Supplementary Materials

Synthesis of 3-Acyl-4-quinolones via Reductive Ring Transformation of 4-(2-Nitrobenzoyl)isoxazoles

Pavlos Pelagias, Jan P. Sandler and Franz Bracher *

Department of Pharmacy, Center for Drug Research, Ludwig-Maximilians University, Munich 81377, Germany

* Correspondence: franz.bracher@cup.lmu.de

1. 2D NMR Spectra of Compounds 14a and 14b

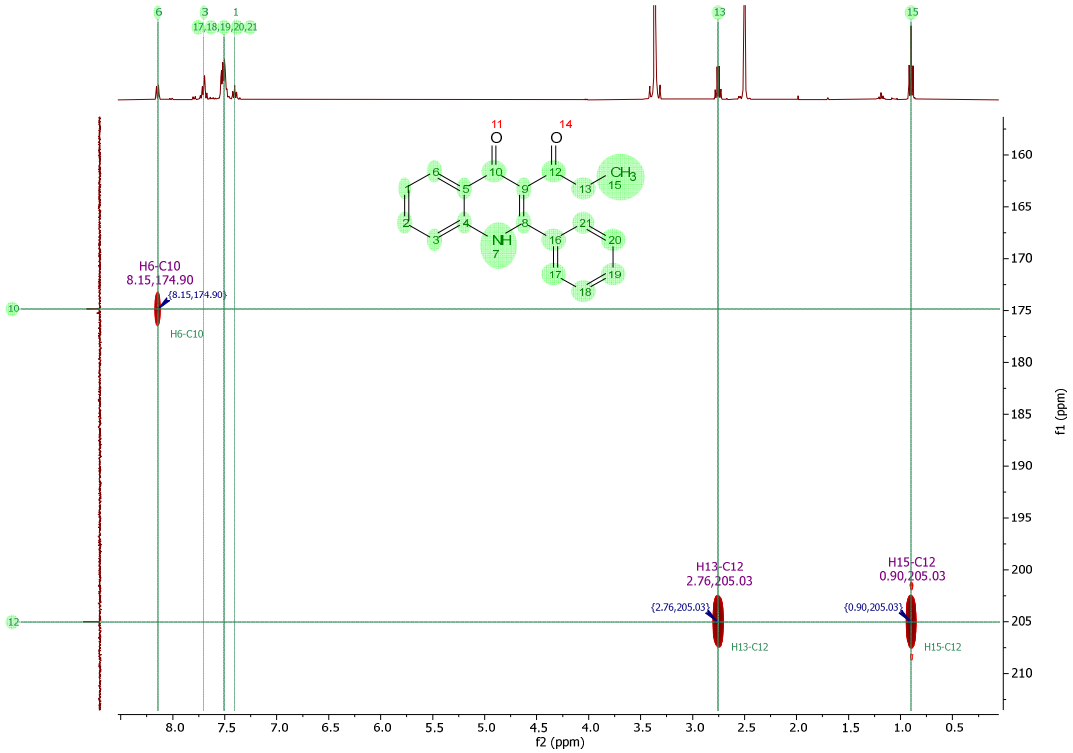


Figure S1. Key HMBC correlations (DMSO-d_6, 400 MHz) observed for **14a**. Cross-peaks confirm long-range couplings between the methylene (H13) and methyl (H15) protons of the ethyl group and the ketone carbon (C12, δ 205.0 ppm). Atom numbering above follows MestReNova software and does not reflect formal IUPAC conventions.

