

Biotransformation of guttiferones, *Symphonia globulifera* metabolites, by *Bipolaris cactivora*, an endophytic fungus isolated from its leaves

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Figure S1: HRMS in positive mode of 3,16-oxy-guttiferone C 7

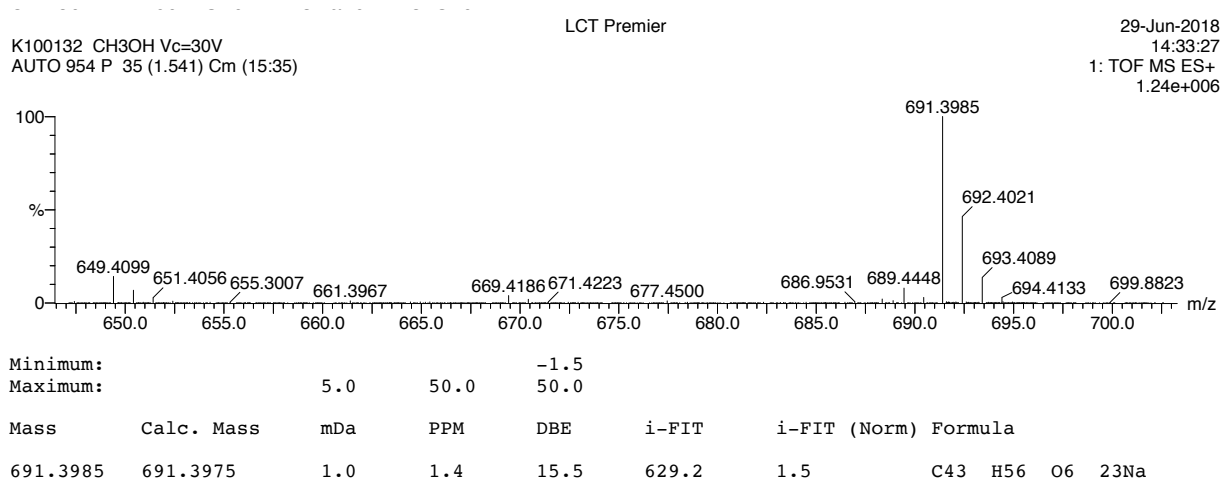


Figure S2: HRMS in negative mode of 1,16-oxy-guttiferone C 8

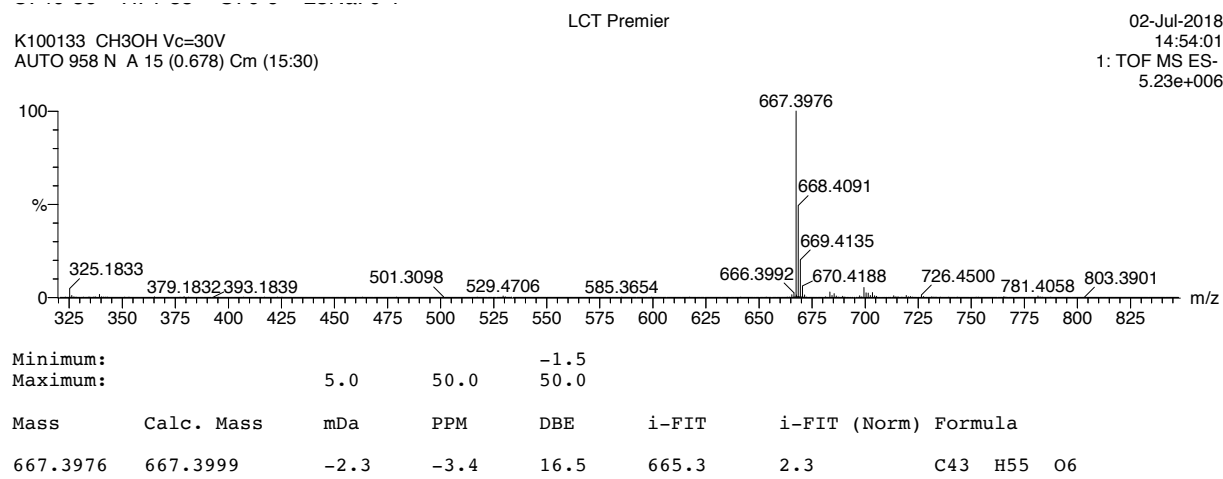


Table S1. NMR Spectroscopic Data (¹H, 400 MHz) and (¹³C 100 MHz) in CD₃OD for oxyguttiterone C 7 and 8

