-03



IS341C02\_002001r

Normalized Intensity



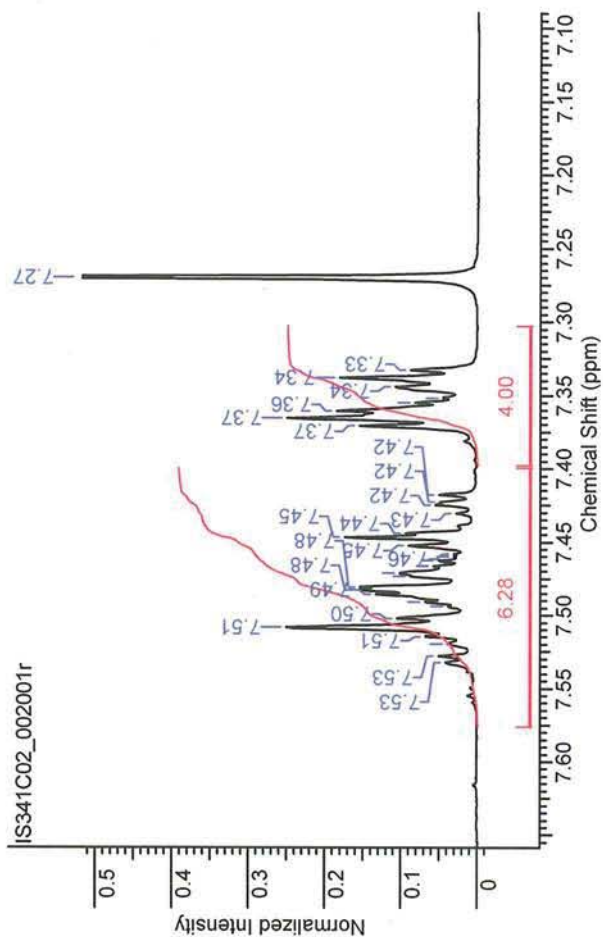
7.27

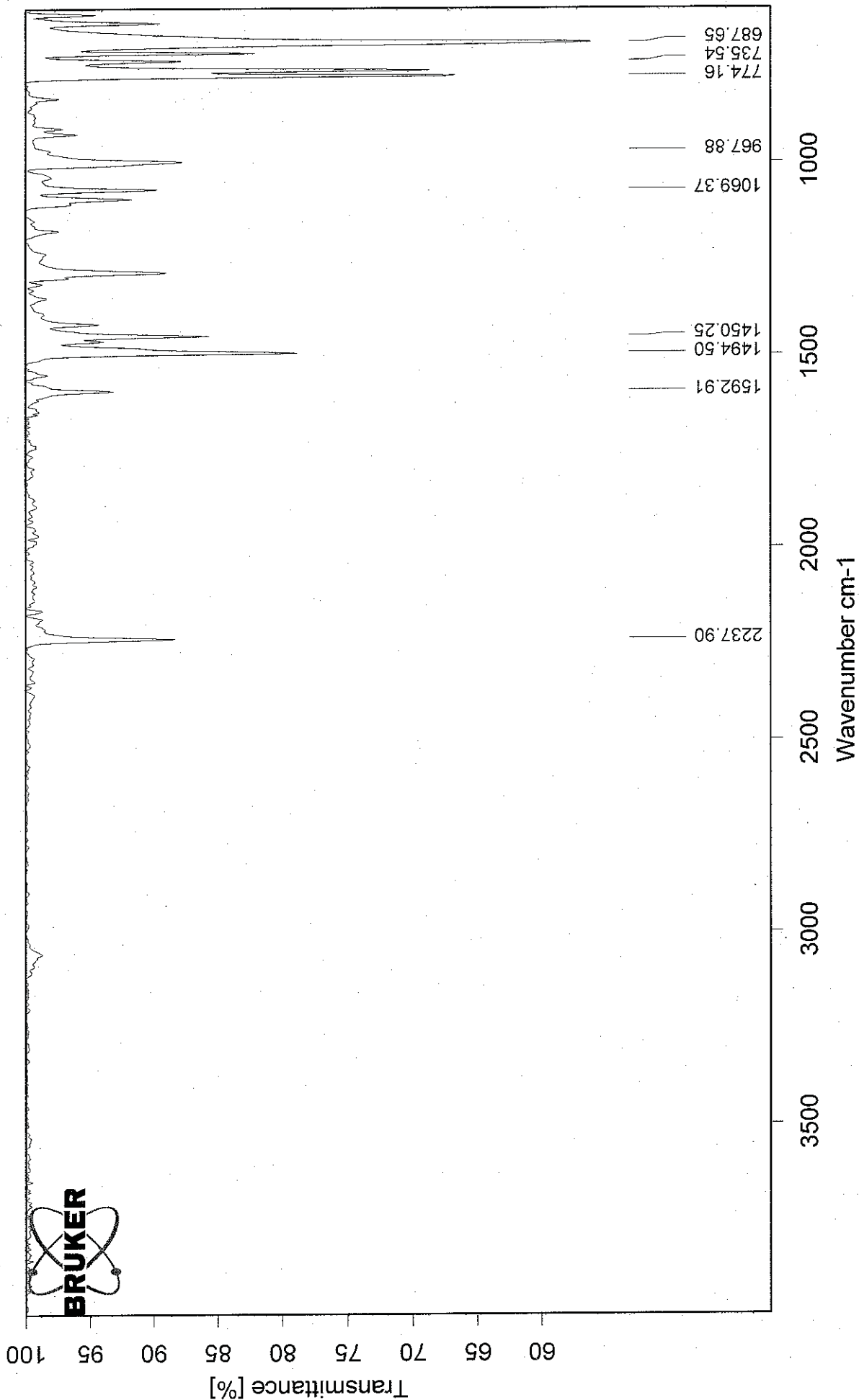
30.07.2012 08:29:20

1.57

IS341C02\_002001r

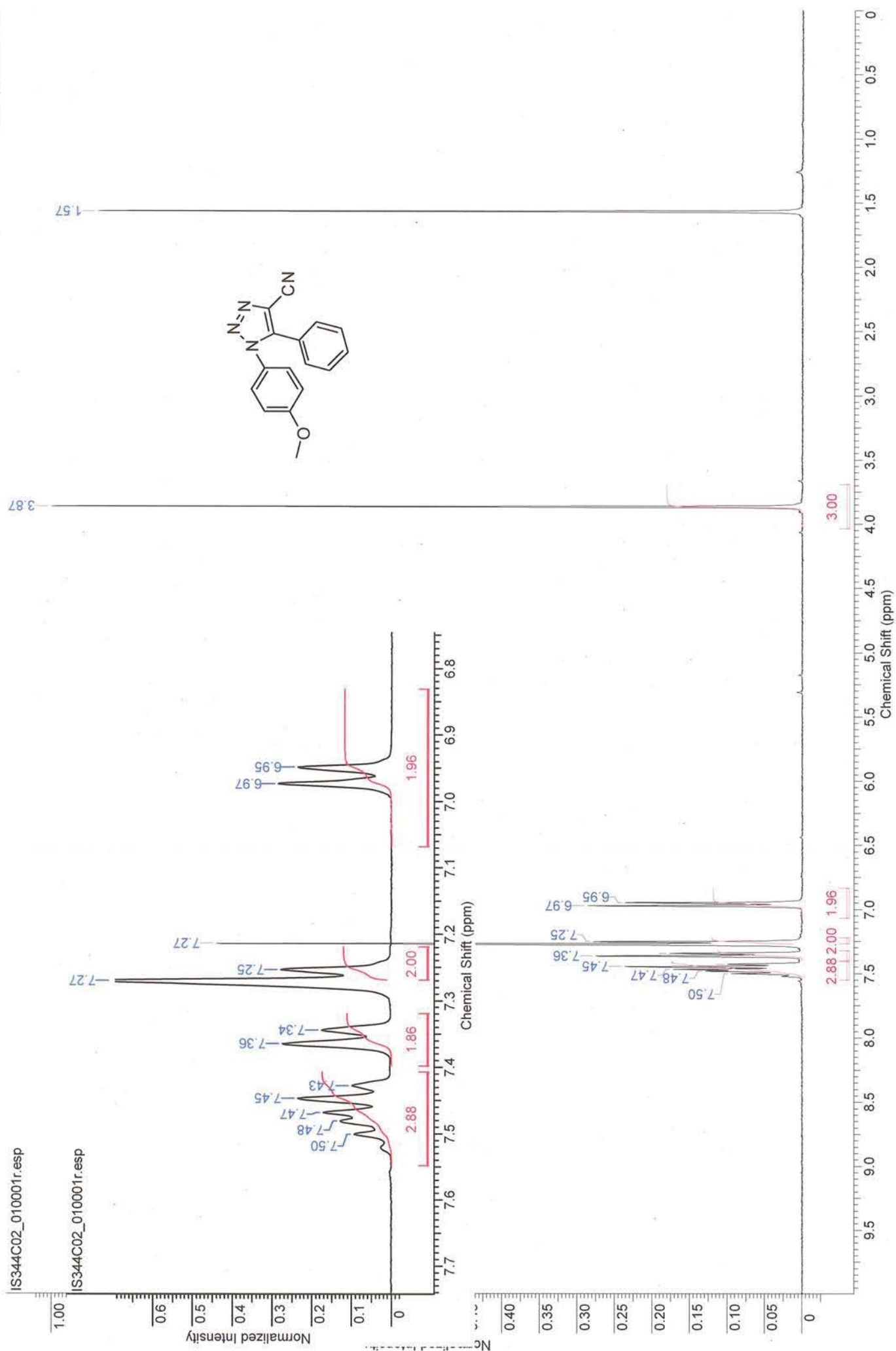
Normalized Intensity

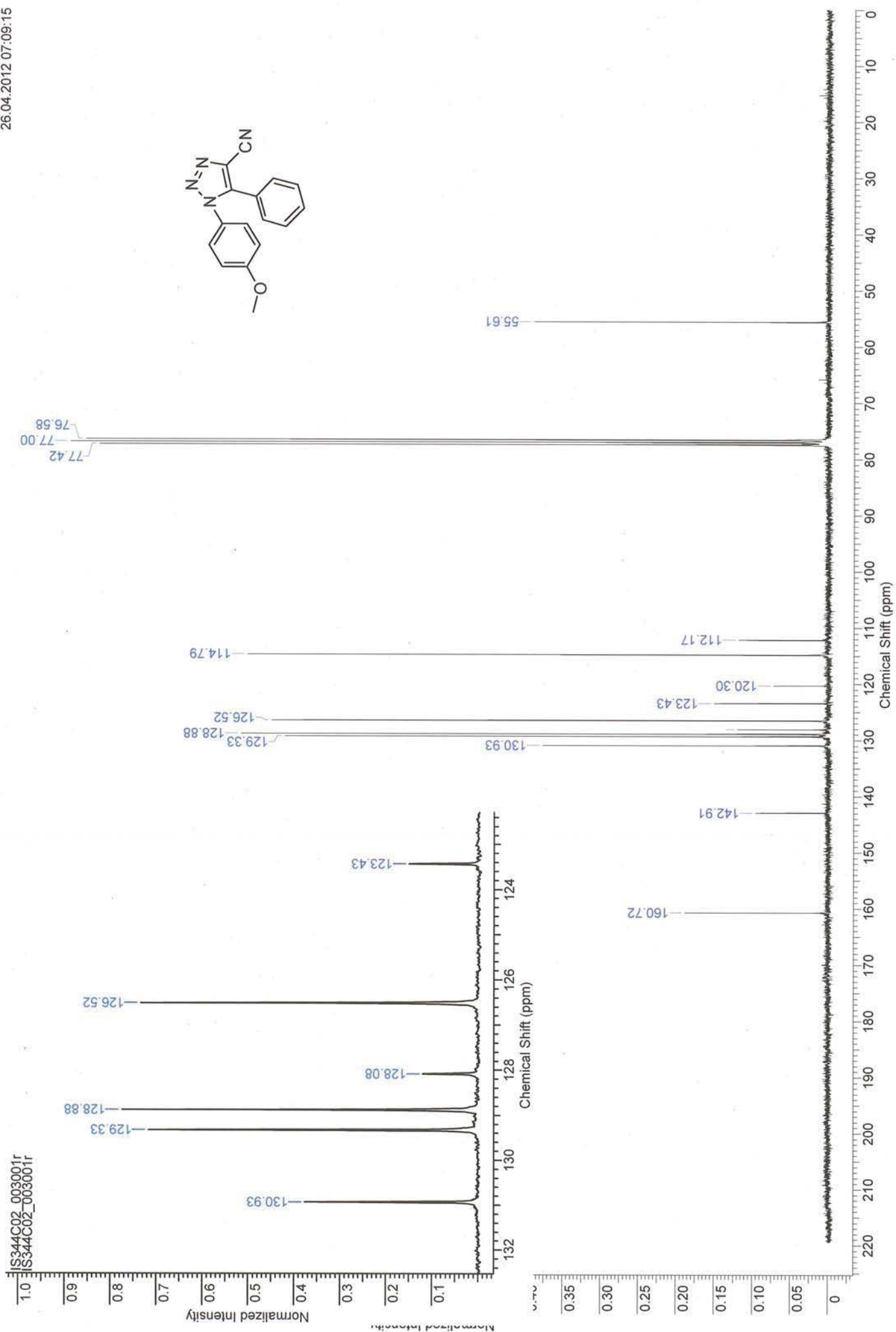


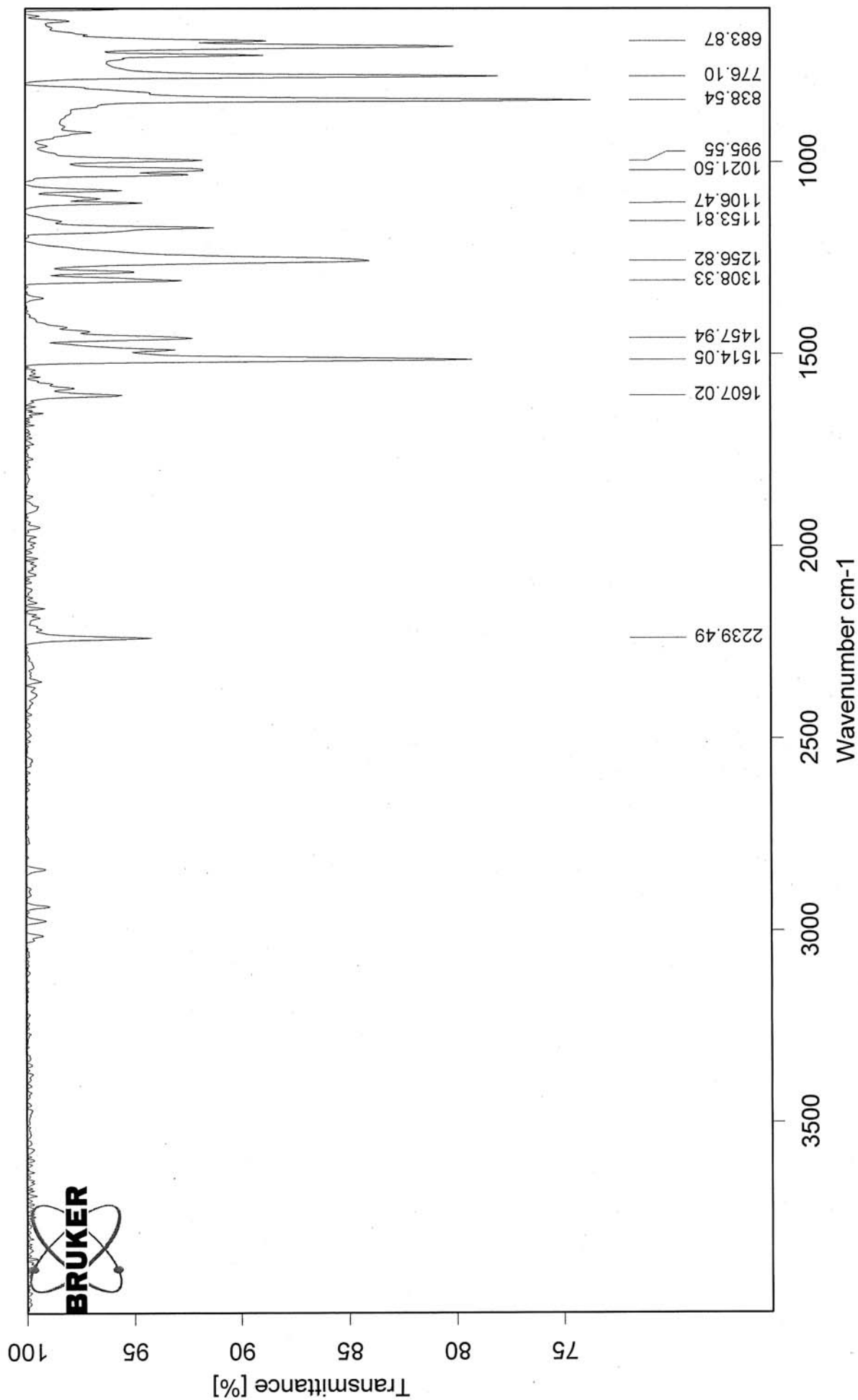


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ESI-MS: IS344CO2

XMASS Mass Analysis for /Data/UNI\_FR/ALIM6523\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

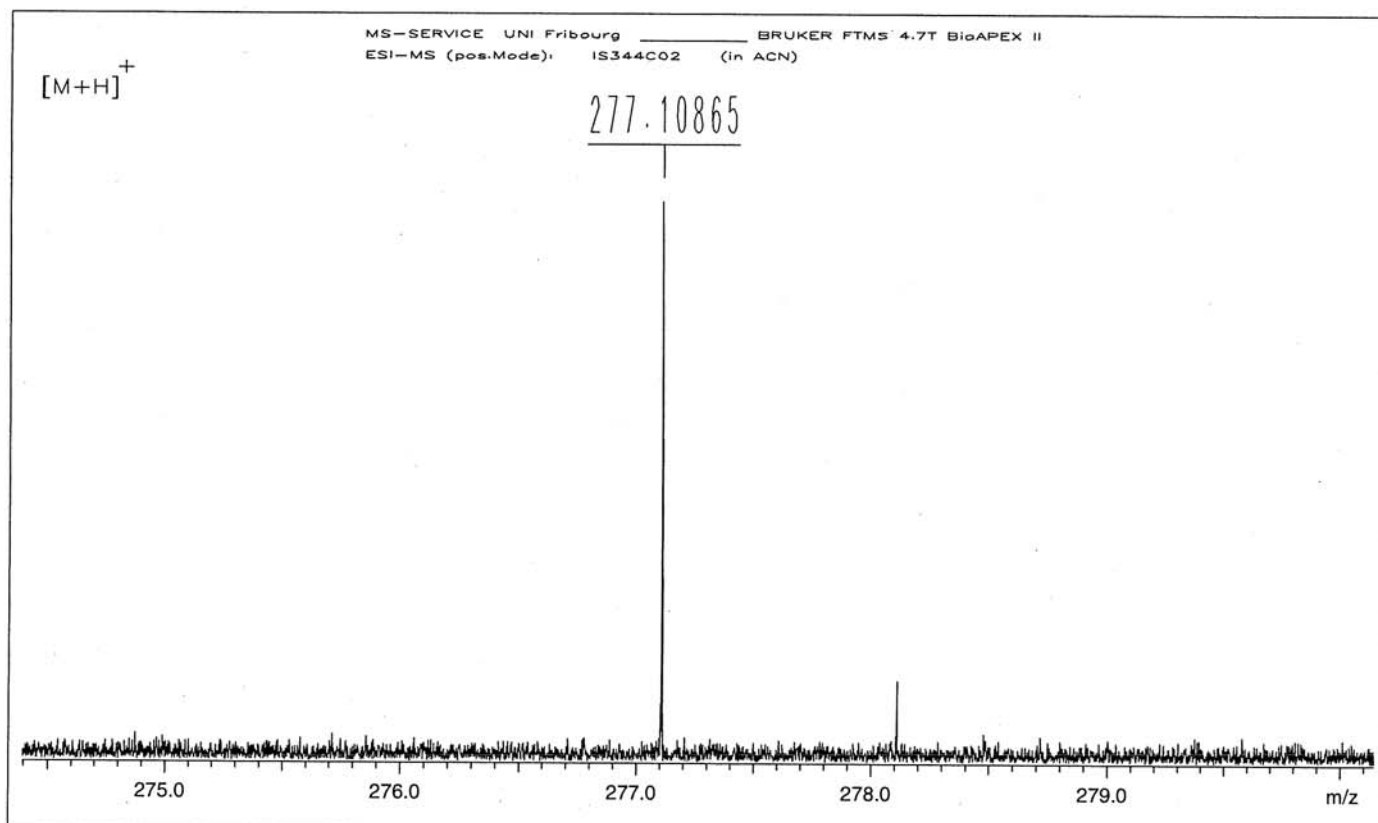
Ion mass = 277.1086490

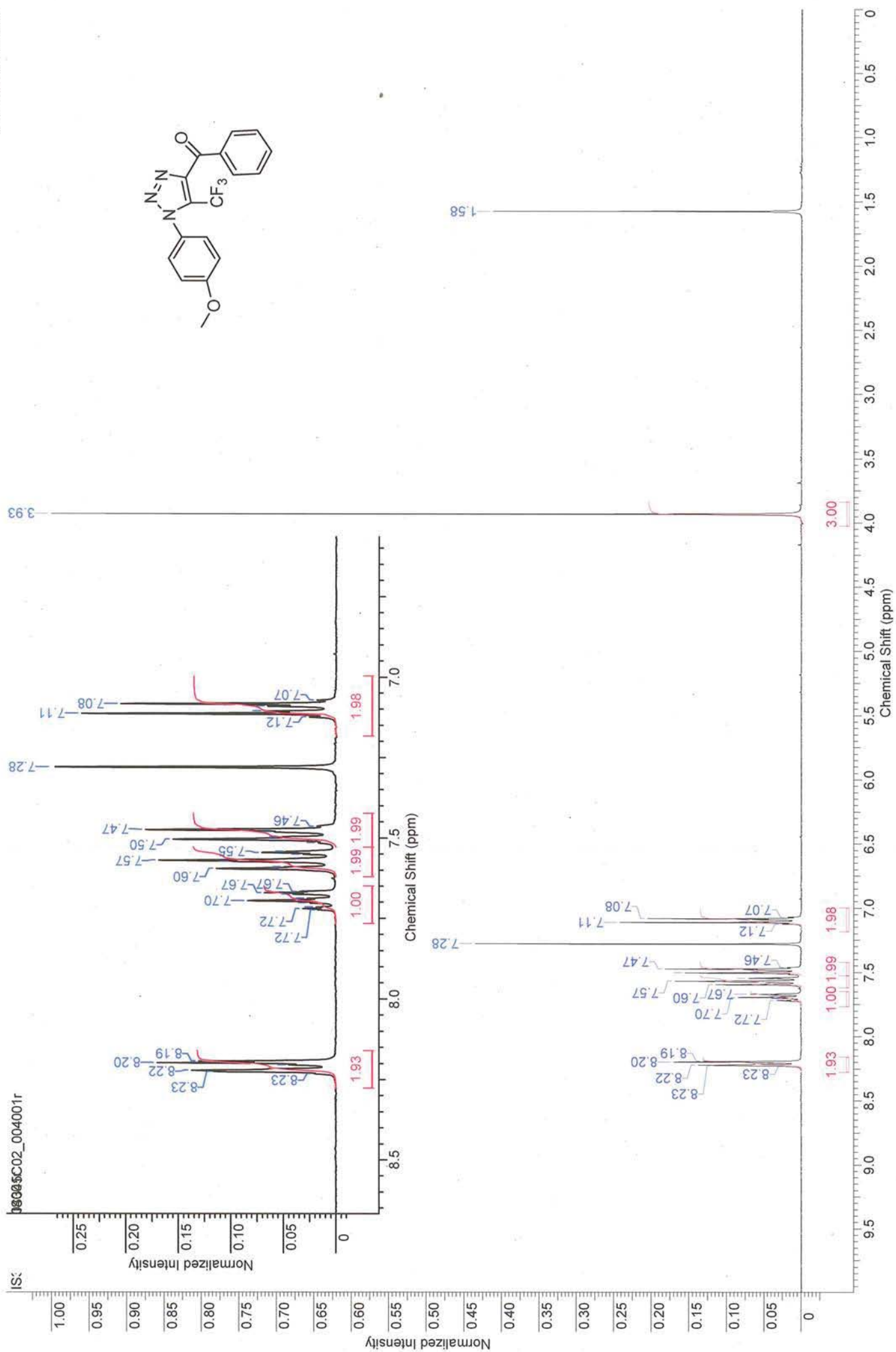
Charge = +1

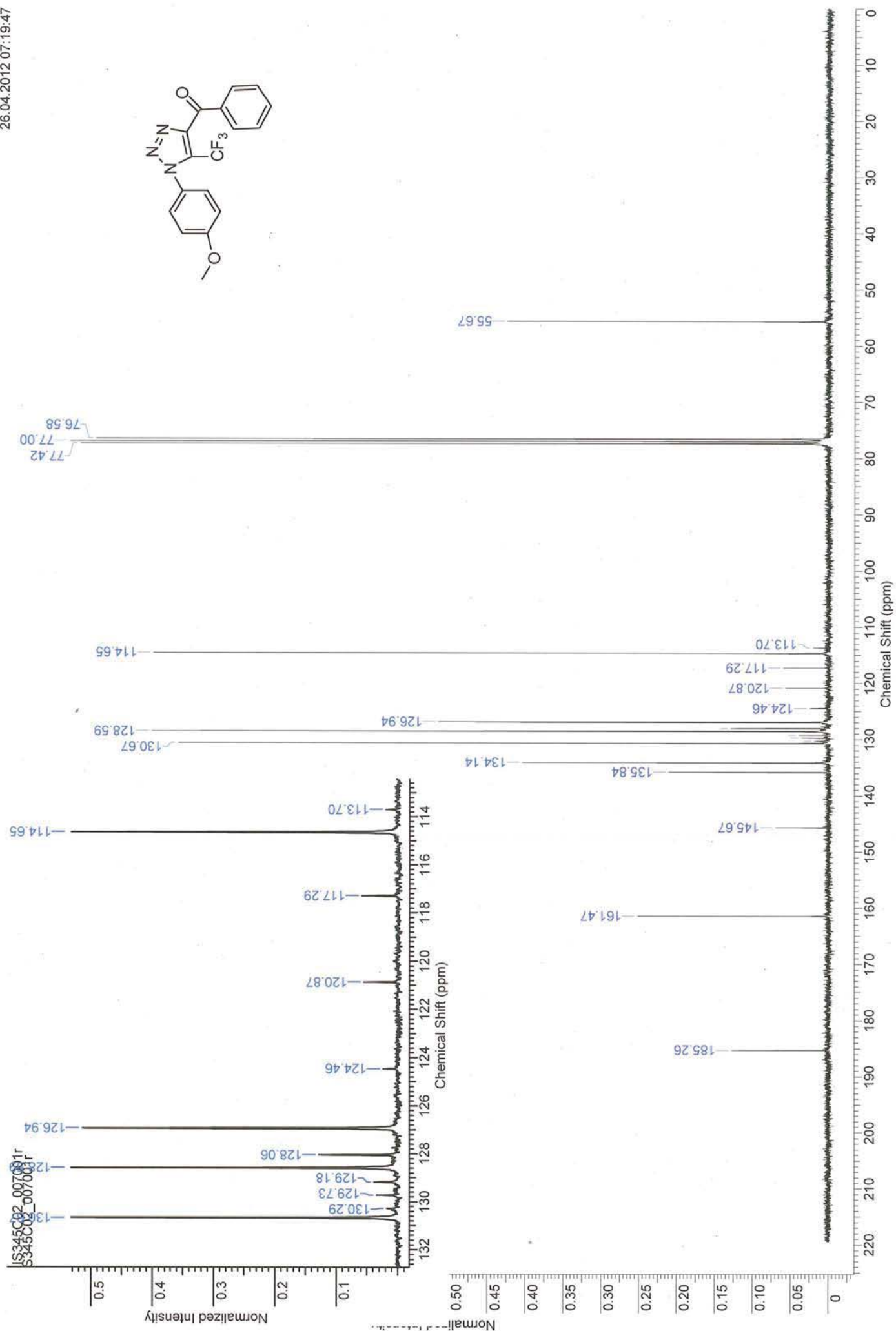
#	C	H	N	O	mass	DBE	error
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\*\*\* Mass Analysis for mass 277.1086490

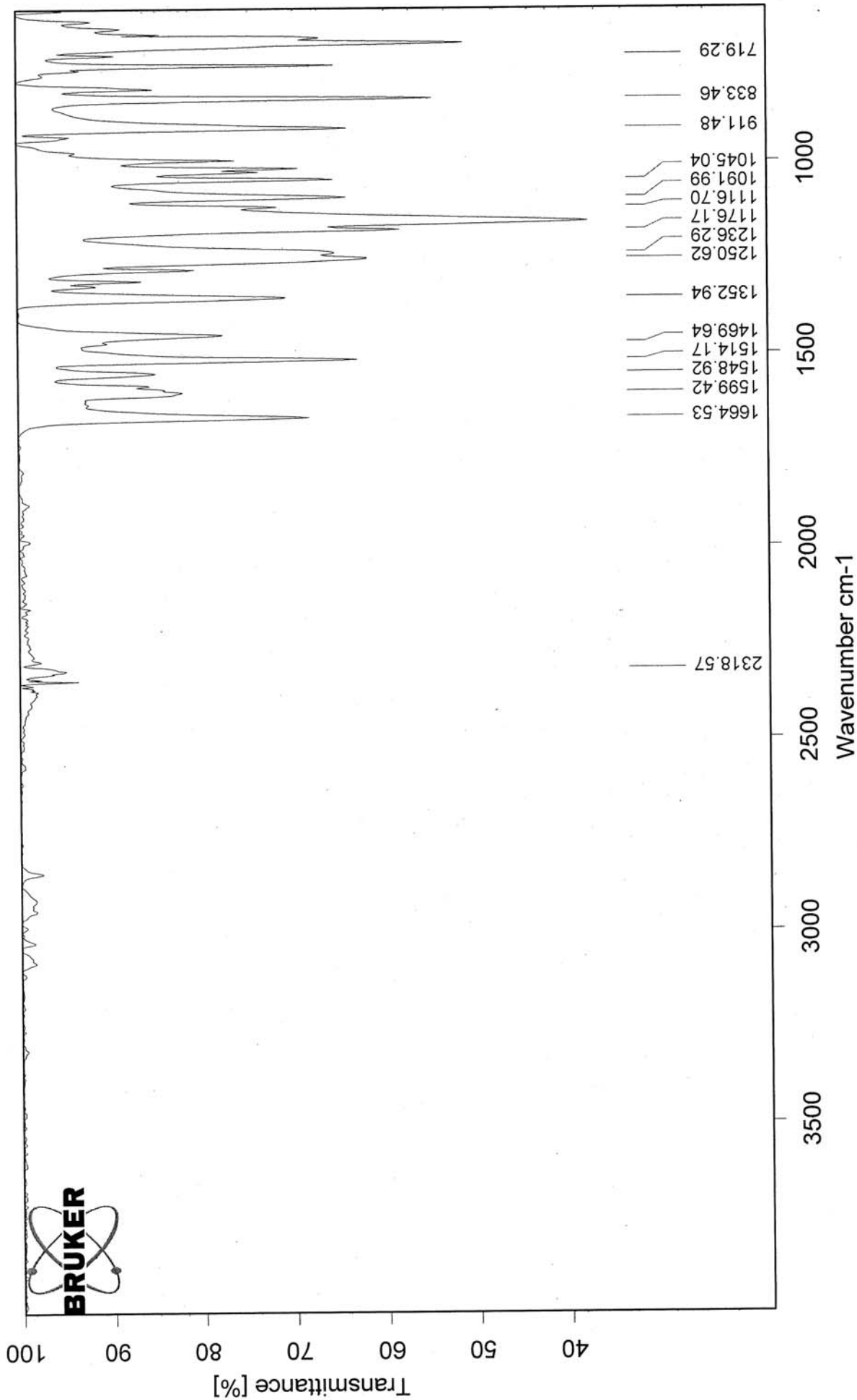
1	16	13	4	1	277.1083875	12.5	2.615e-04
2	18	15	1	2	277.1097302	12.0	1.081e-03
3	5	13	10	4	277.1115754	4.5	2.926e-03
4	6	19	3	9	277.1115806	-1.0	2.932e-03
5	13	15	3	4	277.1057074	8.0	2.942e-03
6	7	15	7	5	277.1129180	4.0	4.269e-03
7	11	13	6	3	277.1043647	8.5	4.284e-03
8	9	17	4	6	277.1142607	3.5	5.612e-03
9	10	17	2	7	277.1030273	3.5	5.622e-03
10	9	11	9	2	277.1030221	9.0	5.627e-03











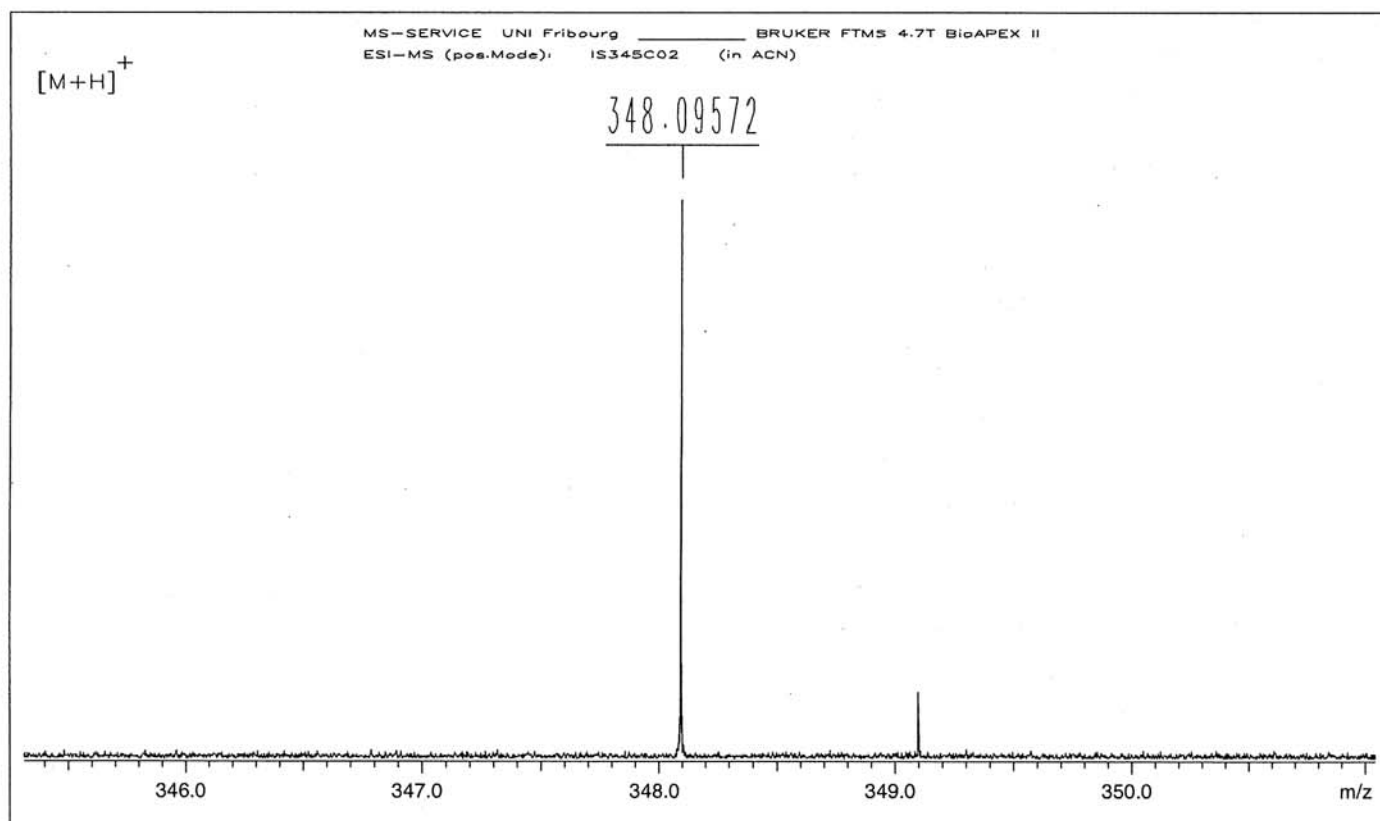
ESI-MS: IS345CO2

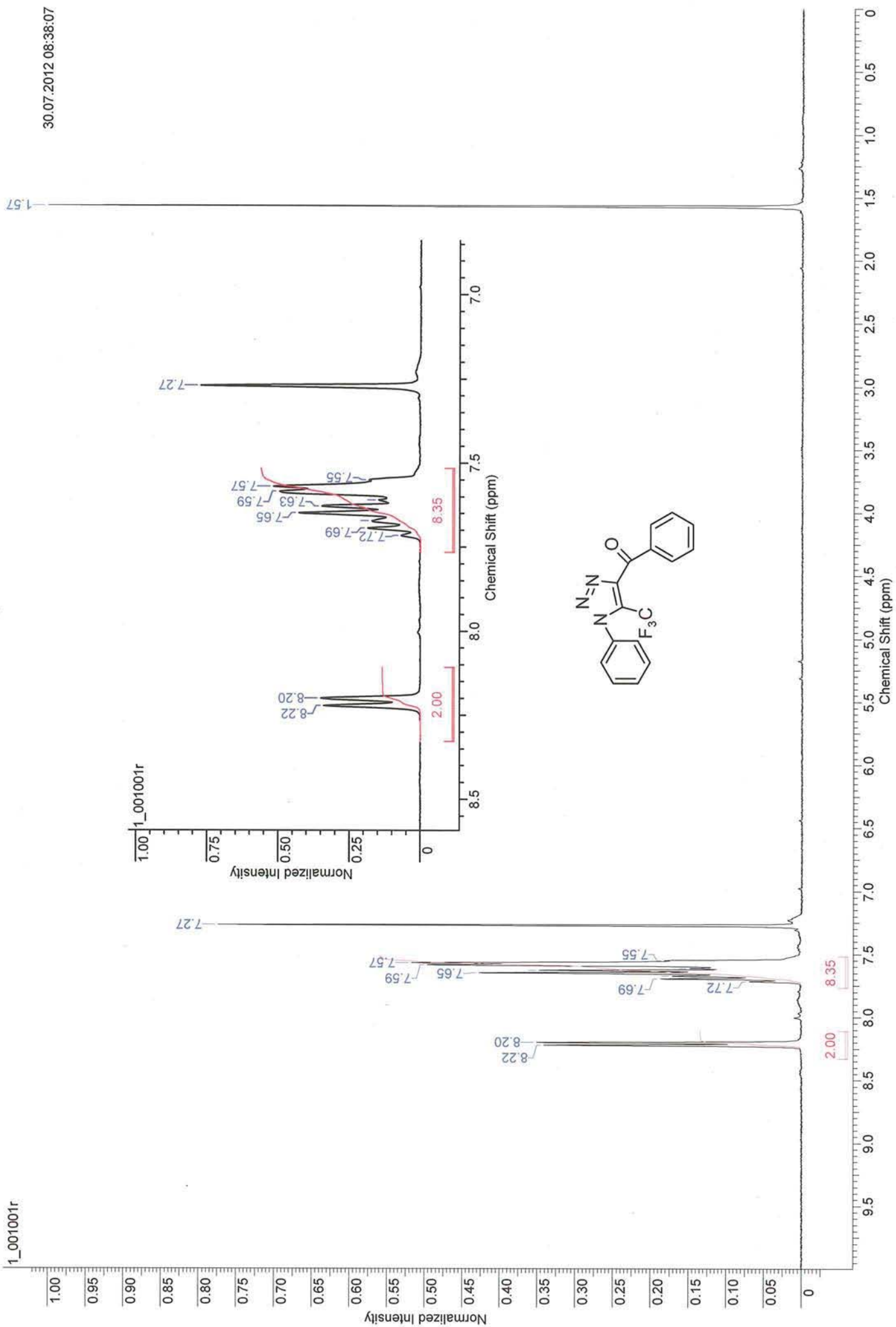
XMASS Mass Analysis for /Data/UNI\_FR/ALIM6524\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

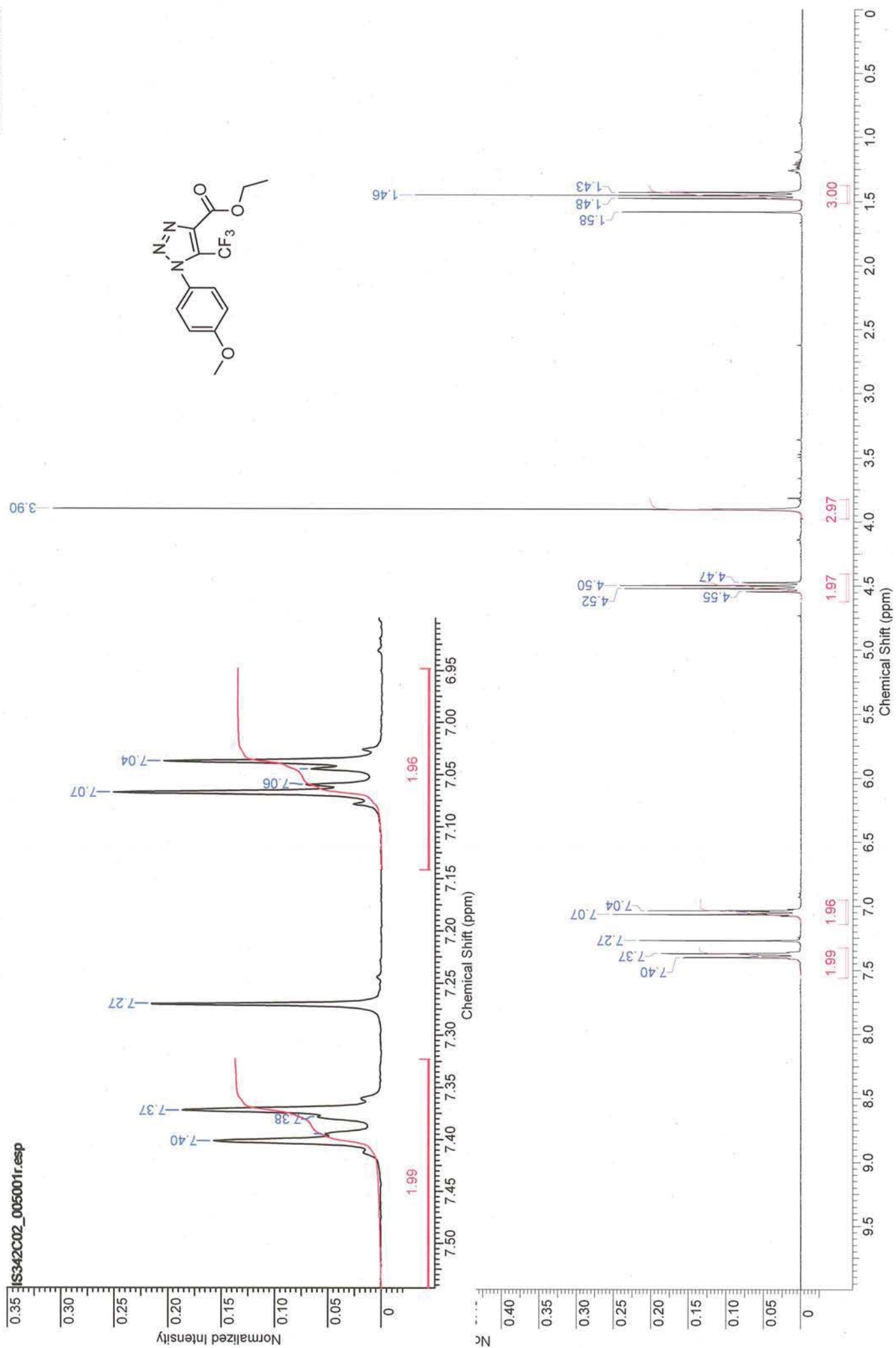
**Ion mass = 348.0957160**

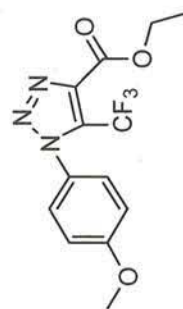
**Charge = +1**

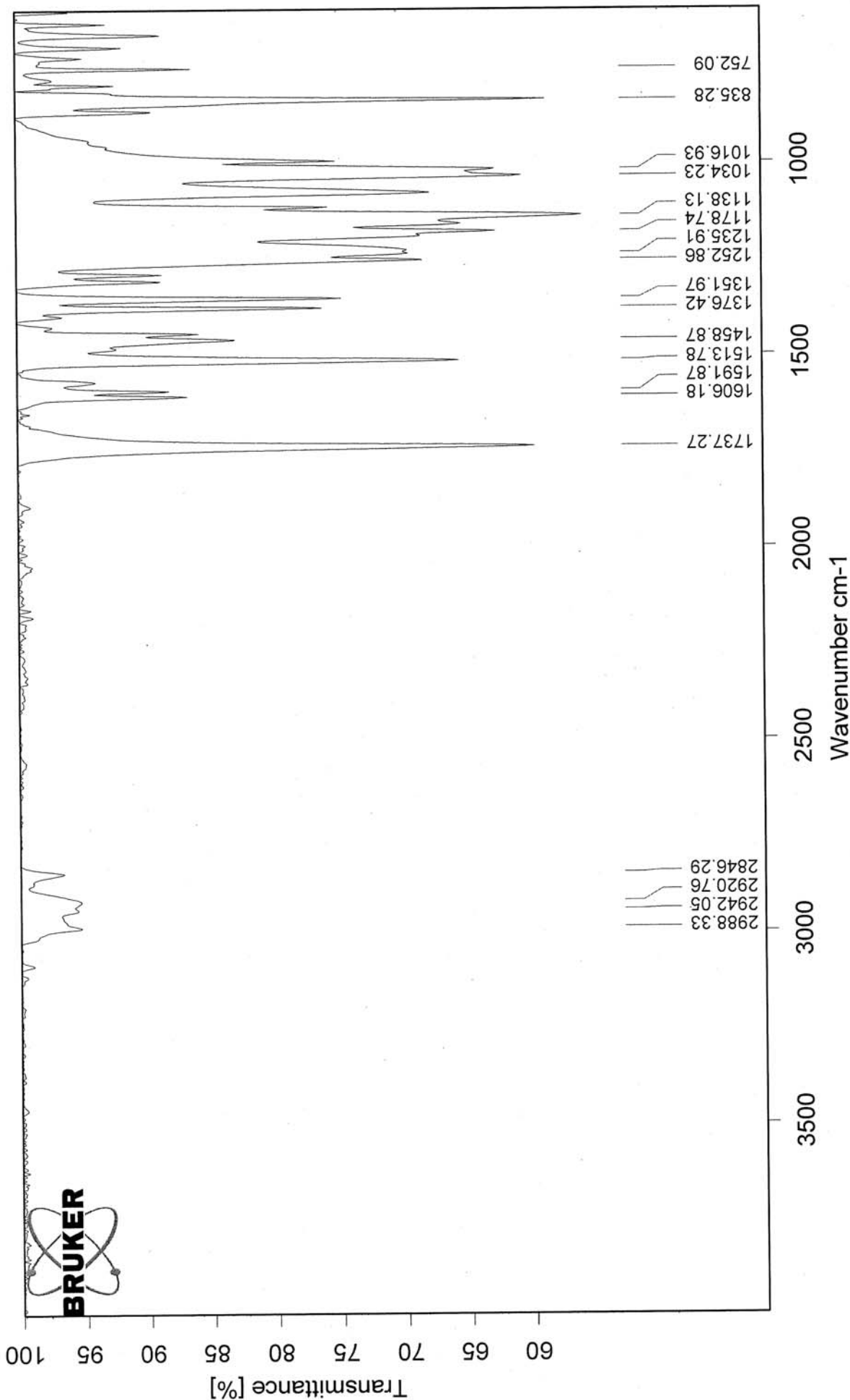
#	C	H	F	N	O	mass	DBE	error
*** Mass Analysis for mass 348.0957160								
1	17	13	3	3	2	348.0954377	11.5	2.783e-04
2	8	16	2	5	8	348.0961453	2.5	4.293e-04
3	12	12	4	6	2	348.0952379	8.0	4.781e-04
4	12	11	1	9	3	348.0963399	11.5	6.239e-04
5	13	17	1	2	8	348.0963452	6.0	6.292e-04
6	9	13	5	6	3	348.0963807	4.0	6.647e-04
7	8	17	5	2	7	348.0950433	-1.0	6.727e-04
8	7	11	5	9	2	348.0950381	4.5	6.779e-04
9	11	15	1	5	7	348.0950025	6.5	7.135e-04
10	14	14	4	3	3	348.0965806	7.5	8.646e-04











11/04/2012

yellow solid

IS342C02

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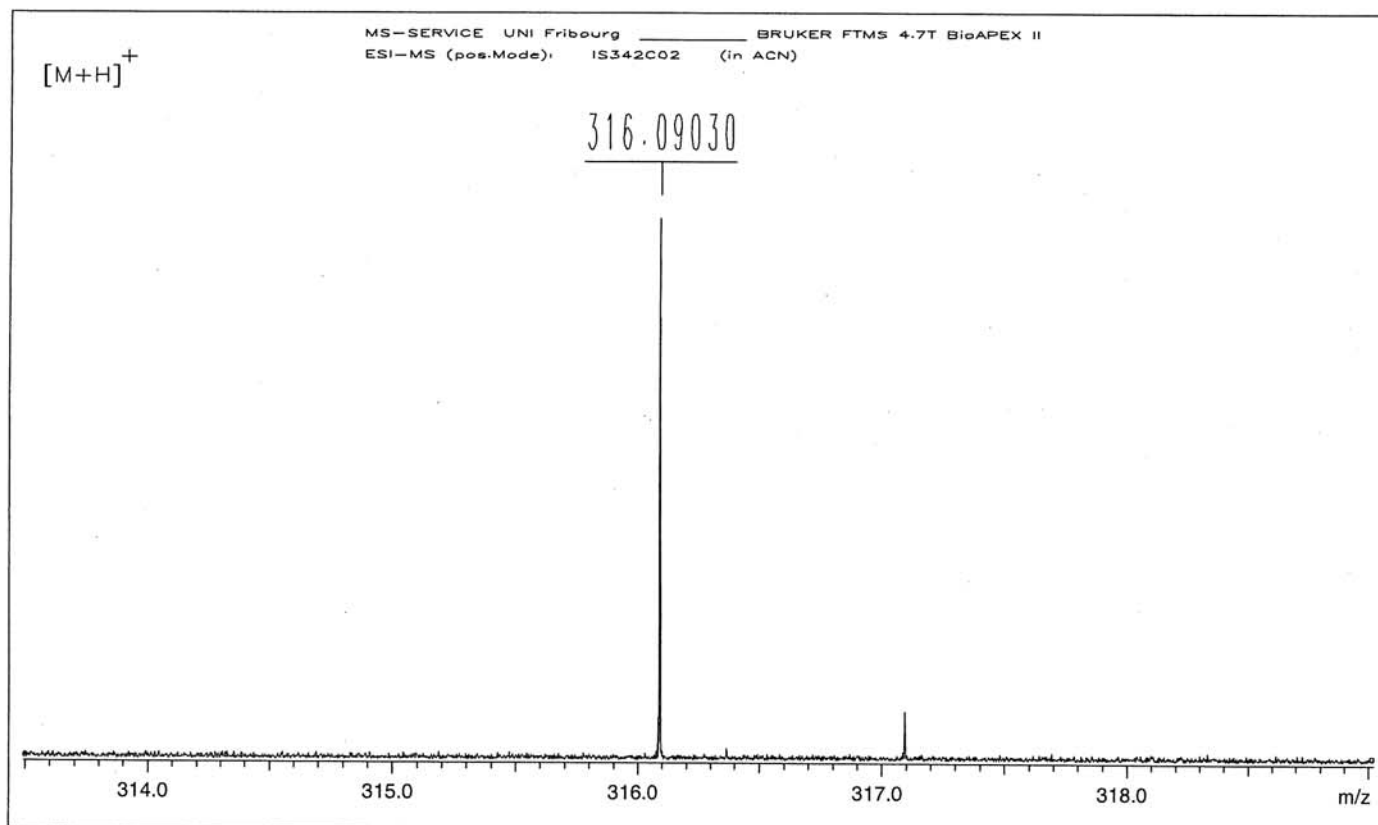
ESI-MS: IS342CO2

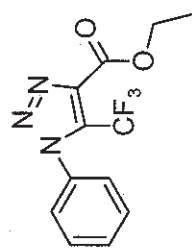
XMASS Mass Analysis for /Data/UNI\_FR/ALIM6522\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

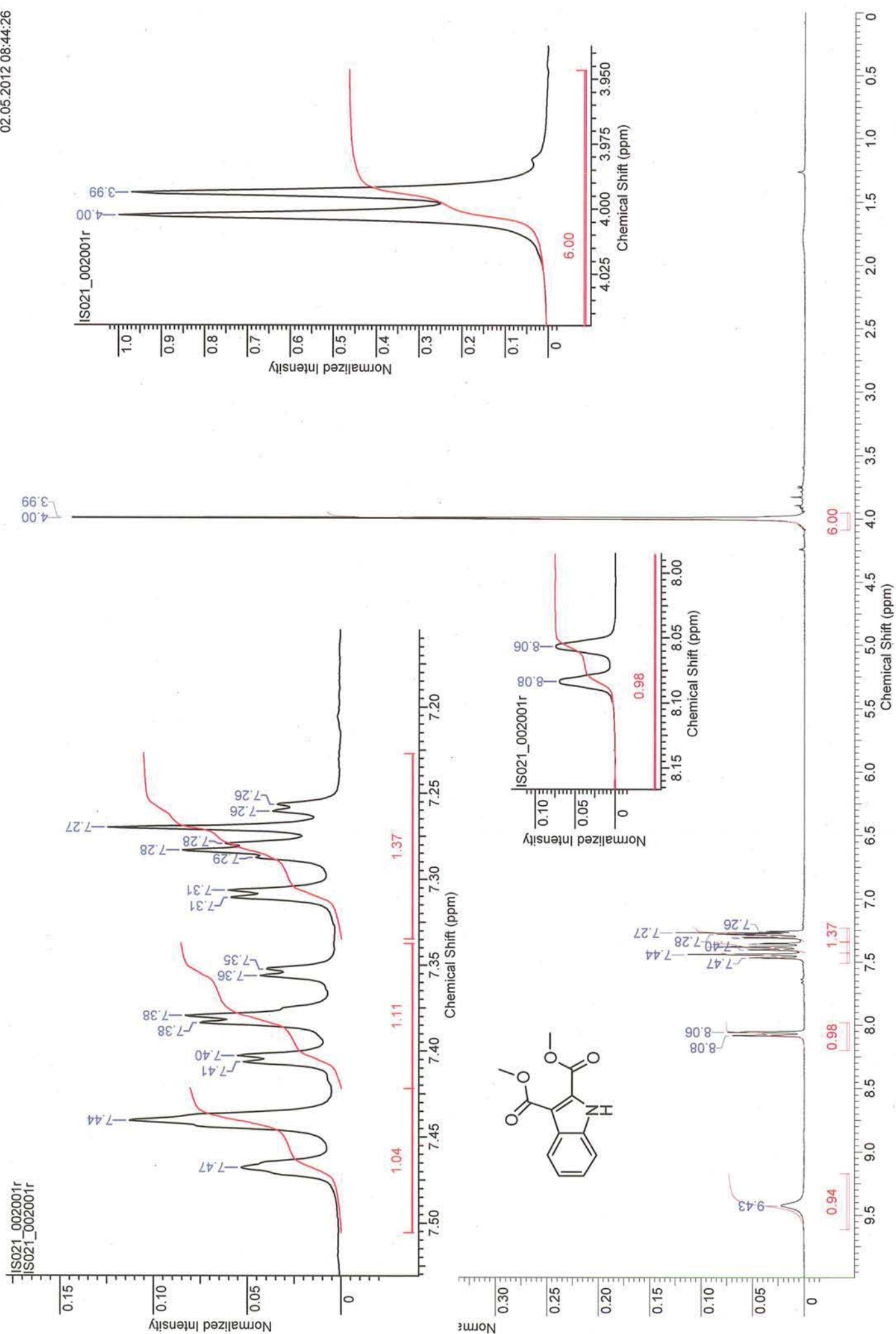
Ion mass = 316.0902960

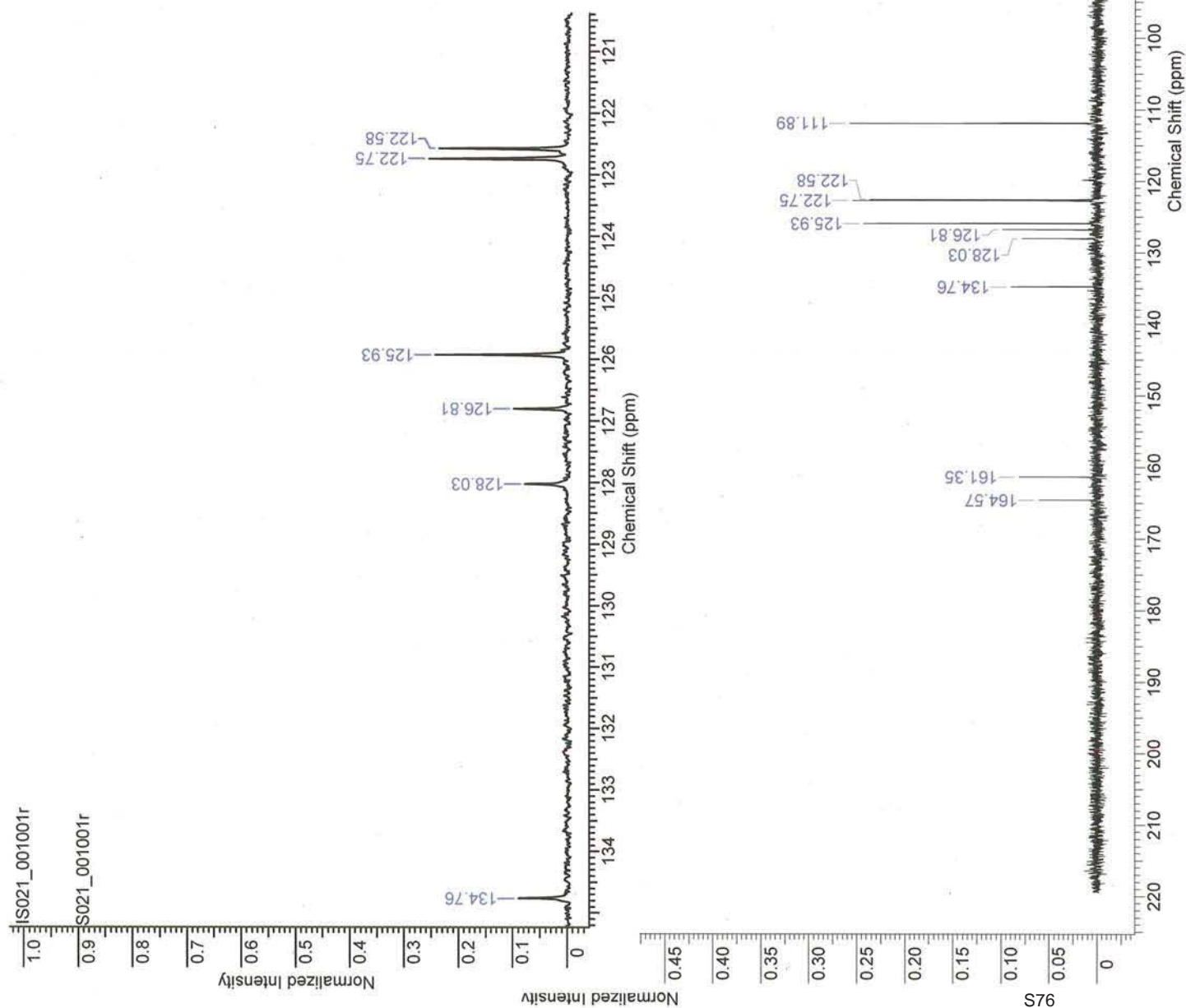
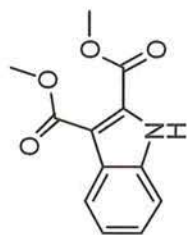
Charge = +1

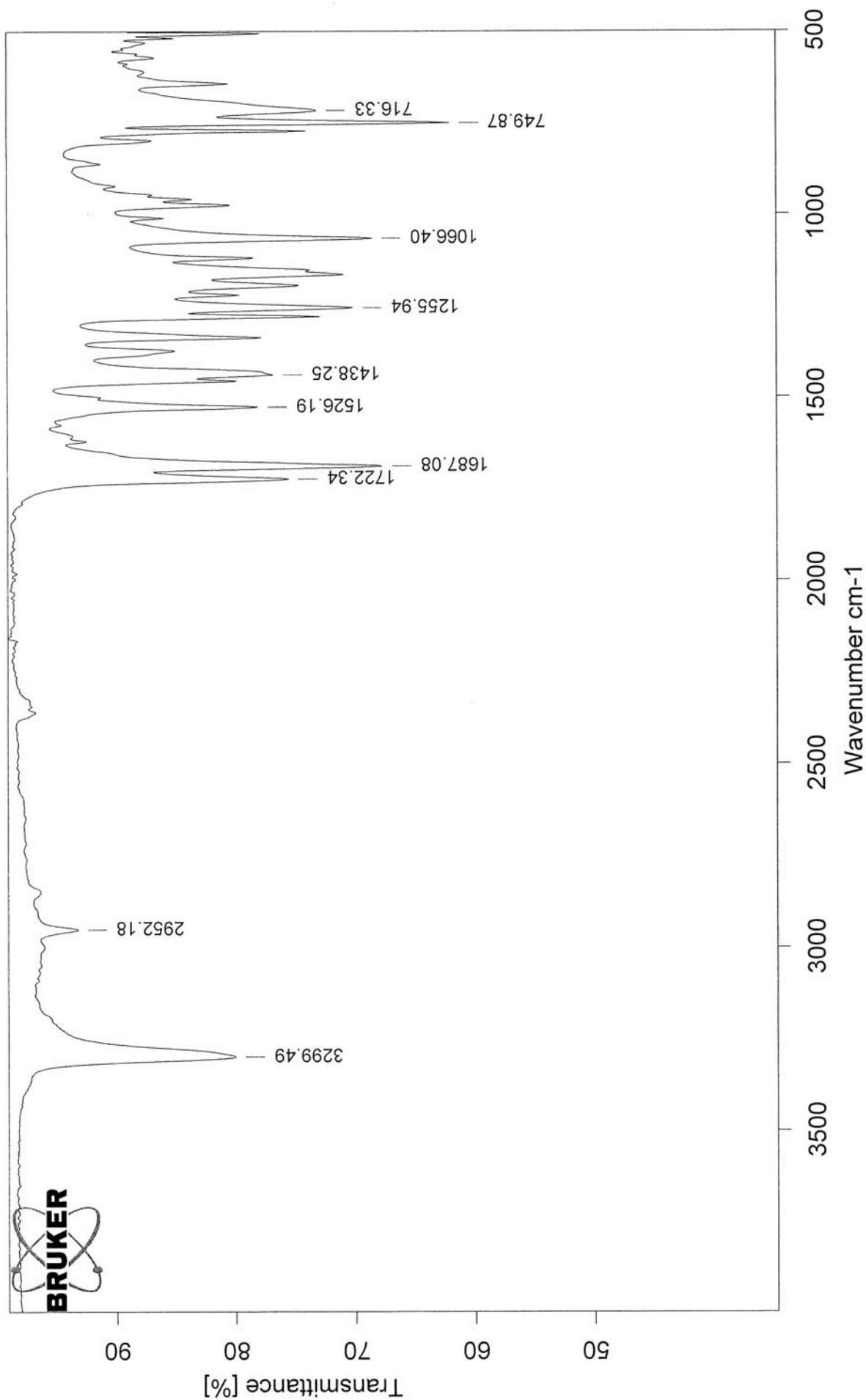
#	C	H	F	N	O	mass	DBE	error
*** Mass Analysis for mass 316.0902960								
1	13	13	3	3	3	316.0903523	7.5	5.632e-05
2	8	12	4	6	3	316.0901525	4.0	1.435e-04
3	7	15	1	5	8	316.0899171	2.5	3.789e-04
4	8	11	1	9	4	316.0912545	7.5	9.585e-04
5	9	17	1	2	9	316.0912598	2.0	9.638e-04
6	5	13	5	6	4	316.0912954	0.0	9.994e-04
7	16	12	2	3	2	316.0892095	11.5	1.087e-03
8	10	14	4	3	4	316.0914952	3.5	1.199e-03
9	11	11	3	6	2	316.0890096	8.0	1.286e-03
10	7	16	4	2	7	316.0888151	-1.0	1.481e-03











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is-021

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ESI-MS: is-021

XMASS Mass Analysis for /Data/UNI\_FR/ALIM4616\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

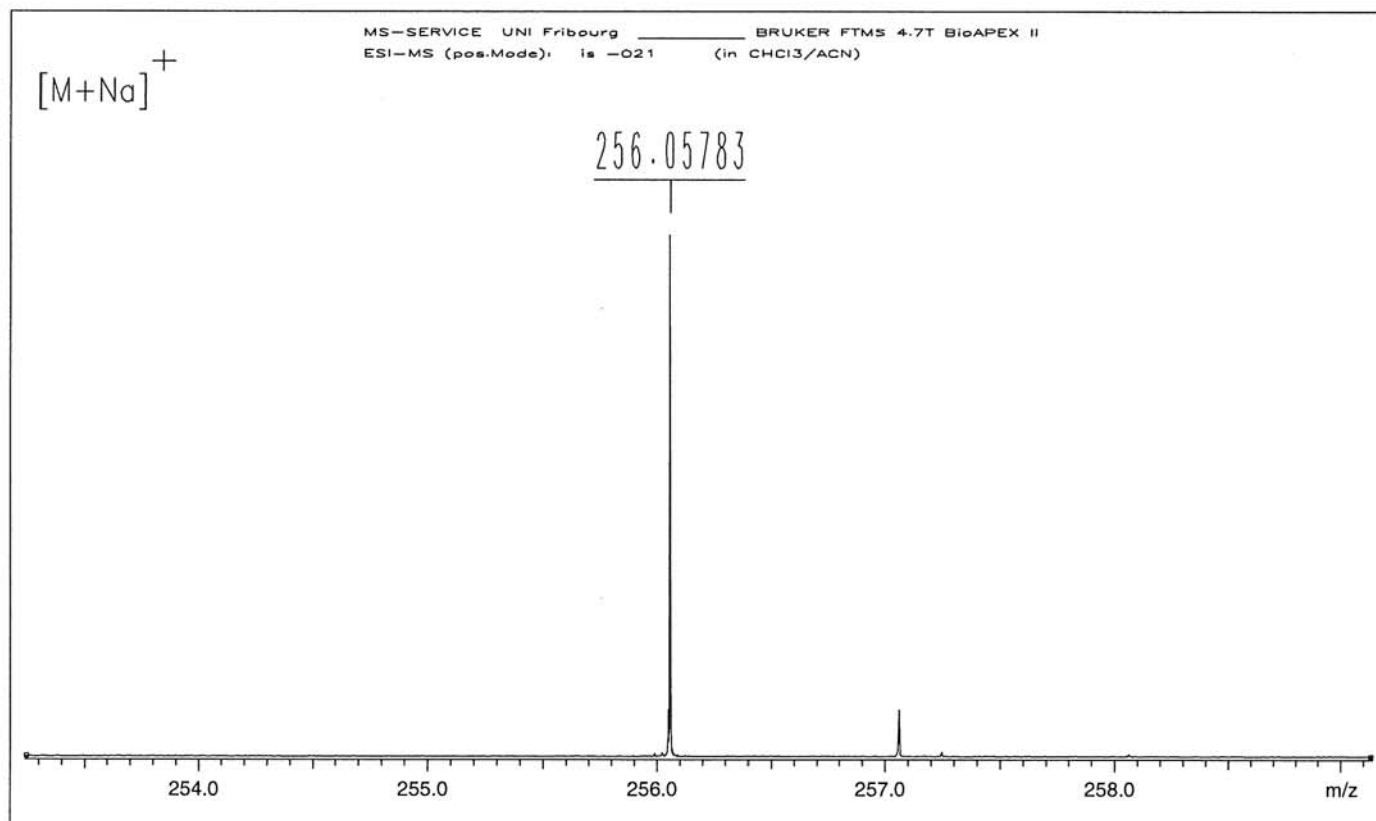
Ion mass = 256.0578260

Charge = +1

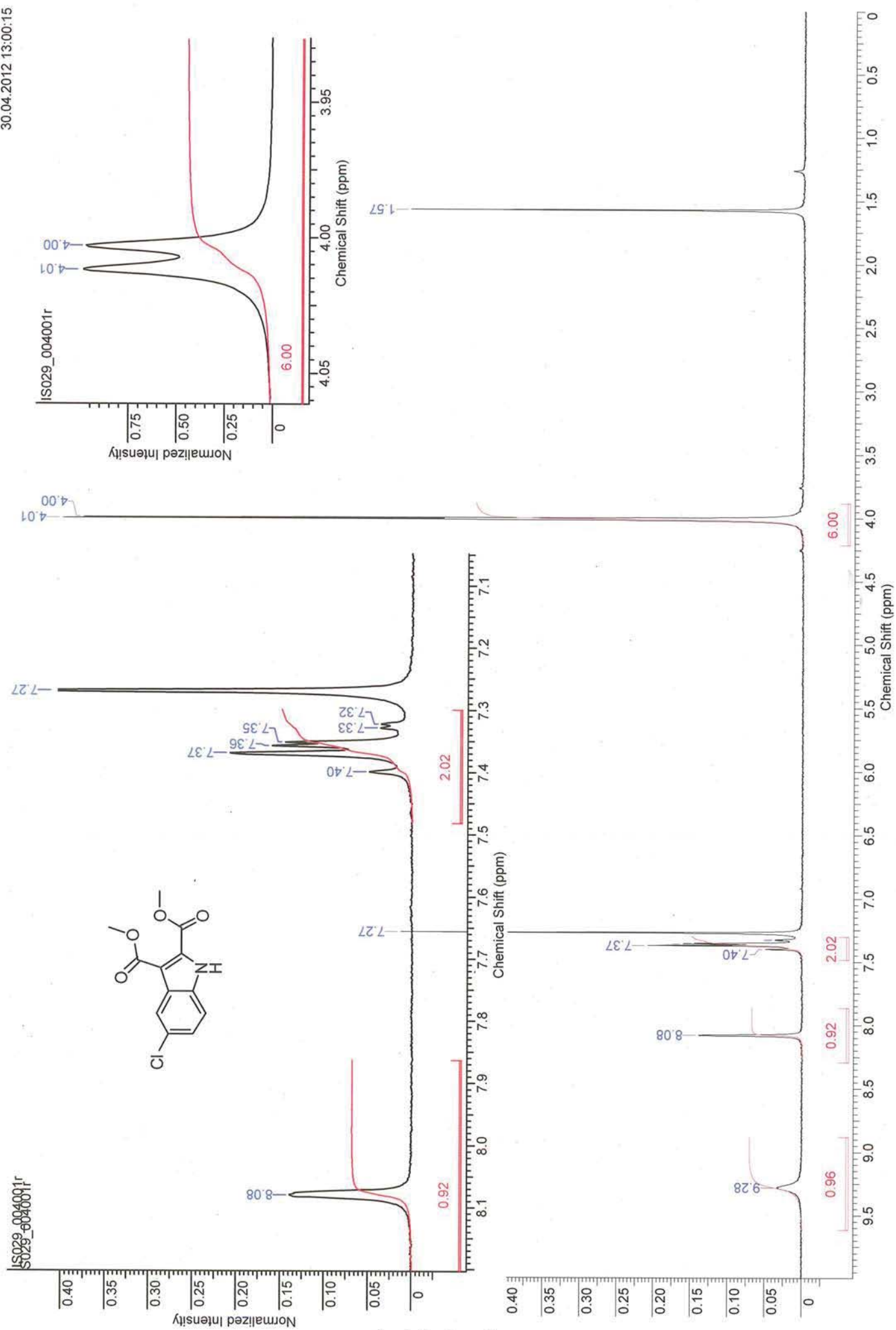
#	C	H	N	O	Na	mass	DBE	error
---	---	---	---	---	----	------	-----	-------

