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Briaviodiol A (4)

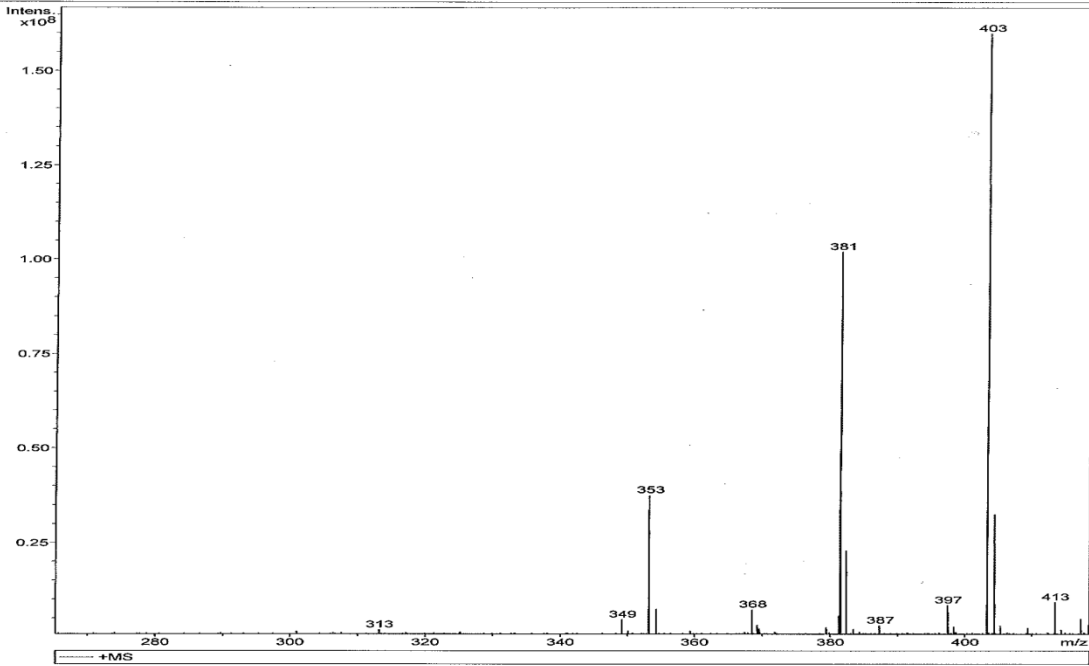
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FT-MS

Analysis Info

Analysis Name D:\Data\2\BVG74512_000004.d
Method broadband first signal
Sample Name BVG-7-4-5-1-2
Comment ESI Positive

7/12/2017 11:39:47 AM
Instrument: FT-MS solarix



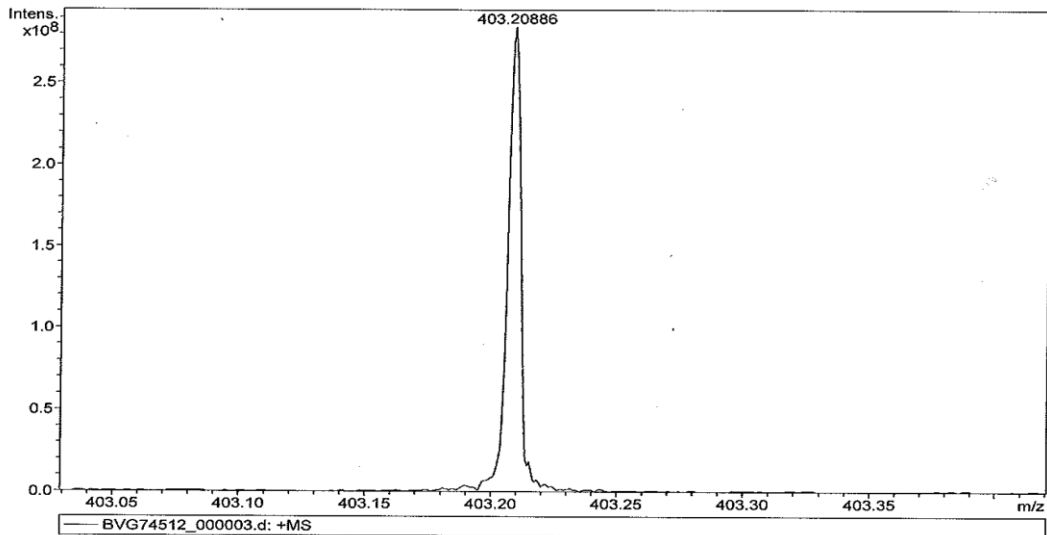
S 1-1 ESIMS spectrum of 1

Mass Spectrum SmartFormula Report

Analysis Info

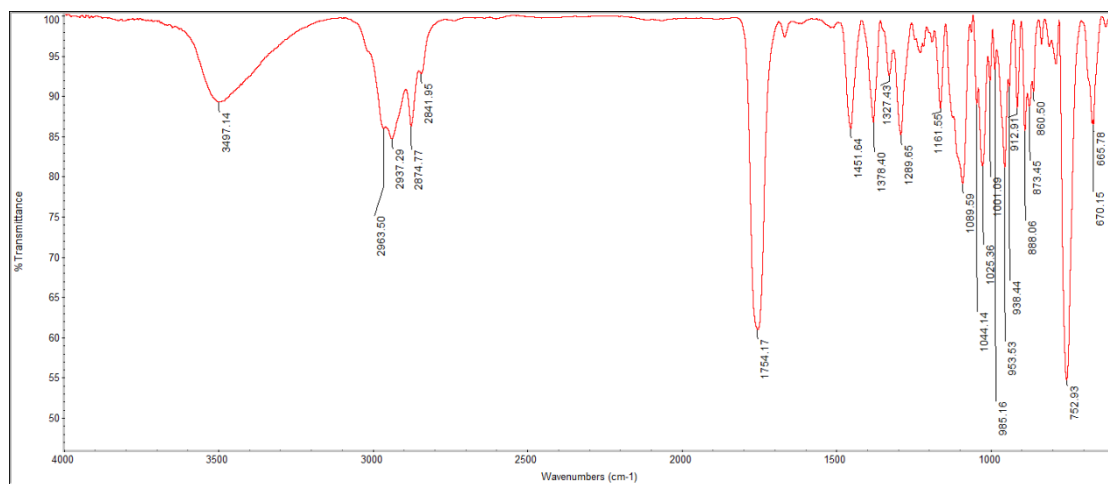
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Sample Name BVG-7-4-5-1-2
Comment ESI Positive

7/12/2017 11:38:53 AM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solarix

