

Supplementary Material

Muscarine-like compounds derived from a pyrolysis product of cellulose

Andrea Defant, Ines Mancini,* Rosanna Matucci, Cristina Bellucci, Federico Dosi,

Danilo Malferrari and Daniele Fabbri

Figure S1. Overlapped energy-minimized structures of (+)-muscarine (light gray) and of compound **4** (gray). Hydrogen atoms are omitted to simplify the view.

Figure S2. ¹H-NMR spectrum (CD₃OD, 400 MHz) of 1-((2*S*,4*R*)-4-hydroxy-4-(methoxycarbonyl)tetrahydrofuran-2-yl)-*N,N,N*-trimethylmethan- aminium iodide (**4**).

Figure S3. ¹³C-NMR spectrum (CD₃OD, 100 MHz) of compound **4**.

Figure S4. ¹H-NMR spectrum (CDCl₃, 400 MHz) of *N*-(((2*S*,4*R*)-4-hydroxy-4-(methoxycarbonyl)tetrahydrofuran-2-yl)methyl)-*N*-methyl cyclohexanaminium 4-methylbenzenesulfonate (**5**).

Figure S5. ¹³C-NMR spectrum (CDCl₃, 100 MHz) of compound **5**.

Figure S6. ¹H-NMR spectrum (CDCl₃, 400 MHz) of pure 1-(((2*S*,4*R*)-4-Hydroxy-4-(methoxycarbonyl)tetrahydrofuran-2-yl)methyl)pyrrolidin-1-ium 4-methylbenzenesulfonate (**6**).

Figure S7. ¹³C-NMR spectrum (CDCl₃, 100 MHz) of pure compound **6**.

Figure S8. ¹H-NMR spectrum (CDCl₃, 400 MHz) of 1-(((2*S*,4*R*)-4-Hydroxy-4-(methoxycarbonyl)tetrahydrofuran-2-yl)methyl)piperidin-1-ium 4-methylbenzenesulfonate (**7**).

Figure S9. ¹³C-NMR spectrum (CDCl₃, 100 MHz) of compound **7**.

Figure S10. ¹H-NMR spectrum (CDCl₃, 400 MHz) of 1-(((2*S*,4*R*)-4-hydroxy-4-(piperidine-1-carbonyl)tetrahydrofuran-2-yl)methyl)piperidin-1-ium (**8**).

Figure S11. ¹³C-NMR spectrum (CDCl₃, 100 MHz) of compound **8**.

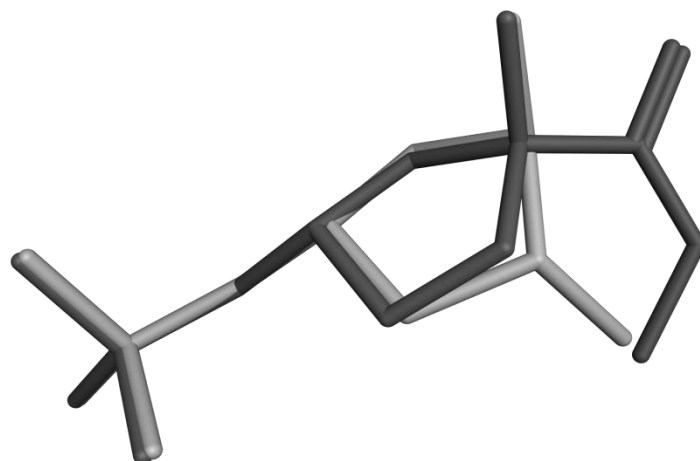


Figure S1. Overlapped energy-minimized structures of muscarine (light gray) and of compound 4 (gray). Hydrogen atoms are omitted to simplify the view.

