

Coordination and structural studies of crowned-porphyrins

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Bernard Boitrel**

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Page S26: ^1H NMR (500 MHz) ^{13}C - ^1H HMQC-2D map of **3** (298 K, CDCl_3).

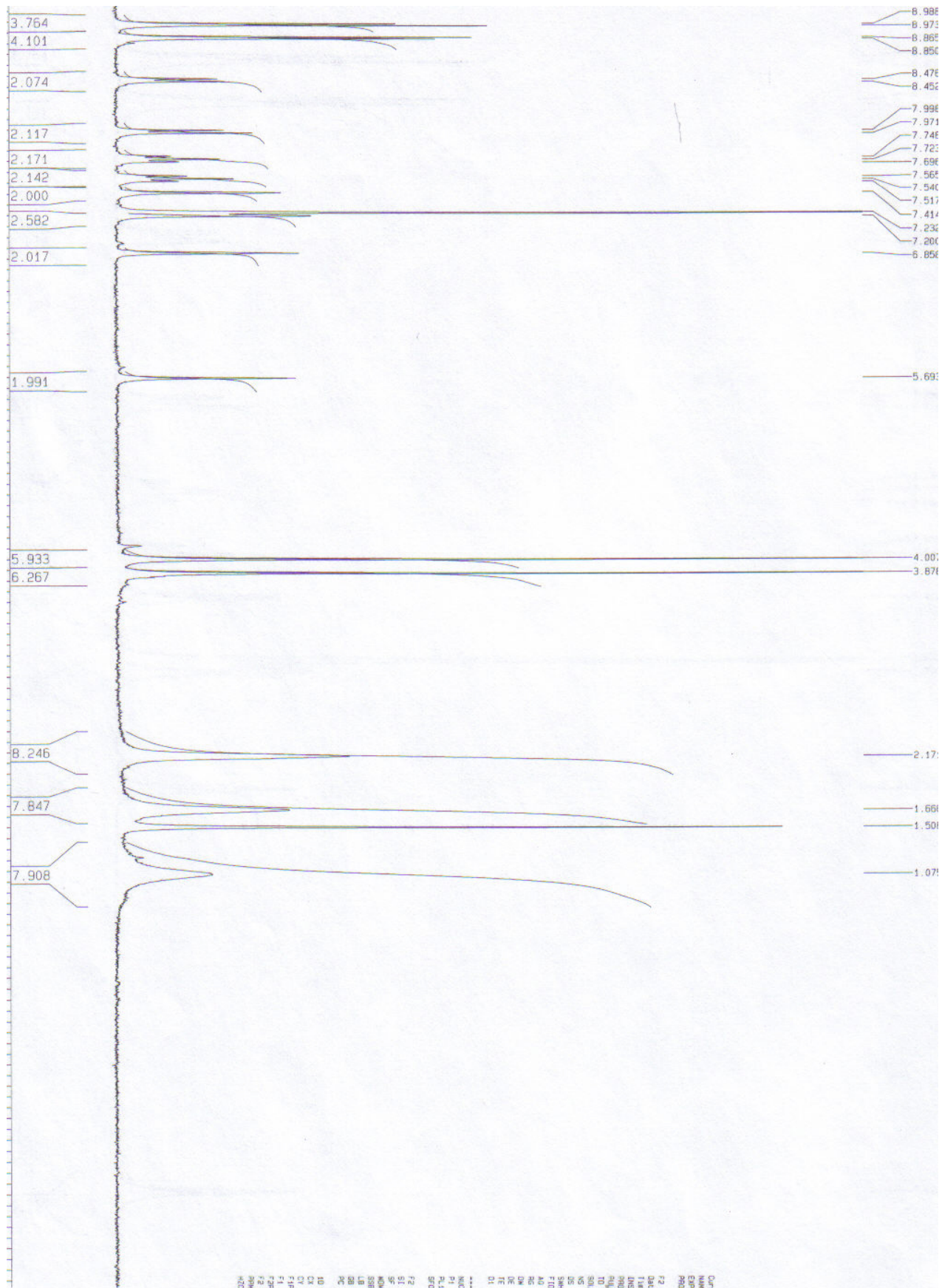
Page S27: ^1H NMR (500 MHz) ^{13}C - ^1H HMBC-2D map of **3** (298 K, CDCl_3).

Page S28: ^1H NMR (500 MHz) ^{13}C - ^1H HMBC-2D map (aromatic domain) of **3** (298 K, CDCl_3).

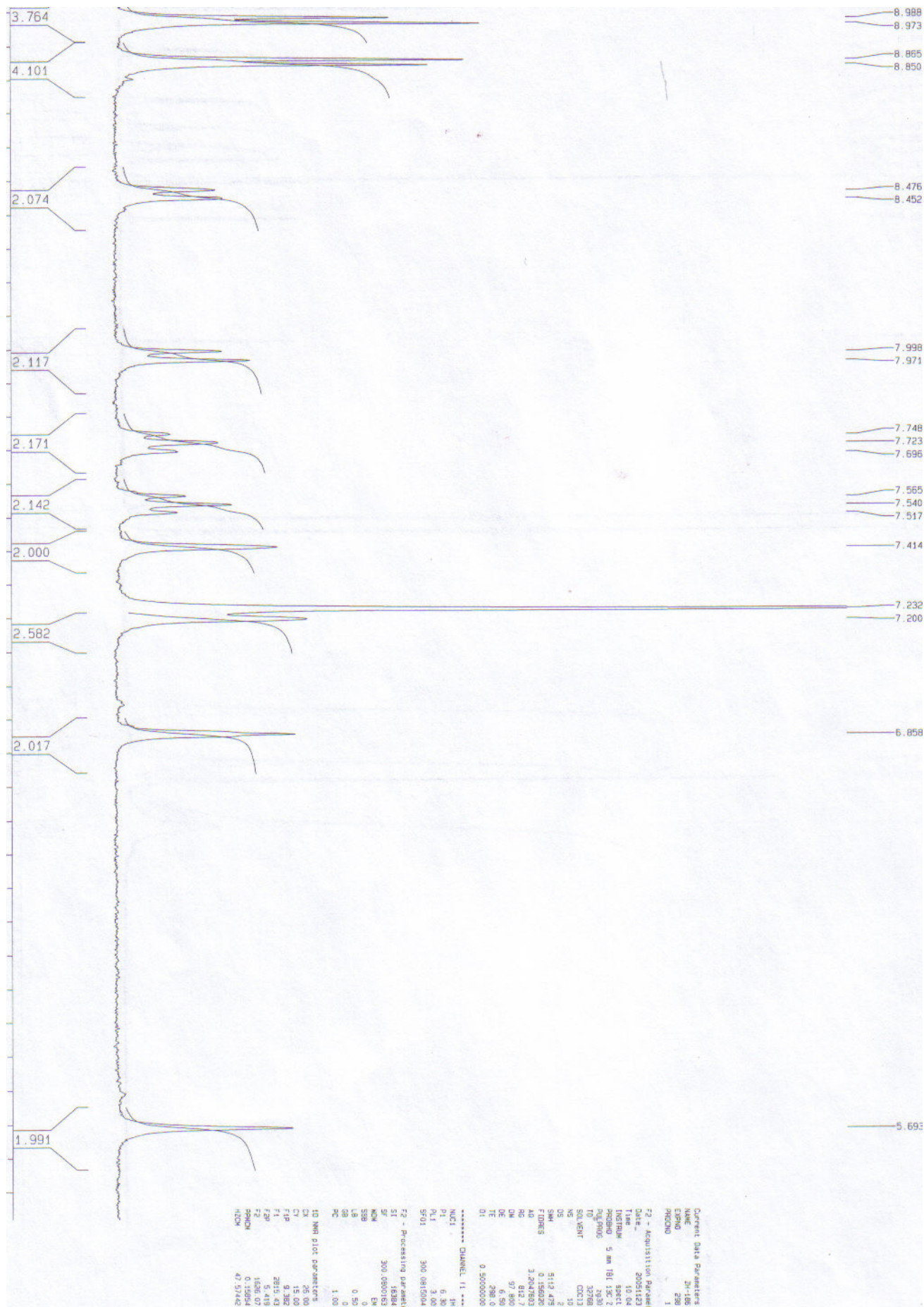
Page S29: Low resolution mass spectrum of **3**.

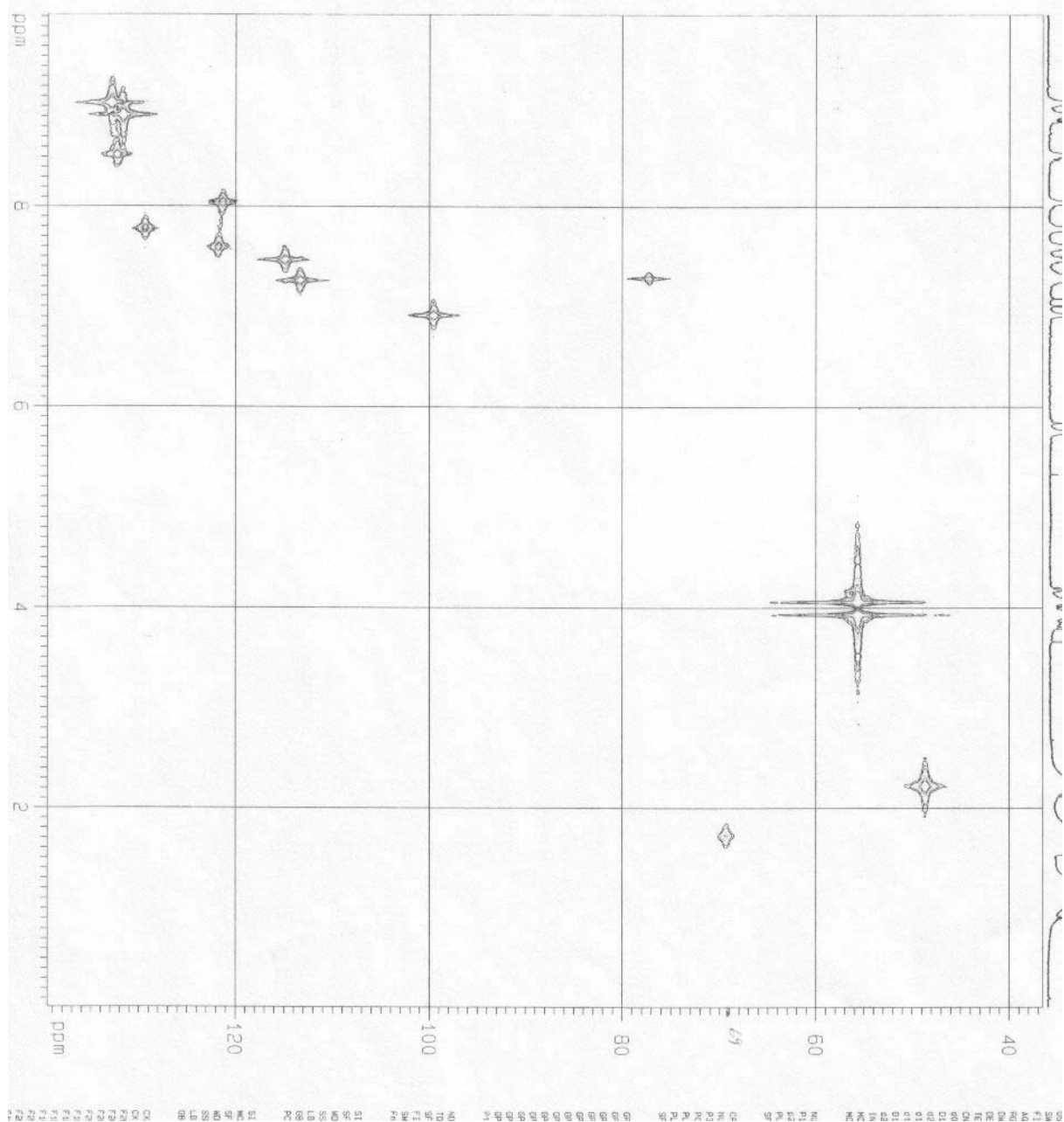
Page S30: Low resolution mass spectrum (zoomed view) of **3**.

