

Bio-guided isolation of new compounds from *Baccharis* spp. as antifungal against *Botrytis cinerea*.

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Isolation procedure:

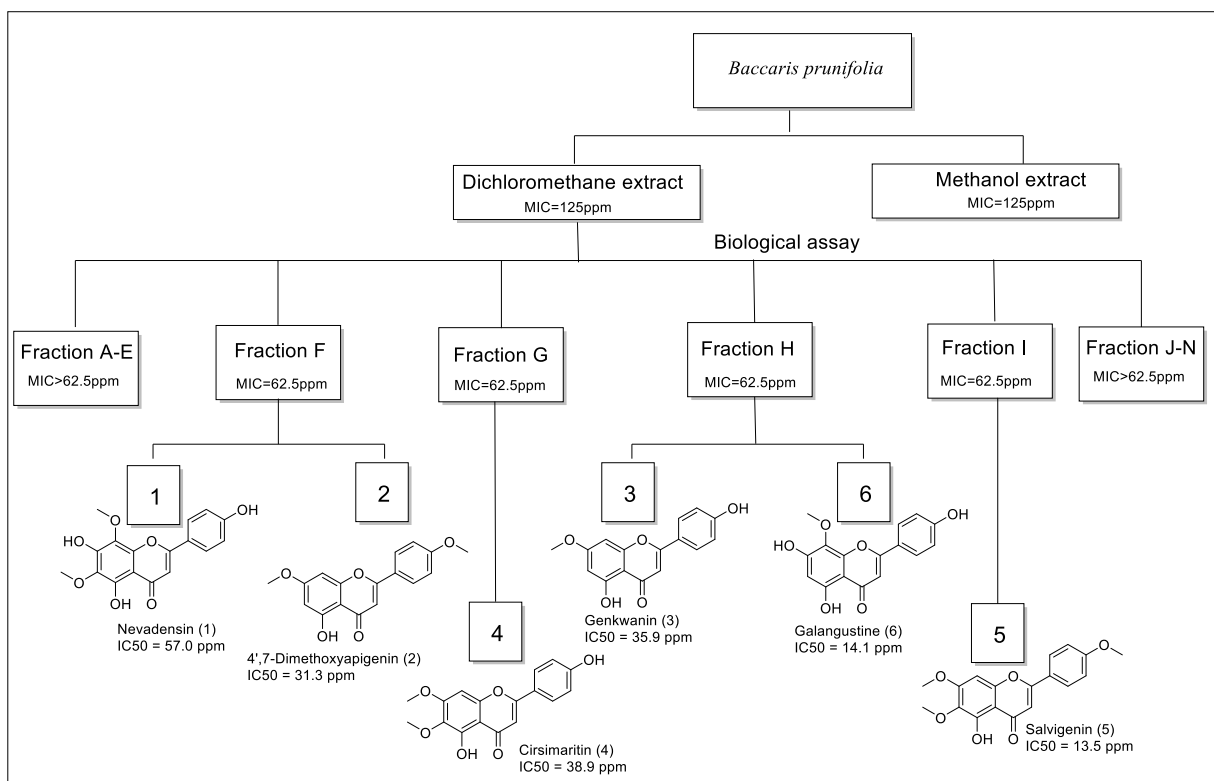


Figure SI- 1: Scheme of the bio-guided isolated compounds from *Baccharis prunifolia*.

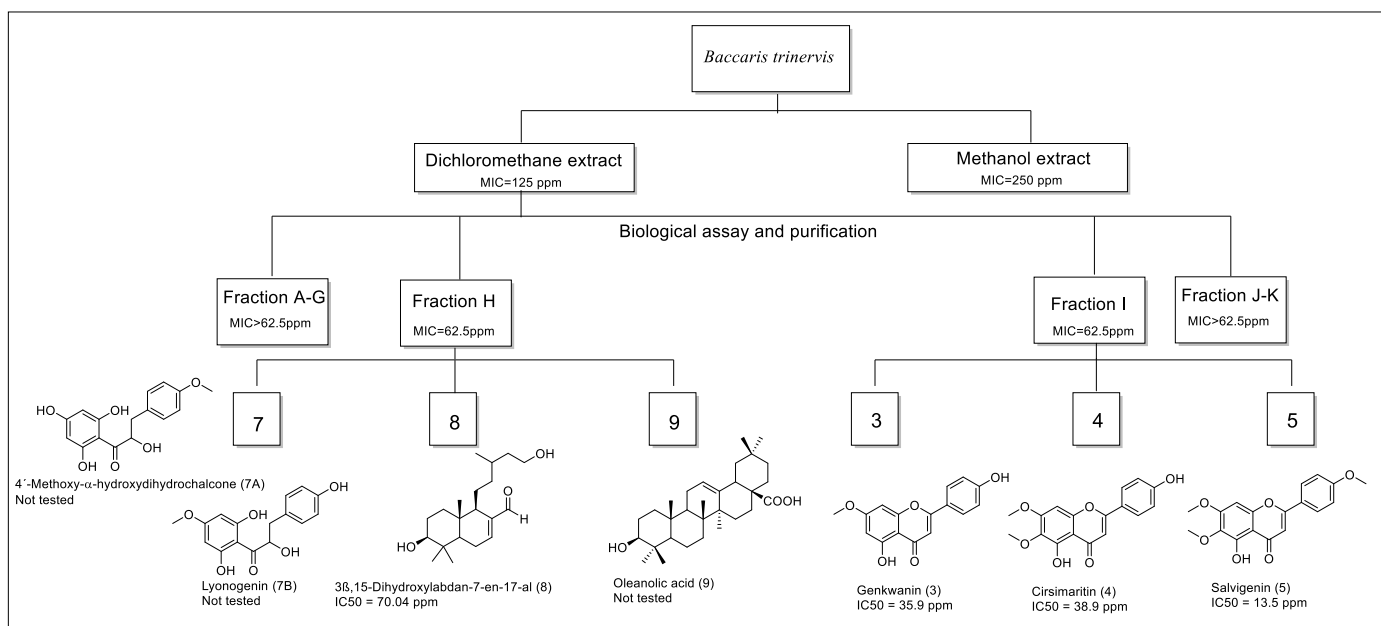


Figure SI- 2: Scheme of the bio-guides isolated compounds from *Baccharis trinervis*.

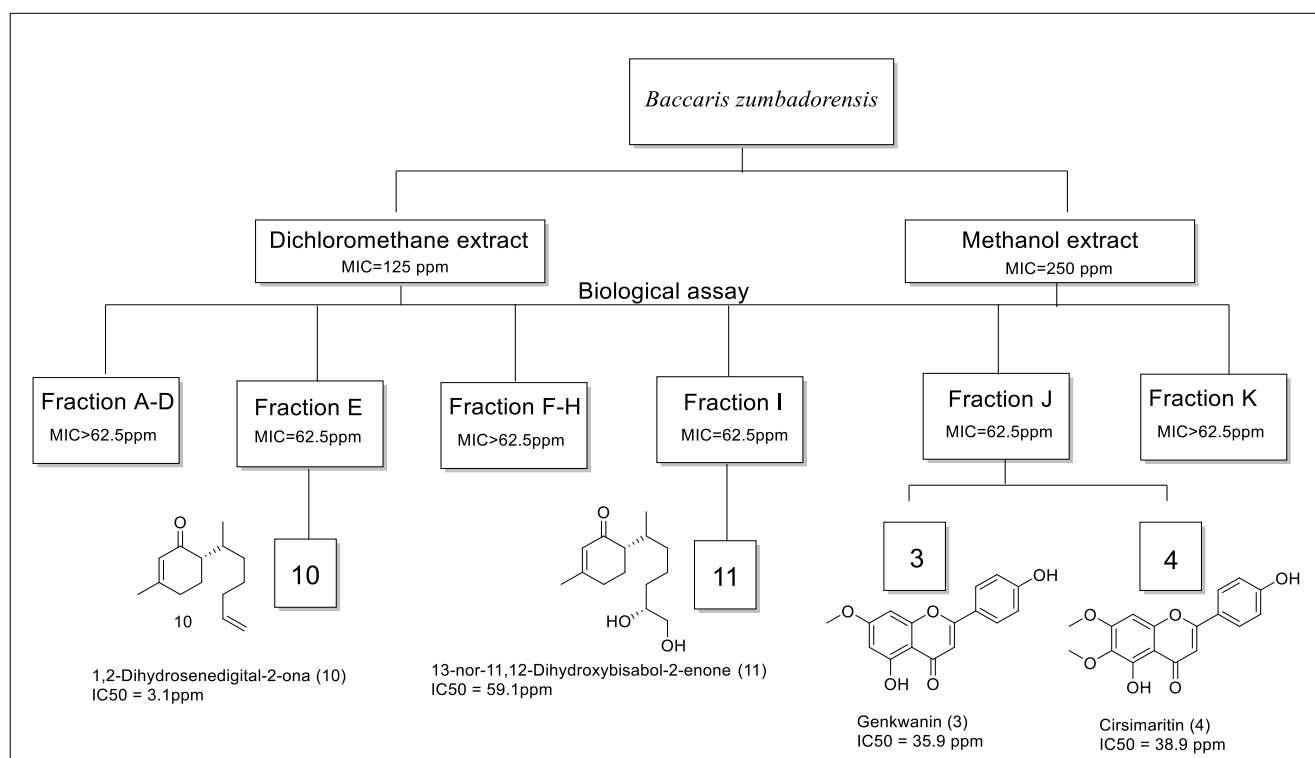
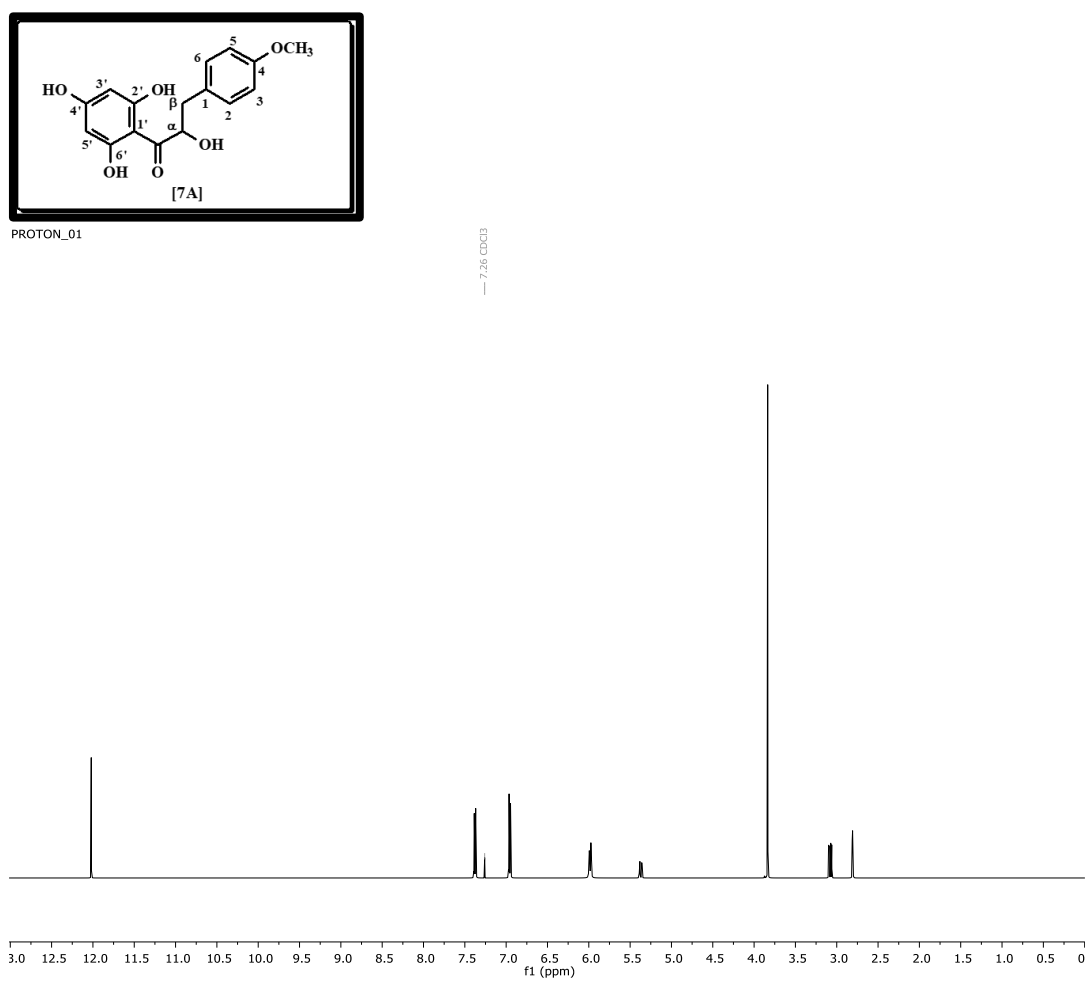


Figure SI- 3: Scheme of the bio-guided isolated compounds from *Baccharis Zumbadorensis*.

1- NMR spectroscopic data



CARBON_01

— 77.00 CDCl₃

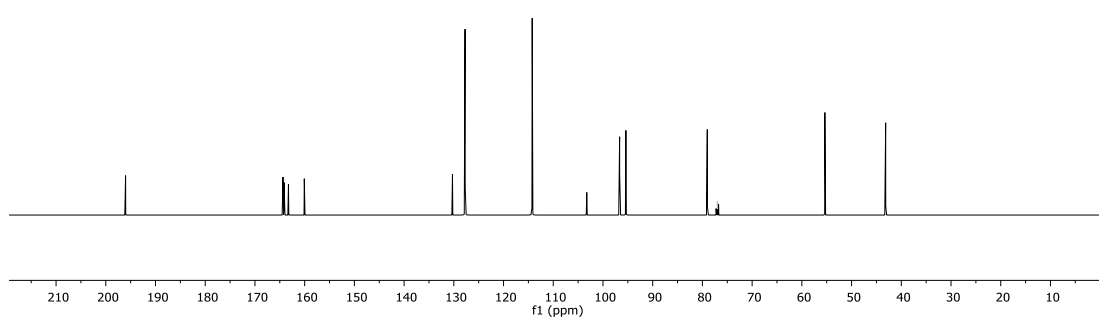


Figure SI- 5: ¹³C-NMR spectrum of compound **7A** in CDCl₃ (100MHz).

