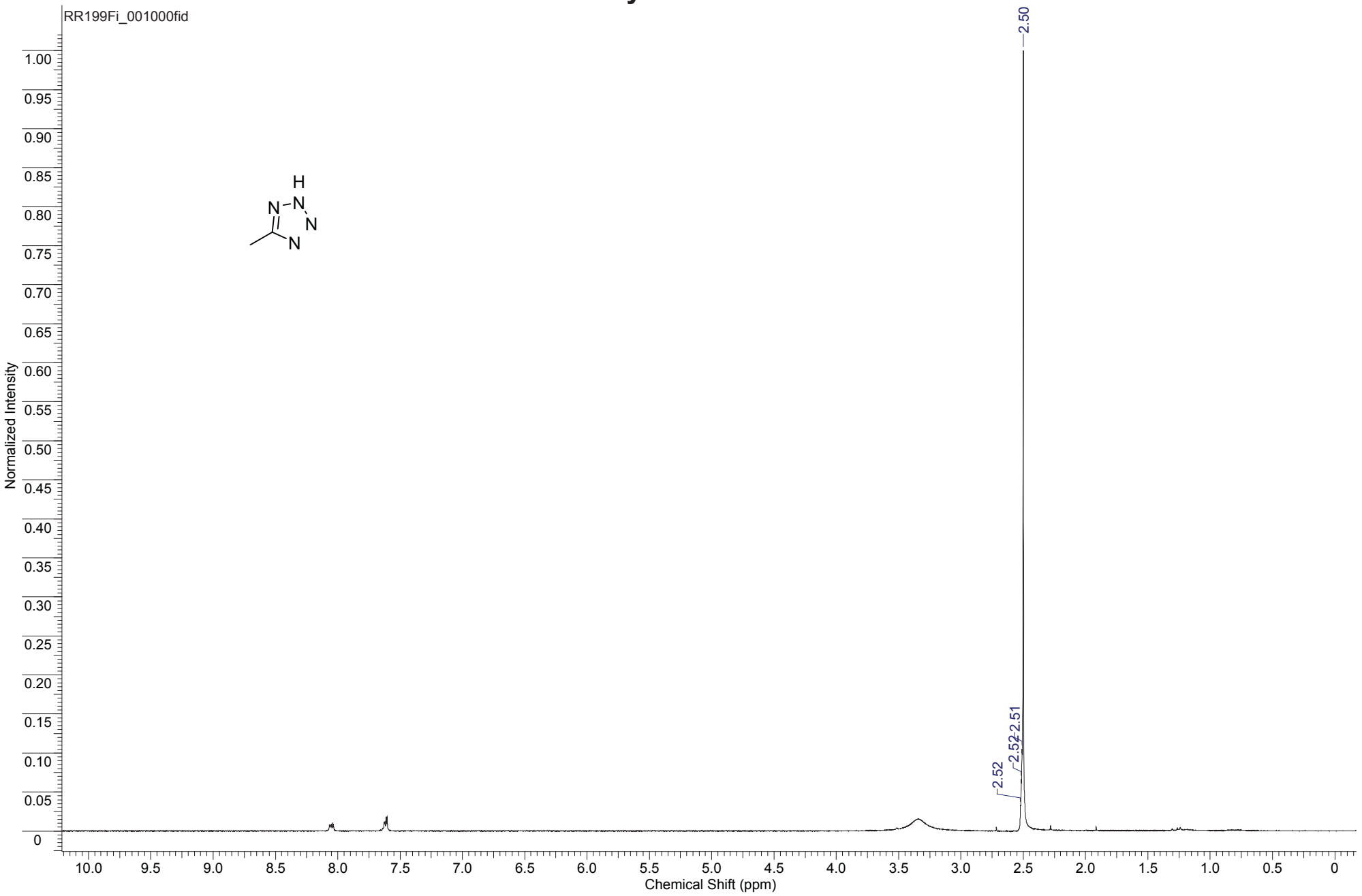
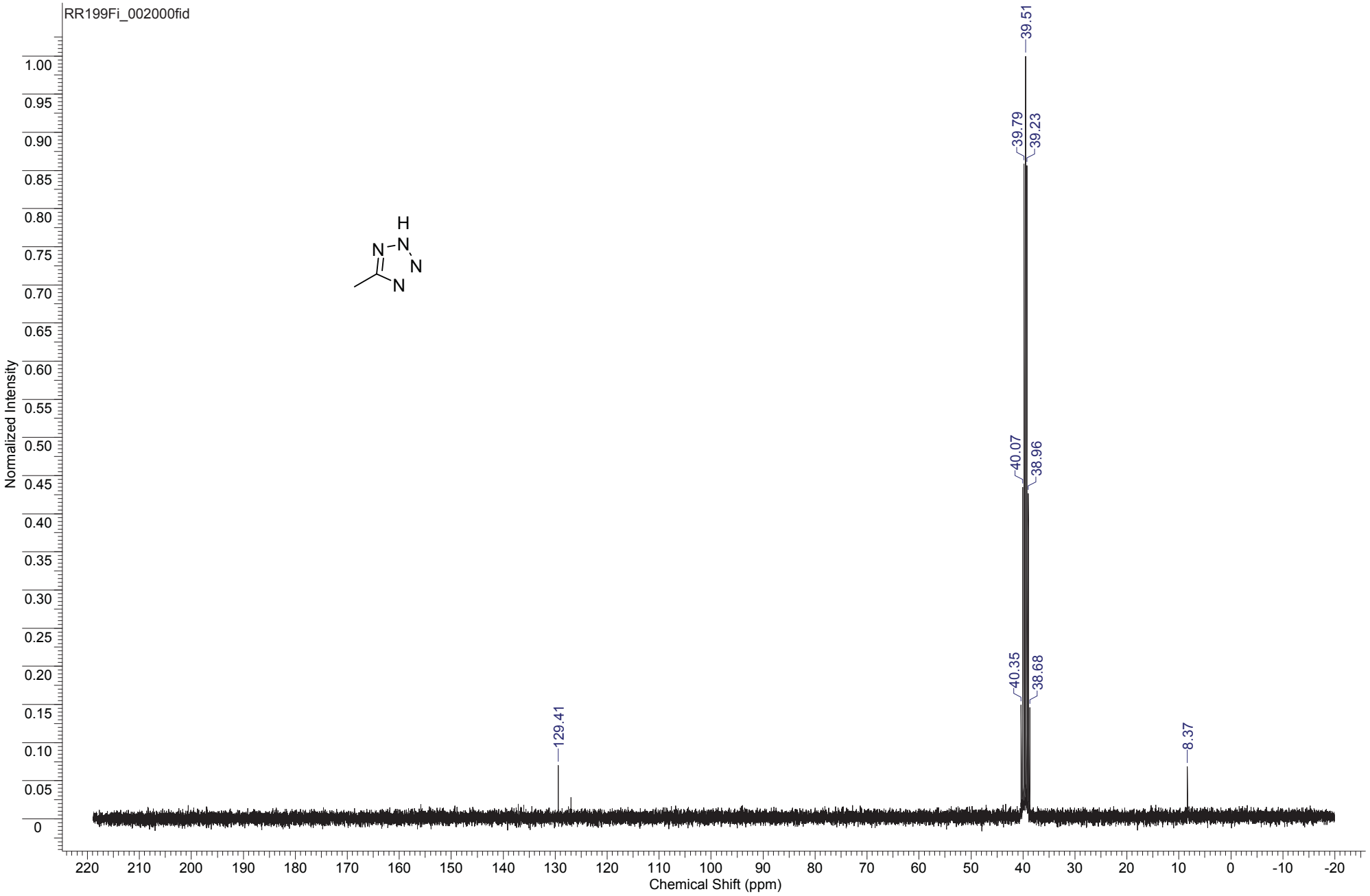
Index

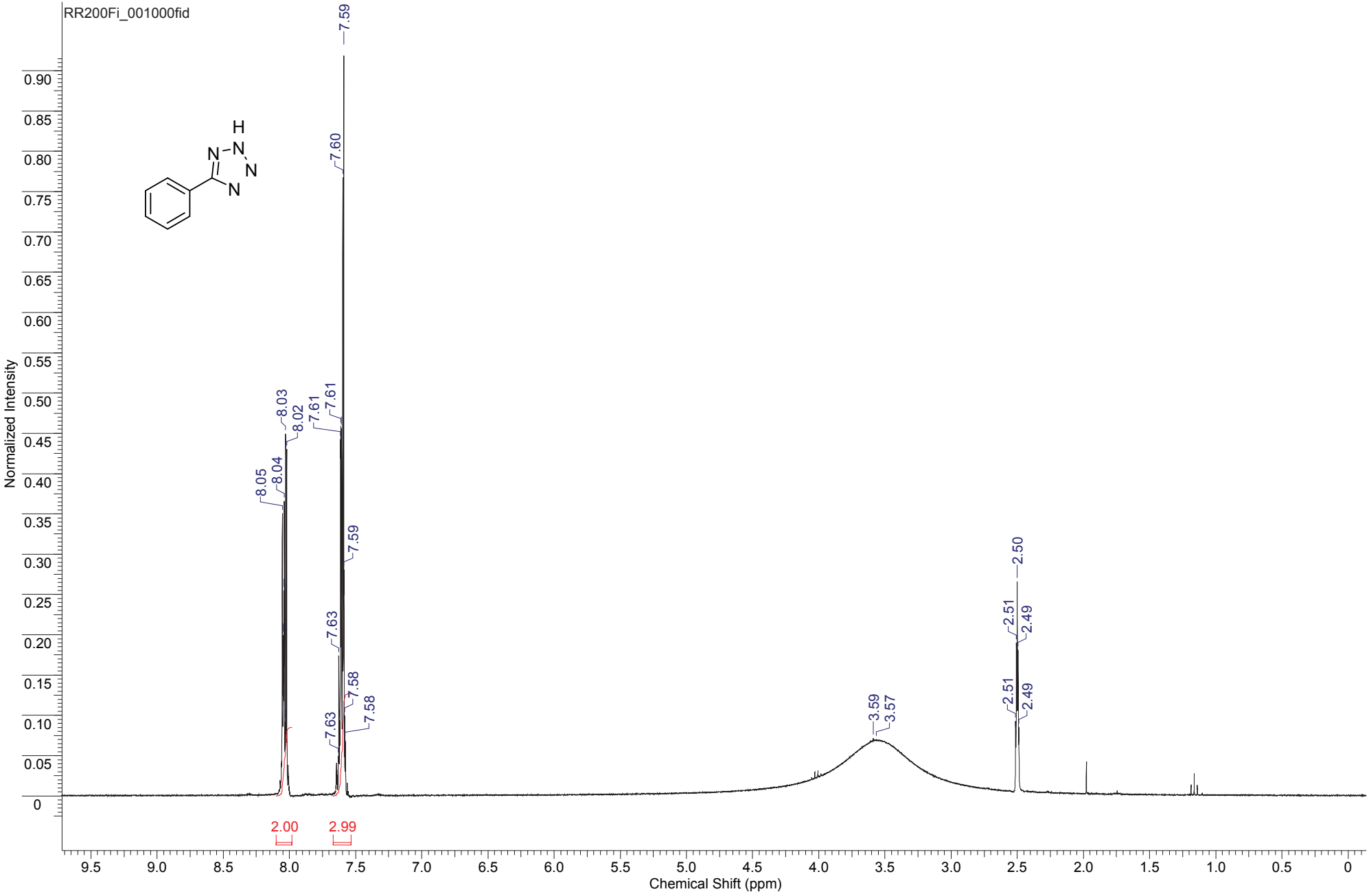
5-methyl-2H-tetrazole



5-methyl-2H-tetrazole



5-phenyl-2H-tetrazole



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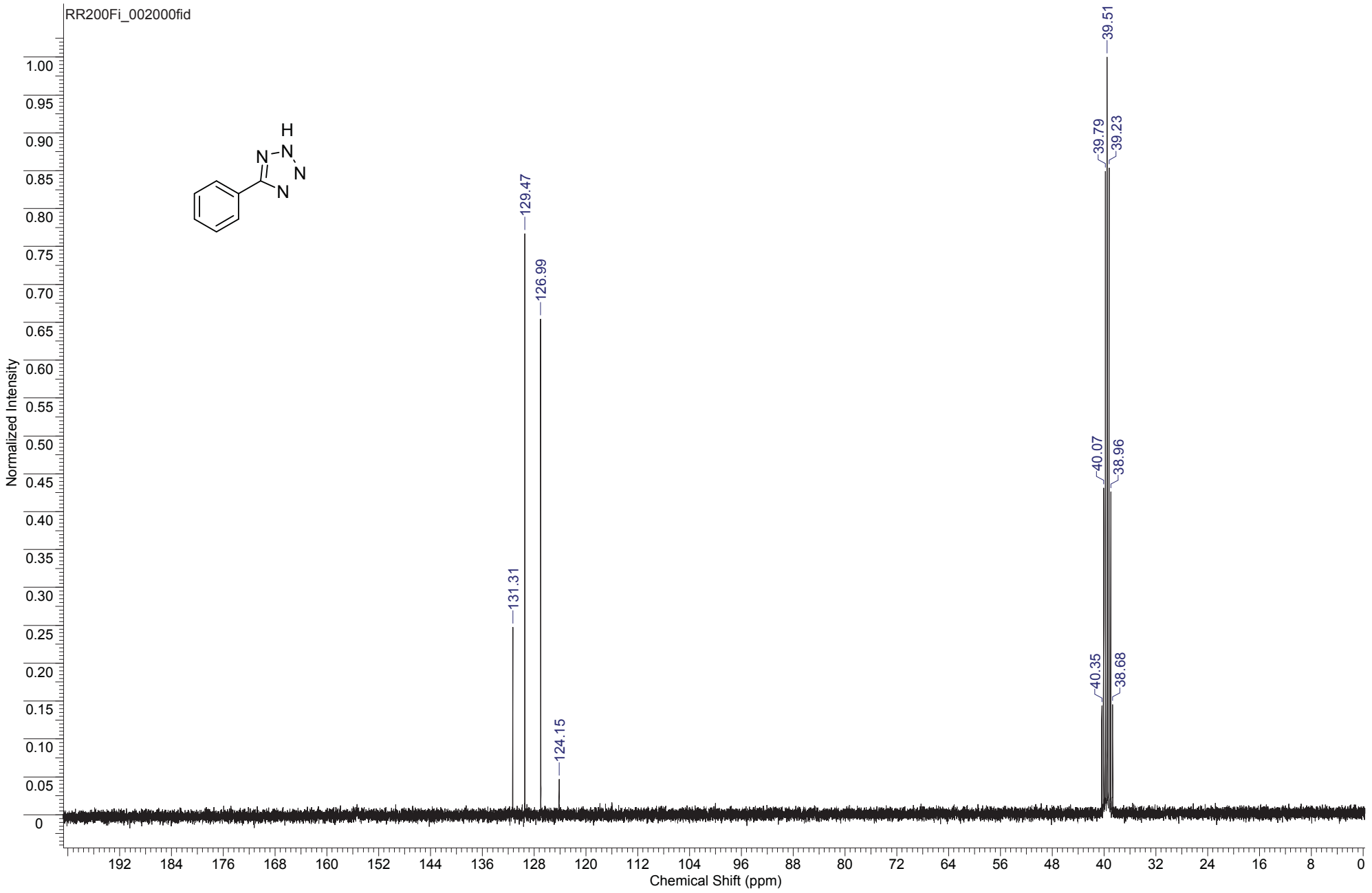
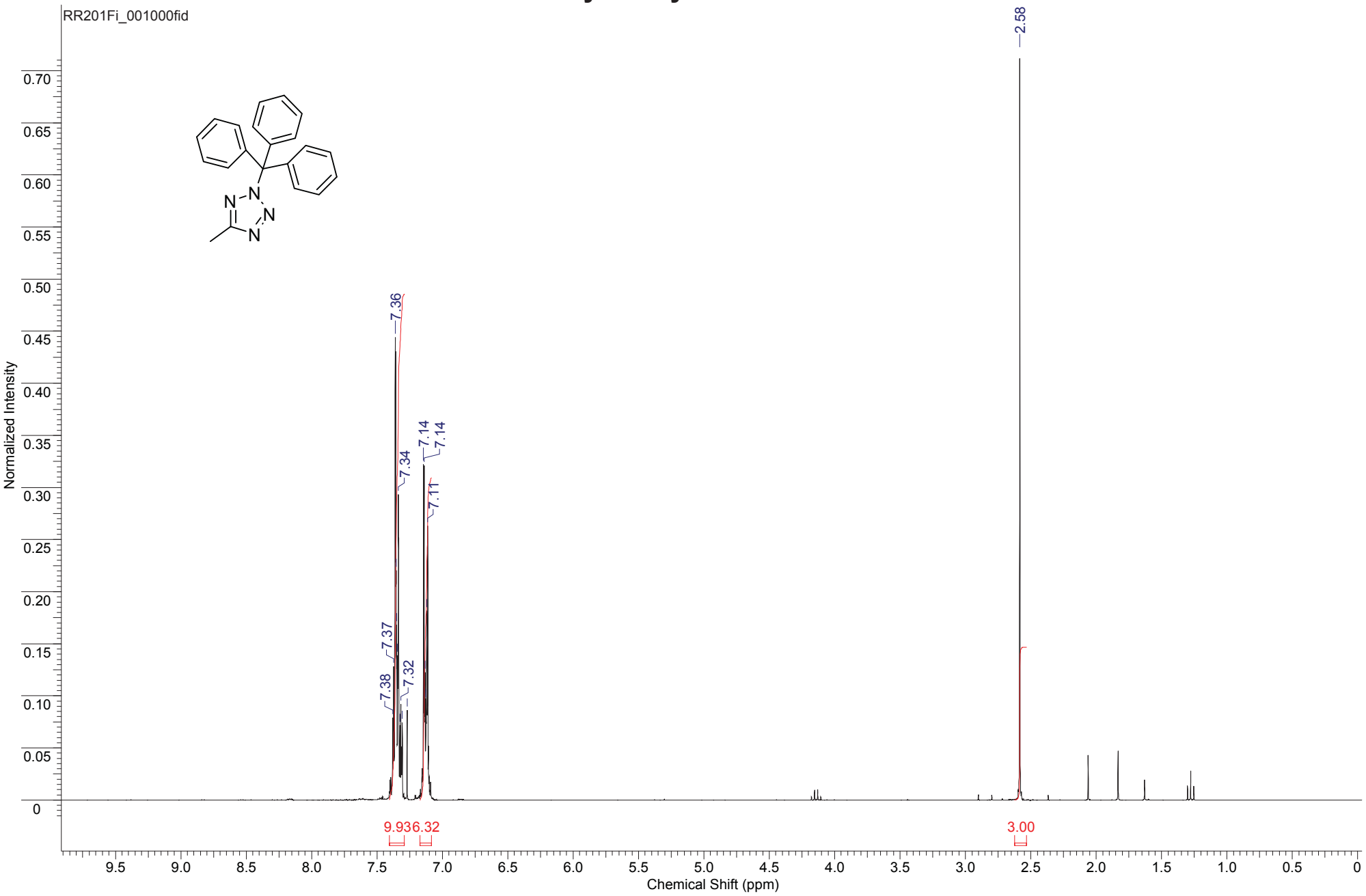


5-methyl-2-trityl-2H-tetrazole



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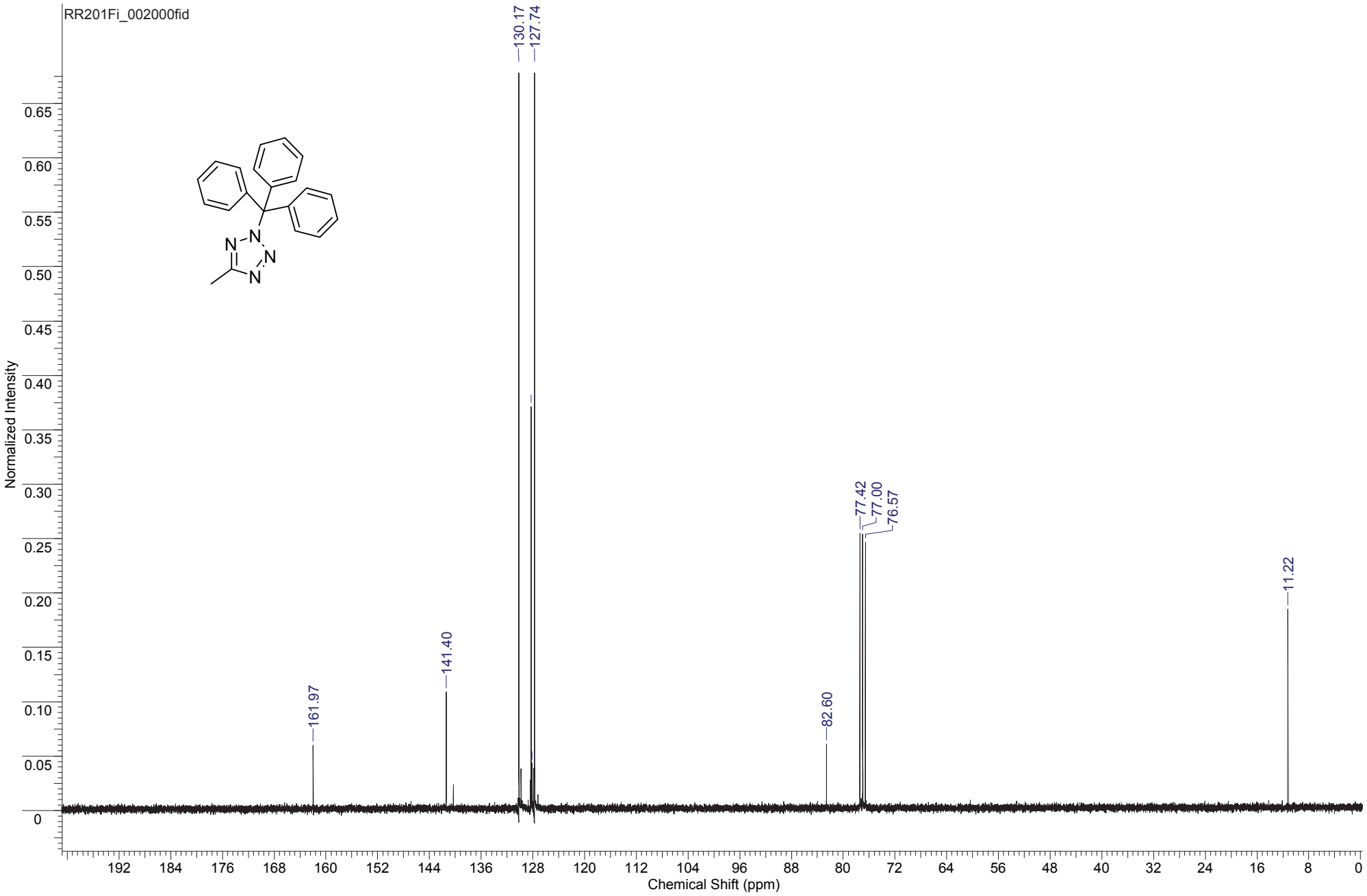
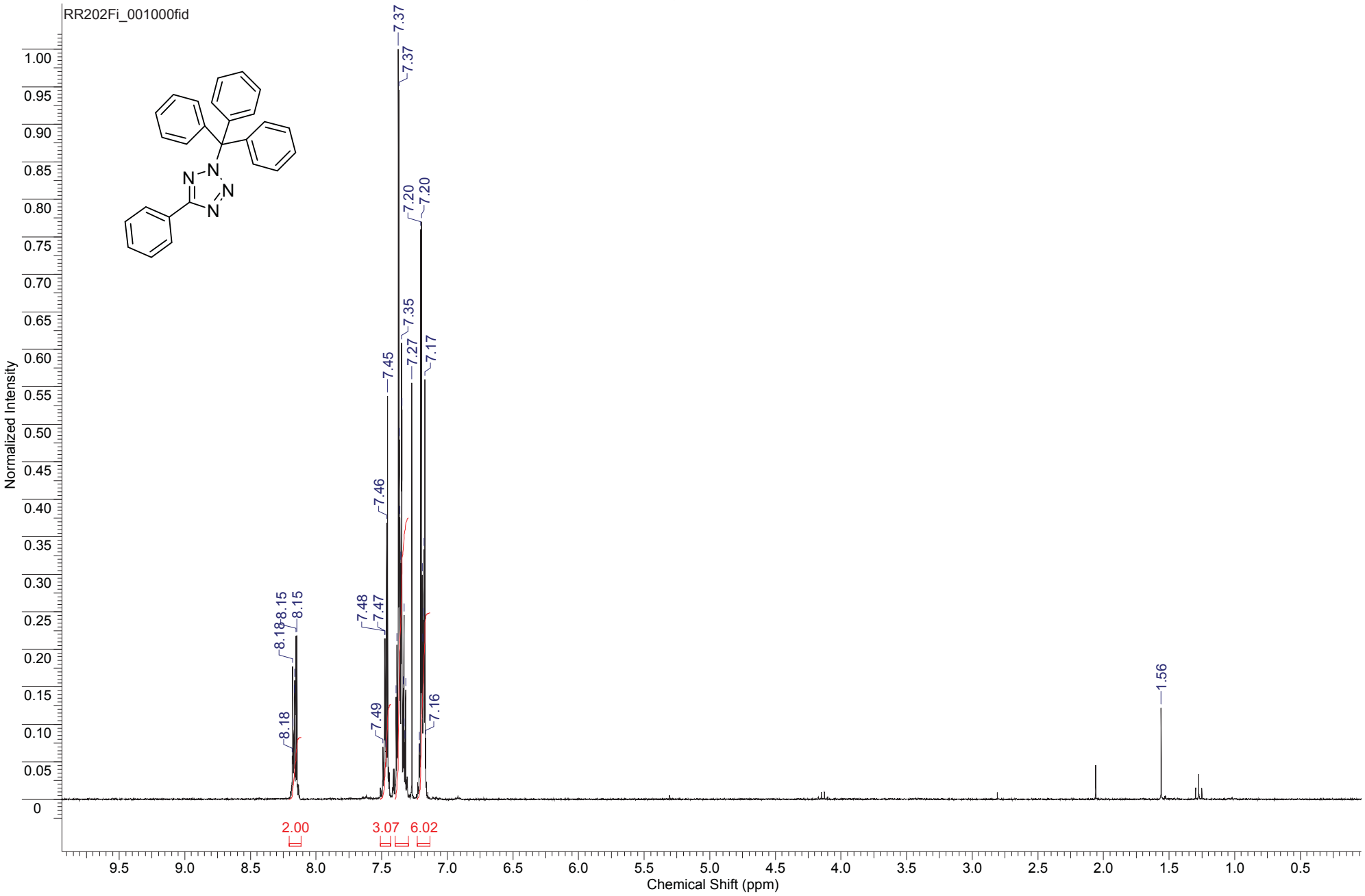
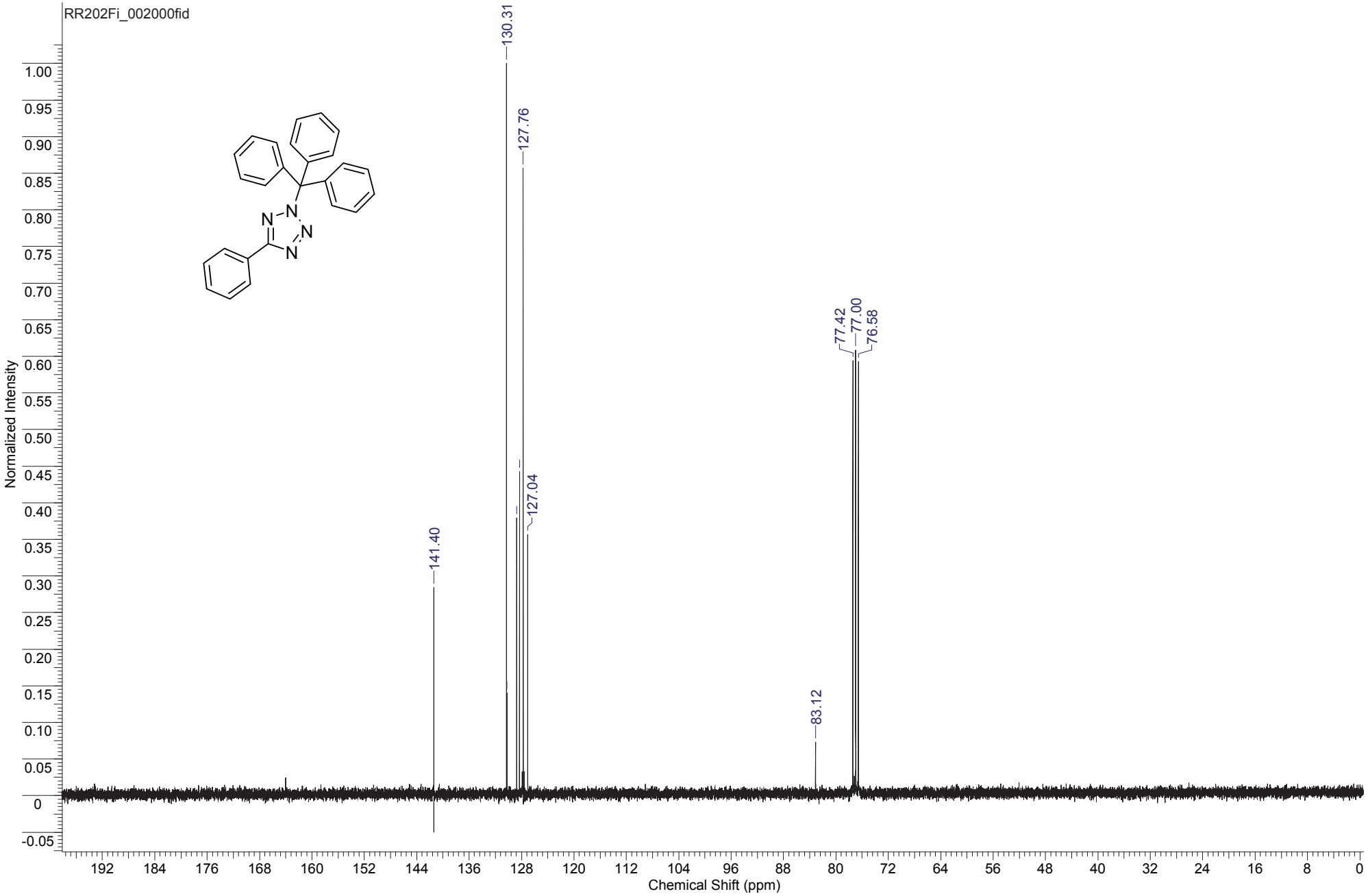


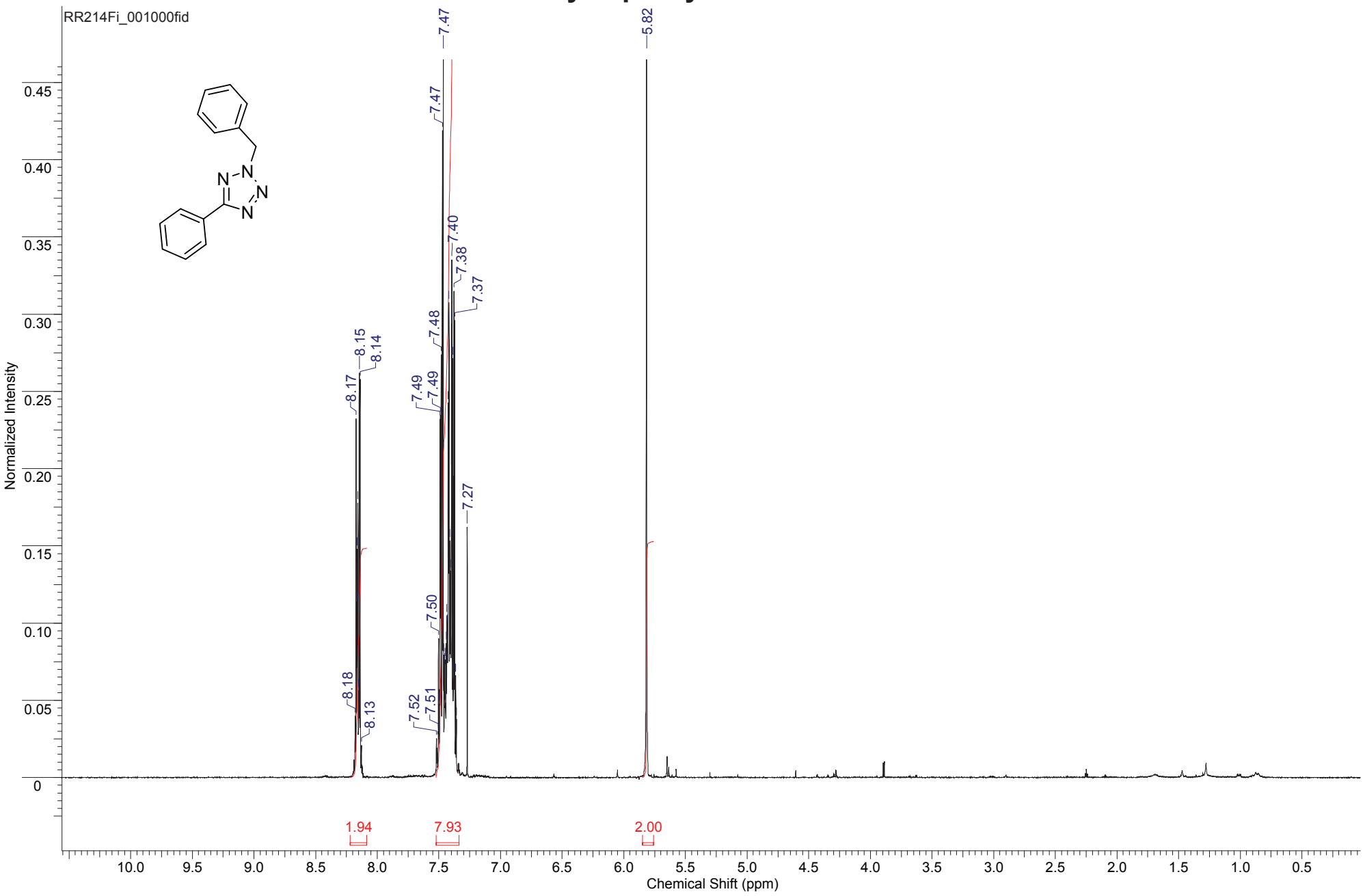
5-phenyl-2-trityl-2H-tetrazole



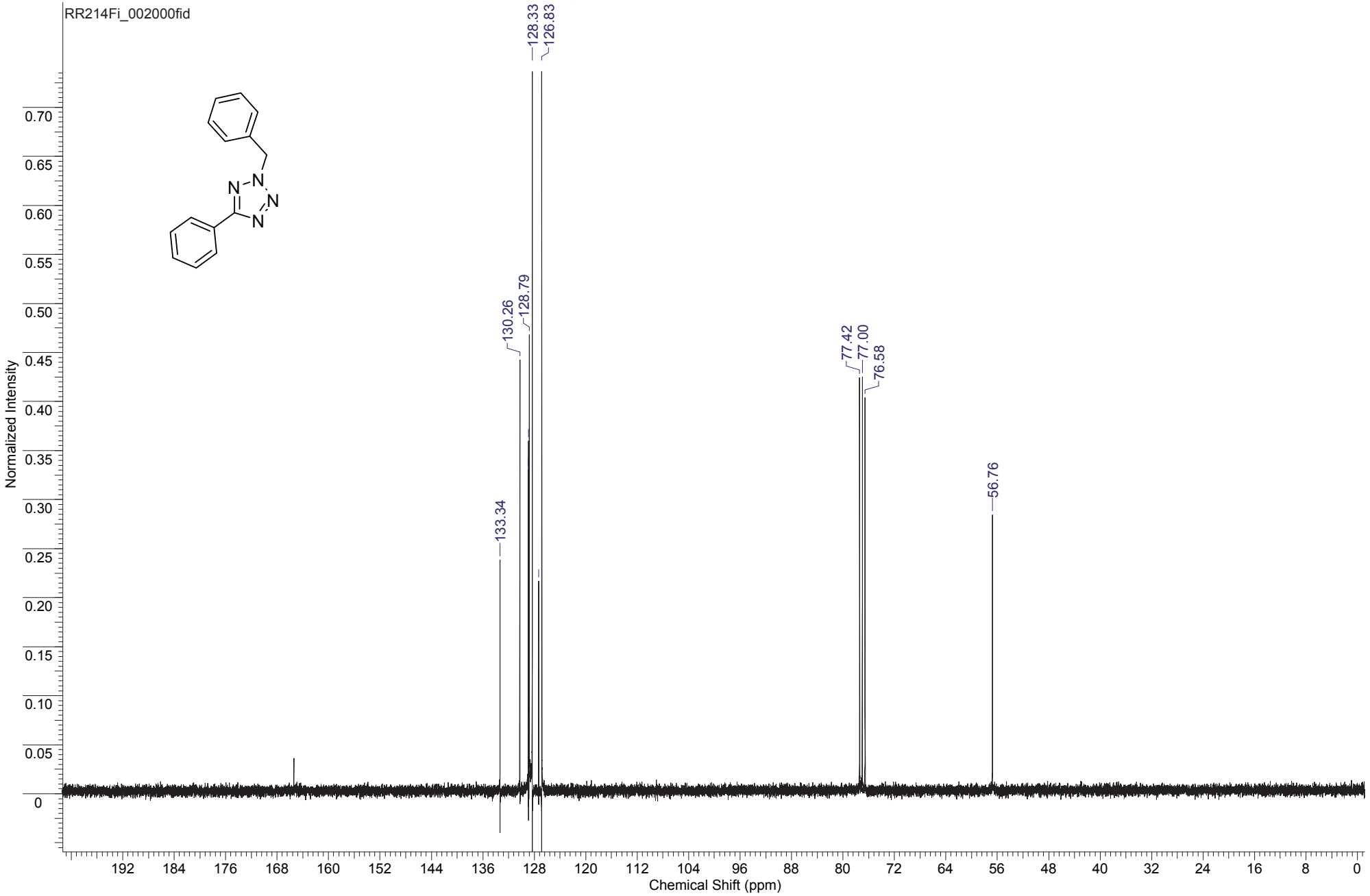
5-phenyl-2-trityl-2H-tetrazole



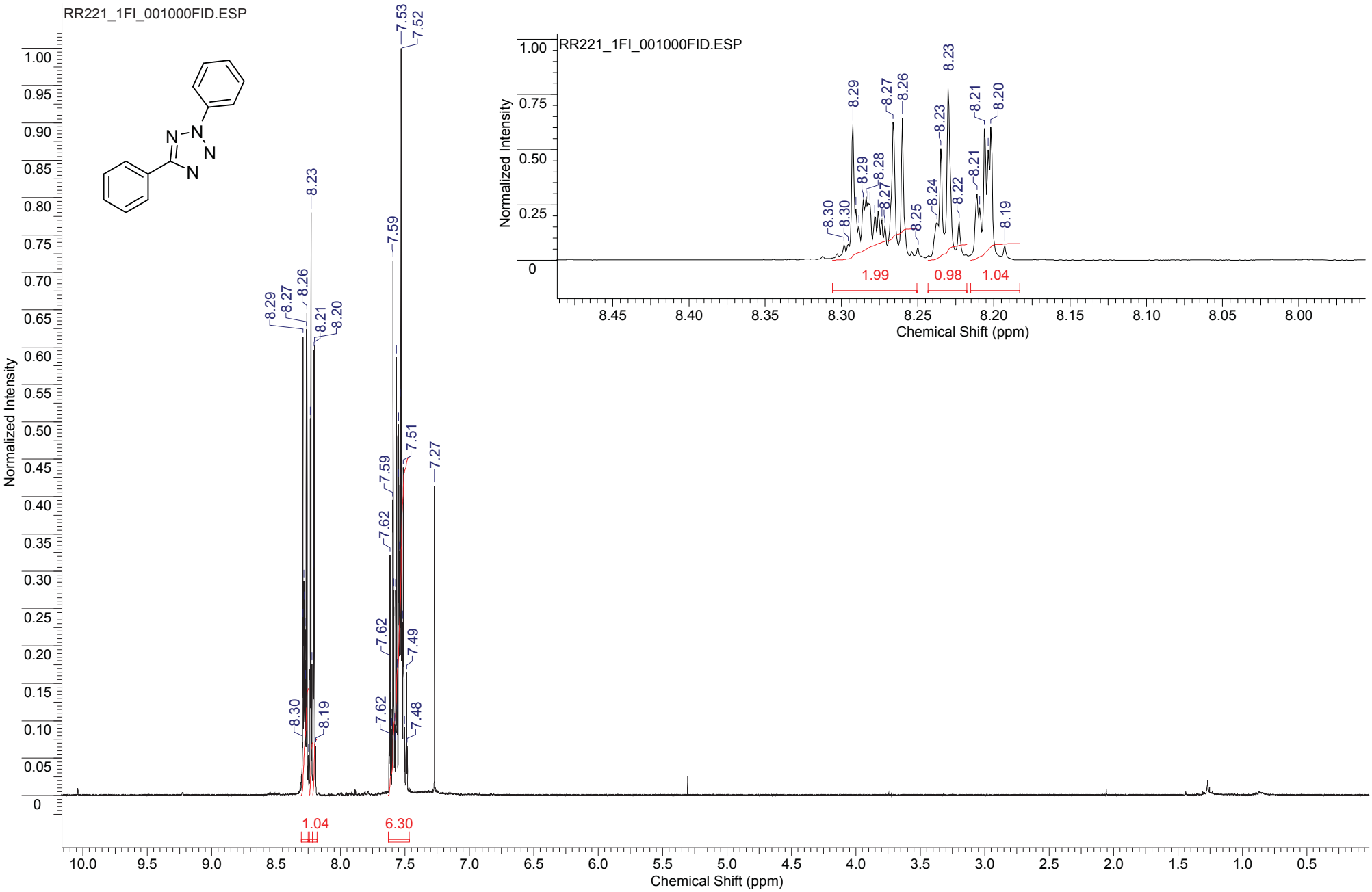
2-benzyl-5-phenyl-2H-tetrazole



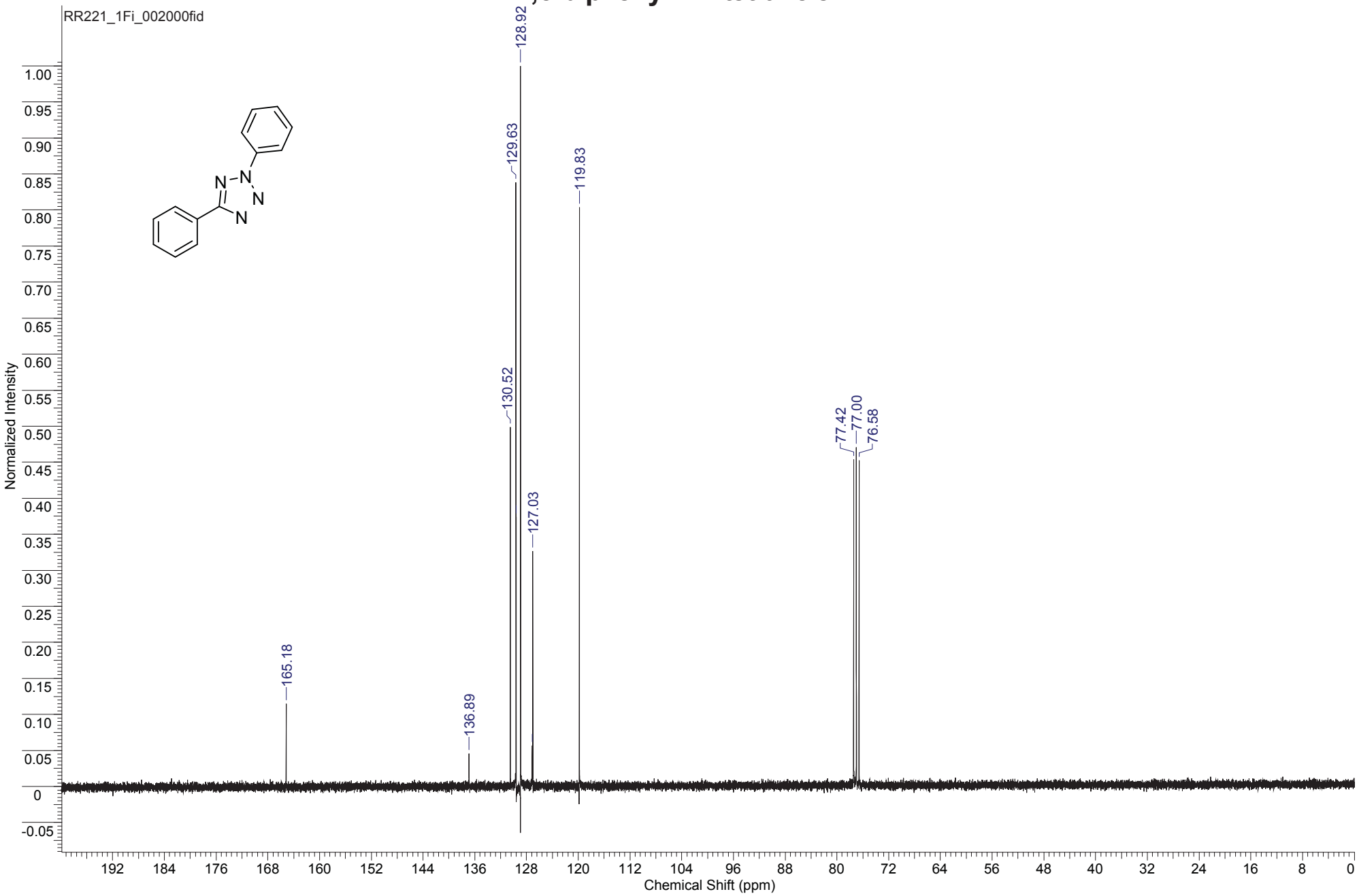
2-benzyl-5-phenyl-2H-tetrazole

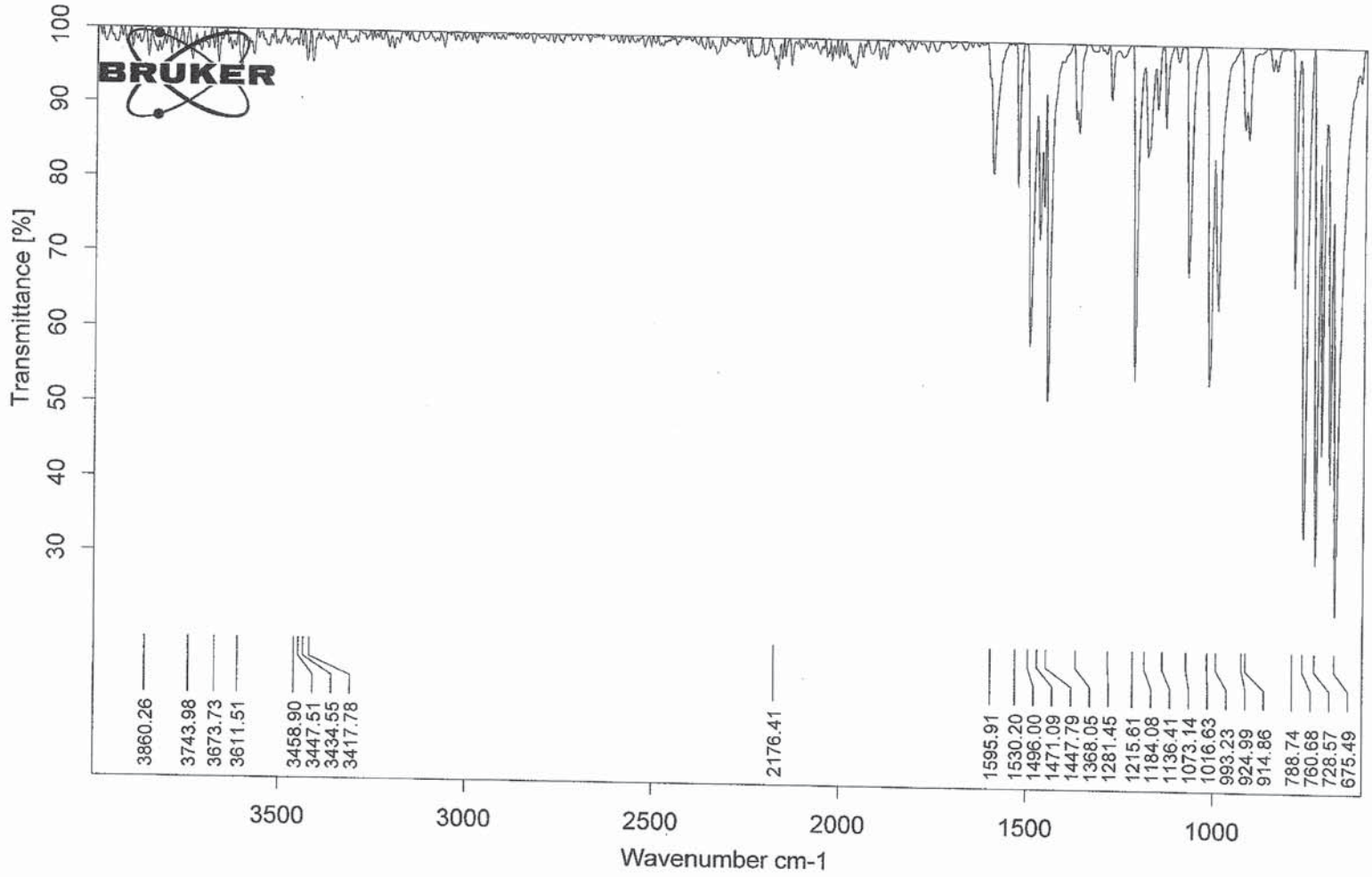


2,5-diphenyl-2H-tetrazole



2,5-diphenyl-2H-tetrazole





U:\IR\Tetrazole 1.0	Tetrazole 1	pink solid	22.05.2015

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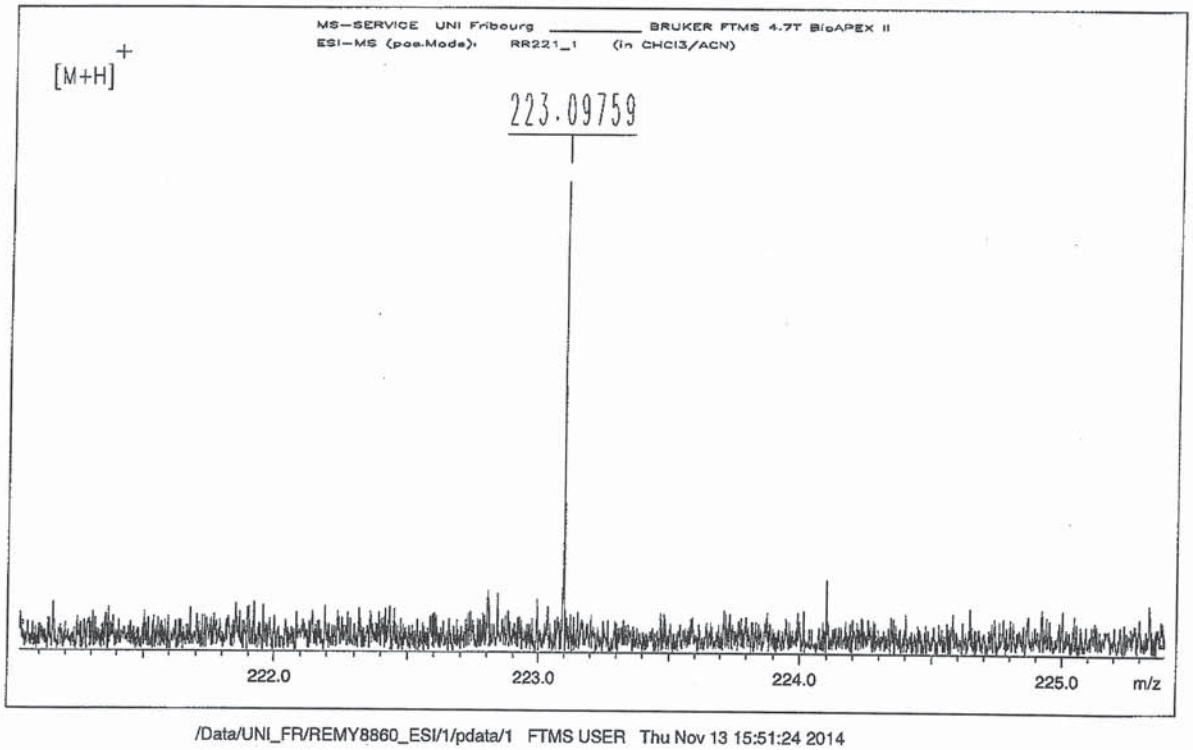
ESI-MS: RR221_1

XMASS Mass Analysis for /Data/UNI_FR/REMY8860_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 223.0975890

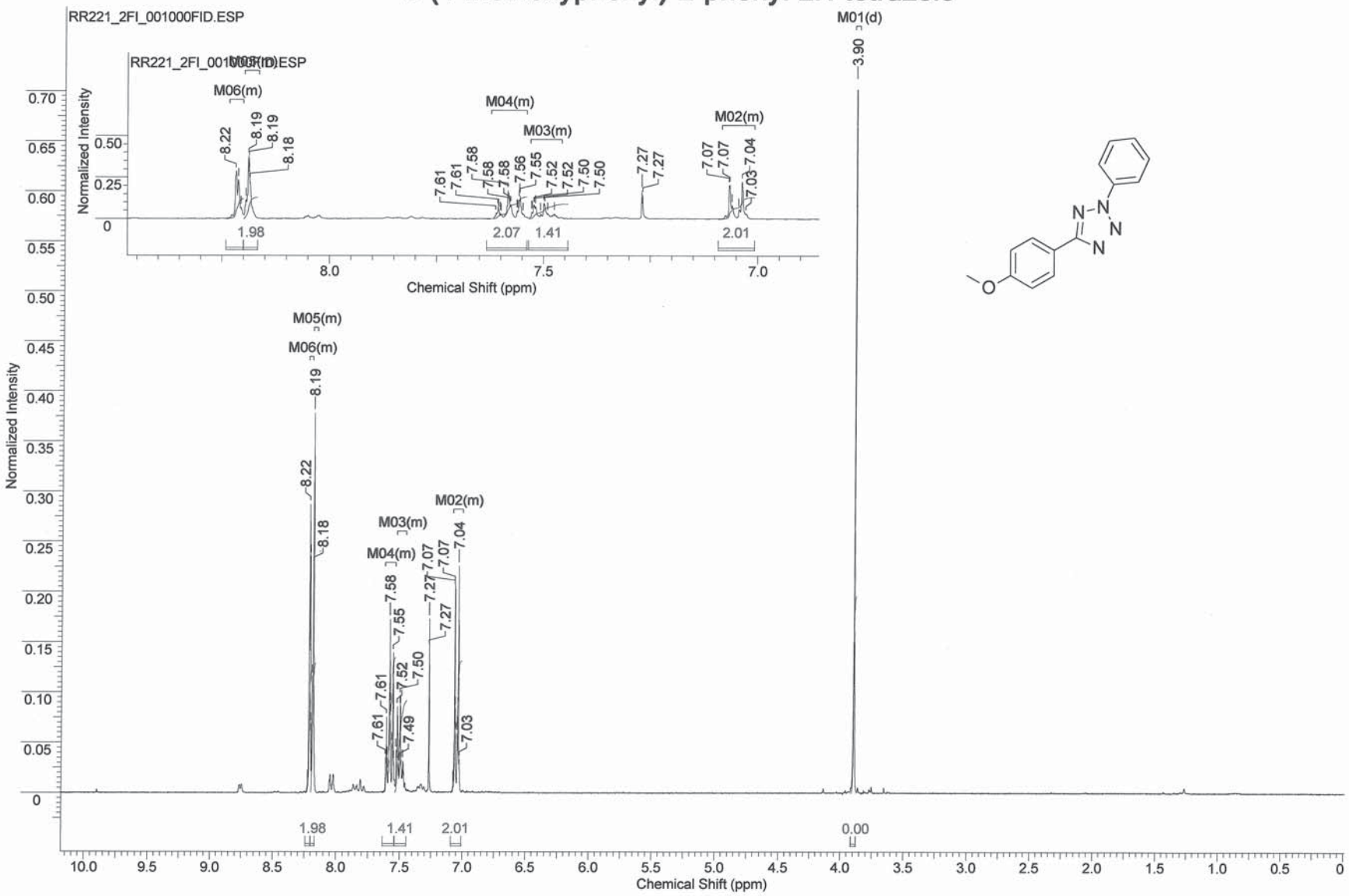
Charge = +1

#	C	H	N	mass	DBE	error
*** Mass Analysis for mass 223.0975890						
1	13	11	4	223.0978228	10.5	2.338e-04
2	12	9	5	223.0852467	11.0	1.234e-02
3	14	13	3	223.1103989	10.0	1.281e-02
4	6	11	10	223.1162668	6.5	1.868e-02
5	11	7	6	223.0726707	11.5	2.492e-02
6	15	15	2	223.1229749	9.5	2.539e-02
7	7	13	9	223.1288429	6.0	3.125e-02
8	10	5	7	223.0600946	12.0	3.749e-02
9	16	17	1	223.1355510	9.0	3.796e-02
10	8	15	8	223.1414189	5.5	4.383e-02

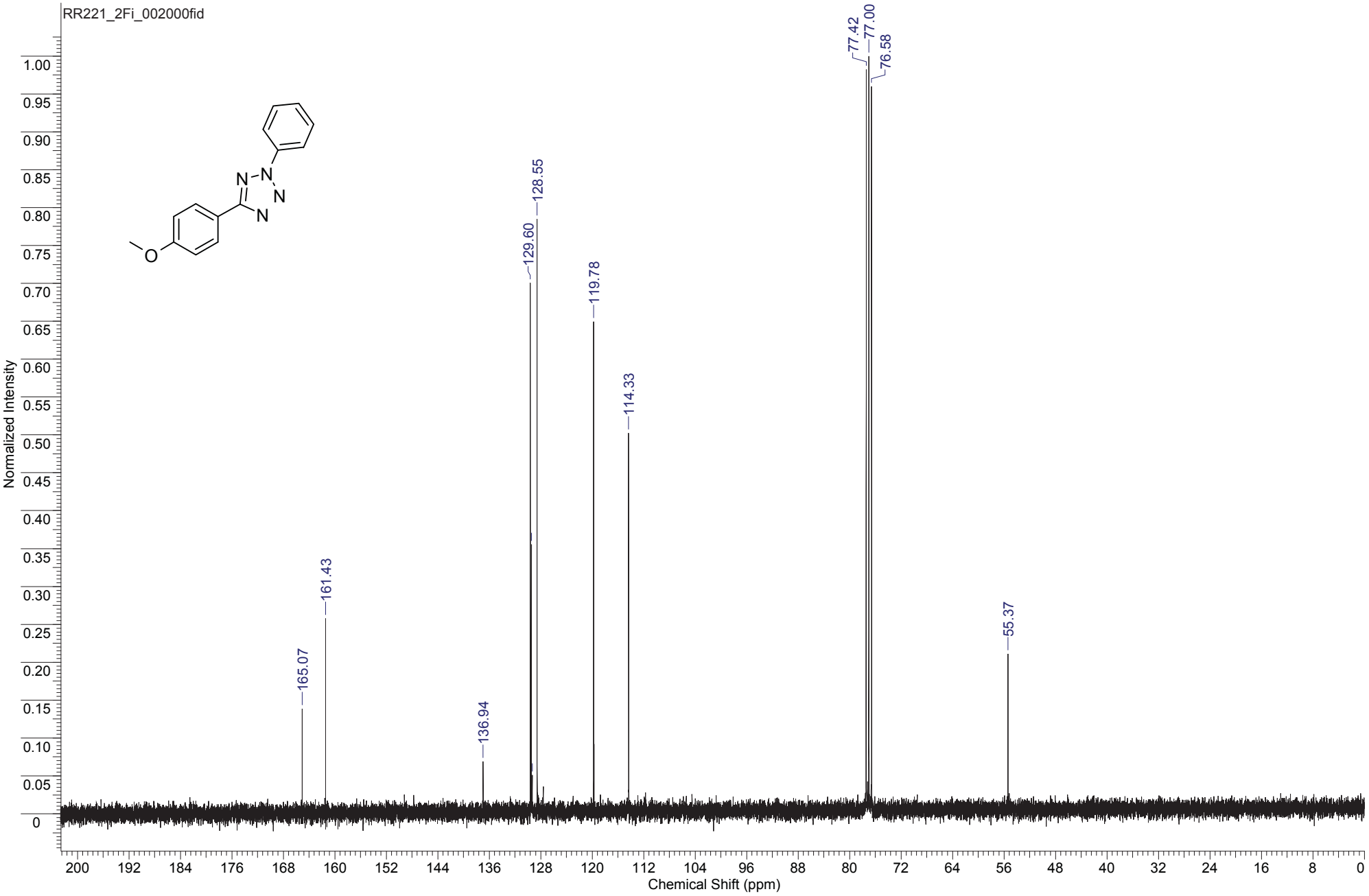


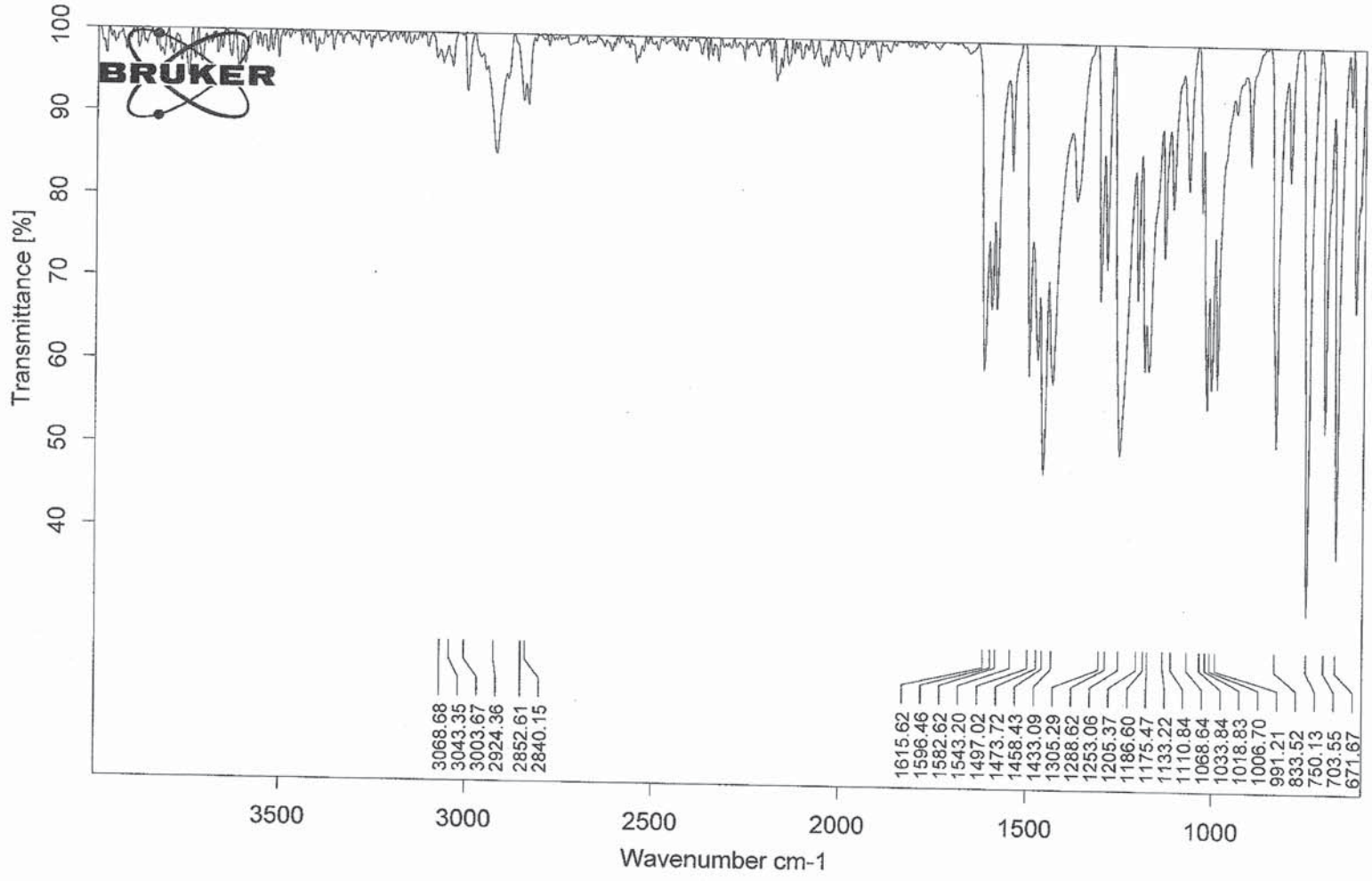
/Data/UNI_FR/REMY8860_ESI/1/pdata/1 FTMS USER Thu Nov 13 15:51:24 2014

5-(4-methoxyphenyl)-2-phenyl-2H-tetrazole



5-(4-methoxyphenyl)-2-phenyl-2H-tetrazole





U:\IR\Tetrazole 2.0	Tetrazole 2	yellow solid	22.05.2015

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Mass Spectrometry Service
Department of Chemistry

BRUKER FTMS 4.7T BioAPEX II

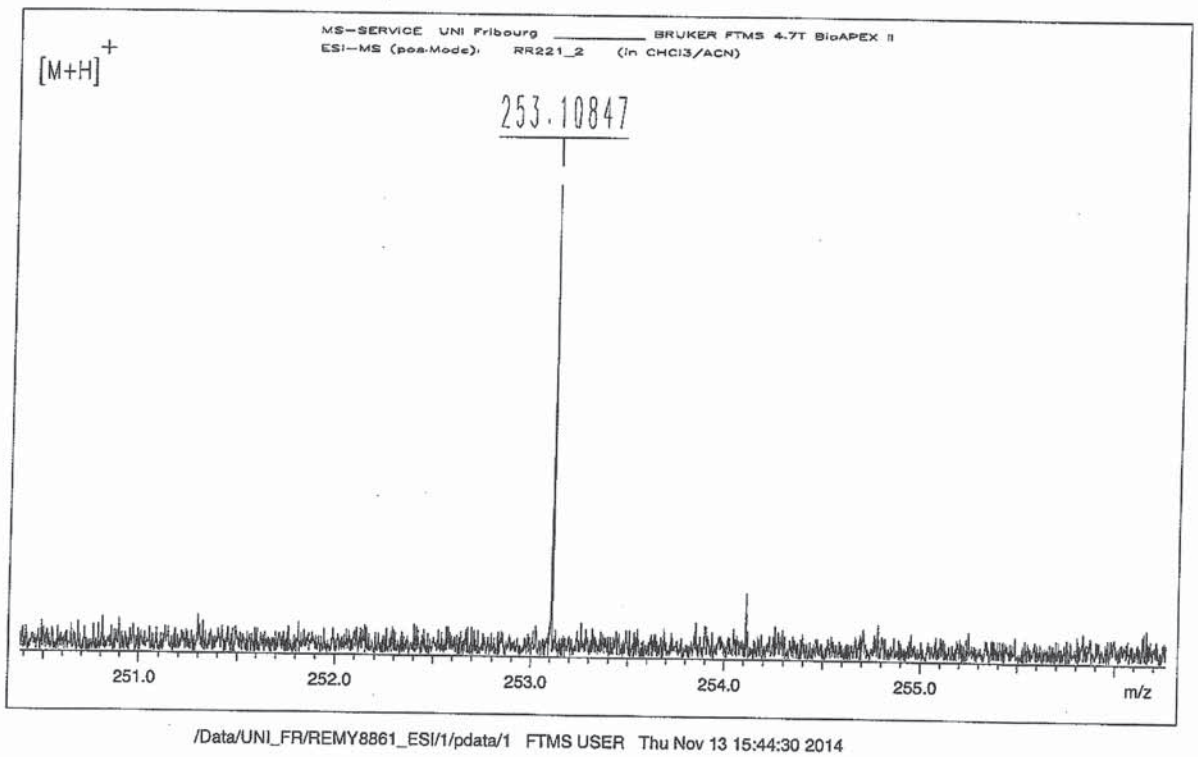
ESI-MS: RR221_2

XMASS Mass Analysis for /Data/UNI_FR/REMY8861_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

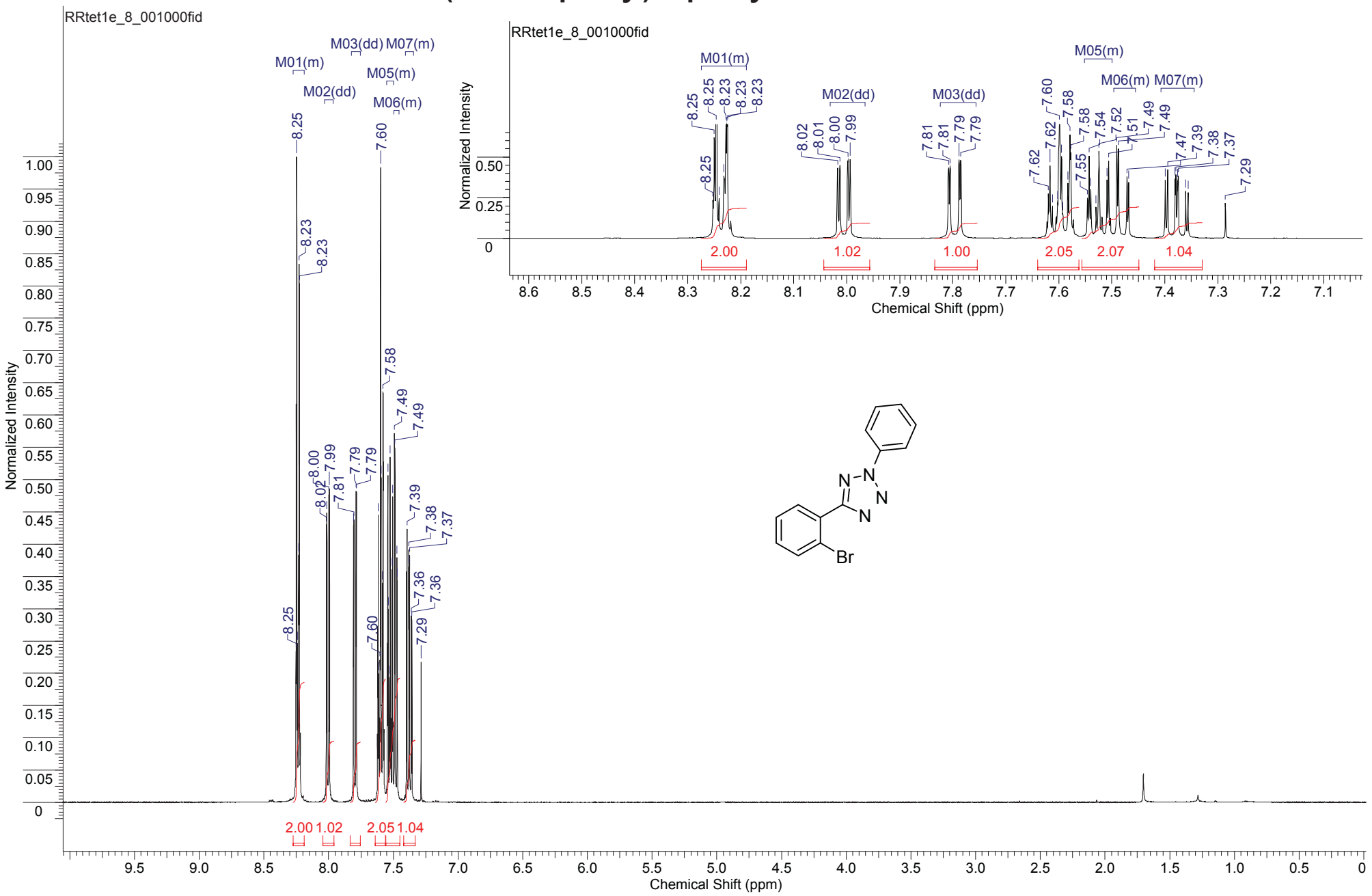
Ion mass = 253.1084680

Charge = +1

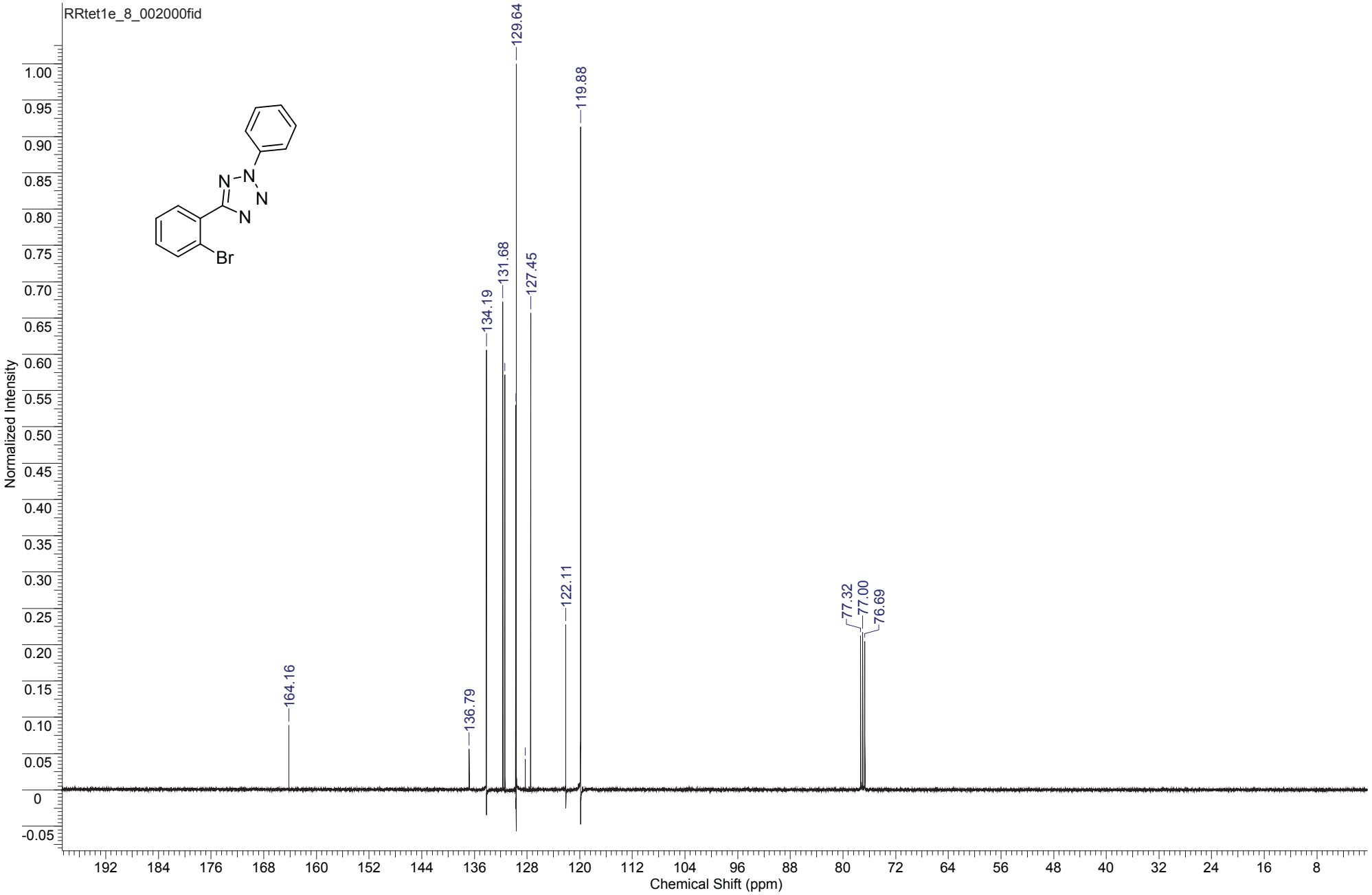
#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 253.1084680							
1	14	13	4	1	253.1083875	10.5	8.052e-05
2	16	15	1	2	253.1097302	10.0	1.262e-03
3	11	15	3	4	253.1057074	6.0	2.761e-03
4	9	13	6	3	253.1043647	6.5	4.103e-03
5	5	15	7	5	253.1129180	2.0	4.450e-03
6	8	17	2	7	253.1030273	1.5	5.441e-03
7	7	11	9	2	253.1030221	7.0	5.446e-03
8	7	17	4	6	253.1142607	1.5	5.793e-03
9	6	15	5	6	253.1016847	2.0	6.783e-03
10	8	13	8	2	253.1155981	6.5	7.130e-03

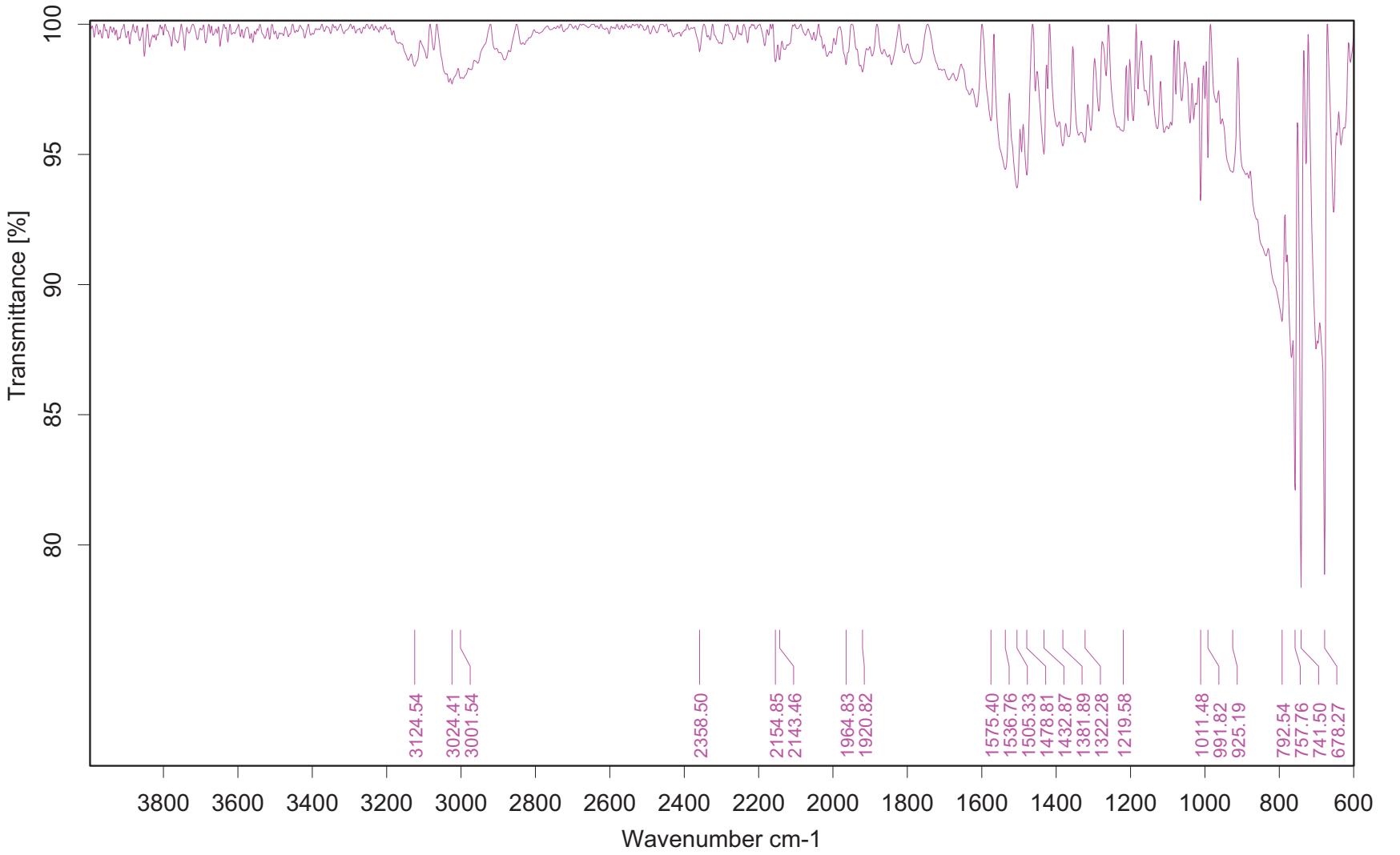


5-(2-bromophenyl)-2-phenyl-2H-tetrazole



5-(2-bromophenyl)-2-phenyl-2H-tetrazole





C:\Users\remyr\Desktop\IR 7 decembre	RRtet1e.2	Date: 22.08.2017, 14:05:55

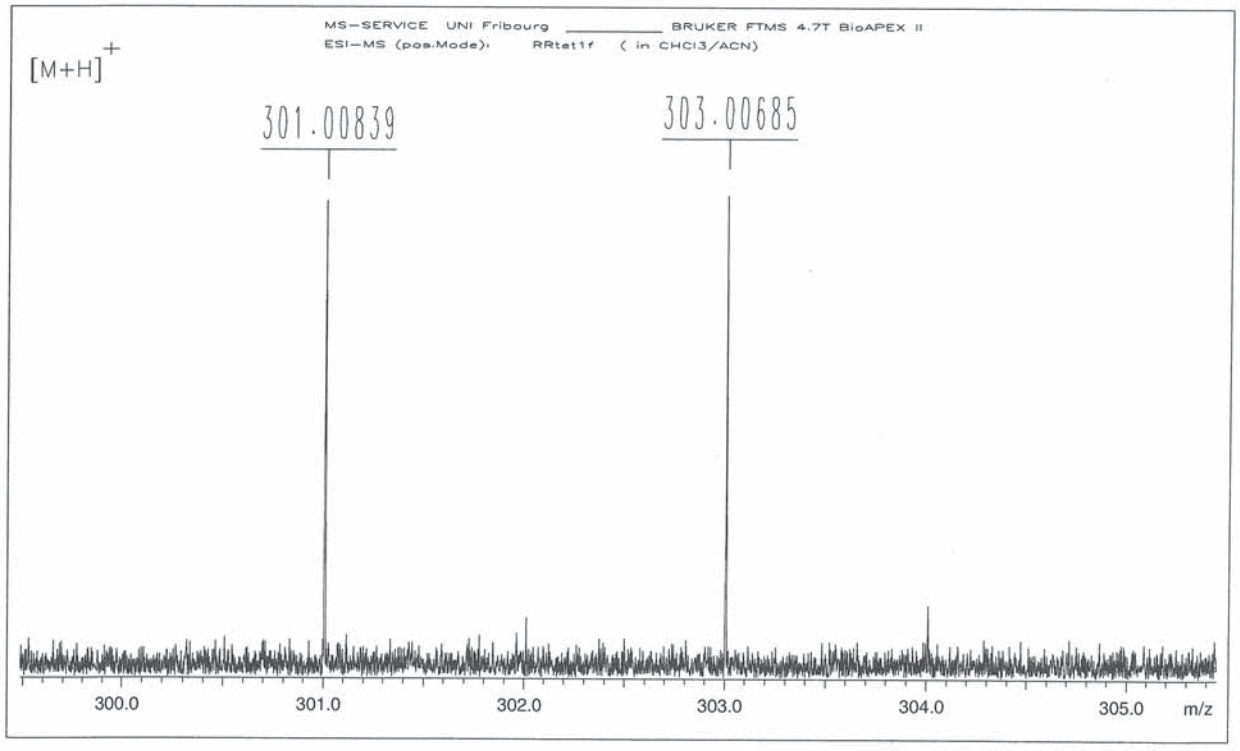
ESI-MS: RRtet1f

XMASS Mass Analysis for /Data/UNI_FR/REMY2026_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

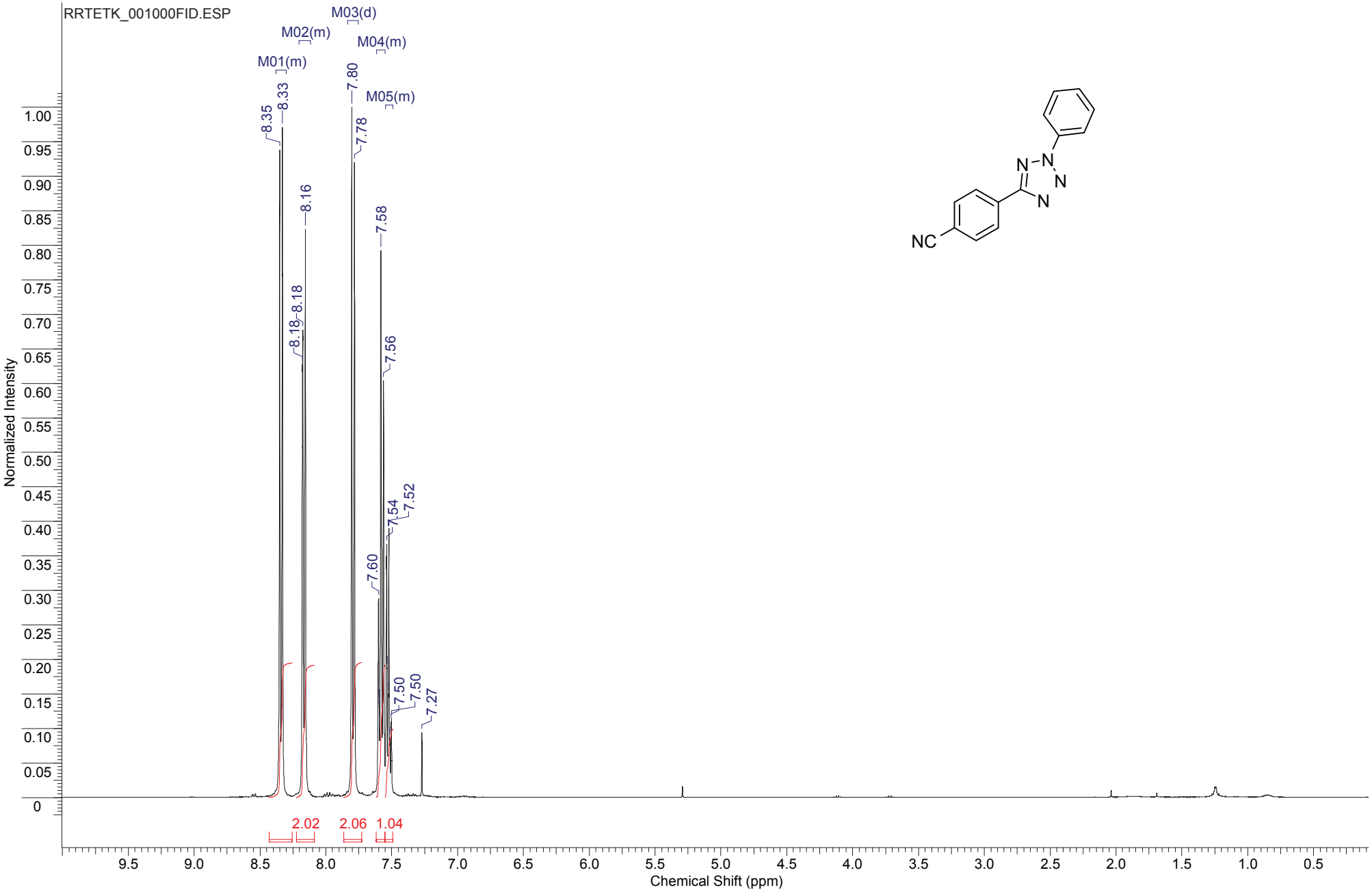
Ion mass [1] = 301.0083930
Ion mass [2] = 303.0068520

Charge = +1

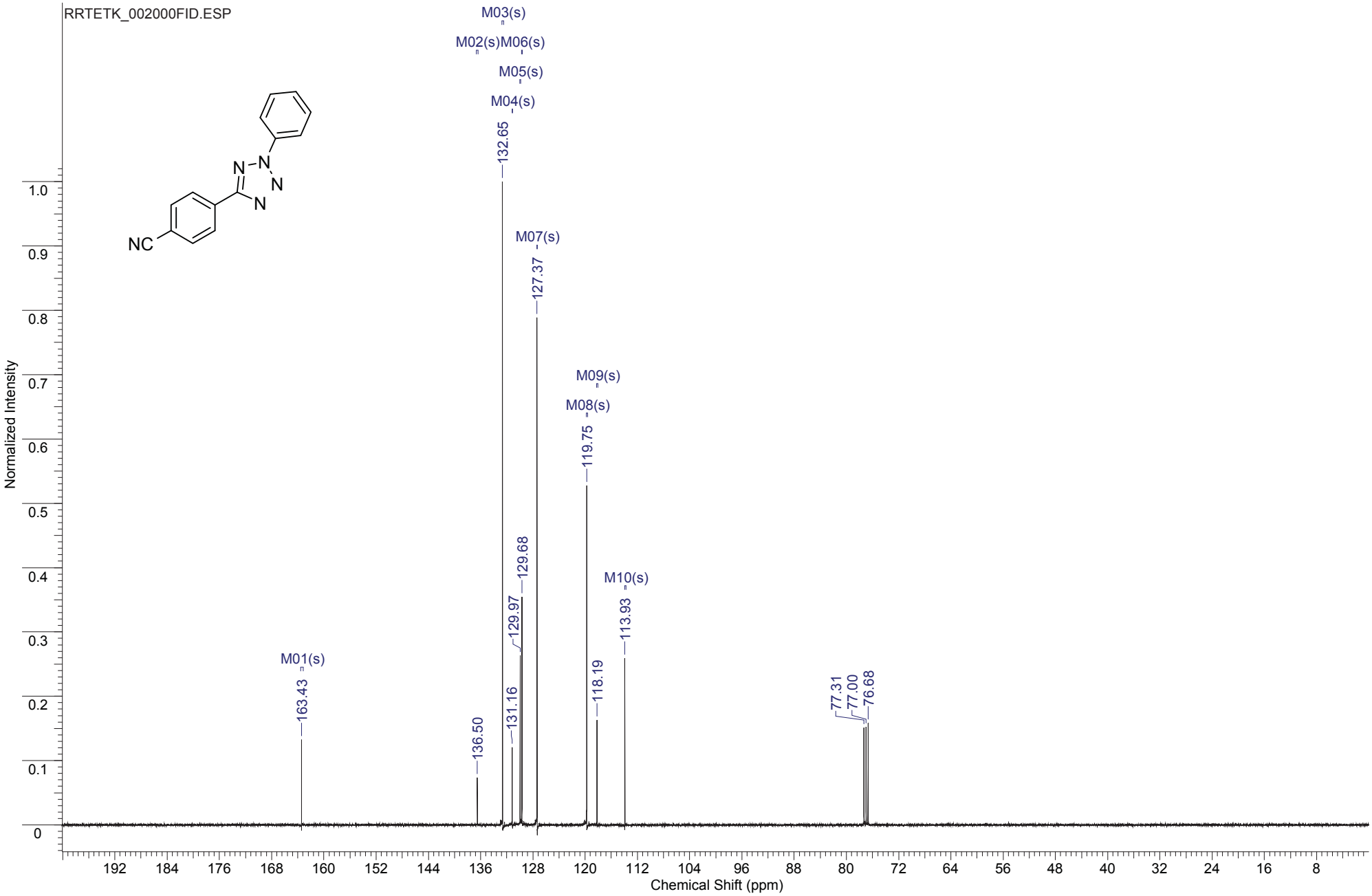
#	C	H	79Br	81Br	N	mass	DBE	error
*** Mass Analysis for mass [1] 301.0083930								
1	**13**	**10**	**1**	**0**	**4**	**301.0083354**	10.5	5.764e-05
2	6	8	0	1	10	301.0090827	7.5	6.897e-04
3	14	10	0	1	3	301.0032148	11.0	5.178e-03
4	15	12	0	1	2	301.0157908	10.5	7.398e-03
5	14	12	1	0	3	301.0209114	10.0	1.252e-02
*** Mass Analysis for mass [2] 303.0068520								
1	**13**	**10**	**0**	**1**	**4**	**303.0062888**	10.5	5.632e-04
2	12	10	1	0	5	303.0114094	10.0	4.557e-03
3	9	21	1	1	1	303.0014797	-1.0	5.372e-03
4	11	8	1	0	6	302.9988333	10.5	8.019e-03
5	14	12	0	1	3	303.0188648	10.0	1.201e-02