position	3,16 oxyguttiferone C 7			1,16 oxyguttiferone C 8		
	dc, type	dH (J in Hz)	HMBC	dc, type	dH (J in Hz)	HMBC
1	194.5, Cq			178.9, Cq		
2	121.3, Cq			121.0, Cq		
3	176.7, Cq			194.9, Cq		
4	63.3, Cq			73.6, Cq		
5	51.5, Cq			53.7, Cq		
6	53.4, Cq			57.0, Cq		
7	44.8, CH ₂	2.18 m	1, 6, 8, 9, 24	42.4, CH ₂	2.44 d (14) 2.05 dd (14, 7)	1, 5, 6, 8, 9, 24 1, 6, 8, 24
8	41.0, CH	1.89 m	5, 7, 24	40.3, CH	1.87 m	7
9	208.7, Cq			208.4, Cq		
10	173.7, Cq			174.1, Cq		
11	118.2, Cq			118.8, Cq		
12	109.6, CH	7.44 s	10, 13, 14, 16	109.6, CH	7.44 s	10, 13, 14, 16
13	146.9, Cq			146.5, Cq		
14	151.3, Cq			151.0, Cq		
15	103.9, CH	6.94 s	11, 13, 14, 16	104.1, CH	6.91 s	11, 13, 14, 16
16	154.7, Cq			154.6, Cq		
17	26.5, CH ₂	2.89 m	3, 4, 9, 18, 19	26.5, CH ₂	2.65 t (8)	3, 4, 9, 18, 19
18	120.3, CH	4.67 m	20 and 21	119.9, CH	4.76 m	20 and 21
19	135.9, Cq			135.4, Cq		
20	26.1, CH ₃	1.43 s	18, 19, 21	26.2, CH ₃	1.56 s	18, 19, 21
21	18.7, CH ₃	1.77 s	18, 19, 20	18.7, CH ₃	1.73 s	18, 19, 20
22	20.4, CH ₃	1.28 s	4, 5, 6, 23	20.4, CH ₃	1.14 s	4, 5, 6, 23
23	36.5, CH ₃	1.89 m	5, 6, 40	36.2, CH ₂	1.39 m	39
24	30.3, CH ₂	1.89 m	5, 6, 7	30.4, CH ₂	1.87 m	7
25	125.3, CH	4.82 m	27 and 28	125.1, CH ₂	4.76 m	27 and 28
26	133.7, Cq			133.8, Cq		
27	26.0, CH ₃	1.60 s	25, 26, 28	25.9, CH ₃	1.51 s	25, 26, 28
28	18.0, CH ₃	1.33 s	25, 26, 27	18.5, CH ₃	0.98 s	25, 26, 27
29	38.8, CH ₂	2.18 m	1, 7, 8, 9, 30, 31, 34	37.7, CH ₂	2.30 m	8, 9, 30
30	44.1, CH	2.67 h (5)	29, 31, 32, 33, 34	44.7, CH	1.87 m 2.30 m	1, 7, 8, 30, 31, 34
31	150.2, Cq			148.1, Cq		
32	114.7, CH ₂	4.47 s 4.38 m	30 and 33 30 and 33	112.9, CH ₂	4.16 s 4.09 m	30 and 33 30 and 33
33	17.9, CH ₃	1.57 s	30, 31, 32	17.9, CH ₃	1.59 s	30, 31, 32
34	32.5, CH ₂	1.38 s		32.9, CH ₂	1.63 m	
35	36.8, CH ₂	1.89 m	34, 36, 37, 38	36.3, CH ₂	1.87 m	34, 36, 37, 38
36	149.5, Cq			147.0, Cq		
37	110.4, CH ₂	4.64 m 4.61 s	35 and 38 35 and 38	110.7, CH ₂	4.58 s 4.61 s	35 and 38 35 and 38
38	22.6, CH ₃	1.67 s	35 and 37	22.6, CH ₃	1.67 s	35, 36, 37
39	24.1, CH ₂	1.89 m	5, 40, 41	24.2, CH ₂	1.87 m	40
40	125.0, CH	5.10 t	42 and 43	124.8, CH	5.11 t (7)	42 and 43
41	133.0, Cq			132.9, Cq		
42	25.9, CH ₃	1.69 s	40, 41, 43	25.7, CH ₃	1.70 s	40, 41, 43
43	17.8, CH ₃	1.60 s	40, 41, 42	17.7, CH ₃	1.61 s	40, 41, 42

