

## Supporting information

# Exploration of the Divergent Outcomes for the Nenitzescu Reaction of Piperazinone Enaminoesters

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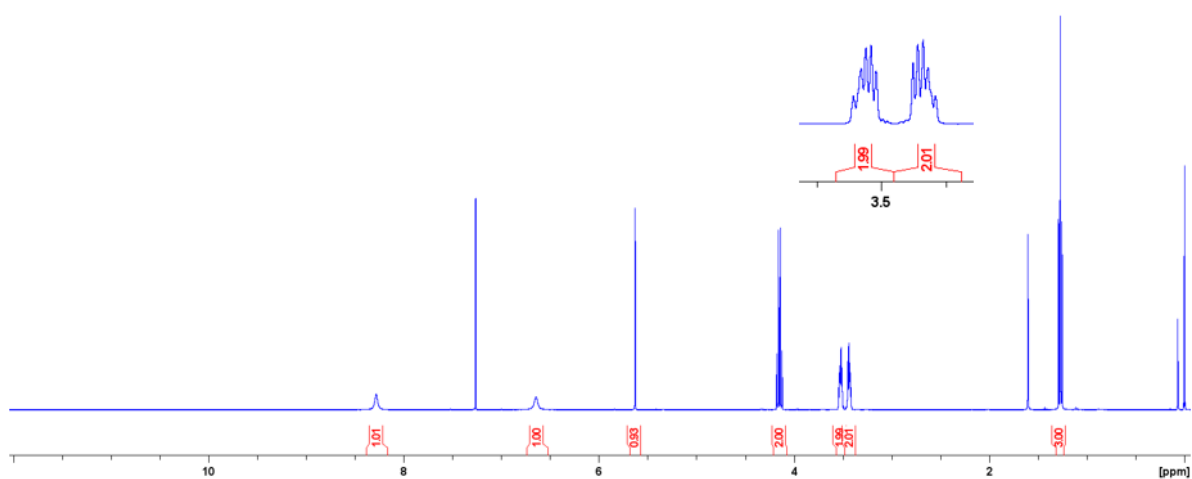
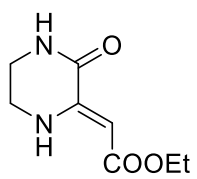
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<sup>2</sup> Biochemistry, Molecular and Structural Biology, Department of Chemistry, KU Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium

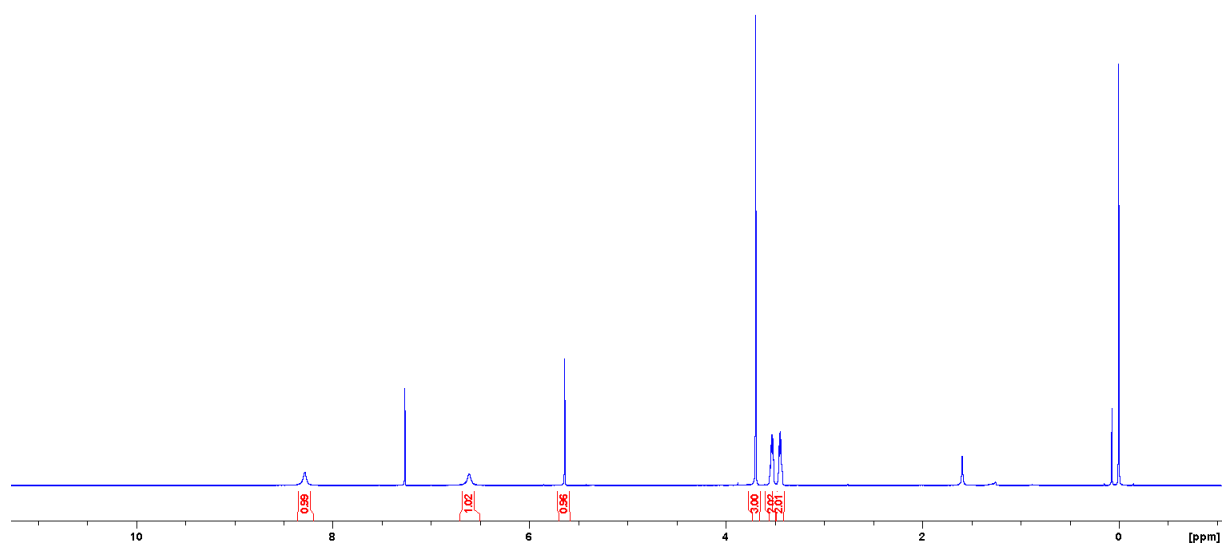
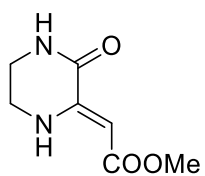
\* Correspondence: wim.dehaen@kuleuven.be

