Supporting Information

Herbarone, a Rearranged Heptaketide Derivative from the Sea Hare Associated Fungus *Torula herbarum*

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Table S1. ^{1}H and ^{13}C NMR Data for **2** and **3**[a]

	2		**3**	
position	δ_C, type	δ_H (*J* in Hz)	δ_C, type	δ_H (*J* in Hz)
1	93.8, CH	5.53 (1H, s)	87.3, CH	6.02 (1H, s)
3	62.0, CH	4.20 (1H, m)	62.9, CH	4.30 (1H, m)
4	29.0, CH_2	2.67 (1H, dd, 19.0, 3.5)	29.0, CH_2	2.68(1H, dd, 19.0, 3.2)
		2.23 (1H, dd, 19.0, 11.0)		2.22(1H, dd, 19.0, 11.0)
4a	140.5, C		140.1, C	
5	184.9, C		184.6, C	
5a	135.7, C		135.7, C	
6	103.2, CH	7.23 (1H, d, 2.4)	103.6, CH	7.27(1H, d, 2.4)
7	164.5, C		164.9, C	
8	104.4, CH	6.72 (1H, d, 2.4)	104.3, CH	6.73(1H, d, 2.4)
9	162.0, C		162.1, C	
9a	114.2, C		114.1, C	
10	180.8, C		182.1, C	
10a	140.9, C		140.5, C	
1’	21.0, CH_3	1.54 (3H, d, 6.4)	21.0, CH_3	1.38 (3H, d, 6.3)
1-OMe	55.9, CH_3	3.57 (3H, s)		
7-OMe	56.4, CH_3	3.95 (3H, s)	56.5, CH_3	3.97(3H, s)
9-OMe	56.3, CH_3	3.94 (3H, s)	56.0, CH_3	3.96 (3H, s)

[a] δ in ppm, in $CDCl_3$, at 400 MHz for ^{1}H and 100 MHz for ^{13}C NMR experiments.

Figure S1. DFT optimized geometries of the six lowest-energy conformers of (5*S*,7*S*,9*S*,11*R*)-**1**.

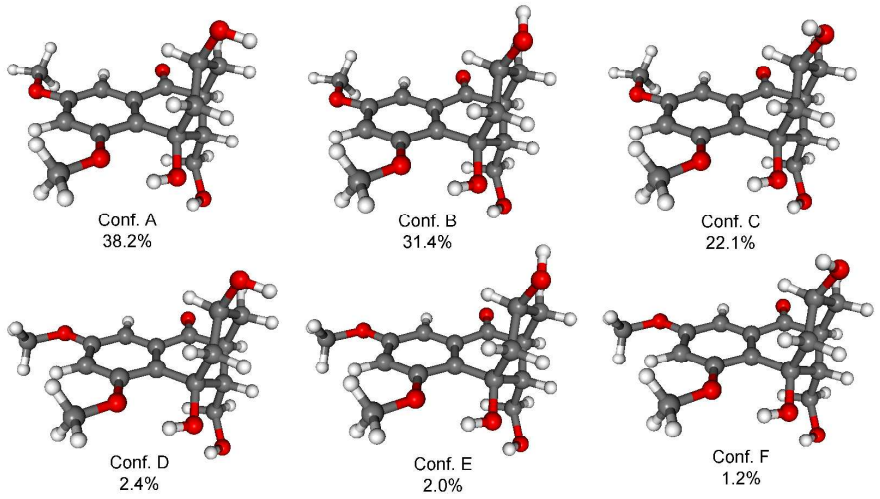


Figure S2. DFT optimized geometries and populations of the six lowest-energy conformers of (1*R*,3*S*)-**2**.

