

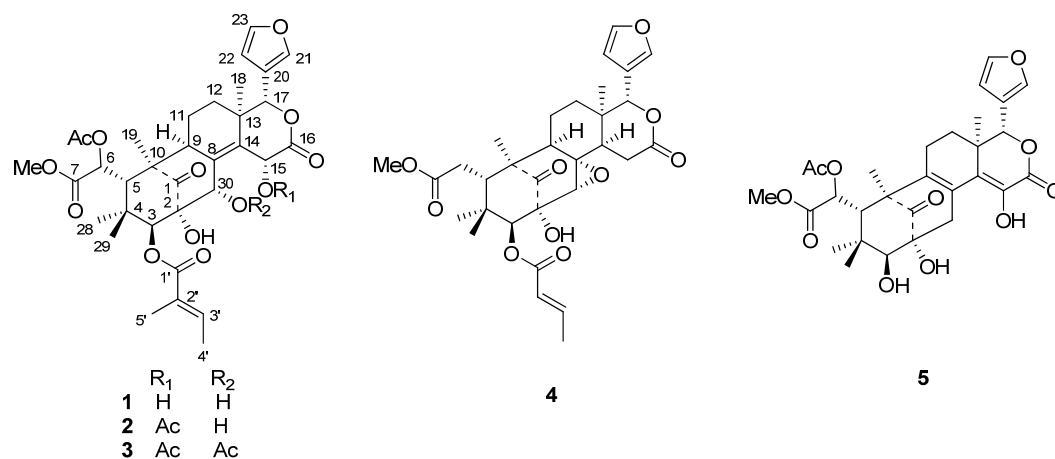
Five new mexicanolide type limonoids from *Heynea trijuga*

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Received 24 May 2012; Accepted 4 June 2012



Structures of compounds **1–5**

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Fig. 5S HMBC NMR spectrum of compound **1** in CDCl_3

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Fig. 29S ^1H -NMR spectrum of compound **4** in CDCl_3

Fig. 30S ^{13}C -NMR spectrum of compound **4** in CDCl_3

Fig. 31S HSQC NMR spectrum of compound **4** in CDCl_3

Fig. 32S HMBC NMR spectrum of compound **4** in CDCl_3

Fig. 33S ^1H - ^1H COSY NMR spectrum of compound **4** in CDCl_3

Fig. 34S ROESY NMR spectrum of compound **4** in CDCl_3

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Fig. 36S UV spectrum of compound **4** in CH_3OH