## NMR Spectra

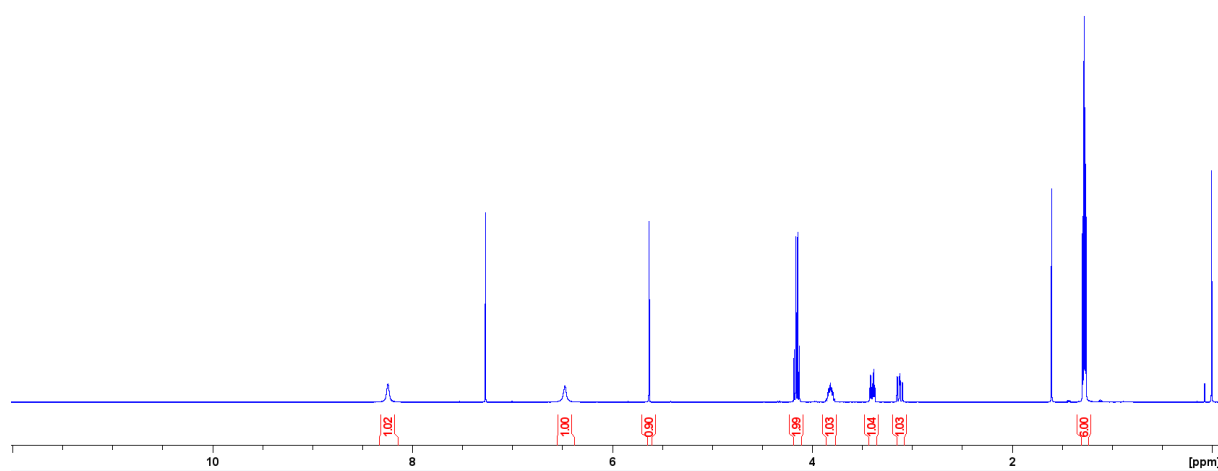
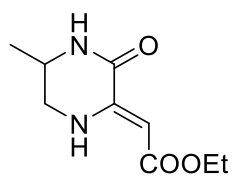
**Ethyl (Z)-2-(3-oxopiperazin-2-ylidene)acetate (15)**



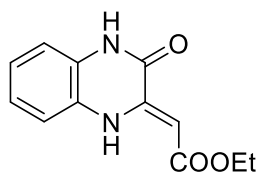
**Methyl (Z)-2-(3-oxopiperazin-2-ylidene)acetate (22)**

