Supporting Information

Brevianamides and mycophenolic acid derivatives from the Deep-Sea-Derived Fungus *Penicillium brevicompactum* DFFSCS025

Xinya Xu,[1] Xiaoyong Zhang,[1] Xuhua Nong,[1] Jie Wang[1], and Shuhua Qi[*,1]

[1] Key Laboratory of Tropical Marine Bio-resources and Ecology, Guangdong Key Laboratory of Marine Materia Medica, RNAM Center for Marine Microbiology, South China Sea Institute of Oceanology, Chinese Academy of Sciences, 164 West Xingang Road, Guangzhou 510301 Guangdong, China; E-Mails: xuxinya@scsio.ac.cn (X.-Y.X.); zhangxiaoyong@scsio.ac.cn (X.-Y.Z.); xhnong@scsio.ac.cn (X.-H.N.); wangjielangjing@126.com (J.W.); shuhuaqi@scsio.ac.cn (S.-H. Q)

***** Author to whom correspondence should be addressed; E-Mail: shuhuaqi@scsio.ac.cn; Tel.: +86-20-8902-2112; Fax: +86-20-8445-8964.

List of contents

Figure S1. ^{1}H NMR spectrum for compound **1**.

Figure S2. ^{13}C NMR spectrum for compound **1**.

Figure S3. HSQC spectrum for compound **1**.

Figure S4. HMBC spectrum for compound **1**.

Figure S5. ^{1}H-^{1}H COSY spectrum for compound **1**.

Figure S6. NOESY spectrum for compound **1**.

Figure S7. HR-ESIMS spectrum for compound **1**.

Figure S8. ^{1}H NMR spectrum for compound **2**.

Figure S9. ^{13}C NMR spectrum for compound **2**.

Figure S10. HSQC spectrum for compound **2**.

Figure S11. HMBC spectrum for compound **2**.

Figure S12. NOESY spectrum for compound **2**.

Figure S13. HR-ESIMS spectrum for compound **2**.

Figure S14. ^{1}H NMR spectrum for compound **3**.

Figure S15. ^{13}C NMR spectrum for compound **3**.

Figure S16. HSQC spectrum for compound **3**.

Figure S17. HMBC spectrum for compound **3**.

Figure S18. HR-ESIMS spectrum for compound **3**.