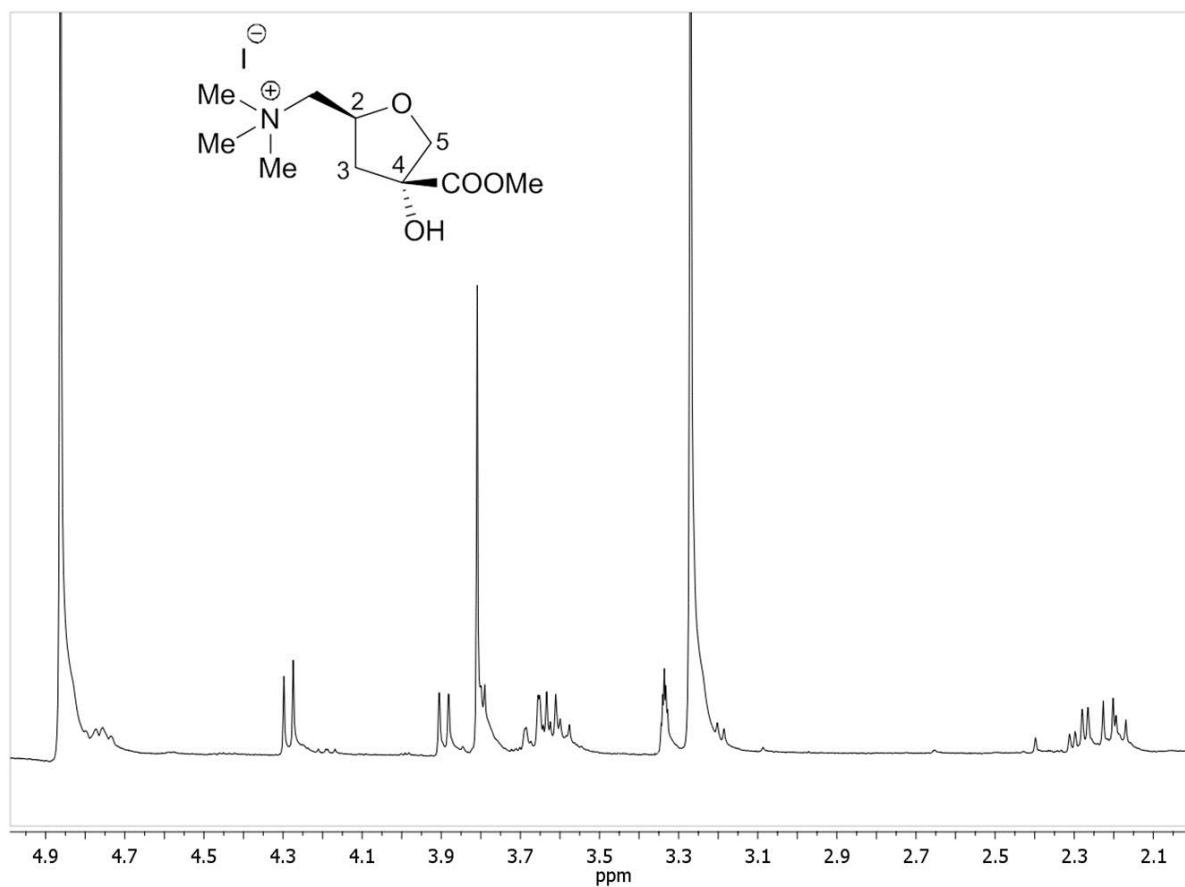


Figure S2. $^1\text{H-NMR}$ spectrum (CD_3OD , 400 MHz) of 1-((2*S*,4*R*)-4-hydroxy-4-(methoxycarbonyl)tetrahydrofuran-2-yl)-*N,N,N*-trimethylmethan-aminium iodide (**4**).

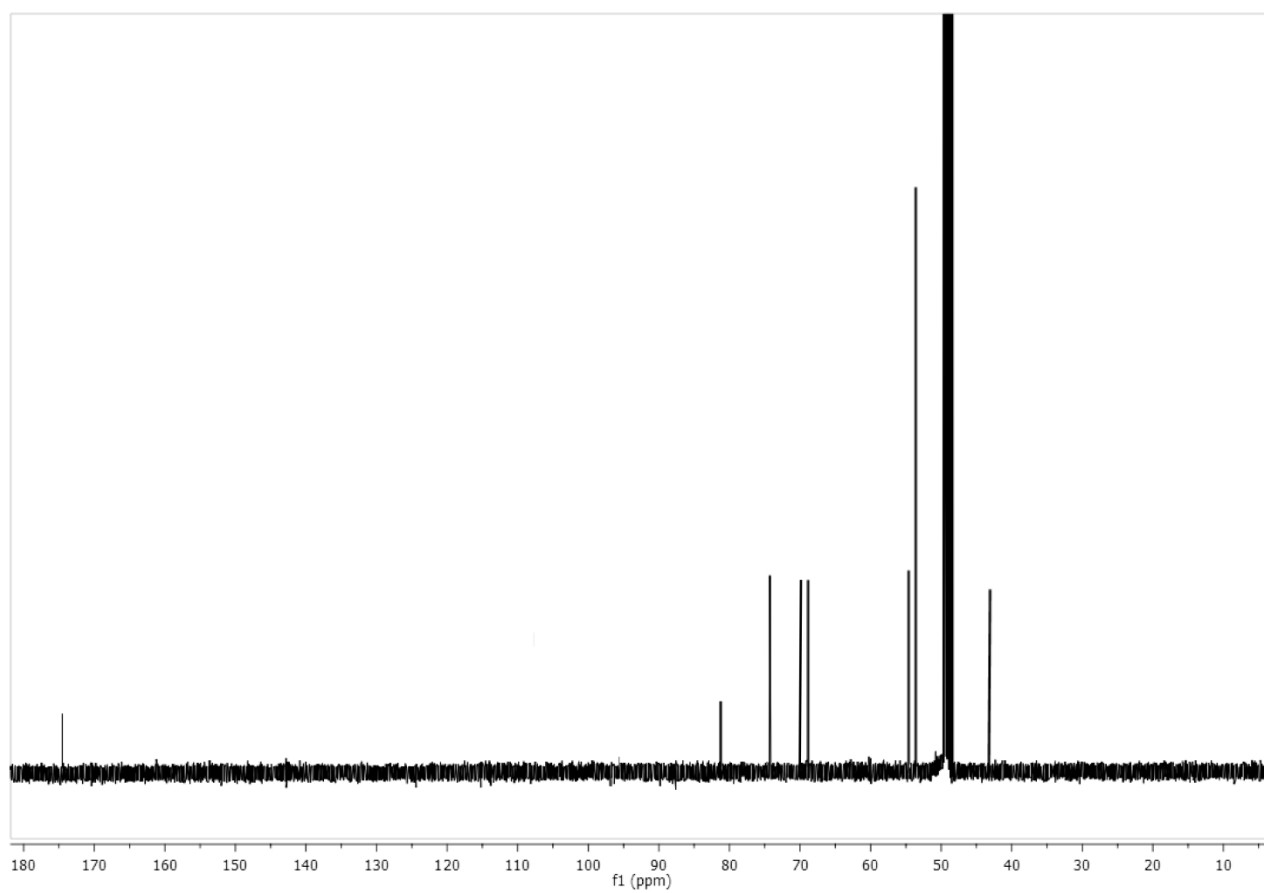
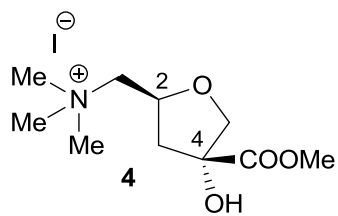


