

Supplementary Information

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Figure S71. TIC and MS spectrum of compound **44c**.
Figure S72. ^1H NMR spectrum of compound **44d**.
Figure S73. TIC and MS spectrum of compound **44d**.

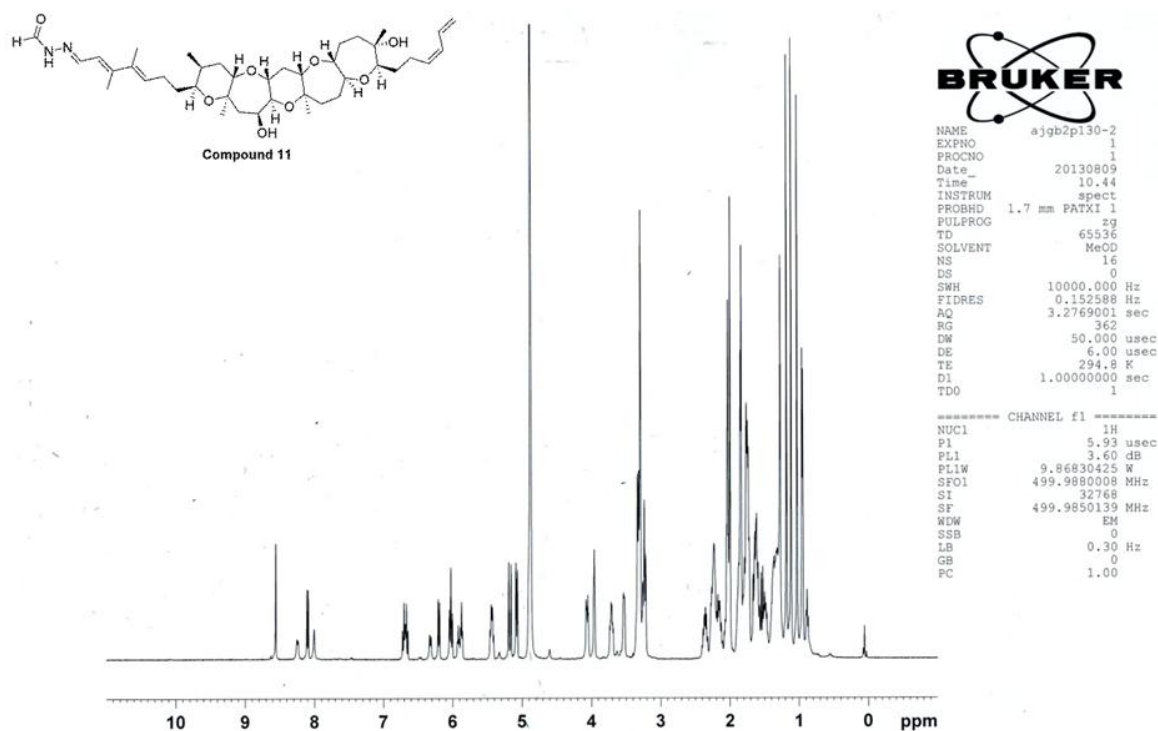
Figure S1. ^1H NMR spectrum of compound 11.

Figure S2. HRMS spectrum of compound 11.

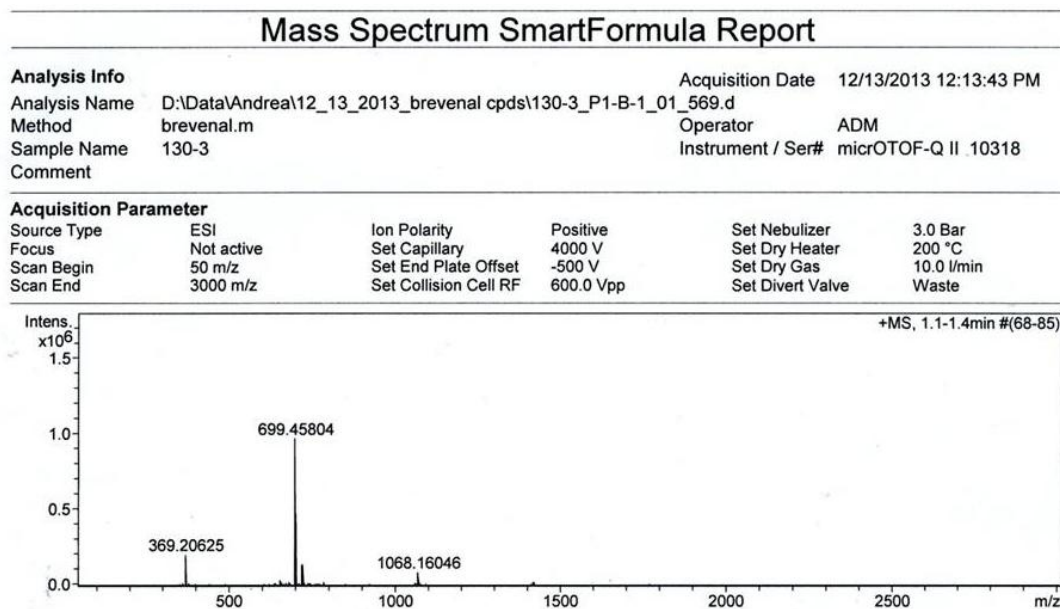
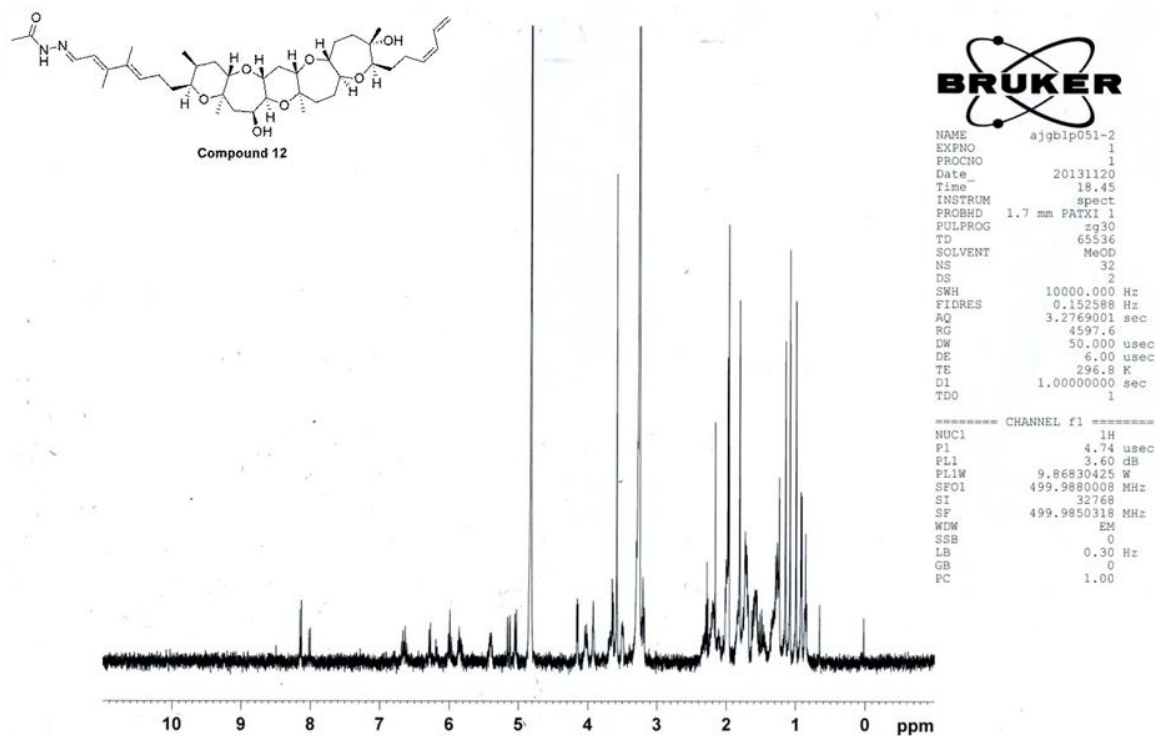


Figure S3. ^1H NMR spectrum of compound 12.**Figure S4.** HRMS spectrum of compound 12.**Mass Spectrum SmartFormula Report**

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Method	brevenal.m	Instrument / Ser#	micrOTOF-Q II 10318
Sample Name	brevenal acet		
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
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Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste

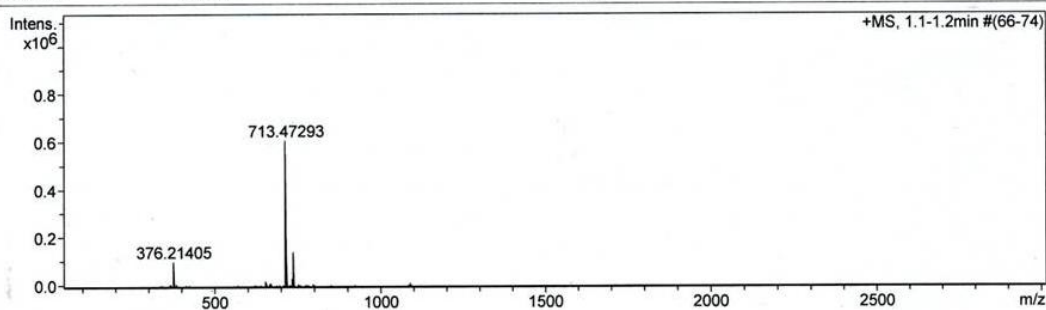
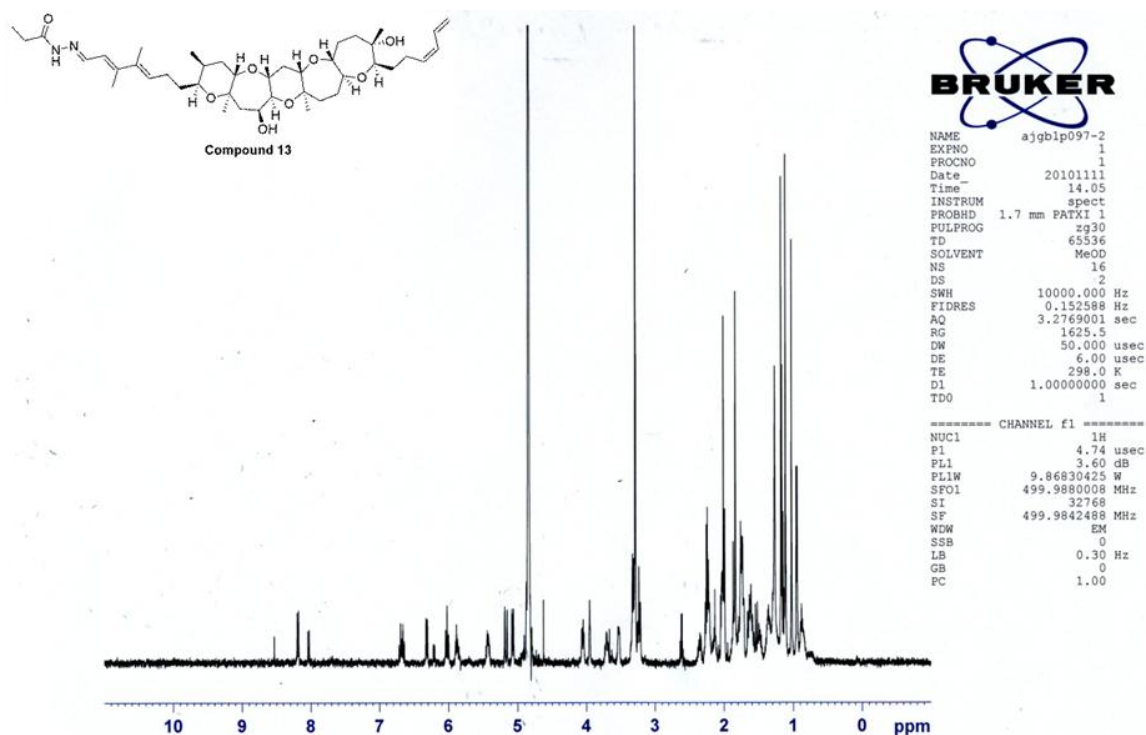


Figure S5. ^1H NMR spectrum of compound 13.**Figure S6.** HRMS spectrum of compound 13.**Mass Spectrum SmartFormula Report**

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Method	brevalen.m	Instrument / Ser#	micrOTOF-Q II 10318
Sample Name	97-2-3		
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
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Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste

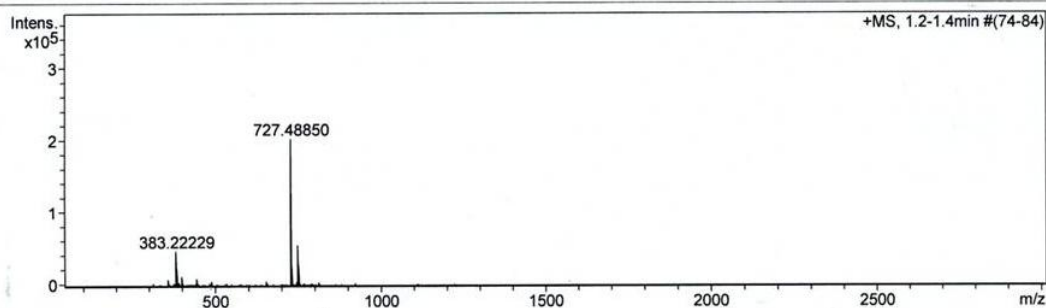


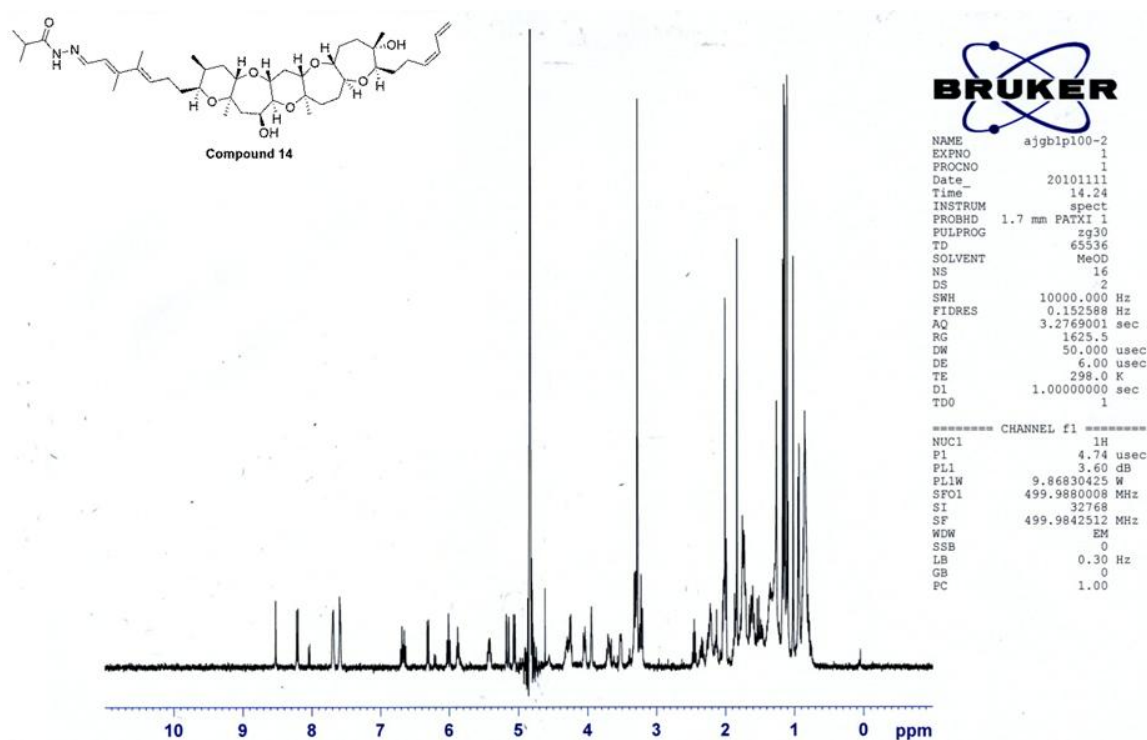
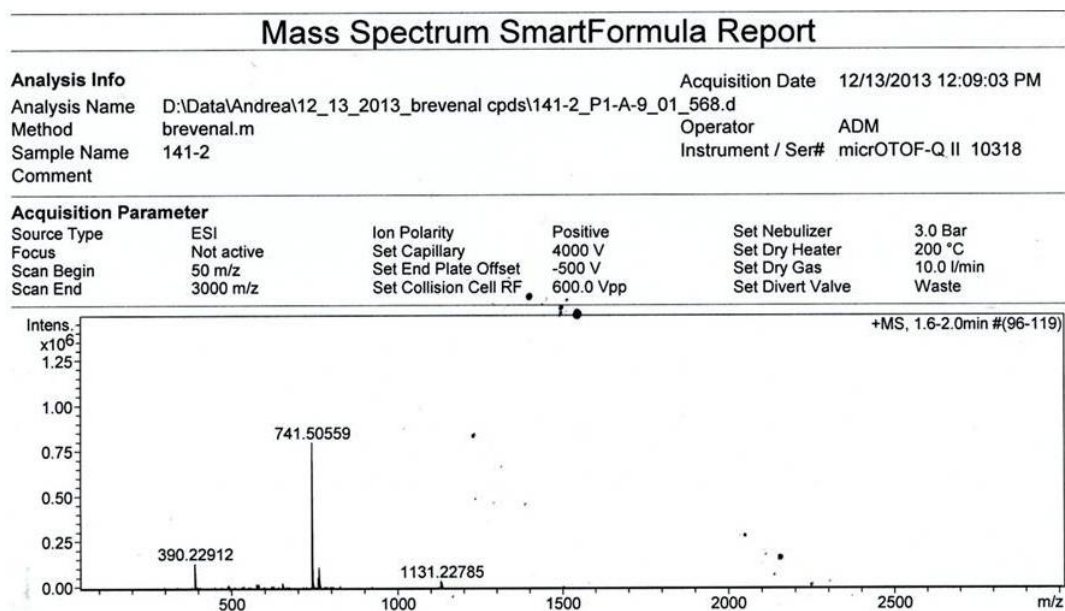
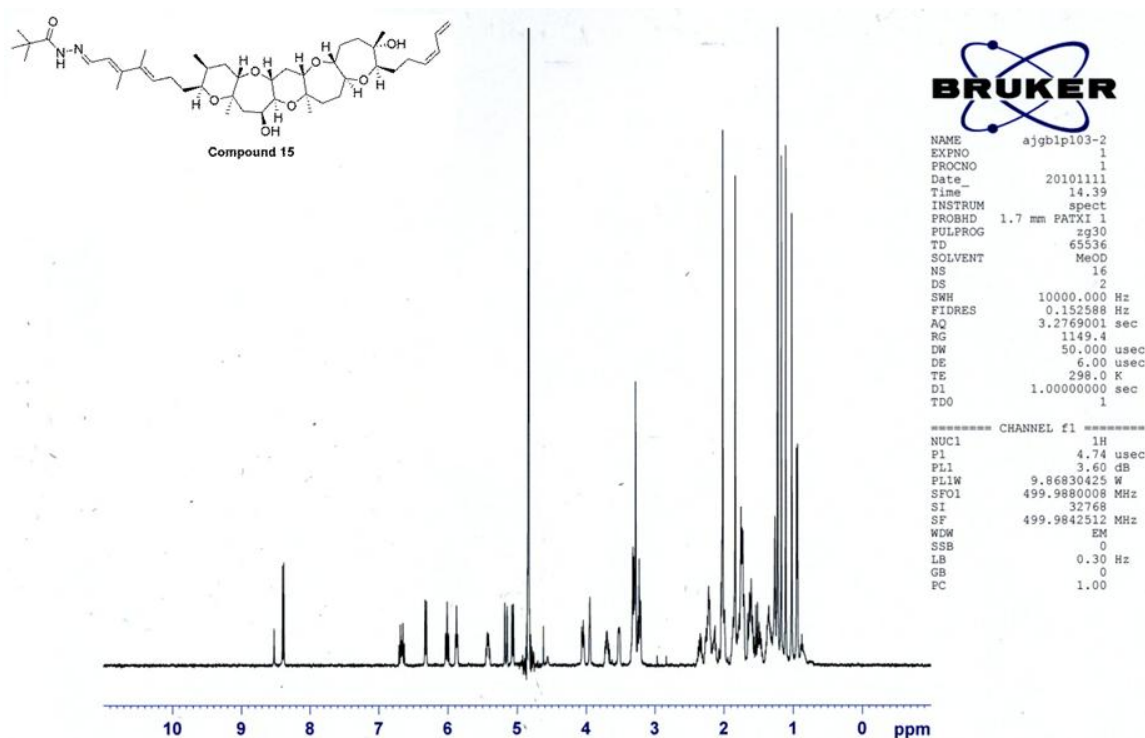
Figure S7. ^1H NMR spectrum of compound 14.**Figure S8.** HRMS spectrum of compound 14.