Figure S1. ^{1}H NMR spectrum for compound **1**

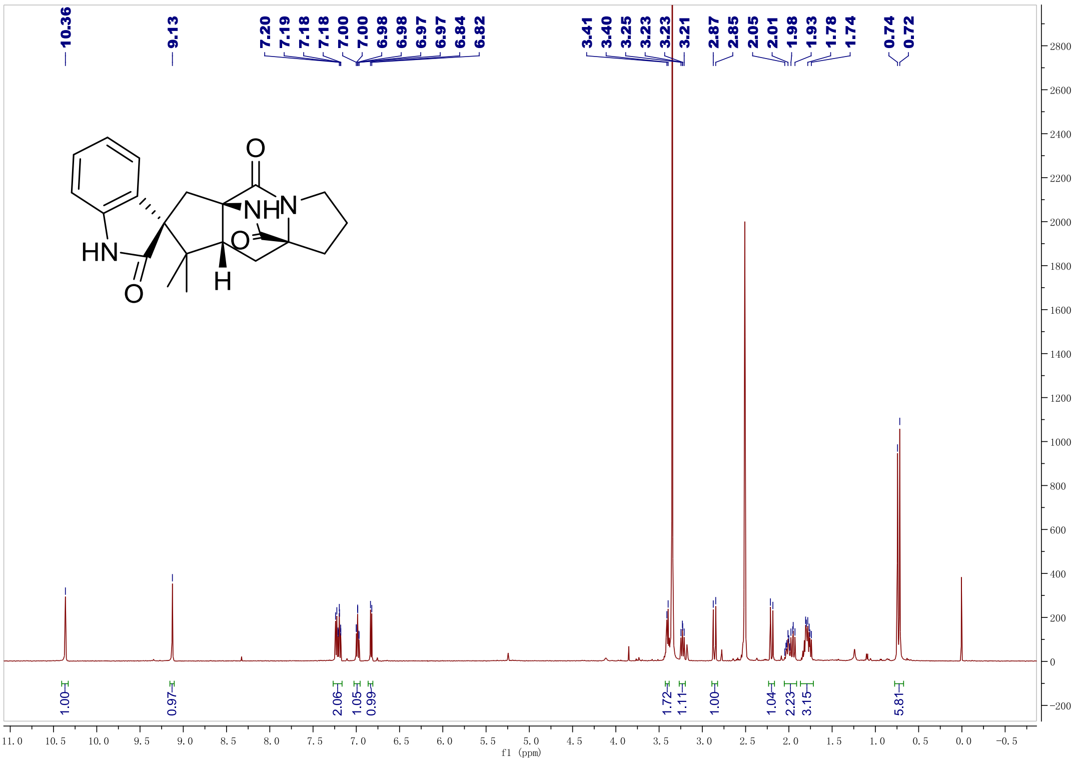


Figure S2. ^{13}C NMR spectrum for compound **1**

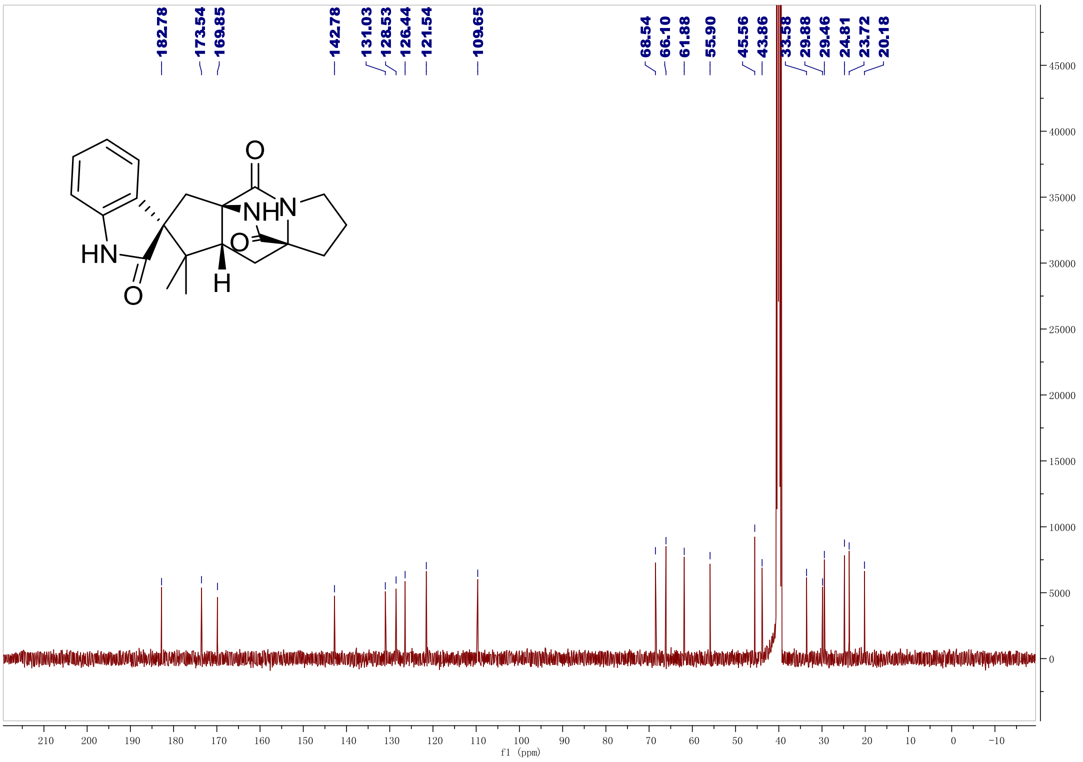


Figure S3. HSQC spectrum for compound **1**

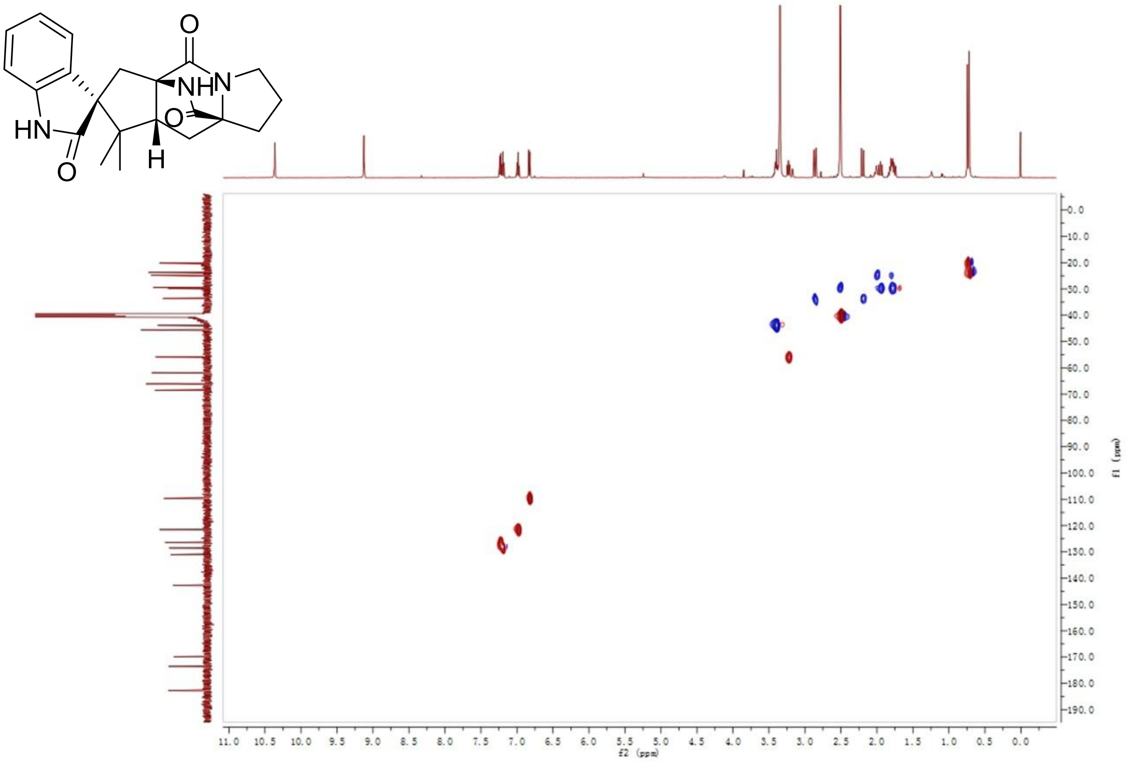


Figure S4. HMBC spectrum for compound **1**

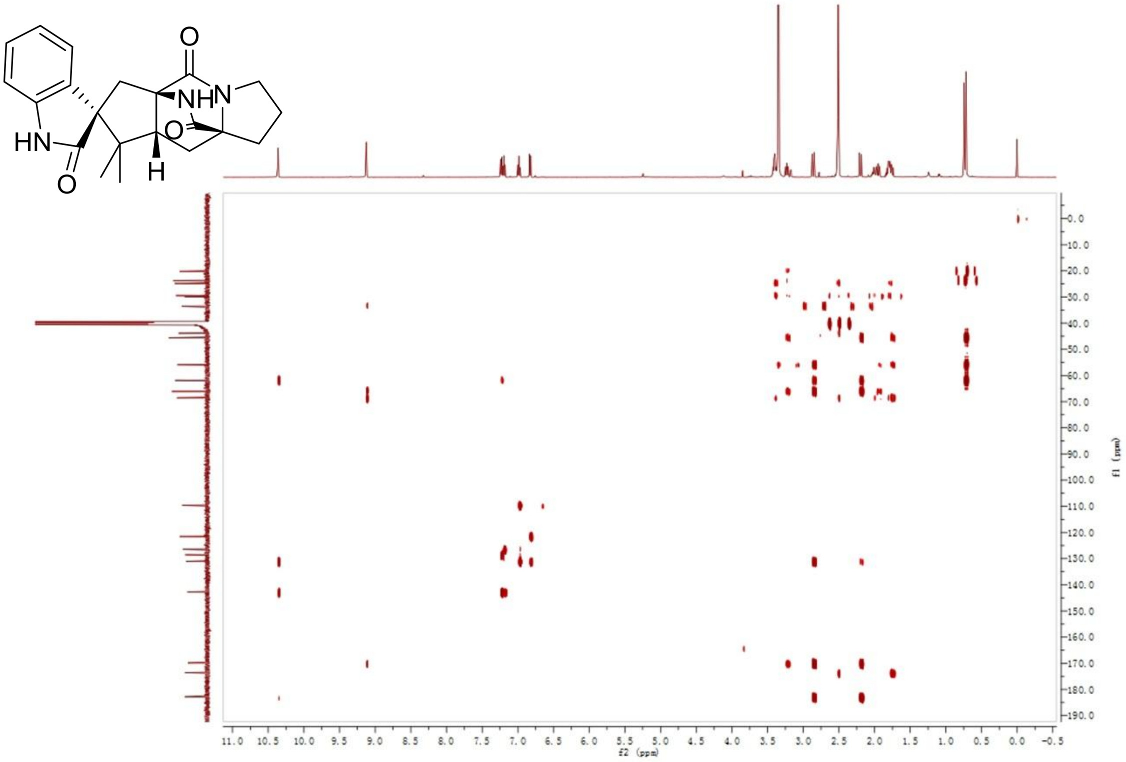


Figure S5. ^1H-^1H COSY spectrum for compound **1**

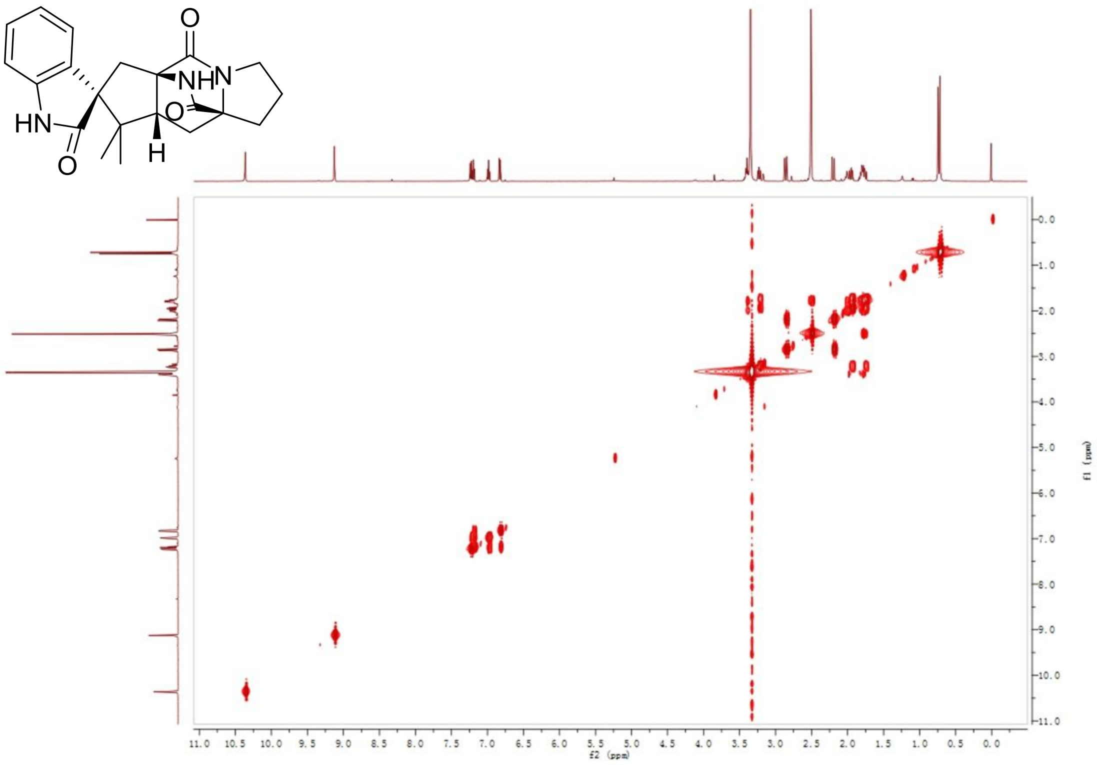


Figure S6. NOESY spectrum for compound **1**

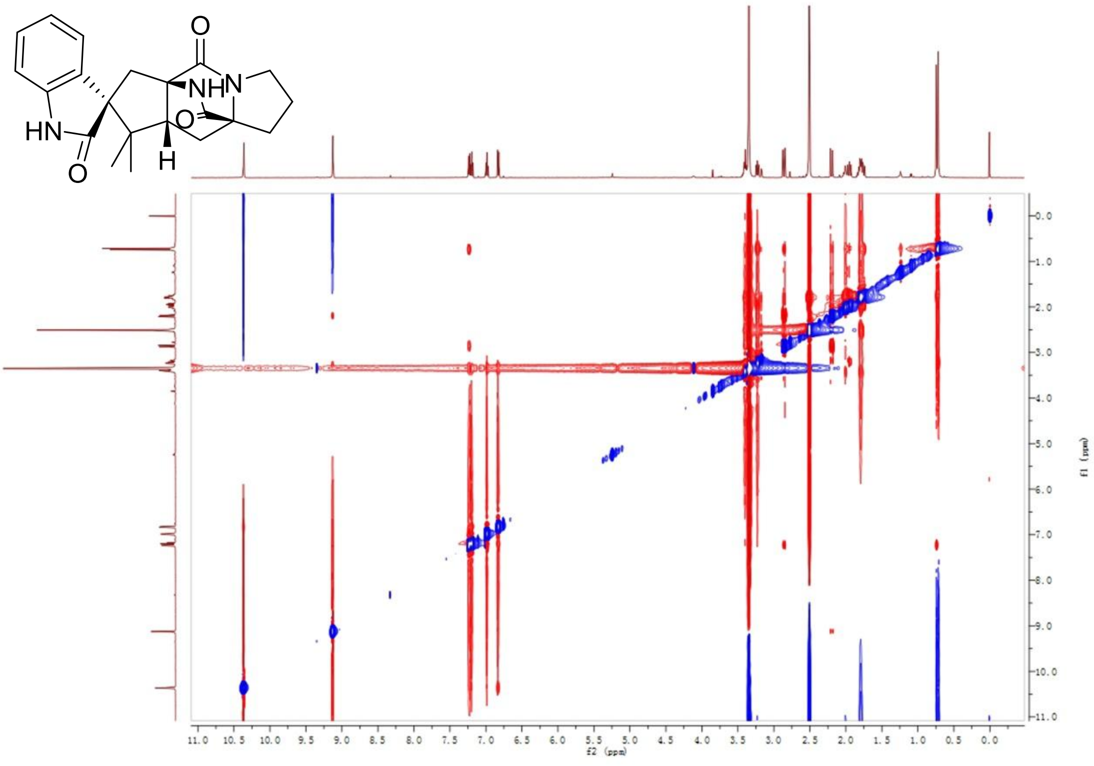
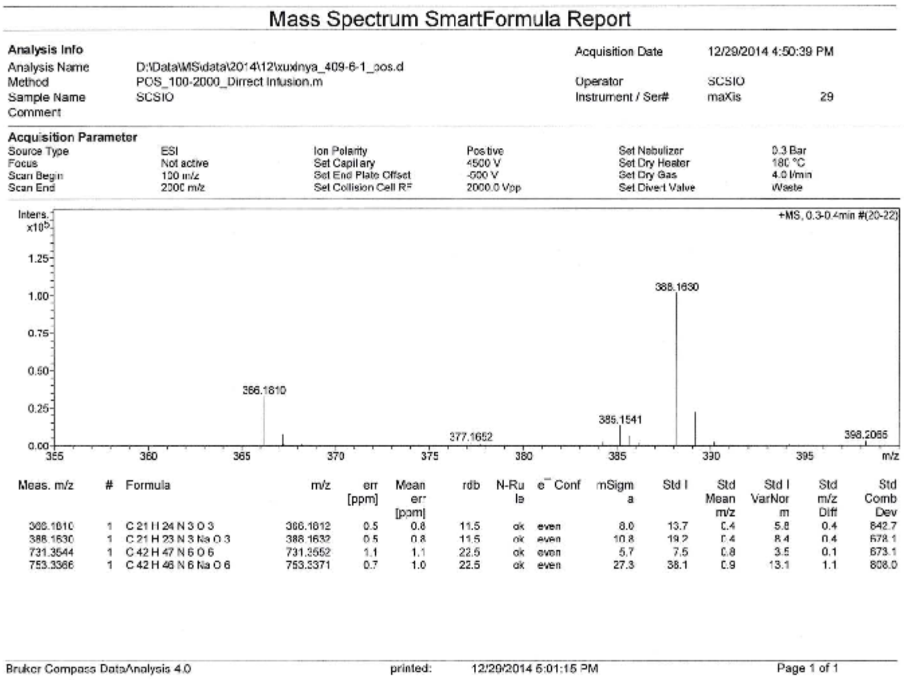


Figure S7. HR-ESIMS spectrum for compound **1**



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388.1630	1	C 21 H 23 N 3 Na O 3	388.1632	0.5	0.8	11.5	ok	even	10.8	19.2	0.4	8.4	0.4	678.1
731.3544	1	C 42 H 47 N 6 O 6	731.3552	1.1	1.1	22.5	ok	even	5.7	7.5	0.8	3.5	0.1	673.1
753.3366	1	C 42 H 46 N 6 Na O 6	753.3371	0.7	1.0	22.5	ok	even	27.3	38.1	0.9	13.1	1.1	808.0