Page S31: High resolution mass spectrum of **3**.

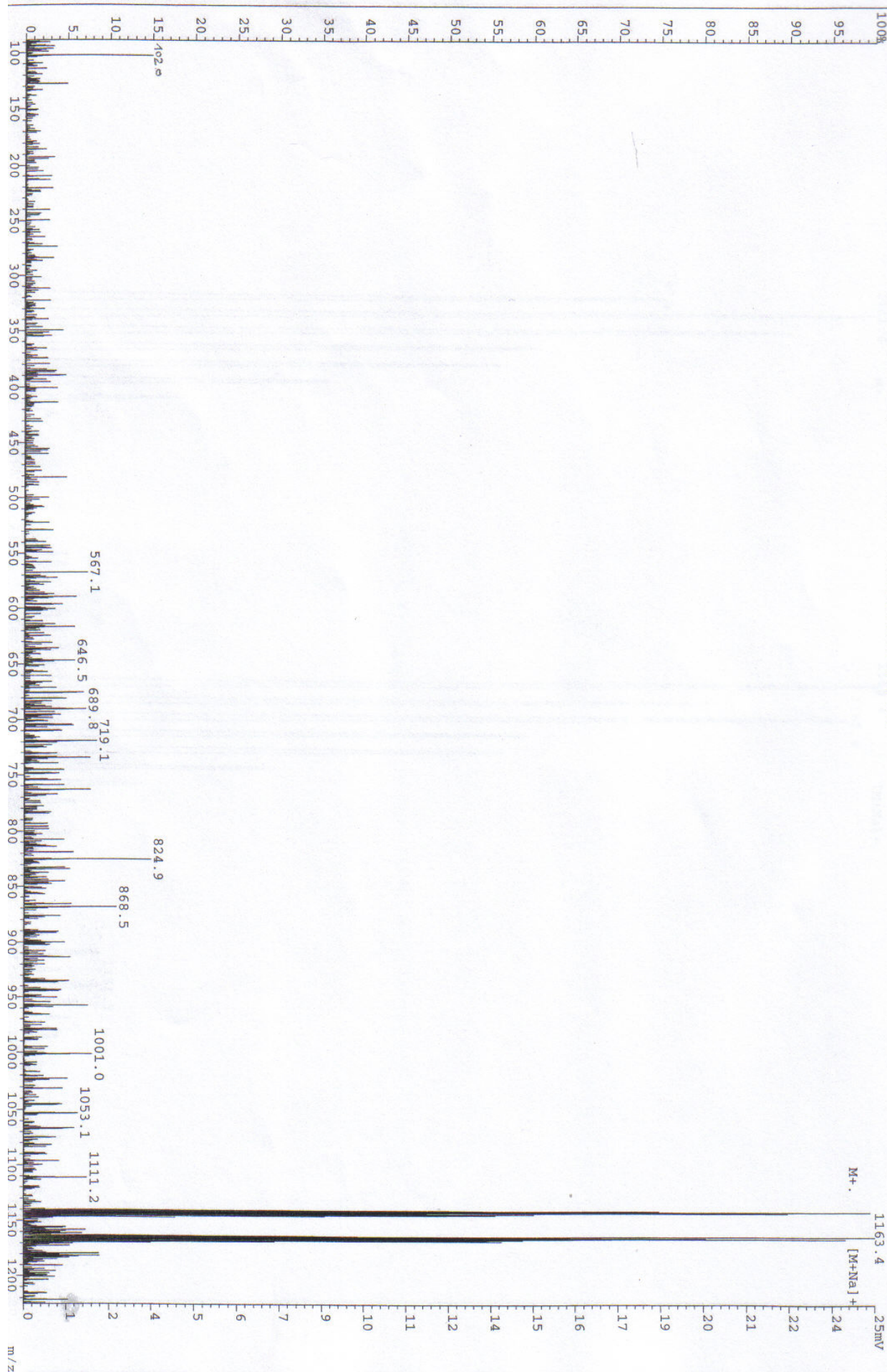


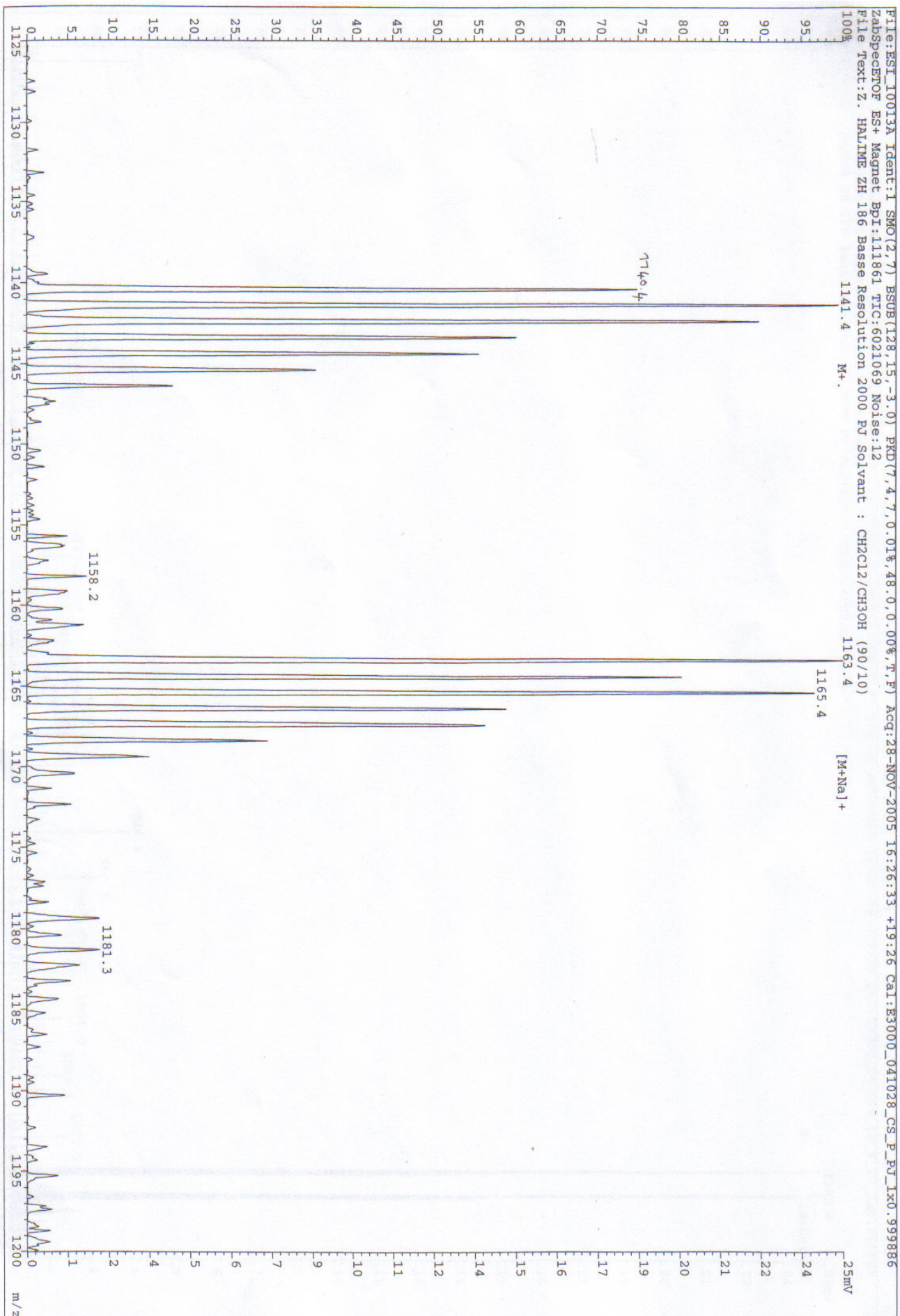
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AQ 3.2047603 sec
RG 812.7
DE 37.700000 sec
TE 300.2 K
D1 0.5000000 sec
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SSB 0
LB 0.50 Hz
GB 0
PC 1.00
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F1 2881.12 Hz
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F2 -883.57 Hz
NUC2 1H
PC2 152.4274 Hz/cm



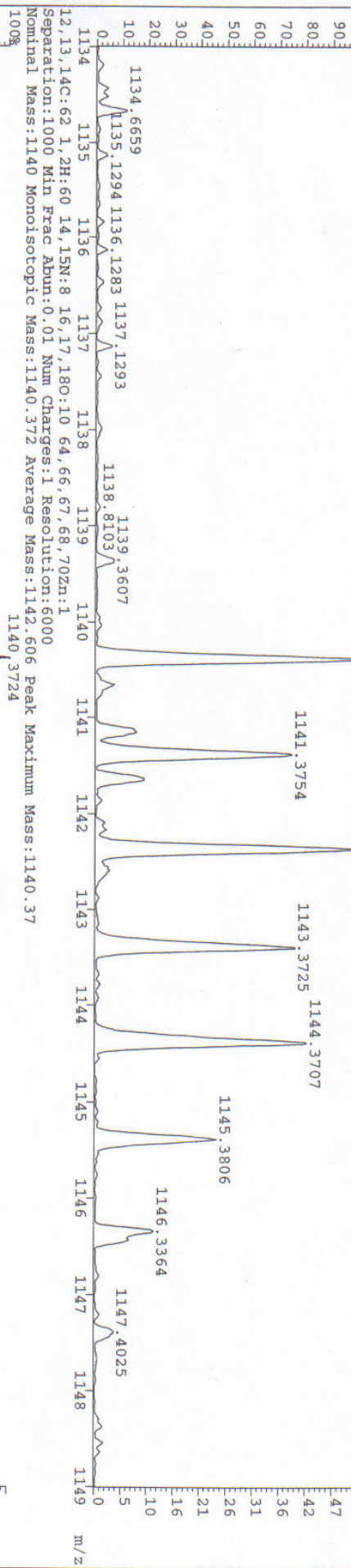
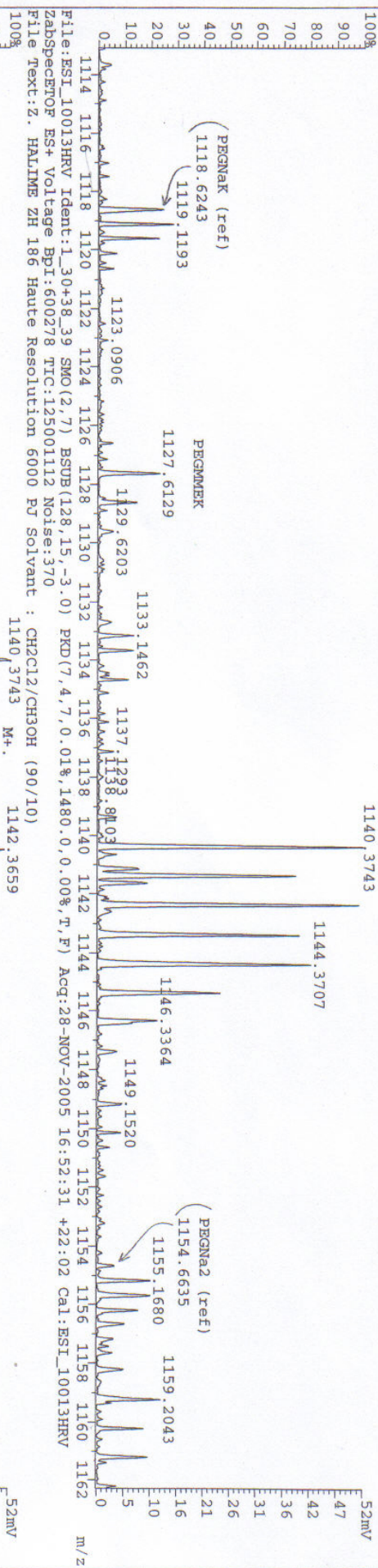


