

Electronic Supplementary Information

Novel phthalide derivatives from the rhizomes of *Ligusticum chuanxiong* and their inhibitory effect against lipopolysaccharide-induced nitric oxide production in RAW 264.7 macrophage cells

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PR China. Tel.: 86 10 82801569; fax: +86 10 82802724. E-mail address:

xwyang@bjmu.edu.cn (X. W. Yang).

Contents

Figure S 1. HRESIMS data of **1**

Figure S 1. IR spectrum of **1**

Figure S 2. UV spectrum of **1** in MeOH

Figure S 3. ¹H NMR spectrum of **1** in CDCl₃

Figure S 5. ¹³C NMR spectrum of **1** in CDCl₃

Figure S 6. DEPT spectrum of **1** in CDCl₃

Figure S 7. ¹H-¹H COSY spectrum of **1** in CDCl₃

Figure S 8. HSQC spectrum of **1** in CDCl₃

Figure S 9. HMBC spectrum of **1** in CDCl₃

Figure S 10. NOESY spectrum of **1** in CDCl₃

Figure S 11. HRESIMS data of **2**

Figure S 14. IR spectrum of **2**

Figure S 15. UV spectrum of **2** in MeOH

Figure S 16. ^1H NMR spectrum of **1** in CDCl_3

Figure S 15. ^{13}C NMR spectrum of **2** in CDCl_3

Figure S 16. DEPT spectrum of **2** in CDCl_3

Figure S 17. ^1H - ^1H COSY spectrum of **2** in CDCl_3

Figure S 18. HSQC spectrum of **2** in CDCl_3

Figure S 19. HMBC spectrum of **2** in CDCl_3

Figure S 20. NOESY spectrum of **2** in CDCl_3

Figure S 21. HRESIMS data of **3**

Figure S 27. IR spectrum of **3**

Figure S 28. UV spectrum of **3** in MeOH

Figure S 29. ^1H NMR spectrum of **3** in CDCl_3

Figure S 25. ^{13}C NMR spectrum of **3** in CDCl_3

Figure S 26. DEPT spectrum of **3** in CDCl_3

Figure S 27. ^1H - ^1H COSY spectrum of **3** in CDCl_3

Figure S 28. HSQC spectrum of **3** in CDCl_3

Figure S 29. HMBC spectrum of **3** in CDCl_3

Figure S 30. NOESY spectrum of **3** in CDCl_3

Figure S 31. HRESIMS data of **4**

Figure S 310. IR spectrum of **4**

Figure S 311. UV spectrum of **4** in MeOH

Figure S 312. ^1H NMR spectrum of **4** in CDCl_3

Figure S 35. ^{13}C NMR spectrum of **4** in CDCl_3

Figure S 36. DEPT spectrum of **4** in CDCl_3

Figure S 37. ^1H - ^1H COSY spectrum of **4** in CDCl_3

Figure S 38. HSQC spectrum of **4** in CDCl_3

Figure S 39. HMBC spectrum of **4** in CDCl_3

Figure S 40. NOESY spectrum of **4** in CDCl_3

Figure S 41. HRESIMS data of **5**

Figure S 413. IR spectrum of **5**

Figure S 414. UV spectrum of **5** in MeOH

Figure S 415. ^1H NMR spectrum of **5** in CDCl_3

Figure S 45. ^{13}C NMR spectrum of **5** in CDCl_3

Figure S 46. DEPT spectrum of **5** in CDCl_3

Figure S 47. ^1H - ^1H COSY spectrum of **5** in CDCl_3

Figure S 48. HSQC spectrum of **5** in CDCl_3

Figure S 49. HMBC spectrum of **5** in CDCl_3

Figure S 50. NOESY spectrum of **5** in CDCl_3

Elemental Composition Report

Single Mass Analysis

Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

752 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

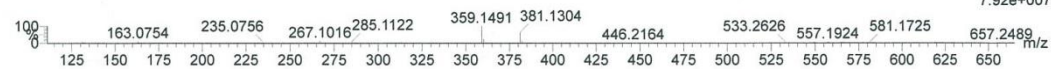
C: 0-100 H: 0-200 N: 0-5 O: 0-30 Si: 0-1

Xevo G2 Q-TOF/YCA166#

15-May-2015

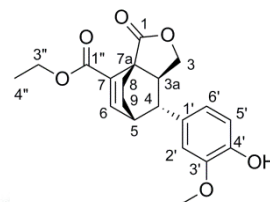
20150508-12 12 (0.220) Cm (10:18-(1:5+27:56))

Waters
 TOF MS ES+
 7.92e+007



Minimum: -1.5
 Maximum: 5.0 2.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
359.1491	359.1495	-0.4	-1.1	9.5	1011.4	0.000	100.00	C20 H23 O6
	359.1486	0.5	1.4	0.5	1027.5	16.096	0.00	C11 H27 N2 O9 Si



Page 1

Figure S 16. HRESIMS data of 1

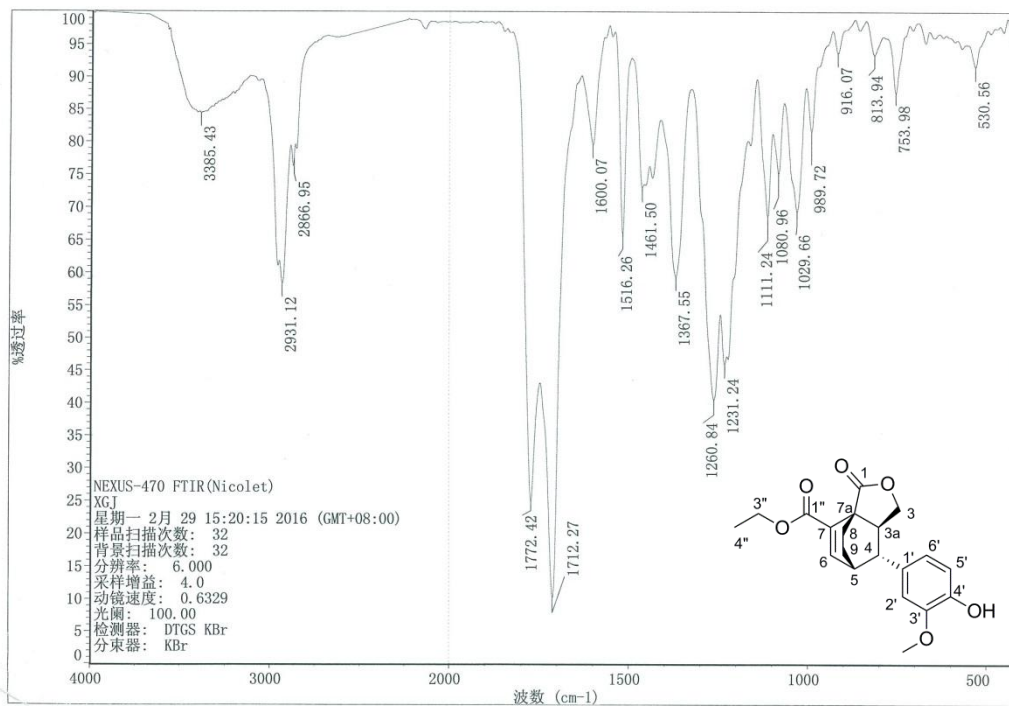
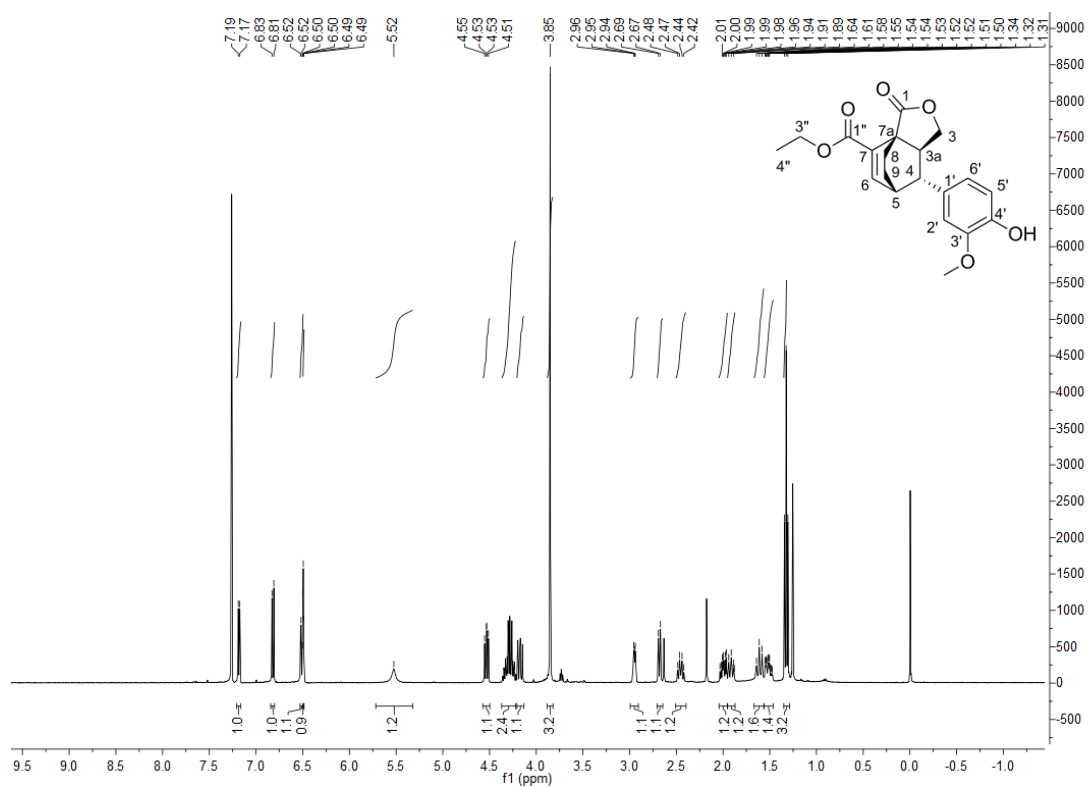
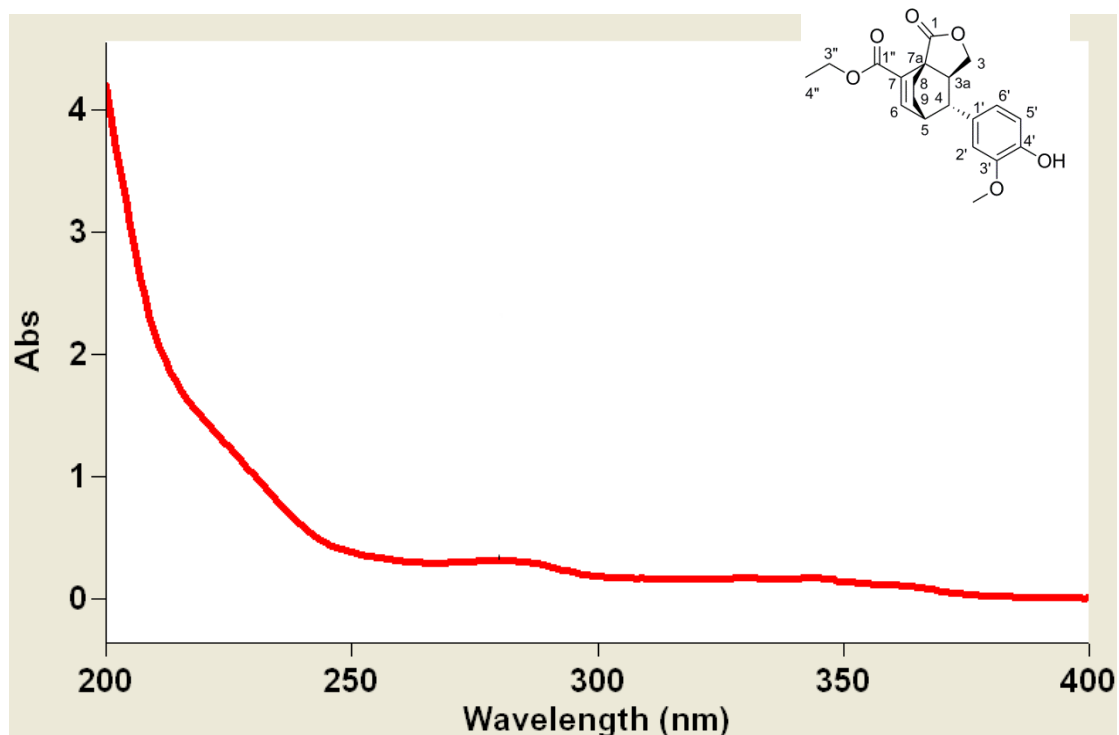