Fig. 37S ESIMS spectrum of compound **5**

Fig. 38S ^1H -NMR spectrum of compound **5** in CDCl_3

Fig. 39S ^{13}C -NMR spectrum of compound **5** in CDCl_3

Fig. 40S HSQC NMR spectrum of compound **5** in CDCl_3

Fig. 41S HMBC NMR spectrum of compound **5** in CDCl_3

Fig. 42S ^1H - ^1H COSY NMR spectrum of compound **5** in CDCl_3

Fig. 43S ROESY NMR spectrum of compound **5** in CDCl_3

Fig. 44S IR spectrum of compound **5**

Fig. 1S ESIMS spectrum of compound **1**

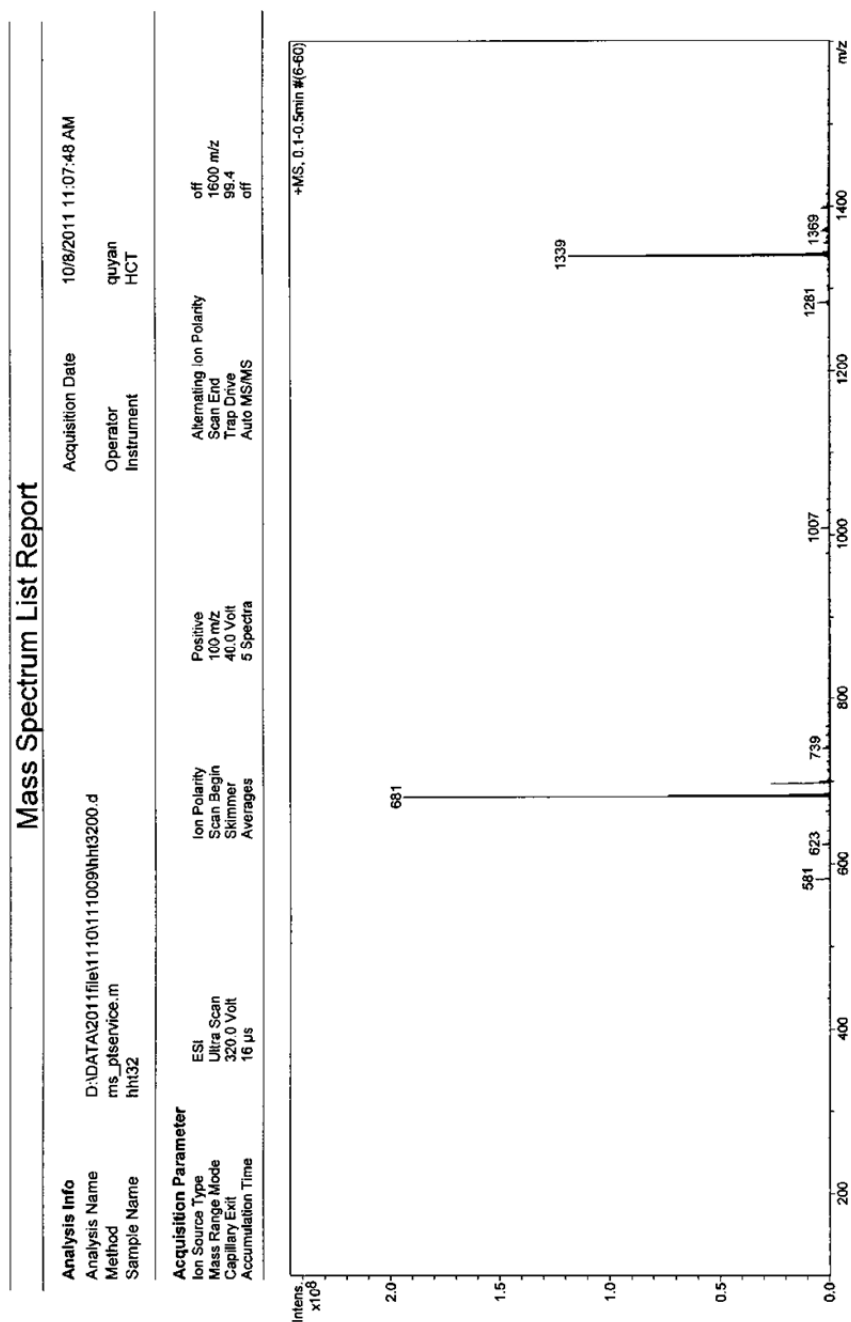


Fig. 2S ^1H -NMR spectrum of compound **1** in CDCl_3

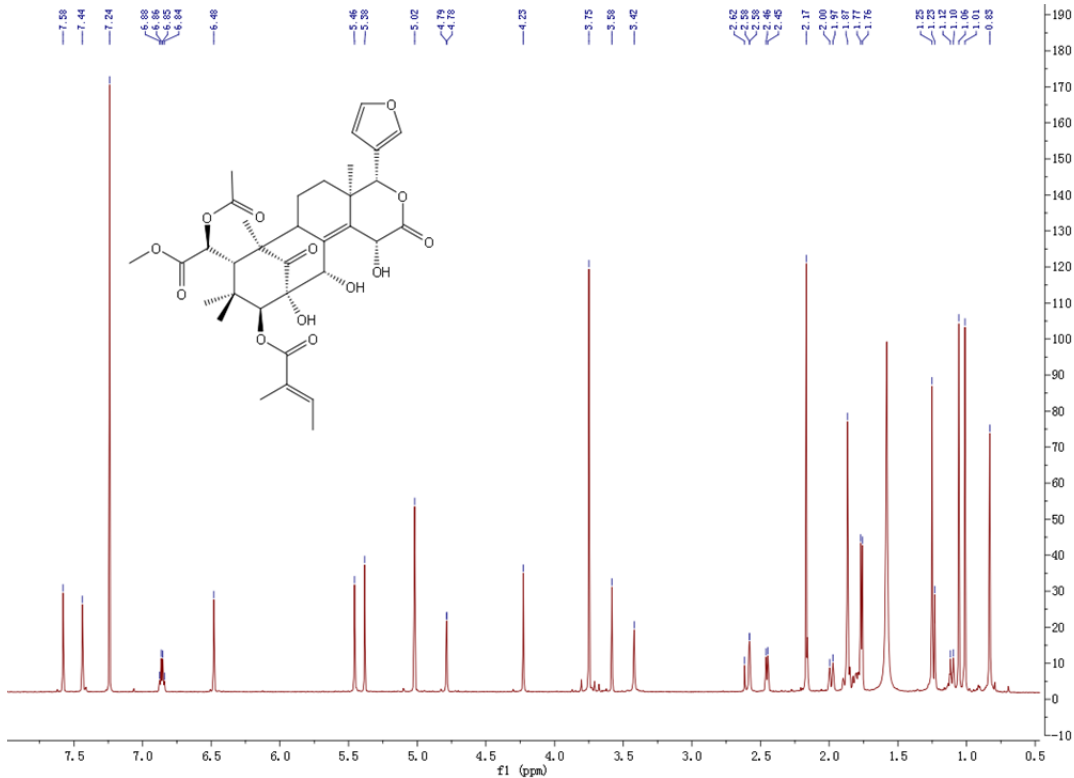


Fig. 3S ^{13}C -NMR spectrum of compound **1** in CDCl_3

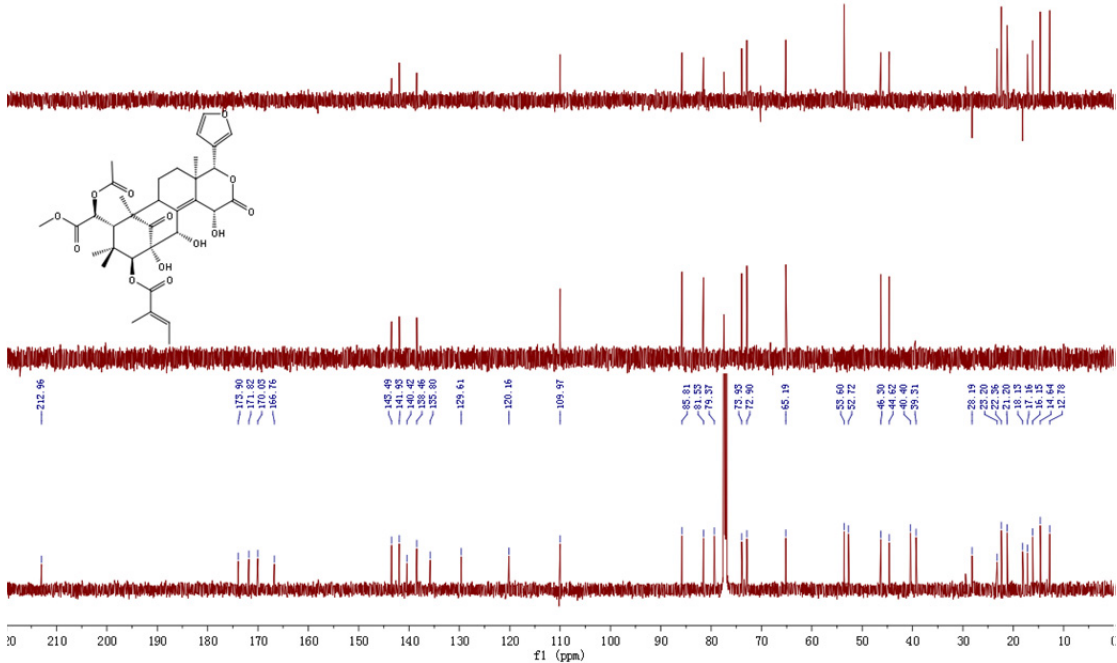


Fig. 4S HSQC NMR spectrum of compound **1** in CDCl₃

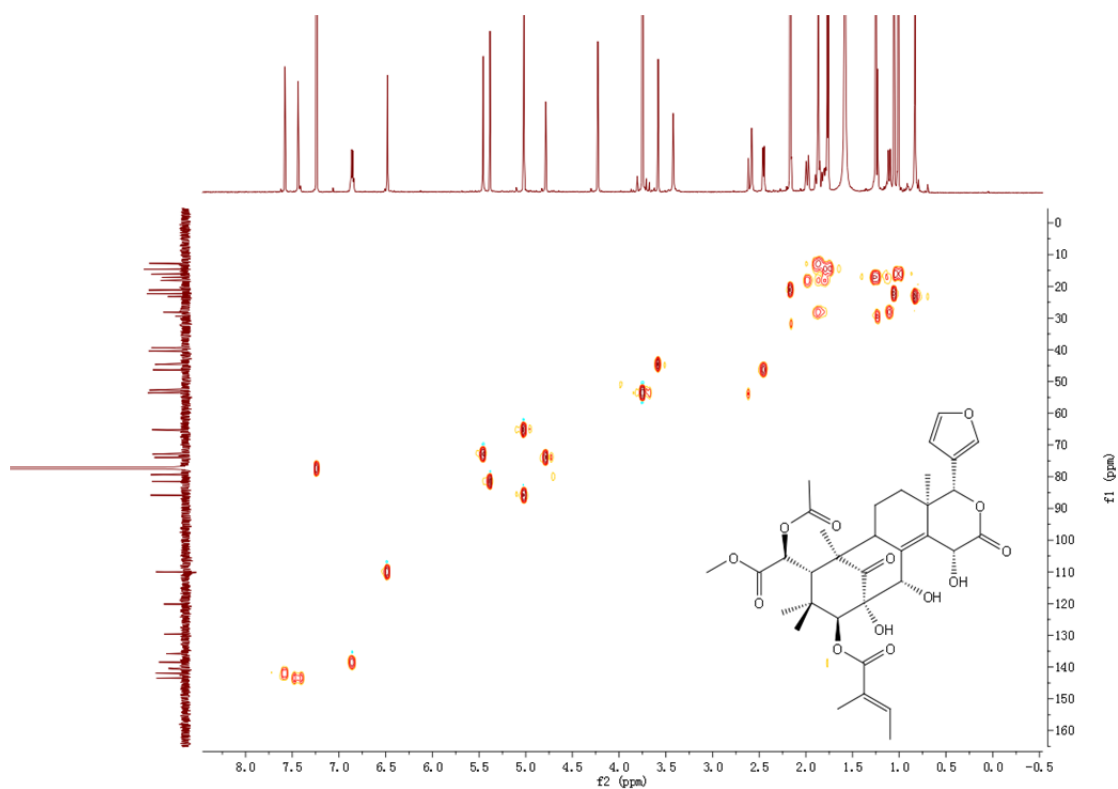


Fig. 5S HMBC NMR spectrum of compound **1** in CDCl₃

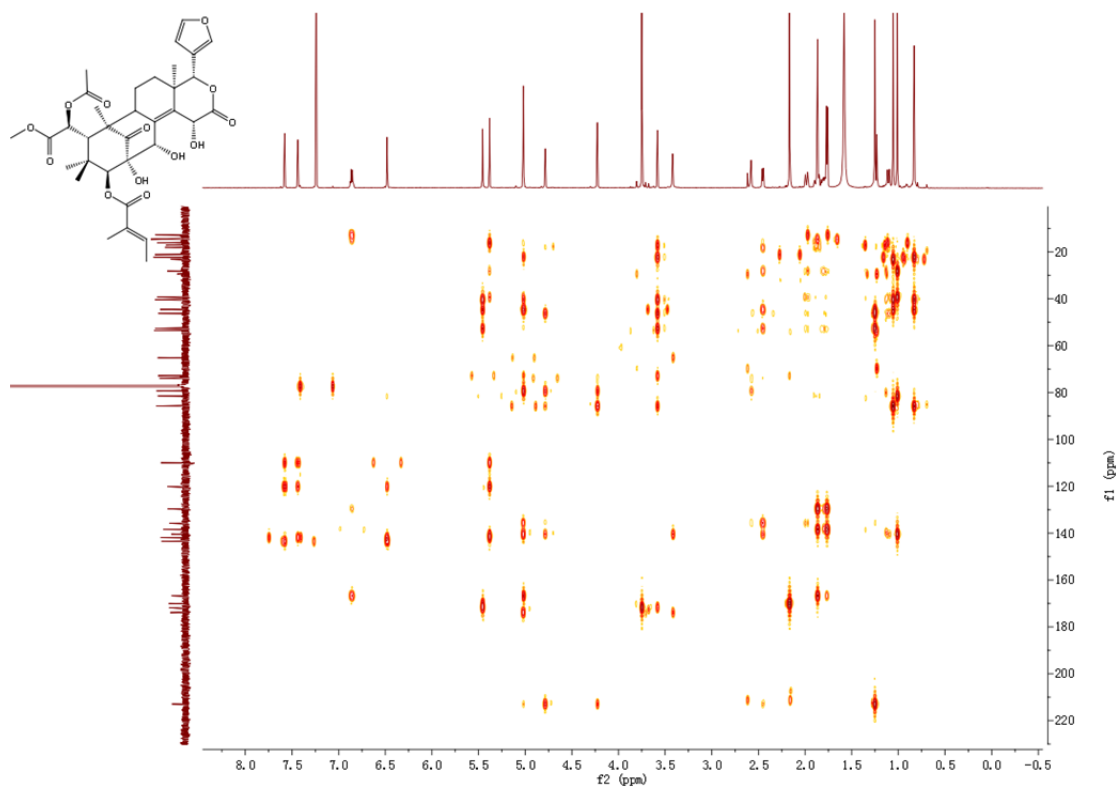


Fig. 6S ¹H-¹H COSY NMR spectrum of compound **1** in CDCl₃

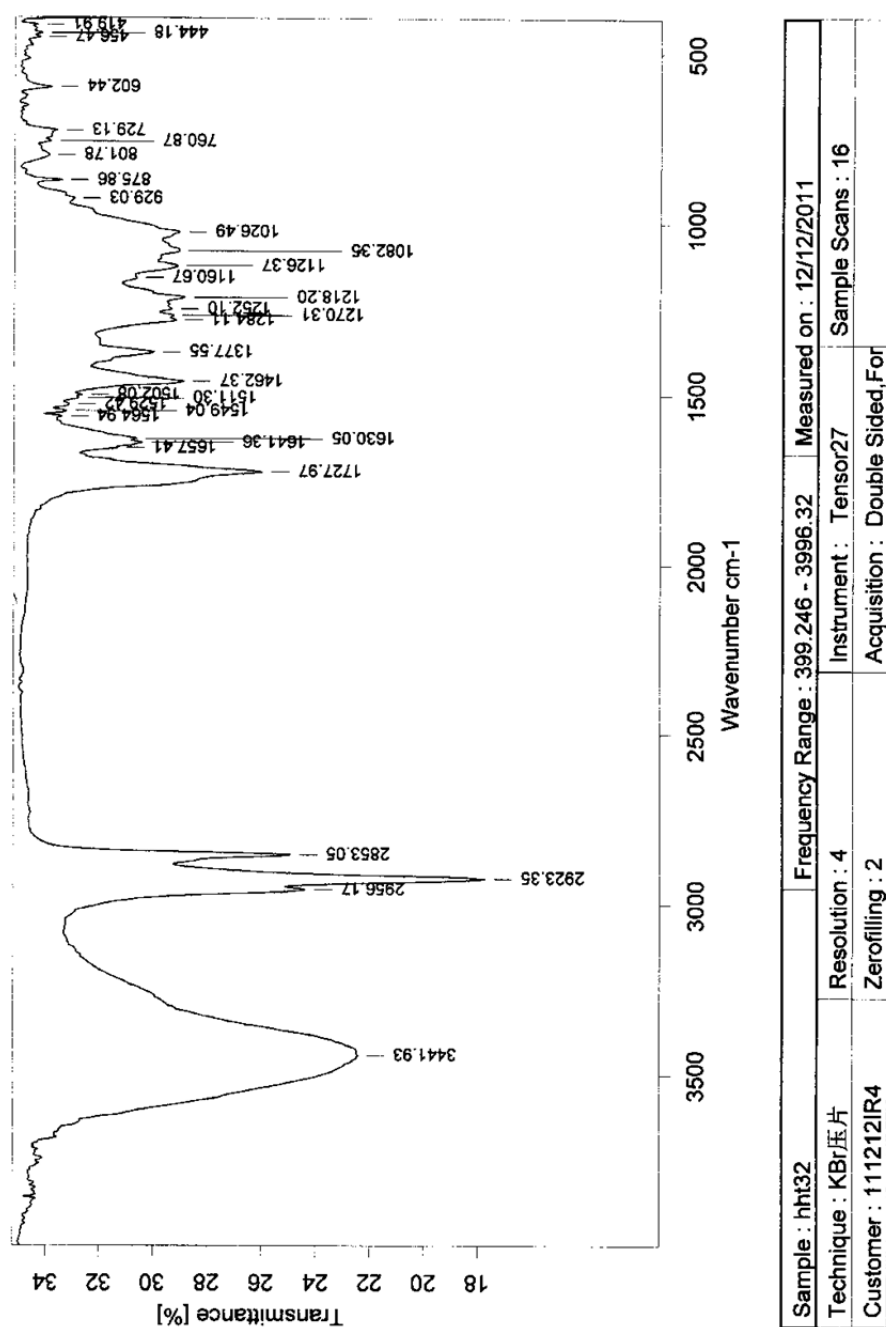
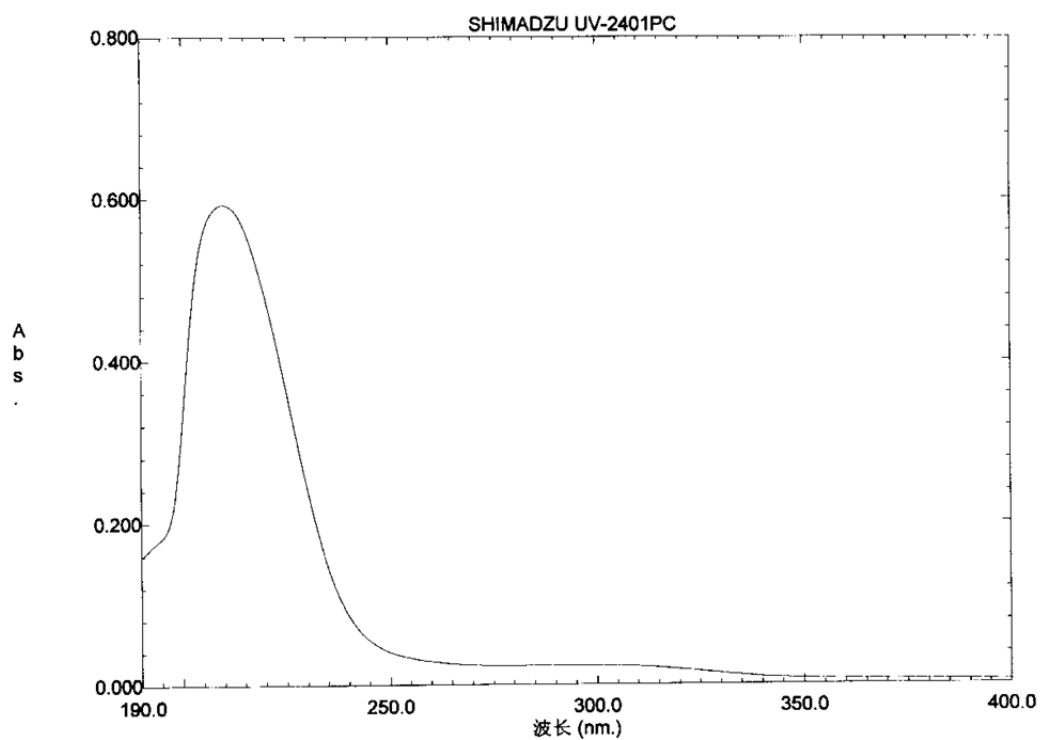


Fig. 9S UV spectrum of compound 1 in CH₃OH



文件名: 12053102
样品名称: HHT32

12053102
样品浓度: 0.0202毫克/毫升
溶剂: 甲醇

创建于: 14:01 12-05-31
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	290.20	0.0236
2	210.00	0.5921

Fig. 10S HREIMS spectrum of compound **2**

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
 Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
 32 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)

Elements Used:

C: 0-200 H: 0-400 O: 12-15

hhf50

12.40.27 24-May-2012

Voltage E1+

KIB
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 700.2729

Autospec Premier
 P7776
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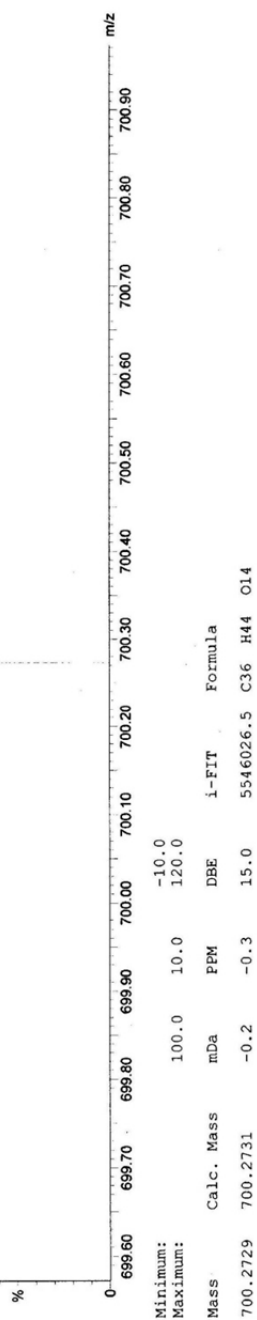


