

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

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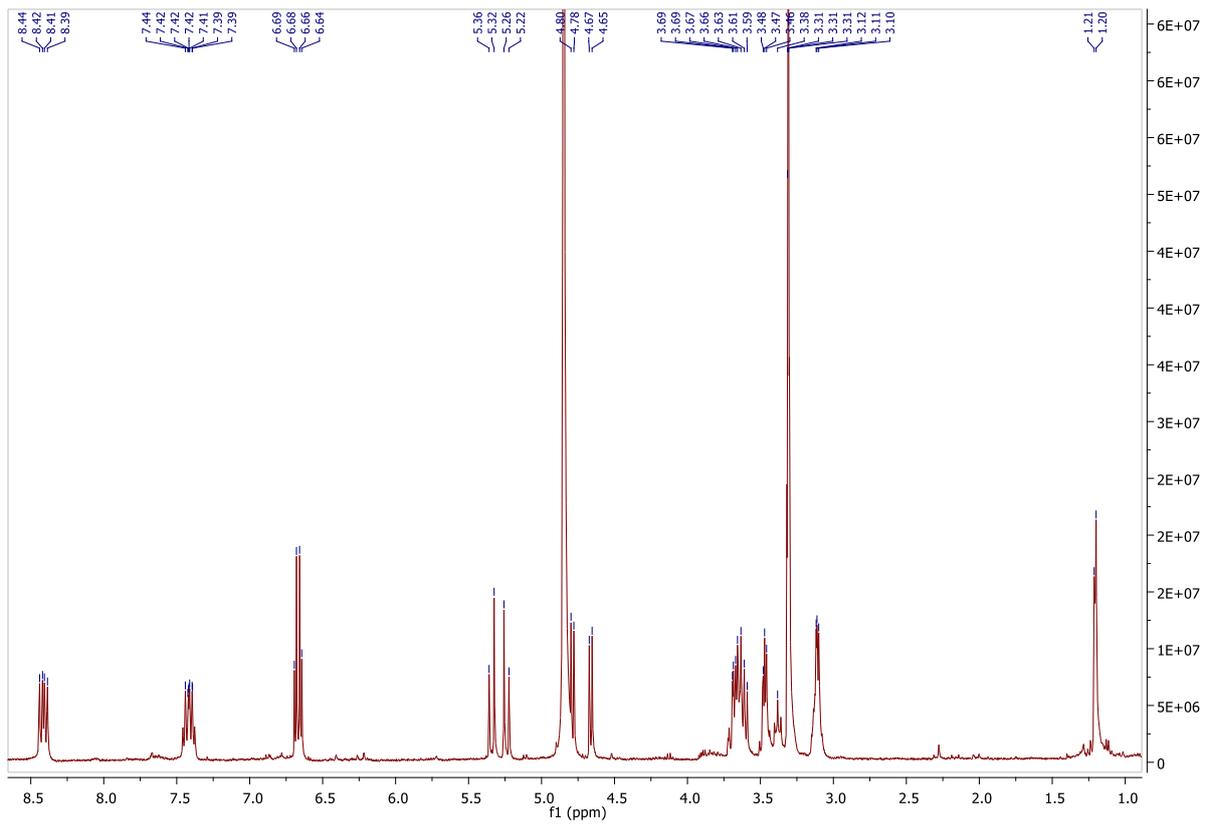


Figure 1: ^1H NMR spectrum of 1 in CD_3OD (600 MHz)