Figure S 17. IR spectrum of 1



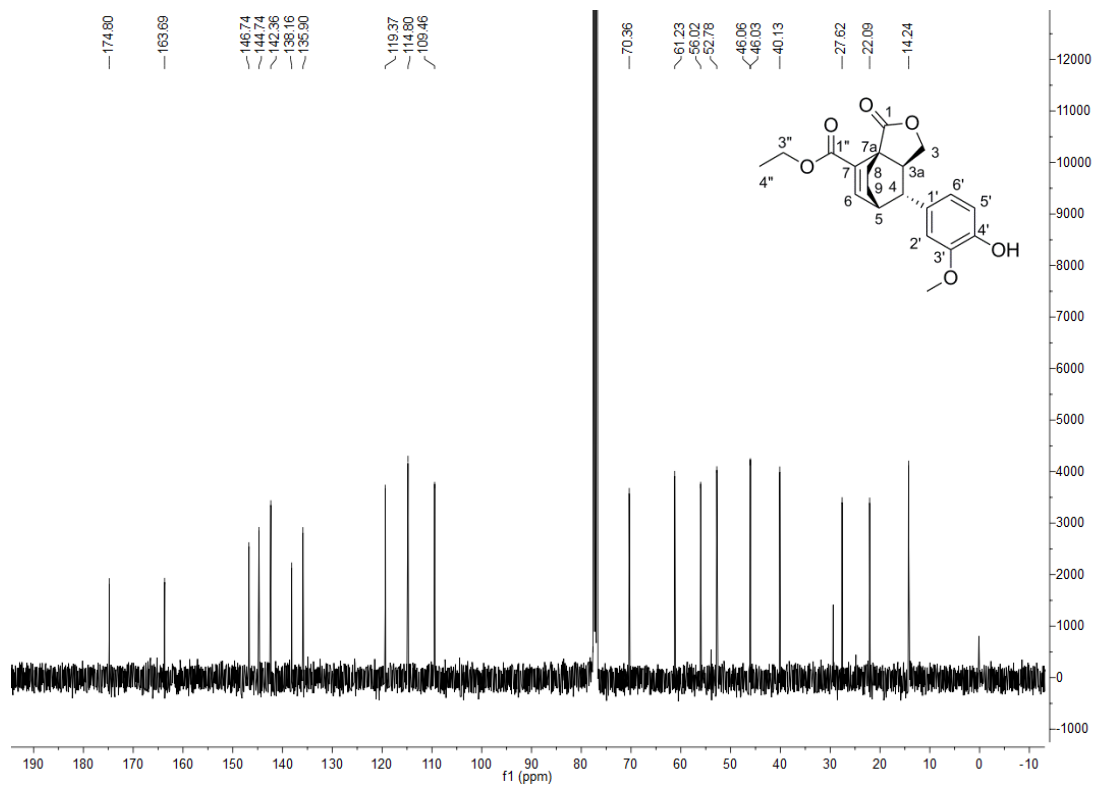


Figure S 20. ^{13}C NMR spectrum of **1** in CDCl_3

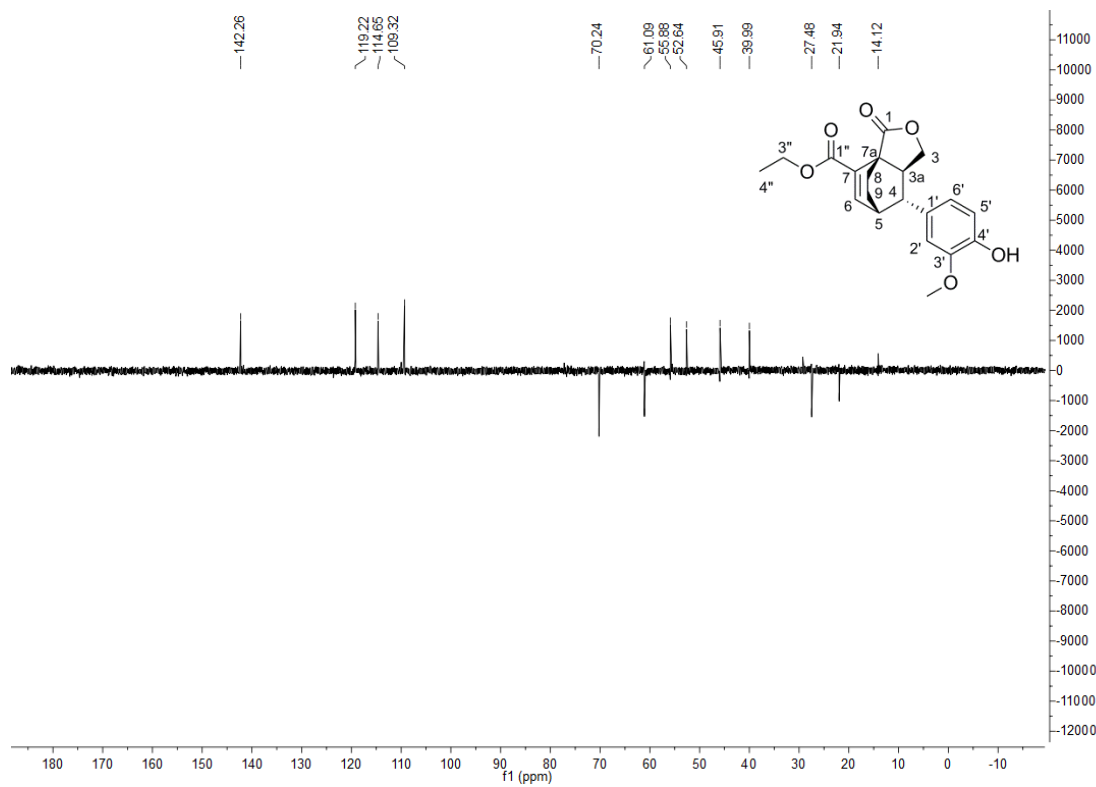


Figure S 21. DEPT 135 spectrum of **1** in CDCl_3

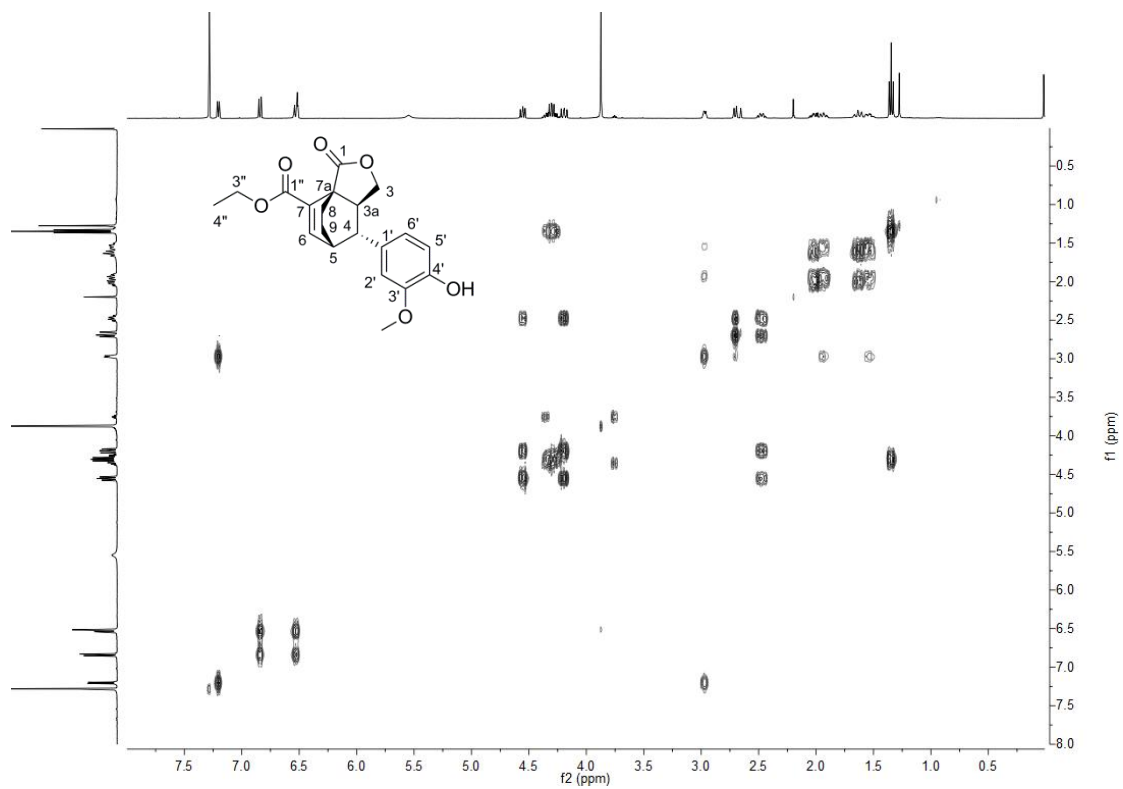


Figure S 22. ^1H - ^1H COSY spectrum of **1** in CDCl_3

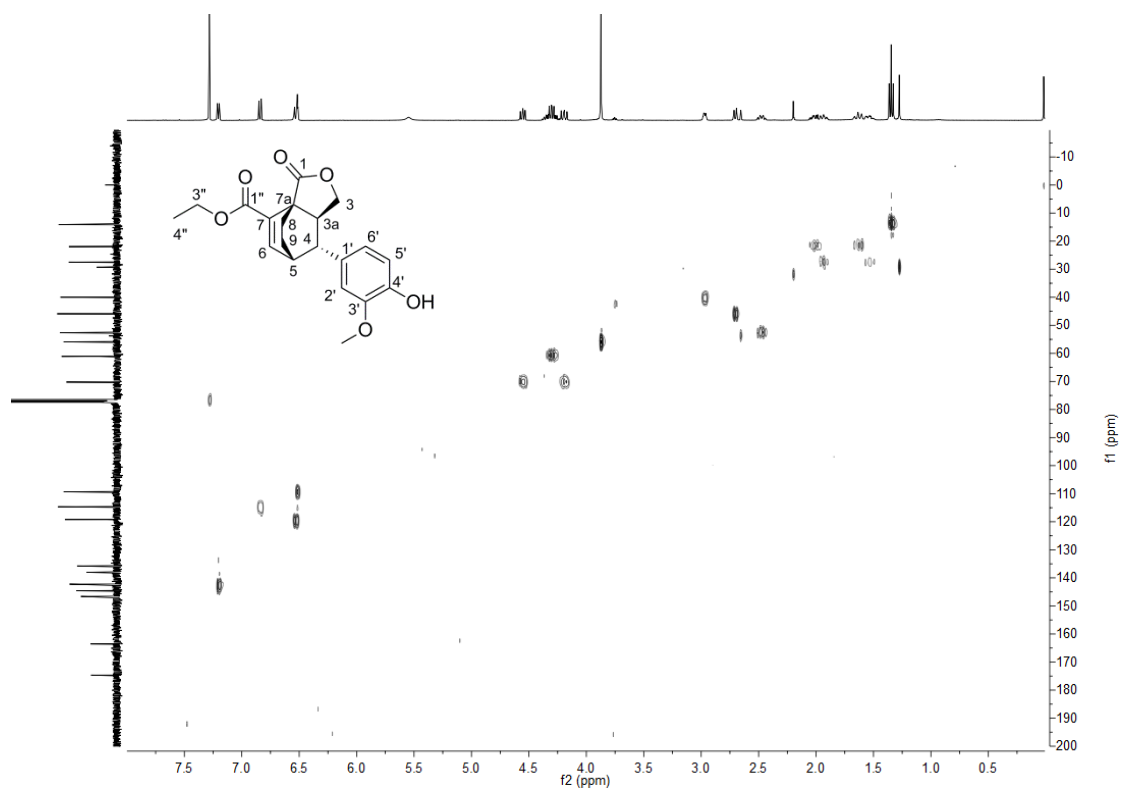


Figure S 23. HSQC spectrum of **1** in CDCl_3

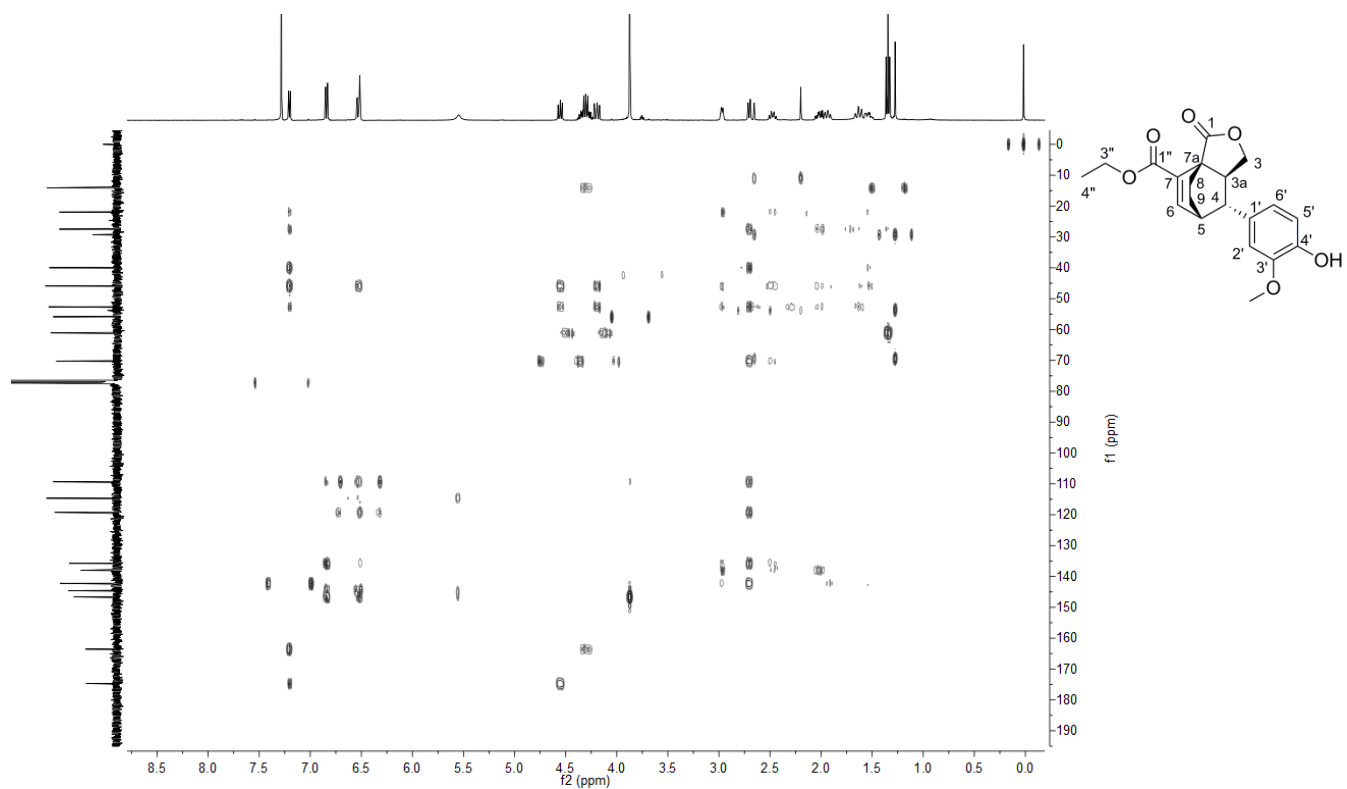


Figure S 24. HMBC spectrum of **1** in CDCl₃

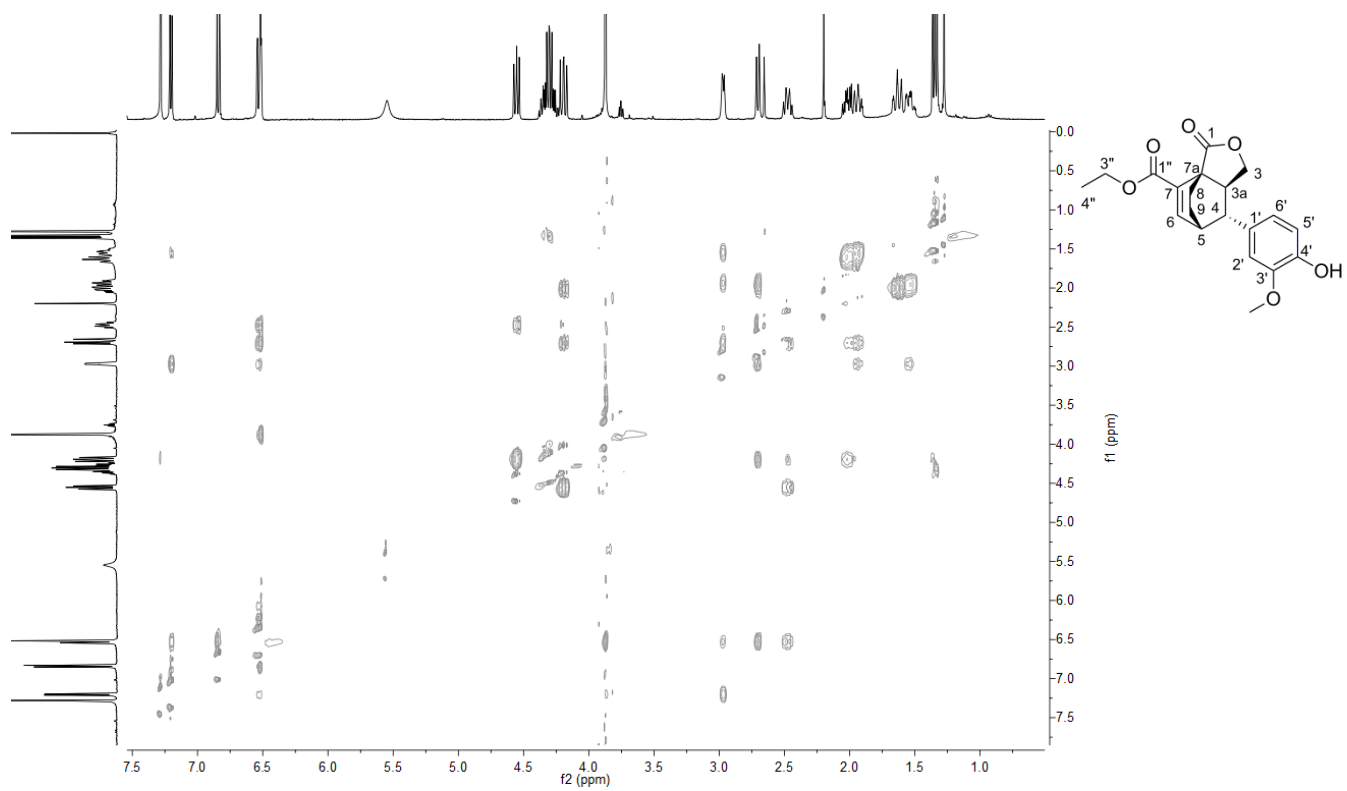


Figure S 25. NOESY spectrum of **1** in CDCl₃

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

84 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

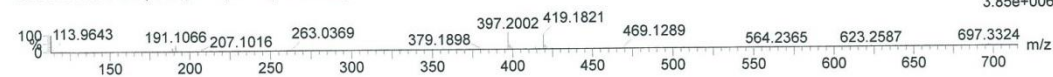
C: 0-100 H: 0-200 O: 0-50

Xevo G2 Q-TOF/YCA166#

CX-20151106-A 13 (0.237) Cm (11:17-(2:7+23:58))

24-Nov-2015

Waters
TOF MS ES+
3.85e+006



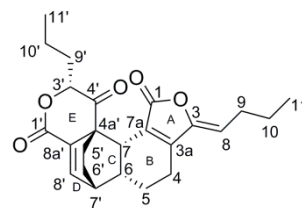
Minimum:

Maximum: 5.0 5.0 -1.5

50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
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397.2002	397.2015	-1.3	-3.3	10.5	408.5	n/a	n/a	C24 H29 O5
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Page 1

