

Bioactive Norditerpenoids and Neolignans from the Roots of *Salvia miltiorrhiza*[†]

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[†] Electronic Supplementary Information (ESI) available: See DOI: 10.1039/x0xx00000x

Supporting Information

Table of Contents

1. Supplementary Figures

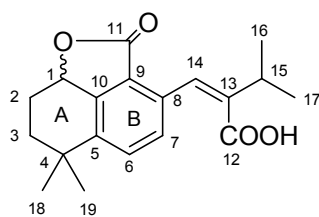
S1	HRESIMS spectrum of 1	4
S2	IR spectrum of 1	5
S3	¹ H NMR spectrum of 1 tested in	6
S4	¹³ C NMR spectrum of 1 tested in C ₅ D ₅ N.....	7
S5	HSQC spectrum of 1 tested in C ₅ D ₅ N.....	8
S6	HMBC spectrum of 1 tested in C ₅ D ₅ N.....	9
S7	Single-crystal X-ray structure of 1	10
S8	HRESIMS spectrum of 2	11
S9	IR spectrum of 2	12
S10	¹ H NMR spectrum of 2 tested in CD ₃ OD.....	13
S11	¹³ C NMR spectrum of 2 tested in CD ₃ OD.....	14
S12	HSQC spectrum of 2 tested in CD ₃ OD.....	15
S13	HMBC correlations and spectrum of 2 tested in CD ₃ OD.....	16
S14	NOESY spectrum of 2 tested in CD ₃ OD.....	17
S15	HRESIMS spectrum of 3	18
S16	IR spectrum of 3	19
S17	¹ H NMR spectrum of 3 tested in CD ₃ OD.....	20
S18	¹³ C NMR spectrum of 3 tested in CD ₃ OD.....	21
S19	HSQC spectrum of 3 tested in CD ₃ OD.....	22
S20	HMBC spectrum of 3 tested in CD ₃ OD.....	23
S21	NOESY spectrum of 3 tested in CD ₃ OD.....	24
S22	HRESIMS spectrum of 4	25
S23	IR spectrum of 4	26
S24	¹ H NMR spectrum of 4 tested in DMSO- <i>d</i> ₆	27
S25	¹³ C NMR spectrum of 4 tested in DMSO- <i>d</i> ₆	28
S26	HSQC spectrum of 4 tested in DMSO- <i>d</i> ₆	29
S27	HMBC spectrum of 4 tested in DMSO- <i>d</i> ₆	30
S28	NOESY spectrum of 4 tested in DMSO- <i>d</i> ₆	31
S29	HRESIMS spectrum of 5 tested in CD ₃ OD.....	32
S30	¹ H NMR spectrum of 5 tested in CD ₃ OD.....	33
S31	¹³ C NMR spectrum of 5 tested in CD ₃ OD.....	34
S32	HMBC spectrum of 5 tested in DMSO- <i>d</i> ₆	35
S33	Single-crystal X-ray data of 1	36
S34	The chiral HPLC chromatogram of 1	47
S35	The chiral HPLC chromatogram of 2	47
S36	The chiral HPLC chromatogram of 3	48
S37	The chiral HPLC chromatogram of 4	48
S38	The CD spectra of 1 in MeOH.....	49
S39	The CD spectra of 1a in MeOH.....	50
S40	The CD spectra of 1b in MeOH.....	51

S41	The CD spectra of 2a in MeOH.....	52
S42	The CD spectra of 2b in MeOH.....	53
S43	The CD spectra of 3a in MeOH.....	54
S44	The CD spectra of 3b in MeOH.....	55
S45	The calculated CD spectra of 3a and 3b in MeOH.....	56
S46	The CD spectra of 4a in MeOH.....	57
S47	The CD spectra of 4b in MeOH.....	58
S48	The calculated CD spectra of 4a and 4b in MeOH.....	59
S49	ES-MS spectrum of 1	60
S50	ES-MS spectrum of 2	63
S51	ES-MS spectrum of 3	66
S52	ES-MS spectrum of 4	69

Supplementary Tables

1	Conformations of 1a and 1b	71
2	Conformations of 2a and 2b	72
3	Conformations of 3a and 3b	73
4	Conformations of 4a and 4b	74
5	The toxic effect of isolates in H9c2 cells after 24 h incubation.....	75
6	The cytoprotective effects of the isolates assessed using LDH leakage assays	76
7	The toxic effect of isolates in LPS-induced N9 cell viability.....	77

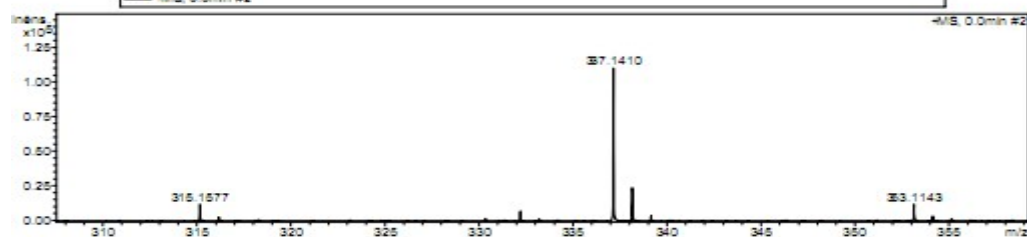
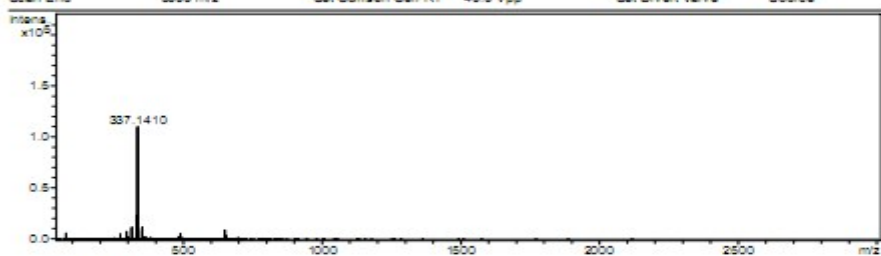
S1 HRESIMS spectrum of 1



Compound Mass Spectrum List Report

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 Operator: Bruker Customer
 Instrument / Ser#: micrOTOF-Q 125

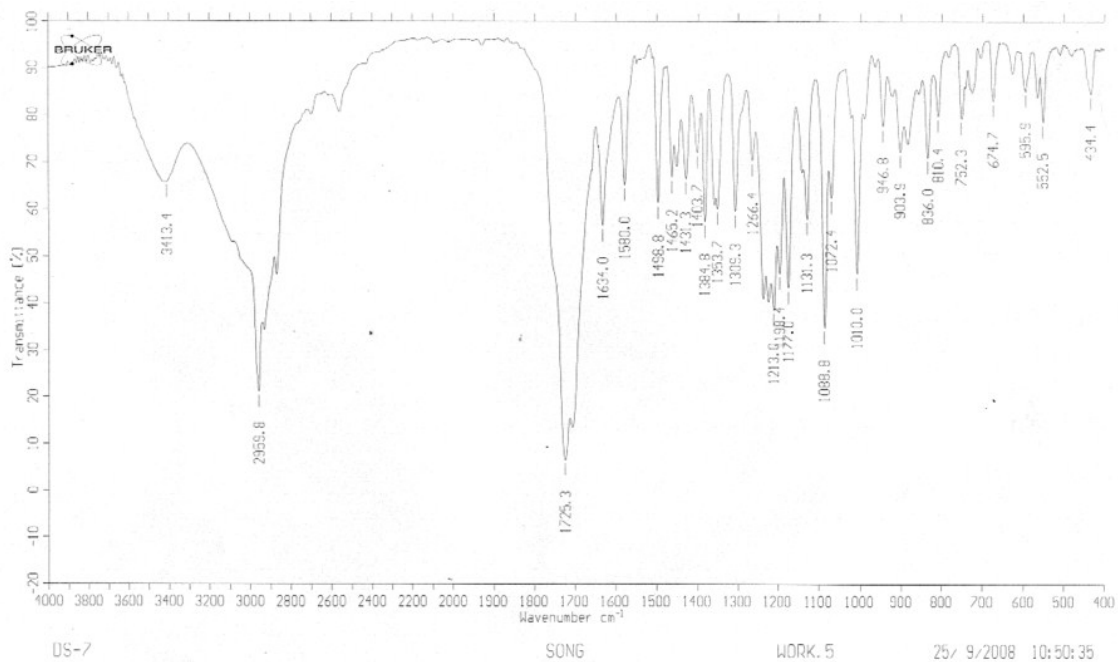
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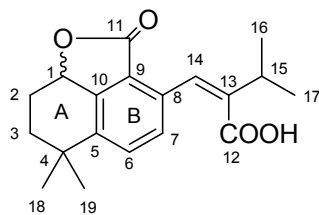
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S2 IR spectrum of 1



S3 ¹H NMR spectrum of 1 tested in C₅D₅N



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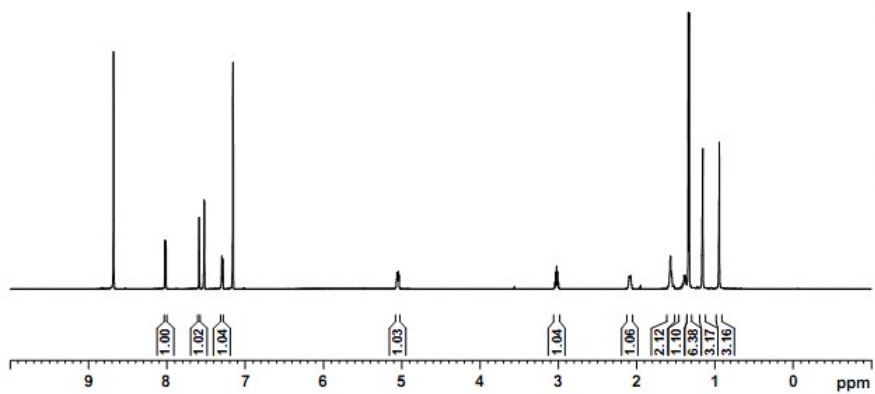
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3.0000
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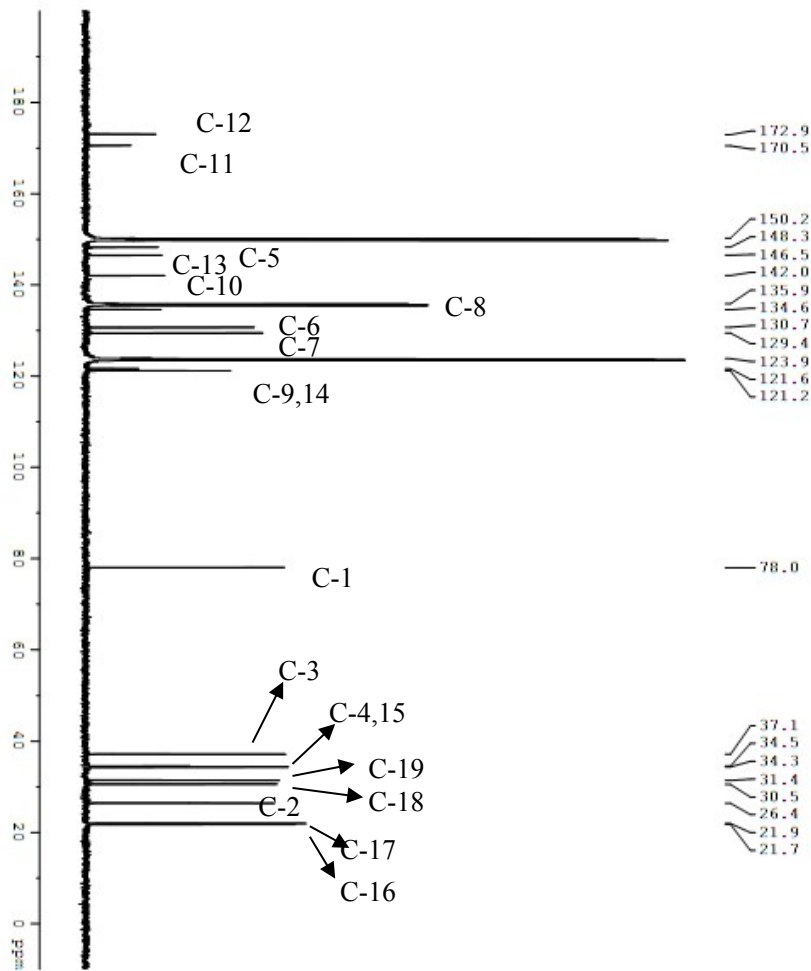
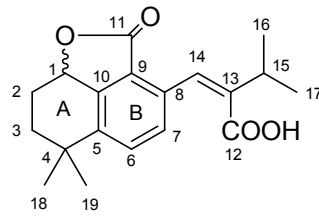


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SOLVENT       Pye
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FIDRES        0.274432 Hz
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RG            320
AQ           0.000000 sec
DE           6.50 usec
TE            300.2 K
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NUC2           1
H2O           1.00000000 sec
----- CHANNEL f1 -----
NUC1           1H
P1            11.00 usec
PL1           +1.00 dB
PC1           34.70088872 W
SFO1          800.1300000 MHz
SF            800.1300000 MHz
WDW           EM
SSB           0
GB            0
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RG            1.00
  
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S4 ¹³C NMR spectrum of 1 tested in C₅D₅N



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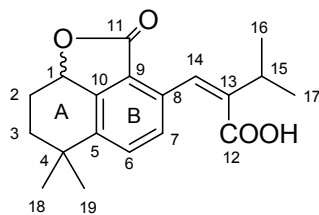
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TE: 300.2
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D11: 0.0000000
TD0: 1

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LB1: 1.0000000
GB1: 0
PC1: 1.0000000
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PL15: 1.0000000
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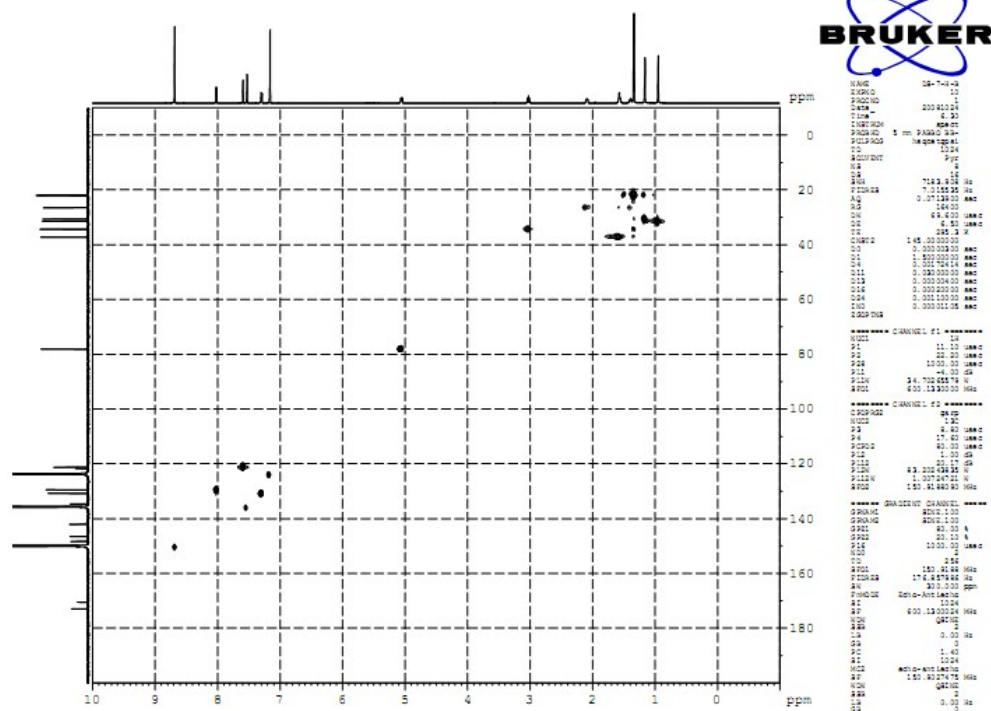
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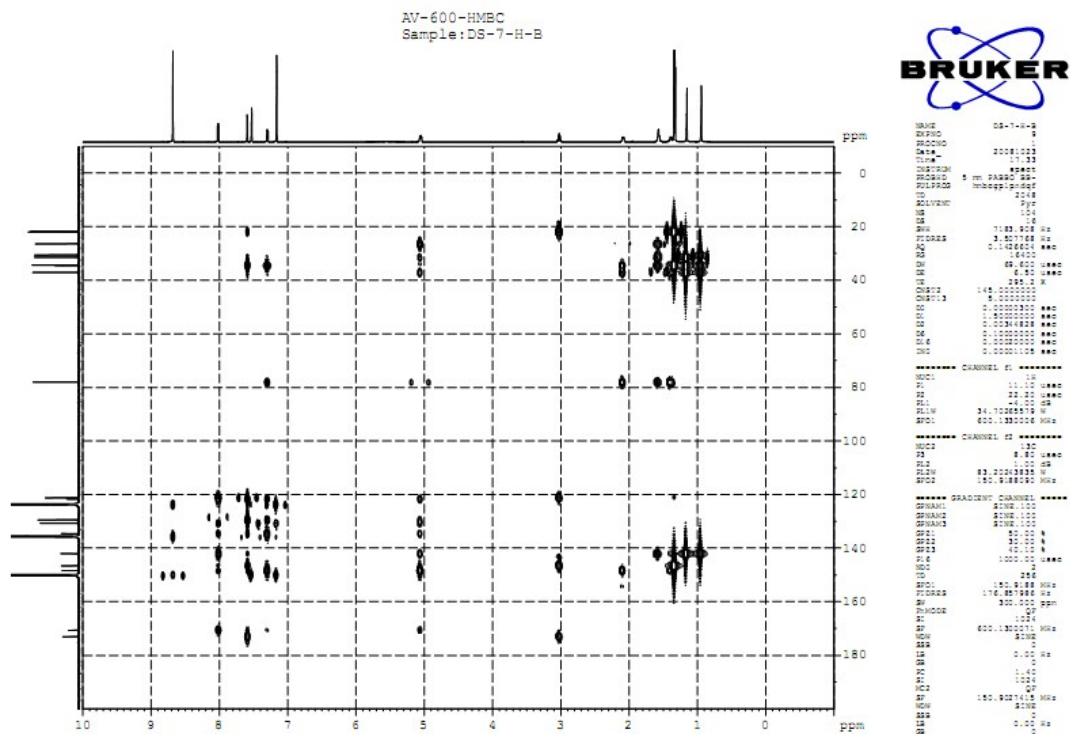
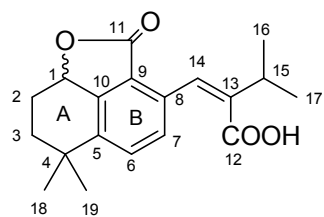
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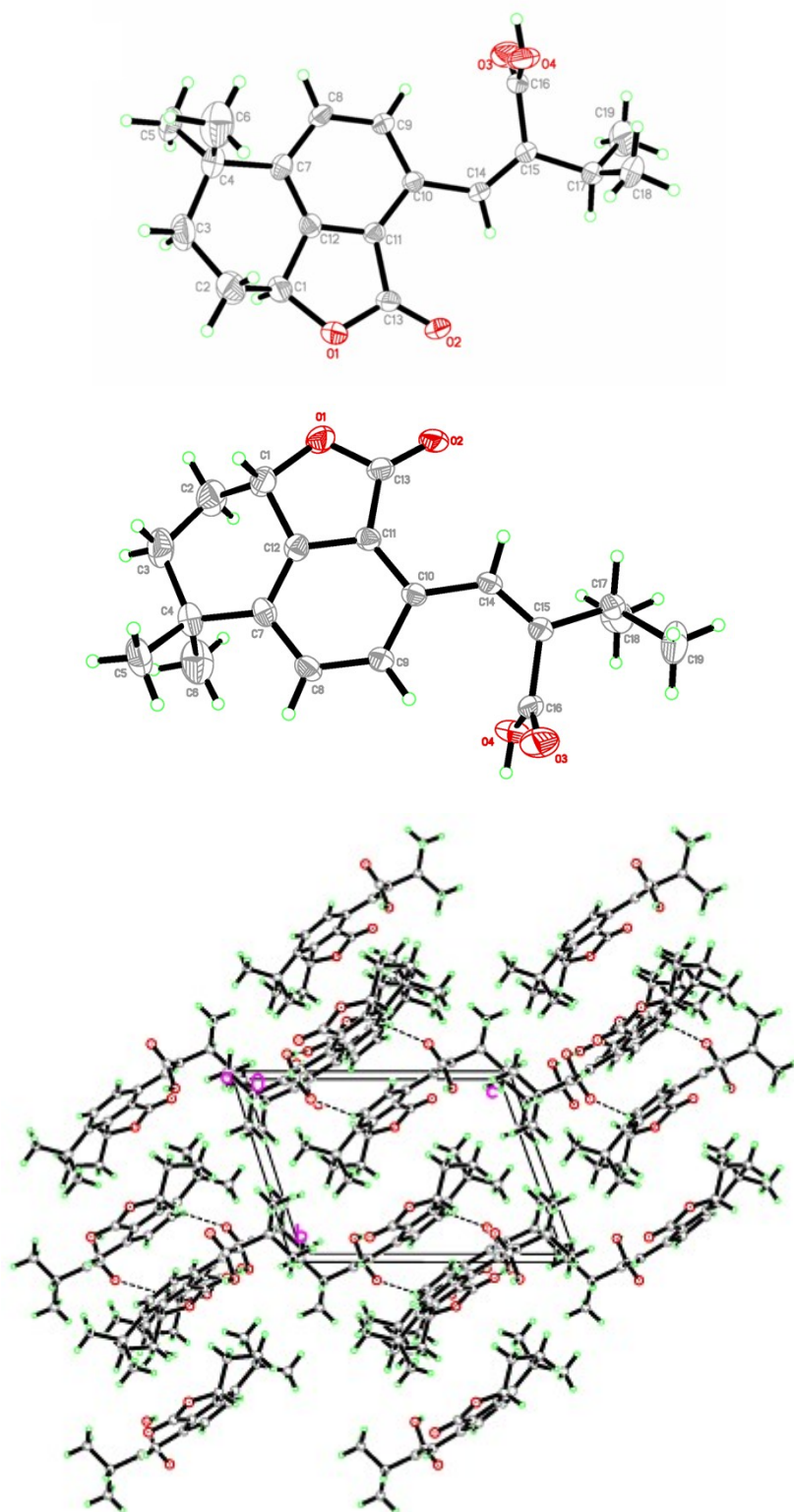
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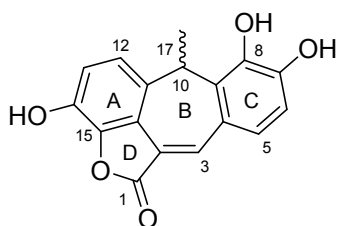
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S7 Single-crystal X-ray structure of 1



S8 HRESIMS spectrum of 2



Compound Mass Spectrum List Report

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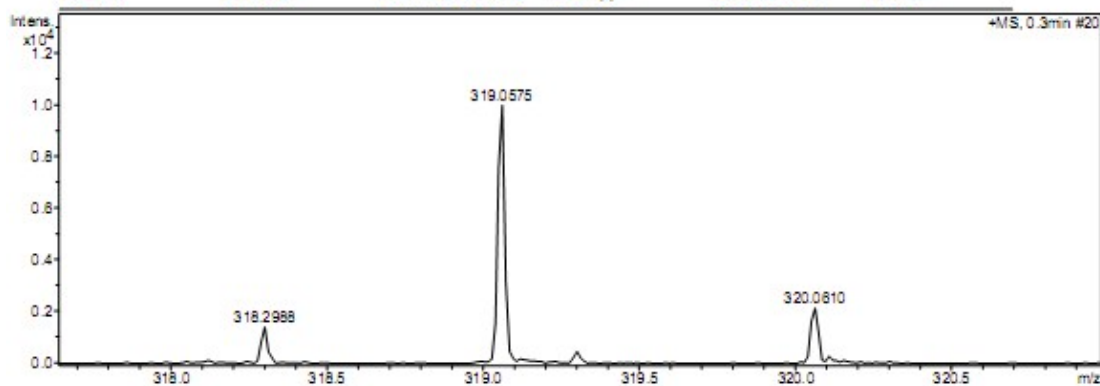
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Operator Bruker Customer
 Instrument / Ser# micrOTOF-Q 125

