

Cyclisation Modes in Anilides of *N*-Protected 3-Oxo-4-phenylaminobutyric Acid Under Knorr Conditions

Plamen Angelov and Yordanka Mollova-Sapundzhieva

angelov@uni-plovdiv.bg

Supplementary Information

Primary unprocessed NMR data, including 2D spectra, is available for download at: <https://doi.org/10.5281/zenodo.14175517>

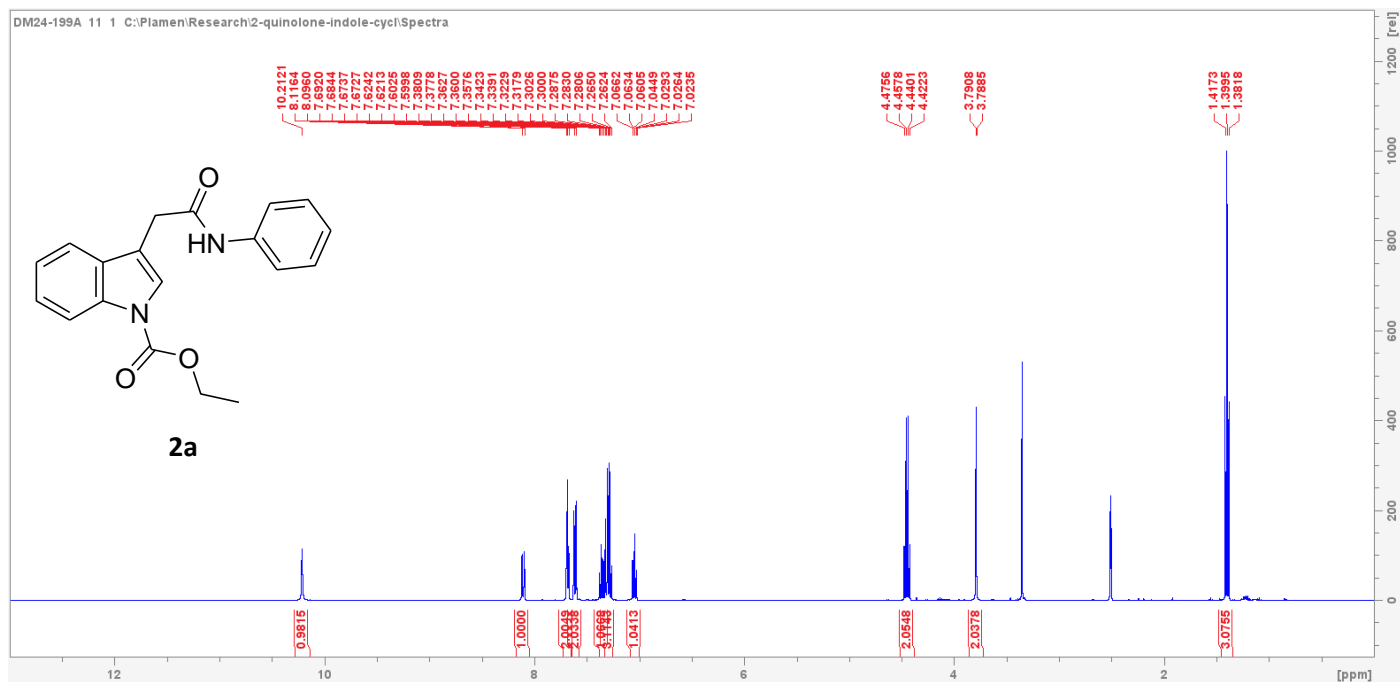


Figure S1. ^1H NMR spectrum of 3-Phenylcarbamoylmethylindole-1-carboxylic acid ethyl ester (**2a**)

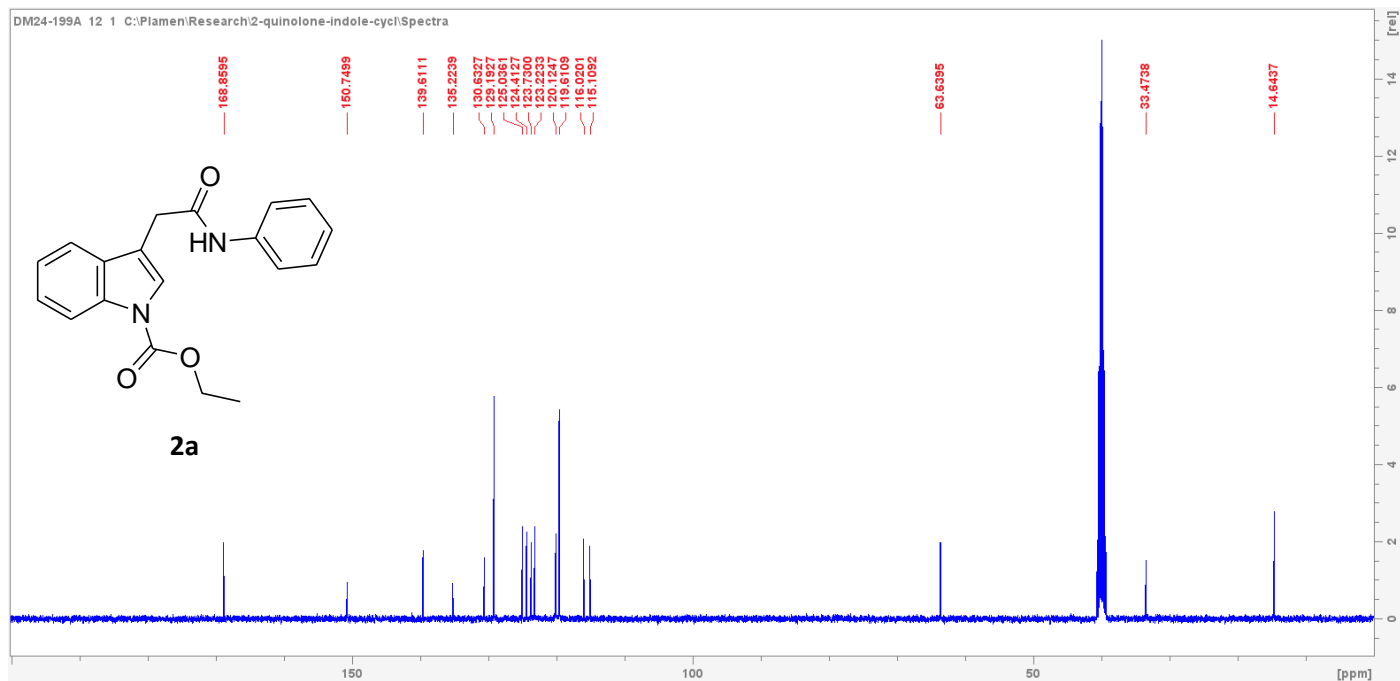


Figure S2. ^{13}C NMR spectrum of 3-Phenylcarbamoylmethylindole-1-carboxylic acid ethyl ester (**2a**)