Fig. 11S ¹H-NMR spectrum of compound **2** in CDCl₃

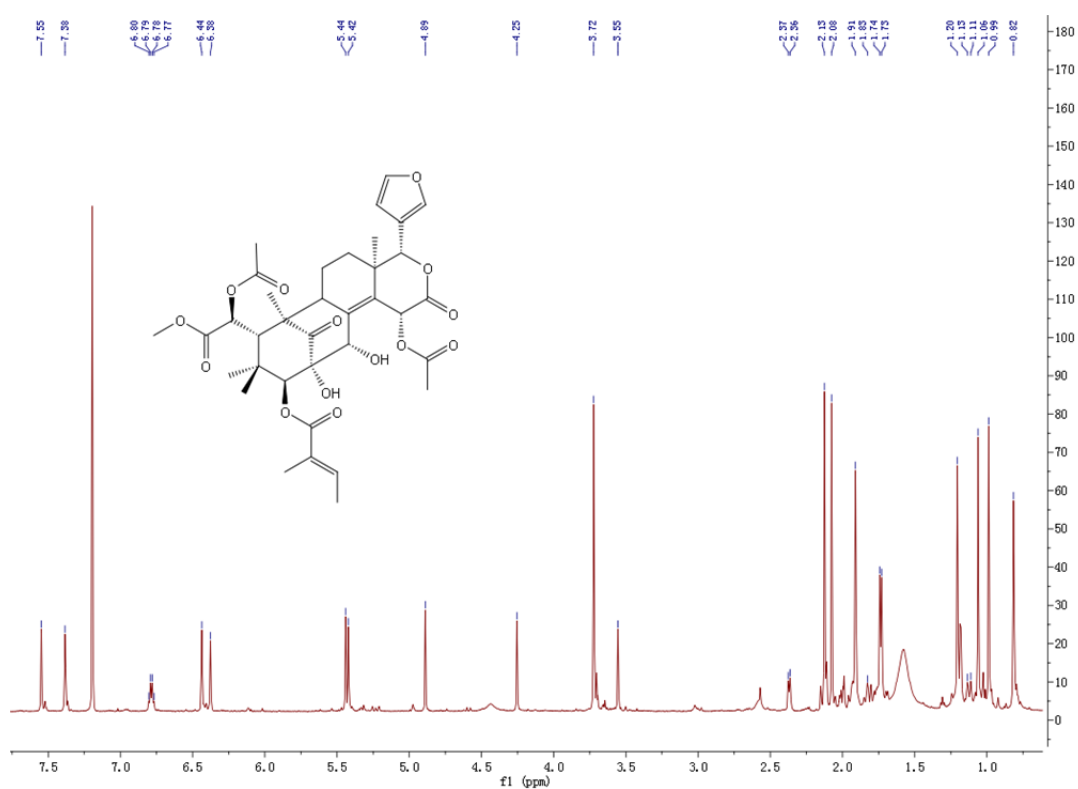


Fig. 12S ^{13}C -NMR spectrum of compound **2** in CDCl_3

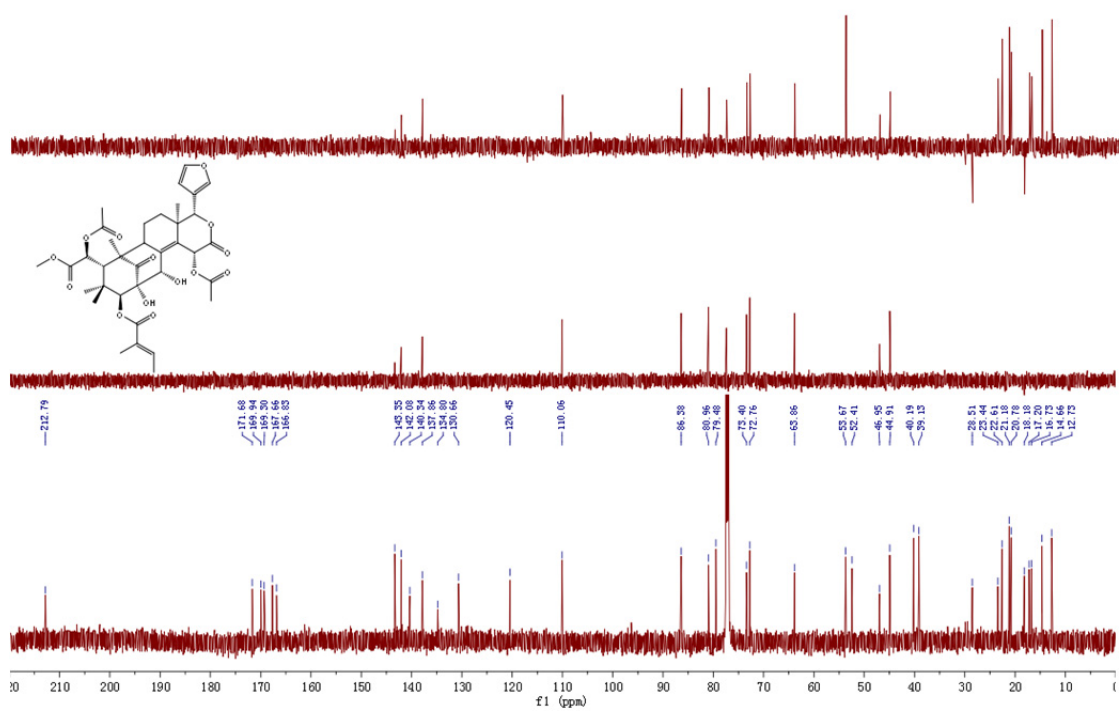


Fig. 13S HSQC NMR spectrum of compound **2** in CDCl_3

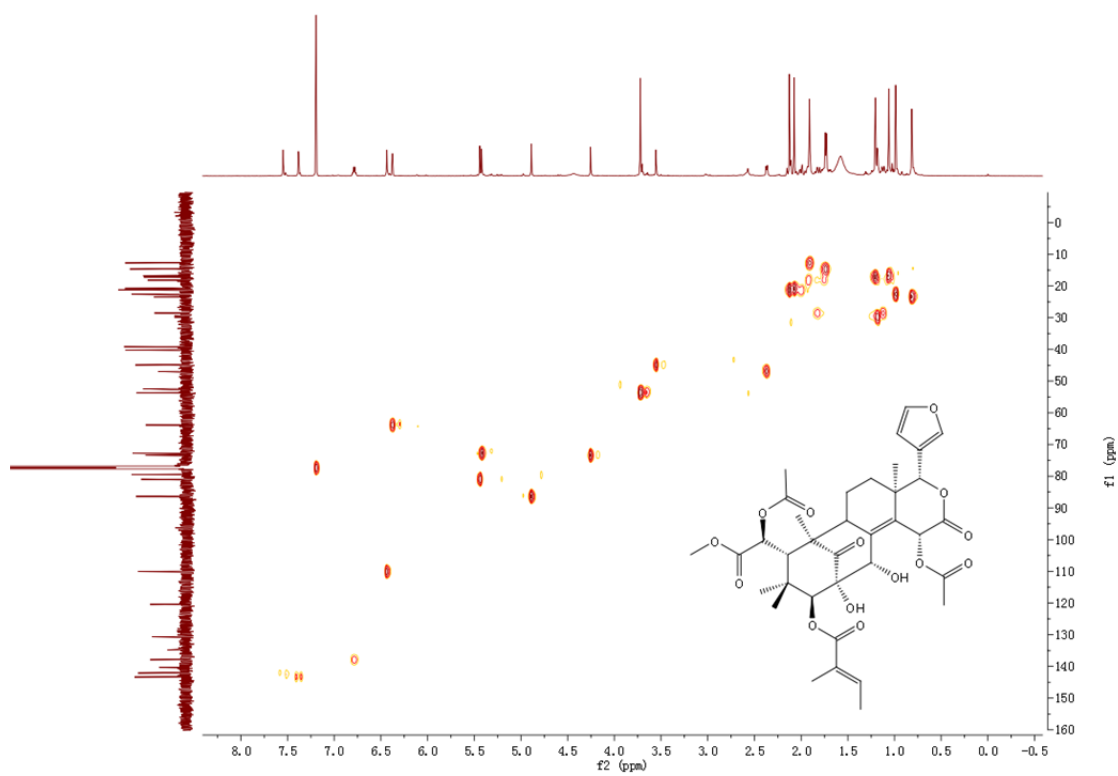


Fig. 14S HMBC NMR spectrum of compound **2** in CDCl_3

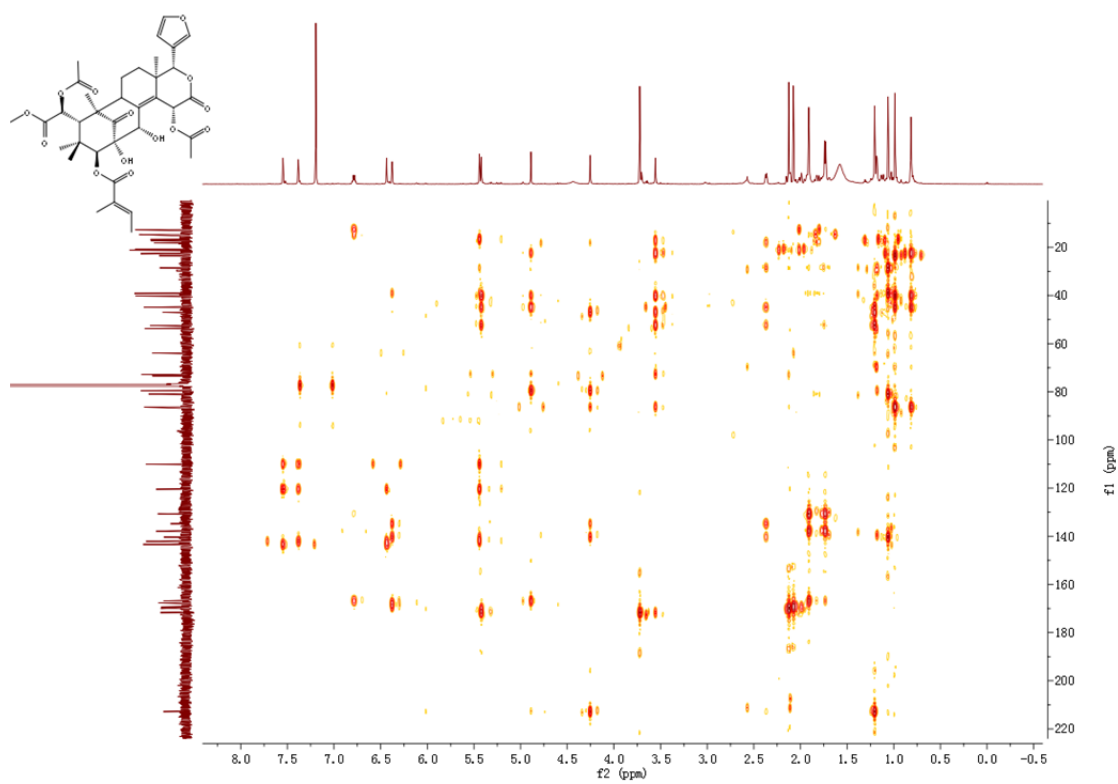


Fig. 15S ^1H - ^1H COSY NMR spectrum of compound **2** in CDCl_3

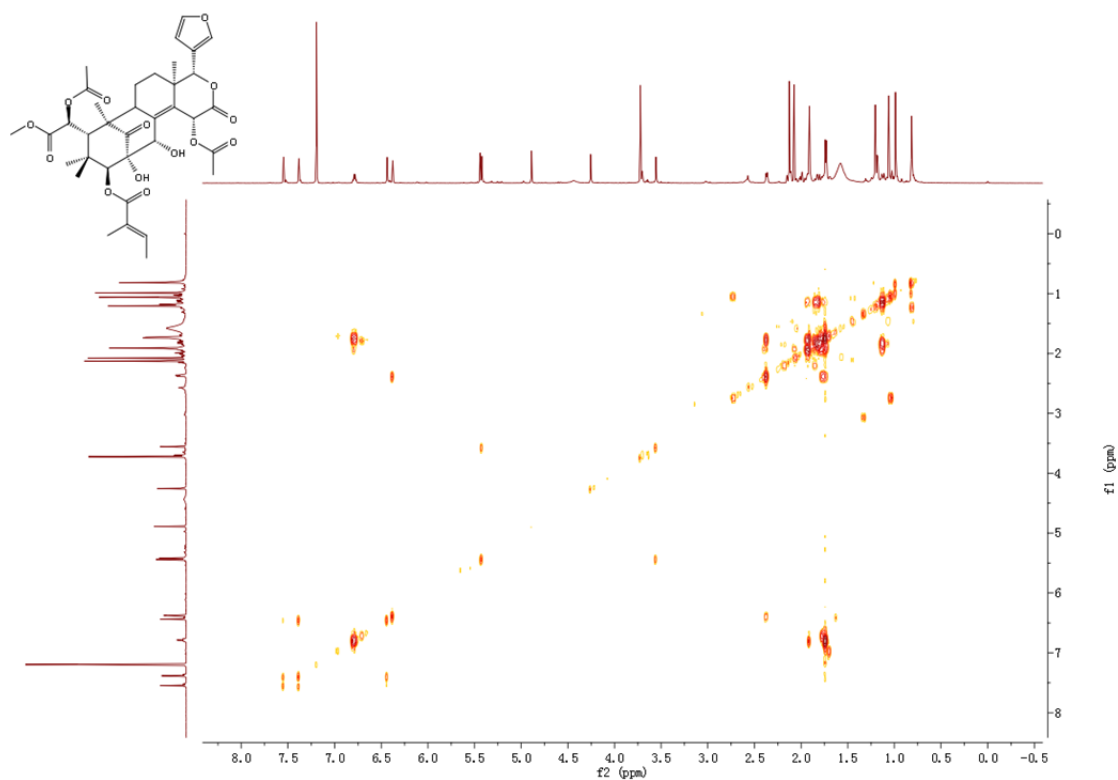


Fig. 16S ROESY NMR spectrum of compound **2** in CDCl_3

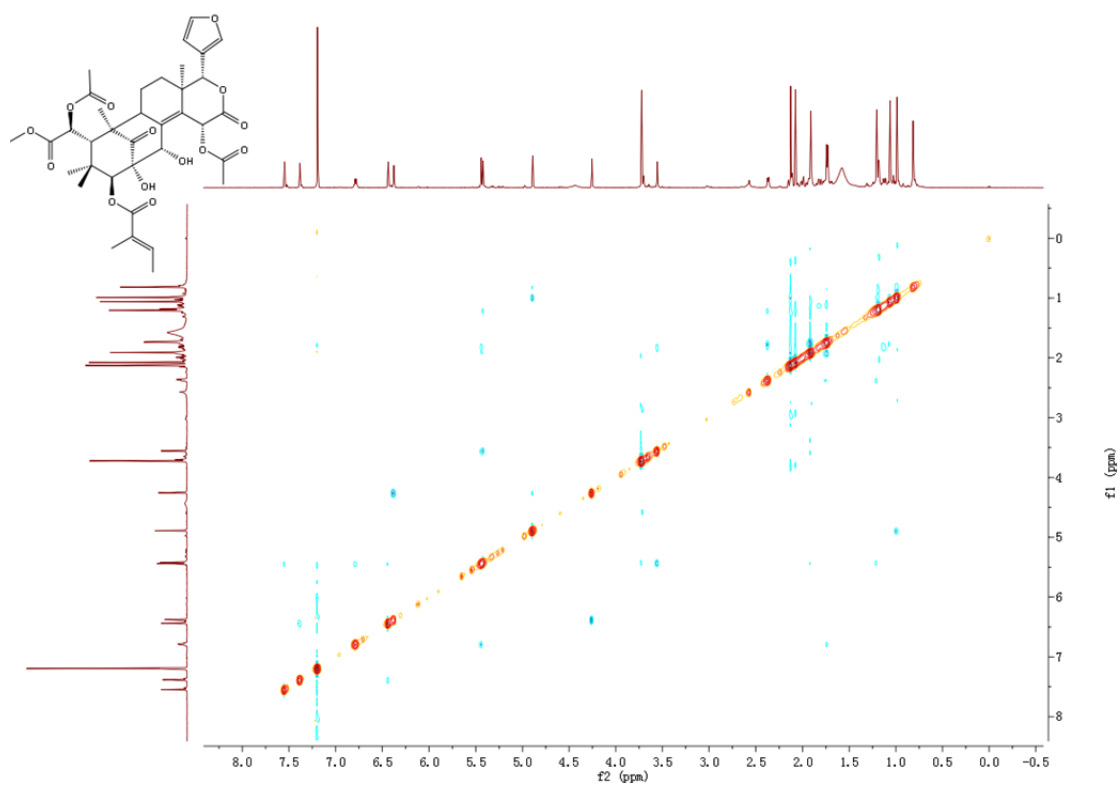


Fig. 17S IR spectrum of compound **2**

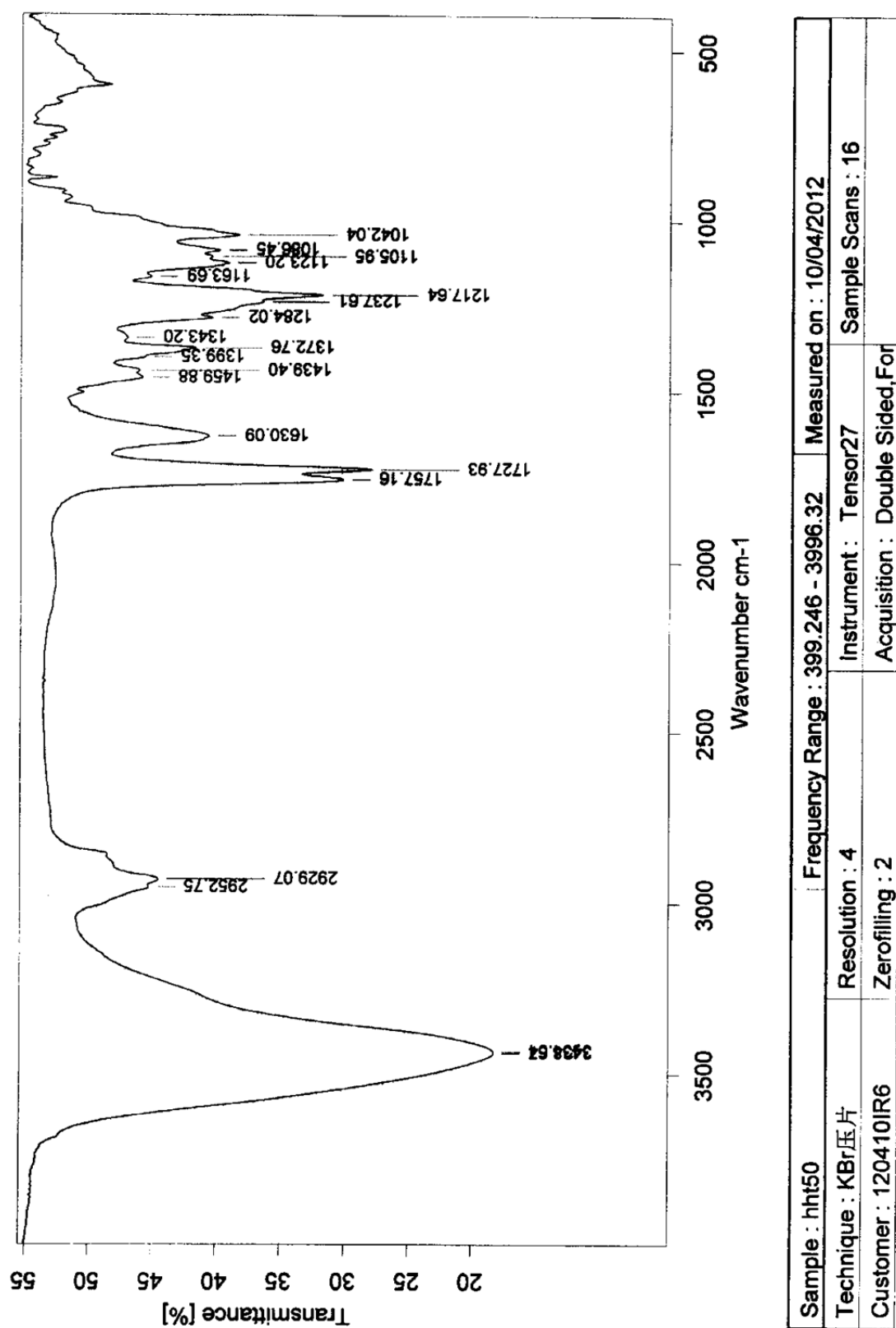
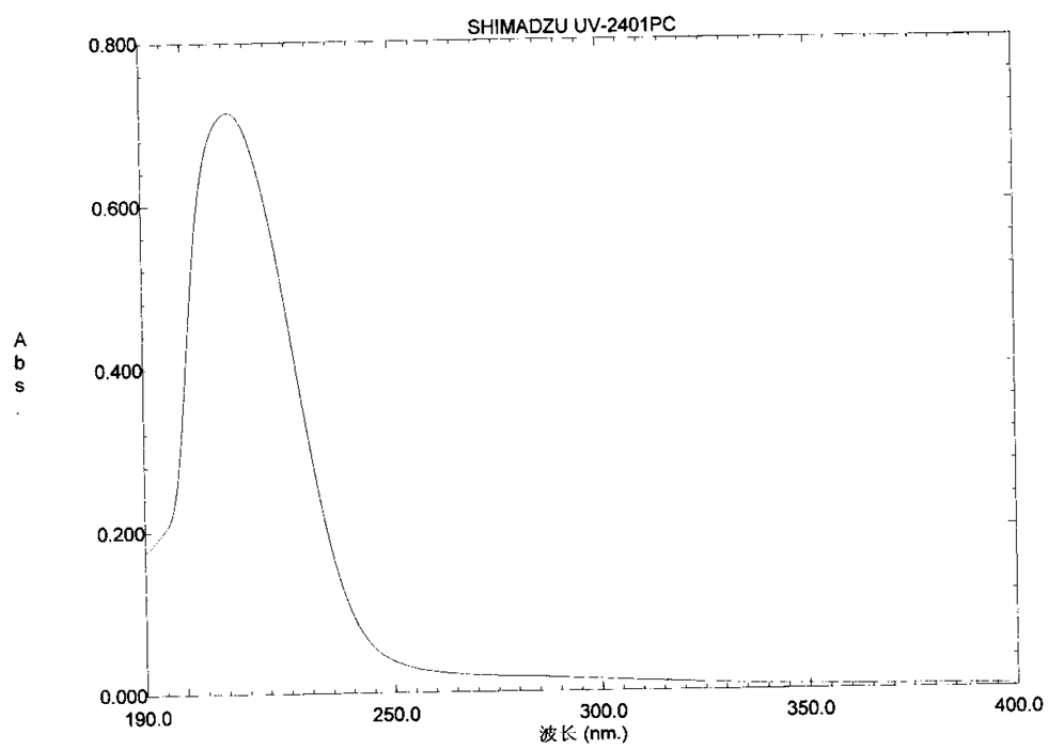


