

# Oxonitrogenated Derivatives of Eremophilans and Eudesmans: Antiproliferative and Anti-*Trypanosoma cruzi* Activity

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## 1. NMR spectra of natural sesquiterpene tessaric acid (1), ilicic acid (2) and ilicic alcohol (3)

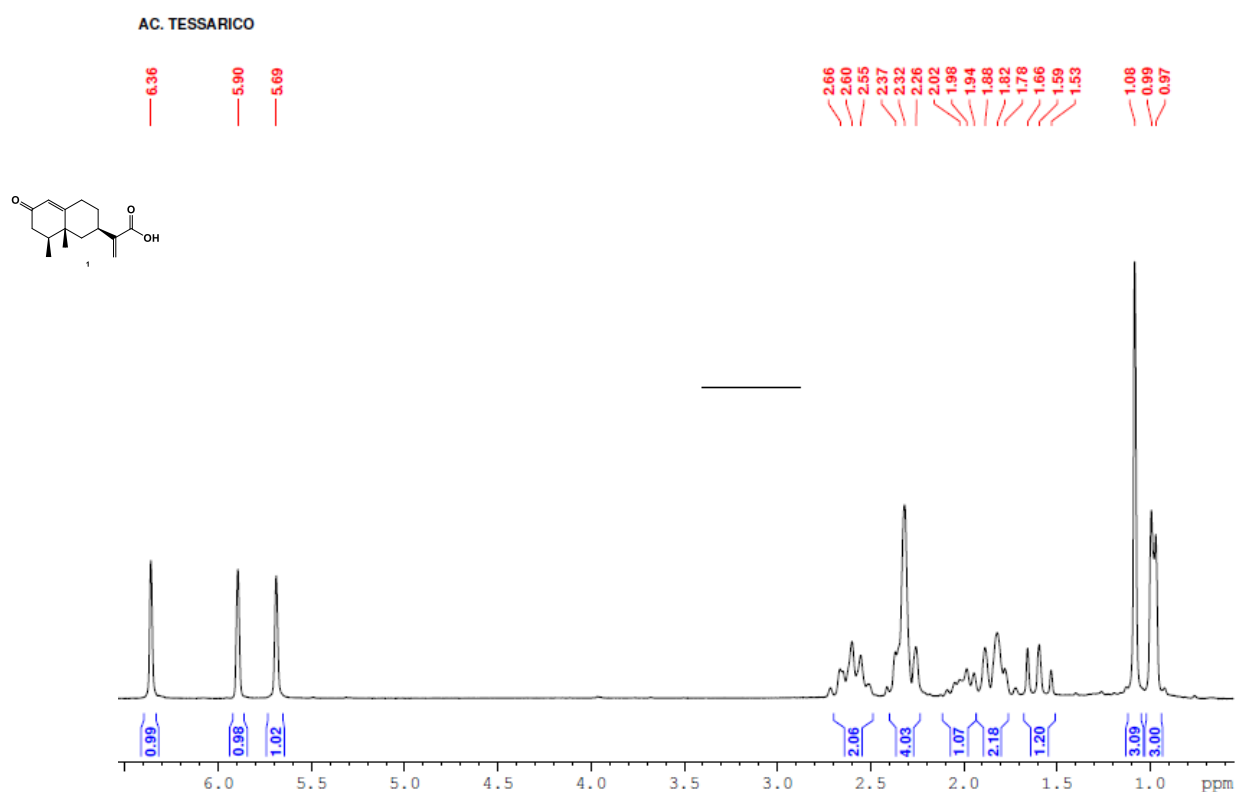


Figure S1. <sup>1</sup>H-NMR of 1.

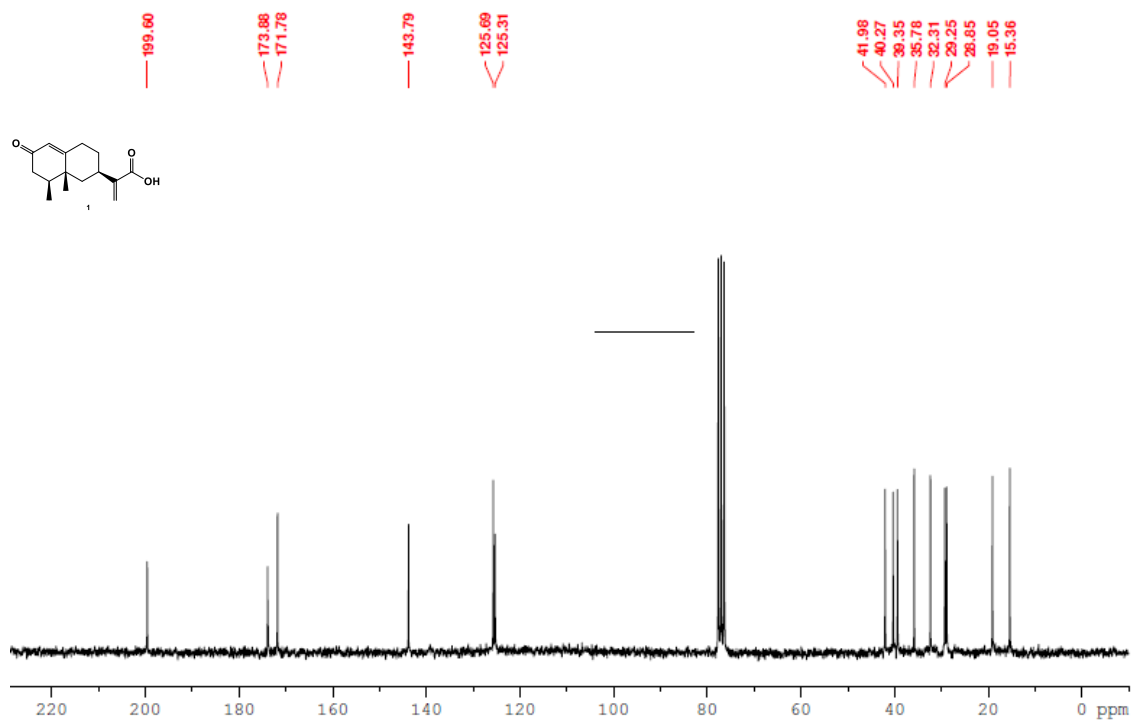


Figure S2.  $^{13}\text{C}$ -NMR of 1.

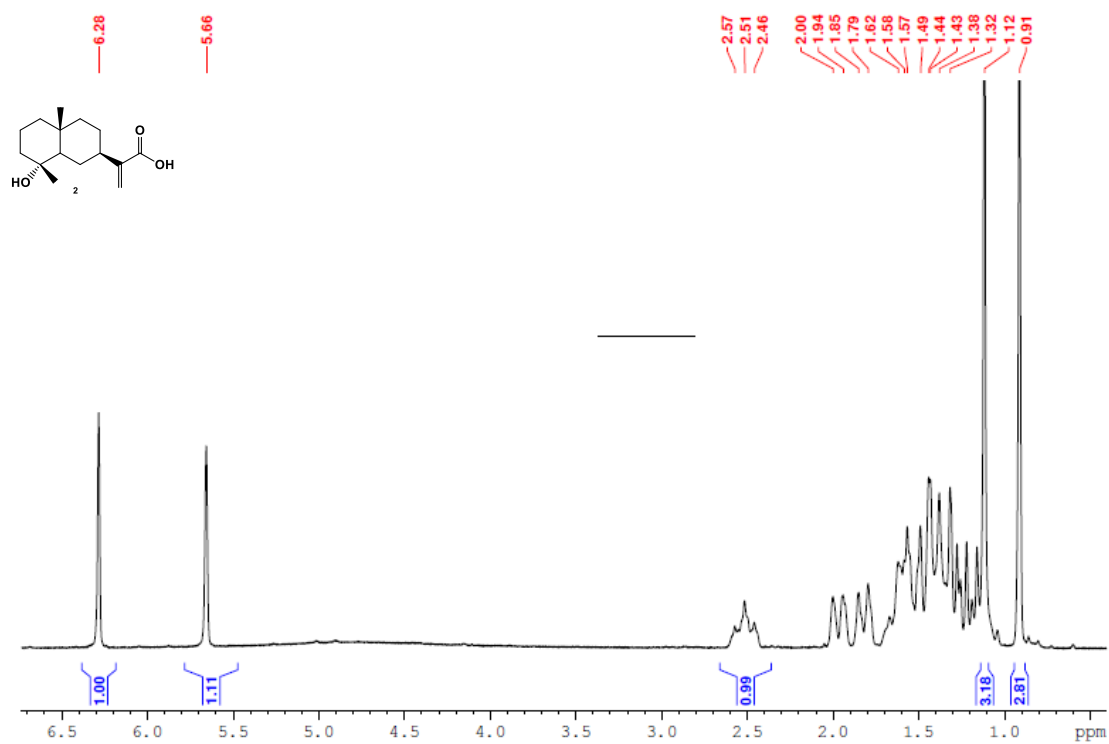


Figure S3.  $^1\text{H}$ -NMR of 2.

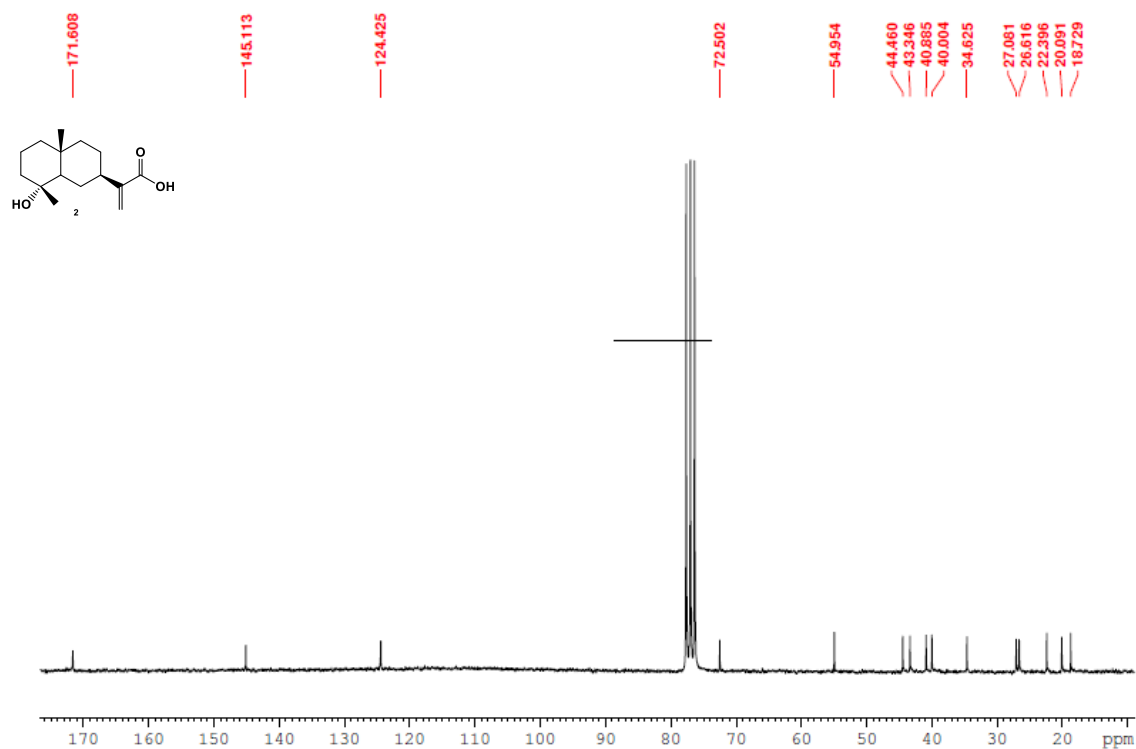


Figure S4. <sup>13</sup>C-NMR of 2.

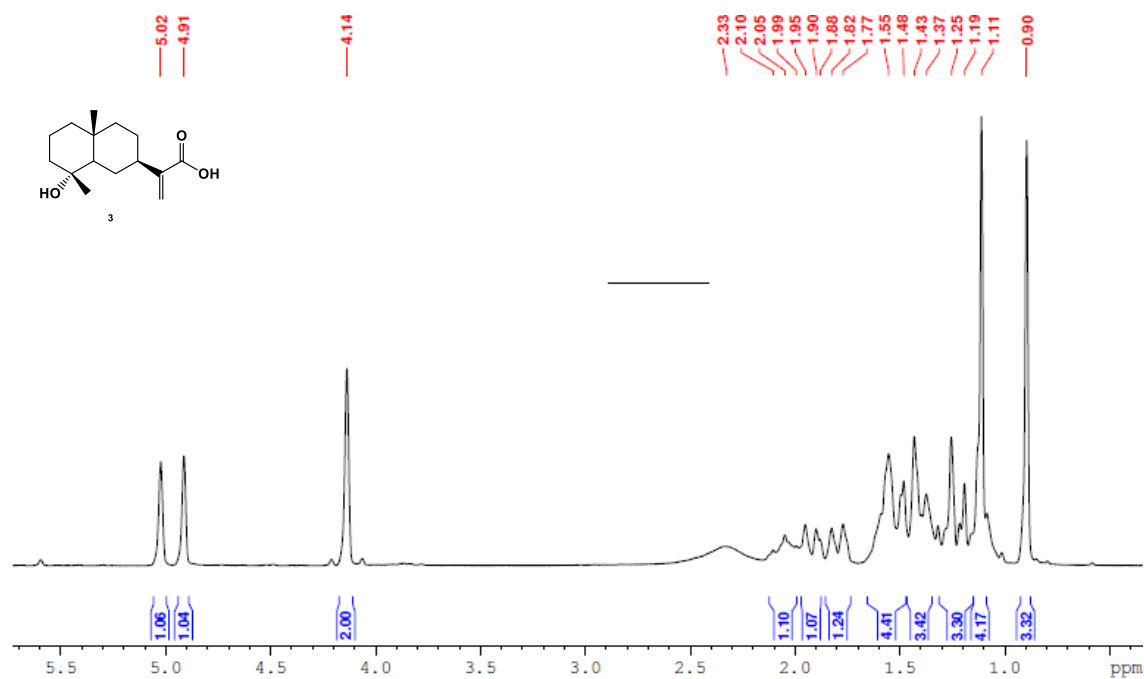


Figure S5. <sup>1</sup>H-NMR of 3.

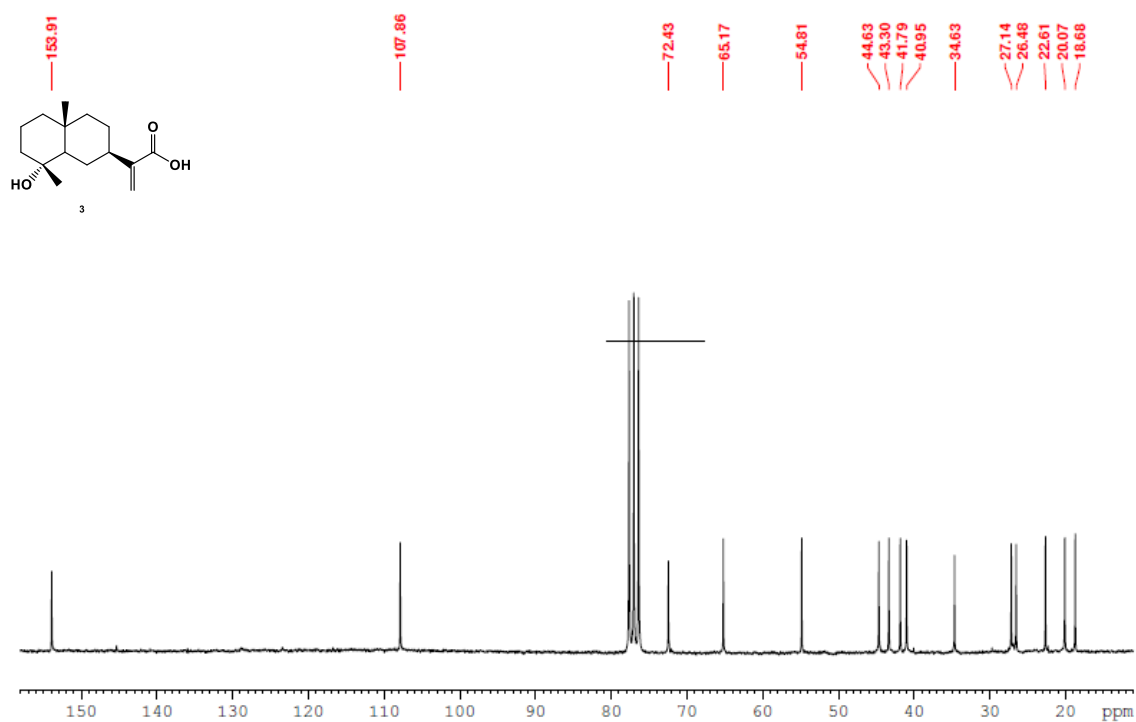


Figure S6.  $^{13}\text{C}$ -NMR of 3.

## 2. NMR spectra of tessaric acid derivatives

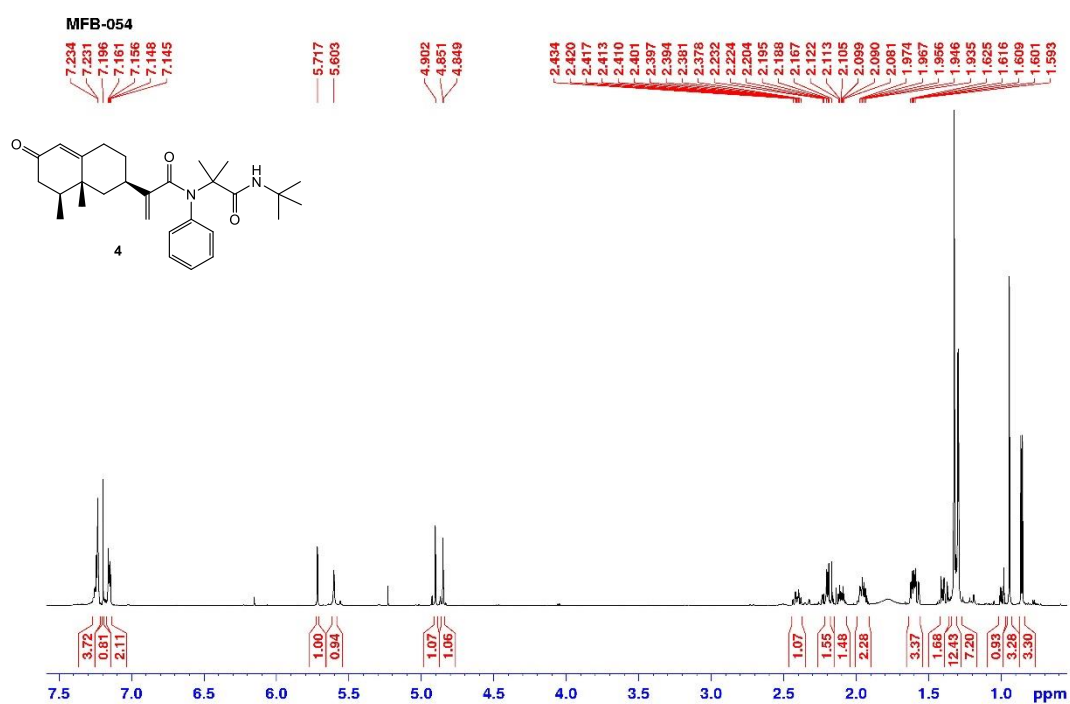


Figure S7.  $^1\text{H}$ -NMR of 4.

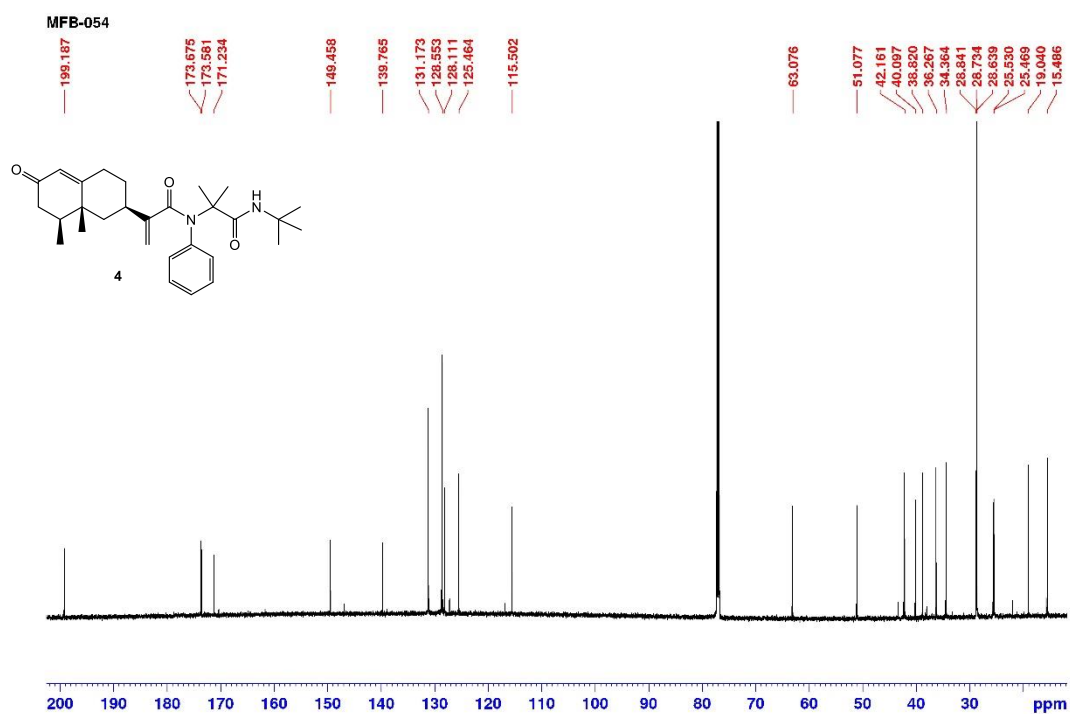


Figure S8. <sup>13</sup>C-NMR of 4.

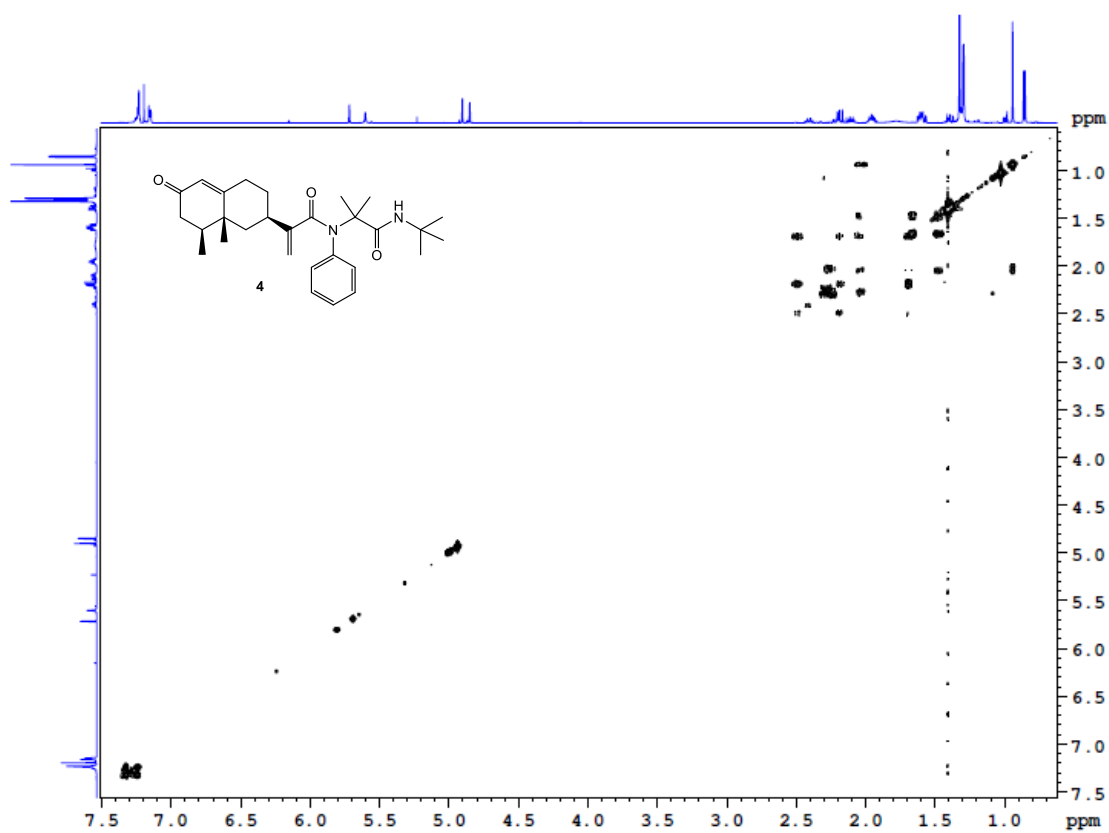


Figure S9. COSY of 4.

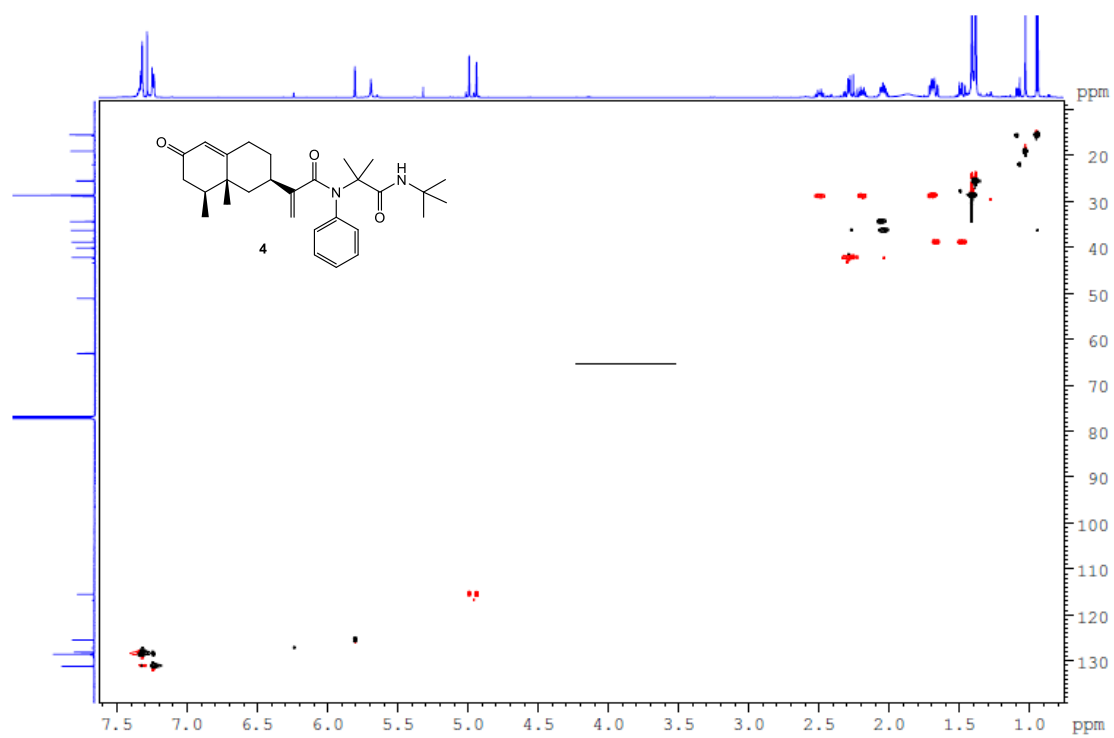


Figure S10. HSQC of 4.

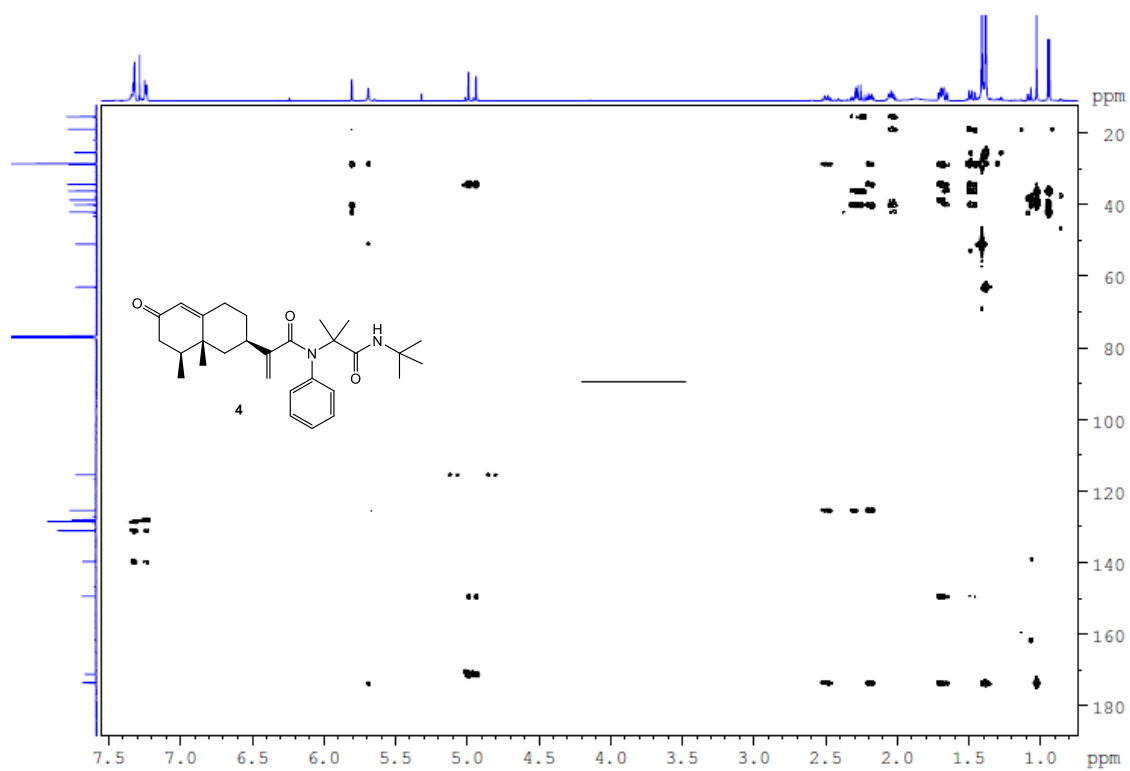


Figure S11. HMBC of 4.

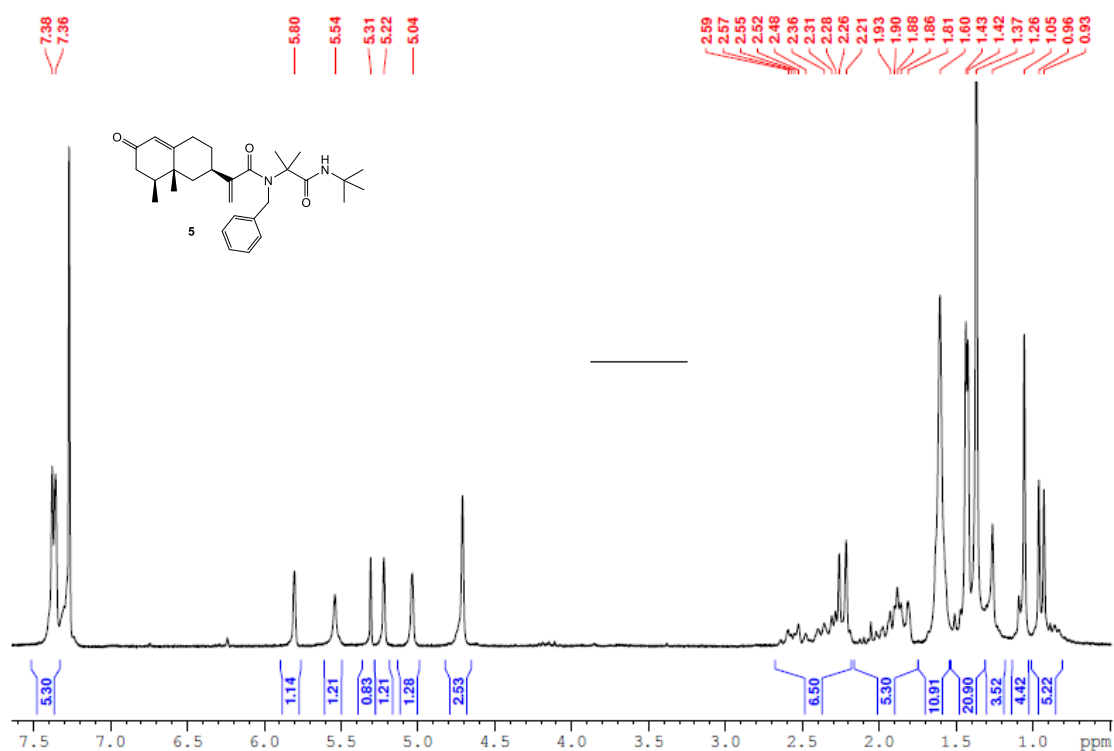


Figure S12. <sup>1</sup>H-NMR of 5.