Figure S3. ¹³C-NMR spectrum (CD₃OD, 100 MHz) of compound **4**.

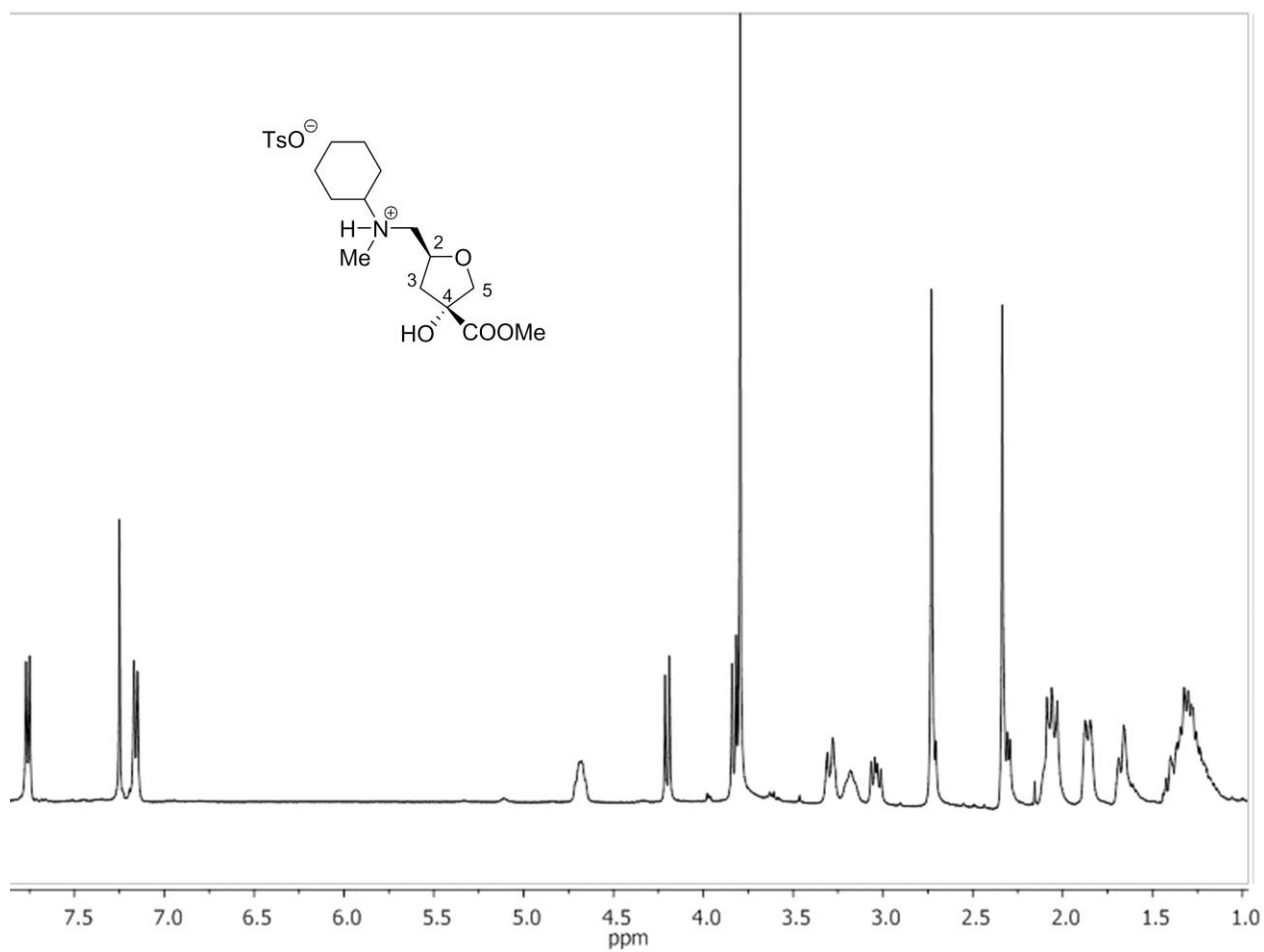


Figure S4. ¹H-NMR spectrum (CDCl₃, 400 MHz) of N-(((2S,4R)-4-hydroxy-4-(methoxycarbonyl)tetrahydrofuran-2-yl)methyl)-N-methyl cyclohexanaminium 4-methyl benzene sulfonate (**5**).