Fig. 18S UV spectrum of compound 2 in CH₃OH



文件名: HHT50

HHT50 — —

创建于: 14:30 12-04-06
数据: 原始

样品浓度: 0.0317毫克/毫升
溶剂: 甲醇

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否	波长 (nm.)	Abs.
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Fig. 19S HRESIMS spectrum of compound **3**

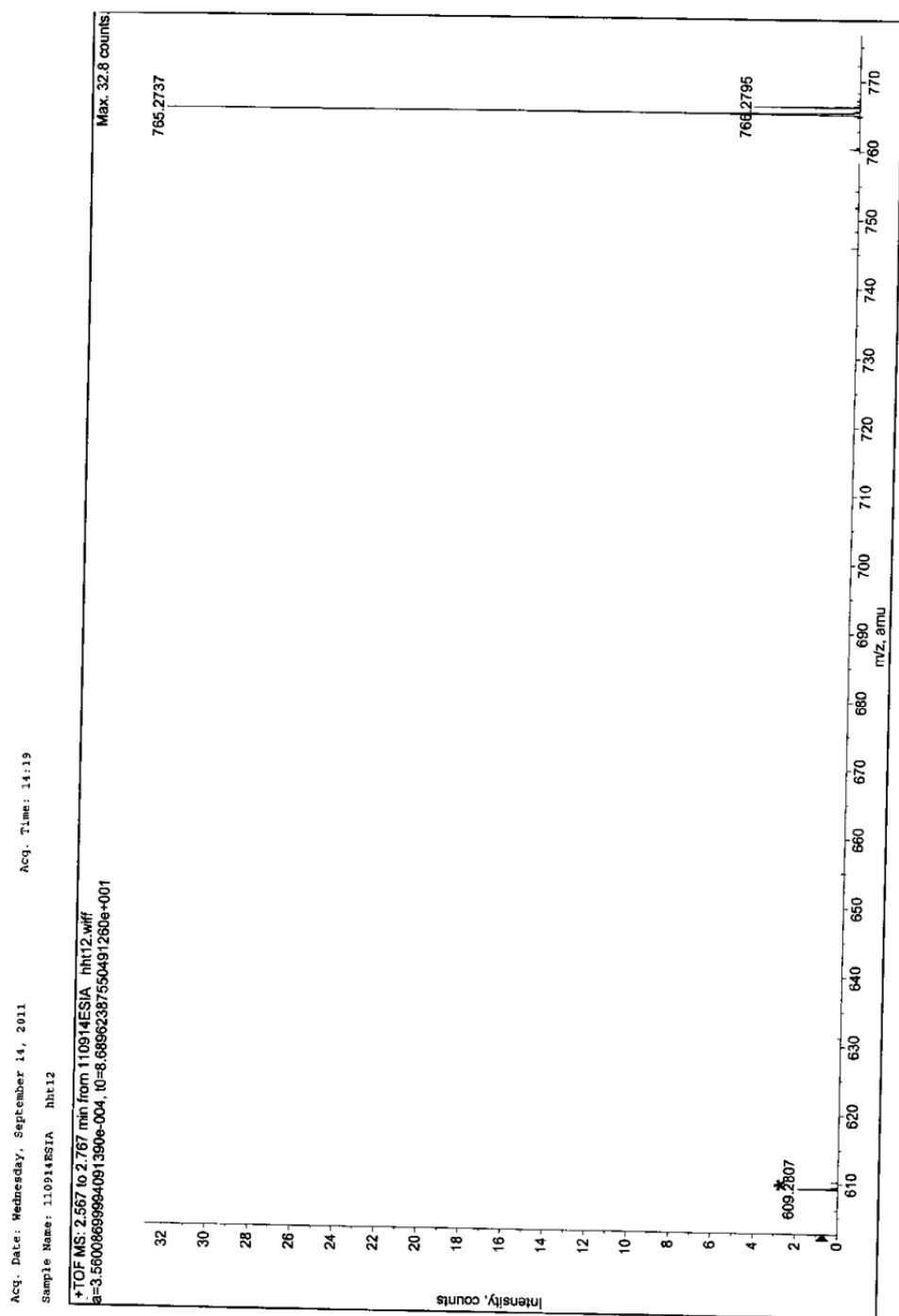


Fig. 20S ^1H -NMR spectrum of compound **3** in CDCl_3

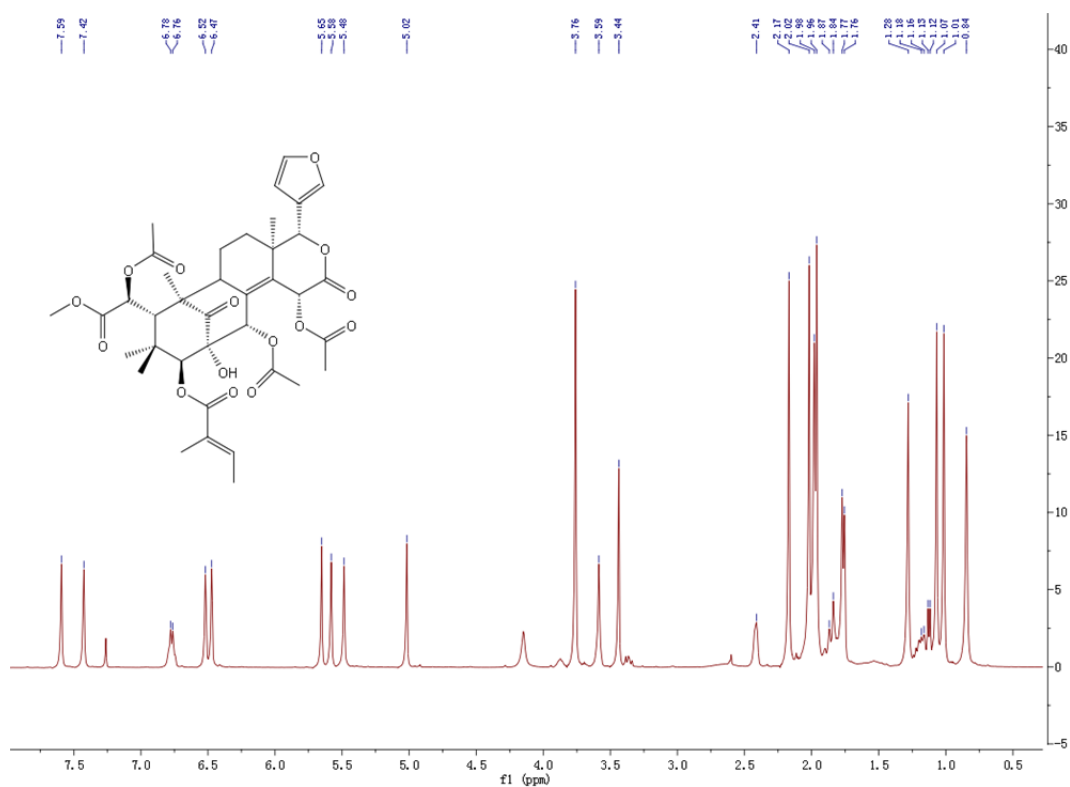


Fig. 21S ^{13}C -NMR spectrum of compound **3** in CDCl_3

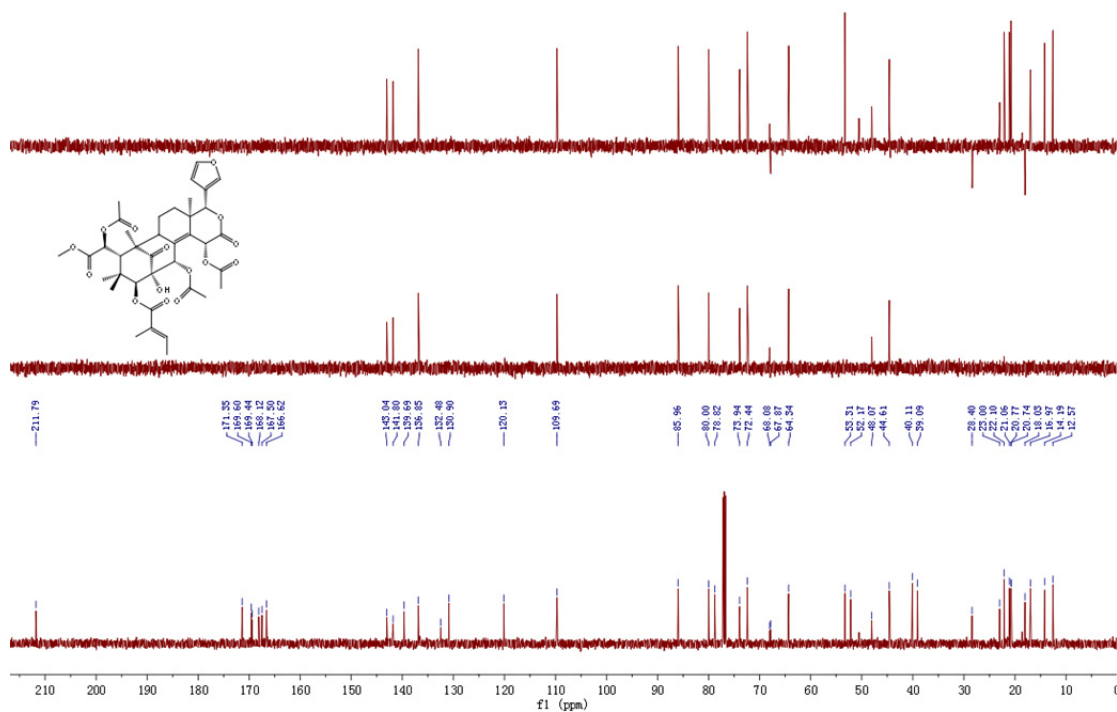


Fig. 22S HSQC NMR spectrum of compound **3** in CDCl_3