Figure S 26. HRESIMS data of **2**

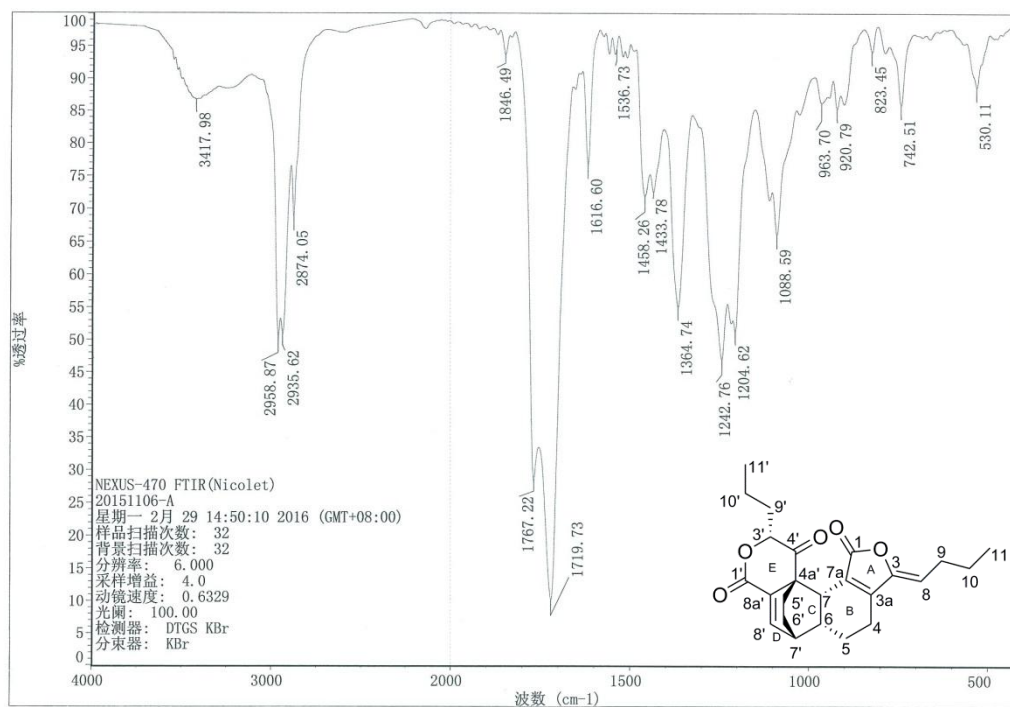


Figure S 27. IR spectrum of **2**

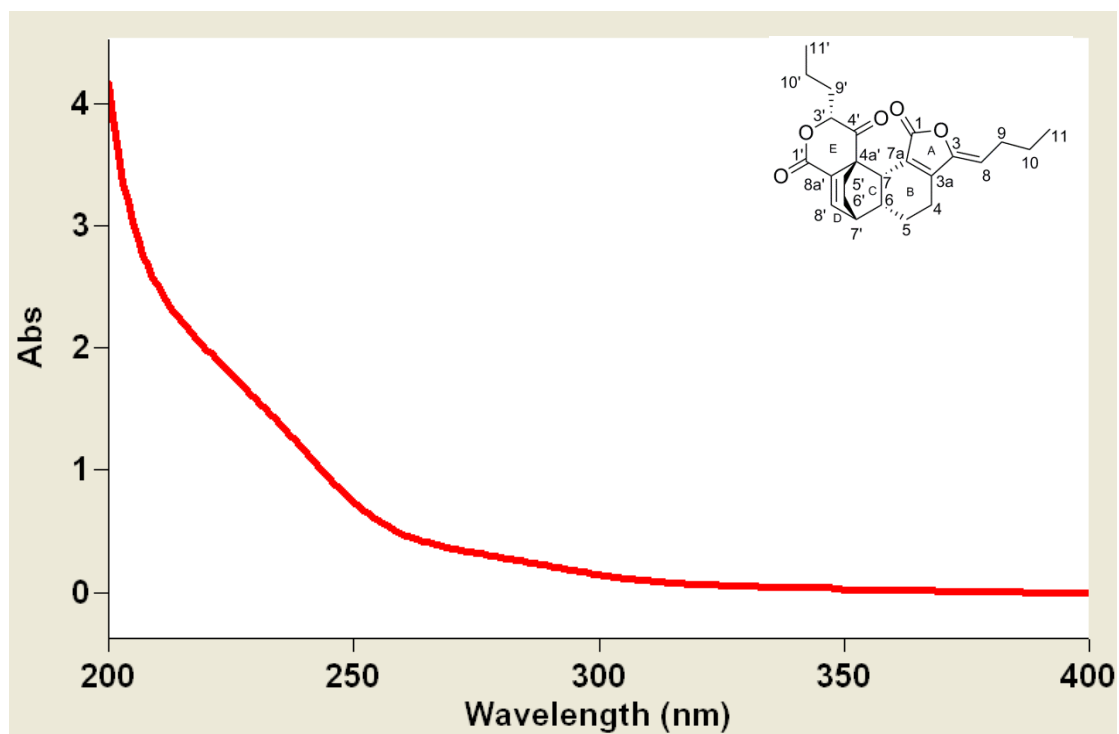


Figure S 28. UV spectrum of **2** in MeOH

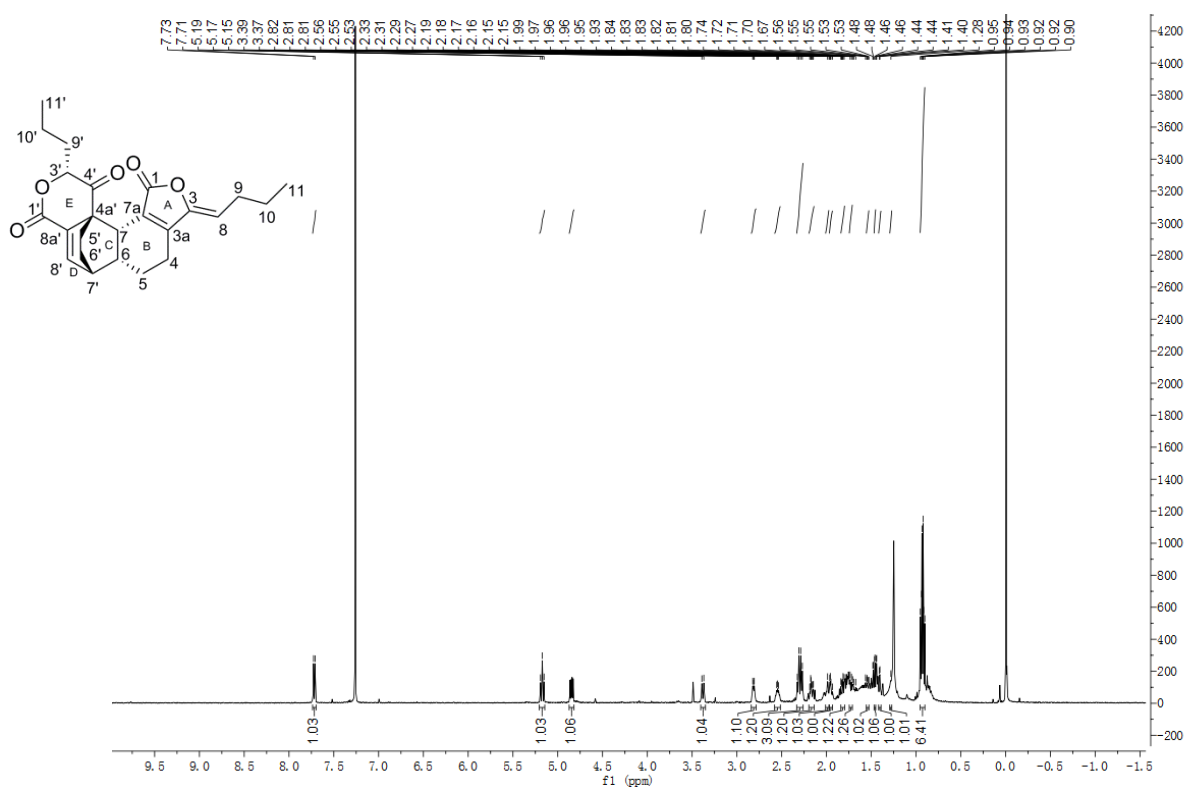


Figure S 29. ¹H NMR spectrum of **2** in CDCl₃

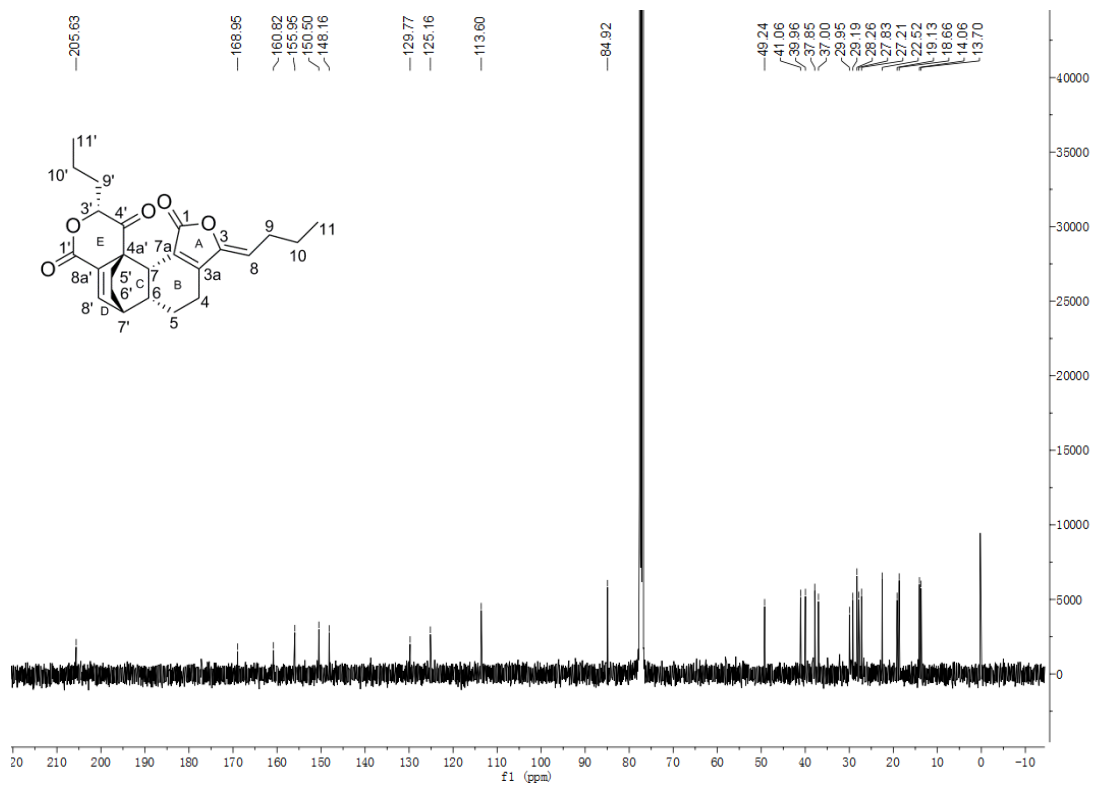


Figure S 30. ^{13}C NMR spectrum of **2** in CDCl_3

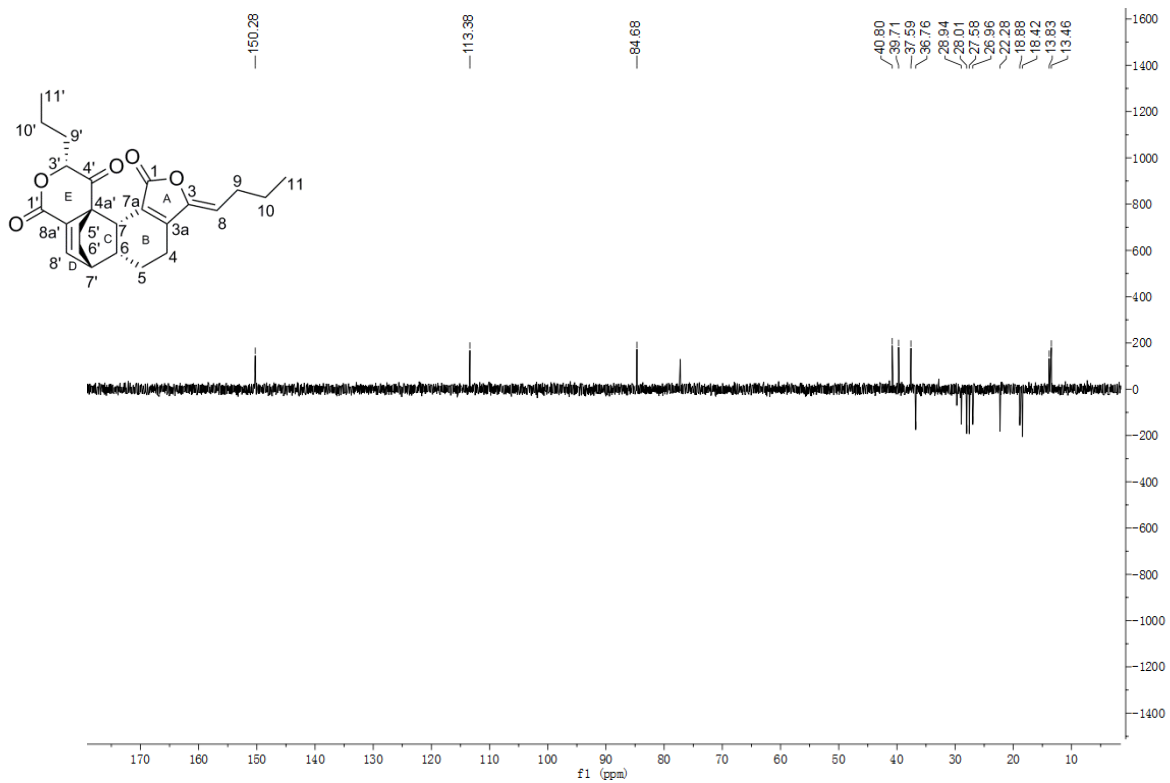


Figure S 31. DEPT spectrum of **2** in CDCl_3

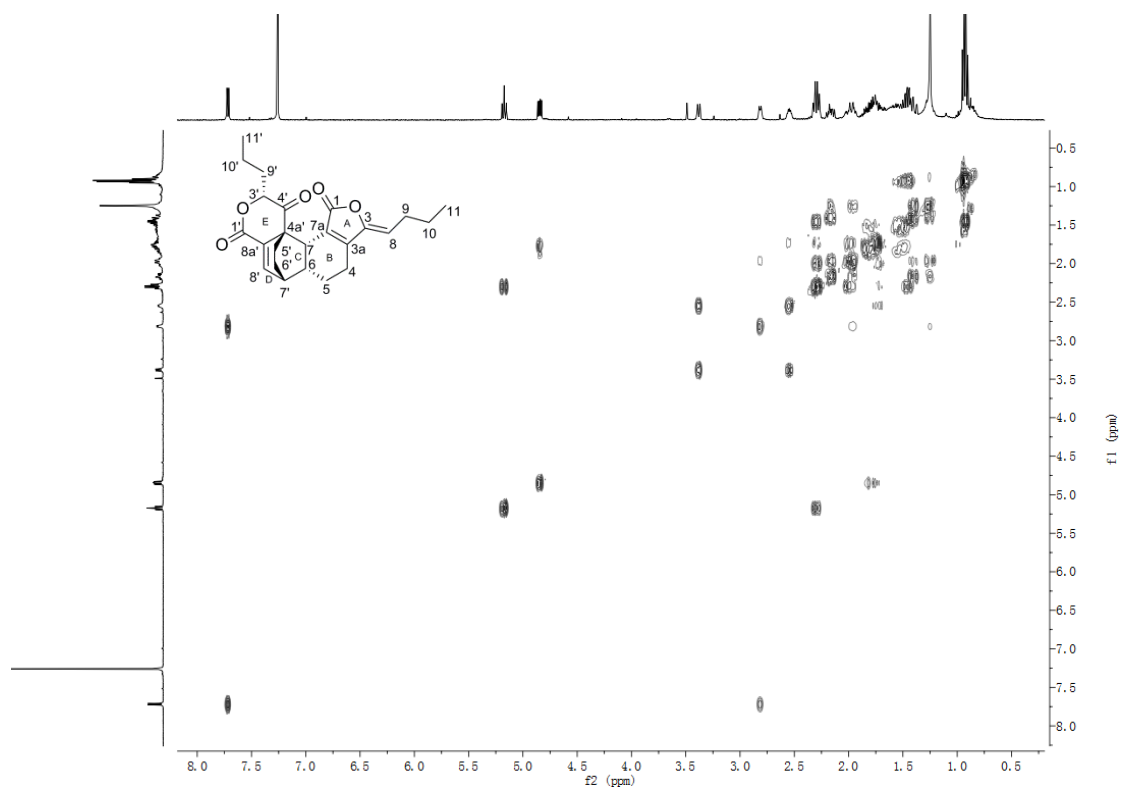


Figure S 32. ^1H - ^1H COSY spectrum of **2** in CDCl_3

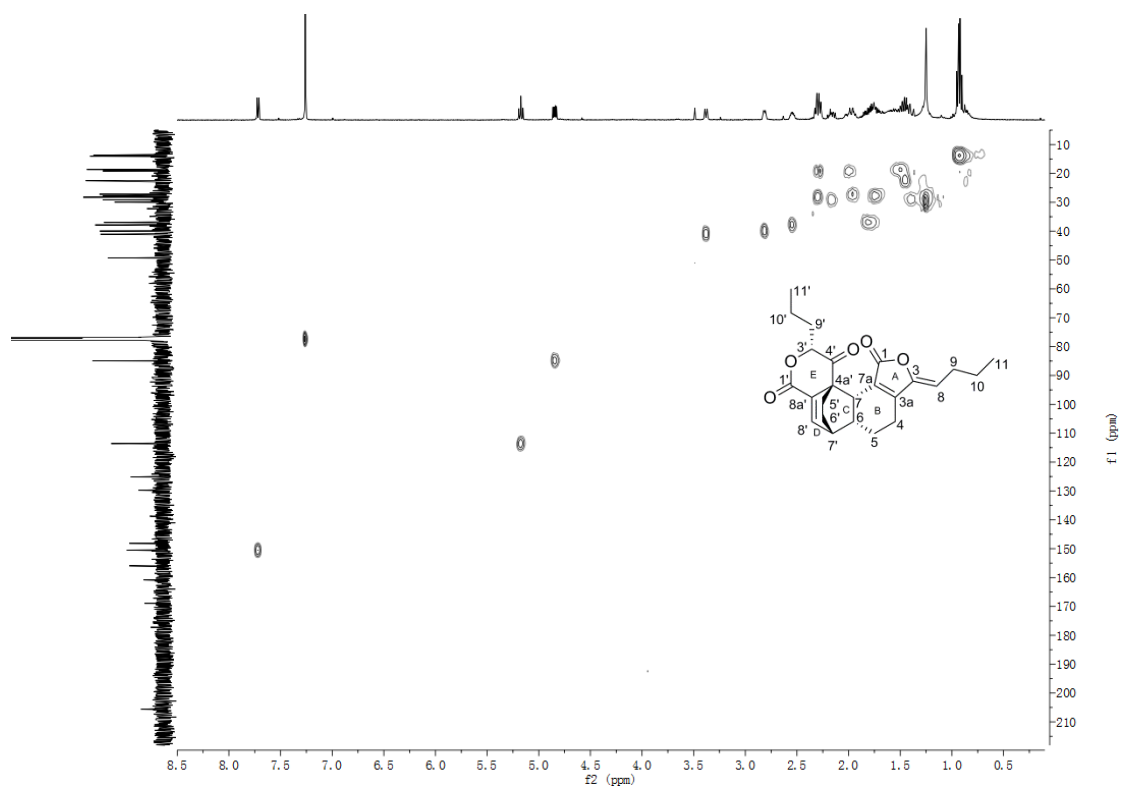


Figure S 33. HSQC spectrum of **2** in CDCl_3

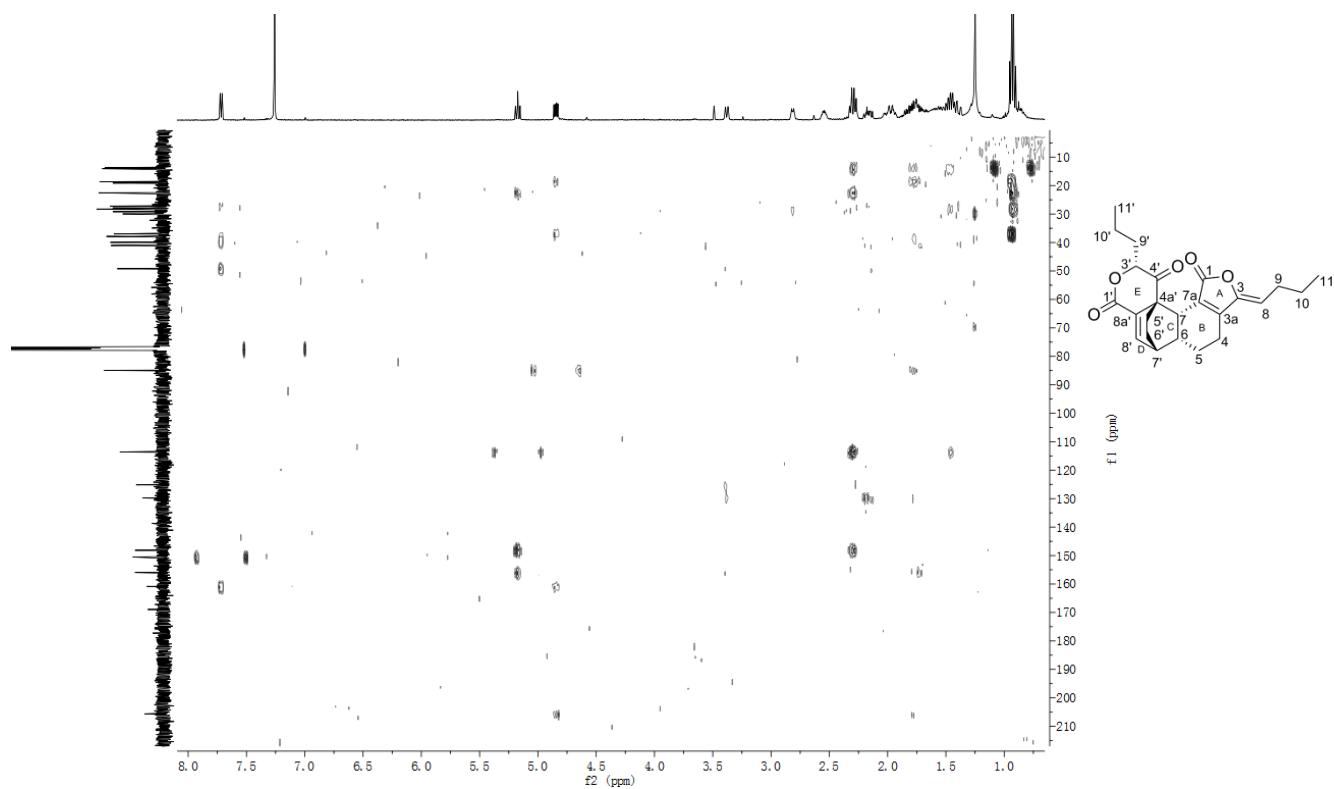