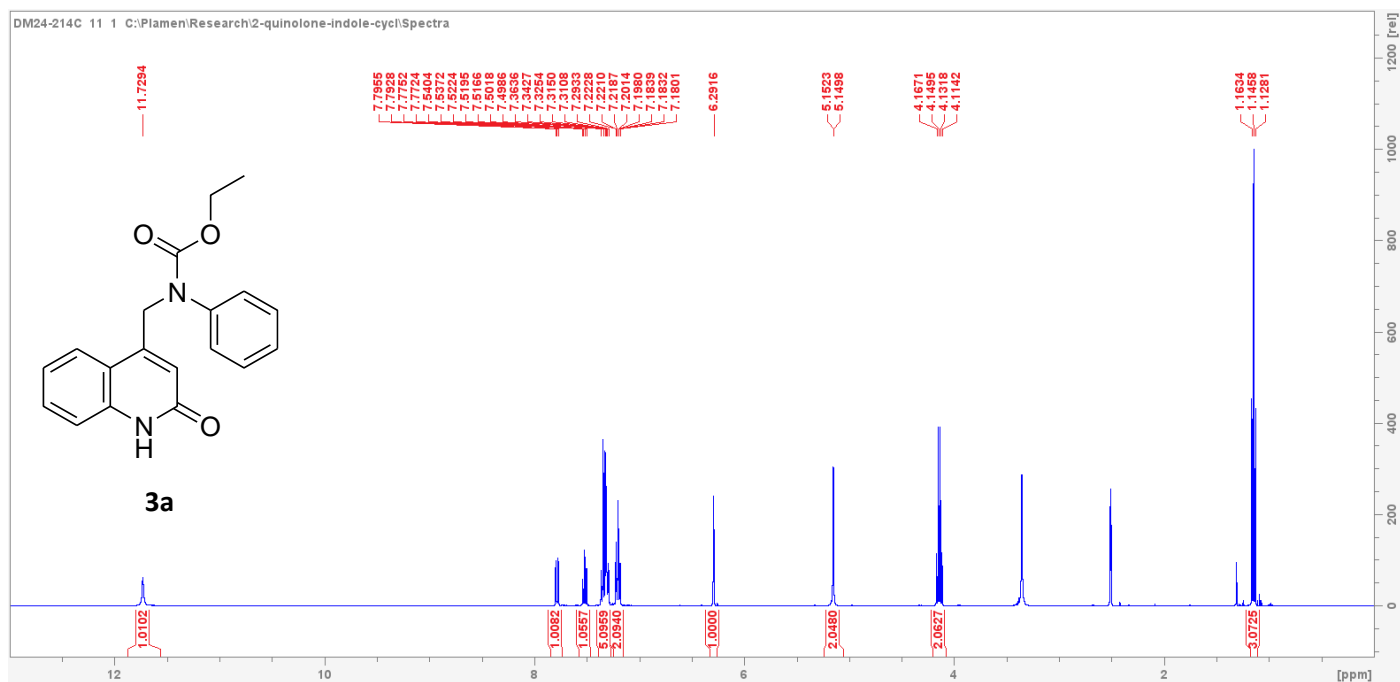


Figure S3. ¹H NMR spectrum of (2-Oxo-1,2-dihydroquinolin-4-ylmethyl)-phenylcarbamic acid ethyl ester (**3a**)

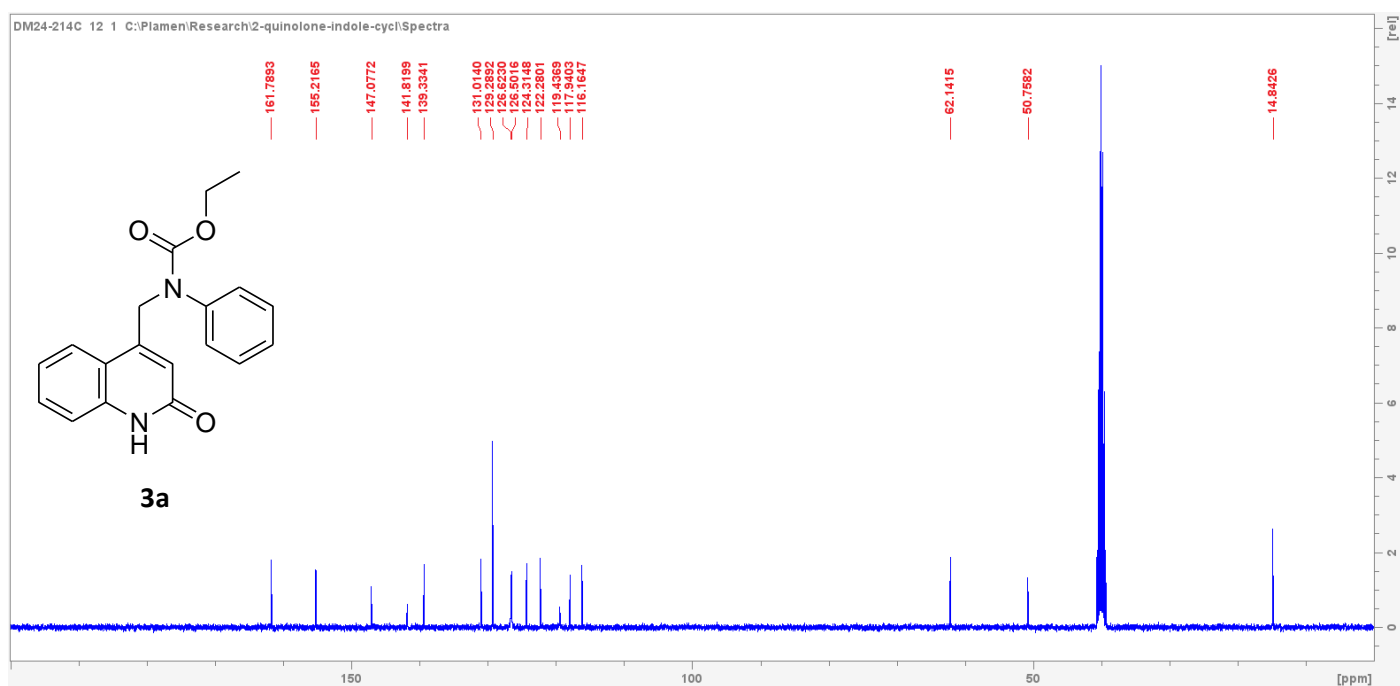


Figure S4. ¹³C NMR spectrum of (2-Oxo-1,2-dihydroquinolin-4-ylmethyl)-phenylcarbamic acid ethyl ester (**3a**)

