Supporting Information

Two halosesquiterpenes from *Laurencia composita*

Xiao-Dong Li,[a,c] Feng-Ping Miao,[a] Xiao-Rui Liang,[b] Bin-Gui Wang[c] and Nai-Yun Ji*[a]

[a]*Key Laboratory of Coastal Biology and Bioresource Utilization, Yantai Institute of Coastal Zone Research, Chinese Academy of Sciences, Yantai 264003, China. E-mail address: nyji@yic.ac.cn; Tel: +86 535 2109176*
[b]*Naval Aeronautical and Astronautical University, Yantai 264001, China*
[c]*Institute of Oceanology, Chinese Academy of Sciences, Qingdao 266071, China*

Contents

Table S1. Charge distributions, bond lengths, and angles around C-9 of **1** (X = Cl) and **2** (X = Br) in water

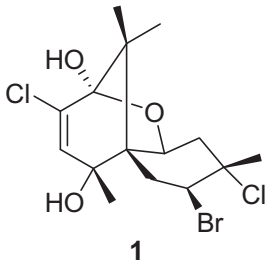
		1	**2**
charge	X-9	0.177051 e	0.220535 e
	C-9	–0.159760 e	0.016631 e
	C-8	–0.304566 e	–0.413107 e
bond length	X-9–C-9	1.77 Å	1.92 Å
	C-9–C-8	1.33 Å	1.33 Å
bond angle	∠X-9–C-9–C-8	120.90°	120.57°
	∠X-9–C-9–C-10	116.87°	116.77°

Table S2. Absolute and relative free energies (hartree) of conformers of **1** and **2**

	solvent	absolute energy	relative energy
1	chloroform	–4301.781356	0
	methanol	–4301.785217	0
	water	–4301.785692	0
2	chloroform	–6413.318621	0
	methanol	–6413.322903	0
	water	–6413.323427	0

Table S3. Bioassay results of **1** and **2**

	1	**2**	$K_2Cr_2O_7$	chloramphenicol
A. salina (LC_{50}, μmol/L; 24h)	219.9	305.7	70.7	
H. akashiwo (EC_{50}, μmol/L; 24h)	39.2	45.0	45.9	
V. ichthyoenteri (inhibitory diameter, mm; 24h)	0	0		28
P. mirabilis (inhibitory diameter, mm; 24h)	0	0		26
E. cloacae (inhibitory diameter, mm; 24h)	0	0		22
B. cereus (inhibitory diameter, mm; 24h)	6.0	0		20



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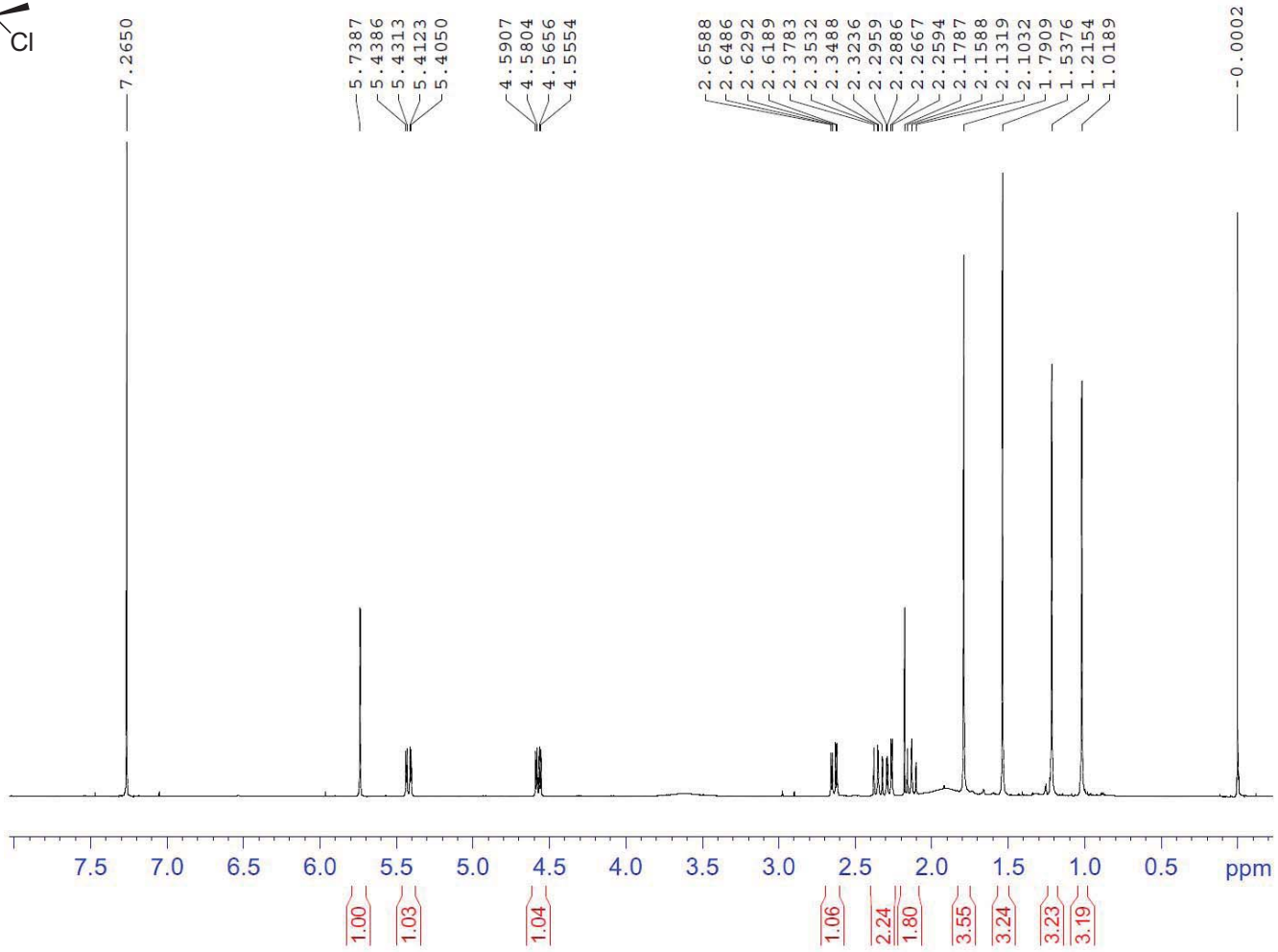

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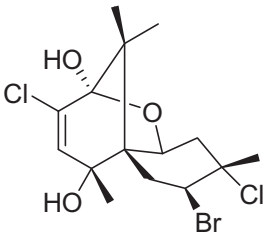
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	144
DW	48.400 usec
DE	6.50 usec
TE	293.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.40 usec
PL1	0.35 dB
PL1W	19.76737595 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300110 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



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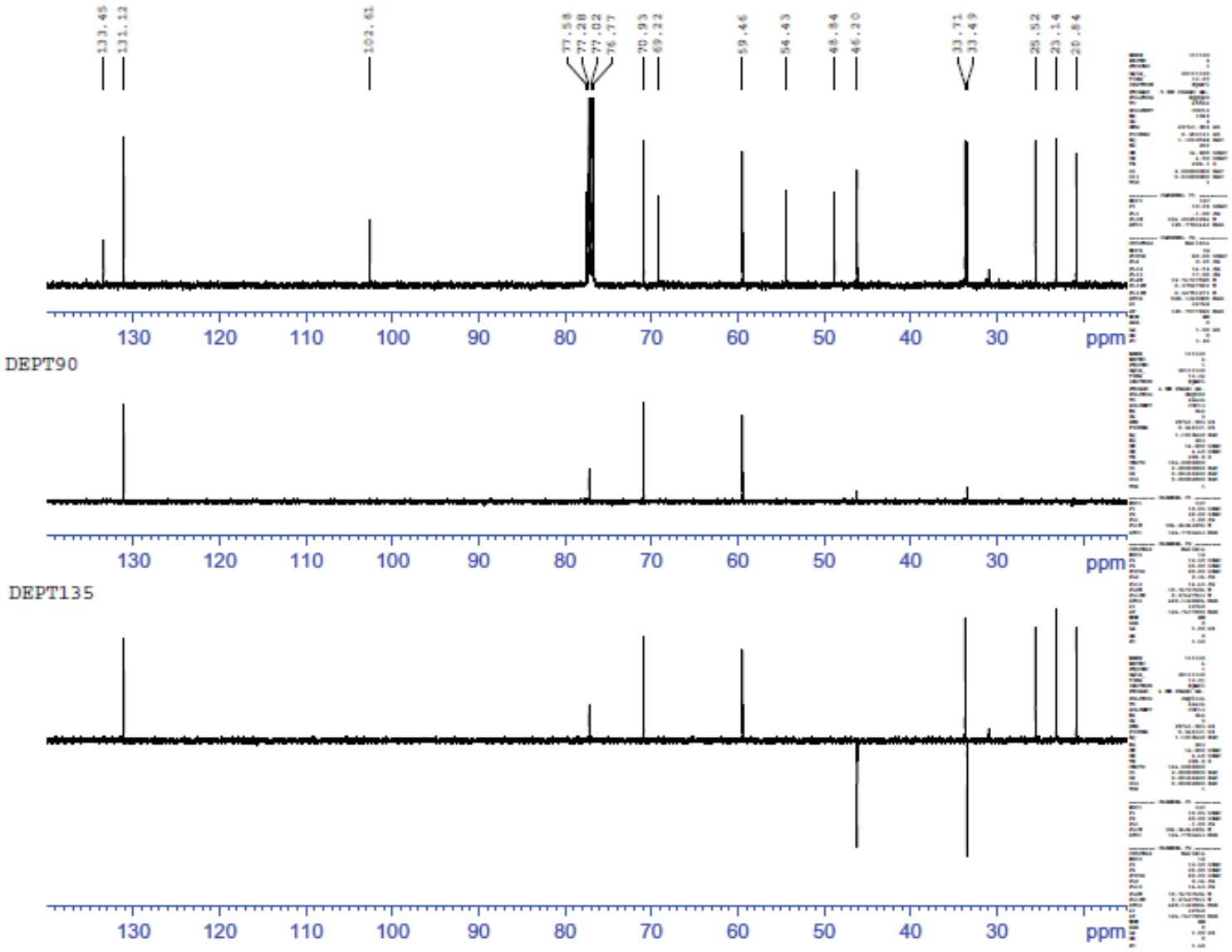