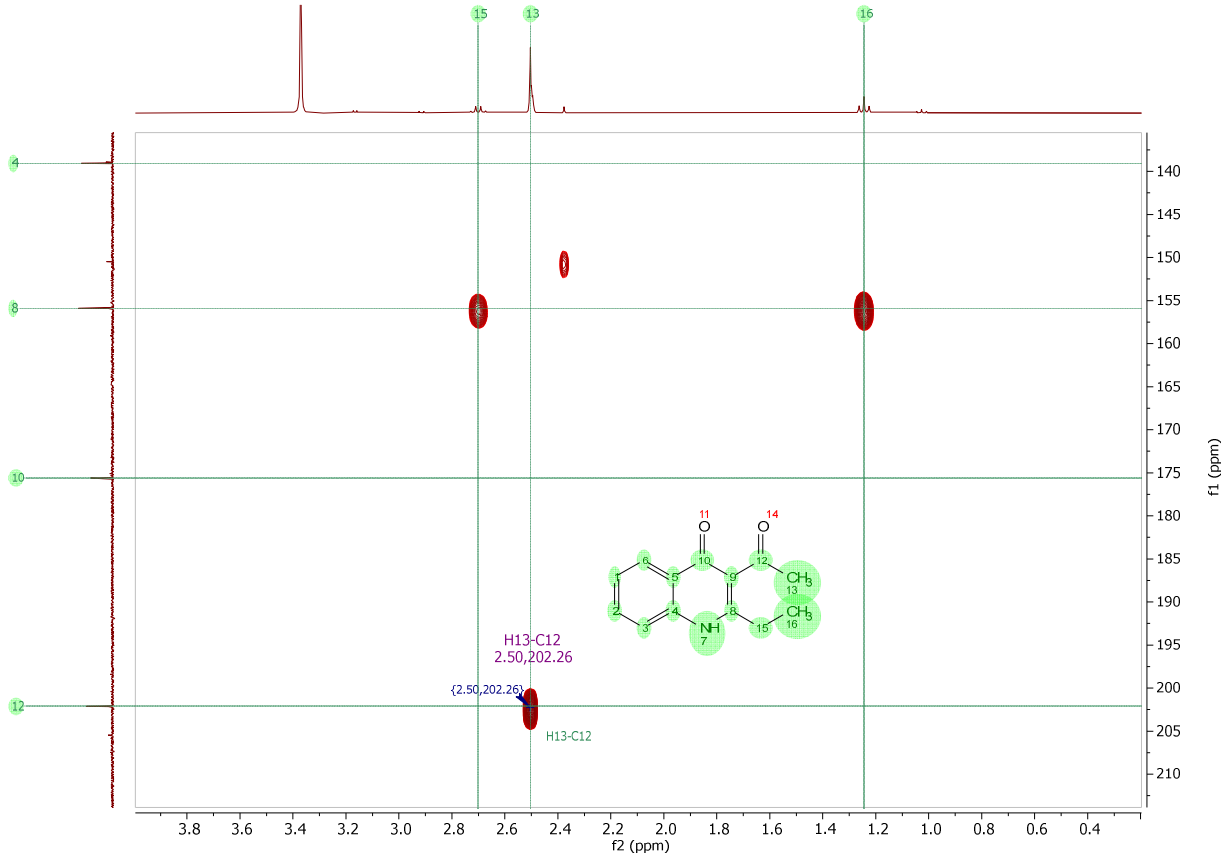


Figure S2. HMBC spectrum of **14b** (DMSO-d_6, 400 MHz, 2D HMBC). A key cross-peak is observed between the methyl singlet at δ 2.50 ppm (H13) and the carbonyl carbon at δ 202.3 ppm (C12), confirming the methyl group's direct attachment to the carbonyl group, forming an acetyl fragment at C9. Atom numbering follows the MestReNova assignment scheme and does not reflect formal IUPAC nomenclature. In IUPAC terms, the acetyl group at C9 is located at position 3 and the ketone carbon C10 is position 4 of the quinolone scaffold.

2. NMR spectra of novel compounds

Chemical shifts of solvent peaks are indicated in red.