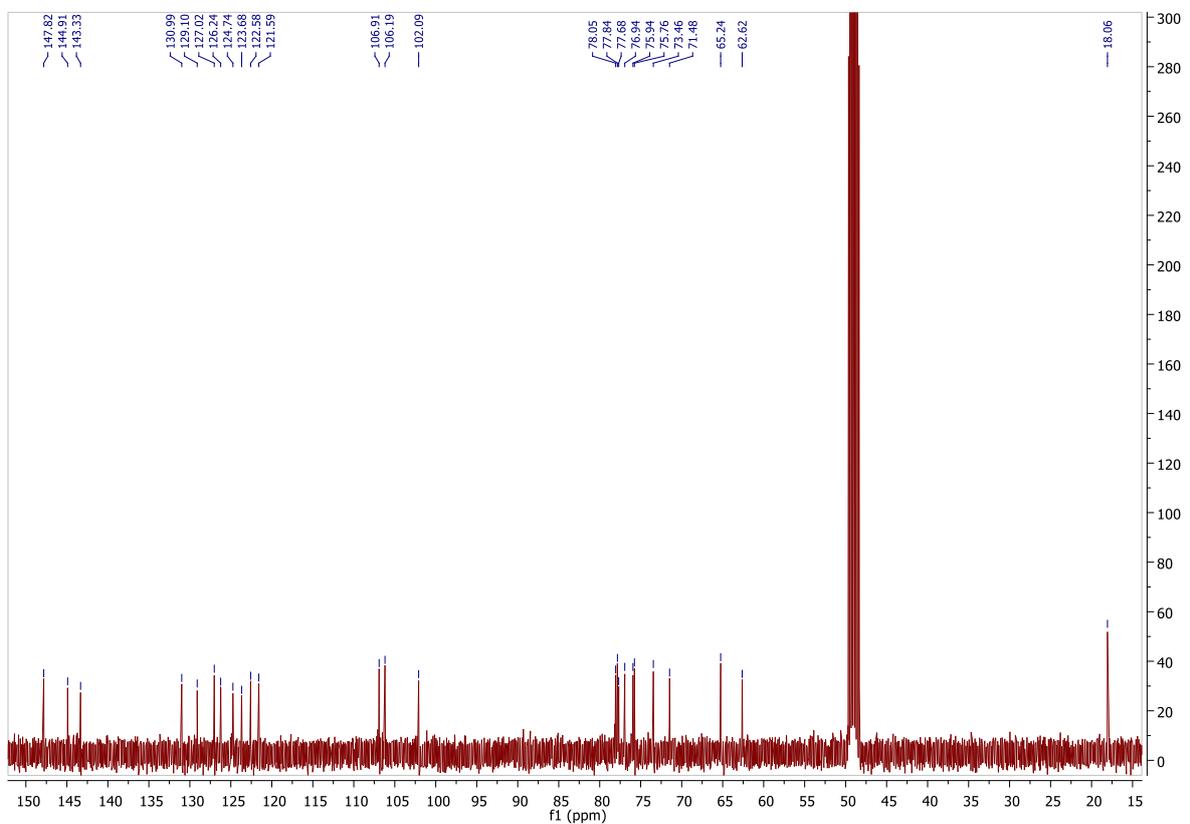


Figure 2: ^{13}C NMR spectrum of 1 in CD_3OD (125 MHz)

