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Supporting Information

New Conjugated *meso*-Tetrafluorenylporphyrin-Cored Derivatives as Fluorescent Two-Photon Photosensitizers for Singlet Oxygen Generation

Dandan Yao,[a, b] Xu Zhang,[a, b] Amédée Triadon,[a] Nicolas Richy,[a] Olivier Mongin,[a] Mireille Blanchard-Desce,[c] Frédéric Paul,[a] and Christine O. Paul-Roth*[a, b]

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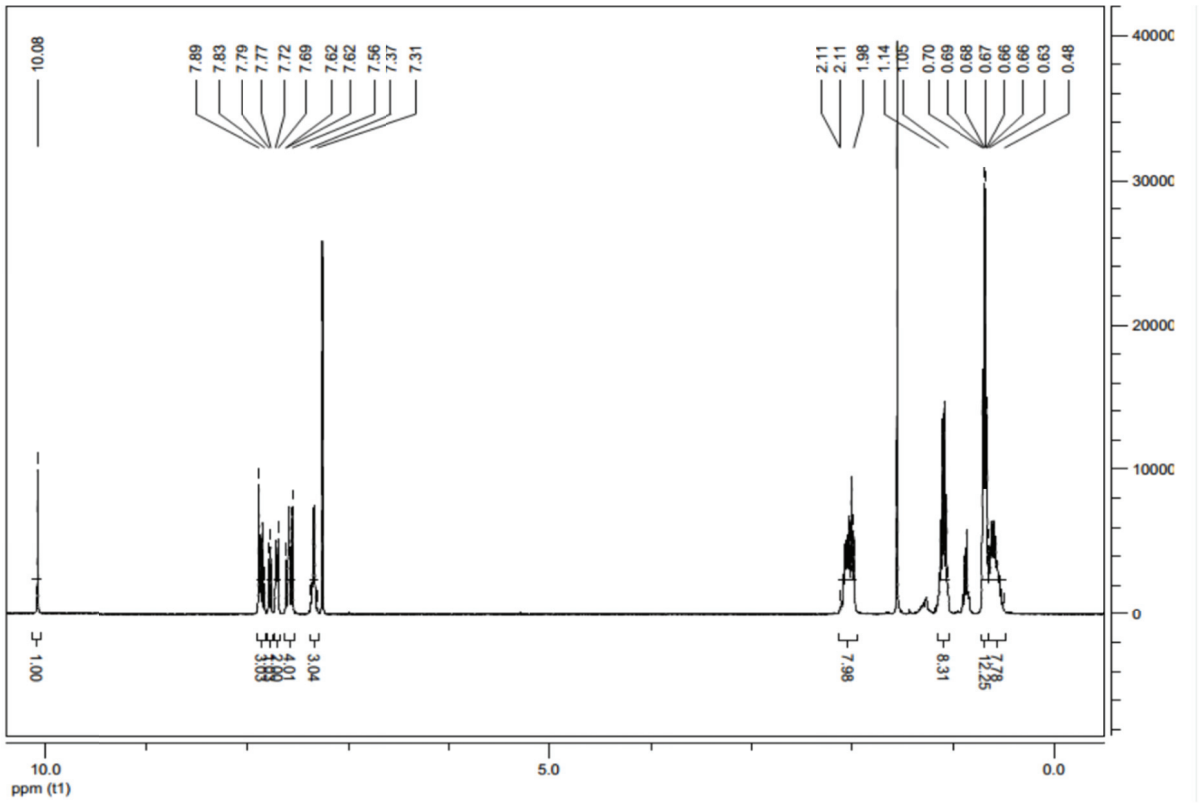
1. **^{1}H NMR Spectra of the Dendrons D1, D2, D3, and of TFP1, TFP2, TFP3.**

D1:



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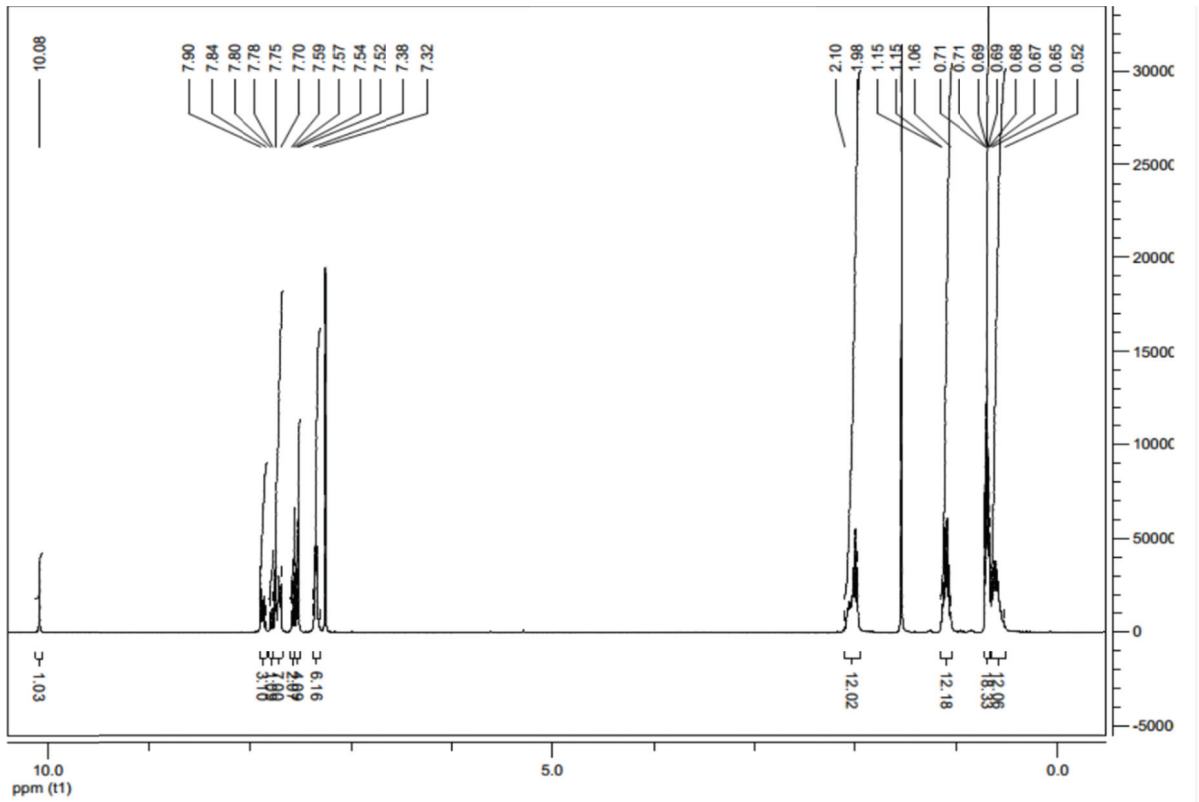

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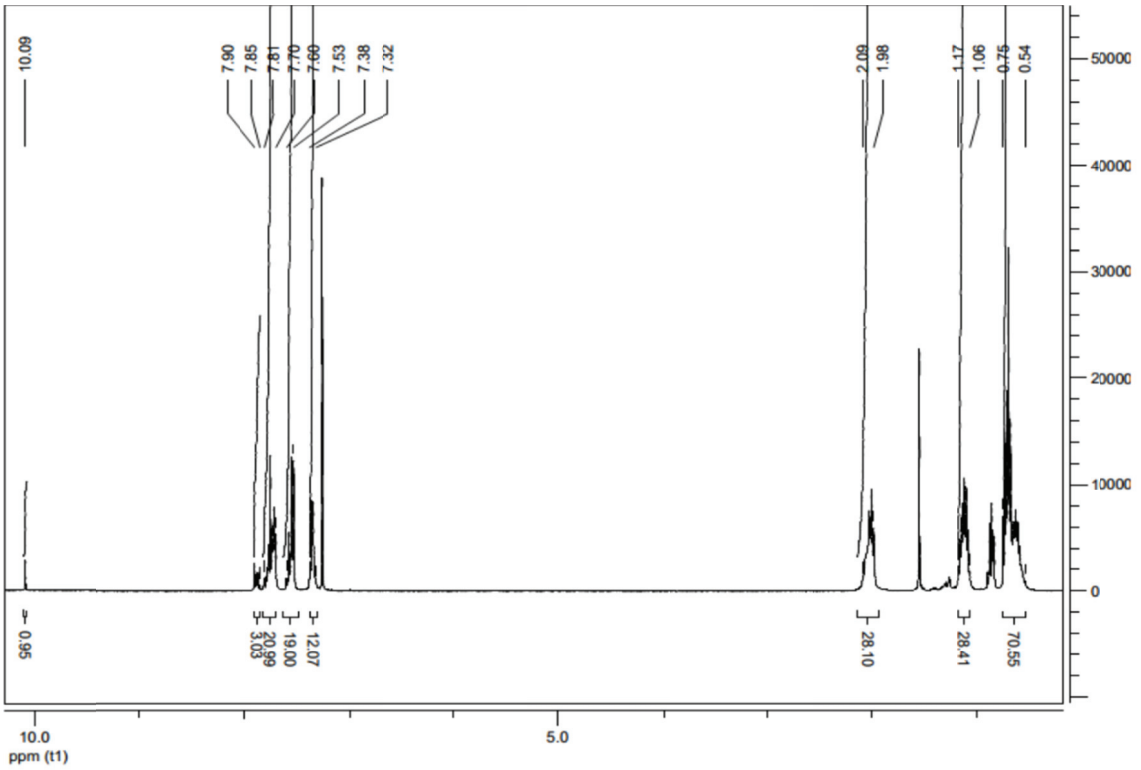
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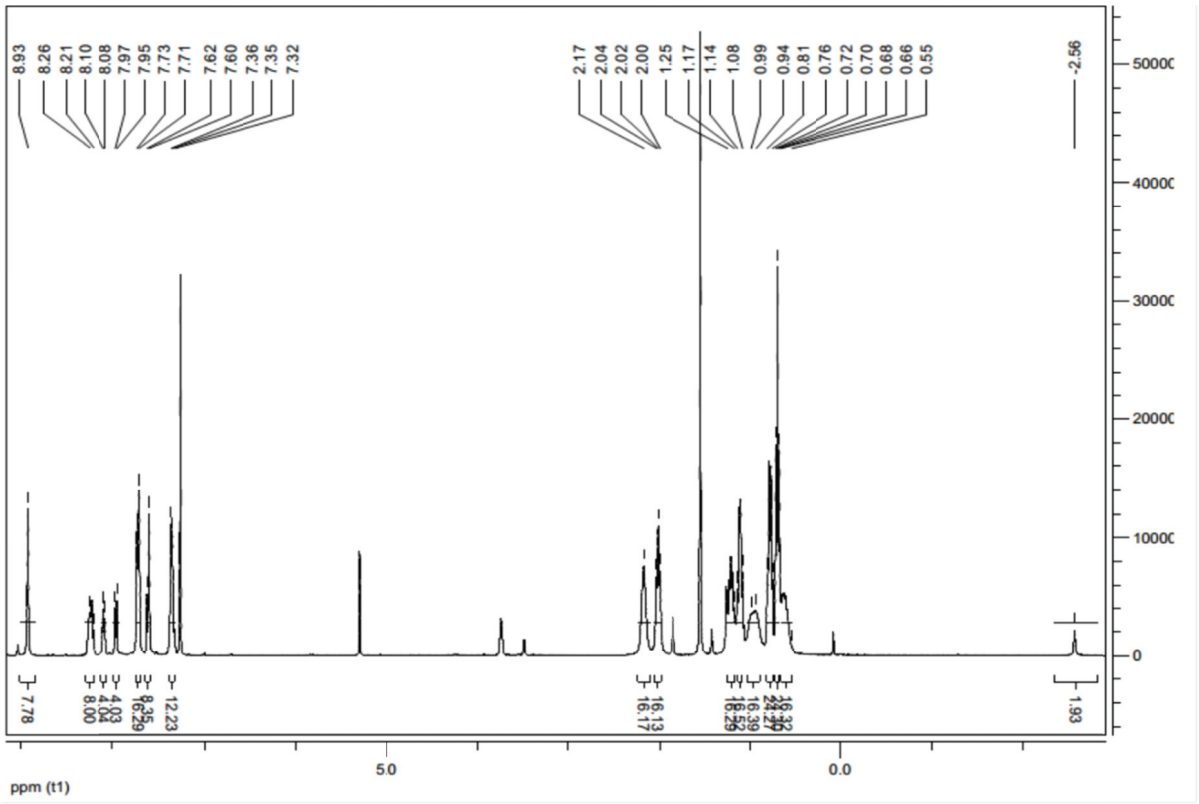
7.90
7.85
7.81
7.70
7.60
7.53
7.38
7.32
2.09
1.98
1.17
1.06
0.75
0.54
50000
40000
30000
20000
10000
0
0.95
3.03
20.99
19.00
12.07
28.10
28.41
70.55
10.0
ppm (t1)
5.0