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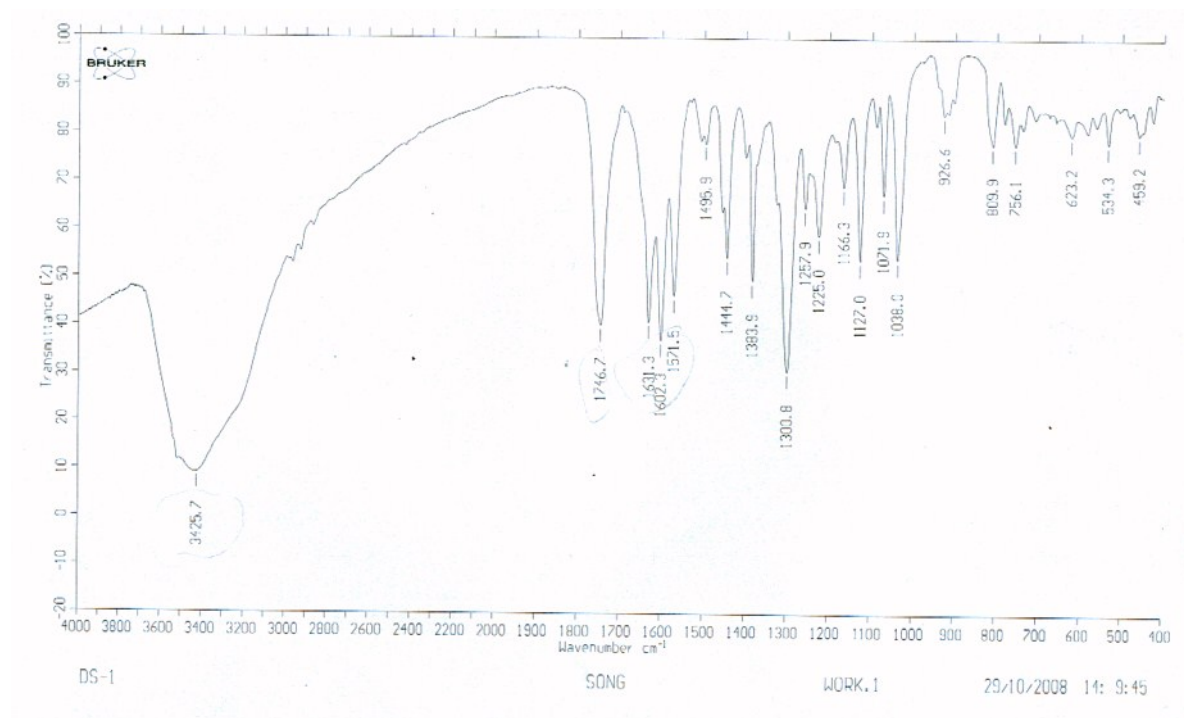
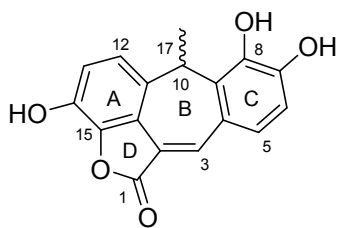
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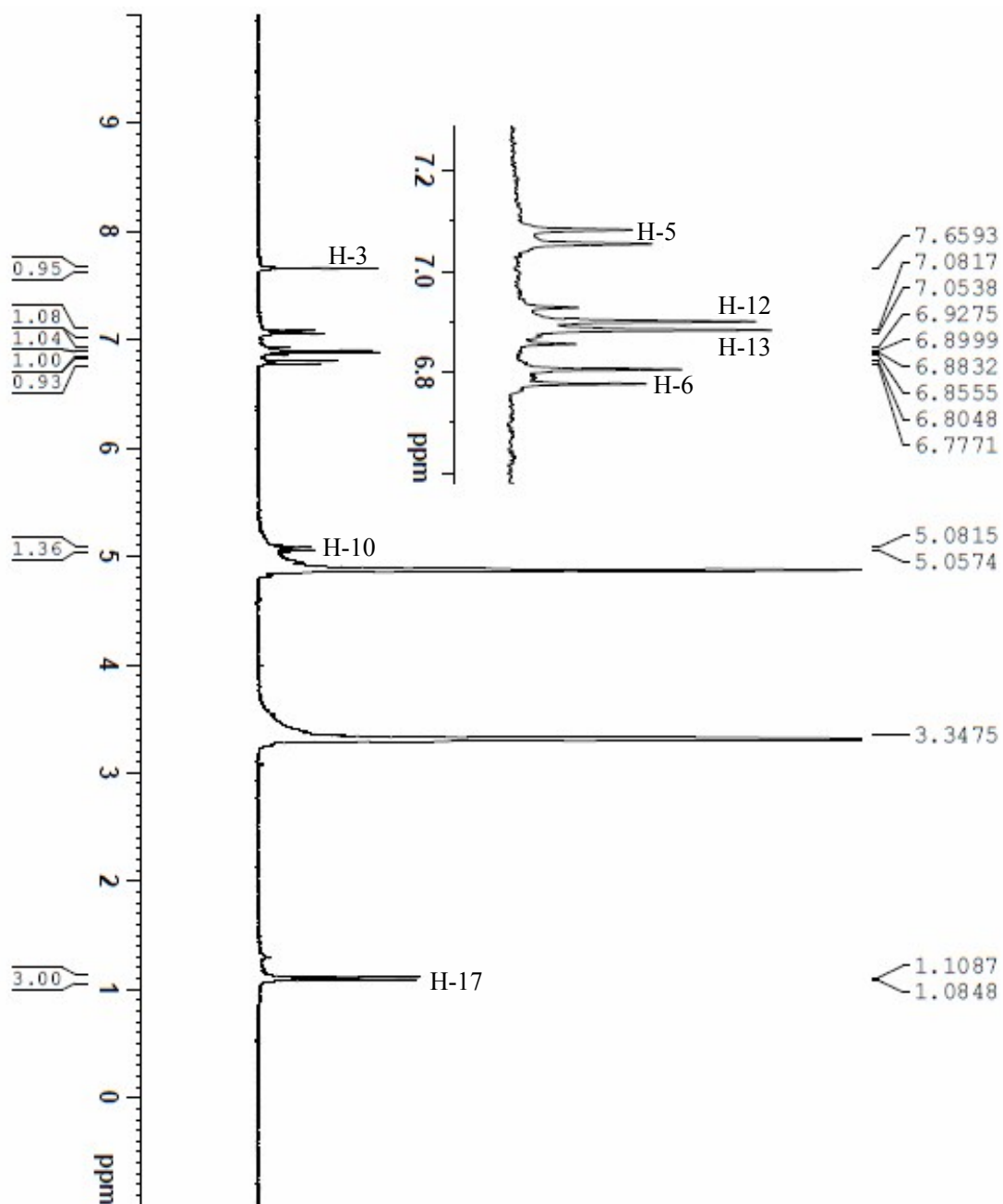
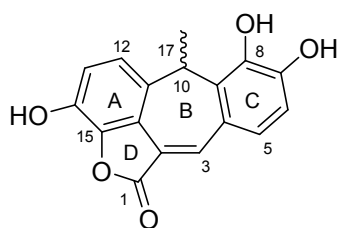
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3	320.0810	2129

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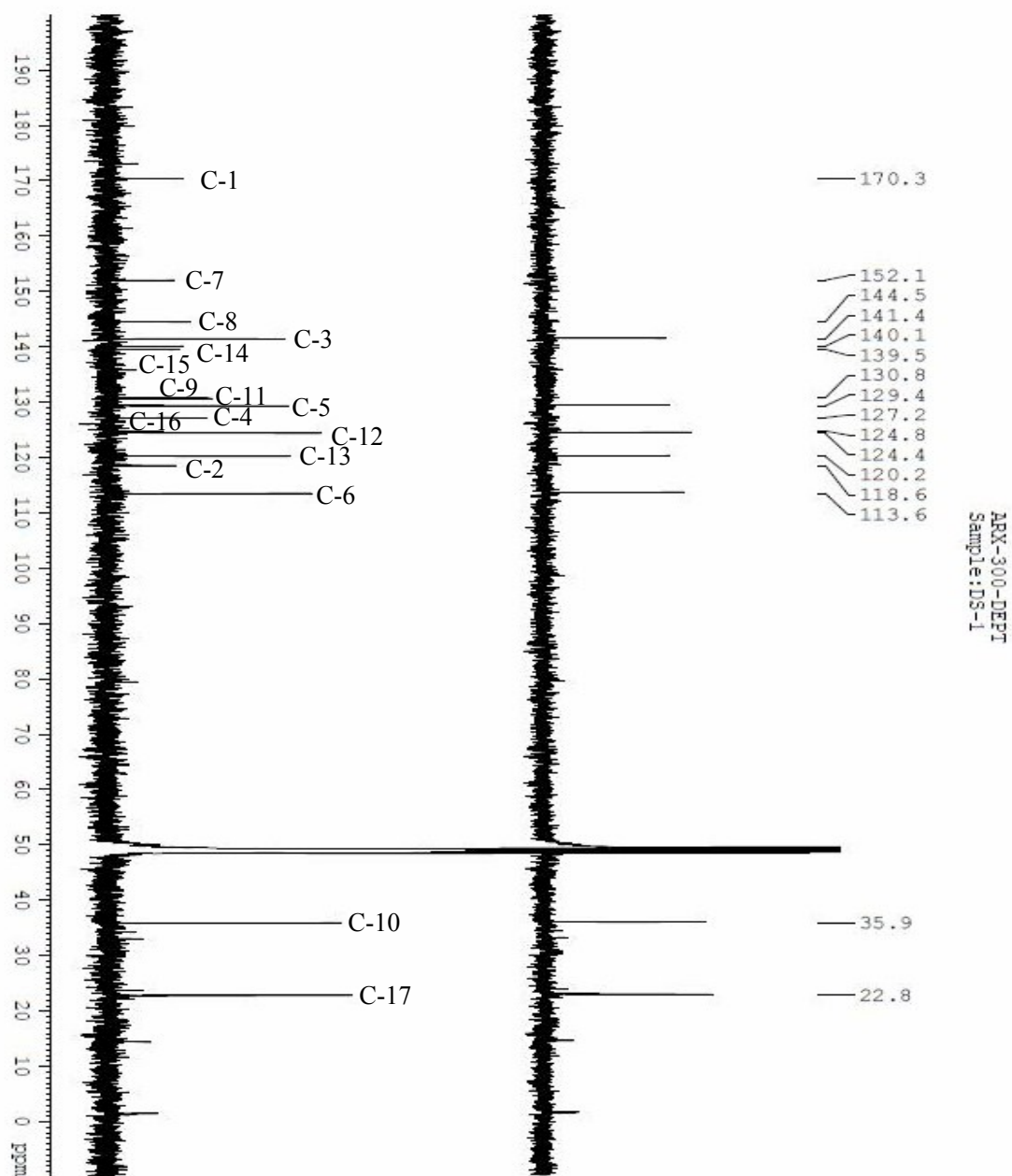
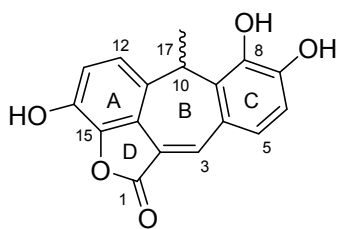
S9 IR spectrum of 2



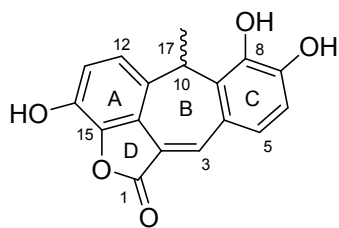
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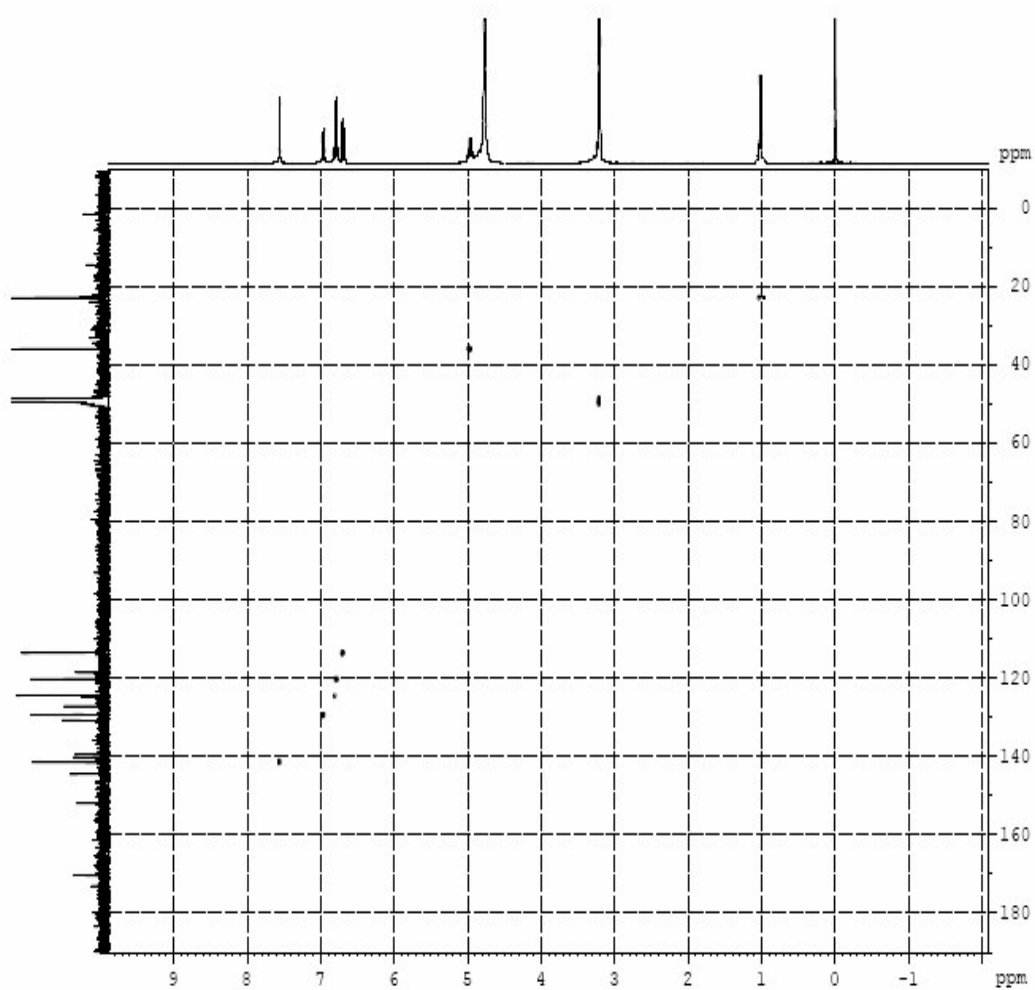
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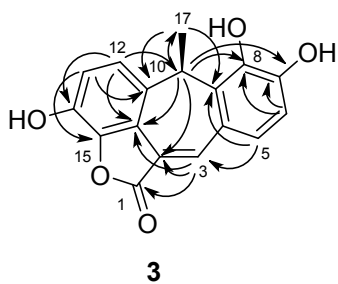
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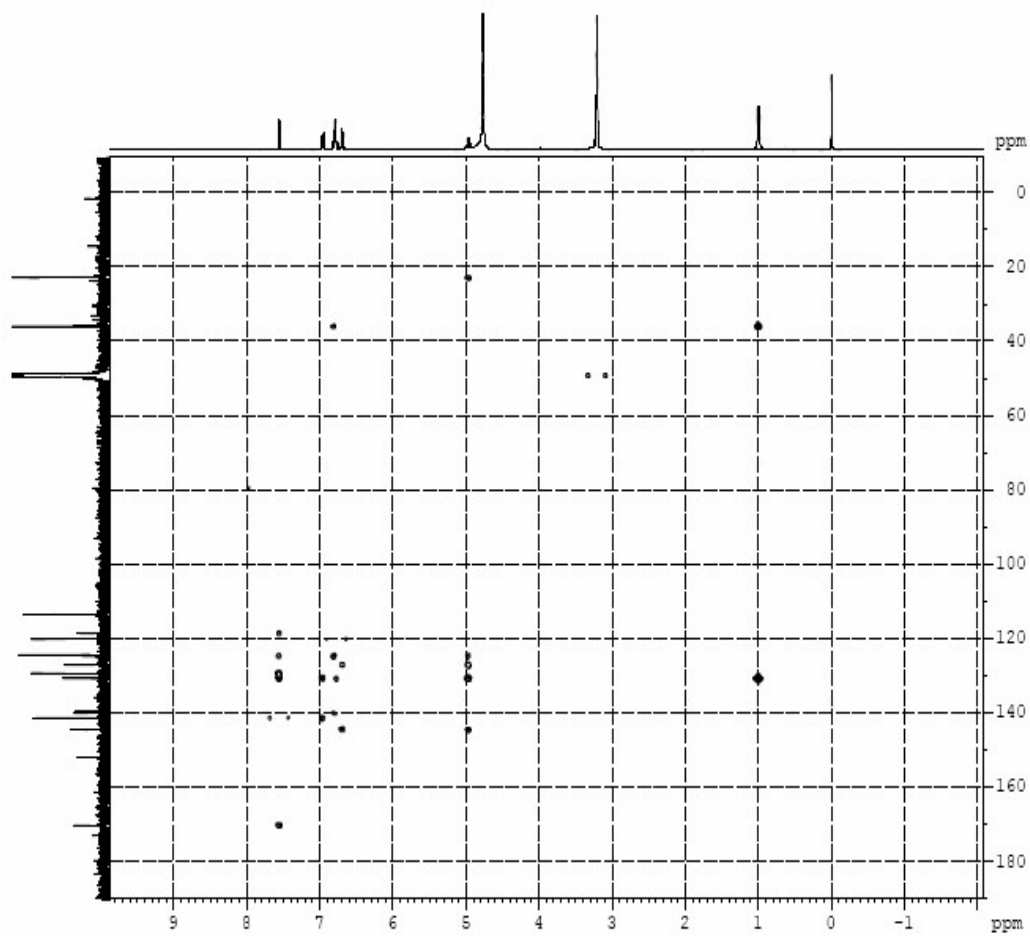
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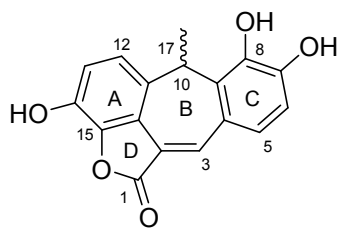
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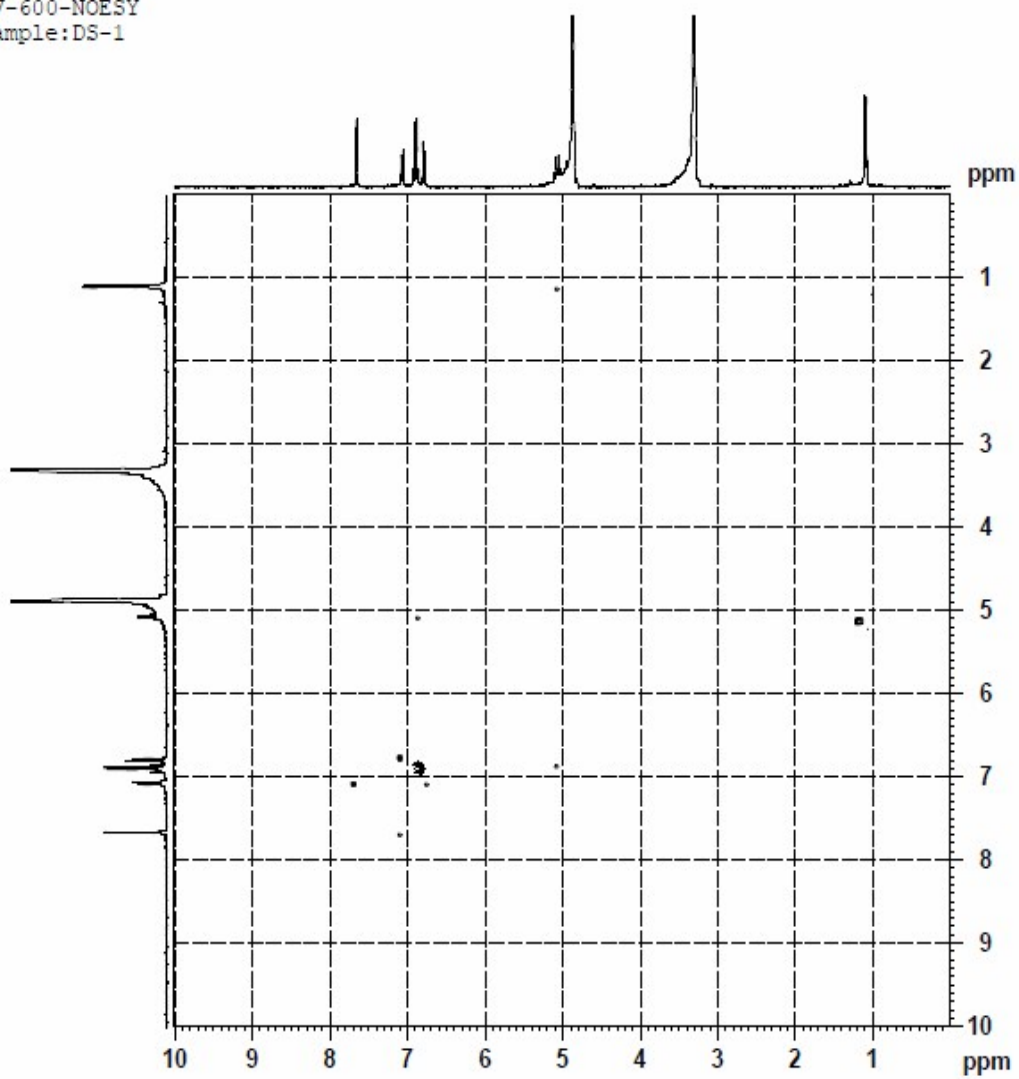
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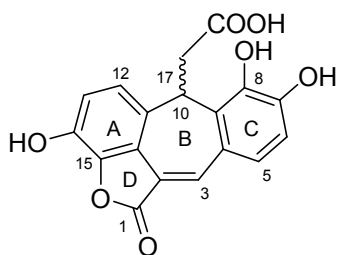
S14 NOESY spectrum of 2 tested in CD₃OD



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S15 HRESIMS spectrum of 3



Compound Mass Spectrum List Report

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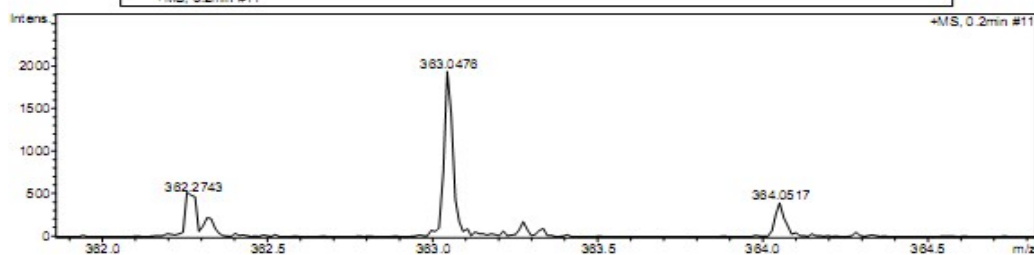
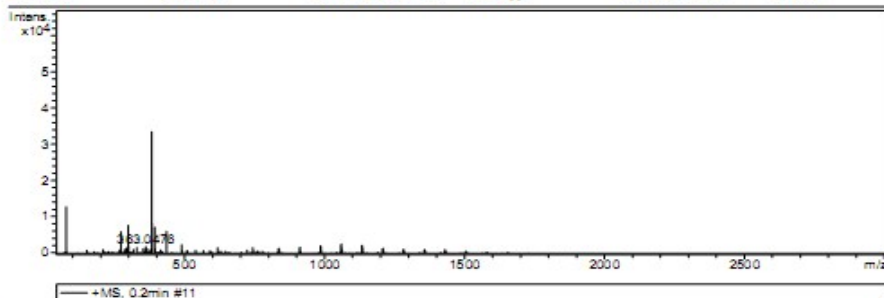
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 Instrument / Ser# micrOTOF-Q 125