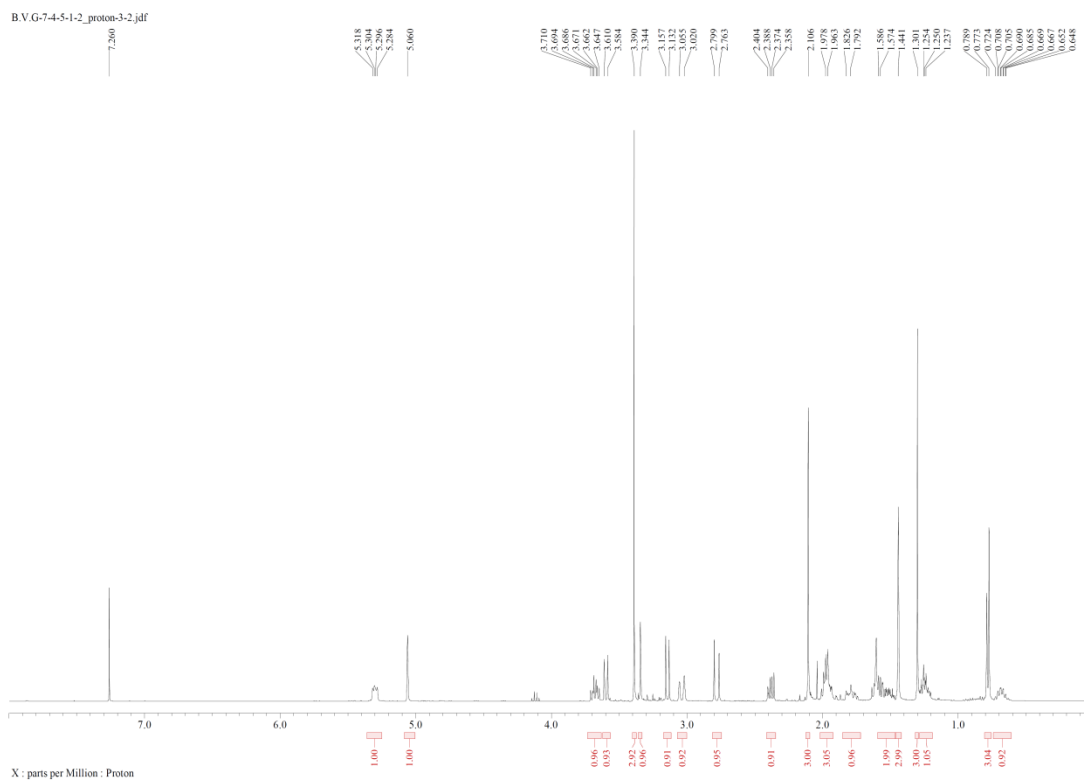


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
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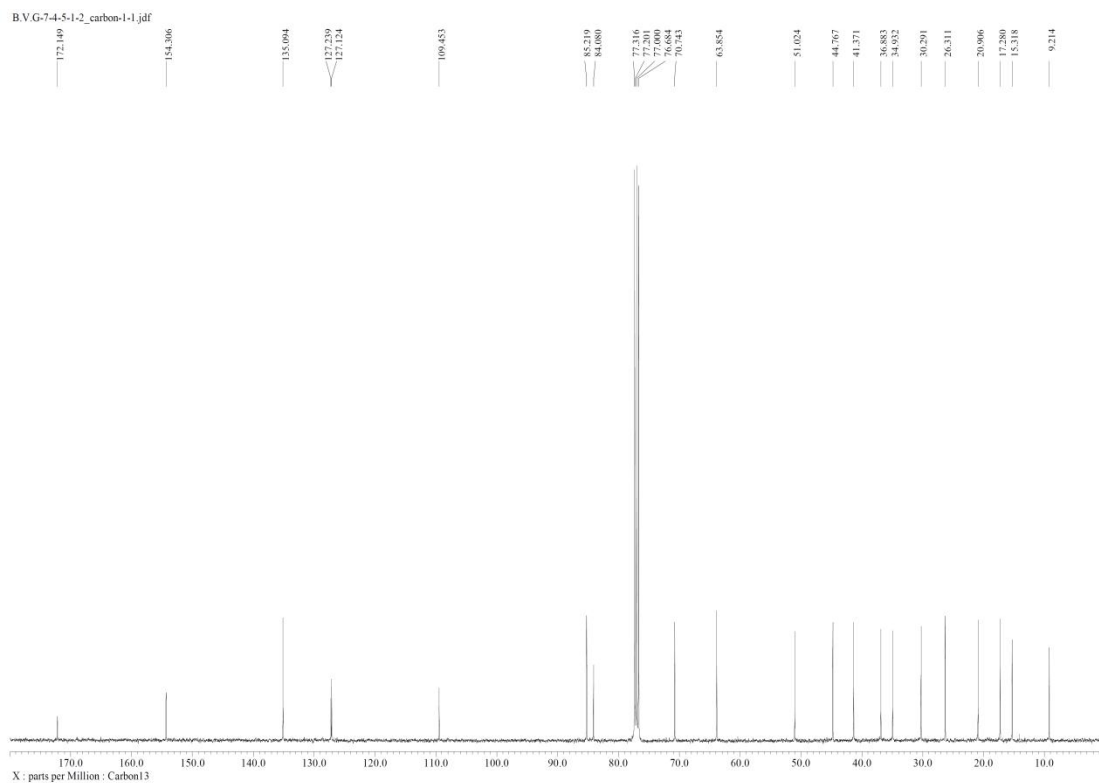
S 1-2 HRESIMS spectrum of 1



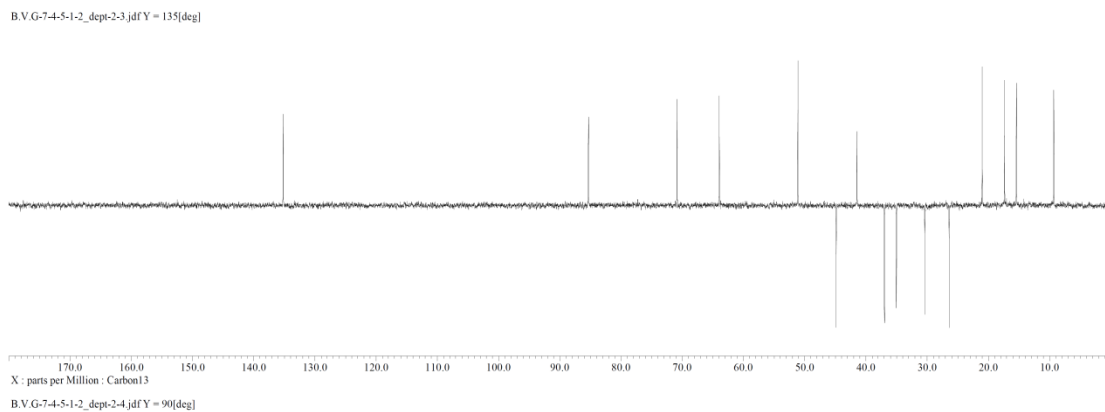
S 1-3 IR spectrum of **1**



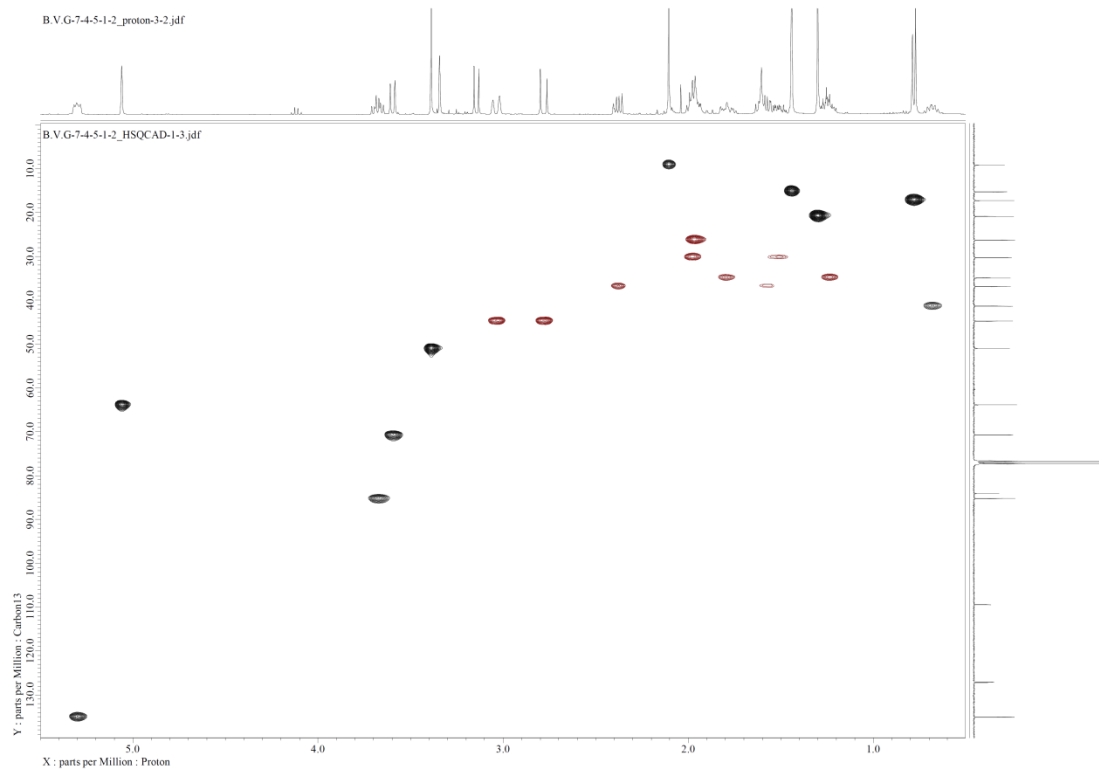
S 1-4 ^1H NMR spectrum of **1** (400 MHz, CDCl_3)



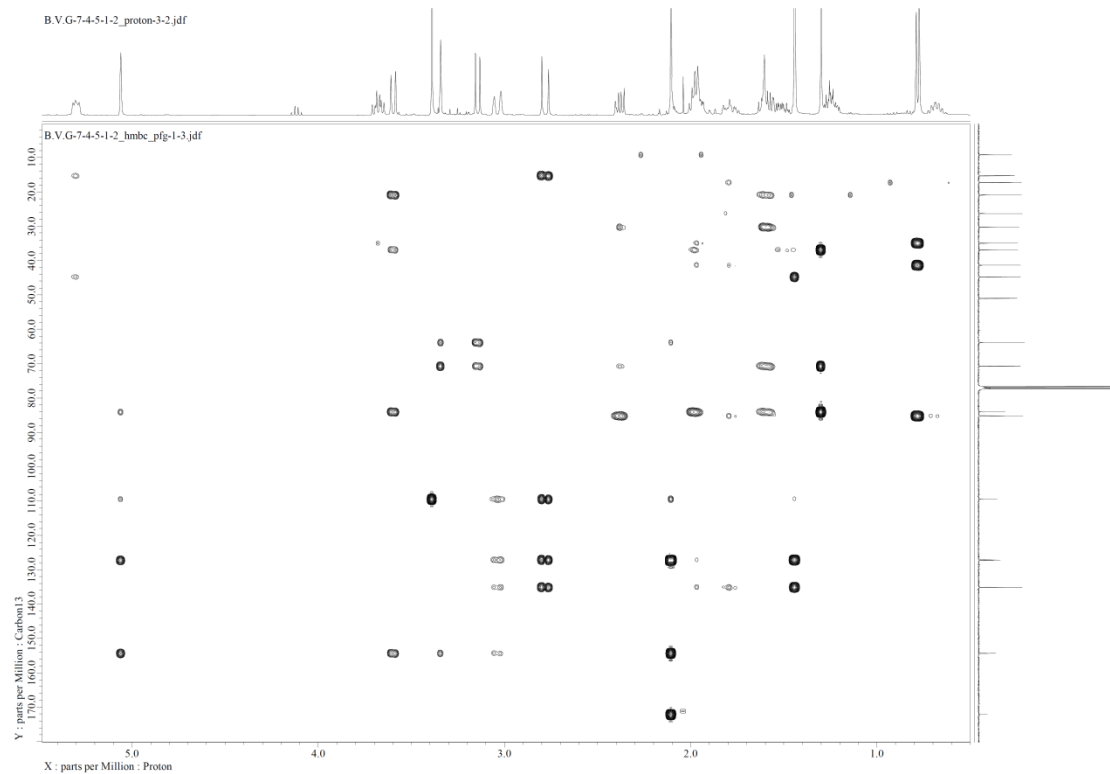
S 1-5 ^{13}C NMR spectrum of **1** (100 MHz, CDCl_3)