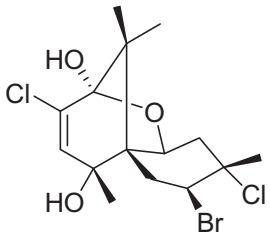

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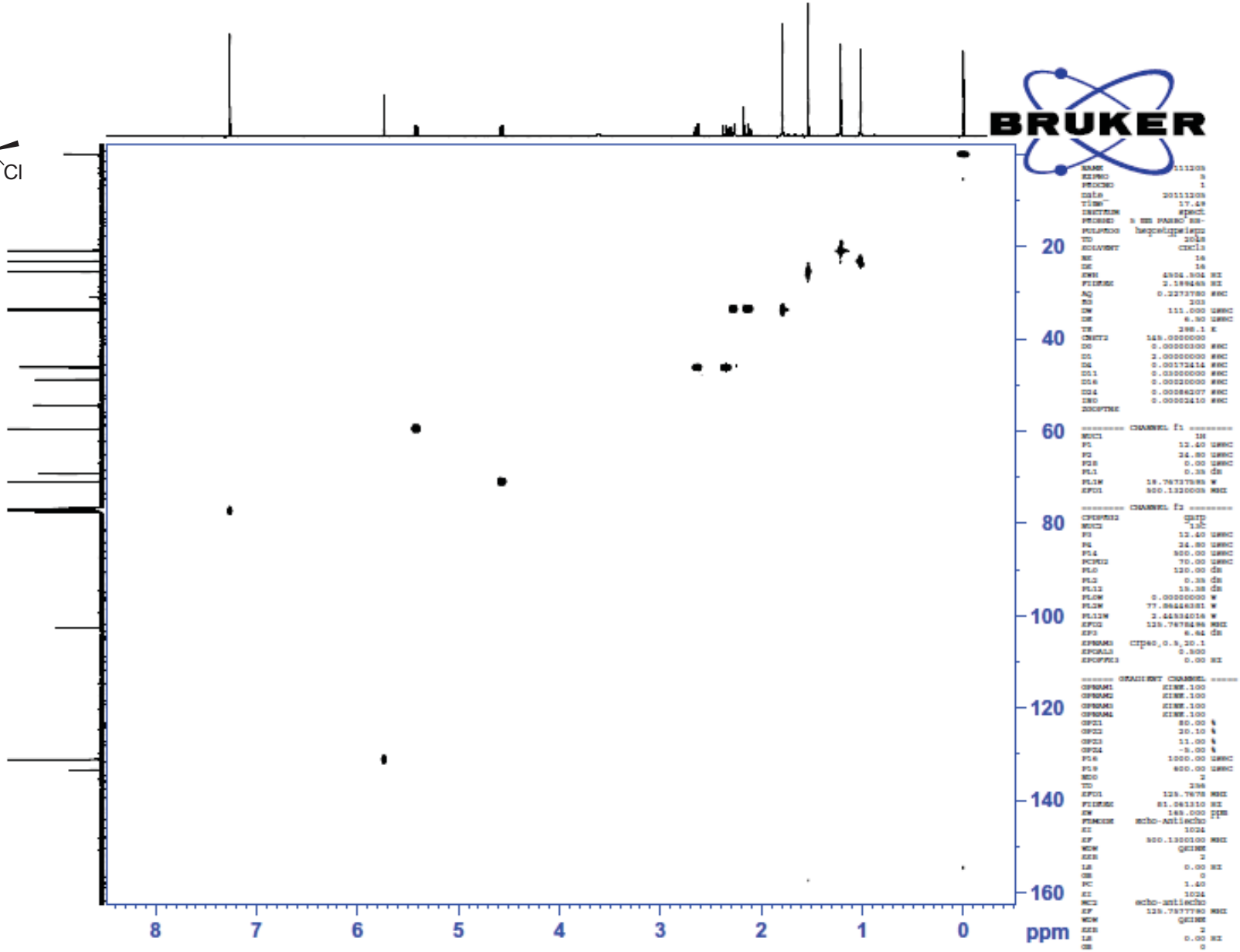

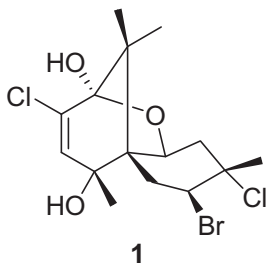

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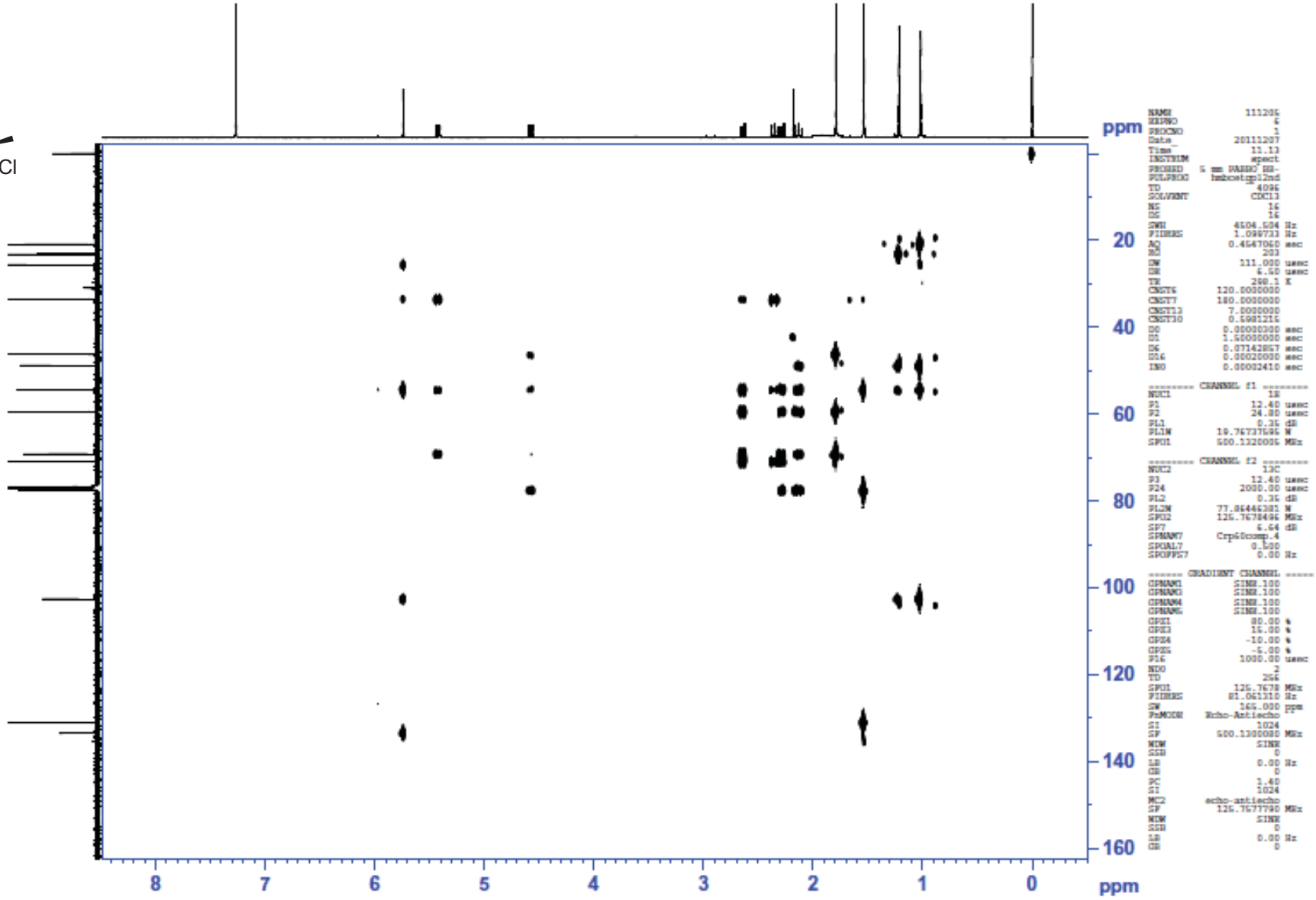

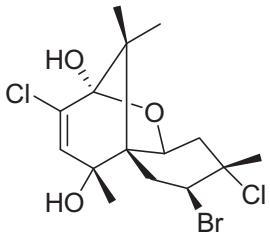

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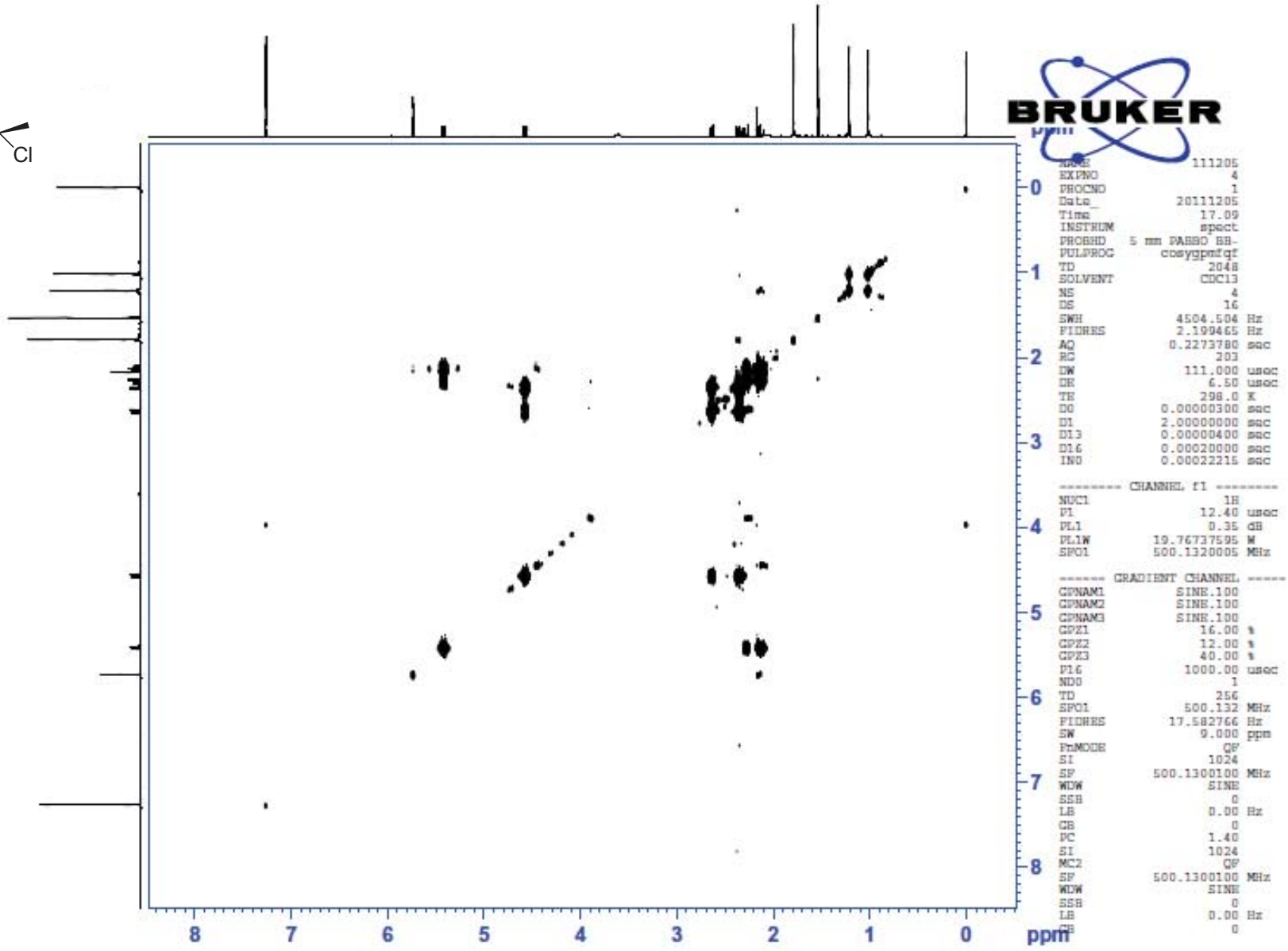