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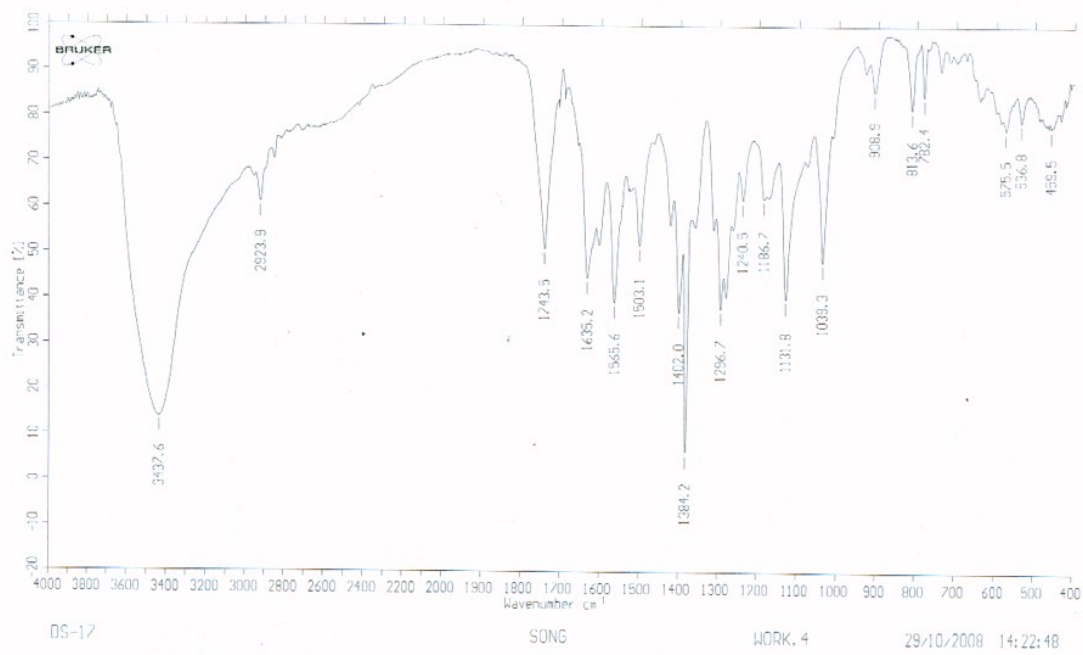
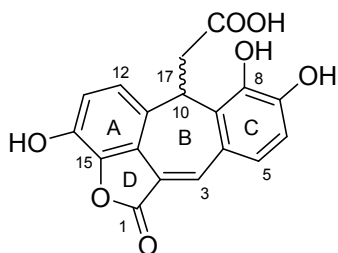
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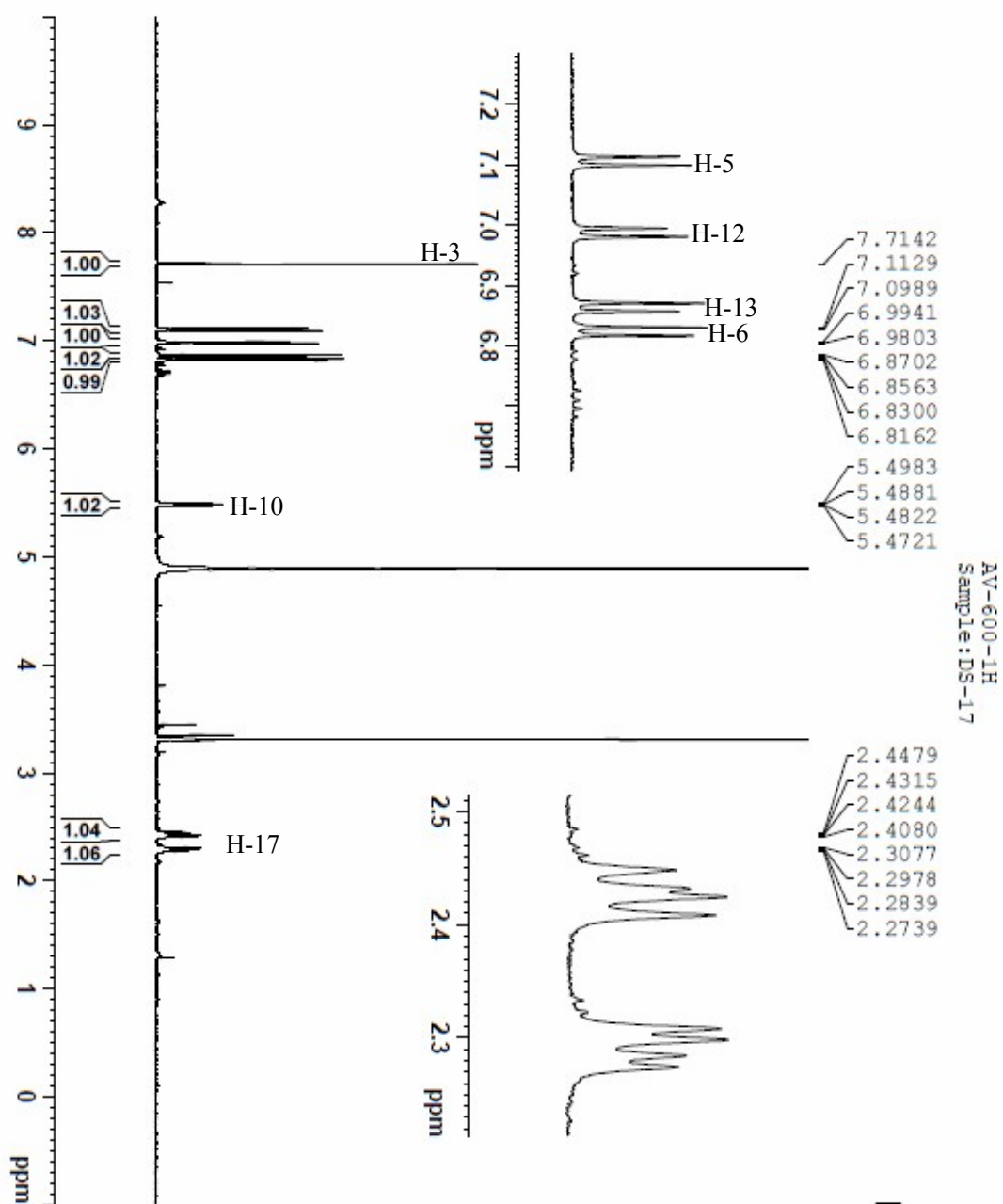
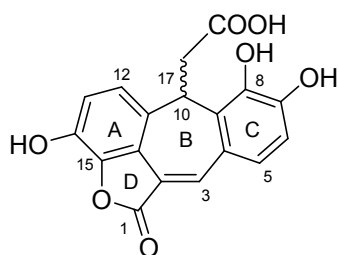
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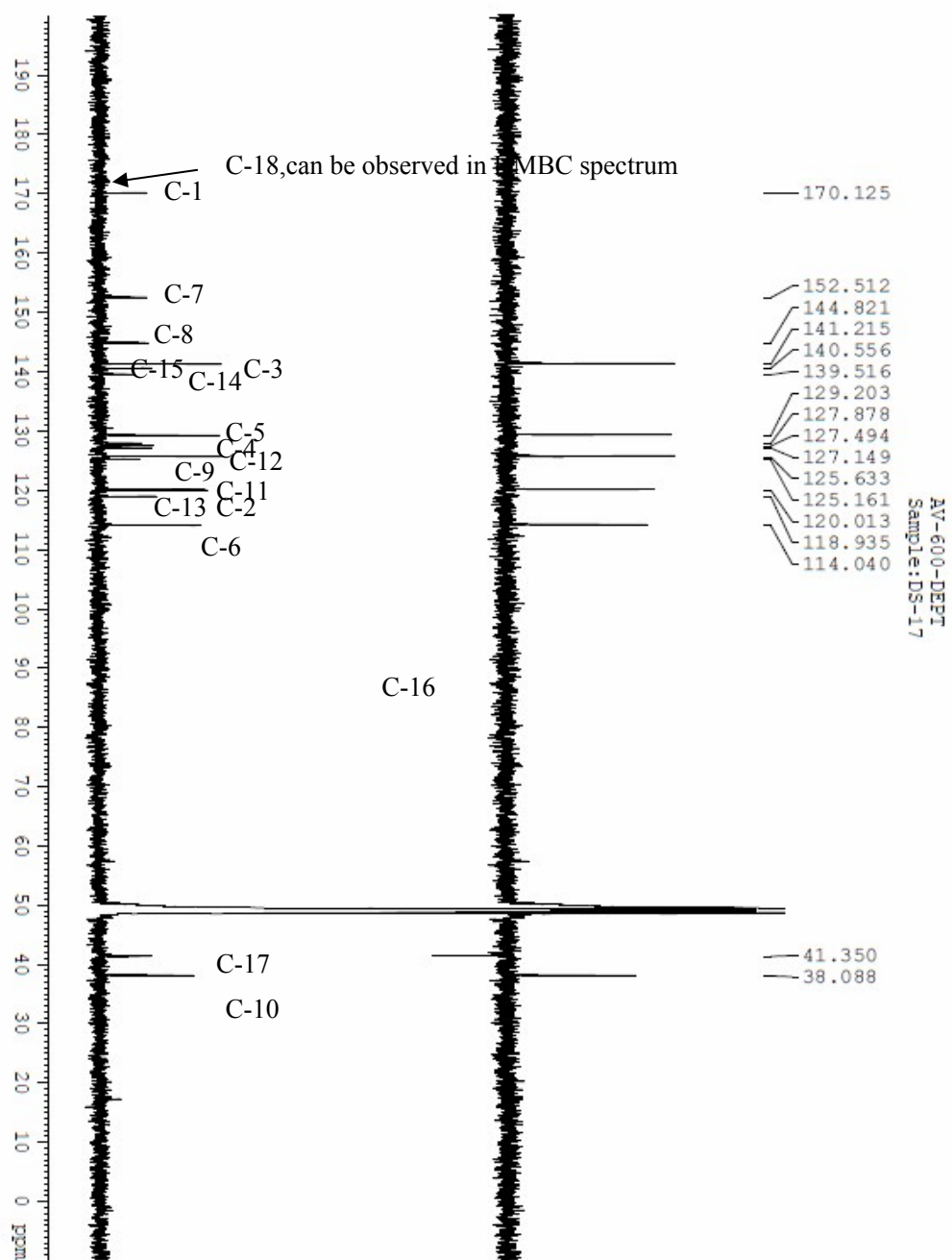
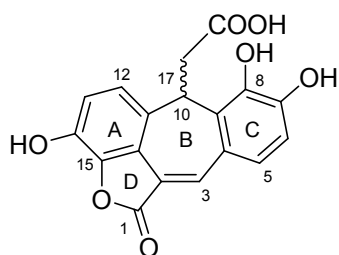
S16 IR spectrum of 3 tested in CD₃OD



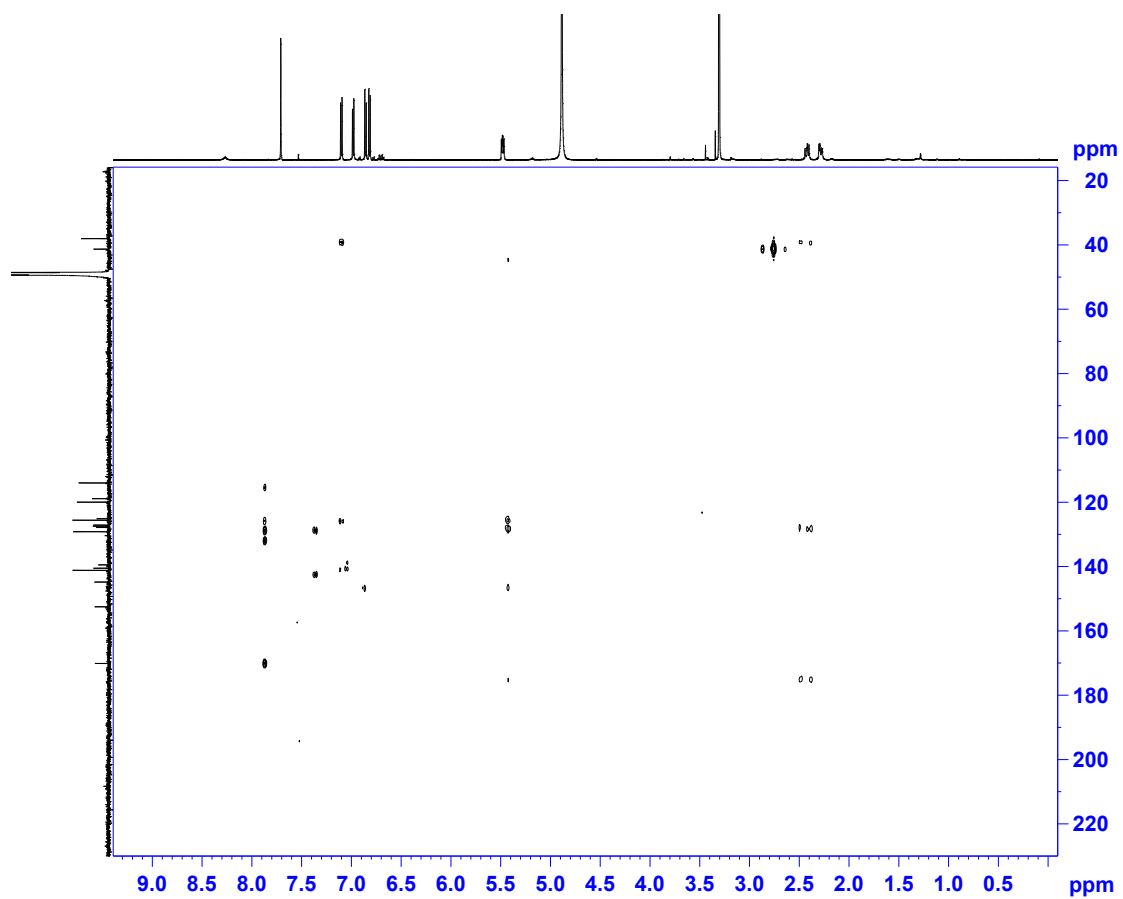
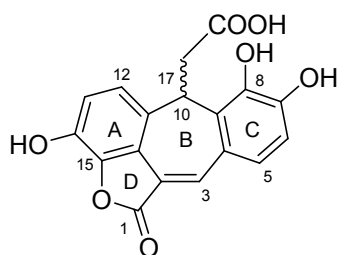
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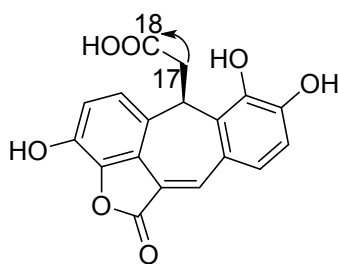
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S 19 HSQC spectrum of 3 tested in CD₃OD

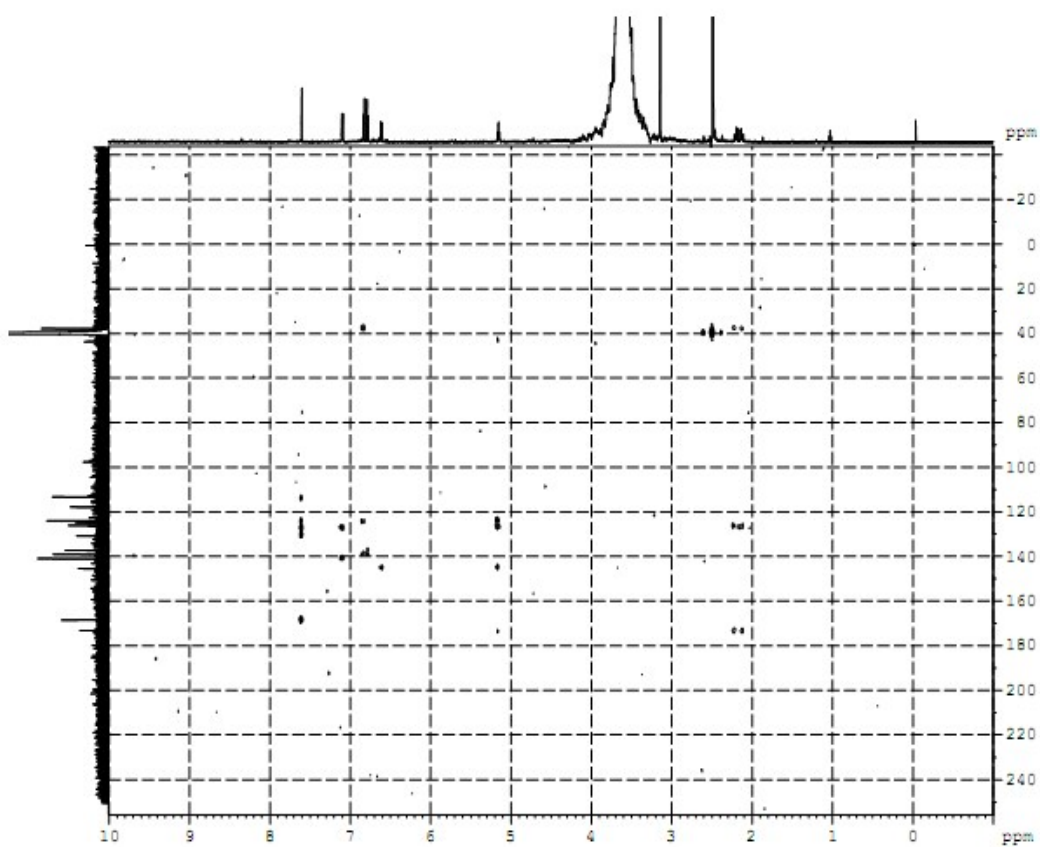


S20 HMBC spectrum of 3 tested in CD₃OD

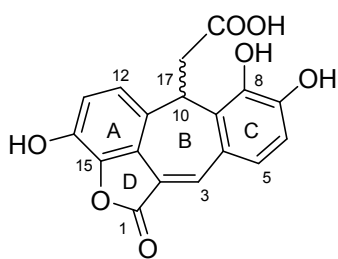


4

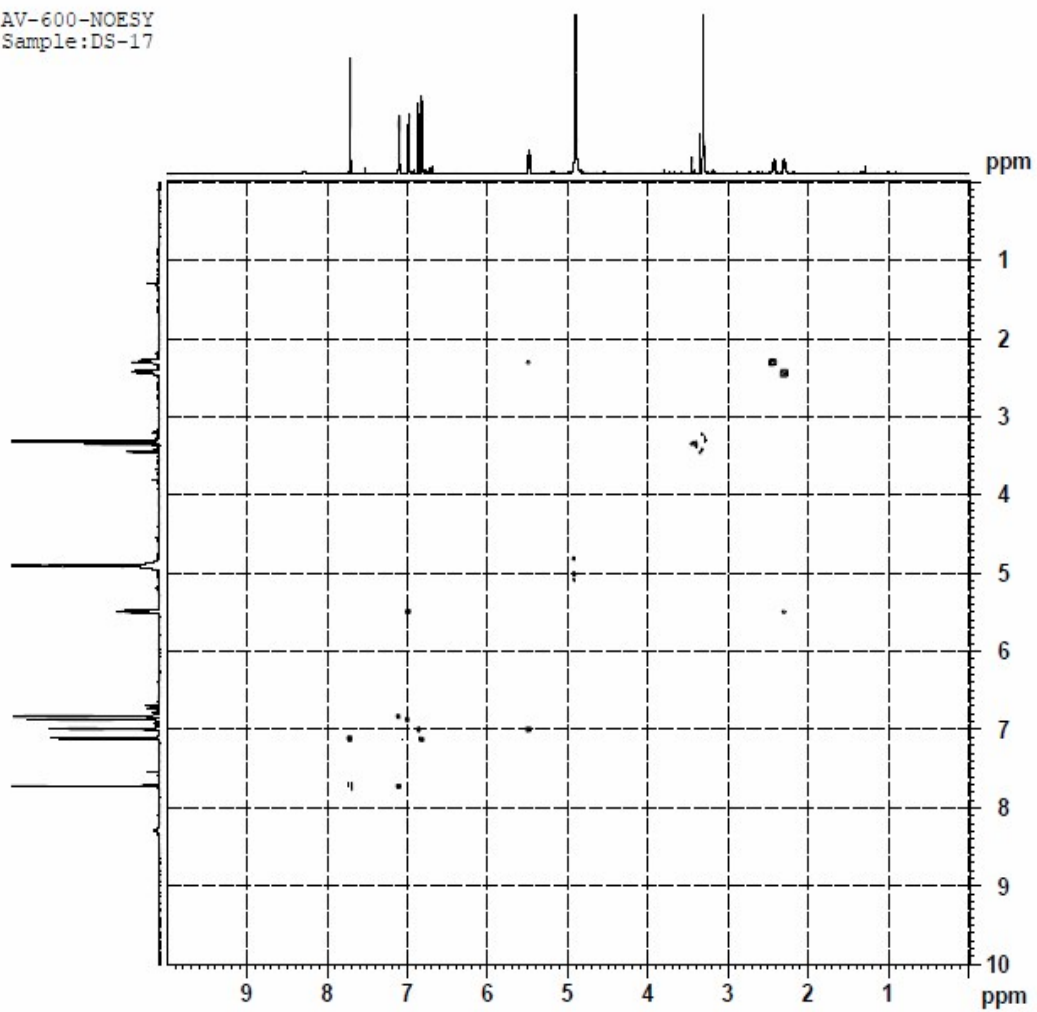
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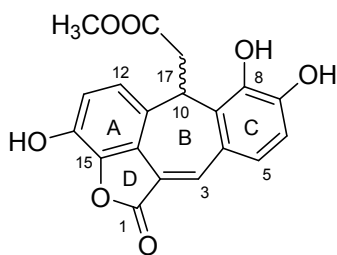
S21 NOESY spectrum of 3 tested in CD₃OD



AV-600-NOESY
Sample: DS-17



S22 HRESIMS spectrum of 4



Compound Mass Spectrum List Report

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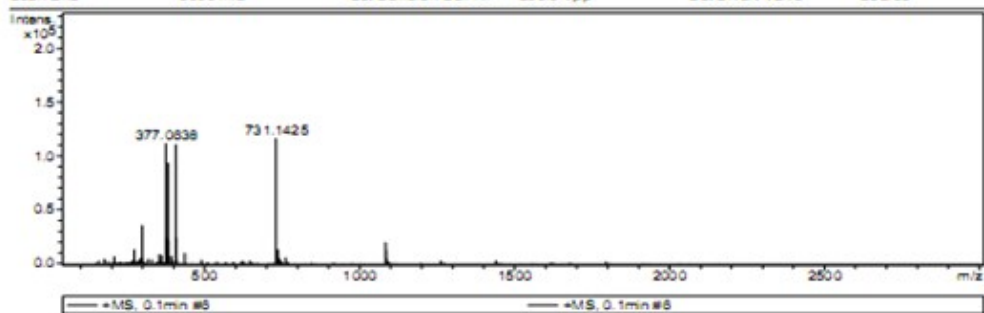
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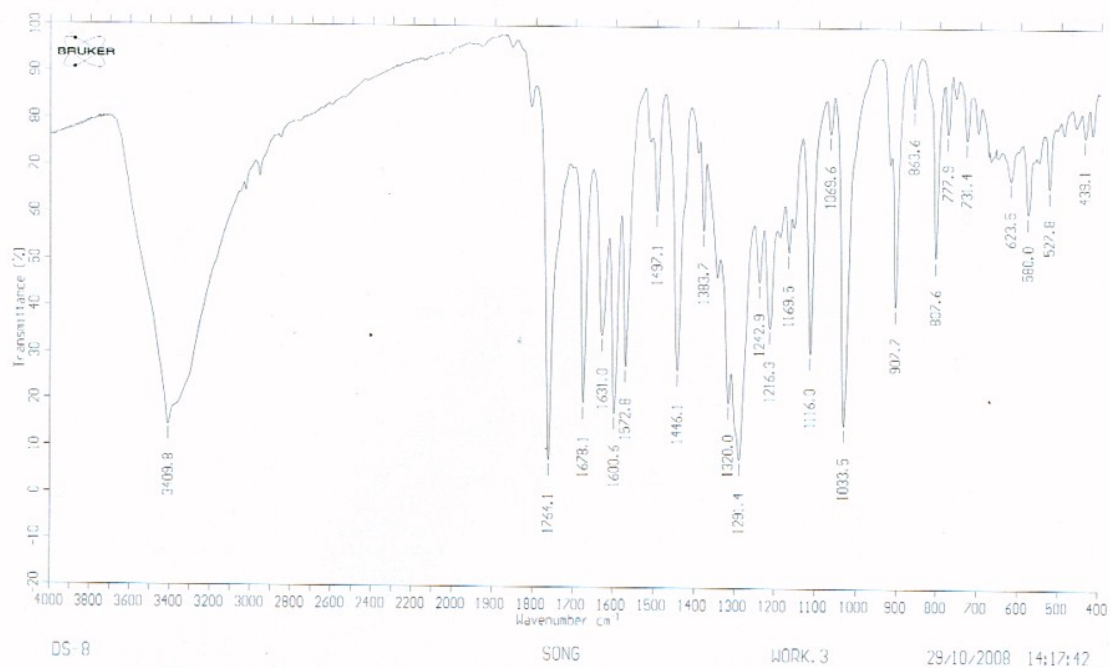
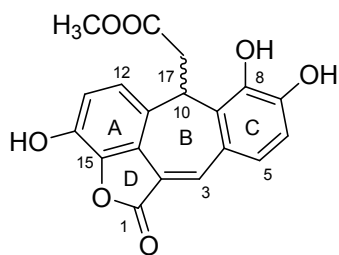
Operator Bruker Customer
Instrument / Ser# micrOTOF-Q 125

