

Supporting information to MS/MS-guided isolation of clarinoside, a new anti-inflammatory pentalogin derivative

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Figure 1: ¹ H NMR spectrum of 1 in CD ₃ OD (600 MHz).....	2
Figure 2: ¹³ C NMR spectrum of 1 in CD ₃ OD (125 MHz)	2
Figure 3: COSY spectrum of 1 in CD ₃ OD	3
Figure 4: TOCSY spectrum of 1 in CD ₃ OD	3
Figure 5: HSQC spectrum of 1 in CD ₃ OD.....	4
Figure 6: HMBC spectrum of 1 in CD ₃ OD.....	4
Figure 7: ¹ H NMR spectrum of 1 after H ₂ SO ₄ hydrolysis.	5
Figure 8: ¹ H NMR spectrum of 1 after H ₂ SO ₄ hydrolysis (enlargement).	6
Figure 9: ¹ H NMR spectrum of 1 after H ₂ SO ₄ hydrolysis (enlargement)	6
Figure 10: ¹ H NMR spectrum of 1 after H ₂ SO ₄ hydrolysis (enlargement)	7
Figure 11: HRMS/MS spectrum of 1	7
Figure 12 : FTIR spectrum of 1	8
Figure 13: Energy profile of both C5-O and C10-O bonds.....	8

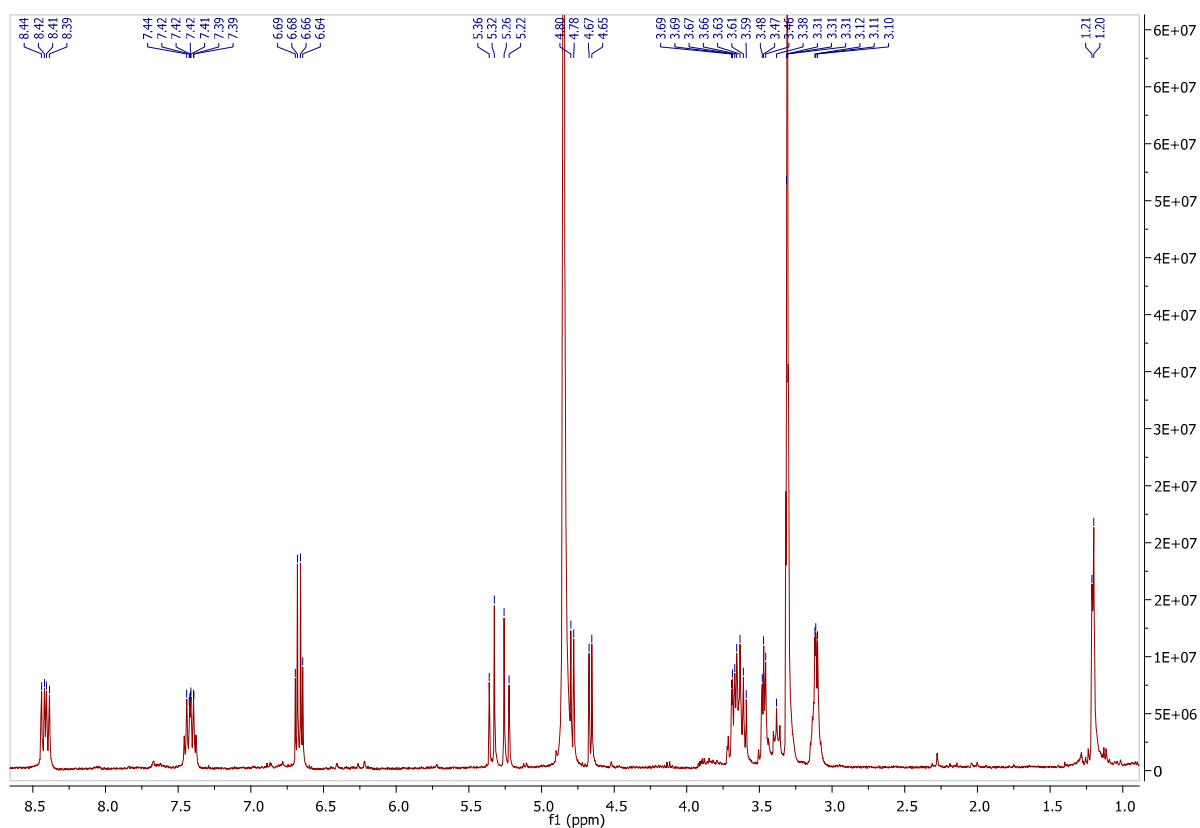


Figure 1: ^1H NMR spectrum of **1** in CD_3OD (600 MHz)