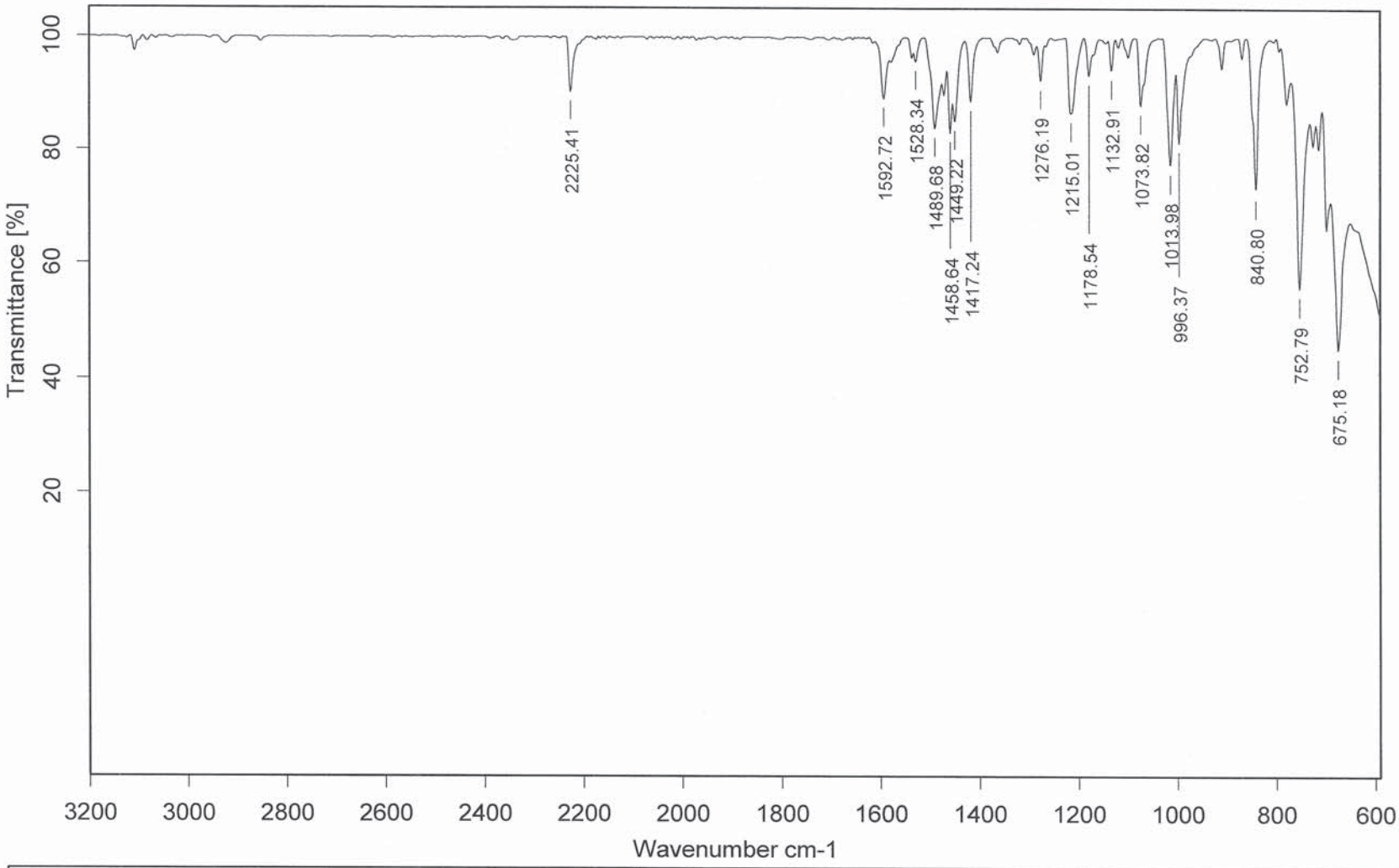


4-(2-phenyl-2H-tetrazol-5-yl)benzonitrile



4-(2-phenyl-2H-tetrazol-5-yl)benzonitrile





C:\Users\remyr\Documents\Bruker\OPUS_7.5.18	tetraz1k.0	Date: 07.12.2016, 14:40:03

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BRUKER FTMS 4.7T BioAPEX II

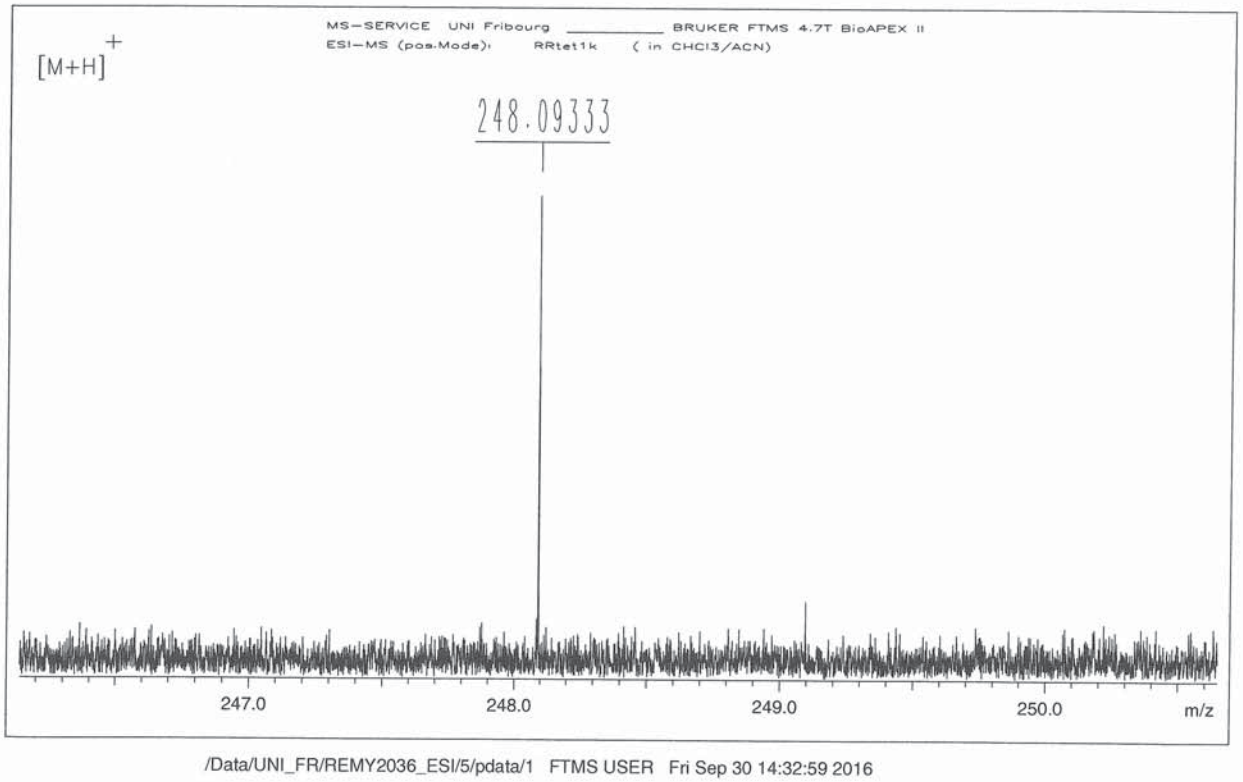
ESI-MS: RRtet1k

XMASS Mass Analysis for /Data/UNI_FR/REMY2036_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

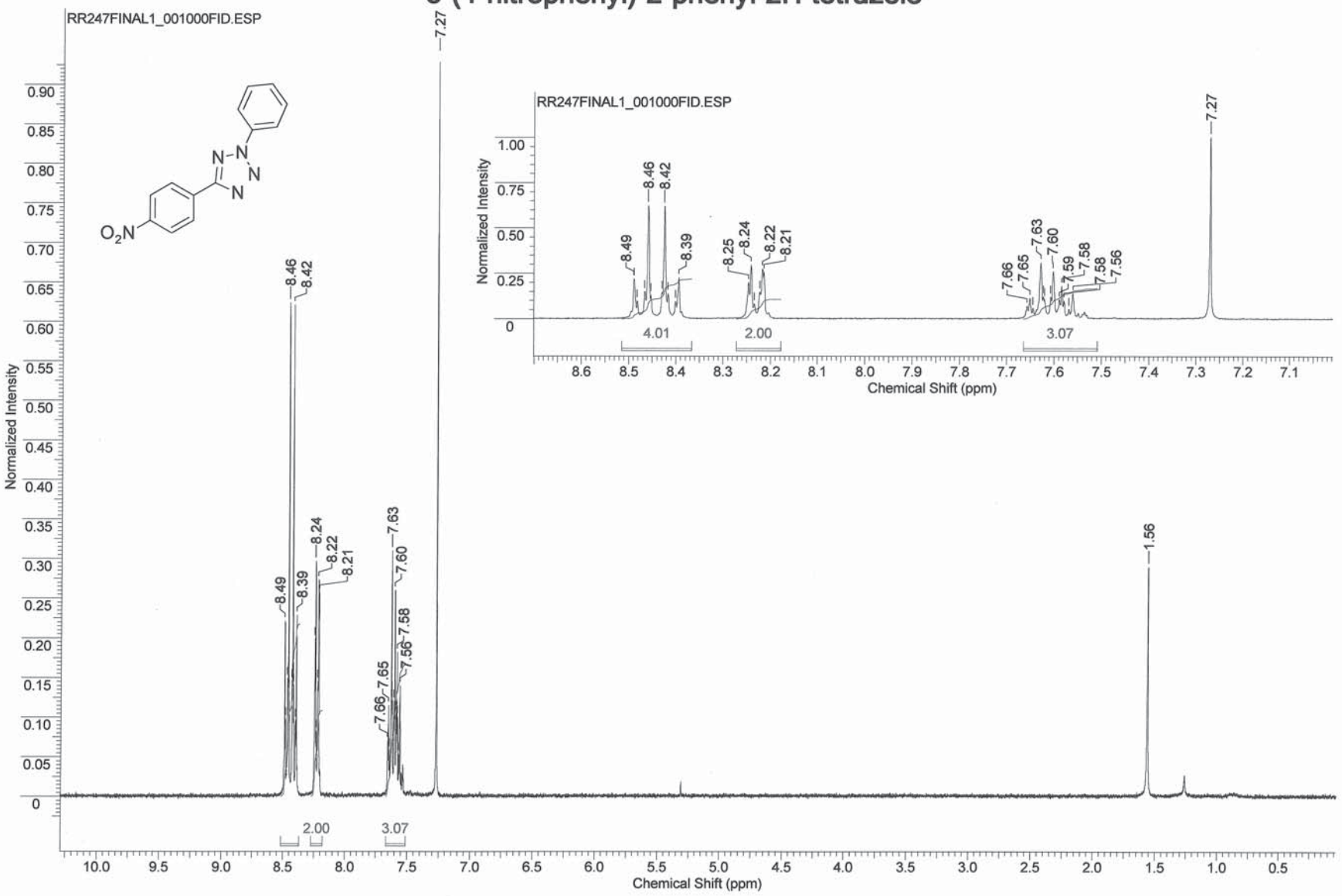
Ion mass = 248.0933300

Charge = +1

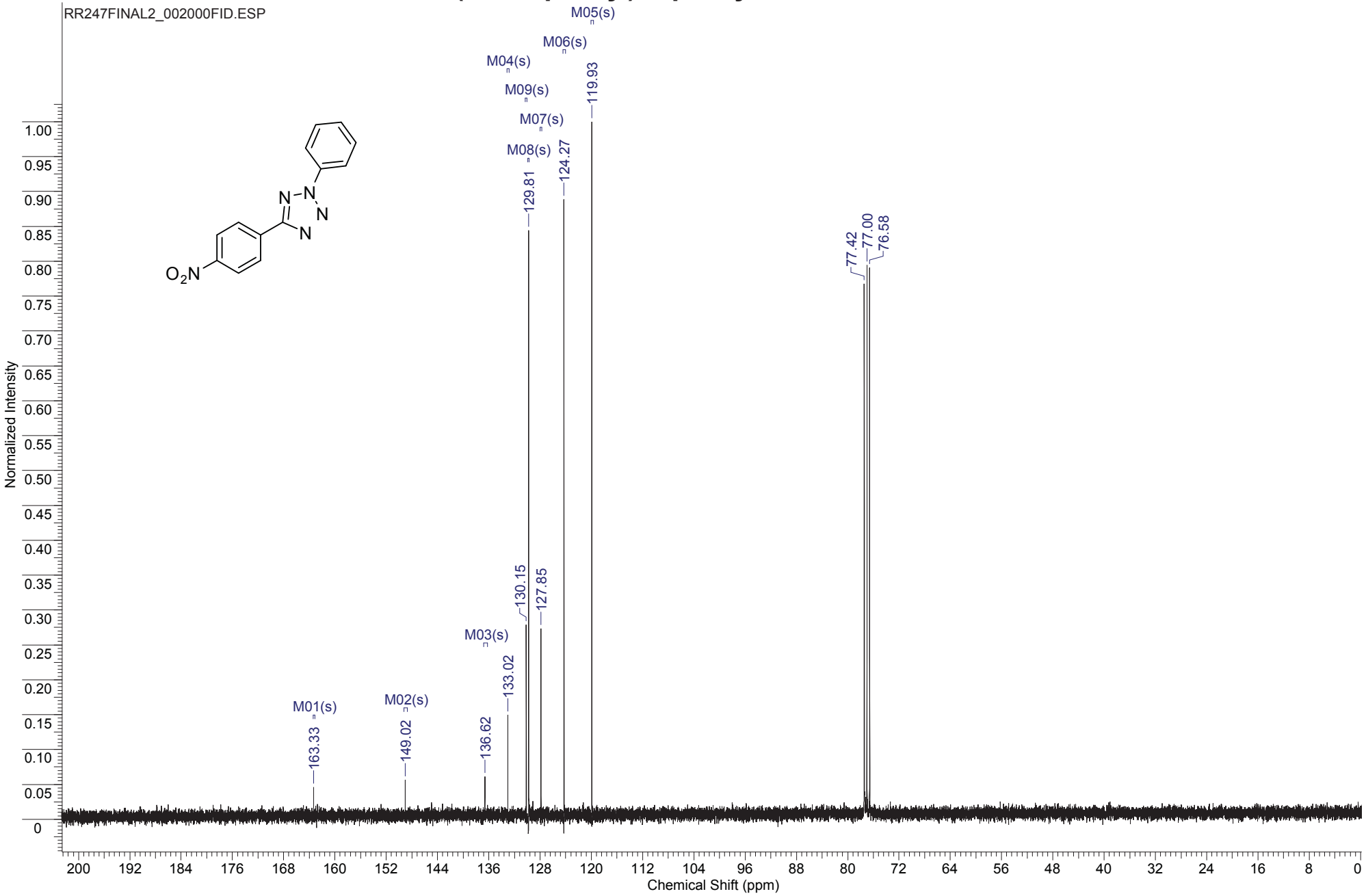
#	C	H	N	mass	DBE	error
*** Mass Analysis for mass 248.0933300						
1	**14**	**10**	**5**	**248.0930718**	12.5	2.582e-04
2	15	12	4	248.1056478	12.0	1.232e-02
3	13	8	6	248.0804957	13.0	1.283e-02
4	16	14	3	248.1182239	11.5	2.489e-02
5	12	6	7	248.0679196	13.5	2.541e-02
6	8	12	10	248.1240919	8.0	3.076e-02
7	17	16	2	248.1307999	11.0	3.747e-02
8	11	4	8	248.0553436	14.0	3.799e-02
9	9	14	9	248.1366679	7.5	4.334e-02
10	19	6	1	248.0494756	17.5	4.385e-02

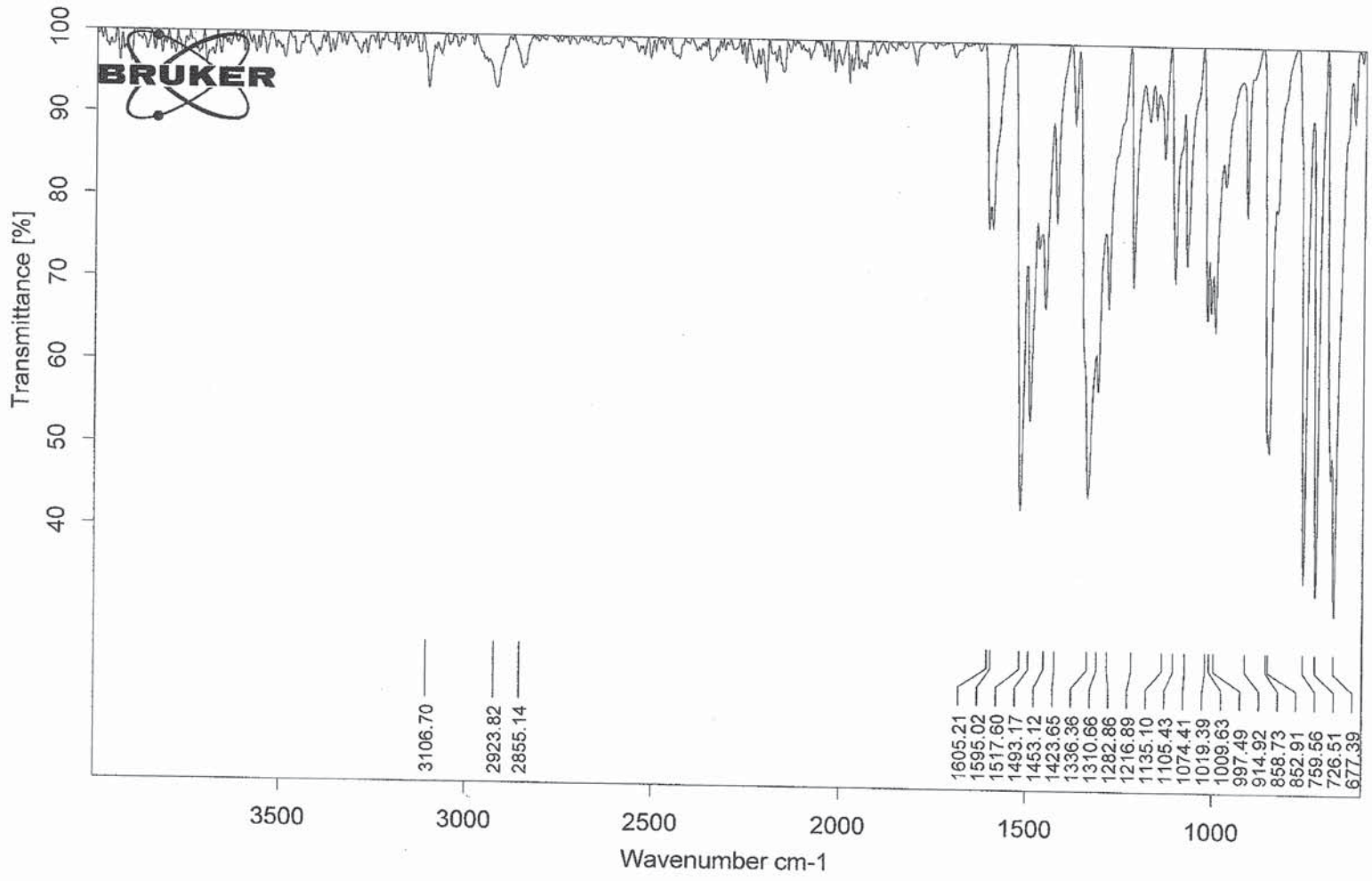


5-(4-nitrophenyl)-2-phenyl-2H-tetrazole



5-(4-nitrophenyl)-2-phenyl-2H-tetrazole





U:\IR\Tetrazole 3.0	Tetrazole 3	red solid	22.05.2015

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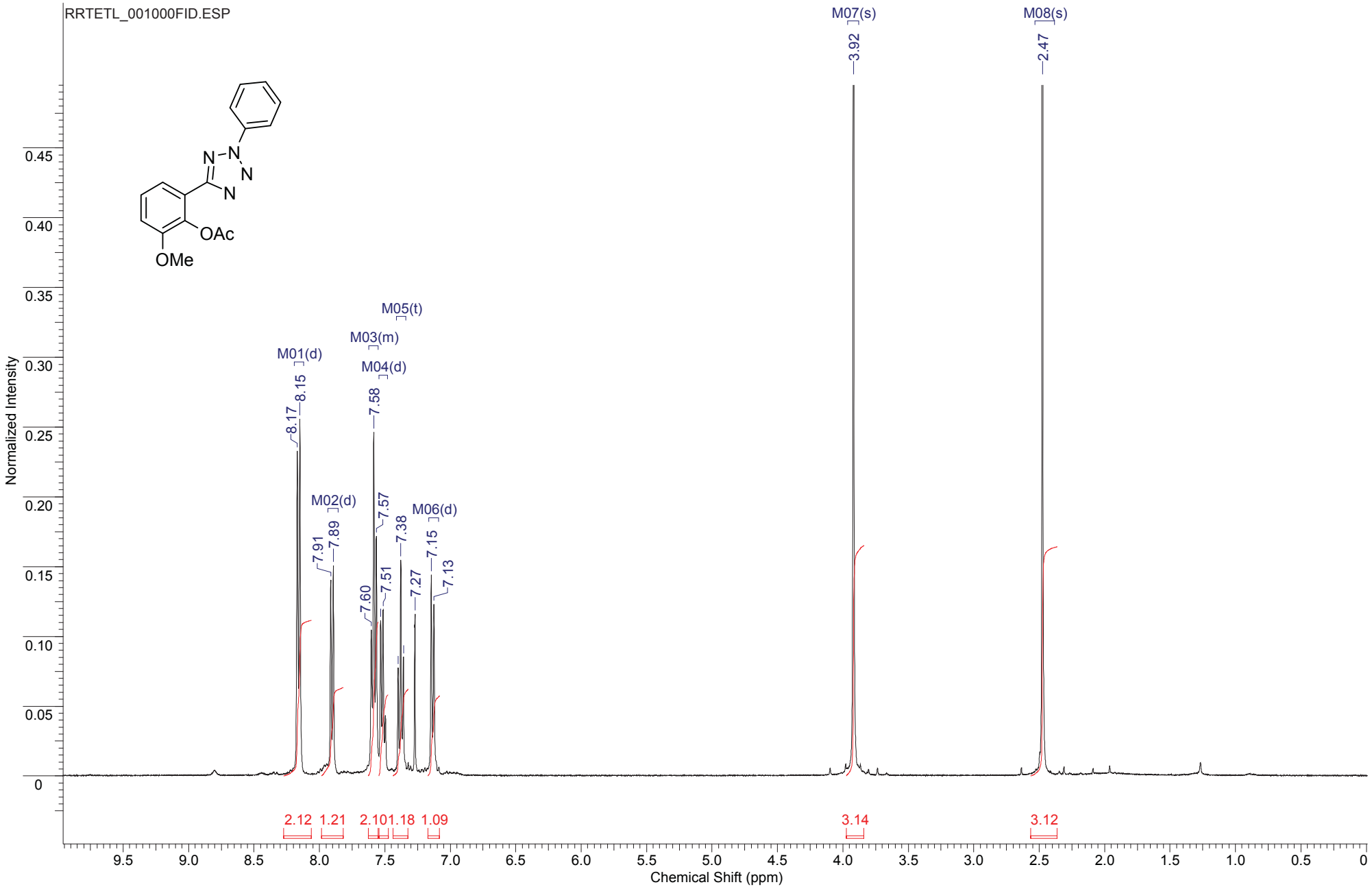
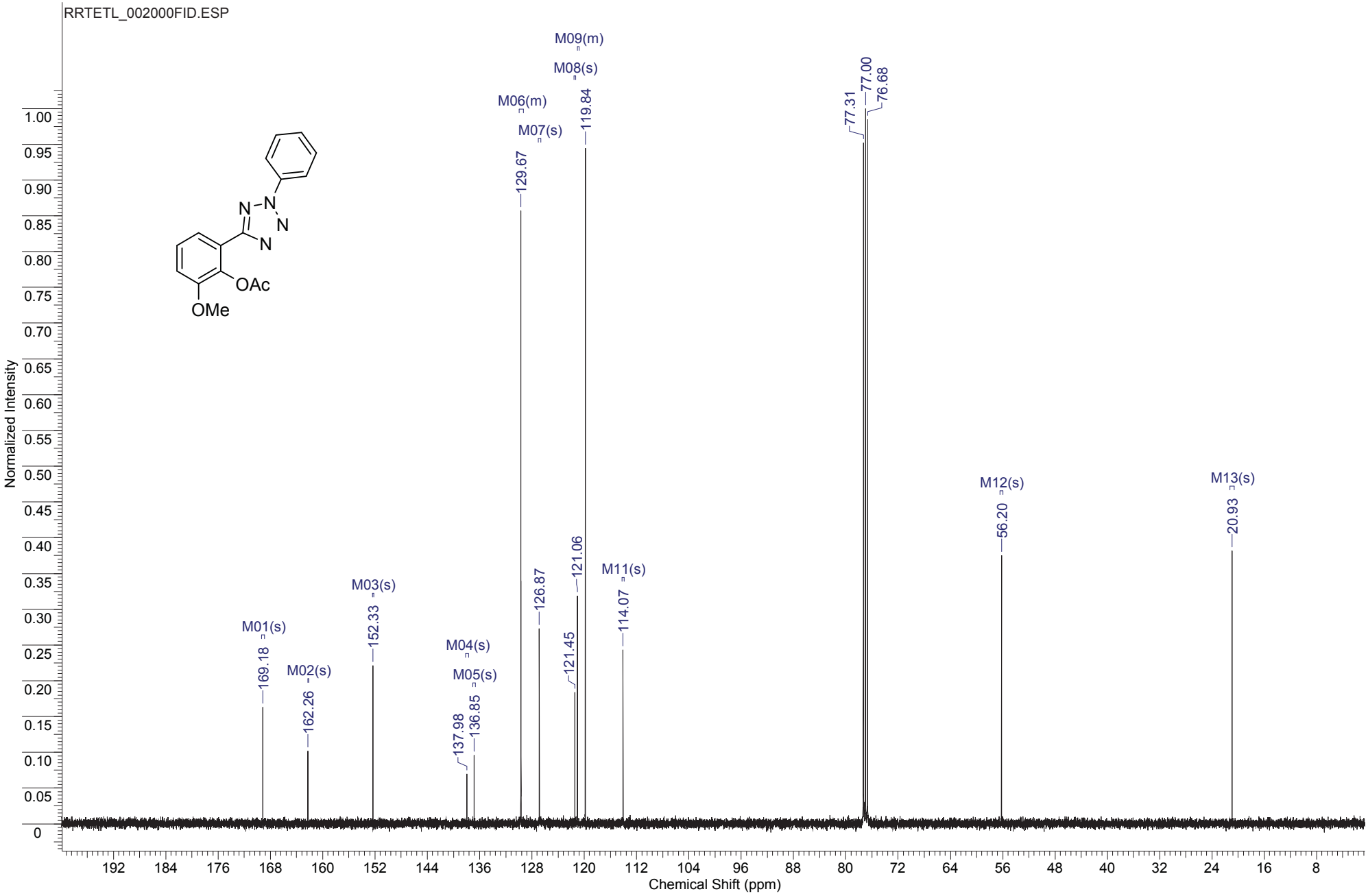
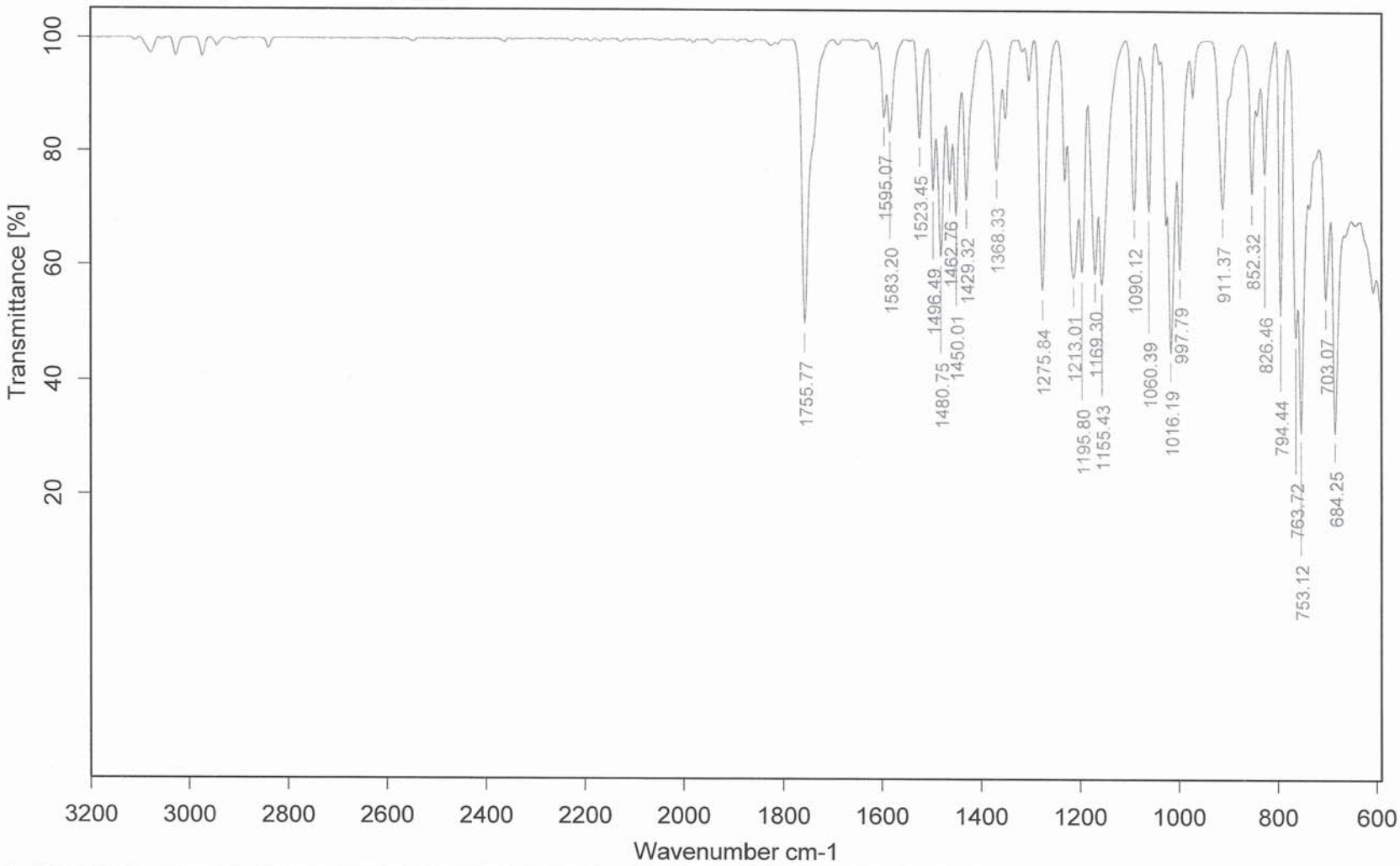
2-methoxy-6-(2-phenyl-2H-tetrazol-5-yl)phenyl acetate



2-methoxy-6-(2-phenyl-2H-tetrazol-5-yl)phenyl acetate





C:\Users\remyr\Documents\Bruker\OPUS_7.5.18	tetraz1l.0	Date: 07.12.2016, 14:45:37

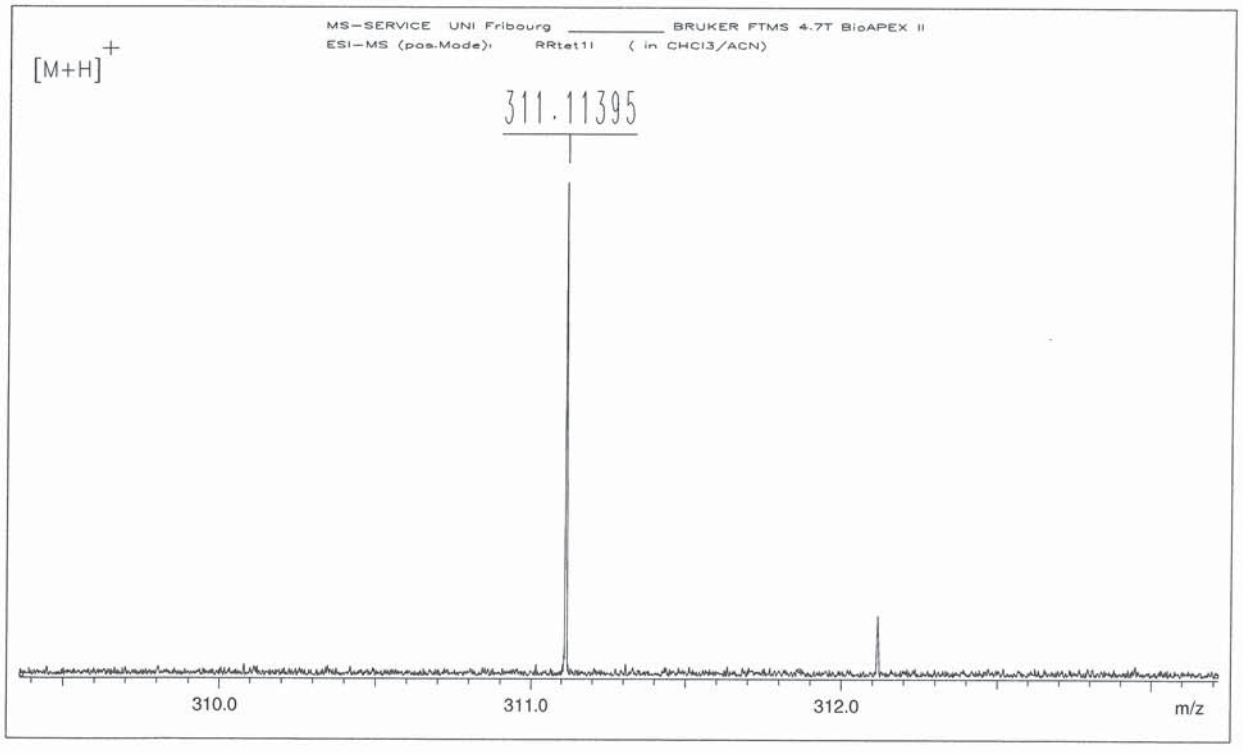
ESI-MS: RRtet1I

XMASS Mass Analysis for /Data/UNI_FR/REMY2037_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 311.1139510

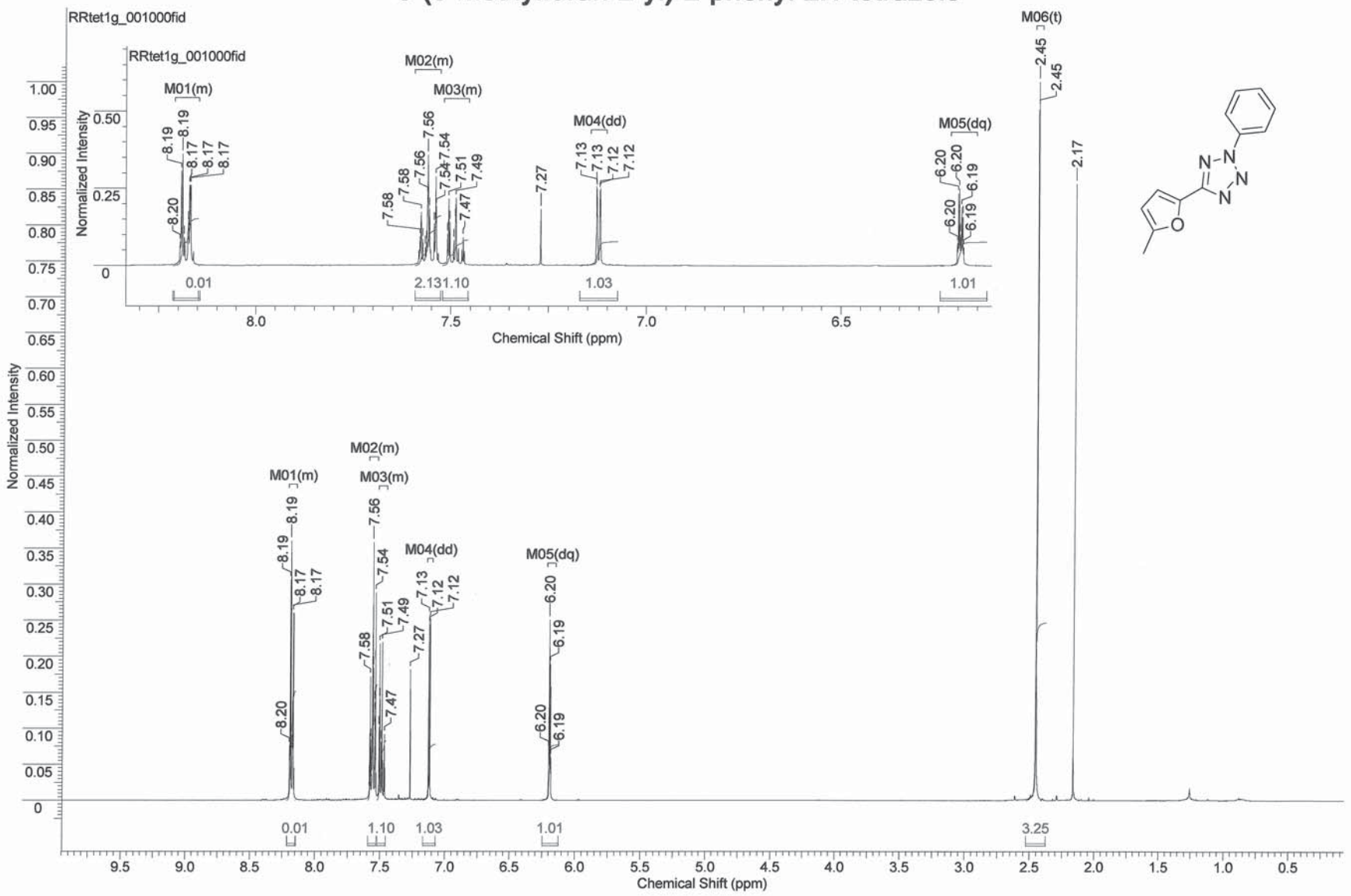
Charge = +1

#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 311.1139510							
1	**16**	**15**	**4**	**3**	**311.1138668**	11.5	8.421e-05
2	2	17	9	9	311.1143746	-1.0	4.236e-04
3	18	17	1	4	311.1152095	11.0	1.258e-03
4	14	13	7	2	311.1125241	12.0	1.427e-03
5	4	19	6	10	311.1157173	-1.5	1.766e-03
6	13	17	3	6	311.1111867	7.0	2.764e-03
7	12	11	10	1	311.1111814	12.5	2.770e-03
8	5	15	10	6	311.1170547	3.5	3.104e-03
9	21	15	2	1	311.1178895	15.5	3.939e-03
10	11	15	6	5	311.1098440	7.5	4.107e-03

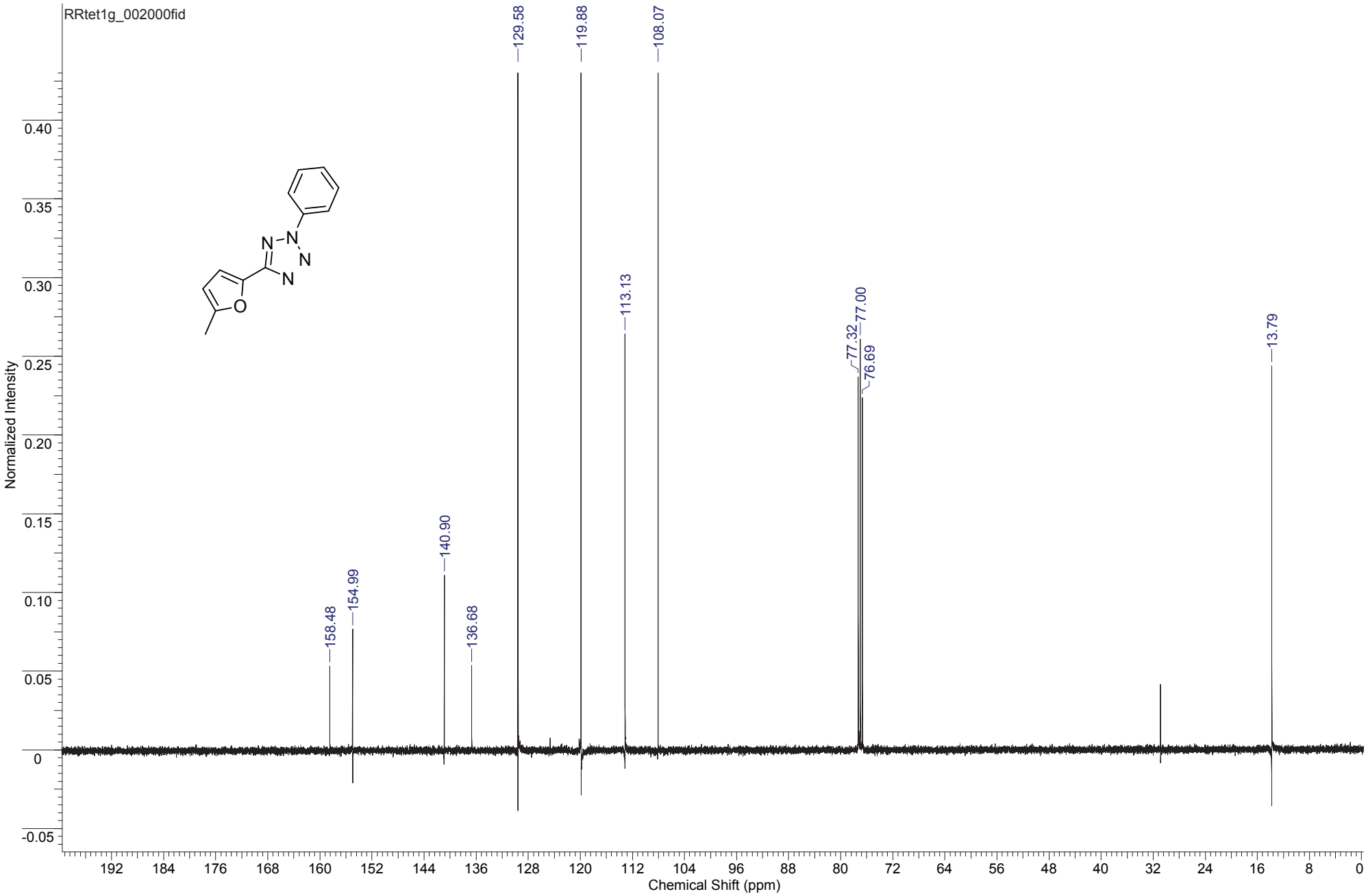


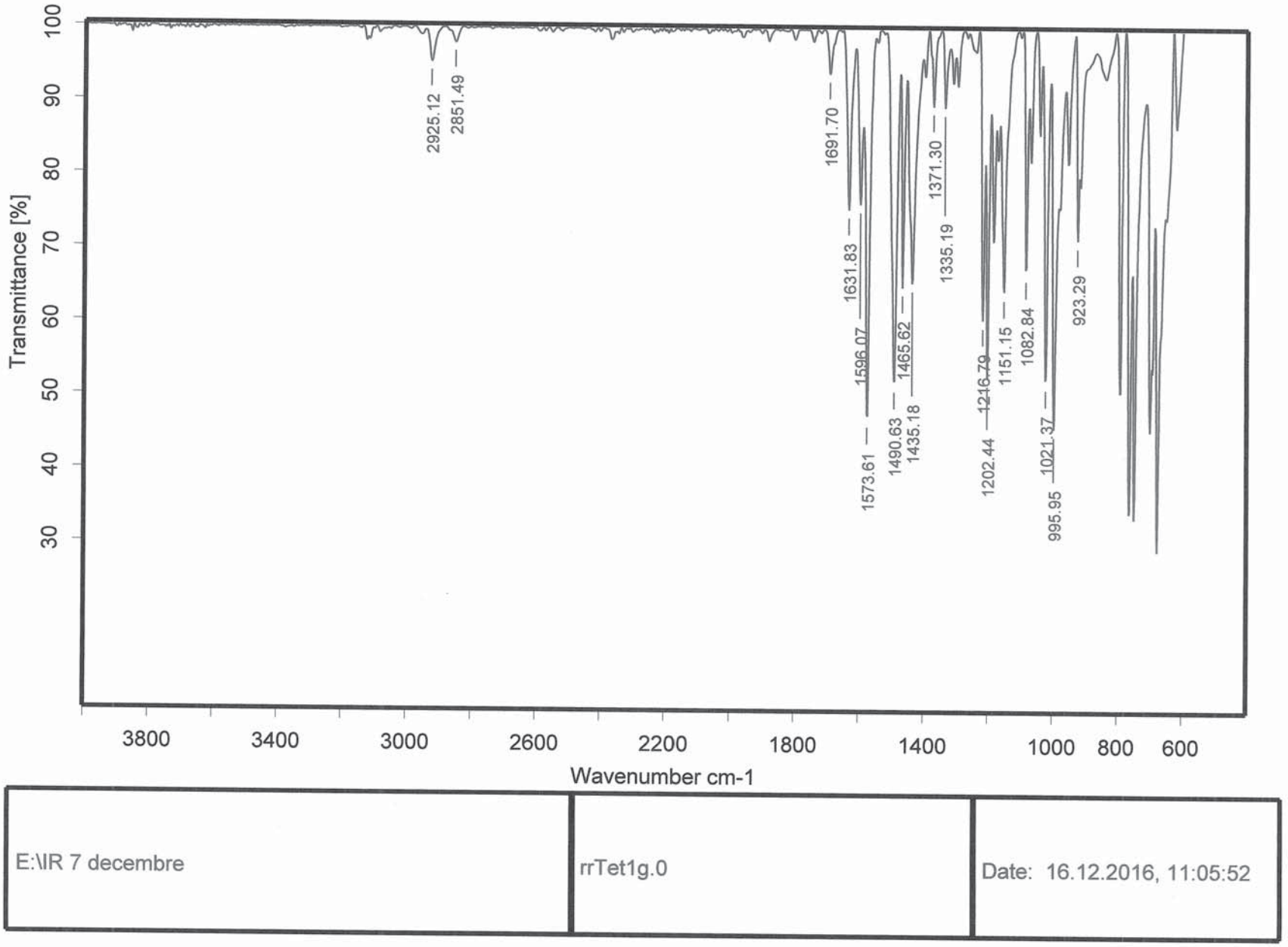
/Data/UNI_FR/REMY2037_ESI/5/pdata/1 FTMS USER Fri Sep 30 14:36:59 2016

5-(5-methylfuran-2-yl)-2-phenyl-2H-tetrazole



5-(5-methylfuran-2-yl)-2-phenyl-2H-tetrazole

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Mass Spectrometry Service
Department of Chemistry

BRUKER FTMS 4.7T BioAPEX II

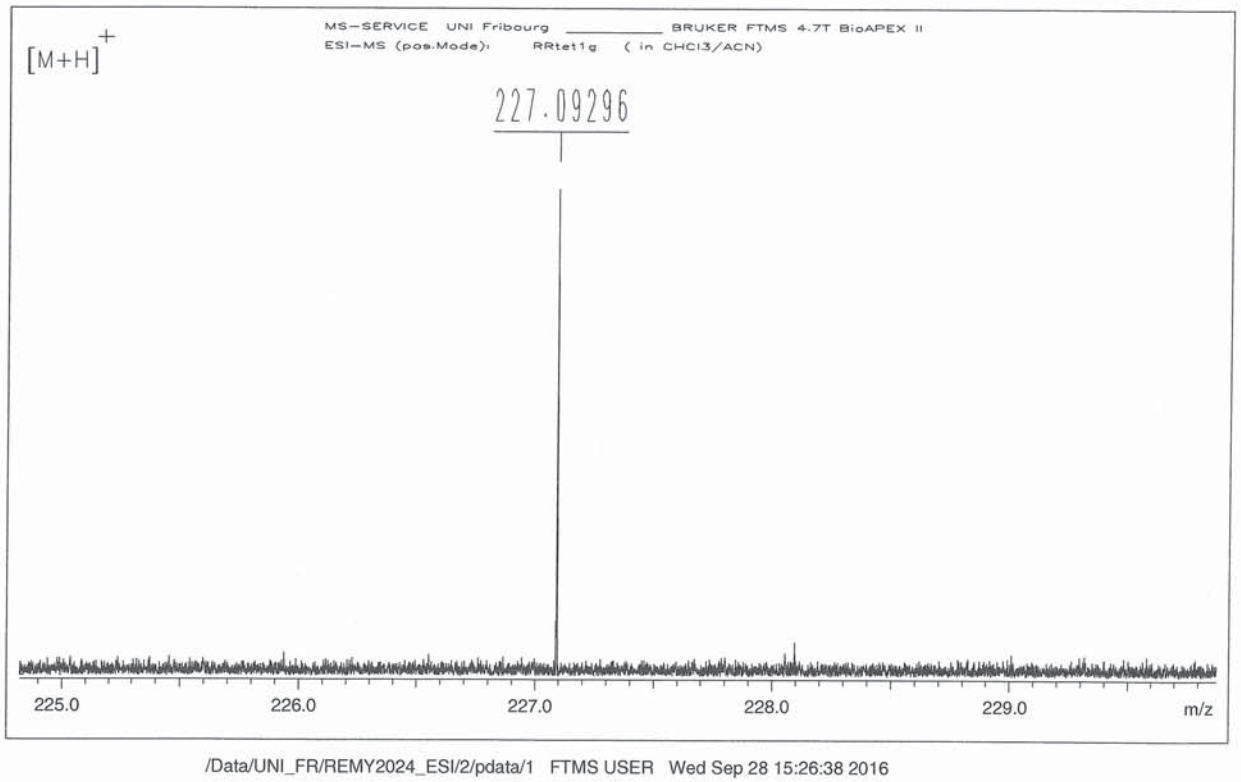
ESI-MS: RRtet1g

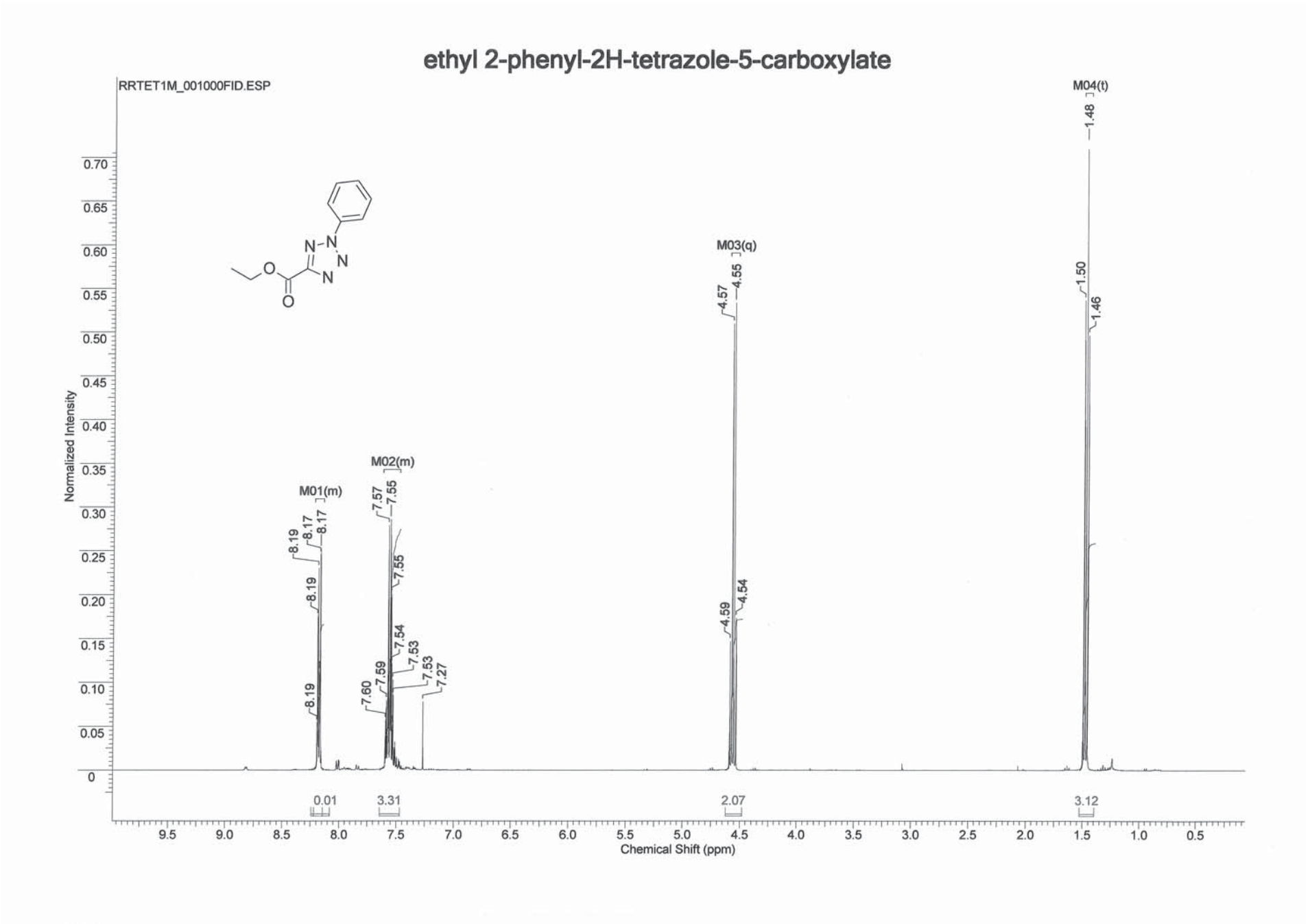
XMASS Mass Analysis for /Data/UNI_FR/REMY2024_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 227.0929560

Charge = +1

#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 227.0929560							
1	**12**	**11**	**4**	**1**	**227.0927374**	9.5	2.186e-04
2	14	13	1	2	227.0940801	9.0	1.124e-03
3	9	13	3	4	227.0900573	5.0	2.899e-03
4	7	11	6	3	227.0887147	5.5	4.241e-03
5	6	15	2	7	227.0873773	0.5	5.579e-03
6	5	9	9	2	227.0873720	6.0	5.584e-03
7	5	15	4	6	227.0986107	0.5	5.655e-03
8	6	11	8	2	227.0999481	5.5	6.992e-03
9	7	17	1	7	227.0999533	0.0	6.997e-03
10	8	13	5	3	227.1012907	5.0	8.335e-03




ethyl 2-phenyl-2H-tetrazole-5-carboxylate
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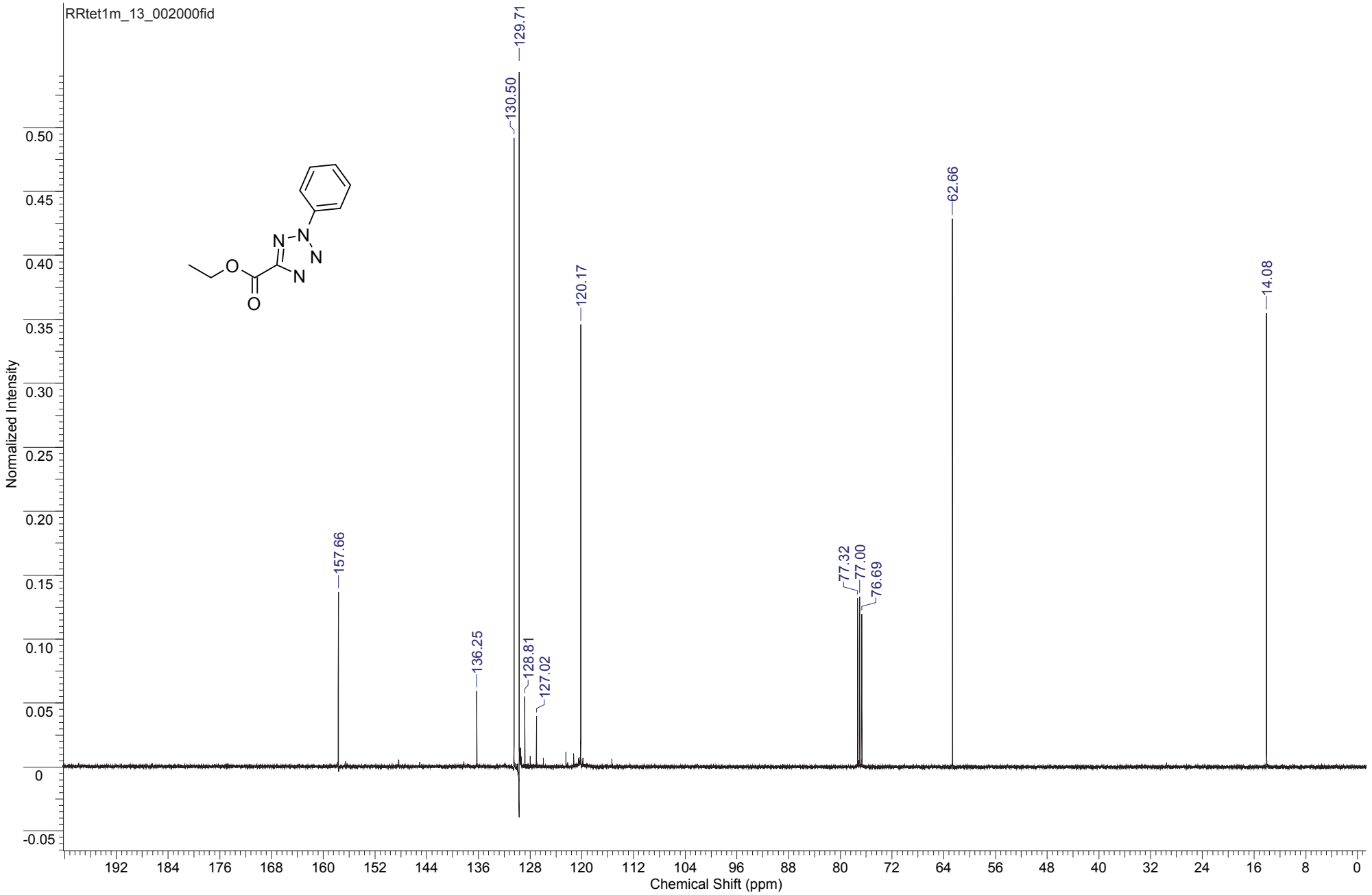
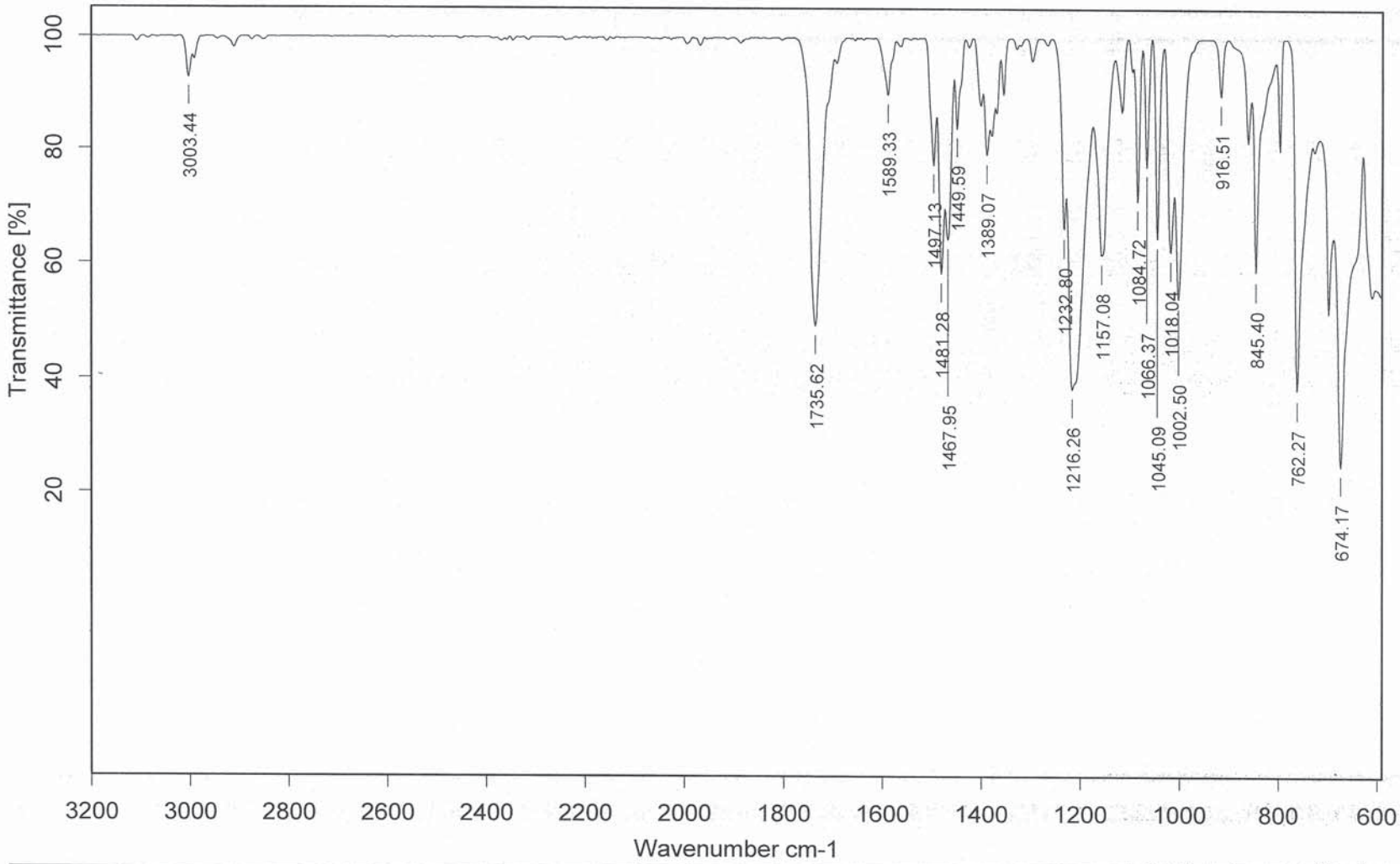
M03(q)
M02(m)
M01(m)
Normalized Intensity
Chemical Shift (ppm)
0.01
3.31
2.07
3.12

ethyl 2-phenyl-2H-tetrazole-5-carboxylate





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BRUKER **FTMS 4.7T BioAPEX II**

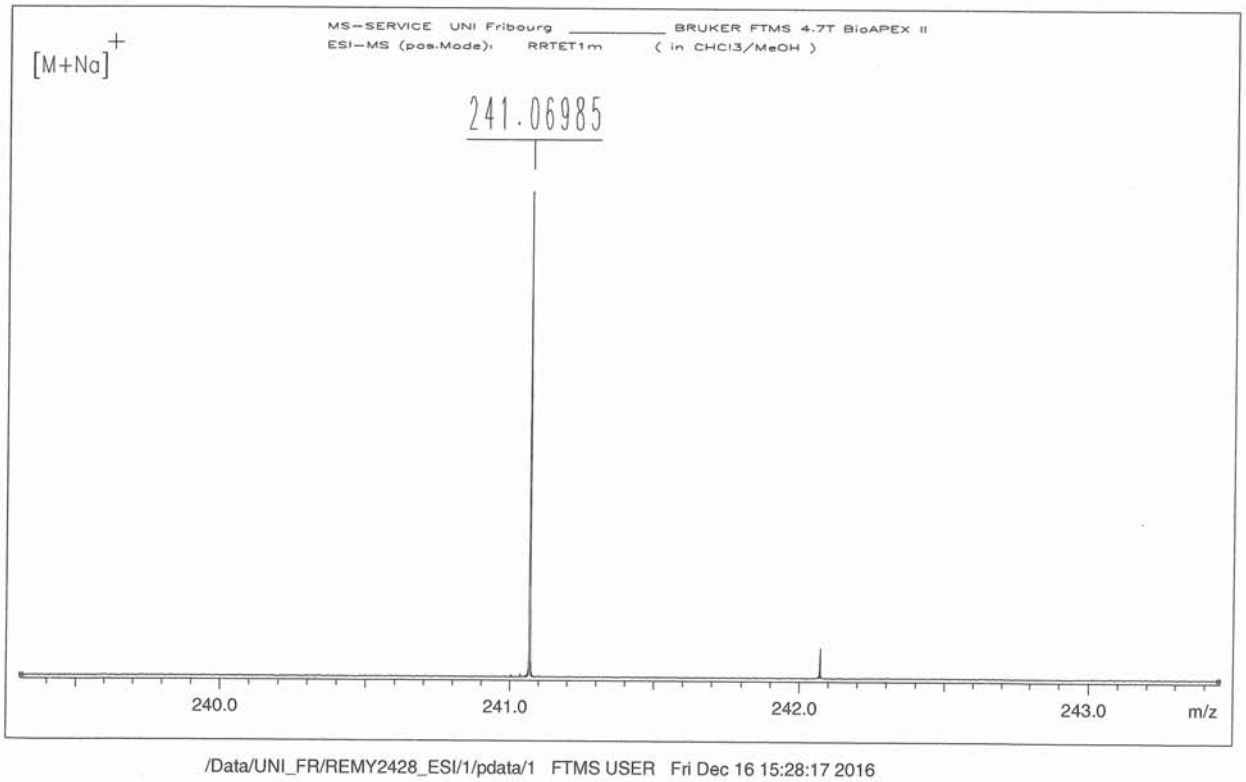
ESI-MS: RRTET1m

XMASS Mass Analysis for /Data/UNI_FR/REMY2428_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

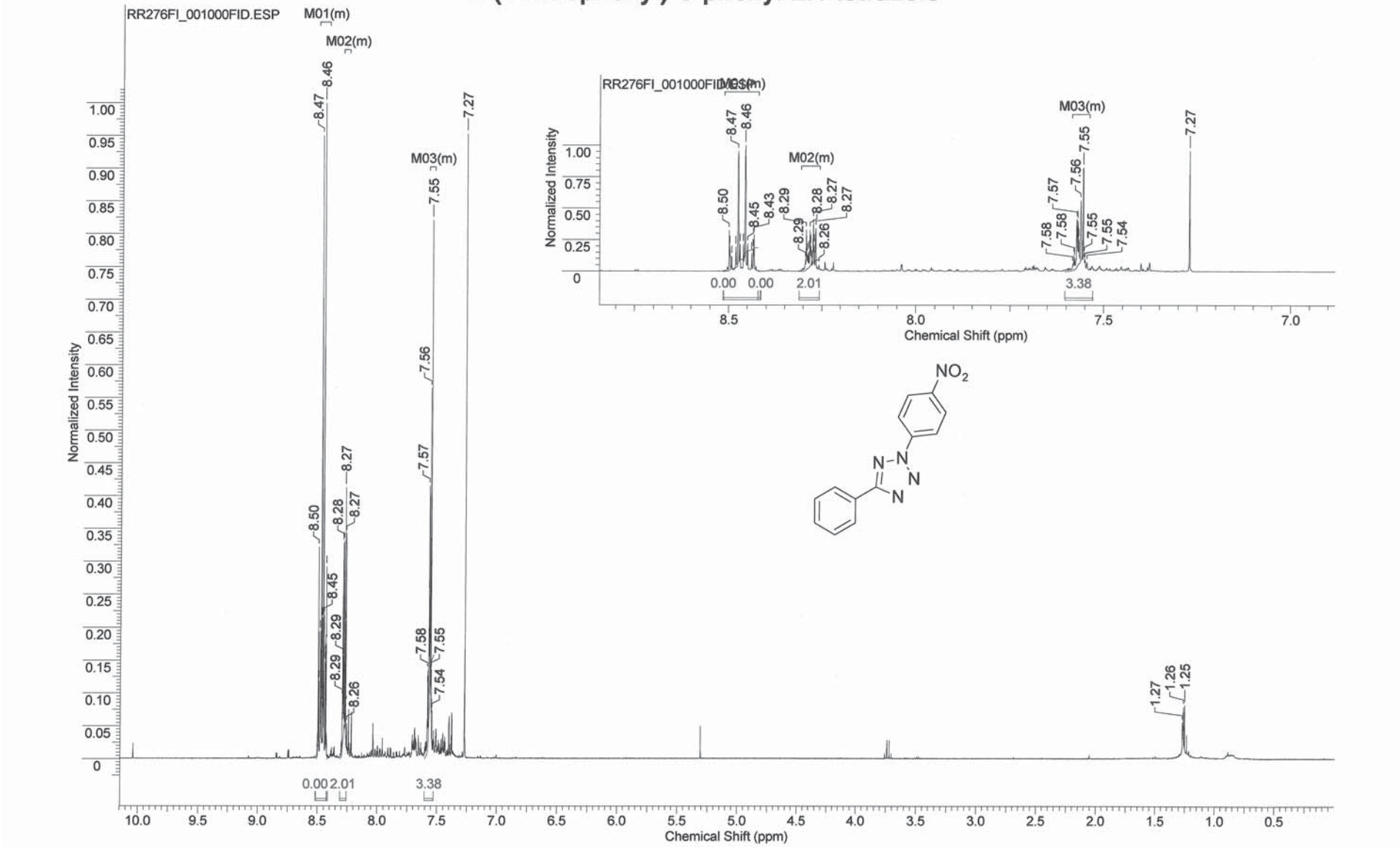
Ion mass = 241.0698460

Charge = +1

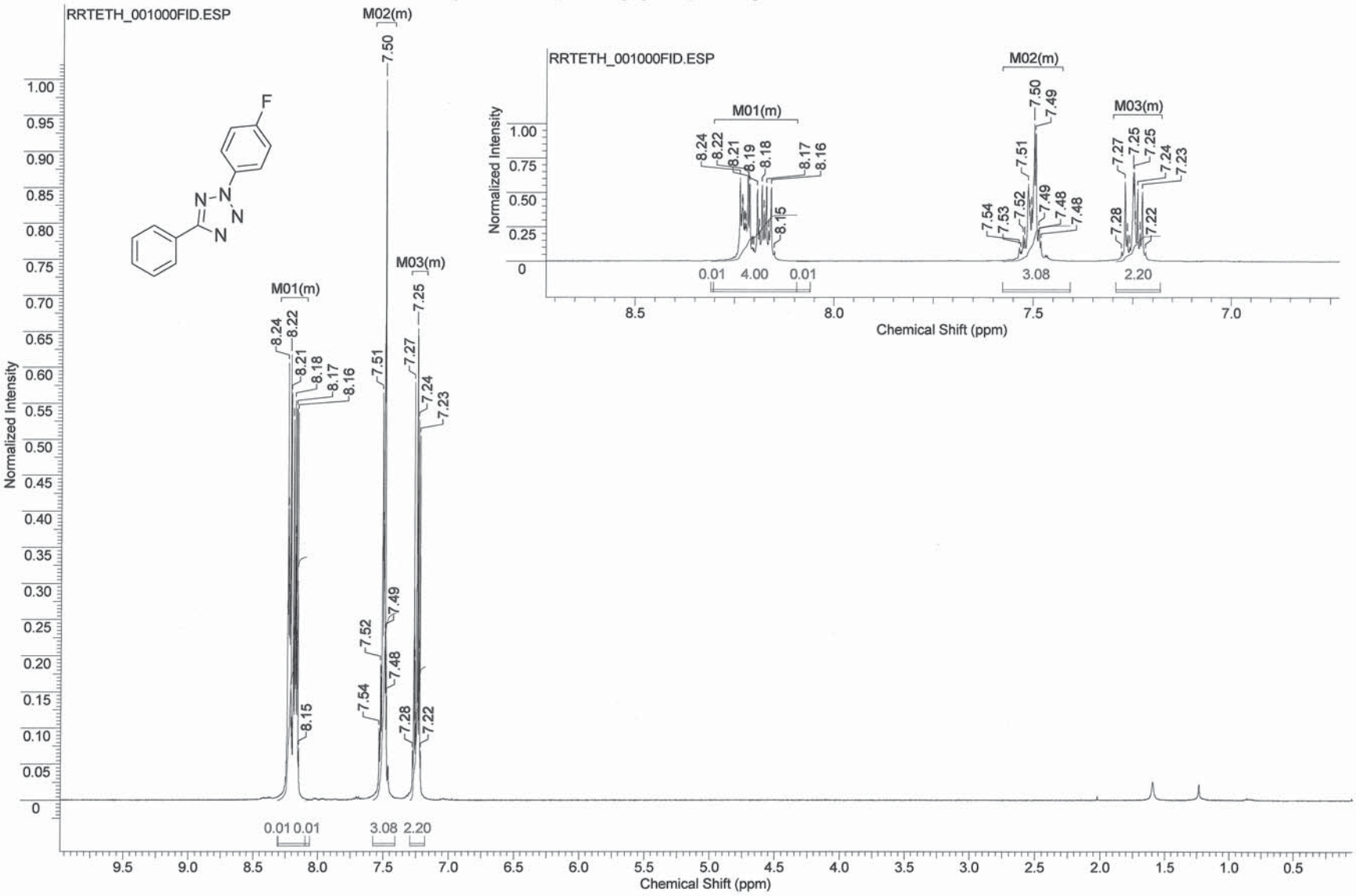
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 241.0698460								
1	**10**	**10**	**4**	**2**	**1**	**241.0695967**	7.5	2.493e-04
2	9	11	3	5	0	241.0693219	6.0	5.241e-04
3	10	7	7	1	0	241.0706593	11.0	8.133e-04
4	12	12	1	3	1	241.0709393	7.0	1.093e-03
5	8	8	7	1	1	241.0682540	8.0	1.592e-03
6	7	9	6	4	0	241.0679792	6.5	1.867e-03
7	12	9	4	2	0	241.0720020	10.5	2.156e-03
8	7	12	3	5	1	241.0669166	3.0	2.929e-03
9	6	13	2	8	0	241.0666418	1.5	3.204e-03
10	5	7	9	3	0	241.0666366	7.0	3.209e-03



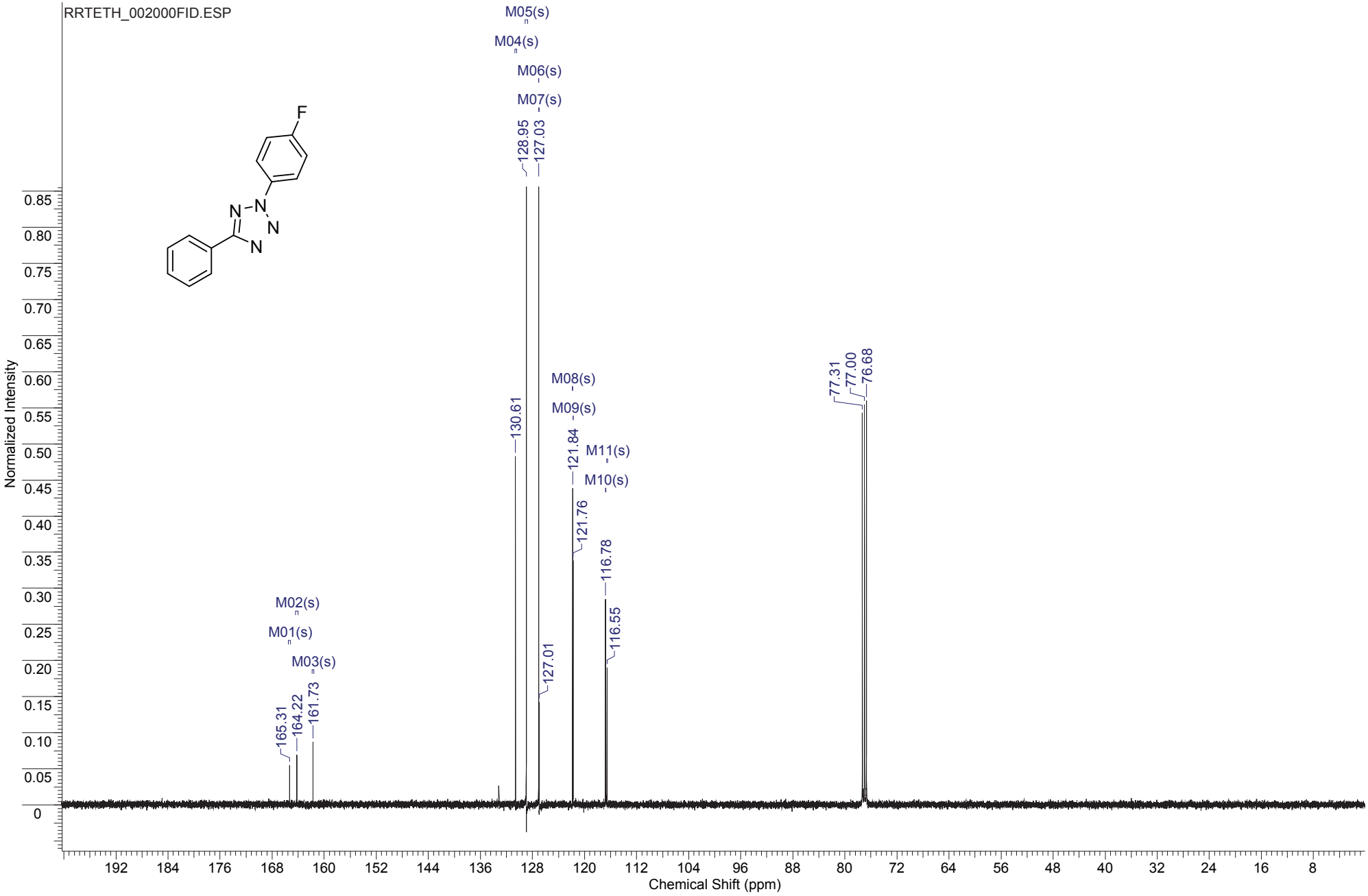
2-(4-nitrophenyl)-5-phenyl-2H-tetrazole

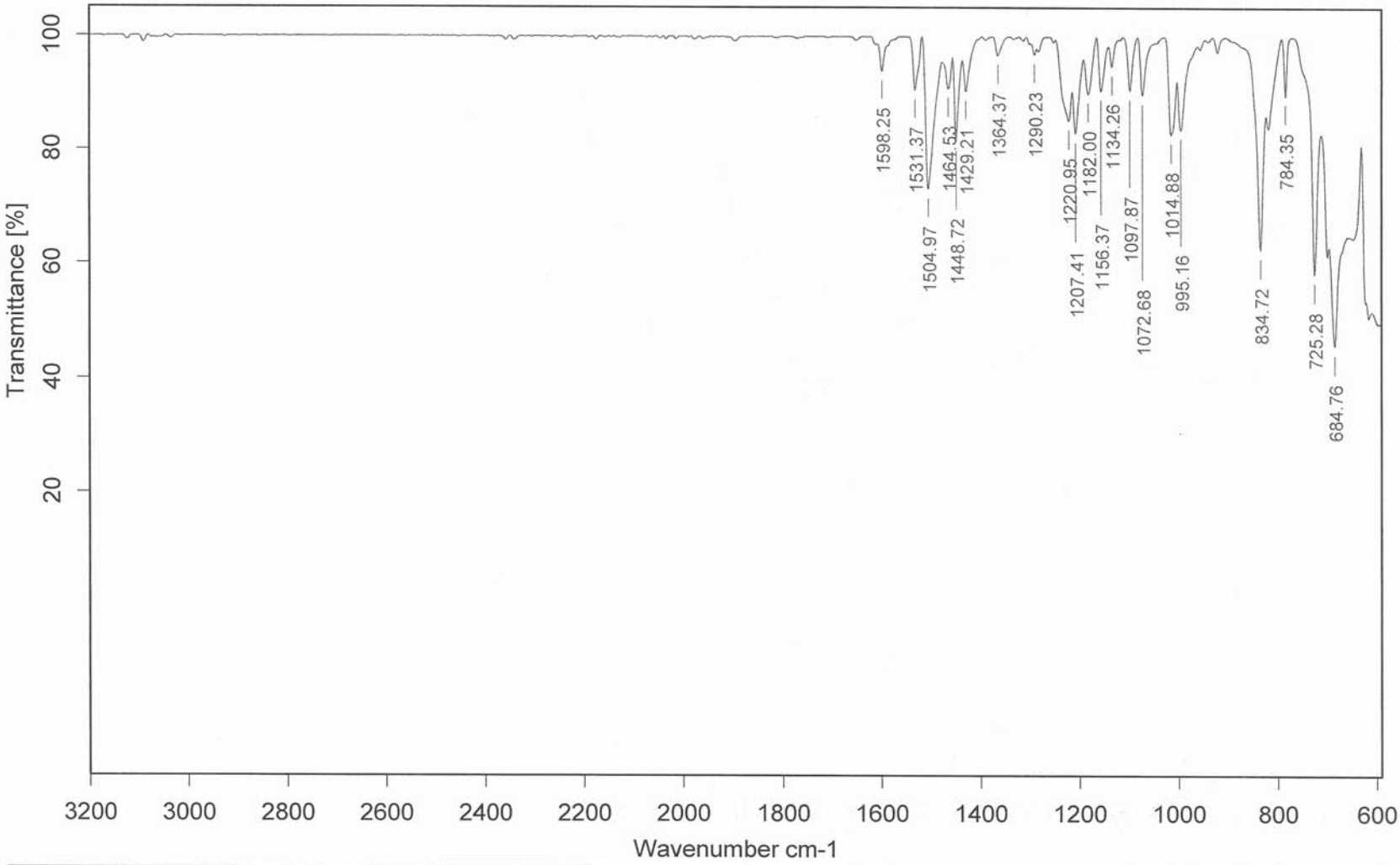


2-(4-fluorophenyl)-5-phenyl-2H-tetrazole



2-(4-fluorophenyl)-5-phenyl-2H-tetrazole





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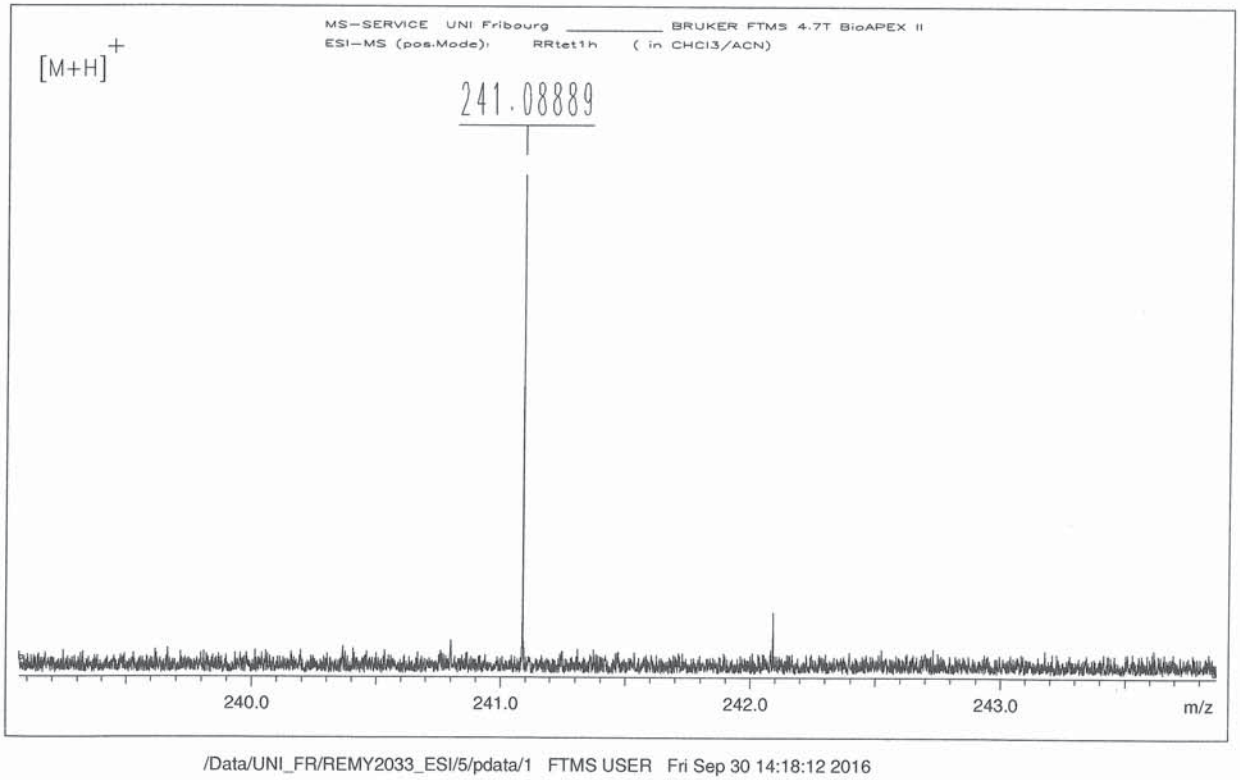
ESI-MS: RRtet1h

XMASS Mass Analysis for /Data/UNI_FR/REMY2033_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

