

Supporting Information

Antibiotic abietane-type diterpenoids from *Plectranthus punctatus*

Negera Abdissa, Marcel Frese, and Norbert Sewald

Table of contents

Contents	Page
Spectroscopic data for 6β, 7β-dihydroxy-12-methylroyleanone (1)	
Figure S1: ¹ H NMR spectrum of 6 β , 7 β -dihydroxy-12-methylroyleanone (1)	S2
Figure S2: ¹³ C NMR spectrum of 6 β , 7 β -dihydroxy-12-methylroyleanone (1)	S2
Figure S3: ¹³ C DEPT NMR spectrum of 6 β , 7 β -dihydroxy-12-methylroyleanone (1)	S3
Figure S4: COSY spectrum of 6 β , 7 β -dihydroxy-12-methylroyleanone (1)	S3
Figure S5: HMQC spectrum of 6 β , 7 β -dihydroxy-12-methylroyleanone (1)	S4
Figure S6: HMBC spectrum of 6 β , 7 β -dihydroxy-12-methylroyleanone (1)	S4
Figure S7: NOESY spectrum of 6 β , 7 β -dihydroxy-12-methylroyleanone (1)	S5
Figure S8: HRESIMS spectra of 6 β , 7 β -dihydroxy-12-methylroyleanone (1)	S5
Spectroscopic data for 6β-acetoxy-6α-methoxy-7-oxoroyleanone (2)	
Figure S9: ¹ H NMR spectrum of 6 β -acetoxy-6 α -methoxy-7-oxoroyleanone (2)	S6
Figure S10: ¹³ C NMR spectrum of 6 β -acetoxy-6 α -methoxy-7-oxoroyleanone (2)	S6
Figure S11: COSY spectrum of 6 β -acetoxy-6 α -methoxy-7-oxoroyleanone (2)	S7
Figure S12: HMQC spectrum of 6 β -acetoxy-6 α -methoxy-7-oxoroyleanone (2)	S7
Figure S13: HMBC spectrum of 6 β -acetoxy-6 α -methoxy-7-oxoroyleanone (2)	S8
Figure S14: HRESIMS spectra of 6 β -acetoxy-6 α -methoxy-7-oxoroyleanone (2)	S8
Spectroscopic data for 8α,9α-epoxy-6-deoxycoleon U (3)	
Figure S15: ¹ H NMR spectrum of 8 α ,9 α -epoxy-6-deoxycoleon U (3)	S9
Figure S16: ¹³ C NMR spectrum of 8 α ,9 α -epoxy-6-deoxycoleon U (3)	S9
Figure S17: COSY spectrum of 8 α ,9 α -epoxy-6-deoxycoleon U (3)	S10
Figure S18: NOESY spectrum of 8 α ,9 α -epoxy-6-deoxycoleon U (3)	S10
Figure S19: HMQC spectrum of 8 α ,9 α -epoxy-6-deoxycoleon U (3)	S11
Figure S20: HMBC spectrum of 8 α ,9 α -epoxy-6-deoxycoleon U (3)	S11
Figure S21: HRESIMS spectra of 8 α ,9 α -epoxy-6-deoxycoleon U (3)	S12
Figure S22: IR spectra of 8 α ,9 α -epoxy-6-deoxycoleon U (3)	S12
Spectroscopic data for 6,12-dihydroxysapriparaquinone (4)	
Figure S23: ¹ H NMR spectrum of 6,12-dihydroxysapriparaquinone (4)	S13
Figure S24: ¹³ C NMR spectrum of 6,12-dihydroxysapriparaquinone (4)	S13
Figure S25: ¹³ C DEPT NMR spectrum of 6,12-dihydroxysapriparaquinone (4)	S14
Figure S26: COSY spectrum of 6,12-dihydroxysapriparaquinone (4)	S14
Figure S27: HMQC spectrum of 6,12-dihydroxysapriparaquinone (4)	S15
Figure S28: HMBC spectrum of 6,12-dihydroxysapriparaquinone (4)	S15
Figure S29: HRESIMS spectra 6,12-dihydroxysapriparaquinone (4)	S16

OC3_SchroederDa_0430_1.nd
13C(1H)_DEPT135 Acetone (C:\NMRData\Service_aktuell) OC3 16

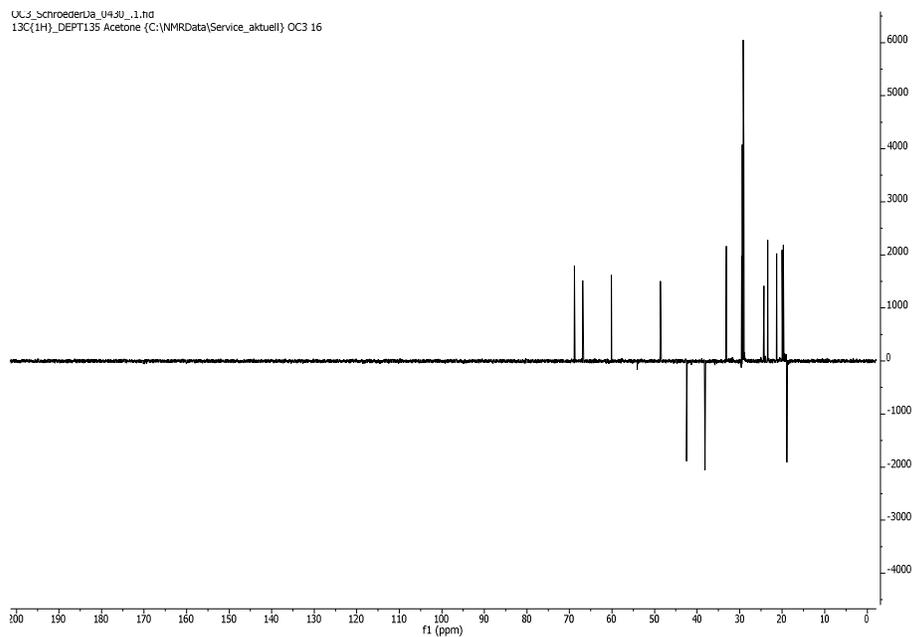


Figure S3. The ^{13}C DEPT NMR spectrum of 6 β , 7 β -dihydroxy-12-methylroyleanone (**1**) observed at 125 MHz in acetone- d_6 solution at 25 °C.

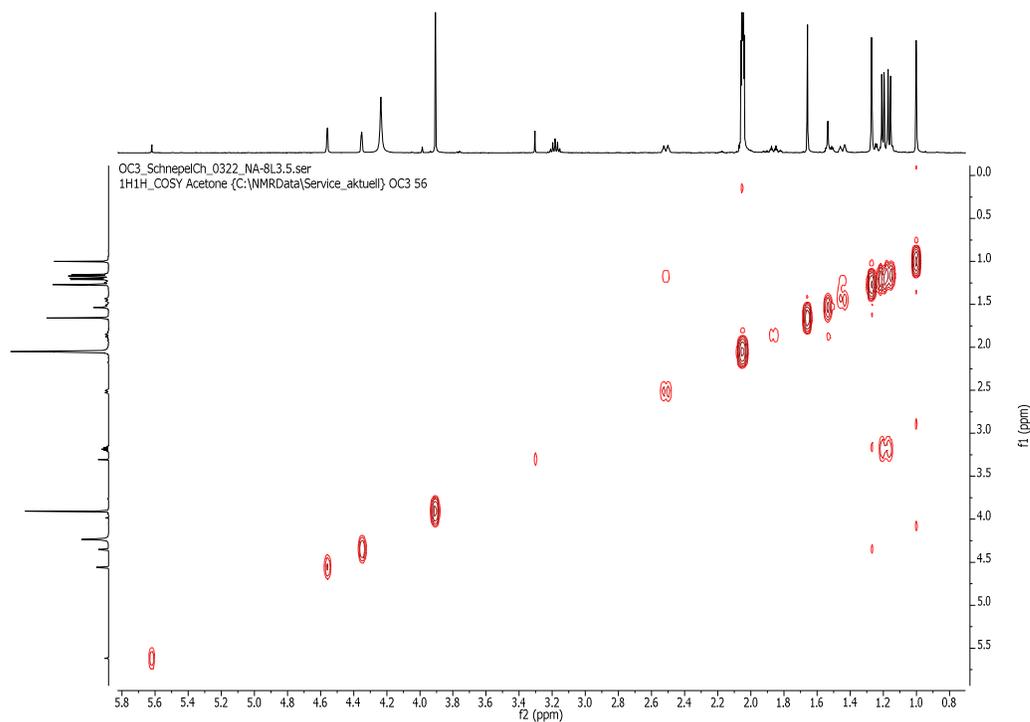


Figure S4. The COSY spectrum of 6 β , 7 β -dihydroxy-12-methylroyleanone (**1**) observed at 500 MHz in acetone- d_6 solution at 25 °C.