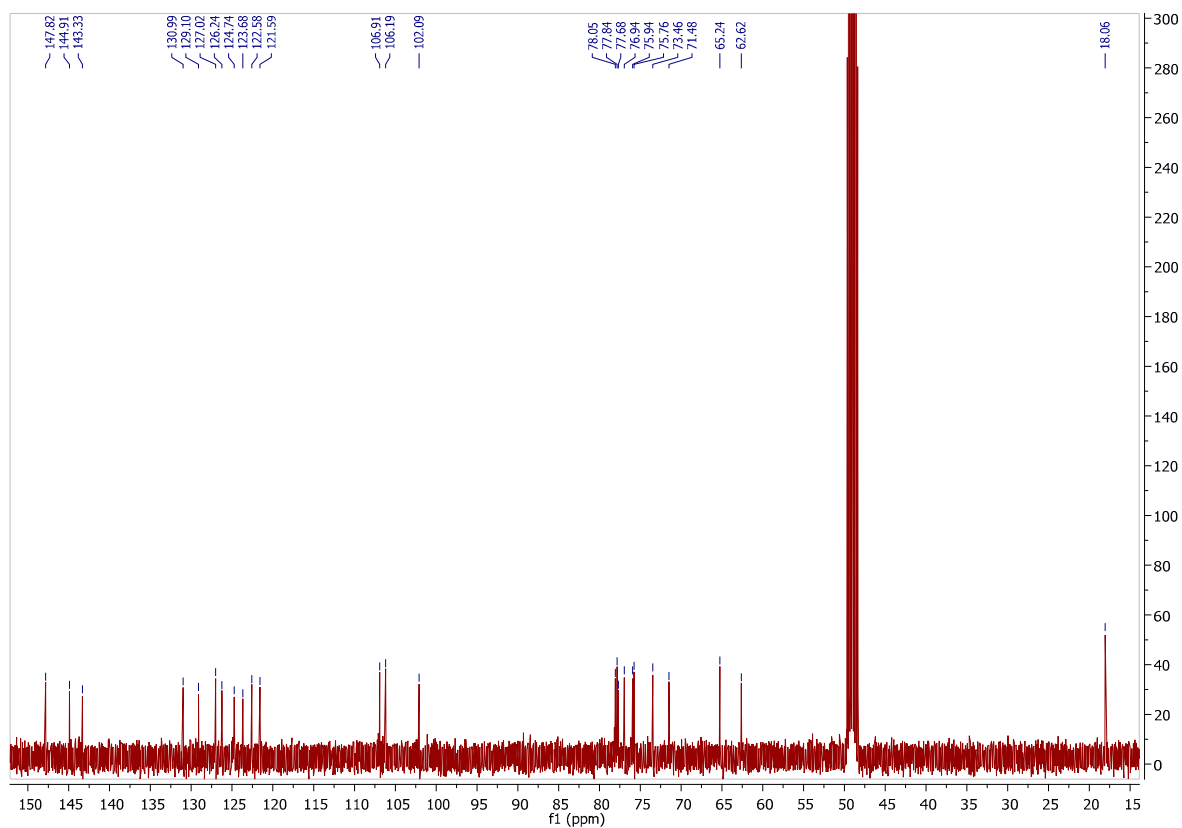


Figure 2: ^{13}C NMR spectrum of **1** in CD_3OD (125 MHz)