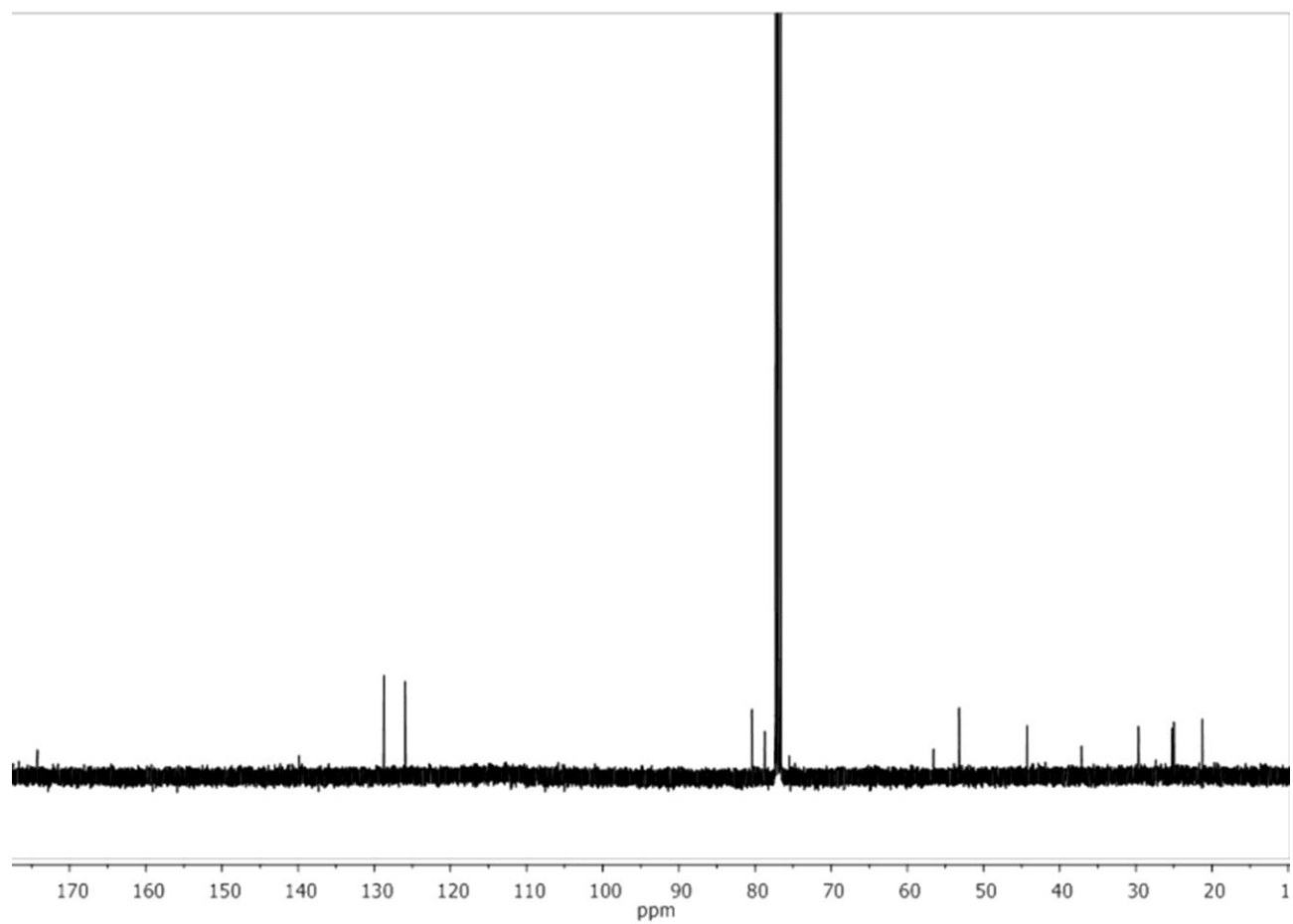


Figure S5. ^{13}C -NMR spectrum (CDCl_3 , 100 MHz) of compound **5**.