TFP1: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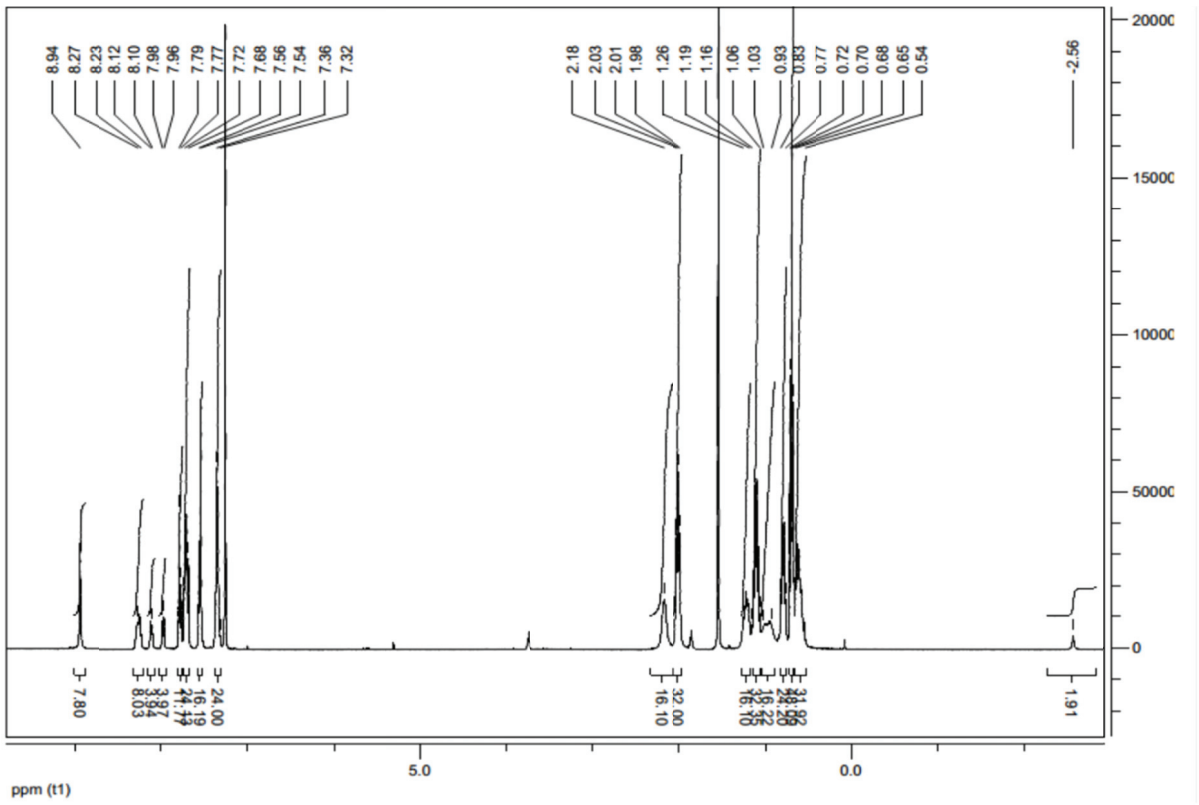
8.26
8.21
8.10
8.08
7.97
7.95
7.73
7.71
7.62
7.60
7.36
7.35
7.32
2.17
2.04
2.02
2.00
1.25
1.17
1.14
1.08
0.99
0.94
0.81
0.76
0.72
0.70
0.68
0.66
0.55
-2.56
7.78
8.00
4.03
4.04
8.29
8.25
12.23
16.13
16.17
16.29
16.39
1.93
5.0
0.0
ppm (t1)

TFP2: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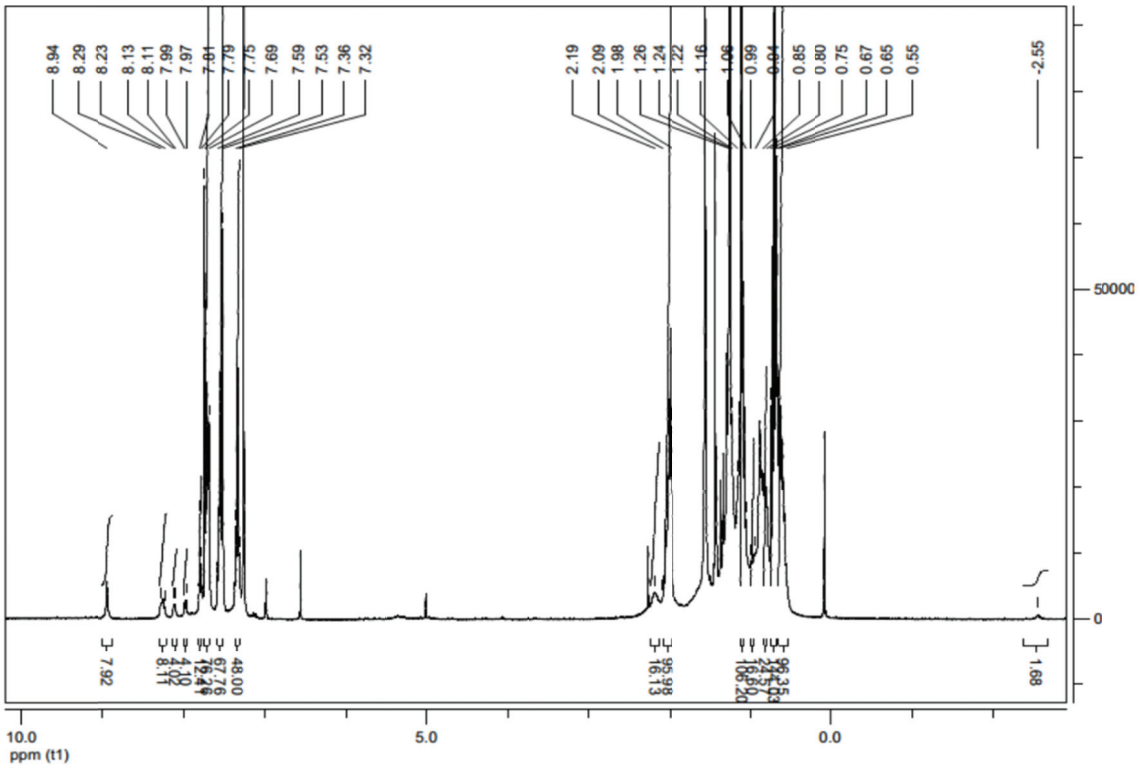
8.27
8.23
8.12
8.10
7.98
7.96
7.79
7.77
7.72
7.68
7.56
7.54
7.36
7.32
2.18
2.03
2.01
1.98
1.26
1.19
1.16
1.06
1.03
0.93
0.83
0.77
0.72
0.70
0.68
0.65
0.54
-2.56
7.80
8.03
3.97
3.94
16.19
24.00
16.10
32.00
16.35
16.22
1.91
5.0
0.0
ppm (t1)

TFP3: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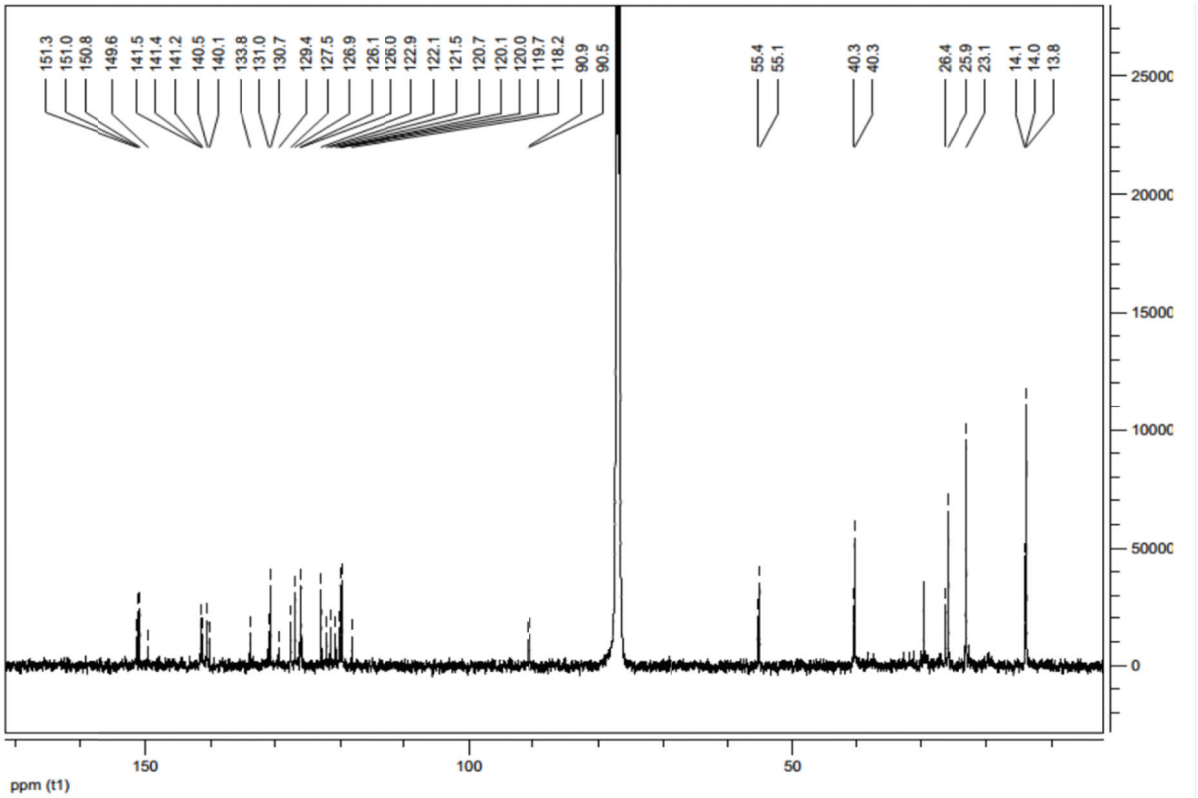
8.29
8.23
8.13
8.11
7.99
7.97
7.81
7.79
7.75
7.69
7.59
7.53
7.36
7.32
2.19
2.09
1.98
1.26
1.24
1.22
1.16
1.06
0.99
0.94
0.85
0.80
0.75
0.67
0.65
0.55
-2.55
50000
0
7.92
8.11
48.00
16.13
1.68
10.0
ppm (t1)
5.0
0.0

2. ^{13}C NMR Spectra of TFP1, TFP2 and TFP3.

TFP1:



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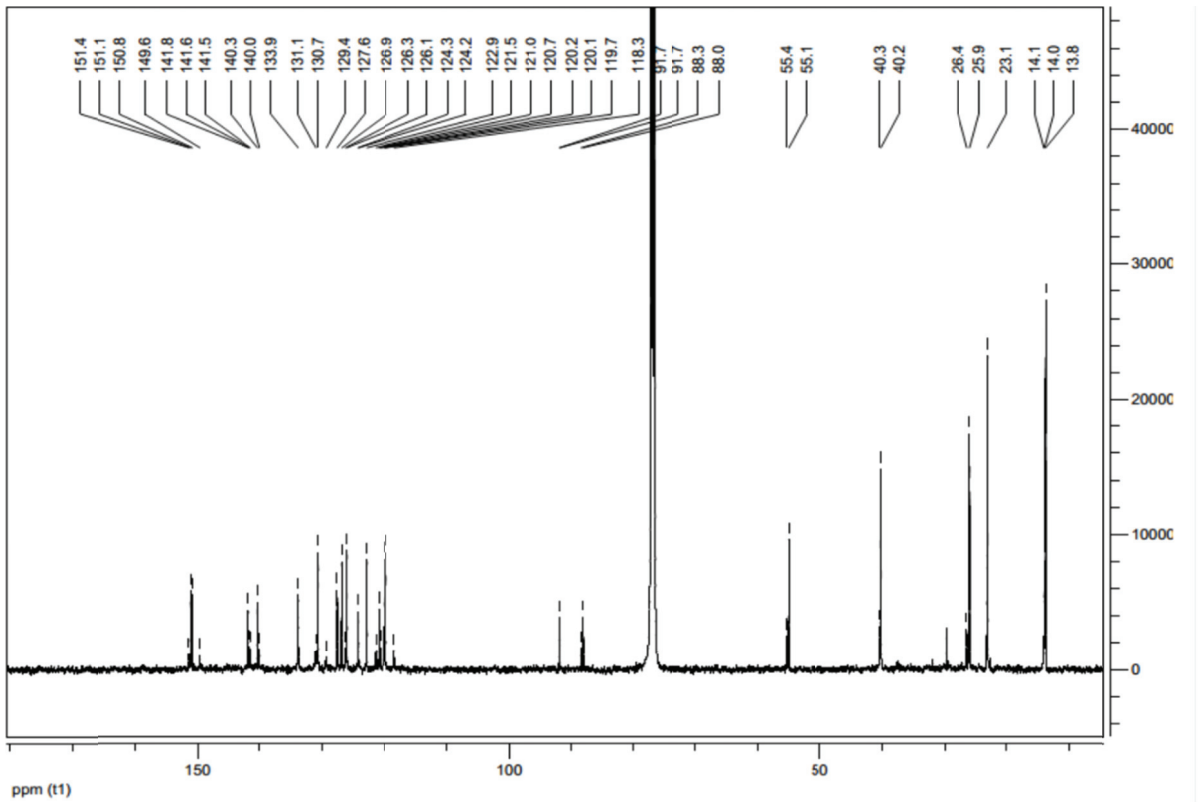
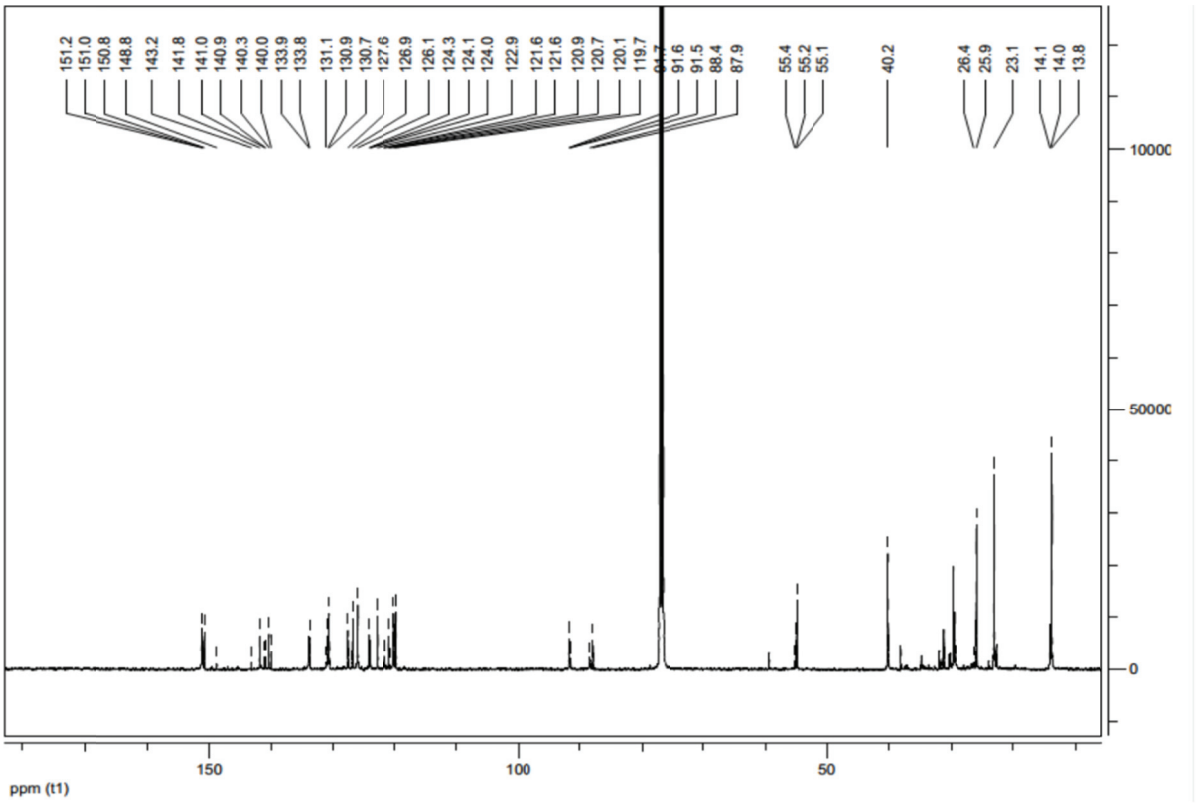
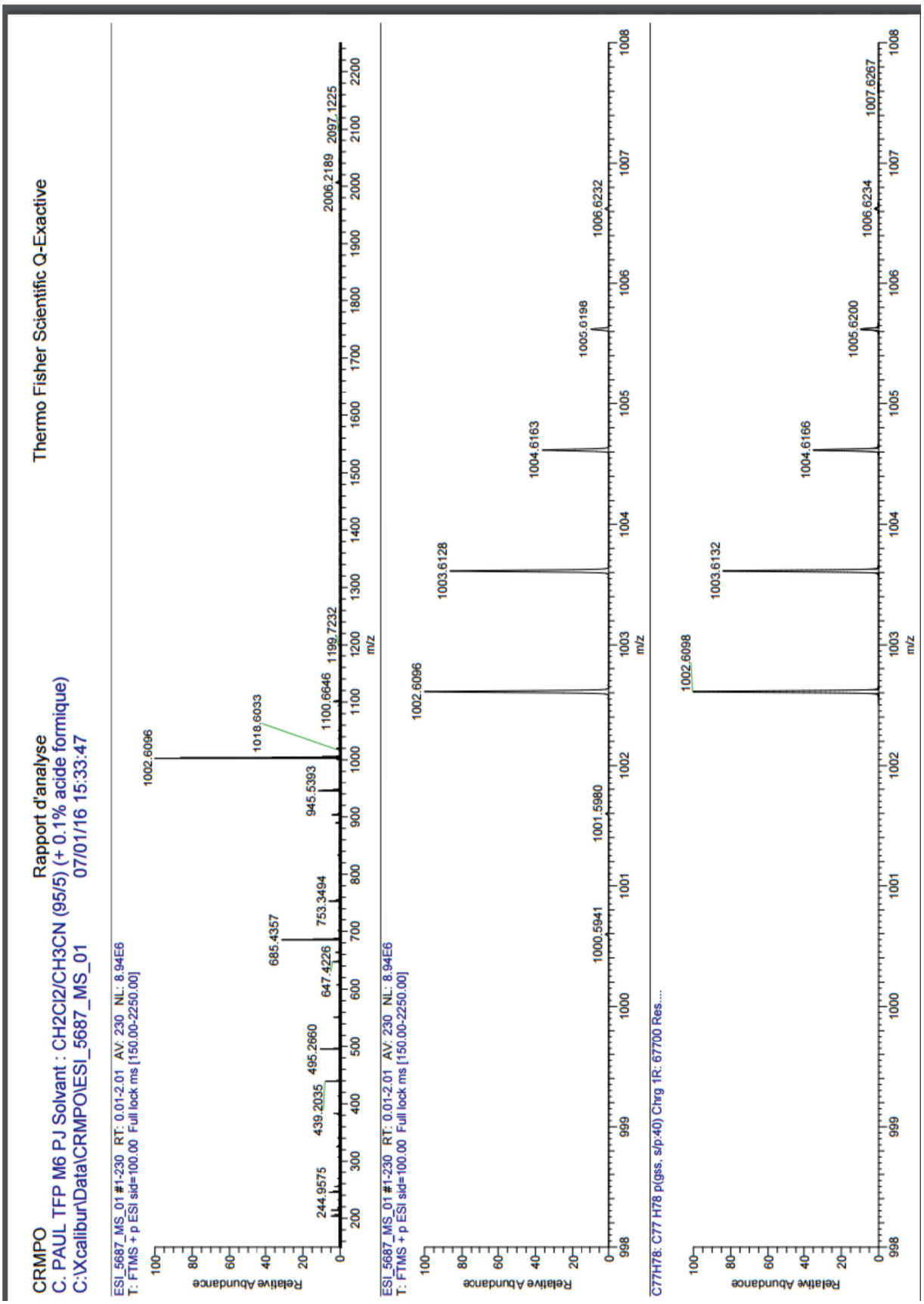


TFP3:

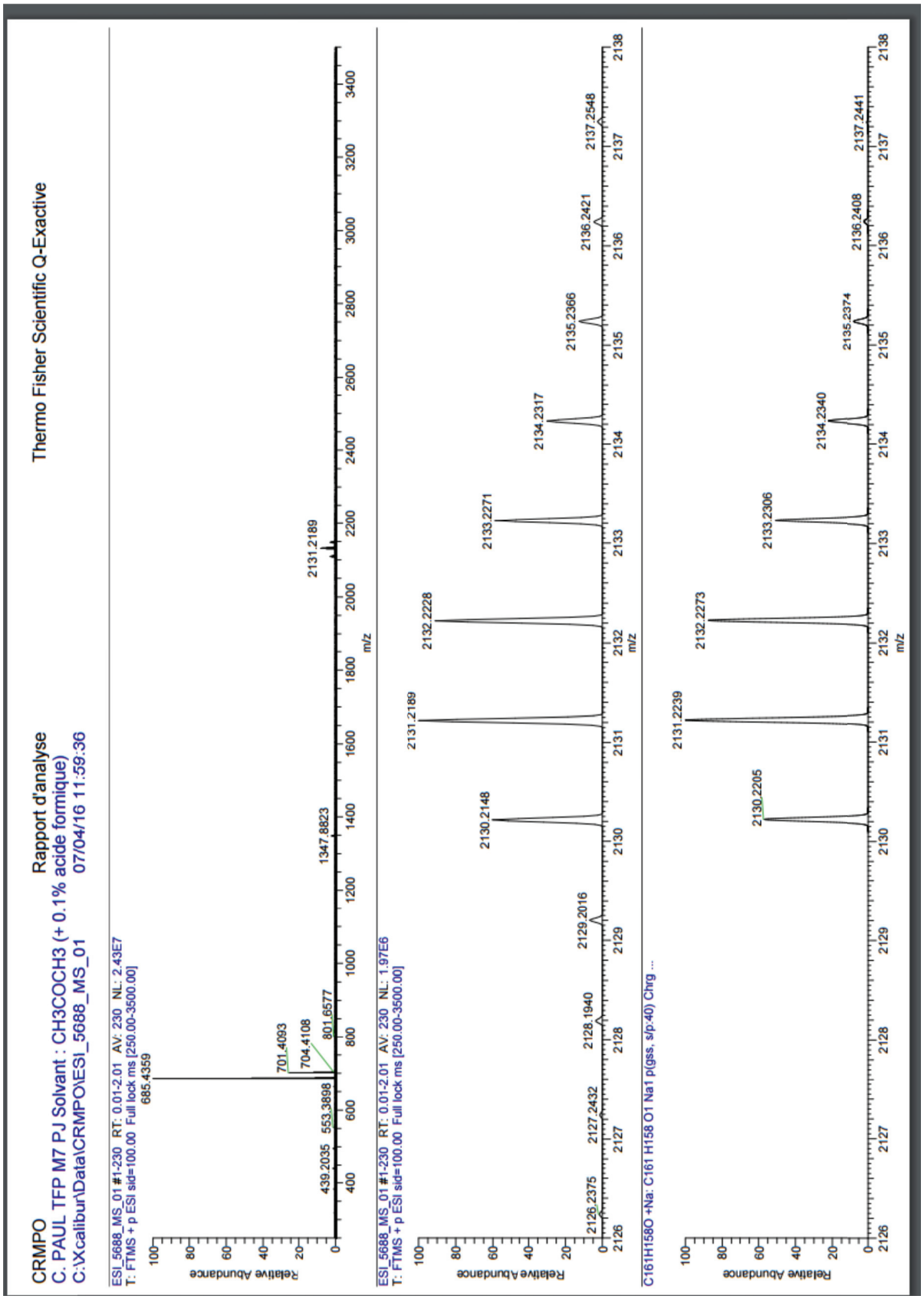

151.2
151.0
150.8
148.8
143.2
141.8
141.0
140.9
140.3
140.0
133.9
133.8
131.1
130.9
130.7
127.6
126.9
126.1
124.3
124.1
124.0
122.9
121.6
121.6
120.9
120.7
120.1
119.7
91.6
91.5
88.4
87.9
55.4
55.2
55.1
40.2
26.4
25.9
23.1
14.1
14.0
13.8
10000
50000
0
150
100
50
ppm (t1)

3. HR Mass spectra of **Intermediate 6,7, 9, Dendron1**, **Dendron2**, **Dendron3**, and **TFP1**, **TFP2**, **TFP3**

Intermediate 6:



Intermediate 7:



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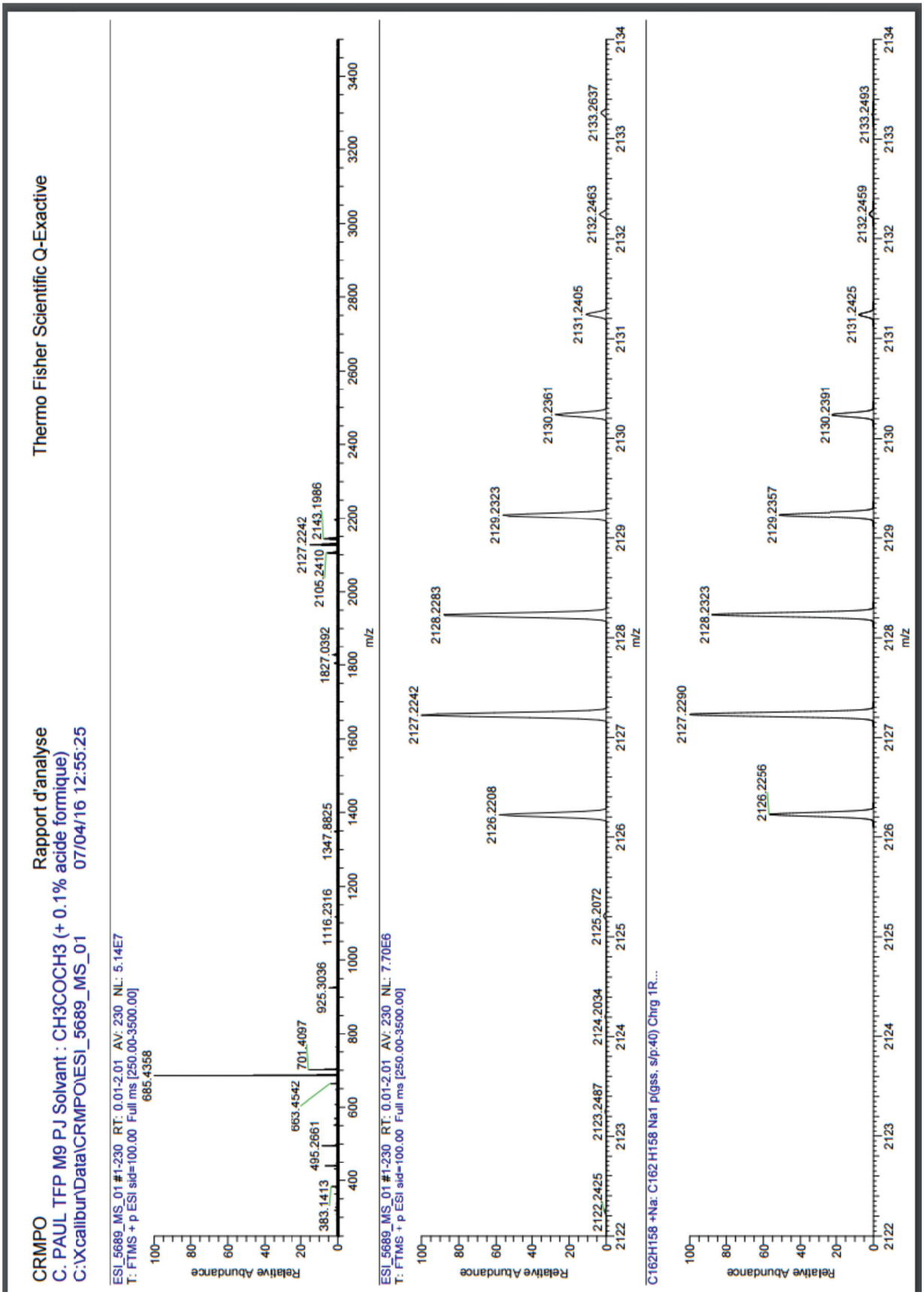

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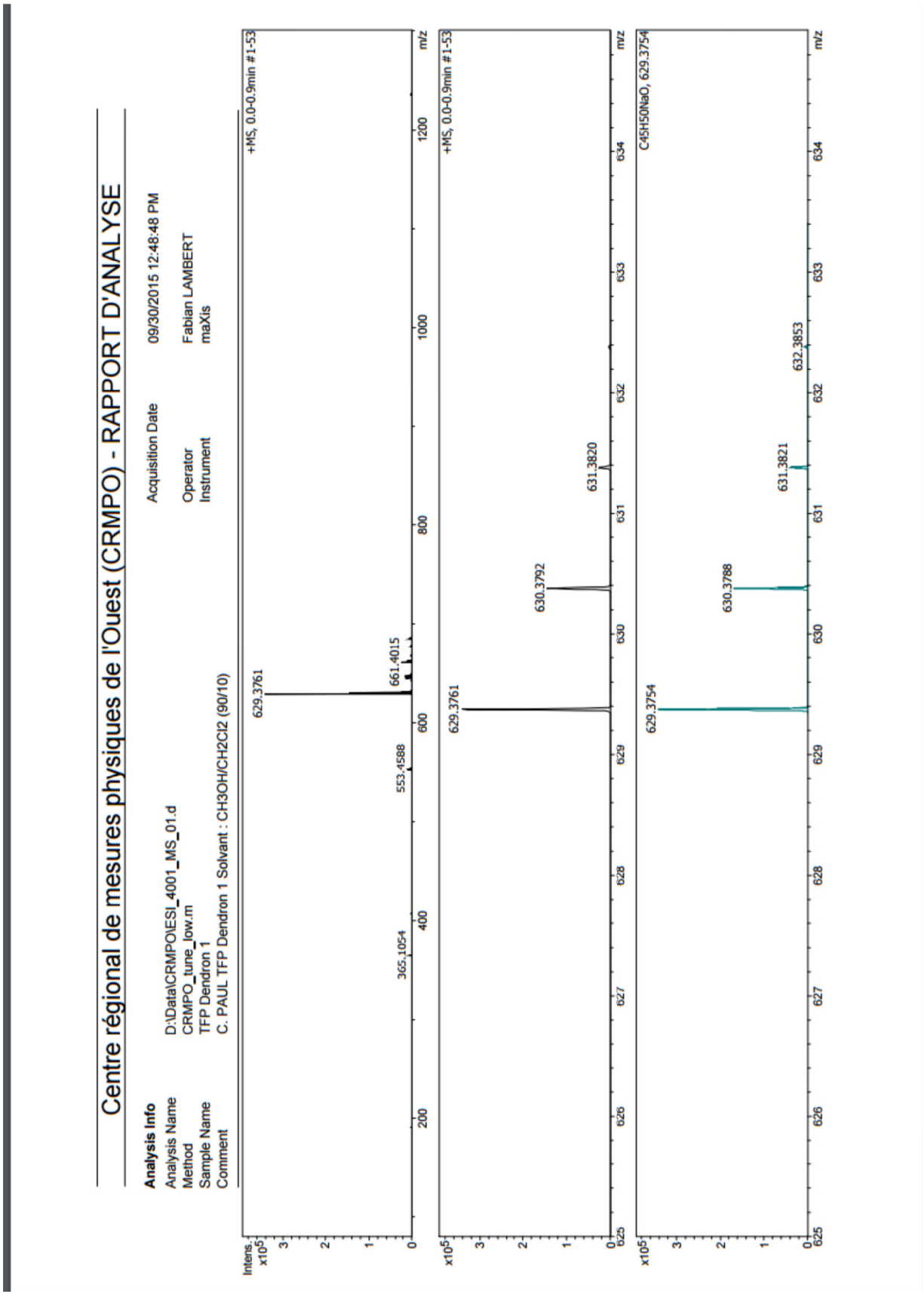
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Method CRMPO_tune_low.m
Sample Name TFP Dendron 1
Comment C. PAUL TFP Dendron 1 Solvant : CH3OH/CH2Cl2 (90/10)
Acquisition Date 09/30/2015 12:48:48 PM
Operator Fabian LAMBERT
Instrument maXis
+MS, 0.0-0.9min #1-53
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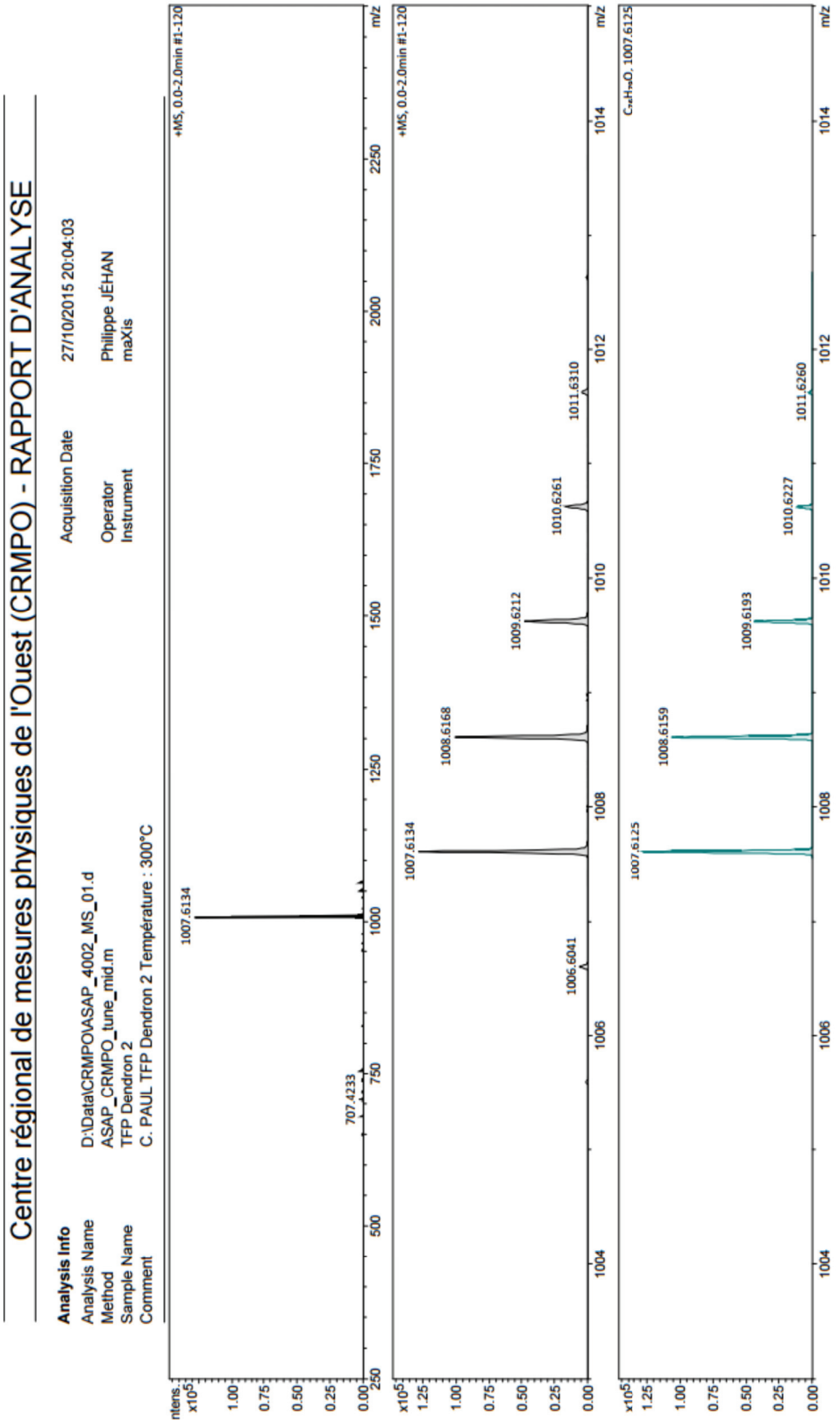
661.4015
553.4588
365.1054
630.3792
631.3820
C45H50NaO, 629.3754
629.3754
630.3788
631.3821
632.3853
Intens.
x10^5
m/z

Dendron 2: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Comment C. PAUL TFP Dendron 2 Température : 300°C
Acquisition Date 27/10/2015 20:04:03
Operator Philippe JÉHAN
Instrument maXis
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1008.6168
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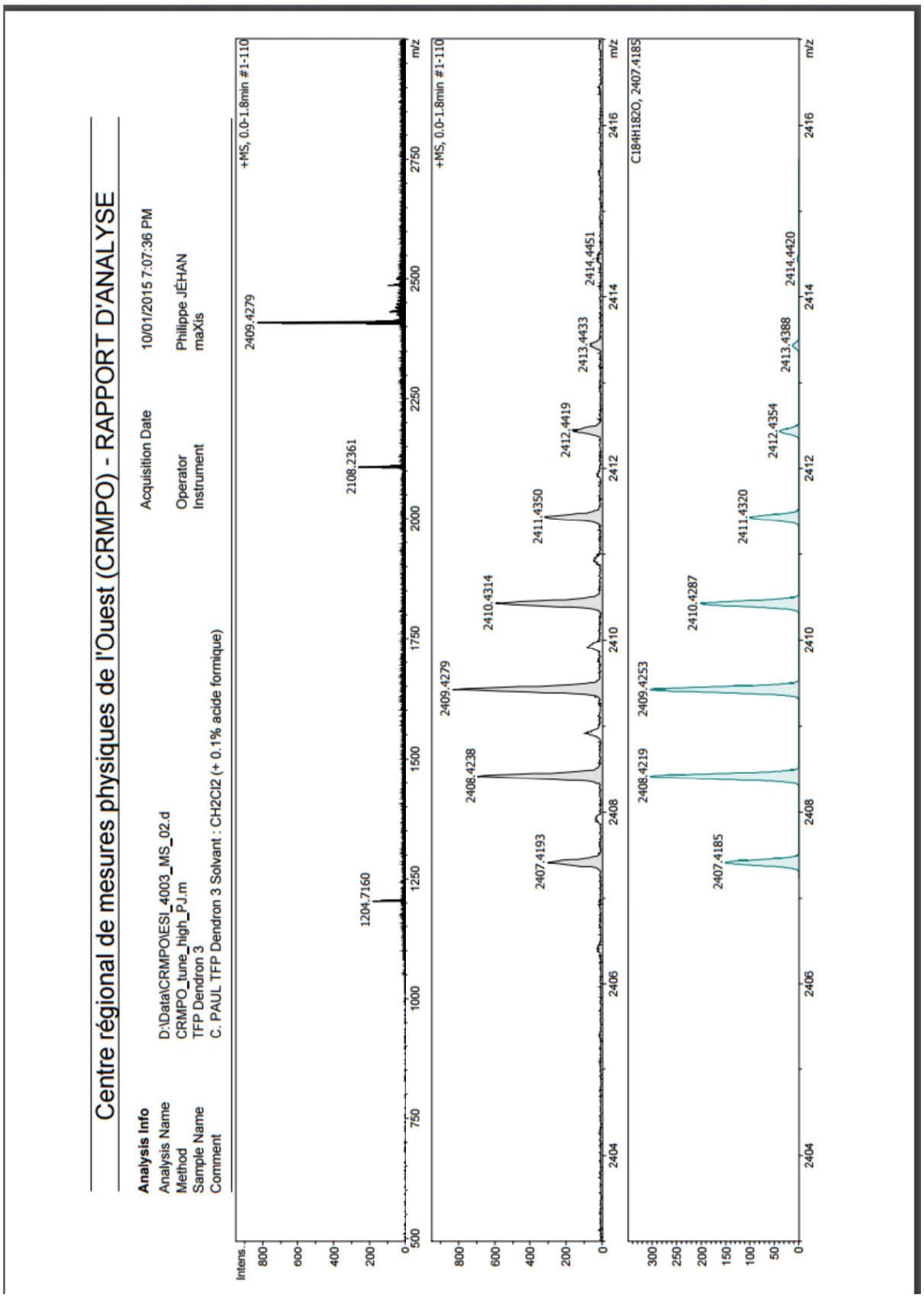
1010.6261
1011.6310
1007.6125
1008.6159
1009.6193
1010.6227
1011.6260
C₄₈H₄₂O₂ 1007.6125
m/z