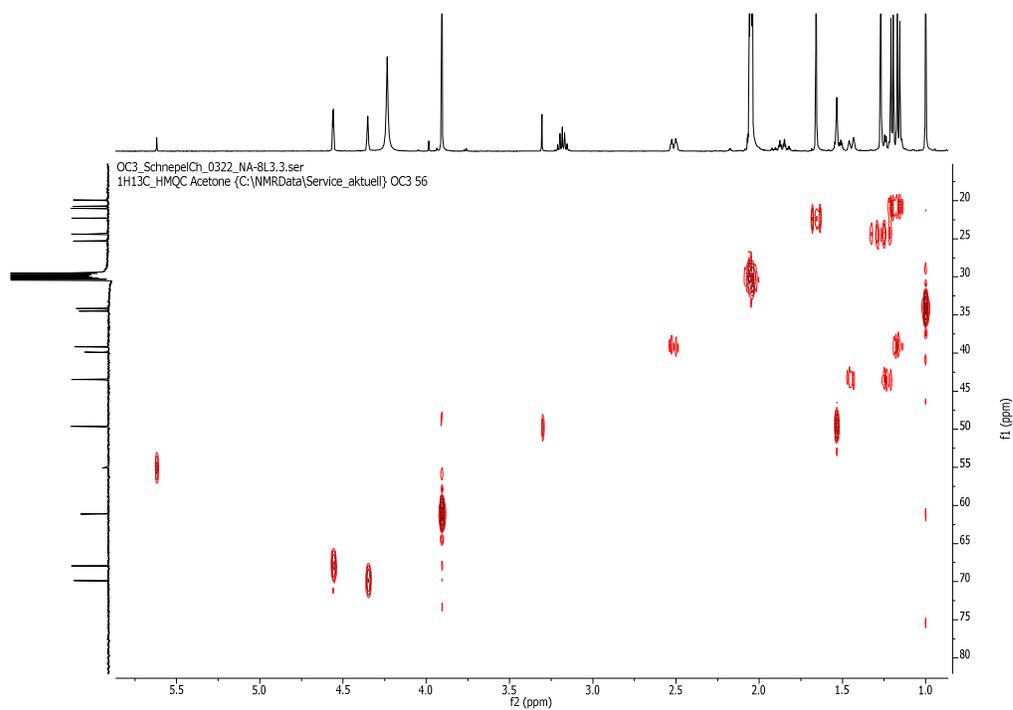


Figure S5. The HSQC spectrum of 6 β , 7 β -dihydroxy-12-methyloleanone (**1**) observed at 500 and 125 MHz in acetone-*d*₆ solution at 25 °C.

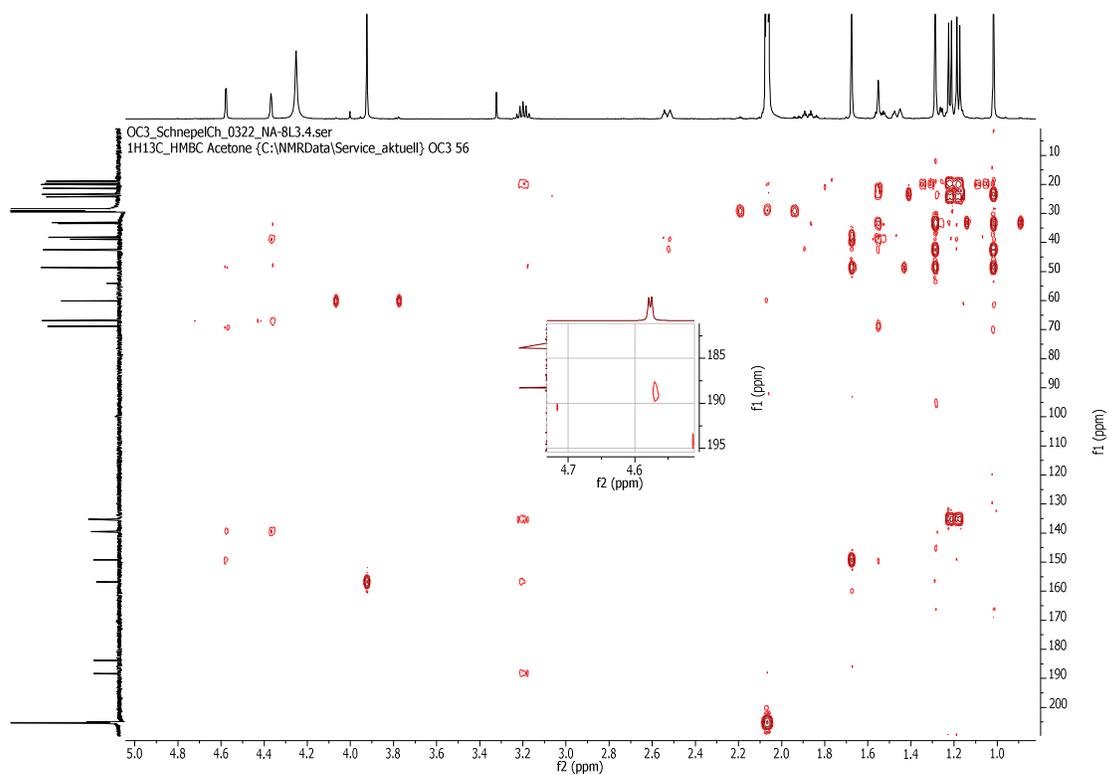


Figure S6. The HMBC spectrum of 6 β , 7 β -dihydroxy-12-methyloleanone (**1**) observed at 500 and 125 MHz in acetone-*d*₆ solution at 25 °C.

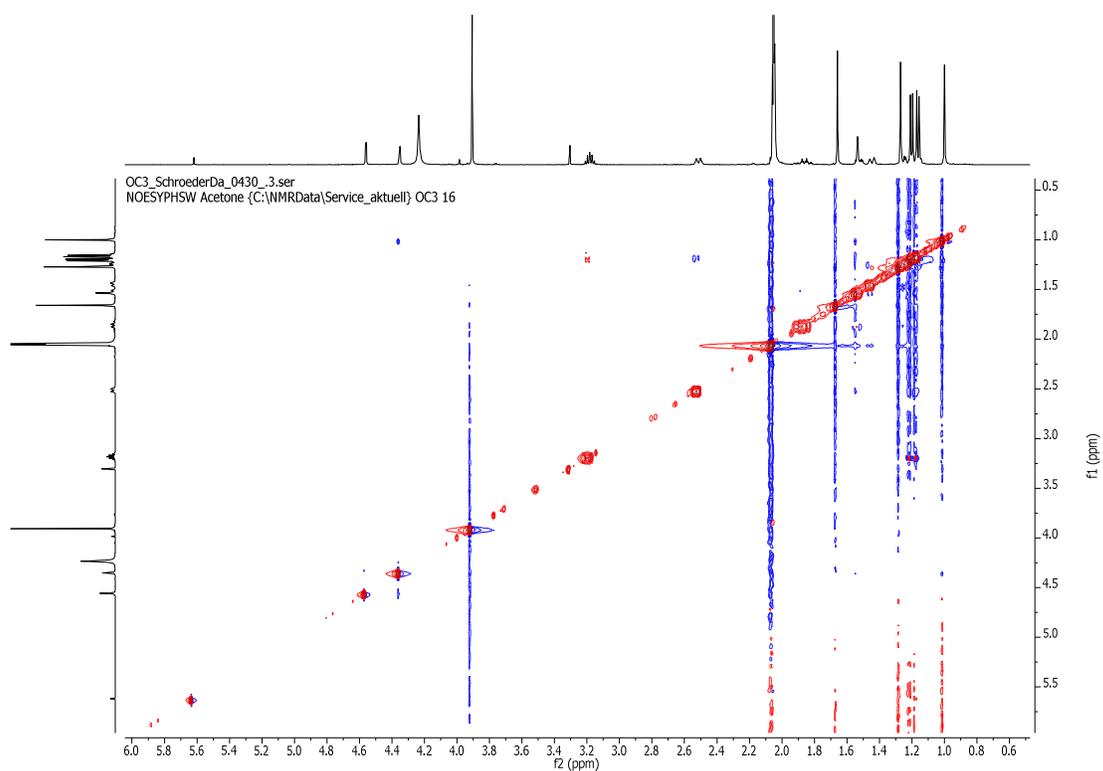


Figure S7. The NOESY spectrum of 6 β , 7 β -dihydroxy-12-methylroyleanone (**1**) observed at 500 MHz in acetone- d_6 solution at 25 °C.