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ZabspecTOP ES+ Magnet BpI:111861 TIC:6021069 Noise:12
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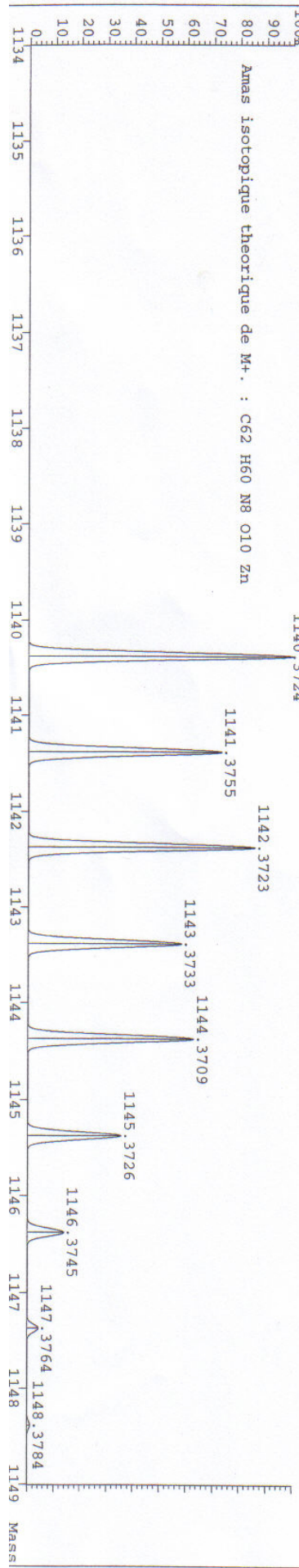