Figure S9. ^1H NMR spectrum of compound 15.**Figure S10.** HRMS spectrum of compound 15.**Mass Spectrum SmartFormula Report**

Analysis Info		Acquisition Date	12/20/2013 10:01:33 AM
Analysis Name	D:\Data\Andrea\12_20_2013_breval cpds 2\103-2-5_P1-A-8_01_581.d	Operator	ADM
Method	breval.m	Instrument / Ser#	micrOTOF-Q II 10318
Sample Name	103-2-5		
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
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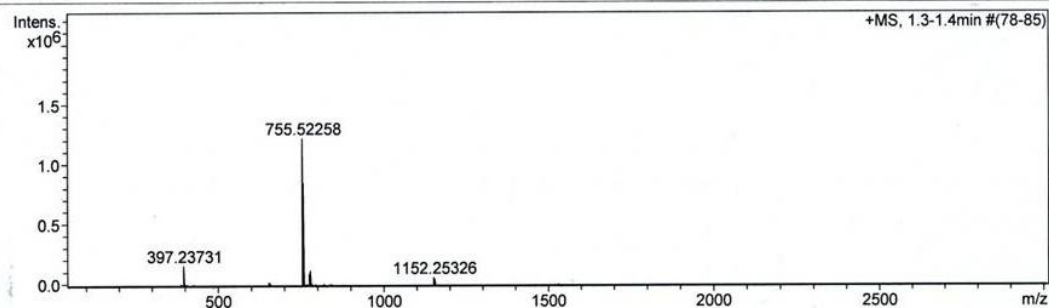


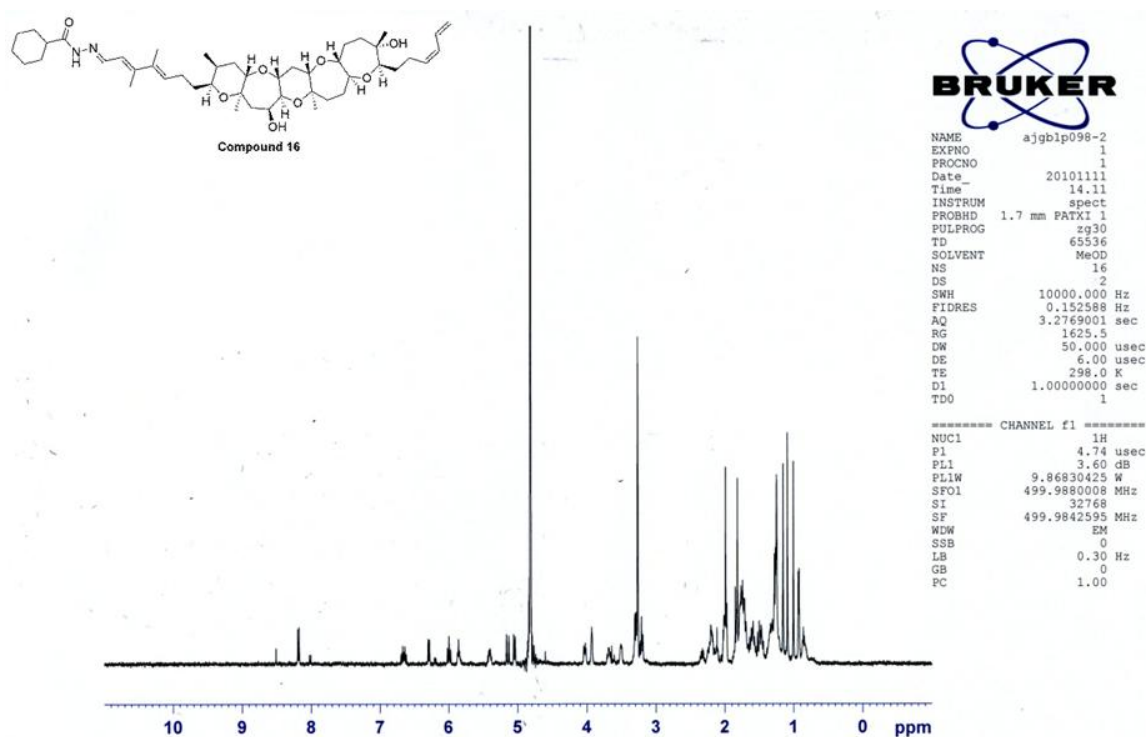
Figure S11. ^1H NMR spectrum of compound 16.

Figure S12. HRMS spectrum of compound 16.

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	12/20/2013 9:56:50 AM
Analysis Name	D:\Data\Andrea\12_20_2013_breval cpds 2\98-2-4_P1-A-7_01_580.d	Operator	ADM
Method	breval.m	Instrument / Ser#	micrOTOF-Q II 10318
Sample Name	98-2-4		
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
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Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste

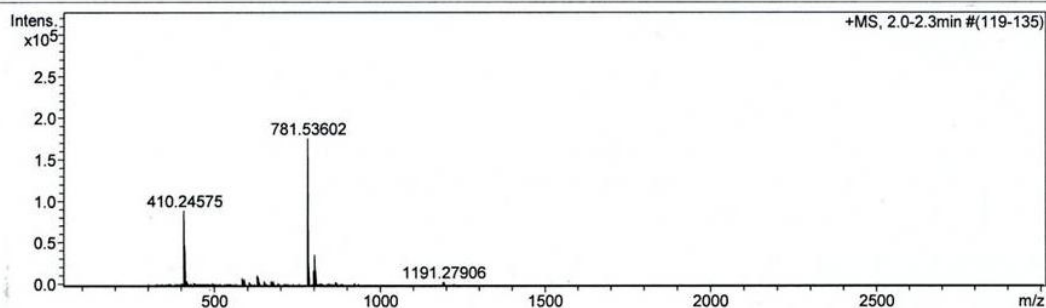


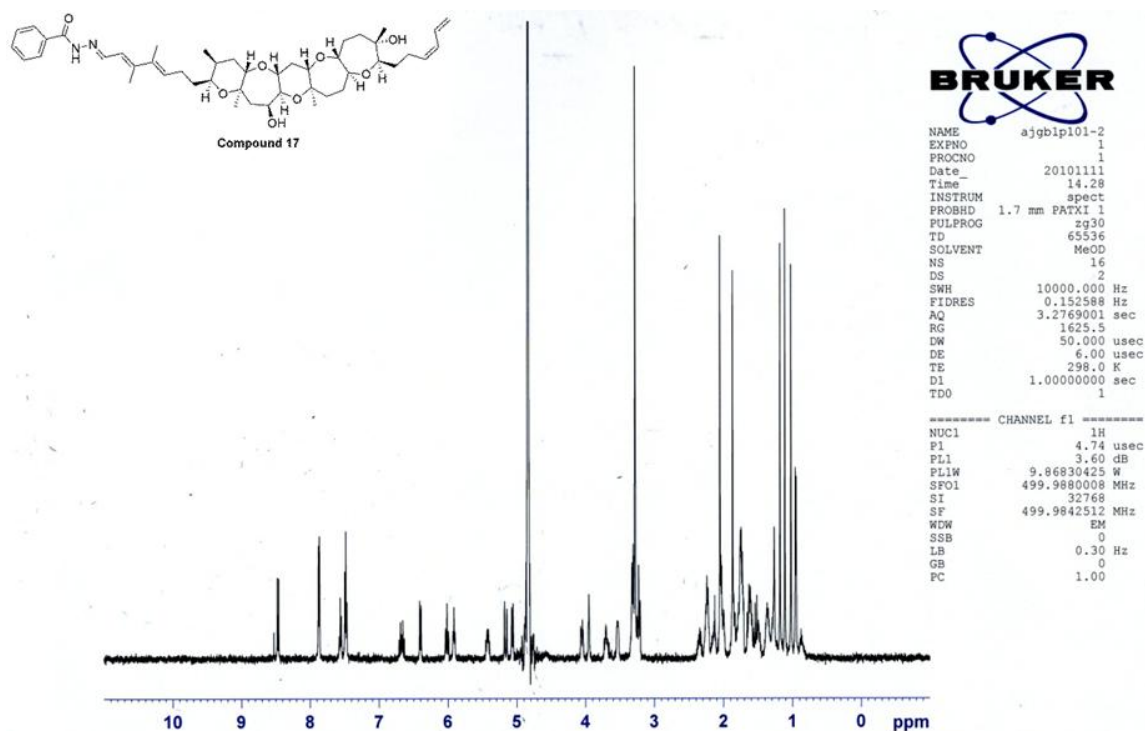
Figure S13. ^1H NMR spectrum of compound 17.

Figure S14. HRMS spectrum of compound 17.

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	12/20/2013 10:48:14 AM
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Method	breval.m	Instrument / Ser#	micrOTOF-Q II 10318
Sample Name	101-2-6		
Comment			

Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
Focus	Not active	Set Capillary	4000 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp
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		Set Dry Gas	10.0 l/min
		Set Divert Valve	Waste

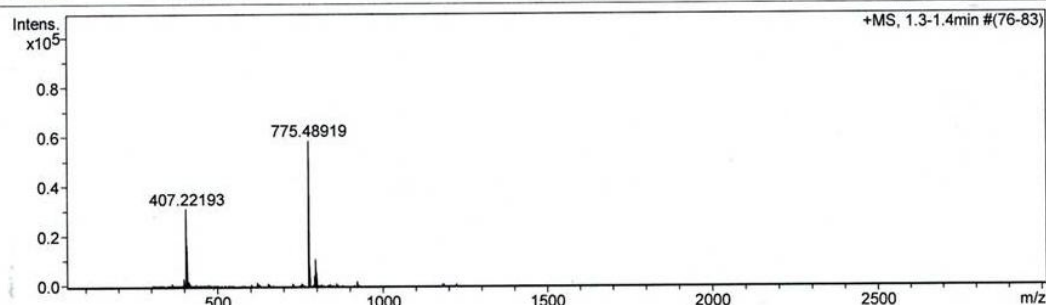


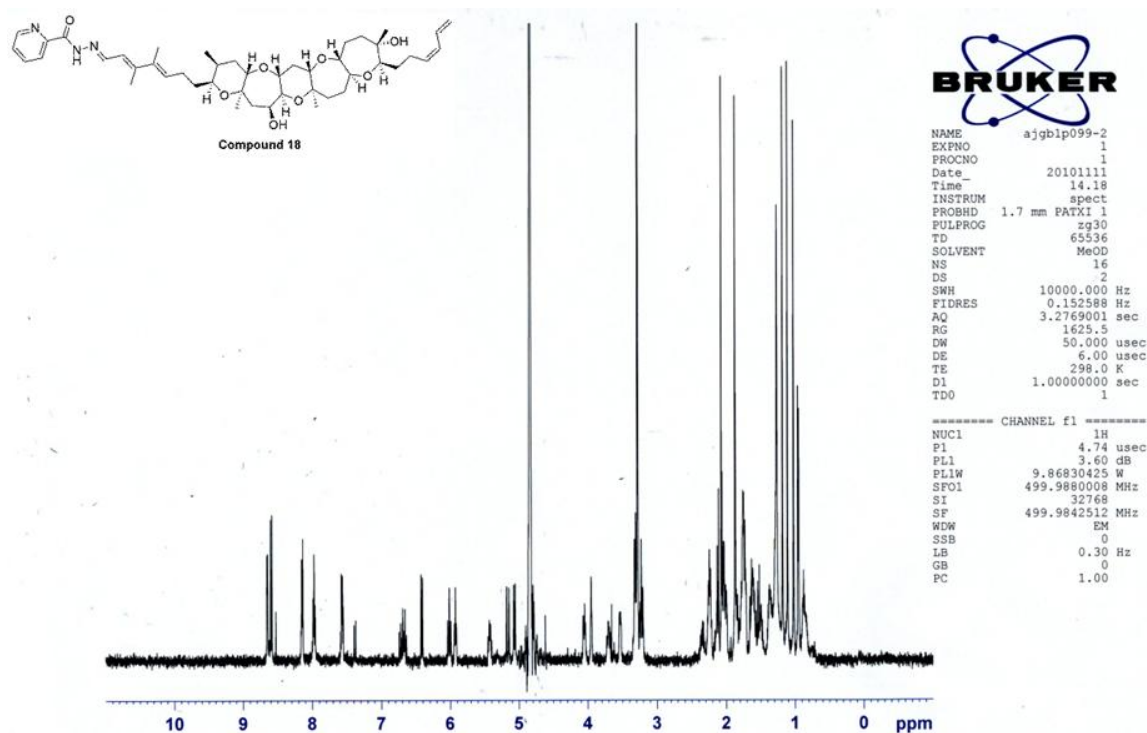
Figure S15. ^1H NMR spectrum of compound 18.

Figure S16. HRMS spectrum of compound 18.

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	12/20/2013 10:29:33 AM
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Method	breval.m	Instrument / Ser#	micrOTOF-Q II 10318
Sample Name	pico-3		
Comment			

Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
Focus	Not active	Set Capillary	4000 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp
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		Set Dry Gas	10.0 l/min
		Set Divert Valve	Waste

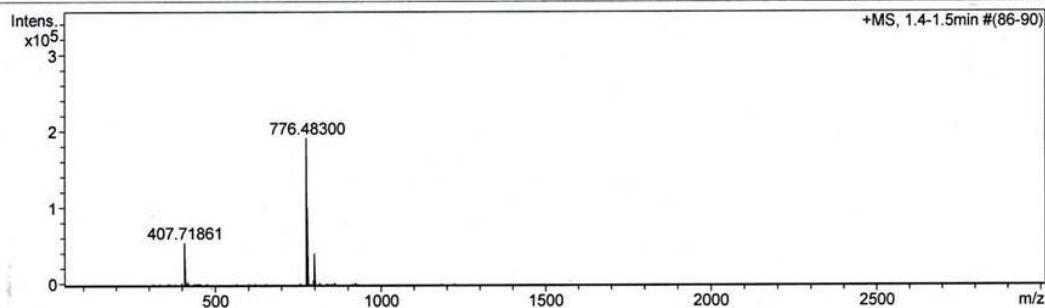


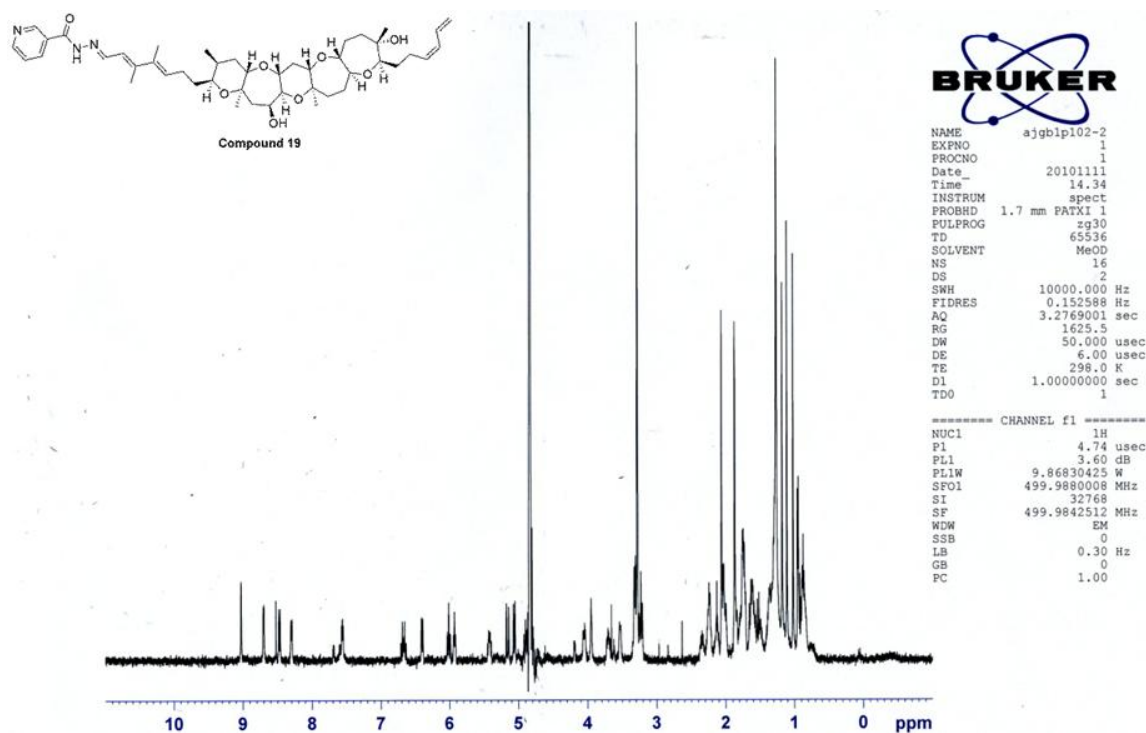
Figure S17. ^1H NMR spectrum of compound 19.

