

New Mono- and Diesters With Imidazoquinolinone Ring - Synthesis, Structure Characterization and Molecular Modeling

Iwona Zarzyka ^{1,*}, Antonin Klásek ², Karol Hęclik ¹, Antonin Lyčka ³, Radek Bartošík ², and Lucjan Dobrowolski, ¹

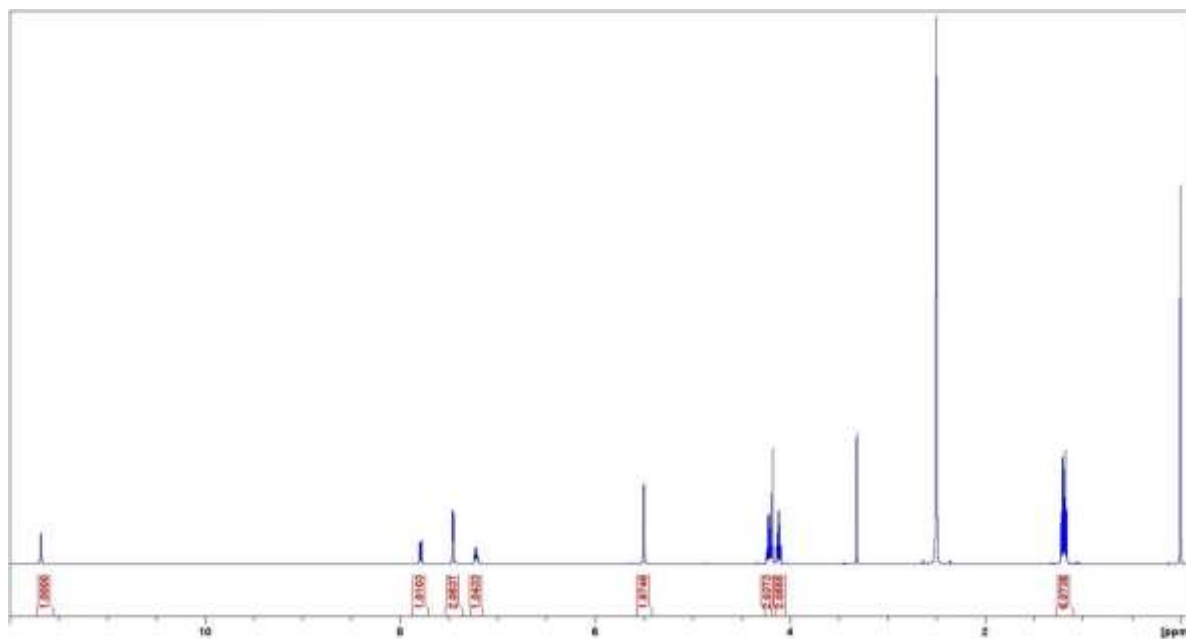


Fig. 1S. ¹H-NMR spectrum of ethyl 2-((4-oxo-4,5-dihydro-3H-imidazo[4,5-c]quinolin-2-yl)thio)acetate (4a)