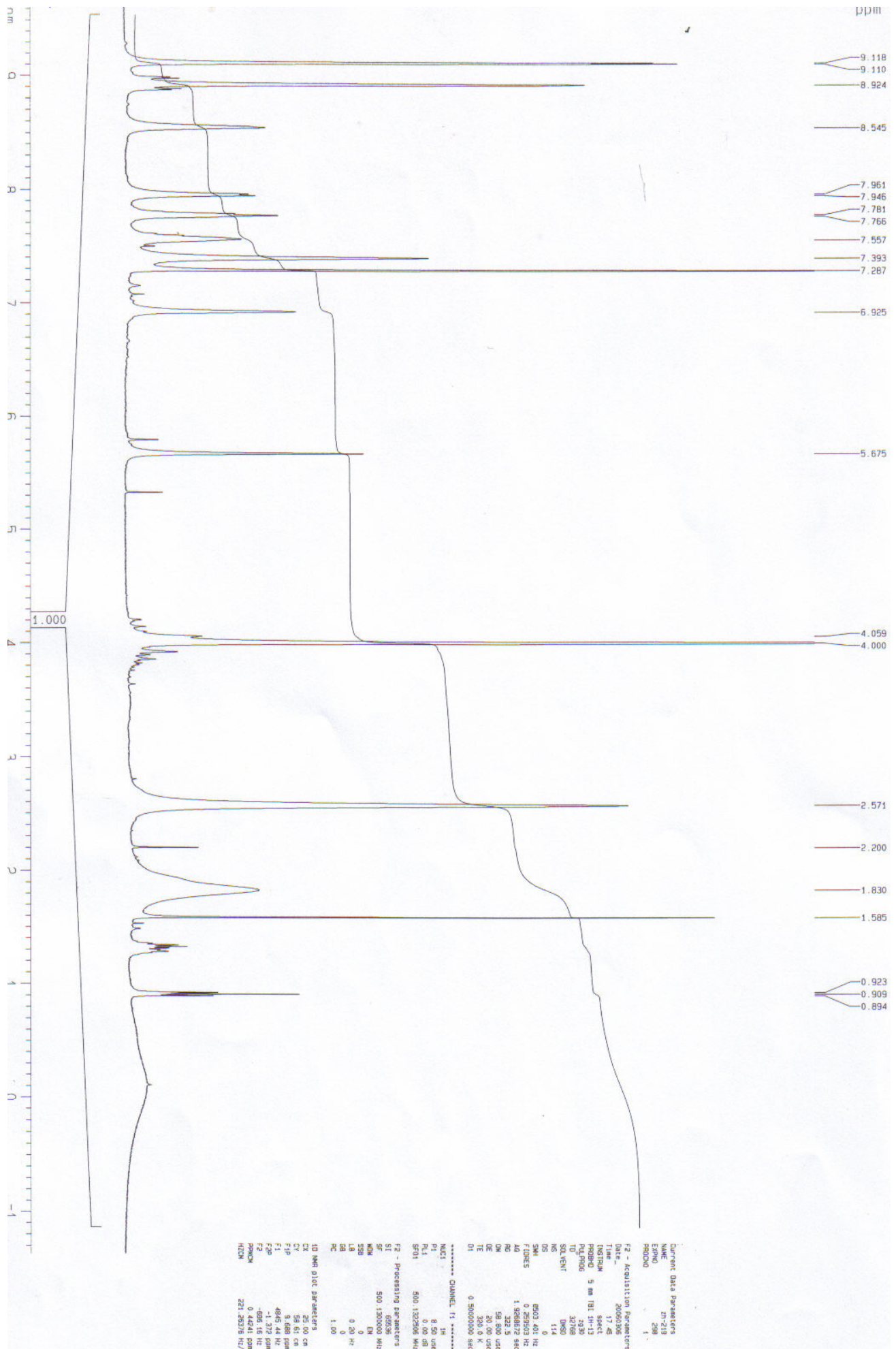


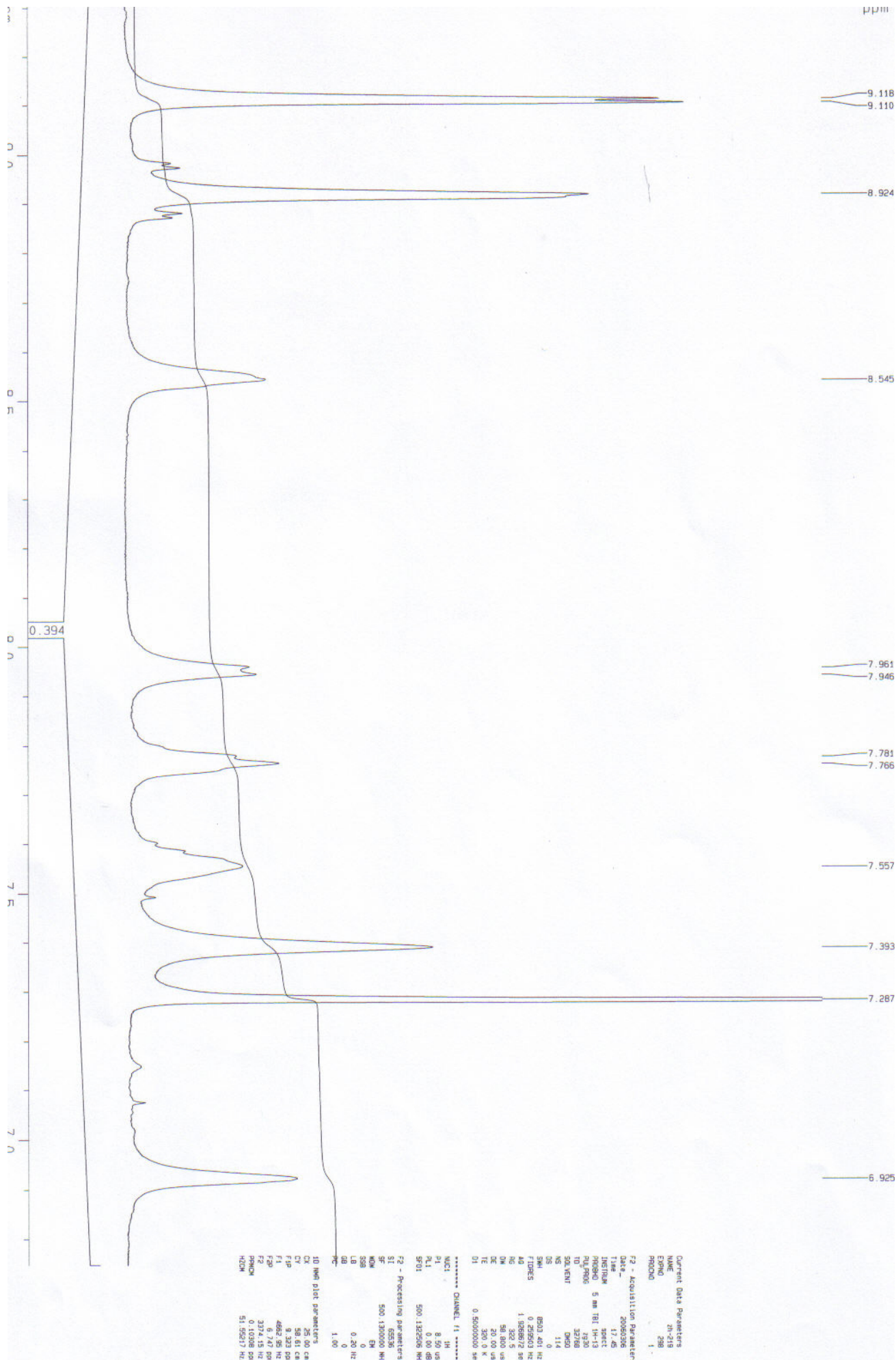
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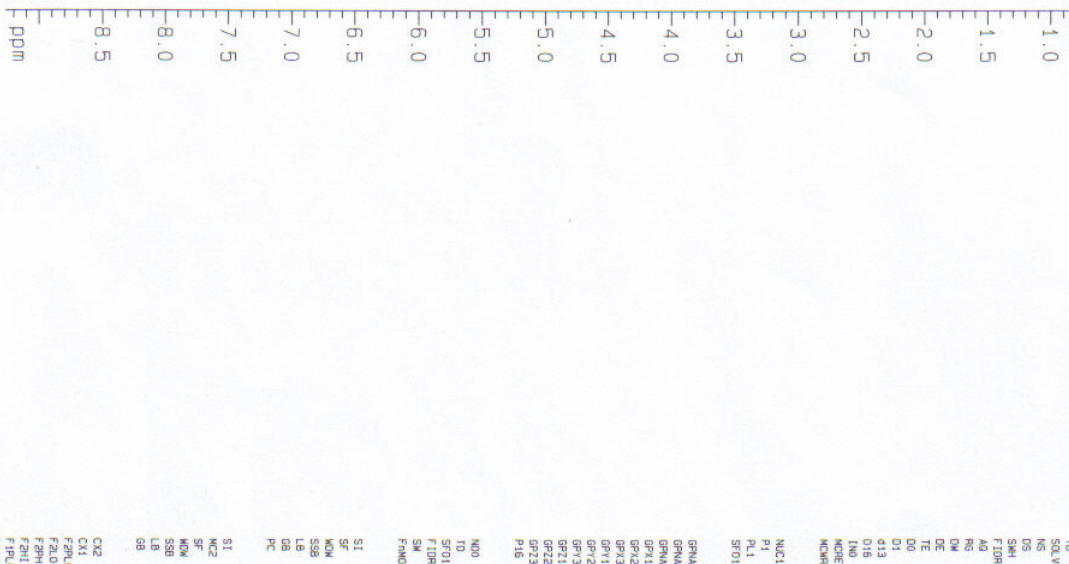
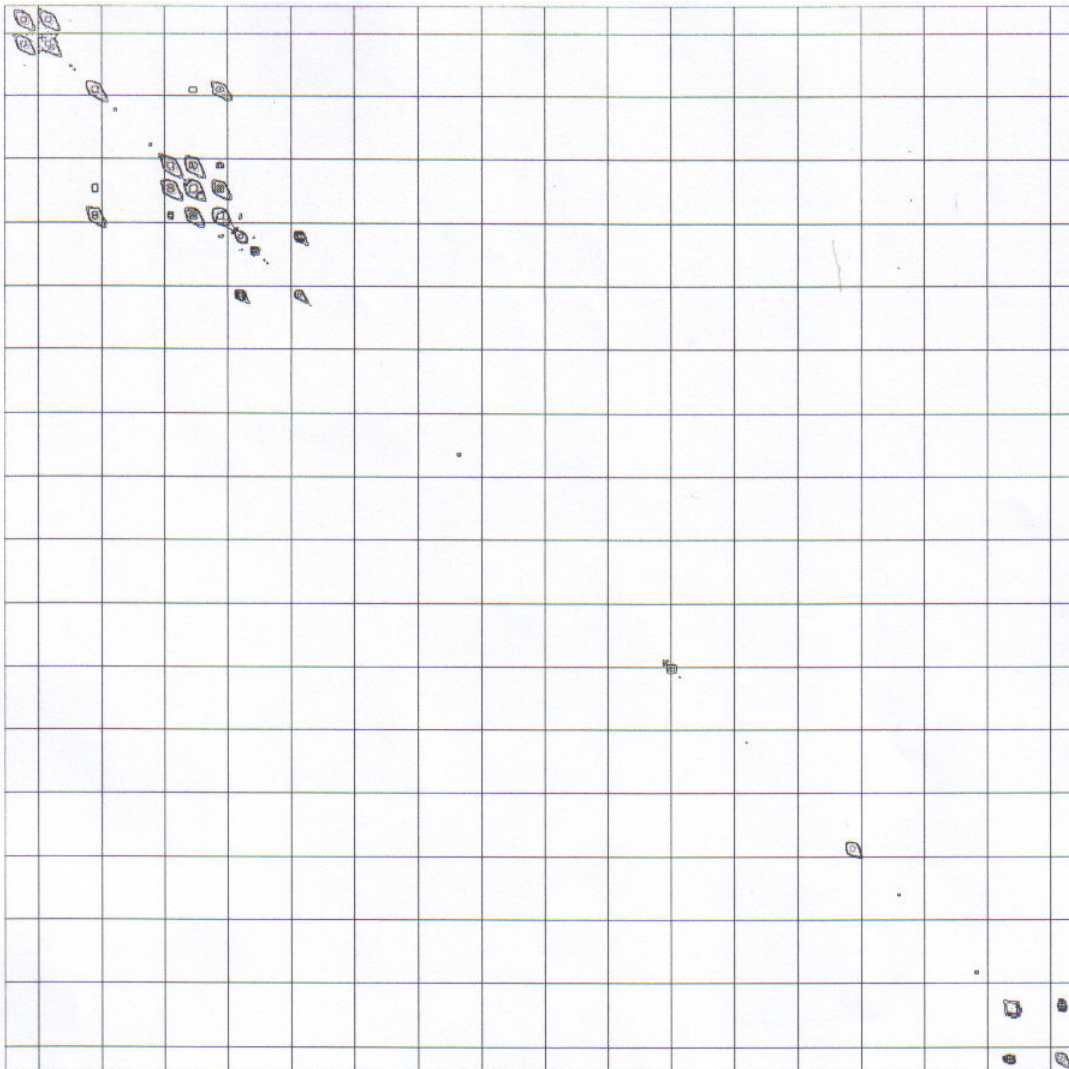


Amas isotopique theorique de M+ : C62 H60 N8 O10 Zn









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EXPNO 10
PROCNO 1

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SOLVENT csg/psd
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DS 16
SWH 5482.456 Hz
FIDRES 2.679560 Hz
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RG 26008
RM 91.200 usec
DE 150.0 usec
TE 300.0 K
D0 0.00000000 sec
D1 1.00000000 sec
d13 0.0000400 sec
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IN0 0.00018240 sec
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NMRK 1.00000000 sec

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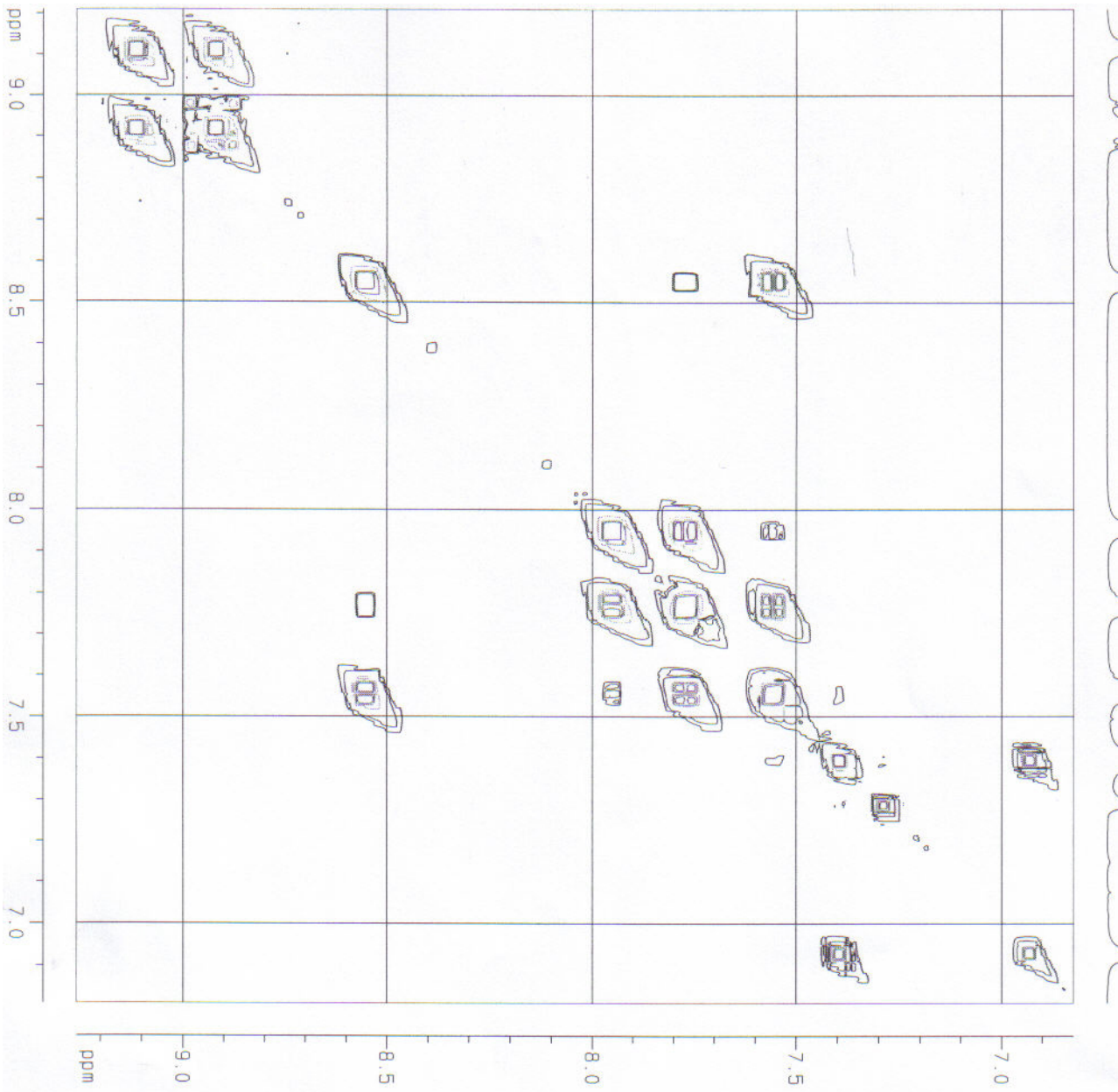
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GPA91 0.00 %
GPA92 0.00 %
GPA93 0.00 %
GPA94 0.00 %
GPA95 0.00 %
GPA96 0.00 %
GPA97 0.00 %
GPA98 0.00 %
GPA99 0.00 %
GPA100 0.00 %

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F2 - Processing Parameters
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SF 500.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing Parameters
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SF 500.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