Acquisition Parameter

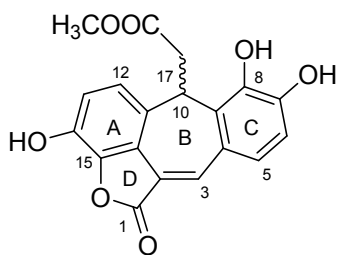
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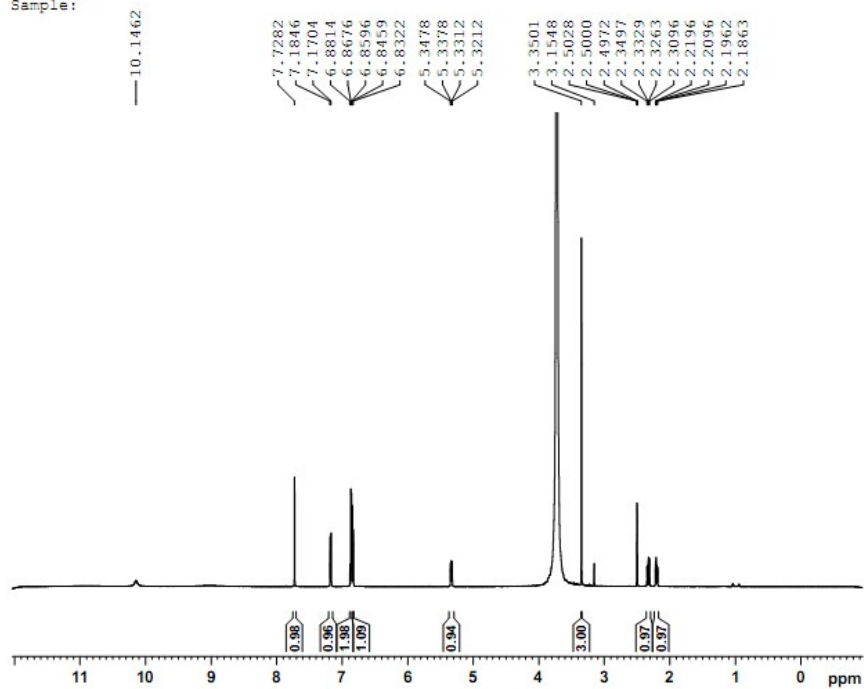
S23 IR spectrum of 4



S24 ¹H NMR spectrum of 4 tested in DMSO-d6



AV-600-1H
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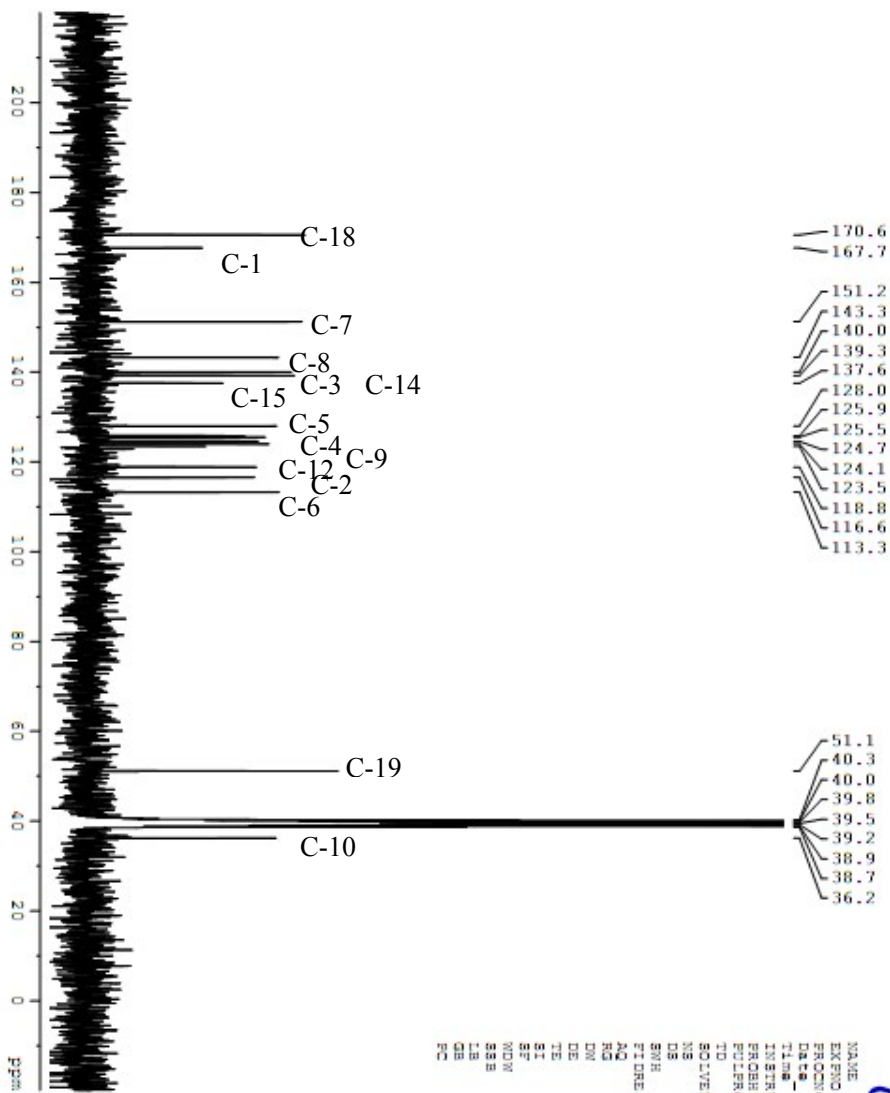
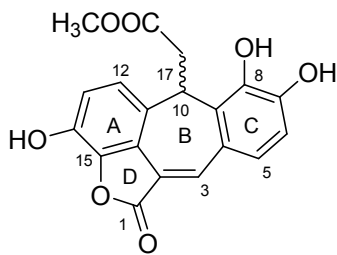


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PROCNO        1
Date_         20080111
Time          13.28
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PROBHD        5 mm BBOBO 90
PULPROG       zg30
PC            65536
SOLVENT       DMSO
DS            4
DE            2
SWH           7788.162 Hz
FIDRES        0.118838 Hz
AQ            4.207553 sec
RG            25.4
SD            64.000 usec
LR            6.50 usec
GB            296.4 K
SI            1.00000000 sec
DDO           1

----- CHANNEL f1 -----
NUC1          1H
P1            11.00 usec
PL1           -4.00 dB
PULSEW       34.70265579 W
SFO1          600.132296 MHz
SI            32768
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PC            1.00
    
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S25 ¹³C NMR spectrum of 4 tested in DMSO-d6



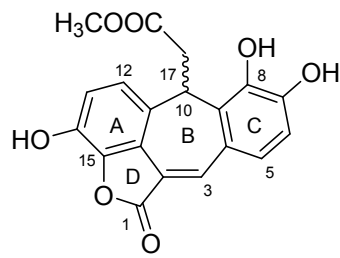
ARX-300
Sample: DS-8



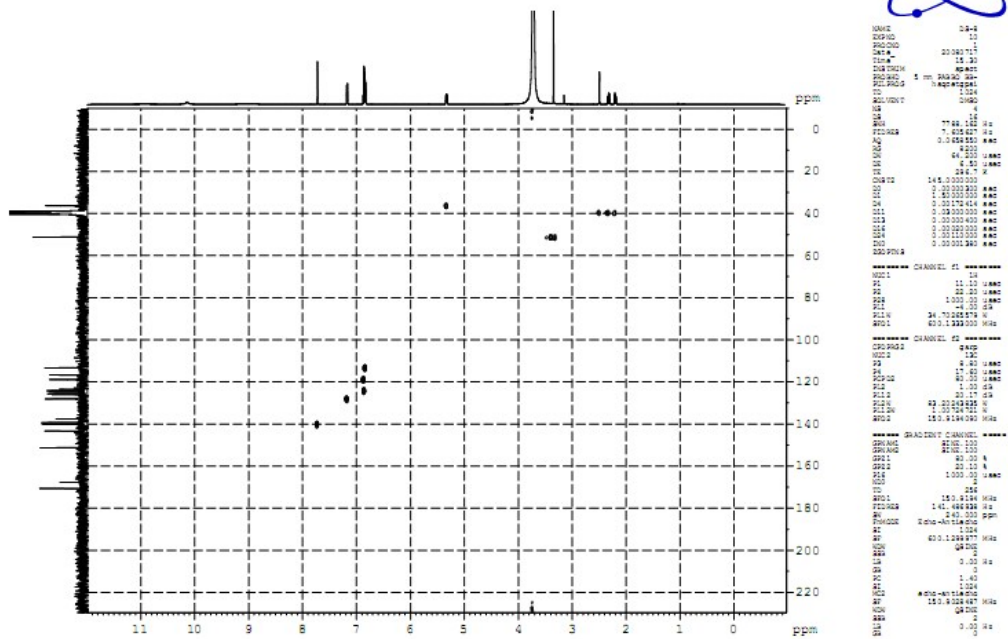
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PROCNO       1
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TIME         9.28
INSTRUM      spect
PROBHD       5 mm QNP 1H
PULPROG      zgpg30
TD           65536
SOLVENT      DMSO
NS           192
DS           4
SWH          24727.773 Hz
FIDRES       1.297163 Hz
AQ           0.2604980 sec
RG           24800
DE           24.000 usec
TE           31.43 usec
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WDW          EM
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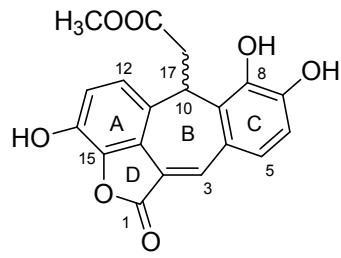
S26 HSQC spectrum of 4 tested in DMSO-d6



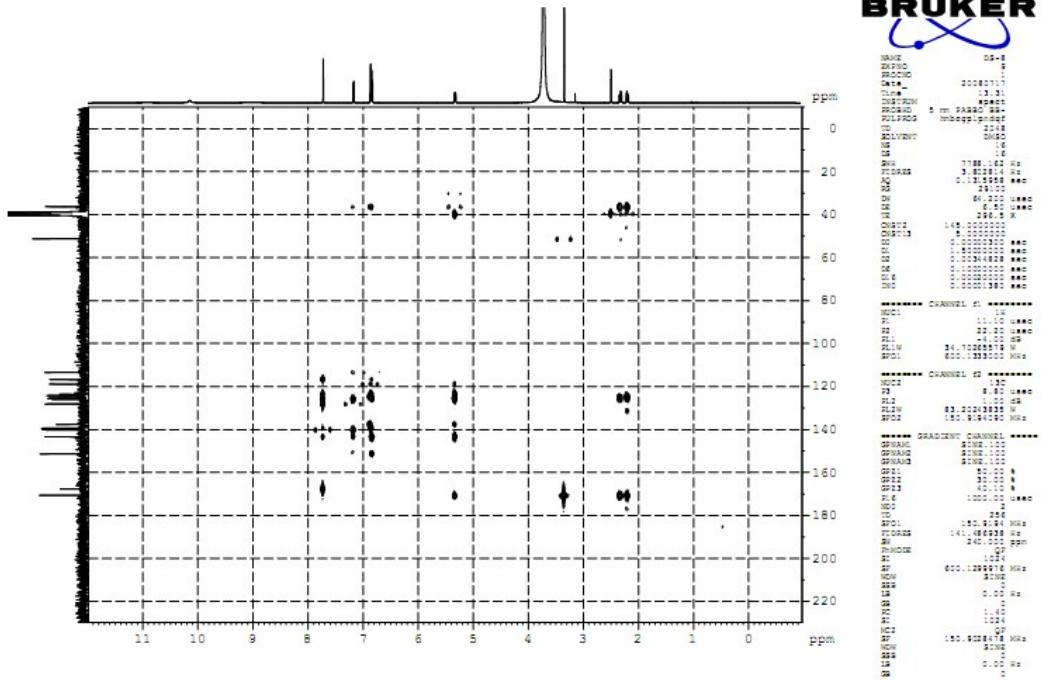
AV-600-HSQC
Sample: DS-8



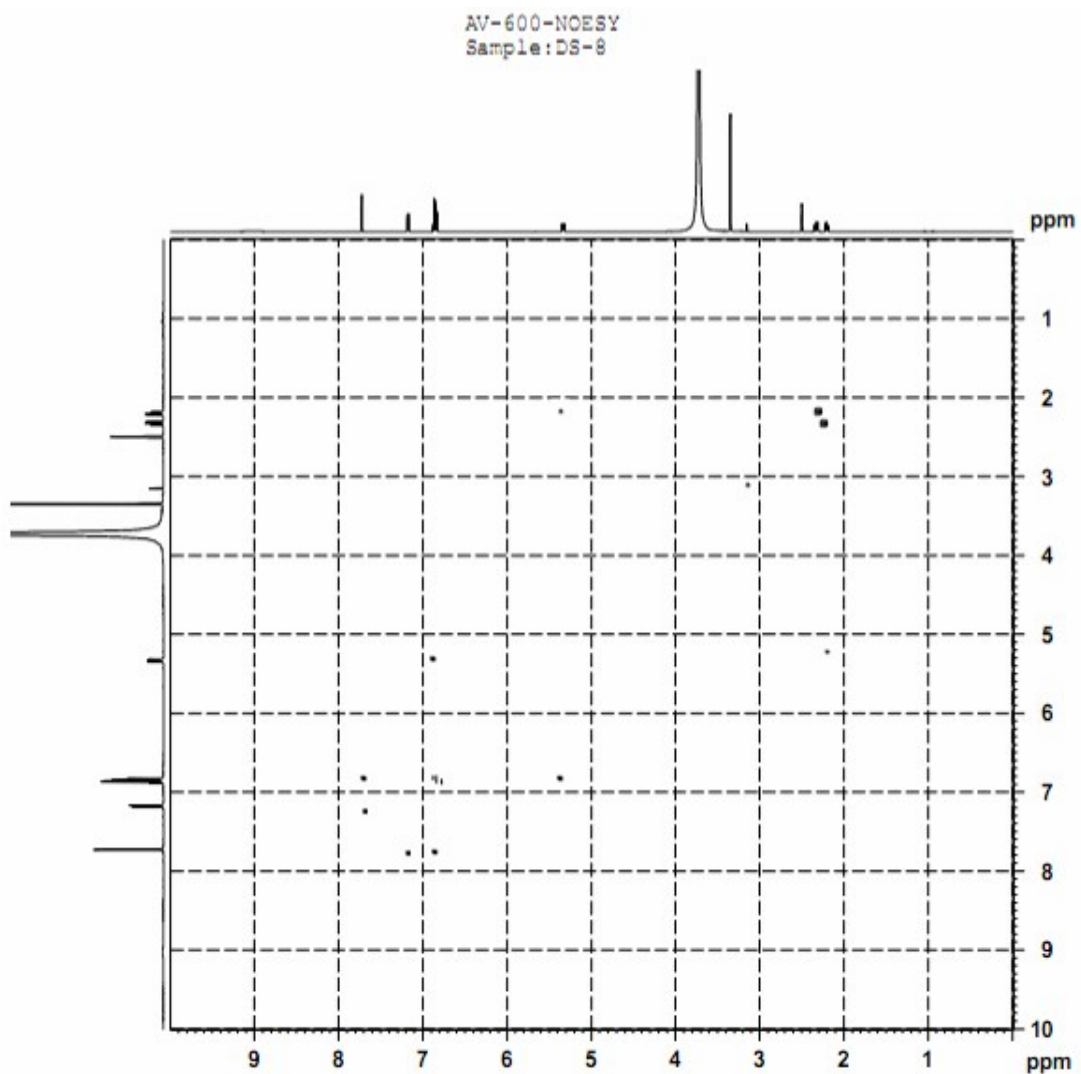
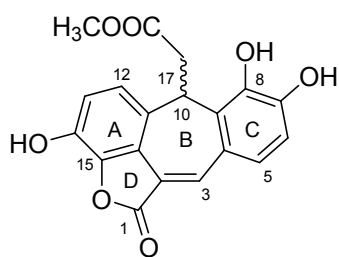
S27 HMBC spectrum of 4 tested in DMSO-d6



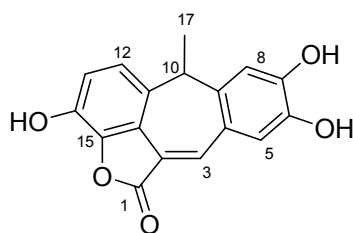
AV-600-HMBC
Sample: DS-8



S28 NOESY spectrum of 4 tested in DMSO-d6



S29 HRESIMS spectrum of 5



Mass Spectrum Molecular Formula Report

Analysis Info

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 Sample Name nafa-2
 Comment

Acquisition Date 4/26/2011 11:38:49 AM

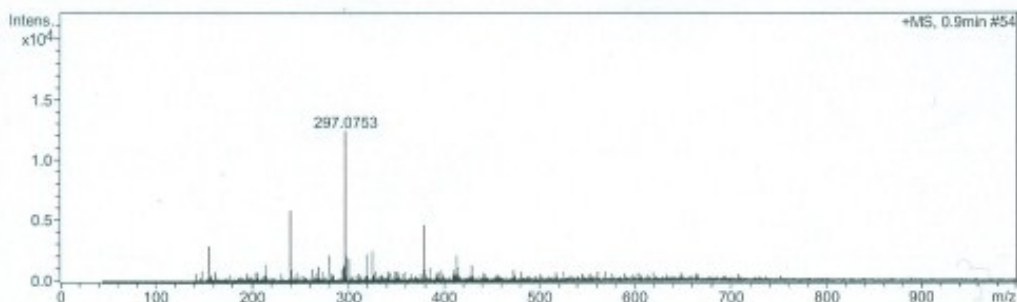
Operator Bruker Customer
 Instrument / Ser# micrOTOF-Q 125

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source

Generate Molecular Formula Parameter

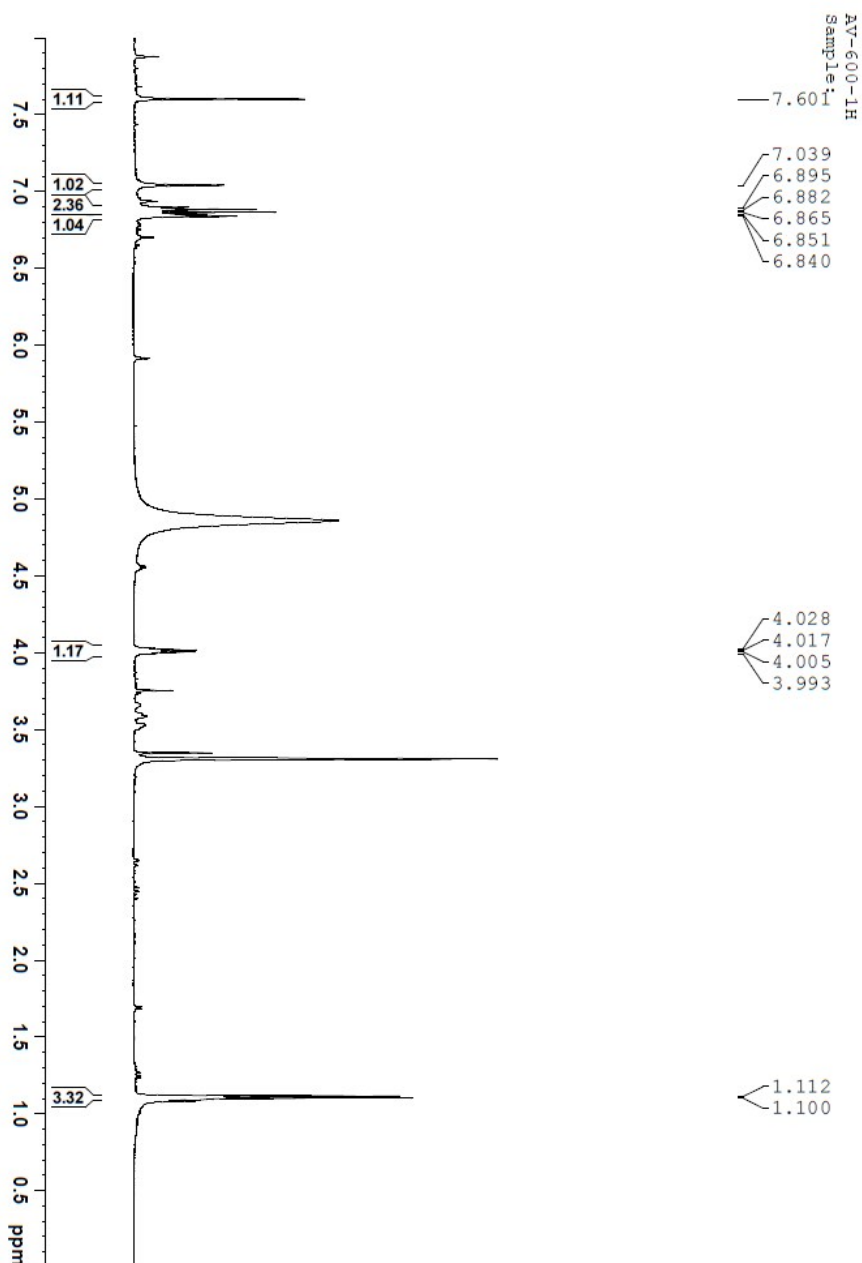
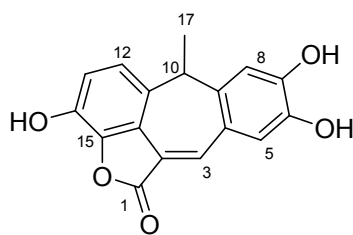
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Formula, max.					
Measured m/z	297.075	Tolerance	4 mDa	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nitrogen Rule	no	Electron Configuration	both		
Filter H/C Ratio	no	Minimum	0	Maximum	3
Estimate Carbon	yes				



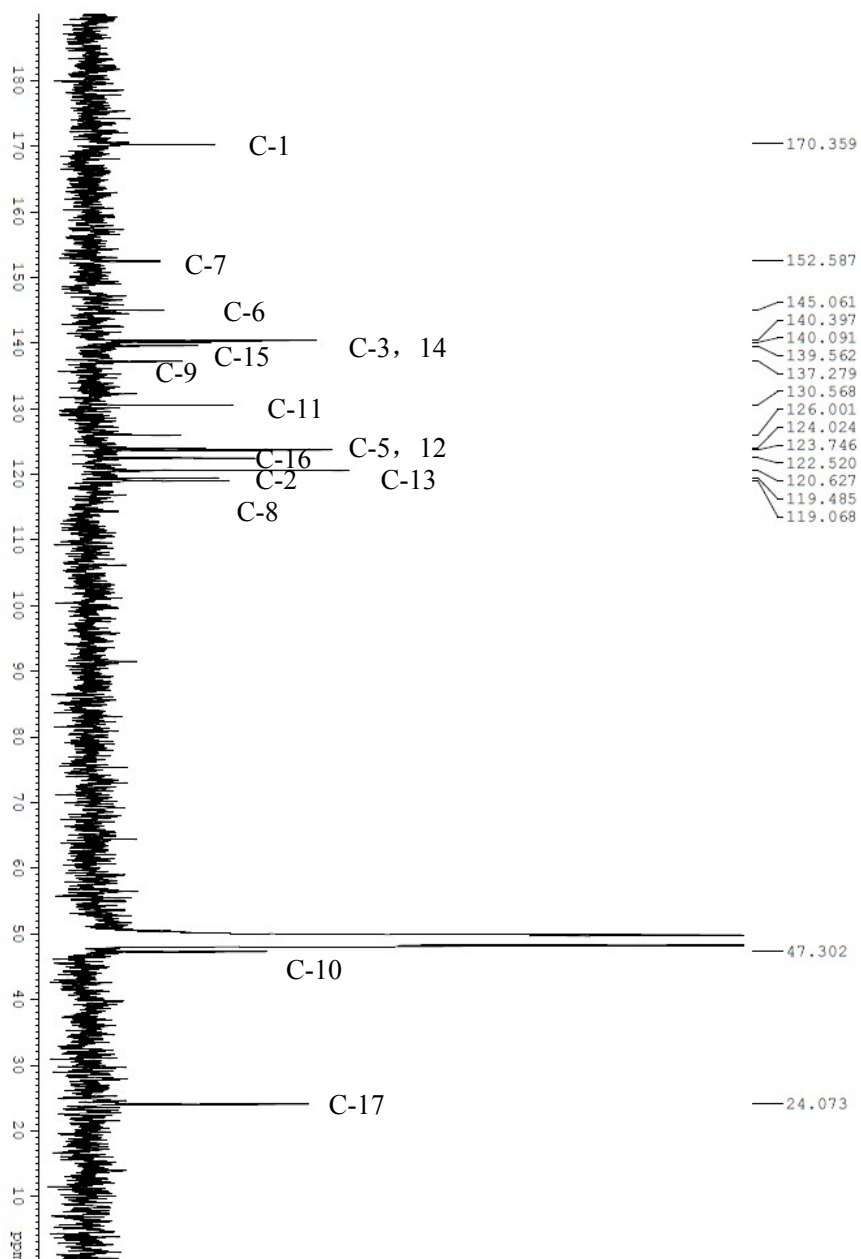
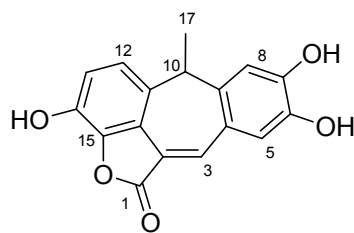
#	m/z	I
1	297.0753	12430