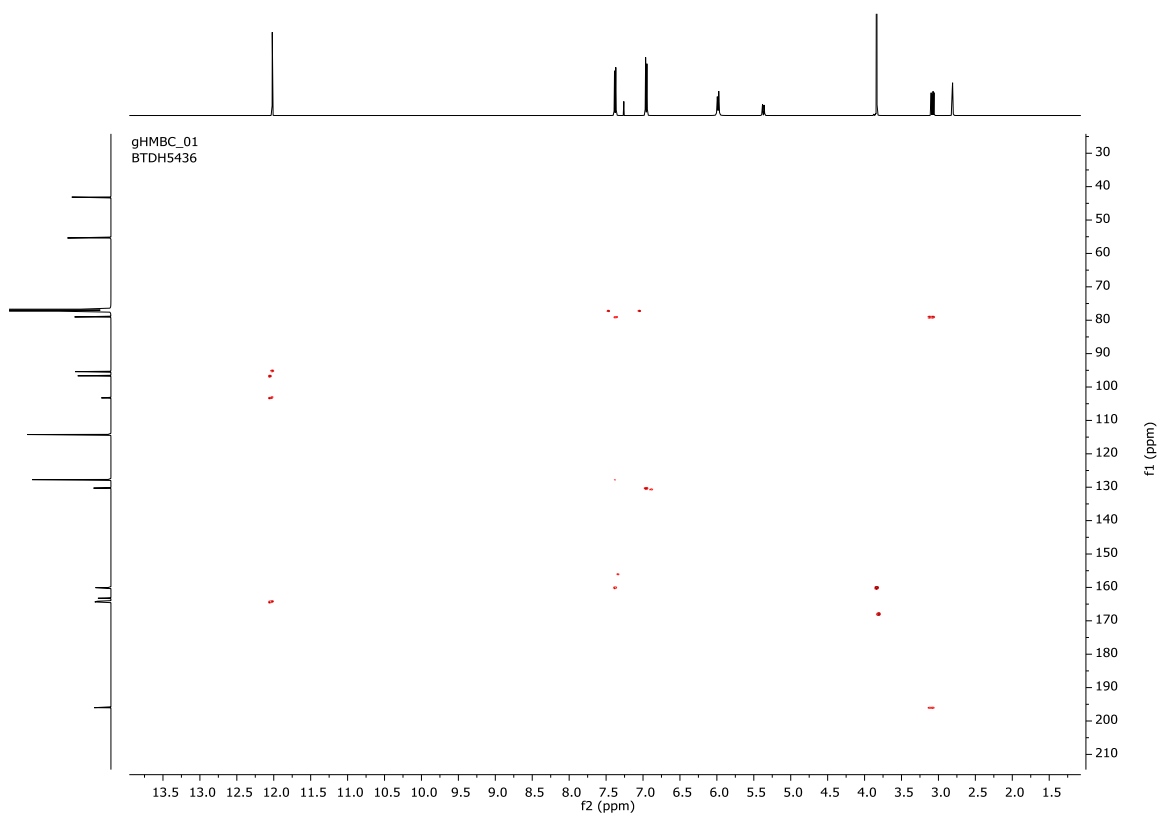


Figure SI- 6: gHMBC spectrum of compound **7A** in CDCl₃.

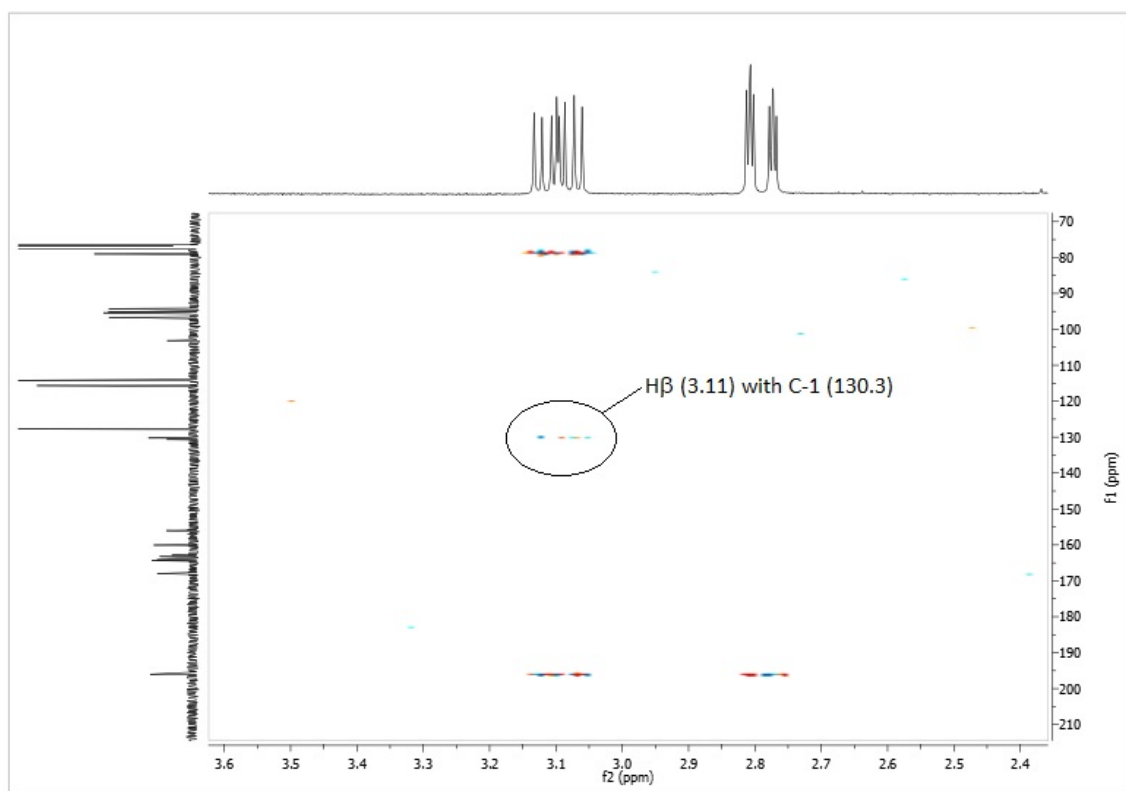


Figure SI-6a: gHMBC spectrum of compound **7A**; Correlation between H-1 (3.11) and C1 (130,3) in compound **7A**.

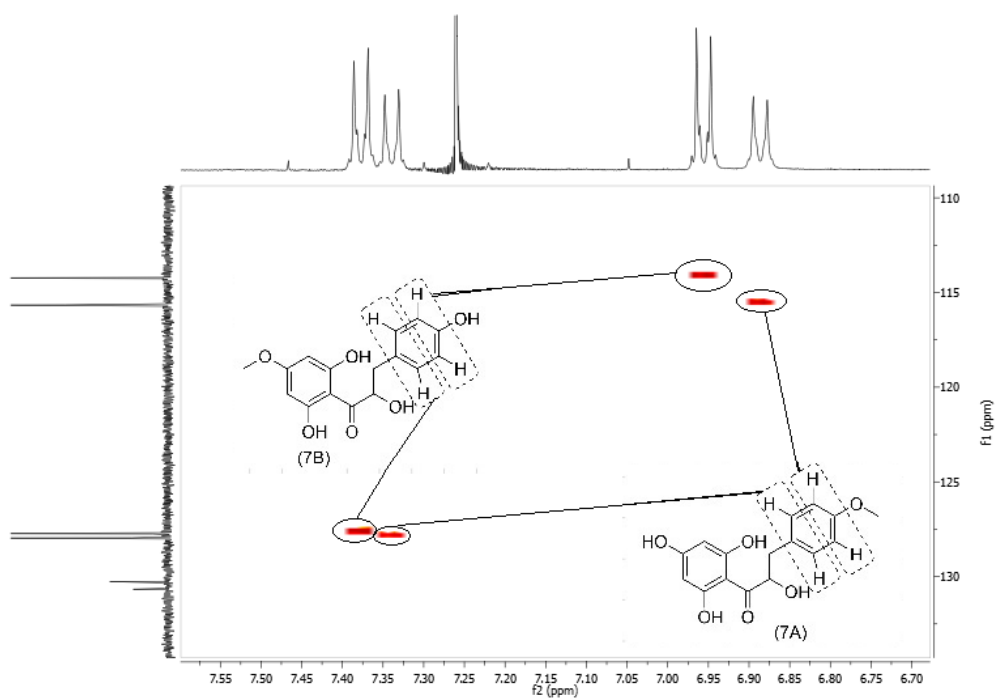


Figure SI-6b: gHMBC spectrum of compound **7A**; Correlation between H2/H6 with C2/C6 and H3/H5 with C3/C5 in compounds **7A** and **7B**.

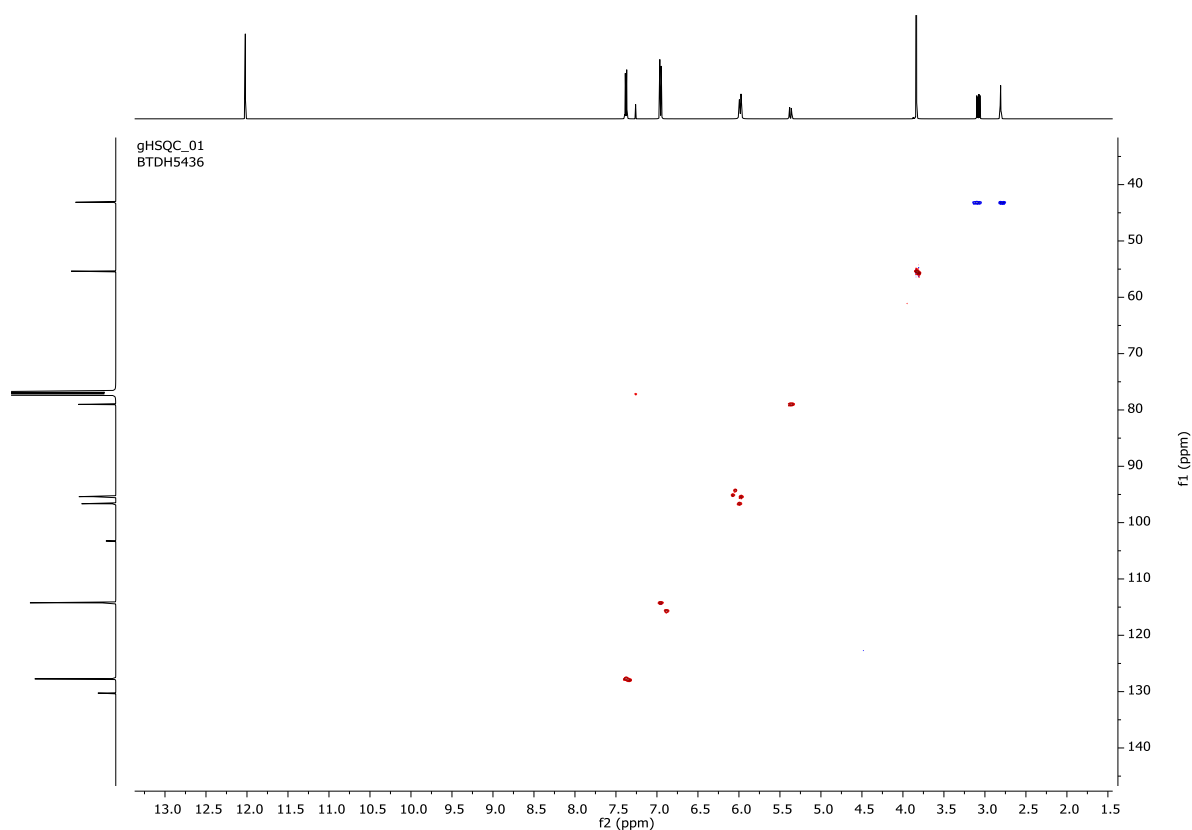


Figure SI- 7: gHSQC spectrum of compound **7A** in CDCl_3 .

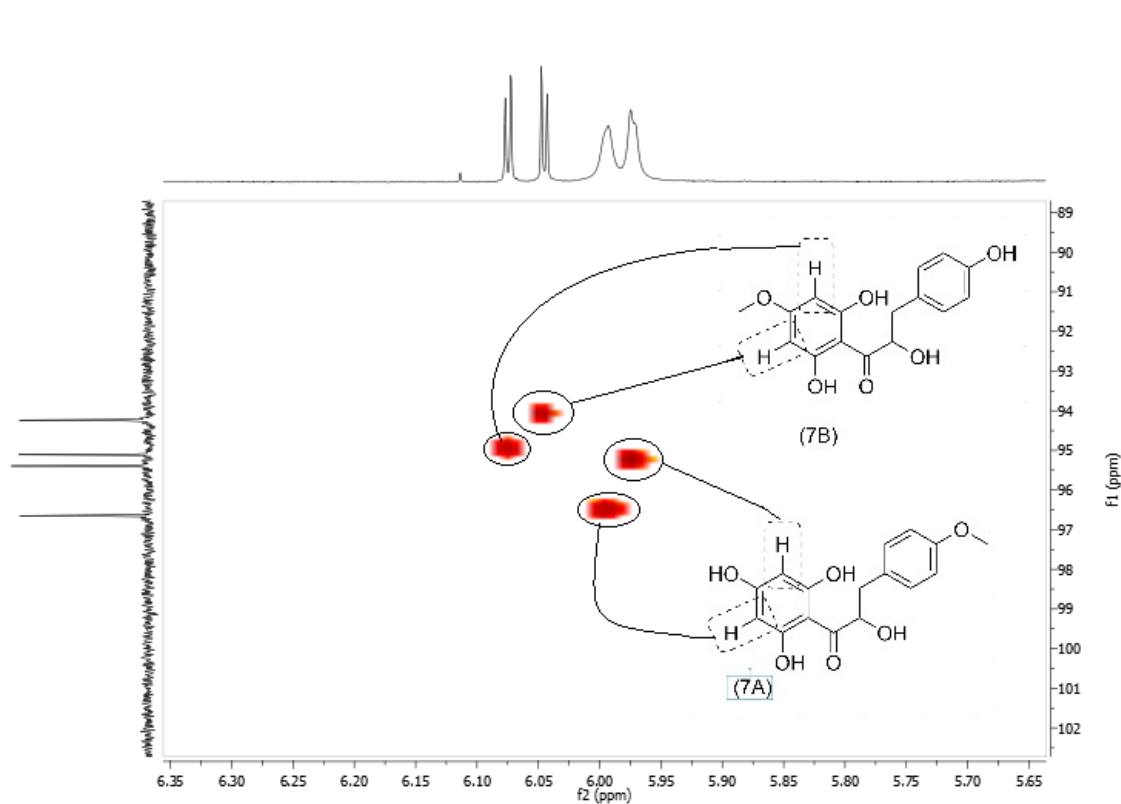


Figure SI- 7a: gHSQC spectrum of compound **7A**;HSQC correlations between H3'(5.99) with C3' (96.65) and H5'(5.98) with C5' (95.32) in compound **7A** and correlations between H3'(6.08) with C3' (95.09) and H5'(6.05) with C5' (94.19) in compound **7B**.

