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

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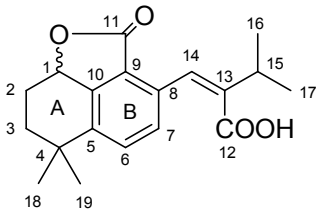
Supplementary Tables

S1 HRESIMS spectrum of 1



Compound Mass Spectrum List Report

Analysis Info

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Sample Name	DUI	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

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Focus	Active	Set Capillary	4500 V	Set Dry Heater	190 °C
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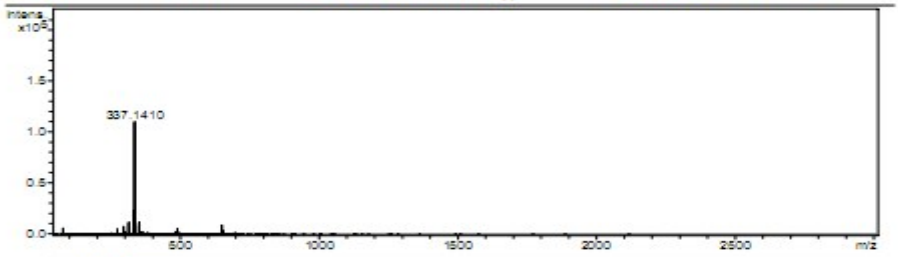
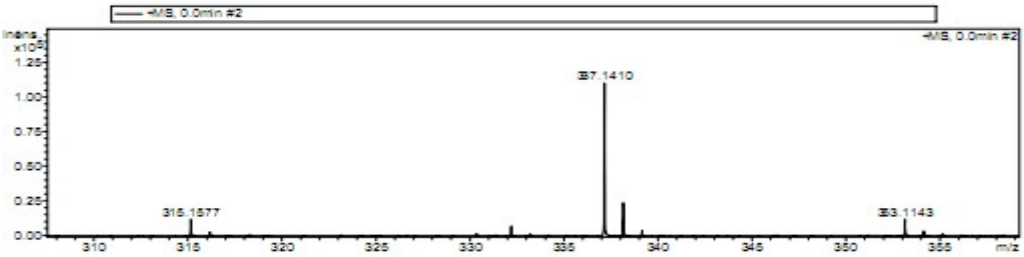
Scan End	3000 m/z	Set Collision Cell RF	40.0 Vpp	Set Divert Valve	Source





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2	337.1410	110106
3	353.1143	11725

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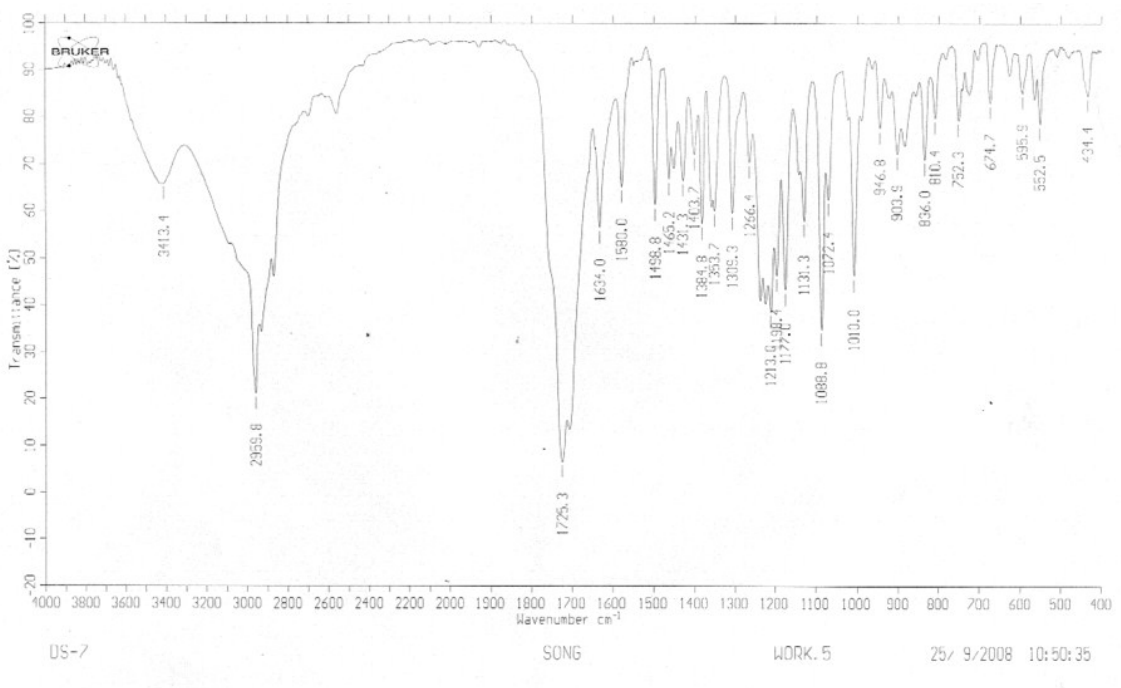

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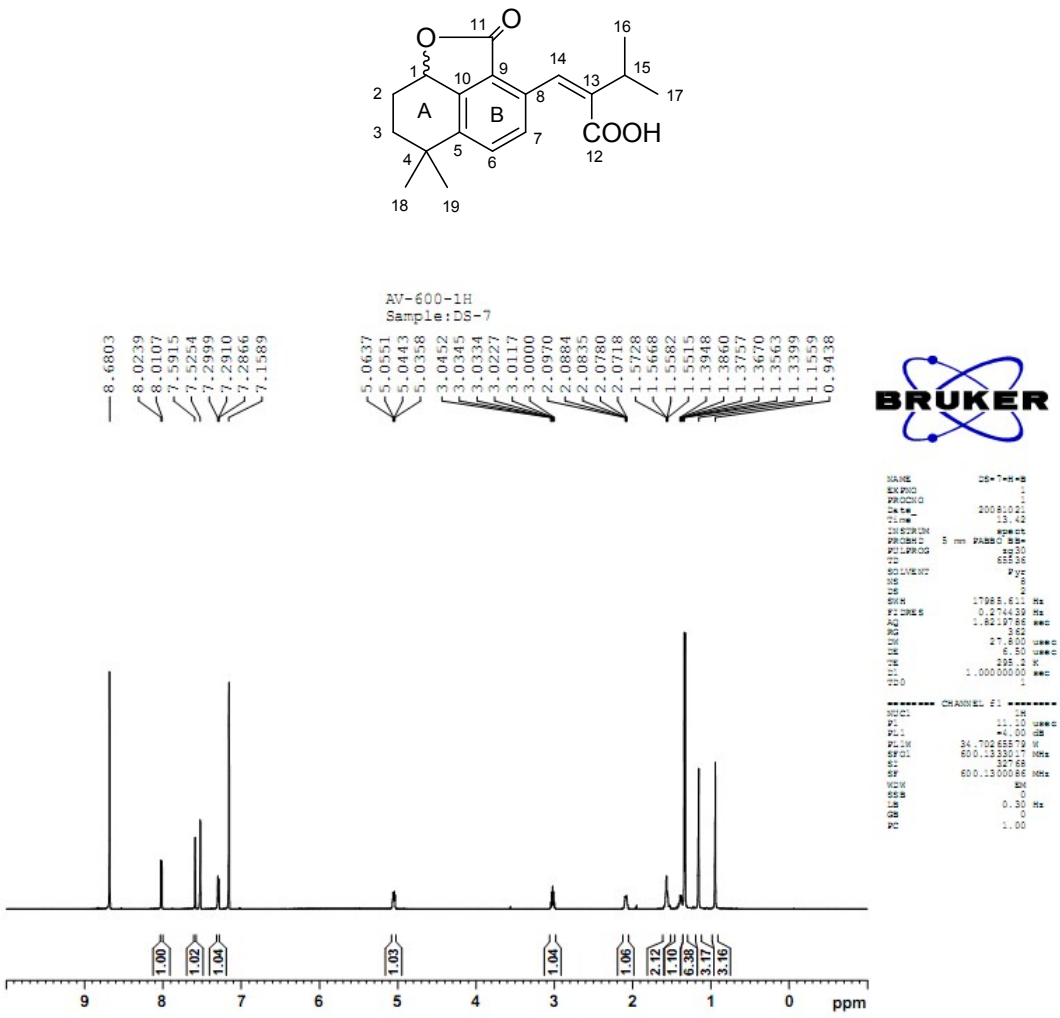

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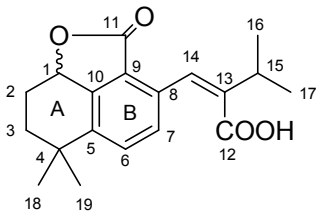
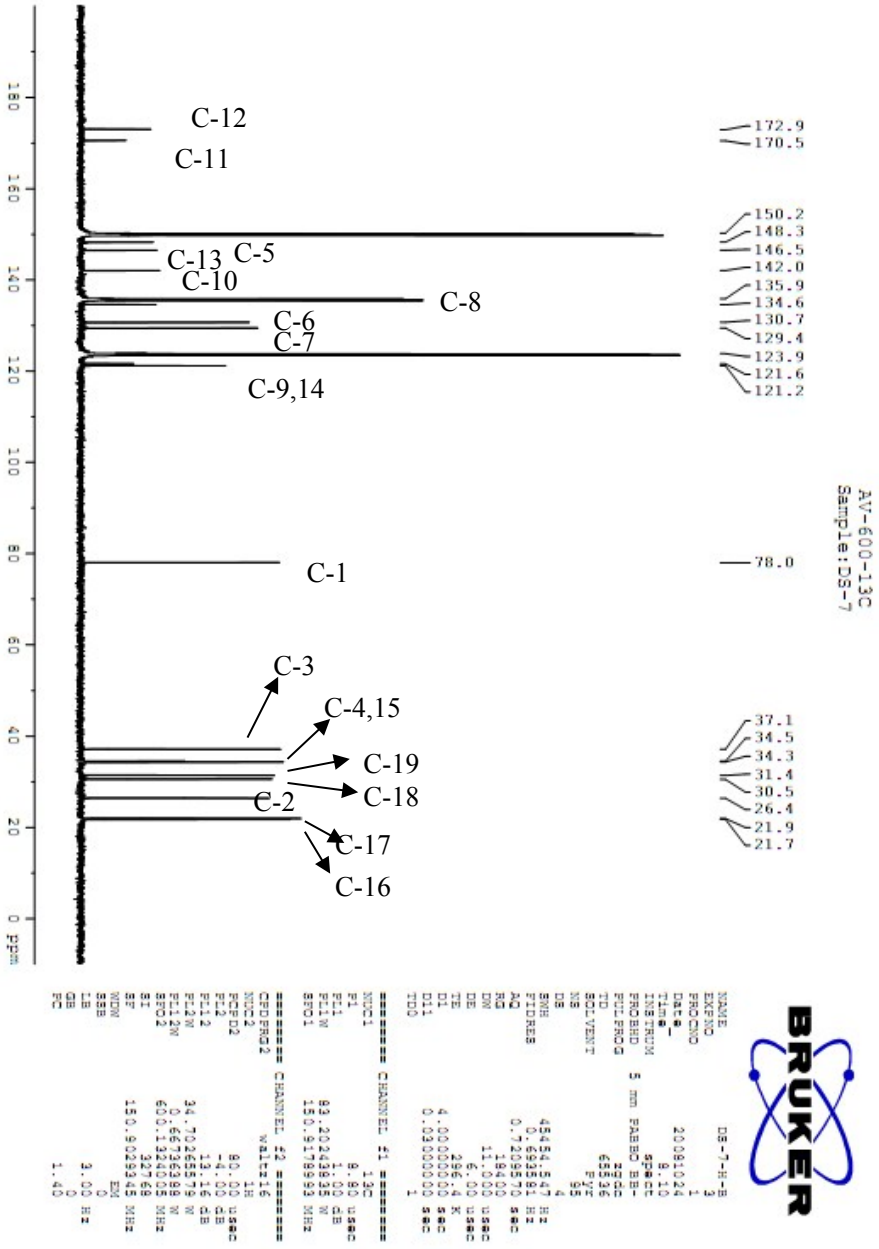
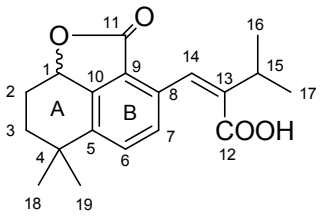
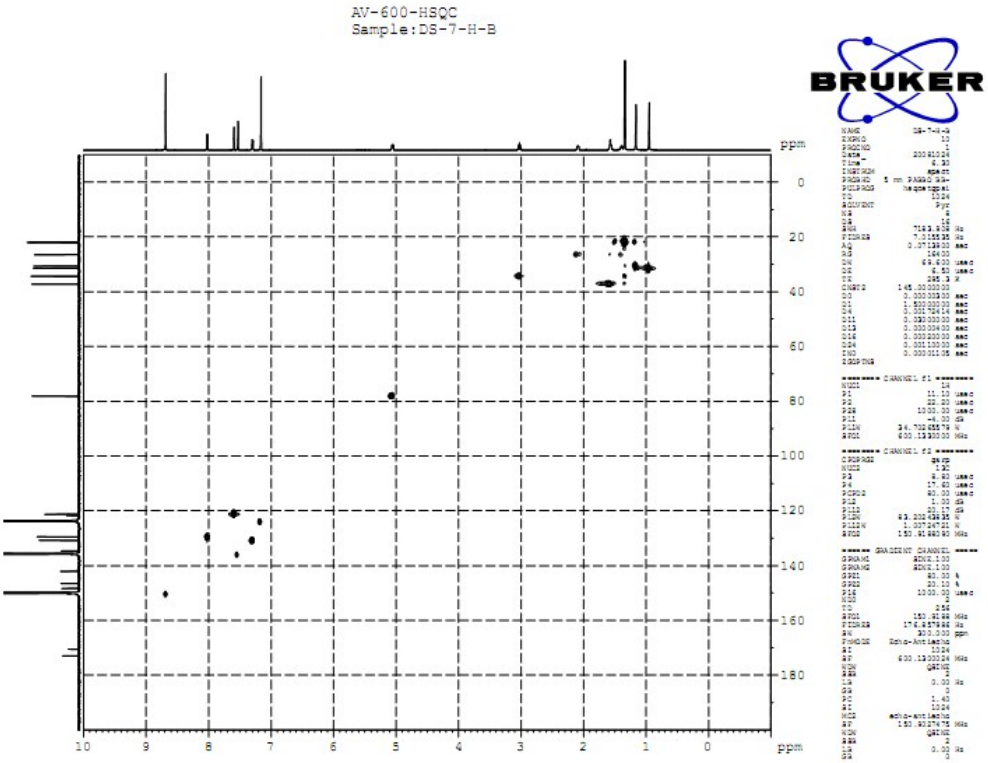




S5 HSQC spectrum of 1 tested in C_5D_5N





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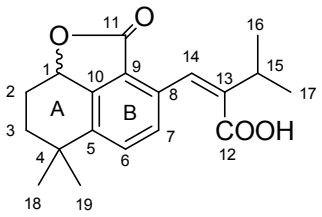
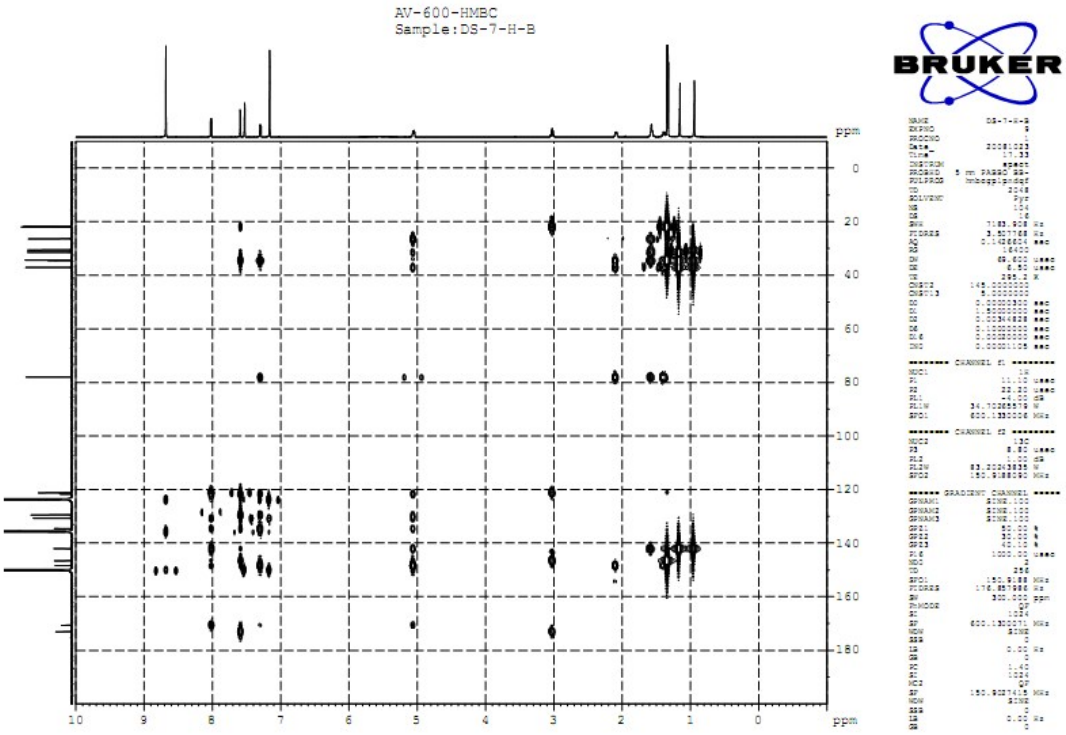
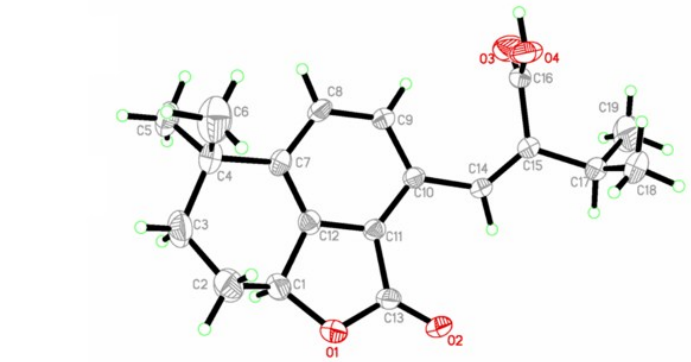
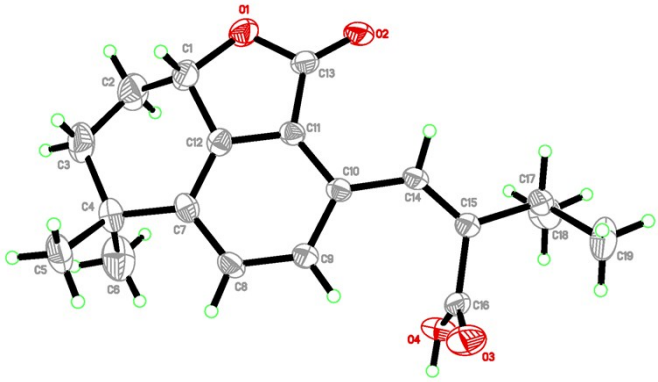
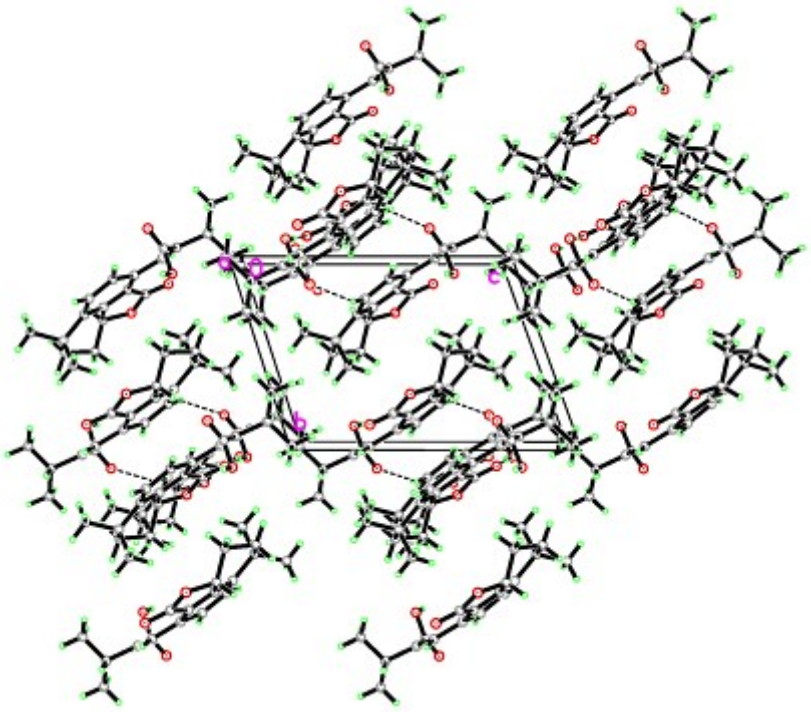




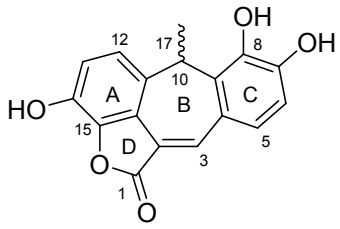
S7 Single-crystal X-ray structure of 1







S8 HRESIMS spectrum of 2



Compound Mass Spectrum List Report

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Comment			

Acquisition Parameter

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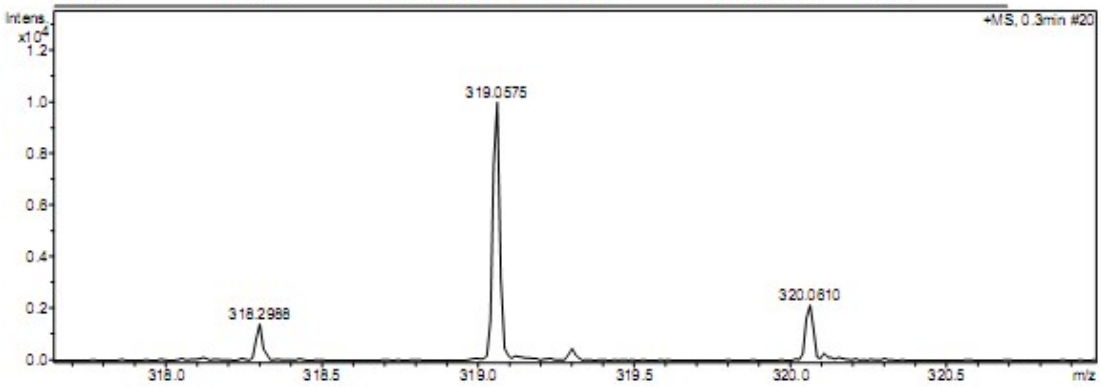
Focus	Active	Set Capillary	4500 V	Set Dry Heater	190 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	120.0 Vpp	Set Divert Valve	Source



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2	319.0575	9978
3	320.0810	2129

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e
C 17 H 12 Na 1 O 5	0.022	319.0577	0.54	0.52	0.17	11.50	ok	even

