

Supplementary Materials

New Water-Soluble Condensed Heterocyclic Compounds with Antimicrobial Activity Based on Annulation Reactions of 8-Quinolinesulfenyl Halides with Natural Products and Alkenes

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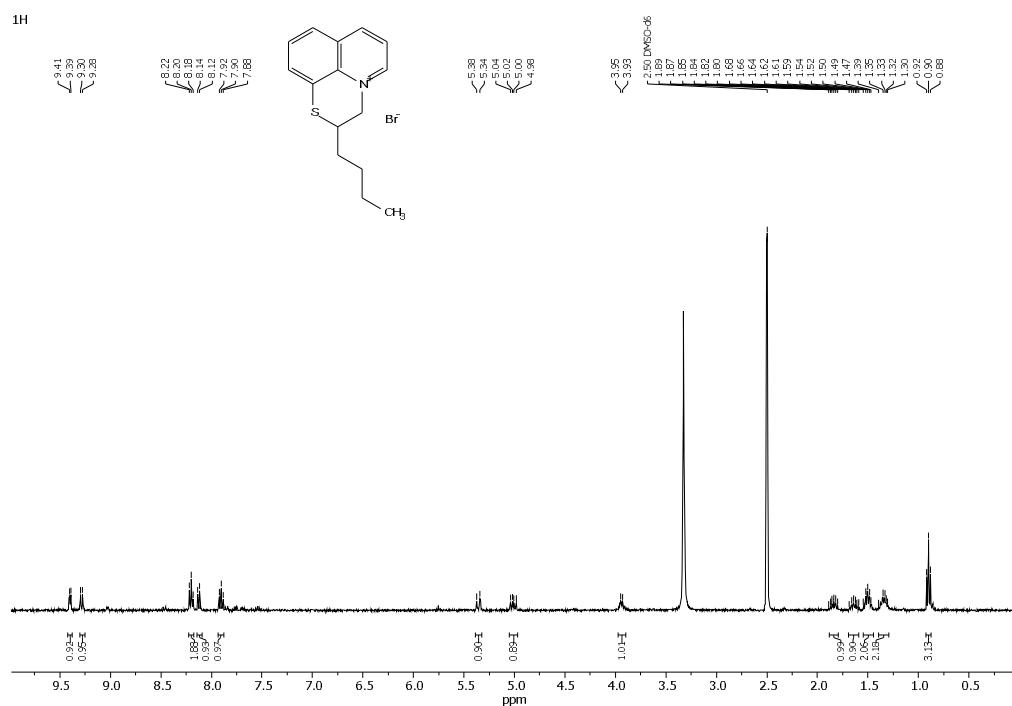
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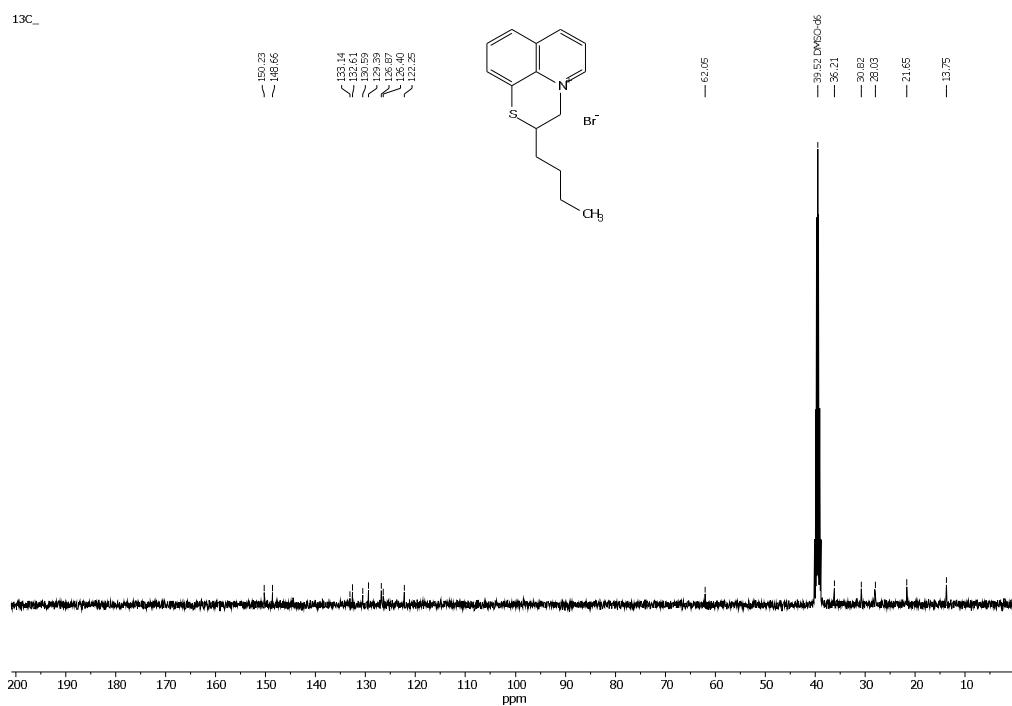
Experimental (General Information)

¹H (400.1 MHz) and ¹³C (100.6 MHz) NMR spectra were recorded on a Bruker DPX-400 spectrometer (Bruker BioSpin GmbH, Rheinstetten, Germany) in 2-5% solution in D₂O or DMSO-*d*₆. ¹H and ¹³C chemical shifts (δ) are reported in parts per million (ppm), relative to tetramethylsilane (external) or to the residual solvent peaks of D₂O (δ = 4.79) and DMSO-*d*₆ (δ = 2.50 and 39.52 ppm for ¹H and ¹³C NMR, respectively). Elemental analysis was performed on a Thermo Scientific FLASH 2000 Organic Elemental Analyzer (Thermo Fisher Scientific Inc., Milan, Italy). Melting points were determined on a Kofler Hot-Stage Microscope PolyTherm A apparatus (Wagner & Munz GmbH, München, Germany). Absolute solvents were used in the reactions.