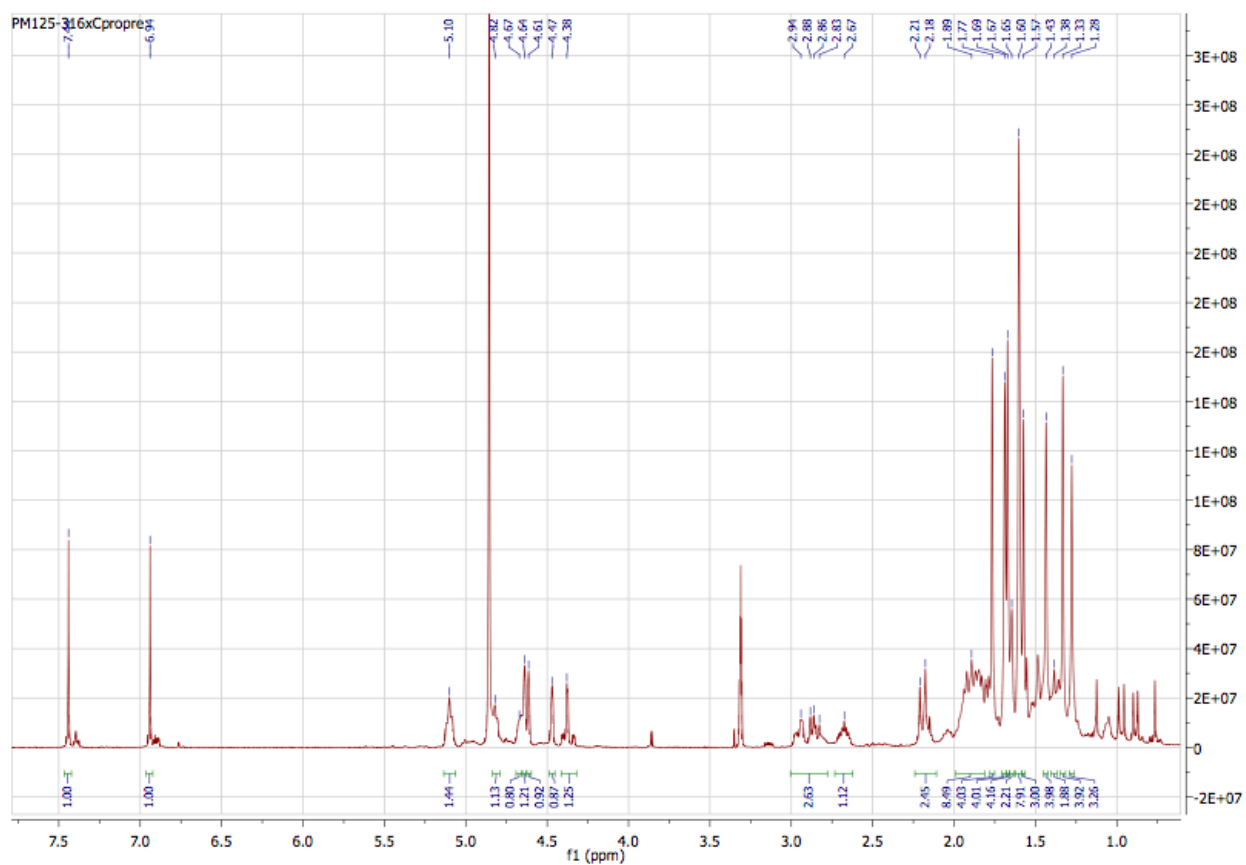
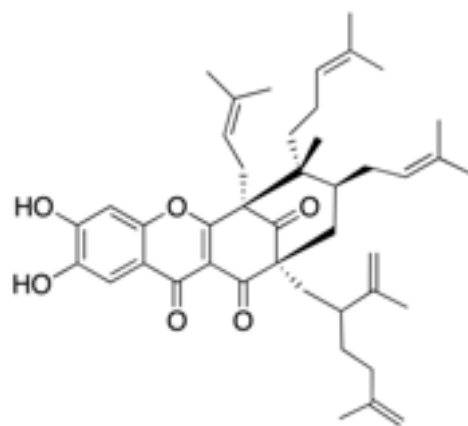
Figure S4: ^1H NMR spectrum (400MHz, CD_3OD) of 3,16-oxyguttiferone C 7