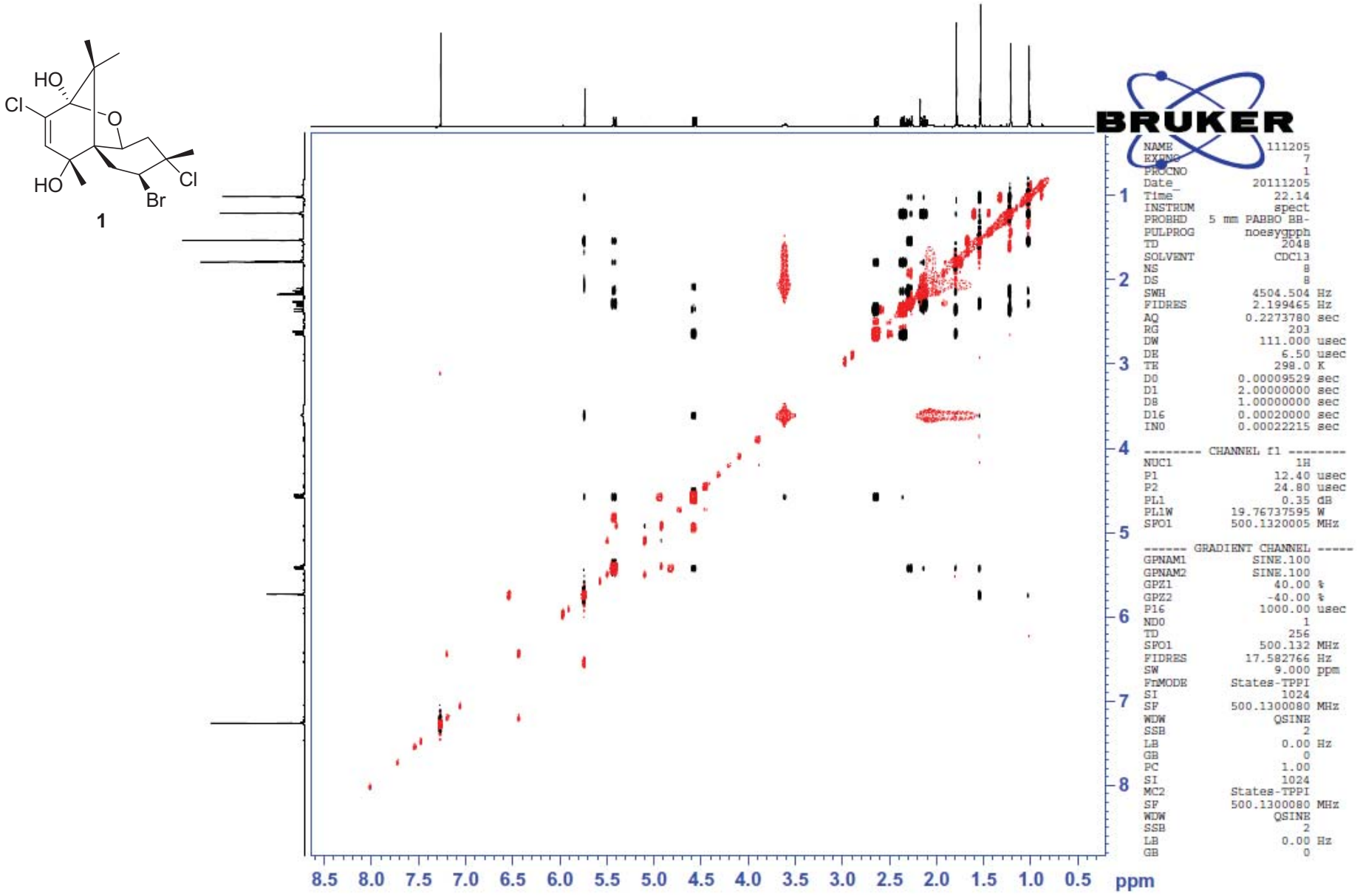

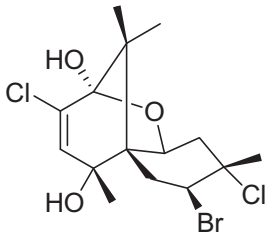

1

Elemental Composition Report

Single Mass Analysis

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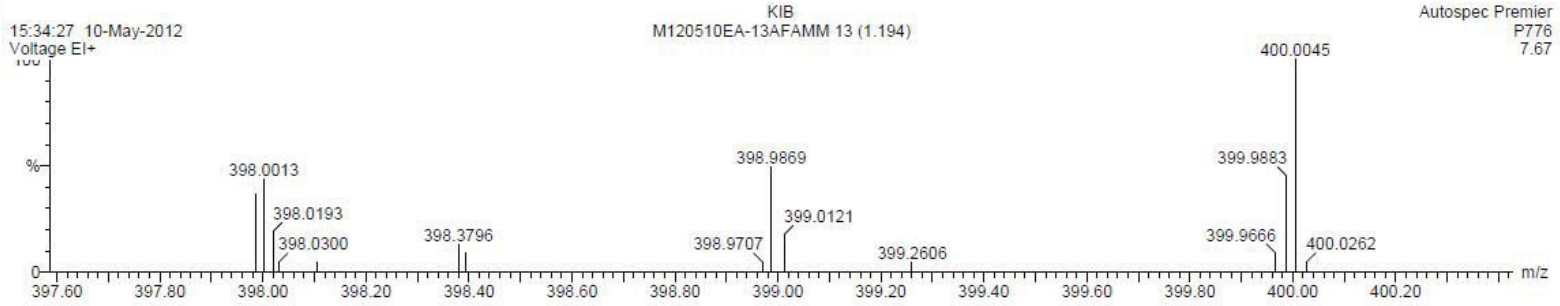
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

16 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 0-4 Cl: 2-2 Br: 1-1



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Maximum:		100.0	10.0	120.0		
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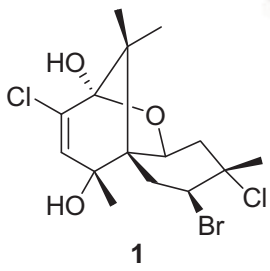

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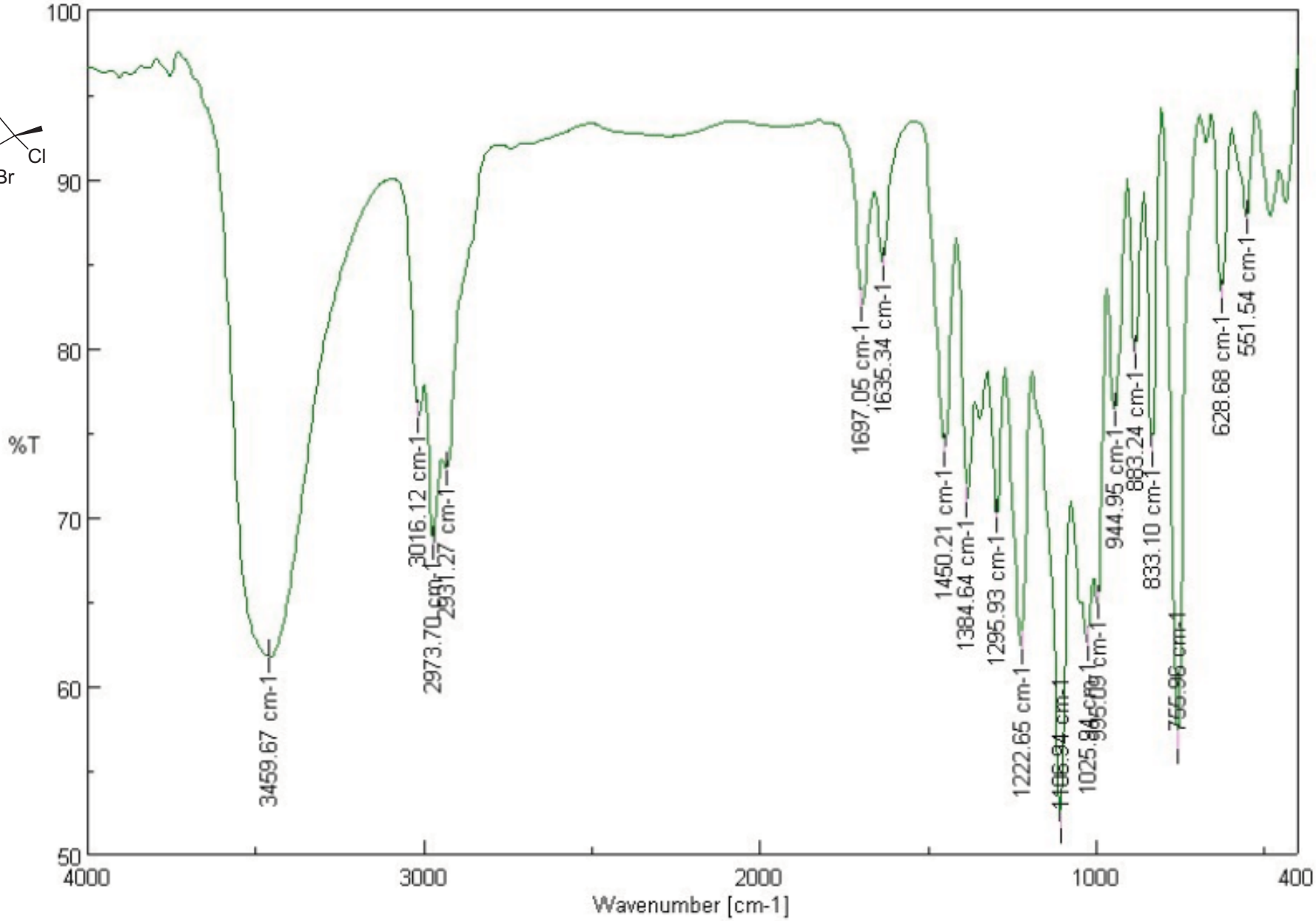