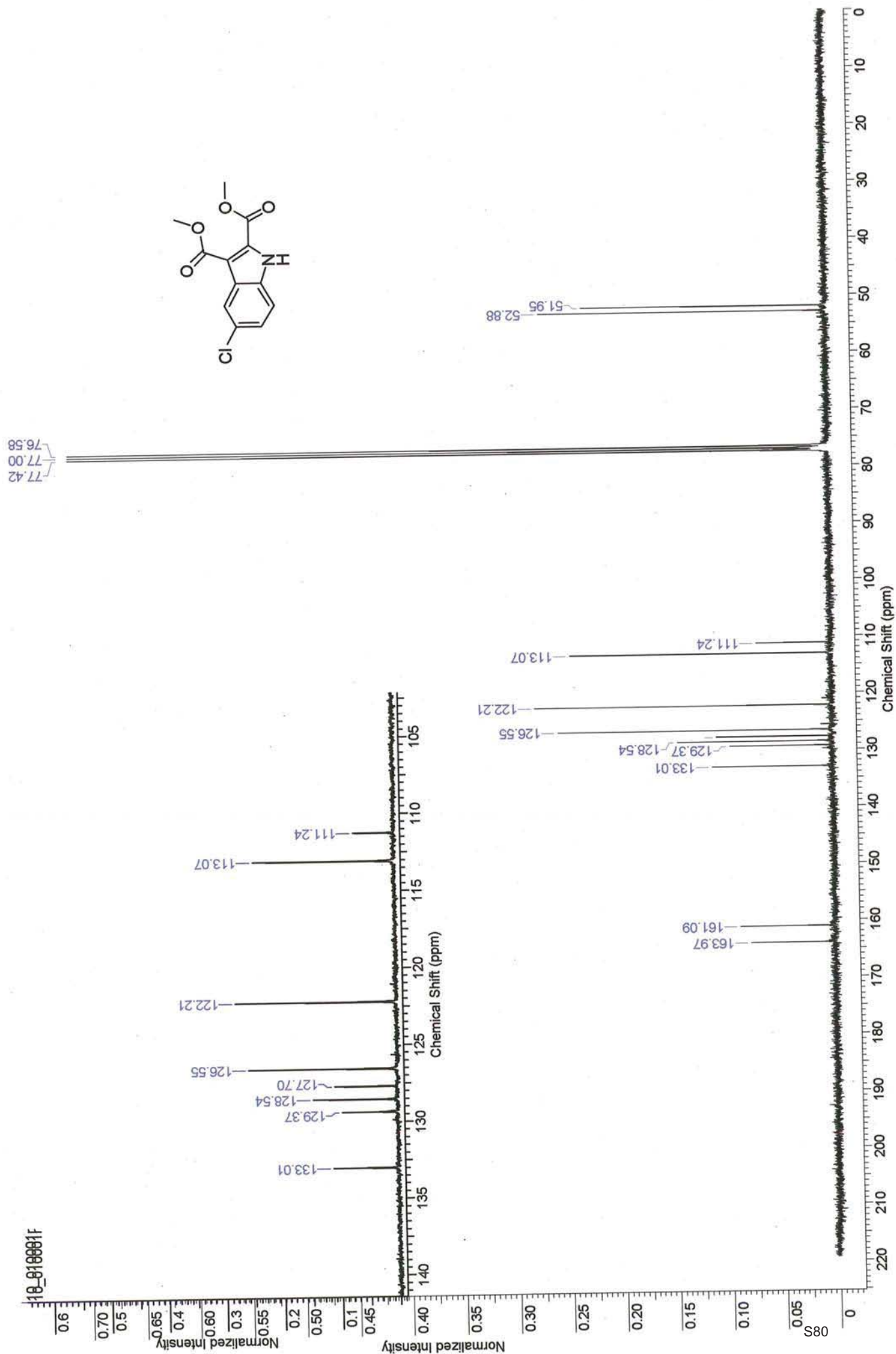
\*\*\* Mass Analysis for mass 256.0578260

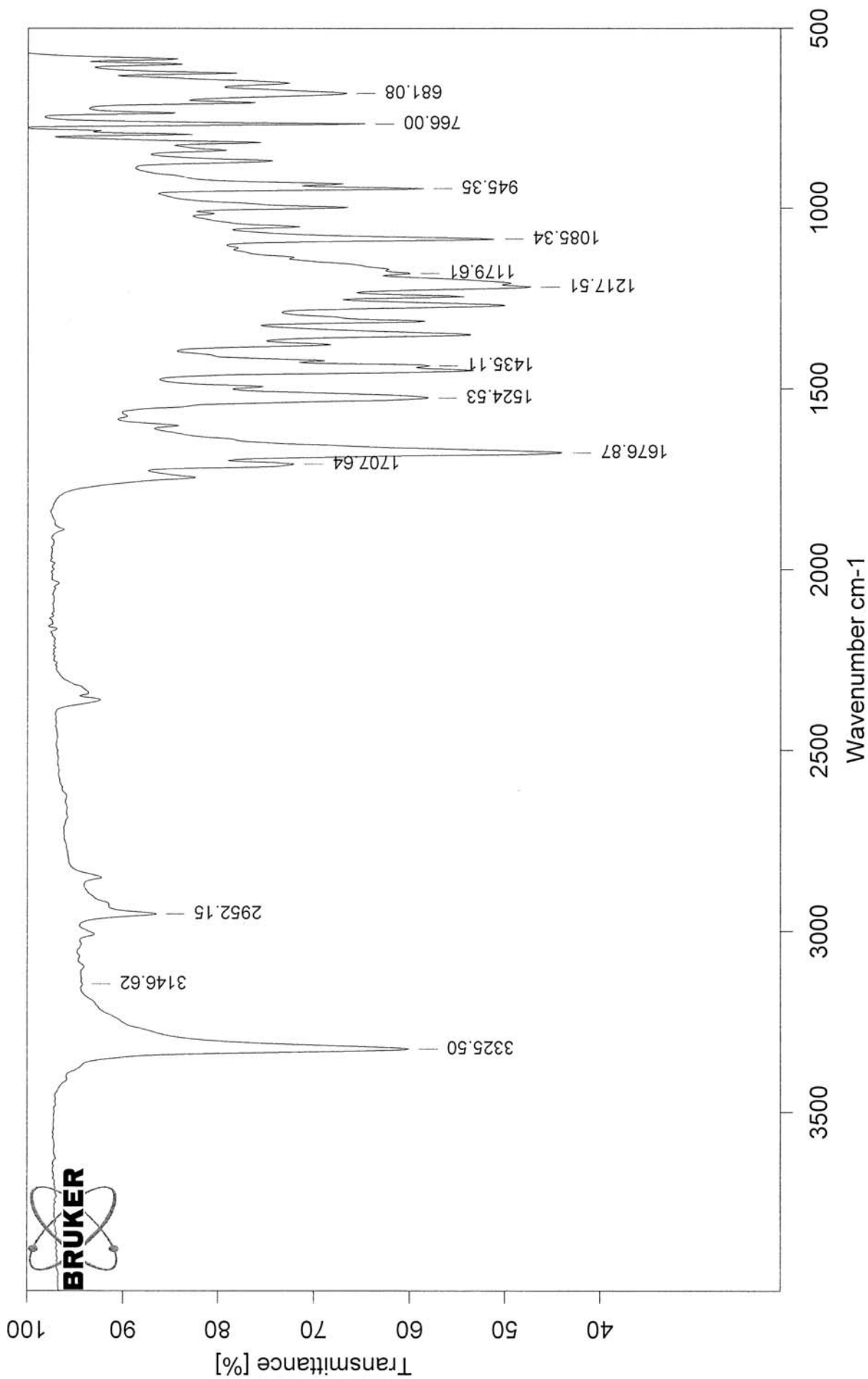
1	12	11	1	4	1	256.0580289	7.5	2.029e-04
2	10	9	4	3	1	256.0566863	8.0	1.140e-03
3	12	8	4	3	0	256.0590916	11.0	1.266e-03
4	9	10	3	6	0	256.0564115	6.5	1.415e-03
5	14	10	1	4	0	256.0604342	10.5	2.608e-03
6	15	9	2	1	1	256.0607090	12.0	2.883e-03
7	7	11	3	6	1	256.0540062	3.5	3.820e-03
8	6	12	2	9	0	256.0537314	2.0	4.095e-03
9	17	8	2	1	0	256.0631143	15.0	5.288e-03
10	5	15	1	9	1	256.0639022	-1.5	6.076e-03











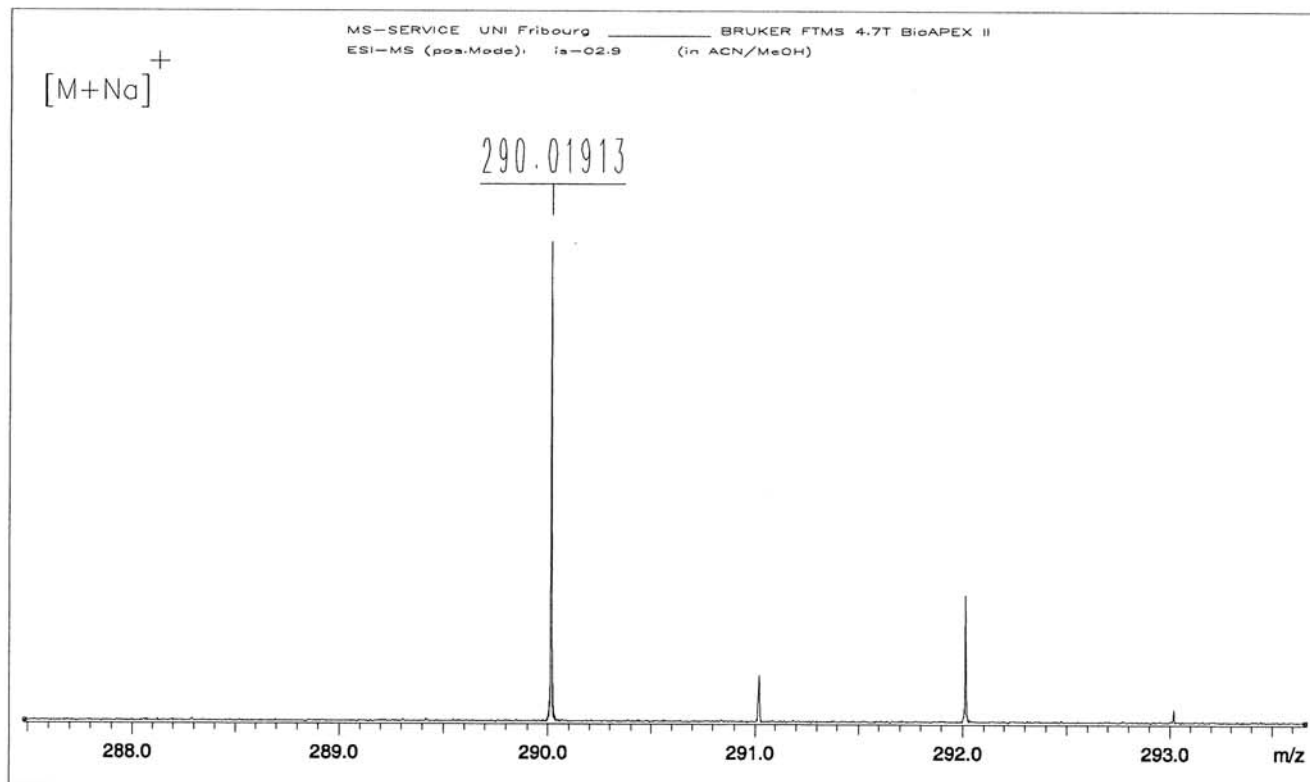
ESI-MS: is-029

XMASS Mass Analysis for /Data/UNI\_FR/ALIM4617\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

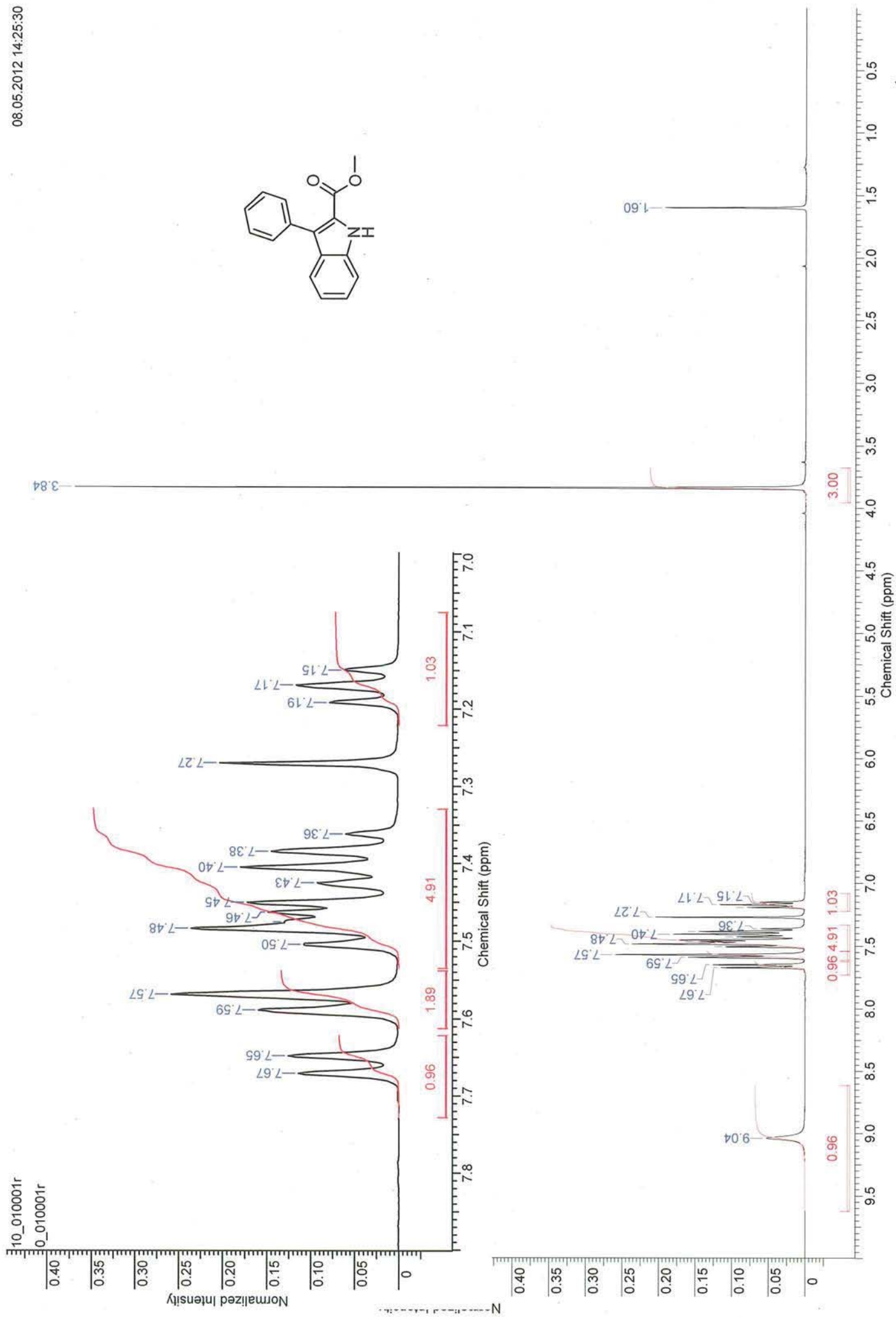
**Ion mass = 290.0191340**

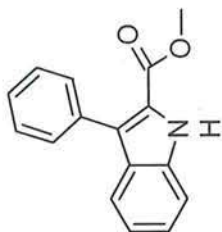
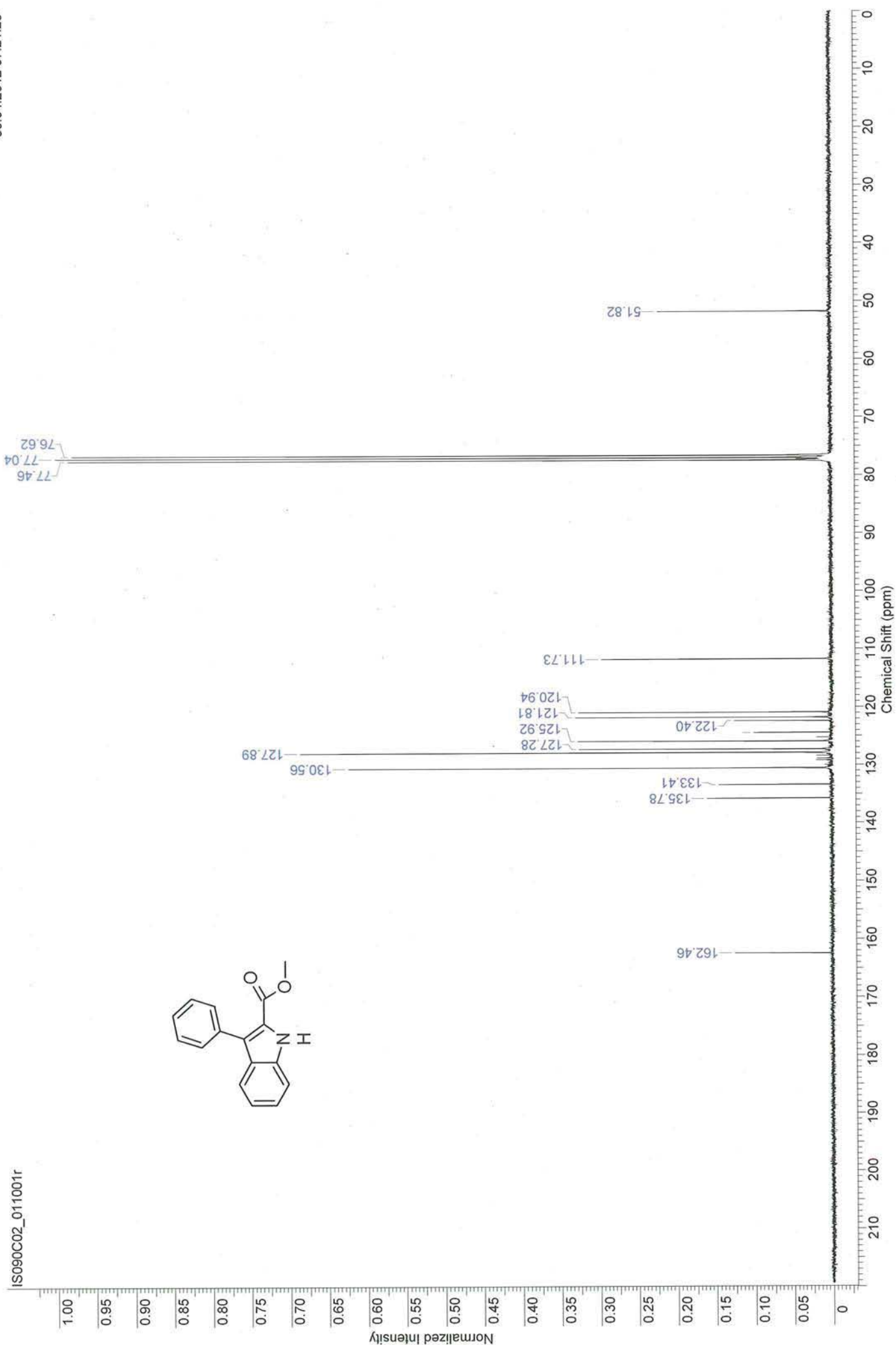
**Charge = +1**

#	C	H	35Cl	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 290.0191340									
1	12	10	1	1	4	1	290.0190566	7.5	7.739e-05
2	10	5	1	7	2	0	290.0187766	11.5	3.574e-04
3	12	7	1	4	3	0	290.0201192	11.0	9.852e-04
4	10	8	1	4	3	1	290.0177139	8.0	1.420e-03
5	14	9	1	1	4	0	290.0214619	10.5	2.328e-03
6	15	8	1	2	1	1	290.0217367	12.0	2.603e-03
7	11	12	2	2	3	0	290.0219491	6.0	2.815e-03
8	17	7	1	2	1	0	290.0241420	15.0	5.008e-03
9	15	10	2	1	1	0	290.0133958	10.5	5.738e-03
10	16	5	1	3	1	0	290.0115659	15.5	7.568e-03

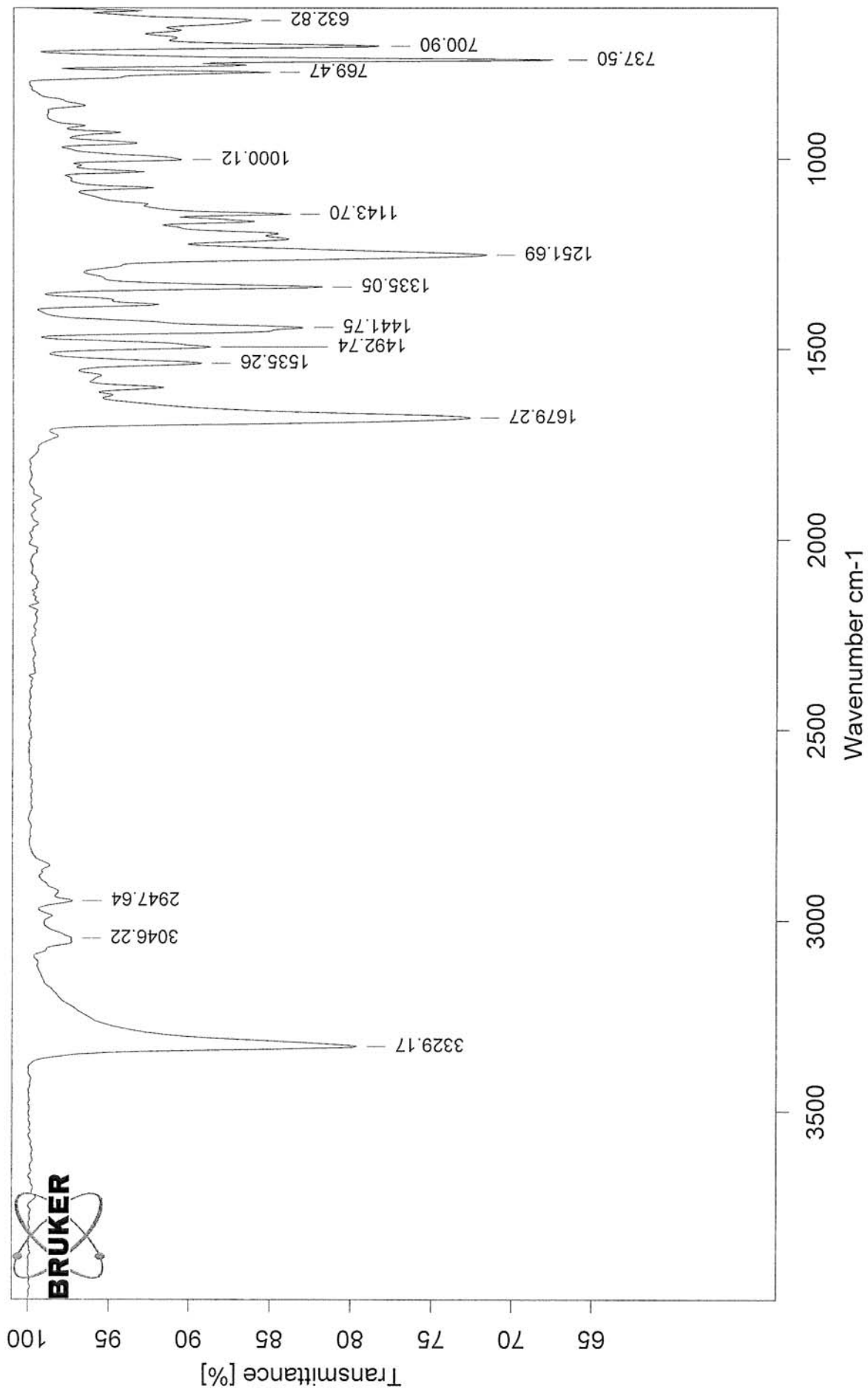


/Data/UNI FR/ALIM4617 ESI/2/pdata/1 FTMS USER Mon Jan 4 10:40:37 2010









U:\IR\_spectra\IS090.1

IS090

white yellow solid

09/07/2010

ESI-MS: IS090

XMASS Mass Analysis for /Data/UNI\_FR/ALIM4973\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

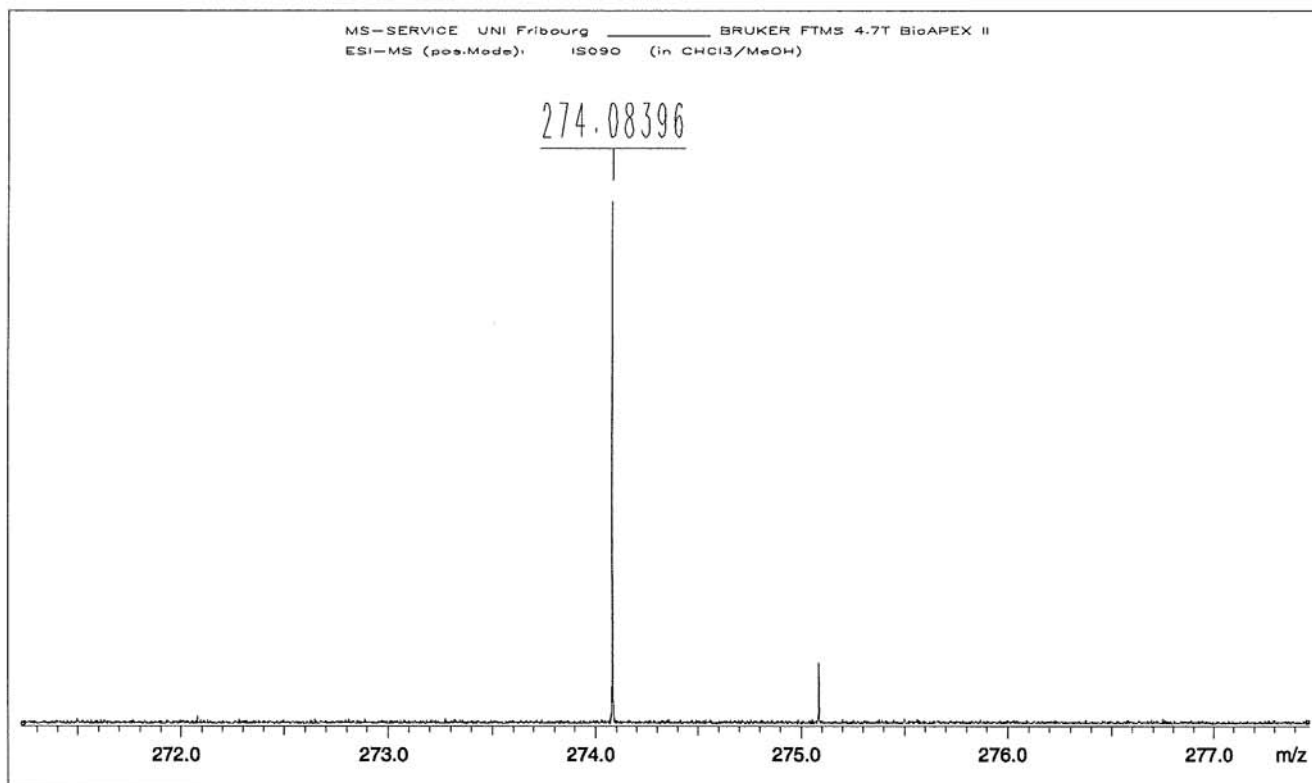
Ion mass = 274.0839610

Charge = +1

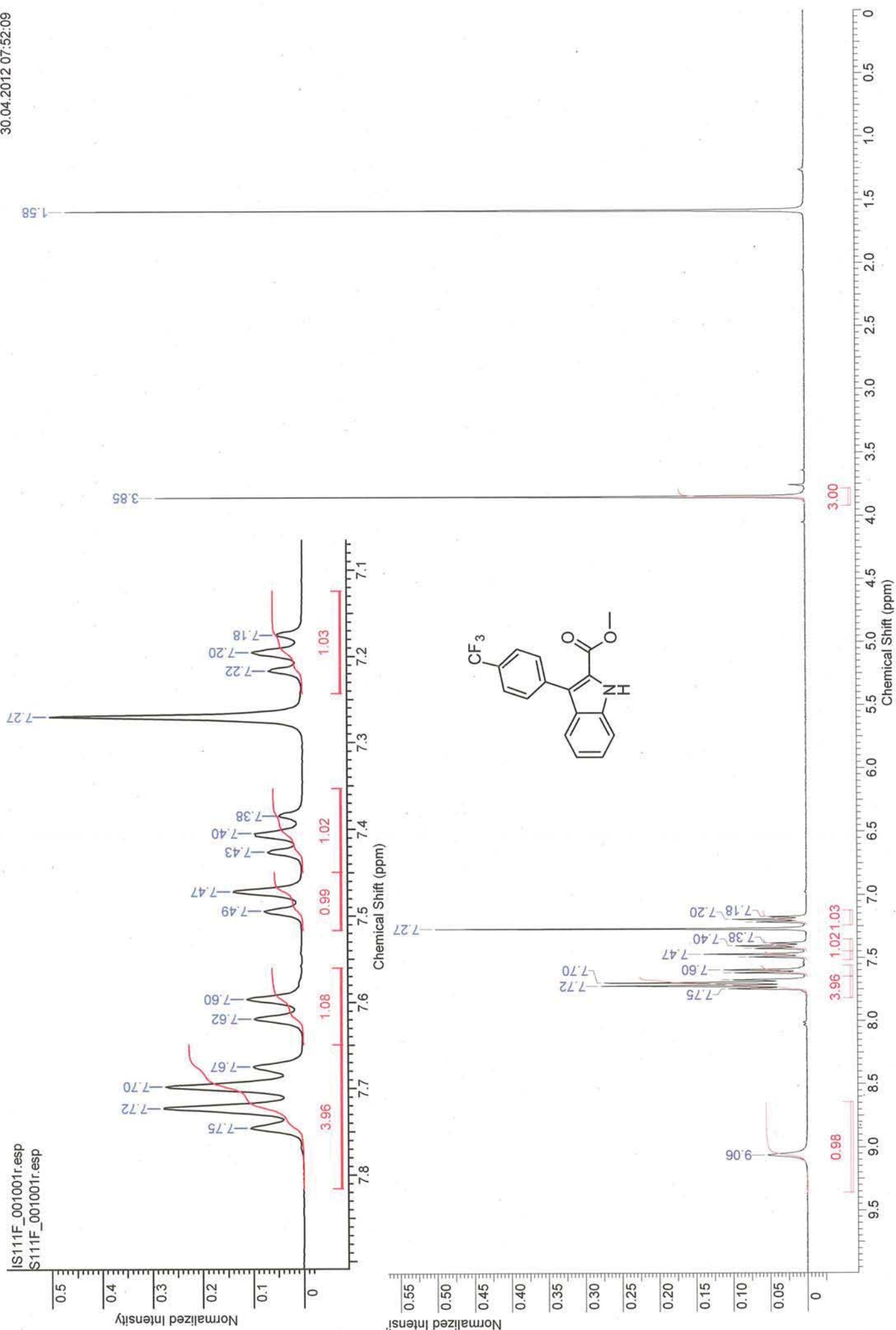
#	C	H	N	O	Na	mass	DBE	error
---	---	---	---	---	----	------	-----	-------

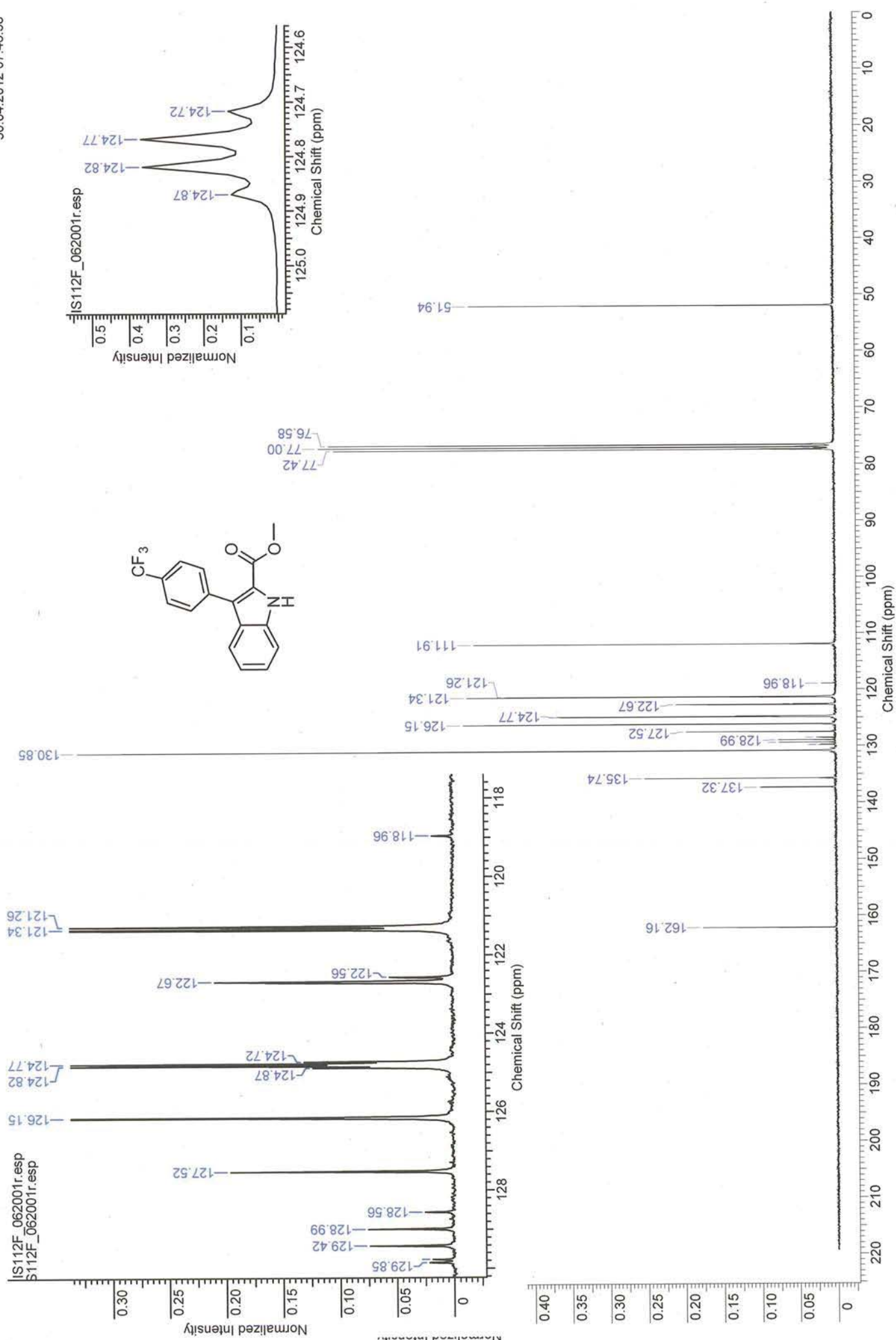
\*\*\* Mass Analysis for mass 274.0839610

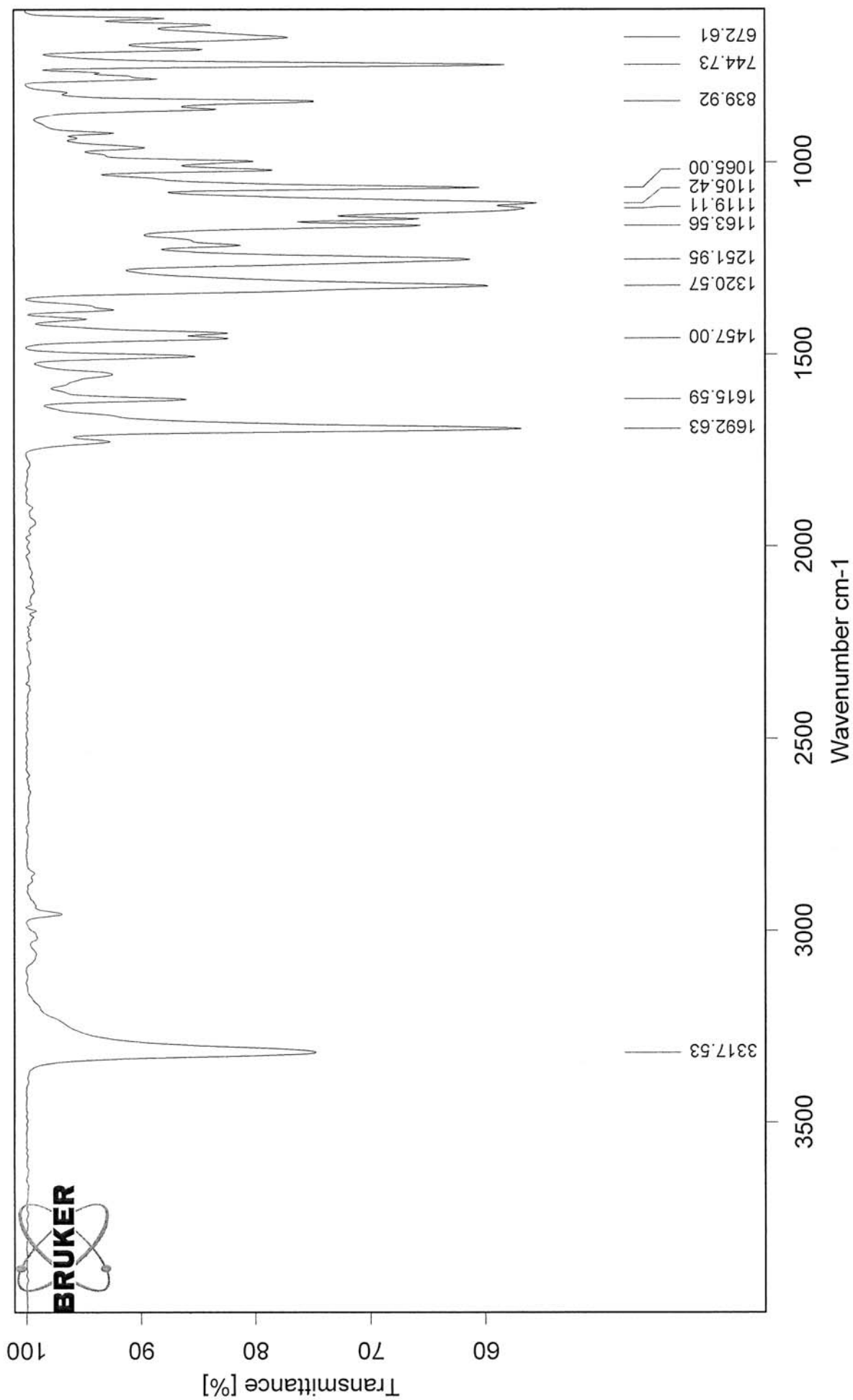
1	16	13	1	2	1	274.0838498	10.5	1.112e-04
2	16	10	4	1	0	274.0849124	14.0	9.514e-04
3	14	11	4	1	1	274.0825071	11.0	1.454e-03
4	13	12	3	4	0	274.0822323	9.5	1.729e-03
5	18	12	1	2	0	274.0862551	13.5	2.294e-03
6	11	10	6	3	0	274.0808896	10.0	3.071e-03
7	5	13	7	5	1	274.0870377	2.5	3.077e-03
8	11	13	3	4	1	274.0798270	6.5	4.134e-03
9	5	10	10	4	0	274.0881003	6.0	4.139e-03
10	6	16	3	9	0	274.0881055	0.5	4.145e-03



/Data/UNI\_FR/ALIM4973\_ESI/1/pdata/1 FTMS USER Thu Jul 8 11:57:50 2010









FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

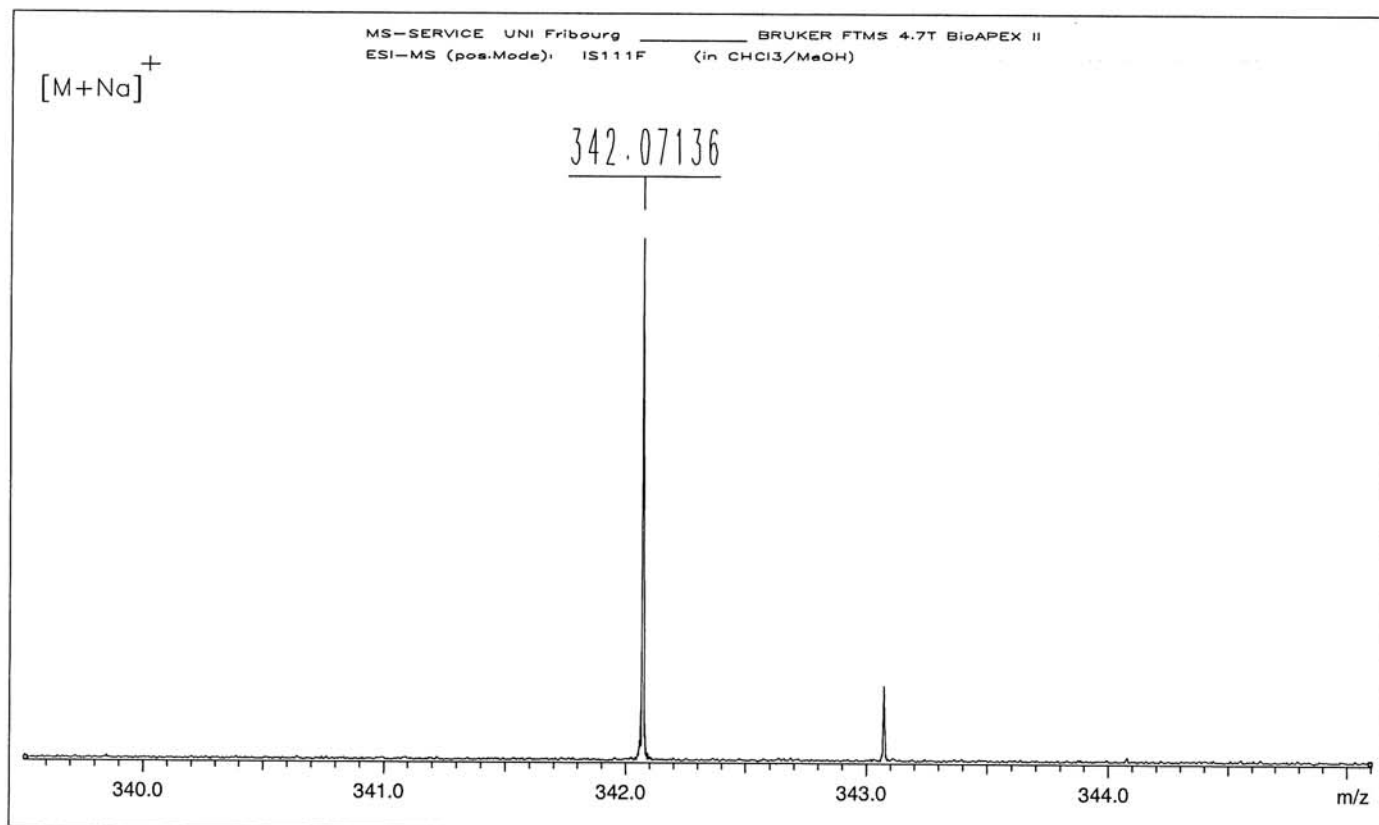
ESI-MS: IS111F

XMASS Mass Analysis for /Data/UNI\_FR/ALIM5098\_ESI/3/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

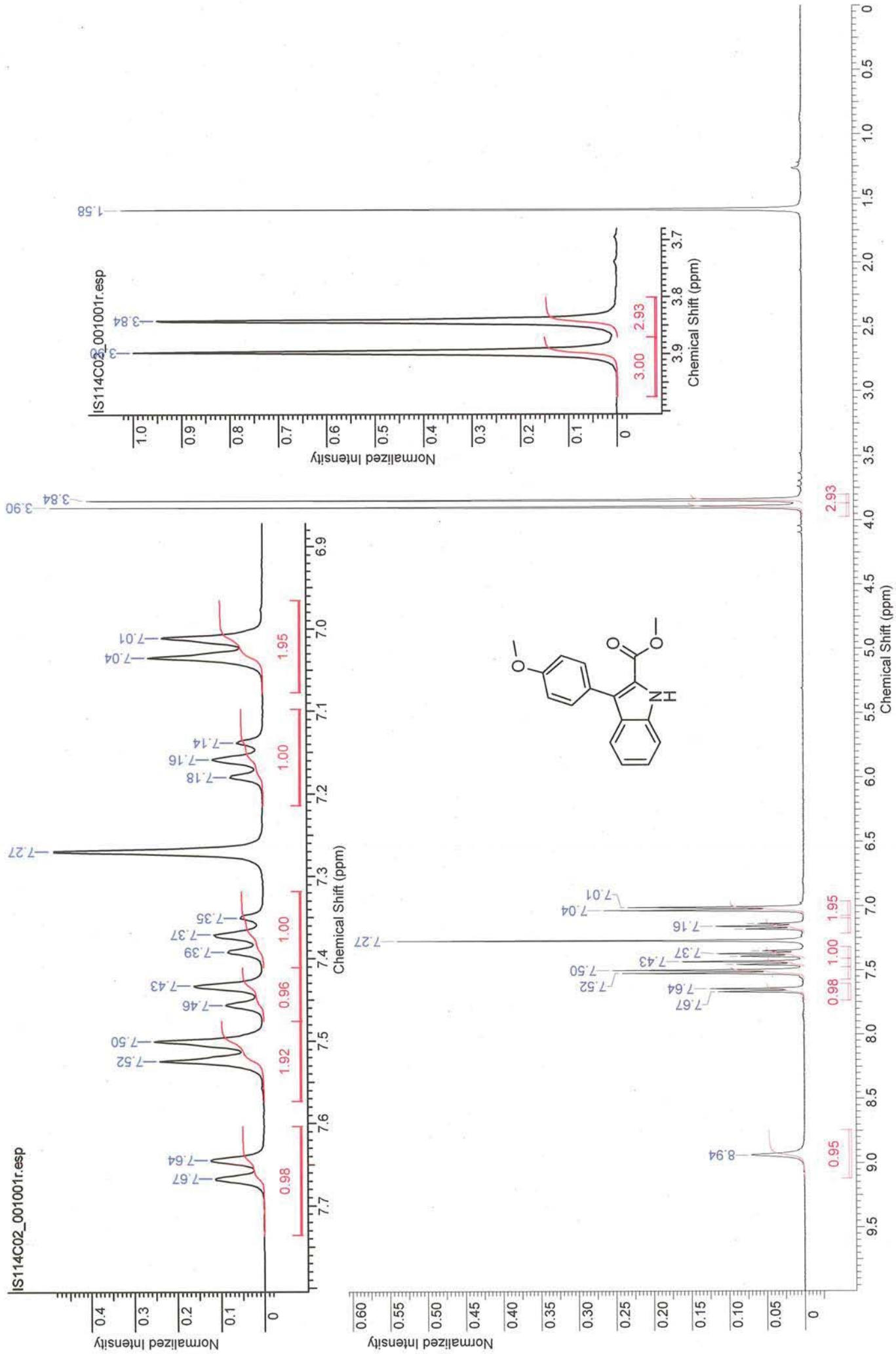
Ion mass = 342.0713610

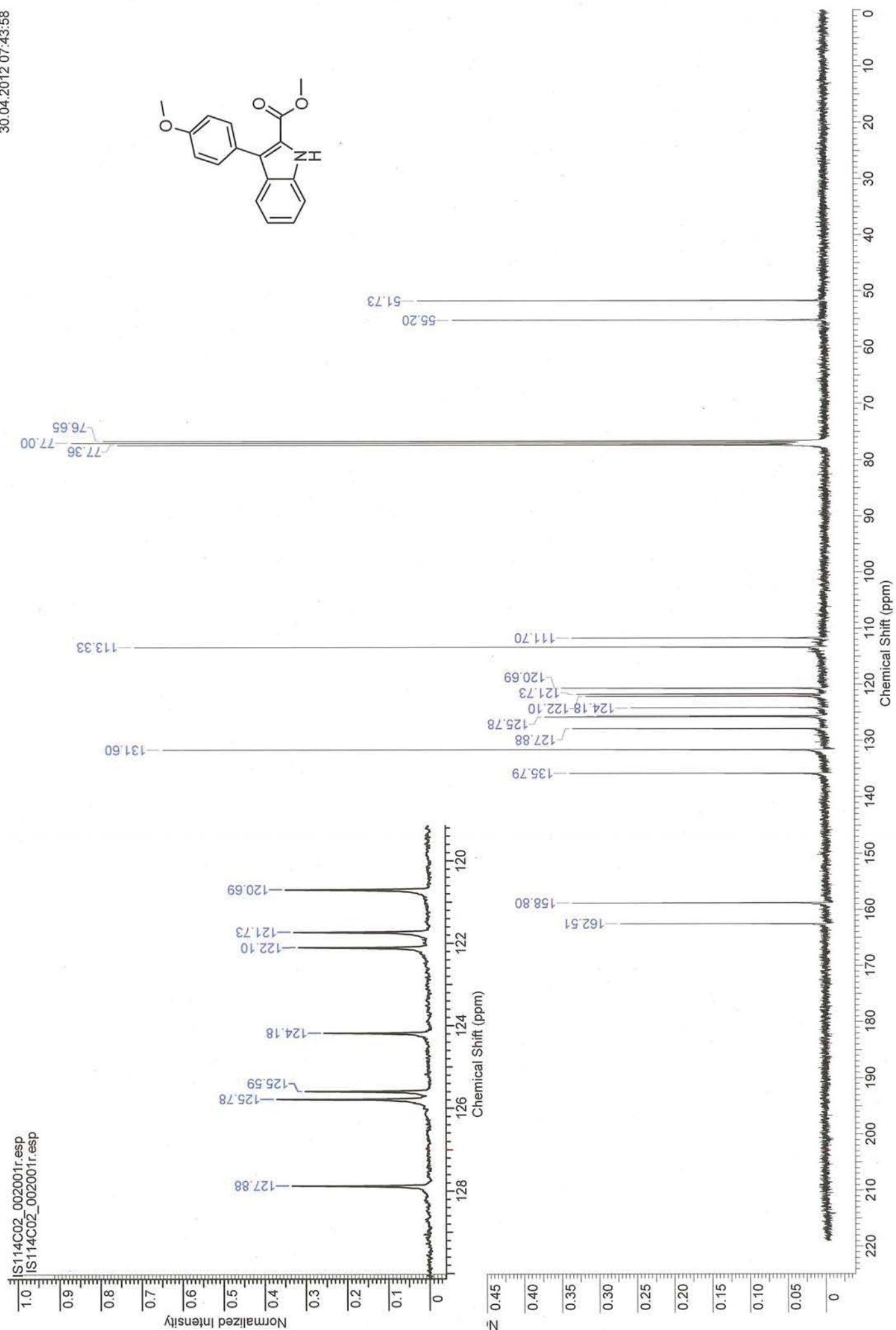
Charge = +1

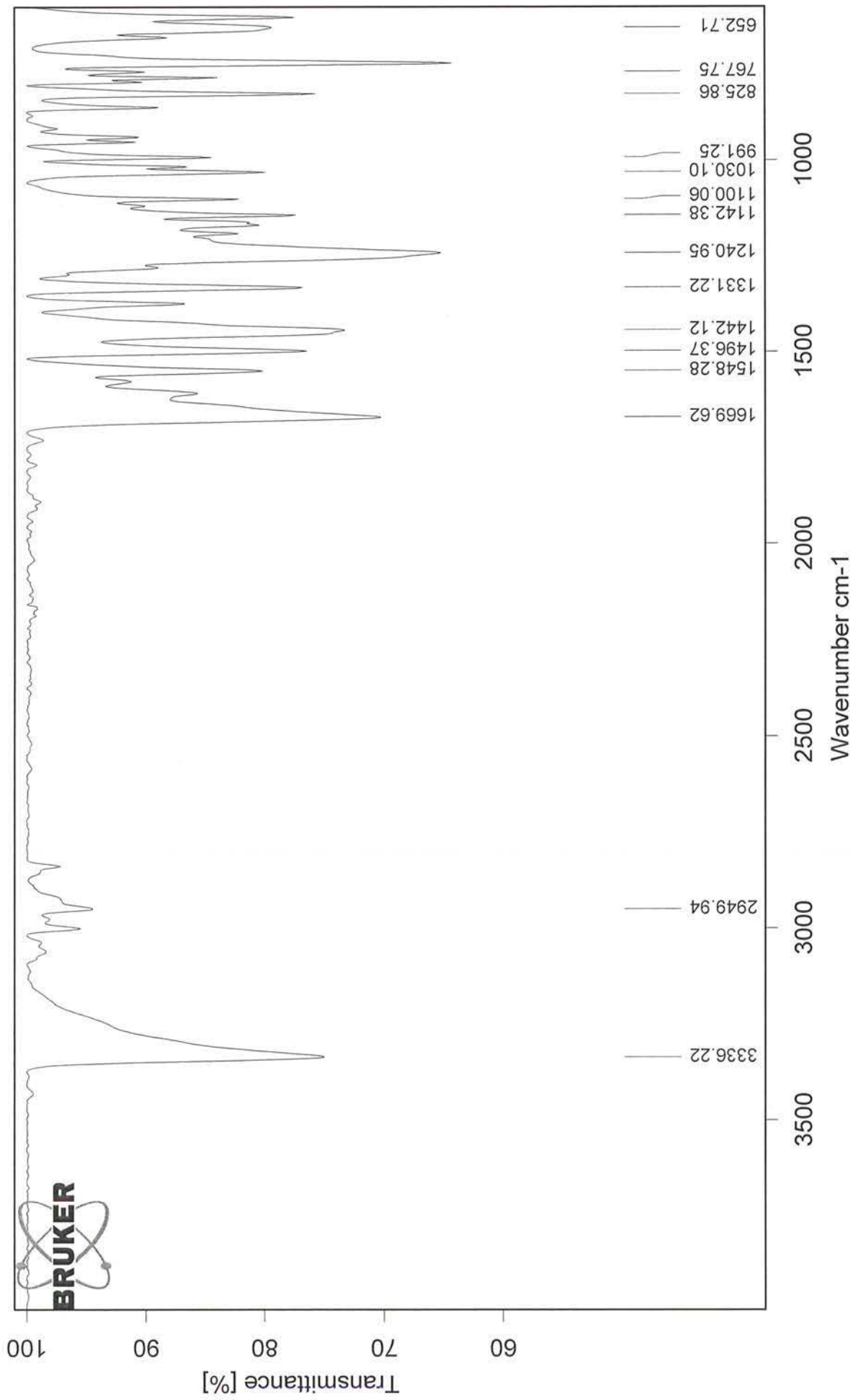
#	C	H	F	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 342.0713610									
1	17	12	3	1	2	1	342.0712343	10.5	1.267e-04
2	12	11	4	4	2	1	342.0710345	7.0	3.265e-04
3	11	12	4	3	5	0	342.0707597	5.5	6.013e-04
4	9	12	5	4	3	1	342.0721774	3.0	8.164e-04
5	17	9	3	4	1	0	342.0722970	14.0	9.360e-04
6	14	13	4	1	3	1	342.0723772	6.5	1.016e-03
7	22	10	2	1	1	0	342.0724968	17.5	1.136e-03
8	20	11	2	1	1	1	342.0700915	14.5	1.270e-03
9	15	10	3	4	1	1	342.0698917	11.0	1.469e-03
10	14	11	3	3	4	0	342.0696169	9.5	1.744e-03











U:\IR_spectra\IS114F.0	white solid	12/11/2010
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ESI-MS: IS114F

XMASS Mass Analysis for /Data/UNI\_FR/ALIM5099\_ESI/3/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

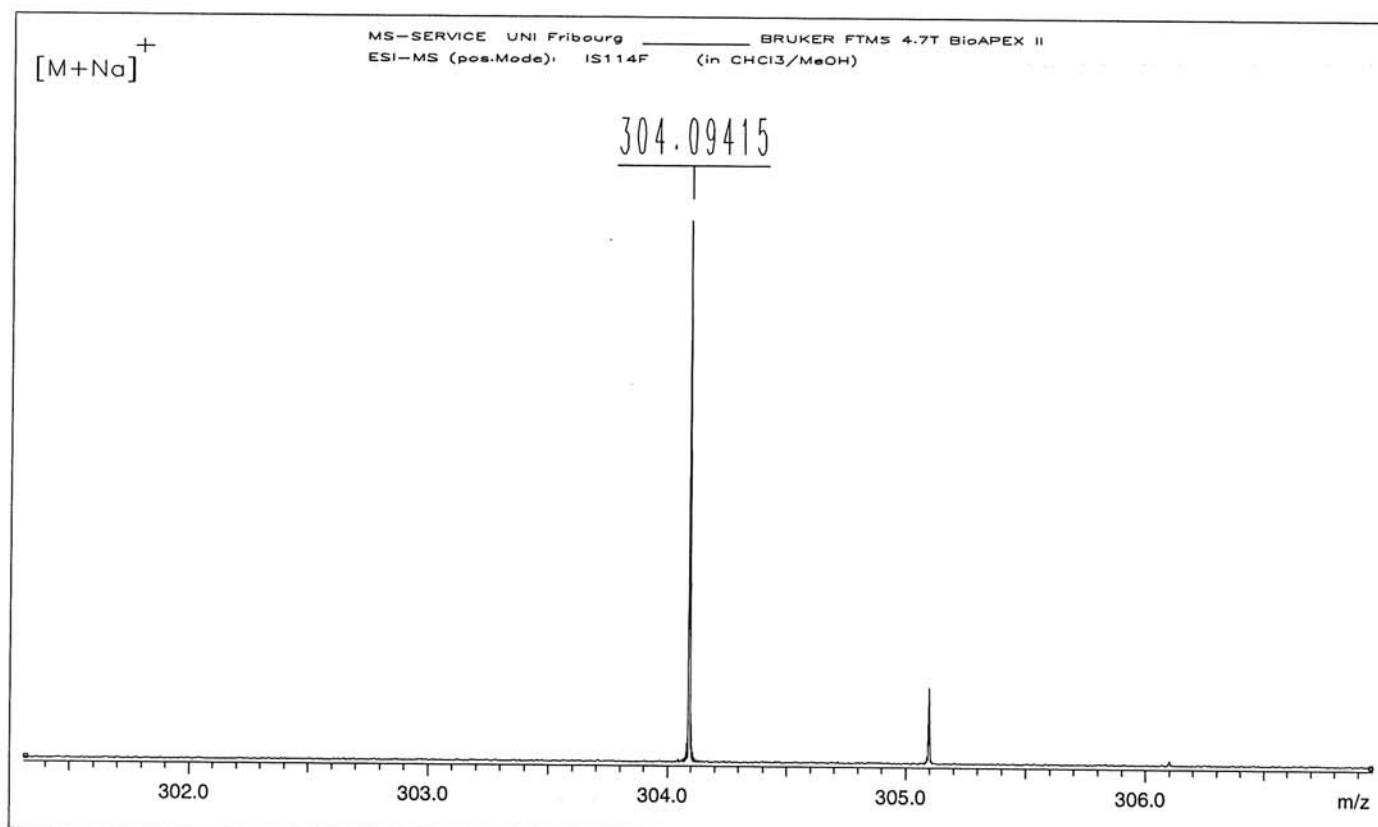
Ion mass = 304.0941460

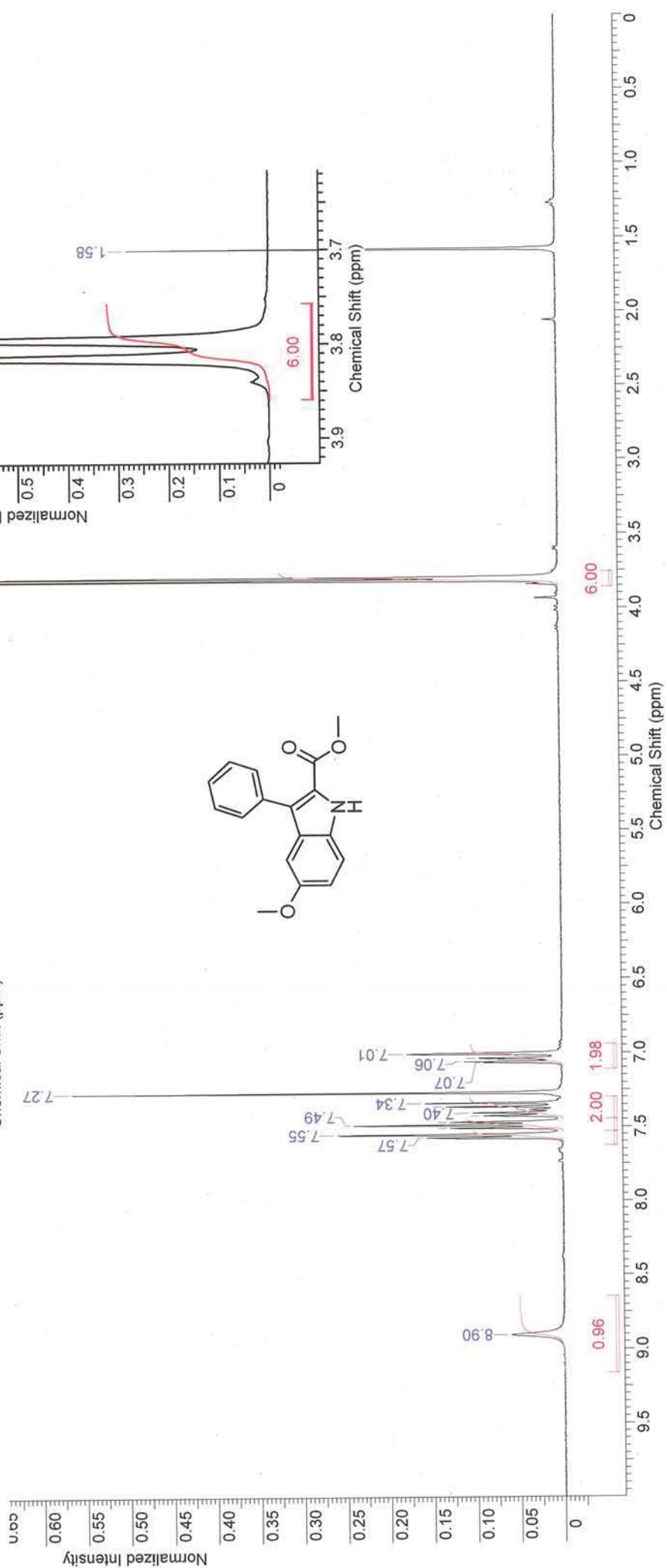
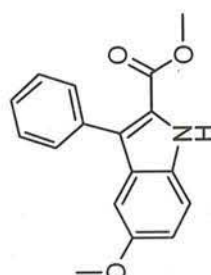
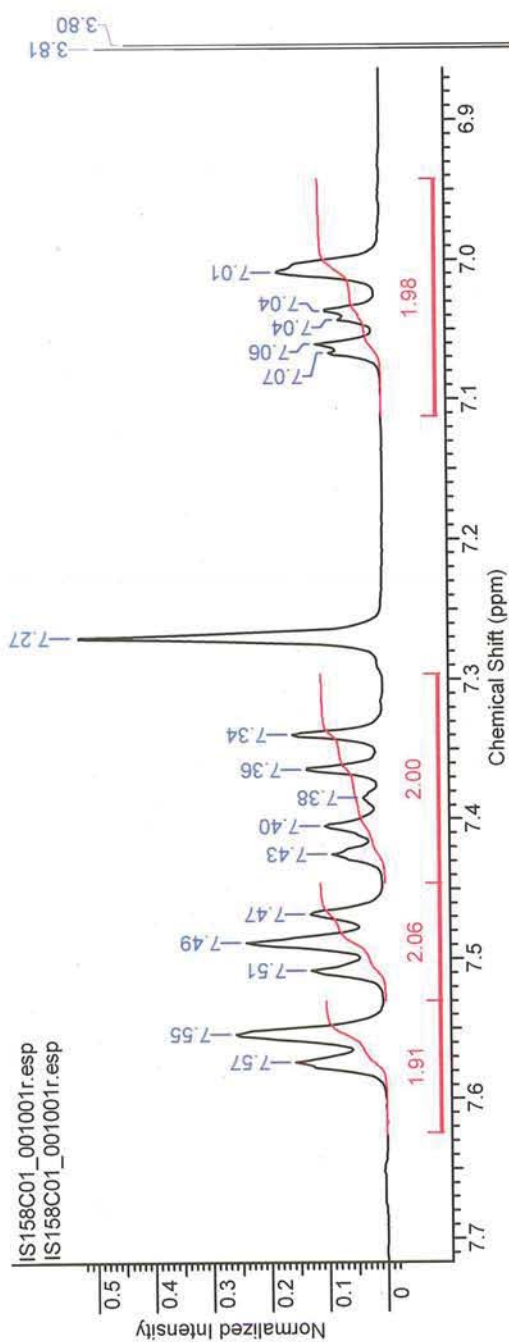
Charge = +1

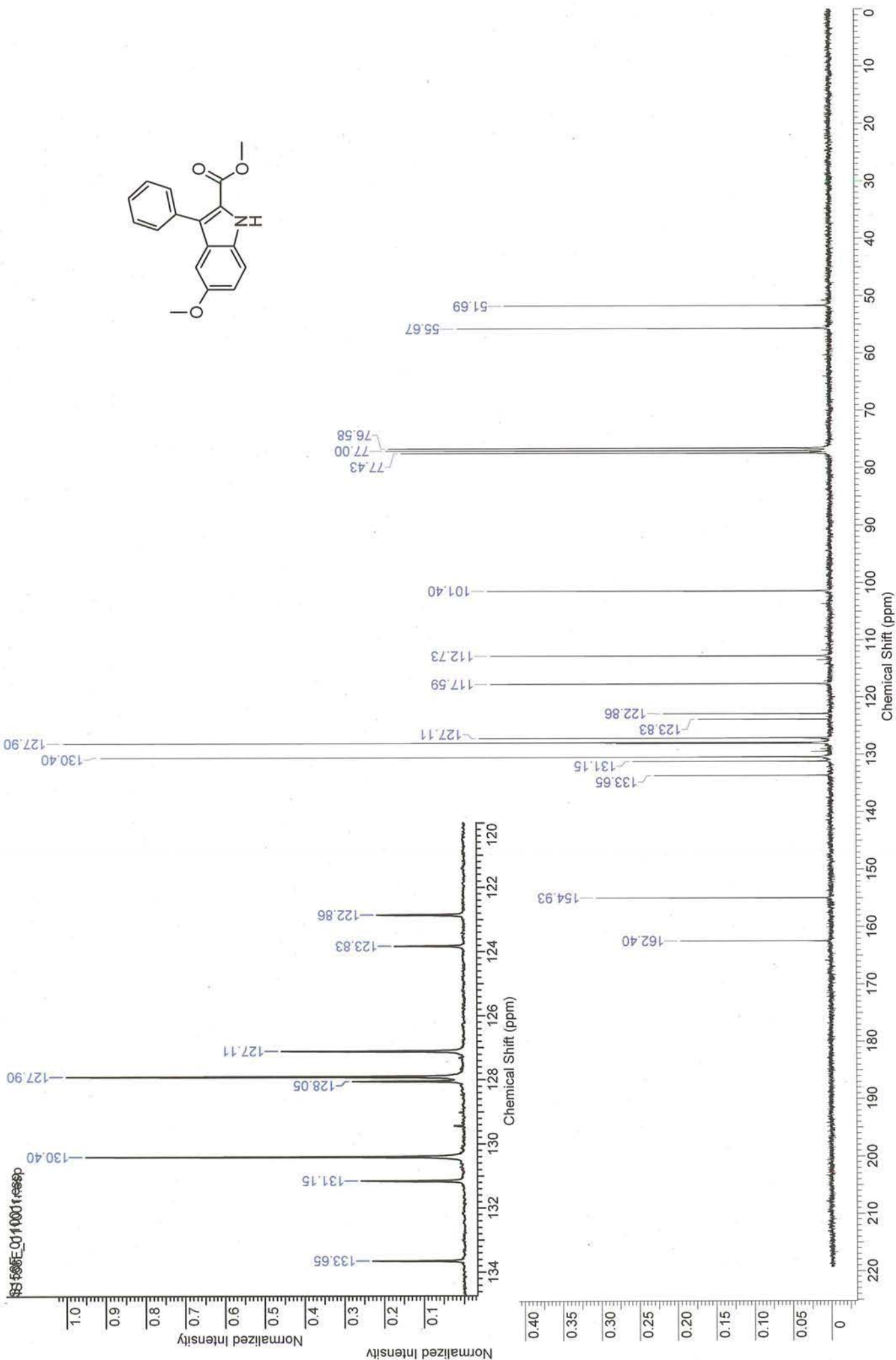
#	C	H	N	O	Na	mass	DBE	error
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\*\*\* Mass Analysis for mass 304.0941460