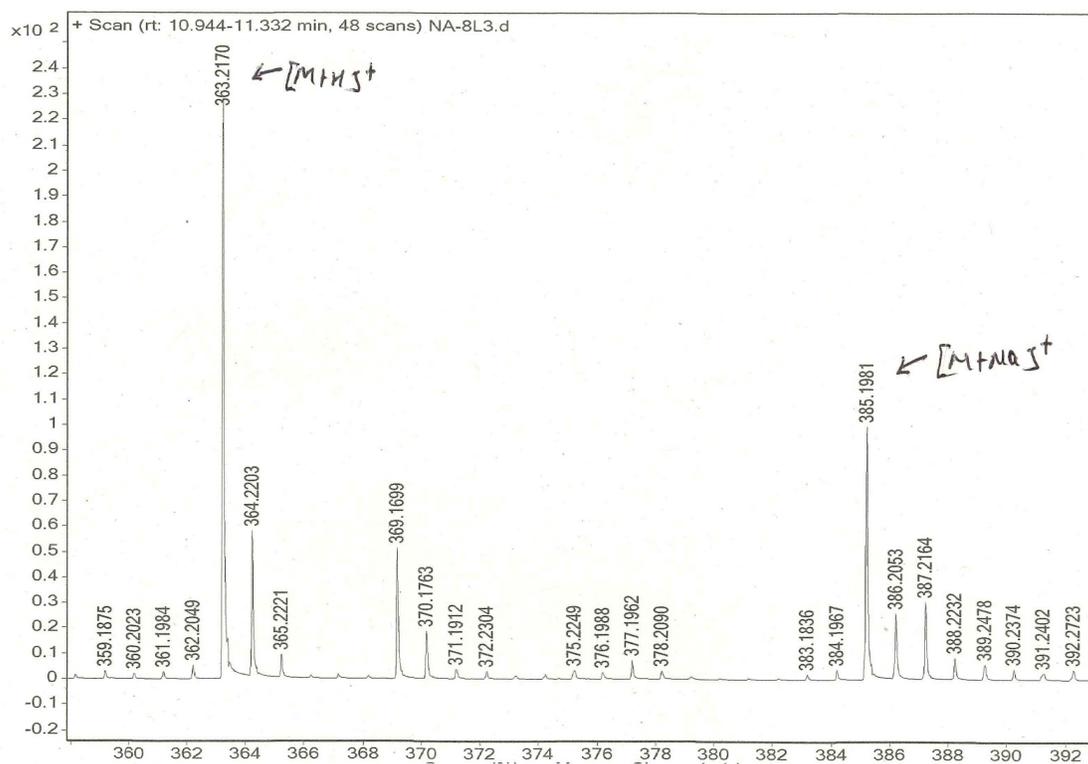


Figure S8. The HRMS of 6 β , 7 β -dihydroxy-12-methylroyleanone (**1**).

Spectroscopic data for 6 β -acetoxy-6 α -methoxy-7-oxoroleanone (2)

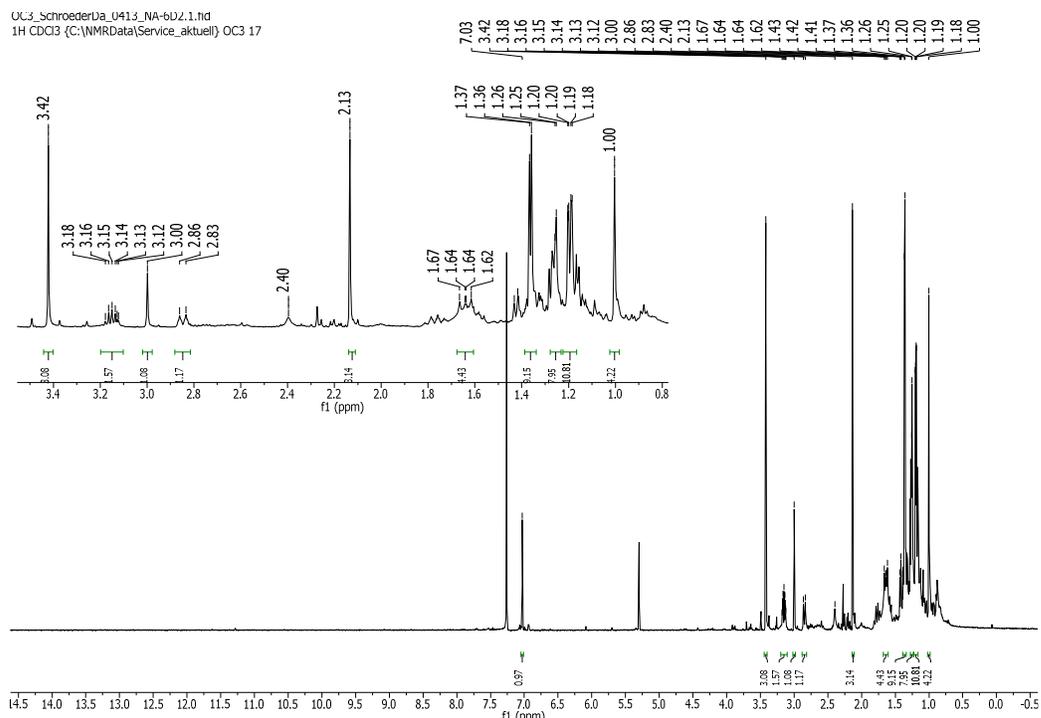


Figure S9. The ^1H NMR of 6 β -acetoxy-6 α -methoxy-7-oxoroleanone (**2**) observed at 500 MHz in CDCl_3 solution at 25 $^\circ\text{C}$. Assignments are given in Table 1.

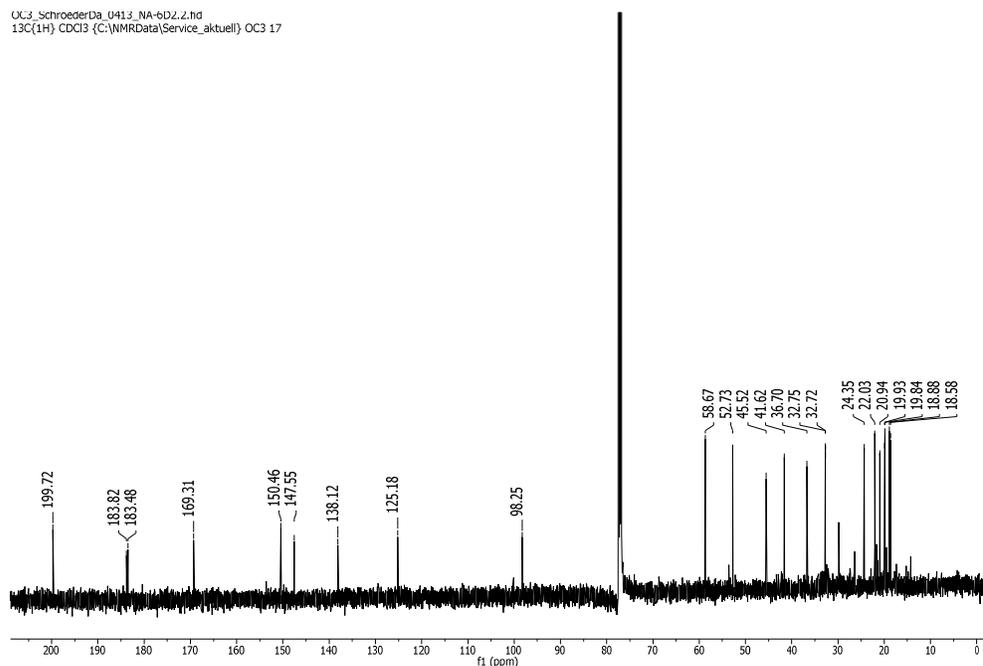


Figure S10. The ^{13}C NMR spectrum of 6 β -acetoxy-6 α -methoxy-7-oxoroleanone (**2**) observed at 125 MHz in CDCl_3 solution at 25 $^\circ\text{C}$. Assignments are given in Table 1.