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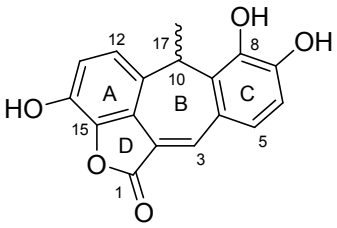
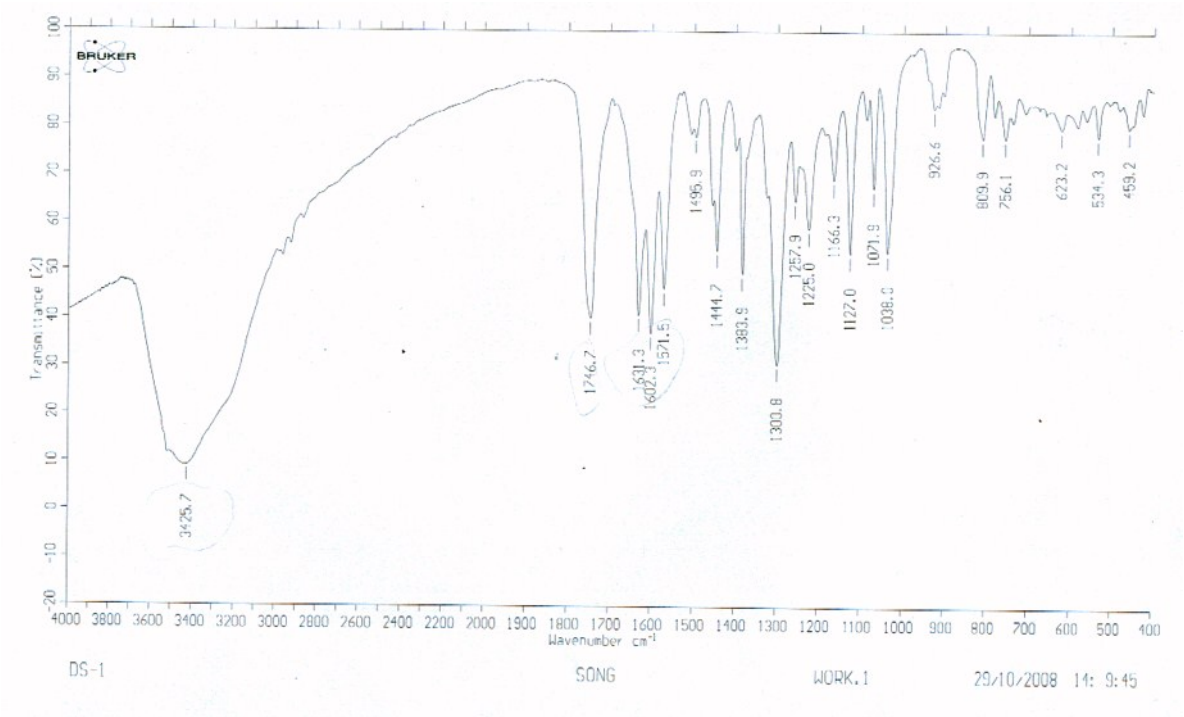
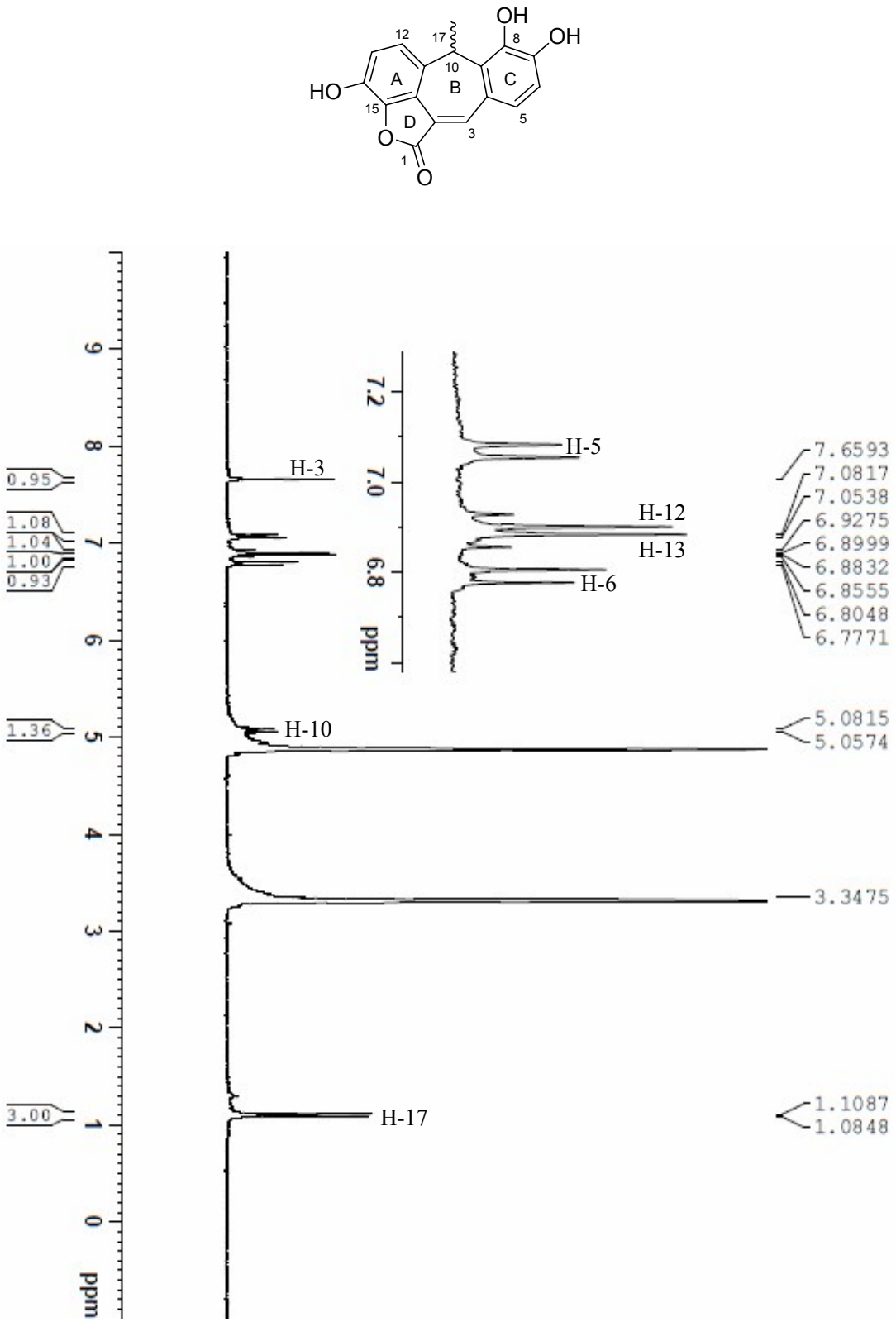




S10 ^{1}H NMR spectrum of 2 tested in CD_3OD



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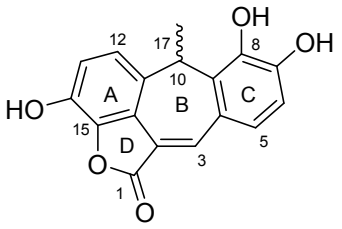

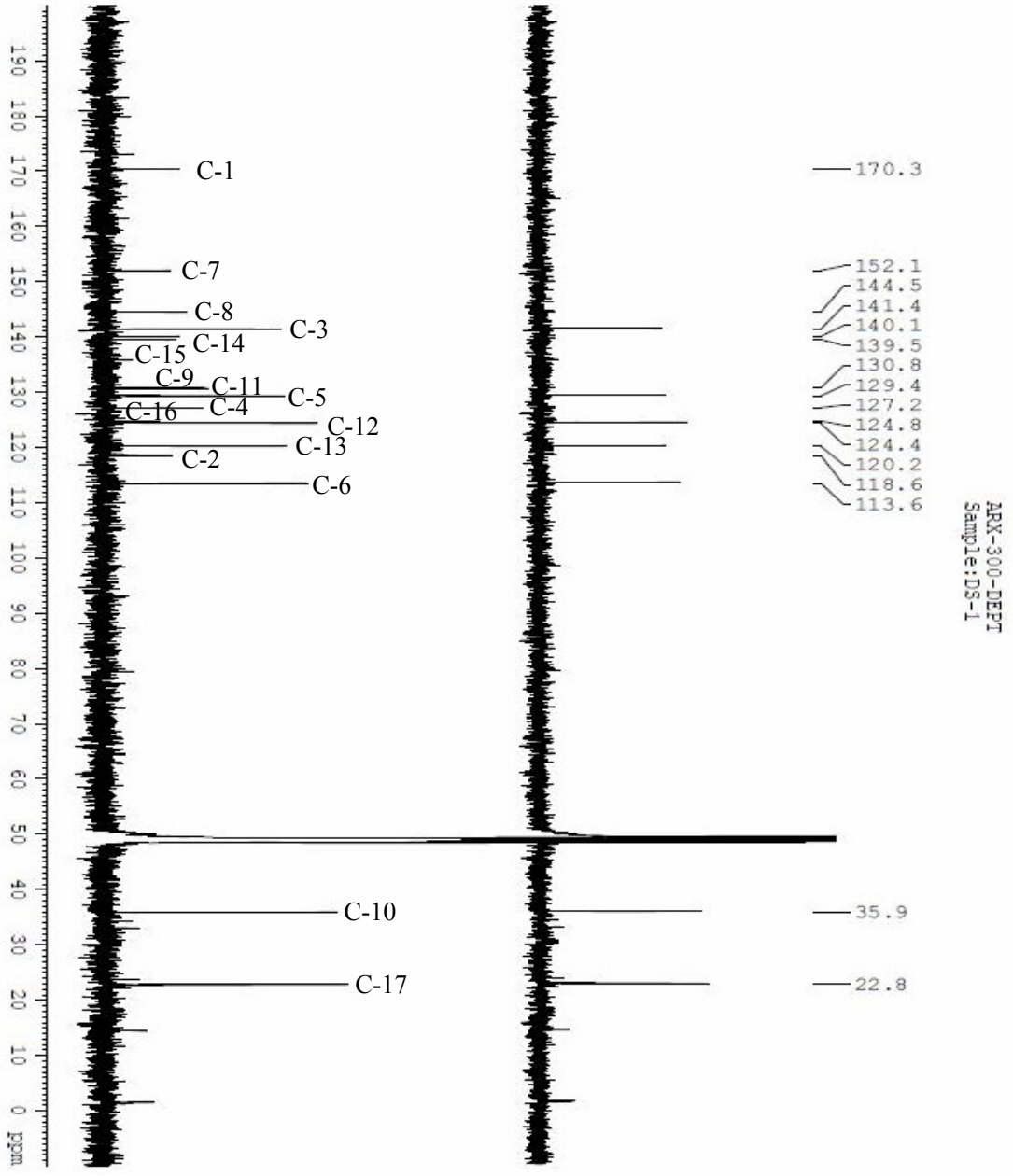

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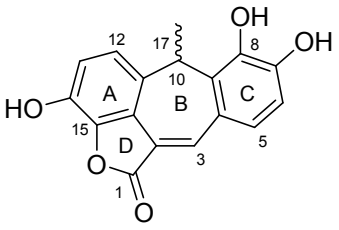
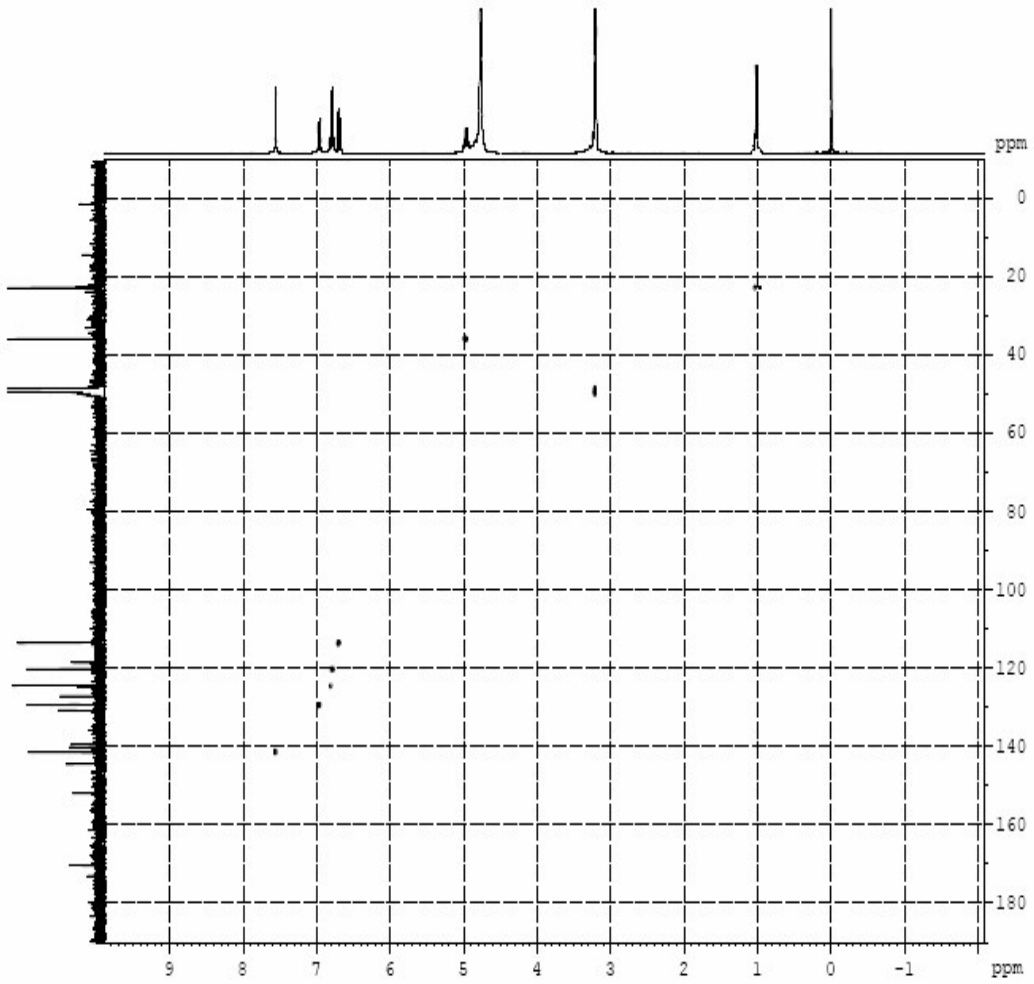


AV-600-HSQC
Sample:DS-1



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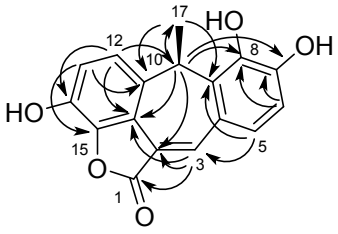

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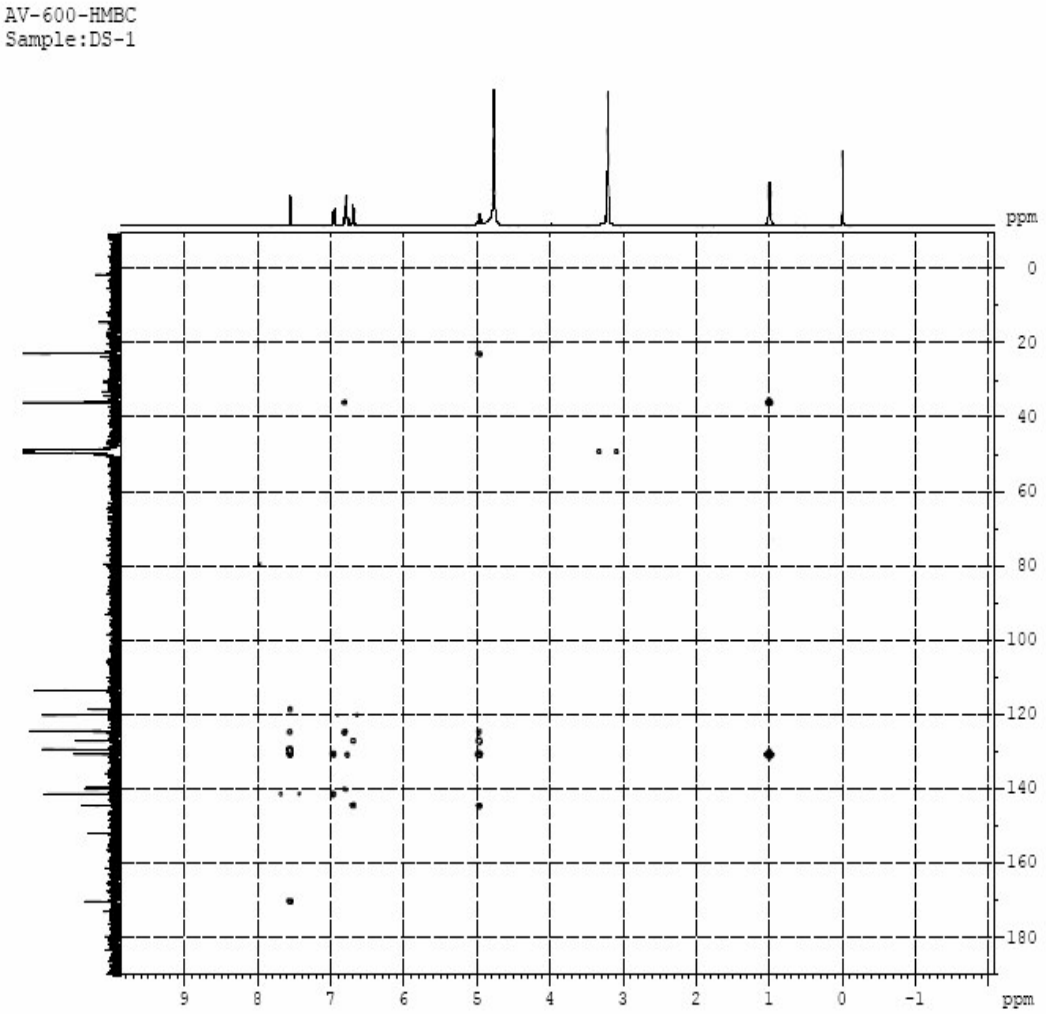

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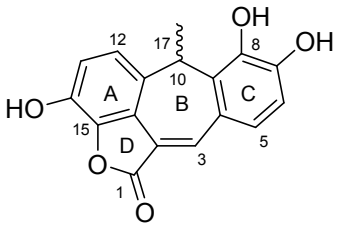
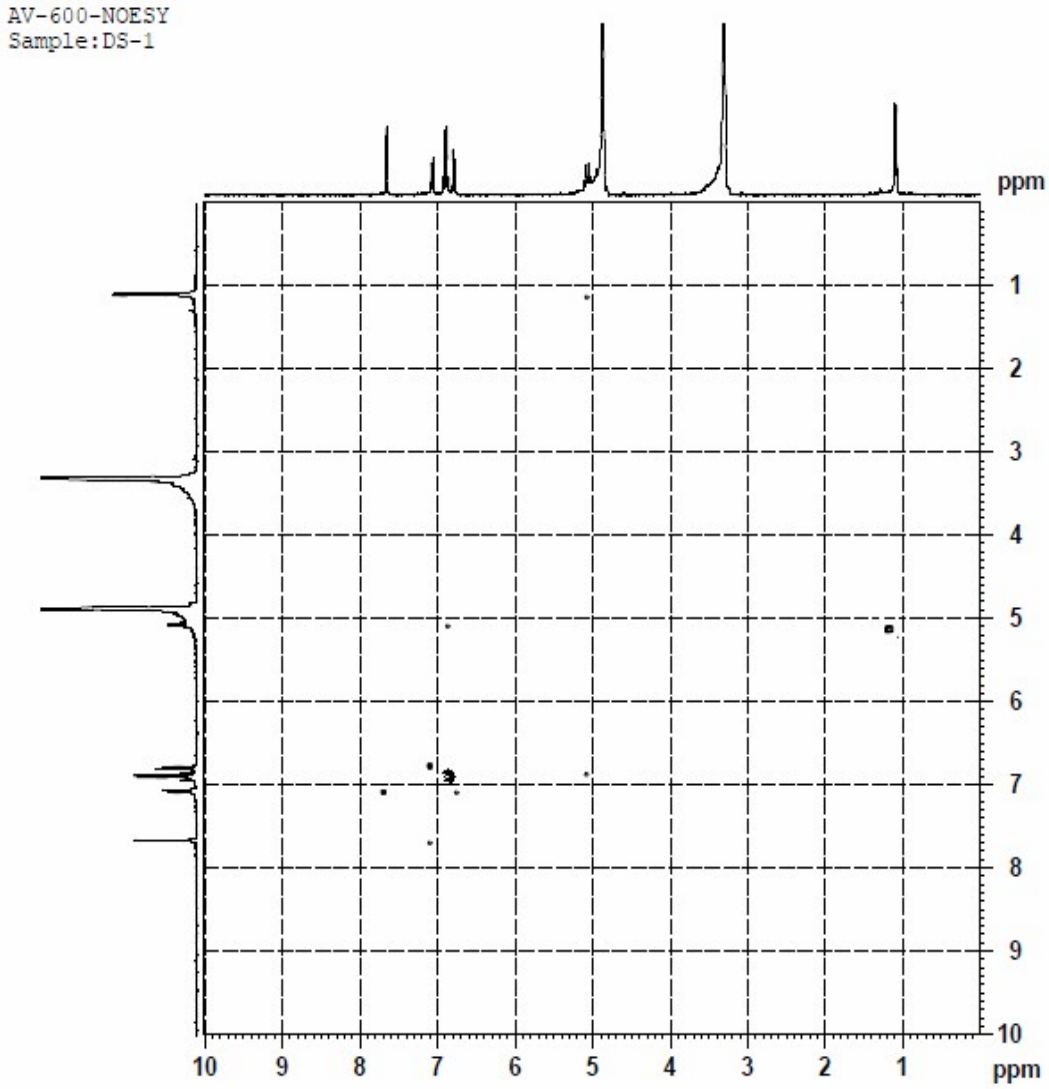
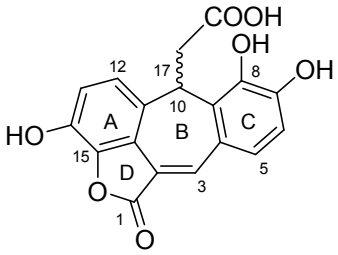




S15 HRESIMS spectrum of 3



Compound Mass Spectrum List Report

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Sample Name	DUI	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