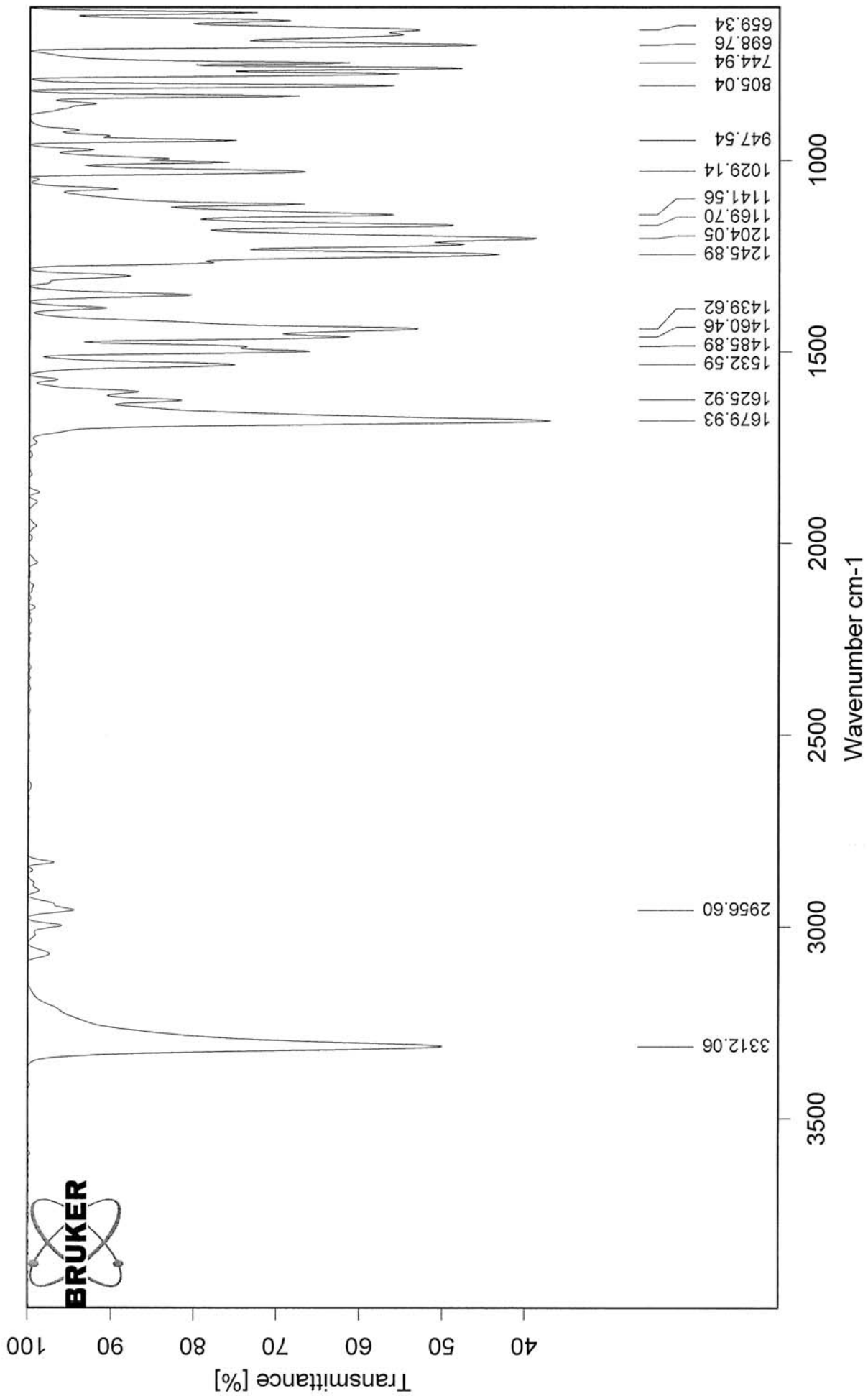
1	17	15	1	3	1	304.0944144	10.5	2.684e-04
2	15	13	4	2	1	304.0930718	11.0	1.074e-03
3	17	12	4	2	0	304.0954771	14.0	1.331e-03
4	14	14	3	5	0	304.0927970	9.5	1.349e-03
5	5	19	3	10	1	304.0962649	-2.5	2.119e-03
6	19	14	1	3	0	304.0968197	13.5	2.674e-03
7	12	15	3	5	1	304.0903917	6.5	3.754e-03
8	11	16	2	8	0	304.0901169	5.0	4.029e-03
9	7	18	3	10	0	304.0986702	0.5	4.524e-03
10	8	17	4	7	1	304.0989450	2.0	4.799e-03











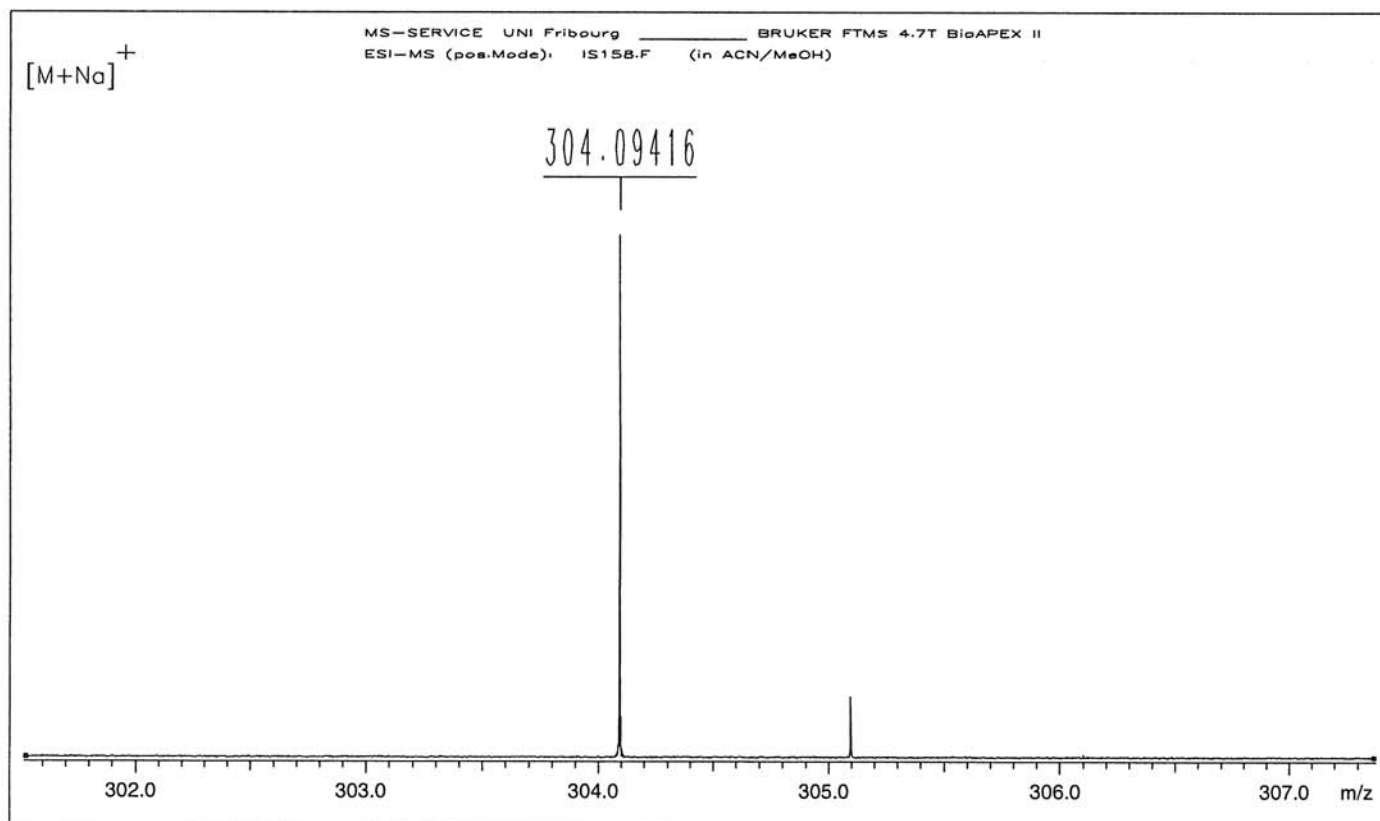
ESI-MS: IS158.F

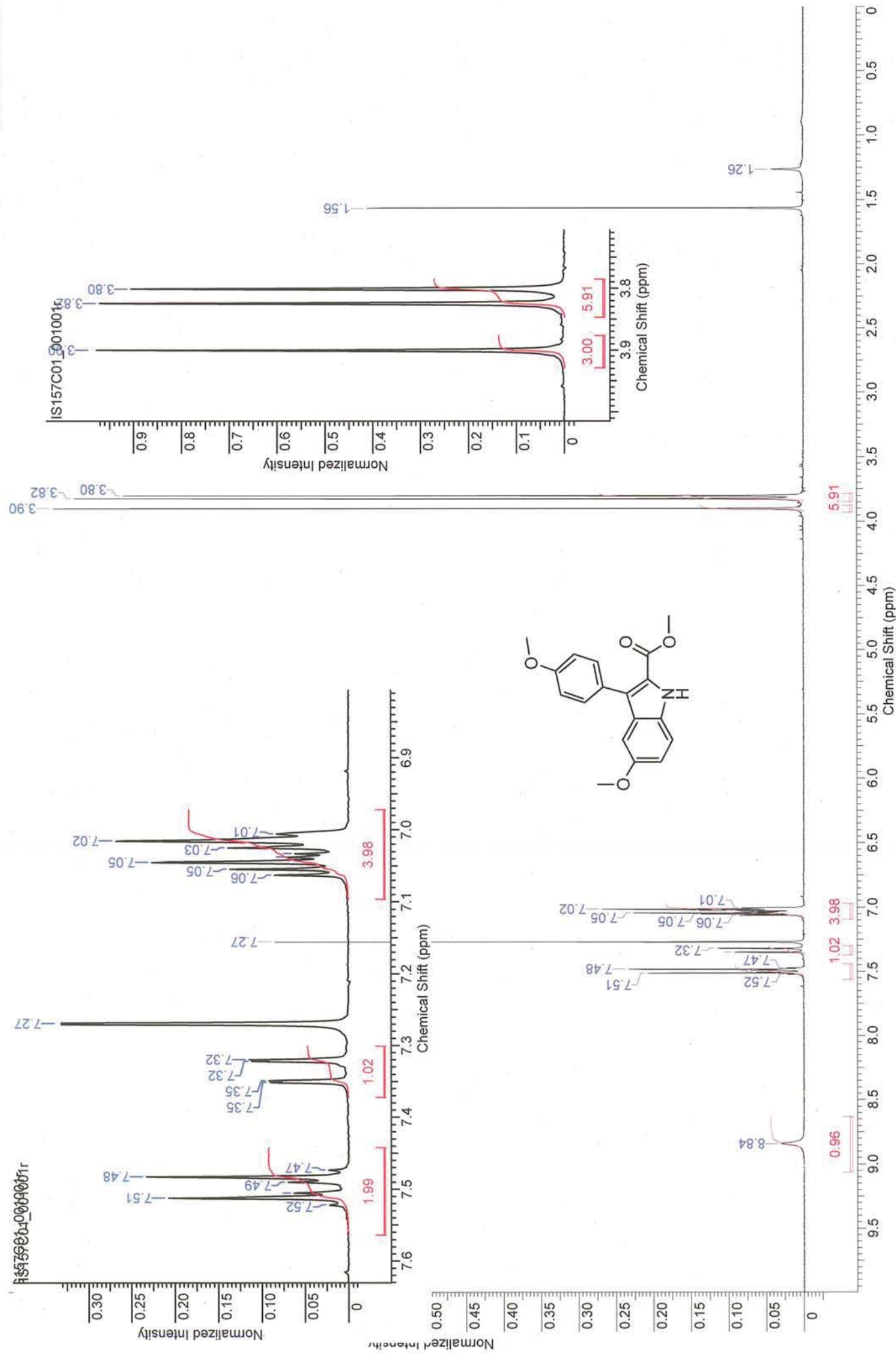
XMASS Mass Analysis for /Data/UNI\_FR/ALIM5318\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

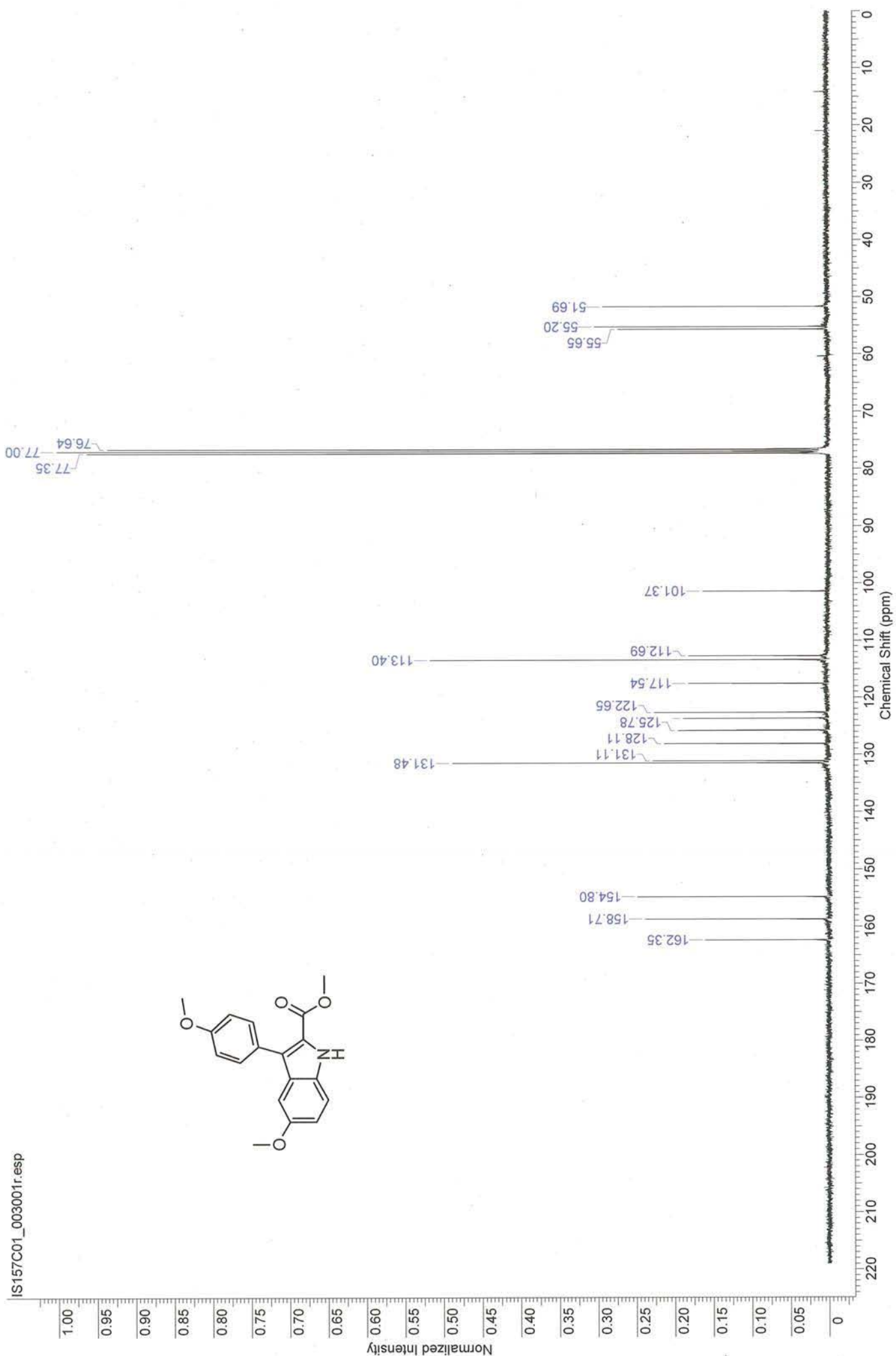
**Ion mass = 304.0941630**

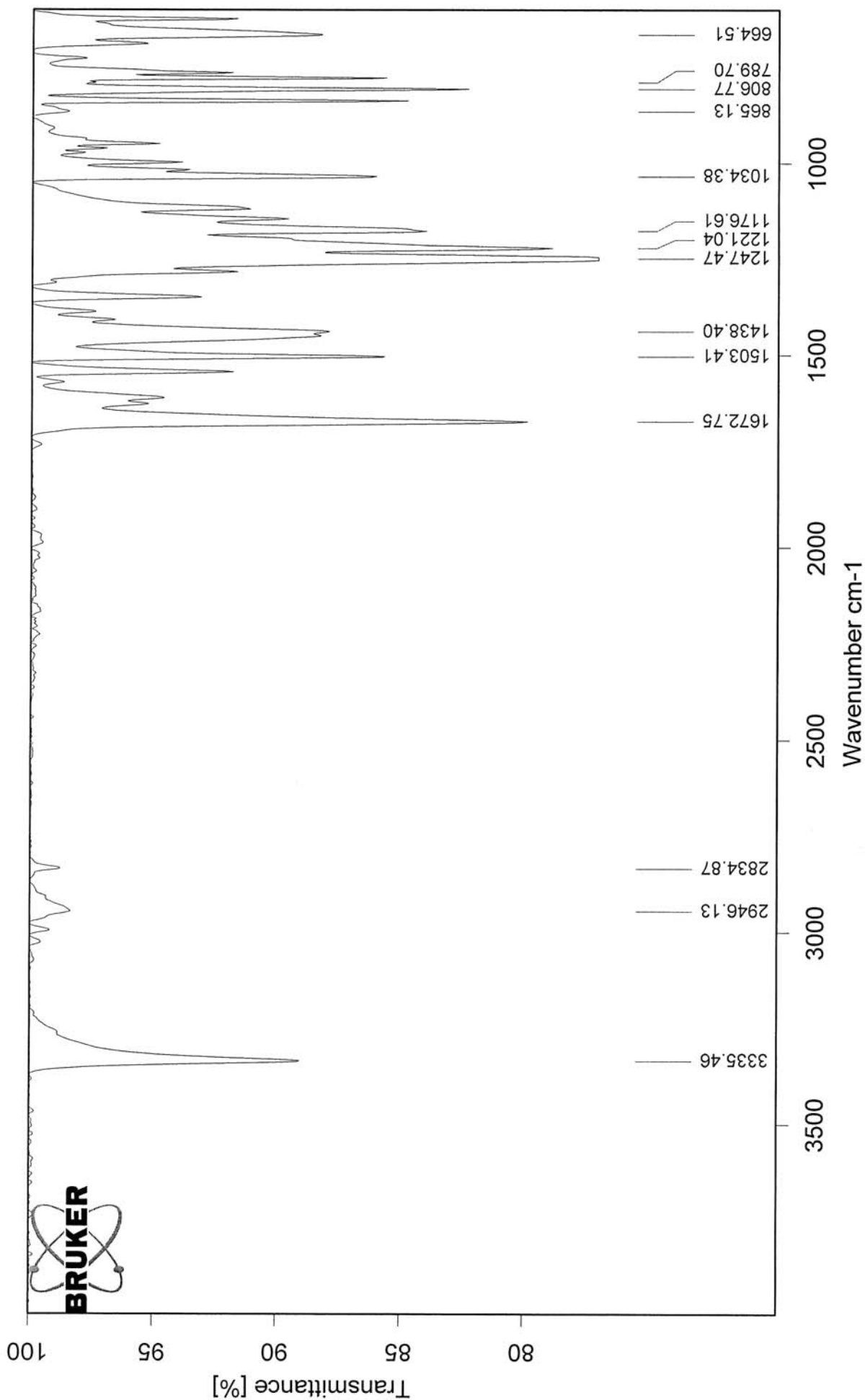
**Charge = +1**

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 304.0941630								
1	17	15	1	3	1	304.0944144	10.5	2.514e-04
2	15	13	4	2	1	304.0930718	11.0	1.091e-03
3	17	12	4	2	0	304.0954771	14.0	1.314e-03
4	14	14	3	5	0	304.0927970	9.5	1.366e-03
5	5	19	3	10	1	304.0962649	-2.5	2.102e-03
6	19	14	1	3	0	304.0968197	13.5	2.657e-03
7	12	12	6	4	0	304.0914543	10.0	2.709e-03
8	5	16	6	9	0	304.0973276	1.0	3.165e-03
9	12	15	3	5	1	304.0903917	6.5	3.771e-03
10	11	16	2	8	0	304.0901169	5.0	4.046e-03









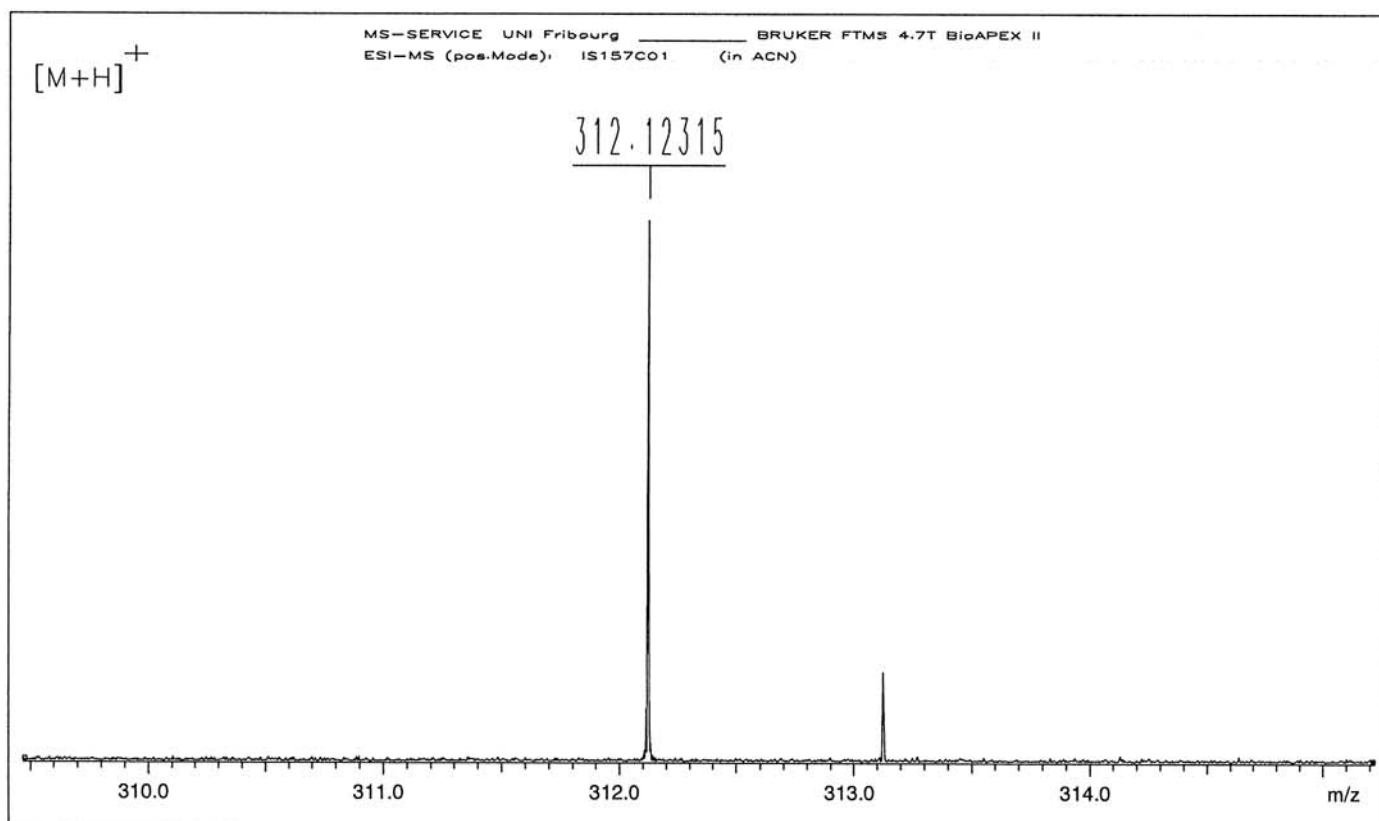
ESI-MS: IS157C01

XMASS Mass Analysis for /Data/UNI\_FR/ALIM5301\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

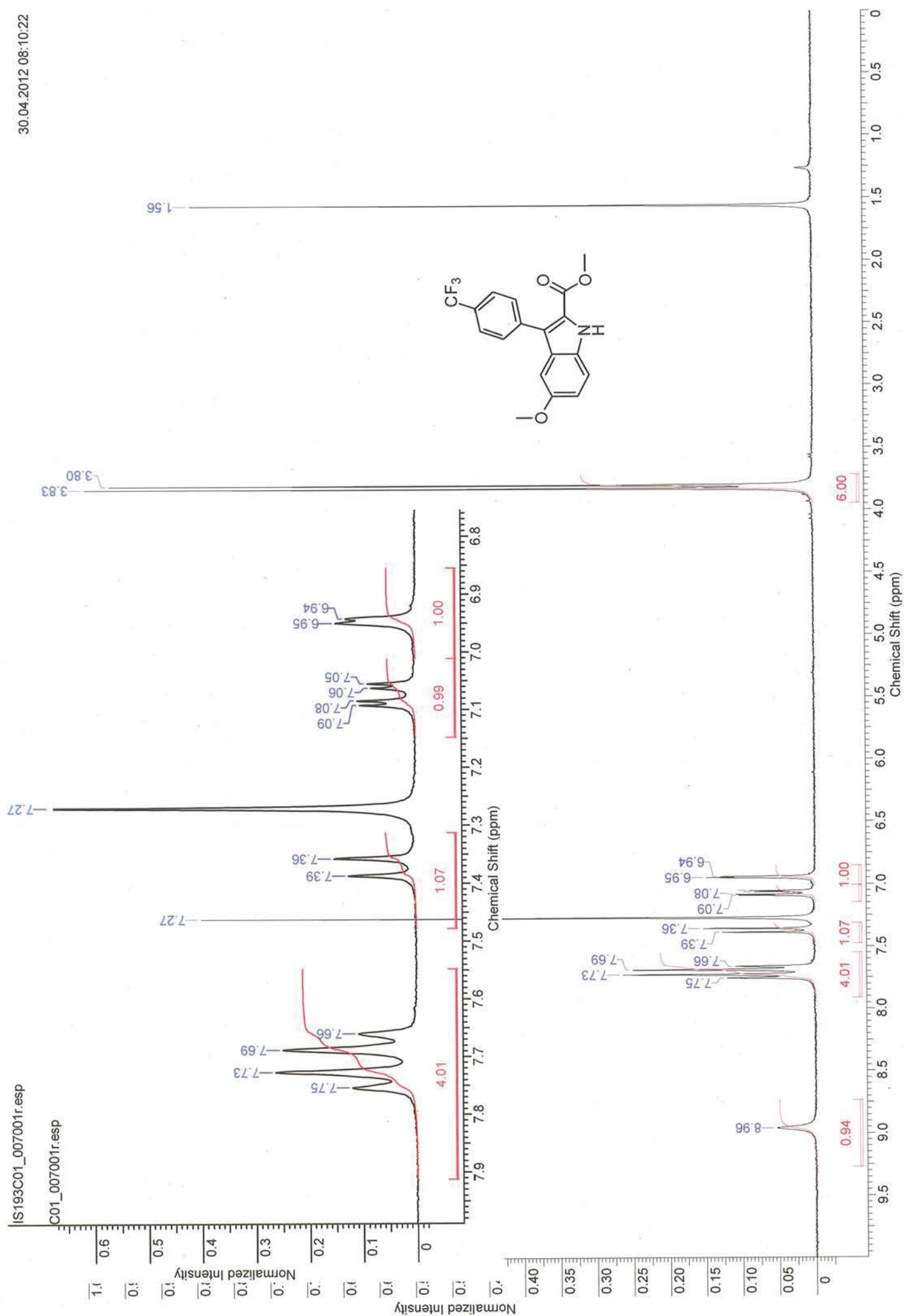
Ion mass = 312.1231460

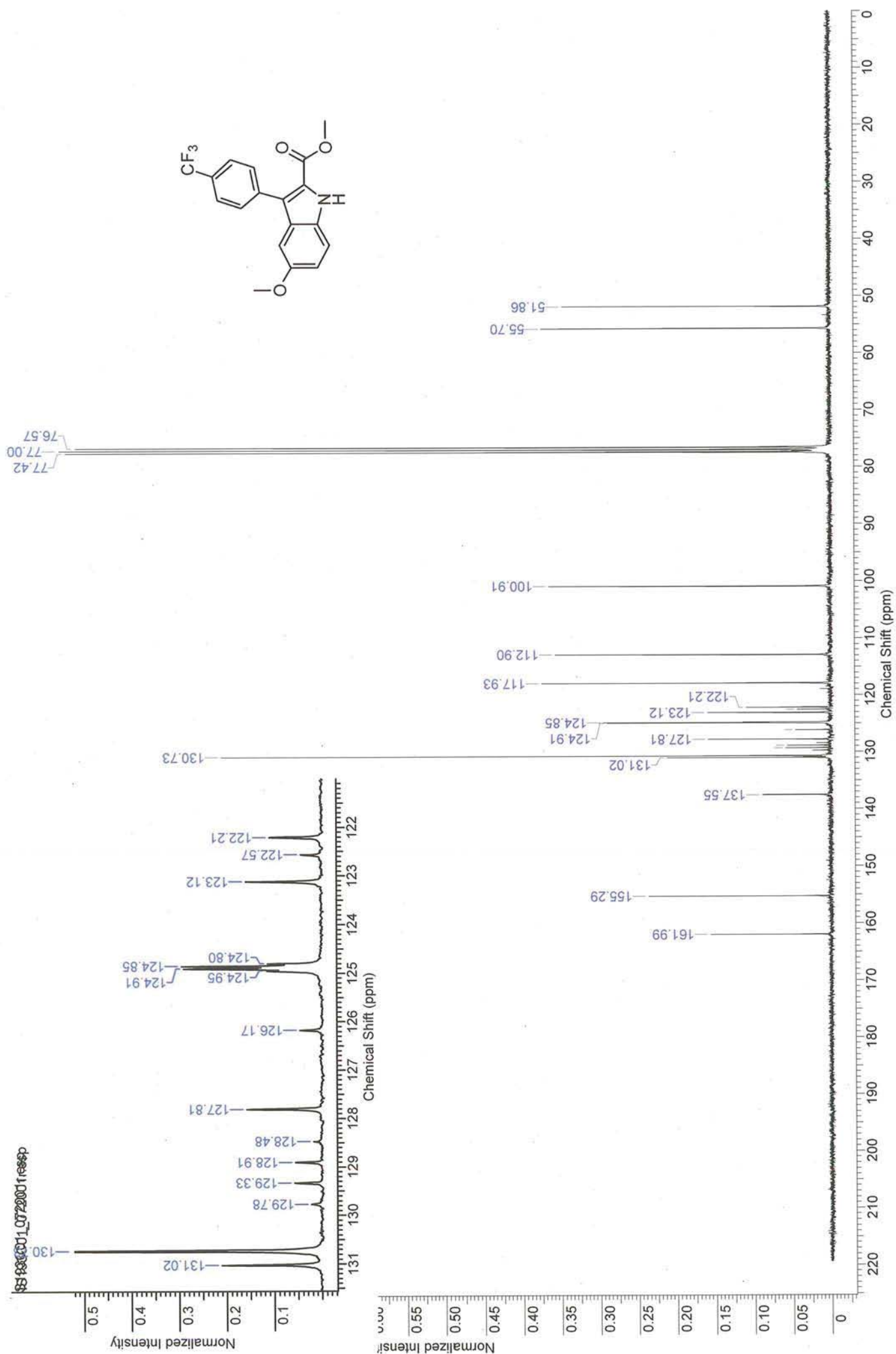
Charge = +1

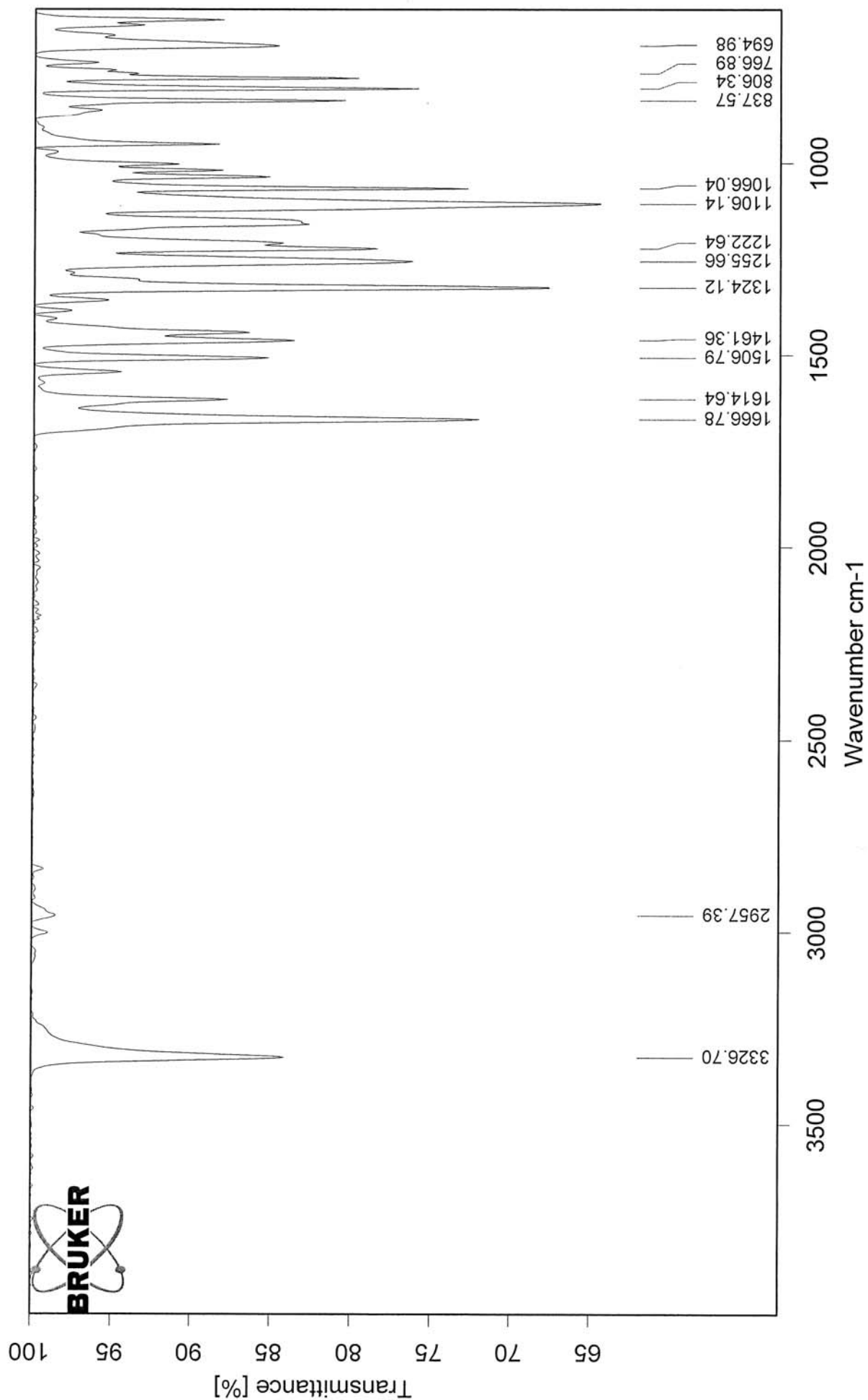
#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 312.1231460							
1	18	18	1	4	312.1230345	10.5	1.115e-04
2	16	16	4	3	312.1216918	11.0	1.454e-03
3	5	16	10	6	312.1248797	3.0	1.734e-03
4	21	16	2	1	312.1257146	15.0	2.569e-03
5	14	14	7	2	312.1203491	11.5	2.797e-03
6	7	18	7	7	312.1262224	2.5	3.076e-03
7	13	18	3	6	312.1190117	6.5	4.134e-03
8	12	12	10	1	312.1190065	12.0	4.140e-03
9	9	20	4	8	312.1275651	2.0	4.419e-03
10	11	16	6	5	312.1176691	7.0	5.477e-03











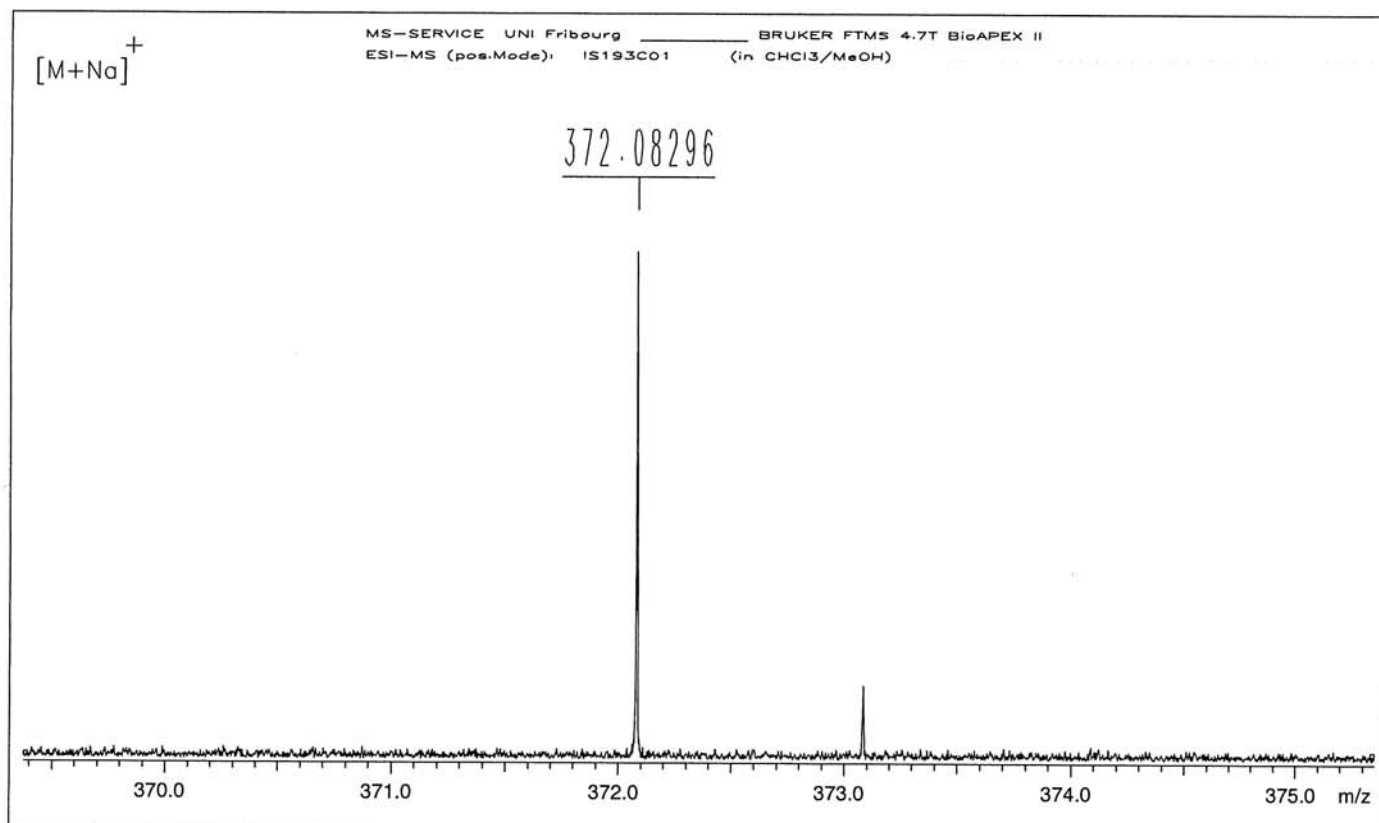
ESI-MS: IS193C01

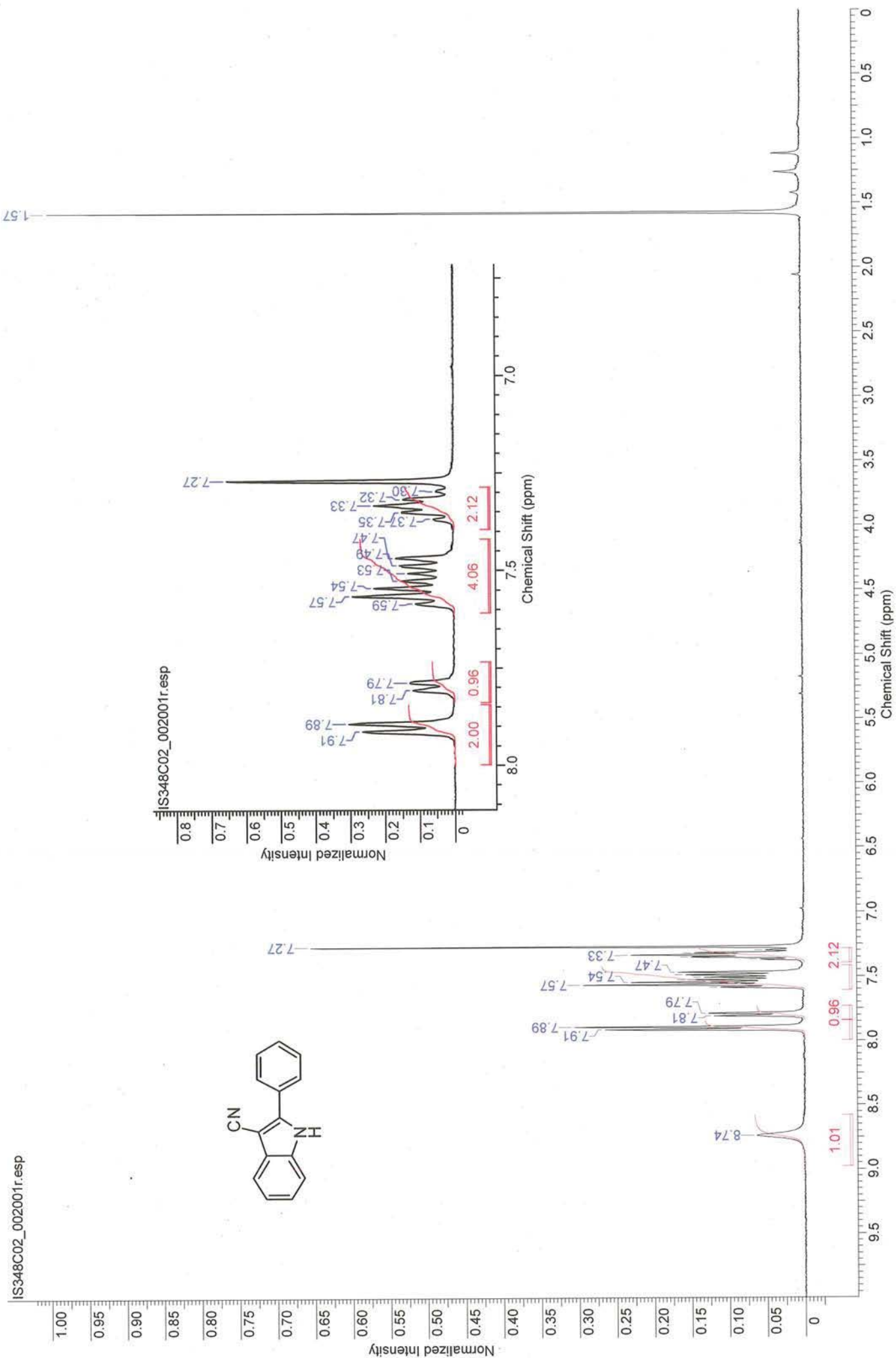
XMASS Mass Analysis for /Data/UNI\_FR/ALIM5470\_ESI/5/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

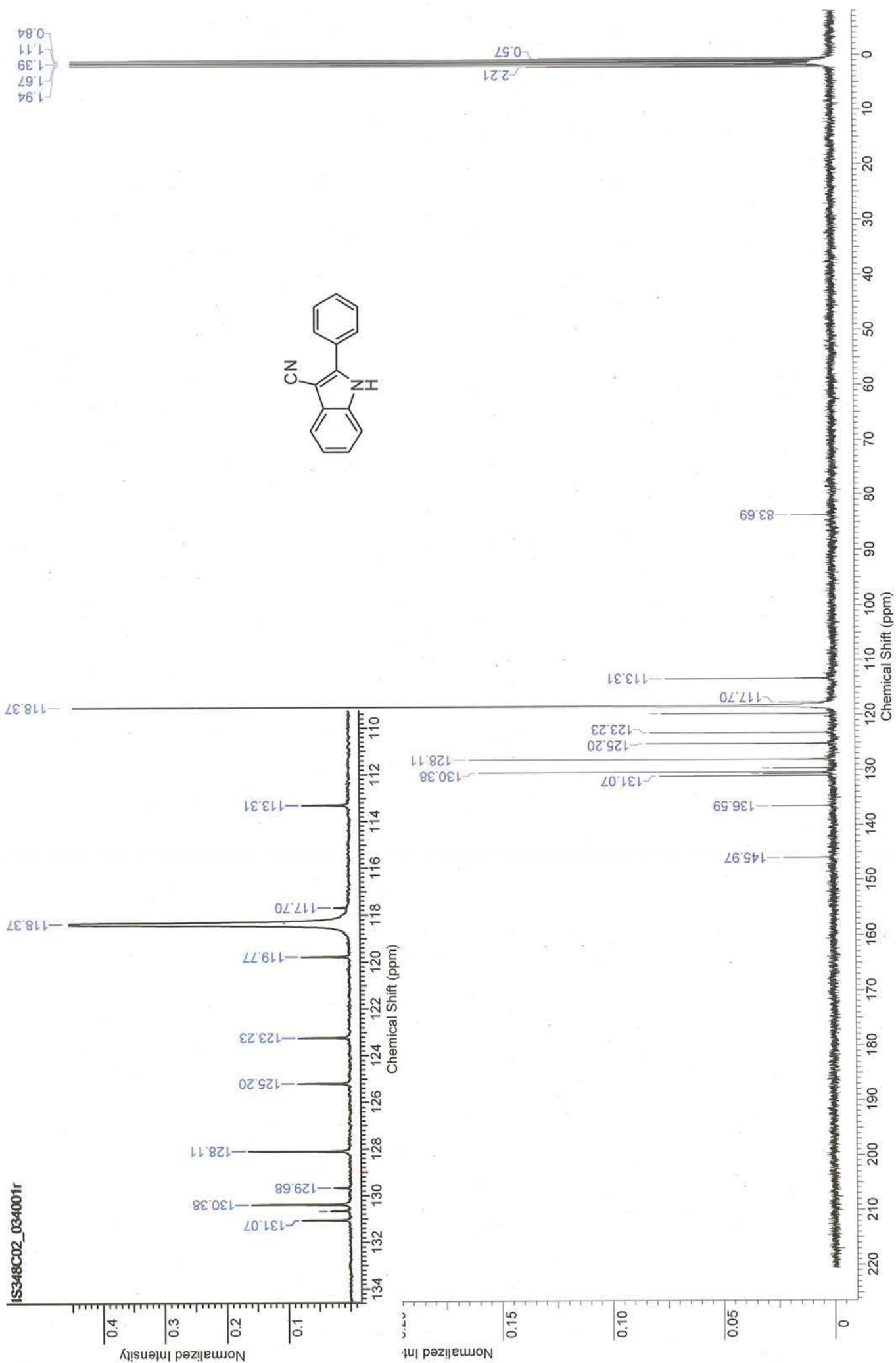
**Ion mass = 372.0829640**

**Charge = +1**

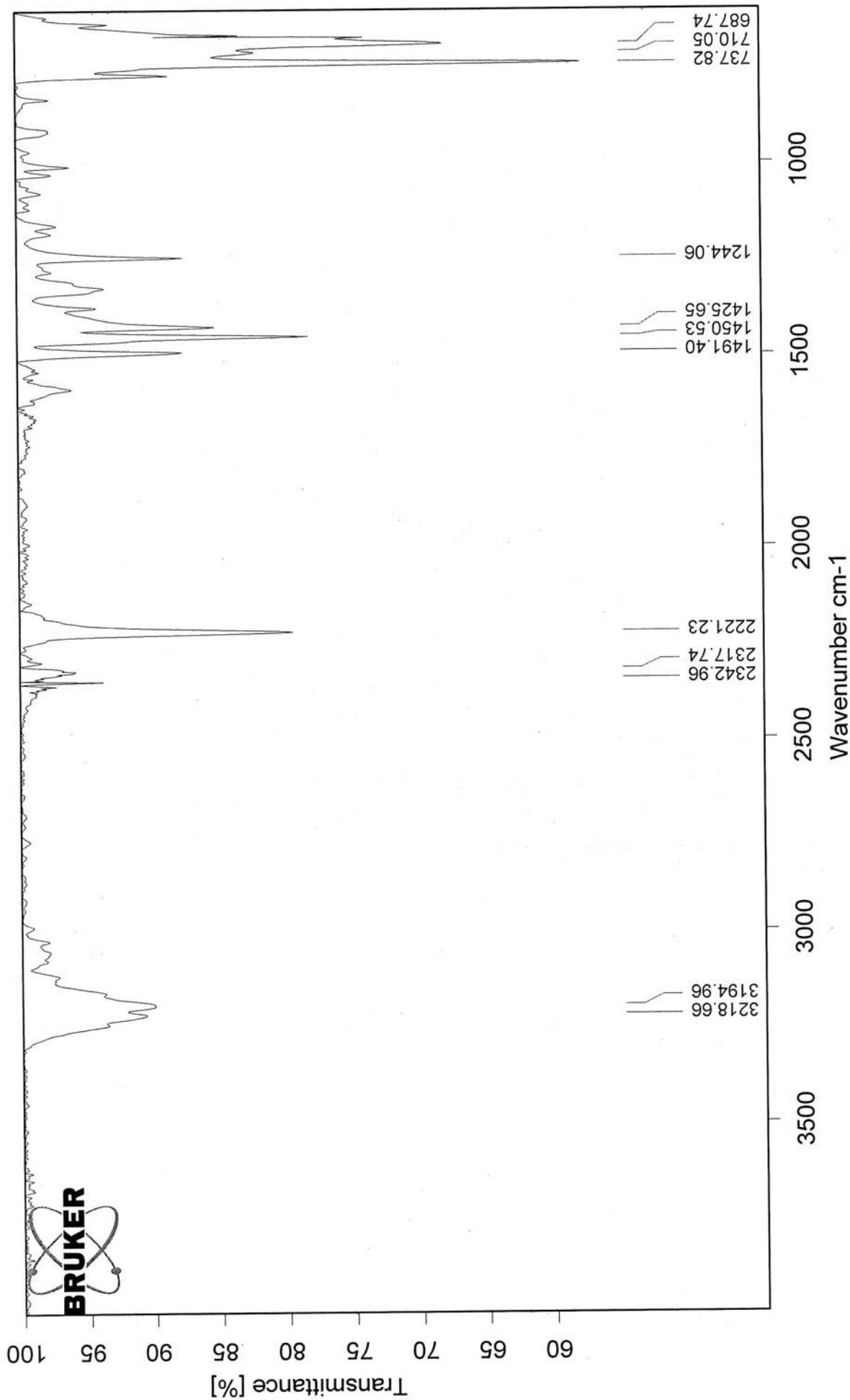
#	C	H	F	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 372.0829640									
1	18	14	3	1	3	1	372.0817990	10.5	1.165e-03
2	20	13	3	1	3	0	372.0842043	13.5	1.240e-03
3	17	16	1	1	6	1	372.0853865	9.5	2.423e-03
4	15	13	3	3	5	0	372.0801816	9.5	2.782e-03
5	18	12	2	3	4	0	372.0790387	13.5	3.925e-03
6	19	15	1	1	6	0	372.0877918	12.5	4.828e-03
7	20	14	1	2	3	1	372.0880666	14.0	5.103e-03
8	13	14	3	3	5	1	372.0777763	6.5	5.188e-03
9	17	15	2	2	4	1	372.0892095	10.0	6.245e-03
10	16	13	2	3	4	1	372.0766334	10.5	6.331e-03











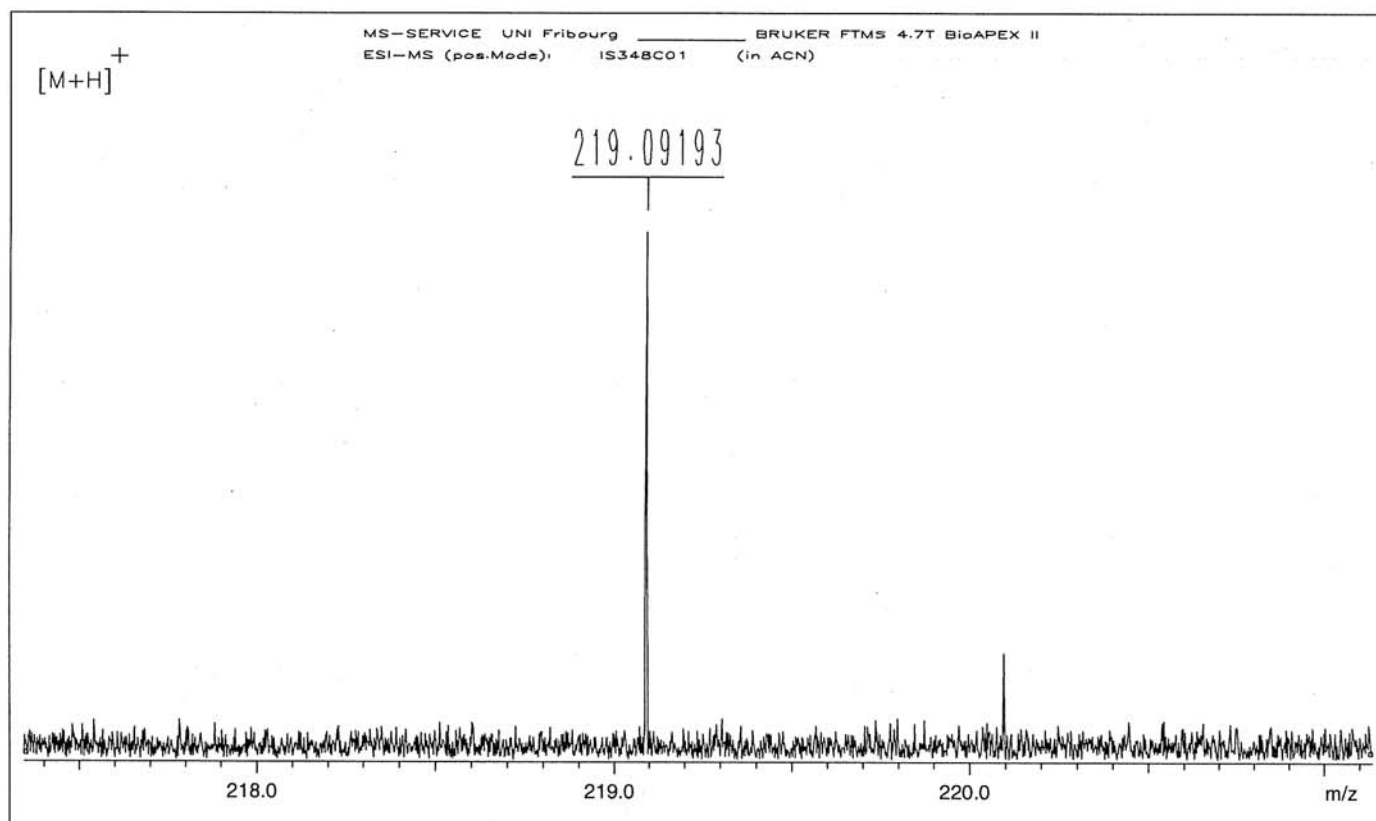
ESI-MS: IS348C01

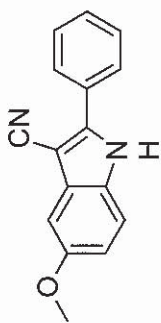
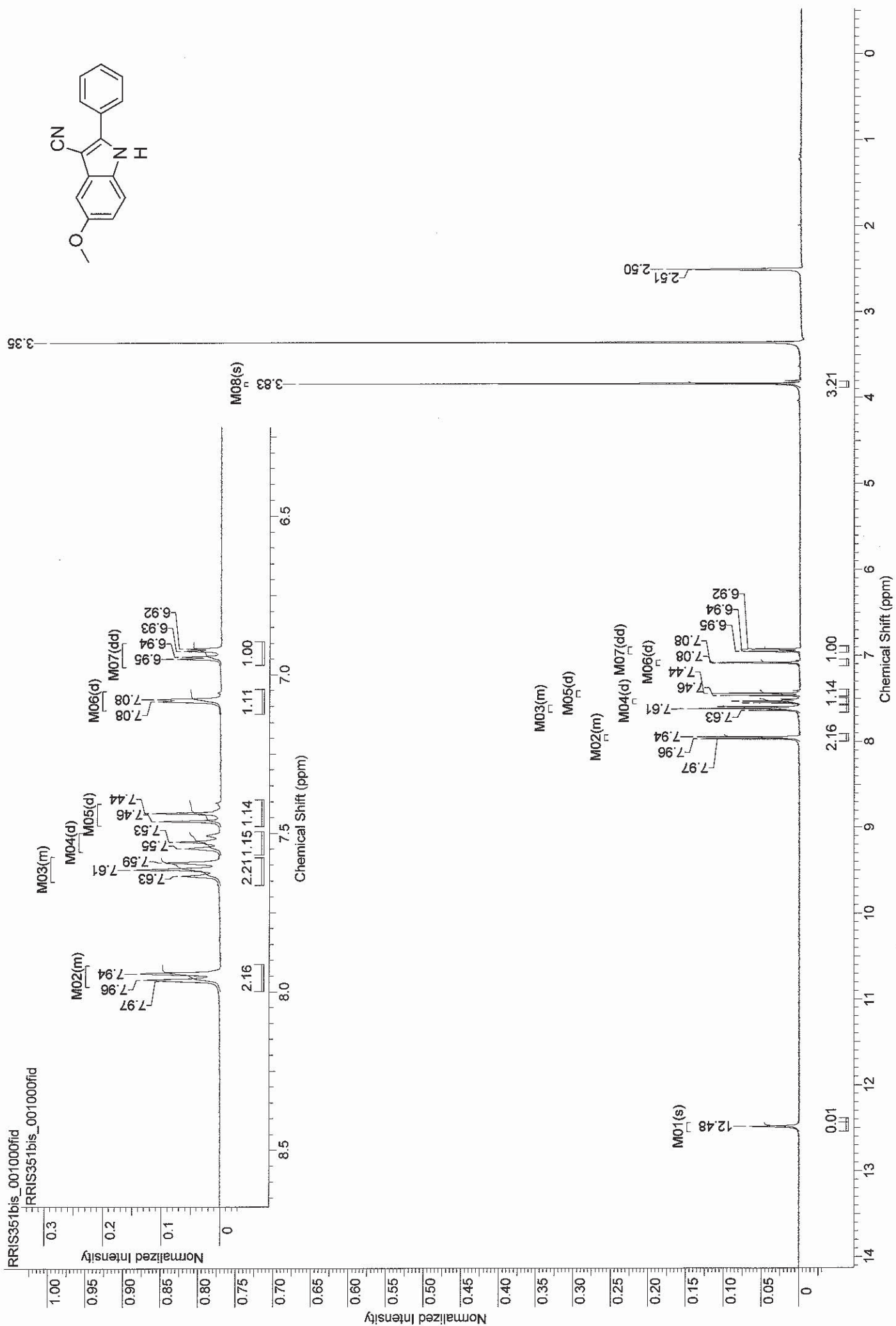
XMASS Mass Analysis for /Data/UNI\_FR/ALIM6535\_ESI/10/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

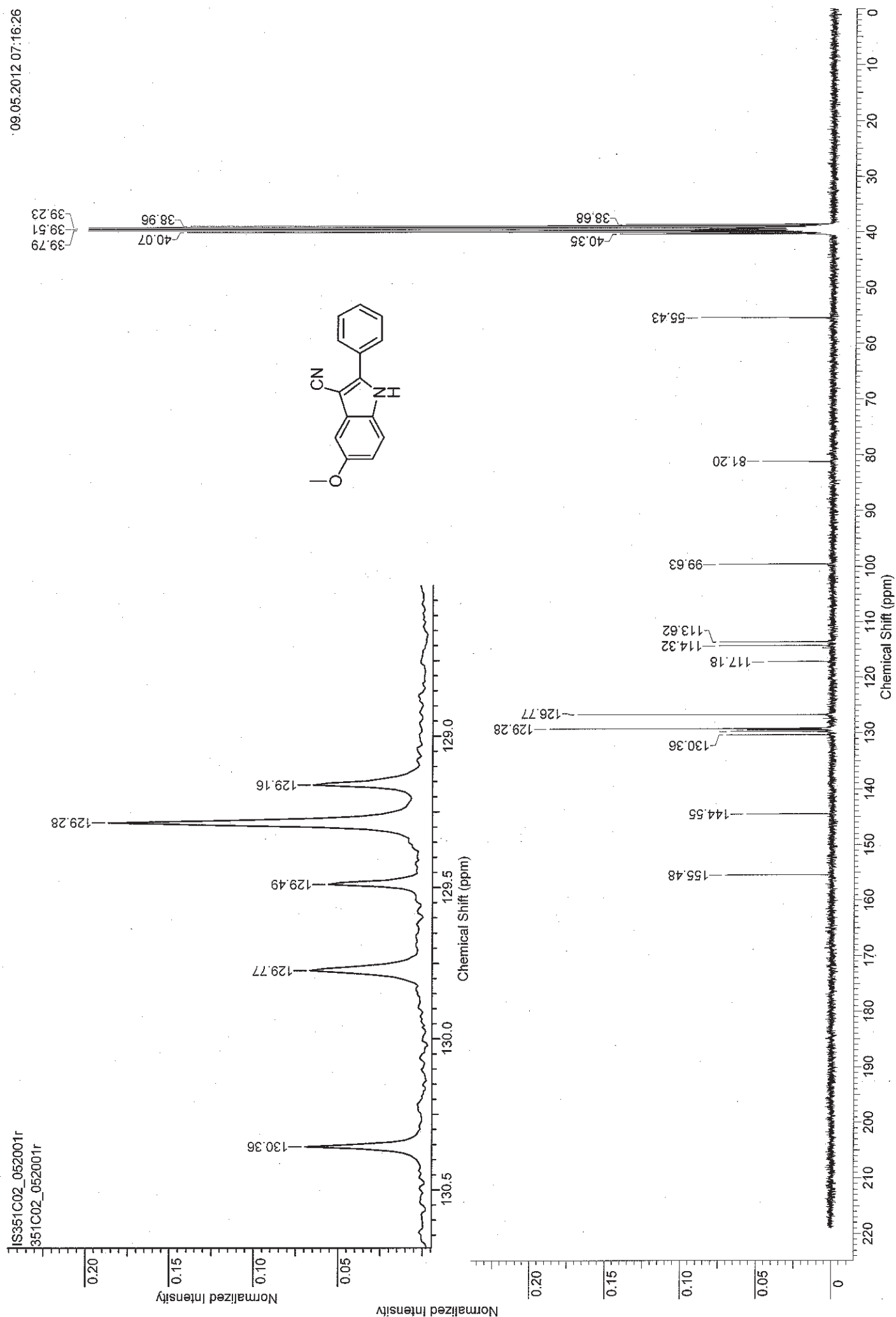
Ion mass = 219.0919320

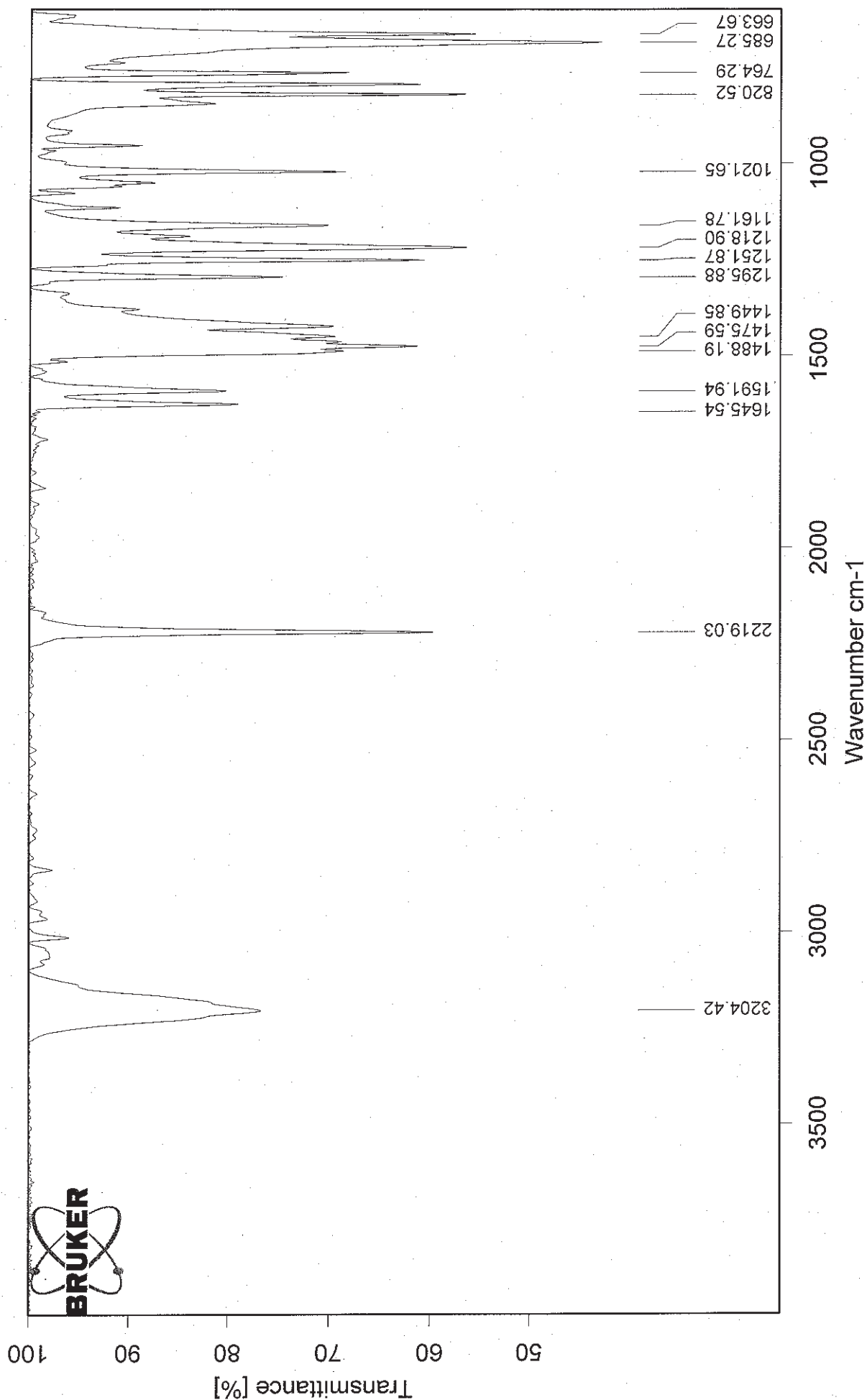
Charge = +1

#	C	H	N	mass	DBE	error
*** Mass Analysis for mass 219.0919320						
1	15	11	2	219.0916748	11.5	2.572e-04
2	7	9	9	219.0975428	8.0	5.611e-03
3	6	7	10	219.0849667	8.5	6.965e-03
4	16	13	1	219.1042508	11.0	1.232e-02
5	14	9	3	219.0790987	12.0	1.283e-02
6	8	11	8	219.1101188	7.5	1.819e-02
7	13	7	4	219.0665227	12.5	2.541e-02
8	9	13	7	219.1226949	7.0	3.076e-02
9	12	5	5	219.0539466	13.0	3.799e-02
10	10	15	6	219.1352709	6.5	4.334e-02









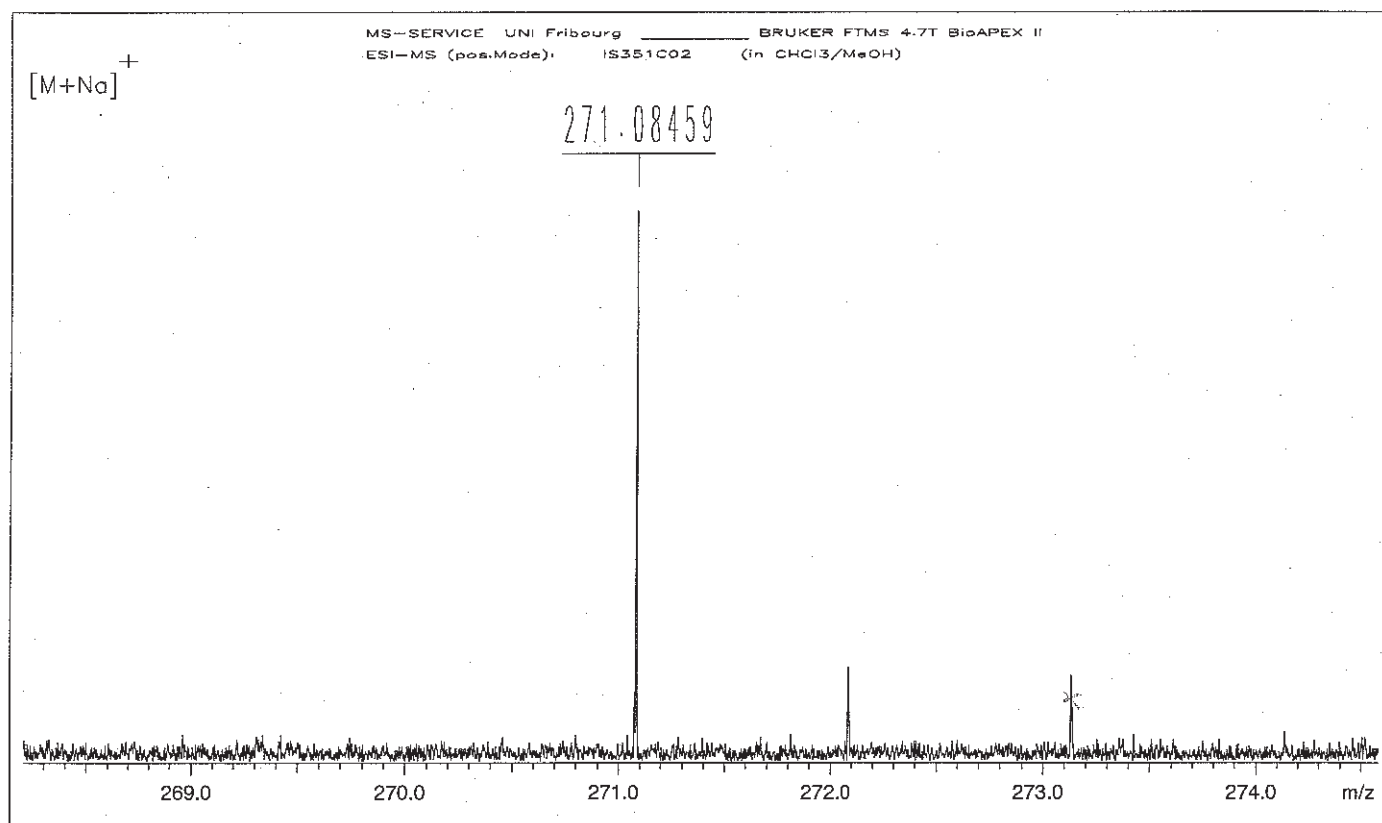
ESI-MS: IS351C02

XMASS Mass Analysis for /Data/UNI\_FR/ALIM6555\_ESI/4/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