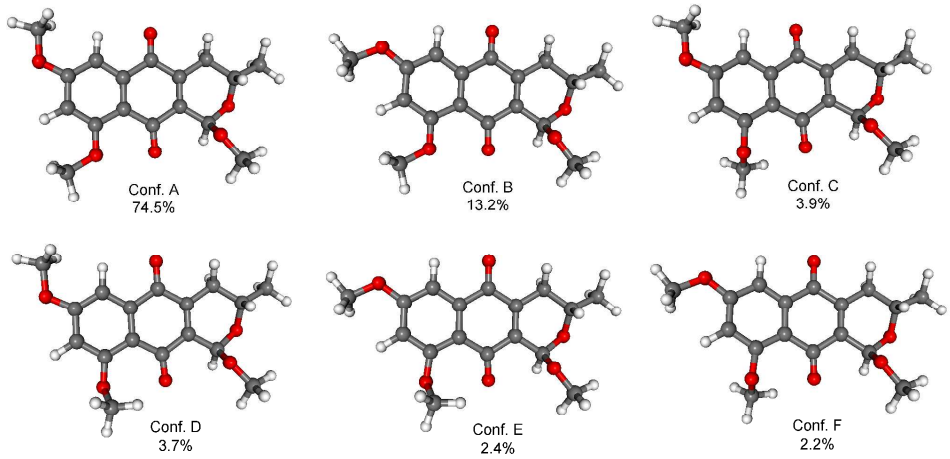


Figure S3. DFT optimized geometries of the seven lowest-energy conformers of (*R*)-**5**.

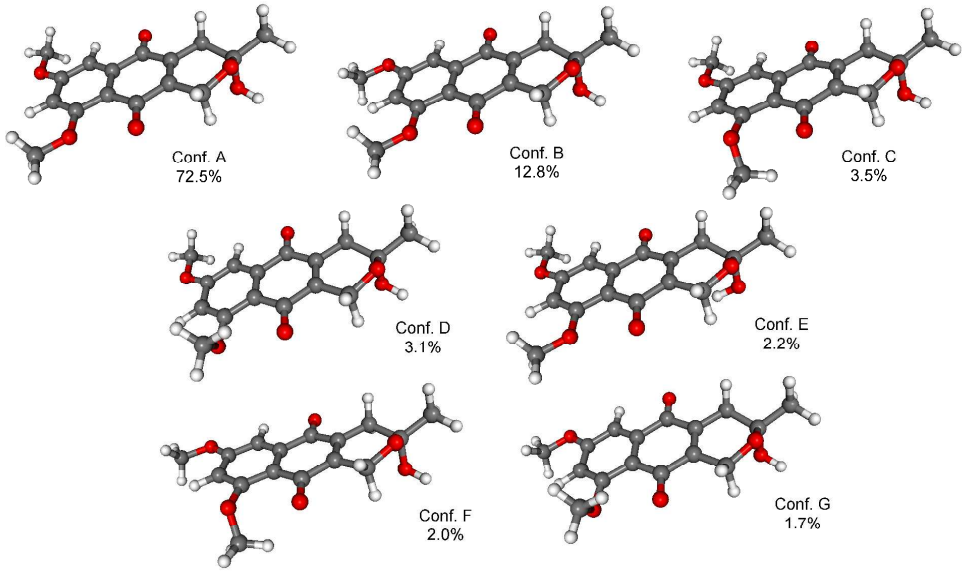


Figure S4. DFT optimized geometries and populations of the six lowest-energy conformers of (*R*)-**4**.