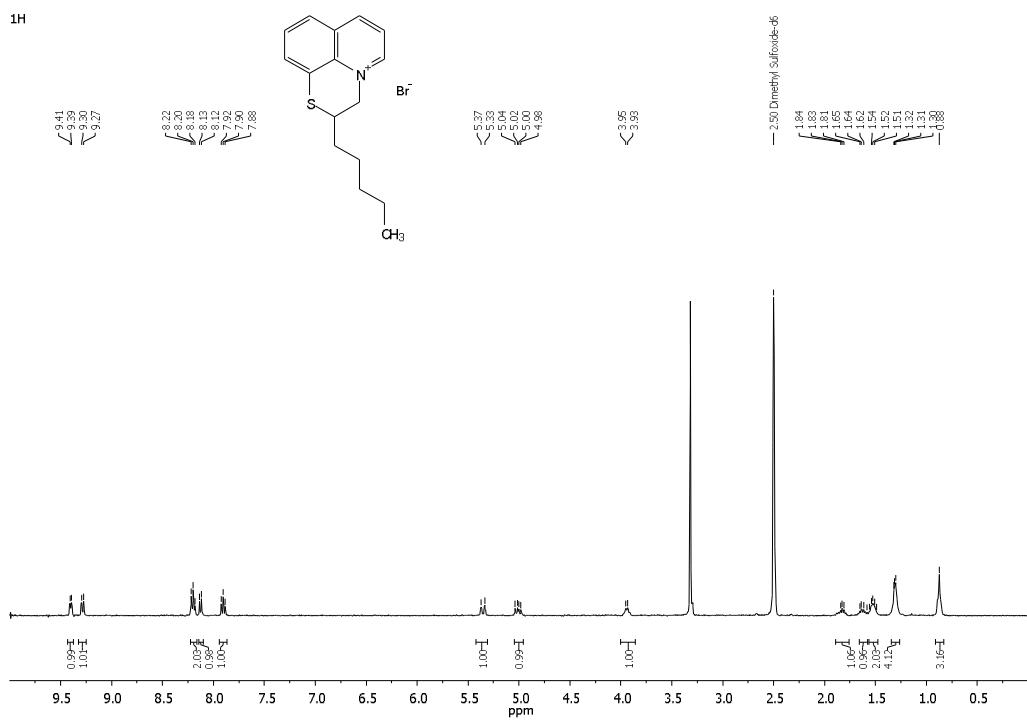
Examples of ^1H - and ^{13}C -NMR spectra



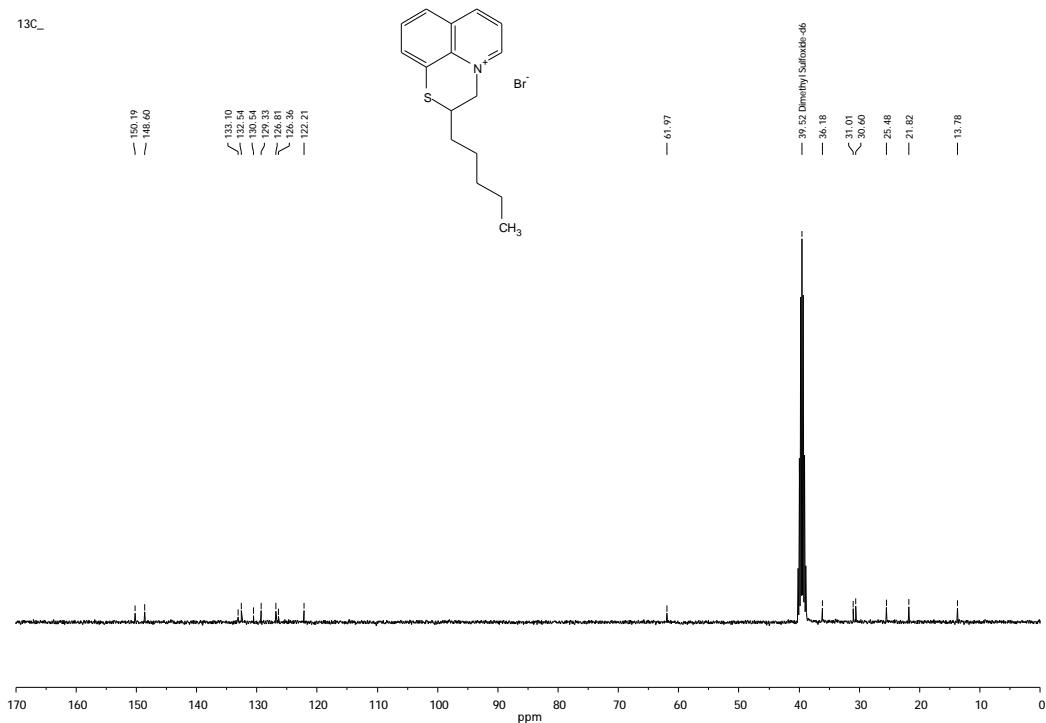
¹H-NMR (DMSO-d₆) spectrum of 2-butyl-2*H*,3*H*-[1,4]thiazino[2,3,4-*ij*]quinolin-4-i um bromide (5)



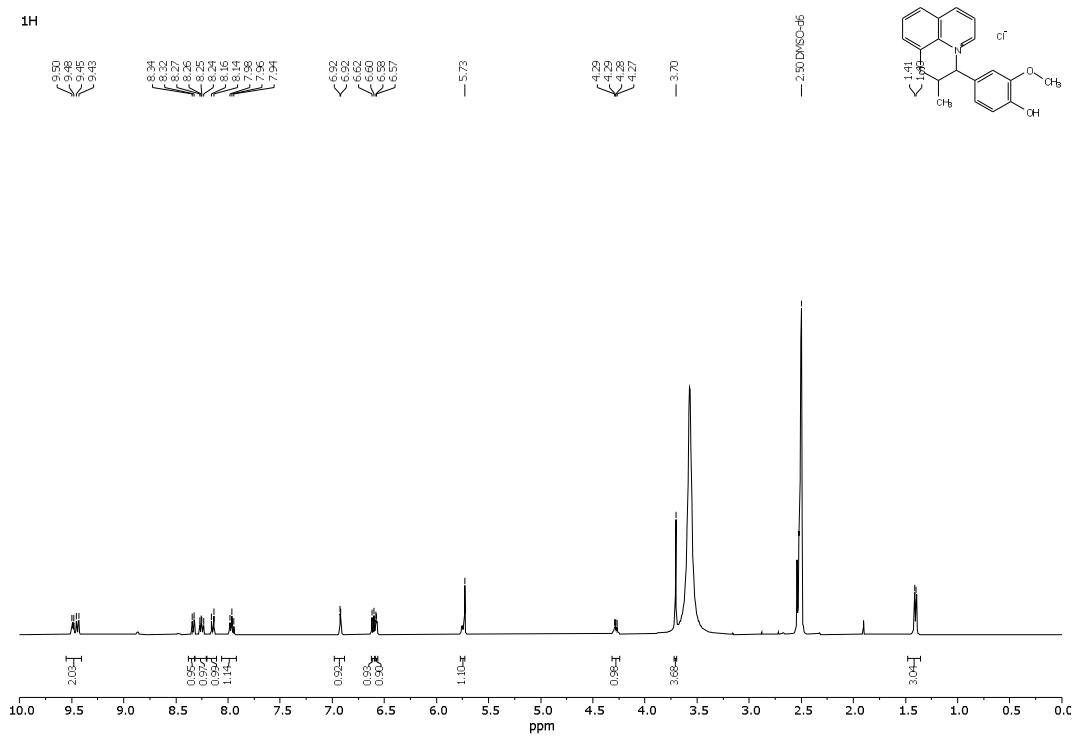
¹³C-NMR (DMSO-*d*₆) spectrum of 2-butyl-2*H*,3*H*-[1,4]thiazino[2,3,4-*ij*]quinolin-4-i um bromide (5)



