Supplementary Information

Figure S1. ESI (+) MS (top) and fragmentation MS/MS spectraon *m/z* 353 $[M + Na]^+$ (bottom) of compound **13**.

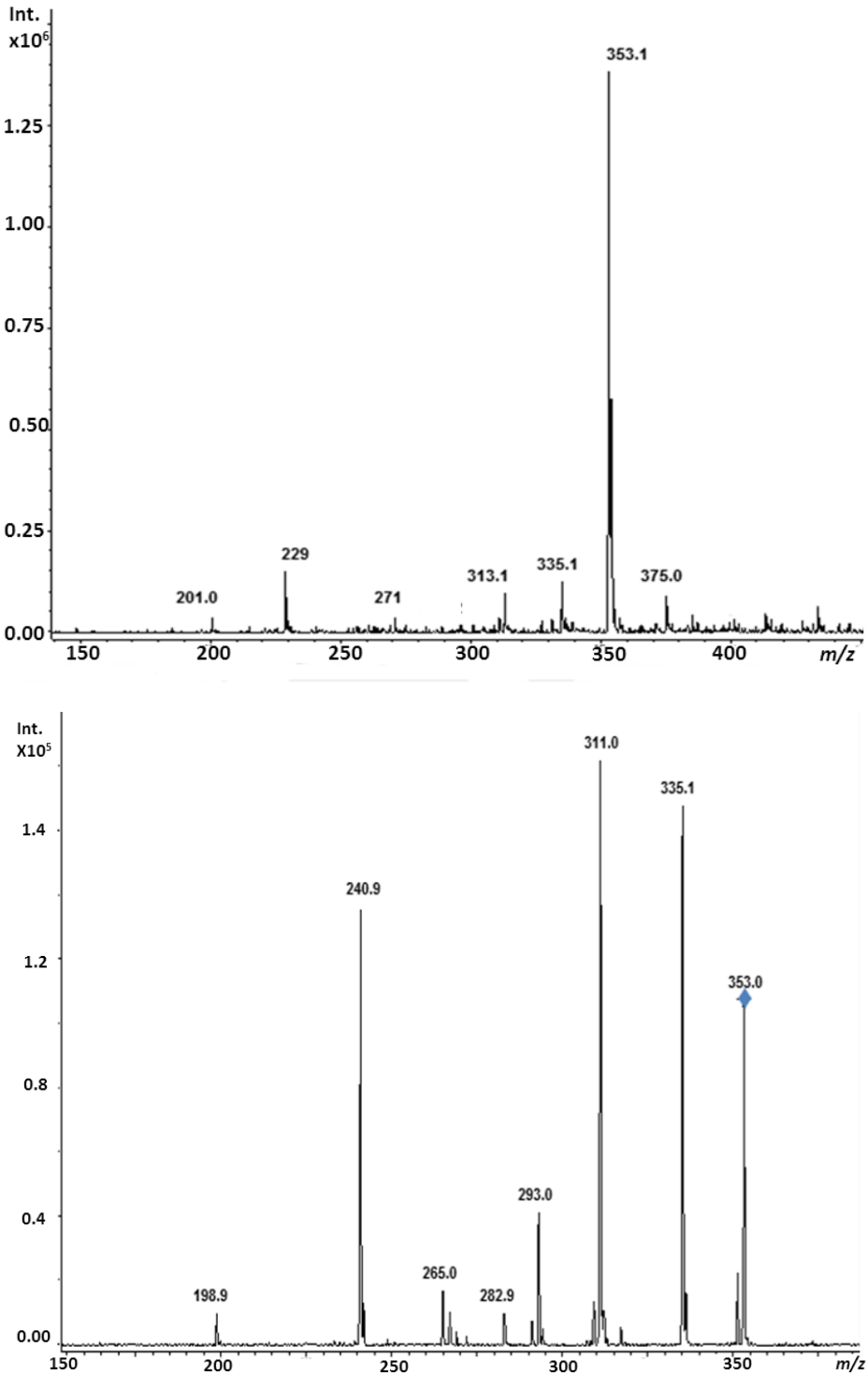


Figure S2. ESI (−) MS (top) and MS/MS spectraon *m/z* 329 [M − H]$^-$ (bottom) of compound **13**.

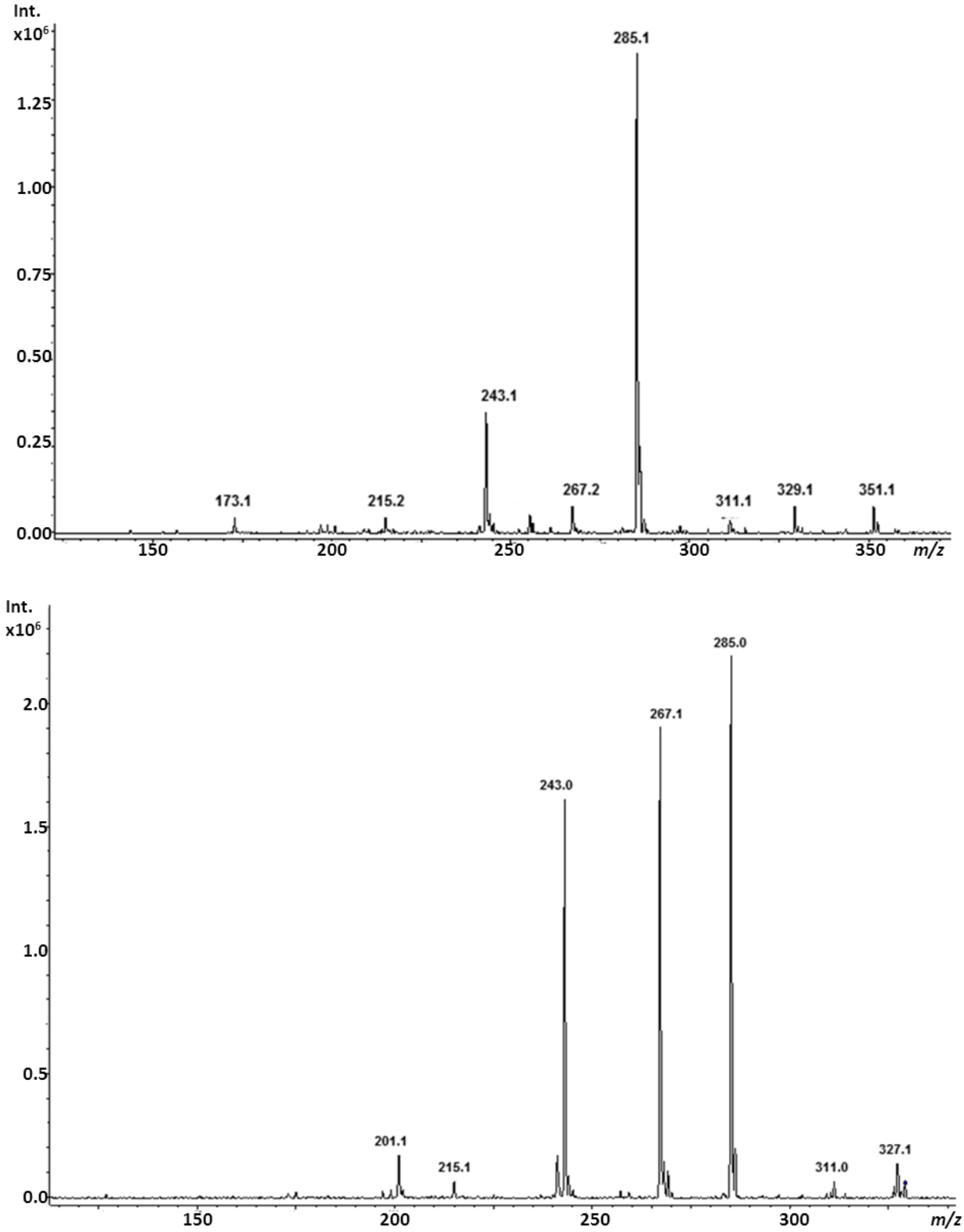


Figure S3. ^{1}H-NMR spectrum of **13** (400 MHz, in $CDCl_3$).