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CX2 15.00 cm
CY2 15.00 cm
F2B0 9.216 cm
F2B1 0.807 ppm
F2B2 403.47 Hz
F2B3 5.264 ppm
F2B4 4633.10 Hz
F2B5 0.823 ppm
F2B6 411.50 Hz
F2B7 0.56077 ppm/cm
F2B8 280.49531 Hz/cm



```

INSTRUM spect
PROBHD 5 mm TBI HX-13
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SOLVENT CDCl3
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DS 16
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FIDRES 2.676980 Hz
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RG 26008
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DE 6.00 usec
TE 300.0 K
D0 0.00000000 sec
D1 0.00000000 sec
d13 0.00000000 sec
D16 0.00050000 sec
TNO 0.00018240 sec
MCRESIT 0.00000000 sec
MCNEX 1.00000000 sec

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P1 8.50 usec
PL1 0.00 dB
SFO1 500.1322506 MHz

***** GRADIENT CHANNEL *****
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GRANA2 size:100
GRANA3 size:100
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GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
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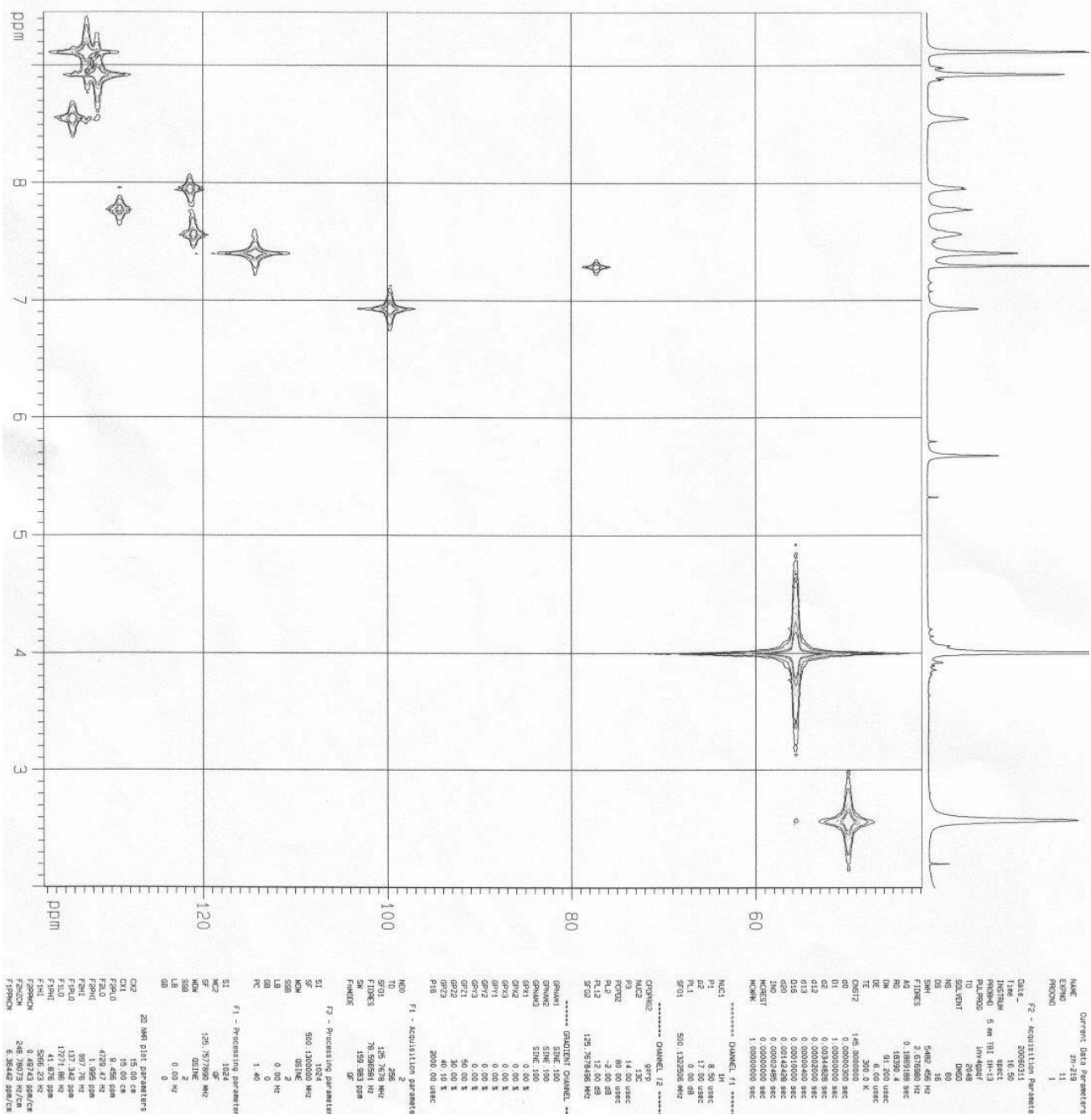