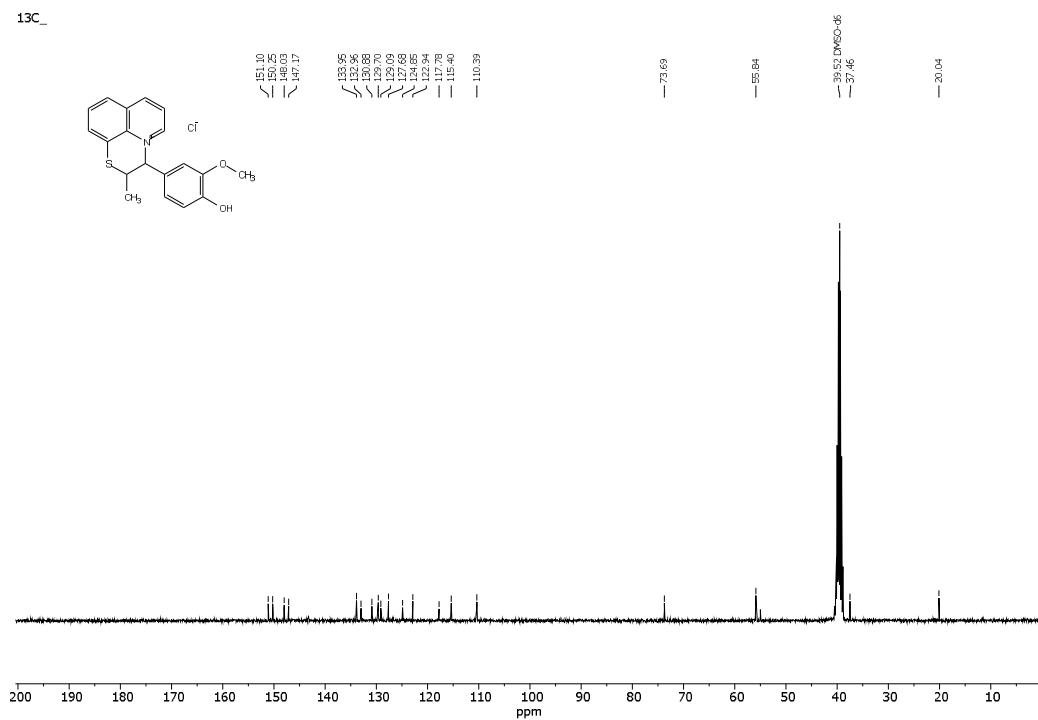
¹H-NMR (DMSO-d₆) spectrum of 2-pentyl-2*H*,3*H*-[1,4]thiazino[2,3,4-*ij*]quinolin-4-i um bromide (6)



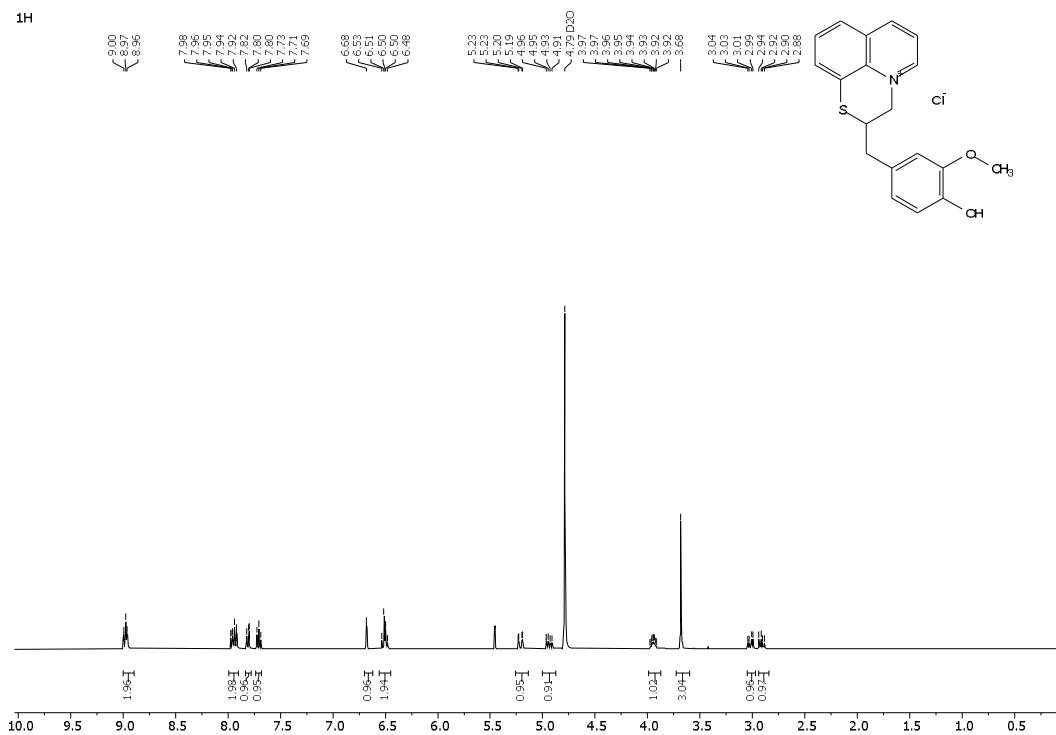
¹³C-NMR (DMSO-*d*₆) spectrum of 2-pentyl-2*H*,3*H*-[1,4]thiazino[2,3,4-*ij*]quinolin-4-i um bromide (**6**)