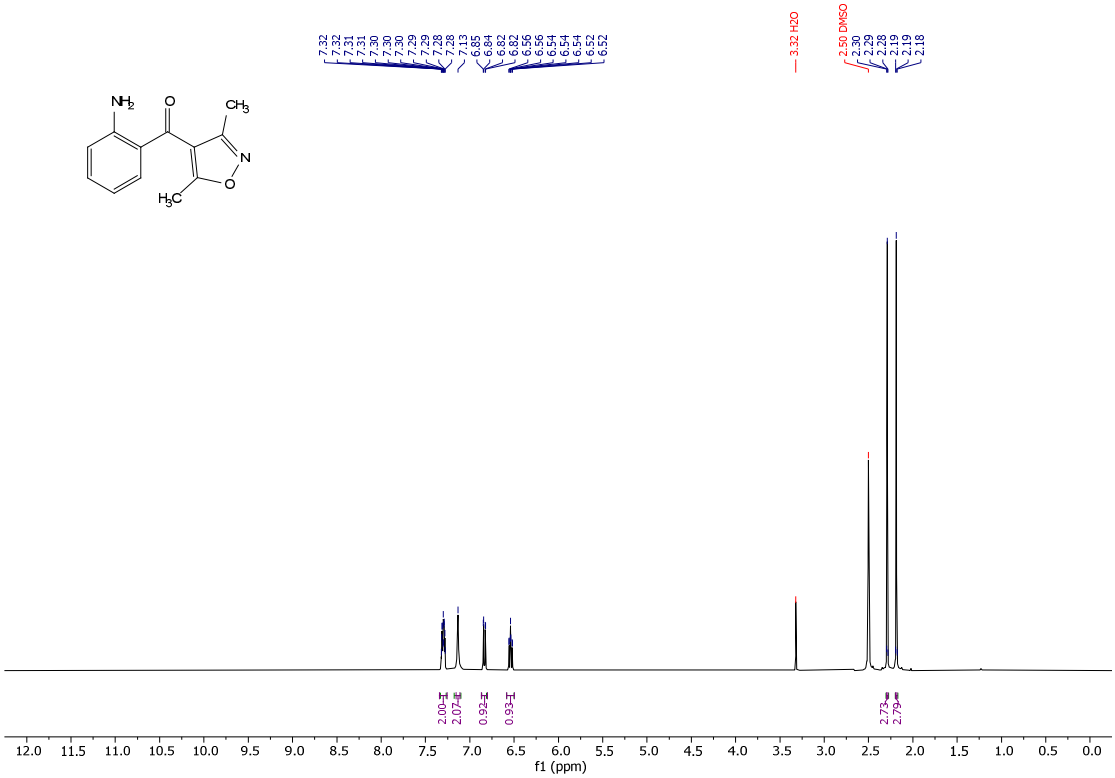


Figure S3A. ¹H NMR spectrum of (2-aminophenyl)(3,5-dimethylisoxazol-4-yl)methanone (**8**) in DMSO-d_6.

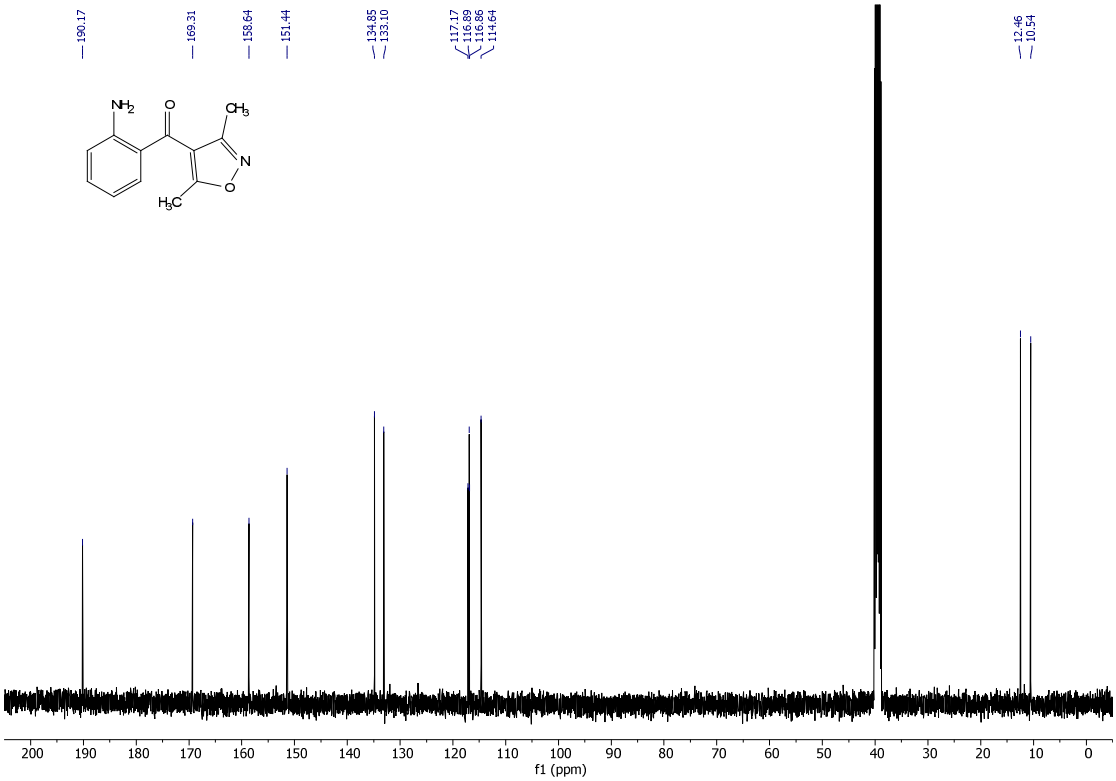


Figure S3B. *¹C NMR spectrum of (2-aminophenyl)(3,5-dimethylisoxazol-4-yl)methanone (**8**) in DMSO-d_6.*