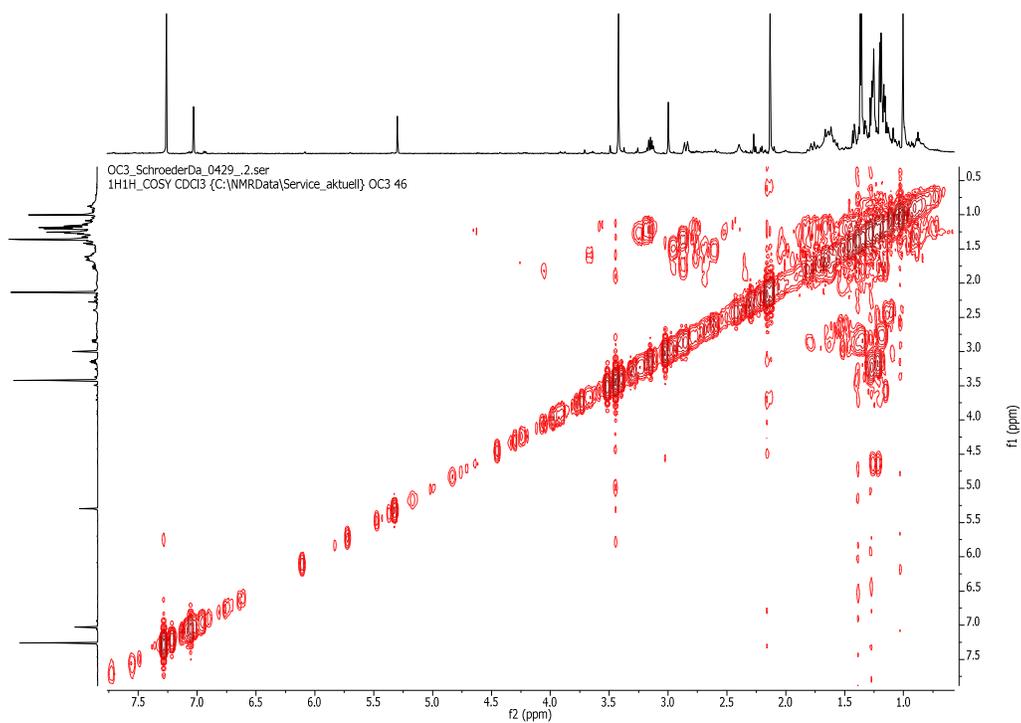


Figure S11. The COSY spectrum of 6 β -acetoxy-6 α -methoxy-7-oxoroleanone (**2**) observed at 500 MHz in CDCl₃ solution at 25 °C.

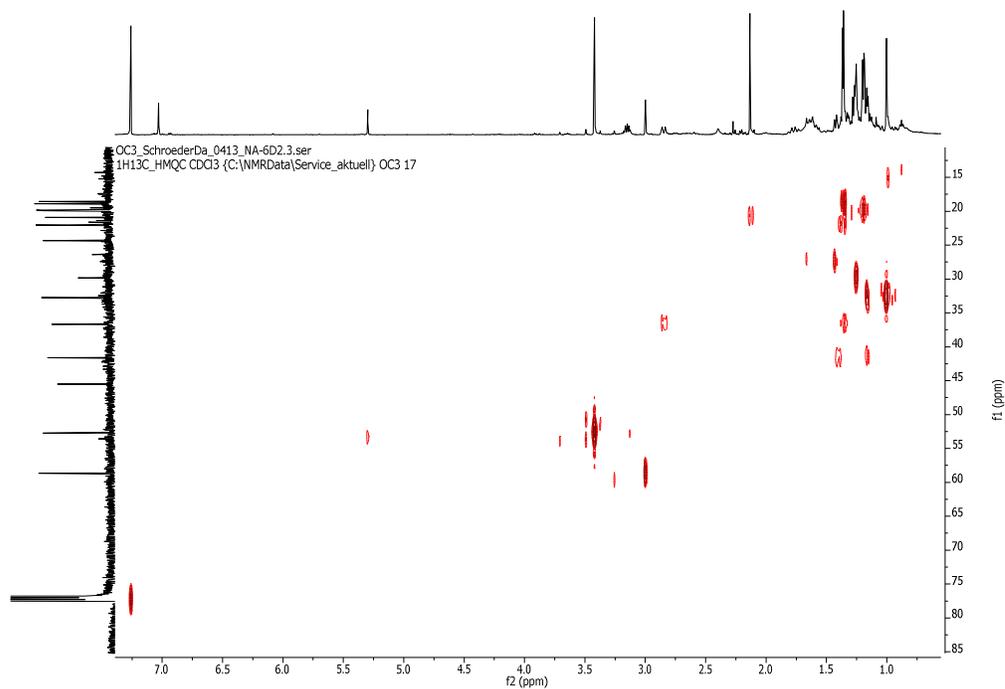


Figure S12. The HSQC spectrum of 6 β -acetoxy-6 α -methoxy-7-oxoroleanone (**2**) observed at 500 and 125 MHz in CDCl₃ solution at 25 °C.

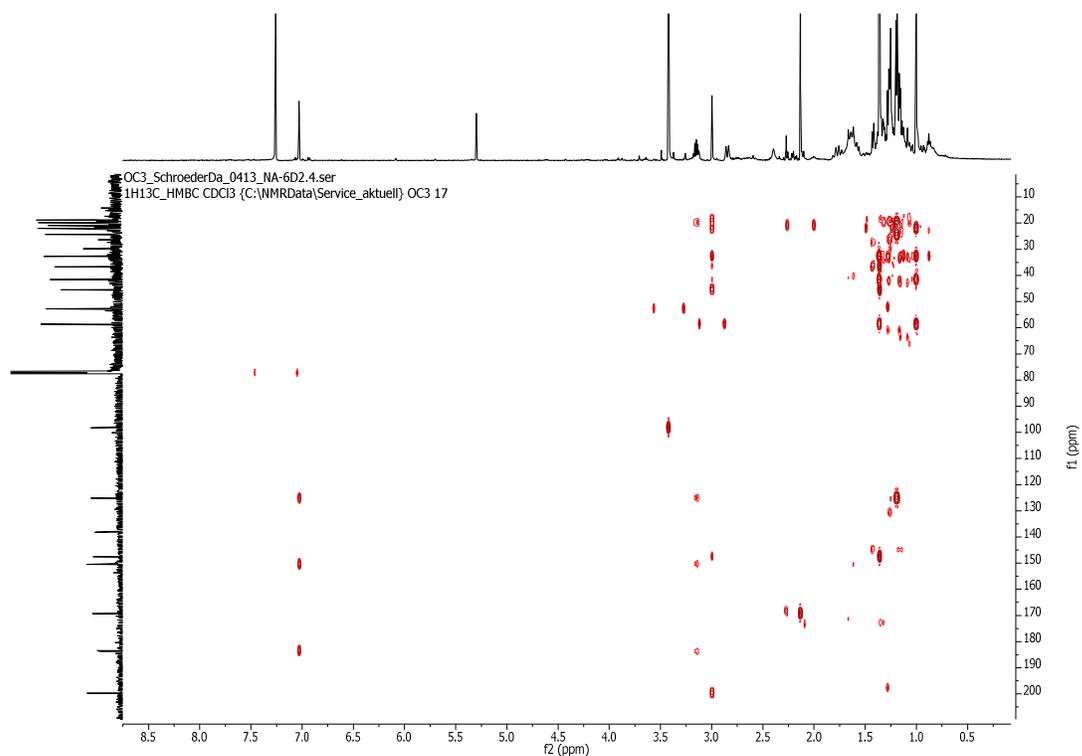


Figure S13. The HMBC spectrum of 6 β -acetoxy-6 α -methoxy-7-oxoroyleanone (**2**) observed at 500 and 125 MHz in CDCl₃ solution at 25 °C.

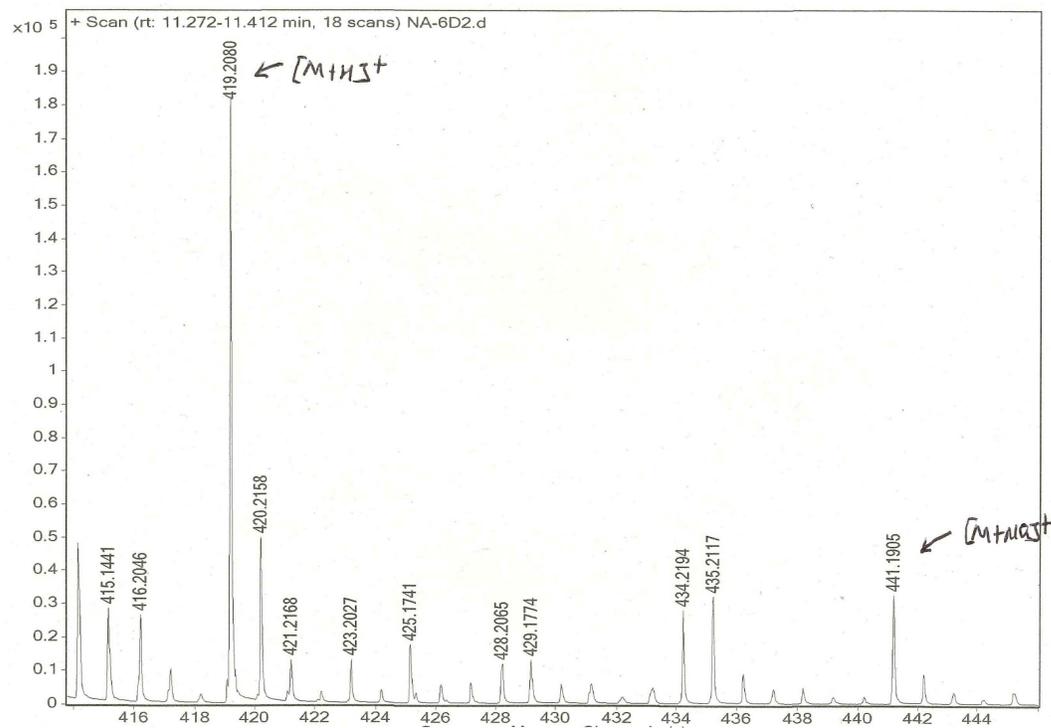


Figure S14. The HRESIMS of 6 β -acetoxy-6 α -methoxy-7-oxoroyleanone (**2**)