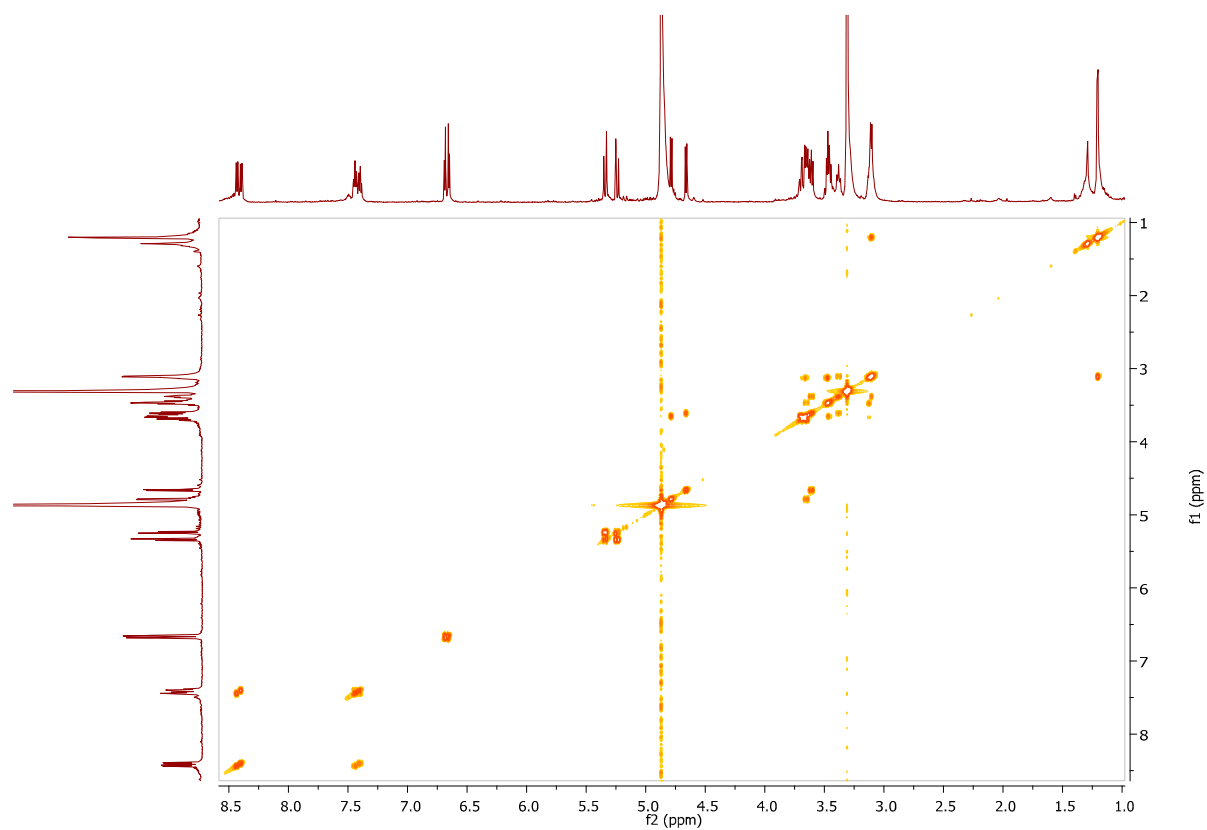


Figure 3: COSY spectrum of **1** in CD₃OD

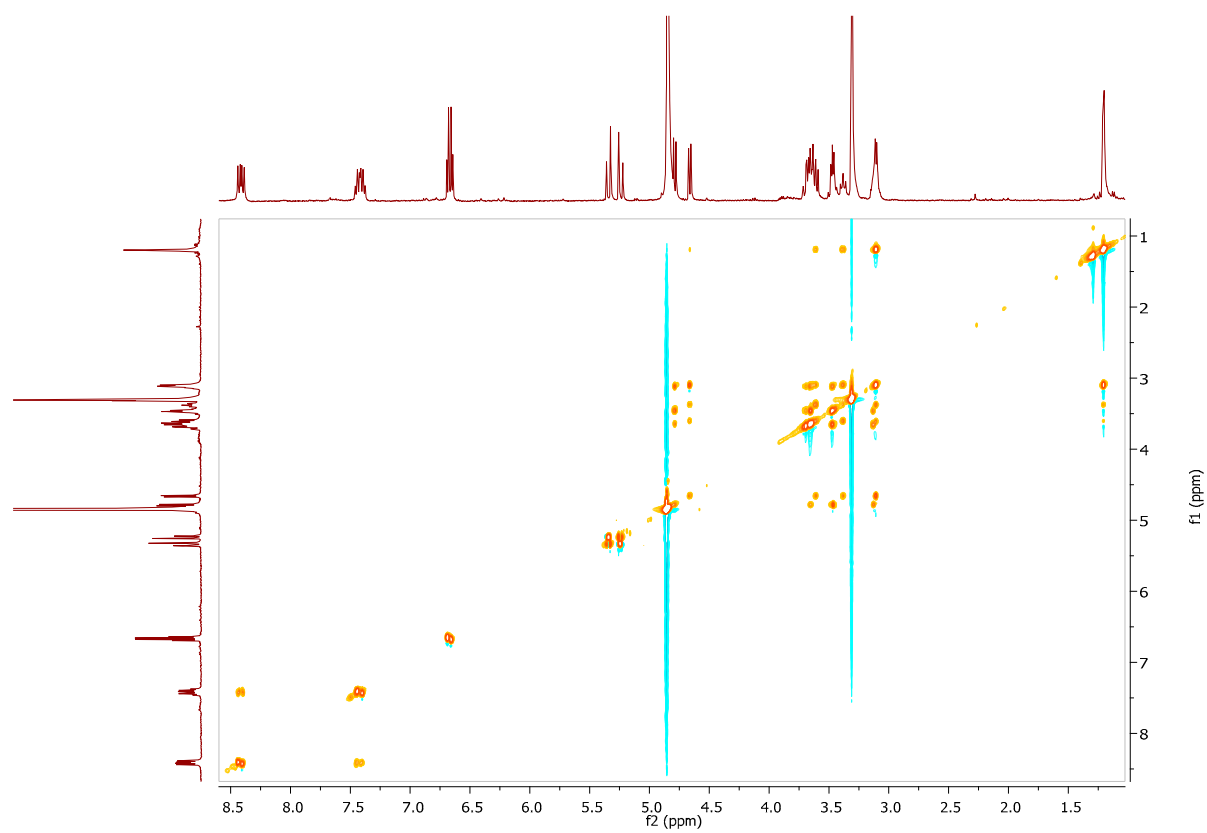