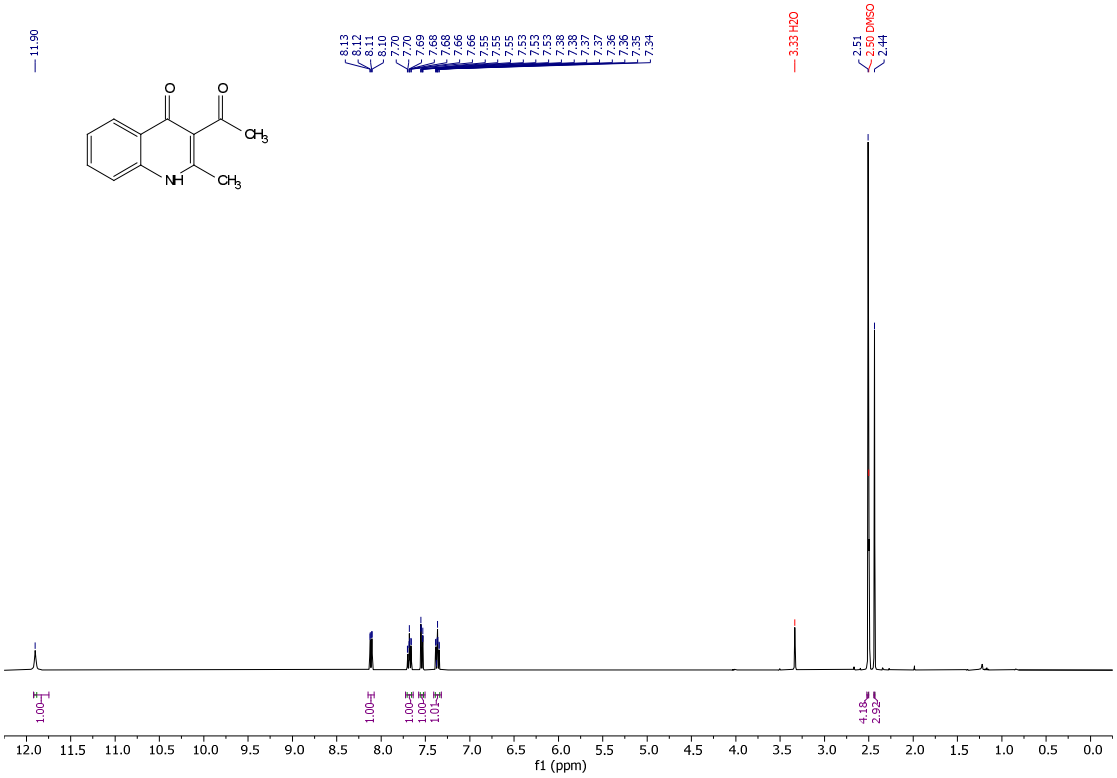


Figure S4A. *[1] H NMR spectrum of 1-(2-methyl-1,4-dihydroquinolin-3-yl)ethan-1-one (**5**) in DMSO-d6.*

