Supplementary data

Cytotoxicity of new diterpene alkaloids, ceylonamides G-I, isolated from Indonesian marine sponge of *Spongia* sp.

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Ceylonamide G (1)

HR-ESI-MS

Elemental Composition Report **Page 1**

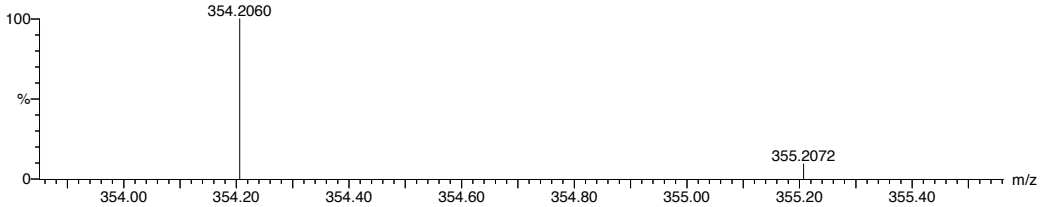
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
340 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 20-20 H: 17-32 N: 0-2 O: 0-10 Na: 0-1 S: 0-5

24-Feb-2017
19:21:38
TOF MS ES+

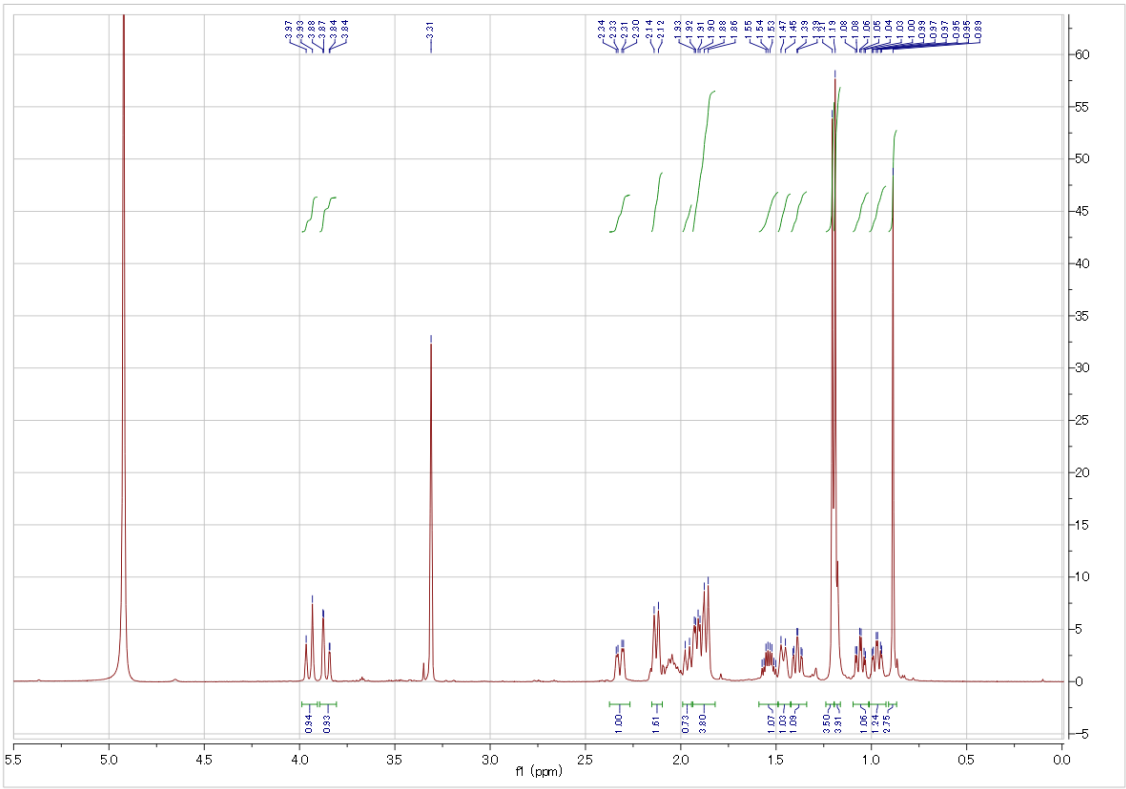
TJ-7-05C24-FR E3-2-2 POG-1 25 (0.472) AM (Cen,4, 80.00, Ar,5000.0,556.28,0.18); Sm (SG, 2x3.00)