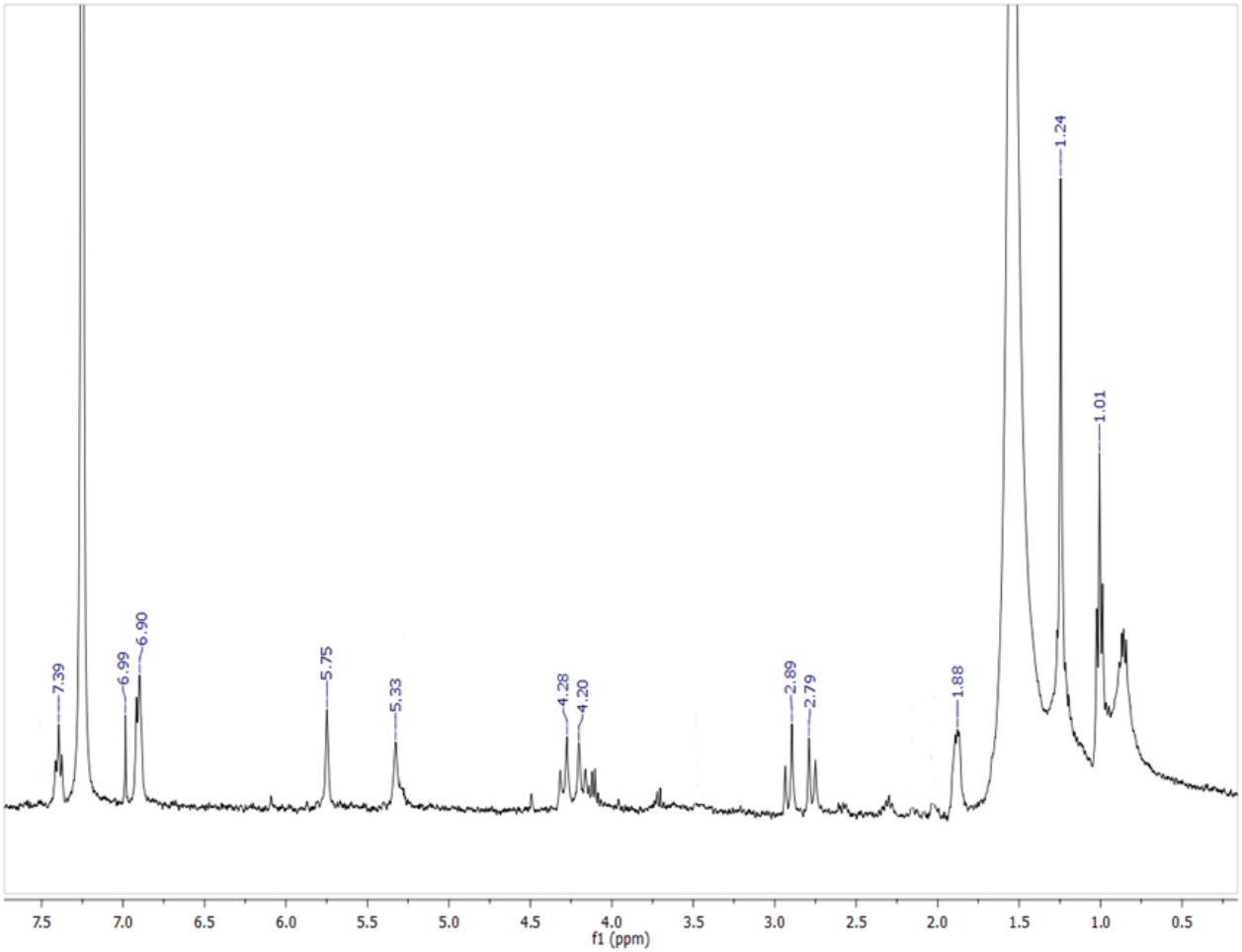


Figure S4. ^{1}H-NMR spectrum of **13** (400 MHz, in CD_3OD).

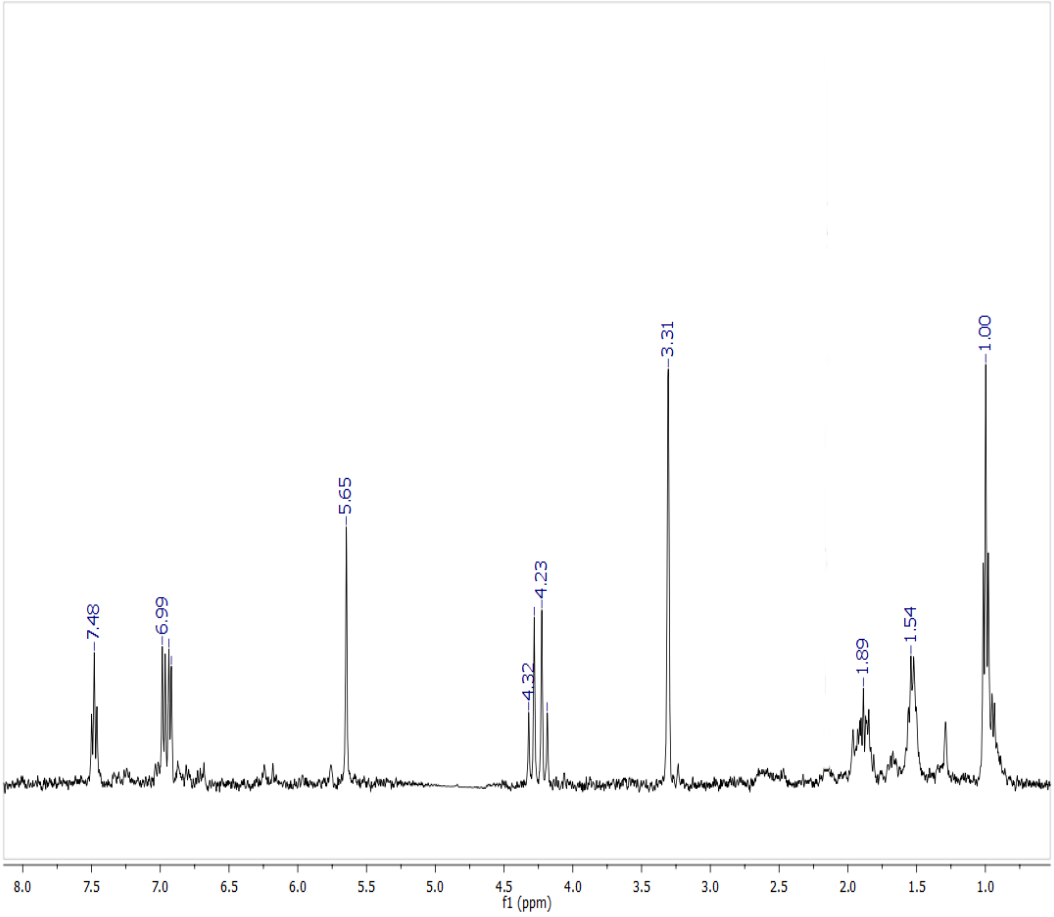


Figure S5. HSQC spectrum of **13** in CD_3OD.