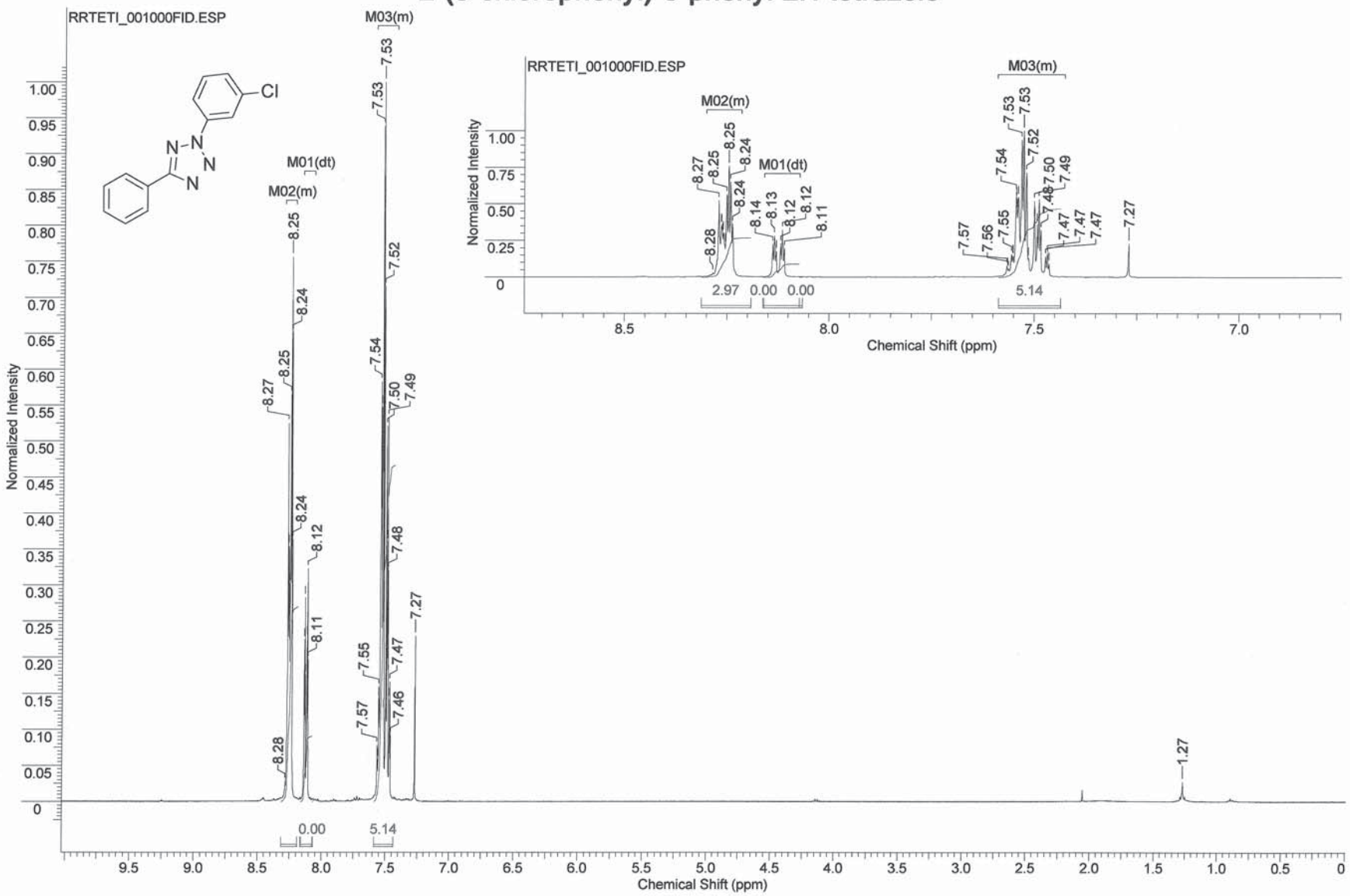
Ion mass = 241.0888890

Charge = +1

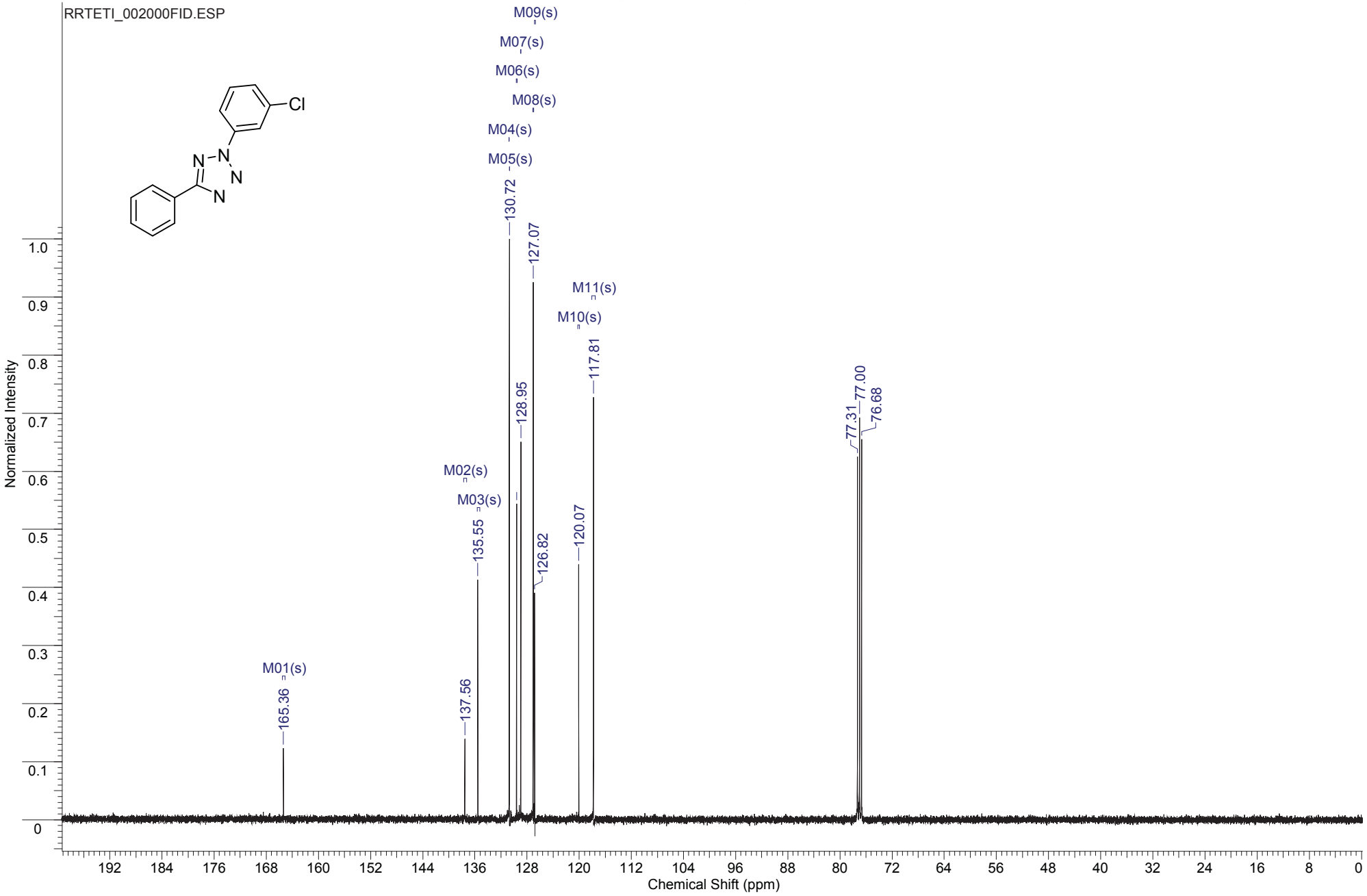
#	C	H	F	N	mass	DBE	error
*** Mass Analysis for mass 241.0888890							
1	**13**	**10**	**1**	**4**	**241.0884010**	10.5	4.880e-04
2	8	9	2	7	241.0882011	7.0	6.879e-04
3	12	12	3	2	241.0947094	6.5	5.820e-03
4	11	10	3	3	241.0821334	7.0	6.756e-03
5	9	11	2	6	241.1007772	6.5	1.189e-02
6	14	12	1	3	241.1009770	10.0	1.209e-02
7	12	8	1	5	241.0758249	11.0	1.306e-02
8	7	7	2	8	241.0756251	7.5	1.326e-02
9	6	10	1	10	241.1068450	6.5	1.796e-02
10	13	14	3	1	241.1072855	6.0	1.840e-02

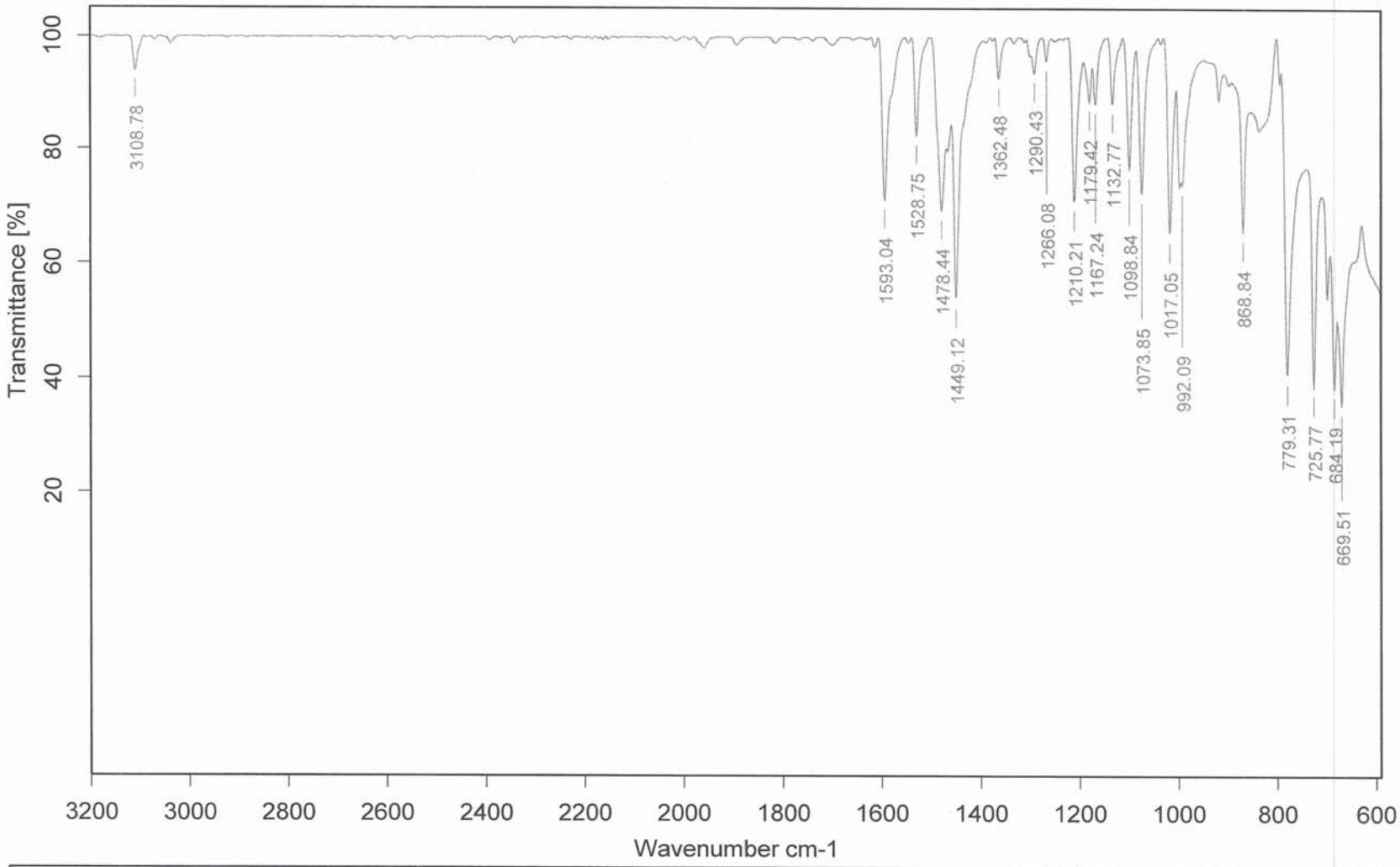


2-(3-chlorophenyl)-5-phenyl-2H-tetrazole



2-(3-chlorophenyl)-5-phenyl-2H-tetrazole





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BRUKER FTMS 4.7T BioAPEX II

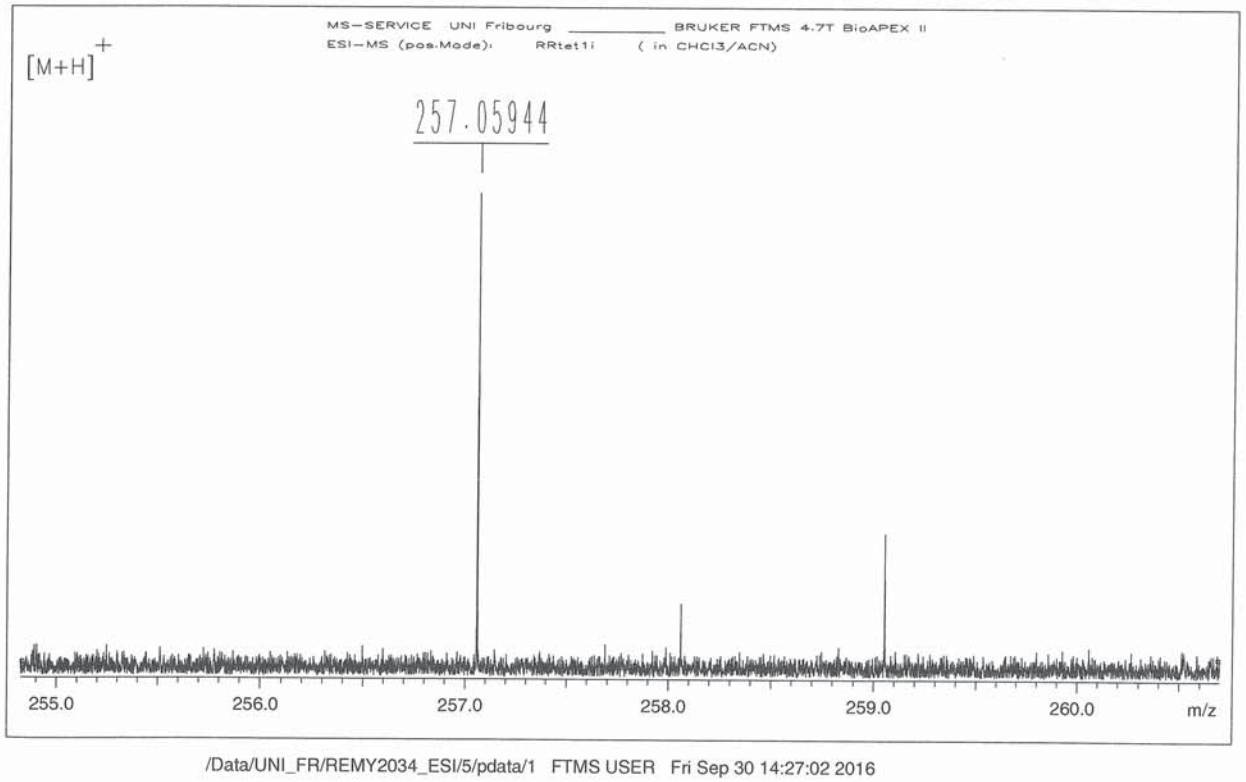
ESI-MS: RRtet1i

XMASS Mass Analysis for /Data/UNI_FR/REMY2034_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

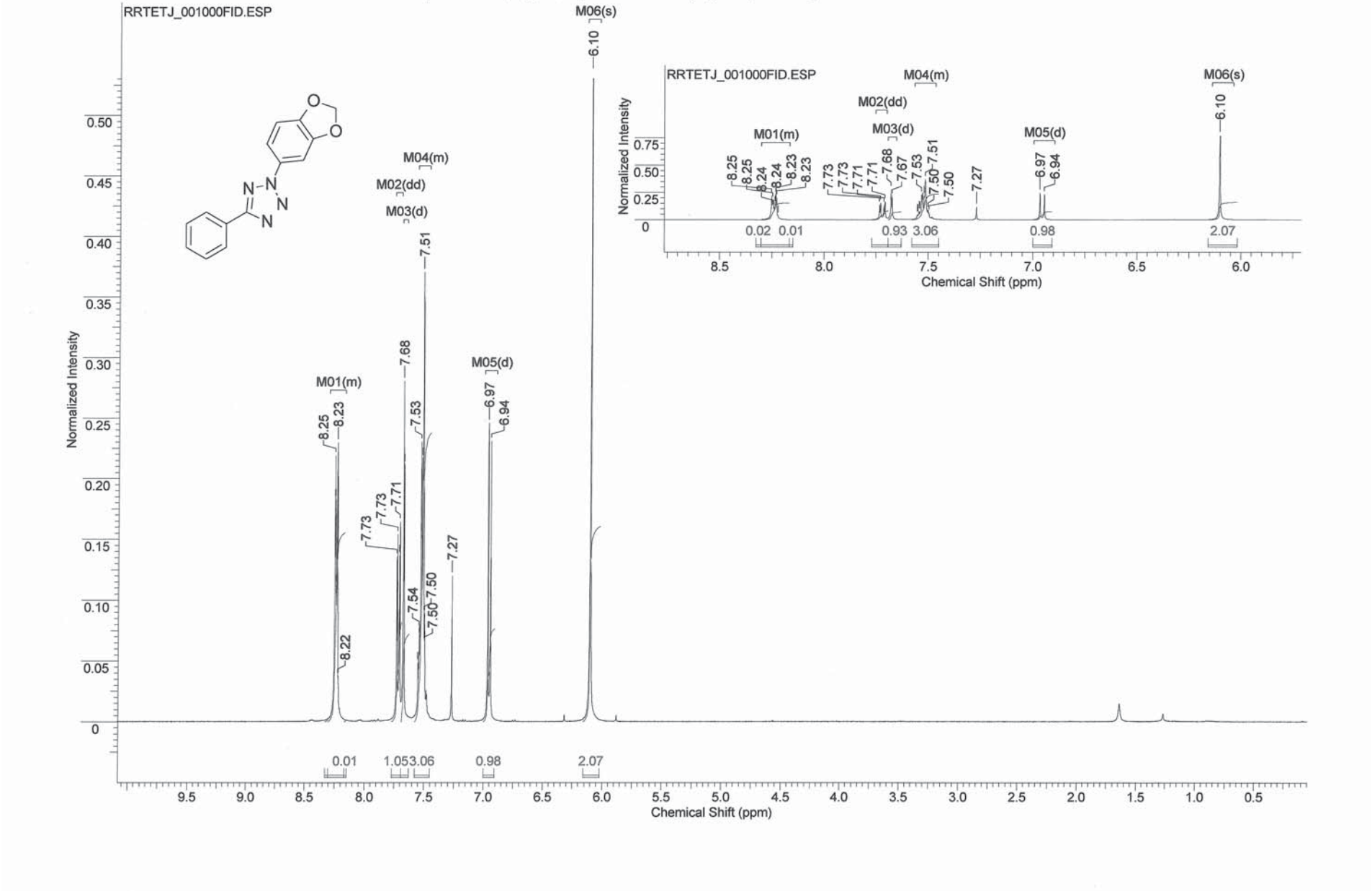
Ion mass = 257.0594380

Charge = +1

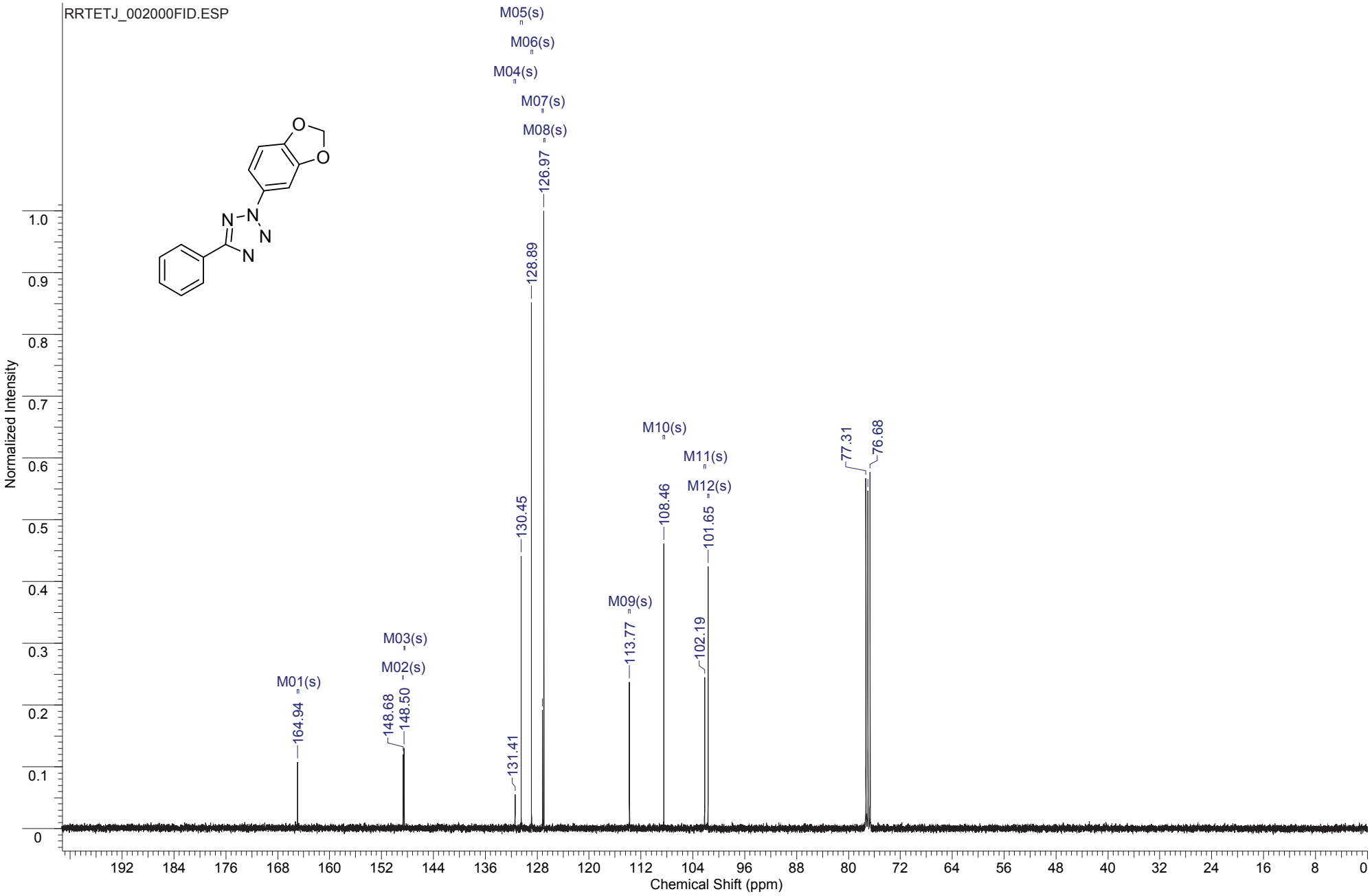
#	C	H	35Cl	N	mass	DBE	error
*** Mass Analysis for mass 257.0594380							
1	**13**	**10**	**1**	**4**	**257.0588505**	10.5	5.875e-04
2	14	5	0	6	257.0570206	15.5	2.417e-03
3	15	7	0	5	257.0695967	15.0	1.016e-02
4	14	12	1	3	257.0714265	10.0	1.199e-02
5	12	8	1	5	257.0462744	11.0	1.316e-02
6	13	3	0	7	257.0444446	16.0	1.499e-02
7	16	9	0	4	257.0821727	14.5	2.273e-02
8	15	14	1	2	257.0840026	9.5	2.456e-02
9	11	6	1	6	257.0336984	11.5	2.574e-02
10	20	3	0	1	257.0260005	20.0	3.344e-02

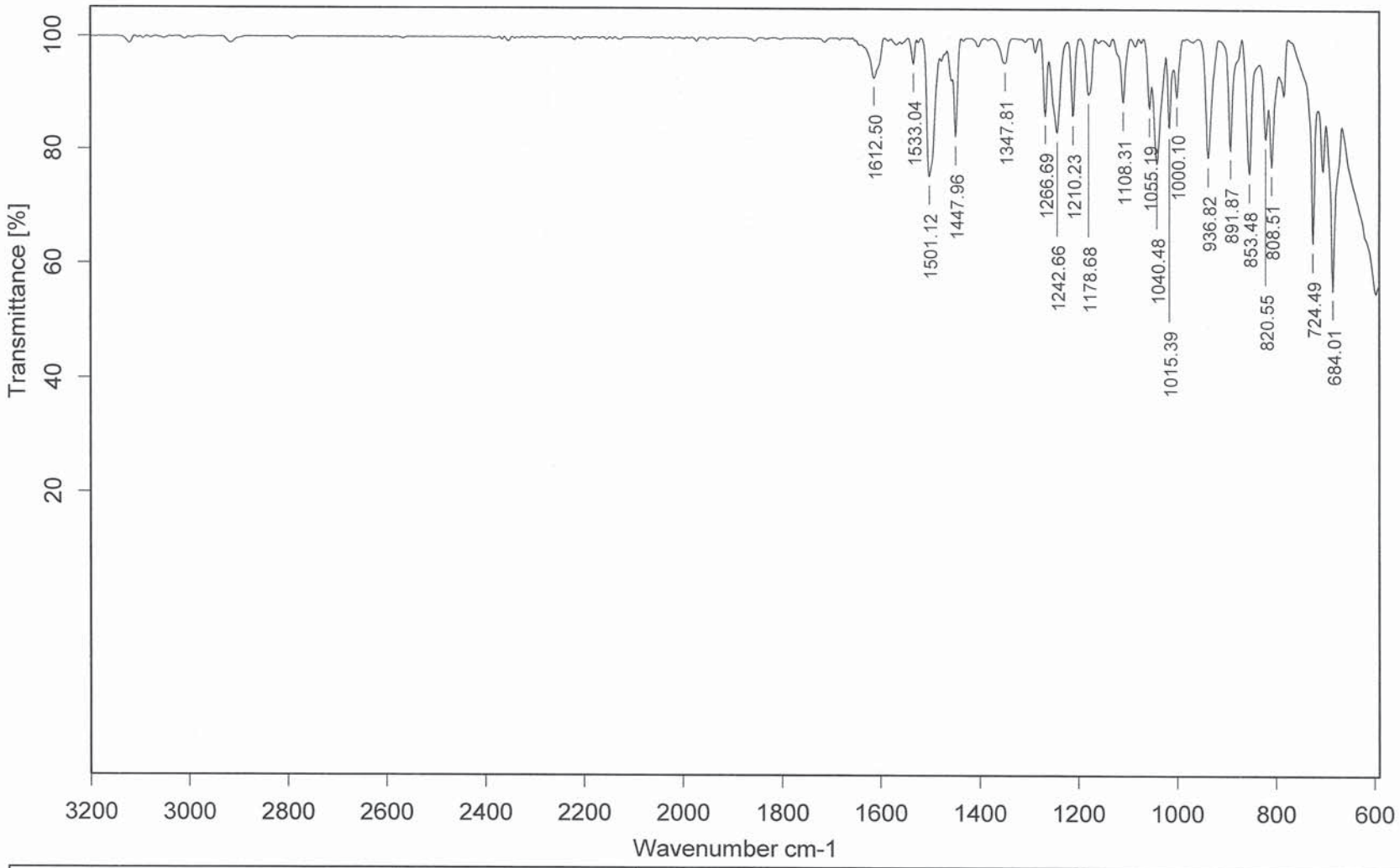


2-(benzo[d][1,3]dioxol-5-yl)-5-phenyl-2H-tetrazole



2-(benzo[d][1,3]dioxol-5-yl)-5-phenyl-2H-tetrazole





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BRUKER **FTMS 4.7T BioAPEX II**

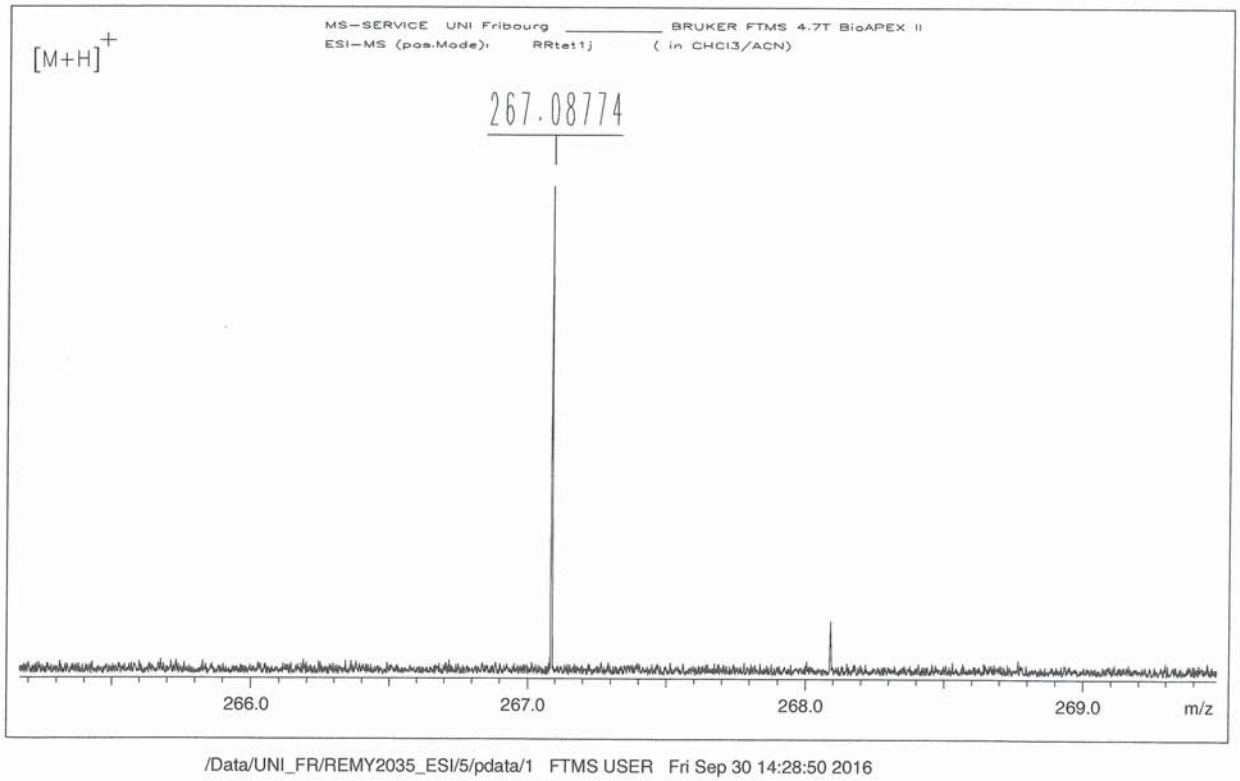
ESI-MS: RRtet1j

```
XMASS Mass Analysis for /Data/UNI_FR/REMY2035_ESI/5/pdata/1/massanal.res:
        XMASS Mass Analysis Constraints
```

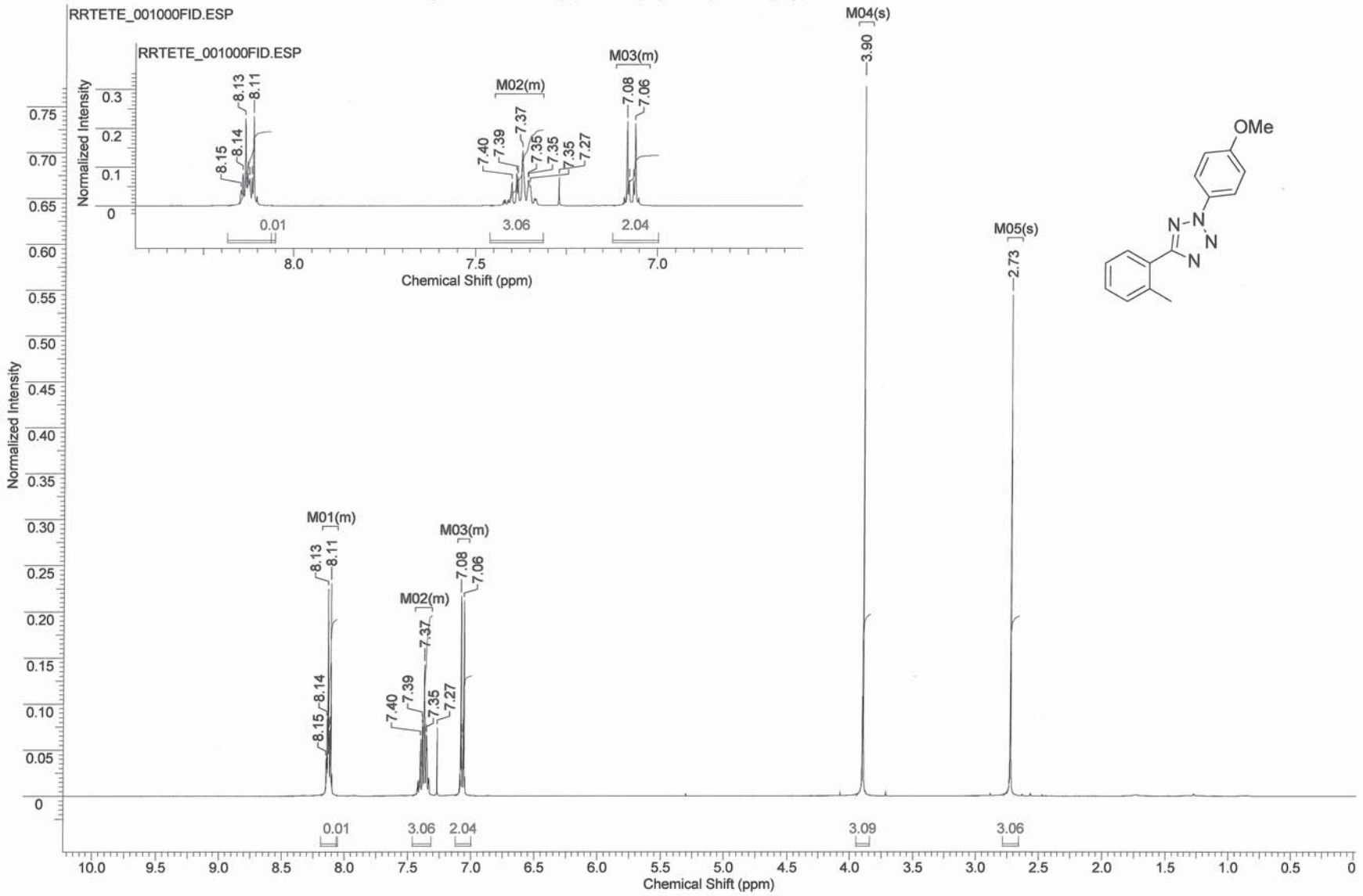
Ion mass = 267.0877420

Charge = +1

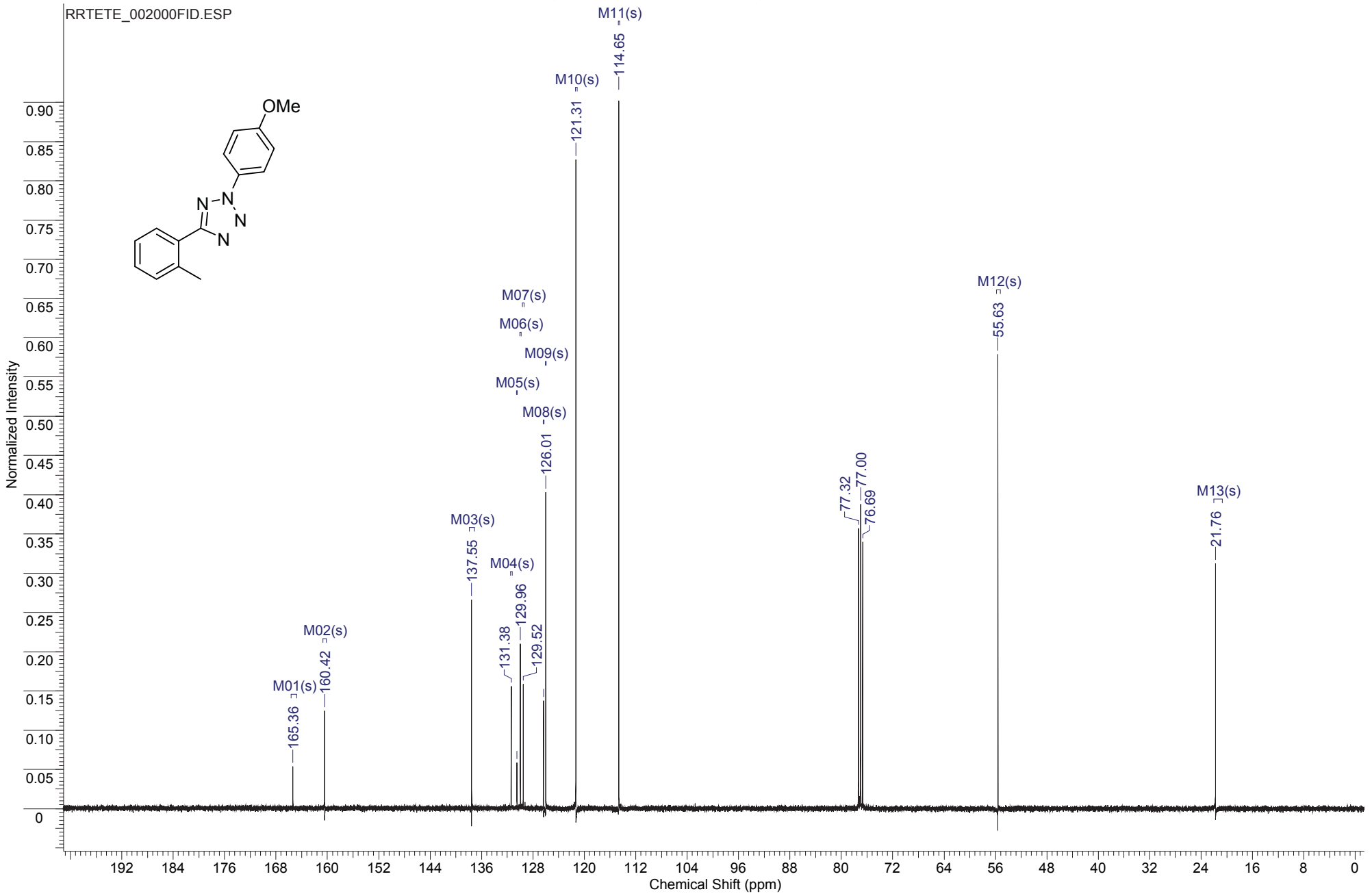
#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 267.0877420							
1	**14**	**11**	**4**	**2**	**267.0876520**	11.5	8.996e-05
2	16	13	1	3	267.0889947	11.0	1.253e-03
3	12	9	7	1	267.0863094	12.0	1.433e-03
4	11	13	3	5	267.0849720	7.0	2.770e-03
5	9	11	6	4	267.0836293	7.5	4.113e-03
6	5	13	7	6	267.0921826	3.0	4.441e-03
7	8	15	2	8	267.0822919	2.5	5.450e-03
8	7	15	4	7	267.0935253	2.5	5.783e-03
9	6	13	5	7	267.0809492	3.0	6.793e-03
10	8	11	8	3	267.0948627	7.5	7.121e-03

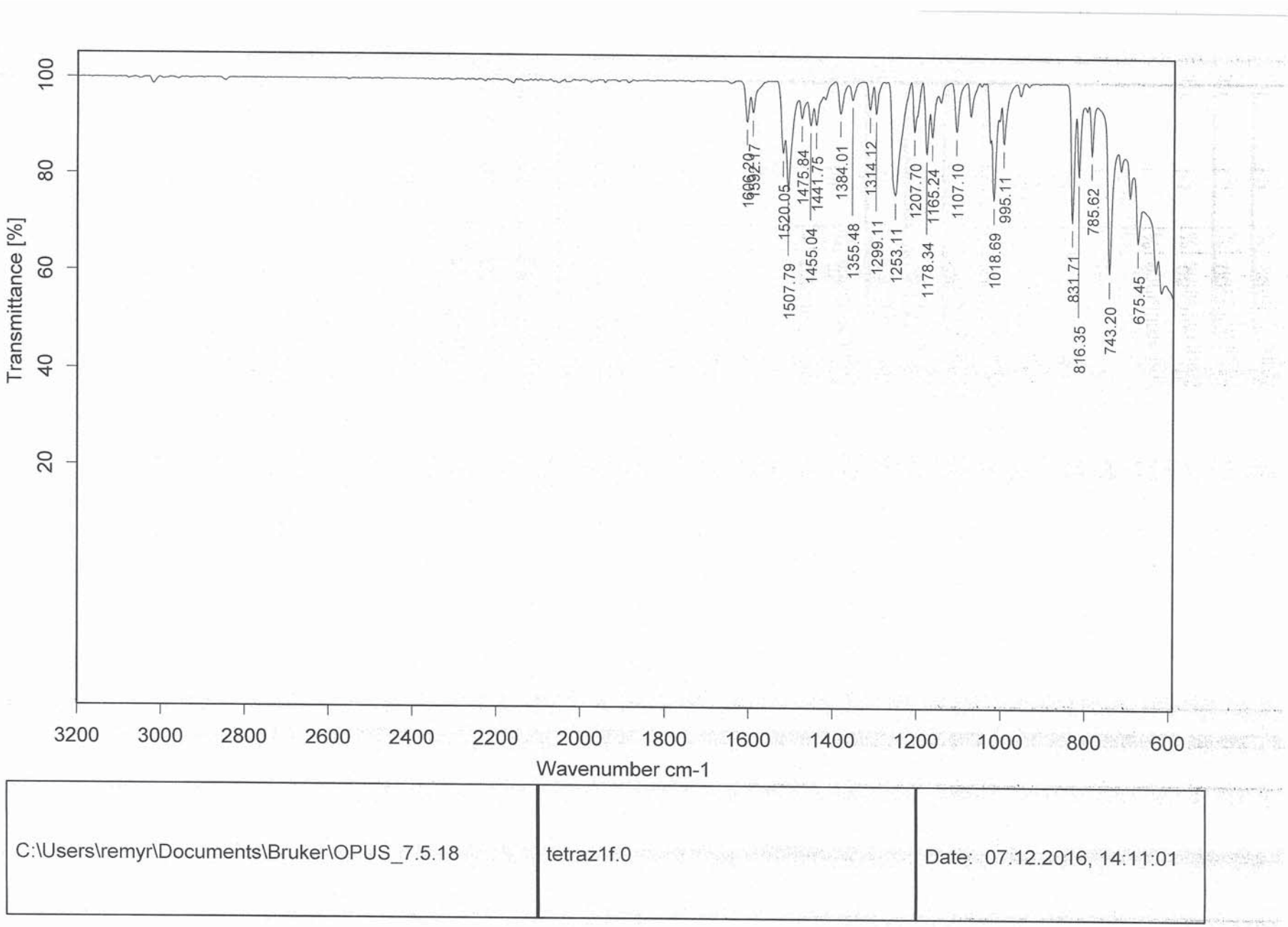


2-(4-methoxyphenyl)-5-(o-tolyl)-2H-tetrazole



2-(4-methoxyphenyl)-5-(o-tolyl)-2H-tetrazole

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1441.75
1384.01
1355.48
1314.12
1299.11
1253.11
1207.70
1178.34
1165.24
1107.10
1018.69
995.11
831.71
816.35
785.62
743.20
675.45
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3000
2800
2600
2400
2200
2000
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1600
1400
1200
1000
800
600
Wavenumber cm-1
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tetraz1f.0
Date: 07.12.2016, 14:11:01

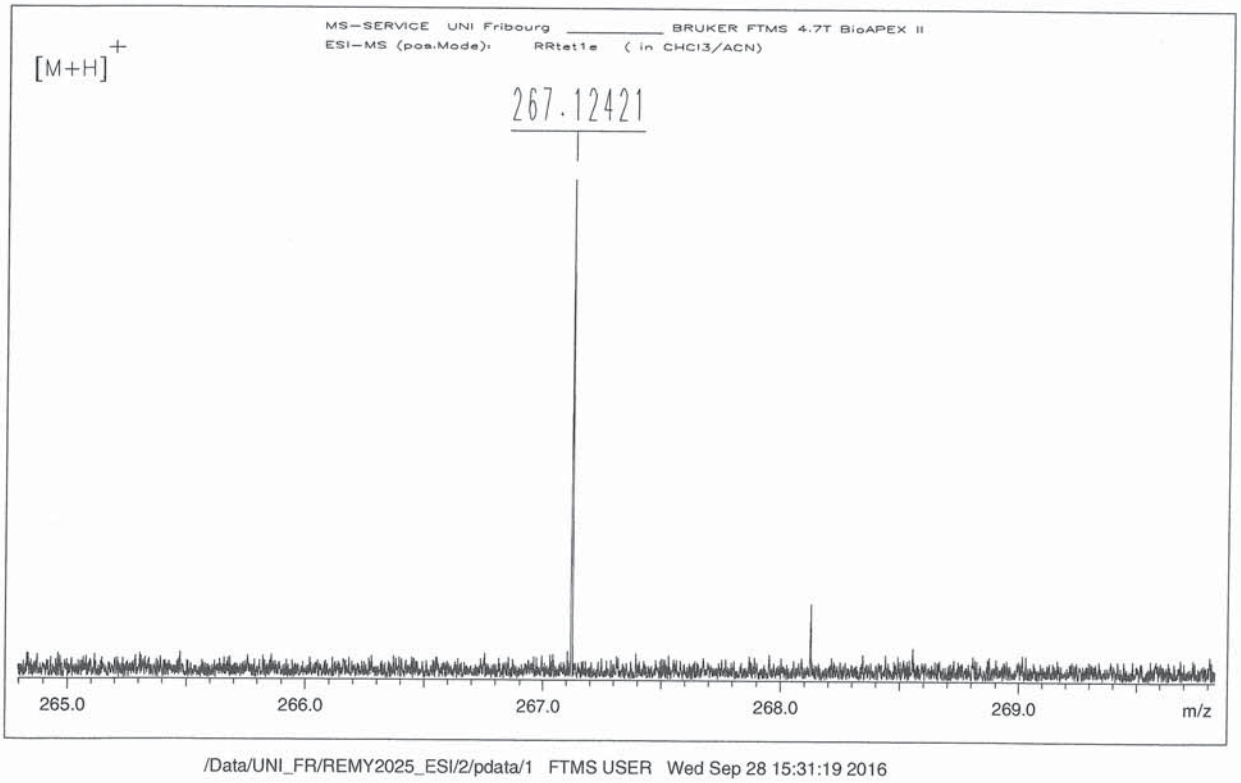
ESI-MS: RRtet1e

XMASS Mass Analysis for /Data/UNI_FR/REMY2025_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

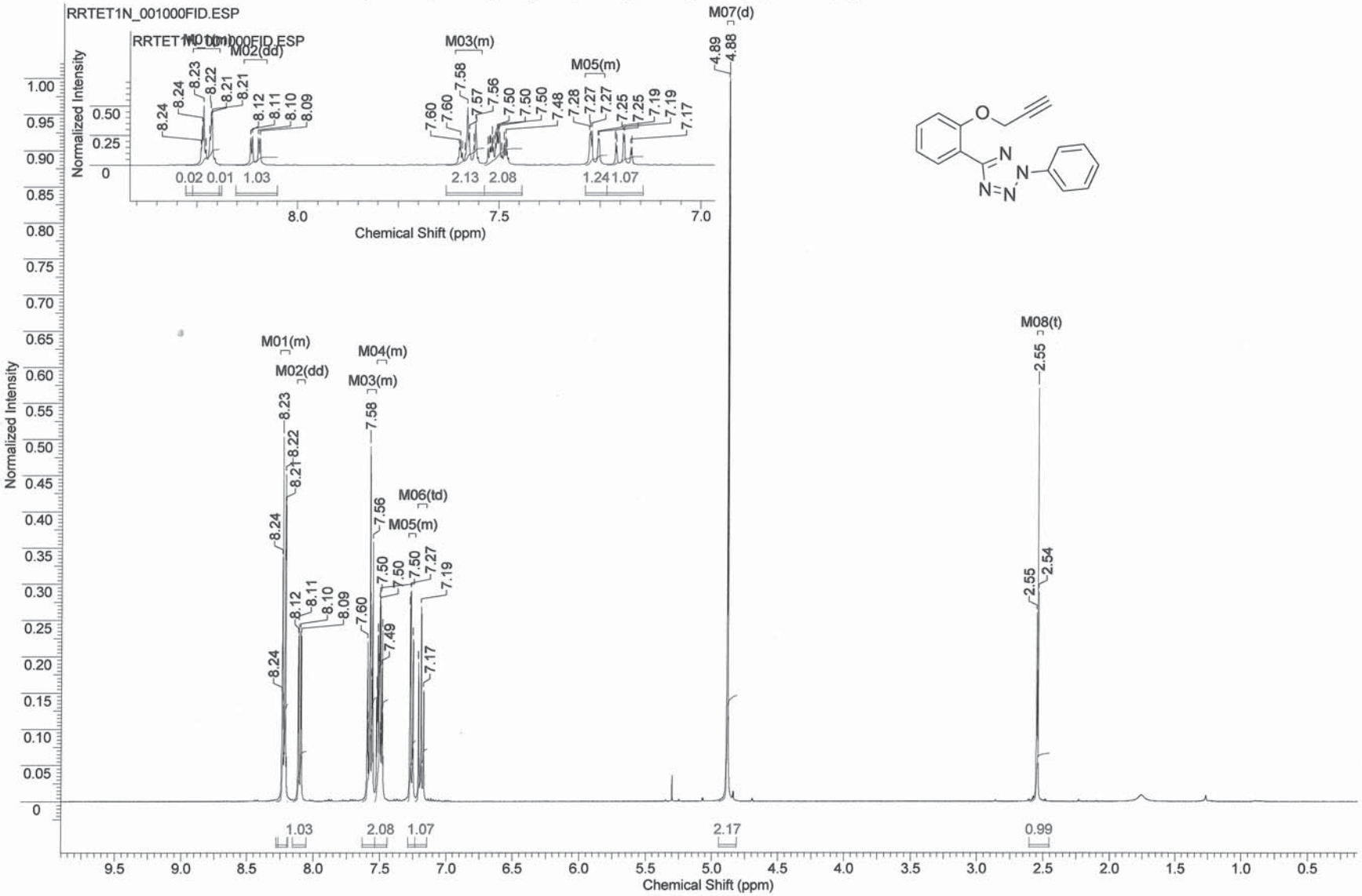
Ion mass = 267.1242050

Charge = +1

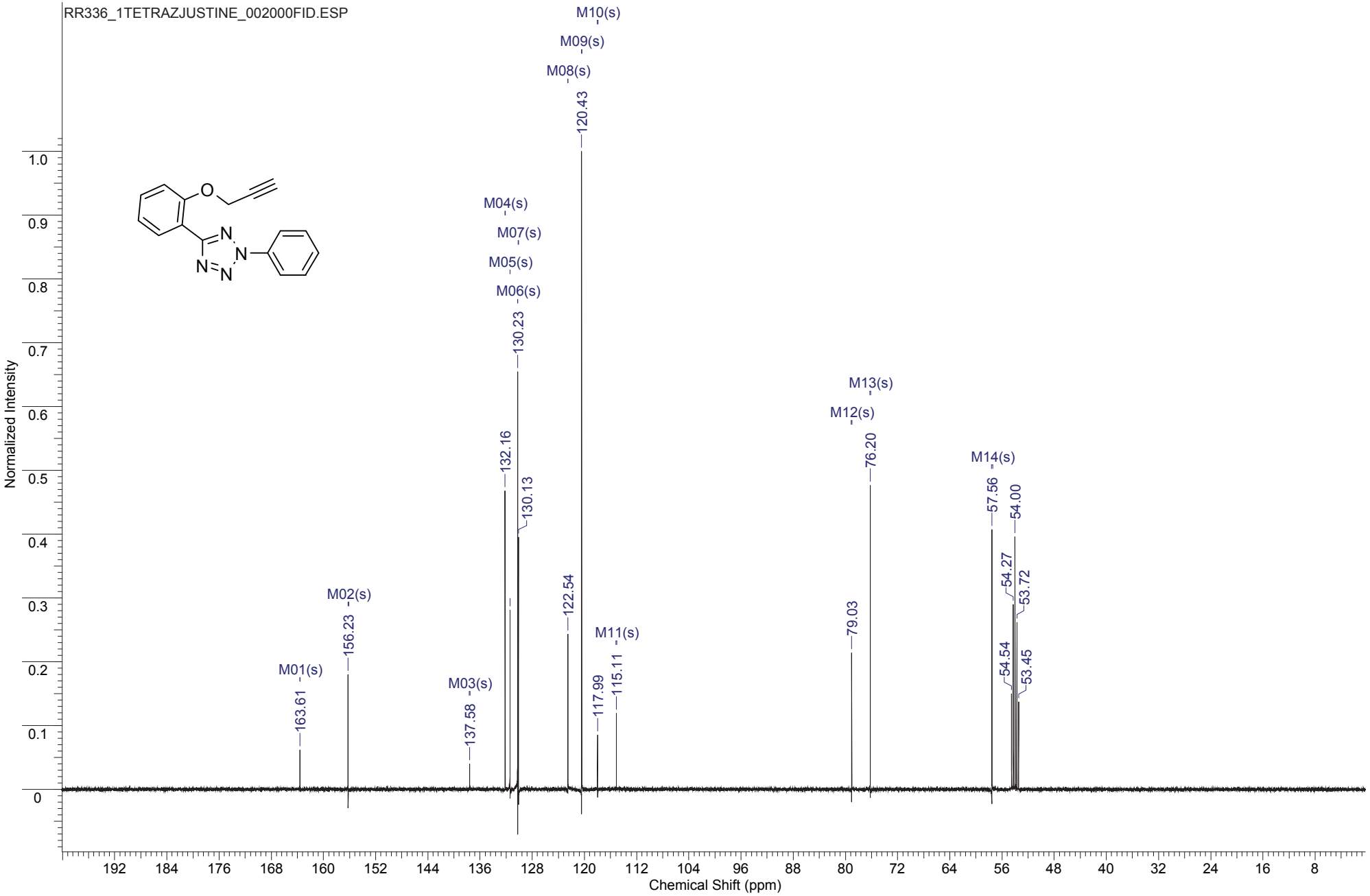
#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 267.1242050							
1	**15**	**15**	**4**	**1**	**267.1240375**	10.5	1.675e-04
2	17	17	1	2	267.1253802	10.0	1.175e-03
3	12	17	3	4	267.1213575	6.0	2.848e-03
4	10	15	6	3	267.1200148	6.5	4.190e-03
5	6	17	7	5	267.1285681	2.0	4.363e-03
6	9	19	2	7	267.1186774	1.5	5.528e-03
7	8	13	9	2	267.1186721	7.0	5.533e-03
8	8	19	4	6	267.1299108	1.5	5.706e-03
9	7	17	5	6	267.1173347	2.0	6.870e-03
10	9	15	8	2	267.1312482	6.5	7.043e-03

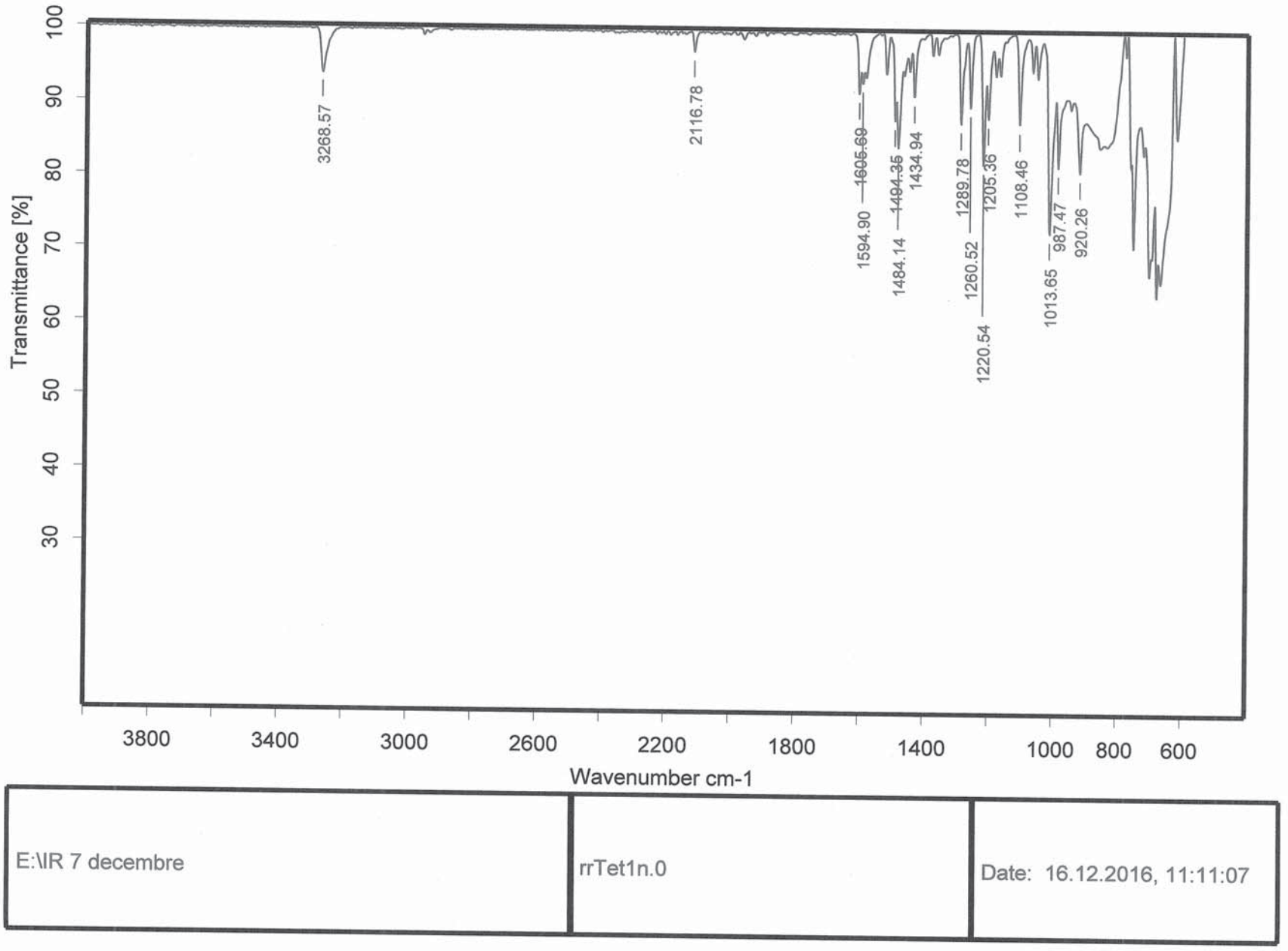


2-phenyl-5-(2-(prop-2-yn-1-yloxy)phenyl)-2H-tetrazole



2-phenyl-5-(2-(prop-2-yn-1-yloxy)phenyl)-2H-tetrazole




Transmittance [%]
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1289.78
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1220.54
1205.36
1108.46
1013.65
987.47
920.26
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3000
2600
2200
1800
1400
1000
800
600
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BRUKER FTMS 4.7T BioAPEX II

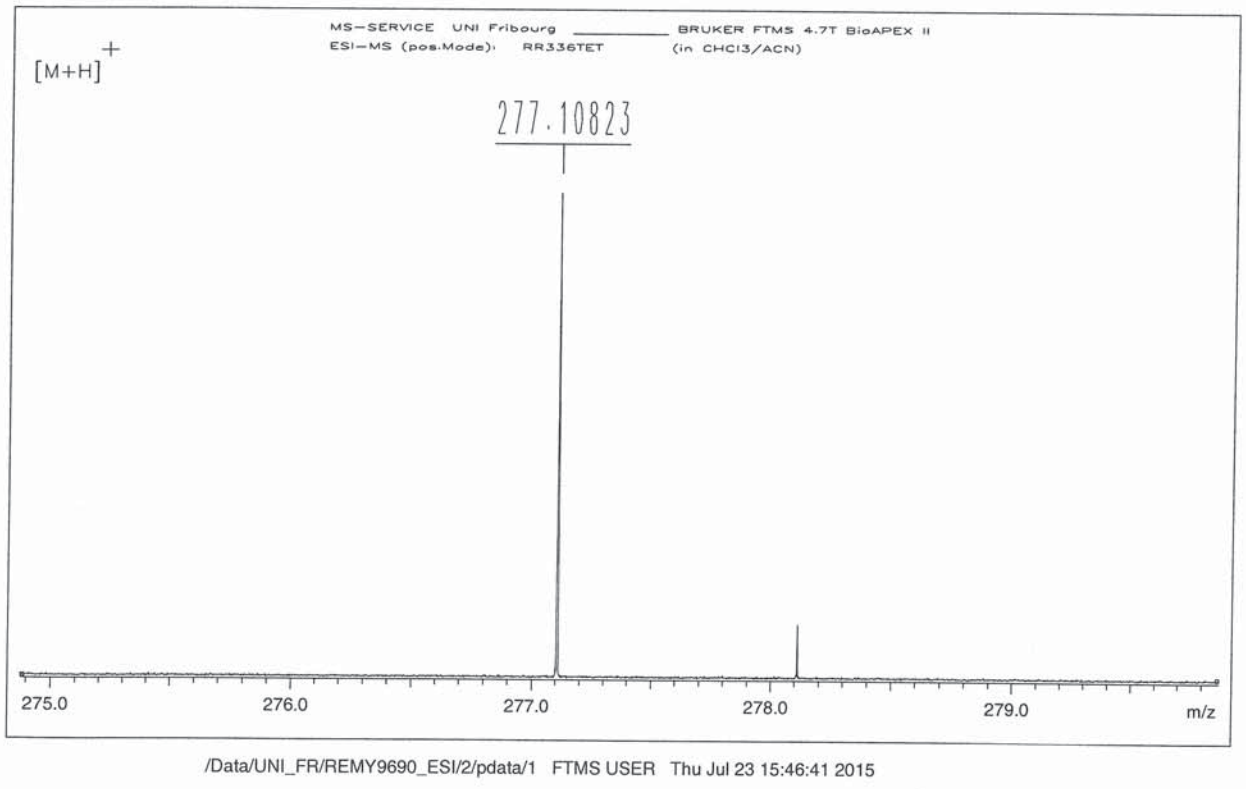
ESI-MS: RR336TET

XMASS Mass Analysis for /Data/UNI_FR/REMY9690_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 277.1082300

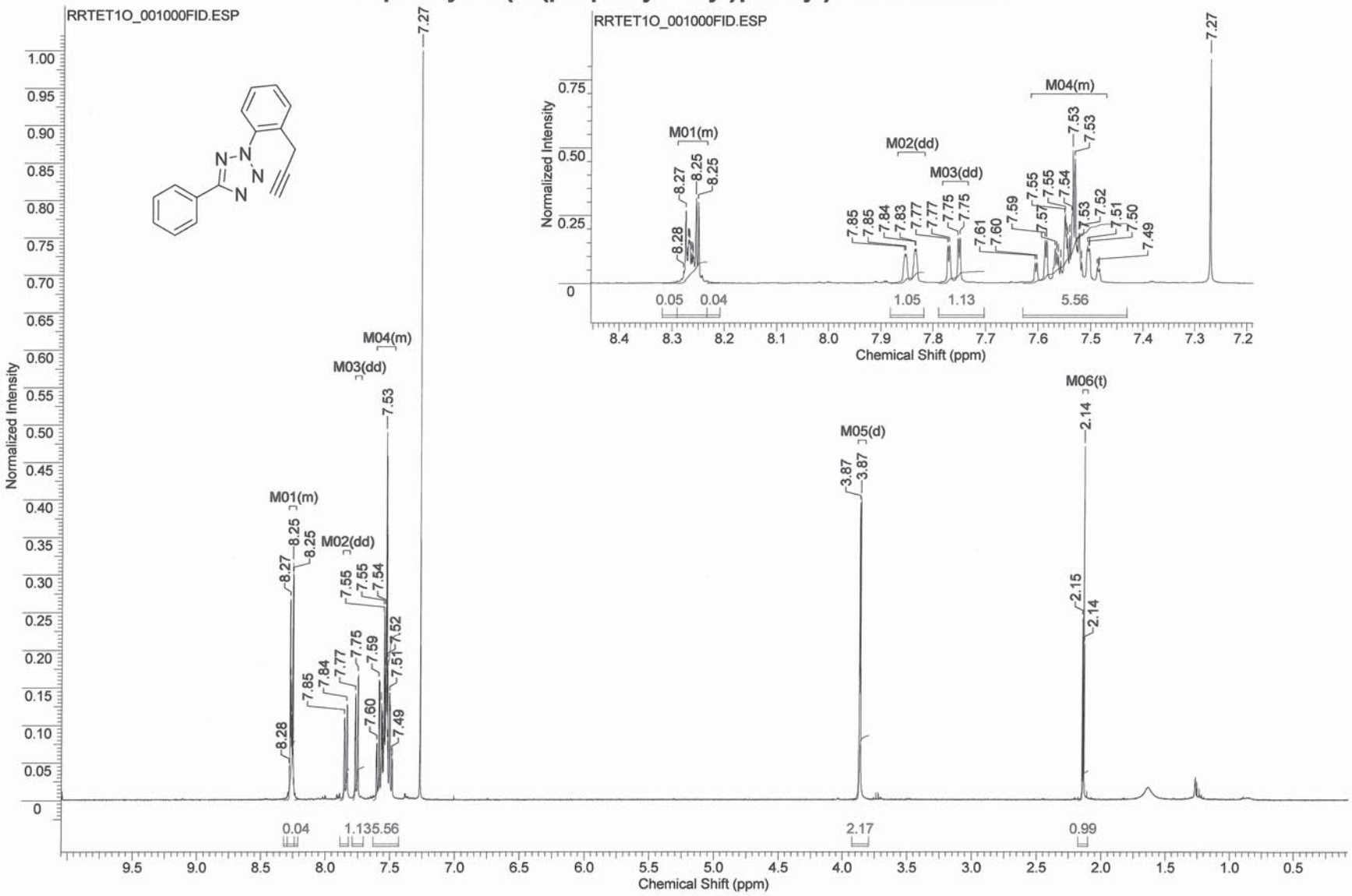
Charge = +1

#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 277.1082300							
1	**16**	**13**	**4**	**1**	**277.1083875**	**12.5**	**1.575e-04**
2	18	15	1	2	277.1097302	12.0	1.500e-03
3	13	15	3	4	277.1057074	8.0	2.523e-03
4	5	13	10	4	277.1115754	4.5	3.345e-03
5	6	19	3	9	277.1115806	-1.0	3.351e-03
6	11	13	6	3	277.1043647	8.5	3.865e-03
7	7	15	7	5	277.1129180	4.0	4.688e-03
8	10	17	2	7	277.1030273	3.5	5.203e-03
9	9	11	9	2	277.1030221	9.0	5.208e-03
10	9	17	4	6	277.1142607	3.5	6.031e-03

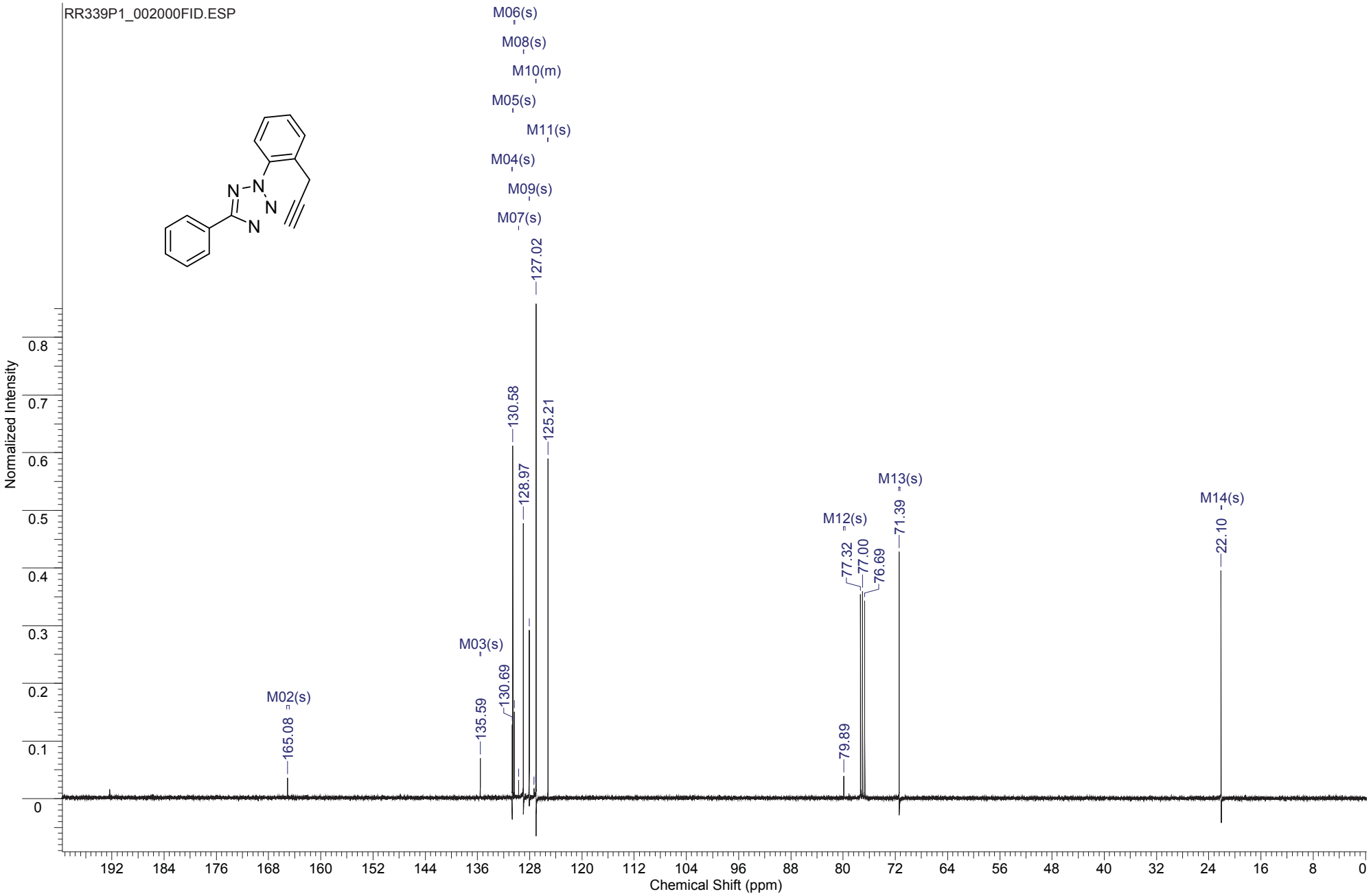


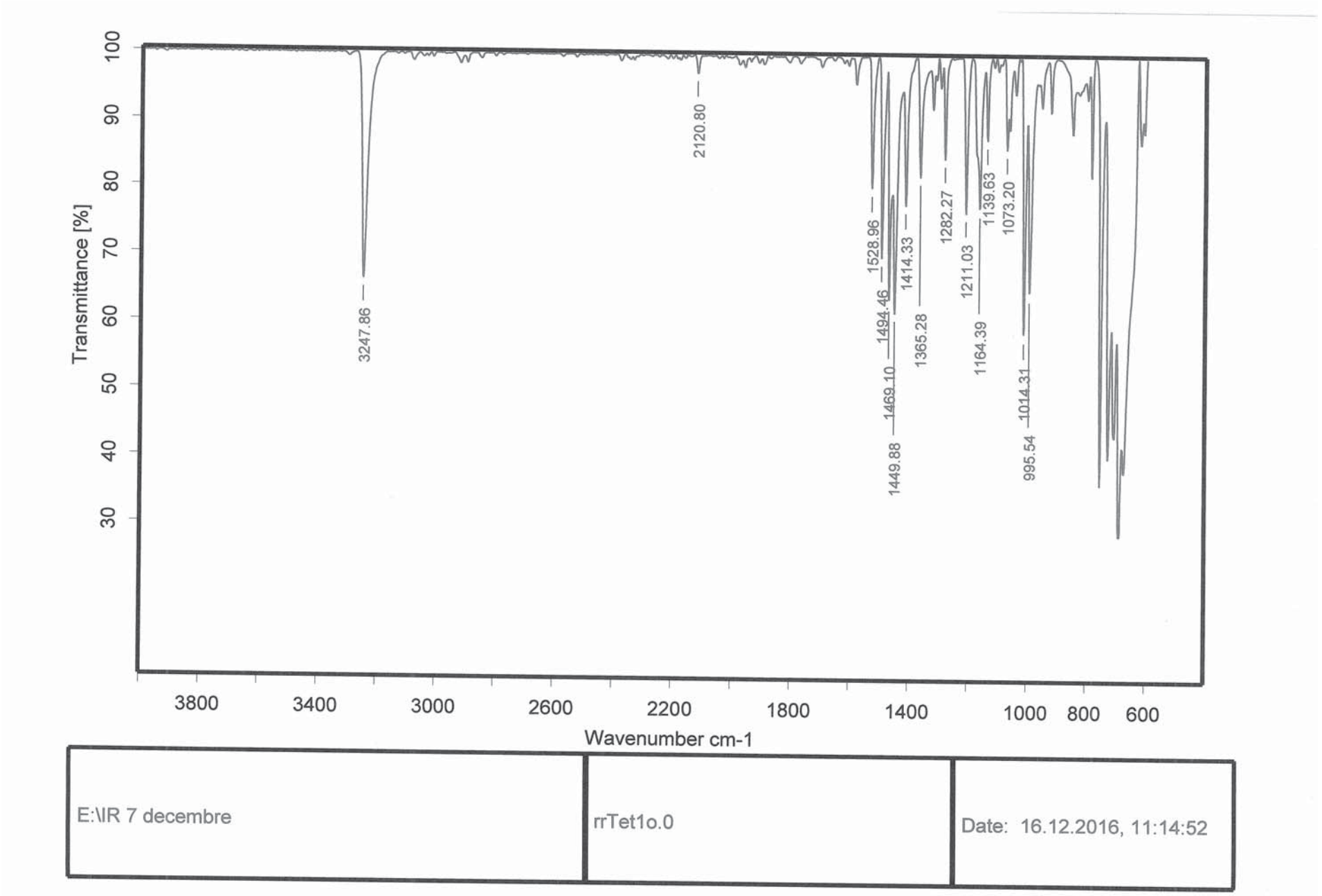
/Data/UNI_FR/REMY9690_ESI/2/pdata/1 FTMS USER Thu Jul 23 15:46:41 2015

5-phenyl-2-(2-(prop-2-yn-1-yl)phenyl)-2H-tetrazole



5-phenyl-2-(2-(prop-2-yn-1-yl)phenyl)-2H-tetrazole




Transmittance [%]
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50
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3400
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2600
2200
1800
1400
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800
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Wavenumber cm-1
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rrTet1o.0
Date: 16.12.2016, 11:14:52

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BRUKER FTMS 4.7T BioAPEX II

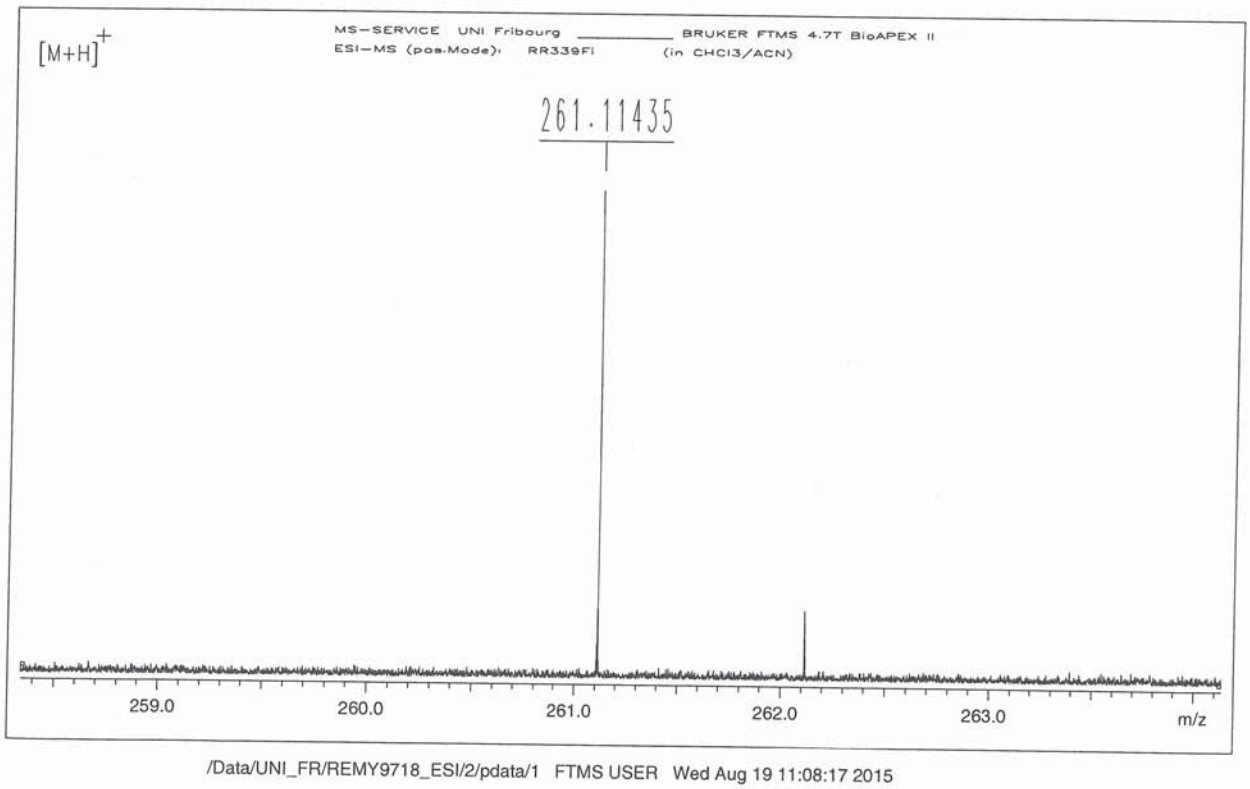
ESI-MS: RR339Fi

XMASS Mass Analysis for /Data/UNI_FR/REMY9718_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 261.1143520

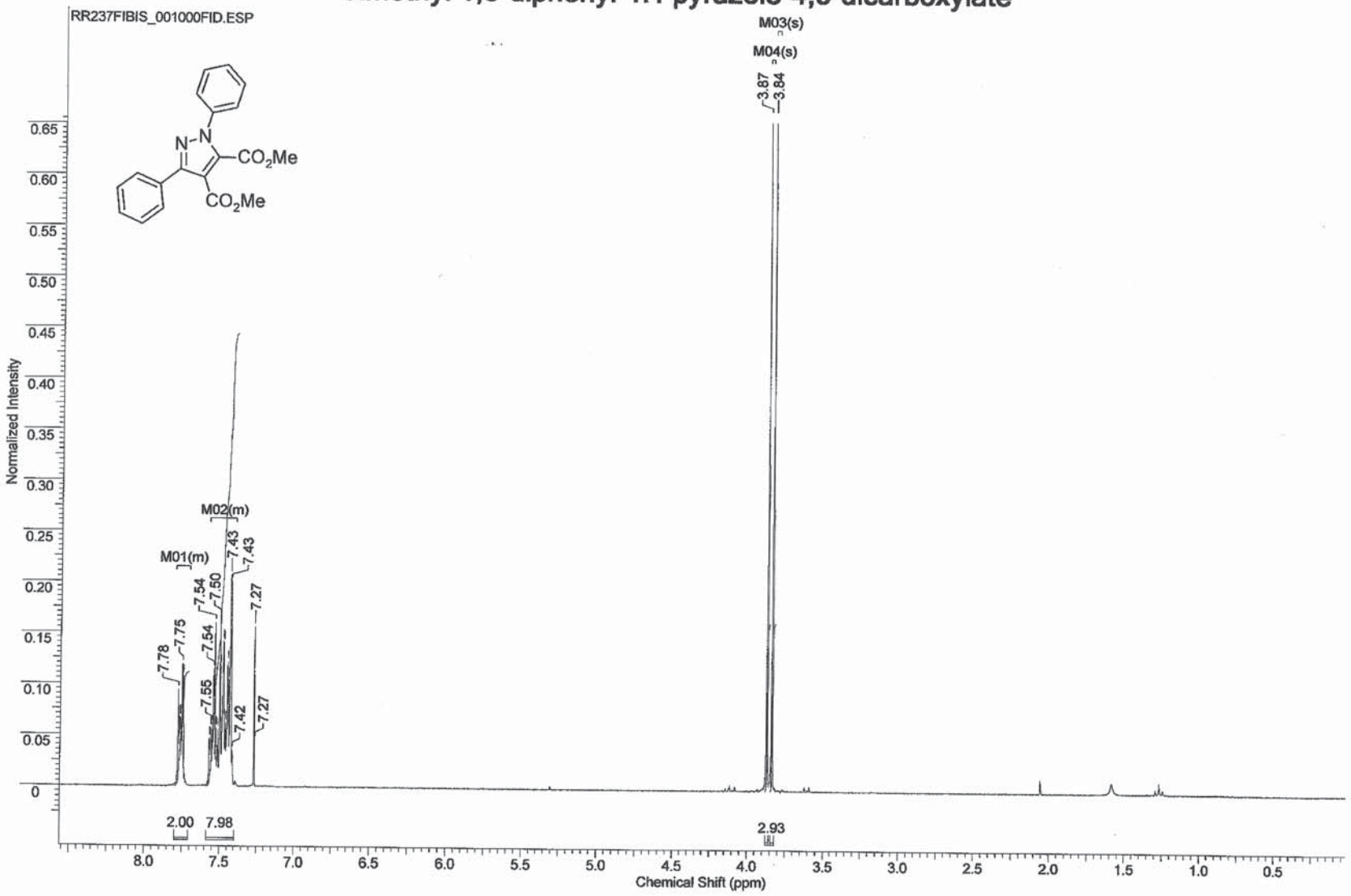
Charge = +1

#	C	H	N	mass	DBE	error
*** Mass Analysis for mass 261.1143520						
1	**16**	**13**	**4**	**261.1134729**	**12.5**	**8.791e-04**
2	17	15	3	261.1260489	12.0	1.170e-02
3	15	11	5	261.1008968	13.0	1.346e-02
4	9	13	10	261.1319169	8.5	1.756e-02
5	18	17	2	261.1386250	11.5	2.427e-02
6	14	9	6	261.0883207	13.5	2.603e-02
7	10	15	9	261.1444929	8.0	3.014e-02
8	19	19	1	261.1512010	11.0	3.685e-02
9	13	7	7	261.0757447	14.0	3.861e-02
10	11	17	8	261.1570690	7.5	4.272e-02

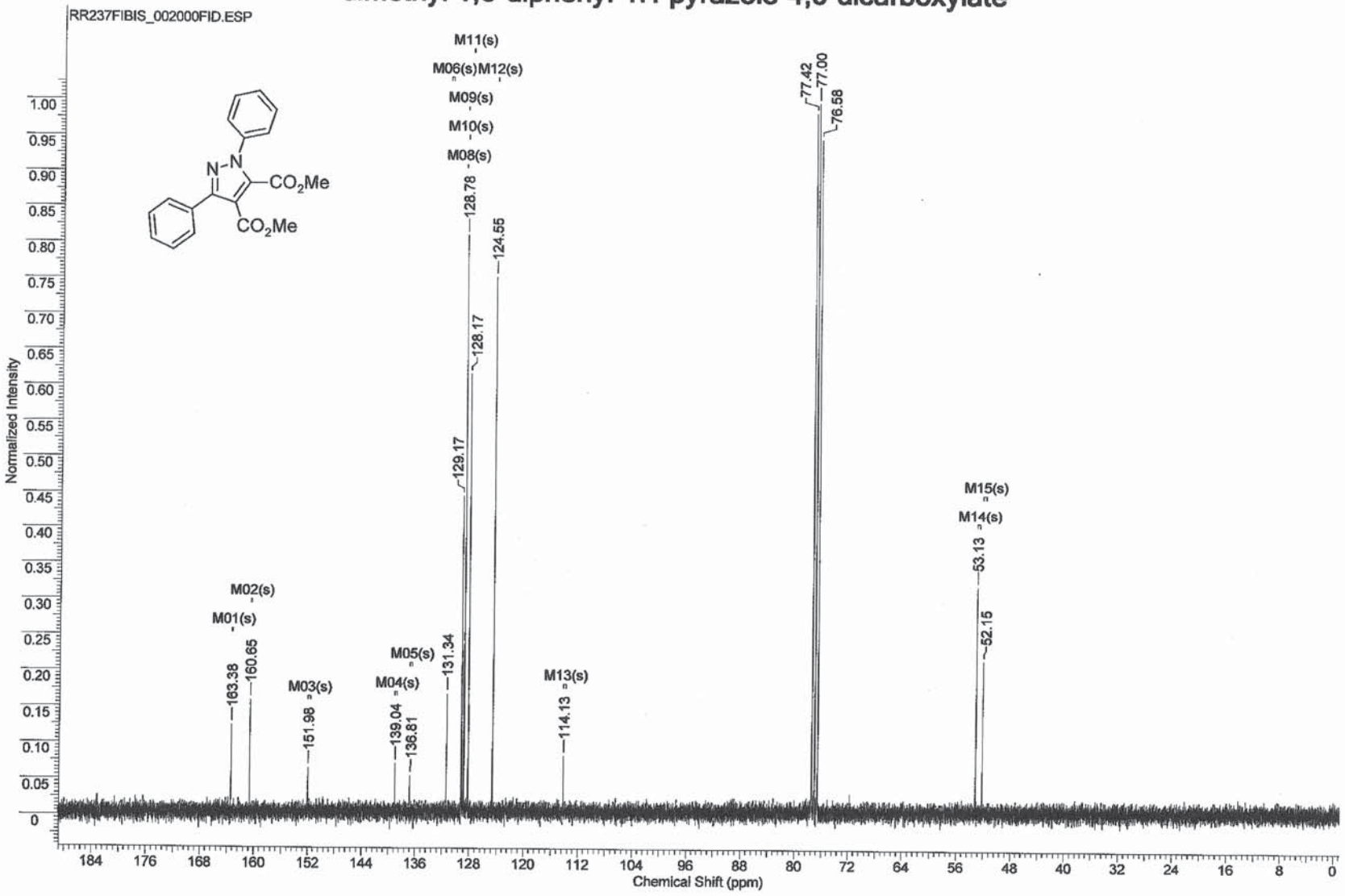


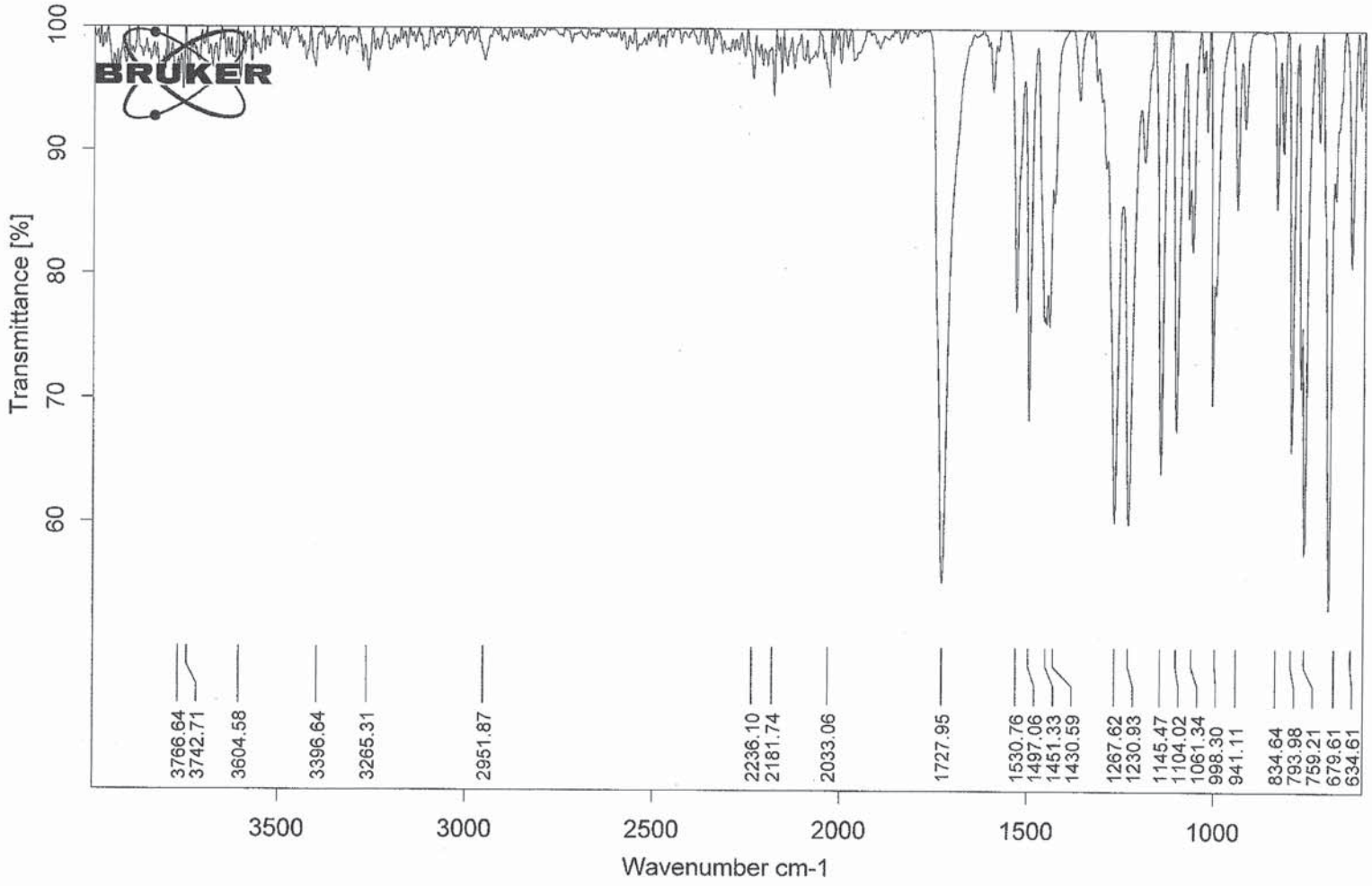
/Data/UNI_FR/REMY9718_ESI/2/pdata/1 FTMS USER Wed Aug 19 11:08:17 2015

dimethyl 1,3-diphenyl-1H-pyrazole-4,5-dicarboxylate



dimethyl 1,3-diphenyl-1H-pyrazole-4,5-dicarboxylate





U:\IR\tetraz1 avec DMAD pyrazole.0	tetraz1 avec DMAD pyrazole	yellow solid	22.05.2015

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BRUKER FTMS 4.7T BioAPEX II

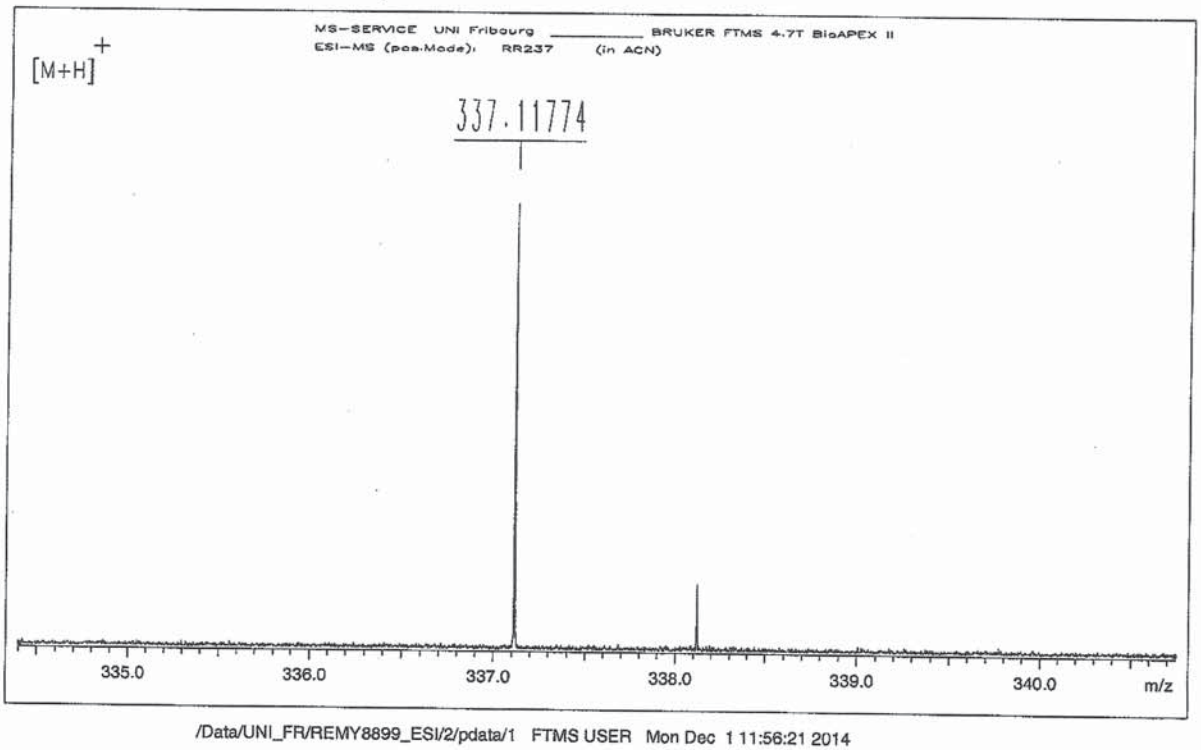
ESI-MS: RR237

XMASS Mass Analysis for /Data/UNI_FR/REMY8899_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