Bruker Compass DataAnalysis 4.0   printed: 12/29/2014 5:01:15 PM   Page 1 of 1

Figure S8. ^{1}H NMR spectrum for compound **2**

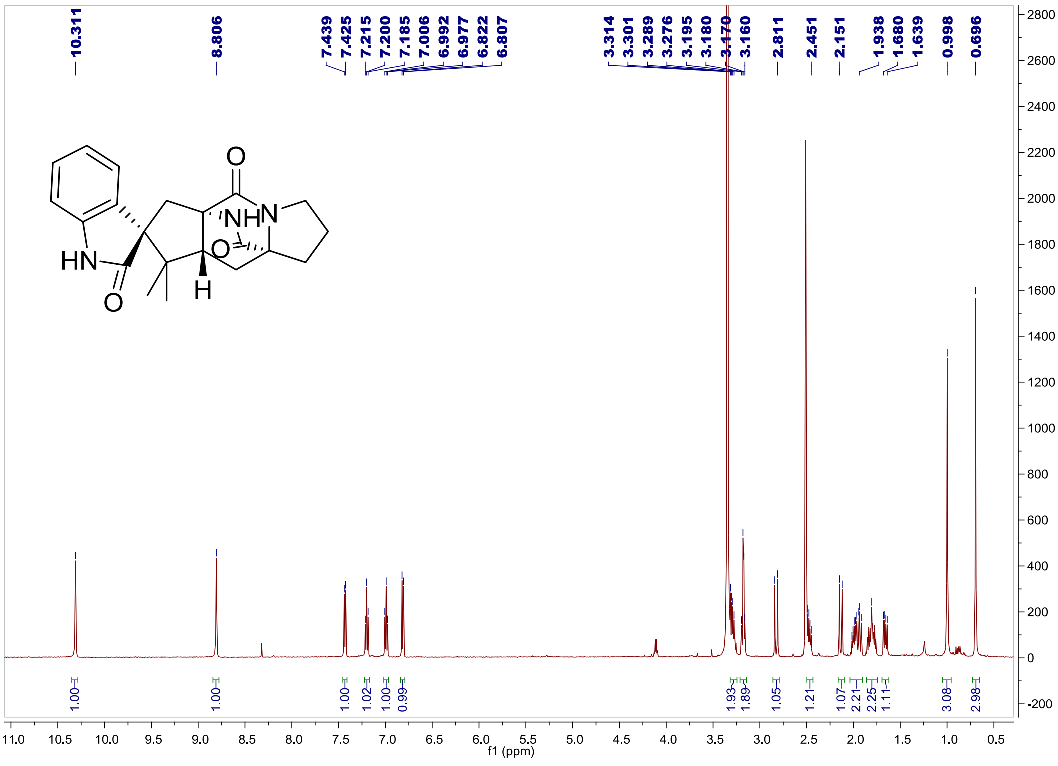


Figure S9. ^{13}C NMR spectrum for compound **2**

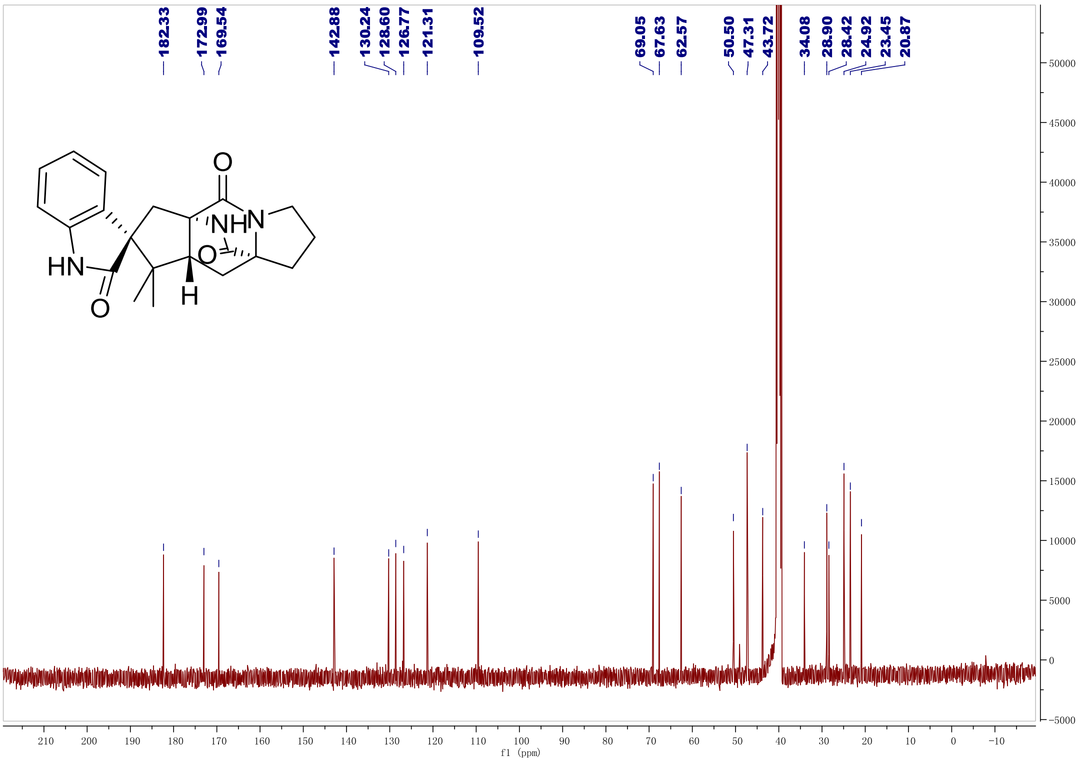


Figure S10. HSQC spectrum for compound **2**

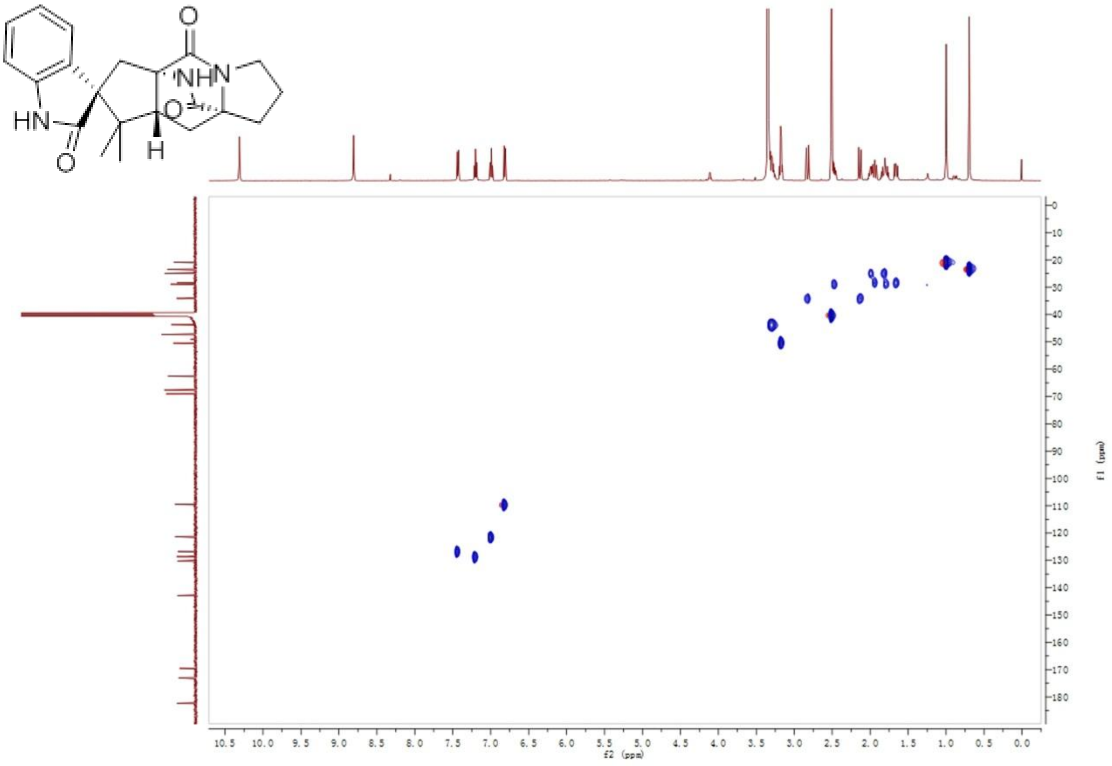


Figure S11. HMBC spectrum for compound **2**

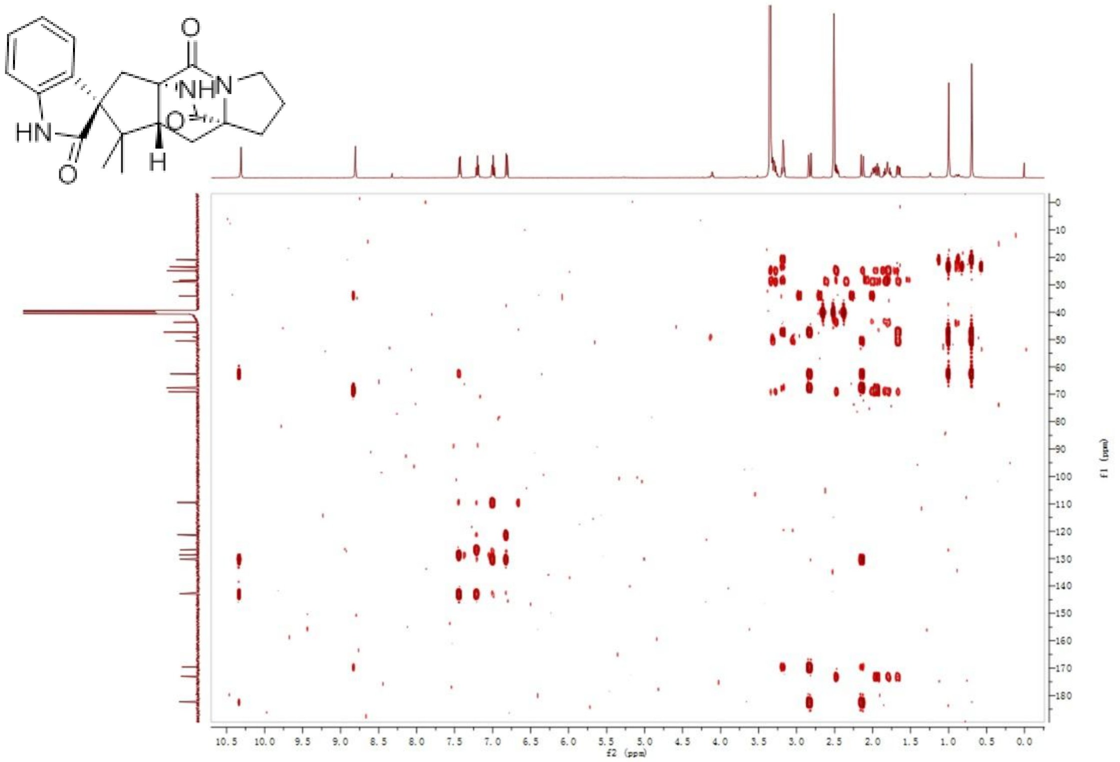


Figure S12. NOESY spectrum for compound **2**

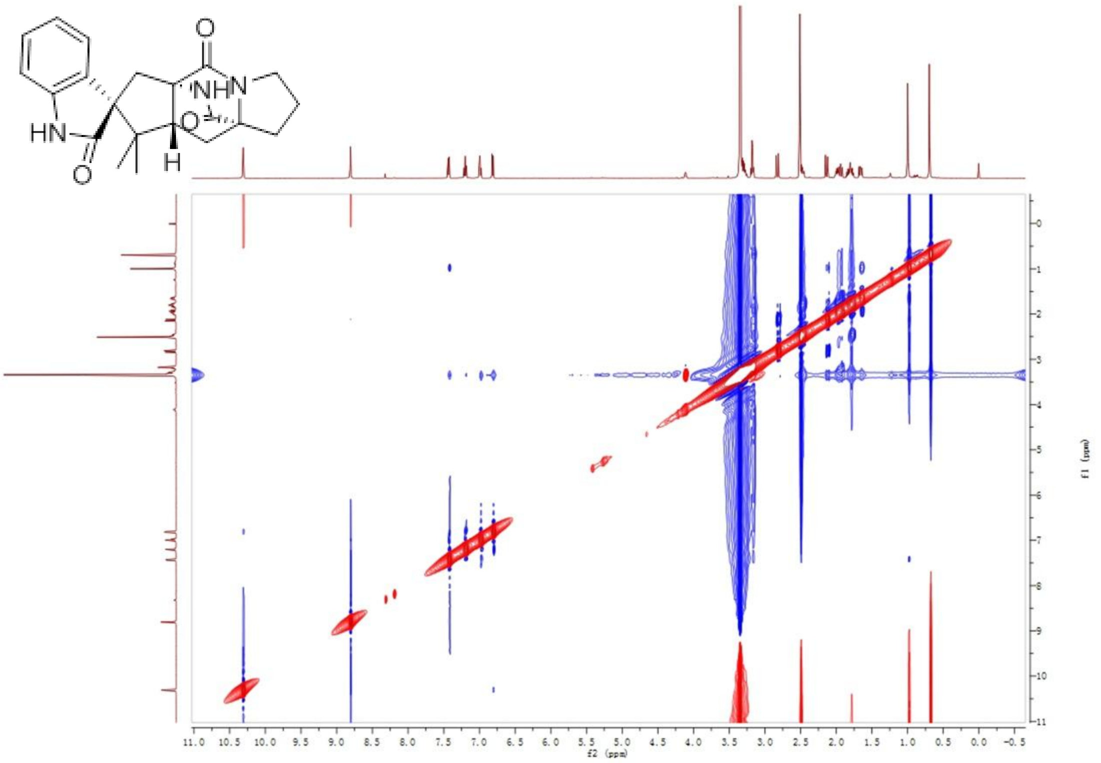
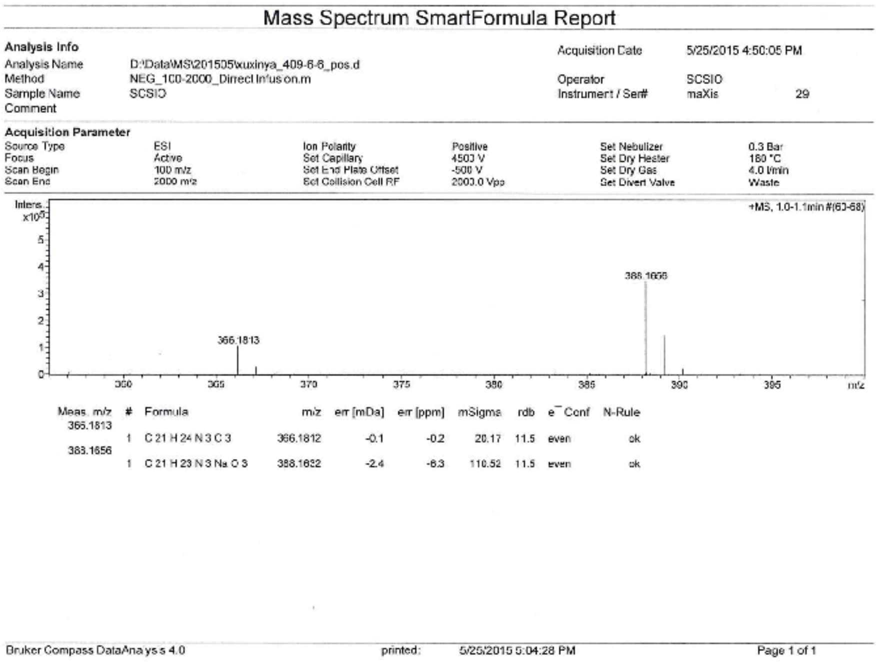


Figure S13. HR-ESIMS spectrum for compound **2**



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388.1656									
	1	C 21 H 23 N 3 Na O 3	388.1632	-2.4	-6.3	110.52	11.5	even	ok

Bruker Compass DataAnalysis 4.0 printed: 5/25/2015 5:04:28 PM Page 1 of 1

Figure S14. ^{1}H NMR spectrum for compound **3**

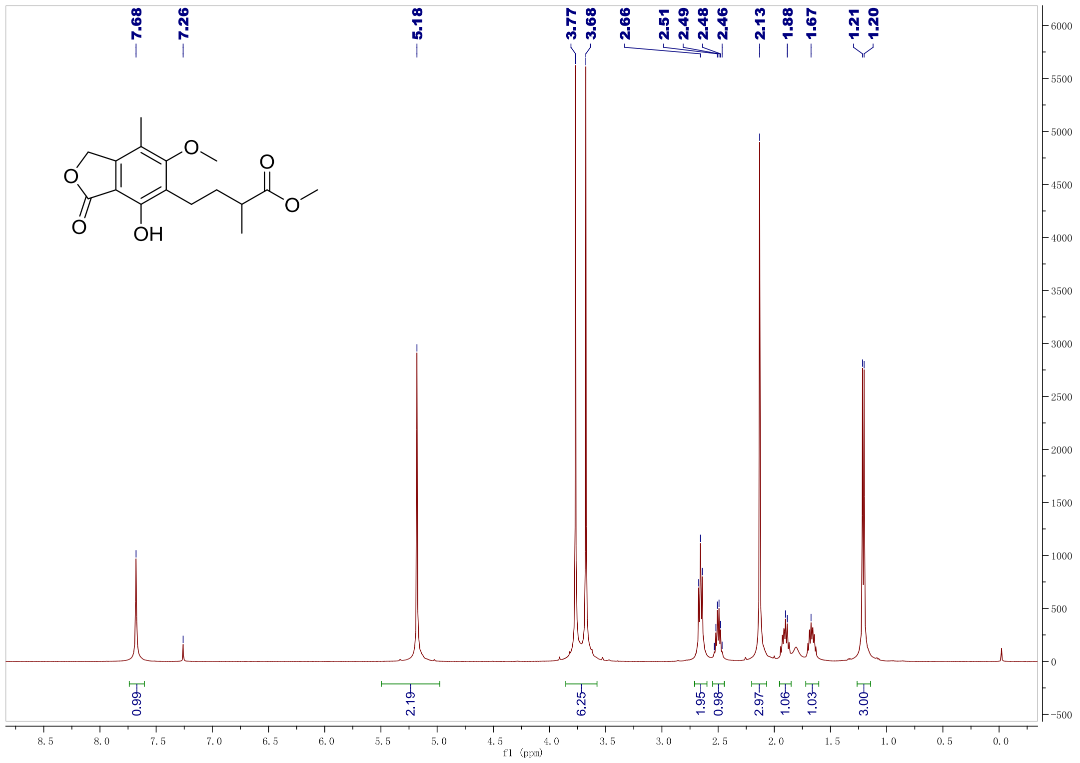


Figure S15. ^{13}C NMR spectrum for compound **3**

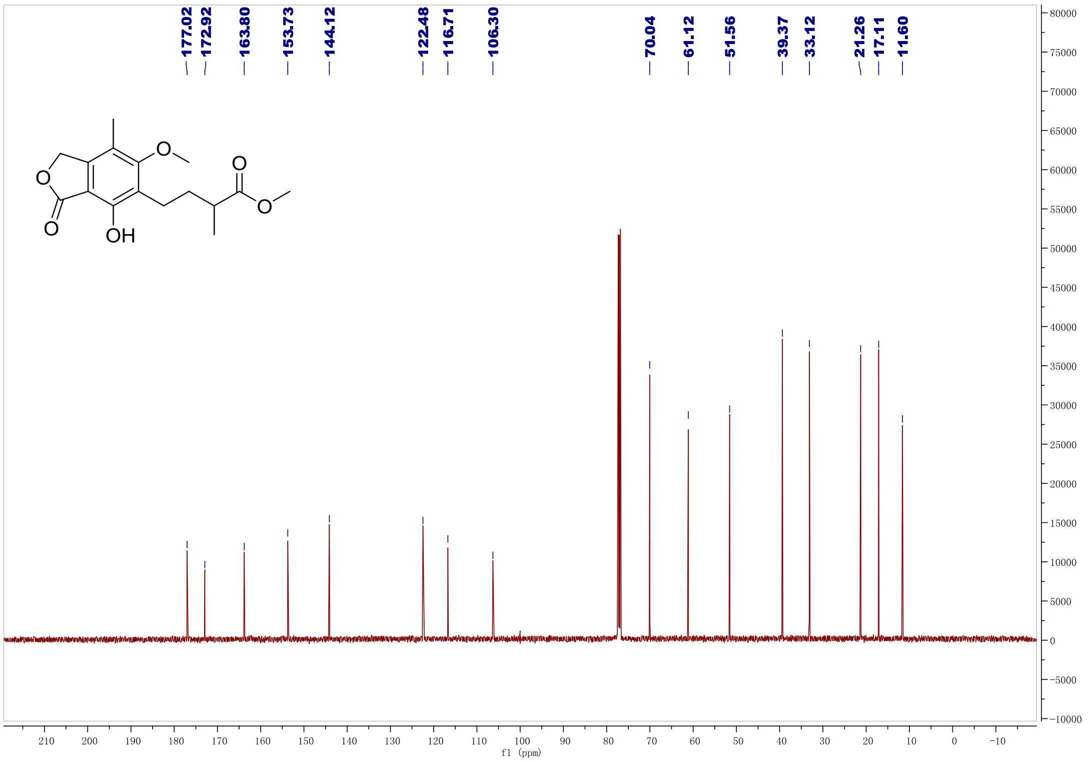


Figure S16. HSQC spectrum for compound **3**

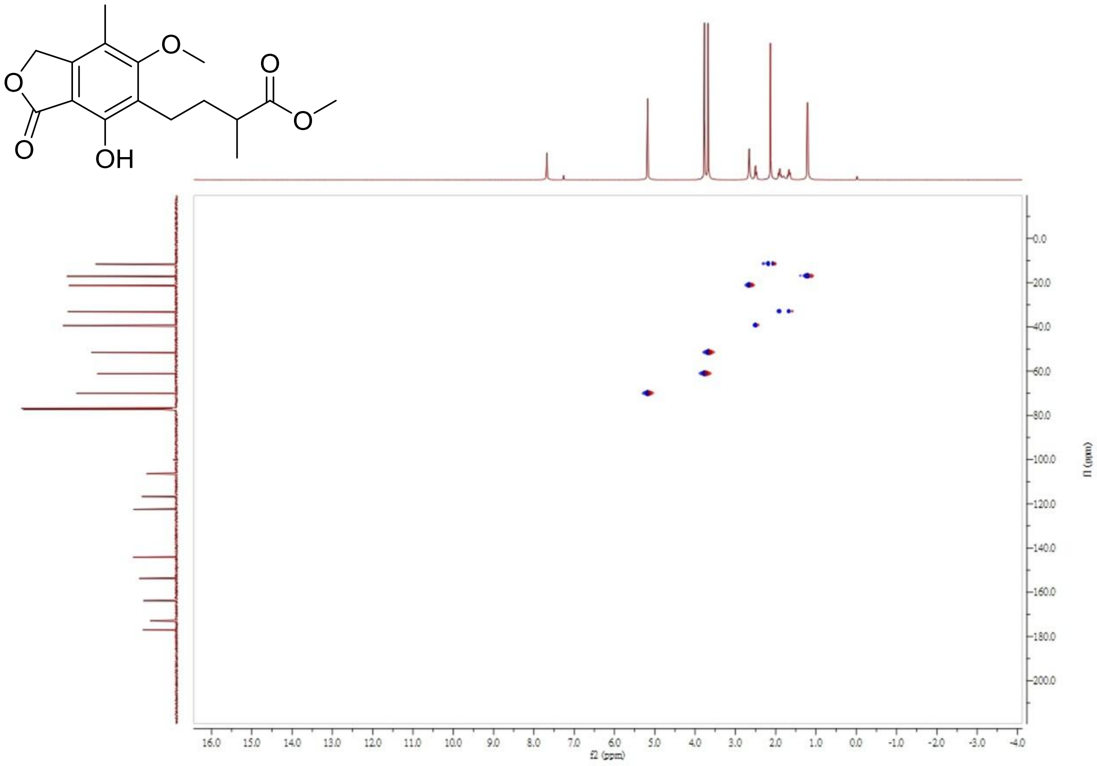


Figure S17. HMBC spectrum for compound **3**

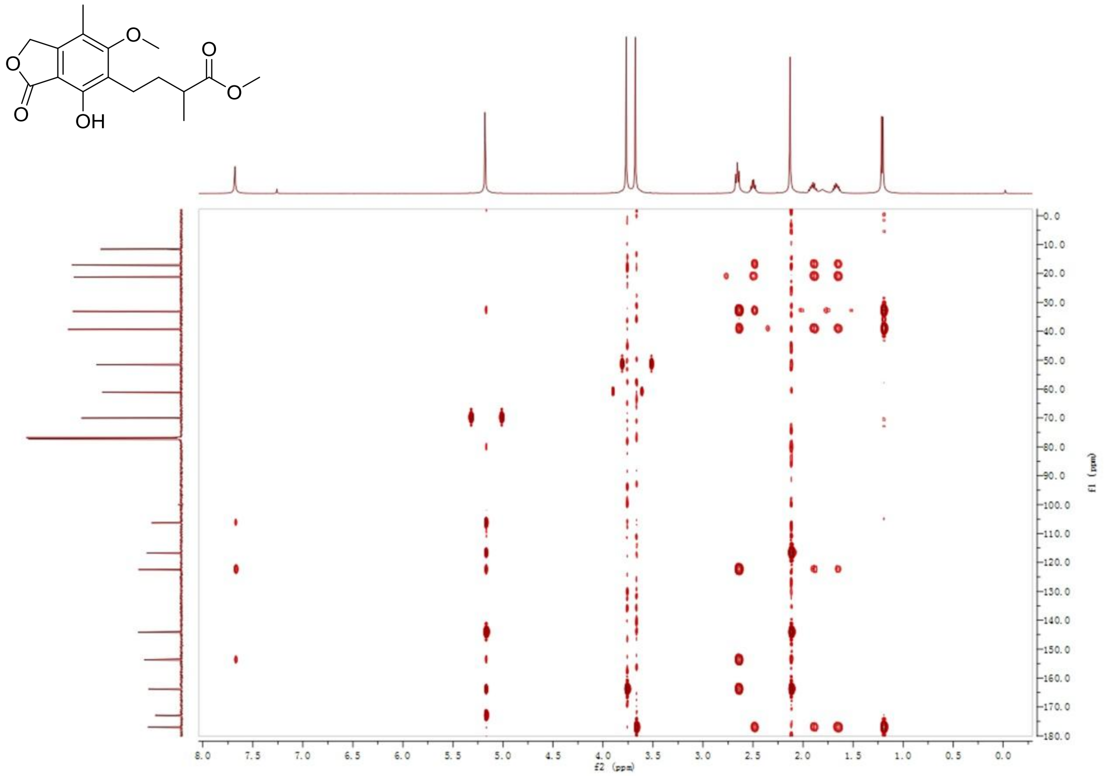
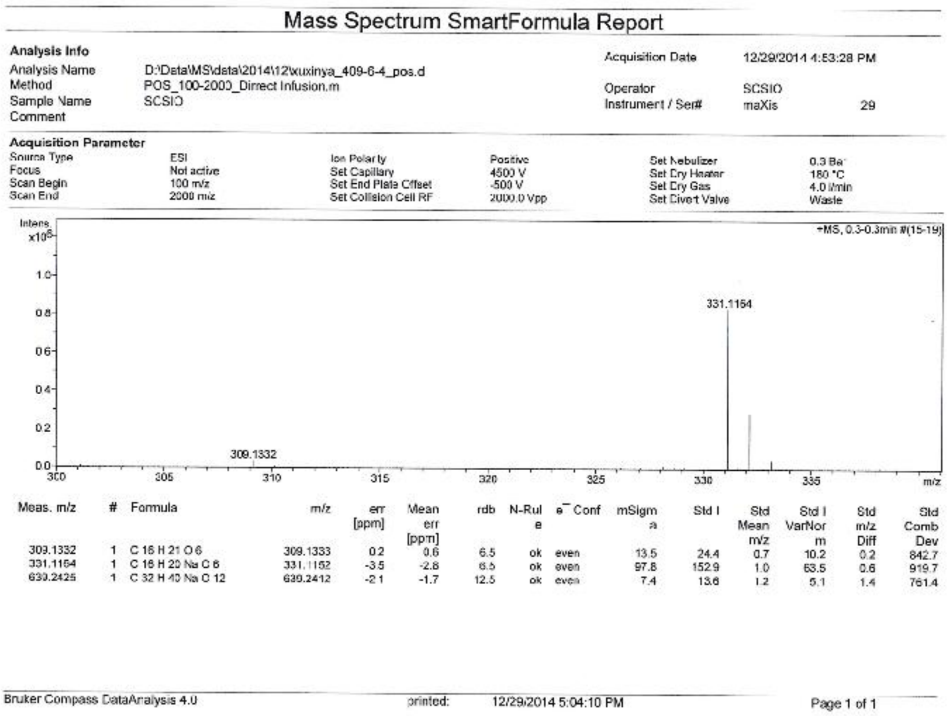