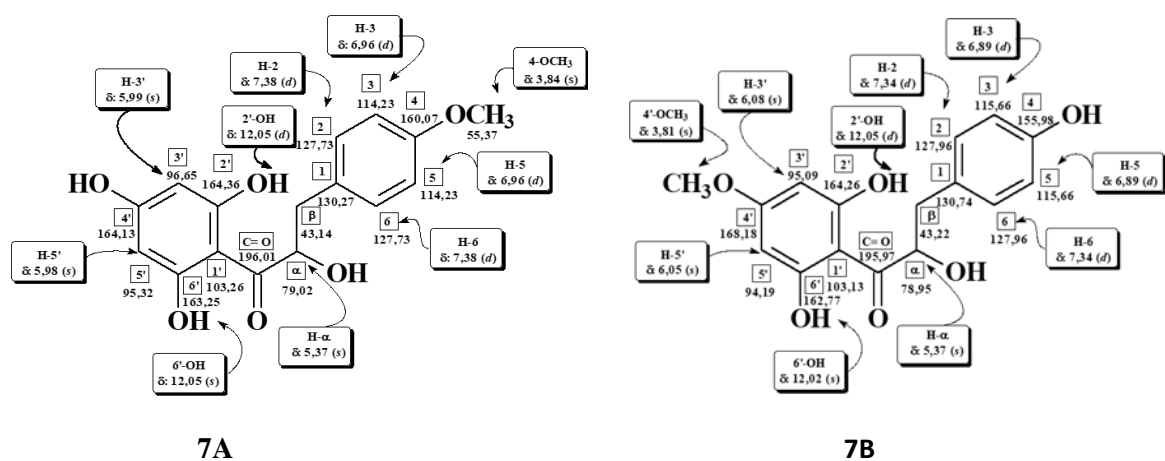
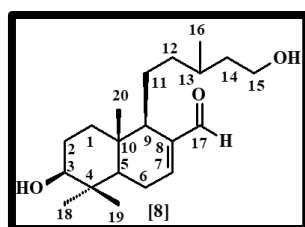


Figure SI- 7b: gHSQC correlations in **7A** and **7B**.



PROTON_01
Gradient Shimming

— 7.26 CDCl₃

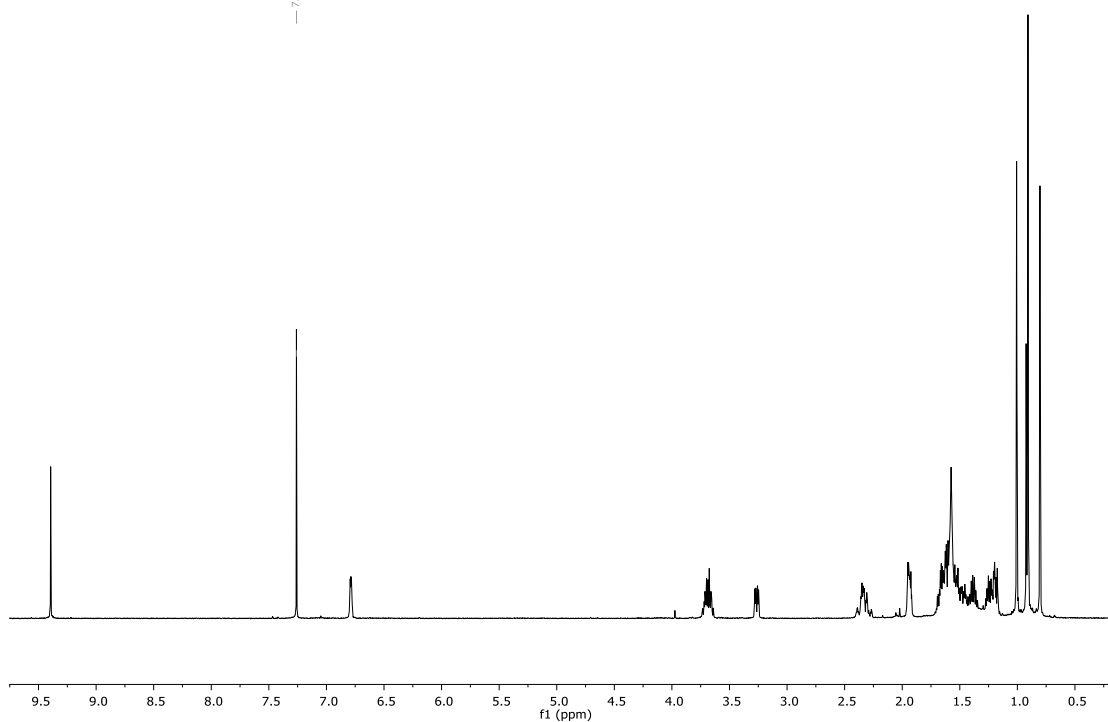


Figure SI- 8: ¹H-NMR spectrum of compound **8** in CDCl₃ (400MHz).

CARBON_01
Gradient Shimming

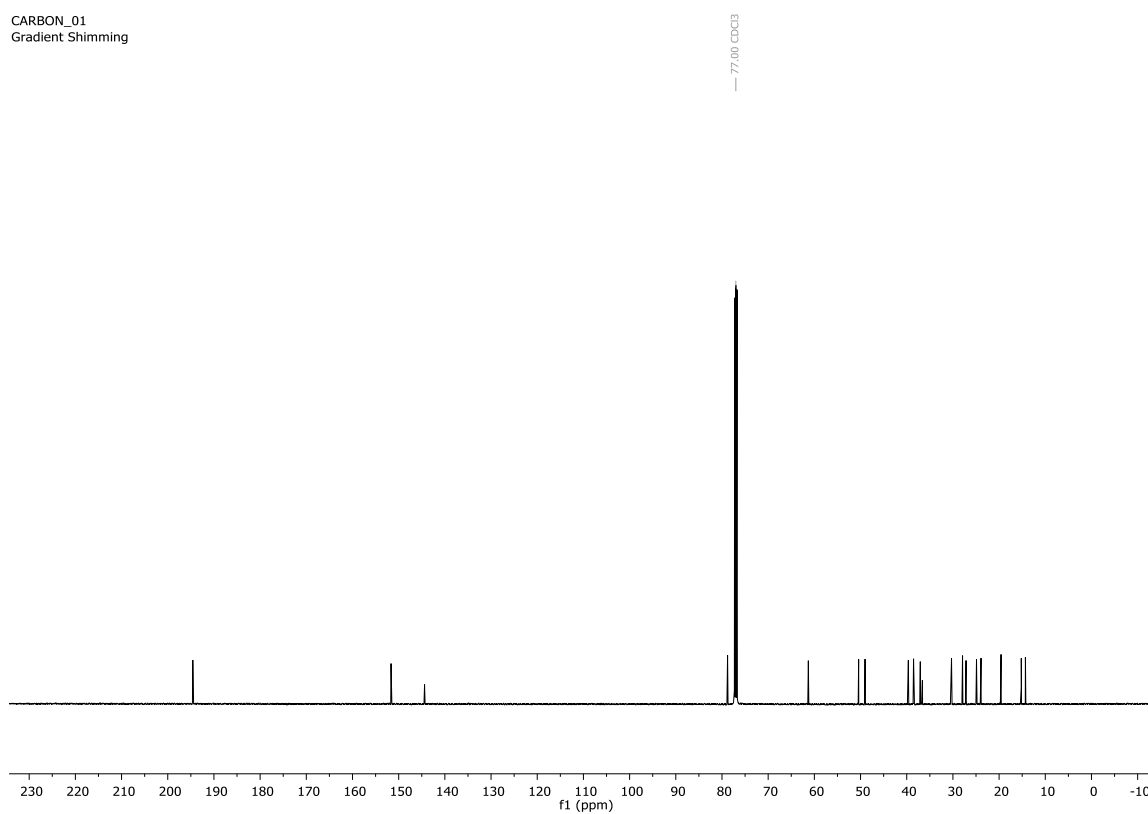


Figure SI- 9: ^{13}C - NMR spectrum of compound **8** in CDCl_3 (100MHz).

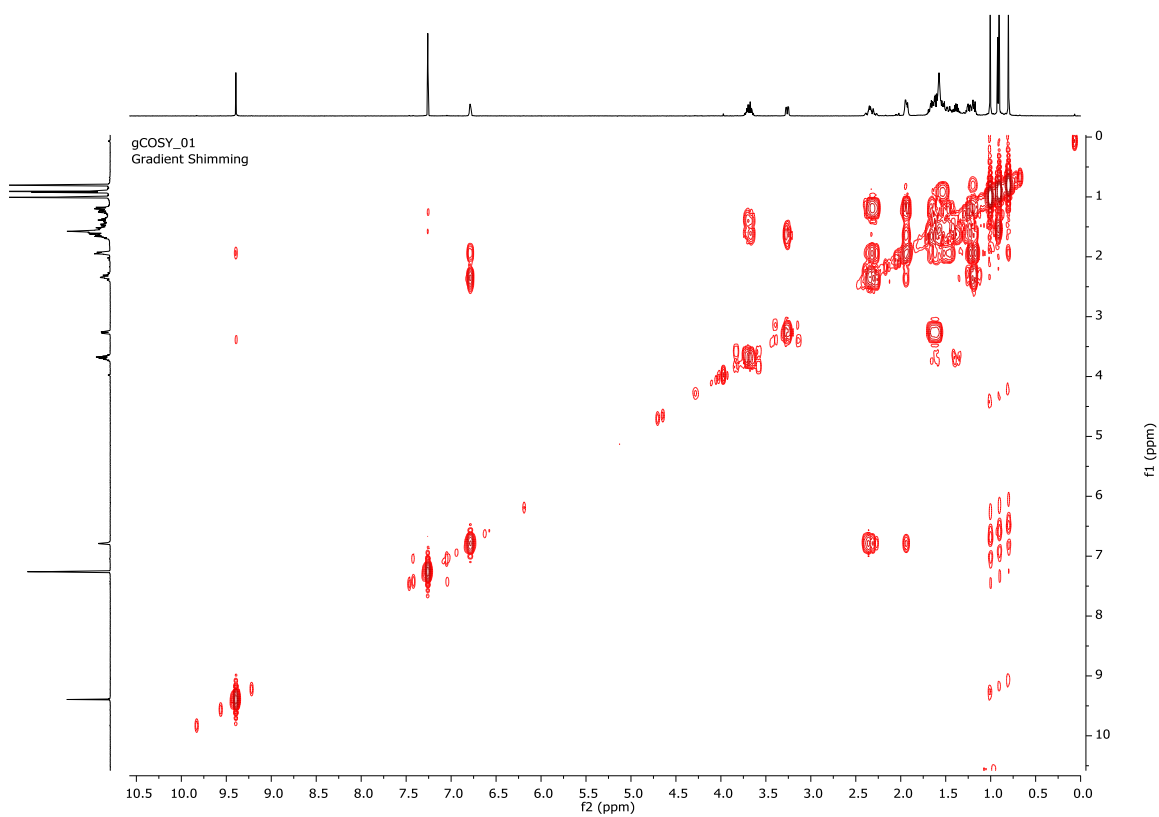


Figure SI-10: gCOSY spectrum of compound **8** in CDCl_3 (400MHz).

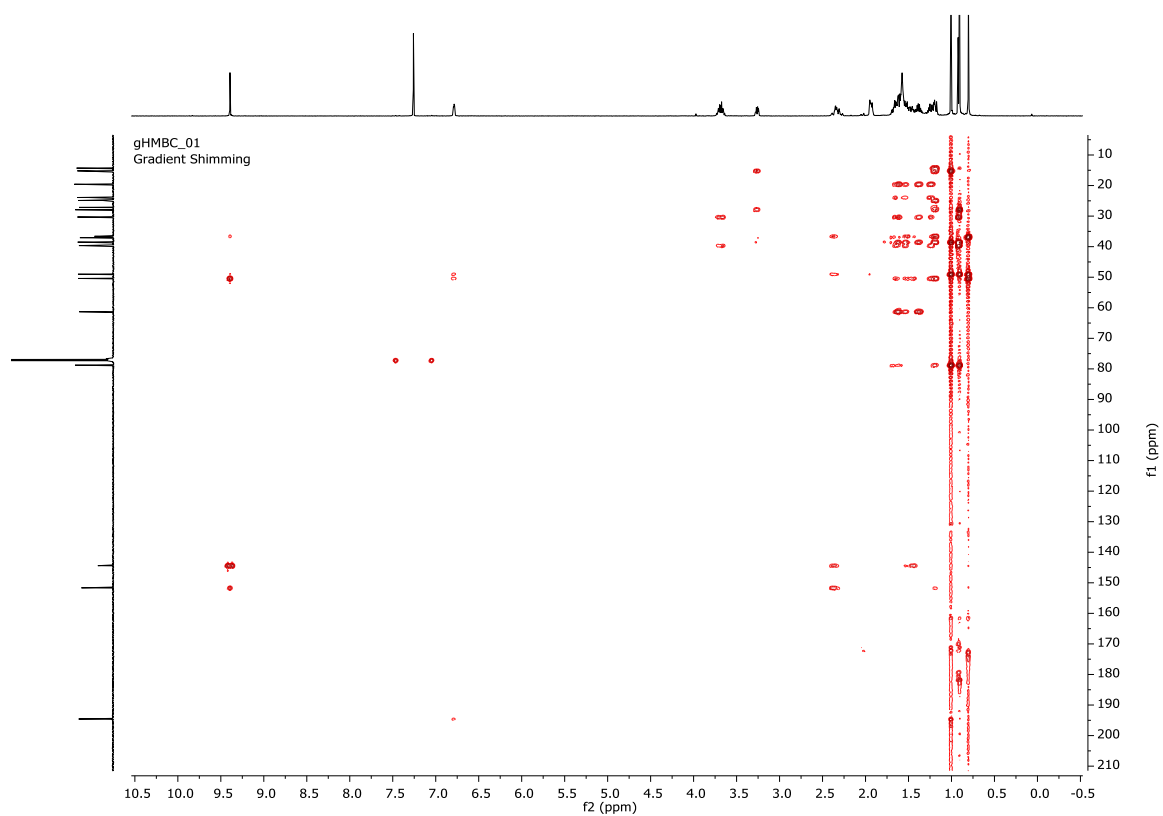


Figure SI-11: gHMBC spectrum of compound **8** in CDCl_3 .