Dendron 3: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Sample Name TFP Dendron 3
Comment C. PAUL TFP Dendron 3 Solvant : CH2Cl2 (+ 0.1% acide formique)
Acquisition Date 10/01/2015 7:07:36 PM
Operator Philippe JÉHAN
Instrument maXis
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2108.2361
2409.4279
2413.4433
2414.4451
+MS, 0.0-1.8min #1-110
2407.4193
2408.4238
2409.4279
2410.4314
2411.4350
2412.4419
C184H182O, 2407.4185
2407.4185
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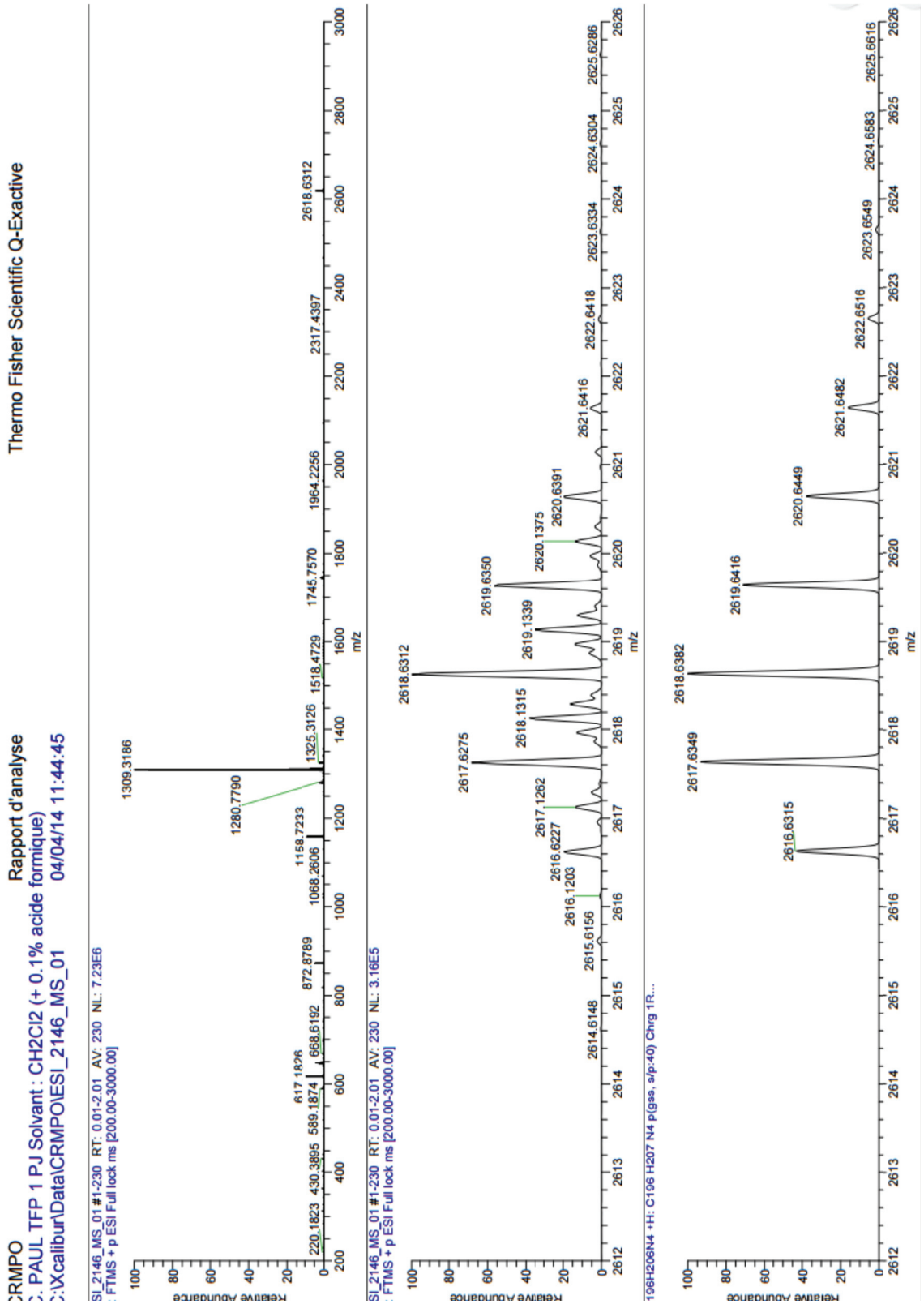
2414.4420
m/z

TFP1:


Thermo Fisher Scientific Q-Exactive
Rapport d'analyse
CRMPO
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SI_2146_MS_01 #1-230 RT: 0.01-2.01 AV: 230 NL: 3.16E5
FTMS + p ESI Full lock ms [200.00-3000.00]
196H206N4 +H: C196 H207 N4 p(gas, a/p:40) Chrg 1R:...
Relative Abundance
m/z

Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

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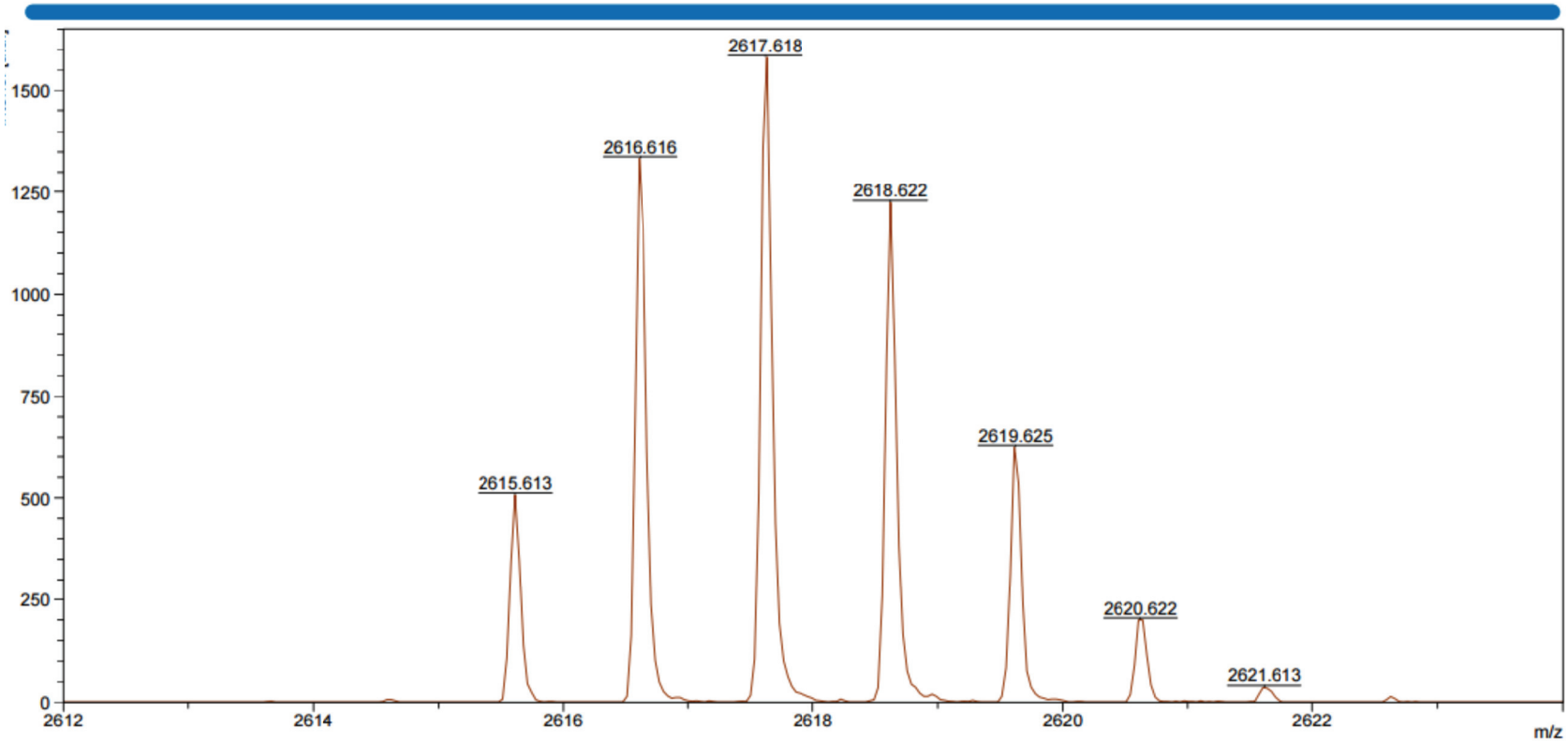

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Bruker Daltonics

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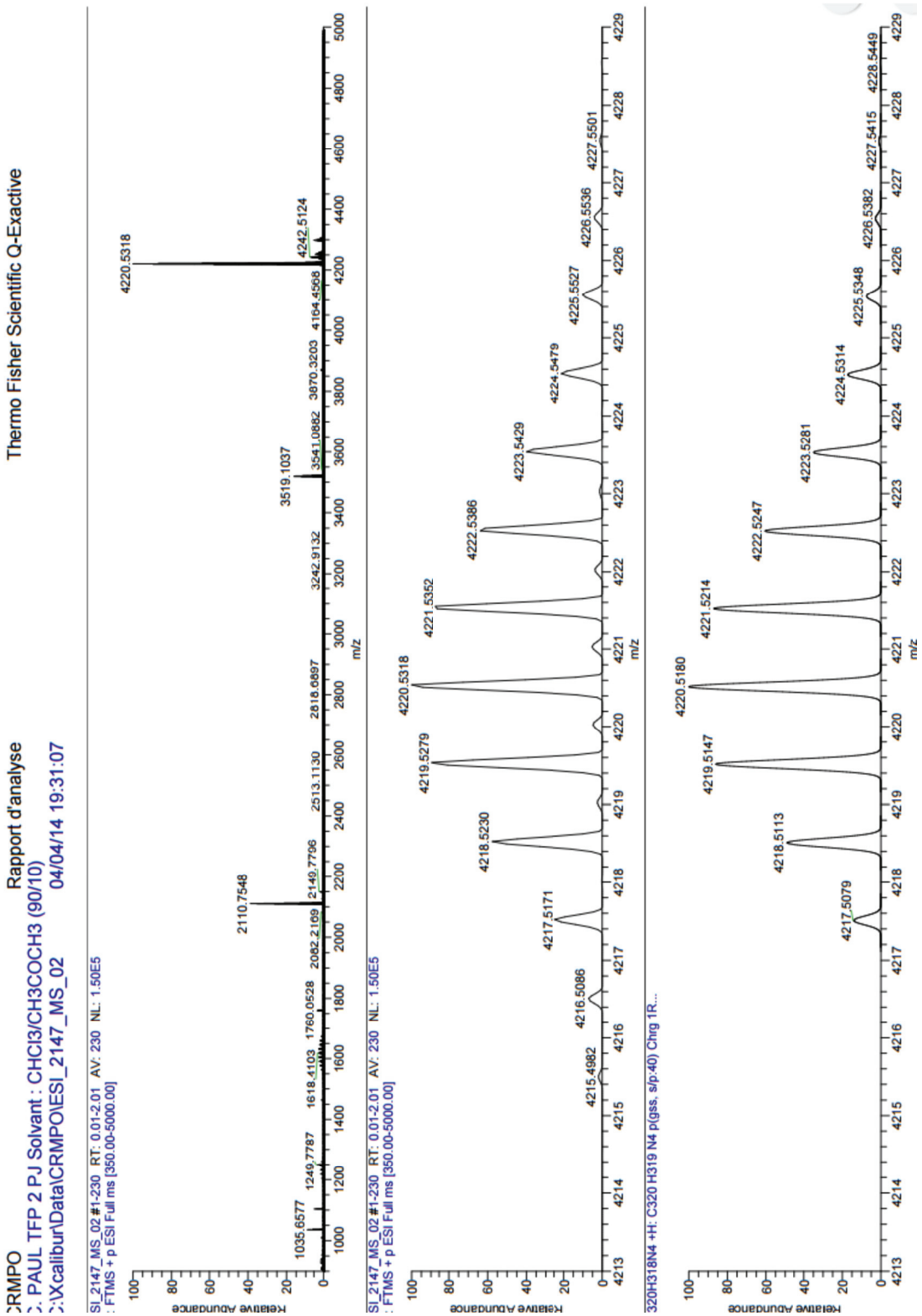
CRMPO
Rapport d'analyse
Thermo Fisher Scientific Q-Exactive
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Relative Abundance
m/z
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4242.5124
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4221.5352
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4216.5086
4224.5479
4215.4982
4225.5527
4226.5536
4227.5501
320H318N4 +H: C320 H319 N4 p(gss, s/p:40) Chrg 1R...
4220.5180
4221.5214
4219.5147
4222.5247
4218.5113
4223.5281
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4224.5314
4225.5348
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Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