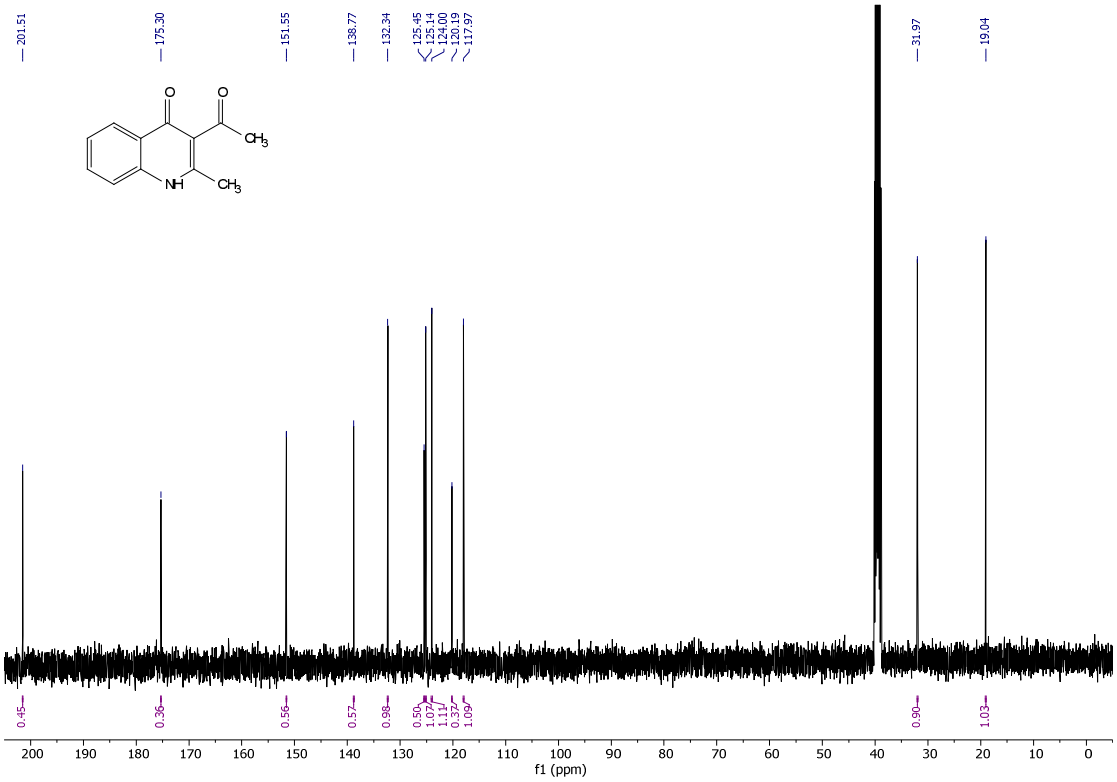


Figure S4B. *[13] C NMR spectrum of 1-(2-methyl-1,4-dihydroquinolin-3-yl)ethan-1-one (**5**) in DMSO-d6.*