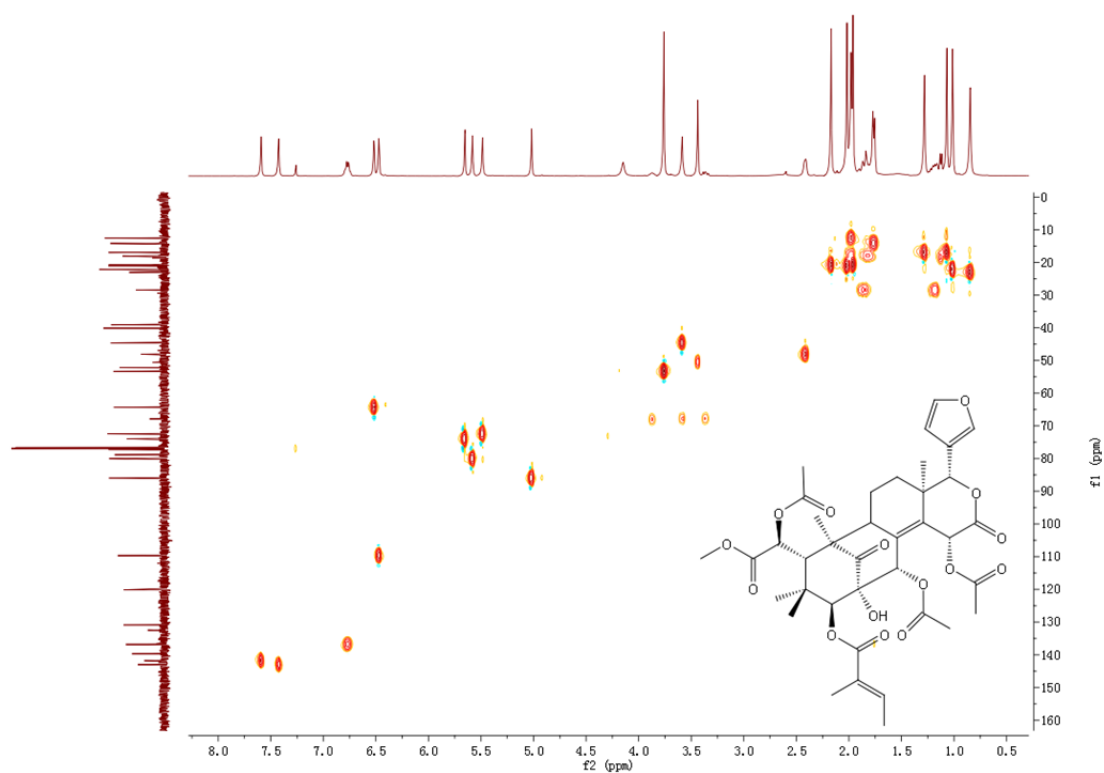


Fig. 23S HMBC NMR spectrum of compound **3** in CDCl₃

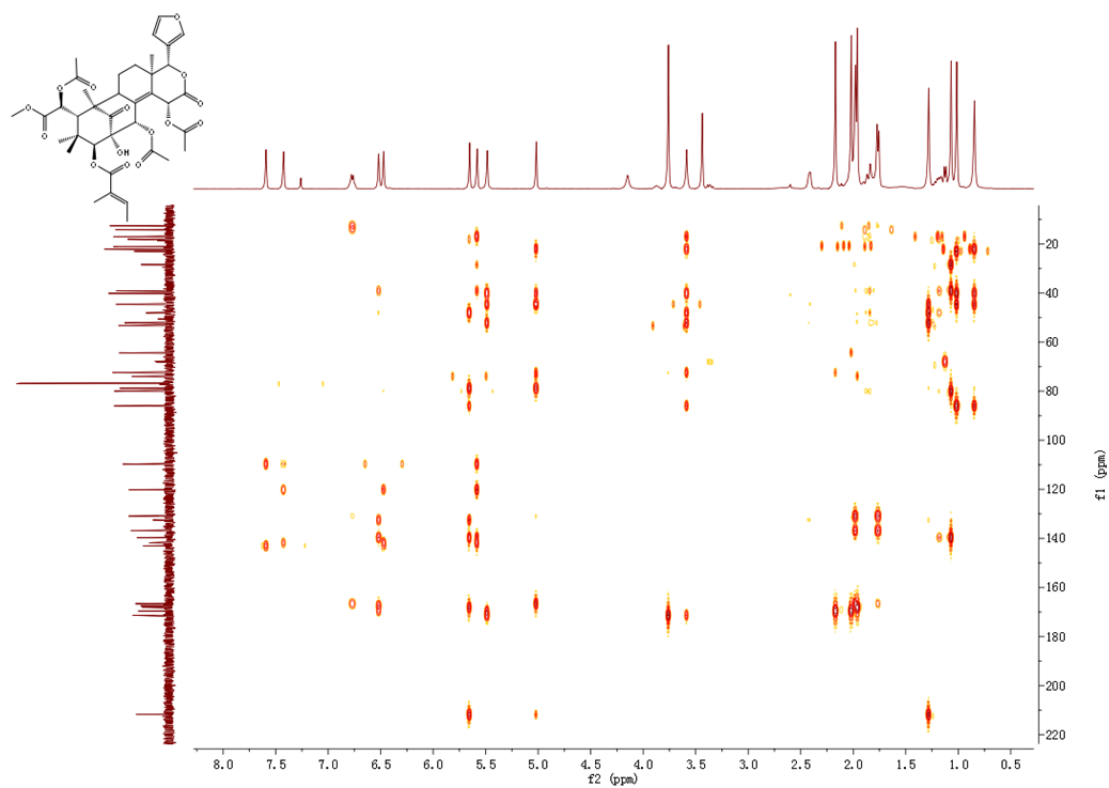


Fig. 24S ¹H-¹H COSY NMR spectrum of compound **3** in CDCl₃

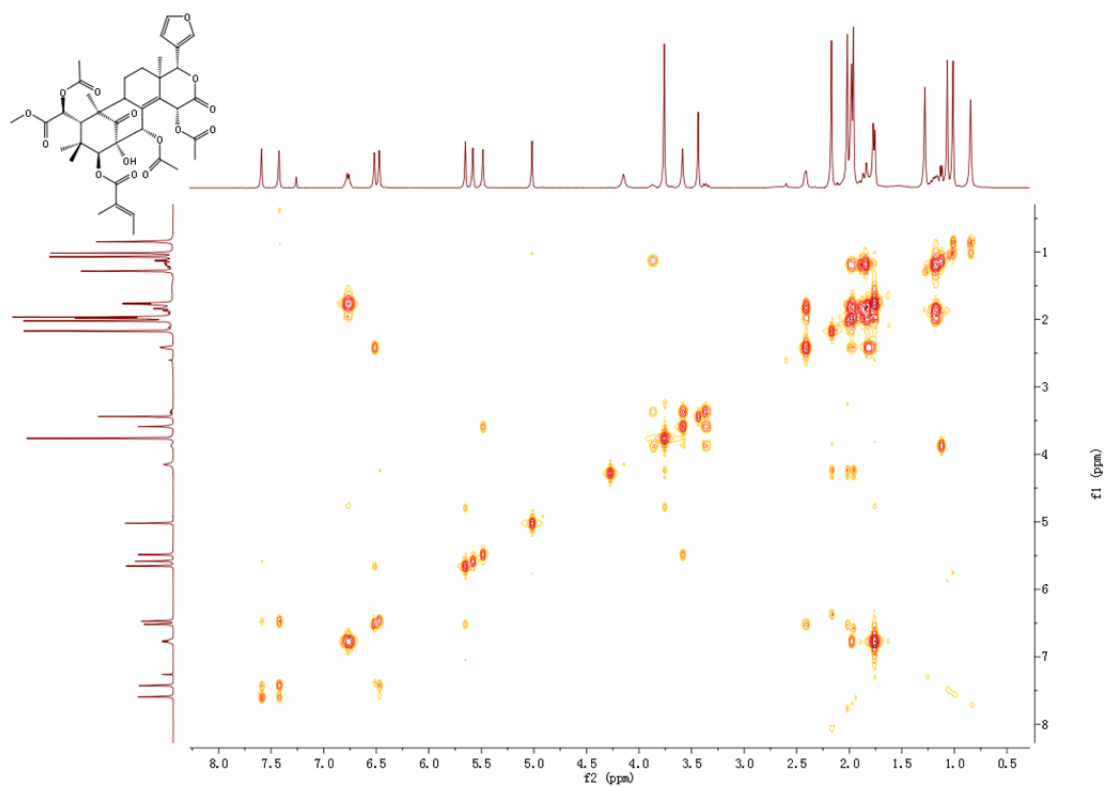


Fig. 25S ROESY NMR spectrum of compound **3** in CDCl_3

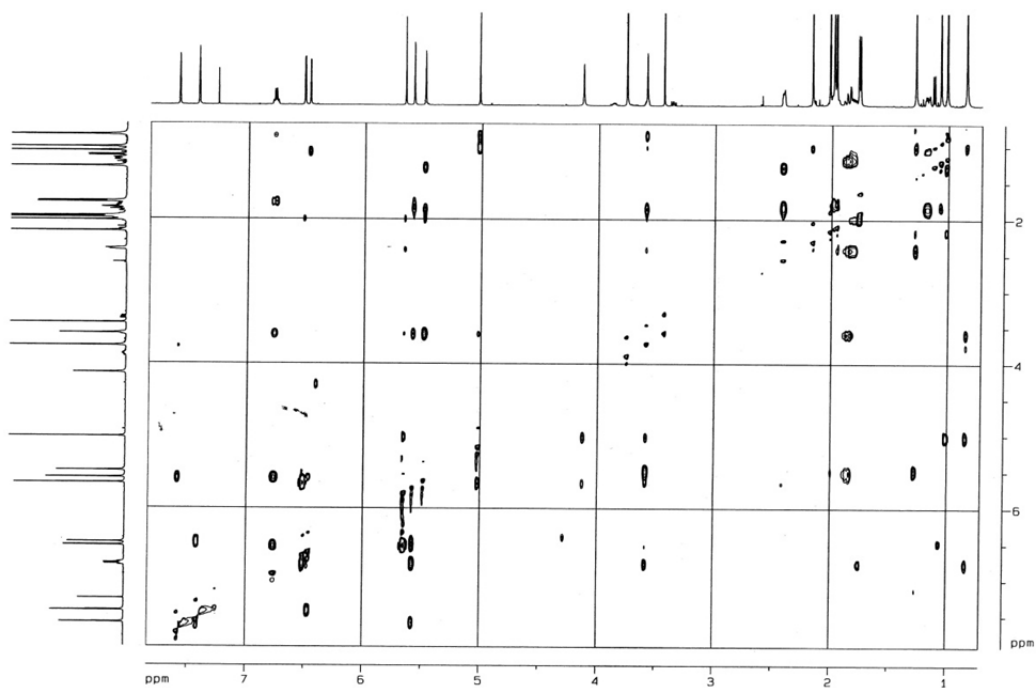


Fig. 26S IR spectrum of compound **3**

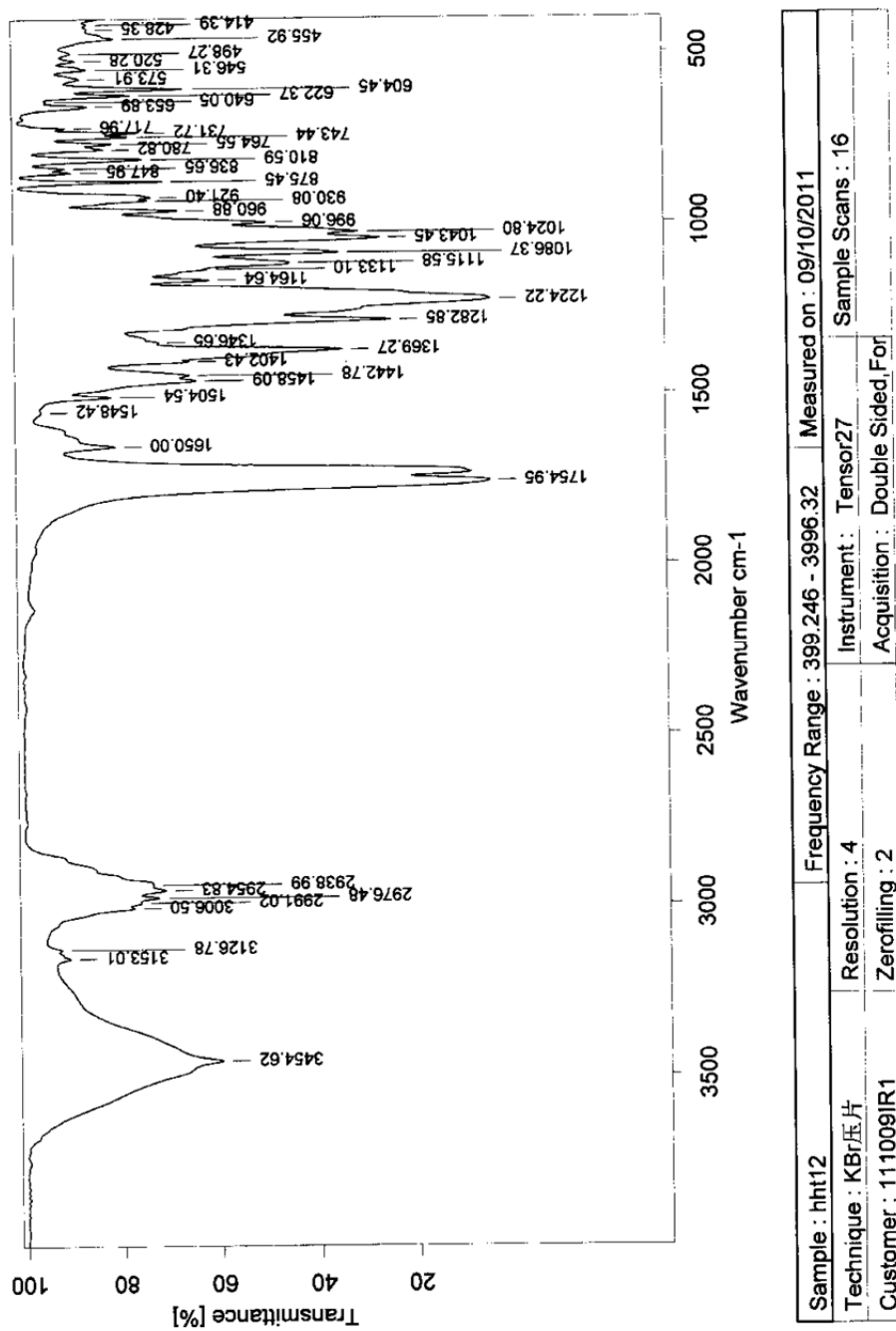
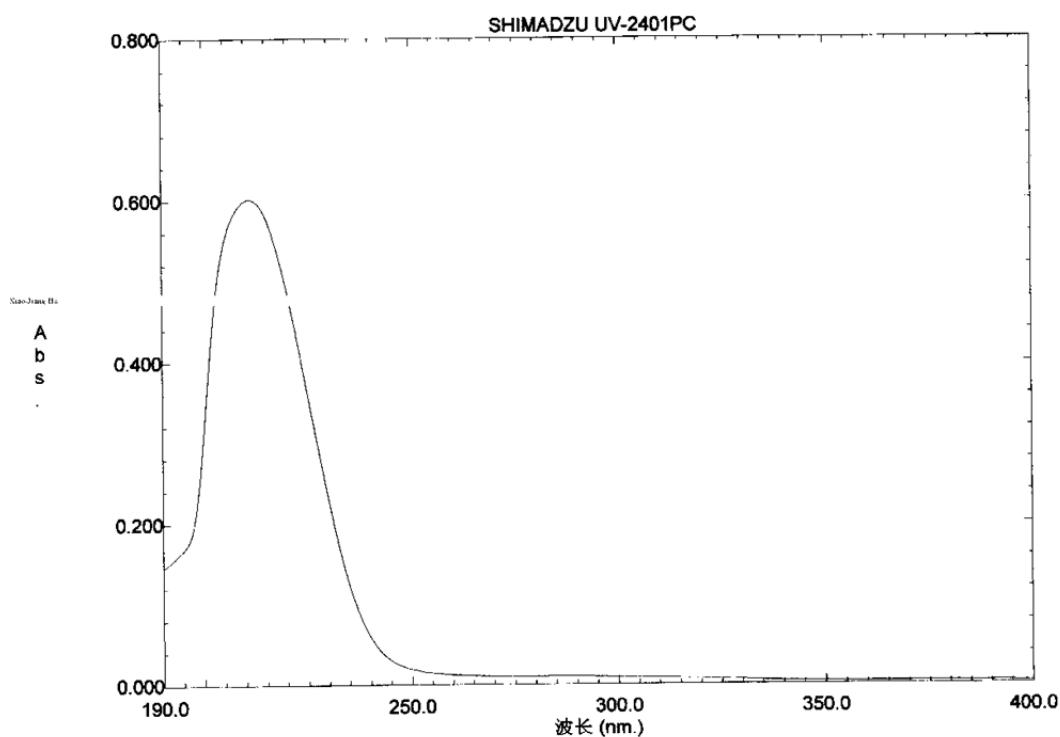


Fig. 27S UV spectrum of compound **3** in CH₃OH



文件名: 12053100

样品名称: HHT12

创建于: 13:42 12-05-31

数据: 原始

12053100

样品浓度: 0.0182毫克/毫升

溶剂: 甲醇

测量模式: Abs.