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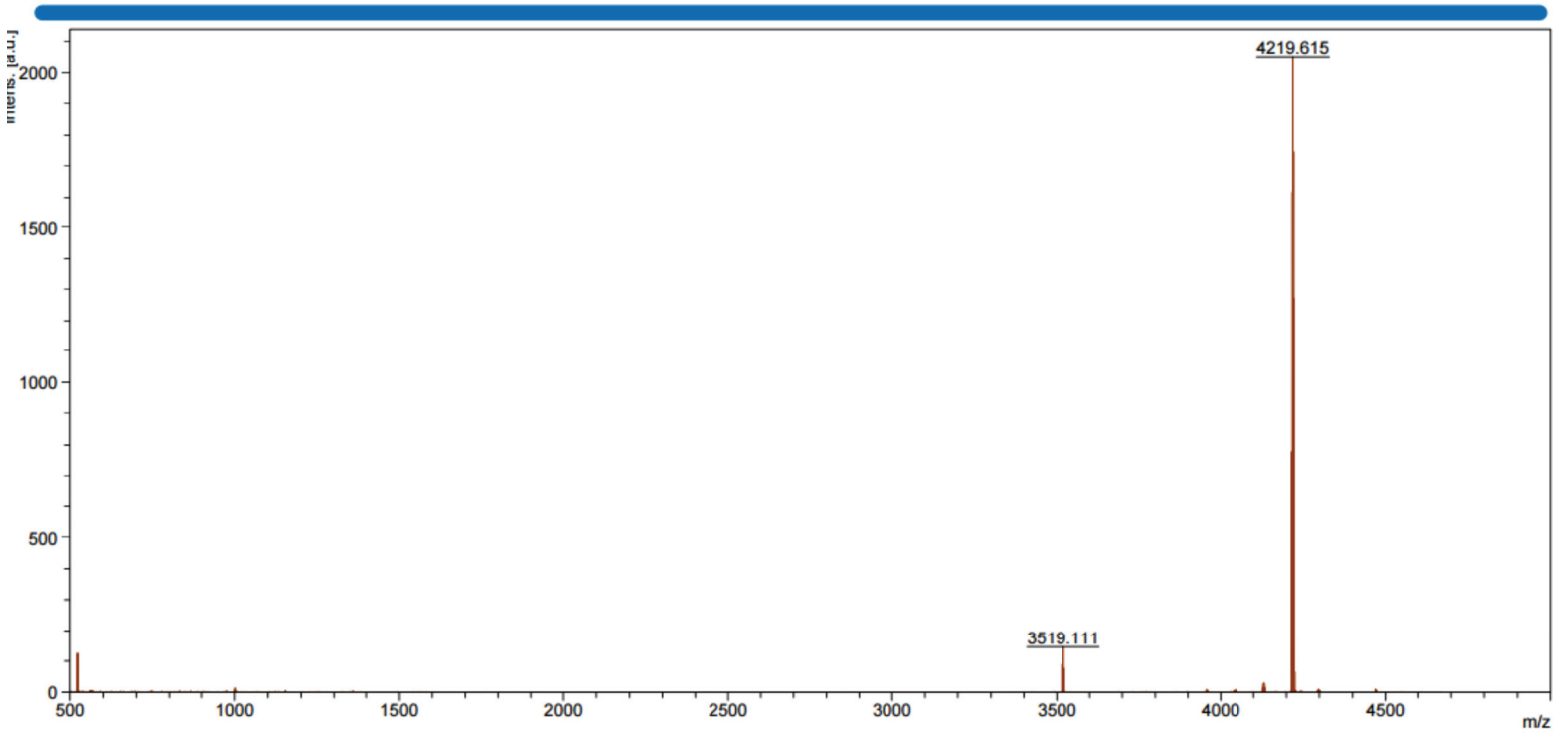

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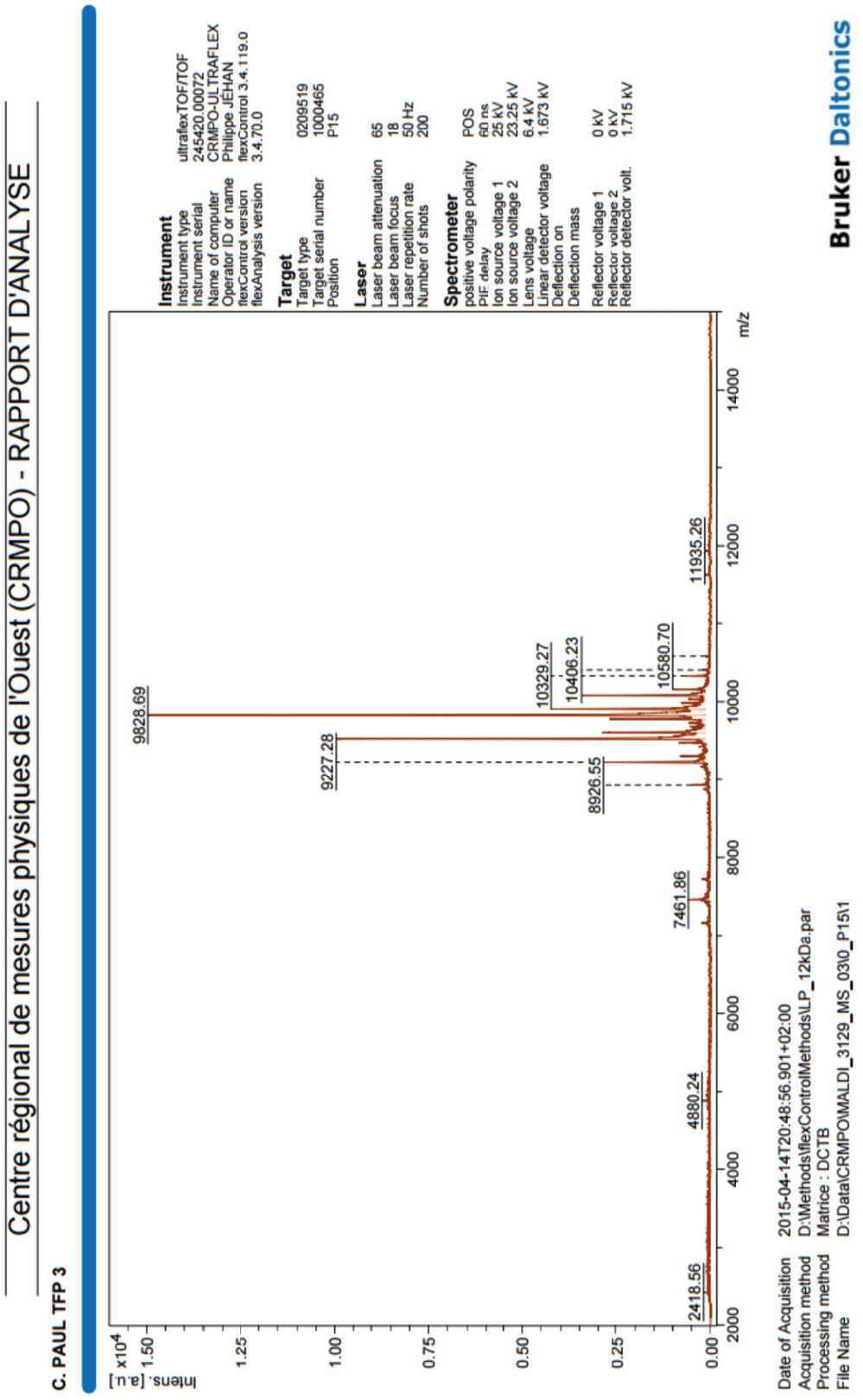
Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE
C. PAUL TFP 3
Instrument
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Instrument serial 245420.00072
Name of computer CRMPO-ULTRAFLEX
Operator ID or name Philippe JEHAN
flexControl version flexControl 3.4.119.0
flexAnalysis version 3.4.70.0
Target
Target type 0209519
Target serial number 1000465
Position P15
Laser
Laser beam attenuation 65
Laser beam focus 18
Laser repetition rate 50 Hz
Number of shots 200
Spectrometer
positive voltage polarity POS
PIF delay 60 ns
Ion source voltage 1 25 kV
Ion source voltage 2 23.25 kV
Lens voltage 6.4 kV
Linear detector voltage 1.673 kV
Deflection on
Deflection mass
Reflector voltage 1 0 kV
Reflector voltage 2 0 kV
Reflector detector volt. 1.715 kV
Intens. [a.u.]
x10^4
1.50
1.25
1.00
0.75
0.50
0.25
0.00
2000
4000
6000
8000
10000
12000
14000
m/z
2418.56
4880.24
7461.86
8926.55
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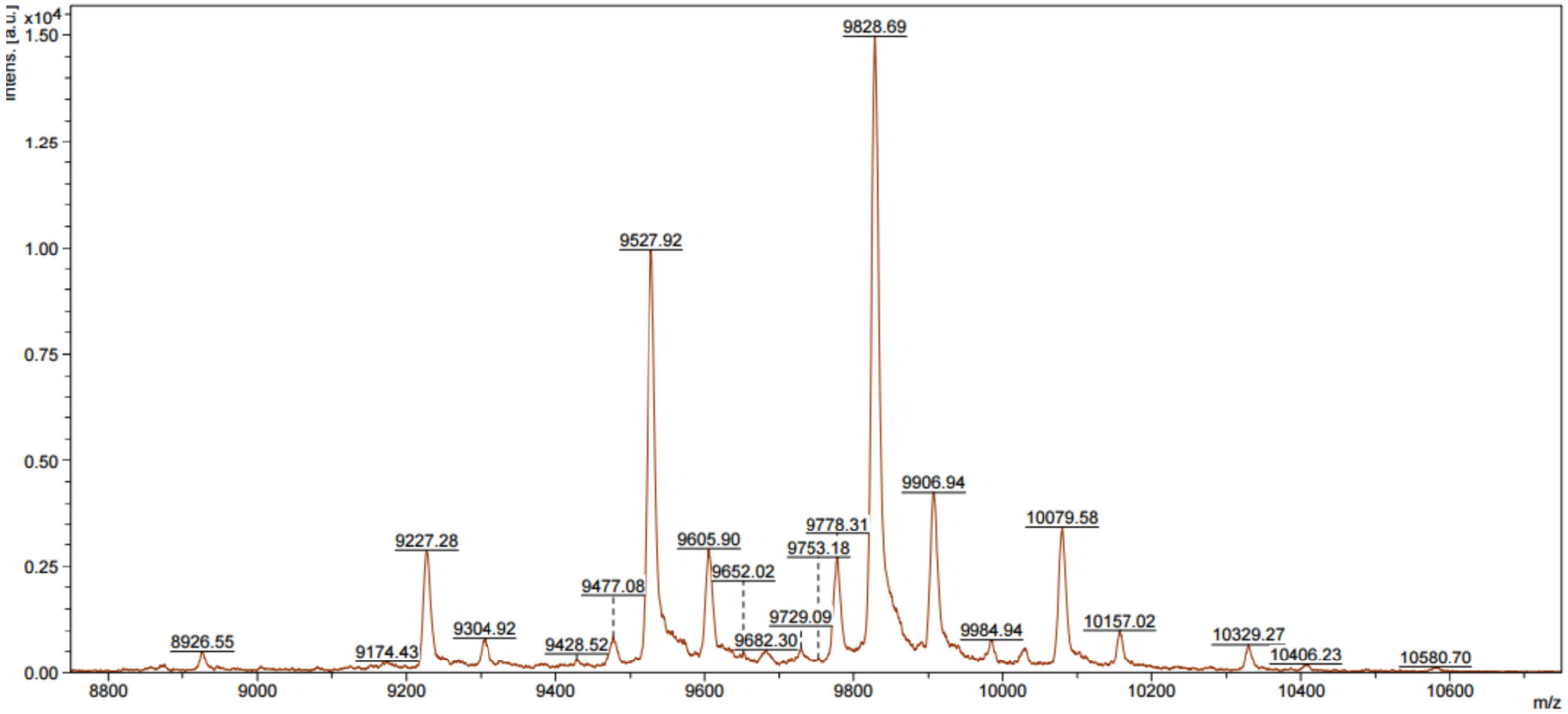
Bruker Daltonics

Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

C. PAUL TFP 3



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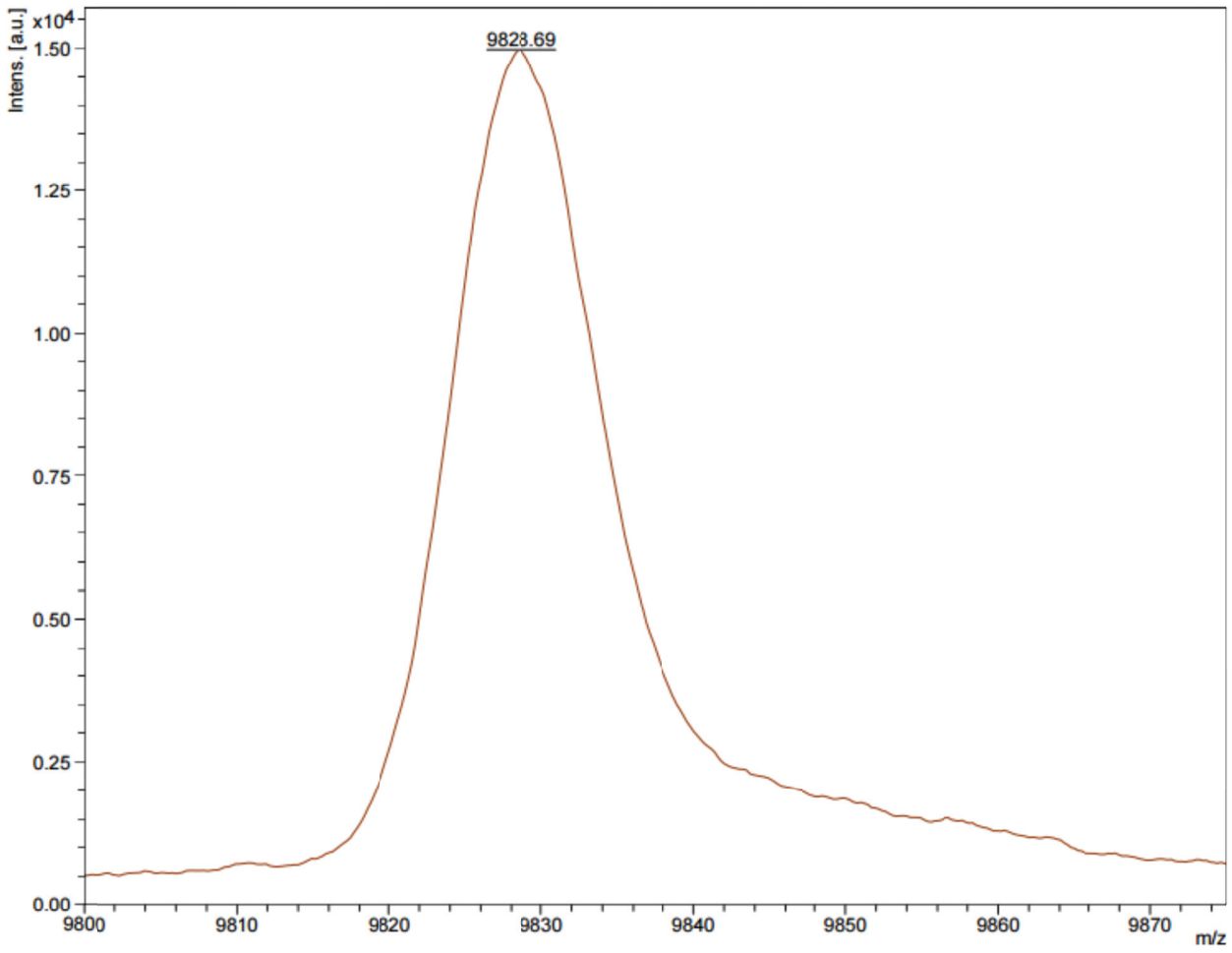
Bruker Daltonics

Centre régional de mesures physiques de l'Ouest (CRMPO)
RAPPORT D'ANALYSE

C. PAUL TFP 3



Acquisition Parameter

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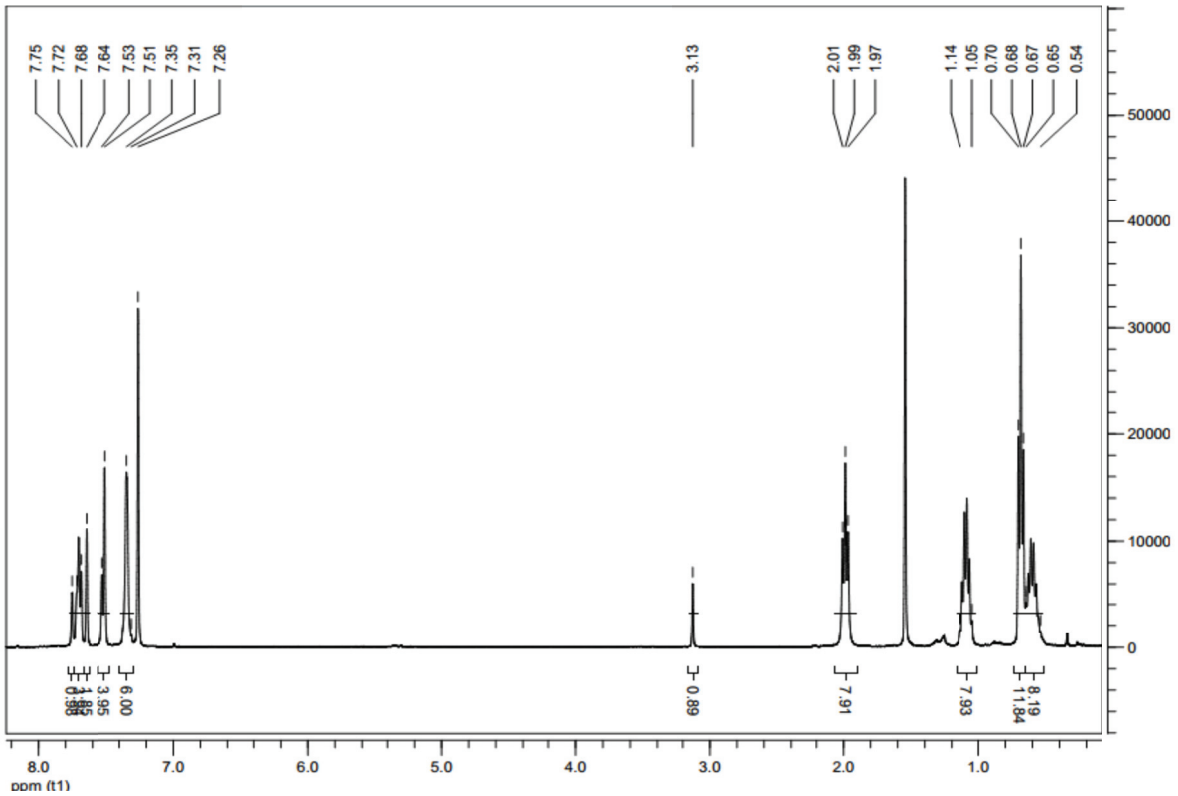
Aquisition operation mode	Linear
Voltage polarity	POS

4. ^{1}H NMR Spectra of Intermediate Compounds 3, 5, 6, 7, 8 and 9.

Compound 3:



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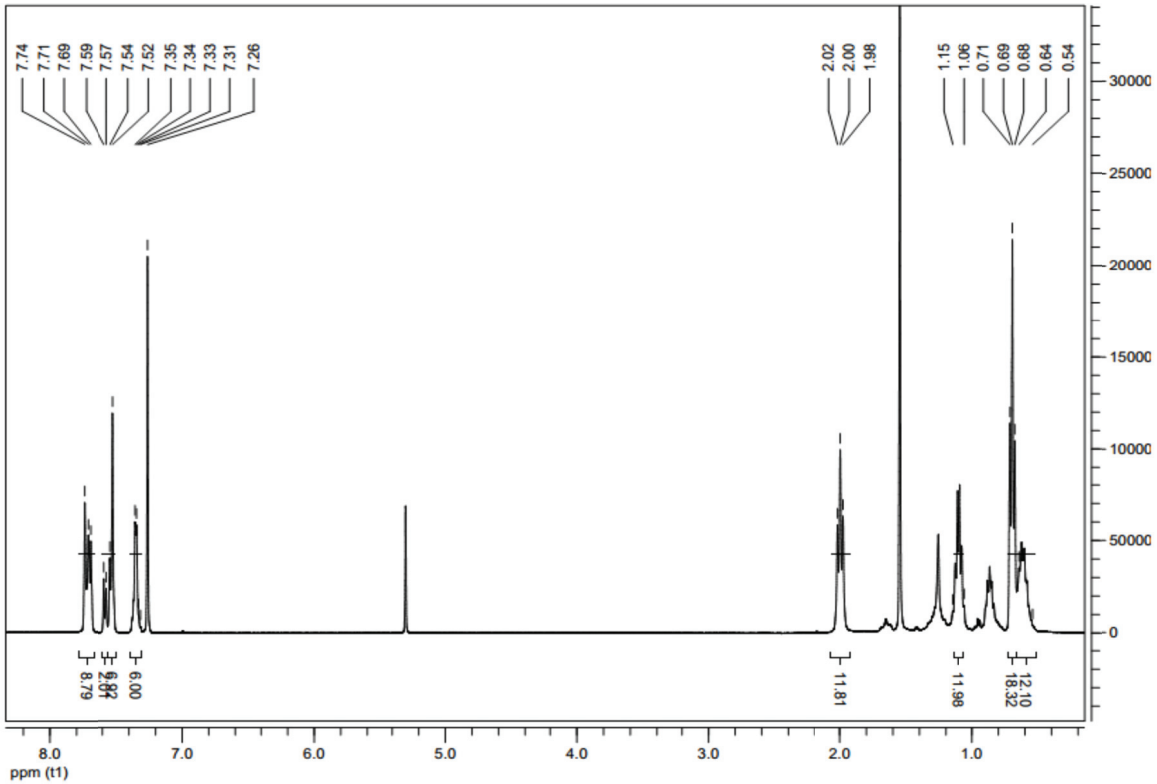
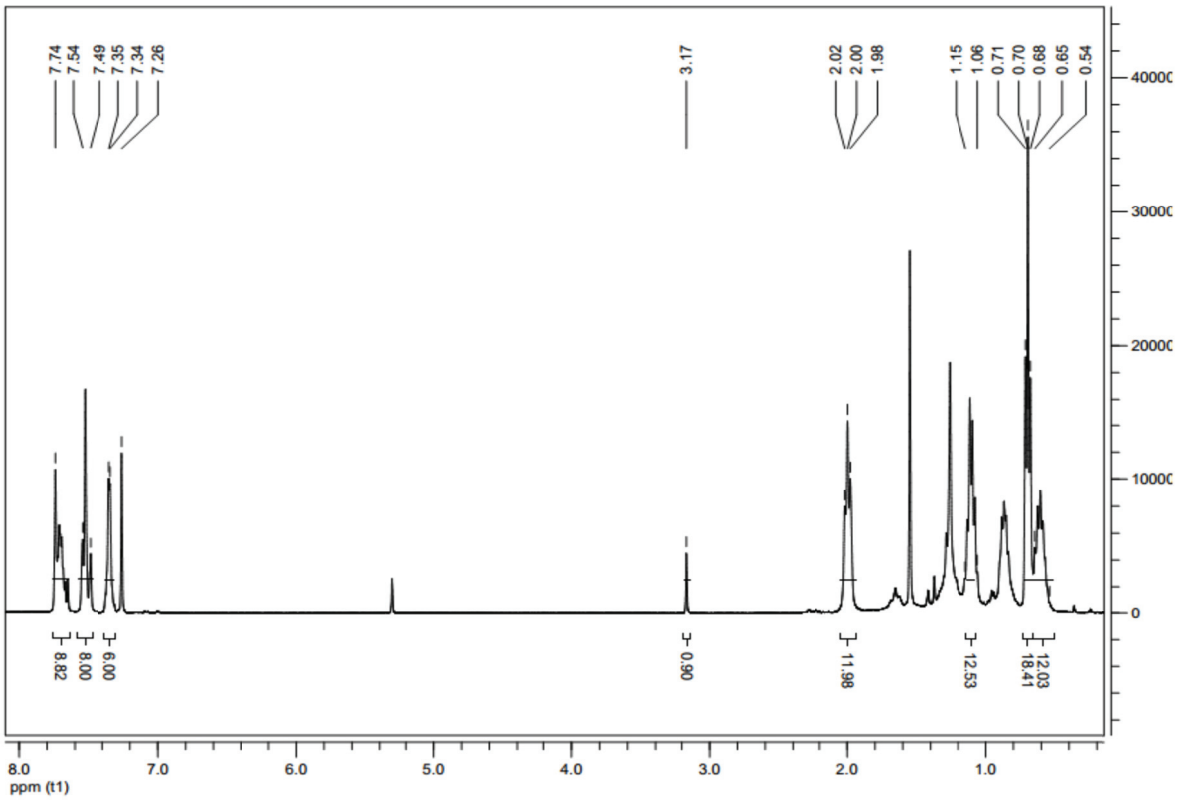
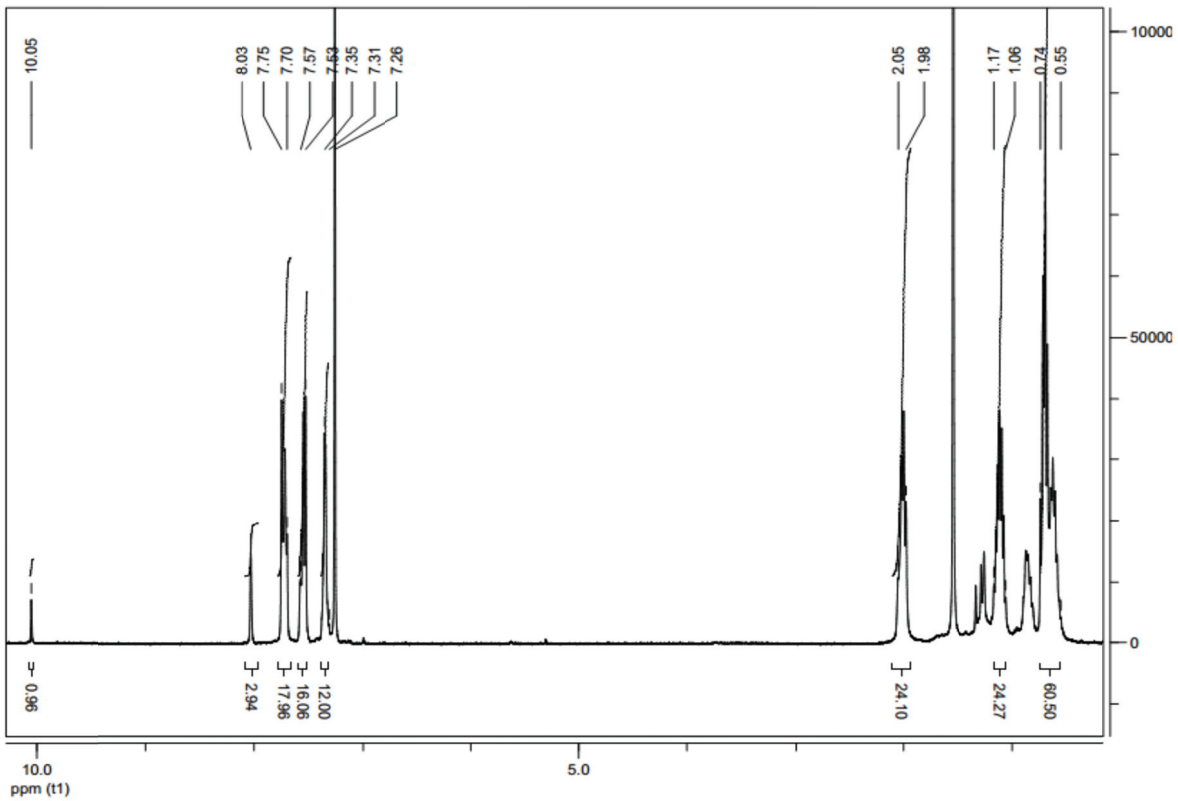