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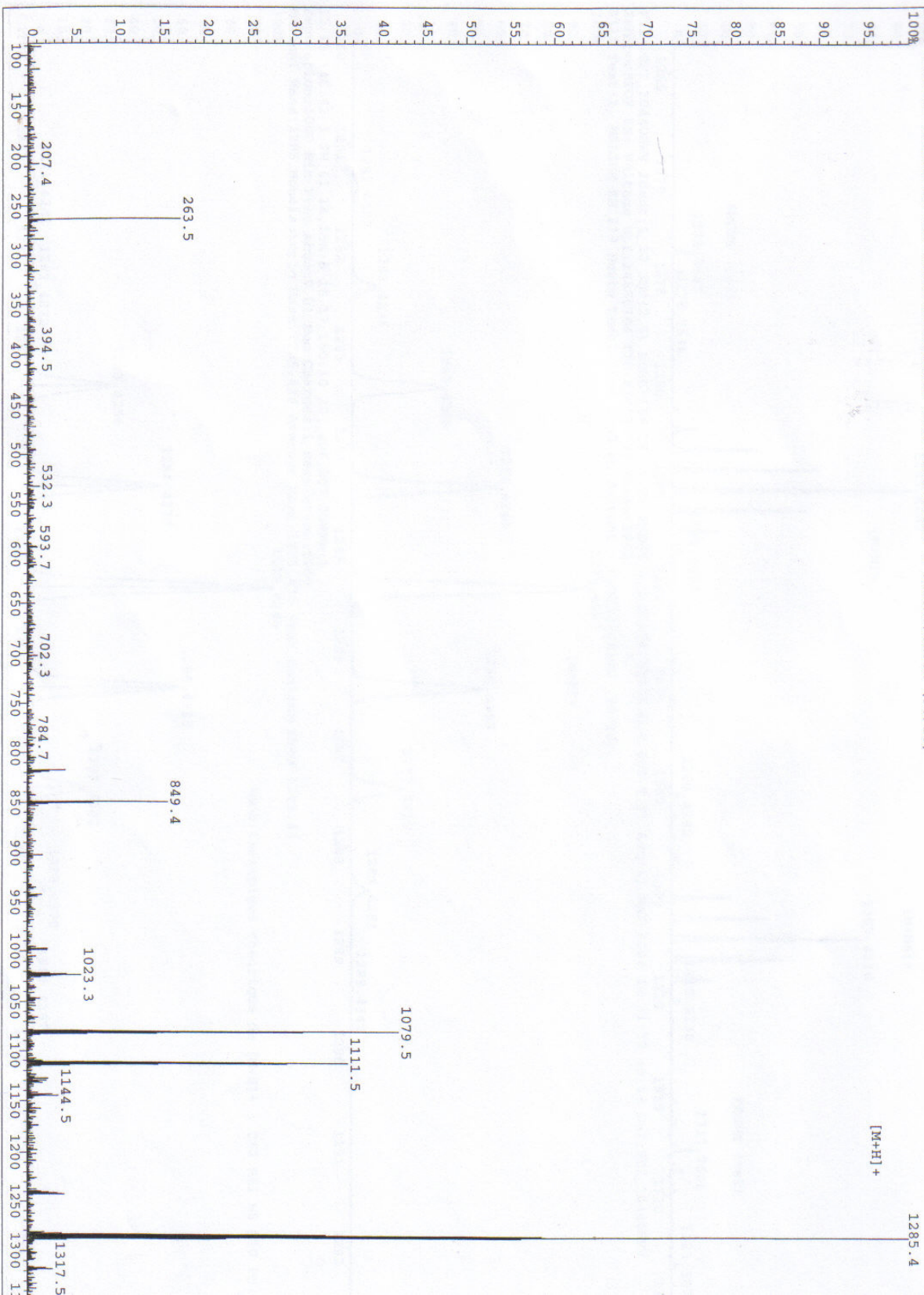
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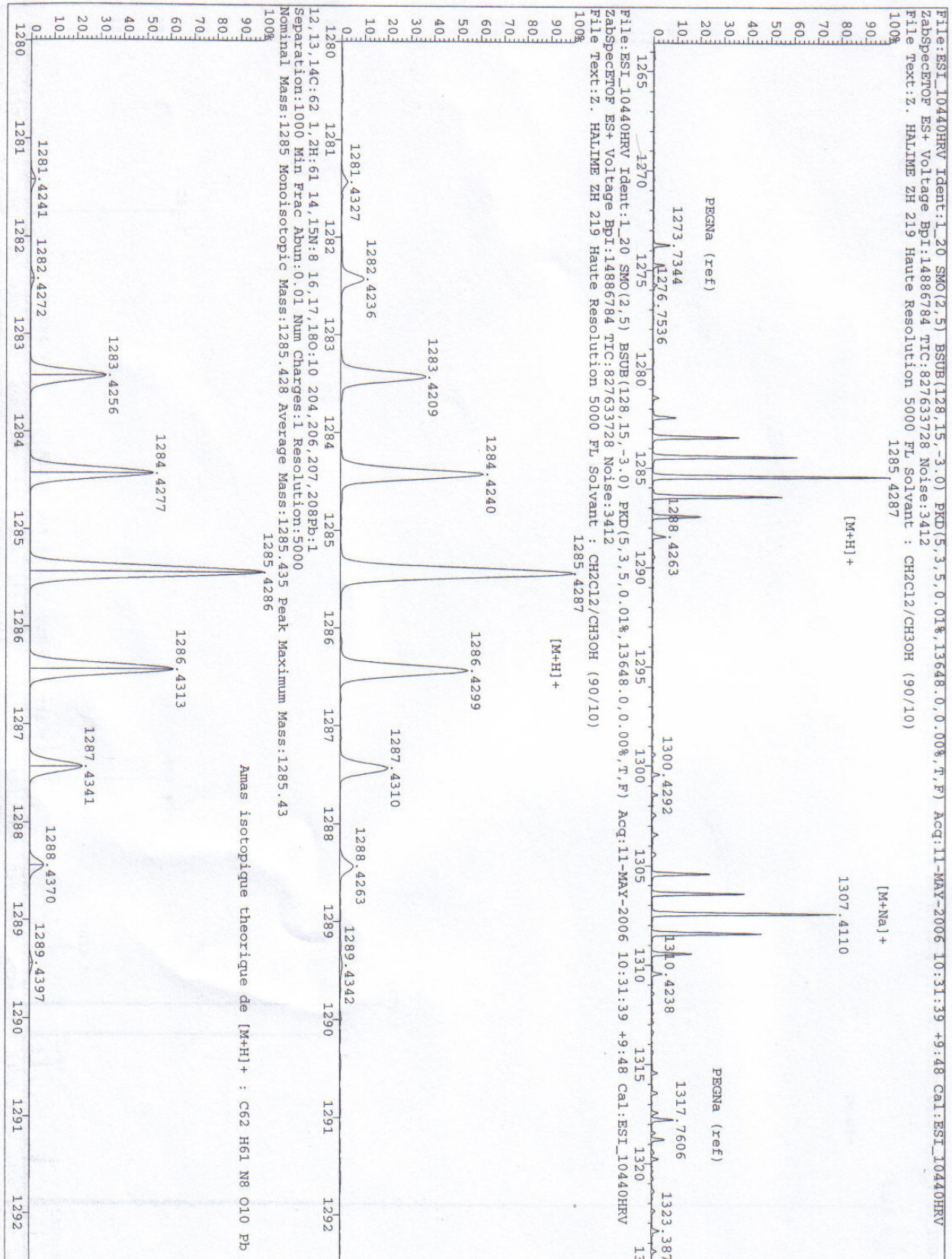
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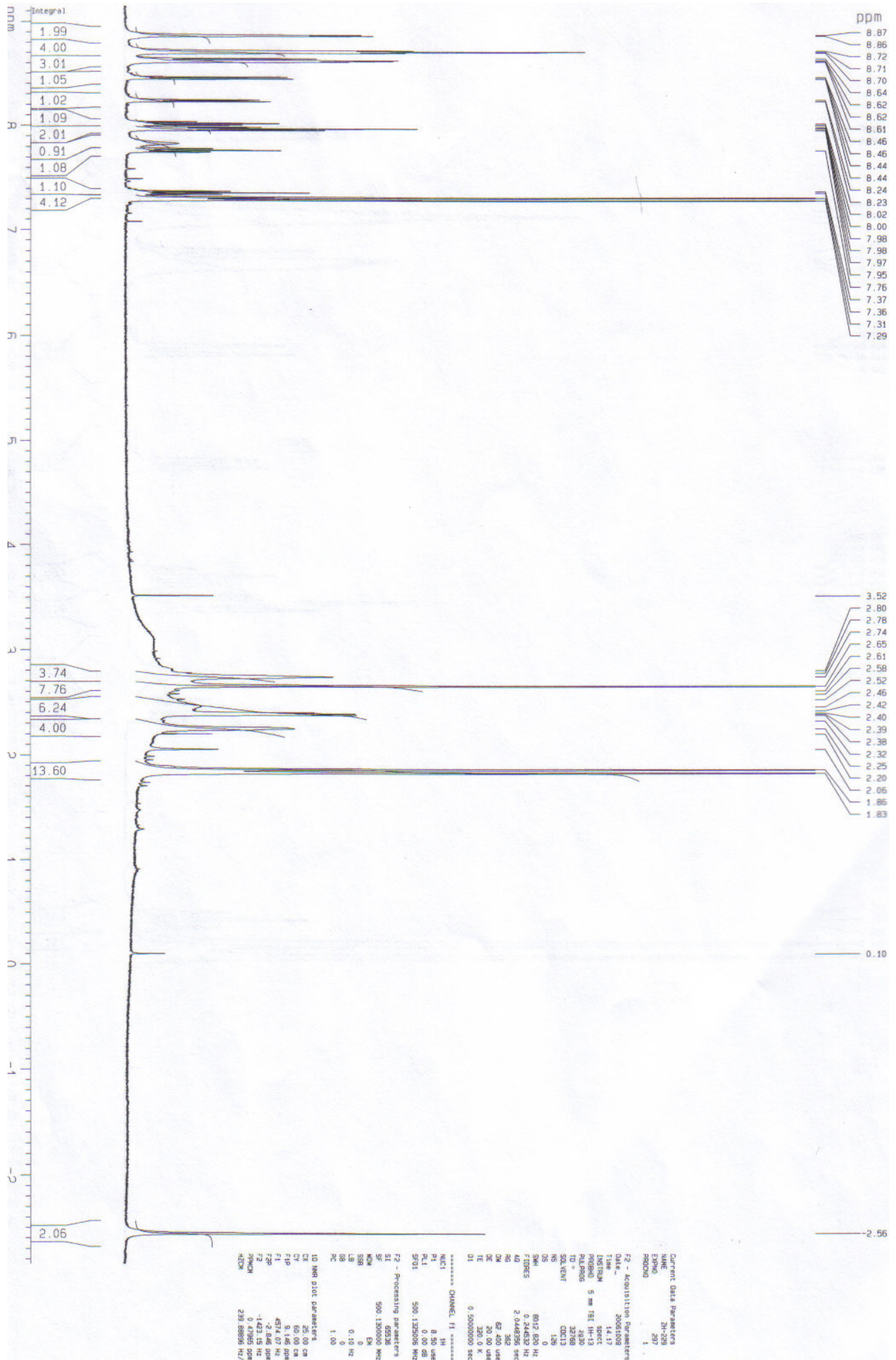
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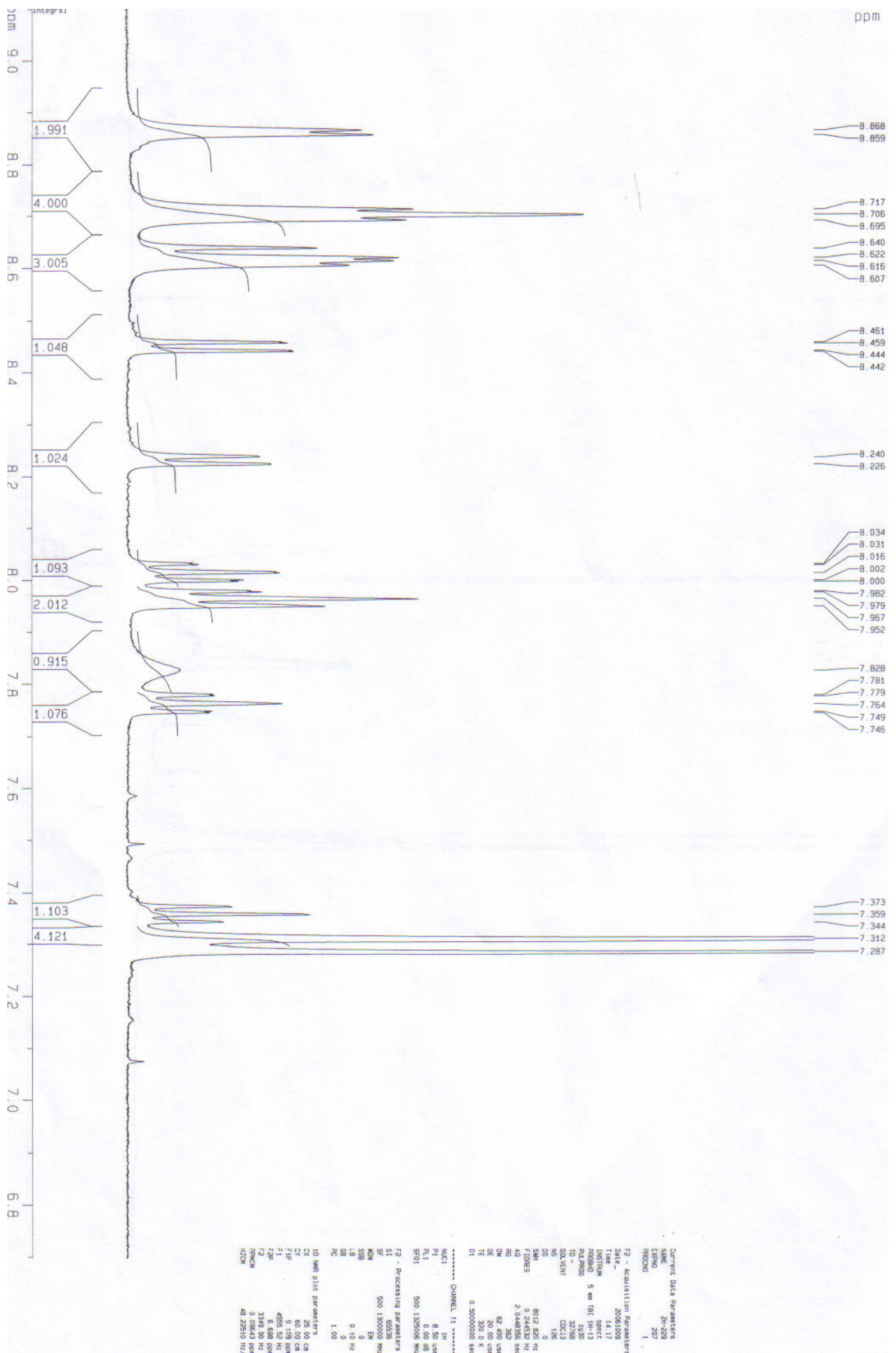


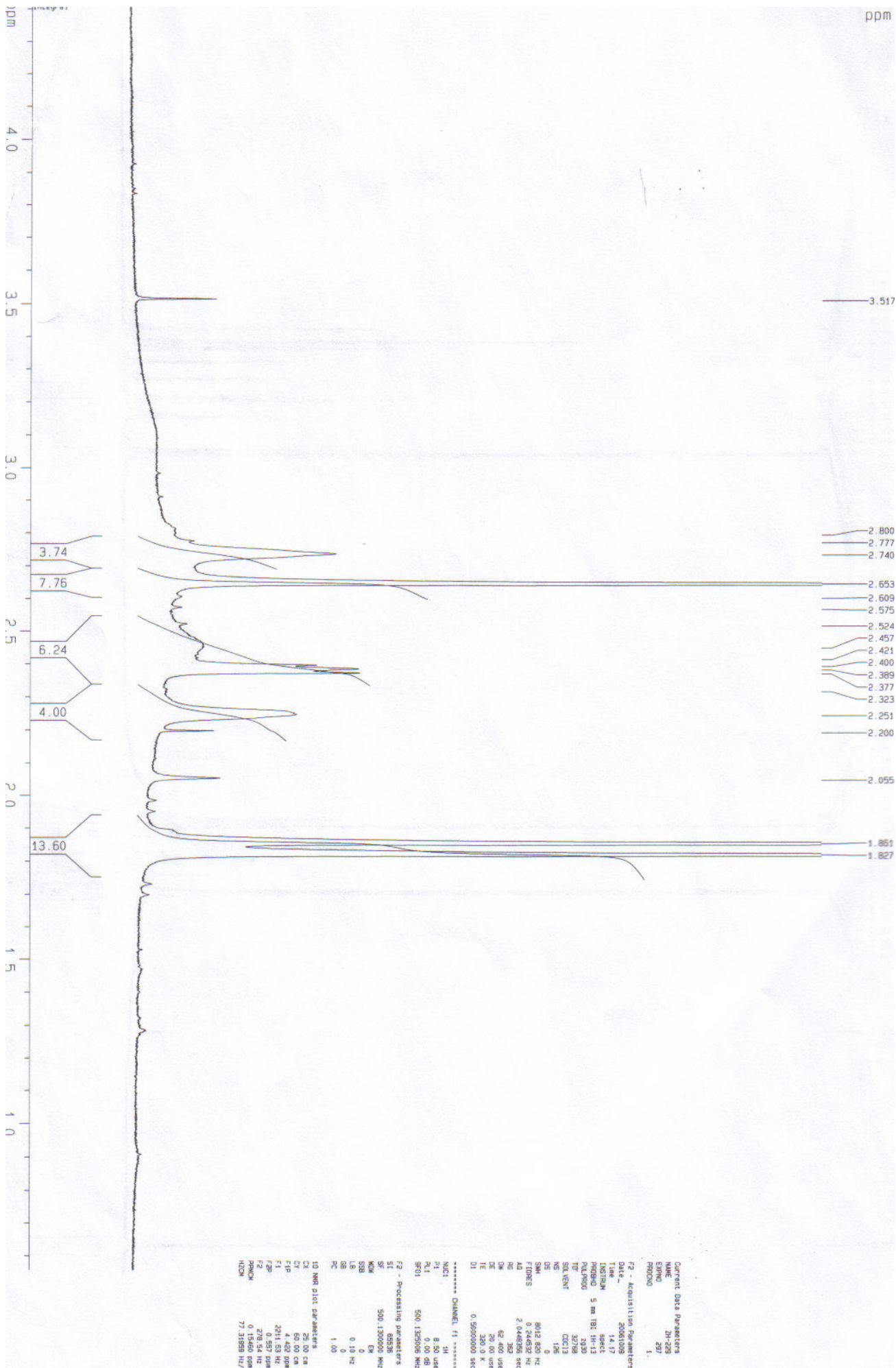
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ZabsSpecOf ES+ Magnet Bpt:177844 TIC:13375490 Noise:7
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100%

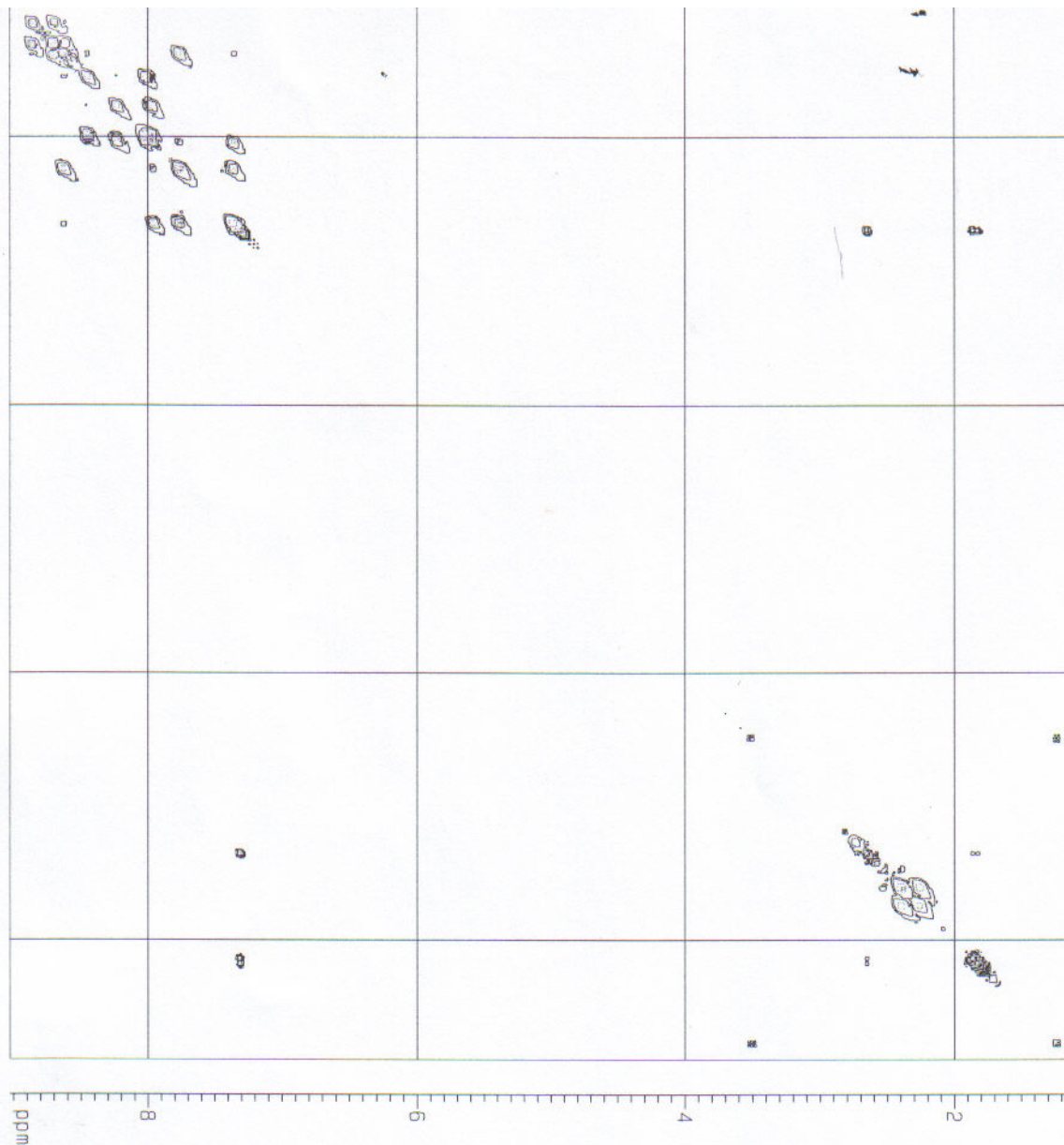












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D12 0.0005000 sec

TNO 0.0018240 sec

NOEST 0.0000000 sec

NOH2K 1.0000000 sec

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GRAB2 sine 100

GRAB3 sine 100

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GPX2 0.00 %

GPX3 0.00 %

GPY1 0.00 %

GPY2 0.00 %

GPY3 0.00 %

GPZ1 16.00 %

GPZ2 12.00 %

GPZ3 40.00 %

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TO 256