Figure S18. HRMS spectrum of compound 19.

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	12/20/2013 10:10:51 AM
Analysis Name	D:\Data\Andrea\12_20_2013_brevenal cpds 2\142-2-4_P1-B-1_01_583.d	Operator	ADM
Method	brevenal.m	Instrument / Ser#	micrOTOF-Q II 10318
Sample Name	142-2-4		
Comment			

Acquisition Parameter					
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Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
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Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste

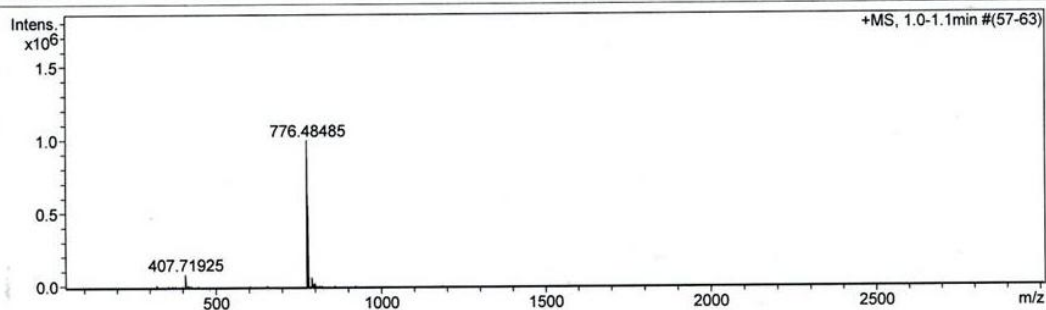


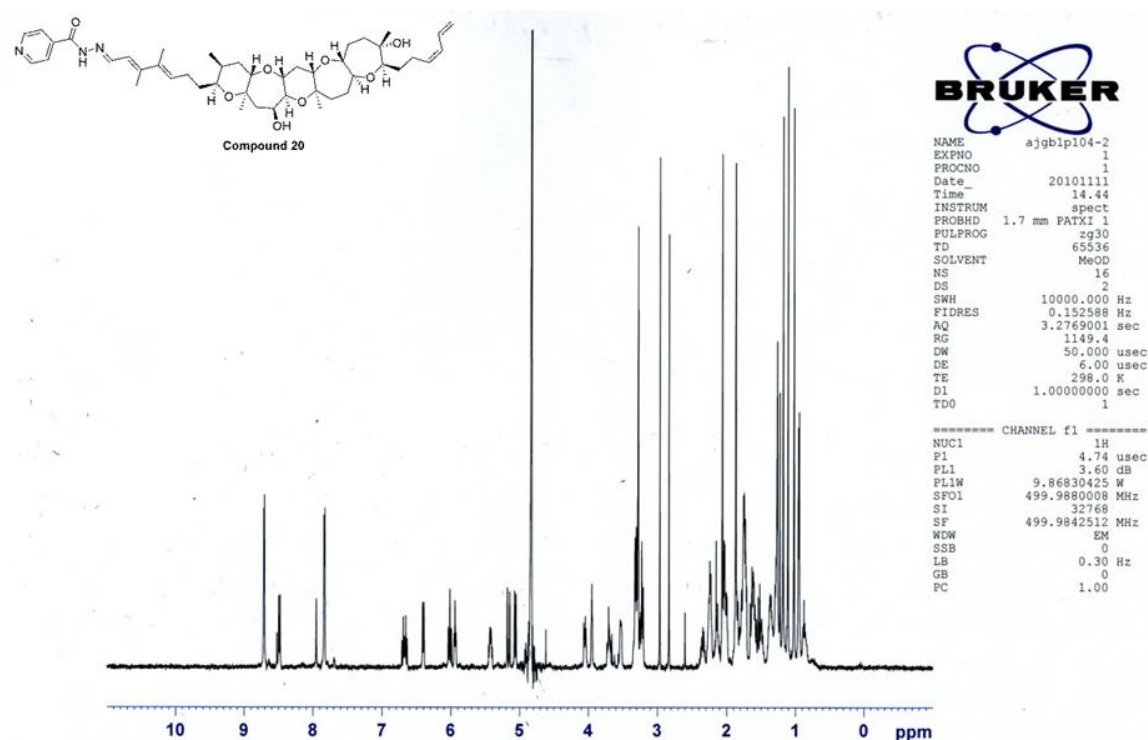
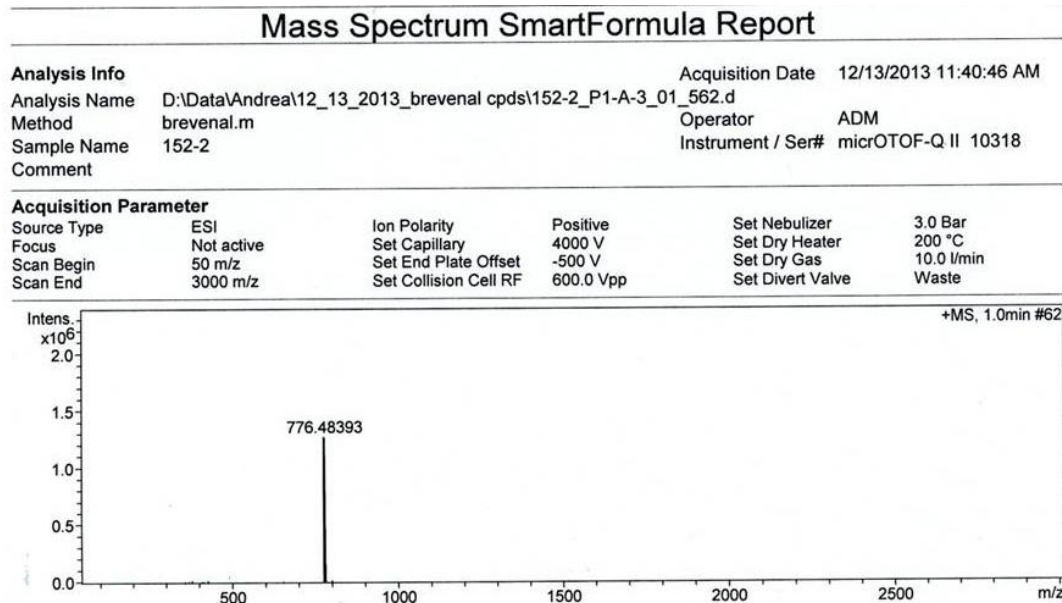
Figure S19. ¹H NMR spectrum of compound 20.

Figure S20. HRMS spectrum of compound 20.



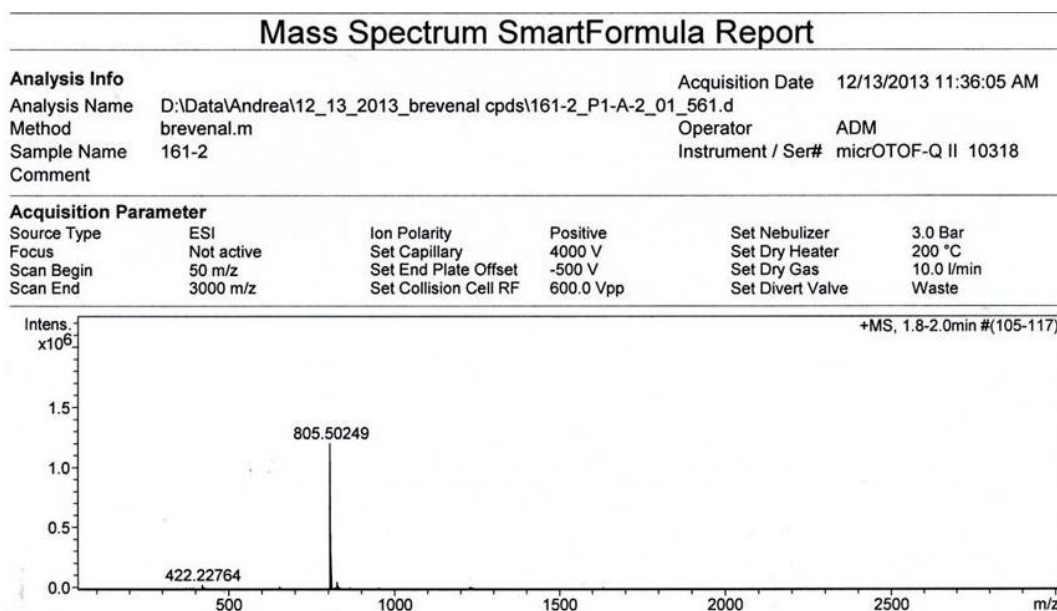
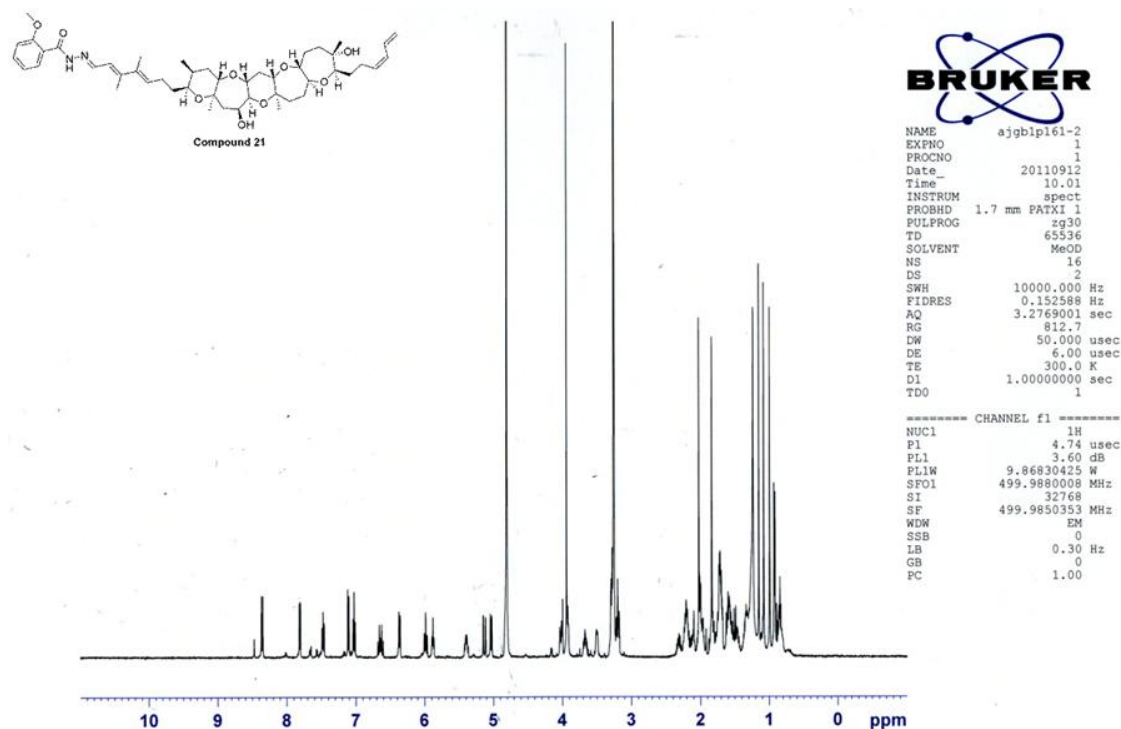


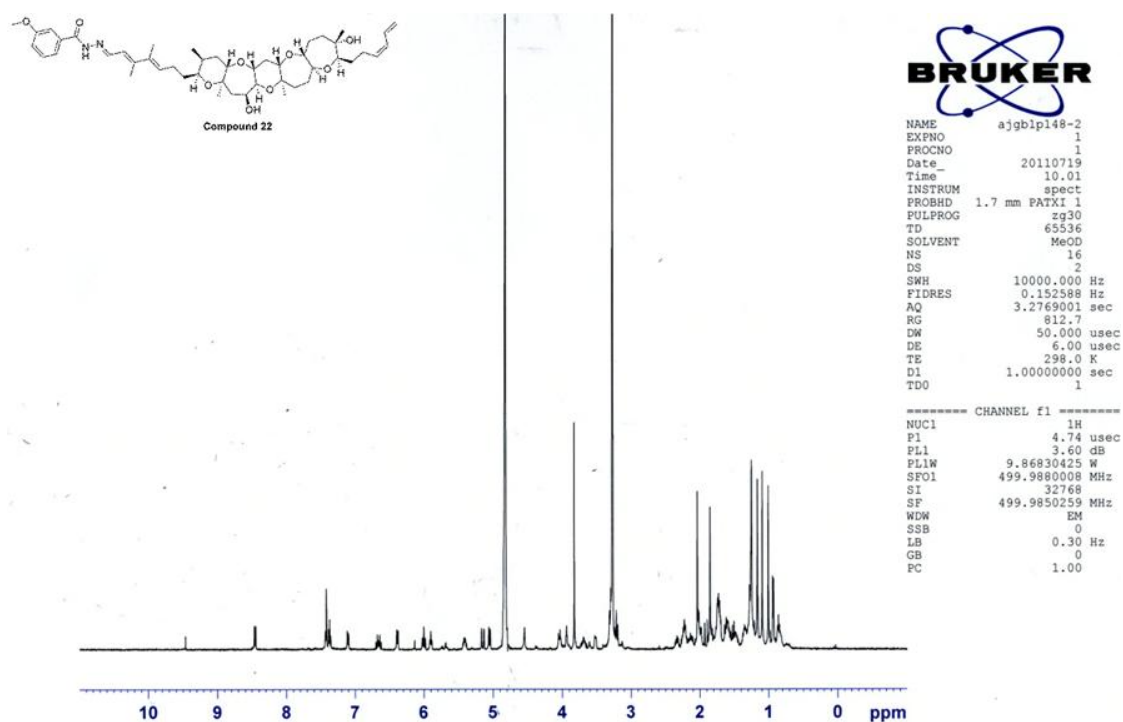
Figure S23. ^1H NMR spectrum of compound 22.

Figure S24. HRMS spectrum of compound 22.

Mass Spectrum SmartFormula Report

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Method	brevenal.m	Instrument / Ser#	micrOTOF-Q II 10318
Sample Name	148-2		
Comment			

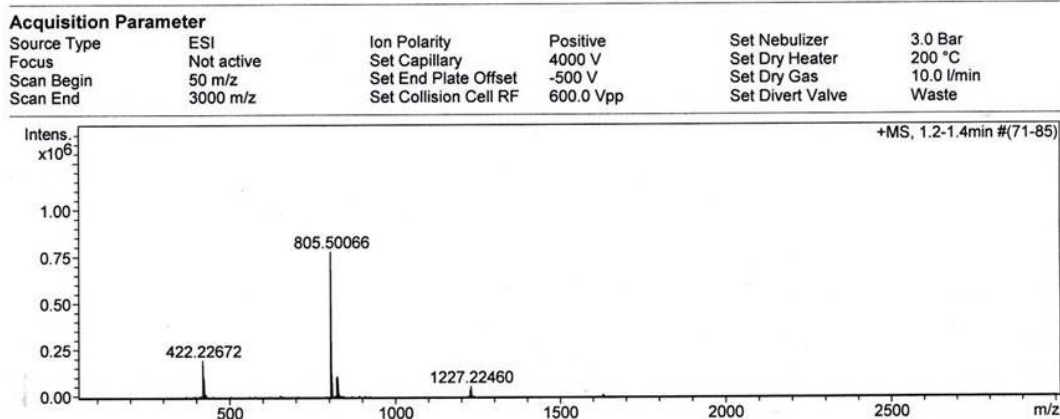


Figure S27. ^1H NMR spectrum of compound **24**.

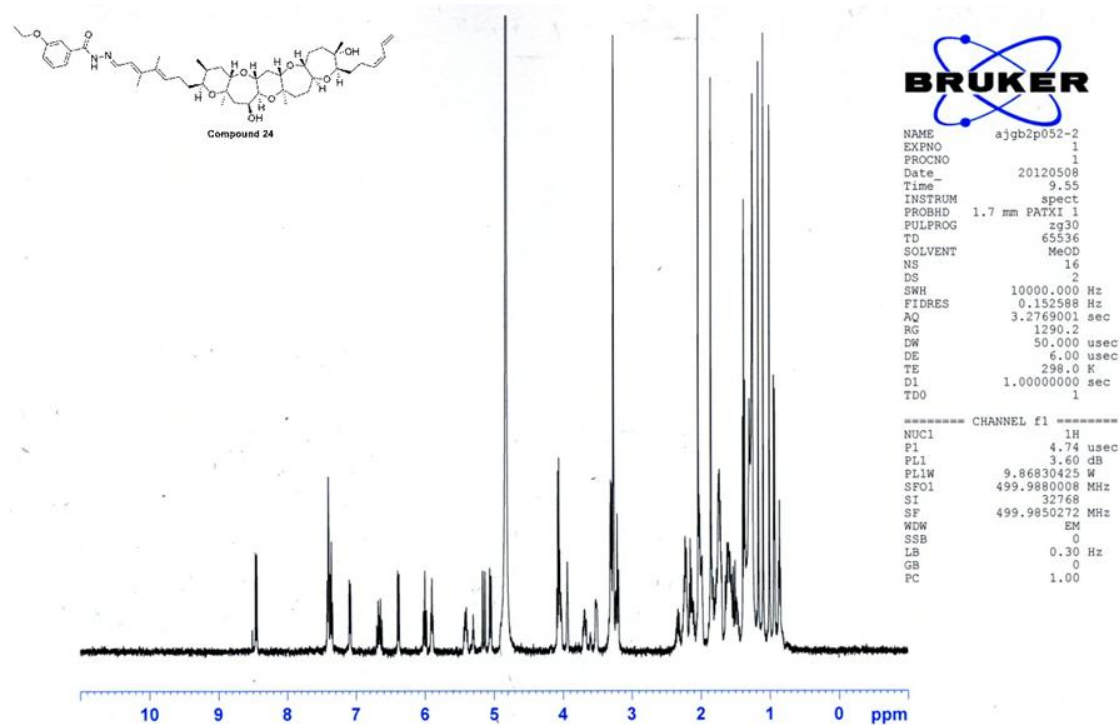


Figure S28. HRMS spectrum of compound **24**.

