

Supporting Information

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A New Angular Naphthopyrone from Crinoid *Colobometra perspinosa*

Hsu-Ming Chung^{1*}, Ling-Tsung Hsiao¹, Zong-You Li^{1,2} and

Zhi-Hong Wen²

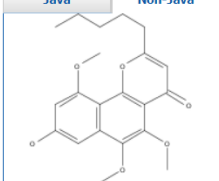
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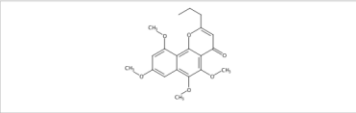
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

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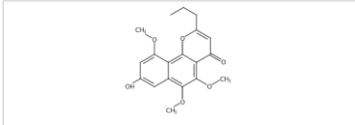
~1 




C₂₀ H₂₂ O₆
 4H-Naphtho[1,2-b]pyran-4-one, 5,6,8,10-tetramethoxy-2-propyl-
[Key Physical Properties](#)



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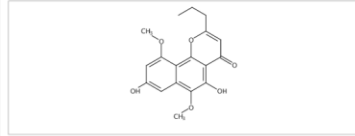
~14  ~3 




C₁₉ H₂₀ O₆
 4H-Naphtho[1,2-b]pyran-4-one, 8-hydroxy-5,6,10-trimethoxy-2-propyl-
[Key Physical Properties](#)
[Spectra](#)
[Experimental Properties](#)


Score: 90
☐ 3. 111397-48-9 

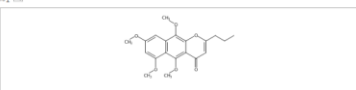
~13  ~6 




C₁₉ H₁₈ O₆
 4H-Naphtho[1,2-b]pyran-4-one, 5,8-dihydroxy-6,10-dimethoxy-2-propyl-
[Key Physical Properties](#)
[Spectra](#)
[Experimental Properties](#)


Score: 86
☐ 4. 60658-79-9 

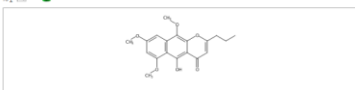
~1 




C₂₀ H₂₂ O₆
 4H-Naphtho[2,3-b]pyran-4-one, 5,6,8,10-tetramethoxy-2-propyl-
[Key Physical Properties](#)



Score: 85
☐ 5. 111397-50-3 

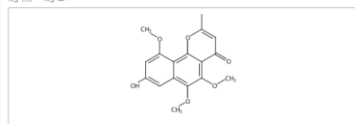
~1 



C₁₉ H₂₀ O₆
 4H-Naphtho[2,3-b]pyran-4-one, 5-hydroxy-6,8,10-trimethoxy-2-propyl-
[Key Physical Properties](#)
[Experimental Properties](#)

Score: 85
☐ 6. 1172585-04-4 

~3  ~3 



C₁₇ H₁₆ O₆
 4H-Naphtho[1,2-b]pyran-4-one, 8-hydroxy-5,6,10-trimethoxy-2-methyl-
[Key Physical Properties](#)