Figure S 34. HMBC spectrum of **2** in CDCl₃

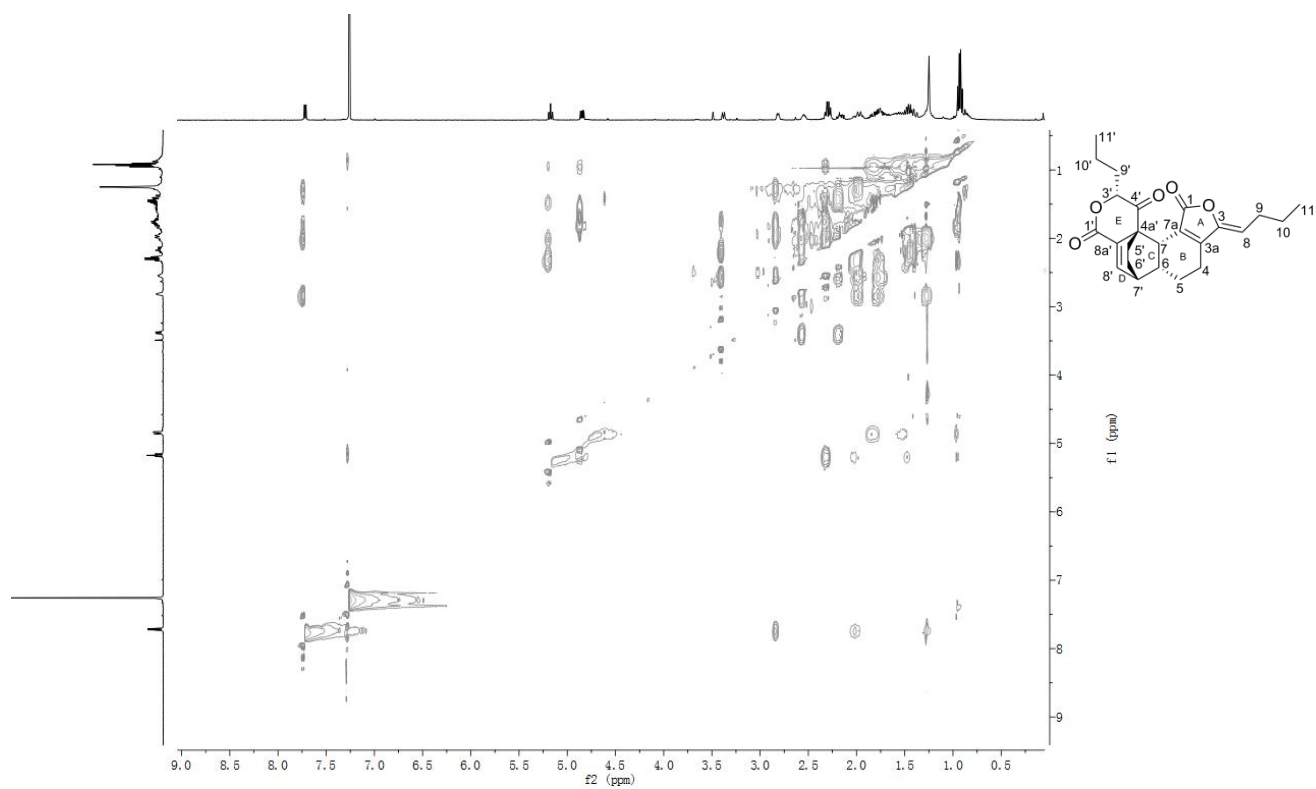


Figure S 35. NOESY spectrum of **2** in CDCl₃

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

66 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

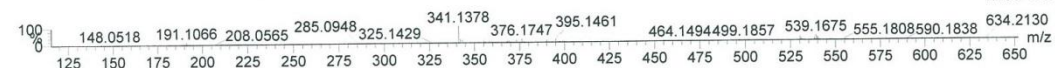
C: 0-100 H: 0-200 O: 0-50

Xevo G2 Q-TOF/YCA166#

20151119-A 13 (0.237) Cm (11:18-(2:8+24:55))

24-Nov-2015

Waters
TOF MS ES+
1.19e+007



Minimum:

Maximum: 5.0 5.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
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341.1378	341.1389	-1.1	-3.2	10.5	564.3	n/a	n/a	C20 H21 O5
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Figure S 36. HRESIMS data of **3**