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FIDRES 21.415844 Hz

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FMKQCE GP

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WDW SINE

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GB 0.00 Hz

GB 0

PC 1.40

F1 - Processing parameter

SI 2048

SF 500.1300000 MHz

WDW SINE

SSB 0

GB 0.00 Hz

GB 0

20 NMR plot parameters

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CH1 15.00 cm

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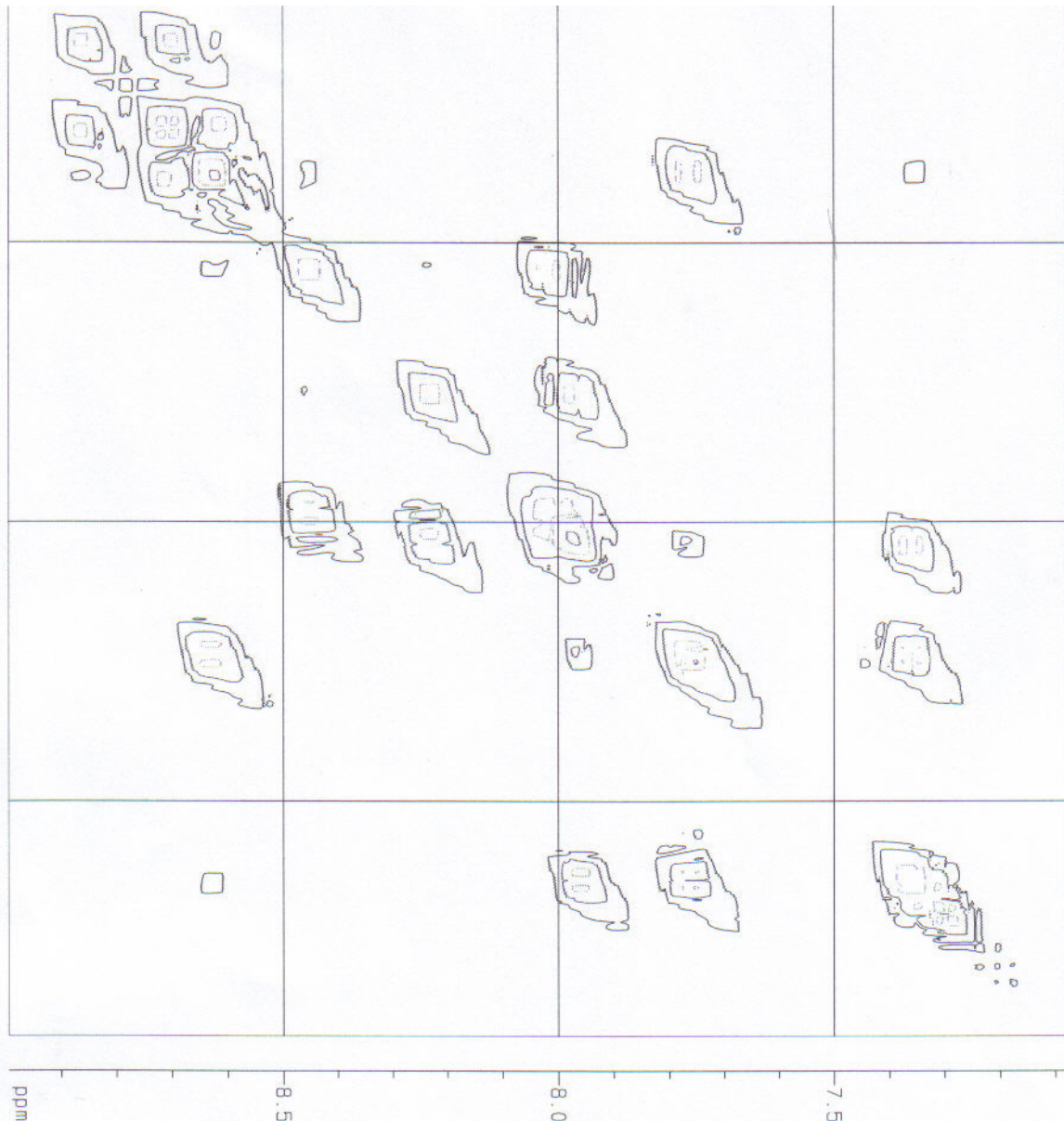
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F2HI 542.67 Hz

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TD 2048
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GPZ3 40.00 %
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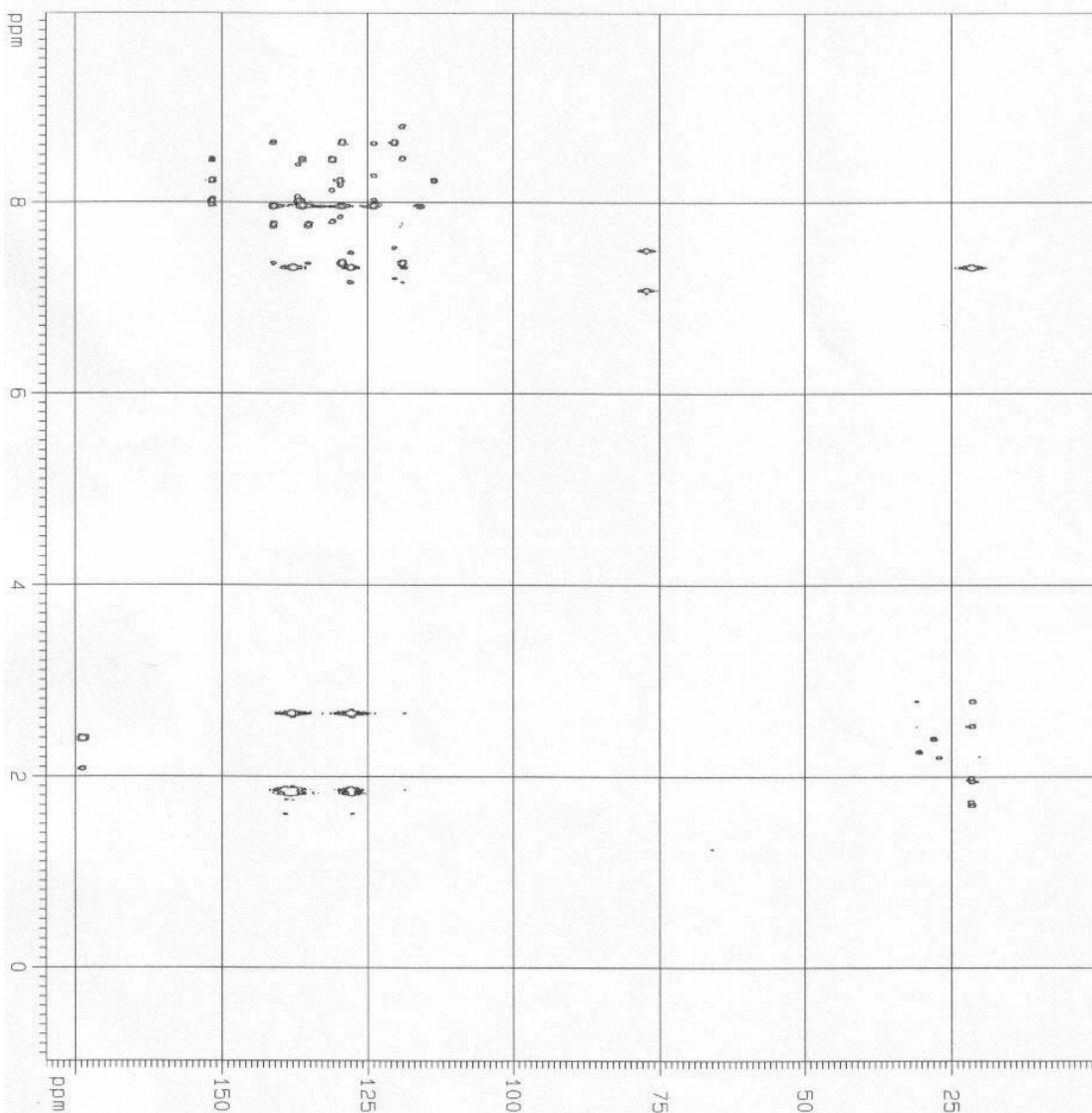
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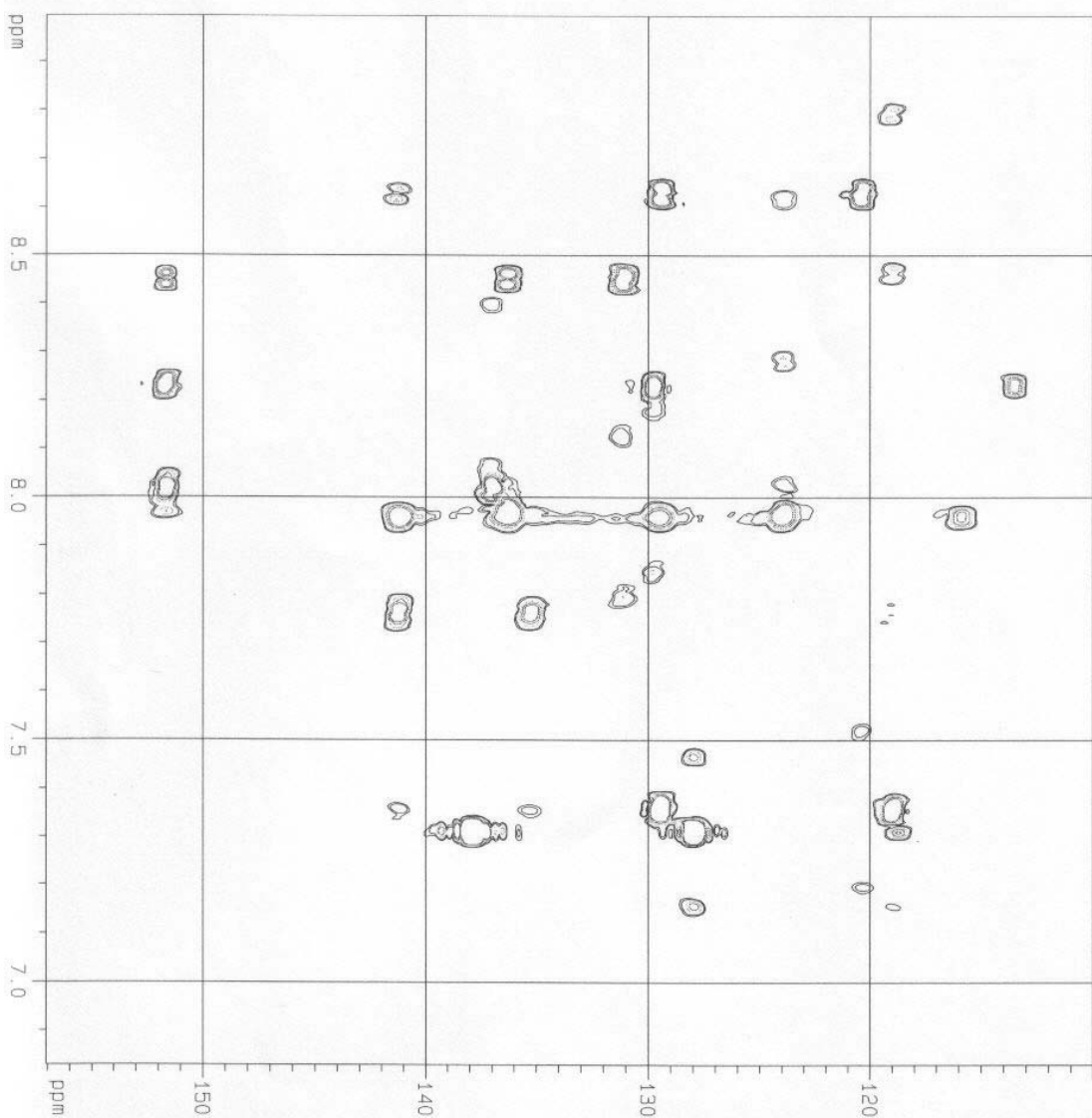
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LB 0.00 Hz
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PC 1.40

F1 - Processing Parameters
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MC2 2048