Figure S1: Scifinder Search Results of 1

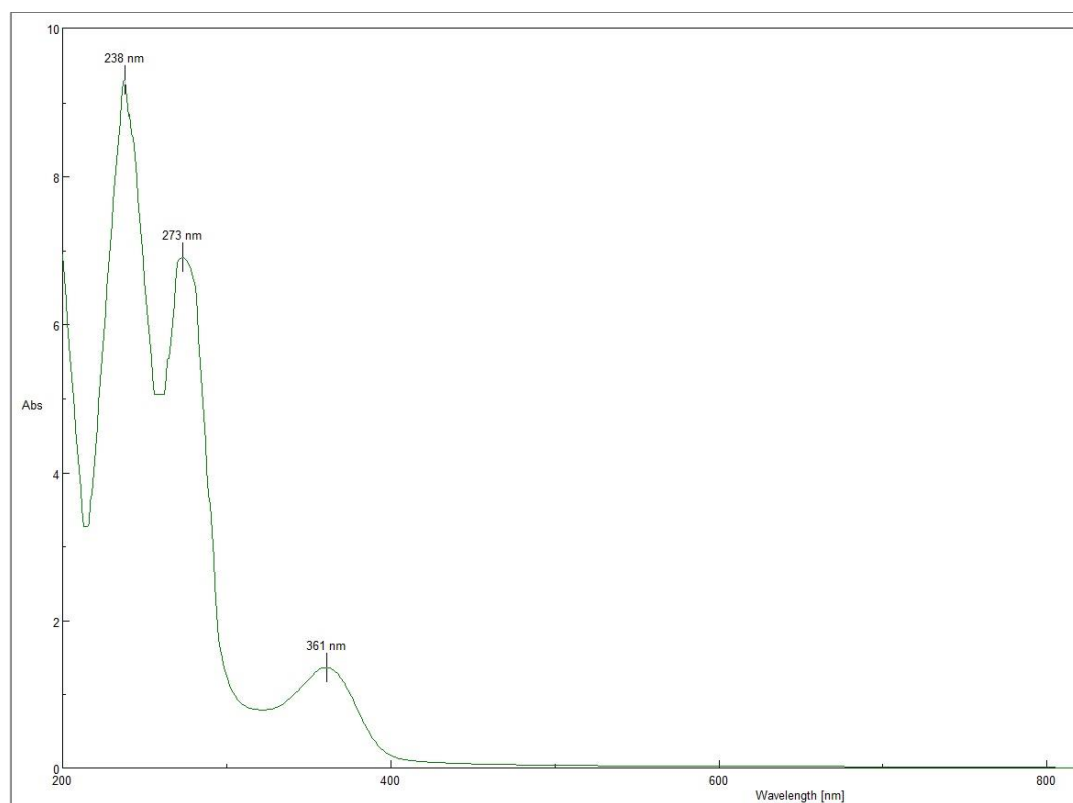


Figure S2: UV spectrum of **1** in EtOH

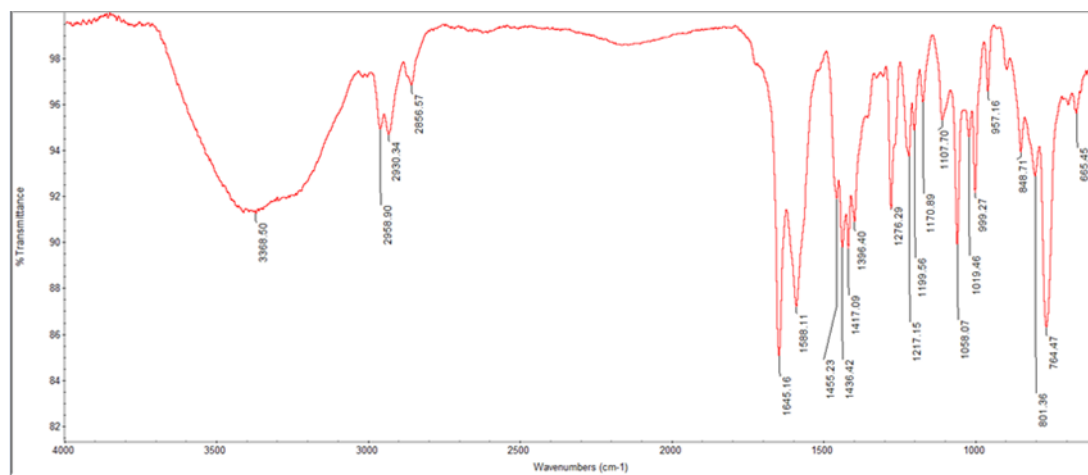


Figure S3: IR Spectrum of **1** in CDCl₃

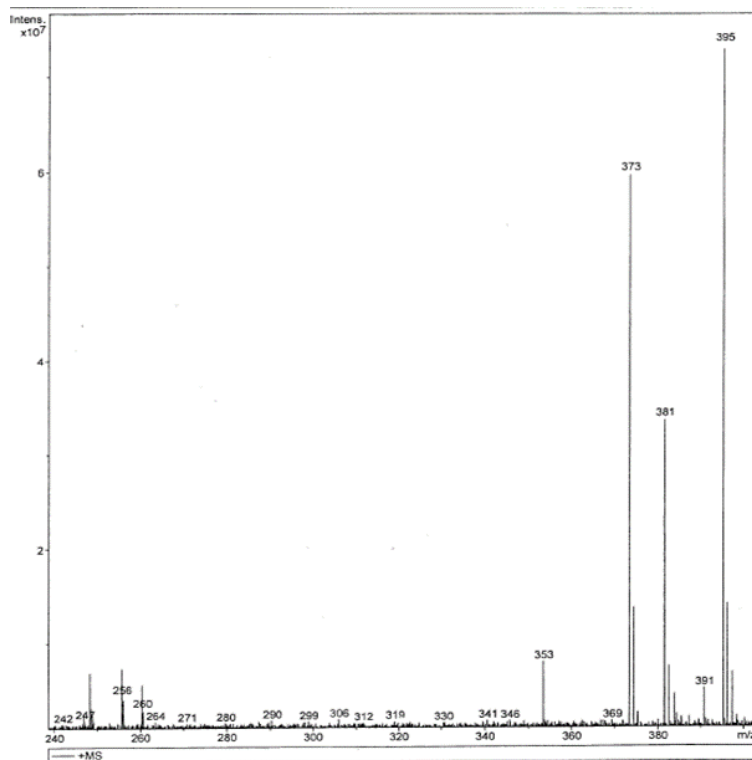


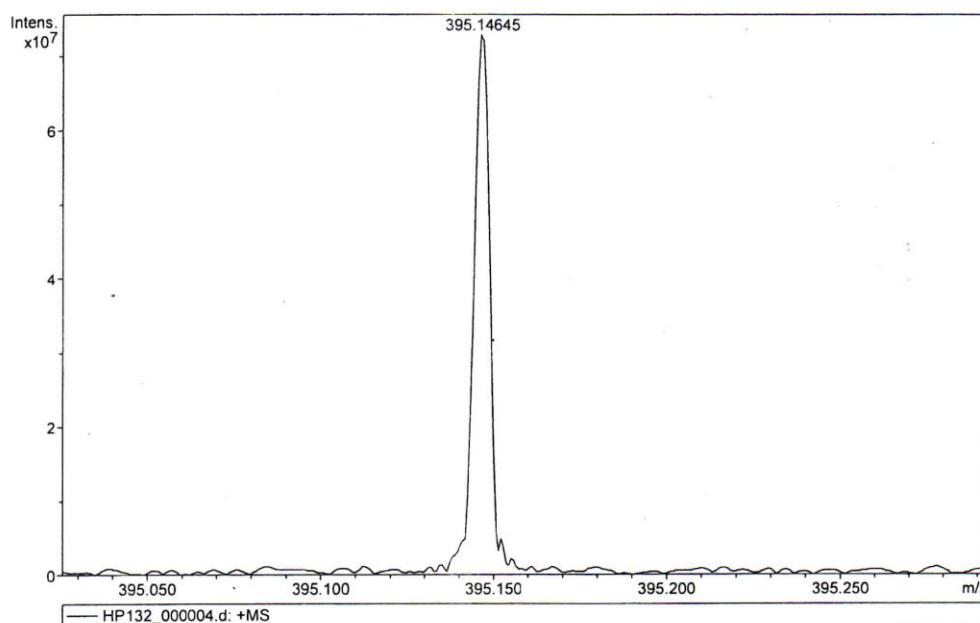
Figure S4: ESIMS spectrum of 1

Mass Spectrum SmartFormula Report