2.17e+002

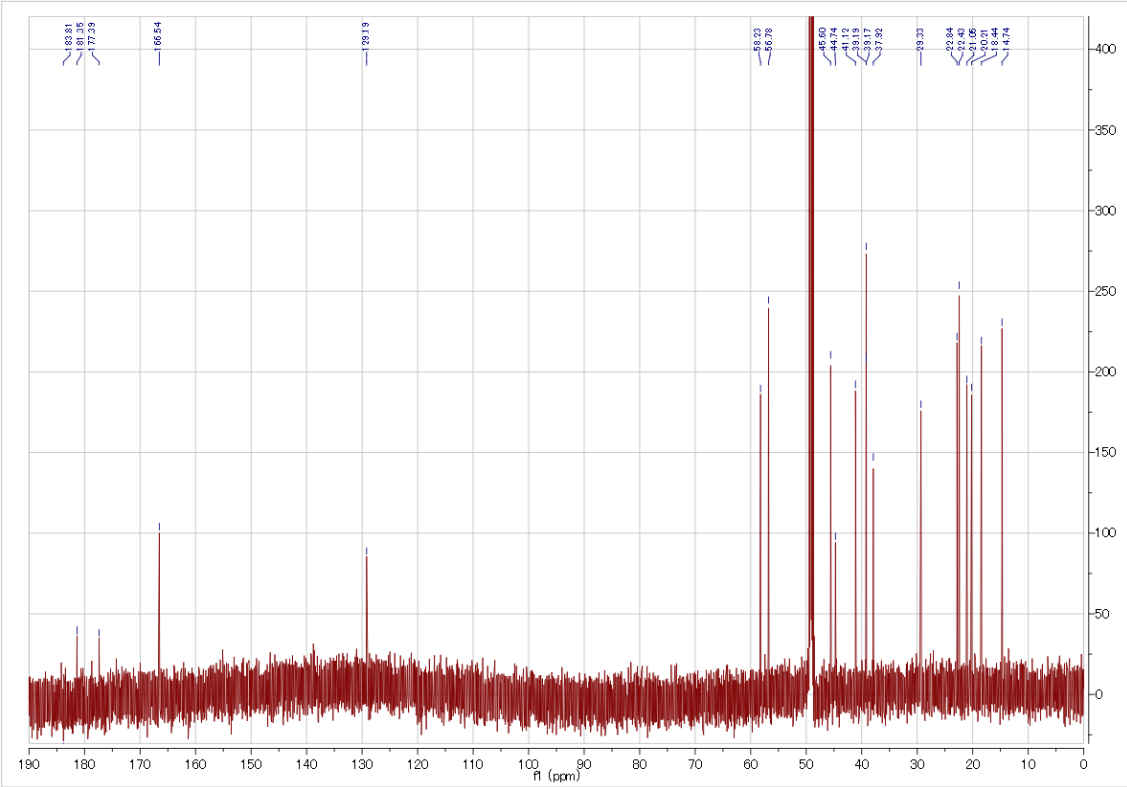


Minimum:				-1.5		
Maximum:		20.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
354.2060	354.2045	1.5	4.2	6.5	n/a	C20 H29 N O3 Na

^{1}H-NMR (CD_3OD)



^{13}C-NMR (CD_3OD)



Ceylonamide H (2)