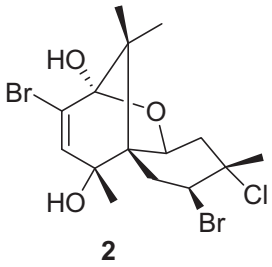

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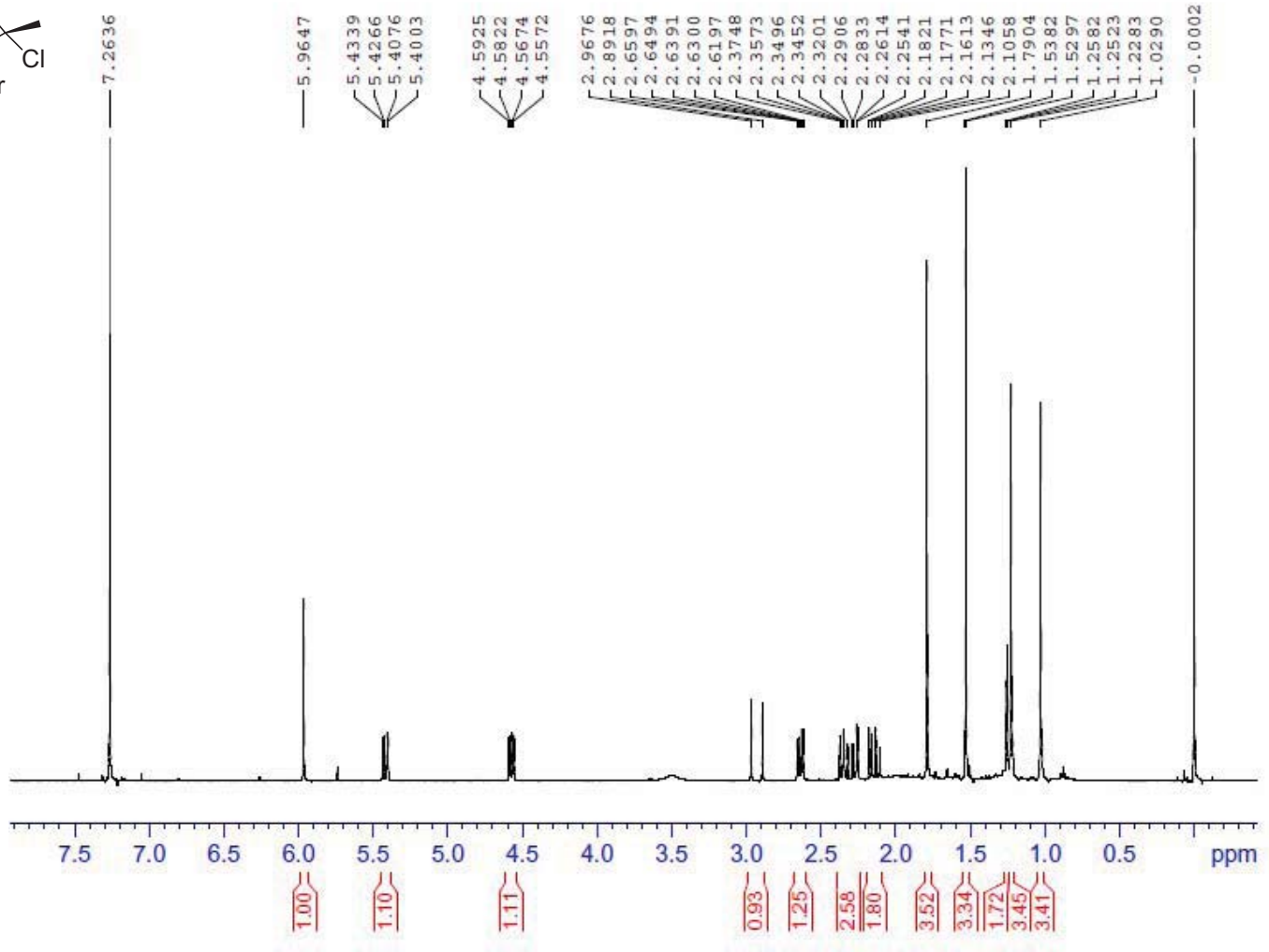


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TD                   65536
SOLVENT              CDC13
NS                       8
DS                       0
SWH              10330.578 Hz
FIDRES           0.157632 Hz
AQ               3.1719923 sec
RG                     144
DW                  48.400 usec
DE                   6.50 usec
TE                  293.6 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.40 usec
PL1                   0.35 dB
PL1W         19.76737595 W
SFO1         500.1330885 MHz
SI                   32768
SF           500.1300118 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
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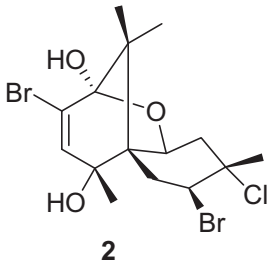

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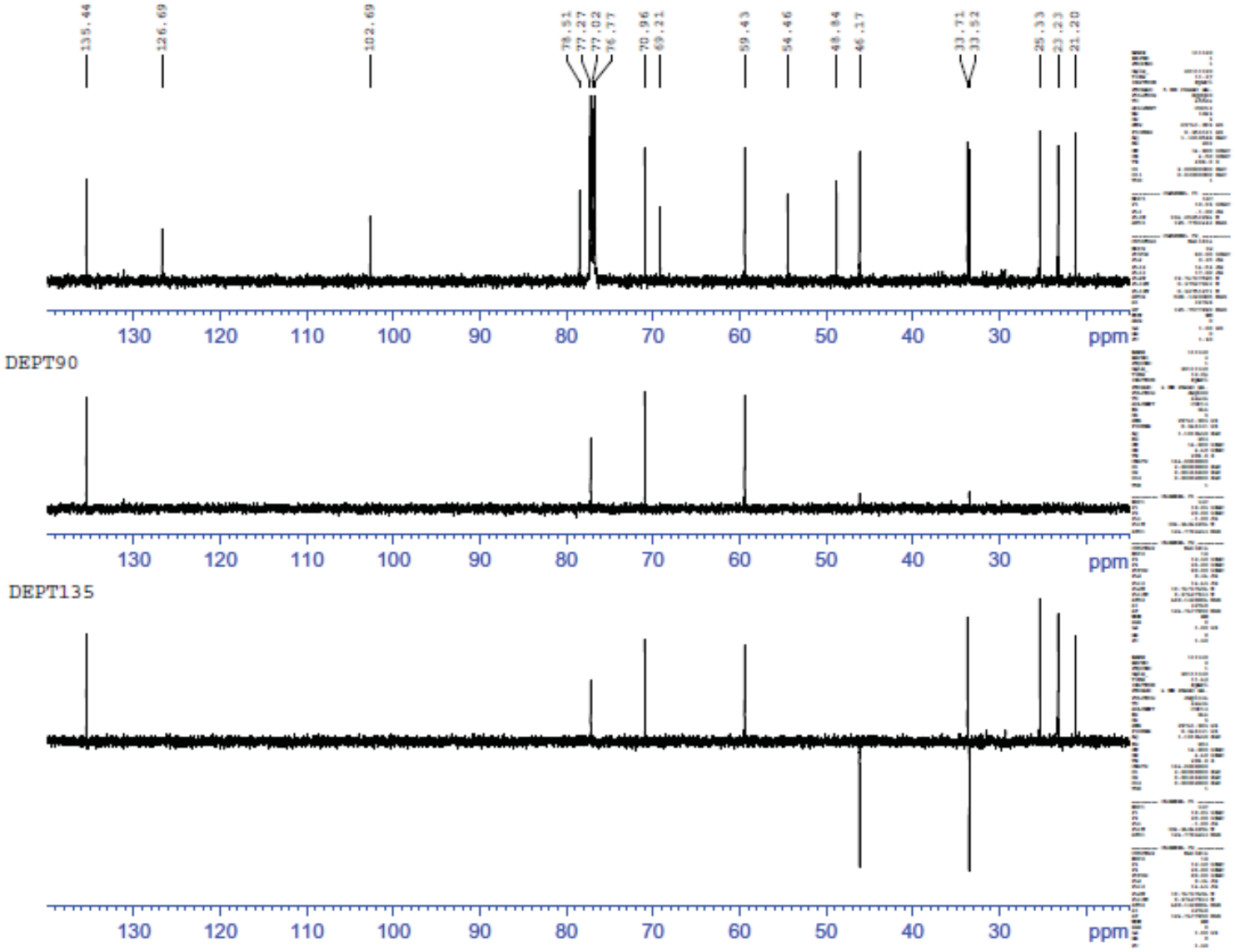