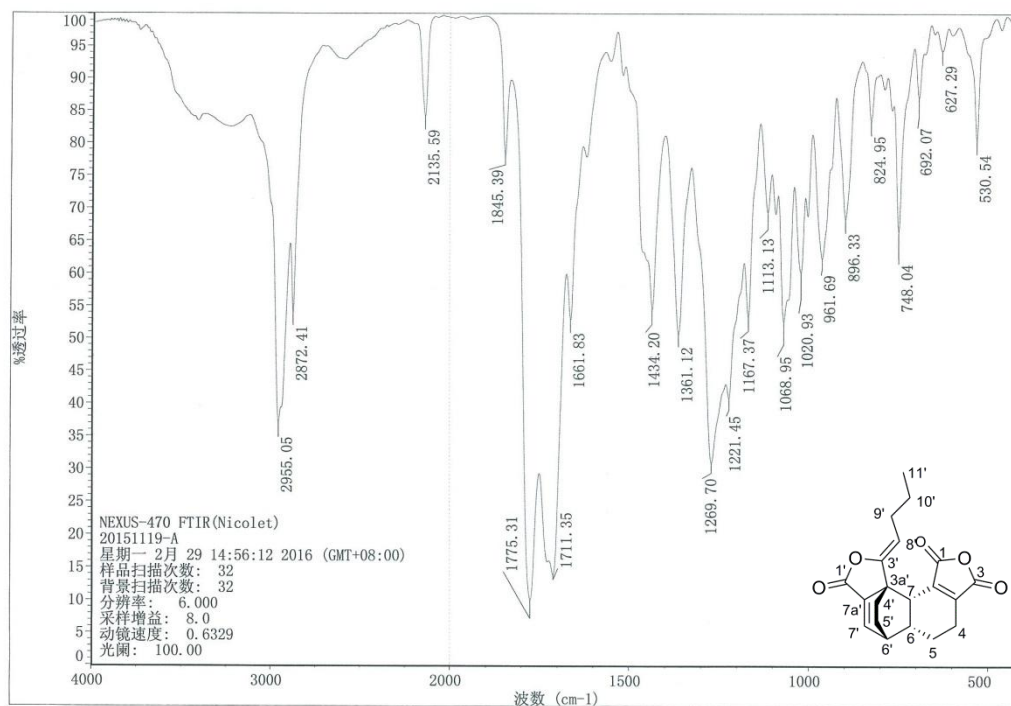


Figure S 37. IR spectrum of **3**

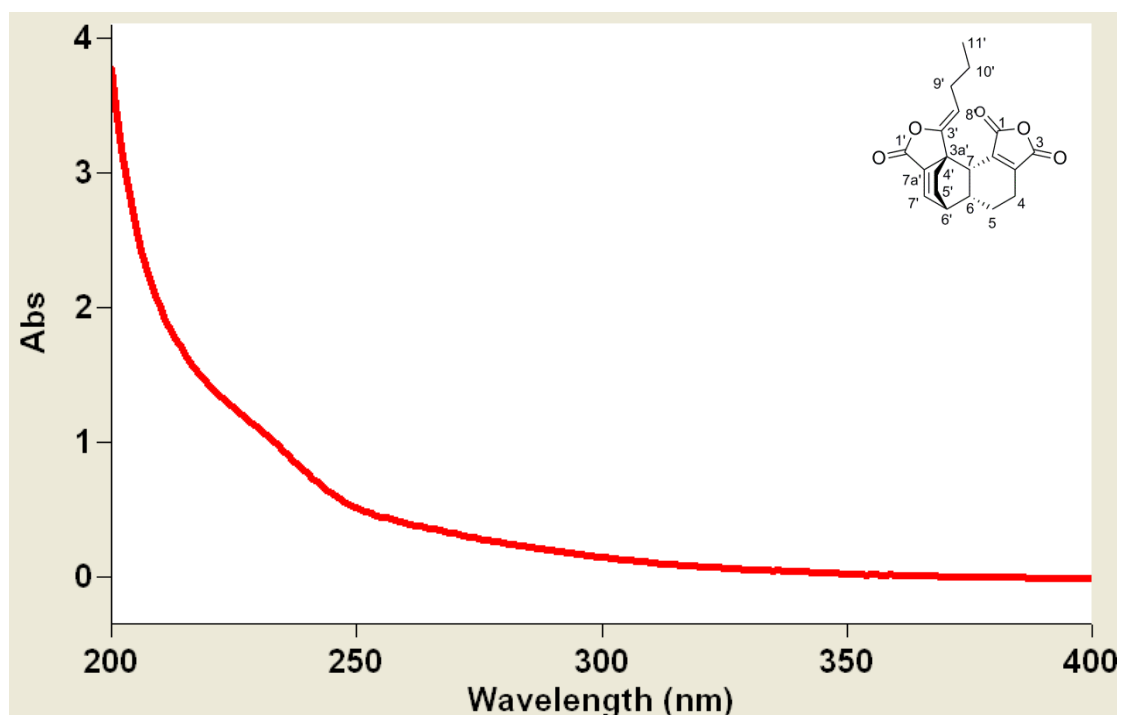


Figure S 38. UV spectrum of **3** in MeOH

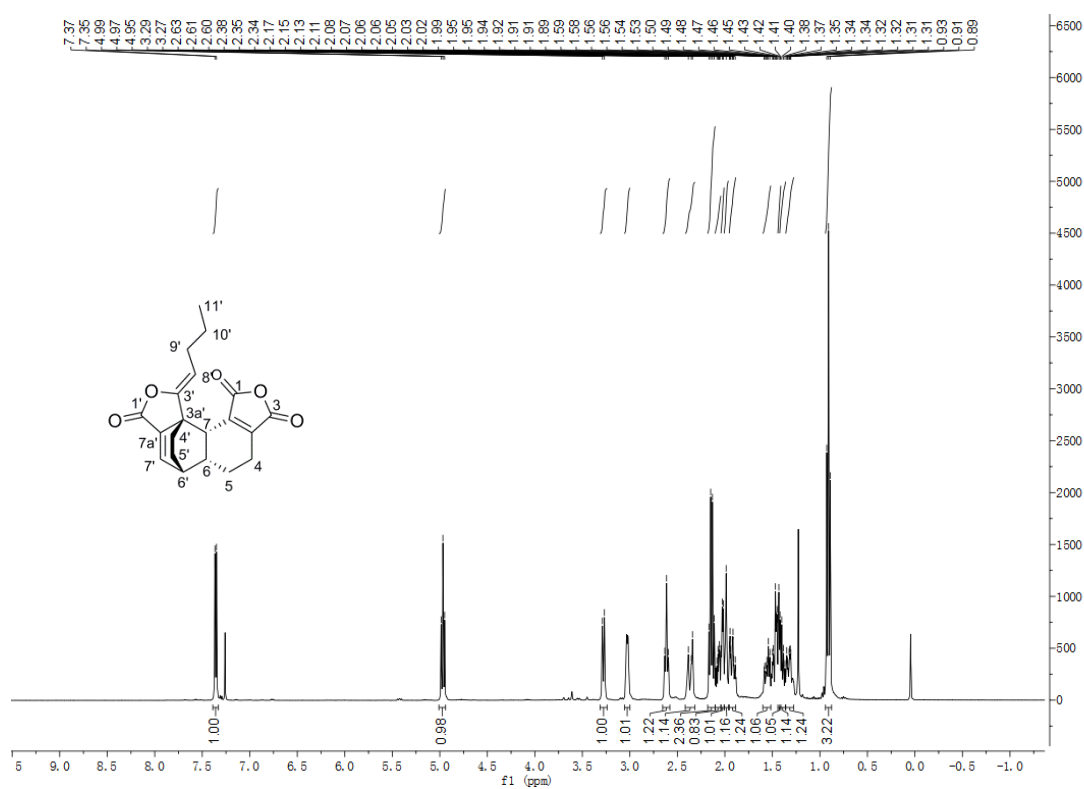


Figure S 39. ¹H NMR spectrum of **3** in CDCl₃

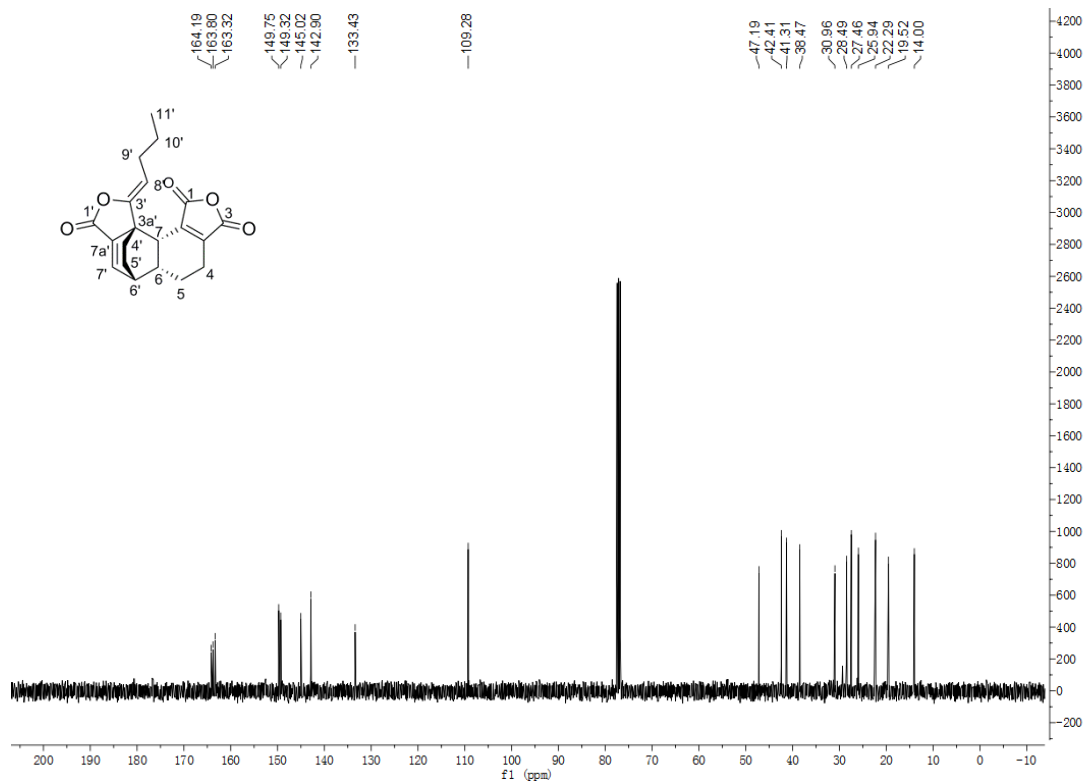


Figure S 40. ^{13}C NMR spectrum of **3** in CDCl_3

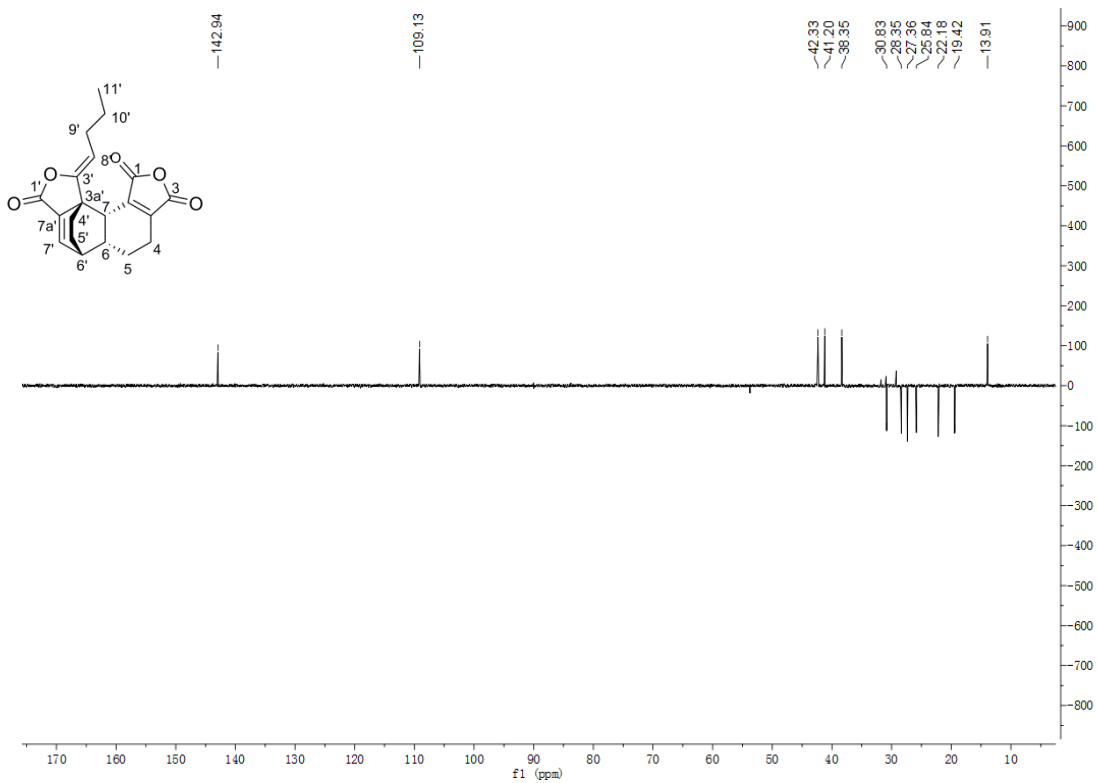


Figure S 41. DEPT spectrum of **3** in CDCl_3

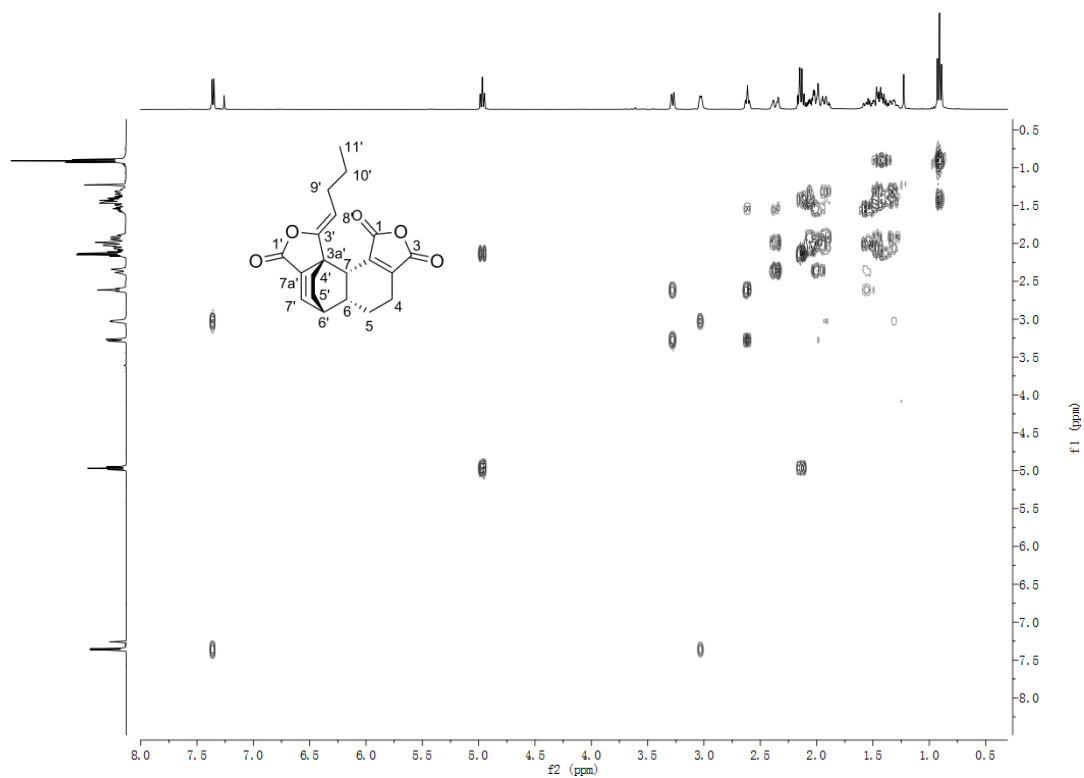


Figure S 42. ^1H - ^1H COSY spectrum of **3** in CDCl_3

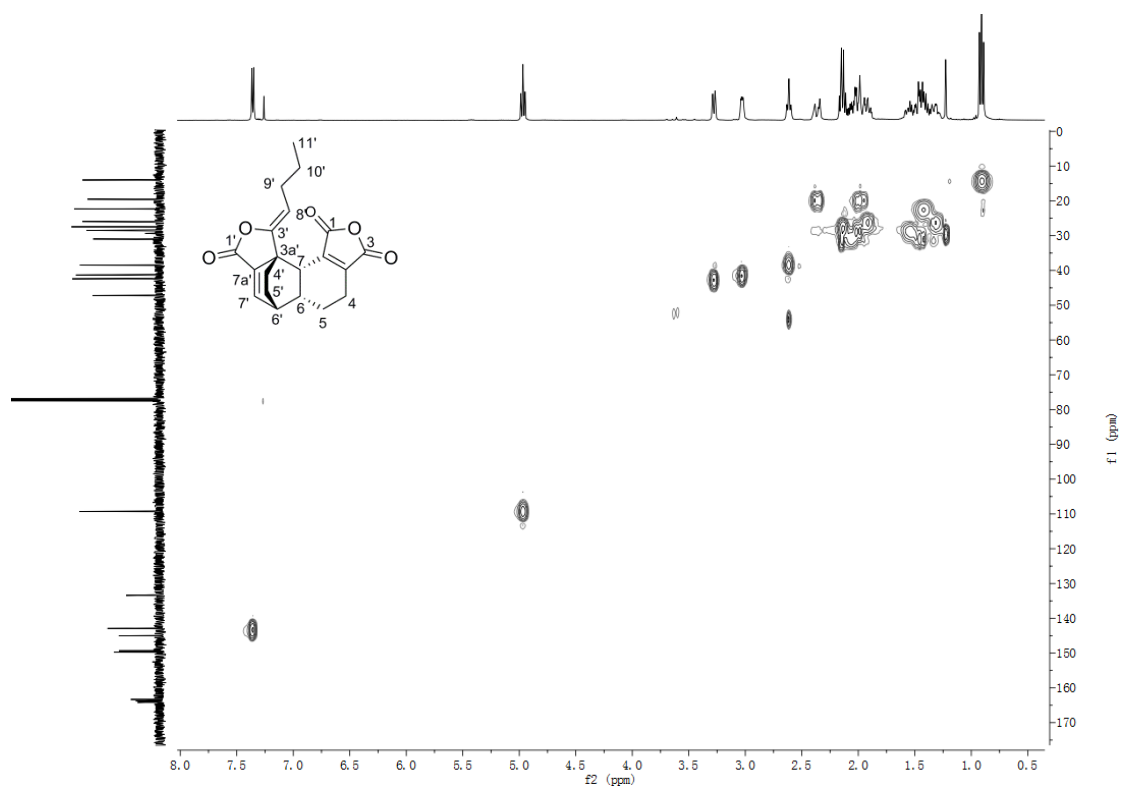


Figure S 43. HSQC spectrum of **3** in CDCl_3

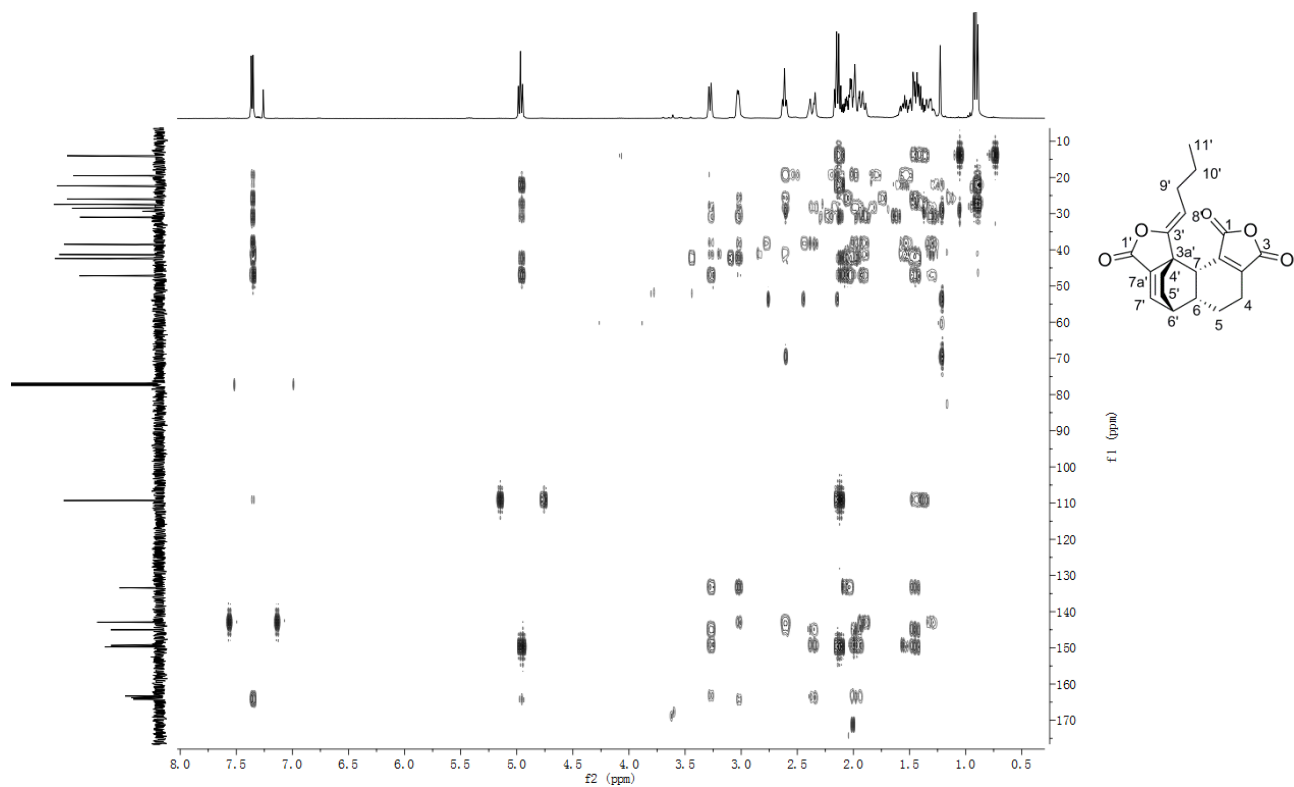


Figure S 44. HMBC spectrum of **3** in CDCl₃

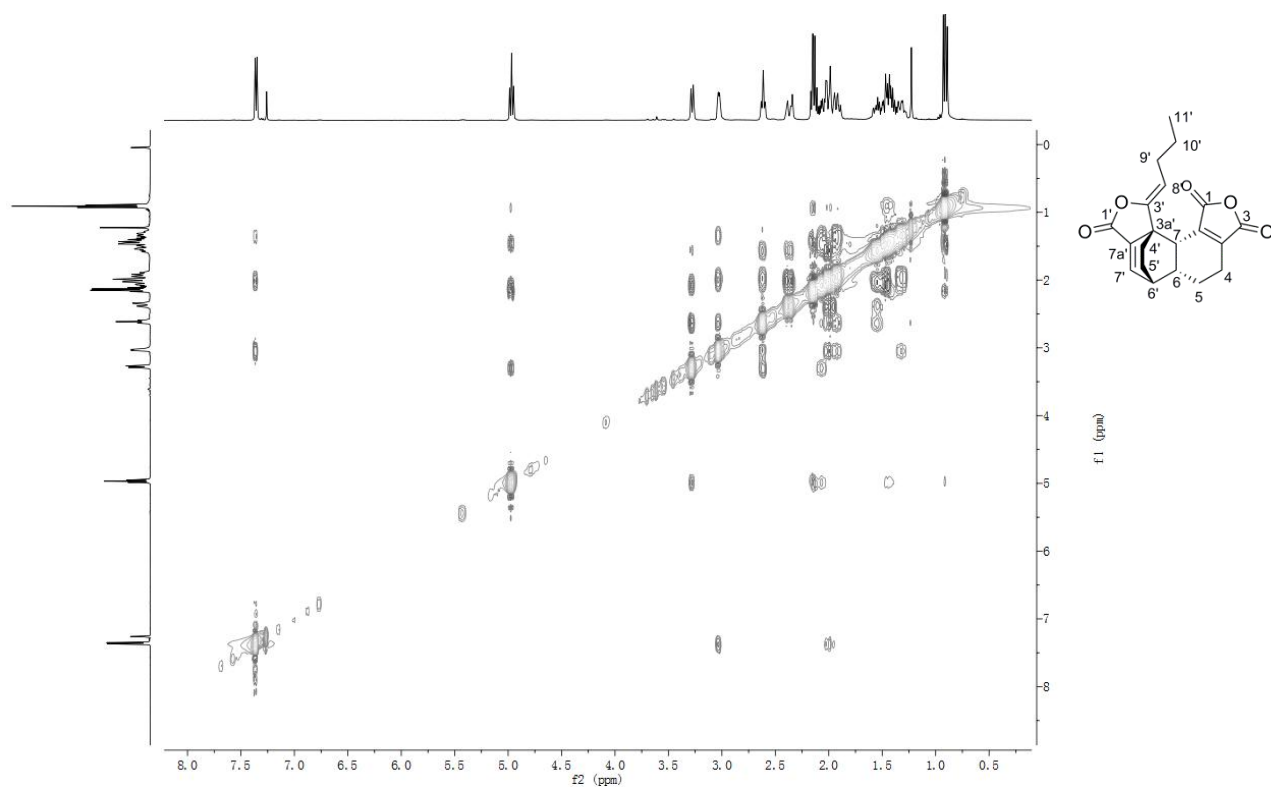


Figure S 45. NOESY spectrum of **3** in CDCl₃

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

194 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

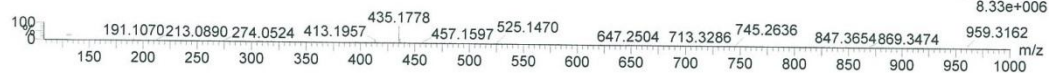
C: 0-100 H: 0-200 O: 0-50 Na: 0-1

Xevo G2 Q-TOF/YCA166#

24-Nov-2015

20151119-C POS 13 (0.237) Cm (11:16-(1:7+22:39))

Waters
 TOF MS ES+
 8.33e+006



Minimum: -1.5
 Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
435.1778	435.1784	-0.6	-1.4	10.5	416.7	n/a	n/a	C ₂₄ H ₂₈ O ₆ Na