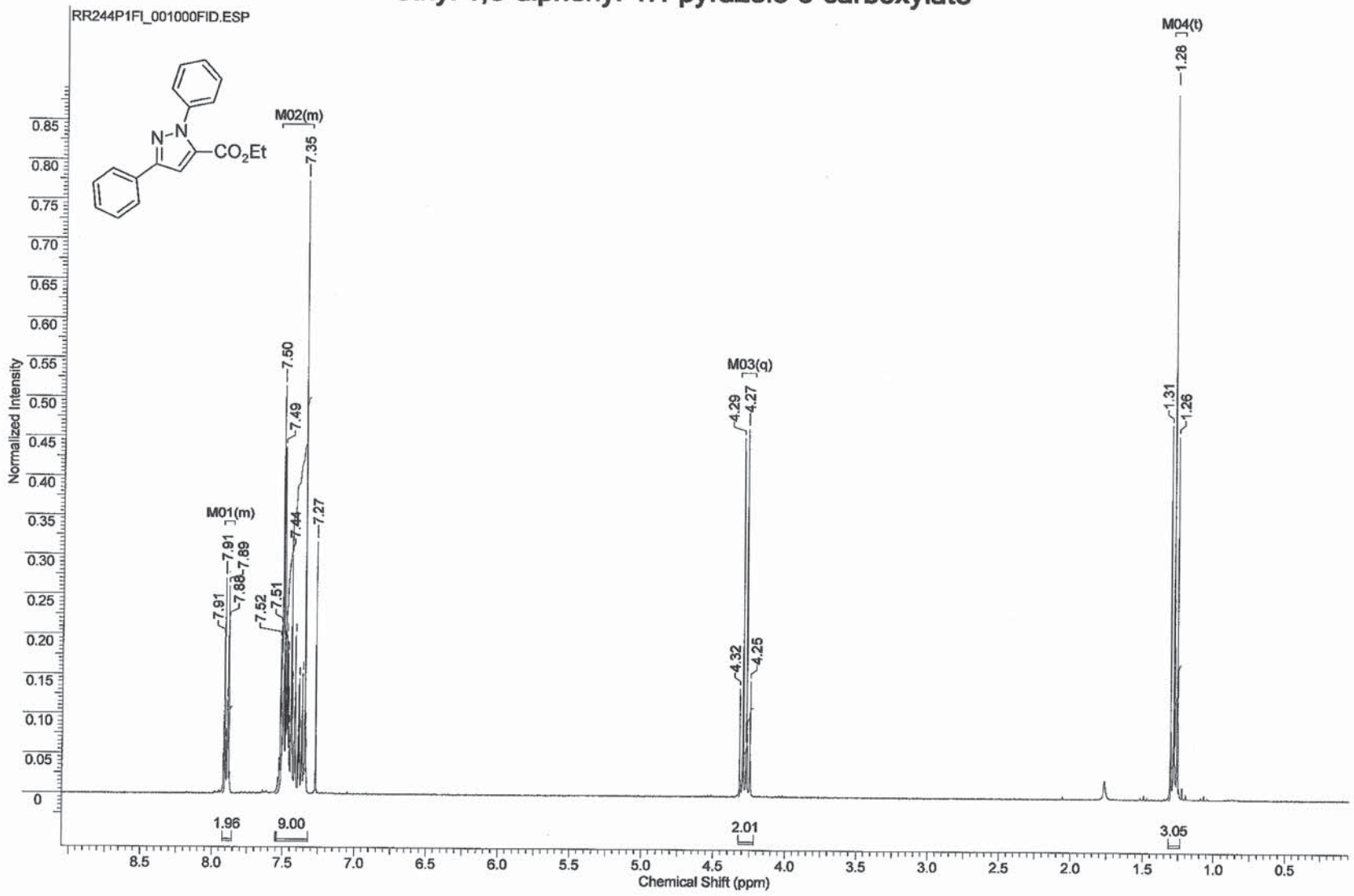
Ion mass = 337.1177390

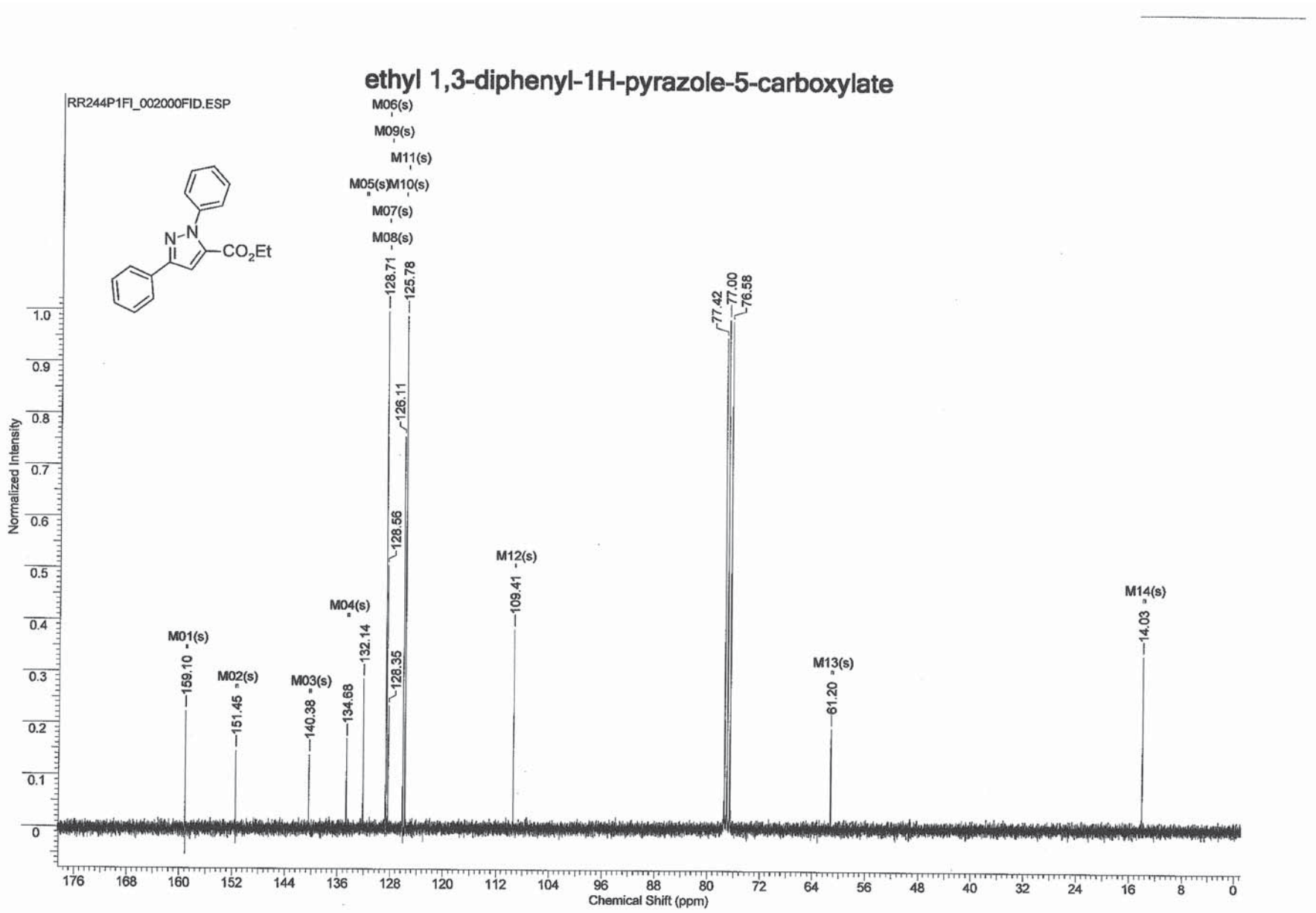
Charge = +1

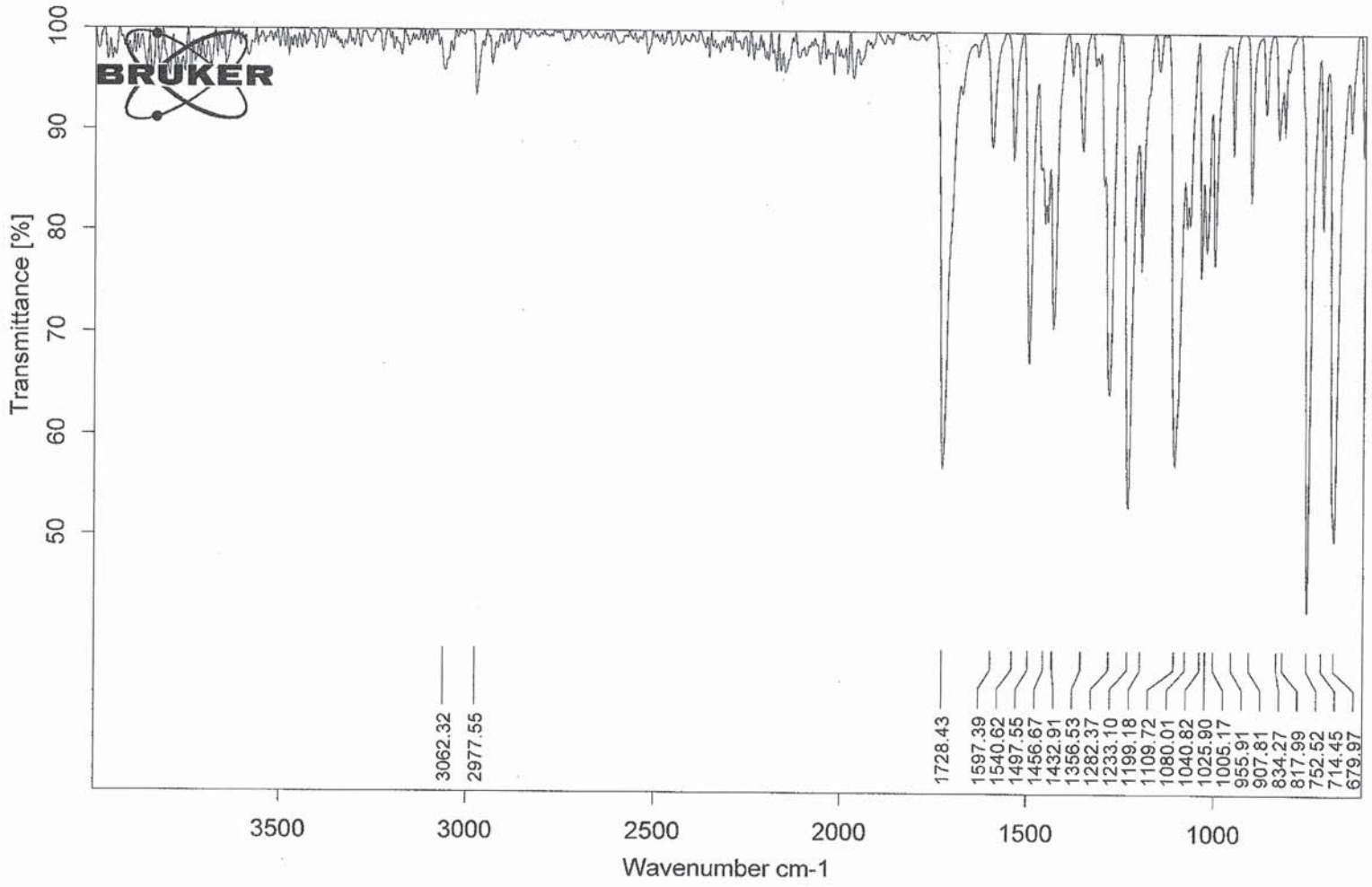
#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 337.1177390							
1	19	17	2	4	337.1182835	12.5	5.445e-04
2	17	15	5	3	337.1169408	13.0	7.982e-04
3	5	19	7	10	337.1187913	0.0	1.052e-03
4	16	19	1	7	337.1156034	8.0	2.136e-03
5	15	13	8	2	337.1155981	13.5	2.141e-03
6	22	15	3	1	337.1209635	17.0	3.225e-03
7	14	17	4	6	337.1142607	8.5	3.478e-03
8	8	17	8	7	337.1214714	4.5	3.732e-03
9	12	15	7	5	337.1129180	9.0	4.821e-03
10	10	19	5	8	337.1228140	4.0	5.075e-03



ethyl 1,3-diphenyl-1H-pyrazole-5-carboxylate




ethyl 1,3-diphenyl-1H-pyrazole-5-carboxylate
RR244P1FI_002000FID.ESP
CO2Et
M01(s)
M02(s)
M03(s)
M04(s)
M05(s)
M06(s)
M07(s)
M08(s)
M09(s)
M10(s)
M11(s)
M12(s)
M13(s)
M14(s)
159.10
151.45
140.38
134.68
132.14
128.71
128.56
128.35
126.11
125.78
109.41
77.42
77.00
76.58
61.20
14.03
Normalized Intensity
Chemical Shift (ppm)



U:\IR\RR244P1.0	RR244P1	yellow solid	22.05.2015

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BRUKER **FTMS 4.7T BioAPEX II**

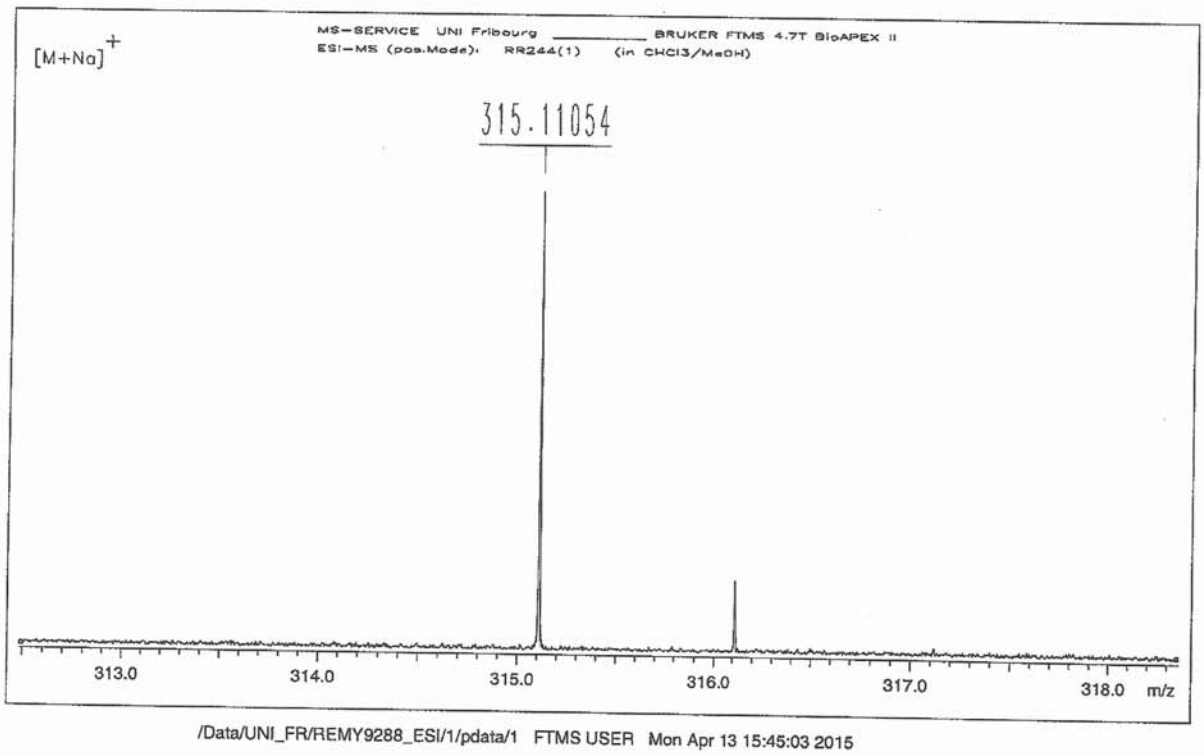
ESI-MS: RR244(1)

XMASS Mass Analysis for /Data/UNI_FR/REMY9288_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

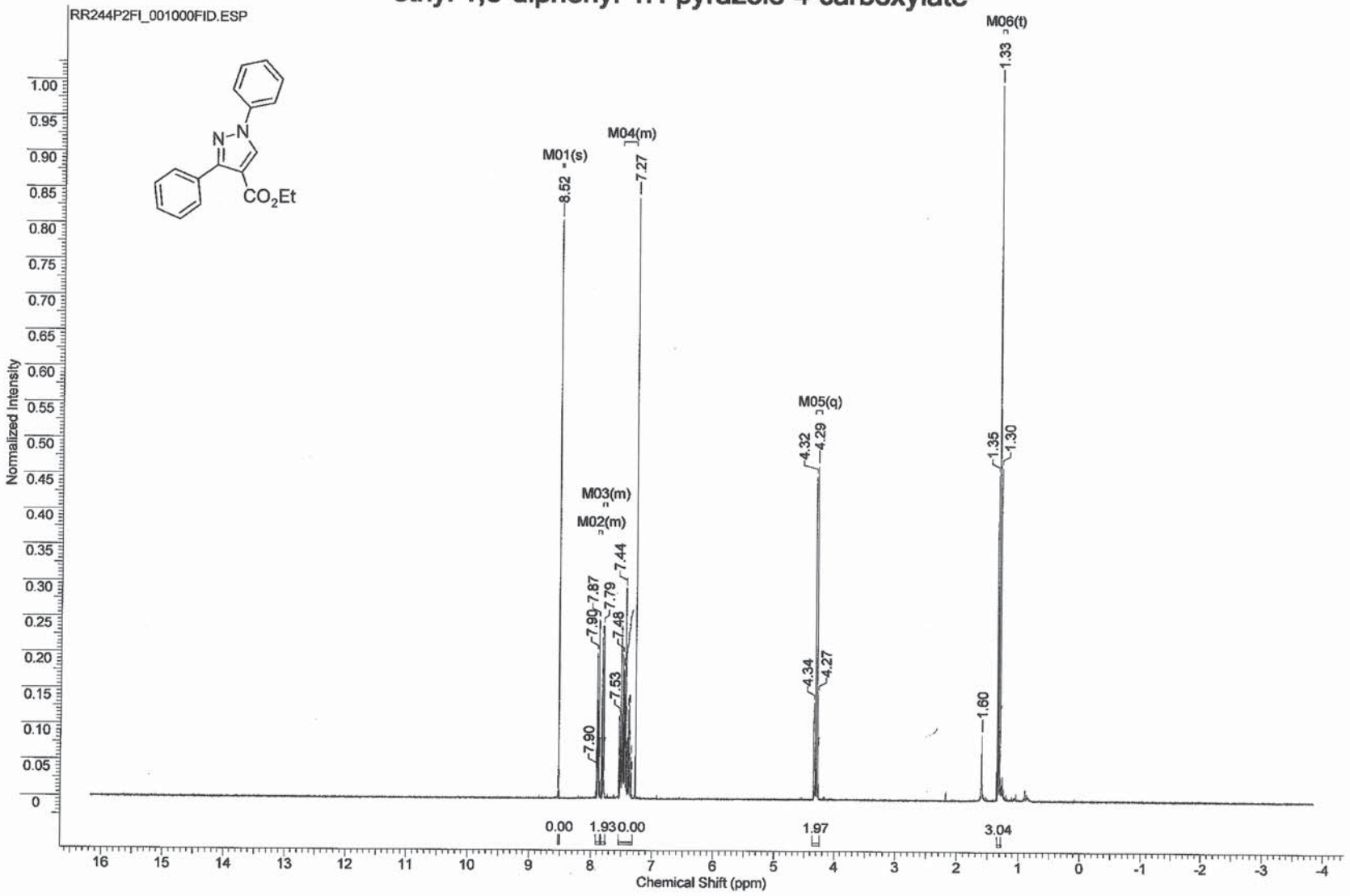
Ion mass = 315.1105350

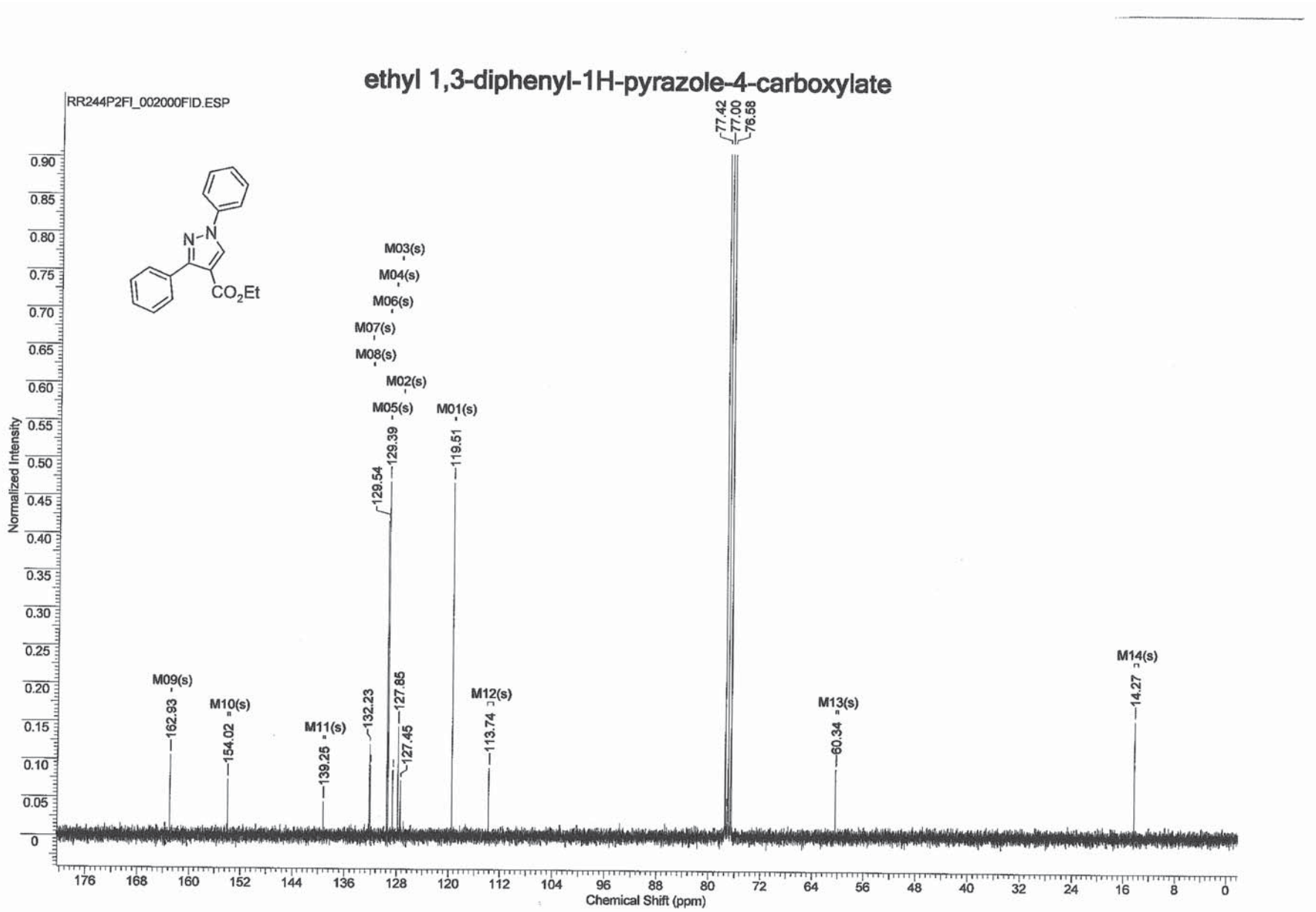
Charge = +1

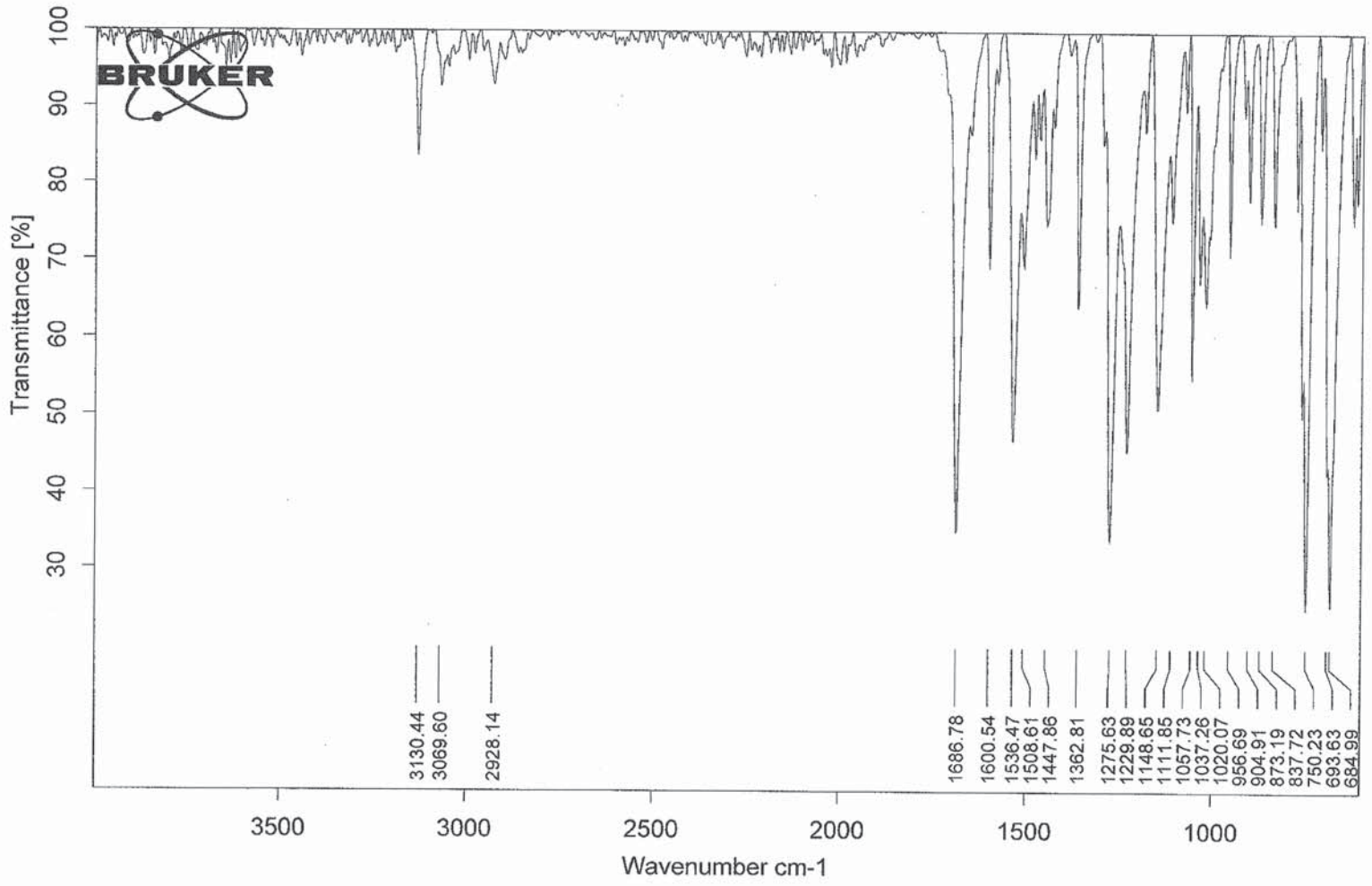
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 315.1105350								
1	**18**	**16**	**2**	**2**	**1**	**315.1103989**	**11.5**	**1.361e-04**
2	17	17	1	5	0	315.1101241	10.0	4.109e-04
3	18	13	5	1	0	315.1114615	15.0	9.265e-04
4	16	14	5	1	1	315.1090562	12.0	1.479e-03
5	15	15	4	4	0	315.1087814	10.5	1.754e-03
6	20	15	2	2	0	315.1128042	14.5	2.269e-03
7	15	18	1	5	1	315.1077188	7.0	2.816e-03
8	13	13	7	3	0	315.1074387	11.0	3.096e-03
9	13	16	4	4	1	315.1063761	7.5	4.159e-03
10	9	18	5	6	1	315.1149294	3.0	4.394e-03



ethyl 1,3-diphenyl-1H-pyrazole-4-carboxylate




ethyl 1,3-diphenyl-1H-pyrazole-4-carboxylate
RR244P2FI_002000FID.ESP
CO2Et
Normalized Intensity
Chemical Shift (ppm)
M01(s)
M02(s)
M03(s)
M04(s)
M05(s)
M06(s)
M07(s)
M08(s)
M09(s)
M10(s)
M11(s)
M12(s)
M13(s)
M14(s)
77.42
77.00
76.58
129.54
129.39
119.51
162.93
154.02
139.25
132.23
127.85
127.45
113.74
60.34
14.27



U:\IR\RR244P2.0	RR244P2	yellow solid	22.05.2015

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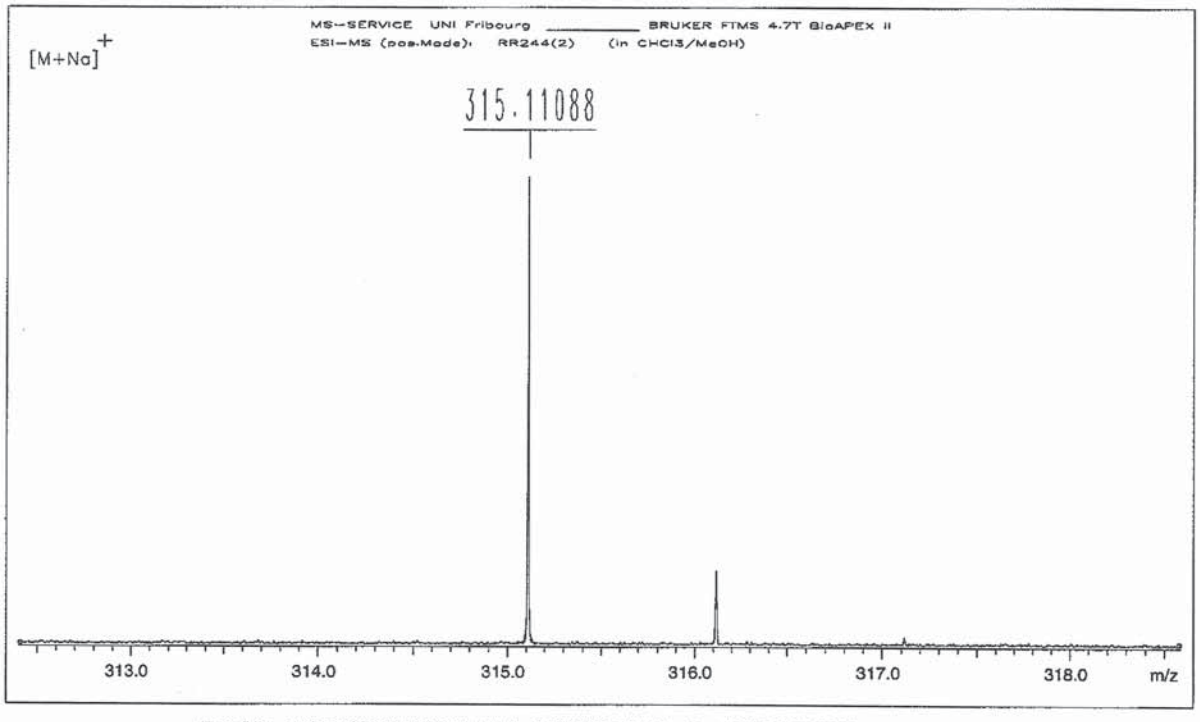
ESI-MS: RR244(2)

XMASS Mass Analysis for /Data/UNI_FR/REMY9287_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 315.1108840

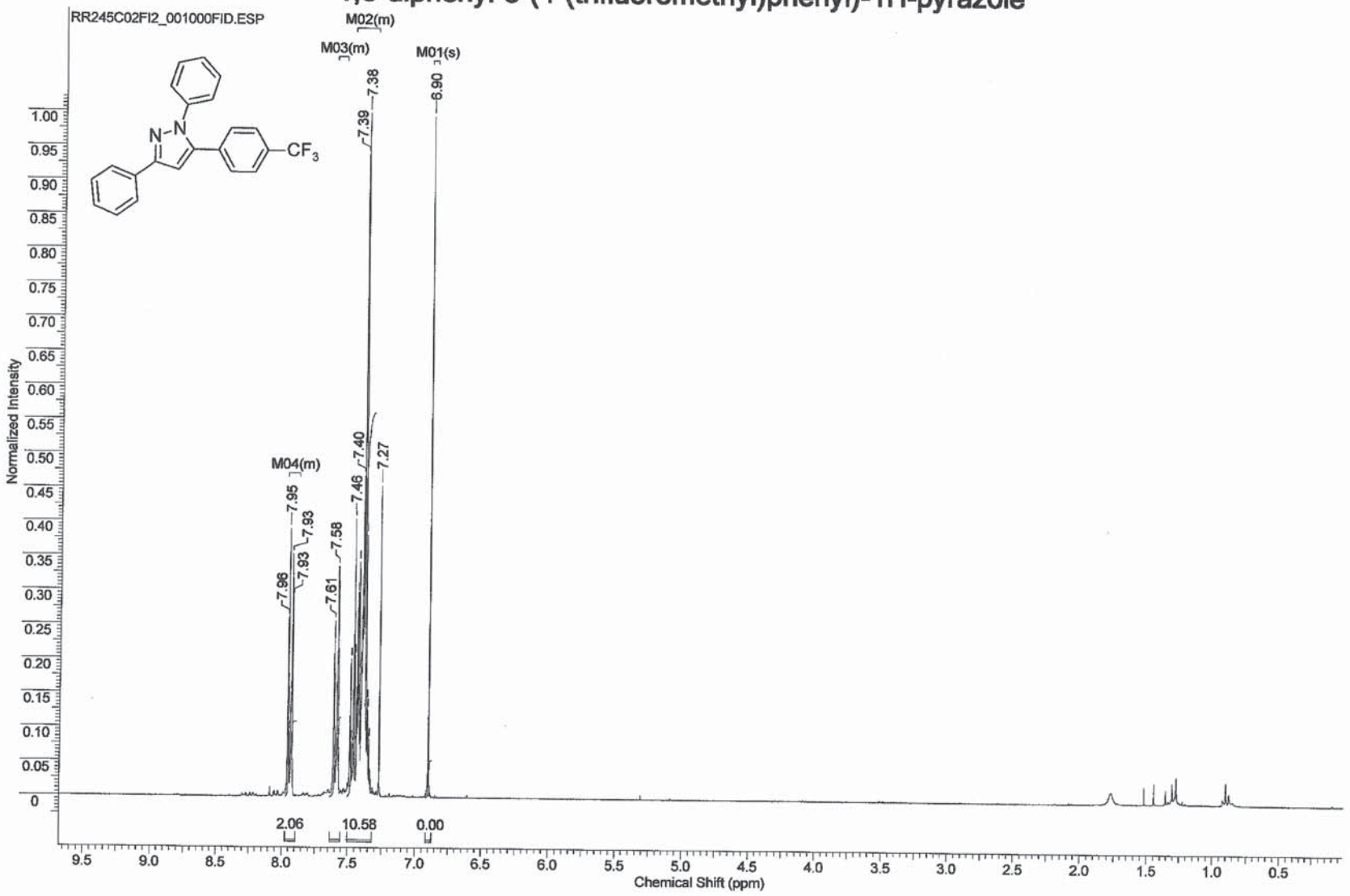
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 315.1108840								
1	**18**	**16**	**2**	**2**	**1**	**315.1103989**	**11.5**	**4.851e-04**
2	18	13	5	1	0	315.1114615	15.0	5.775e-04
3	17	17	1	5	0	315.1101241	10.0	7.599e-04
4	16	14	5	1	1	315.1090562	12.0	1.828e-03
5	20	15	2	2	0	315.1128042	14.5	1.920e-03
6	15	15	4	4	0	315.1087814	10.5	2.103e-03
7	15	18	1	5	1	315.1077188	7.0	3.165e-03
8	13	13	7	3	0	315.1074387	11.0	3.445e-03
9	9	18	5	6	1	315.1149294	3.0	4.045e-03
10	13	16	4	4	1	315.1063761	7.5	4.508e-03

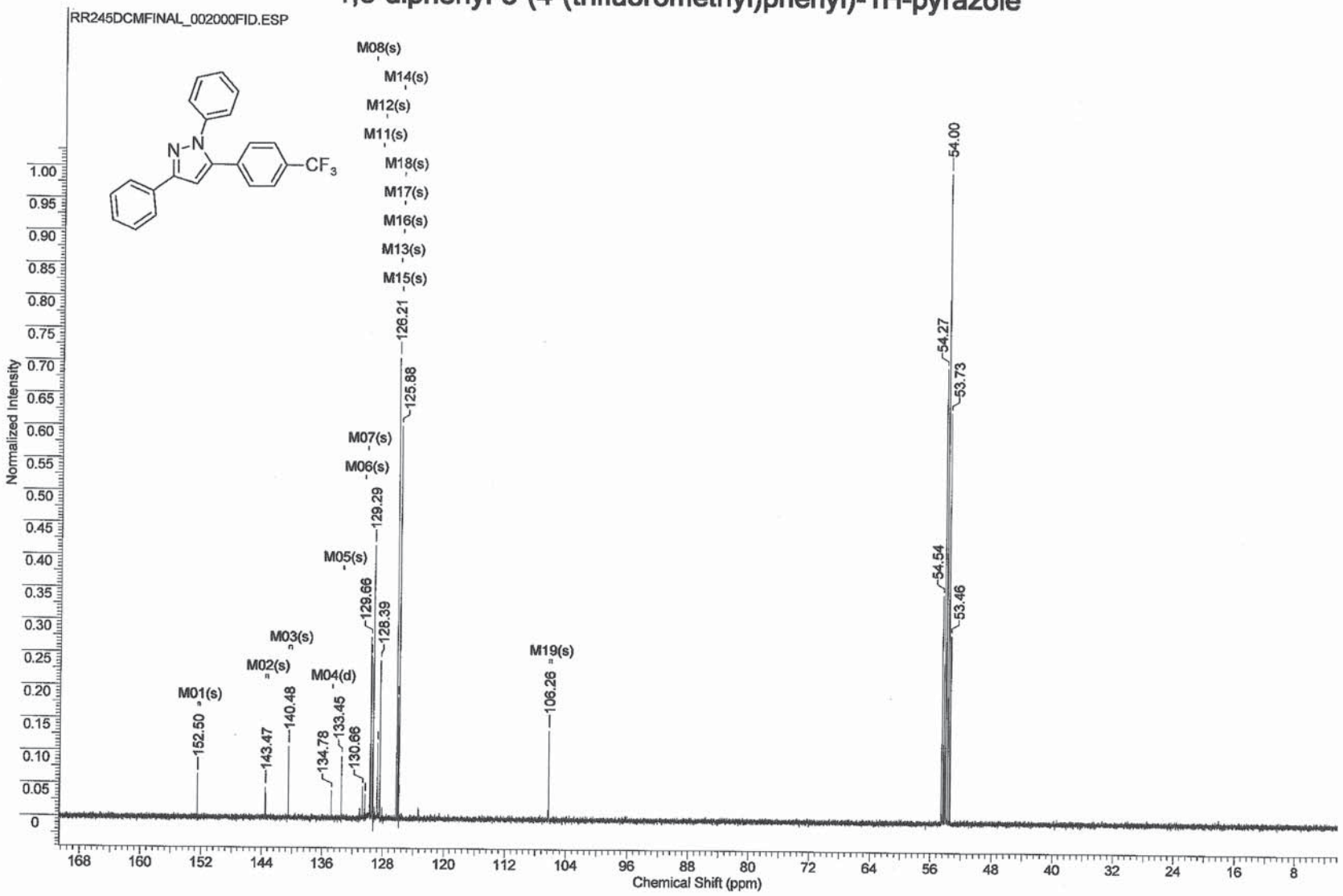


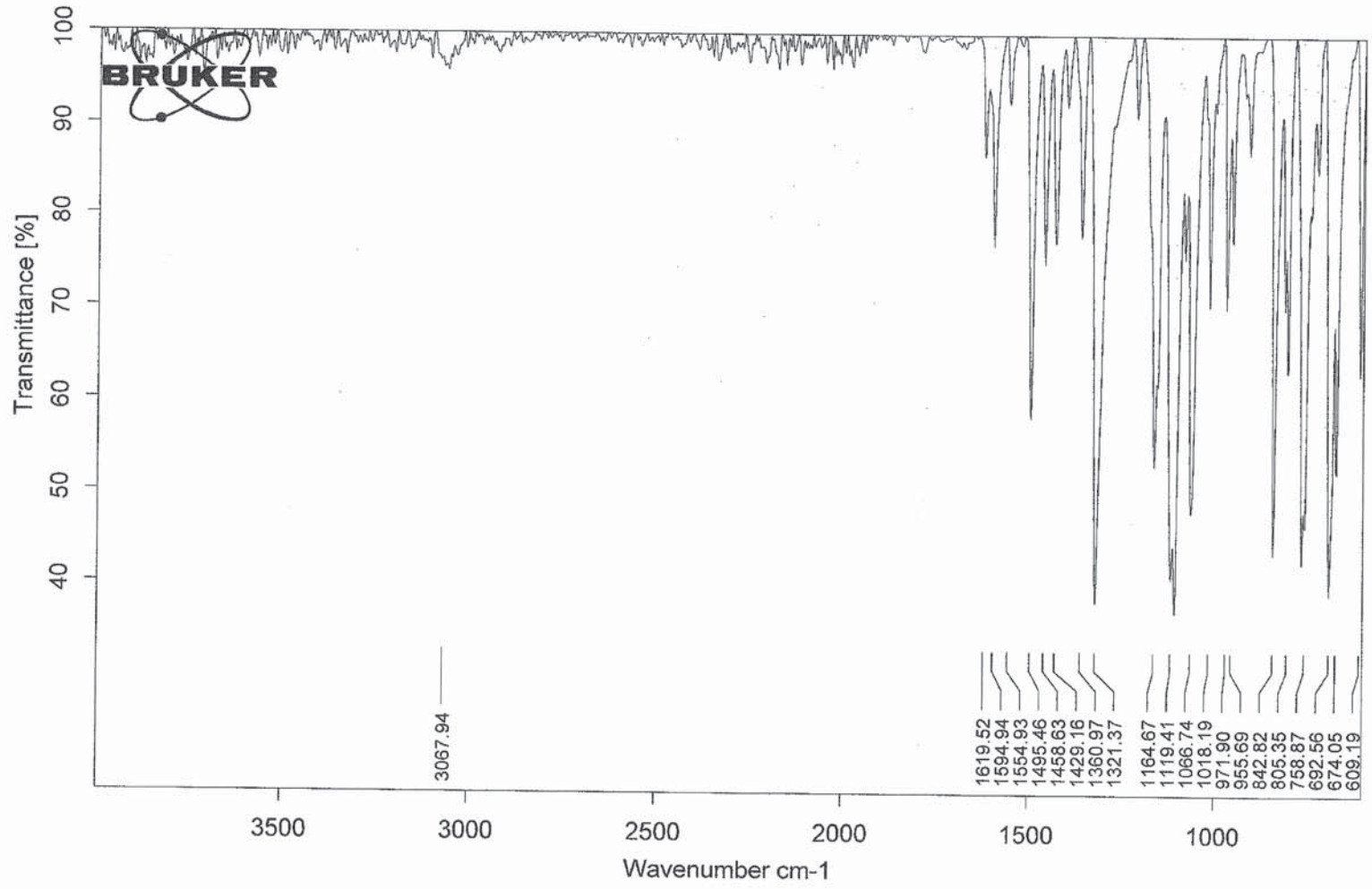
/Data/UNI_FR/REMY9287_ESI/1/pdata/1 FTMS USER Mon Apr 13 15:52:21 2015

1,3-diphenyl-5-(4-(trifluoromethyl)phenyl)-1H-pyrazole



1,3-diphenyl-5-(4-(trifluoromethyl)phenyl)-1H-pyrazole





U:\IR\RR245P2.0	RR245P2	yellow solid	22.05.2015

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BRUKER **FTMS 4.7T BioAPEX II**

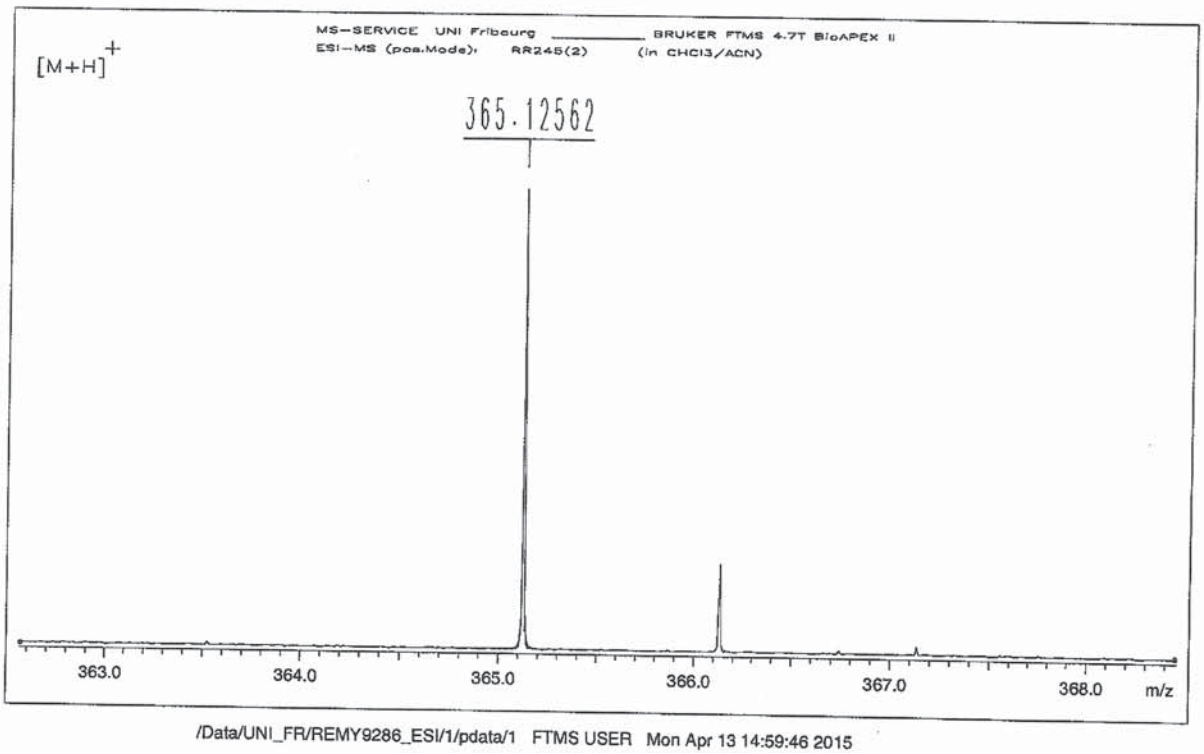
ESI-MS: RR245(2)

XMASS Mass Analysis for /Data/UNI_FR/REMY9286_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

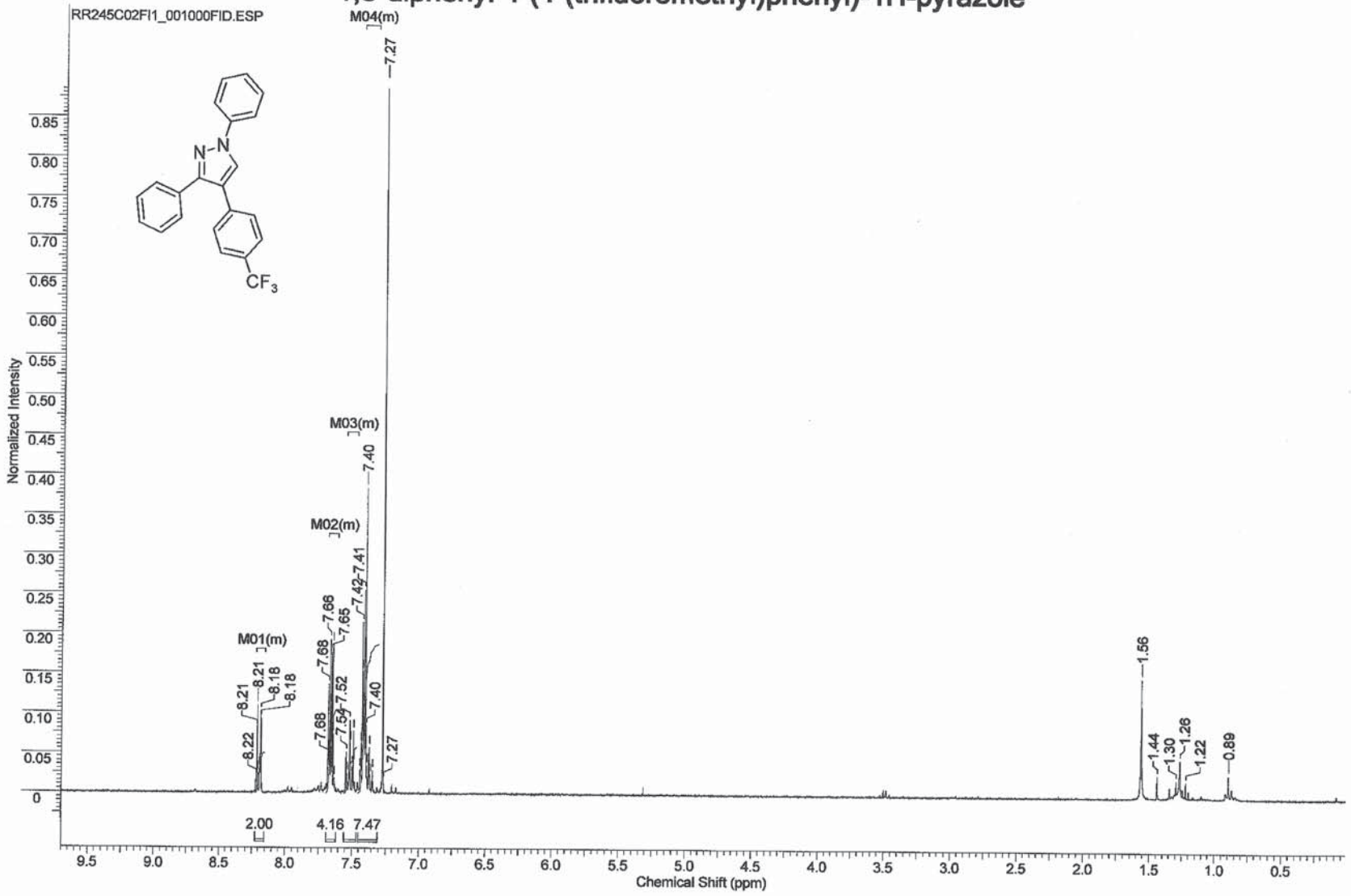
Ion mass = 365.1256240

Charge = +1

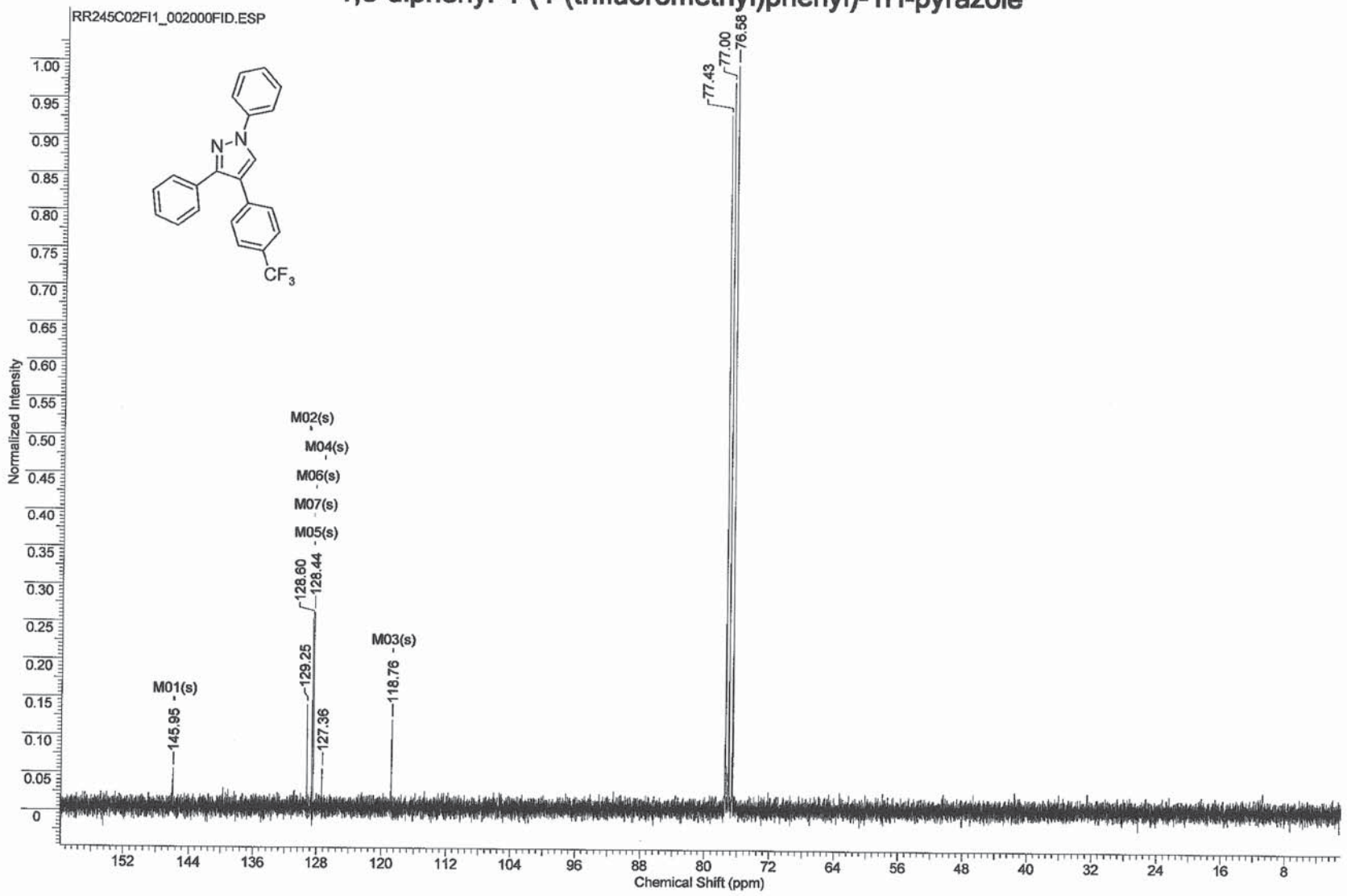
#	C	H	F	N	mass	DBE	error
*** Mass Analysis for mass 365.1256240							
1	**22**	**16**	**3**	**2**	**365.1260095**	**14.5**	**3.855e-04**
2	20	16	5	1	365.1197419	11.0	5.882e-03
3	15	15	6	4	365.1195421	7.5	6.082e-03
4	16	17	6	3	365.1321182	7.0	6.494e-03
5	21	14	3	3	365.1134335	15.0	1.219e-02
6	18	17	4	4	365.1383858	10.5	1.276e-02
7	23	18	3	1	365.1385856	14.0	1.296e-02
8	19	14	5	2	365.1071659	11.5	1.846e-02
9	17	19	6	2	365.1446942	6.5	1.907e-02
10	20	12	3	4	365.1008574	15.5	2.477e-02

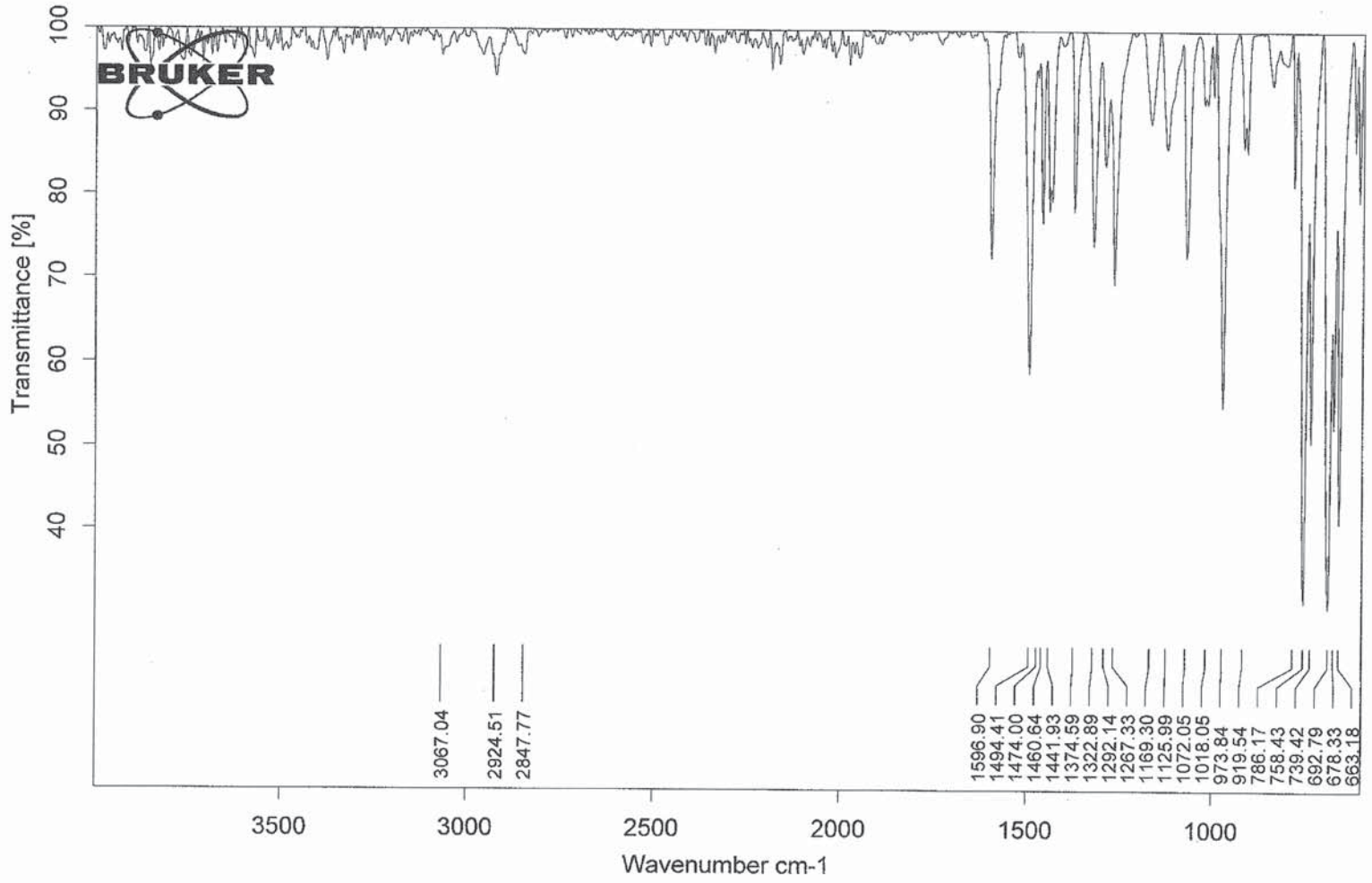


1,3-diphenyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrazole



1,3-diphenyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrazole





U:\IR\RR245P1.0	RR245P1	yellow solid	22.05.2015

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BRUKER FTMS 4.7T BioAPEX II

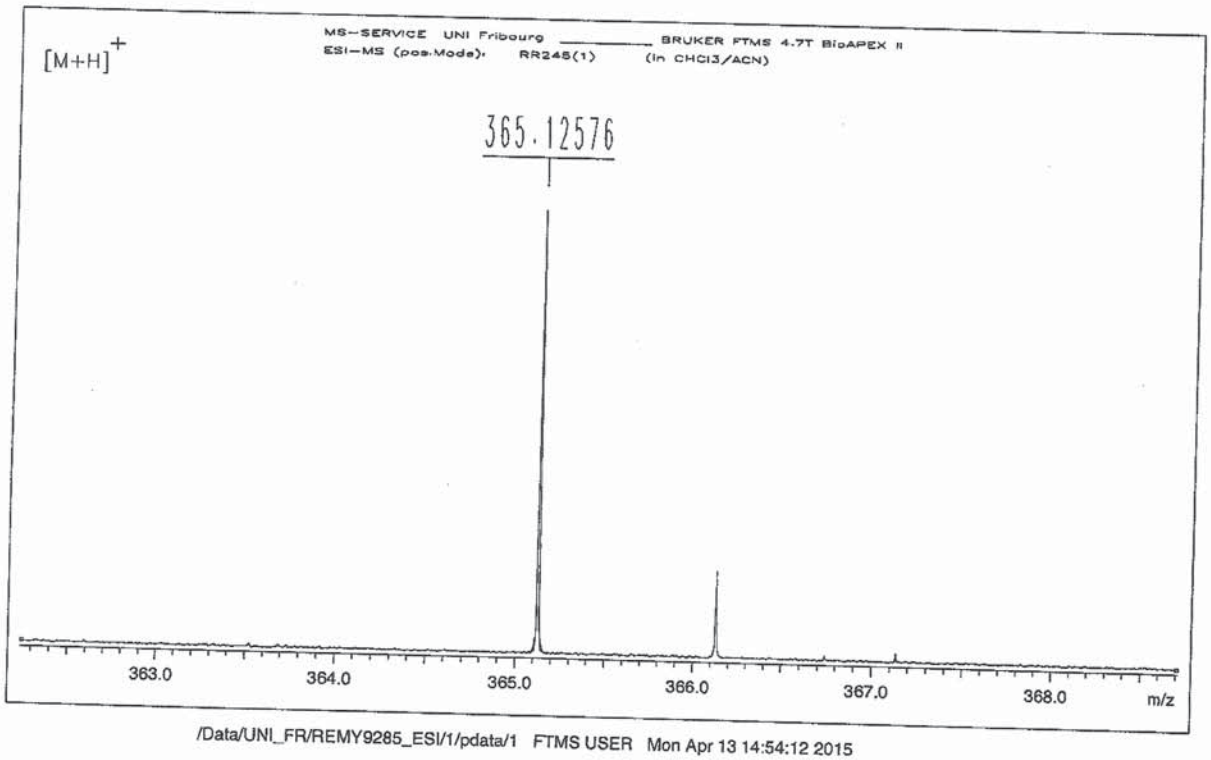
ESI-MS: RR245(1)

XMASS Mass Analysis for /Data/UNI_FR/REMY9285_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

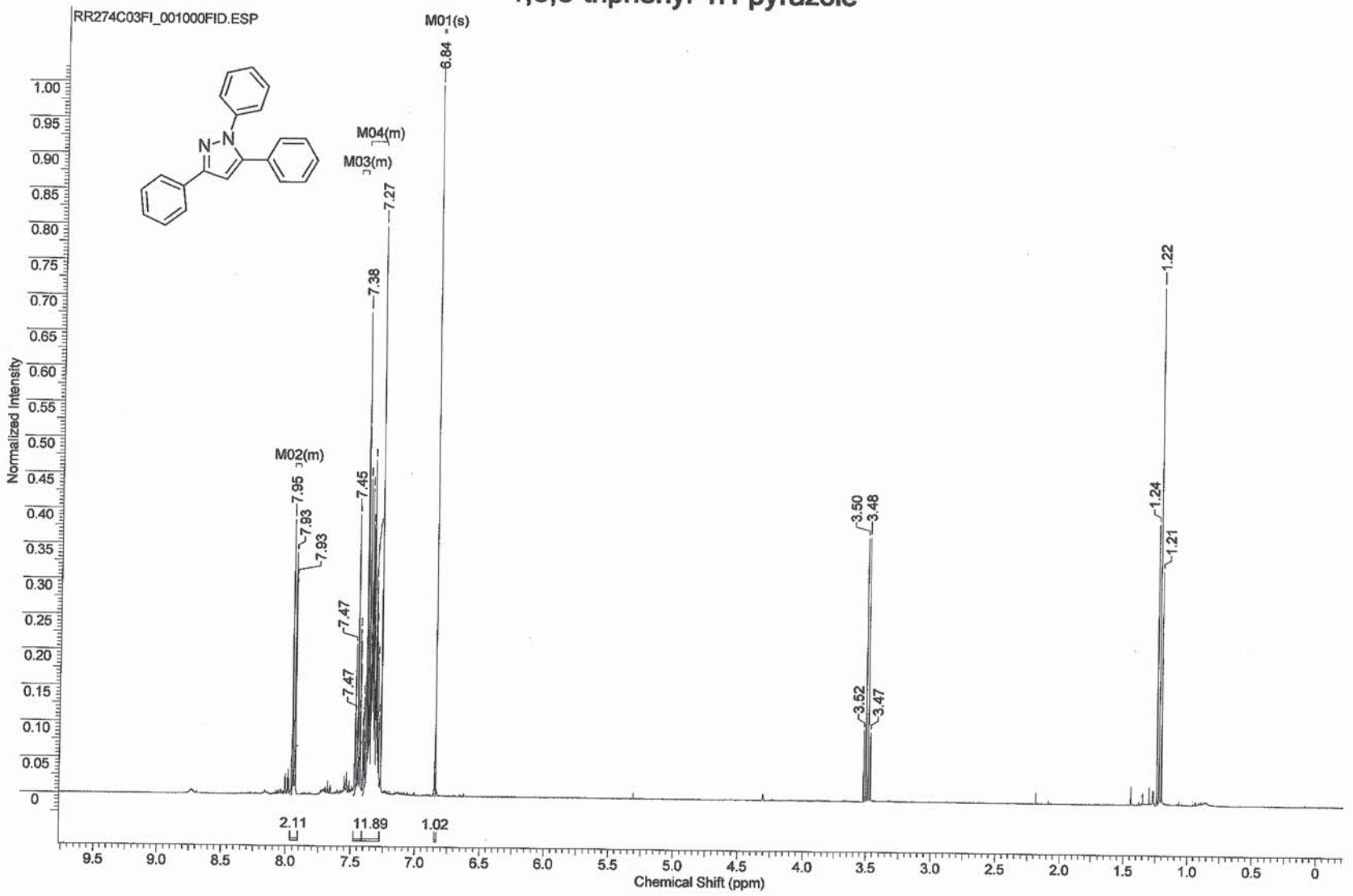
Ion mass = 365.1257590

Charge = +1

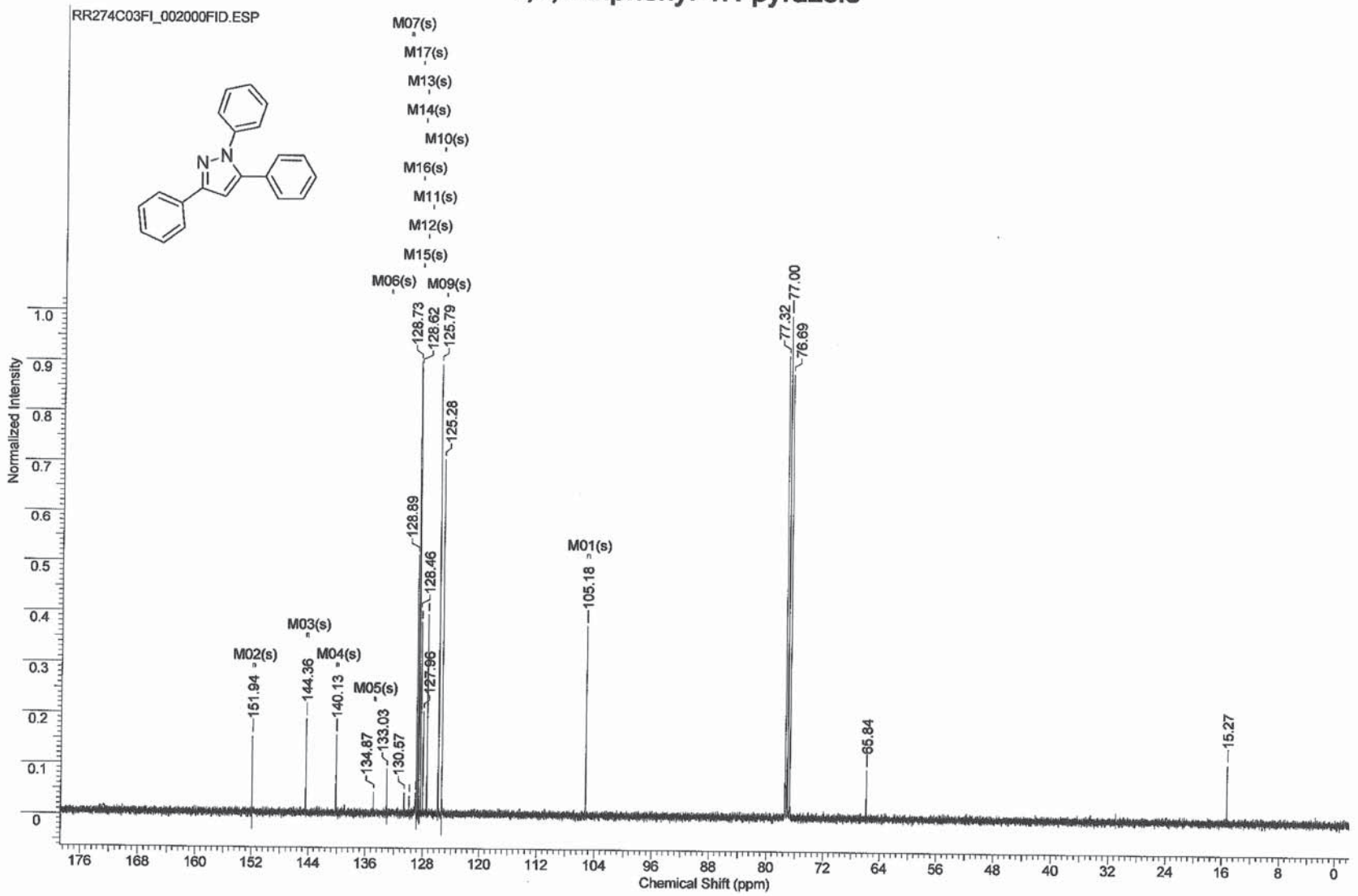
#	C	H	F	N	mass	DBE	error
*** Mass Analysis for mass 365.1257590							
1	**22**	**16**	**3**	**2**	**365.1260095**	**14.5**	**2.505e-04**
2	20	16	5	1	365.1197419	11.0	6.017e-03
3	15	15	6	4	365.1195421	7.5	6.217e-03
4	16	17	6	3	365.1321182	7.0	6.359e-03
5	21	14	3	3	365.1134335	15.0	1.233e-02
6	18	17	4	4	365.1383858	10.5	1.263e-02
7	23	18	3	1	365.1385856	14.0	1.283e-02
8	19	14	5	2	365.1071659	11.5	1.859e-02
9	17	19	6	2	365.1446942	6.5	1.894e-02
10	20	12	3	4	365.1008574	15.5	2.490e-02

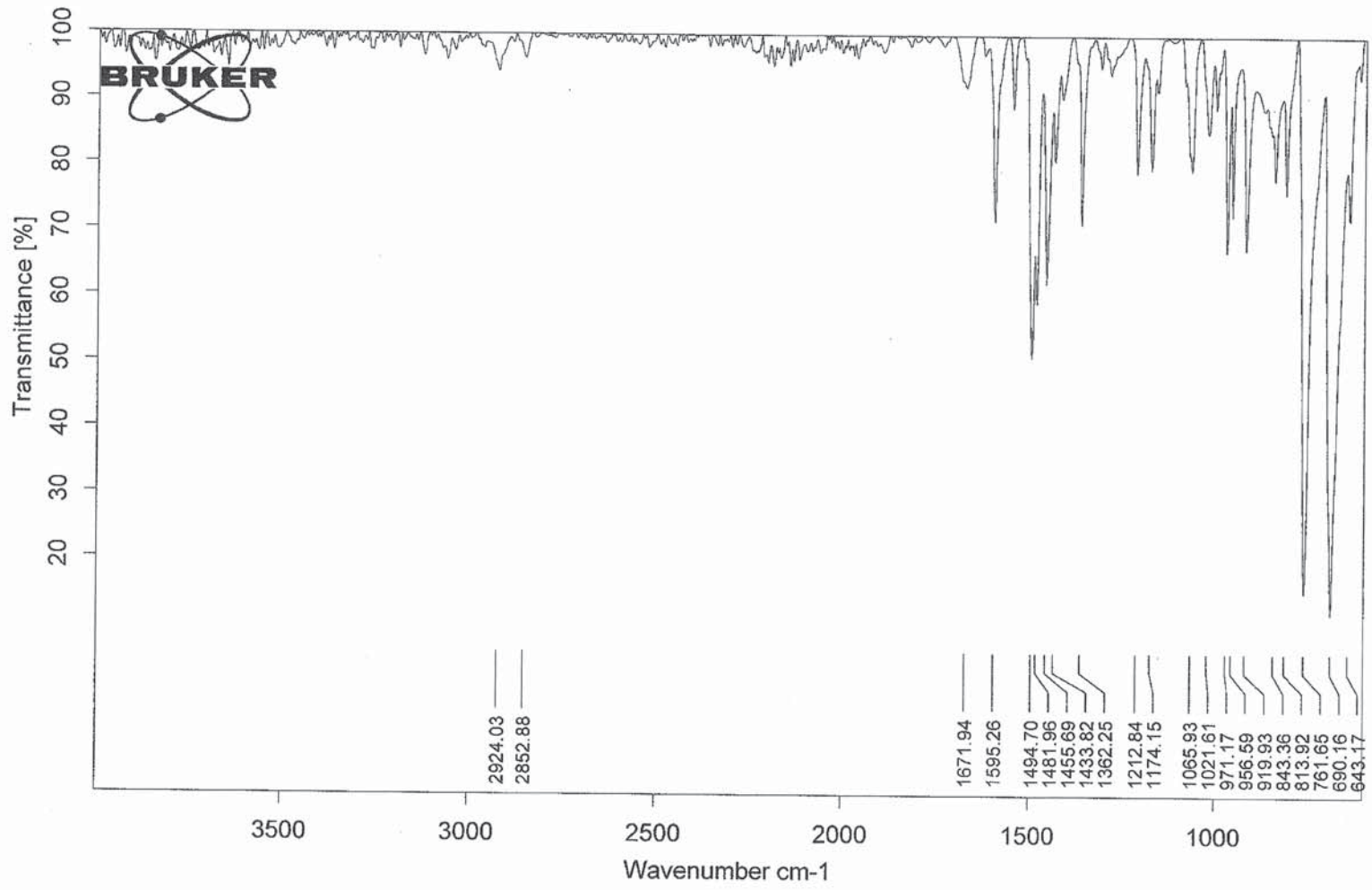


1,3,5-triphenyl-1H-pyrazole



1,3,5-triphenyl-1H-pyrazole





U:\IR\RR274maj.0	RR274maj	yellow solid	22.05.2015

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BRUKER **FTMS 4.7T BioAPEX II**

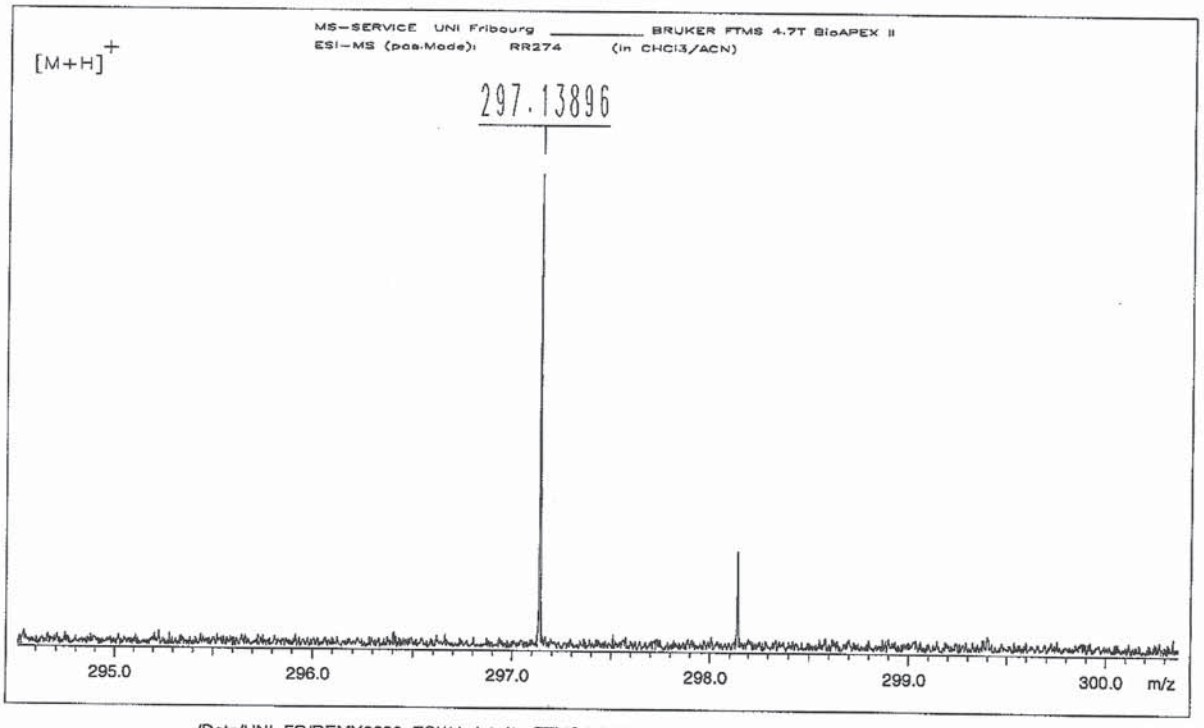
ESI-MS: RR274

XMASS Mass Analysis for /Data/UNI_FR/REMY9298_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 297.1389600

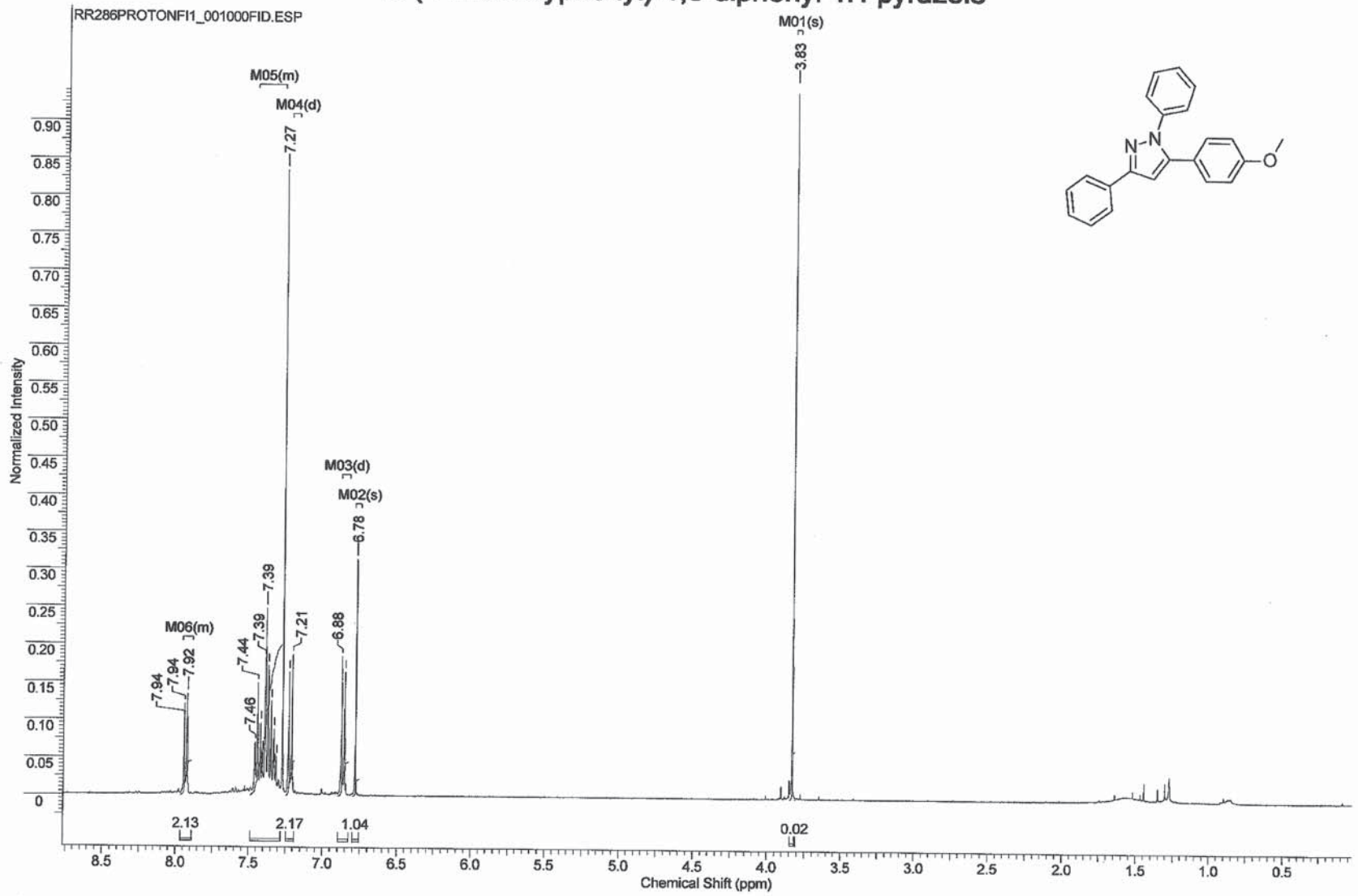
Charge = +1

#	C	H	N	mass	DBE	error
*** Mass Analysis for mass 297.1389600						
1	**21**	**17**	**2**	**297.1386250**	**14.5**	**3.350e-04**
2	13	15	9	297.1444929	11.0	5.533e-03
3	12	13	10	297.1319169	11.5	7.043e-03
4	22	19	1	297.1512010	14.0	1.224e-02
5	20	15	3	297.1260489	15.0	1.291e-02
6	14	17	8	297.1570690	10.5	1.811e-02
7	19	13	4	297.1134729	15.5	2.549e-02
8	15	19	7	297.1696451	10.0	3.069e-02
9	18	11	5	297.1008968	16.0	3.806e-02
10	16	21	6	297.1822211	9.5	4.326e-02

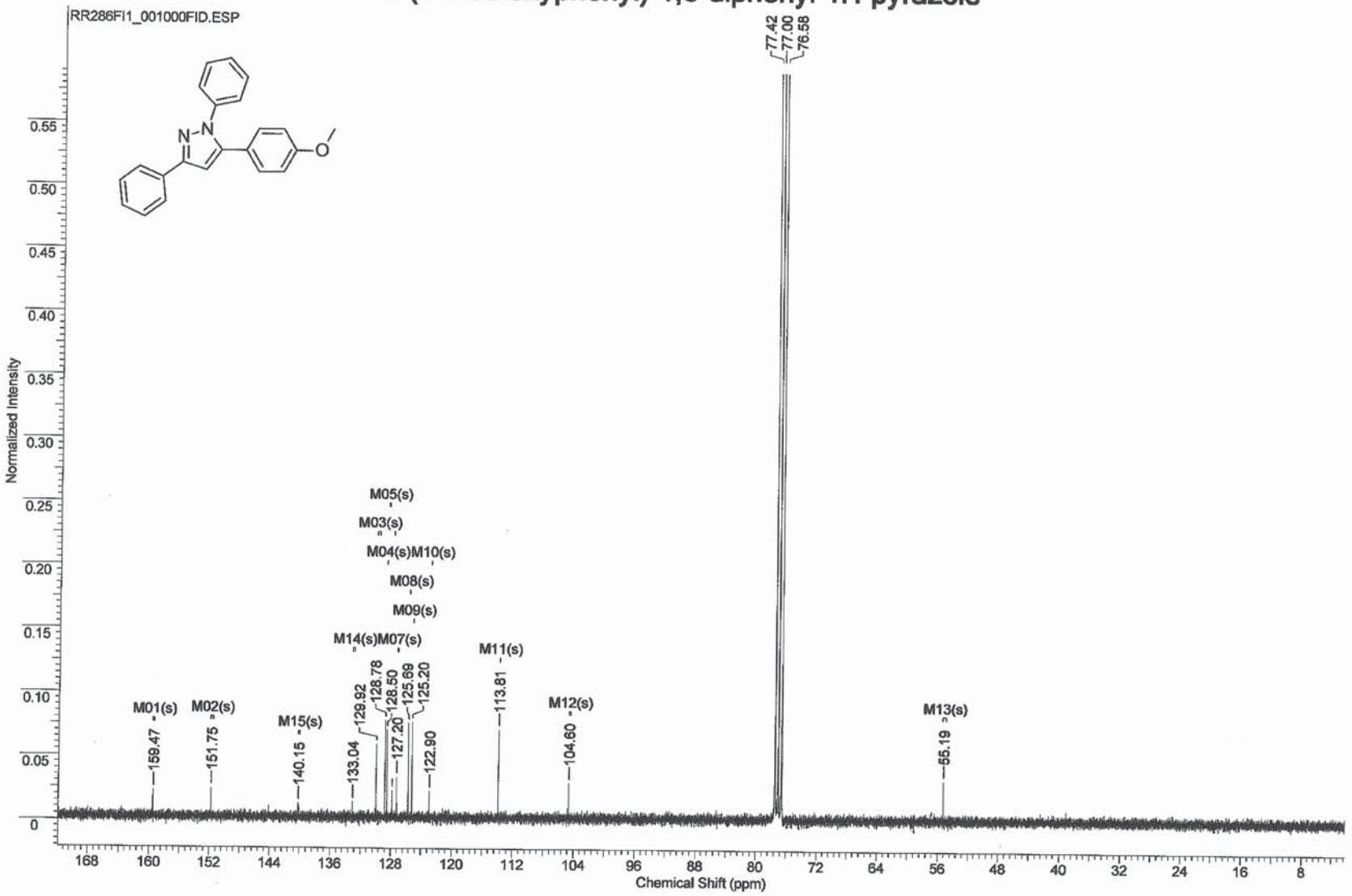


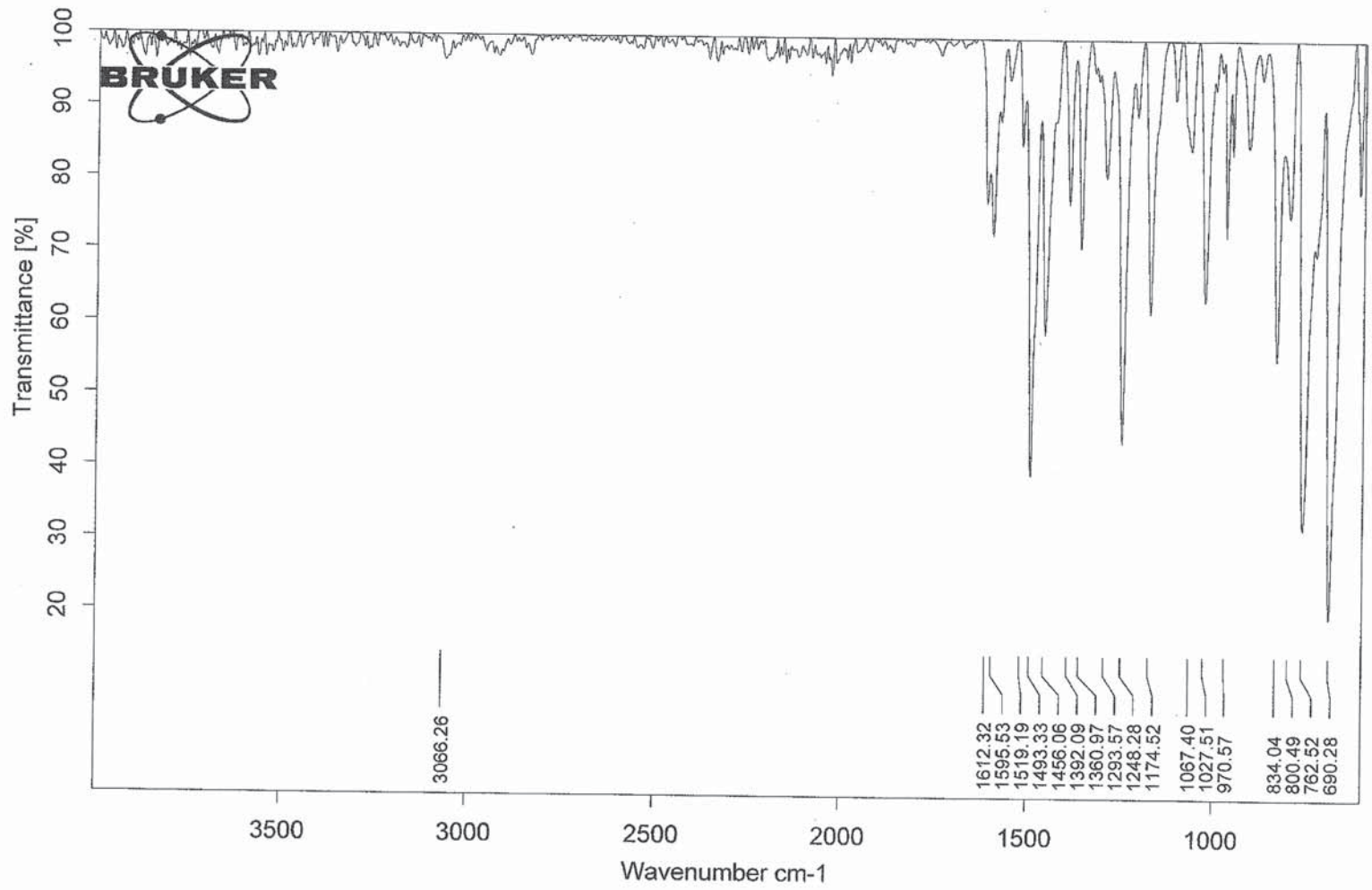
/Data/UNI_FR/REMY9298_ESI/1/pdata/1 FTMS USER Mon Apr 13 15:09:18 2015