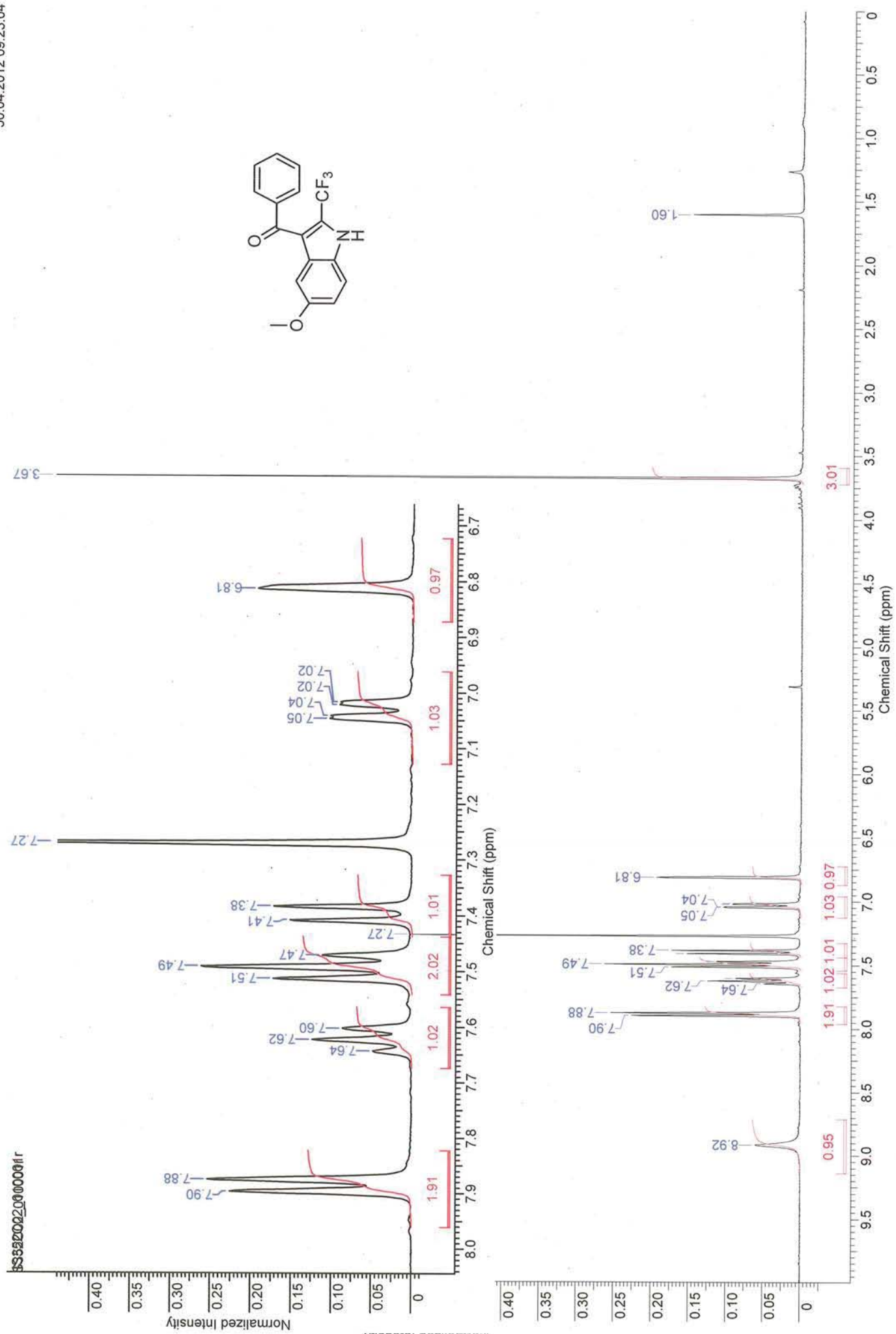
Ion mass = 271.0845900

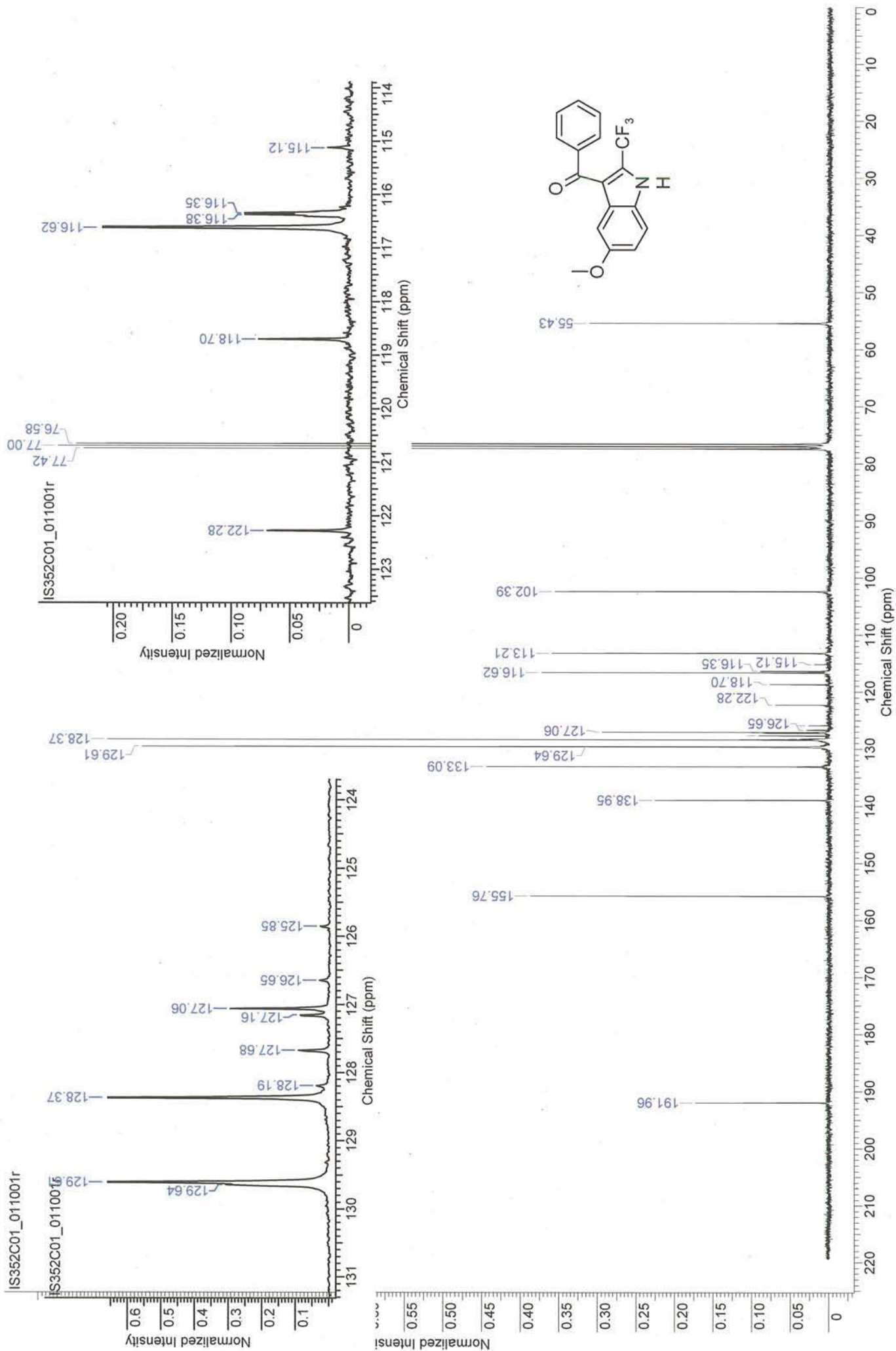
Charge = +1

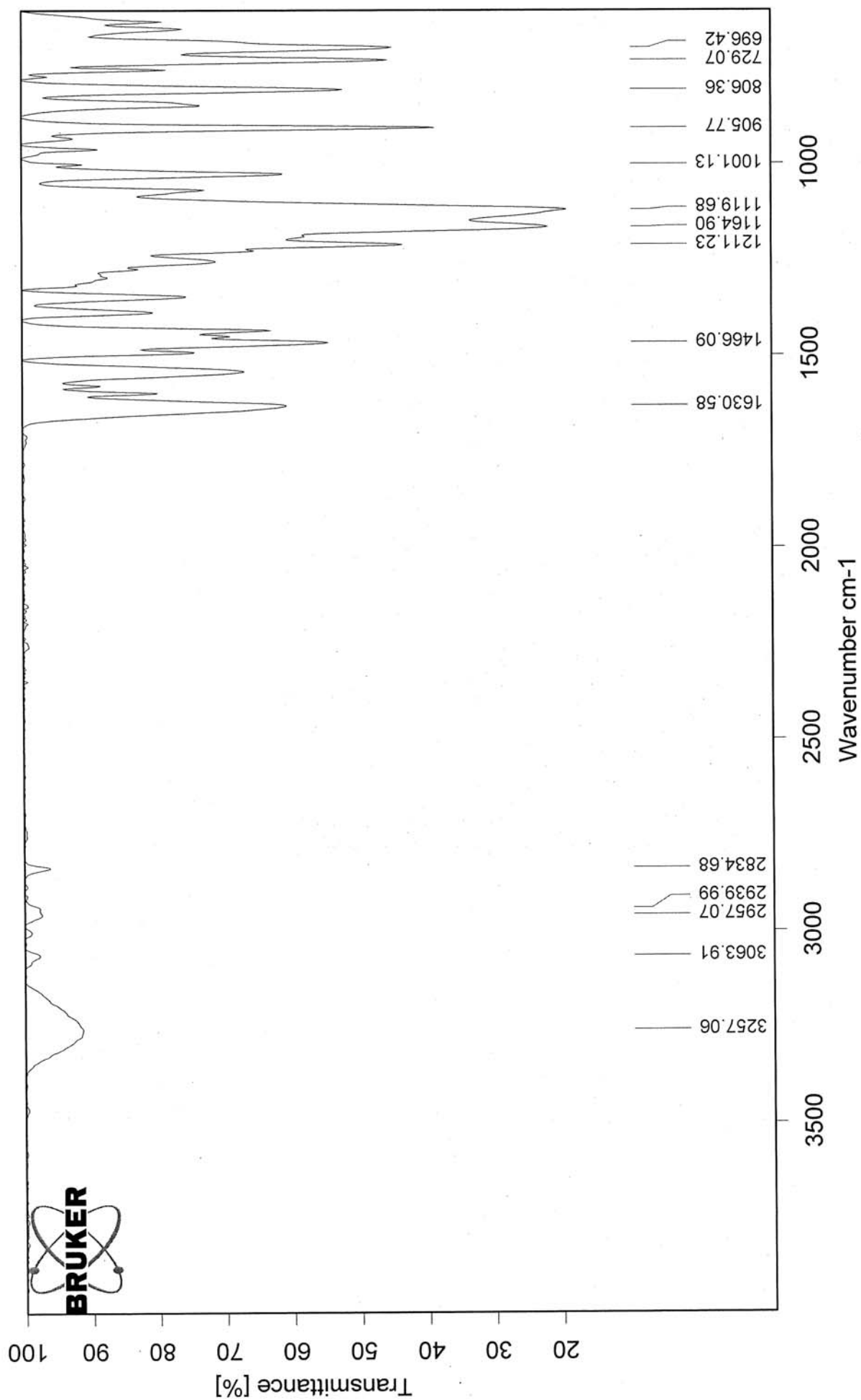
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 271.0845900								
1	16	12	2	1	1	271.0841841	11.5	4.059e-04
2	15	13	1	4	0	271.0839093	10.0	6.807e-04
3	18	11	2	1	0	271.0865894	14.5	1.999e-03
4	13	11	4	3	0	271.0825667	10.5	2.023e-03
5	5	12	8	4	1	271.0873720	3.5	2.782e-03
6	6	18	1	9	1	271.0873773	-2.0	2.787e-03
7	13	14	1	4	1	271.0815040	7.0	3.086e-03
8	11	9	7	2	0	271.0812240	11.0	3.366e-03
9	6	15	4	8	0	271.0884399	1.5	3.850e-03
10	7	14	5	5	1	271.0887147	3.0	4.125e-03











brown liquid

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IS352C01

19/04/2012

ESI-MS: IS352C01

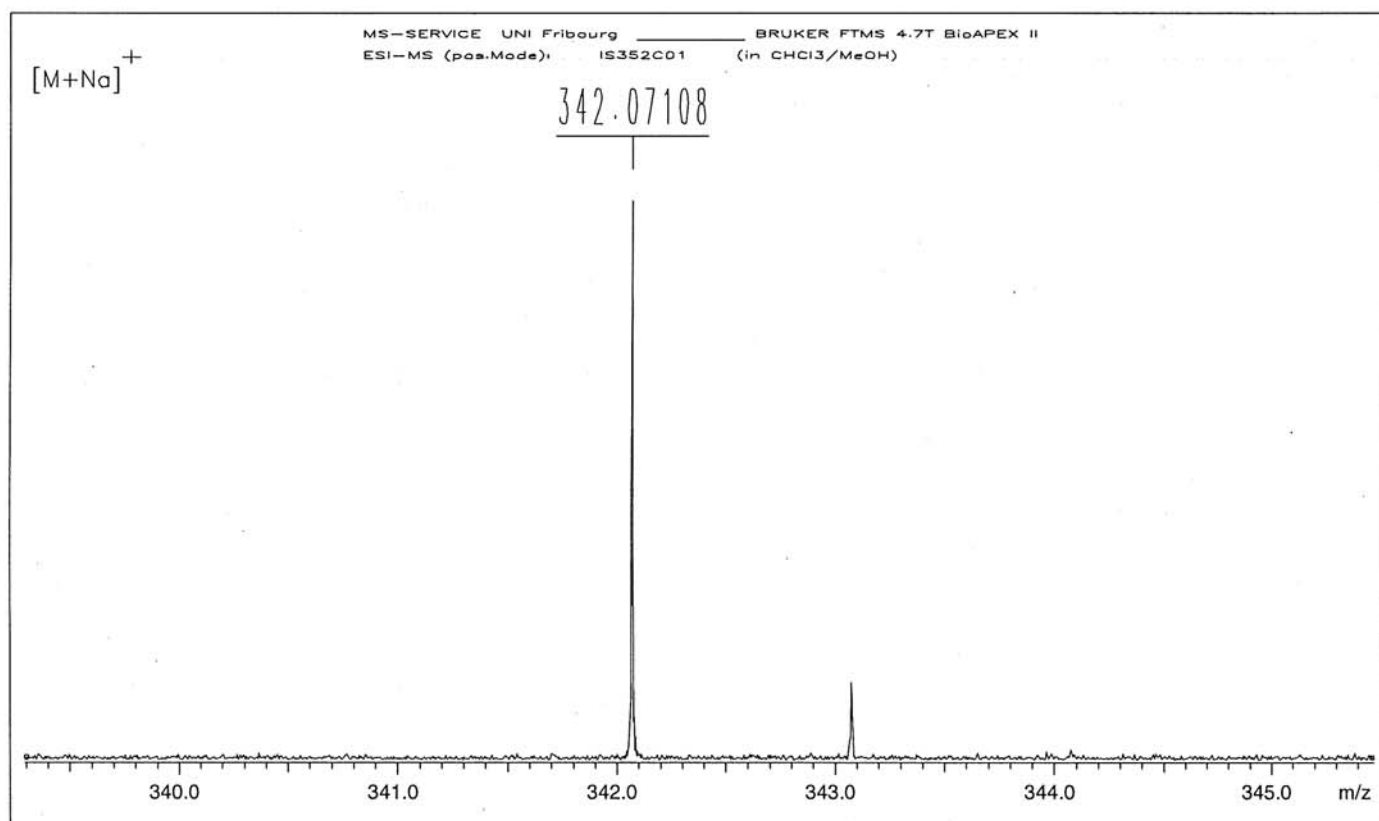
XMASS Mass Analysis for /Data/UNI\_FR/ALIM6554\_ESI/4/pdata/1/massanal.res:

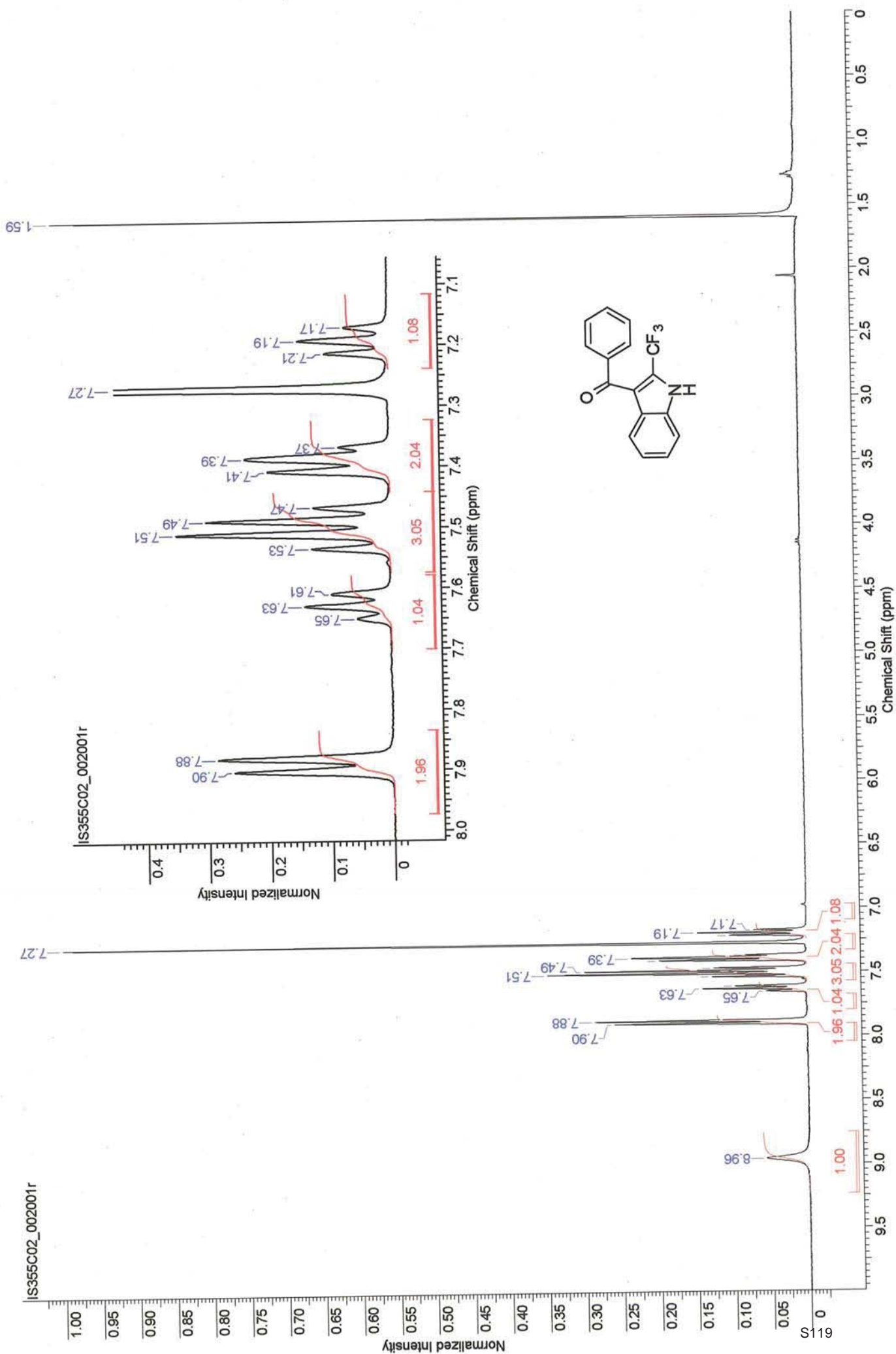
XMASS Mass Analysis Constraints

Ion mass = 342.0710770

Charge = +1

#	C	H	F	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 342.0710770									
1	17	12	3	1	2	1	342.0712343	10.5	1.573e-04
2	11	12	4	3	5	0	342.0707597	5.5	3.173e-04
3	20	11	2	1	1	1	342.0700915	14.5	9.855e-04
4	14	13	4	1	3	1	342.0723772	6.5	1.300e-03
5	22	10	2	1	1	0	342.0724968	17.5	1.420e-03
6	14	11	3	3	4	0	342.0696169	9.5	1.460e-03
7	11	14	5	1	4	1	342.0735200	2.5	2.443e-03
8	19	11	3	1	2	0	342.0736396	13.5	2.563e-03
9	17	10	2	3	3	0	342.0684740	13.5	2.603e-03
10	9	13	4	3	5	1	342.0683544	2.5	2.723e-03

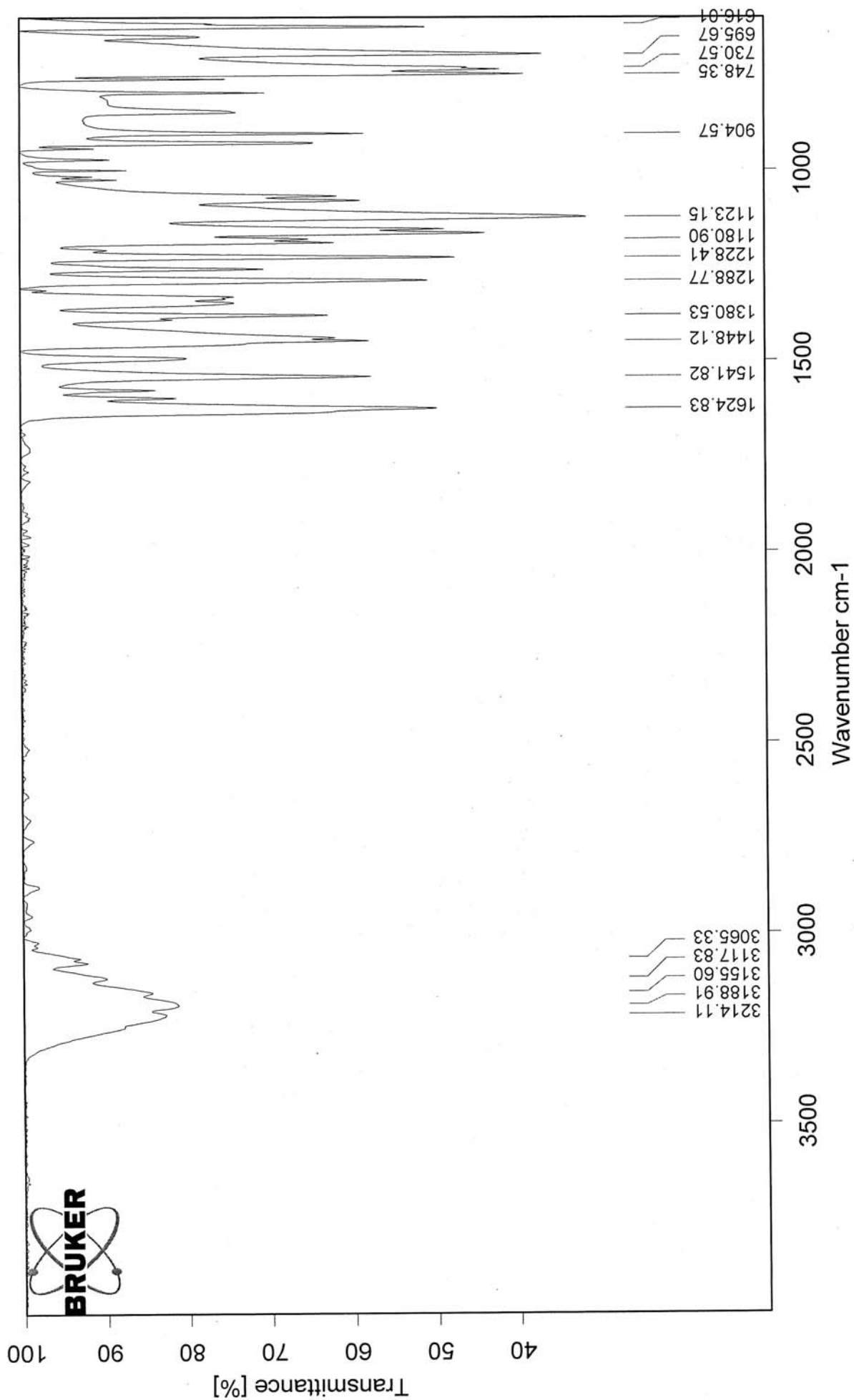












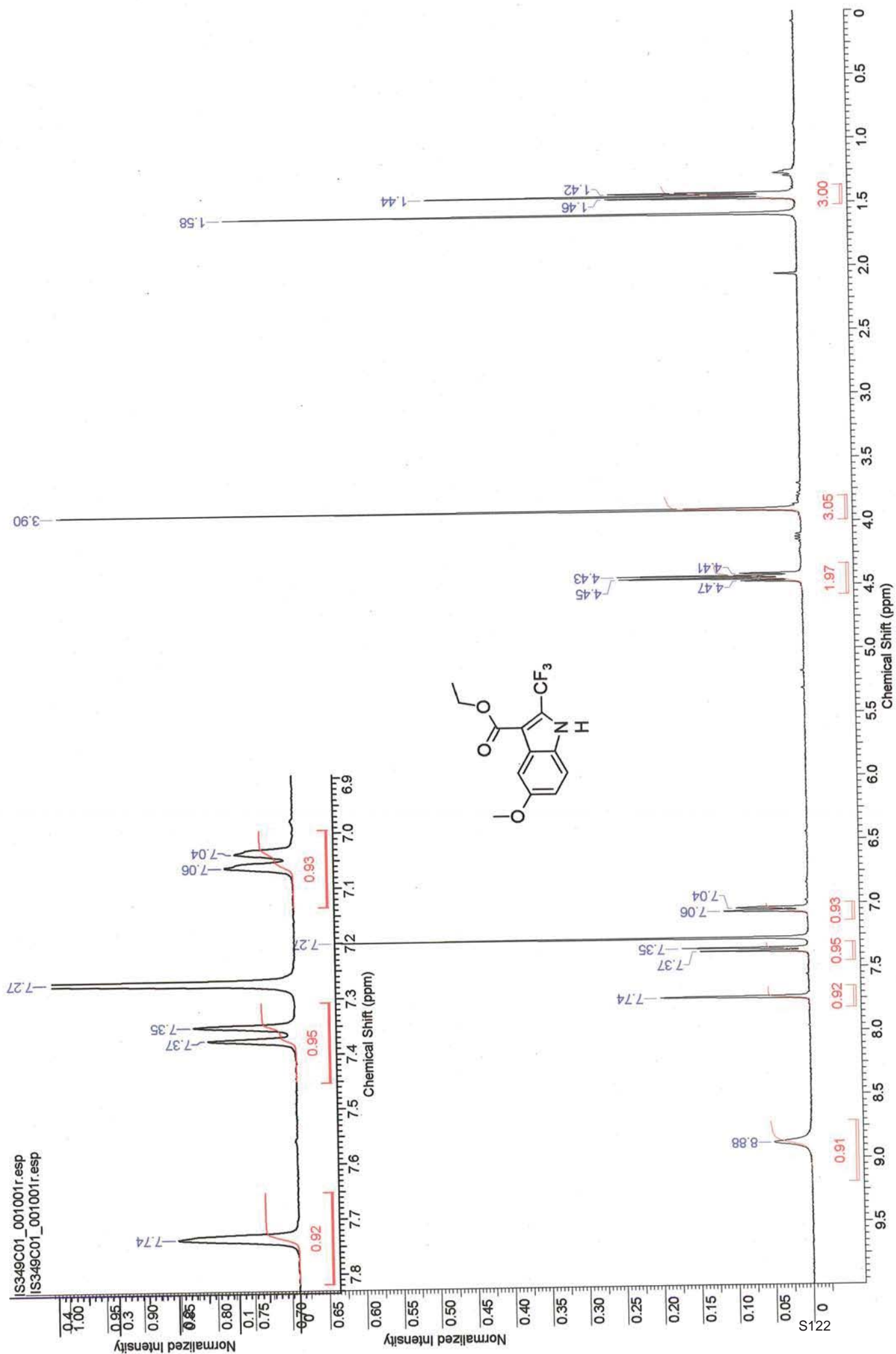
121S

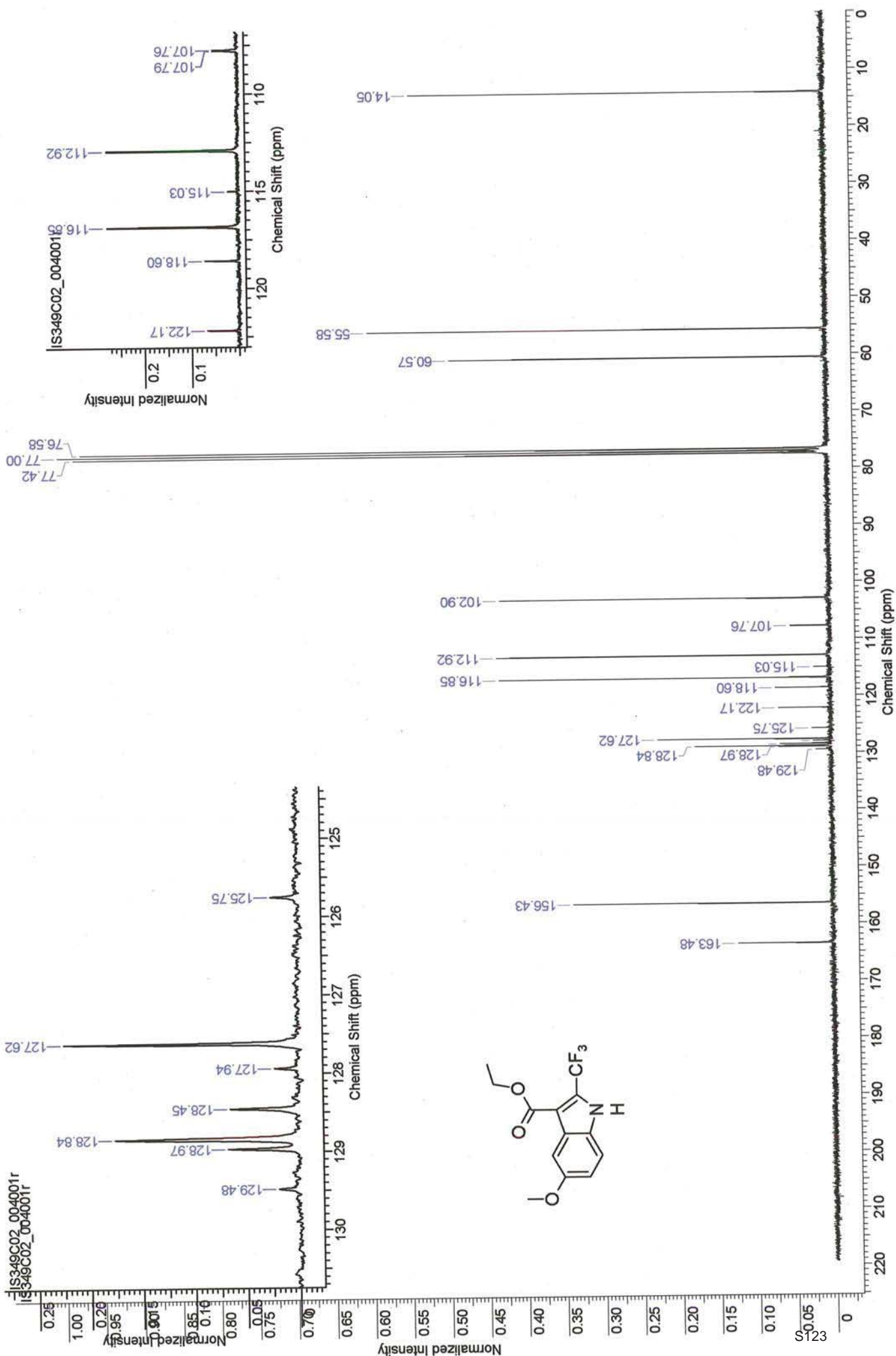
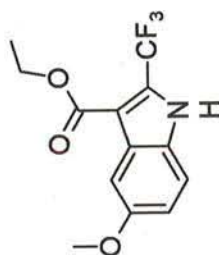
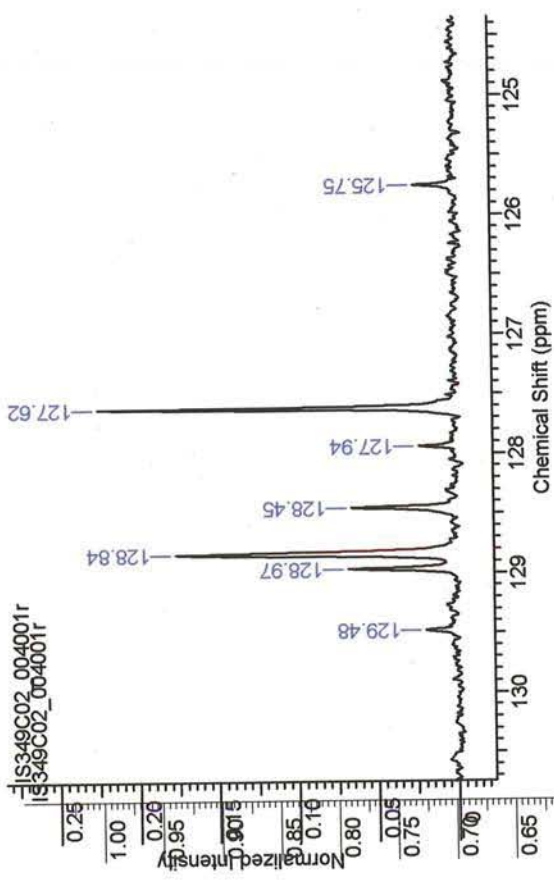
U:\DOCTORAT\CHARACTERISATION\IR\_SPECTRA\IS355C02.0

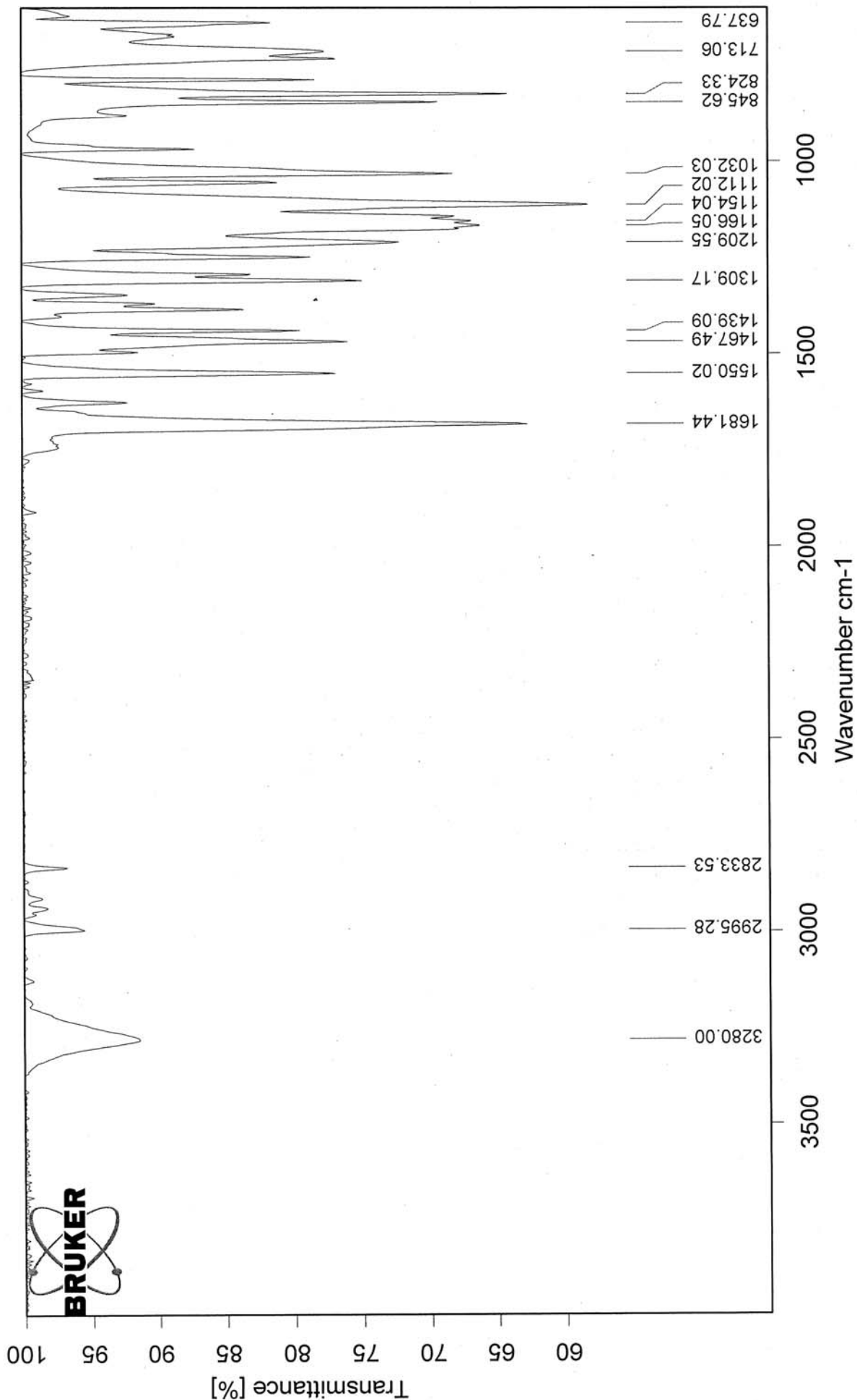
IS355C02

white solid

03/05/2012







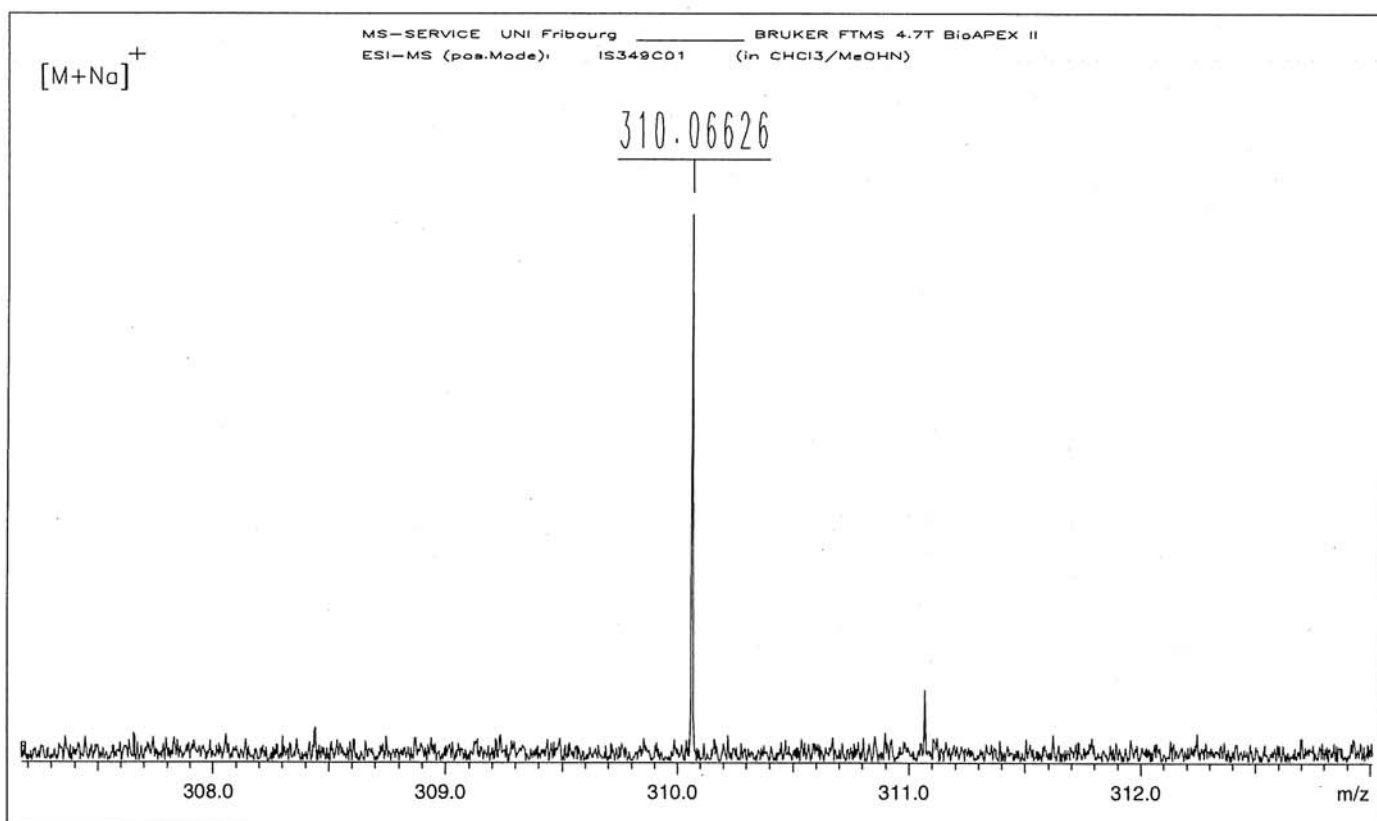
ESI-MS: IS349C01

XMASS Mass Analysis for /Data/UNI\_FR/ALIM6545\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

Ion mass = 310.0662590

Charge = +1

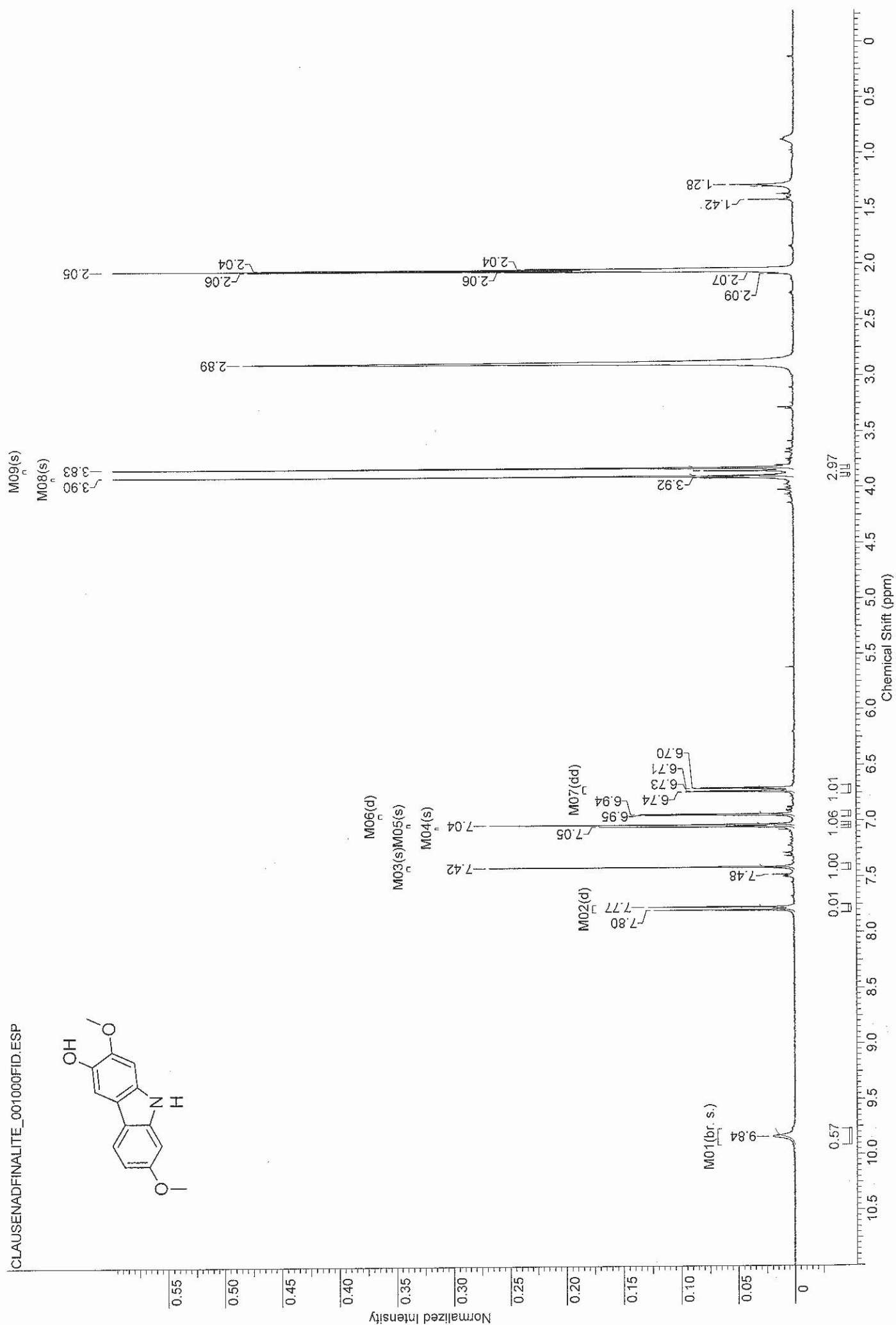
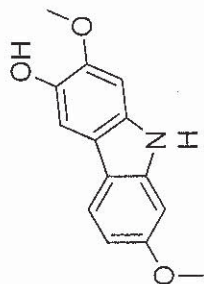
#	C	H	F	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 310.0662590									
1	13	12	3	1	3	1	310.0661489	6.5	1.101e-04
2	13	10	6	1	1	0	310.0661096	6.5	1.494e-04
3	16	8	2	4	1	0	310.0660687	14.0	1.903e-04
4	8	11	4	4	3	1	310.0659491	3.0	3.099e-04
5	7	12	4	3	6	0	310.0656744	1.5	5.846e-04
6	5	12	5	4	4	1	310.0670920	-1.0	8.330e-04
7	13	9	3	4	2	0	310.0672116	10.0	9.526e-04
8	10	13	4	1	4	1	310.0672918	2.5	1.033e-03
9	18	10	2	1	2	0	310.0674114	13.5	1.152e-03
10	16	11	2	1	2	1	310.0650061	10.5	1.253e-03

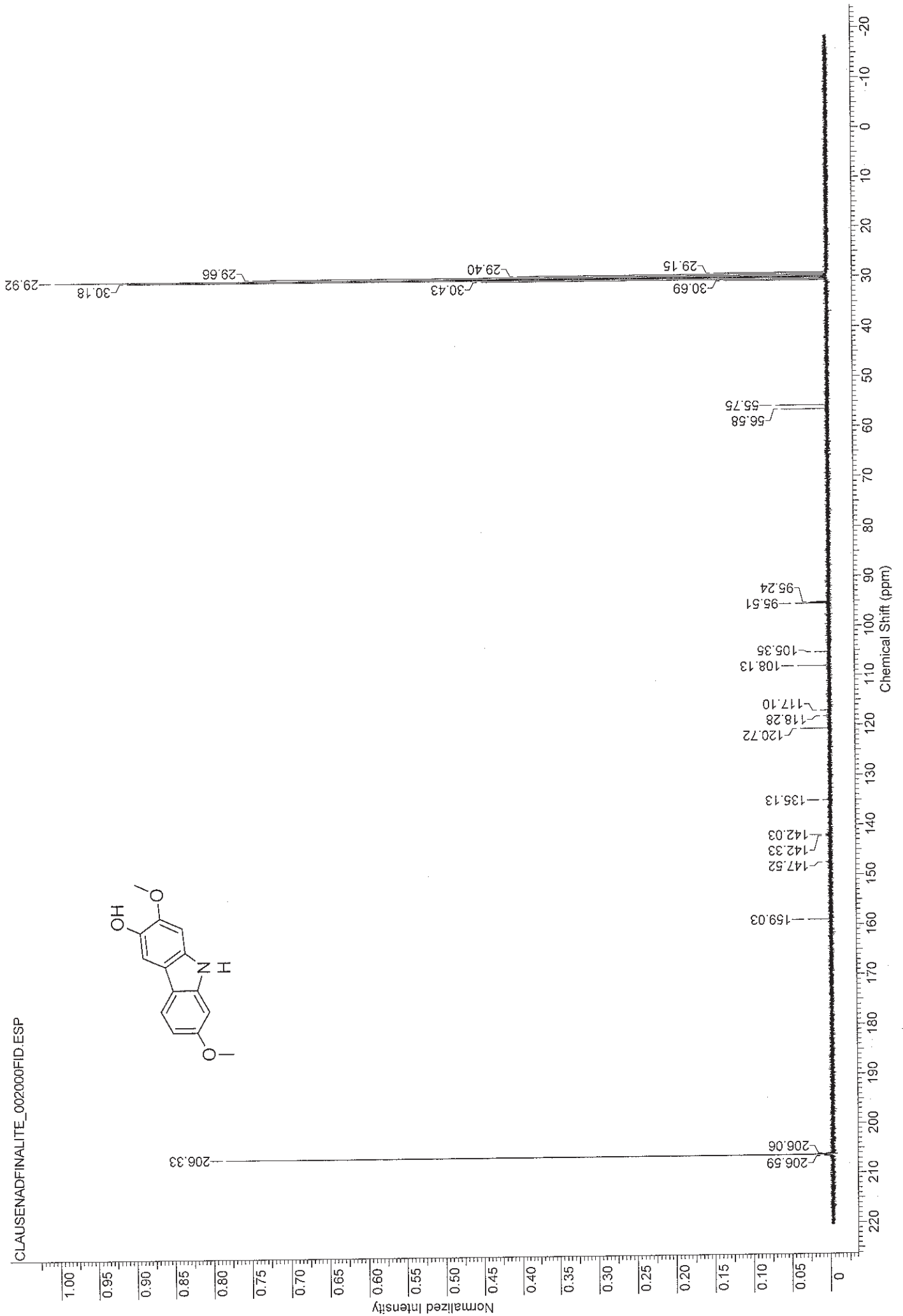


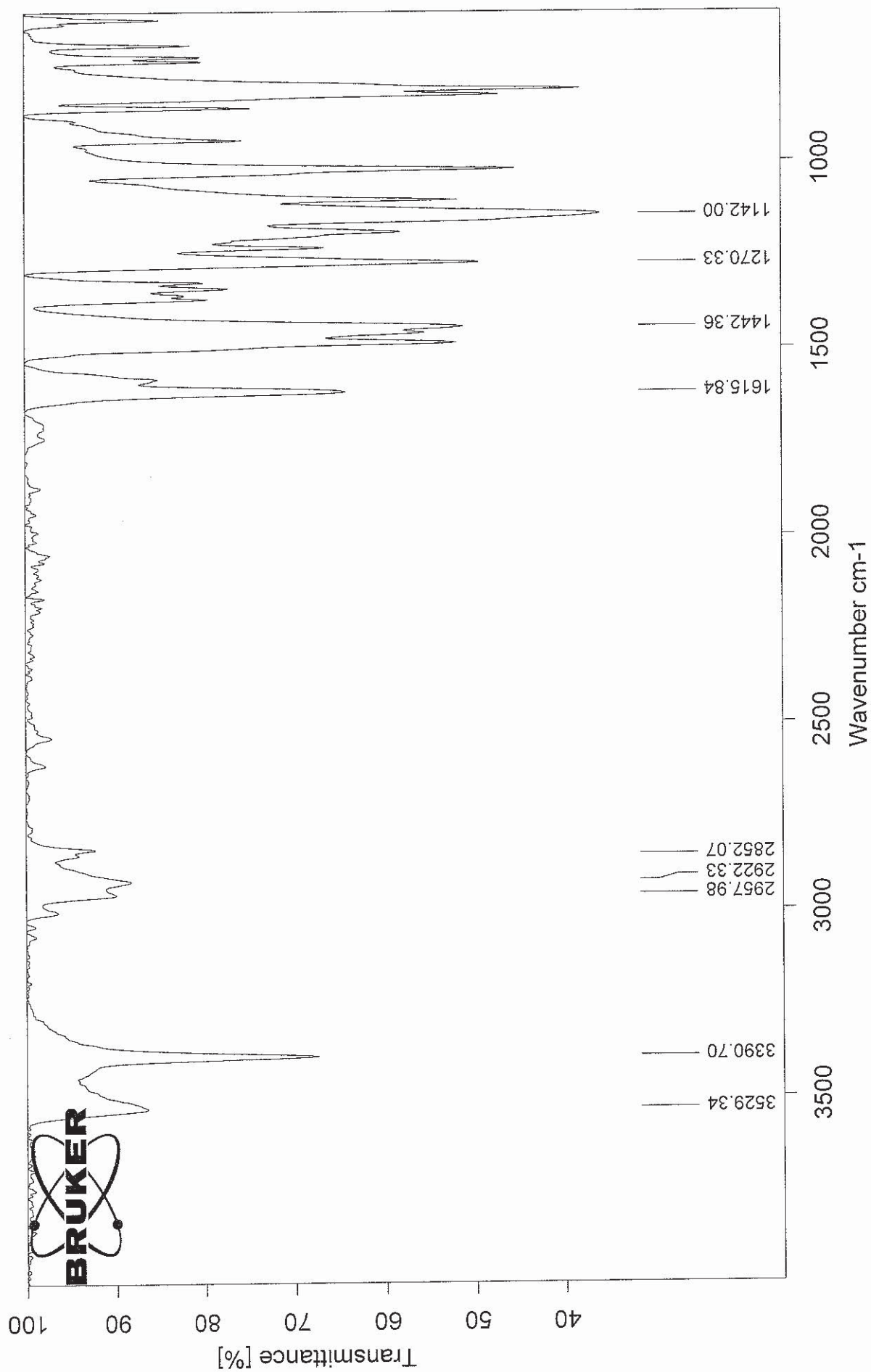












U:\IR\Clausenawalline D.0

Clausenawalline D

brown solid

18.11.2013

ESI-MS: RR073A

XMASS Mass Analysis for /Data/UNI\_FR/REMY7660\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

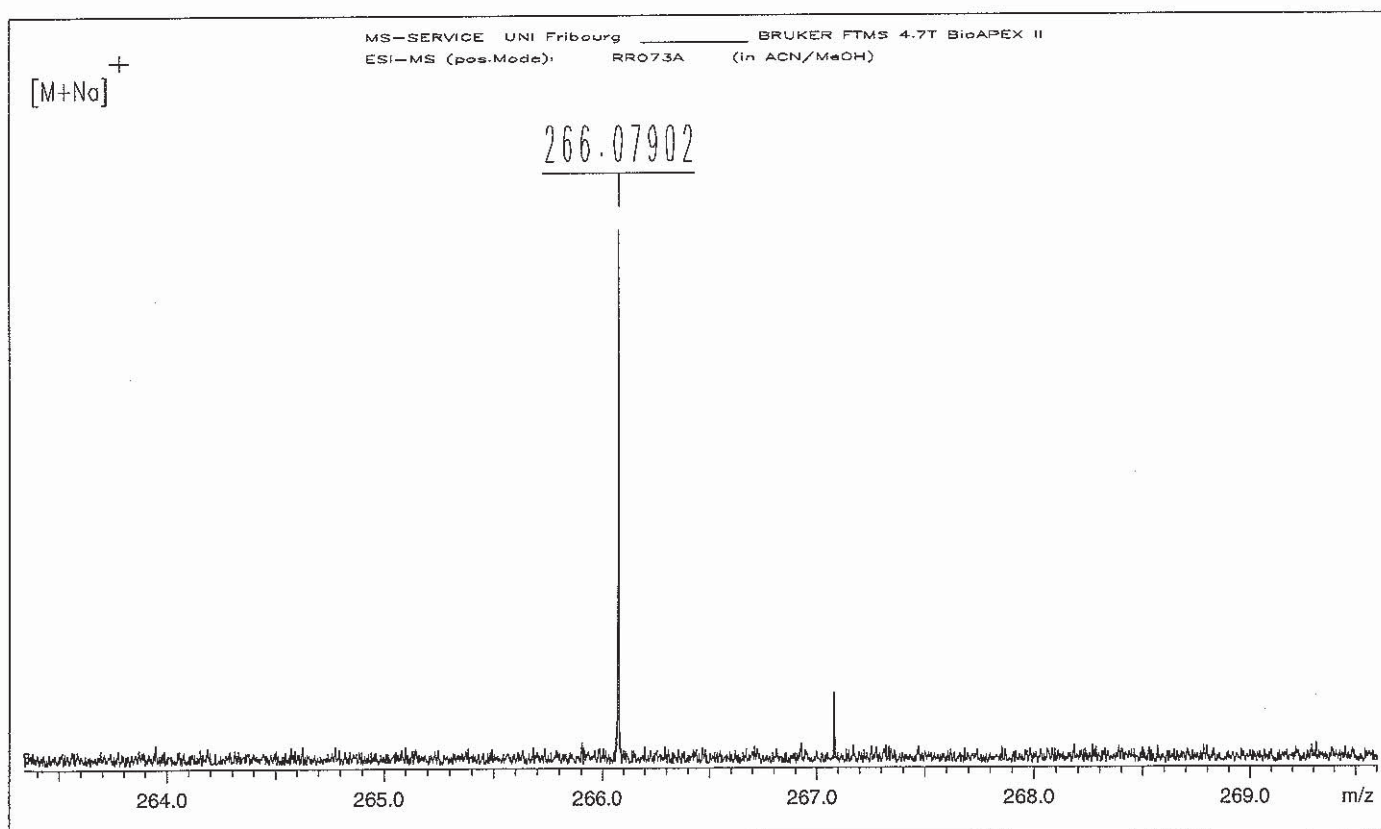
Ion mass = 266.0790200

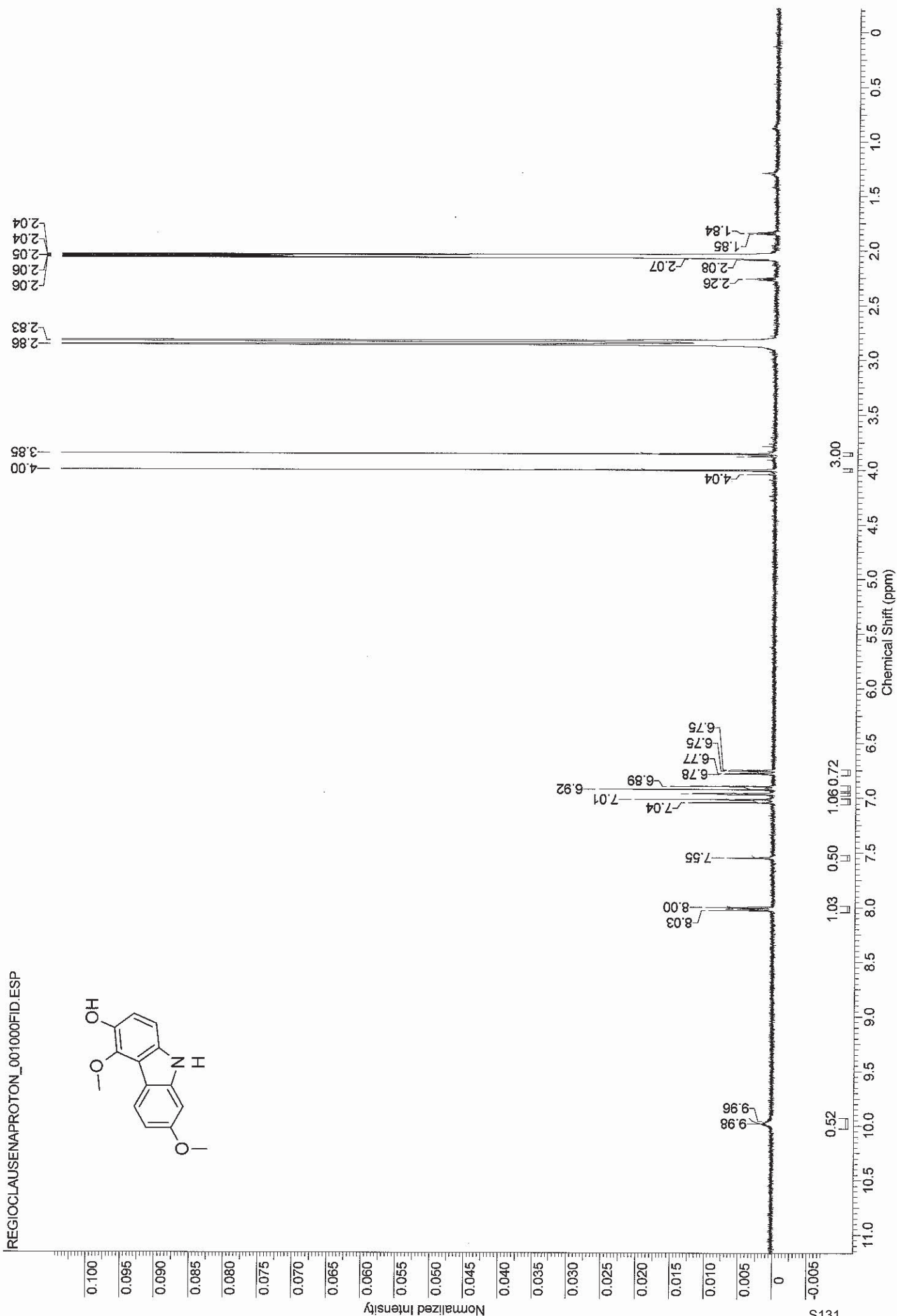
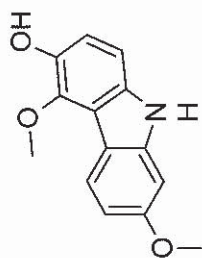
Charge = +1

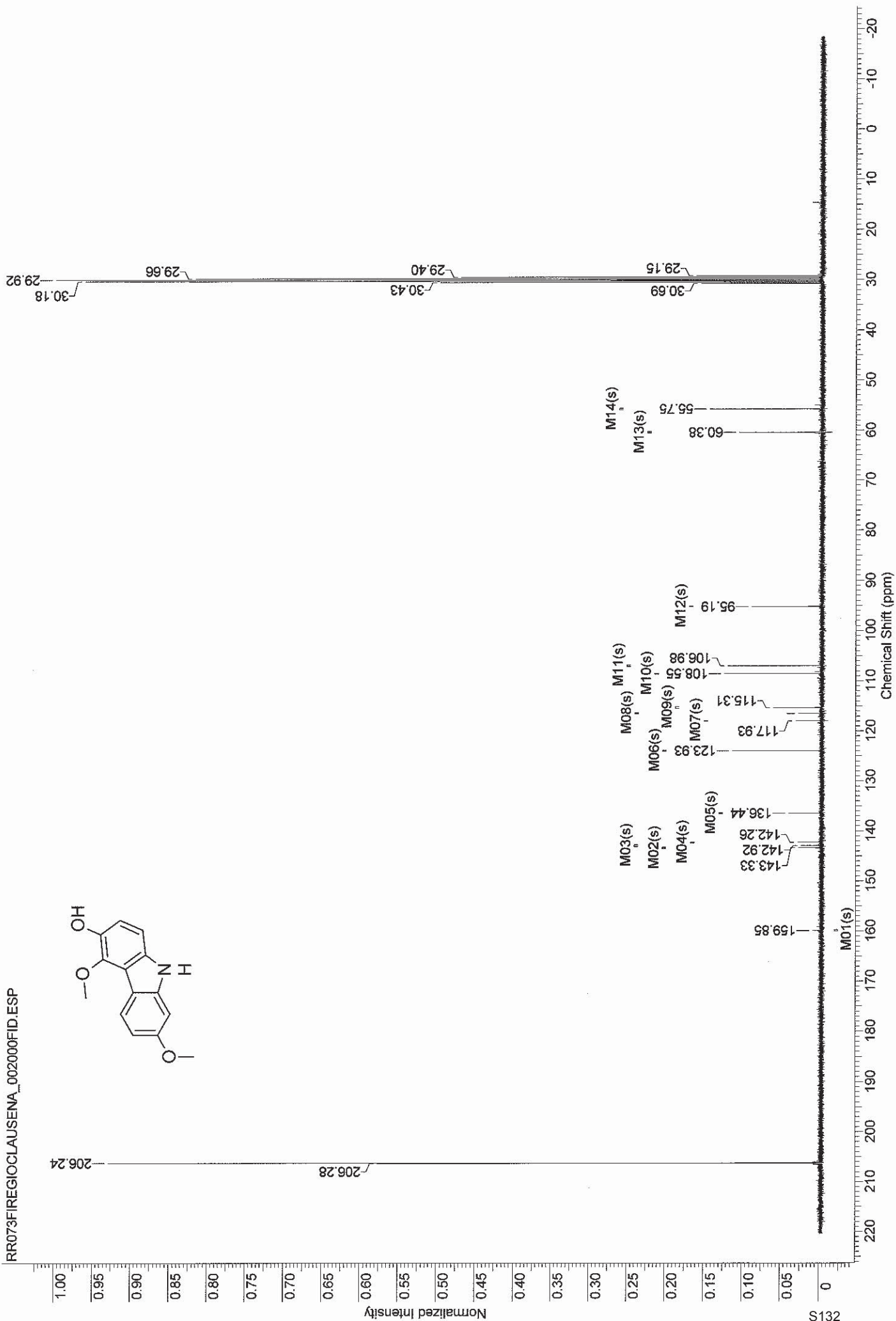
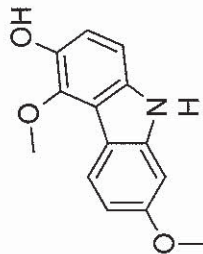
#	C	H	N	O	Na	mass	DBE	error
---	---	---	---	---	----	------	-----	-------

\*\*\* Mass Analysis for mass 266.0790200

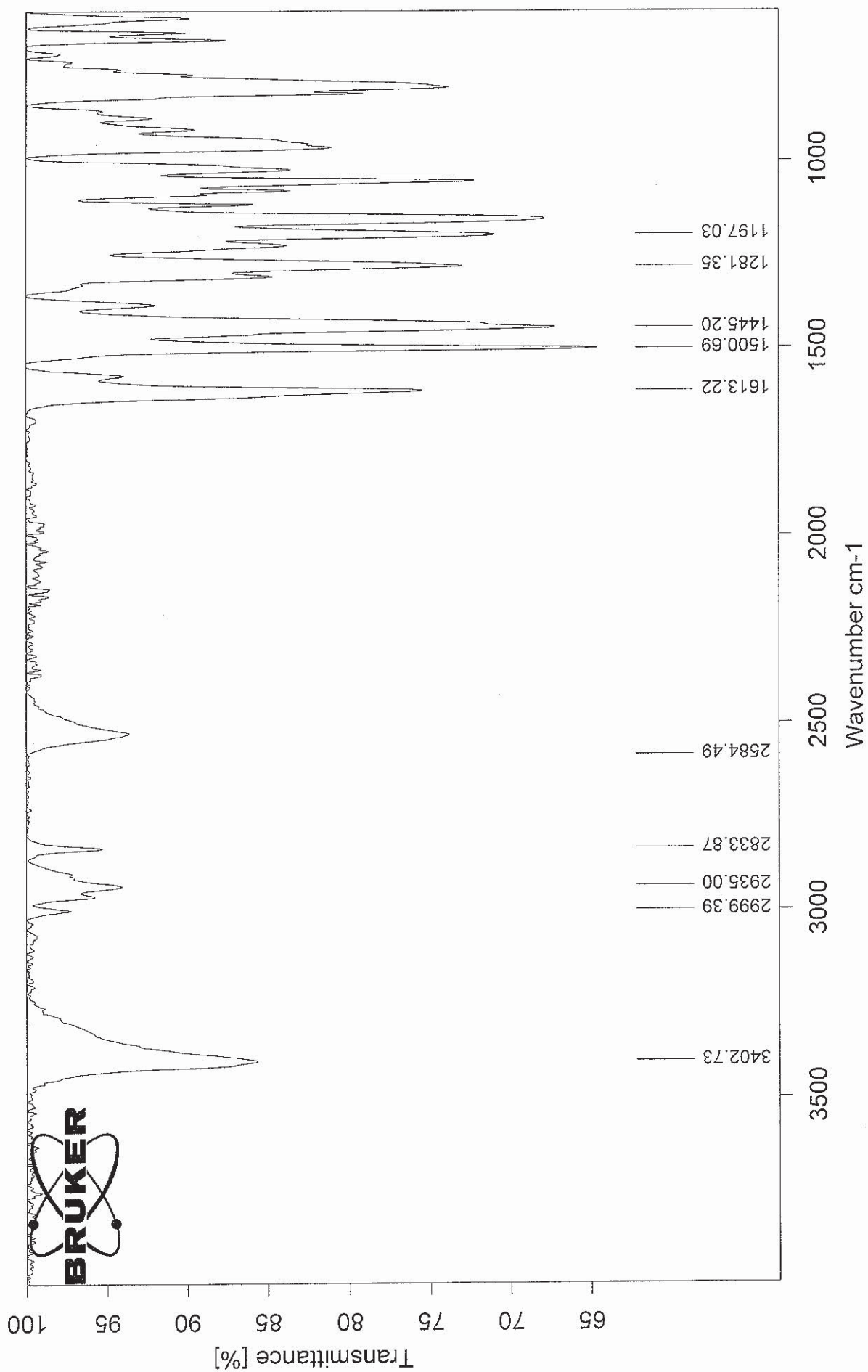
1	14	13	1	3	1	266.0787644	8.5	2.556e-04
2	12	8	7	1	0	266.0784843	12.5	5.357e-04
3	14	10	4	2	0	266.0798270	12.0	8.070e-04
4	12	11	4	2	1	266.0774217	9.0	1.598e-03
5	11	12	3	5	0	266.0771469	7.5	1.873e-03
6	16	12	1	3	0	266.0811697	11.5	2.150e-03
7	10	9	7	1	1	266.0760790	9.5	2.941e-03
8	9	10	6	4	0	266.0758043	8.0	3.216e-03
9	5	15	4	7	1	266.0832949	0.0	4.275e-03
10	9	13	3	5	1	266.0747416	4.5	4.278e-03