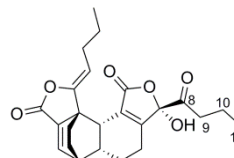


Figure S 46. HRESIMS data of 4

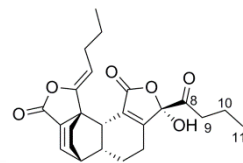
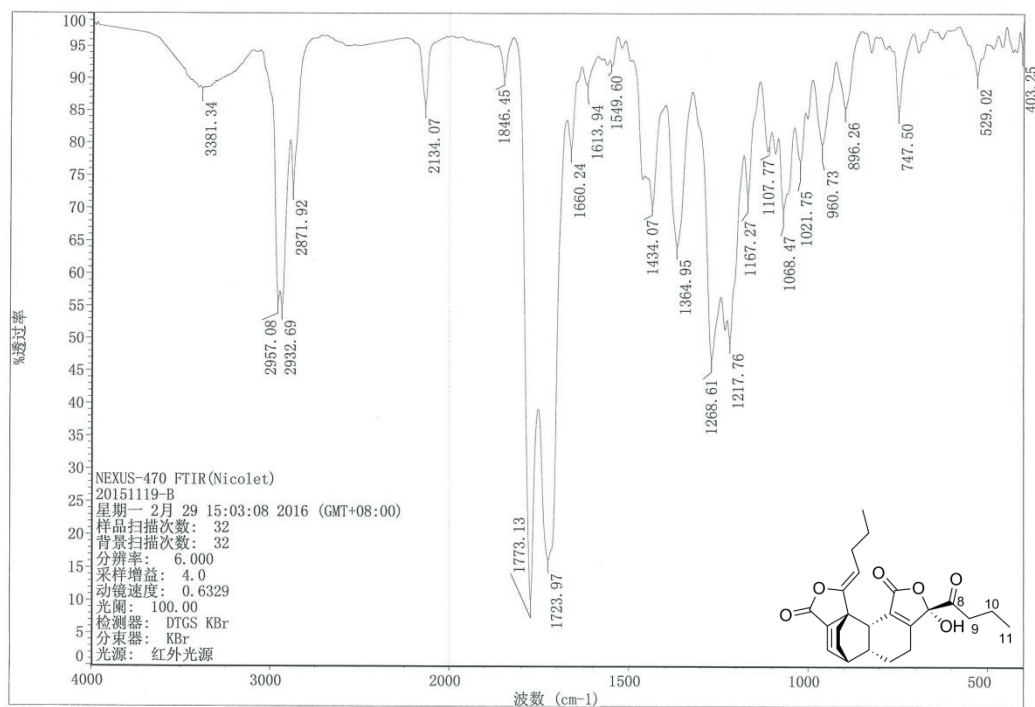
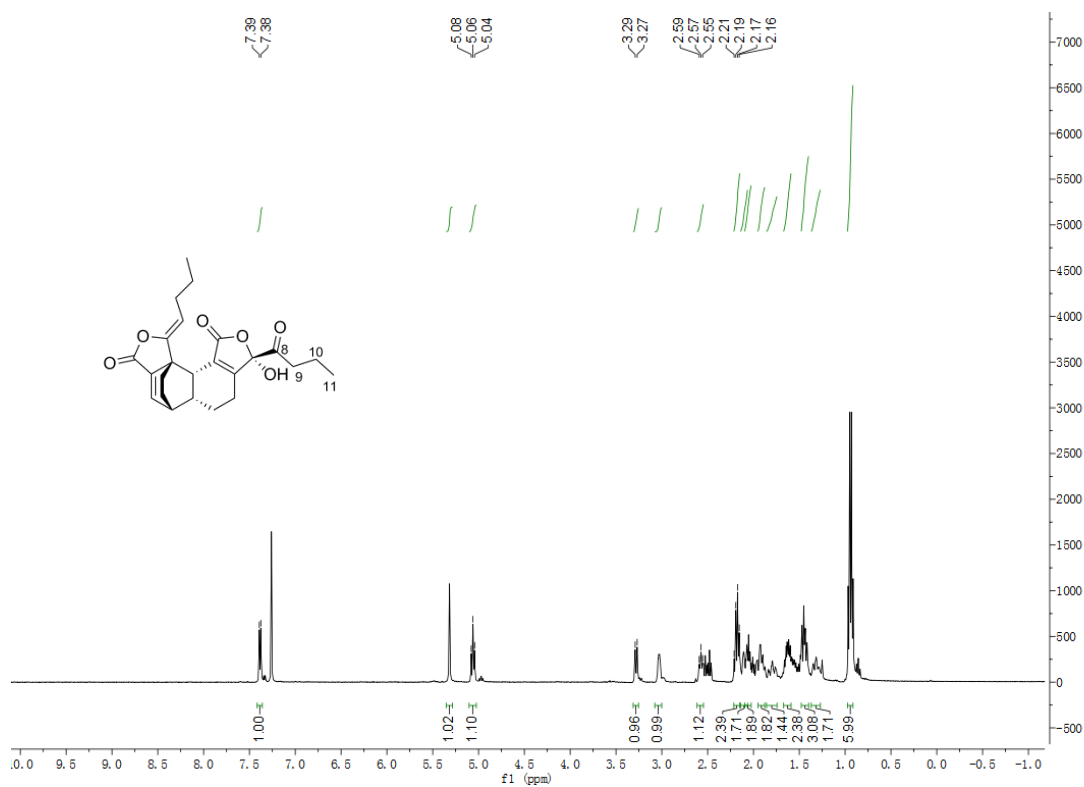
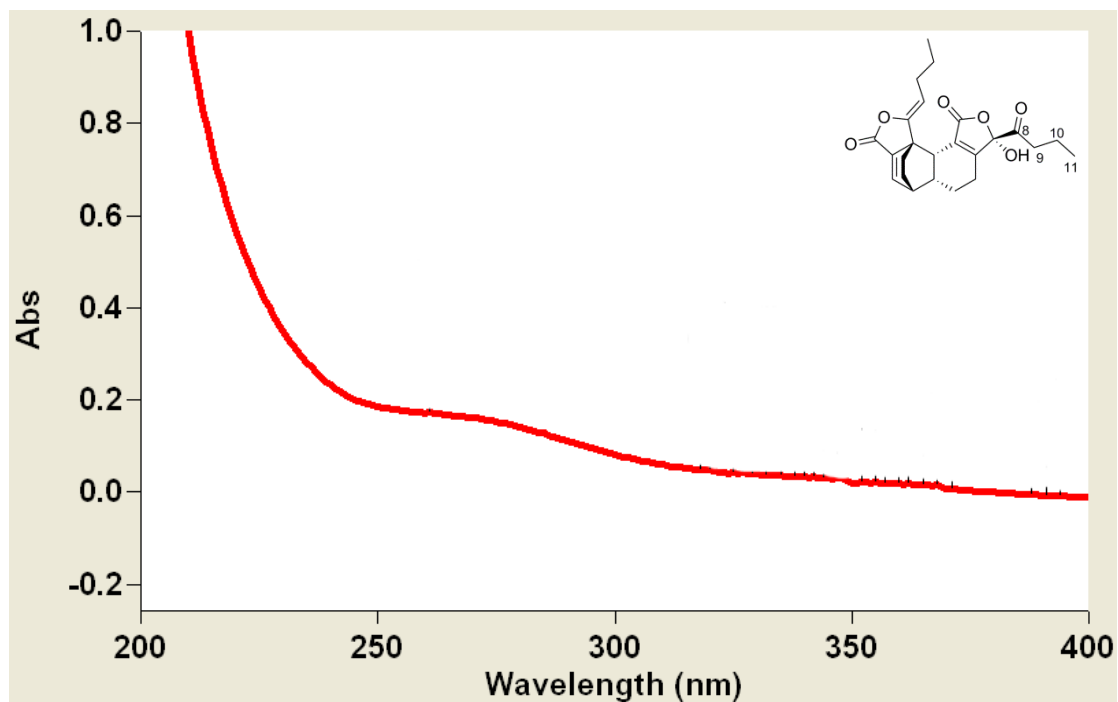