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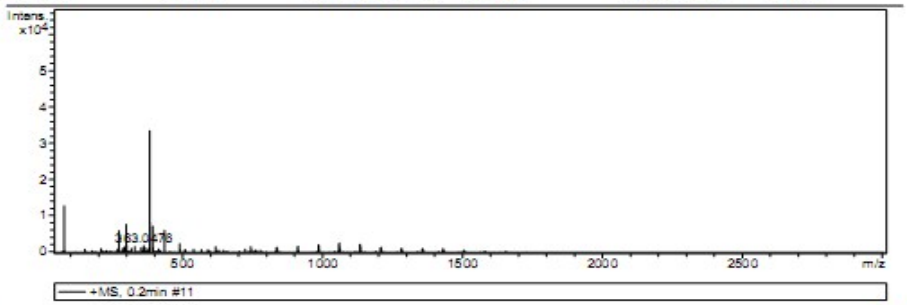
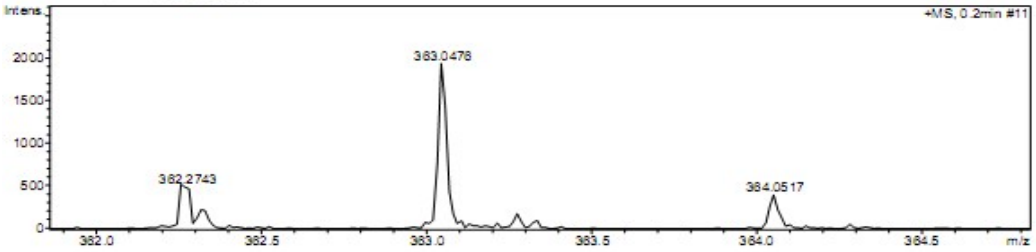
Scan End	3000 m/z	Set Collision Cell RF	90.0 Vpp	Set Divert Valve	Source





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3	384.0517	391

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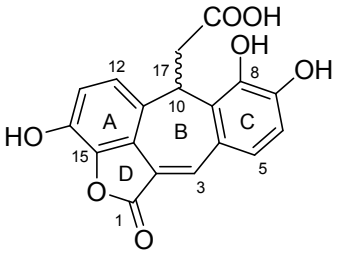
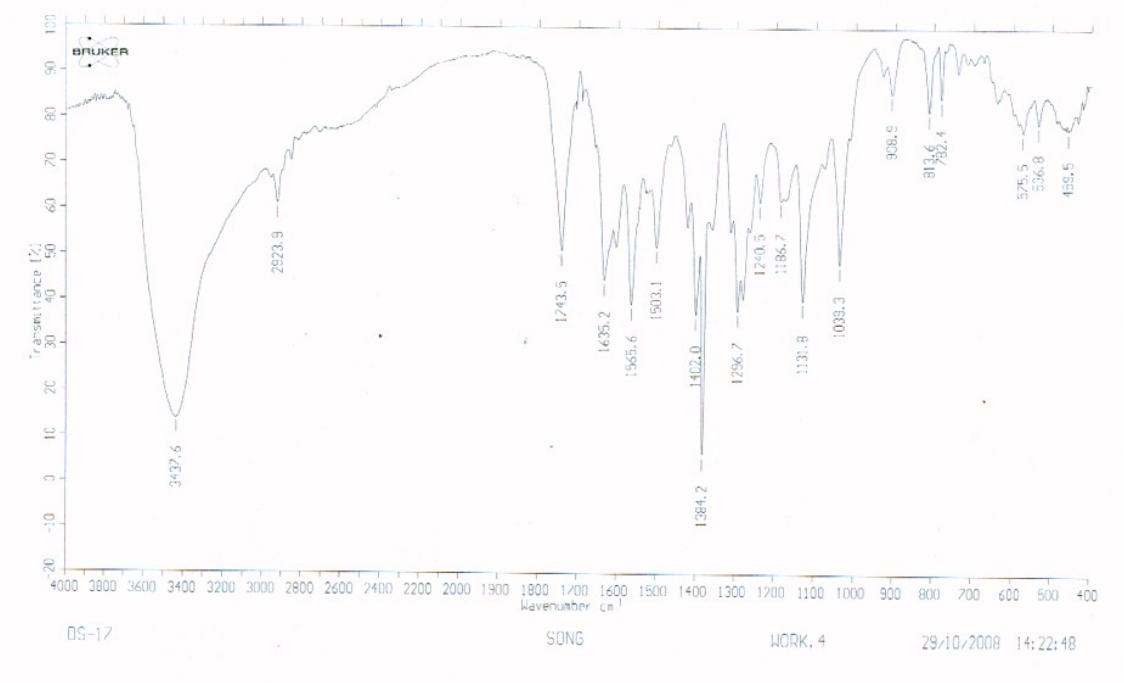
S16 IR spectrum of 3 tested in CD_3OD





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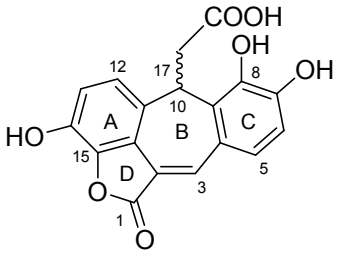

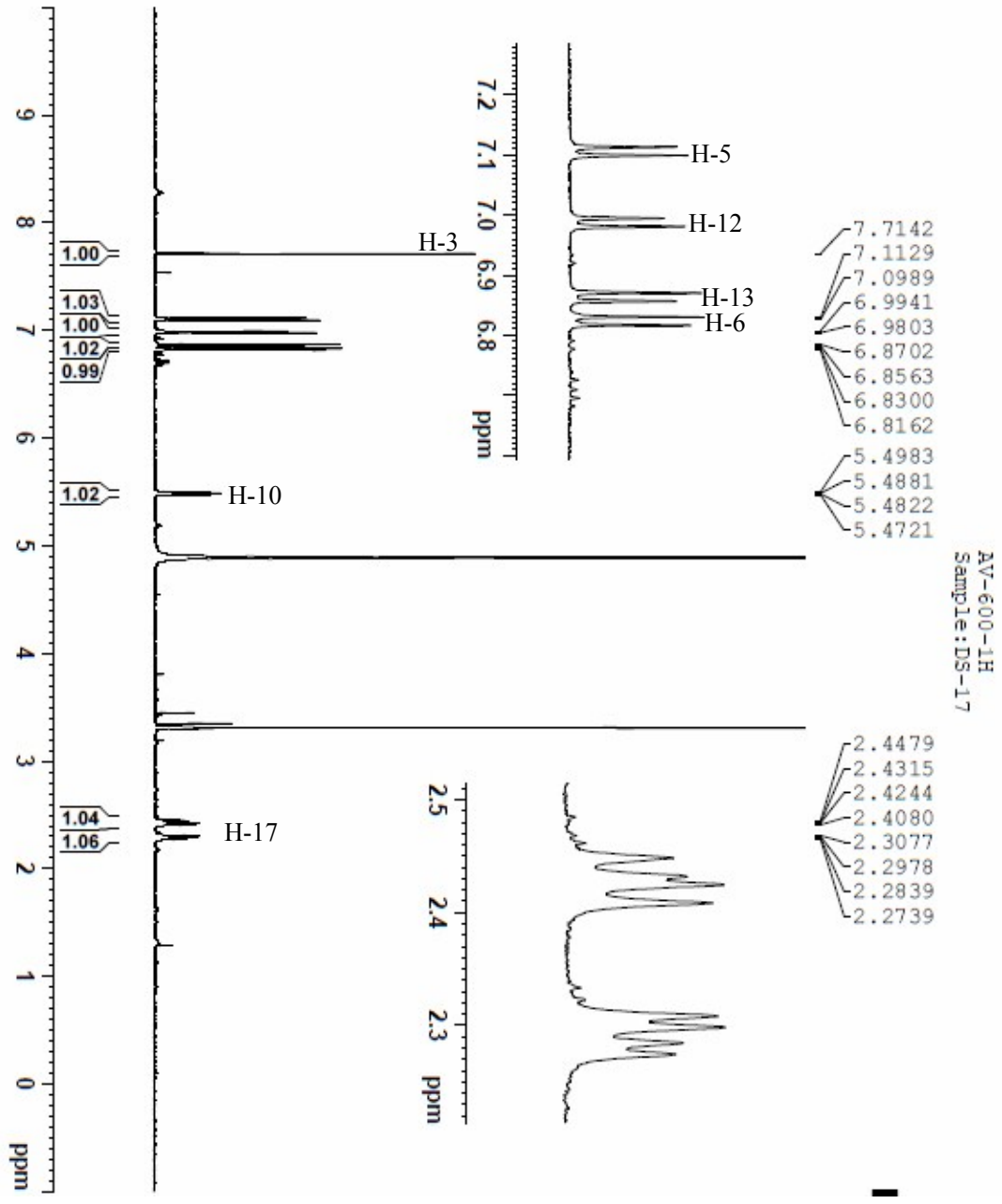

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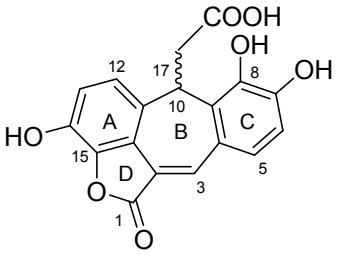

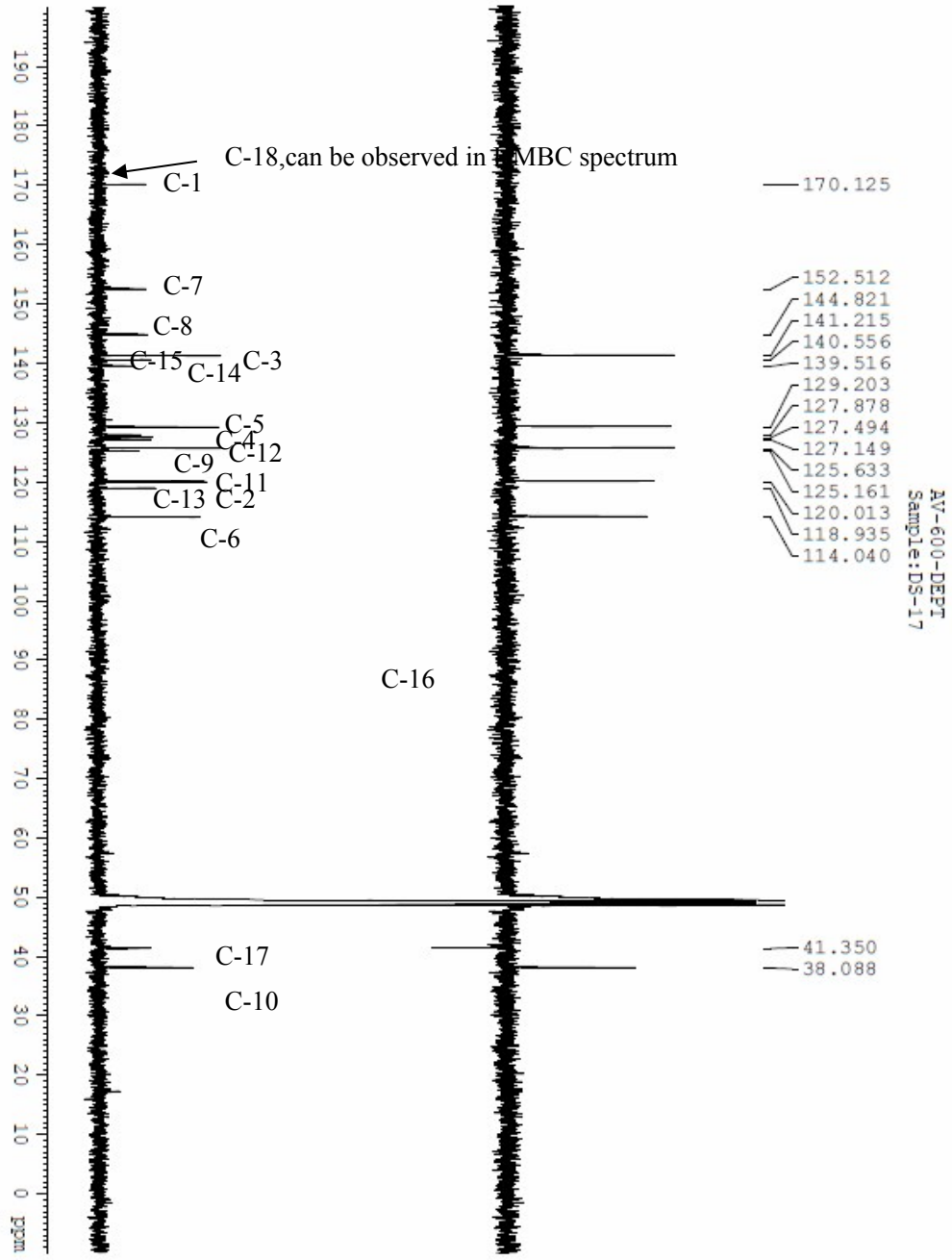

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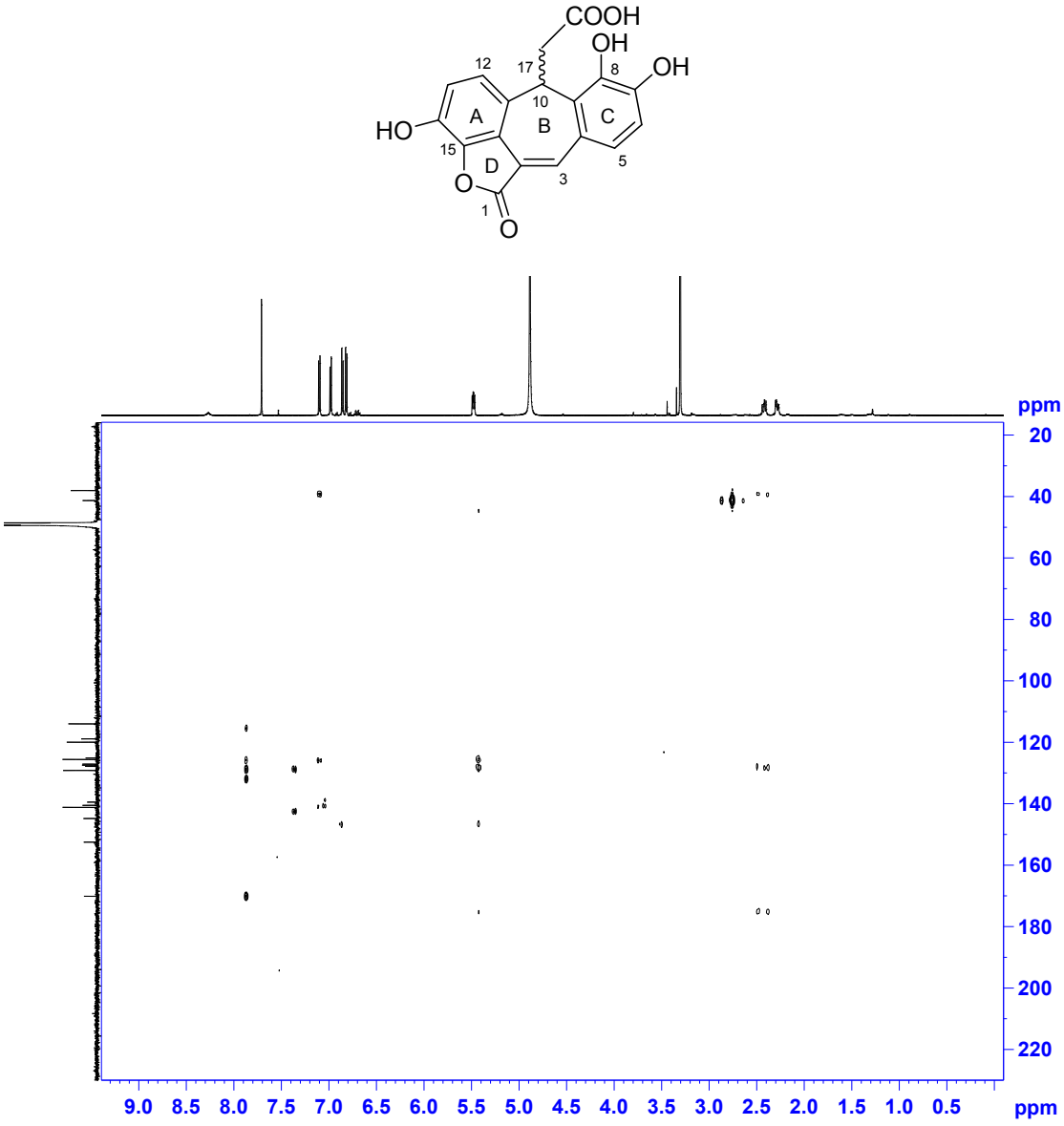

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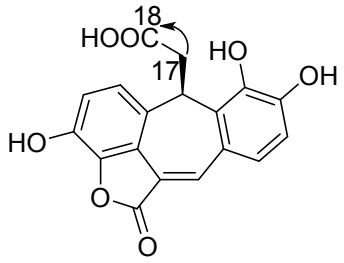

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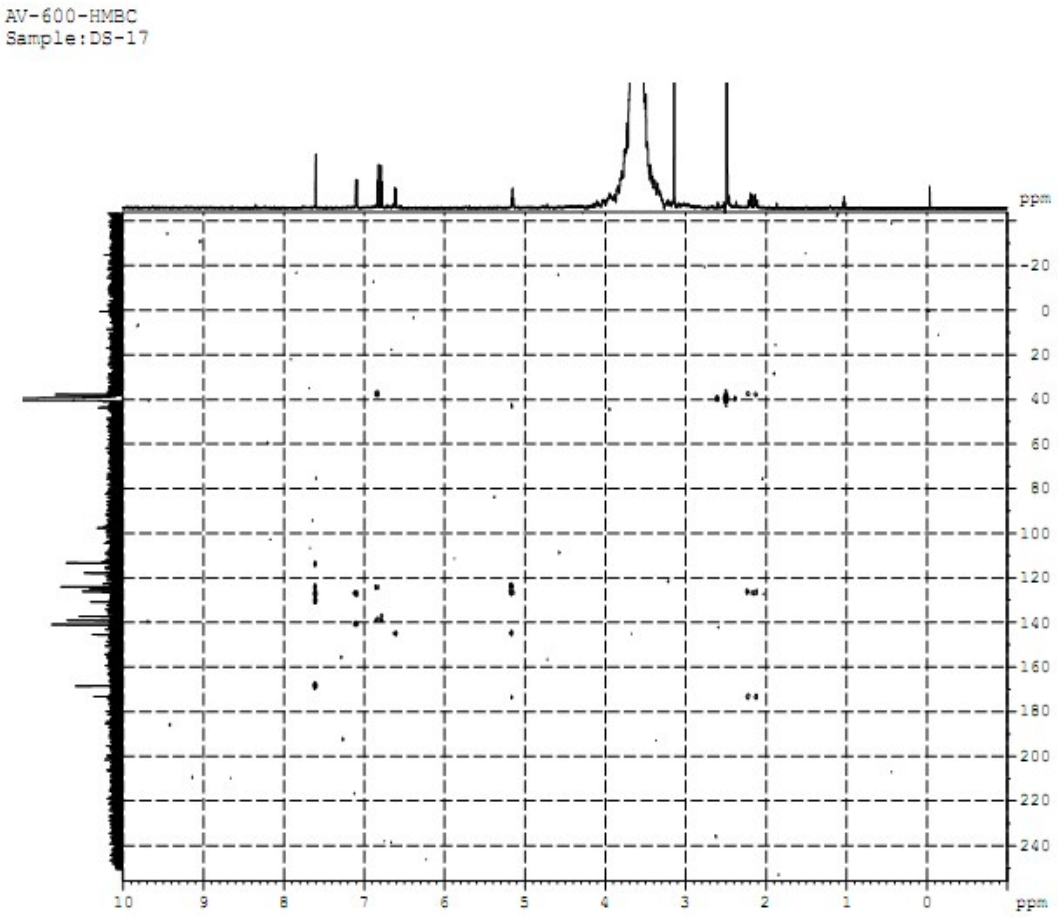

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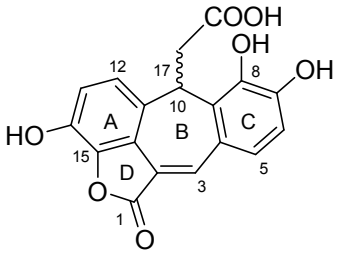
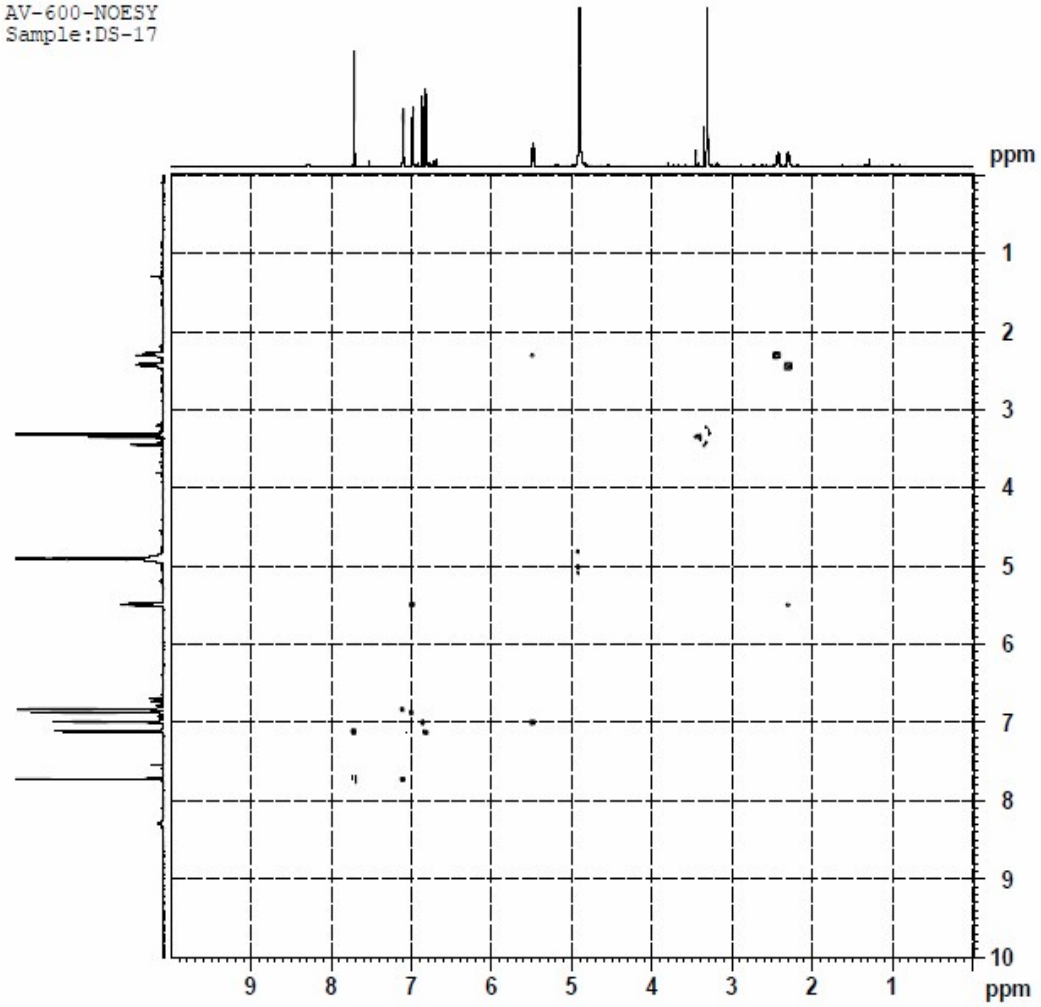
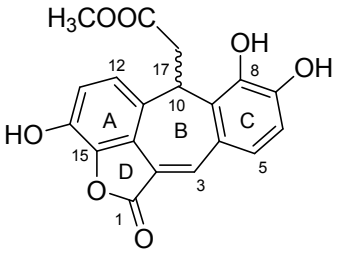
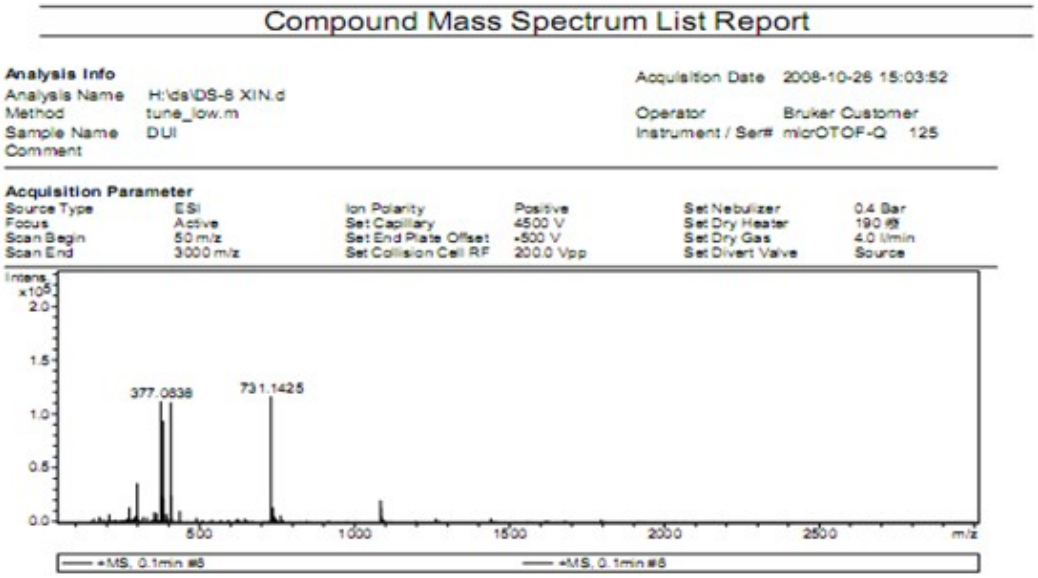