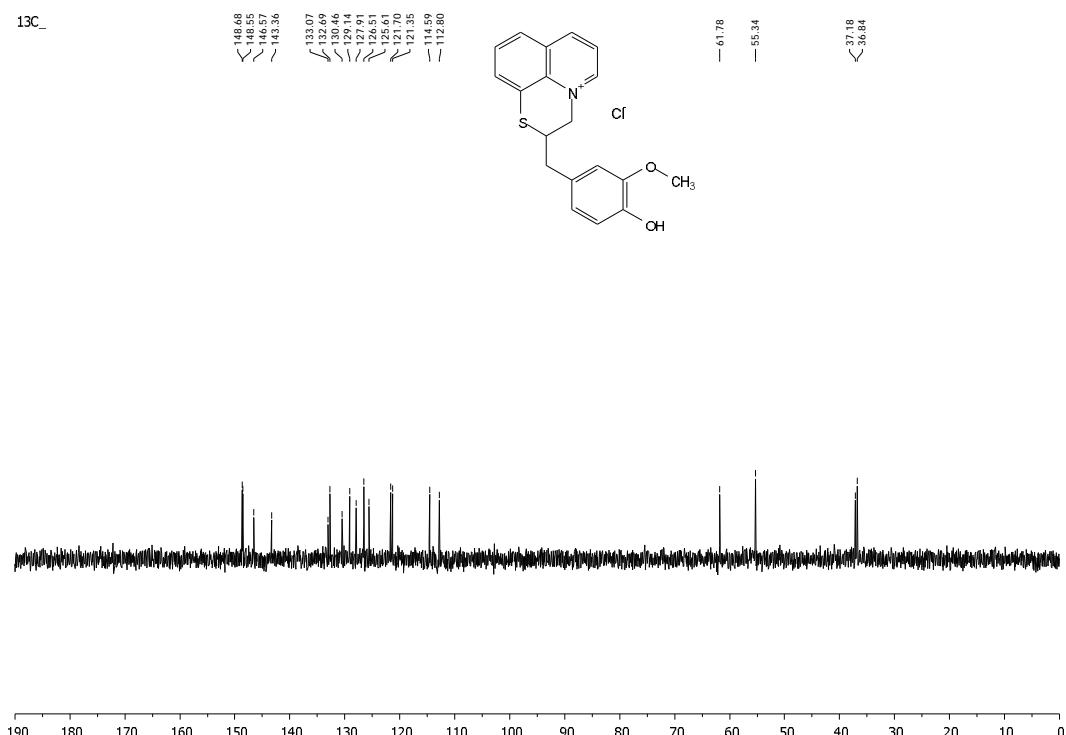
¹H-NMR (DMSO-*d*₆) spectrum of 3-(4-hydroxy-3-methoxyphenyl)-2-methyl-2*H*,3*H*-[1,4]thiazino[2,3,4-*ij*]quinolin-4-i um (7)



¹³C-NMR (DMSO-*d*₆) spectrum of 3-(4-hydroxy-3-methoxyphenyl)-2-methyl-2*H*,3*H*-[1,4]thiazino[2,3,4-*ij*]quinolin-4-i um (7)



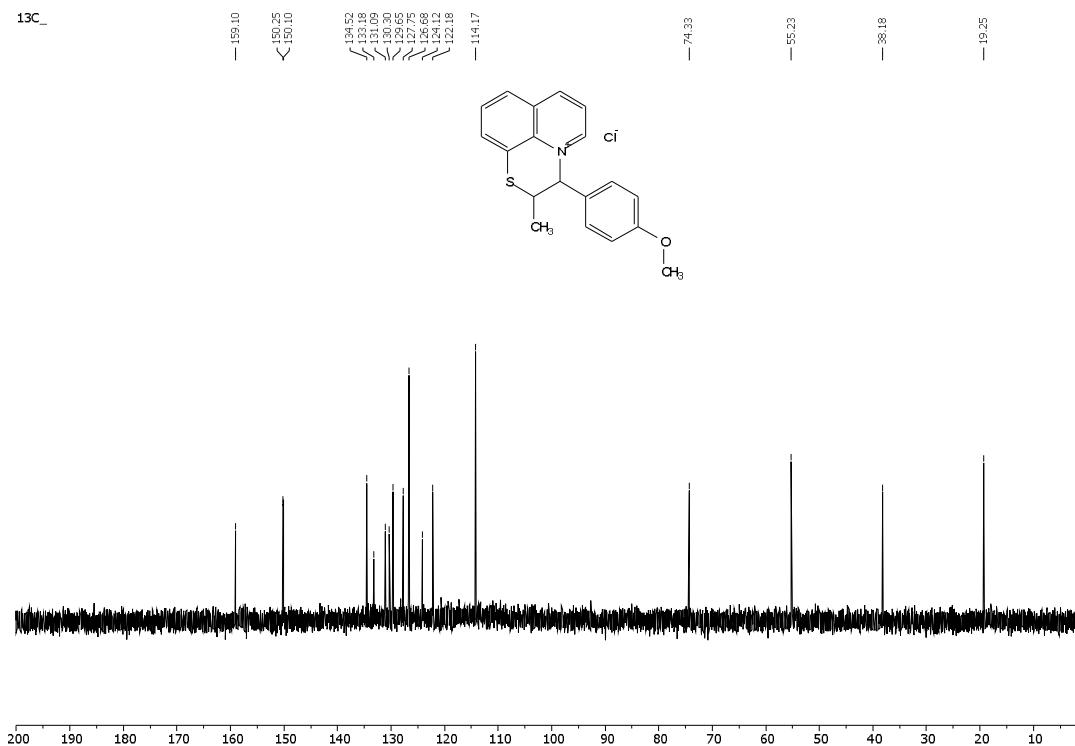
¹H-NMR (D_2O) spectrum of 2-[(4-hydroxy-3-methoxyphenyl)methyl]-2*H*,3*H*-[1,4]thiazino[2,3,4-*i*]quinolin-4-i um chloride (8)



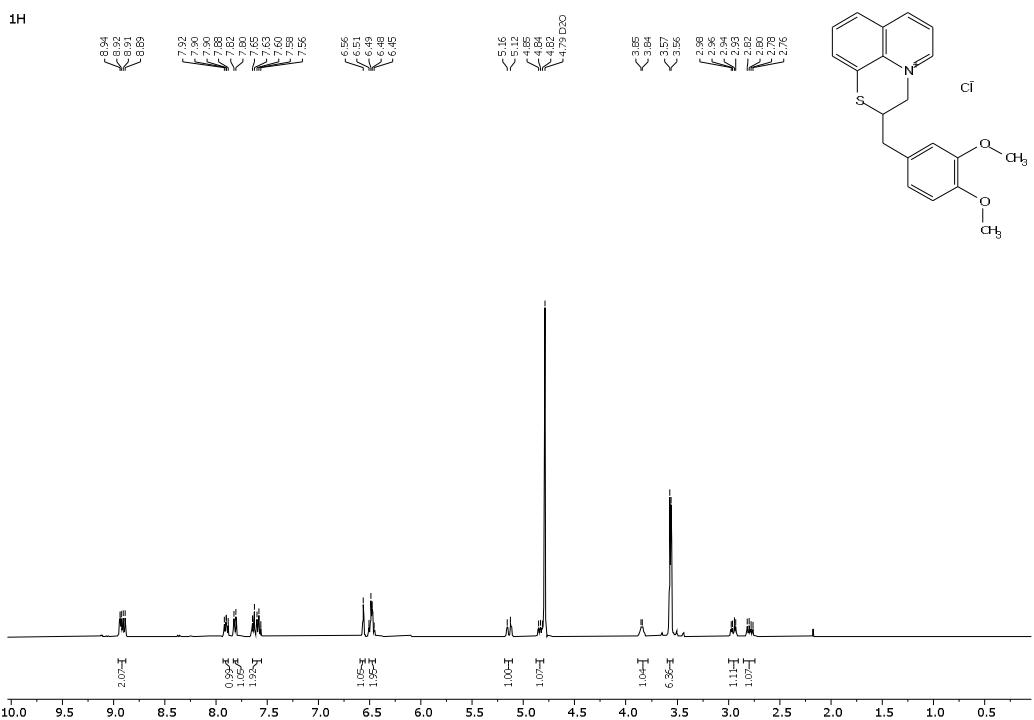
¹³C-NMR (D_2O) spectrum of 2-[(4-hydroxy-3-methoxyphenyl)methyl]-2*H*,3*H*-[1,4]thiazino[2,3-*i*]quinolin-4-i um chloride (8)