5-(4-methoxyphenyl)-1,3-diphenyl-1H-pyrazole



5-(4-methoxyphenyl)-1,3-diphenyl-1H-pyrazole





U:\IR\RR286P1.0	RR286P1	brown solid	22.05.2015

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FTMS 4.7T BioAPEX II

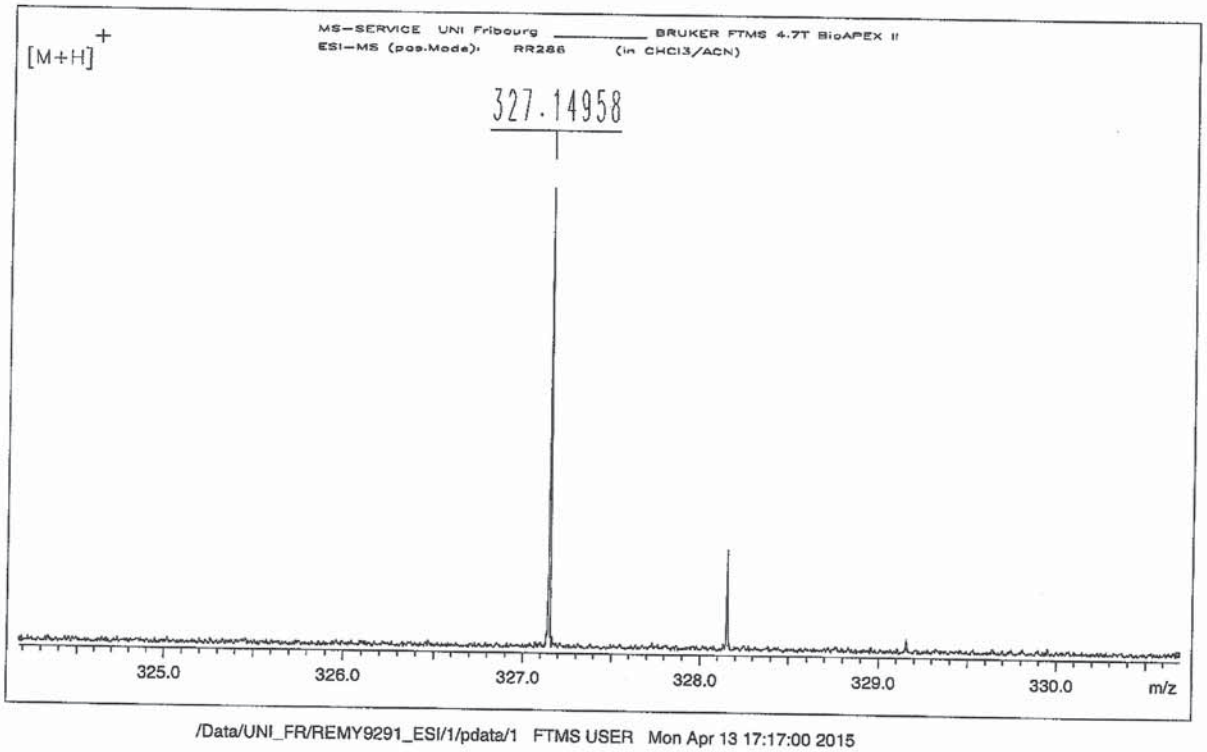
ESI-MS: RR286

XMASS Mass Analysis for /Data/UNI_FR/REMY9291_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 327.1495780

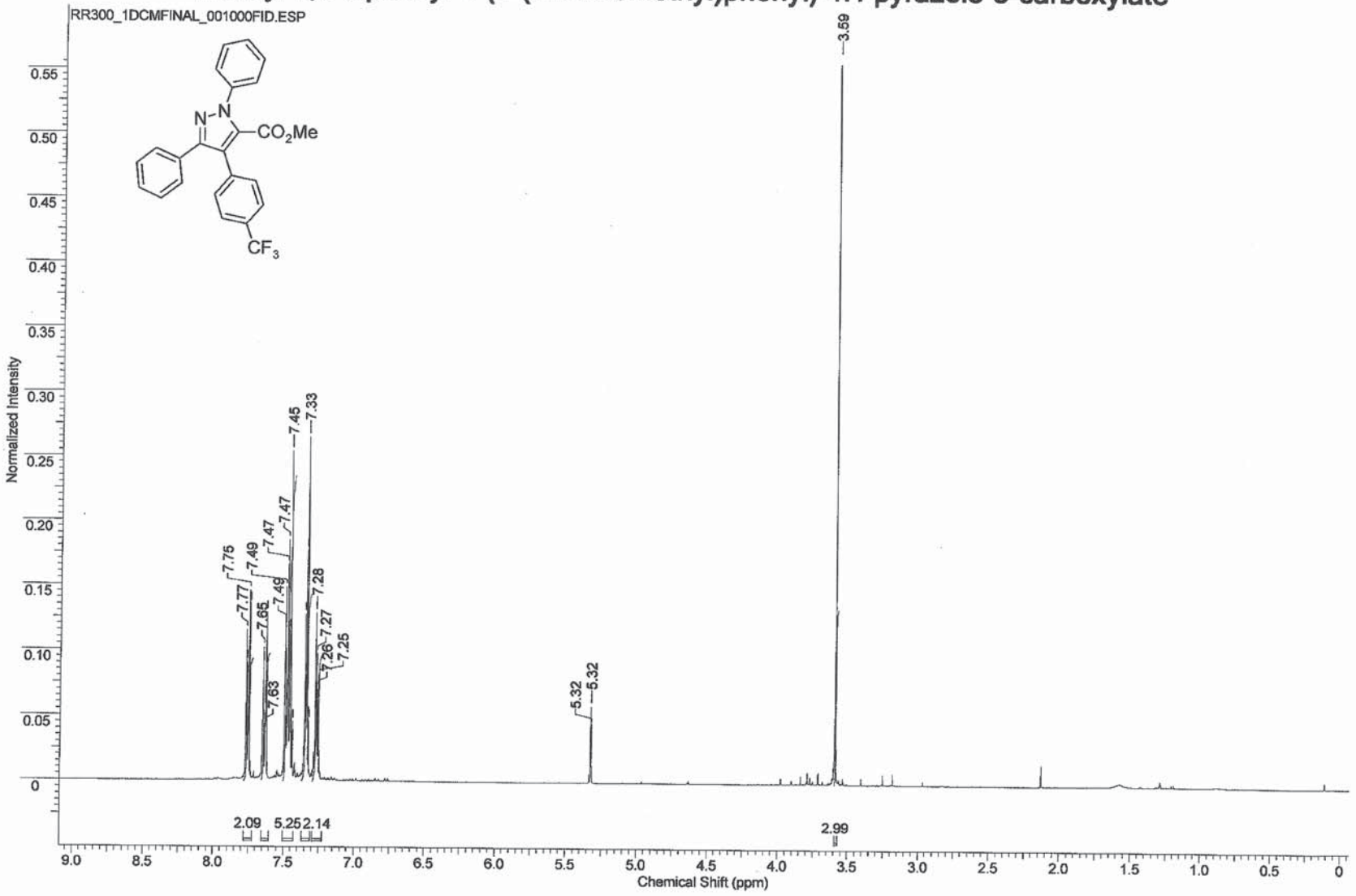
Charge = +1

#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 327.1495780							
1	**22**	**19**	**2**	**1**	**327.1491897**	**14.5**	**3.883e-04**
2	6	19	10	6	327.1483548	2.5	1.223e-03
3	11	19	8	4	327.1523776	6.5	2.800e-03
4	19	21	1	4	327.1465096	10.0	3.068e-03
5	13	21	5	5	327.1537202	6.0	4.142e-03
6	17	19	4	3	327.1451669	10.5	4.411e-03
7	14	17	9	1	327.1550576	11.0	5.480e-03
8	15	23	2	6	327.1550629	5.5	5.485e-03
9	15	17	7	2	327.1438242	11.0	5.754e-03
10	16	19	6	2	327.1564003	10.5	6.822e-03

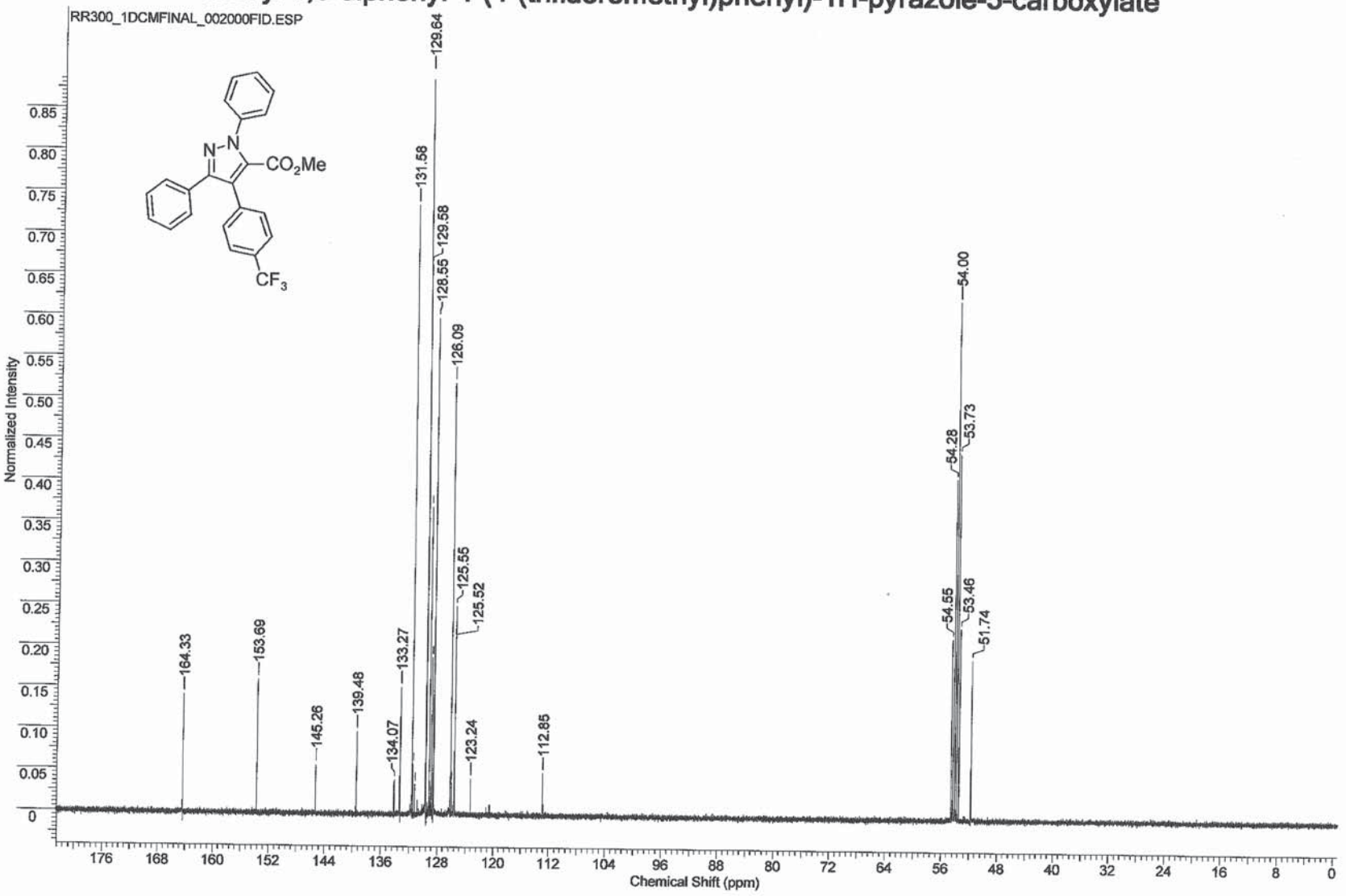


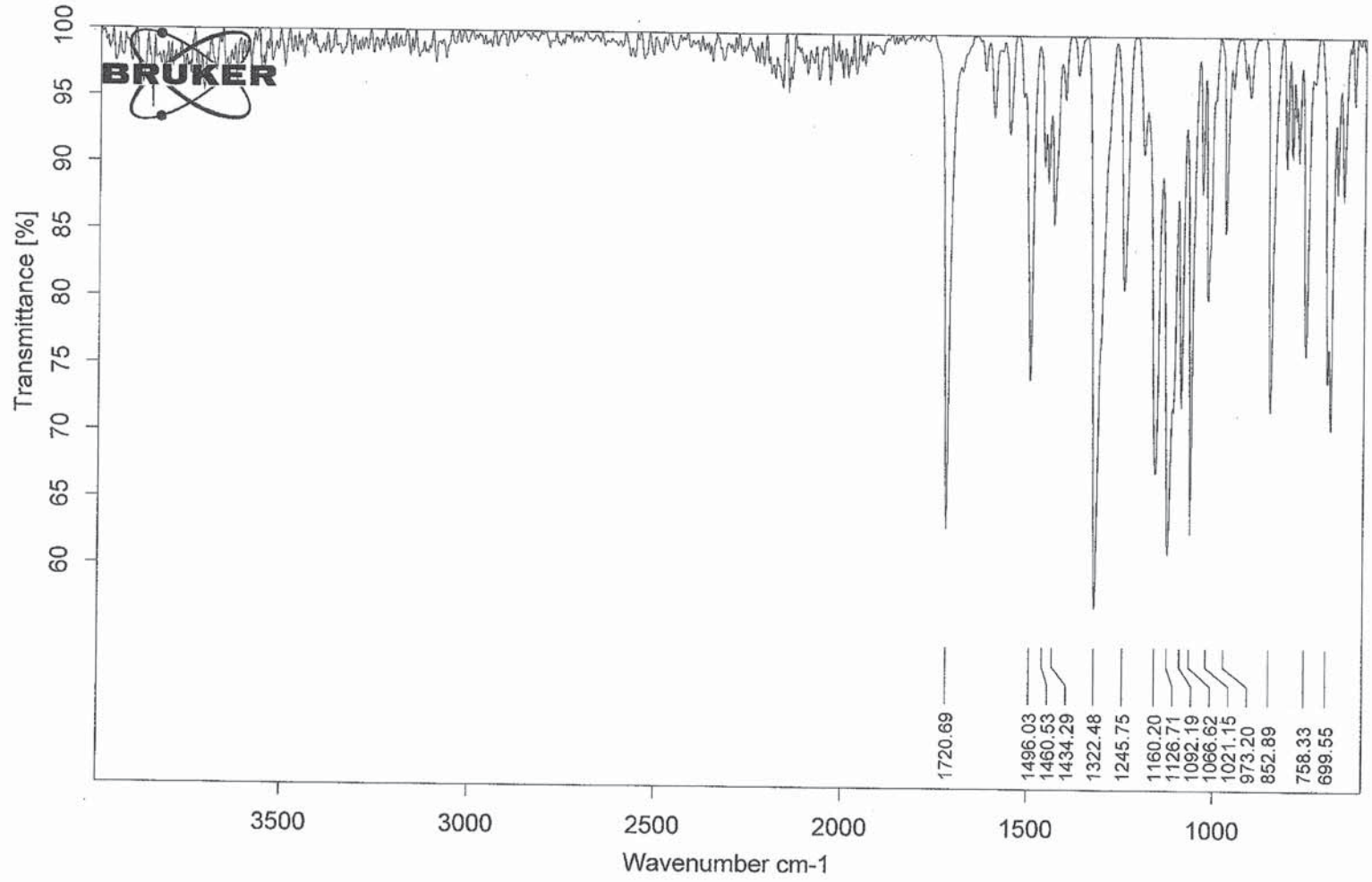
/Data/UNI_FR/REMY9291_ESI/1/pdata/1 FTMS USER Mon Apr 13 17:17:00 2015

methyl 1,3-diphenyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrazole-5-carboxylate



methyl 1,3-diphenyl-4-(4-(trifluoromethyl)phenyl)-1H-pyrazole-5-carboxylate





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BRUKER FTMS 4.7T BioAPEX II

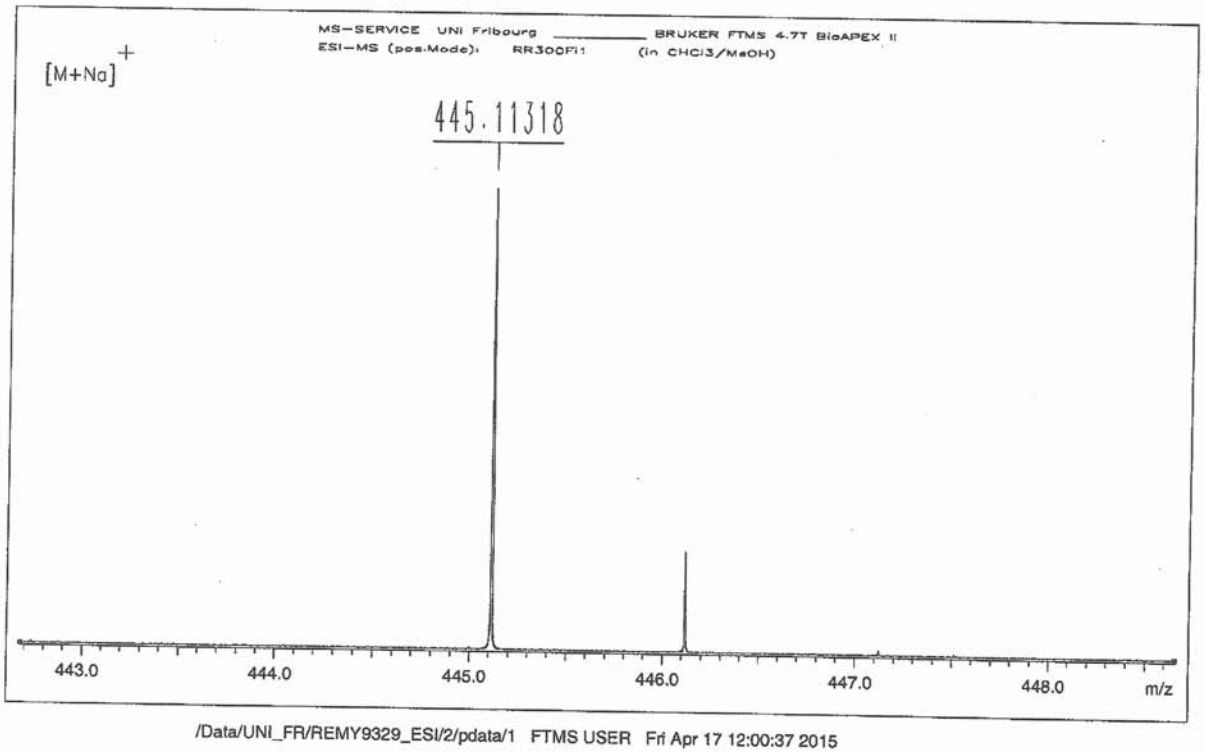
ESI-MS: RR300Fi1

XMASS Mass Analysis for /Data/UNI_FR/REMY9329_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 445.1131810

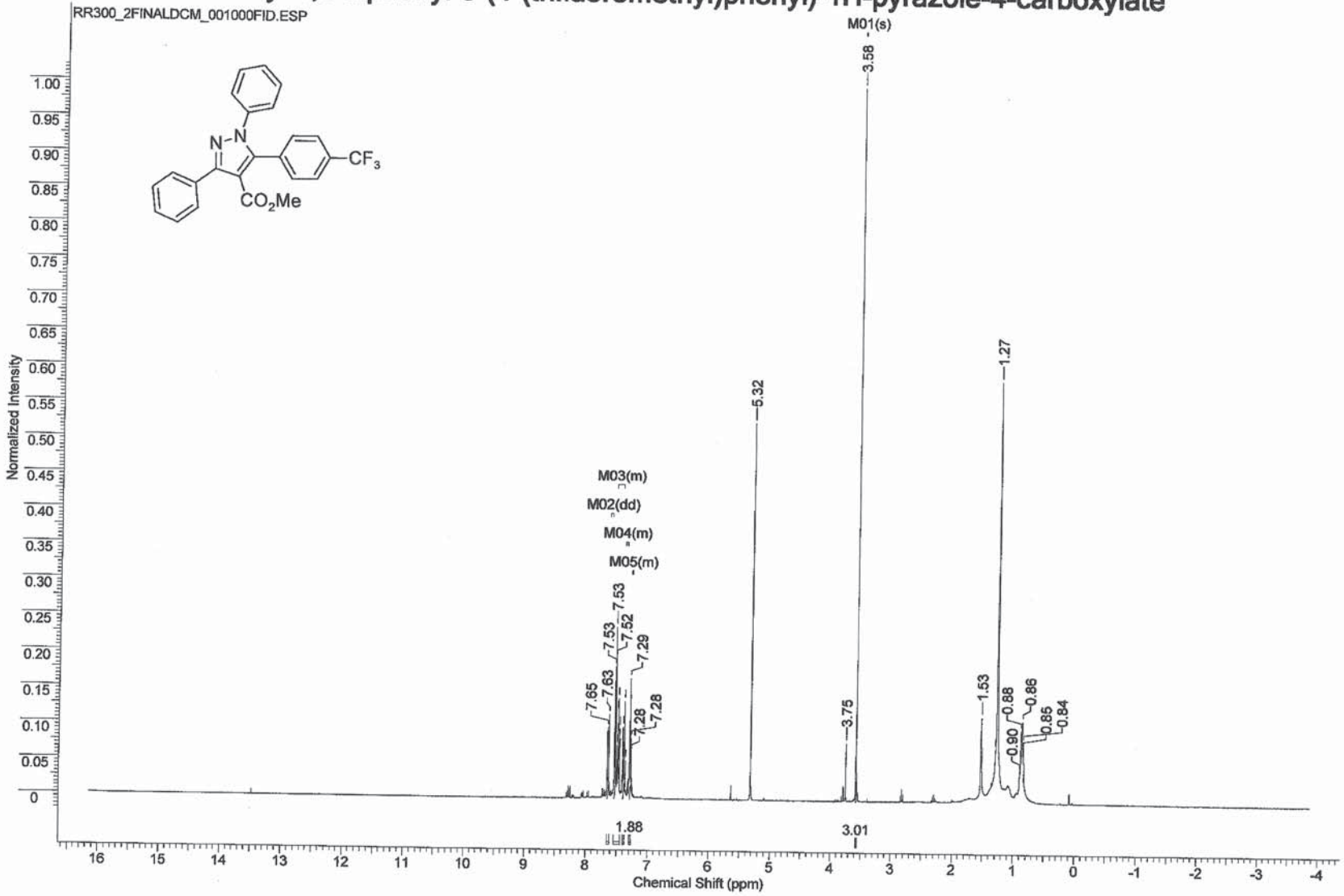
Charge = +1

#	C	H	F	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 445.1131810									
1	**24**	**17**	**3**	**2**	**2**	**1**	**445.1134335**	**15.5**	**2.525e-04**
2	27	16	2	2	1	1	445.1122906	19.5	8.904e-04
3	26	17	2	1	4	0	445.1120159	18.0	1.165e-03
4	21	16	3	4	4	0	445.1118160	14.5	1.365e-03
5	21	18	4	2	3	1	445.1145763	11.5	1.395e-03
6	29	15	2	2	1	0	445.1146959	22.5	1.515e-03
7	29	16	1	1	3	0	445.1108730	22.0	2.308e-03
8	24	15	2	4	3	0	445.1106732	18.5	2.508e-03
9	18	19	5	2	4	1	445.1157192	7.5	2.538e-03
10	26	16	3	2	2	0	445.1158388	18.5	2.658e-03

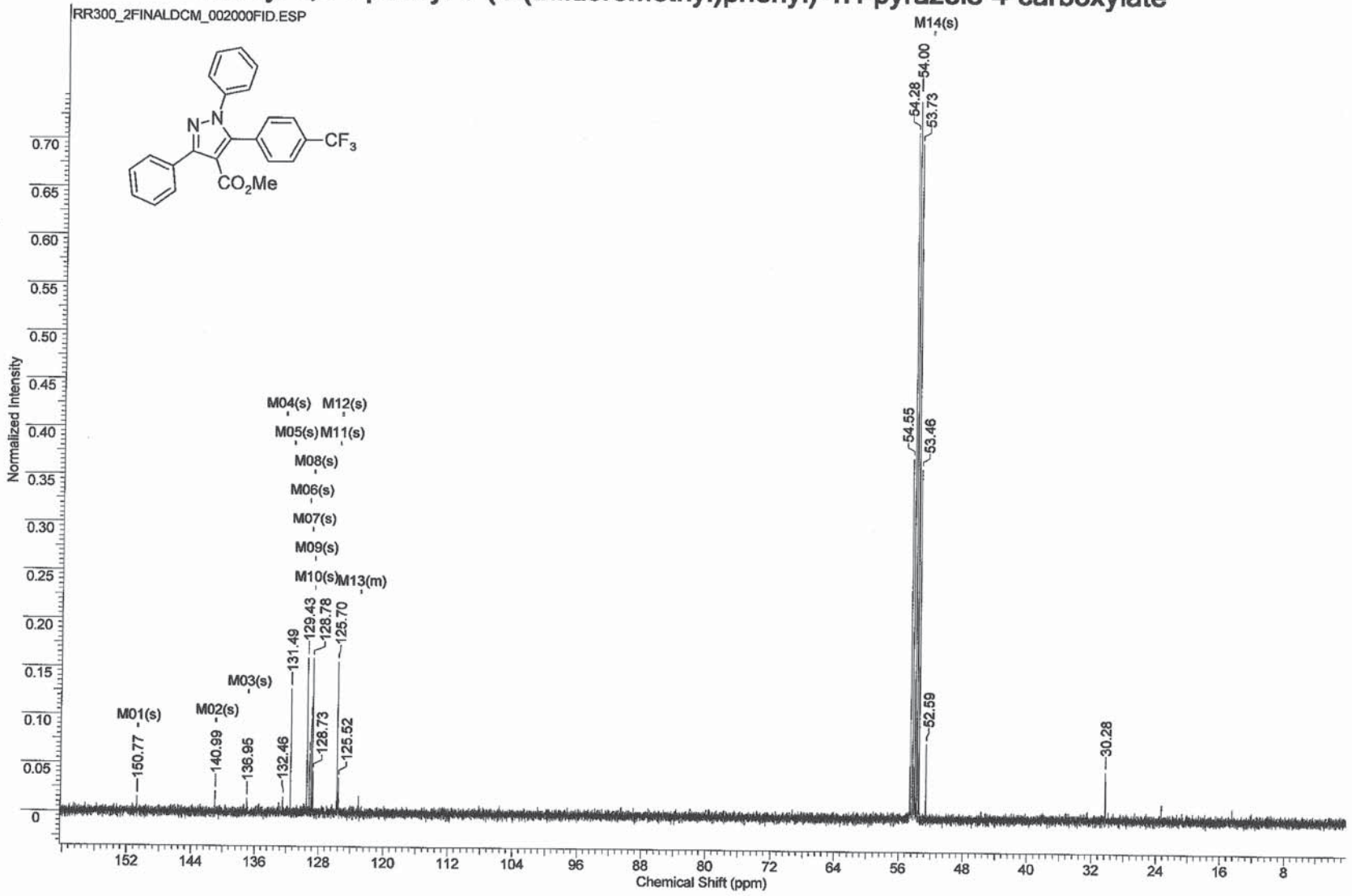


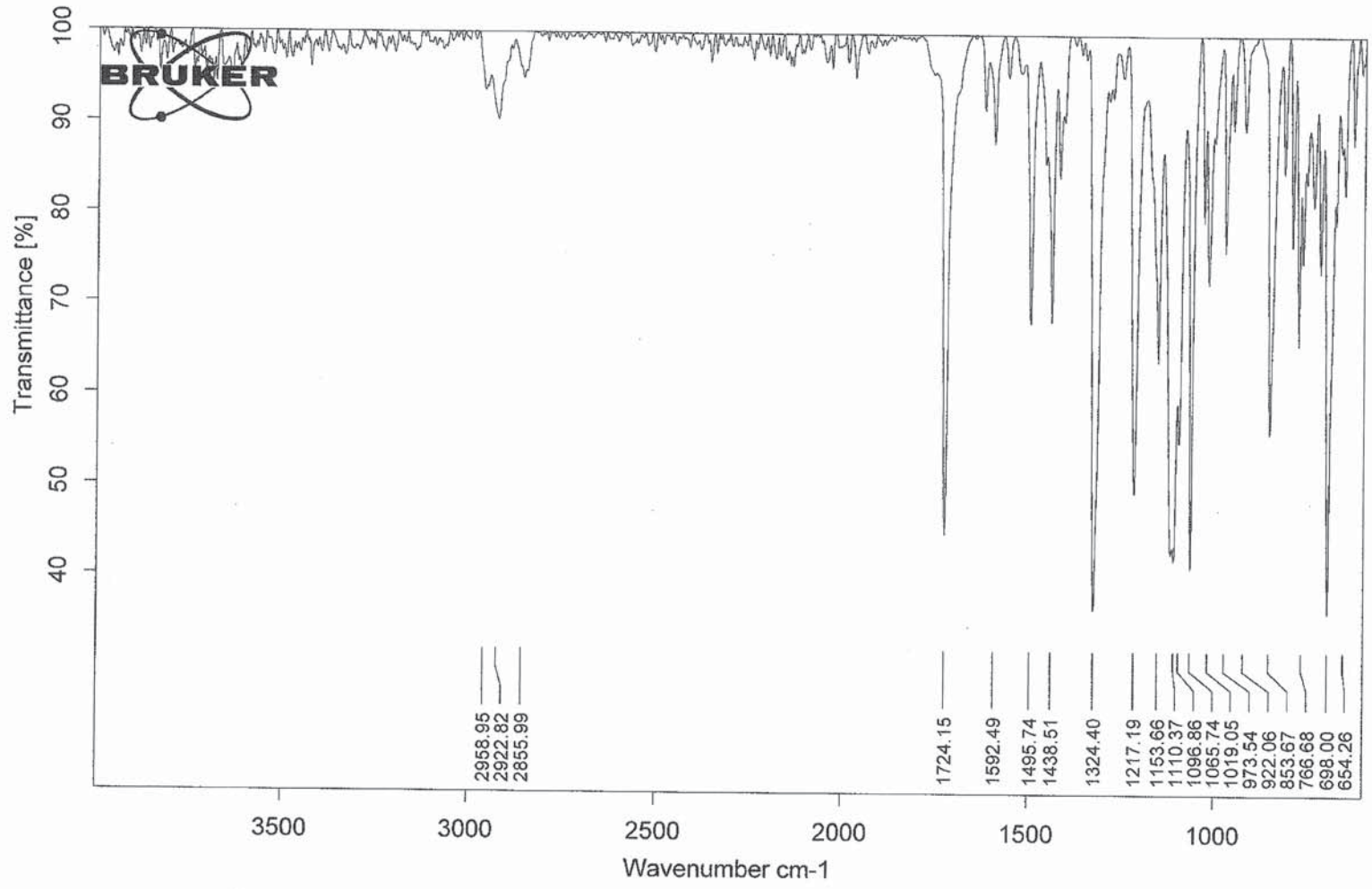
/Data/UNI_FR/REMY9329_ESI/2/pdata/1 FTMS USER Fri Apr 17 12:00:37 2015

methyl 1,3-diphenyl-5-(4-(trifluoromethyl)phenyl)-1H-pyrazole-4-carboxylate



methyl 1,3-diphenyl-5-(4-(trifluoromethyl)phenyl)-1H-pyrazole-4-carboxylate





U:\IR\RR300P2.0	RR300P2	clear brow solid	22.05.2015

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BRUKER FTMS 4.7T BioAPEX II

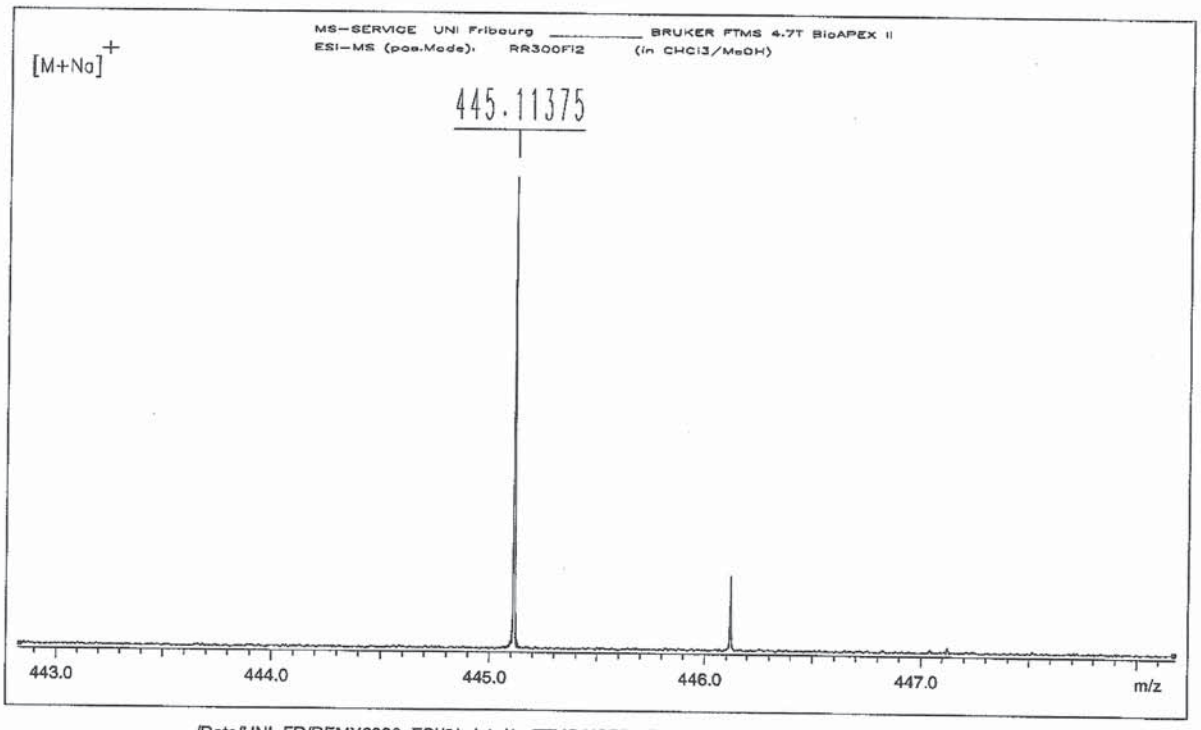
ESI-MS: RR300Fi2

XMASS Mass Analysis for /Data/UNI_FR/REMY9328_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 445.1137470

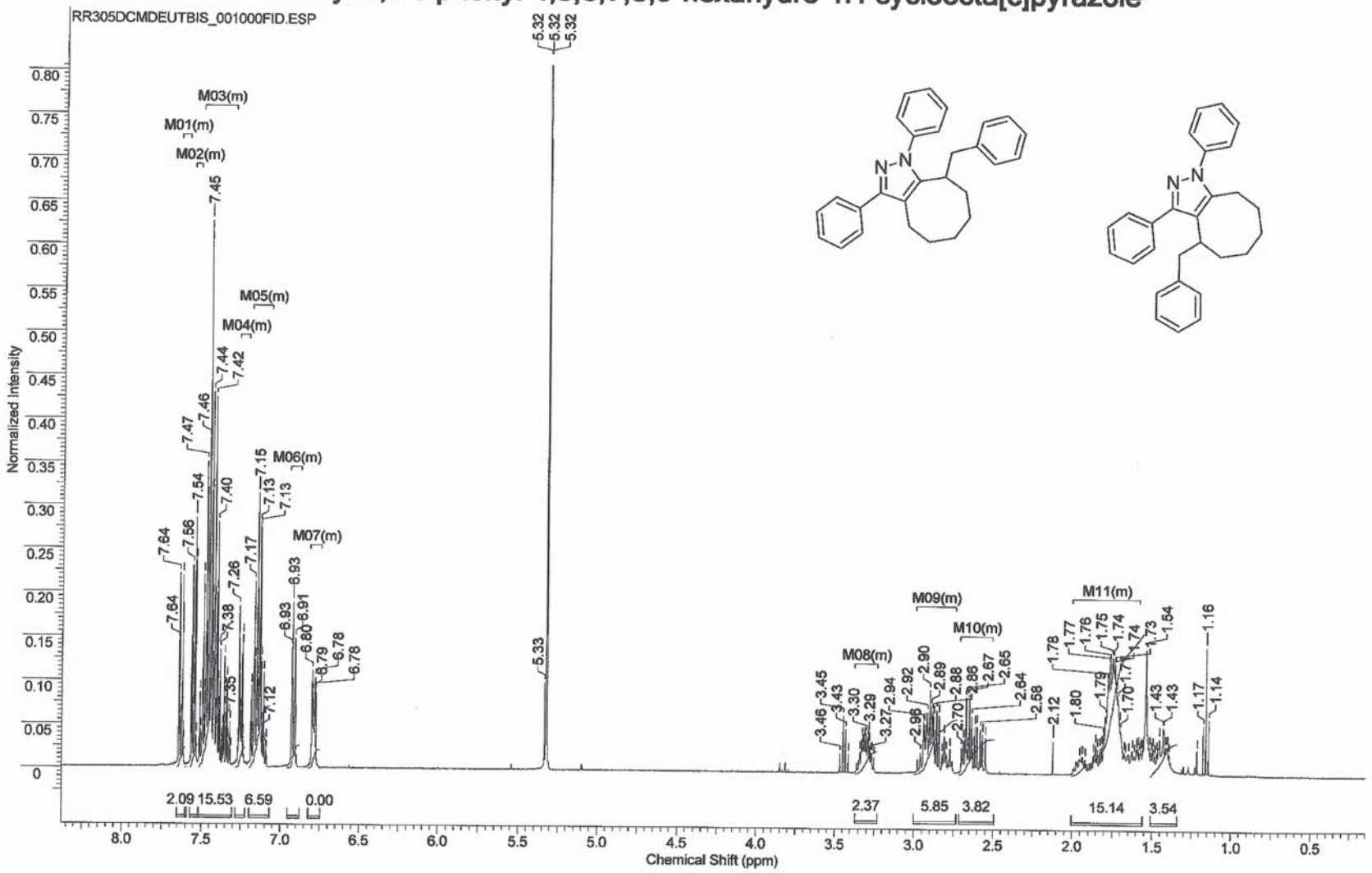
Charge = +1

#	C	H	F	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 445.1137470									
1	**24**	**17**	**3**	**2**	**2**	**1**	**445.1134335**	**15.5**	**3.135e-04**
2	21	18	4	2	3	1	445.1145763	11.5	8.293e-04
3	29	15	2	2	1	0	445.1146959	22.5	9.489e-04
4	27	16	2	2	1	1	445.1122906	19.5	1.456e-03
5	26	17	2	1	4	0	445.1120159	18.0	1.731e-03
6	21	16	3	4	4	0	445.1118160	14.5	1.931e-03
7	18	19	5	2	4	1	445.1157192	7.5	1.972e-03
8	26	16	3	2	2	0	445.1158388	18.5	2.092e-03
9	29	16	1	1	3	0	445.1108730	22.0	2.874e-03
10	24	15	2	4	3	0	445.1106732	18.5	3.074e-03

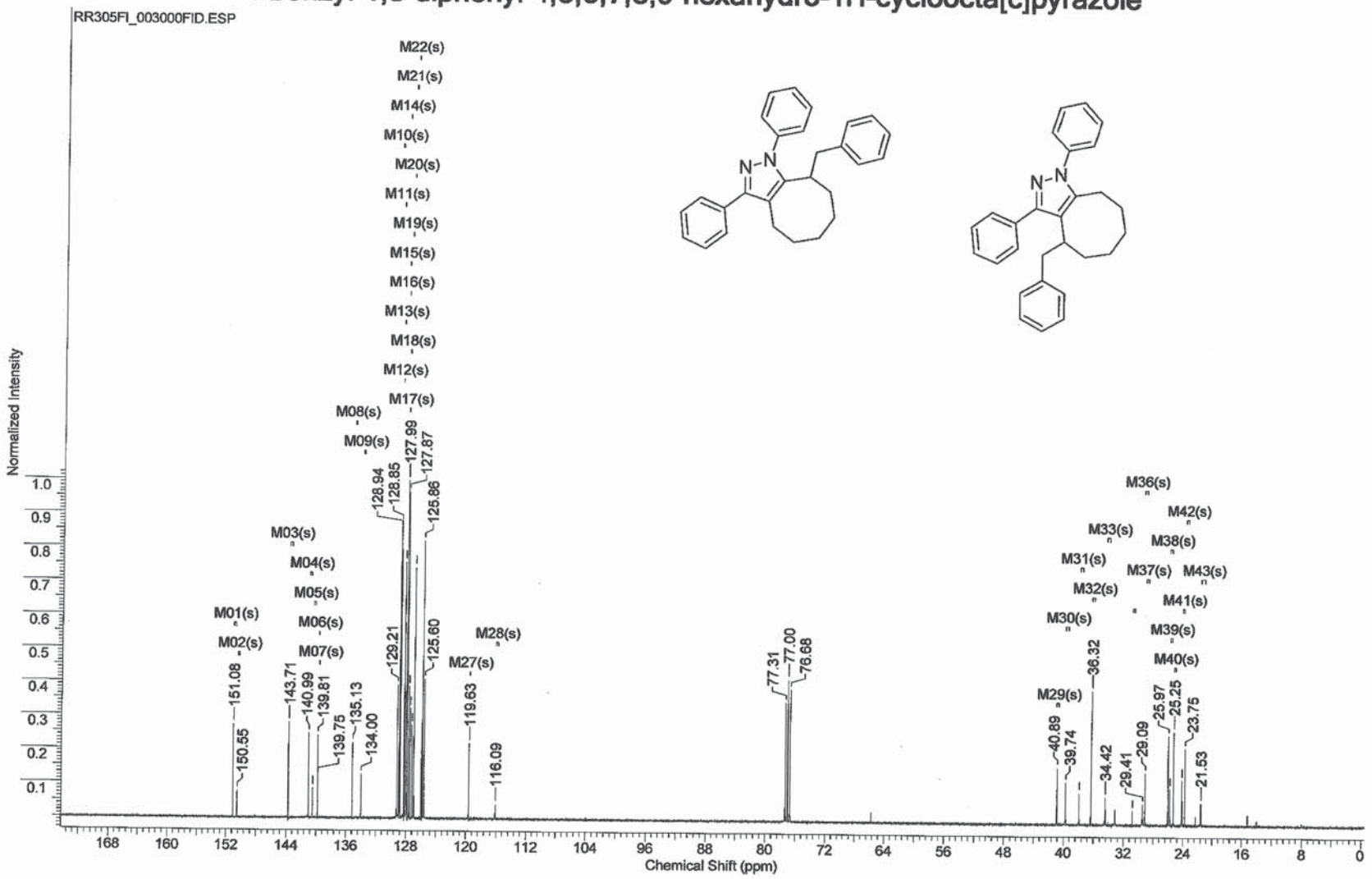


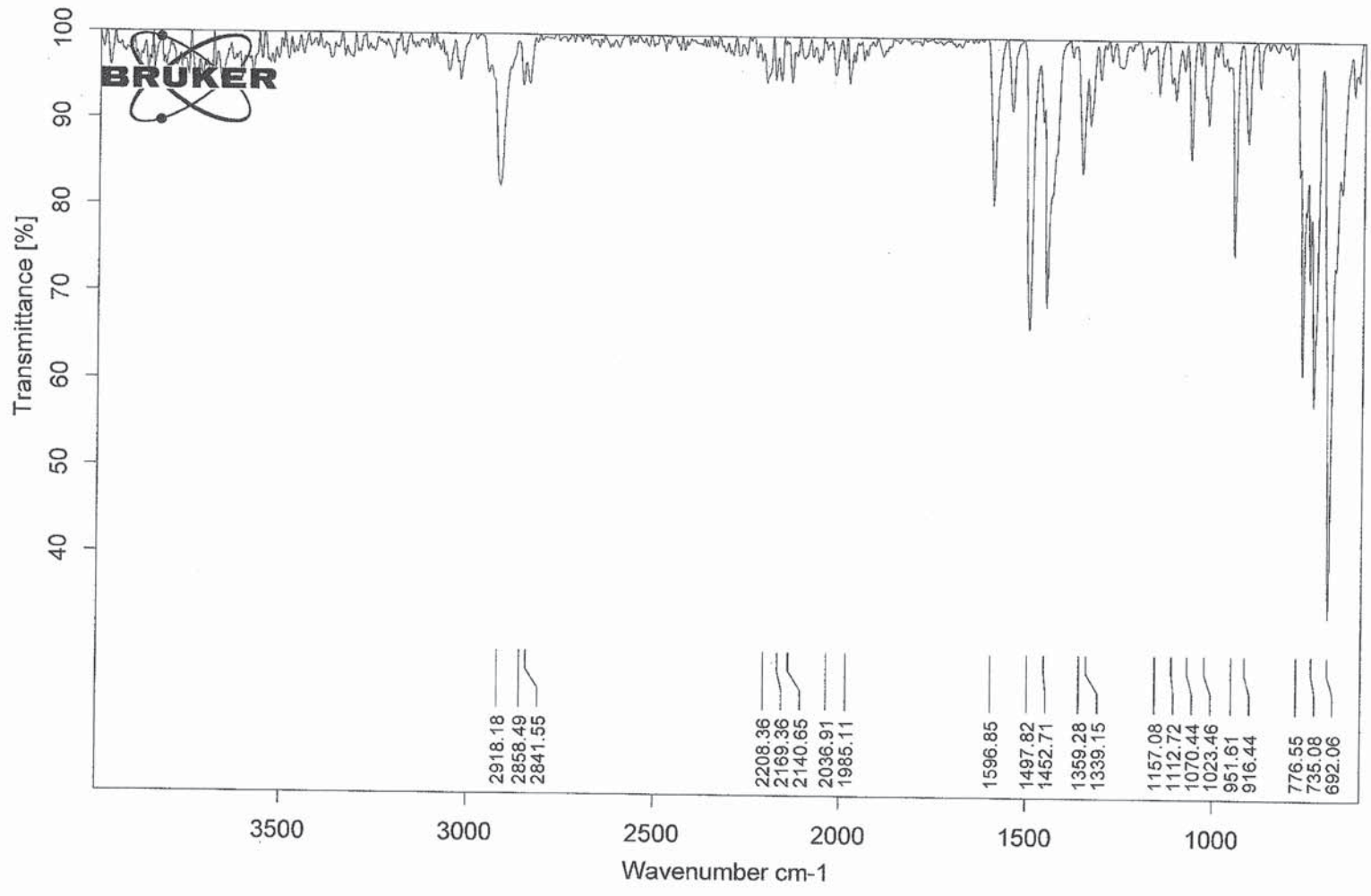
/Data/UNI_FR/REMY9328_ESI/2/pdata/1 FTMS USER Fri Apr 17 12:06:30 2015

9-benzyl-1,3-diphenyl-4,5,6,7,8,9-hexahydro-1H-cycloocta[c]pyrazole and 4-benzyl-1,3-diphenyl-4,5,6,7,8,9-hexahydro-1H-cycloocta[c]pyrazole



9-benzyl-1,3-diphenyl-4,5,6,7,8,9-hexahydro-1H-cycloocta[c]pyrazole and 4-benzyl-1,3-diphenyl-4,5,6,7,8,9-hexahydro-1H-cycloocta[c]pyrazole





U:\IR\RR305mix.0	RR305mix	yellow solid	22.05.2015

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BRUKER FTMS 4.7T BioAPEX II

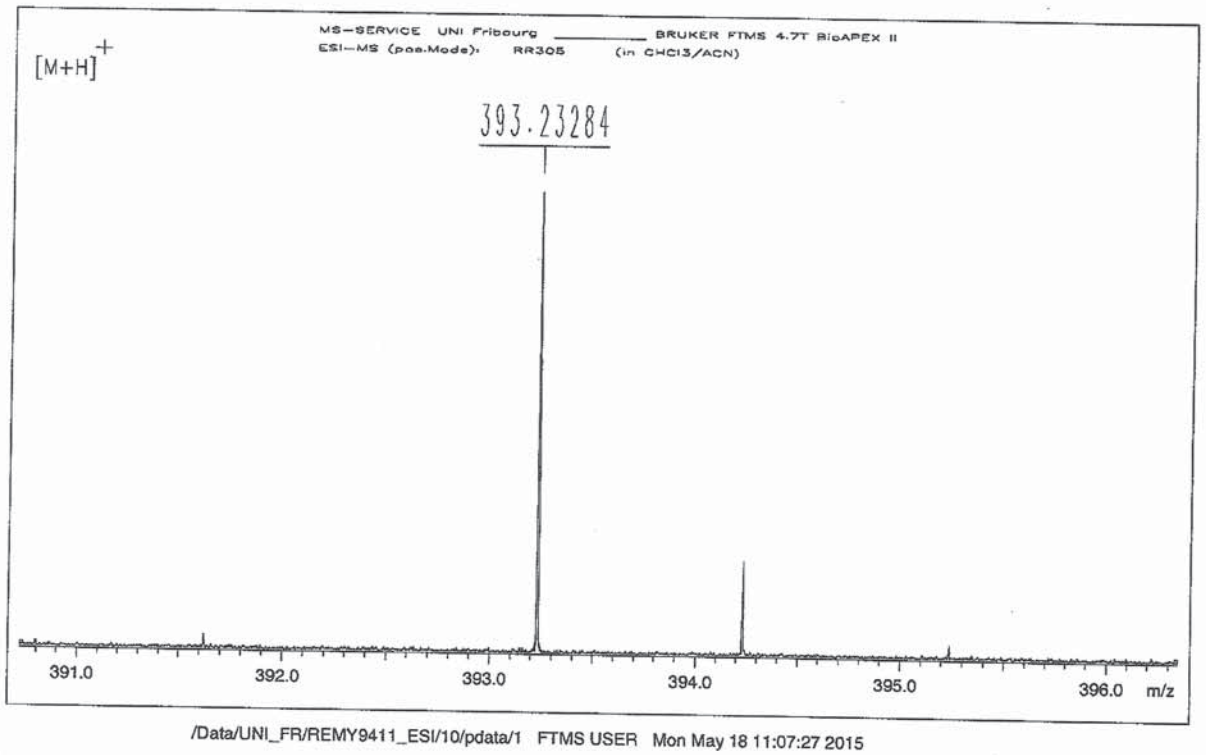
ESI-MS: RR305

XMASS Mass Analysis for /Data/UNI_FR/REMY9411_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 393.2328390

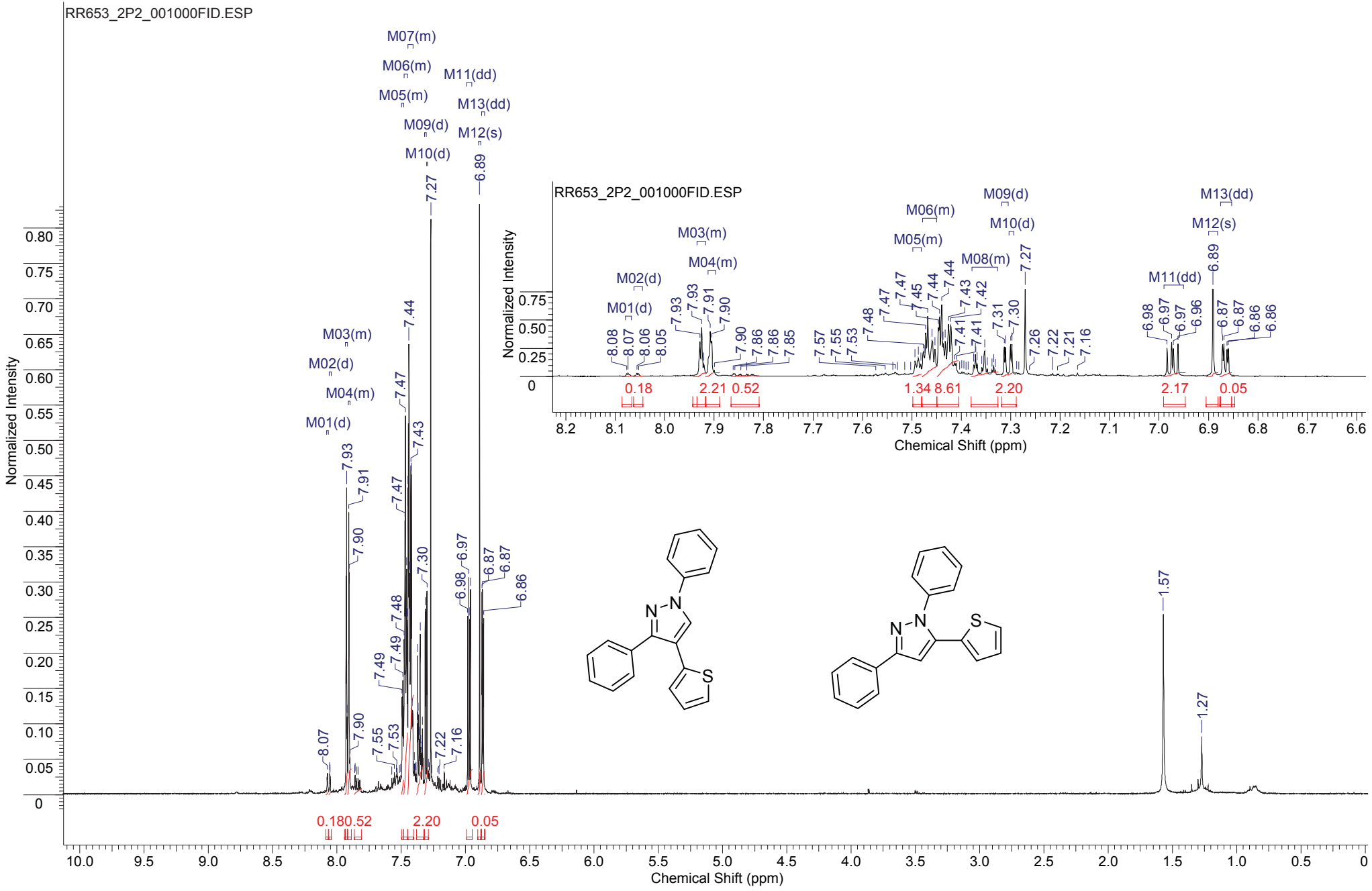
Charge = +1

#	C	H	N	mass	DBE	error
*** Mass Analysis for mass 393.2328390						
1	**28**	**29**	**2**	**393.2325254**	**15.5**	**3.136e-04**
2	20	27	9	393.2383933	12.0	5.554e-03
3	19	25	10	393.2258173	12.5	7.022e-03
4	29	31	1	393.2451014	15.0	1.226e-02
5	27	27	3	393.2199493	16.0	1.289e-02
6	21	29	8	393.2509694	11.5	1.813e-02
7	26	25	4	393.2073732	16.5	2.547e-02
8	22	31	7	393.2635455	11.0	3.071e-02
9	25	23	5	393.1947972	17.0	3.804e-02
10	23	33	6	393.2761215	10.5	4.328e-02

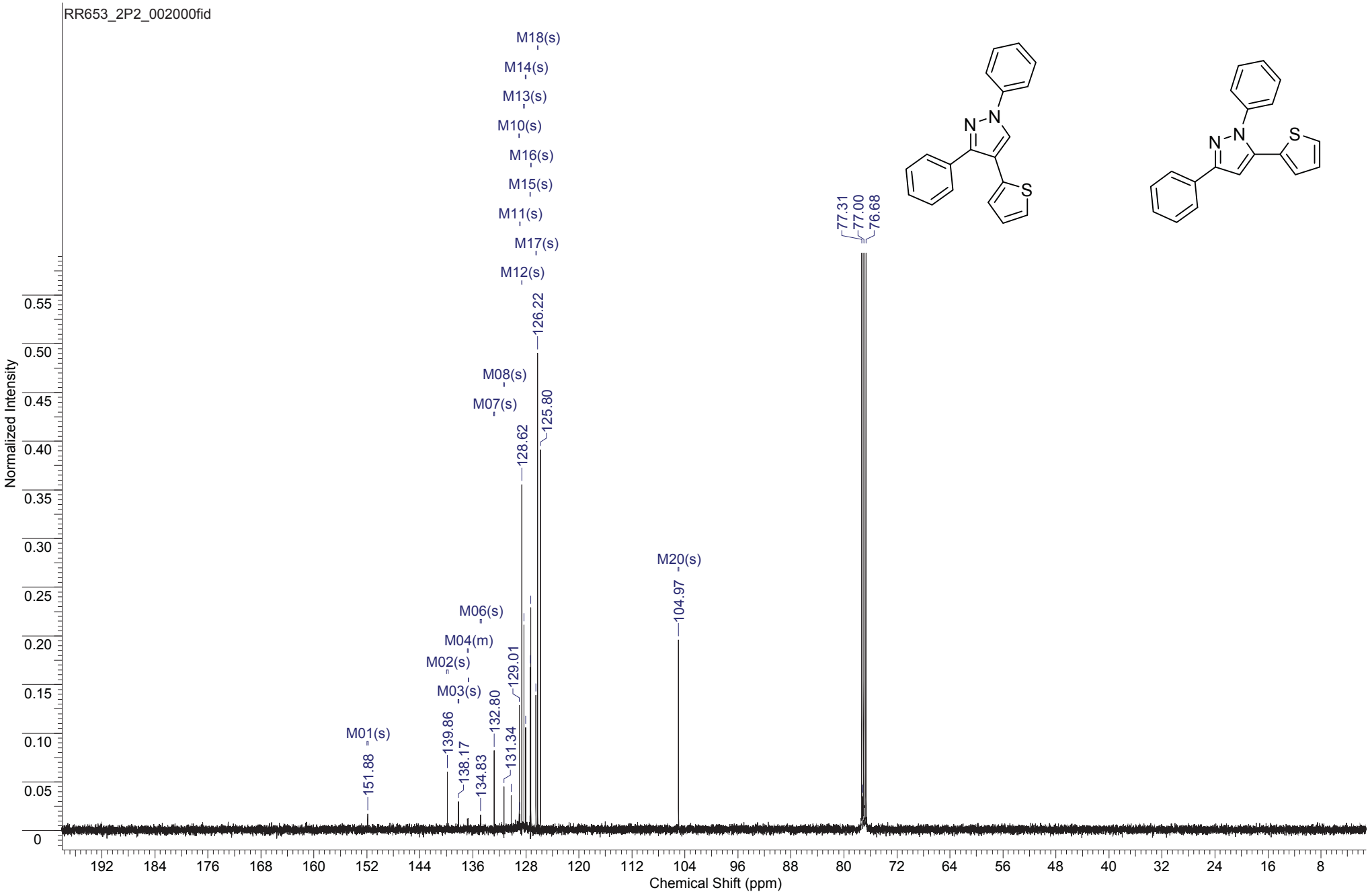


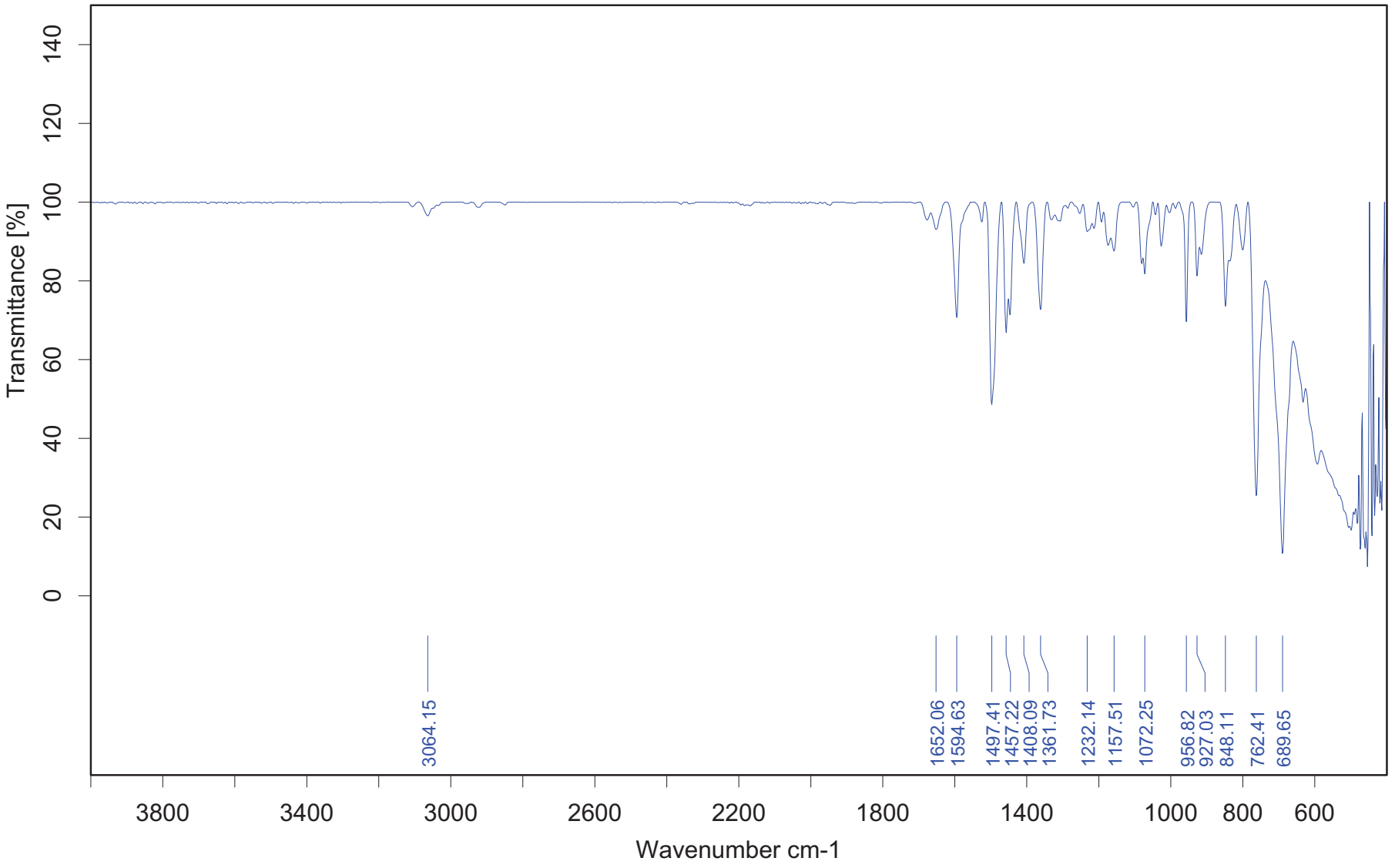
/Data/UNI_FR/REMY9411_ESI/10/pdata/1 FTMS USER Mon May 18 11:07:27 2015

1,3-diphenyl-5-(thiophen-2-yl)-1H-pyrazole and 1,3-diphenyl-4-(thiophen-2-yl)-1H-pyrazole



1,3-diphenyl-5-(thiophen-2-yl)-1H-pyrazole and 1,3-diphenyl-4-(thiophen-2-yl)-1H-pyrazole





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Comment 1

Comment 2 **RR653_2Fi in DCTB**

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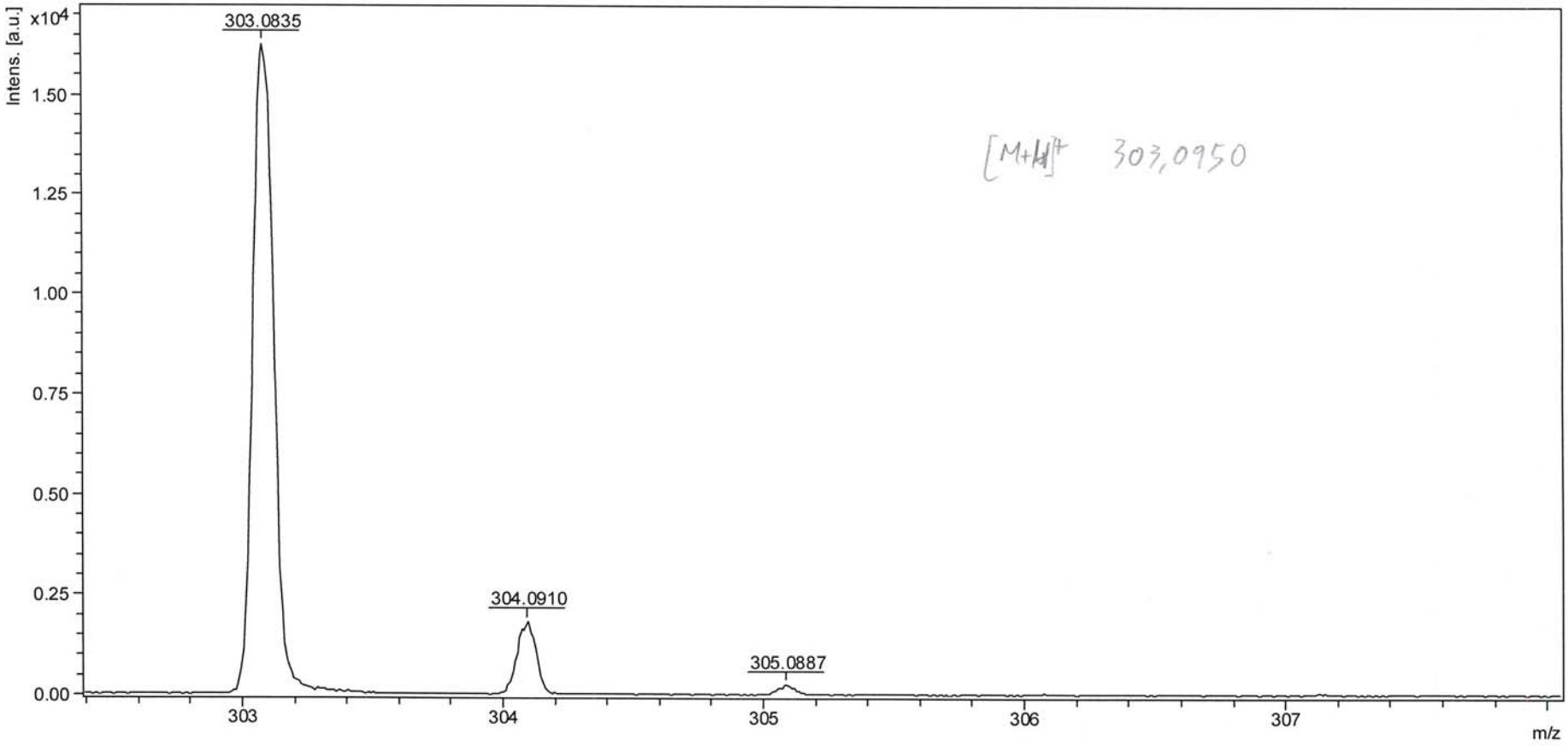
Department of Chemistry



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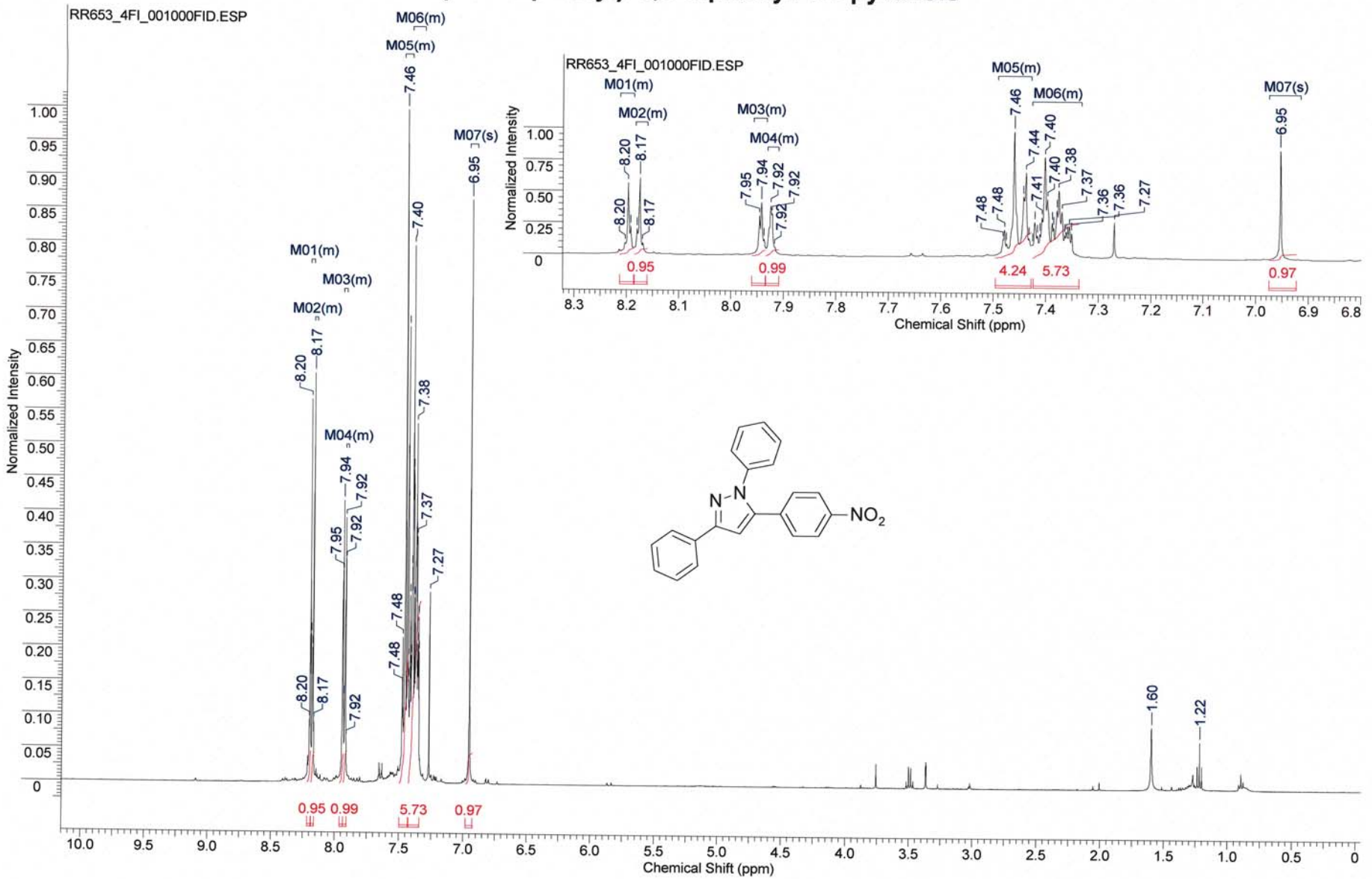
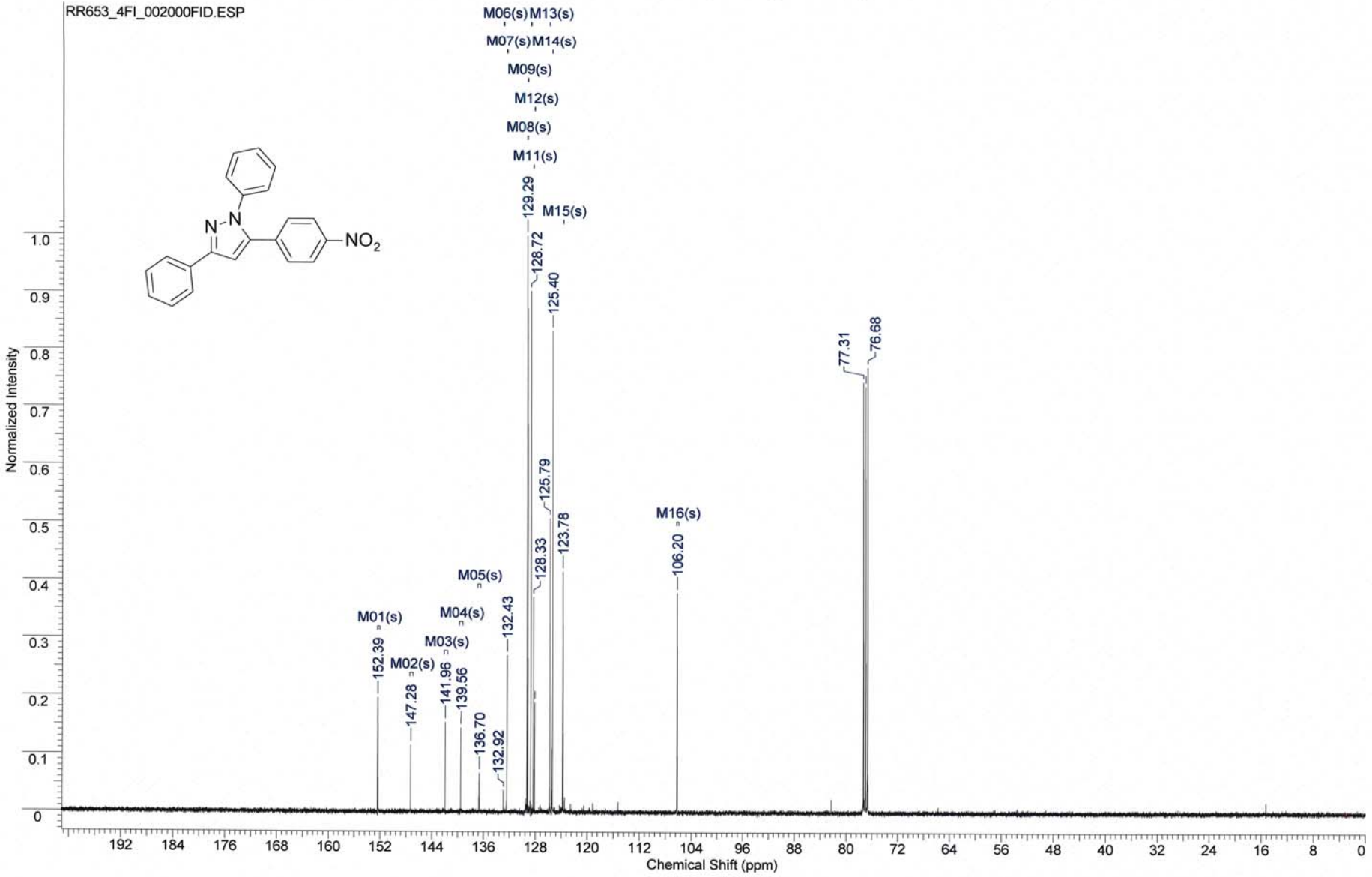
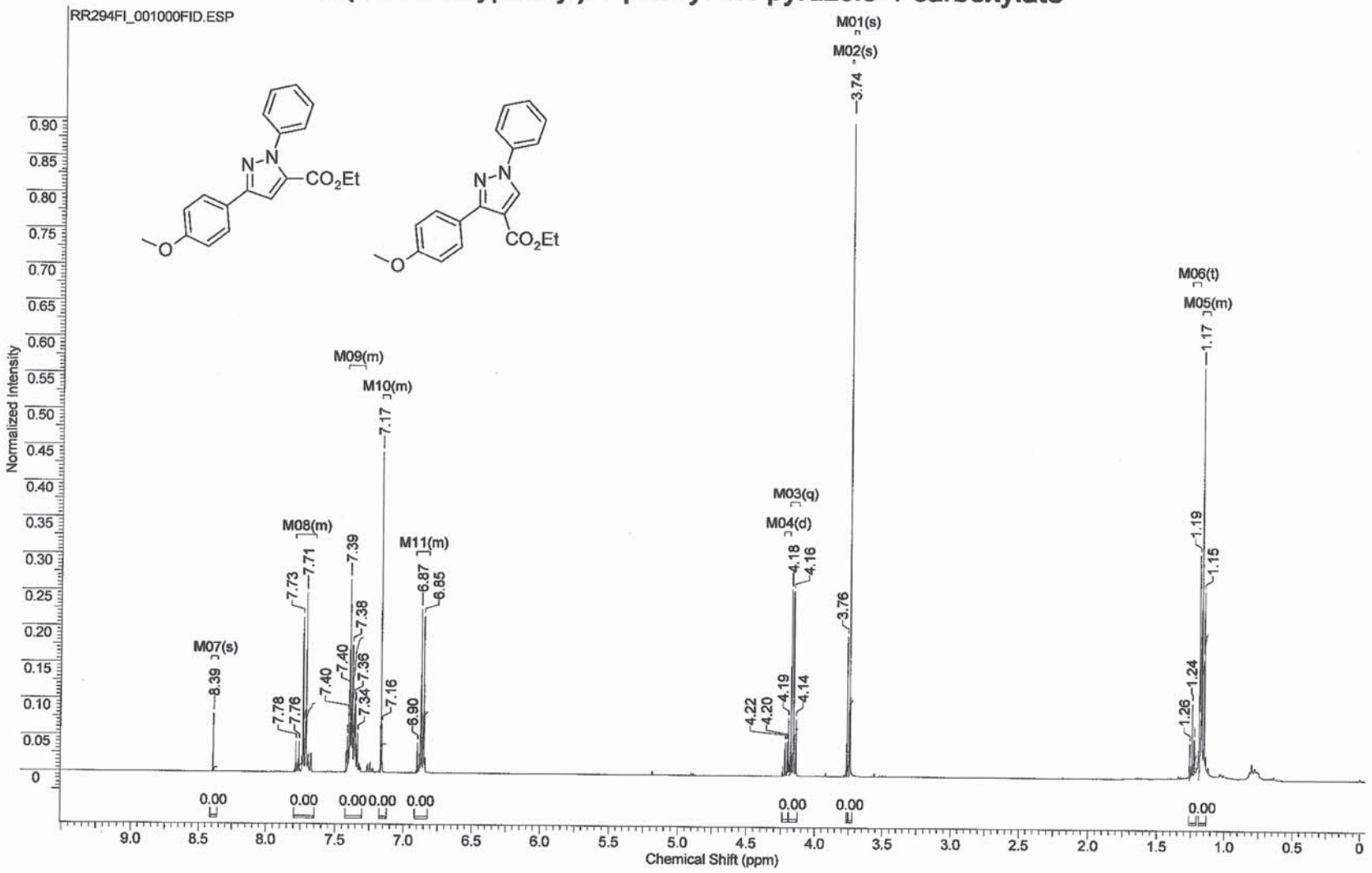
5-(4-nitrophenyl)-1,3-diphenyl-1H-pyrazole



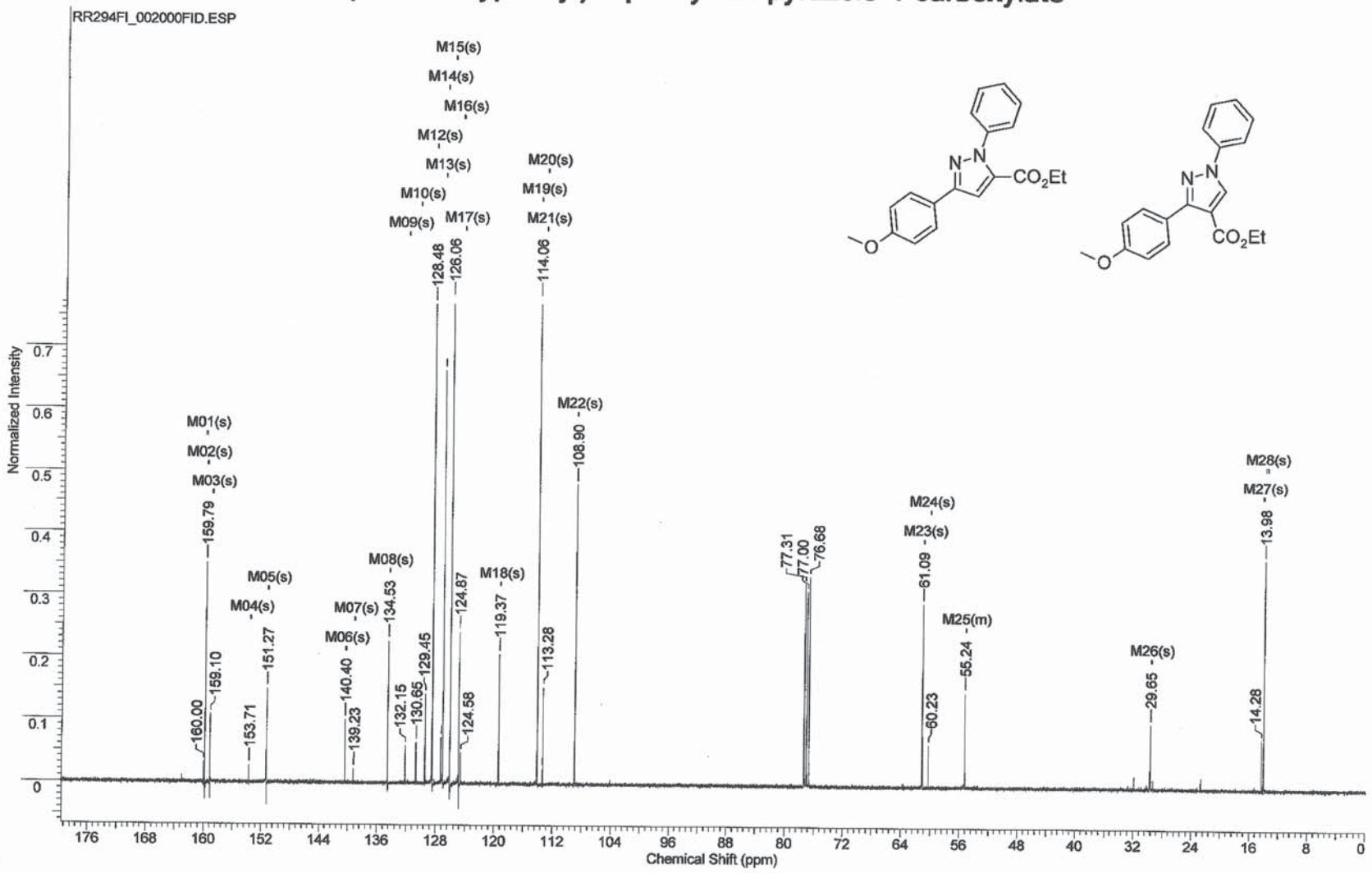
5-(4-nitrophenyl)-1,3-diphenyl-1H-pyrazole

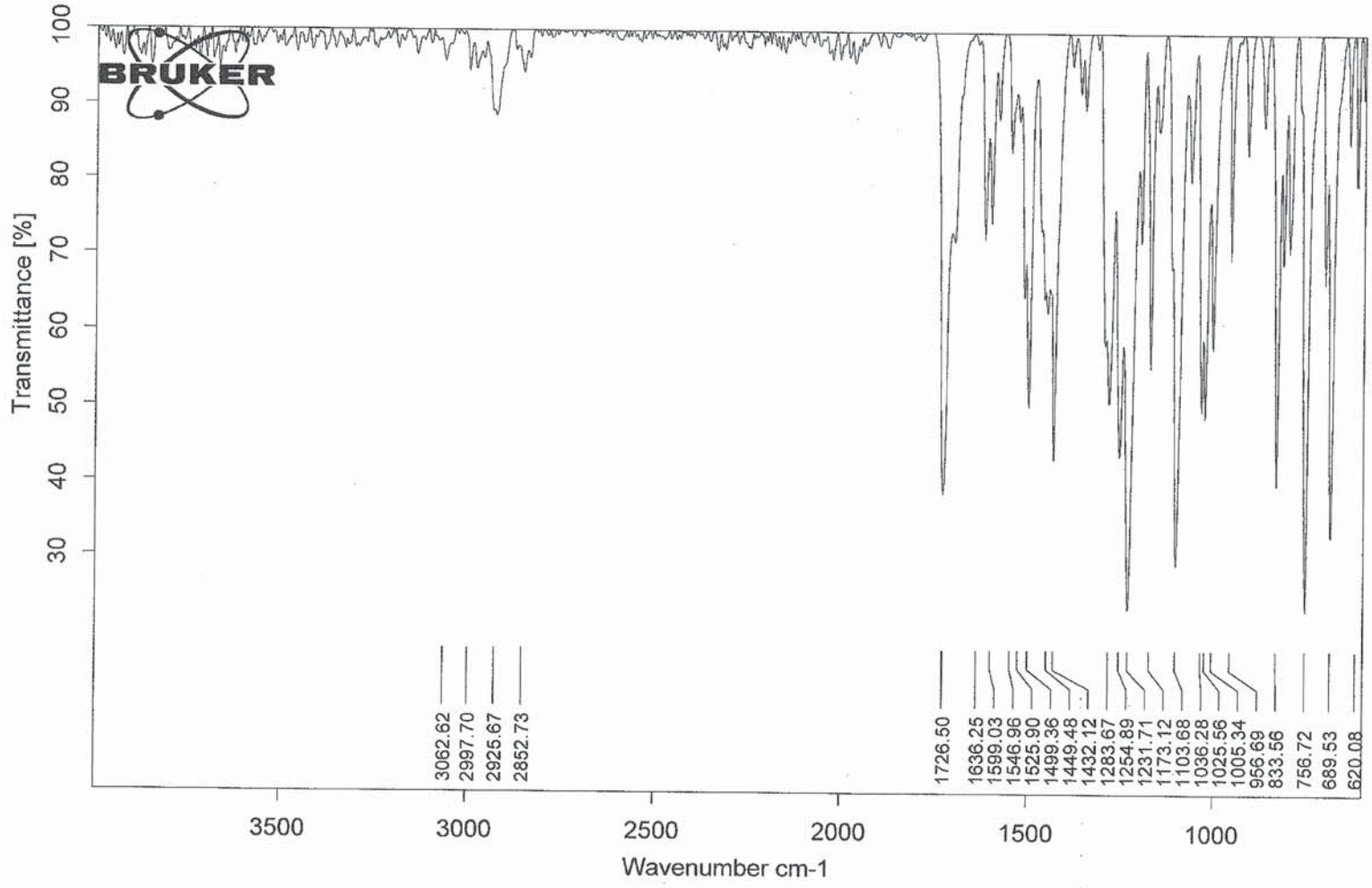


ethyl 3-(4-methoxyphenyl)-1-phenyl-1H-pyrazole-5-carboxylate and ethyl 3-(4-methoxyphenyl)-1-phenyl-1H-pyrazole-4-carboxylate



ethyl 3-(4-methoxyphenyl)-1-phenyl-1H-pyrazole-5-carboxylate and ethyl 3-(4-methoxyphenyl)-1-phenyl-1H-pyrazole-4-carboxylate





U:\IR\RR294mix.0	RR294mix	yellow solid	22.05.2015

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BRUKER **FTMS 4.7T BioAPEX II**

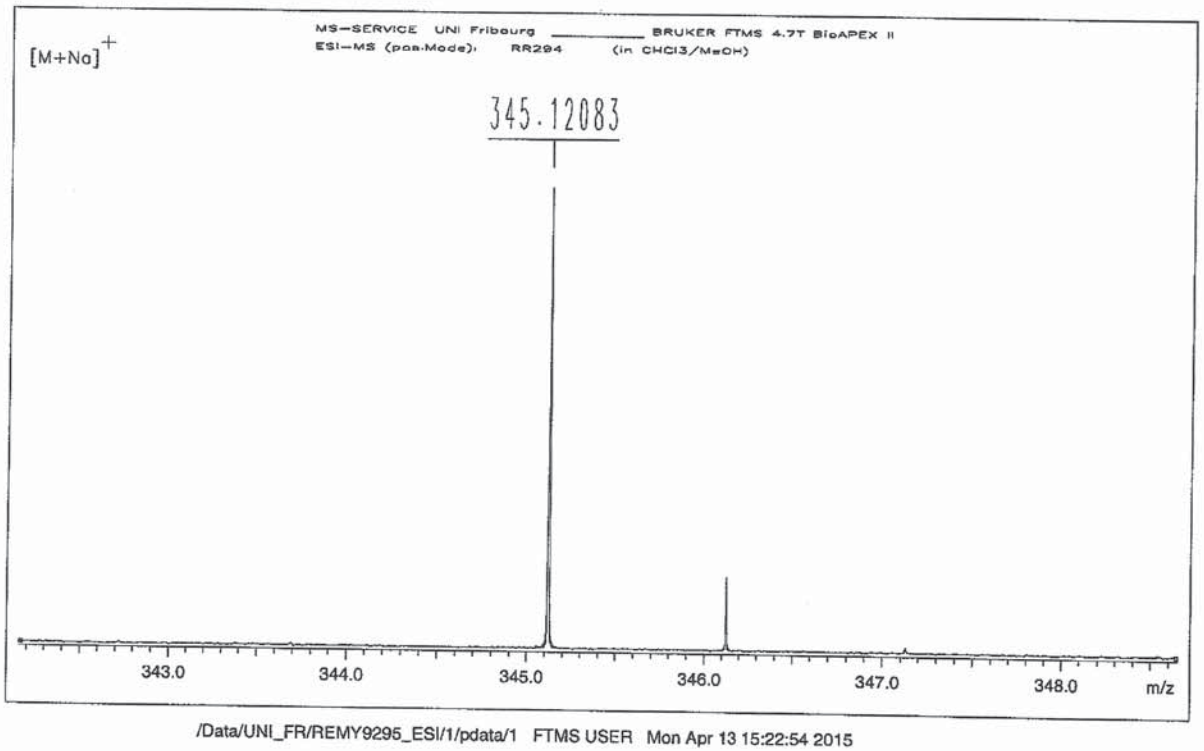
ESI-MS: RR294

XMASS Mass Analysis for /Data/UNI_FR/REMY9295_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