U:\IR\4,7-dimethoxy-9H-carbazol-3-ol.0

4,7-dimethoxy-9H-carbazol-3-ol

brown solid

18.11.2013

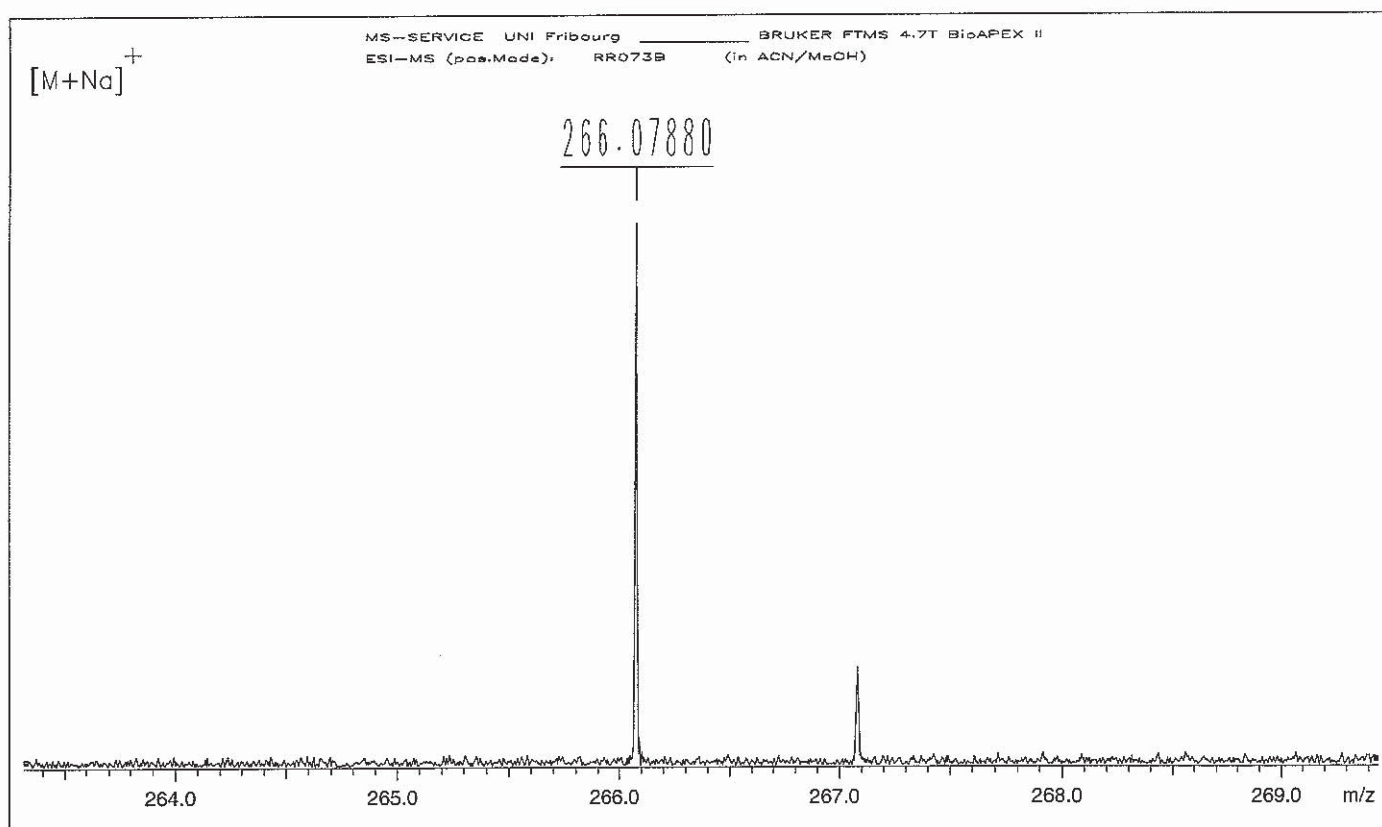
ESI-MS: RR073B

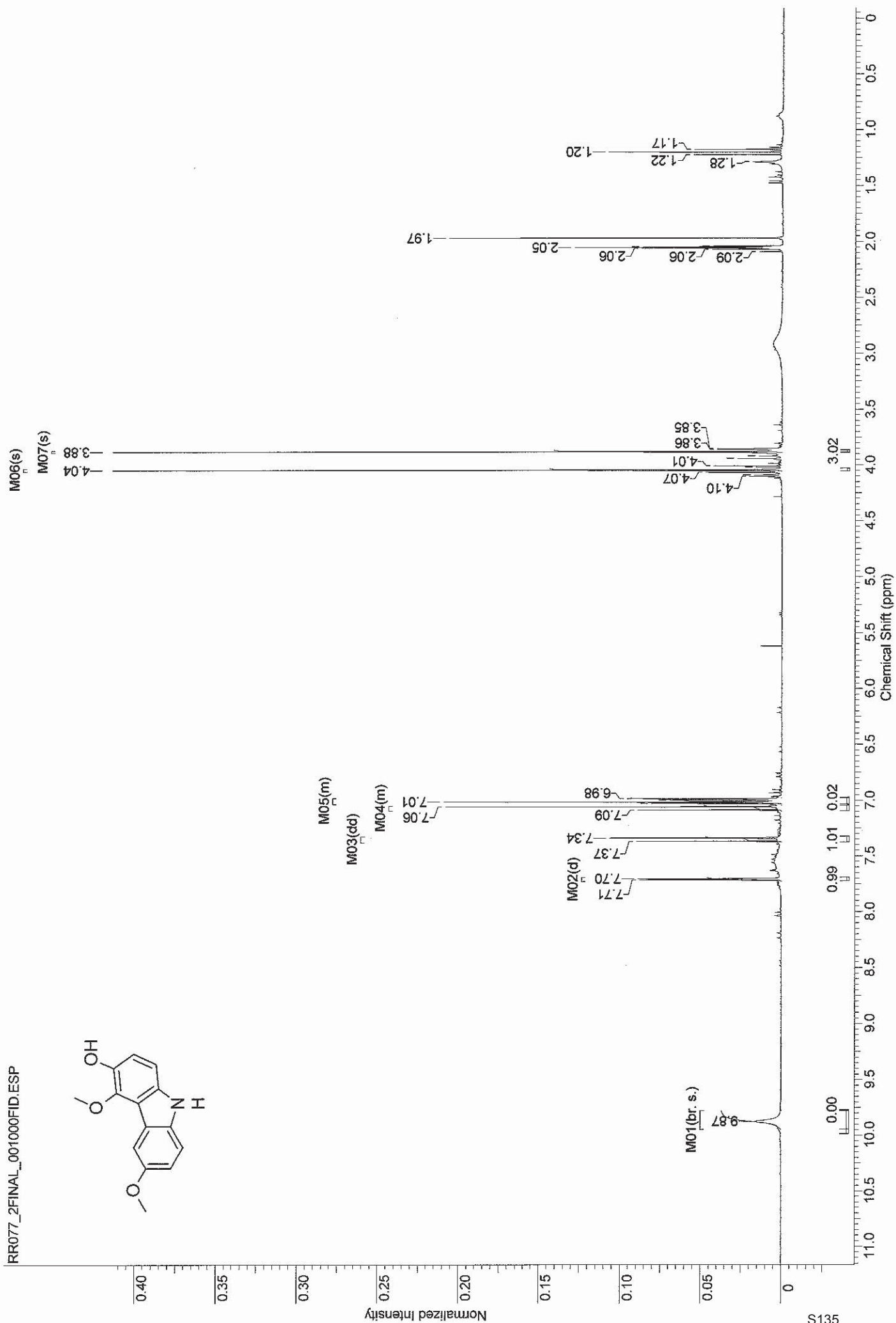
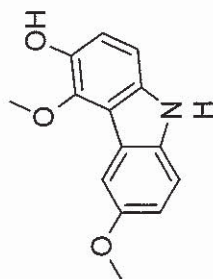
XMASS Mass Analysis for /Data/UNI\_FR/REMY7721\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

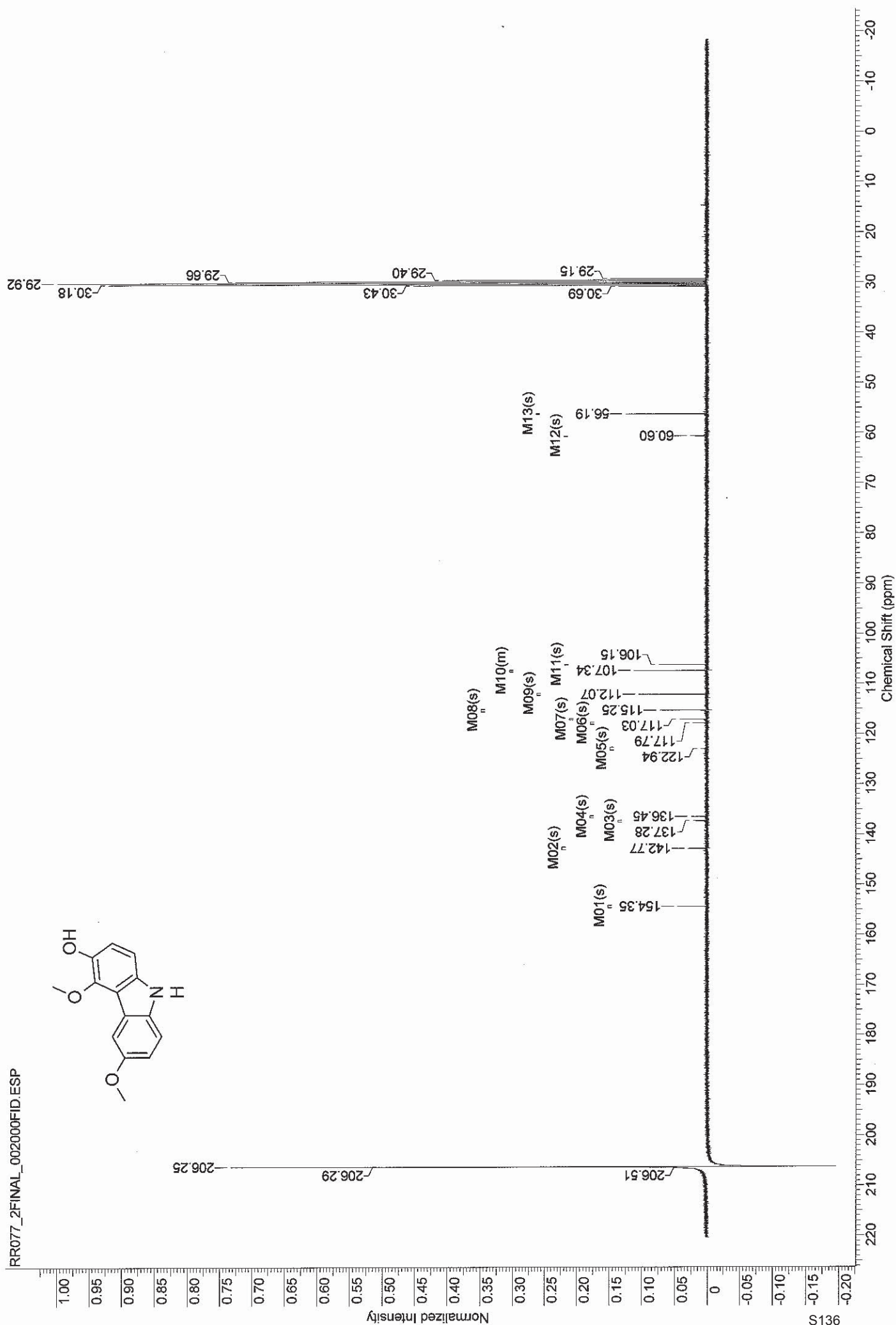
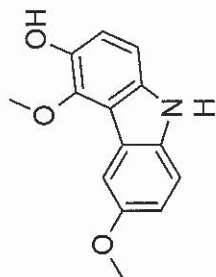
Ion mass = 266.0788000

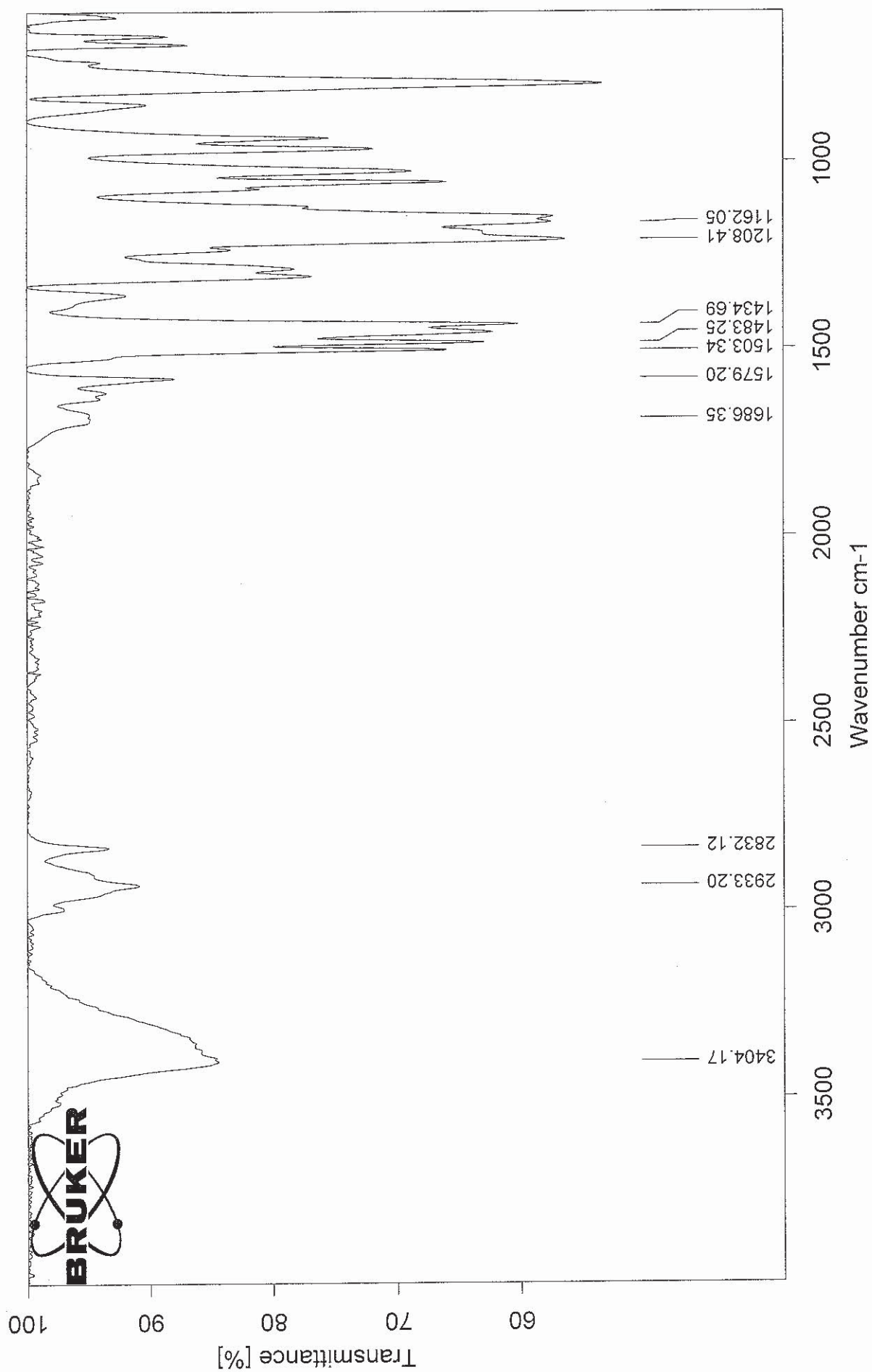
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 266.0788000								
1	14	13	1	3	1	266.0787644	8.5	3.562e-05
2	14	10	4	2	0	266.0798270	12.0	1.027e-03
3	12	11	4	2	1	266.0774217	9.0	1.378e-03
4	11	12	3	5	0	266.0771469	7.5	1.653e-03
5	16	12	1	3	0	266.0811697	11.5	2.370e-03
6	9	13	3	5	1	266.0747416	4.5	4.058e-03
7	5	15	4	7	1	266.0832949	0.0	4.495e-03
8	6	12	5	7	0	266.0731242	3.5	5.676e-03
9	7	14	4	7	0	266.0857002	3.0	6.900e-03
10	8	13	5	4	1	266.0859750	4.5	7.175e-03









U:\IR\4,6-dimethoxy-9H-carbazol-3-ol.0

4,6-dimethoxy-9H-carbazol-3-ol

brown solid

18.11.2013

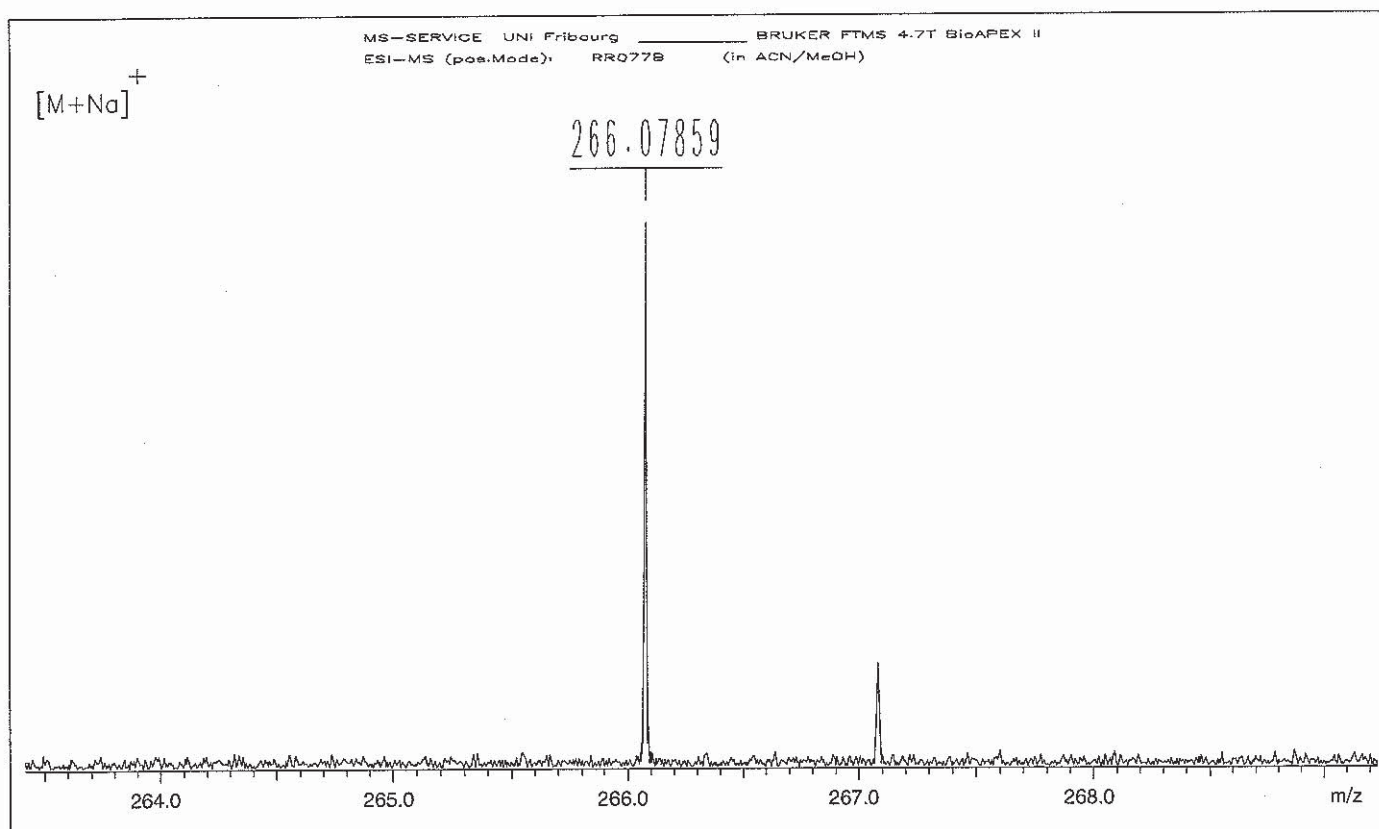
ESI-MS: RR077B

XMASS Mass Analysis for /Data/UNI\_FR/REMY7722\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

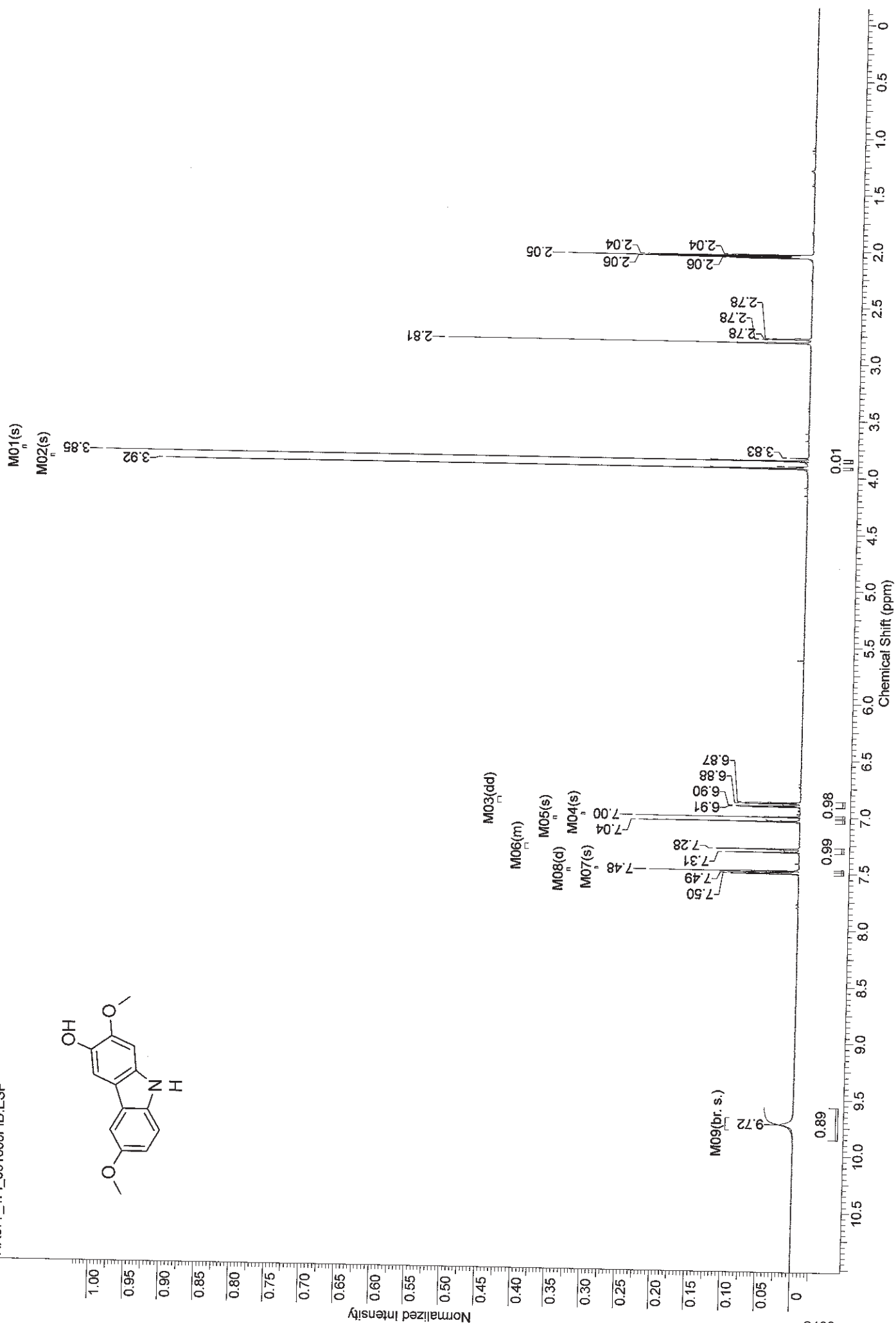
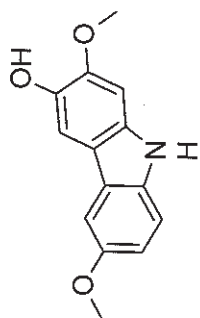
Ion mass = 266.0785860

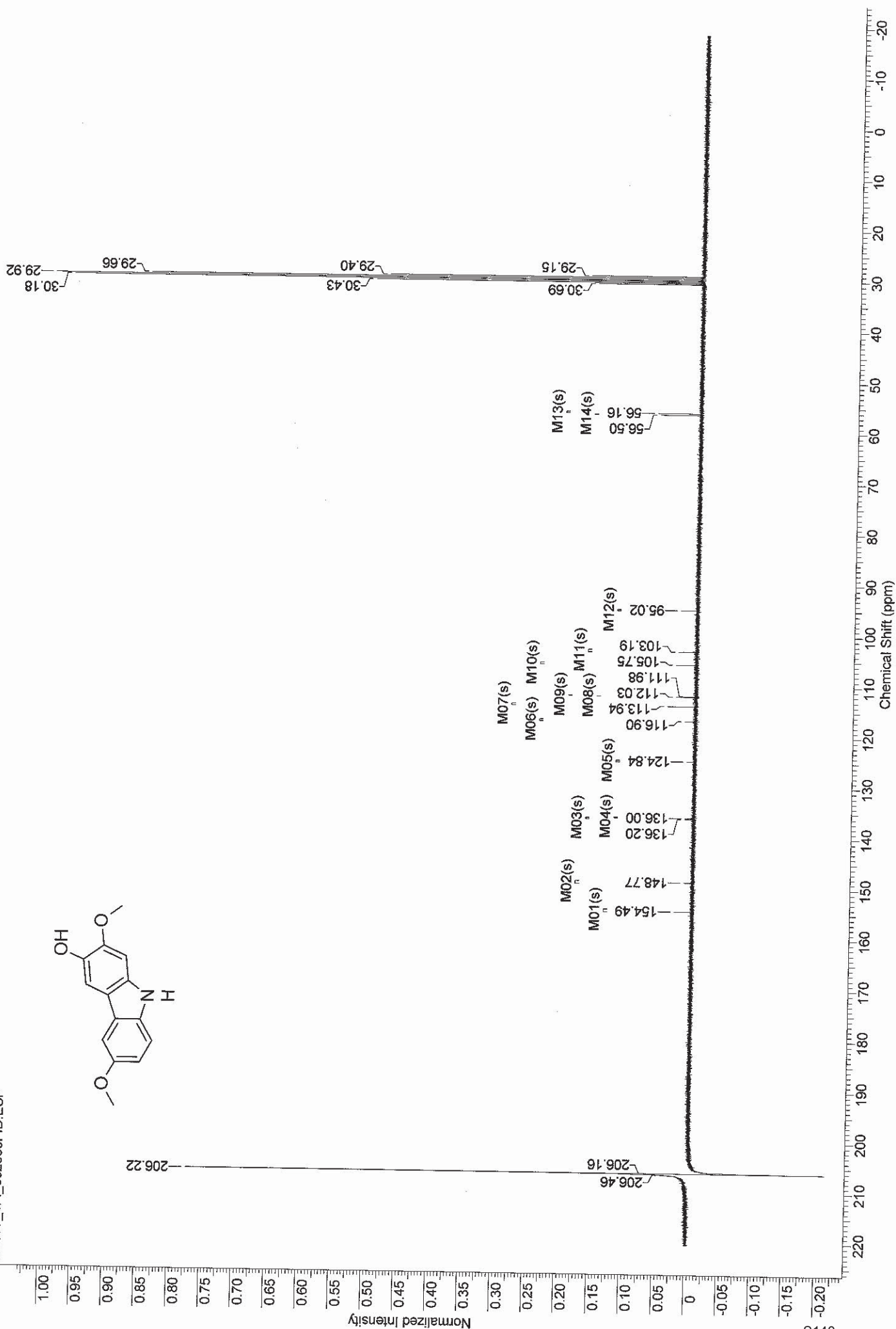
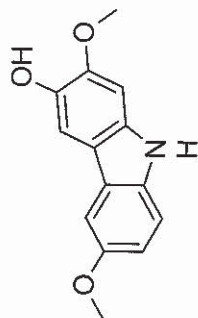
Charge = +1

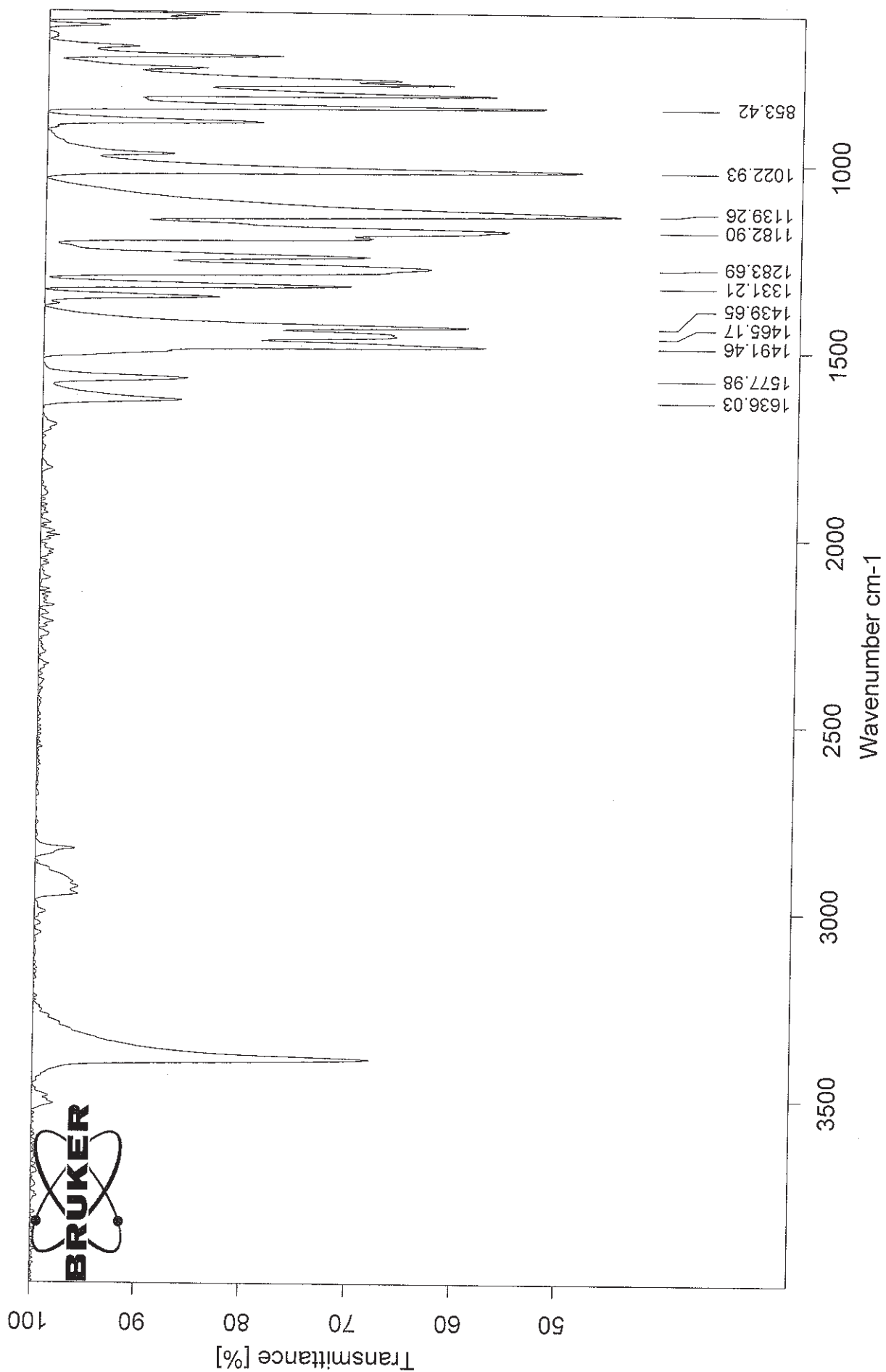
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 266.0785860								
1	14	13	1	3	1	266.0787644	8.5	1.784e-04
2	12	11	4	2	1	266.0774217	9.0	1.164e-03
3	14	10	4	2	0	266.0798270	12.0	1.241e-03
4	11	12	3	5	0	266.0771469	7.5	1.439e-03
5	16	12	1	3	0	266.0811697	11.5	2.584e-03
6	9	13	3	5	1	266.0747416	4.5	3.844e-03
7	5	15	4	7	1	266.0832949	0.0	4.709e-03
8	6	12	5	7	0	266.0731242	3.5	5.462e-03
9	7	14	4	7	0	266.0857002	3.0	7.114e-03
10	8	13	5	4	1	266.0859750	4.5	7.389e-03











ESI-MS: RR077A

XMASS Mass Analysis for /Data/UNI\_FR/REMY7661\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

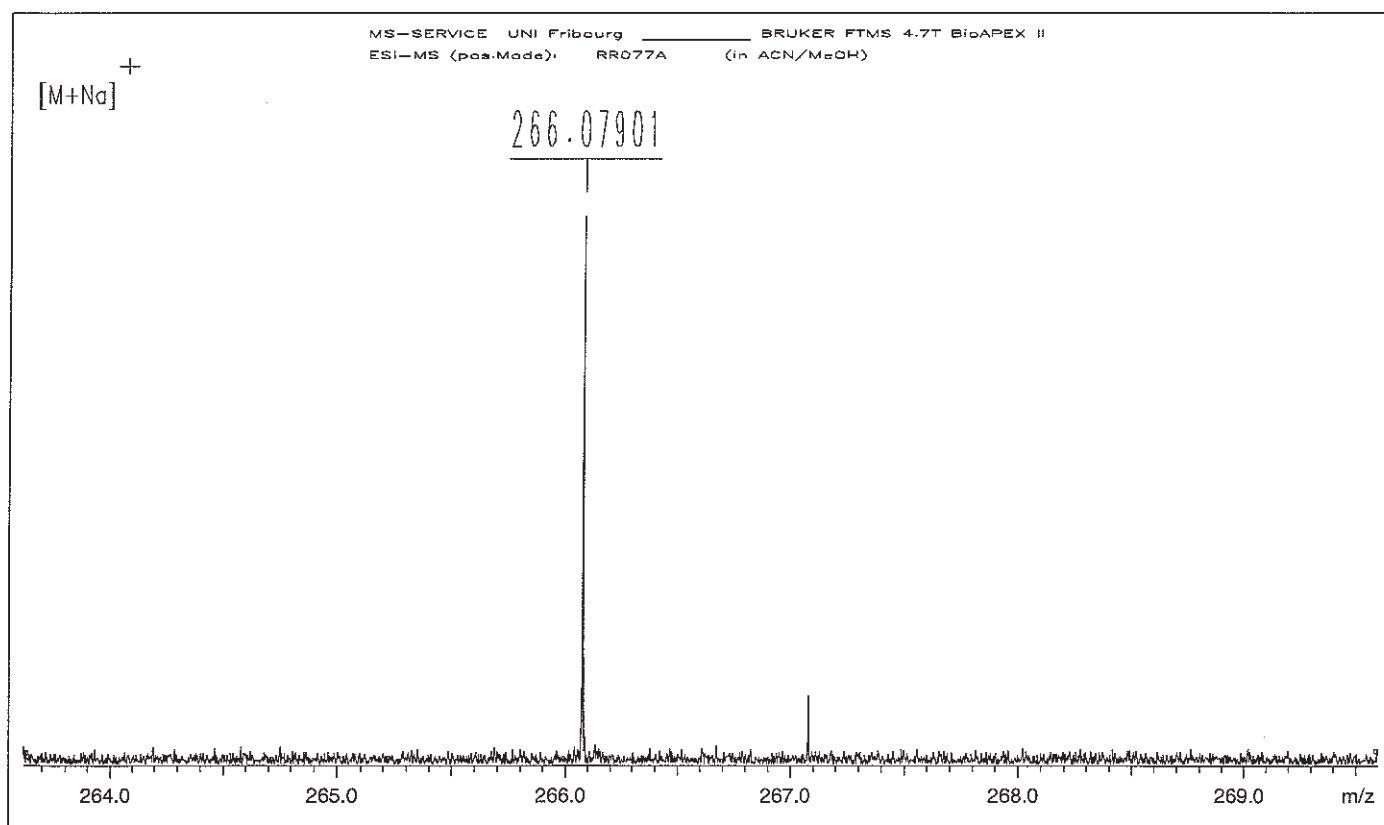
Ion mass = 266.0790090

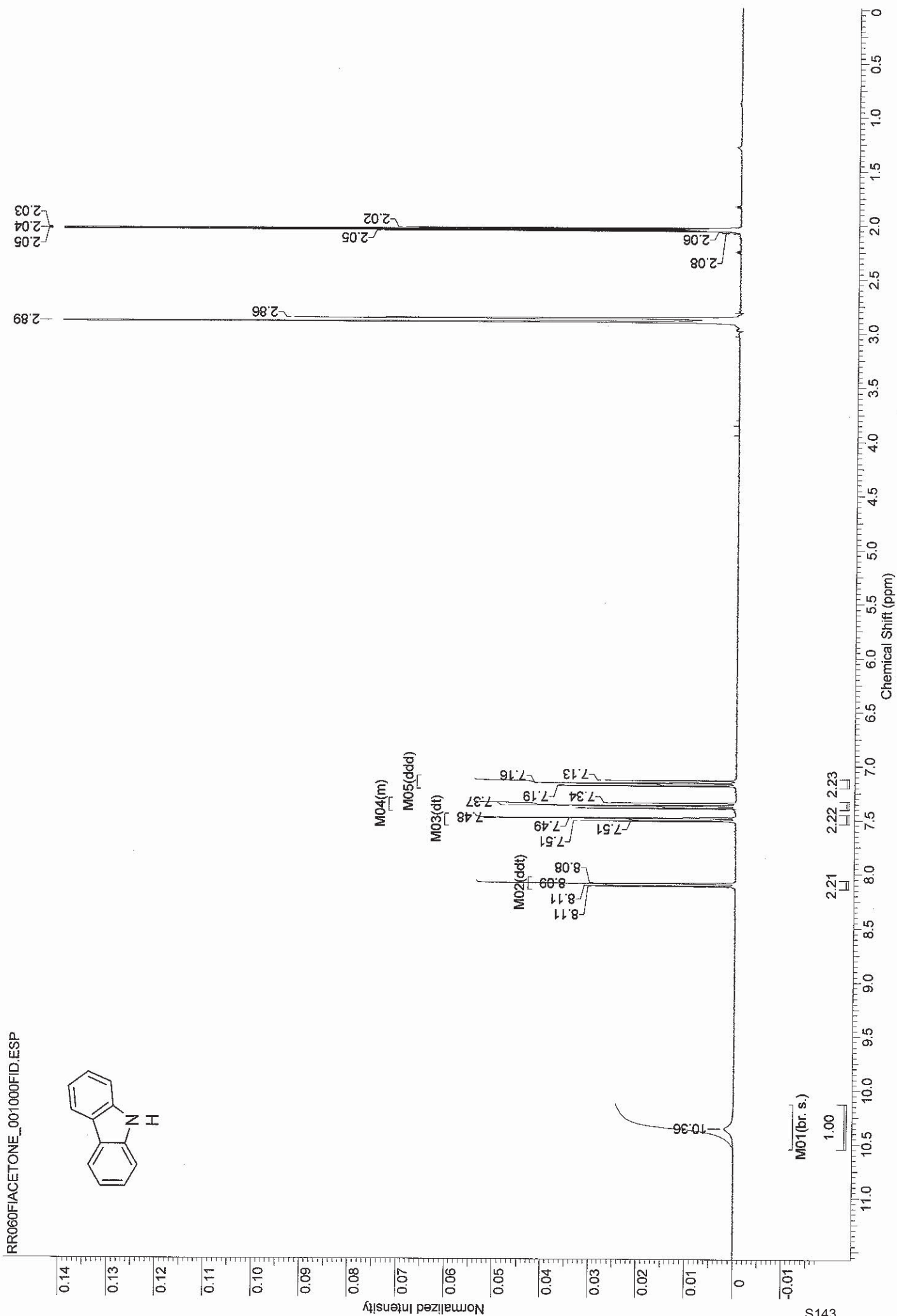
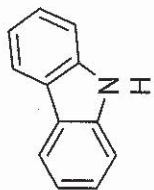
Charge = +1

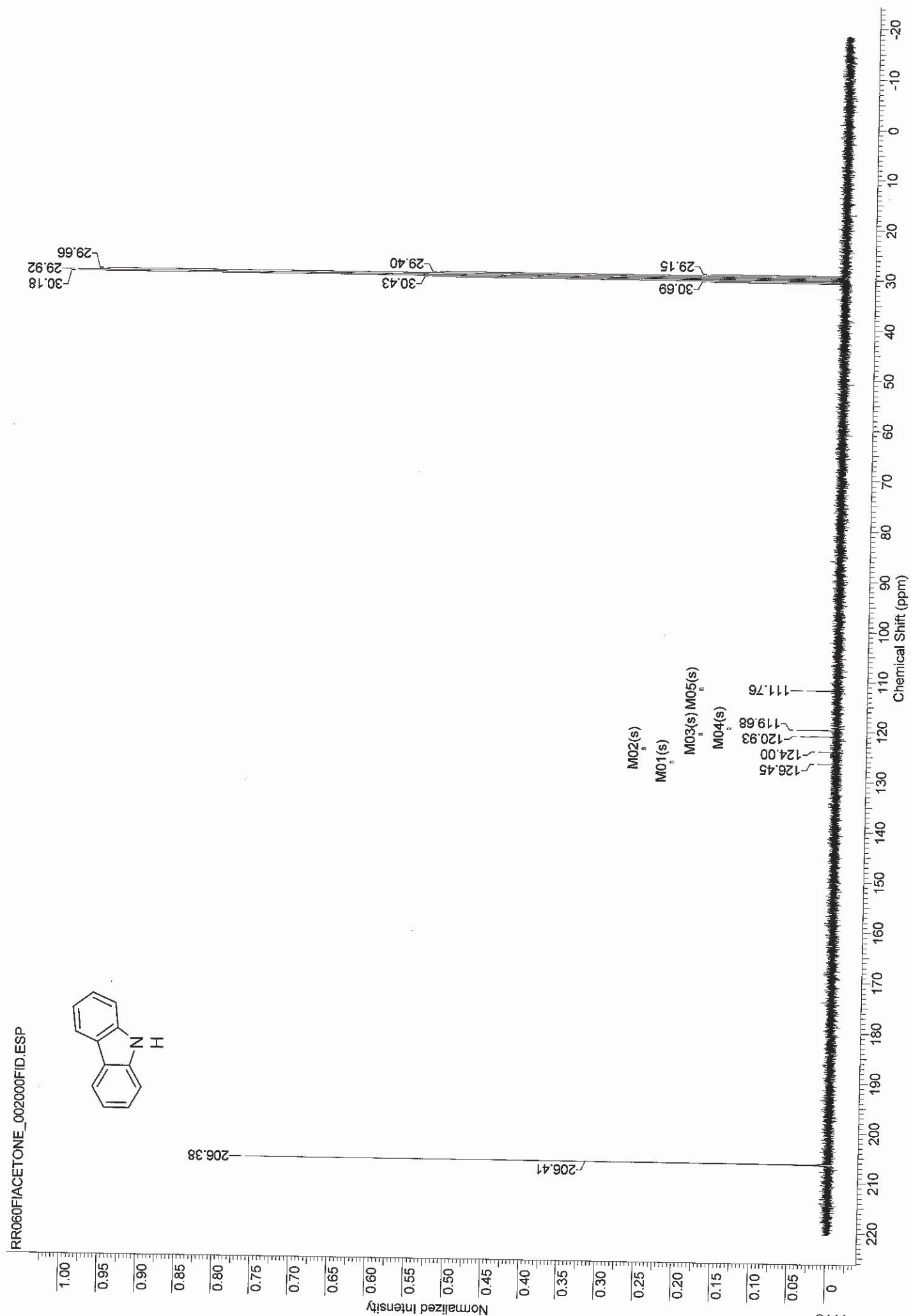
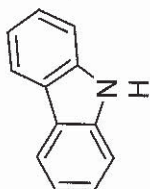
#	C	H	N	O	Na	mass	DBE	error
---	---	---	---	---	----	------	-----	-------

\*\*\* Mass Analysis for mass 266.0790090

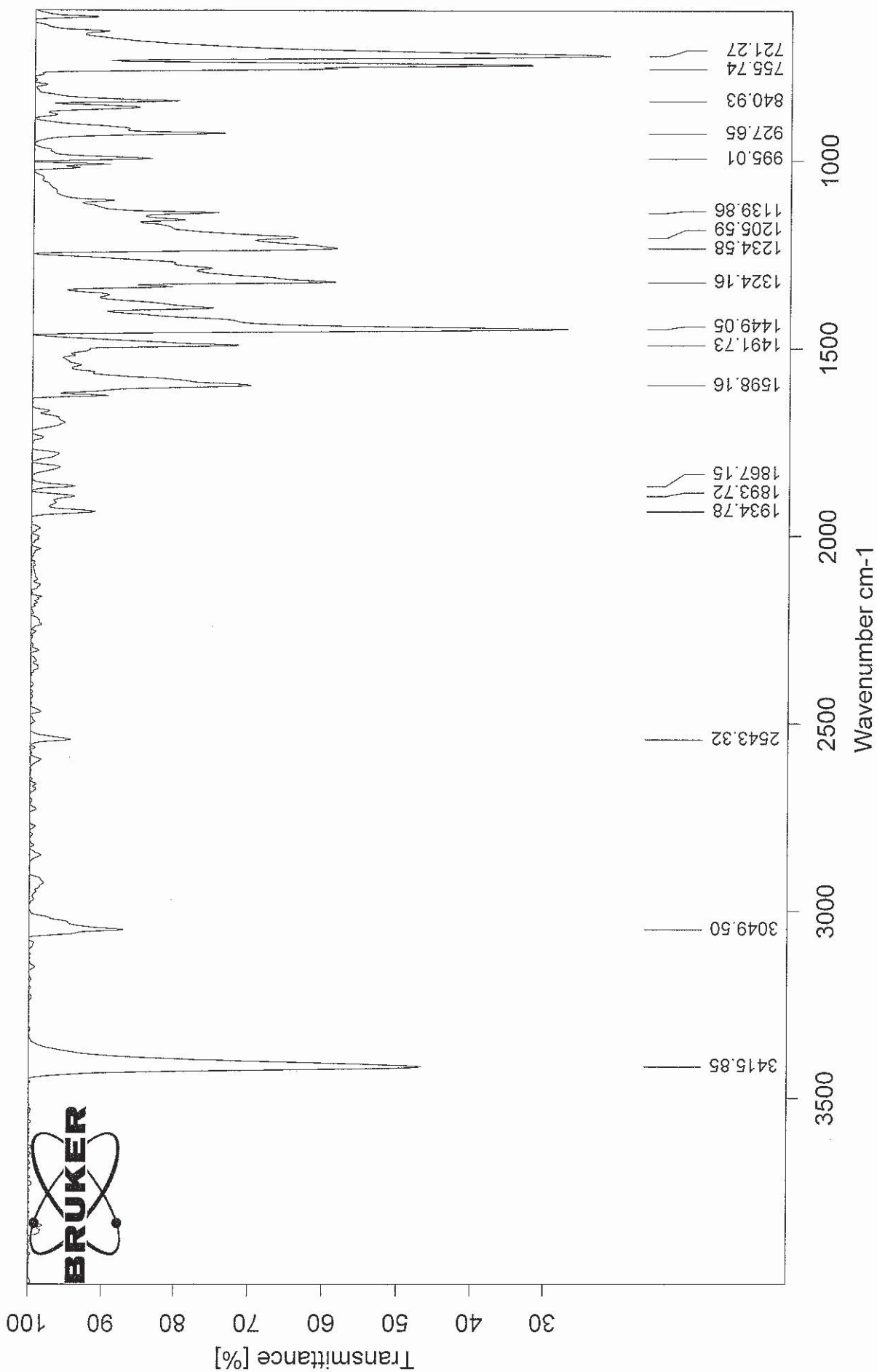
1	14	13	1	3	1	266.0787644	8.5	2.446e-04
2	12	8	7	1	0	266.0784843	12.5	5.247e-04
3	14	10	4	2	0	266.0798270	12.0	8.180e-04
4	12	11	4	2	1	266.0774217	9.0	1.587e-03
5	11	12	3	5	0	266.0771469	7.5	1.862e-03
6	16	12	1	3	0	266.0811697	11.5	2.161e-03
7	10	9	7	1	1	266.0760790	9.5	2.930e-03
8	9	10	6	4	0	266.0758043	8.0	3.205e-03
9	9	13	3	5	1	266.0747416	4.5	4.267e-03
10	5	15	4	7	1	266.0832949	0.0	4.286e-03











Comment 1

Comment 2

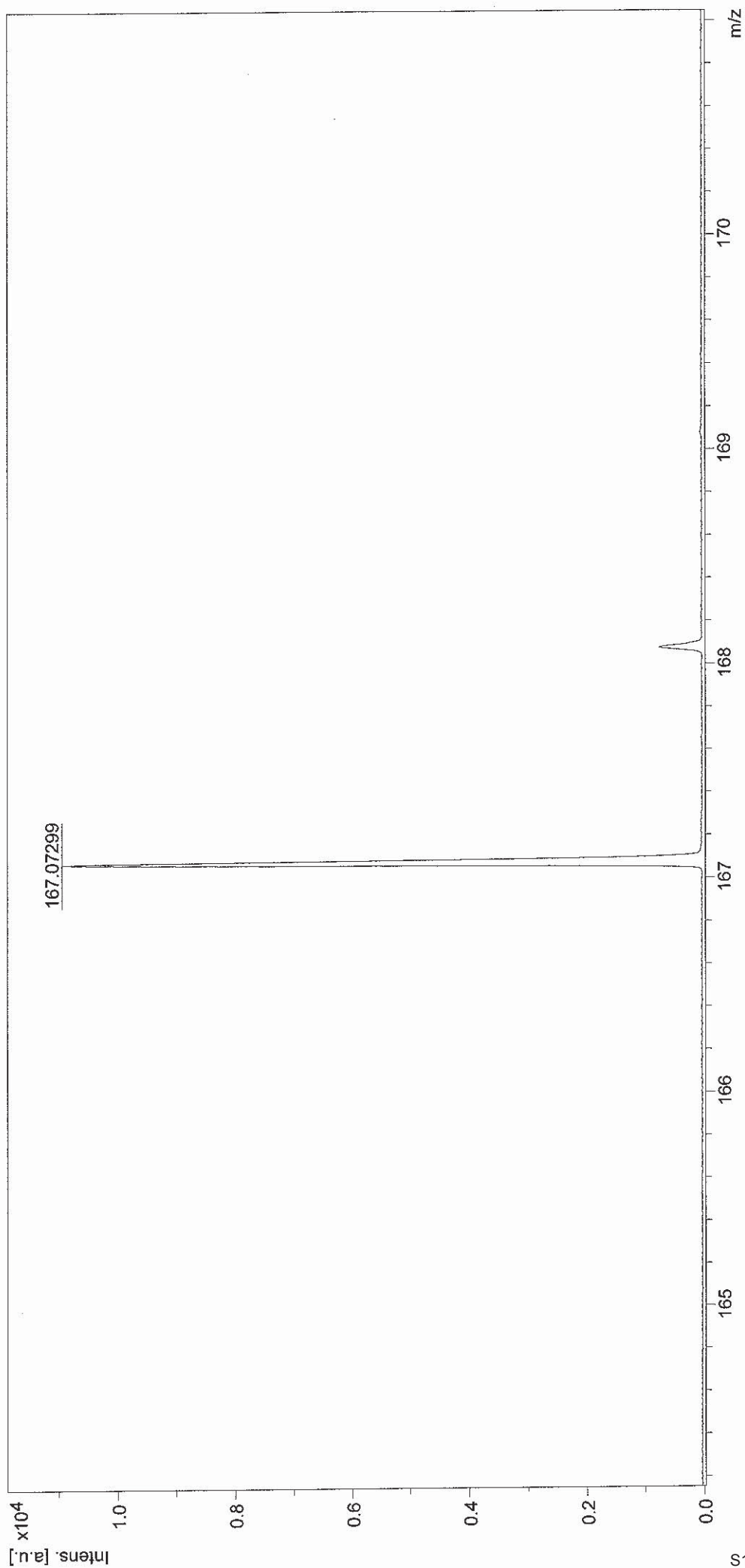
**RR061M in DCTB**

Instrument type: MALDI-TOF BRUKER ultrafleXtreme

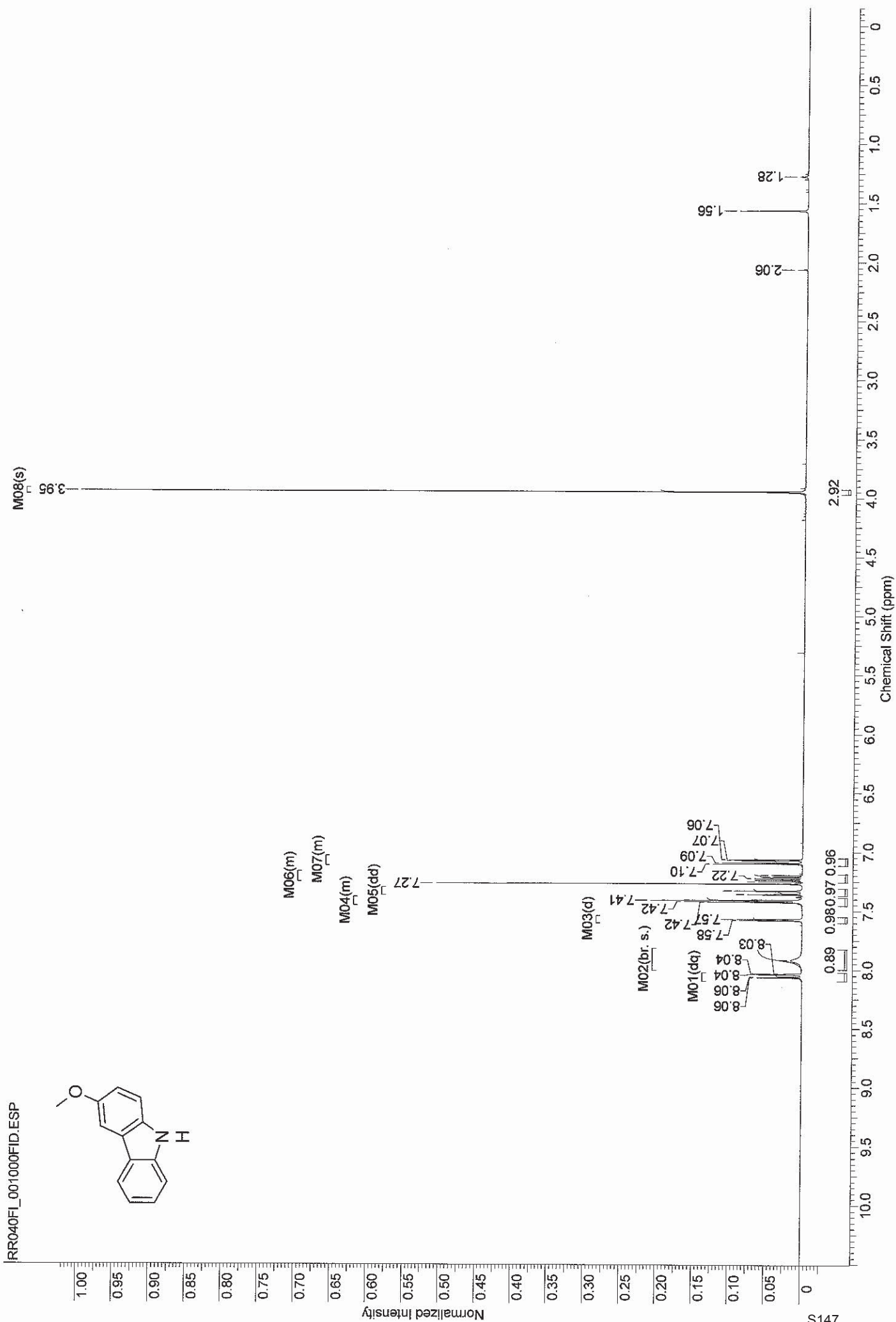
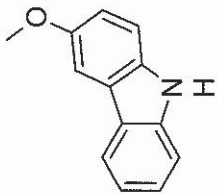
Mass spectrometry service

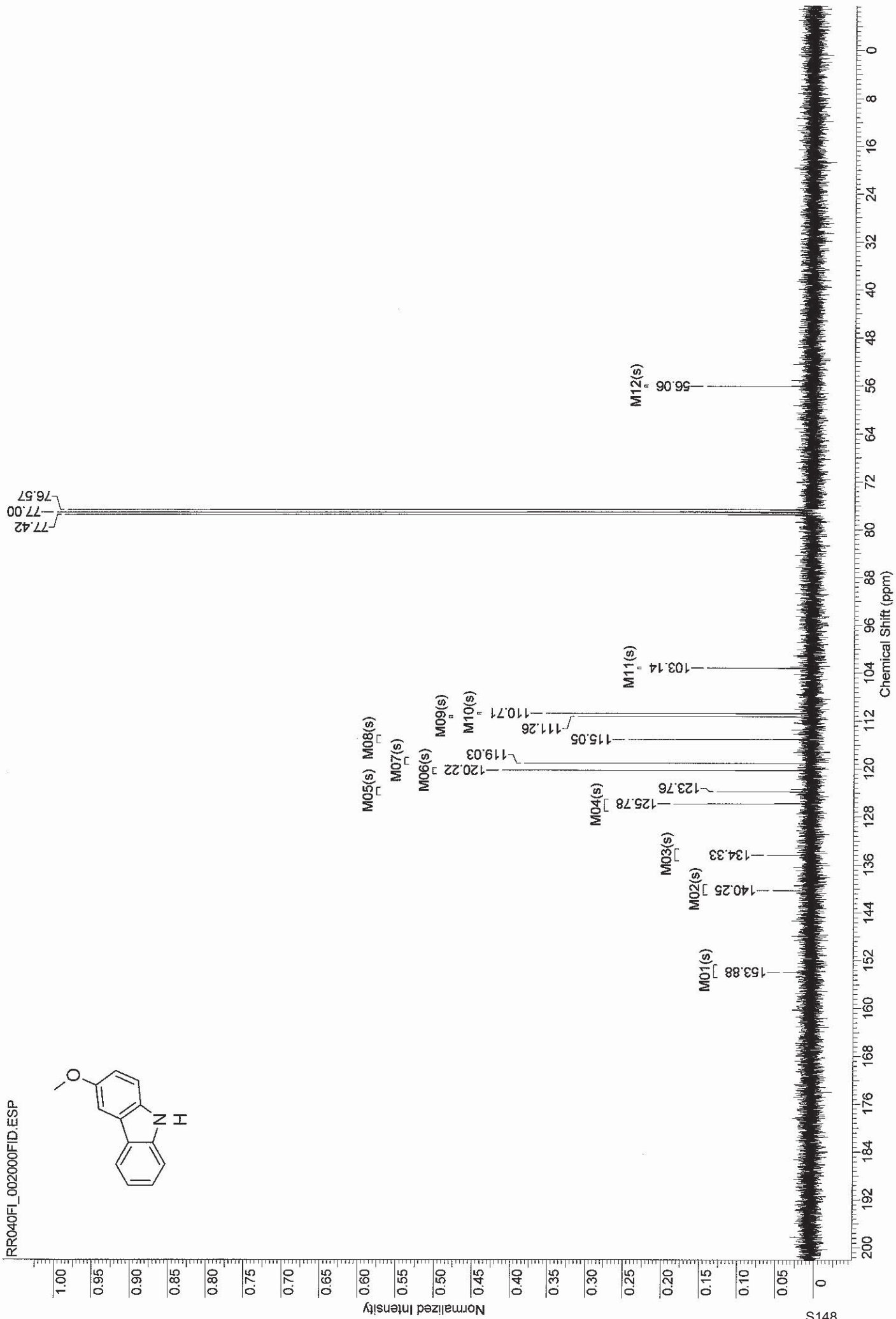
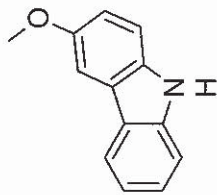
University of Fribourg

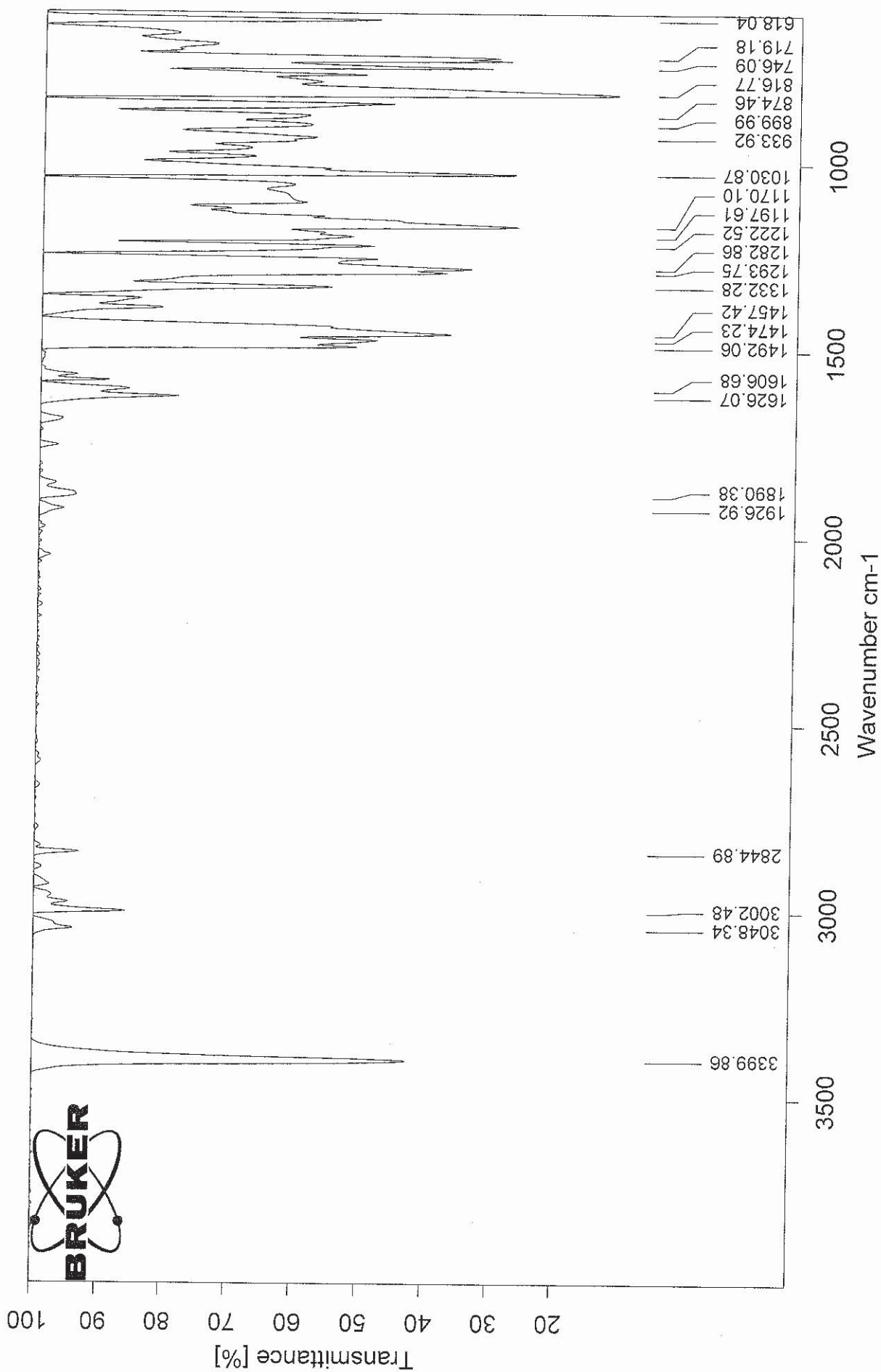
Department of Chemistry



S146







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Acquisition method name

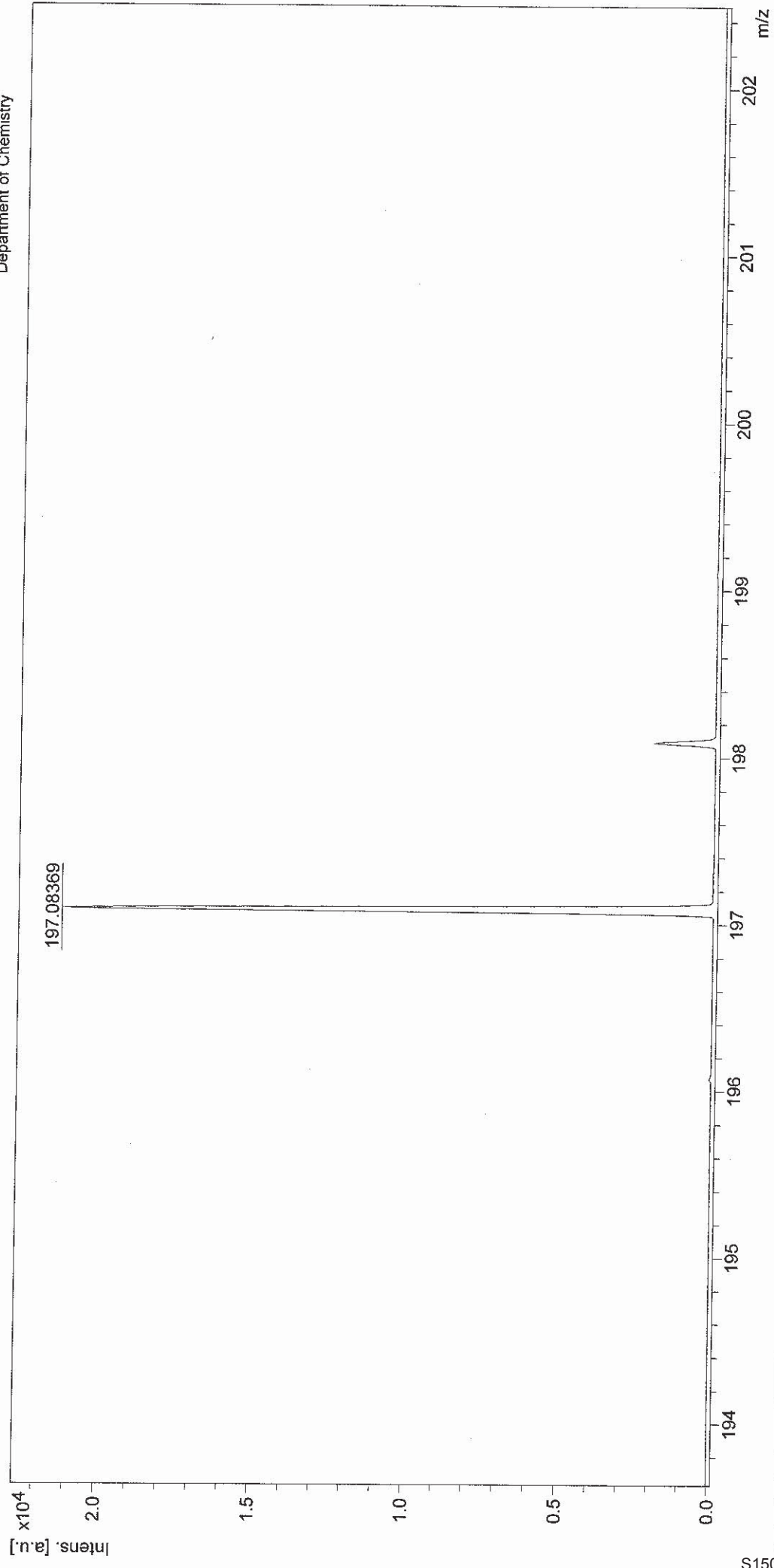
D:\Methods\MS\_SERVICE\_2013\RP\_150-2000\_Da.par

Comment 1

Comment 2 **RR040M in DCTB**

Mass spectrometry service  
University of Fribourg  
Department of Chemistry

Instrument type: MALDI-TOF BRUKER ultraflexXtreme

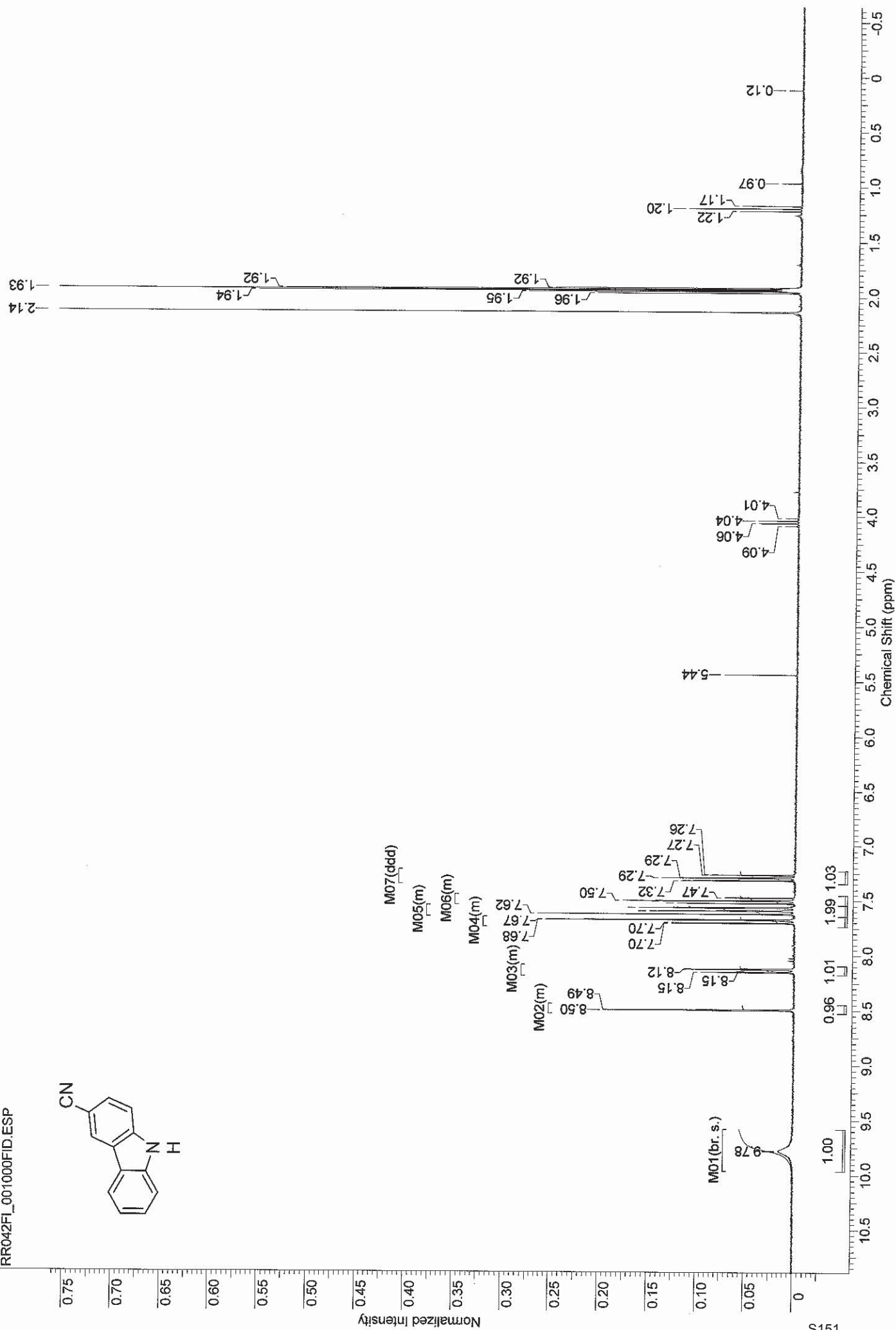
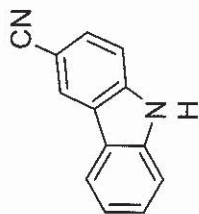