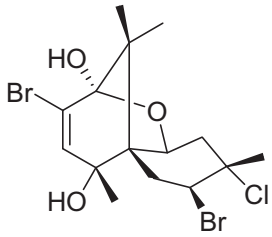

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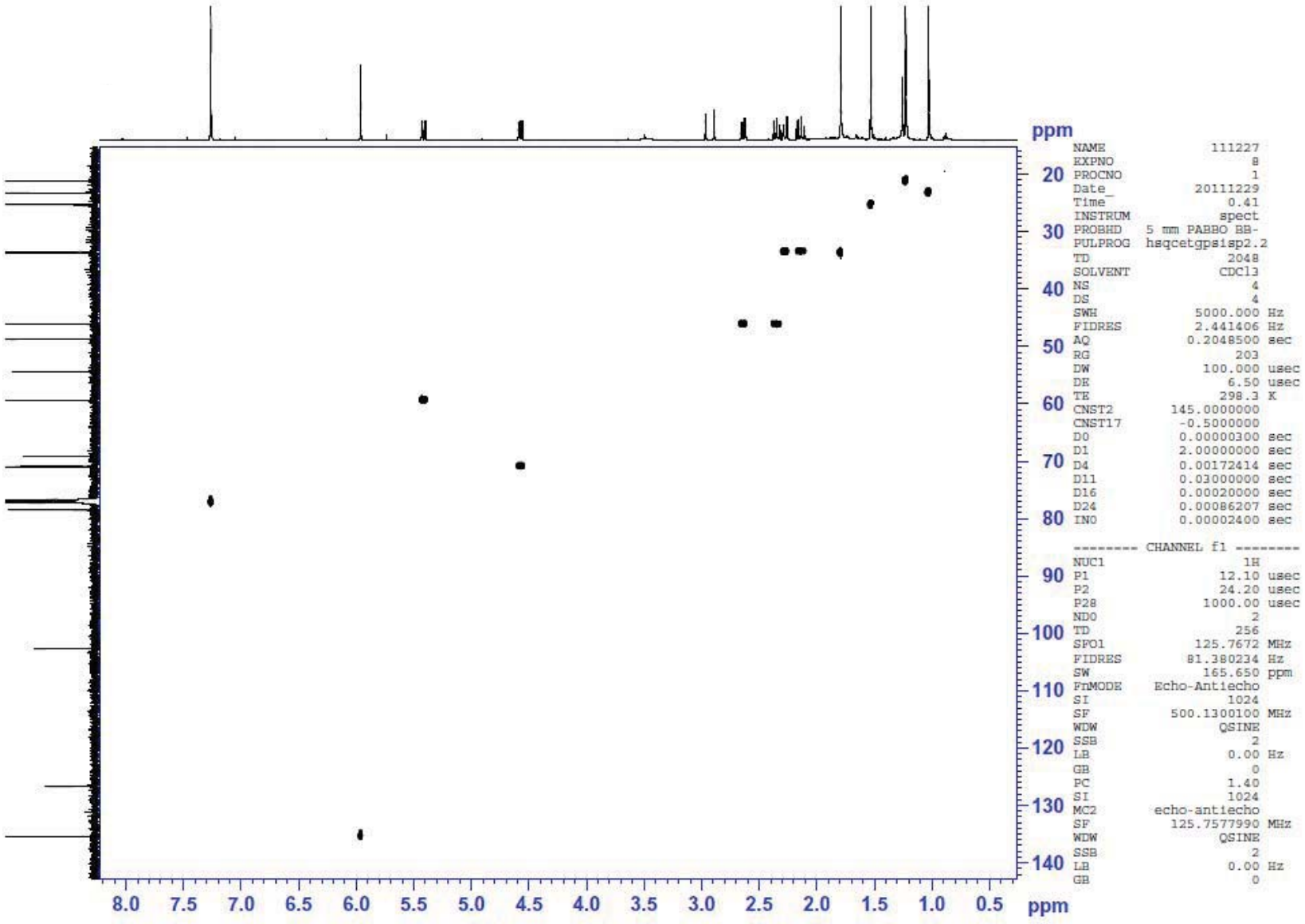

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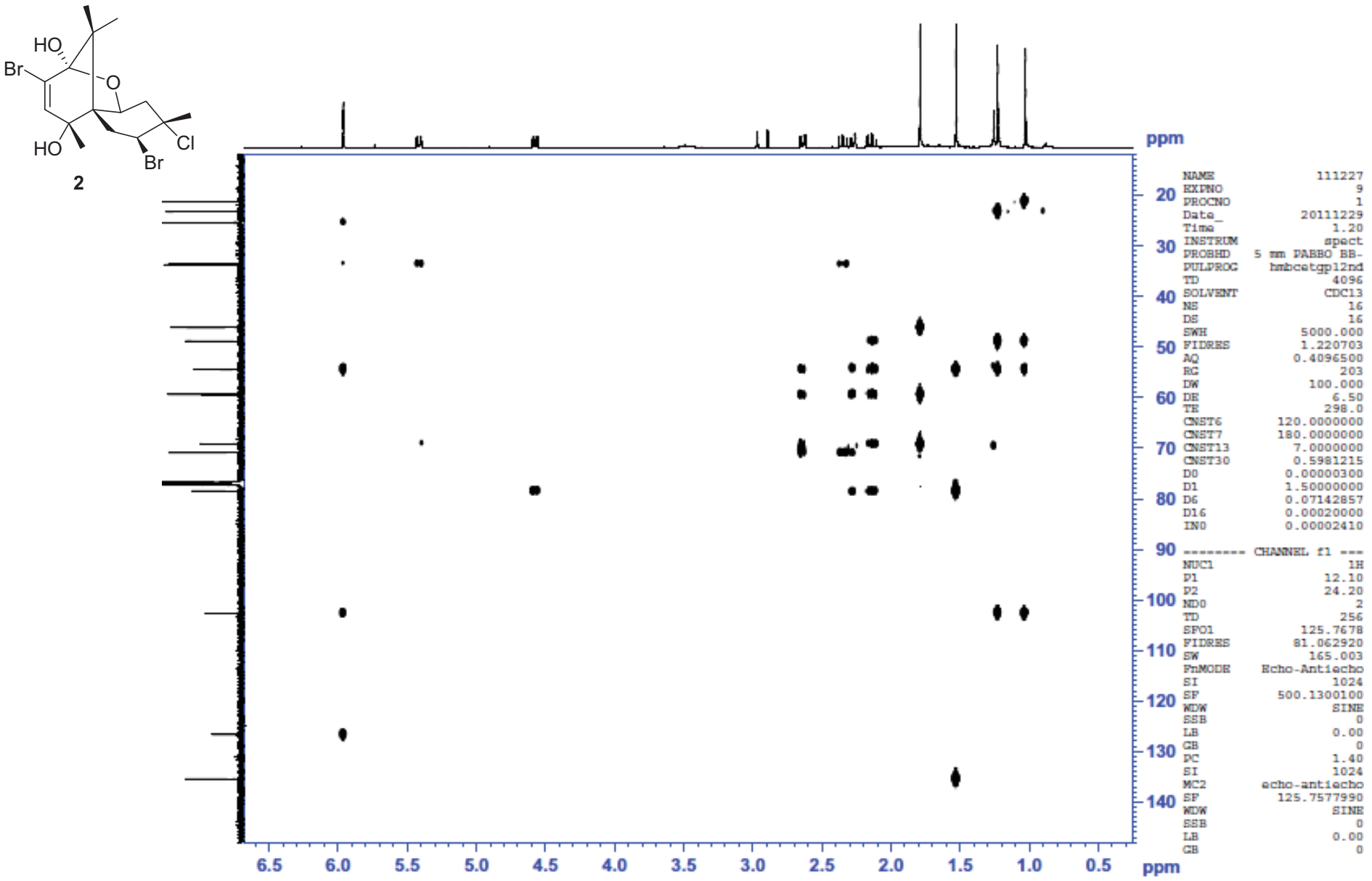
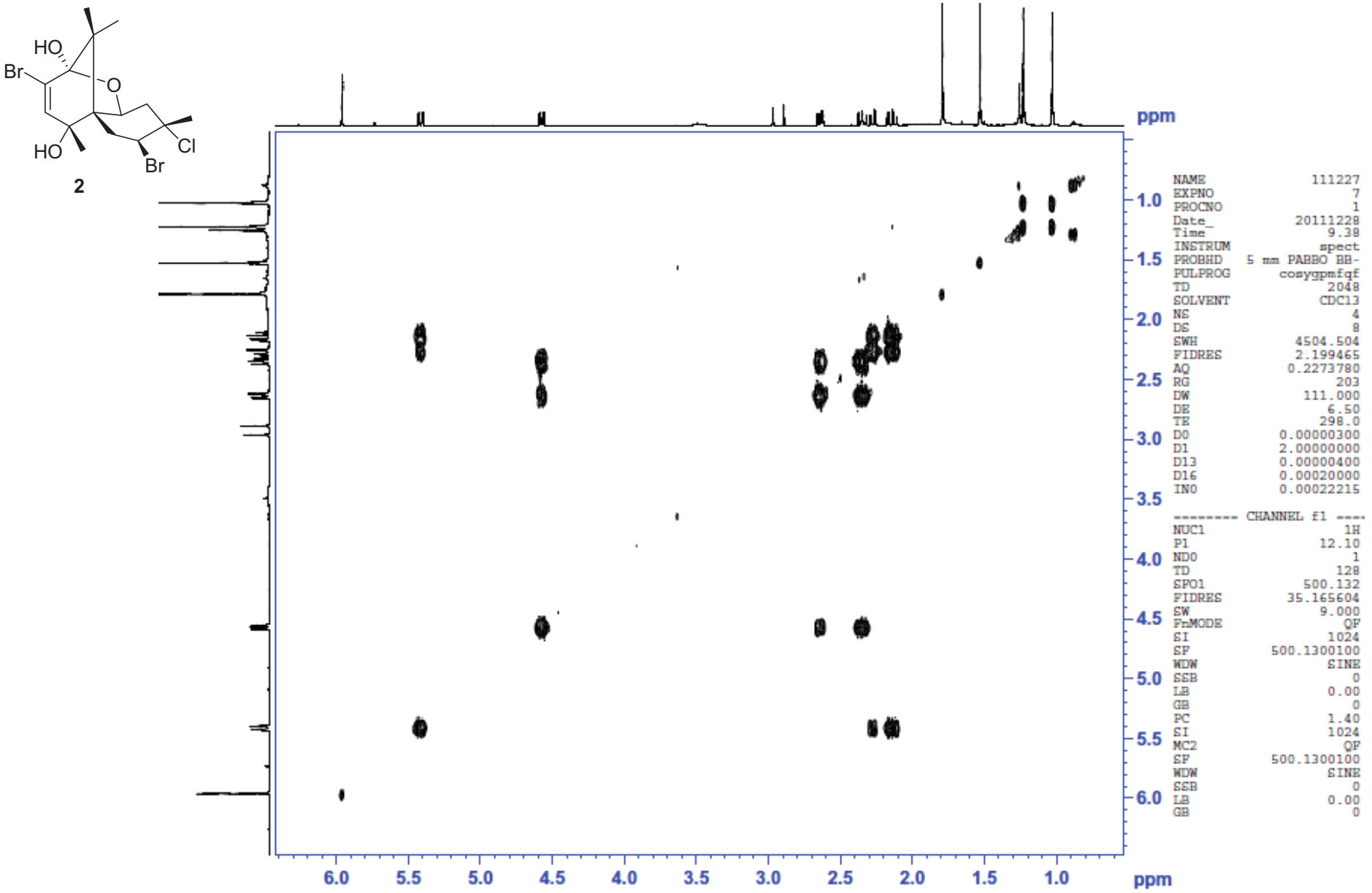
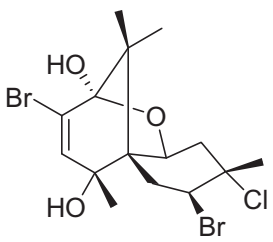
TD	2048
SOLVENT	CDCl3
NS	4
DS	4
SWH	5000.000 Hz
FIDRES	2.441406 Hz
AQ	0.2048500 sec
RG	203
DW	100.000 usec
DE	6.50 usec
TE	298.3 K
CNST2	145.0000000
CNST17	-0.5000000
D0	0.00000300 sec
D1	2.00000000 sec
D4	0.00172414 sec
D11	0.03000000 sec
D16	0.00020000 sec
D24	0.00086207 sec
IN0	0.00002400 sec
-------- CHANNEL f1 --------	
NUC1	1H
P1	12.10 usec
P2	24.20 usec
P28	1000.00 usec
ND0	2
TD	256
SFO1	125.7672 MHz
FIDRES	81.380234 Hz
SW	165.650 ppm
FnMODE	Echo-Antiecho
SI	1024
SF	500.1300100 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	125.7577990 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0