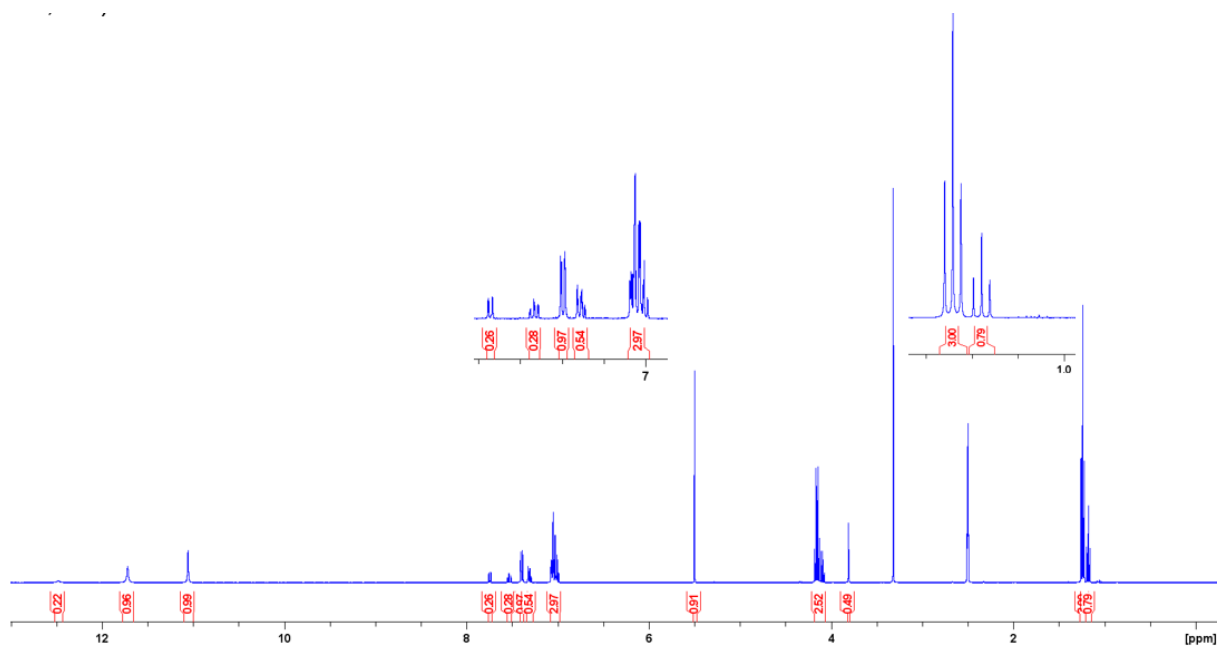


**Ethyl (Z)-2-(5-methyl-3-oxopiperazin-2-ylidene)acetate (23)**

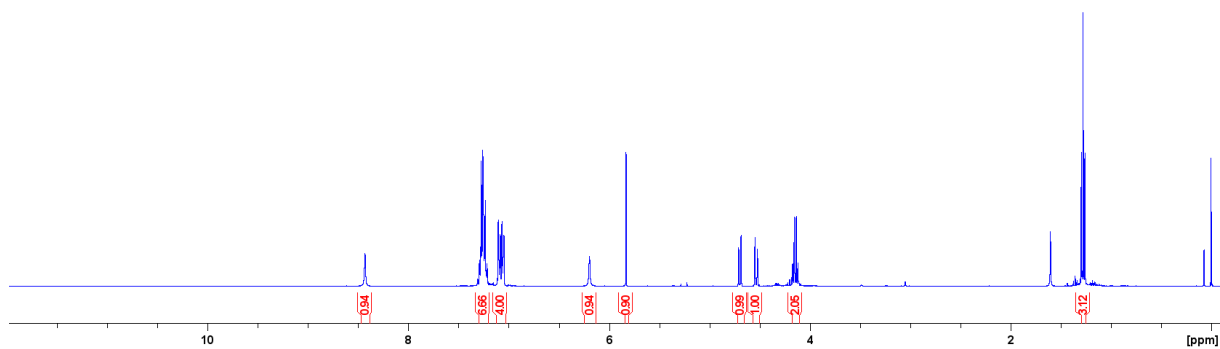
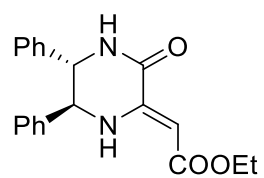