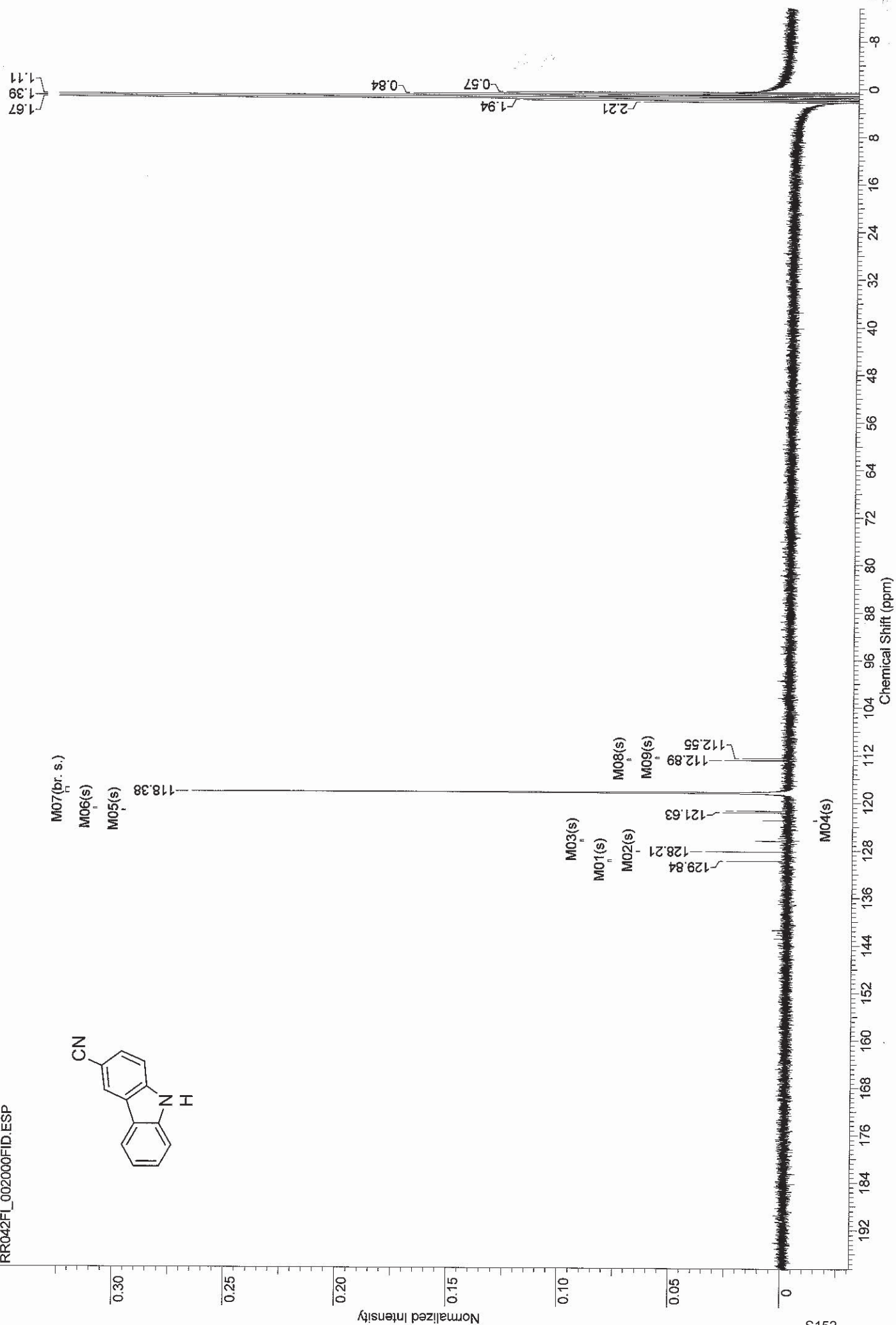
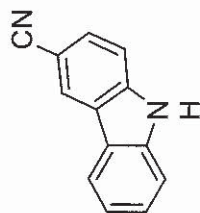
S150

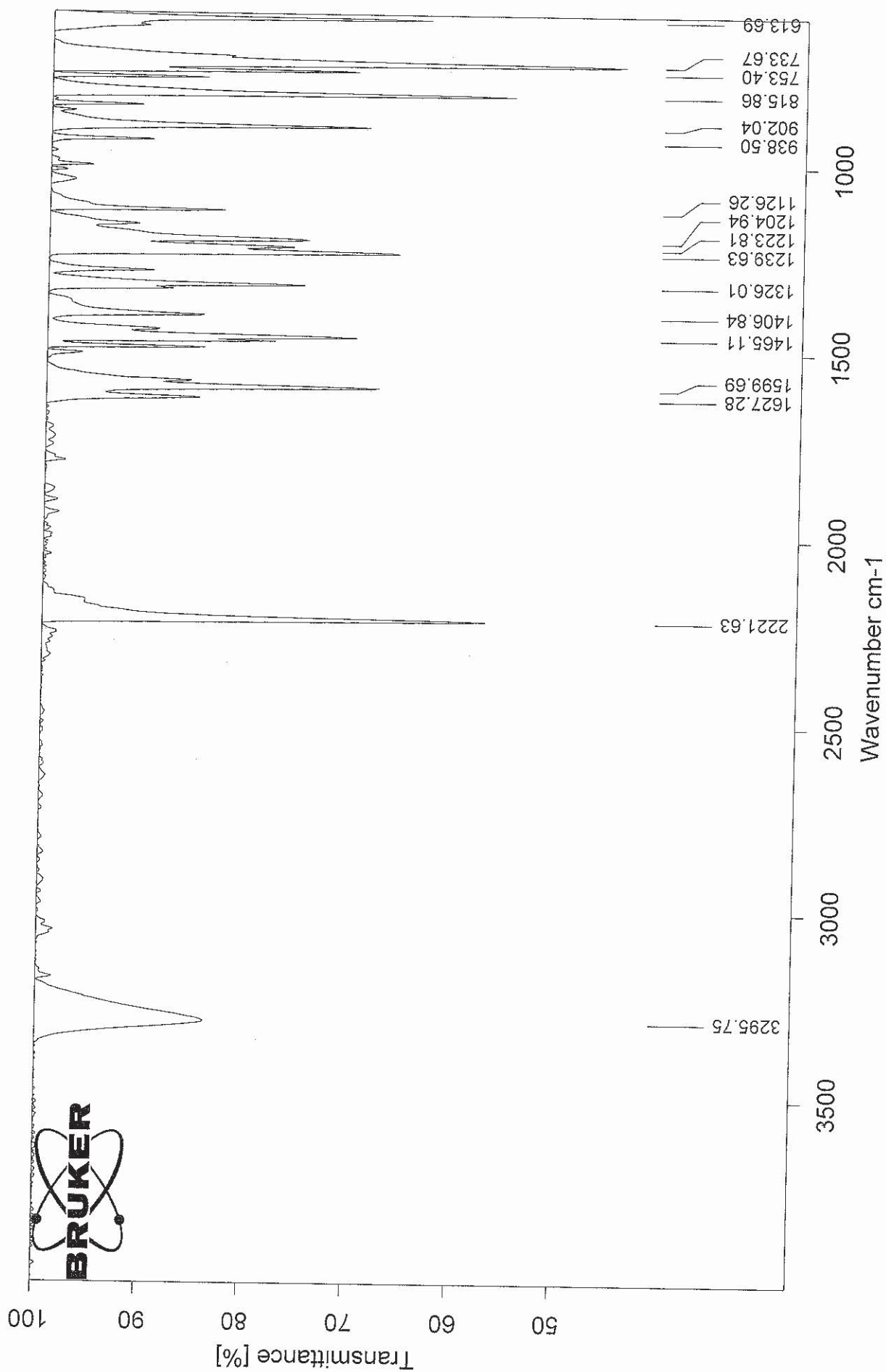
Brucker Daltonics flexAnalysis

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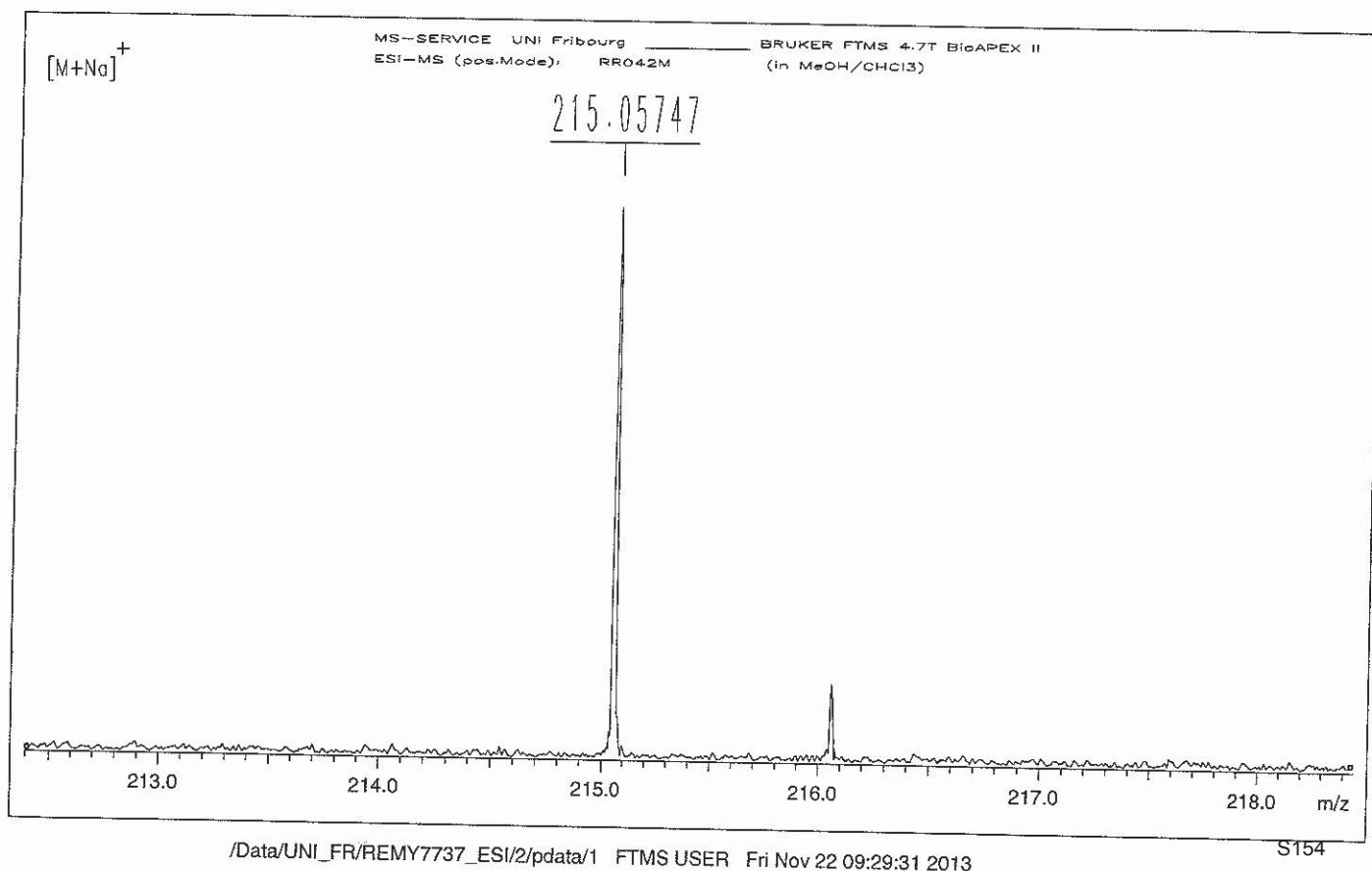
ESI-MS: RR042M

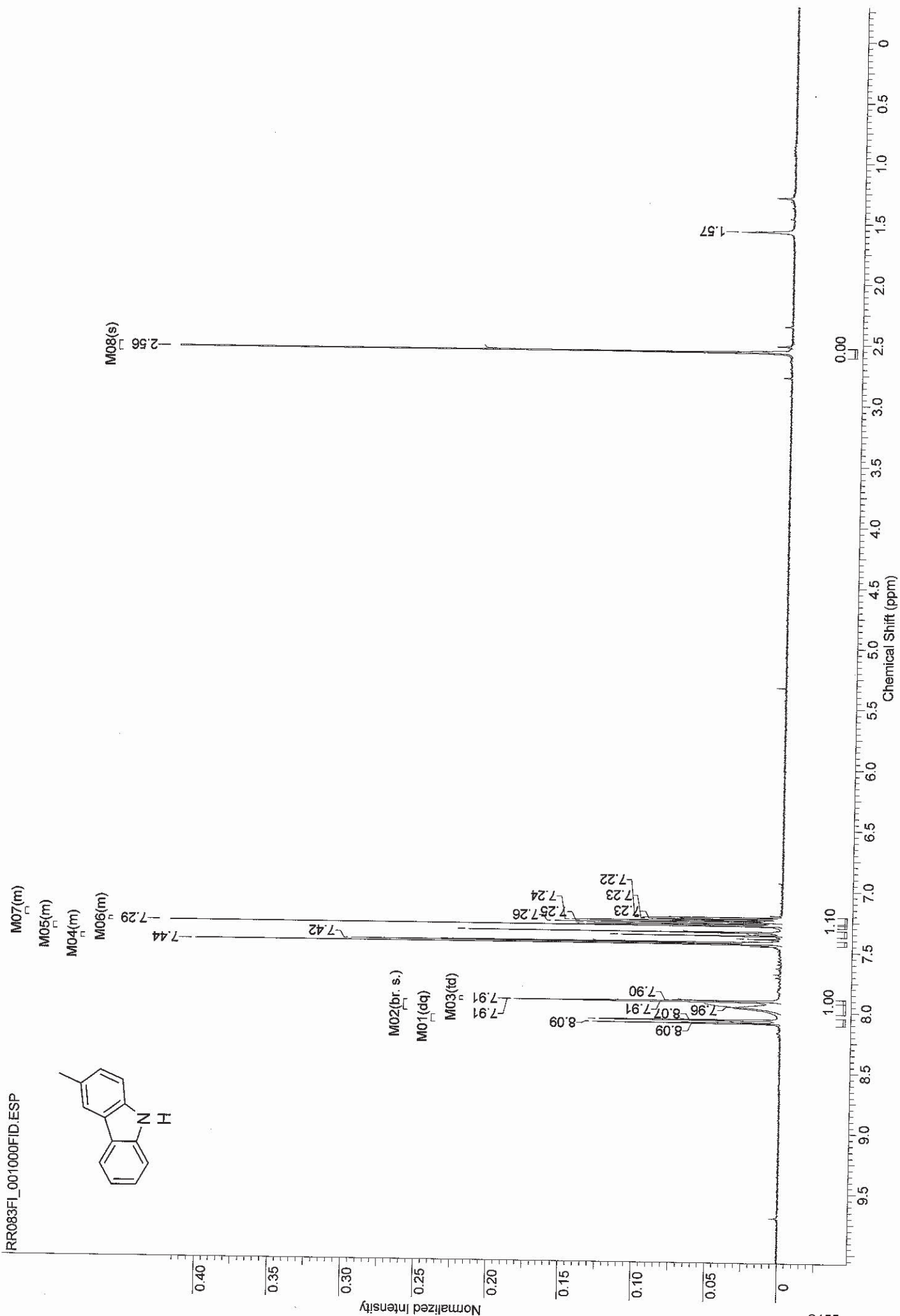
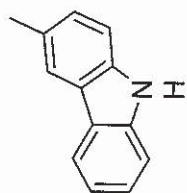
XMASS Mass Analysis for /Data/UNI\_FR/REMY7737\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

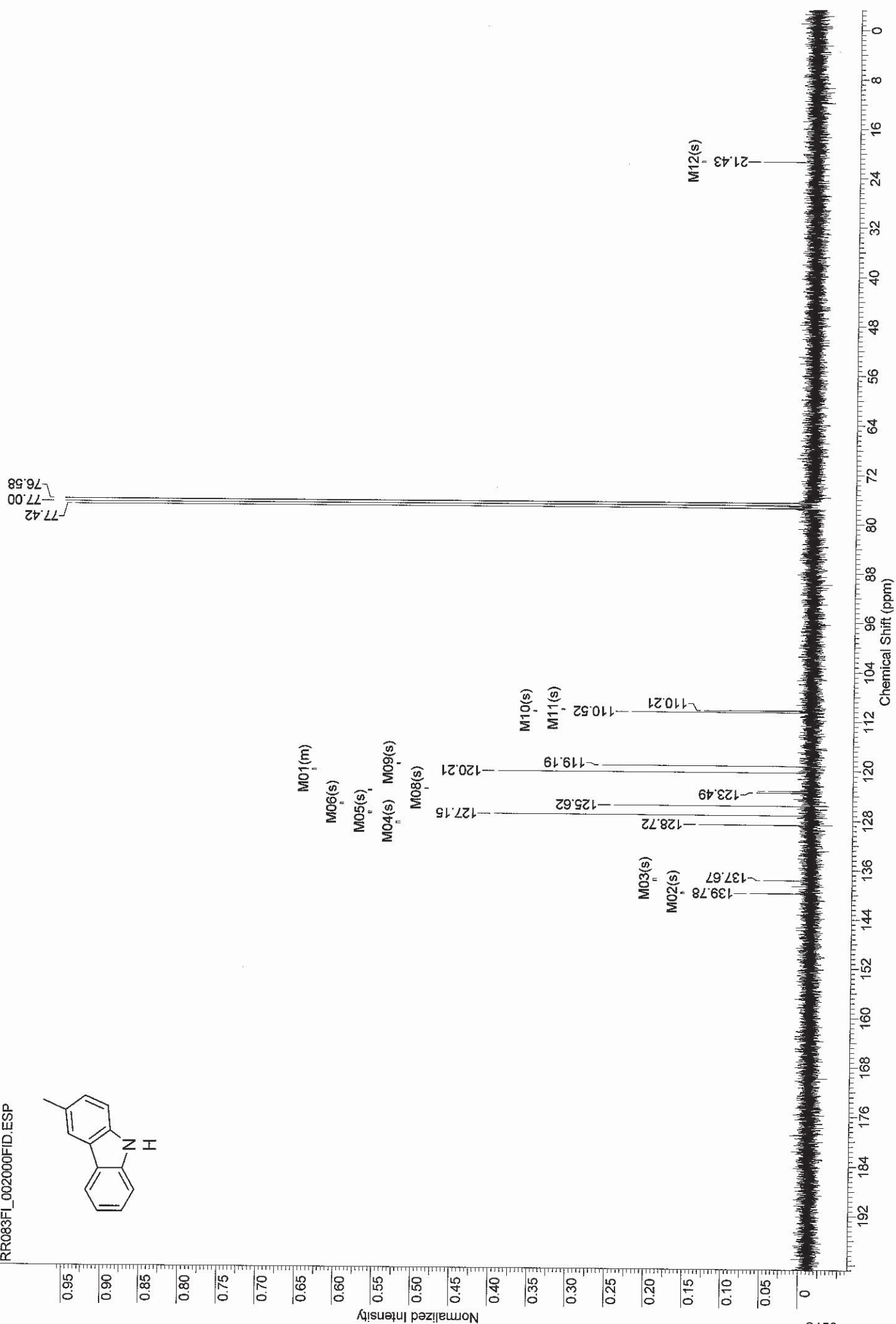
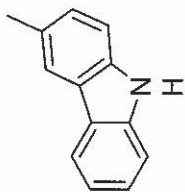
Ion mass = 215.0574740

Charge = +1

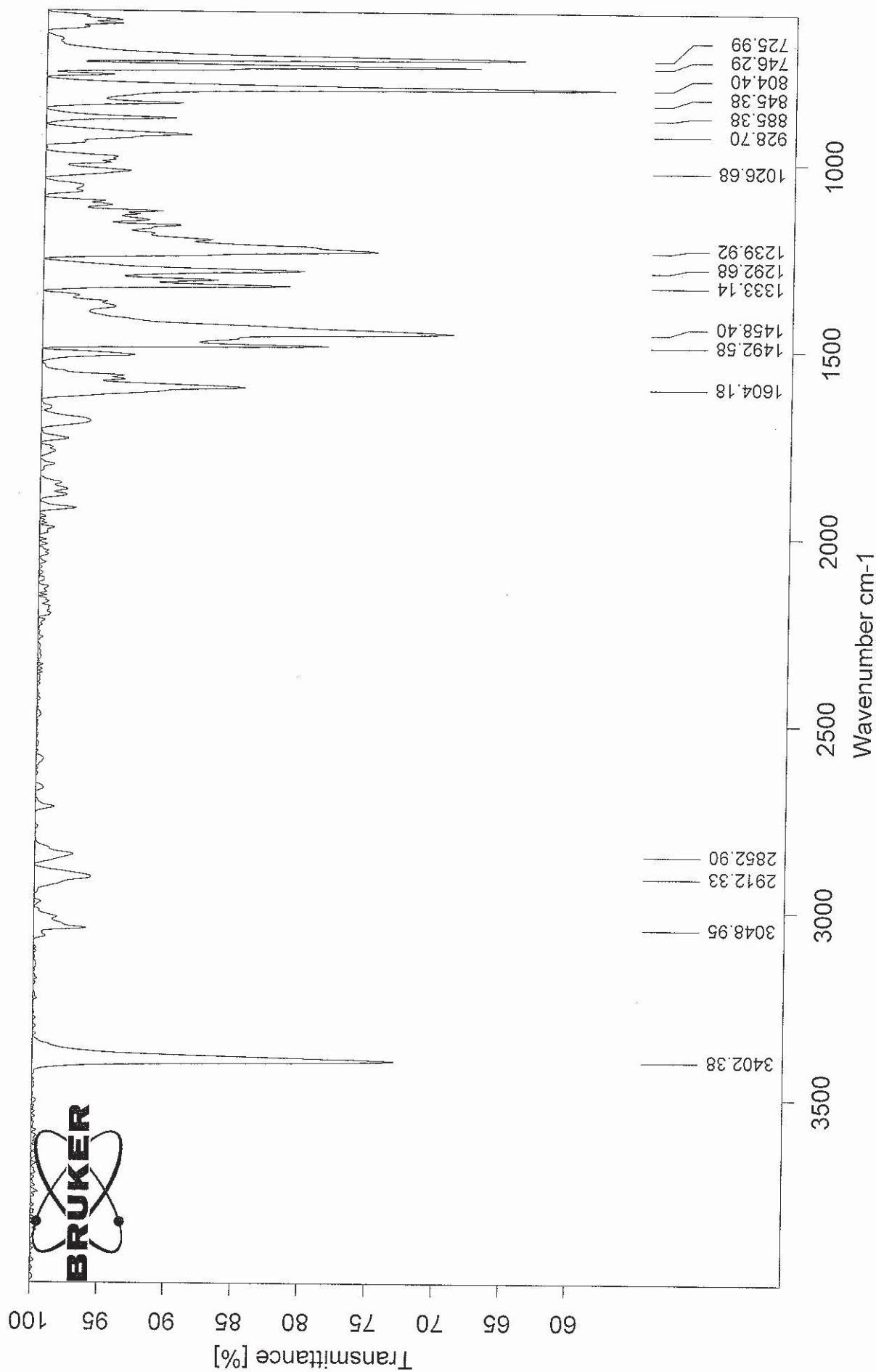
#	C	H	N	Na	mass	DBE	error
*** Mass Analysis for mass 215.0574740							
1	13	8	2	1	215.0579694	10.5	4.954e-04
2	15	7	2	0	215.0603747	13.5	2.901e-03
3	6	3	10	0	215.0536666	10.5	3.807e-03
4	5	6	9	1	215.0638373	7.0	6.363e-03
5	7	5	9	0	215.0662426	10.0	8.769e-03
6	14	5	3	0	215.0477986	14.0	9.675e-03
7	12	6	3	1	215.0453933	11.0	1.208e-02
8	14	10	1	1	215.0705454	10.0	1.307e-02
9	16	9	1	0	215.0729507	13.0	1.548e-02
10	6	8	8	1	215.0764134	6.5	1.894e-02











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24.04.2013

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Acquisition method name

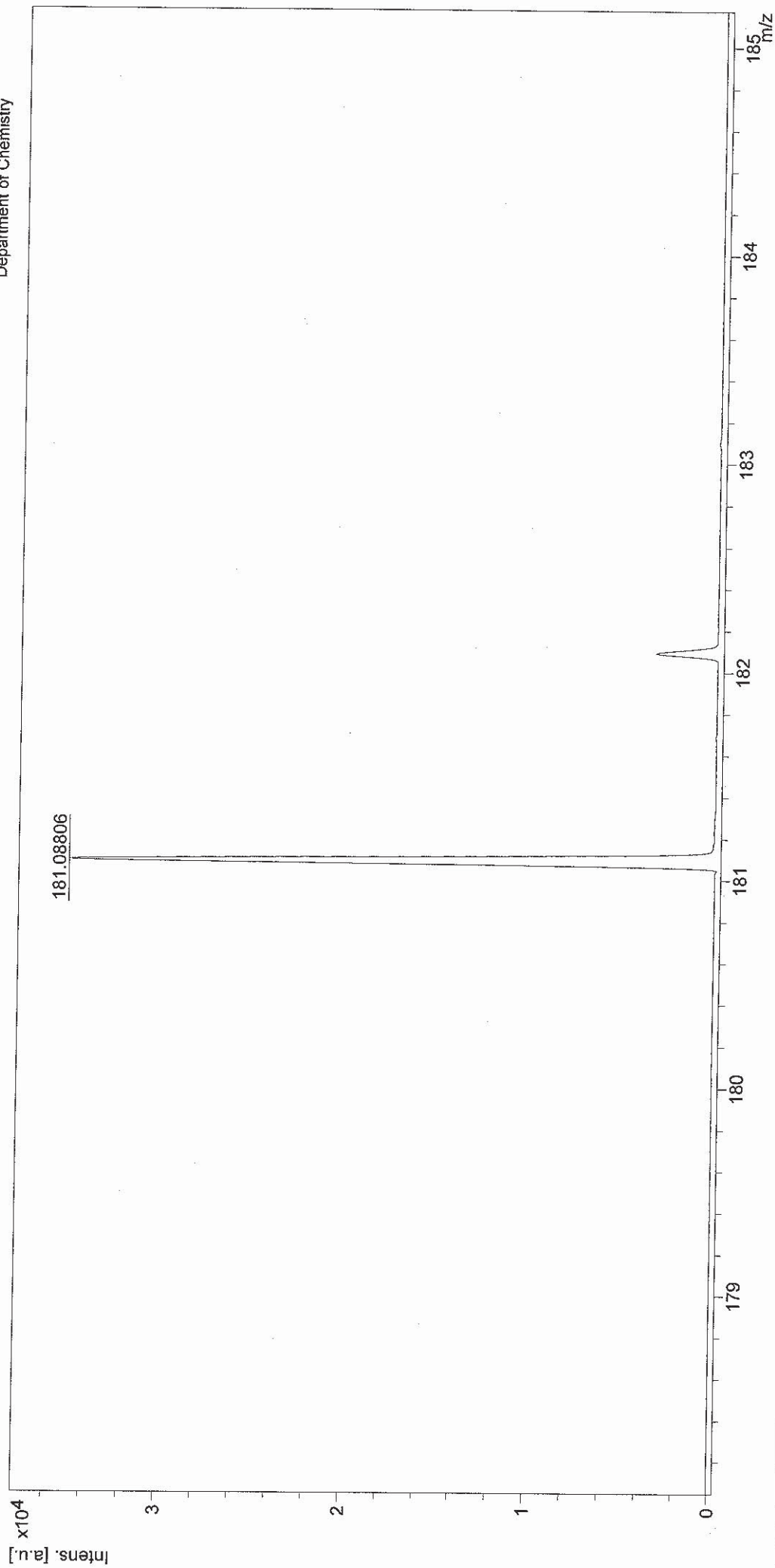
D:\Methods\MS\_SERVICE\_2013\RP\_150-2000\_Da.par

Comment 1

Comment 2 **RR083M in DCTB**

Instrument type: MALDI-TOF BRUKER ultrafleXtreme

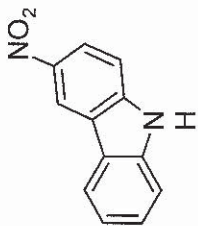
Mass spectrometry service  
University of Fribourg  
Department of Chemistry



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Brucker Daltonics flexAnalysis

printed: 11/22/2013 8:17:14 AM



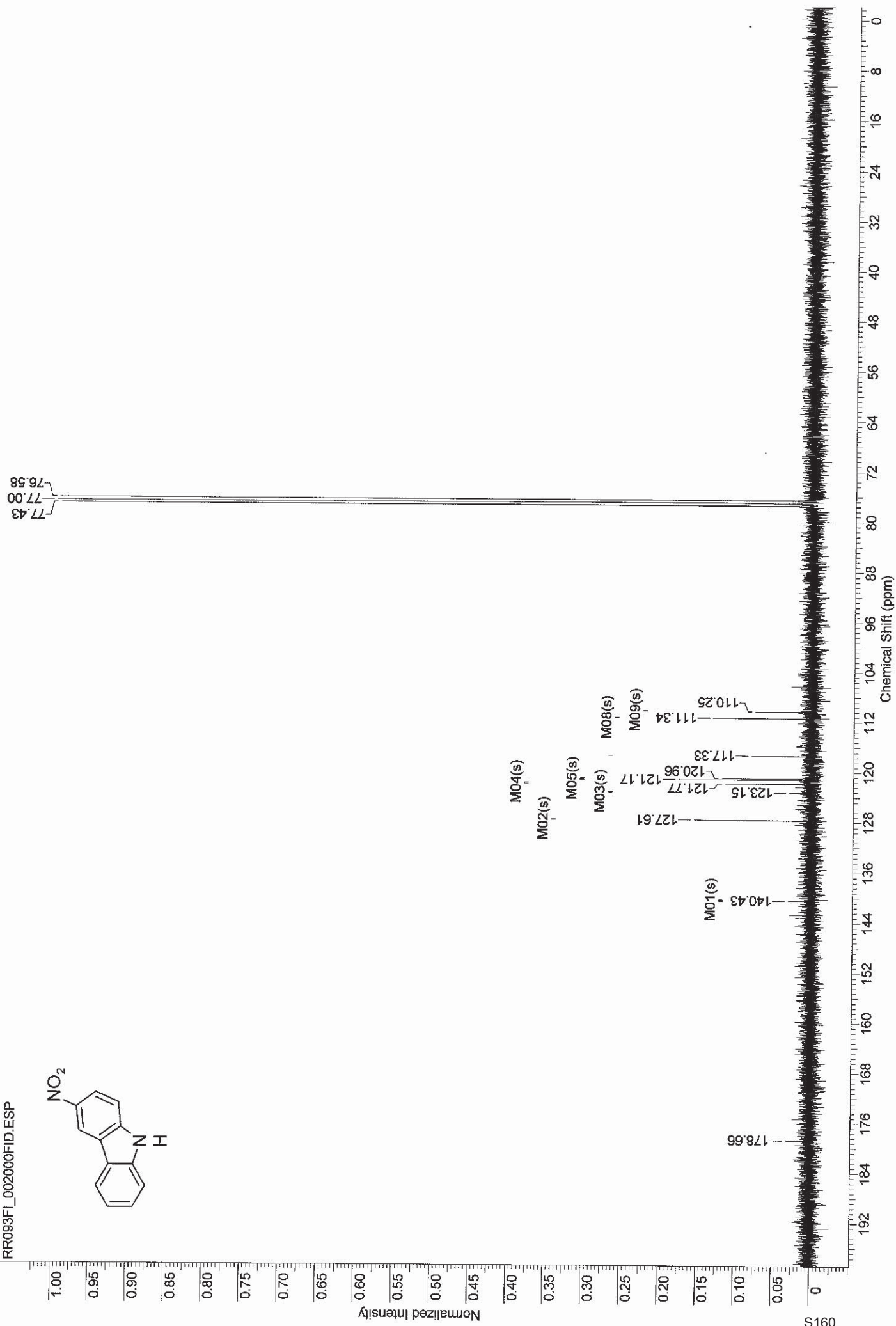
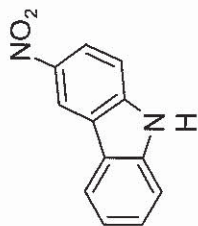
M08(m)  
M07(m)  
M06(dd)  
M05(m)

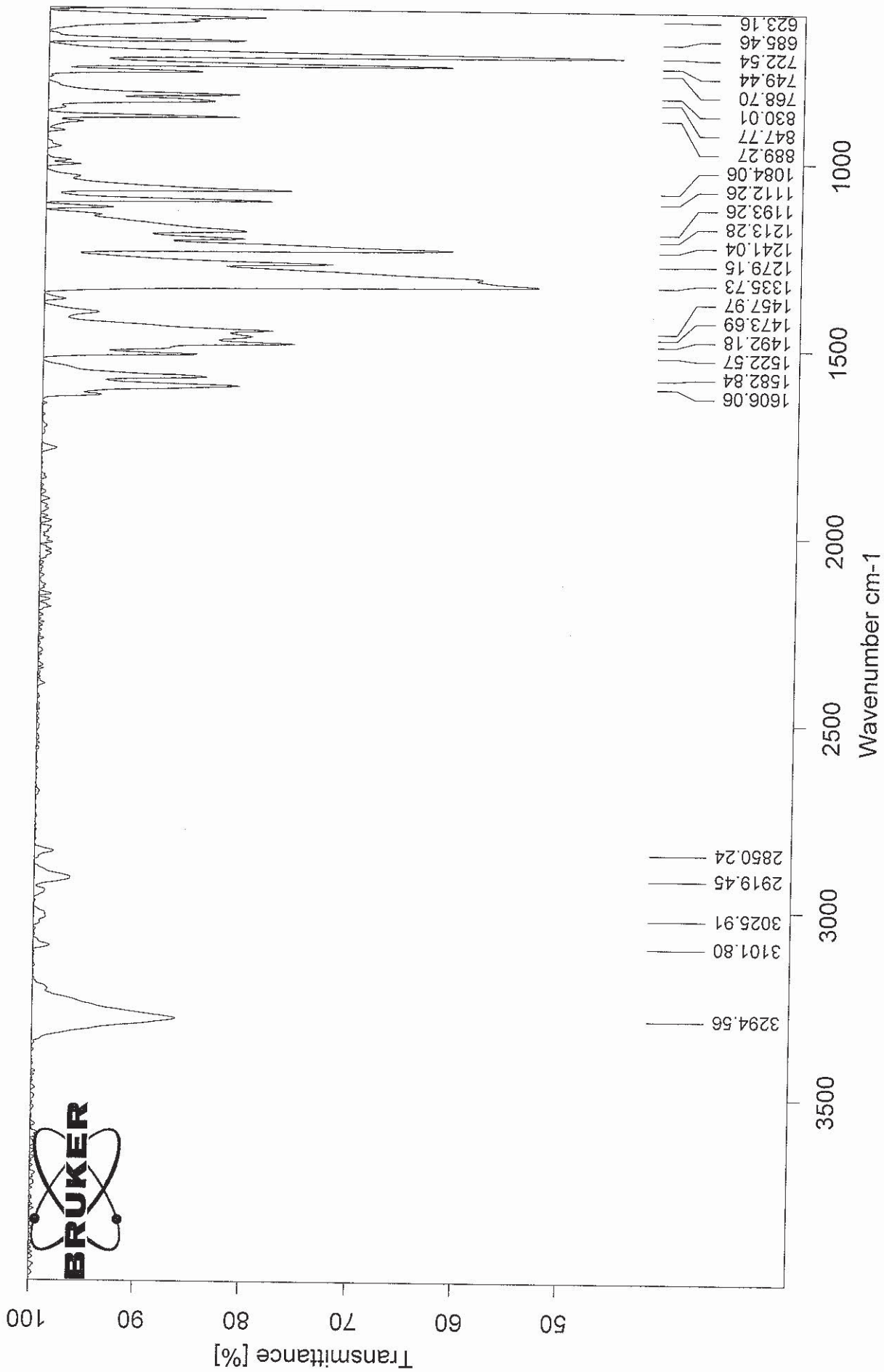
7.27

M02(m)

M01(d)  
9.03  
9.02  
8.54  
8.52  
8.51  
8.39  
8.36  
8.17  
8.15  
8.14  
8.11  
8.08  
7.58  
7.55  
7.54  
7.53  
7.53  
7.50  
7.37

2.06  
1.58  
1.30  
1.29  
1.27  
1.26  
0.89  
0.86  
0.84







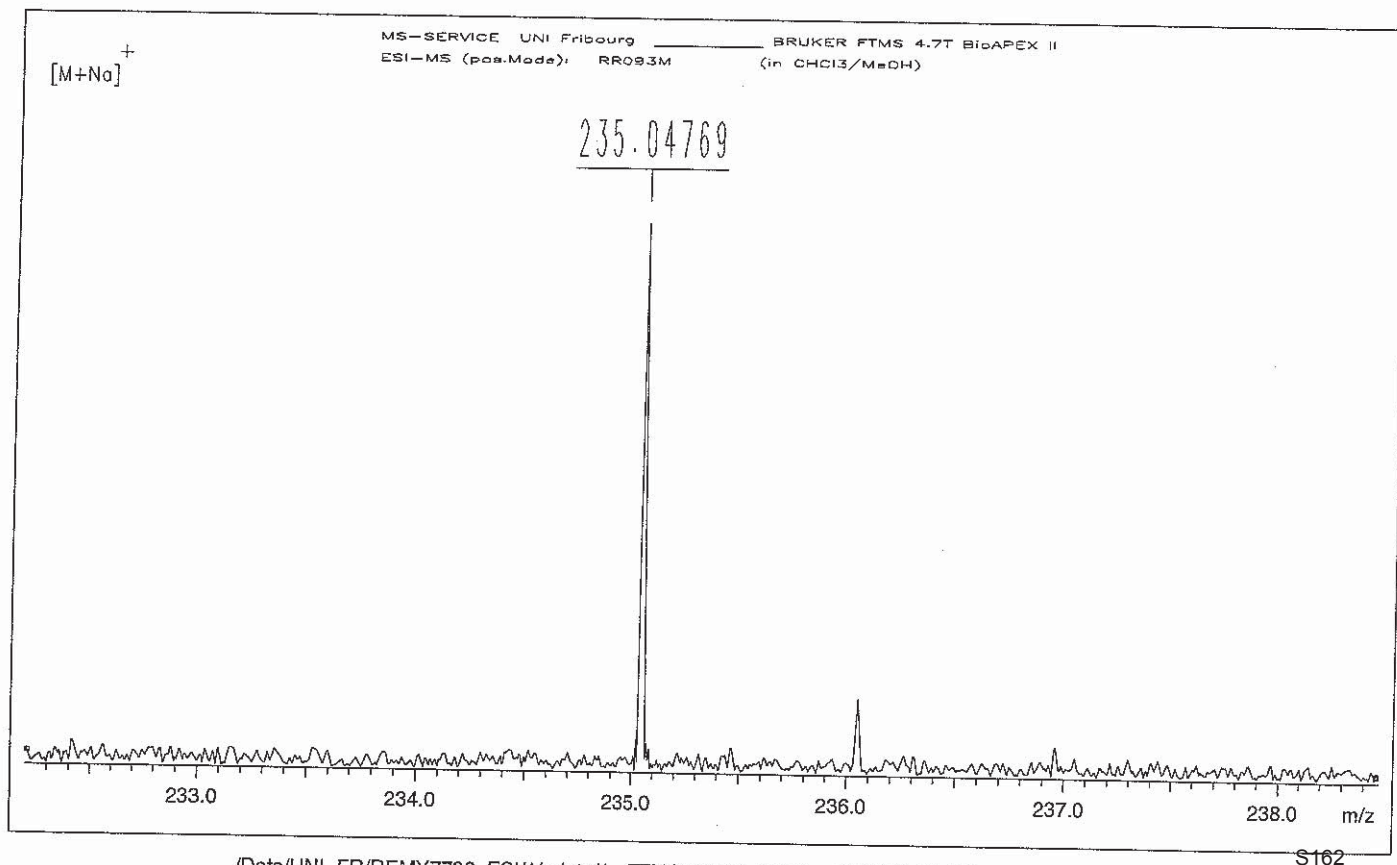
ESI-MS: RR093M

XMASS Mass Analysis for /Data/UNI\_FR/REMY7736\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

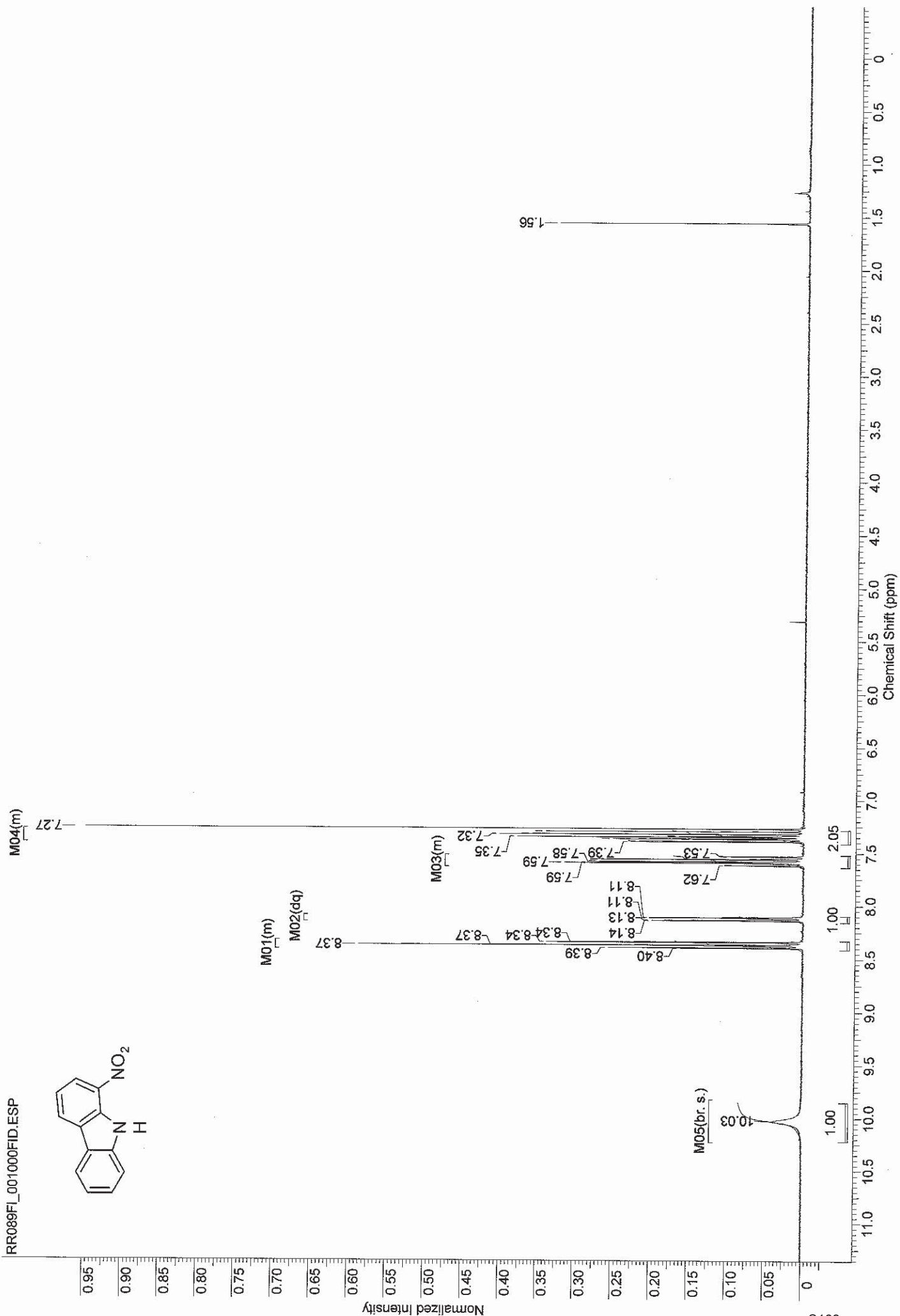
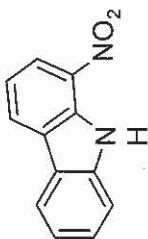
Ion mass = 235.0476920

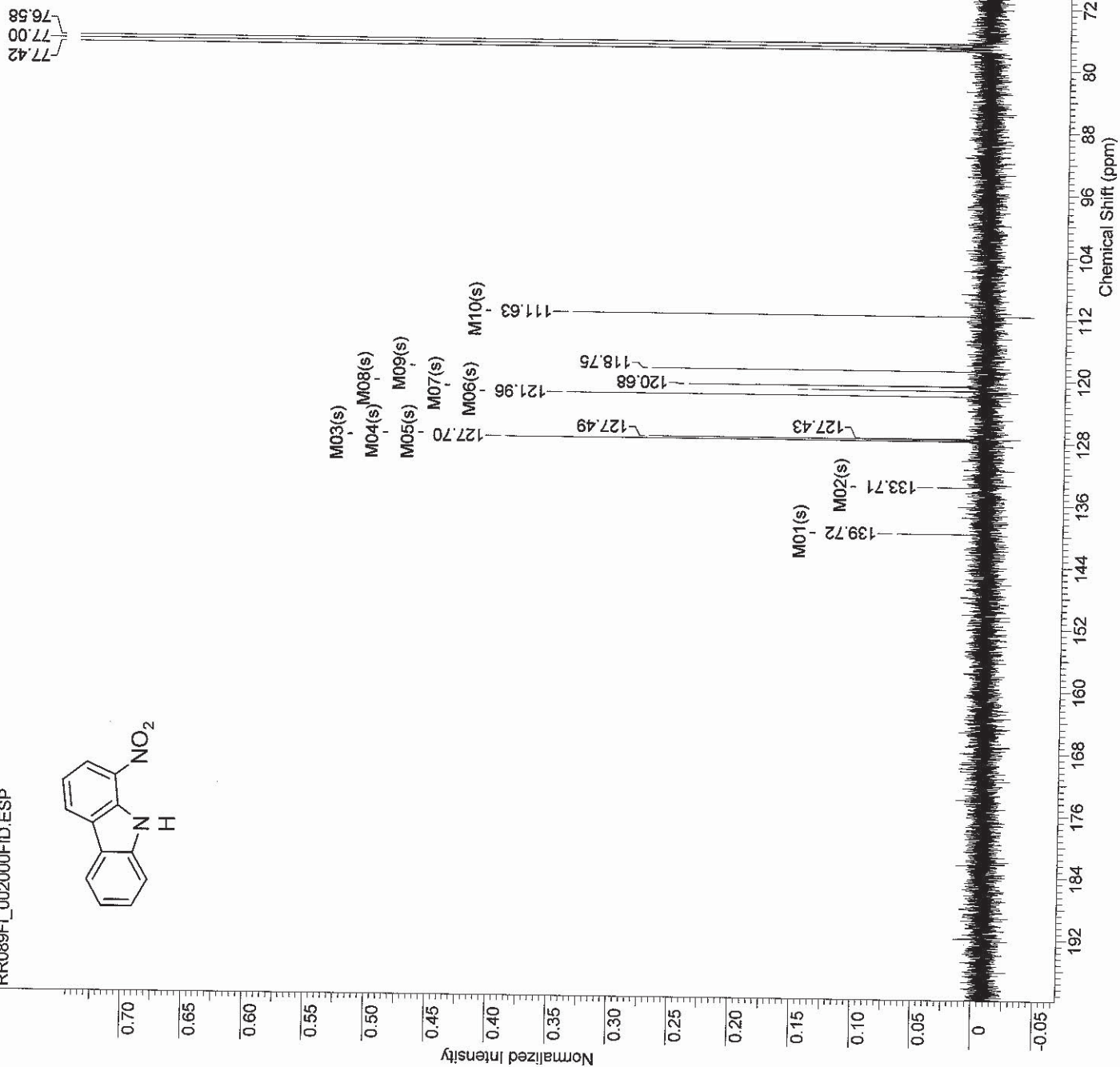
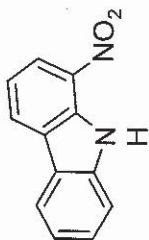
Charge = +1

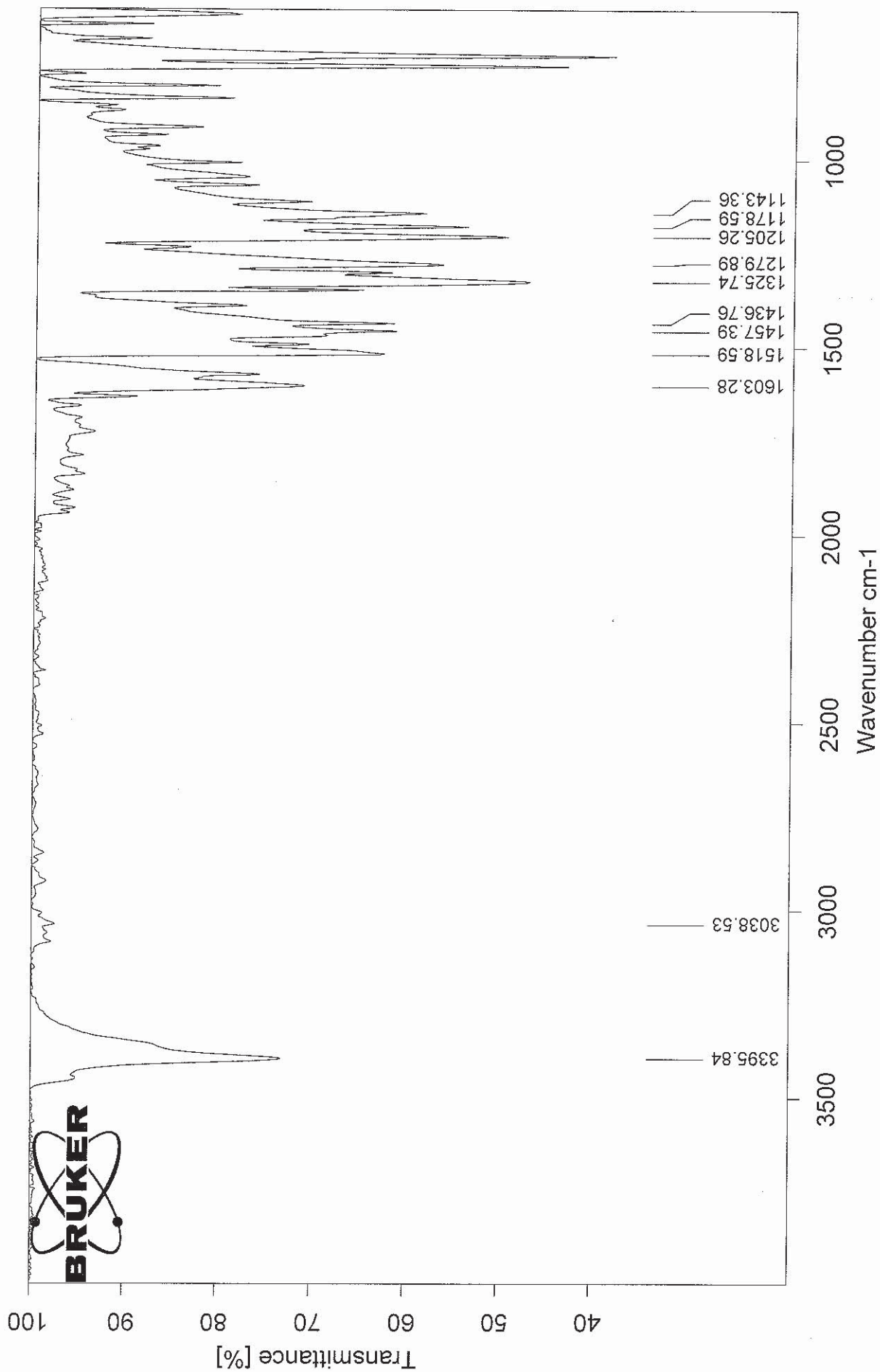
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 235.0476920								
1	12	8	2	2	1	235.0477986	9.5	1.066e-04
2	11	9	1	5	0	235.0475238	8.0	1.682e-04
3	12	5	5	1	0	235.0488612	13.0	1.169e-03
4	10	6	5	1	1	235.0464559	10.0	1.236e-03
5	9	7	4	4	0	235.0461812	8.5	1.511e-03
6	14	7	2	2	0	235.0502039	12.5	2.512e-03
7	9	10	1	5	1	235.0451185	5.0	2.573e-03
8	7	5	7	3	0	235.0448385	9.0	2.854e-03
9	7	8	4	4	1	235.0437759	5.5	3.916e-03
10	6	9	3	7	0	235.0435011	4.0	4.191e-03











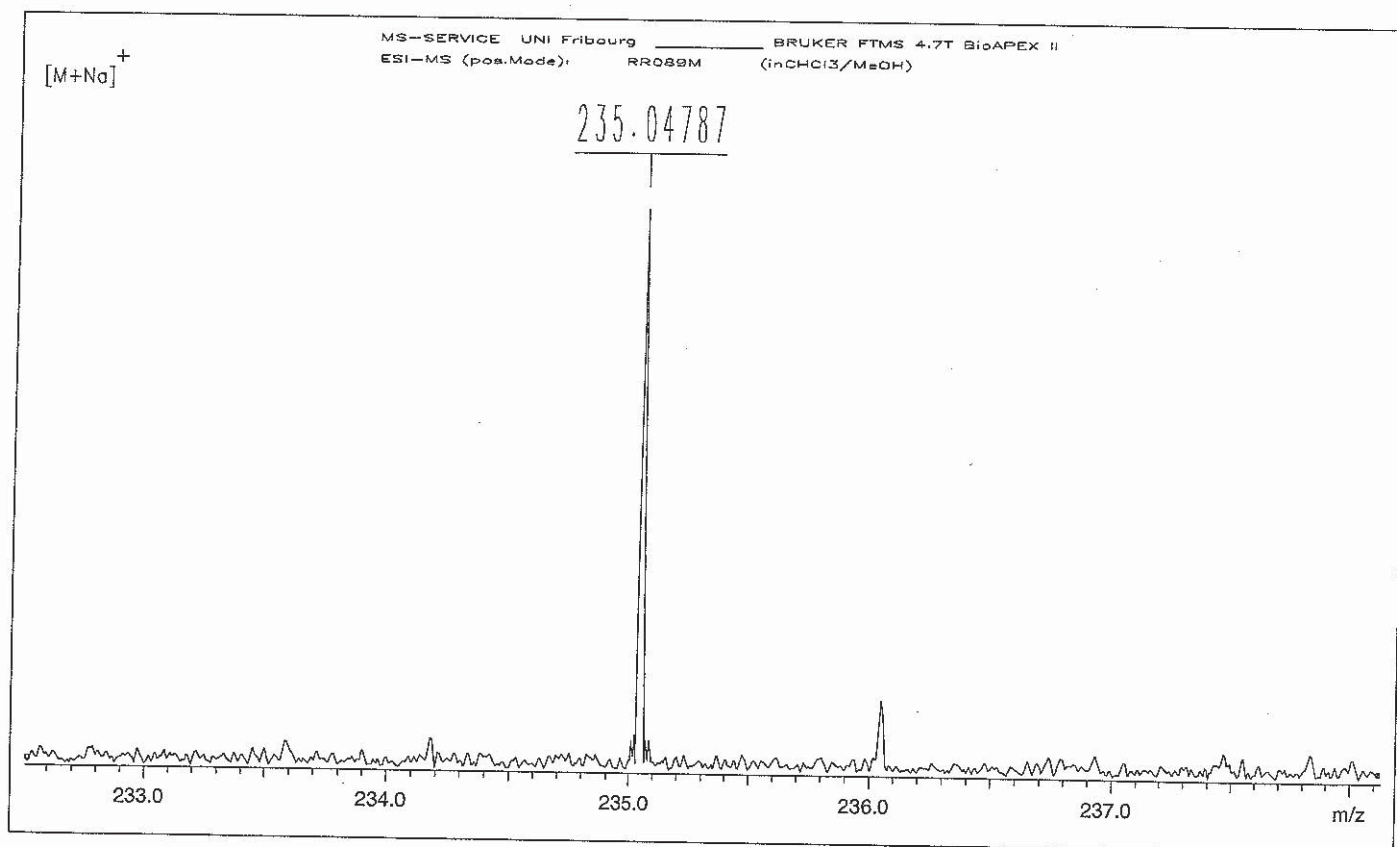
ESI-MS: RR0893M

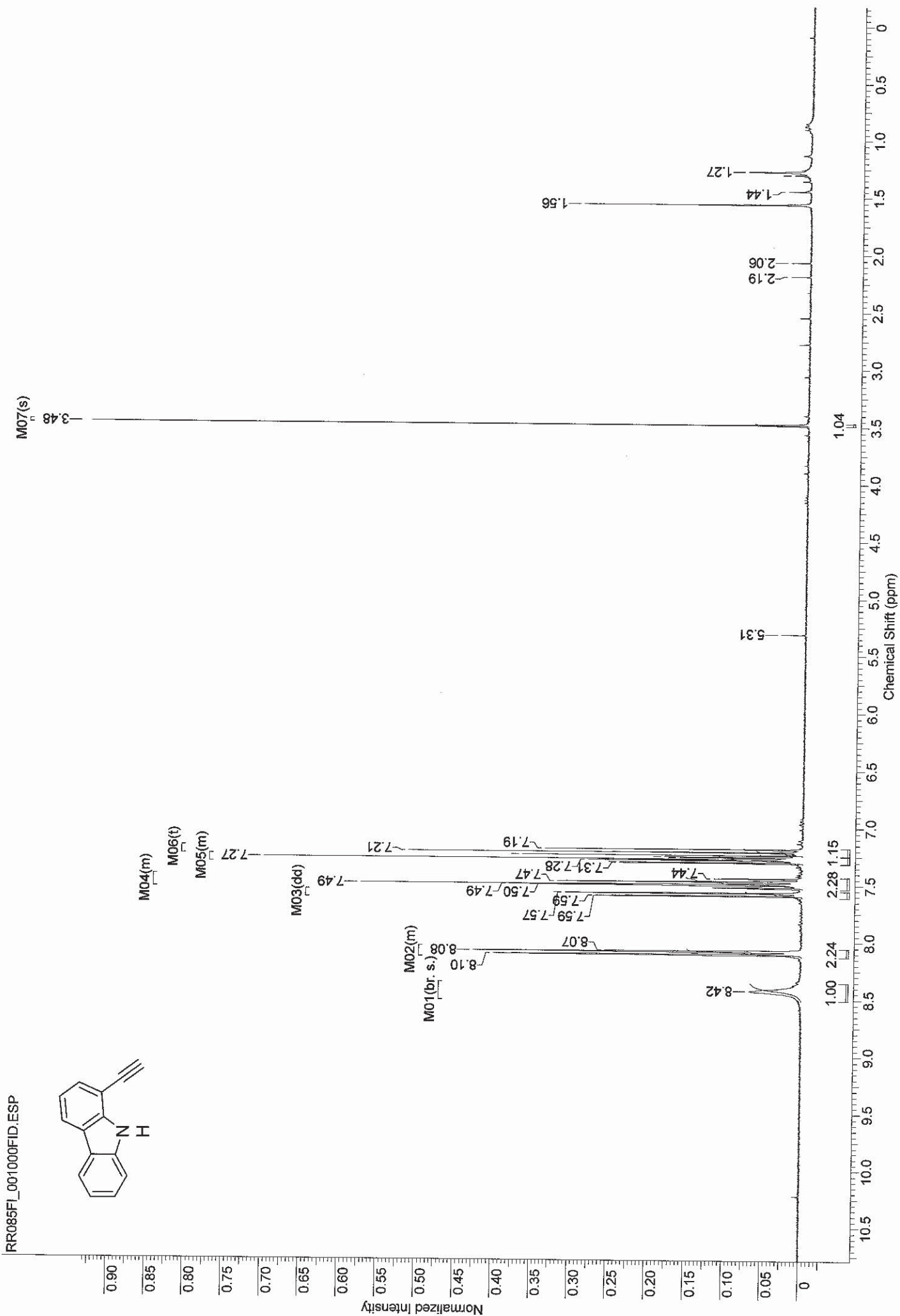
XMASS Mass Analysis for /Data/UNI\_FR/REMY7735\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

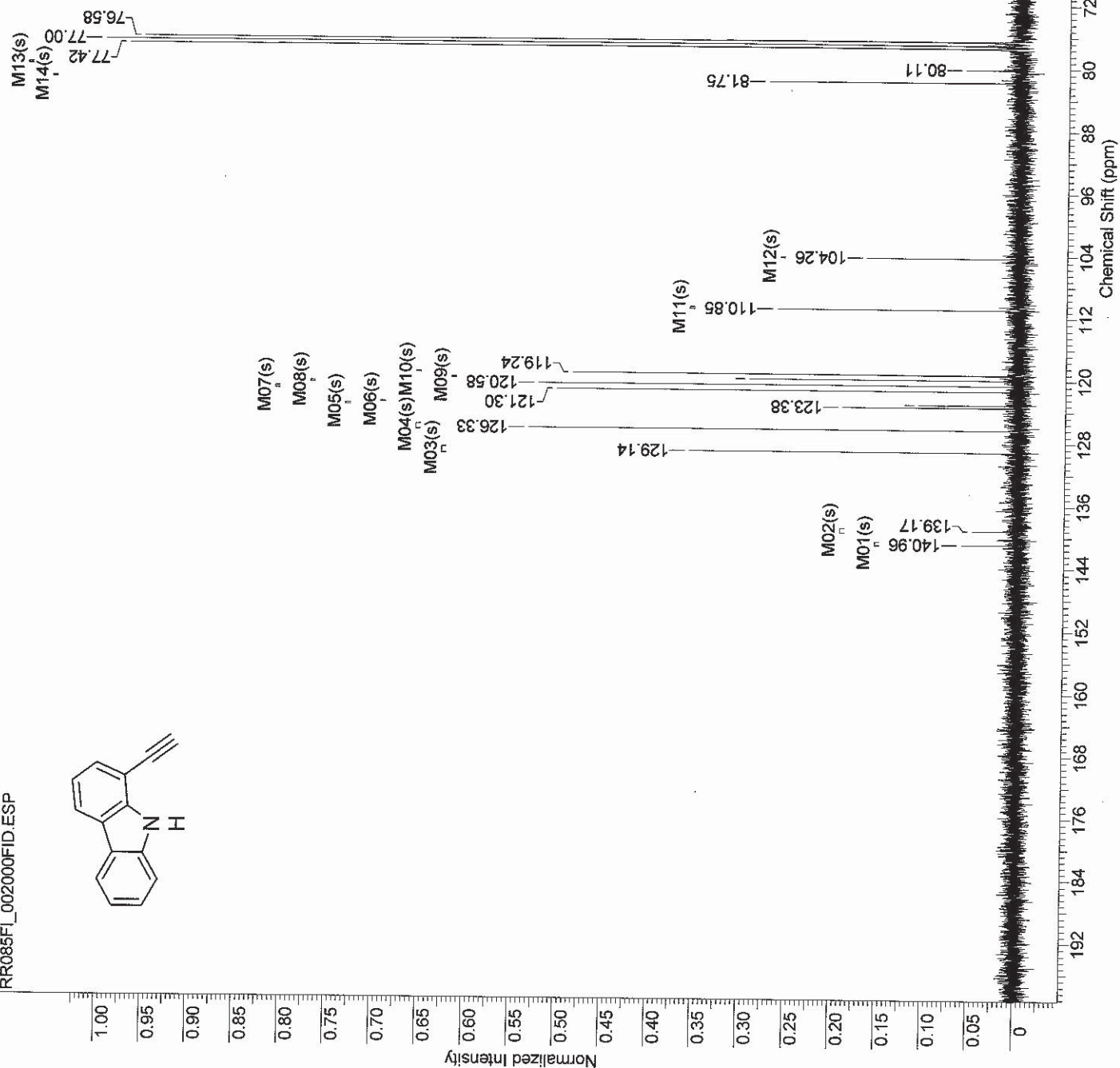
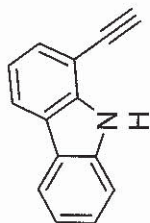
Ion mass = 235.0478660

Charge = +1

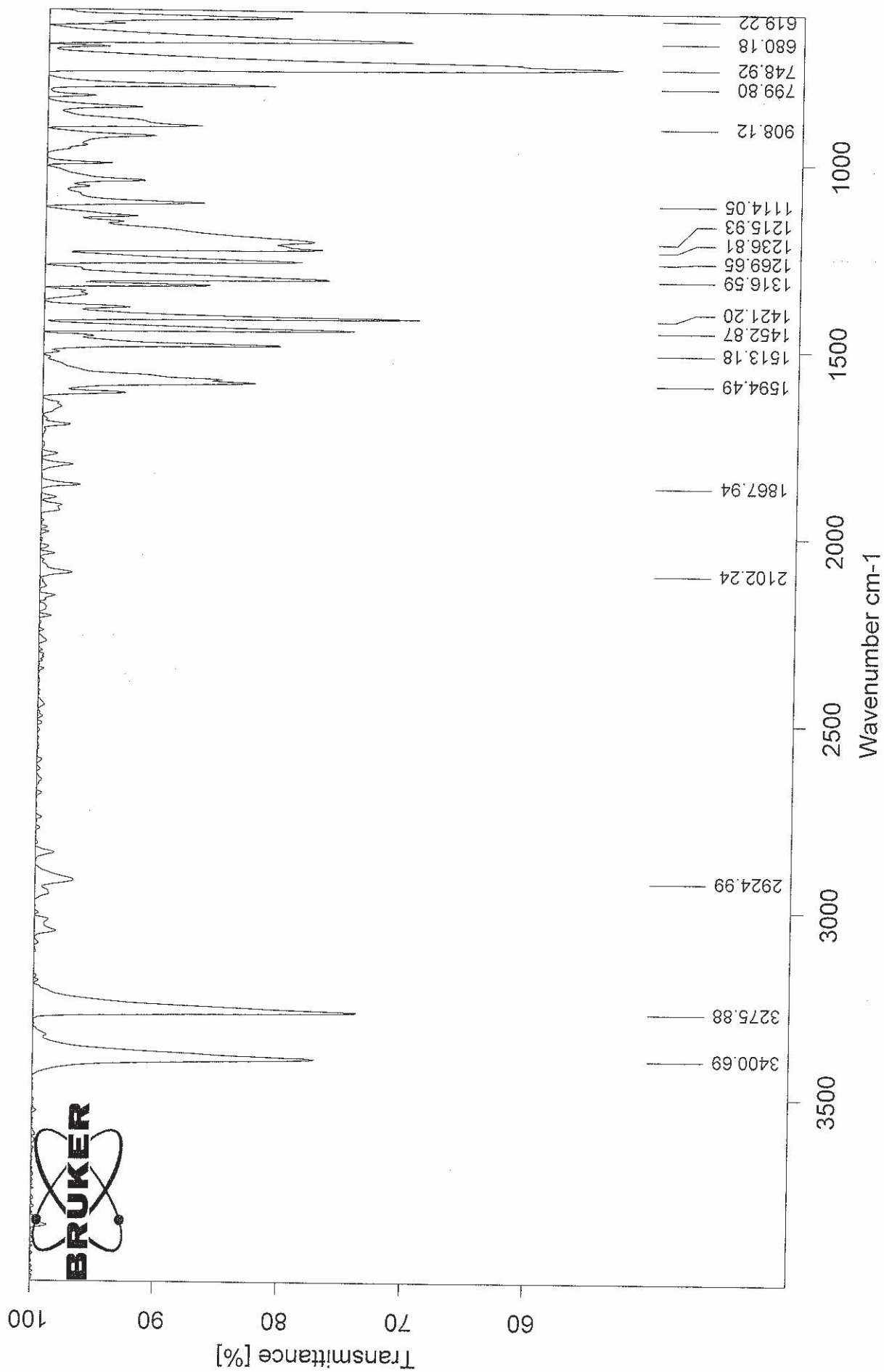
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 235.0478660								
1	12	8	2	2	1	235.0477986	9.5	6.740e-05
2	11	9	1	5	0	235.0475238	8.0	3.422e-04
3	12	5	5	1	0	235.0488612	13.0	9.952e-04
4	10	6	5	1	1	235.0464559	10.0	1.410e-03
5	9	7	4	4	0	235.0461812	8.5	1.685e-03
6	14	7	2	2	0	235.0502039	12.5	2.338e-03
7	9	10	1	5	1	235.0451185	5.0	2.747e-03
8	7	5	7	3	0	235.0448385	9.0	3.028e-03
9	7	8	4	4	1	235.0437759	5.5	4.090e-03
10	6	9	3	7	0	235.0435011	4.0	4.365e-03