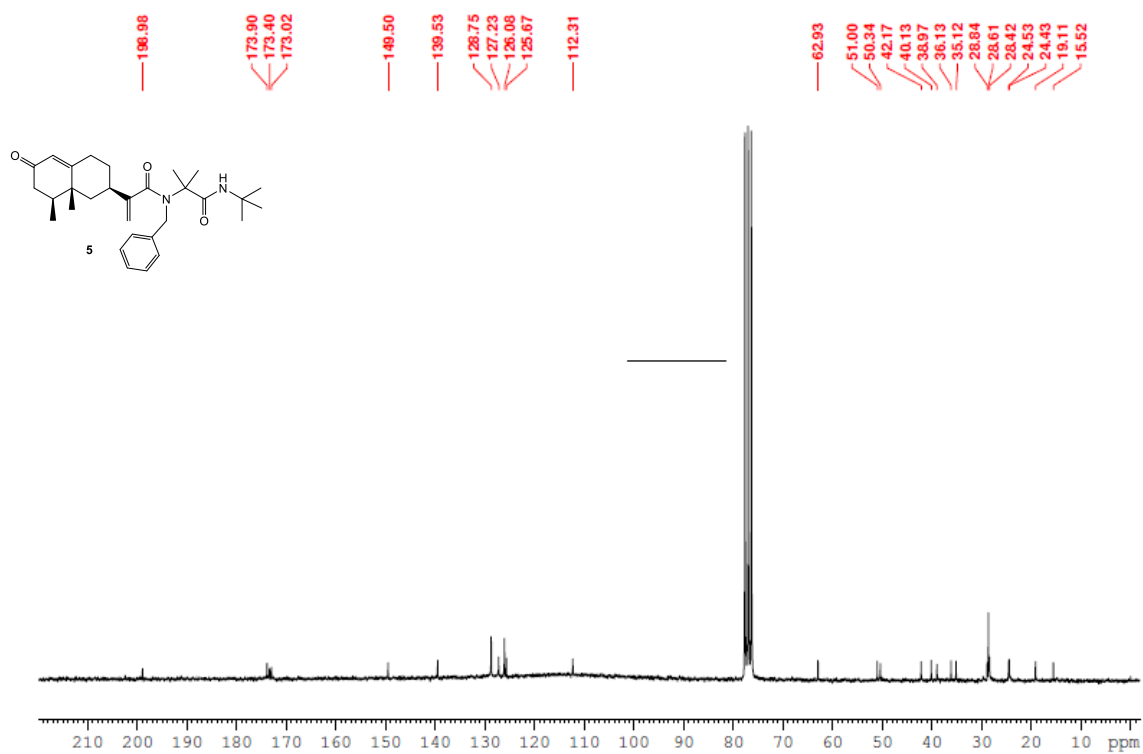


Figure S13. <sup>13</sup>C-NMR of 5.

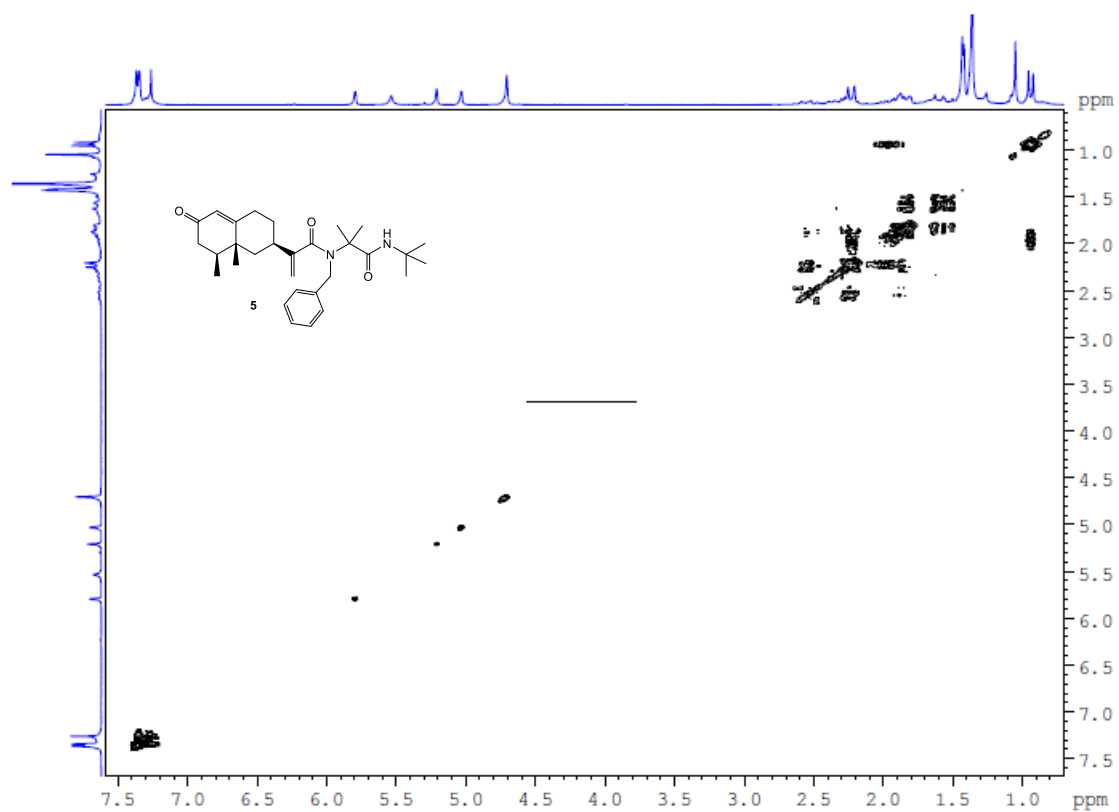


Figure S14. COSY of 5.

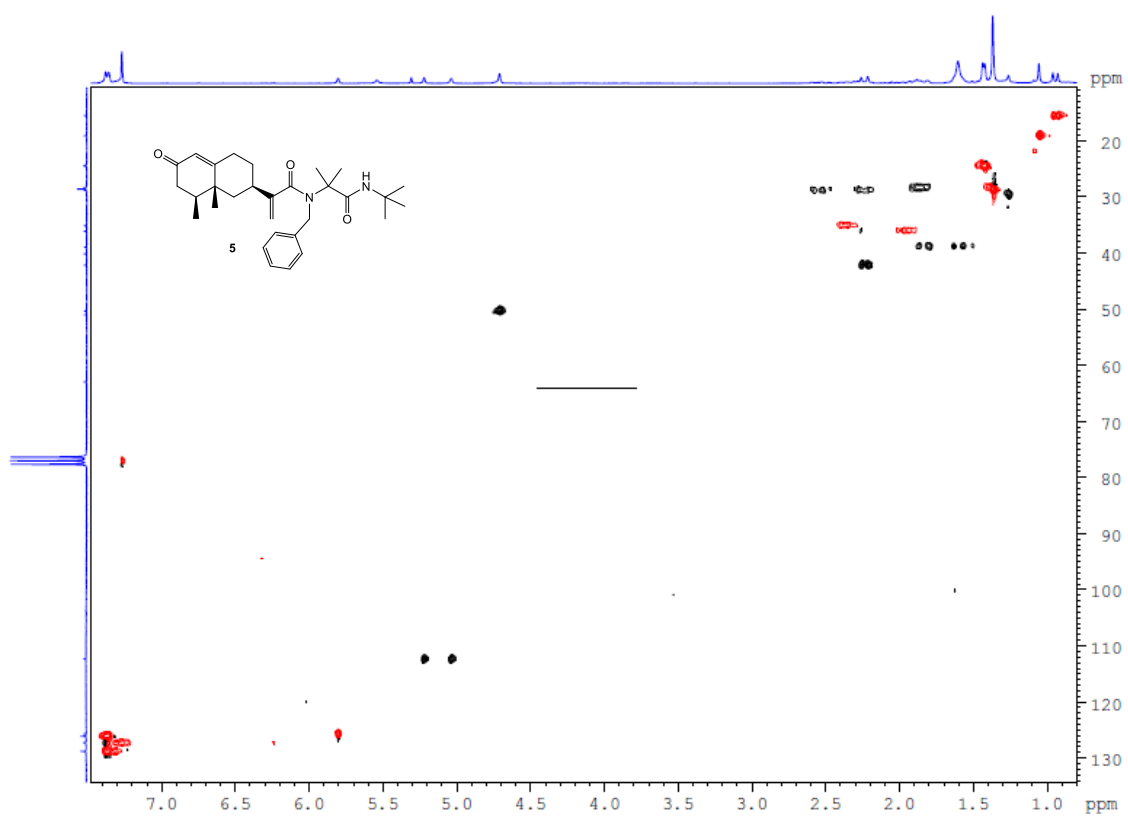


Figure S15. HSQC of 5.



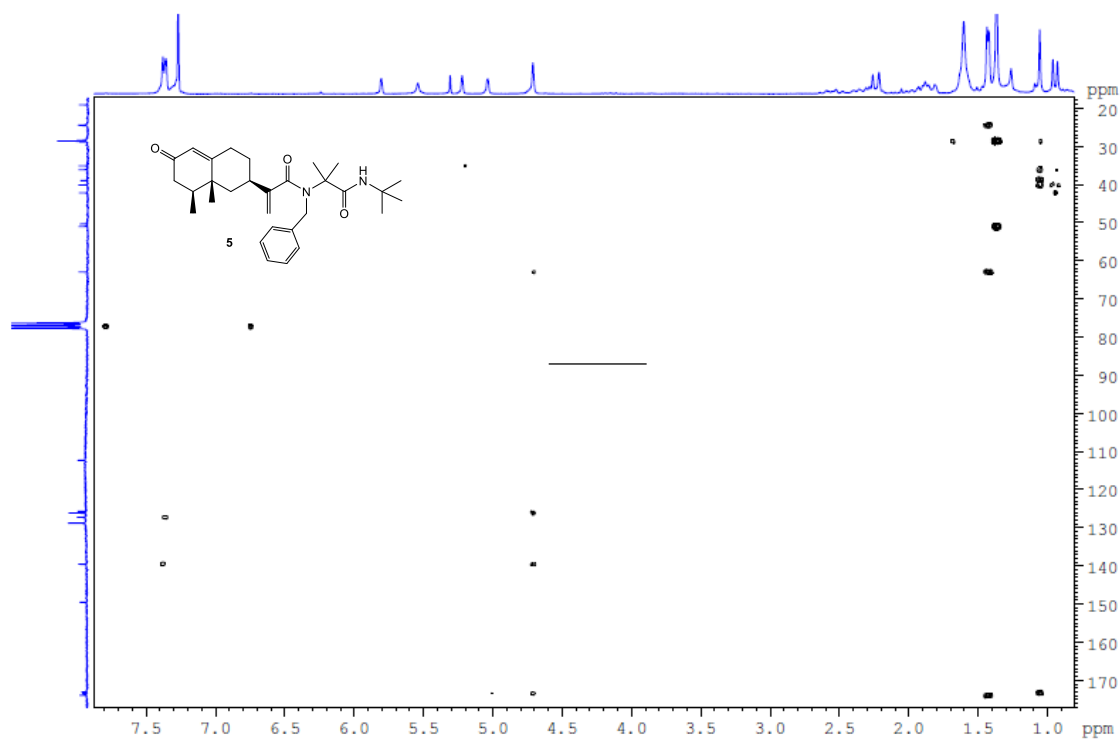


Figure S16. HMBC of 5.

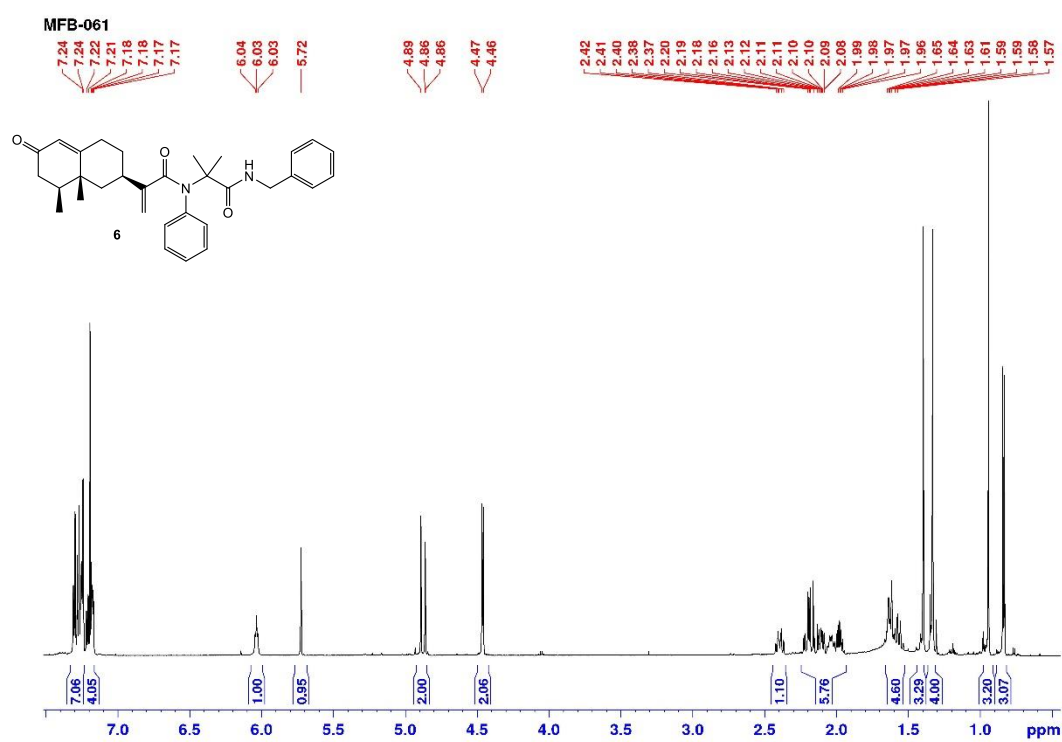


Figure S17.  $^1\text{H}$ -NMR of 6.

MFB-061

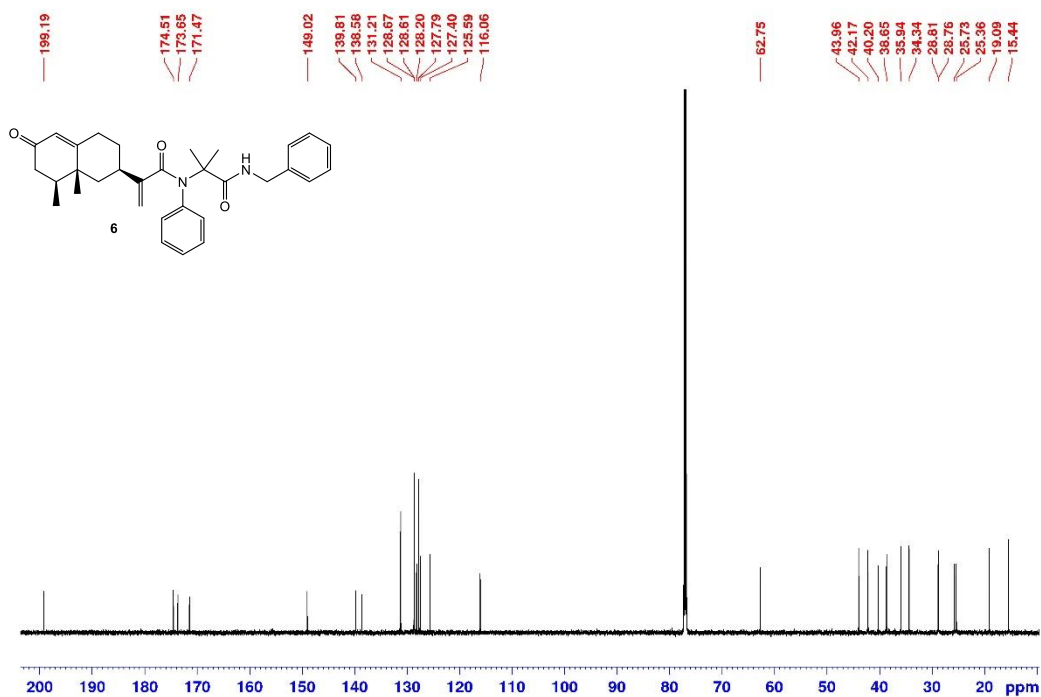


Figure S18.  $^{13}\text{C}$ -NMR of 6.

MFB-061

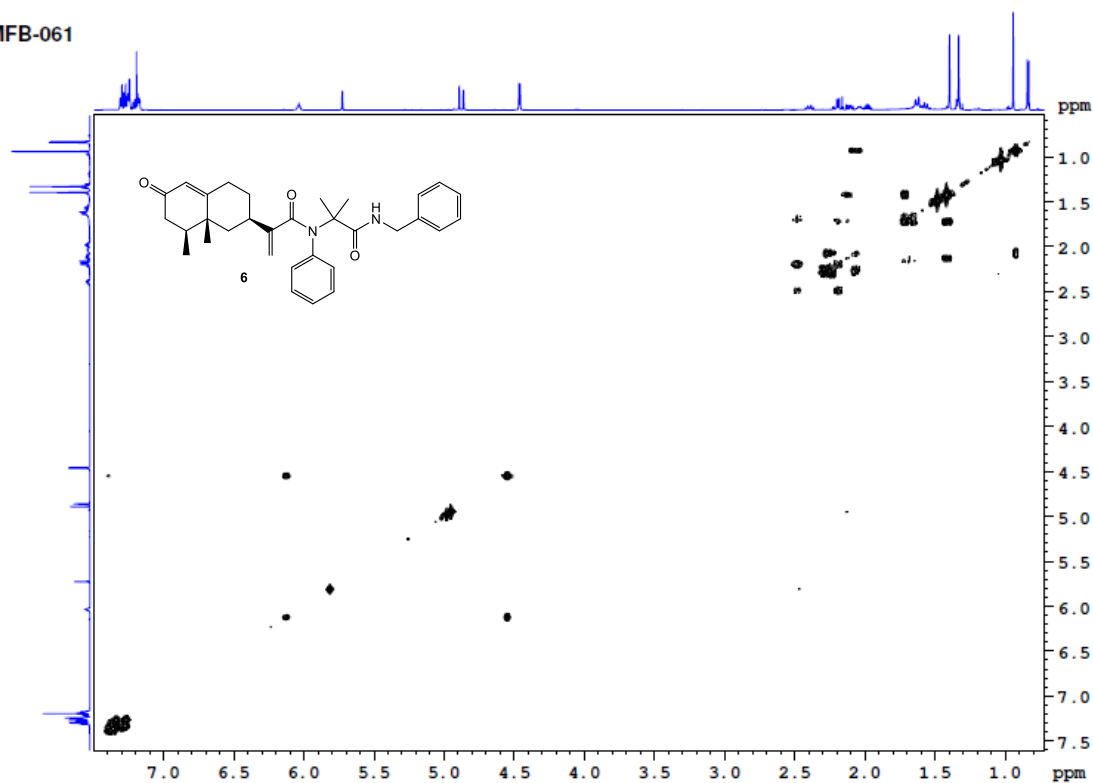


Figure S19. COSY of 6.

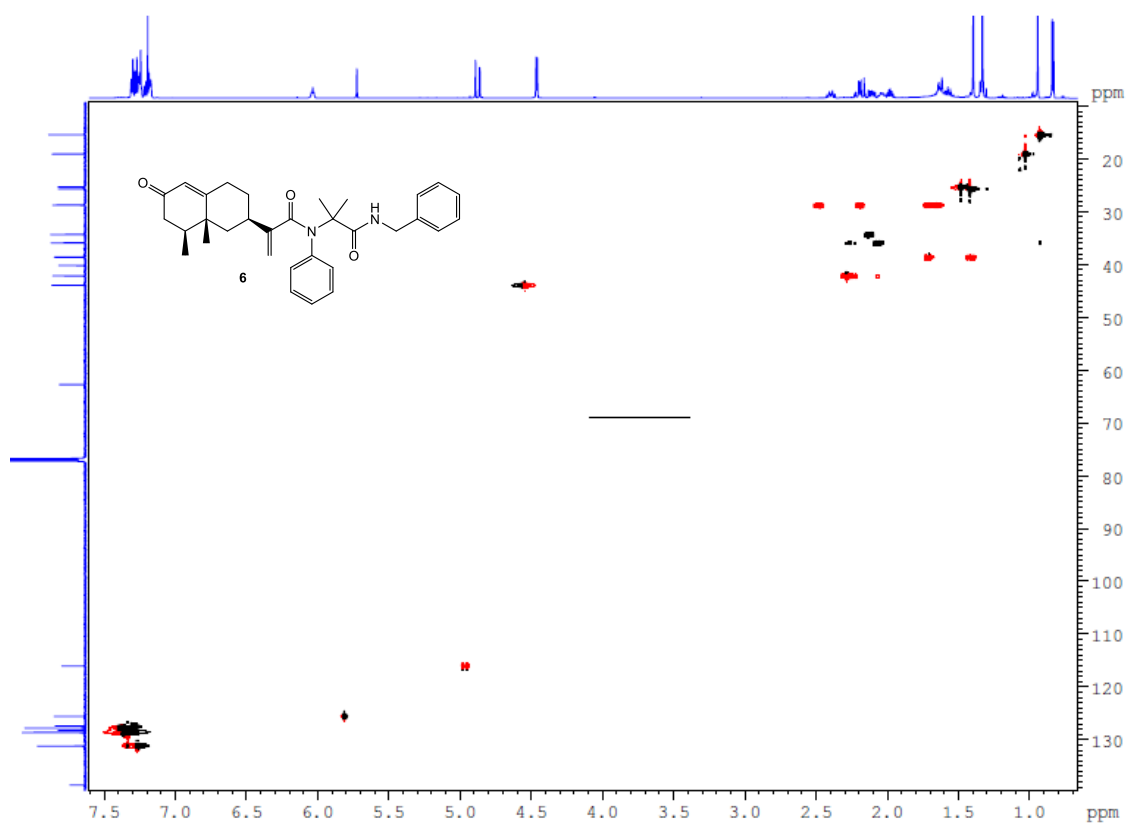


Figure S20. HSQC of 6.

mfb-061

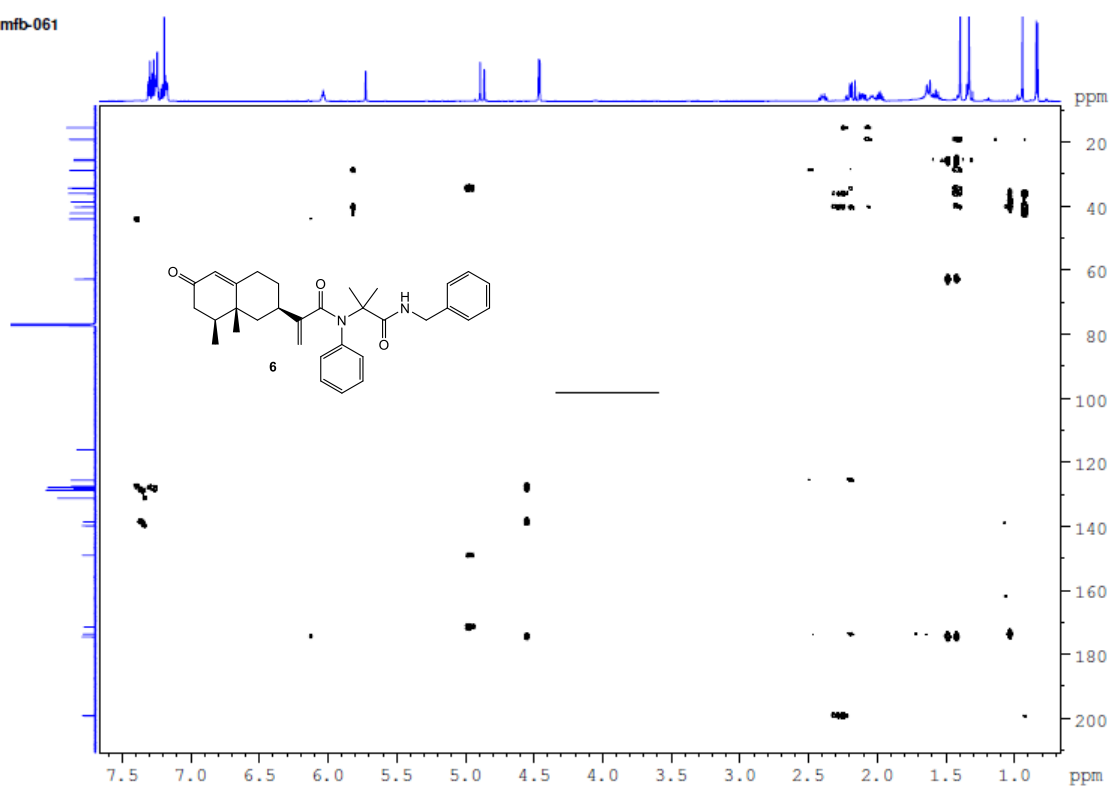


Figure S21. HMBC of 6.

mtb060

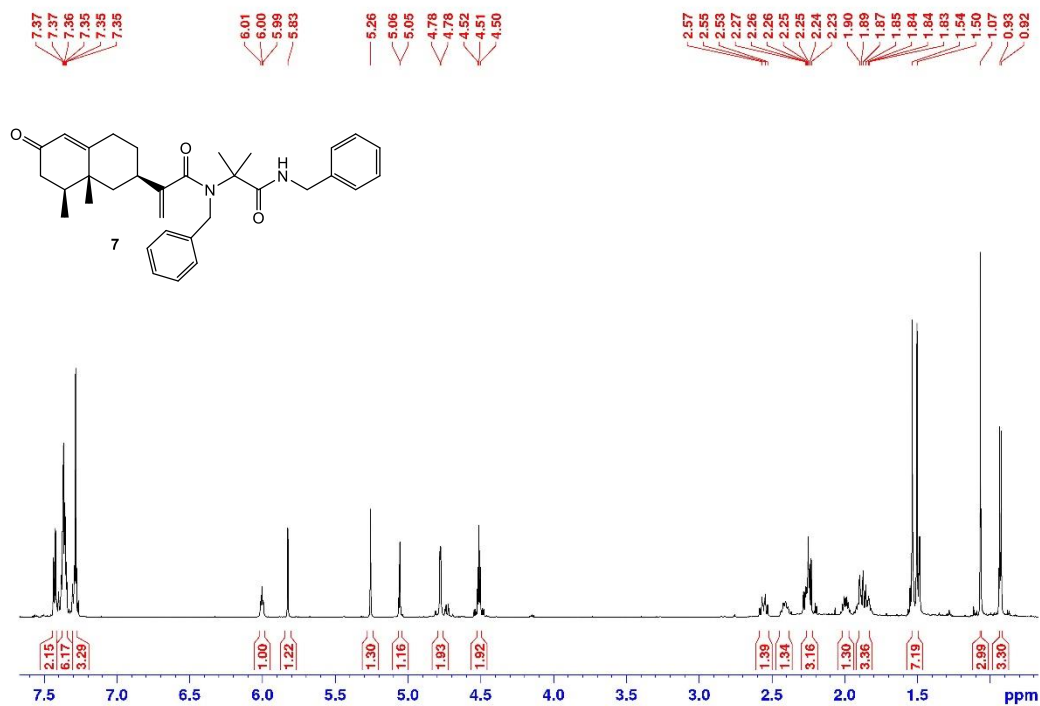


Figure S22. <sup>1</sup>H-NMR of 7.

mtb-060

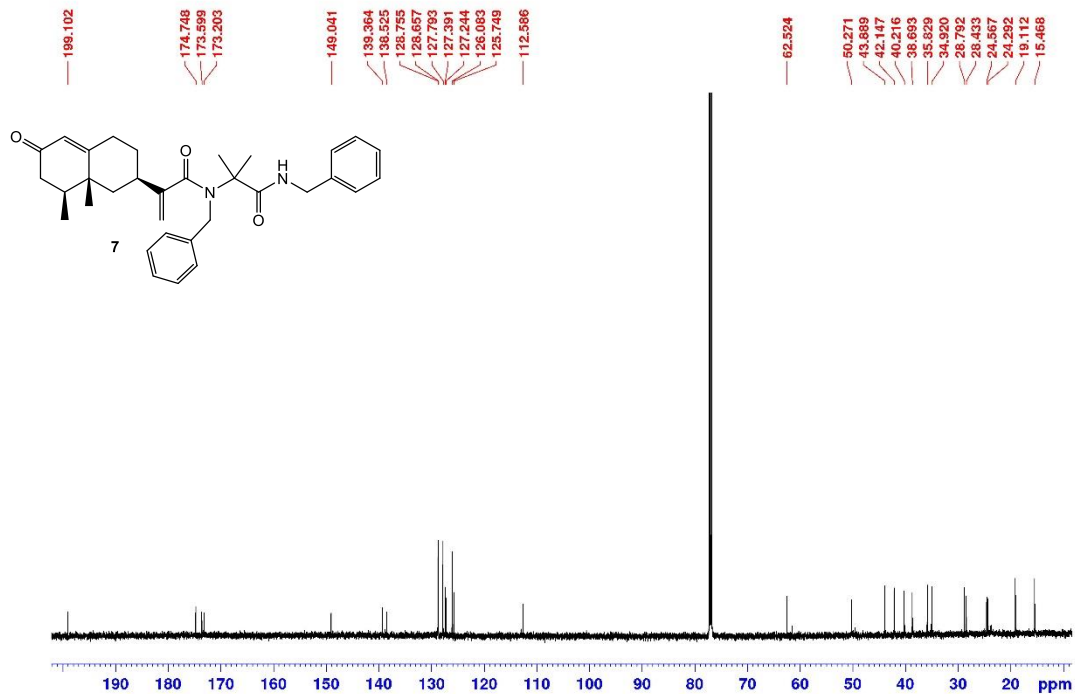


Figure S23. <sup>13</sup>C-NMR of 7.

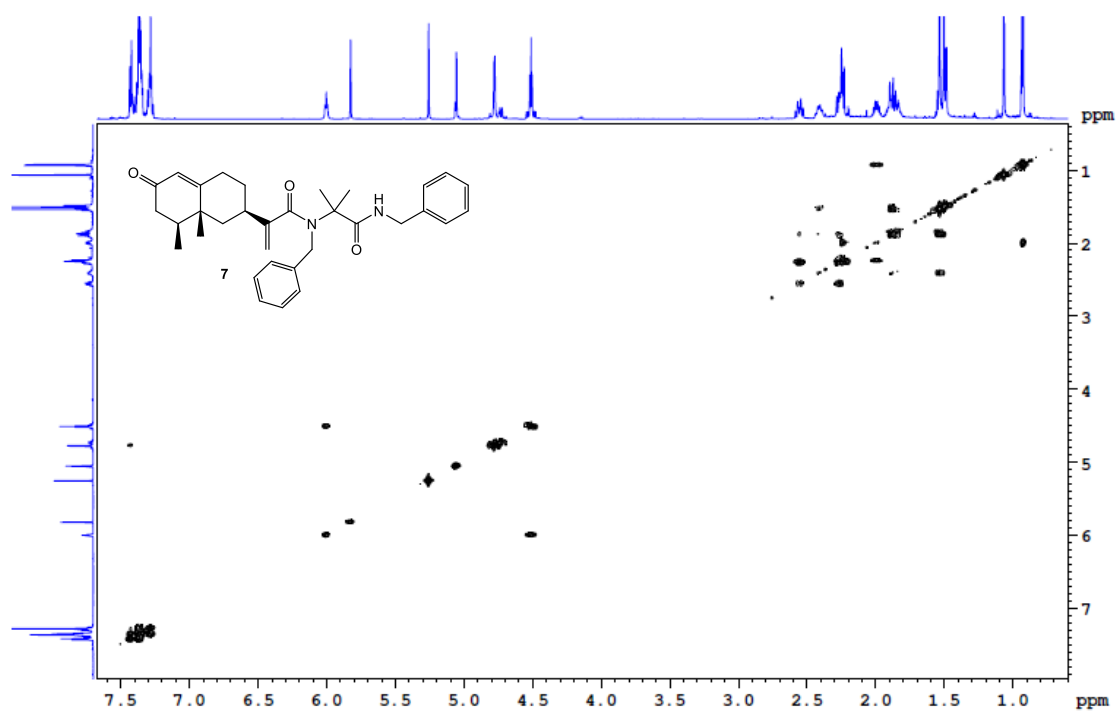


Figure S24. COSY of 7.