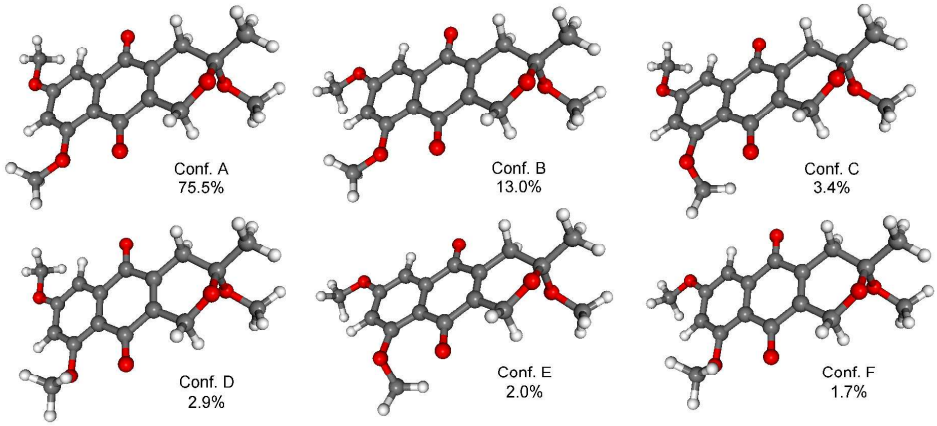
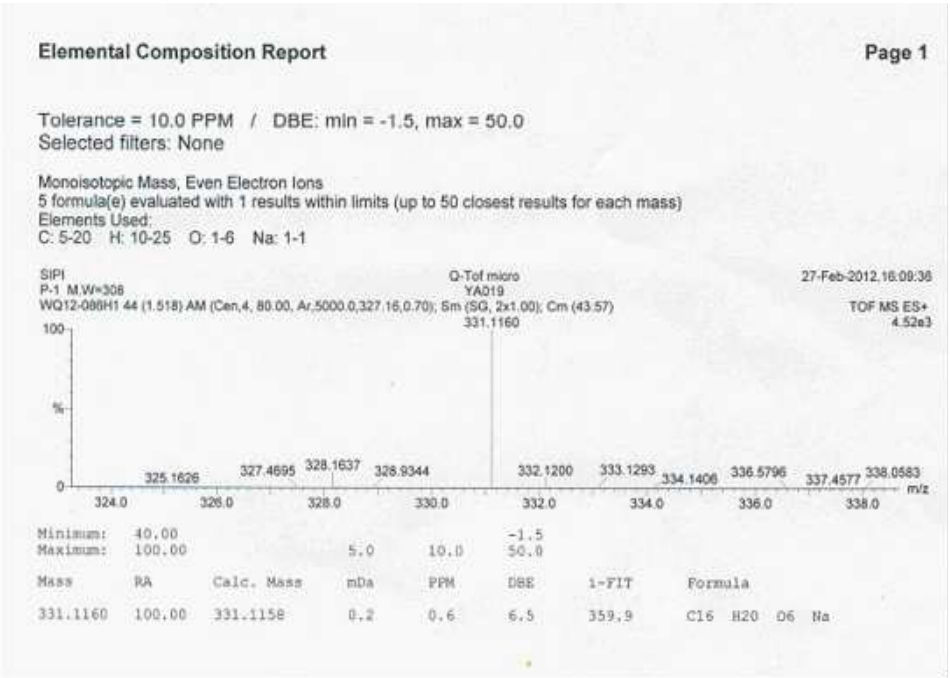


Figure S5. HRESIMS of herbarone (**1**) in $CDCl_3$



Elemental Composition Report Page 1

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 5-20 H: 10-25 O: 1-6 Na: 1-1

SIPI
P-1 M.W=308
WQ12-086H1 44 (1.518) AM (Cen,4, 80.00, Ar,5000.0,327.16,0.70); Sm (SG, 2x1.00); Cm (43.57)
Q-Tof micro
YA019
27-Feb-2012,16:09:36
TOF MS ES+
4.52e3

Minimum:	40.00				-1.5		
Maximum:	100.00		5.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
331.1160	100.00	331.1158	0.2	0.6	6.5	359.9	C16 H20 O6 Na

Figure S6. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of herbarone (**1**)