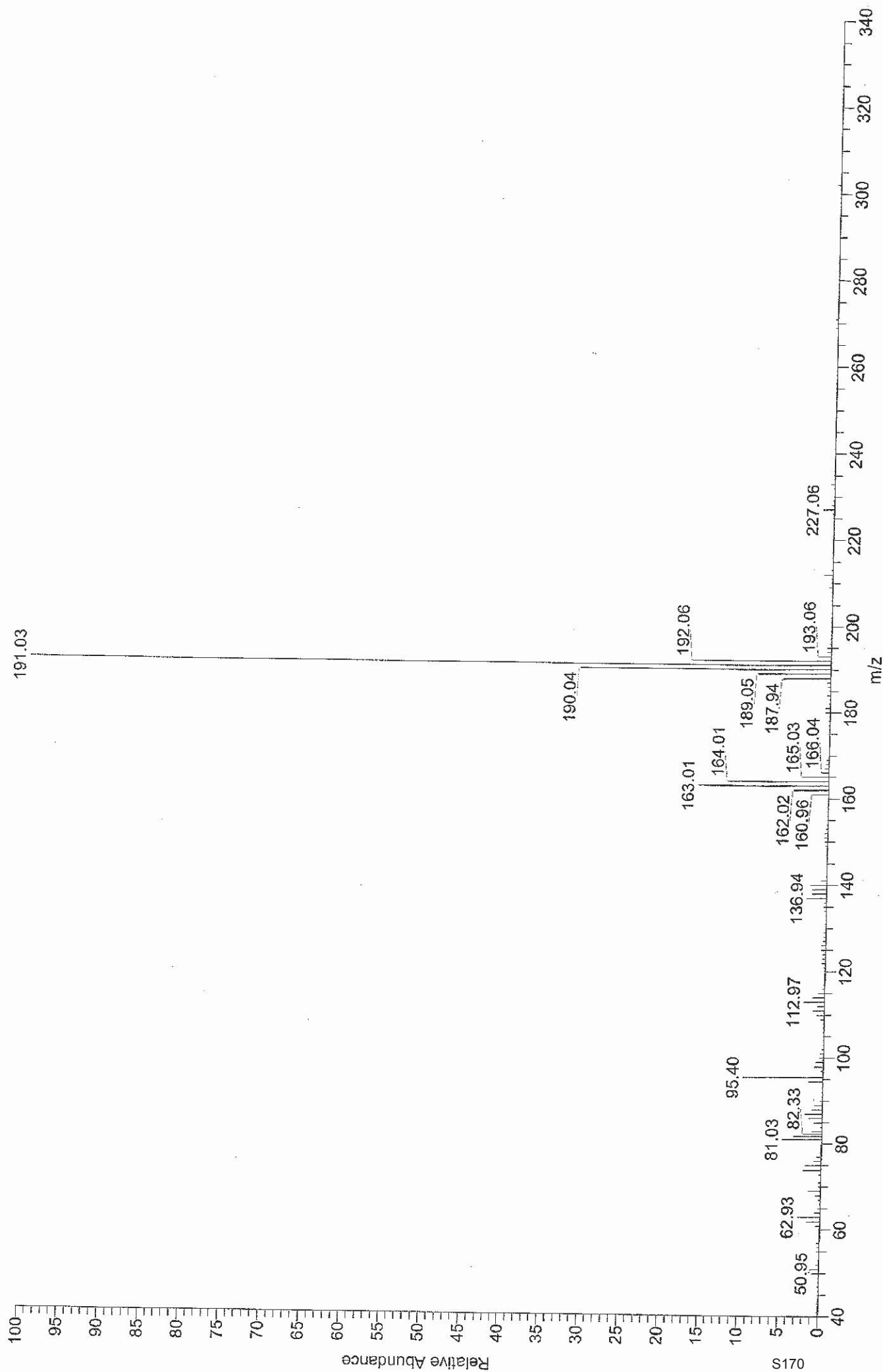


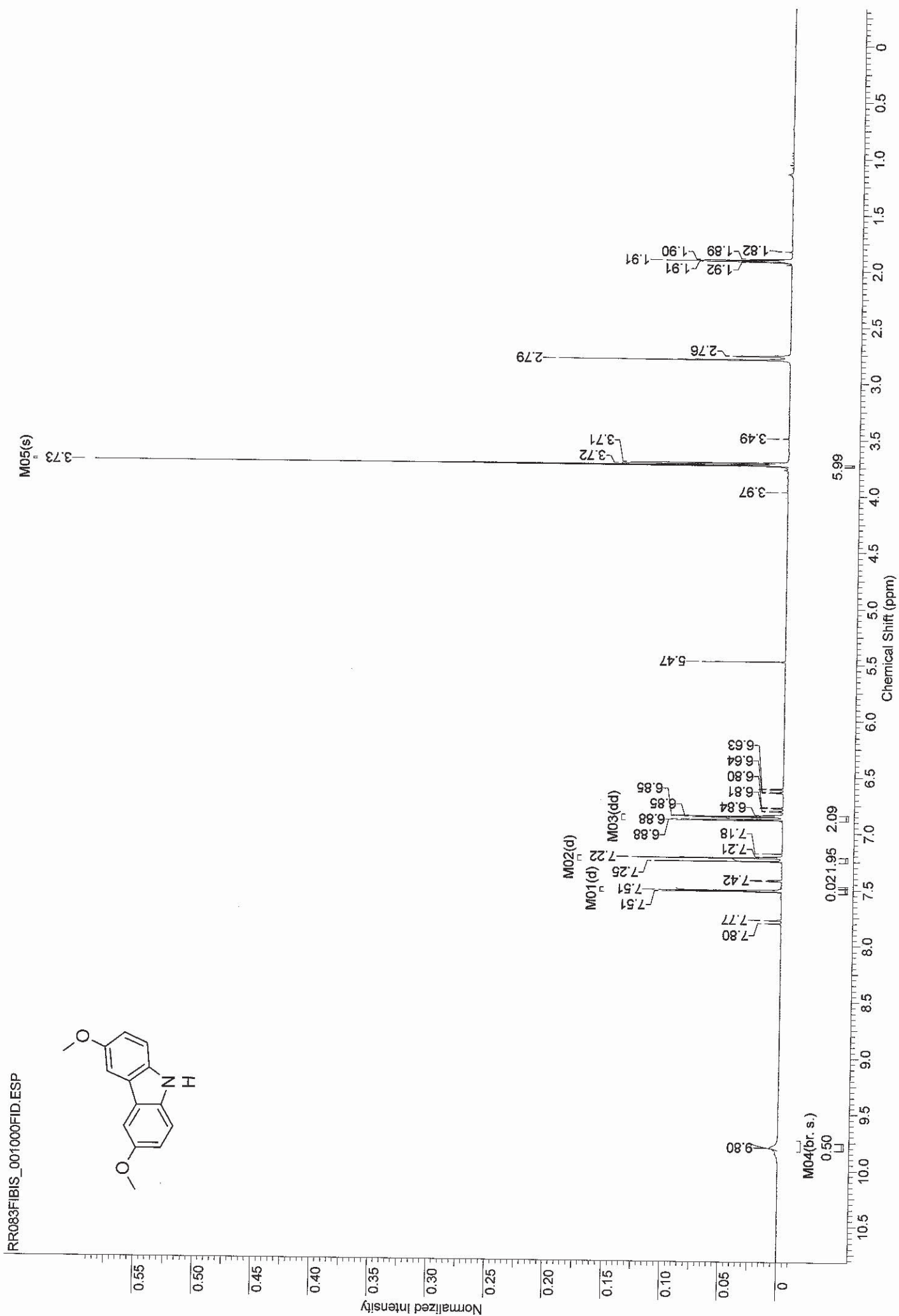
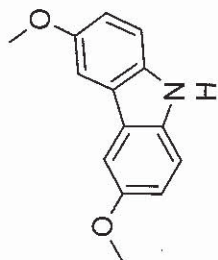


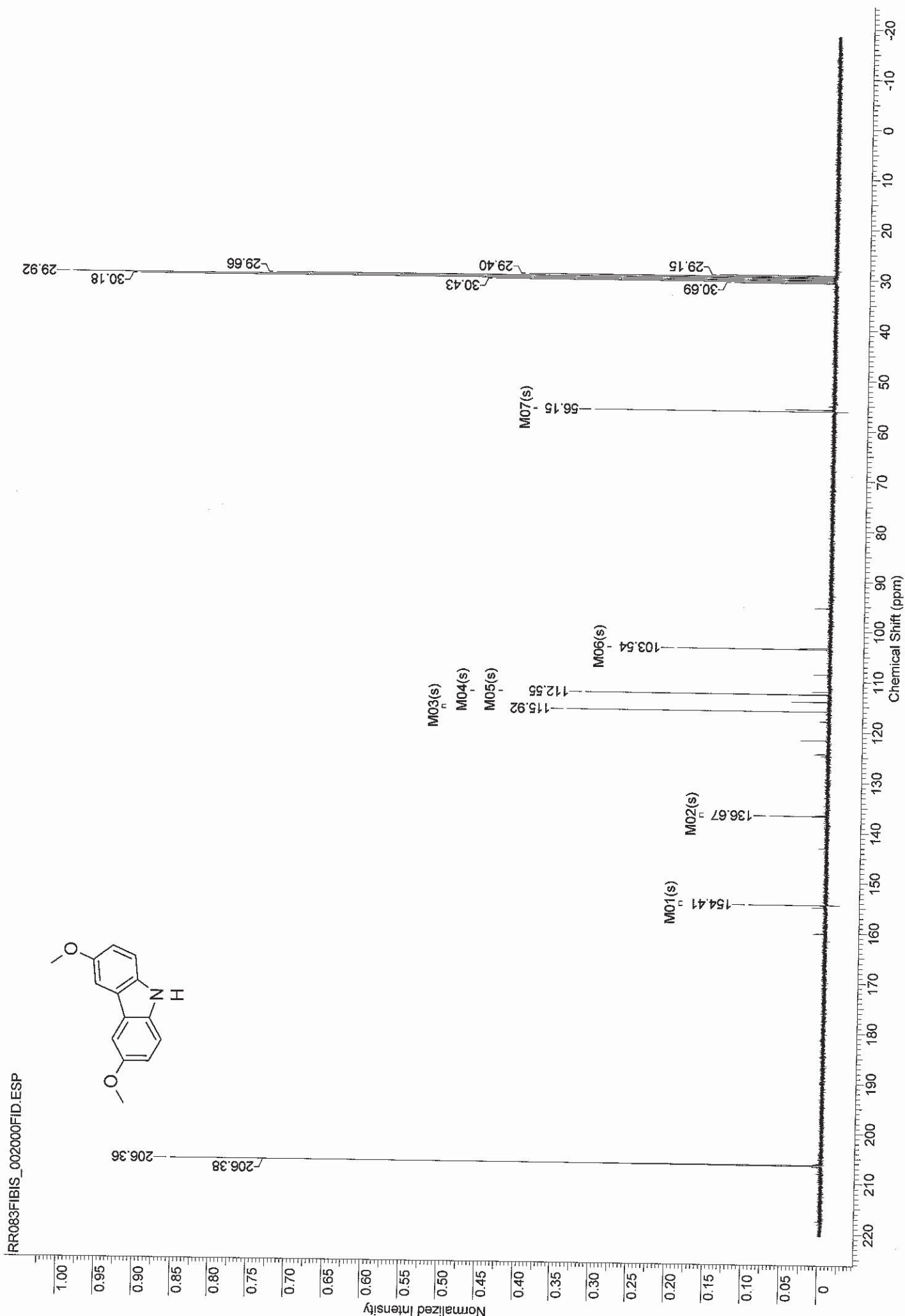


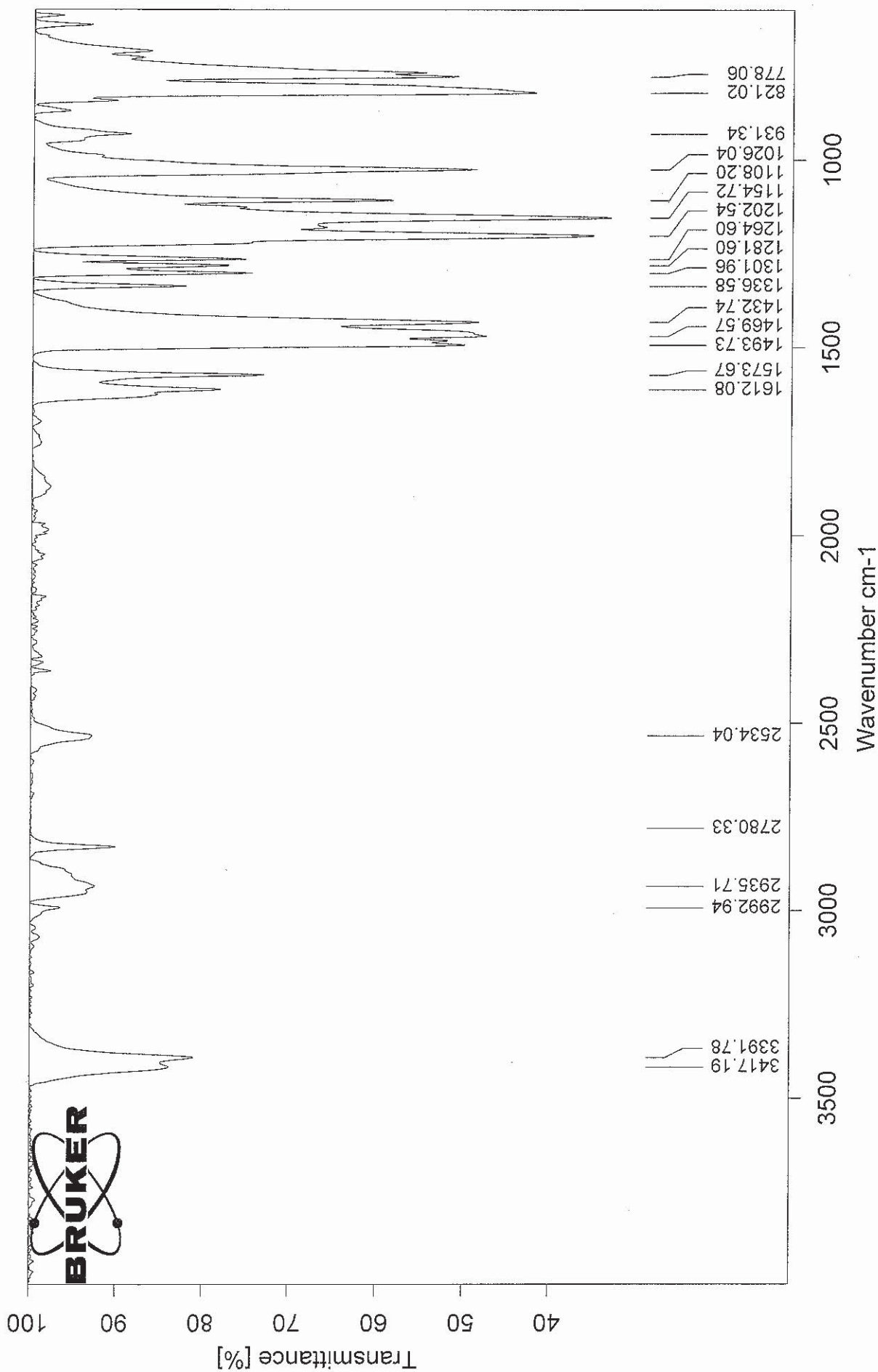


REMY7813\_EI #51-65 RT: 0.55-0.69 AV: 15 NL: 7.33E8  
T: + c Full ms [40.00-650.00]





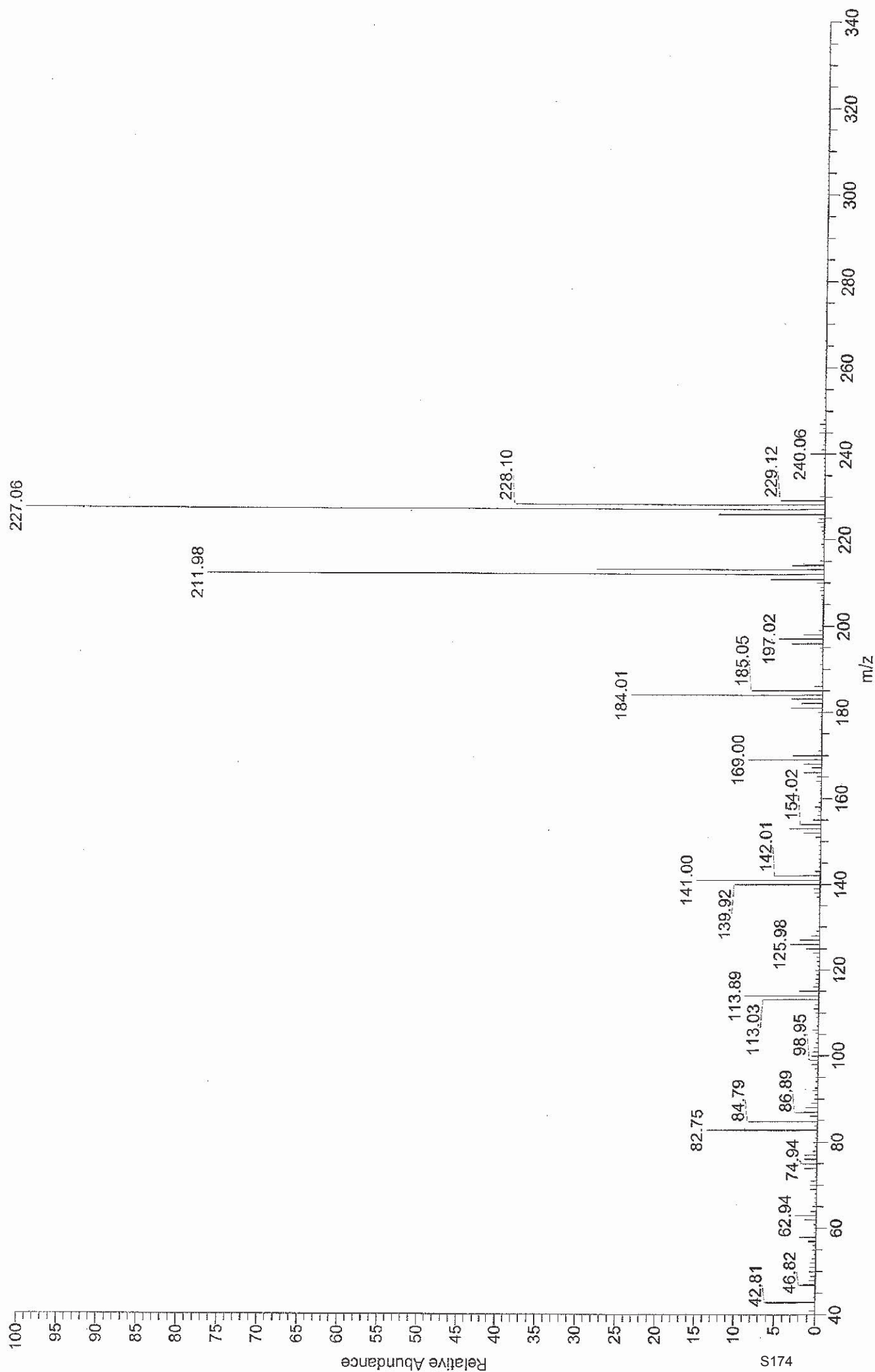




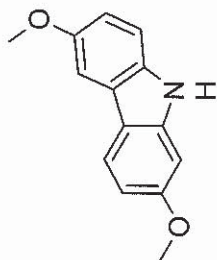
U:\IR\RR083D.0 RR083D brown solid

10.12.2013

REMY7812\_EI #61-82 RT: 0.67-0.89 AV: 22 NL: 3.95E8  
T: + c Full ms [40.00-650.00]







M07(s)

M08(s)

3.88  
3.85

M05(dd)

M03(m)

M06(dd)

M04(d)

M02(d)

M01(dd)

M09(br. s.)

3.06

0.99

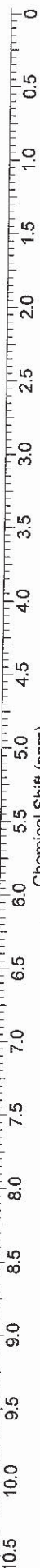
0.99

1.00

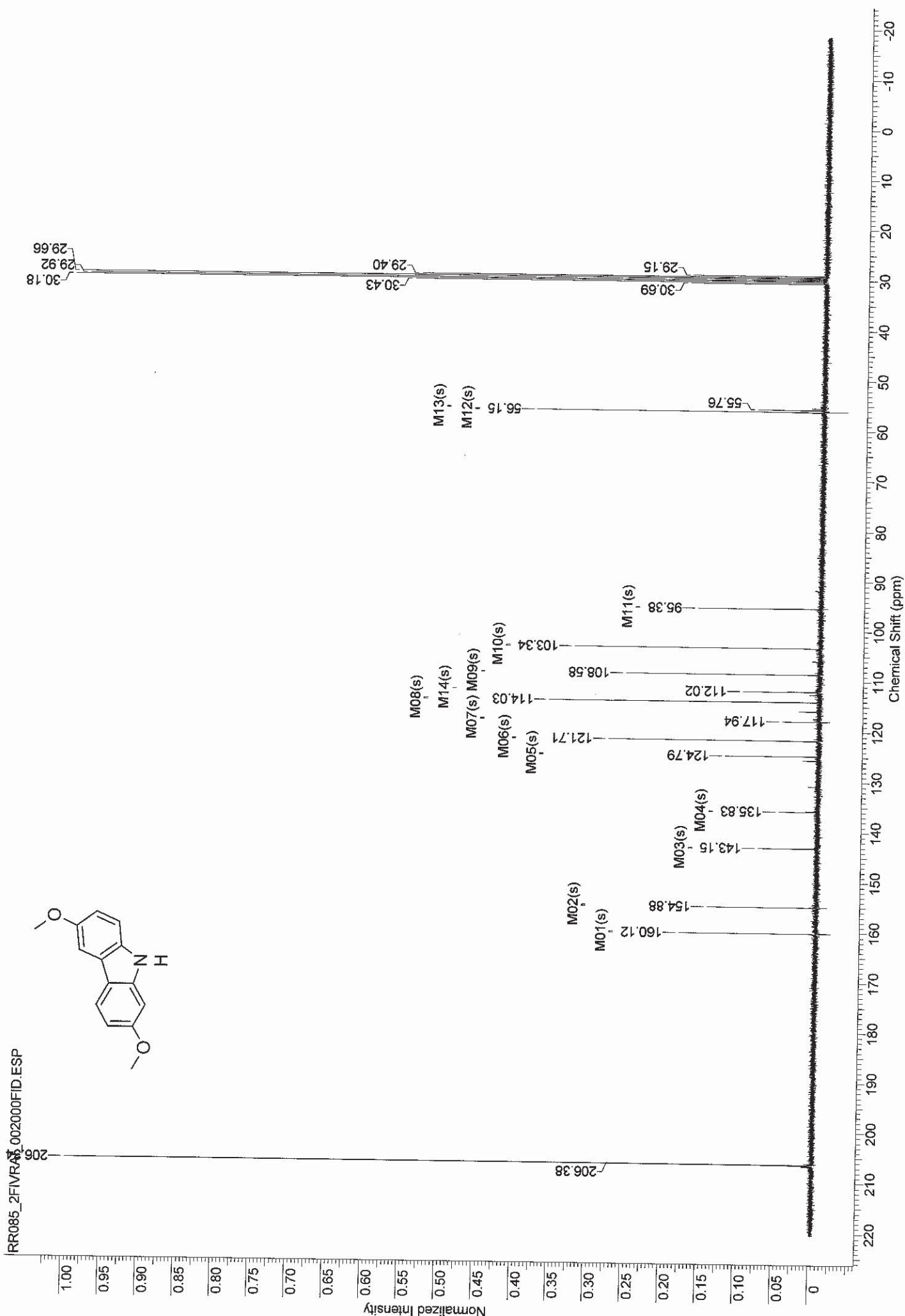
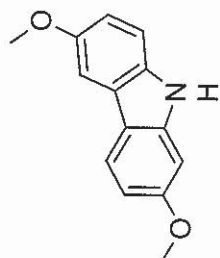
0.67

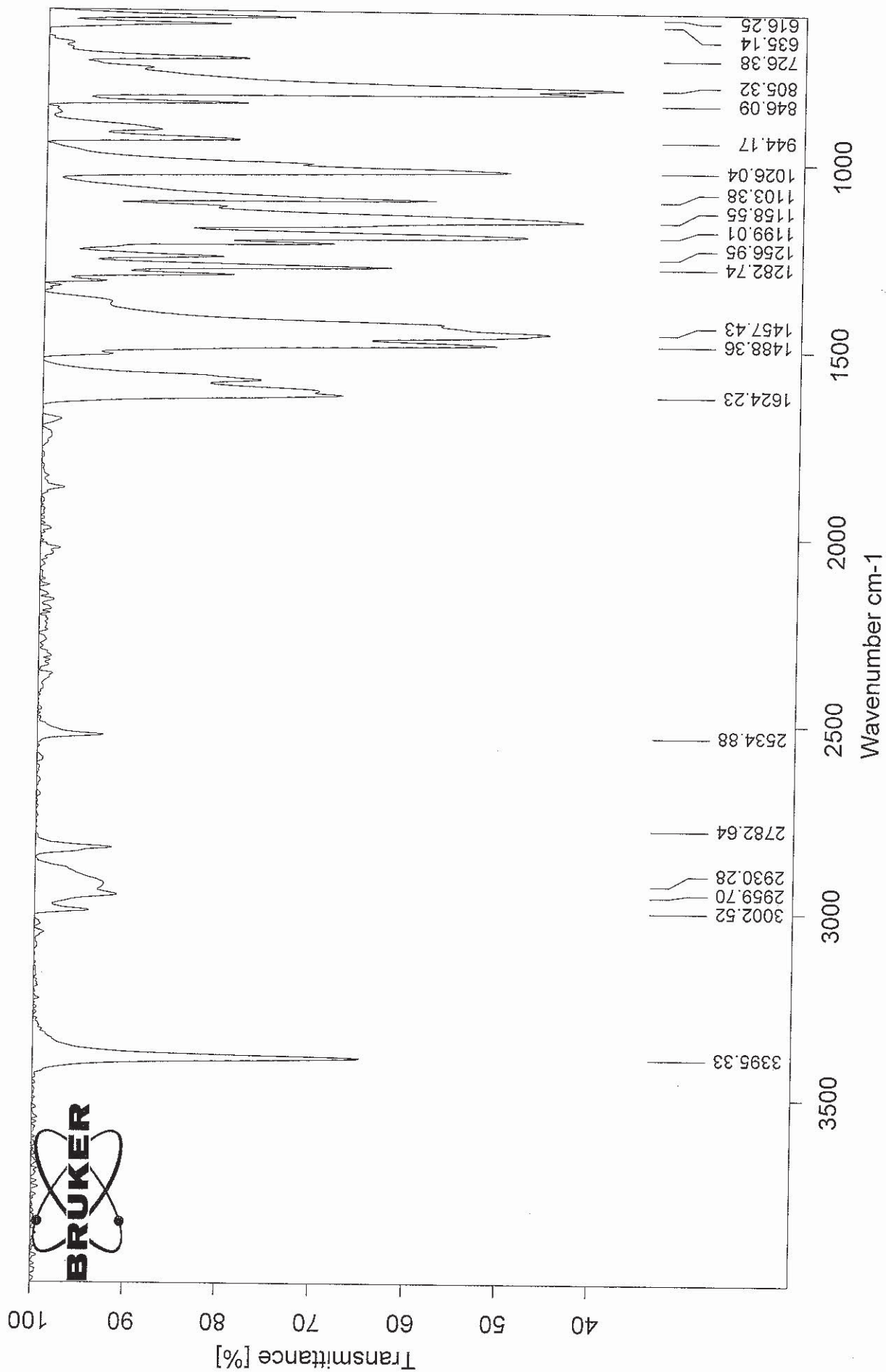
S175

Chemical Shift (ppm)

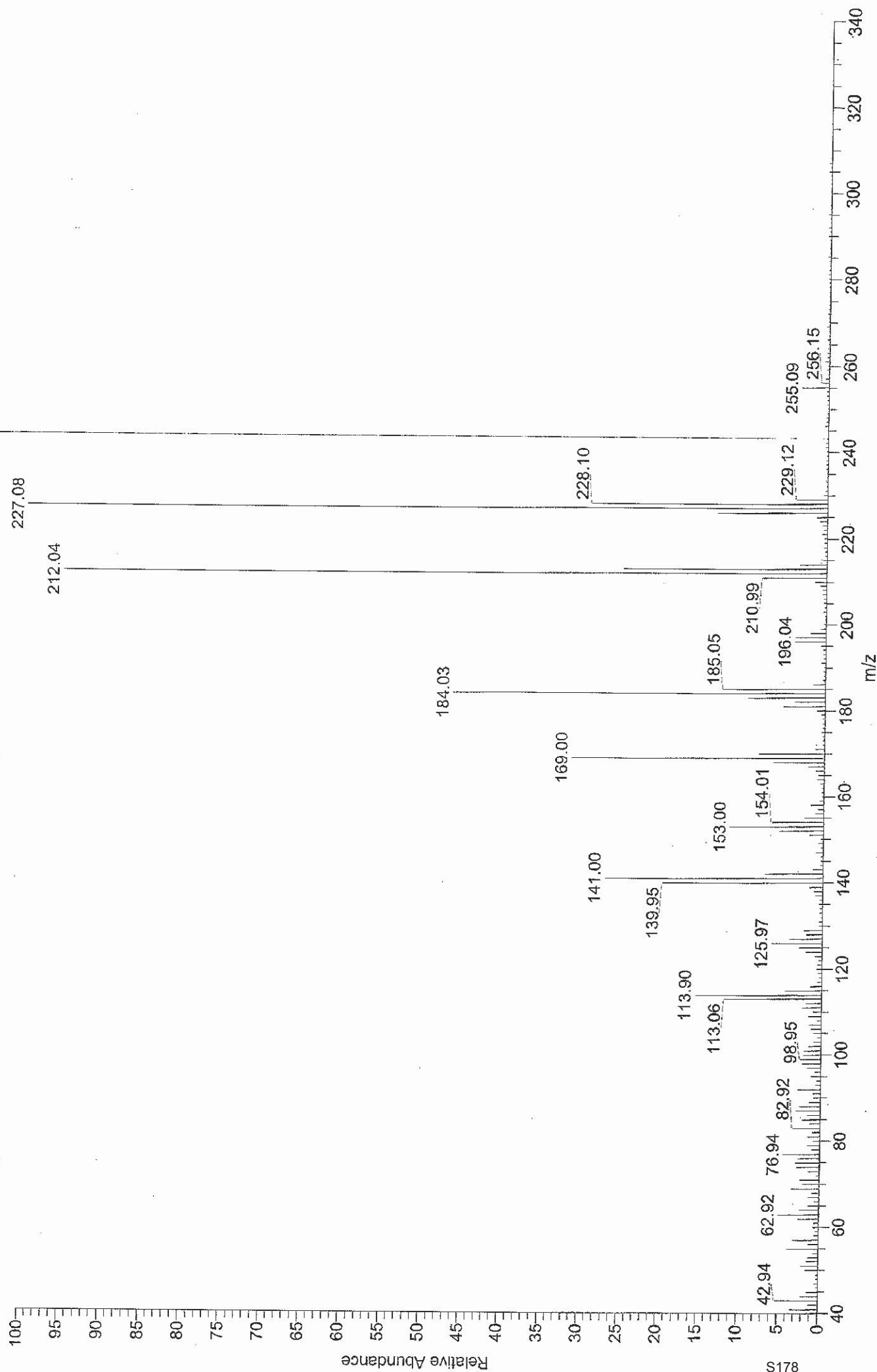


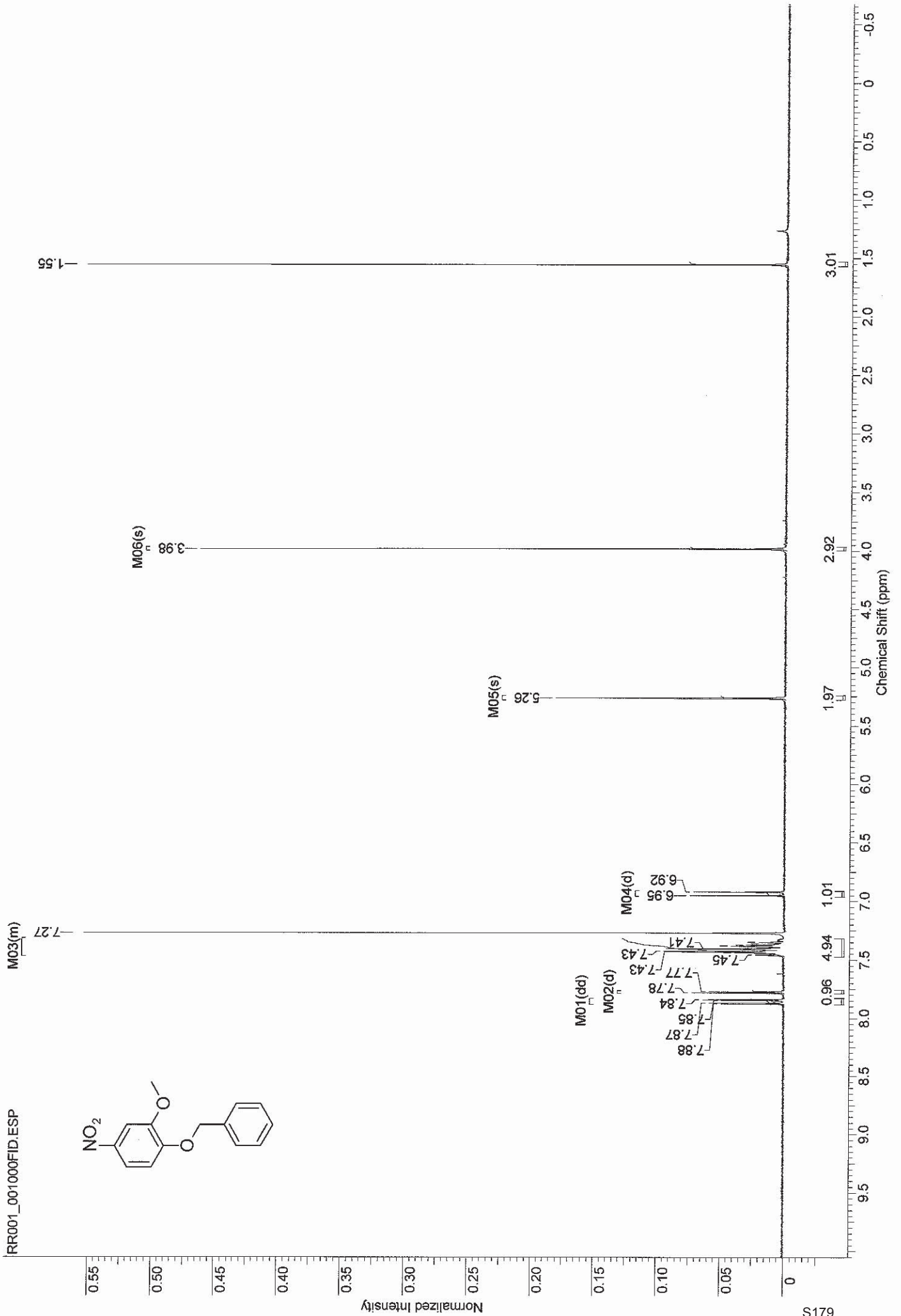
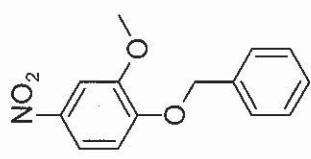
RR085\_2FVRA1.002000FID.ESP

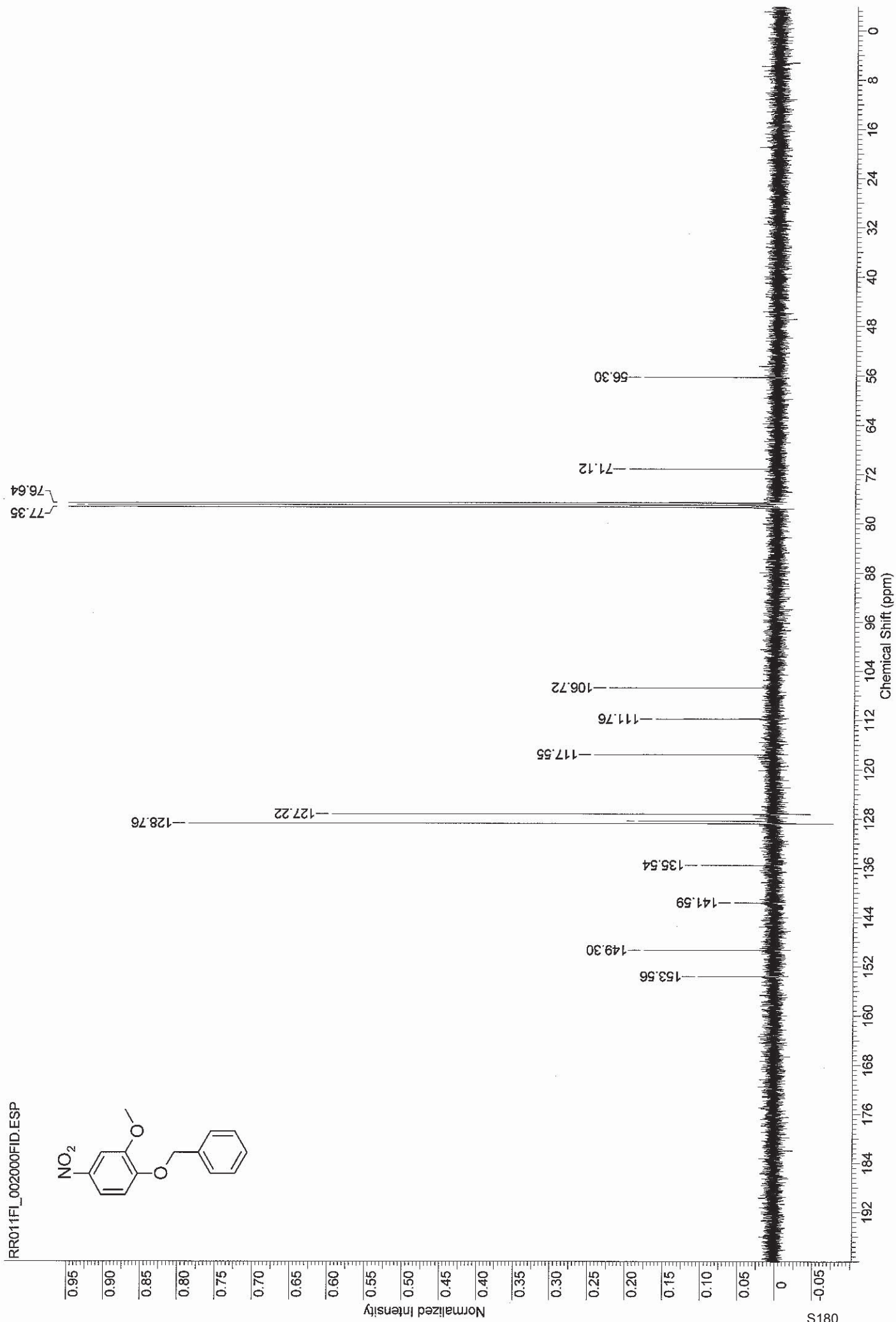
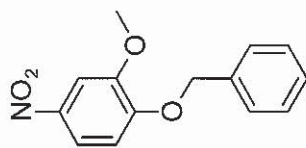




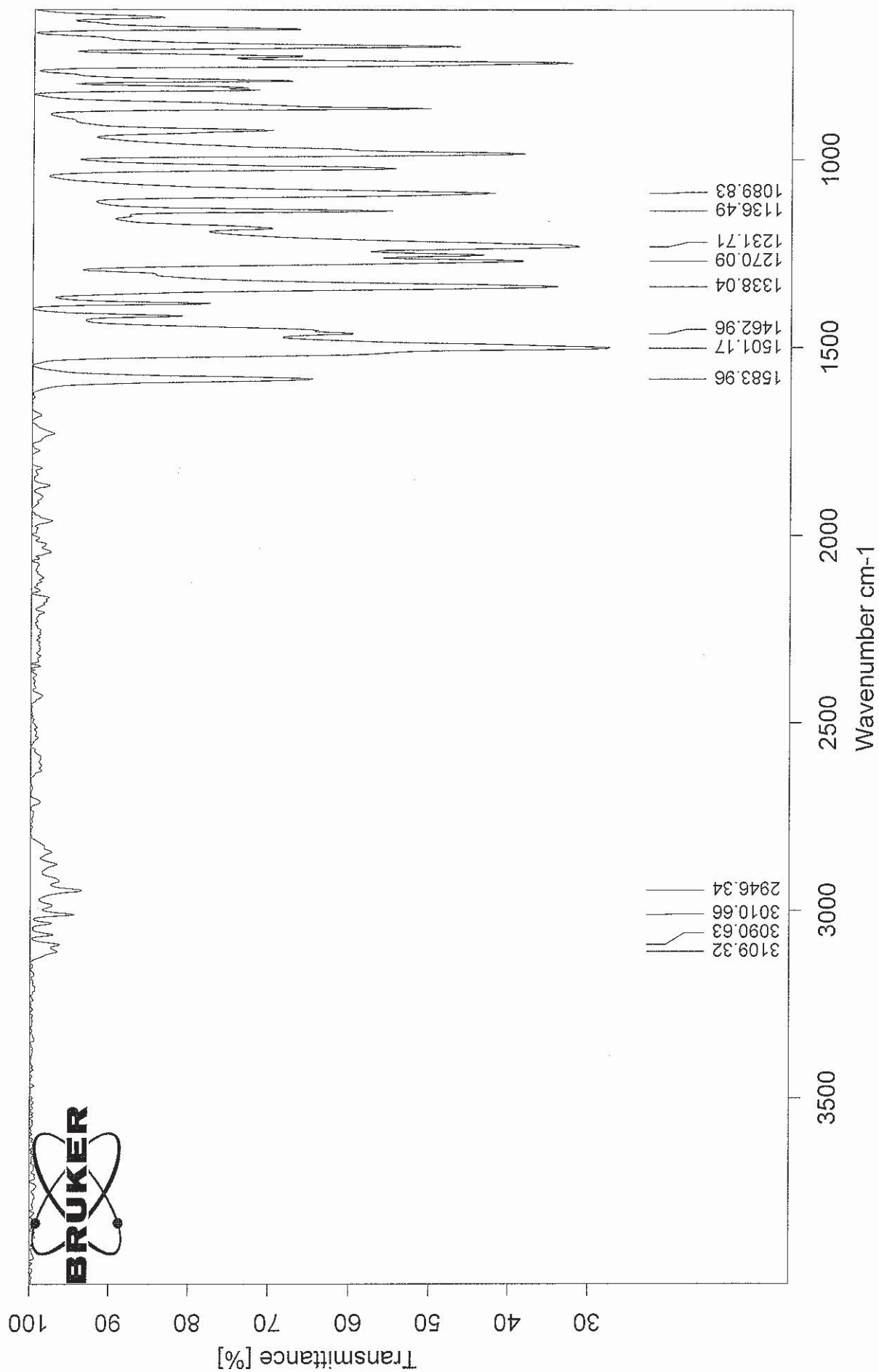
REMY7811\_EI#75-93 RT: 0.81-1.00 AV: 19 NL: 5.67E7  
T: + c Full ms [40.00-650.00]











U:IR11-(benzyloxy)-2-methoxy-4-nitrobenzene.0

1-(benzyloxy)-2-methoxy-4-nitrobenzene

yellow solid

18.11.2013



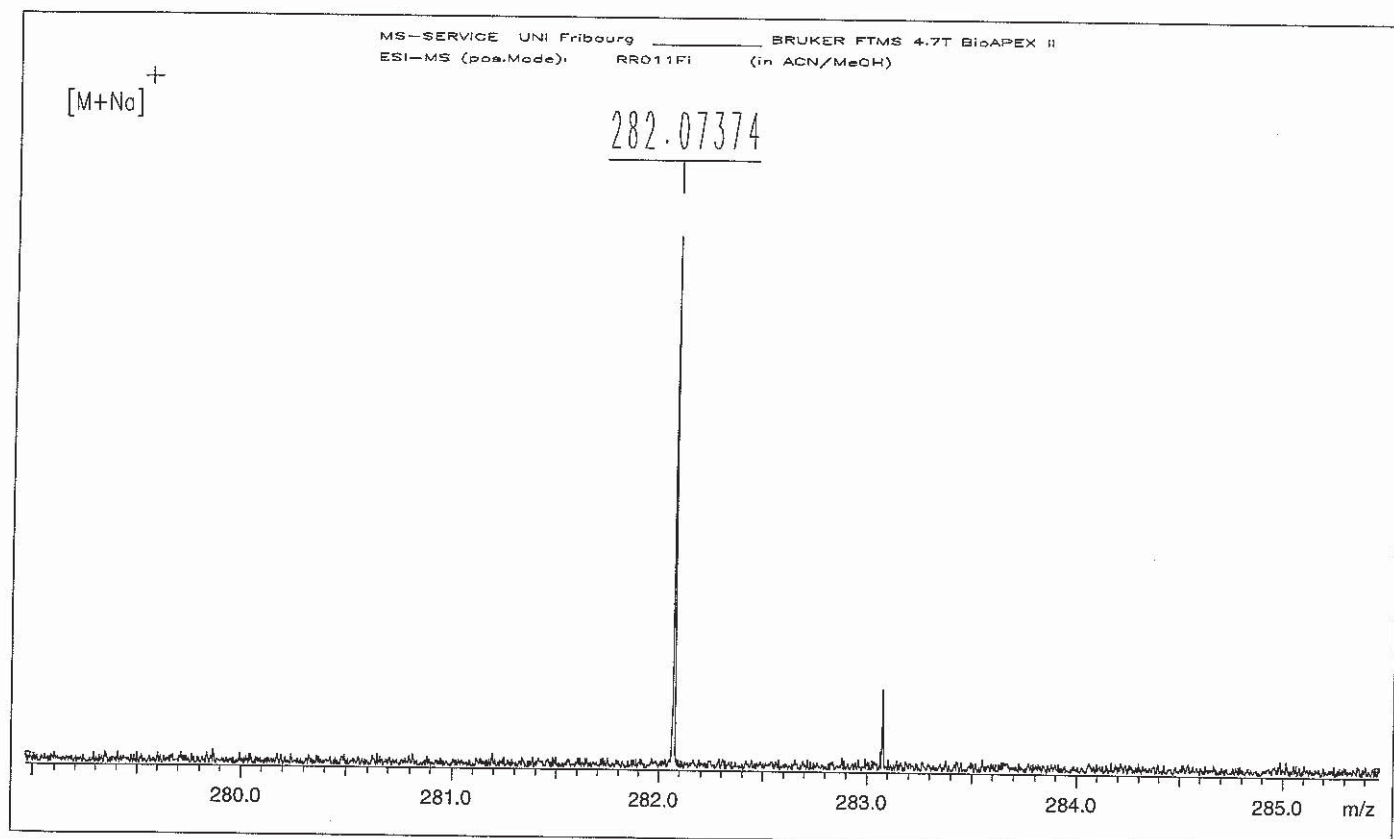
ESI-MS: RR011Fi

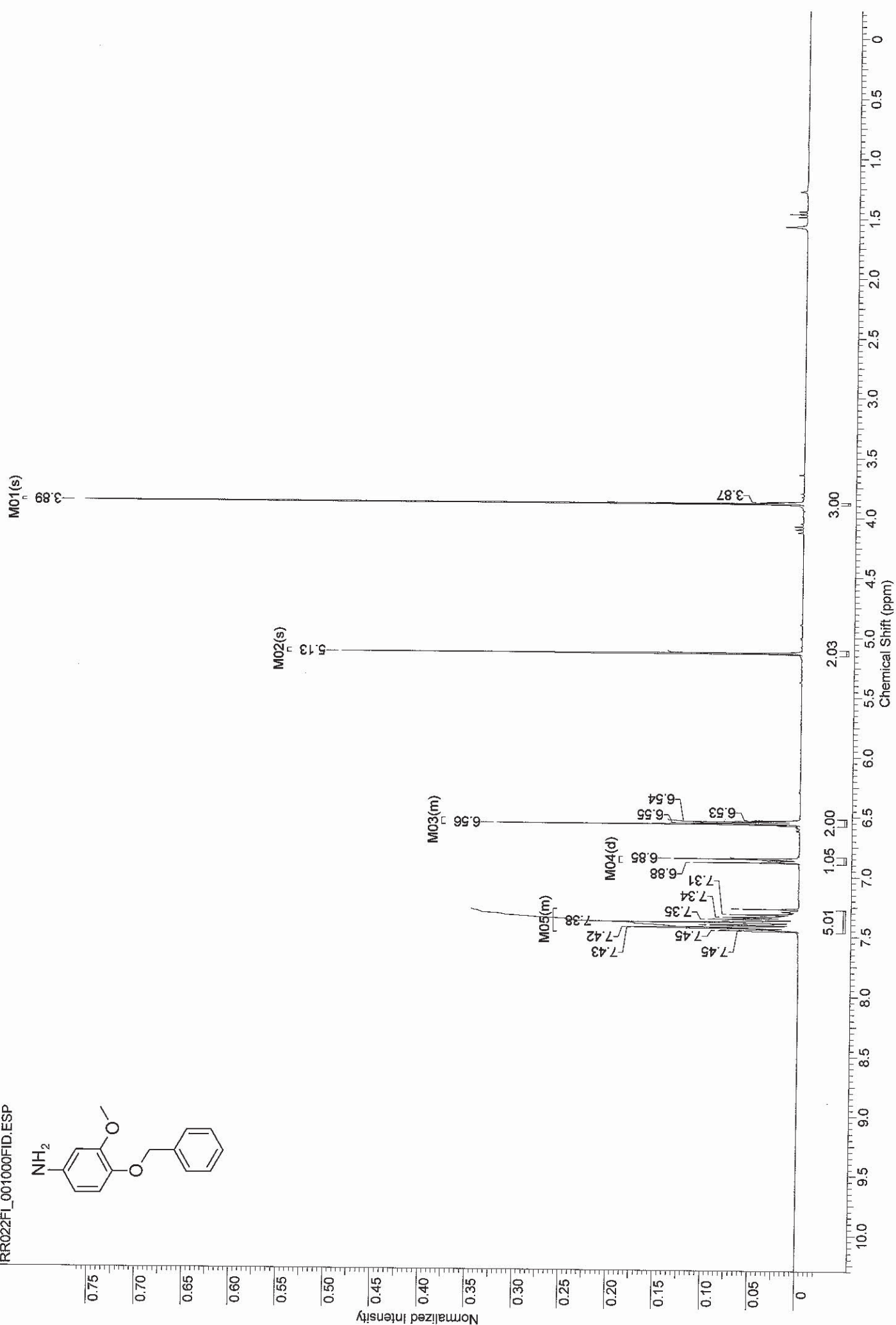
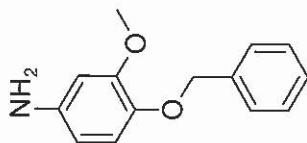
XMASS Mass Analysis for /Data/UNI\_FR/REMY7655\_ESI/2/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

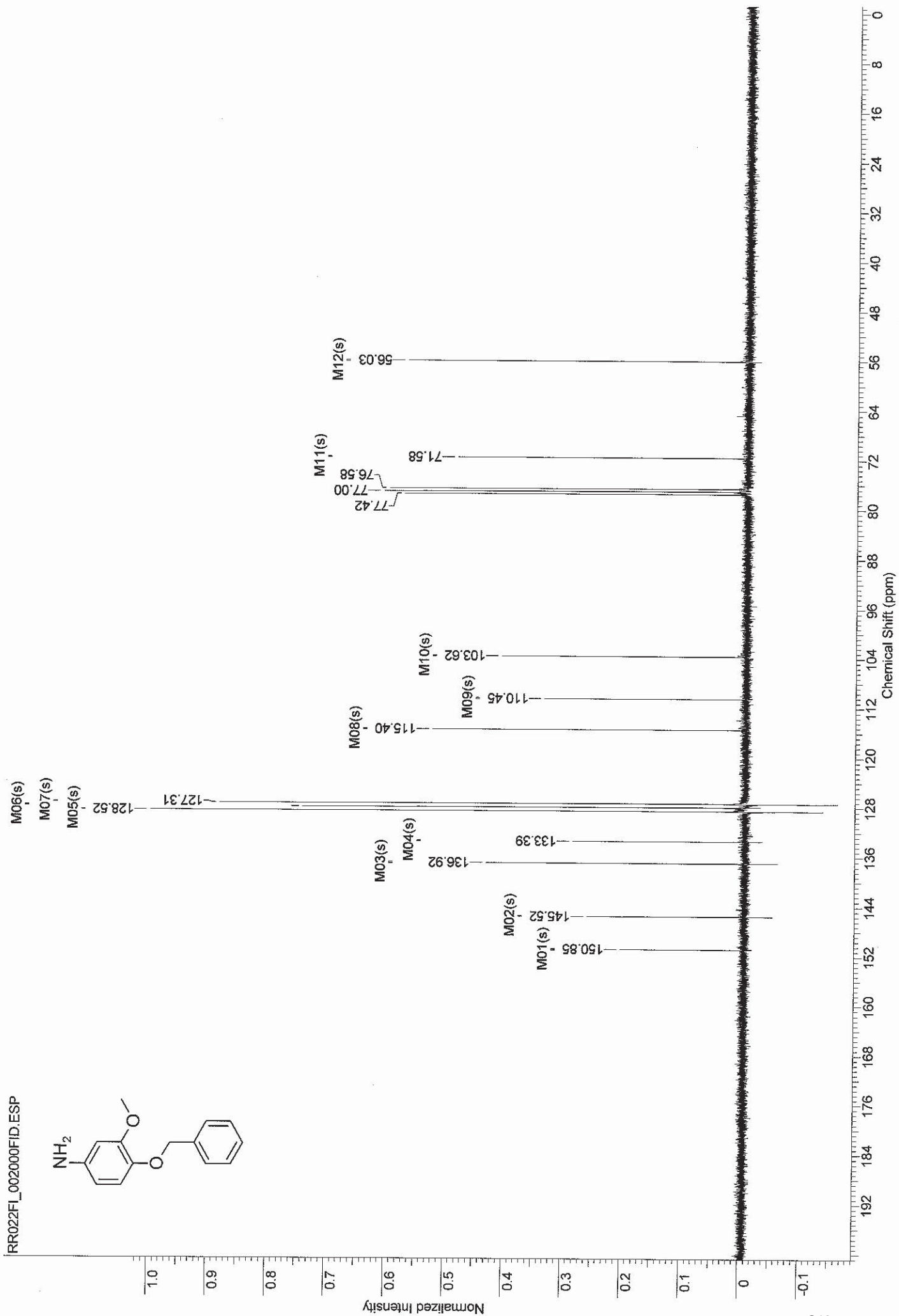
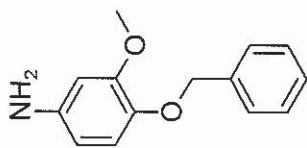
Ion mass = 282.0737410

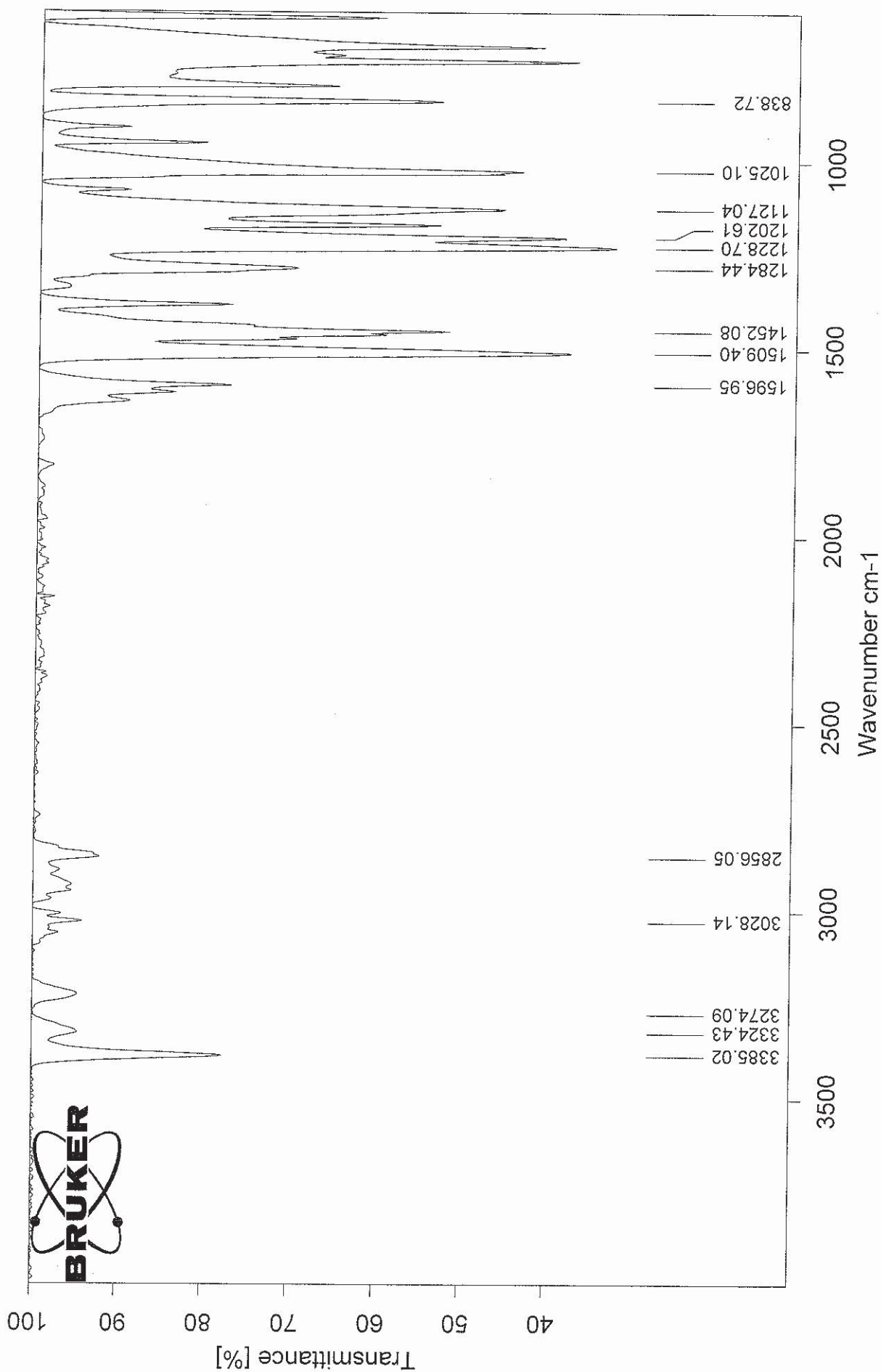
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 282.0737410								
1	14	13	1	4	1	282.0736790	8.5	6.200e-05
2	12	8	7	2	0	282.0733990	12.5	3.420e-04
3	14	10	4	3	0	282.0747416	12.0	1.001e-03
4	12	11	4	3	1	282.0723363	9.0	1.405e-03
5	11	12	3	6	0	282.0720616	7.5	1.679e-03
6	10	6	10	1	0	282.0720563	13.0	1.685e-03
7	16	12	1	4	0	282.0760843	11.5	2.343e-03
8	17	11	2	1	1	282.0763591	13.0	2.618e-03
9	10	9	7	2	1	282.0709937	9.5	2.747e-03
10	9	10	6	5	0	282.0707189	8.0	3.022e-03









U:\IR\4-(benzyloxy)-3-methoxyaniline.0

4-(benzyloxy)-3-methoxyaniline

brown solid

18.11.2013

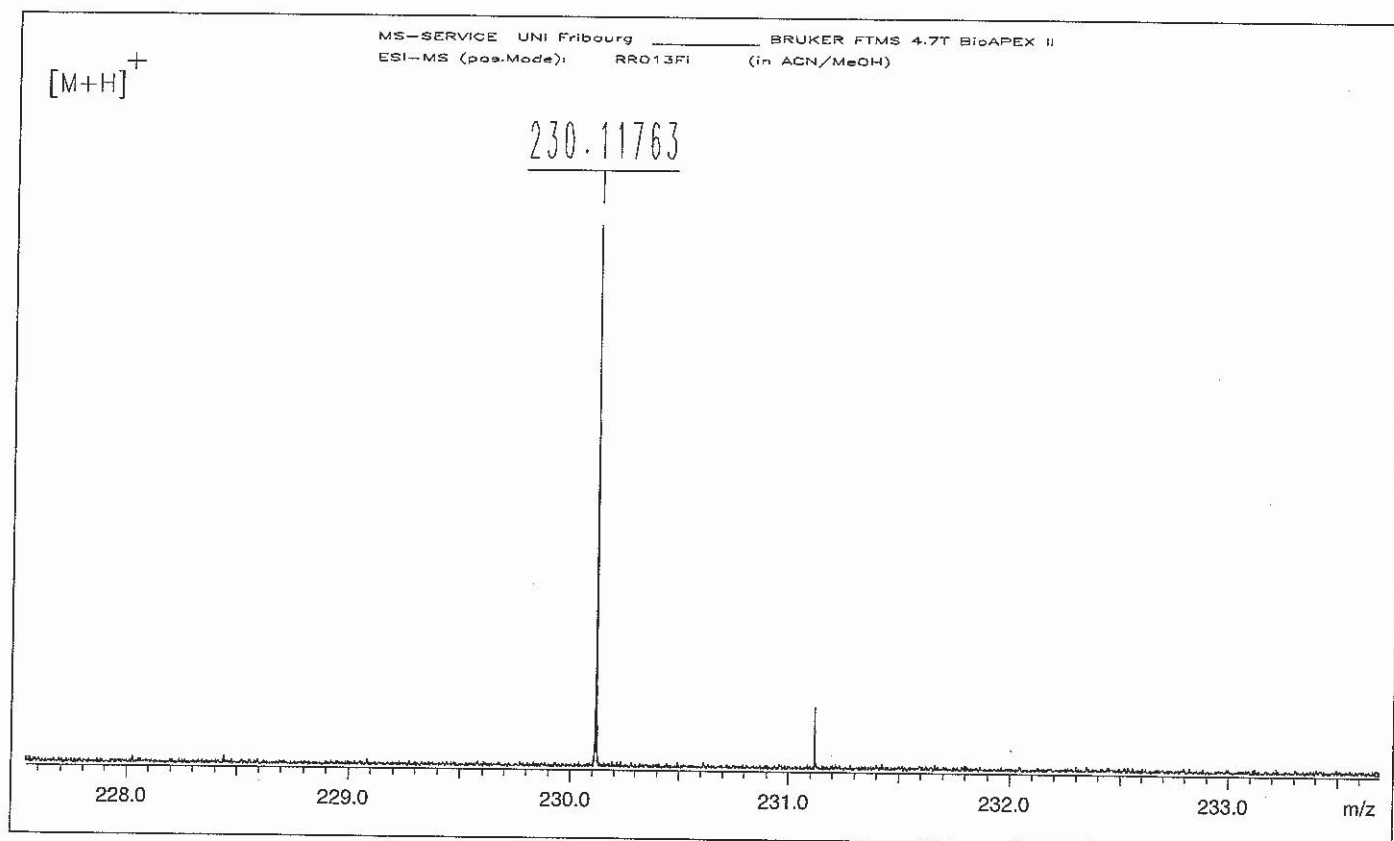
ESI-MS: RR013Fi

XMASS Mass Analysis for /Data/UNI\_FR/REMY7651\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

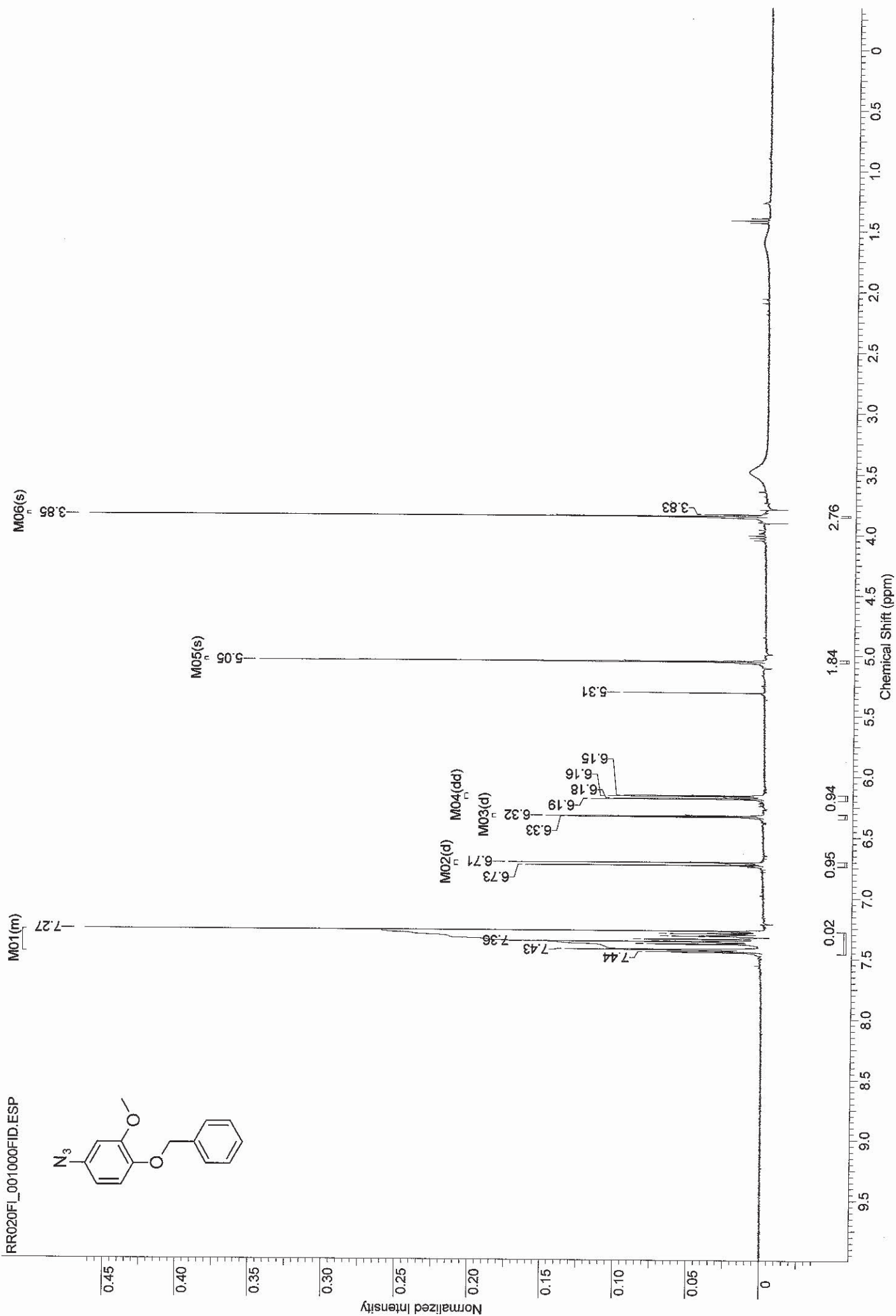
Ion mass = 230.1176290

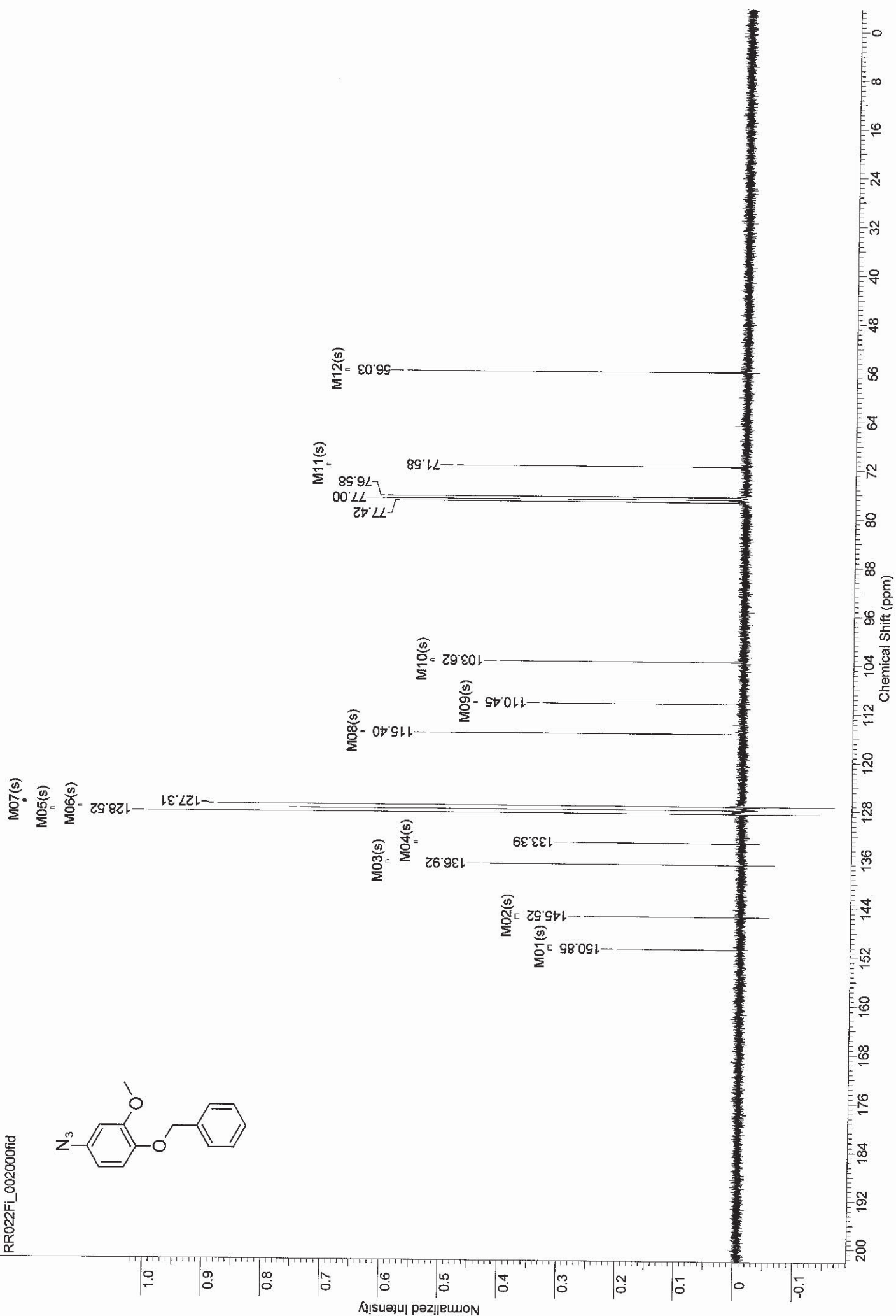
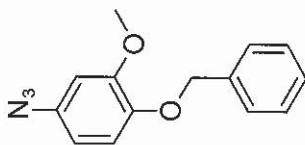
Charge = +1