**Ethyl (Z)-2-(3-oxo-3,4-dihydroquinoxalin-2(1H)-ylidene)acetate (24)**

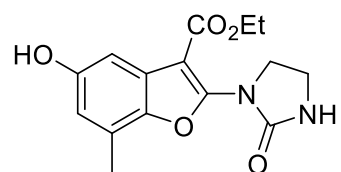


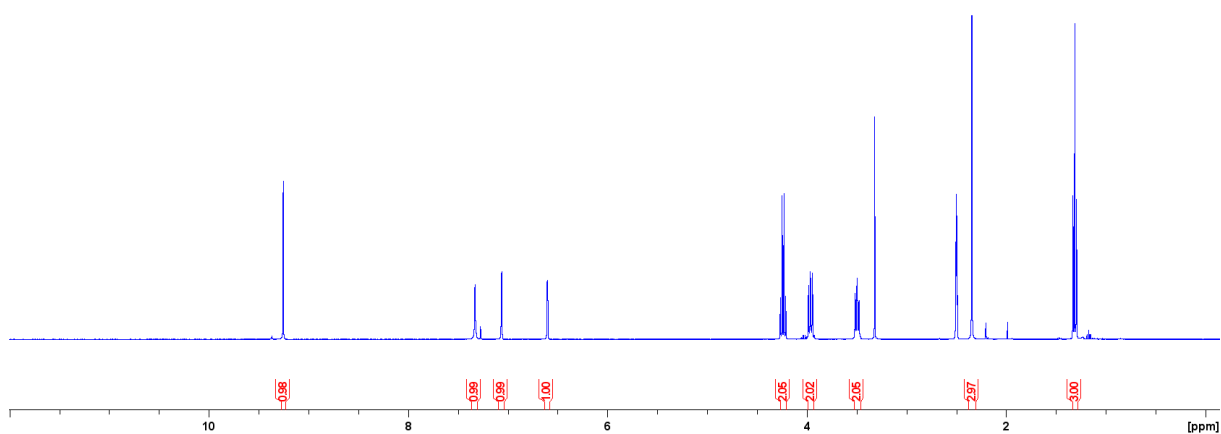


**Ethyl (Z)-2-((5S,6S)-3-oxo-5,6-diphenylpiperazin-2-ylidene)acetate (25)**

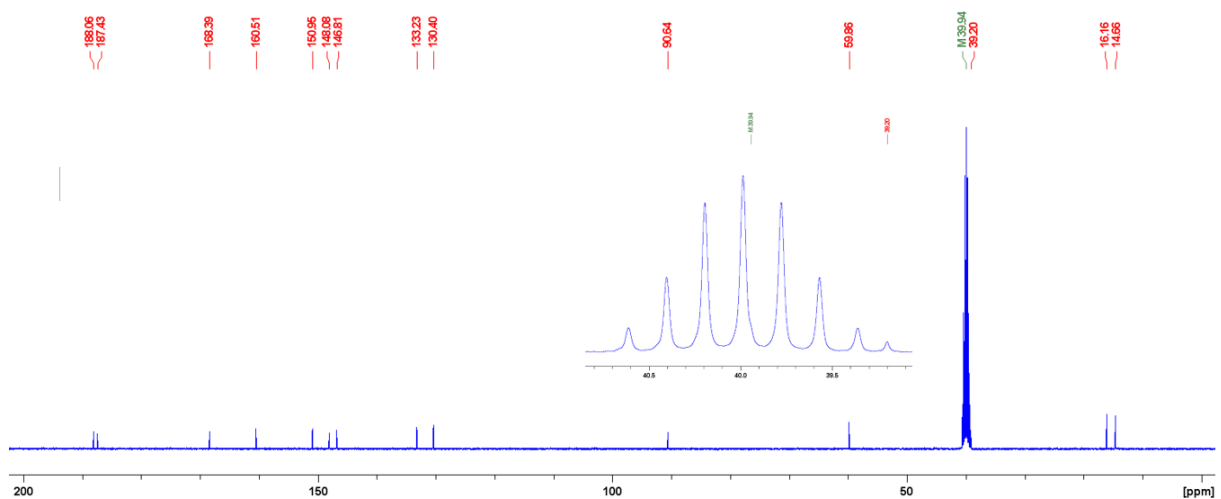
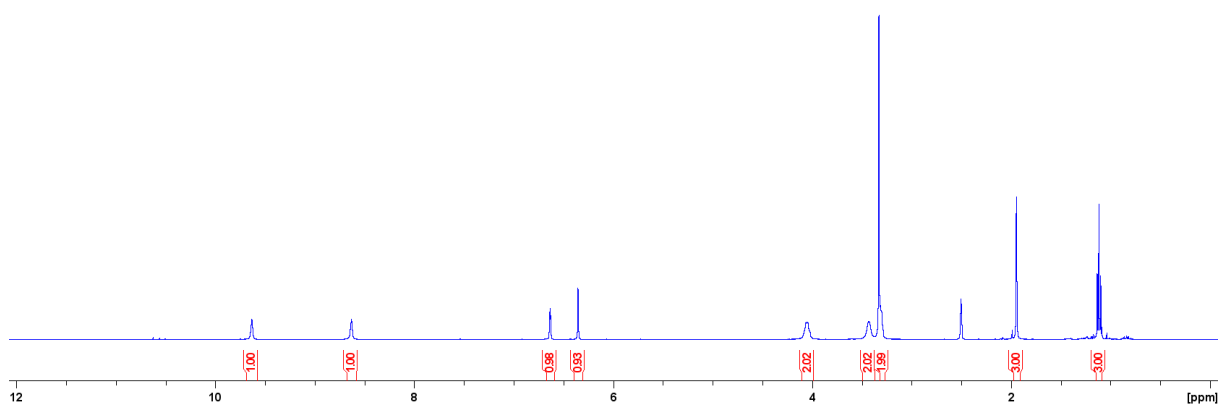
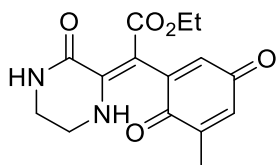