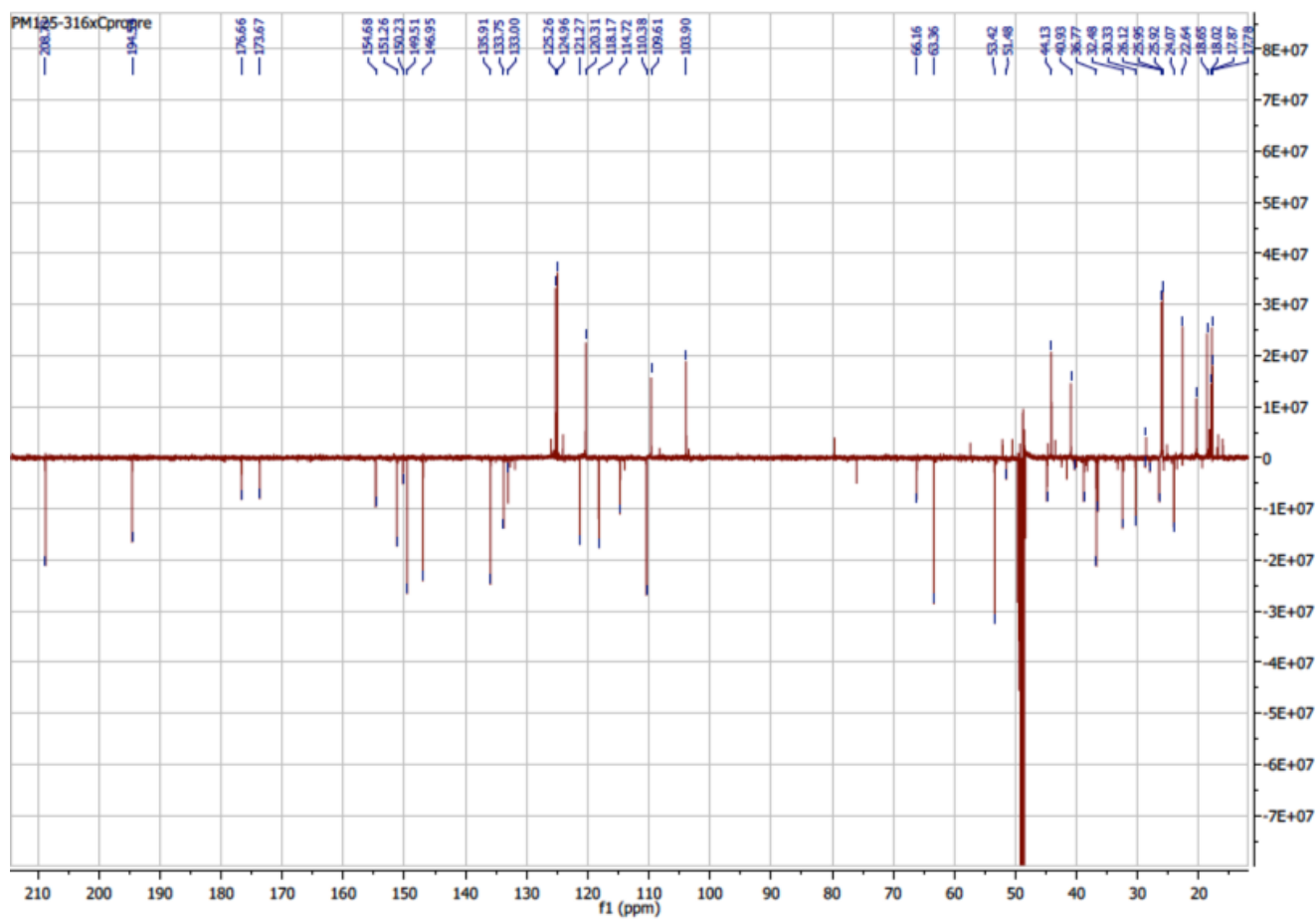
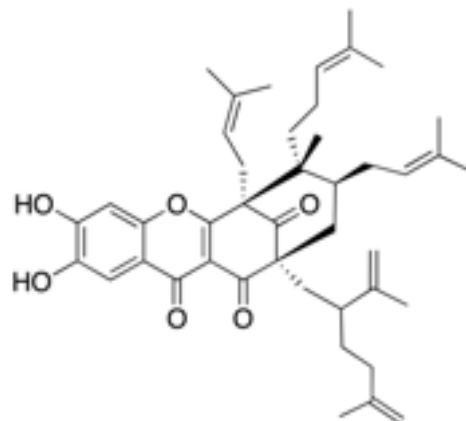
Figure S5: ^{13}C NMR spectrum (100MHz, CD_3OD) of 3,16-oxyguttiferone C 7