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	12/13/2013 11:54:54 AM
Analysis Name	D:\Data\Andrea\12_13_2013_breval cpds\52-2_P1-A-6_01_565.d		
Method	breval.m	Operator	ADM
Sample Name	52-2	Instrument / Ser#	microTOF-Q II 10318
Comment			

Acquisition Parameter					
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Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste

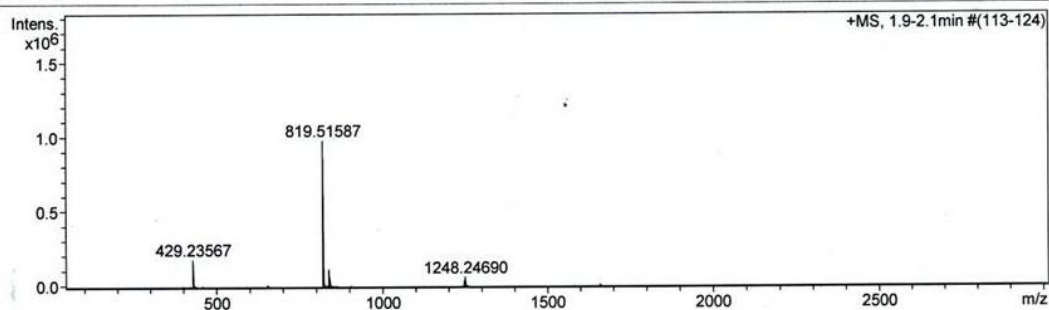


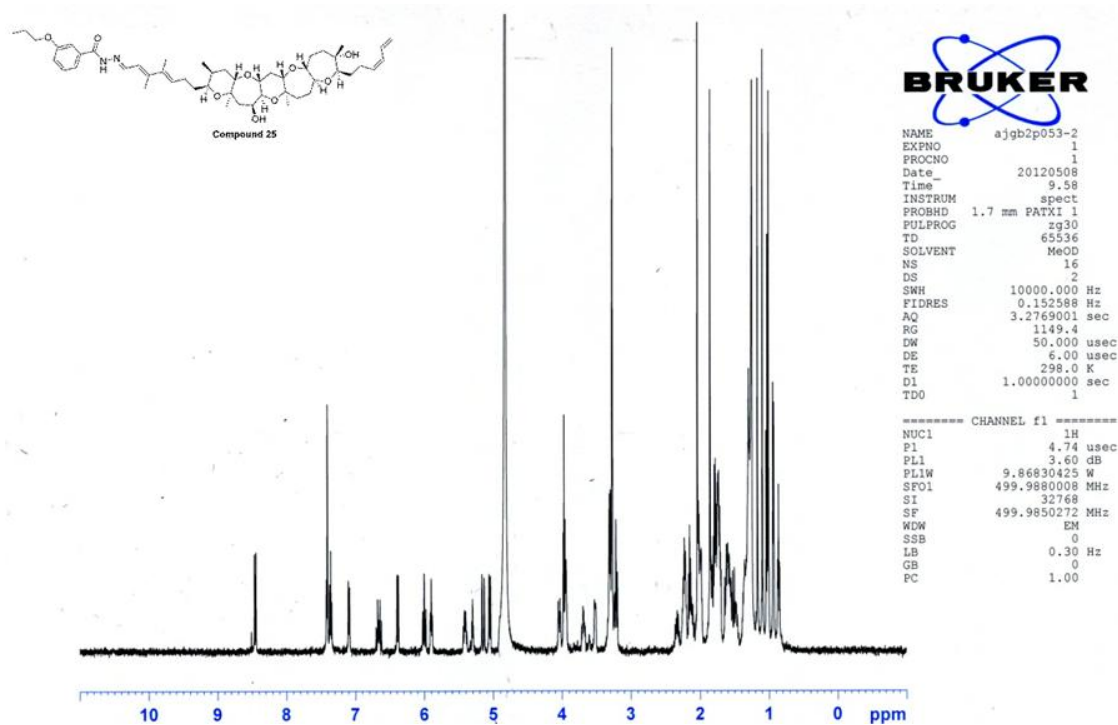
Figure S29. ^1H NMR spectrum of compound 25.

Figure S30. HRMS spectrum of compound 25.

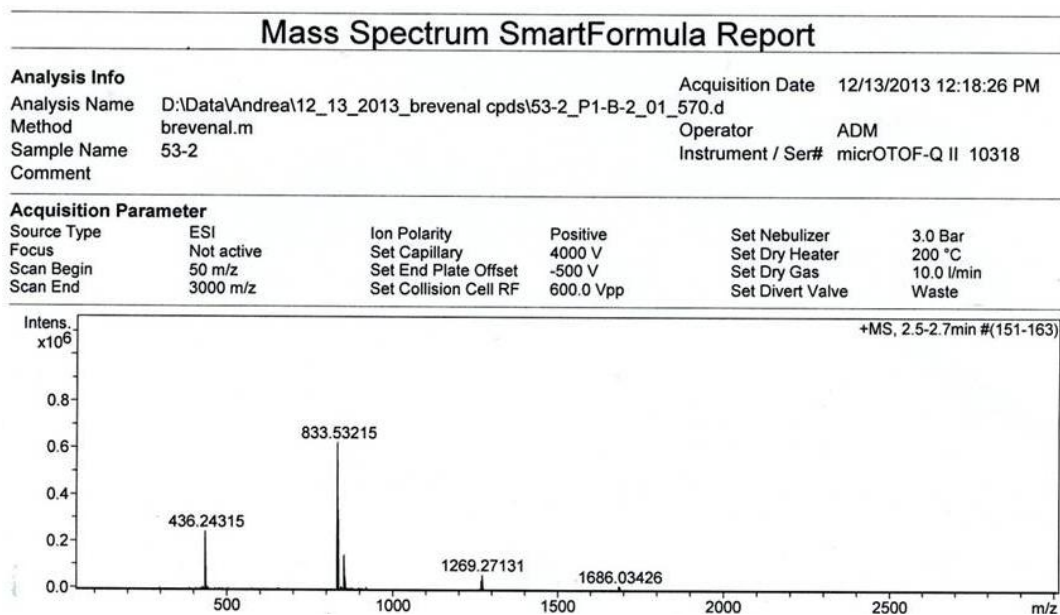


Figure S33. ^1H NMR spectrum of compound **27**.

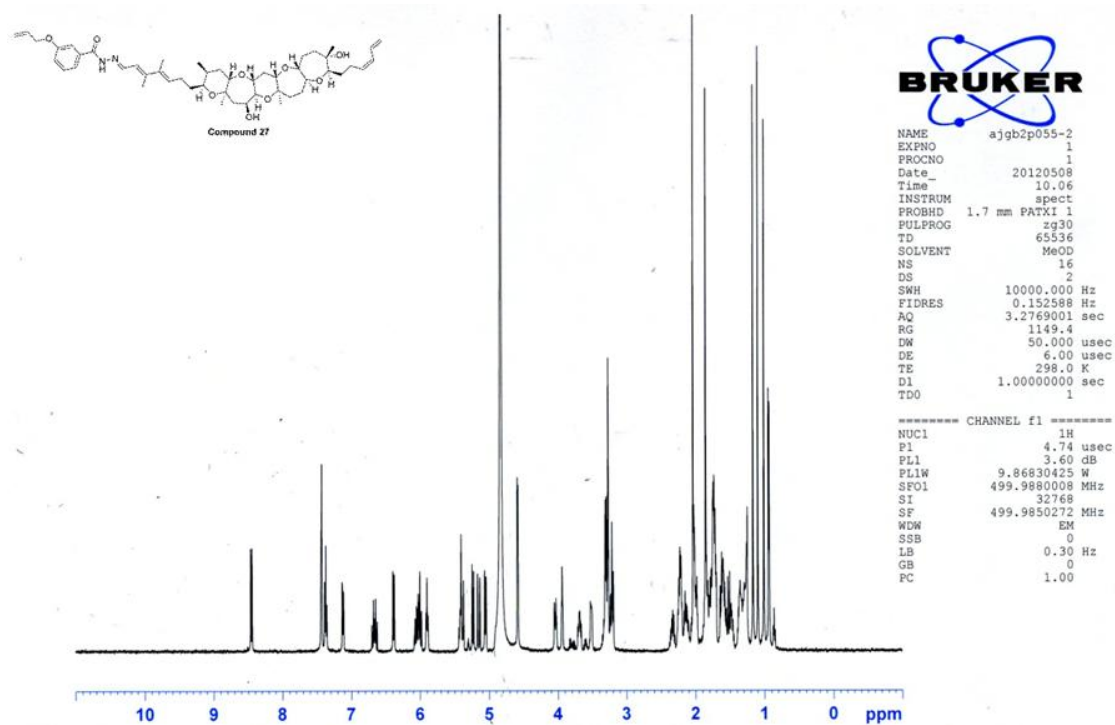
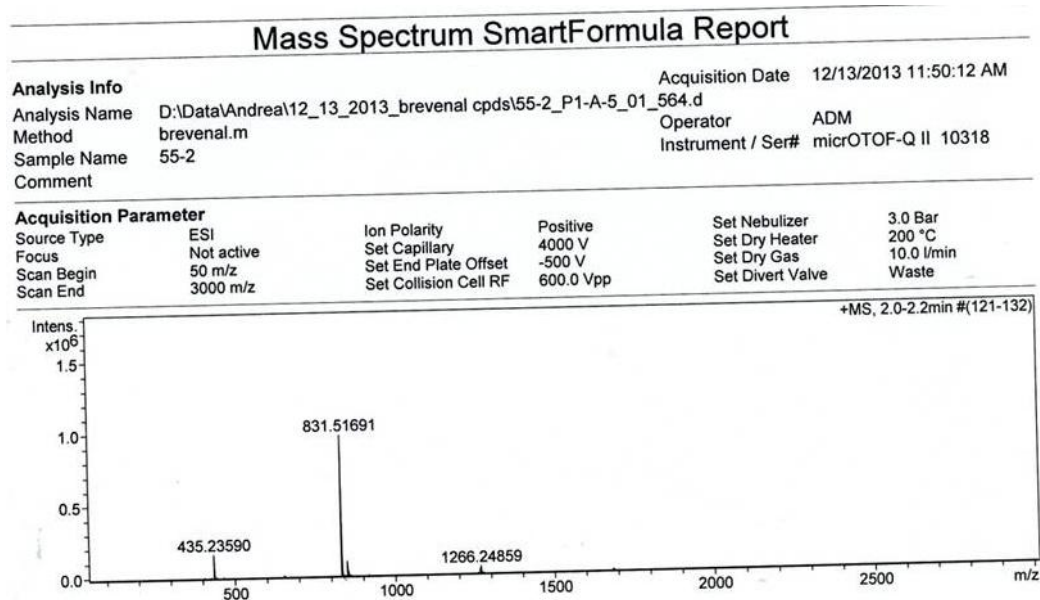


Figure S34. HRMS spectrum of compound **27**.



Analysis Info

Analysis Name

Method

Sample Name

Comment

Acquisition Date 12/13/2013 11:50:12 AM

564.d

Operator ADM
Instrument / Ser# micrOTOF-Q II 10318

Acquisition ParameterSource Type

Focus

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Scan End

Scan END

ES

Not active
EO m/z

3000 m/z

Ion Polarity

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Set Collision Cell BESet Collision Cell RFPositive4000 V

-500 V
600.0 V

000.0 vppSet NebulizerSet Dry HeaterSet Dry GasSet Divert Valve3.0 Bar200 °C10.0 l/min
Wastewaste

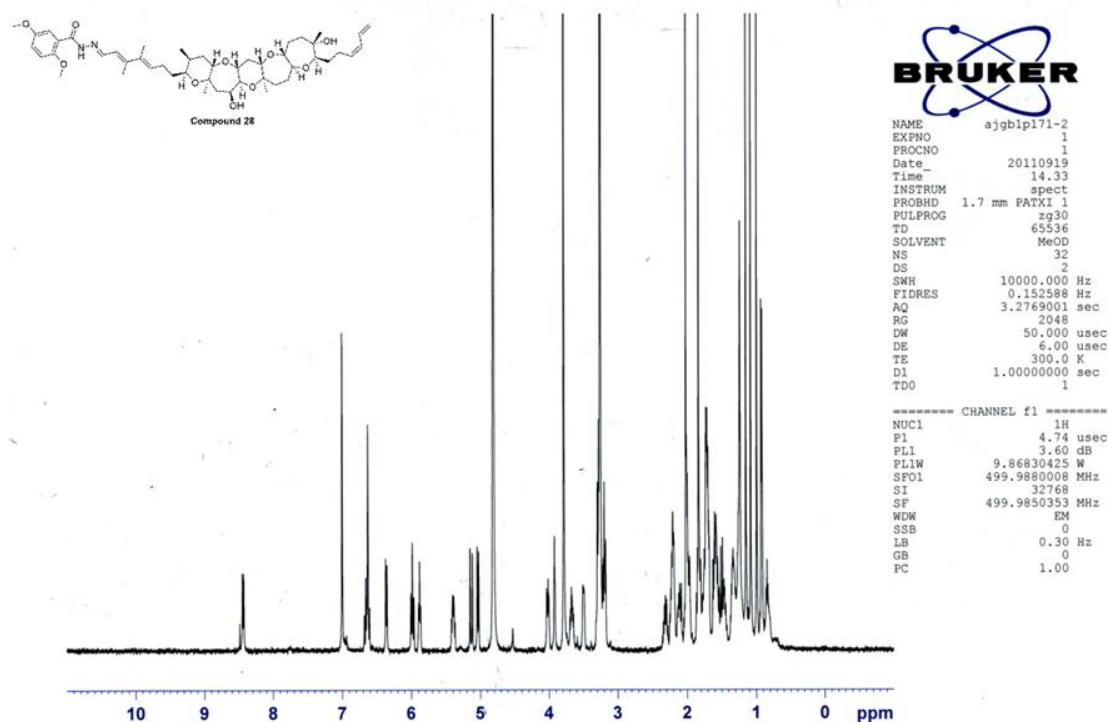
Figure S35. ^1H NMR spectrum of compound 28.

Figure S36. HRMS spectrum of compound 28.

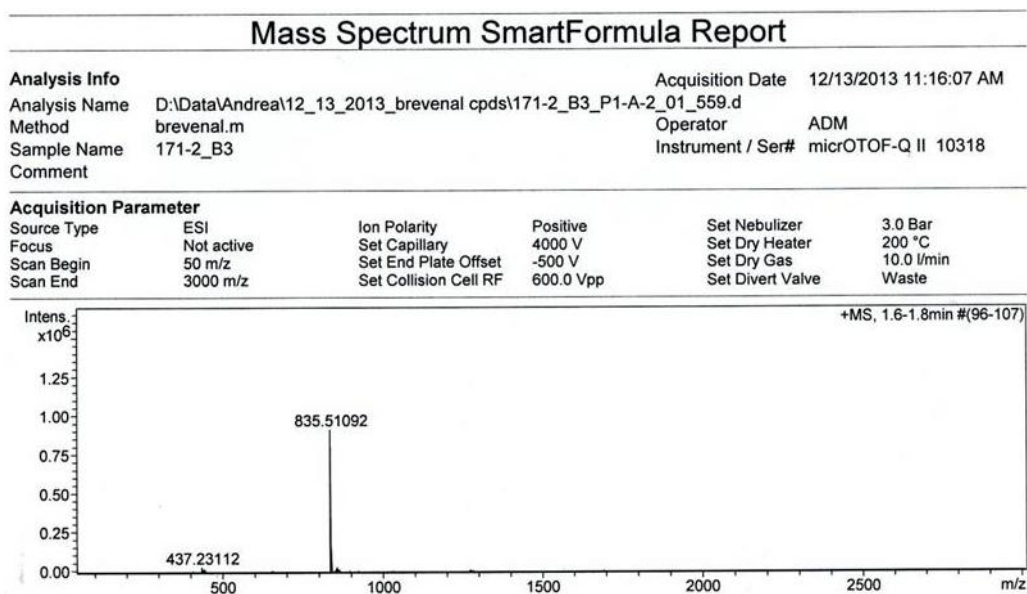


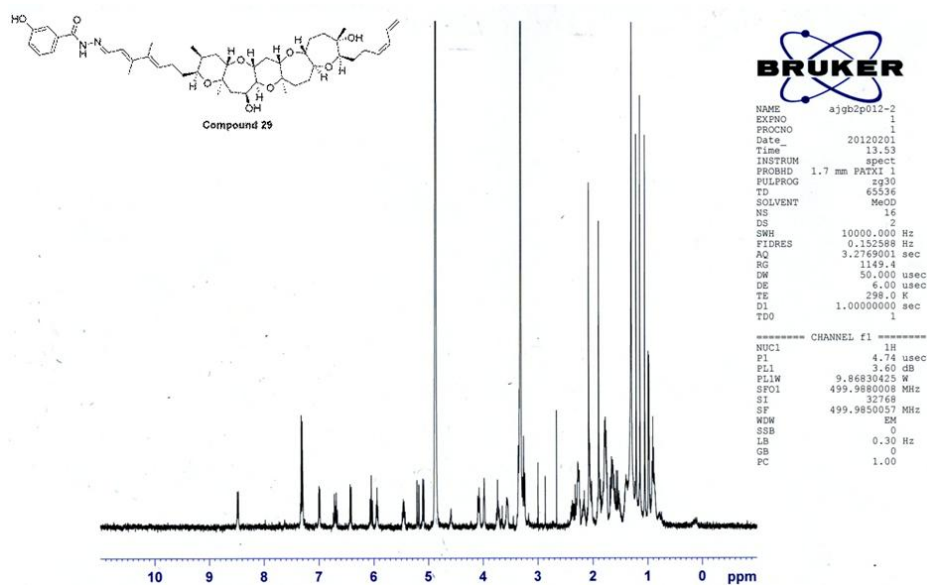
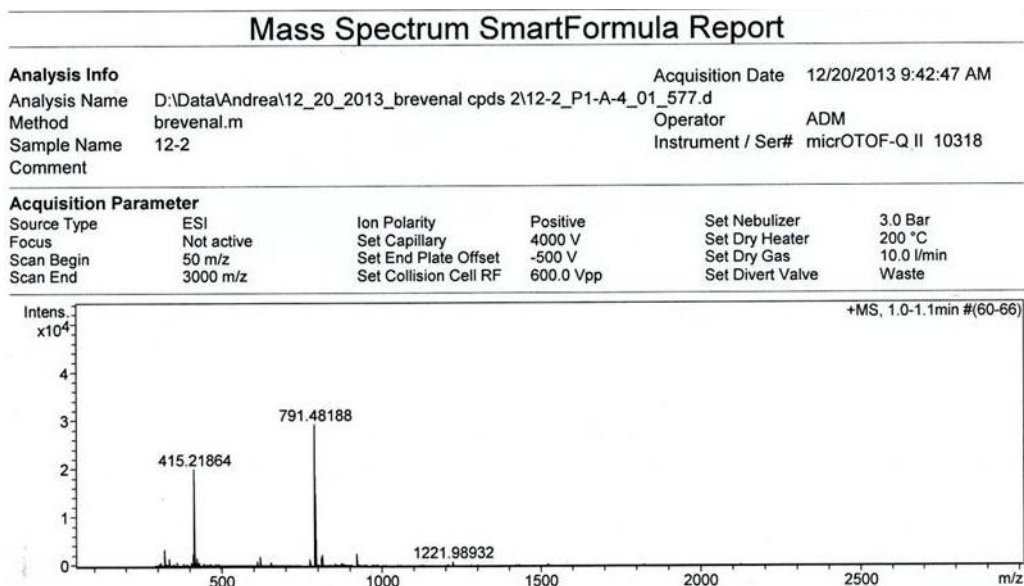
Figure S37. ^1H NMR spectrum of compound 29.