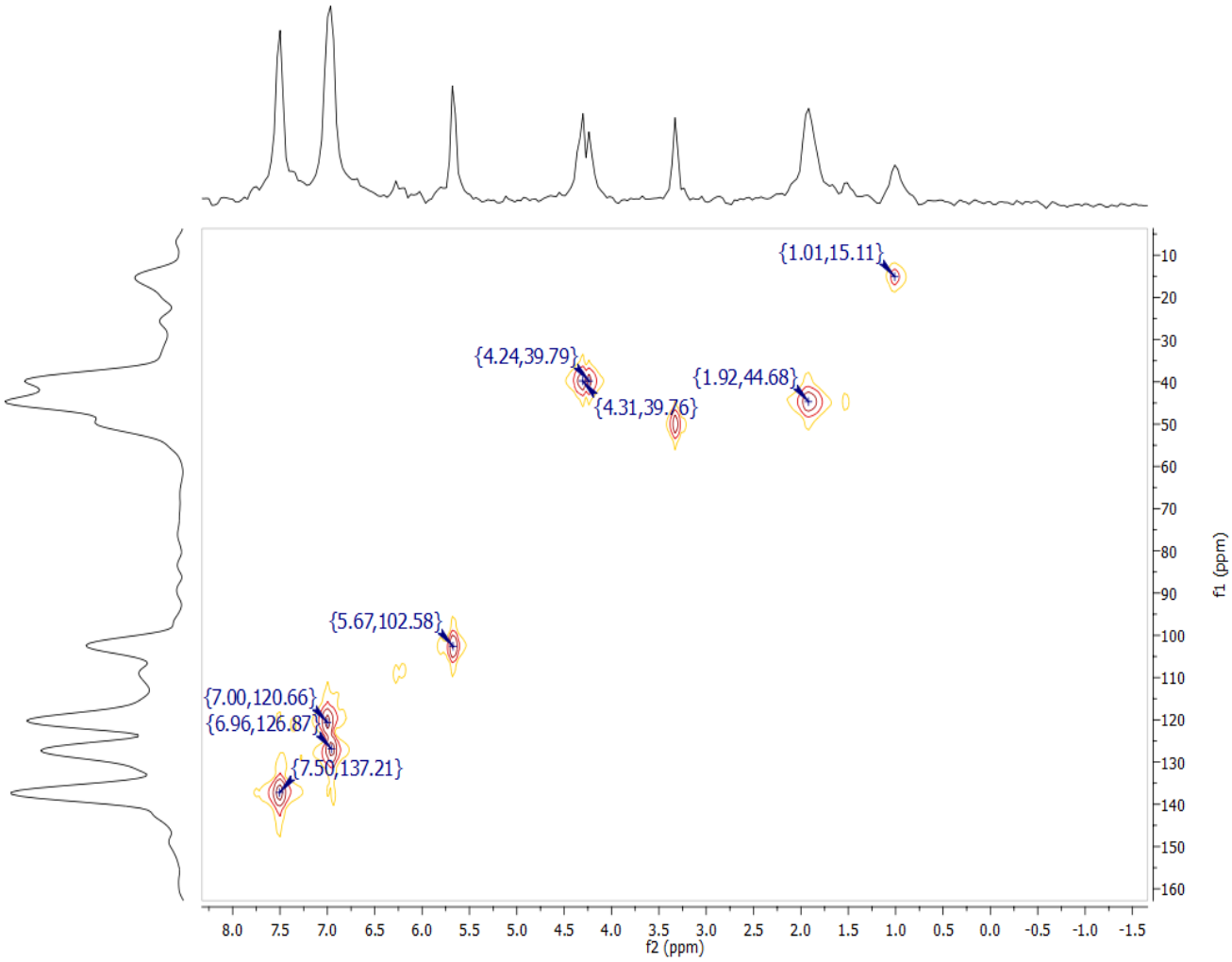


Figure S6. HMBC spectrum of **13** in CD_3OD.

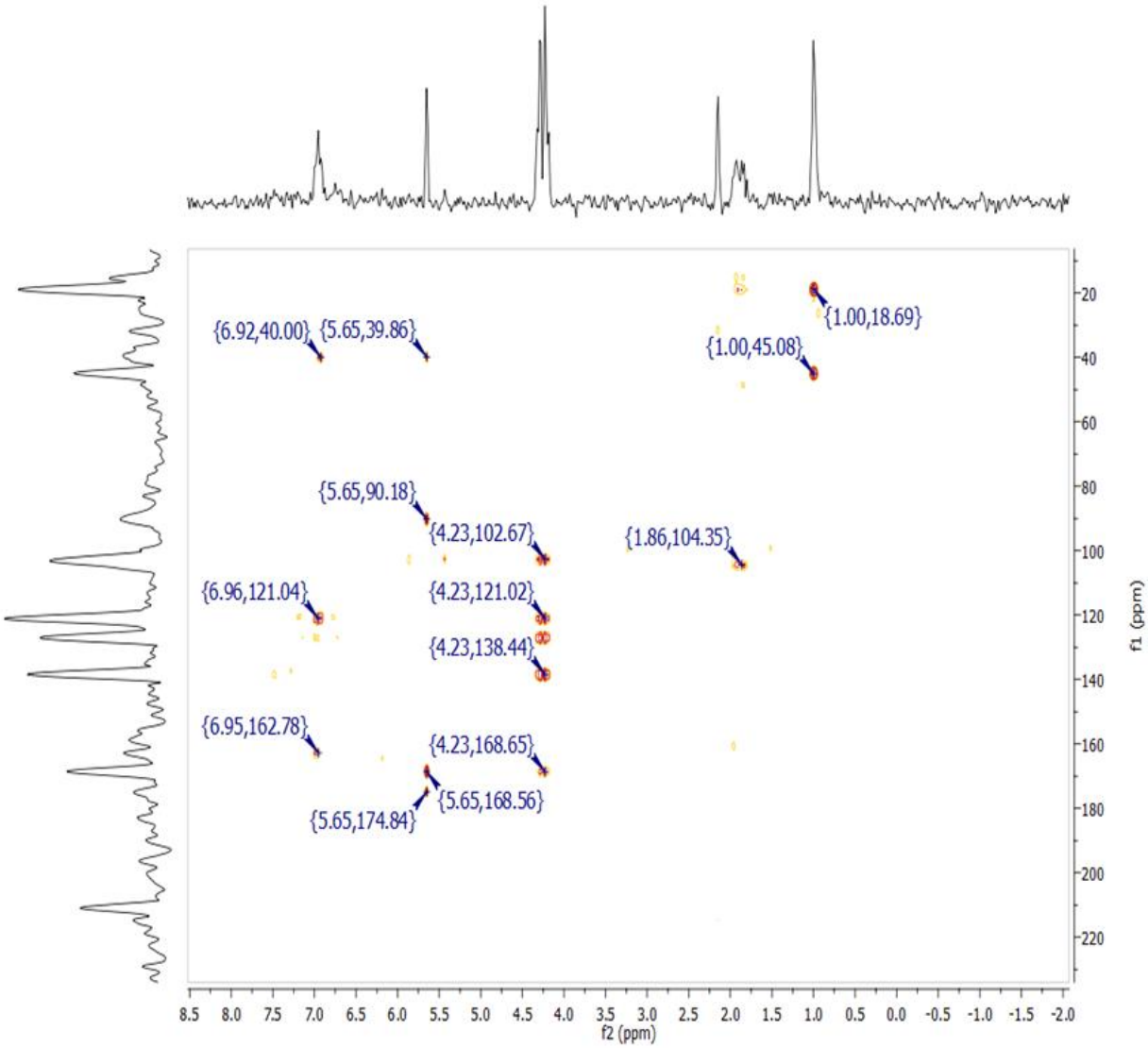


Figure S7. ESI (+) MS and MS/MS spectra on *m/z* 358 $[M + Na]^+$ of deuterated **13** from a CD_3OD solution.