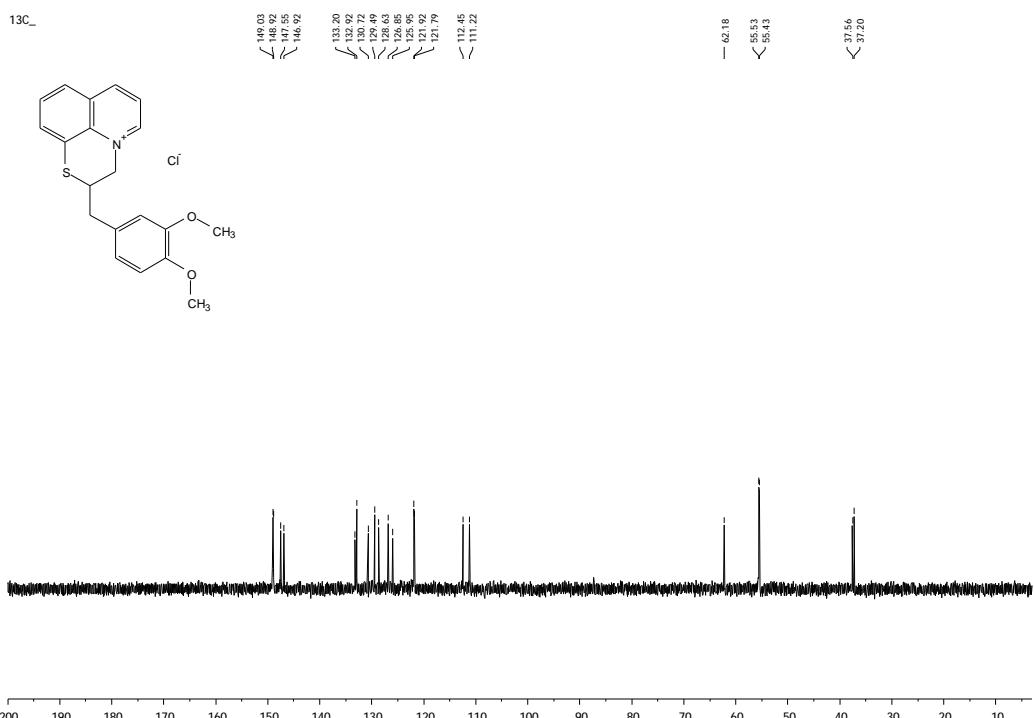
¹H-NMR (D₂O) spectrum of 3-(4-methoxyphenyl)-2-methyl-2H,3H-[1,4]thiazino[2,3,4-*ij*]quinolin-4-iun chloride (9)



¹³C-NMR (D₂O) spectrum of 3-(4-methoxyphenyl)-2-methyl-2H,3H-[1,4]thiazino[2,3,4-*ij*]quinolin-4-iun chloride (9)

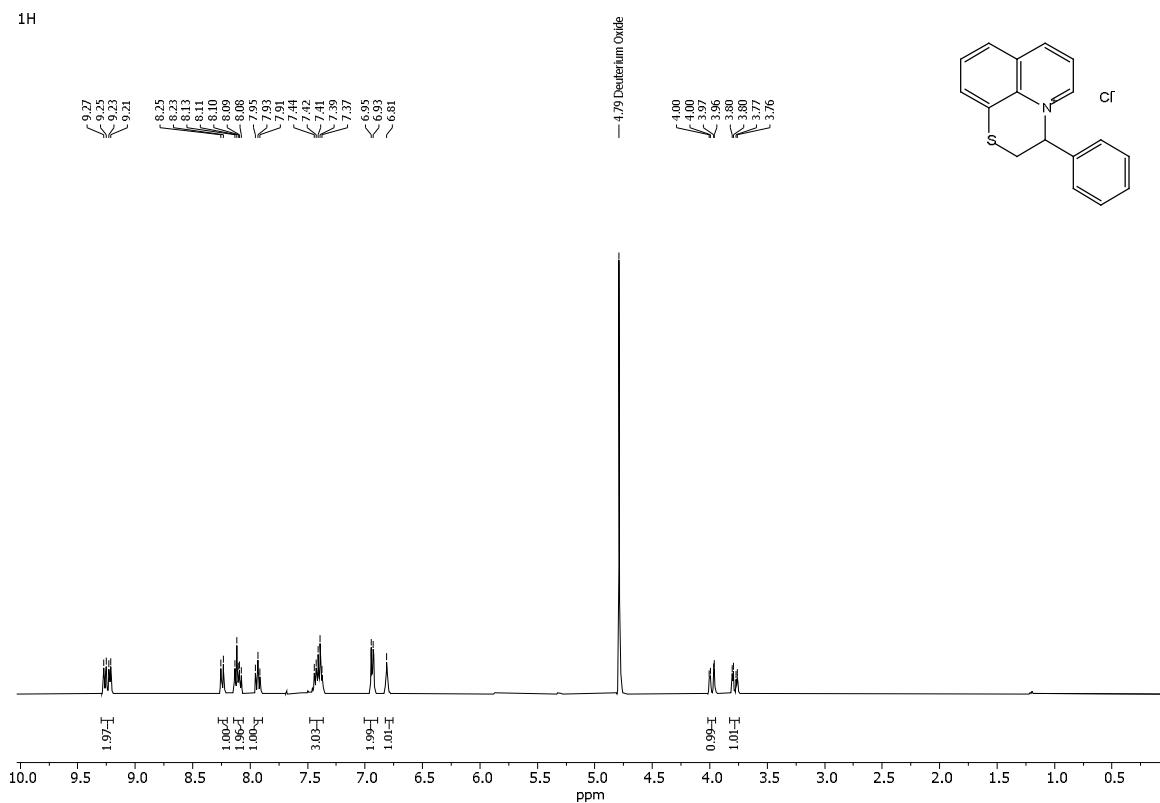


¹H-NMR (D₂O) spectrum of 2-[{(3,4-dimethoxyphenyl)methyl]-2*H*,3*H*-[1,4]thiazino[2,3-*i*]quinolin-4-i um chloride (10)