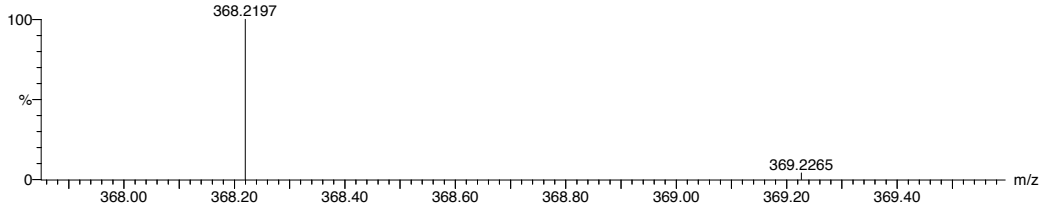
HR-ESI-MS

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

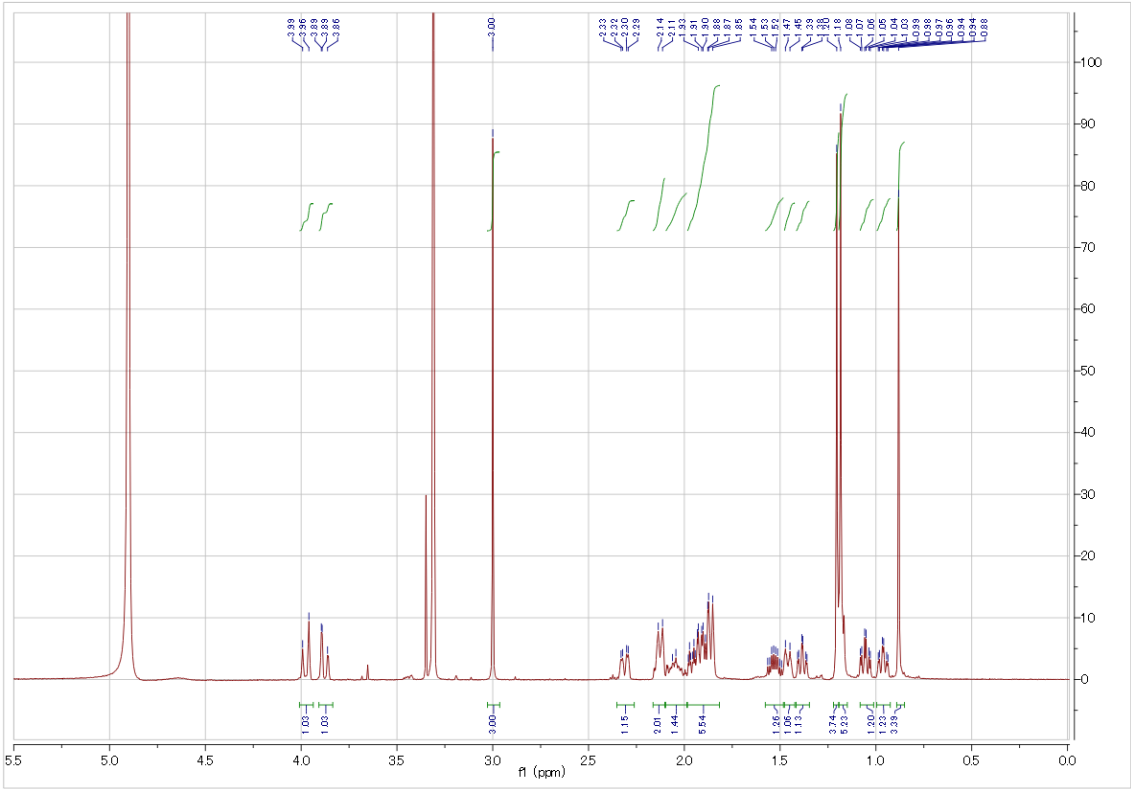
Monoisotopic Mass, Even Electron Ions
261 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 15-40 H: 30-60 N: 0-6 O: 0-10 Na: 0-1

02-Mar-2017 F
20:59:12
TJ-7-05C24-FR E3-6-2 F POG-1 99 (1.844) AM (Cen,4, 80.00, Ar,5000.0,556.28,0.18); Sm (SG, 2x3.00) TOF MS ES+
7.50e+002