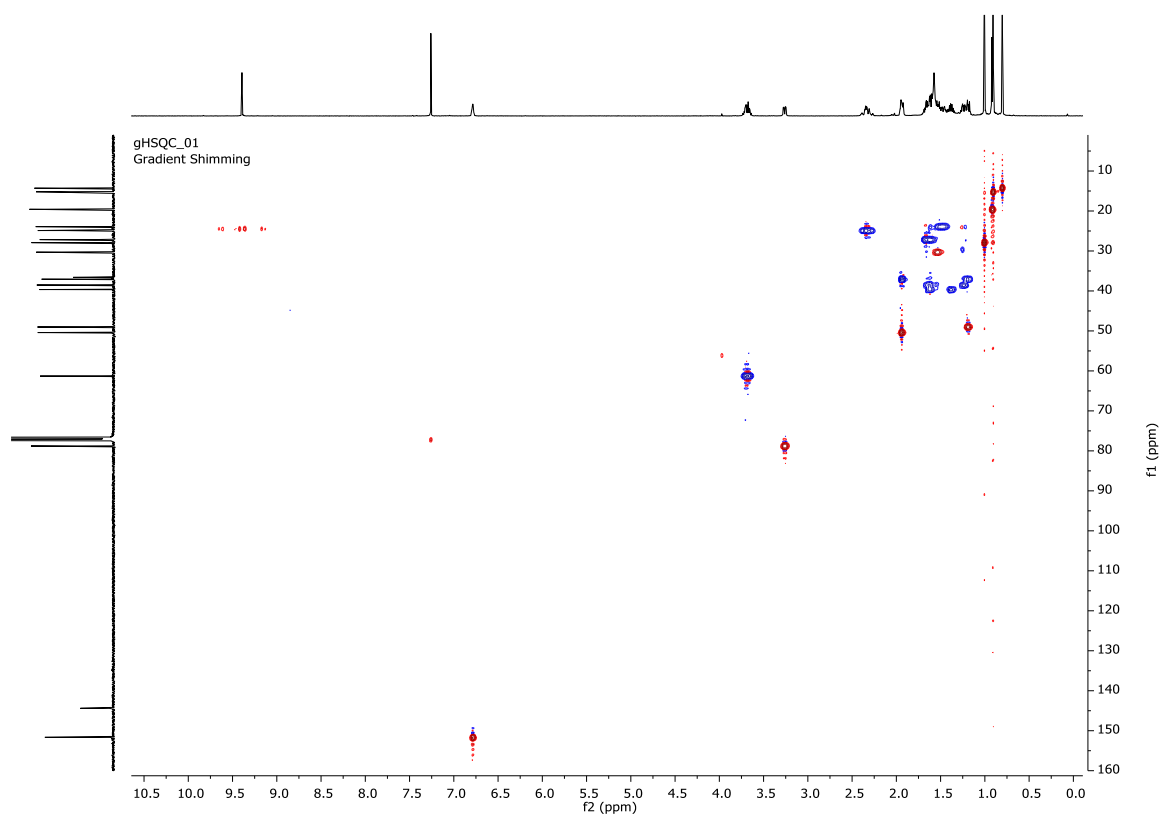
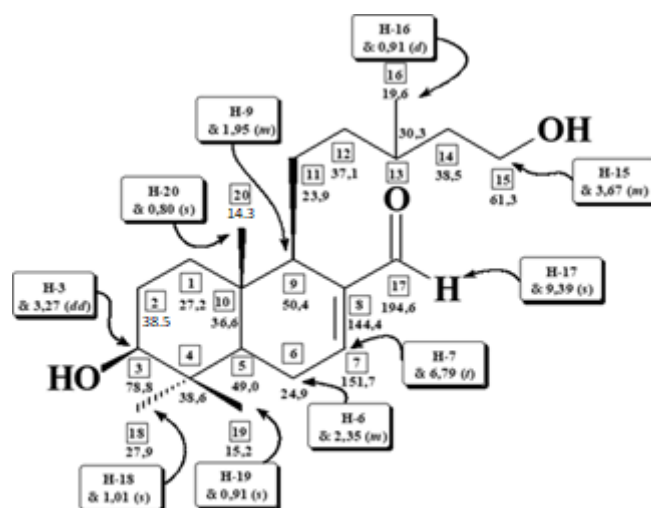


Figure SI-12: gHSQC spectrum of compound **8** in CDCl_3 .



8

Figure SI- 12a: gHSQC correlations of compound **8**.

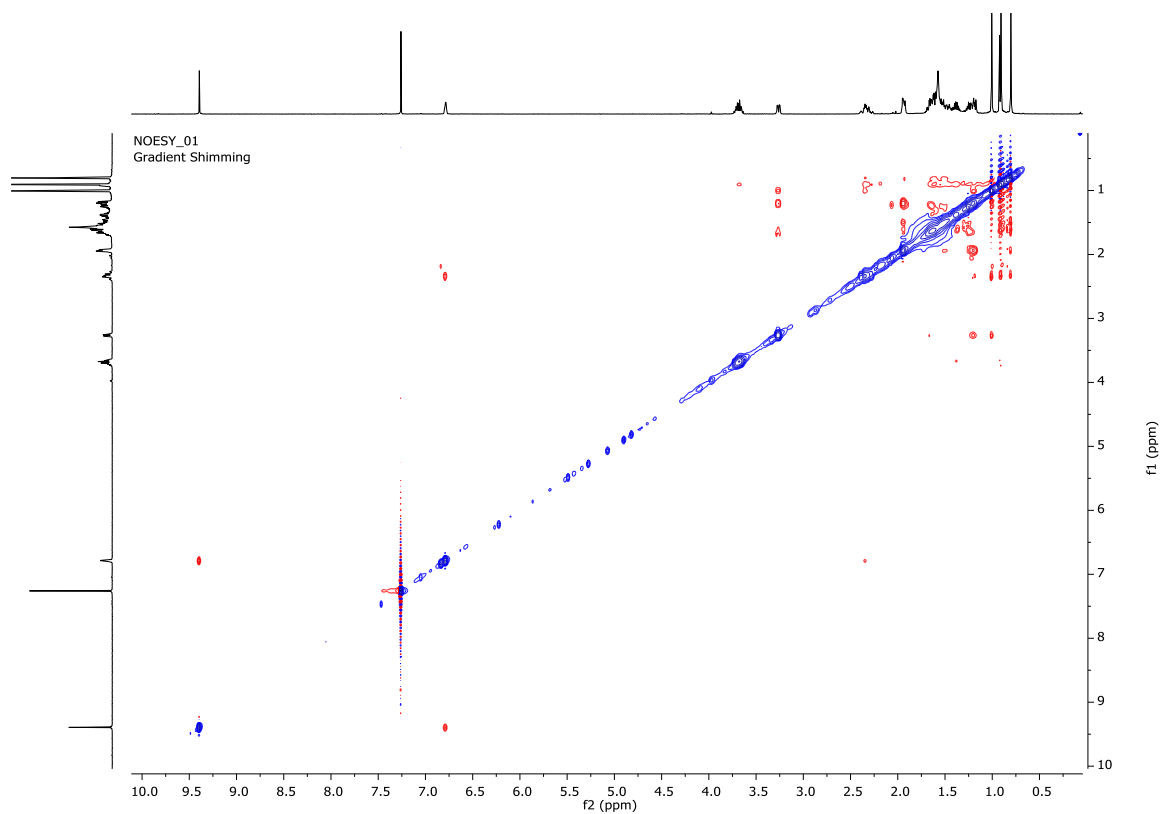


Figure SI-13: NOESY spectrum of compound **8** in CDCl₃.

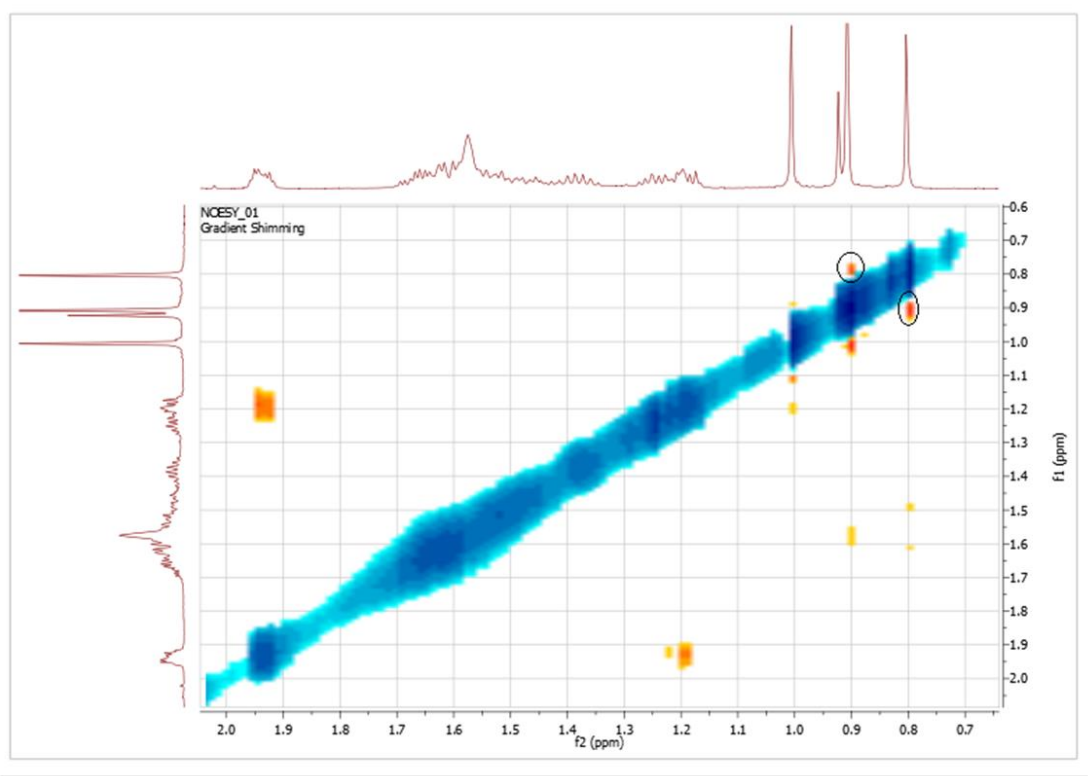
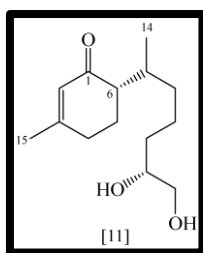


Figure SI-13a: NOESY spectrum of compound **8**; Correlation between H19 and H20.



PROTON_03
Gradient Shimming

7.26

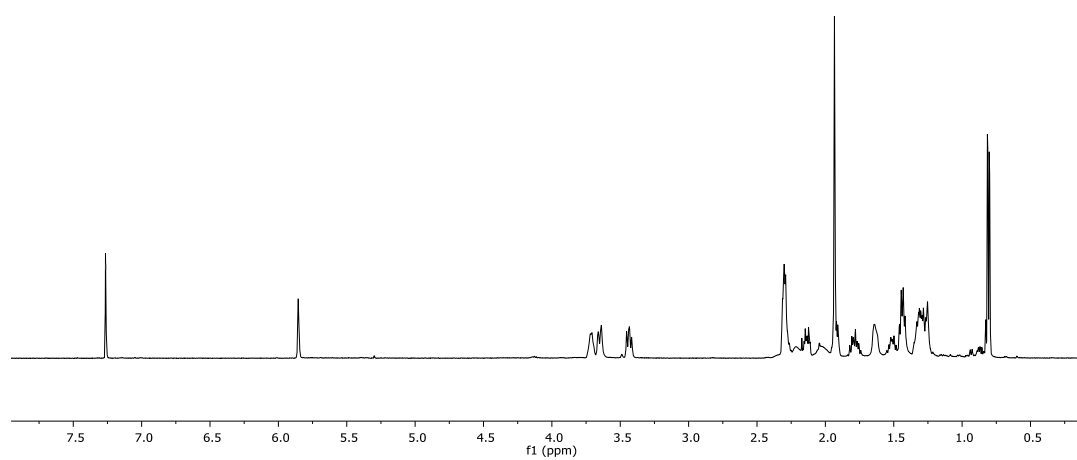


Figure SI-14: ^1H -NMR spectrum of compound **11** in CDCl_3 (400MHz).