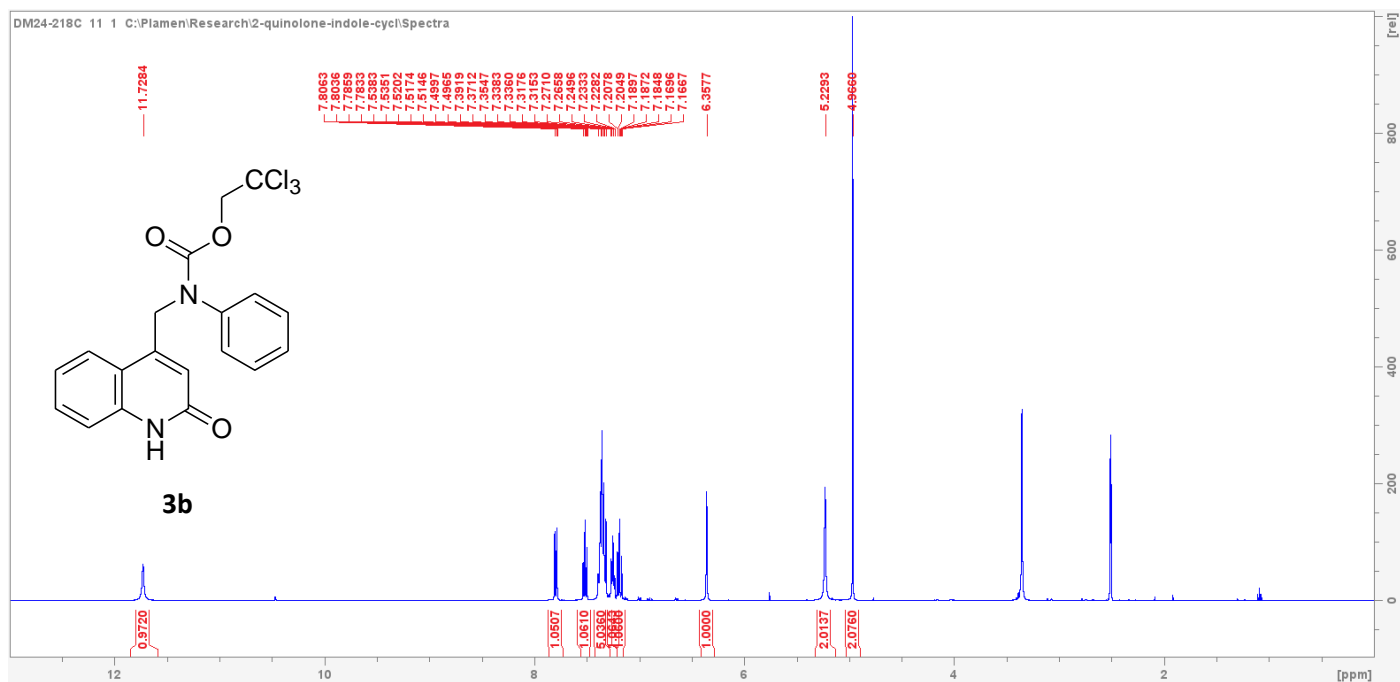


Figure S5. ^1H NMR spectrum of (2-Oxo-1,2-dihydroquinolin-4-ylmethyl)-phenylcarbamic acid 2,2,2-trichloroethyl ester (**3b**)

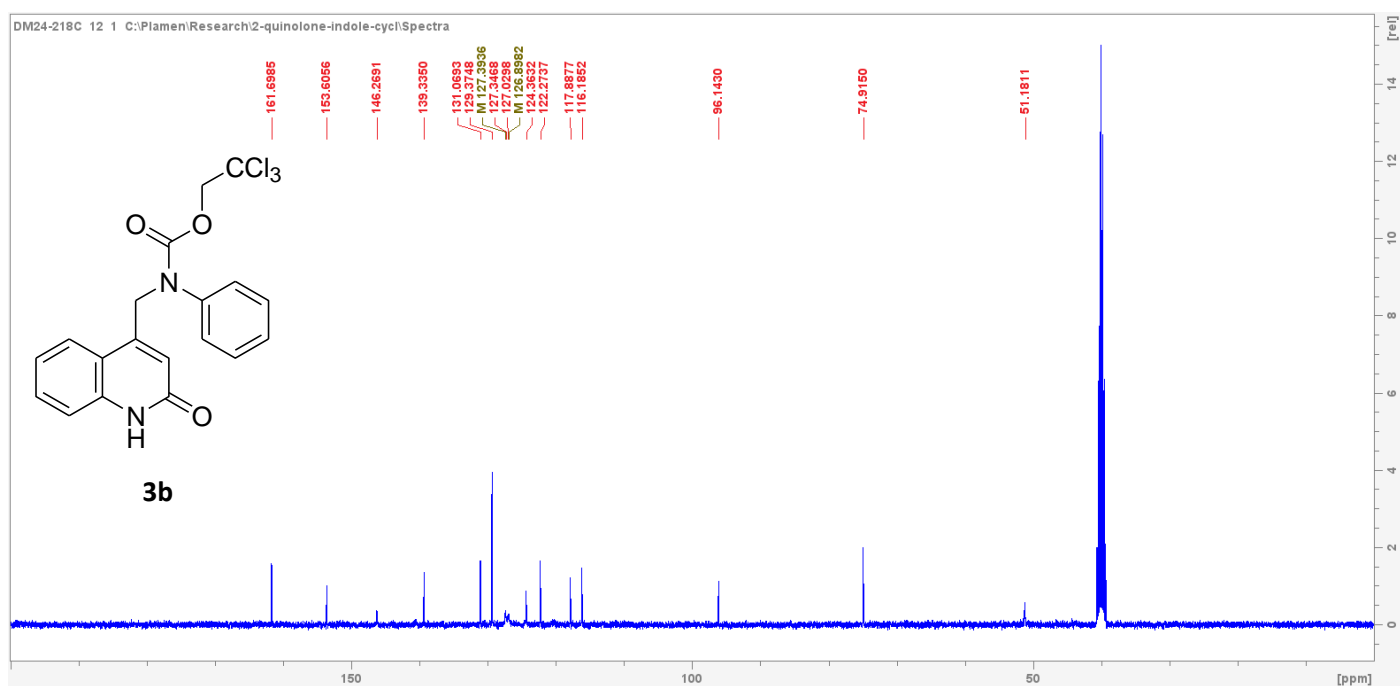


Figure S6. ^{13}C NMR spectrum of (2-Oxo-1,2-dihydroquinolin-4-ylmethyl)-phenylcarbamic acid 2,2,2-trichloroethyl ester (**3b**)

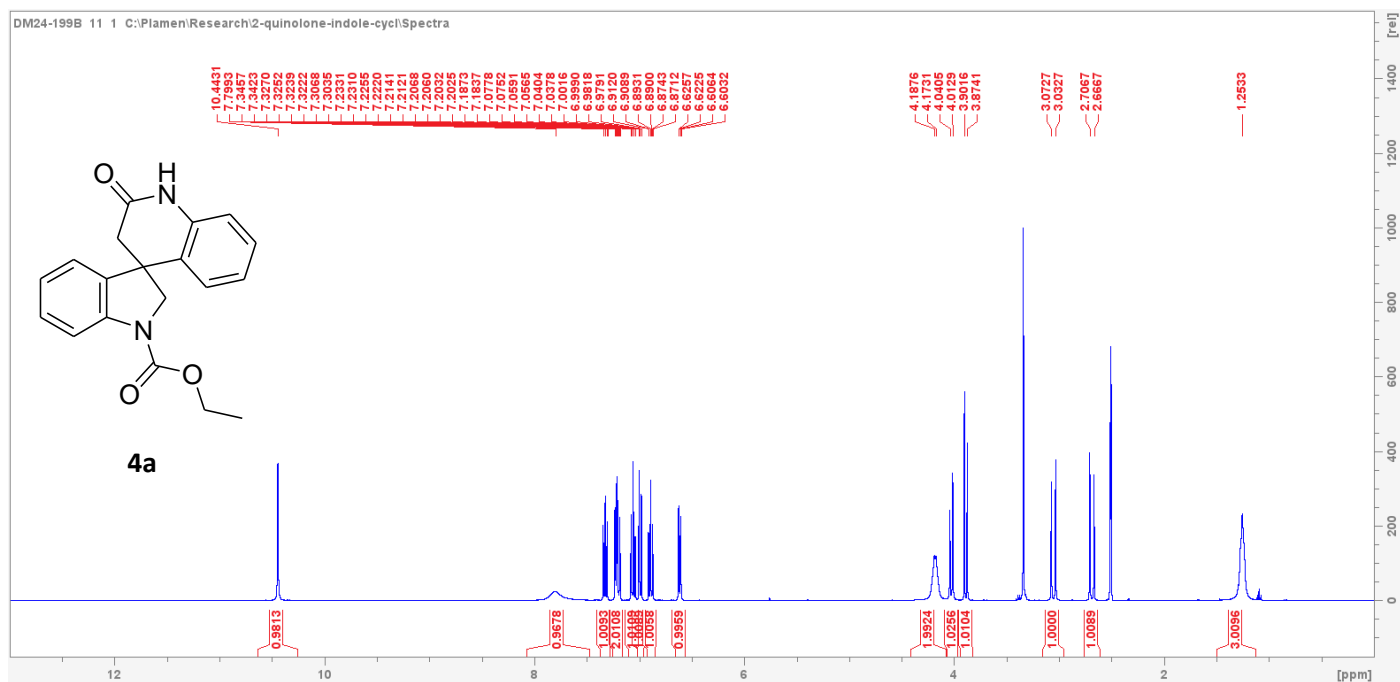


Figure S7. ^1H NMR spectrum of Ethyl 2'-oxo-2',3'-dihydro-1'H-spiro[indole-3,4'-quinoline]-1(2H)-carboxylate (**4a**)