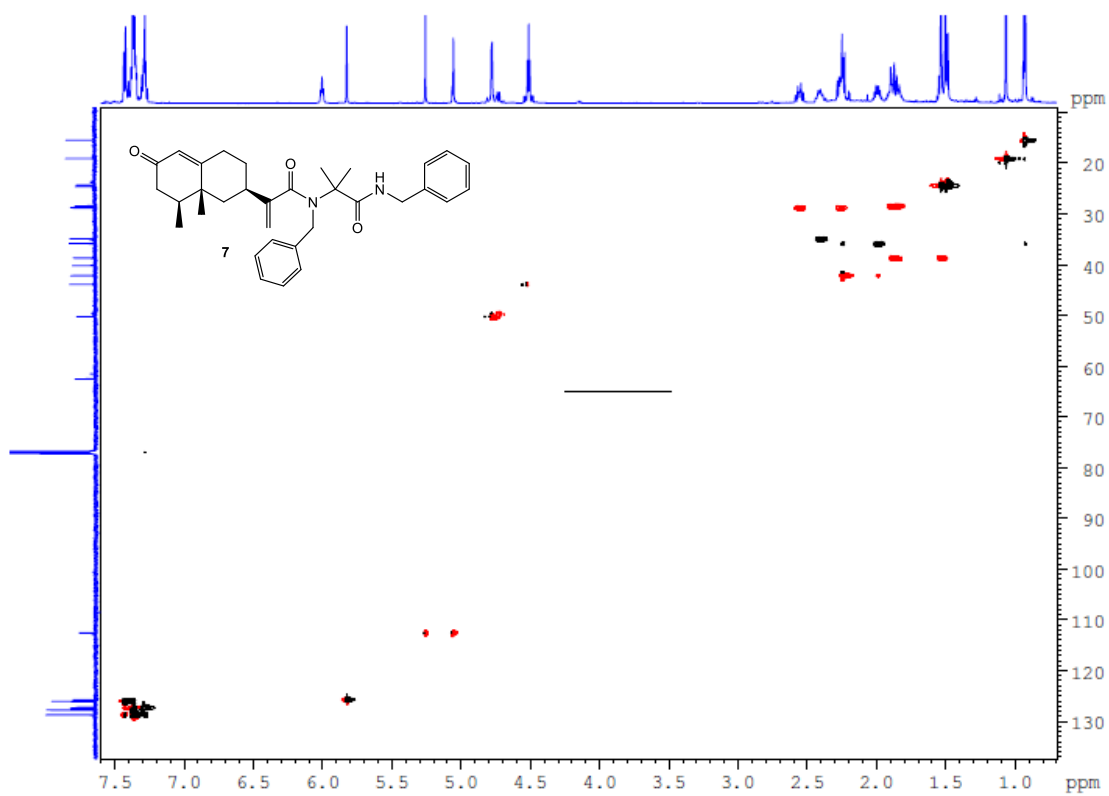


Figure S25. HSQC of 7.

mfb-060

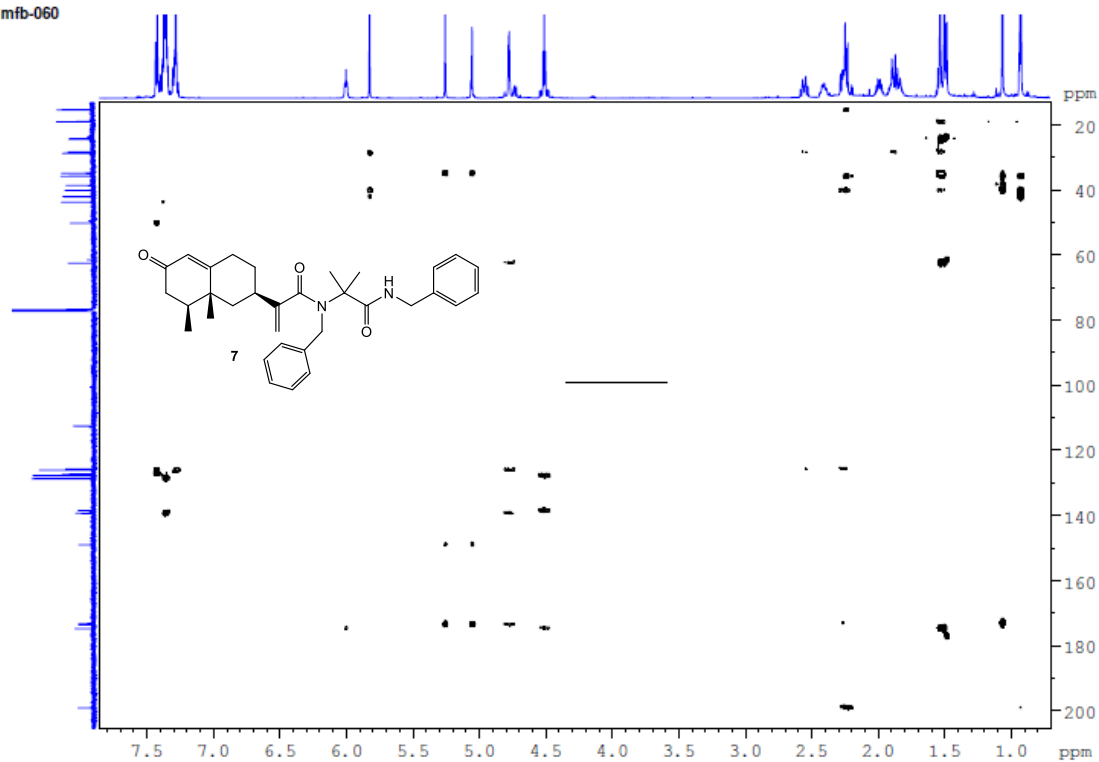


Figure S26. HMBC of 7.

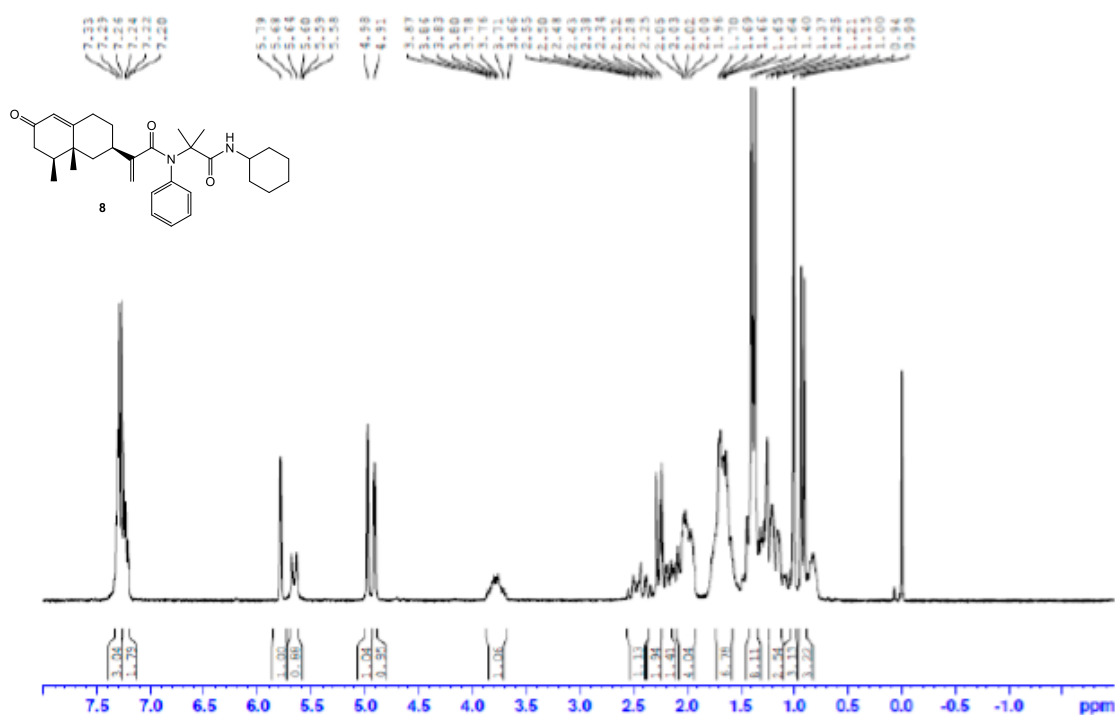


Figure S27.  $^1\text{H}$ -NMR of 8.

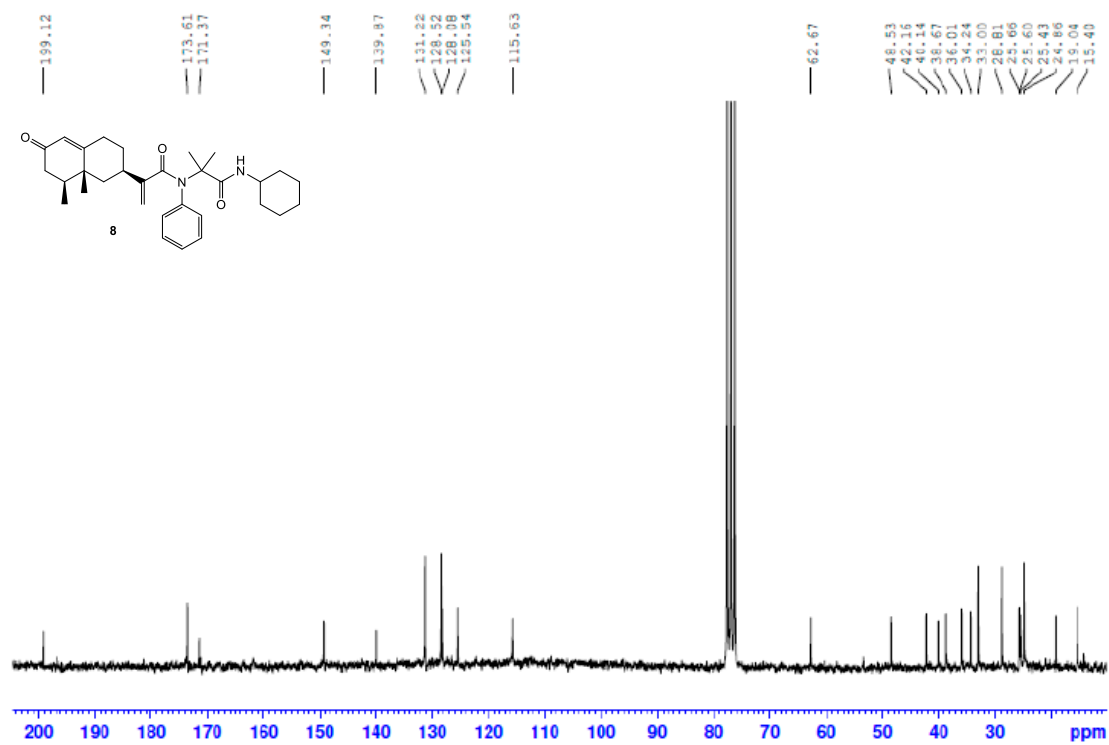


Figure S28. <sup>13</sup>C-NMR of 8.

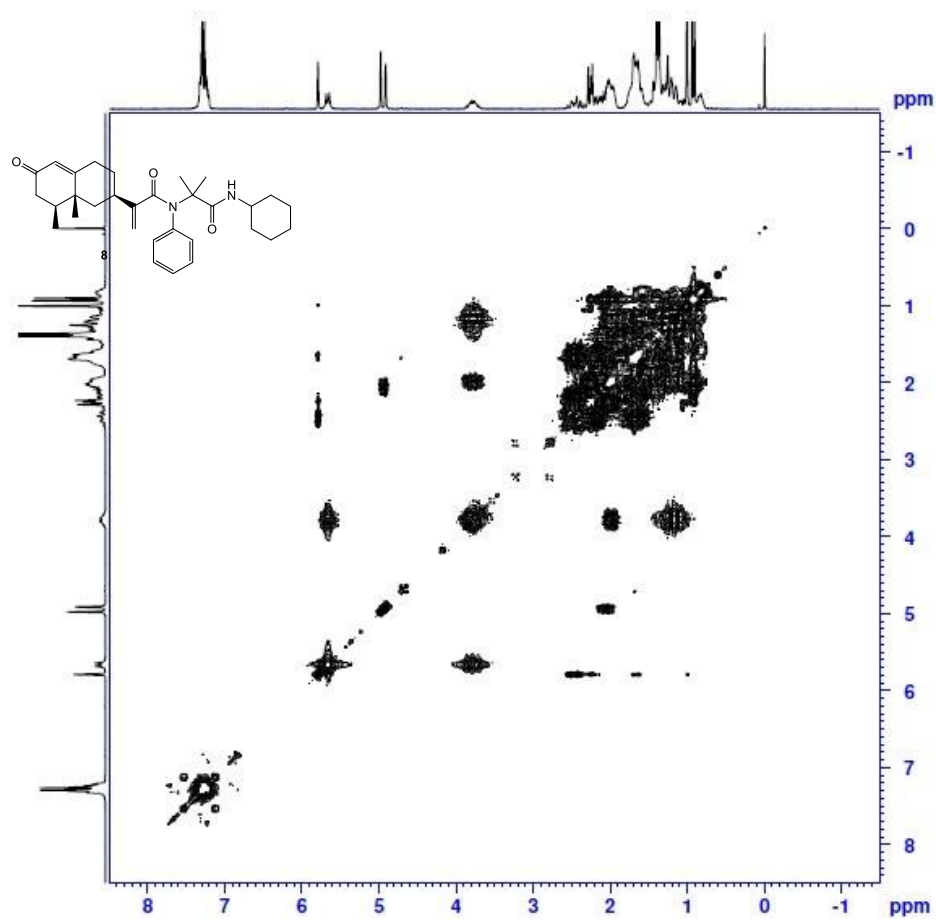


Figure S29. COSY of 8.

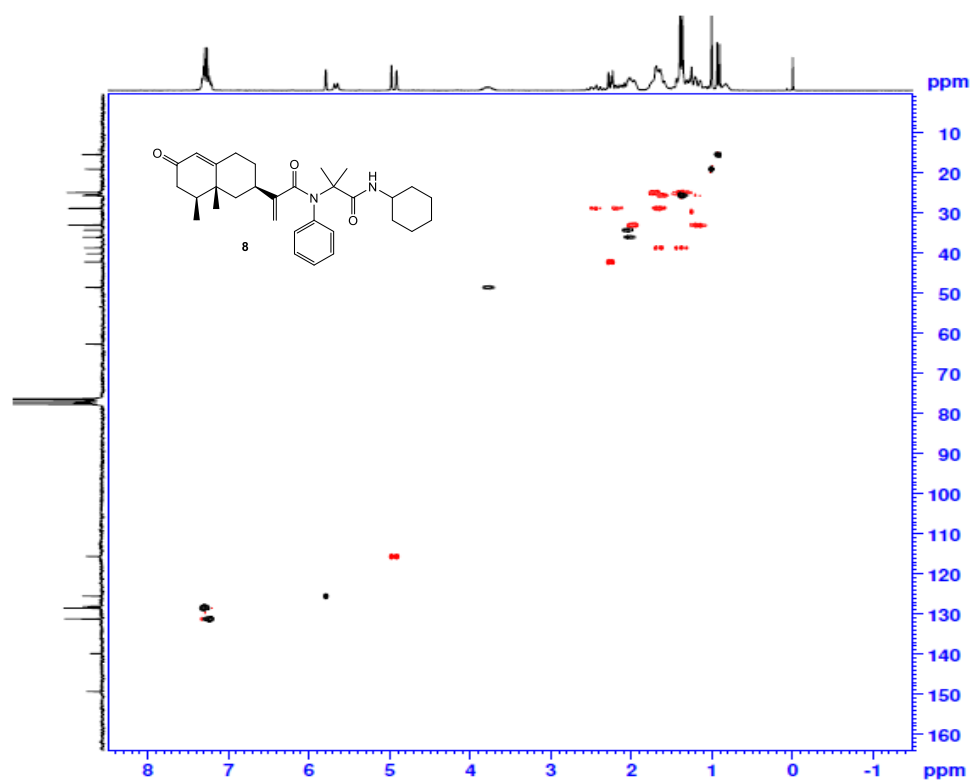


Figure S30. HSQC of 8.

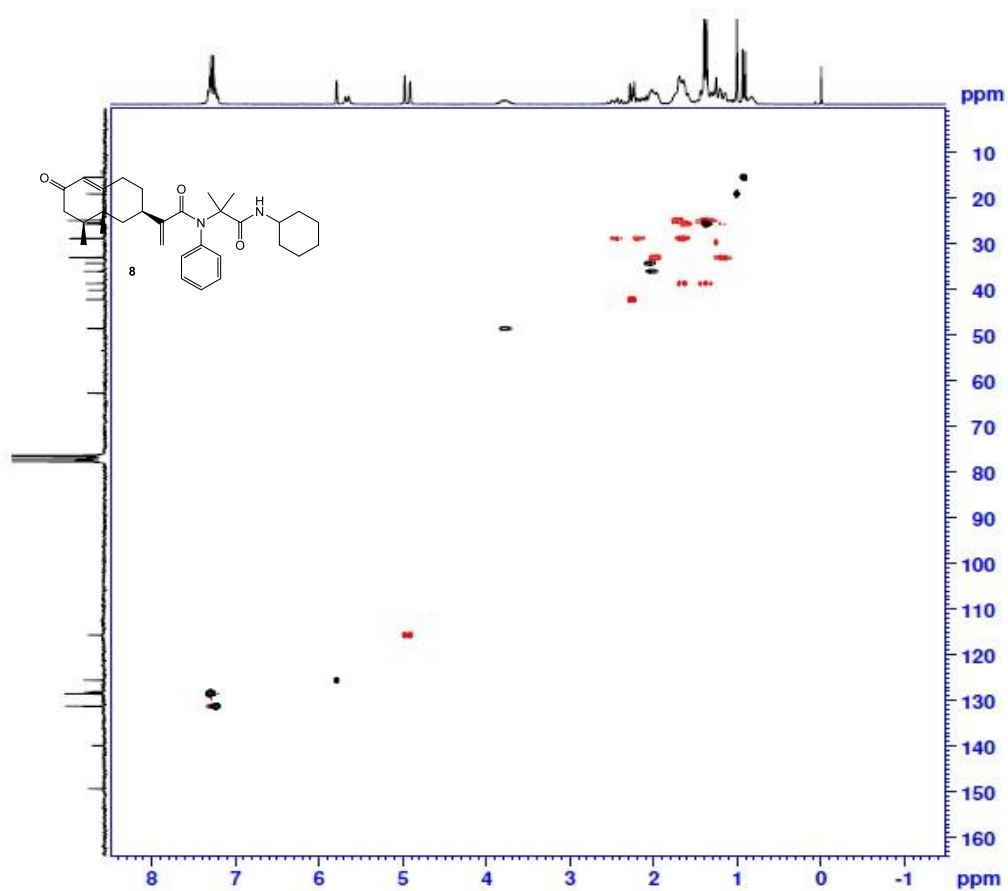


Figure S31. HSQC of 8.



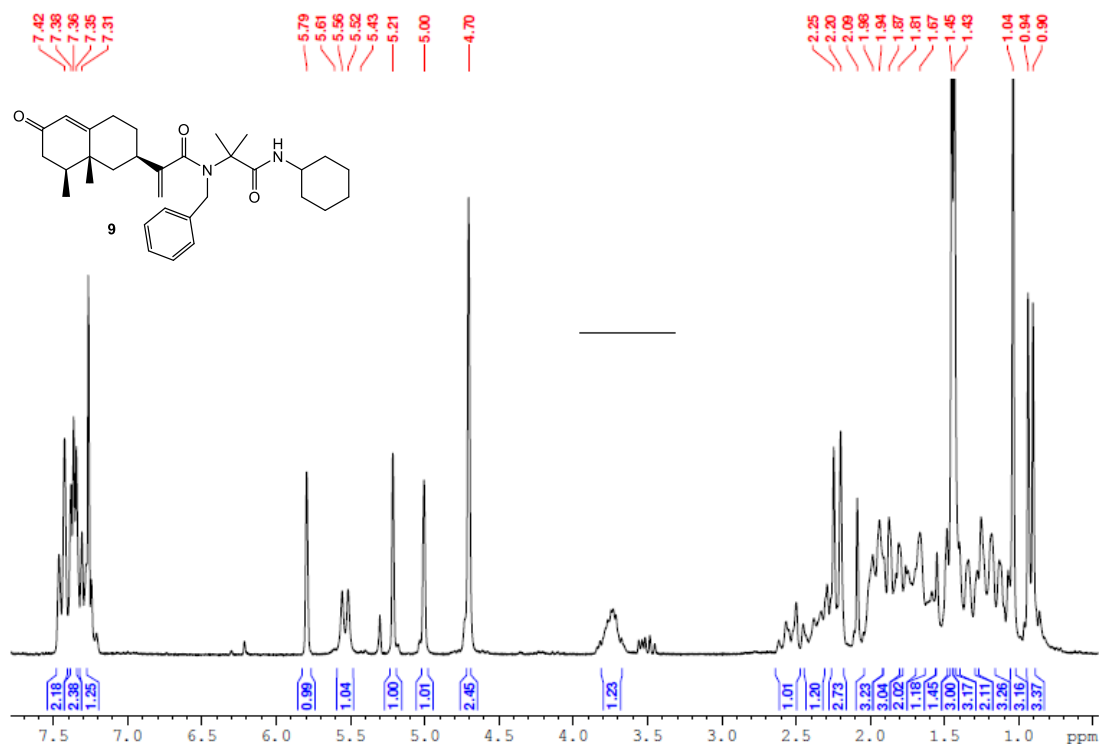


Figure S32. <sup>1</sup>H-NMR of 9.

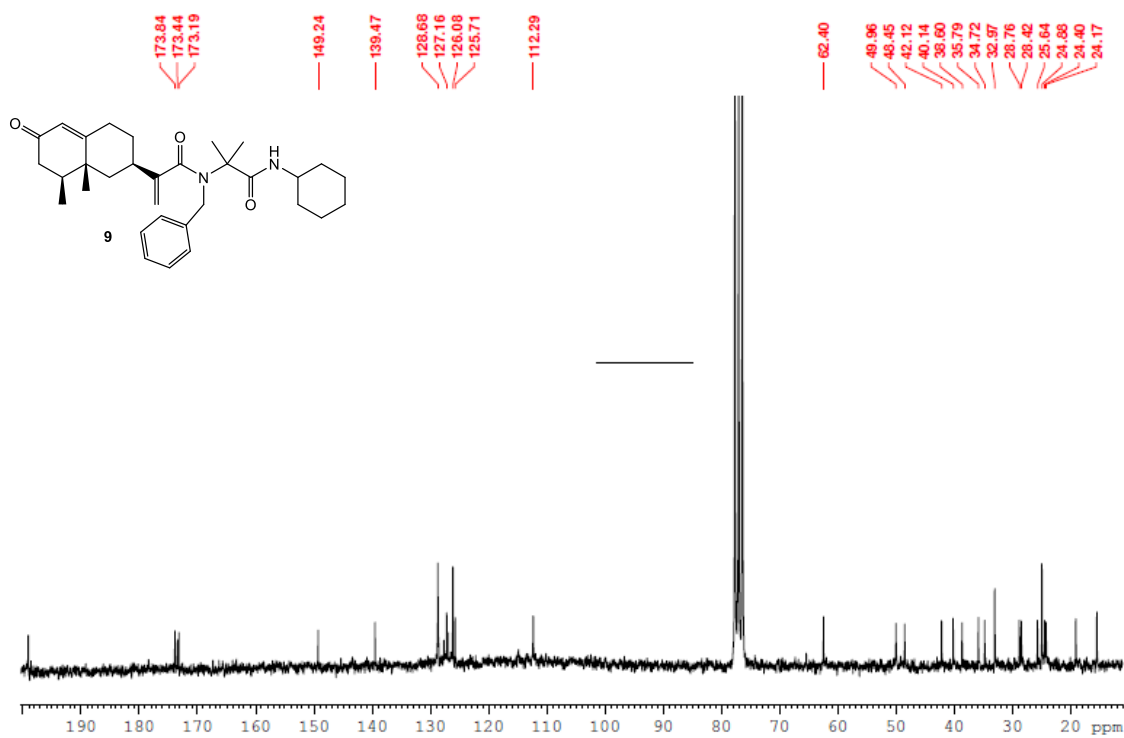


Figure S33. <sup>13</sup>C-NMR of 9.

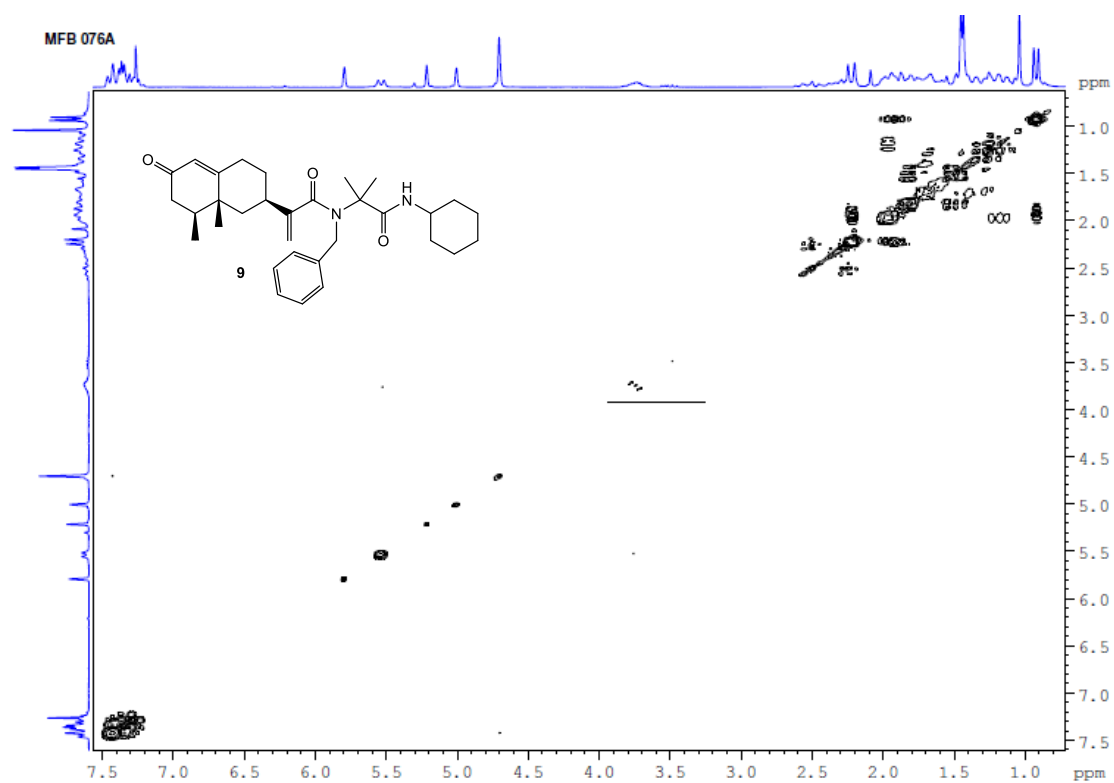


Figure S34. COSY of 9.

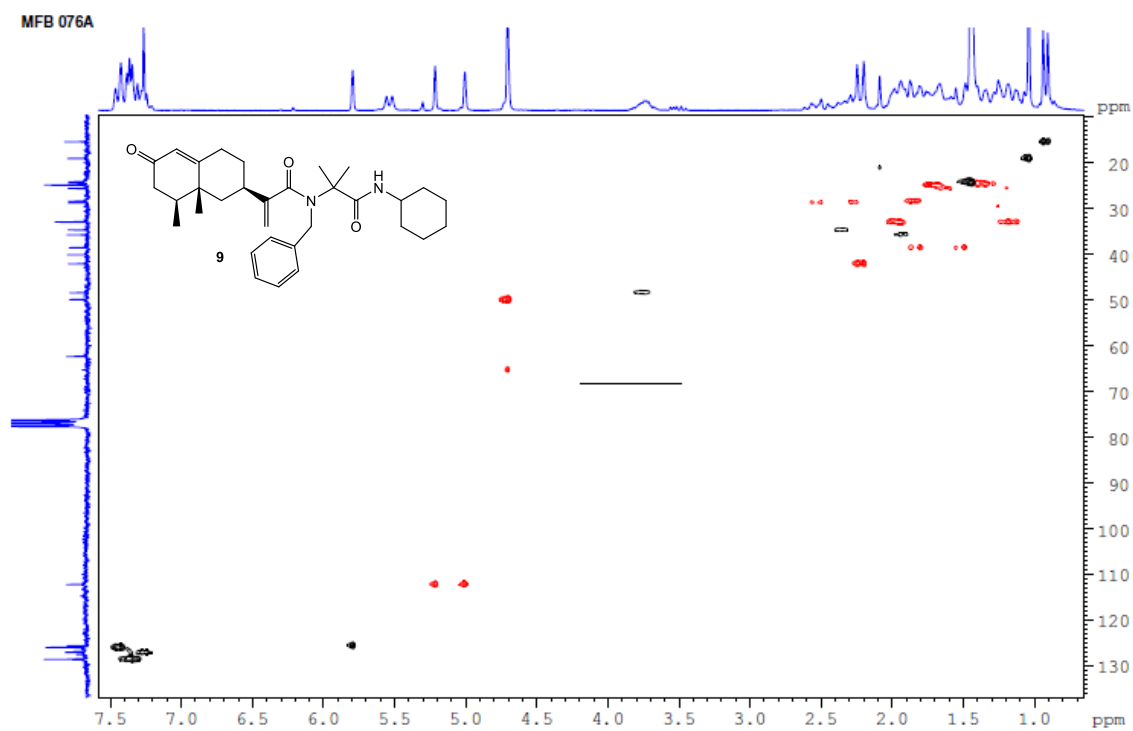


Figure S35. HSQC of 9.

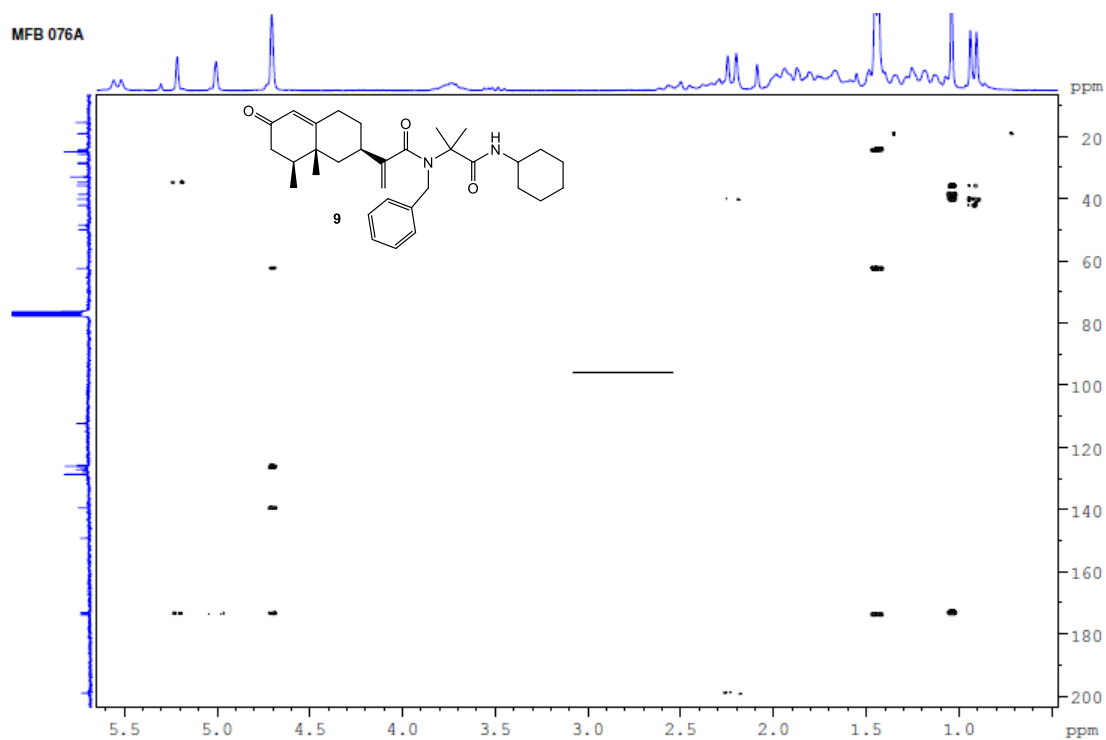


Figure S36. HMBC of 9.