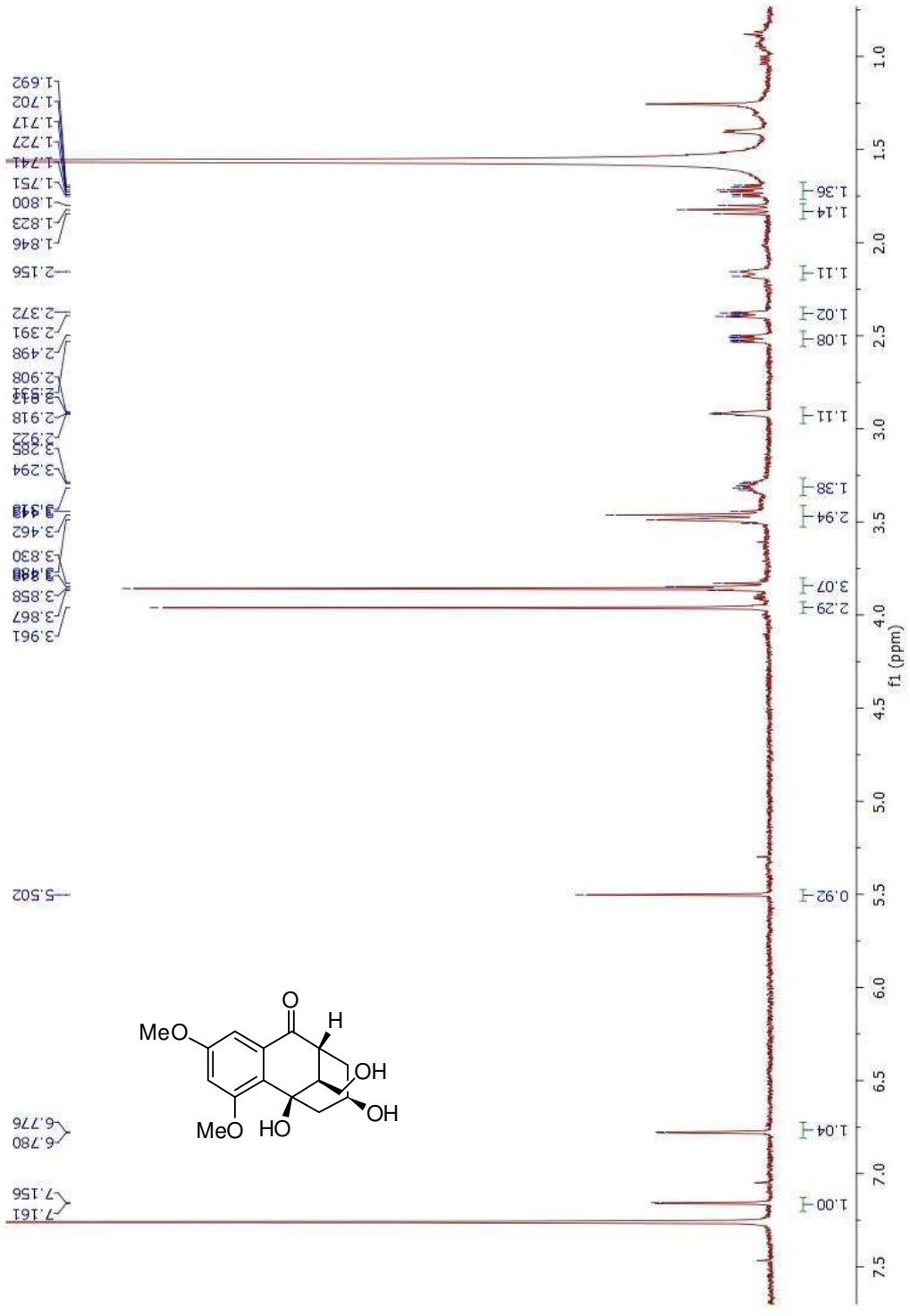


Figure S7. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of herbarone (**1**)