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 Method broadband first signal
 Sample Name HP-13-2
 Comment ESI Positive

9/6/2016 3:25:10 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
395.14645	1	C ₂₁ H ₂₄ NaO ₆	100.00	395.14651	0.06	0.16	21.2	9.5	even		ok

Figure S5: HRESIMS spectrum of **1**

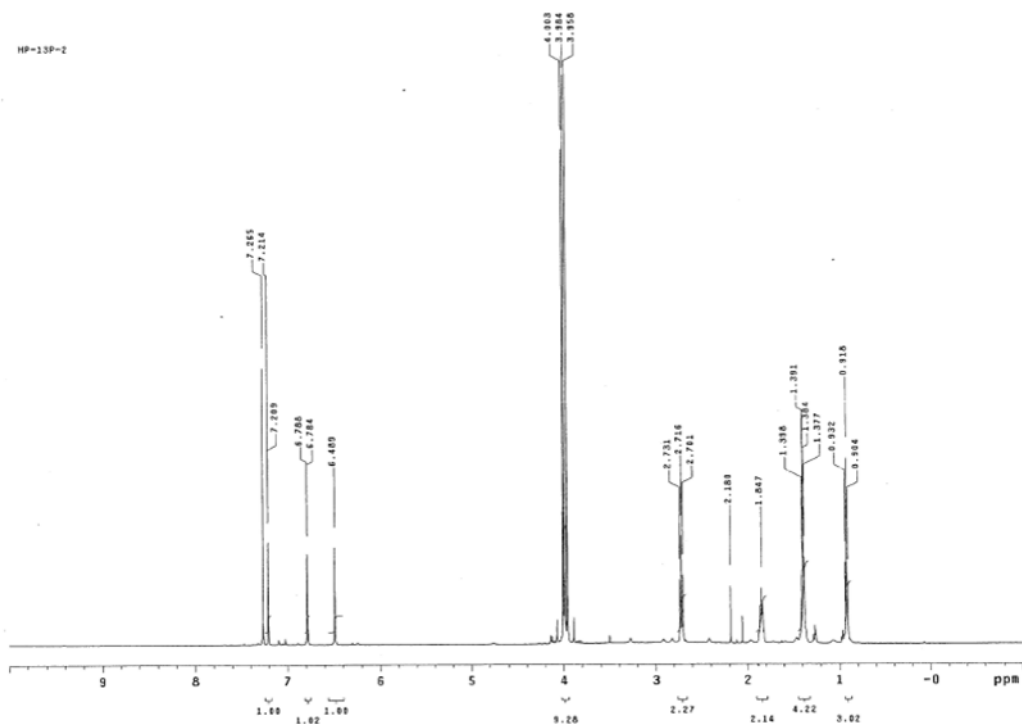


Figure S6: ^1H NMR Spectrum of **1** in CDCl_3 (500 MHz)