CARBON_01
Gradient Shimming

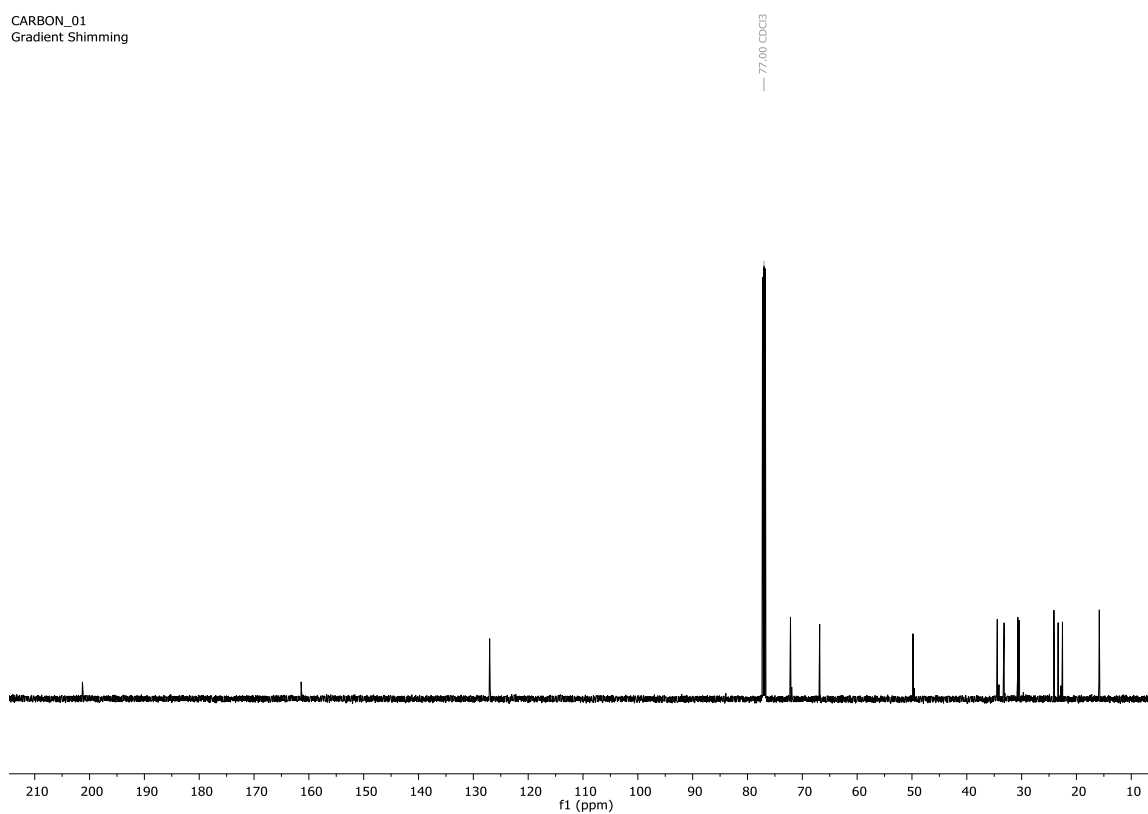


Figure SI-15: ^{13}C - NMR spectrum of compound **11** in CDCl_3 (100MHz).

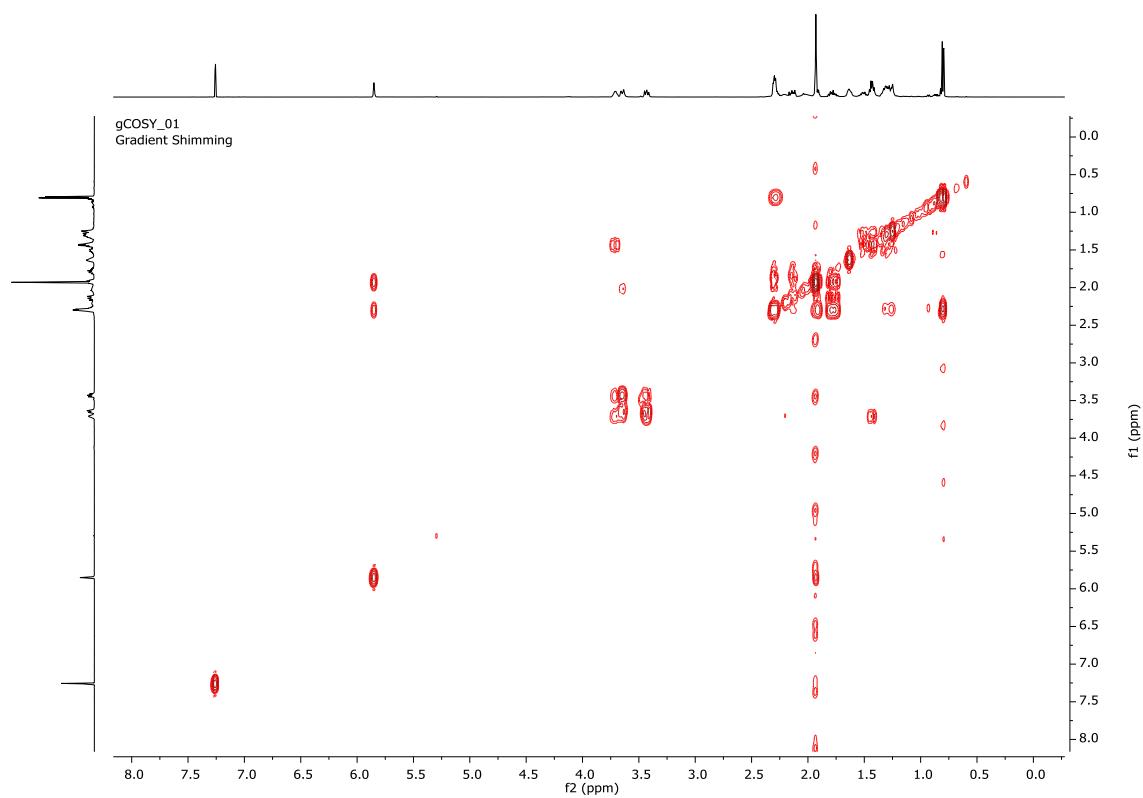


Figure SI-16: gCOSY spectrum of compound **11** in CDCl_3 .

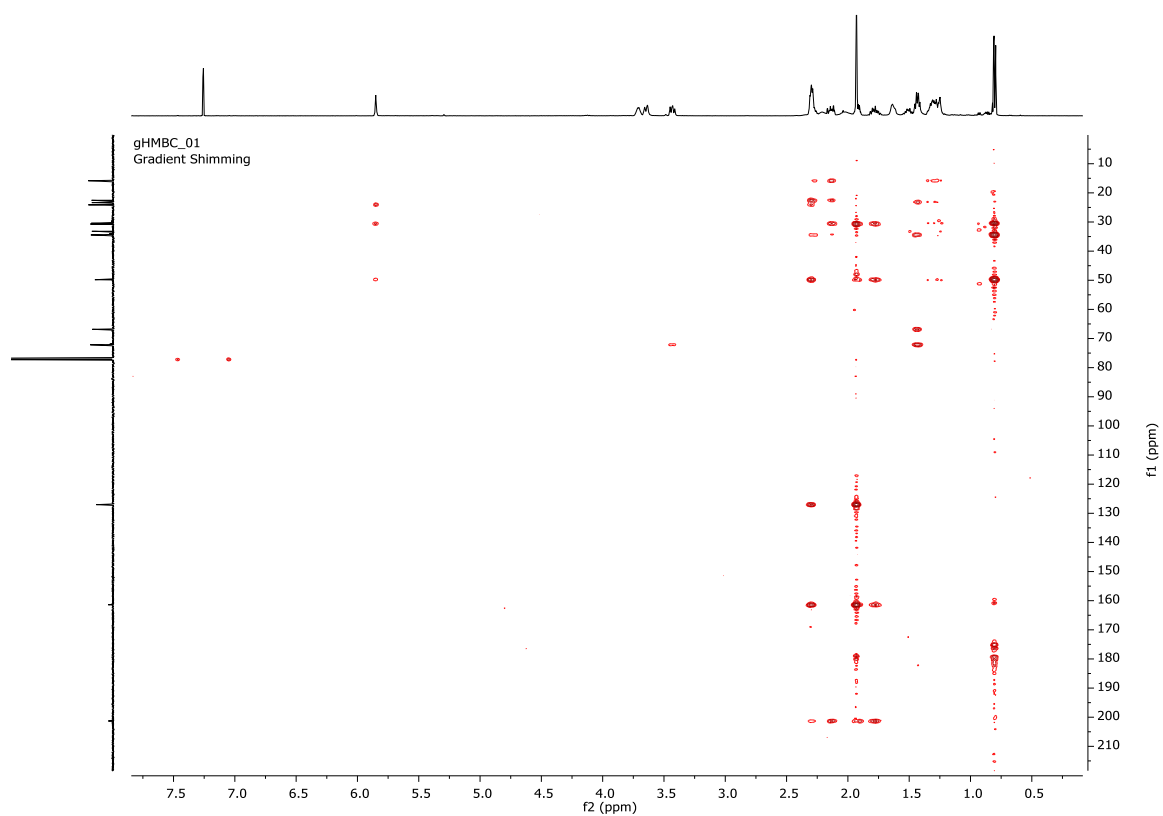


Figure SI-17: gHMBC spectrum of compound **11** in CDCl_3 .

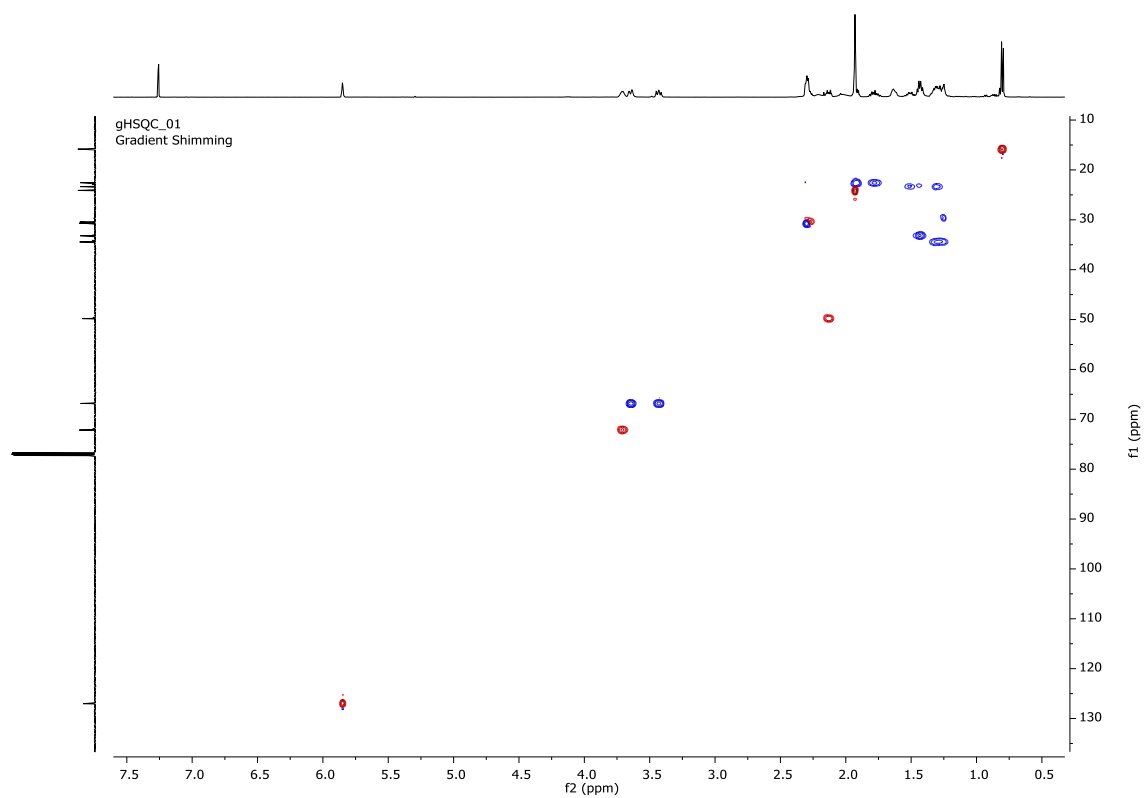


Figure SI-18: gHSQC spectrum of compound **11** in CDCl_3 .

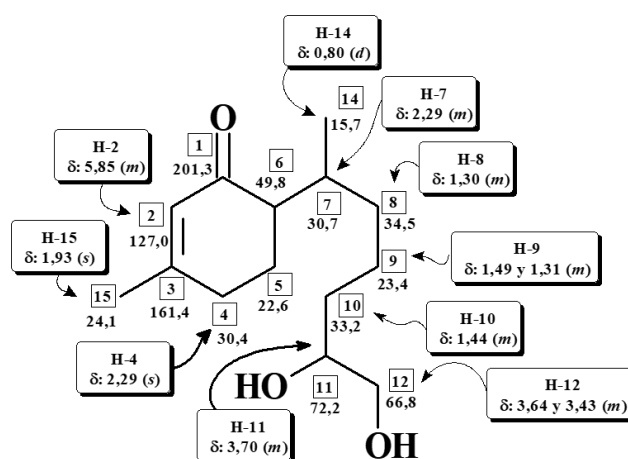
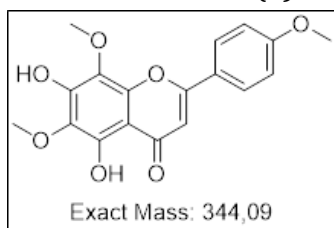


Figure SI-18a: gHSQC correlations of compound 11.

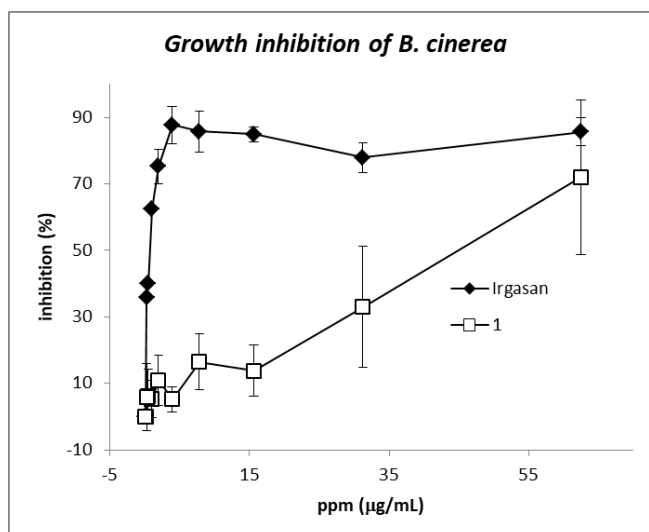
2- Antifungal activity against *Botrytis cinerea* UCA 992.

Microplate bioassay. Compound 1, 2, 3, 4, 5, 6, 8, 10 and 11

SI- 19- Nevadensin (1).