Figure S38. HRMS spectrum of compound 29.



Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	12/20/2013 9:42:47 AM
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Method	brevenal.m	Instrument / Ser#	micrOTOF-Q II 10318
Sample Name	12-2		
Comment			

Acquisition Parameter		Ion Polarity	Positive	Set Nebulizer	3.0 Bar
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Scan End	3000 m/z				

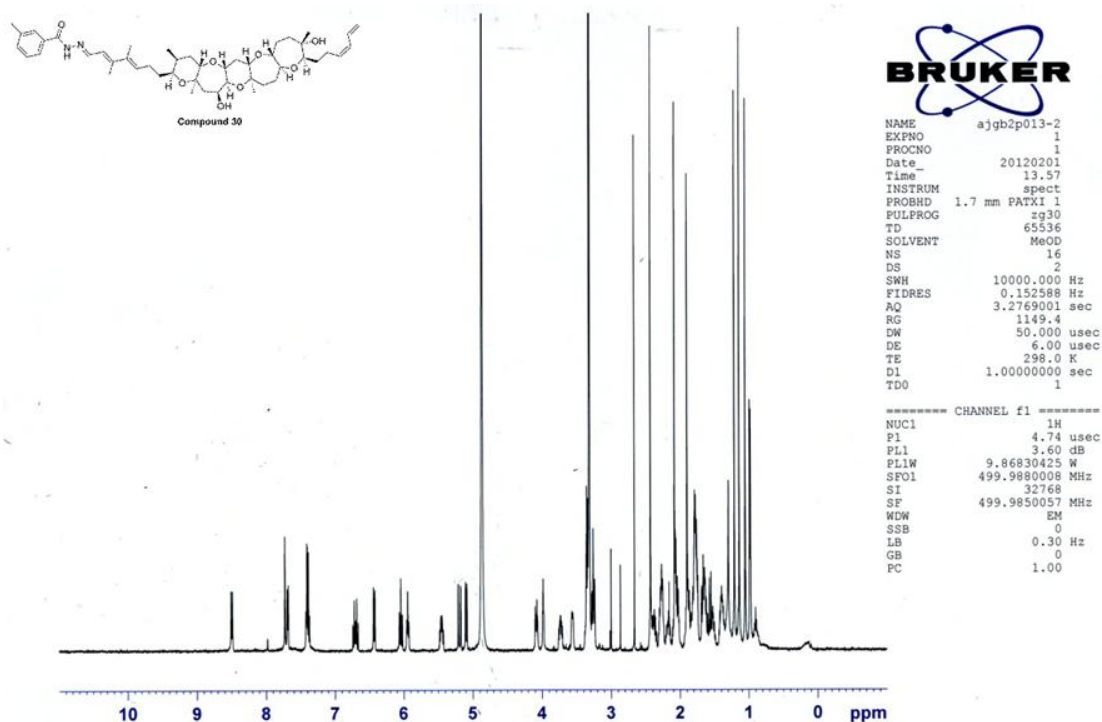
Figure S39. ^1H NMR spectrum of compound 30.

Figure S40. HRMS spectrum of compound 30.

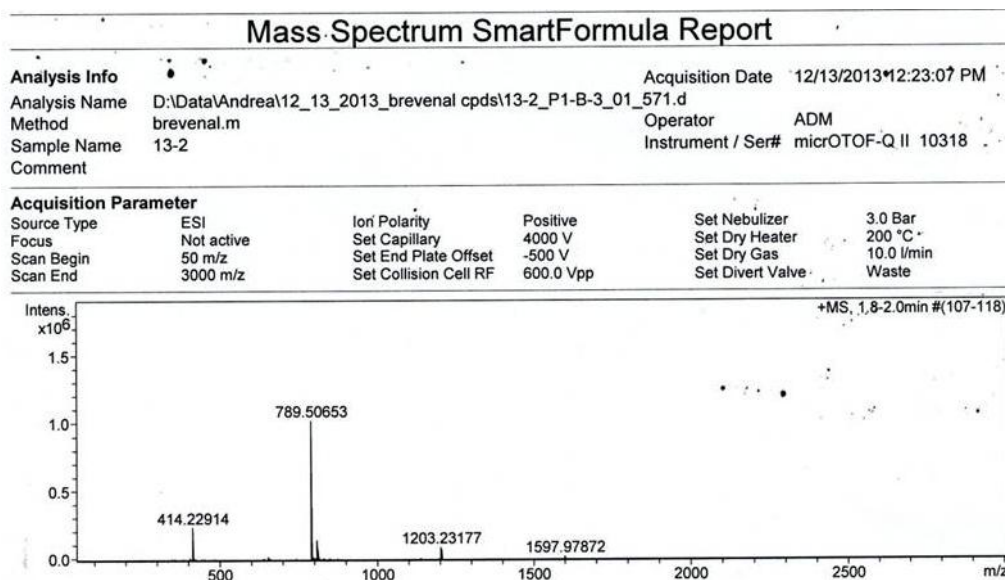


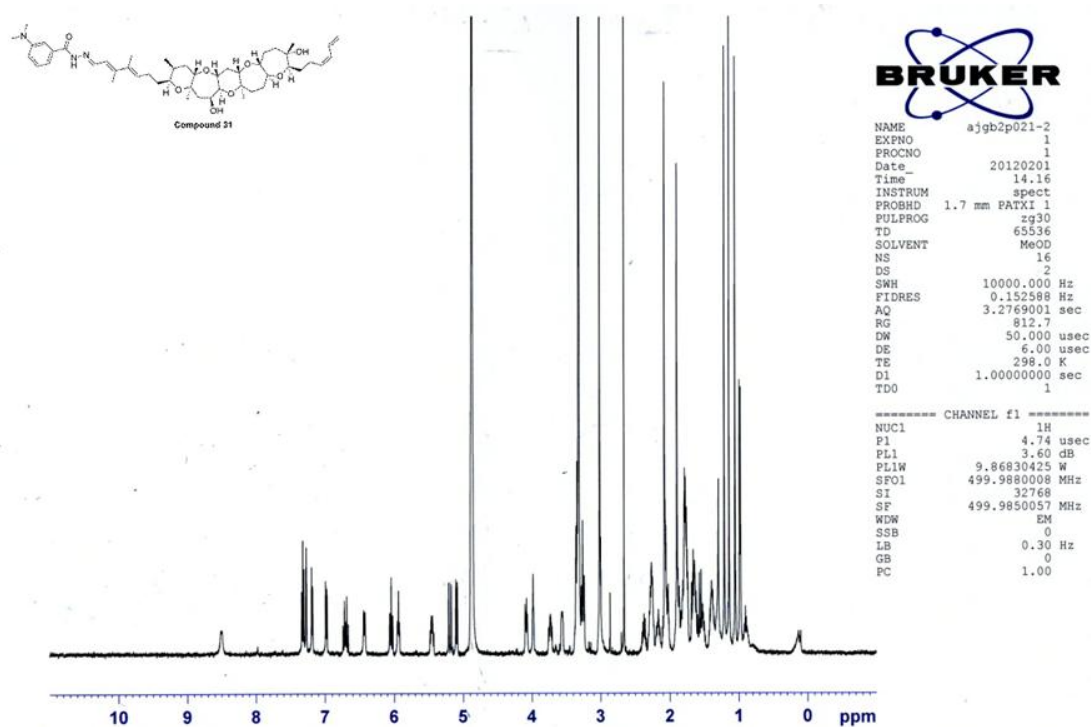
Figure S41. ¹H NMR spectrum of compound 31.

Figure S42. HRMS spectrum of compound 31.

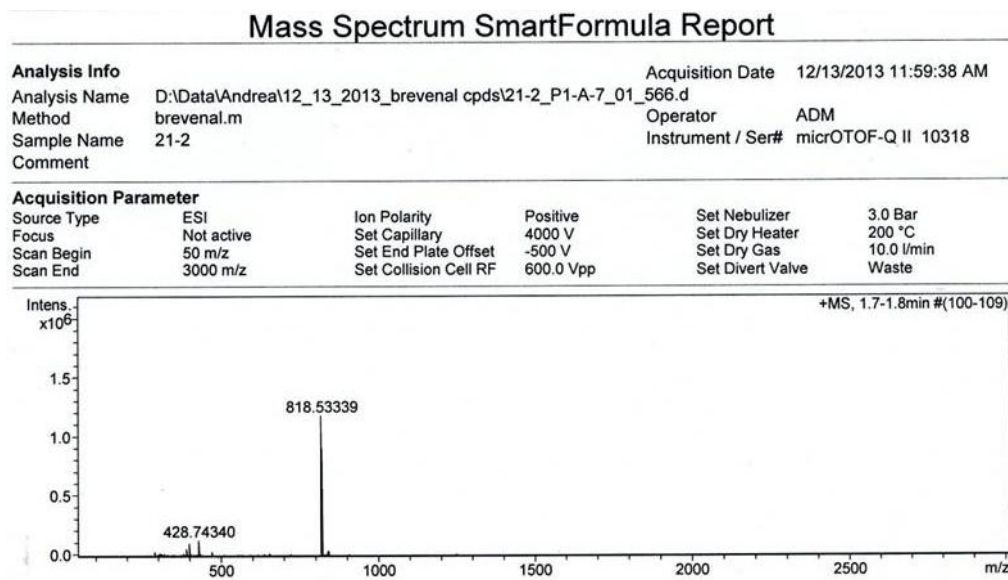


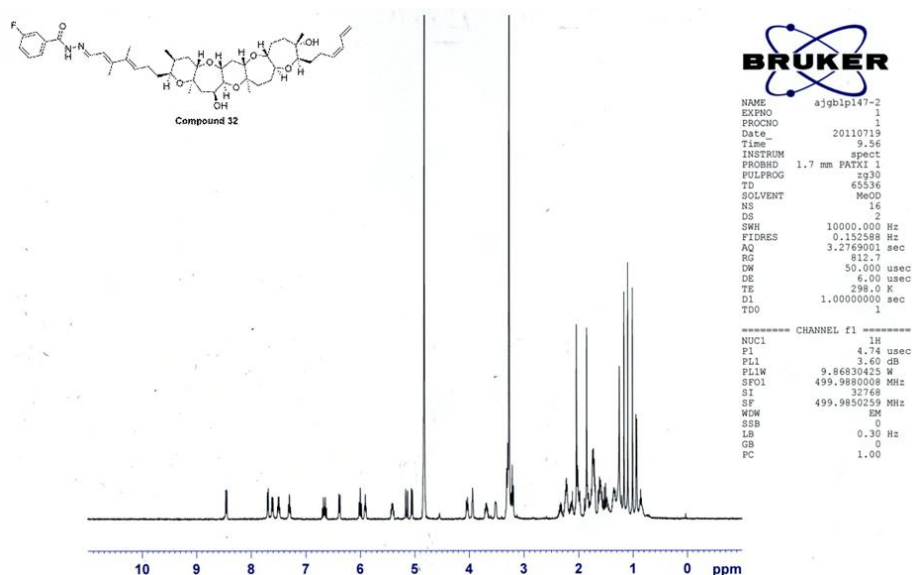
Figure S43. ^1H NMR spectrum of compound 32.

Figure S44. HRMS spectrum of compound 32.

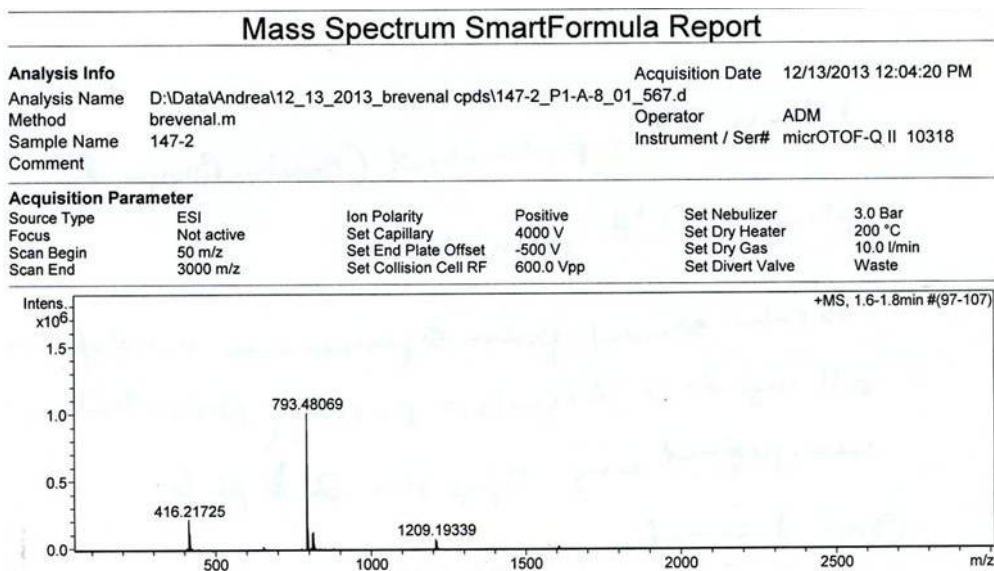


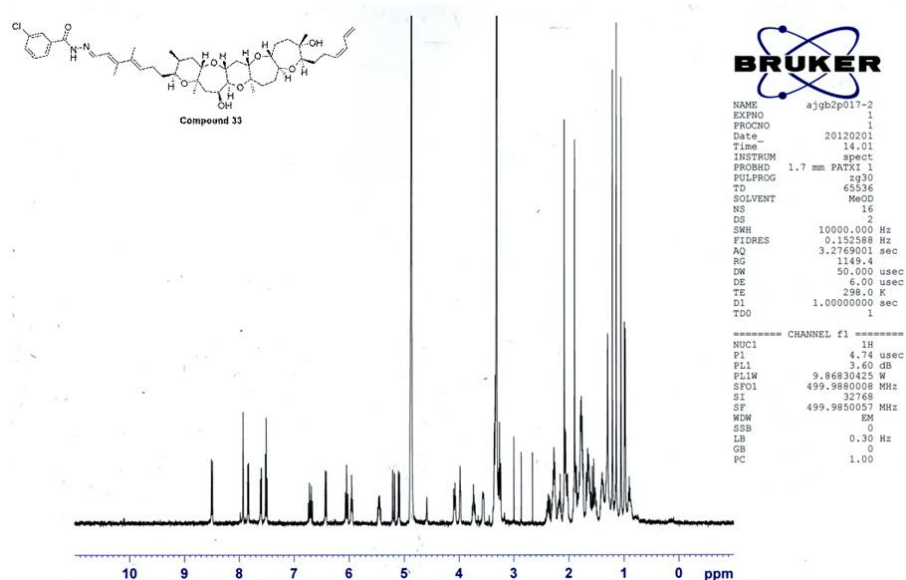
Figure S45. ^1H NMR spectrum of compound 33.

Figure S46. HRMS spectrum of compound 33.

Mass Spectrum SmartFormula Report

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Method	brevenal.m	Instrument / Ser#	micrOTOF-Q II 10318
Sample Name	P124.2		
Comment			

Acquisition Parameter

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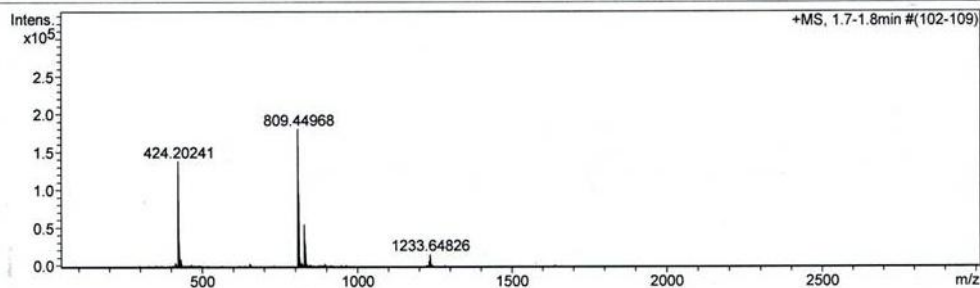


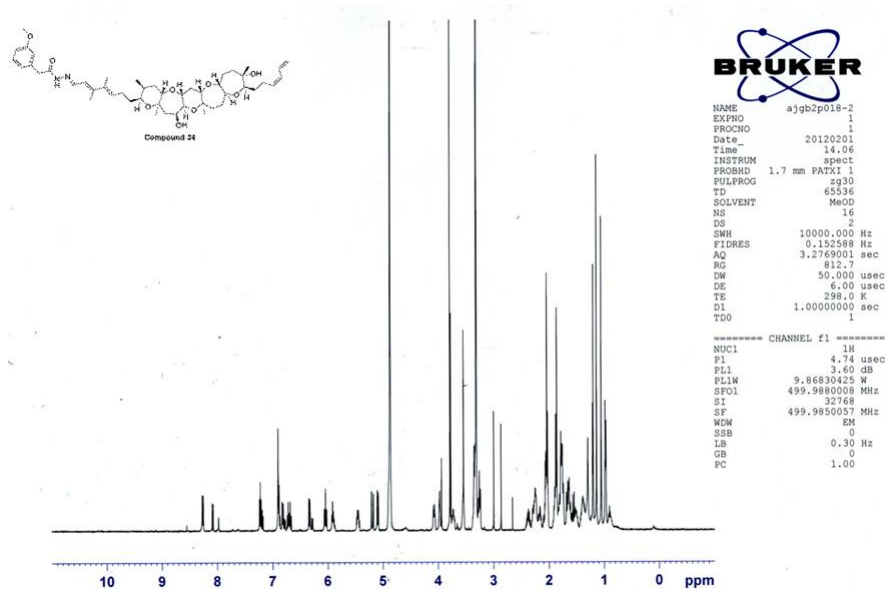
Figure S47. ^1H NMR spectrum of compound 34.

Figure S48. HRMS spectrum of compound 34.