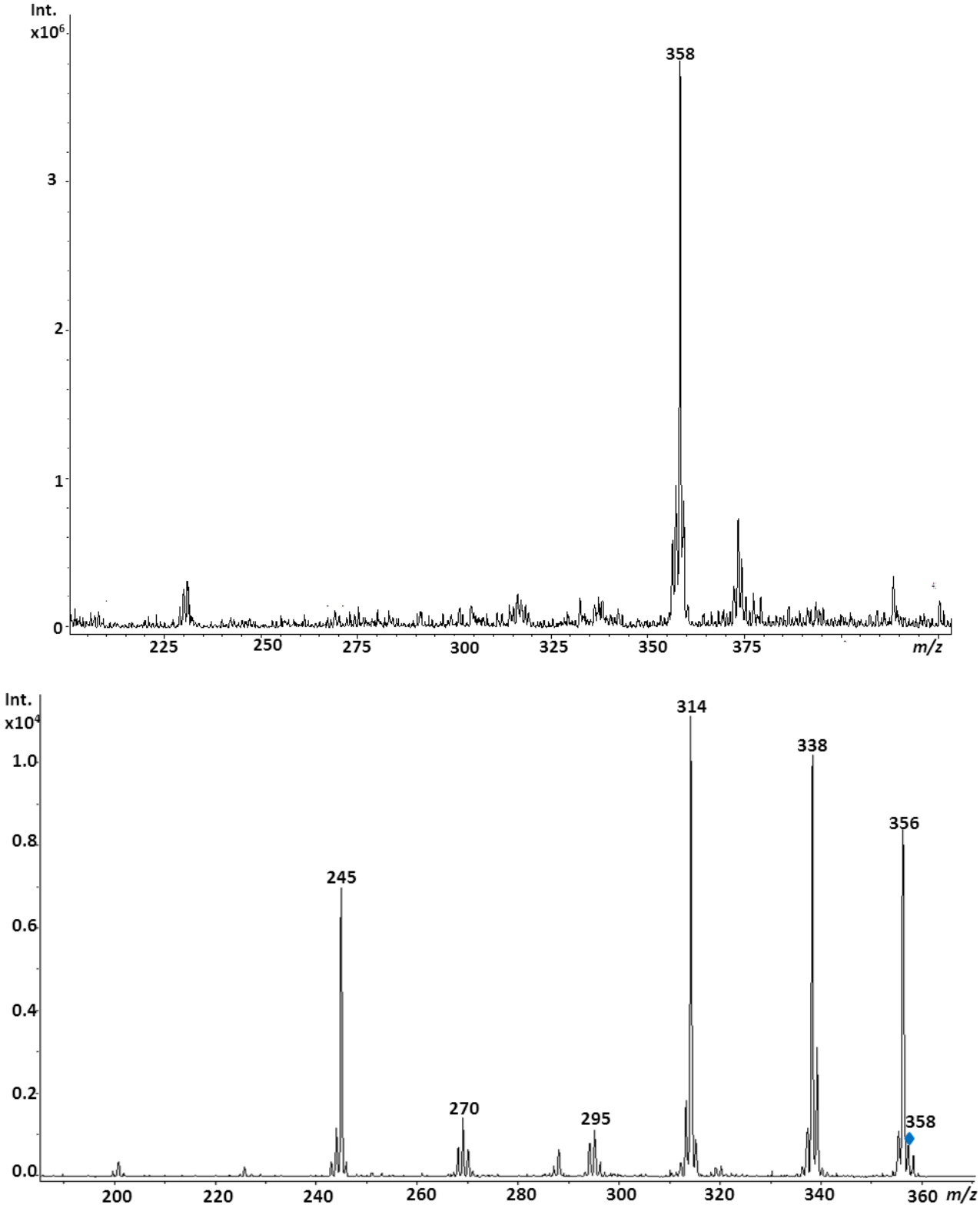


Figure S8. ESI (−) MS and MS/MS spectra on *m/z* 332 $[M - H]^-$ of deuterated **13** from a CD_3OD solution.

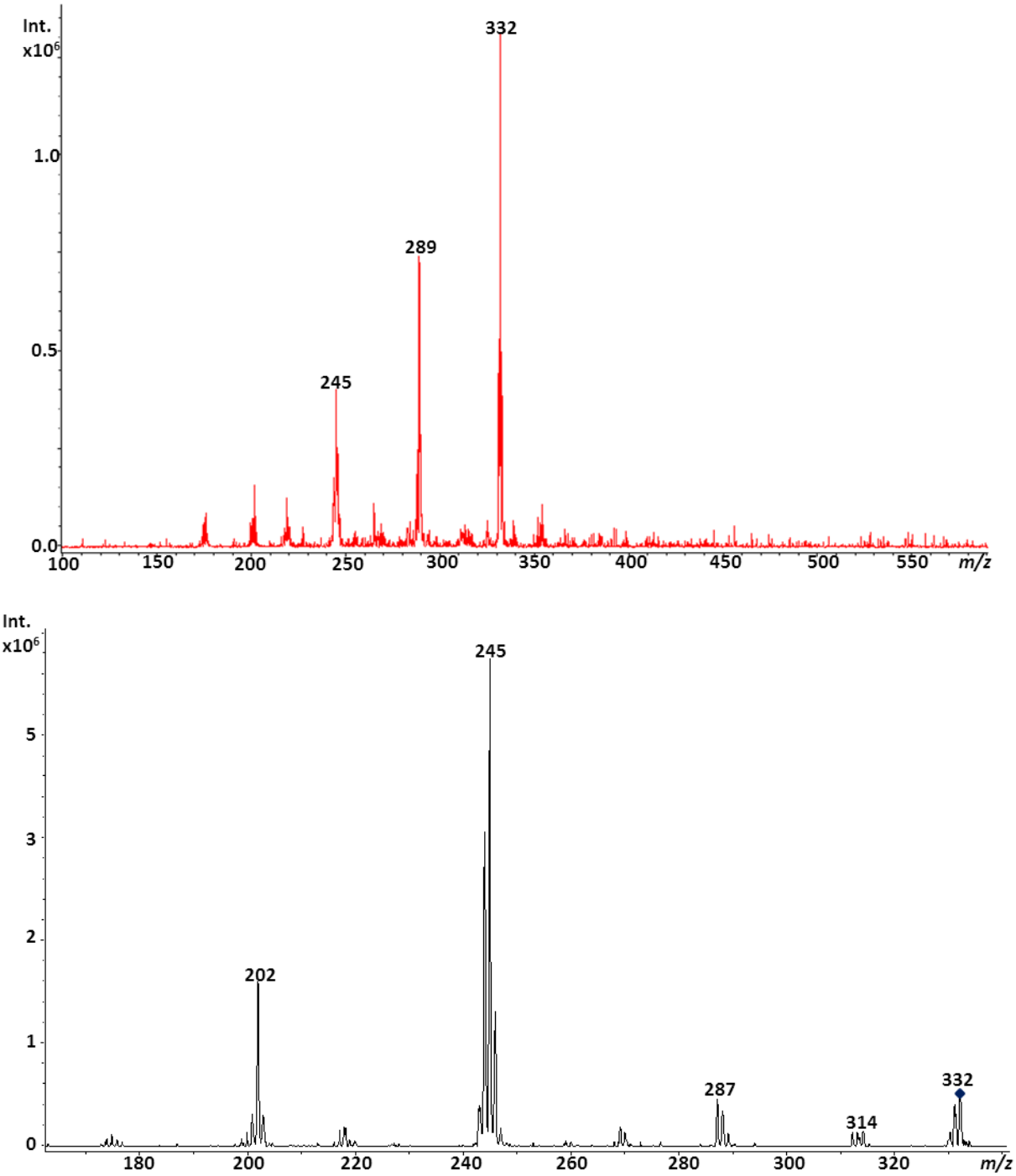


Figure S9. ^{1}H-NMR spectrum of **7** (400 MHz, in acetone-d_6).