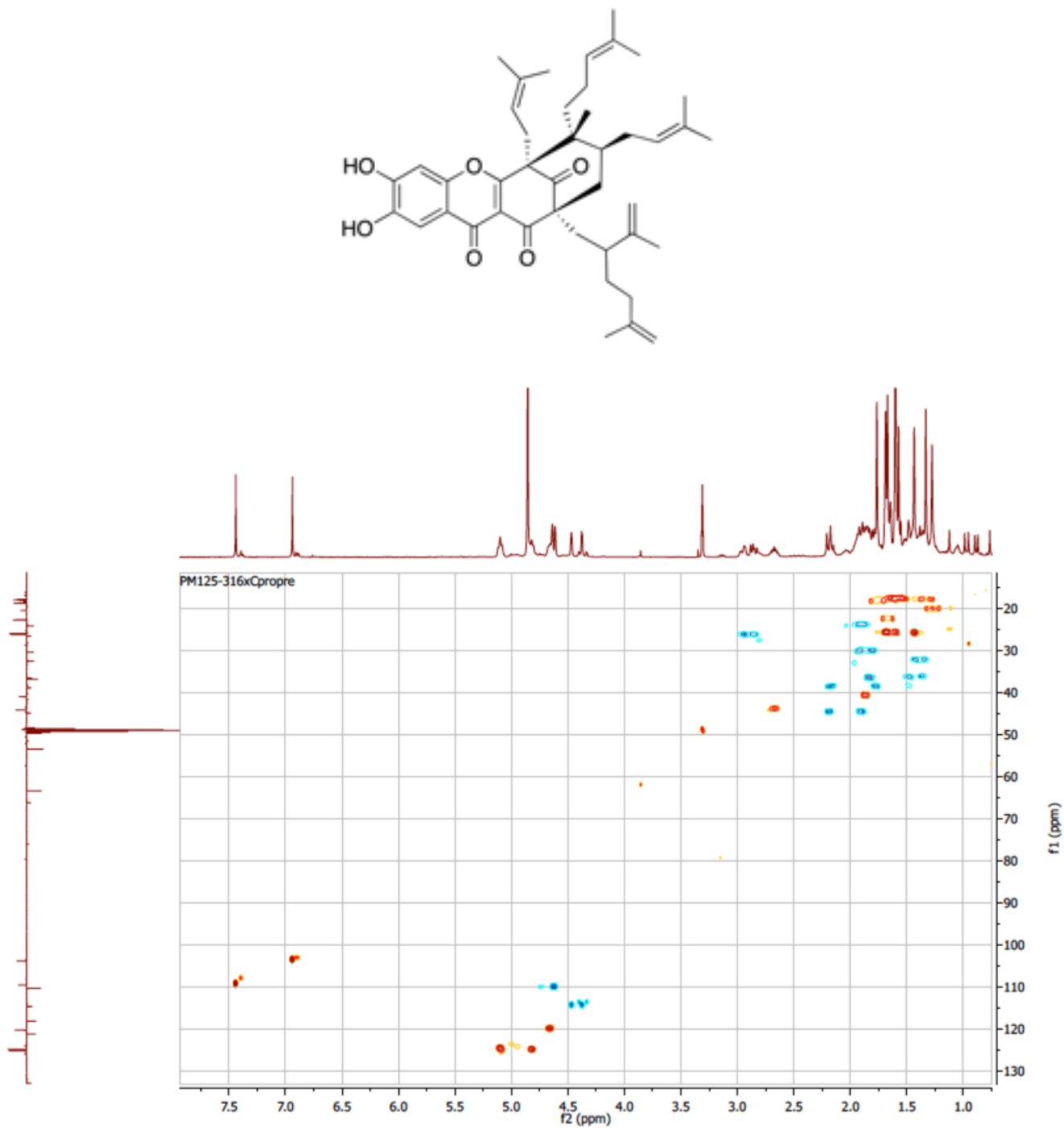
Figure S6: HSQC spectrum of 3,16-oxyguttiferone C 7 (CD₃OD)