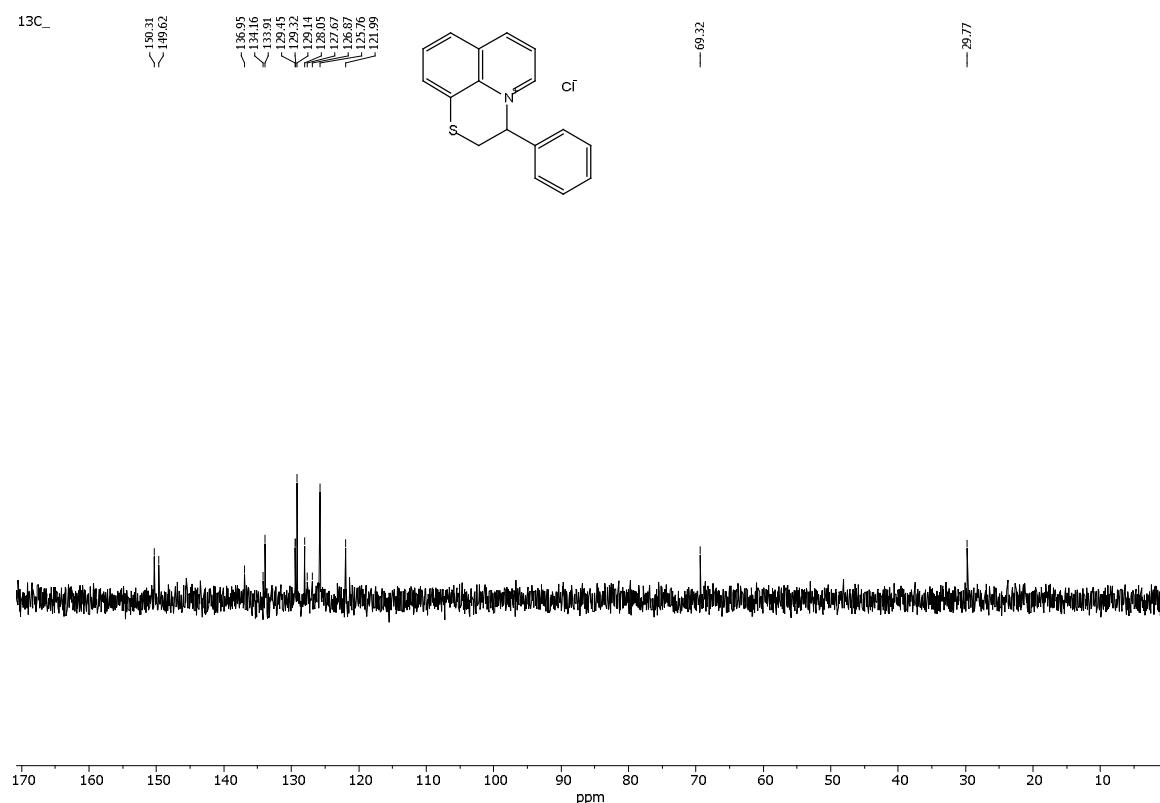
¹³C-NMR (D₂O) spectrum of 2-[{(3,4-dimethoxyphenyl)methyl]-2*H*,3*H*-[1,4]thiazino[2,3-*i*]quinolin-4-i um chloride (10)

¹H

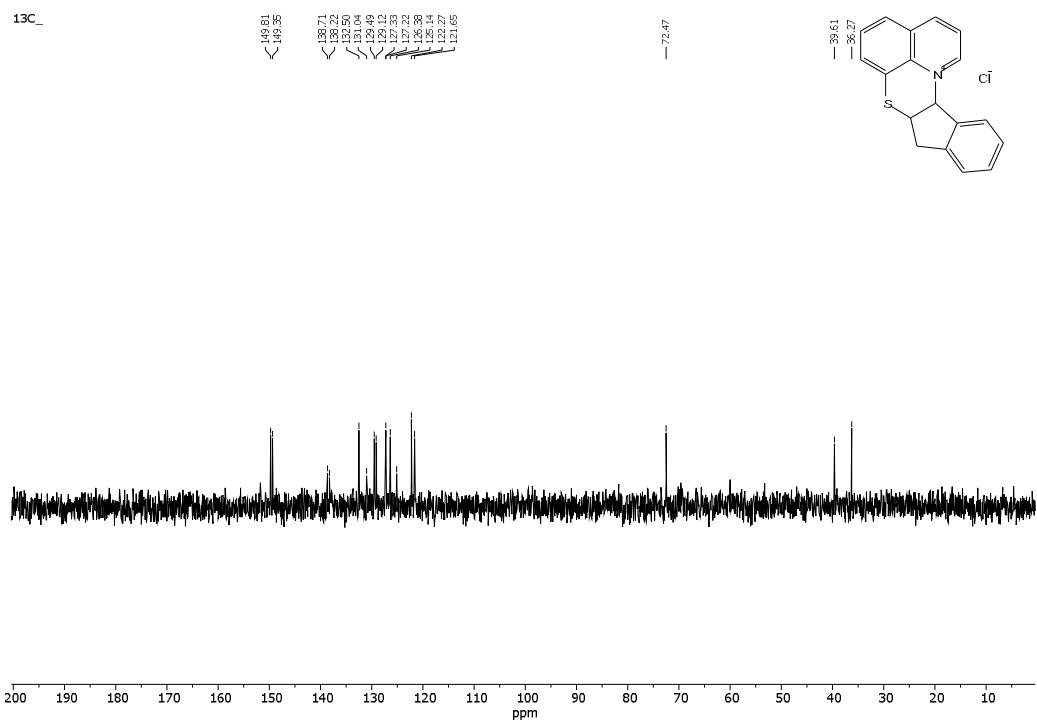
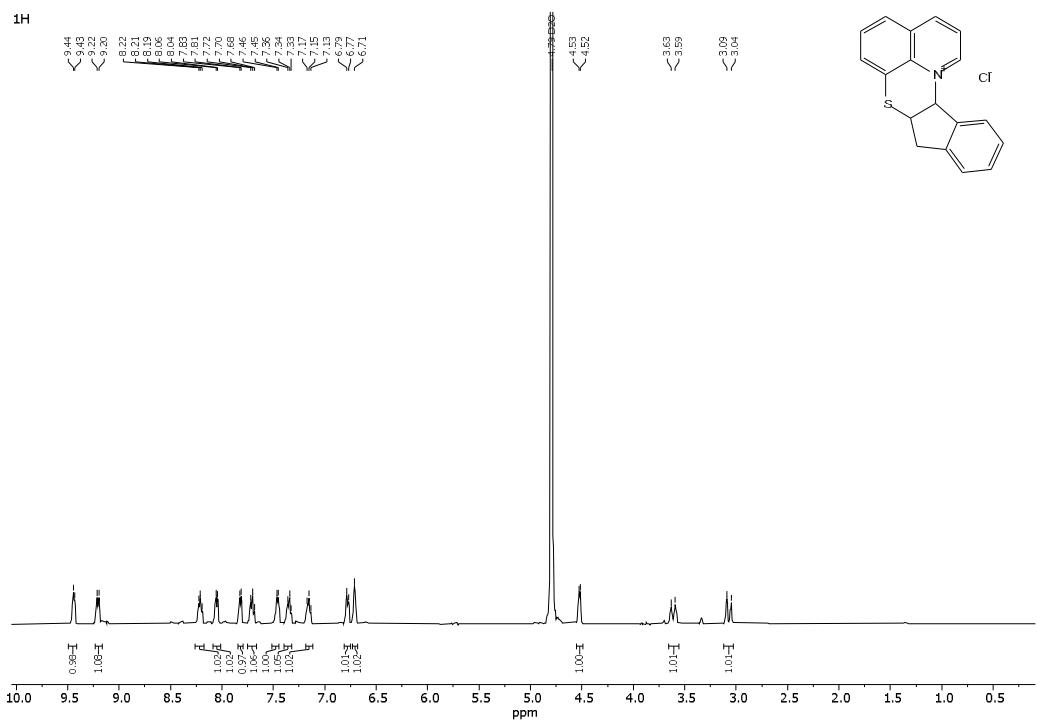