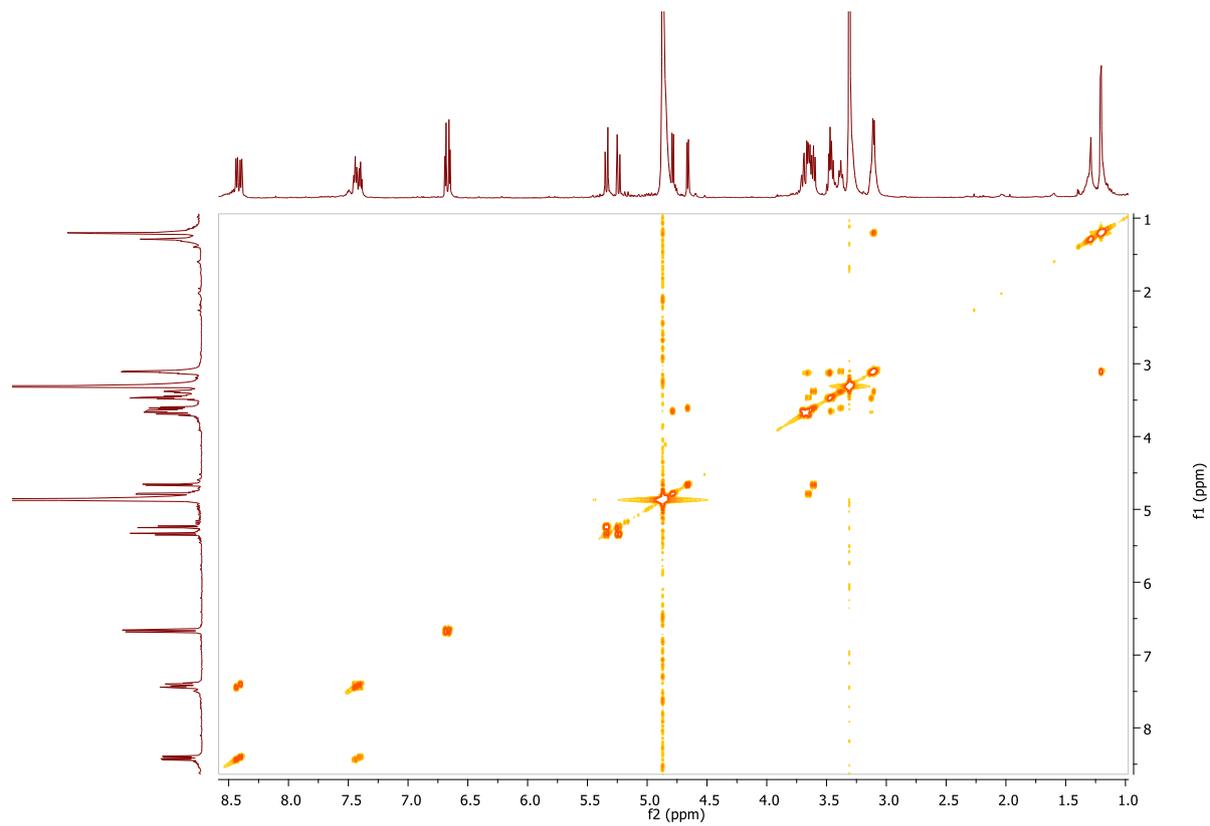


Figure 3: COSY spectrum of **1** in CD₃OD

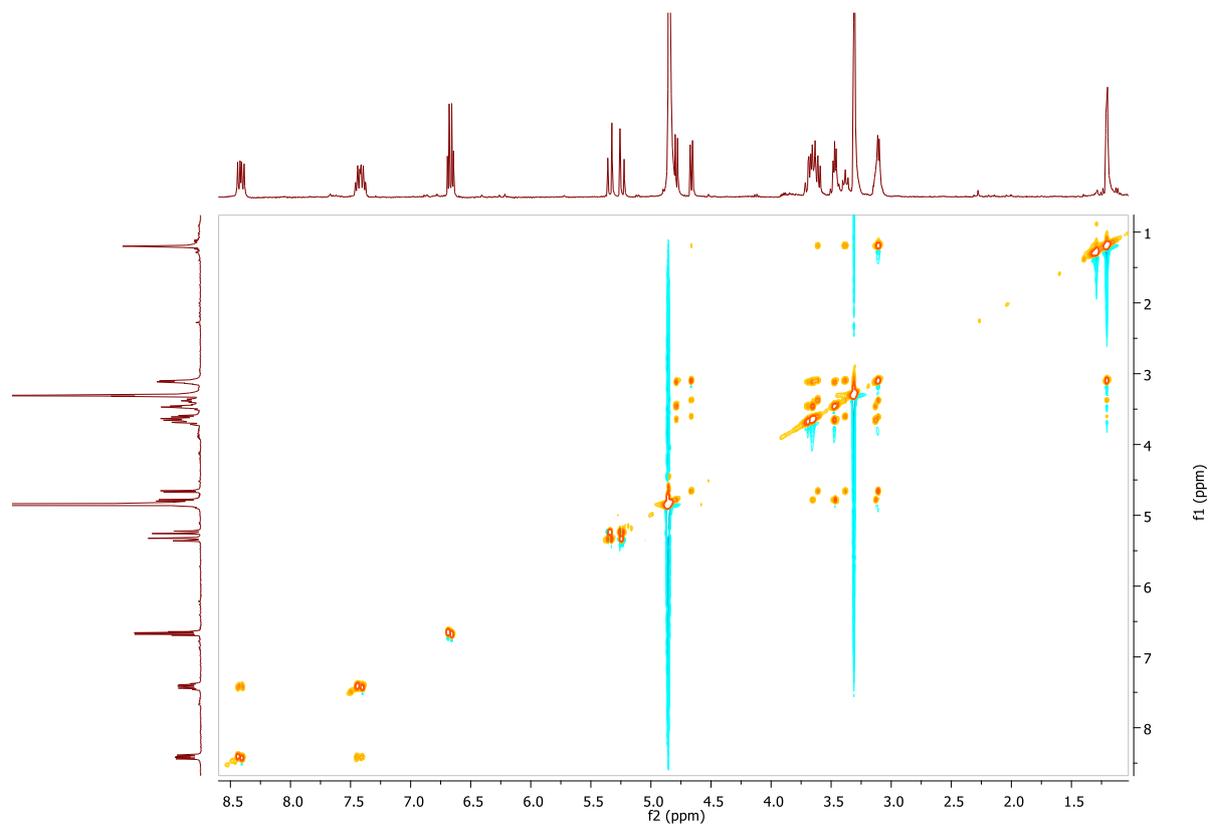