Figure S7: HMBC spectrum of 3,16-oxyguttiferone C 7 (CD₃OD)

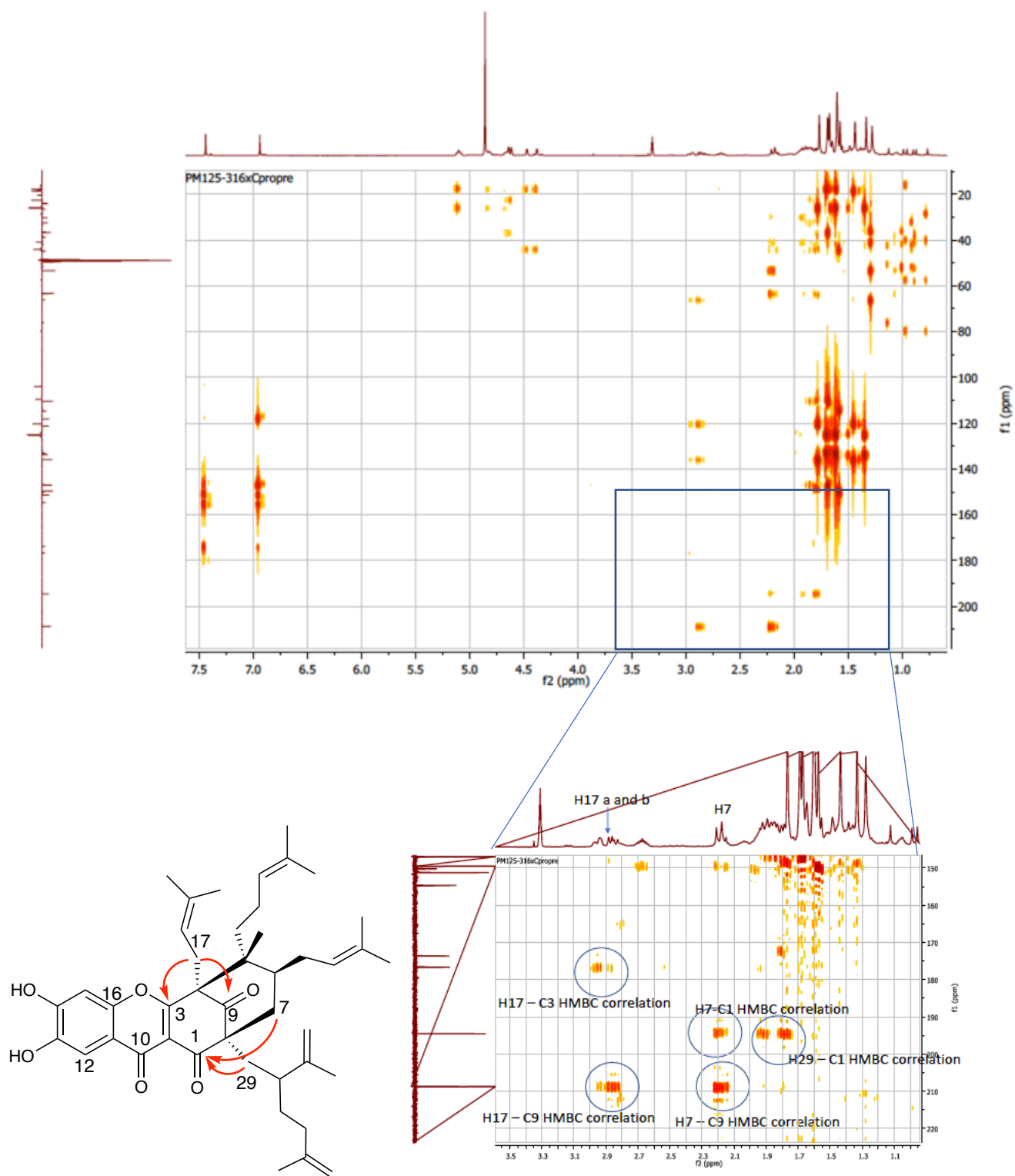


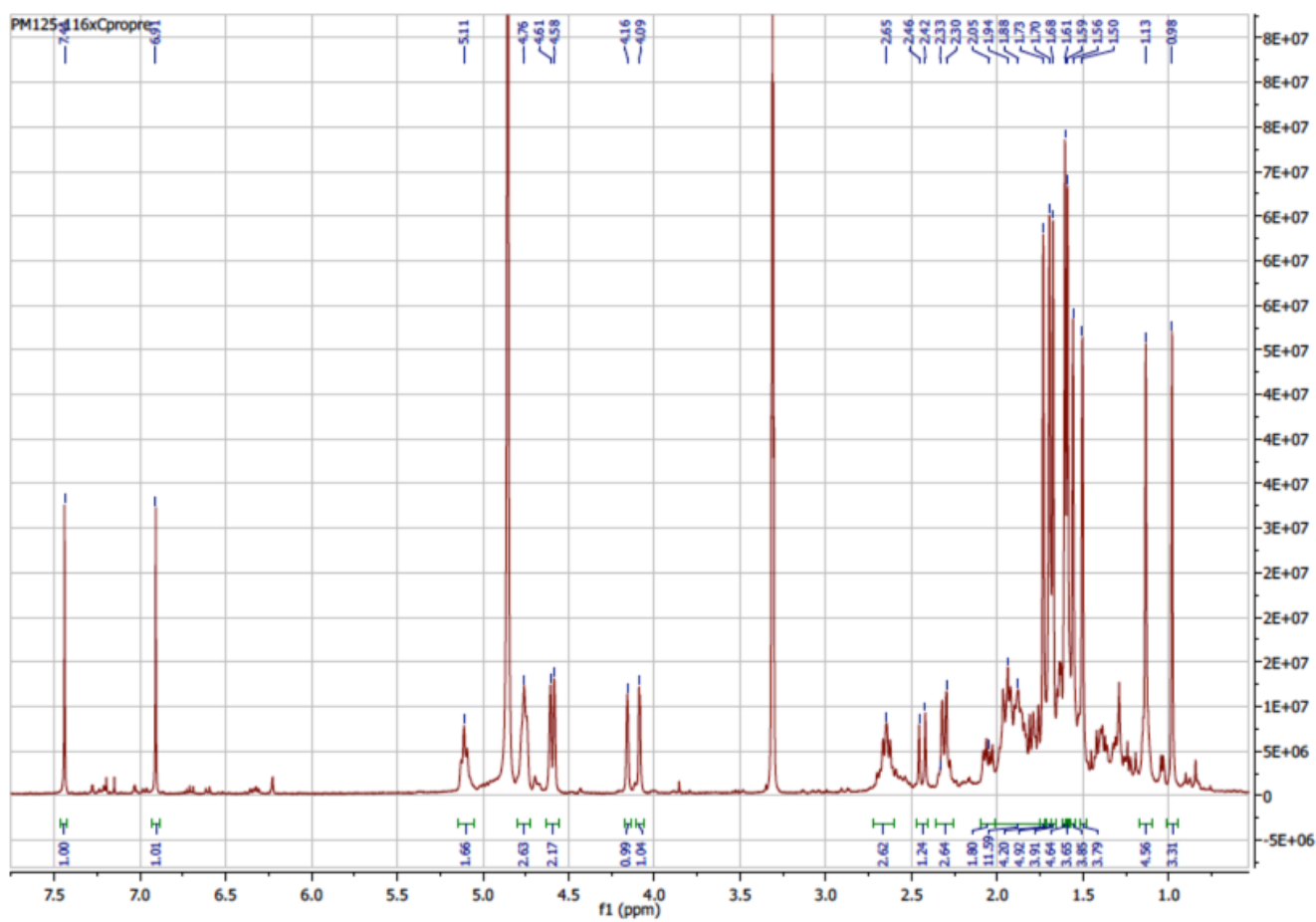
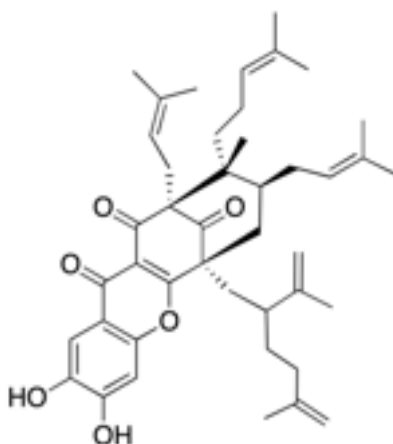
Figure S8: ^1H NMR spectrum (400MHz, CD_3OD) of 1,16-oxyguttiferone C 8