IC₅₀ (ppm)	57.03
EC ₅₀ Lower (ppm)	27.51
EC ₅₀ Upper (ppm)	118.2
IC₅₀ (μM)	165.70
EC ₅₀ Lower (μM)	80,0
EC ₅₀ Upper (μM)	343,5



Conc. (ppm)	62,50	31,25	15,63	7,81	3,91	1,95	0,98	0,49	0,24	0,12	0,06
Inhibition (%)	72,05	32,97	13,74	16,44	5,17	10,90	5,19	6,12	5,83	0,00	0,00
Standard deviation	23,30	18,21	7,72	8,46	3,68	7,65	5,63	8,06	10,10	0,00	0,00

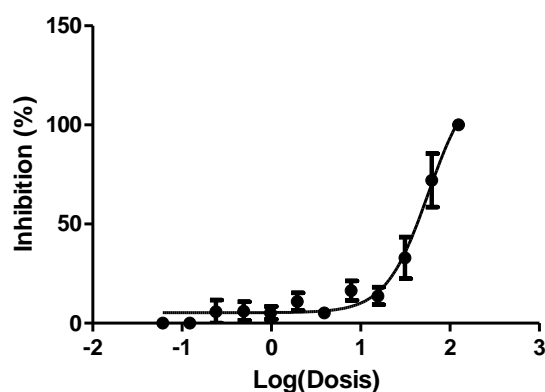
Log EC₅₀= 1.756

EC₅₀ = 57.03 ppm

EC₅₀ lower 95% confidence limit = 27.51 ppm

EC₅₀ upper 95% confidence limit = 118.2 ppm

Transform of Prune rows of Data 1

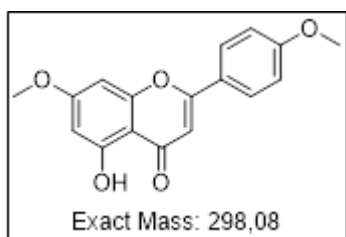


Error estandar LogEC₅₀=0.1551

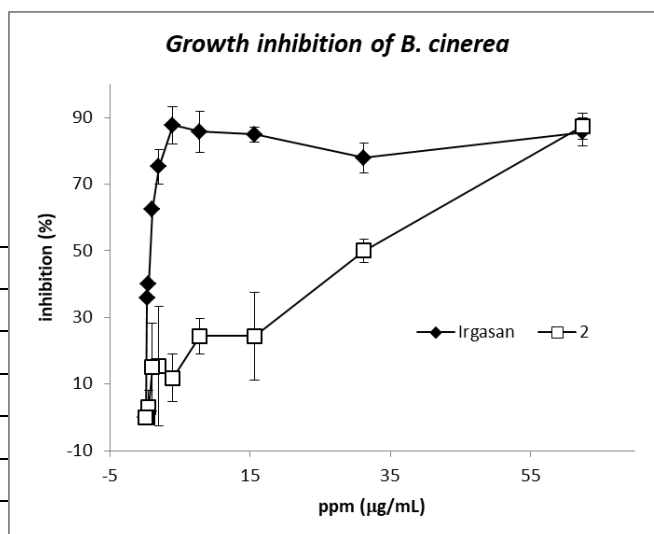
(debe ser <0.5; EC₅₀ valido)

R²=0.8659

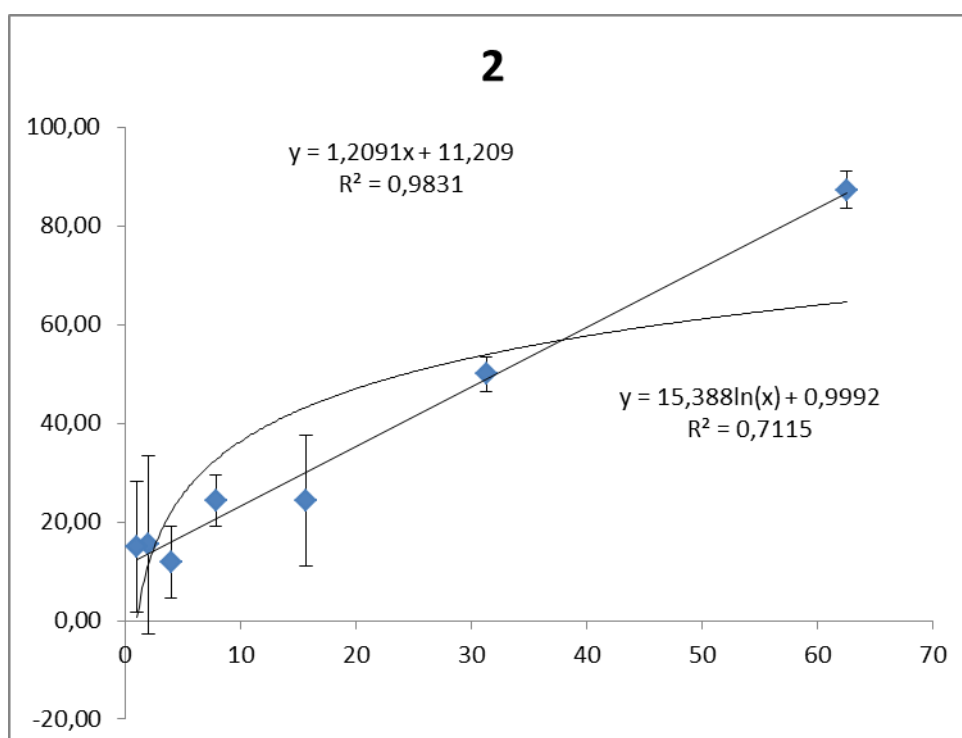
SI- 20- 4',7-Dimethoxyapigenin (2).



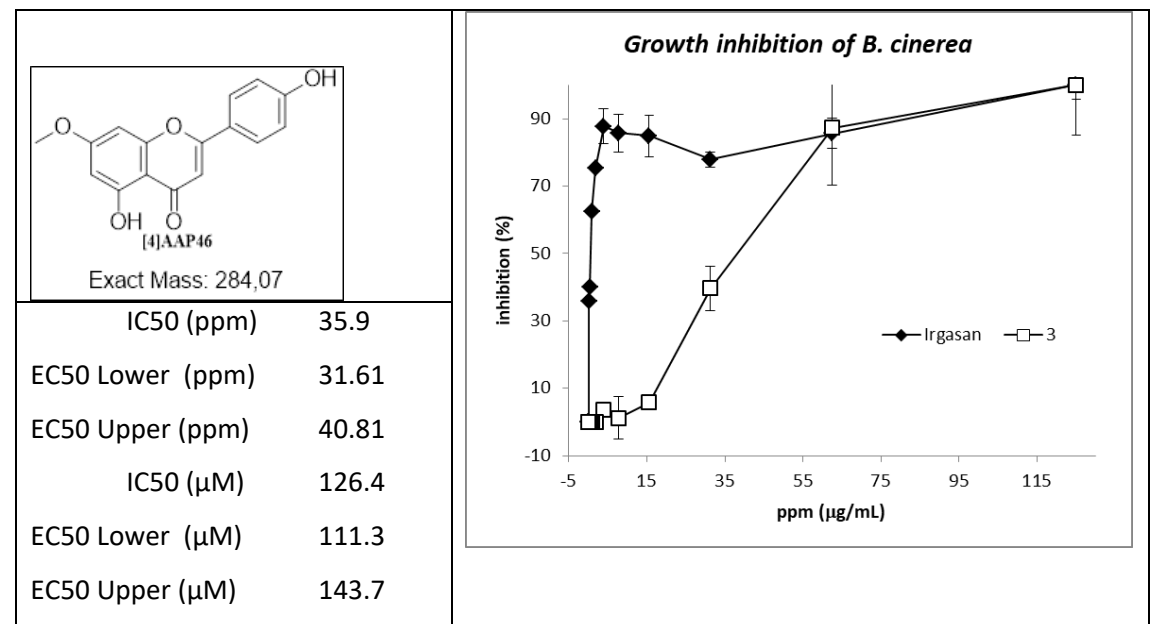
IC50 (ppm)	31.25
EC50 Lower (ppm)	
EC50 Upper (ppm)	
IC50 (μM)	104
EC50 Lower (μM)	
EC50 Upper (μM)	



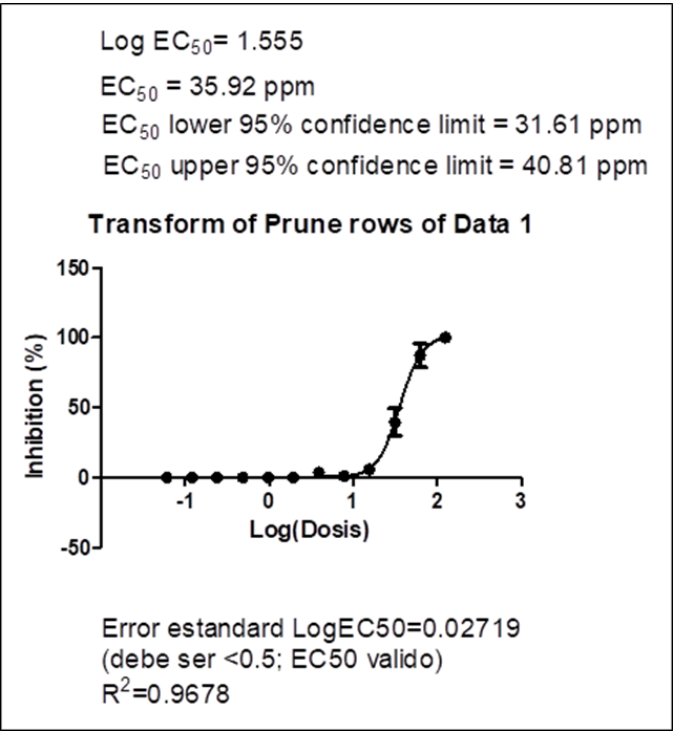
Conc. (ppm)	62,50	31,25	15,63	7,81	3,91	1,95	0,98	0,49	0,24	0,12	0,06
Inhibition (%)	87,42	49,98	24,35	24,34	11,85	15,38	15,10	2,94	0,00	0,00	0,00
Standard deviation	3,89	3,62	13,24	5,24	7,17	17,99	13,27	5,09	0,00	0,00	0,00



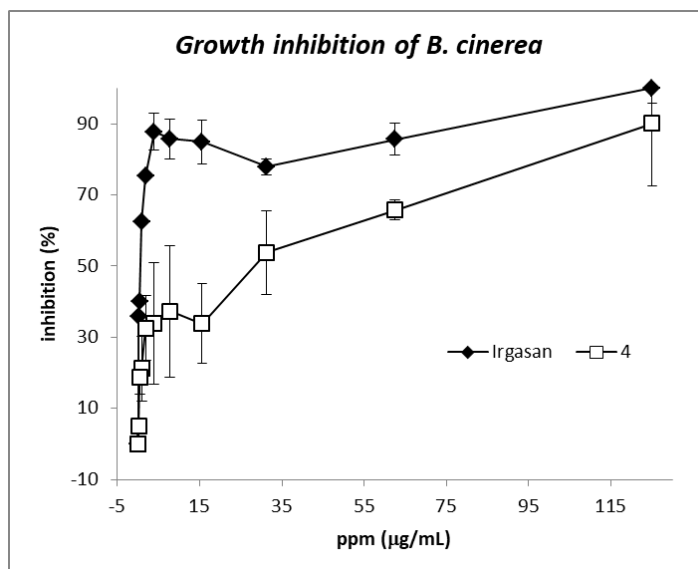
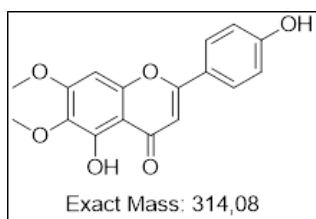
SI-21- Genkwanin (3).



Conc. (ppm)	62,50	31,25	15,6 3	7,81	3,91	1,95	0,98	0,49	0,24	0,12	0,06
Inhibition (%)	87,28	39,64	5,77	1,16	3,69	0,00	0,00	0,00	0,00	0,00	0,00
Standard deviation	14,74	17,09	6,53	2,02	6,39	0,00	0,00	0,00	0,00	0,00	0,00

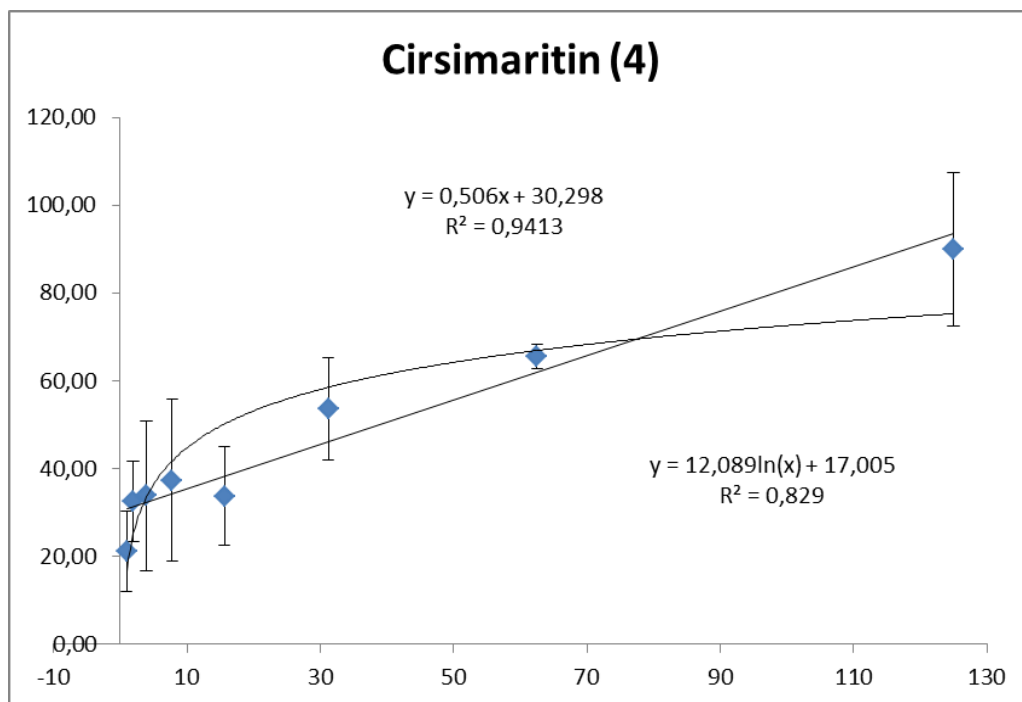


SI- 22- Cirsimaritin (4).