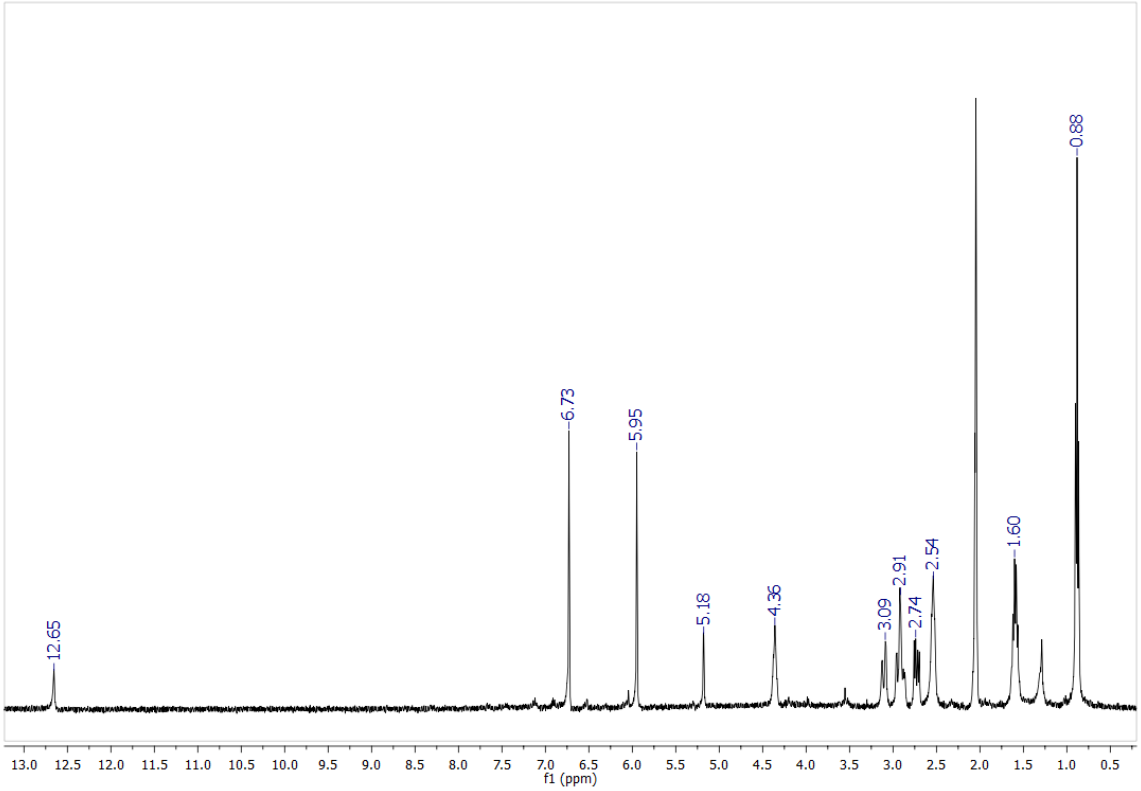


Figure S10. ^{1}H-NMR spectrum of **9** (400 MHz, in acetone-d_6).

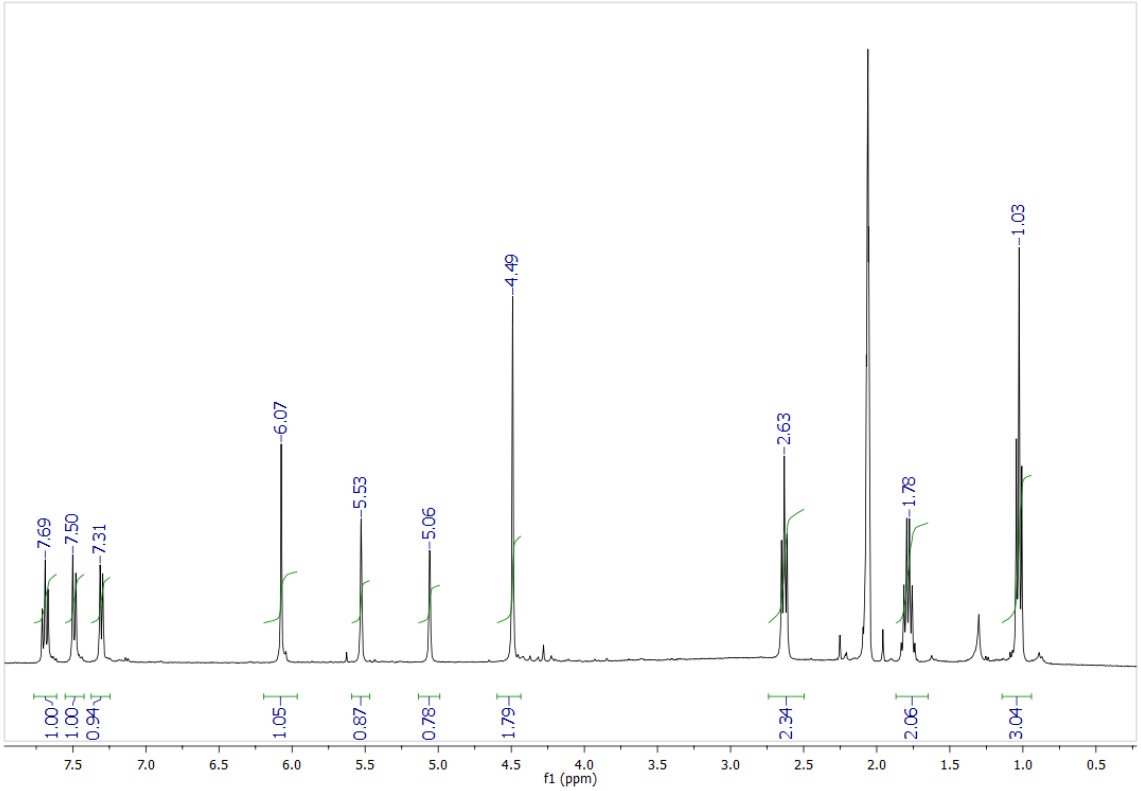


Figure S11. ^{1}H-NMR spectrum of **11** (400 MHz, in CD_3OD).

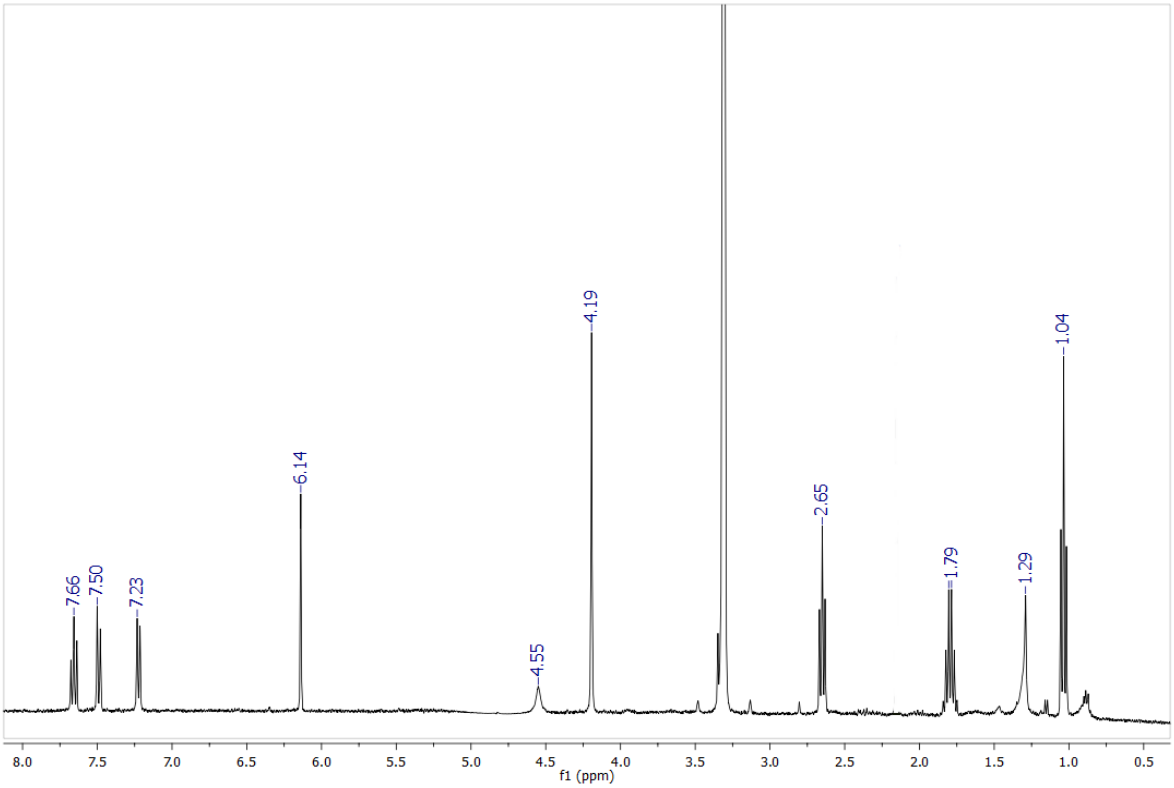


Figure S12. DFTcalculated IR spectra of 4-hydroxy α-pyrone form (**A**) and 2-hydroxy γ-pyroneform (**B**) of the compound **7**.