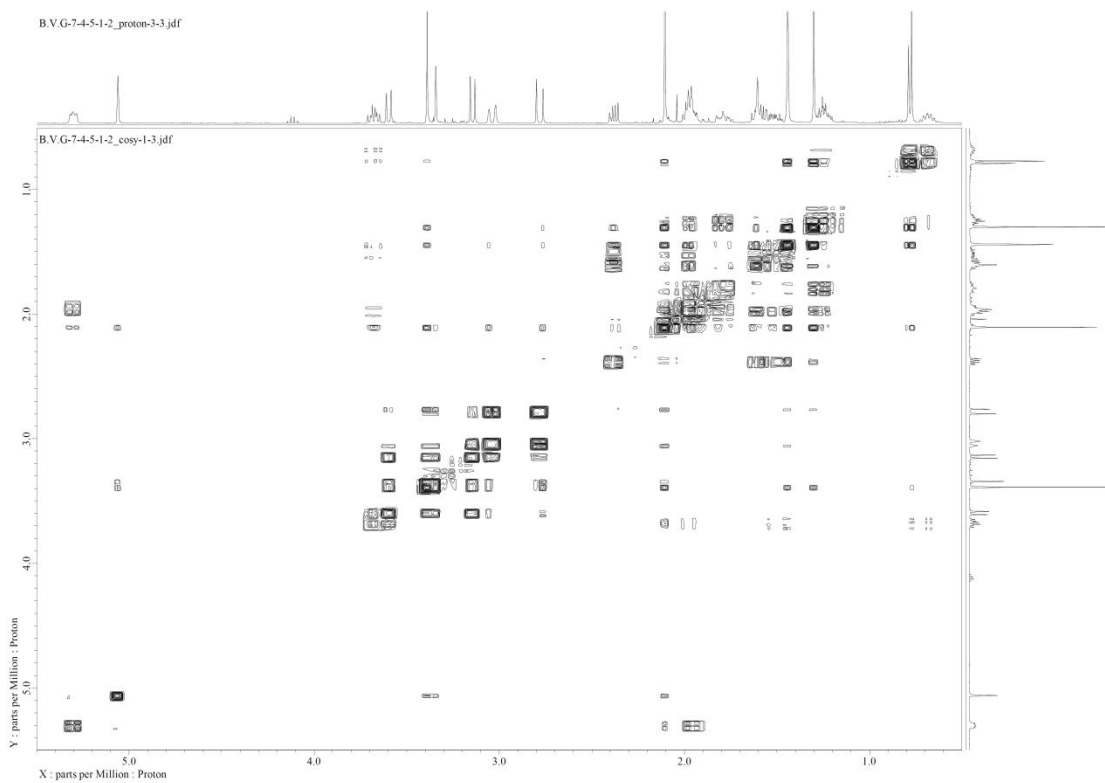
S 1-6 DEPT spectrum of **1**



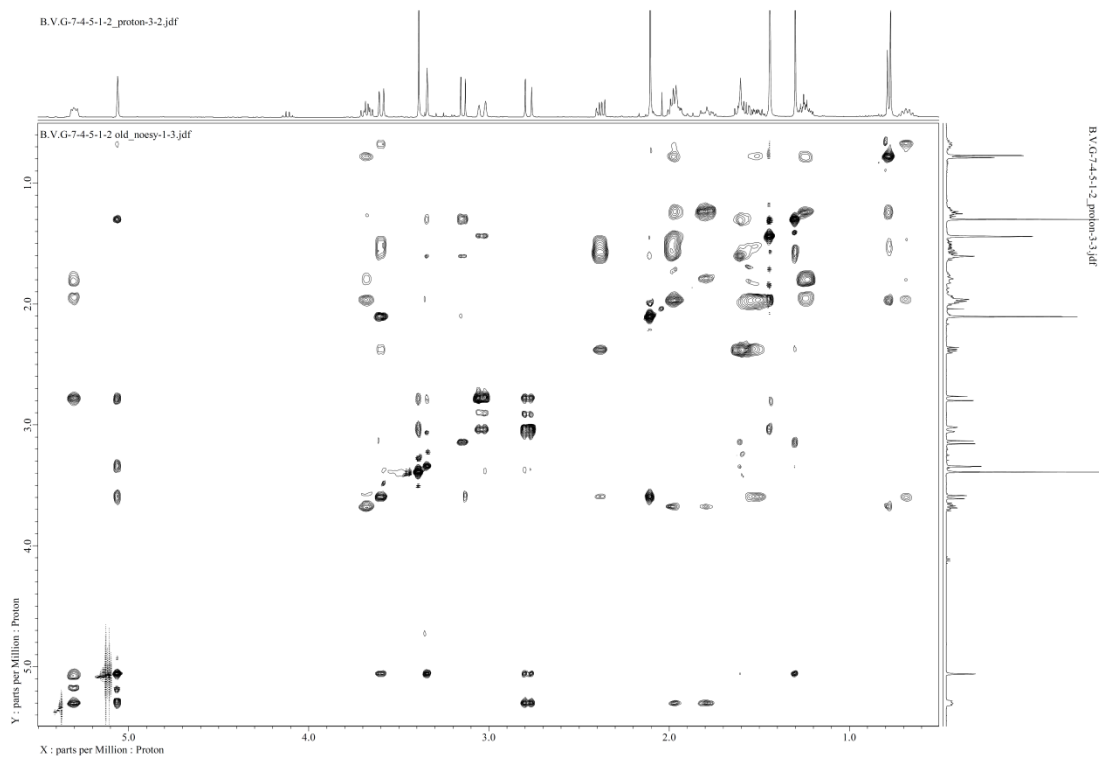
S 1-7 HSQC spectrum of **1**



S 1-8 HMBC spectrum of **1**



S 1-9 ^1H - ^1H COSY spectrum of **1**



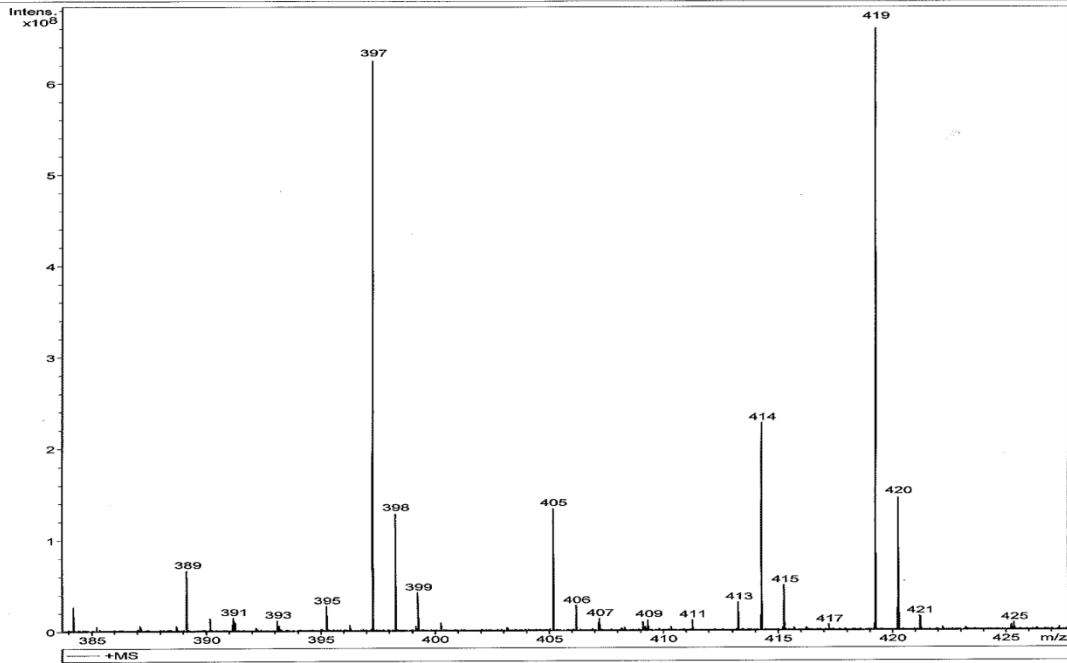
S 1-10 NOESY spectrum of **1**

FT-MS

Analysis Info

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 Sample Name BVG-7-8-6-1
 Comment ESI Positive

1/17/2018 3:54:26 PM
 Instrument: FT-MS solarix



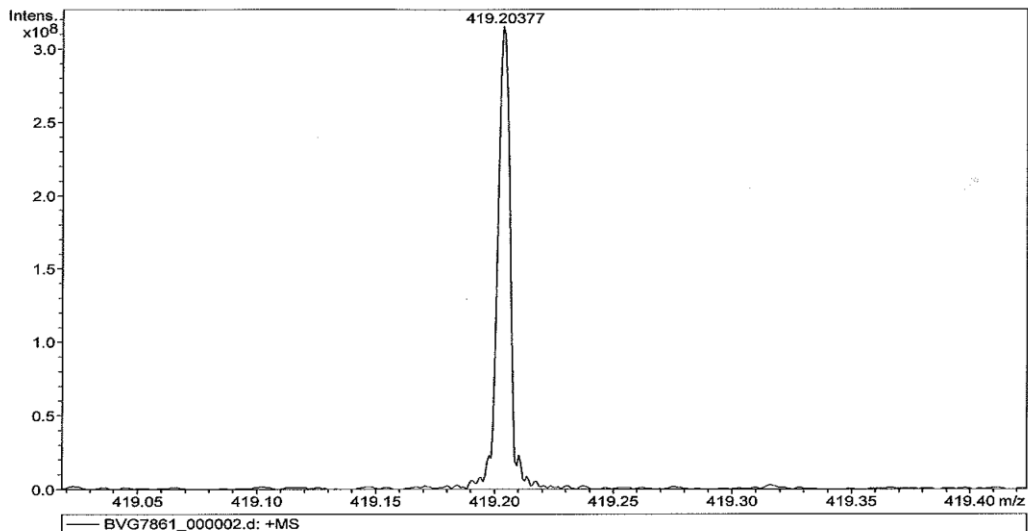
S 2-1 ESIMS spectrum of 2

Mass Spectrum SmartFormula Report

Analysis Info

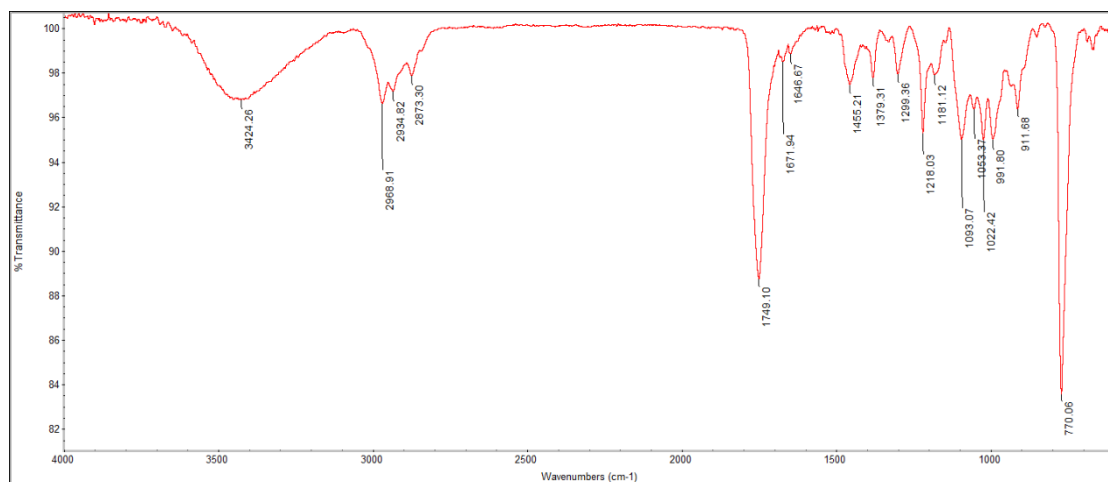
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 Comment ESI Positive