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 17 H 13 O 5	0.013	297.0757	1.67	1.48	0.50	11.50	ok	even

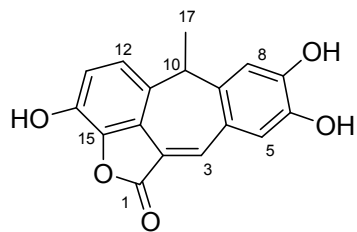
S30 ¹H NMR spectrum of 5 tested in MeOD



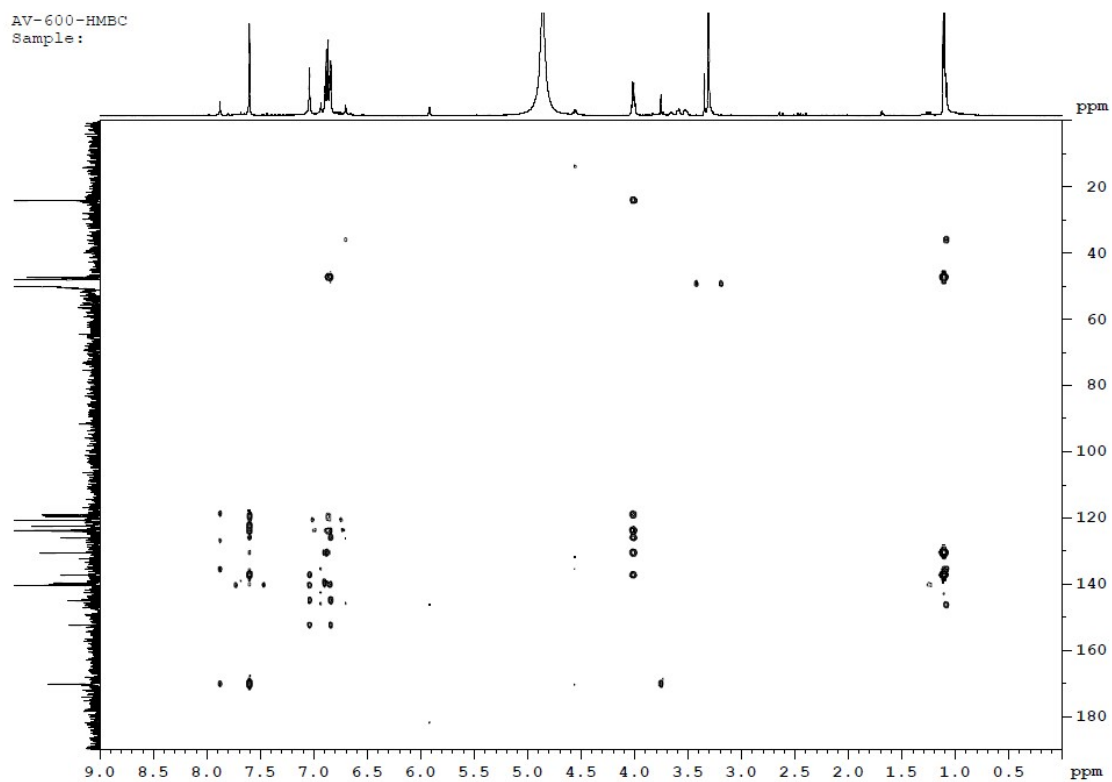
S31 ^{13}C NMR spectrum of 5 in MeOD



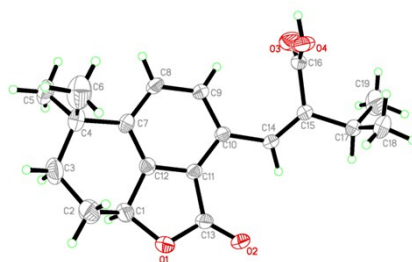
S32 HMBC spectrum of 5 tested in DMSO-D6



AV-600-HMBC
Sample:



S33 Single-crystal X-ray data of 1



1

Table 1. Crystal data and structure refinement for shelxl.

Identification code	shelxl	
Empirical formula	C ₁₉ H ₂₂ O ₄	
Formula weight	314.37	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	triclinic, P-1	
Unit cell dimensions	a = 8.424(5) Å	alpha = 71.63(2)
deg.	b = 9.093(7) Å	beta = 89.35(2)
deg.	c = 12.323(7) Å	gamma = 74.44(3)
deg.		
Volume	860.1(9) Å ³	
Z, Calculated density	2, 1.214 Mg/m ³	
Absorption coefficient	0.084 mm ⁻¹	
F(000)	336	
Crystal size	0.14 x 0.13 x 0.13 mm	
Theta range for data collection	3.15 to 27.48 deg.	
Limiting indices	-10<=h<=9, -11<=k<=11, -15<=l<=15	
Reflections collected / unique	8499 / 3891 [R(int) = 0.0220]	
Completeness to theta = 27.48	98.8 %	
Max. and min. transmission	0.9895 and 0.9883	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3891 / 0 / 213	

Goodness-of-fit on F^2	1.118
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0458, wR2 = 0.1268
R indices (all data)	R1 = 0.0641, wR2 = 0.1355
Largest diff. peak and hole	0.221 and -0.150 e. \AA^{-3}

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for shelxl.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	2222(2)	3226(2)	4136(1)	56(1)
C(2)	1860(3)	4979(2)	3447(2)	78(1)
C(3)	2906(3)	5028(2)	2418(2)	77(1)
C(4)	4817(2)	4404(2)	2690(1)	56(1)
C(5)	5614(3)	3942(3)	1686(1)	75(1)
C(6)	5461(4)	5731(2)	2877(2)	95(1)
C(7)	5259(2)	2981(2)	3797(1)	43(1)
C(8)	6859(2)	2162(2)	4297(1)	46(1)
C(9)	7163(2)	1104(2)	5413(1)	45(1)
C(10)	5898(2)	838(2)	6135(1)	37(1)
C(11)	4300(2)	1597(2)	5598(1)	38(1)
C(12)	4022(2)	2551(2)	4461(1)	41(1)
C(13)	2667(2)	1785(2)	6064(1)	46(1)
C(14)	6120(2)	-75(2)	7363(1)	41(1)
C(15)	7453(2)	-606(2)	8097(1)	42(1)
C(16)	9119(2)	-458(2)	7733(1)	45(1)
C(17)	7375(2)	-1357(2)	9378(1)	59(1)
C(18)	7336(3)	-131(3)	9981(2)	88(1)
C(19)	8759(3)	-2898(3)	9913(2)	105(1)
O(1)	1495(1)	2811(2)	5229(1)	61(1)

0(2)	2309(1)	1208(2)	7027(1)	61(1)
0(3)	10092(1)	-1479(2)	7453(1)	75(1)
0(4)	9386(1)	891(2)	7757(1)	62(1)

Table 3. Bond lengths [Å] and angles [deg] for shelx1.

C(1)-O(1)	1.456(2)
C(1)-C(12)	1.481(2)
C(1)-C(2)	1.499(3)
C(1)-H(1)	0.9800
C(2)-C(3)	1.532(3)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.558(3)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(7)	1.521(2)
C(4)-C(5)	1.522(3)
C(4)-C(6)	1.527(3)
C(5)-H(5A)	0.9600
C(5)-H(5B)	0.9600
C(5)-H(5C)	0.9600
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600
C(7)-C(12)	1.381(2)
C(7)-C(8)	1.393(2)
C(8)-C(9)	1.387(2)
C(8)-H(8)	0.9300
C(9)-C(10)	1.403(2)
C(9)-H(9)	0.9300
C(10)-C(11)	1.401(2)

C(10)-C(14)	1.465(2)
C(11)-C(12)	1.379(2)
C(11)-C(13)	1.472(2)
C(13)-O(2)	1.2081(19)
C(13)-O(1)	1.352(2)
C(14)-C(15)	1.330(2)
C(14)-H(14)	0.9300
C(15)-C(16)	1.496(2)
C(15)-C(17)	1.518(2)
C(16)-O(3)	1.2002(19)
C(16)-O(4)	1.314(2)
C(17)-C(18)	1.516(3)
C(17)-C(19)	1.522(3)
C(17)-H(17)	0.9800
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
O(4)-H(4)	0.8200
O(1)-C(1)-C(12)	103.35(12)
O(1)-C(1)-C(2)	117.58(14)
C(12)-C(1)-C(2)	109.25(15)
O(1)-C(1)-H(1)	108.8
C(12)-C(1)-H(1)	108.8
C(2)-C(1)-H(1)	108.8
C(1)-C(2)-C(3)	105.09(15)
C(1)-C(2)-H(2A)	110.7
C(3)-C(2)-H(2A)	110.7
C(1)-C(2)-H(2B)	110.7

C (3)-C (2)-H(2B)	110. 7
H(2A)-C (2)-H(2B)	108. 8
C (2)-C (3)-C (4)	116. 45 (15)
C (2)-C (3)-H(3A)	108. 2
C (4)-C (3)-H(3A)	108. 2
C (2)-C (3)-H(3B)	108. 2
C (4)-C (3)-H(3B)	108. 2
H(3A)-C (3)-H(3B)	107. 3
C (7)-C (4)-C (5)	111. 26 (14)
C (7)-C (4)-C (6)	106. 98 (14)
C (5)-C (4)-C (6)	109. 57 (18)
C (7)-C (4)-C (3)	110. 28 (14)
C (5)-C (4)-C (3)	109. 10 (15)
C (6)-C (4)-C (3)	109. 61 (17)
C (4)-C (5)-H(5A)	109. 5
C (4)-C (5)-H(5B)	109. 5
H(5A)-C (5)-H(5B)	109. 5
C (4)-C (5)-H(5C)	109. 5
H(5A)-C (5)-H(5C)	109. 5
H(5B)-C (5)-H(5C)	109. 5
C (4)-C (6)-H(6A)	109. 5
C (4)-C (6)-H(6B)	109. 5
H(6A)-C (6)-H(6B)	109. 5
C (4)-C (6)-H(6C)	109. 5
H(6A)-C (6)-H(6C)	109. 5
H(6B)-C (6)-H(6C)	109. 5
C (12)-C (7)-C (8)	114. 74 (12)
C (12)-C (7)-C (4)	119. 73 (14)
C (8)-C (7)-C (4)	125. 01 (14)
C (9)-C (8)-C (7)	121. 97 (13)
C (9)-C (8)-H(8)	119. 0
C (7)-C (8)-H(8)	119. 0

C(8)-C(9)-C(10)	122.77(13)
C(8)-C(9)-H(9)	118.6
C(10)-C(9)-H(9)	118.6
C(11)-C(10)-C(9)	114.25(12)
C(11)-C(10)-C(14)	119.64(12)
C(9)-C(10)-C(14)	126.05(12)
C(12)-C(11)-C(10)	121.96(12)
C(12)-C(11)-C(13)	106.11(12)
C(10)-C(11)-C(13)	131.38(13)
C(11)-C(12)-C(7)	123.42(13)
C(11)-C(12)-C(1)	110.10(13)
C(7)-C(12)-C(1)	125.85(13)
O(2)-C(13)-O(1)	120.92(13)
O(2)-C(13)-C(11)	129.67(14)
O(1)-C(13)-C(11)	109.39(13)
C(15)-C(14)-C(10)	130.24(13)
C(15)-C(14)-H(14)	114.9
C(10)-C(14)-H(14)	114.9
C(14)-C(15)-C(16)	122.85(12)
C(14)-C(15)-C(17)	122.00(13)
C(16)-C(15)-C(17)	115.11(12)
O(3)-C(16)-O(4)	124.52(14)
O(3)-C(16)-C(15)	122.60(16)
O(4)-C(16)-C(15)	112.88(12)
C(18)-C(17)-C(15)	110.14(15)
C(18)-C(17)-C(19)	111.30(18)
C(15)-C(17)-C(19)	113.29(16)
C(18)-C(17)-H(17)	107.3
C(15)-C(17)-H(17)	107.3
C(19)-C(17)-H(17)	107.3
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5

H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(13)-O(1)-C(1)	110.06(12)
C(16)-O(4)-H(4)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for shelxl.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^*^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(1)	48(1)	69(1)	46(1)	-18(1)	-1(1)	-7(1)
C(2)	67(1)	69(1)	69(1)	-7(1)	0(1)	11(1)
C(3)	85(1)	66(1)	51(1)	0(1)	-5(1)	3(1)
C(4)	75(1)	47(1)	39(1)	-8(1)	4(1)	-16(1)
C(5)	95(1)	85(1)	37(1)	-11(1)	11(1)	-23(1)
C(6)	147(2)	56(1)	81(1)	-10(1)	-4(1)	-42(1)
C(7)	54(1)	44(1)	34(1)	-16(1)	9(1)	-15(1)

C(8)	45(1)	57(1)	39(1)	-16(1)	16(1)	-19(1)
C(9)	36(1)	57(1)	39(1)	-13(1)	8(1)	-11(1)
C(10)	35(1)	42(1)	37(1)	-15(1)	7(1)	-14(1)
C(11)	37(1)	45(1)	36(1)	-18(1)	8(1)	-15(1)
C(12)	43(1)	44(1)	37(1)	-17(1)	3(1)	-9(1)
C(13)	35(1)	64(1)	46(1)	-22(1)	5(1)	-16(1)
C(14)	35(1)	52(1)	37(1)	-12(1)	10(1)	-17(1)
C(15)	37(1)	50(1)	37(1)	-12(1)	6(1)	-13(1)
C(16)	32(1)	61(1)	37(1)	-13(1)	3(1)	-7(1)
C(17)	46(1)	85(1)	37(1)	-4(1)	4(1)	-23(1)
C(18)	83(1)	143(2)	44(1)	-36(1)	18(1)	-35(1)
C(19)	100(2)	104(2)	64(1)	17(1)	-11(1)	-3(1)
O(1)	36(1)	87(1)	53(1)	-21(1)	4(1)	-7(1)
O(2)	40(1)	99(1)	48(1)	-21(1)	15(1)	-29(1)
O(3)	48(1)	80(1)	90(1)	-33(1)	19(1)	-2(1)
O(4)	46(1)	82(1)	73(1)	-35(1)	25(1)	-33(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for shelxl.

	x	y	z	U(eq)
H(1)	1892	2655	3661	67
H(2A)	2169	5579	3896	94
H(2B)	694	5436	3194	94
H(3A)	2636	6134	1907	92
H(3B)	2582	4392	2004	92
H(5A)	6794	3578	1842	112
H(5B)	5326	4865	1002	112
H(5C)	5225	3093	1579	112

H(6A)	4892	6082	3470	142
H(6B)	5271	6626	2178	142
H(6C)	6624	5319	3102	142
H(8)	7750	2330	3870	56
H(9)	8252	547	5694	54
H(14)	5179	-323	7680	49
H(17)	6329	-1642	9488	71
H(18A)	8369	135	9922	132
H(18B)	7161	-577	10774	132
H(18C)	6453	826	9626	132
H(19A)	8722	-3669	9538	157
H(19B)	8621	-3338	10714	157
H(19C)	9806	-2661	9824	157
H(4)	10291	941	7522	93

Table 6. Torsion angles [deg] for shelxl.

O(1)-C(1)-C(2)-C(3)	175.14(15)
C(12)-C(1)-C(2)-C(3)	57.9(2)
C(1)-C(2)-C(3)-C(4)	-63.2(2)
C(2)-C(3)-C(4)-C(7)	36.4(2)
C(2)-C(3)-C(4)-C(5)	158.91(18)
C(2)-C(3)-C(4)-C(6)	-81.1(2)
C(5)-C(4)-C(7)-C(12)	-128.50(17)
C(6)-C(4)-C(7)-C(12)	111.86(19)
C(3)-C(4)-C(7)-C(12)	-7.3(2)
C(5)-C(4)-C(7)-C(8)	60.2(2)
C(6)-C(4)-C(7)-C(8)	-59.5(2)
C(3)-C(4)-C(7)-C(8)	-178.62(15)
C(12)-C(7)-C(8)-C(9)	-5.3(2)
C(4)-C(7)-C(8)-C(9)	166.46(15)

$C(7) - C(8) - C(9) - C(10)$	-3.1(2)
$C(8) - C(9) - C(10) - C(11)$	6.4(2)
$C(8) - C(9) - C(10) - C(14)$	-170.85(14)
$C(9) - C(10) - C(11) - C(12)$	-1.46(19)
$C(14) - C(10) - C(11) - C(12)$	175.99(12)
$C(9) - C(10) - C(11) - C(13)$	-171.76(15)
$C(14) - C(10) - C(11) - C(13)$	5.7(2)
$C(10) - C(11) - C(12) - C(7)$	-7.3(2)
$C(13) - C(11) - C(12) - C(7)$	165.18(13)
$C(10) - C(11) - C(12) - C(1)$	-178.56(13)
$C(13) - C(11) - C(12) - C(1)$	-6.12(16)
$C(8) - C(7) - C(12) - C(11)$	10.4(2)
$C(4) - C(7) - C(12) - C(11)$	-161.82(13)
$C(8) - C(7) - C(12) - C(1)$	-179.73(14)
$C(4) - C(7) - C(12) - C(1)$	8.1(2)
$O(1) - C(1) - C(12) - C(11)$	9.66(17)
$C(2) - C(1) - C(12) - C(11)$	135.60(15)
$O(1) - C(1) - C(12) - C(7)$	-161.38(14)
$C(2) - C(1) - C(12) - C(7)$	-35.4(2)
$C(12) - C(11) - C(13) - O(2)$	-178.14(16)
$C(10) - C(11) - C(13) - O(2)$	-6.7(3)
$C(12) - C(11) - C(13) - O(1)$	-0.14(17)
$C(10) - C(11) - C(13) - O(1)$	171.30(14)
$C(11) - C(10) - C(14) - C(15)$	-164.62(15)
$C(9) - C(10) - C(14) - C(15)$	12.5(2)
$C(10) - C(14) - C(15) - C(16)$	-5.6(2)
$C(10) - C(14) - C(15) - C(17)$	172.21(15)
$C(14) - C(15) - C(16) - O(3)$	-89.8(2)
$C(17) - C(15) - C(16) - O(3)$	92.24(19)
$C(14) - C(15) - C(16) - O(4)$	90.31(18)
$C(17) - C(15) - C(16) - O(4)$	-87.64(17)
$C(14) - C(15) - C(17) - C(18)$	-100.14(19)

C(16)-C(15)-C(17)-C(18)	77.84(18)
C(14)-C(15)-C(17)-C(19)	134.48(19)
C(16)-C(15)-C(17)-C(19)	-47.5(2)
O(2)-C(13)-O(1)-C(1)	-175.33(15)
C(11)-C(13)-O(1)-C(1)	6.46(17)
C(12)-C(1)-O(1)-C(13)	-9.71(17)
C(2)-C(1)-O(1)-C(13)	-130.12(17)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for shelxl [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4)...O(2)#1	0.82	1.85	2.6684(19)	175.1

Symmetry transformations used to generate equivalent atoms:

#1 x+1, y, z

S34.The chiral HPLC chromatogram of 1.

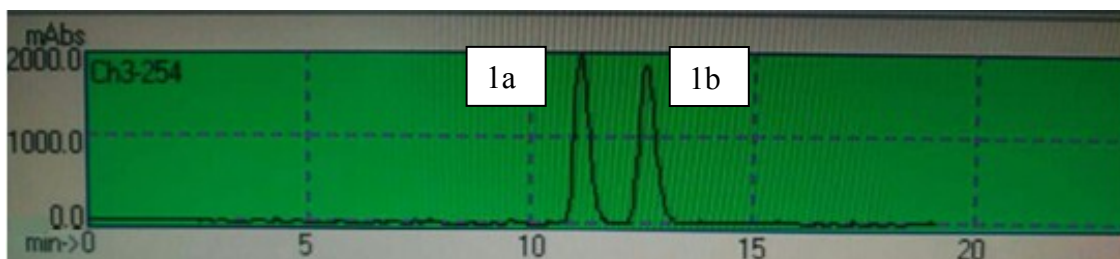


Figure S34.The chiral HPLC chromatogram of 1.

S35.The chiral HPLC chromatogram of 2.

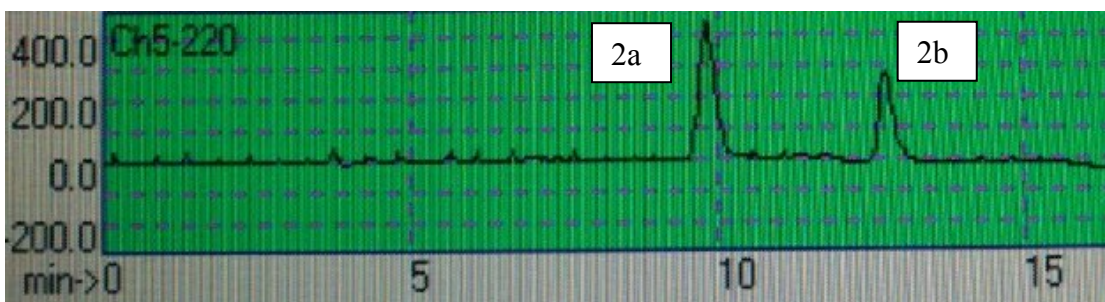


Figure S35.The chiral HPLC chromatogram of 2.

S36.The chiral HPLC chromatogram of 3.

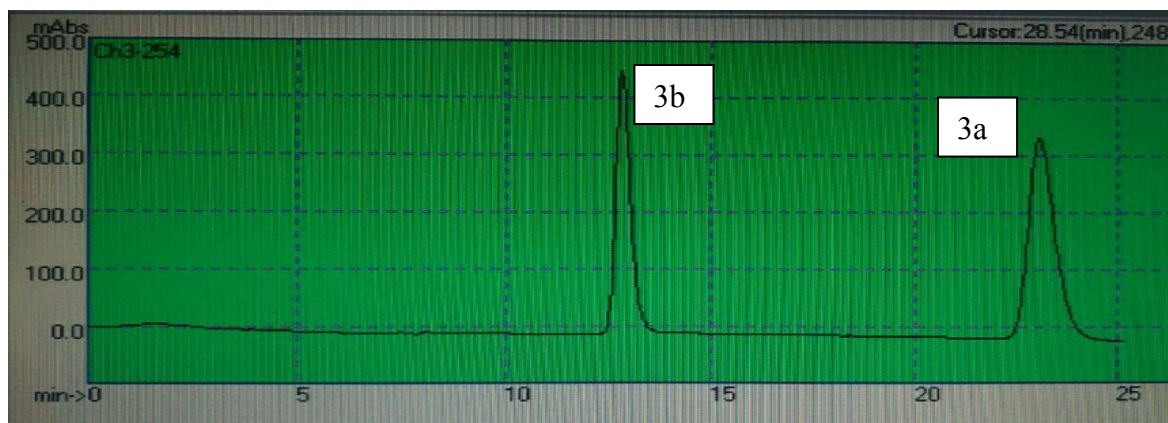


Figure S36.The chiral HPLC chromatogram of 3.

S37.The chiral HPLC chromatogram of 4.