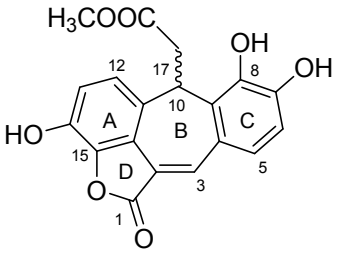


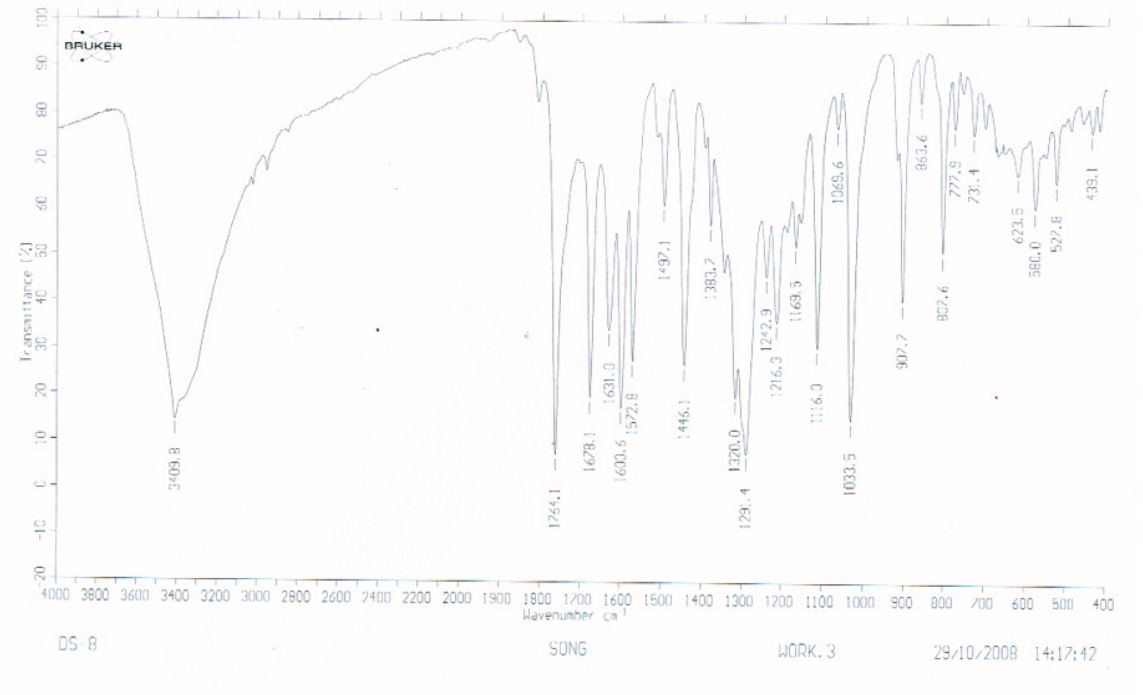
S22 HRESIMS spectrum of 4



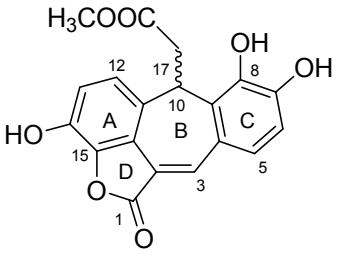


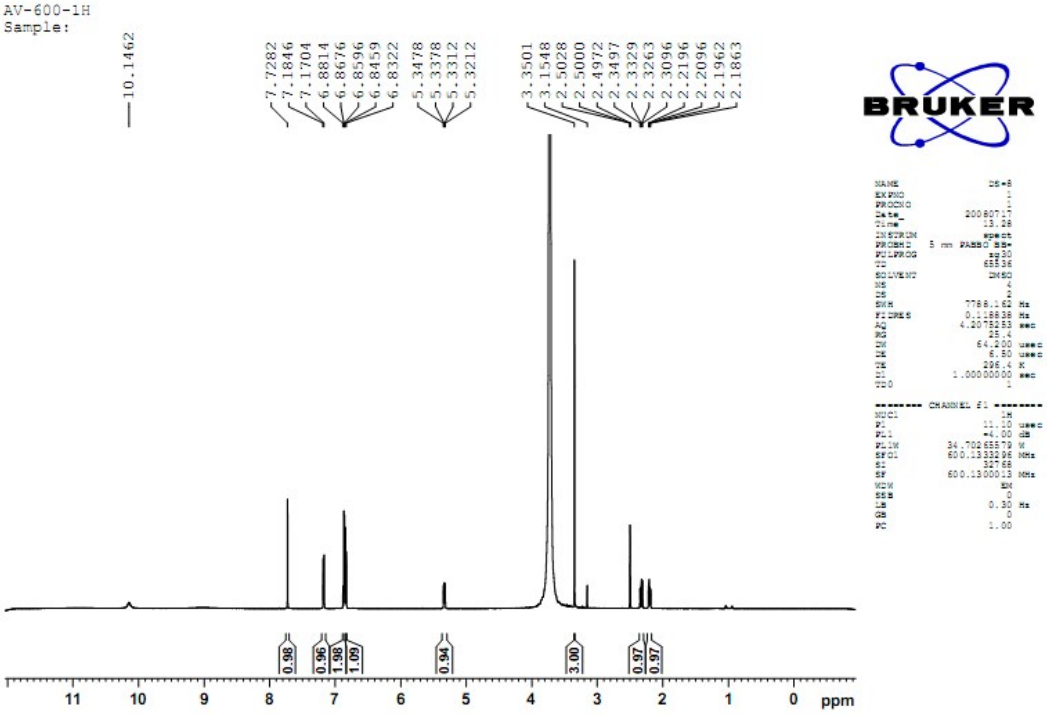
S23 IR spectrum of 4



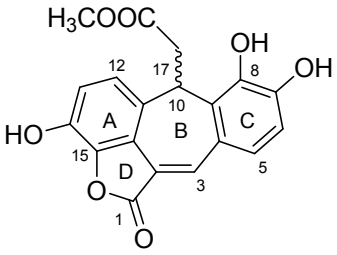


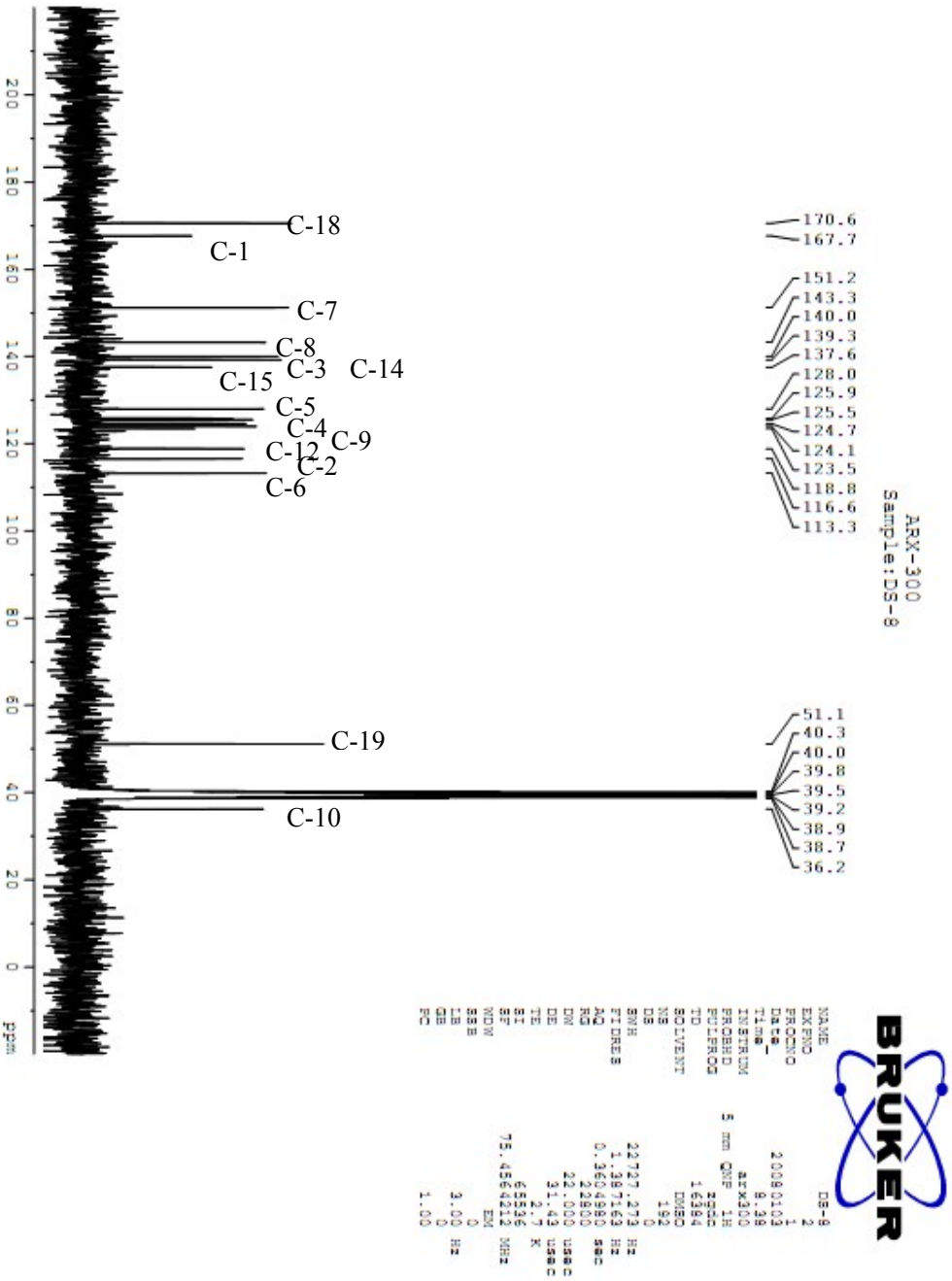
S24 ^{1}H NMR spectrum of 4 tested in DMSO-d6



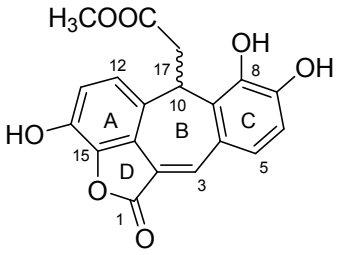


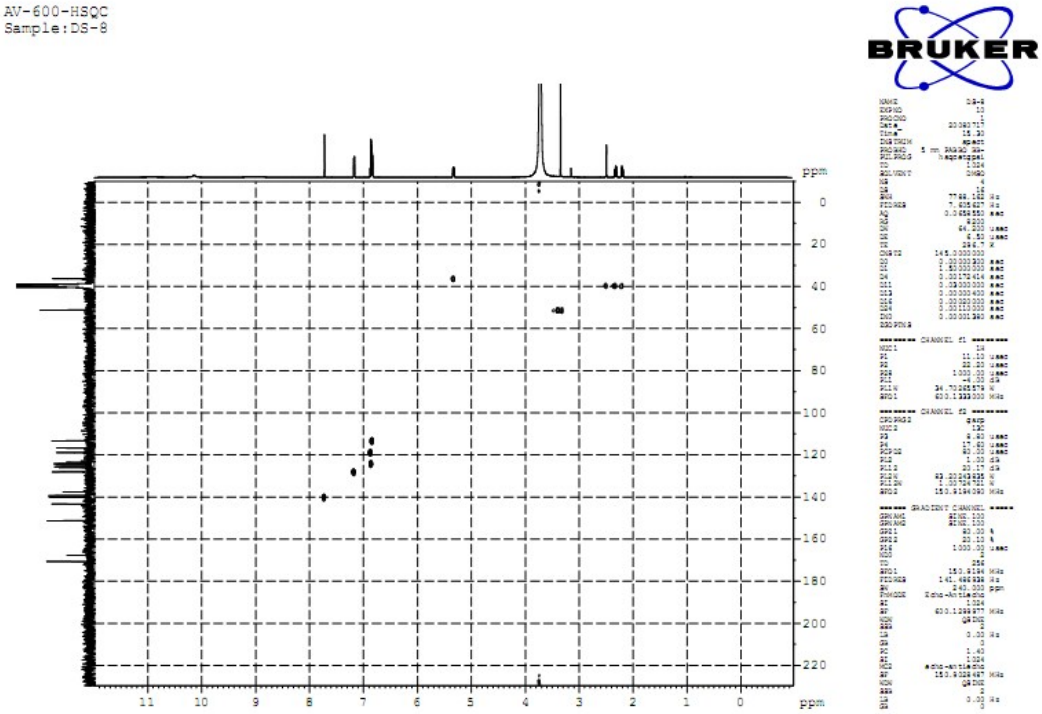
S25 ^{13}C NMR spectrum of 4 tested in DMSO-d6



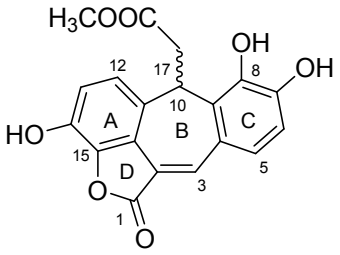


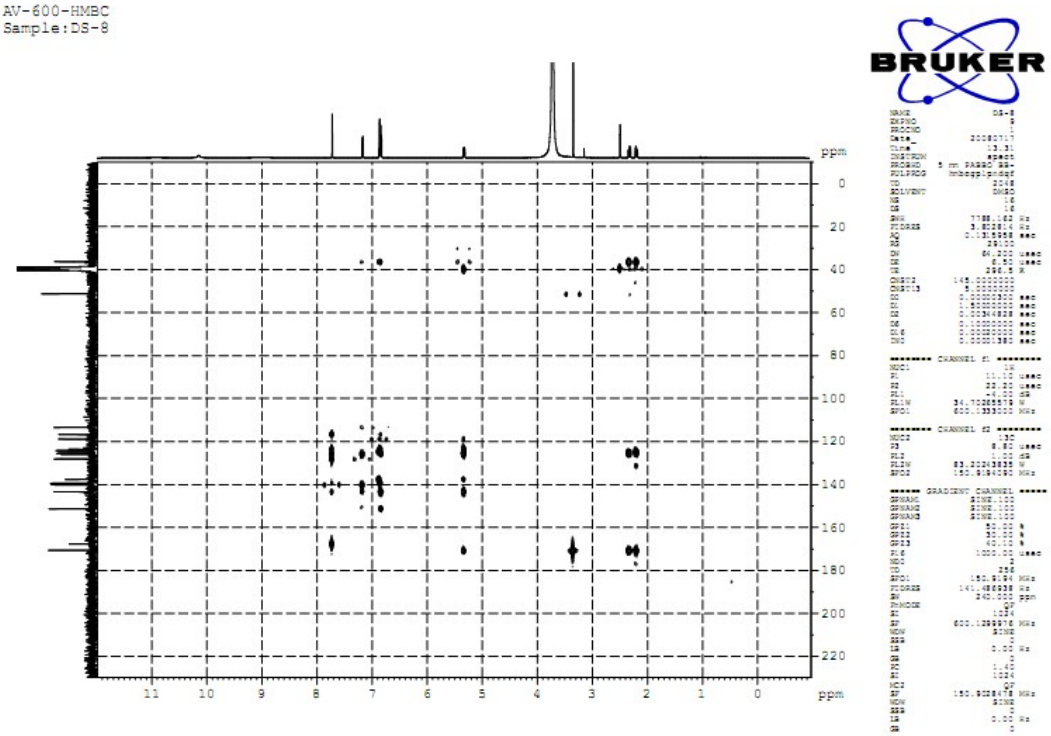
S26 HSQC spectrum of 4 tested in DMSO-d6



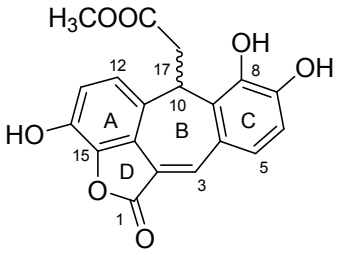


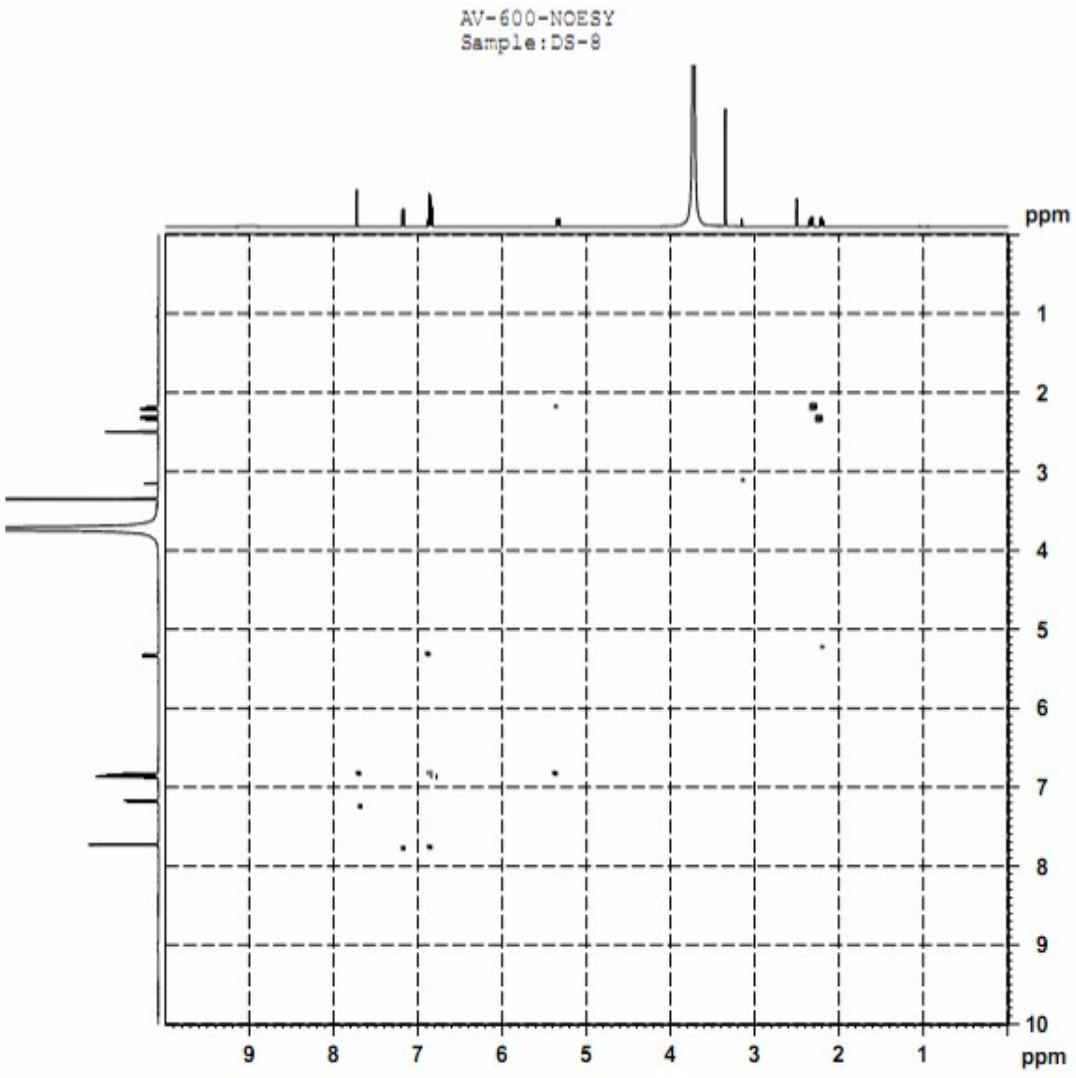
S27 HMBC spectrum of 4 tested in DMSO-d6



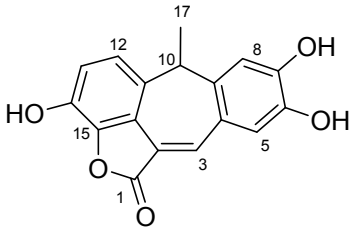


S28 NOESY spectrum of 4 tested in DMSO-d6





S29 HRESIMS spectrum of 5



Mass Spectrum Molecular Formula Report

Analysis Info

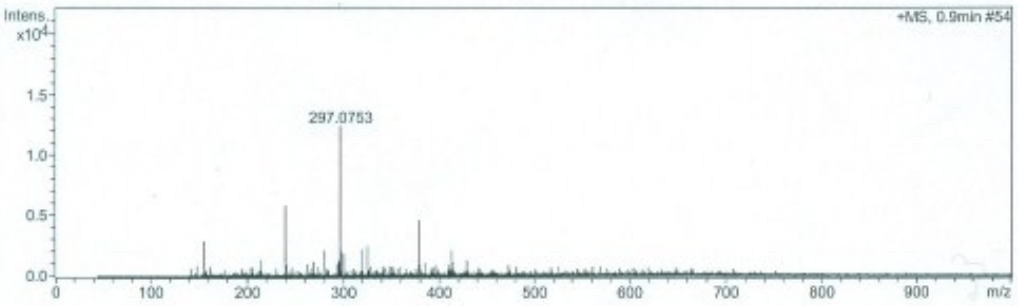
Analysis Name	D:\Data\20110426\dsg-3.d	Acquisition Date	4/26/2011 11:38:49 AM
Method	tune_50-1000_POS_20110328.m	Operator	Bruker Customer
Sample Name	nafa-2	Instrument / Ser#	micrOTOF-Q 125
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
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