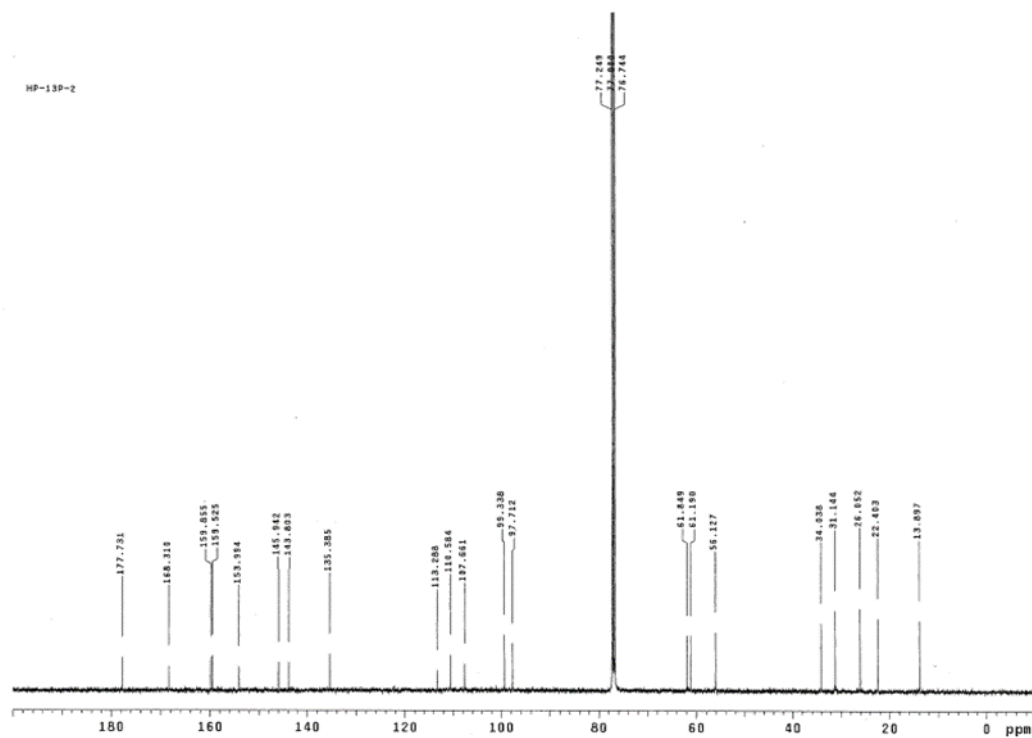


Figure S7: ^{13}C NMR Spectrum of **1** in CDCl_3 (125 MHz)

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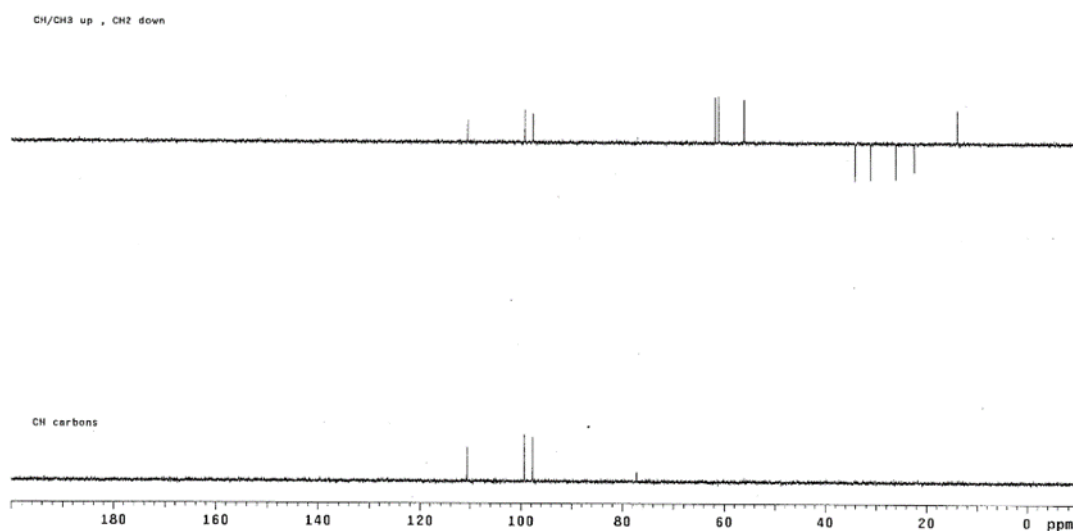