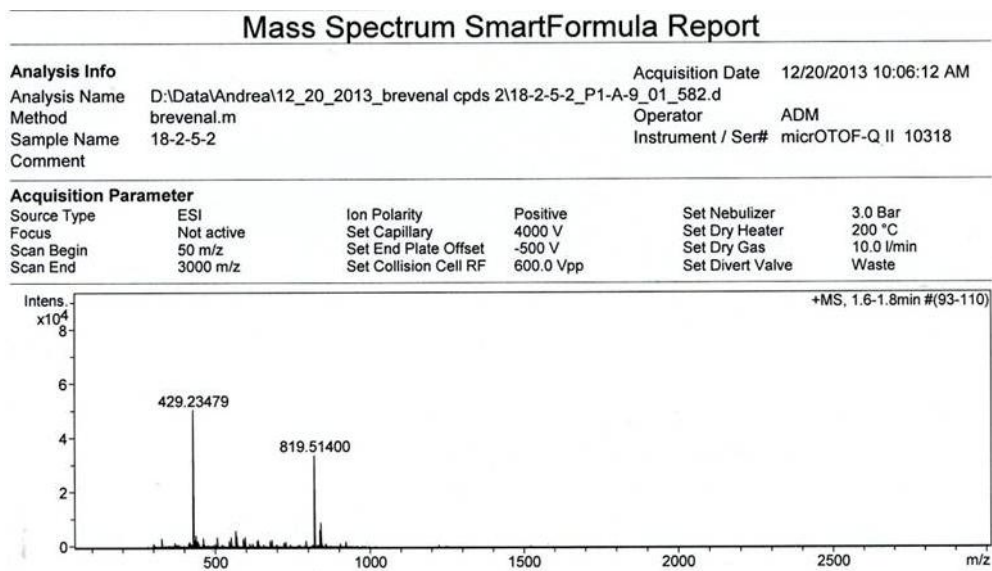


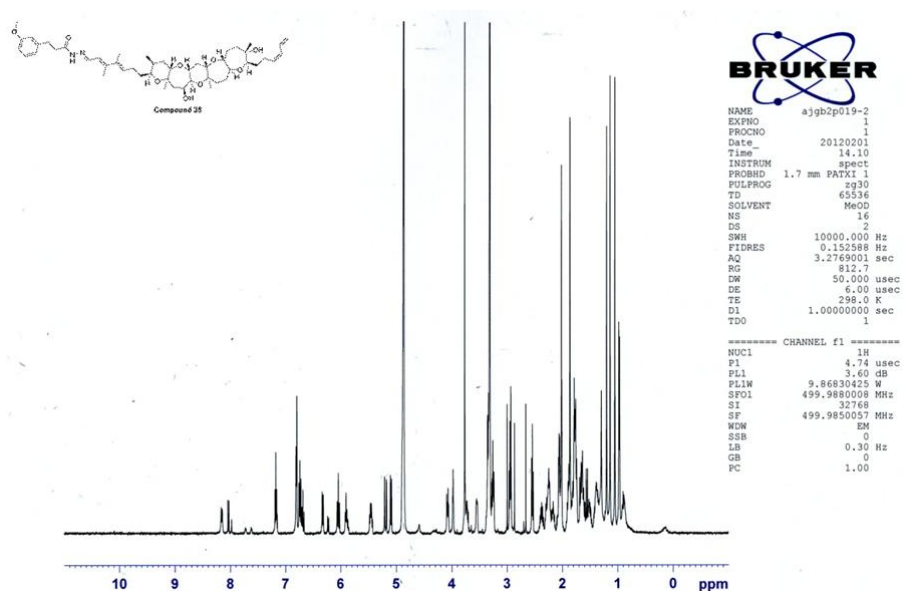
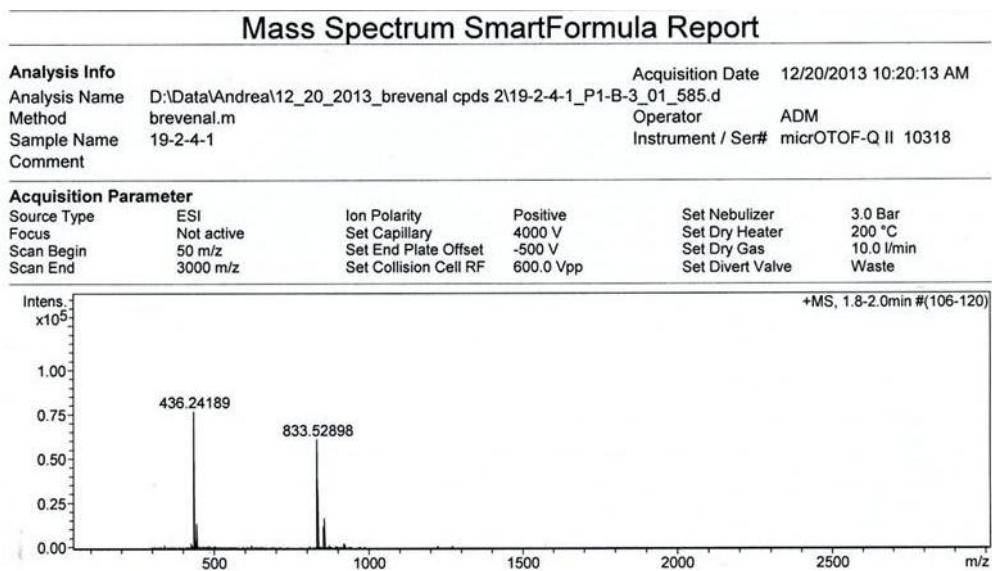
Figure S49. ^1H NMR spectrum of compound 35.**Figure S50.** HRMS spectrum of compound 35.

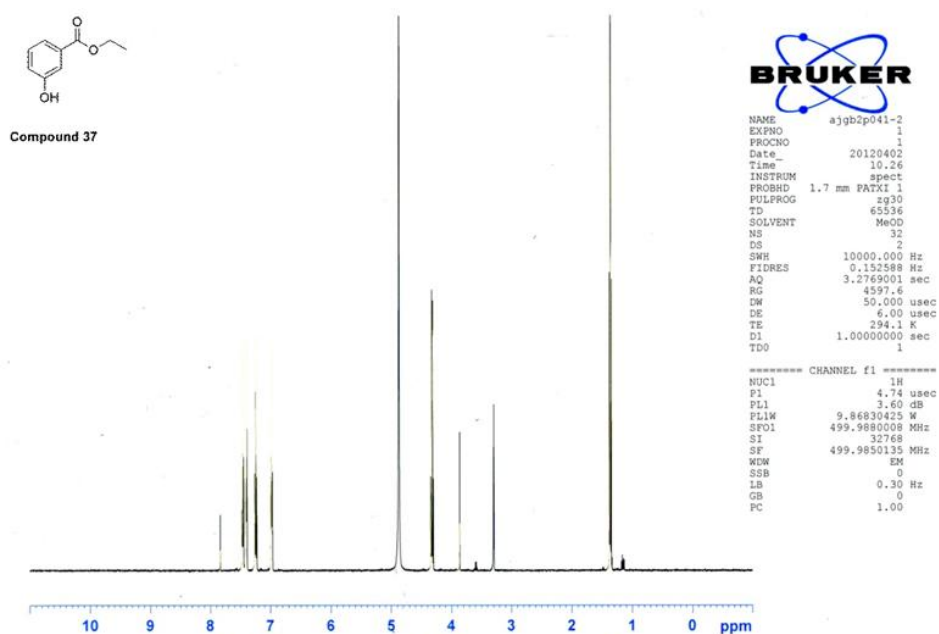
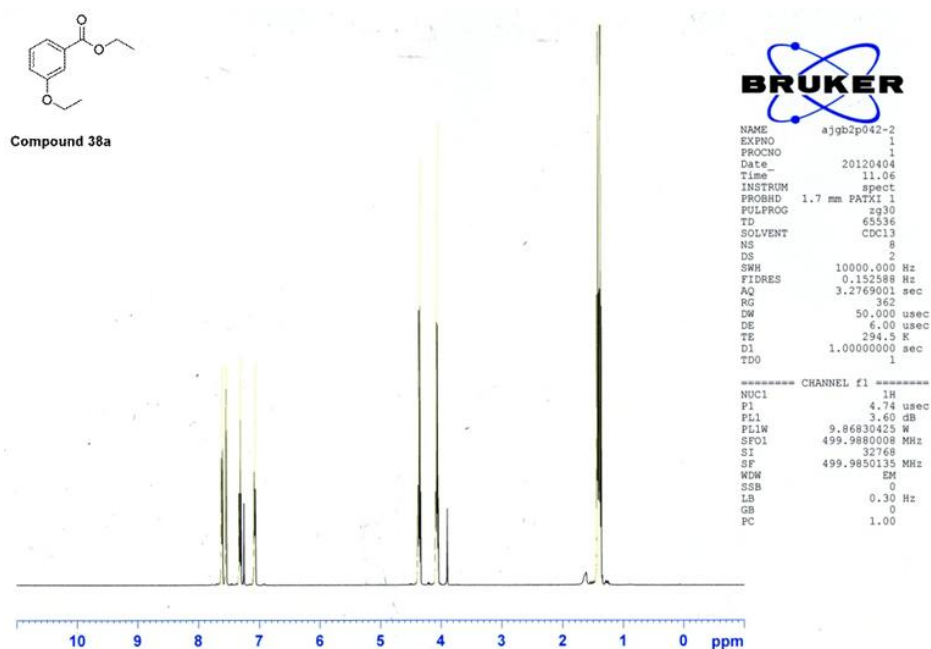
Figure S51. ^1H NMR spectrum of compound 37.**Figure S52.** ^1H NMR spectrum of compound 38a.

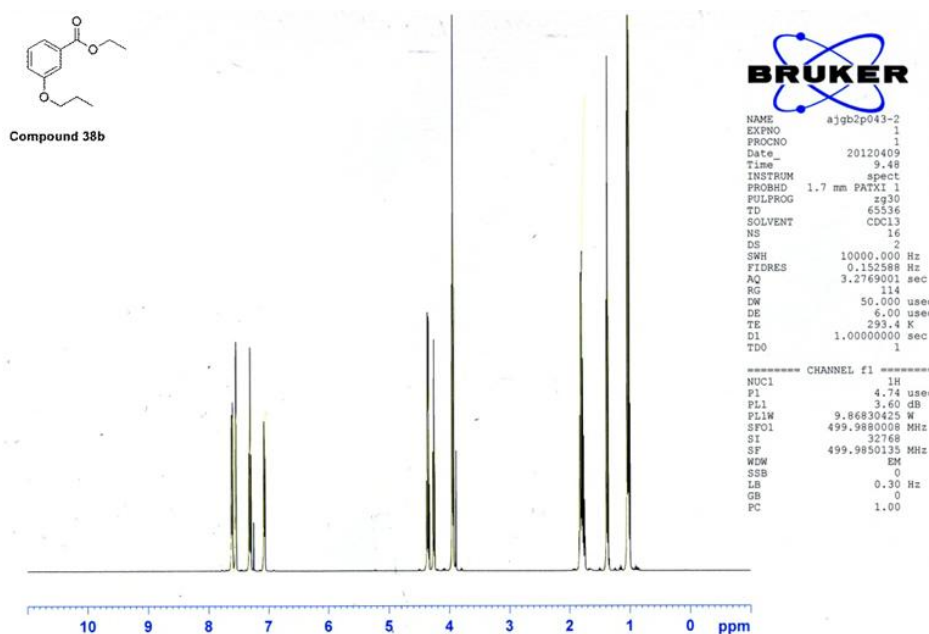
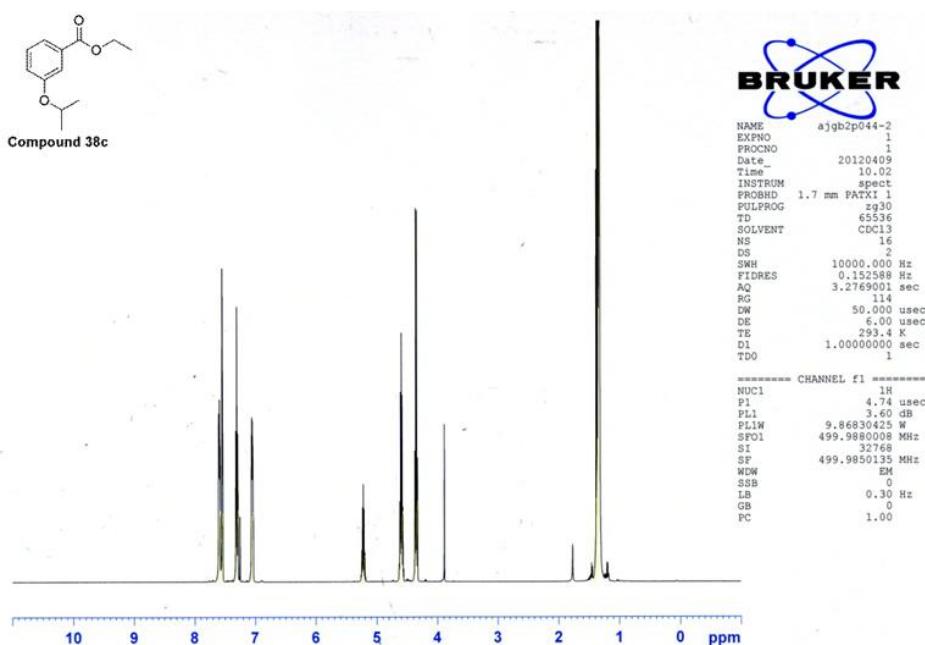
Figure S53. ^1H NMR spectrum of compound 38b.Figure S54. ^1H NMR spectrum of compound 38c.

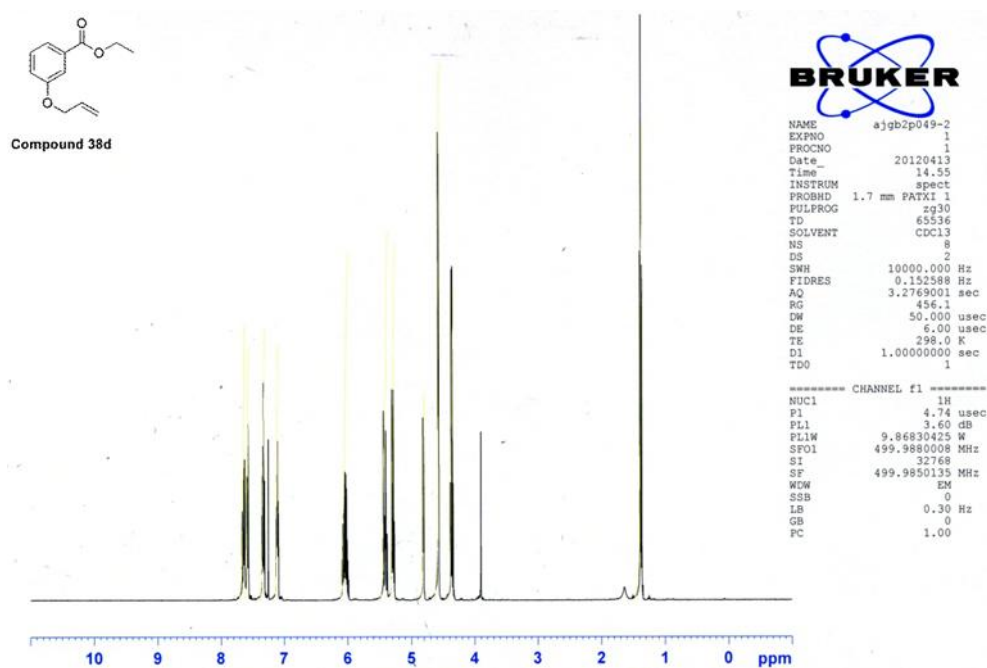
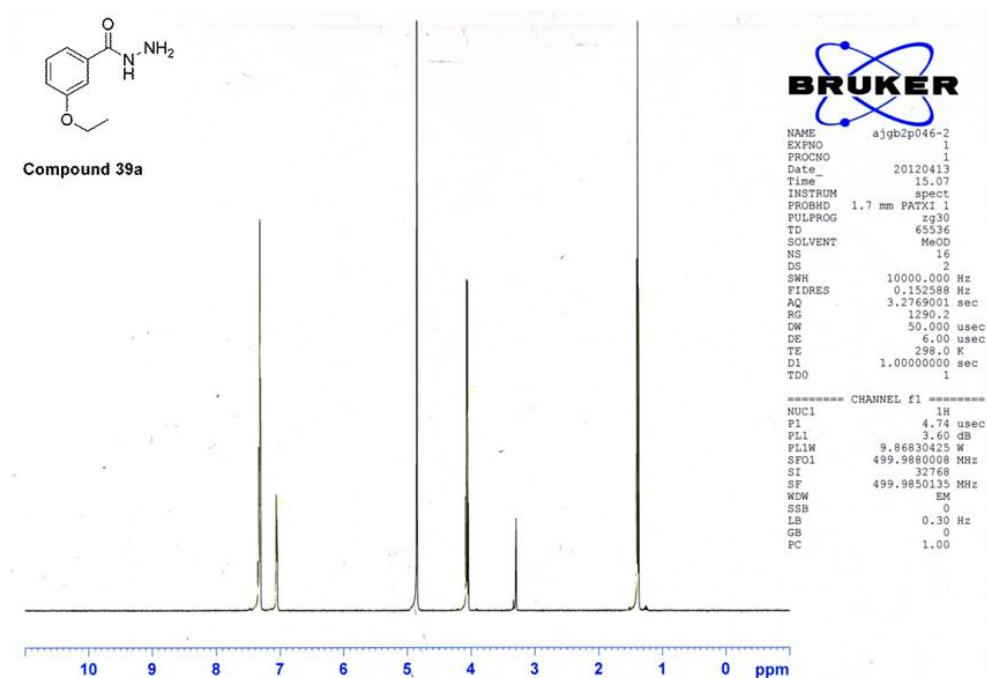
Figure S55. ^1H NMR spectrum of compound 38d.Figure S56. ^1H NMR spectrum of compound 39a.

Figure S57. TIC and MS spectrum of compound 39a.