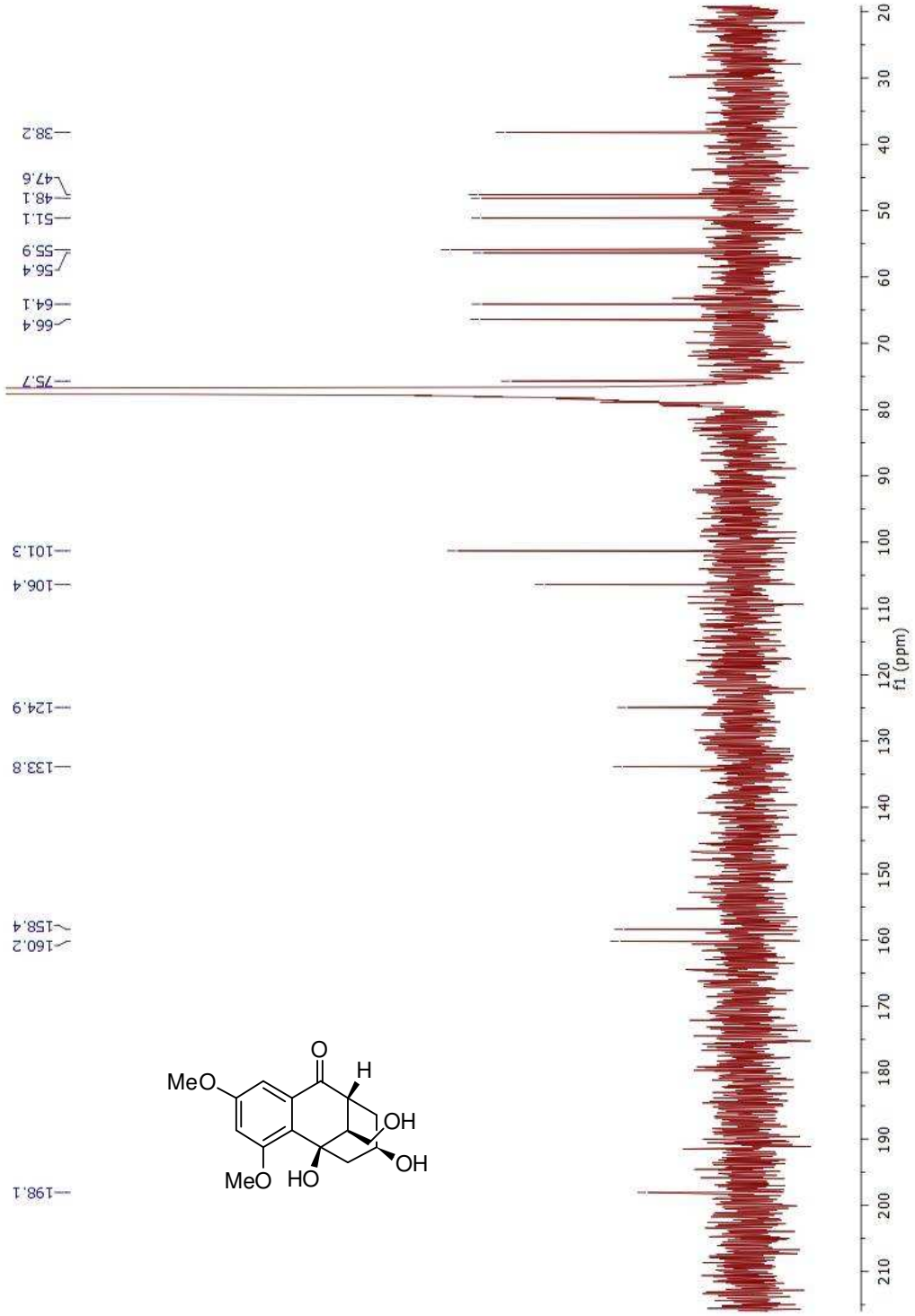


Figure S8. DEPT (125 MHz, $CDCl_3$) spectrum of herbarone (**1**)