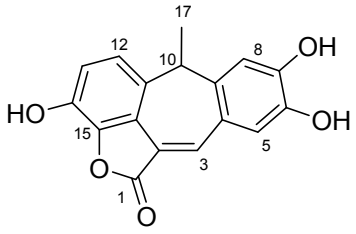
Formula, min.	C17H12O5				
Formula, max.					
Measured m/z	297.075	Tolerance	4 mDa	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nirogen Rule	no	Electron Configuration	both		
Filter H/C Ratio	no	Minimum	0	Maximum	3
Estimate Carbon	yes				

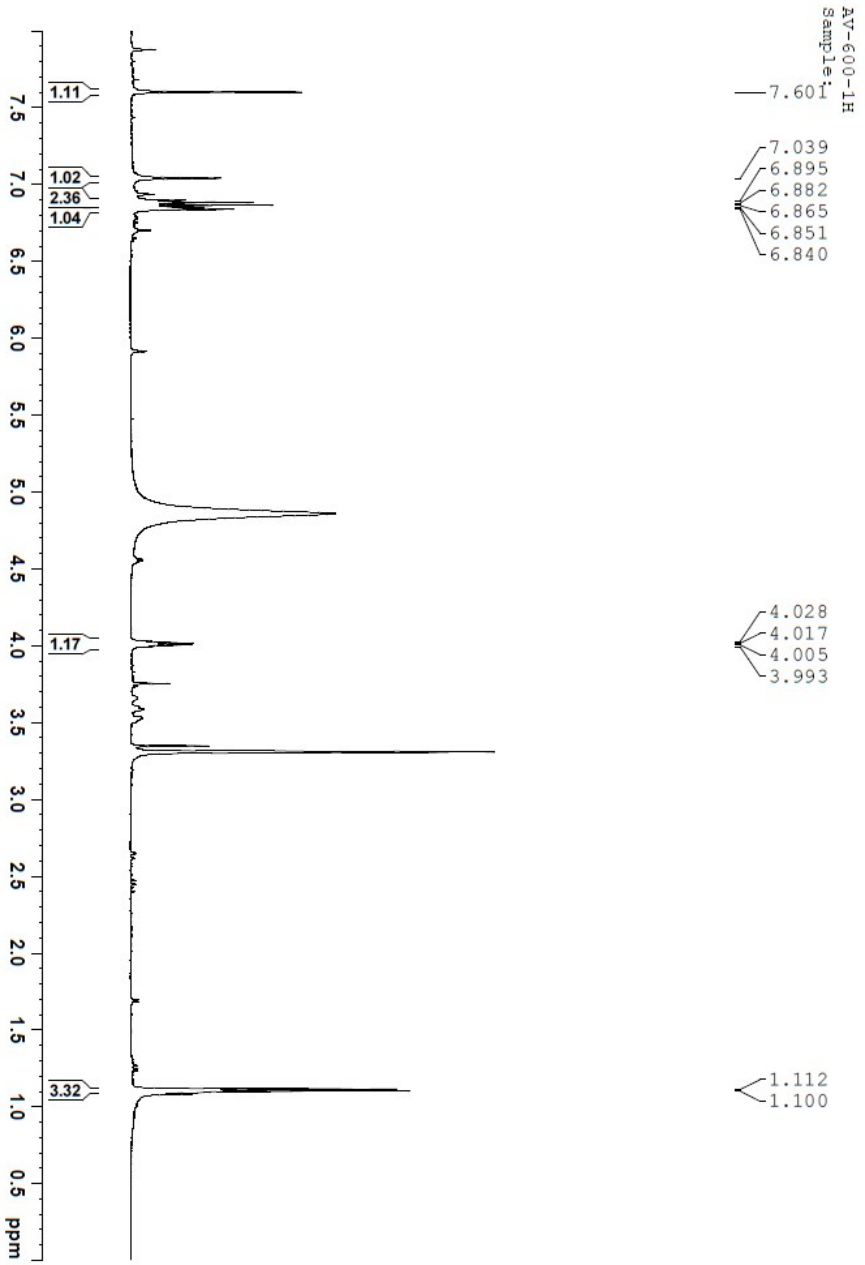


#	m/z	I
1	297.0753	12430

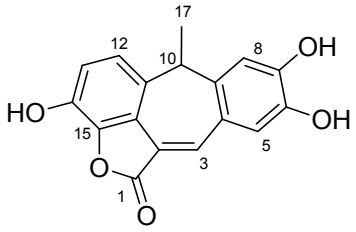
Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e⁻
C 17 H 13 O 5	0.013	297.0757	1.67	1.48	0.50	11.50	ok	even

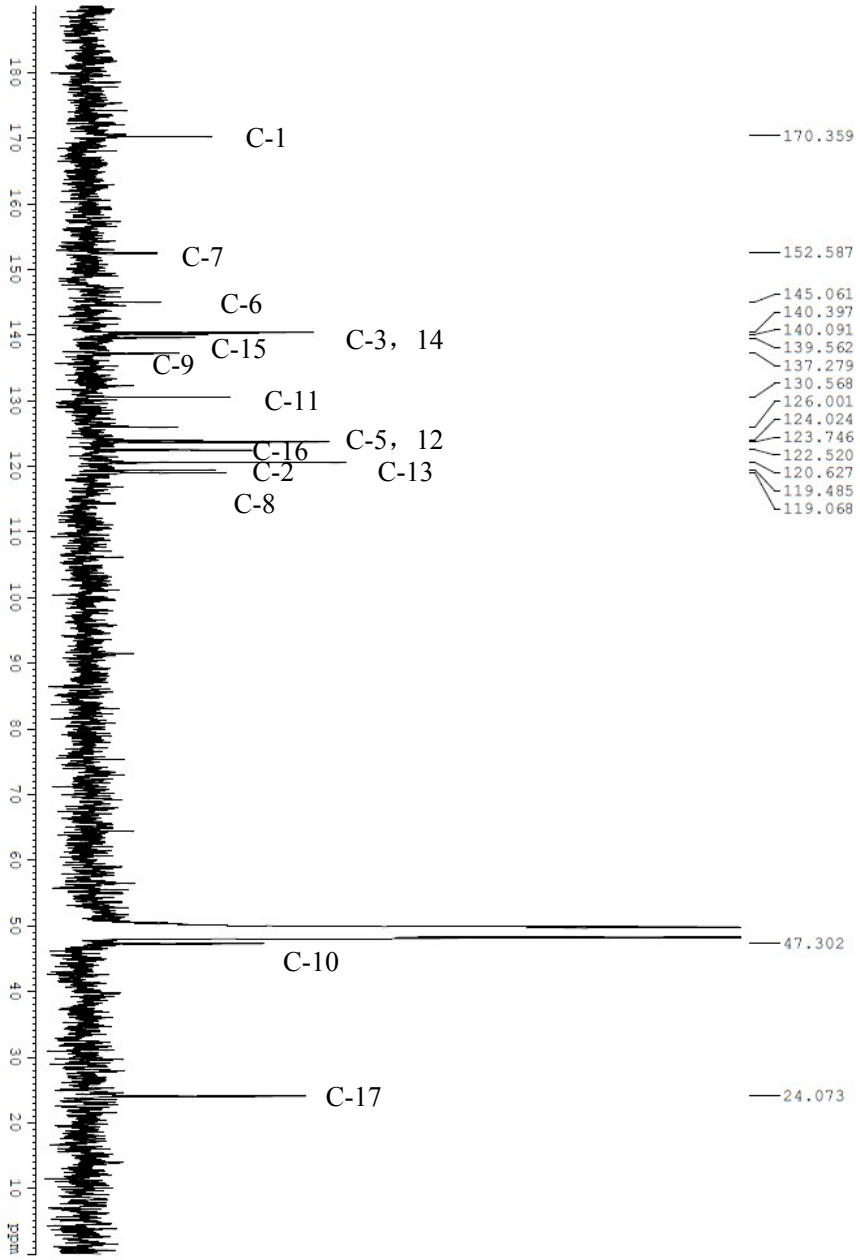
S30 ^{1}H NMR spectrum of 5 tested in MeOD



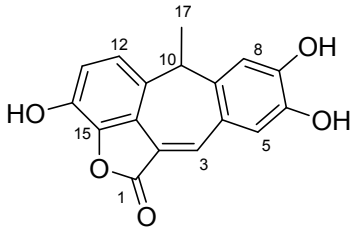


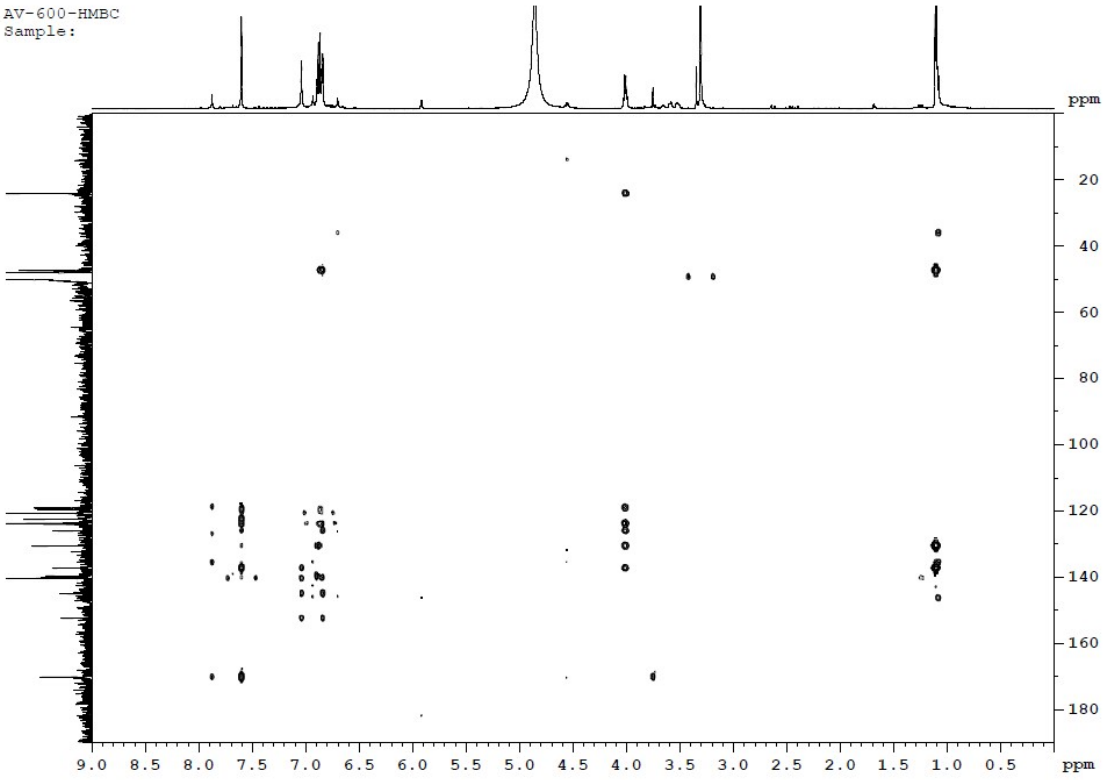
S31 ^{13}C NMR spectrum of 5 in MeOD



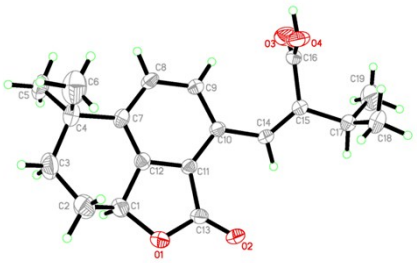


S32 HMBC spectrum of 5 tested in DMSO-D6





S33 Single-crystal X-ray data of 1



1

Table 1. Crystal data and structure refinement for shelxl.

Identification code	shelxl
Empirical formula	C19 H22 O4
Formula weight	314.37
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	triclinic, P-1
Unit cell dimensions	a = 8.424(5) A alpha = 71.63(2) deg.
	b = 9.093(7) A beta = 89.35(2) deg.
	c = 12.323(7) A gamma = 74.44(3) deg.
Volume	860.1(9) A^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>2sigma(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.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 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)

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

Table 3. Bond lengths [A] and angles [deg] for shelxl.

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 (Å^2 x 10^3) for shelxl. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	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 (x 10^4) and isotropic displacement parameters (A^2 x 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.

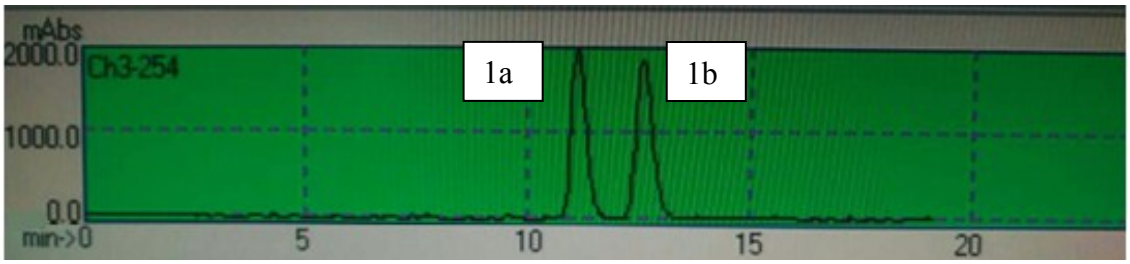


Figure S34.The chiral HPLC chromatogram of 1.

S35.The chiral HPLC chromatogram of 2.

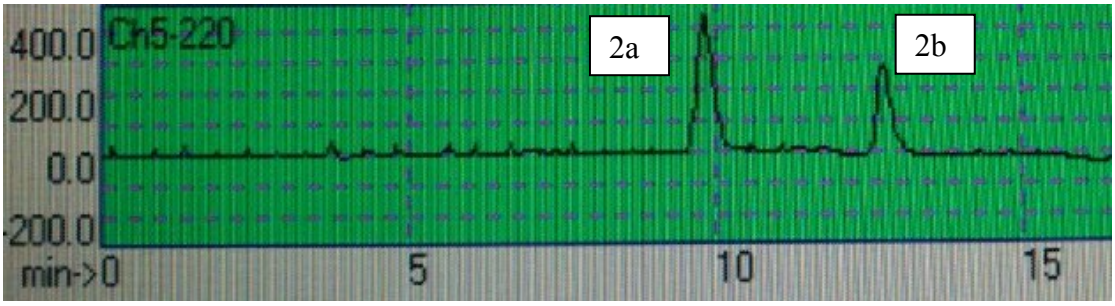


Figure S35.The chiral HPLC chromatogram of 2.

S36.The chiral HPLC chromatogram of 3.

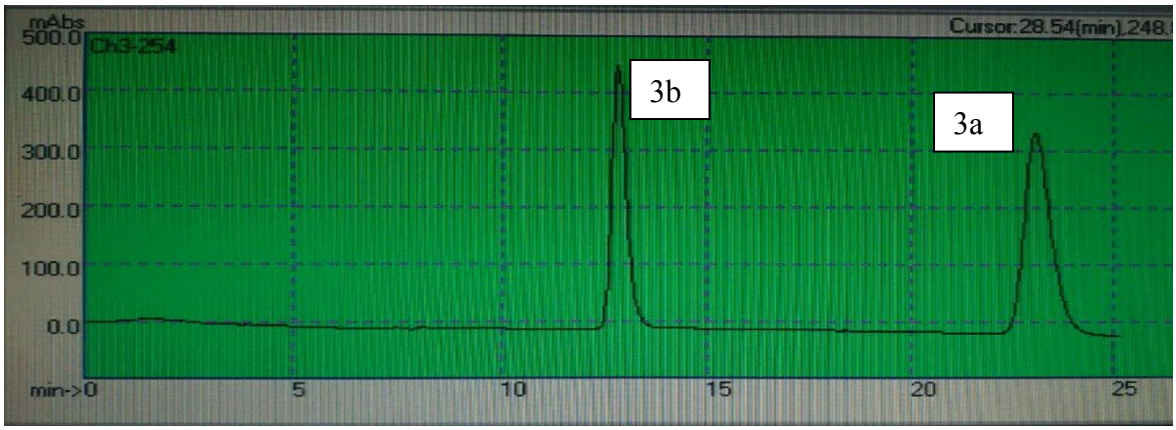


Figure S36.The chiral HPLC chromatogram of 3.

S37.The chiral HPLC chromatogram of 4.

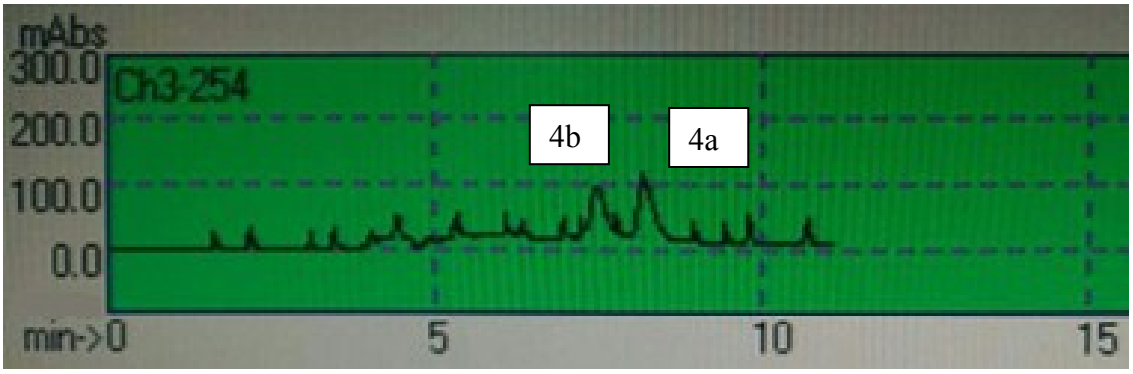
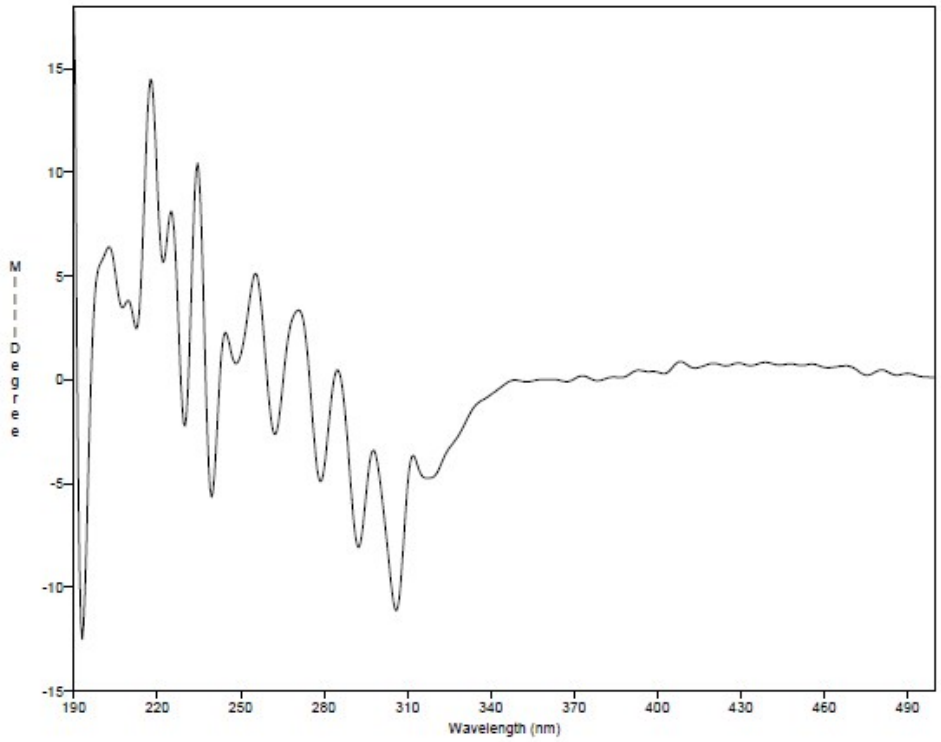
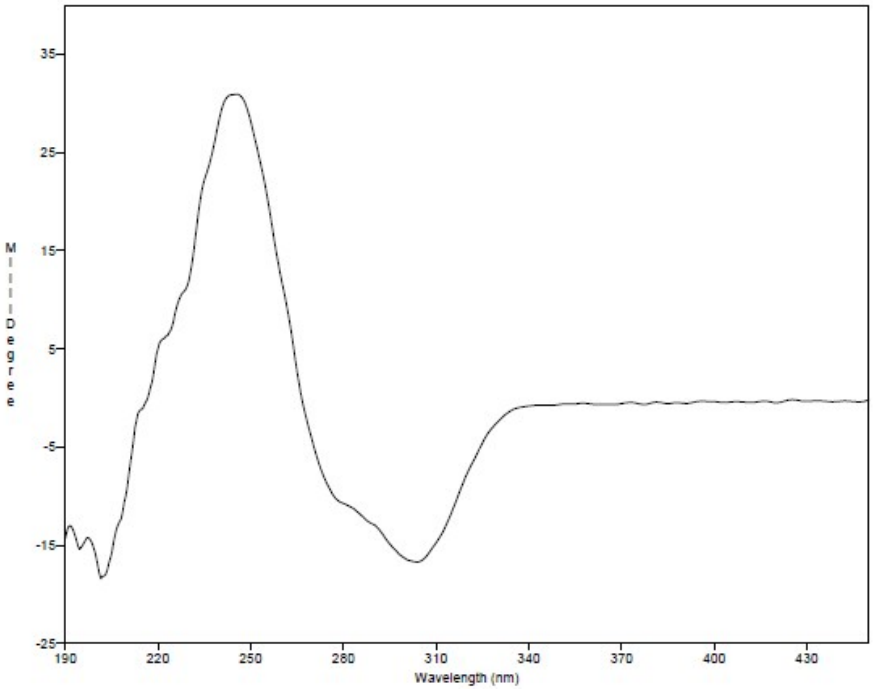


Figure S37.The chiral HPLC chromatogram of 4.

S38 The CD spectra of 1 in MeOH.

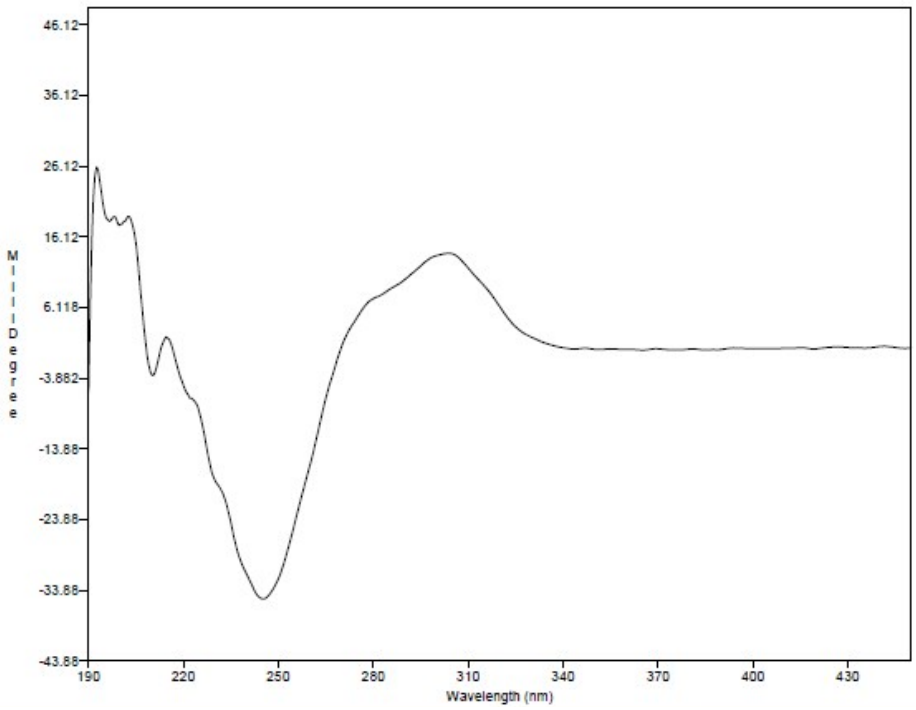


S39 The CD spectra of 1a in MeOH.



