Supplementary data

HRMS of fraction 2 demonstrating the calculated molecular mass (341.04) and the formula (C11, H19, N, O5, S3) of the compound.

Single Mass Analysis

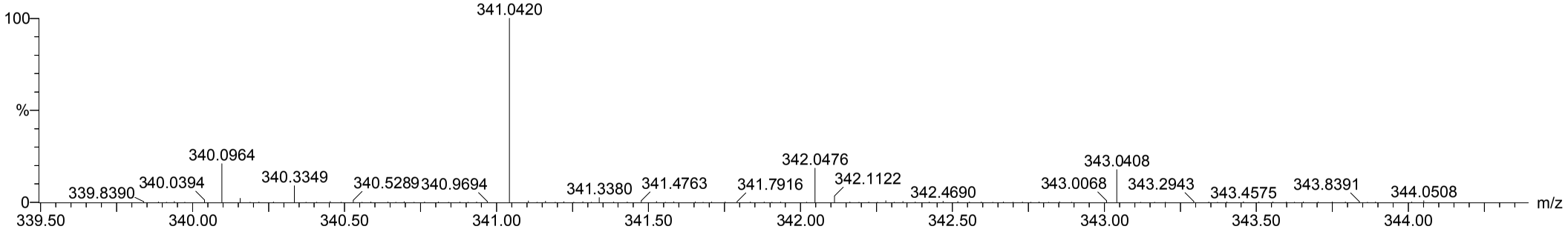
Tolerance = 20.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
48 formula(e) evaluated with 6 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 10-15 H: 17-20 N: 0-2 O: 0-6 S: 0-3

13-Jun-2013
cli_5716p 169 (1.459) Cm (151:256-87:117)

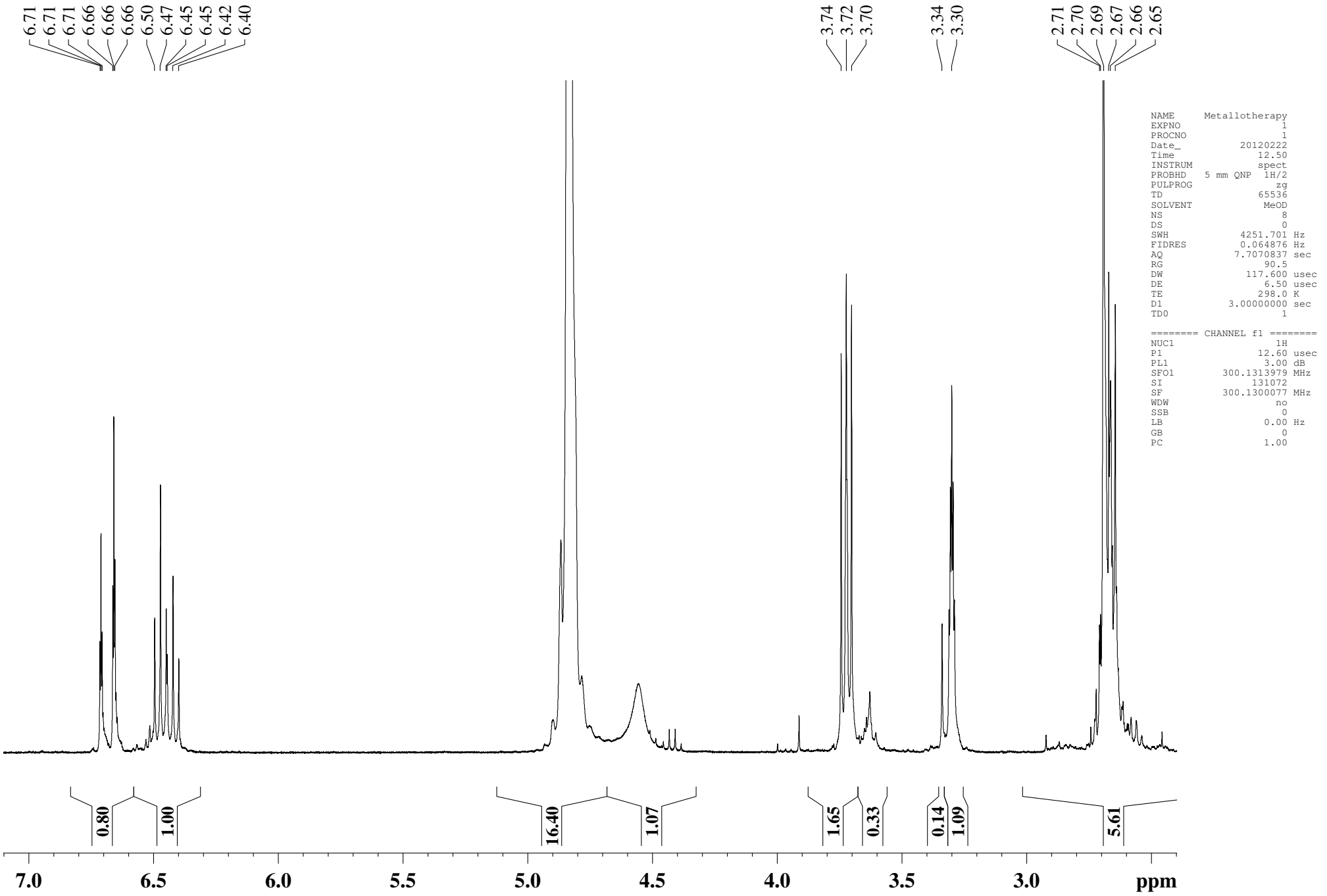
sample

Galilee Society
TOF MS ES+
7.40e+004



Minimum:				-1.5		
Maximum:		20.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
341.0420	341.0425	-0.5	-1.5	3.0	233.3	C11 H19 N O5 S3
	341.0452	-3.2	-9.4	7.5	132.8	C14 H17 N2 O2 S3
	341.0340	8.0	23.5	7.5	283.8	C15 H17 O3 S3
	341.0517	-9.7	-28.4	7.5	972.8	C15 H17 O5 S2
	341.0300	12.0	35.2	3.5	716.0	C10 H17 N2 O5 S3
	341.0578	-15.8	-46.3	7.0	693.0	C15 H19 N O2 S3