1/17/2018 3:53:21 PM
 Operator: YU HSIAO-CHING
 Instrument: BRUKER FT-MS solarix

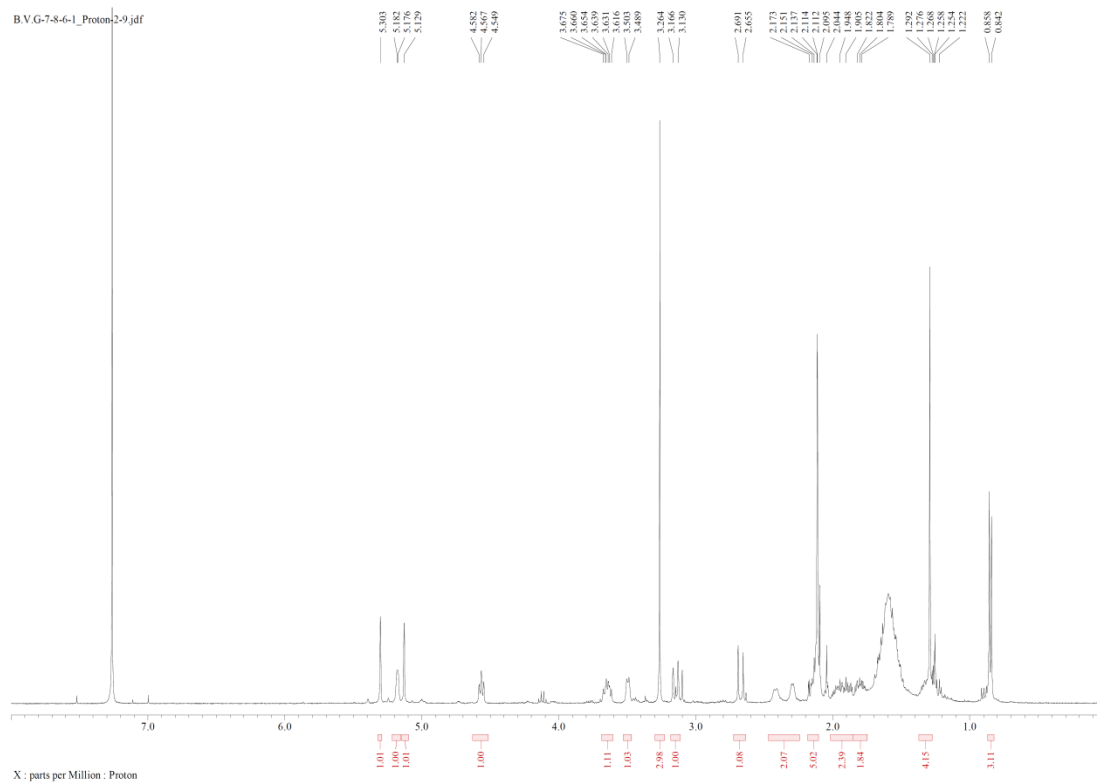


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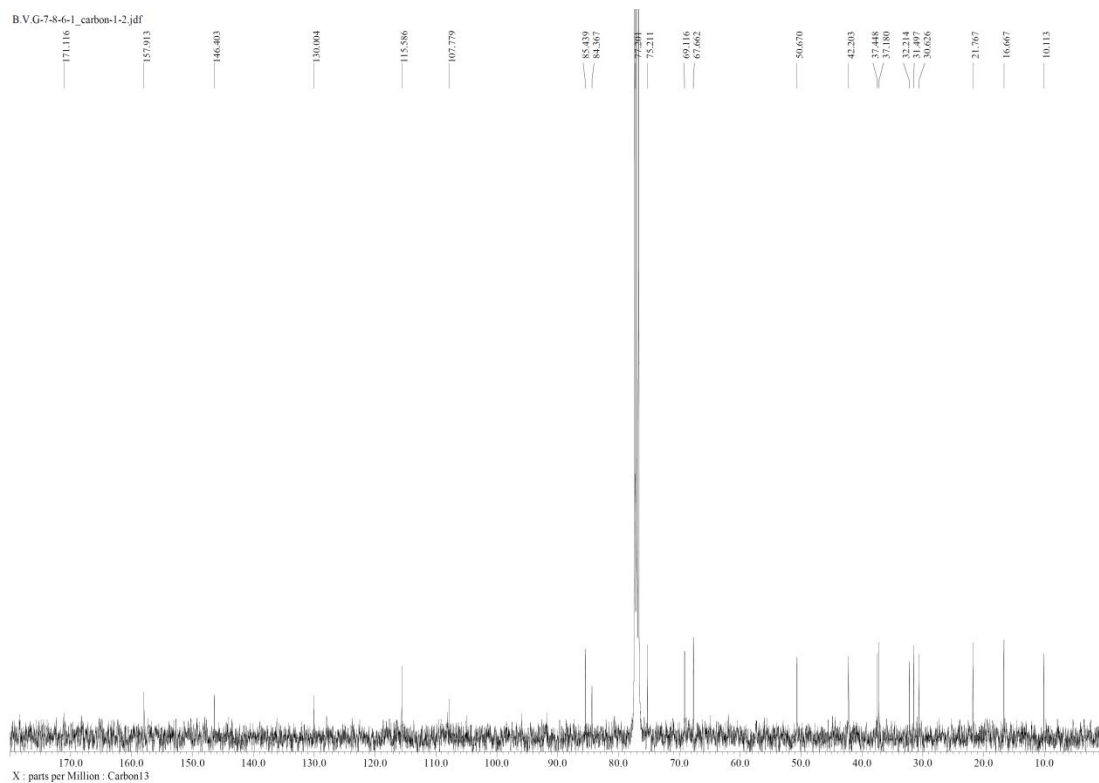
S 2-2 HRESIMS spectrum of 2



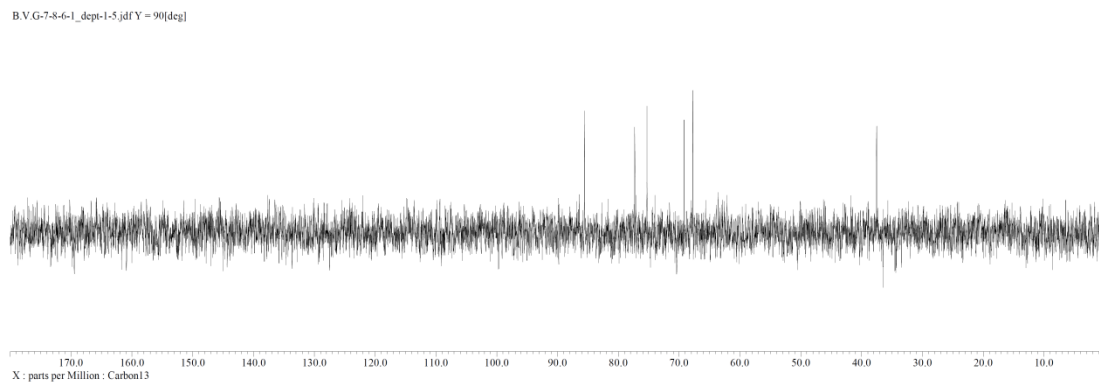
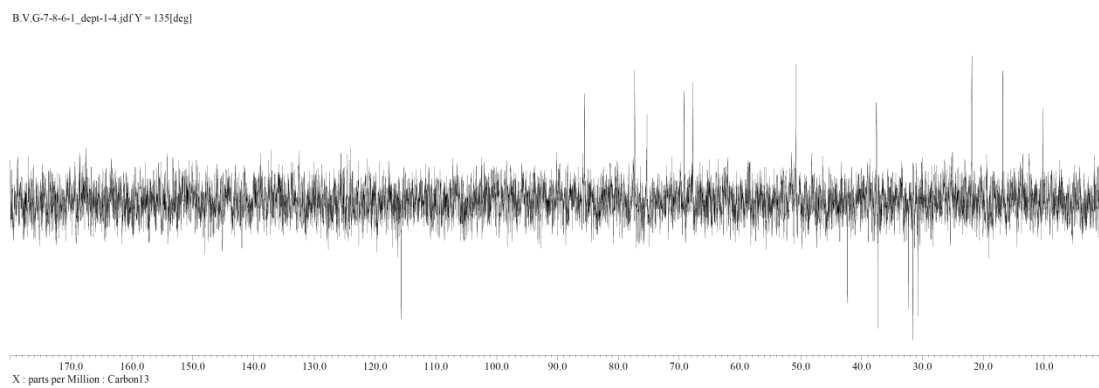
S 2-3 IR spectrum of 2



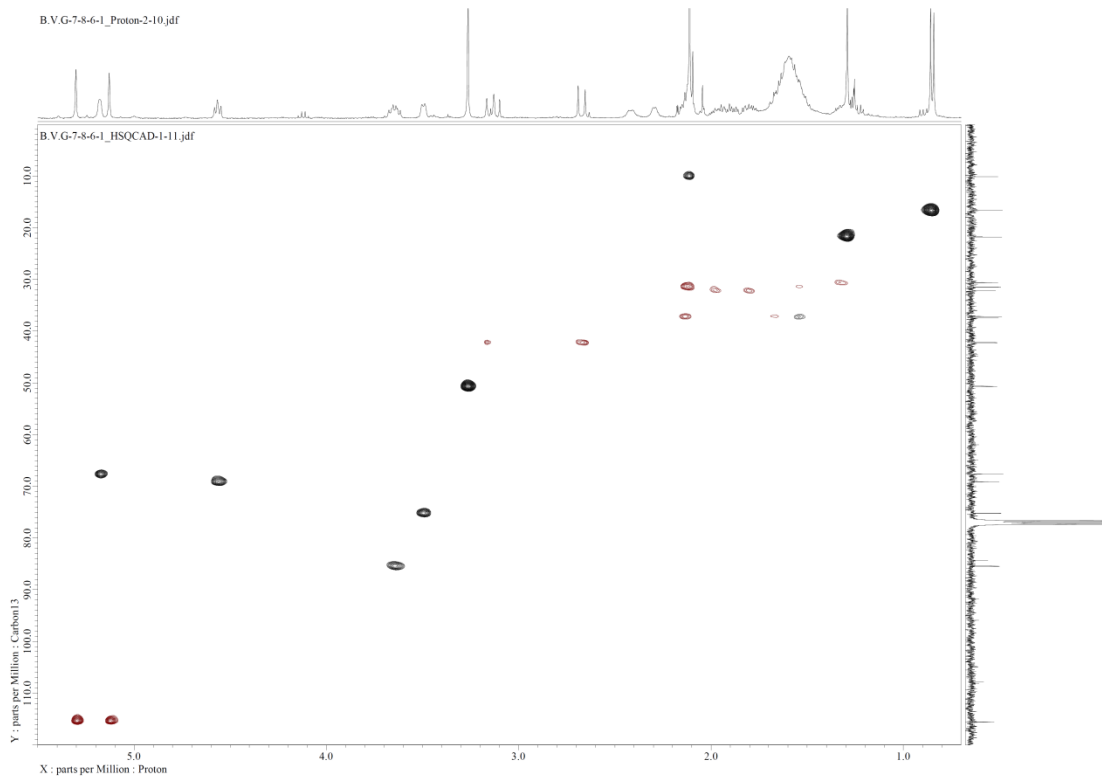
S 2-4 ¹H NMR spectrum of 2 (400 MHz, CDCl₃)