Figure 4: TOCSY spectrum of **1** in CD₃OD

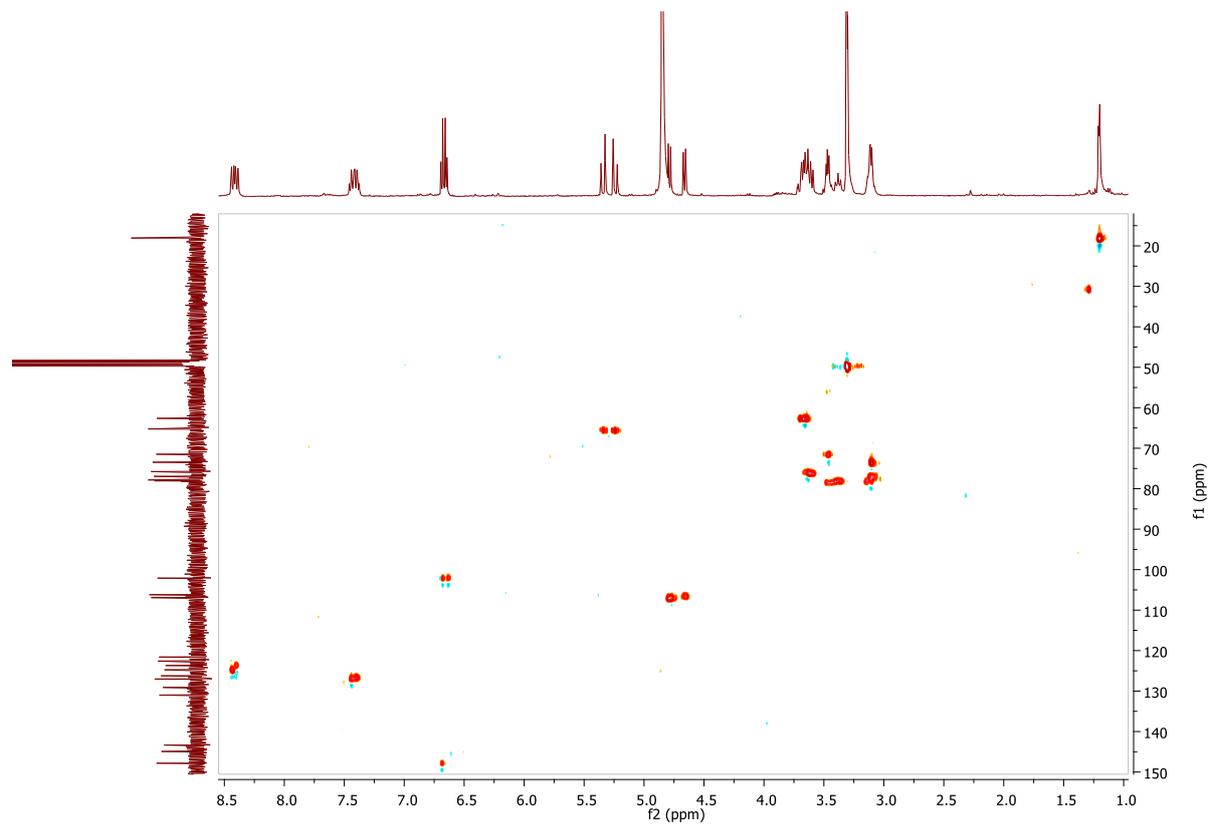


Figure 5: HSQC spectrum of **1** in CD₃OD

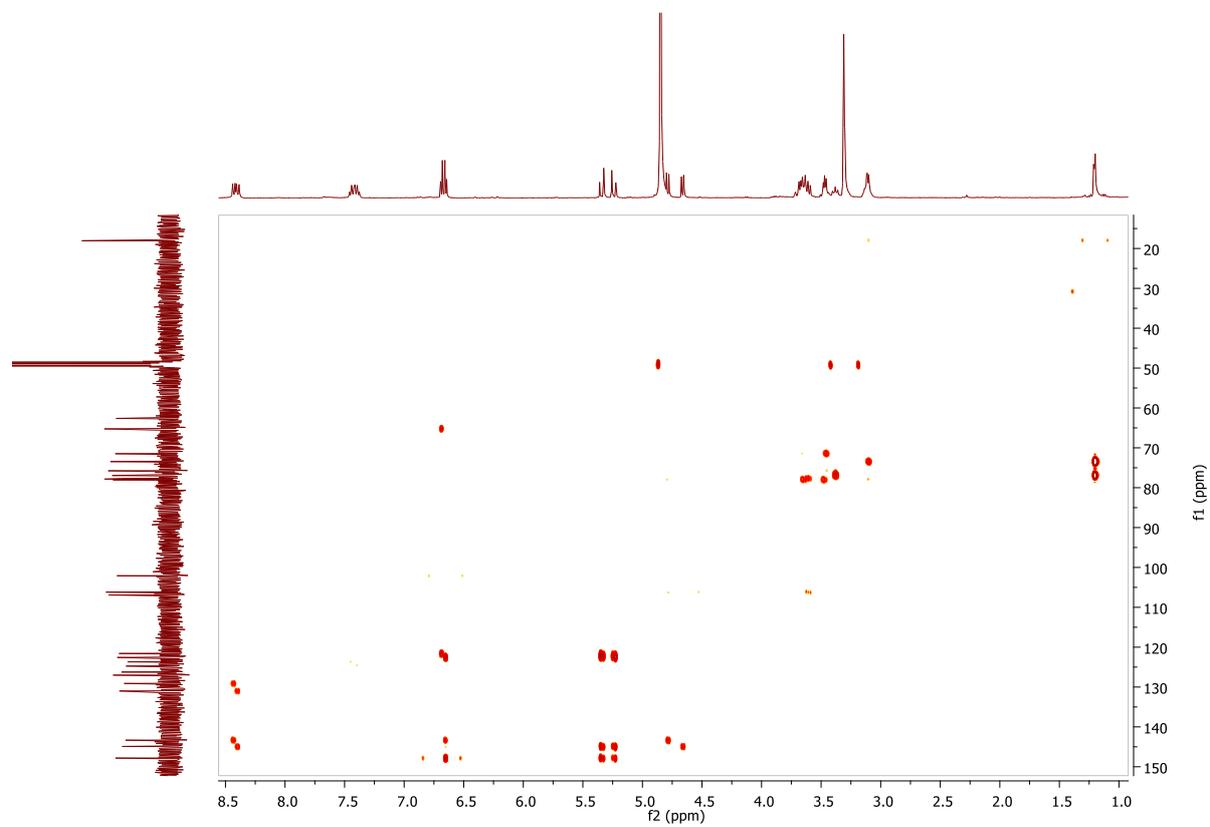