### 3. NMR spectra of Illicic acid derivatives

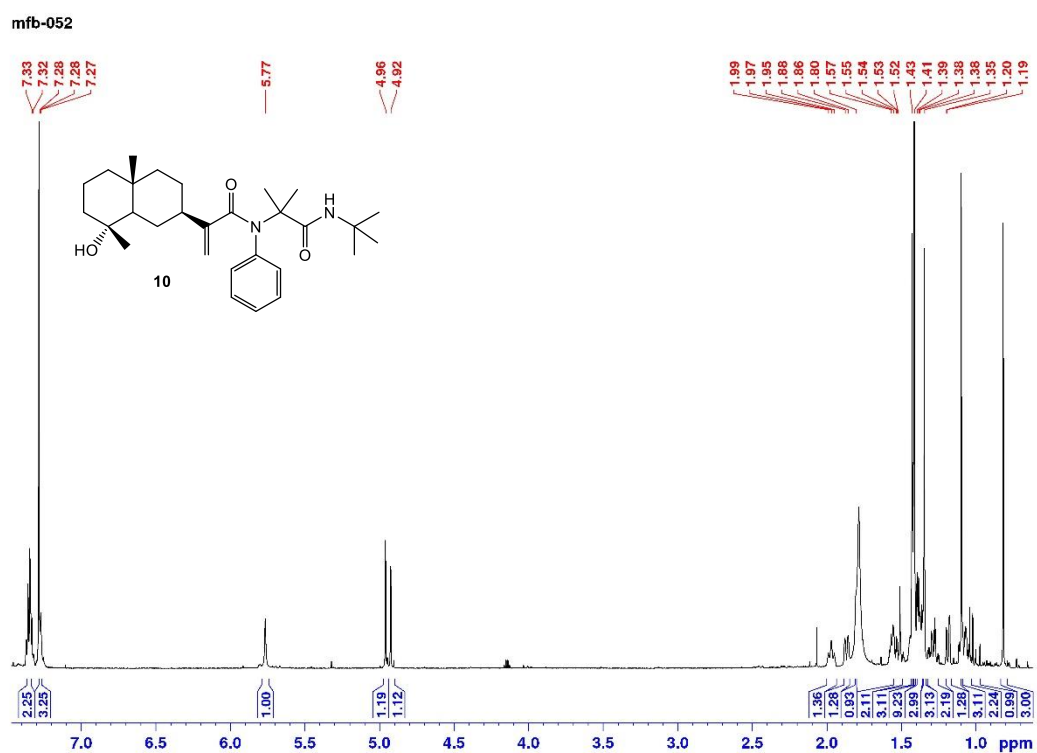


Figure S37. <sup>1</sup>H-NMR of 10.

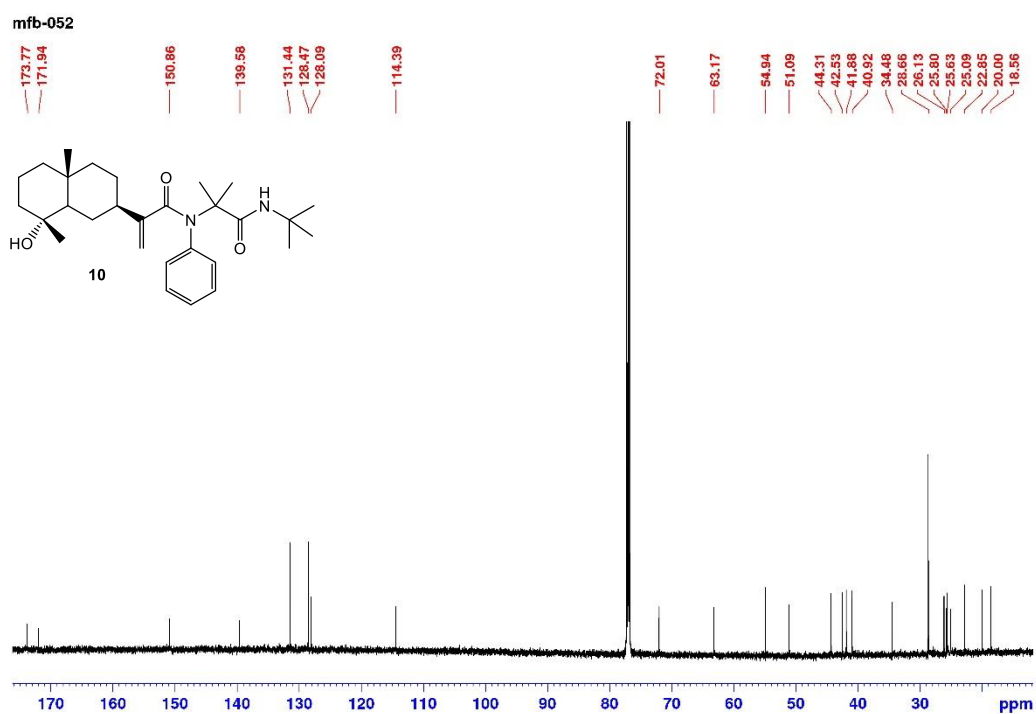


Figure S38. <sup>13</sup>C-NMR of 10.

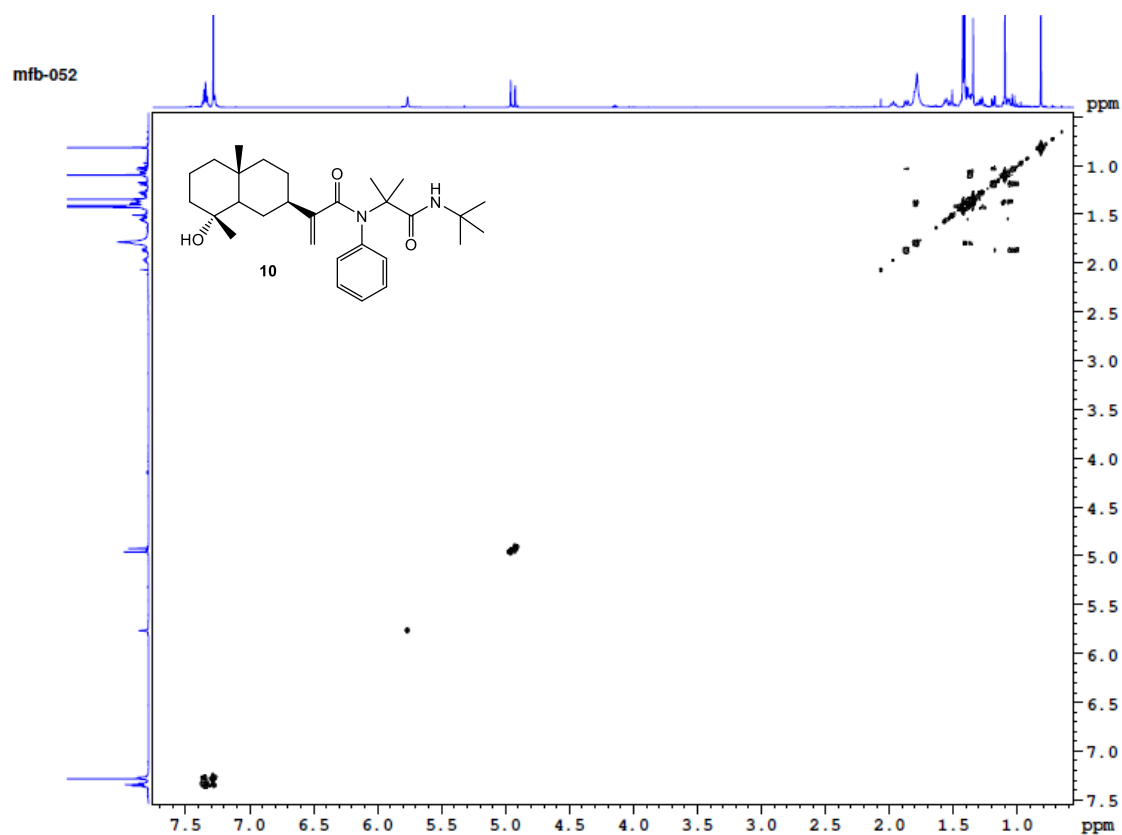
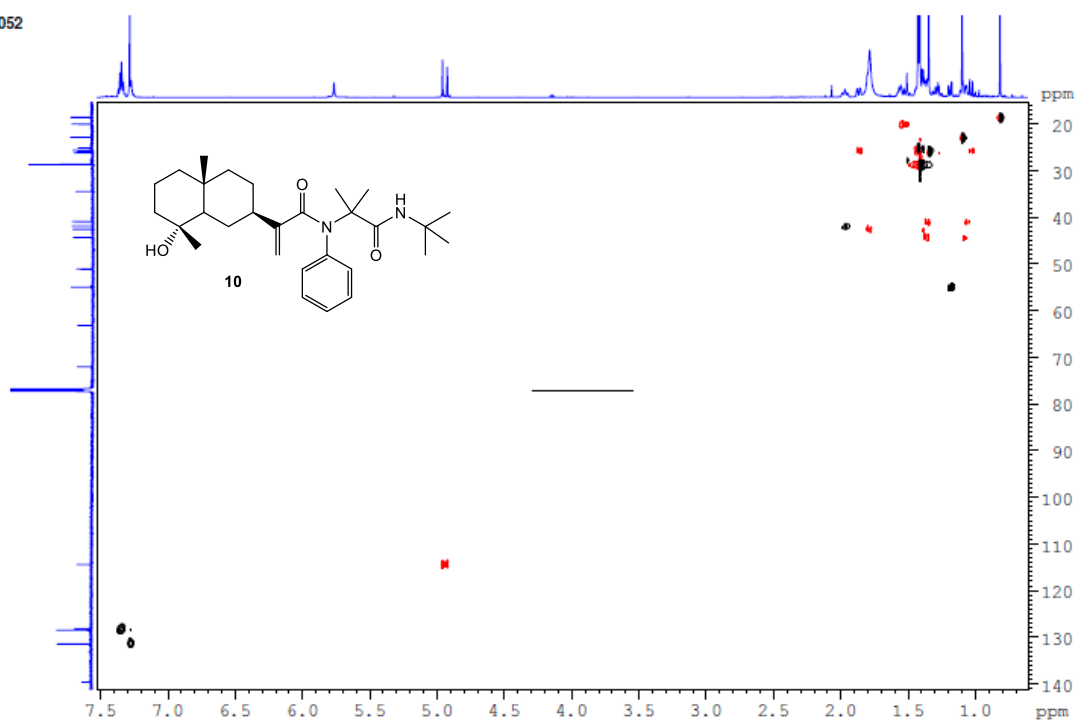
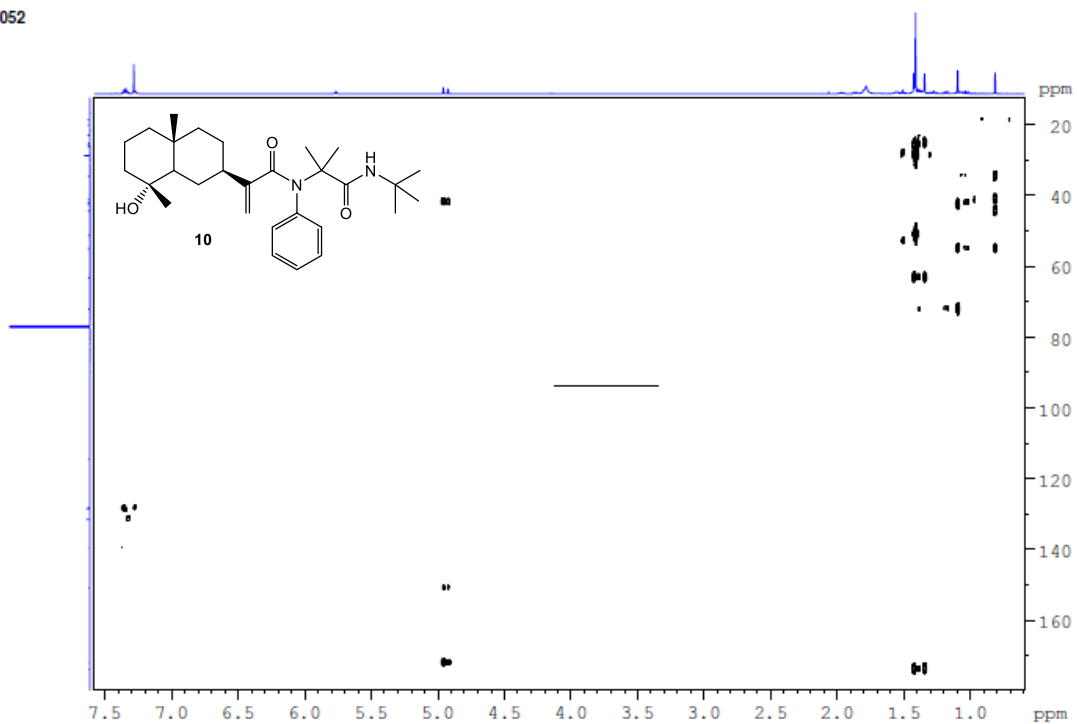


Figure S39. COSY of 10.

mfb-052



mfb-052



mfb-053

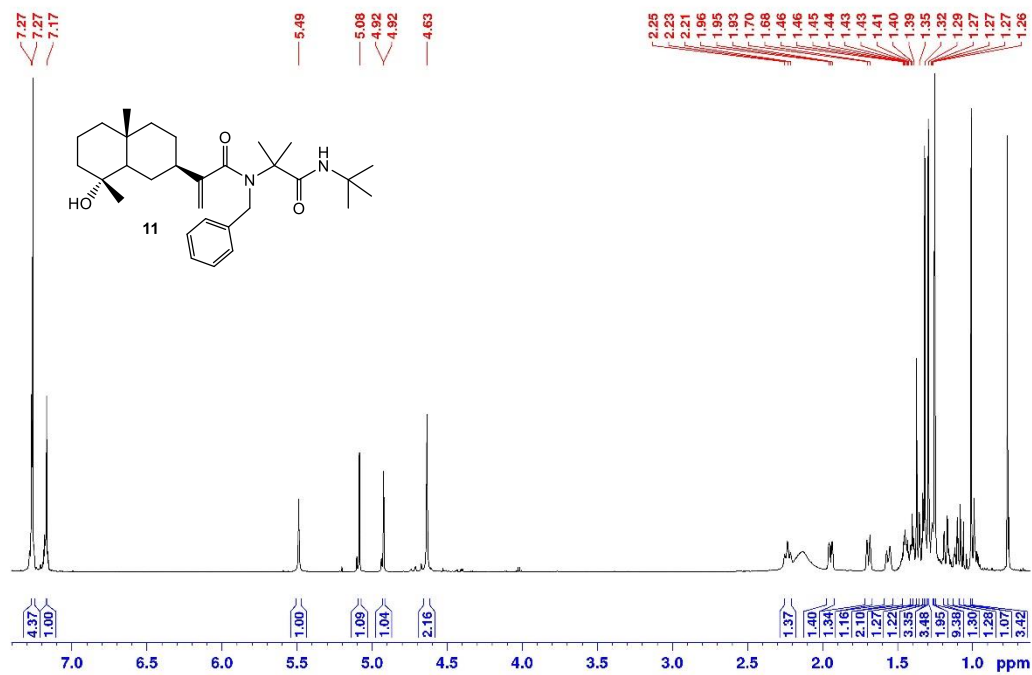


Figure S42. <sup>1</sup>H-NMR of 11.

mfb-053

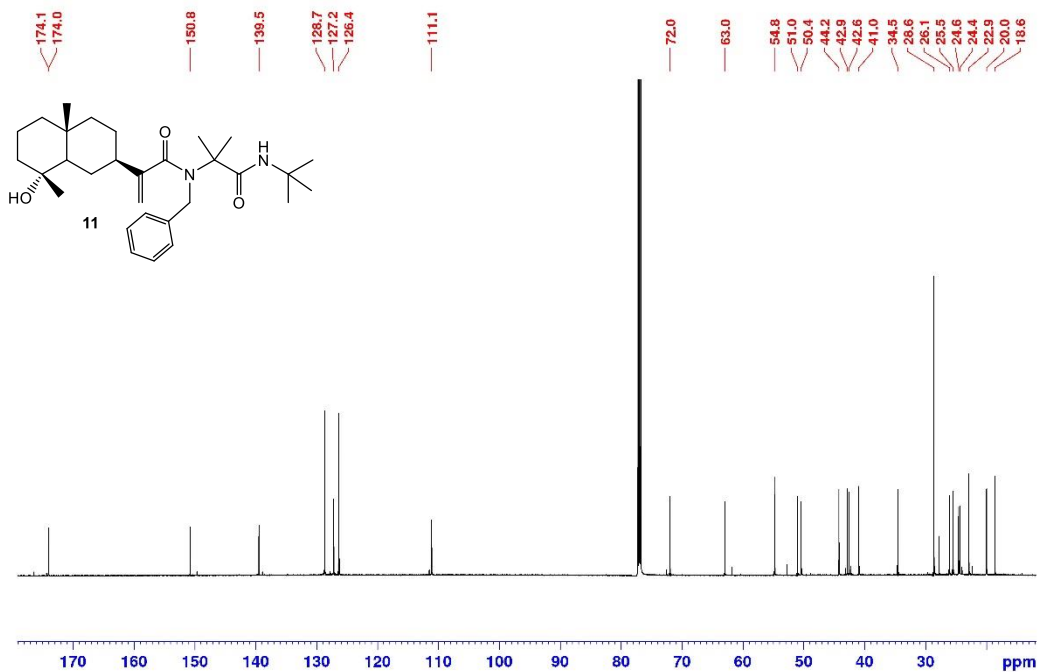


Figure S43. <sup>13</sup>C-NMR of 11.

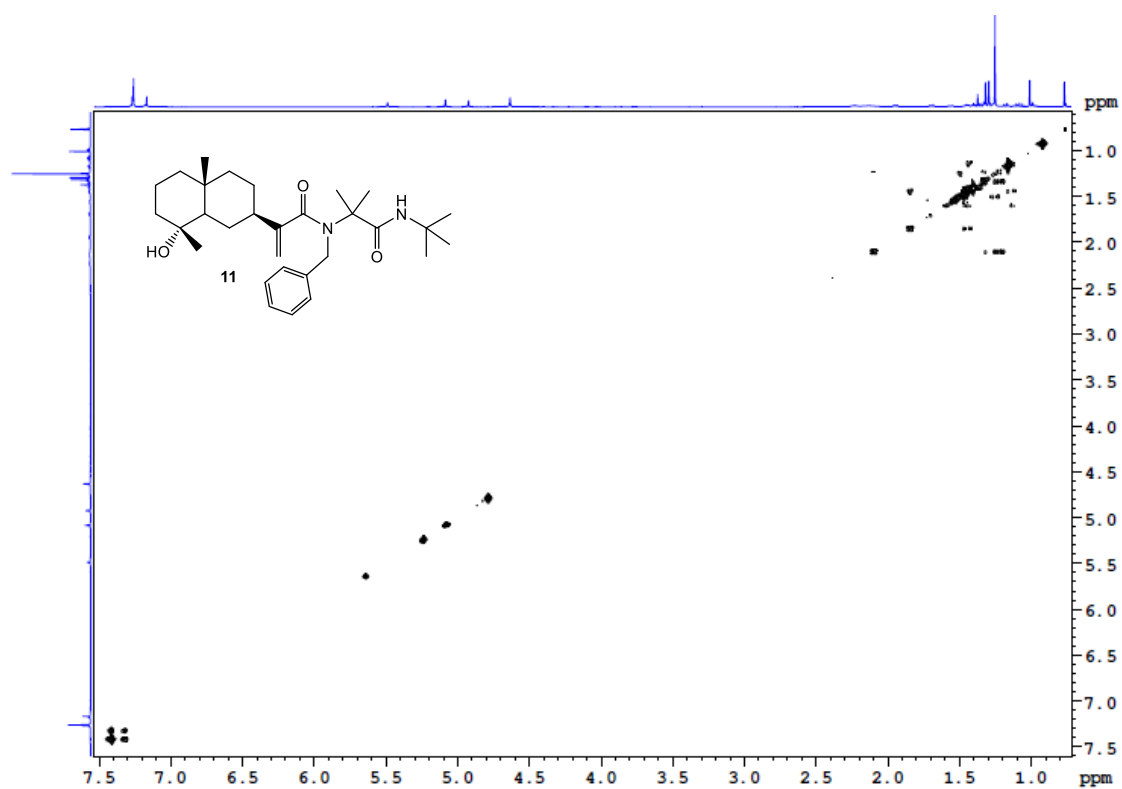


Figure S44. COSY of 11.

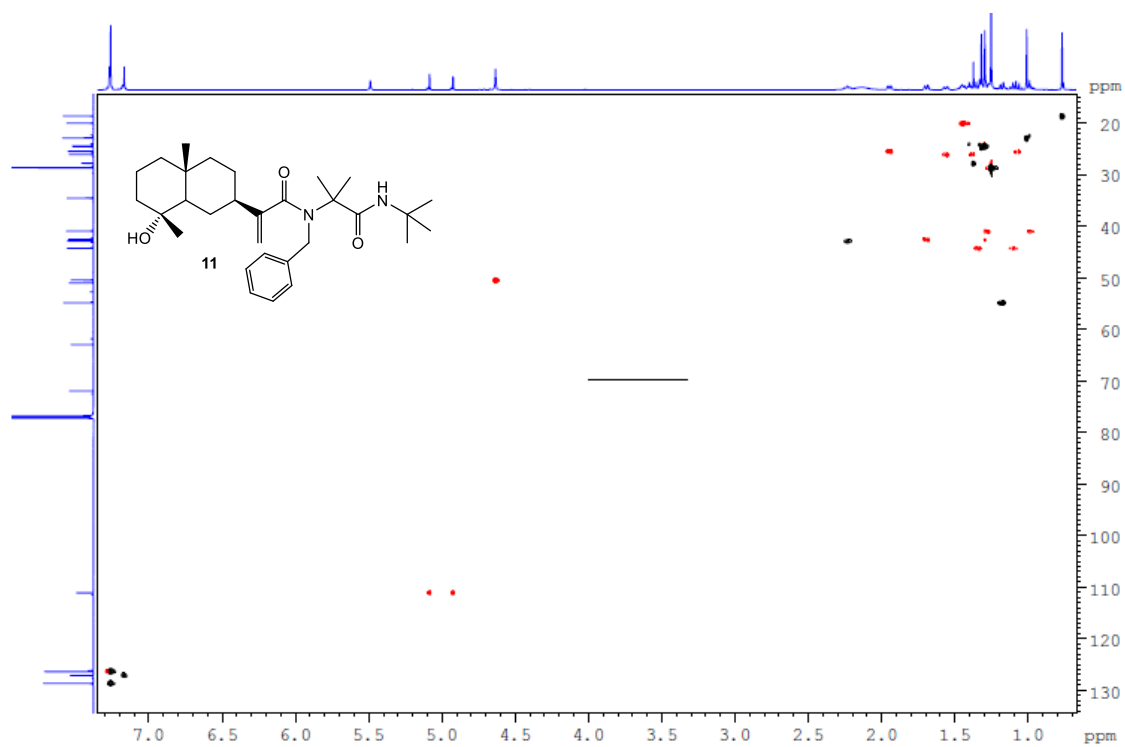


Figure S45. HSQC of 11.

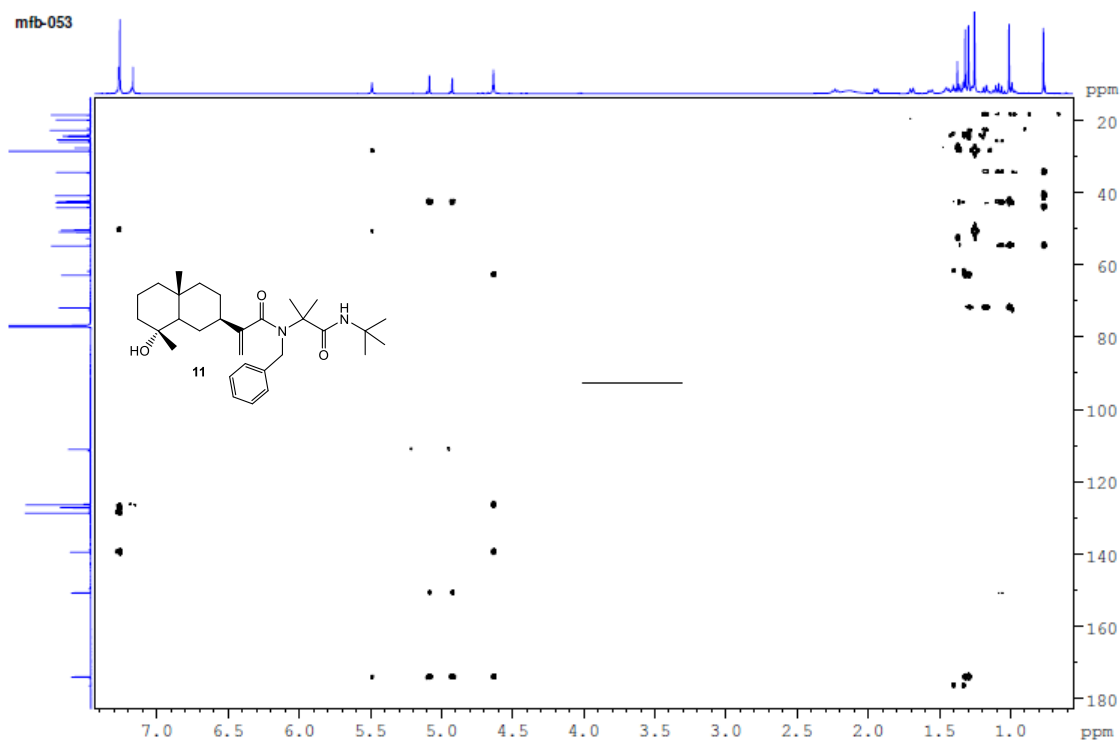


Figure S46. HMBC of 11.

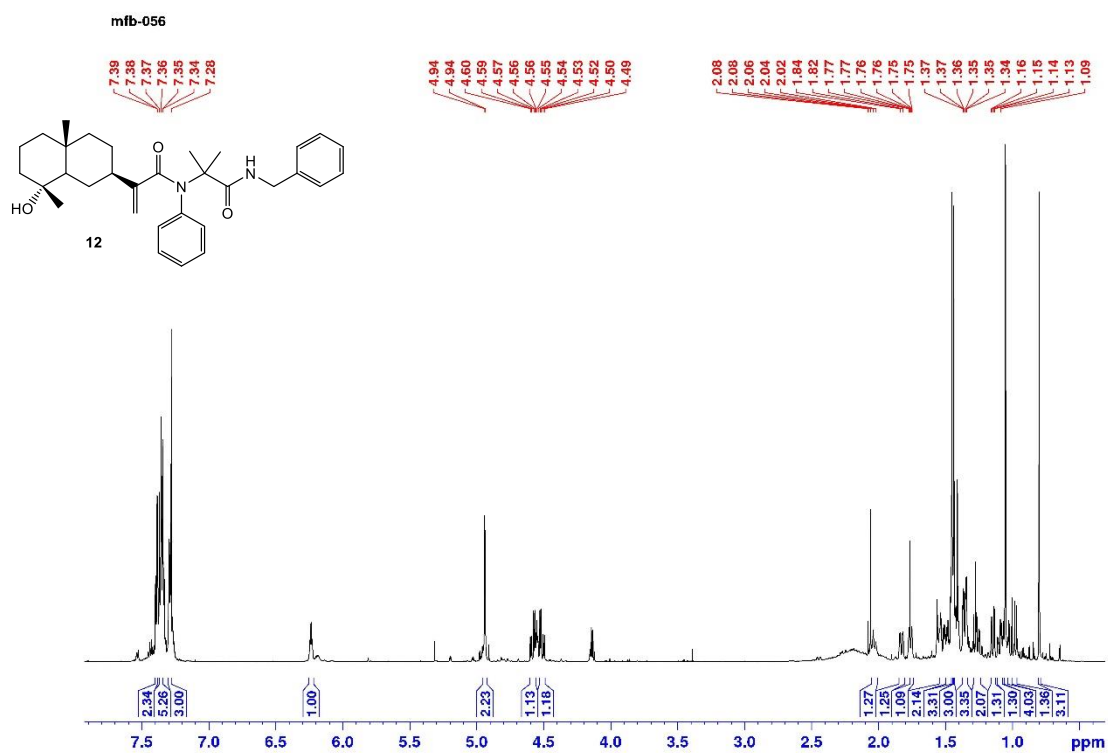


Figure S47.  $^1\text{H}$ -NMR of 12.



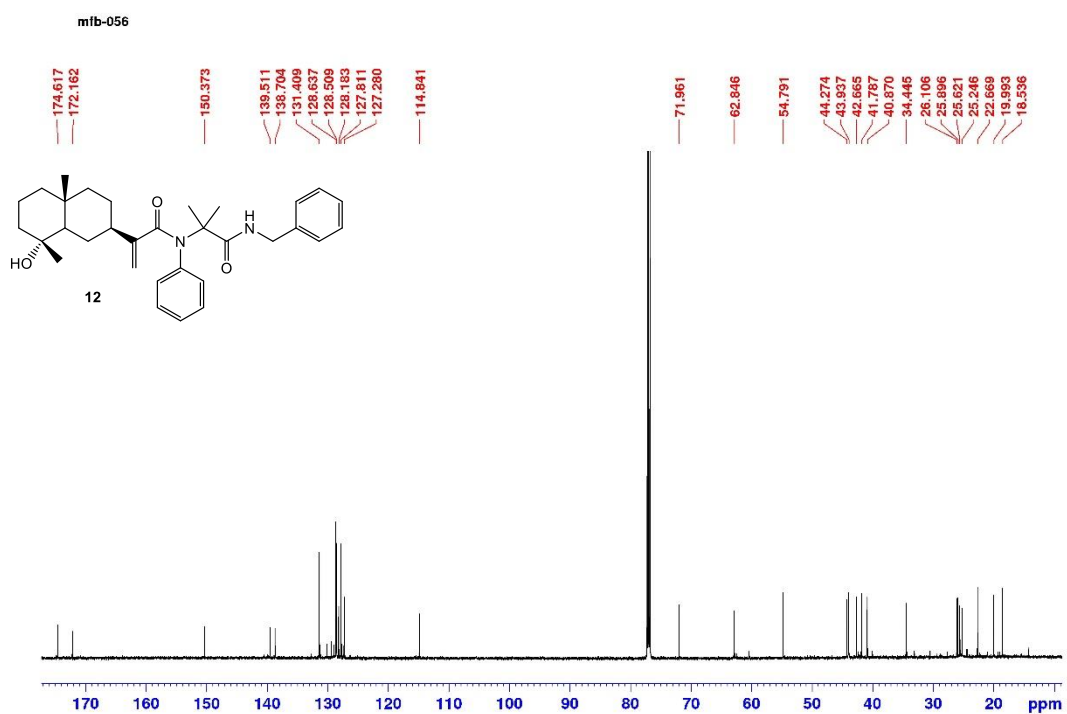


Figure S48.  $^{13}\text{C}$ -NMR of 12.