**Ethyl 5-hydroxy-7-methyl-2-(2-oxoimidazolidin-1-yl)benzofuran-3-carboxylate (19)**

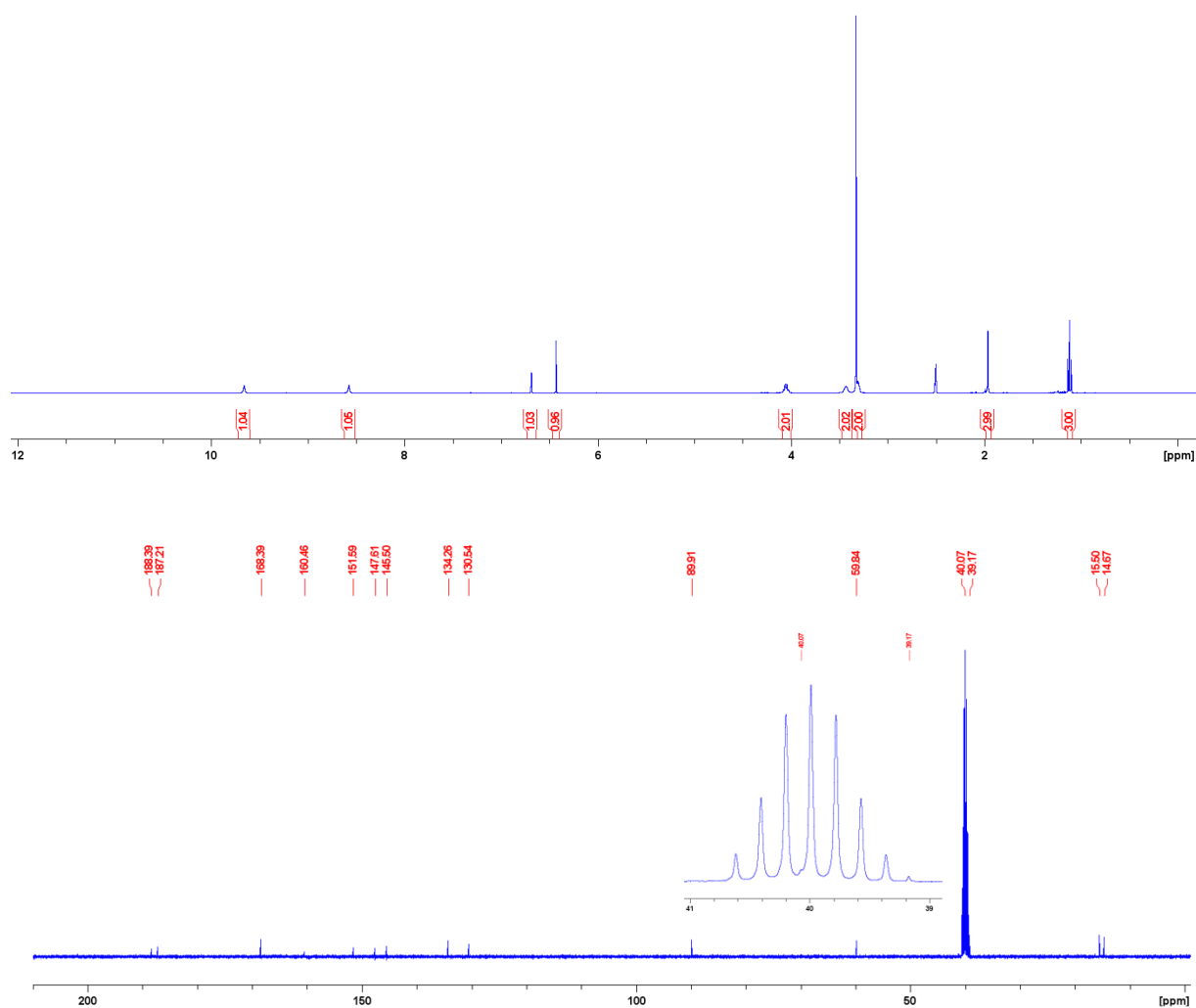
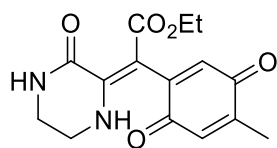




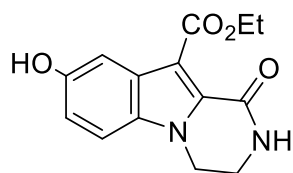
**Ethyl-2-(5-methyl-3,6-dioxocyclohexa-1,4-dien-1-yl)-2-(3-oxopiperazin-2-ylidene)acetate (20a)**