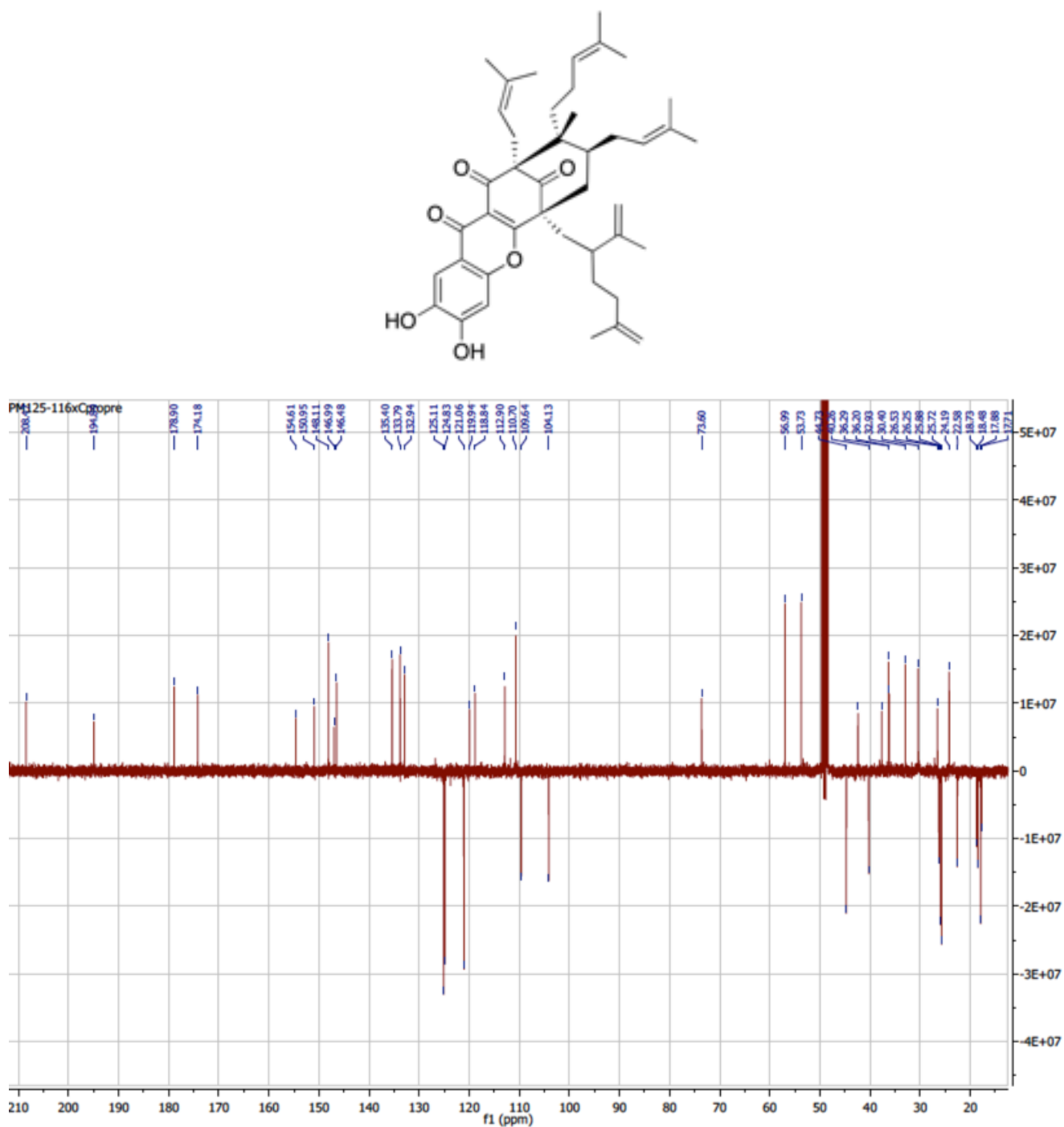
Figure S9: ^{13}C NMR spectrum (100MHz, CD_3OD) of 1,16-oxyguttiferone C 8

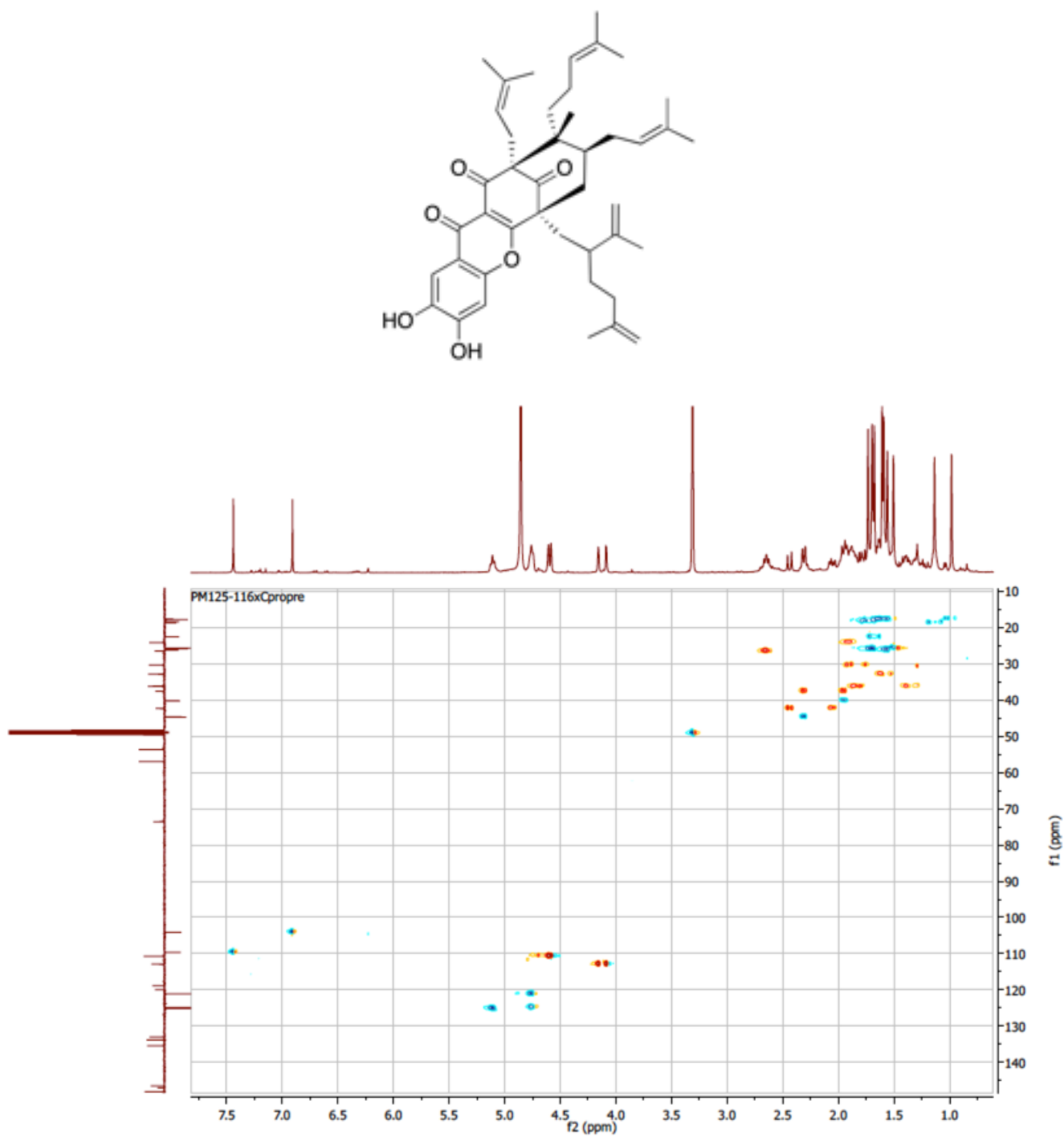
Figure S10: HSQC spectrum of 1,16-oxyguttiferone C **8** (CD₃OD)