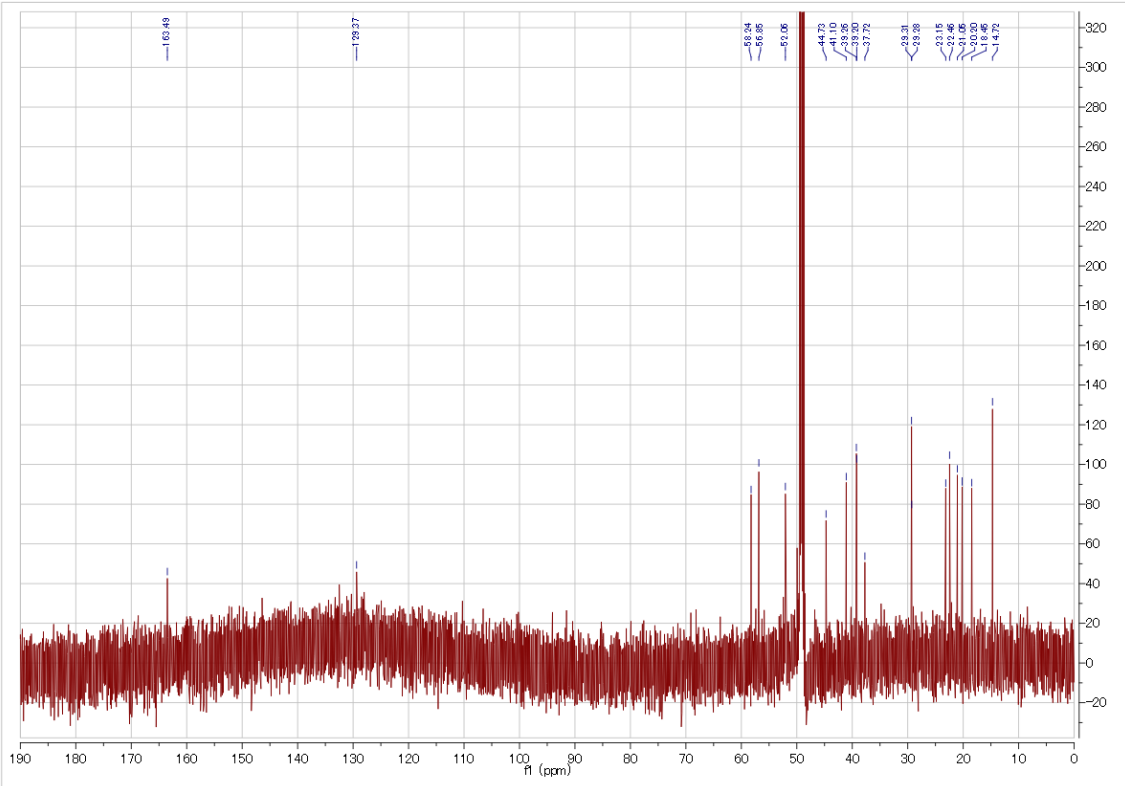


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
368.2197	368.2202	-0.5	-1.4	6.5	n/a	C21 H31 N O3 Na
	368.2185	1.2	3.3	5.5	n/a	C18 H30 N3 O5

^{1}H-NMR (CD_3OD)



^{13}C-NMR (CD_3OD)



Ceylonamide I (3)