Figure S8: DEPT Spectrum of **1** in CDCl_3

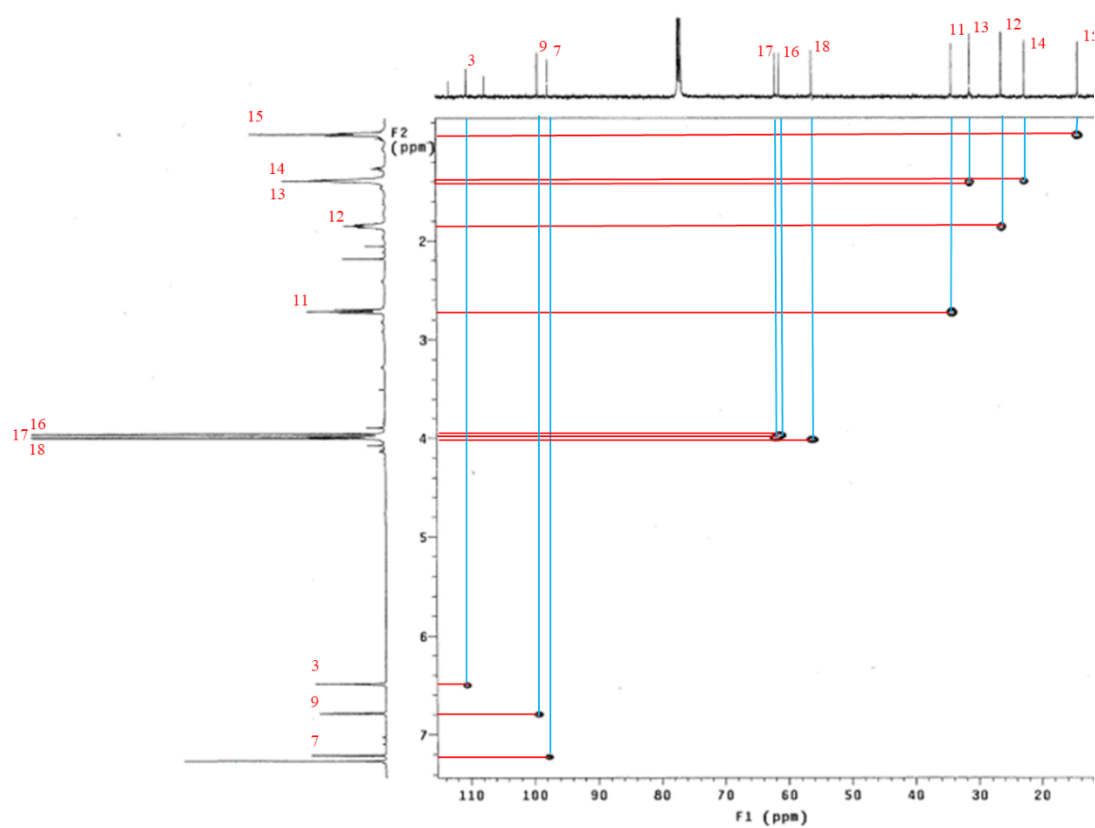


Figure S9: HMBC Spectrum of **1** in CDCl_3

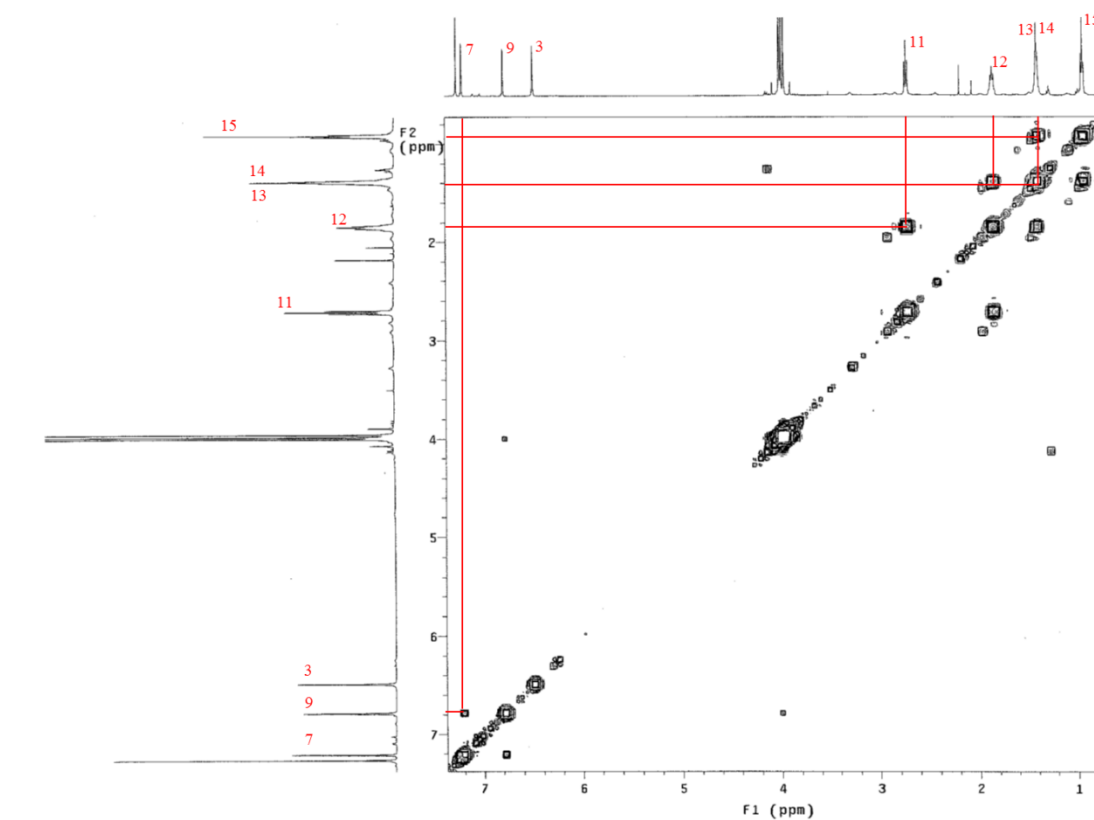