Figure 4: TOCSY spectrum of **1** in CD₃OD

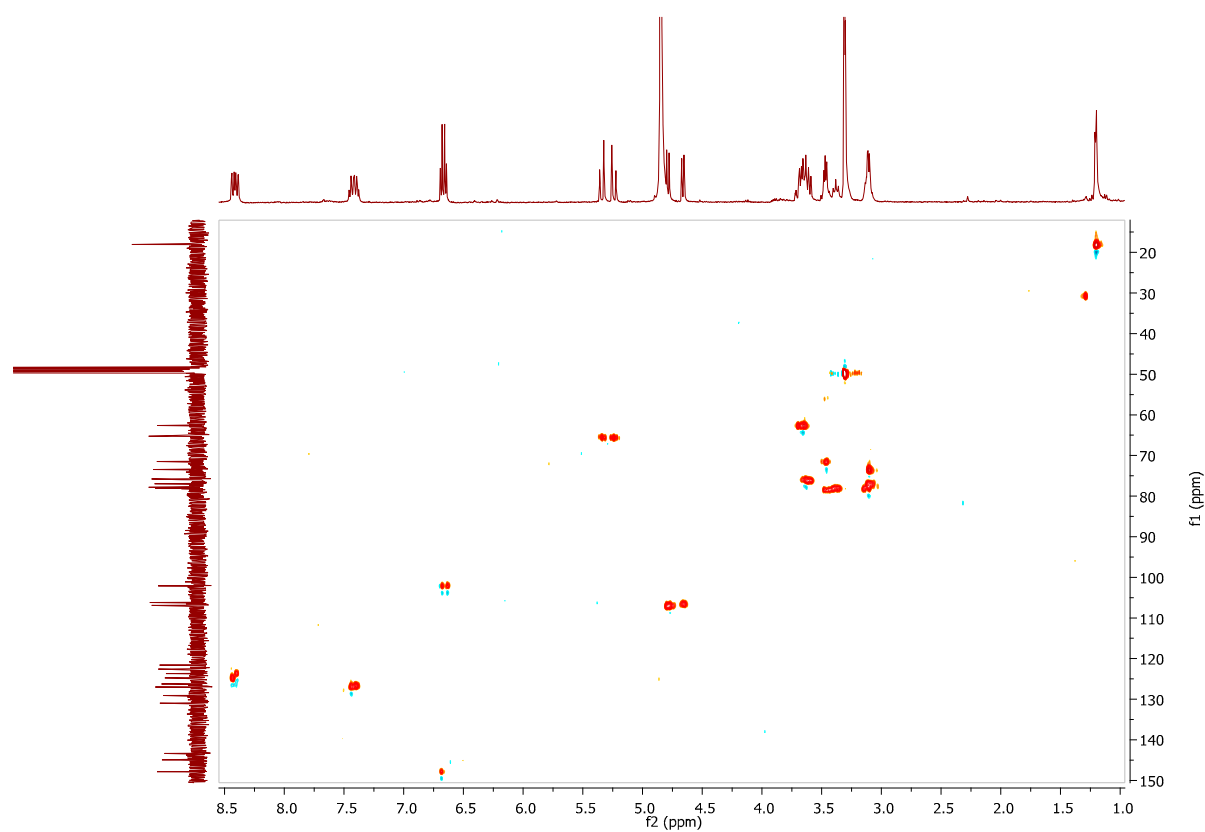


Figure 5: HSQC spectrum of **1** in CD₃OD

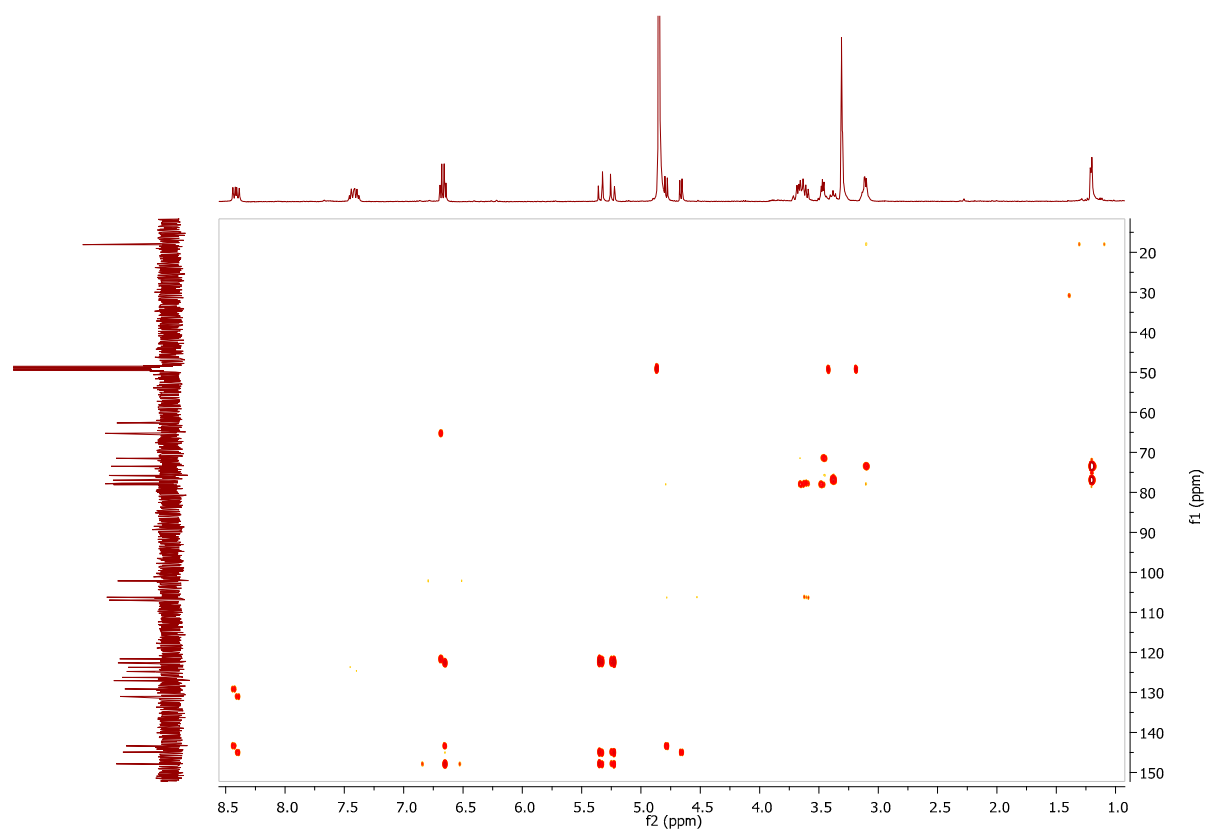