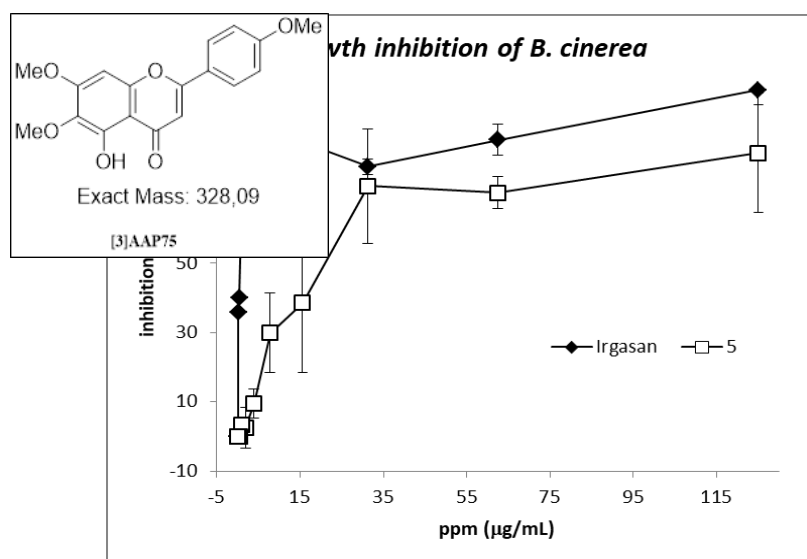


IC50 (ppm)	38.9
EC50 Lower (ppm)	
EC50 Upper (ppm)	
IC50 (μM)	123.9
EC50 Lower (μM)	
EC50 Upper (μM)	

Conc. (ppm)	62,50	31,25	15,63	7,81	3,91	1,95	0,98	0,49	0,24	0,12	0,06
Inhibition (%)	65,68	53,76	33,84	37,32	33,86	32,60	21,21	18,73	4,95	0,00	0,00
Standard deviation	17,50	2,80	11,70	11,14	18,47	17,02	9,13	9,09	4,73	0,00	0,00

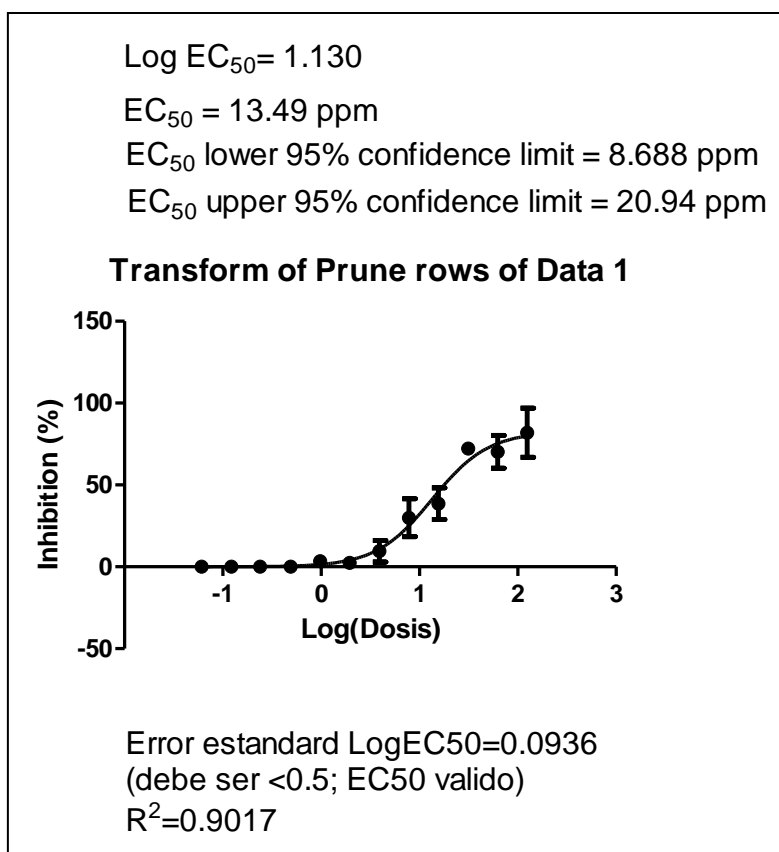


SI- 23- Salvigenin (5).

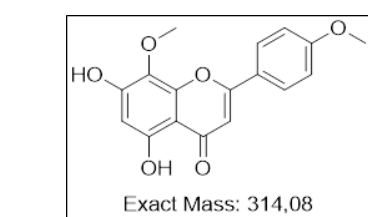


IC50 (ppm)	13.49
EC50 Lower (ppm)	8.69
EC50 Upper (ppm)	20.94
IC50 (μM)	41.1
EC50 Lower (μM)	26.5
EC50 Upper (μM)	63.8

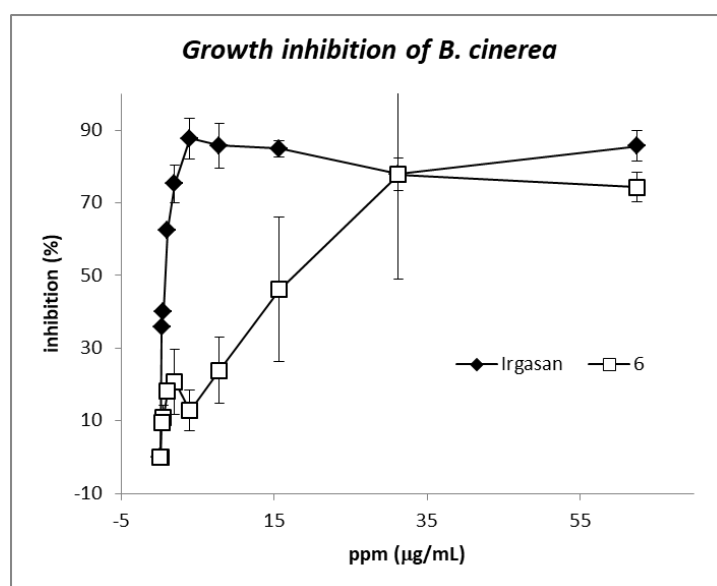
Conc. (ppm)	62,50	31,25	15,63	7,81	3,91	1,95	0,98	0,49	0,24	0,12	0,06
Inhibition (%)	70,31	72,27	38,61	29,94	9,56	2,42	3,36	0,00	0,00	0,00	0,00
Standard deviation	17,35	4,60	16,65	20,08	11,41	4,19	5,81	0,00	0,00	0,00	0,00



SI- 24- Galangustin (6).



IC₅₀ (ppm)	14.06
EC ₅₀ Lower (ppm)	9.41
EC ₅₀ Upper (ppm)	21.01
IC₅₀ (μM)	44.8
EC ₅₀ Lower (μM)	30.0
EC ₅₀ Upper (μM)	66.9



Conc. (ppm)	62,50	31,25	15,63	7,81	3,91	1,95	0,98	0,49	0,24	0,12	0,06
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Inhibition (%)	74,32	77,75	46,17	23,89	12,78	20,79	18,14	10,97	9,54	0,00	0,00
Standard deviation	16,89	4,08	28,83	19,90	9,10	5,67	8,96	1,47	3,23	0,00	0,00

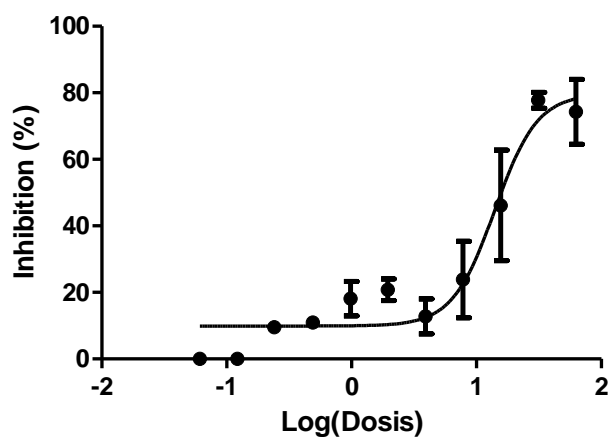
Log EC₅₀ = 1.148

EC₅₀ = 14.06 ppm

EC₅₀ lower 95% confidence limit = 9.408 ppm

EC₅₀ upper 95% confidence limit = 21.01 ppm

Transform of Prune rows of Data 1

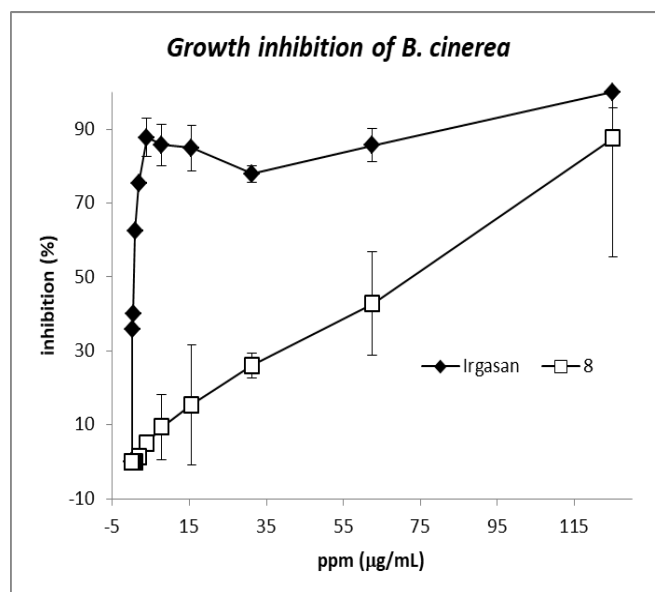
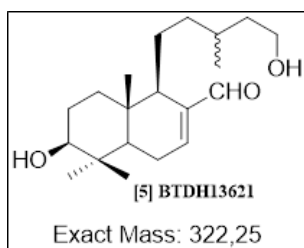


Error estandard LogEC₅₀=0.08533

(debe ser <0.5; EC₅₀ valido)

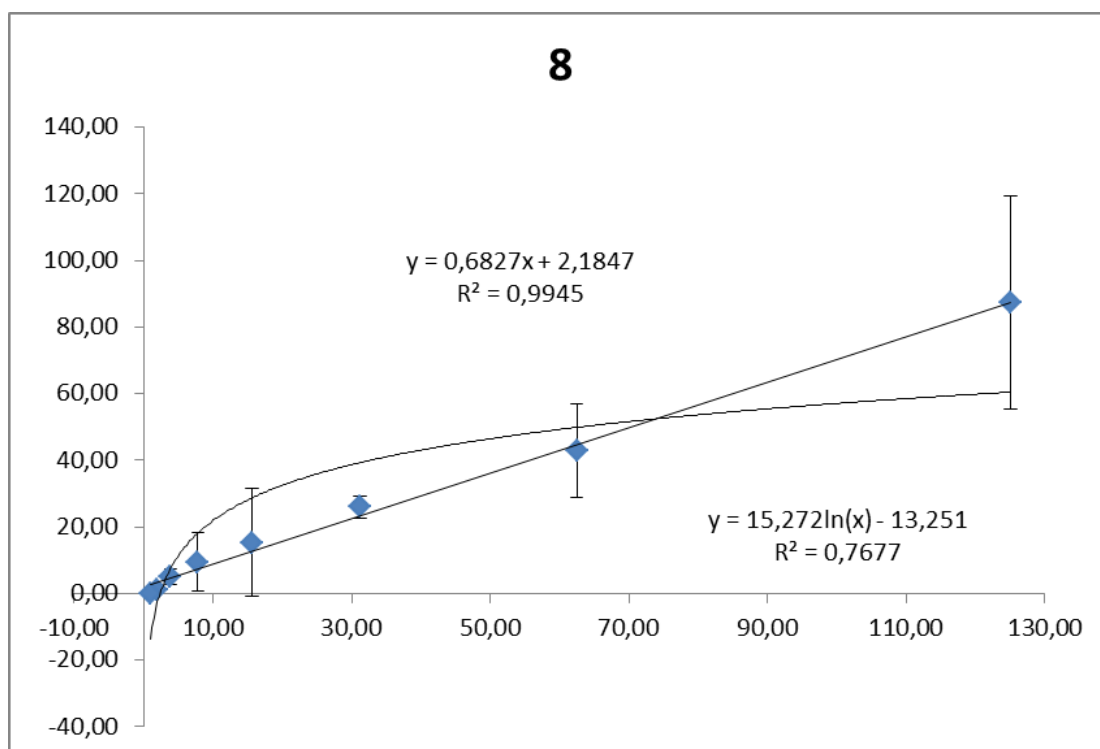
R²=0.8164

SI- 25- 3β,15-Dihydroxylabdan-7-en-17-al (8).

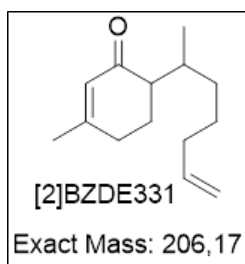


IC ₅₀ (ppm)	70.04
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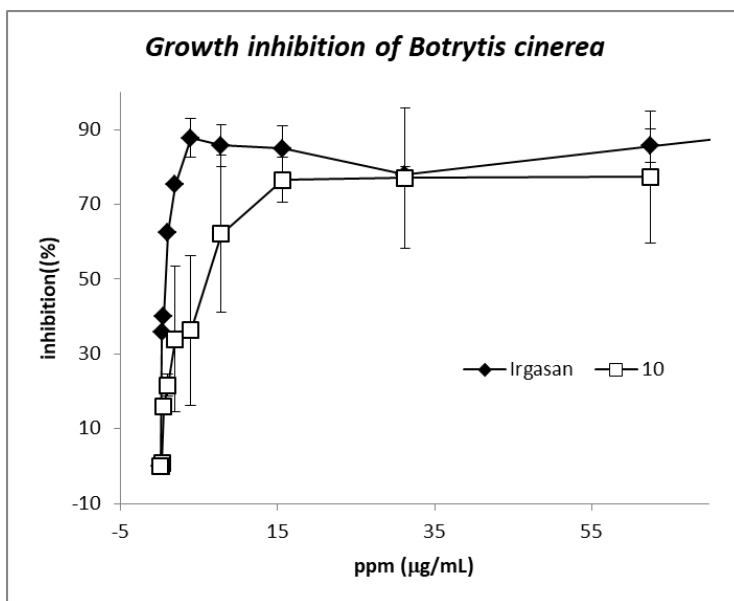
EC50 Lower (ppm)											
EC50 Upper (ppm)											
IC50 (μM)	246.6										
EC50 Lower (μM)											
EC50 Upper (μM)											
Conc. (ppm)	125,00	62,50	31,25	15,63	7,81	3,91	1,95	0,98	0,49	0,24	0,12
Inhibition (%)	87,54	42,80	26,03	15,38	9,37	5,07	1,30	0,00	0,00	0,00	0,00
Standard deviation	5,50	32,02	14,00	3,41	16,23	8,78	2,25	0,00	0,00	0,00	0,00



SI- 26- 1,2-Dyhidrosenedigital-2-ona (10).