Figure 6: HMBC spectrum of **1** in CD₃OD

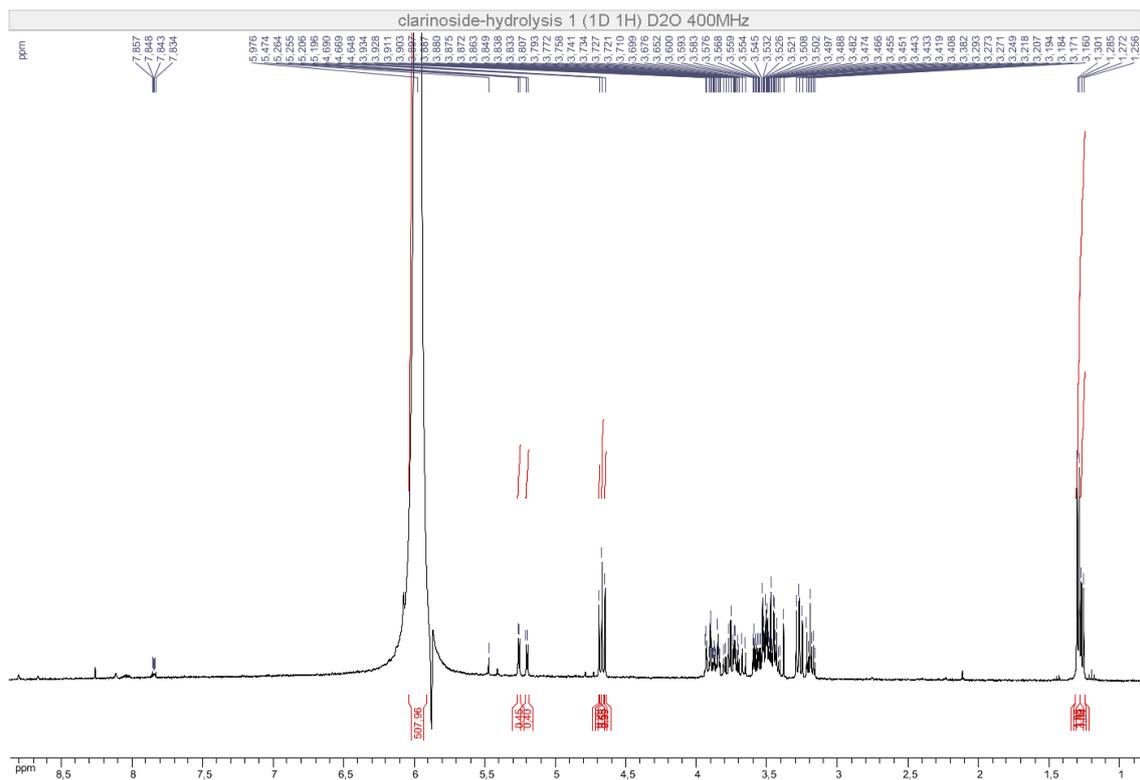


Figure 7: ^1H NMR spectrum of **1** after H_2SO_4 hydrolysis.