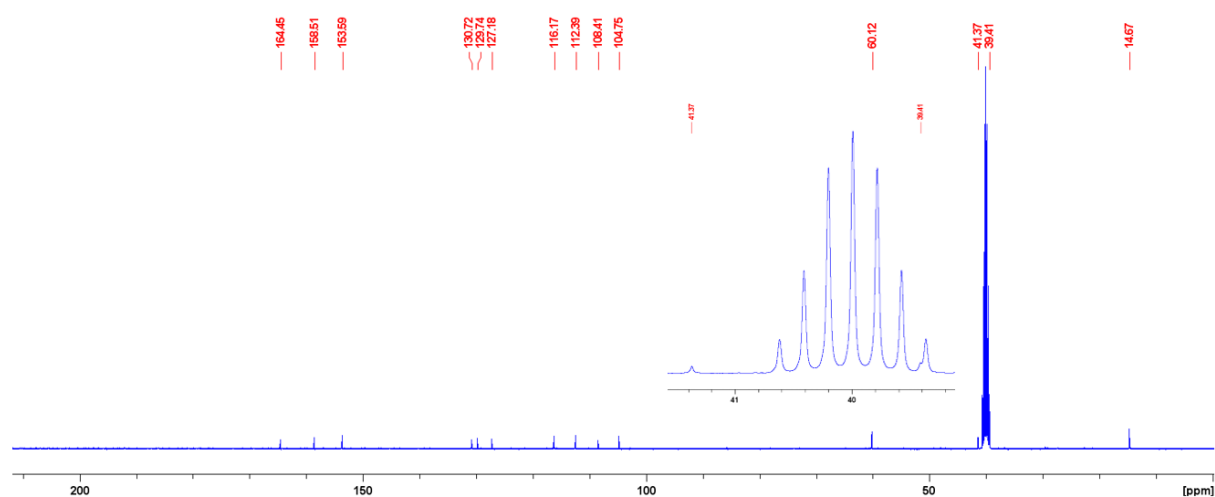
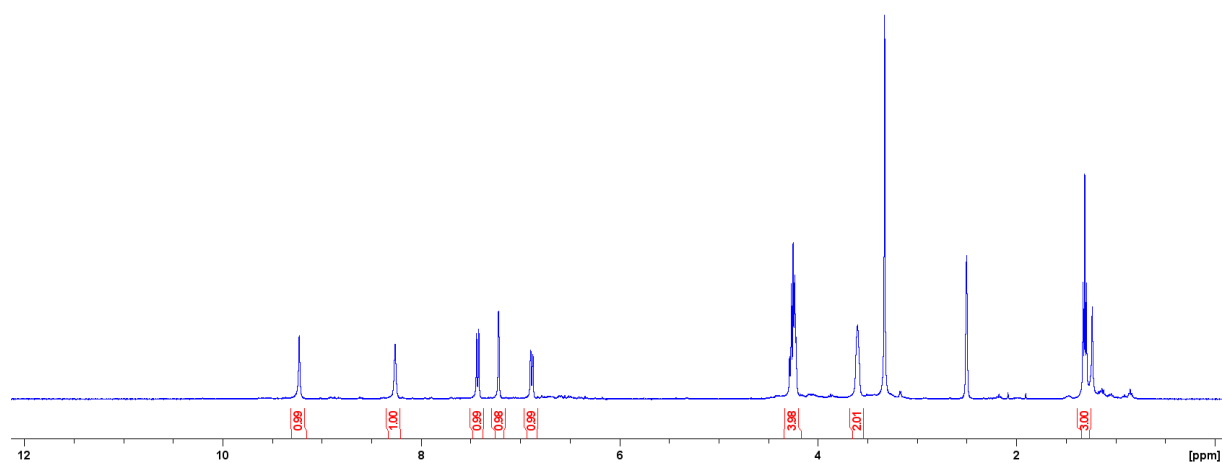


**Ethyl-2-(4-methyl-3,6-dioxocyclohexa-1,4-dien-1-yl)-2-(3-oxopiperazin-2-ylidene)acetate (20b)**

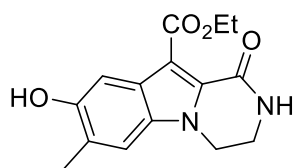
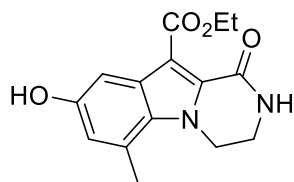


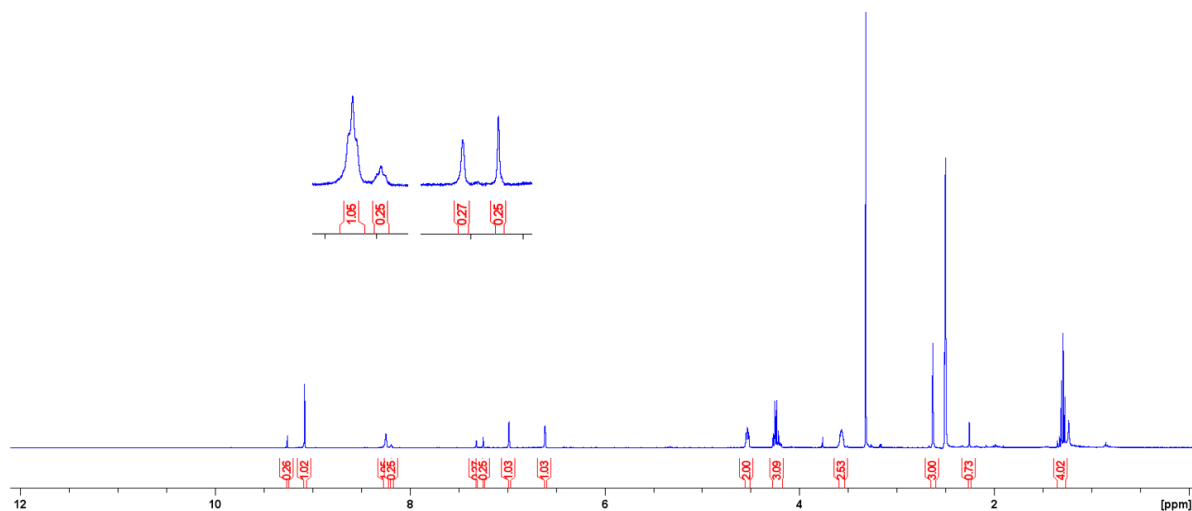
**Ethyl 8-hydroxy-1-oxo-1,2,3,4-tetrahydropyrazino[1,2-a]indole-10-carboxylate (27)**