Figure S18. HR-ESIMS spectrum for compound **3**



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Instrument / Ser# maXis 29

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Set Dry Gas 4.0 l/min
Set Divert Valve Waste

Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
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331.1164	1	C 16 H 20 Na O 6	331.1152	-3.5	-2.8	6.5	ok	even	97.8	152.9	1.0	63.5	0.6	919.7
639.2425	1	C 32 H 40 Na O 12	639.2412	-2.1	-1.7	12.5	ok	even	7.4	13.6	1.2	5.1	1.4	761.4

Bruker Compass DataAnalysis 4.0 printed: 12/29/2014 5:04:10 PM Page 1 of 1

Figure S19. ^{1}H NMR spectrum for compound **4**

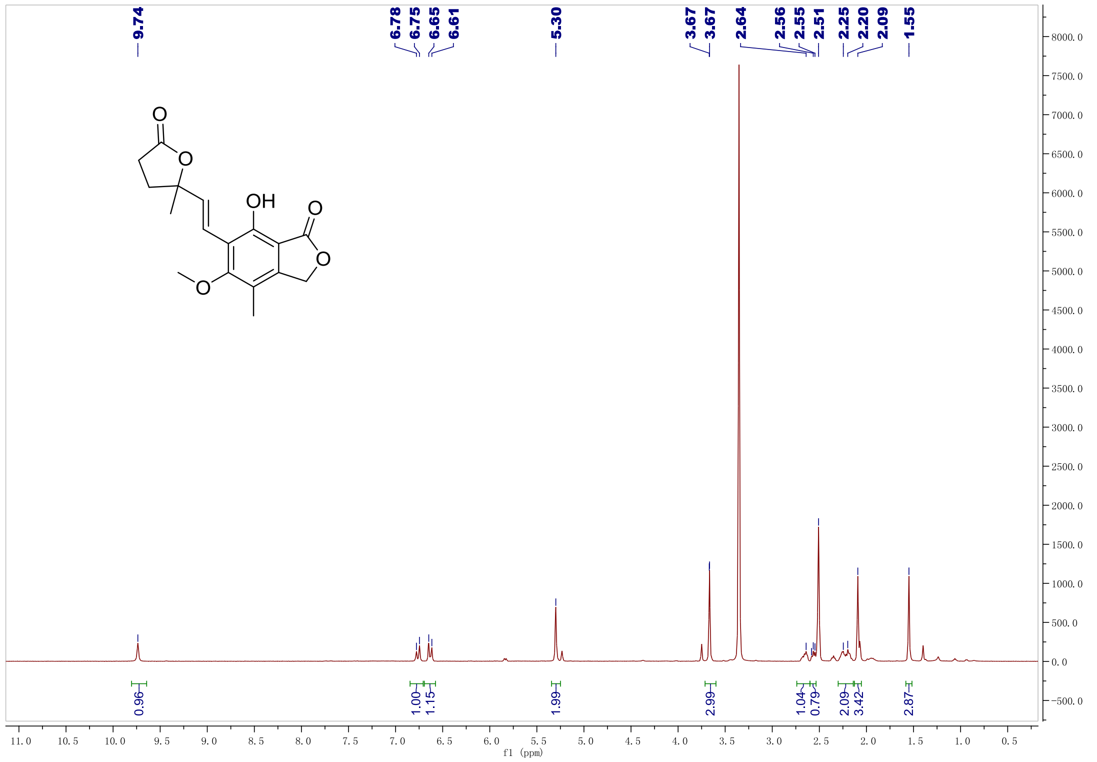


Figure S20. ^{13}C NMR spectrum for compound **4**

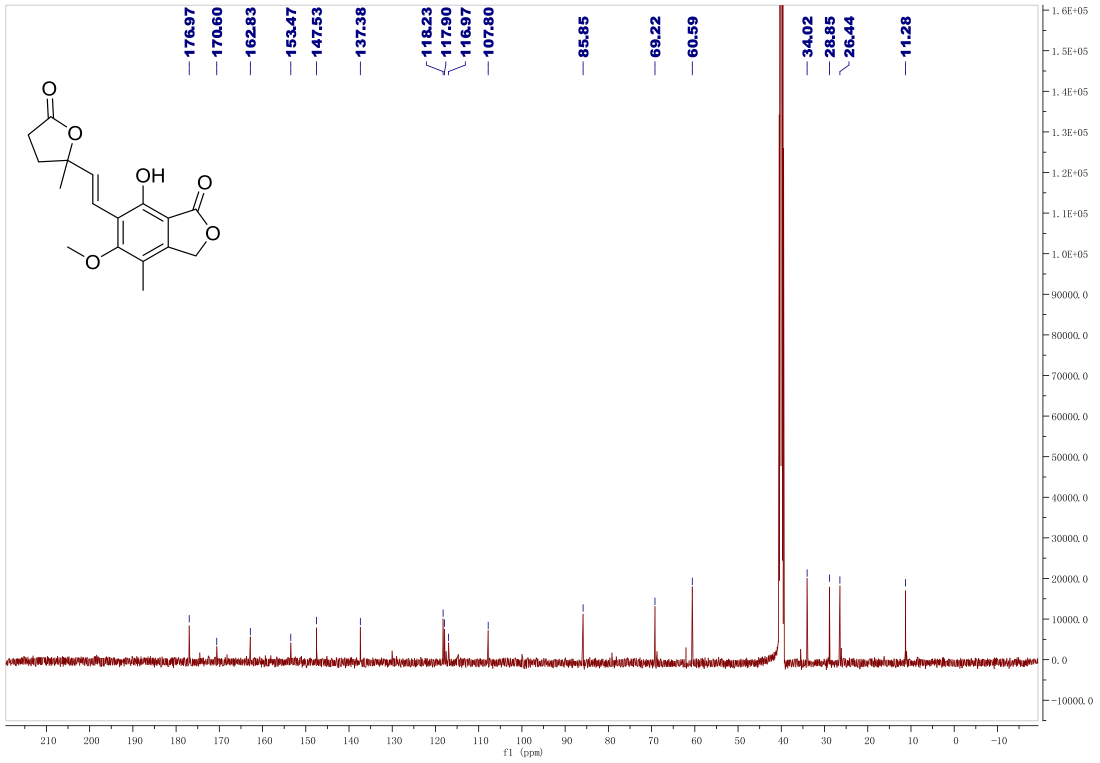


Figure S21. HSQC spectrum for compound **4**

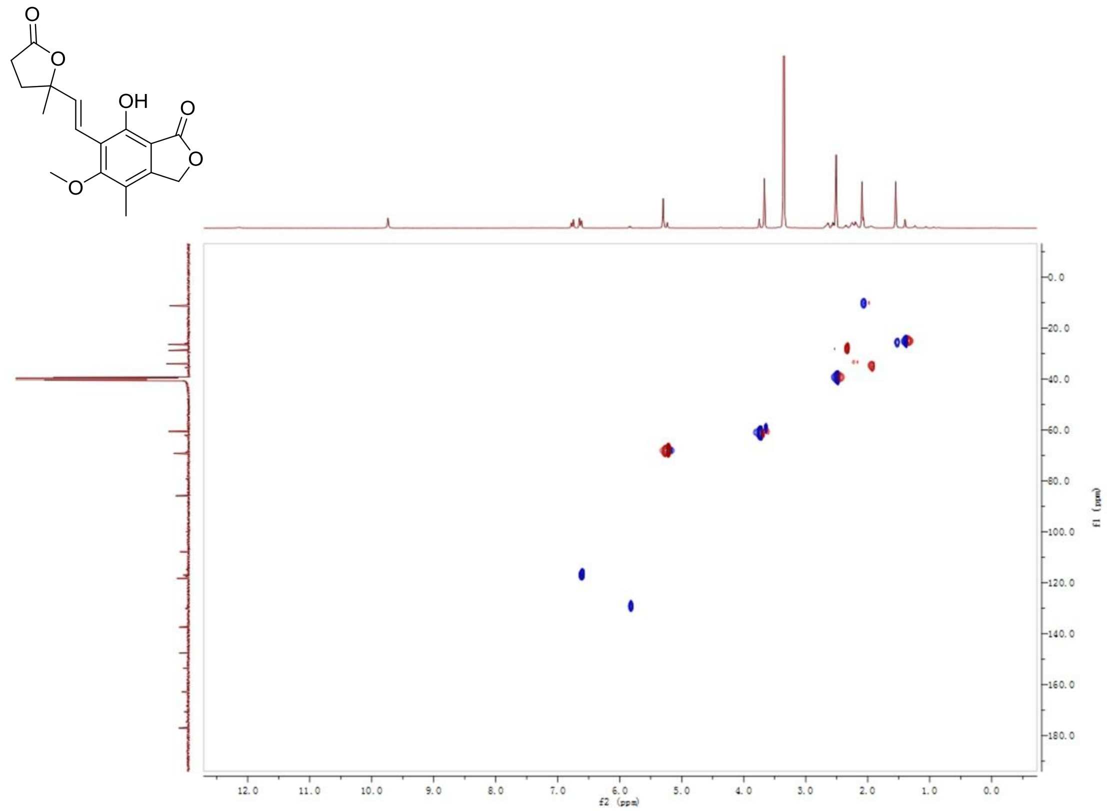
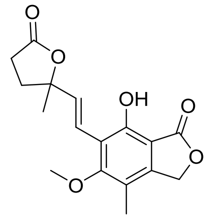


Figure S22. HMBC spectrum for compound **4**



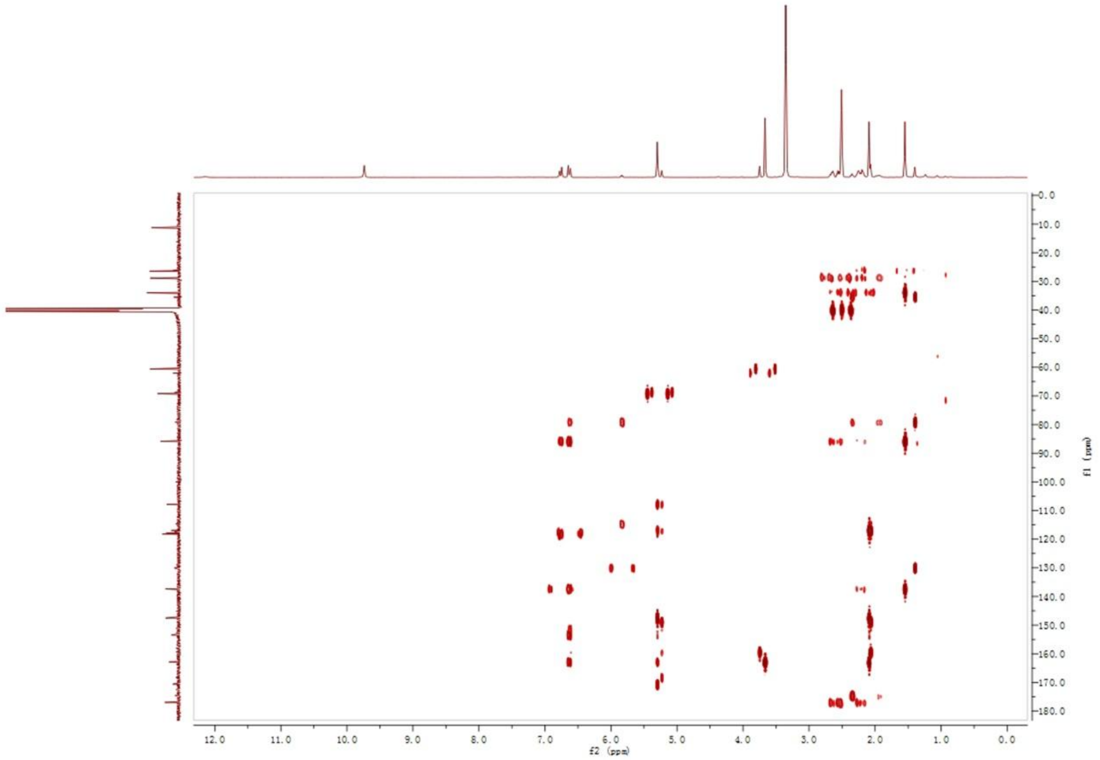
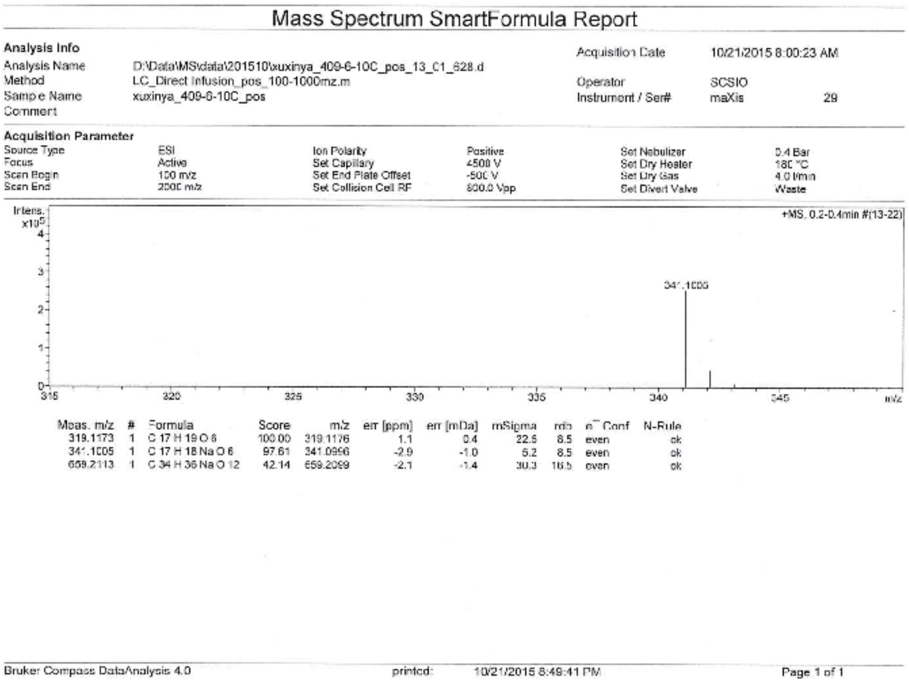


Figure S23. HR-ESIMS spectrum for compound **4**



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341.1005	1	C 17 H 18 Na O 6	97.61	341.0996	-2.9	-1.0	5.2	8.5	even	ok
659.2113	1	C 34 H 36 Na O 12	42.14	659.2099	-2.1	-1.4	30.3	16.5	even	ok