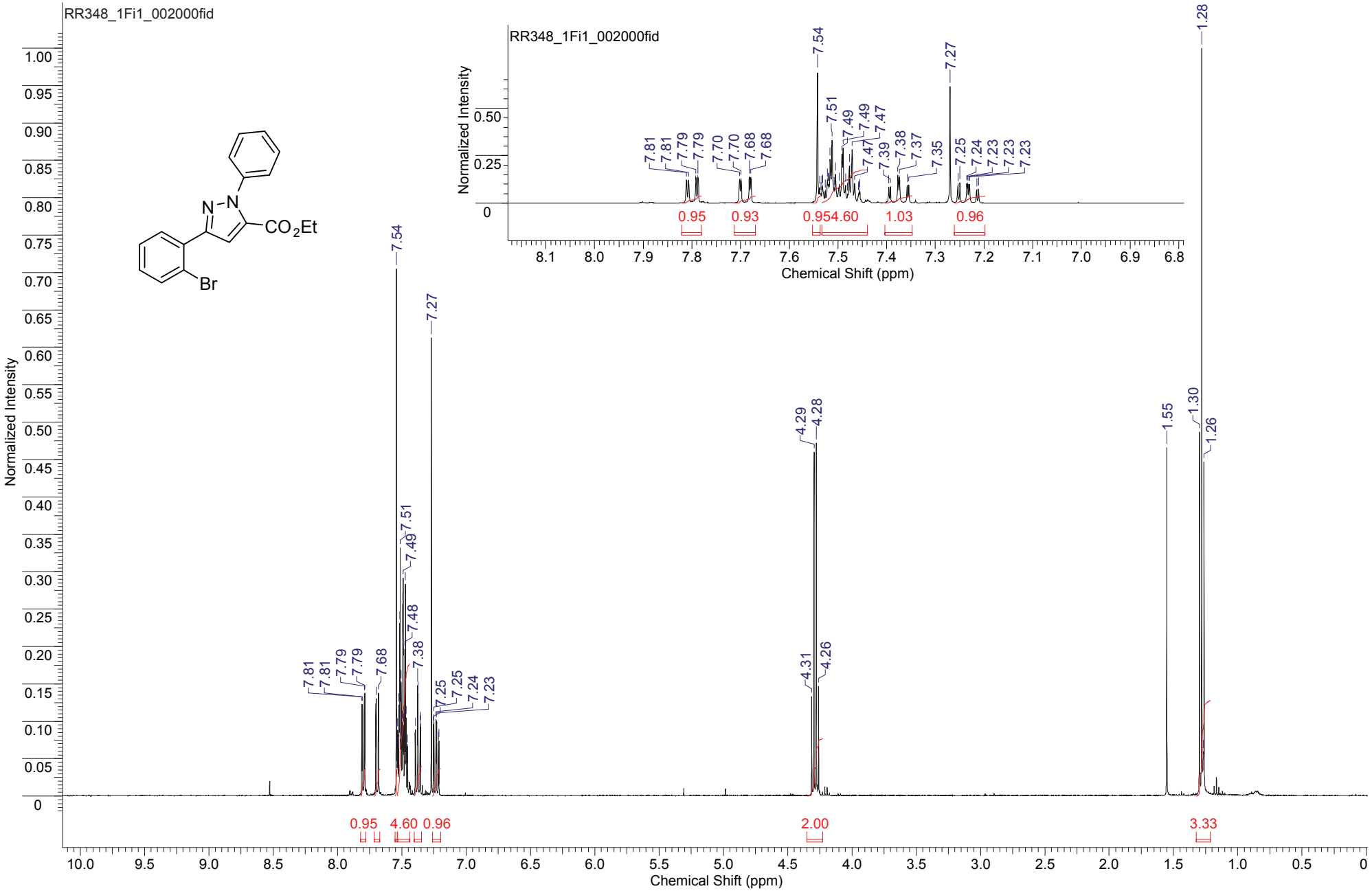
Ion mass = 345.1208330

Charge = +1

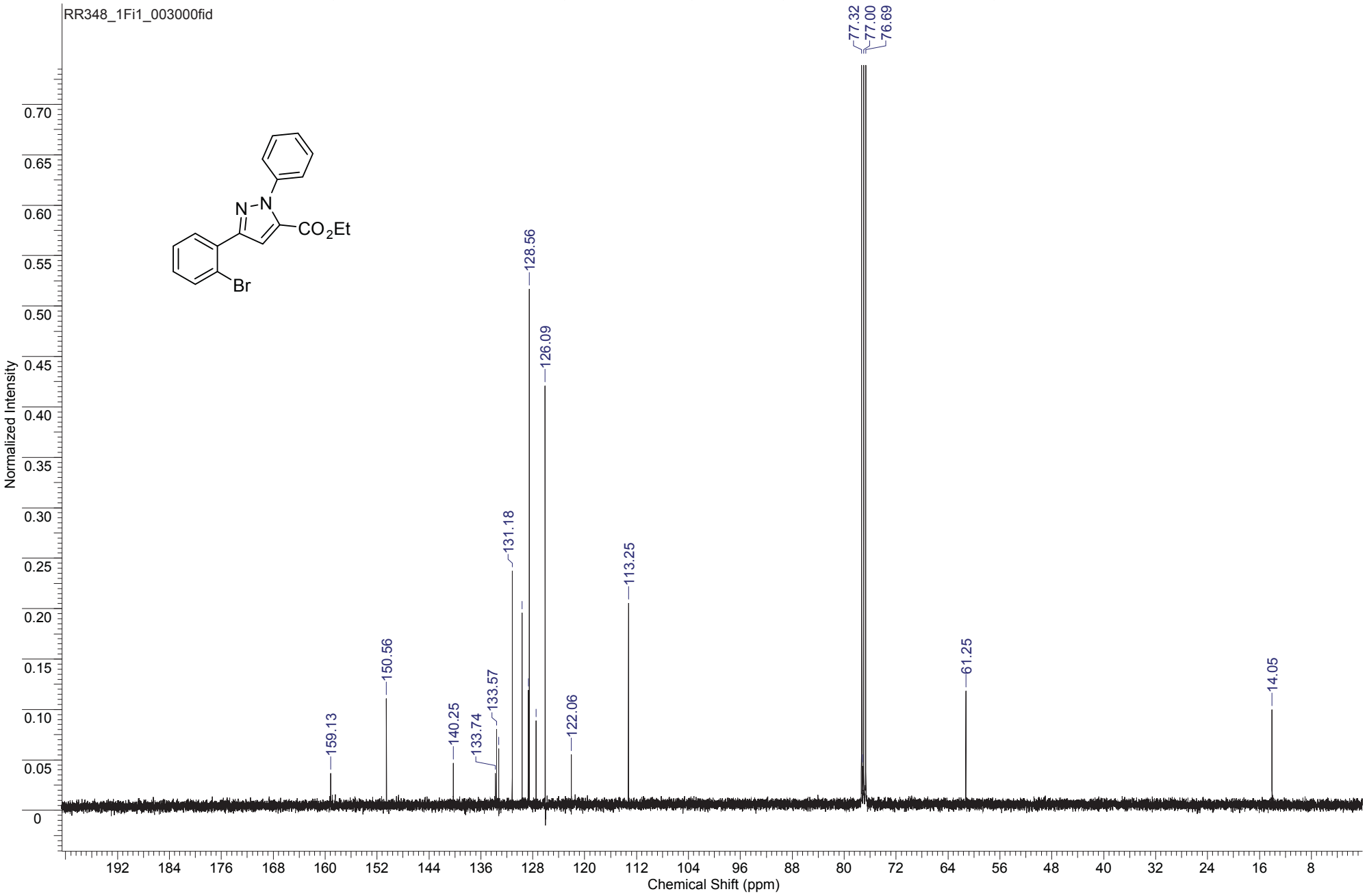
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 345.1208330								
1	**19**	**18**	**2**	**3**	**1**	**345.1209635**	**11.5**	**1.305e-04**
2	18	19	1	6	0	345.1206888	10.0	1.442e-04
3	17	13	8	1	0	345.1206835	15.5	1.495e-04
4	19	15	5	2	0	345.1220262	15.0	1.193e-03
5	17	16	5	2	1	345.1196209	12.0	1.212e-03
6	16	17	4	5	0	345.1193461	10.5	1.487e-03
7	21	17	2	3	0	345.1233688	14.5	2.536e-03
8	16	20	1	6	1	345.1182835	7.0	2.550e-03
9	15	14	8	1	1	345.1182782	12.5	2.555e-03
10	14	15	7	4	0	345.1180034	11.0	2.830e-03

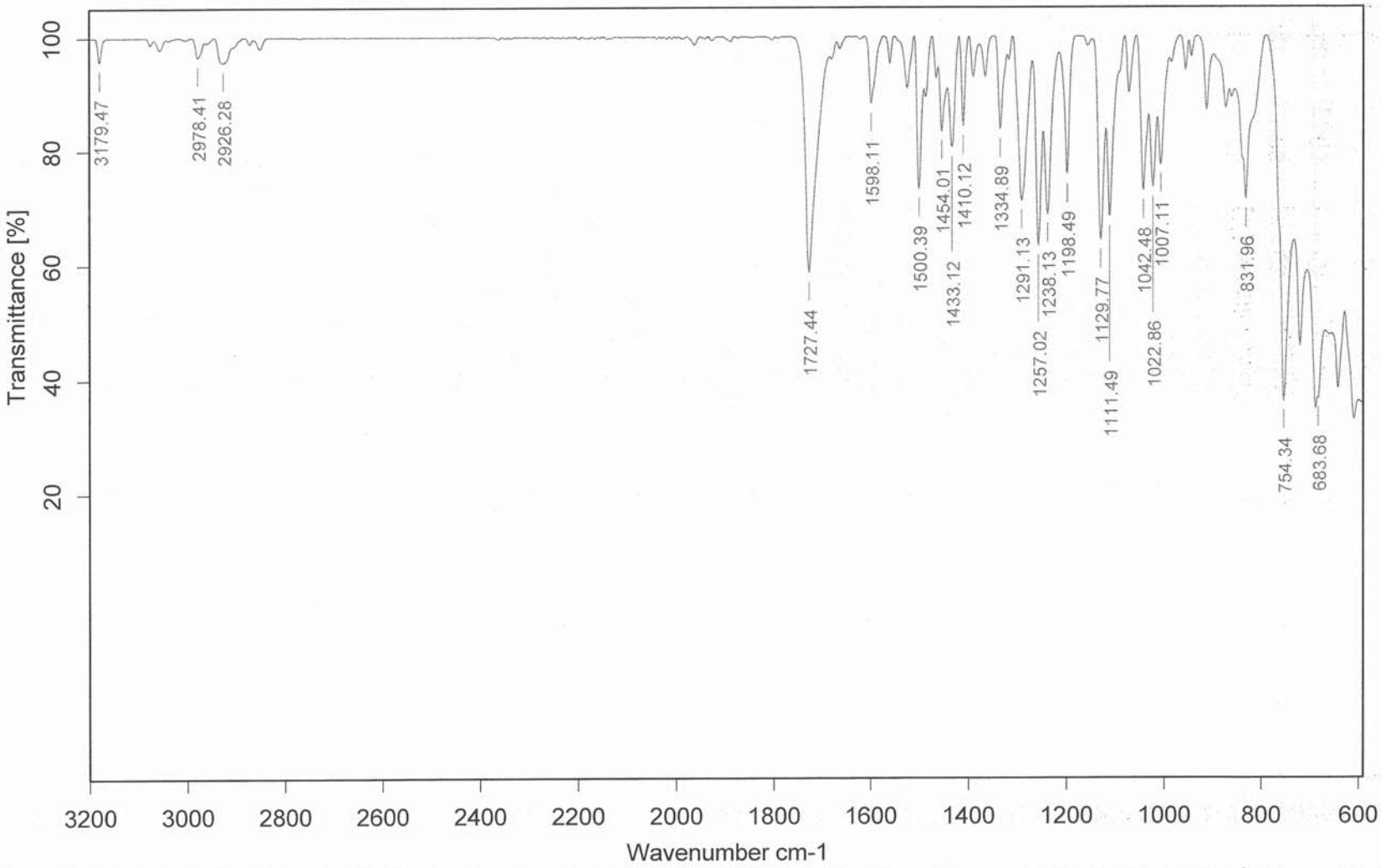


ethyl 3-(2-bromophenyl)-1-phenyl-1H-pyrazole-5-carboxylate



ethyl 3-(2-bromophenyl)-1-phenyl-1H-pyrazole-5-carboxylate





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Mass Spectrometry Service
Department of Chemistry

BRUKER **FTMS 4.7T BioAPEX II**

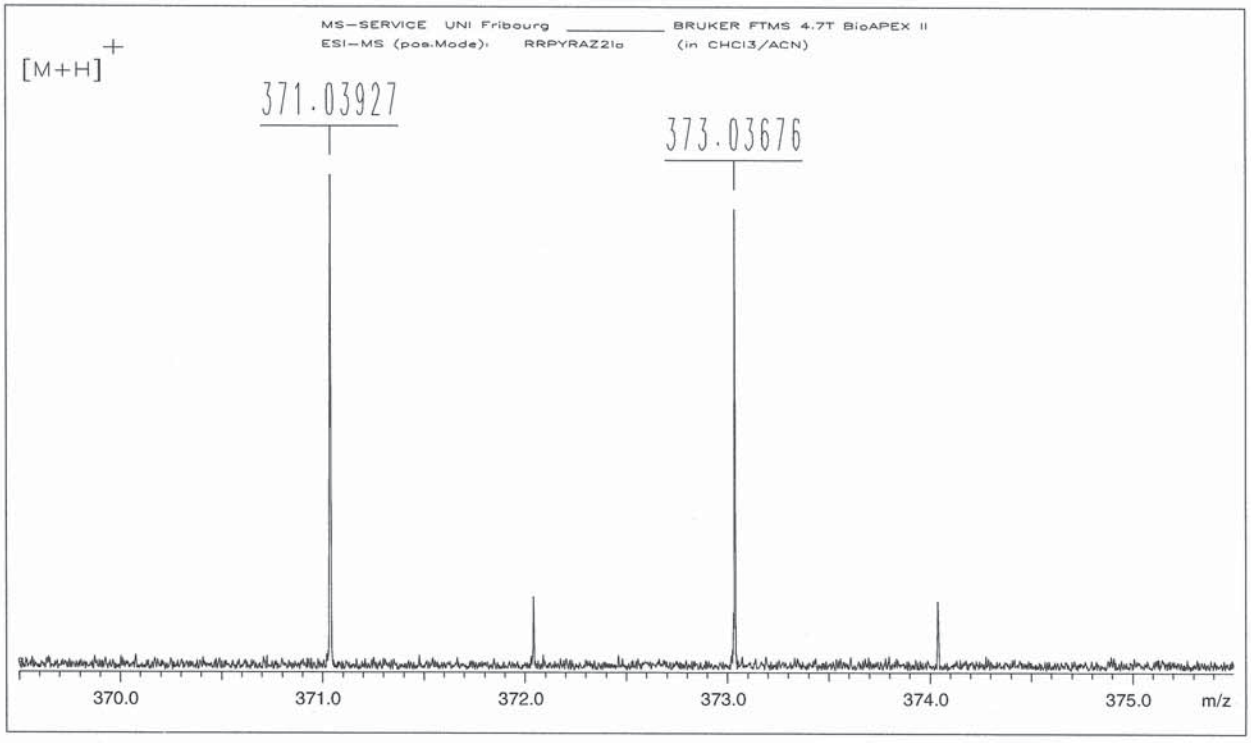
ESI-MS: RRPYRAZ2la

XMASS Mass Analysis for /Data/UNI_FR/REMY2406_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass [1] = 371.0392720
Ion mass [2] = 373.0367570

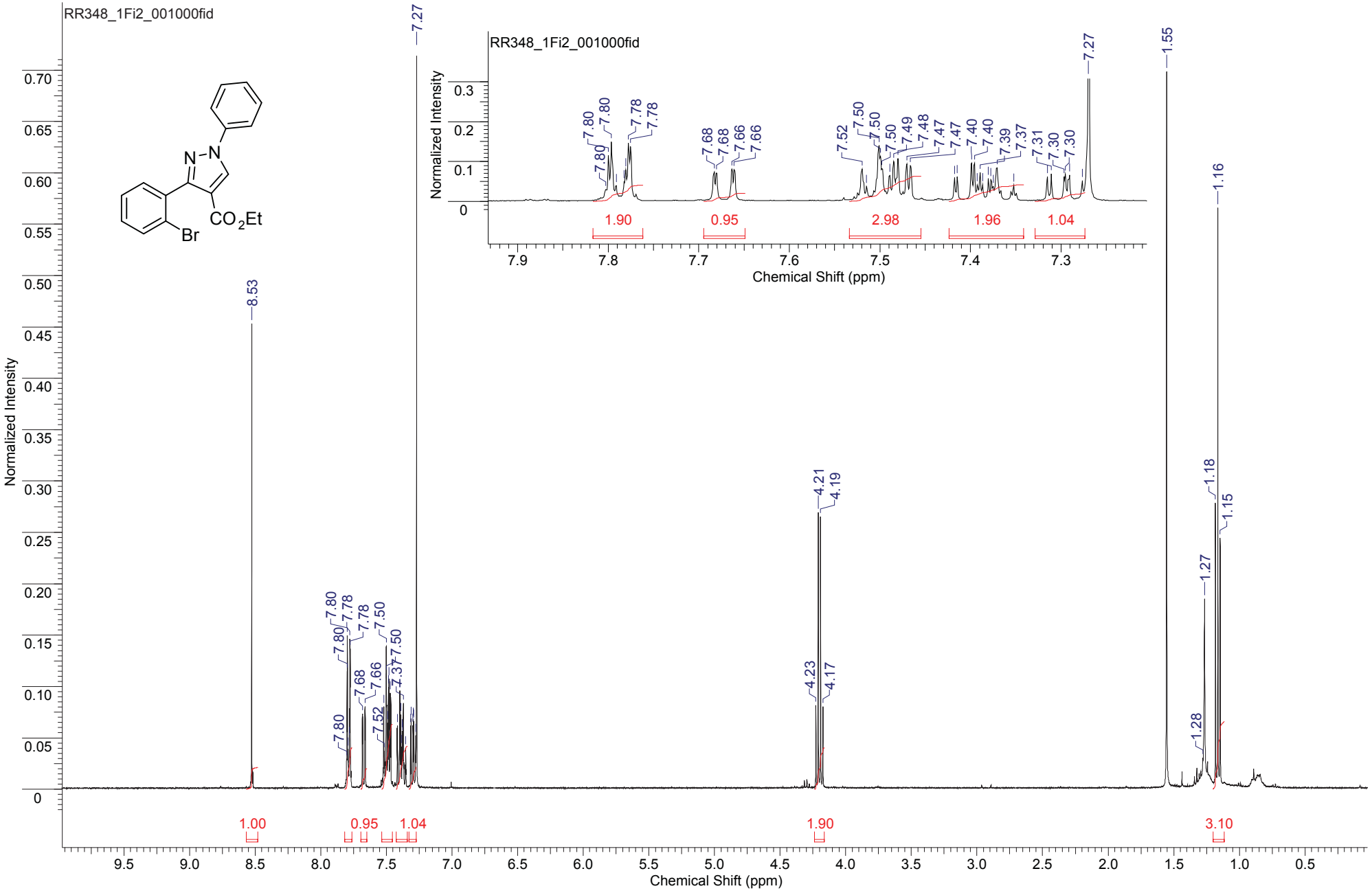
Charge = +1

#	C	H	79Br	81Br	N	O	mass	DBE	error
*** Mass Analysis for mass [1] 371.0392720									
1	**18**	**16**	**1**	**0**	**2**	**2**	**371.0389668**	11.5	3.052e-04
2	28	5	0	0	1	1	371.0365652	27.0	2.707e-03
3	15	18	0	1	2	4	371.0423995	7.5	3.127e-03
4	13	16	1	0	4	4	371.0349440	7.5	4.328e-03
5	19	16	0	1	1	2	371.0338462	12.0	5.426e-03
*** Mass Analysis for mass [2] 373.0367570									
1	**18**	**16**	**0**	**1**	**2**	**2**	**373.0369202**	11.5	1.632e-04
2	24	7	0	0	1	4	373.0369591	22.0	2.021e-04
3	22	5	0	0	4	3	373.0356165	22.5	1.141e-03
4	27	5	0	0	2	1	373.0396392	26.5	2.882e-03
5	13	16	0	1	4	4	373.0328974	7.5	3.860e-03

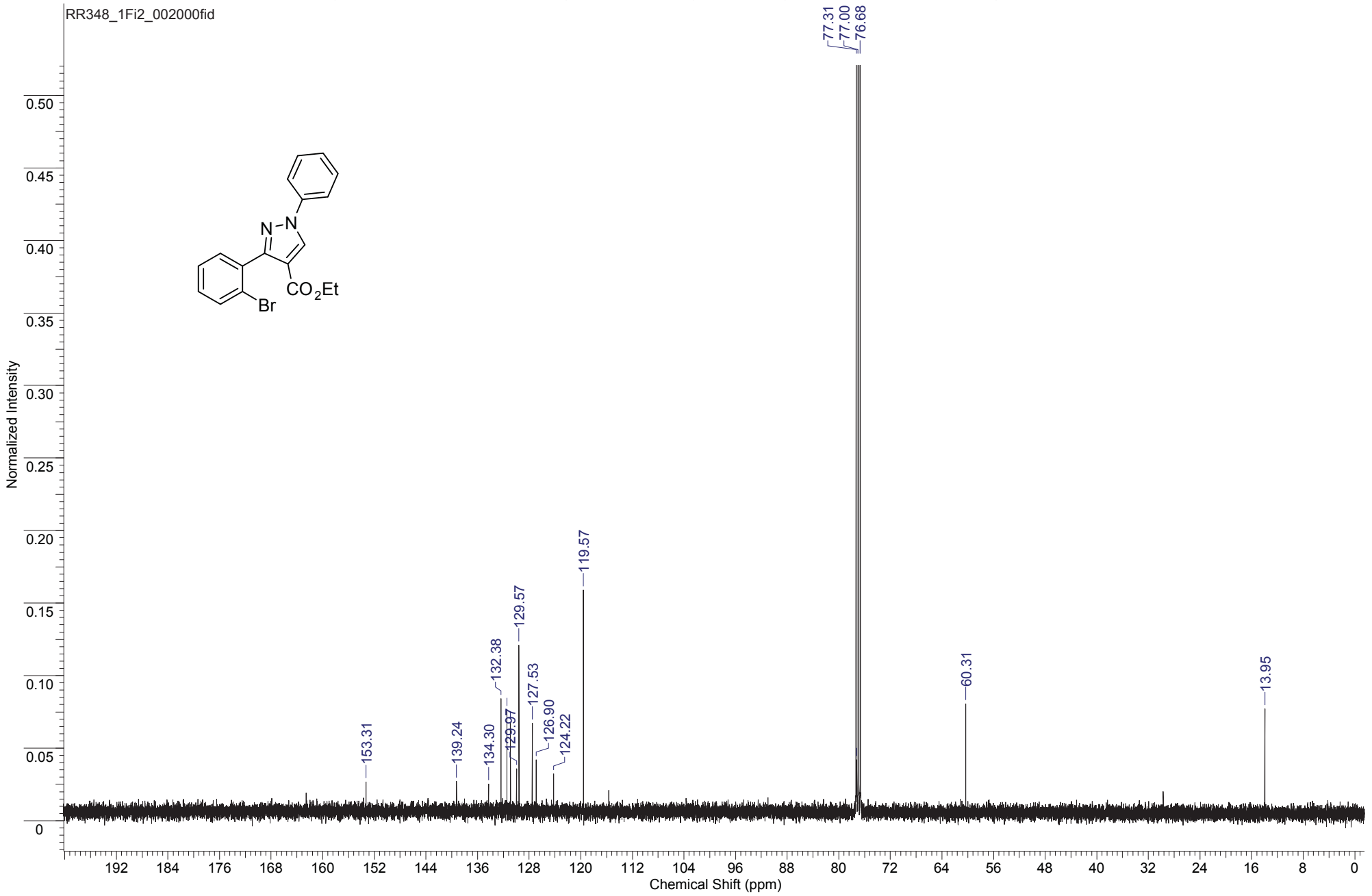


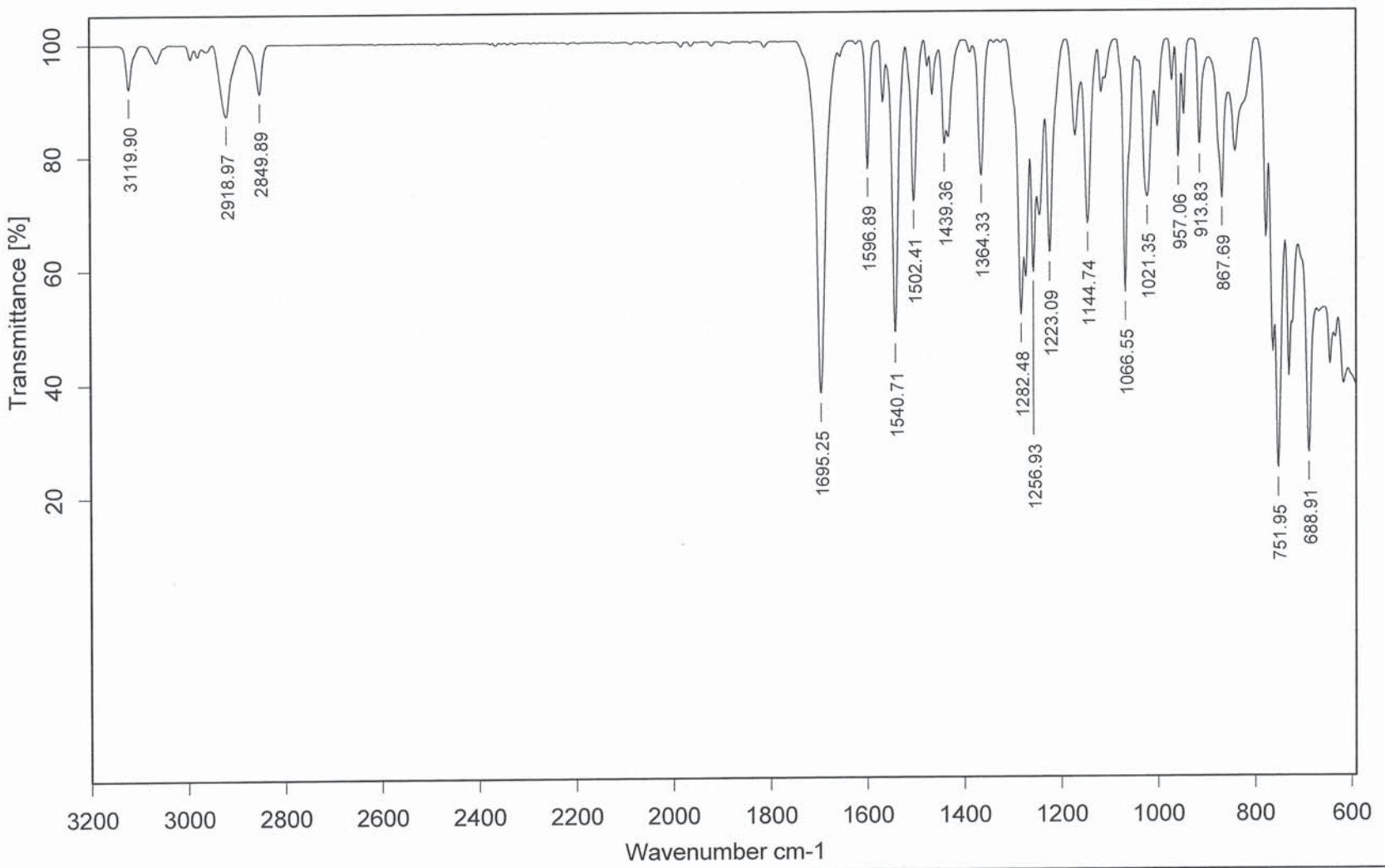
/Data/UNI_FR/REMY2406_ESI/2/pdata/1 FTMS USER Wed Dec 14 13:41:24 2016

ethyl 3-(2-bromophenyl)-1-phenyl-1H-pyrazole-4-carboxylate



ethyl 3-(2-bromophenyl)-1-phenyl-1H-pyrazole-4-carboxylate





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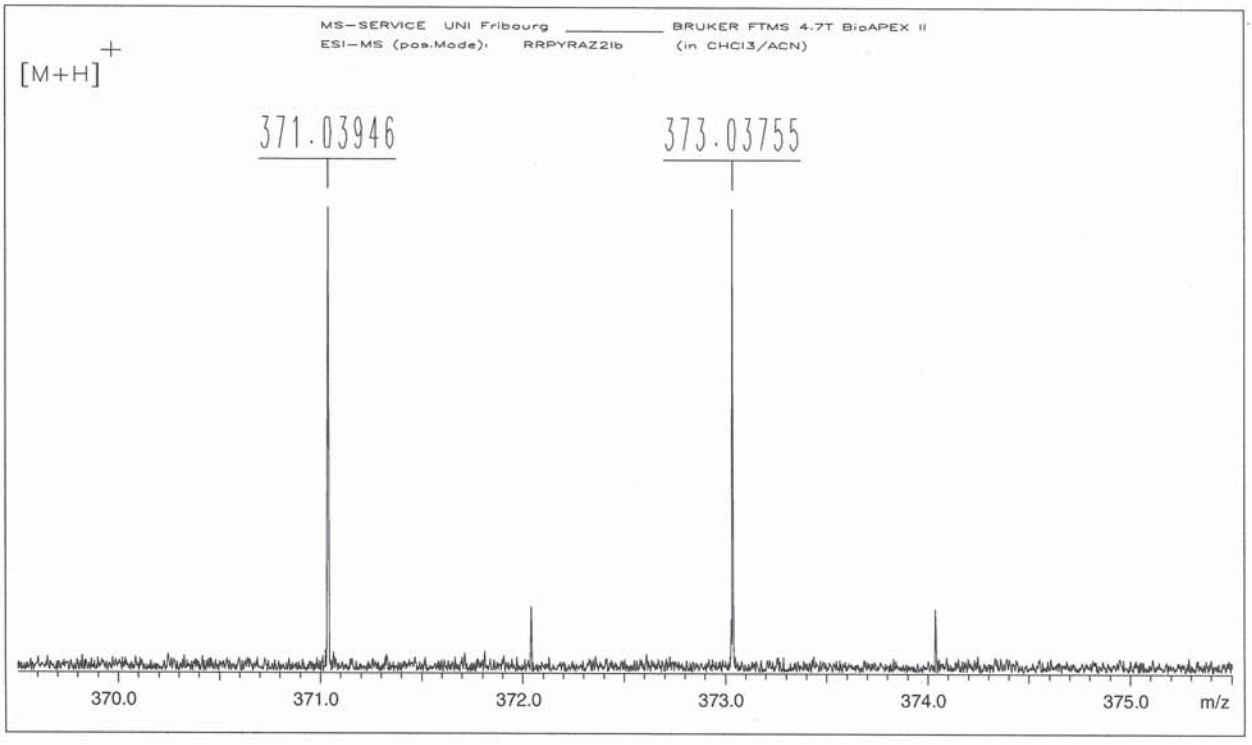
ESI-MS: RRPYRAZ2b

XMASS Mass Analysis for /Data/UNI_FR/REMY2407_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

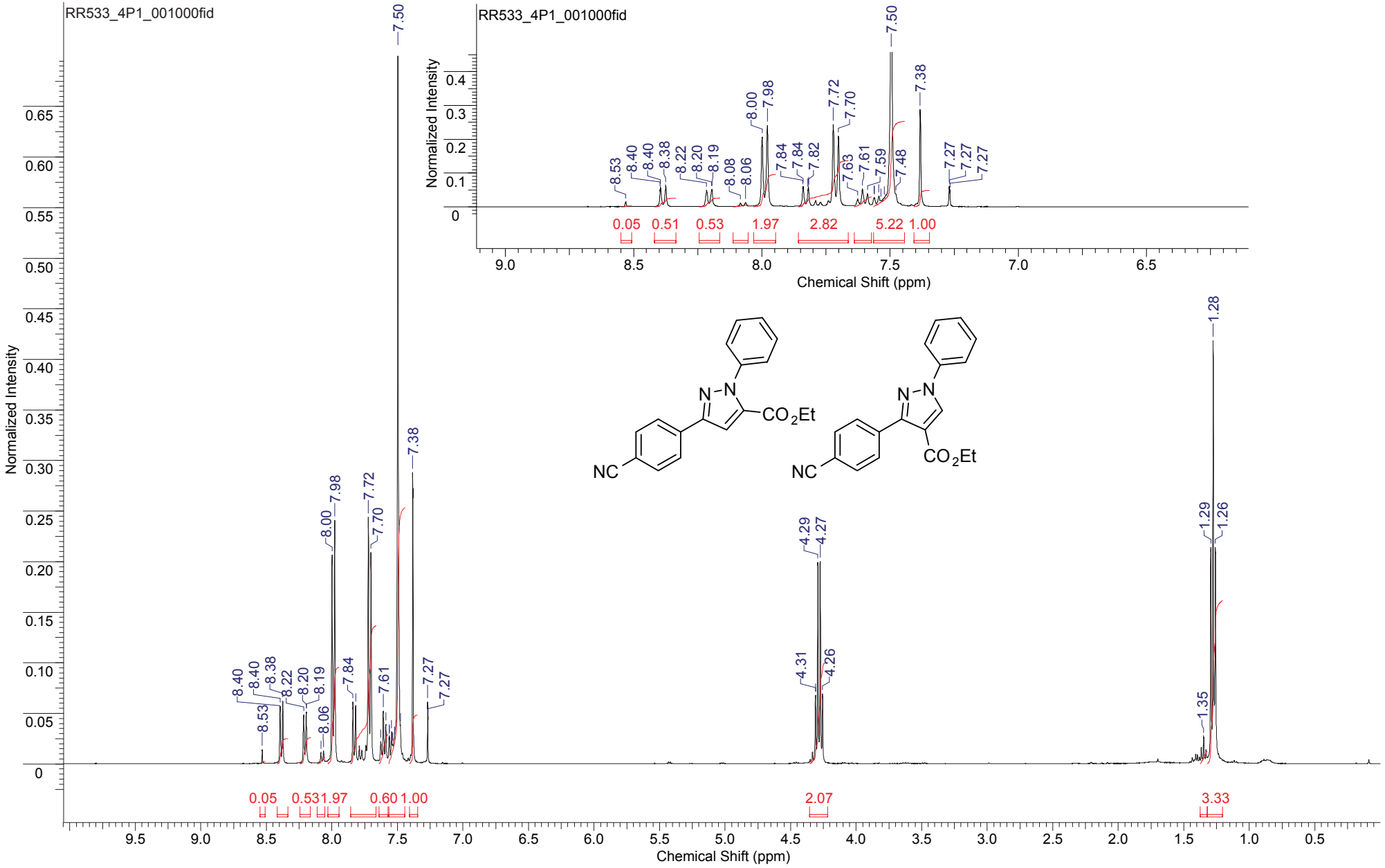
Ion mass [1] = 371.0394570
Ion mass [2] = 373.0375520

Charge = +1

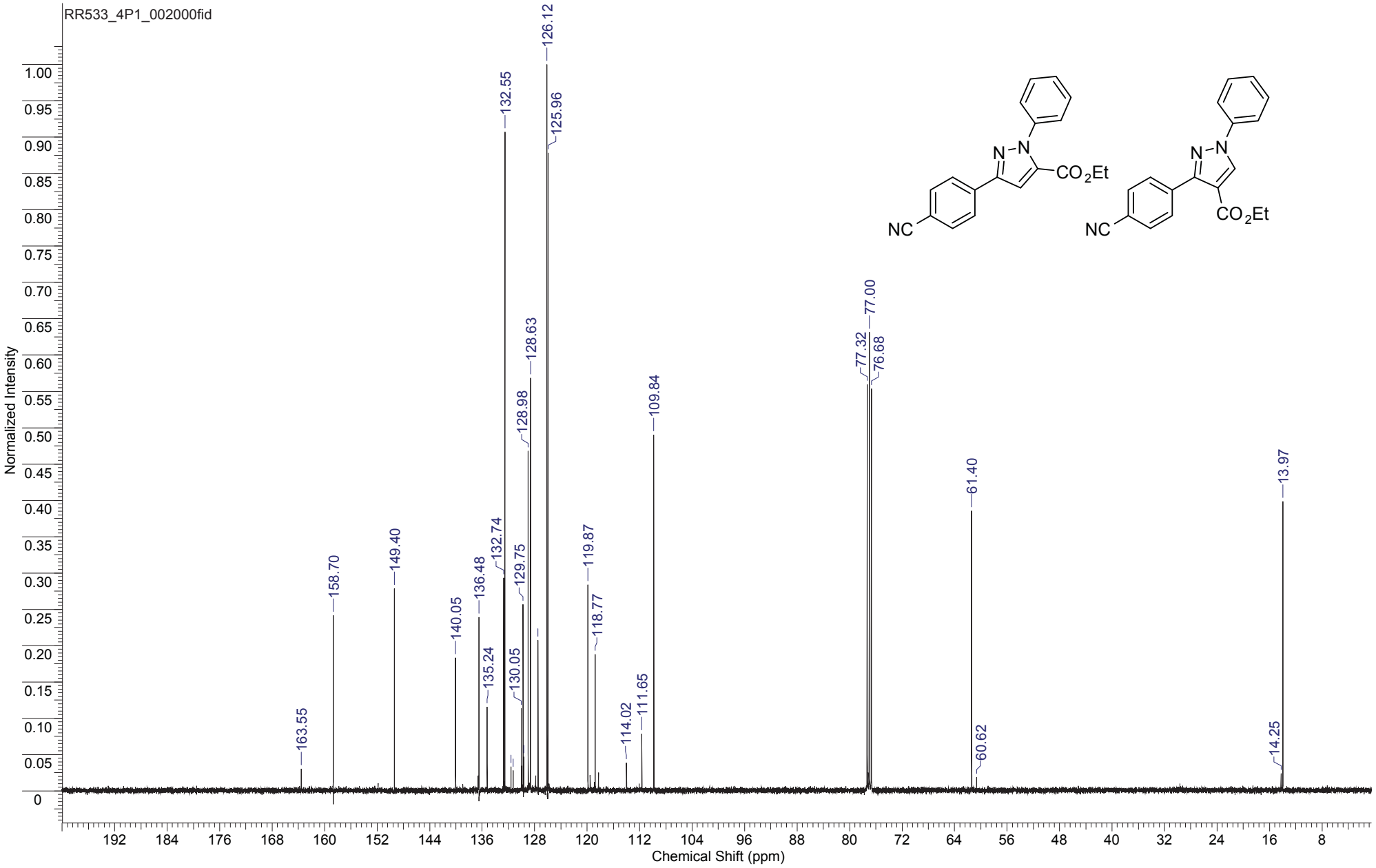
#	C	H	79Br	81Br	N	O	mass	DBE	error
*** Mass Analysis for mass [1] 371.0394570									
1	**18**	**16**	**1**	**0**	**2**	**2**	**371.0389668**	11.5	4.902e-04
2	28	5	0	0	1	1	371.0365652	27.0	2.892e-03
3	15	18	0	1	2	4	371.0423995	7.5	2.942e-03
4	13	16	1	0	4	4	371.0349440	7.5	4.513e-03
5	19	16	0	1	1	2	371.0338462	12.0	5.611e-03
*** Mass Analysis for mass [2] 373.0375520									
1	**18**	**16**	**0**	**1**	**2**	**2**	**373.0369202**	11.5	6.318e-04
2	22	5	0	0	4	3	373.0356165	22.5	1.936e-03
3	27	5	0	0	2	1	373.0396392	26.5	2.087e-03
4	17	16	1	0	3	2	373.0420408	11.0	4.489e-03
5	13	16	0	1	4	4	373.0328974	7.5	4.655e-03

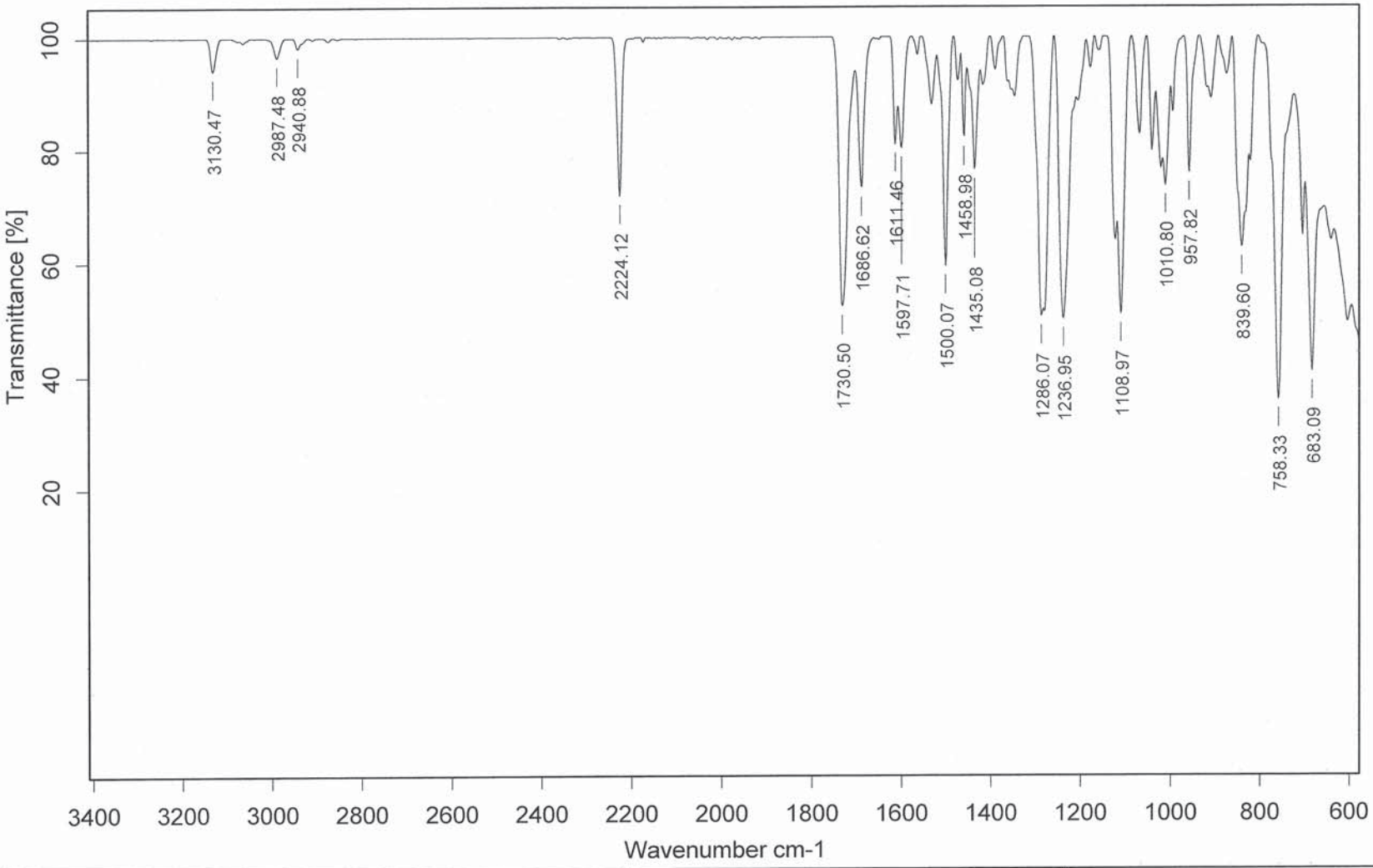


ethyl 3-(4-cyanophenyl)-1-phenyl-1H-pyrazole-5-carboxylate and ethyl 3-(4-cyanophenyl)-1-phenyl-1H-pyrazole-4-carboxylate



ethyl 3-(4-cyanophenyl)-1-phenyl-1H-pyrazole-5-carboxylate and ethyl 3-(4-cyanophenyl)-1-phenyl-1H-pyrazole-4-carboxylate





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BRUKER **FTMS 4.7T BioAPEX II**

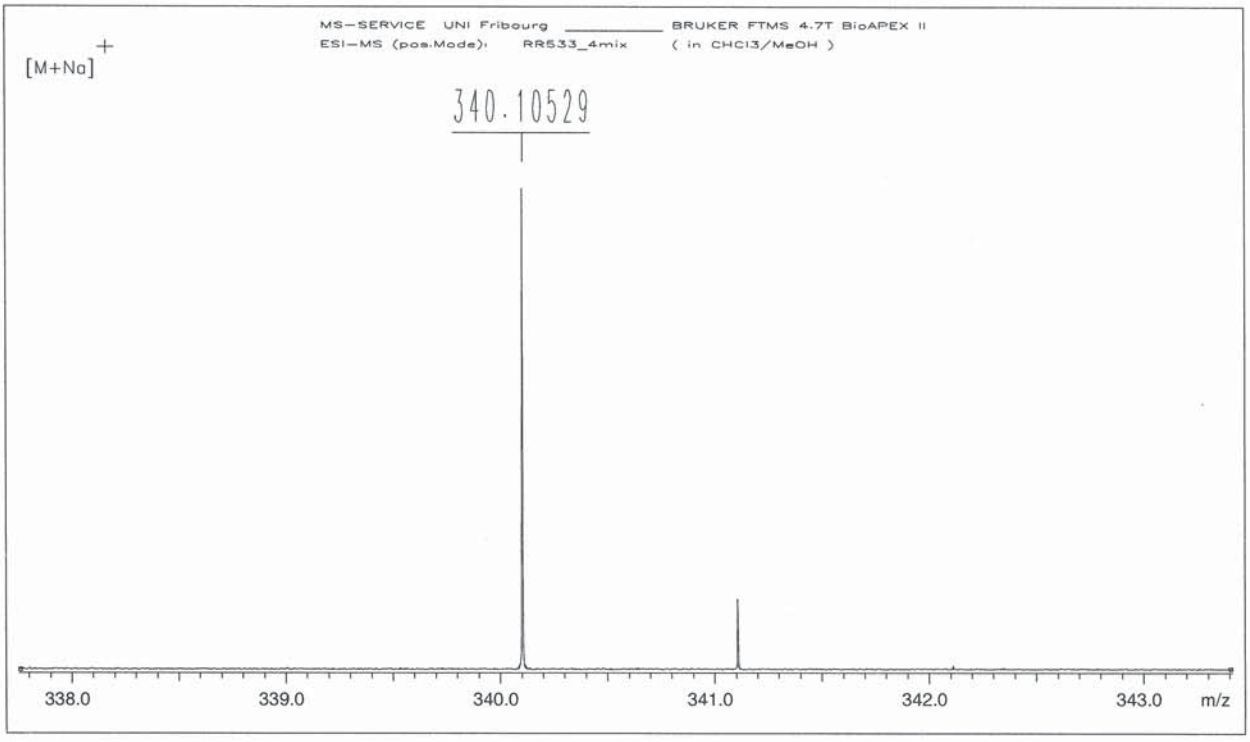
ESI-MS: RR533_4mix

XMASS Mass Analysis for /Data/UNI_FR/REMY2207_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 340.1052860

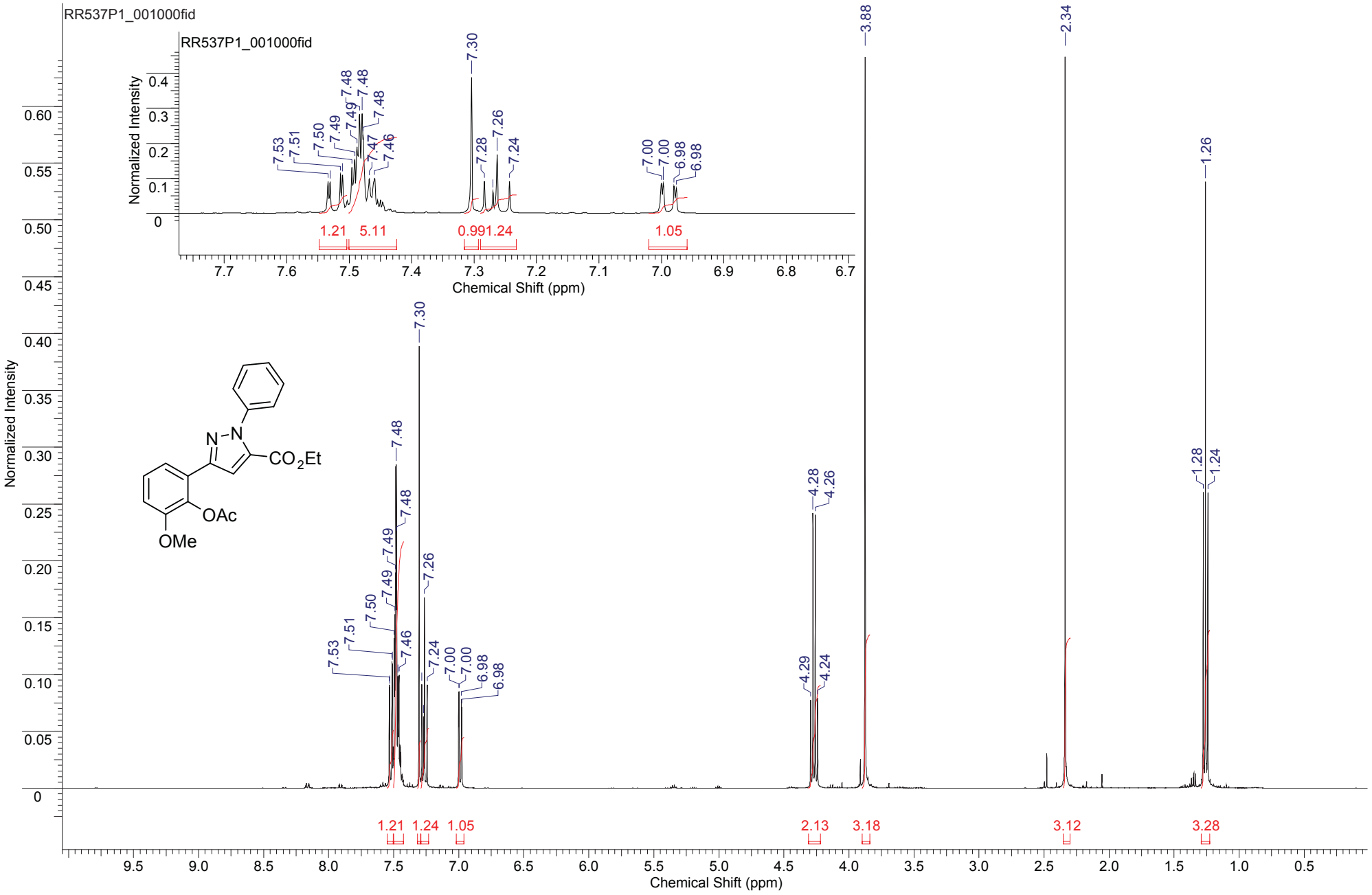
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 340.1052860								
1	**19**	**15**	**3**	**2**	**1**	**340.1056478**	13.5	3.618e-04
2	17	13	6	1	1	340.1043052	14.0	9.808e-04
3	16	14	5	4	0	340.1040304	12.5	1.256e-03
4	19	12	6	1	0	340.1067105	17.0	1.424e-03
5	14	12	8	3	0	340.1026877	13.0	2.598e-03
6	21	14	3	2	0	340.1080531	16.5	2.767e-03
7	14	15	5	4	1	340.1016251	9.5	3.661e-03
8	12	13	8	3	1	340.1002824	10.0	5.004e-03
9	11	13	10	2	1	340.1115158	10.0	6.230e-03
10	13	15	7	3	1	340.1128585	9.5	7.572e-03

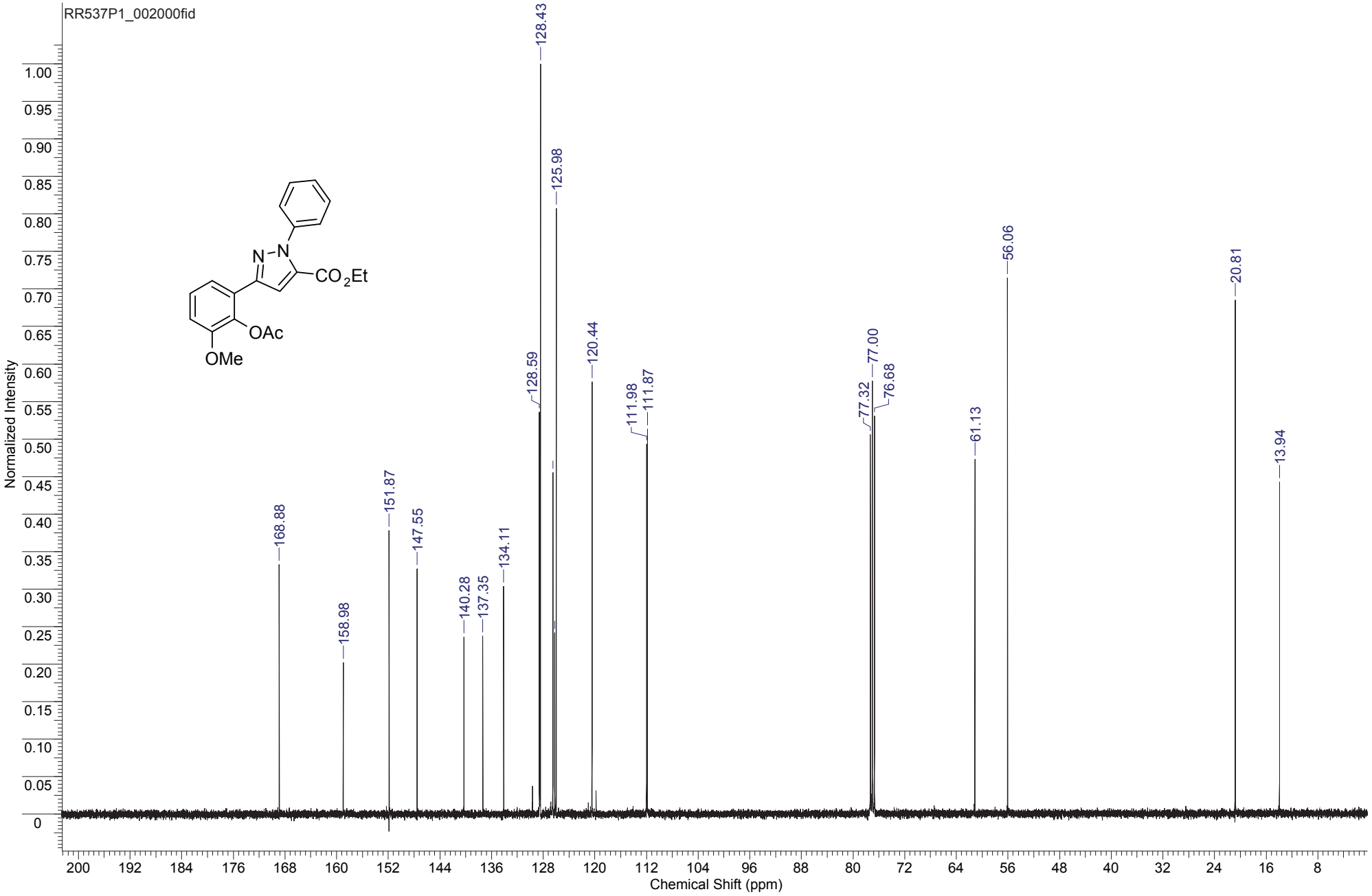


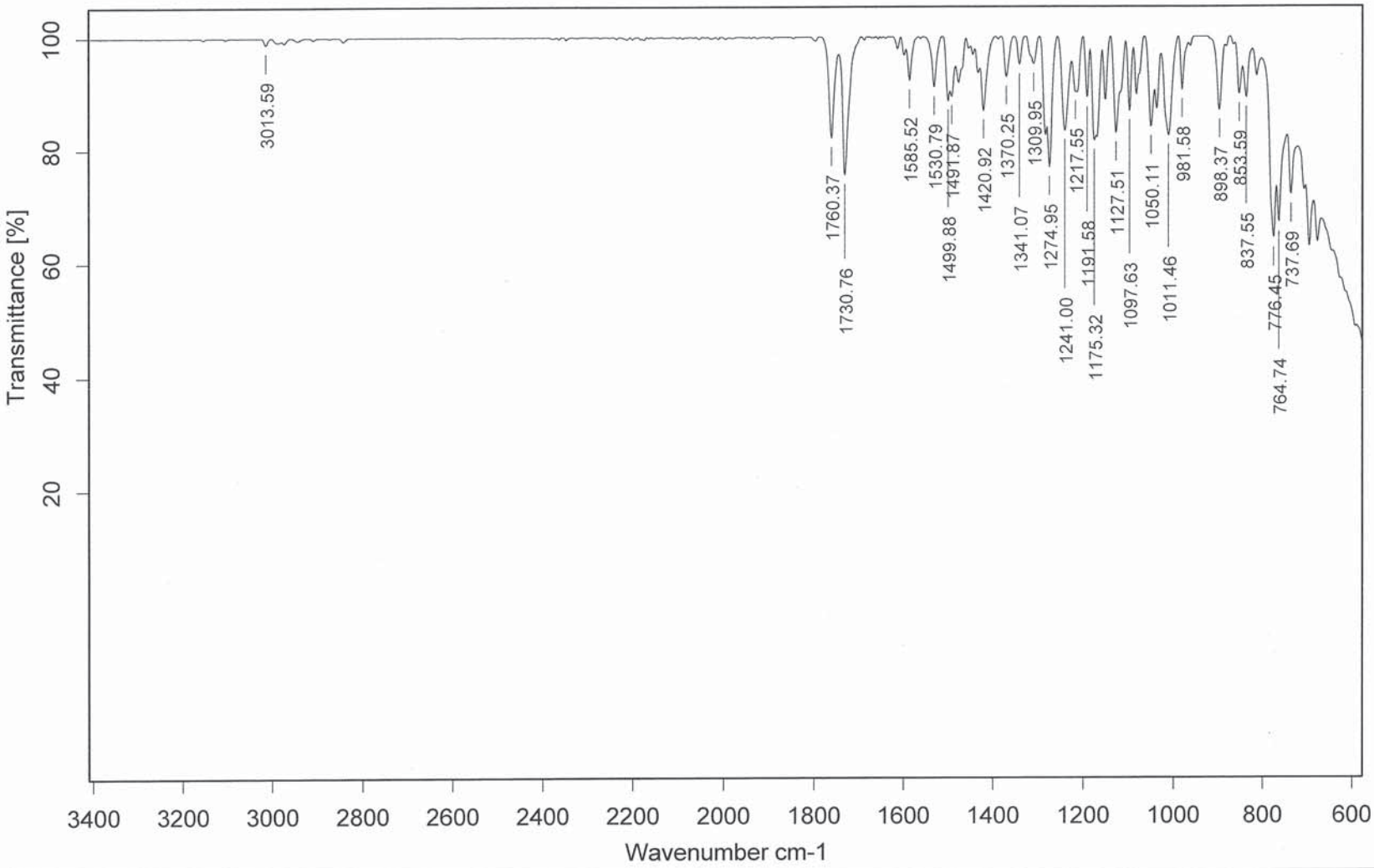
/Data/UNI_FR/REMY2207_ESI/2/pdata/1 FTMS USER Fri Oct 28 15:16:13 2016

ethyl 3-(2-acetoxy-3-methoxyphenyl)-1-phenyl-1H-pyrazole-5-carboxylate



ethyl 3-(2-acetoxy-3-methoxyphenyl)-1-phenyl-1H-pyrazole-5-carboxylate





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BRUKER **FTMS 4.7T BioAPEX II**

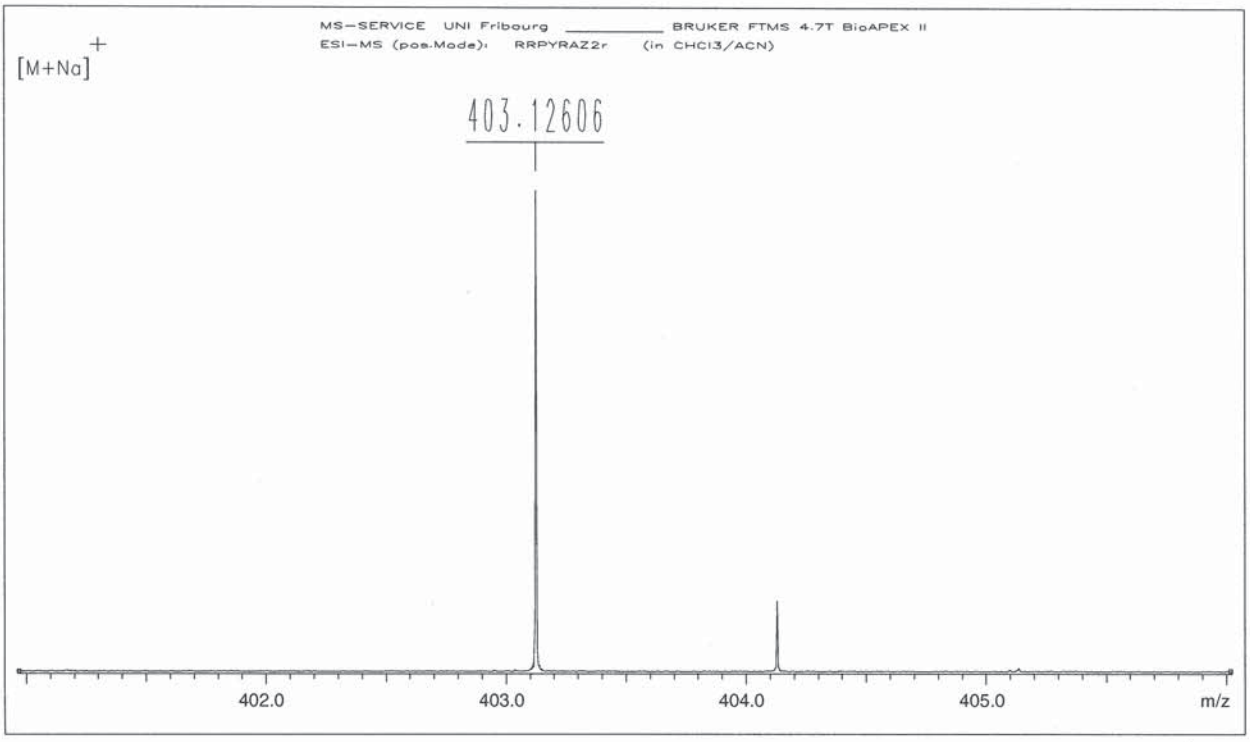
ESI-MS: RRPYRAZ2r

XMASS Mass Analysis for /Data/UNI_FR/REMY2410_ESI/4/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 403.1260580

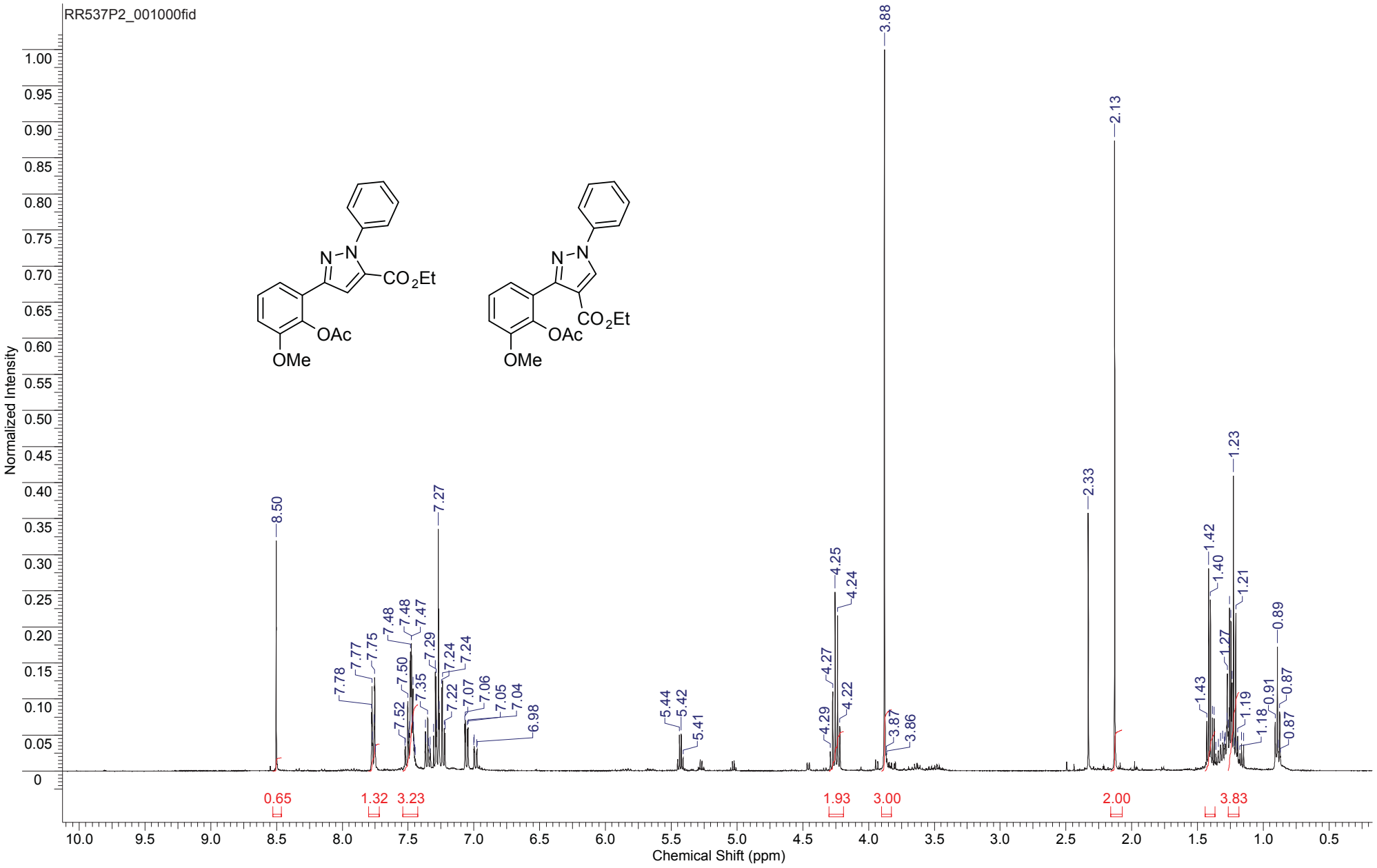
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 403.1260580								
1	**21**	**20**	**2**	**5**	**1**	**403.1264429**	12.5	3.849e-04
2	19	18	5	4	1	403.1251002	13.0	9.578e-04
3	18	19	4	7	0	403.1248254	11.5	1.233e-03
4	21	17	5	4	0	403.1275055	16.0	1.447e-03
5	23	19	2	5	0	403.1288482	15.5	2.790e-03
6	24	18	3	2	1	403.1291229	17.0	3.065e-03
7	16	20	4	7	1	403.1224201	8.5	3.638e-03
8	26	17	3	2	0	403.1315282	20.0	5.470e-03
9	27	17	1	3	0	403.1202948	20.0	5.763e-03
10	25	15	4	2	0	403.1189522	20.5	7.106e-03

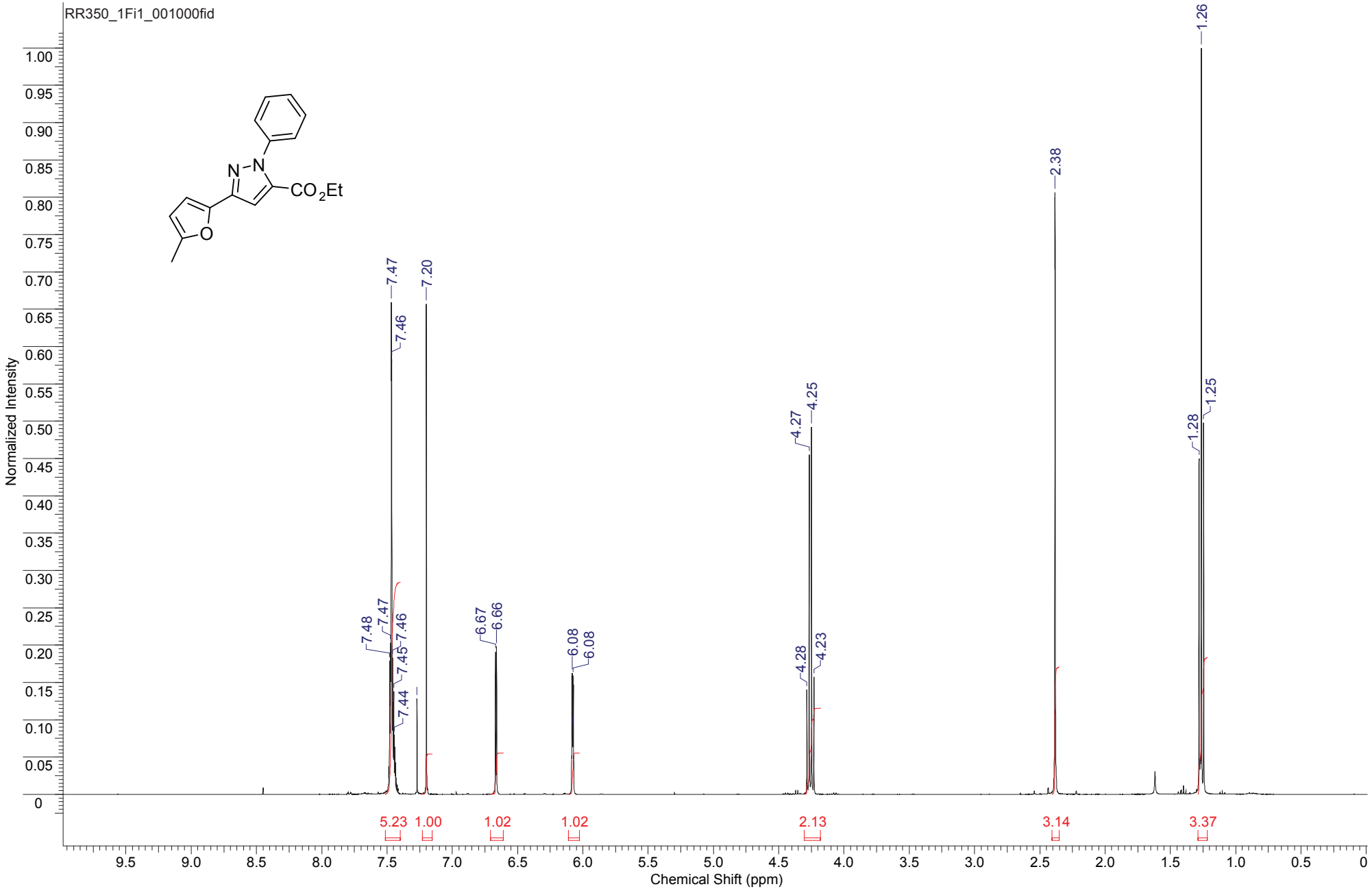


/Data/UNI_FR/REMY2410_ESI/4/pdata/1 FTMS USER Wed Dec 14 14:21:12 2016

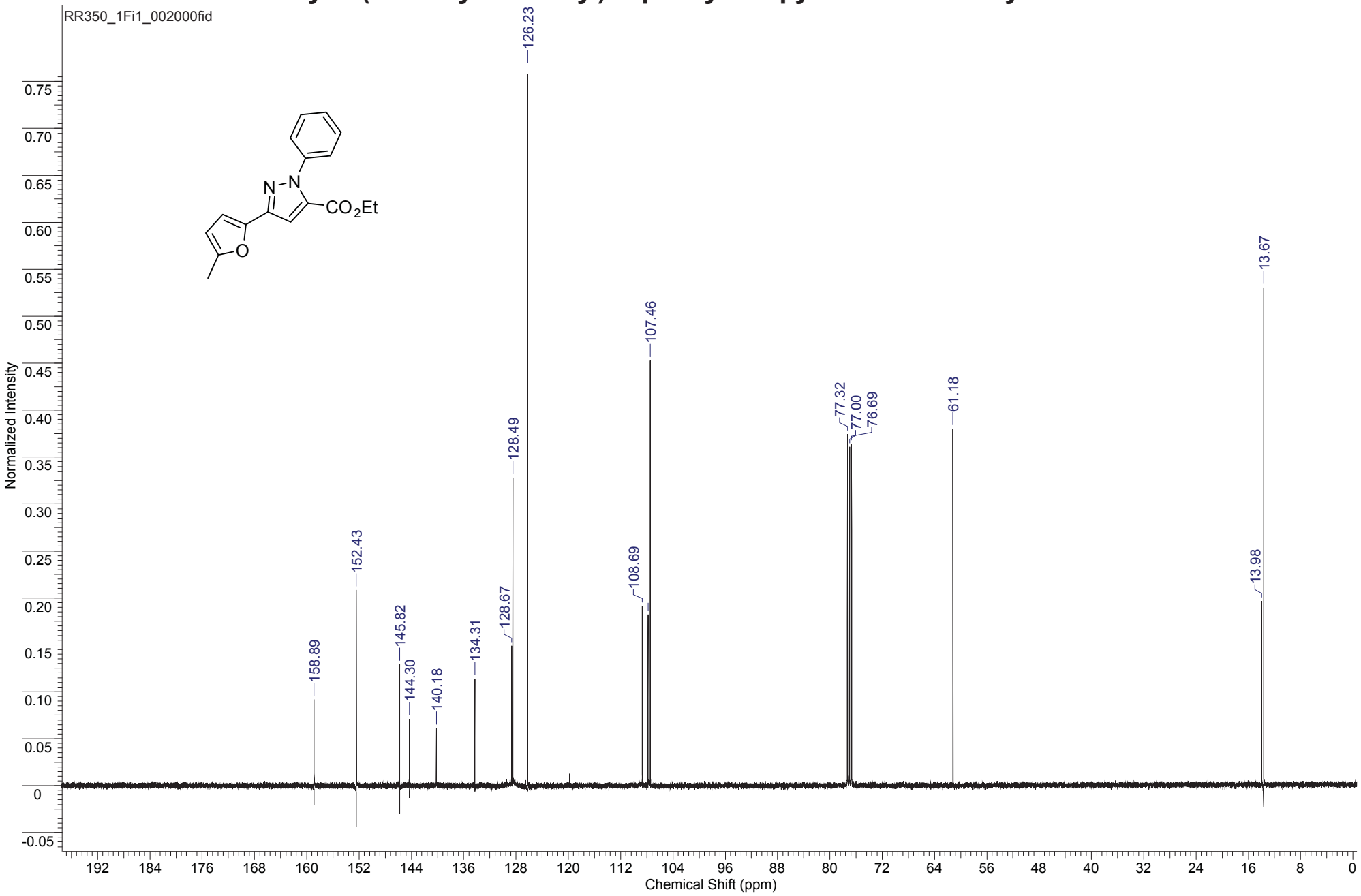
ethyl 3-(2-acetoxy-3-methoxyphenyl)-1-phenyl-1H-pyrazole-5-carboxylate and ethyl 3-(2-acetoxy-3-methoxyphenyl)-1-phenyl-1H-pyrazole-4-carboxylate

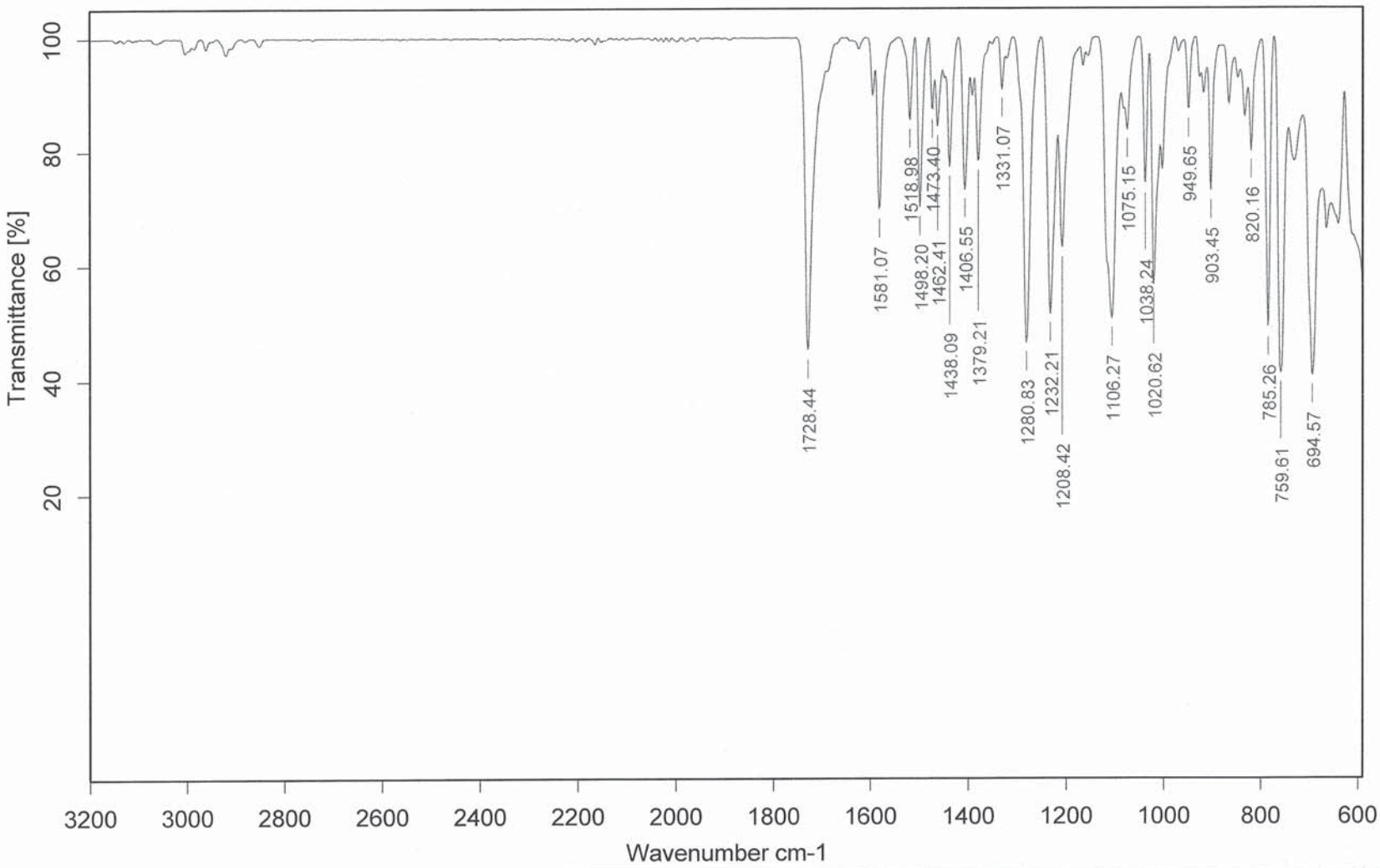


ethyl 3-(5-methylfuran-2-yl)-1-phenyl-1H-pyrazole-5-carboxylate



ethyl 3-(5-methylfuran-2-yl)-1-phenyl-1H-pyrazole-5-carboxylate





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FTMS 4.7T BioAPEX II

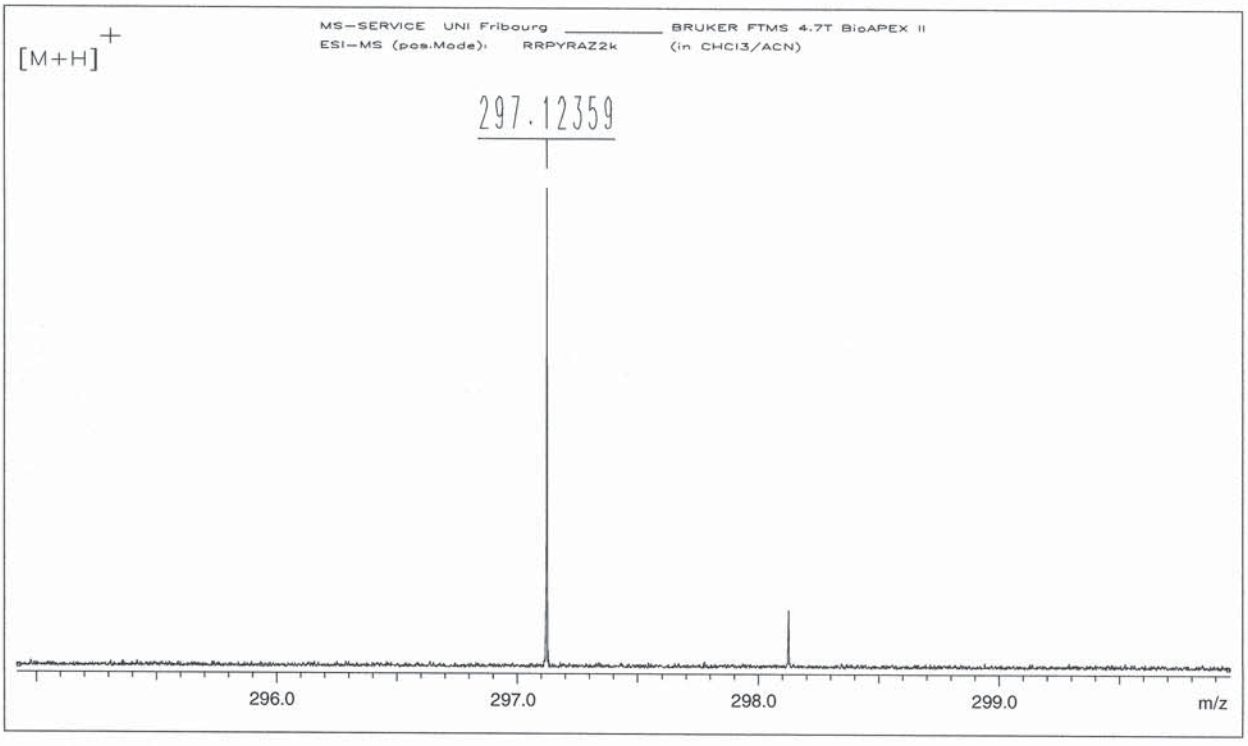
ESI-MS: RRPYRAZ2k

XMASS Mass Analysis for /Data/UNI_FR/REMY2405_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 297.1235870

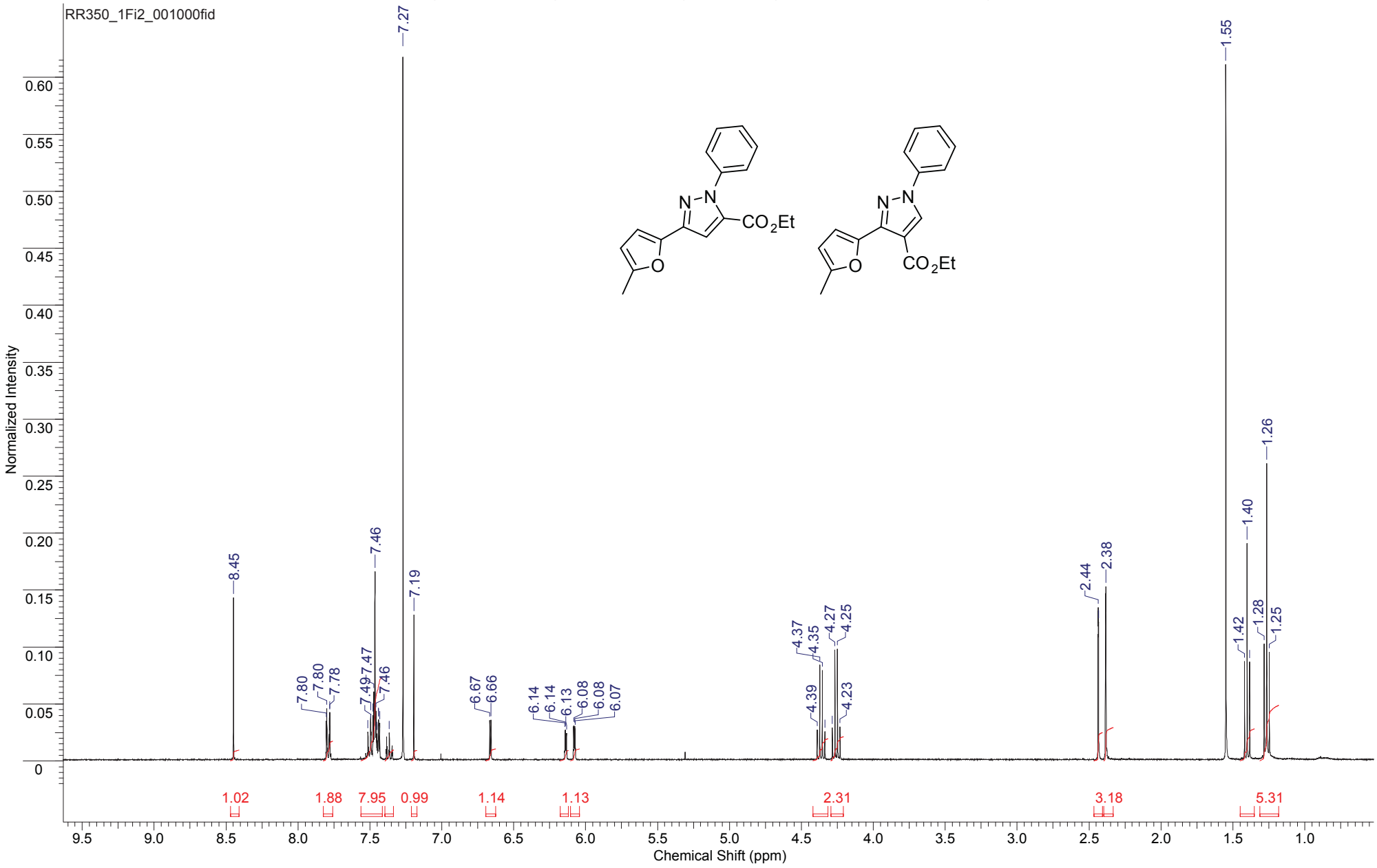
Charge = +1

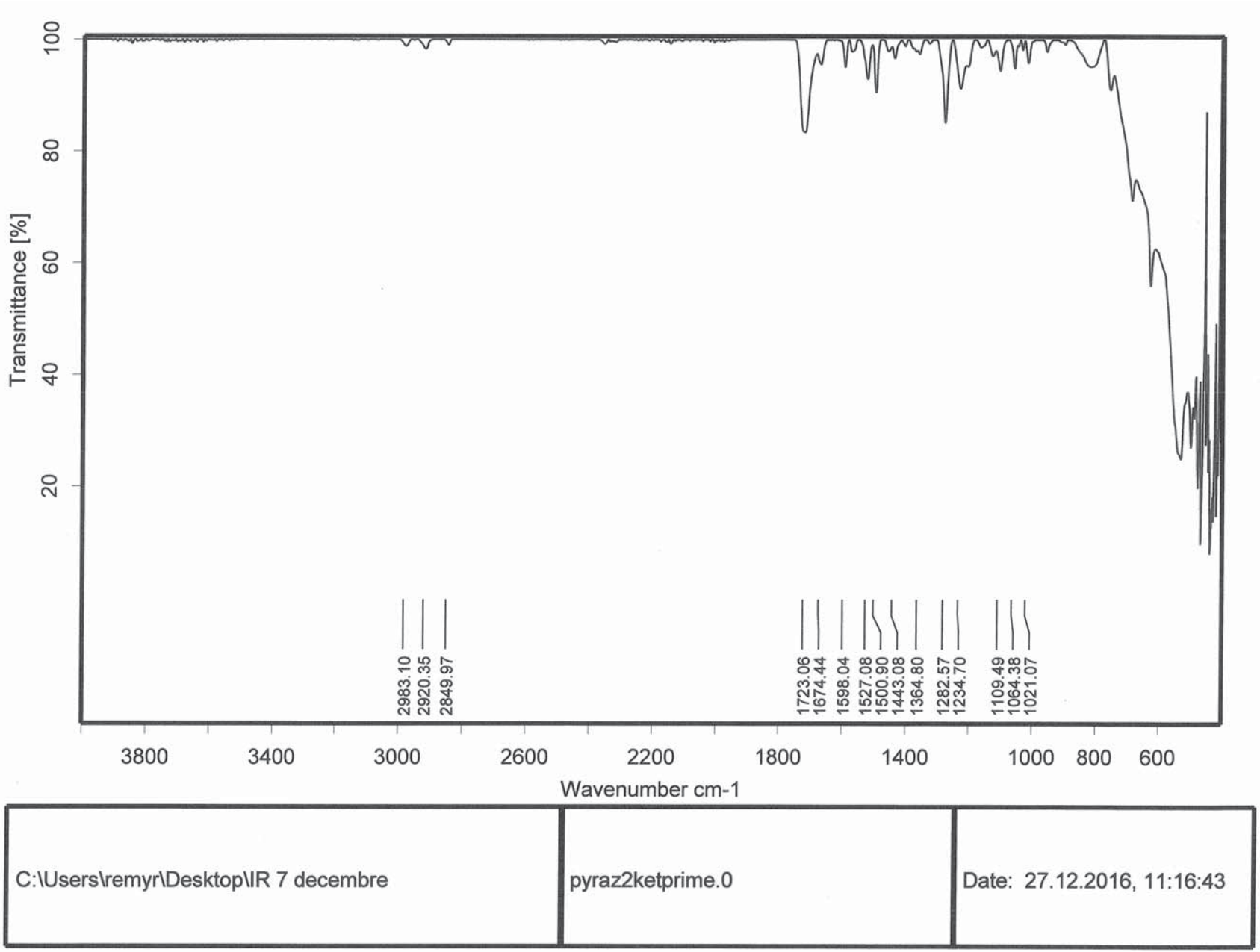
#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 297.1235870							
1	**17**	**17**	**2**	**3**	**297.1233688**	10.5	2.182e-04
2	21	15	1	1	297.1148155	15.0	8.771e-03
3	16	17	4	2	297.1346022	10.5	1.102e-02
4	18	19	1	3	297.1359449	10.0	1.236e-02
5	16	15	3	3	297.1107928	11.0	1.279e-02
6	20	13	2	1	297.1022395	15.5	2.135e-02
7	17	19	3	2	297.1471783	10.0	2.359e-02
8	17	15	1	4	297.0995594	11.0	2.403e-02
9	15	13	4	3	297.0982167	11.5	2.537e-02
10	13	21	4	4	297.1557316	5.5	3.214e-02



/Data/UNI_FR/REMY2405_ESI/2/pdata/1 FTMS USER Wed Dec 14 13:49:15 2016

ethyl 3-(5-methylfuran-2-yl)-1-phenyl-1H-pyrazole-5-carboxylate and ethyl 3-(5-methylfuran-2-yl)-1-phenyl-1H-pyrazole-4-carboxylate