Figure 6: HMBC spectrum of **1** in CD₃OD

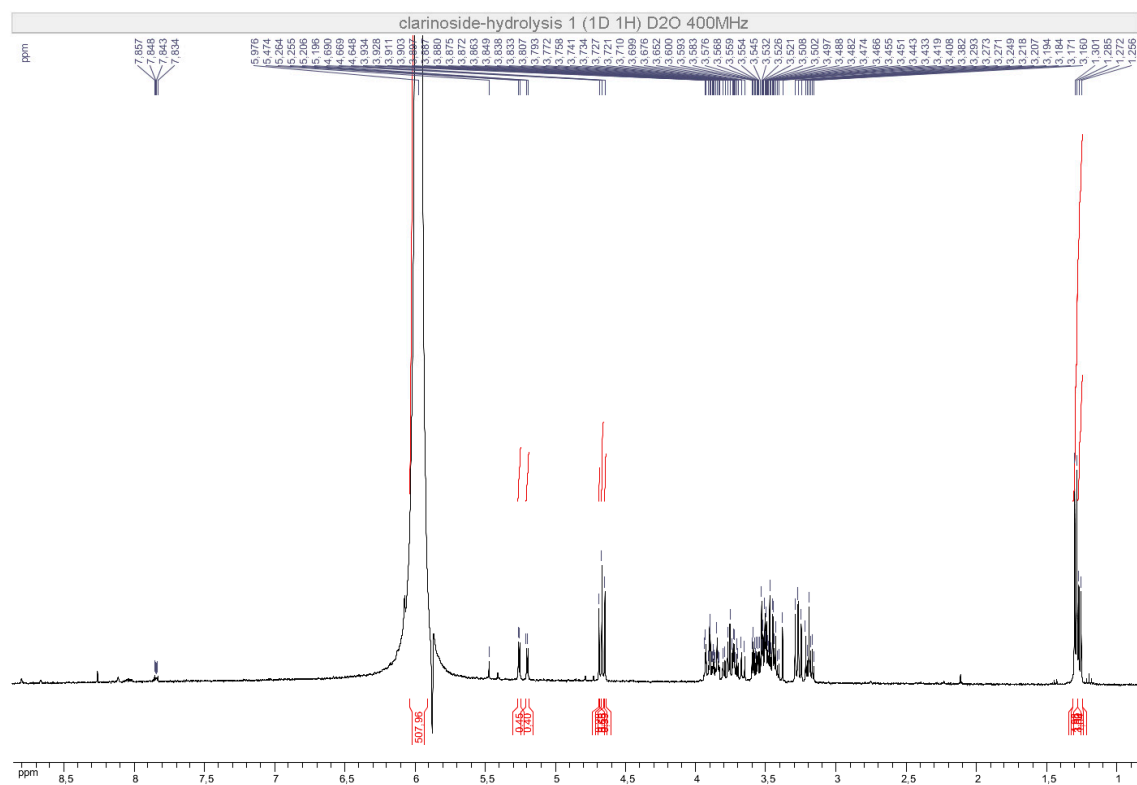


Figure 7: ^1H NMR spectrum of **1** after H_2SO_4 hydrolysis.