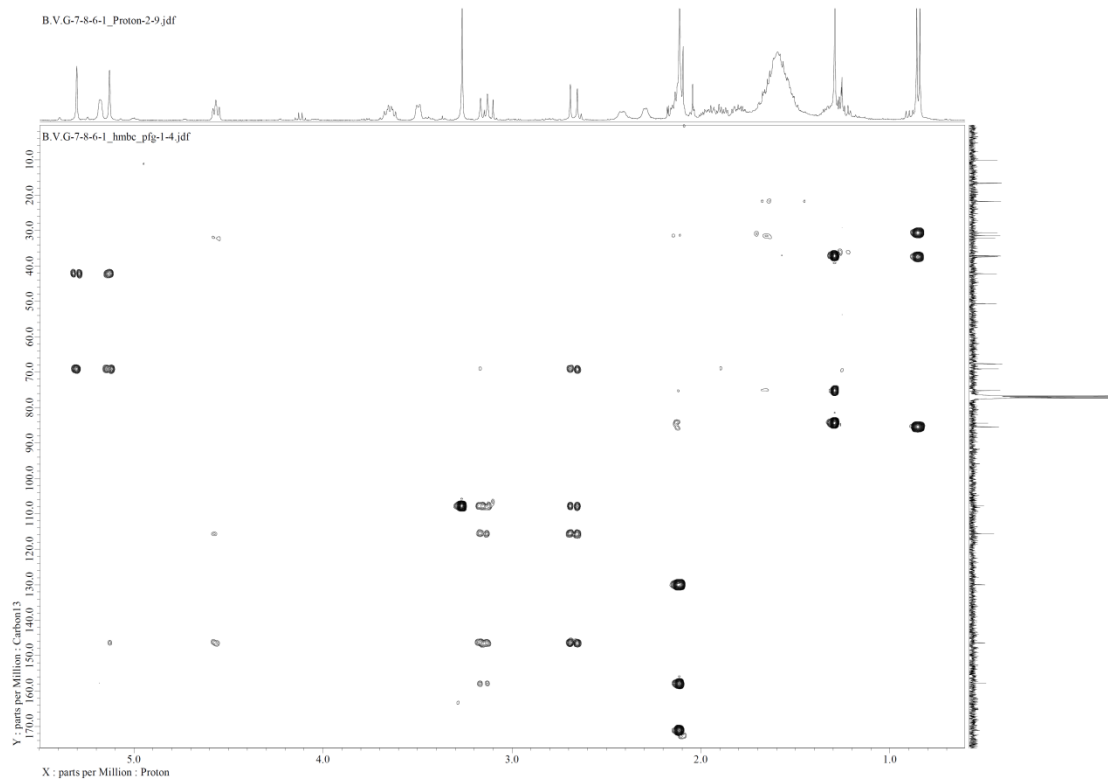
S 2-5 ^{13}C NMR spectrum of **2** (100 MHz, CDCl_3)