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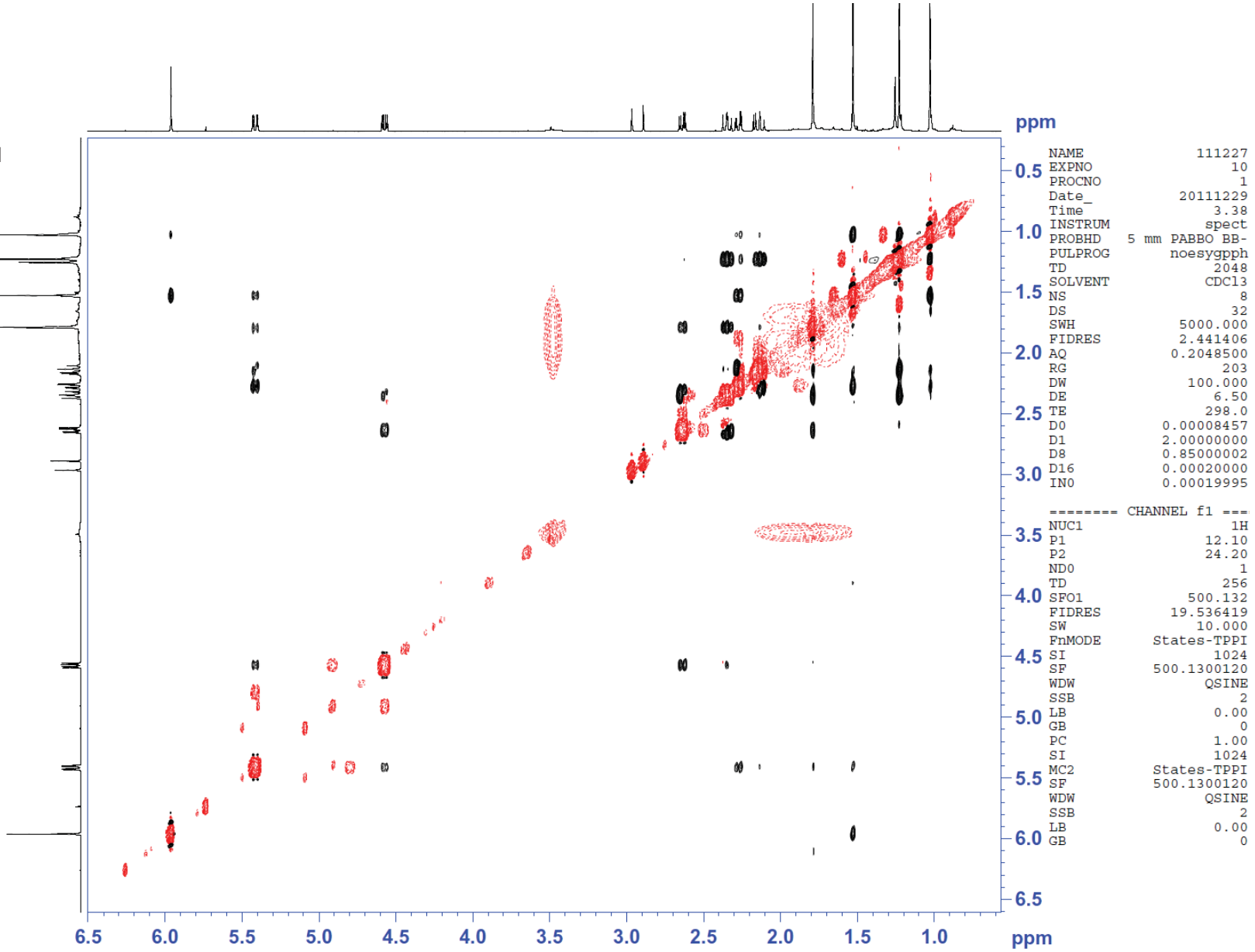

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TD	2048
SOLVENT	CDCl3
NS	8
DS	32
SWH	5000.000
FIDRES	2.441406
AQ	0.2048500
RG	203
DW	100.000
DE	6.50
TE	298.0
D0	0.00008457
D1	2.00000000
D8	0.85000002
D16	0.00020000
IN0	0.00019995
======== CHANNEL f1 ===	
NUC1	1H
P1	12.10
P2	24.20
ND0	1
TD	256
SFO1	500.132
FIDRES	19.536419
SW	10.000
FnMODE	States-TPPI
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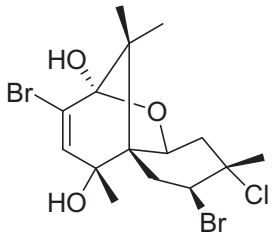
SF	500.1300120
WDW	QSINE
SSB	2
LB	0.00
GB	0
PC	1.00
SI	1024
MC2	States-TPPI
SF	500.1300120
WDW	QSINE
SSB	2
LB	0.00
GB	0



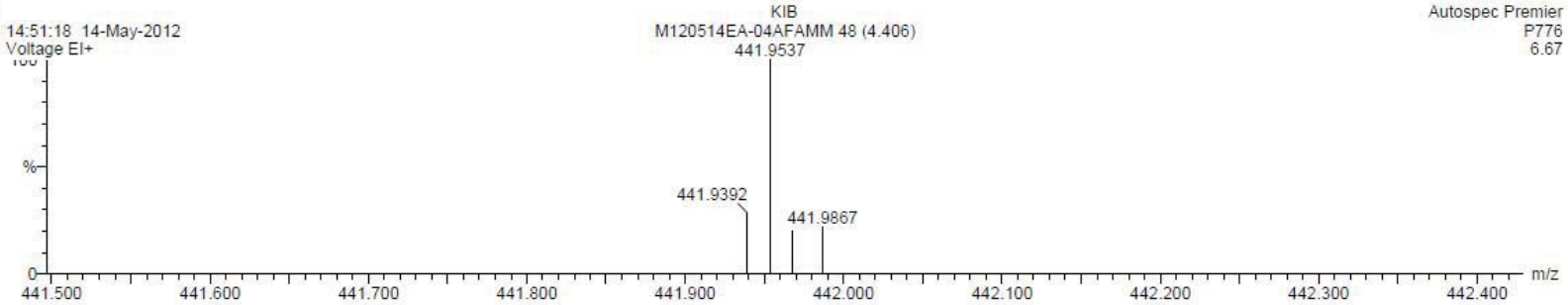
2

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = 0.5, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 O: 1-4 Cl: 1-1 Br: 2-2



Minimum:				0.5		
Maximum:		100.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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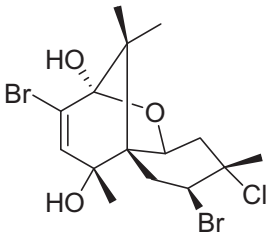

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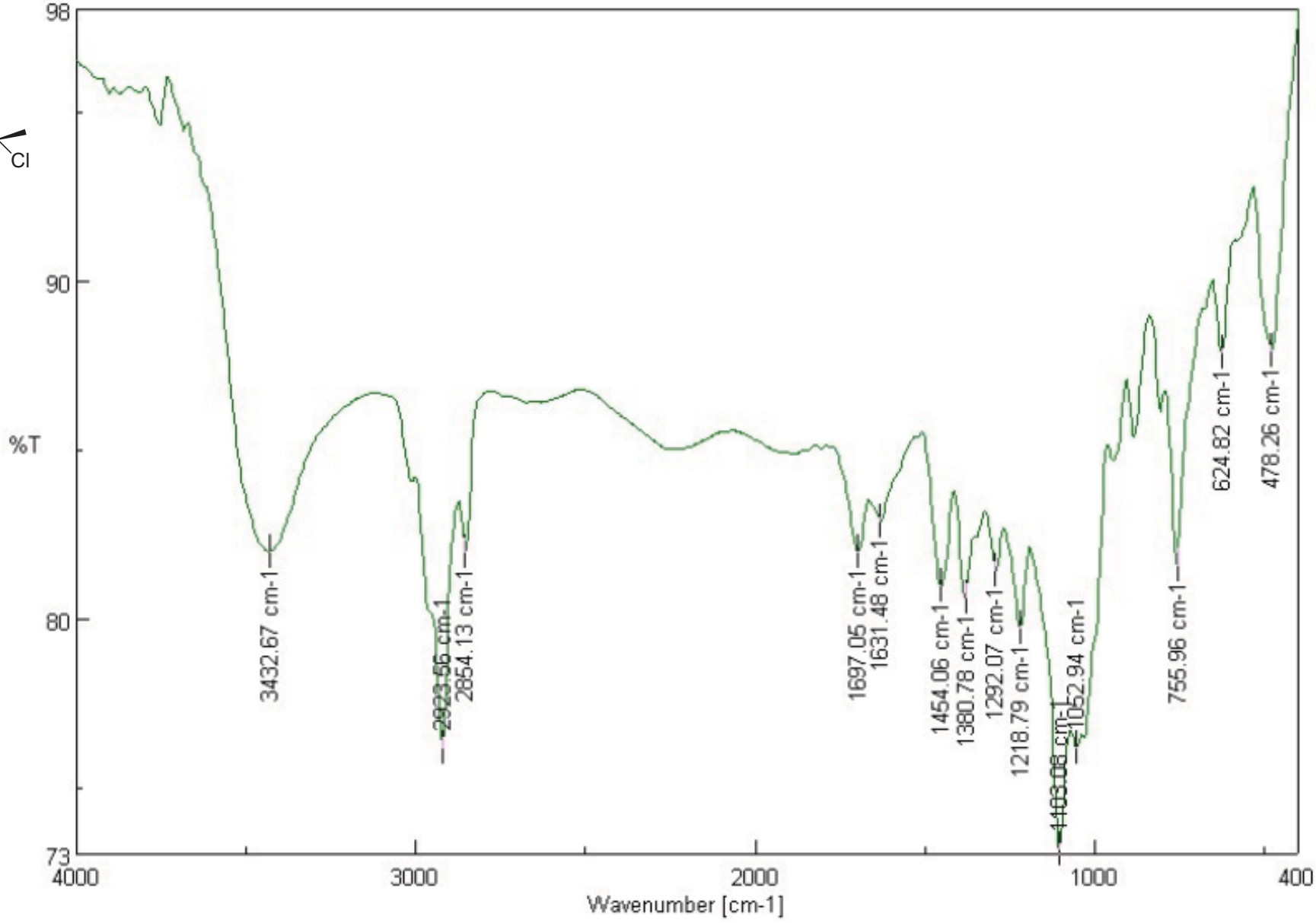