扫描速度: 中速

狭缝: 5.0

采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	211.20	0.6016

Fig. 28S ESIMS spectrum of compound **4**

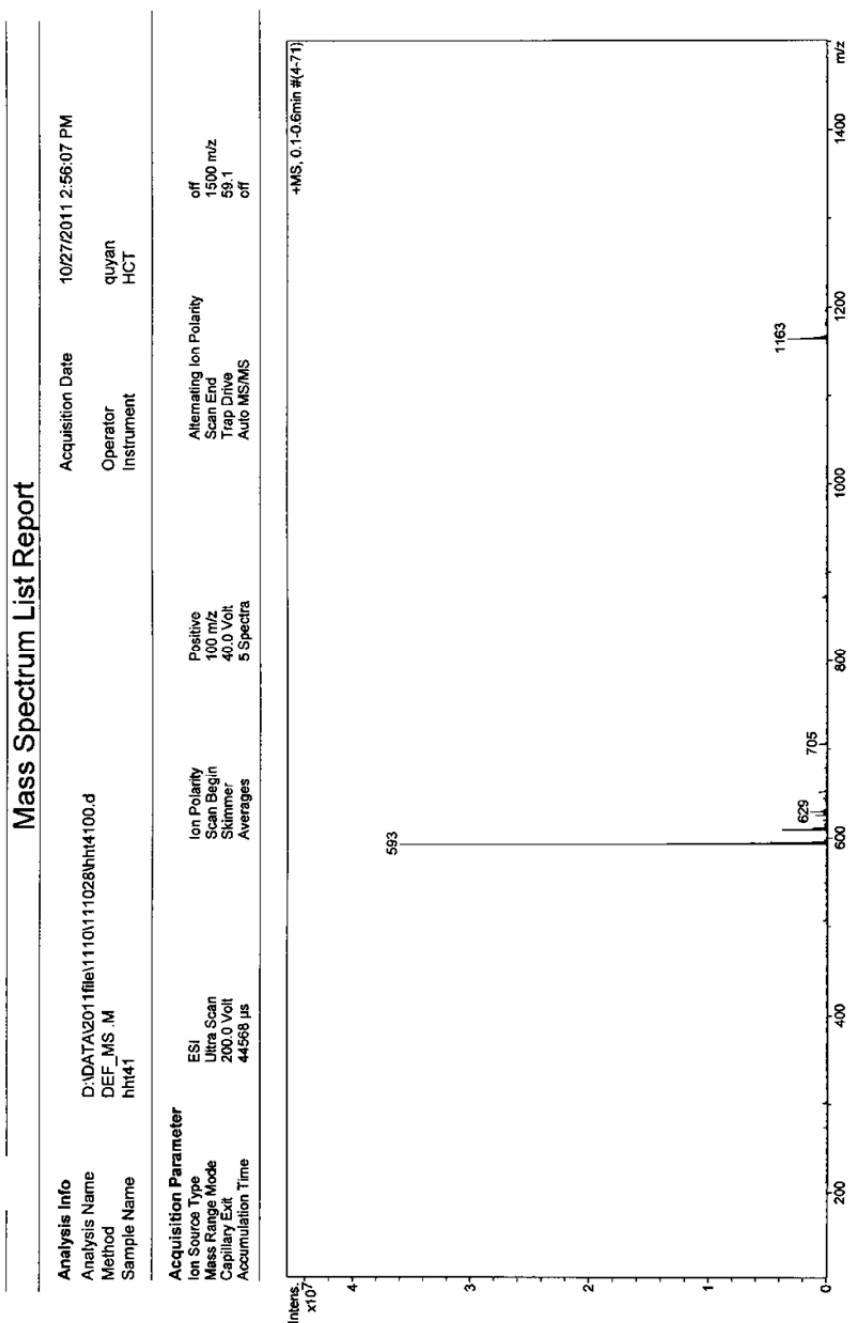


Fig. 29S ^1H -NMR spectrum of compound **4** in CDCl_3

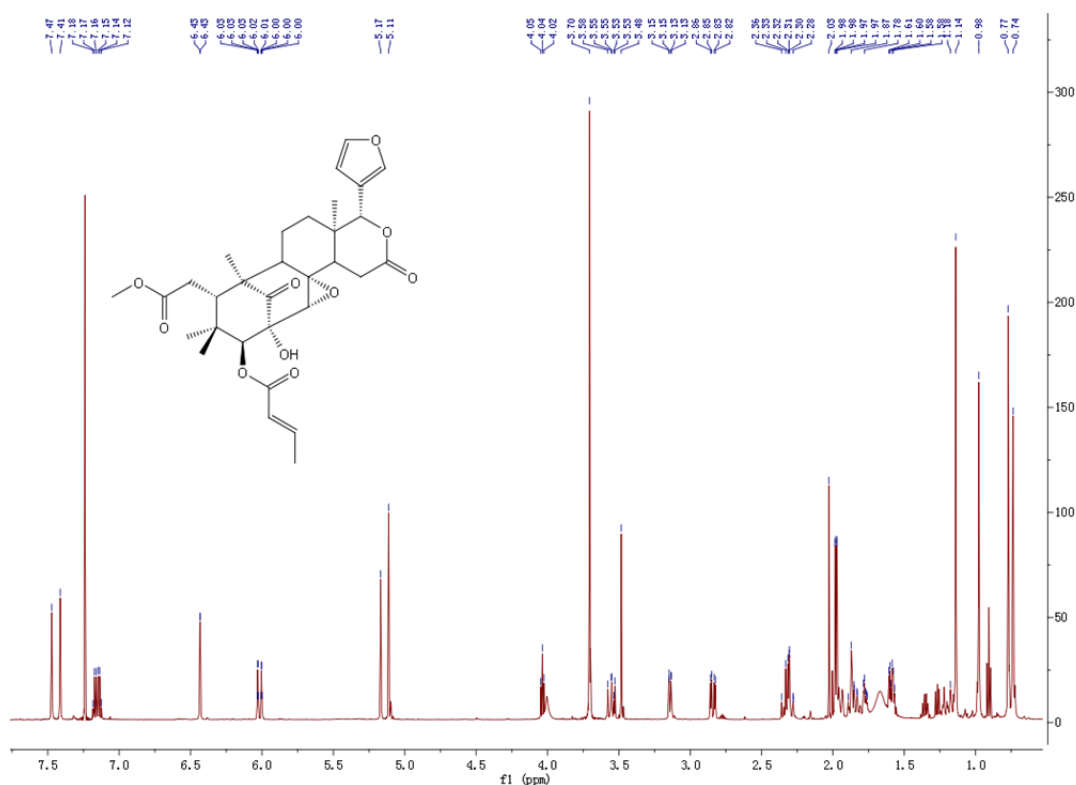


Fig. 30S ^{13}C -NMR spectrum of compound **4** in CDCl_3

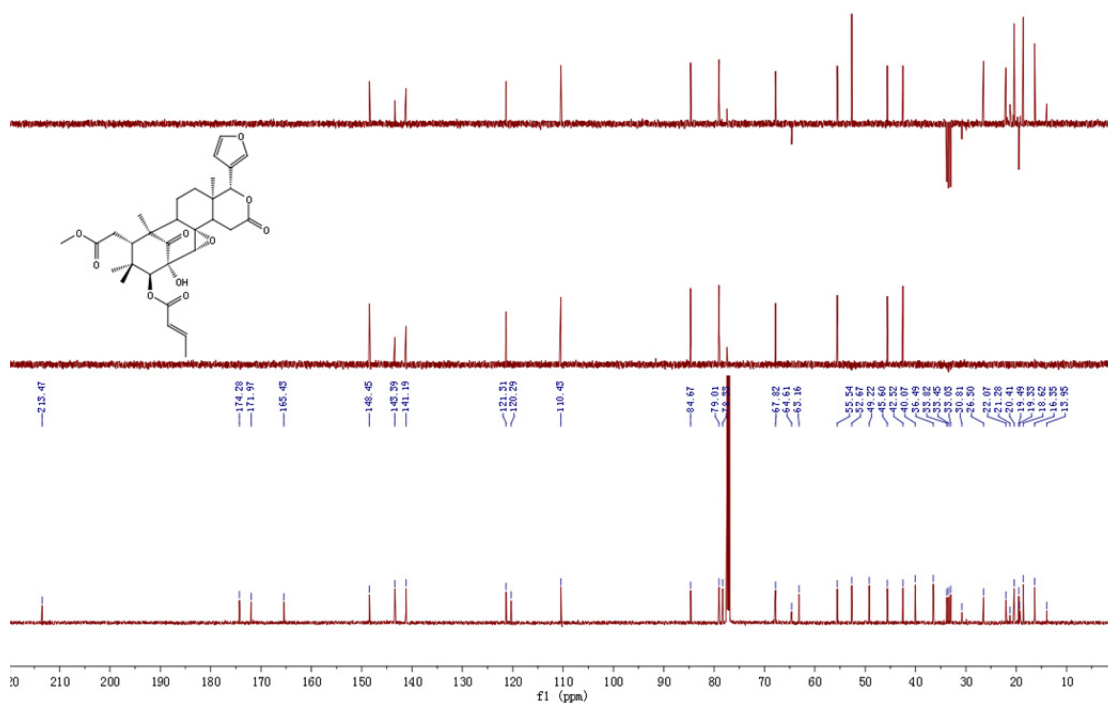


Fig. 31S HSQC NMR spectrum of compound **4** in CDCl_3

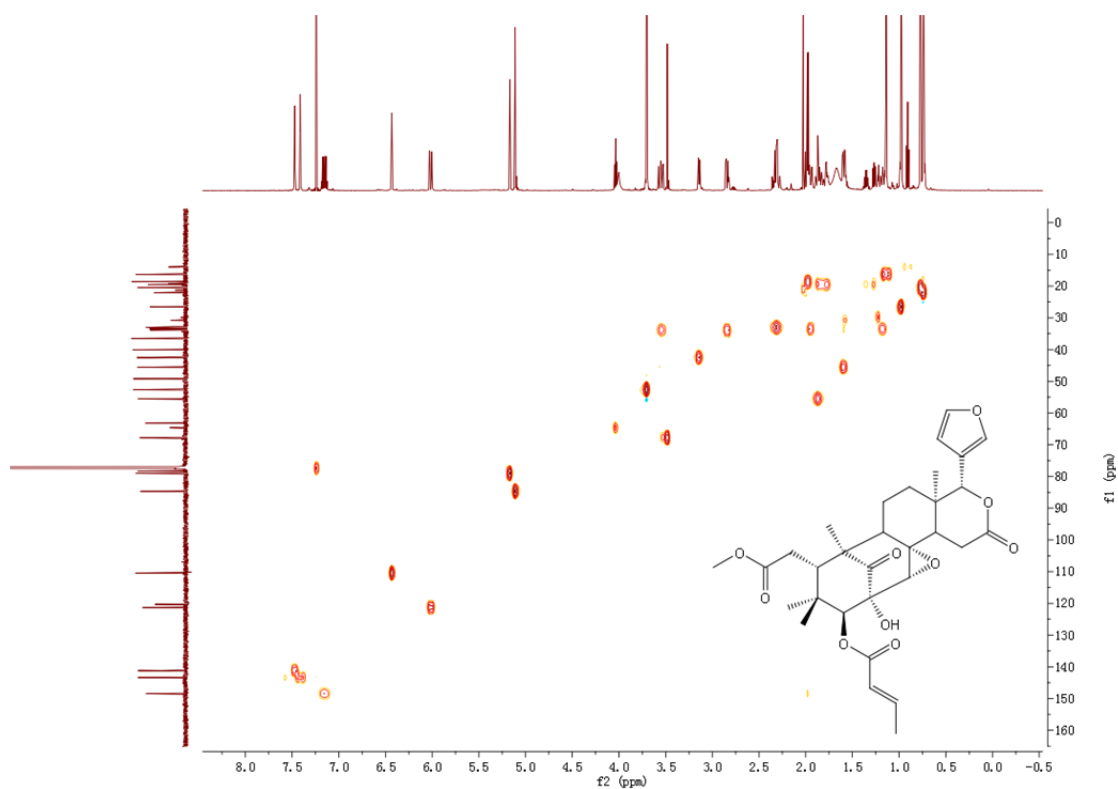


Fig. 32S HMBC NMR spectrum of compound **4** in CDCl_3

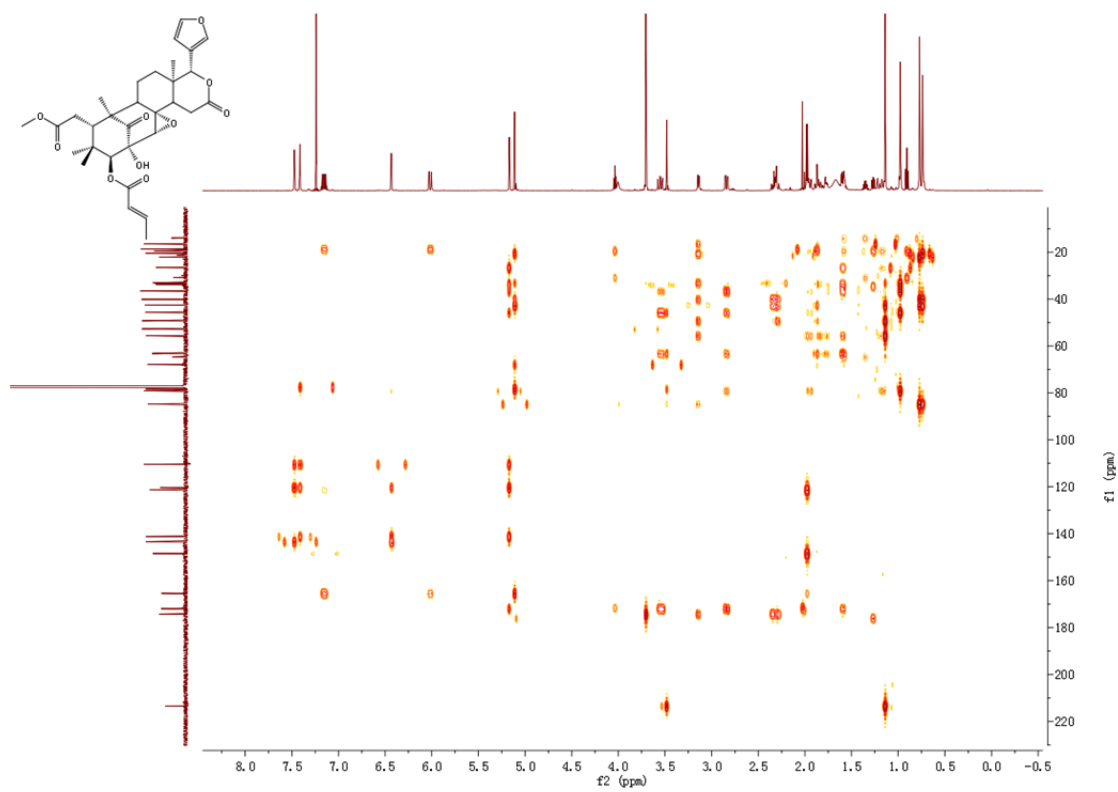


Fig. 33S ^1H - ^1H COSY NMR spectrum of compound **4** in CDCl_3

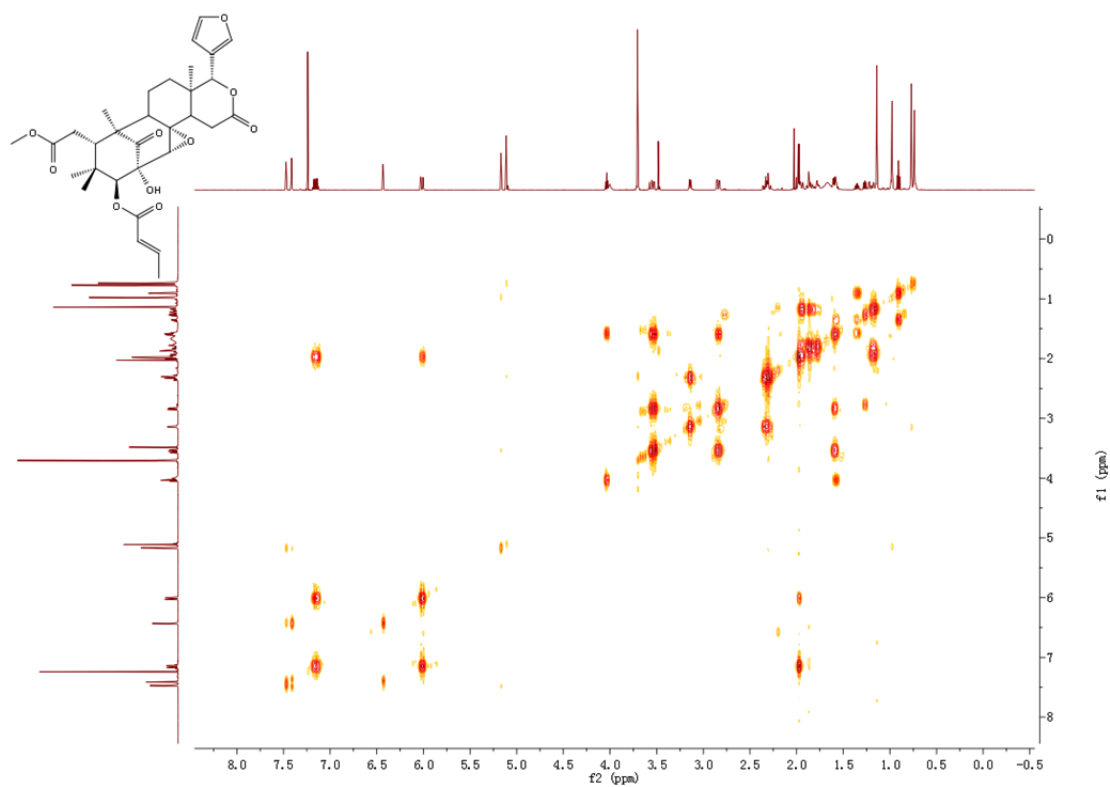


Fig. 34S ROESY NMR spectrum of compound **4** in CDCl₃

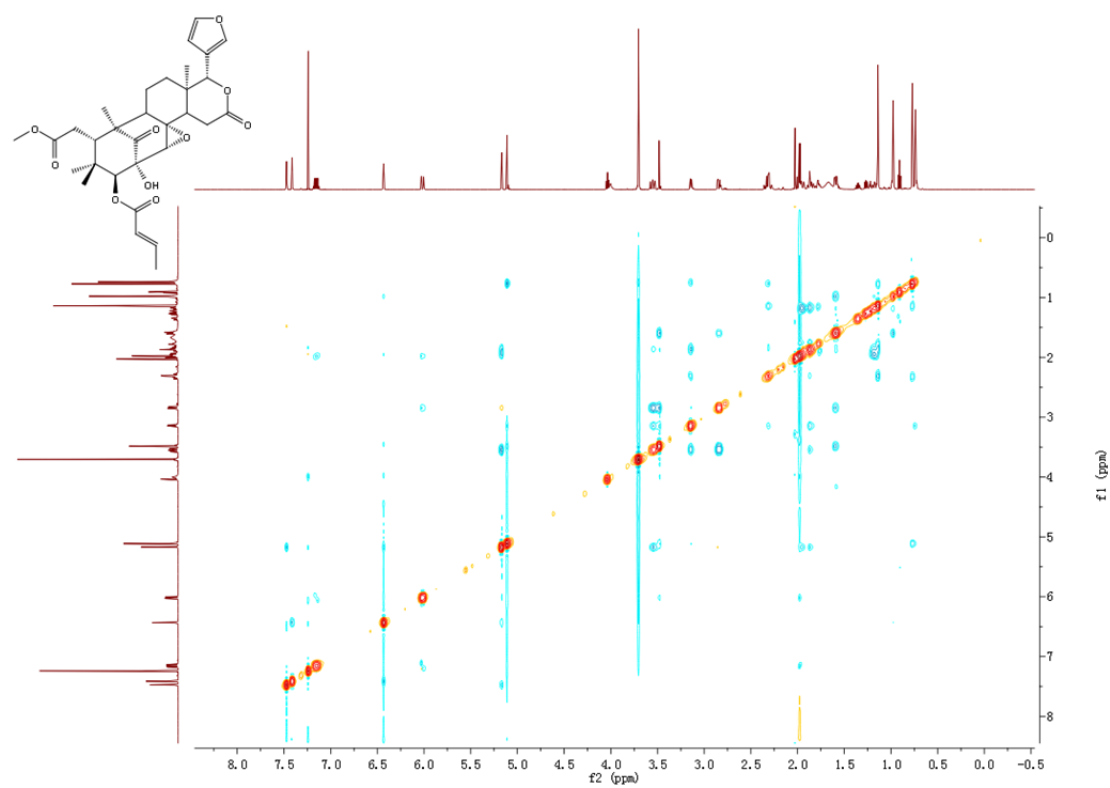
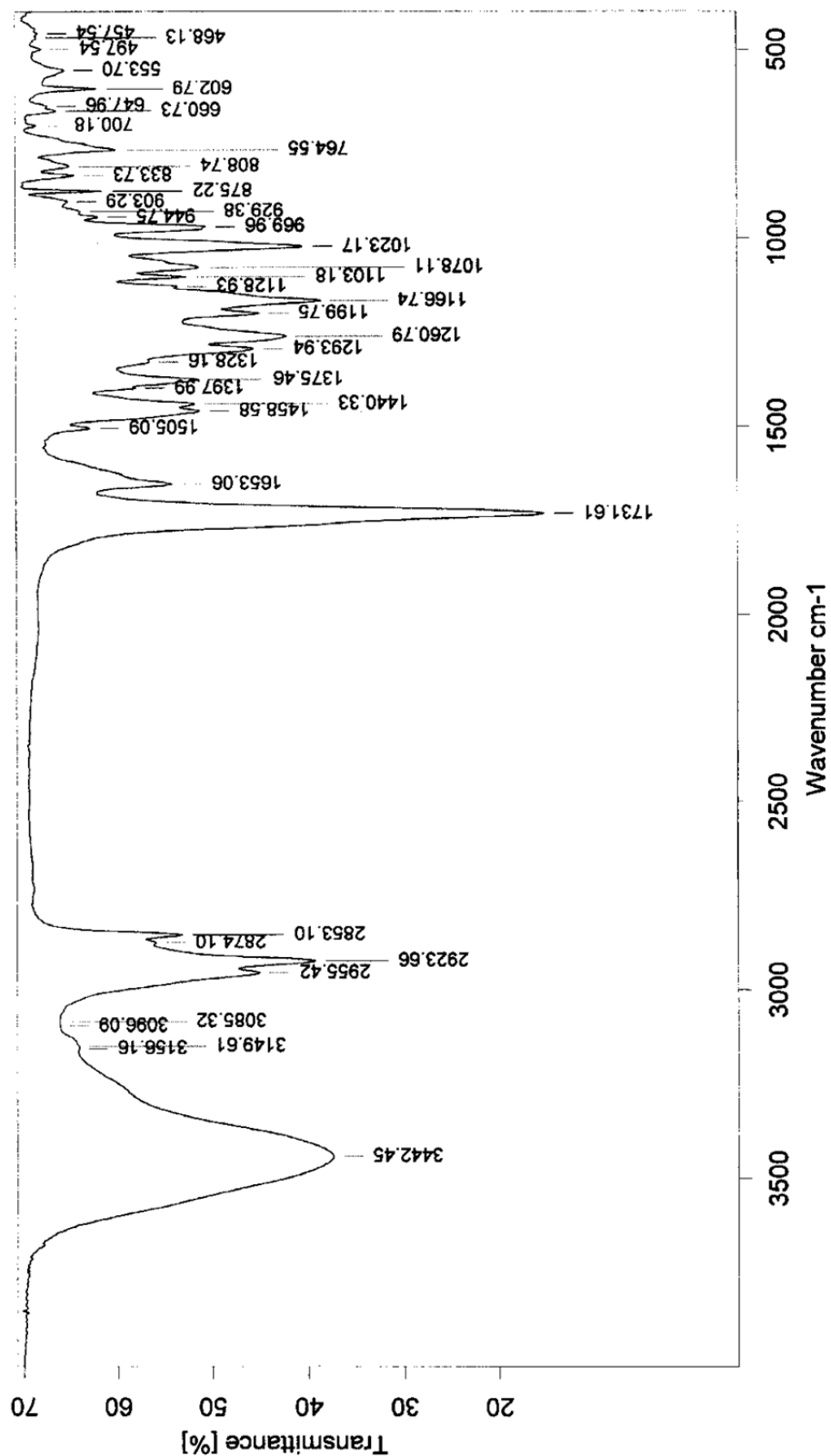