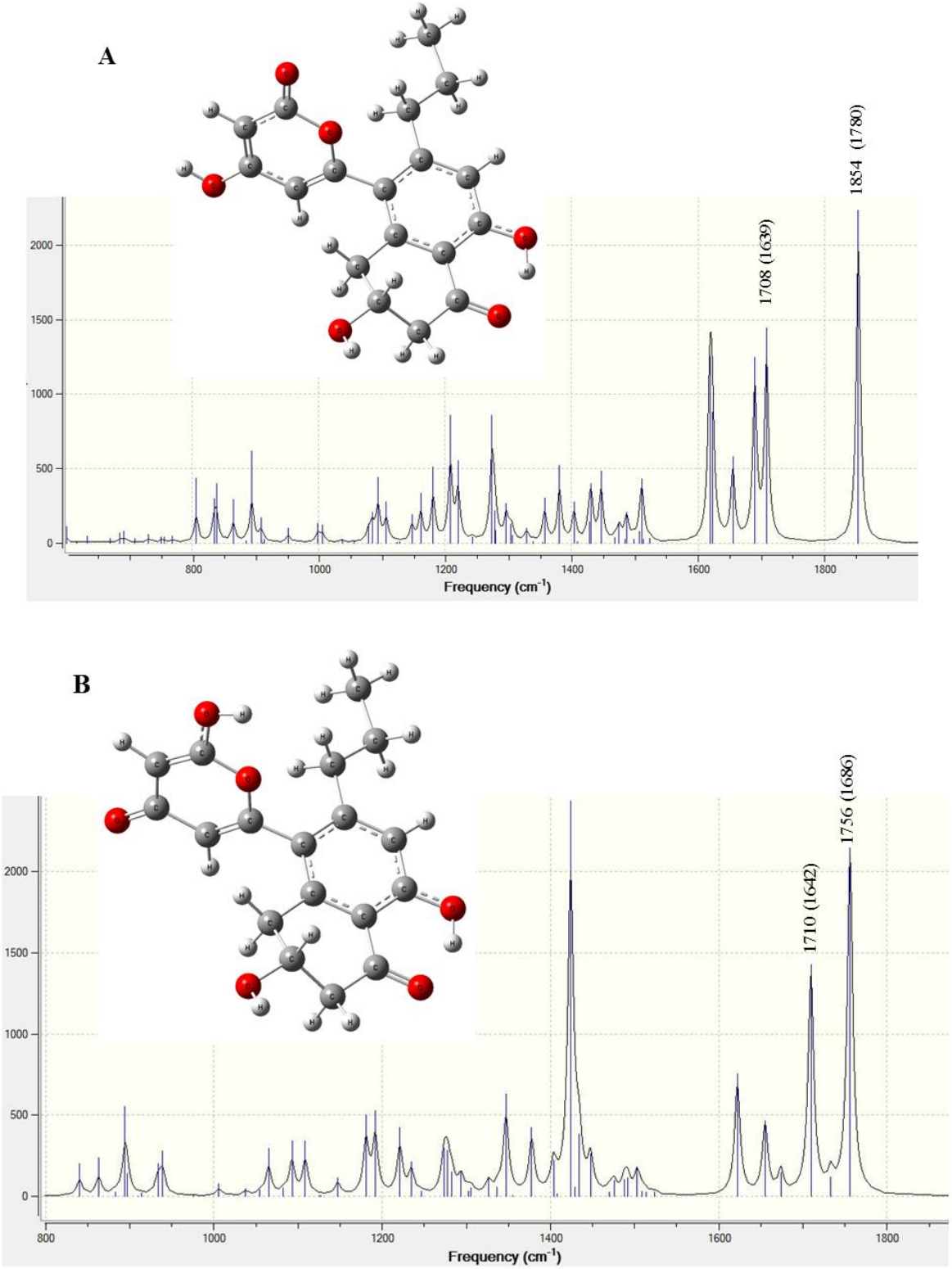


Figure S13. Experimental FT-IR spectrum of compound **7**.

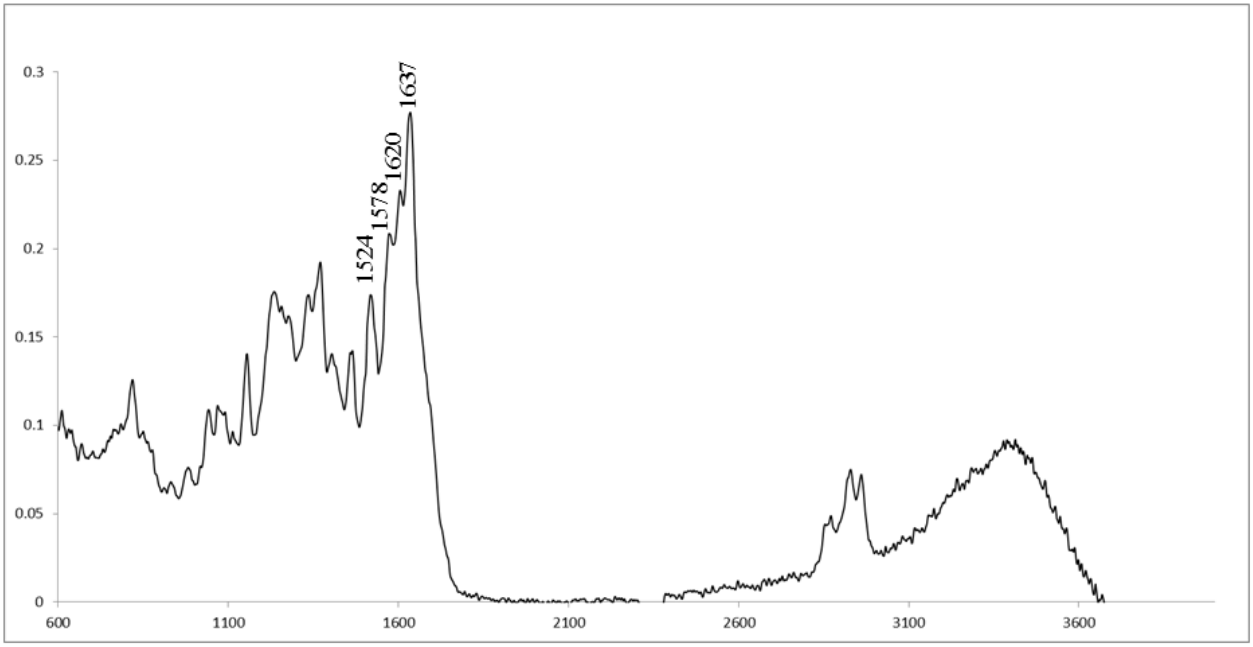
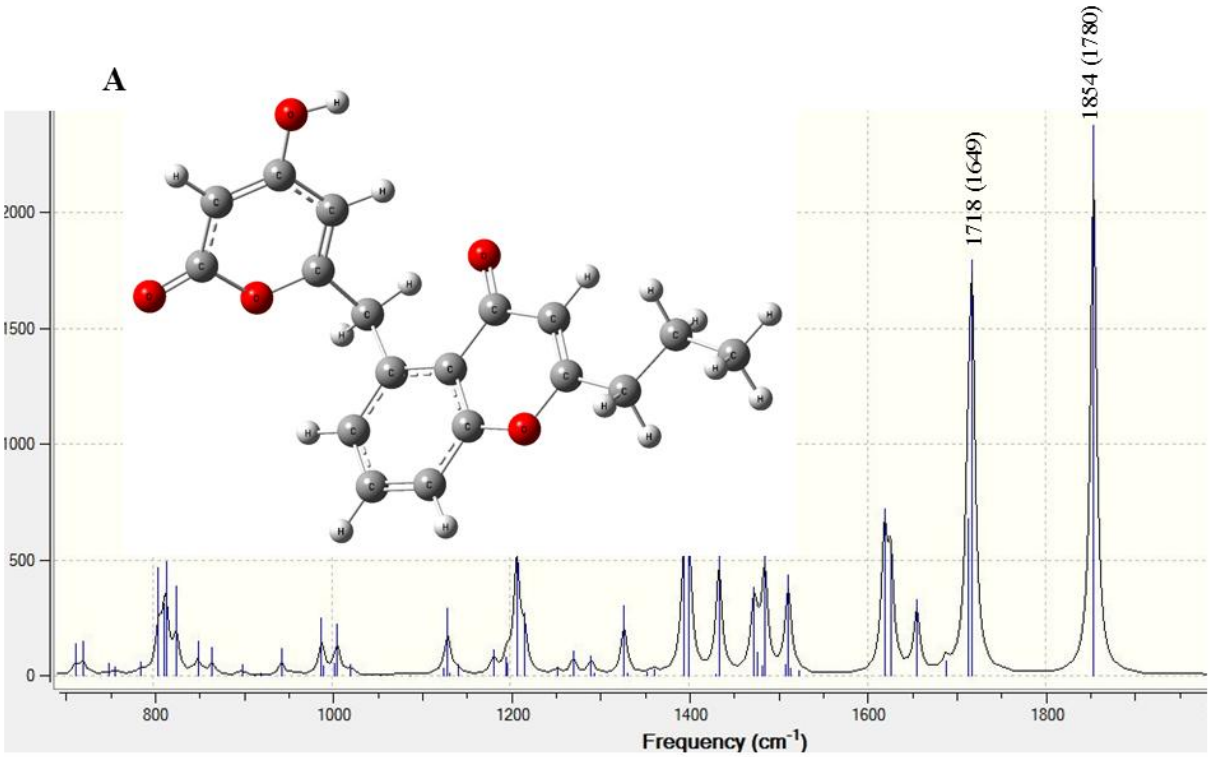