Bruker Compass DataAnalysis 4.0 printed: 10/21/2015 8:49:41 PM Page 1 of 1

Figure S24. ^{1}H NMR spectrum for compound **6**

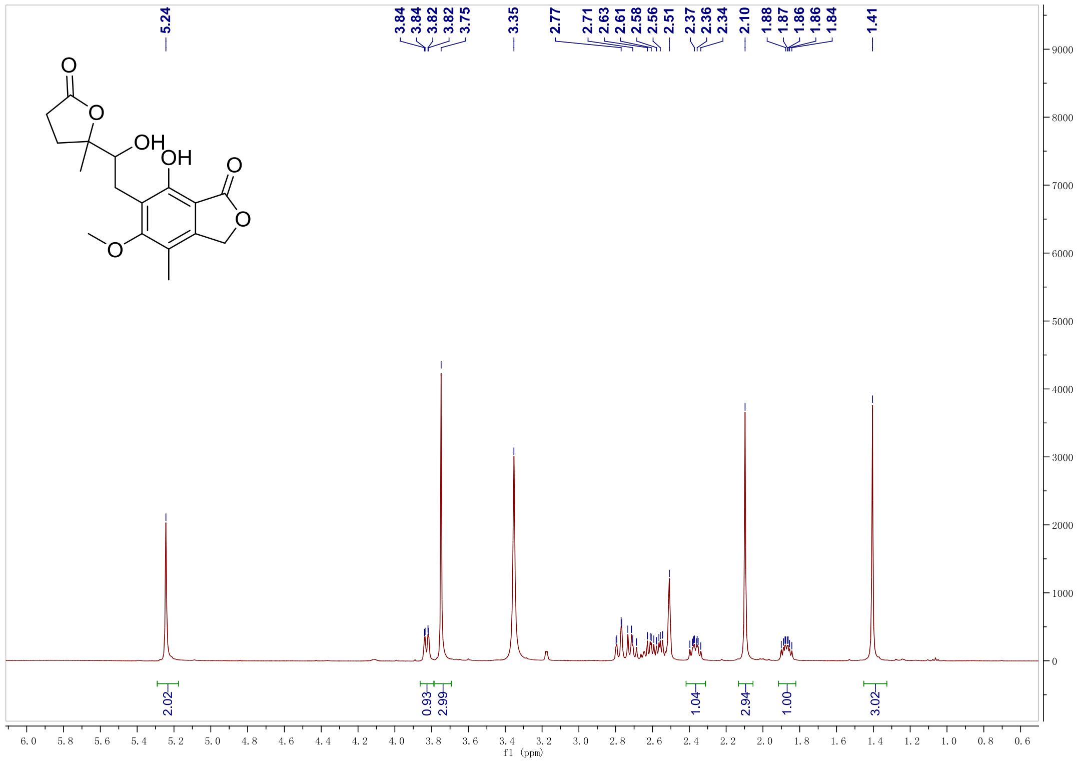


Figure S25. ^{13}C NMR spectrum for compound **6**

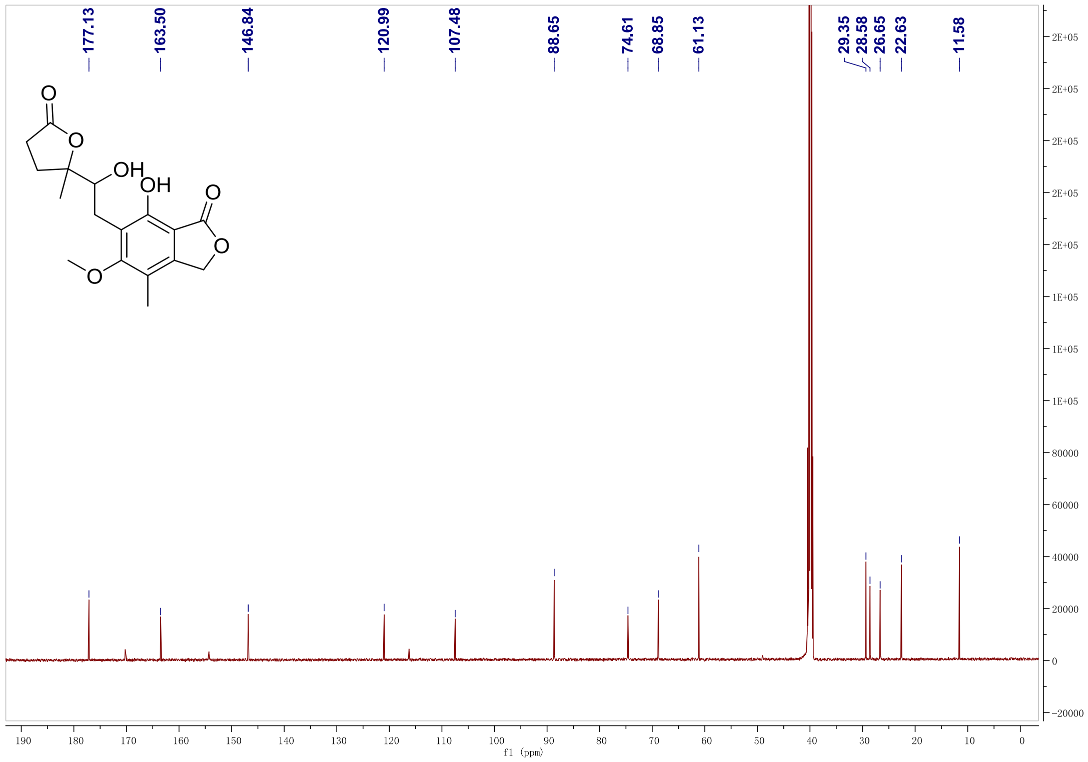


Figure S26. HSQC spectrum for compound **6**

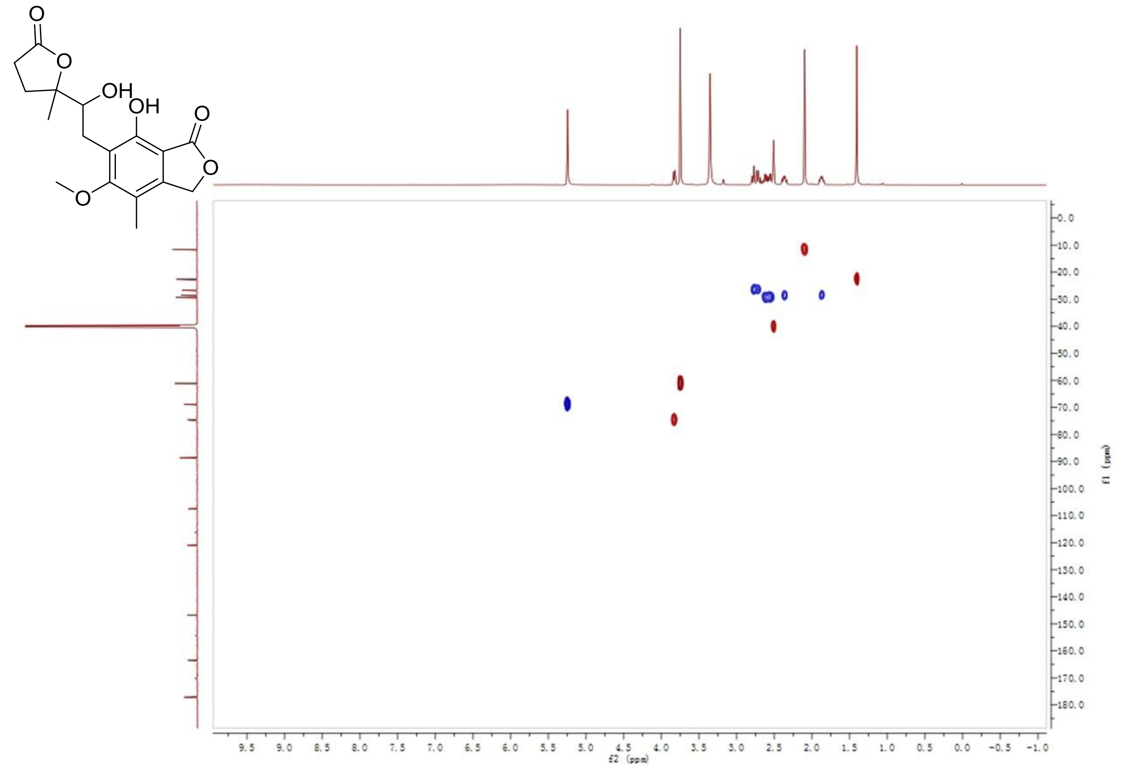


Figure S27. HMBC spectrum for compound **6**

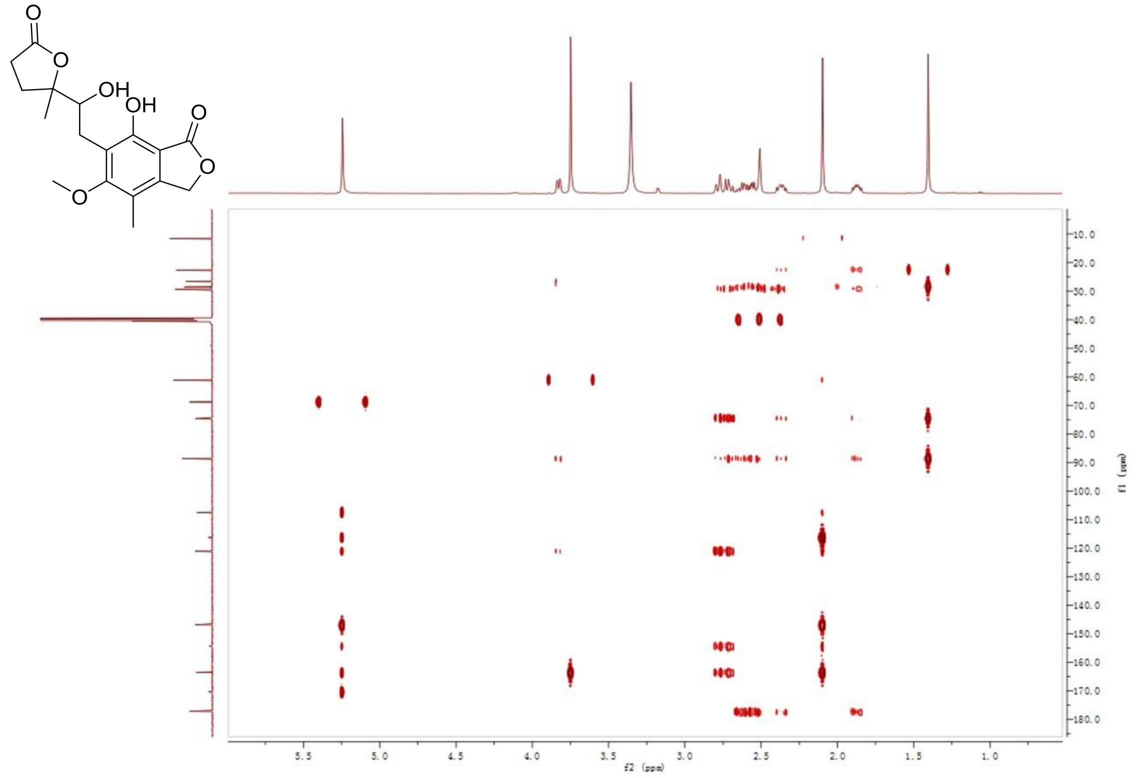
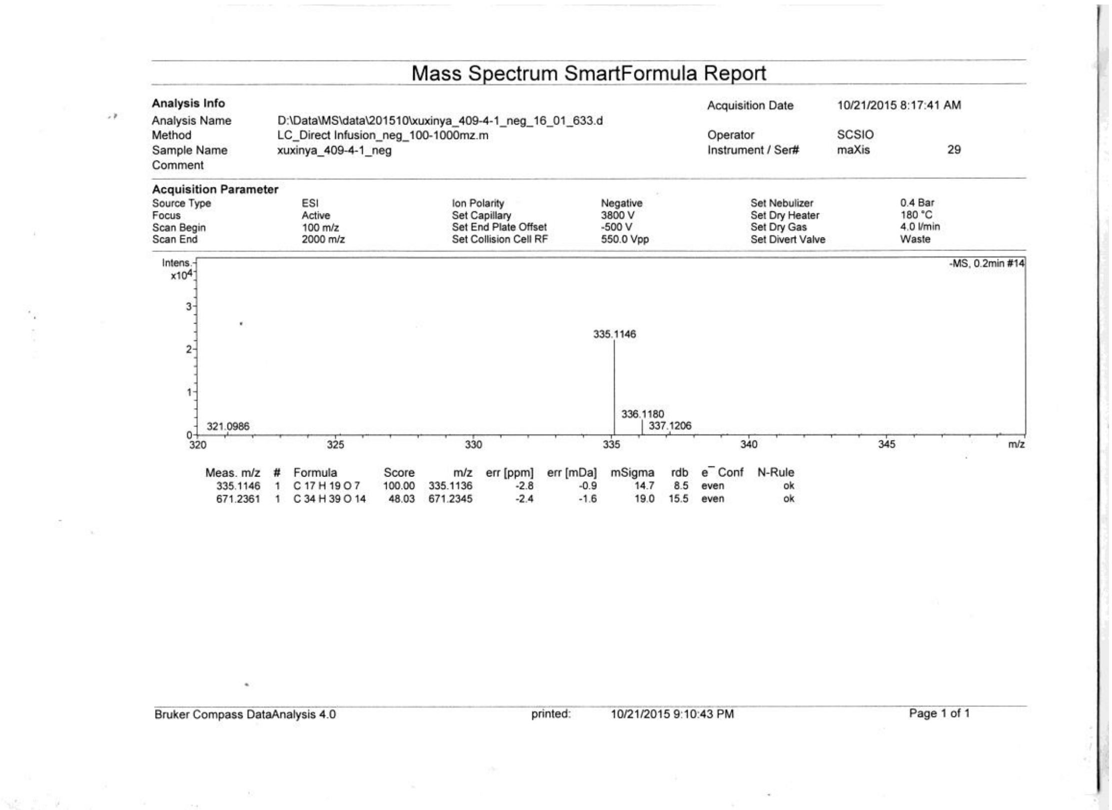


Figure S28. HR-ESIMS spectrum for compound **6**.



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671.2361	1	C 34 H 39 O 14	48.03	671.2345	-2.4	-1.6	19.0	15.5	even	ok

Bruker Compass DataAnalysis 4.0 printed: 10/21/2015 9:10:43 PM Page 1 of 1

Figure S29. Original CD spectrum for compound 6 (MeOH, 200 μg/mL)