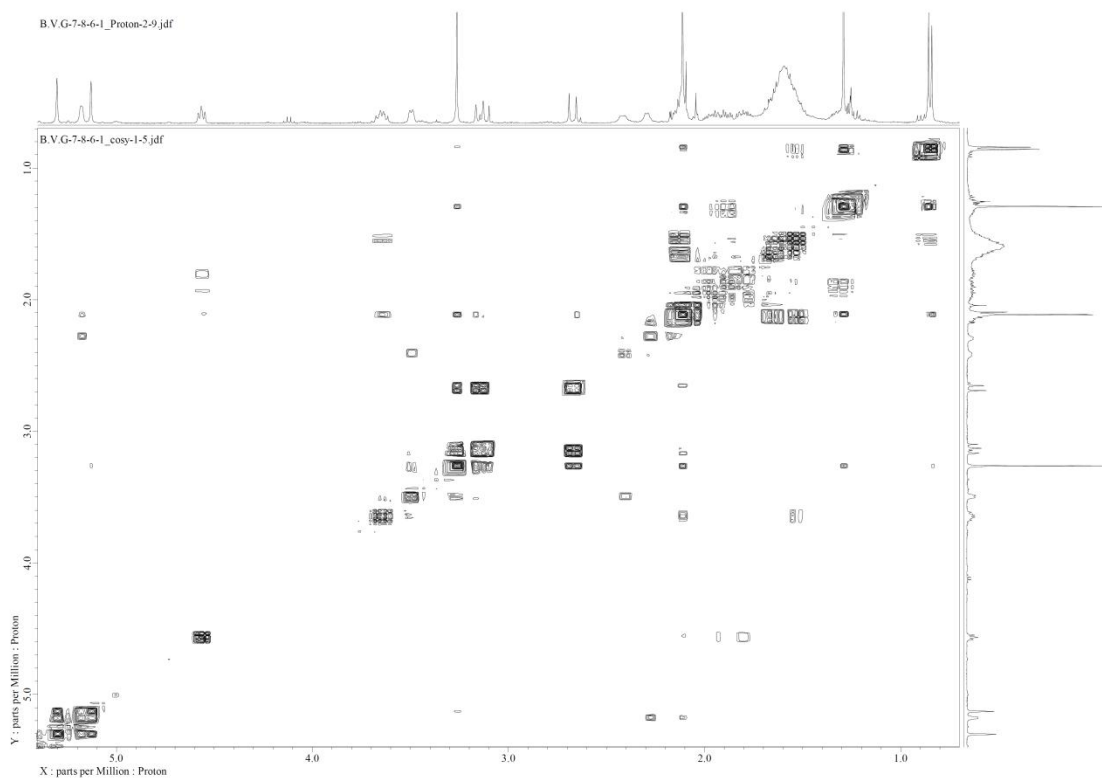
S 2-6 DEPT spectrum of **2**



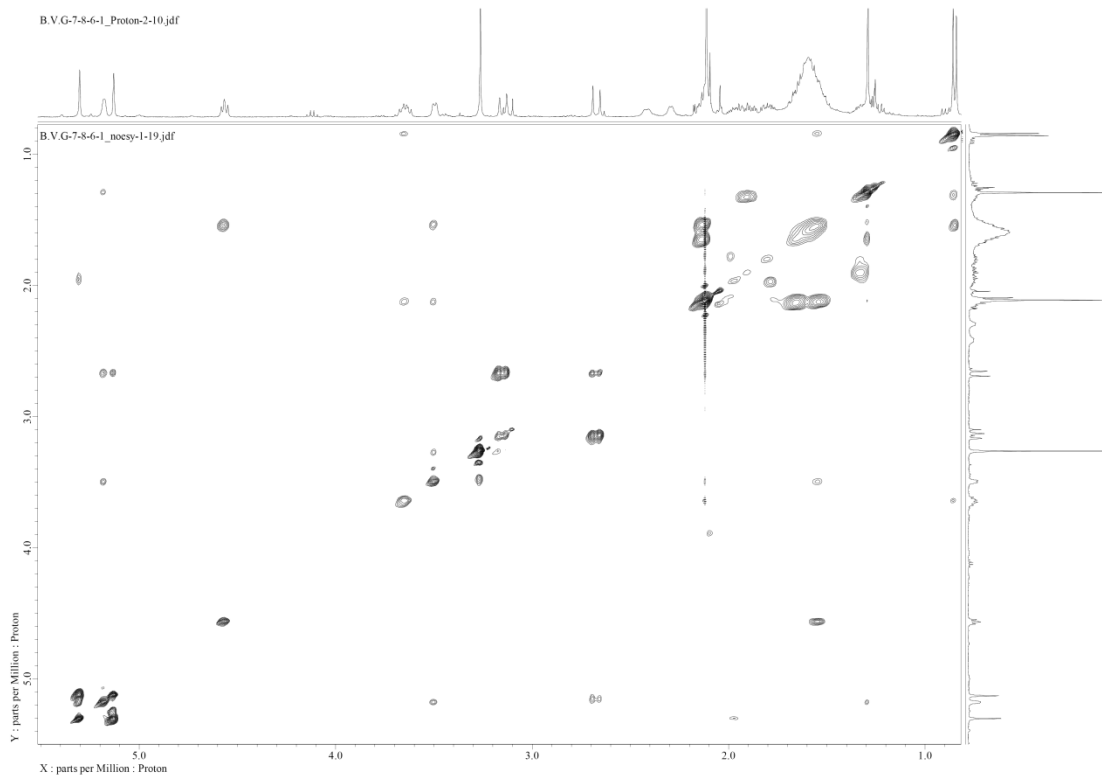
S 2-7 HSQC spectrum of **2**



S 2-8 HMBC spectrum of **2**



S 2-9 ^1H - ^1H COSY spectrum of **2**



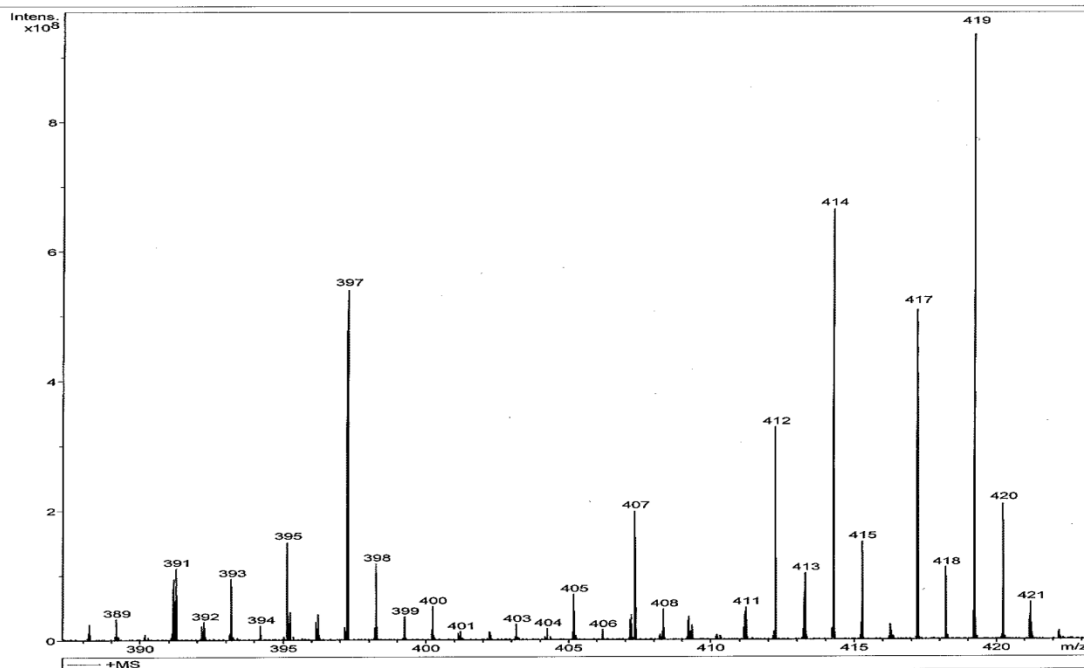
S 2-10 NOESY spectrum of **2**

FT-MS

Analysis Info

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 Sample Name BVG-7-4-10-5
 Comment ESI Positive

1/17/2018 3:32:24 PM
 Instrument: FT-MS solarix



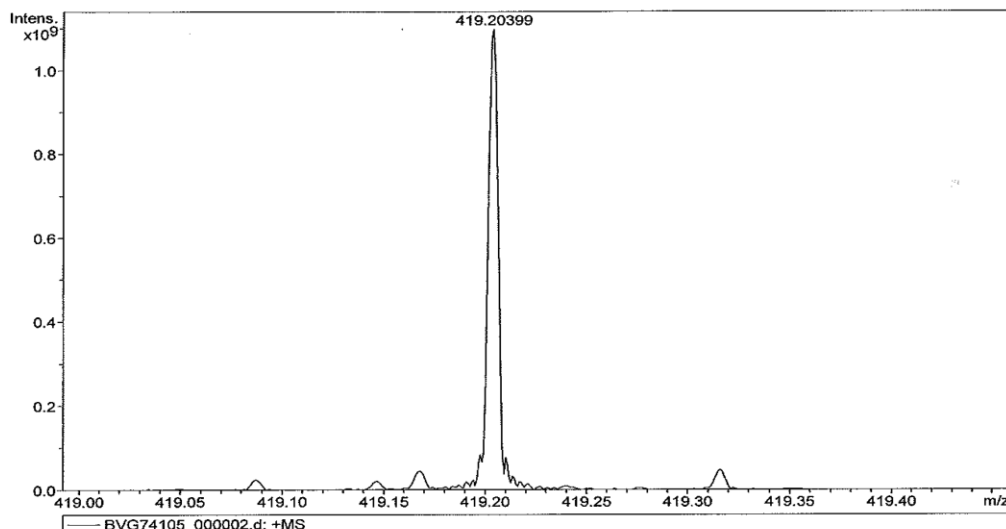
S 3-1 ESIMS spectrum of 3

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Analysis Info

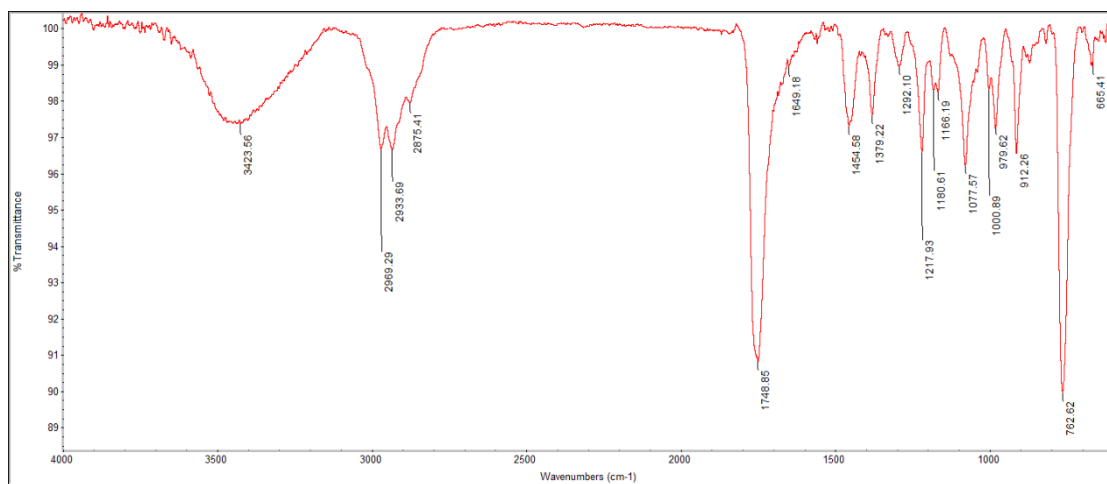
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 Comment ESI Positive

1/17/2018 3:31:24 PM
 Operator: YU HSIAO-CHING
 Instrument: BRUKER FT-MS solarix

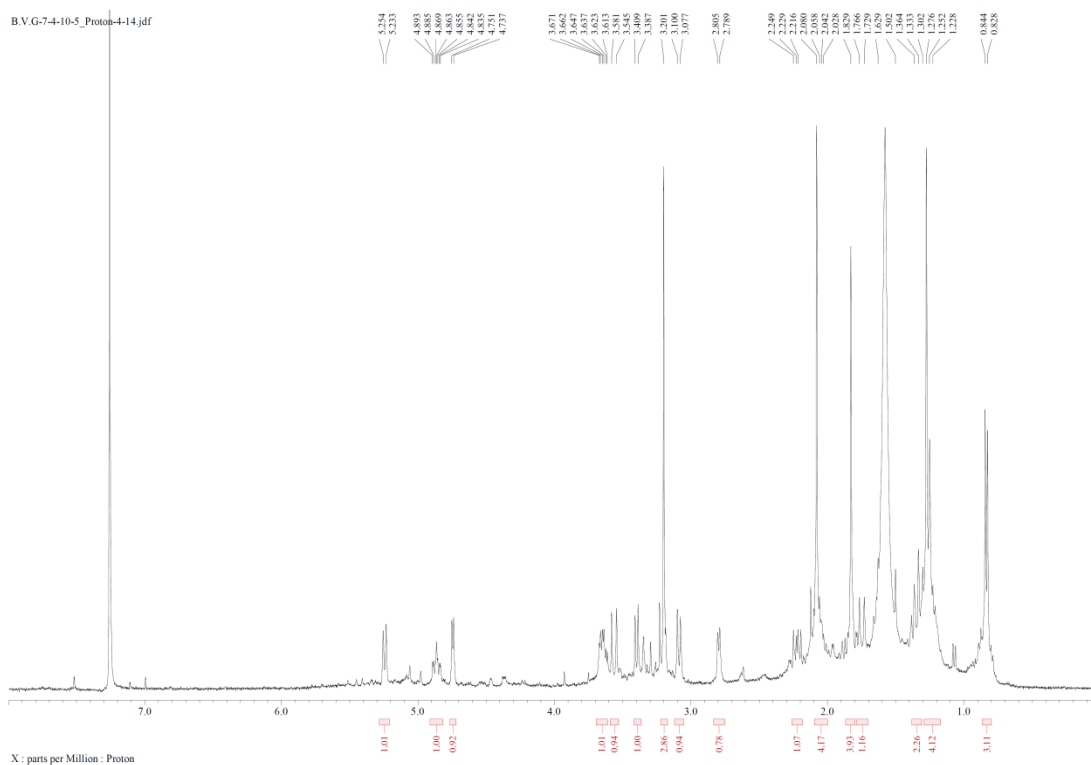


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
419.20399	1	C 21 H 32 Na O 7	100.00	419.20402	0.03	0.08	12.7	5.5	even	ok