Figure S14. DFT calculated IR spectra of the compound **9** in 4-hydroxy α-pyrone form (**A**) and 2-hydroxy γ-pyroneform (**B**).



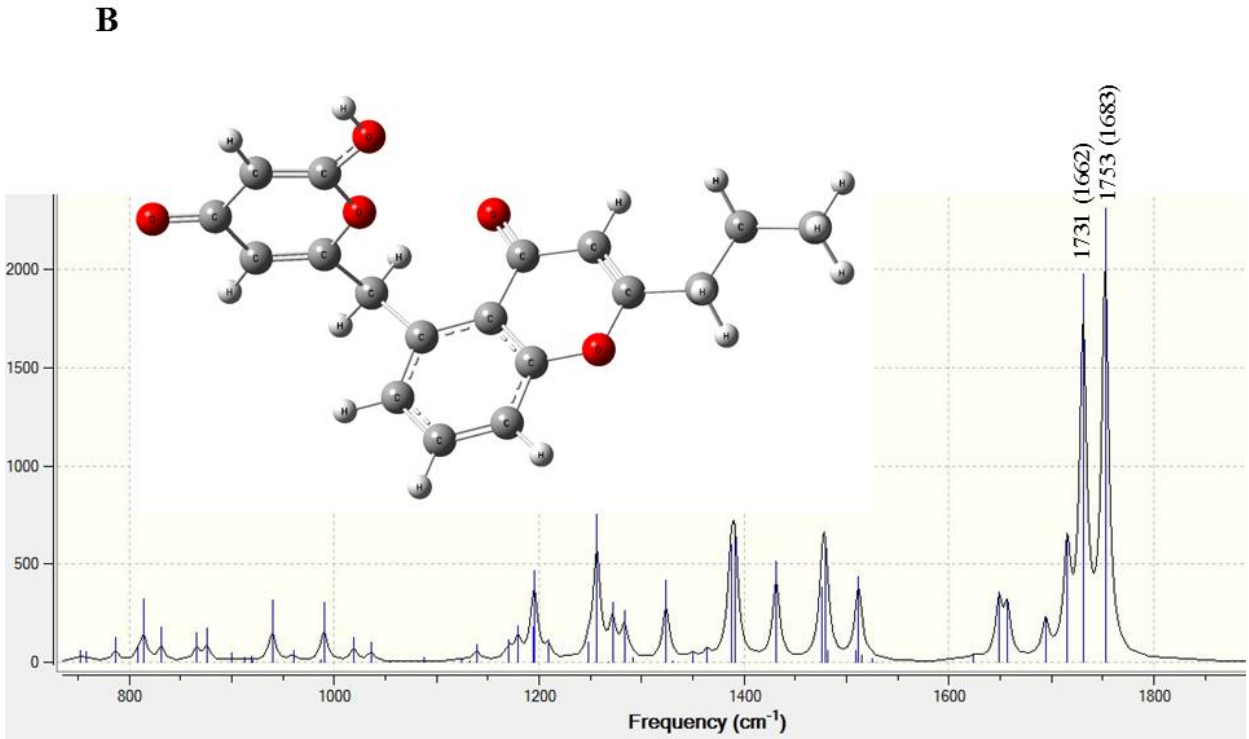


Figure S15. Experimental FT-IR spectrum of compound **9**.

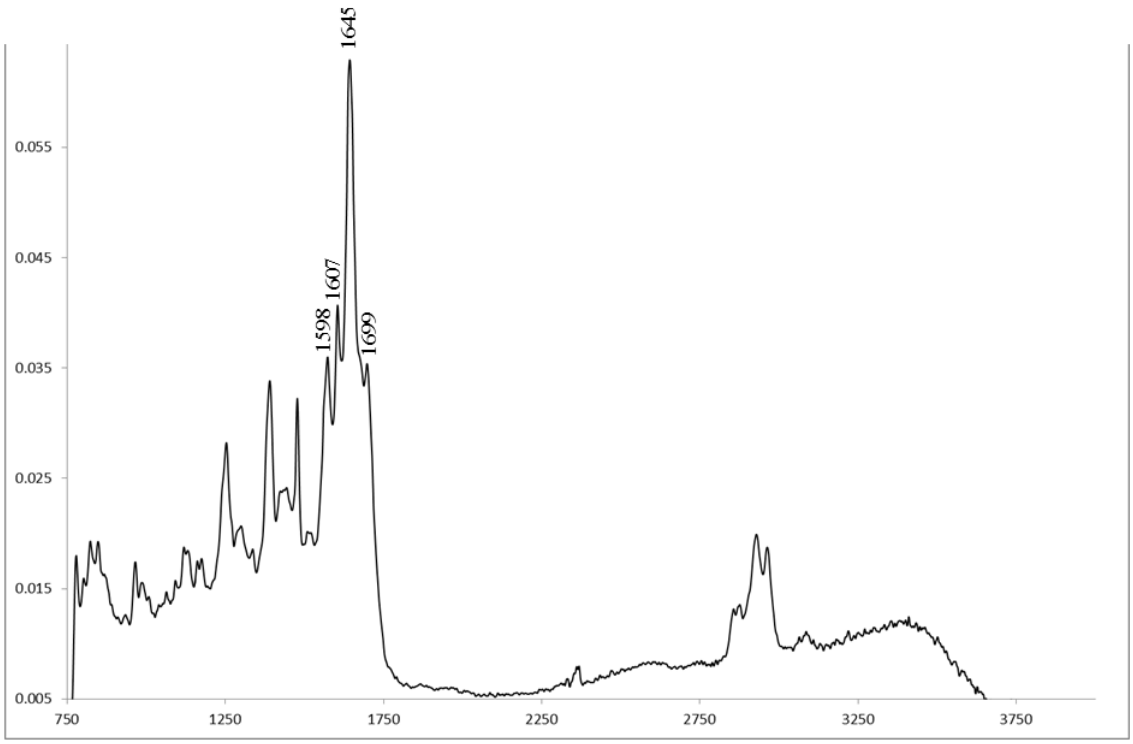


Figure S16. DFT calculated IR spectra of the compound **13** in 4-hydroxy α-pyrone form (**A**) and 2-hydroxy γ-pyrone form (**B**).