Figure S 47. IR spectrum of 4



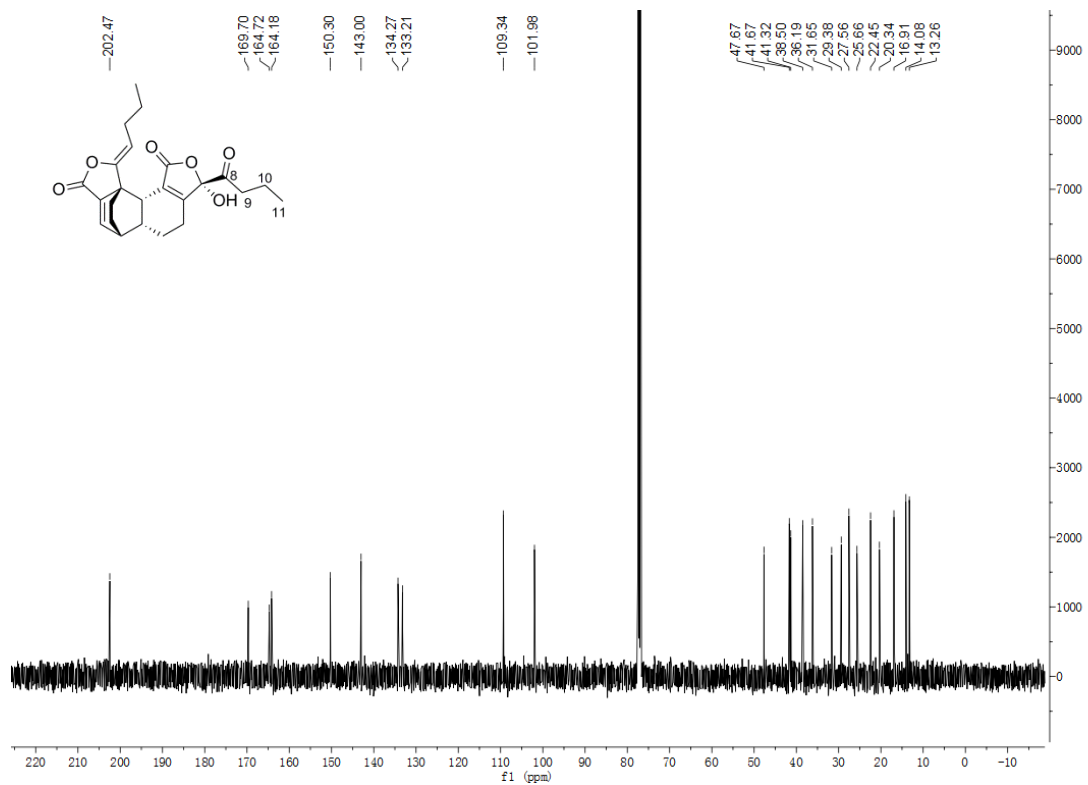


Figure S 50. ^{13}C NMR spectrum of **4** in CDCl_3

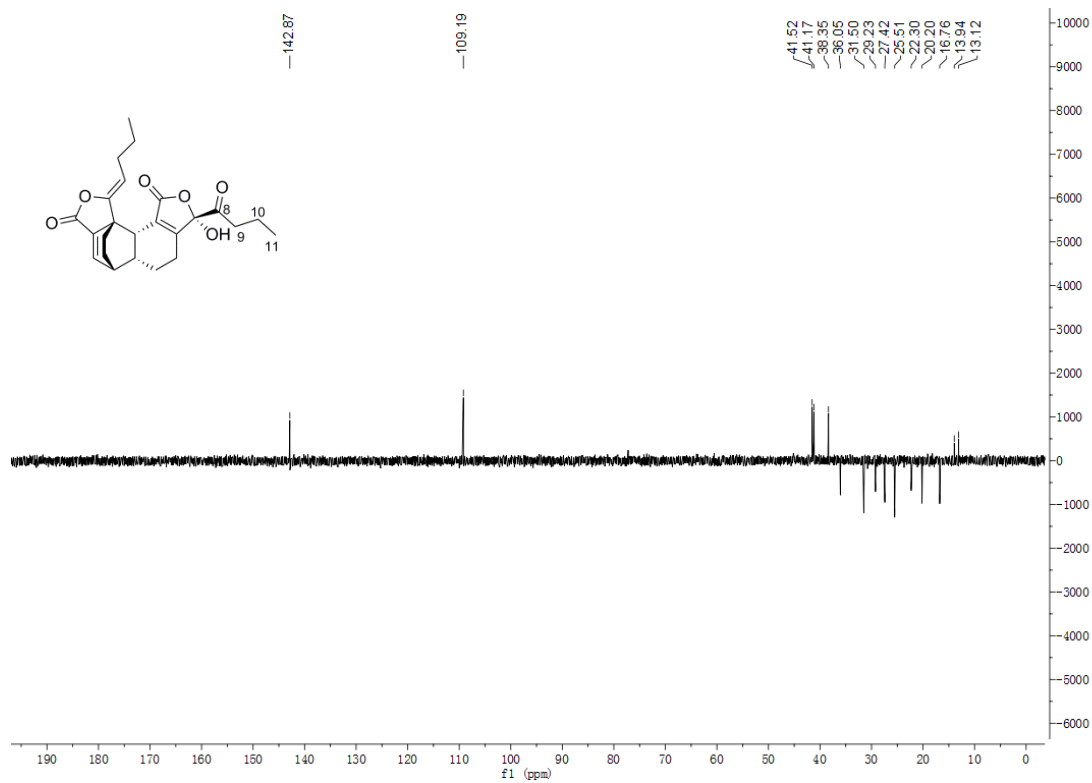


Figure S 51. DEPT spectrum of **4** in CDCl_3

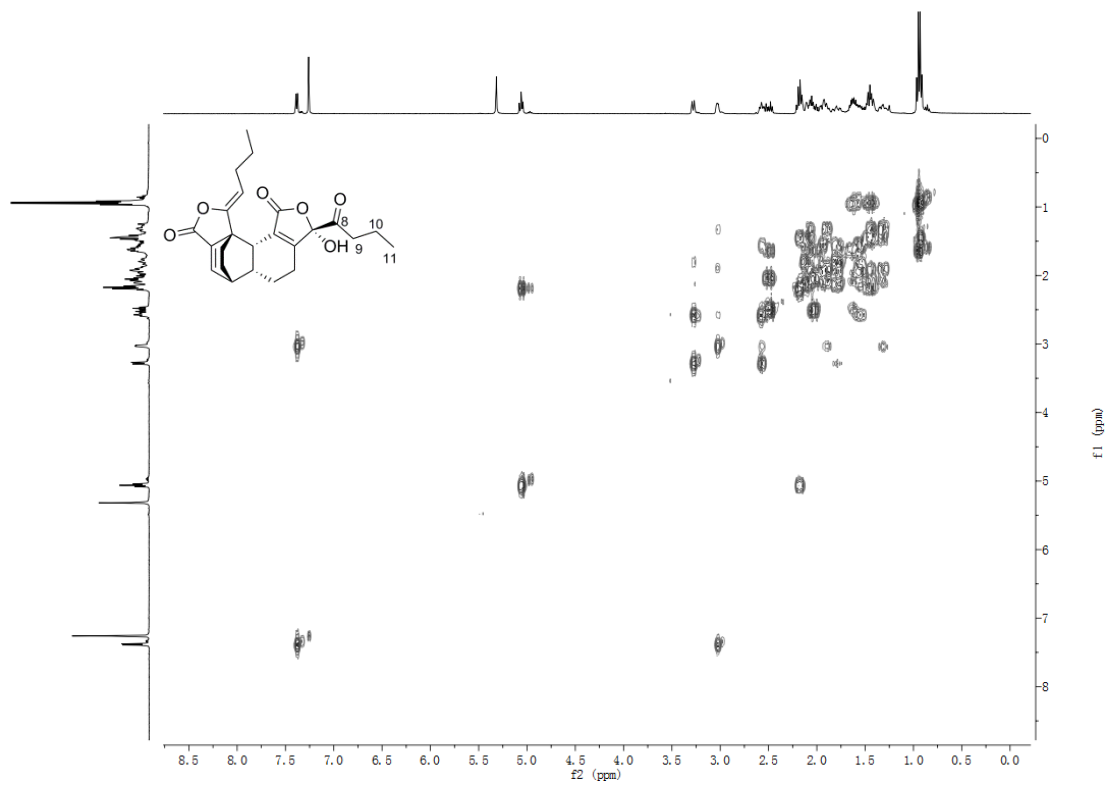


Figure S 52. ^1H - ^1H COSY spectrum of **4** in CDCl_3

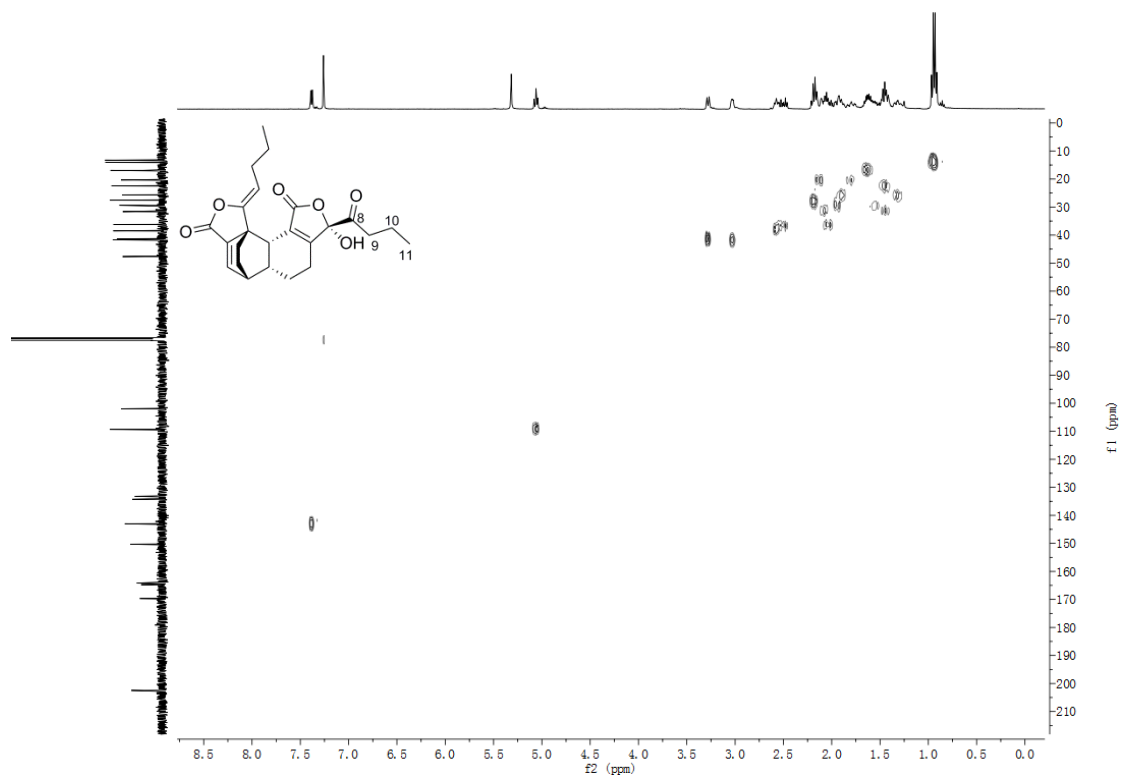


Figure S 53. HSQC spectrum of **4** in CDCl_3

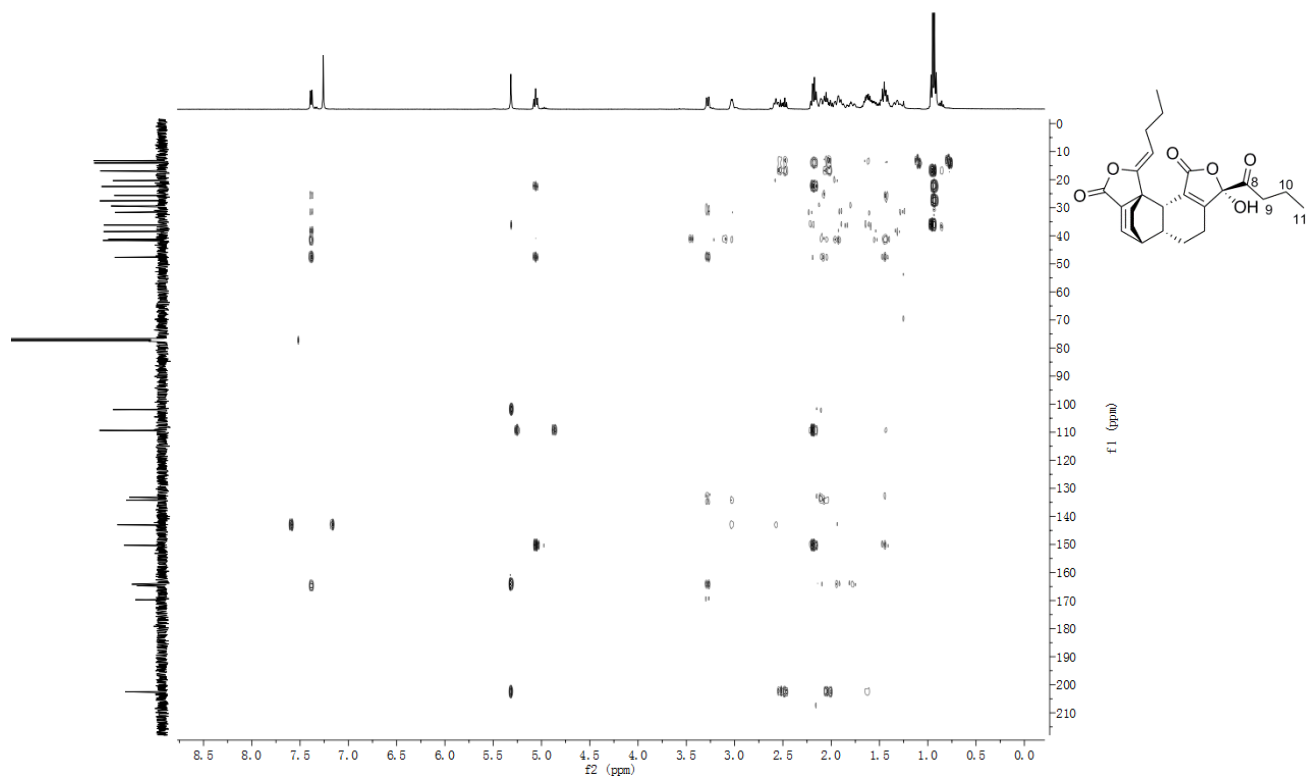


Figure S 54. HMBC spectrum of **4** in CDCl₃

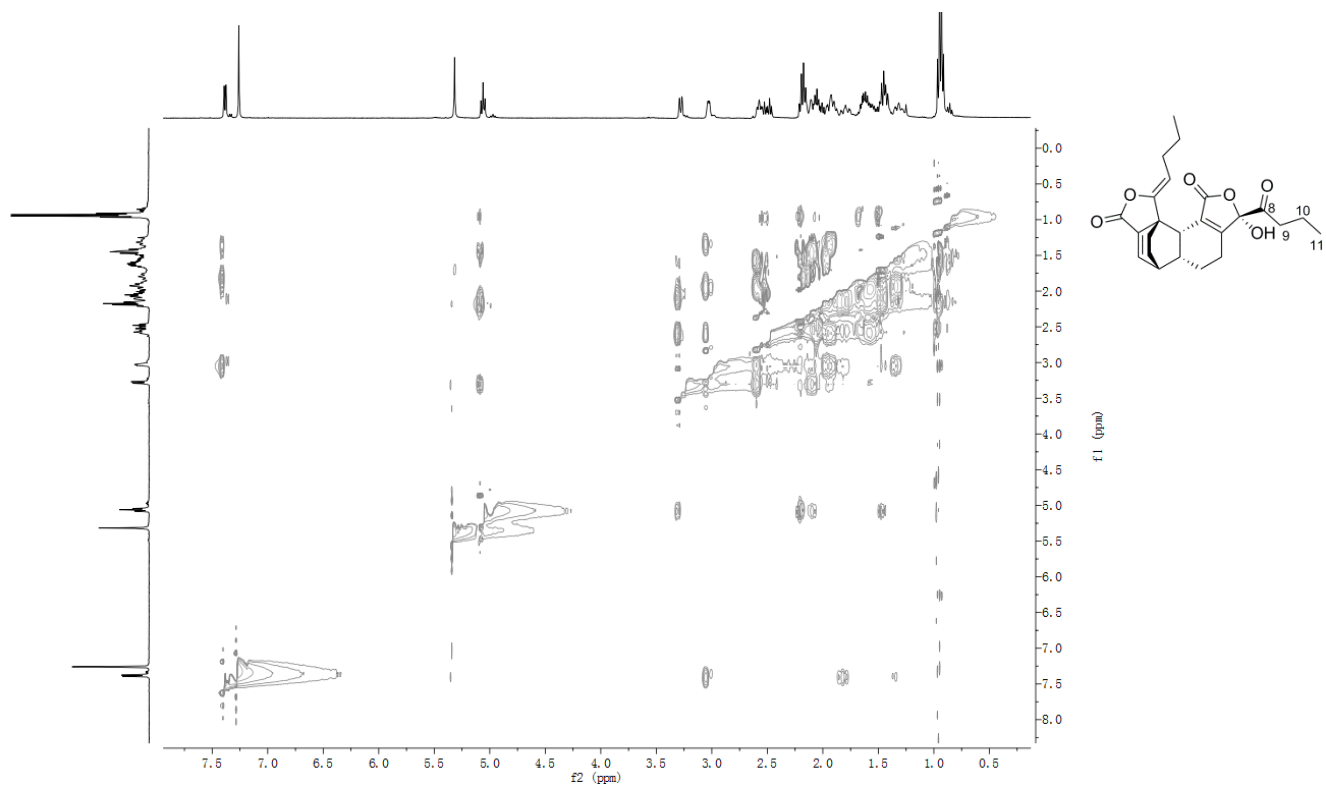


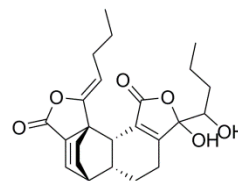
Figure S 55. NOESY spectrum of **4** in CDCl₃

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions

178 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

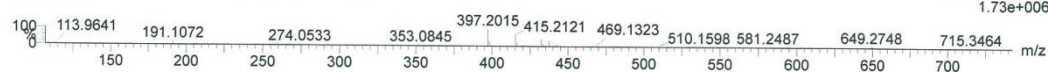
C: 0-100 H: 0-200 O: 0-50 Na: 0-1

Xevo G2 Q-TOF/YCA166#

21-Dec-2015

20151123-A HRMS 12 (0.233) Cm (10:15-(2:8+21:54))

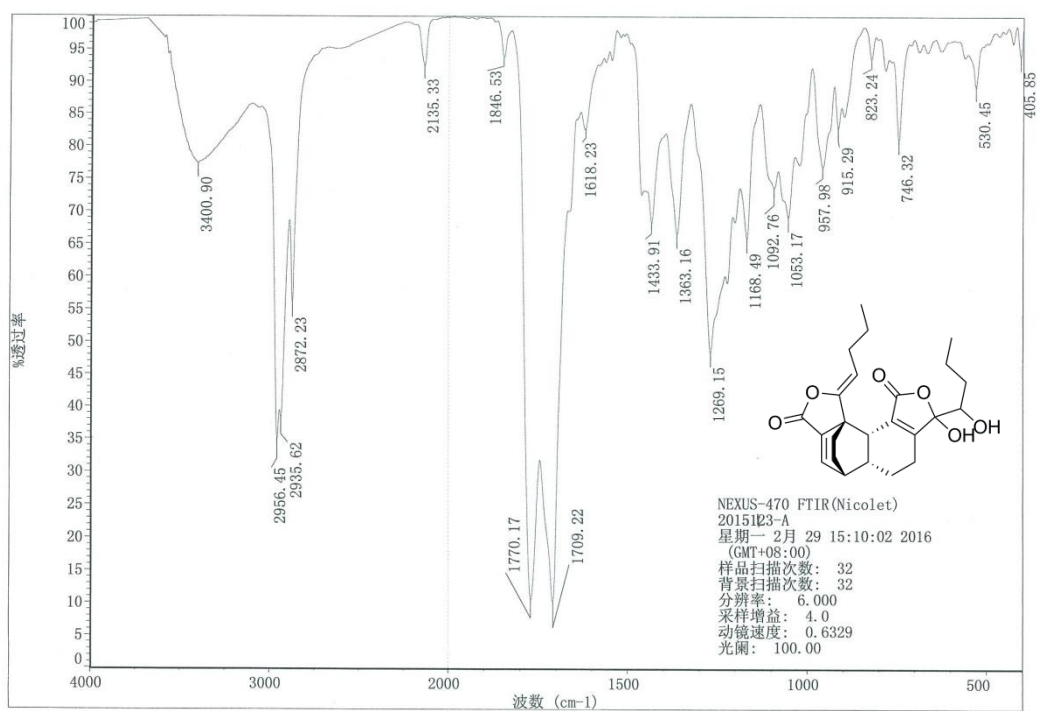
Waters
 1: TOF MS ES+
 1.73e+006



Minimum: -1.5
 Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
415.2121	415.2121	0.0	0.0	9.5	390.1	n/a	n/a	C24 H31 O6

Figure S 56. HRESIMS data of **5**



NEXUS-470 FTIR(Nicolet)
 2015123-A
 星期一 2月 29 15:10:02 2016
 (GMT+08:00)
 样品扫描次数: 32
 背景扫描次数: 32
 分辨率: 6.000
 采样增益: 4.0
 动镜速度: 0.6329
 光阑: 100.00