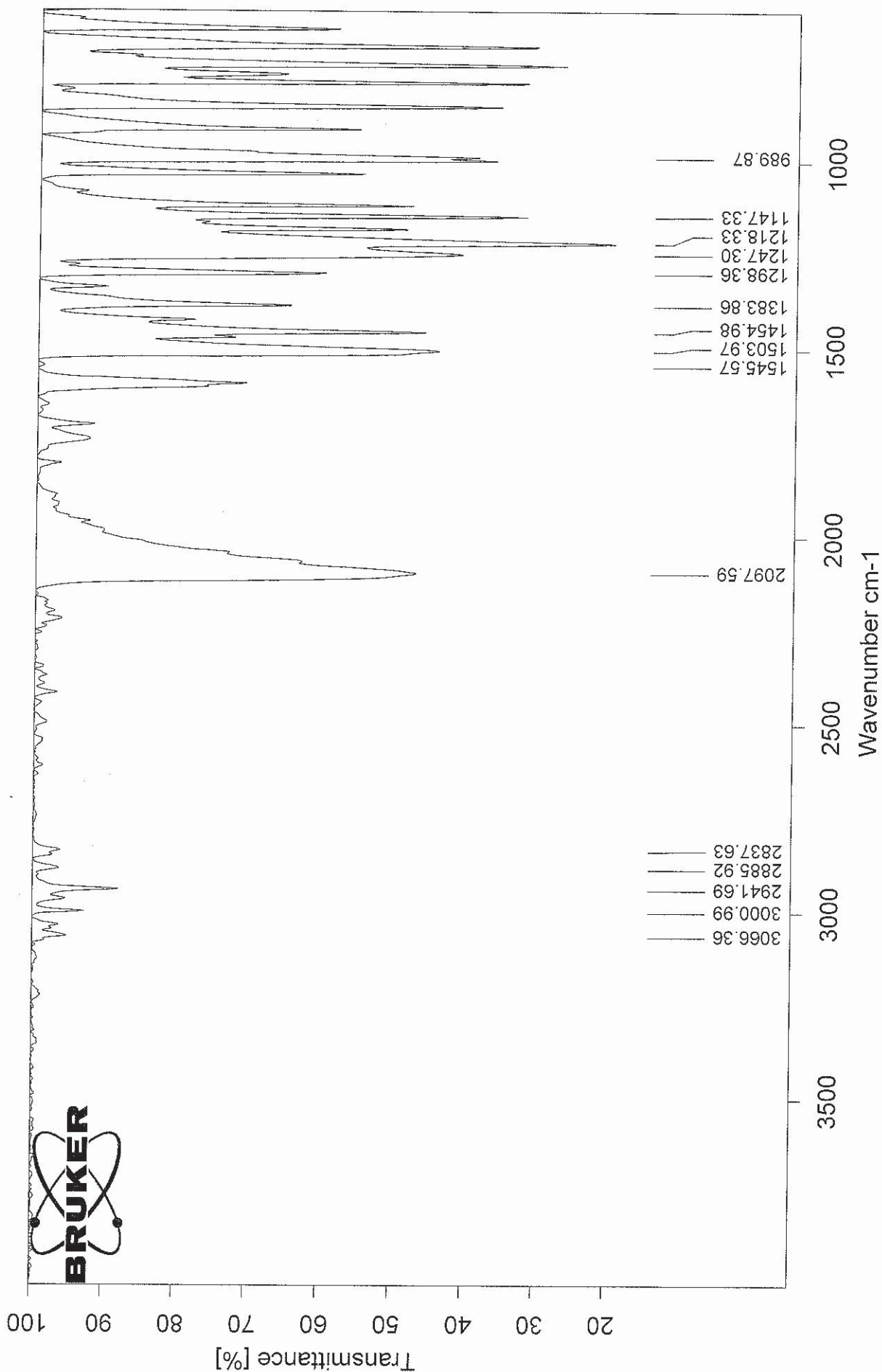
#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 230.1176290							
1	14	16	1	2	230.1175552	7.5	7.382e-05
2	12	14	4	1	230.1162125	8.0	1.416e-03
3	9	16	3	4	230.1135324	3.5	4.097e-03
4	5	18	4	6	230.1220858	-1.0	4.457e-03
5	7	14	6	3	230.1121898	4.0	5.439e-03
6	6	14	8	2	230.1234232	4.0	5.794e-03
7	7	20	1	7	230.1234284	-1.5	5.799e-03
8	6	18	2	7	230.1108524	-1.0	6.777e-03
9	5	12	9	2	230.1108471	4.5	6.782e-03
10	8	16	5	3	230.1247658	3.5	7.137e-03











ESI-MS: RR014Fi

XMASS Mass Analysis for /Data/UNI\_FR/REMY7654\_ESI/1/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

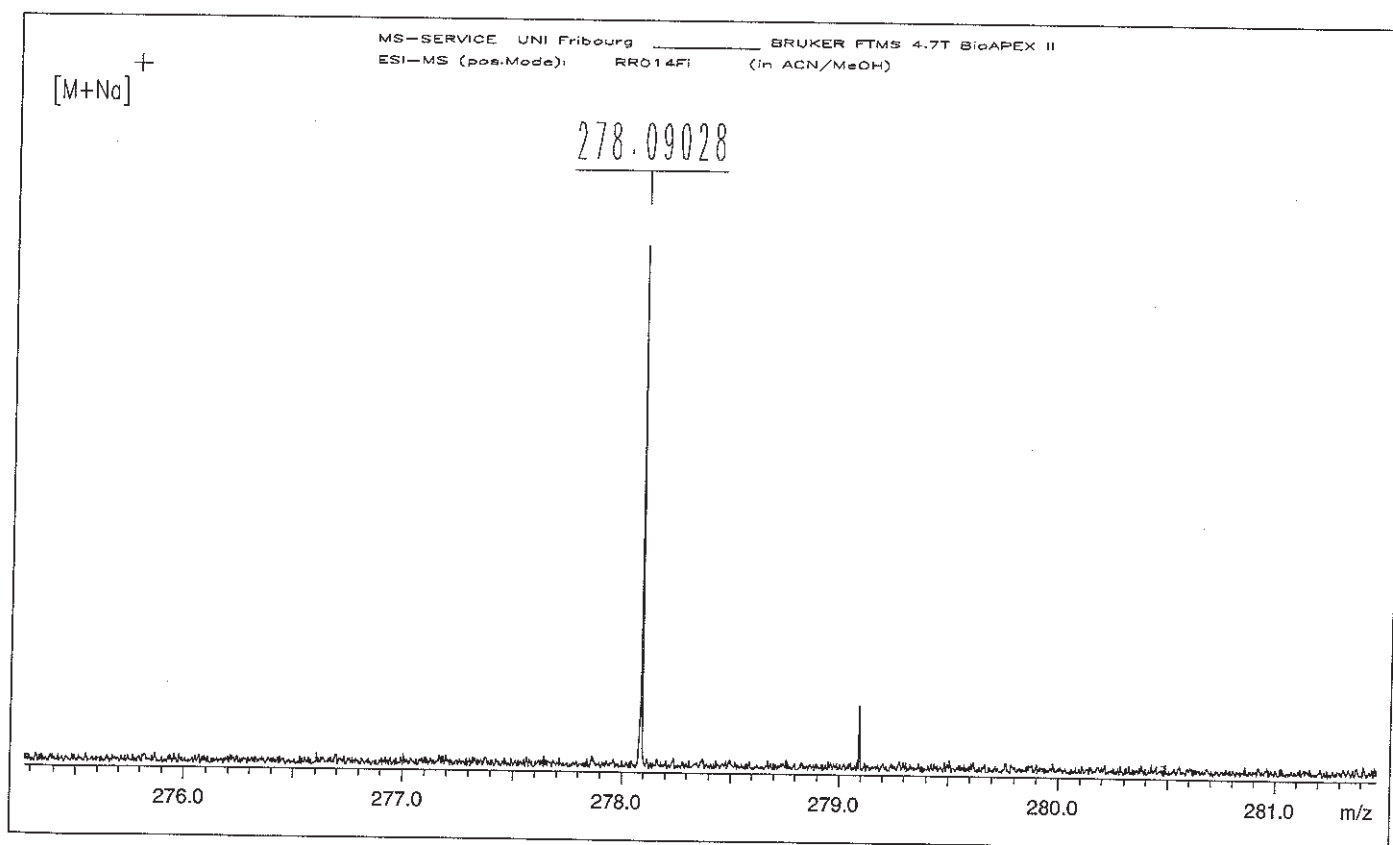
Ion mass = 278.0902750

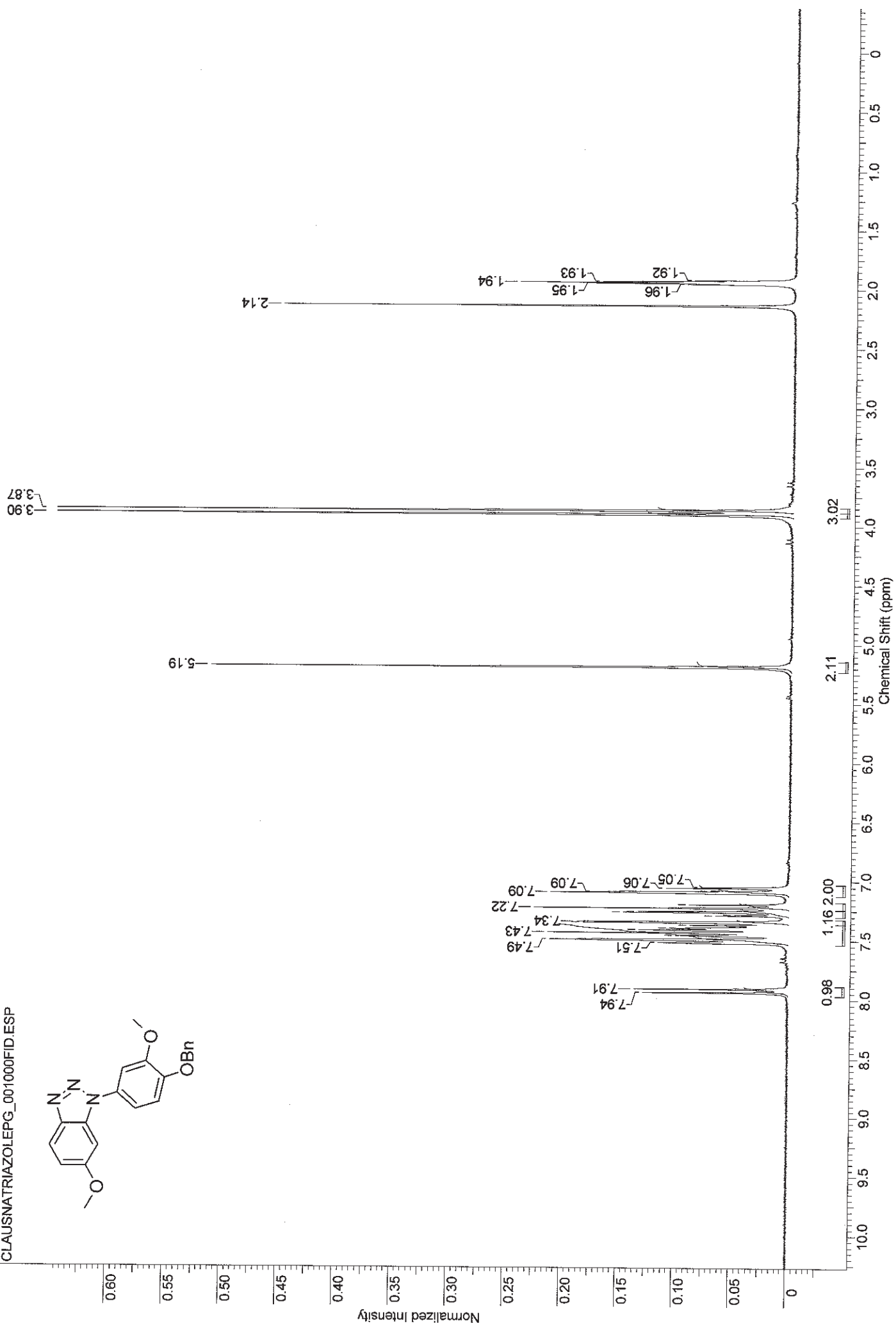
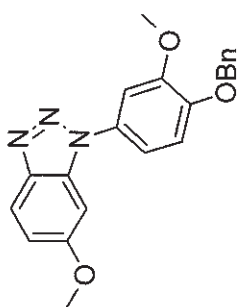
Charge = +1

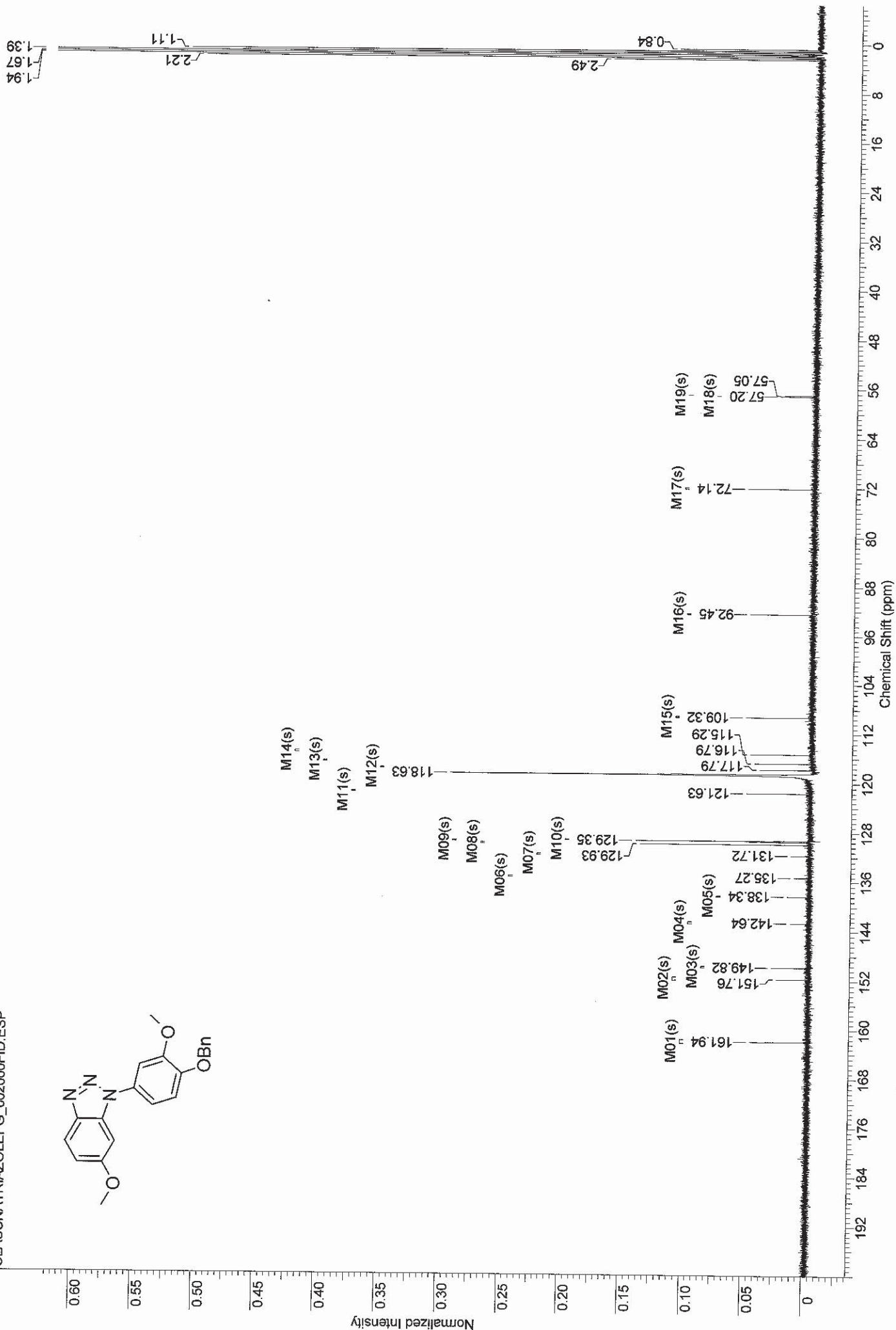
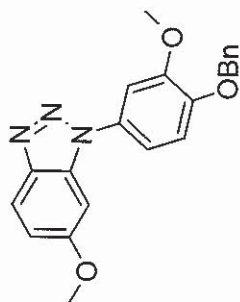
#	C	H	N	O	Na	mass	DBE	error
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\*\*\* Mass Analysis for mass 278.0902750

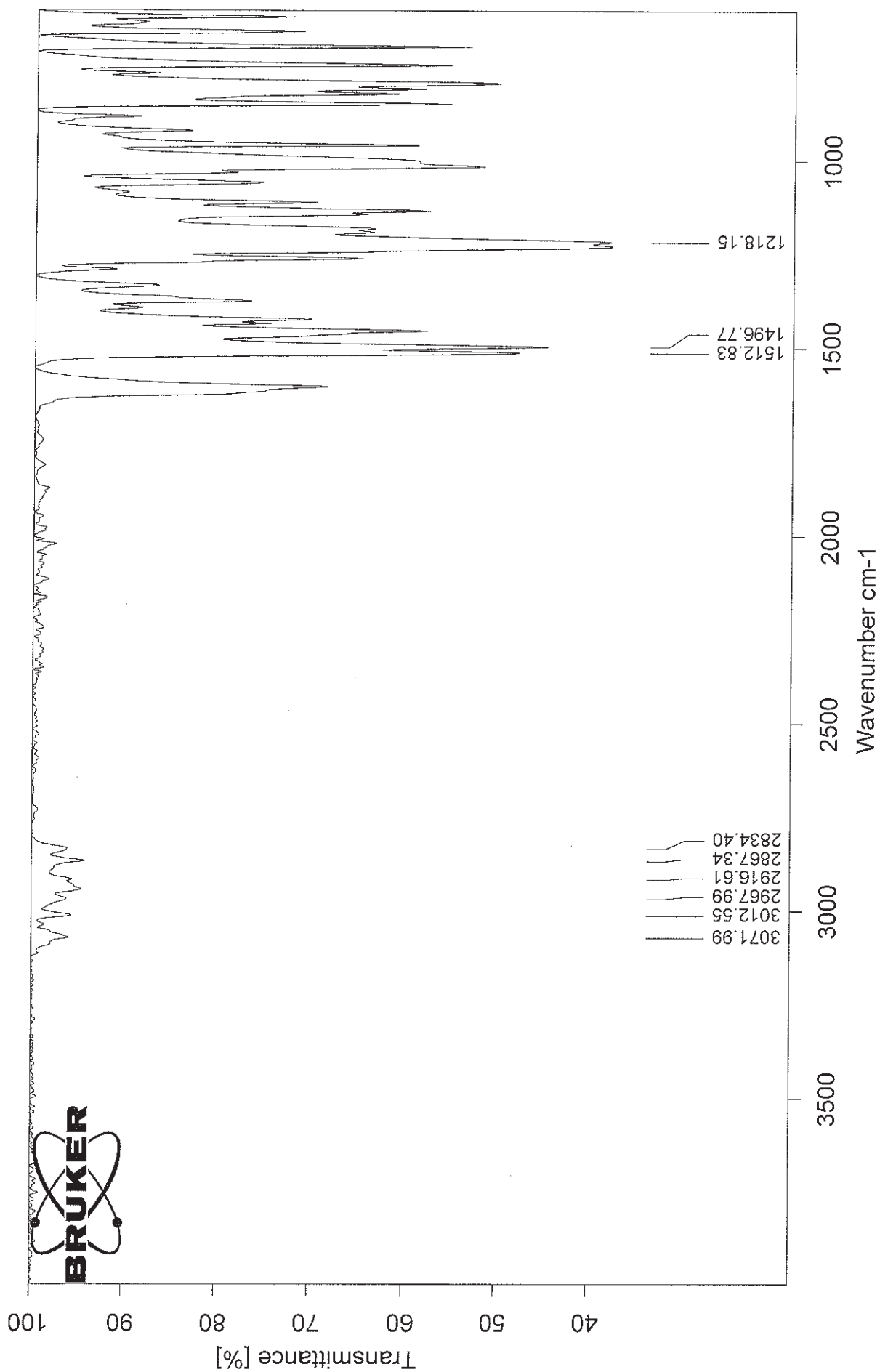
1	14	13	3	2	1	278.0899978	9.5	2.772e-04
2	13	14	2	5	0	278.0897230	8.0	5.520e-04
3	14	10	6	1	0	278.0910604	13.0	7.854e-04
4	12	11	6	1	1	278.0886551	10.0	1.620e-03
5	11	12	5	4	0	278.0883803	8.5	1.895e-03
6	16	12	3	2	0	278.0924031	12.5	2.128e-03
7	11	15	2	5	1	278.0873177	5.0	2.957e-03
8	10	16	1	8	0	278.0870429	3.5	3.232e-03
9	9	10	8	3	0	278.0870376	9.0	3.237e-03
10	5	15	6	6	1	278.0945283	1.0	4.253e-03











ESI-MS: RR042Fi

XMASS Mass Analysis for /Data/UNI\_FR/REMY7650\_ESI/3/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

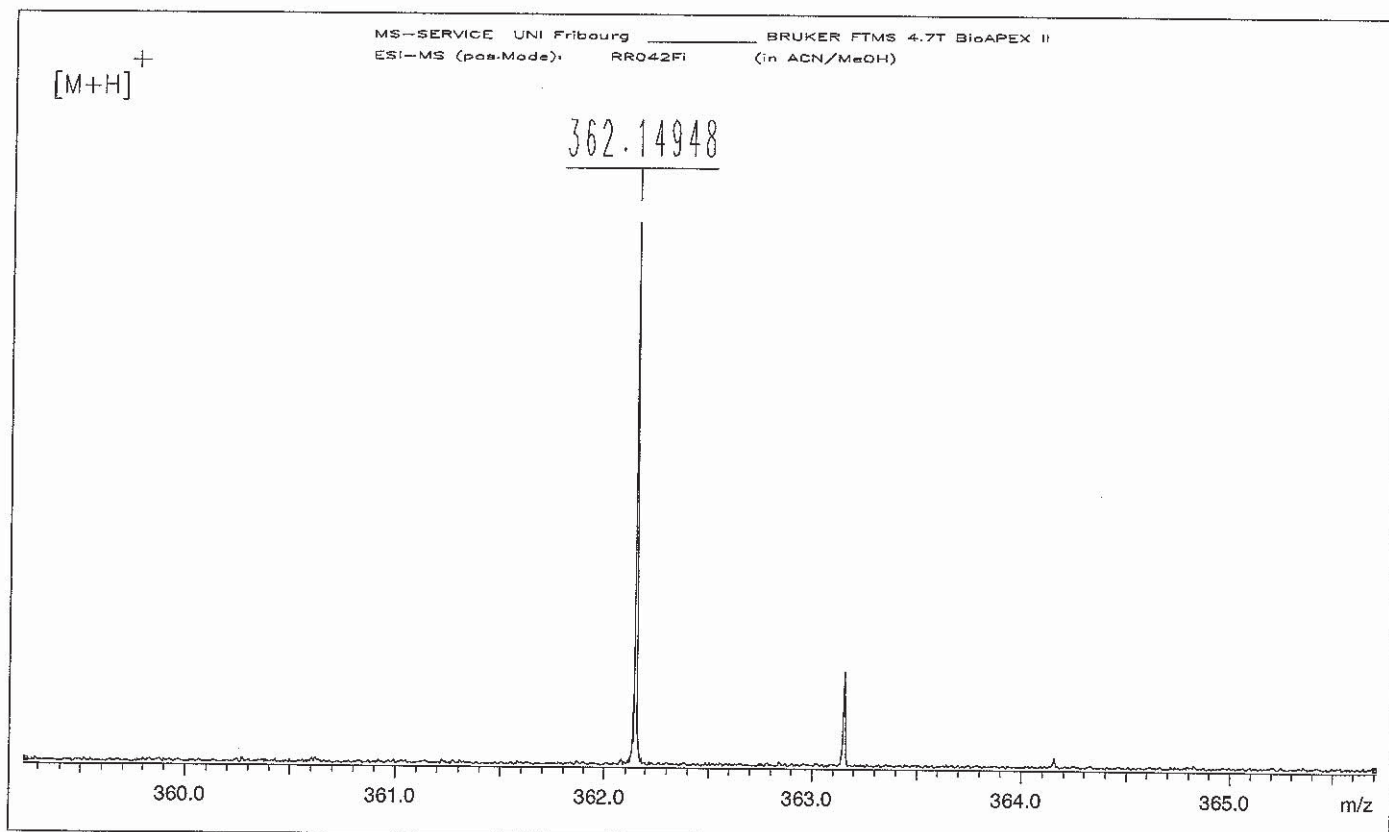
Ion mass = 362.1494770

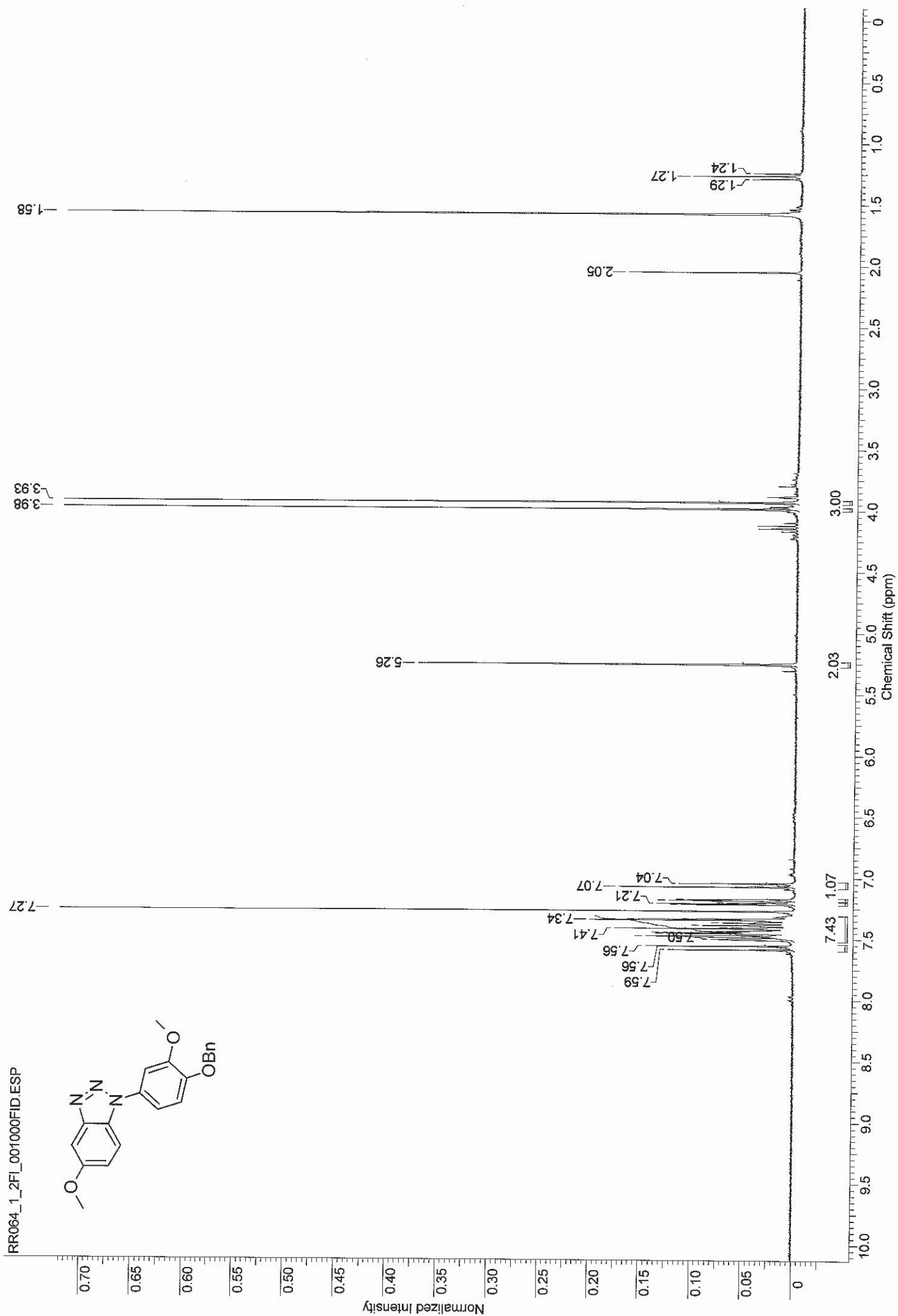
Charge = +1

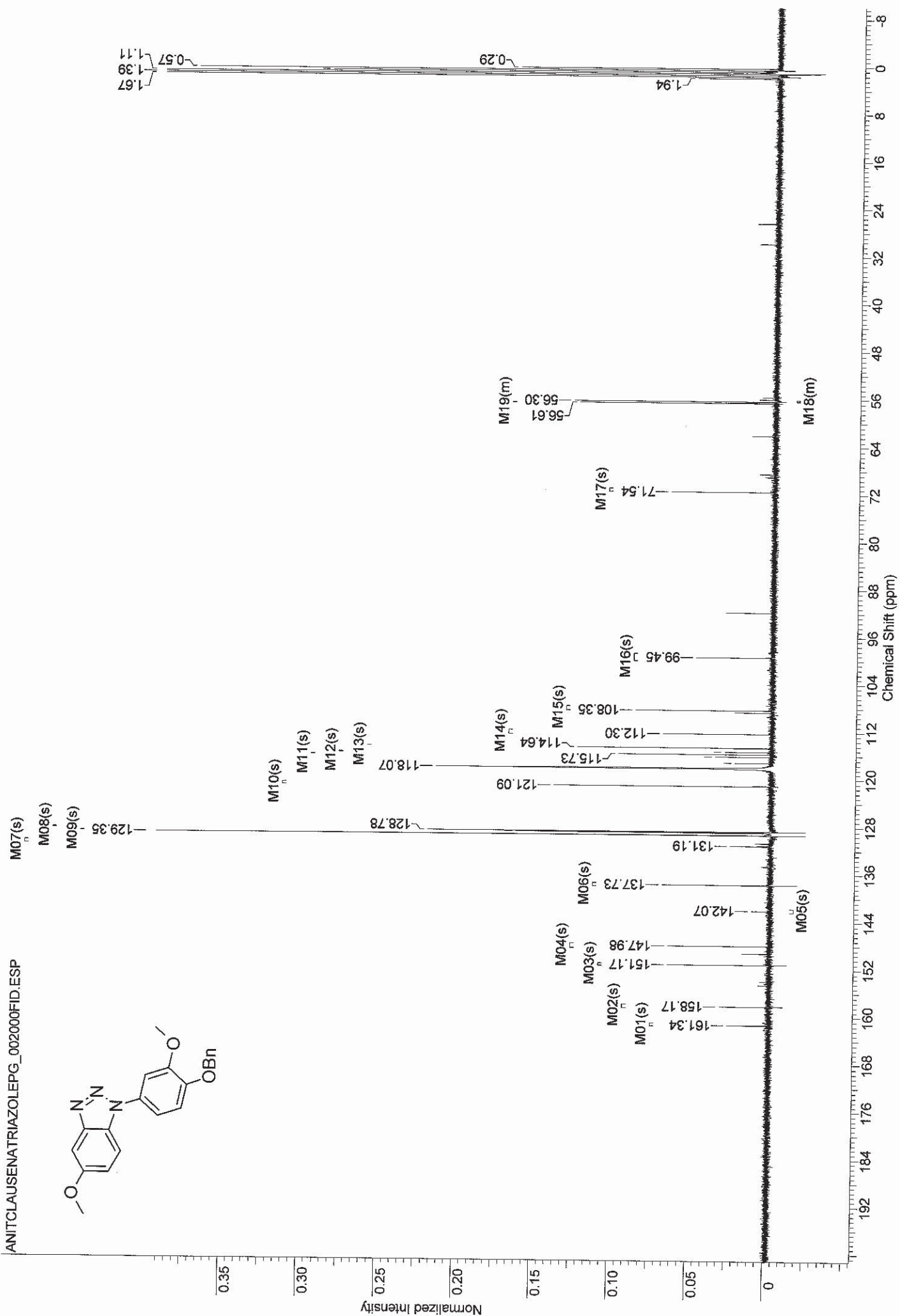
#	C	H	N	O	mass	DBE	error
---	---	---	---	---	------	-----	-------

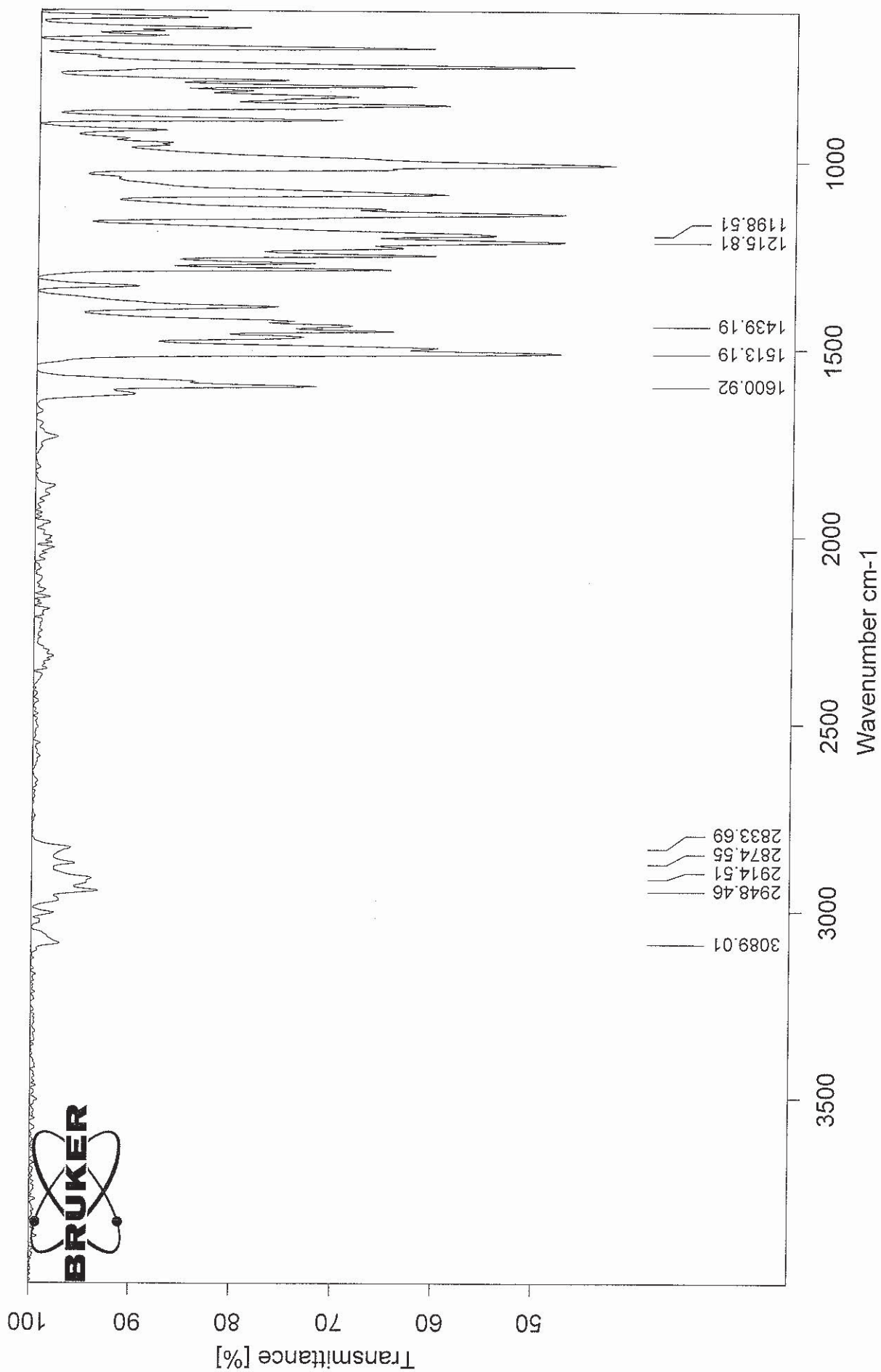
\*\*\* Mass Analysis for mass 362.1494770

1	21	20	3	3	362.1499179	13.5	4.409e-04
2	19	18	6	2	362.1485753	14.0	9.017e-04
3	7	22	8	9	362.1504258	1.0	9.488e-04
4	18	22	2	6	362.1472379	9.0	2.239e-03
5	17	16	9	1	362.1472326	14.5	2.244e-03
6	9	24	5	10	362.1517684	0.5	2.291e-03
7	16	20	5	5	362.1458952	9.5	3.582e-03
8	10	20	9	6	362.1531058	5.5	3.629e-03
9	15	24	1	9	362.1445578	4.5	4.919e-03
10	14	18	8	4	362.1445525	10.0	4.924e-03









U:\IR\1-(4-(benzyloxy)-3-methoxyphenyl)-5-methoxy-1Hbenzo[d][1,2,3]triazole.0

1-(4-(benzyloxy)-3-methoxyphenyl)-5-methoxy-1Hbenzo[d][1,2,

18.11.2013



ESI-MS: RR044Fi

XMASS Mass Analysis for /Data/UNI\_FR/REMY7649\_ESI/3/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

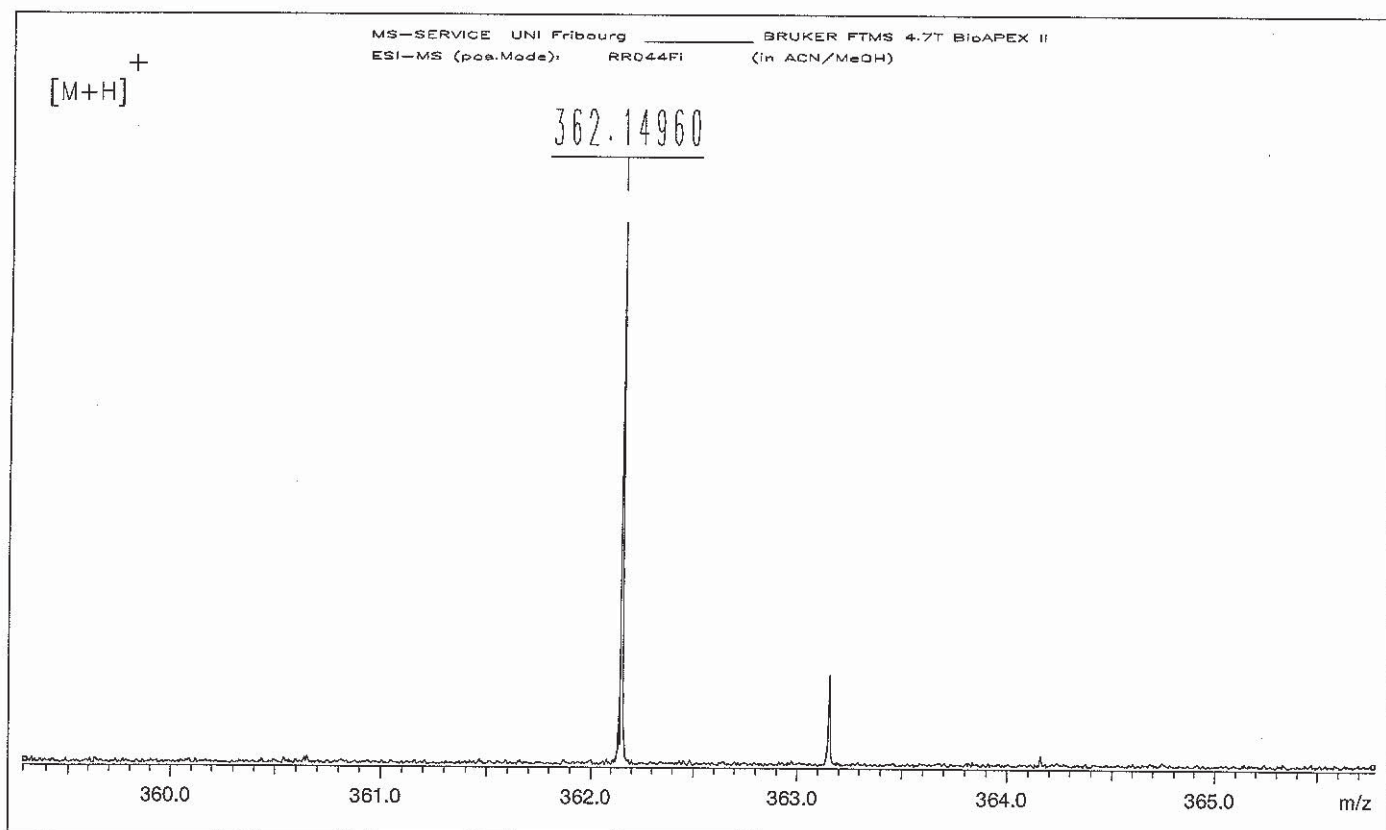
Ion mass = 362.1496000

Charge = +1

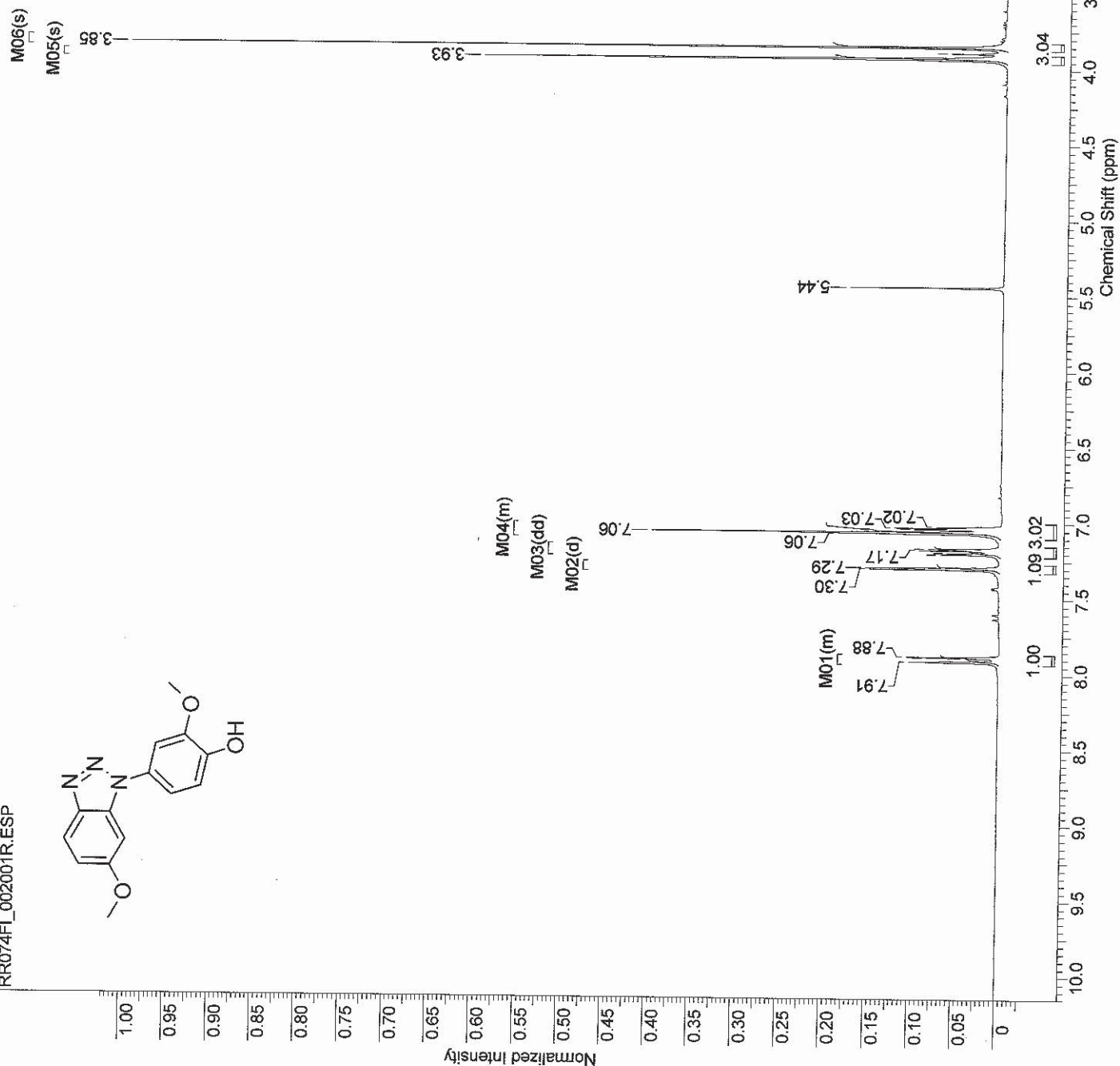
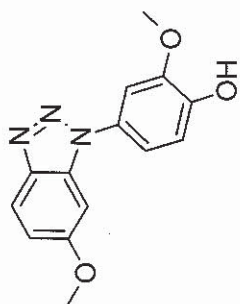
#	C	H	N	O	mass	DBE	error
---	---	---	---	---	------	-----	-------

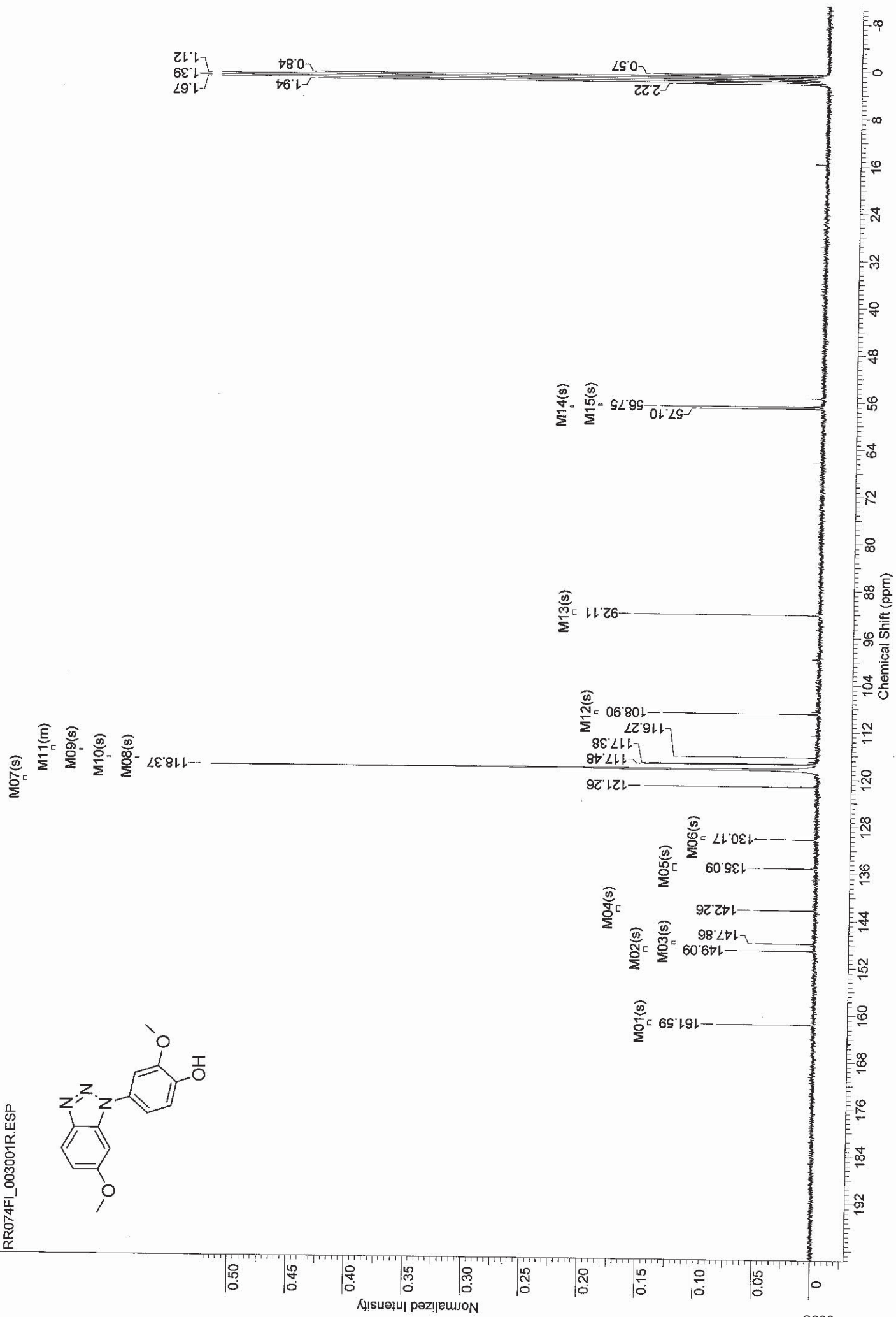
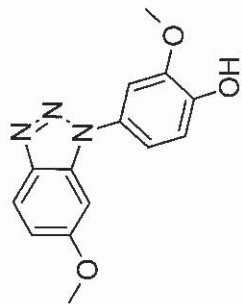
\*\*\* Mass Analysis for mass 362.1496000

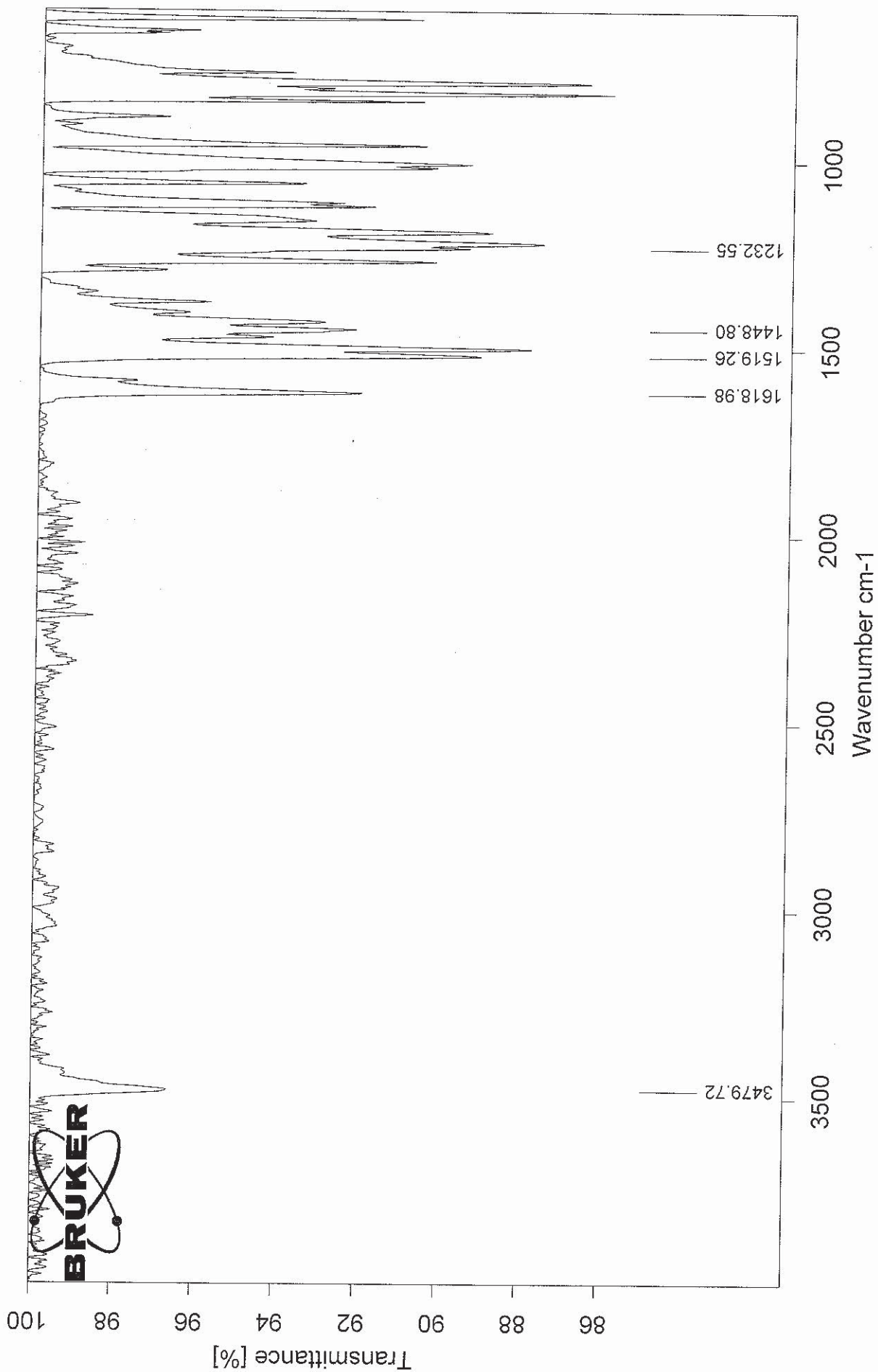
1	21	20	3	3	362.1499179	13.5	3.179e-04
2	7	22	8	9	362.1504258	1.0	8.258e-04
3	19	18	6	2	362.1485753	14.0	1.025e-03
4	9	24	5	10	362.1517684	0.5	2.168e-03
5	18	22	2	6	362.1472379	9.0	2.362e-03
6	17	16	9	1	362.1472326	14.5	2.367e-03
7	10	20	9	6	362.1531058	5.5	3.506e-03
8	16	20	5	5	362.1458952	9.5	3.705e-03
9	12	22	6	7	362.1544485	5.0	4.849e-03
10	15	24	1	9	362.1445578	4.5	5.042e-03













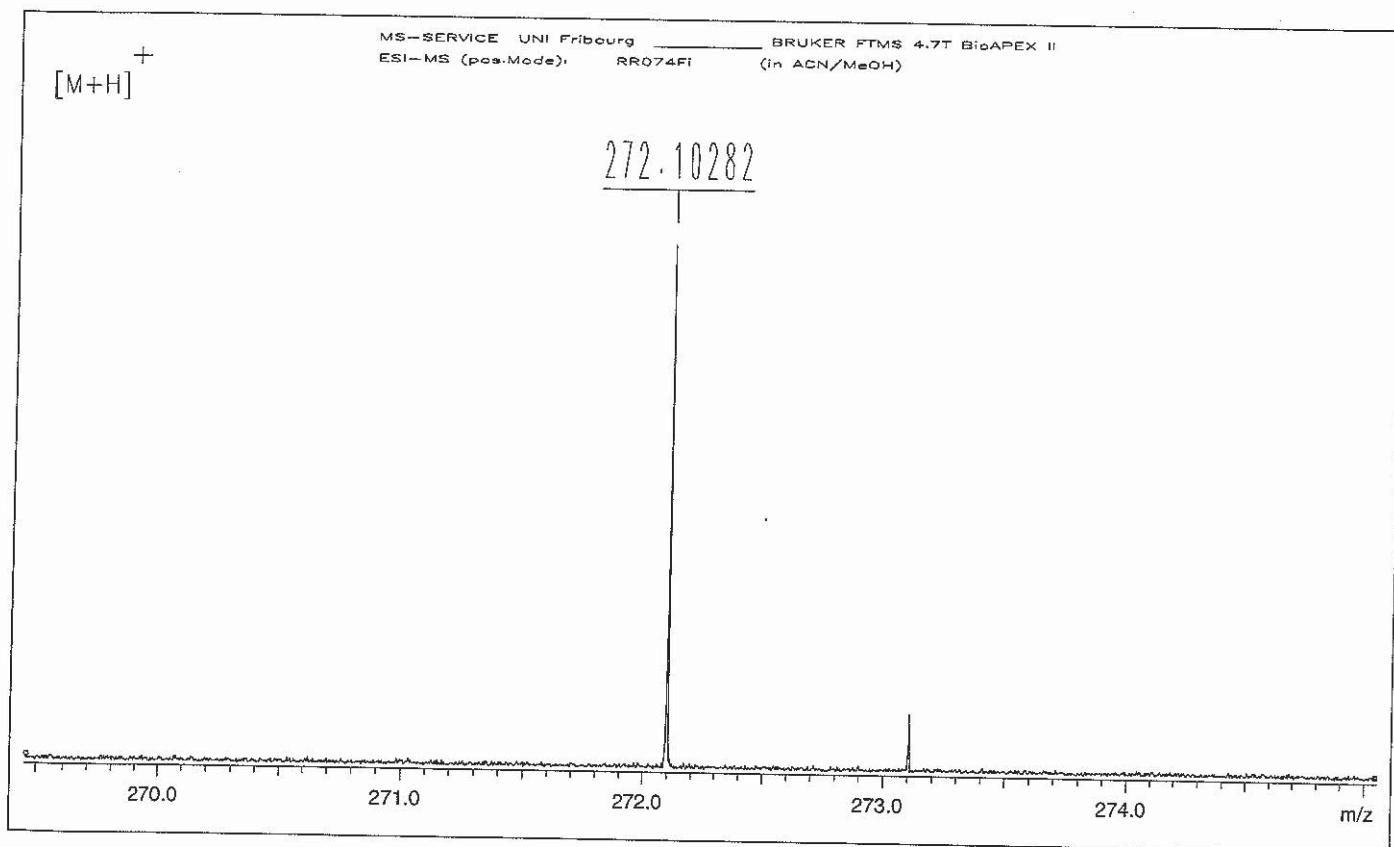
ESI-MS: RR074Fi

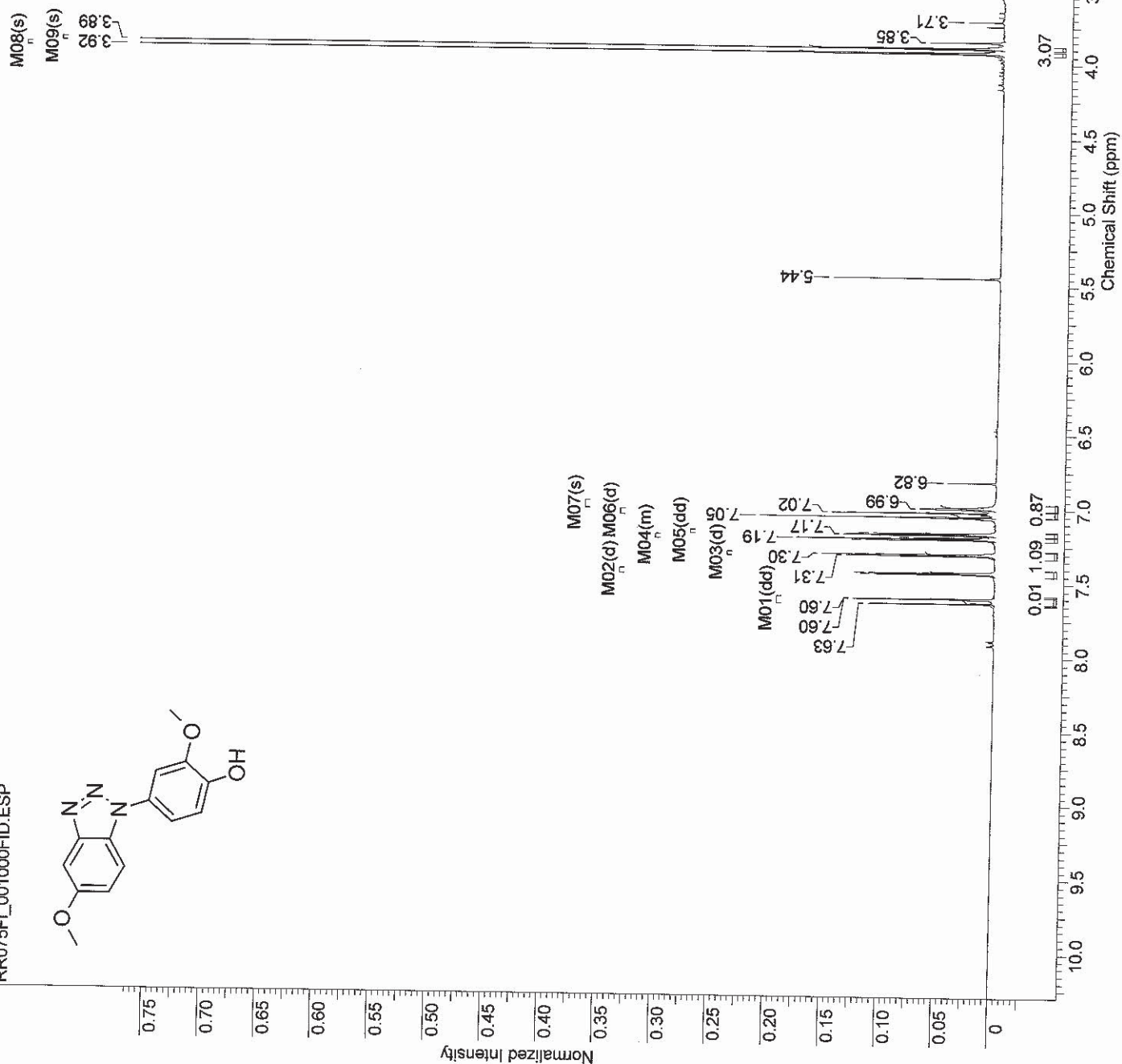
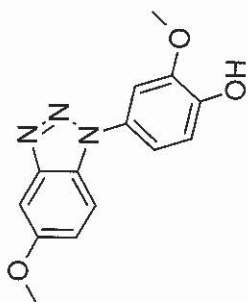
XMASS Mass Analysis for /Data/UNI\_FR/REMY7652\_ESI/3/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

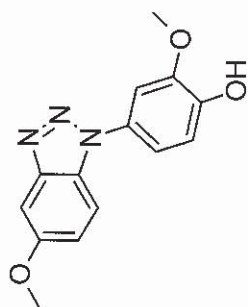
Ion mass = 272.1028240

Charge = +1

#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 272.1028240							
1	14	14	3	3	272.1029678	9.5	1.438e-04
2	12	12	6	2	272.1016251	10.0	1.199e-03
3	11	16	2	6	272.1002877	5.0	2.536e-03
4	10	10	9	1	272.1002824	10.5	2.542e-03
5	9	14	5	5	272.0989450	5.5	3.879e-03
6	19	14	1	1	272.1069905	13.5	4.166e-03
7	5	16	6	7	272.1074983	1.0	4.674e-03
8	8	18	1	9	272.0976076	0.5	5.216e-03
9	7	12	8	4	272.0976023	6.0	5.222e-03
10	6	12	10	3	272.1088357	6.0	6.012e-03

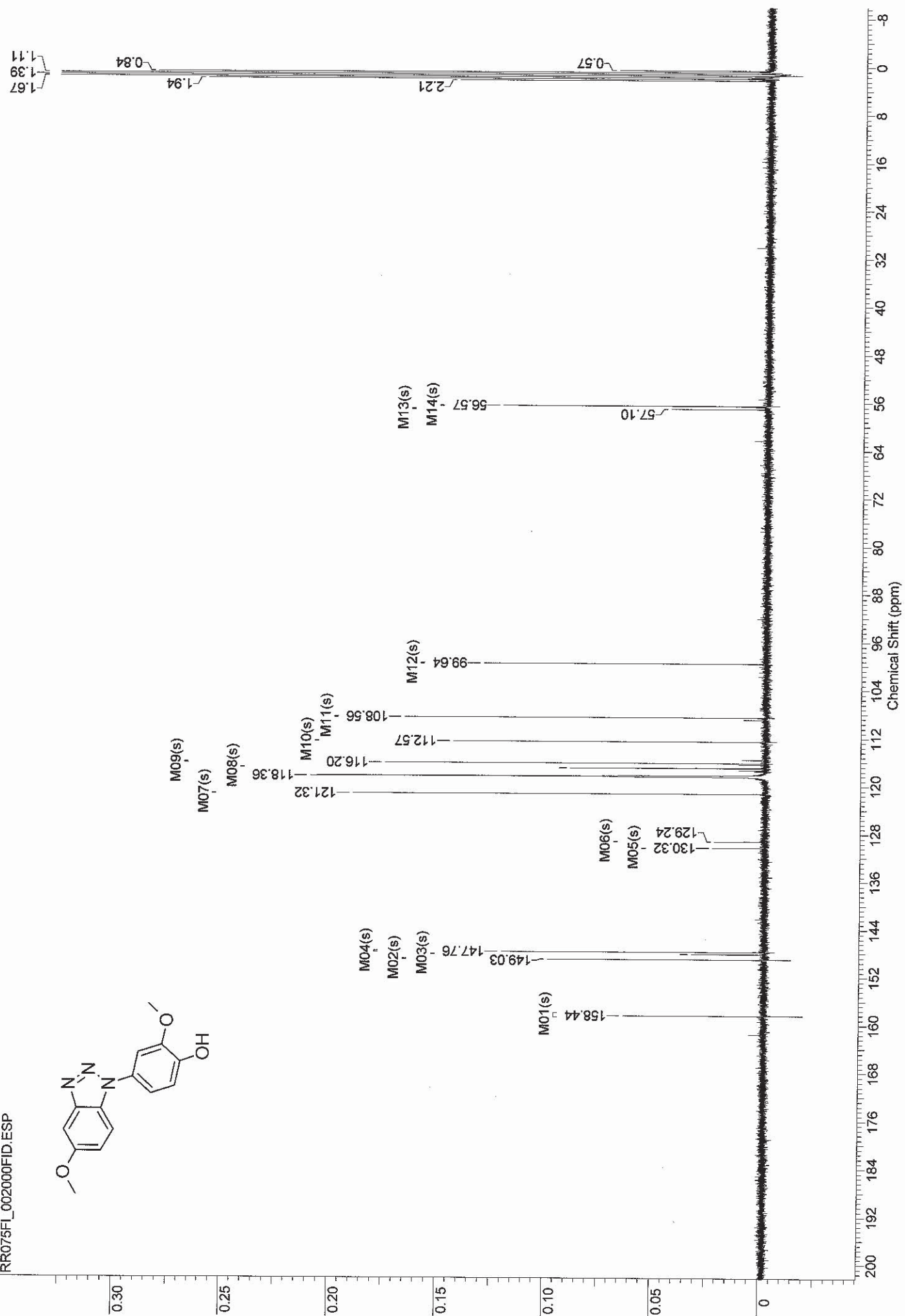




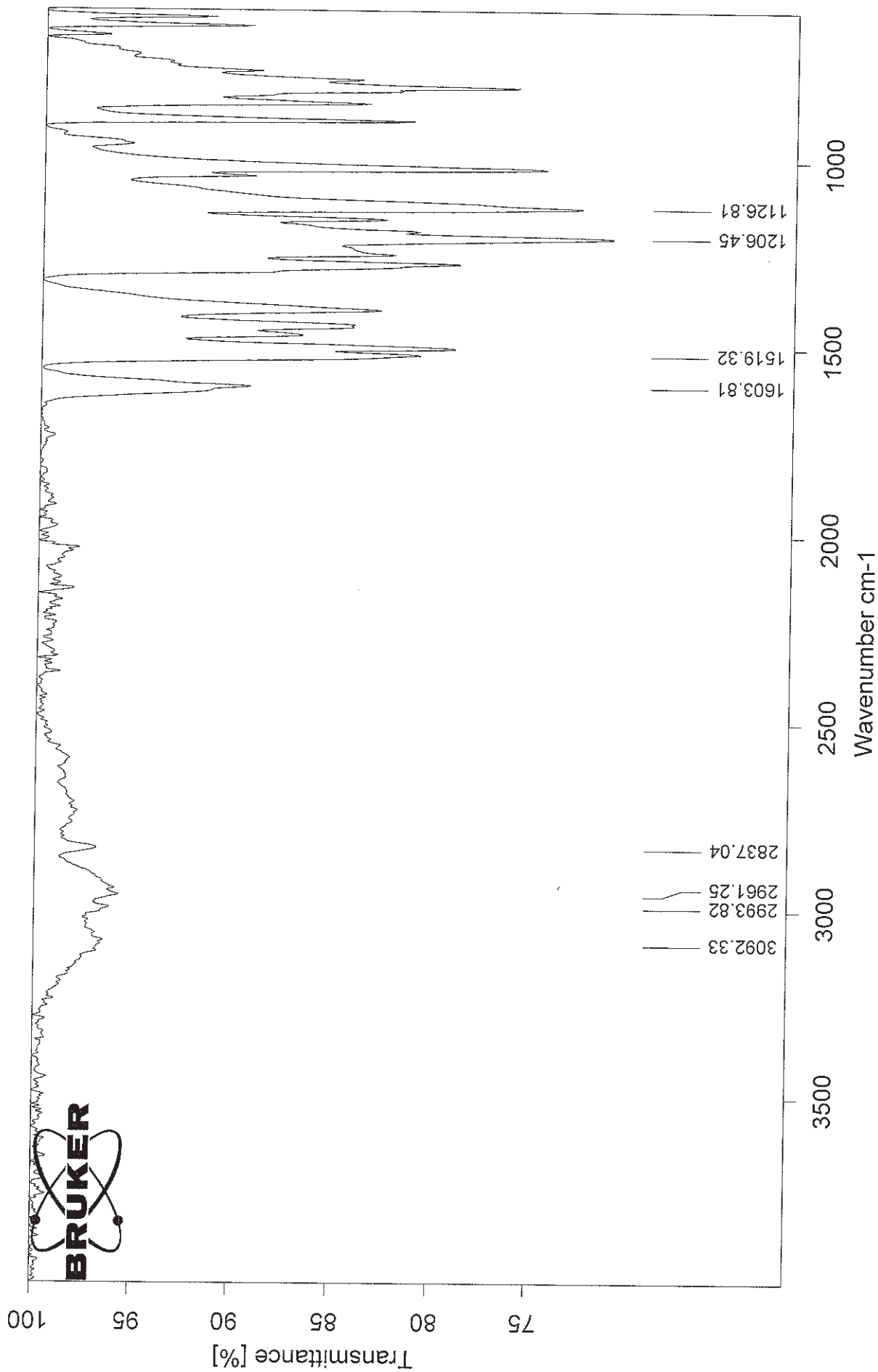


Normalized Intensity

S204









ESI-MS: RR075Fi

XMASS Mass Analysis for /Data/UNI\_FR/REMY7653\_ESI/4/pdata/1/massanal.res:  
XMASS Mass Analysis Constraints

Ion mass = 272.1028760

Charge = +1

#	C	H	N	O	mass	DBE	error
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\*\*\* Mass Analysis for mass 272.1028760

1	14	14	3	3	272.1029678	9.5	9.175e-05
2	12	12	6	2	272.1016251	10.0	1.251e-03
3	11	16	2	6	272.1002877	5.0	2.588e-03
4	10	10	9	1	272.1002824	10.5	2.594e-03
5	9	14	5	5	272.0989450	5.5	3.931e-03
6	19	14	1	1	272.1069905	13.5	4.114e-03
7	5	16	6	7	272.1074983	1.0	4.622e-03
8	8	18	1	9	272.0976076	0.5	5.268e-03
9	7	12	8	4	272.0976023	6.0	5.274e-03
10	6	12	10	3	272.1088357	6.0	5.960e-03