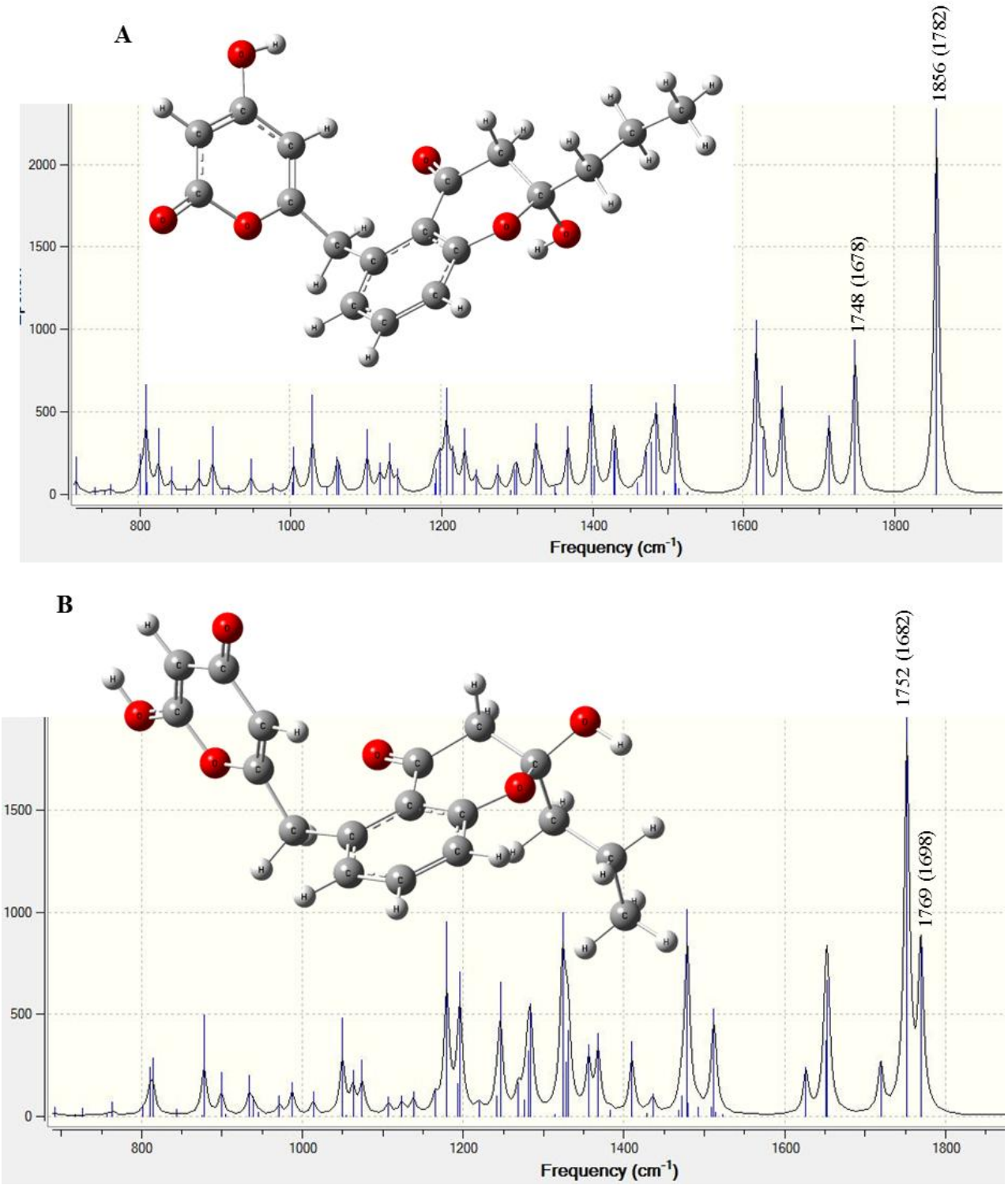


Figure S17. Experimental FT-IR spectrum of compound **13**.

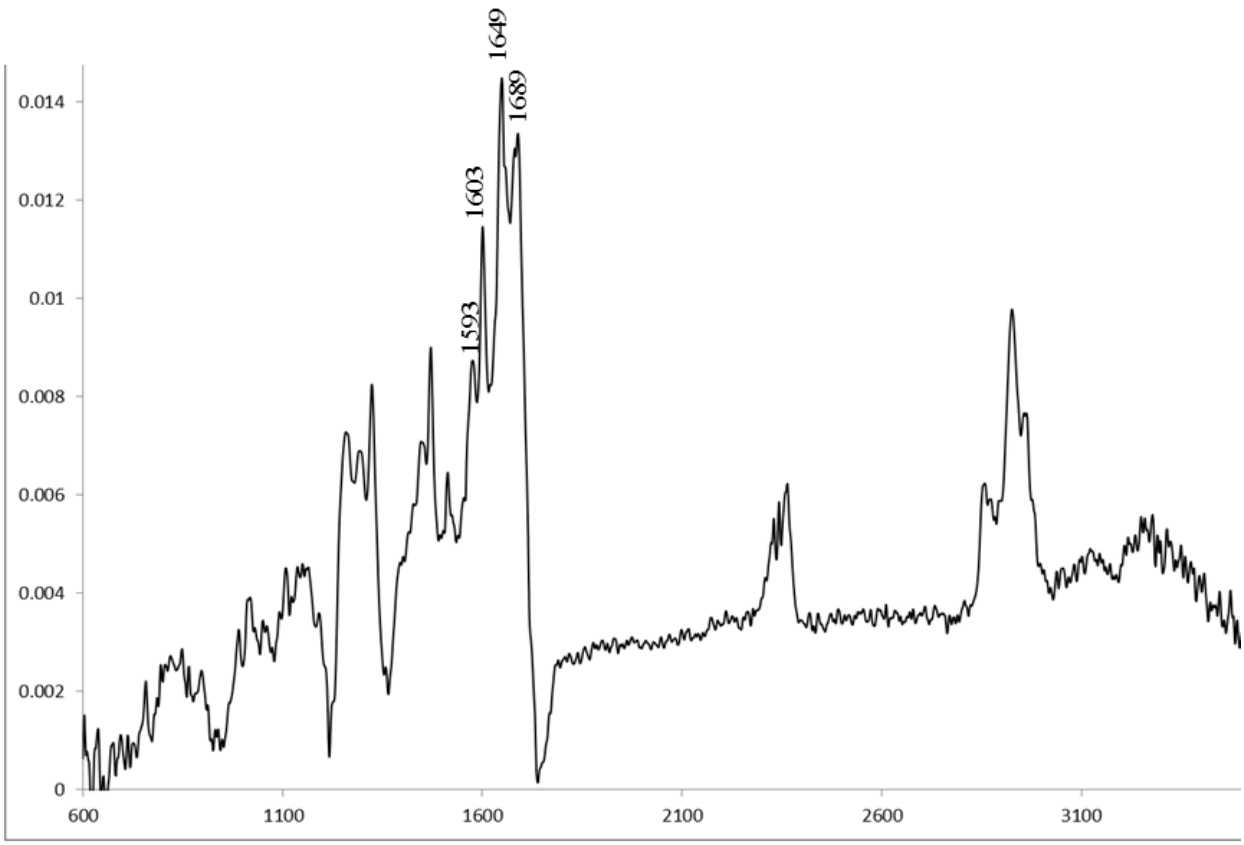


Table S1. Antibacterial activities at 100 µL/well of compounds **9**, **11** and **13**.

Compounds	Inhibition Zone ± SD (mm)				
	***E. coli* ATCC 25922**	***S. aureus* ATCC 25923**	***MRSA* ATCC 43300**	***B. subtilis* ATCC 6633**	***P. aeruginosa* ATCC 27853**
9	-	-	08.34 ± 1.04	-	11.07 ± 1.23
11	08.08 ± 0.41	-	08.27 ± 0.38	-	07.61 ± 0.71
13	12.44 ± 0.84	-	15.033 ± 0.57	-	13.56 ± 0.84
Vancomycin (30 µg/disc)	ND	20.05 ± 0.60	ND	ND	ND
Erythromycin(15 µg/disc)	ND	25.26 ± 0.64	14.63 ± 0.27	ND	ND
Gentamicin (10 µg/disc)	23.37 ± 0.5	25.78 ± 0.30	ND	ND	18.88 ± 0.27

-: No activity observed; ND: not determined.