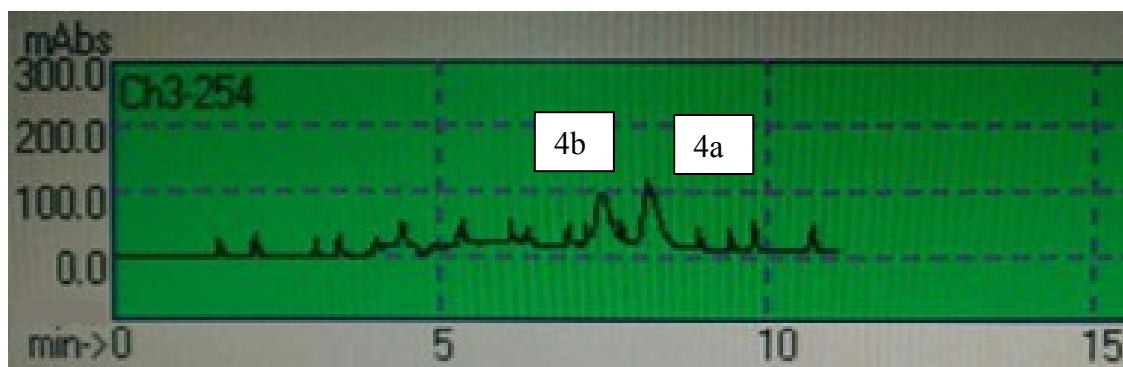
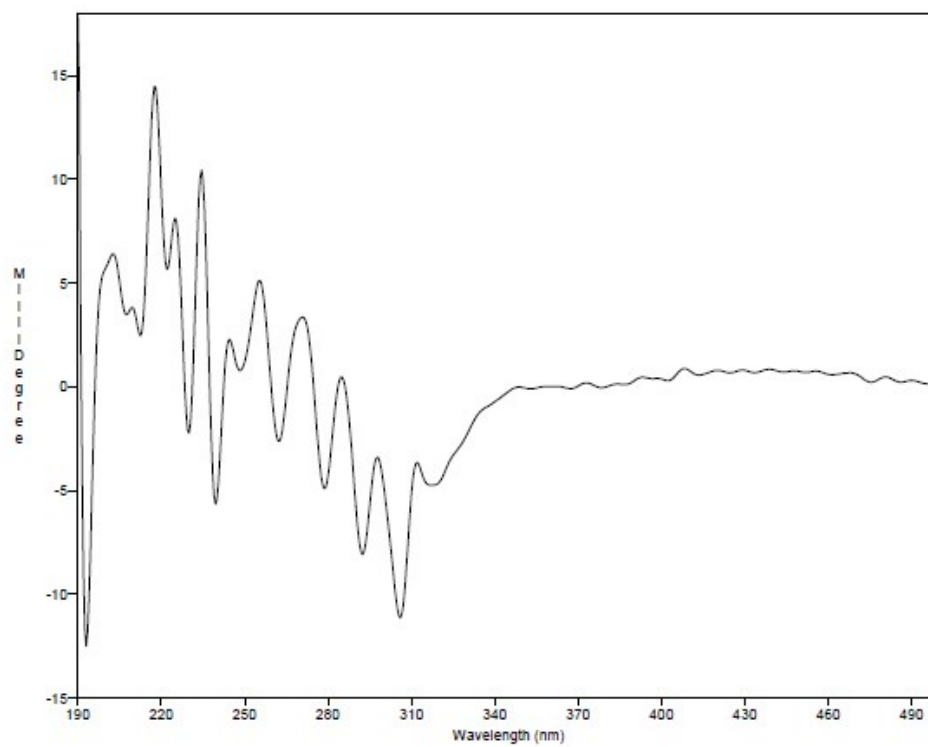
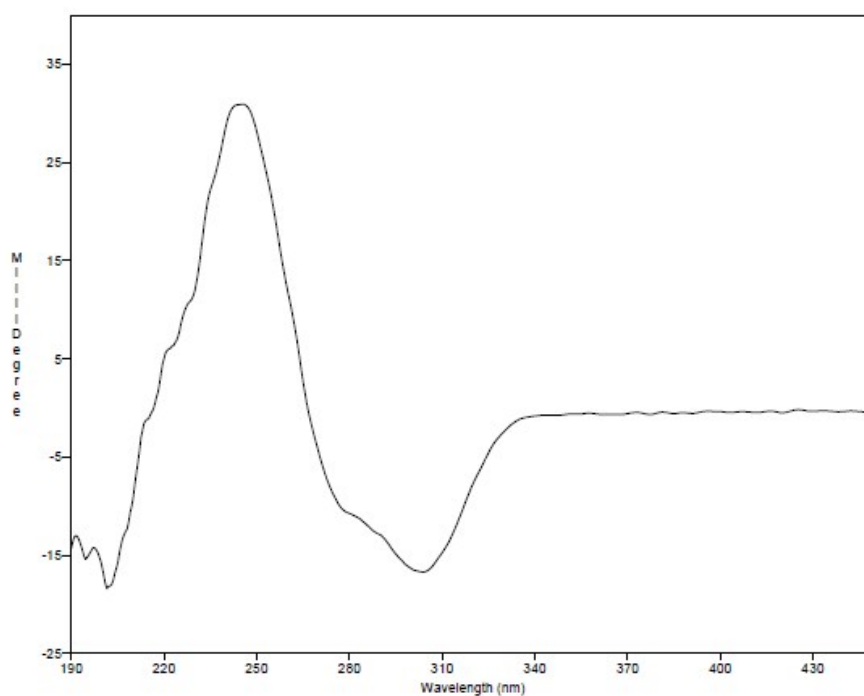


Figure S37.The chiral HPLC chromatogram of 4.

S38 The CD spectra of 1 in MeOH.

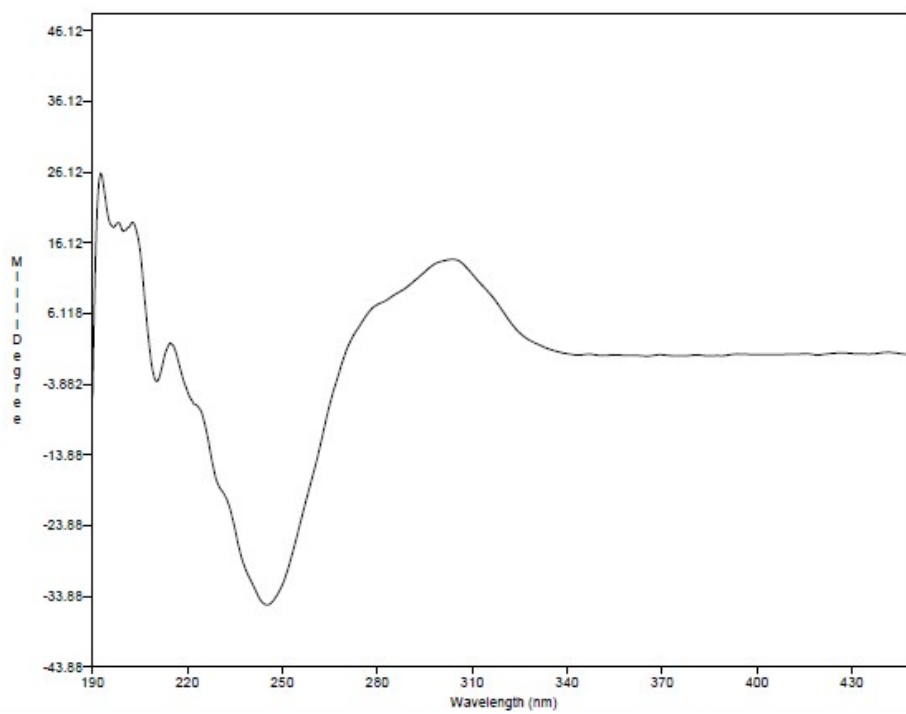


S39 The CD spectra of 1a in MeOH.



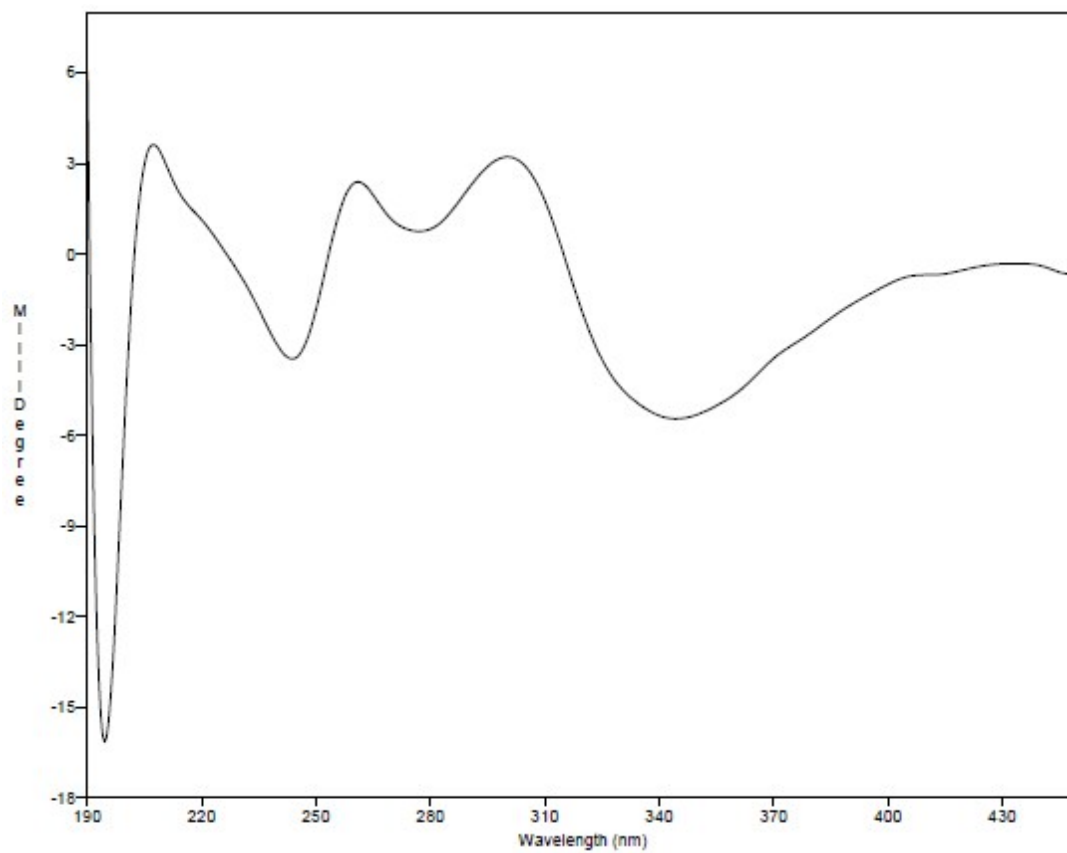
CD spectrum of 1a

S40 The CD spectra of 1b in MeOH.



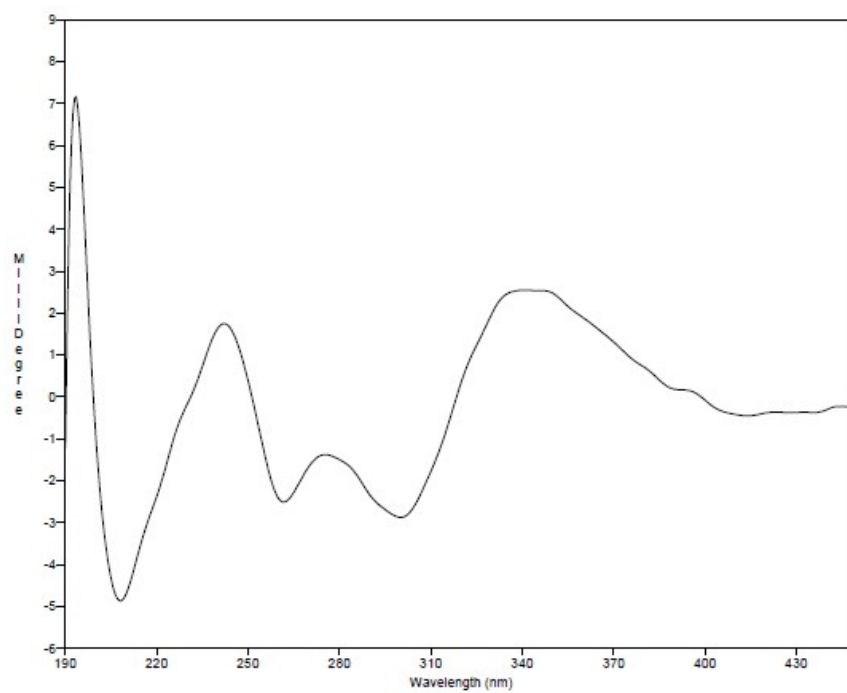
CD spectrum of 1

S41 The CD spectra of 2a in MeOH.



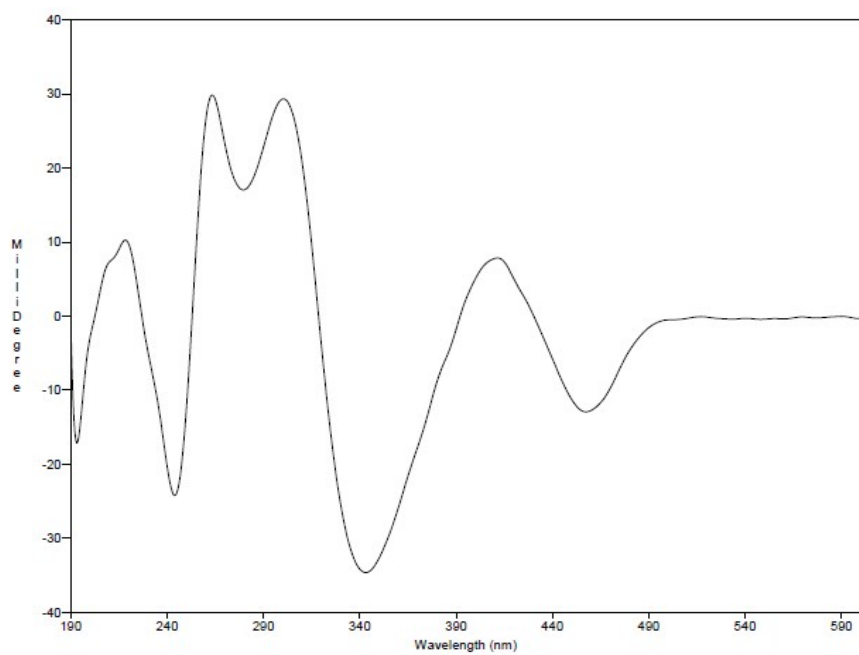
CD spectrum of **2a**

S42 The CD spectra of 2b in MeOH.



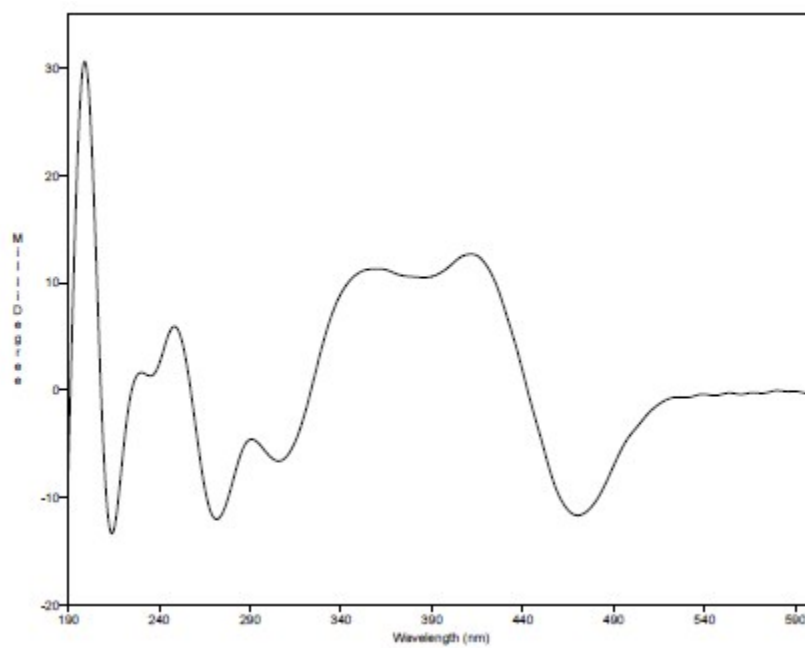
CD spectrum of 2b

S43 The CD spectra of 3a in MeOH.



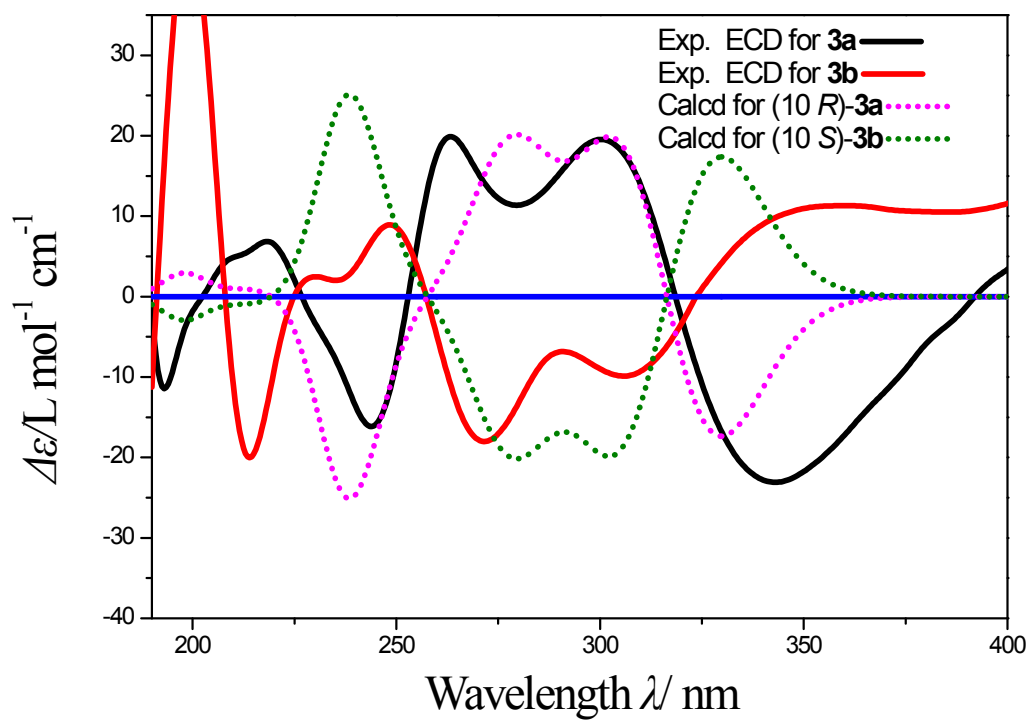
CD spectrum of 3a

S44 The CD spectra of **3b** in MeOH.

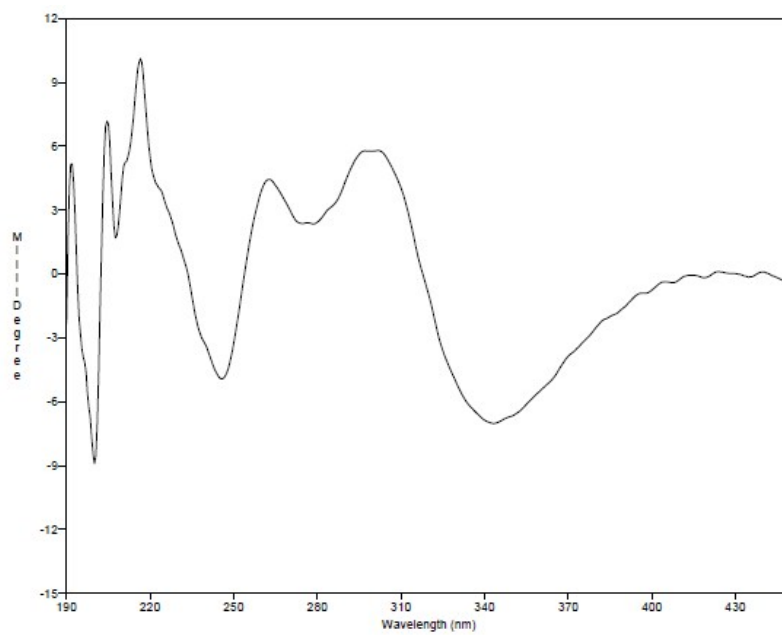


CD spectrum of **3b**

S45 The calculated CD spectra of 3a and 3b in MeOH.

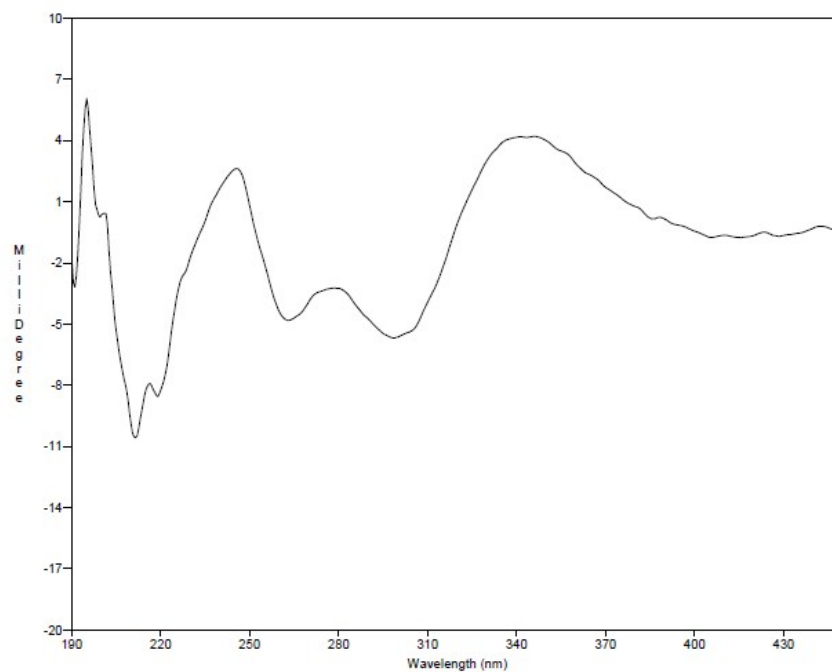


S46 The CD spectra of 4a in MeOH.