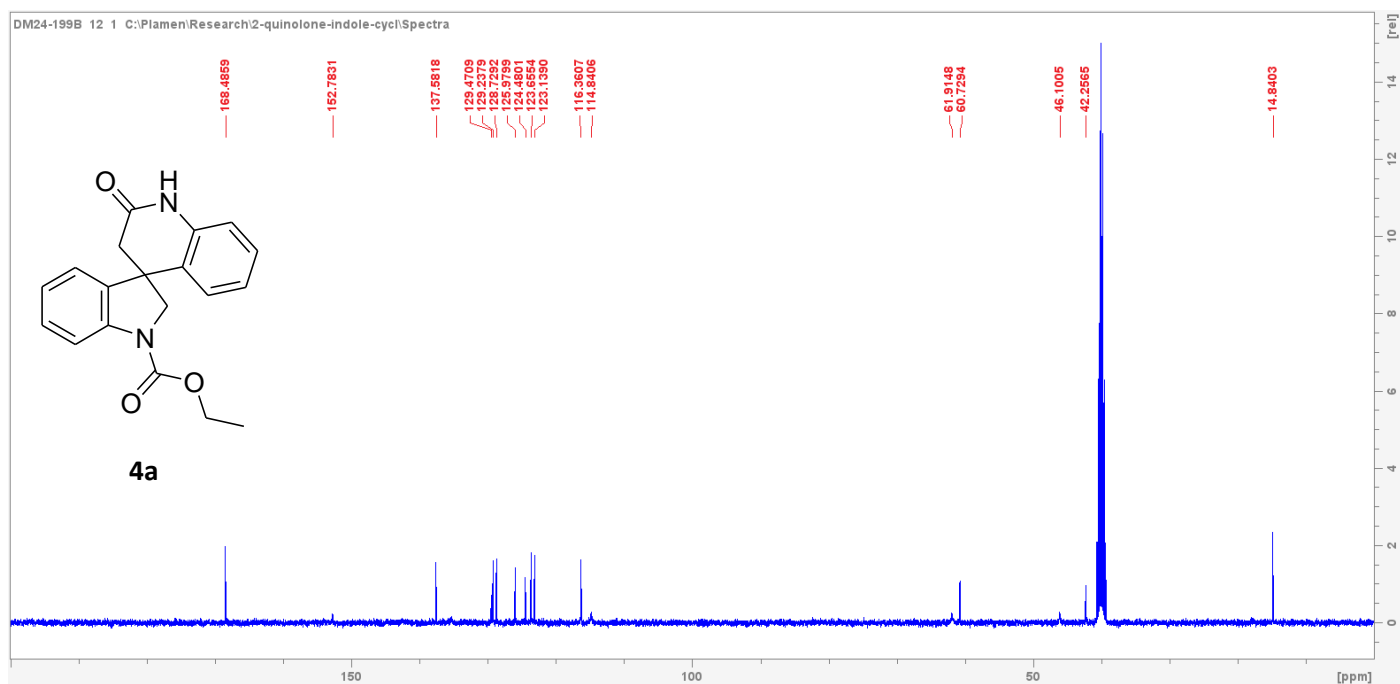
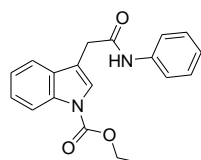


Figure S8. ^{13}C NMR spectrum of Ethyl 2'-oxo-2',3'-dihydro-1'H-spiro[indole-3,4'-quinoline]-1(2H)-carboxylate (**4a**)



Figure S9. ^1H COSY NMR spectrum of 3-Phenylcarbamoylmethylindole-1-carboxylic acid ethyl ester (**2a**)



2a

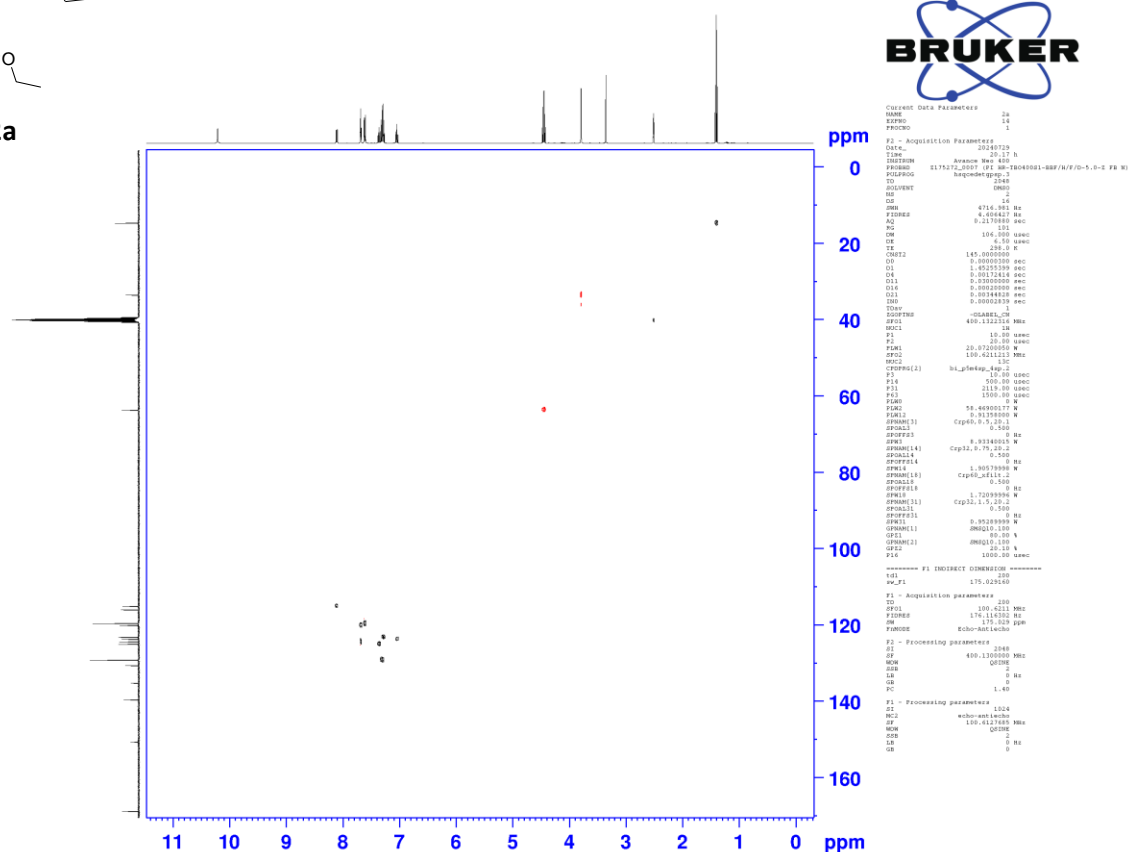
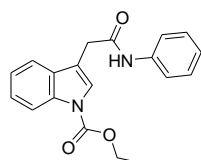


Figure S10. HSQC spectrum of 3-Phenylcarbamoylmethylindole-1-carboxylic acid ethyl ester (2a)