Cartesian coordinates for energy-minimized conformer of **1** optimized by the B3LYP/6-31+G(d,p) basis set in chloroform

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.130100	-0.005700	-0.629400
2	6	0	-2.393400	-0.754300	-1.449100
3	6	0	-0.961100	-1.161300	-1.126900
4	6	0	-0.504900	-0.456000	0.212900
5	6	0	-1.637300	-0.588500	1.318400
6	6	0	-2.601400	0.479000	0.728800
7	6	0	0.905400	-0.901300	0.672100
8	6	0	1.993600	-0.191000	-0.142200
9	6	0	2.056200	1.331500	0.146200
10	6	0	0.660200	1.848900	0.566800
11	6	0	-0.512200	1.101000	-0.060200
12	6	0	-0.781400	-2.688400	-1.193000
13	8	0	-0.131000	-0.605200	-2.184500
14	8	0	-1.748200	1.610800	0.487000
15	6	0	-2.312900	-1.958500	1.521600
16	6	0	-1.184300	-0.137700	2.727200
17	17	0	-4.730700	0.560700	-1.112100
18	8	0	-3.592900	0.826100	1.628400
19	6	0	3.084400	1.782700	1.182800
20	17	0	2.527000	2.162300	-1.463500
21	35	0	3.737800	-1.106400	0.143700
22	1	0	-2.775100	-1.057100	-2.421100
23	1	0	1.025400	-1.980400	0.567300
24	1	0	1.048500	-0.679700	1.731900
25	1	0	1.816600	-0.351300	-1.199700
26	1	0	0.606300	1.770300	1.655300
27	1	0	0.587000	2.913000	0.328500
28	1	0	-0.511300	1.283900	-1.136000
29	1	0	-1.221200	-3.060000	-2.126100
30	1	0	0.281400	-2.943800	-1.203800
31	1	0	-1.257700	-3.220700	-0.372300
32	1	0	-0.260500	-1.128300	-2.988300
33	1	0	-1.579300	-2.709800	1.830600
34	1	0	-3.045700	-1.868100	2.329300
35	1	0	-2.844000	-2.327000	0.645200
36	1	0	-2.063900	-0.054100	3.369300
37	1	0	-0.681900	0.827900	2.743100
38	1	0	-0.522800	-0.885800	3.173000
39	1	0	-4.264000	1.365700	1.182300
40	1	0	4.105000	1.624600	0.835200
41	1	0	2.944000	2.844800	1.401000
42	1	0	2.944300	1.214400	2.108800

Cartesian coordinates for energy-minimized conformer of **1** optimized by the B3LYP/6-31+G(d,p) basis set in methanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.130100	-0.018900	-0.632200
2	6	0	-2.393100	-0.785000	-1.434900
3	6	0	-0.960400	-1.183400	-1.103100
4	6	0	-0.505700	-0.450500	0.223100
5	6	0	-1.640300	-0.560300	1.329300
6	6	0	-2.604200	0.493900	0.715600
7	6	0	0.903400	-0.888400	0.694300
8	6	0	1.989500	-0.192900	-0.134500
9	6	0	2.056400	1.331600	0.134400
10	6	0	0.659400	1.860800	0.535500
11	6	0	-0.511000	1.100400	-0.080400
12	6	0	-0.776500	-2.710900	-1.136300
13	8	0	-0.134300	-0.646300	-2.175200
14	8	0	-1.749500	1.622400	0.451500
15	6	0	-2.315200	-1.926500	1.558100
16	6	0	-1.189000	-0.082200	2.729500
17	17	0	-4.731300	0.538500	-1.128900
18	8	0	-3.597500	0.863600	1.605500
19	6	0	3.078900	1.794300	1.170800
20	17	0	2.543900	2.138500	-1.488600
21	35	0	3.736600	-1.105000	0.151700
22	1	0	-2.773600	-1.109700	-2.399800
23	1	0	1.021500	-1.969200	0.608800
24	1	0	1.046300	-0.646700	1.749600
25	1	0	1.806200	-0.368900	-1.188500
26	1	0	0.601200	1.804900	1.625000
27	1	0	0.590200	2.920000	0.275400
28	1	0	-0.507700	1.261600	-1.159700
29	1	0	-1.218900	-3.105500	-2.058000
30	1	0	0.287100	-2.962600	-1.145800
31	1	0	-1.246200	-3.225400	-0.300600
32	1	0	-0.250000	-1.200300	-2.960800
33	1	0	-1.581500	-2.670000	1.883800
34	1	0	-3.049500	-1.821000	2.362800
35	1	0	-2.843500	-2.313500	0.688000
36	1	0	-2.068900	0.011600	3.370000
37	1	0	-0.685000	0.882800	2.729000
38	1	0	-0.528100	-0.821700	3.189700
39	1	0	-4.285900	1.363700	1.139400
40	1	0	4.101800	1.629500	0.833100
41	1	0	2.938900	2.858900	1.376100
42	1	0	2.929600	1.237700	2.102300

Cartesian coordinates for energy-minimized conformer of **1** optimized by the B3LYP/6-31+G(d,p) basis set in water

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.130189	-0.020535	-0.632504
2	6	0	-2.393105	-0.788906	-1.433035
3	6	0	-0.960359	-1.186119	-1.100089
4	6	0	-0.505868	-0.449788	0.224338
5	6	0	-1.640626	-0.556699	1.330564
6	6	0	-2.604634	0.495776	0.713859
7	6	0	0.902971	-0.886798	0.697002
8	6	0	1.989014	-0.193188	-0.133602
9	6	0	2.056453	1.331482	0.132898
10	6	0	0.659257	1.862376	0.531115
11	6	0	-0.510930	1.100335	-0.083118
12	6	0	-0.775710	-2.713582	-1.129330
13	8	0	-0.134685	-0.651037	-2.173916
14	8	0	-1.749821	1.623855	0.447022
15	6	0	-2.315423	-1.922512	1.562709
16	6	0	-1.189589	-0.075075	2.729658
17	17	0	-4.731393	0.535666	-1.130911
18	8	0	-3.598132	0.868093	1.602560
19	6	0	3.077829	1.795420	1.169750
20	17	0	2.546732	2.135339	-1.491627
21	35	0	3.736291	-1.104807	0.152712
22	1	0	-2.773581	-1.116399	-2.397002
23	1	0	1.020848	-1.967768	0.613924
24	1	0	1.045843	-0.642565	1.751627
25	1	0	1.804861	-0.371201	-1.187051
26	1	0	0.600423	1.809845	1.620717
27	1	0	0.590630	2.920848	0.267890
28	1	0	-0.507671	1.258760	-1.162779
29	1	0	-1.217598	-3.110855	-2.050080
30	1	0	0.288069	-2.964665	-1.137844
31	1	0	-1.245296	-3.225930	-0.292310
32	1	0	-0.250179	-1.207503	-2.957866
33	1	0	-1.581507	-2.664957	1.890345
34	1	0	-3.049834	-1.815078	2.367000
35	1	0	-2.843332	-2.311853	0.693430
36	1	0	-2.069582	0.020224	3.369803
37	1	0	-0.685101	0.889620	2.726967
38	1	0	-0.528948	-0.813616	3.191713
39	1	0	-4.288446	1.363589	1.134313
40	1	0	4.101167	1.629439	0.833762
41	1	0	2.938141	2.860387	1.373146
42	1	0	2.926689	1.240439	2.101924

Cartesian coordinates for energy-minimized conformer of **2** optimized by the B3LYP/6-31+G(d,p) basis set in chloroform

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.742800	-0.101500	-0.382100
2	6	0	-2.033700	-0.652100	-1.365200
3	6	0	-0.570800	-1.045300	-1.199700
4	6	0	-0.064700	-0.572700	0.221100
5	6	0	-1.119700	-0.967500	1.340000
6	6	0	-2.160700	0.141100	1.015700
7	6	0	1.389100	-1.019000	0.512100
8	6	0	2.390400	-0.114900	-0.217100
9	6	0	2.410000	1.327900	0.348400
10	6	0	1.023200	1.686400	0.933000
11	6	0	-0.156300	1.006500	0.245900
12	6	0	-0.335100	-2.523100	-1.557300
13	8	0	0.168700	-0.263400	-2.179100
14	8	0	-1.370800	1.340200	0.952500
15	6	0	-0.598200	-0.760900	2.781600
16	6	0	-1.726900	-2.383600	1.318000
17	35	0	-4.509100	0.563300	-0.709600
18	8	0	-3.108900	0.259700	2.014400
19	6	0	3.479900	1.628700	1.397000
20	17	0	2.747900	2.466300	-1.098200
21	35	0	4.186300	-0.974300	-0.215300
22	1	0	-2.455700	-0.779600	-2.358500
23	1	0	1.547000	-2.053000	0.202800
24	1	0	1.592100	-0.987000	1.584600
25	1	0	2.148500	-0.085700	-1.273200
26	1	0	1.042600	1.405800	1.989100
27	1	0	0.892200	2.771000	0.903000
28	1	0	-0.237200	1.385400	-0.774400
29	1	0	-0.808700	-2.737200	-2.522400
30	1	0	0.734700	-2.718700	-1.664600
31	1	0	-0.745000	-3.220700	-0.829800
32	1	0	-0.000400	-0.626600	-3.060400
33	1	0	-1.436900	-0.850200	3.475600
34	1	0	0.126400	-1.537800	3.040900
35	1	0	-0.142900	0.213500	2.949300
36	1	0	-2.411600	-2.479100	2.166200
37	1	0	-0.946700	-3.141100	1.441800
38	1	0	-2.296900	-2.611800	0.418400
39	1	0	-3.841900	0.814000	1.700600
40	1	0	4.483500	1.589400	0.974300
41	1	0	3.310700	2.622500	1.820100
42	1	0	3.416800	0.890400	2.204000