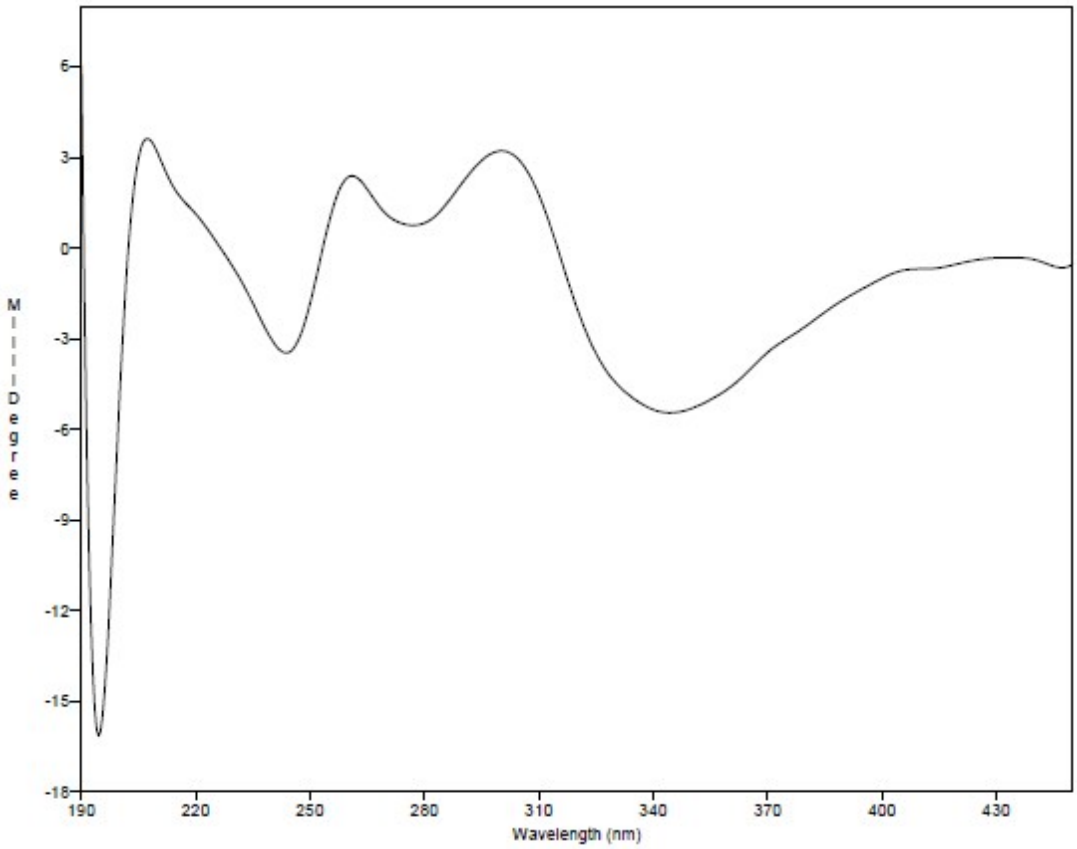
CD spectrum of 1a

S40 The CD spectra of 1b in MeOH.



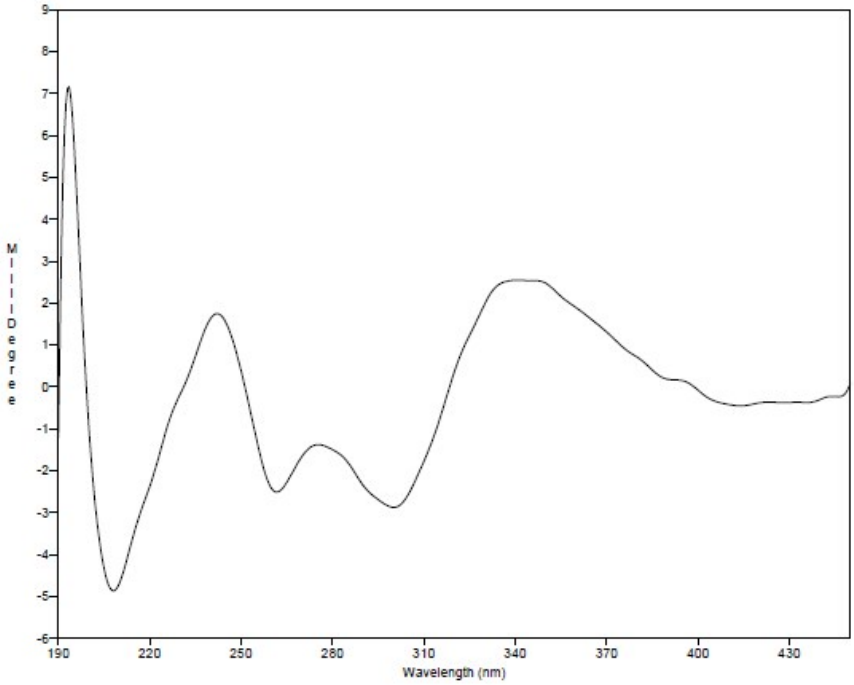
CD spectrum of 1

S41 The CD spectra of 2a in MeOH.



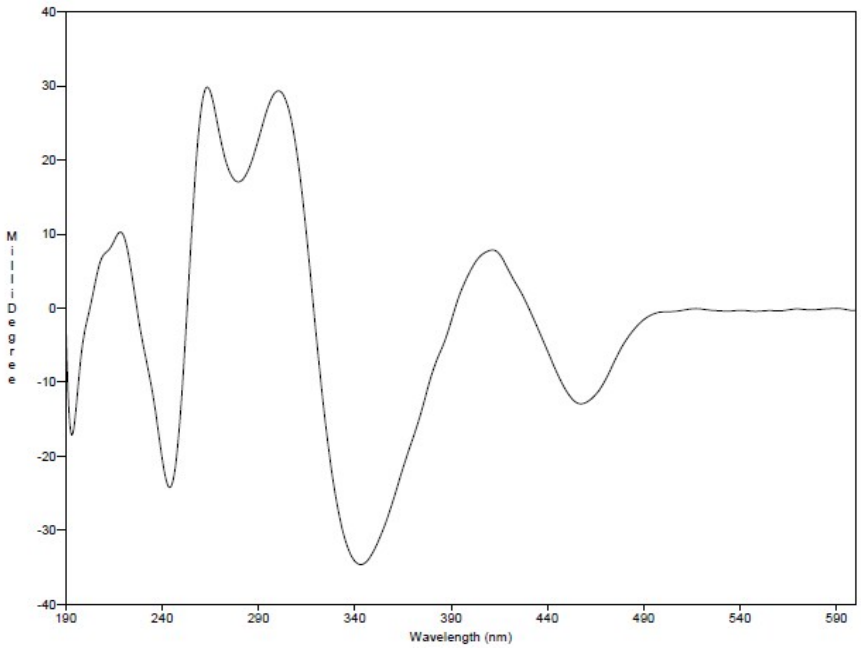
CD spectrum of **2a**

S42 The CD spectra of 2b in MeOH.



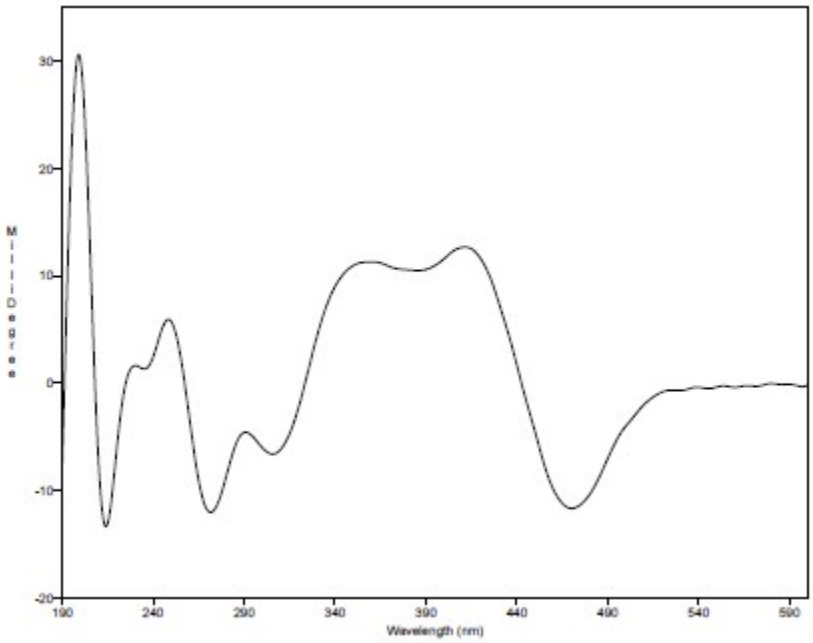
CD spectrum of **2b**

S43 The CD spectra of 3a in MeOH.



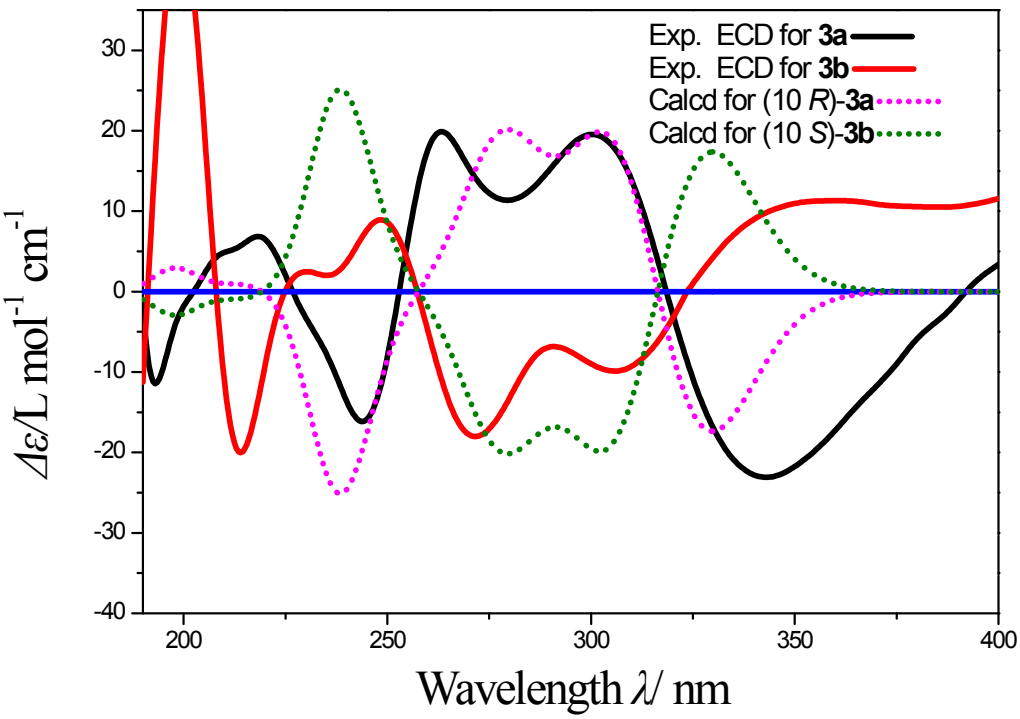
CD spectrum of **3a**

S44 The CD spectra of 3b in MeOH.

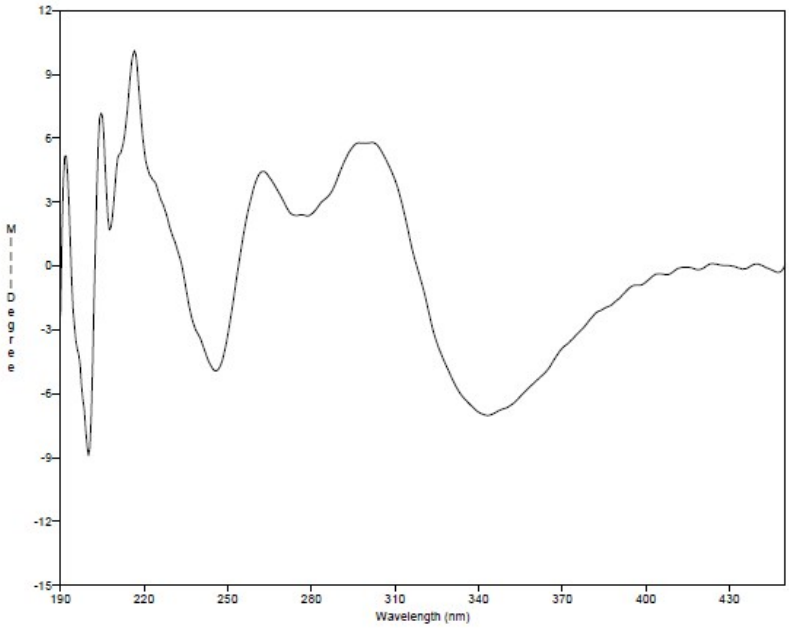


CD spectrum of **3b**

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

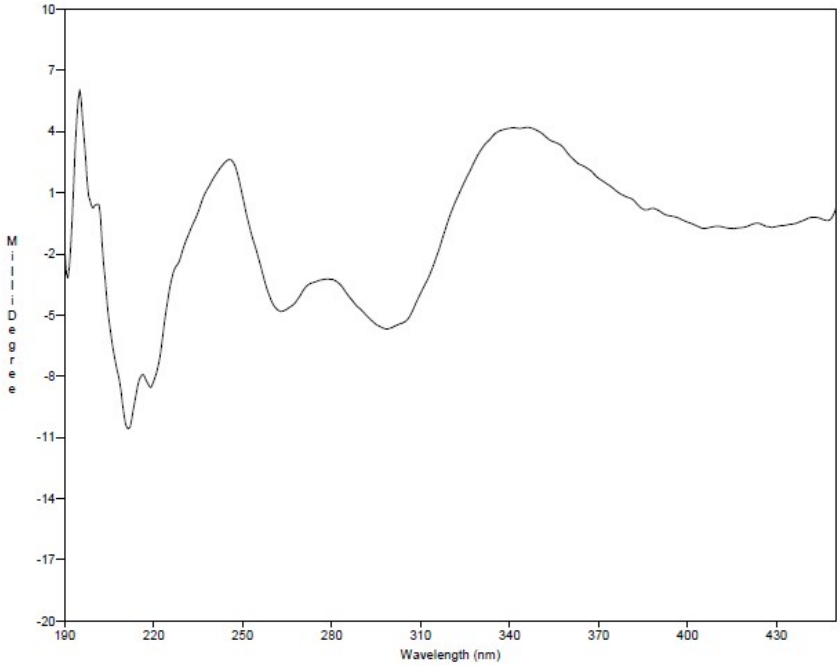


S46 The CD spectra of 4a in MeOH.



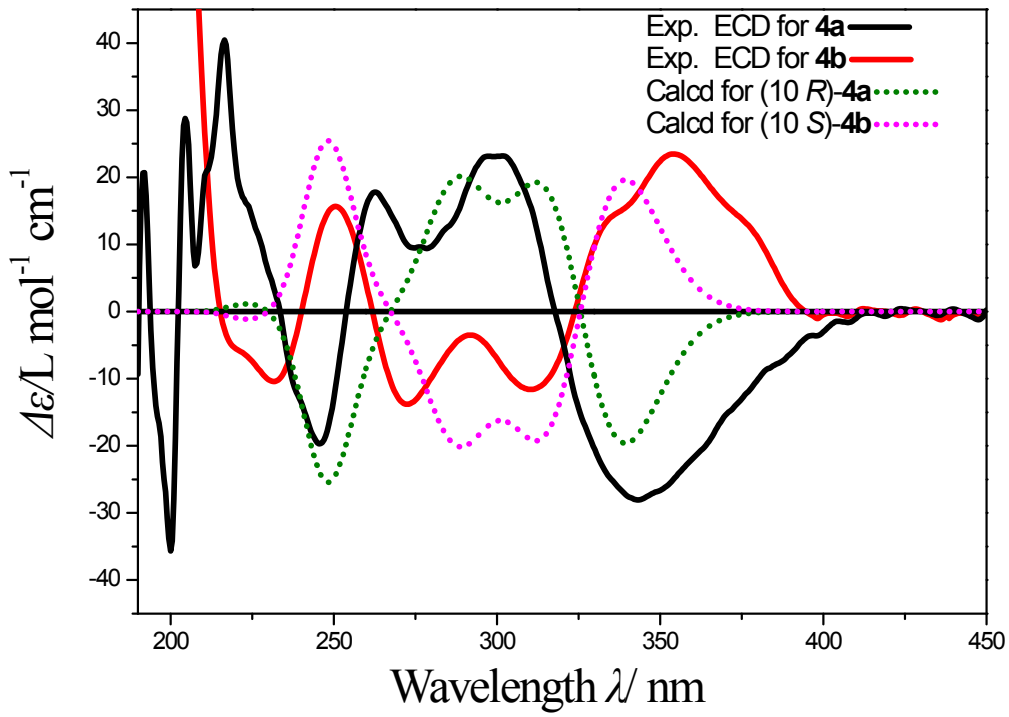
CD spectrum of **4a**

S47 The CD spectra of 4b in MeOH



CD spectrum of **4b**

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



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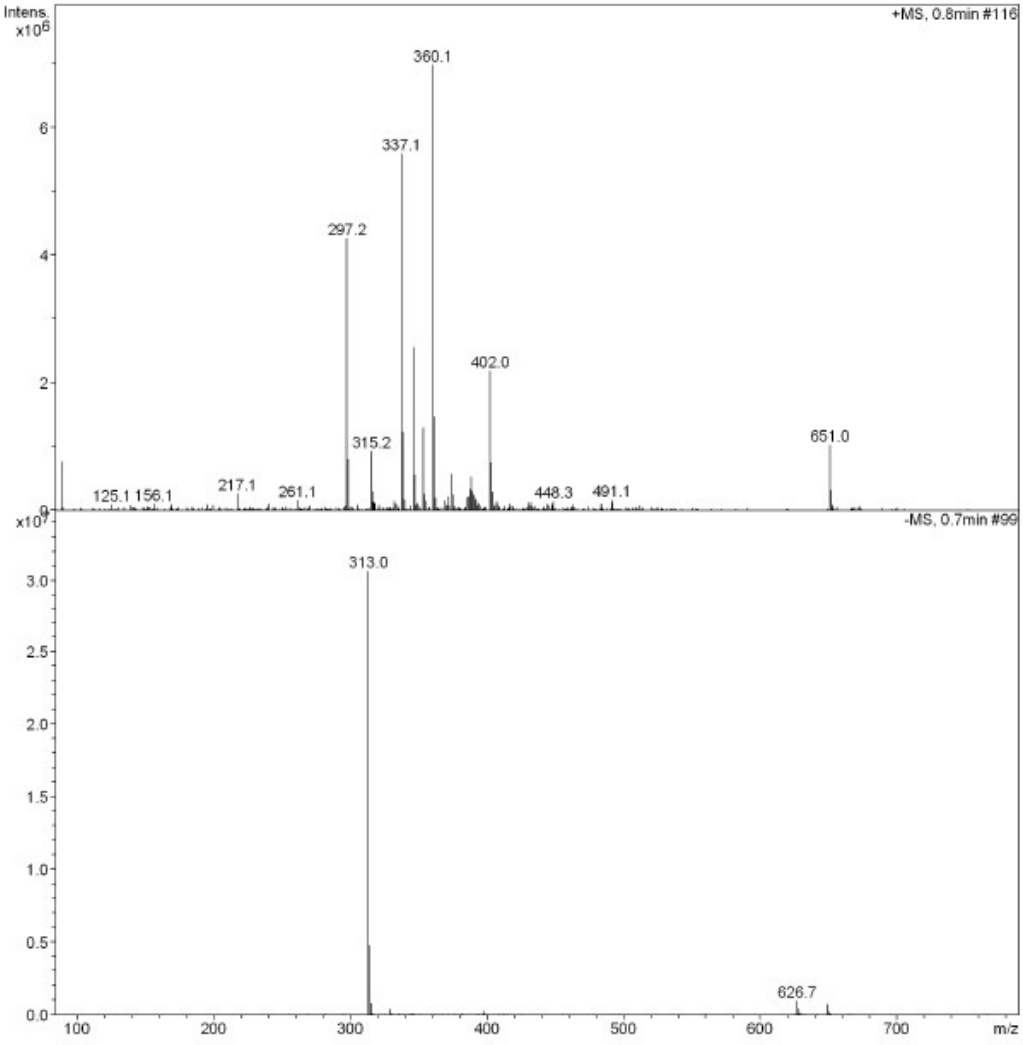
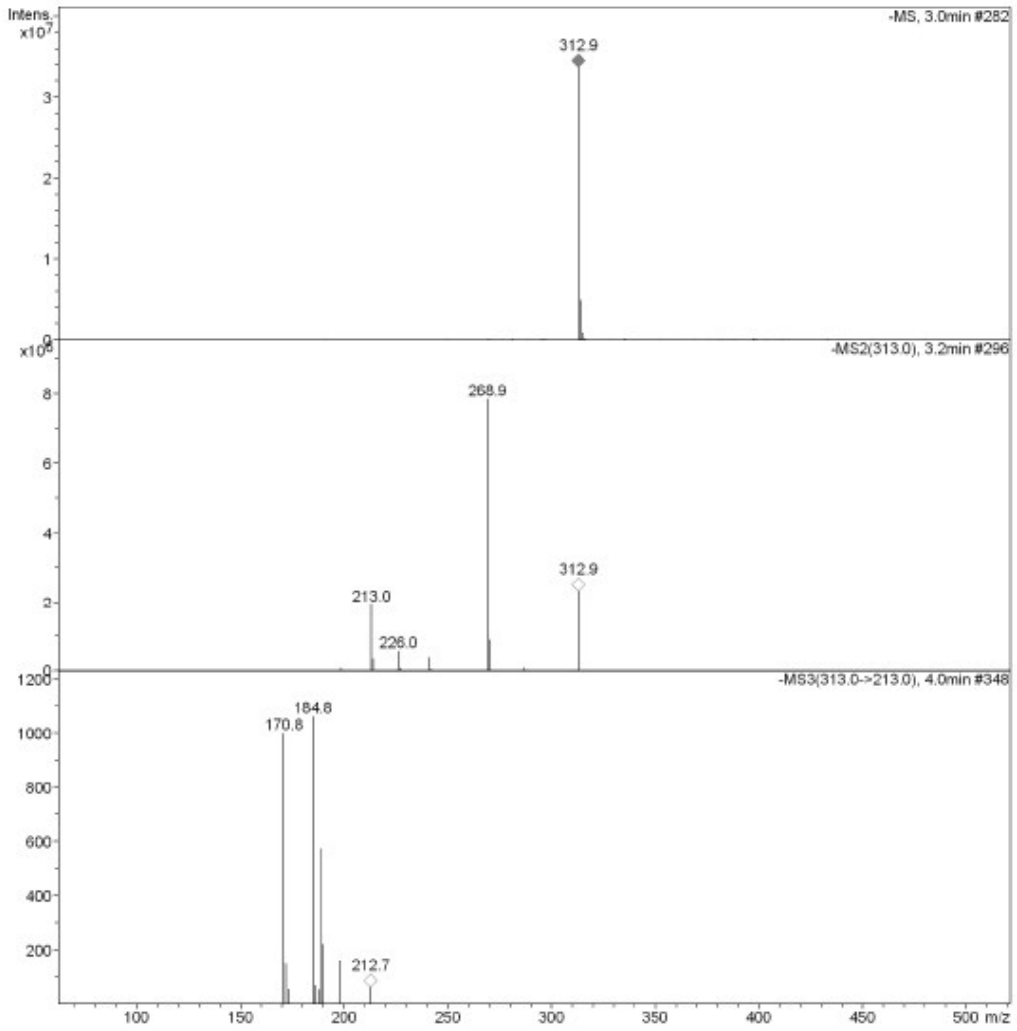
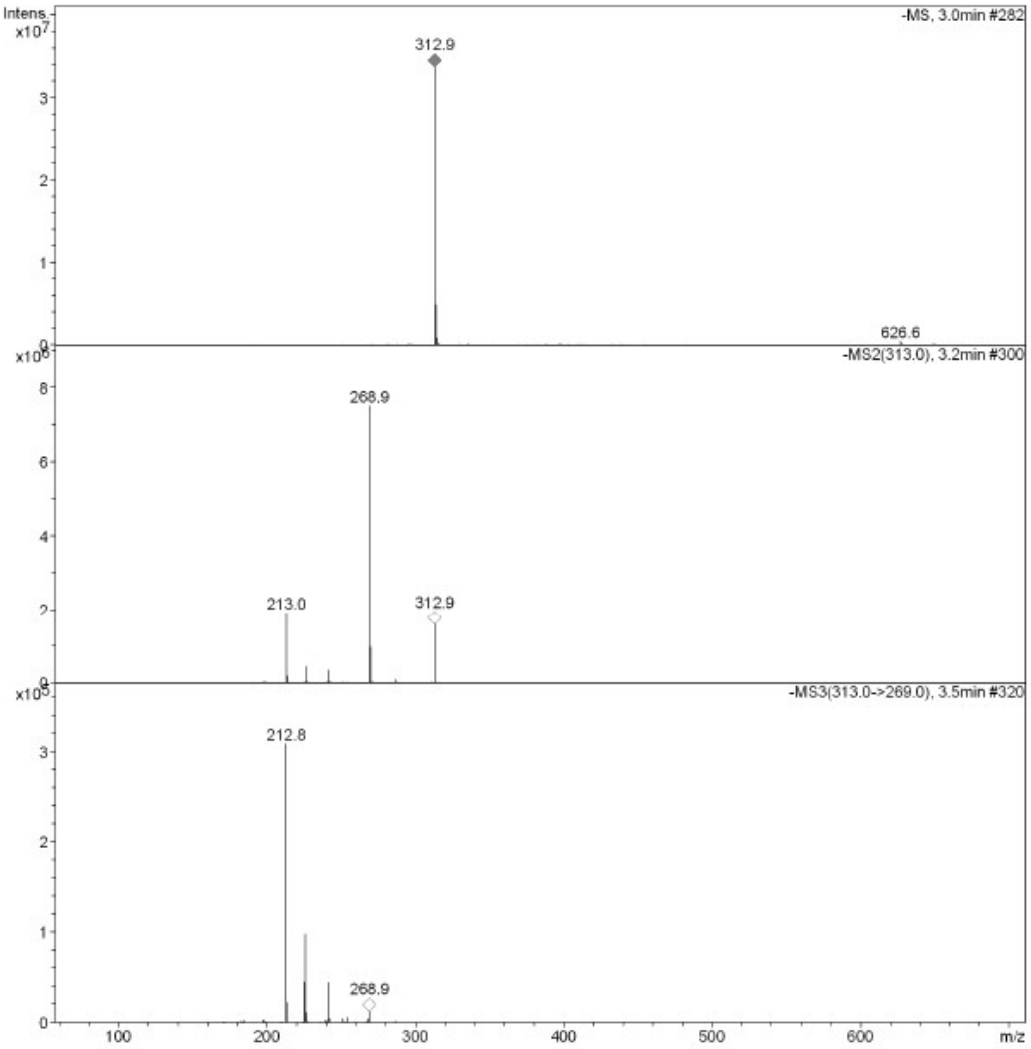
S49 ES-MS spectrum of 1.
Ms