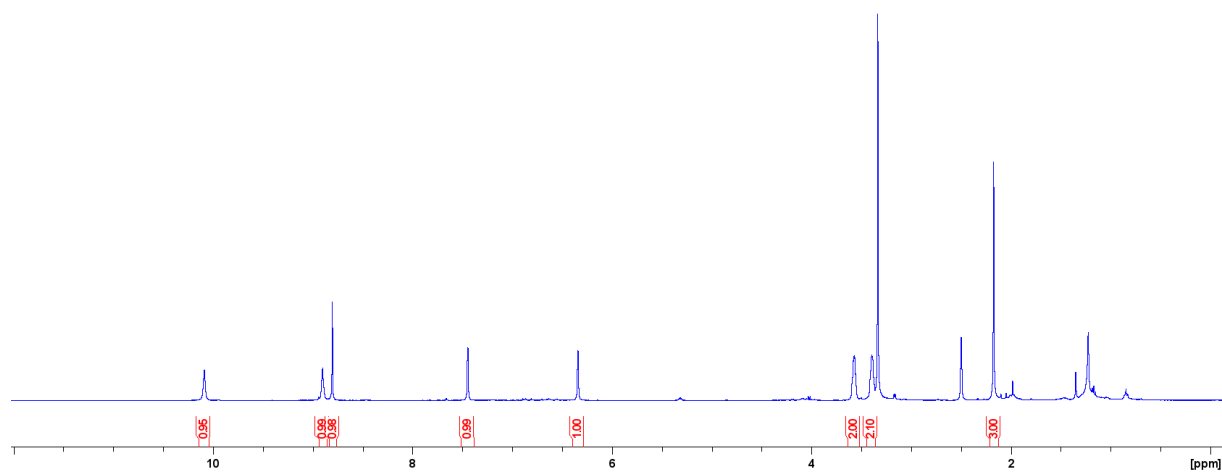
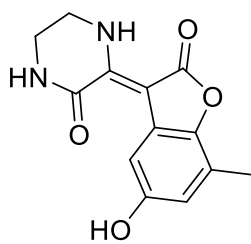


**Ethyl 8-hydroxy-6-methyl-1-oxo-1,2,3,4-tetrahydropyrazino[1,2-a]indole-10-carboxylate (18b) and ethyl 8-hydroxy-7-methyl-1-oxo-1,2,3,4-tetrahydropyrazino[1,2-a]indole-10-carboxylate (18a)**