Cartesian coordinates for energy-minimized conformer of **2** optimized by the B3LYP/6-31+G(d,p) basis set in methanol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.743000	-0.104700	-0.382200
2	6	0	-2.033400	-0.662500	-1.360800
3	6	0	-0.569800	-1.052900	-1.191300
4	6	0	-0.065000	-0.570900	0.226800
5	6	0	-1.121700	-0.957500	1.347300
6	6	0	-2.162500	0.148400	1.013500
7	6	0	1.388300	-1.017300	0.523100
8	6	0	2.388400	-0.117500	-0.212400
9	6	0	2.410800	1.326800	0.346800
10	6	0	1.024000	1.692600	0.925700
11	6	0	-0.154700	1.008200	0.241500
12	6	0	-0.331500	-2.532300	-1.538700
13	8	0	0.164900	-0.274000	-2.178200
14	8	0	-1.371400	1.348600	0.942600
15	6	0	-0.600000	-0.743100	2.787600
16	6	0	-1.729300	-2.373600	1.333800
17	35	0	-4.510200	0.558600	-0.715700
18	8	0	-3.111900	0.279000	2.010900
19	6	0	3.480300	1.633900	1.393200
20	17	0	2.753900	2.458500	-1.110800
21	35	0	4.186300	-0.975000	-0.214500
22	1	0	-2.453700	-0.799300	-2.353300
23	1	0	1.544700	-2.053000	0.219700
24	1	0	1.590700	-0.979200	1.595300
25	1	0	2.142900	-0.094600	-1.267900
26	1	0	1.042900	1.420200	1.983800
27	1	0	0.895500	2.777300	0.887900
28	1	0	-0.234200	1.380400	-0.781400
29	1	0	-0.810100	-2.756200	-2.498700
30	1	0	0.738500	-2.724800	-1.650200
31	1	0	-0.733500	-3.224500	-0.801900
32	1	0	0.022100	-0.666800	-3.051800
33	1	0	-1.438200	-0.829300	3.482800
34	1	0	0.123300	-1.519600	3.050600
35	1	0	-0.141200	0.230600	2.950900
36	1	0	-2.416900	-2.462300	2.180500
37	1	0	-0.949500	-3.129500	1.467200
38	1	0	-2.295300	-2.609700	0.433800
39	1	0	-3.859000	0.805600	1.681700
40	1	0	4.484300	1.591400	0.972000
41	1	0	3.311000	2.629700	1.811100
42	1	0	3.415300	0.900600	2.204300

Cartesian coordinates for energy-minimized conformer of **2** optimized by the B3LYP/6-31+G(d,p) basis set in water

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.743065	-0.105011	-0.382176
2	6	0	-2.033517	-0.664224	-1.359922
3	6	0	-0.569852	-1.054087	-1.190081
4	6	0	-0.065081	-0.570411	0.227537
5	6	0	-1.121899	-0.955794	1.348337
6	6	0	-2.162720	0.149707	1.013269
7	6	0	1.388000	-1.016870	0.524666
8	6	0	2.388081	-0.117864	-0.211808
9	6	0	2.411006	1.326708	0.346409
10	6	0	1.024167	1.693766	0.924135
11	6	0	-0.154456	1.008622	0.240548
12	6	0	-0.330867	-2.533706	-1.535649
13	8	0	0.163909	-0.275870	-2.178491
14	8	0	-1.371364	1.350103	0.940965
15	6	0	-0.600009	-0.740484	2.788507
16	6	0	-1.729503	-2.371949	1.336262
17	35	0	-4.510496	0.557784	-0.716576
18	8	0	-3.112238	0.282235	2.010439
19	6	0	3.480235	1.634612	1.392775
20	17	0	2.755593	2.457375	-1.112732
21	35	0	4.186157	-0.975379	-0.214268
22	1	0	-2.453833	-0.802627	-2.352196
23	1	0	1.544228	-2.052841	0.222154
24	1	0	1.590248	-0.977915	1.596840
25	1	0	2.142196	-0.095836	-1.267203
26	1	0	1.042834	1.422857	1.982579
27	1	0	0.896110	2.778452	0.884919
28	1	0	-0.233898	1.379777	-0.782739
29	1	0	-0.809566	-2.759245	-2.495215
30	1	0	0.739231	-2.725676	-1.647168
31	1	0	-0.731994	-3.225196	-0.797754
32	1	0	0.024614	-0.673032	-3.050725
33	1	0	-1.438162	-0.826105	3.483864
34	1	0	0.122846	-1.517316	3.051760
35	1	0	-0.140337	0.232809	2.951326
36	1	0	-2.417455	-2.459645	2.182804
37	1	0	-0.949657	-3.127501	1.471035
38	1	0	-2.295017	-2.609296	0.436287
39	1	0	-3.861409	0.804617	1.679042
40	1	0	4.484463	1.591175	0.971995
41	1	0	3.311152	2.630901	1.809622
42	1	0	3.414595	0.902266	2.204629

Experimental and calculated ECD data ($\Delta\varepsilon$) for **1** and **2**

wavelength	exptl-1	calcd-1	exptl-2	calcd-2
195	0.477405	-8.62728	-0.91786	-1.41606
196	0.322748	-11.7837	-0.7316	-2.20037
197	-0.16754	-15.3538	-0.9145	-3.23471
198	-0.67283	-19.1185	-0.97368	-4.50582
199	-0.98166	-22.7927	-1.02558	-5.95596
200	-1.21534	-26.0664	-1.02747	-7.48134
201	-1.25964	-28.6558	-1.03401	-8.94227
202	-1.20636	-30.3504	-1.10423	-10.1848
203	-1.10373	-31.0443	-1.13874	-11.0694
204	-0.96769	-30.7435	-1.14118	-11.5003
205	-0.75424	-29.5482	-1.20421	-11.4459
206	-0.47431	-27.6156	-1.17844	-10.9462
207	-0.20037	-25.1179	-1.24452	-10.1038
208	0.091362	-22.2048	-1.24943	-9.0611
209	0.354786	-18.9833	-1.34109	-7.96976
210	0.585838	-15.5169	-1.43406	-6.96061
211	0.771175	-11.8424	-1.53729	-6.12018
212	0.911131	-7.99686	-1.56712	-5.47886
213	0.989973	-4.04305	-1.6764	-5.01178
214	1.05393	-0.08672	-1.63184	-4.6506
215	1.02969	3.721723	-1.56403	-4.30244
216	0.985033	7.200691	-1.44347	-3.87129
217	0.928957	10.16245	-1.2465	-3.27762
218	0.870705	12.44298	-0.98801	-2.47299
219	0.797385	13.92901	-0.75109	-1.44791
220	0.713242	14.57622	-0.48097	-0.23246
221	0.581905	14.41492	-0.25818	1.10942
222	0.470013	13.54327	-0.00517	2.490354
223	0.356707	12.11035	0.27218	3.812507
224	0.269965	10.29359	0.484709	4.980916
225	0.215708	8.275258	0.69342	5.915156
226	0.153388	6.222063	0.858374	6.557876
227	0.099701	4.270642	0.944446	6.879374
228	0.058001	2.519891	1.007998	6.87813
229	-0.01854	1.02975	1.033857	6.577808
230	-0.0807	-0.175	1.045813	6.021712
231	-0.14526	-1.09781	1.046758	5.265882
232	-0.1969	-1.76212	1.009827	4.372018
233	-0.24499	-2.20335	0.953001	3.401185
234	-0.27113	-2.46204	0.885262	2.40897
235	-0.29679	-2.57868	0.823969	1.442345
236	-0.3026	-2.59023	0.756307	0.538219
237	-0.29993	-2.5282	0.694368	-0.27663
238	-0.32039	-2.41793	0.623621	-0.98464
239	-0.33323	-2.27871	0.550832	-1.57603
240	-0.34548	-2.12447	0.457503	-2.04723
241	-0.36696	-1.96463	0.333694	-2.39945
242	-0.39093	-1.80517	0.231825	-2.63748
243	-0.42688	-1.64957	0.14041	-2.76889
244	-0.42944	-1.4996	0.067325	-2.80341
245	-0.40782	-1.35605	0.028441	-2.7525
246	-0.41055	-1.21919	-0.01629	-2.62903
247	-0.40303	-1.08911	-0.05554	-2.44683
248	-0.39081	-0.96594	-0.08394	-2.22027
249	-0.39365	-0.84991	-0.12218	-1.96369
250	-0.41175	-0.74135	-0.15519	-1.69089
251	-0.42323	-0.64064	-0.18544	-1.41452

252	-0.41926	-0.54818	-0.20891	-1.14561
253	-0.37682	-0.46424	-0.22418	-0.89321
254	-0.35041	-0.38899	-0.23465	-0.66416
255	-0.32342	-0.32242	-0.2536	-0.46303
256	-0.29014	-0.2643	-0.24197	-0.29225
257	-0.27297	-0.21427	-0.23276	-0.15231
258	-0.25606	-0.1718	-0.22743	-0.0421
259	-0.2498	-0.13623	-0.22222	0.04068
260	-0.24639	-0.10685	-0.22237	0.099202
261	-0.22994	-0.0829	-0.22294	0.13709
262	-0.21299	-0.06364	-0.20353	0.158116
263	-0.20268	-0.04834	-0.2117	0.165949
264	-0.18898	-0.03635	-0.21484	0.163964
265	-0.16404	-0.02705	-0.21495	0.155118
266	-0.12332	-0.01994	-0.16854	0.141893
267	-0.12598	-0.01455	-0.13747	0.126279
268	-0.10796	-0.01052	-0.08973	0.109798
269	-0.10596	-0.00754	-0.05731	0.093553
270	-0.10553	-0.00535	-0.03759	0.078289
271	-0.11408	-0.00377	-0.03151	0.064458
272	-0.10335	-0.00263	-0.02201	0.052285
273	-0.10386	-0.00182	-0.01208	0.041832
274	-0.07556	-0.00125	0.016833	0.033043
275	-0.07175	-0.00085	0.036513	0.025789
276	-0.06685	-0.00058	0.055071	0.0199
277	-0.04964	-0.00039	0.057647	0.015193
278	-0.04698	-0.00026	0.063491	0.011482
279	-0.04407	-0.00017	0.08379	0.008593
280	-0.03586	-0.00011	0.124062	0.006372
281	-0.05454	-7.30E-05	0.133723	0.004684
282	-0.04792	-4.70E-05	0.139176	0.003413
283	-0.03166	-0.00003	0.153543	0.002467
284	-0.03989	-0.00002	0.155214	0.00177
285	-0.01943	-1.20E-05	0.158746	0.00126
286	-0.01481	-8.00E-06	0.158784	0.00089
287	-0.00343	-5.00E-06	0.167541	0.000625
288	-0.00036	-3.00E-06	0.172438	0.000435
289	-0.01096	-2.00E-06	0.156027	0.000302
290	-0.02047	-1.00E-06	0.151441	0.000207
291	-0.00481	-1.00E-06	0.144521	0.000142
292	-0.01703	0	0.14439	0.000096
293	-0.02147	0	0.146036	0.000065
294	-0.04349	0	0.1371	0.000044
295	-0.0475	0	0.133332	0.000029
296	-0.06544	0	0.132013	0.00002
297	-0.07521	0	0.119376	0.000013
298	-0.07877	0	0.117254	0.000009
299	-0.05561	0	0.097999	0.000006
300	-0.04849	0	0.095586	0.000004
301	-0.03425	0	0.082073	0.000002
302	-0.03114	0	0.058878	0.000002
303	-0.03926	0	0.039819	0.000001
304	-0.05097	0	0.029867	0.000001
305	-0.05559	0	0.009973	0