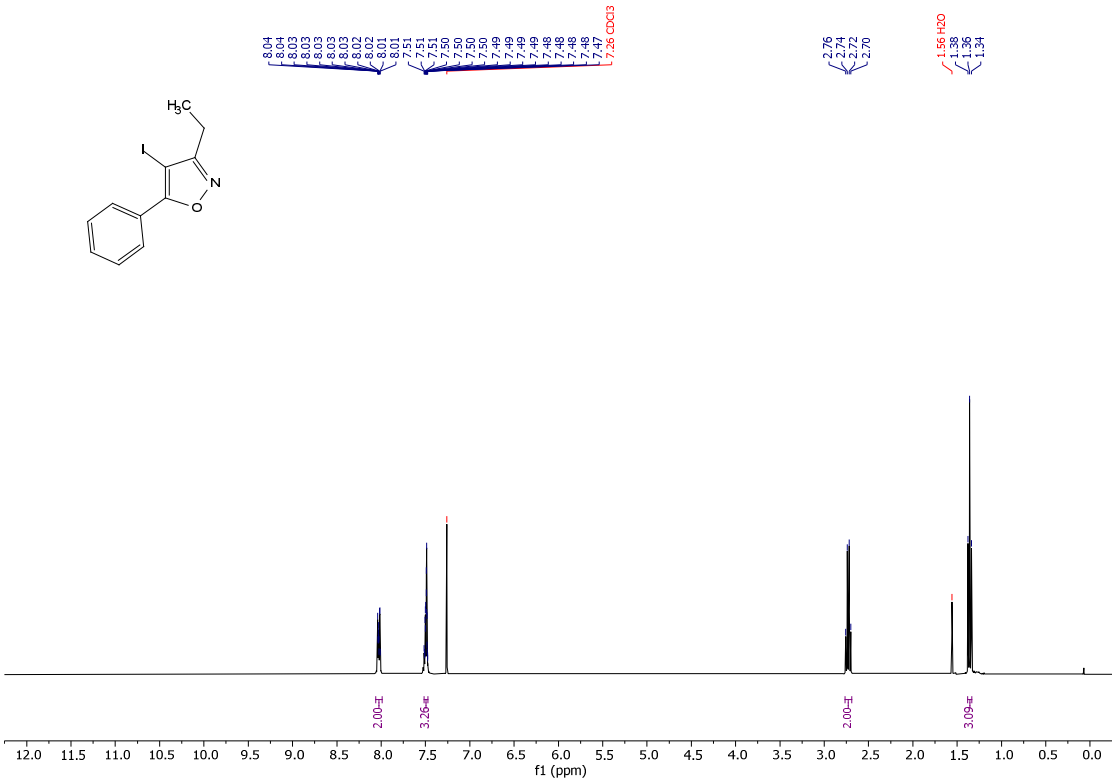


Figure S5A. *^{1}H NMR spectrum of 3-ethyl-4-iodo-5-phenylisoxazole (**10**) in $CDCl_3$.*

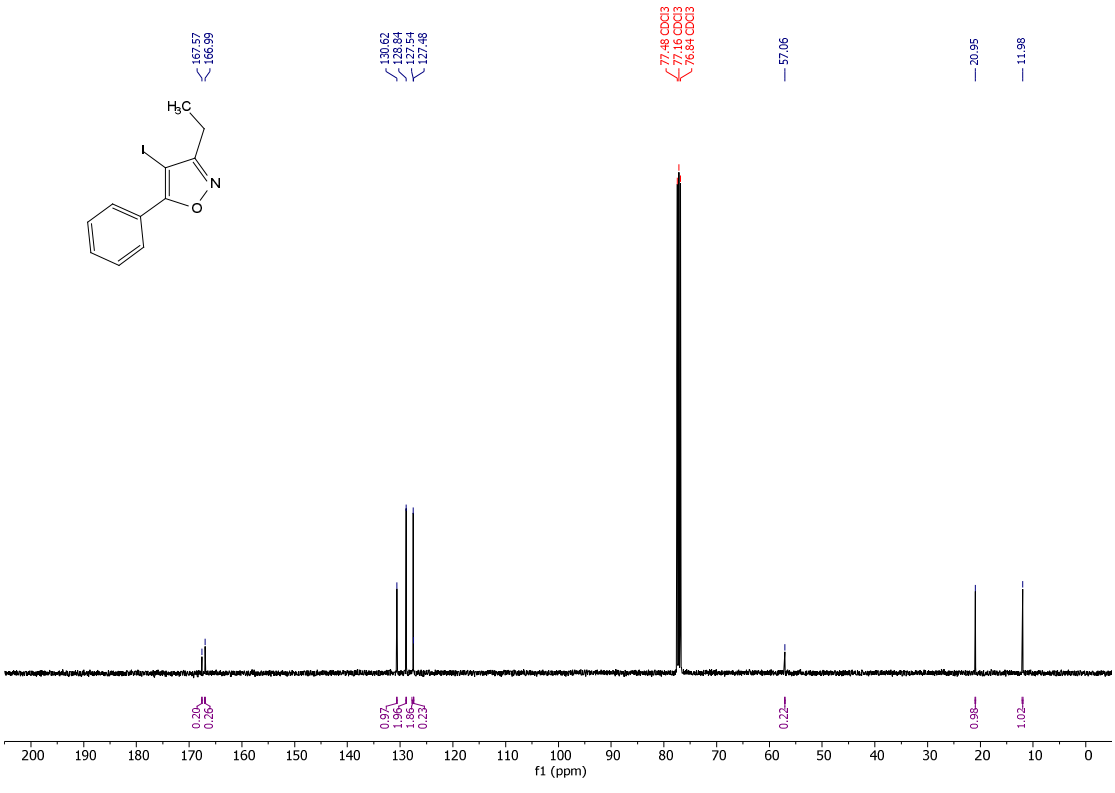


Figure S5B. *^{13}C NMR spectrum of 3-ethyl-4-iodo-5-phenylisoxazole (**10**) in $CDCl_3$.*