^{1}HNMR of fraction 2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6.71
6.71
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6.66
6.66
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6.40
3.74
3.72
3.70
3.34
3.30
2.71
2.70
2.69
2.67
2.66
2.65
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EXPNO 1
PROCNO 1
Date_ 20120222
Time 12.50
INSTRUM spect
PROBHD 5 mm QNP 1H/2
PULPROG zg
TD 65536
SOLVENT MeOD
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FIDRES 0.064876 Hz
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RG 90.5
DW 117.600 usec
DE 6.50 usec
TE 298.0 K
D1 3.00000000 sec
TD0 1
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PL1 3.00 dB
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SI 131072
SF 300.1300077 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
0.80
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1.07
1.65
0.33
0.14
1.09
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6.0
5.5
5.0
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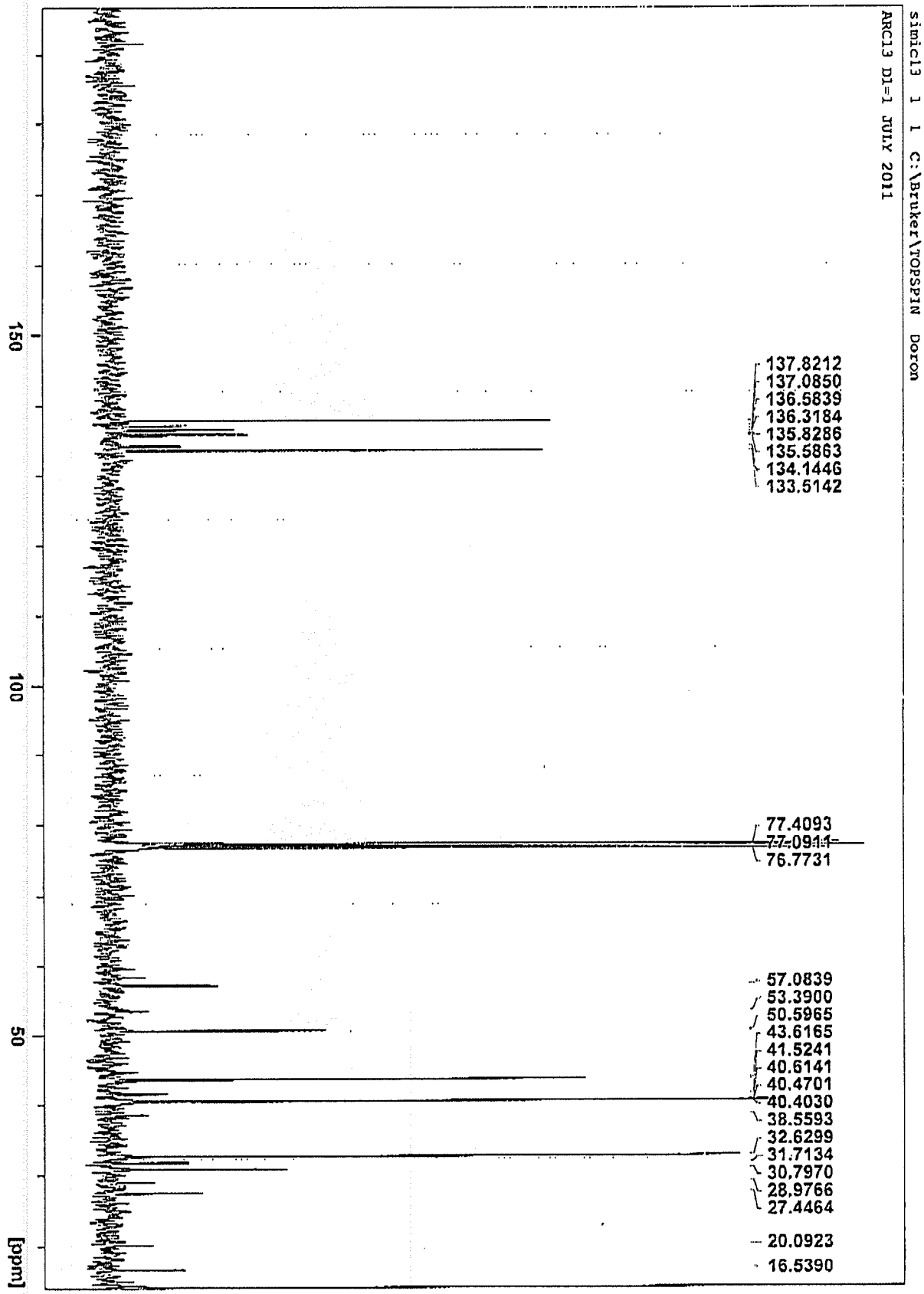
4.0
3.5
3.0
ppm

^{13}CNMR of fraction 2


simic13 1 1 C:\Bruker\TOPSPIN Doron
ARC13 D1=1 JULY 2011
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50.5965
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