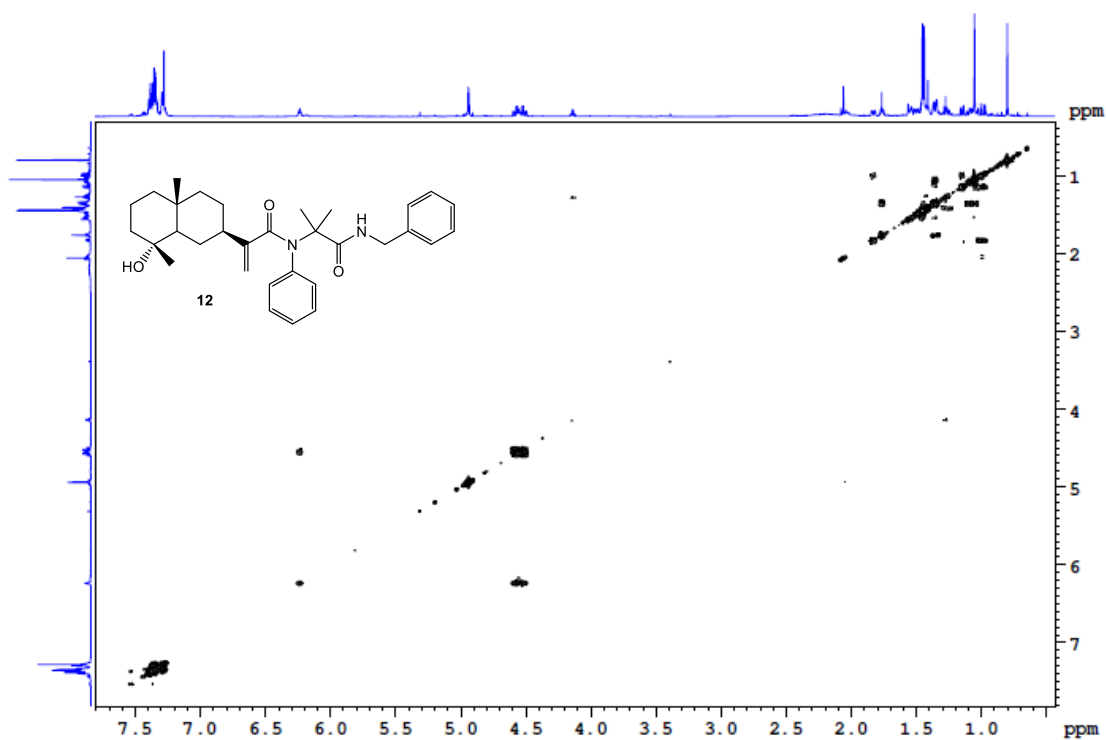


Figure S49. COSY of 12.

mf0-056

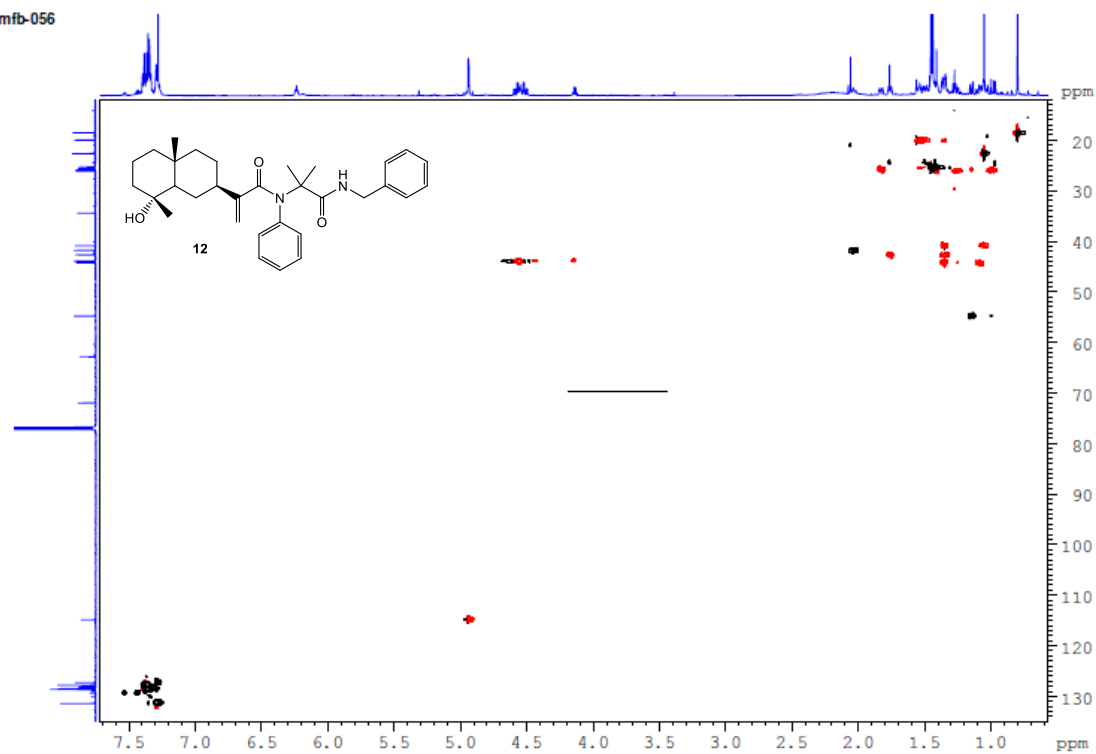


Figure S50. HSQC of 12.

mf0-056

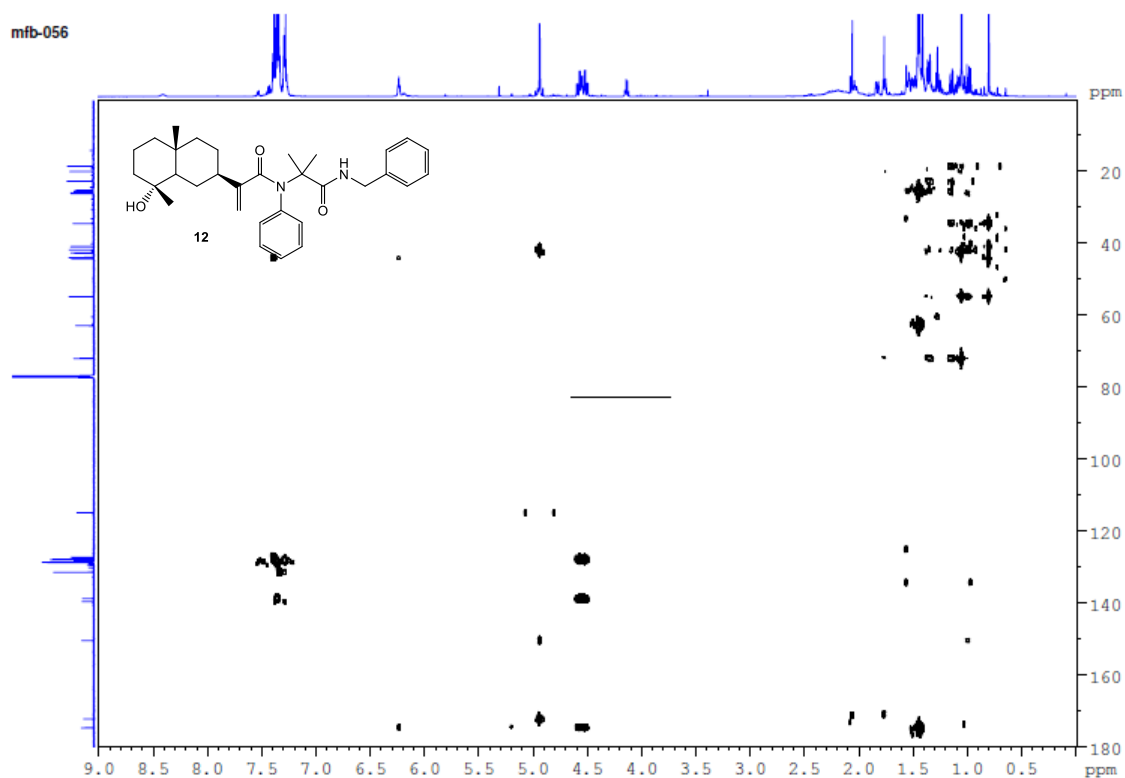


Figure S51. HMBC of 12.

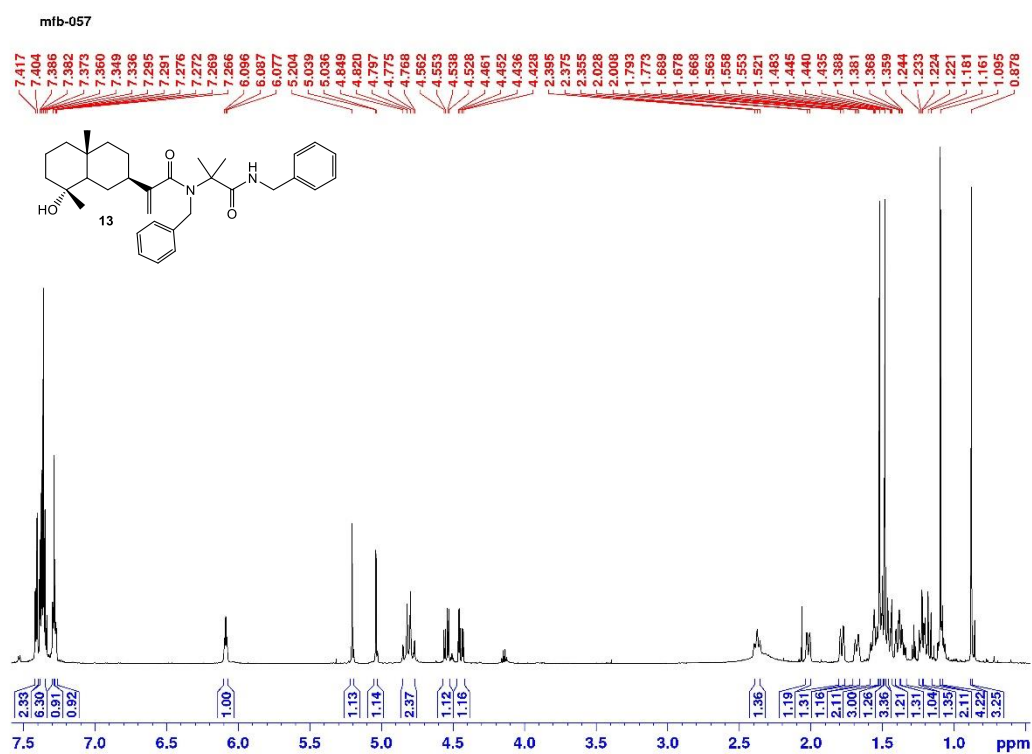


Figure S52. <sup>1</sup>H-NMR of 13.

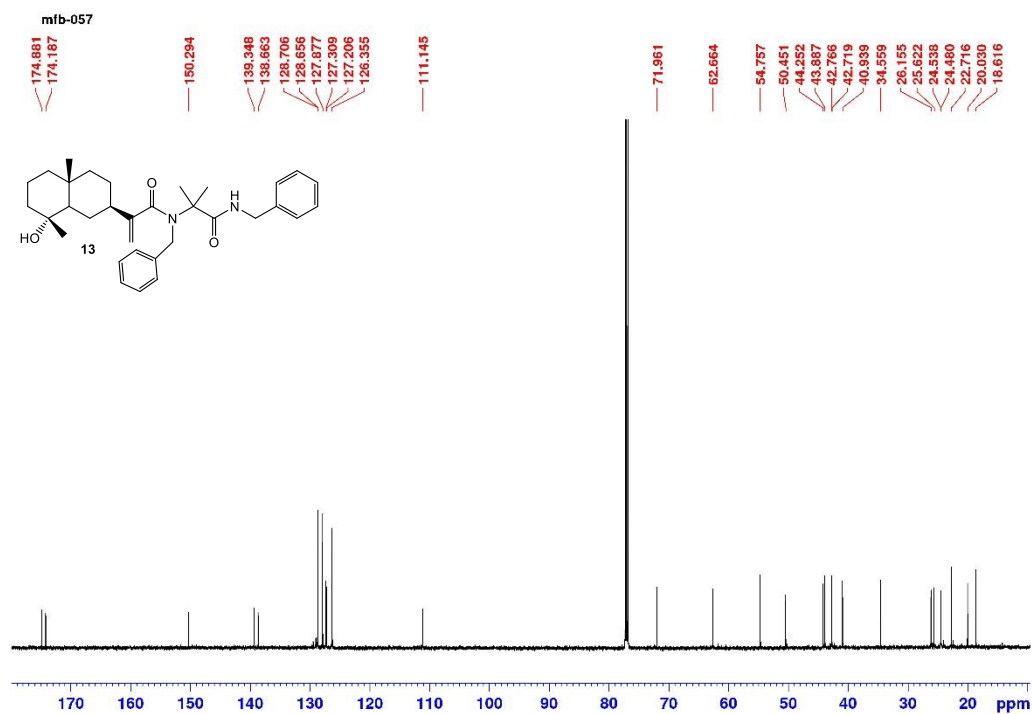
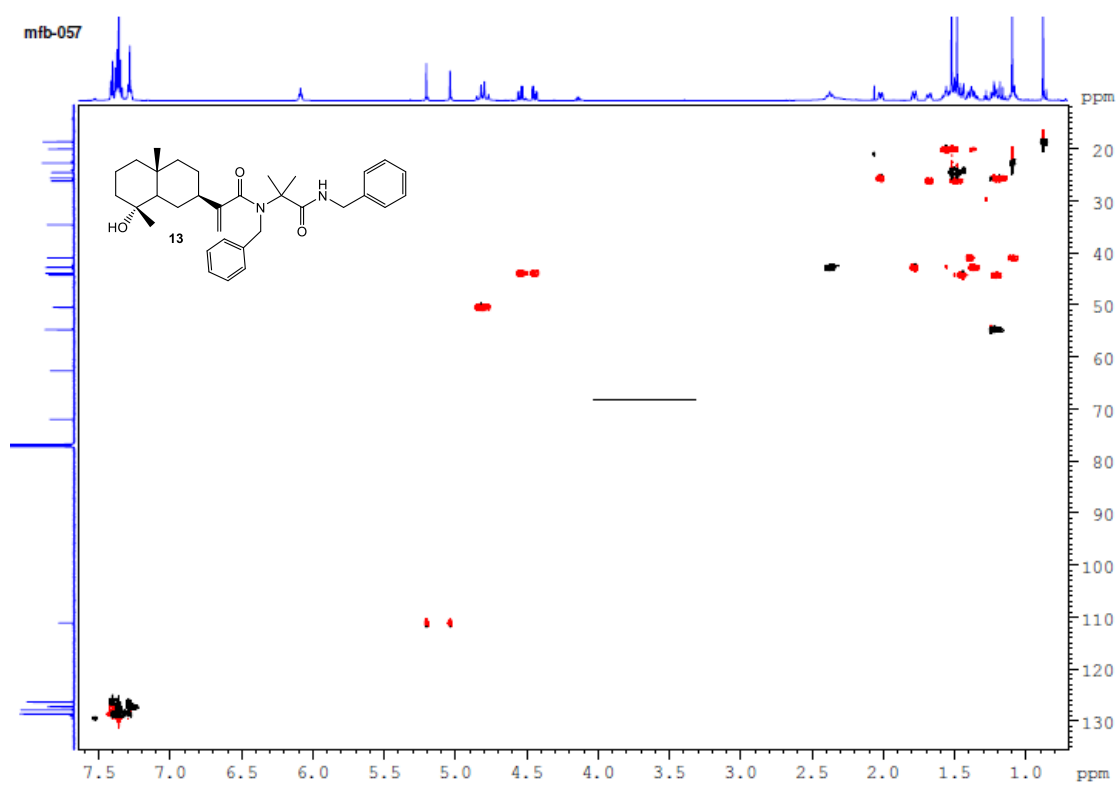
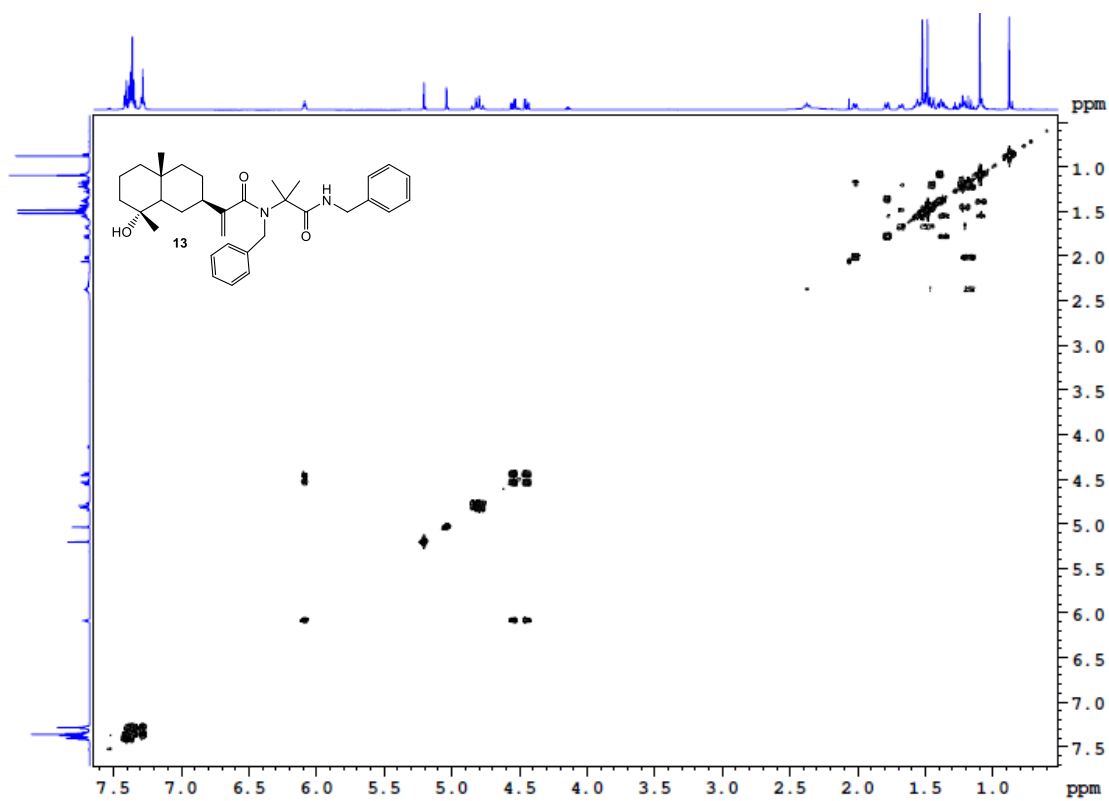


Figure S53. <sup>13</sup>C-NMR of 13.



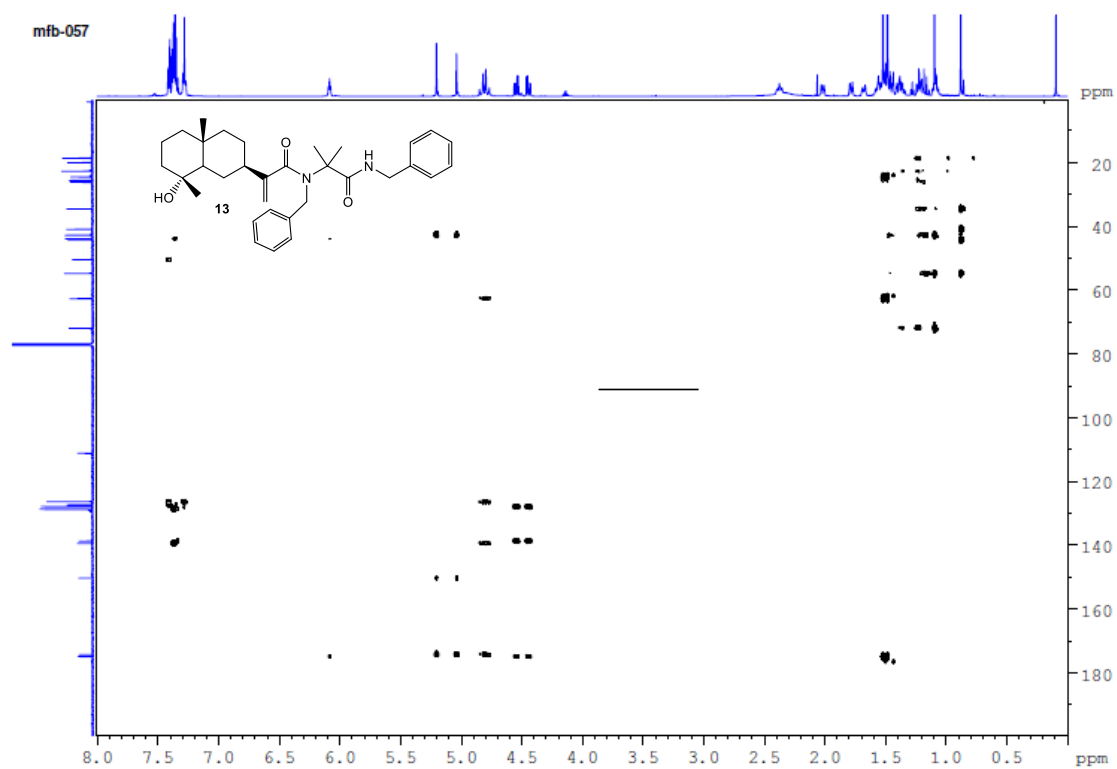


Figure S56. HMBC of 13.

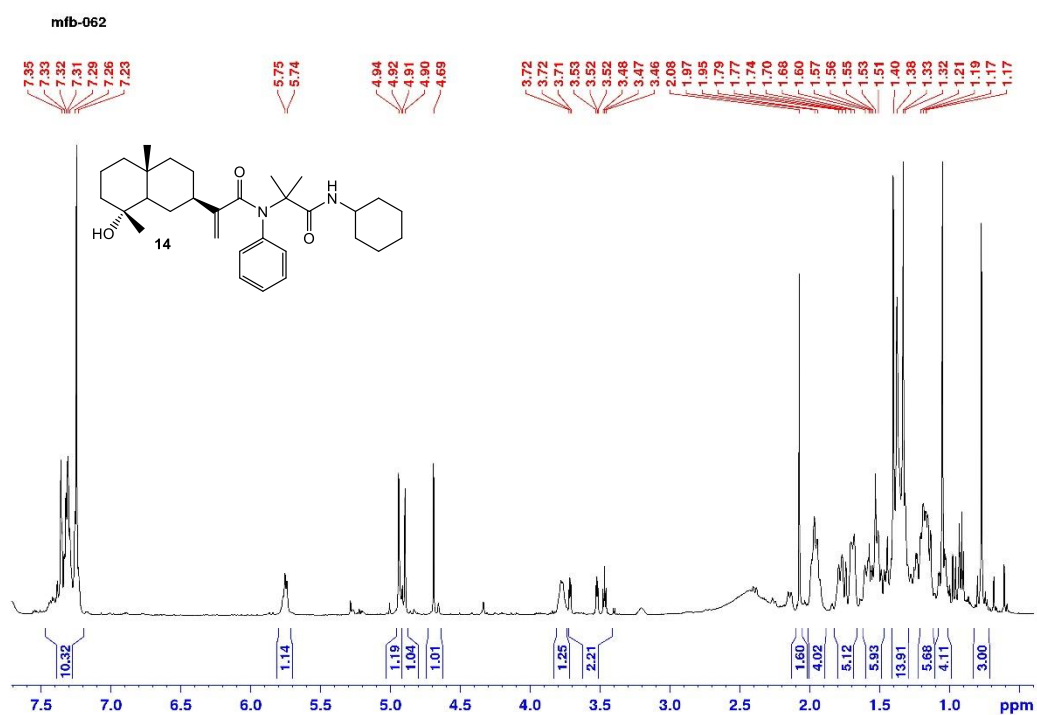


Figure S57.  $^1\text{H}$ -NMR of 14.

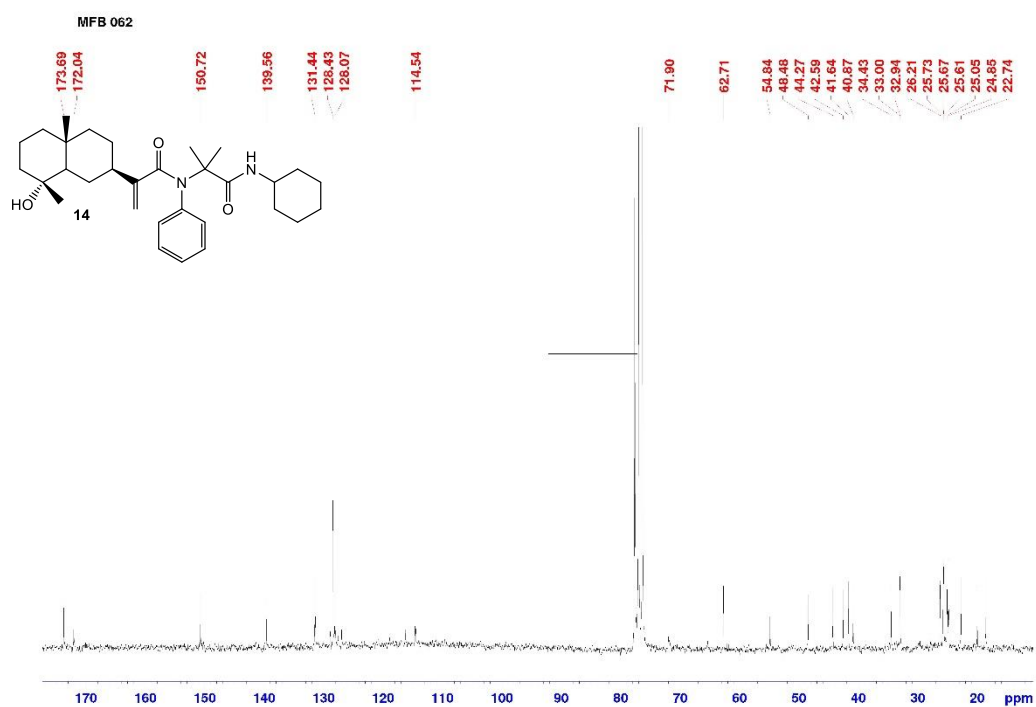


Figure S58.  $^{13}\text{C}$ -NMR of 14.

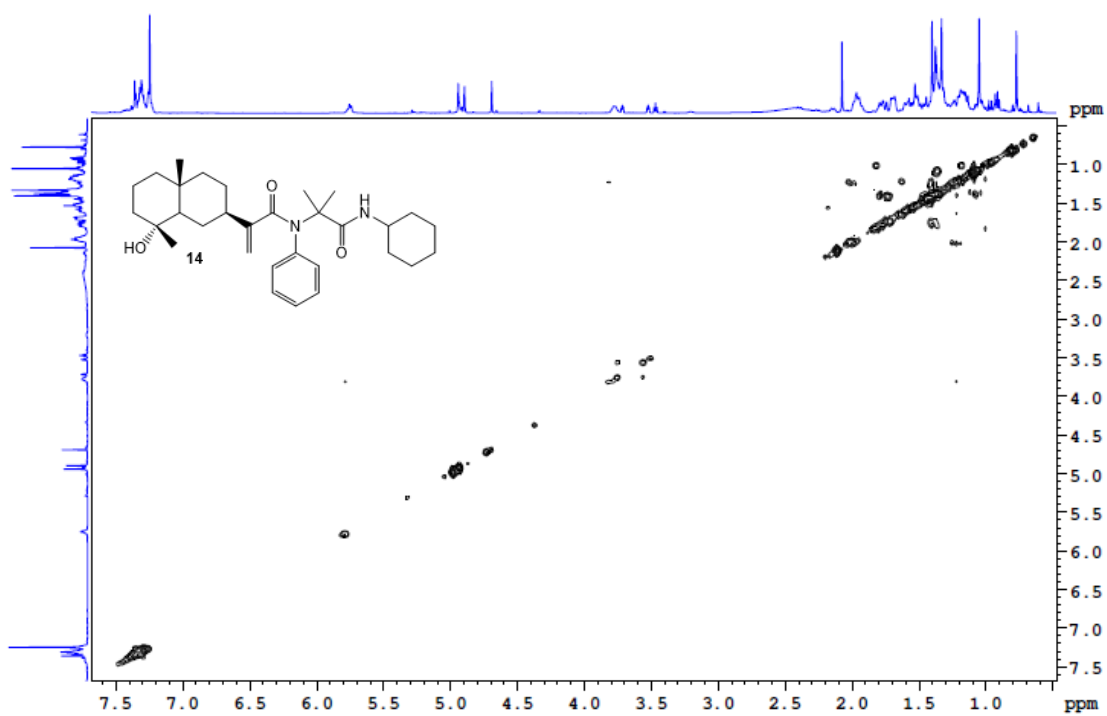


Figure S59. COSY of 14.

mf0-062

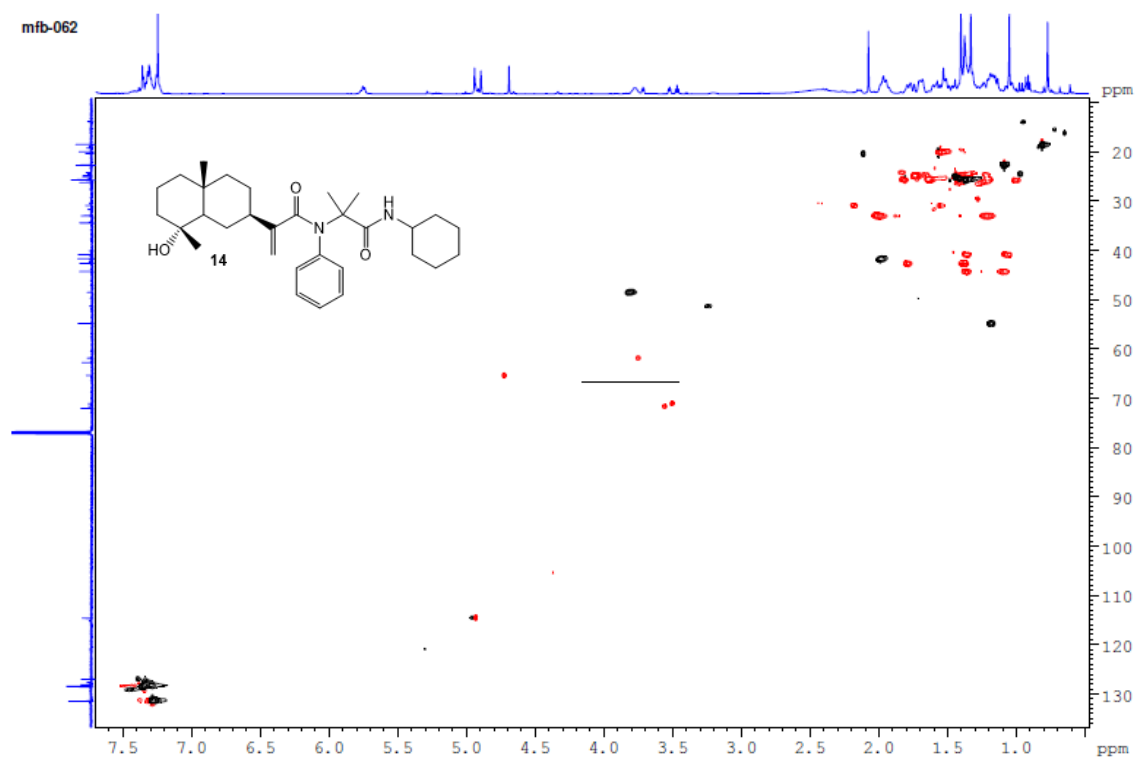


Figure S60. HSQC of 14.

mf0-062

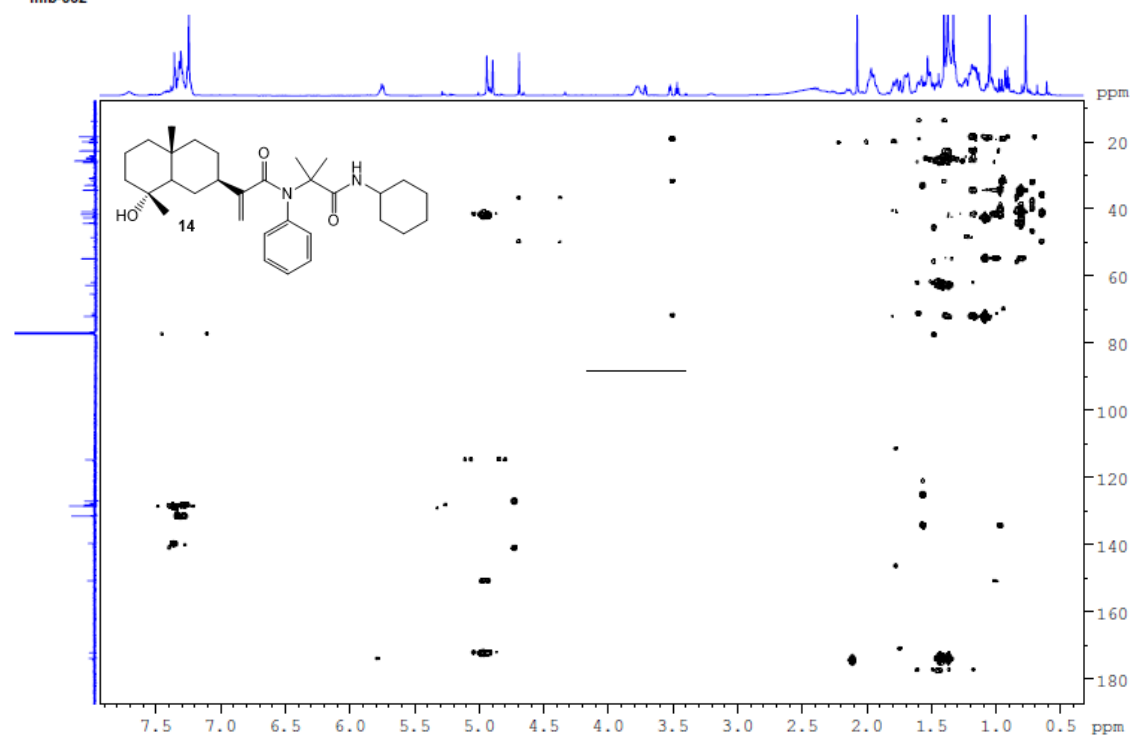


Figure S61. HMBC of 14.