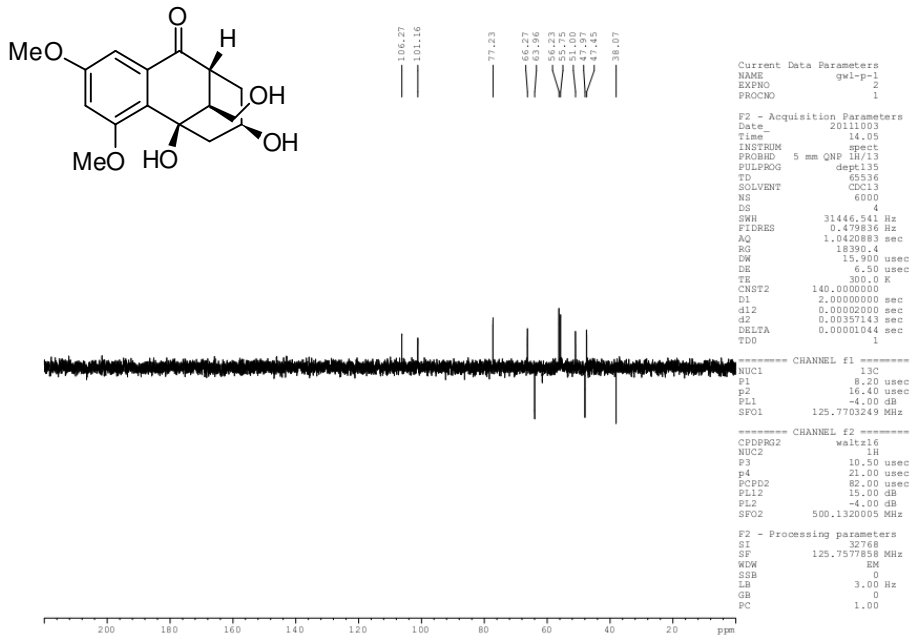
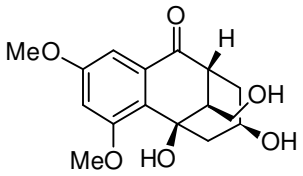
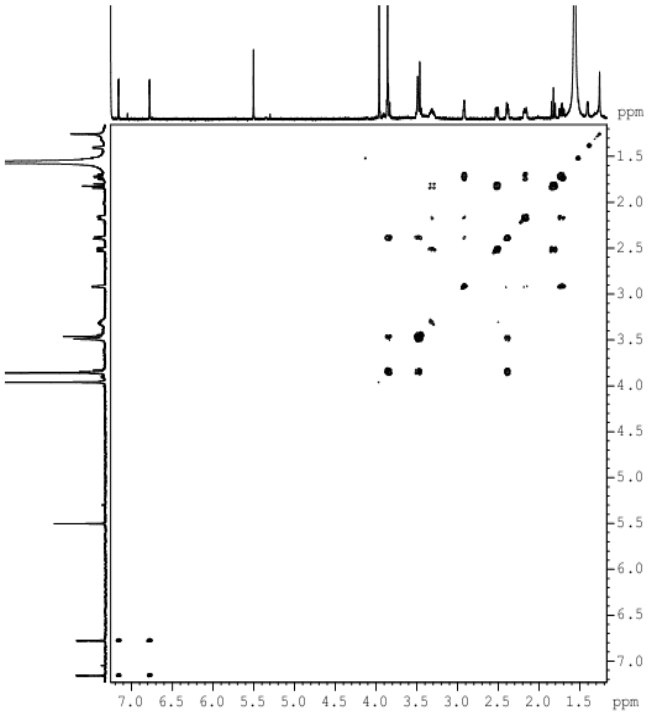


Figure S9. COSY (500 MHz, $CDCl_3$) spectrum of herbarone (**1**)





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PROCNO 1

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TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 4045.307 Hz
FIDRES 3.950495 Hz
AQ 0.1267400 sec
RG 20642.5
DW 123.600 usec
DE 6.50 usec
TE 300.0 K
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D1 2.00000000 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00024720 sec

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P1 10.50 usec
PL1 -4.00 dB
SFO1 500.1318860 MHz

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GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
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TD 512
SFO1 500.1319 MHz
FIDRES 7.900991 Hz
SW 8.088 ppm
FnMODE QF

F2 - Processing parameters
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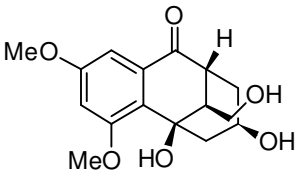
SF 500.1300132 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300132 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

Figure S10. HSQC (500 MHz, $CDCl_3$) spectrum of herbarone (**1**)