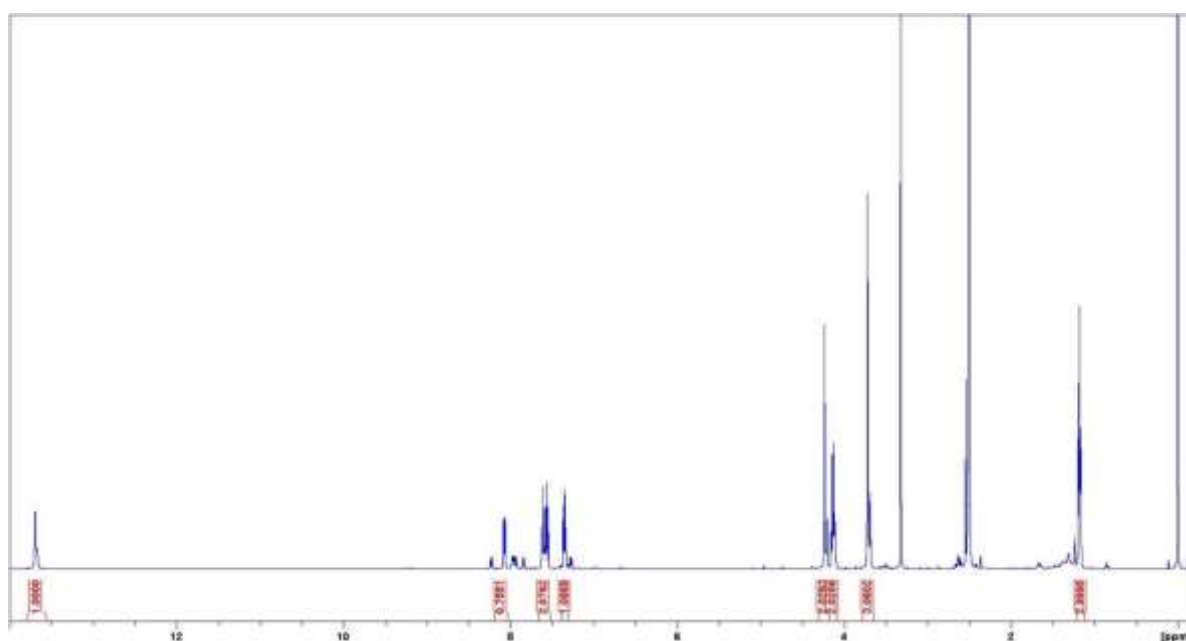


Fig. 2S. $^1\text{H-NMR}$ spectrum of ethyl 2-((4-oxo-5-methyl-4,5-dihydro-3H-imidazo[4,5-c]-quinolin-2-yl)thio)acetate (4b).