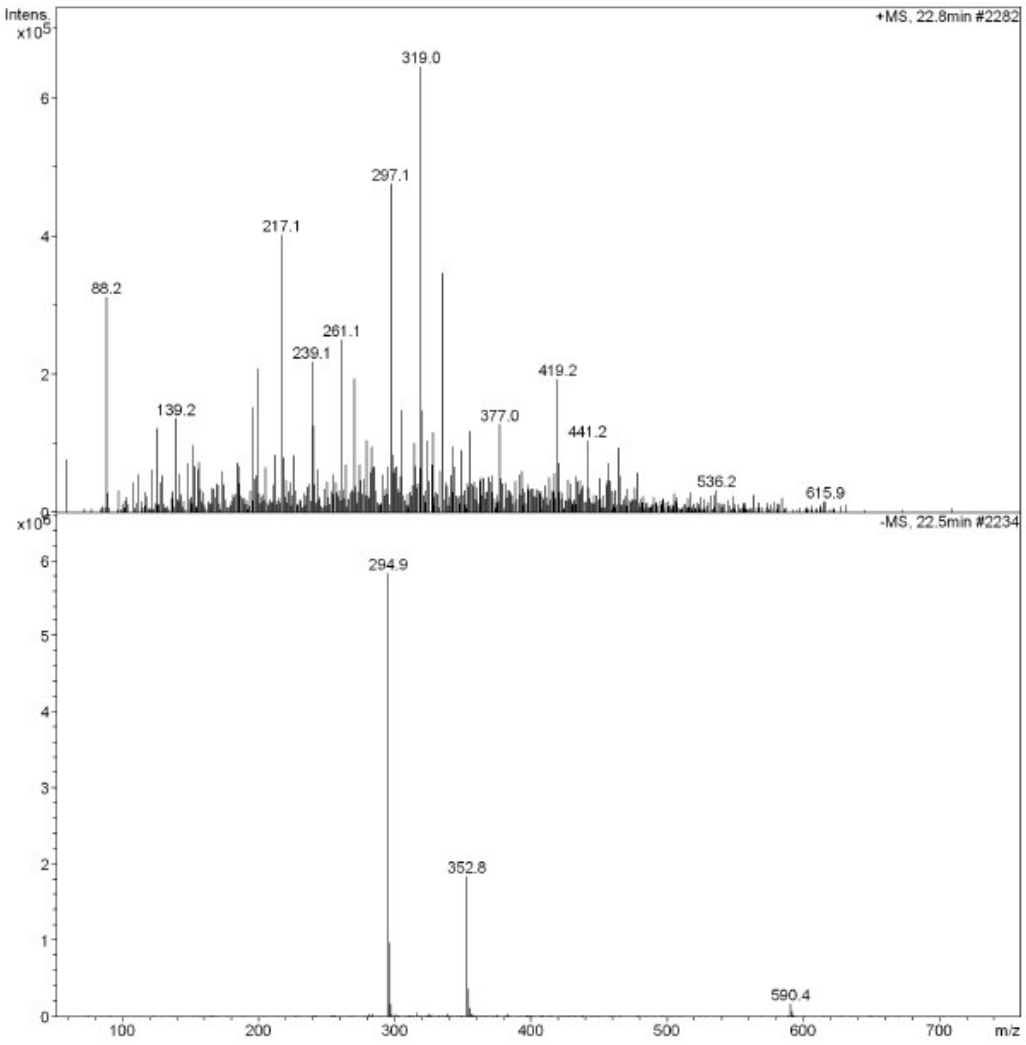
Ms²


Intens.
x10⁷
-MS, 3.0min #282
312.9
x10⁶
-MS2(313.0), 3.2min #296
268.9
312.9
213.0
226.0
-MS3(313.0->213.0), 4.0min #348
184.8
170.8
212.7
100
150
200
250
300
350
400
450
500 m/z

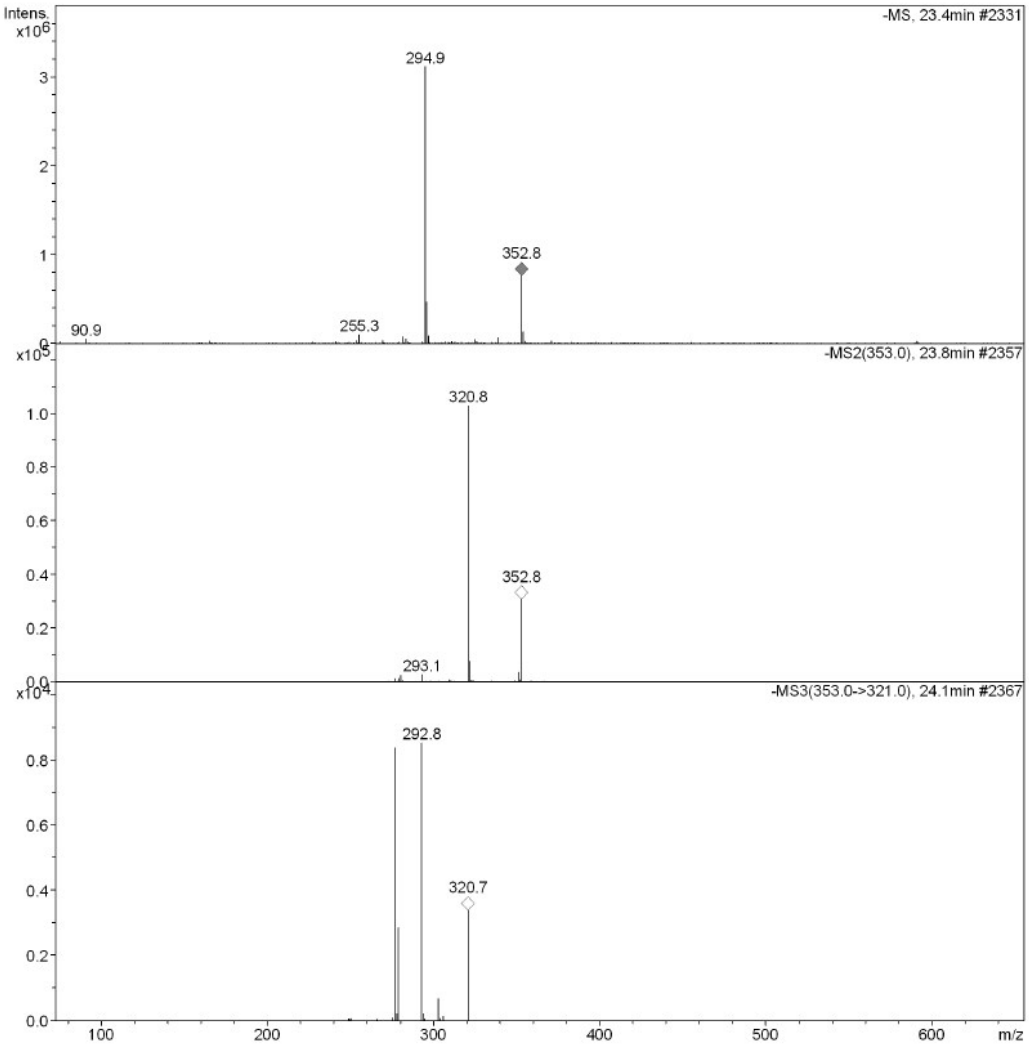
Ms^3


Intens.
x10^7
-MS, 3.0min #282
312.9
626.6
x10^6
-MS2(313.0), 3.2min #300
268.9
213.0
312.9
x10^5
-MS3(313.0->269.0), 3.5min #320
212.8
268.9
100
200
300
400
500
600
m/z

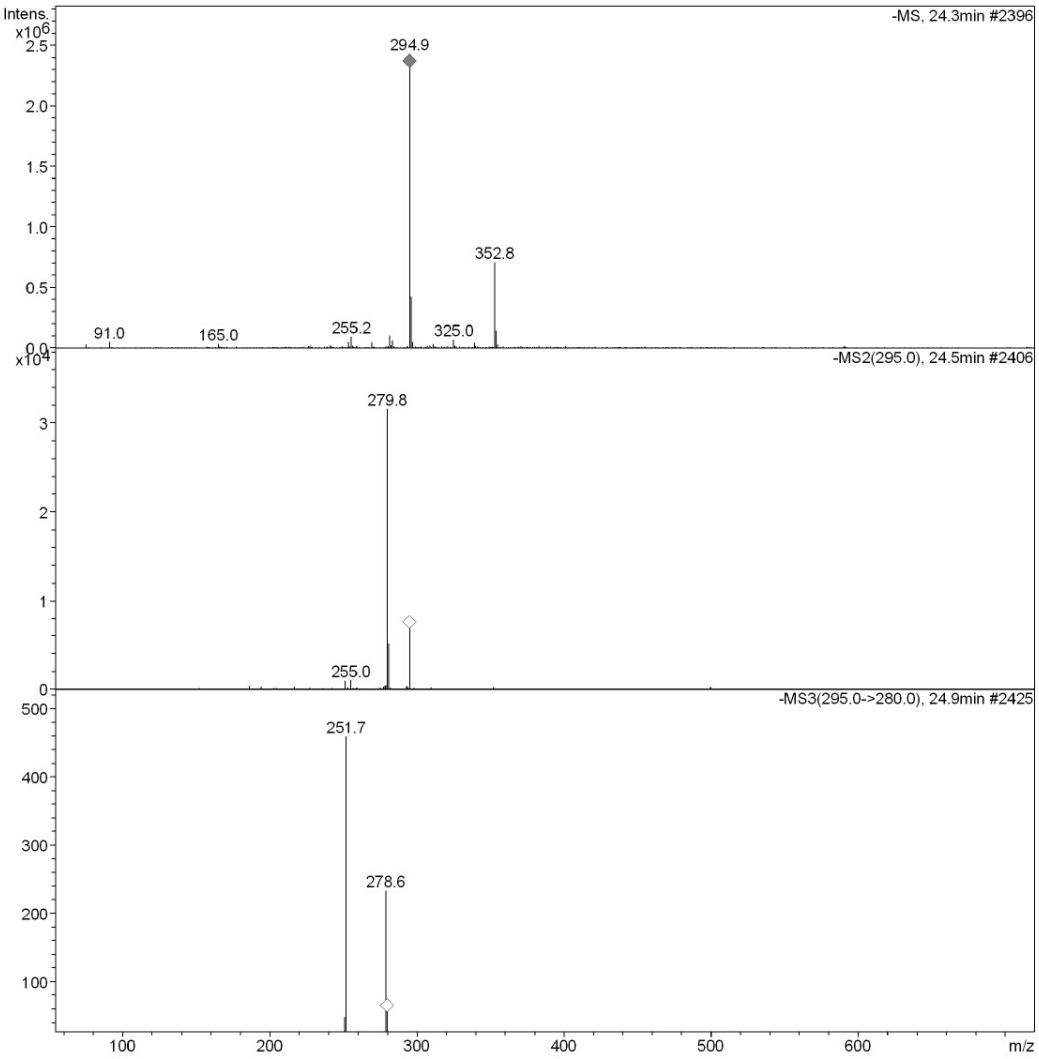
S50 ES-MS spectrum of 2.



Ms²

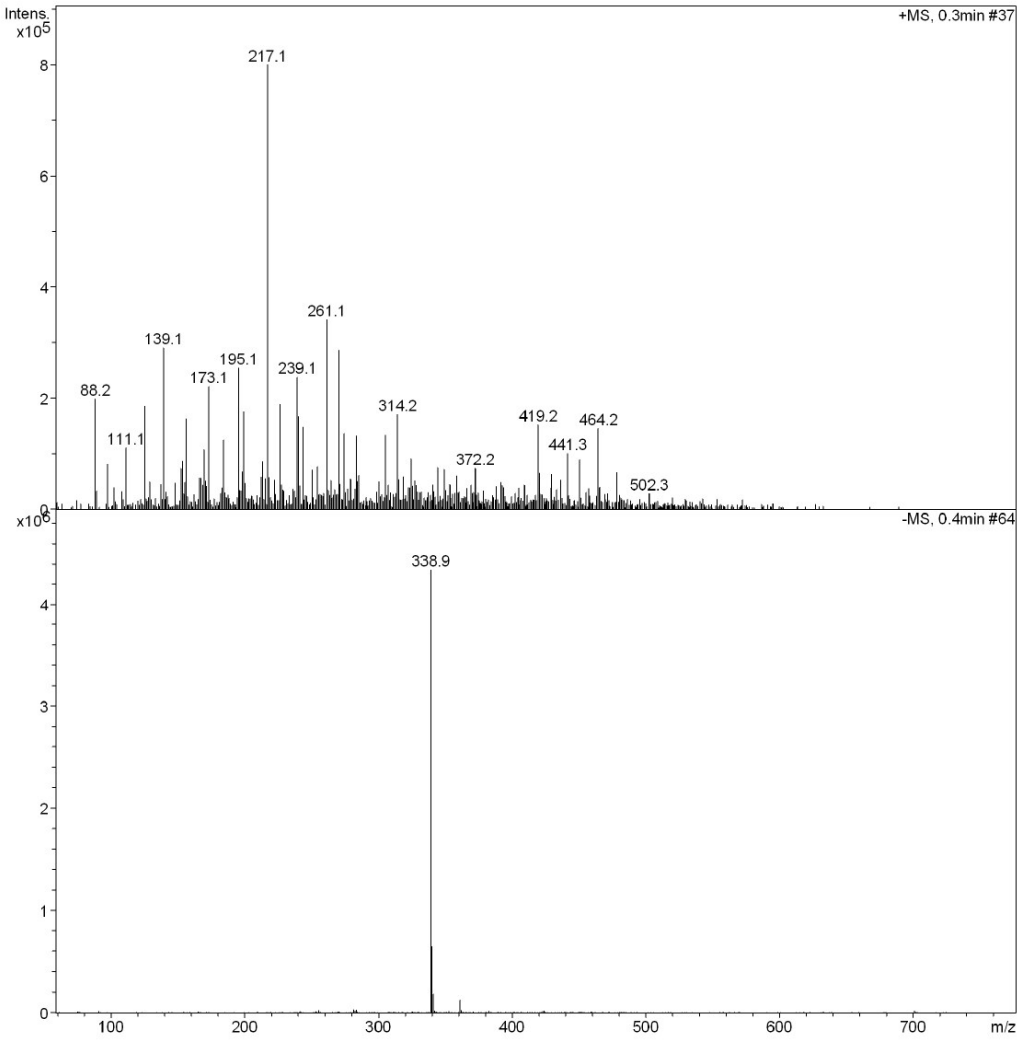

Intens.
x10^6
-MS, 23.4min #2331
294.9
352.8
90.9
255.3
x10^5
-MS2(353.0), 23.8min #2357
320.8
352.8
293.1
x10^4
-MS3(353.0->321.0), 24.1min #2367
292.8
320.7
100
200
300
400
500
600
m/z

Ms³

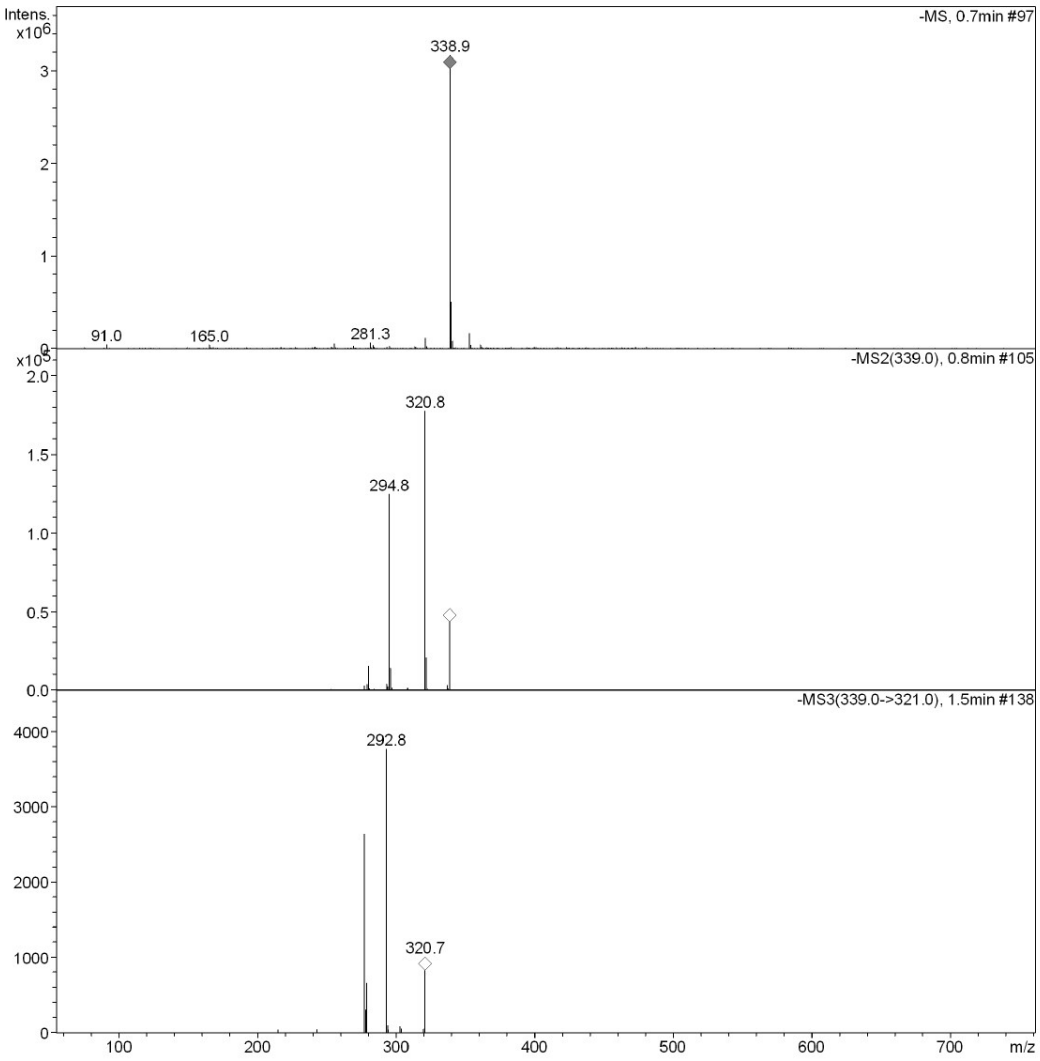

Intens.
x10^6
2.5
2.0
1.5
1.0
0.5
0.0
-MS, 24.3min #2396
294.9
352.8
91.0
165.0
255.2
325.0
x10^4
3
2
1
0
-MS2(295.0), 24.5min #2406
279.8
255.0
500
400
300
200
100
-MS3(295.0->280.0), 24.9min #2425
251.7
278.6
100
200
300
400
500
600
m/z

S51 ES-MS spectrum of 3.