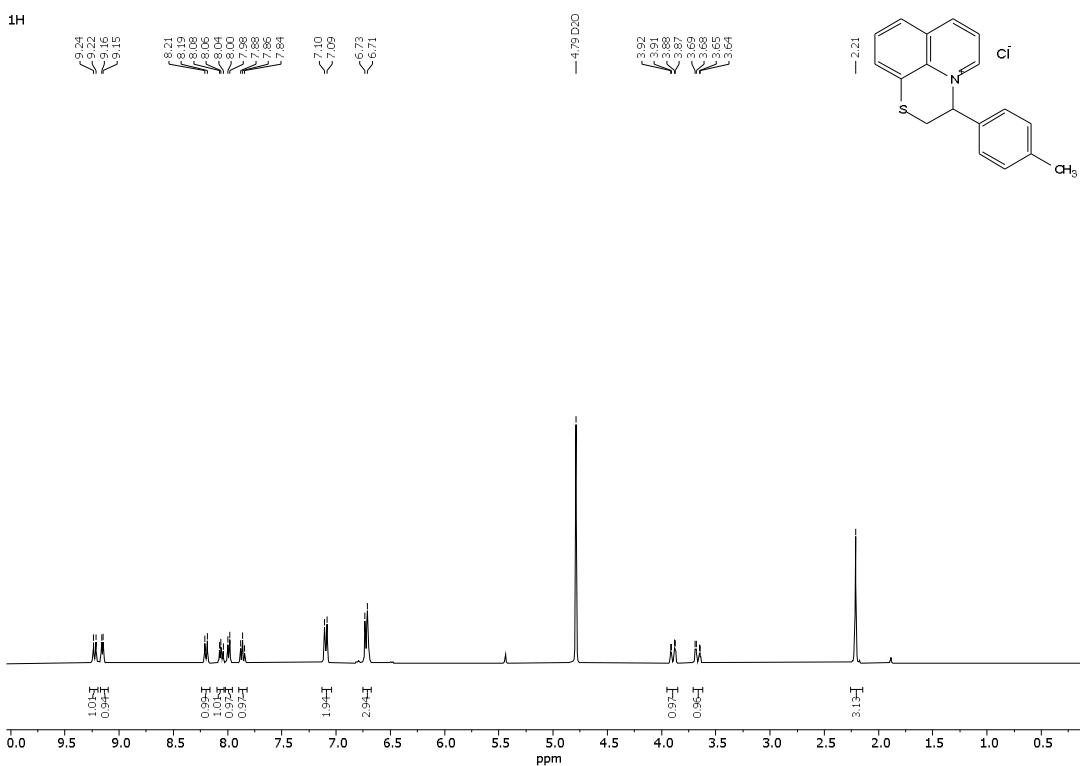
¹H-NMR (D₂O) spectrum of 3-phenyl-2H,3H-[1,4]thiazino[2,3,4-ij]quinolin-4-i um chloride (11)

¹³C₋

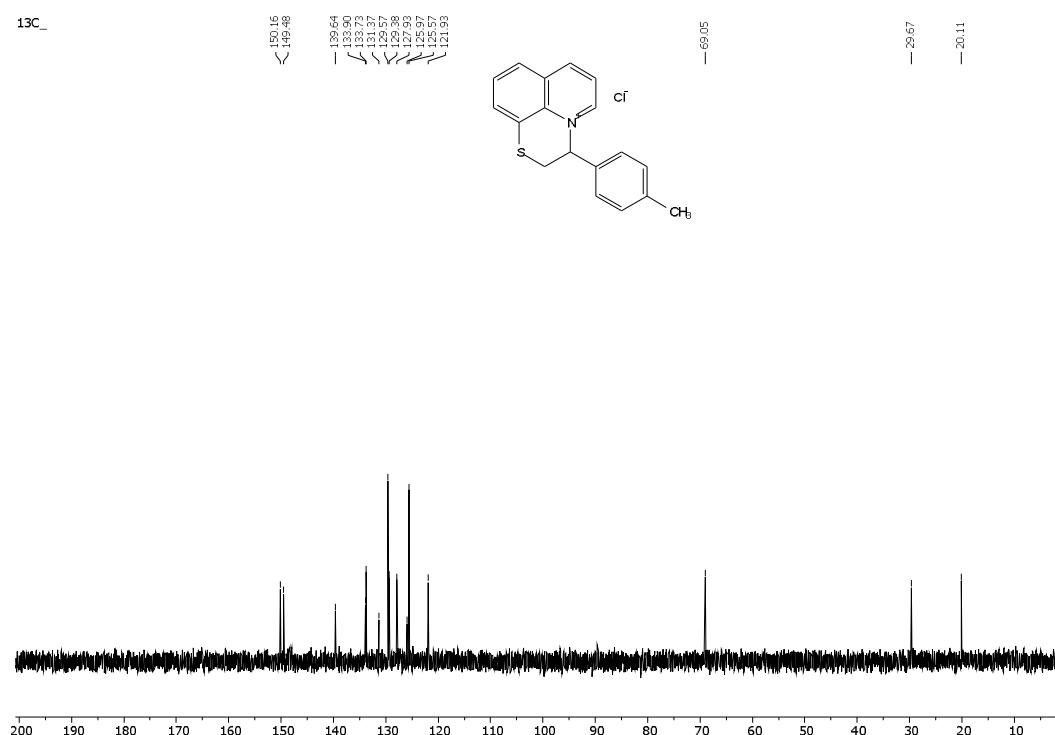


¹³C-NMR (D₂O) spectrum of 3-phenyl-2H,3H-[1,4]thiazino[2,3,4-ij]quinolin-4-i um chloride (11)