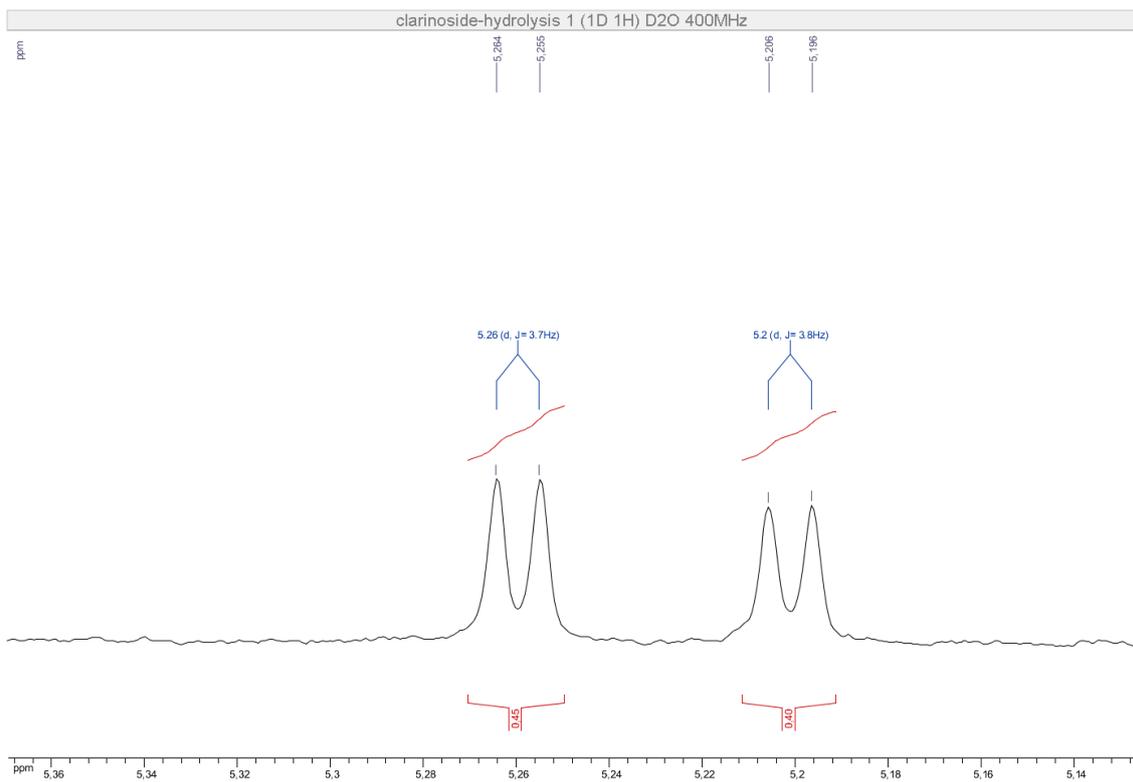


Figure 8: ^1H NMR spectrum of 1 after H_2SO_4 hydrolysis (enlargement).

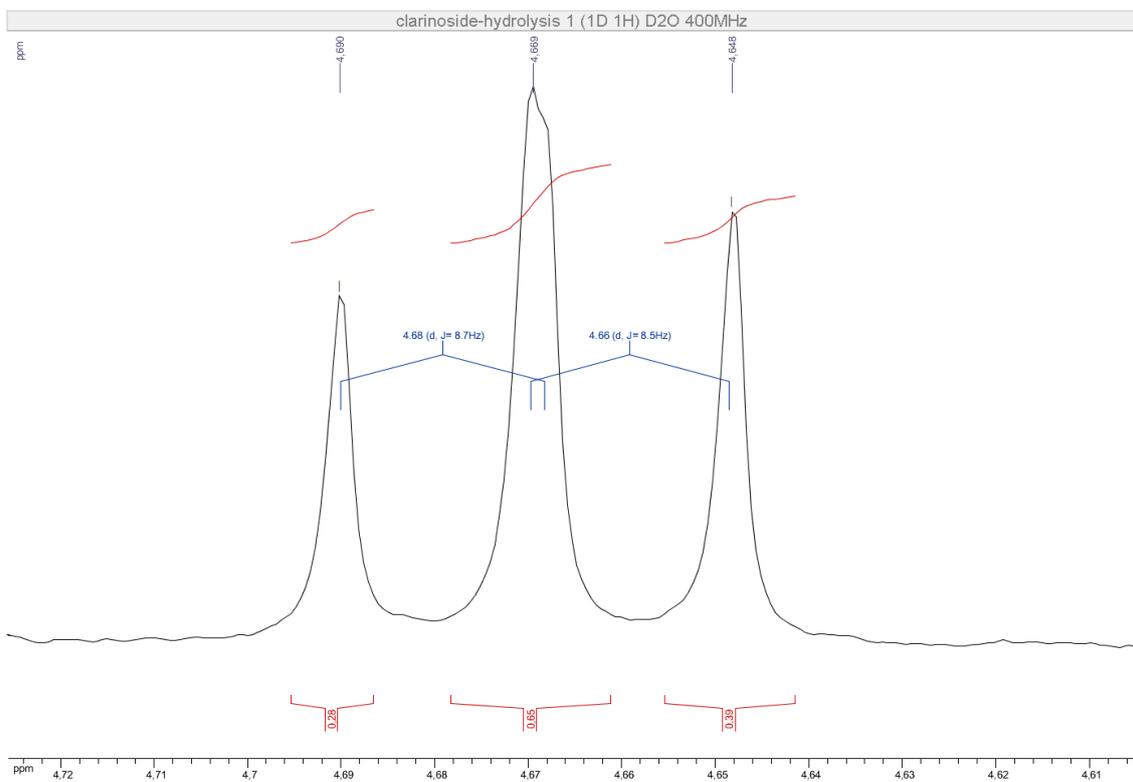


Figure 9: ^1H NMR spectrum of 1 after H_2SO_4 hydrolysis (enlargement)