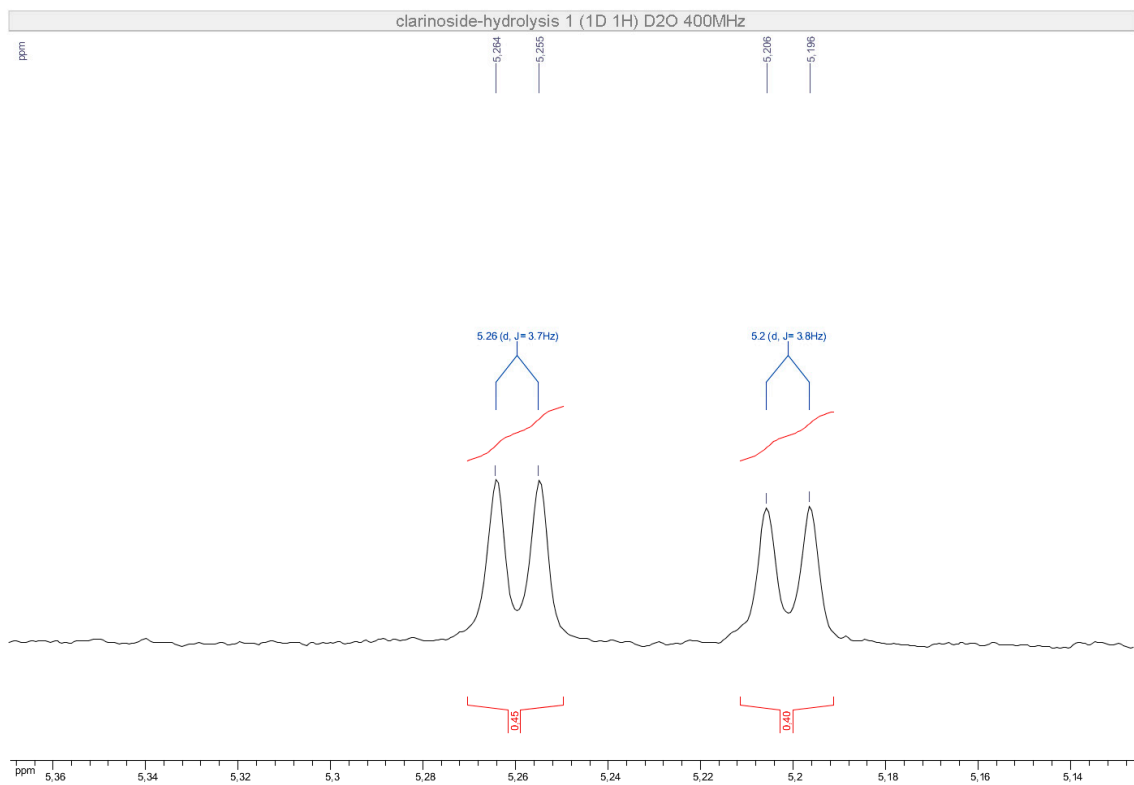


Figure 8: ^1H NMR spectrum of **1** after H_2SO_4 hydrolysis (enlargement).

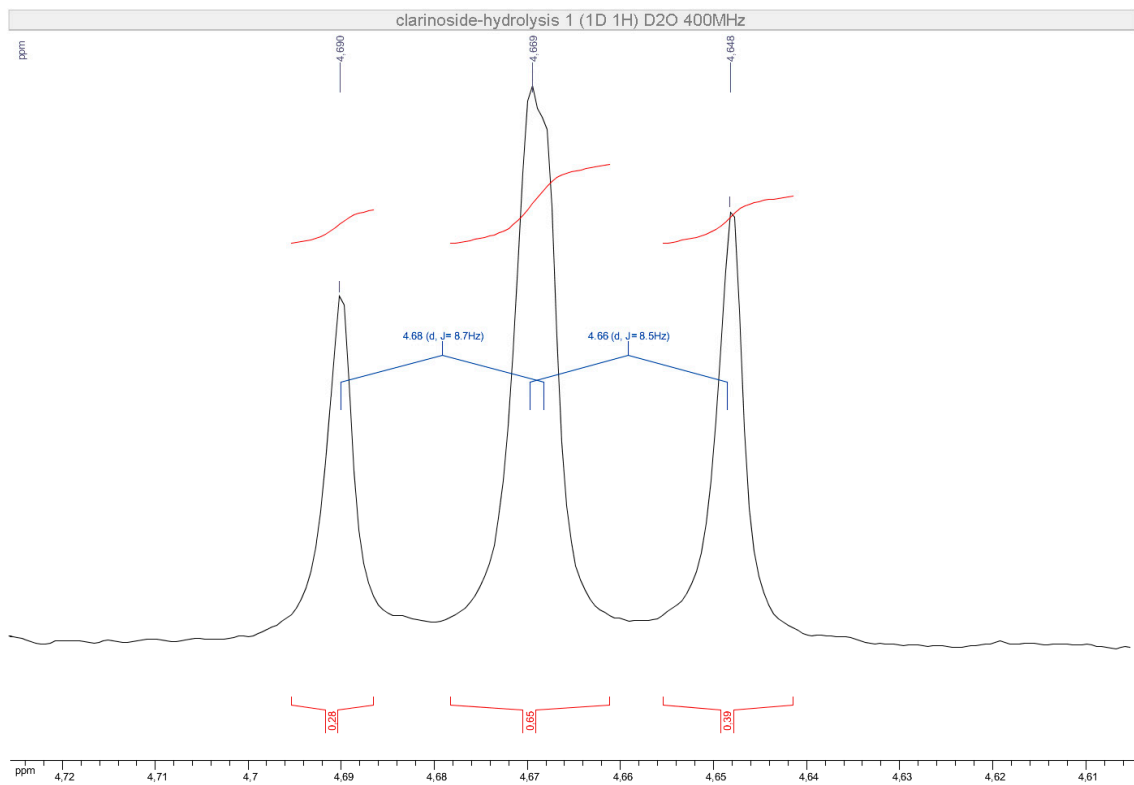


Figure 9: ^1H NMR spectrum of **1** after H_2SO_4 hydrolysis (enlargement)