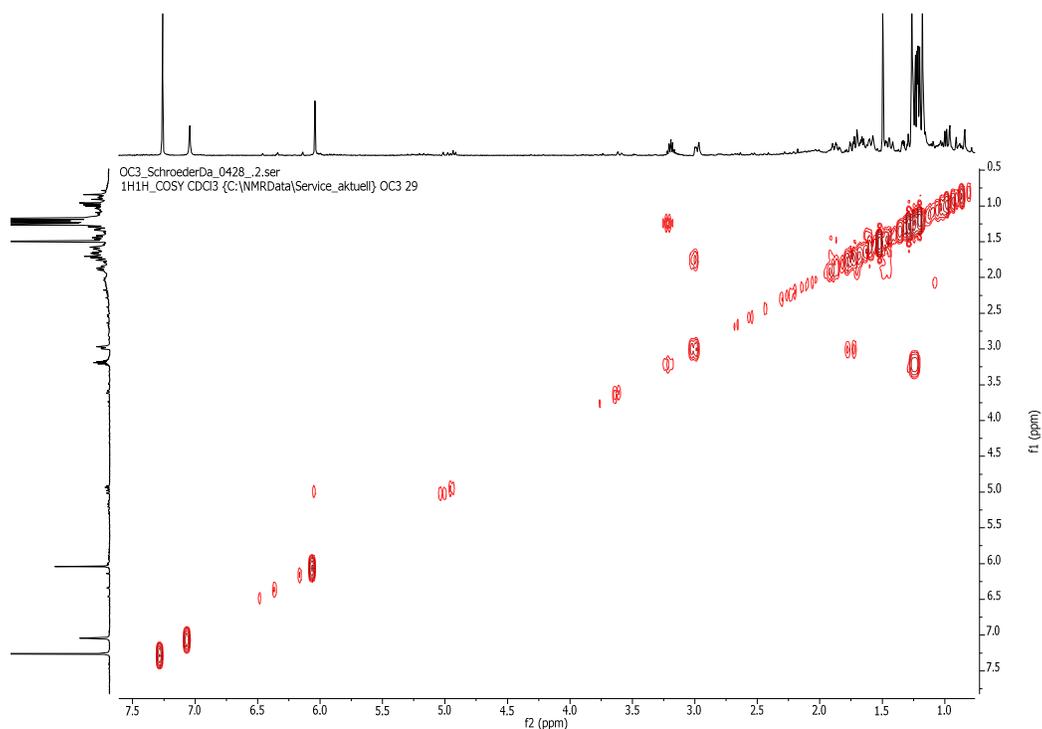


Figure S17. The COSY spectrum of 8 α ,9 α -epoxy-6-deoxycoleon U (**3**) observed at 500 MHz in CDCl₃ solution at 25 °C.

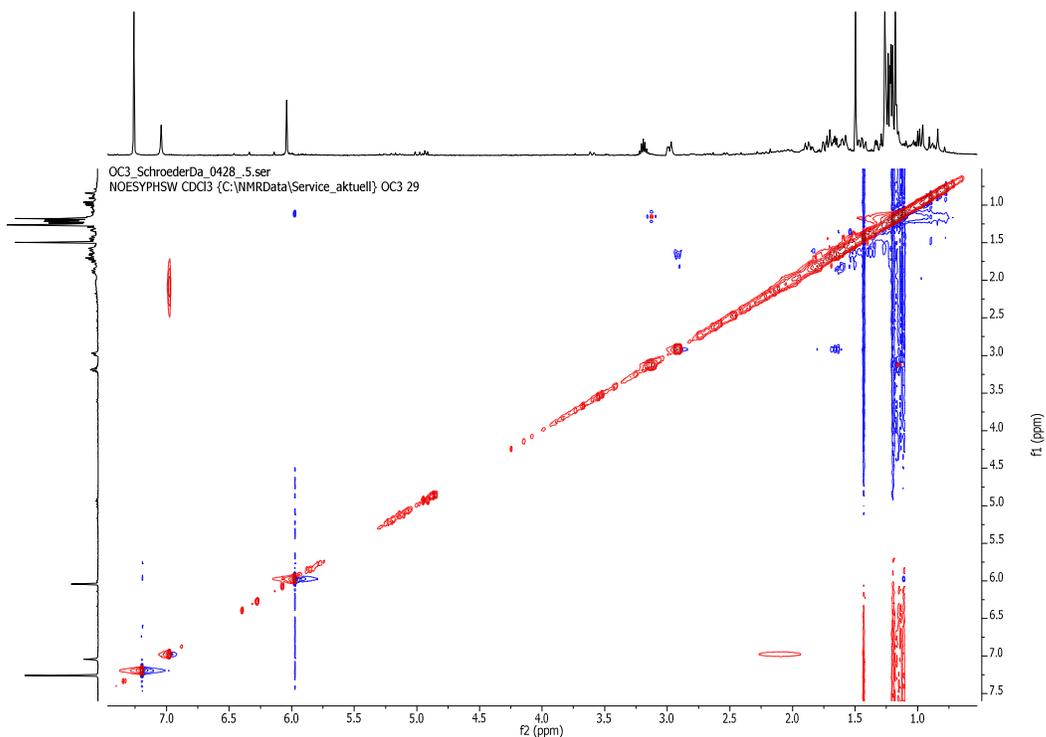


Figure S18. The NOESY spectrum of 8 α ,9 α -epoxy-6-deoxycoleon U (**3**) observed at 500 MHz in CDCl₃ solution at 25 °C.

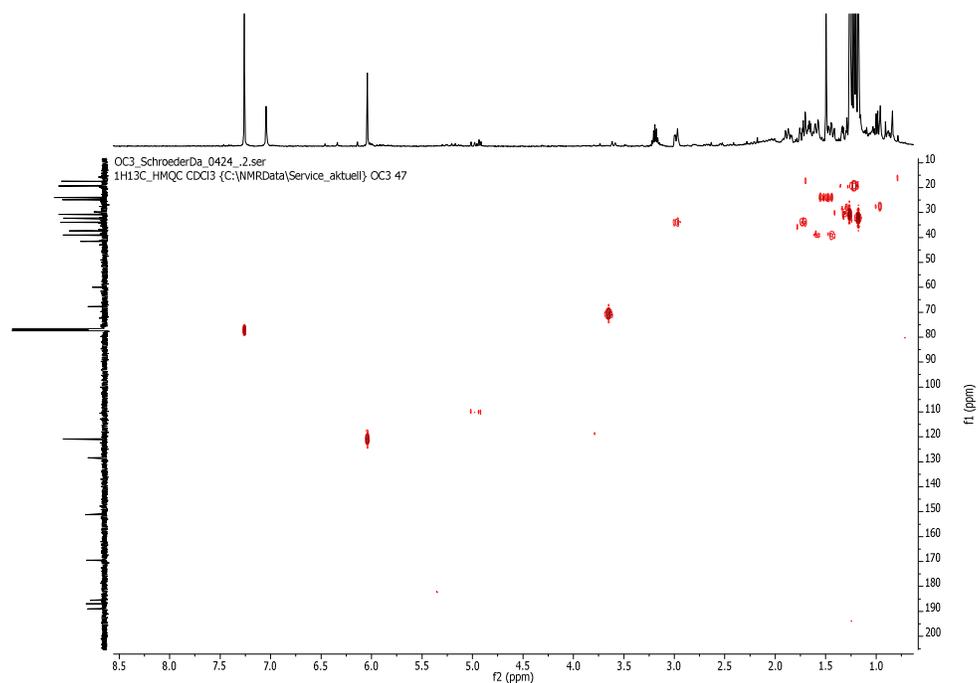


Figure S19. The HSQC spectrum of 8 α ,9 α -epoxy-6-deoxycoleon U (**3**) observed at 500 and 125 MHz in CDCl₃ solution at 25 °C.