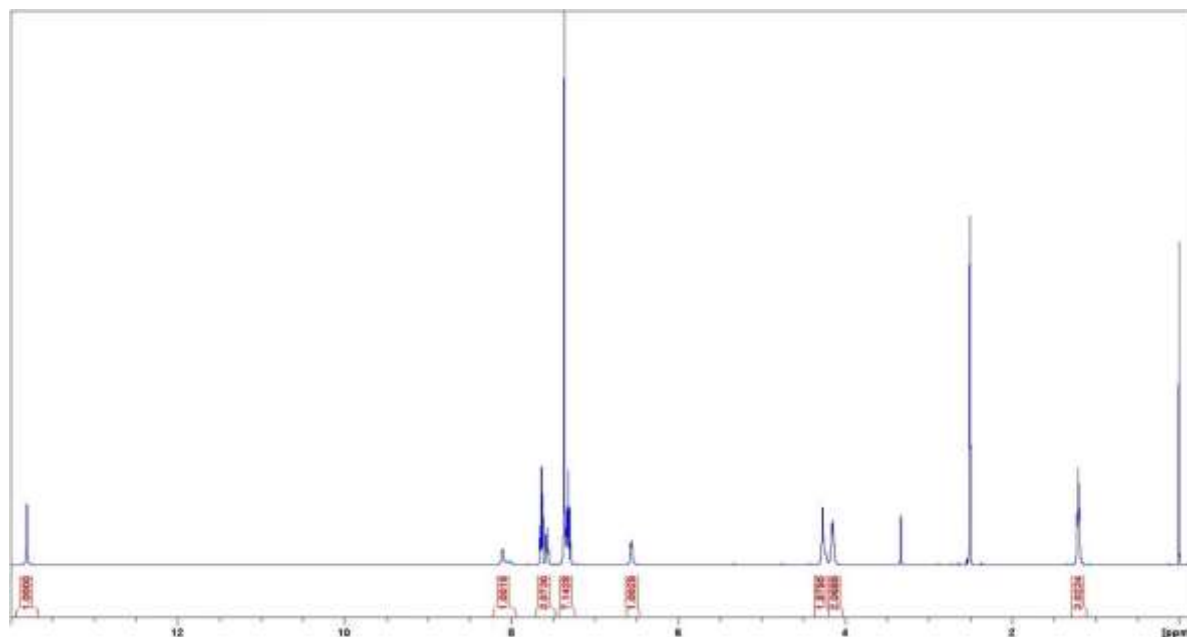


Fig. 3S. $^1\text{H-NMR}$ spectrum of ethyl 2-((4-oxo-5-phenyl-4,5-dihydro-3H-imidazo[4,5-c]-quinolin-2-yl)thio)acetate (4c).

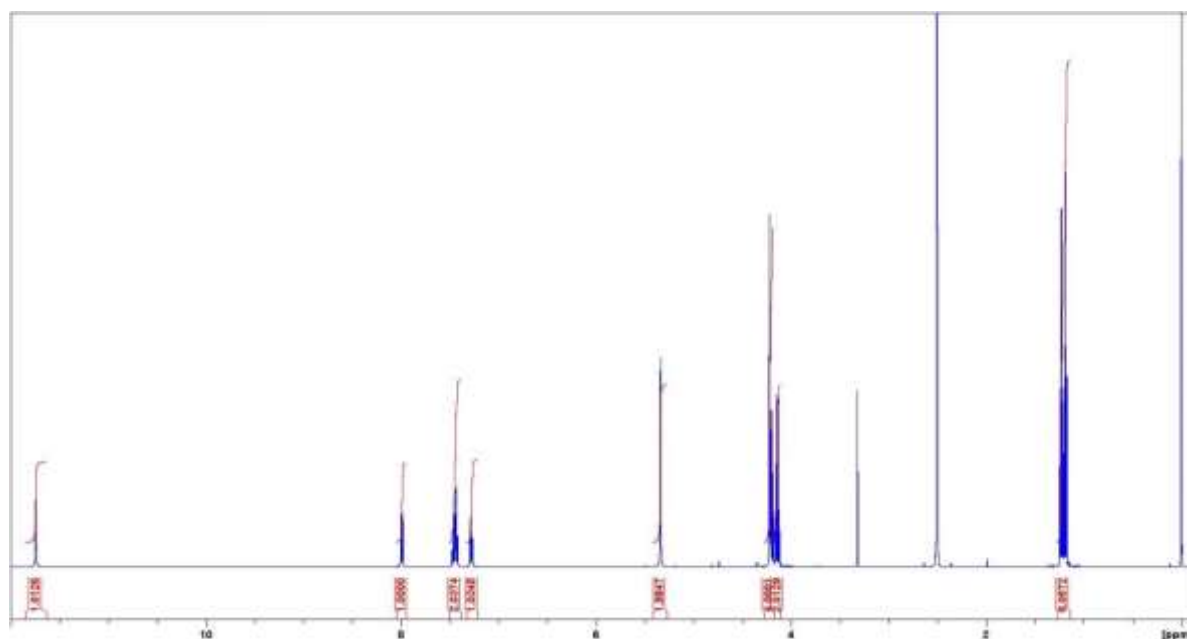


Fig. 4S. $^1\text{H-NMR}$ spectrum of ethyl 2-((3-(2-ethoxy-2-oxoethyl)-4-oxo-4,5-dihydro-3H-imidazo[4,5-c]quinolin-2-yl)thio)acetate (5a).