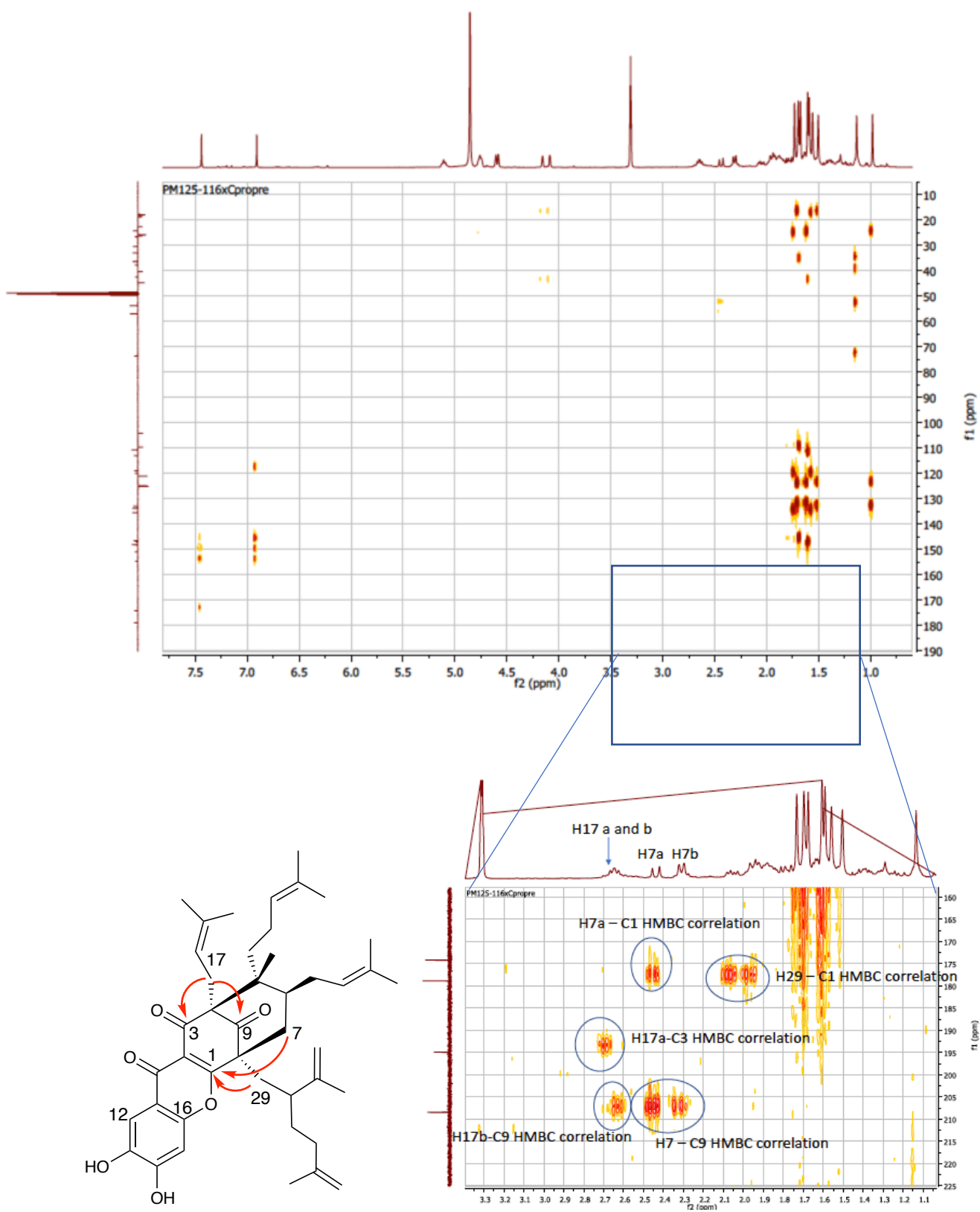
Figure S11: HMBC spectrum of 1,16-oxyguttiferone C **8** (CD₃OD)

Figure S12: HPLC/UV chromatograms of *Bipolaris cactivora* biotransformations after three days incubation time. A: guttiferone A in bioreactor, B: guttiferone C in bioreactor and C: mixture of guttiferone A and C in flask.