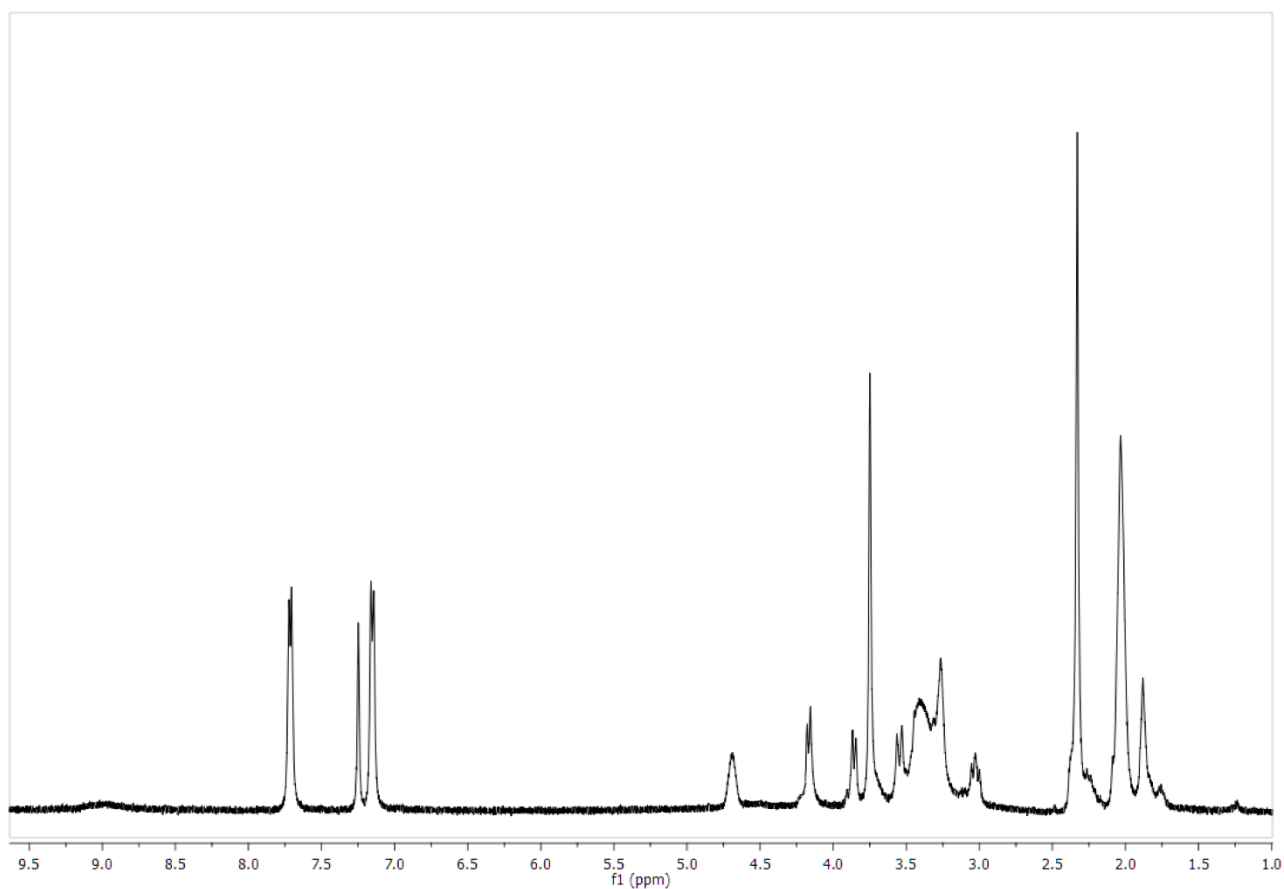


Figure S6. $^1\text{H-NMR}$ spectrum (CDCl_3 , 400 MHz) of pure 1-(((2*S*,4*R*)-4-Hydroxy-4-(methoxycarbonyl)tetrahydrofuran-2-yl)methyl)pyrrolidin-1-ium 4-methylbenzenesulfonate (**6**).

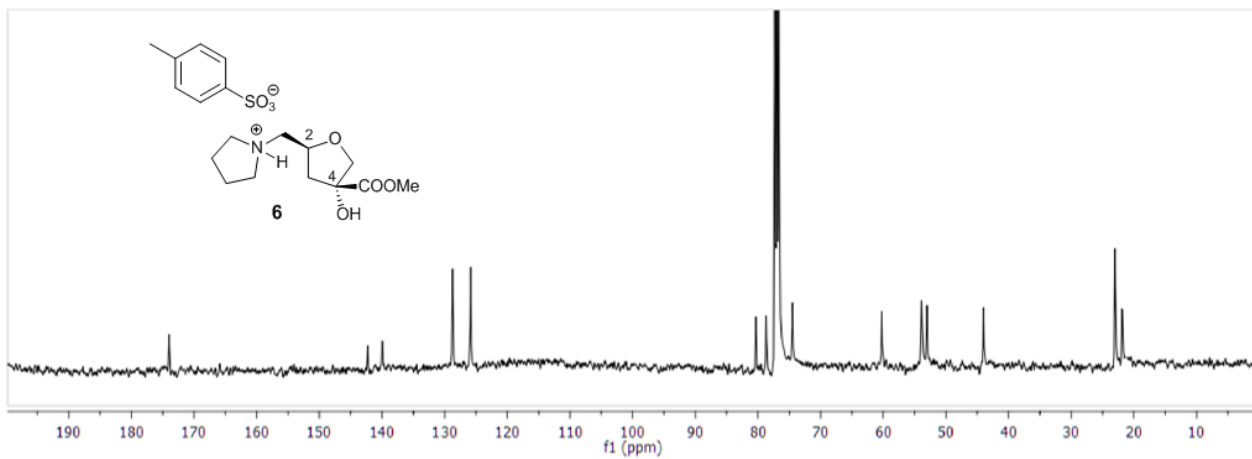


Figure S7. ^{13}C -NMR spectrum (CDCl_3 , 100 MHz) of pure compound **6**.