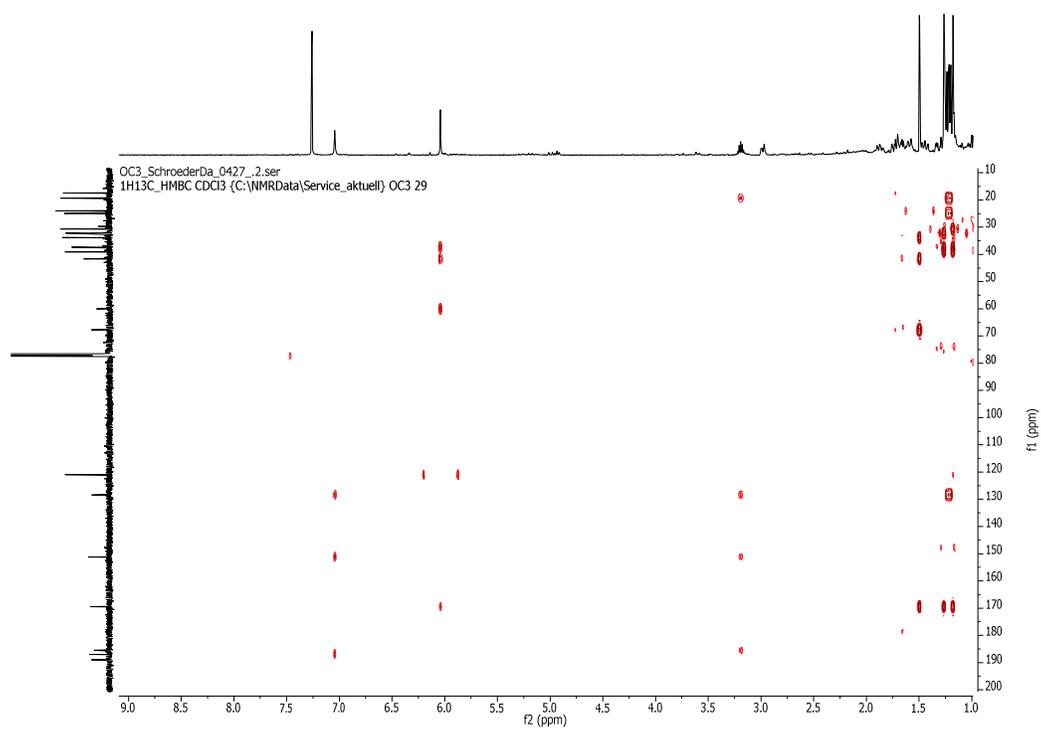


Figure S20. The HMBC spectrum of 8 α ,9 α -epoxy-6-deoxycoleon U (**3**) observed at 500 and 125 MHz in CDCl₃ solution at 25 °C.

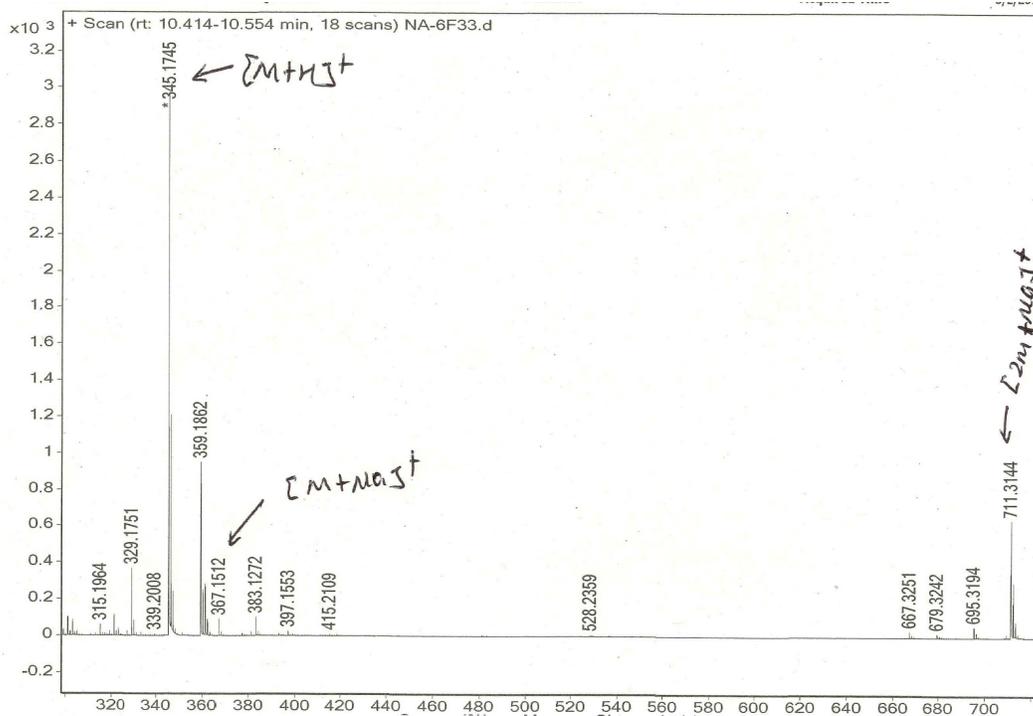


Figure S21. The HRESIMS of 8 α ,9 α -epoxy-6-deoxycoleon U (3).

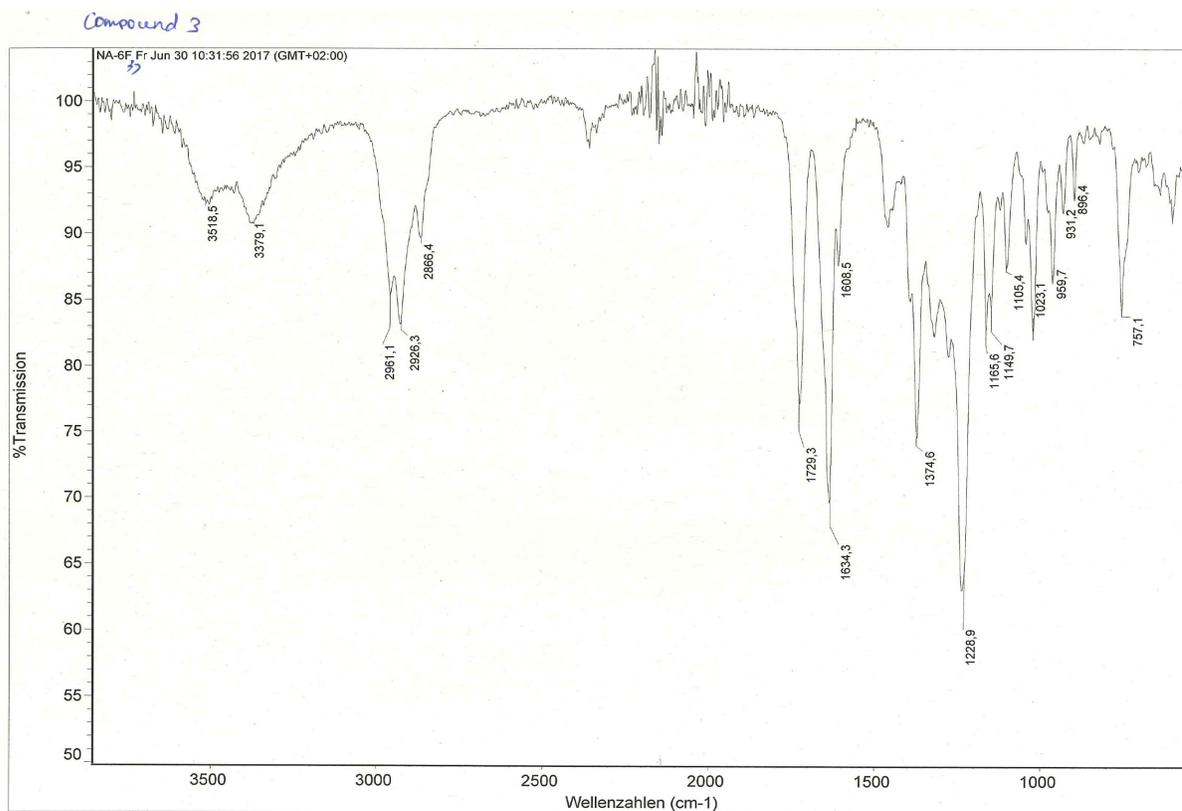


Figure S22. The IR spectra of 8 α ,9 α -epoxy-6-deoxycoleon U (3).