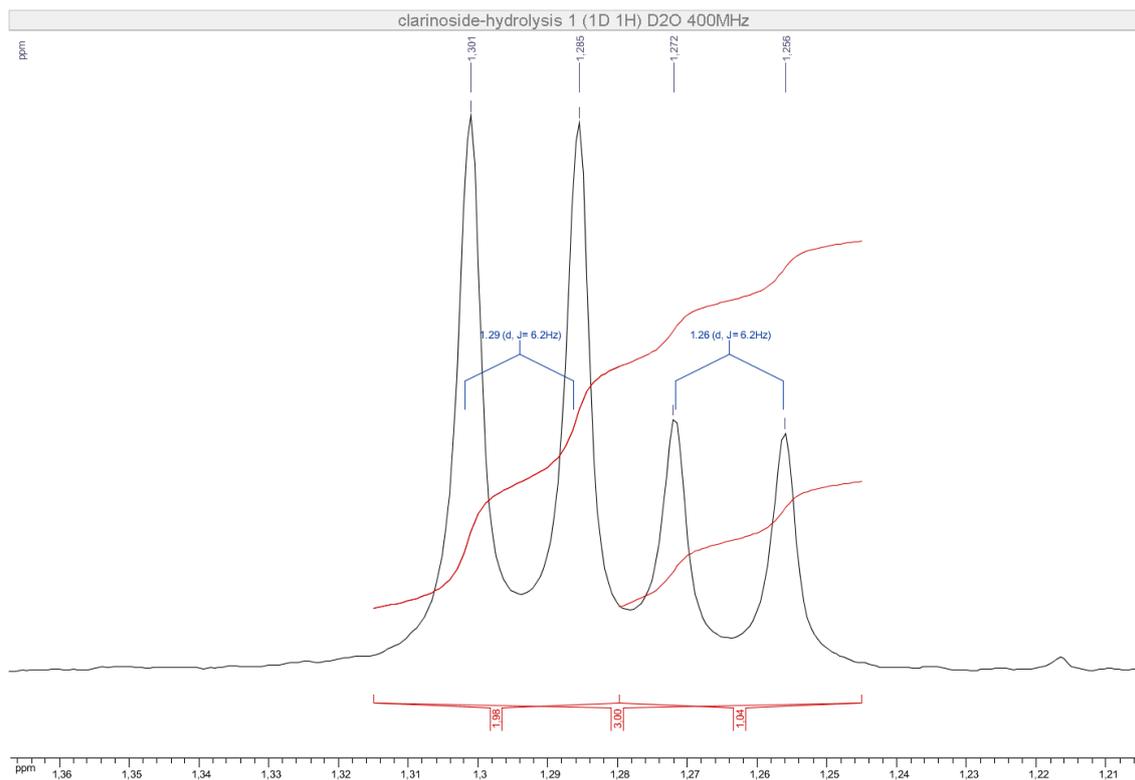


Figure 10: ^1H NMR spectrum of **1** after H_2SO_4 hydrolysis (enlargement)