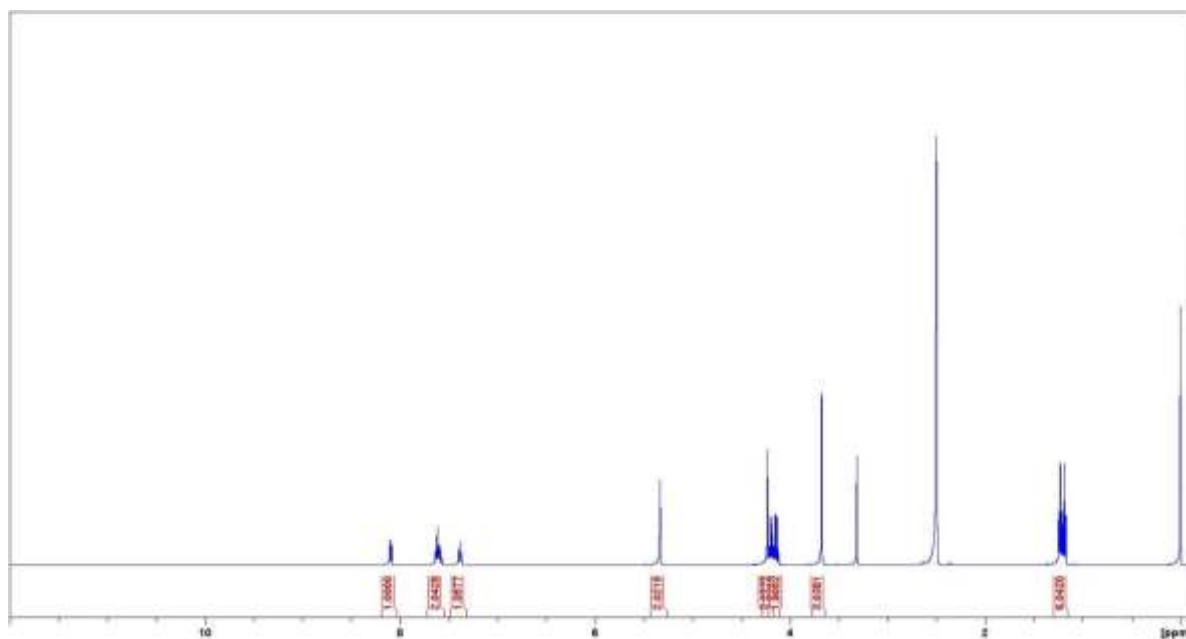


Fig. 5S. ¹H-NMR spectrum of ethyl 2-((3-(2-ethoxy-2-oxoethyl)-4-oxo-5-methyl-4,5-dihydro-3H-imidazo[4,5-c]quinolin-2-yl)thio)- acetate (5b).