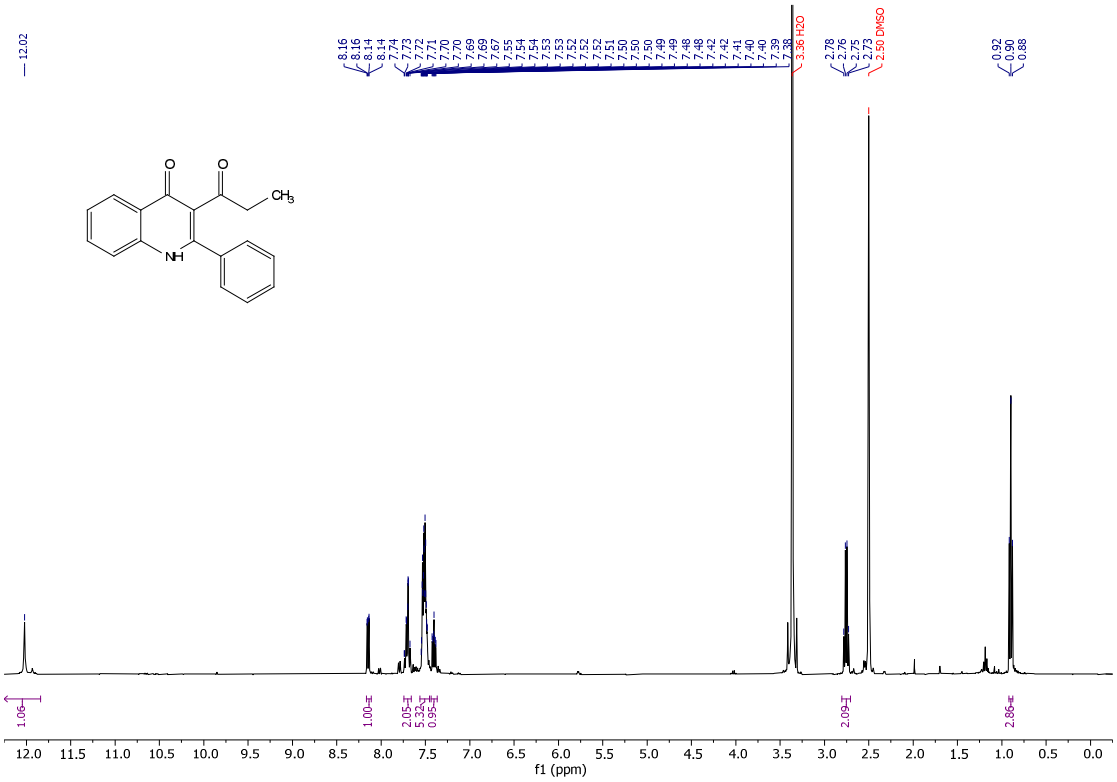


Figure S6A. *^{1}H NMR spectrum of 2-phenyl-3-propionylquinolin-4(1H)-one (**9**) in DMSO-d_6.*