Figure S10: ^1H - ^1H COSY Spectrum of **1** in CDCl_3

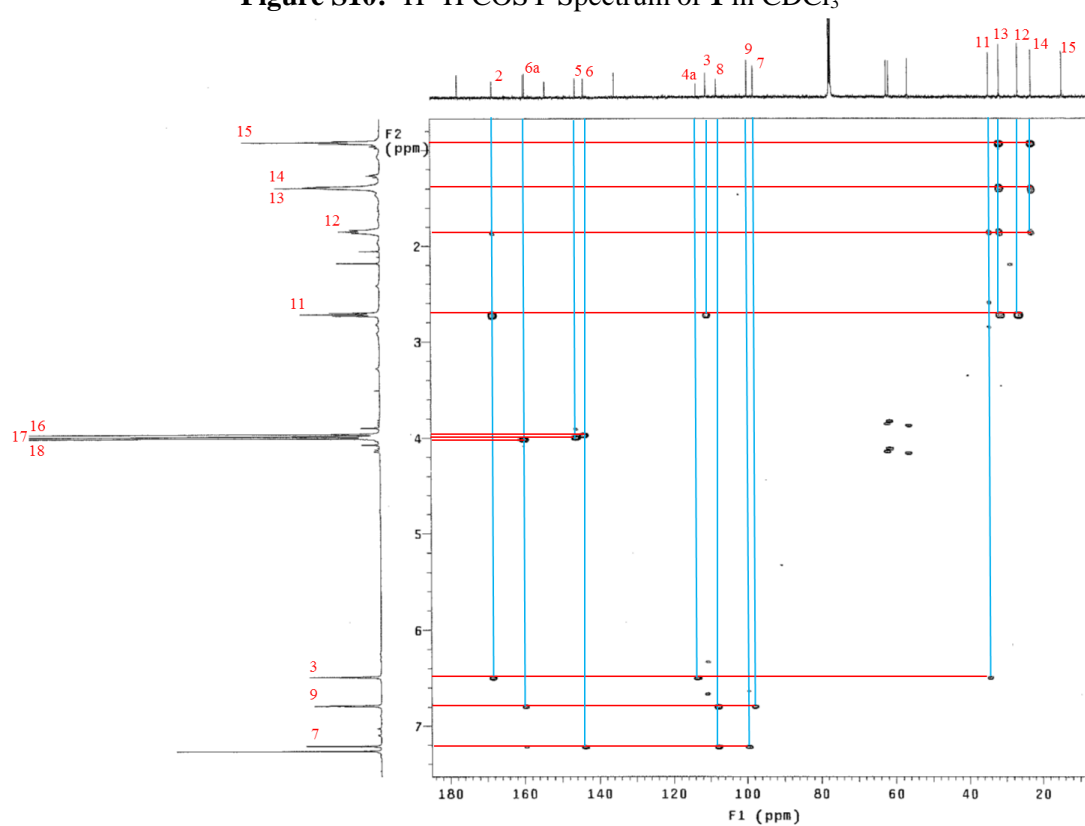


Figure S11: HMBC Spectrum of **1** in CDCl_3

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