IC₅₀ (ppm)	3.12
EC ₅₀ Lower (ppm)	1.36
EC ₅₀ Upper (ppm)	7.15
IC₅₀ (μM)	15.2
EC ₅₀ Lower (μM)	6.6
EC ₅₀ Upper (μM)	34.7



Conc. (ppm)	62,50	31,25	15,63	7,81	3,91	1,95	0,98	0,49	0,24	0,12	0,06
Inhibition (%)	77,31	77,05	76,58	62,14	36,31	33,94	21,62	15,94	0,66	0,00	0,00
Standard deviation	20,87	17,58	18,83	5,93	21,12	20,07	19,54	2,86	1,14	0,00	0,00

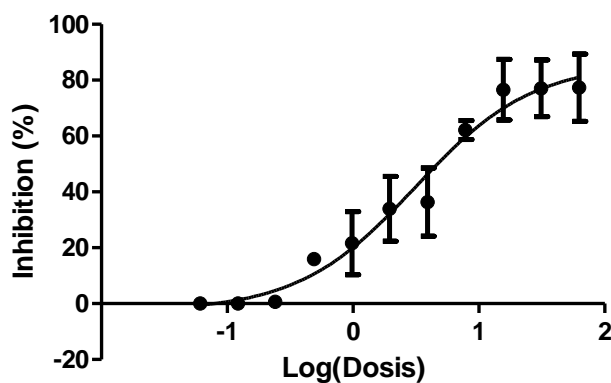
Log EC₅₀= 0.4949

EC₅₀ = 3.126 ppm

EC₅₀ lower 95% confidence limit = 1.365 ppm

EC₅₀ upper 95% confidence limit = 7.156 ppm

Transform of Prune rows of Data 1

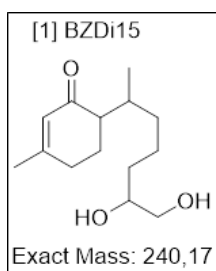


Error estandard LogEC₅₀=0.1759

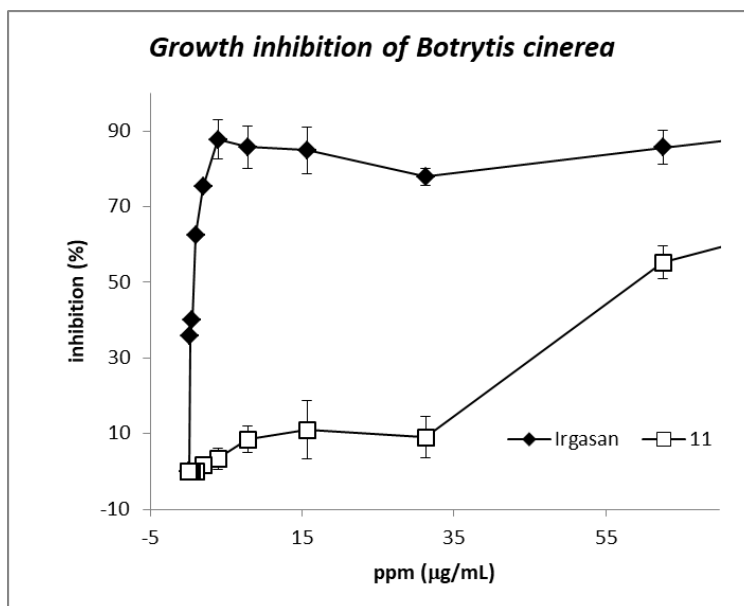
(debe ser <0.5; EC₅₀ valido)

R²=0.8468

SI- 27- 13-nor-11,12-Dihydroxybisabol-2-enone (11).



IC50 (ppm)	59.07
EC50 Lower (ppm)	53.79
EC50 Upper (ppm)	64.87
IC50 (μM)	246.0
EC50 Lower (μM)	224.0
EC50 Upper (μM)	270.1



Conc. (ppm)	125,00	62,50	31,25	15,63	7,81	3,91	1,95	0,98	0,49	0,24	0,12
Inhibition (%)	88,51	55,26	9,04	10,94	8,45	3,34	1,62	0,00	0,00	0,00	0,00
Standard deviation	5,04	11,33	4,32	5,57	7,76	3,57	2,81	0,00	0,00	0,00	0,00

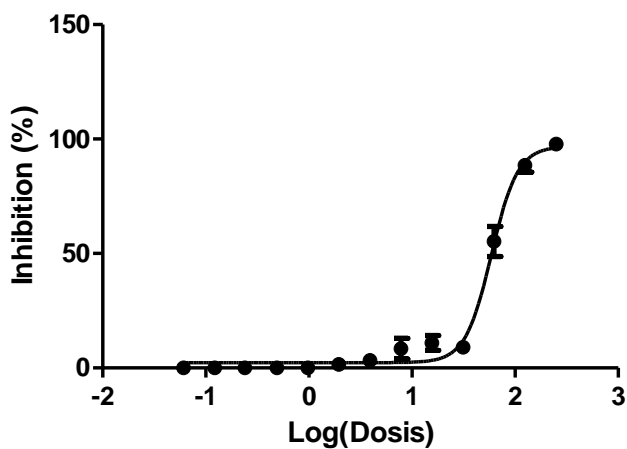
Log EC₅₀= 1.771

EC₅₀ = 59.07 ppm

EC₅₀ lower 95% confidence limit = 53.79 ppm

EC₅₀ upper 95% confidence limit = 64.87 ppm

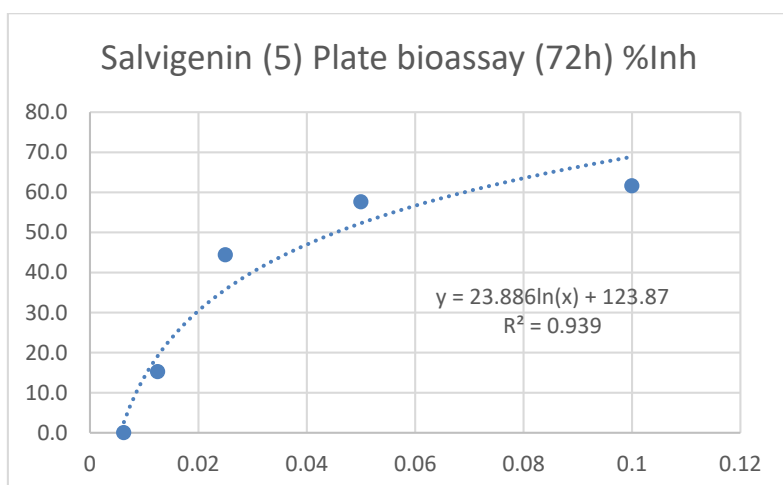
Transform of Prune rows of Data 1



Error estandard LogEC₅₀=0.02001
(debe ser <0.5; EC₅₀ valido)

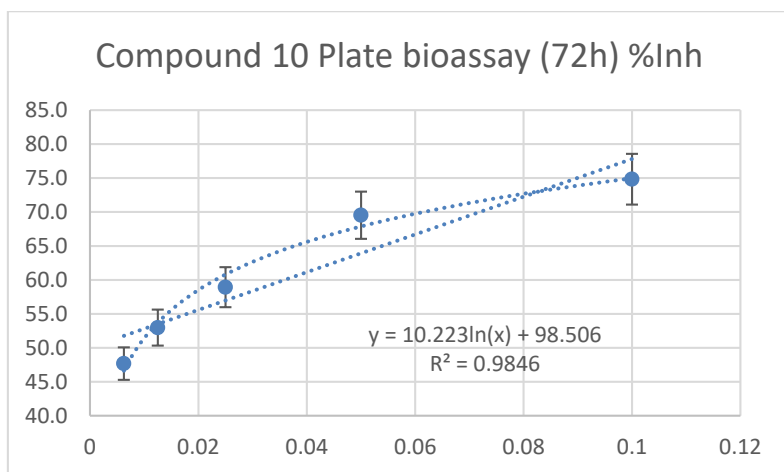
R²=0.9748

SI- 28- Plate bioassay. Compound 5



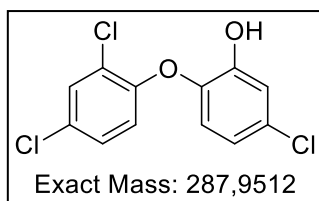
Salvigenin (5) (72h)	
Conc	%Inh
0,1	61,6
0,05	57,6
0,025	44,4
0,0125	15,2
0,00625	0,0
IC50 (ppm)	
14.89	
IC50 (µM)	
45.4	

SI- 29- Plate bioassay. Compound 10

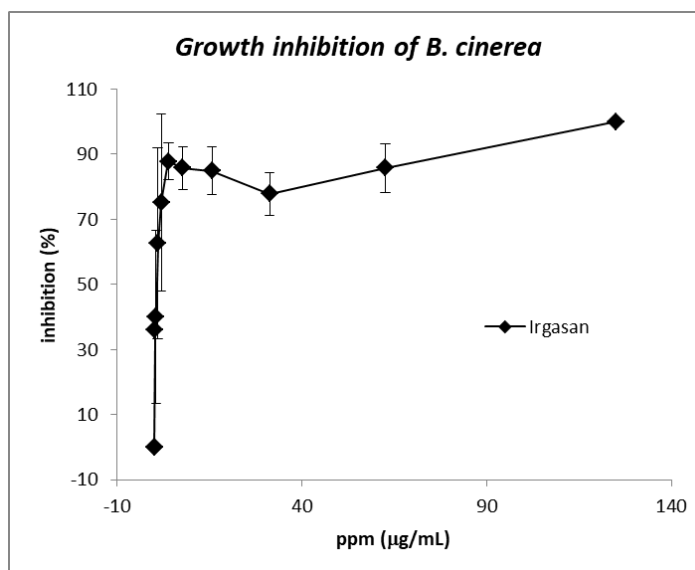


Compound 10 (72h)	
Conc	%Inh
0,1	74,8
0,05	69,5
0,025	58,9
0,0125	53,0
0,00625	47,7
IC50 (ppm)	
1.79	
IC50 (µM)	
8.7	

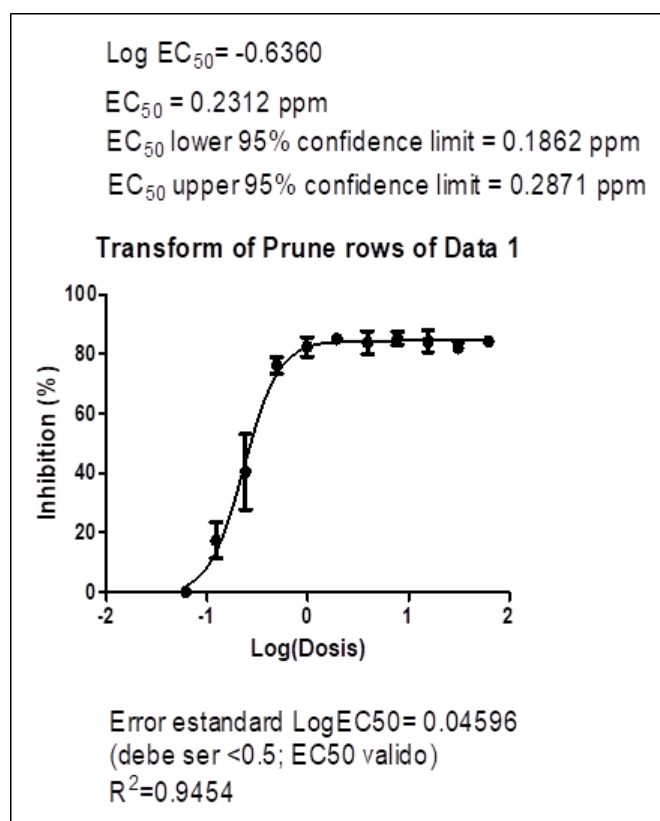
SI- 30- Positive control. Microplate Bioassay (irgasan).



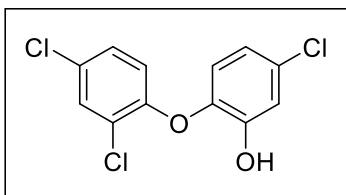
IC50 (ppm)	0.23
EC50 Lower (ppm)	0.19
EC50 Upper (ppm)	0.29
IC50 (μM)	0.80
EC50 Lower (μM)	0.65
EC50 Upper (μM)	1.00



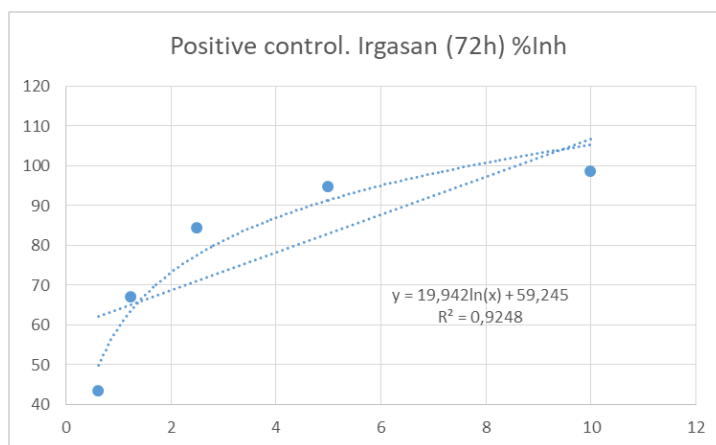
Conc. (ppm)	62,50	31,25	15,63	7,81	3,91	1,95	0,98	0,49	0,24	0,12	0,06
Inhibition (%)	85,69	77,88	84,89	85,73	87,74	75,27	62,52	39,93	35,89	0,00	0,00
Standard deviation	7,55	6,58	7,45	6,51	5,62	27,20	29,32	26,66	16,40	0,00	0,00



SI- 31- Positive control. Plate Bioassay (irgasan).



IC50 (ppm)	0.63
Rango EC50 inferior (ppm)	-
Rango EC50 superior (ppm)	-
IC50 (μM)	2.19
Rango EC50 inferior (μM)	-
Rango EC50 superior (μM)	-



Irgasan (72h)	
Conc	%Inh
10	98,53
5	94,57
2,5	84,32
1,25	66,94
0,625	43,23