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BRUKER **FTMS 4.7T BioAPEX II**

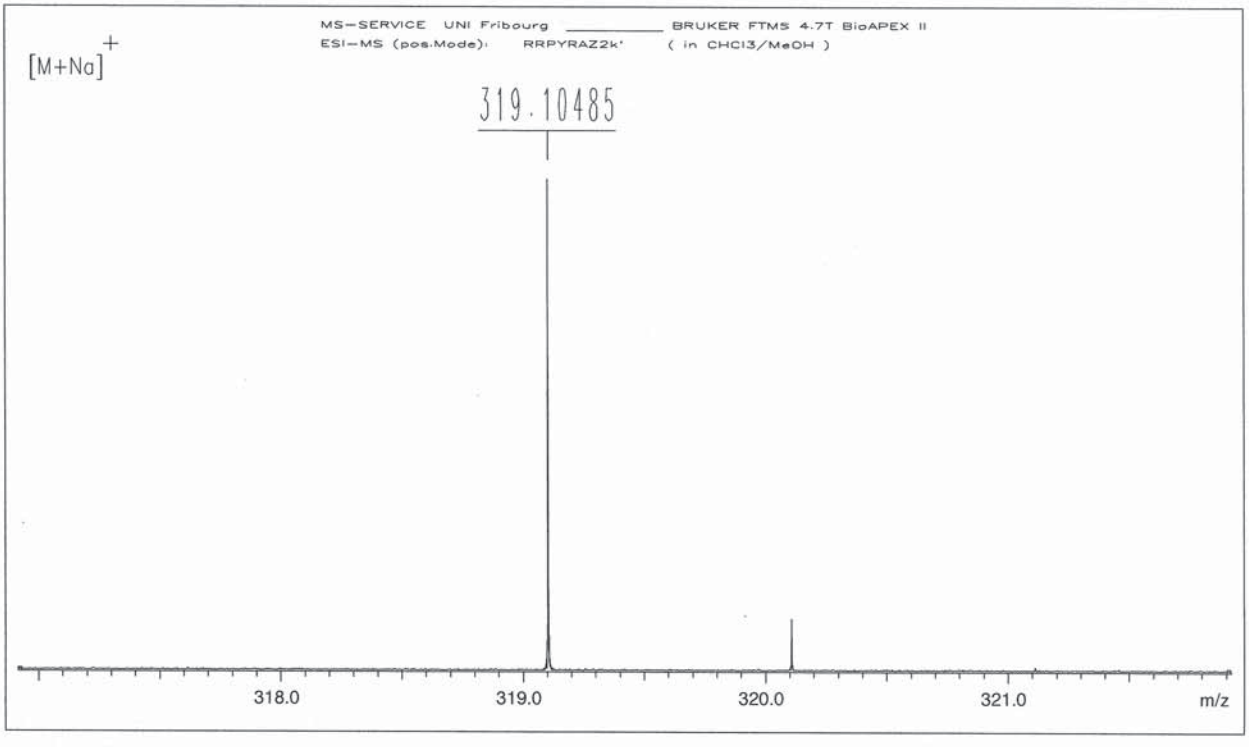
ESI-MS: RRPYRAZ2k'

XMASS Mass Analysis for /Data/UNI_FR/REMY2452_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

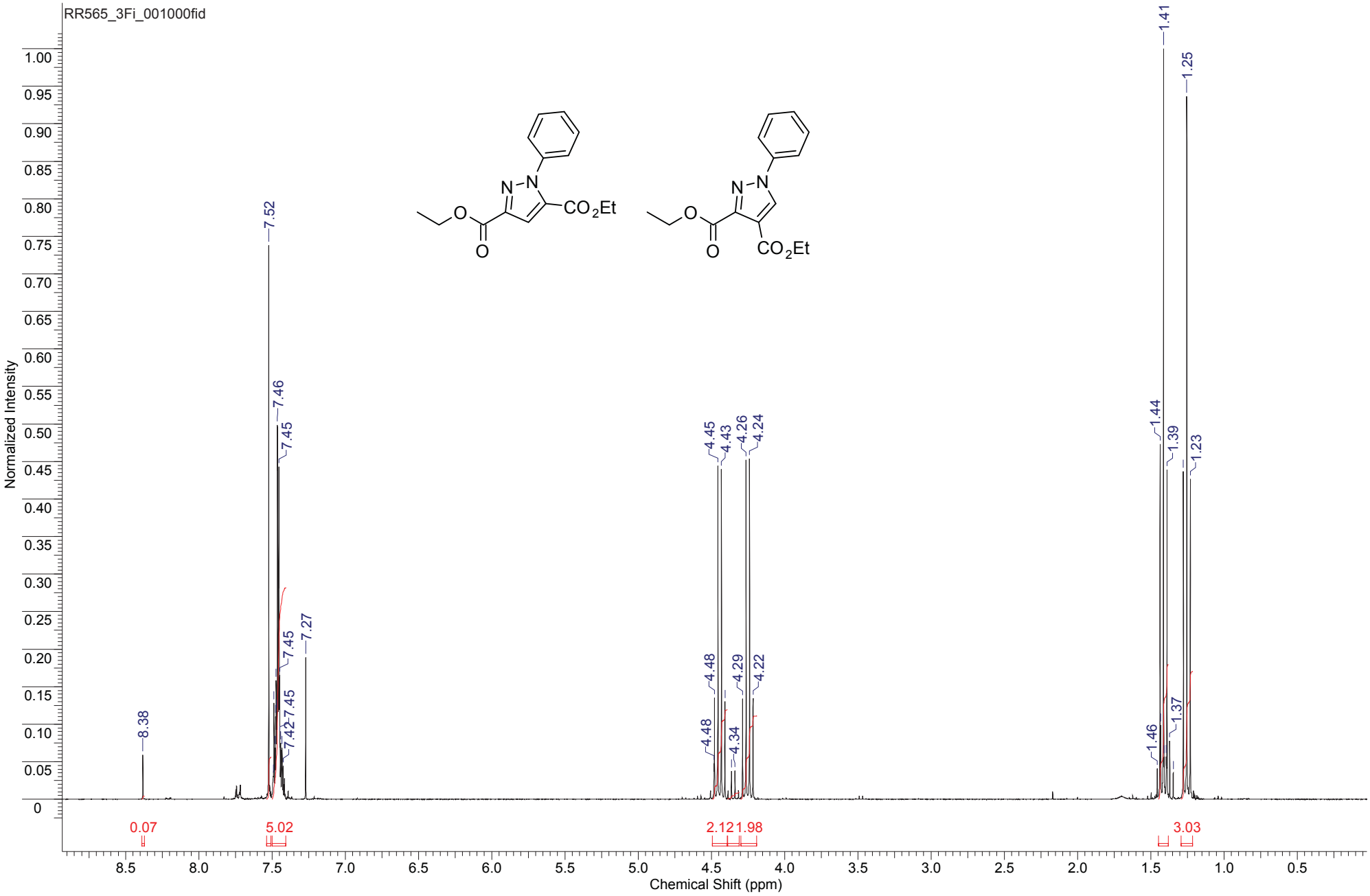
Ion mass = 319.1048550

Charge = +1

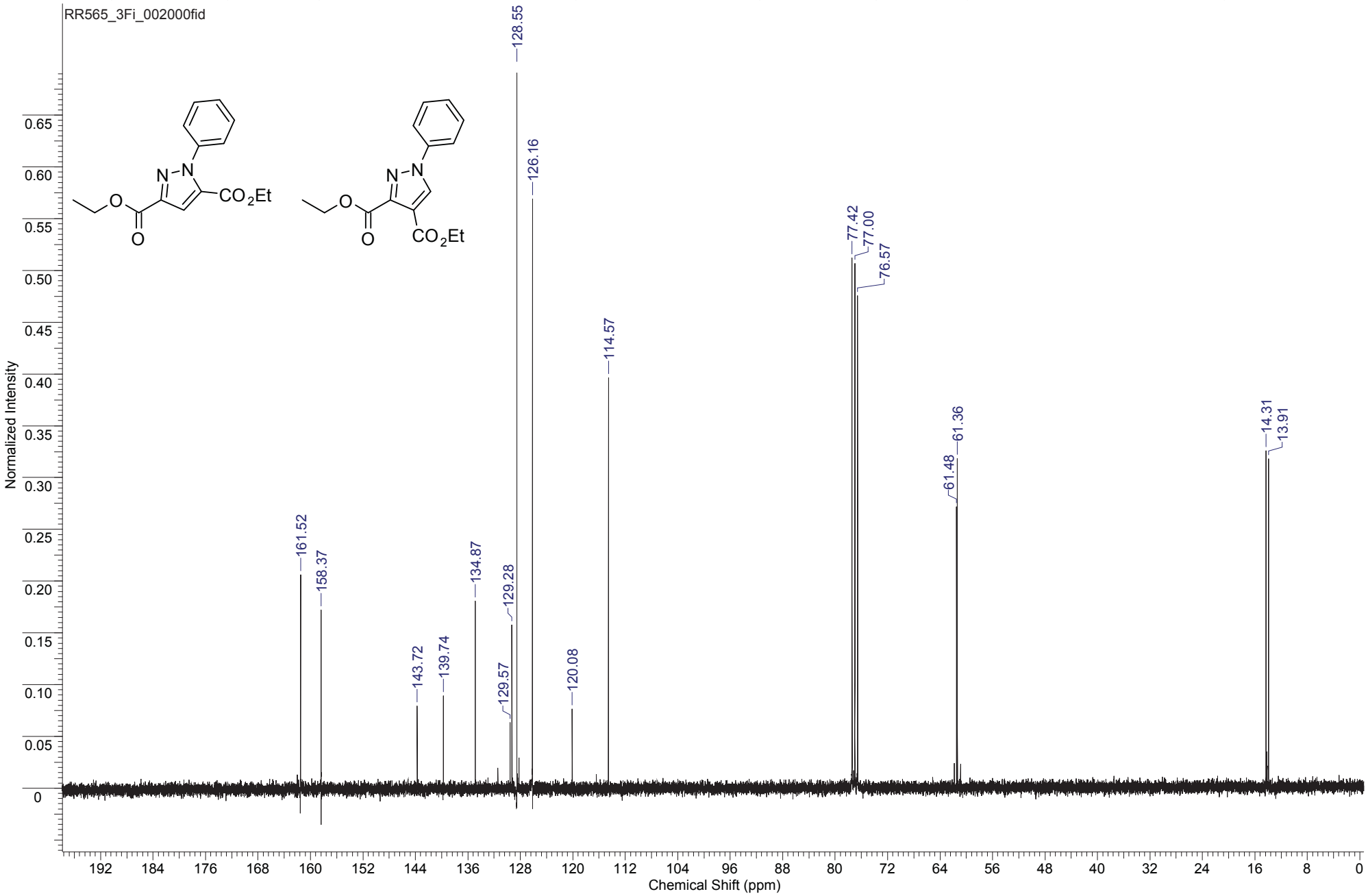
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 319.1048550								
1	**17**	**16**	**2**	**3**	**1**	**319.1053135**	10.5	4.585e-04
2	15	14	5	2	1	319.1039708	11.0	8.842e-04
3	14	15	4	5	0	319.1036960	9.5	1.159e-03
4	17	13	5	2	0	319.1063761	14.0	1.521e-03
5	19	15	2	3	0	319.1077188	13.5	2.864e-03
6	12	16	4	5	1	319.1012907	6.5	3.564e-03
7	23	13	1	1	0	319.0991655	18.0	5.690e-03
8	21	14	1	1	1	319.0967602	15.0	8.095e-03
9	13	18	3	5	1	319.1138668	6.0	9.012e-03
10	18	13	3	3	0	319.0951427	14.0	9.712e-03

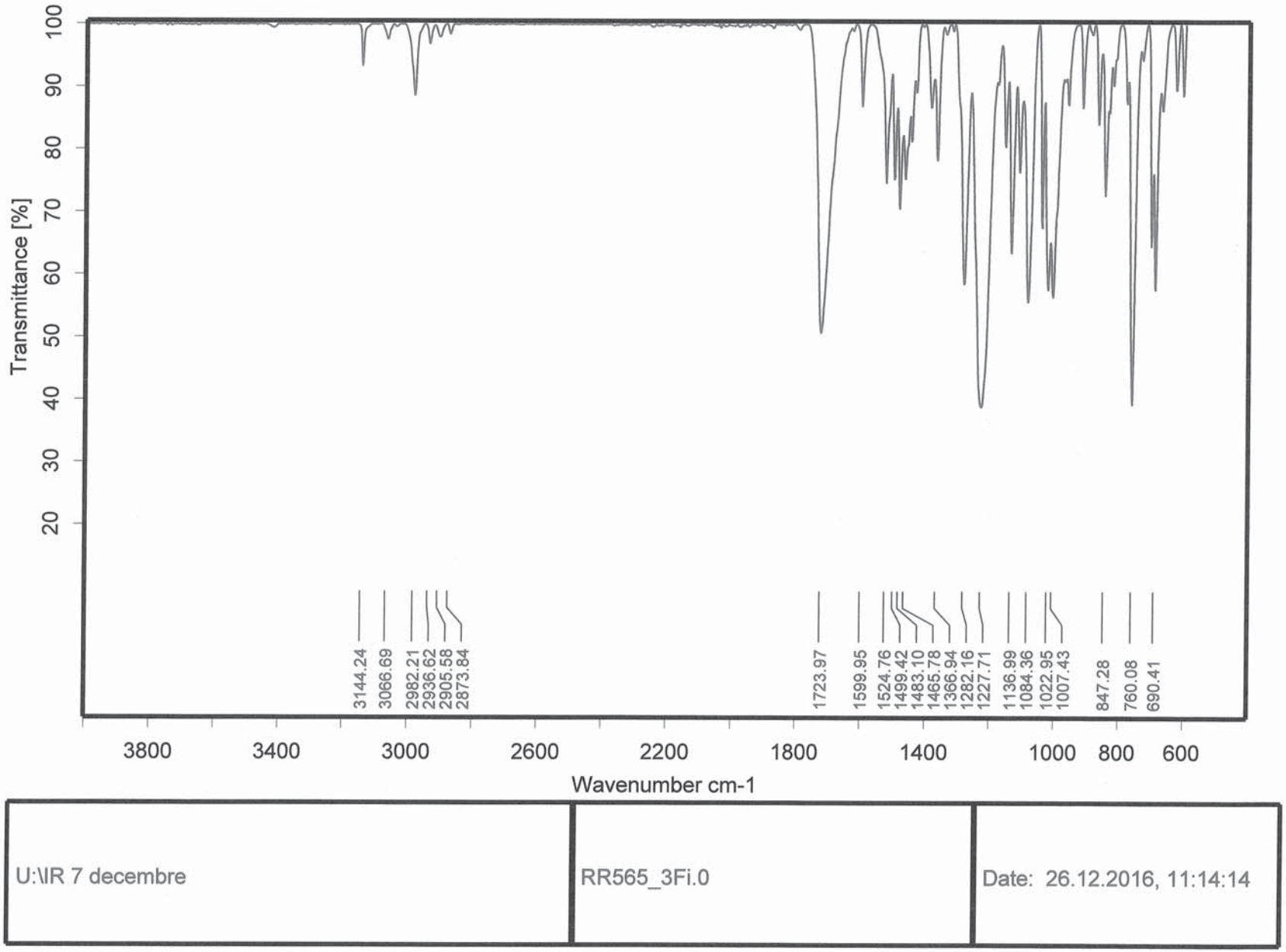


diethyl 1-phenyl-1H-pyrazole-3,5-dicarboxylate and diethyl 1-phenyl-1H-pyrazole-3,4-dicarboxylate



diethyl 1-phenyl-1H-pyrazole-3,5-dicarboxylate and diethyl 1-phenyl-1H-pyrazole-3,4-dicarboxylate

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90
80
70
60
50
40
30
20
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2936.62
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1723.97
1599.95
1524.76
1499.42
1483.10
1465.78
1366.94
1282.16
1227.71
1136.99
1084.36
1022.95
1007.43
847.28
760.08
690.41
3800
3400
3000
2600
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800
600
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BRUKER **FTMS 4.7T BioAPEX II**

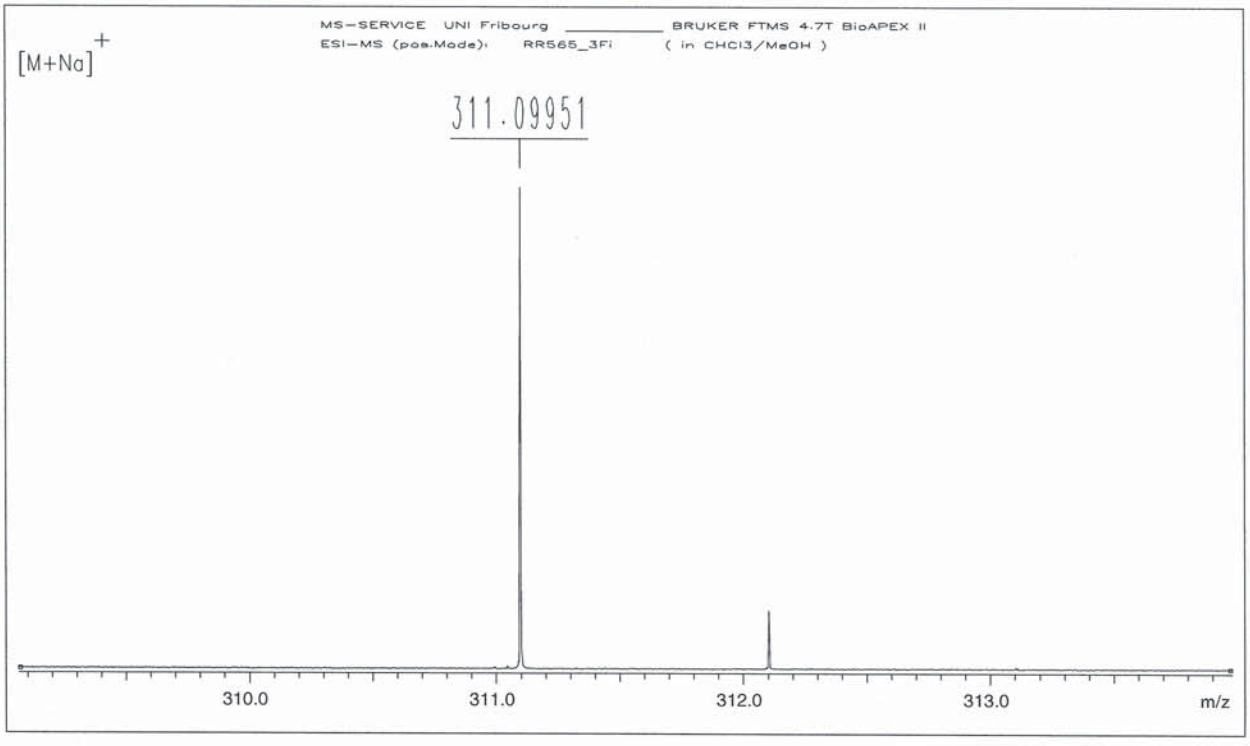
ESI-MS: RR565_3Fi

XMASS Mass Analysis for /Data/UNI_FR/REMY2455_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 311.0995080

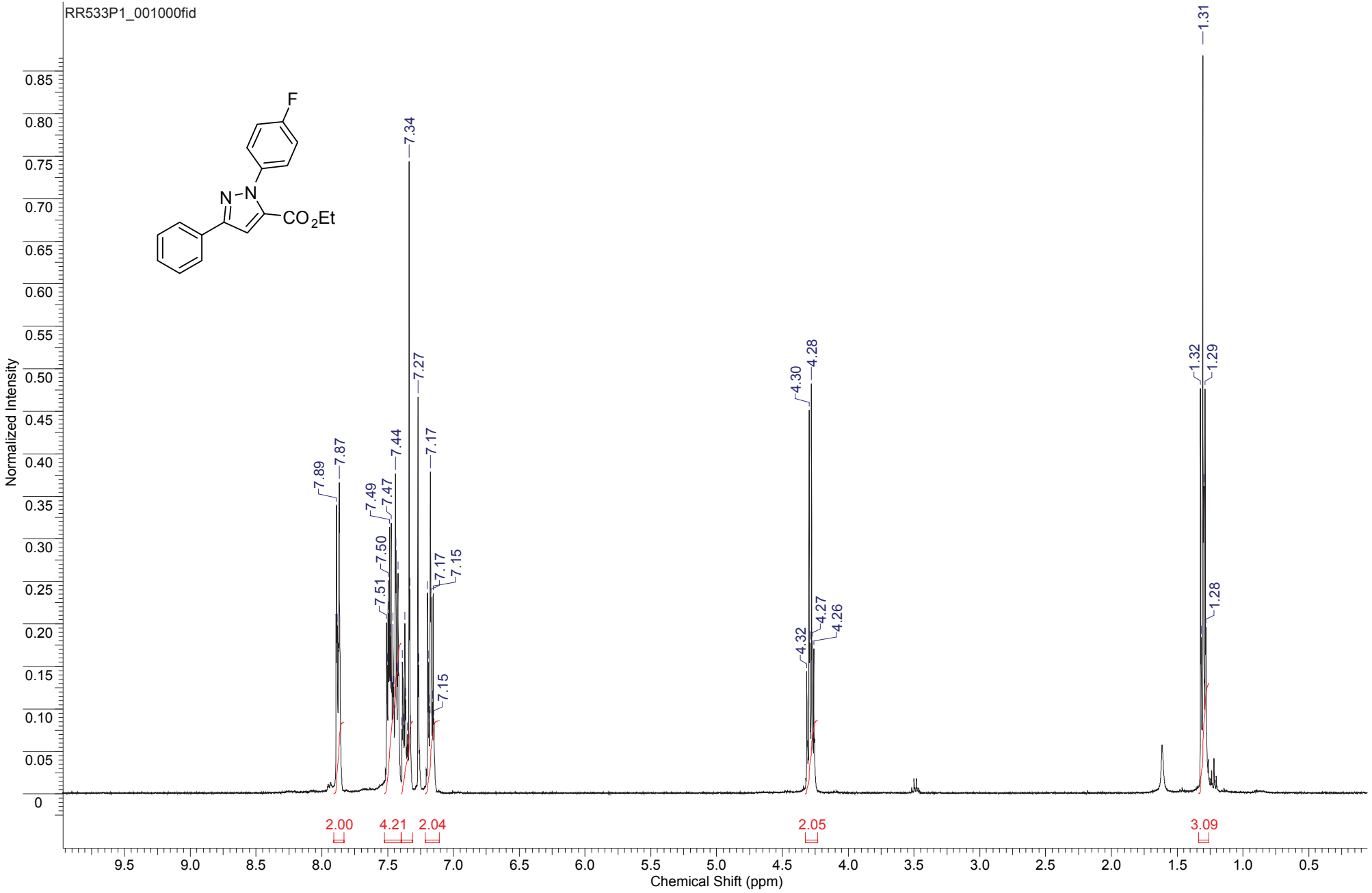
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 311.0995080								
1	**15**	**16**	**2**	**4**	**1**	**311.1002281**	8.5	7.201e-04
2	17	15	2	4	0	311.1026334	11.5	3.125e-03
3	18	14	3	1	1	311.1029082	13.0	3.400e-03
4	21	13	1	2	0	311.0940801	16.0	5.428e-03
5	20	13	3	1	0	311.1053135	16.0	5.805e-03
6	19	11	4	1	0	311.0927374	16.5	6.771e-03
7	19	14	1	2	1	311.0916748	13.0	7.833e-03
8	17	12	4	1	1	311.0903321	13.5	9.176e-03
9	16	13	3	4	0	311.0900573	12.0	9.451e-03
10	14	14	3	4	1	311.0876520	9.0	1.186e-02

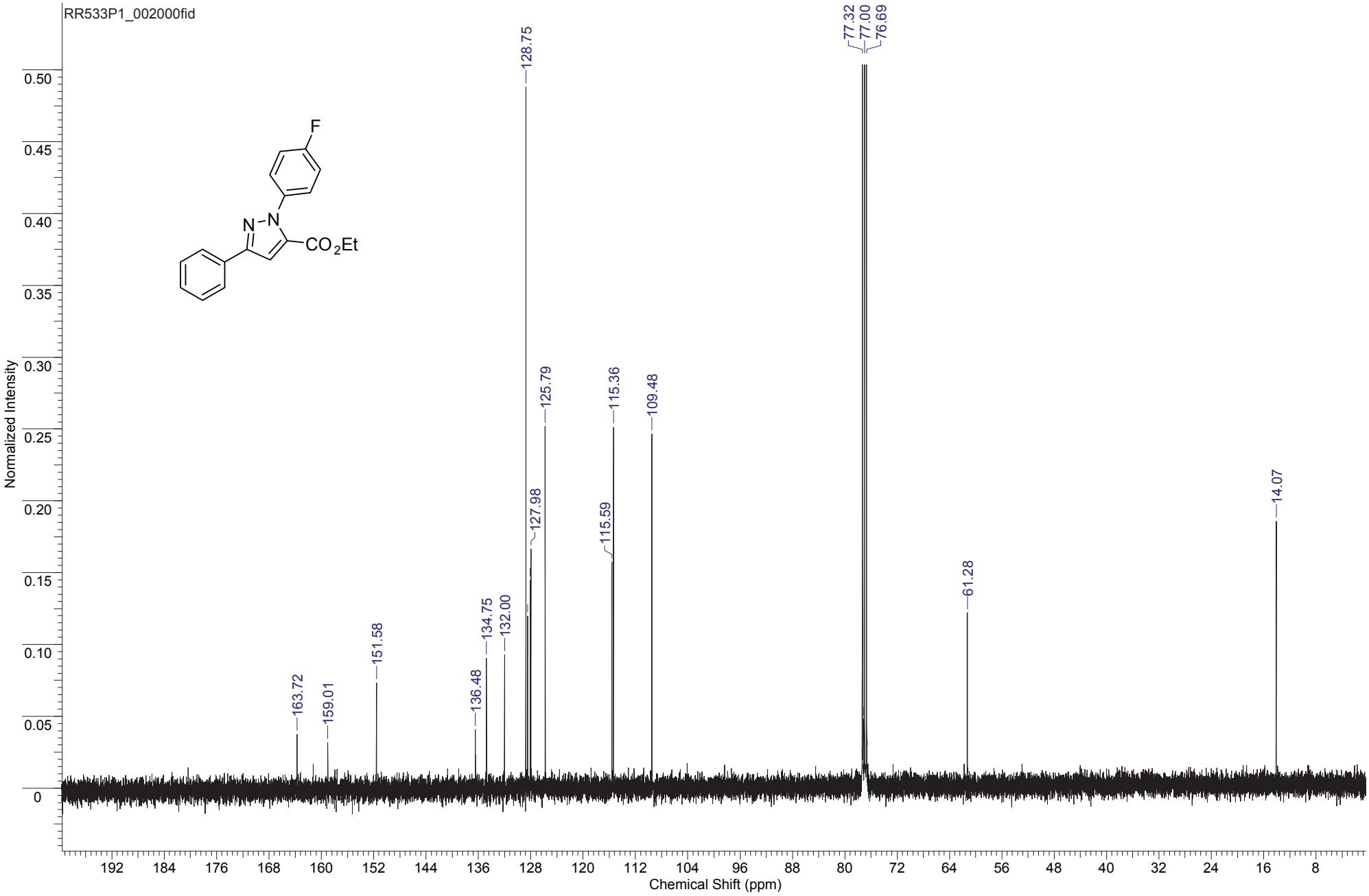


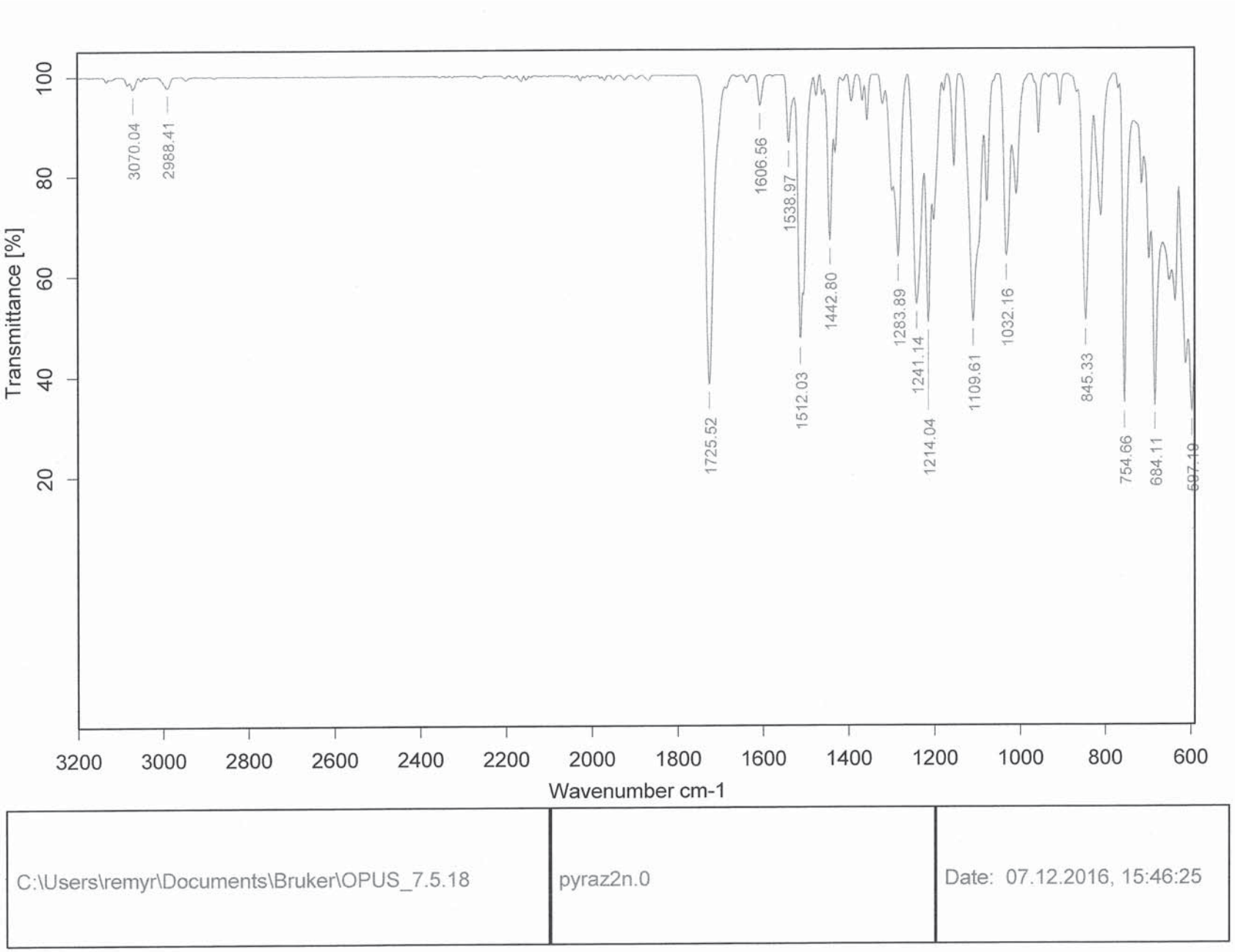
/Data/UNI_FR/REMY2455_ESI/2/pdata/1 FTMS USER Wed Jan 4 17:39:04 2017

ethyl 1-(4-fluorophenyl)-3-phenyl-1H-pyrazole-5-carboxylate



ethyl 1-(4-fluorophenyl)-3-phenyl-1H-pyrazole-5-carboxylate





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BRUKER **FTMS 4.7T BioAPEX II**

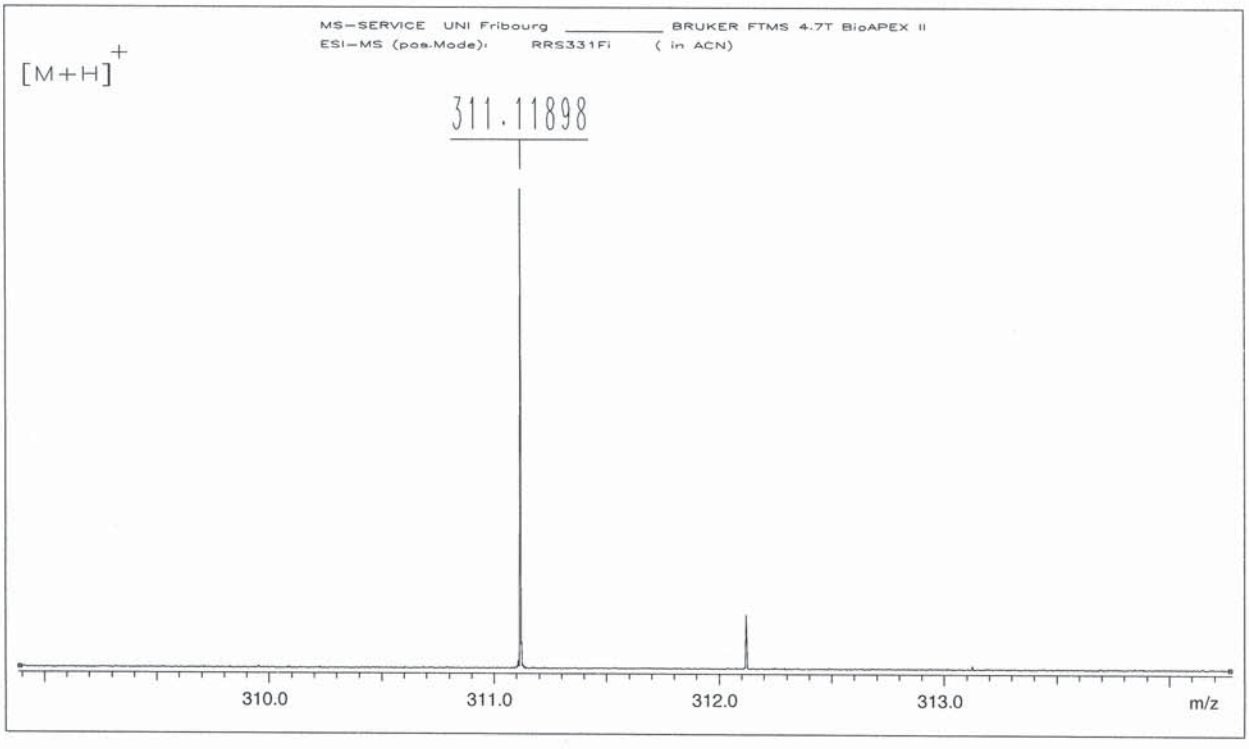
ESI-MS: RR5331Fi

XMASS Mass Analysis for /Data/UNI_FR/REMY2067_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

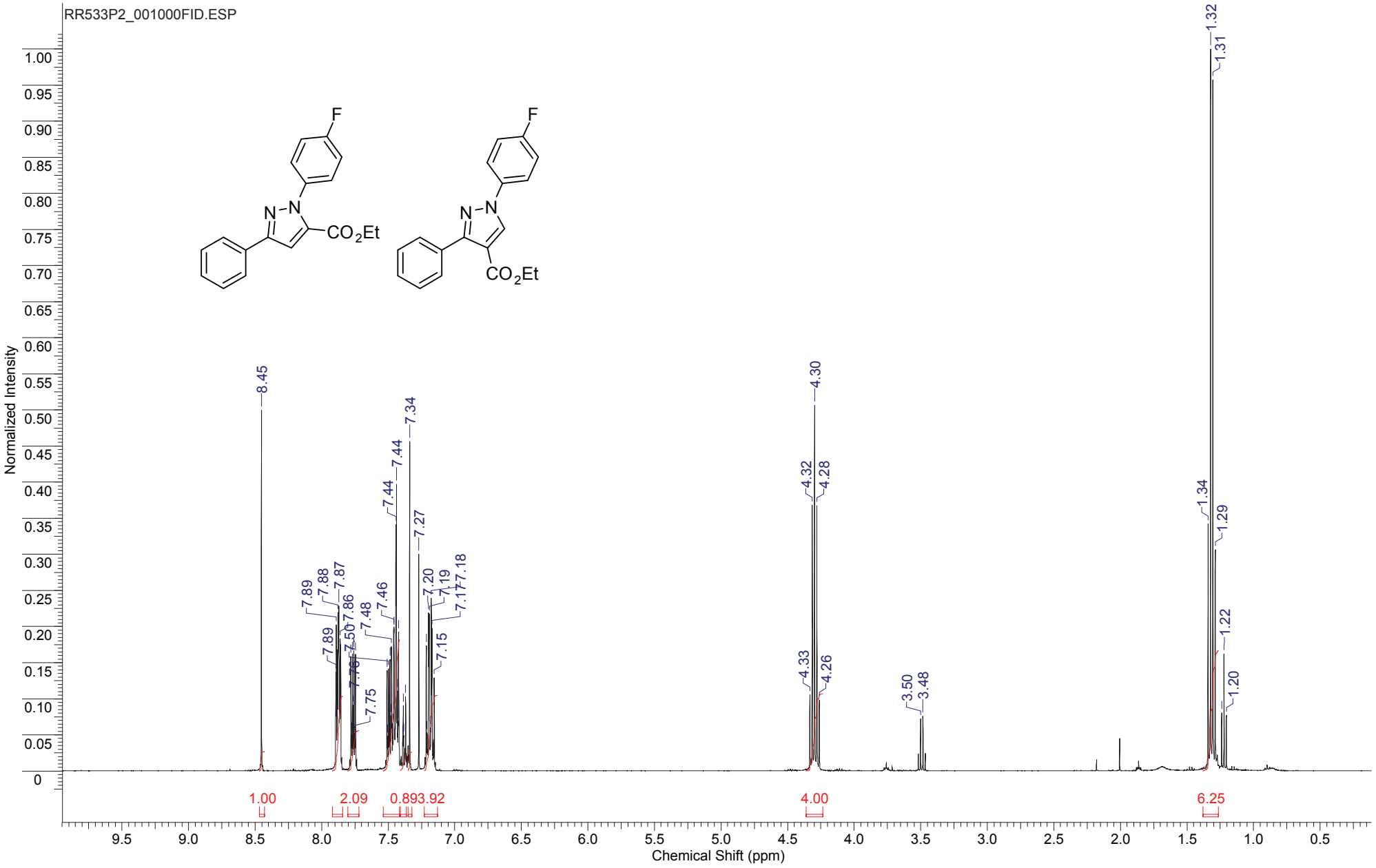
Ion mass = 311.1189830

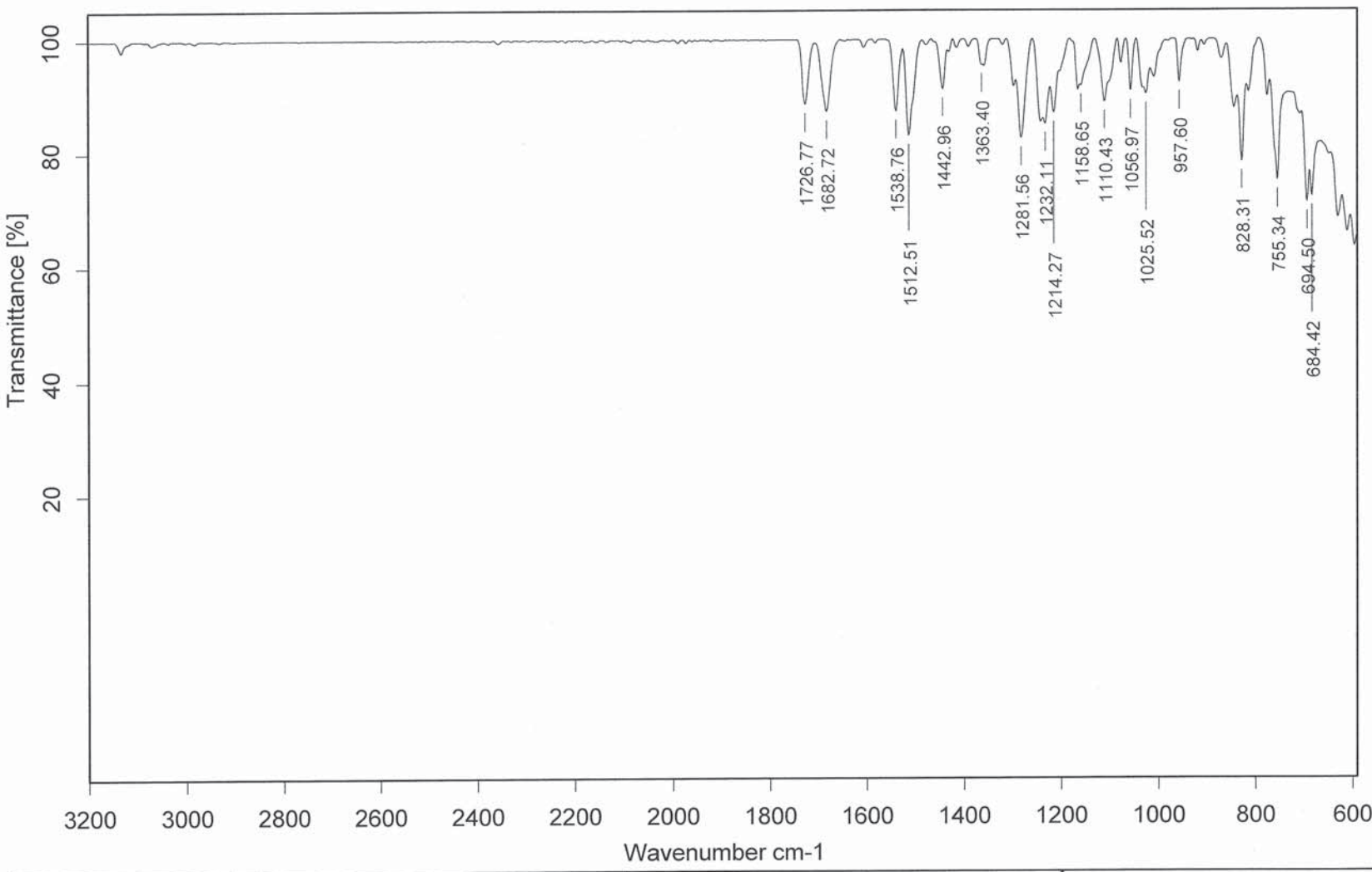
Charge = +1

#	C	H	N	O	F	mass	DBE	error
*** Mass Analysis for mass 311.1189830								
1	**18**	**16**	**2**	**2**	**1**	**311.1190324**	11.5	4.939e-05
2	13	15	5	2	2	311.1188326	8.0	1.504e-04
3	15	17	2	3	2	311.1201752	7.5	1.192e-03
4	16	14	5	1	1	311.1176897	12.0	1.293e-03
5	12	19	1	6	2	311.1174952	3.0	1.488e-03
6	11	13	8	1	2	311.1174899	8.5	1.493e-03
7	6	20	4	9	1	311.1208829	-1.5	1.900e-03
8	15	18	1	5	1	311.1163523	7.0	2.631e-03
9	10	17	4	5	2	311.1161525	3.5	2.831e-03
10	7	16	8	5	1	311.1222203	3.5	3.237e-03



ethyl 1-(4-fluorophenyl)-3-phenyl-1H-pyrazole-5-carboxylate and ethyl 1-(4-fluorophenyl)-3-phenyl-1H-pyrazole-4-carboxylate





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BRUKER **FTMS 4.7T BioAPEX II**

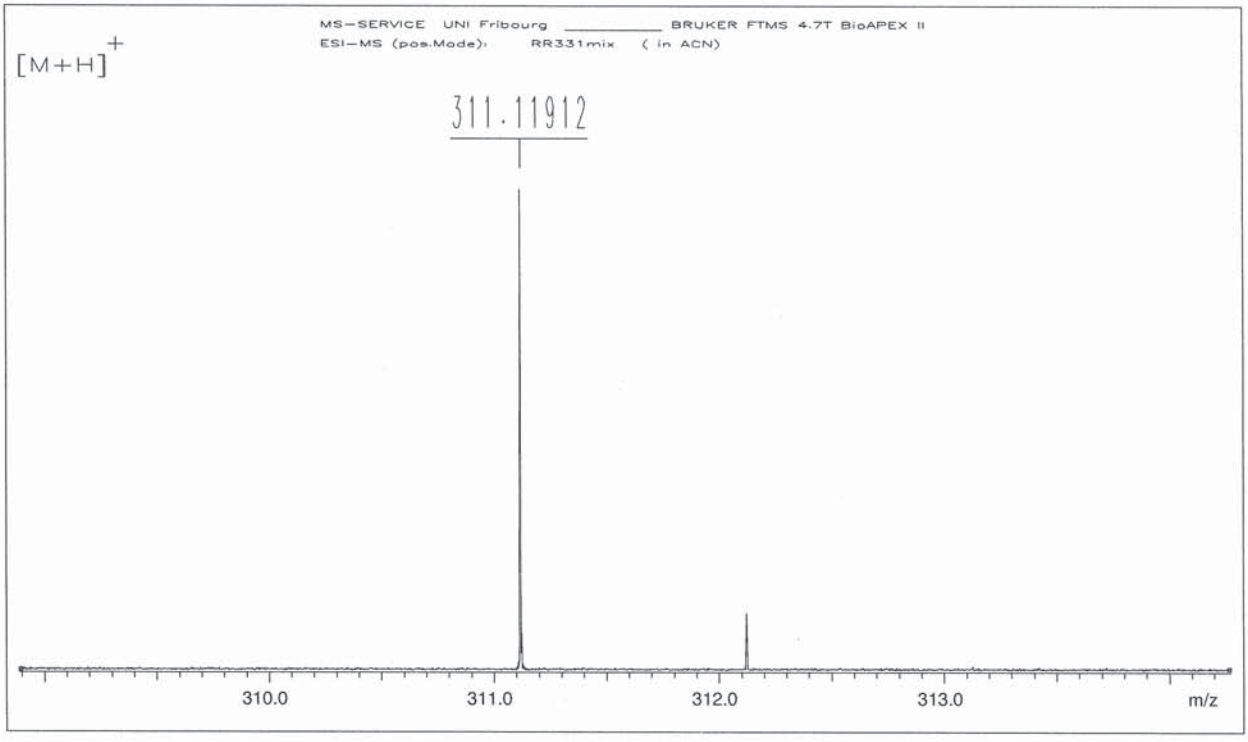
ESI-MS: RR5331mix

XMASS Mass Analysis for /Data/UNI_FR/REMY2066_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 311.1191170

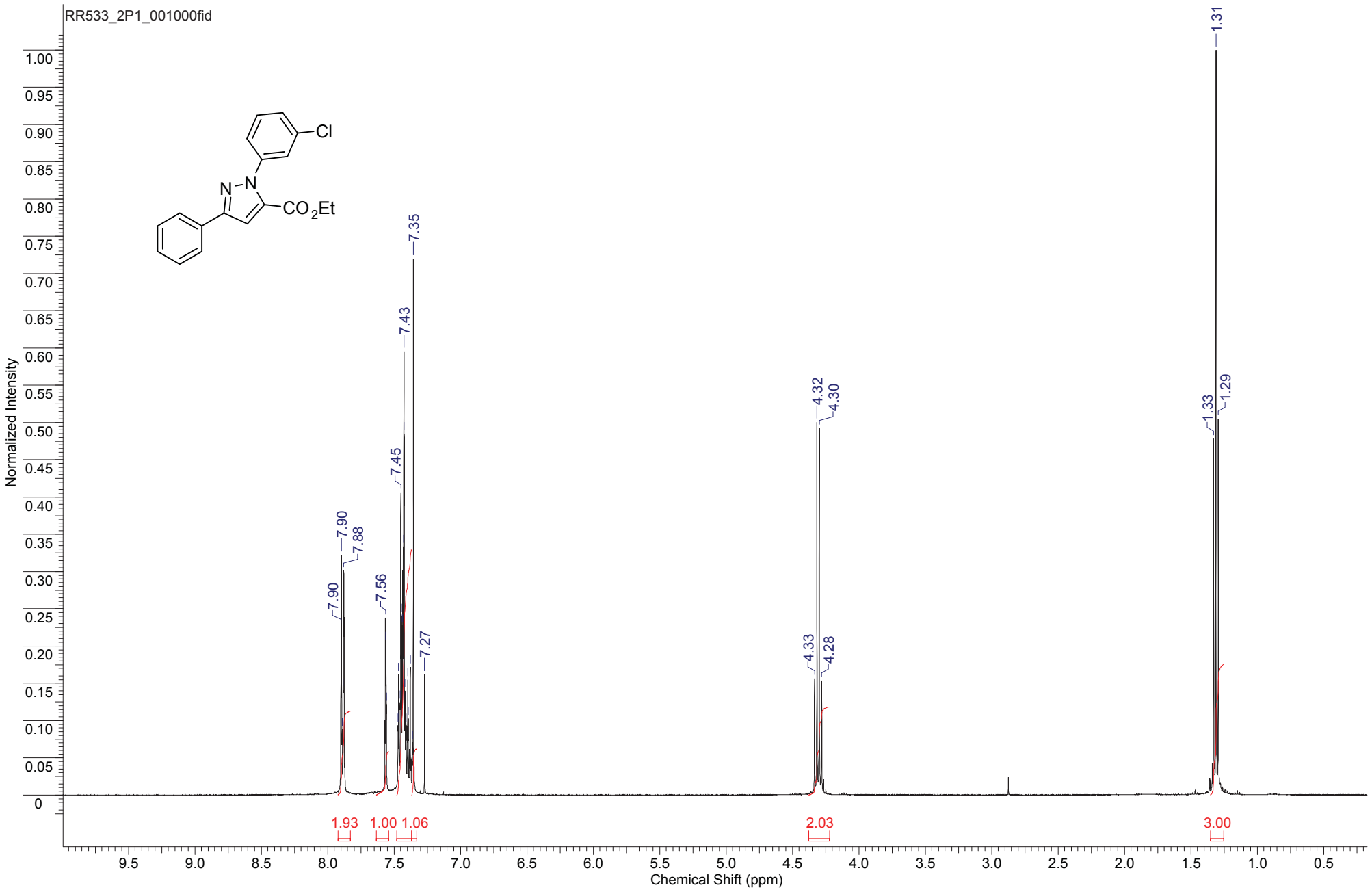
Charge = +1

#	C	H	N	O	F	mass	DBE	error
*** Mass Analysis for mass 311.1191170								
1	**18**	**16**	**2**	**2**	**1**	**311.1190324**	11.5	8.461e-05
2	13	15	5	2	2	311.1188326	8.0	2.844e-04
3	15	17	2	3	2	311.1201752	7.5	1.058e-03
4	16	14	5	1	1	311.1176897	12.0	1.427e-03
5	12	19	1	6	2	311.1174952	3.0	1.622e-03
6	11	13	8	1	2	311.1174899	8.5	1.627e-03
7	6	20	4	9	1	311.1208829	-1.5	1.766e-03
8	15	18	1	5	1	311.1163523	7.0	2.765e-03
9	10	17	4	5	2	311.1161525	3.5	2.965e-03
10	7	16	8	5	1	311.1222203	3.5	3.103e-03

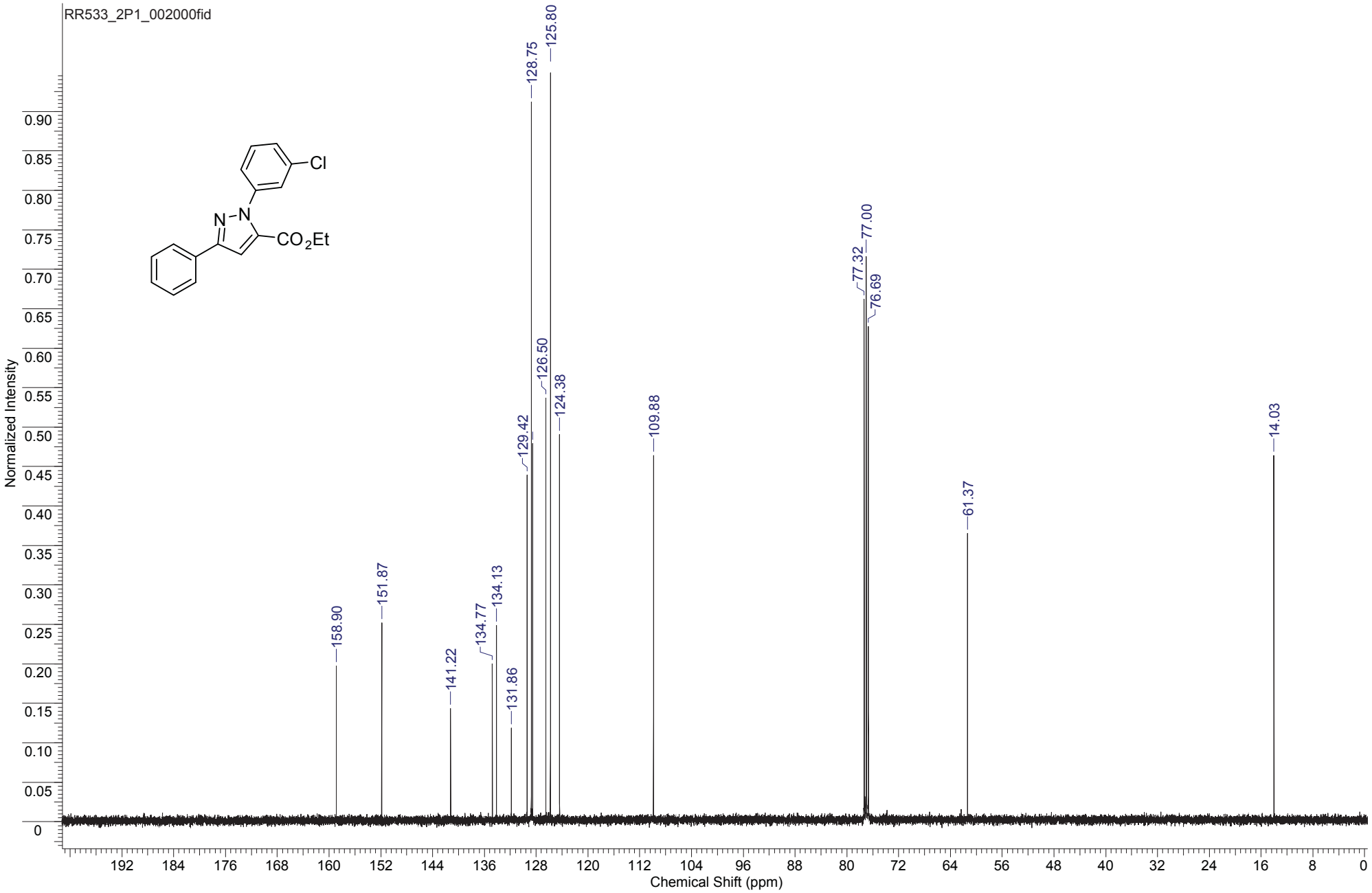


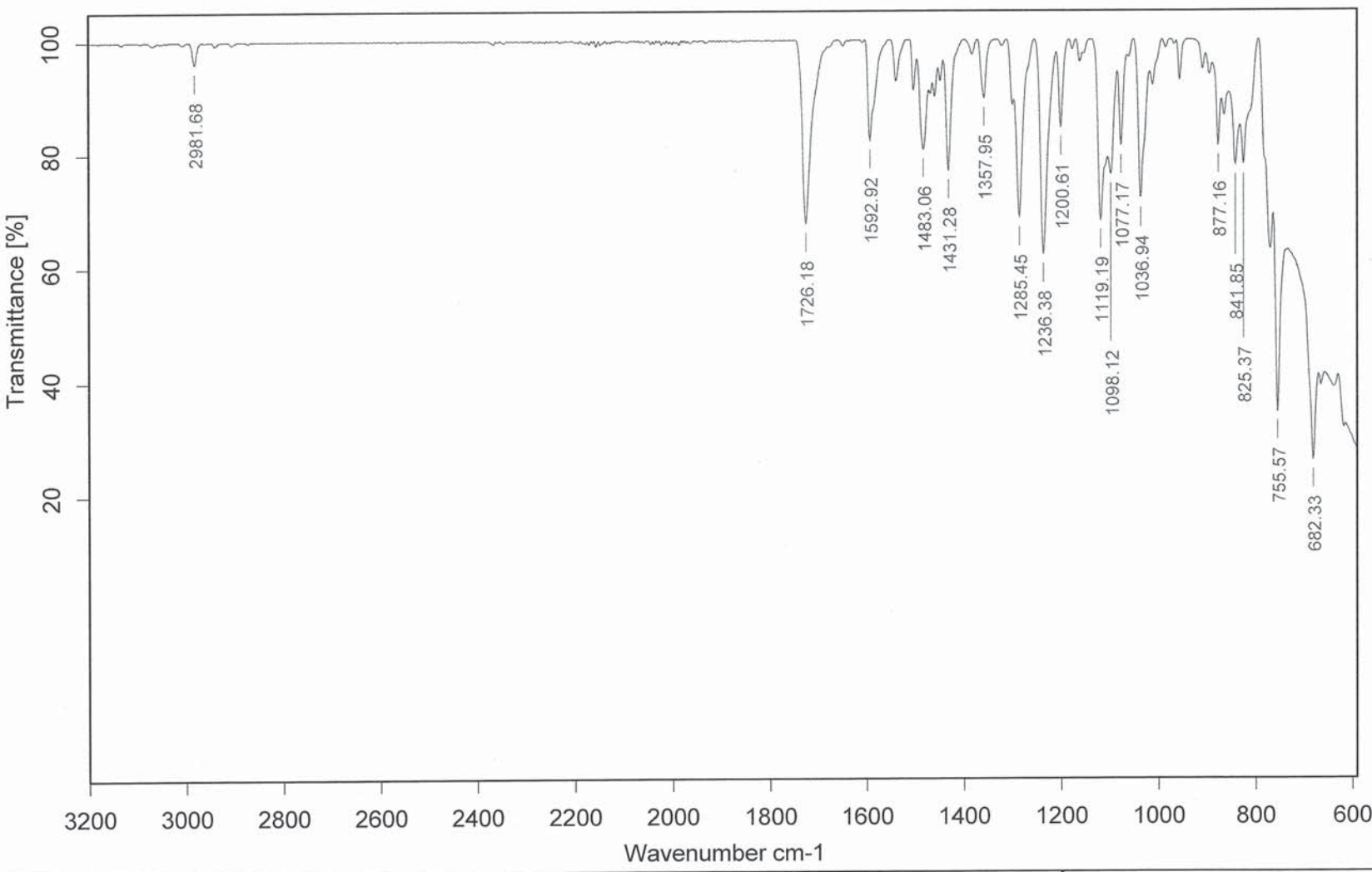
/Data/UNI_FR/REMY2066_ESI/2/pdata/1 FTMS USER Fri Oct 7 11:58:06 2016

ethyl 1-(3-chlorophenyl)-3-phenyl-1H-pyrazole-5-carboxylate



ethyl 1-(3-chlorophenyl)-3-phenyl-1H-pyrazole-5-carboxylate





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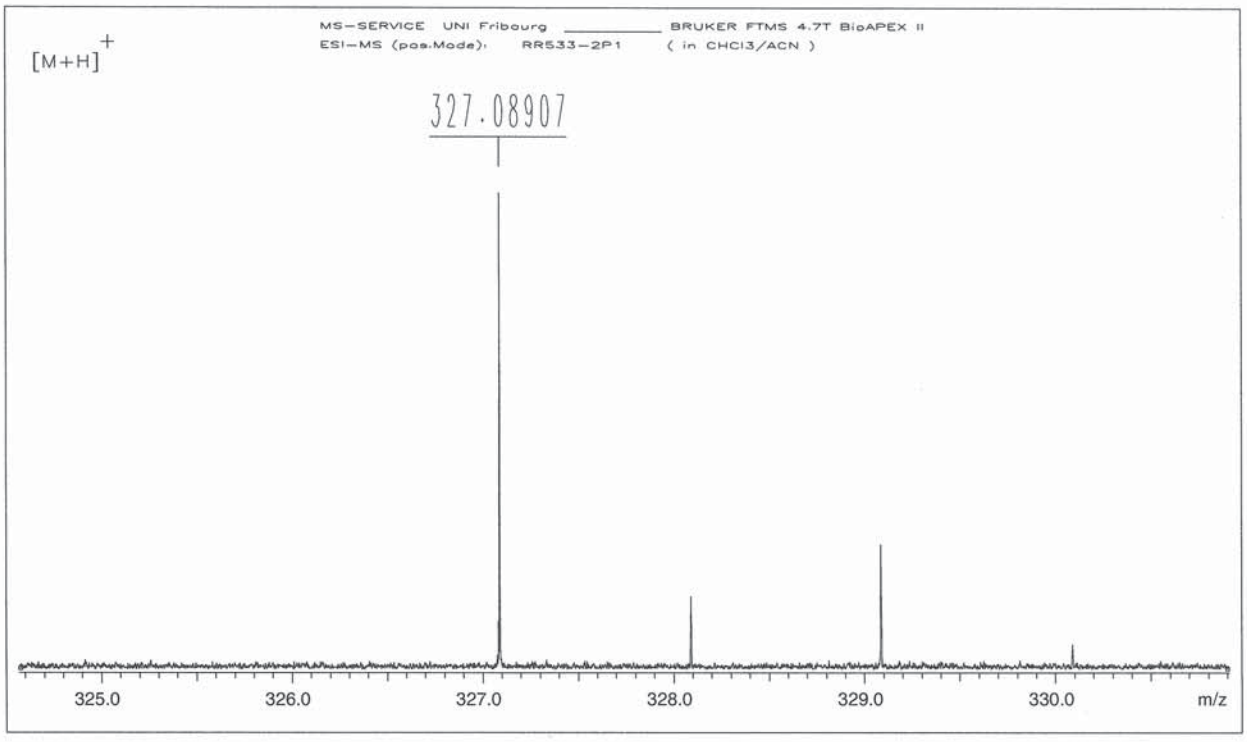
ESI-MS: RR533_2P1

XMASS Mass Analysis for /Data/UNI_FR/REMY2126_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 327.0890660

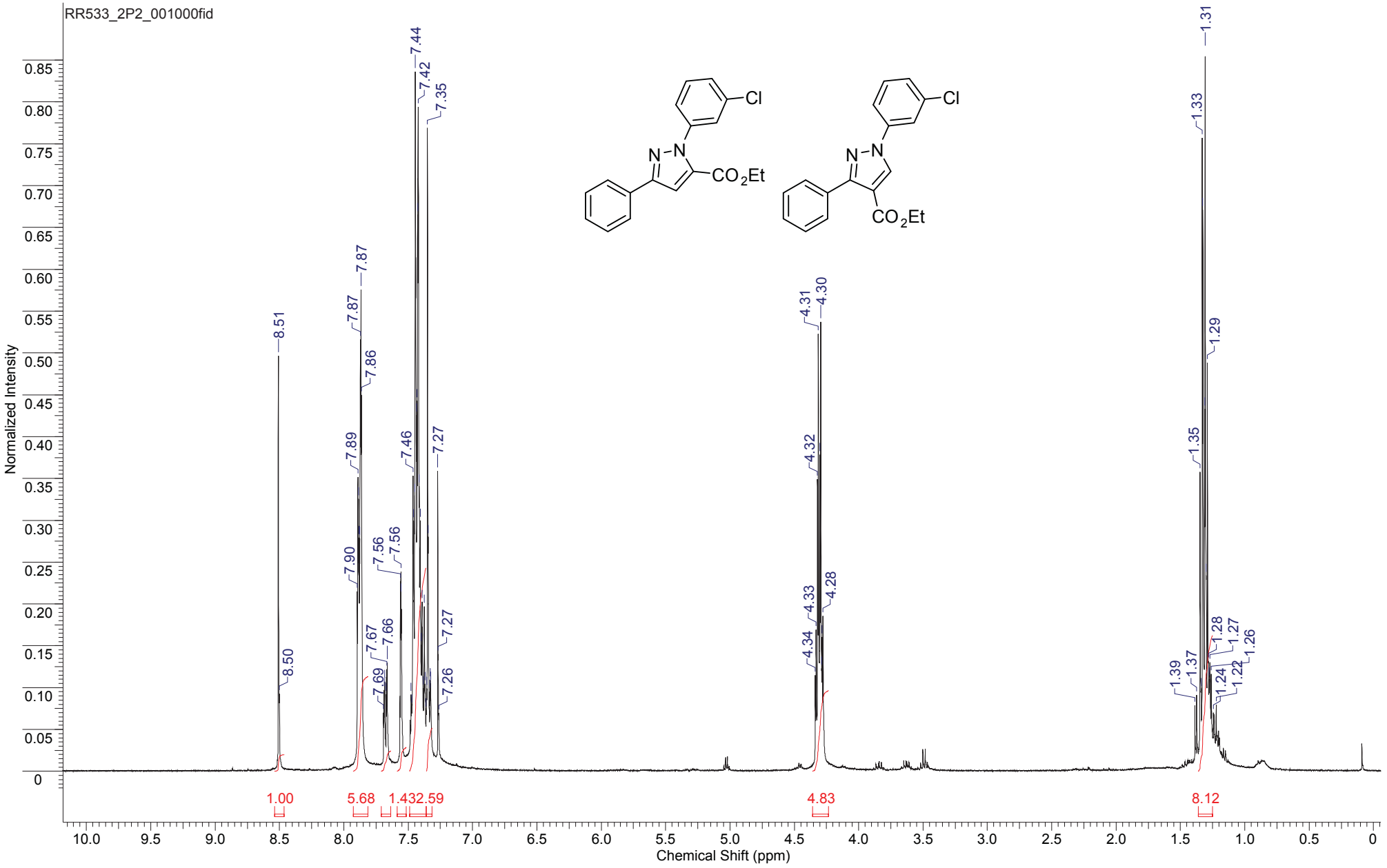
Charge = +1

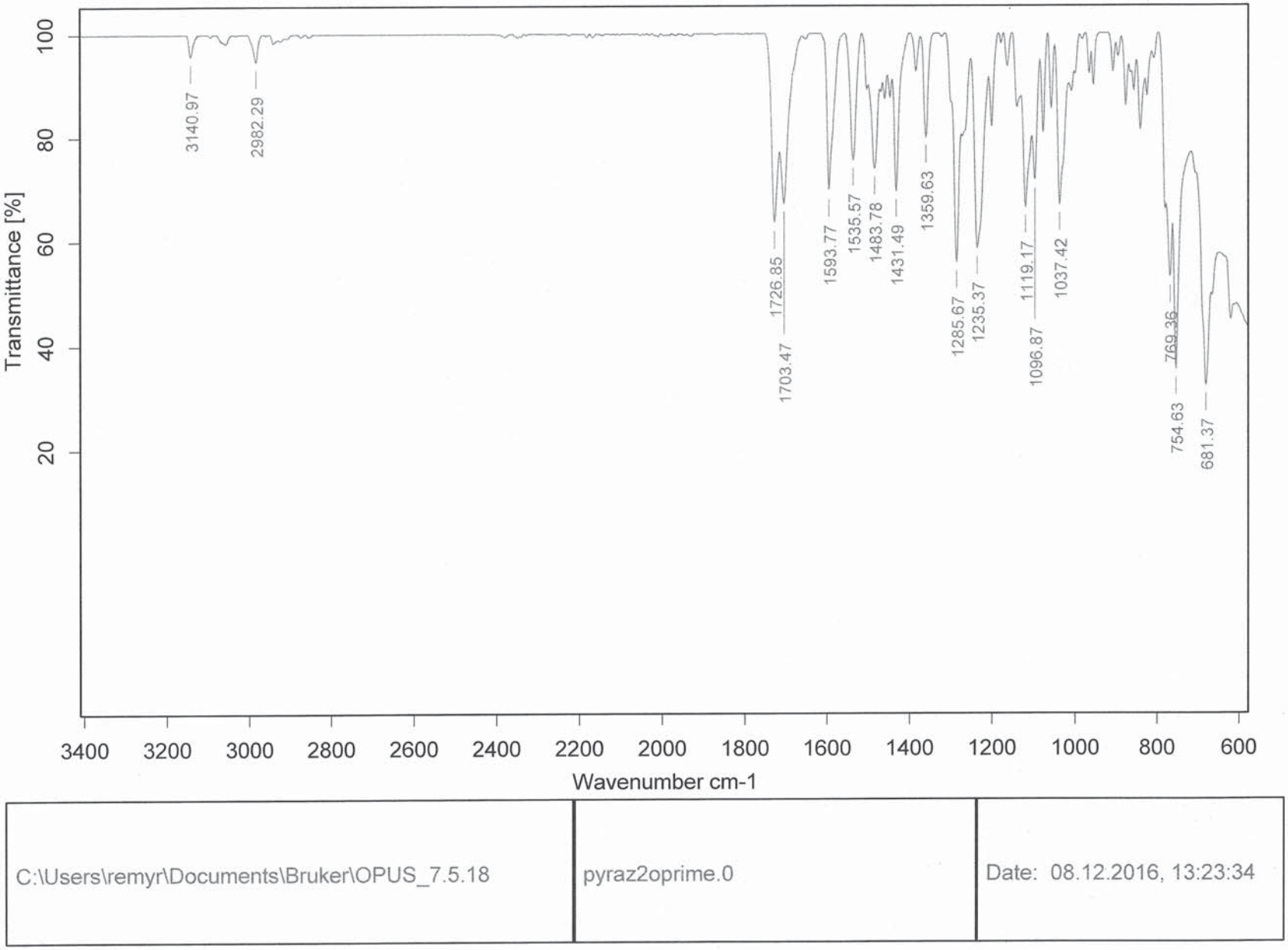
#	C	H	35Cl	N	O	mass	DBE	error
*** Mass Analysis for mass 327.0890660								
1	**18**	**16**	**1**	**2**	**2**	**327.0894819**	11.5	4.159e-04
2	15	19	2	3	1	327.0899691	7.0	9.031e-04
3	16	14	1	5	1	327.0881392	12.0	9.268e-04
4	12	21	2	2	4	327.0872890	2.5	1.777e-03
5	15	18	1	1	5	327.0868018	7.0	2.264e-03
6	6	20	1	4	9	327.0913324	-1.5	2.266e-03
7	10	19	2	5	3	327.0859463	3.0	3.120e-03
8	7	16	1	8	5	327.0926698	3.5	3.604e-03
9	13	16	1	4	4	327.0854592	7.5	3.607e-03
10	8	22	1	1	10	327.0926751	-2.0	3.609e-03



/Data/UNI_FR/REMY2126_ESI/1/pdata/1 FTMS USER Tue Oct 18 08:37:52 2016

ethyl 1-(3-chlorophenyl)-3-phenyl-1H-pyrazole-5-carboxylate and ethyl 1-(3-chlorophenyl)-3-phenyl-1H-pyrazole-4-carboxylate





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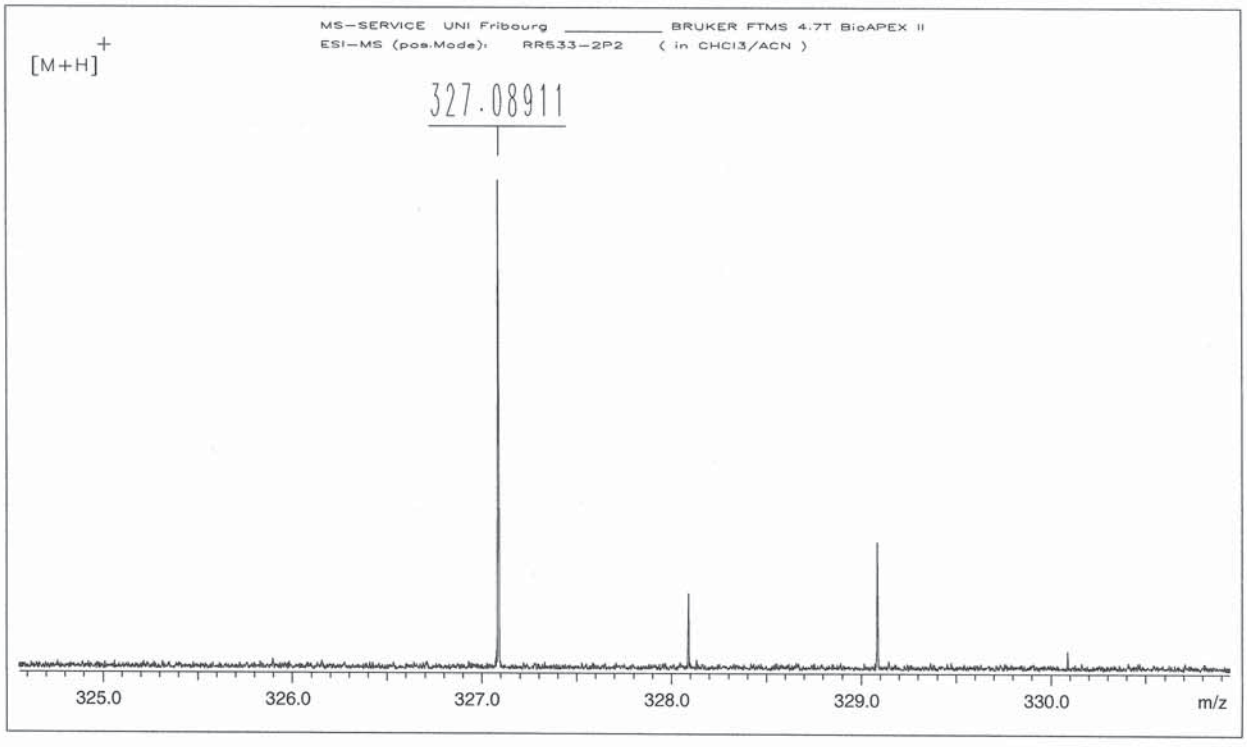
ESI-MS: RR533_2P2

XMASS Mass Analysis for /Data/UNI_FR/REMY2127_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 327.0891120

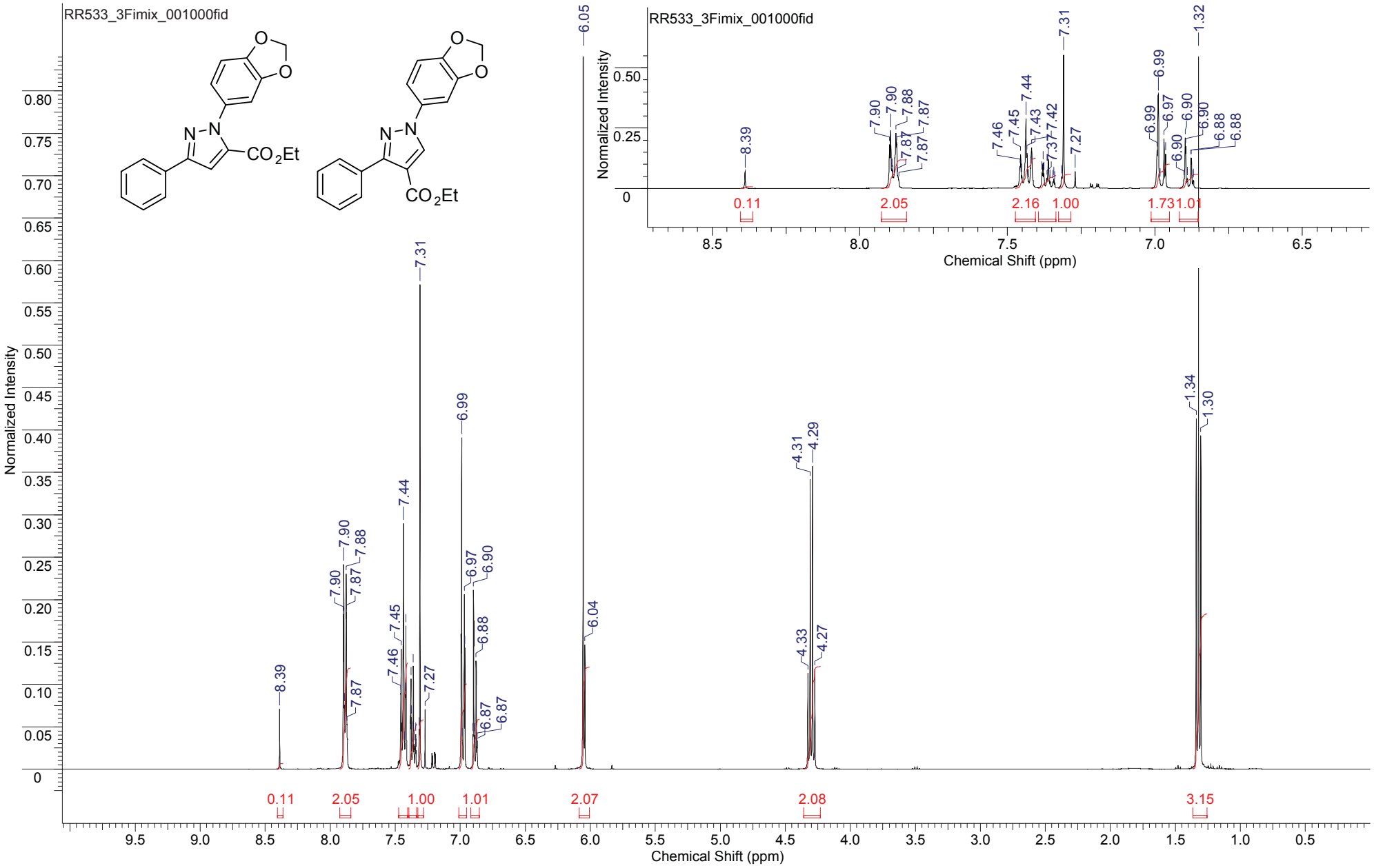
Charge = +1

#	C	H	35Cl	N	O	mass	DBE	error
*** Mass Analysis for mass 327.0891120								
1	**18**	**16**	**1**	**2**	**2**	**327.0894819**	11.5	3.699e-04
2	15	19	2	3	1	327.0899691	7.0	8.571e-04
3	16	14	1	5	1	327.0881392	12.0	9.728e-04
4	12	21	2	2	4	327.0872890	2.5	1.823e-03
5	6	20	1	4	9	327.0913324	-1.5	2.220e-03
6	15	18	1	1	5	327.0868018	7.0	2.310e-03
7	10	19	2	5	3	327.0859463	3.0	3.166e-03
8	7	16	1	8	5	327.0926698	3.5	3.558e-03
9	8	22	1	1	10	327.0926751	-2.0	3.563e-03
10	13	16	1	4	4	327.0854592	7.5	3.653e-03

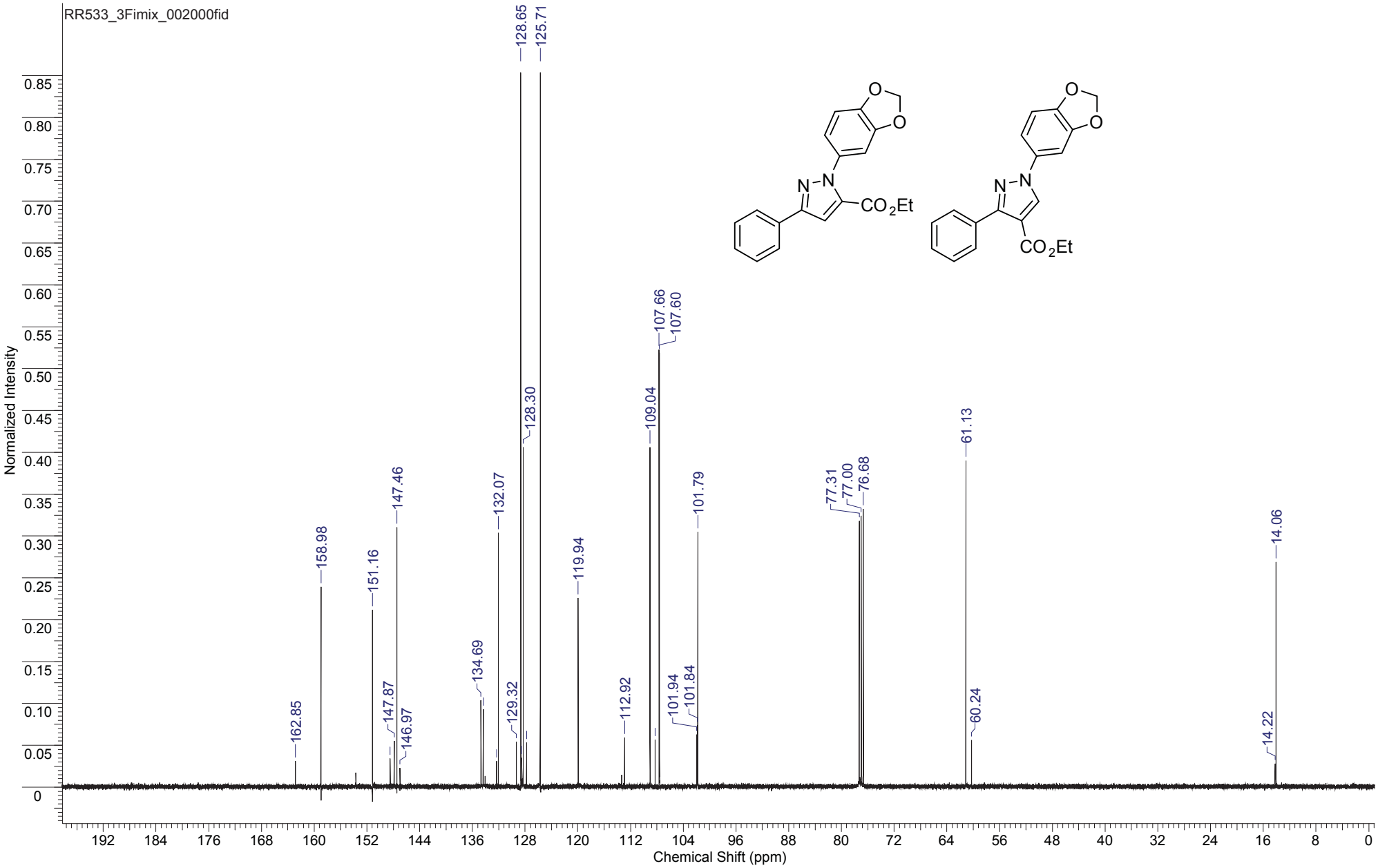


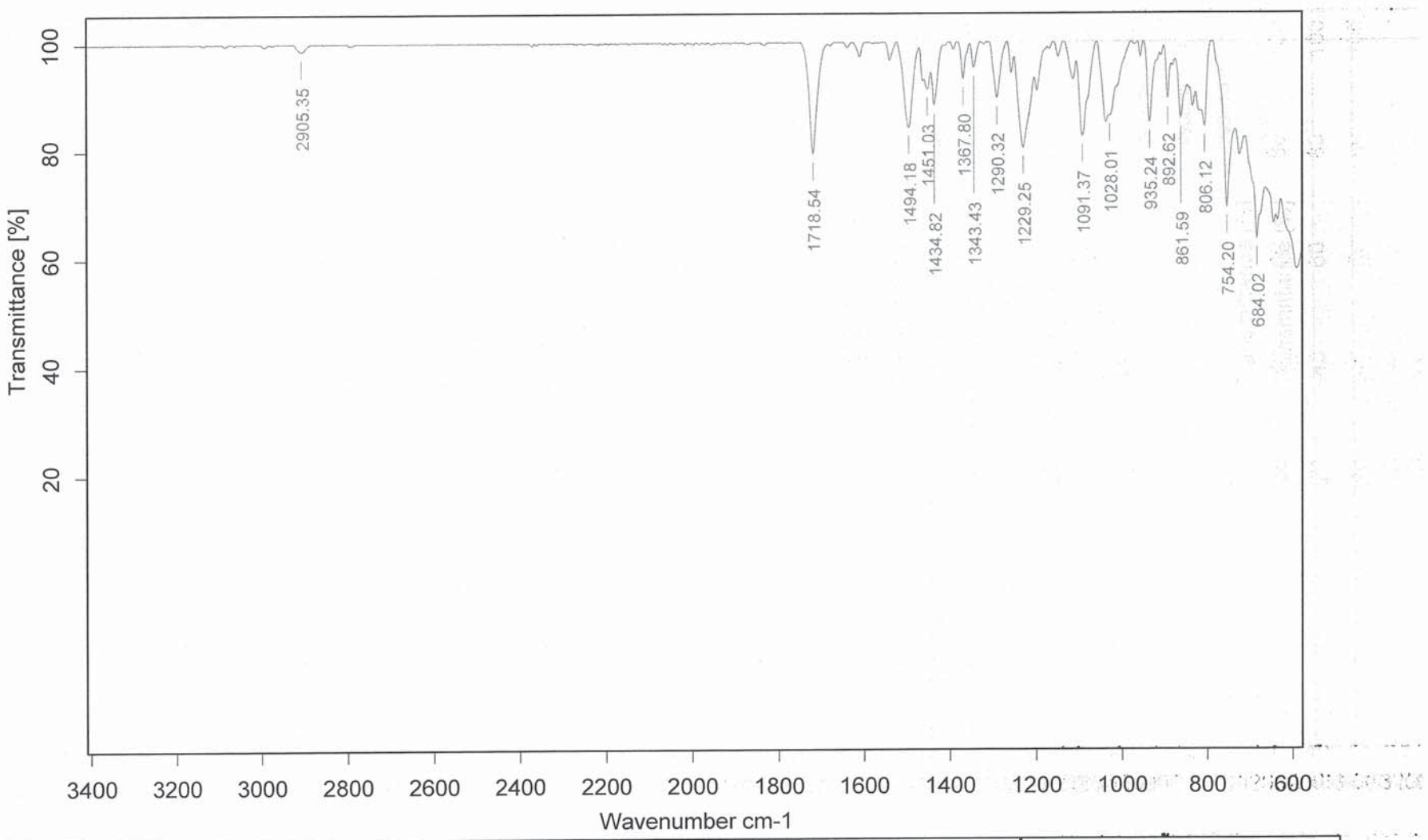
/Data/UNI_FR/REMY2127_ESI/2/pdata/1 FTMS USER Tue Oct 18 08:33:01 2016

ethyl 1-(benzo[d][1,3]dioxol-5-yl)-3-phenyl-1H-pyrazole-5-carboxylate and ethyl 1-(benzo[d][1,3]dioxol-5-yl)-3-phenyl-1H-pyrazole-4-carboxylate



ethyl 1-(benzo[d][1,3]dioxol-5-yl)-3-phenyl-1H-pyrazole-5-carboxylate and ethyl 1-(benzo[d][1,3]dioxol-5-yl)-3-phenyl-1H-pyrazole-4-carboxylate





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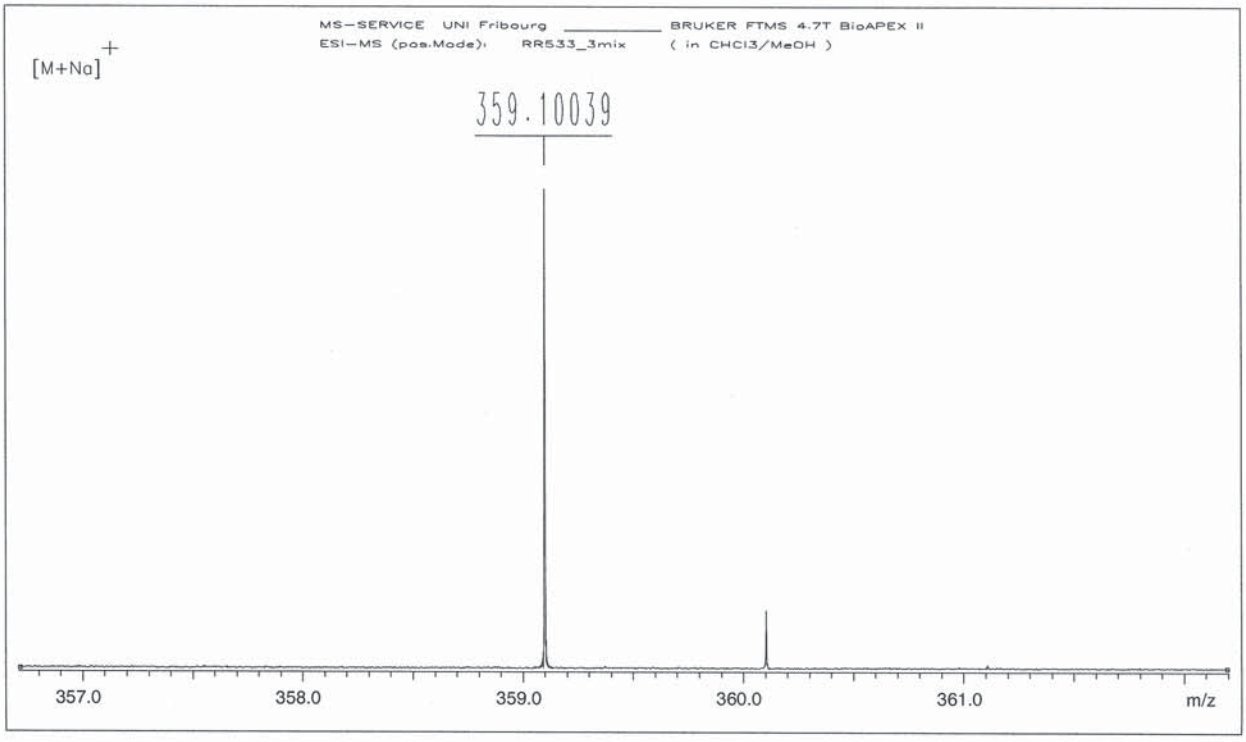
ESI-MS: RR533_3mix

XMASS Mass Analysis for /Data/UNI_FR/REMY2206_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 359.1003870