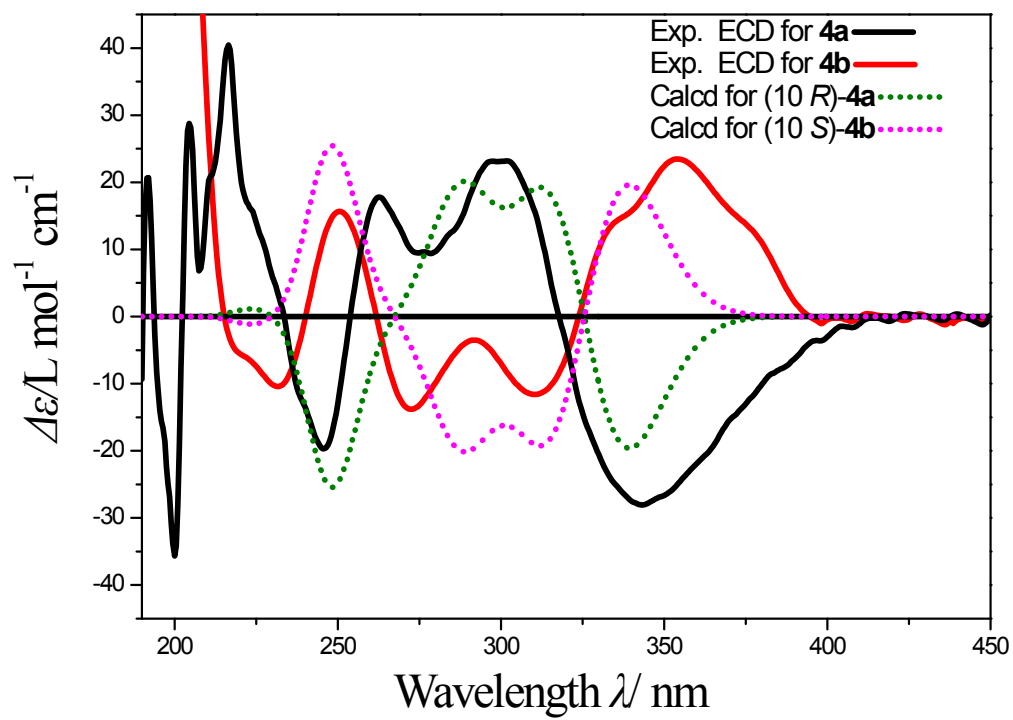
CD spectrum of 4a

S47 The CD spectra of 4b in MeOH



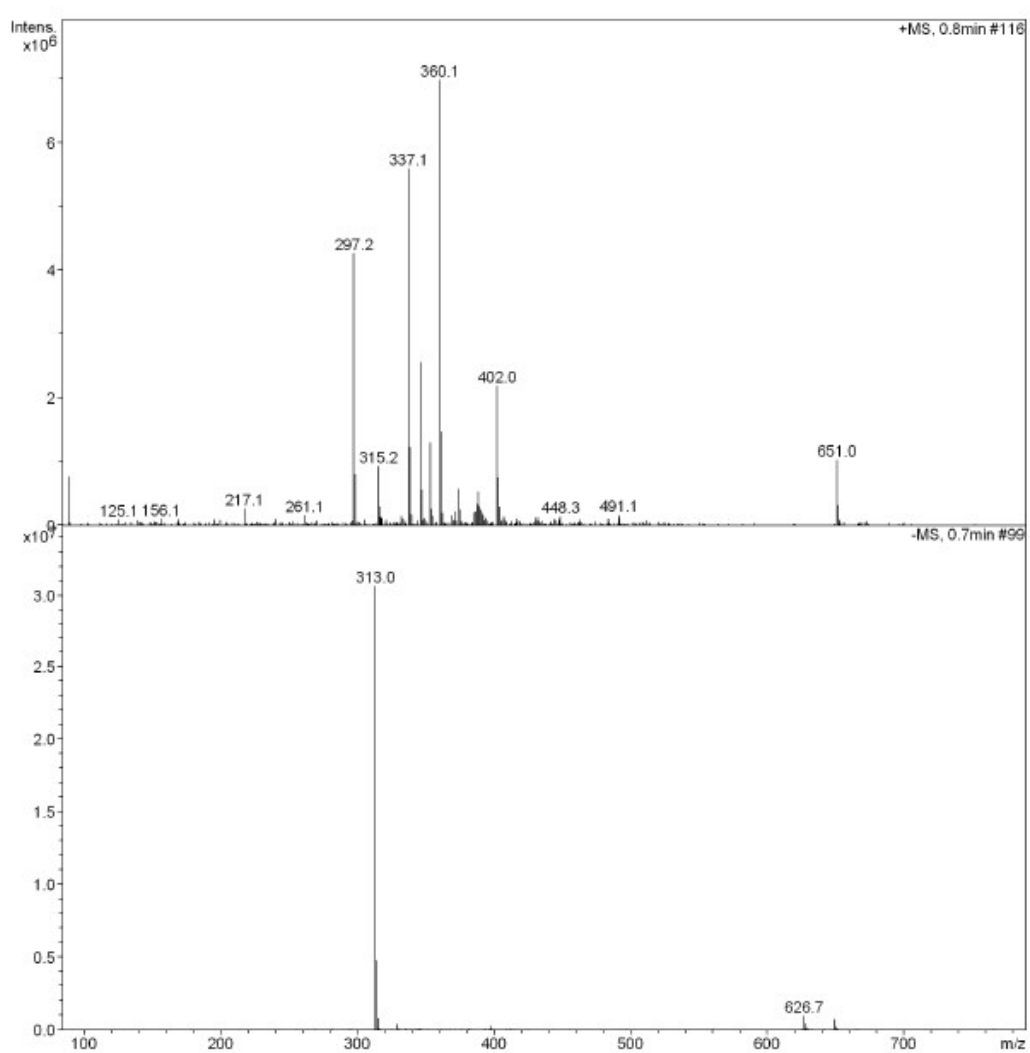
CD spectrum of **4b**

S48 The calculated CD spectra of 4a and 4b in MeOH

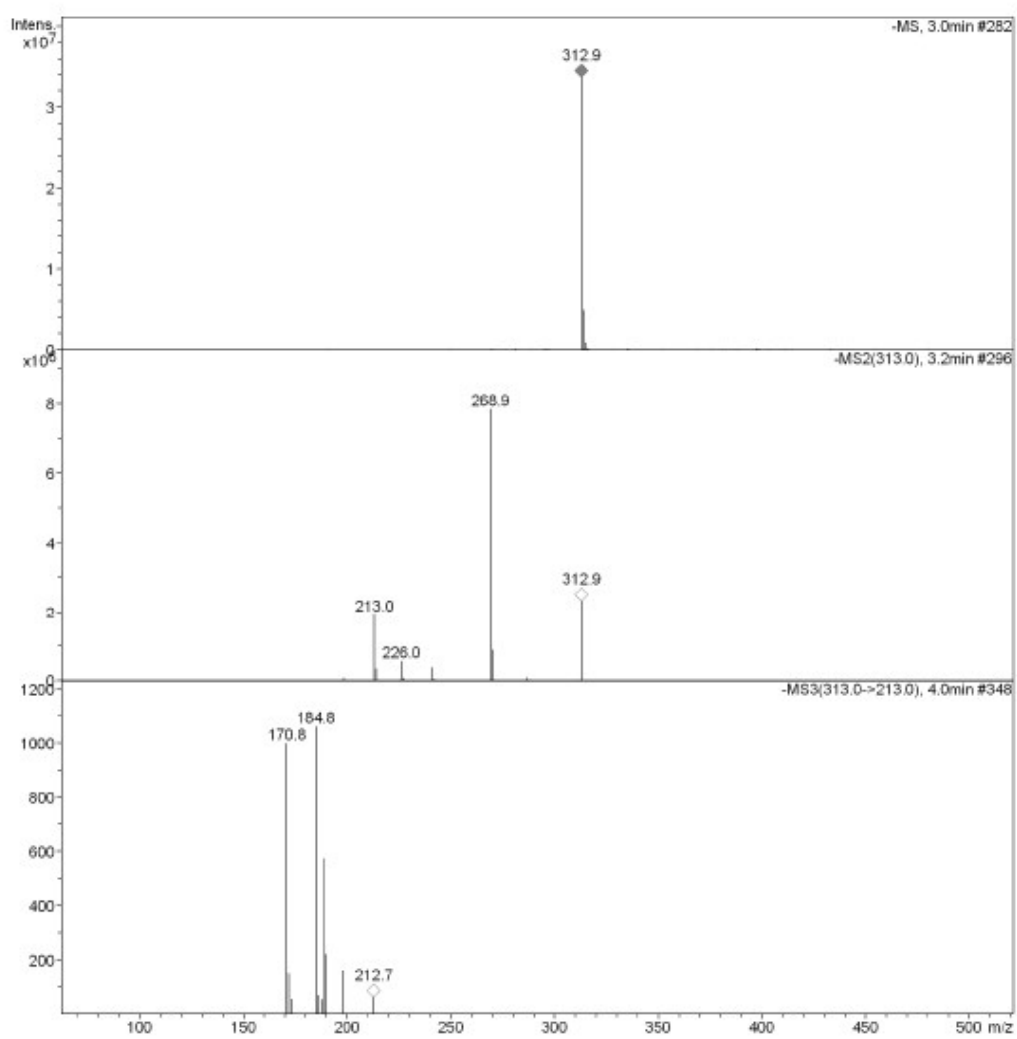


S49 ES-MS spectrum of 1.

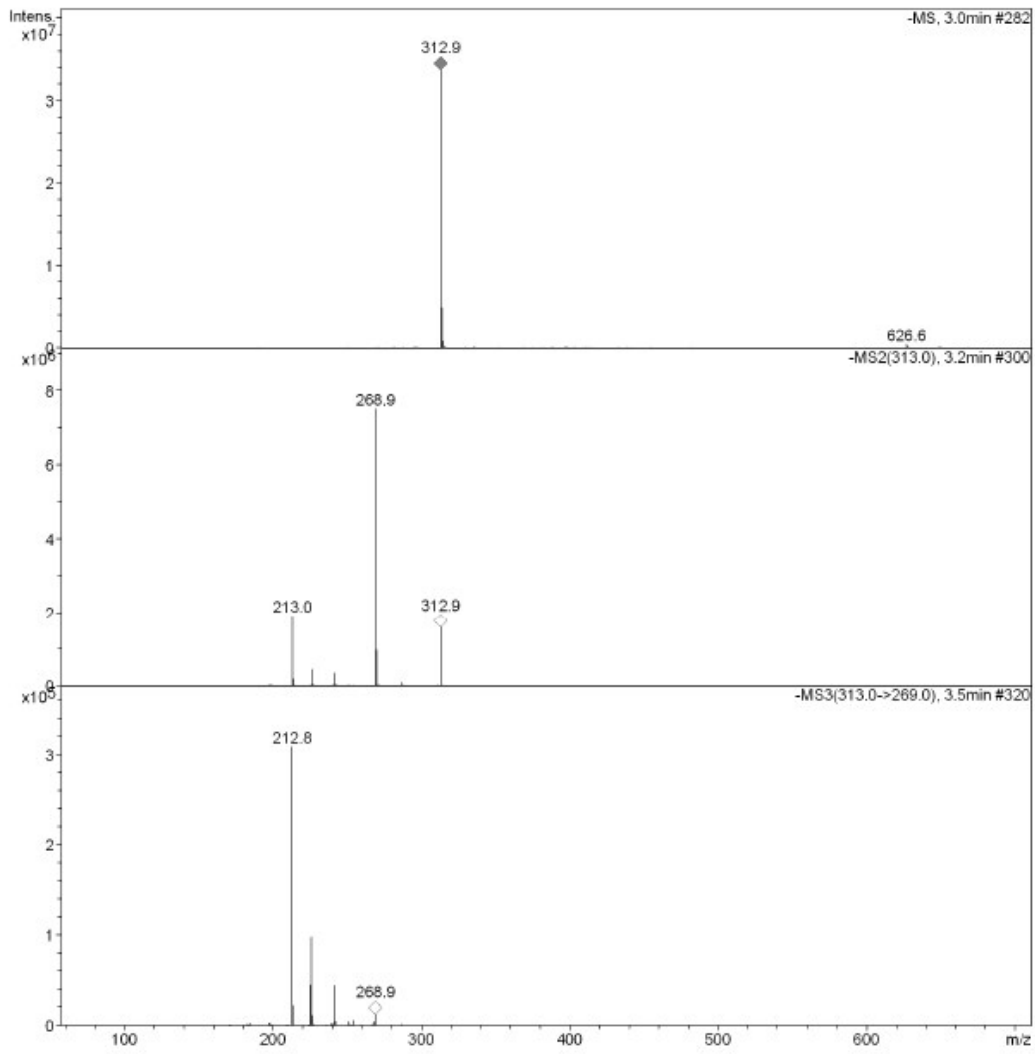
Ms



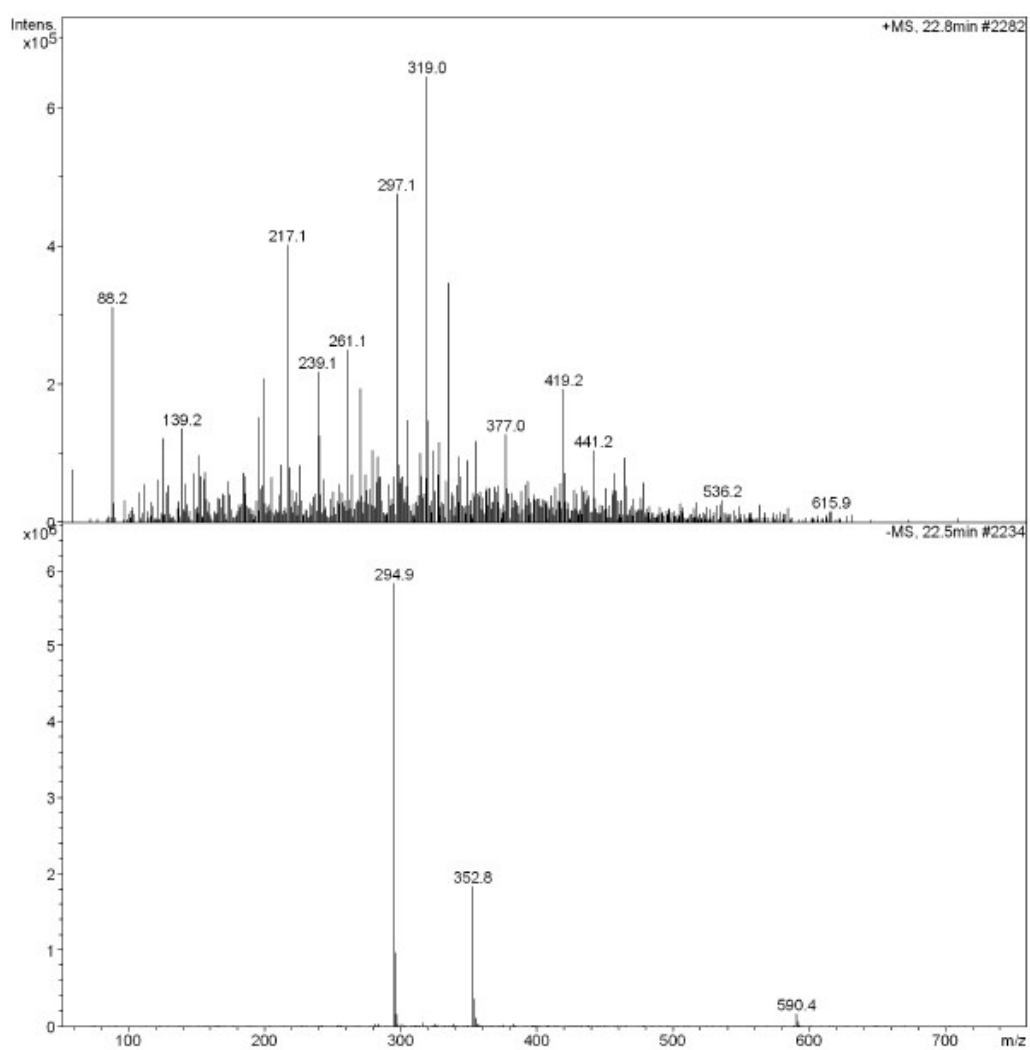
Ms²



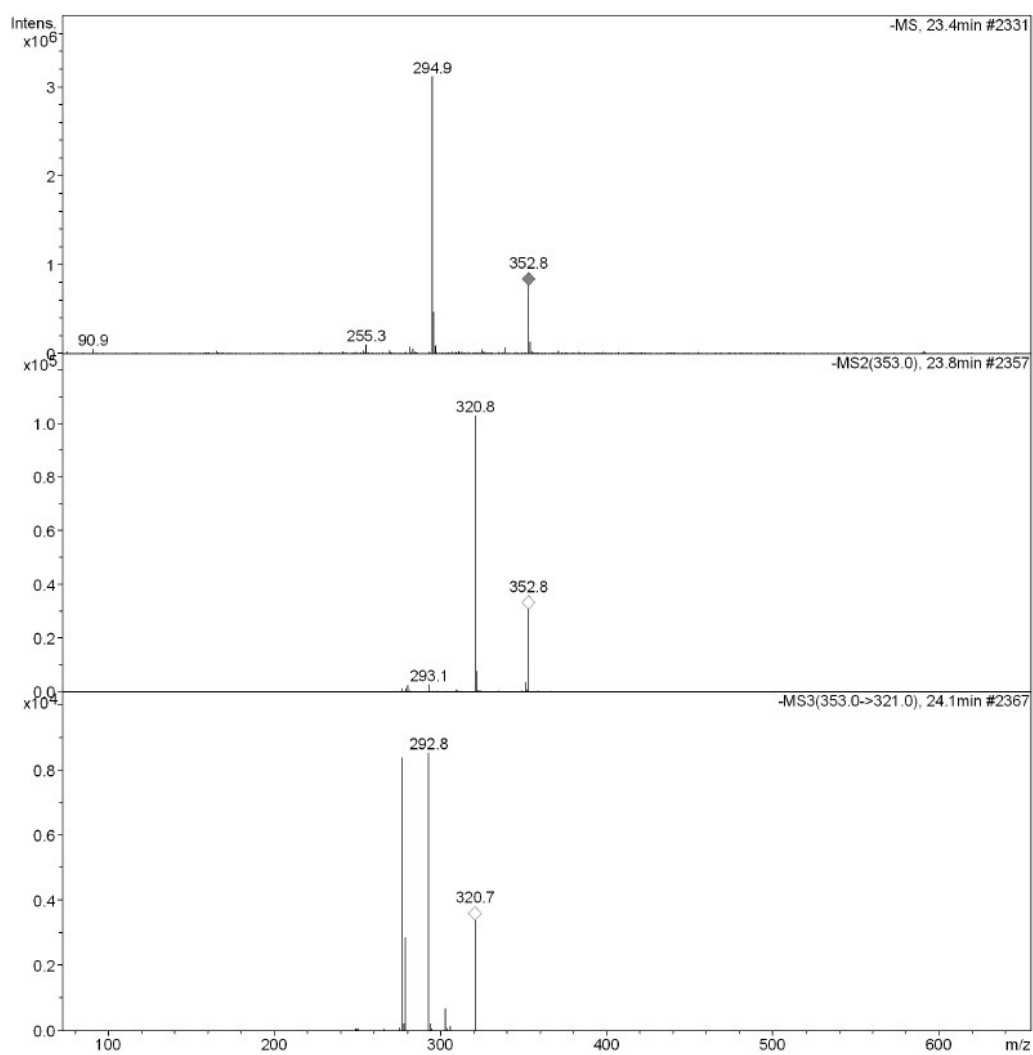
Ms³



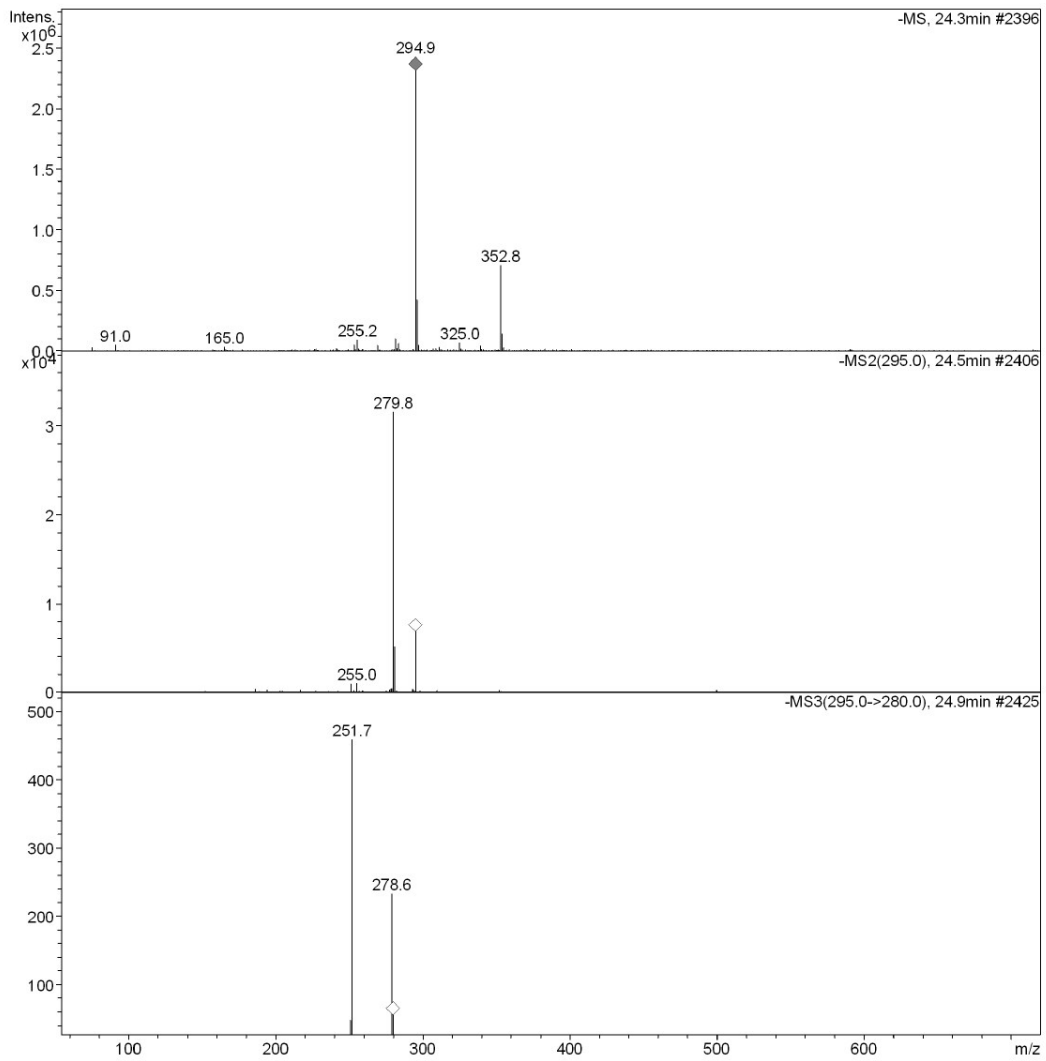
S50 ES-MS spectrum of 2.



Ms²

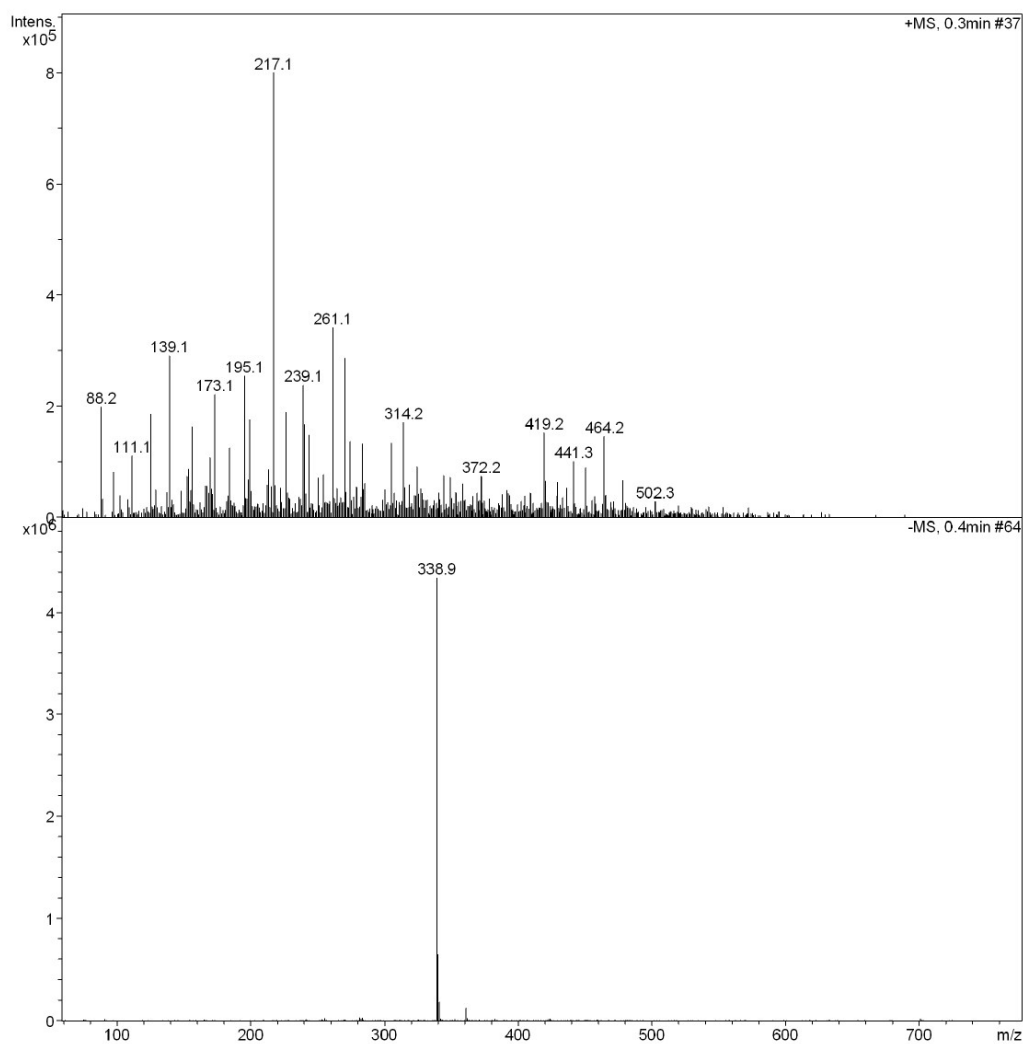


Ms³

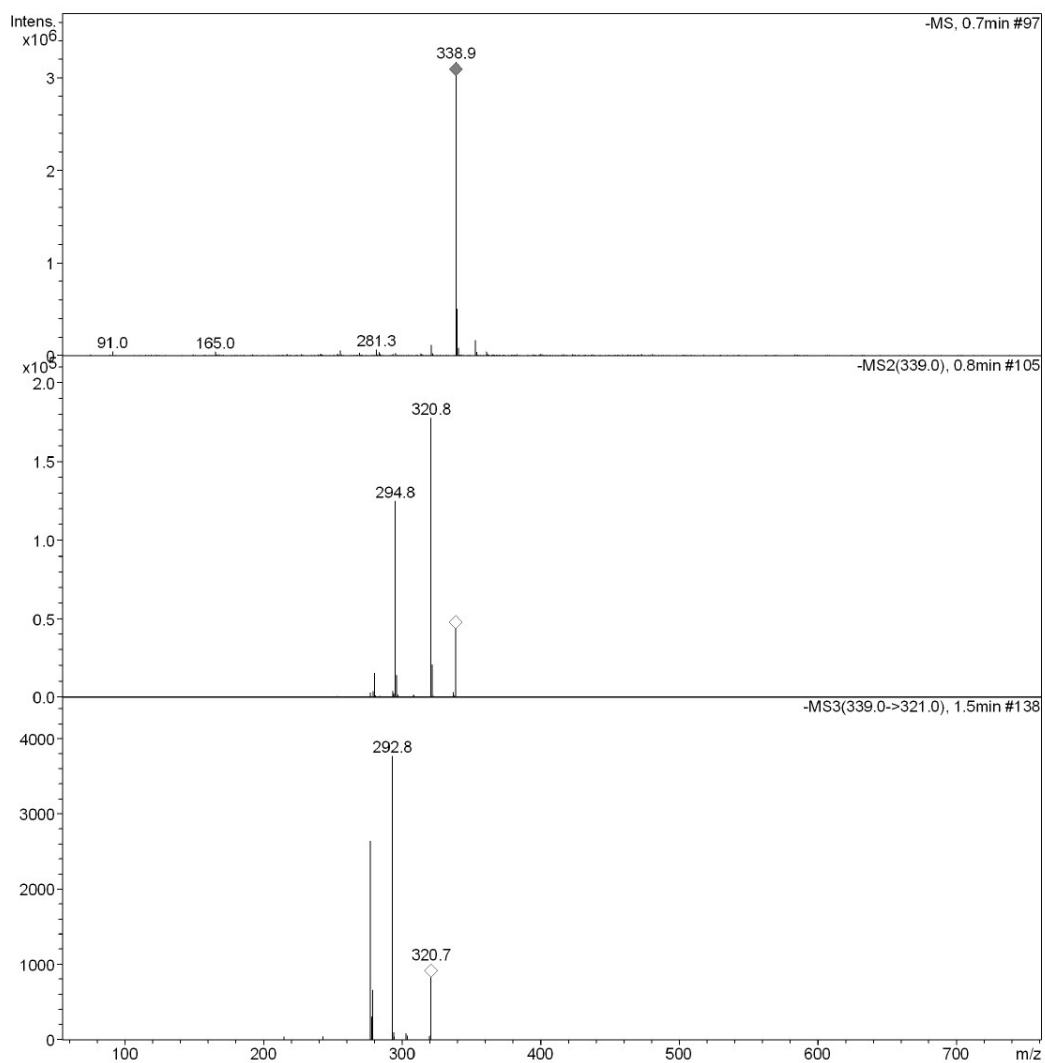


S51 ES-MS spectrum of 3.