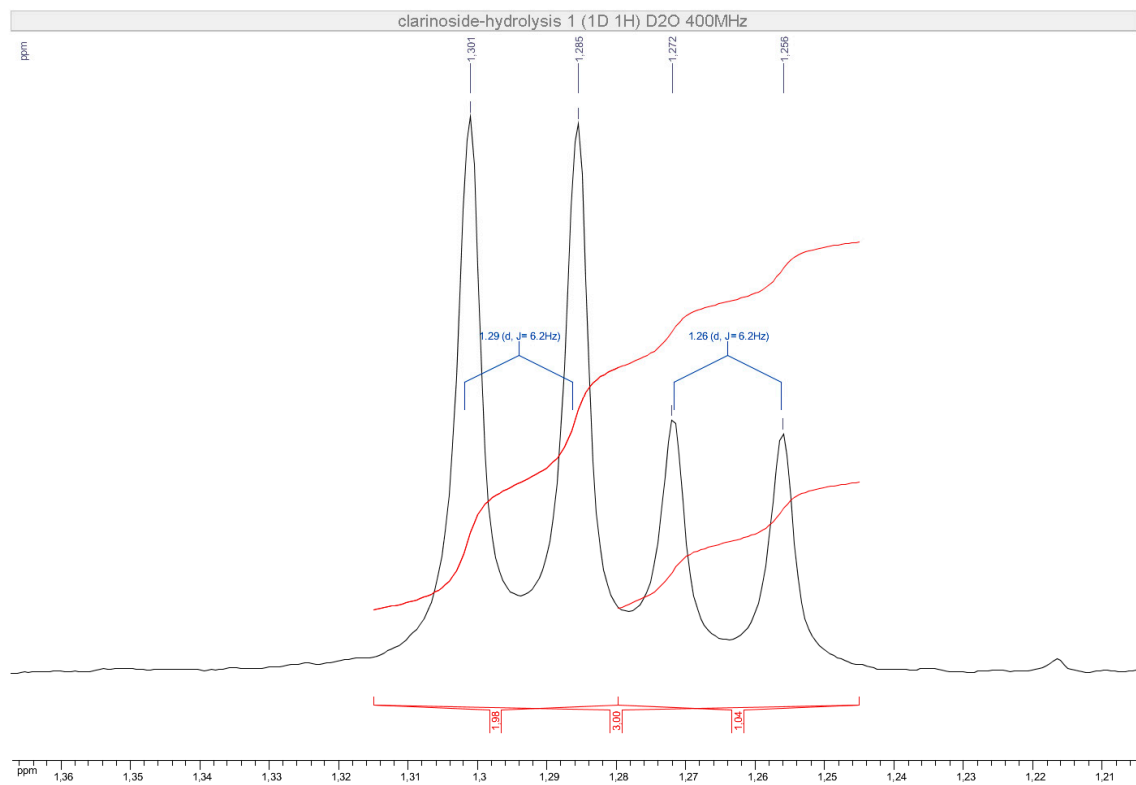


Figure 10: ^1H NMR spectrum of **1** after H_2SO_4 hydrolysis (enlargement)