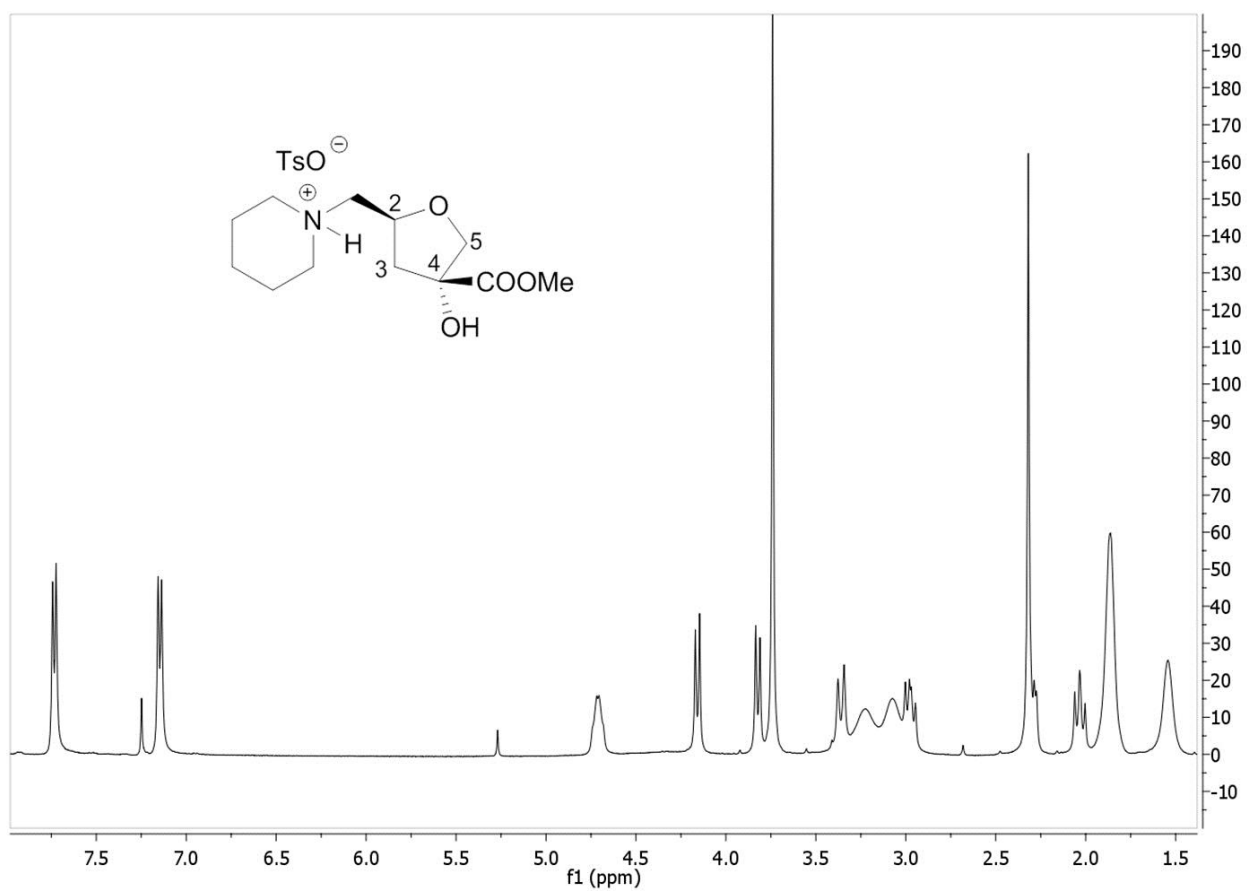


Figure S8. $^1\text{H-NMR}$ spectrum (CDCl_3 , 400 MHz) of 1-(((2S,4R)-4-Hydroxy-4-(methoxycarbonyl)tetrahydrofuran-2-yl)methyl)piperidin-1-ium 4-methylbenzenesulfonate (**7**).