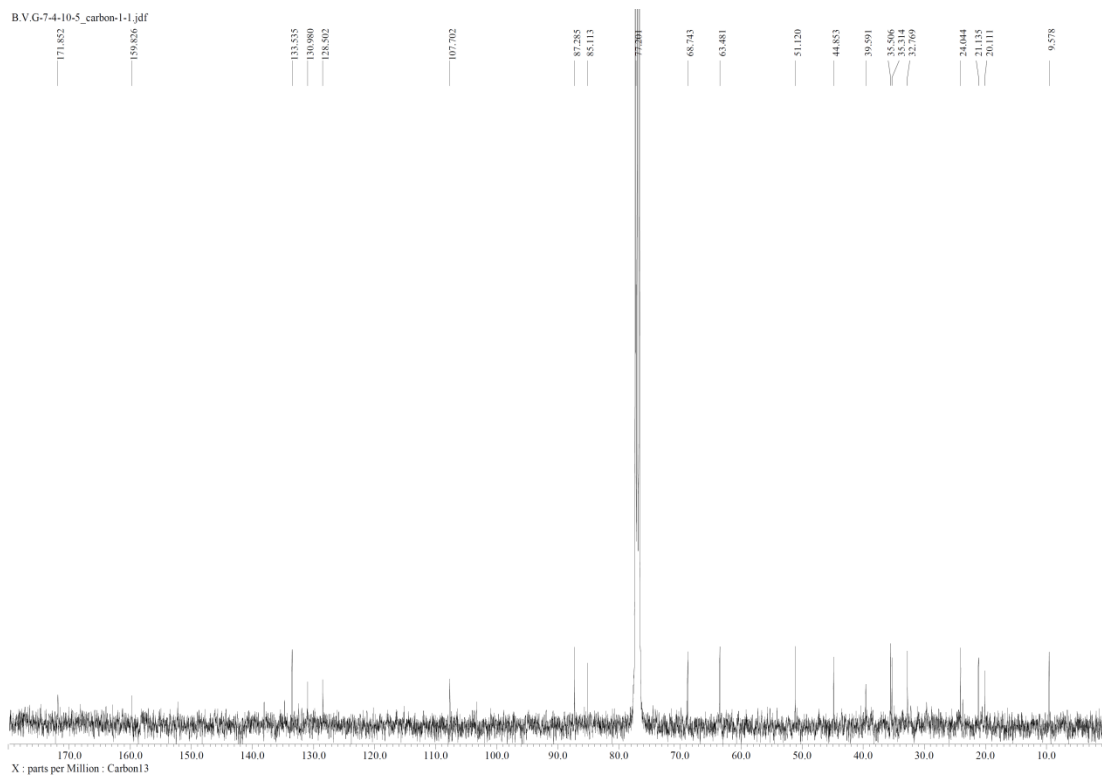
S 3-2 HRESIMS spectrum of 3



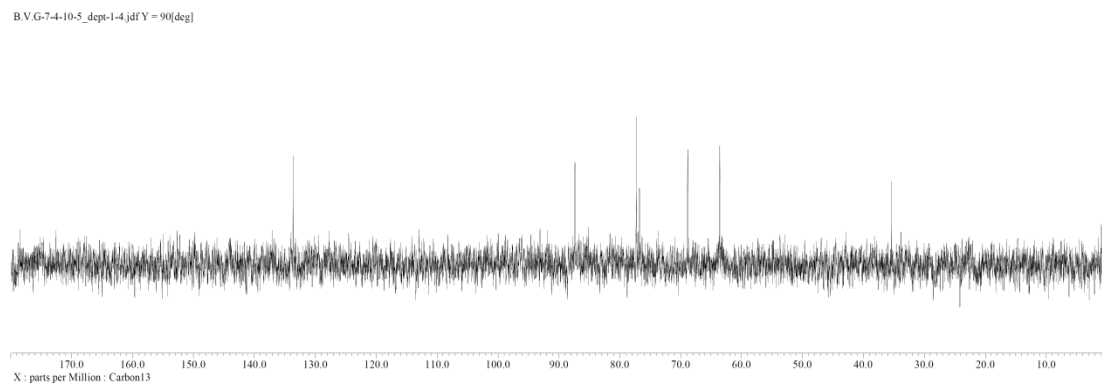
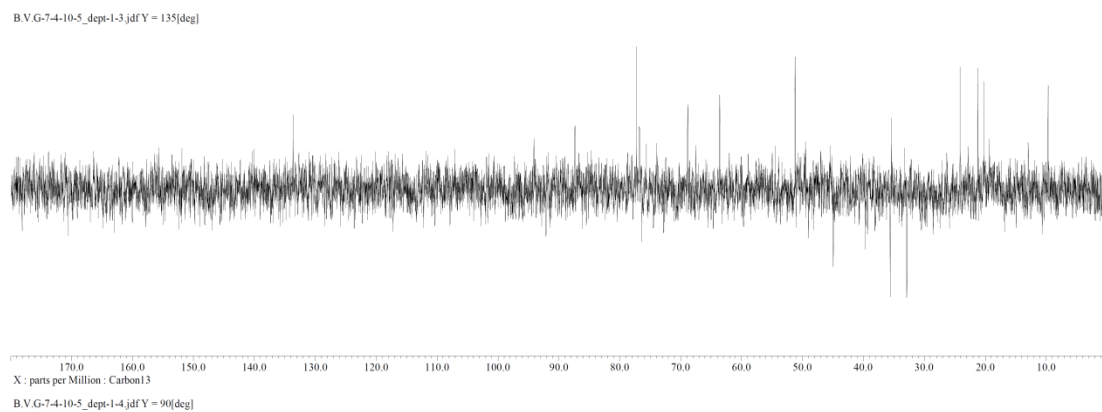
S 3-3 IR spectrum of **3**



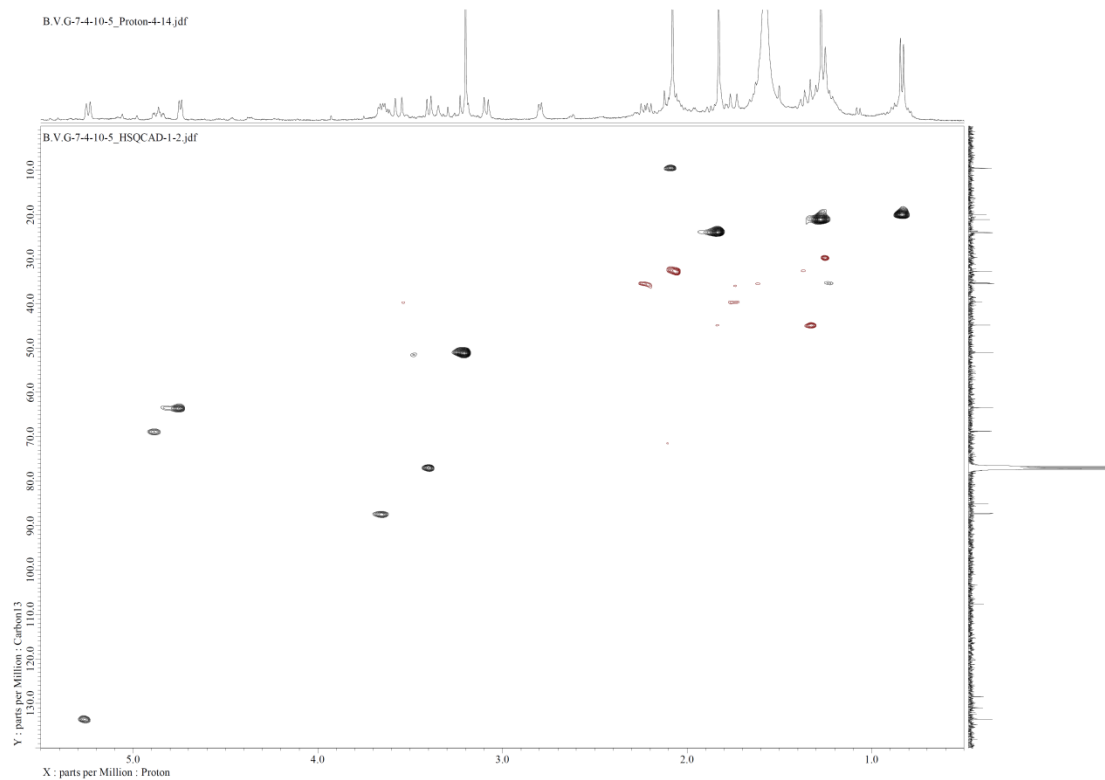
S 3-4 ¹H NMR spectrum of **3** (400 MHz, CDCl₃)



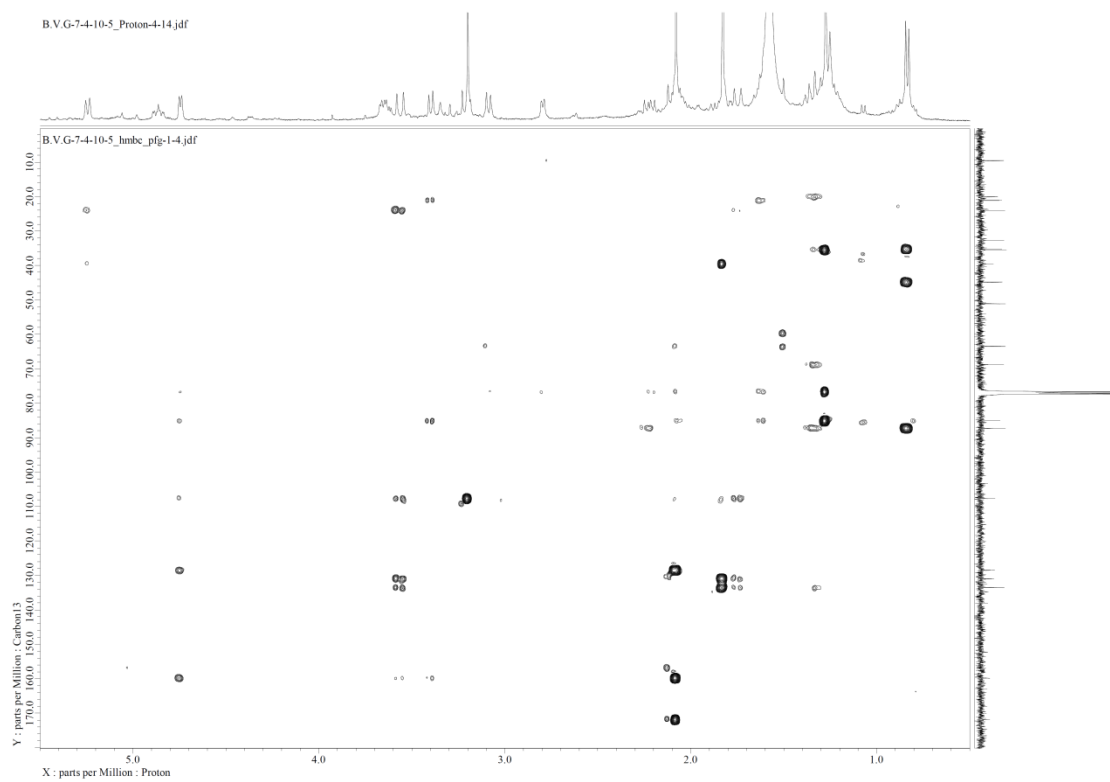
S 3-5 ^{13}C NMR spectrum of **3** (100 MHz, CDCl_3)