2a

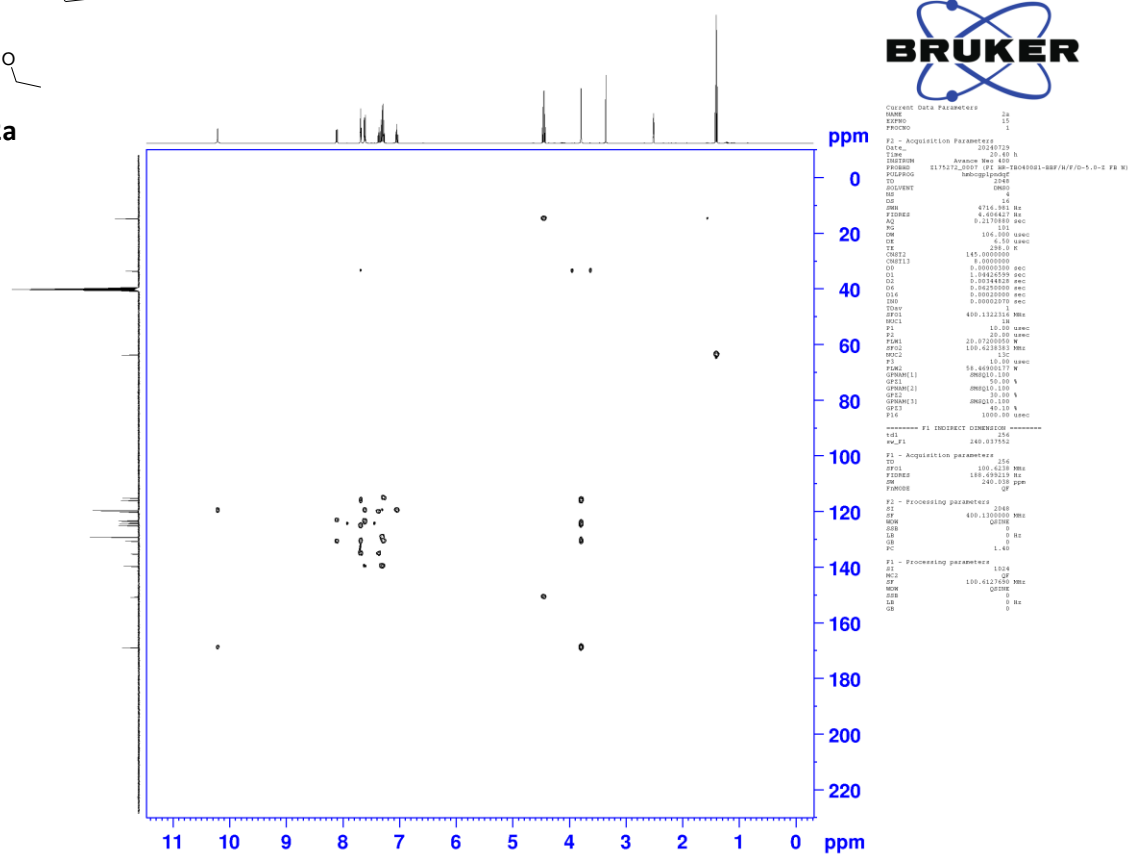


Figure S11. HMBC spectrum of 3-Phenylcarbamoylmethylindole-1-carboxylic acid ethyl ester (2a)



Figure S12. ^1H COSY NMR spectrum of (2-Oxo-1,2-dihydroquinolin-4-ylmethyl)-phenylcarbamic acid ethyl ester (**3a**)

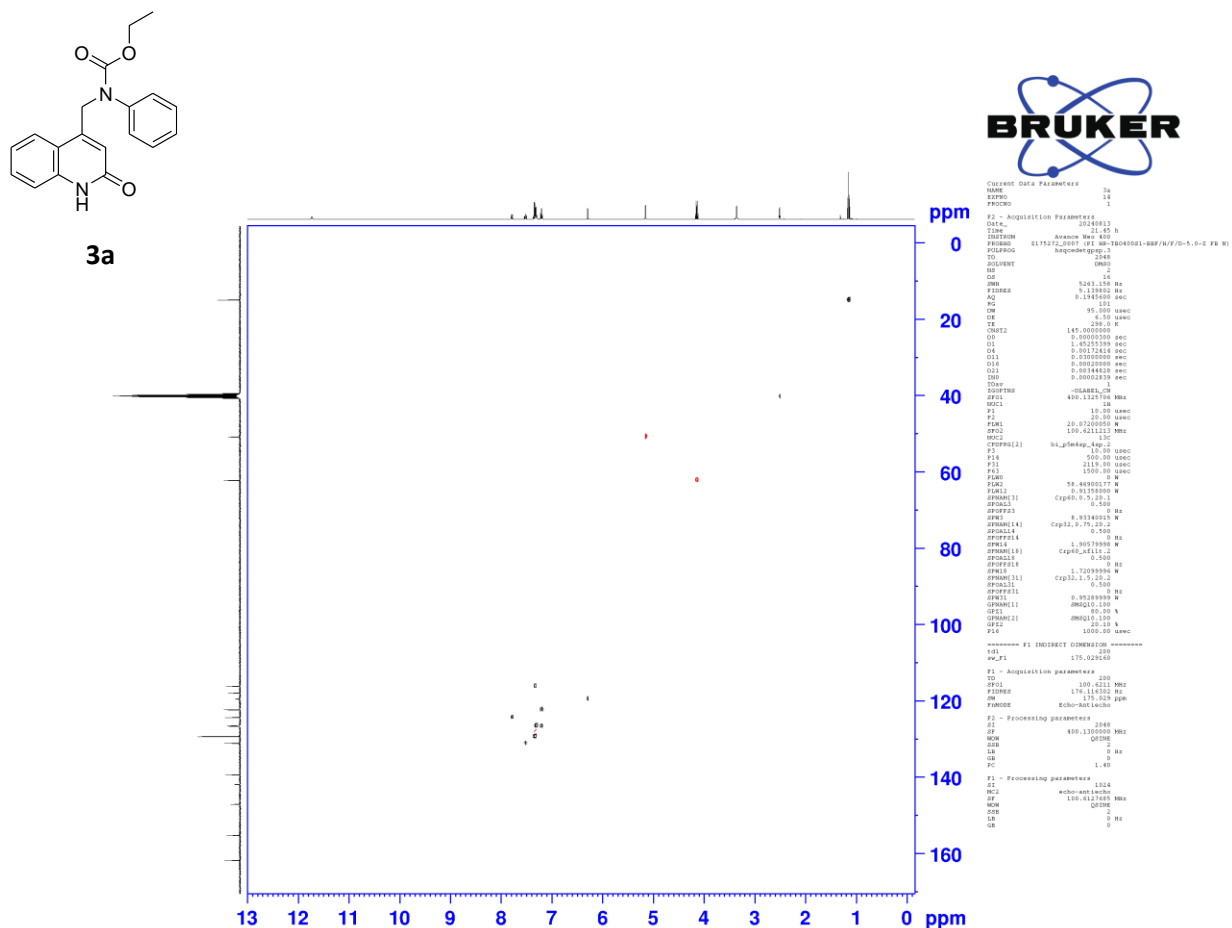
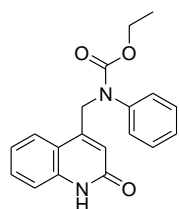


Figure S13. HSQC spectrum of (2-Oxo-1,2-dihydroquinolin-4-ylmethyl)-phenylcarbamic acid ethyl ester (**3a**)