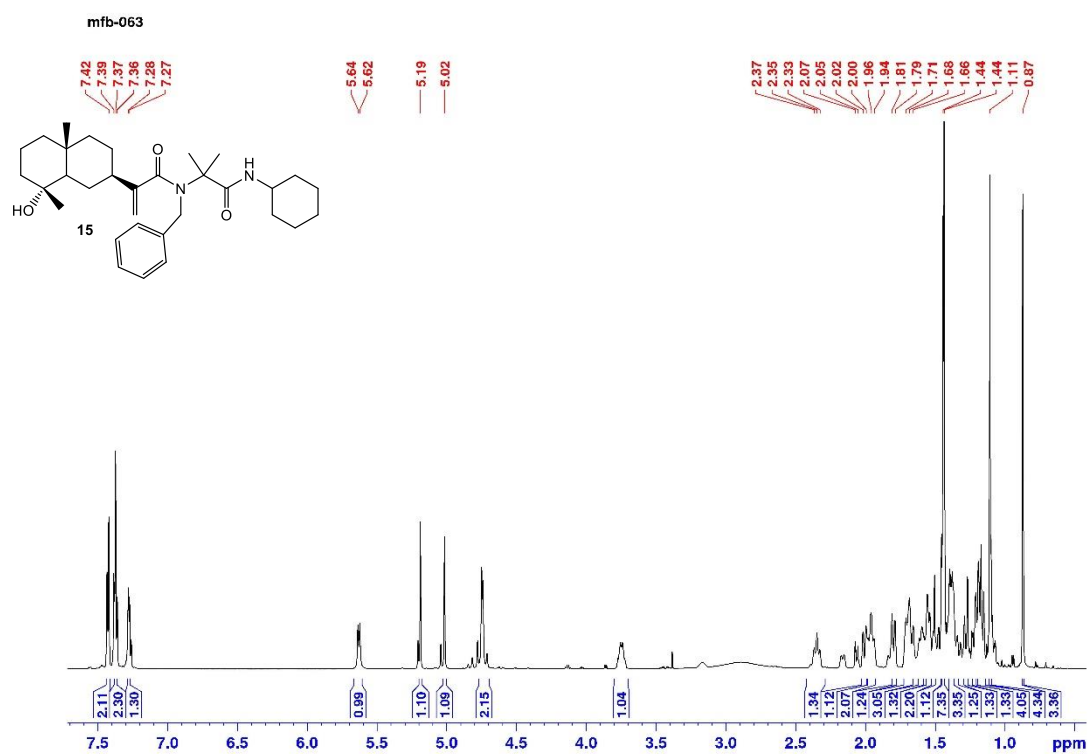


Figure S62. <sup>1</sup>H-NMR of 15.

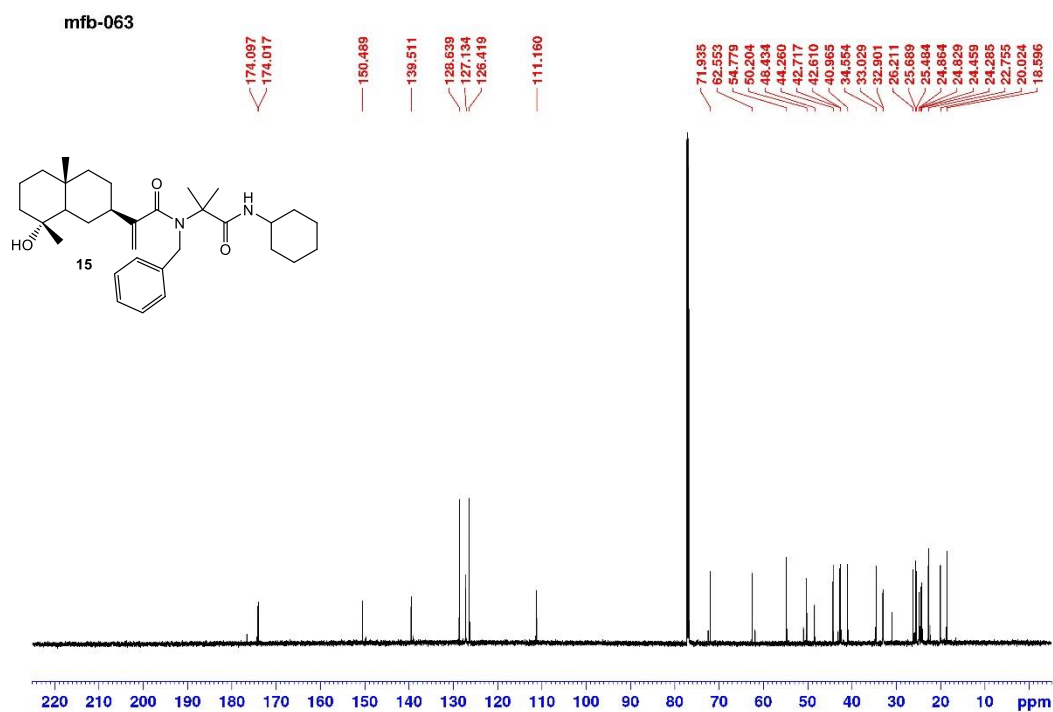


Figure S63. <sup>13</sup>C-NMR of 15.



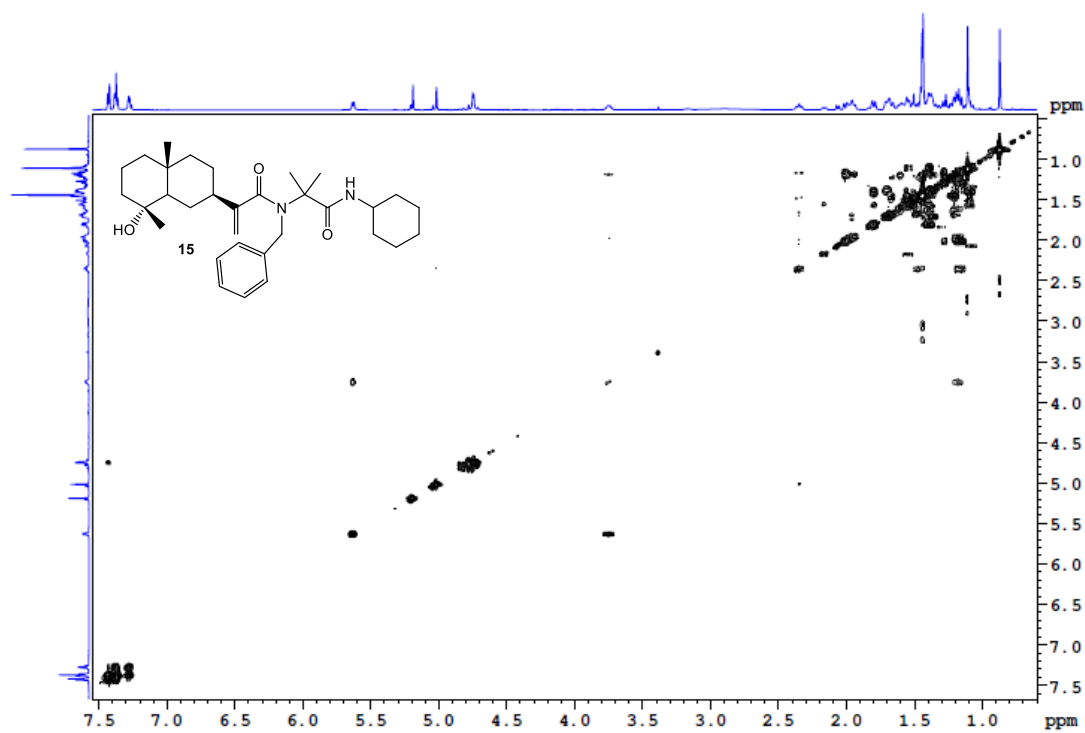


Figure S64. COSY of 15.

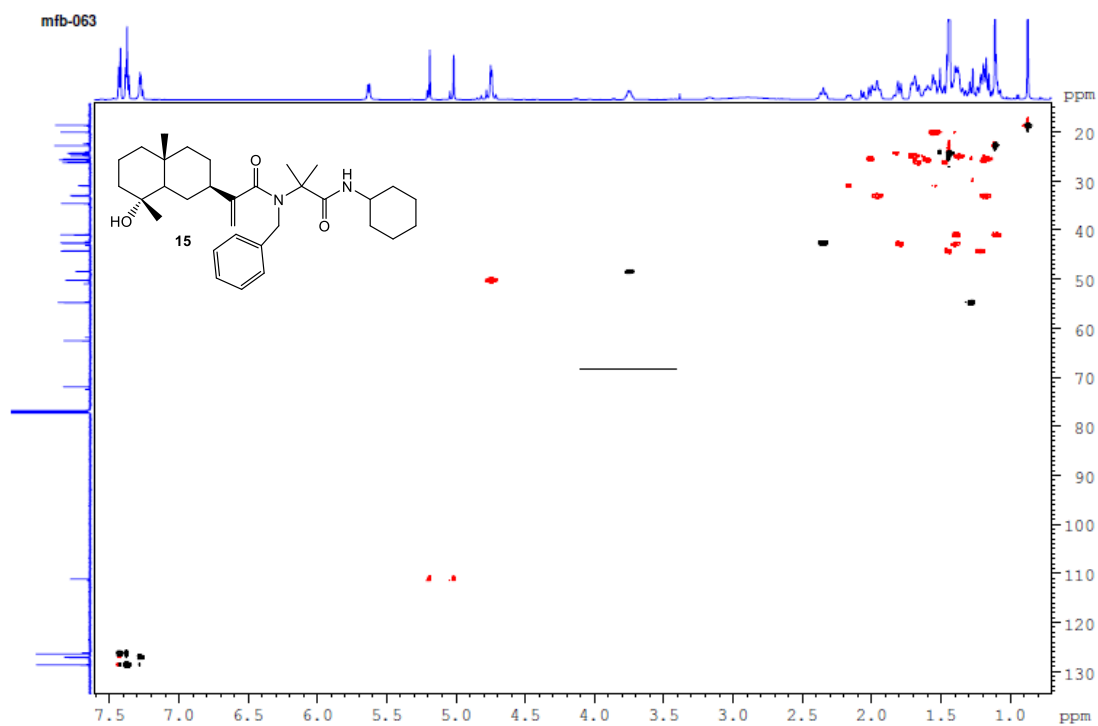


Figure S65. HSQC of 15.

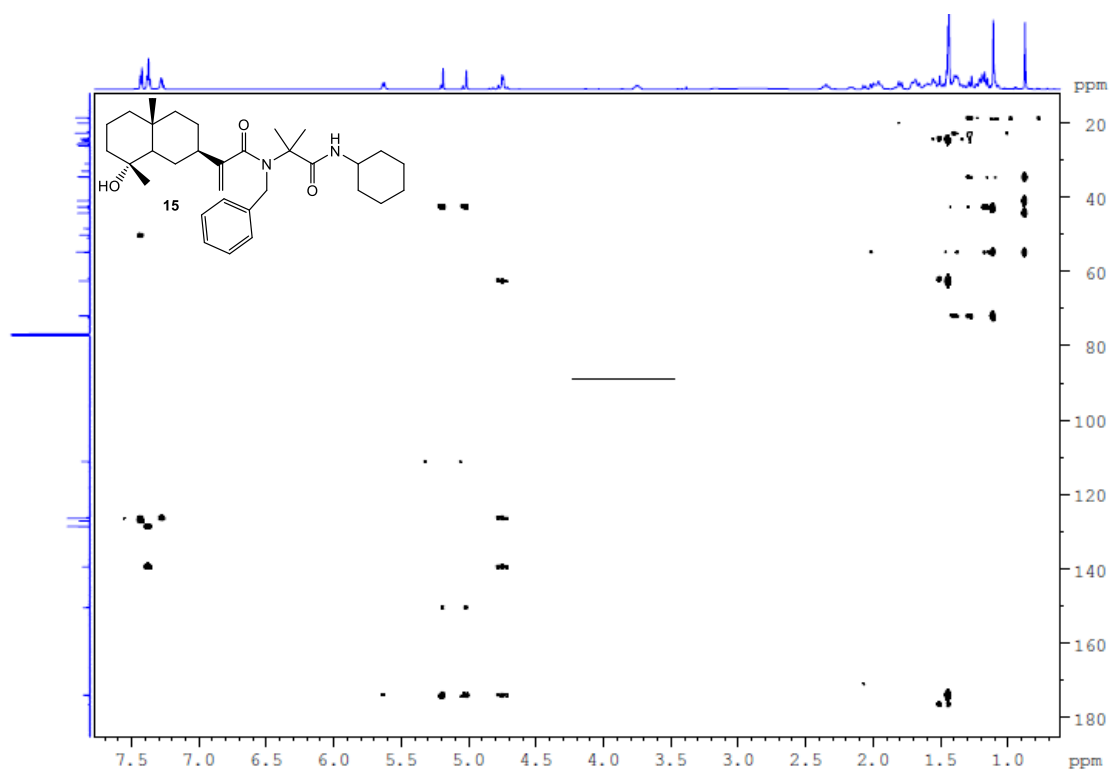


Figure S66. HMBC of 15.

#### 4. NMR spectra of Illic alcohol derivatives

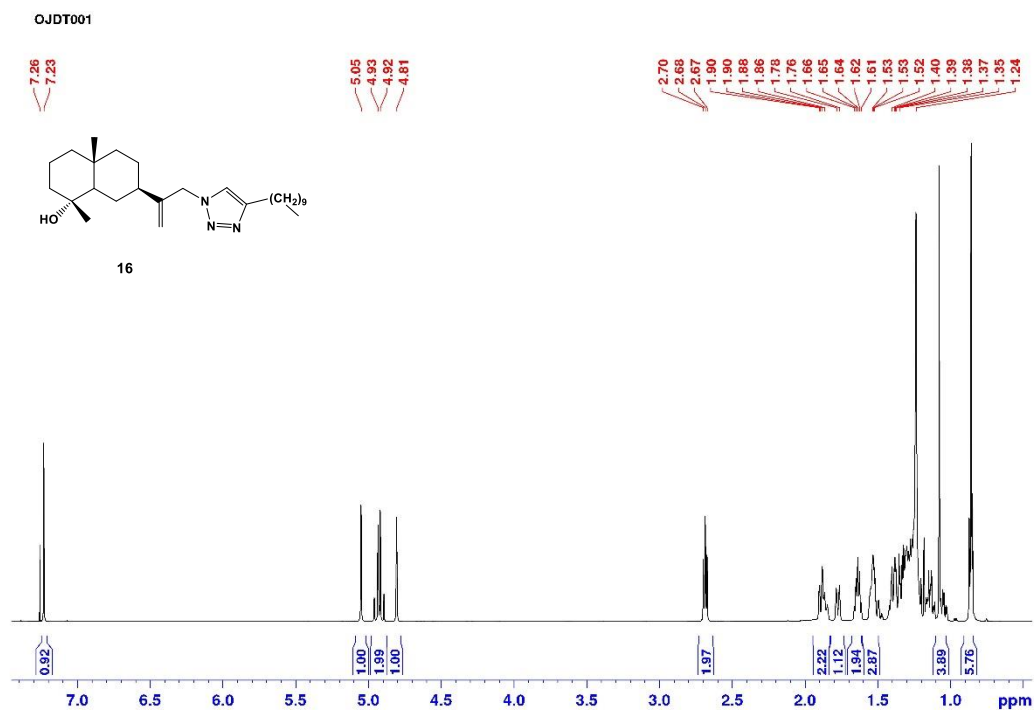


Figure S67.  $^1\text{H}$ -NMR of 16.

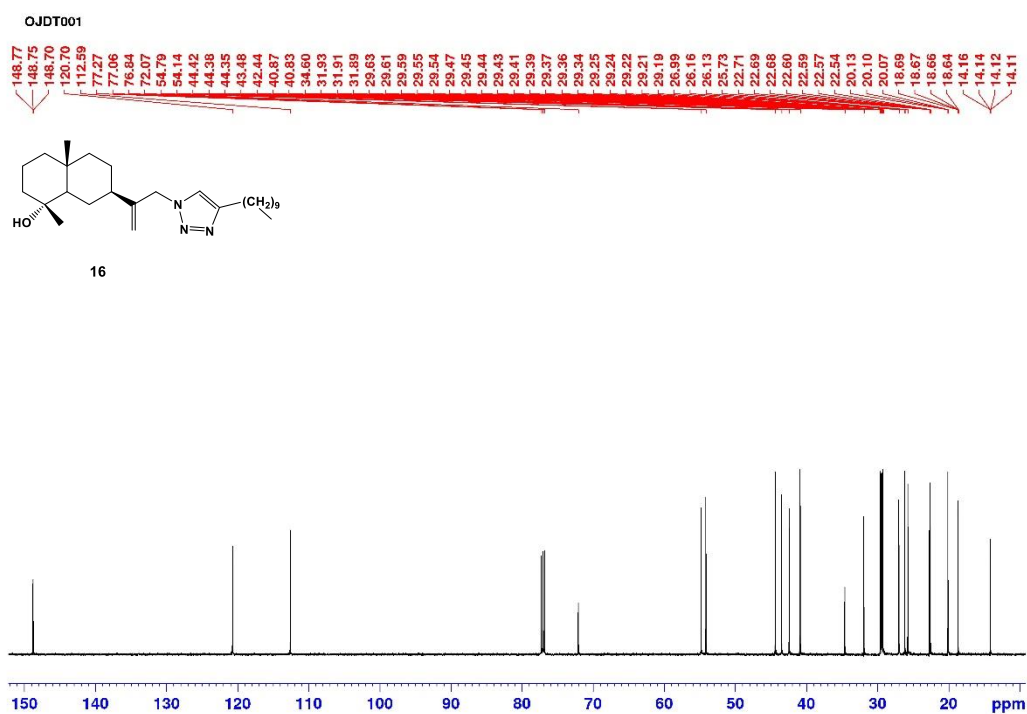


Figure S68.  $^{13}\text{C}$ -NMR of 16.

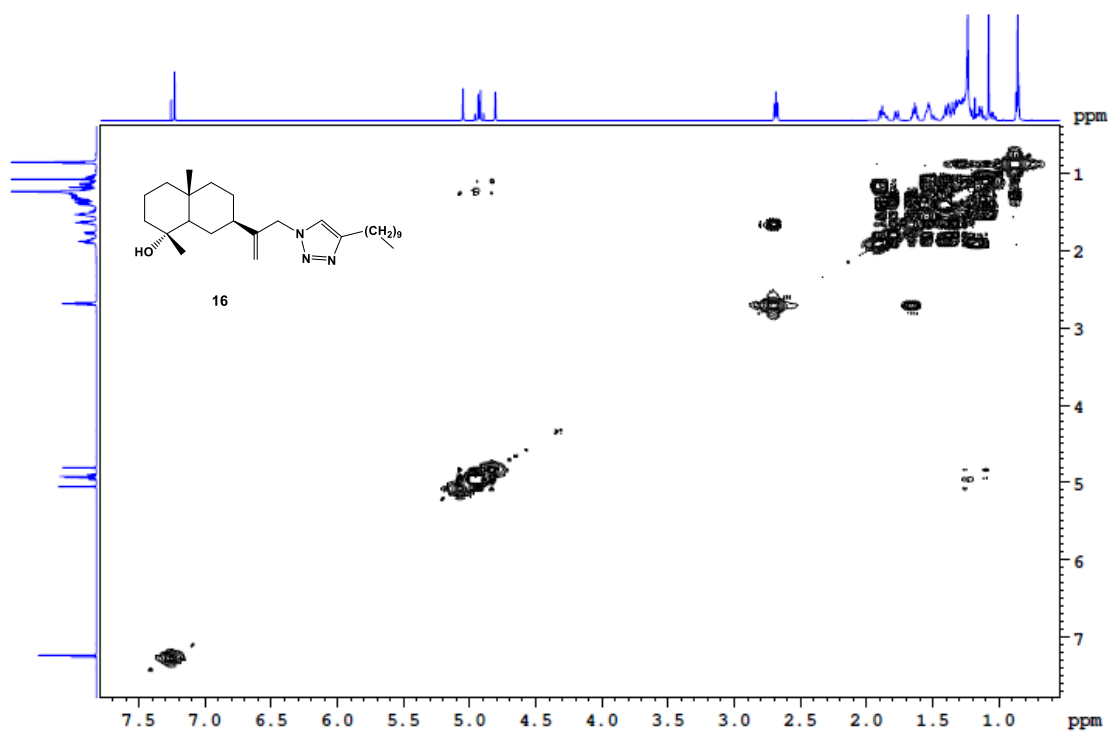


Figure S69. COSY of 16.

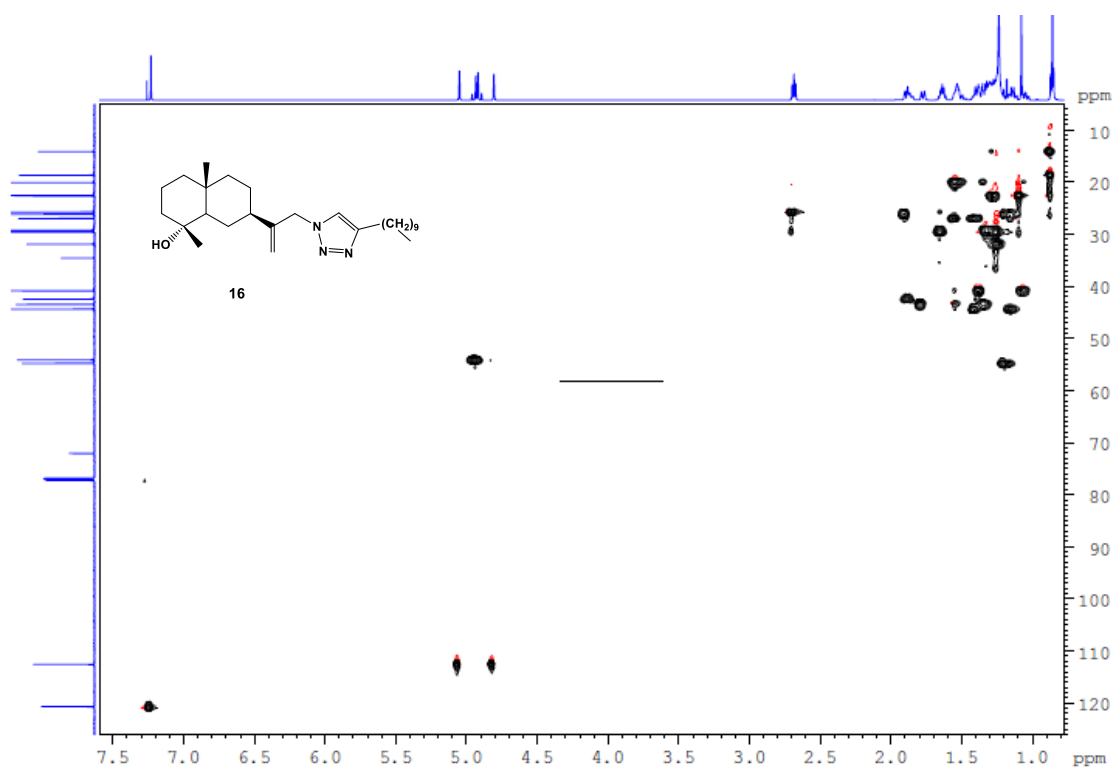


Figure S70. HSQC of 16.

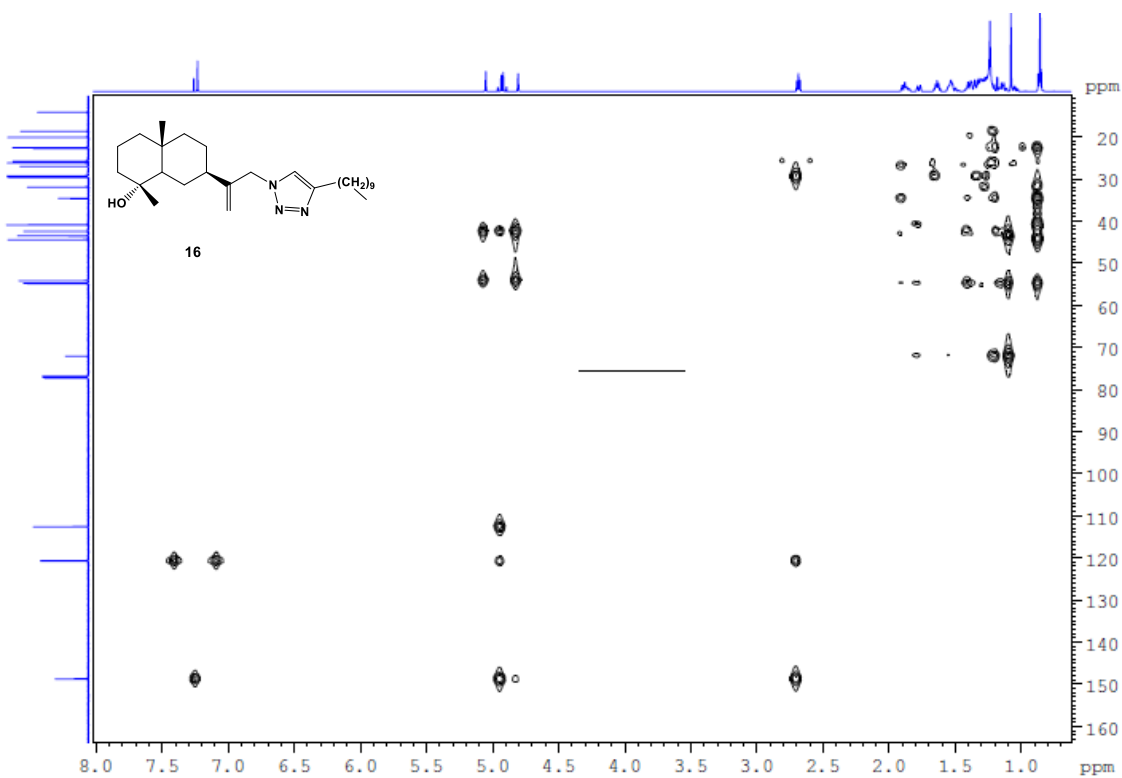


Figure S71. HMBC of 16.

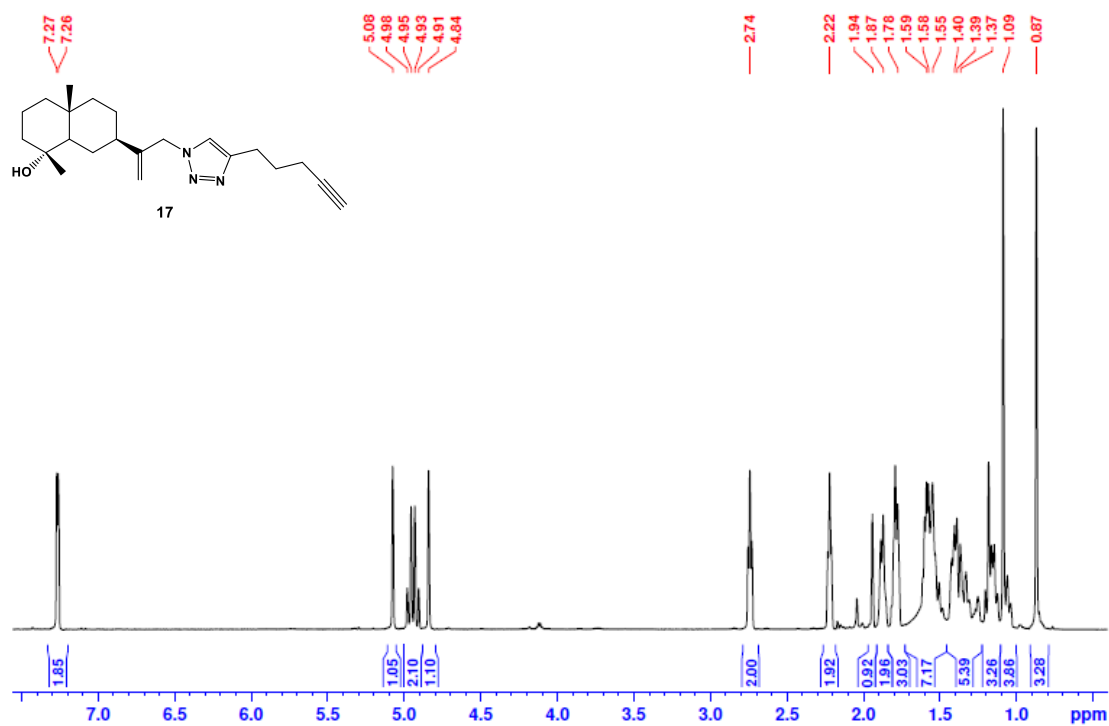


Figure S72. <sup>1</sup>H-NMR of 17.

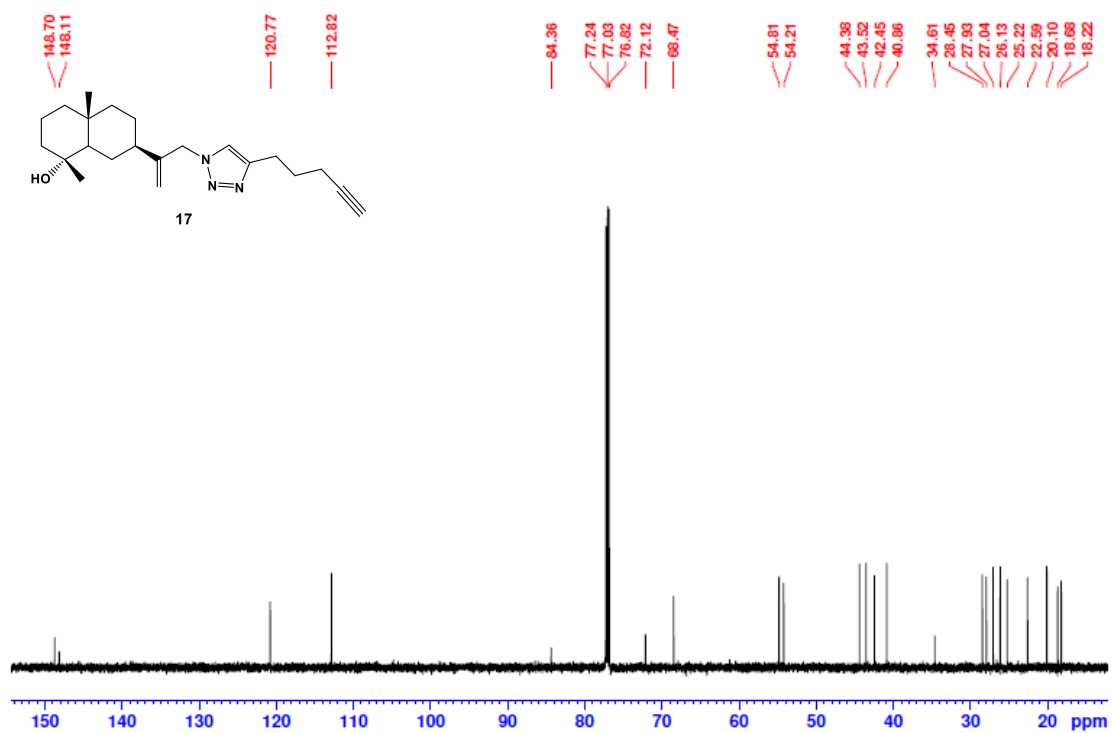


Figure S73. <sup>13</sup>C-NMR of 17.

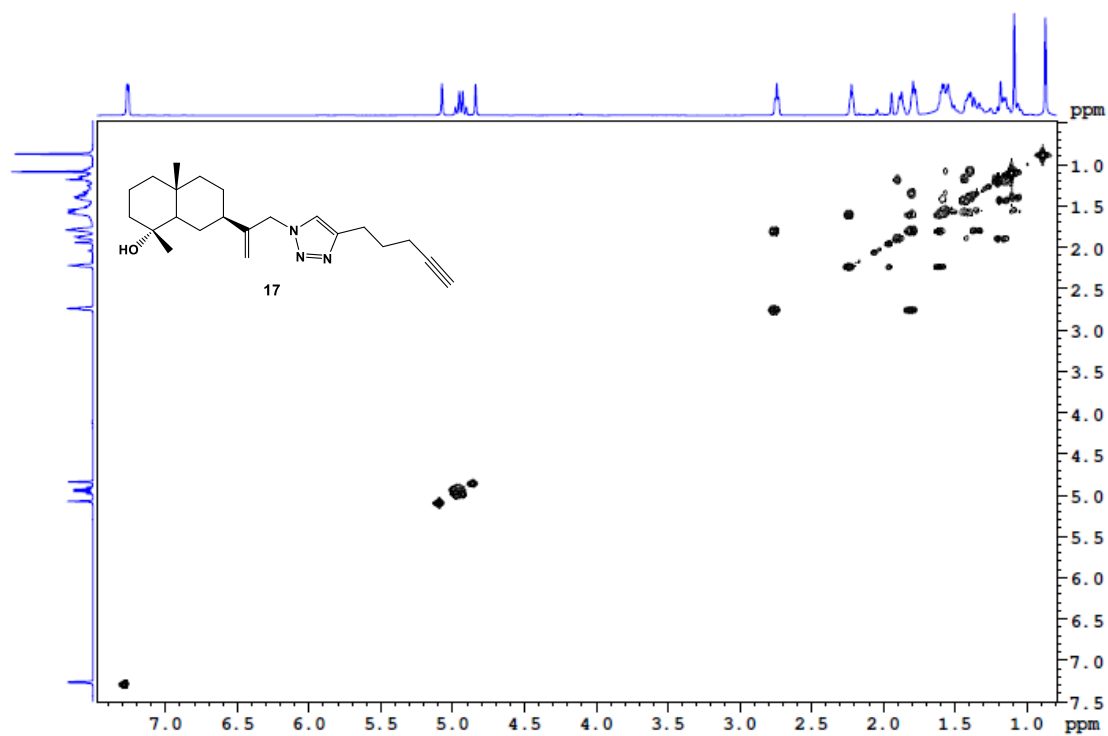


Figure S74. COSY of 17.