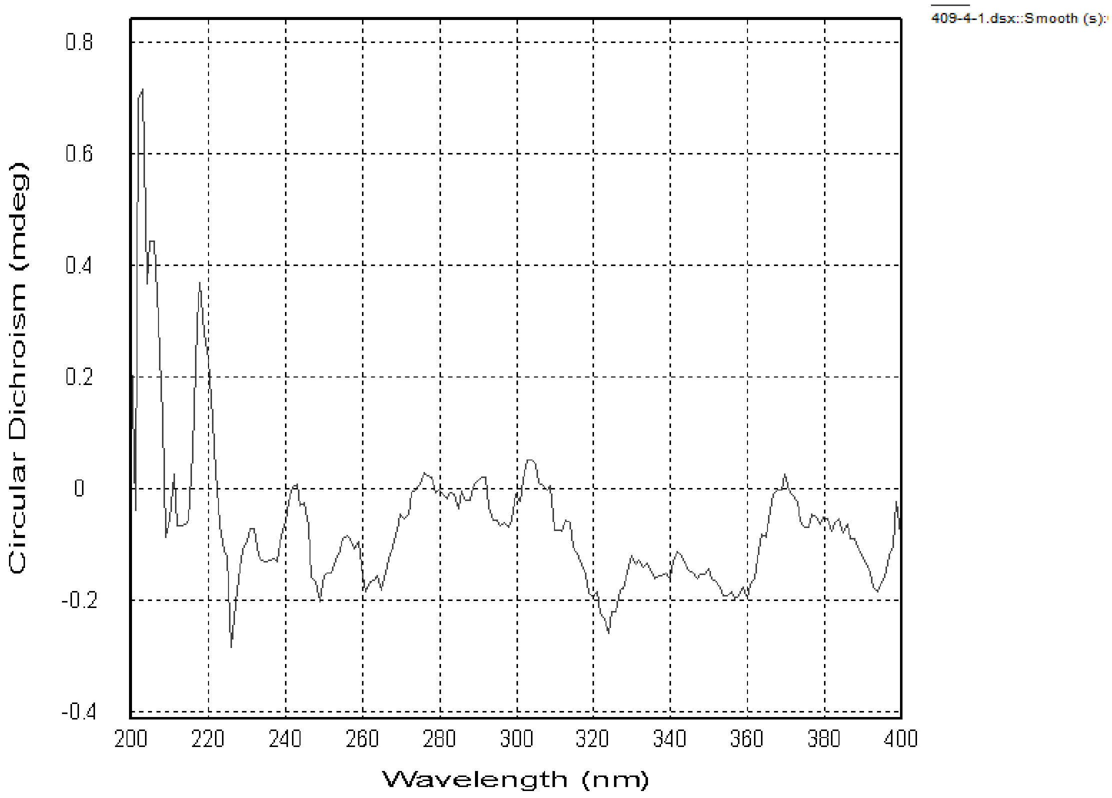


Figure S30. ^{1}H NMR spectrum for compound **8**

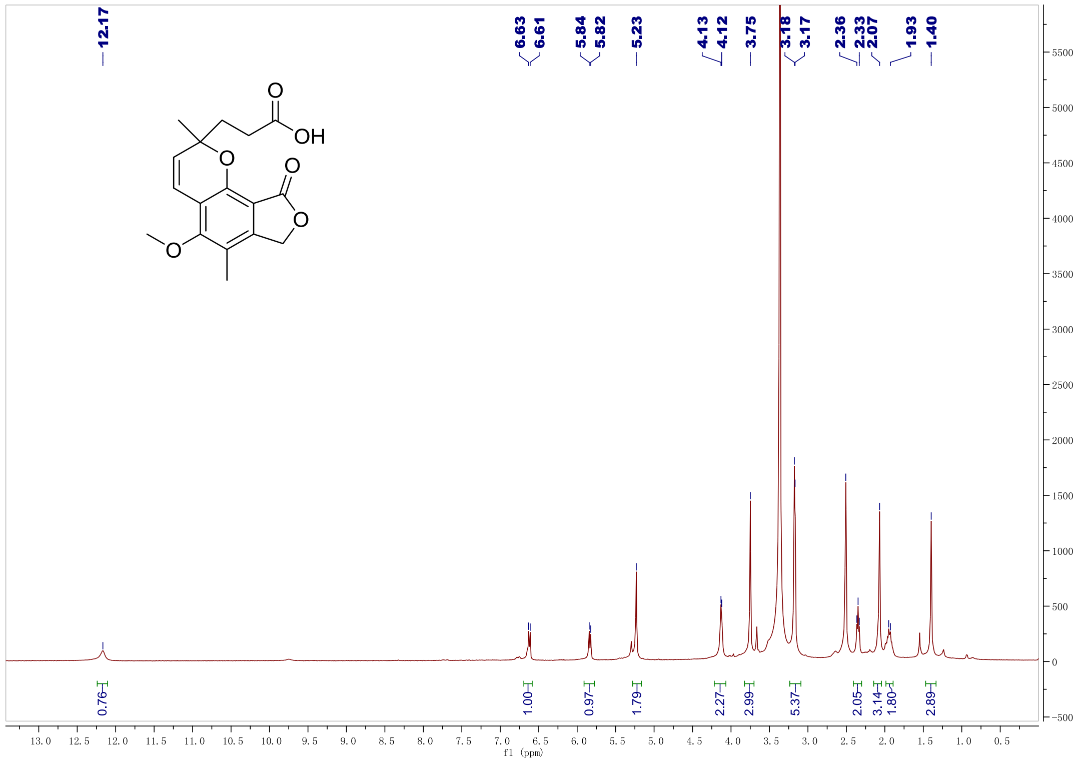


Figure S31. ^{13}C NMR spectrum for compound **8**

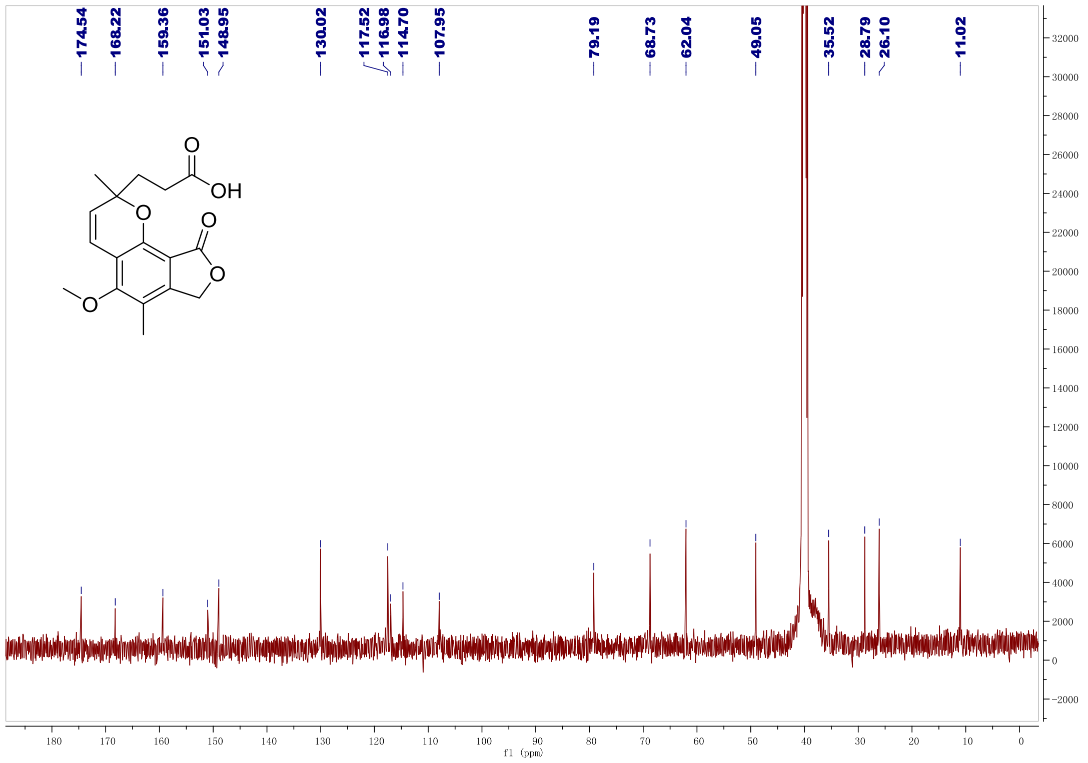


Figure S32. HMBC spectrum for compound **8**

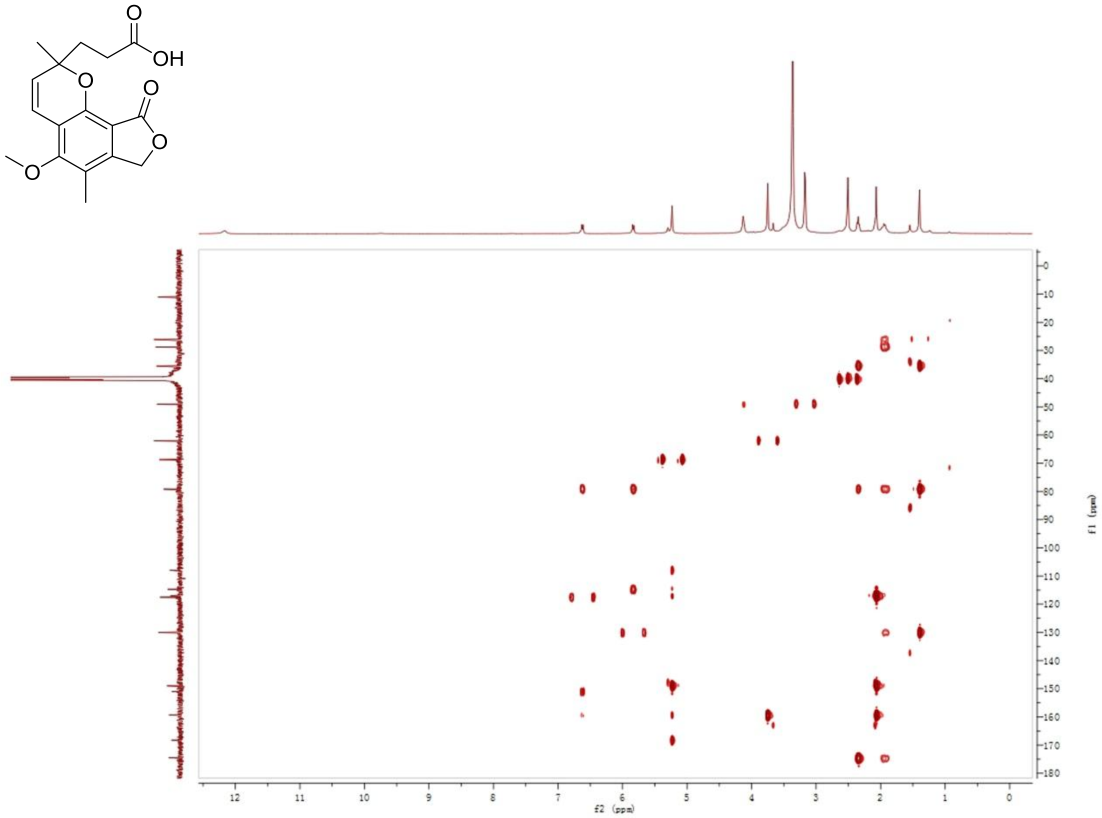
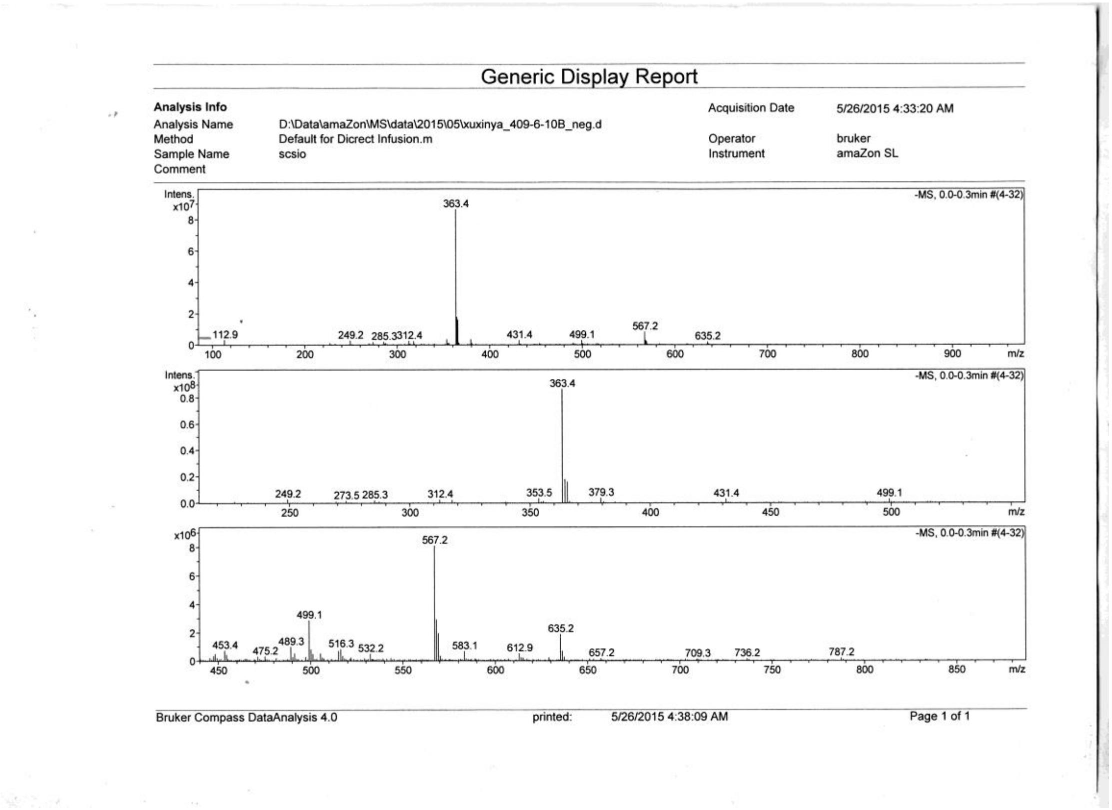


Figure S33. ESIMS spectrum for compound **8**



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Acquisition Date 5/26/2015 4:33:20 AM

Operator bruker
Instrument amaZon SL

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Figure S34. ^{1}H NMR spectrum for compound **9**