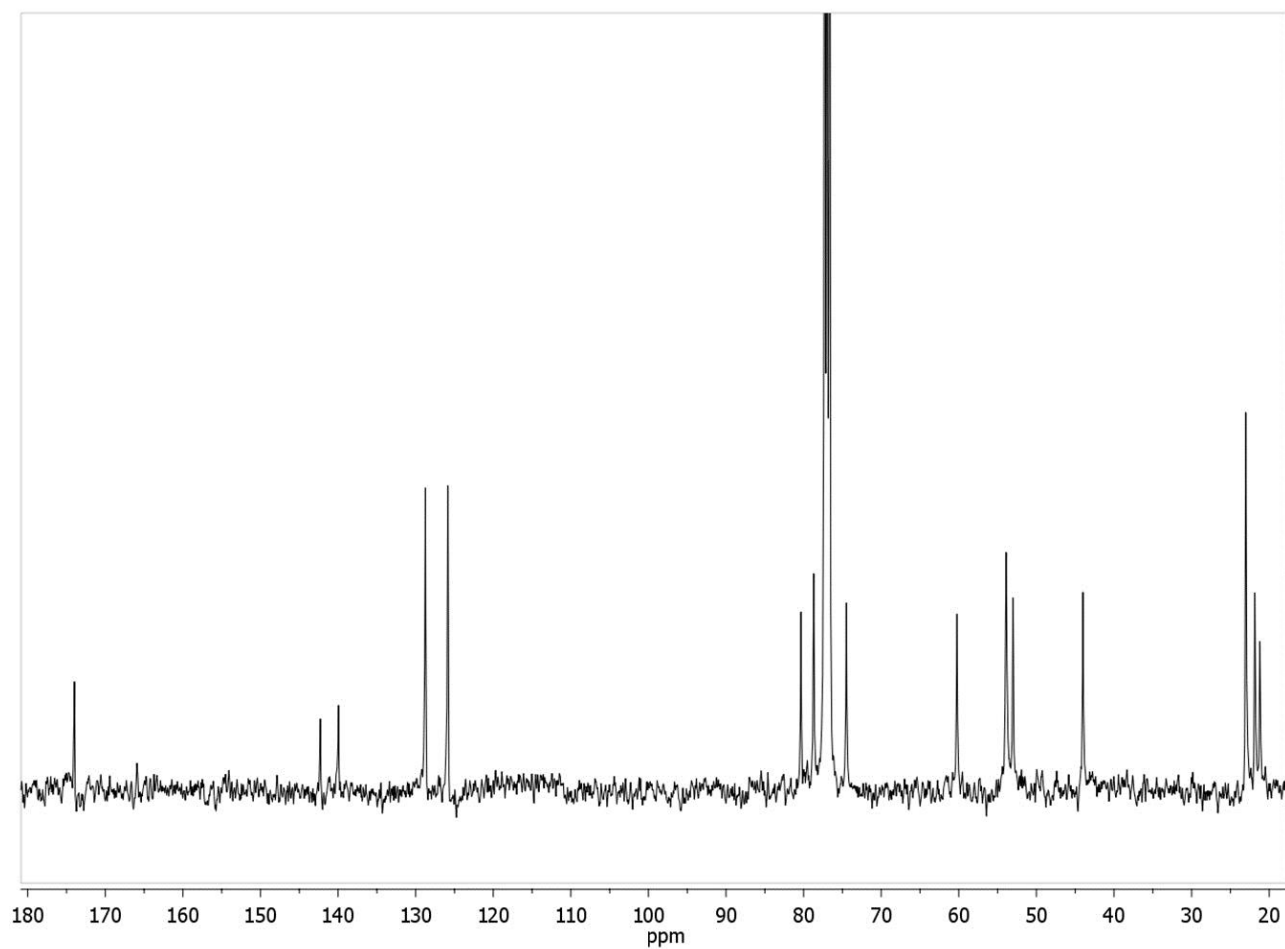


Figure S9. ^{13}C -NMR spectrum (CDCl_3 , 100 MHz) of compound **7**.