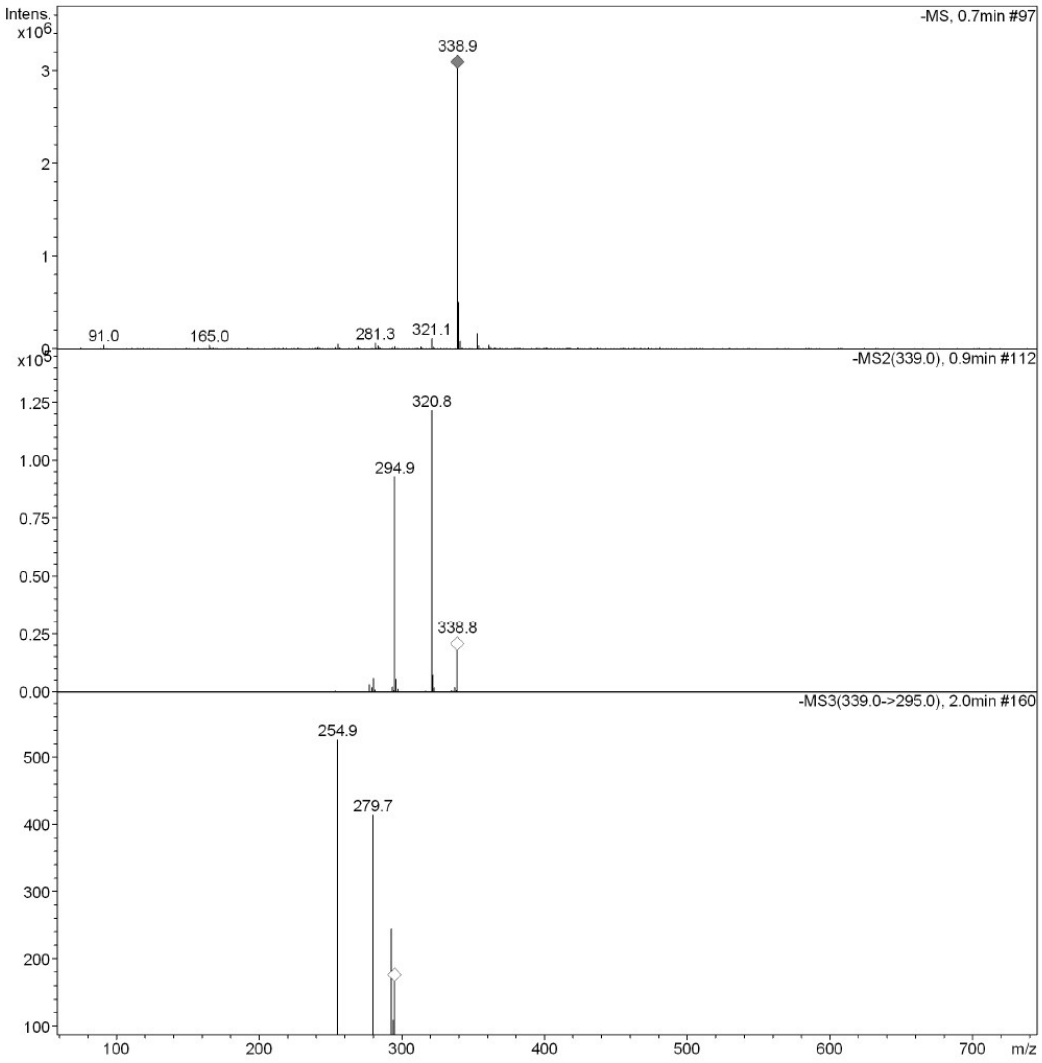
Ms



Ms^2

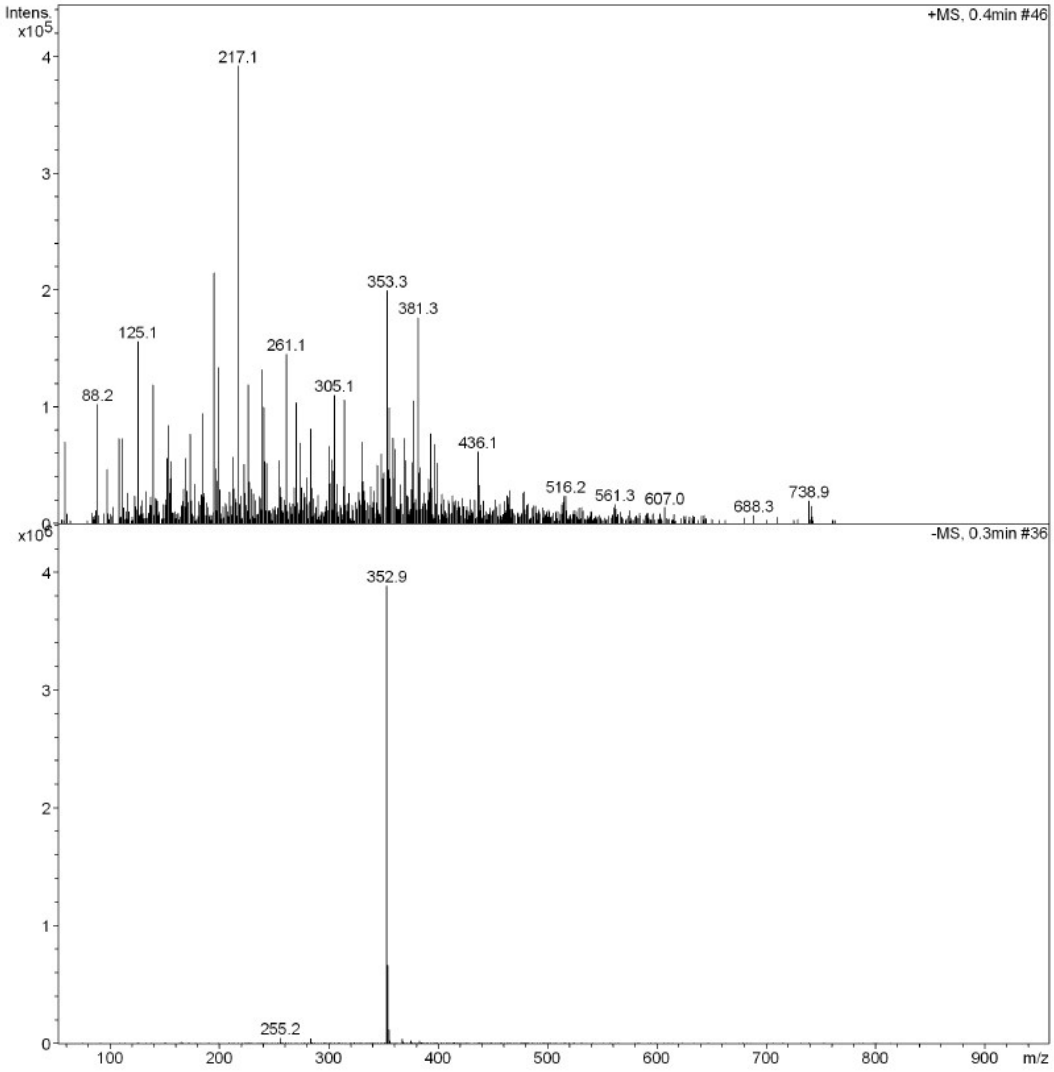

Intens.
x10^6
-MS, 0.7min #97
338.9
91.0
165.0
281.3
x10^5
-MS2(339.0), 0.8min #105
320.8
294.8
-MS3(339.0->321.0), 1.5min #138
292.8
320.7
m/z

Ms³

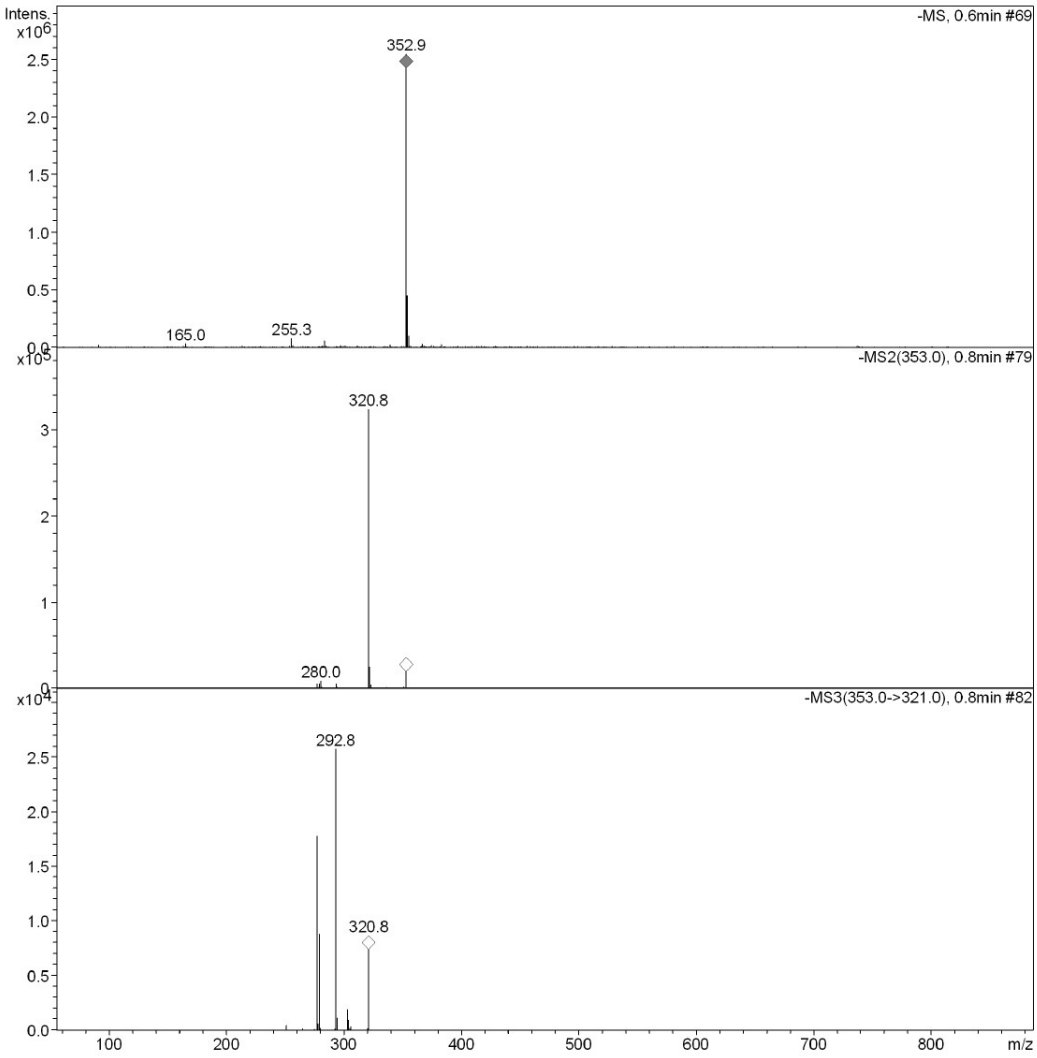

Intens.
x10^6
-MS, 0.7min #97
338.9
91.0
165.0
281.3
321.1
x10^5
-MS2(339.0), 0.9min #112
320.8
294.9
338.8
-MS3(339.0->295.0), 2.0min #160
254.9
279.7
m/z

S52 ES-MS spectrum of 4.

Ms



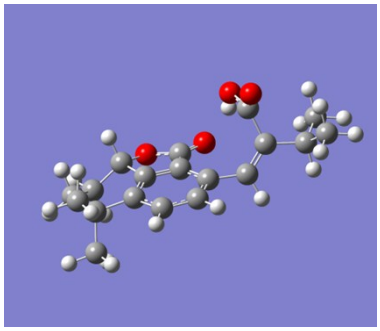
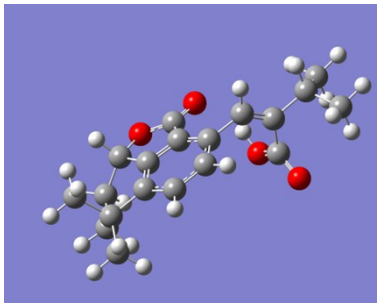
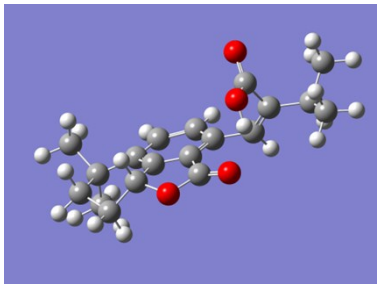
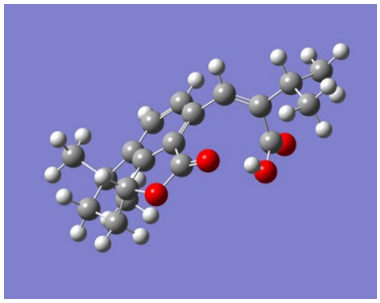
Ms^2


Intens.
x10^6
-MS, 0.6min #69
352.9
165.0
255.3
x10^5
-MS2(353.0), 0.8min #79
320.8
280.0
x10^4
-MS3(353.0->321.0), 0.8min #82
292.8
320.8
m/z

Tables

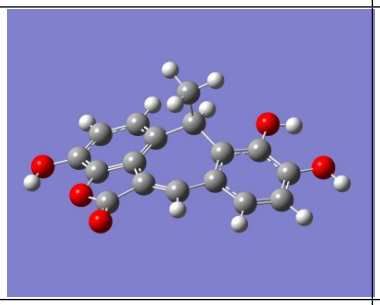
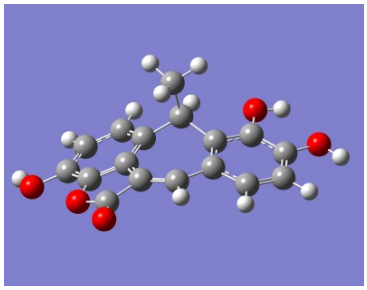
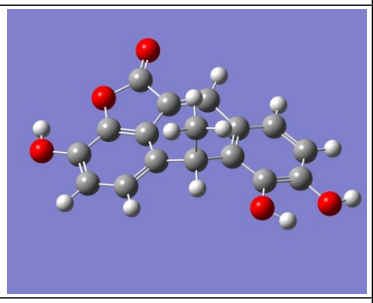
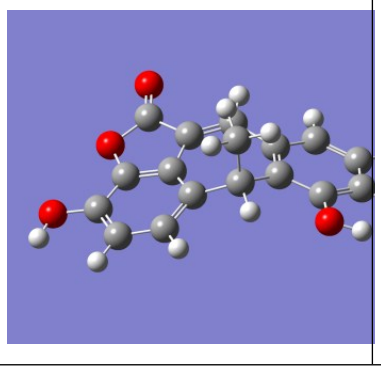
1 Conformations of 1a and 1b

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

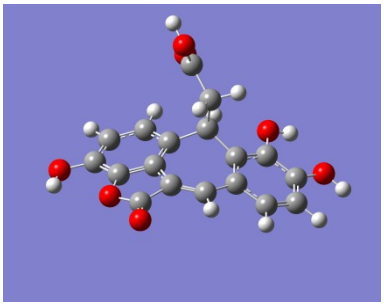
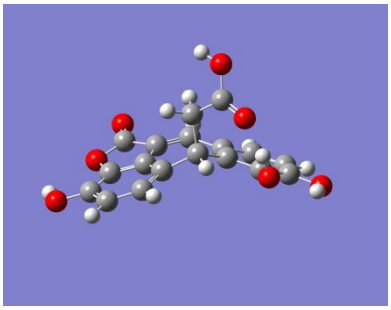
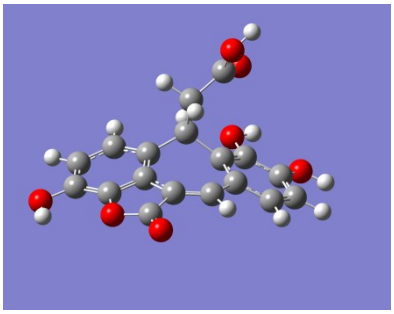
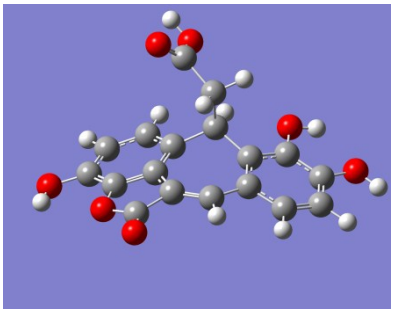
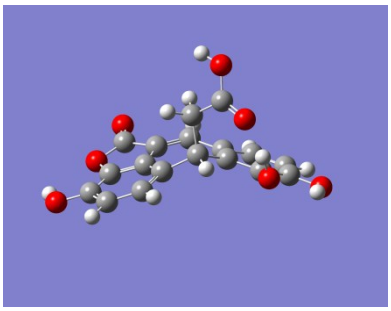
2 Conformations of 2a and 2b

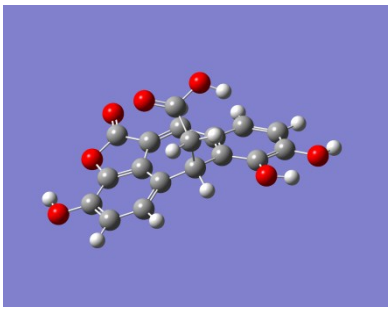
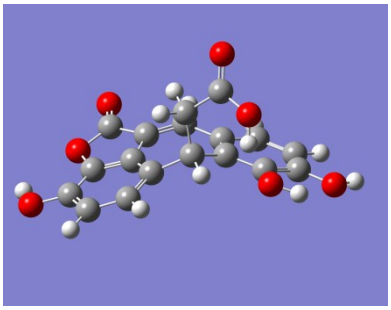
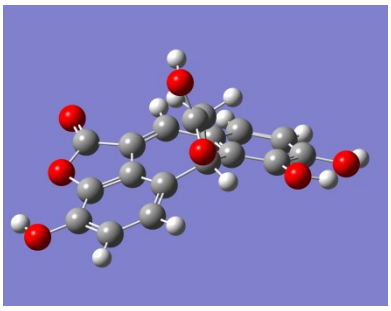
Table S2. Conformations of 2a and 2b were Obtained after the Optimization.

no.	conformer	population (%)
2a-1		75.68
2a-2		24.32
2b-1		75.11
2b-2		24.89

3 Conformations of 3a and 3b

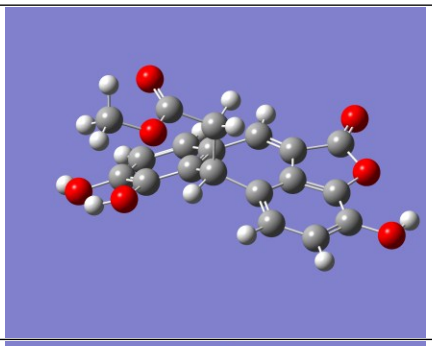
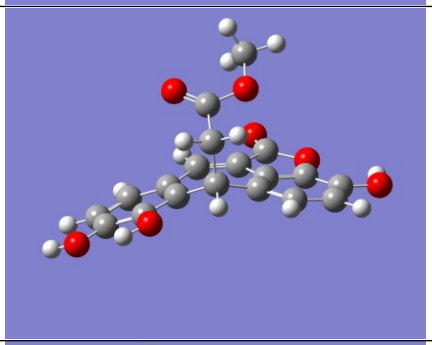
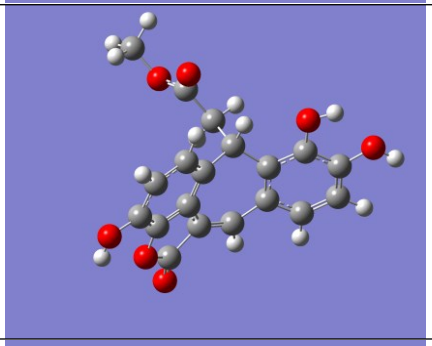
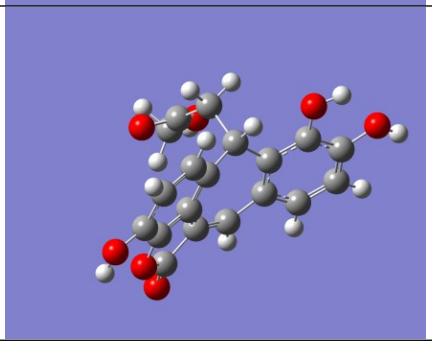
Table S3. Conformations of 3a and 3b were Obtained after the Optimization.

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_2O_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

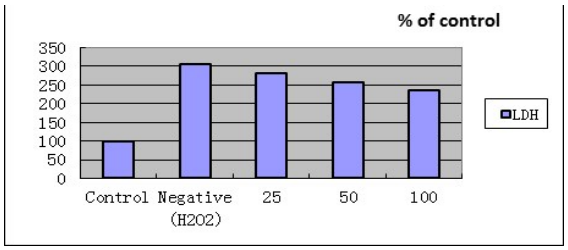
###:P＜0.001 Vs Control；*;P＜0.05 Vs model；**: P＜0.01 Vs model；***:P＜0.001 Vs model

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

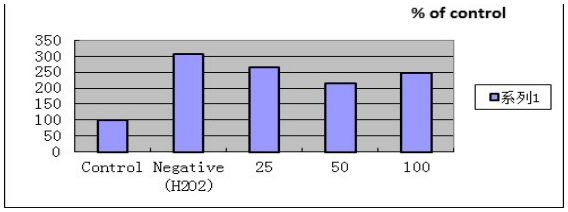
Table S6 Effects of 2-hour isolates pretreatment on LDH activity in each group

	Con (U/L)	H_2O_2(200 μM) (U/L)	Comp. + H_2O_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

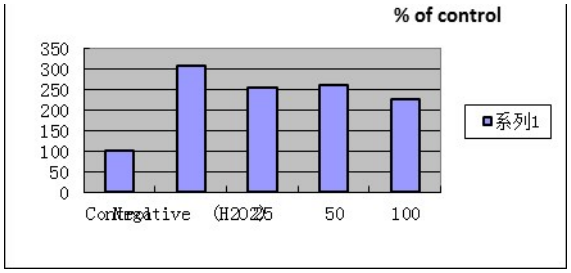
LDH, Lactate dehydrogenase



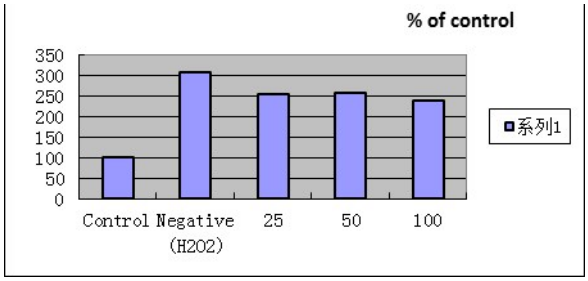
2a



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**