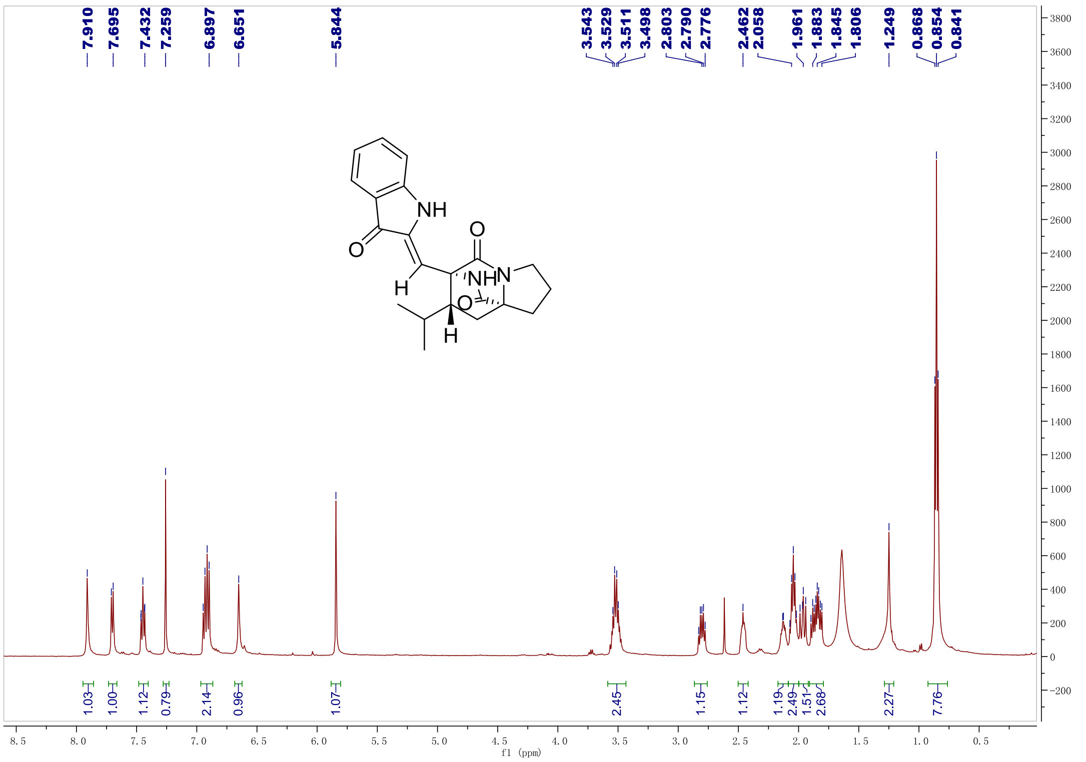


Figure S35. ^{13}C NMR spectrum for compound **9**

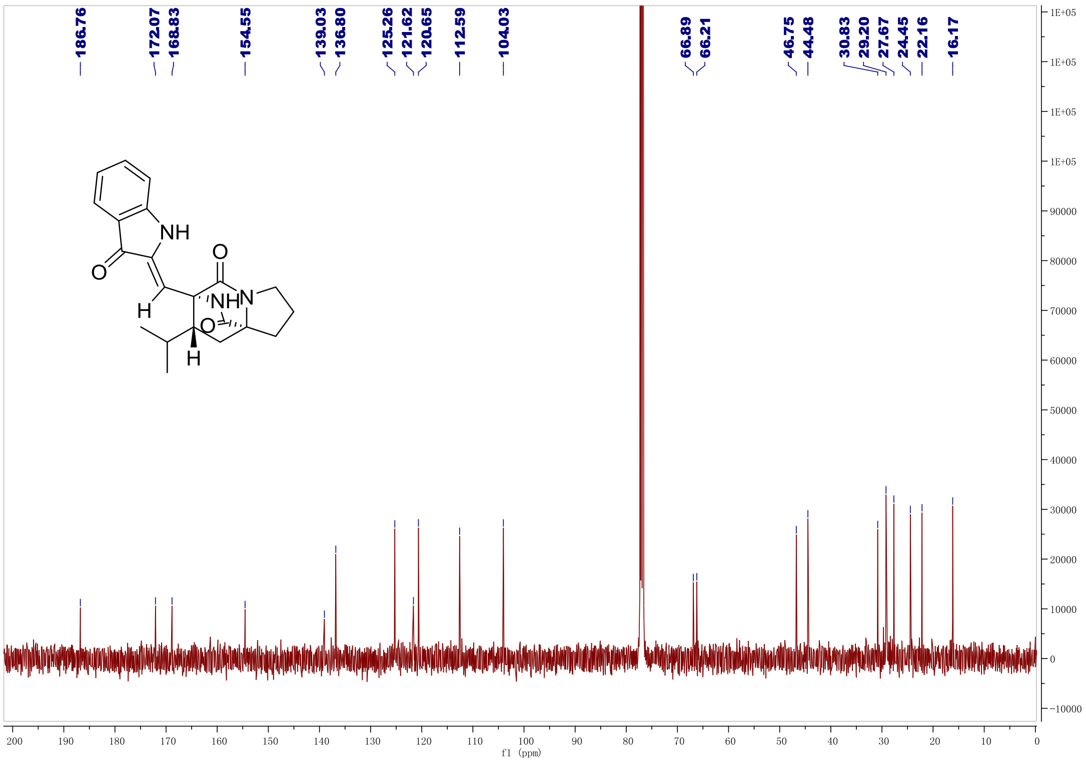


Figure S36. HSQC spectrum for compound **9**

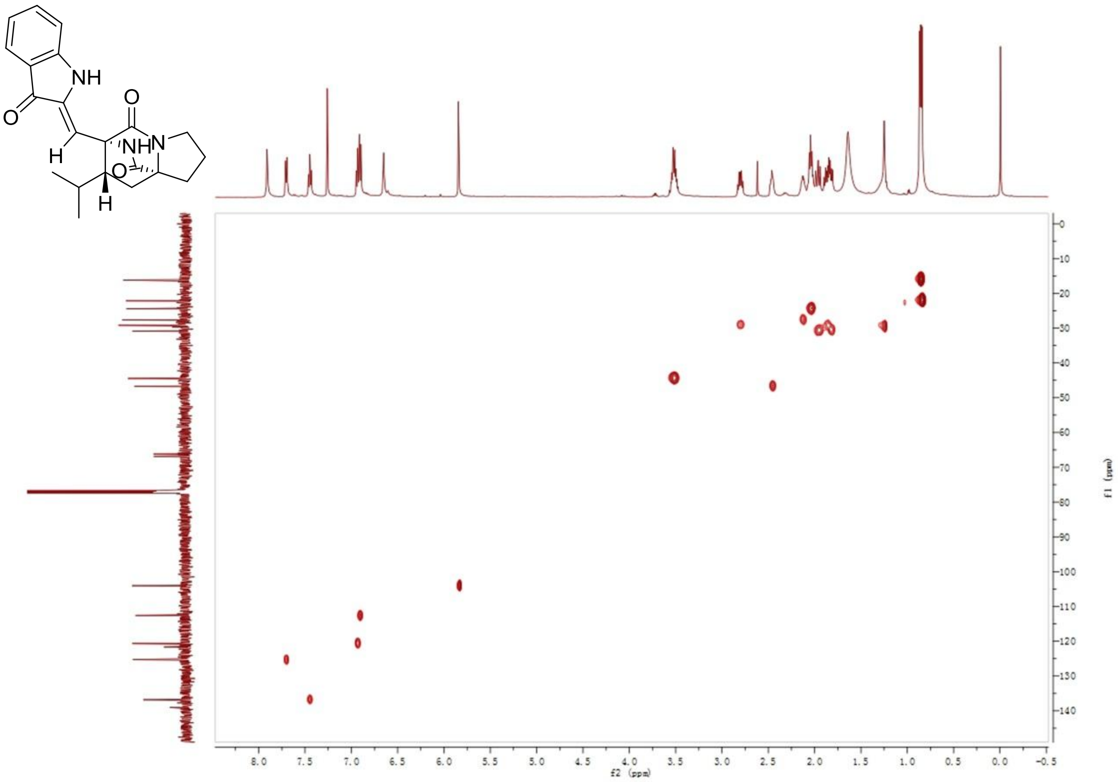


Figure S37. ^{1}H-^{1}H COSY spectrum for compound **9**

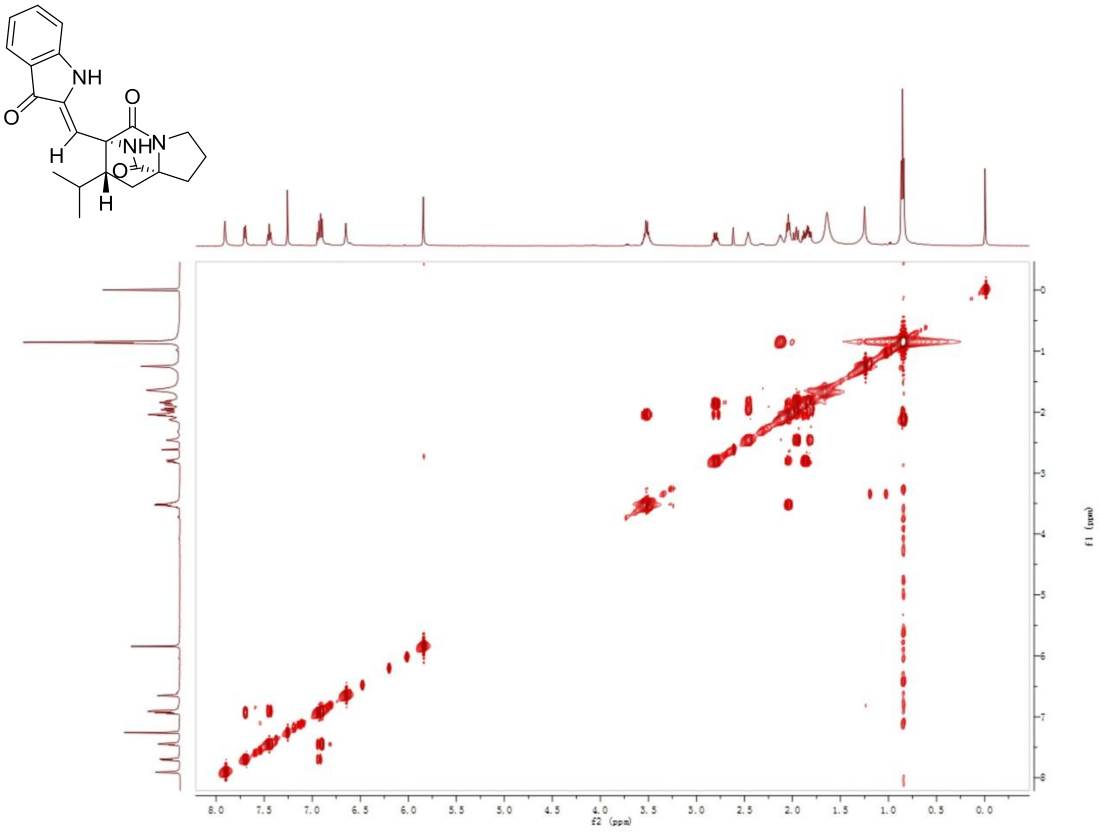


Figure S38. HMBC spectrum for compound **9**

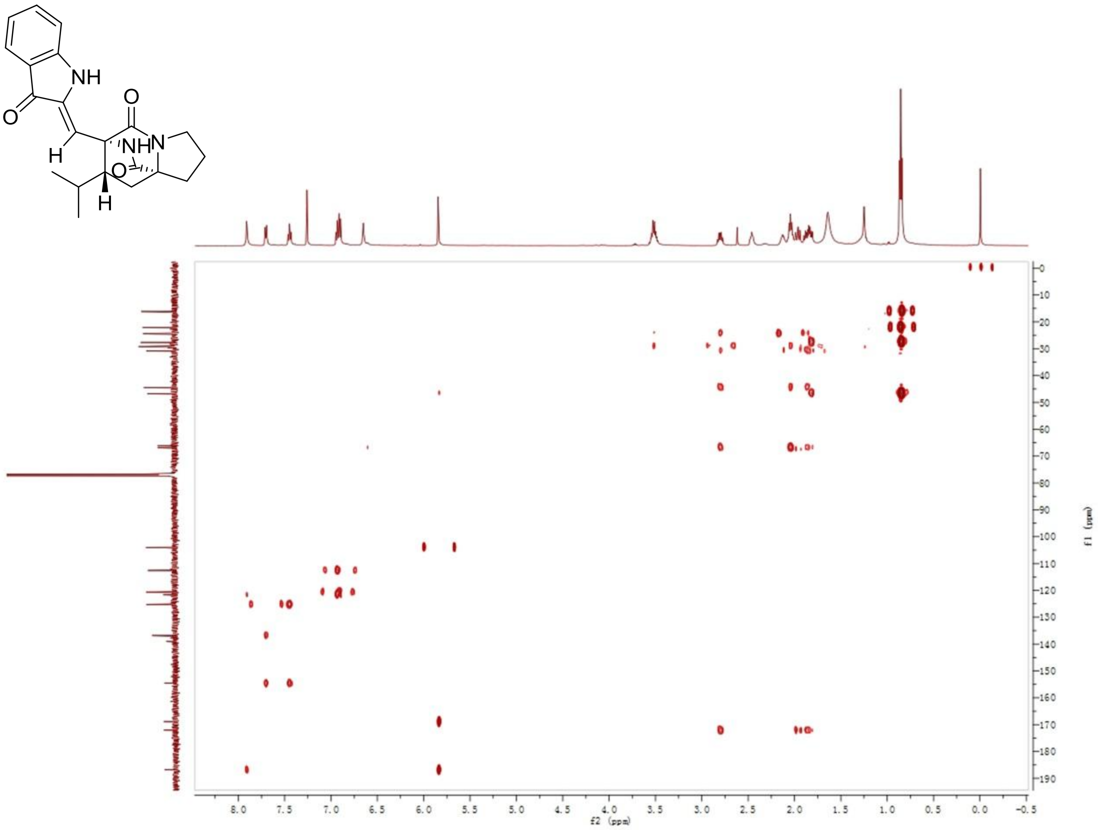


Figure S39. NOESY spectrum for compound **9**

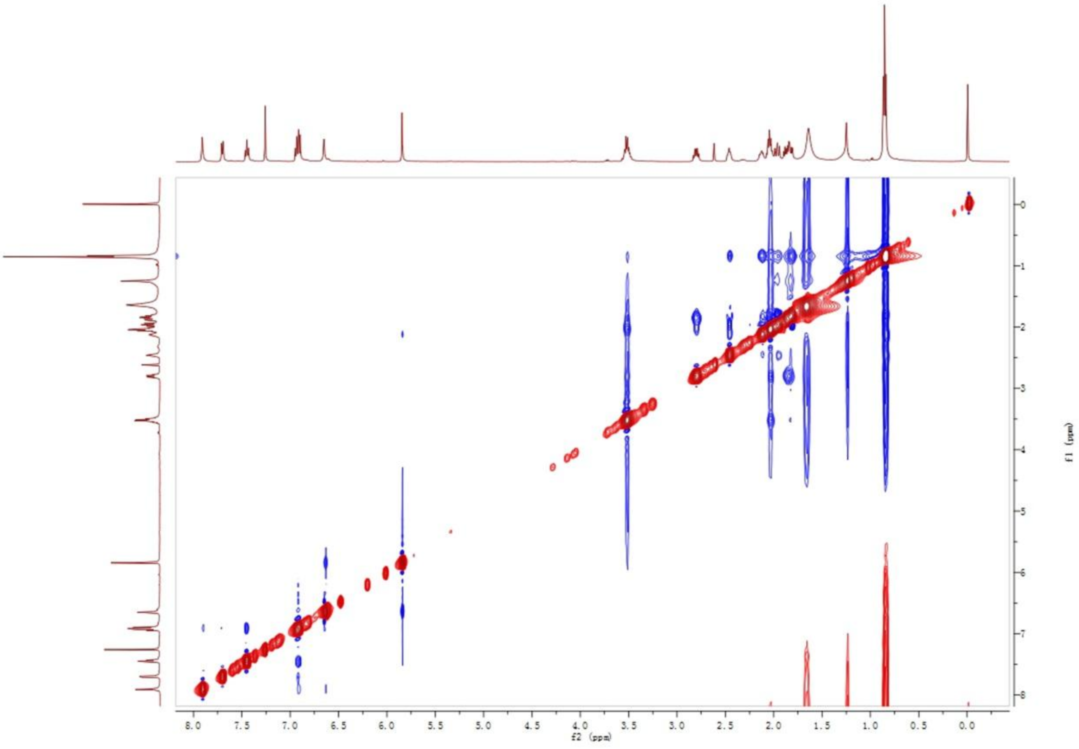
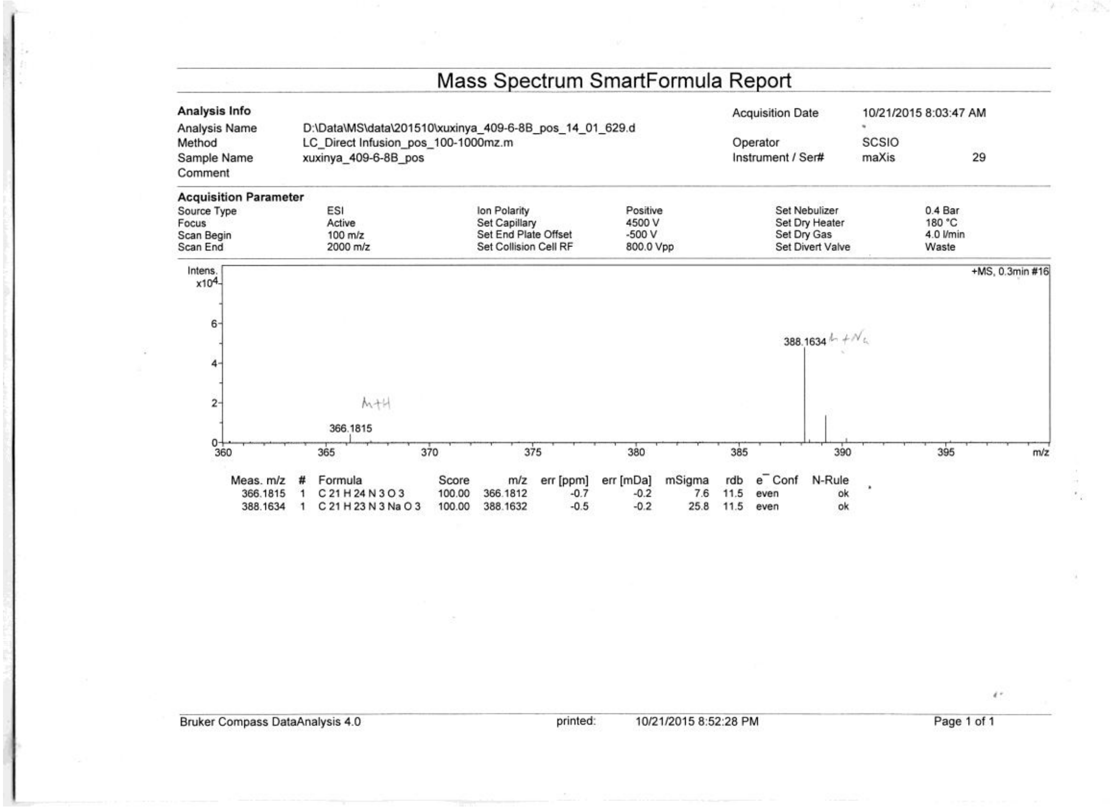