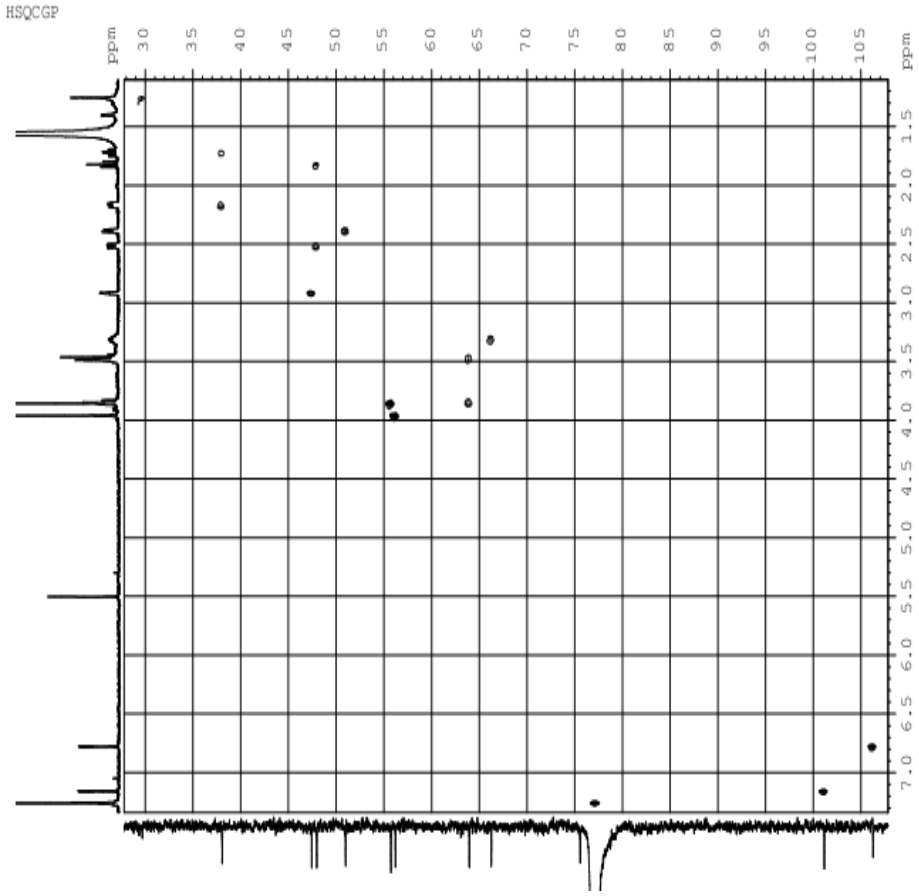
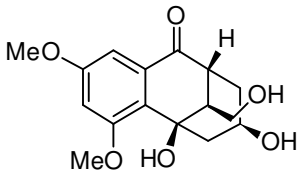


Figure S11. HMBC (500 MHz, $CDCl_3$) spectrum of herbarone (**1**)