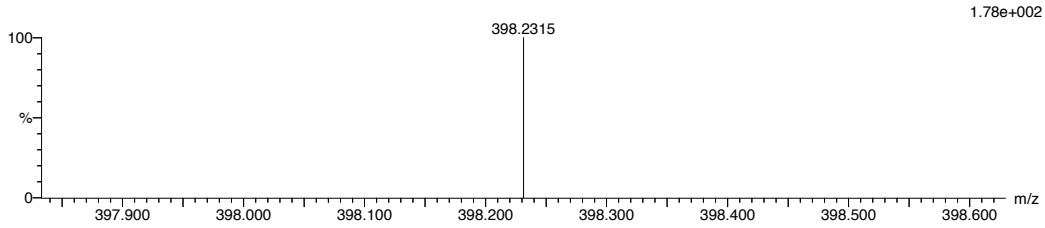
HR-ESI-MS

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

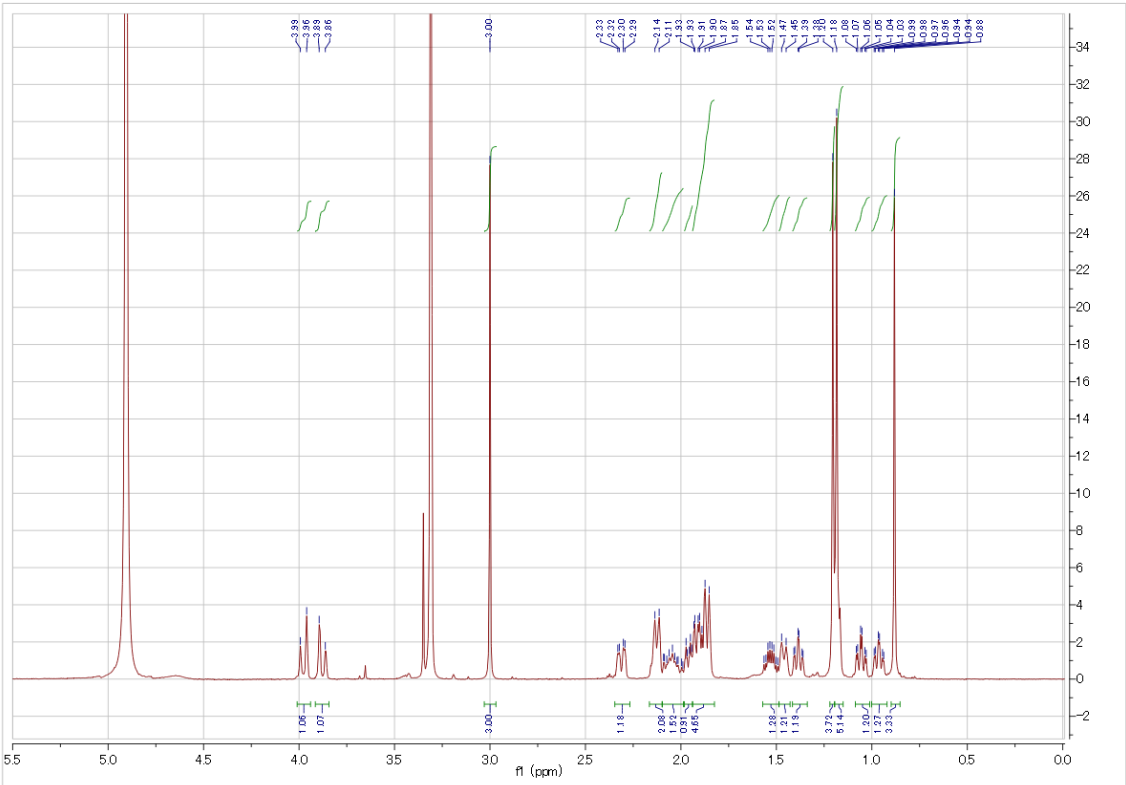
Monoisotopic Mass, Even Electron Ions
710 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 20-23 H: 32-36 N: 0-6 O: 0-10 Na: 0-1 S: 0-5

02-Mar-2017 TJ-7-05C24-FR E3-4-2 POG-1 37 (0.694) AM (Cen,4, 80.00, Ar,5000.0,556.28,0.18); Sm (SG, 2x3.00)
20:27:54
TOF MS ES+