Spectroscopic data for 6,12-dihydroxysapriparaquinone (4)

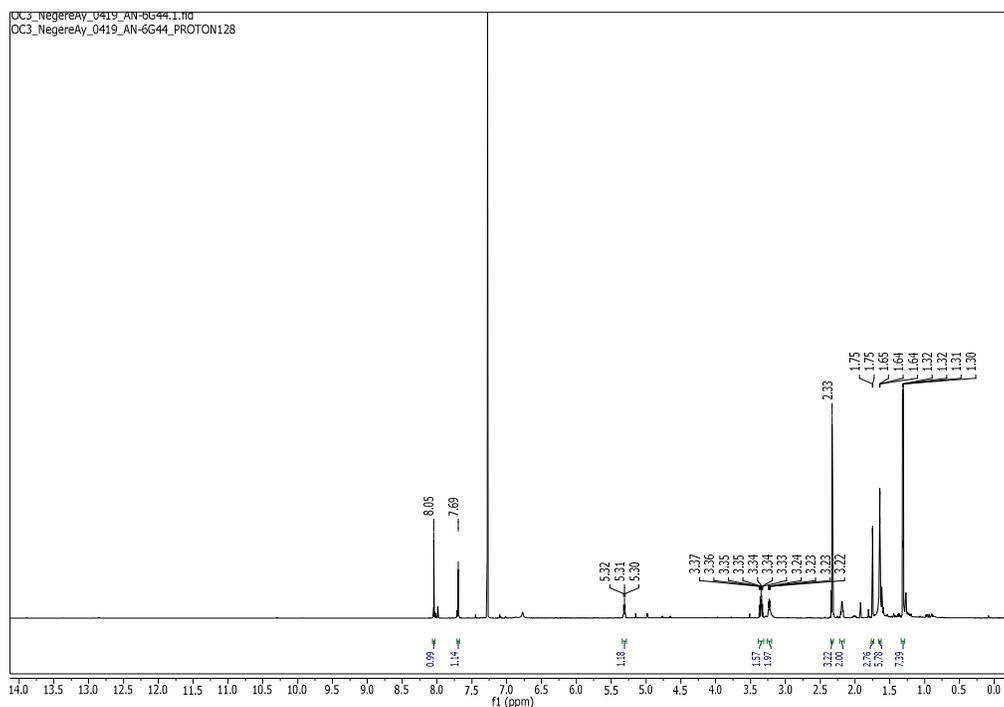


Figure S23. The ^1H NMR of 6,12-dihydroxysapriparaquinone (4) observed at 500 MHz in CDCl_3 solution at 25 °C. Assignment is given in Table 1.

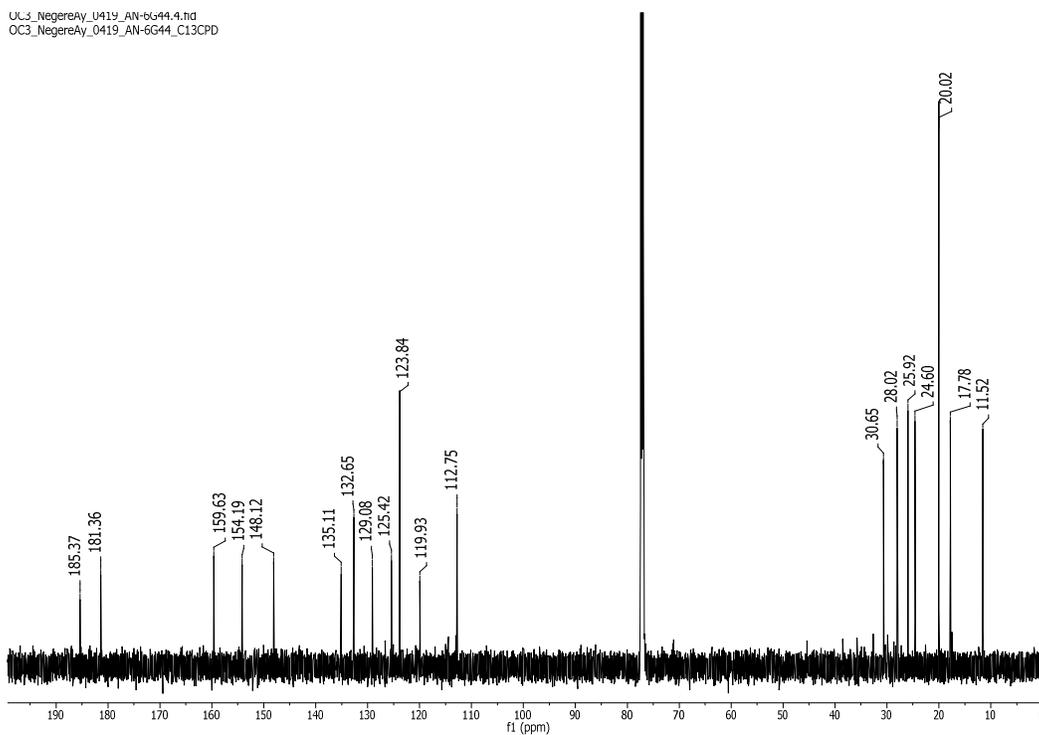


Figure S24. The ^{13}C NMR spectrum 6,12-dihydroxysapriparaquinone (4) observed at 125 MHz in CDCl_3 solution at 25 °C. Assignment is given in Table 1.

OC3_SchroederDa_U429_5.hd
13C(1H)_DEPT135 CDCl3 (C:\NMRData\Service_aktuell)\OC3 43

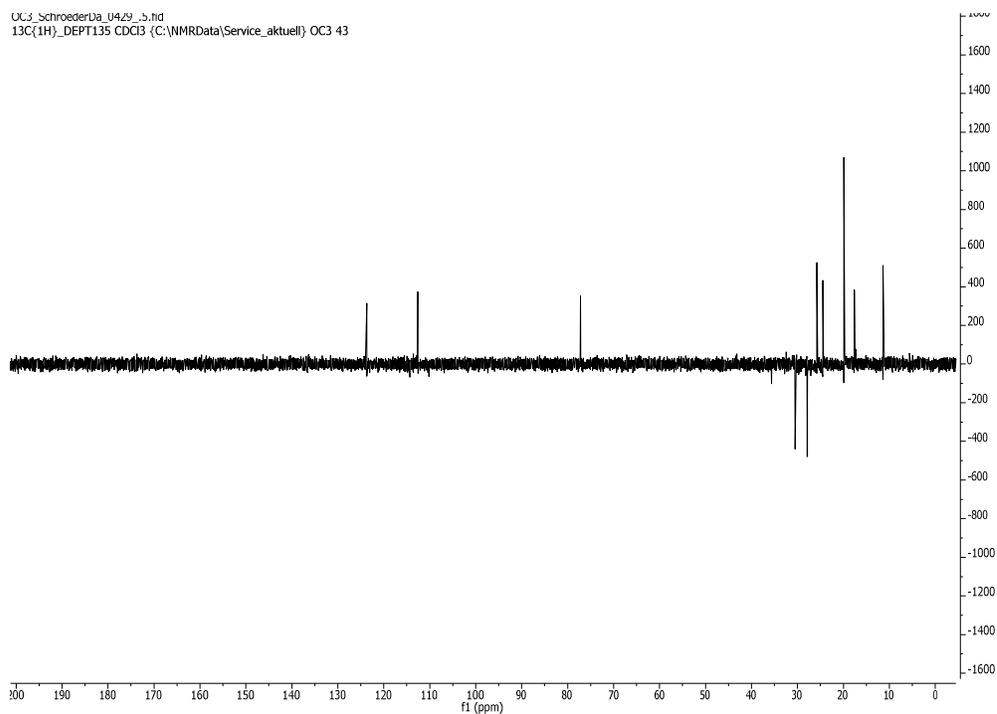


Figure S25. The ^{13}C DEPT NMR spectrum 6,12-dihydroxysapriparaquinone (**4**) observed at 125 MHz in CDCl_3 solution at 25 °C.

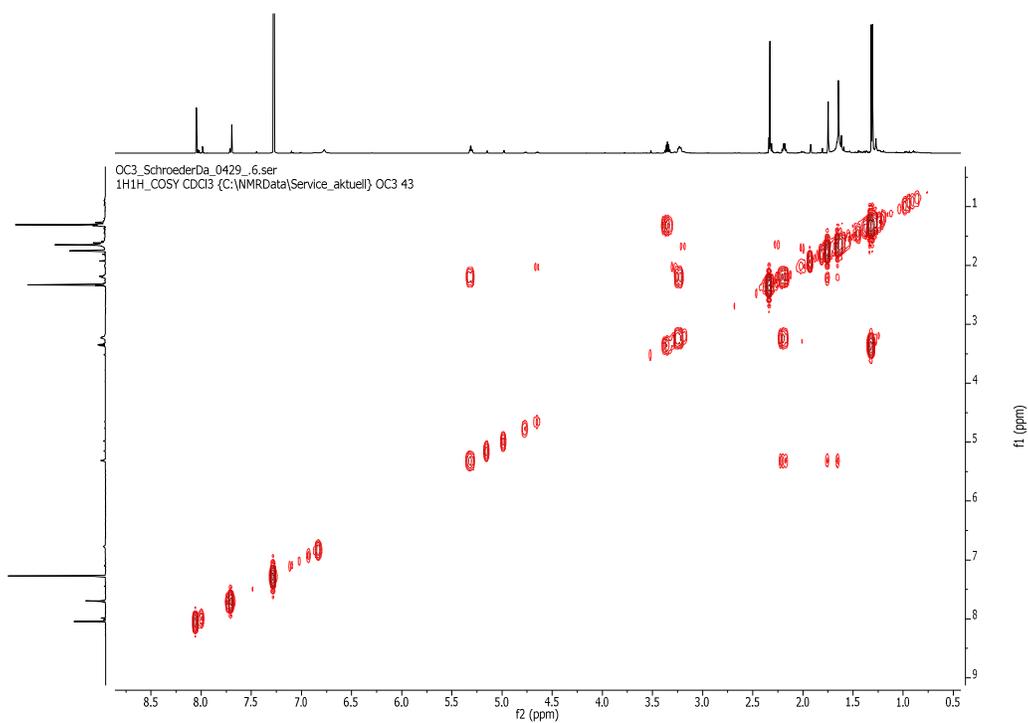


Figure S26. The COSY spectrum of 6,12-dihydroxysapriparaquinone (**4**) observed at 500 MHz in CDCl_3 solution at 25 °C.