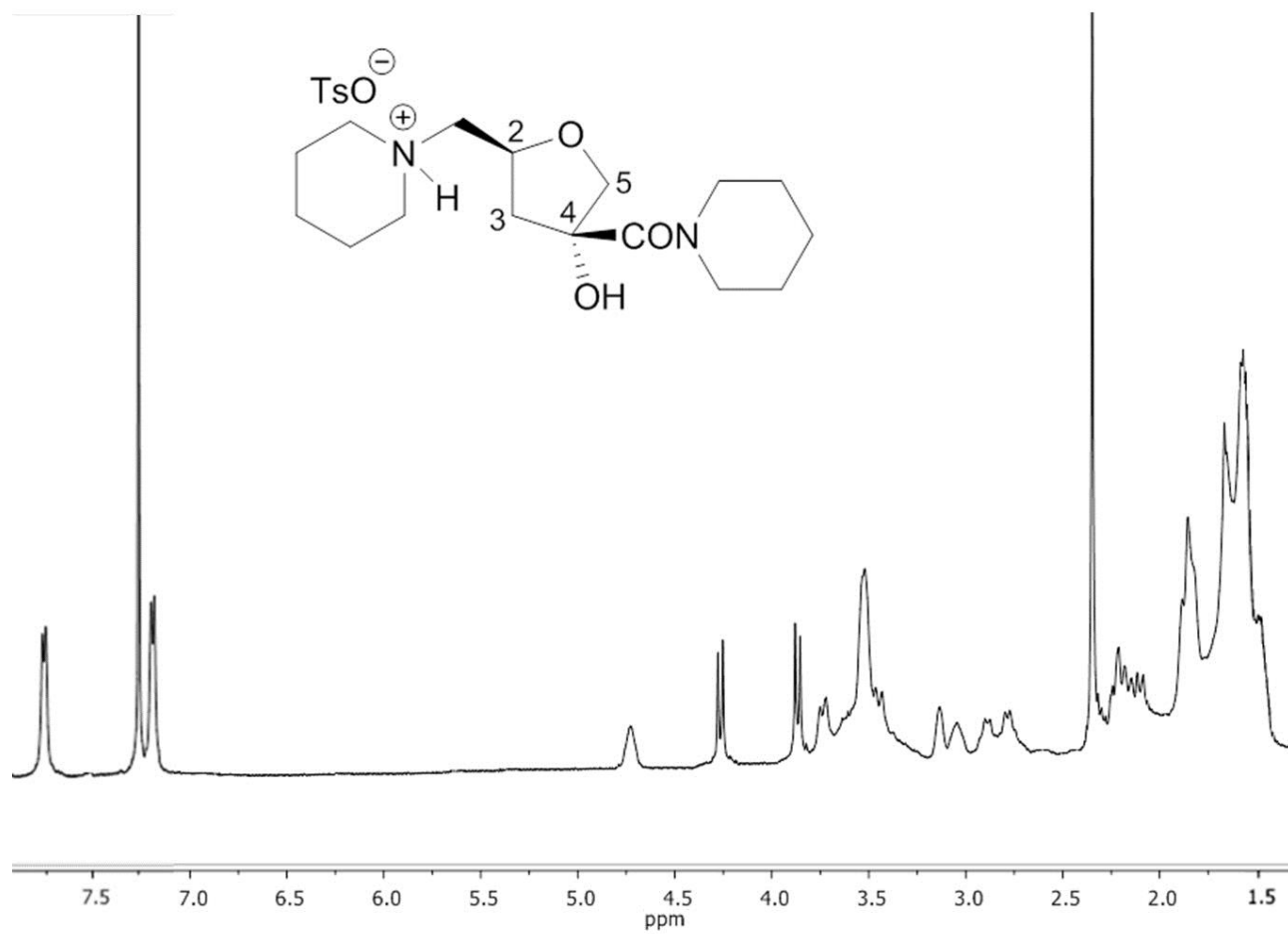


Figure S10. ¹H-NMR spectrum (CDCl₃, 400 MHz) of 1-(((2*S*,4*R*)-4-hydroxy-4-(piperidine-1-carbonyl)tetrahydrofuran-2-yl)methyl)piperidin-1-ium (**8**).

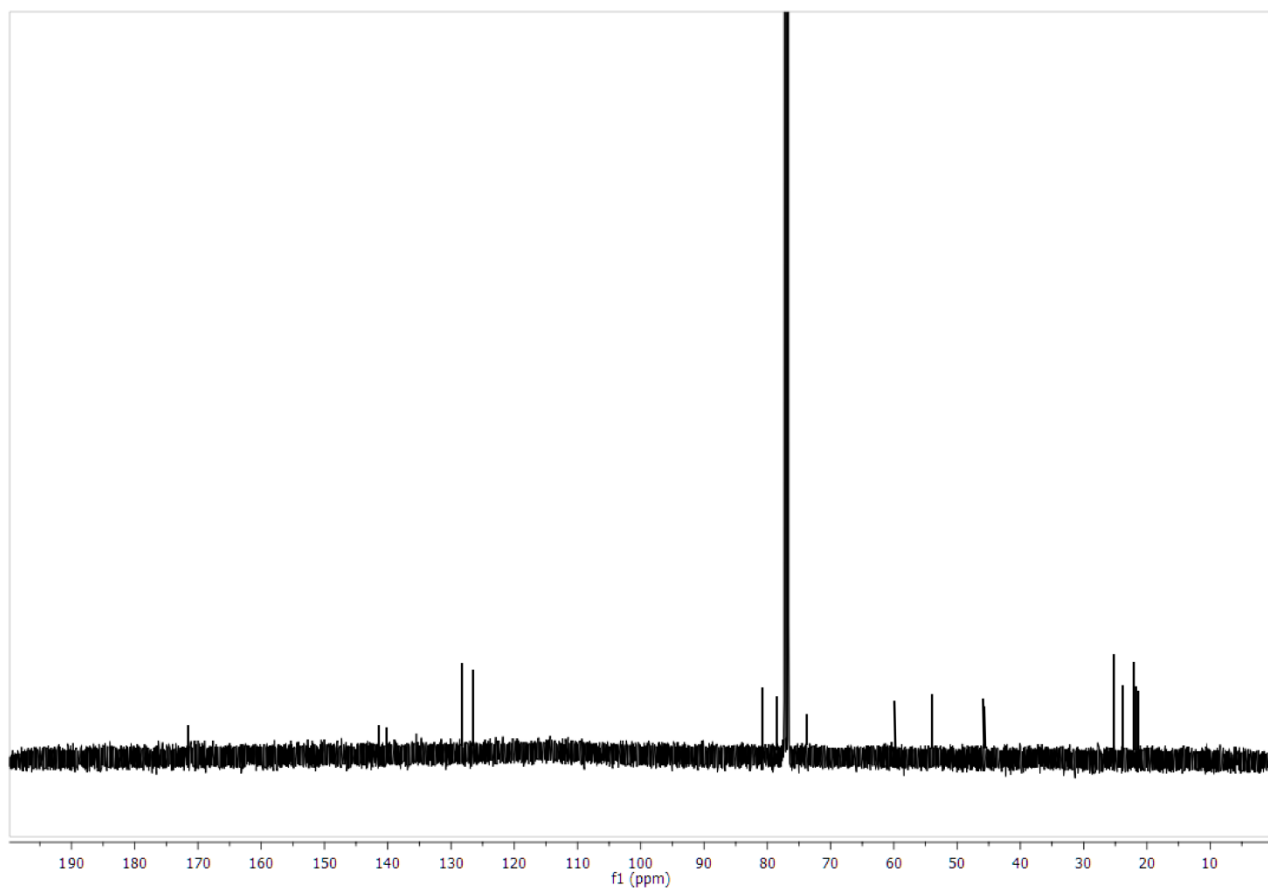
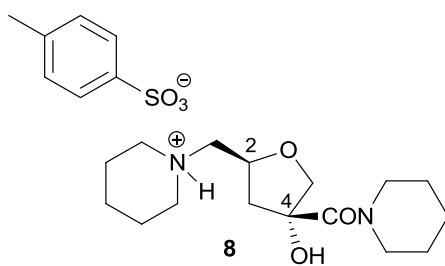


Figure S11. ^{13}C -NMR spectrum (CDCl_3 , 100 MHz) of compound **8**.