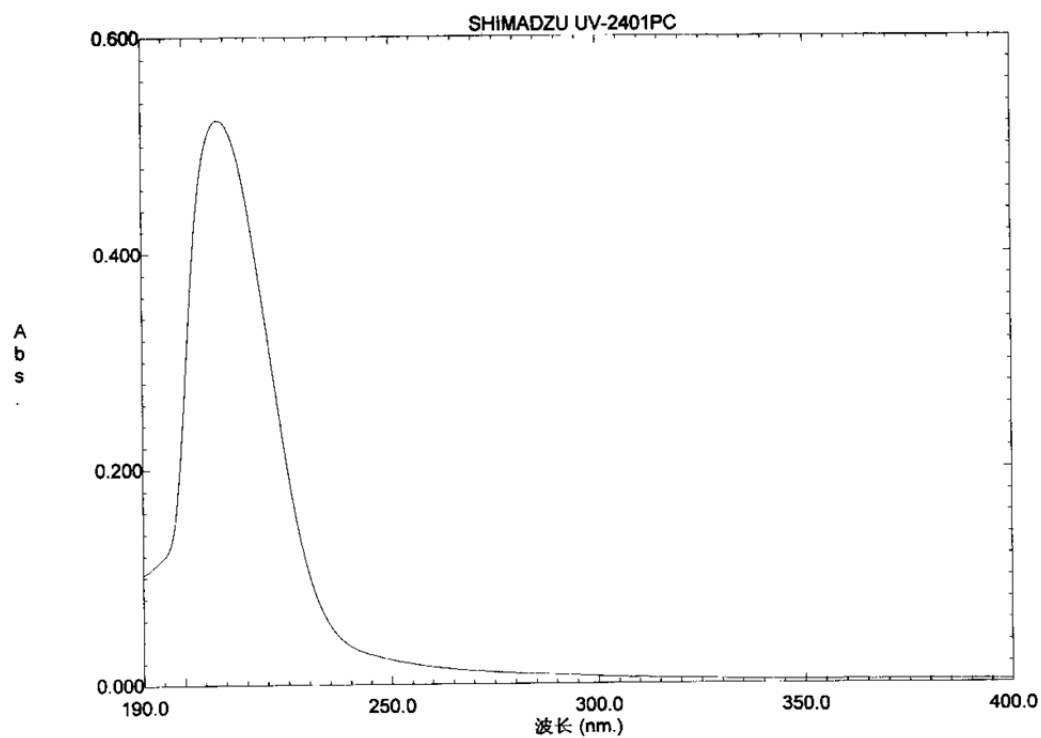


Fig. 35S IR spectrum of compound **4**



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Customer : 111212IR1		Zerofilling : 2		Acquisition : Double Sided, For	
				Sample Scans : 16	

Fig. 36S UV spectrum of compound **4** in CH₃OH



文件名: 12053101
样品名称: HHT41

12053101

创建于: 13:49 12-05-31
数据: 原始

样品浓度: 0.0330毫克/毫升
溶剂: 甲醇

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	208.40	0.5235

Fig. 37S ESIMS spectrum of compound 5

Display Report

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Comment			
Acquisition Parameter			
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Capillary Exit	136.0 Volt	Skimmer	40.0 Volt
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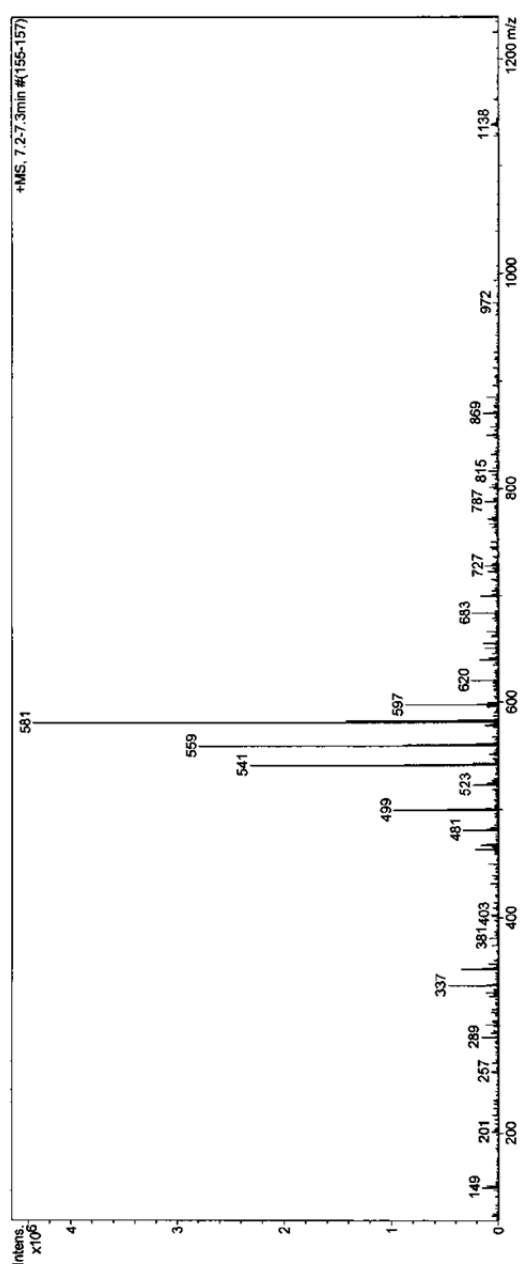