3a

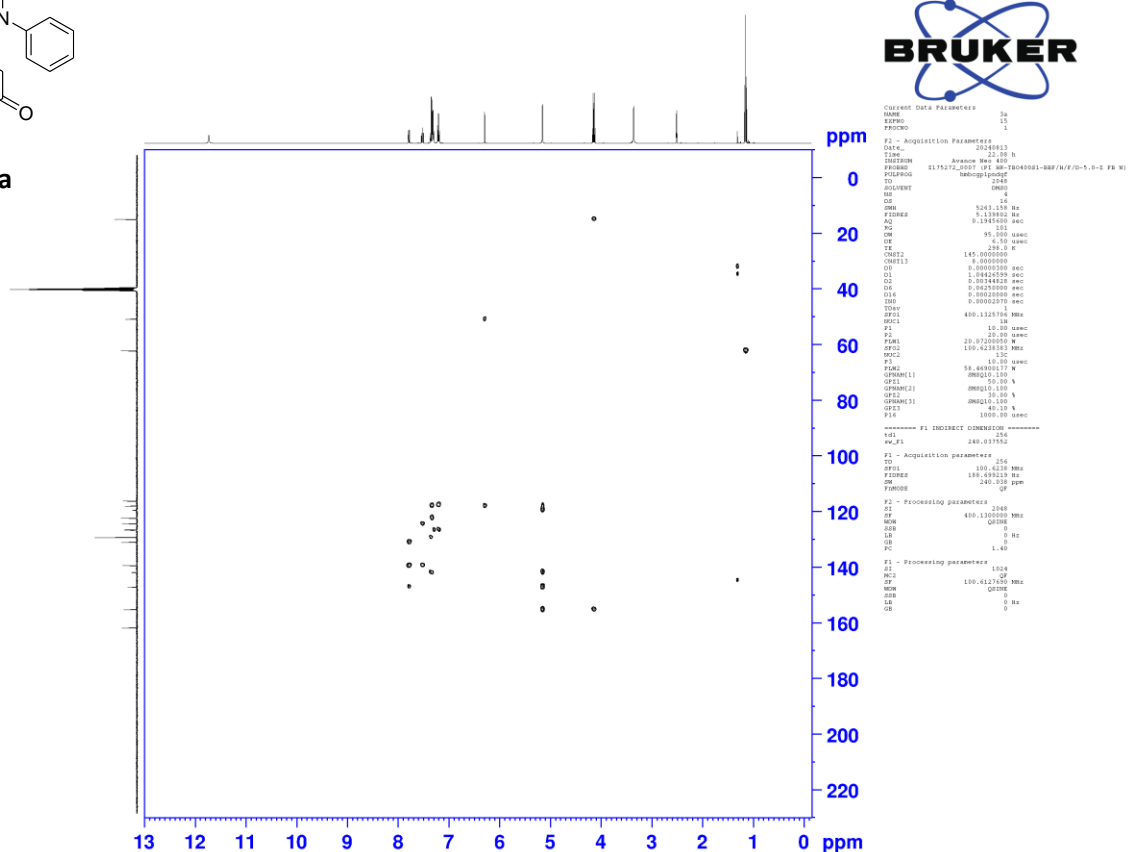


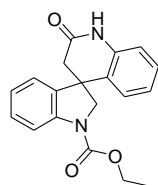
Figure S14. HMBC spectrum of (2-Oxo-1,2-dihydroquinolin-4-ylmethyl)-phenylcarbamic acid ethyl ester (**3a**)



Figure S15. ^1H COSY NMR spectrum of Ethyl 2'-oxo-2',3'-dihydro-1'H-spiro[indole-3,4'-quinoline]-1(2H)-carboxylate (**4a**)



Figure S16. HSQC spectrum of Ethyl 2'-oxo-2',3'-dihydro-1'H-spiro[indole-3,4'-quinoline]-1(2H)-carboxylate (**4a**)



4a

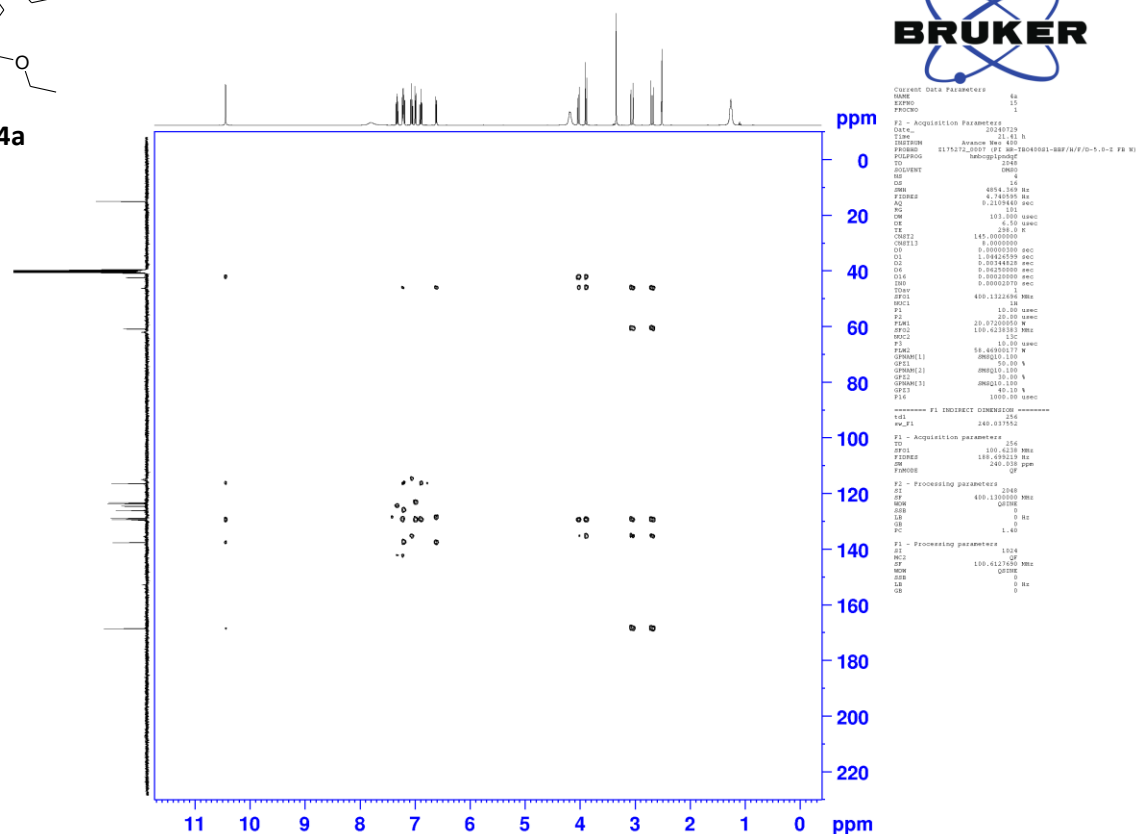


Figure S17. HMBC spectrum of Ethyl 2'-oxo-2',3'-dihydro-1'H-spiro[indole-3,4'-quinoline]-1(2H)-carboxylate (4a)