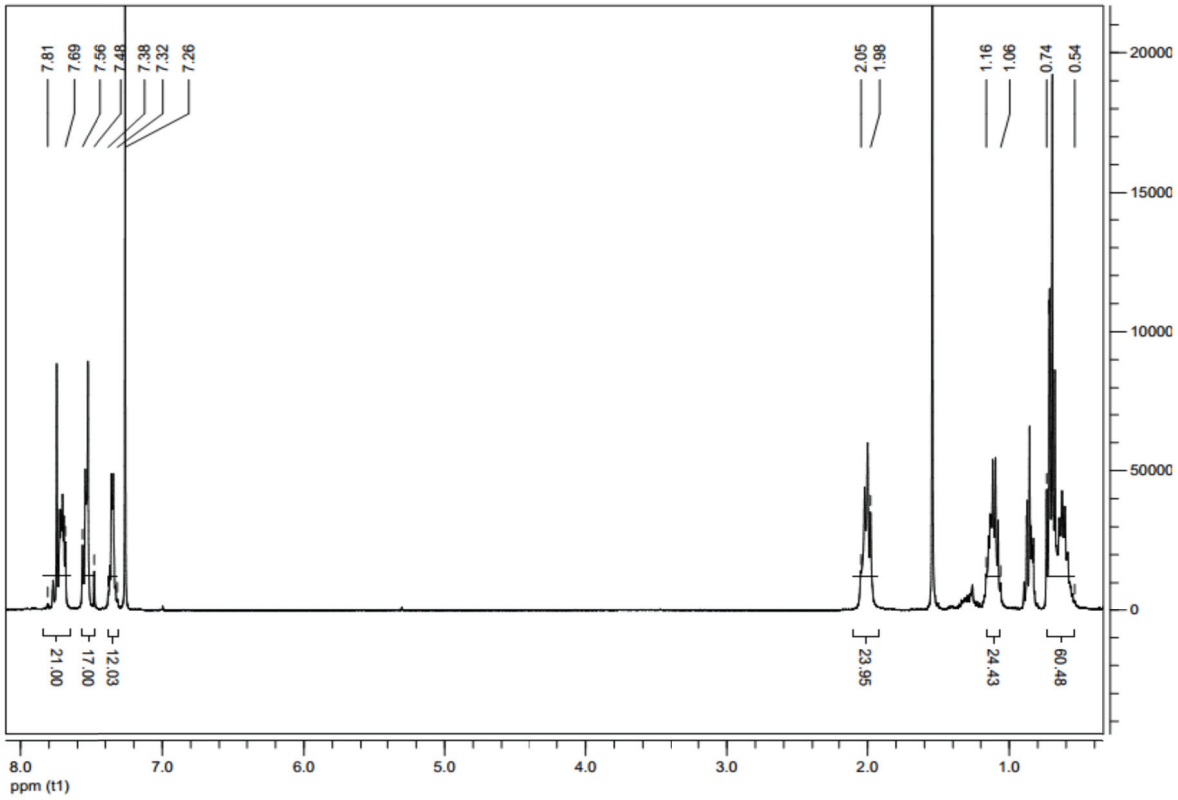
Compound 6:


7.74
7.54
7.49
7.35
7.34
7.26
3.17
2.02
2.00
1.98
1.15
1.06
0.71
0.70
0.68
0.65
0.54
8.82
8.00
9.00
0.90
11.98
12.53
18.41
12.03
ppm (t1)

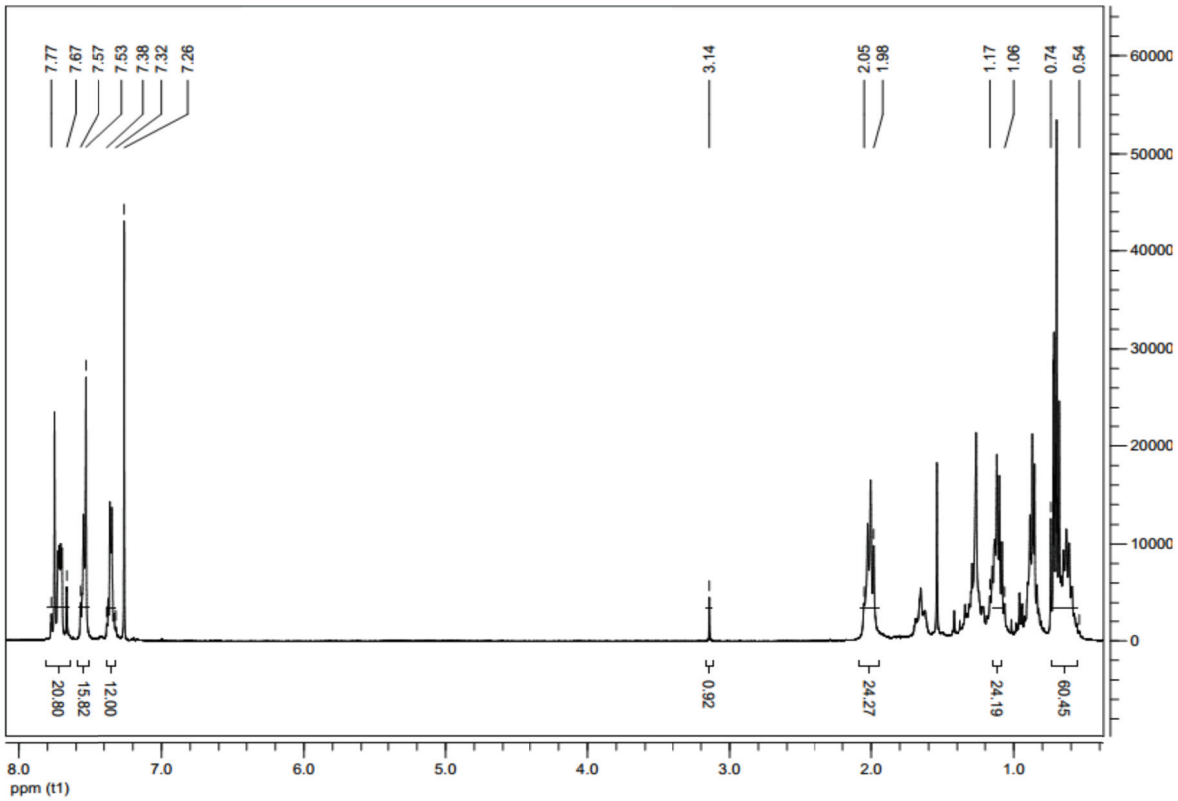
7:


10.05
8.03
7.75
7.70
7.57
7.53
7.35
7.31
7.26
2.05
1.98
1.17
1.06
0.74
0.55
0.96
2.94
17.96
16.06
12.00
24.10
24.27
60.50
ppm (t1)

8:


7.81
7.69
7.56
7.48
7.38
7.32
7.26
2.05
1.98
1.16
1.06
0.74
0.54
21.00
17.00
12.03
23.95
24.43
60.48
20000
15000
10000
50000
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)

9:


7.77
7.67
7.57
7.53
7.38
7.32
7.26
3.14
2.05
1.98
1.17
1.06
0.74
0.54
20.80
15.82
12.00
0.92
24.27
24.19
60.45
60000
50000
40000
30000
20000
10000
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)

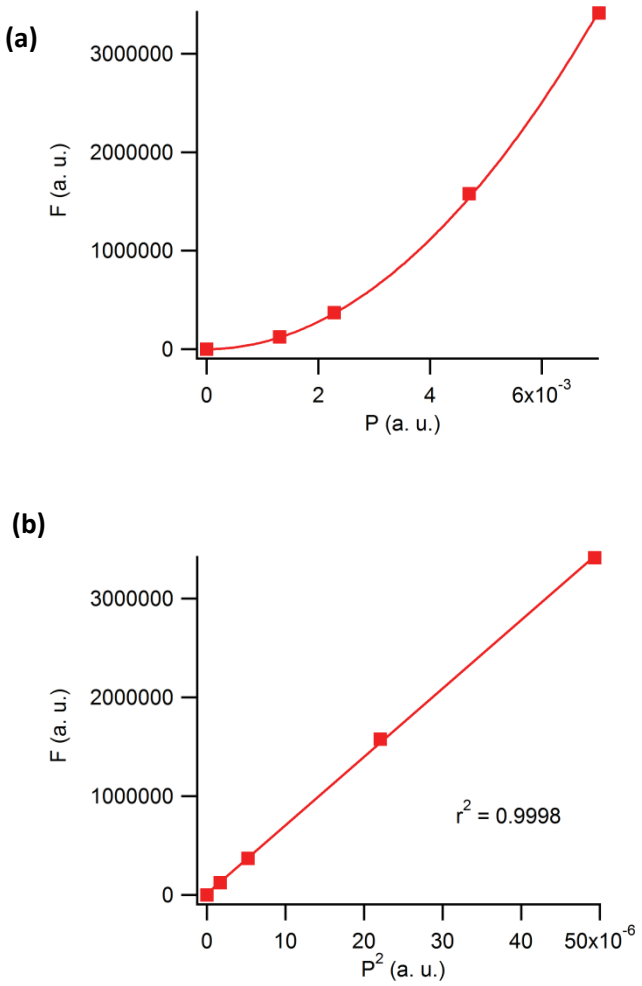


Figure S1. (a) Top: Quadratic Dependence of the Emission Intensity (F) on the Laser Excitation Power (P) for Compound **TFP1** at 790 nm. (b) Bottom: Dependence of F on P^2.