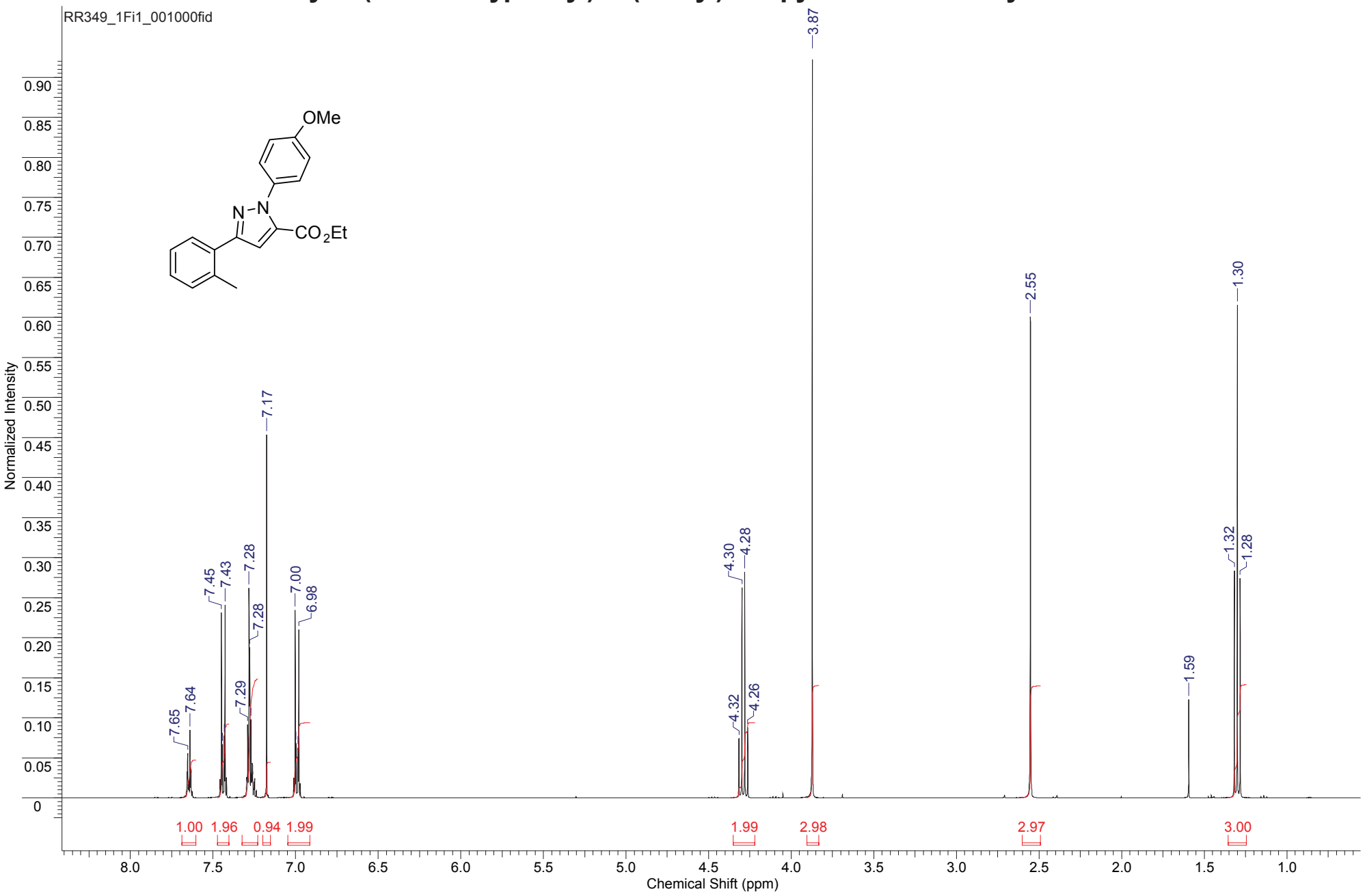
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 359.1003870								
1	**19**	**16**	**2**	**4**	**1**	**359.1002281**	12.5	1.589e-04
2	17	11	8	2	0	359.0999481	16.5	4.389e-04
3	19	13	5	3	0	359.1012907	16.0	9.037e-04
4	17	14	5	3	1	359.0988854	13.0	1.502e-03
5	21	15	2	4	0	359.1026334	15.5	2.246e-03
6	22	14	3	1	1	359.1029082	17.0	2.521e-03
7	15	12	8	2	1	359.0975428	13.5	2.844e-03
8	12	11	10	4	0	359.0959253	12.5	4.462e-03
9	24	13	3	1	0	359.1053135	20.0	4.926e-03
10	11	14	9	4	1	359.1060961	9.0	5.709e-03

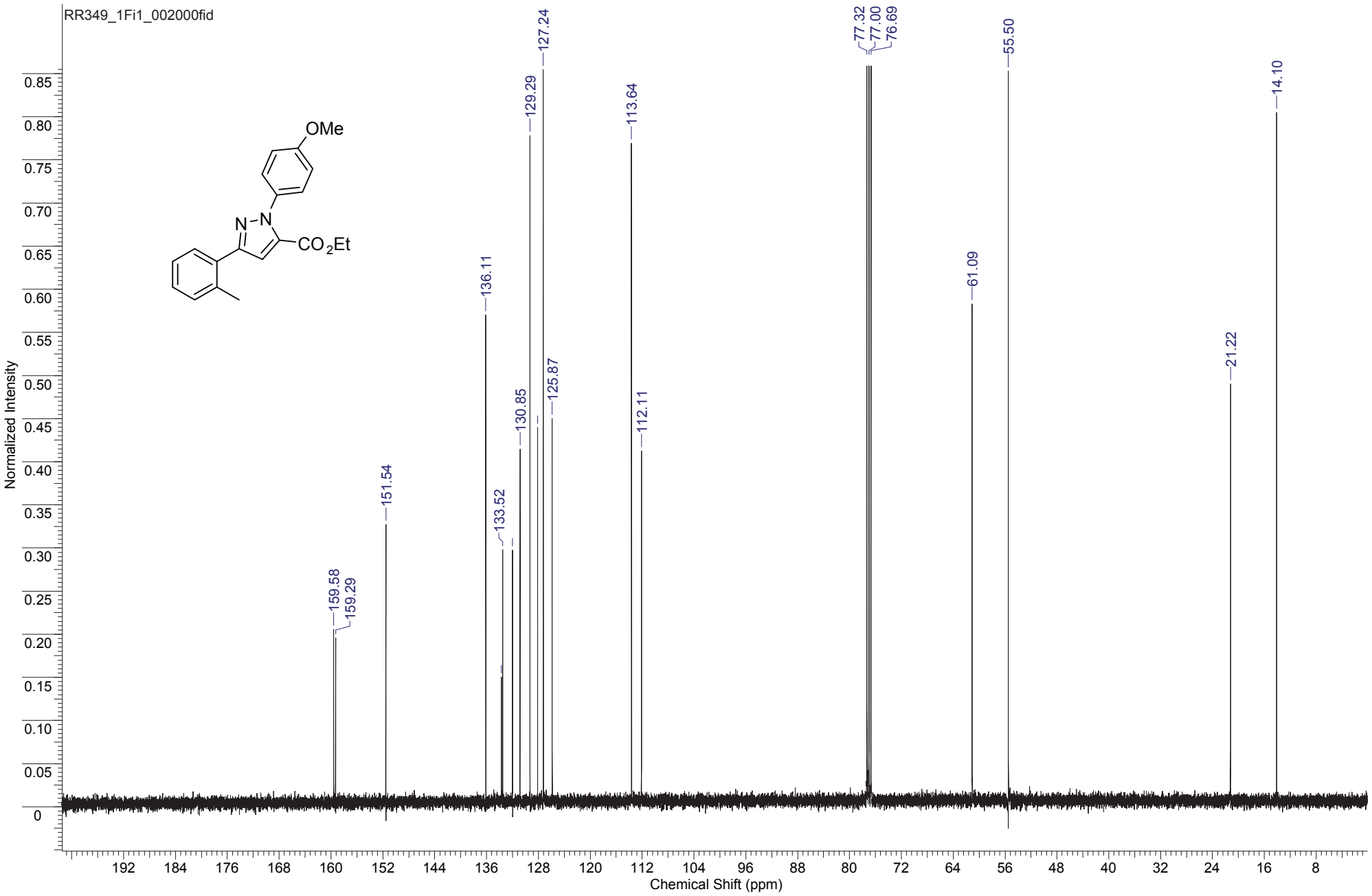


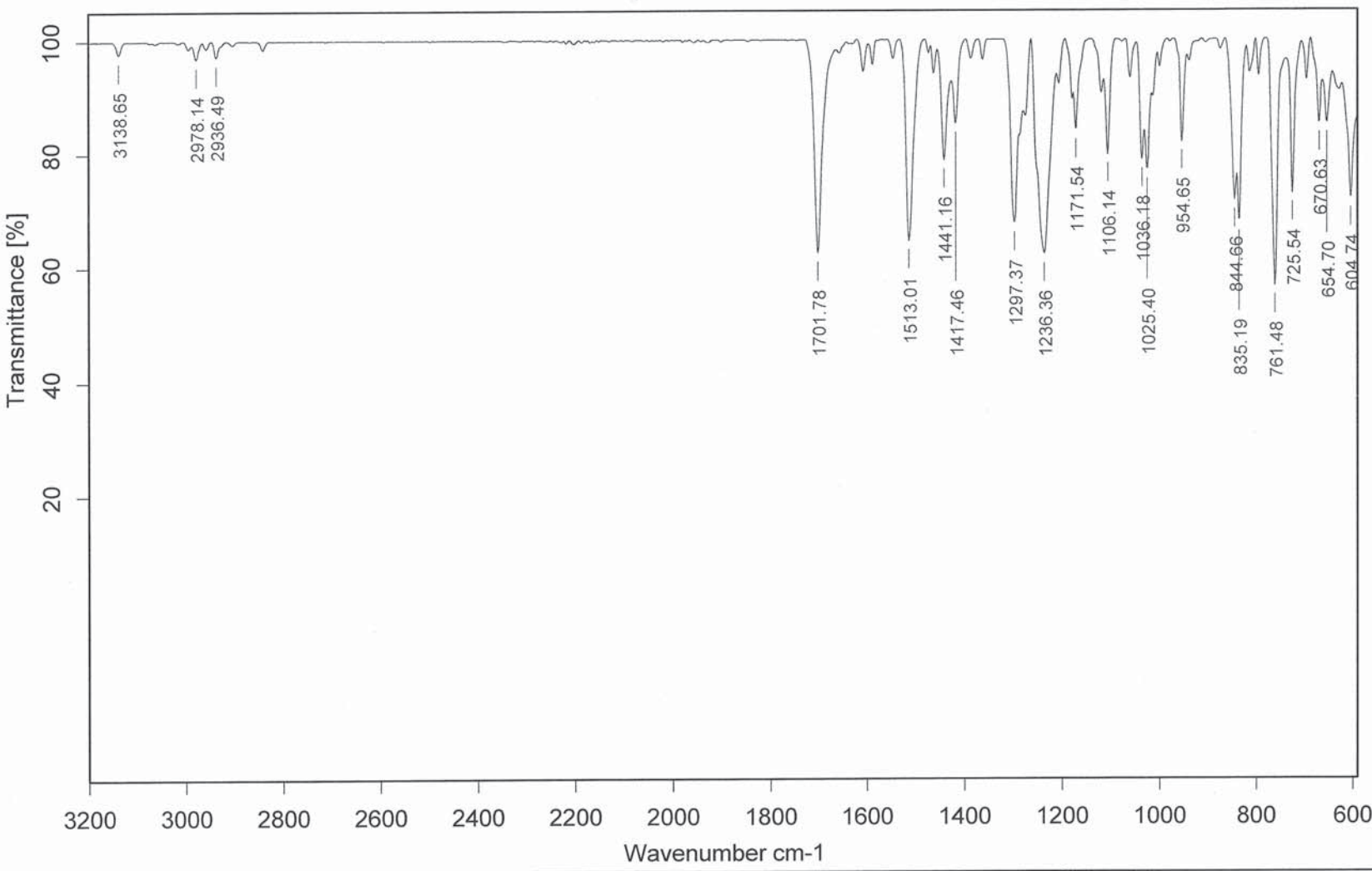
/Data/UNI_FR/REMY2206_ESI/2/pdata/1 FTMS USER Fri Oct 28 15:17:39 2016

ethyl 1-(4-methoxyphenyl)-3-(o-tolyl)-1H-pyrazole-5-carboxylate



ethyl 1-(4-methoxyphenyl)-3-(o-tolyl)-1H-pyrazole-5-carboxylate





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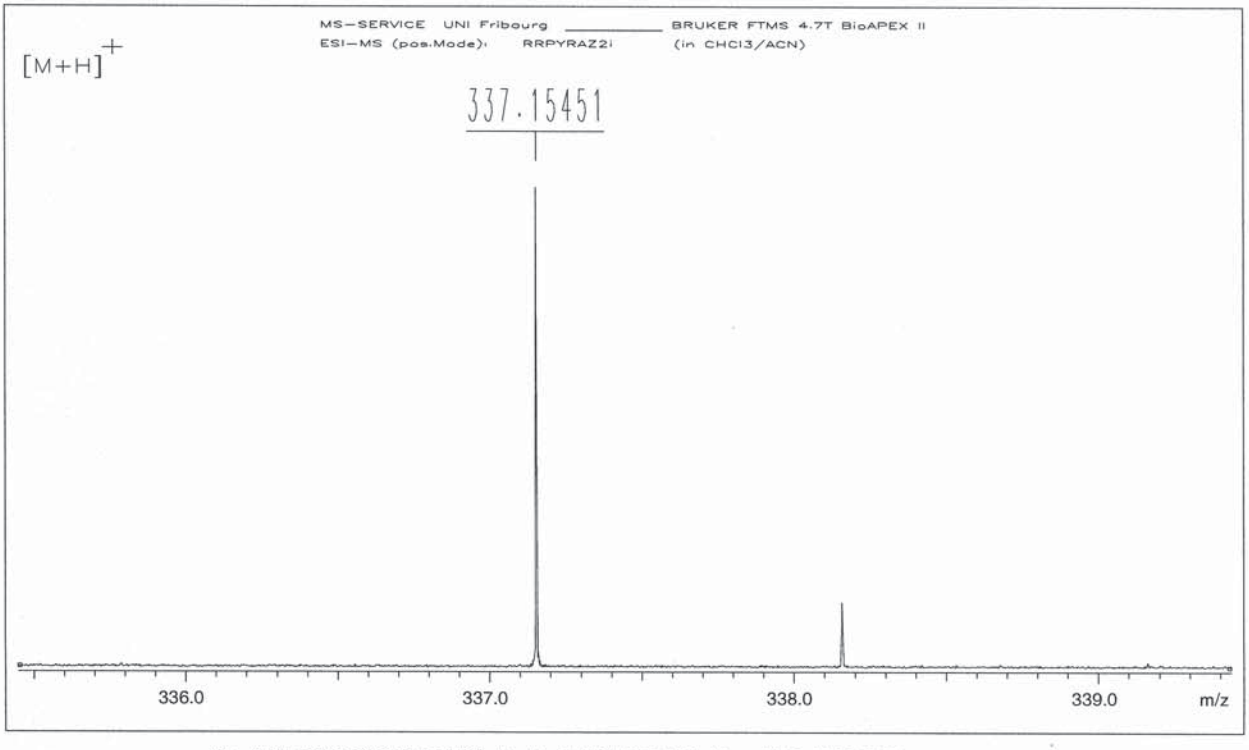
ESI-MS: RRPYRAZ2i

XMASS Mass Analysis for /Data/UNI_FR/REMY2404_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

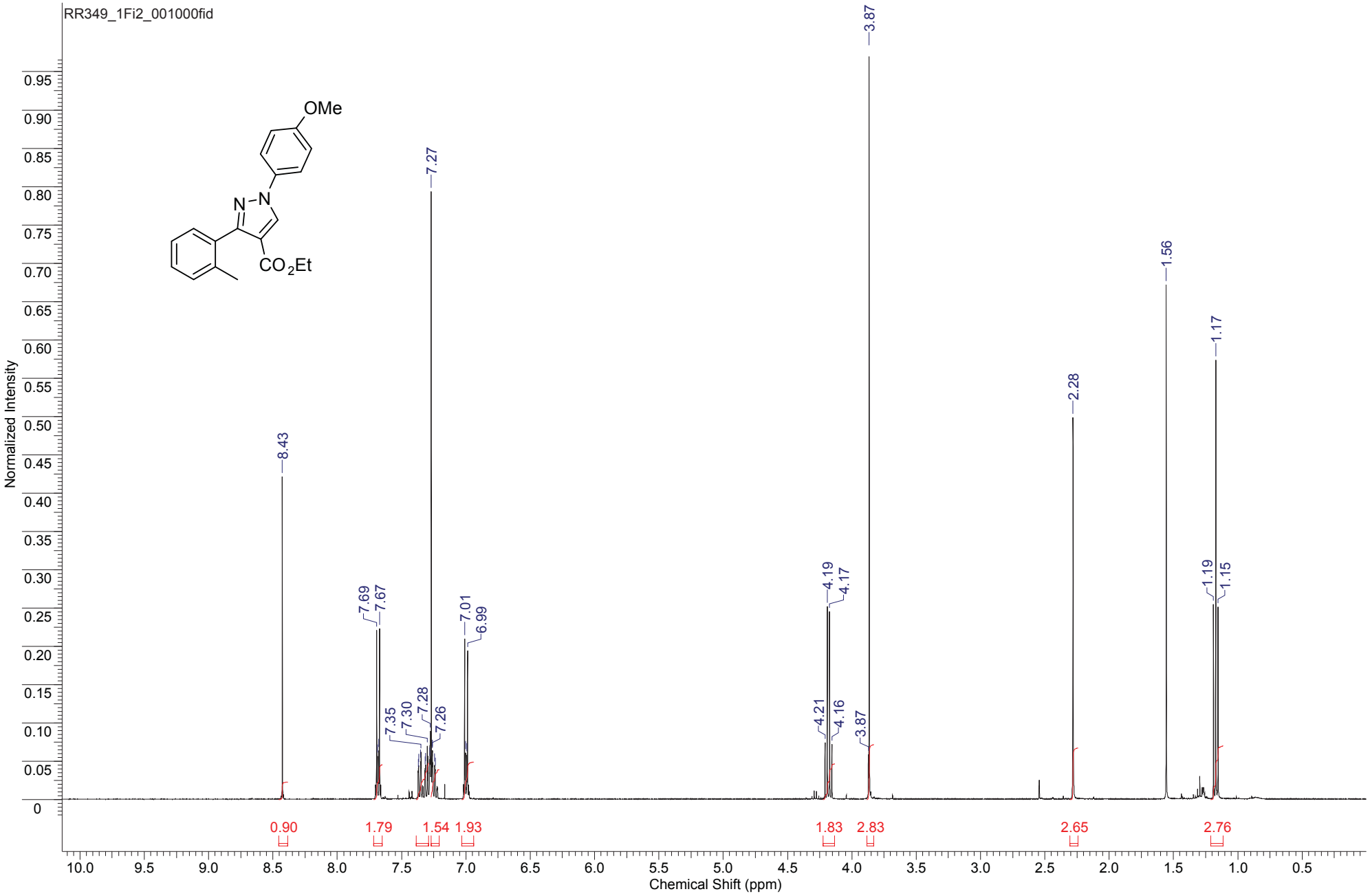
Ion mass = 337.1545120

Charge = +1

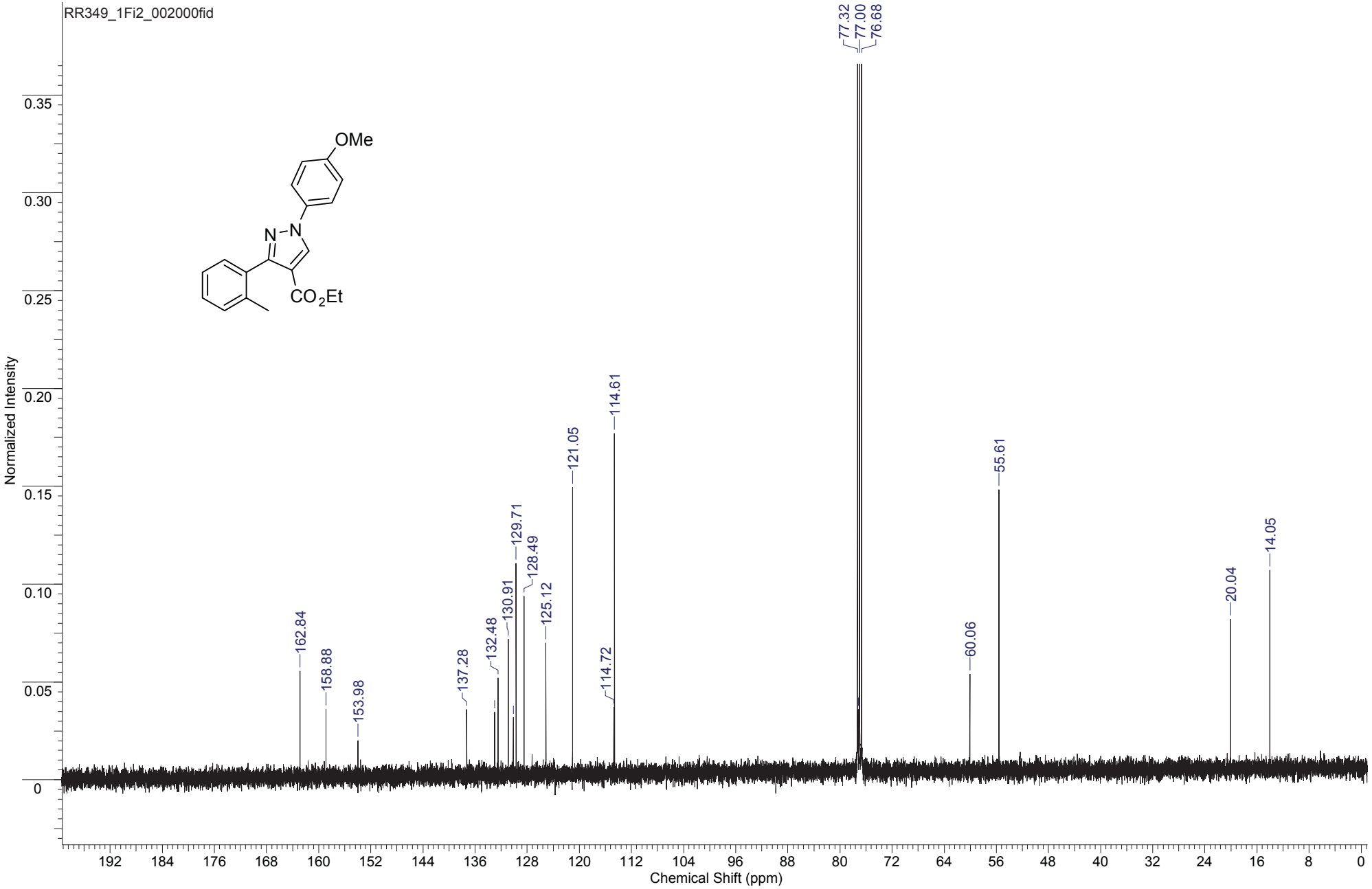
#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 337.1545120							
1	**20**	**21**	**2**	**3**	**337.1546690**	11.5	1.570e-04
2	24	19	1	1	337.1461157	16.0	8.396e-03
3	19	21	4	2	337.1659024	11.5	1.139e-02
4	19	19	3	3	337.1420929	12.0	1.242e-02
5	21	23	1	3	337.1672450	11.0	1.273e-02
6	23	17	2	1	337.1335396	16.5	2.097e-02
7	20	19	1	4	337.1308595	12.0	2.365e-02
8	20	23	3	2	337.1784784	11.0	2.397e-02
9	18	17	4	3	337.1295169	12.5	2.500e-02
10	16	25	4	4	337.1870317	6.5	3.252e-02

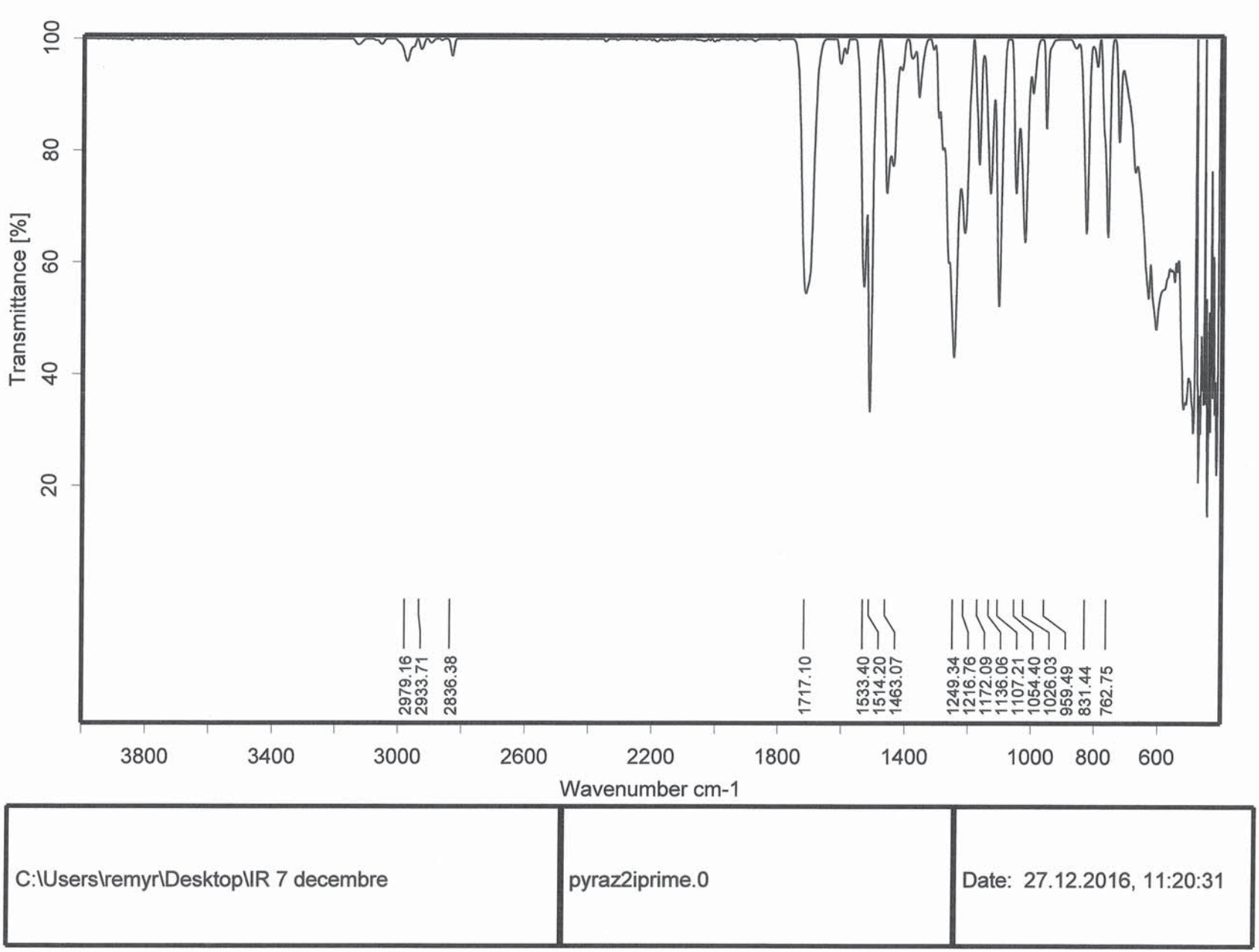


ethyl 1-(4-methoxyphenyl)-3-(o-tolyl)-1H-pyrazole-4-carboxylate



ethyl 1-(4-methoxyphenyl)-3-(o-tolyl)-1H-pyrazole-4-carboxylate





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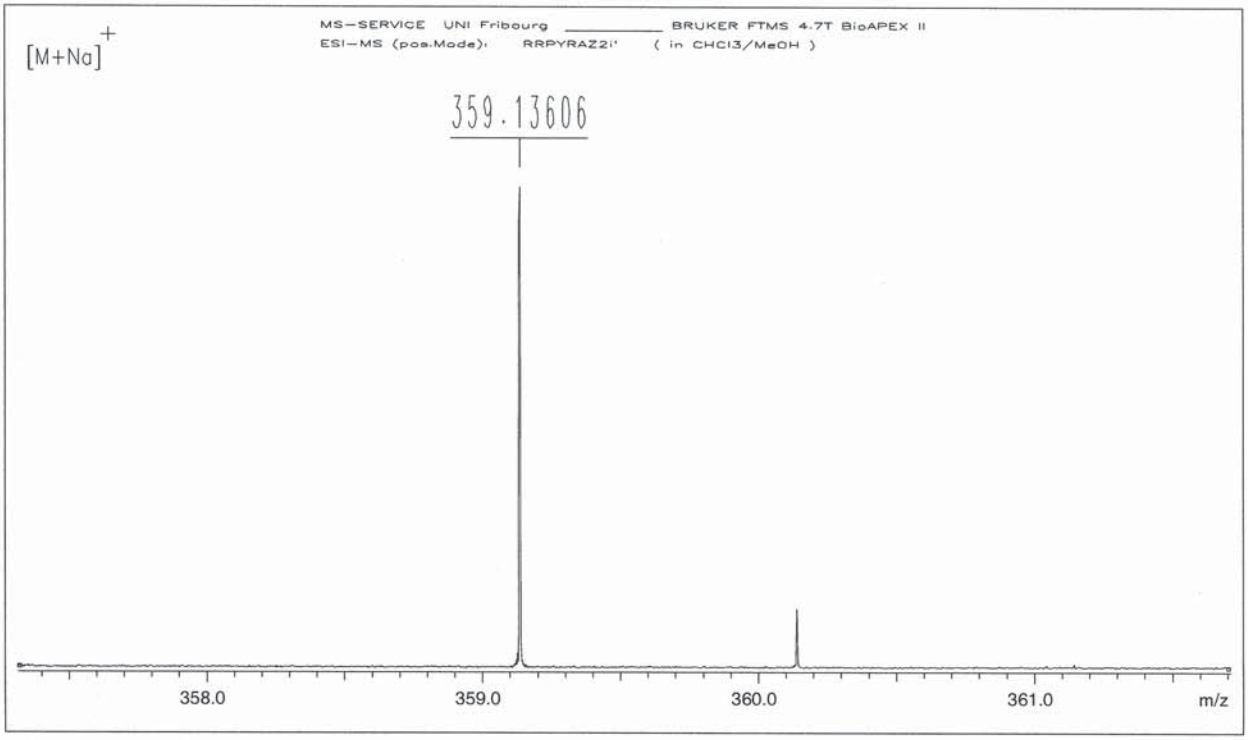
ESI-MS: RRPYRAZ2i'

XMASS Mass Analysis for /Data/UNI_FR/REMY2453_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 359.1360610

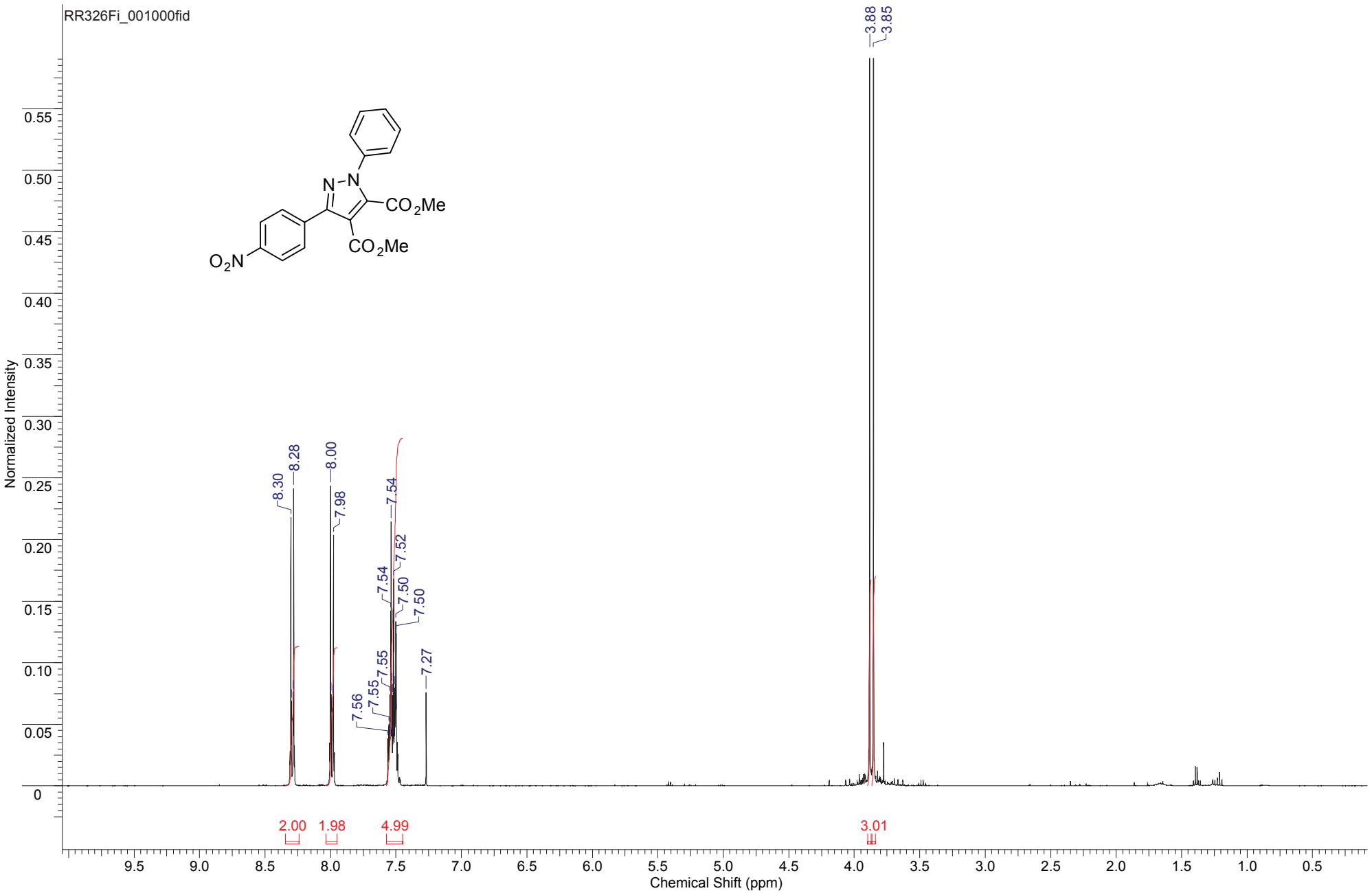
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 359.1360610								
1	**20**	**20**	**2**	**3**	**1**	**359.1366136**	11.5	5.526e-04
2	18	18	5	2	1	359.1352709	12.0	7.901e-04
3	17	19	4	5	0	359.1349962	10.5	1.065e-03
4	20	17	5	2	0	359.1376762	15.0	1.615e-03
5	22	19	2	3	0	359.1390189	14.5	2.958e-03
6	15	20	4	5	1	359.1325909	7.5	3.470e-03
7	26	17	1	1	0	359.1304656	19.0	5.595e-03
8	24	18	1	1	1	359.1280603	16.0	8.001e-03
9	16	22	3	5	1	359.1451669	7.0	9.106e-03
10	21	17	3	3	0	359.1264428	15.0	9.618e-03

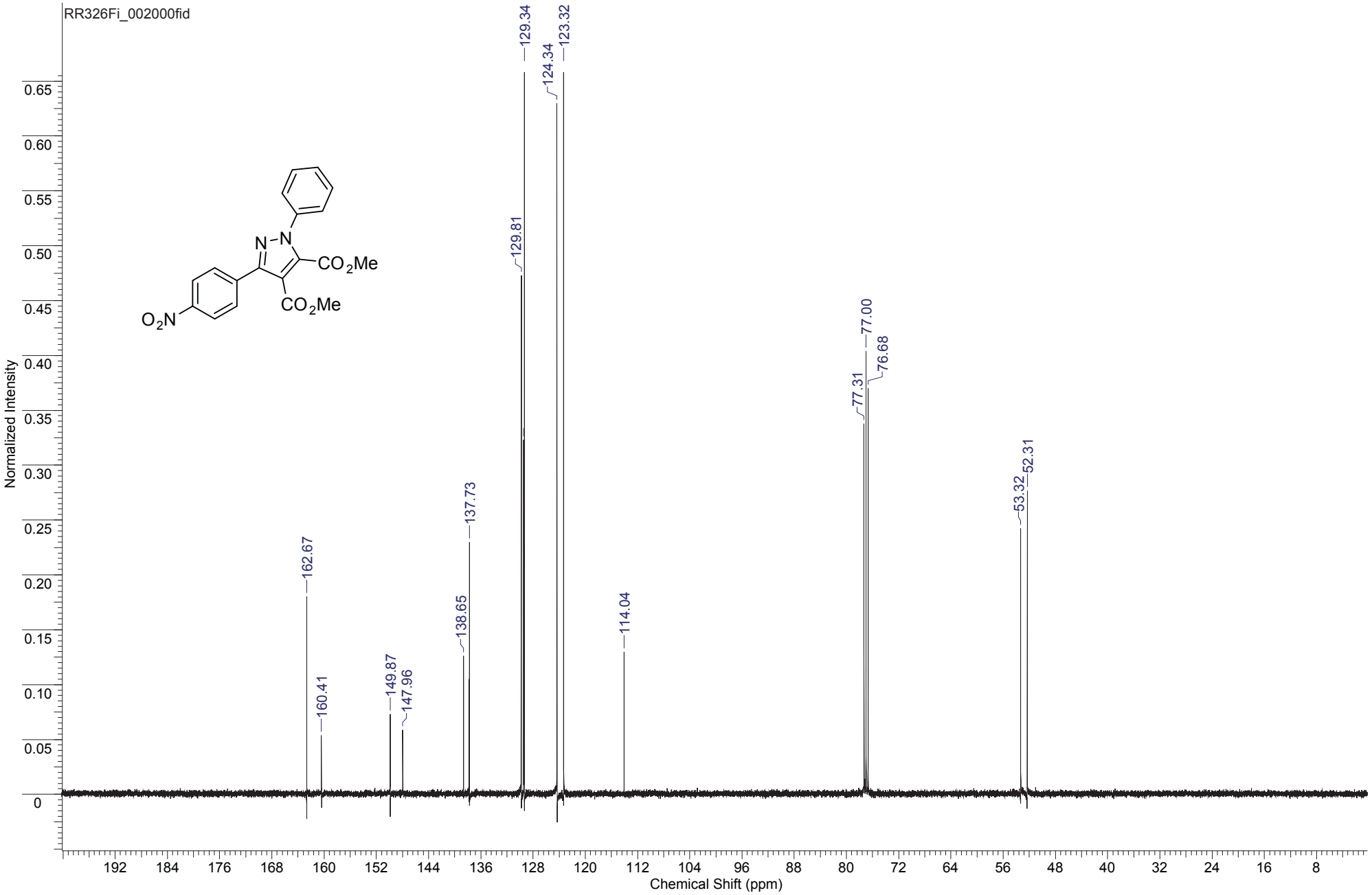


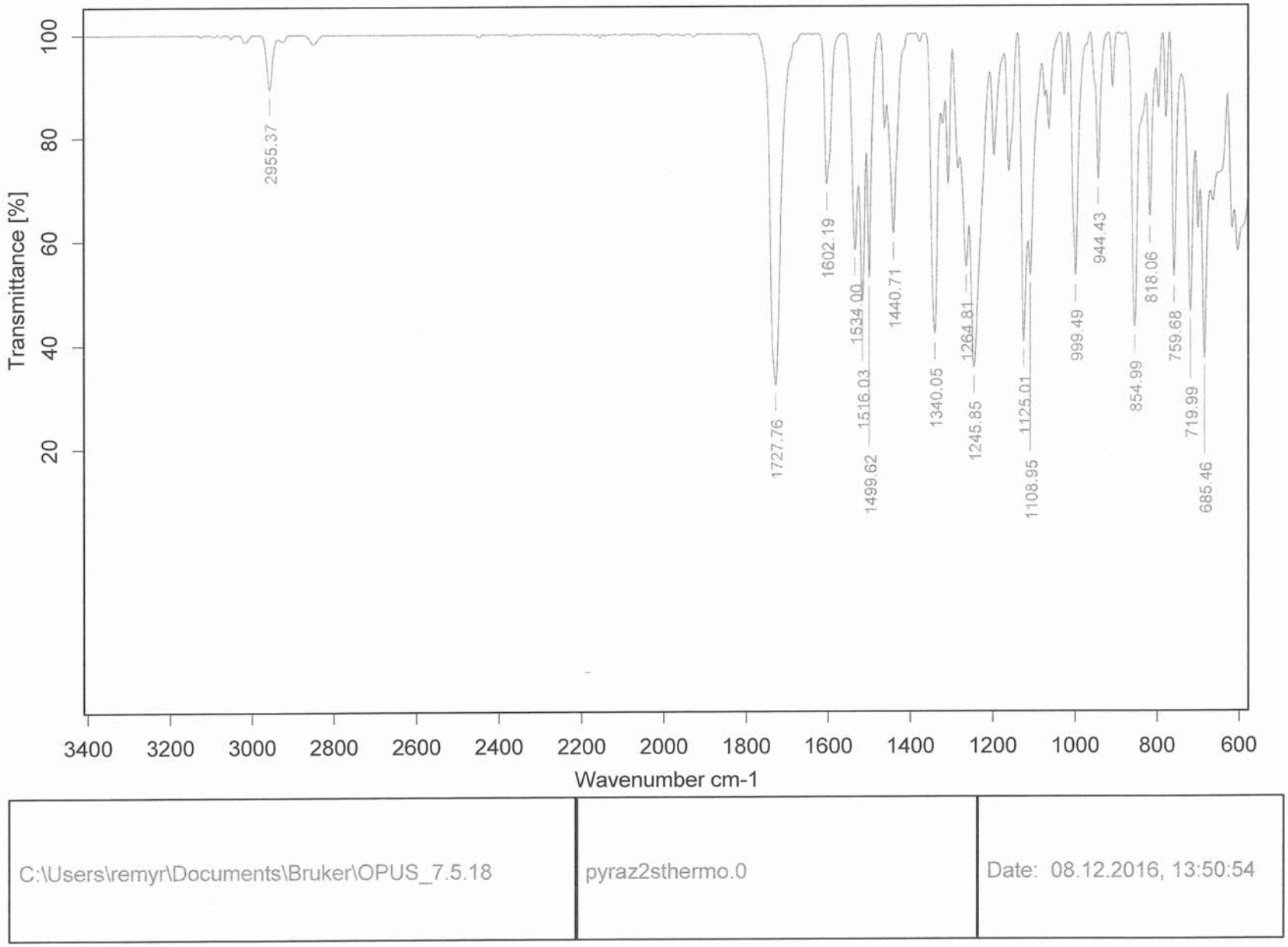
/Data/UNI_FR/REMY2453_ESI/2/pdata/1 FTMS USER Wed Jan 4 17:32:38 2017

dimethyl 3-(4-nitrophenyl)-1-phenyl-1H-pyrazole-4,5-dicarboxylate



dimethyl 3-(4-nitrophenyl)-1-phenyl-1H-pyrazole-4,5-dicarboxylate




Transmittance [%]
100
80
60
40
20
2955.37
1727.76
1602.19
1534.00
1516.03
1499.62
1440.71
1340.05
1264.81
1245.85
1125.01
1108.95
999.49
944.43
854.99
818.06
759.68
719.99
685.46
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
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1200
1000
800
600
Wavenumber cm-1
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pyraz2sthermo.0
Date: 08.12.2016, 13:50:54

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BRUKER **FTMS 4.7T BioAPEX II**

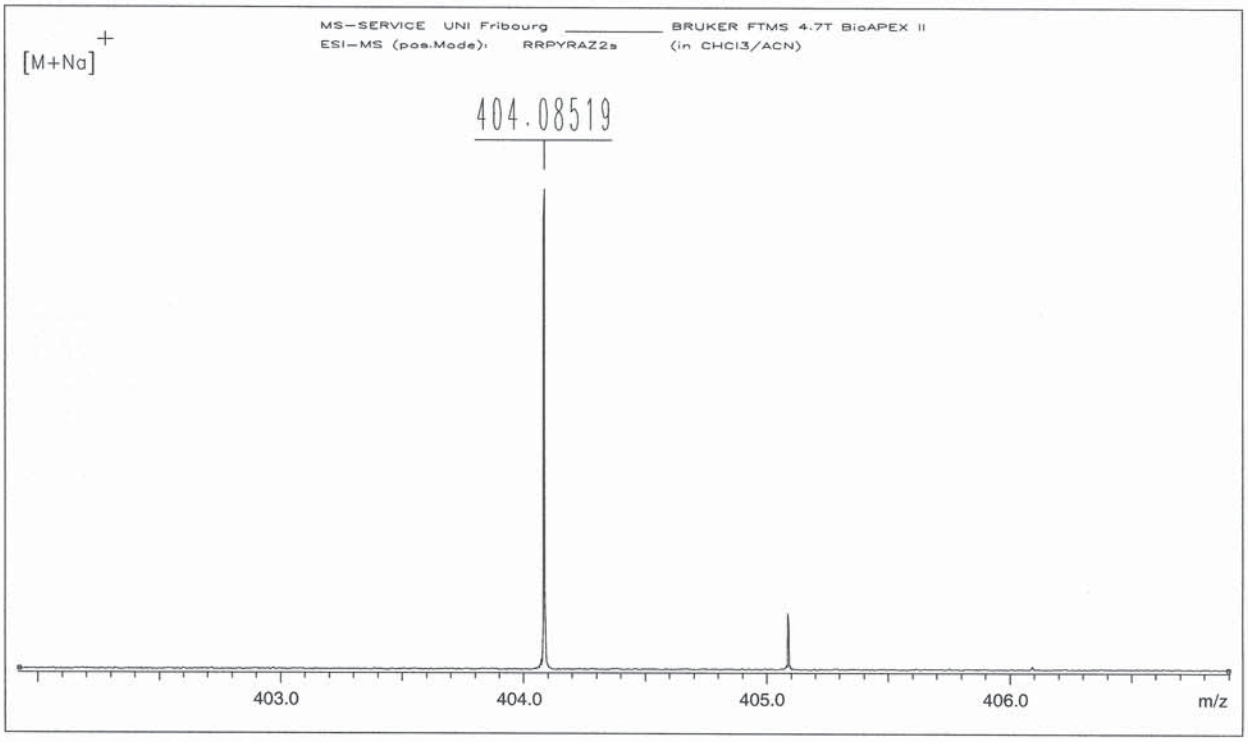
ESI-MS: RRPYRAZ2s Rheuno.

XMASS Mass Analysis for /Data/UNI_FR/REMY2409_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 404.0851900

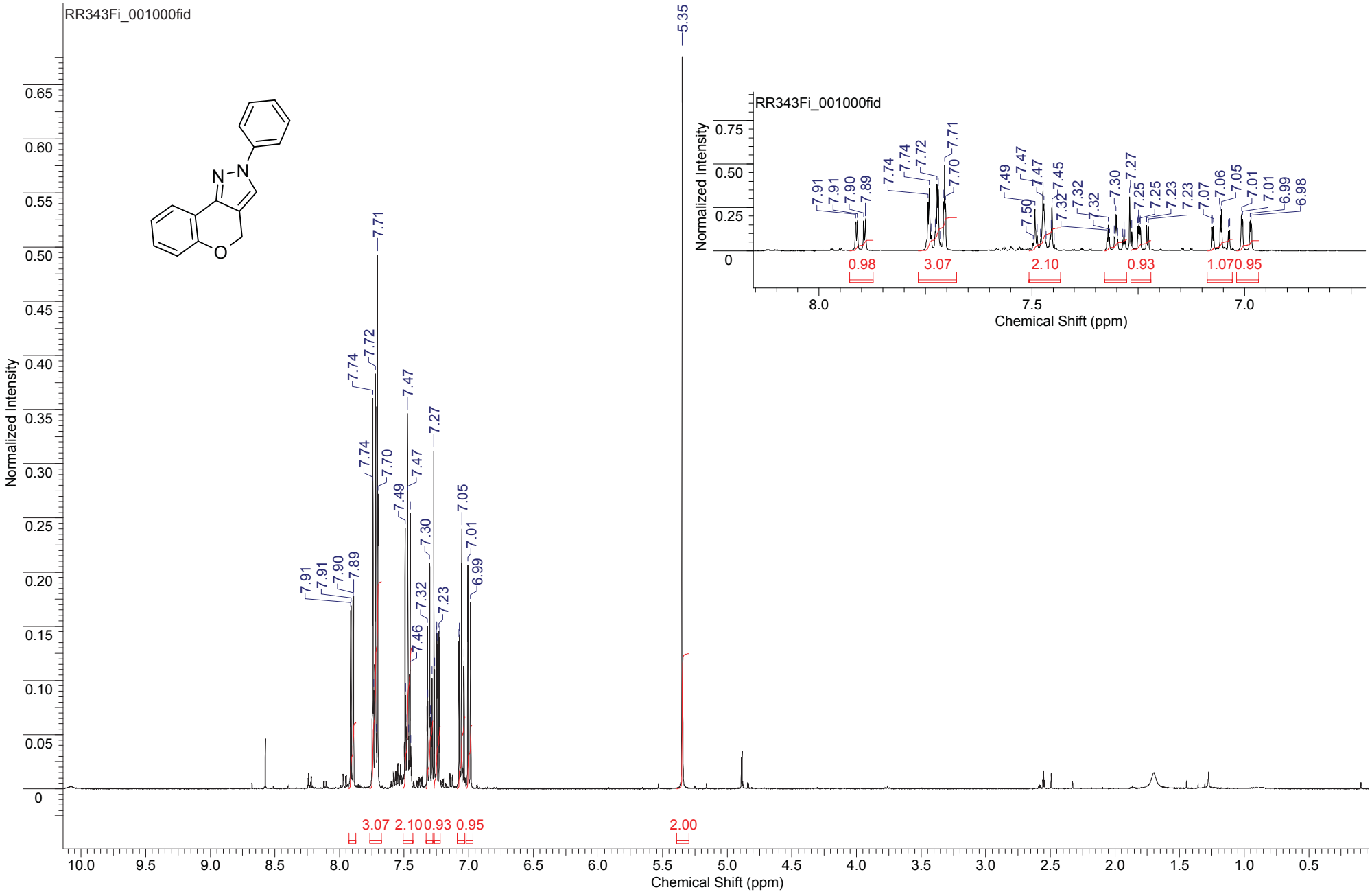
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 404.0851900								
1	**19**	**15**	**3**	**6**	**1**	**404.0853063**	13.5	1.163e-04
2	18	16	2	9	0	404.0850315	12.0	1.585e-04
3	17	10	9	4	0	404.0850263	17.5	1.637e-04
4	19	12	6	5	0	404.0863689	17.0	1.179e-03
5	17	13	6	5	1	404.0839636	14.0	1.226e-03
6	20	11	7	2	1	404.0866437	18.5	1.454e-03
7	16	14	5	8	0	404.0836889	12.5	1.501e-03
8	21	14	3	6	0	404.0877116	16.5	2.522e-03
9	16	17	2	9	1	404.0826262	9.0	2.564e-03
10	15	11	9	4	1	404.0826210	14.5	2.569e-03

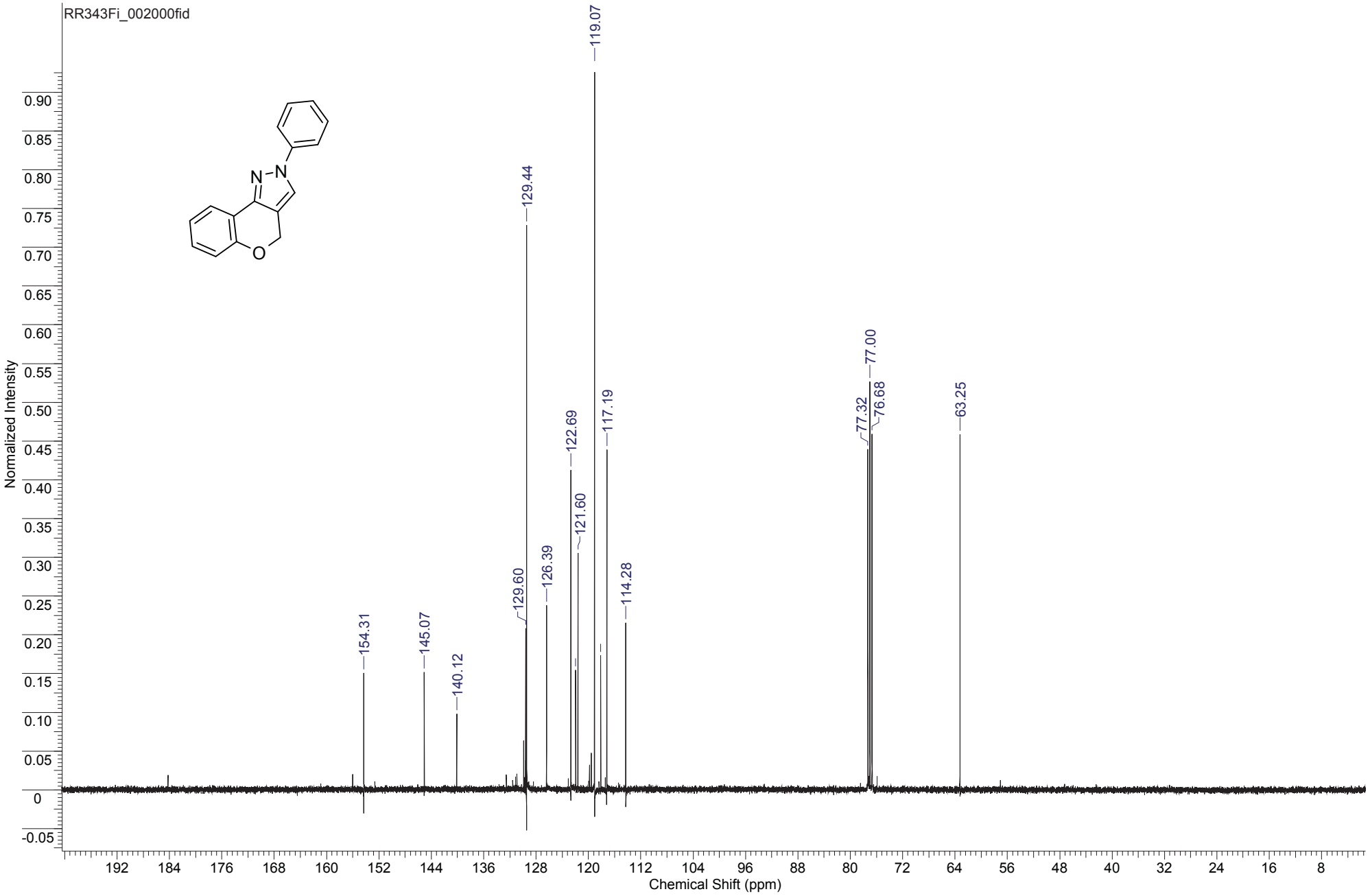


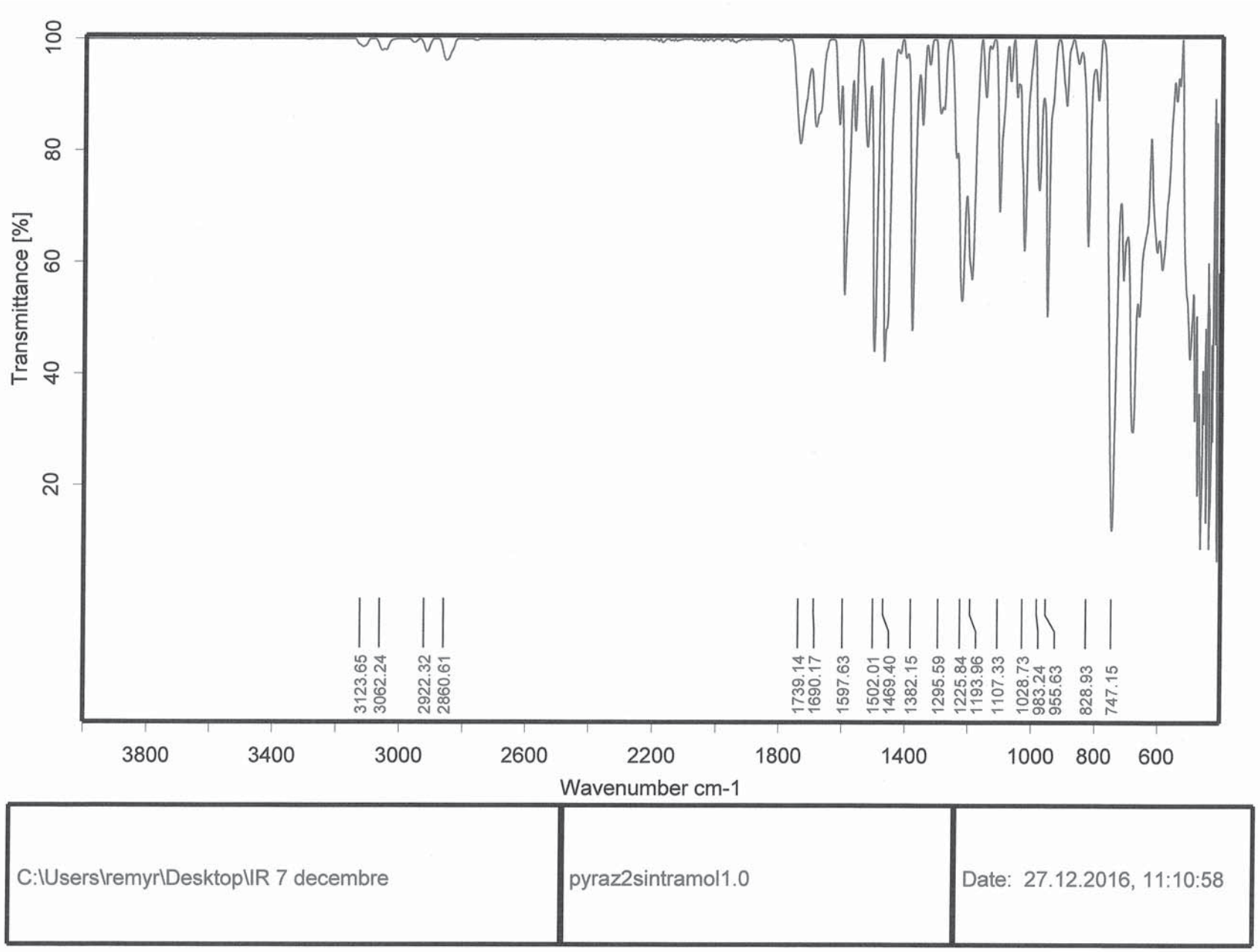
/Data/UNI_FR/REMY2409_ESI/1/pdata/1 FTMS USER Wed Dec 14 14:03:33 2016

2-phenyl-2,4-dihydrochromeno[4,3-c]pyrazole



2-phenyl-2,4-dihydrochromeno[4,3-c]pyrazole





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FTMS 4.7T BioAPEX II

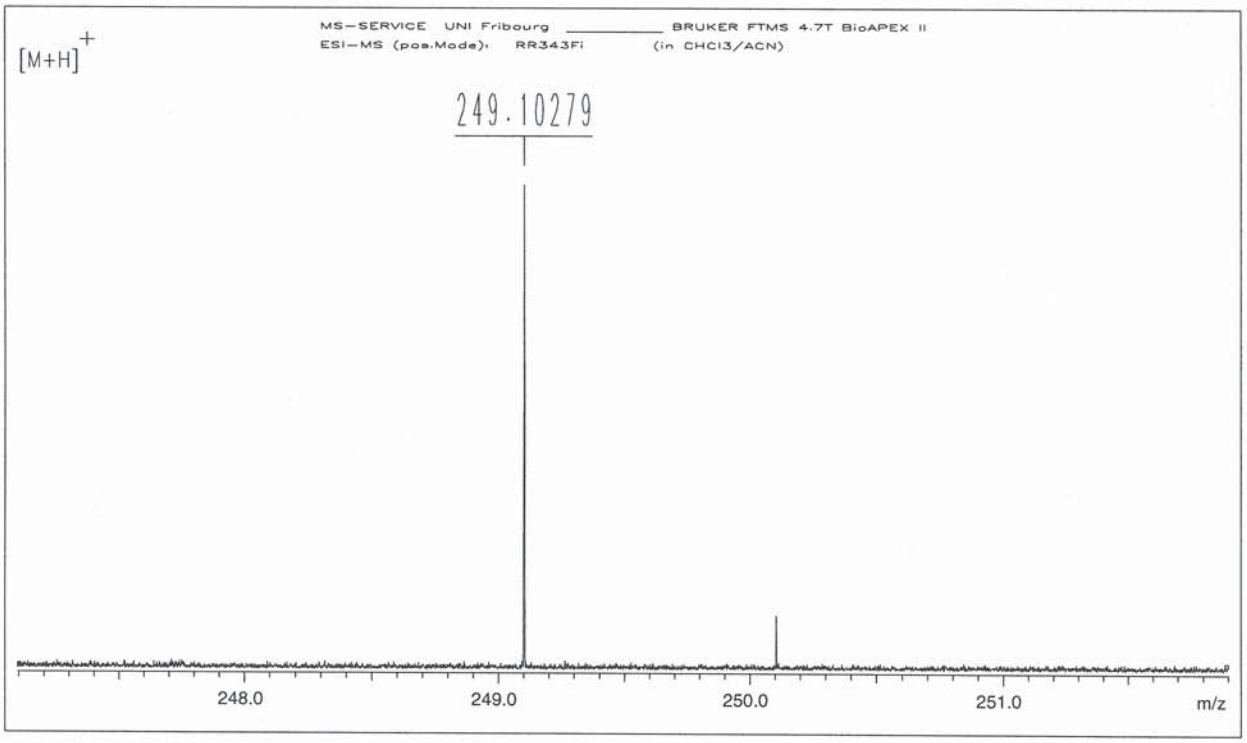
ESI-MS: RR343Fi

XMASS Mass Analysis for /Data/UNI_FR/REMY9720_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 249.1027930

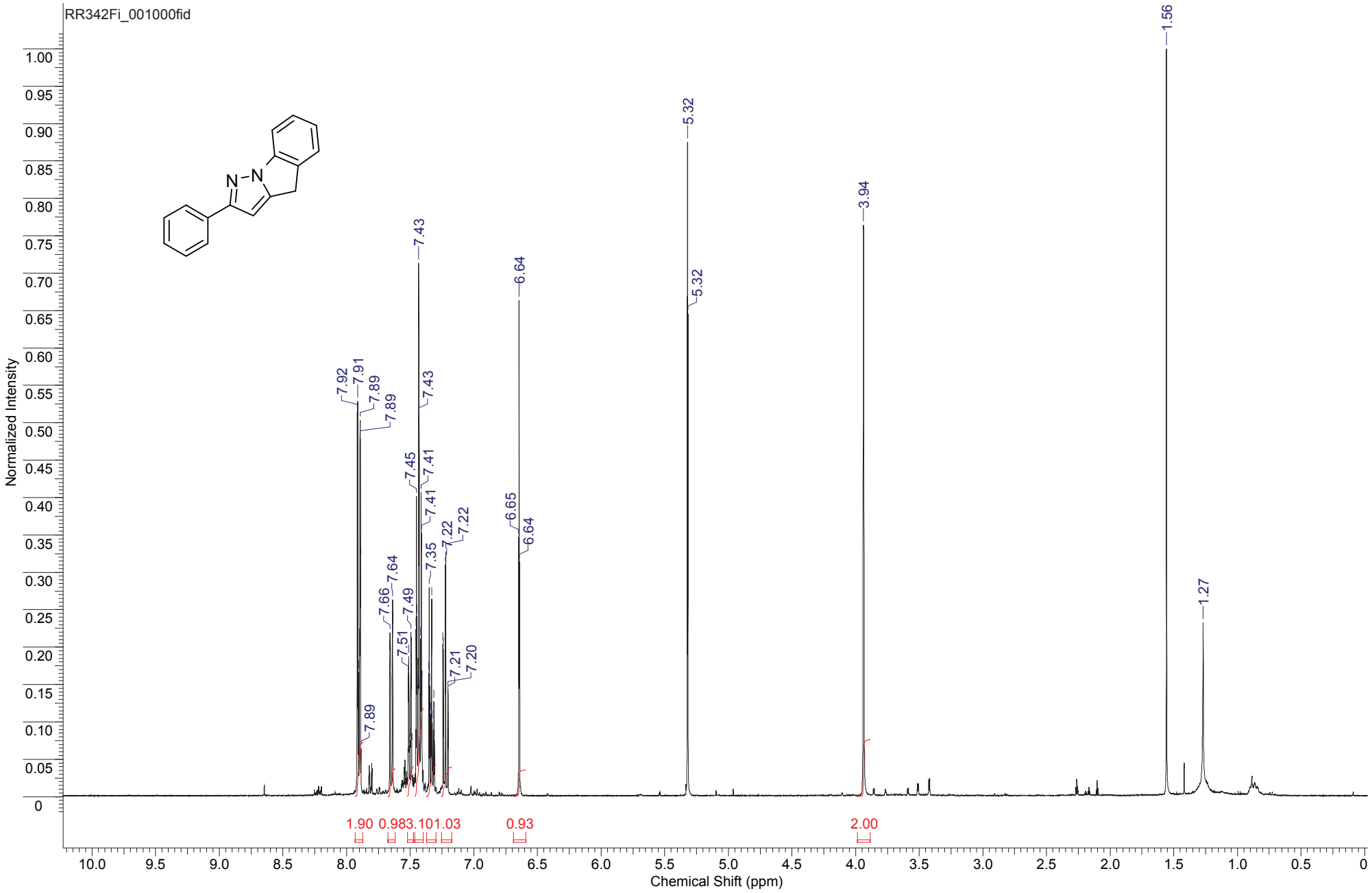
Charge = +1

#	C	H	N	O	mass	DBE	error
*** Mass Analysis for mass 249.1027930							
1	**16**	**13**	**2**	**1**	**249.1022395**	**11.5**	**5.535e-04**
2	13	15	1	4	249.0995594	7.0	3.234e-03
3	11	13	4	3	249.0982167	7.5	4.576e-03
4	12	15	3	3	249.1107928	7.0	8.000e-03
5	17	15	1	1	249.1148155	11.0	1.202e-02
6	15	11	3	1	249.0896634	12.0	1.313e-02
7	12	13	2	4	249.0869833	7.5	1.581e-02
8	13	17	2	3	249.1233688	6.5	2.058e-02
9	16	11	1	2	249.0784300	12.0	2.436e-02
10	14	9	4	1	249.0770874	12.5	2.571e-02

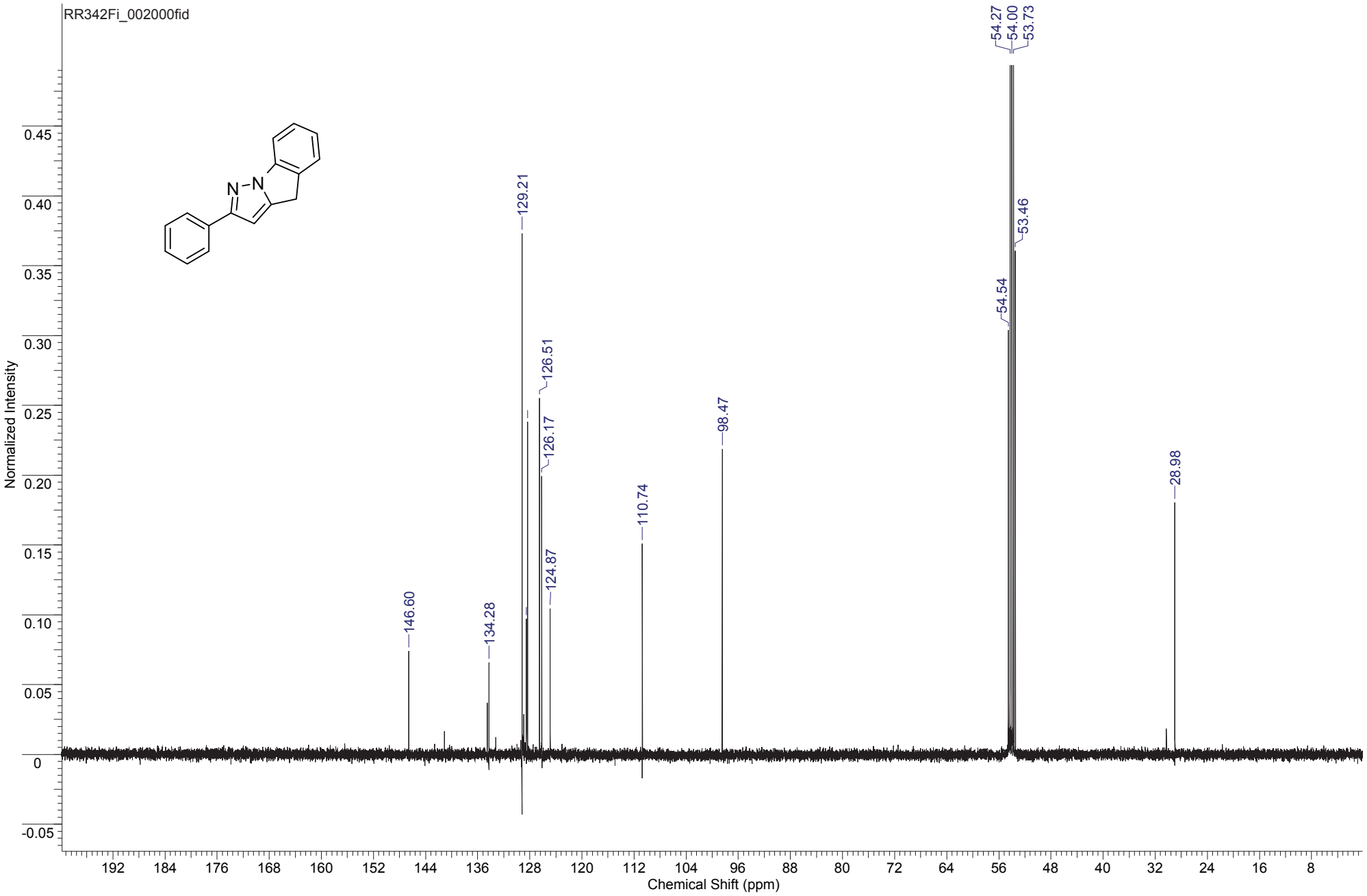


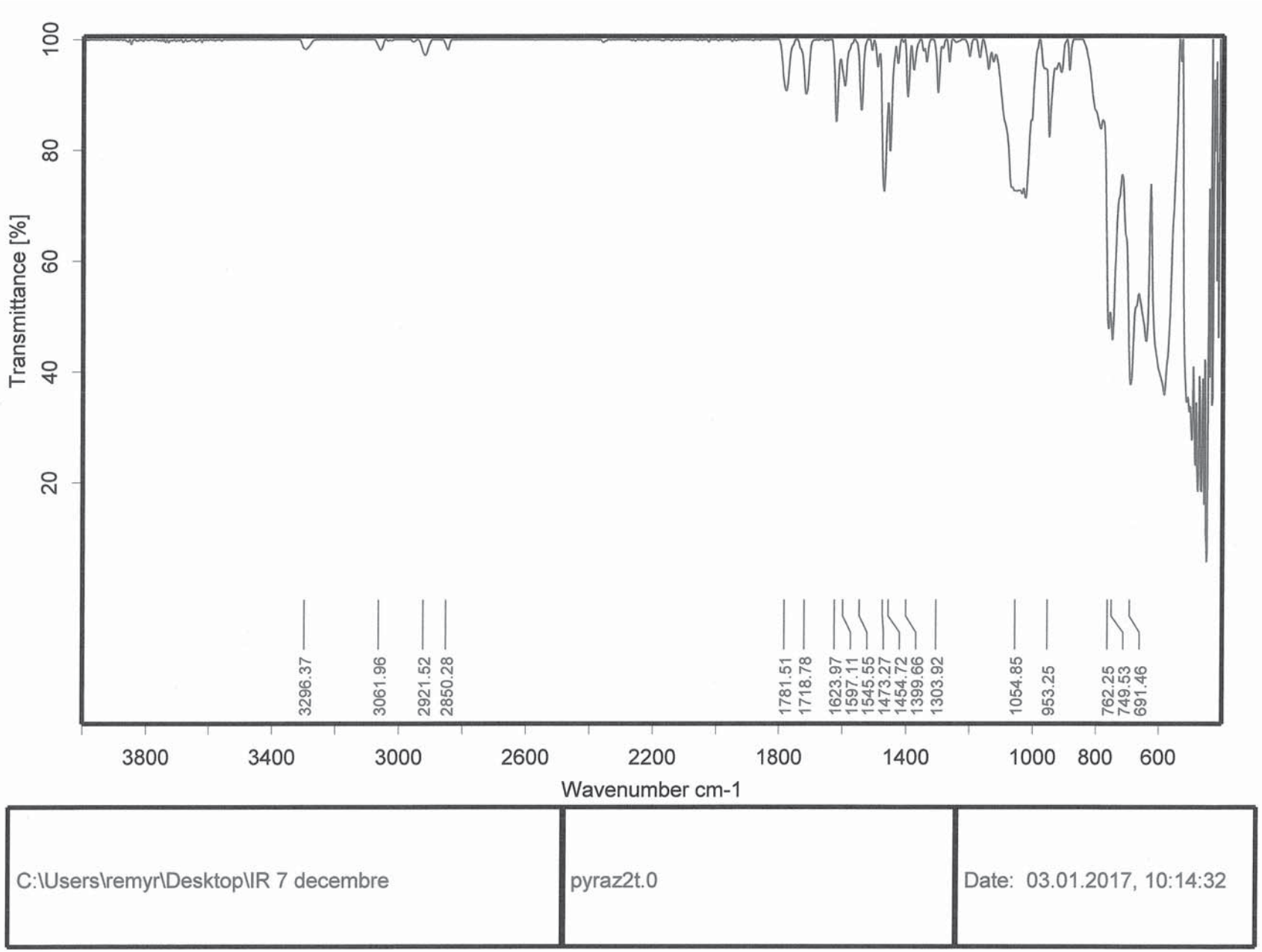
/Data/UNI_FR/REMY9720_ESI/2/pdata/1 FTMS USER Wed Aug 19 10:10:30 2015

2-phenyl-4H-pyrazolo[1,5-a]indole



2-phenyl-4H-pyrazolo[1,5-a]indole





C:\Users\remyr\Desktop\IR 7 decembre	pyraz2t.0	Date: 03.01.2017, 10:14:32

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Mass Spectrometry Service
Department of Chemistry

BRUKER FTMS 4.7T BioAPEX II

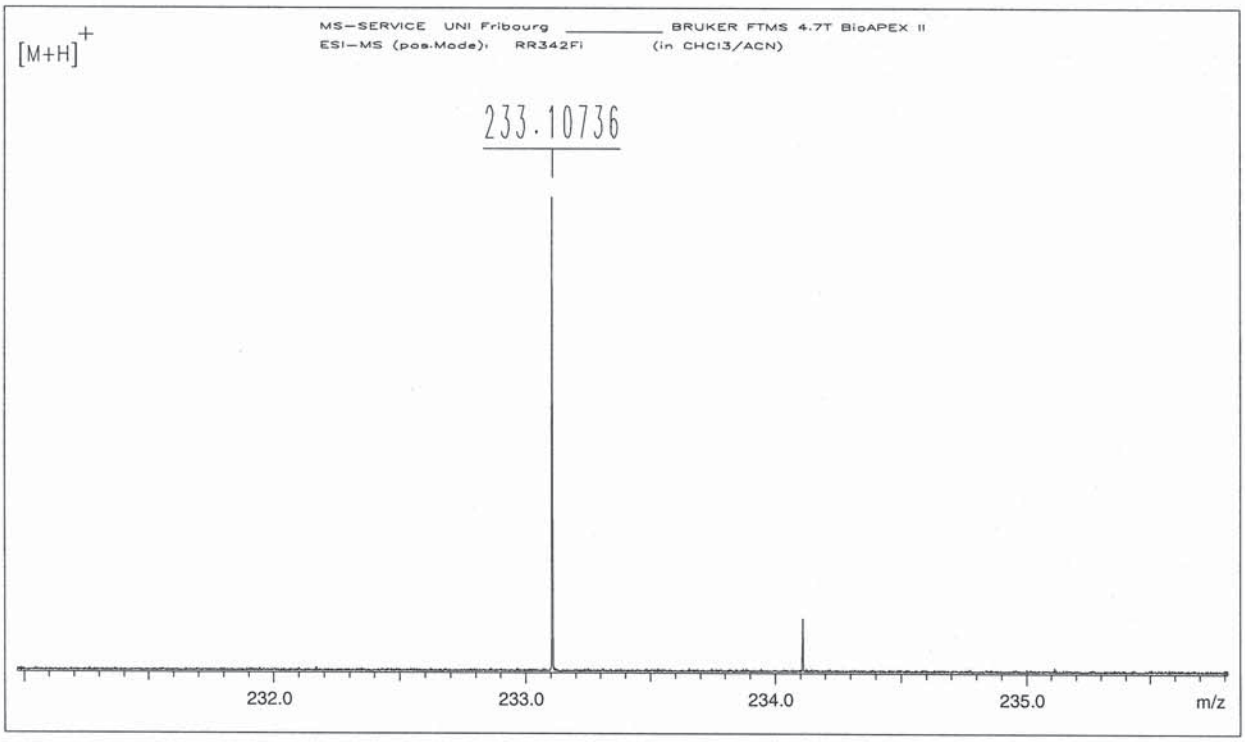
ESI-MS: RR342Fi

XMASS Mass Analysis for /Data/UNI_FR/REMY9719_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 233.1073620

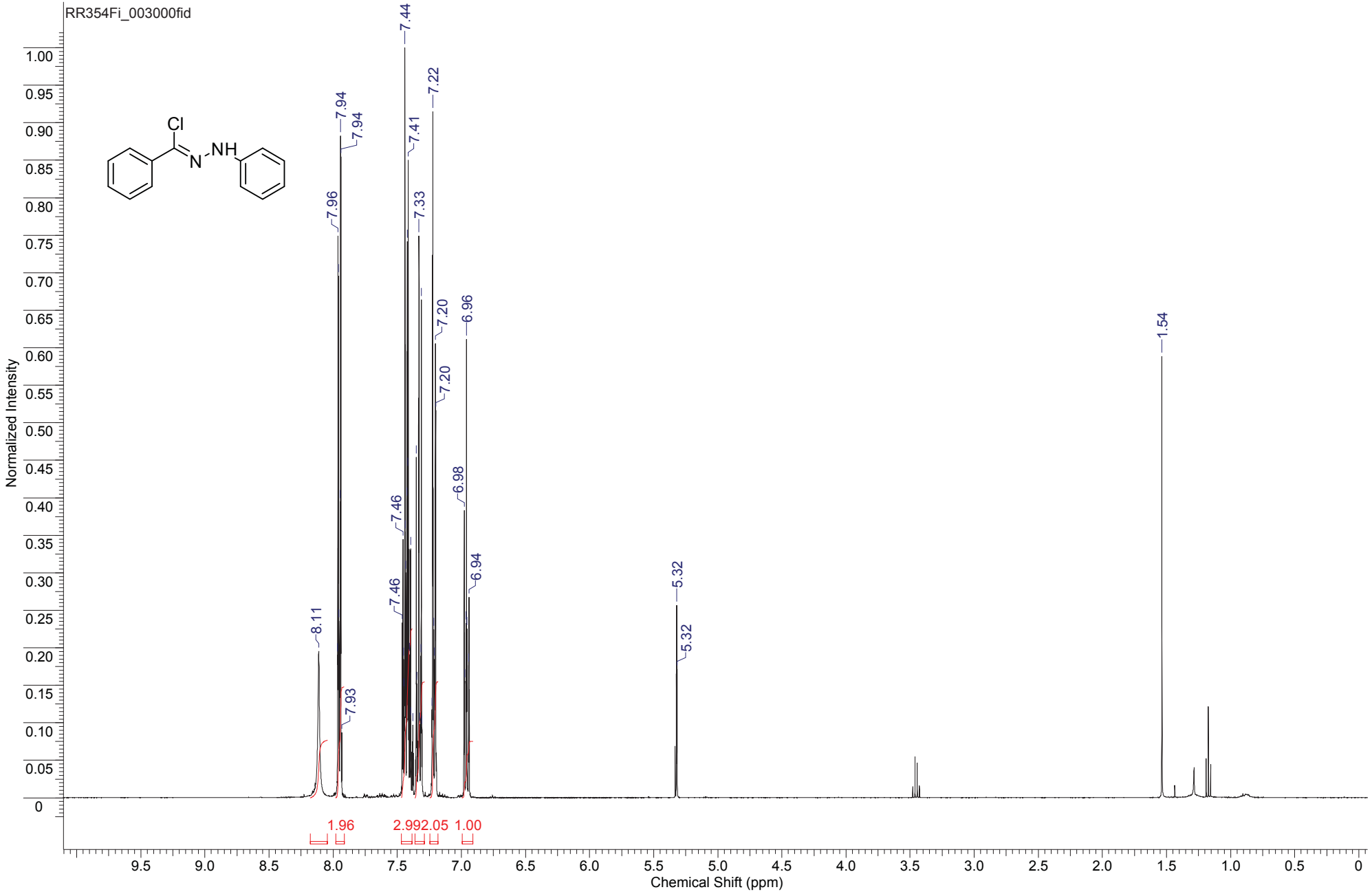
Charge = +1

#	C	H	N	mass	DBE	error
*** Mass Analysis for mass 233.1073620						
1	**16**	**13**	**2**	**233.1073248**	**11.5**	**3.715e-05**
2	8	11	9	233.1131928	8.0	5.831e-03
3	7	9	10	233.1006168	8.5	6.745e-03
4	17	15	1	233.1199009	11.0	1.254e-02
5	15	11	3	233.0947488	12.0	1.261e-02
6	9	13	8	233.1257689	7.5	1.841e-02
7	14	9	4	233.0821727	12.5	2.519e-02
8	10	15	7	233.1383449	7.0	3.098e-02
9	13	7	5	233.0695967	13.0	3.777e-02
10	11	17	6	233.1509210	6.5	4.356e-02

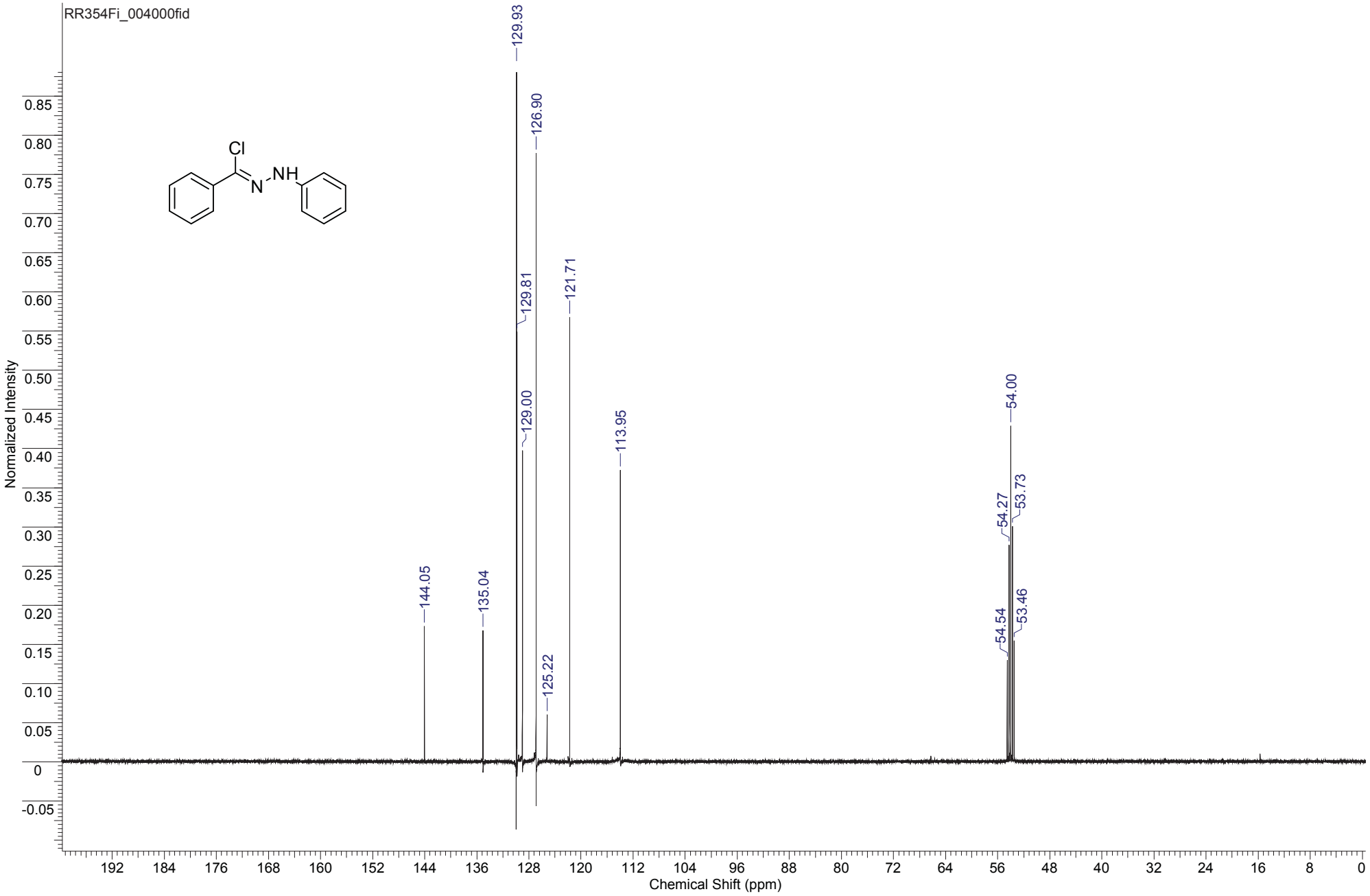


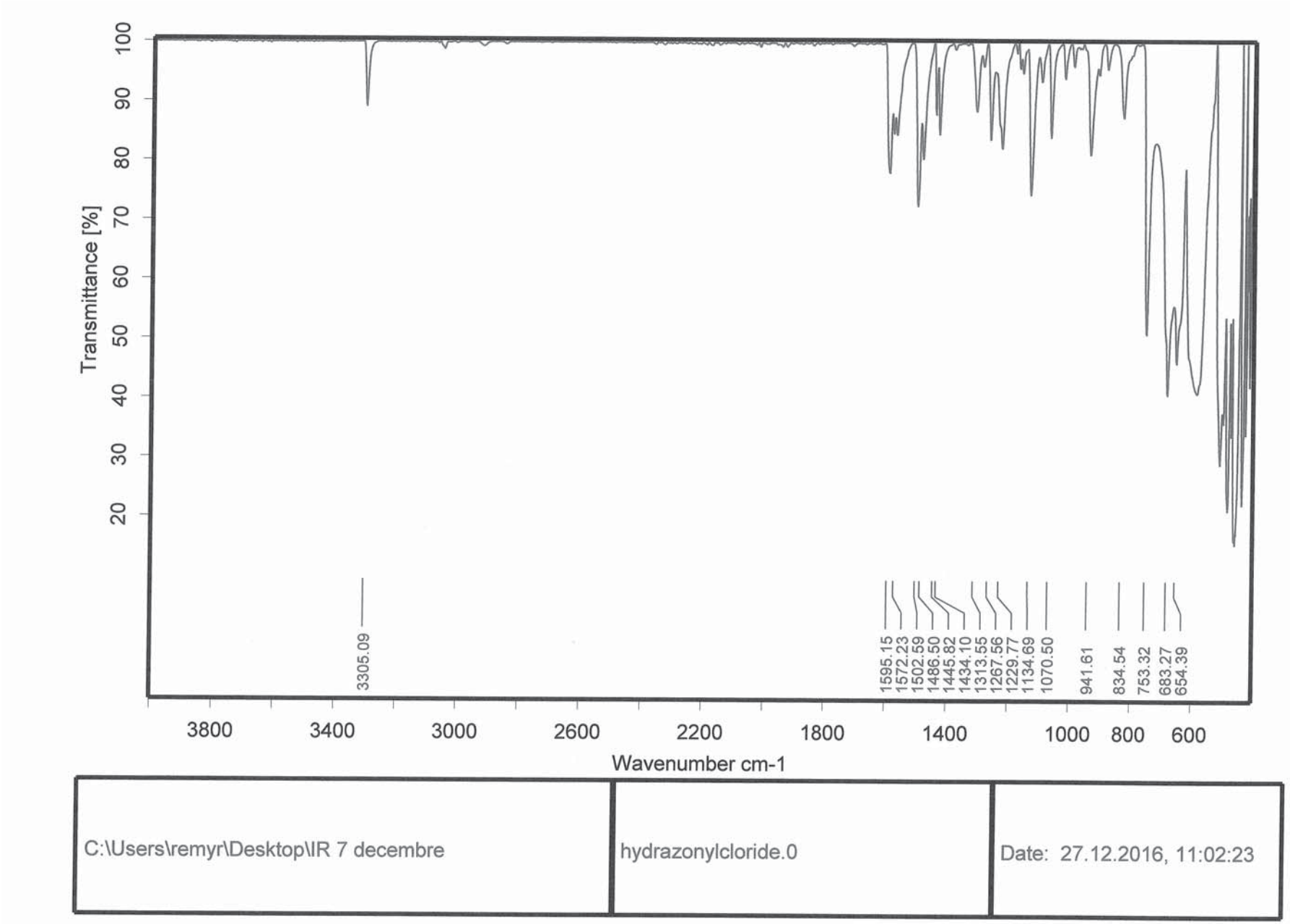
/Data/UNI_FR/REMY9719_ESI/2/pdata/1 FTMS USER Wed Aug 19 11:03:53 2015

(Z)-N'-phenylbenzohydrazonoyl chloride



(Z)-N'-phenylbenzohydrazonoyl chloride




Transmittance [%]
100
90
80
70
60
50
40
30
20
3305.09
1595.15
1572.23
1502.59
1486.50
1445.82
1434.10
1313.55
1267.56
1229.77
1134.69
1070.50
941.61
834.54
753.32
683.27
654.39
3800
3400
3000
2600
2200
1800
1400
1000
800
600
Wavenumber cm-1
C:\Users\remyr\Desktop\IR 7 decembre
hydrazonylcloride.0
Date: 27.12.2016, 11:02:23