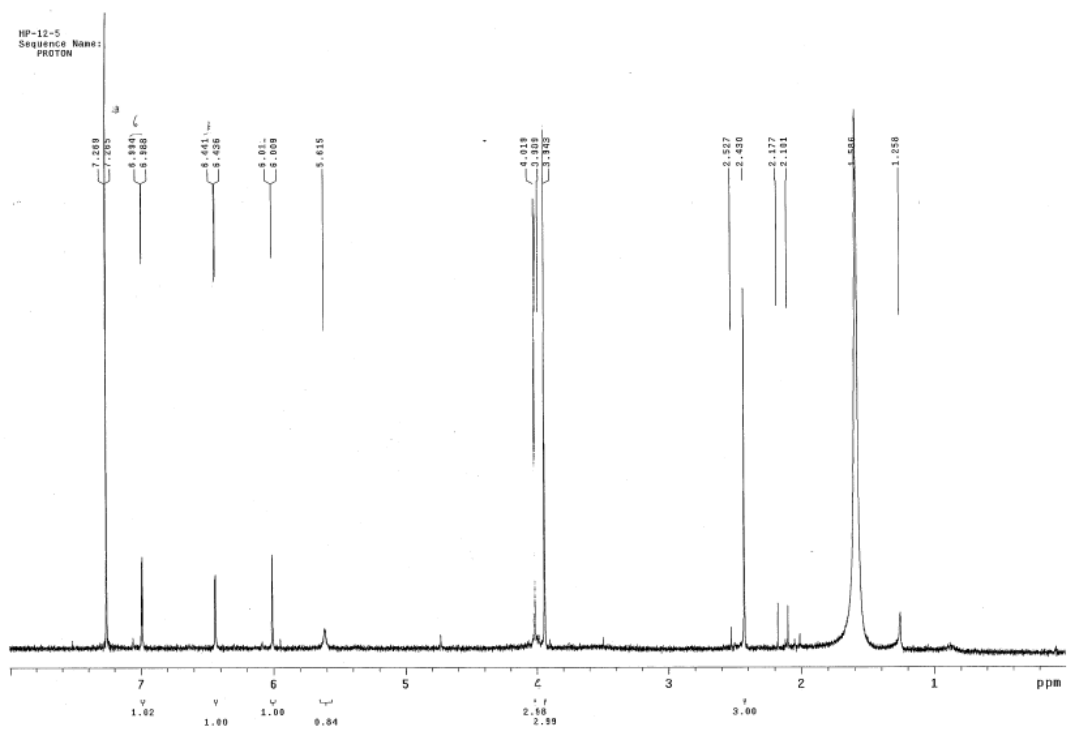


Figure S12: ^1H NMR Spectrum of **2** in CDCl_3 (400 MHz)

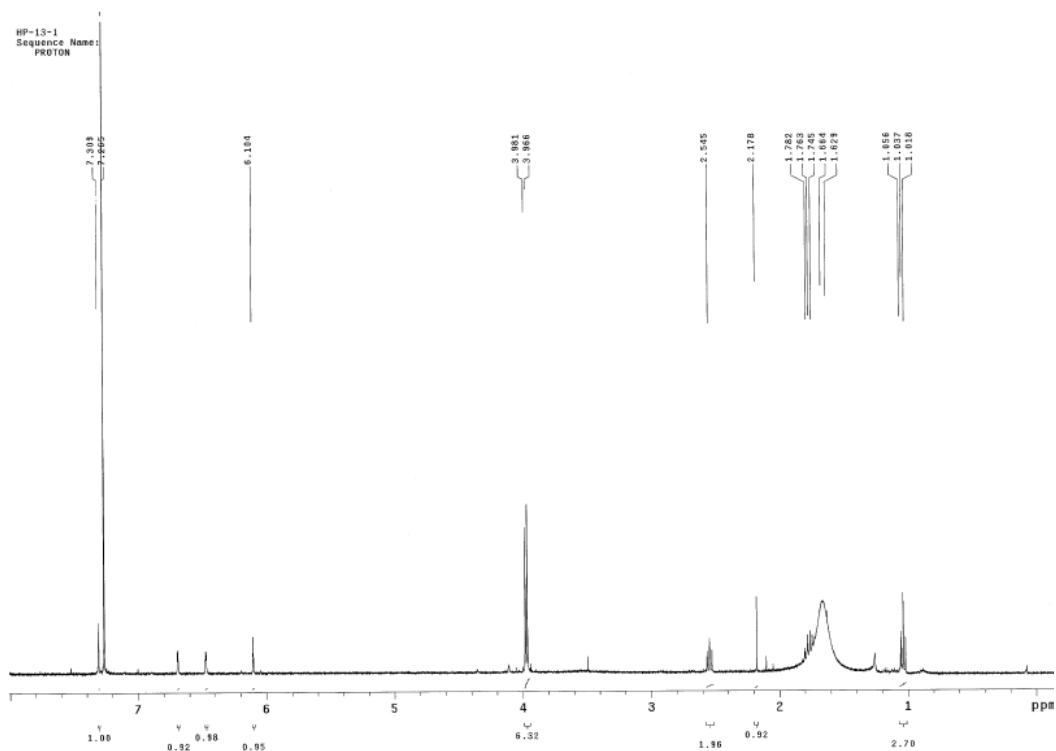


Figure S13: ^1H NMR Spectrum of **3** in CDCl_3 (400 MHz)