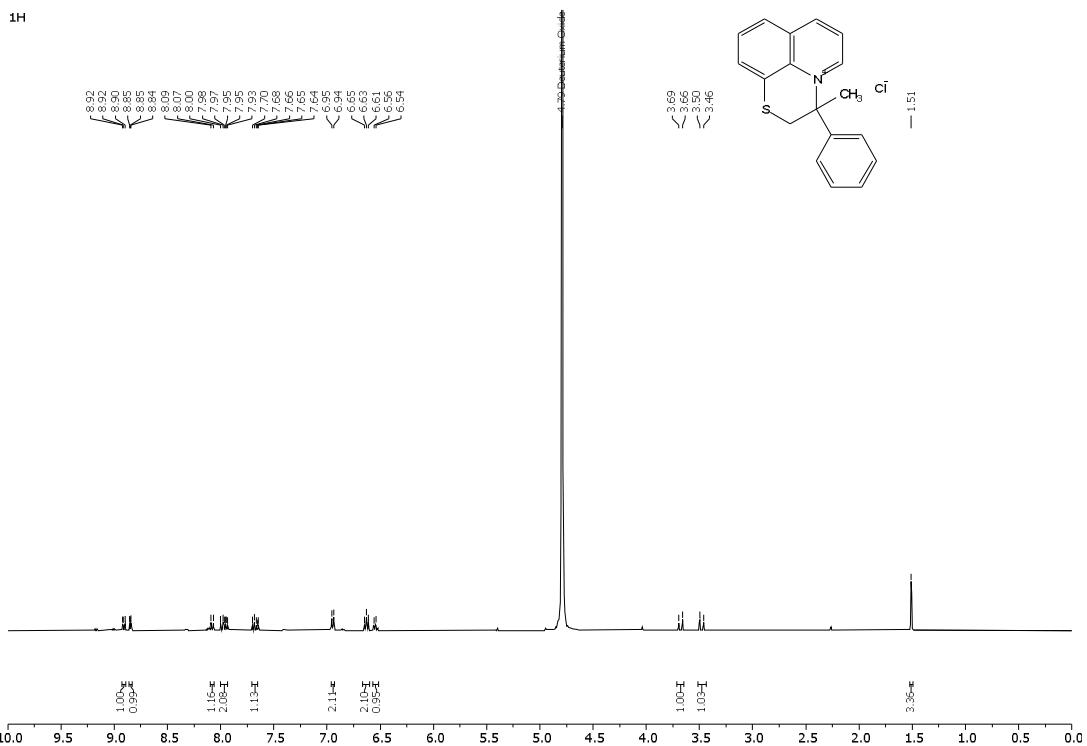




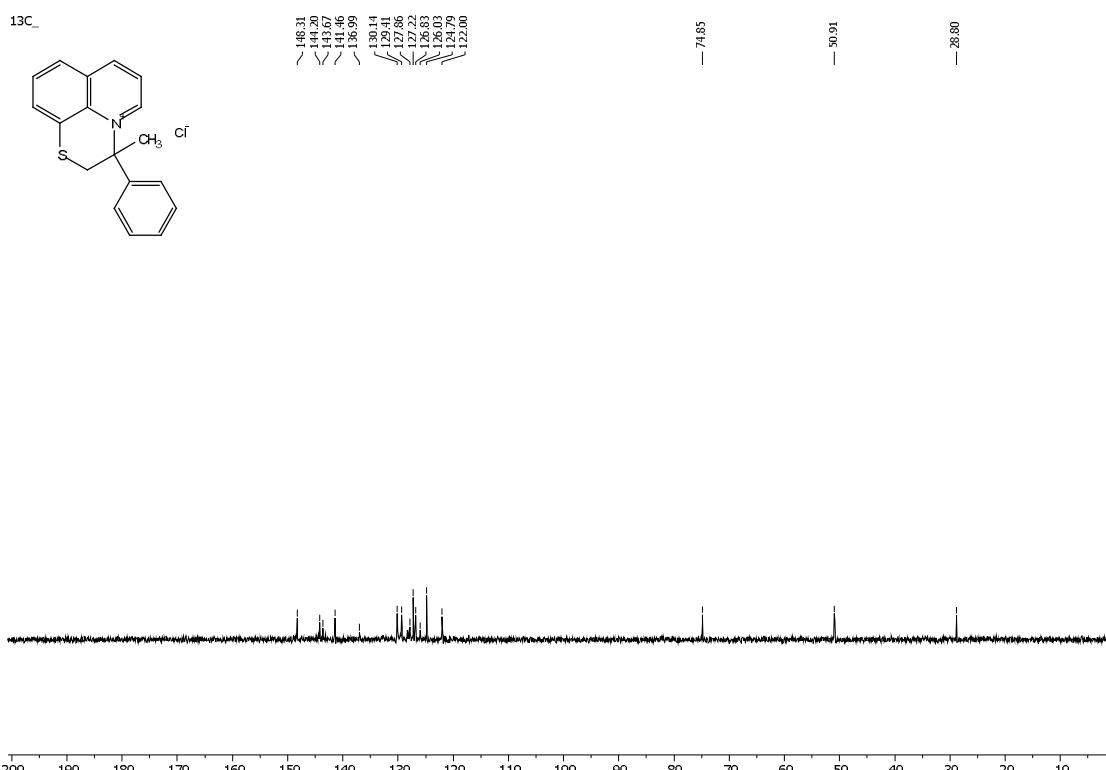
¹H-NMR (D₂O) spectrum of 3-(4-methylphenyl)-2*H*,3*H*-[1,4]thiazino[2,3,4-*ij*]quinolin-4-ium chloride (13)



¹³C-NMR (D₂O) spectrum of 3-(4-methylphenyl)-2*H*,3*H*-[1,4]thiazino[2,3,4-*ij*]quinolin-4-ium chloride (13)



¹H-NMR (D_2O) spectrum of 3-methyl-3-phenyl-2H,3H-[1,4]thiazino[2,3,4-*ij*]quinolin-4-ium chloride (14)



¹³C-NMR (D_2O) spectrum of 3-methyl-3-phenyl-2H,3H-[1,4]thiazino[2,3,4-*ij*]quinolin-4-ium chloride (14)