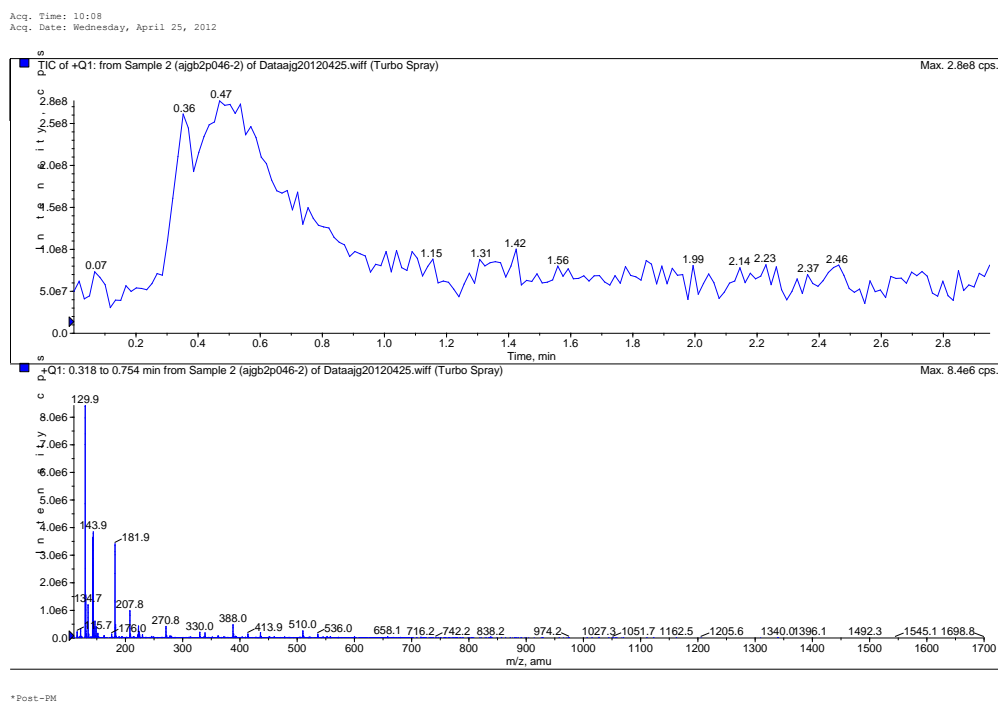
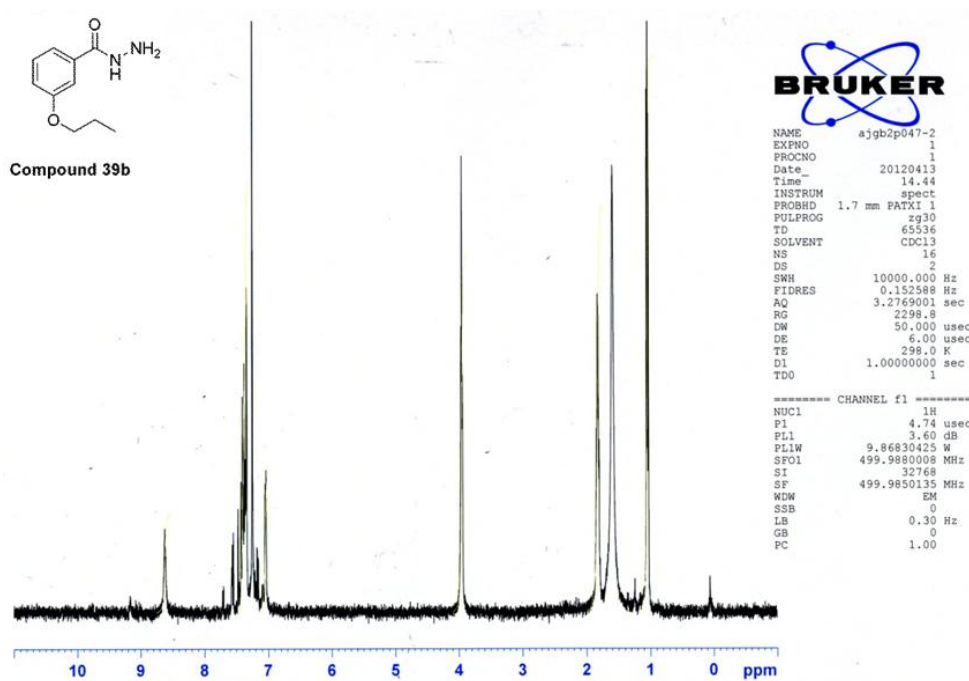
Figure S58. ^1H NMR spectrum of compound 39b.

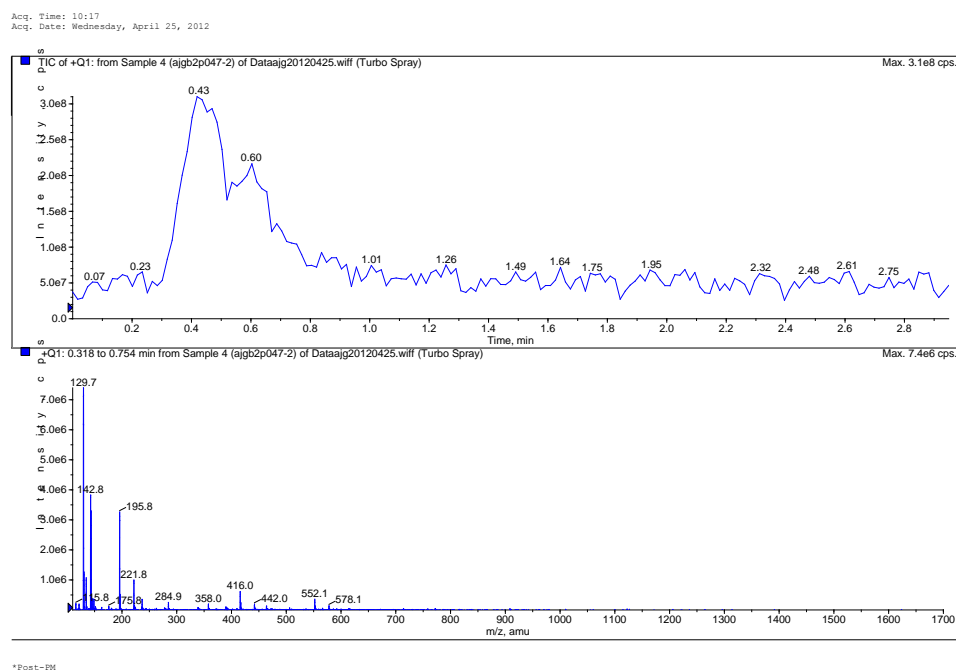
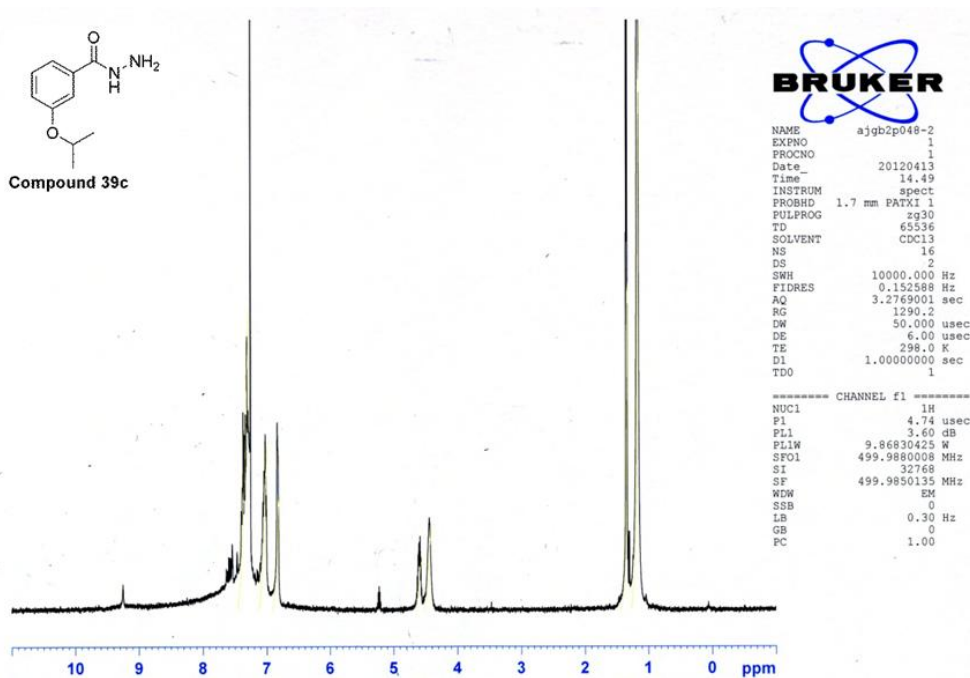
Figure S59. TIC and MS spectrum of compound **39b**.**Figure S60.** ^1H NMR spectrum of compound **39c**.

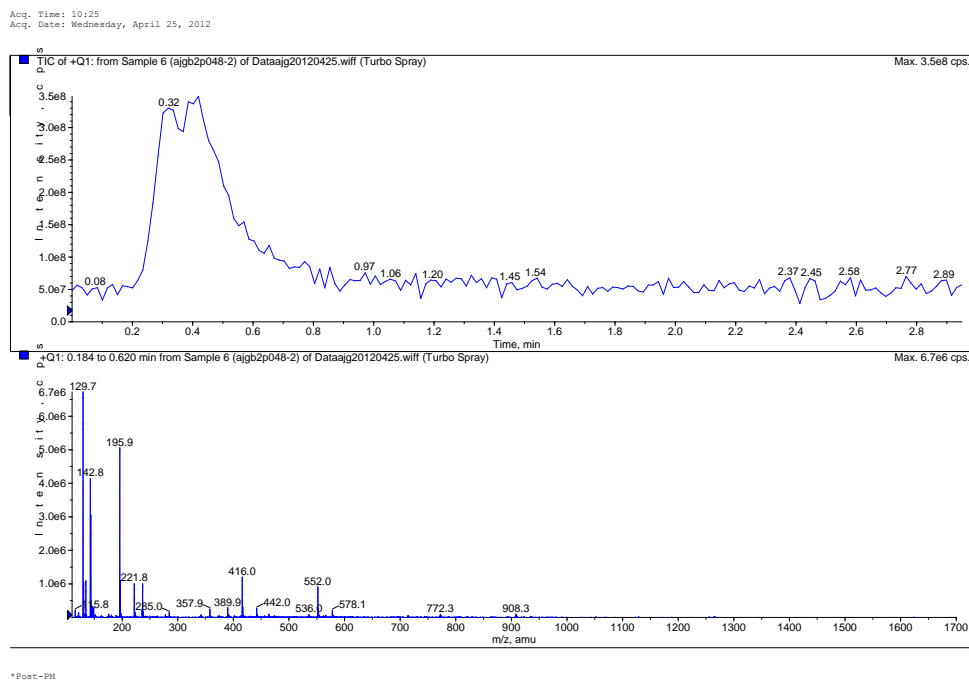
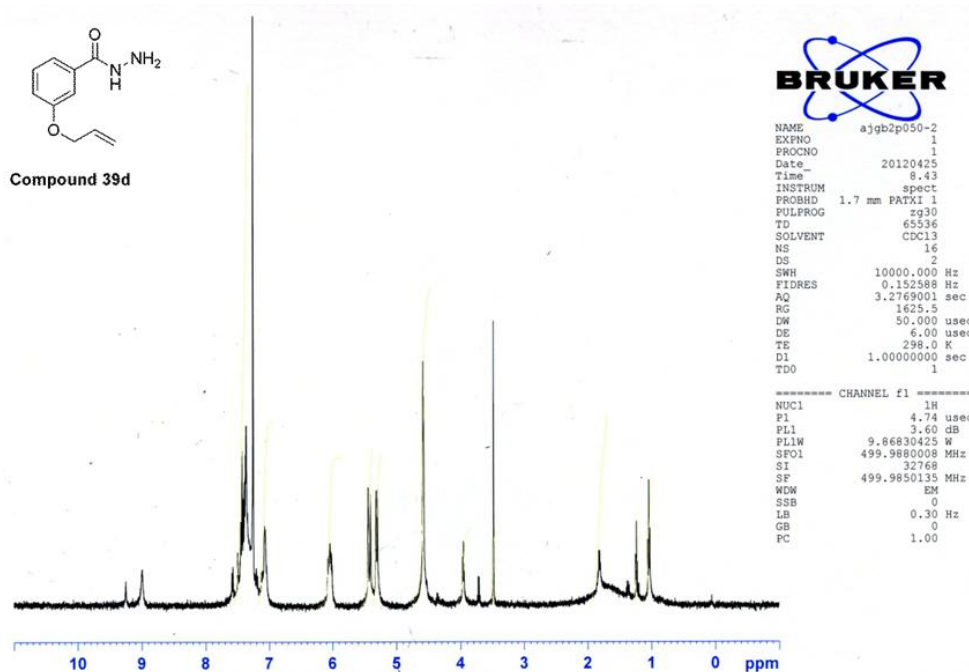
Figure S61. TIC and MS spectrum of compound **39c**.**Figure S62.** ^1H NMR spectrum of compound **39d**.

Figure S63. TIC and MS spectrum of compound 39d.

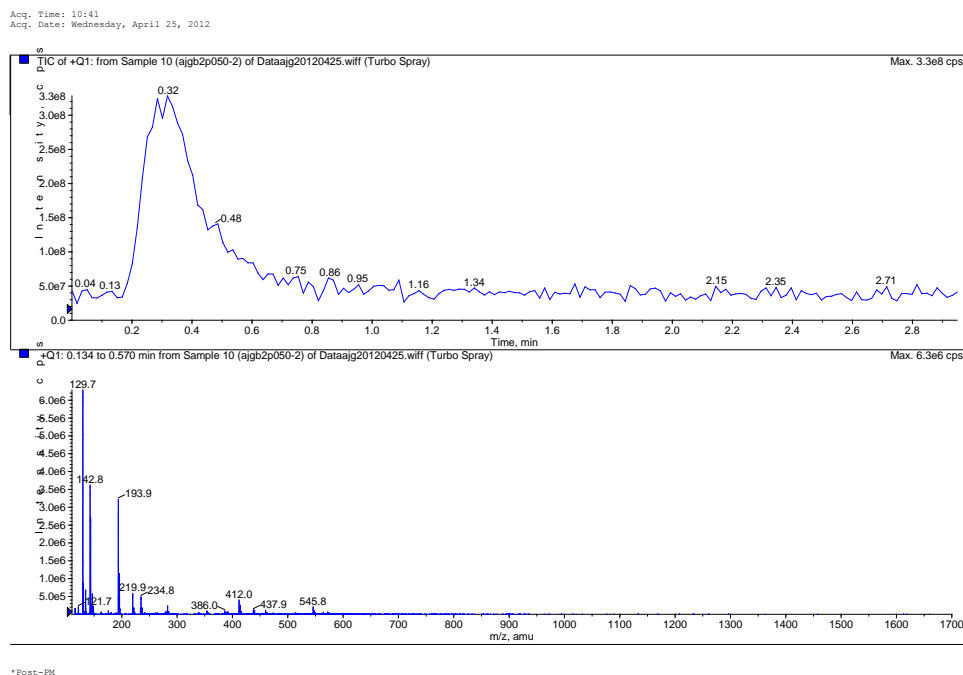
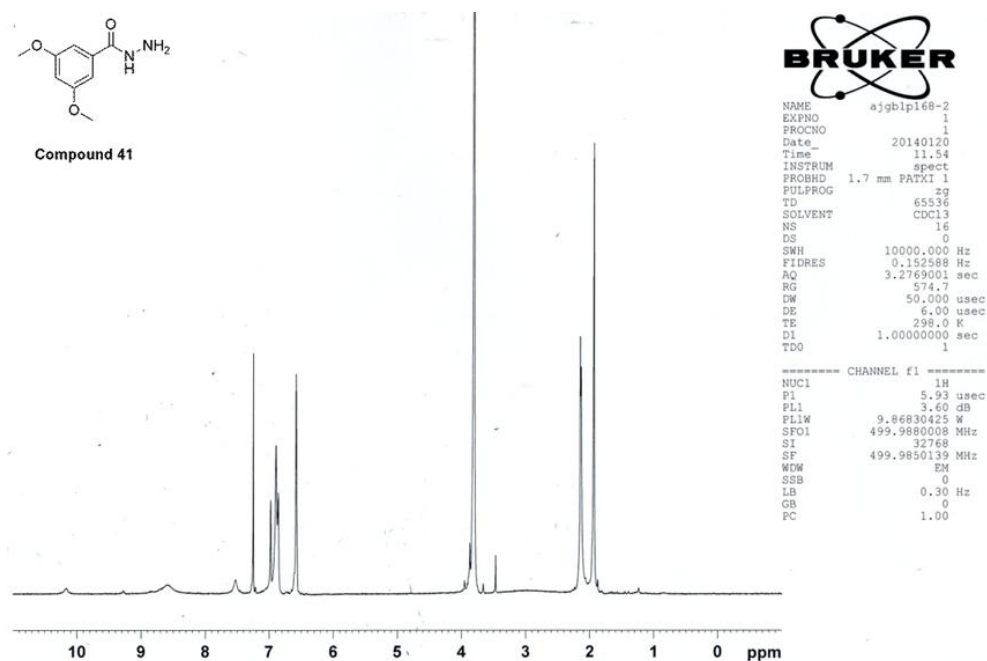
Figure S64. ¹H NMR spectrum of compound 41.

Figure S65. TIC and MS spectrum of compound 41.