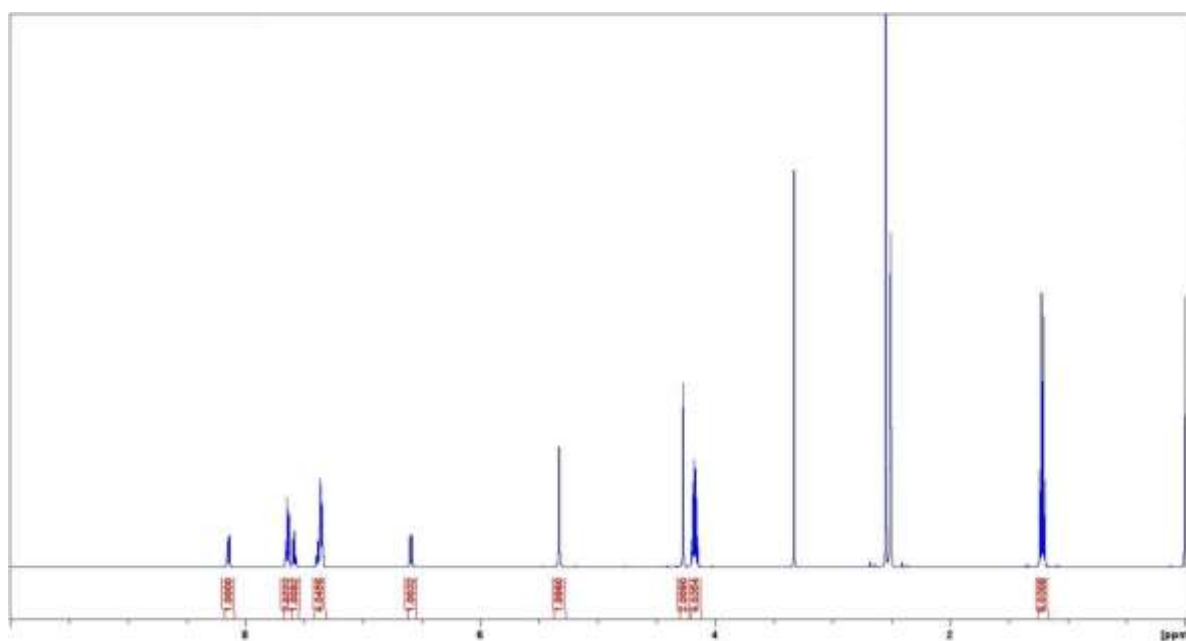

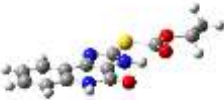






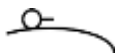
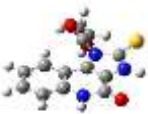






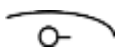



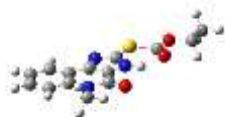
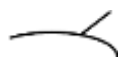


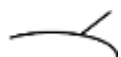
Fig. 6S. ¹H-NMR spectrum of ethyl 2-((3-(2-ethoxy-2-oxoethyl)-4-oxo-5-methyl-4,5-dihydro-3H-imidazo[4,5-c]quinolin-2-yl)thio)- acetate (5c).

Table 1S. Possible conformers of compounds 4

Compound	Conformer symbol	Conformer structure
		
		
		
		
		
4a		
		
		
		
		



4b



4c



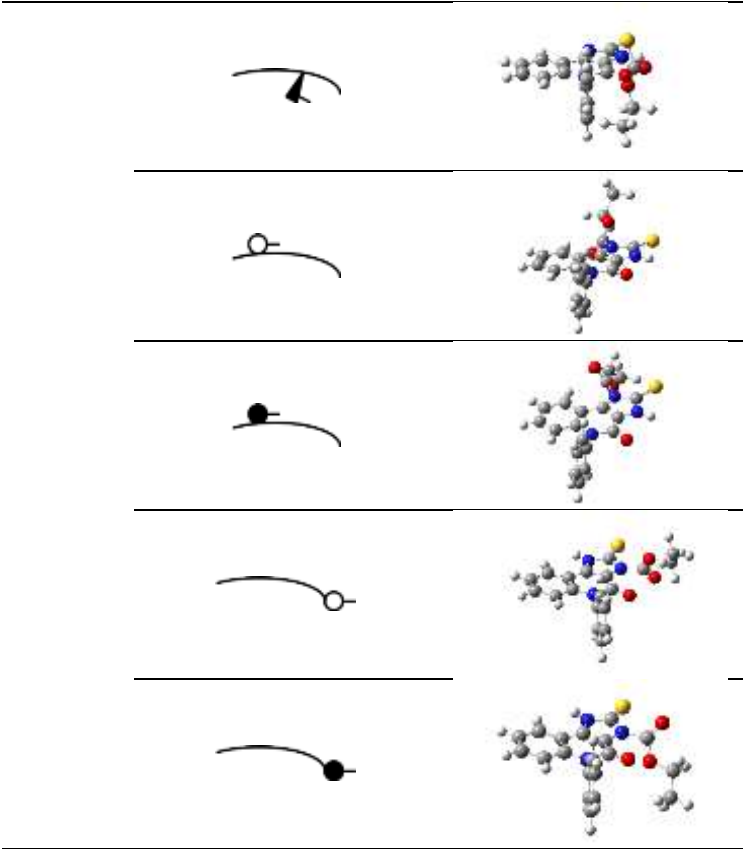


Table 2S. Possible conformers of compounds 5

Compound	Conformer symbol	Conformer structure
5a		
5b		



5c