Figure S40. HR-ESIMS spectrum for compound **9**



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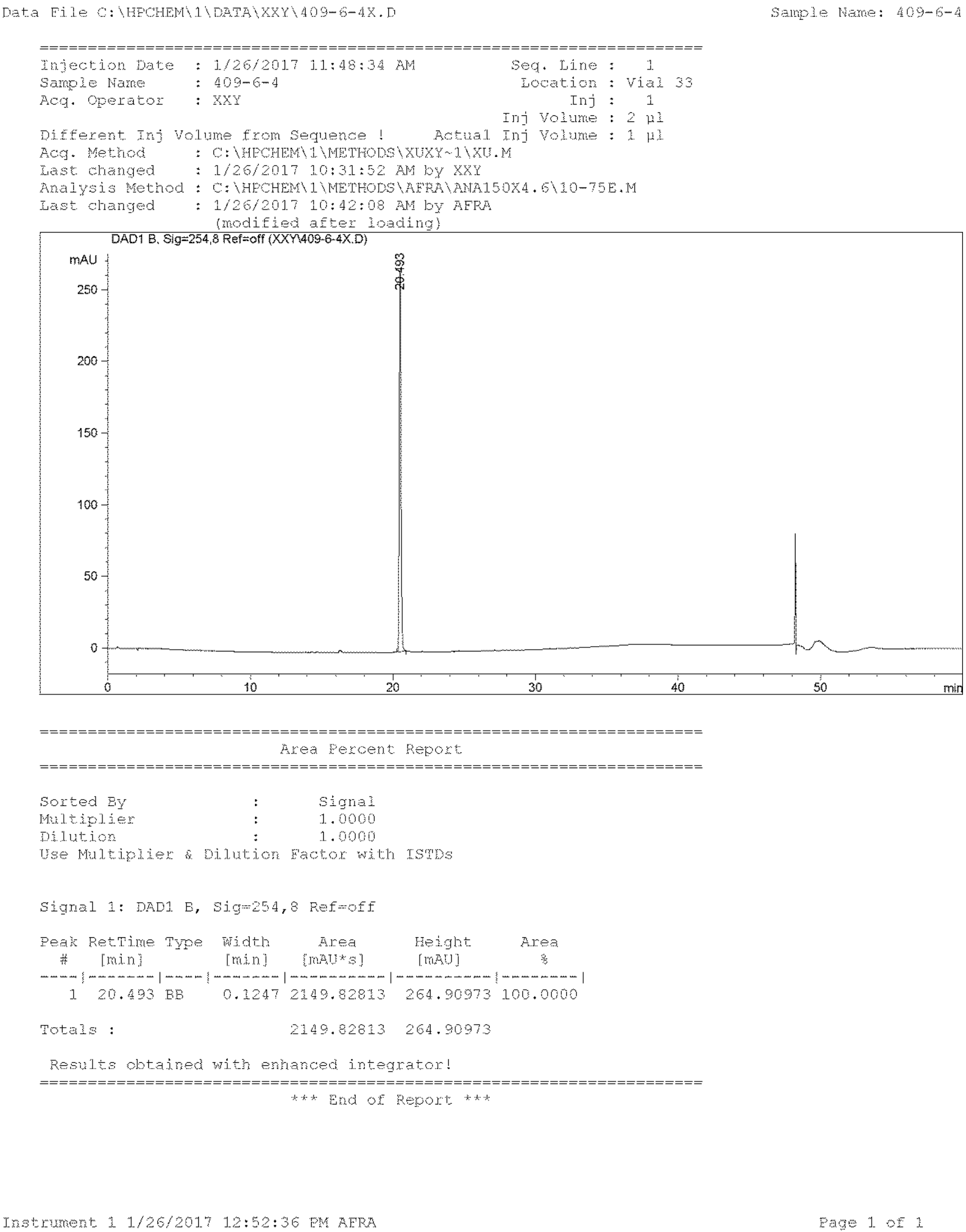
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Waste

Meas. m/z	#	Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
366.1815	1	C 21 H 24 N 3 O 3	100.00	366.1812	-0.7	-0.2	7.6	11.5	even	ok
388.1634	1	C 21 H 23 N 3 Na O 3	100.00	388.1632	-0.5	-0.2	25.8	11.5	even	ok

Bruker Compass DataAnalysis 4.0 printed: 10/21/2015 8:52:28 PM Page 1 of 1

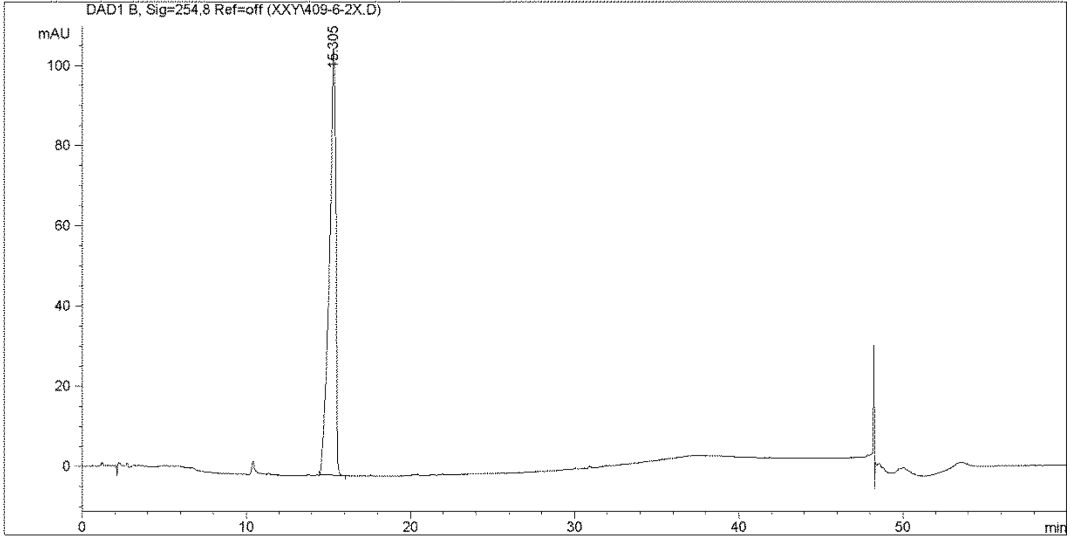
Figure S41. HPLC chromatogram for compounds **3**. HPLC condition: Angilent 1100 HPLC system; Column: Phenomenex® SYNERG I, 150 × 4.6 mm; Mobile phase: ACN/water, v/v; Gradient: 0-35 min, 5% to 100% ACN; 35-45 min, 100% ACN; 45-50 min, 100% to 5% ACN; 50-60 min, 5% ACN; Flow rate: 1 mL/min; Detection: 254 nm; Temperature: 25 ℃).



```
Data File C:\HPCHEM\1\DATA\XXY\409-6-4X.D                                    Sample Name: 409-6-4

   =====================================================================
   Injection Date  : 1/26/2017 11:48:34 AM          Seq. Line :   1
   Sample Name     : 409-6-4                         Location : Vial 33
   Acq. Operator   : XXY                                  Inj :   1
                                                 Inj Volume : 2 µl
   Different Inj Volume from Sequence !     Actual Inj Volume : 1 µl
   Acq. Method     : C:\HPCHEM\1\METHODS\XUXY~1\XU.M
   Last changed    : 1/26/2017 10:31:52 AM by XXY
   Analysis Method : C:\HPCHEM\1\METHODS\AFRA\ANA150X4.6\10-75E.M
   Last changed    : 1/26/2017 10:42:08 AM by AFRA
                     (modified after loading)

   =====================================================================
                            Area Percent Report
   =====================================================================

   Sorted By             :      Signal
   Multiplier            :      1.0000
   Dilution              :      1.0000
   Use Multiplier & Dilution Factor with ISTDs


   Signal 1: DAD1 B, Sig=254,8 Ref=off

   Peak RetTime Type  Width     Area      Height     Area
     #   [min]        [min]   [mAU*s]     [mAU]        %
   ----|-------|----|-------|----------|----------|--------|
      1  20.493 BB    0.1247 2149.82813  264.90973 100.0000

   Totals :                  2149.82813  264.90973

    Results obtained with enhanced integrator!
   =====================================================================
                             *** End of Report ***



Instrument 1 1/26/2017 12:52:36 PM AFRA                                           Page 1 of 1
```

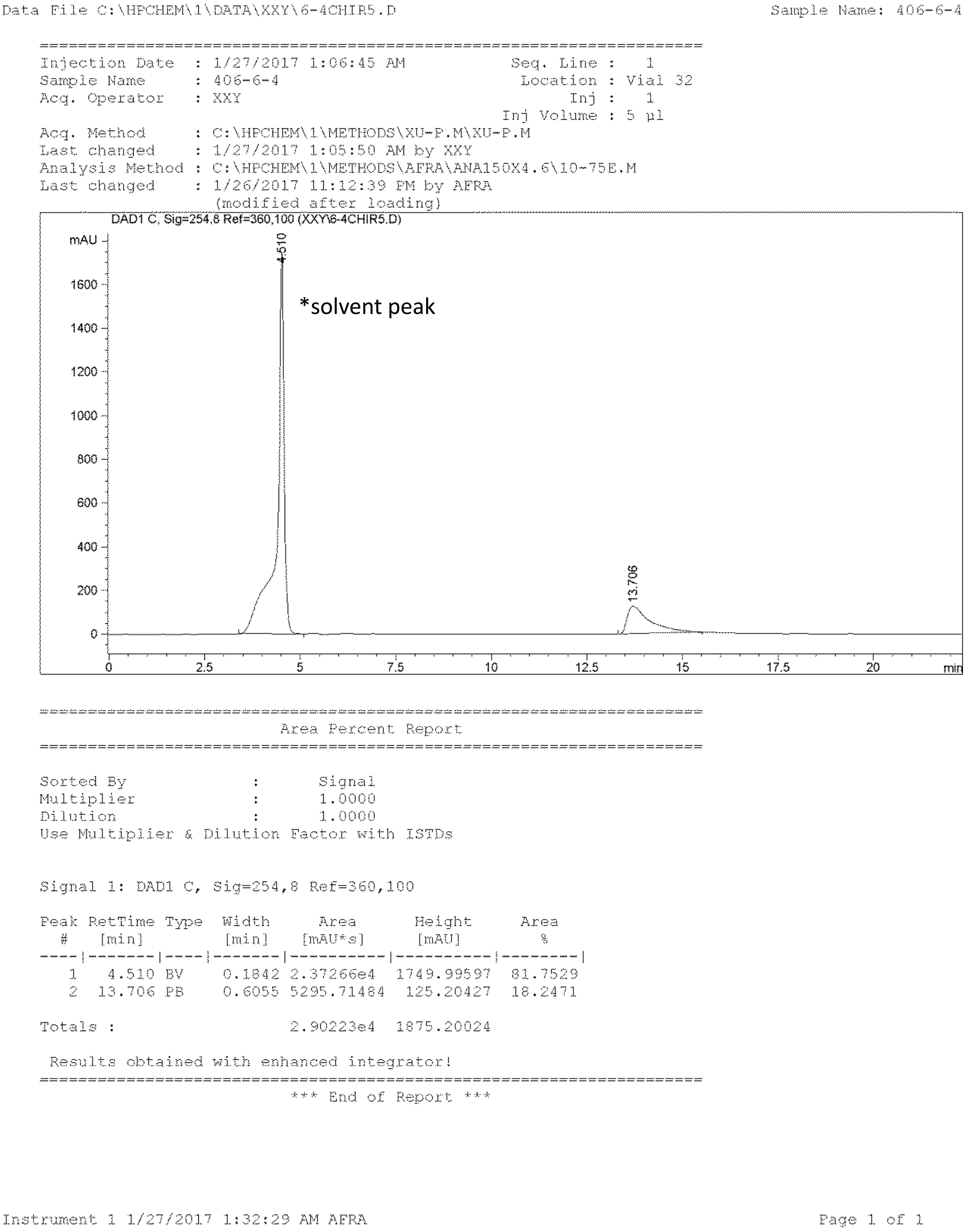
Figure S42. HPLC chromatogram for compound **5**. HPLC condition: same with S41.

```
Data File C:\HPCHEM\1\DATA\XXY\409-6-2X.D                                          Sample Name: 409-6-2

   =====================================================================
   Injection Date  : 1/26/2017 10:34:23 AM           Seq. Line :    1
   Sample Name     : 409-6-2                          Location : Vial 32
   Acq. Operator   : XXY                                   Inj :    1
                                                  Inj Volume : 2 µl
   Acq. Method     : C:\HPCHEM\1\METHODS\XUXY~1\XU.M
   Last changed    : 1/26/2017 10:31:52 AM by XXY
   Analysis Method : C:\HPCHEM\1\METHODS\AFRA\ANA150X4.6\10-75E.M
   Last changed    : 1/26/2017 10:42:08 AM by AFRA
                     (modified after loading)
```



```
   =====================================================================
                         Area Percent Report
   =====================================================================

   Sorted By             :      Signal
   Multiplier            :      1.0000
   Dilution              :      1.0000
   Use Multiplier & Dilution Factor with ISTDs


   Signal 1: DAD1 B, Sig=254,8 Ref=off

   Peak RetTime Type  Width     Area      Height     Area
     #   [min]        [min]   [mAU*s]     [mAU]        %
   ----|-------|----|-------|----------|----------|--------|
      1  15.305 BB    0.3845 2909.28076  106.56707 100.0000

   Totals :                  2909.28076  106.56707

    Results obtained with enhanced integrator!
   =====================================================================
                             *** End of Report ***



Instrument 1 1/26/2017 11:40:08 AM AFRA                                        Page 1 of 1
```

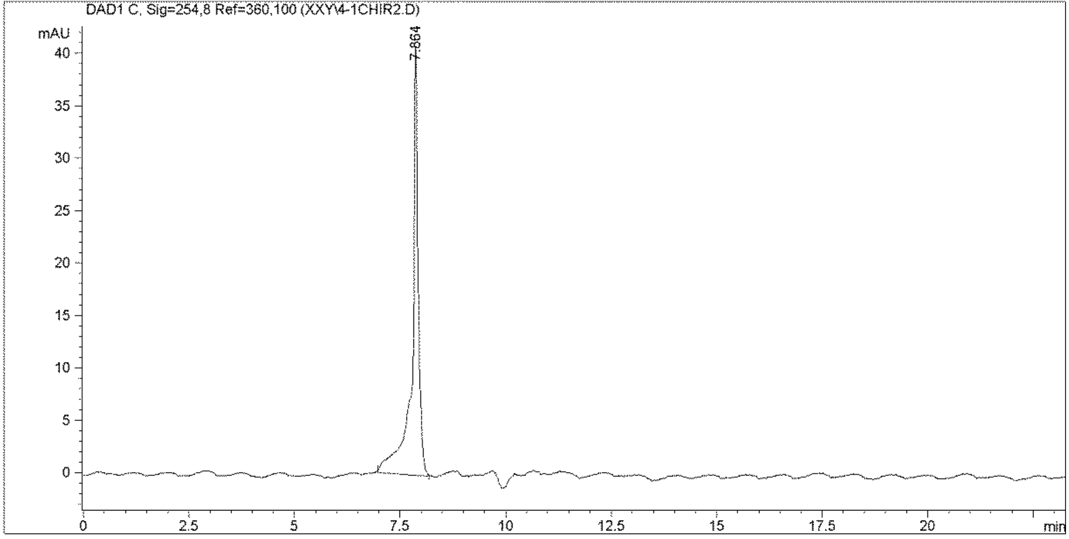
Figure S43. Chiral HPLC chromatogram spectrum for compound **3**. HPLC condition: Angilent 1100 HPLC system; Column: CHIRALPAK® IC, 250 × 4.6 mm; Mobile phase: n-hexane/propan-2-ol 70:30, v/v; Flow rate: 1 mL/min; Detection: 254 nm; Temperature: 25 ℃.



```
Data File C:\HPCHEM\1\DATA\XXY\6-4CHIR5.D                                    Sample Name: 406-6-4

    =====================================================================
    Injection Date  : 1/27/2017 1:06:45 AM           Seq. Line :    1
    Sample Name     : 406-6-4                         Location : Vial 32
    Acq. Operator   : XXY                                  Inj :    1
                                                    Inj Volume : 5 µl
    Acq. Method     : C:\HPCHEM\1\METHODS\XU-P.M\XU-P.M
    Last changed    : 1/27/2017 1:05:50 AM by XXY
    Analysis Method : C:\HPCHEM\1\METHODS\AFRA\ANA150X4.6\10-75E.M
    Last changed    : 1/26/2017 11:12:39 PM by AFRA
                      (modified after loading)

    =====================================================================
                             Area Percent Report
    =====================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 C, Sig=254,8 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1   4.510 BV    0.1842 2.37266e4  1749.99597  81.7529
       2  13.706 PB    0.6055 5295.71484  125.20427  18.2471

    Totals :                  2.90223e4  1875.20024

     Results obtained with enhanced integrator!
    =====================================================================
                              *** End of Report ***



Instrument 1 1/27/2017 1:32:29 AM AFRA                                     Page 1 of 1
```

Figure S44. Chiral HPLC chromatogram spectrum for compound **6**. HPLC condition: Angilent 1100 HPLC system; Column: CHIRALPAK® IC, 250 × 4.6 mm; Mobile phase: n-hexane/propan-2-ol 60:40, v/v; Flow rate: 1 mL/min; Detection: 254 nm; Temperature: 25 ℃).

```
=====================================================================
Injection Date  : 1/27/2017 12:26:17 AM          Seq. Line :    1
Sample Name     : 409-4-1                         Location : Vial 34
Acq. Operator   : XXY                                  Inj :    1
                                                Inj Volume : 5 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2 µl
Acq. Method     : C:\HPCHEM\1\METHODS\XU-P.M\XU-P.M
Last changed    : 1/26/2017 11:59:52 PM by XXY
Analysis Method : C:\HPCHEM\1\METHODS\AFRA\ANA150X4.6\10-75E.M
Last changed    : 1/26/2017 11:12:39 PM by AFRA
                  (modified after loading)
```



```
=====================================================================
                         Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 C, Sig=254,8 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1   7.864 BB    0.1342  414.31332   40.89666 100.0000

Totals :                   414.31332   40.89666

 Results obtained with enhanced integrator!
=====================================================================
                          *** End of Report ***
```