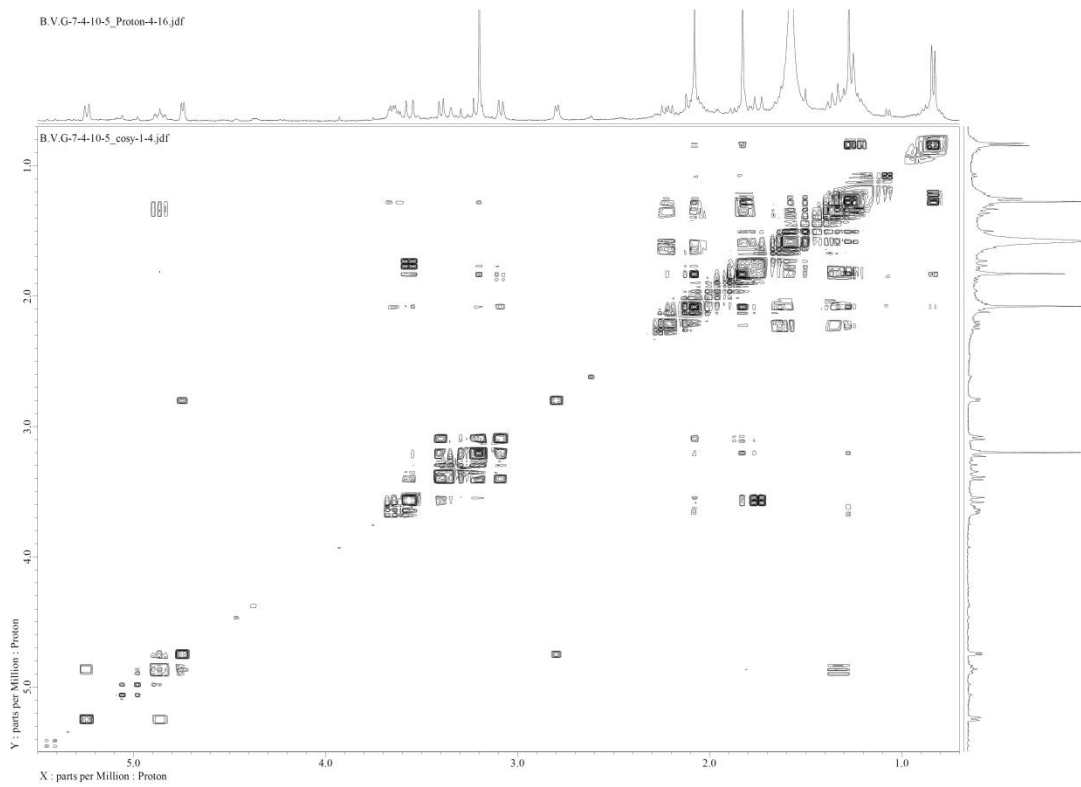
S 3-6 DEPT spectrum of **3**



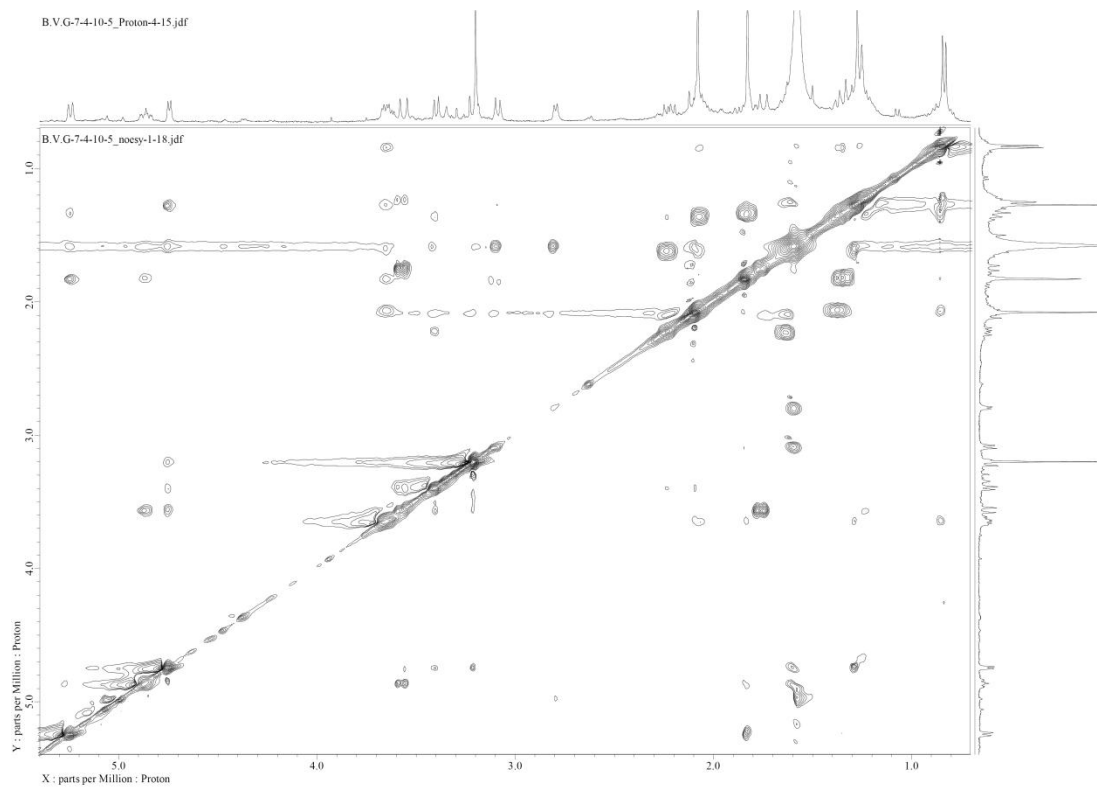
S 3-7 HSQC spectrum of **3**



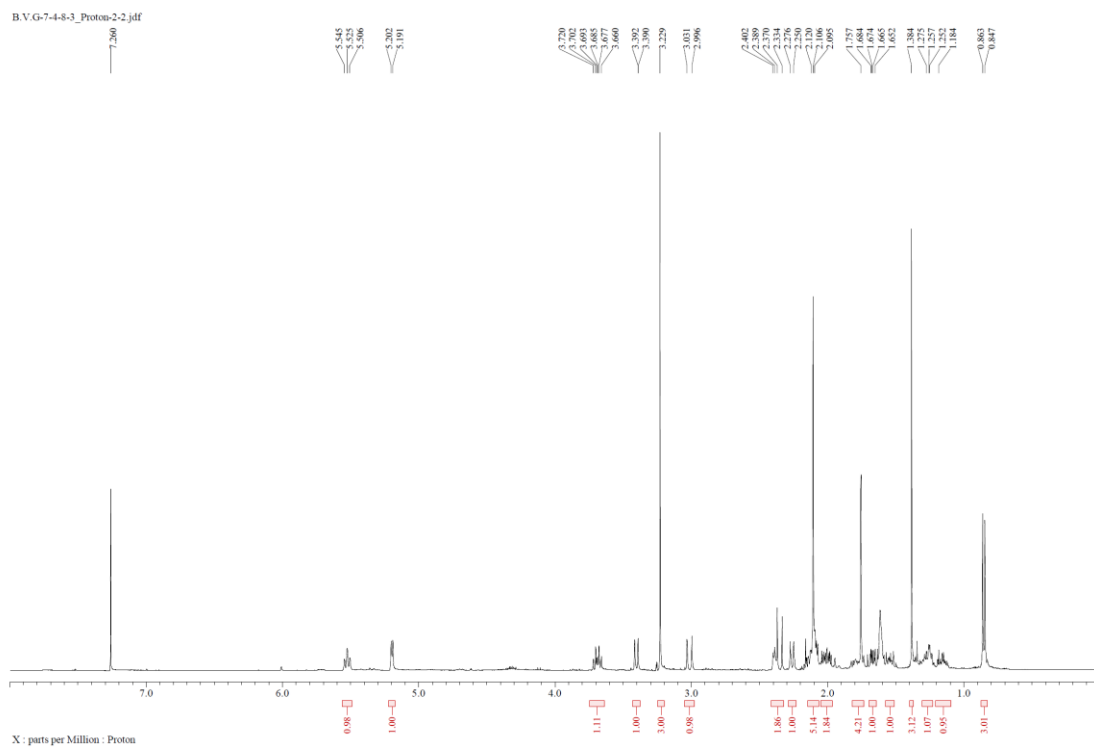
S 3-8 HMBC spectrum of **3**



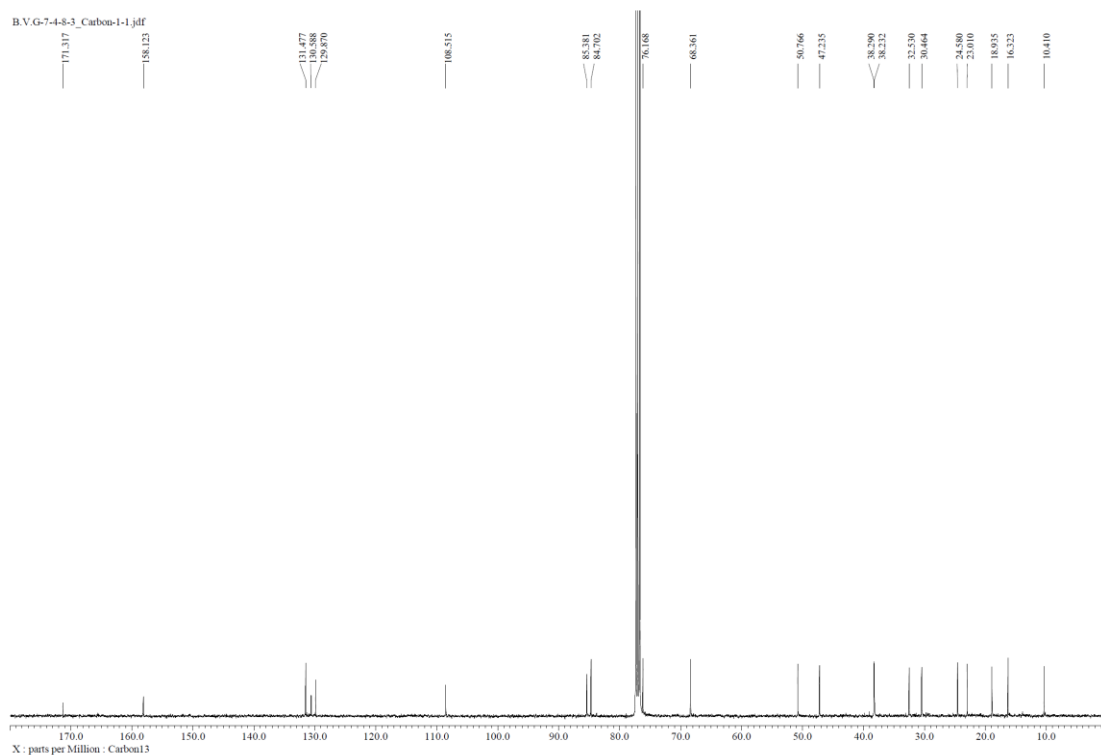
S 3-9 ^1H - ^1H COSY spectrum of **3**



S 3-10 NOESY spectrum of **3**



S 4-1 ^1H NMR spectrum of **4** (400 MHz, CDCl_3)



S 4-2 ^{13}C NMR spectrum of **4** (100 MHz, CDCl_3)