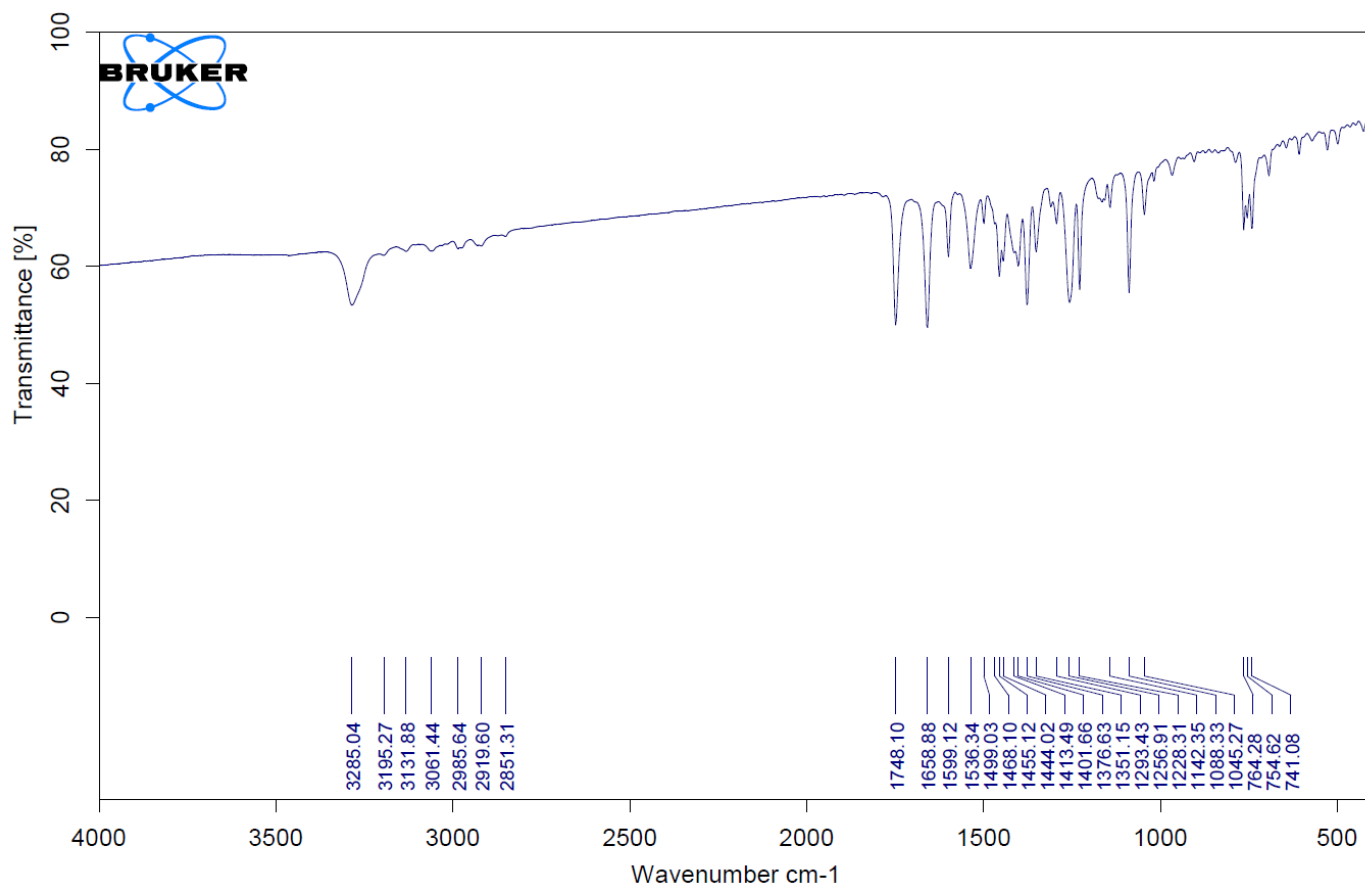


Figure S18. IR spectrum (KBr pellet) of 3-Phenylcarbamoylmethylindole-1-carboxylic acid ethyl ester (2a)

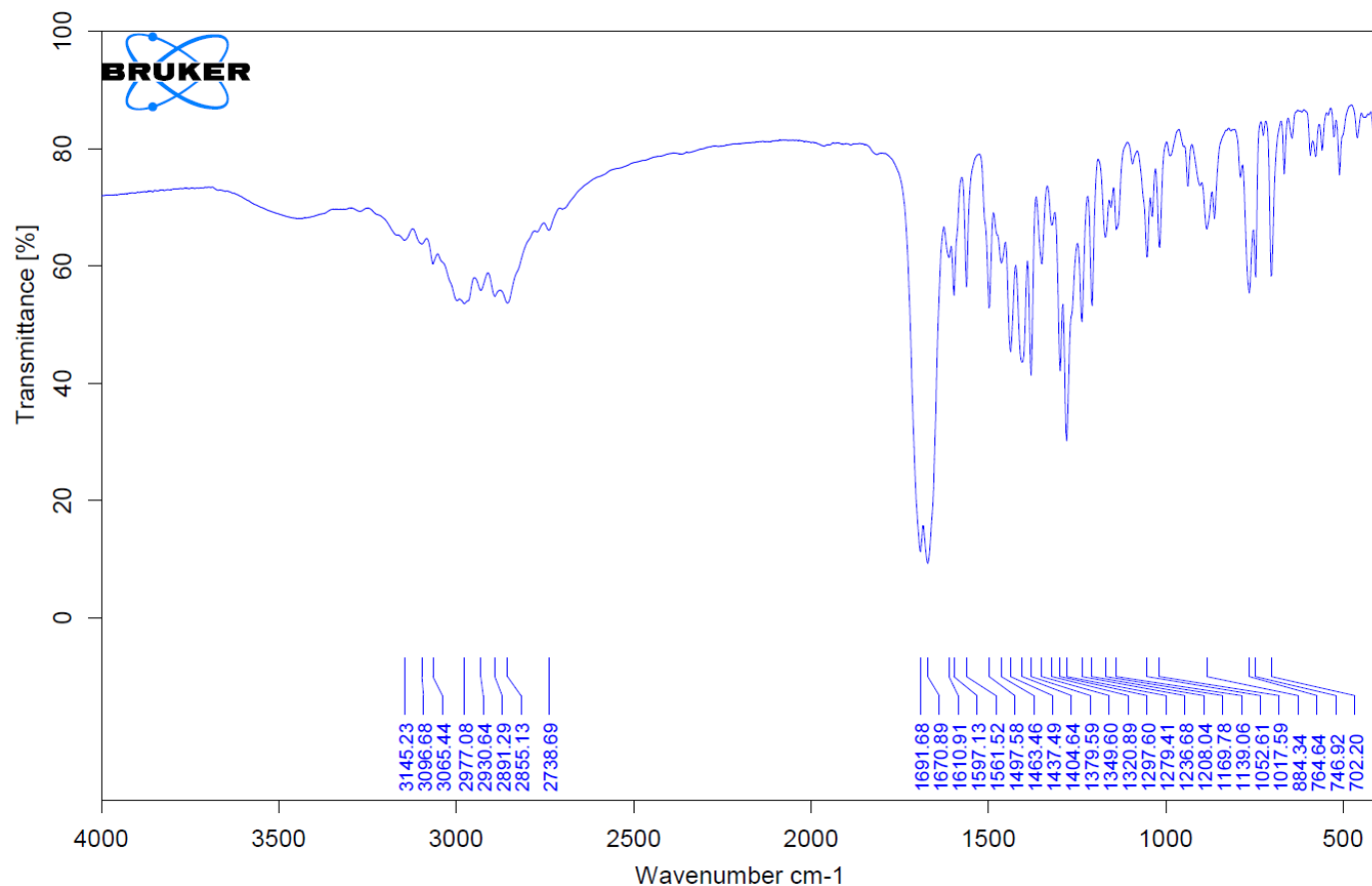


Figure S19. IR spectrum (KBr pellet) of (2-Oxo-1,2-dihydroquinolin-4-ylmethyl)-phenylcarbamic acid ethyl ester (**3a**)