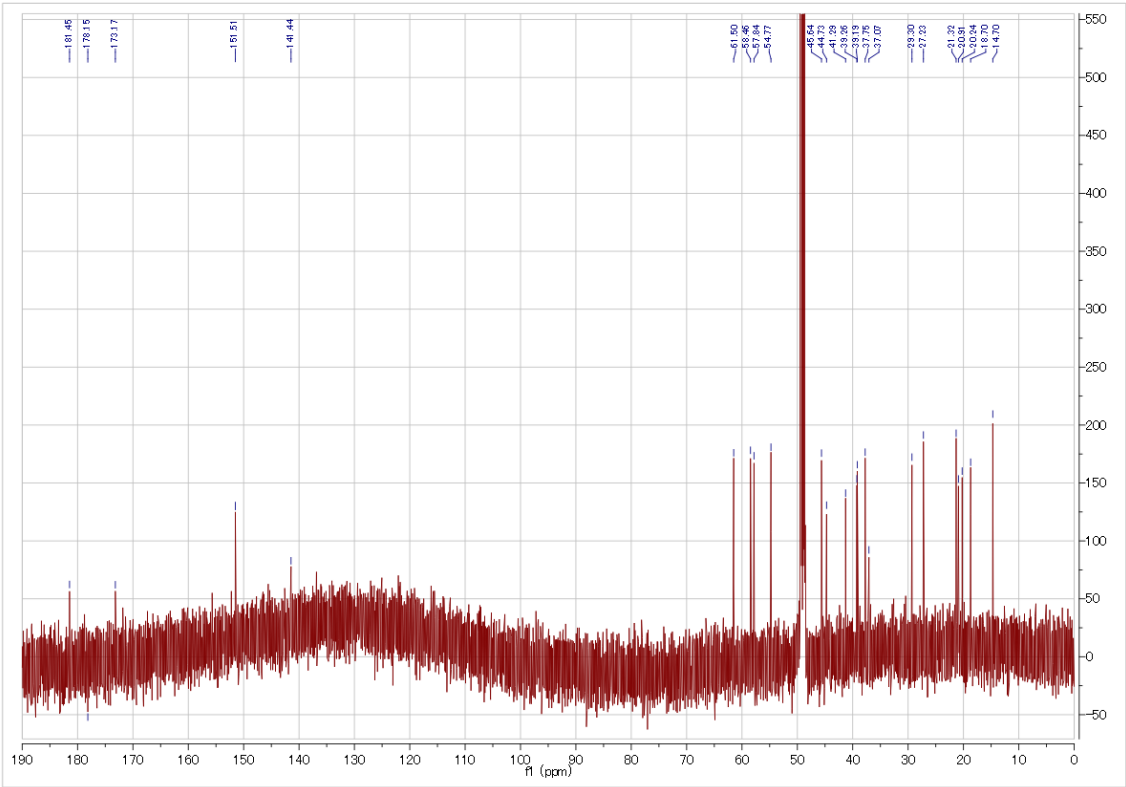
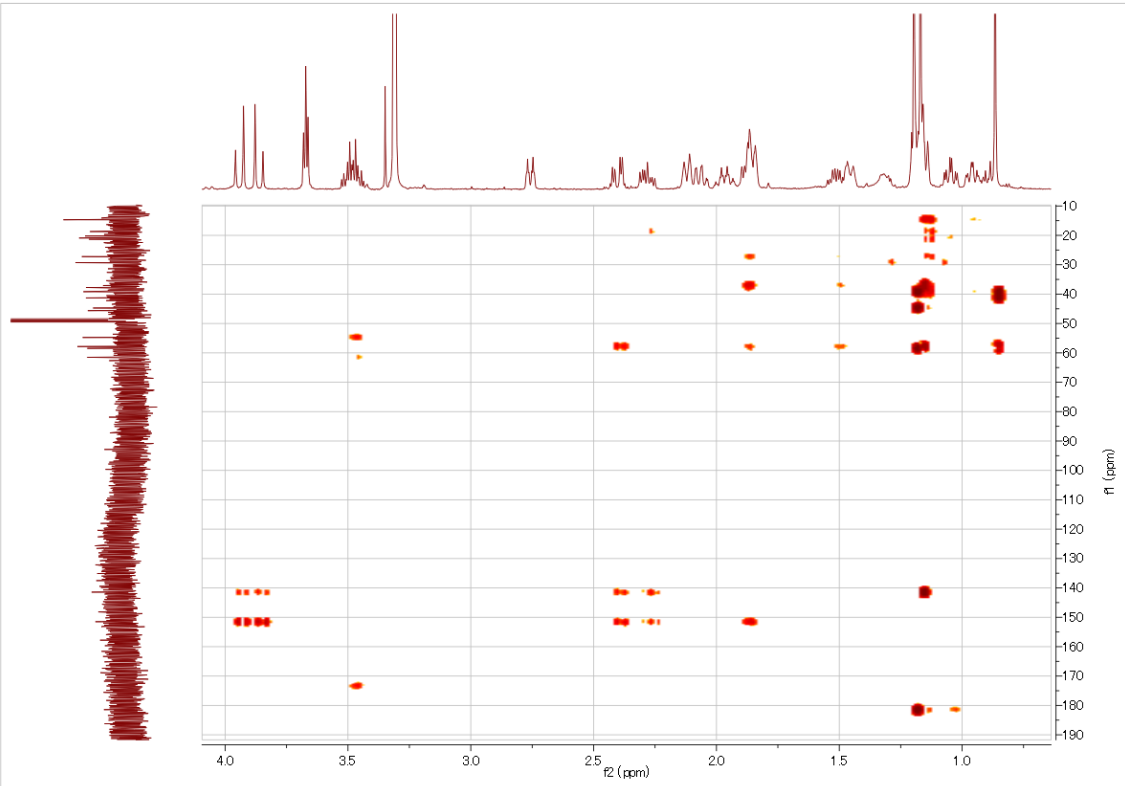


Minimum:				-1.5		
Maximum:		20.0	5.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
398.2315	398.2307	0.8	2.0	6.5	n/a	C22 H33 N O4 Na
	398.2300	1.5	3.8	4.5	n/a	C20 H36 N3 O S2

^{1}H-NMR (CD_3OD)



^{13}C-NMR (CD_3OD)



HMBC (CD_3OD)