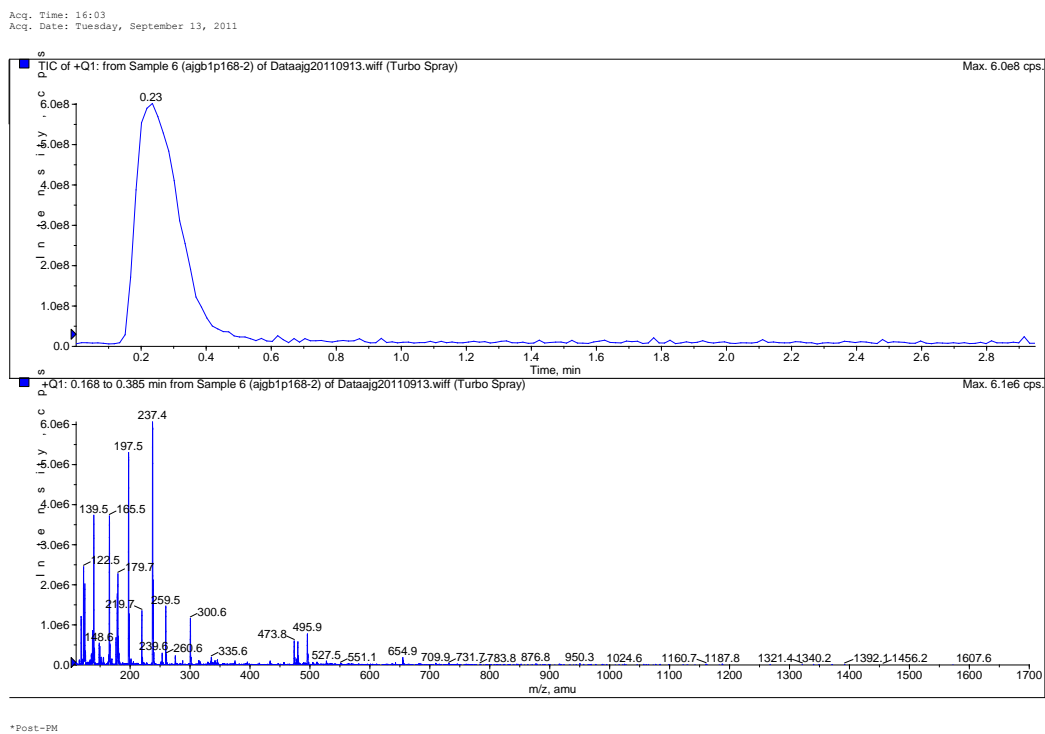
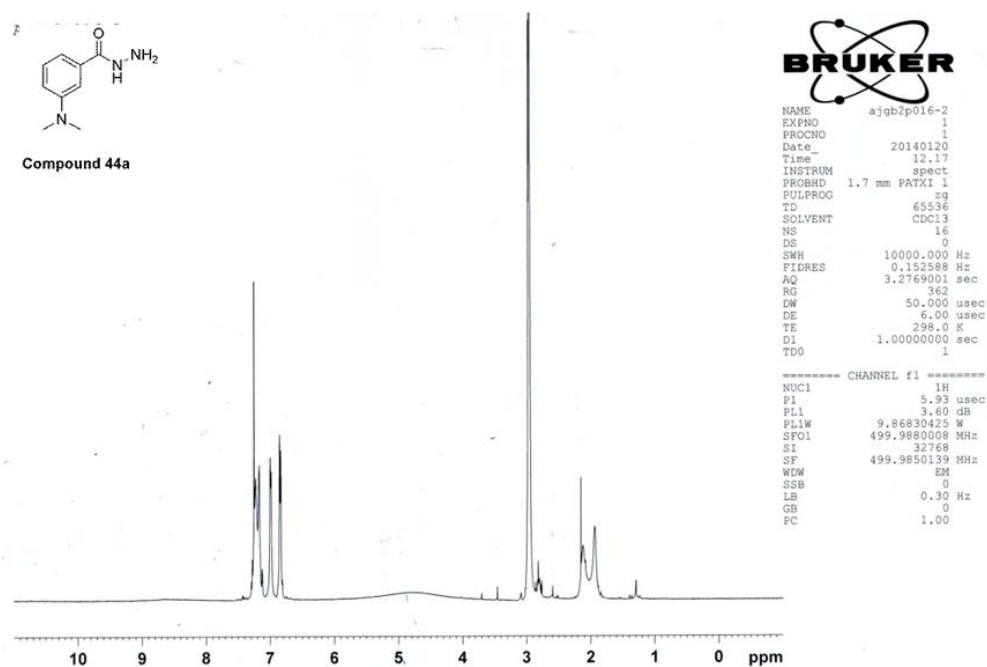
Figure S66. ^1H NMR spectrum of compound 44a.

Figure S67. TIC and MS spectrum of compound 44a.

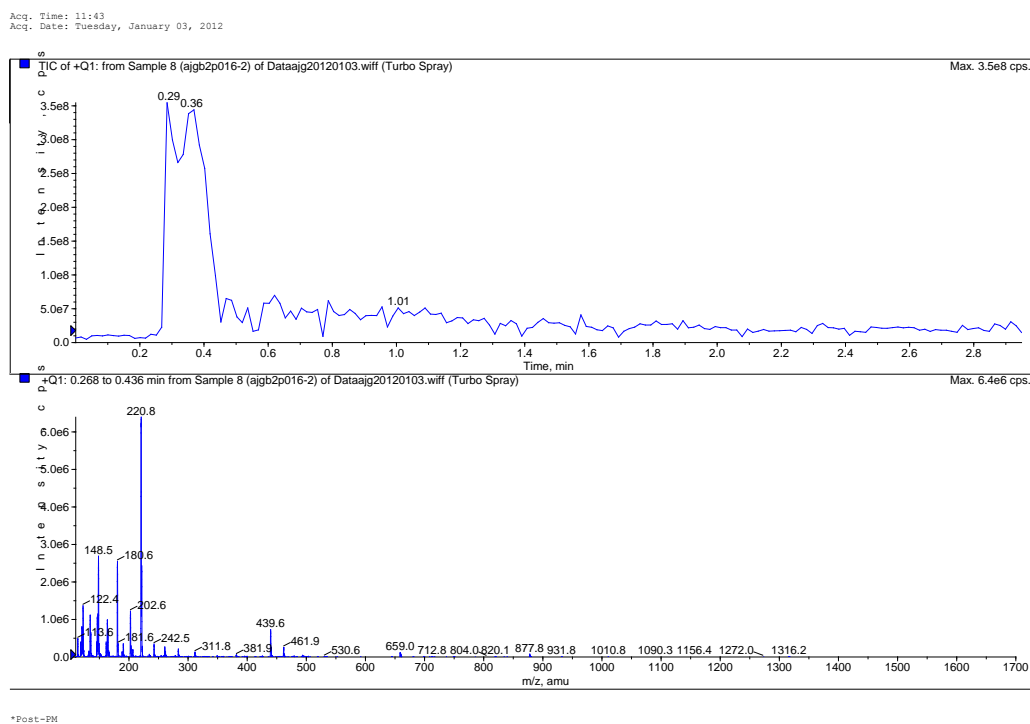
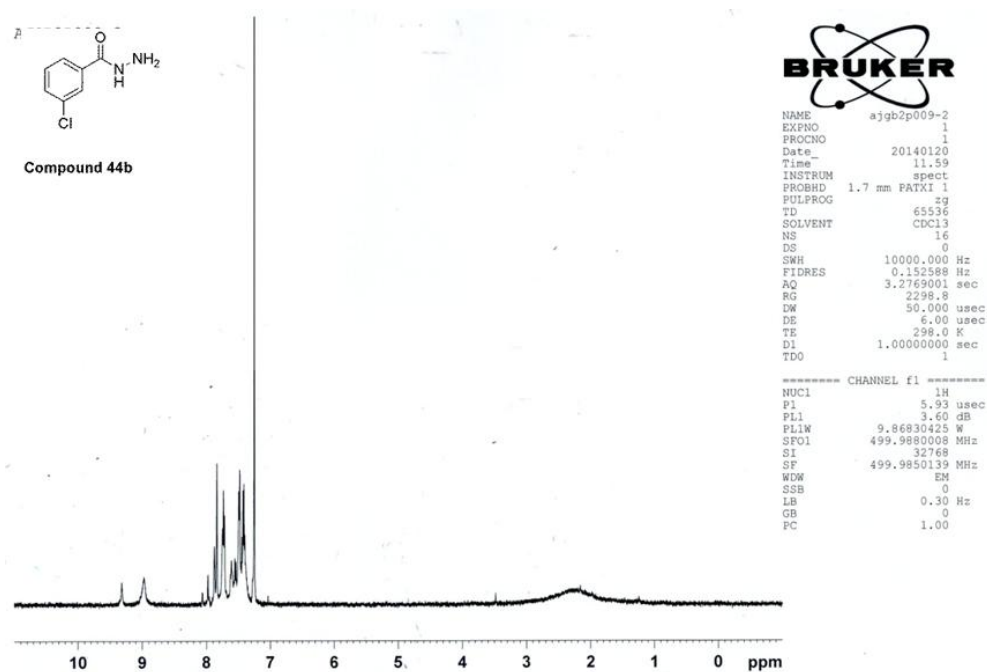
Figure S68. ^1H NMR spectrum of compound 44b.

Figure S69. TIC and MS spectrum of compound 44b.

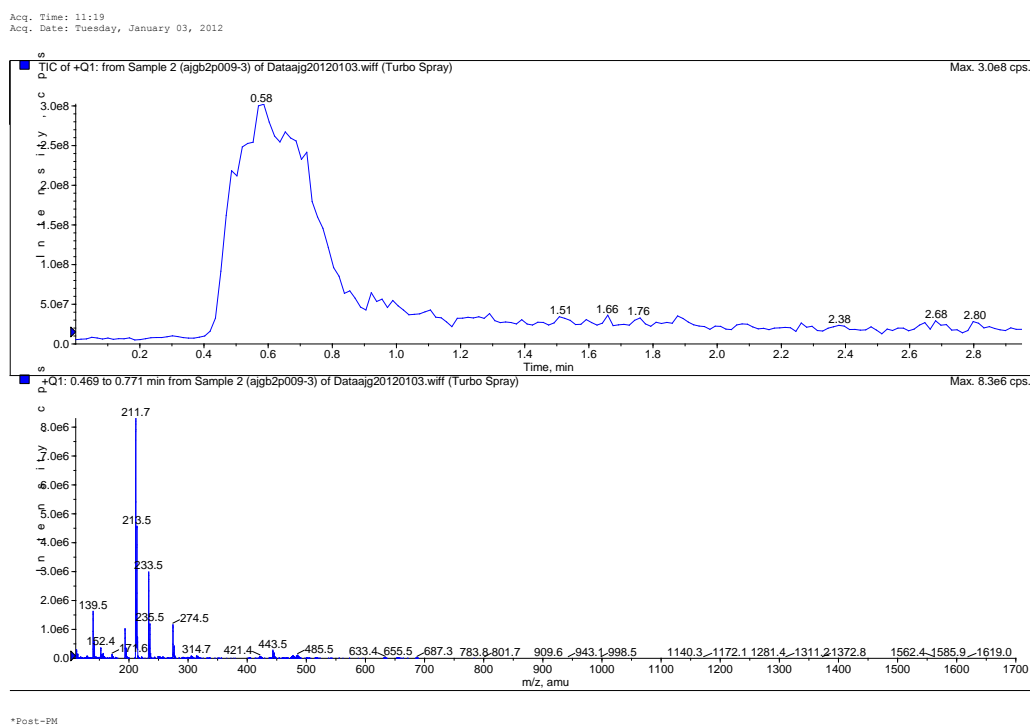
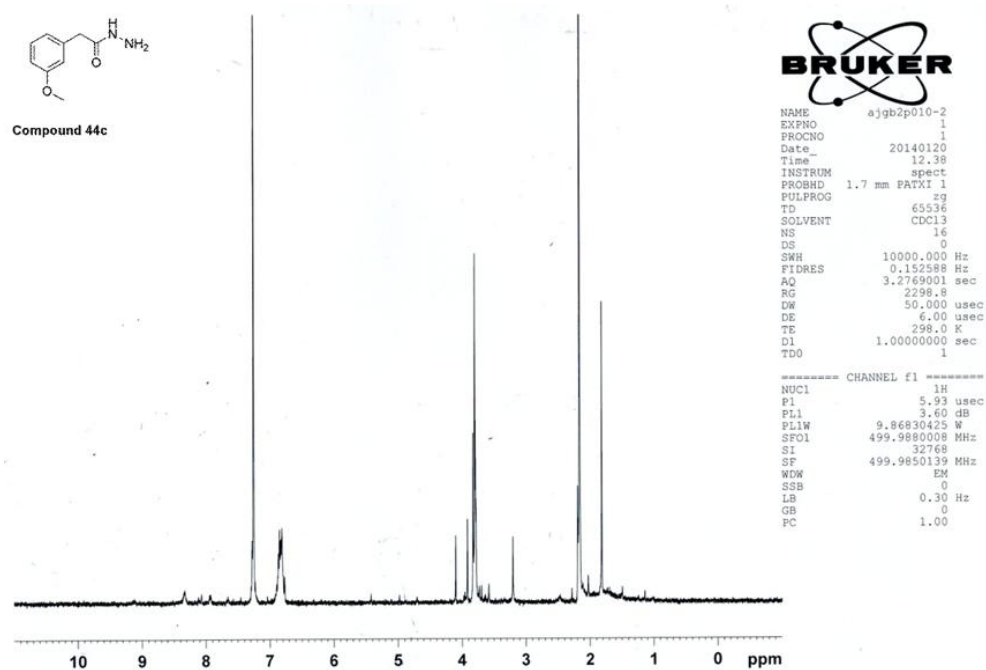
Figure S70. ¹H NMR spectrum of compound 44c.

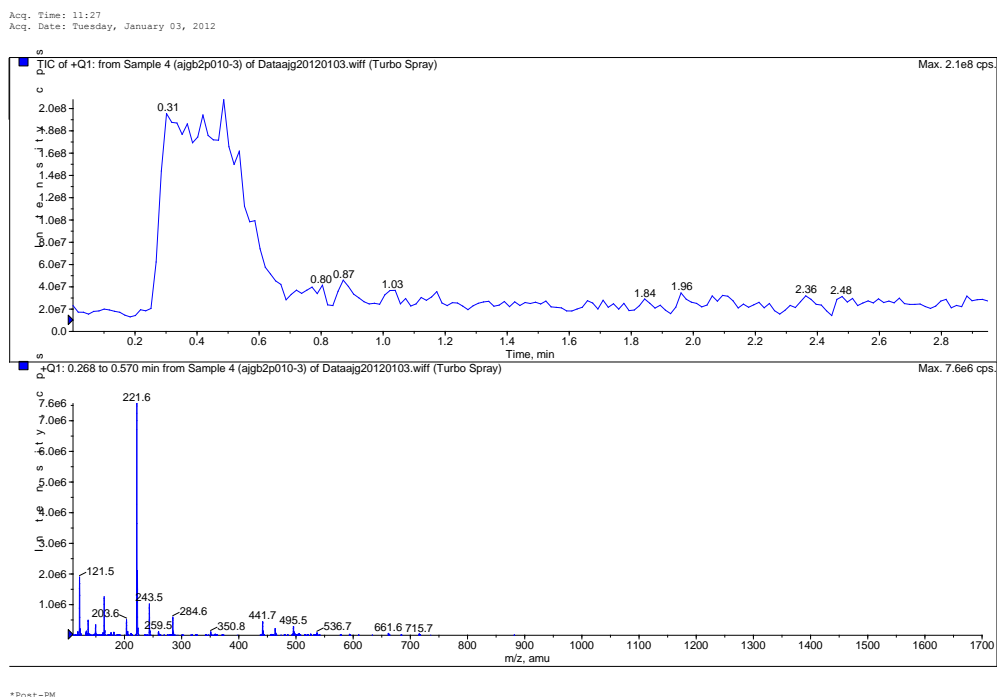
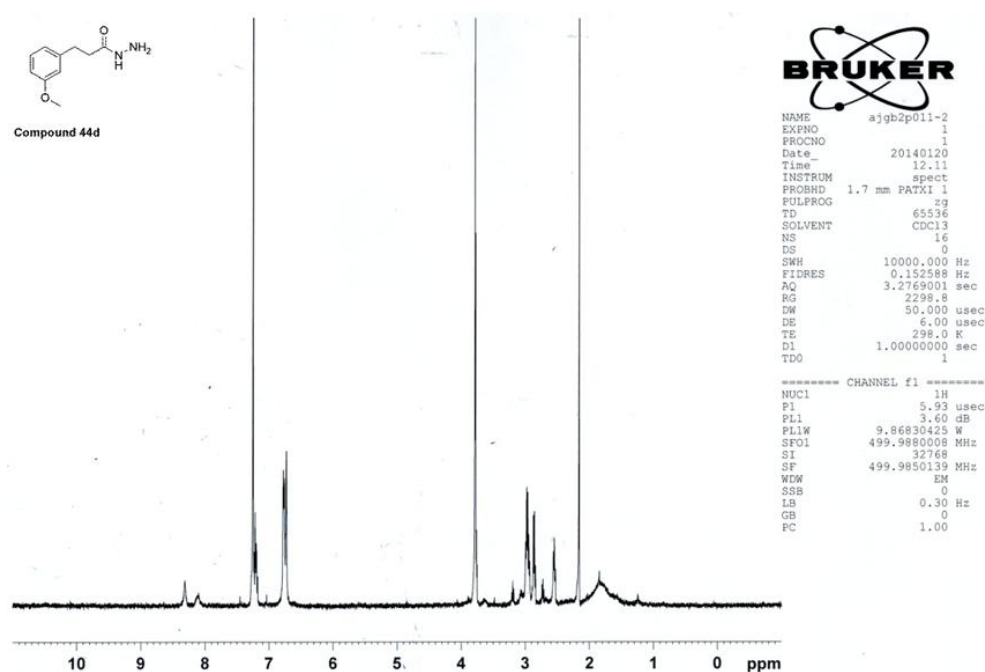
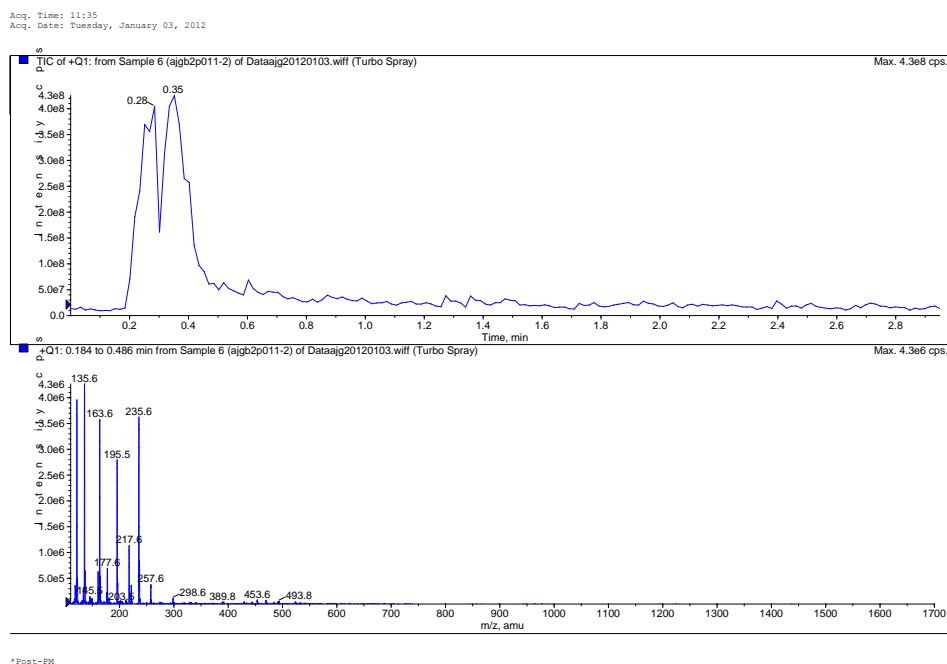
Figure S71. TIC and MS spectrum of compound **44c**.**Figure S72.** ^1H NMR spectrum of compound **44d**.

Figure S73. TIC and MS spectrum of compound **44d**.

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