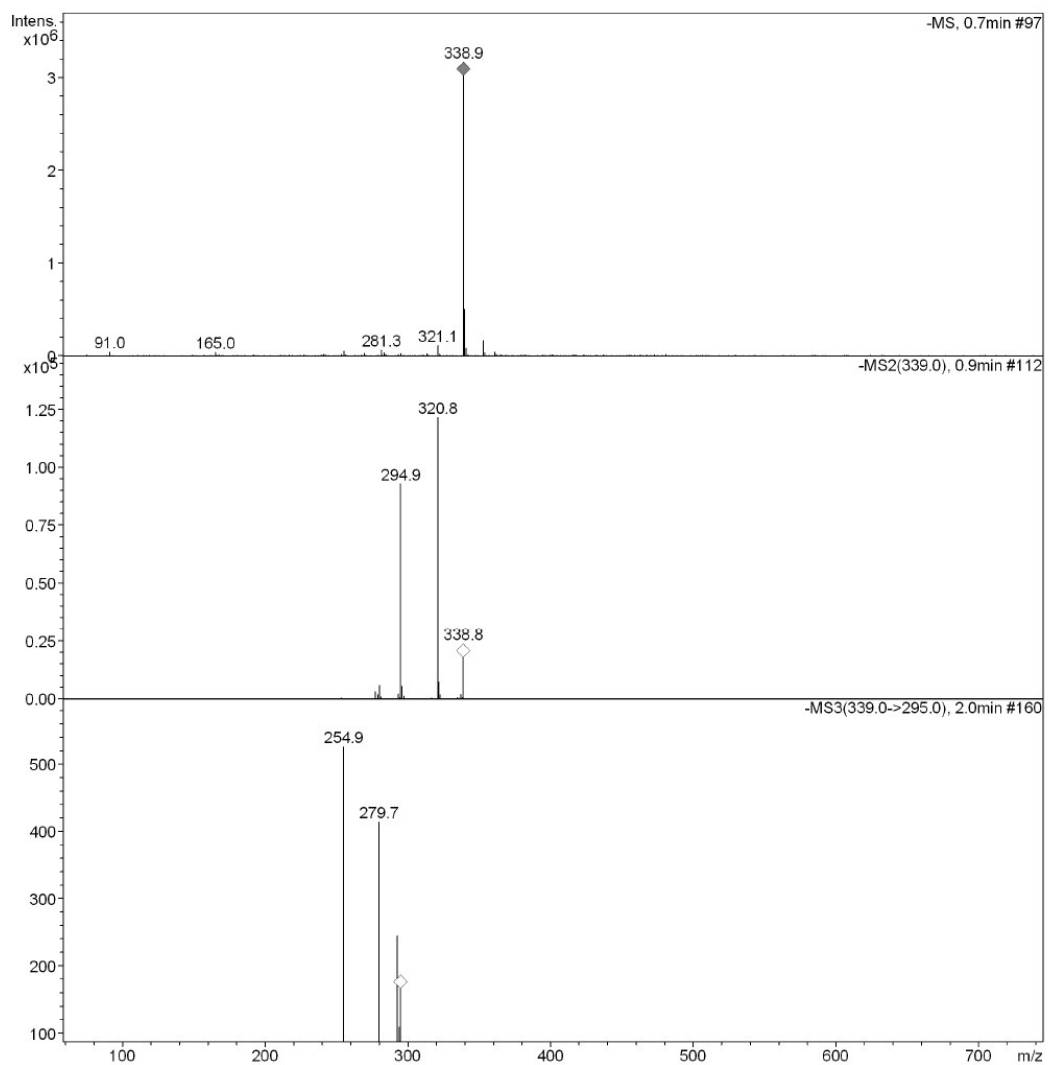
Ms



Ms²

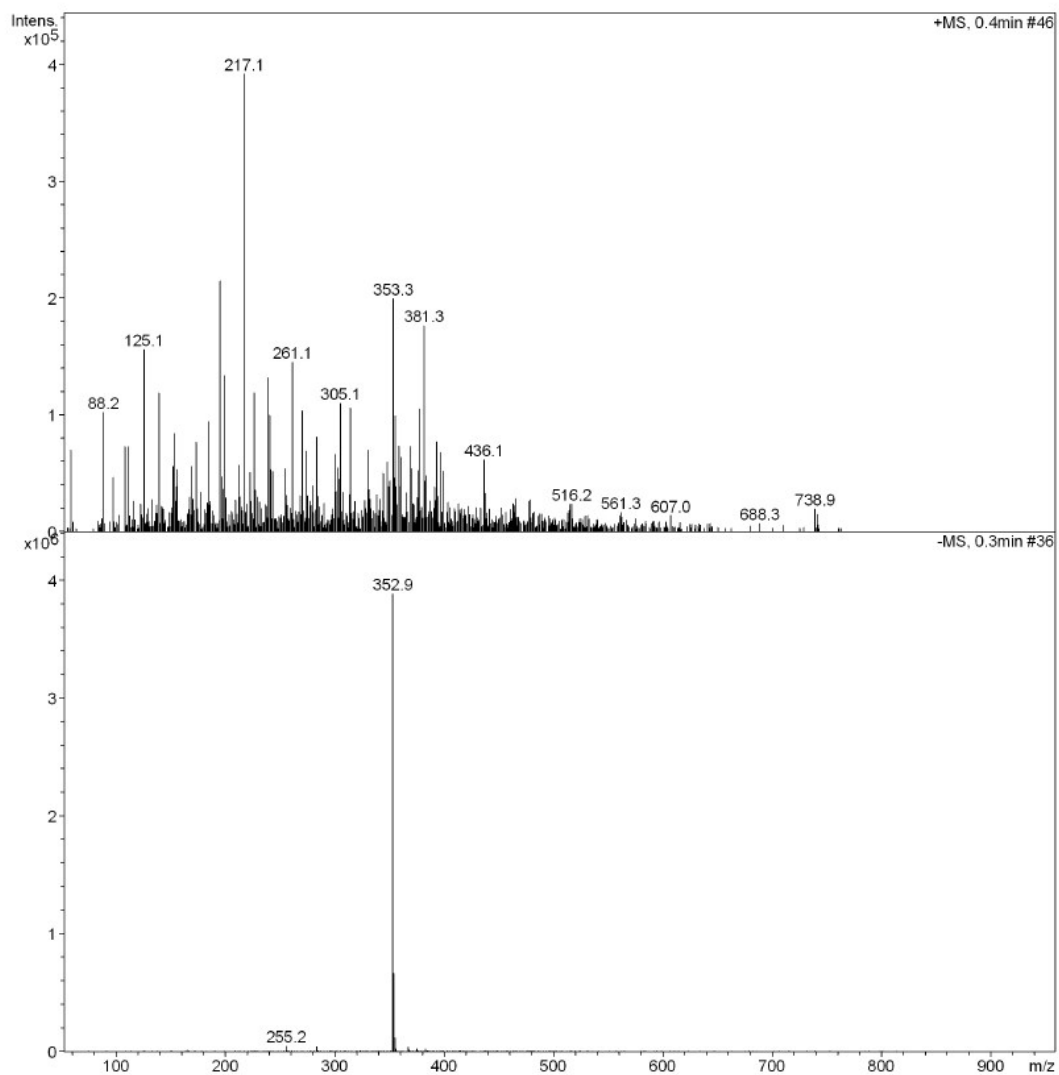


Ms³

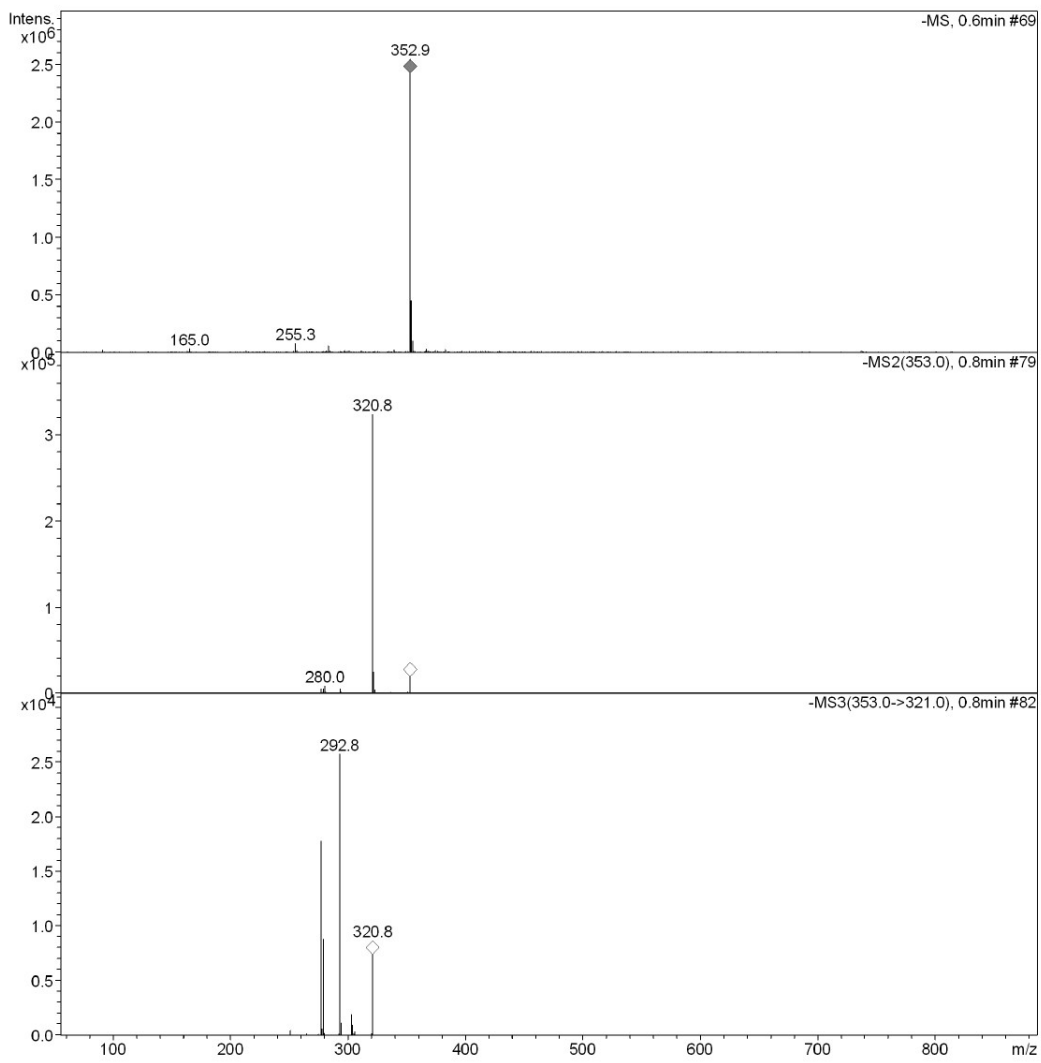


S52 ES-MS spectrum of 4.

Ms



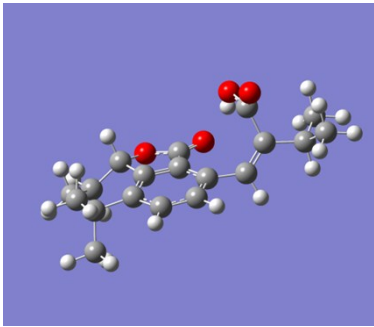
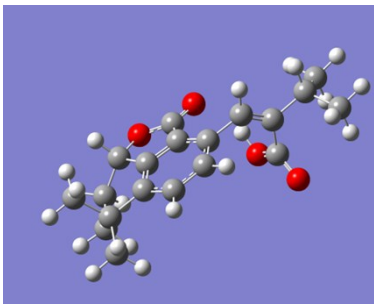
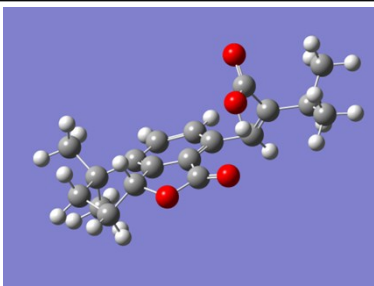
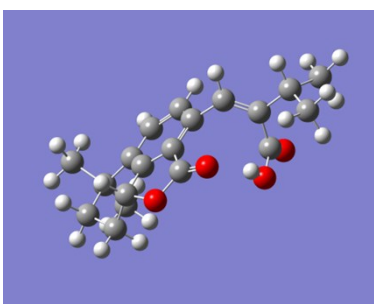
Ms²



Tables

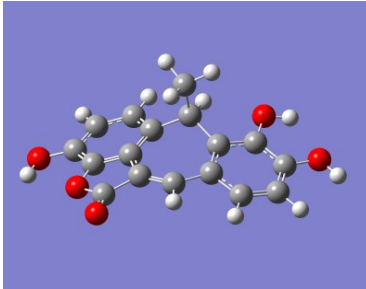
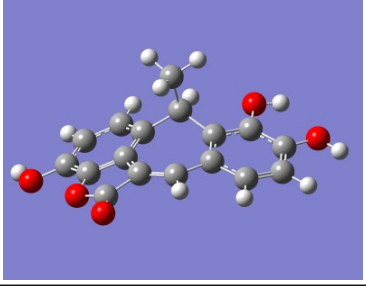
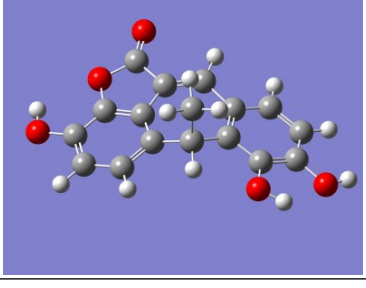
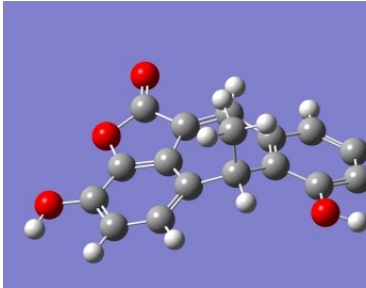
1 Conformations of 1a and 1b

Table S1. Conformations of 1a and 1b were Obtained after the Optimization.

no.	conformer	population (%)
1a-1		99.22
1a-2		0.78
1b-1		98.93
1b-2		1.07

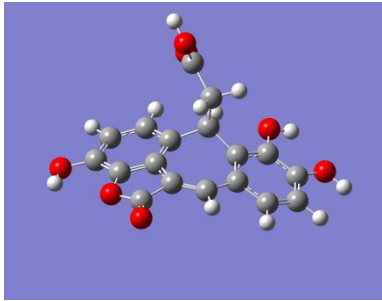
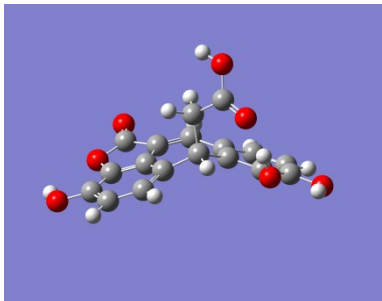
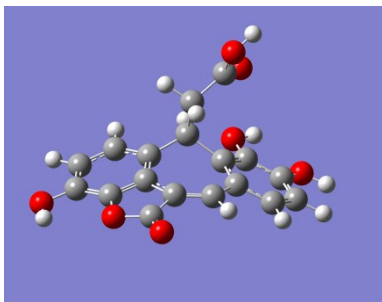
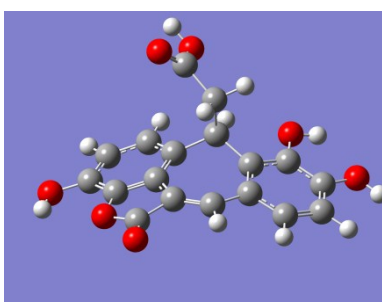
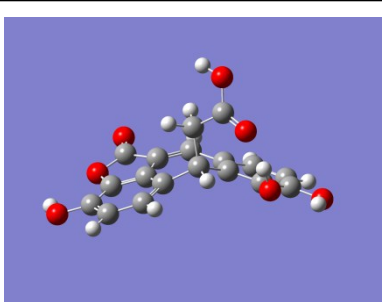
2 Conformations of 2a and 2b

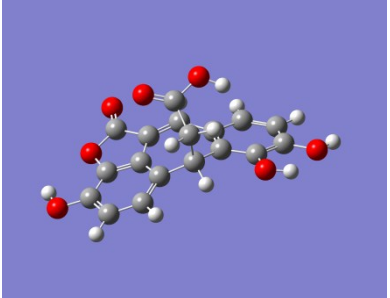

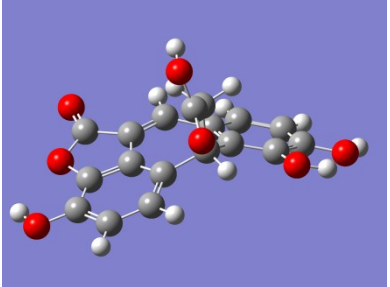
Table S2. Conformations of 2a and 2b were Obtained after the Optimization.

no.	conformer	population (%)
2a-1	 A ball-and-stick model of a complex organic molecule, likely a substituted benzene derivative, shown in a 3D perspective view. The atoms are represented by spheres: carbon (grey), oxygen (red), and hydrogen (white). The molecule is oriented with one oxygen atom pointing upwards and another pointing downwards.	75.68
2a-2	 A ball-and-stick model of the same molecule as 2a-1, but in a different conformation. The oxygen atoms are in different positions, reflecting a rotation around a bond.	24.32
2b-1	 A ball-and-stick model of a different molecule, 2b, shown in a 3D perspective view. It has a similar structure to 2a but with a different arrangement of atoms.	75.11
2b-2	 A ball-and-stick model of the same molecule as 2b-1, but in a different conformation, showing a different orientation of the oxygen atoms.	24.89

3 Conformations of 3a and 3b

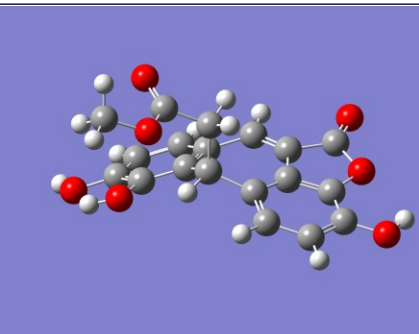
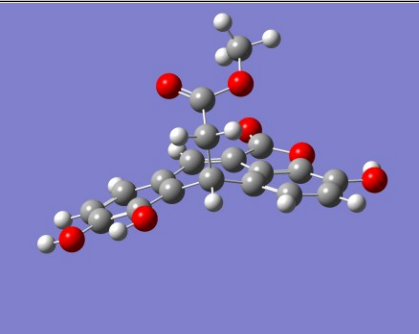


Table S3. Conformations of 3a and 3b were Obtained after the Optimization.

no.	conformer	population (%)
3a-1		53.51
3a-2		12.71...
3a-3		8.88
3a-4		24.91
3b-1		50.30

3b-2		13.55
3b-3		9.35
3b-4		26.80

4 Conformations of 4a and 4a

Table S4. Conformations of 4a and 4b were Obtained after the Optimization.

no.	conformer	population (%)
4a-1		96.55
4a-2		3.45
4b-1		98.97
4b-2		1.03

5 The toxic effect of the isolates in H9c2 cells after 24 h incubation

Table S5 The survival rate of the cell **H9c2** (%) (M±SD)

	CON	Comp. + H ₂ O ₂		
		100μM	50μM	25μM
1a	100±5.78	96.96±3.01	100.47±4.02	101.3±2.24
1b	100±5.78	116.1±5.14*	102.53±2.33	109.26±6.34
2a	100±5.75	91.98±1.76*	90.50±2.04**	95.32±2.66
2b	100±5.75	94.16±1.67	91.79±2.69	97.62±2.77
3a	100±5.75	105.16±1.67	115.21±2.69	105.52±2.77
3b	100±5.75	100.41±6.33	102.87±5.54	101.39±8.39
4a	100±5.78	108.94±4.69	108.305±6.97	103.98±5.66
4b	100±5.78	110.83±9.07	113.01±6.81	112.58±6.92

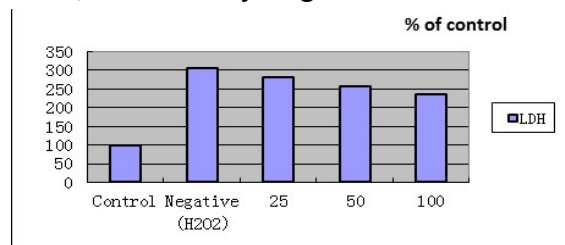
###:P<0.001 Vs Control; *,P<0.05 Vs model; **: P<0.01 Vs model; ***:P<0.001 Vs model

6 The cytoprotective effects of the isolates assessed using LDH leakage assays

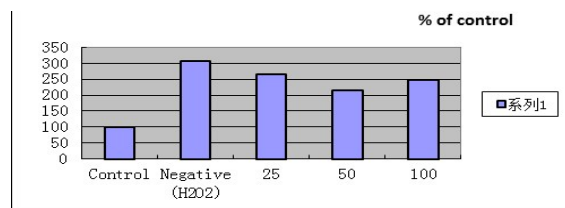
Table S6 Effects of 2-hour isolates pretreatment on LDH activity in each group

	Con (U/L)	H ₂ O ₂ (200 μM) (U/L)	Comp. + H ₂ O ₂ (U/L)		
			25μM	50μM	100μM
Comp.2a	96.67	296.67	273.33	250	226.67
Comp.2b	96.67	296.67	256.67	246.67	240
Comp.3a	96.67	296.67	206.67	253.33	220
Comp.3b	96.67	296.67	246.67	250	230

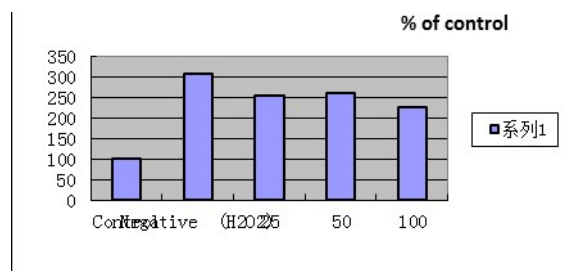
LDH, Lactate dehydrogenase



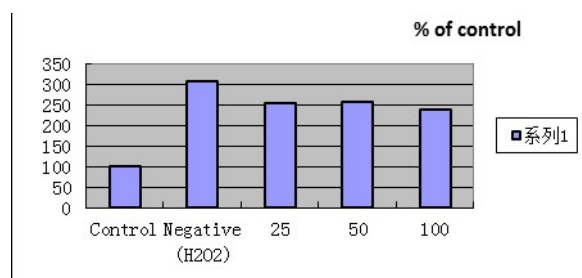
2a



2b



3a



3b

S The toxic effect of isolates in LPS-induced N9 cell viability

Table S7 The survival rate of the cell N9 (%) (M±SD)

	CON	LPS (1 µg/mL)	Comp. + LPS		
			0.3µM	3.0µM	30.0µM
Comp.1a	100±1.34	99.34±1.48	100.14±1.79	98.07±1.89	99.75±1.53
Comp.1b	100±4.06	98.12±2.01	100.34±1.11	99.17±1.09	101.2±0.87
Comp.2a	100±1.54	99.46±0.42	103.18±1.74	99.93±0.89	100.00±2.17
Comp.2b	100±2.04	100.52±10.4	100.03±1.67	99.71±1.41	99.52±0.85
Comp.3a	100±1.00	98.90±2.16	100.29±0.85	100.15±0.36	102.15±1.86
Comp.3b	100±0.91	99.26±0.82	98.69±0.60	101.19±1.20	99.55±1.07
Comp.4a	100±0.59	101.79±0.79	99.46±1.15	98.35±0.76	101.31±0.89
Comp.4b	100±1.18	101.57±2.08	98.76±3.33	99.63±0.87	98.56±0.52
MINO	100±2.5	100.35±1.35	-	-	101.28±0.53 20.0µM

###:P<0.001 Vs Control; *:P<0.05 Vs model; **: P<0.01 Vs model;
***:P<0.001 Vs mod