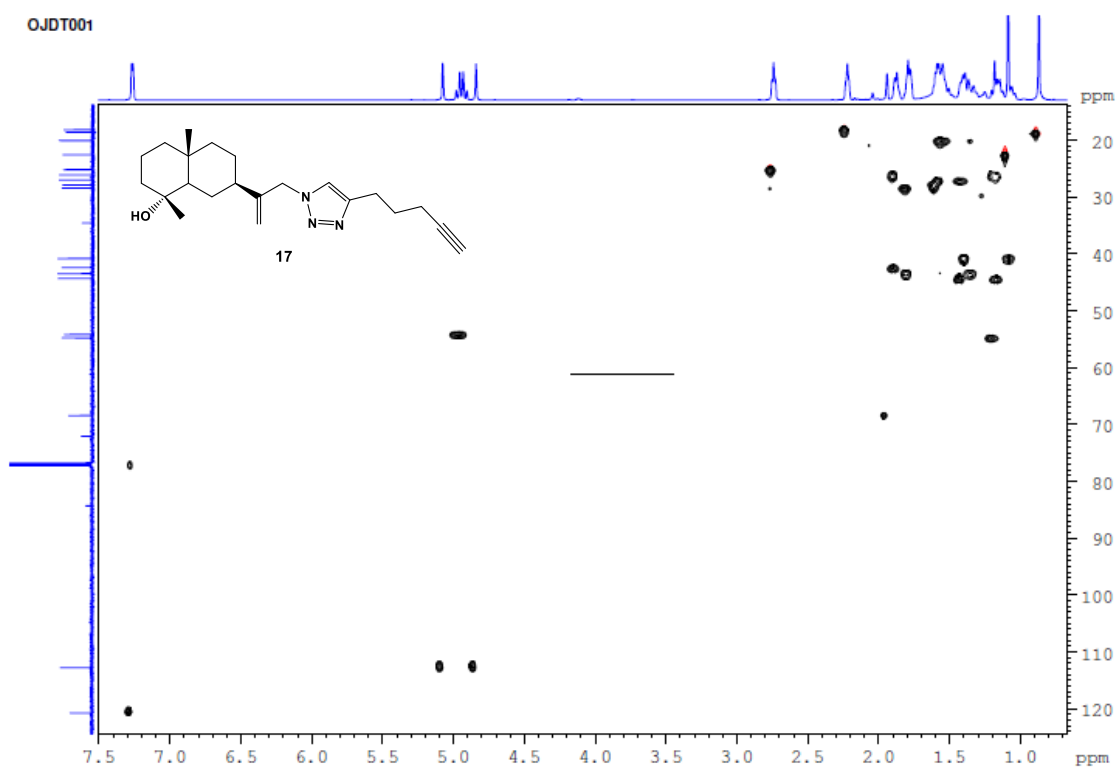
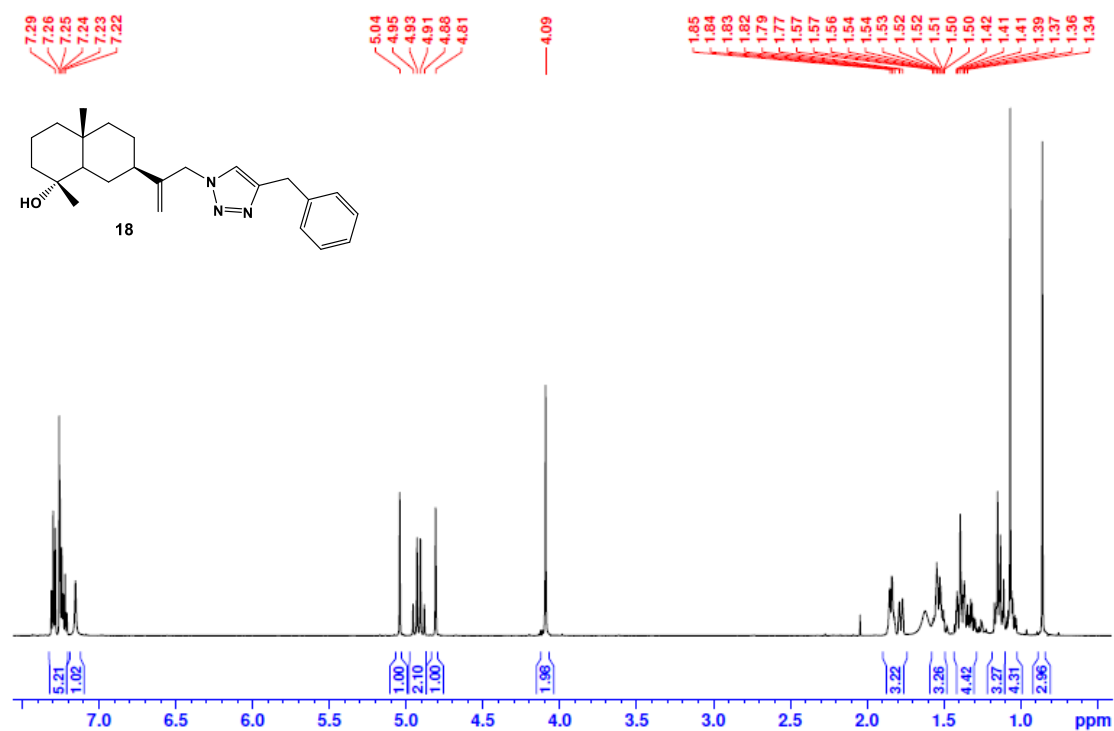
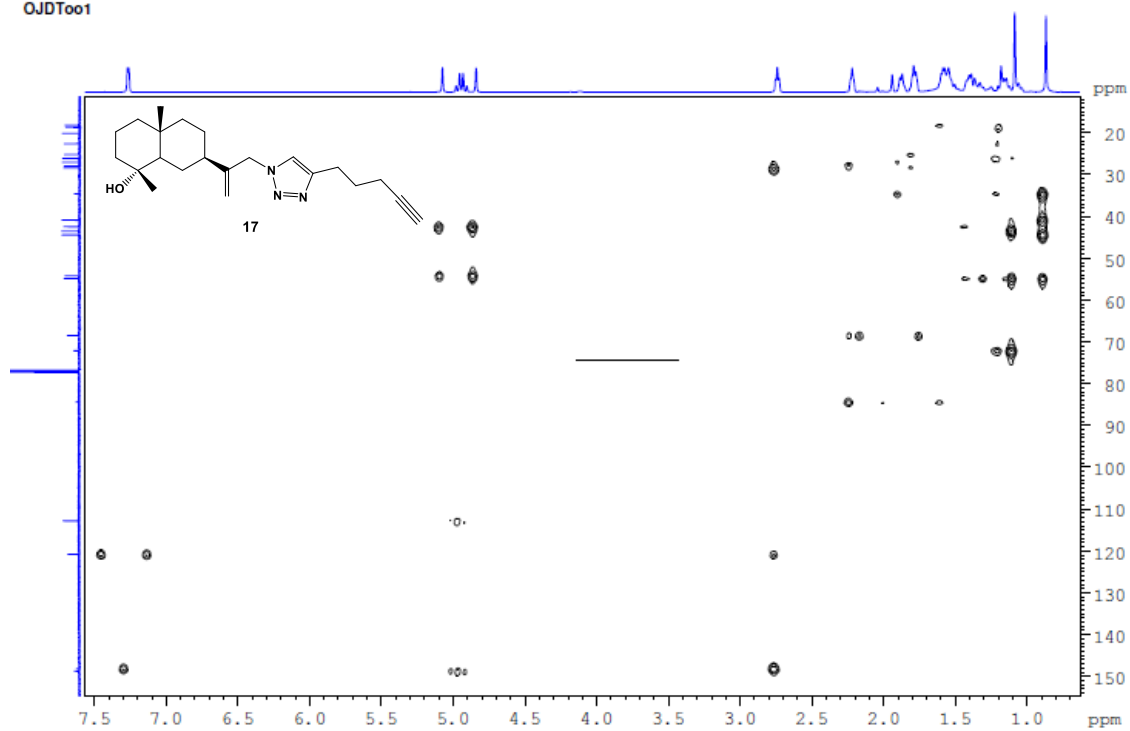


Figure S75. HSQC of 17.



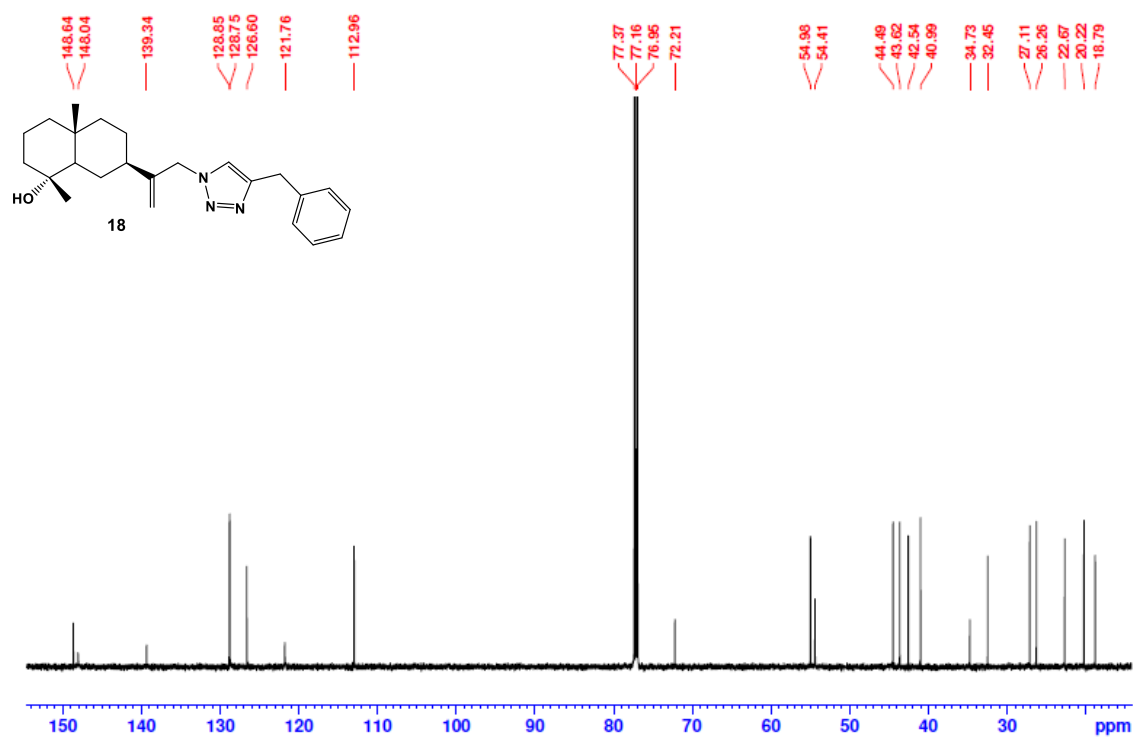


Figure S78.  $^{13}\text{C}$ -NMR of 18.

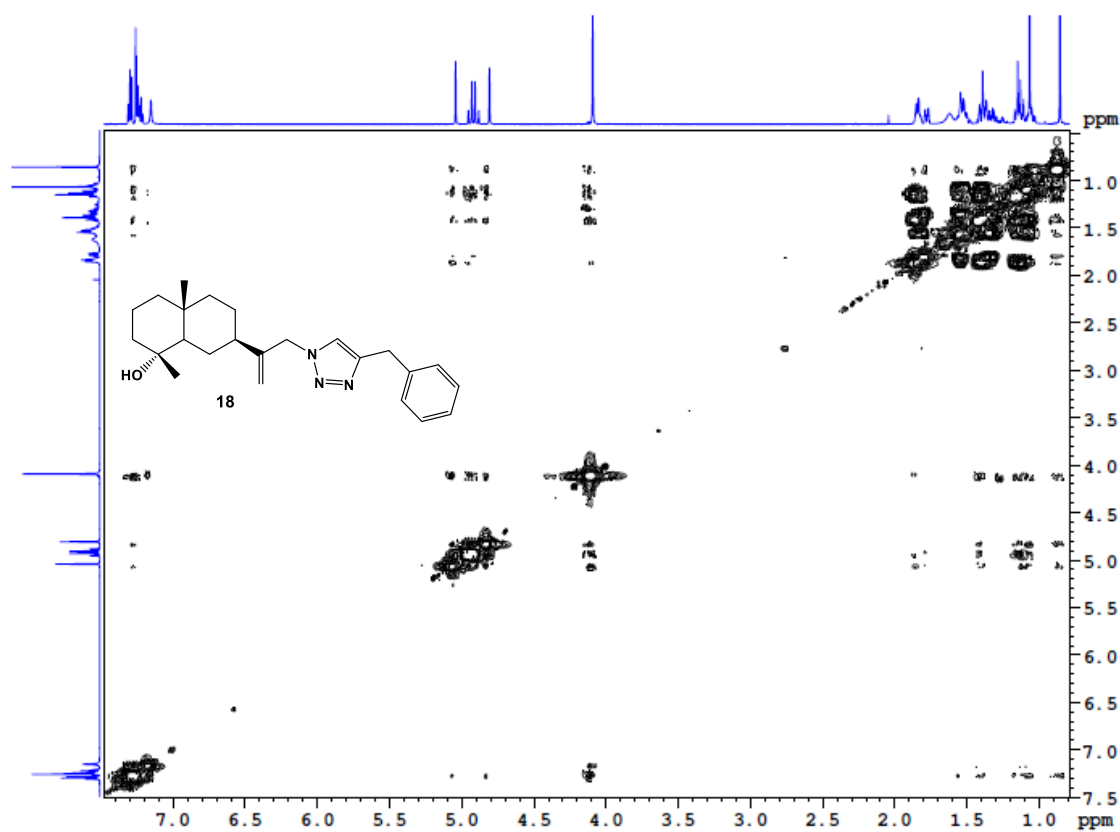


Figure S79. COSY of 18.



OJDT003

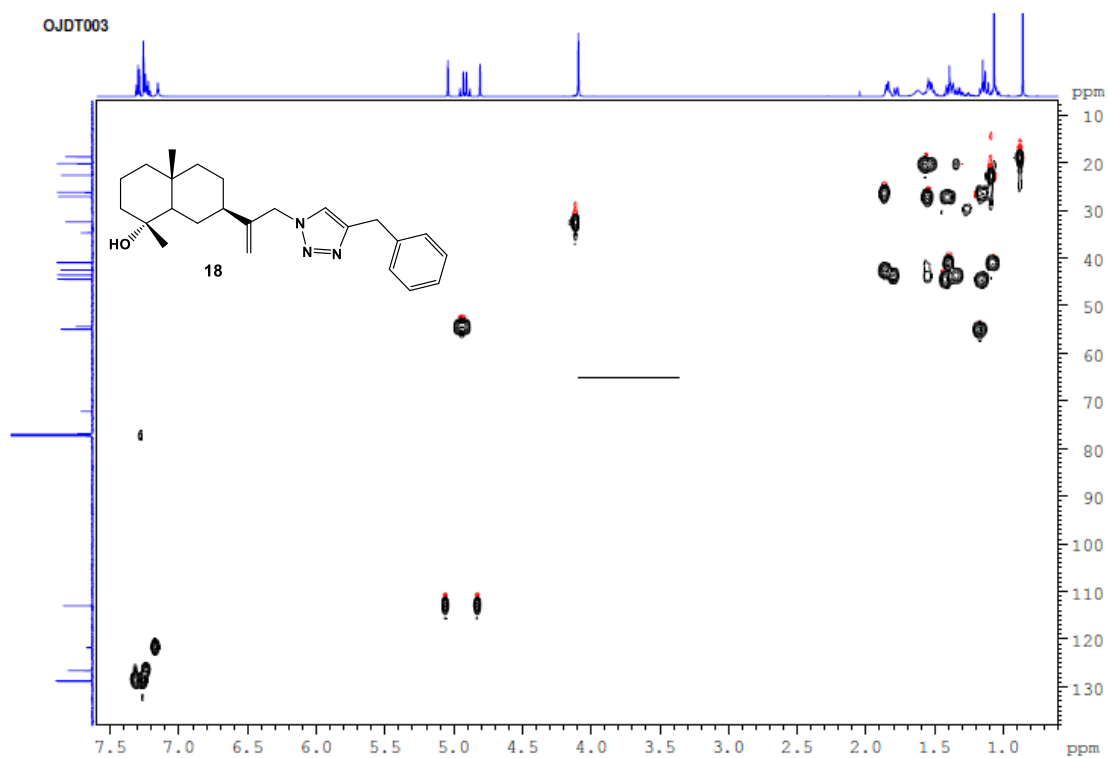


Figure S80. HSQC of 18.

OJDT003

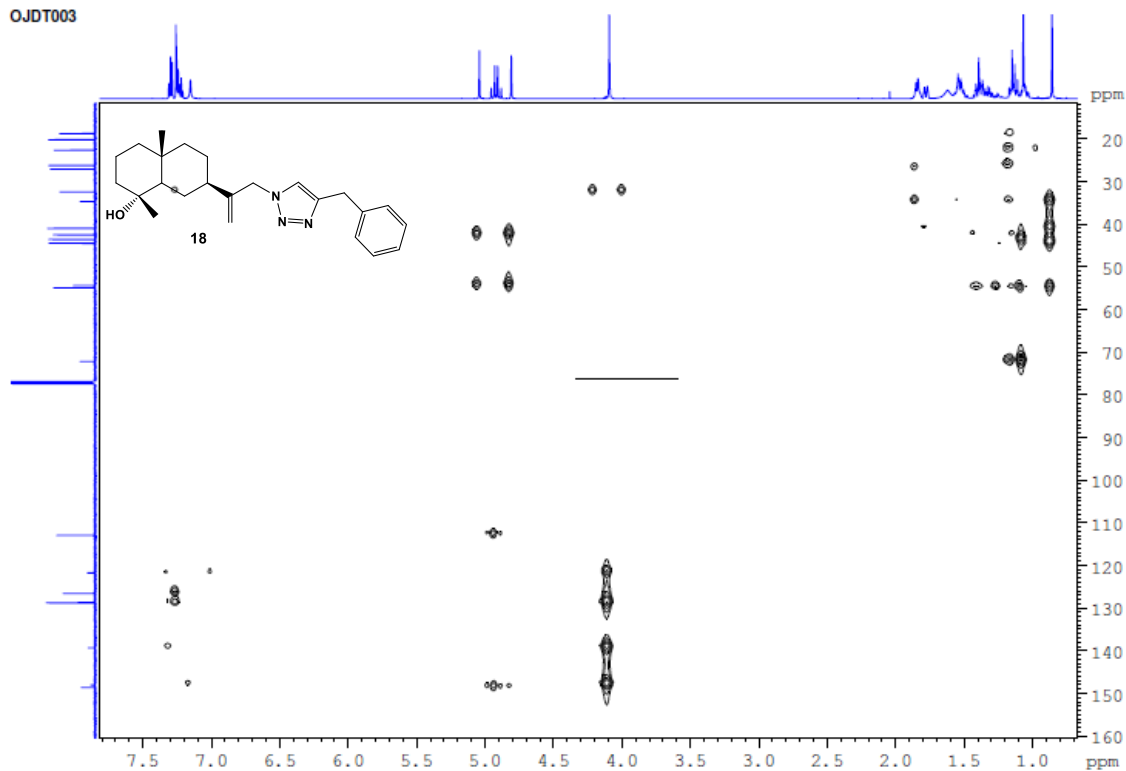


Figure S81. HMBC of 18.

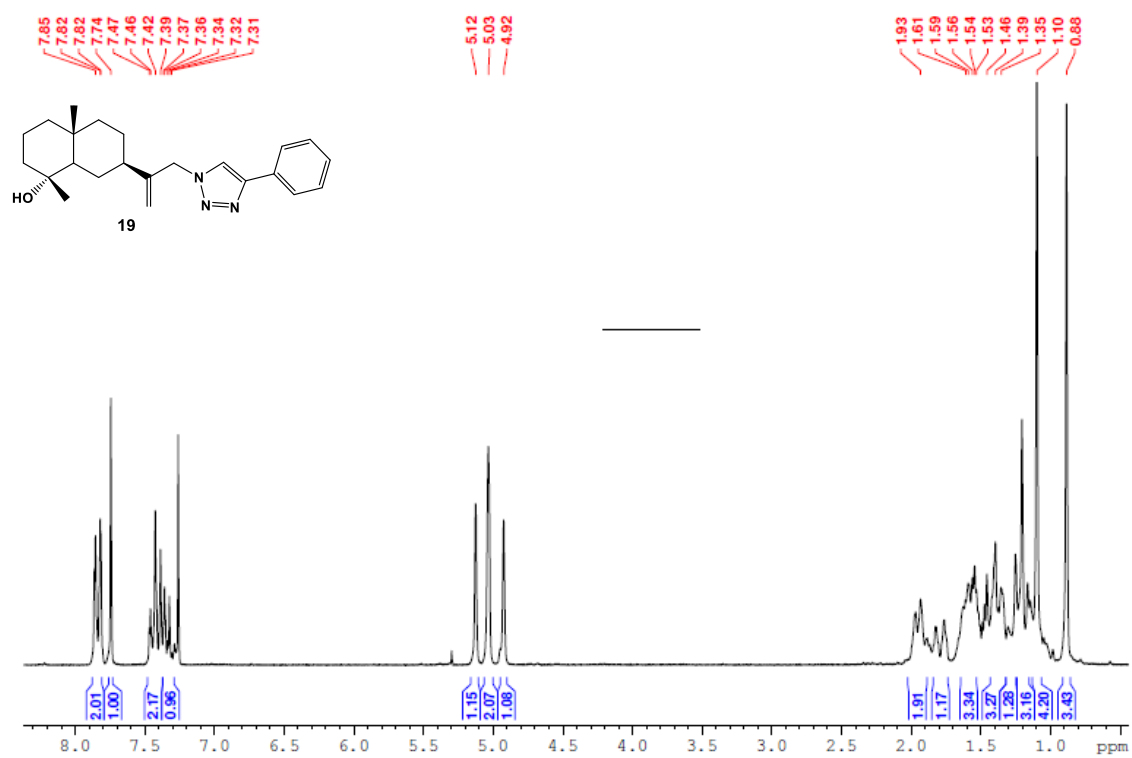


Figure S82. <sup>1</sup>H-NMR of 19.

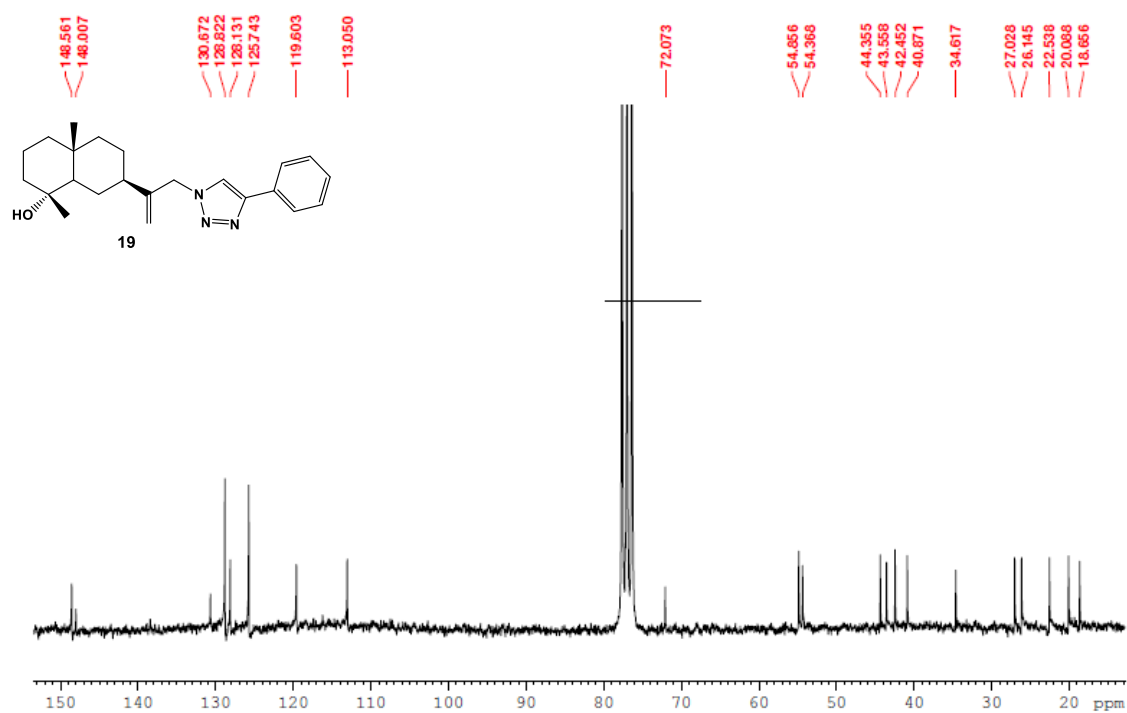


Figure S83. <sup>13</sup>C-NMR of 19.

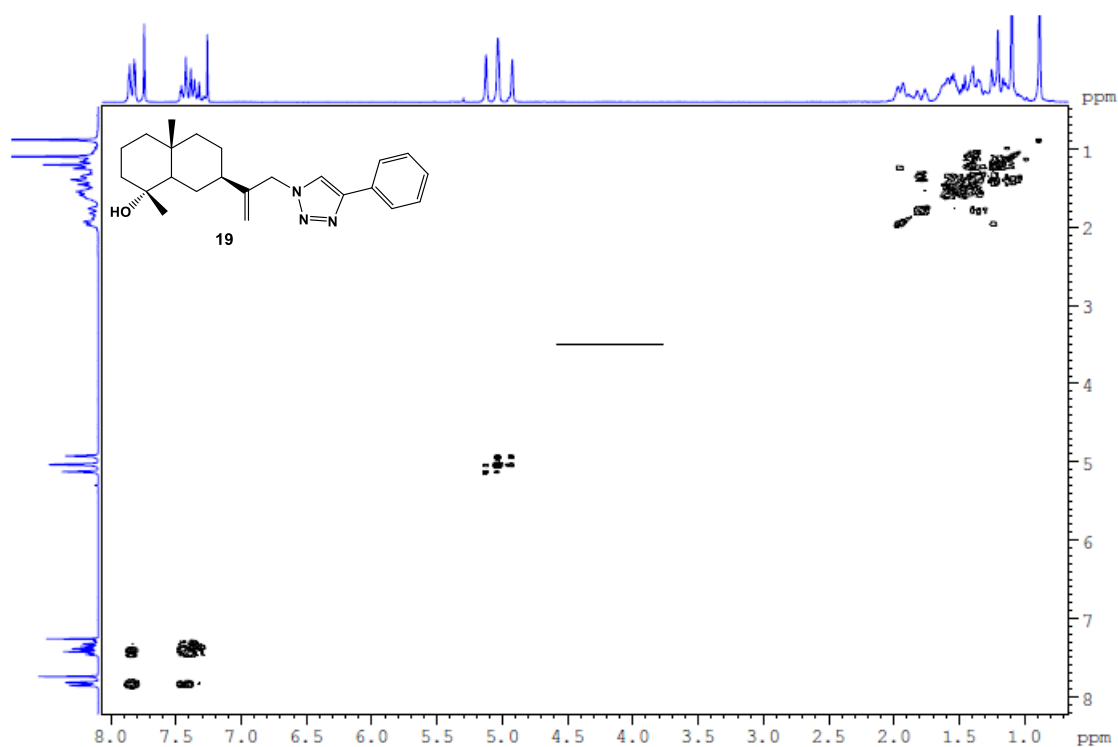


Figure S84. COSY of 19.

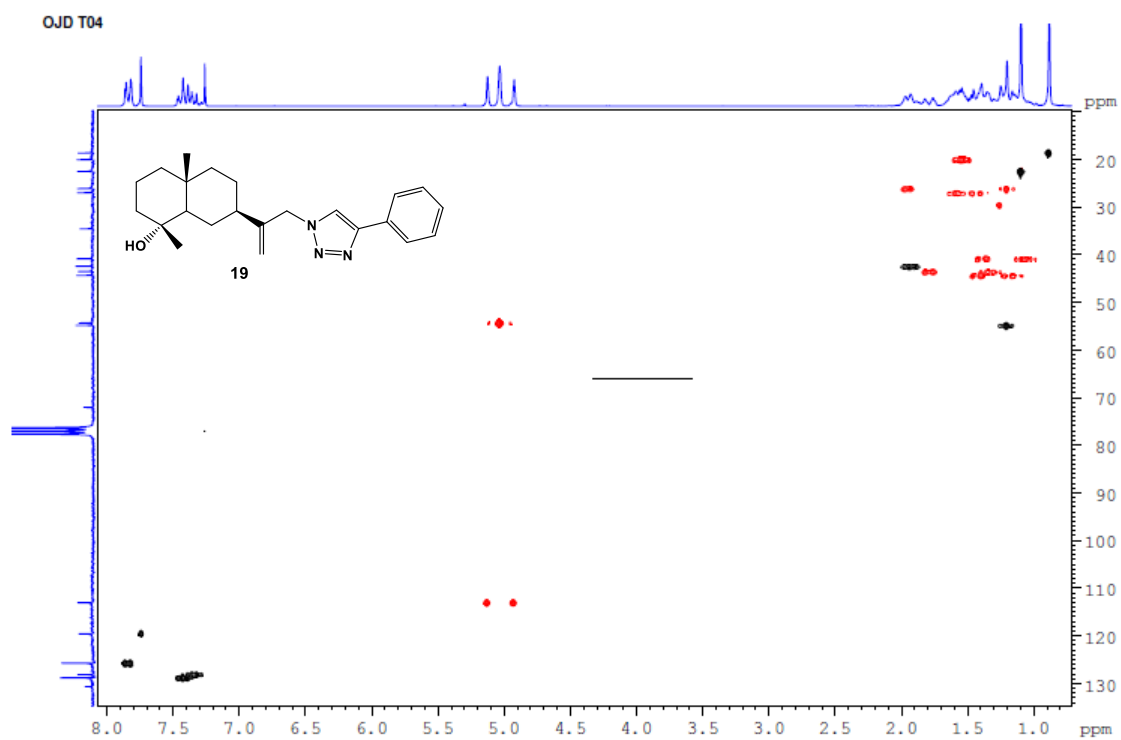


Figure S85. HSQC of 19.

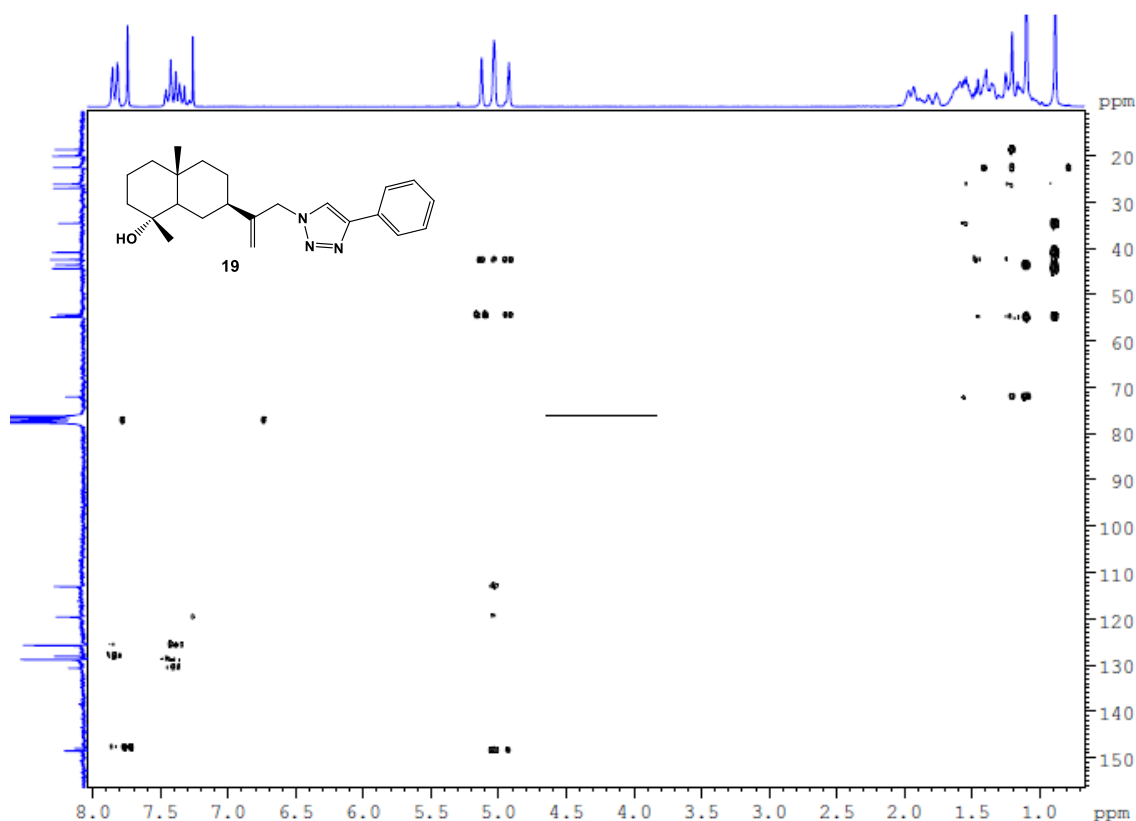
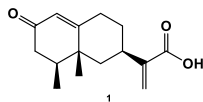


Figure S86. HMBC of 19.