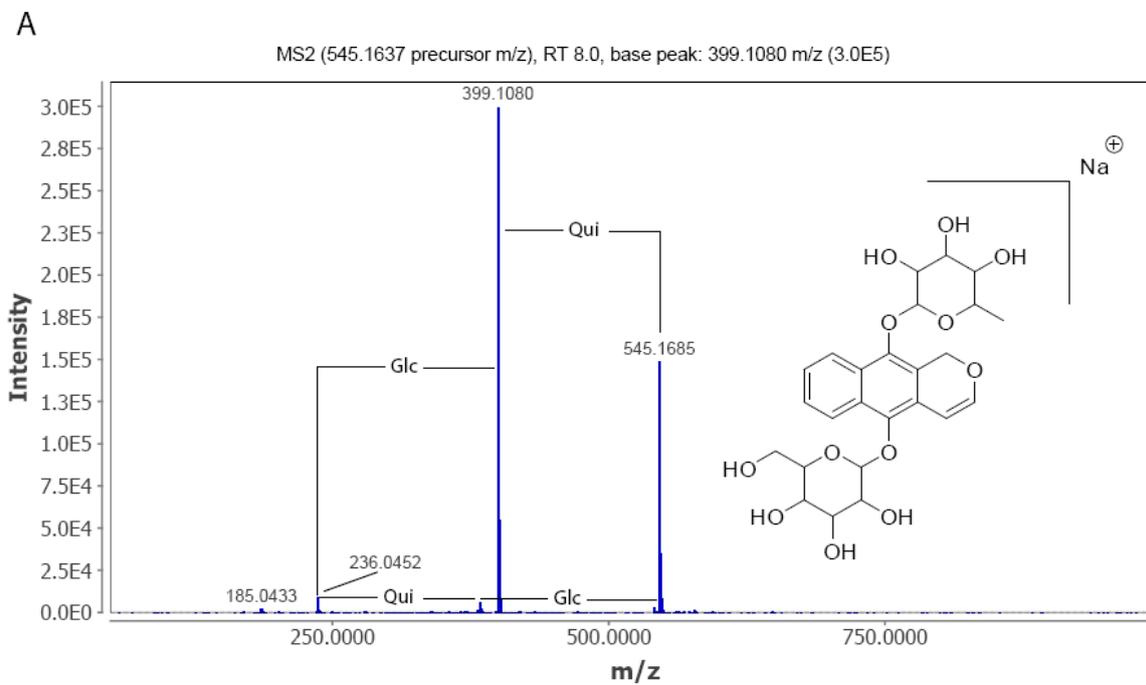


Figure 11: HRMS/MS spectrum of **1**

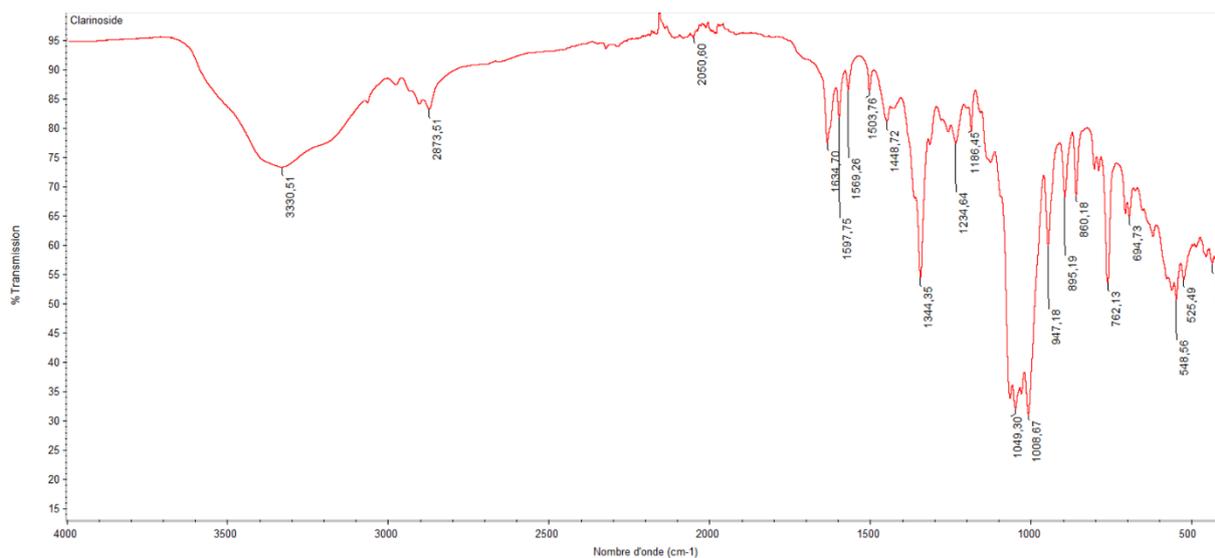


Figure 12 : FTIR spectrum of 1

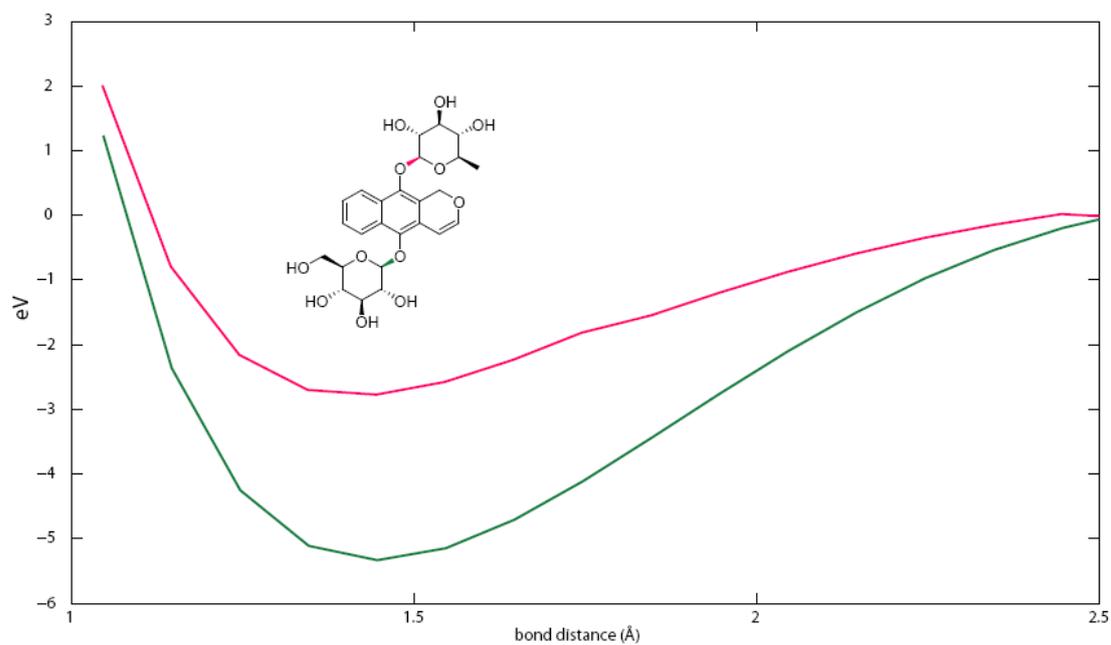


Figure 13: Energy profile of both C5-O and C10-O bonds.