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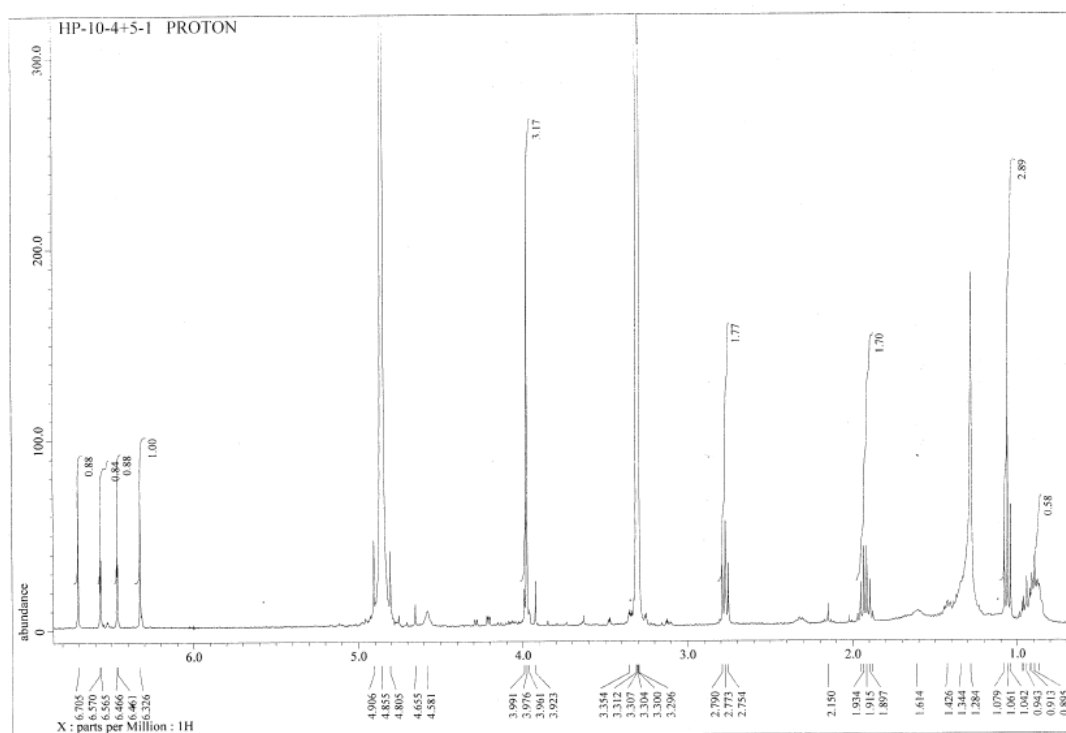


Figure S14: ^1H NMR Spectrum of **4** in MeOH (400 MHz)

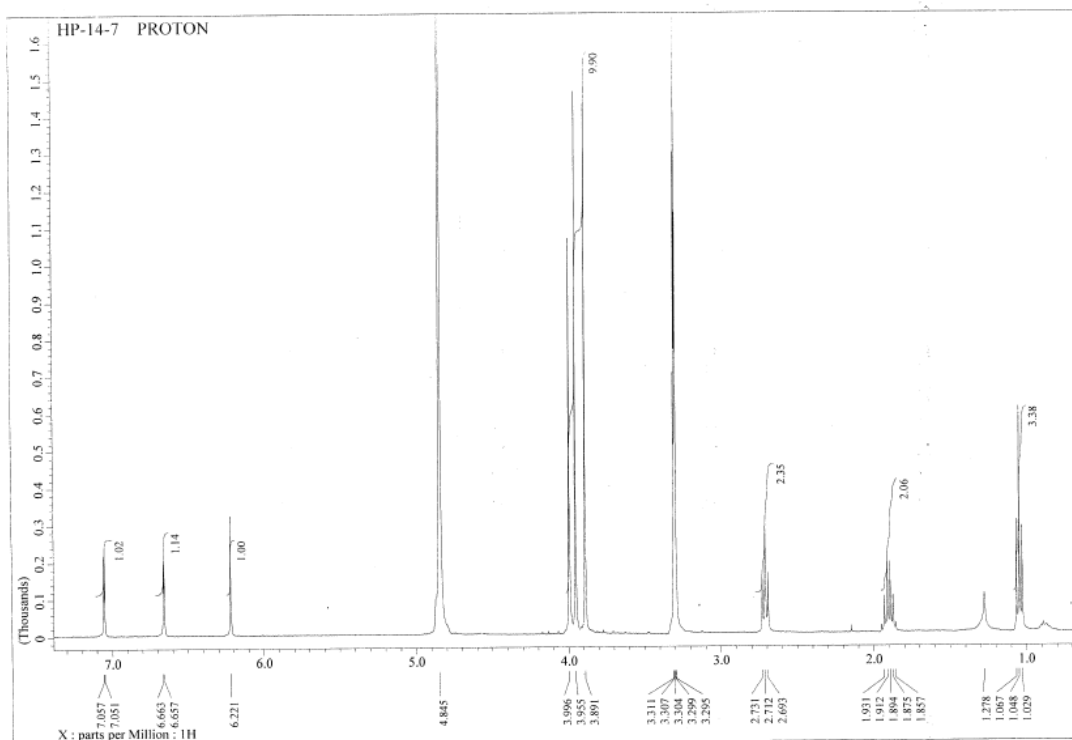


Figure S15: ^1H NMR Spectrum of **5** in MeOH (400 MHz)