## 5. HRMS-ES of compounds 1-15



### Elemental Composition Report

Page 1

#### Multiple Mass Analysis: 3 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 120.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1291 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)

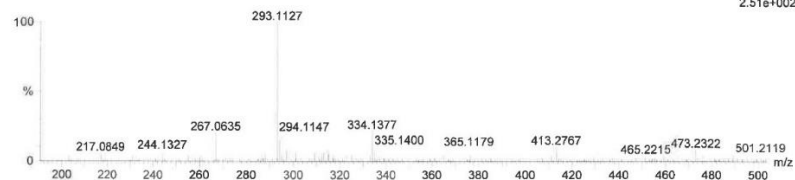
Elements Used:

C: 0-120 H: 0-70 N: 0-5 O: 0-6 Na: 0-2

Oswaldo

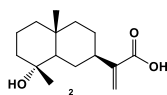
(ESI-18) (206) Oswaldo Donadel (Acido Tessarico) 44 (1.479)

2: TOF MS ES+  
2.51e+002



Minimum:	20.00								
Maximum:	100.00								
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
267.0635	20.16	267.0633	0.2	0.7	8.5	12.7	0.9	C14 H12 O4 Na	
		267.0623	1.2	4.5	10.5	13.0	1.2	C13 H9 N4 Na2	
		267.0647	-1.2	-4.5	13.5	13.1	1.3	C15 H8 N4 Na	
293.1127	100.00	293.1130	-0.3	-1.0	5.5	9.6	1.0	C15 H19 O3 Na2	
		293.1137	-1.0	-3.4	7.5	9.7	1.1	C14 H17 N2 O5	
		293.1113	1.4	4.8	4.5	9.8	1.2	C12 H18 N2 O5 Na	
334.1377	21.34	334.1379	-0.2	-0.6	5.5	15.2	0.0	C14 H21 N3 O5 Na	

Figure S87. HRMS-ES of 1.



# Elemental Composition Report

Page 1

## Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 120.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

824 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-120 H: 0-70 N: 0-5 O: 0-6 Na: 0-2

Oswaldo

(ESI-18) (204) Oswaldo Donadel (Ac Illico) 16 (0.661)

1: TOF MS ES+  
1.62e+004

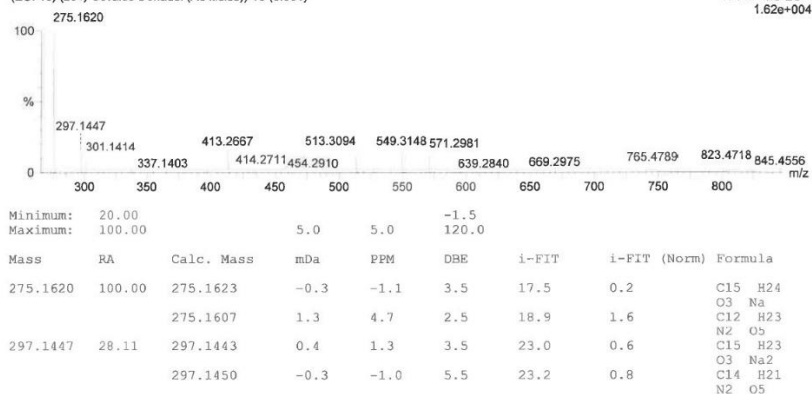
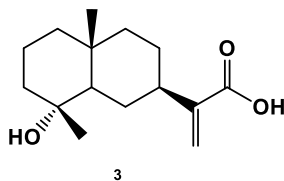


Figure S88. HRMS-ES of 2.



# Elemental Composition Report

Page 1

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 120.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

372 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-120 H: 0-70 N: 0-5 O: 0-6 Na: 0-2

Oswaldo

(ESI-18) (205) Oswaldo Donadel (Alcohol Illico) 19 (0.801)

1: TOF MS ES+  
5.69e+003

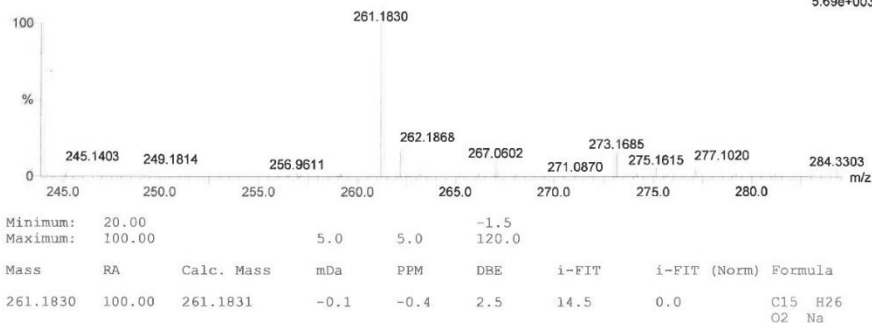
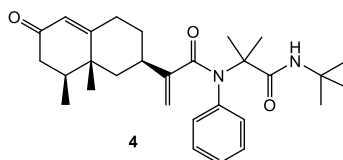


Figure S89. HRMS-ES of 3.



## Elemental Composition Report

Page 1

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 1000.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions  
 1004 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)  
 Elements Used:  
 C: 0-70 H: 0-100 N: 0-4 O: 0-15 Na: 0-1  
 ESI (16-798) Maria F B (MFB-054) 116 (4.052)

2: TOF MS ES+  
 6.58e+001

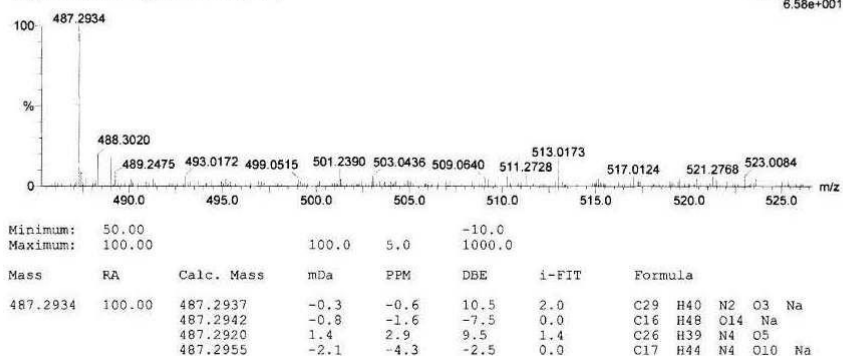
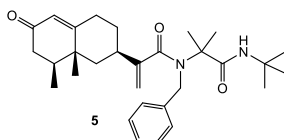


Figure S90. HRMS-ES of 4.



## Elemental Composition Report

Page 1

## Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 1000.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions  
 1304 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)  
 Elements Used:  
 C: 0-70 H: 0-100 N: 0-2 O: 0-16 Na: 0-1  
 ESI (16-867) Maria F (MFB-055A) 61 (2.128)

2: TOF MS ES+  
 1.10e+003

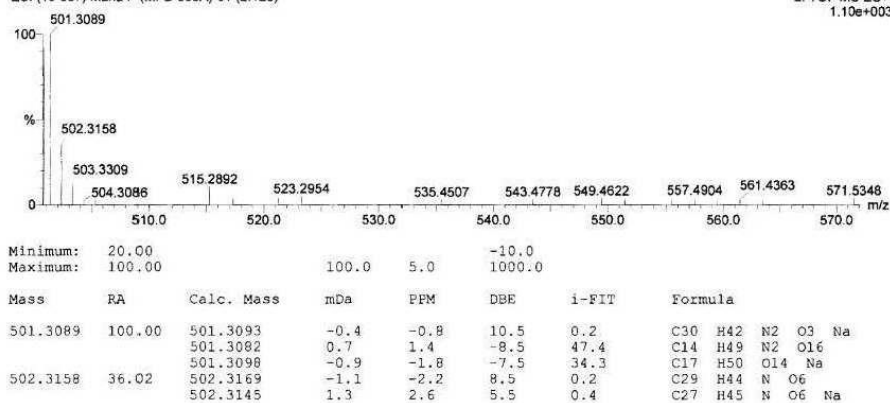
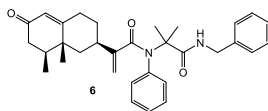


Figure S91. HRMS-ES of 5.



## Elemental Composition Report

Page 1

## Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

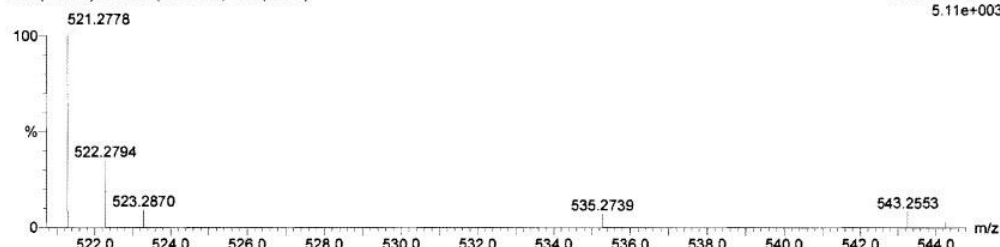
Monoisotopic Mass, Even Electron Ions

1355 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)

Elements Used:

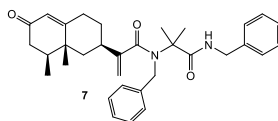
C: 0-70 H: 0-100 N: 0-2 O: 0-16 Na: 0-1

ESI (16-866) Maria F (MFB-061) 130 (4.528)

2: TOF MS ES+  
5.11e+003

Minimum:	20.00								-10.0		
Maximum:	100.00		100.0	5.0					1000.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula				
521.2778	100.00	521.2780	-0.2	-0.4	14.5	2.3	C32	H38	N2	O3	Na
		521.2785	-0.7	-1.3	-3.5	101.7	C19	H46	O14		Na
		521.2769	0.9	1.7	-4.5	150.6	C16	H45	N2	O16	
522.2794	34.95	522.2797	-0.3	-0.6	21.5	58.3	C38	H36	N	O	
		522.2773	2.1	4.0	18.5	46.4	C36	H37	N	O	Na

Figure S92. HRMS-ES of 6.



## Elemental Composition Report

Page 1

## Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

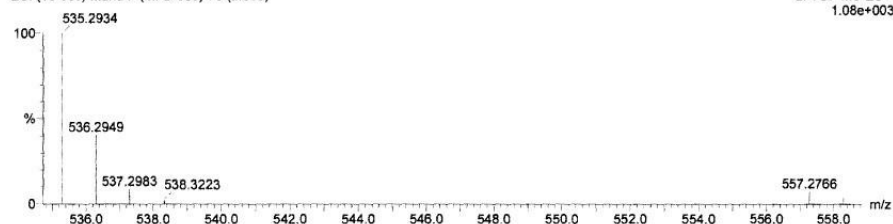
Monoisotopic Mass, Even Electron Ions

1393 formula(e) evaluated with 6 results within limits (all results (up to 1000) for each mass)

Elements Used:

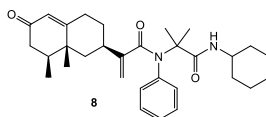
C: 0-70 H: 0-100 N: 0-2 O: 0-16 Na: 0-1

ESI (16-863) Maria F (MFB-060) 76 (2.653)

2: TOF MS ES+  
1.08e+003

Minimum:	20.00							-10.0			
Maximum:	100.00		100.0	5.0				1000.0			
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula				
535.2934	100.00	535.2937	-0.3	-0.6	14.5	0.6	C33	H40	N2	O3	Na
		535.2942	-0.8	-1.5	-3.5	34.3	C20	H48	O14		Na
		535.2926	0.8	1.5	-4.5	46.4	C17	H47	N2	O16	
		535.2961	-2.7	-5.0	17.5	0.2	C35	H39	N2	O3	
536.2949	40.62	536.2953	-0.4	-0.7	21.5	26.9	C39	H38	N	O	
		536.2929	2.0	3.7	18.5	22.9	C37	H39	N	O	Na

Figure S93. HRMS-ES of 7.



## Elemental Composition Report

Page 1

## Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 120.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

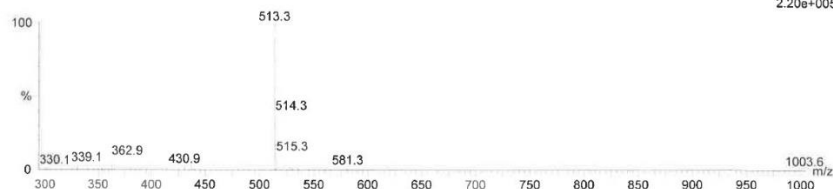
1459 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-120 H: 0-70 N: 0-5 O: 0-6 Na: 0-2

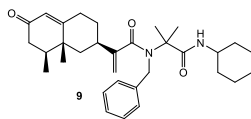
Osvaldo

(ESI-18) (202) Osvaldo Donadel ( MFB 79) 50 (1.688) Cm (50:59)

2: TOF MS ES+  
2.20e+005

Minimum:	20.00								
Maximum:	100.00								
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
513.3099	100.00	513.3077	2.2	4.3	10.5	20.7	0.1	C28 H41	
		513.3093	0.6	1.2	11.5	22.6	2.0	R4 O5	
		513.3117	-1.8	-3.5	14.5	27.0	6.4	C31 H42	
		513.3109	-1.0	-1.9	12.5	27.0	6.5	N2 O3 Na	
		514.3086	1.3	2.5	15.5	34.5	0.6	C33 H41	
		514.3110	-1.1	-2.1	18.5	35.3	1.3	N2 O3	
		514.3121	-2.2	-4.3	3.5	35.8	1.8	C34 H43	
								O Na2	
								C35 H41	
								N O Na	
								C37 H40	
								N O	
								C26 H46	
								N O6 Na2	

Figure S94. HRMS-ES of 8.



## Elemental Composition Report

Page 1

## Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 120.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

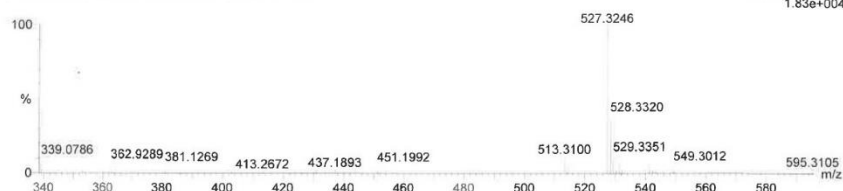
1477 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-120 H: 0-70 N: 0-5 O: 0-6 Na: 0-2

Osvaldo

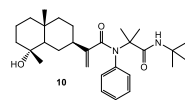
(ESI-18) (203) Osvaldo Donadel ( MFB 76) 36 (1.199)

2: TOF MS ES+  
1.83e+004

Minimum:	20.00								
Maximum:	100.00								
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
527.3246	100.00	527.3250	-0.4	-0.8	11.5	18.2	0.6	C32 H44	
		527.3266	-2.0	-3.8	12.5	19.1	1.6	N2 O3 Na	
		527.3233	1.3	2.5	10.5	19.3	1.7	C35 H45	
		527.3226	2.0	3.8	8.5	20.0	2.5	O Na2	
		528.3314	0.6	1.1	11.5	16.1	1.1	C29 H43	
		528.3325	-0.5	-0.9	9.5	16.1	1.1	N4 O5	
		528.3301	1.9	3.6	6.5	16.8	1.8	C30 H45	
		528.3331	-1.1	-2.1	12.5	17.0	2.0	N2 O3 Na2	
		528.3339	-1.9	-3.6	14.5	18.0	3.0	C30 H43	
								N5 O2 Na	
								C31 H46	
								N O6	
								C29 H47	
								N O6 Na	
								C33 H44	
								N3 Na2	
								C32 H42	
								N5 O2	

Figure S95. HRMS-ES of 9.





# Elemental Composition Report

Page 1

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 1000.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions  
 1008 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)  
 Elements Used:  
 C: 0-70 H: 0-100 N: 0-4 O: 0-15 Na: 0-1  
 ESI (16-800) Mass F B (MPB-052) 81 (2.829)

2 TOF MS ES+  
 1.02e+004

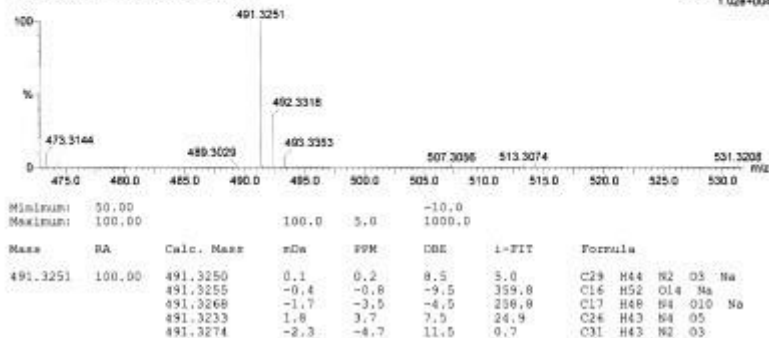
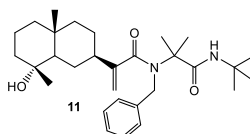


Figure S96. HRMS-ES of 10.



# Elemental Composition Report

Page 1

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 1000.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions  
 1030 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)  
 Elements Used:  
 C: 0-70 H: 0-100 N: 0-4 O: 0-15 Na: 0-1  
 ESI (16-800) Mass F B (MPB-033) 100 (3.462)

2 TOF MS ES+  
 4.51e+002

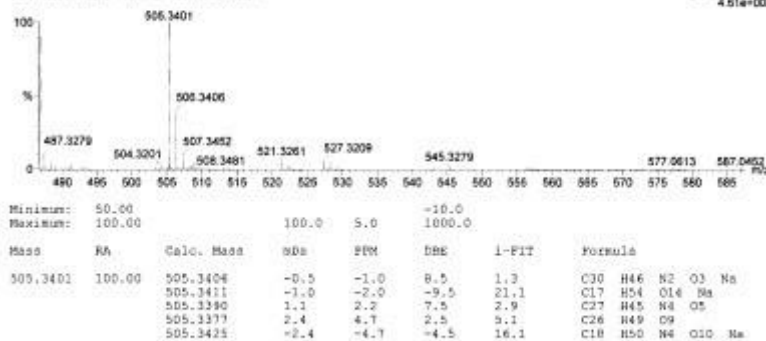
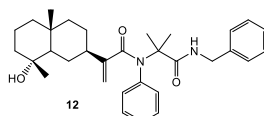


Figure S97. HRMS-ES of 11.



# Elemental Composition Report

Page 1

## Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 2

Monoisotopic Mass, Even Electron Ions

1360 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-70 H: 0-100 N: 0-2 O: 0-16 Na: 0-1

ESI (16-885) Maria F (MFB-056) 70 (3.051)

1: TOF MS ES+  
4.95e+001

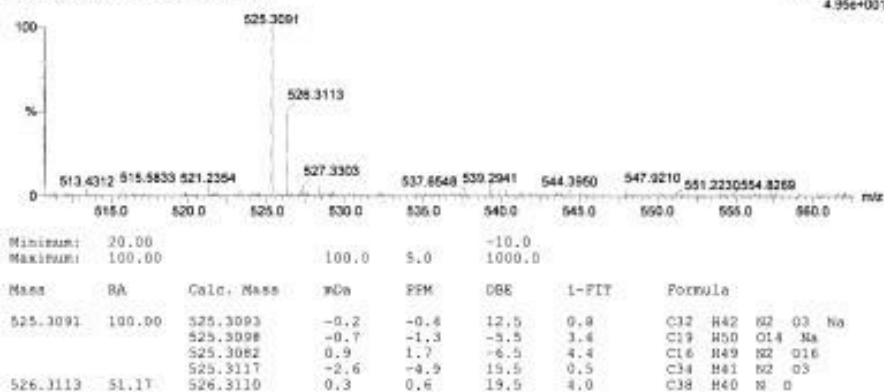
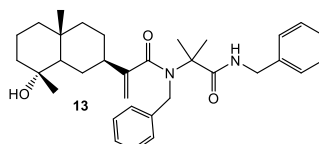


Figure S98. HRMS-ES of 12.



# Elemental Composition Report

Page 1

## Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for I-FIT = 2

Monoisotopic Mass, Even Electron Ions

1389 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-70 H: 0-100 N: 0-2 O: 0-16 Na: 0-1

ESI (16-888) Maria F (MFB-057) 43 (1.898)

1: TOF MS ES+  
5.55e+003

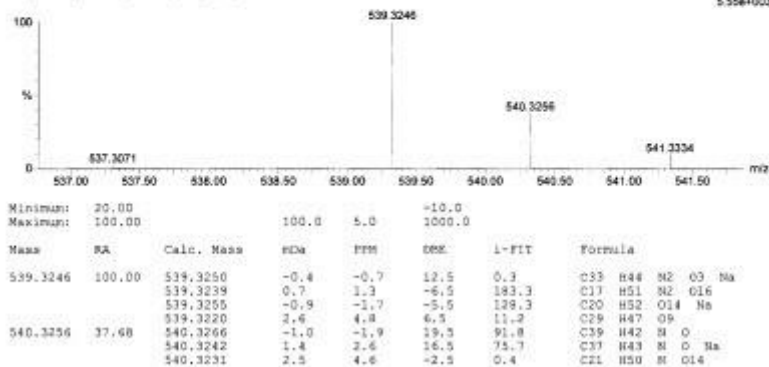
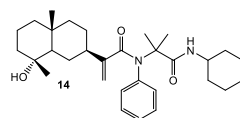


Figure S99. HRMS-ES of 13.



## Elemental Composition Report

Page 1

## Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

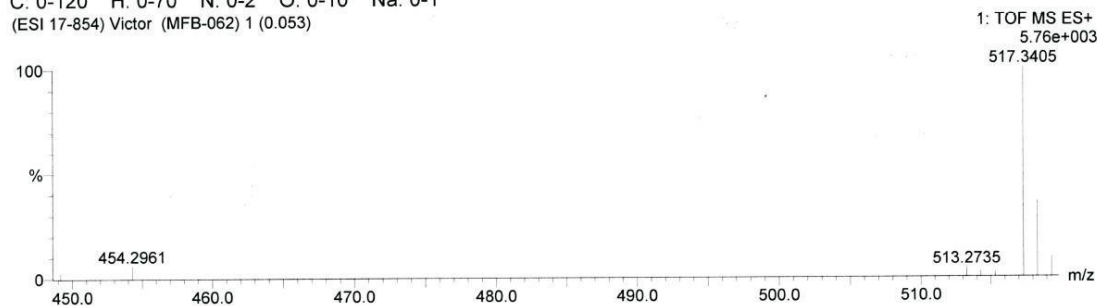
Monoisotopic Mass, Even Electron Ions

792 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

Elements Used:

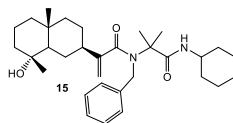
C: 0-120 H: 0-70 N: 0-2 O: 0-10 Na: 0-1

(ESI 17-854) Victor (MFB-062) 1 (0.053)



Minimum:	20.00				-10.0				
Maximum:	100.00		100.0	5.0	1000.0				
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula		
517.3405	100.00	517.3406	-0.1	-0.2	9.5	0.0	C31	H46	N2 O3 Na
		517.3430	-2.5	-4.8	12.5	3.8	C33	H45	N2 O3
518.3444	35.81	518.3458	-1.4	-2.7	4.5	10.9	C28	H49	N O6 Na
		518.3423	2.1	4.1	16.5	59.9	C37	H44	N O

Figure S100. HRMS-ES of 14.



## Elemental Composition Report

Page 1

## Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

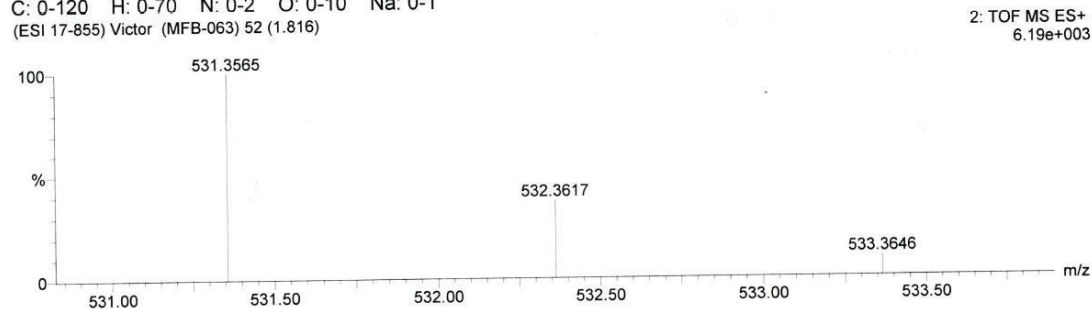
Monoisotopic Mass, Even Electron Ions

792 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

Elements Used:

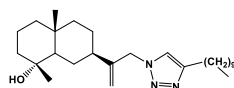
C: 0-120 H: 0-70 N: 0-2 O: 0-10 Na: 0-1

(ESI 17-855) Victor (MFB-063) 52 (1.816)



Minimum:	20.00				-10.0				
Maximum:	100.00		100.0	5.0	1000.0				
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula		
531.3565	100.00	531.3563	0.2	0.4	9.5	0.1	C32	H48	N2 O3 Na
		531.3587	-2.2	-4.1	12.5	3.1	C34	H47	N2 O3
532.3617	37.18	532.3614	0.3	0.6	4.5	18.0	C29	H51	N O6 Na
		532.3638	-2.1	-3.9	7.5	28.9	C31	H50	N O6

Figure S101. HRMS-ES of 15.



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## Elemental Composition Report

Page 1

**Multiple Mass Analysis: 304 mass(es) processed - displaying only valid results**

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

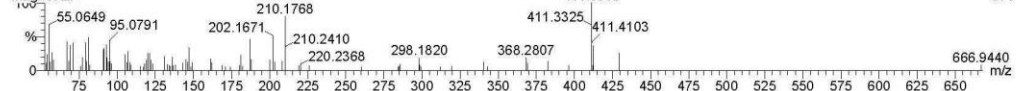
4798 formula(e) evaluated with 92 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-27 H: 1-47 N: 0-3 O: 0-1

23-Oct-14-A 118 (3.003) Cn (Cen,2, 50.00, Ht)

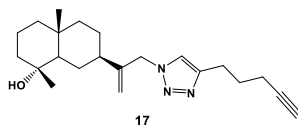
Magnet EI+



Minimum: 0.10  
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
429.3716	25.06	429.3719	-0.3	-0.7	6.0	5546064.0	C27 H47 N3 O
412.3660	36.05	412.3692	-3.2	-7.8	6.5	5546084.0	C27 H46 N3
412.3305	13.25	412.3328	-2.3	-5.6	7.5	5546042.5	C26 H42 N3 O
411.3585	100.00	411.3613	-2.8	-6.8	7.0	2773105.0	C27 H45 N3
411.3325	67.87	411.3375	-5.0	-12.2	7.5	2773053.5	C27 H43 N2 O
		411.3250	7.5	18.2	8.0	2773050.8	C26 H41 N3 O
396.3452	7.20	396.3504	-5.2	-13.1	7.0	5546032.5	C27 H44 N2
		396.3379	7.3	18.4	7.5	5546032.5	C26 H42 N3

Figure S102. HRMS-ES of 16.



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## Elemental Composition Report

Page 1

**Multiple Mass Analysis: 560 mass(es) processed - displaying only valid results**

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

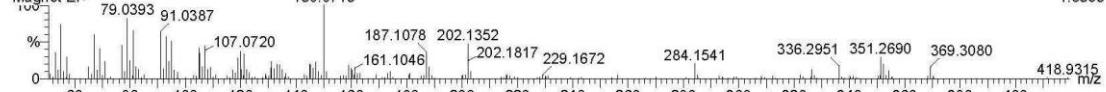
8562 formula(e) evaluated with 251 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-23 H: 2-35 N: 0-3 O: 0-1

23-Oct-14-CAFAMMA 82 (2.087)

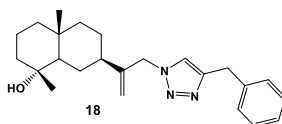
Magnet EI+



Minimum: 0.10  
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
369.2774	12.50	369.2780	-0.6	-1.6	8.0	2773034.8	C23 H35 N3 O
355.2646	1.72	355.2624	2.2	6.2	8.0	5546033.5	C22 H33 N3 O
354.2615	9.32	354.2671	-5.6	-15.8	8.0	2773024.8	C23 H34 N2 O
		354.2545	7.0	19.8	8.5	2773023.5	C22 H32 N3 O
353.2482	4.16	353.2467	1.5	4.2	9.0	78.6	C22 H31 N3 O
351.2690	29.33	351.2674	1.6	4.6	9.0	43.4	C23 H33 N3
351.2496	29.12	351.2436	6.0	17.1	9.5	44.1	C23 H31 N2 O
350.2256	1.59	350.2232	2.4	6.9	10.5	401.7	C22 H28 N3 O
342.2616	0.85	342.2671	-5.5	-16.1	7.0	5546027.5	C22 H34 N2 O
341.2777	2.61	341.2831	-5.4	-15.8	7.0	2773013.3	C22 H35 N3
		341.2719	5.8	17.0	7.0	2773013.0	C23 H35 N O

Figure S103. HRMS-ES of 17.



## Elemental Composition Report

Page 1

### Multiple Mass Analysis: 453 mass(es) processed - displaying only valid results

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

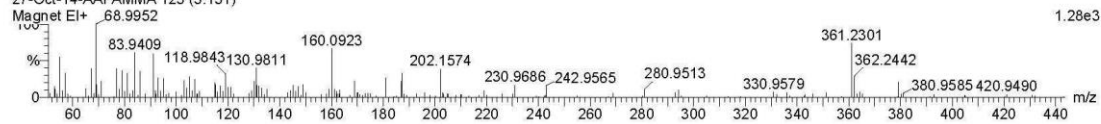
6666 formula(e) evaluated with 165 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-24 H: 2-33 N: 0-3 O: 0-1

27-Oct-14-AAFAMMA 123 (3.131)

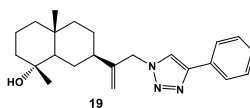
Magnet EI+ 68.9952



Minimum: 0.10  
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
379.2619	17.70	379.2624	-0.5	-1.3	10.0	2773037.5	C24 H33 N3 O
364.2541	1.44	364.2515	2.6	7.1	10.0	2773040.0	C24 H32 N2 O
364.1466	0.89	364.1450	1.6	4.4	17.5	2773045.0	C24 H18 N3 O
363.2478	4.71	363.2436	4.2	11.6	10.5	30.2	C24 H31 N2 O
363.2277	4.16	363.2311	-3.4	-9.4	11.0	61.7	C23 H29 N3 O
362.2208	21.02	362.2232	-2.4	-6.6	11.5	40.8	C23 H28 N3 O
361.2301	73.59	361.2280	2.1	5.8	11.5	3.1	C24 H29 N2 O
351.2405	5.52	351.2436	-3.1	-8.8	9.5	5546051.5	C23 H31 N2 O
346.2078	2.67	346.2045	3.3	9.5	12.0	5546035.0	C23 H26 N2 O
346.1854	1.80	346.1919	-6.5	-18.8	12.5	5546030.0	C22 H24 N3 O

Figure S104. HRMS-ES of 18.



## Elemental Composition Report

Page 1

Tolerance = 5.0 PPM / DBE: min = -10.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

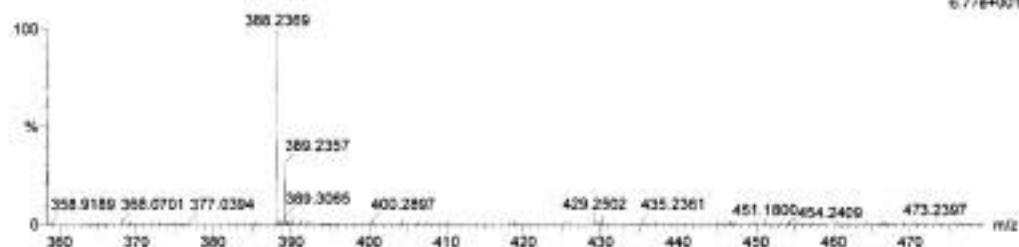
808 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-70 H: 0-100 N: 0-4 O: 0-15 Na: 0-1

ESI (16-799) Mass F.B. (MFB-TQV) 71 (2.484)

2: TOF MS ES+  
6.77e+001



Minimum: 50.00  
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
388.2369	100.00	388.2370	-0.1	-0.3	-8.5	3.7	C10 H38 N O12 Na
		388.2365	0.4	1.0	9.5	0.2	C23 H31 N3 O Na
		388.2358	1.5	3.9	-9.5	4.8	C7 H38 N3 O14

Figure S105. HRMS-ES of 19.