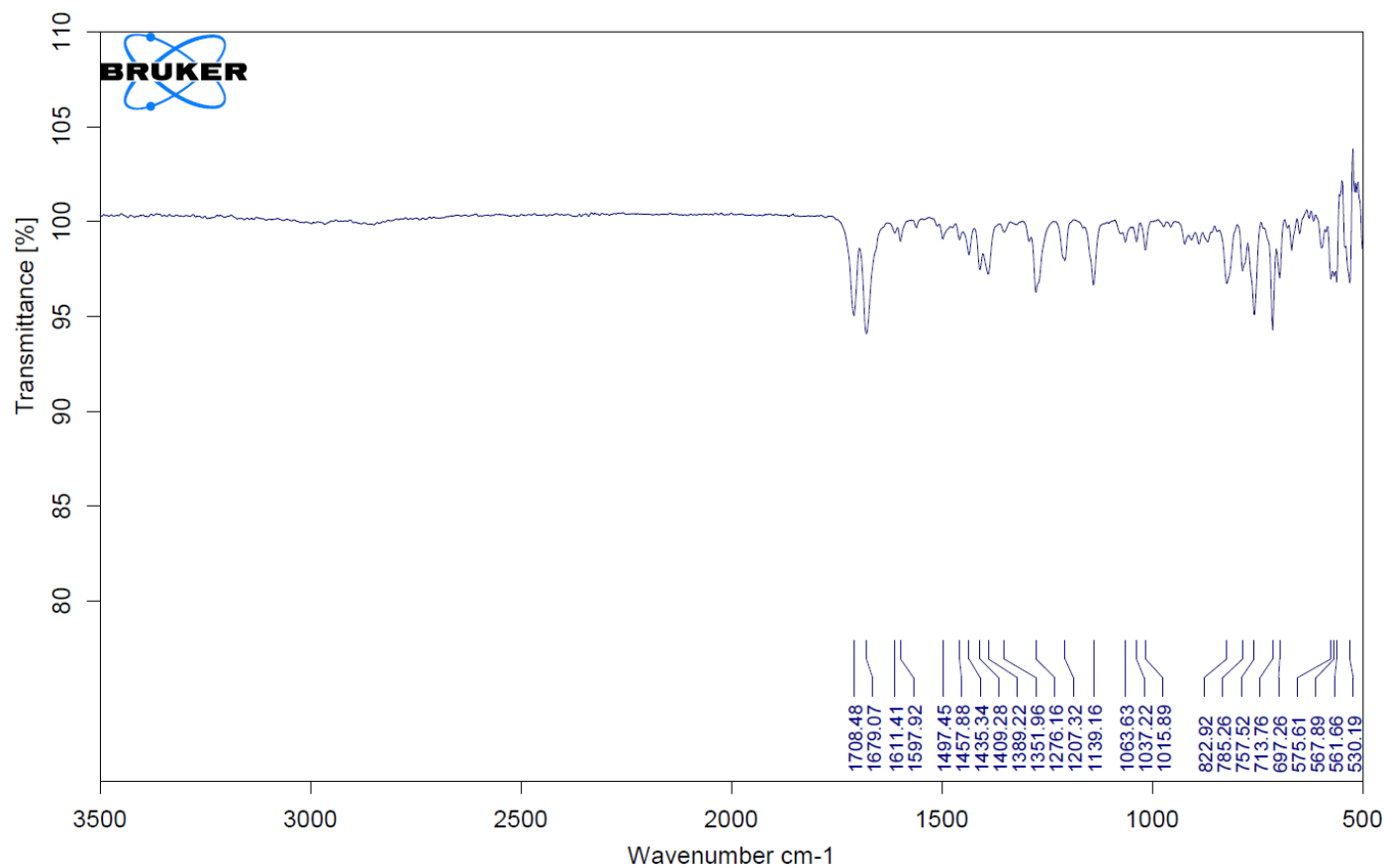


Figure S20. IR spectrum (ATR Ge) of (2-Oxo-1,2-dihydroquinolin-4-ylmethyl)-phenylcarbamic acid 2,2,2-trichloroethyl ester (**3b**)

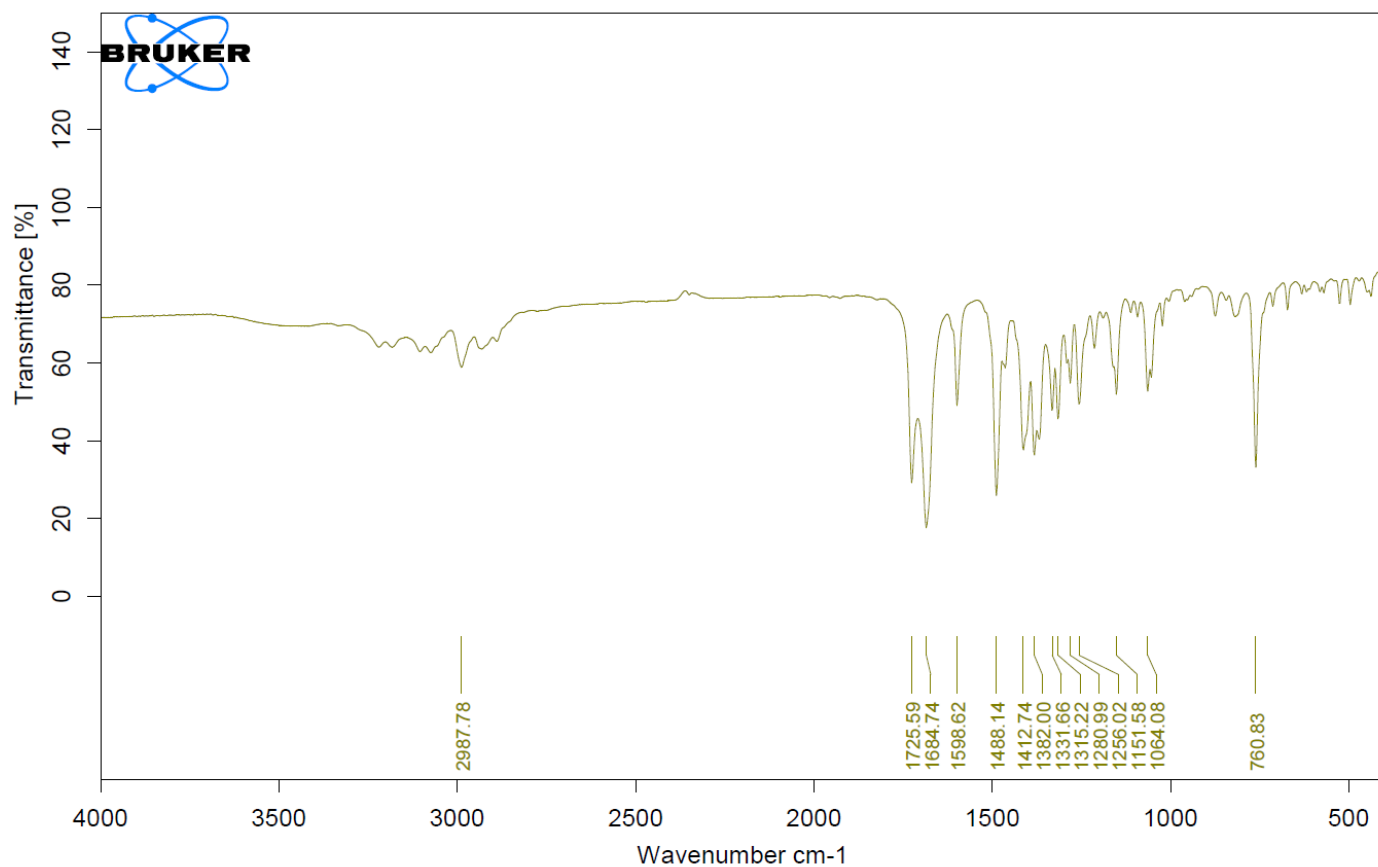


Figure S21. IR spectrum (KBr pellet) of Ethyl 2'-oxo-2',3'-dihydro-1'H-spiro[indole-3,4'-quinoline]-1(2H)-carboxylate (**4a**)