SF 500.130000 MHz
MOM SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
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CX1 15.00 cm
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F2BH 7.080 ppm
F2BL 3540.89 Hz
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FNUC 0.12896 ppm/cm

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[illegible]



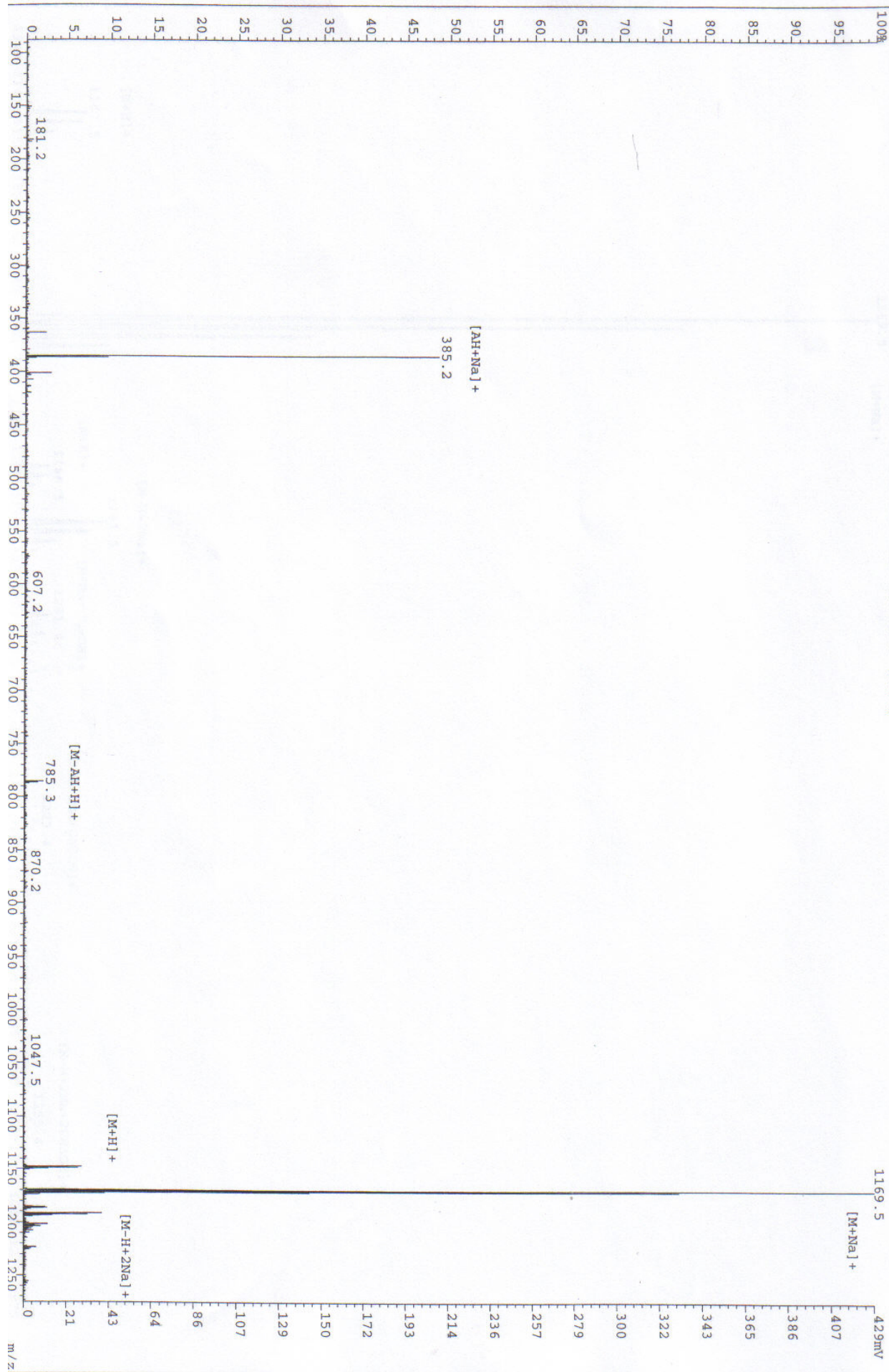
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File: HSL_11147 Ident: I SMO(2,7) B5UB(128,15,-3,0) EKD(7,3,7,0.01%,44.0,0.00%,T,F) Acq: 20-OCT-2006 18:56:37 +17:45 Cal: E3000_061018_CS_P_Pt_1x1_000077
ZabspecTOF ES+ Magnet Bp1: 337952 TIC: 12089712 Noise: 11
File Text: Z. HALIME ZH 229 Basse Resolution 2000 Pt Solvant : CH3OH/CH2Cl2 (95/5)
100%
1169.5

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File:ESI_11147 Ident:1 SMO(2,7) BSUB(128,15,-3,0) PKD(7,3,7,0.01%,44.0,0.00%,T,F) Acq:20-OCT-2006 18:56:37 +17:45 Cal:E3000_061018_CS_P_PJ_1x1.000077
 ZabSpecTOF ES+ Magnet BpI:337952 TIC:12089712 Noise:11
 File Text:Z. HALIME ZH 229 Basse Resolution 2000 PU Solvant : CH3OH/CH2Cl2 (95/5)
 1169.5 [M+Na]⁺