Figure S 57. IR spectrum of **5**

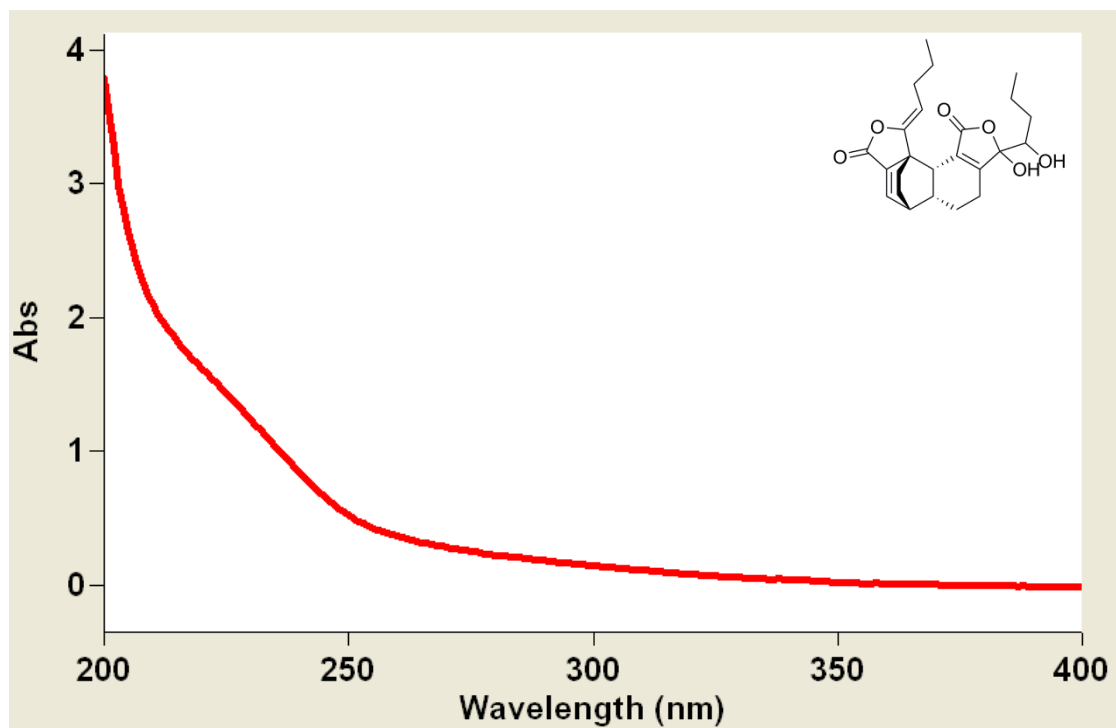


Figure S 58. UV spectrum of **5** in MeOH

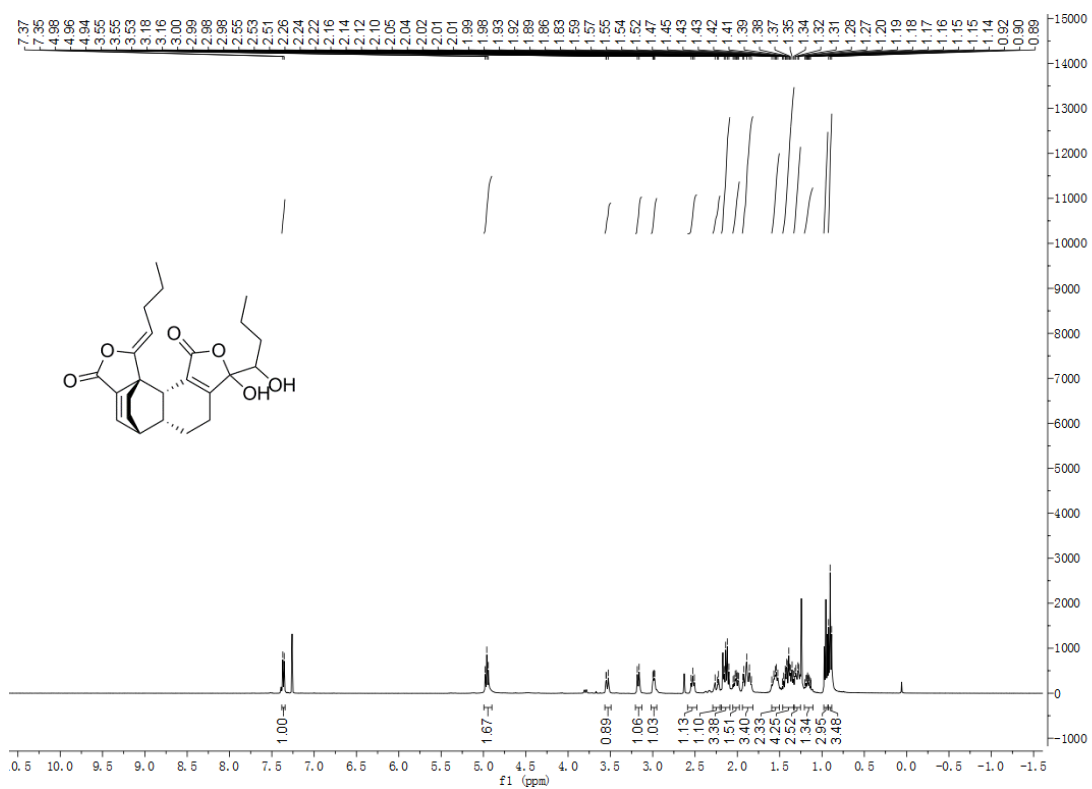


Figure S 59. ¹H NMR spectrum of **5** in CDCl₃

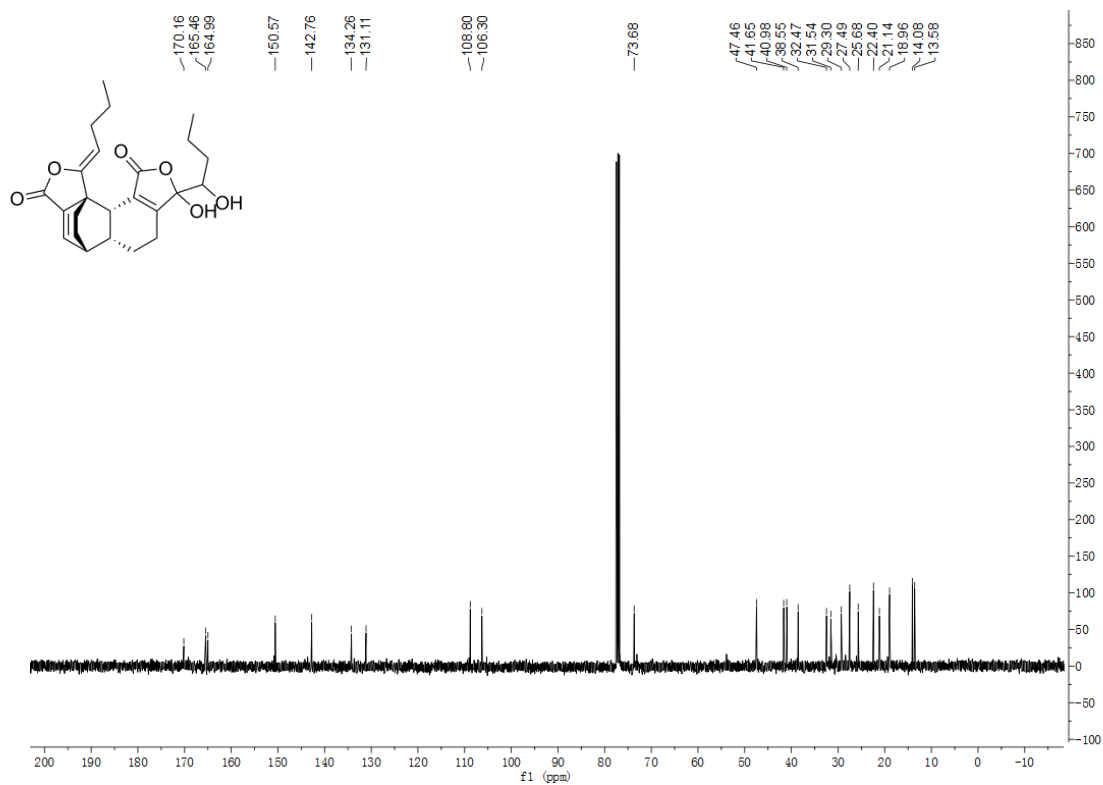


Figure S 60. ^{13}C NMR spectrum of **5** in CDCl₃

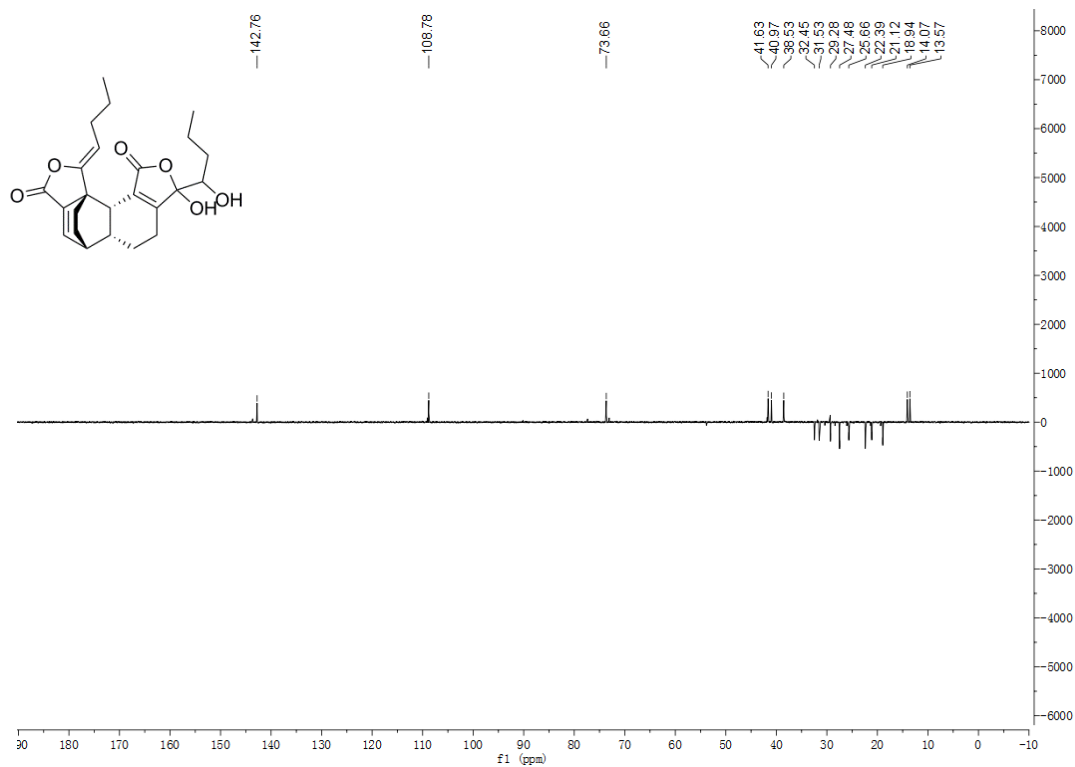
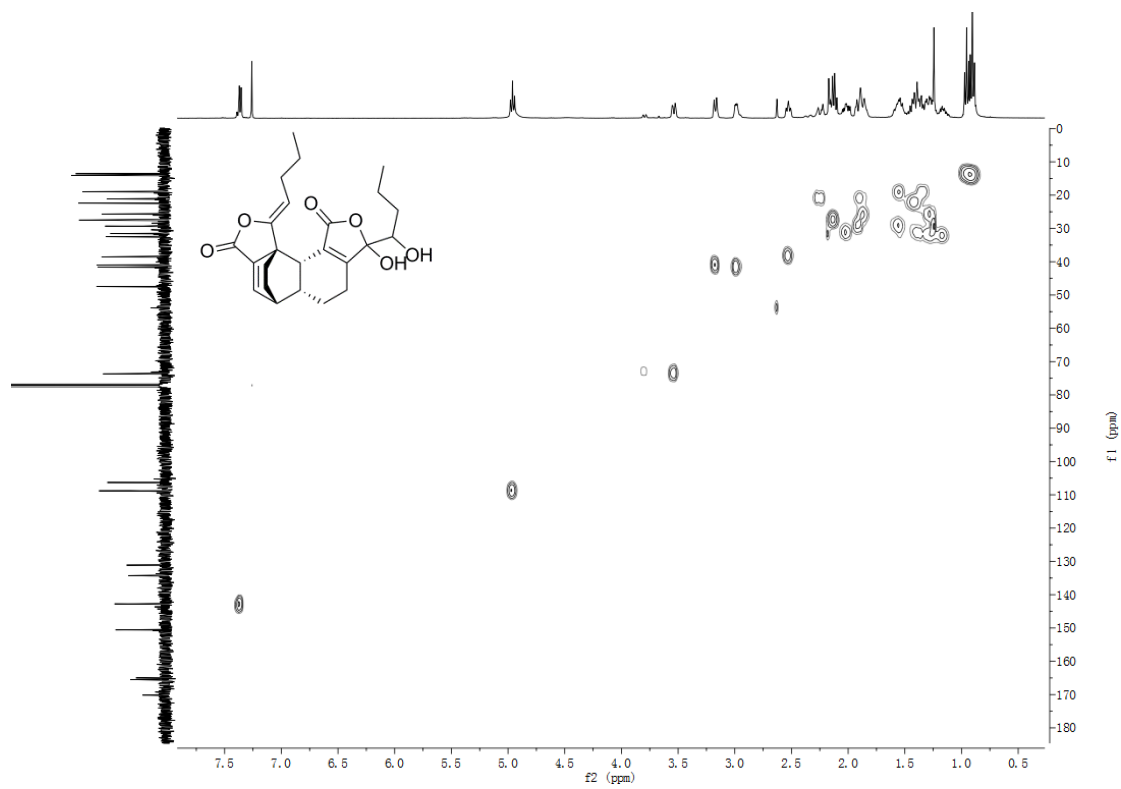
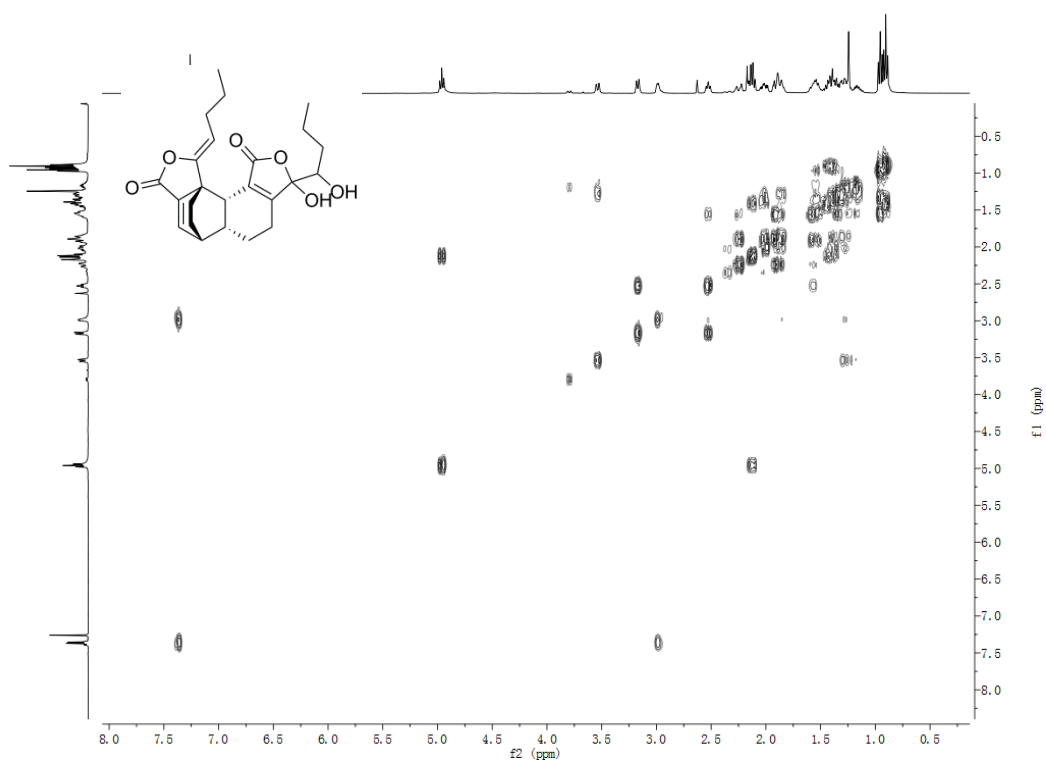


Figure S 61. DEPT spectrum of **5** in CDCl₃



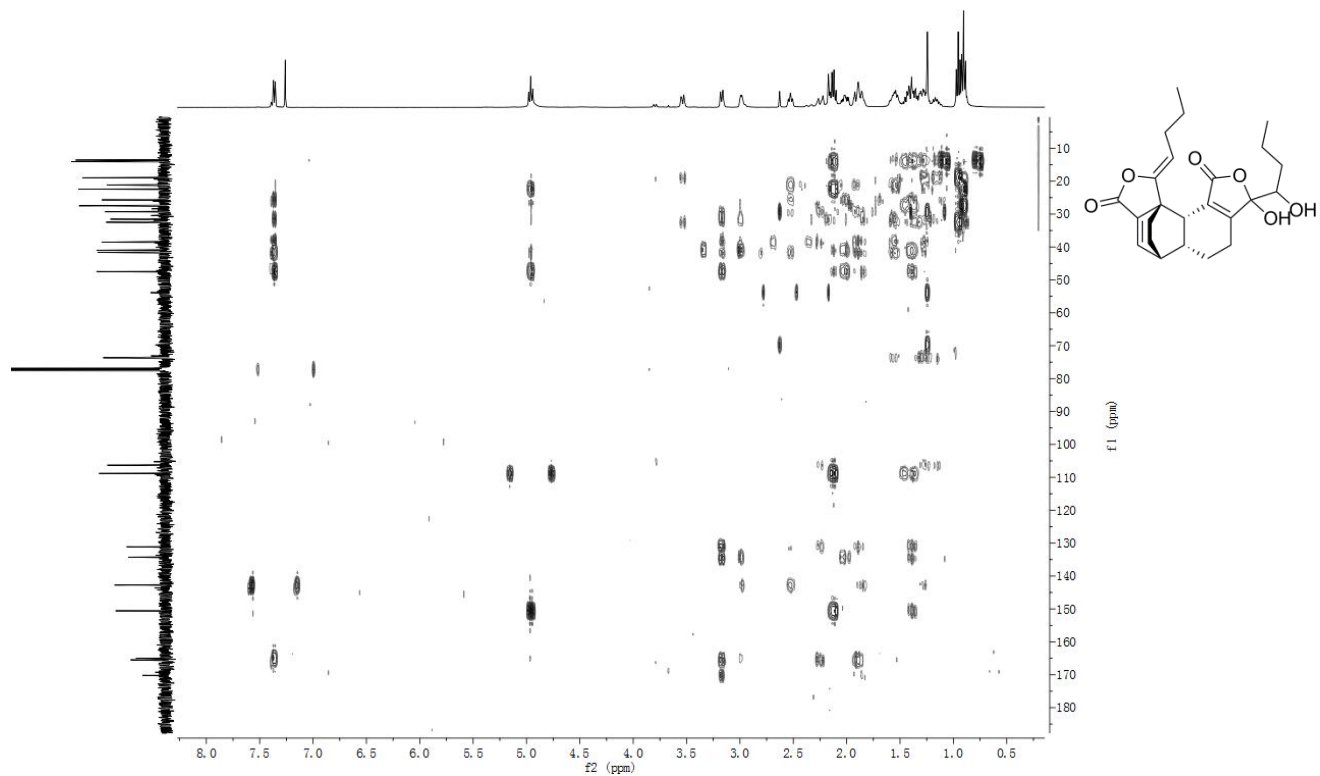


Figure S 64. HMBC spectrum of **5** in CDCl₃

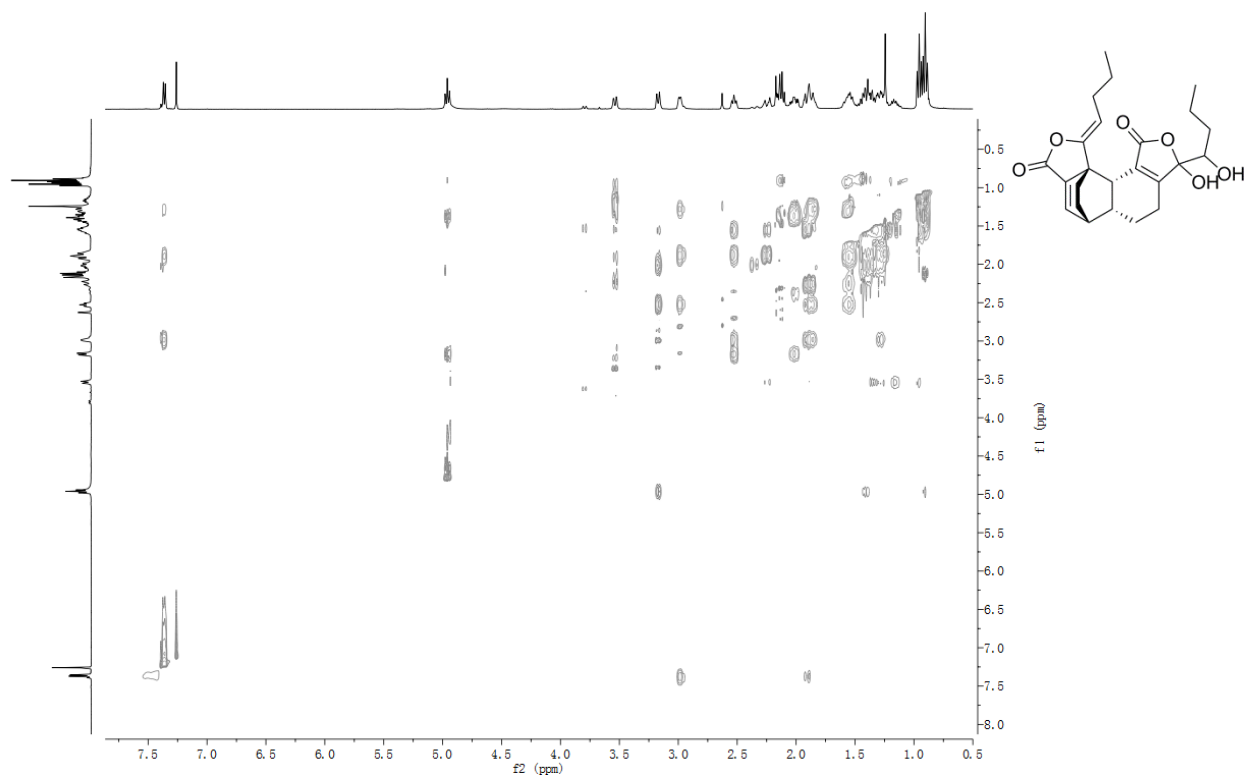


Figure S 65. NOESY spectrum of **5** in CDCl₃