Fig. 38S ^1H -NMR spectrum of compound **5** in CDCl_3

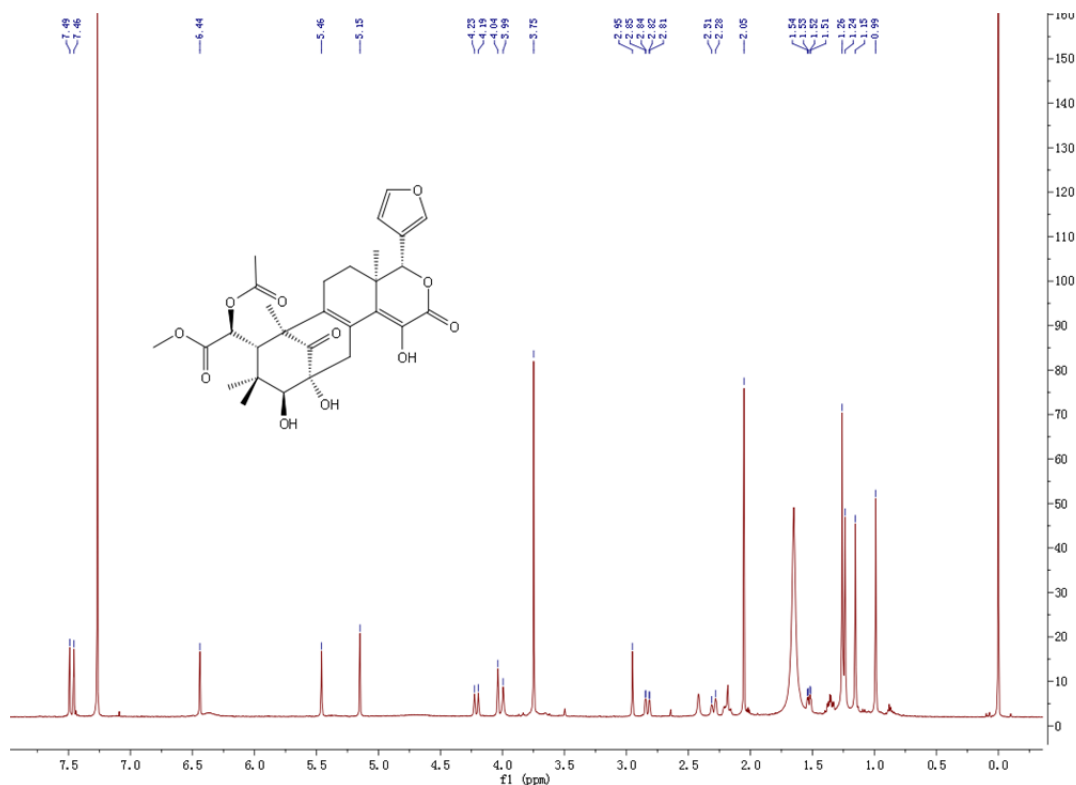


Fig. 39S ^{13}C -NMR spectrum of compound **5** in CDCl_3

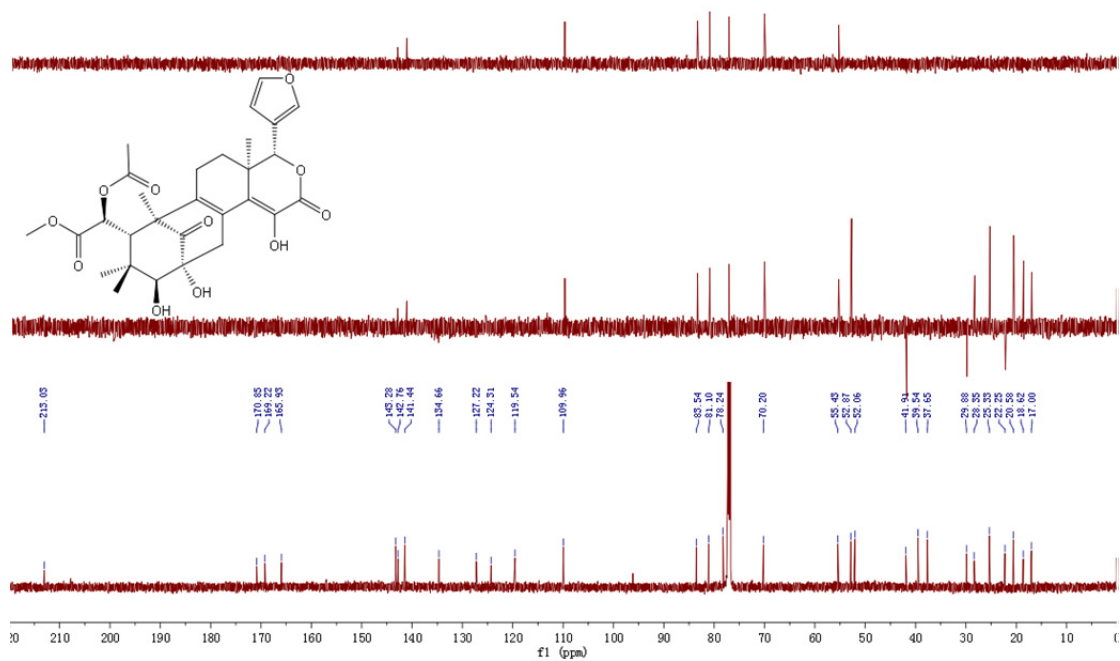


Fig. 40S HSQC NMR spectrum of compound **5** in CDCl_3

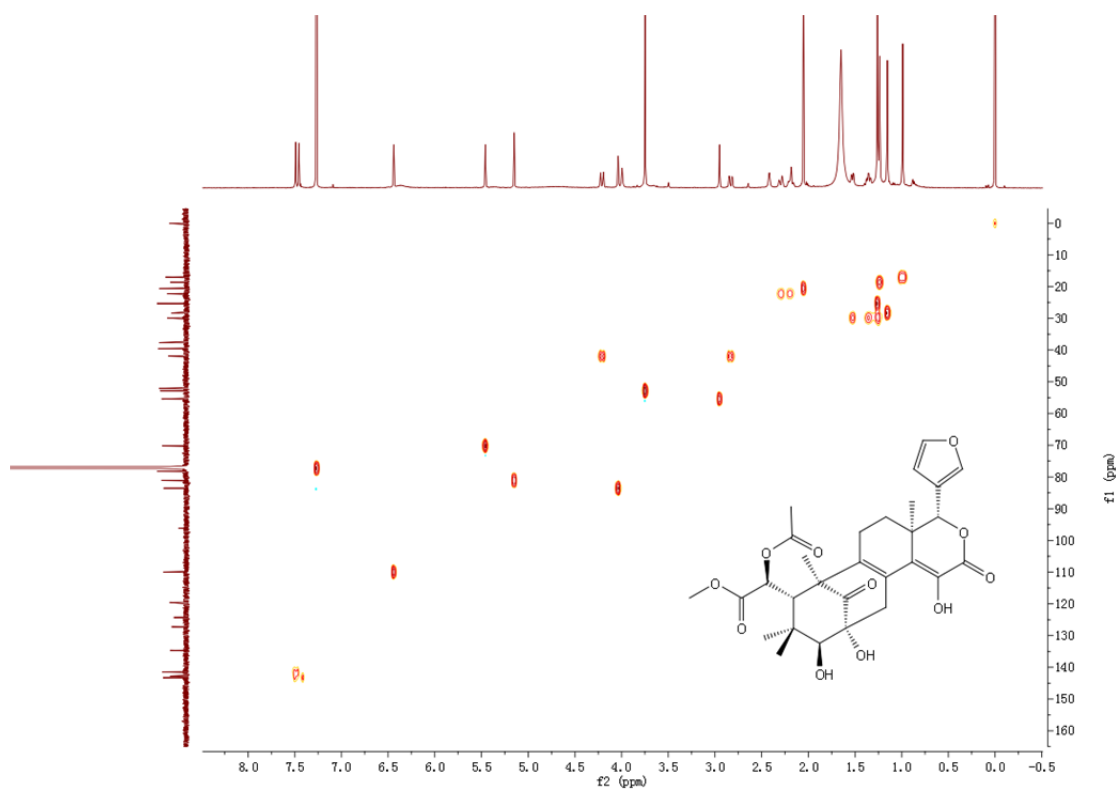


Fig. 41S HMBC NMR spectrum of compound **5** in CDCl₃

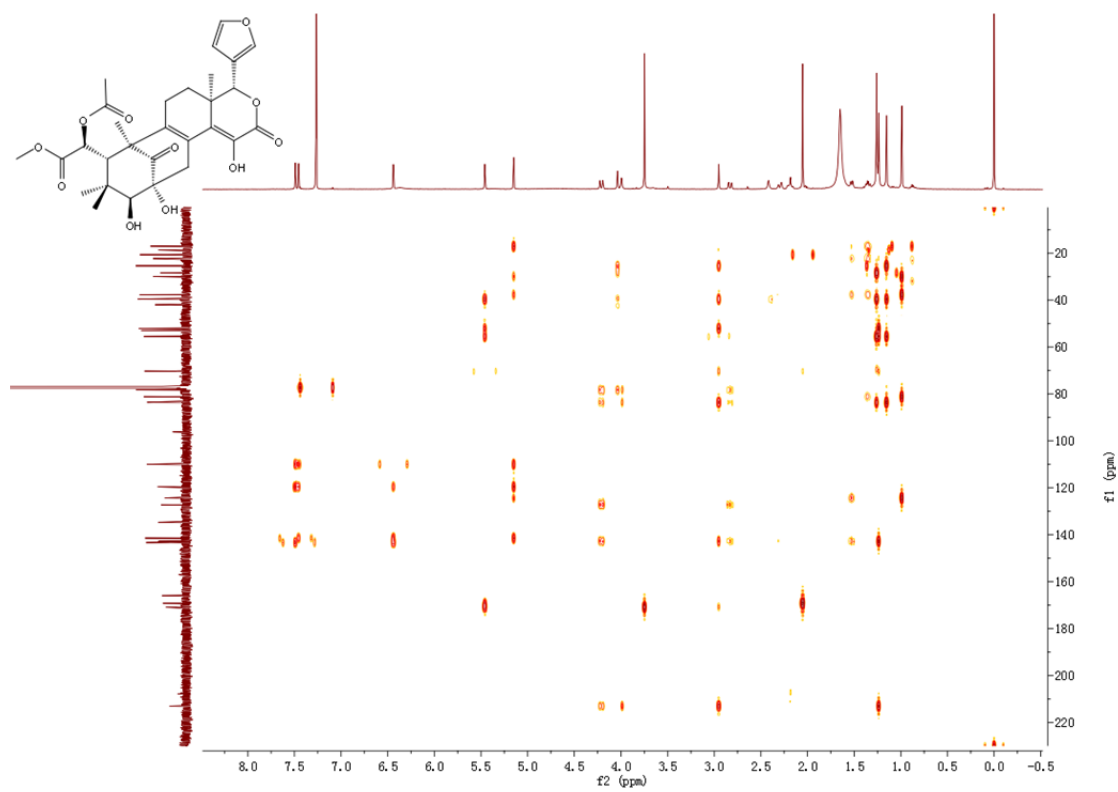


Fig. 42S ¹H-¹H COSY NMR spectrum of compound **5** in CDCl₃

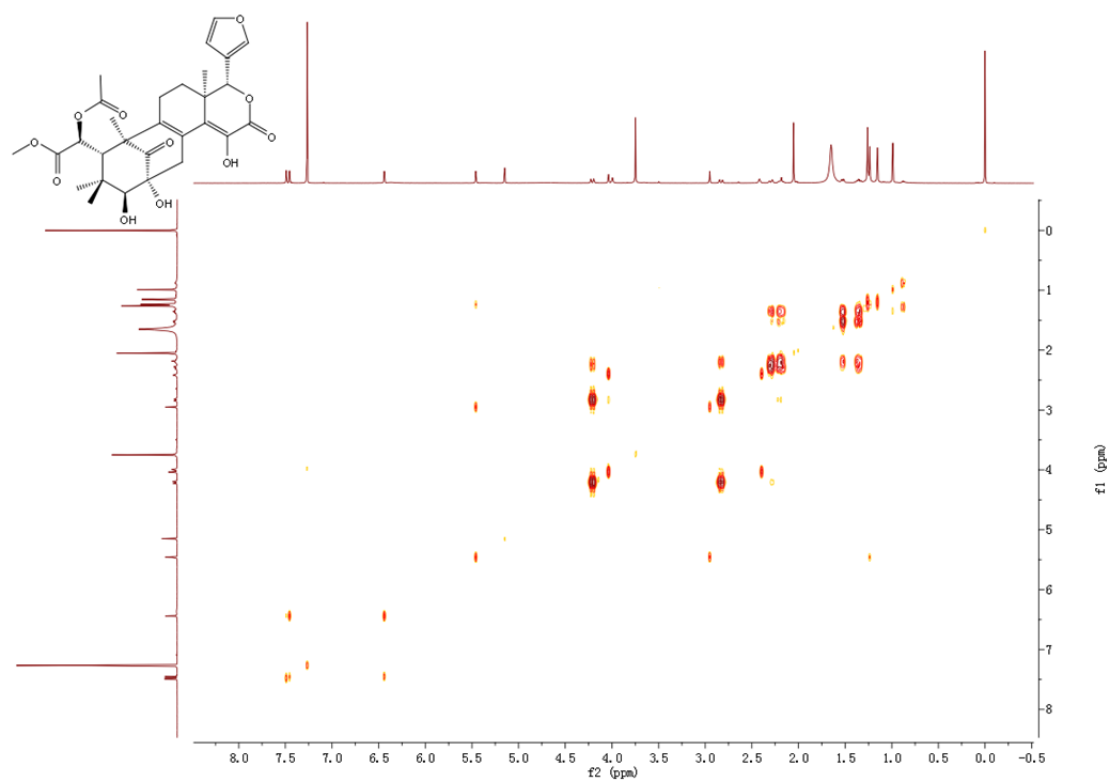


Fig. 43S ROESY NMR spectrum of compound **5** in CDCl₃

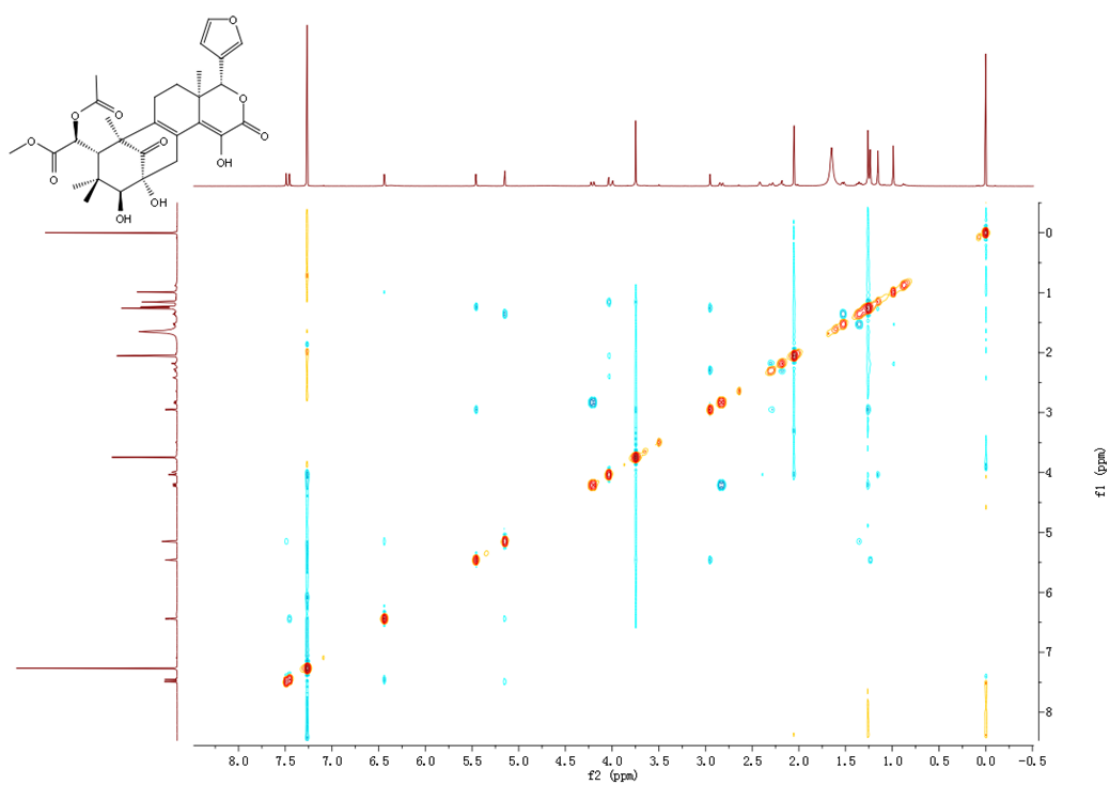
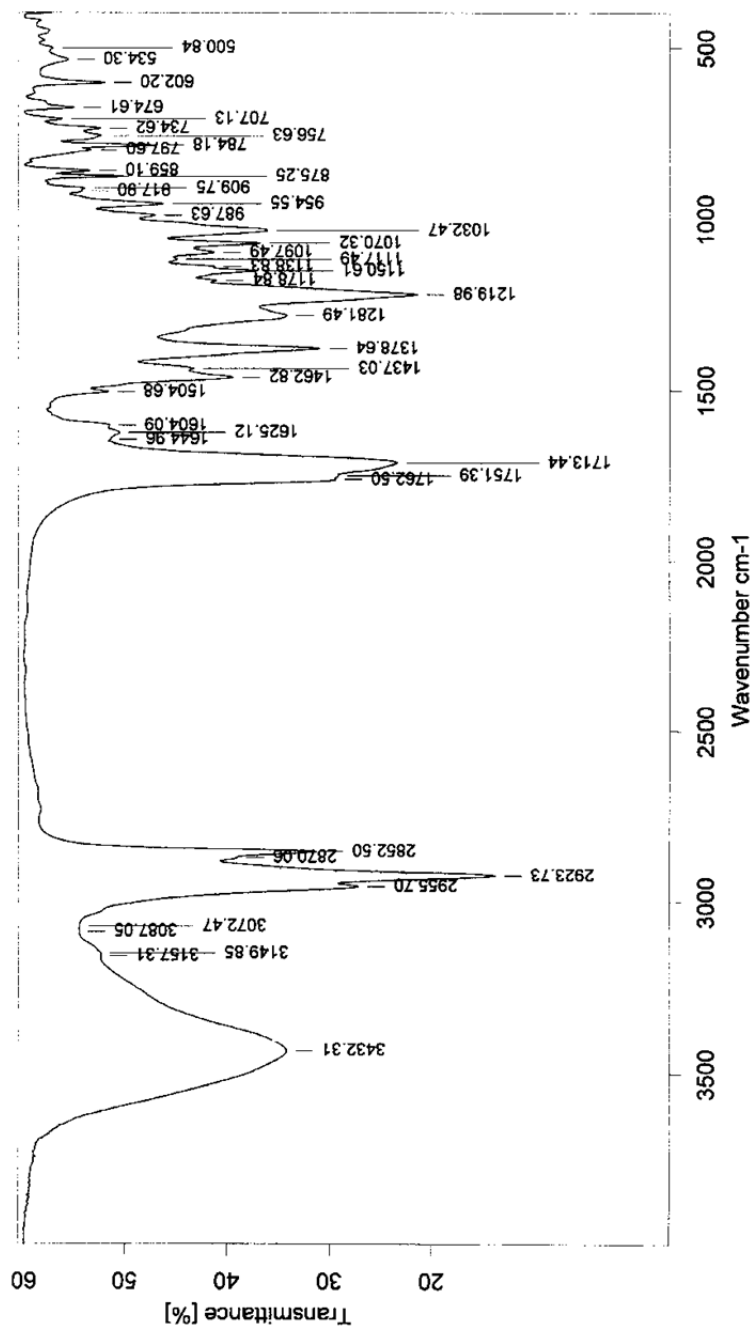


Fig. 44S IR spectrum of compound **5**



Sample : hht37	Frequency Range : 399.246 - 3996.32		Measured on : 12/12/2011	
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