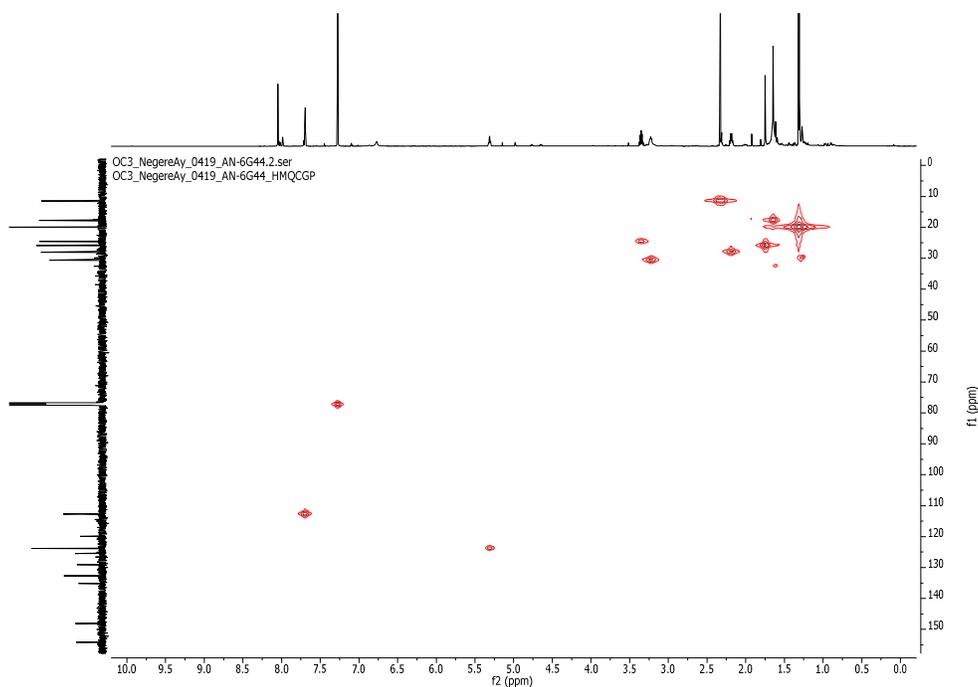


Figure S27. The HSQC spectrum of 6,12-dihydroxysapriparaquinone (**4**) observed at 500 and 125 MHz in CDCl₃ solution at 25 °C.

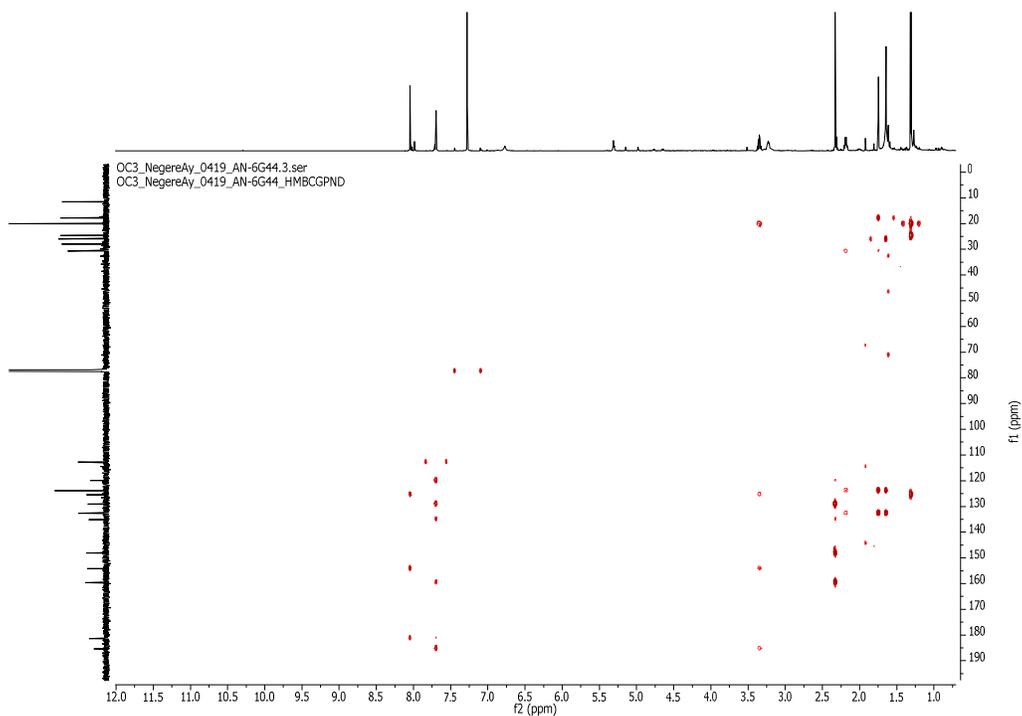


Figure S28. The HMBC spectrum of 6,12-dihydroxysapriparaquinone (**4**) observed at 500 and 125 MHz in CDCl₃ solution at 25 °C.

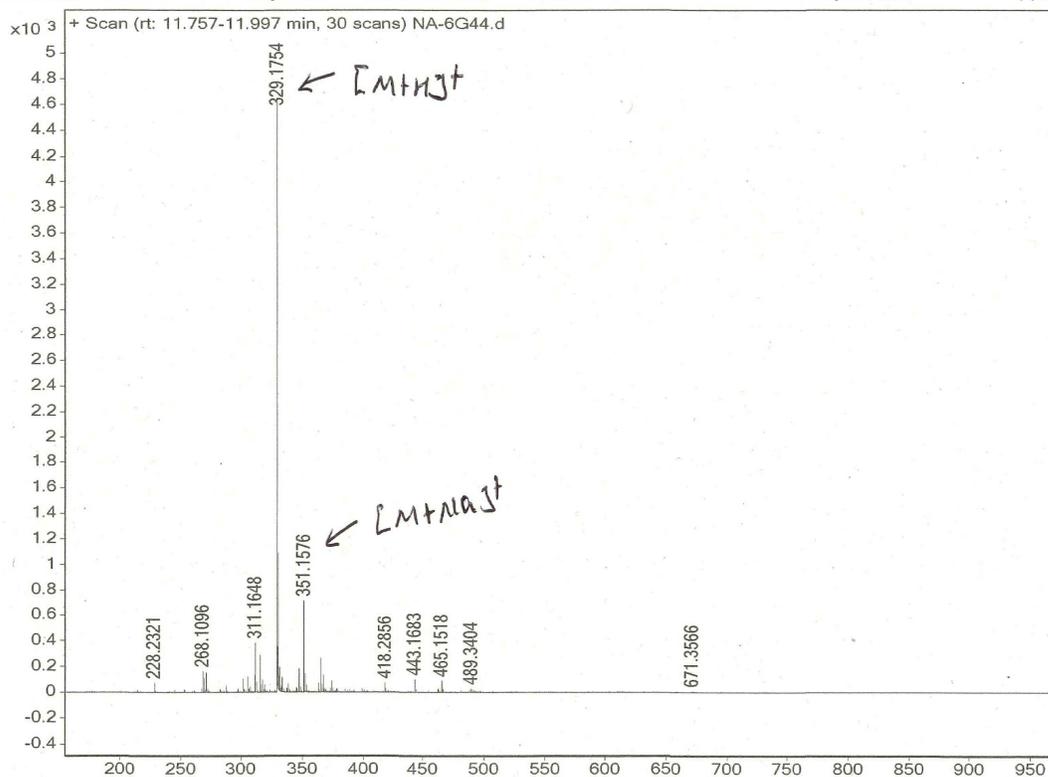


Figure S29: HRESIMS spectra of 6,12-dihydroxysapriparaquinone (**4**)