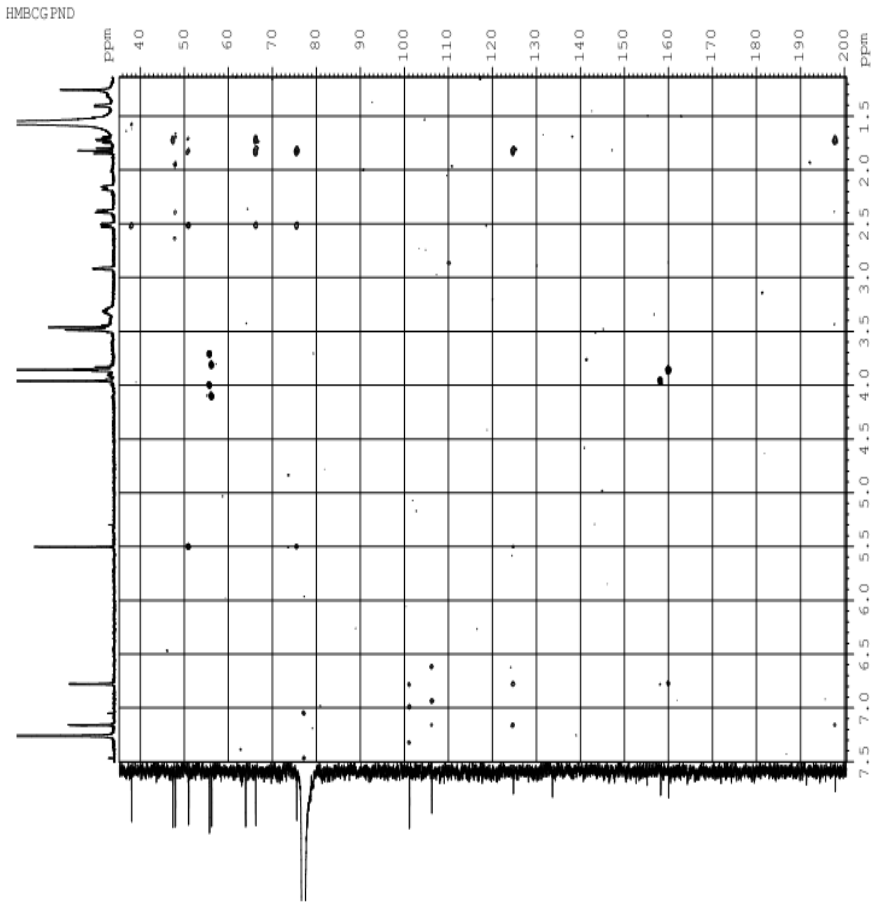
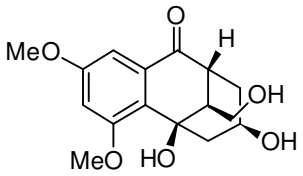
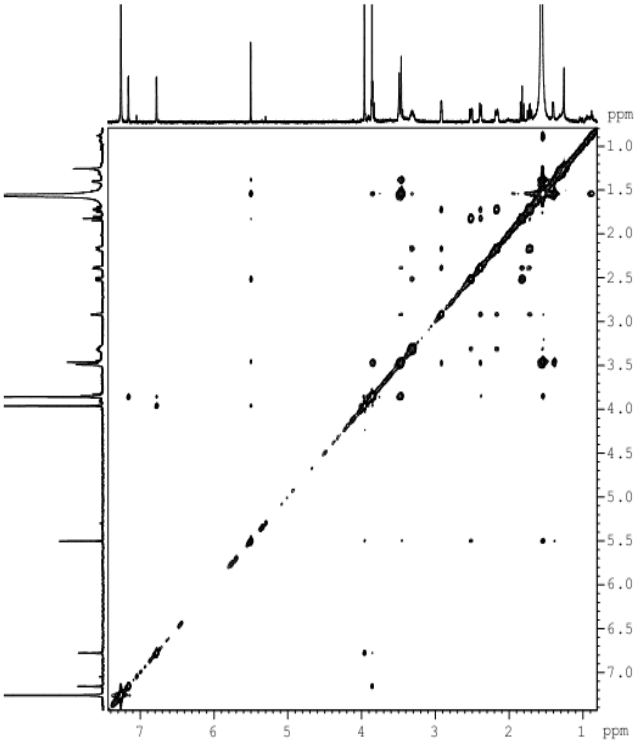


Figure S12. NOESY (500 MHz, $CDCl_3$) spectrum of herbarone (**1**)





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SOLVENT CDCl3
NS 8
DS 16
SWH 4045.307 Hz
FIDRES 3.950495 Hz
AQ 0.1267400 sec
RG 362
DW 123.600 usec
DE 6.50 usec
TE 300.0 K
d0 0.00011023 sec
D1 2.00000000 sec
D16 0.00020000 sec
D8 1.00000000 sec
IN0 0.00024720 sec
STSIGNT 256
TAU 0.49880001 sec

======== CHANNEL f1 ========
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P1 10.50 usec
p2 21.00 usec
PL1 -4.00 dB
SFO1 500.1318860 MHz

====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
NDO 1
TO 512
SFO1 500.1319 MHz
FIDRES 7.900991 Hz
SW 8.088 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 1024
SF 500.1300132 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 States-TPPI
SF 500.1300132 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0