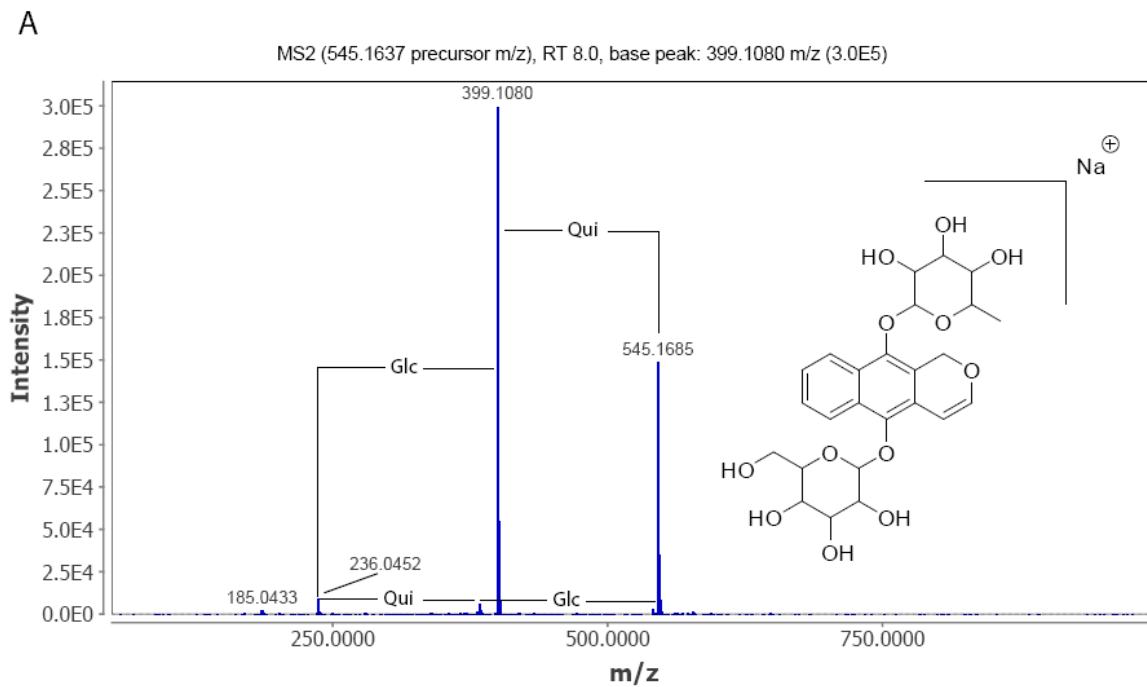


Figure 11: HRMS/MS spectrum of **1**

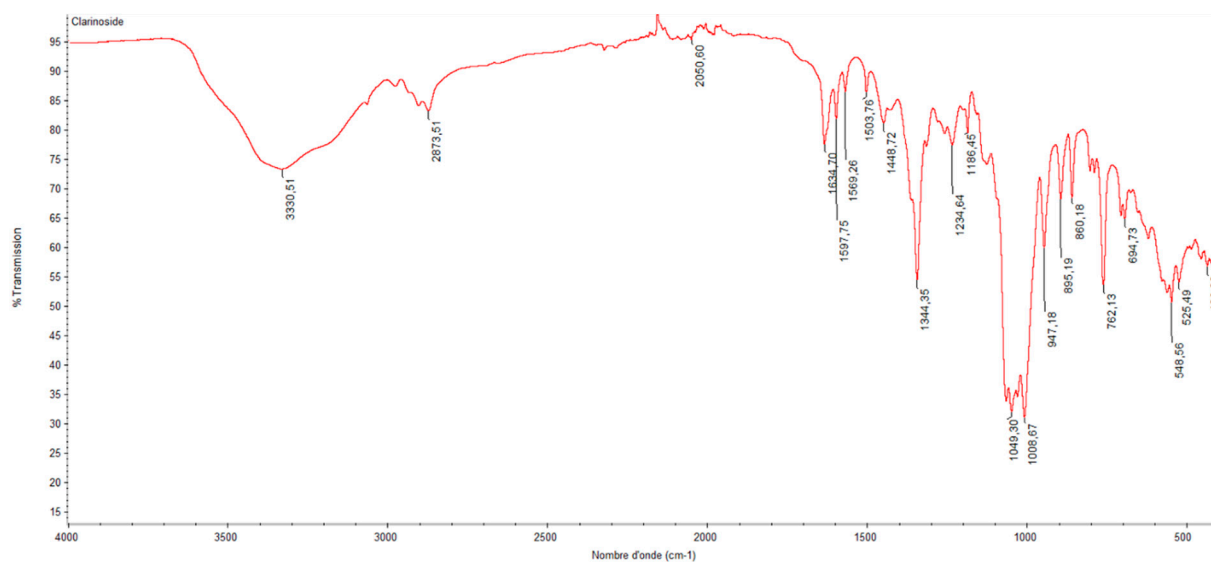


Figure 12 : FTIR spectrum of 1

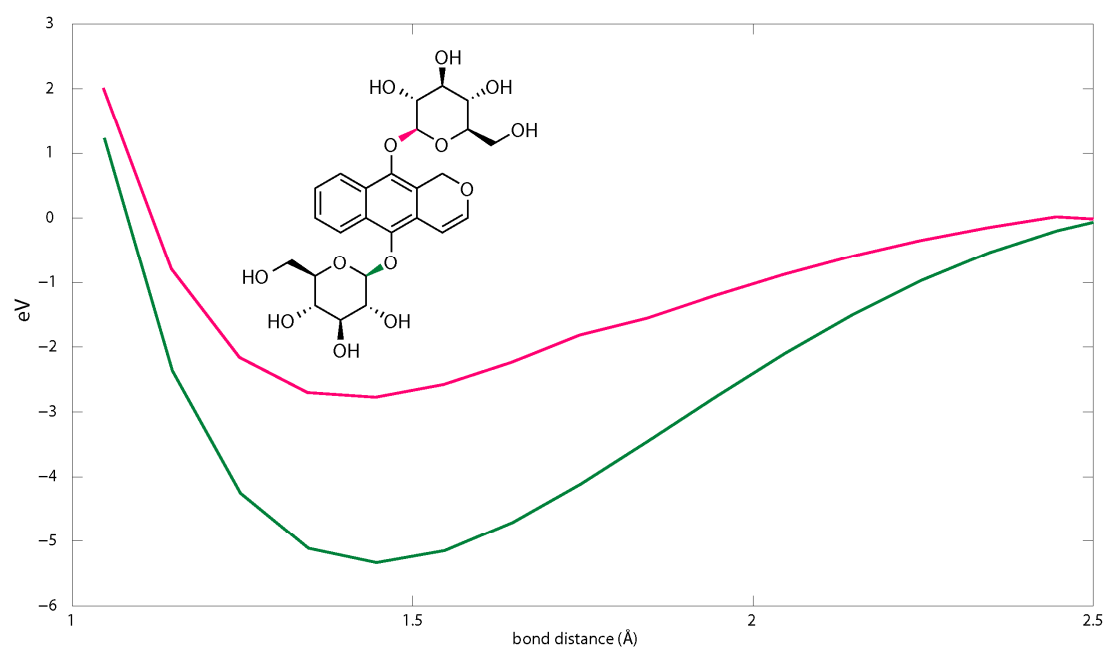


Figure 13: Energy profile of both C5-O and C10-O bonds.

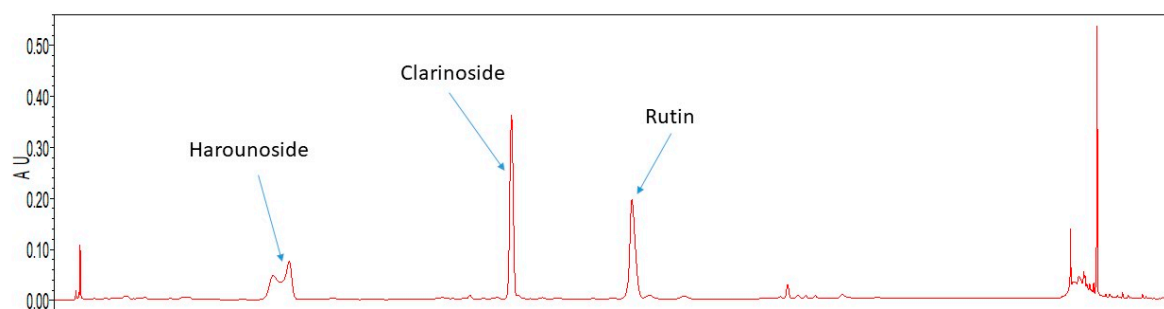


Figure 14: HPLC trace used for the separation (UV 254 nm).