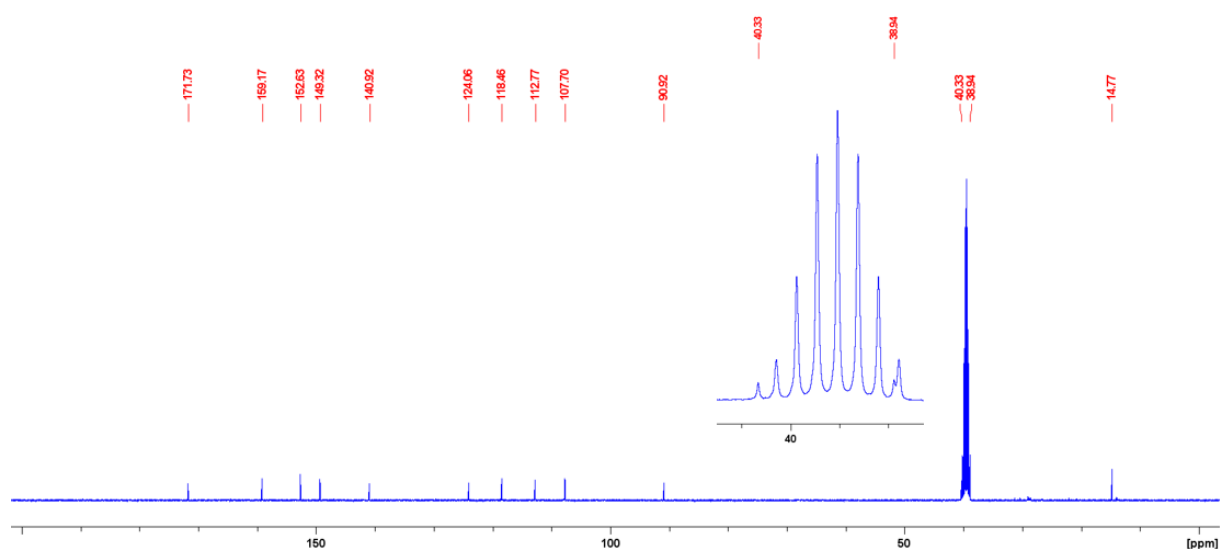




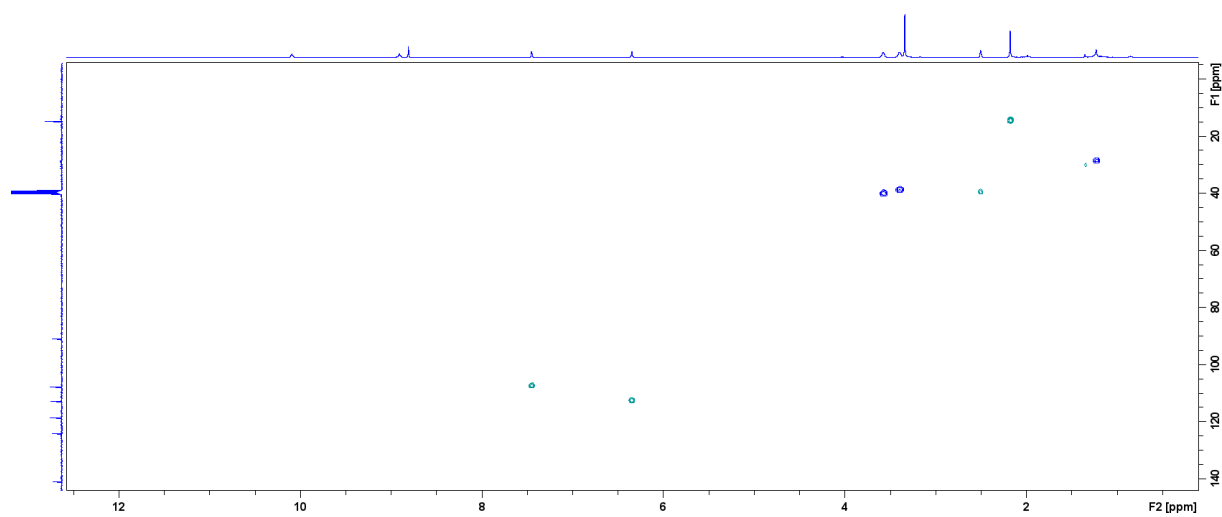
**(Z)-3-(5-Hydroxy-7-methyl-2-oxobenzofuran-3(2H)-ylidene)piperazin-2-one (21a)**



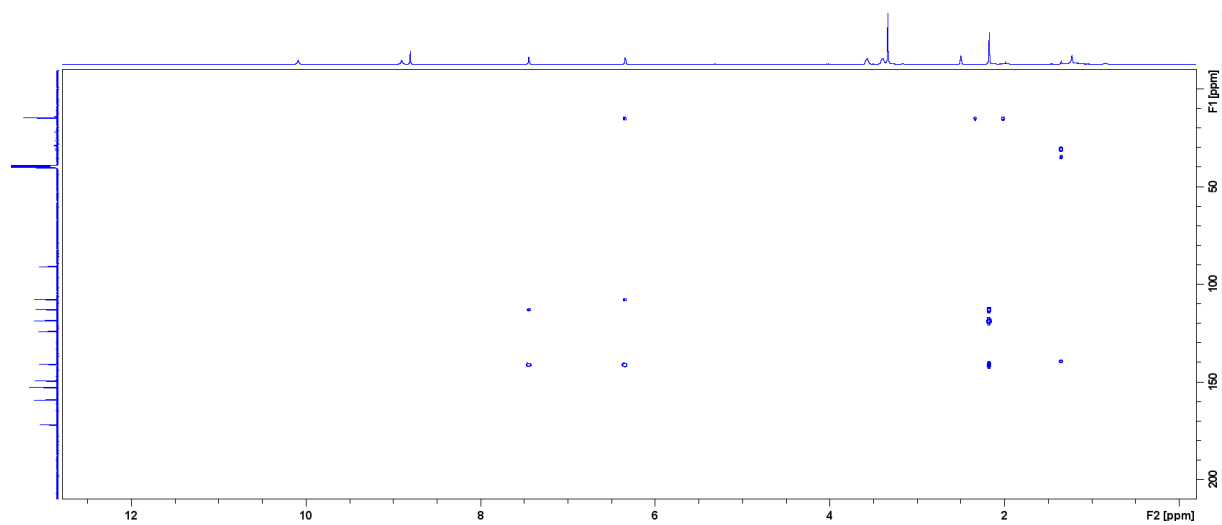




HSQC



HMBC



NOESY