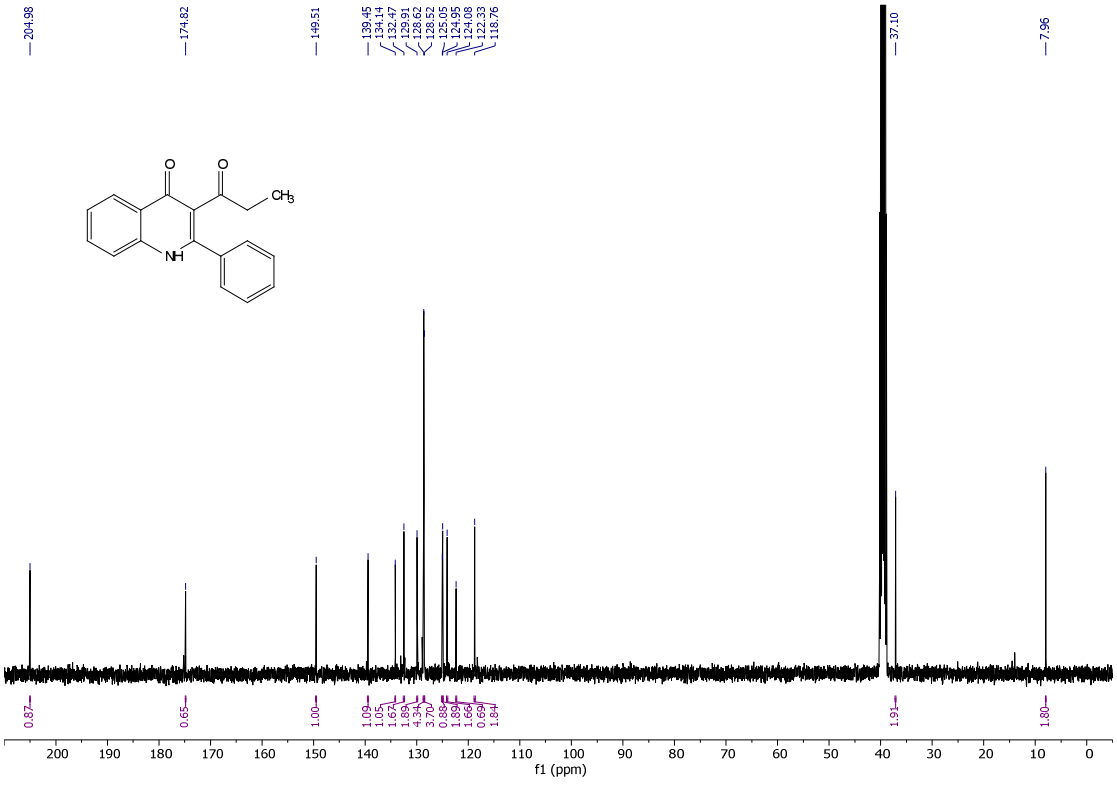


Figure S6B. *^{13}C NMR spectrum of 2-phenyl-3-propionylquinolin-4(1H)-one (**9**) in DMSO-d_6.*

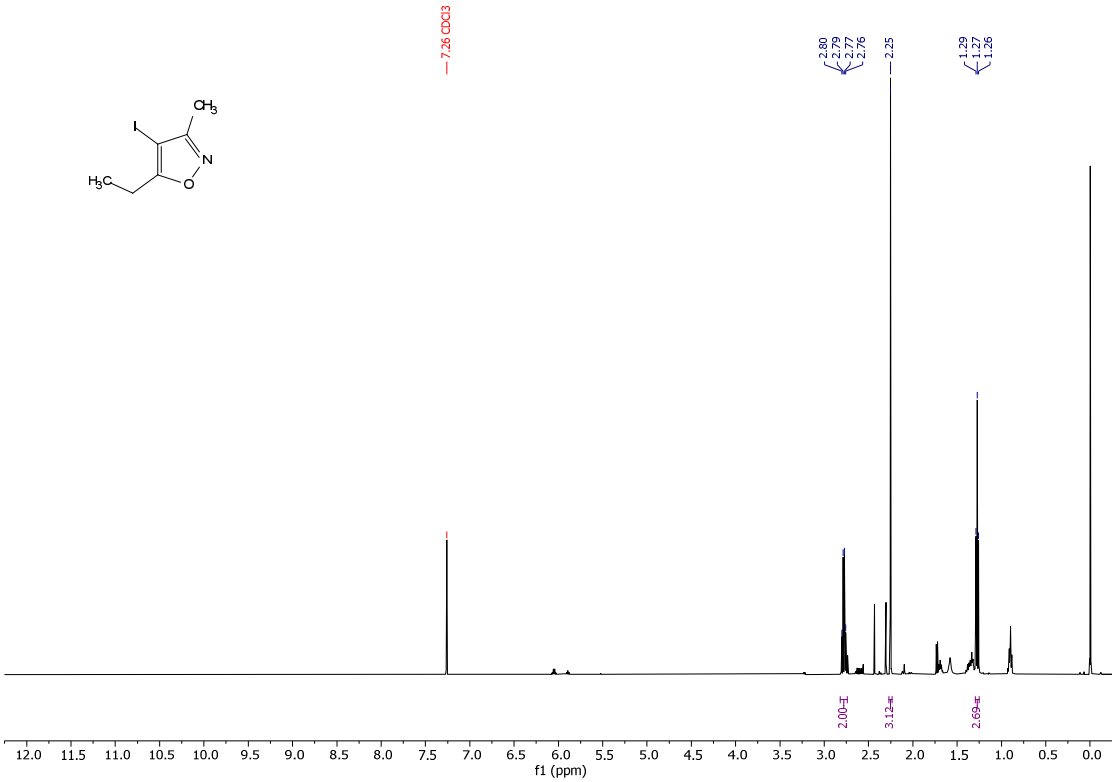


Figure S7A. *^{1}H MMR spectrum of 5-ethyl-4-iodo-3-methylisoxazole (**11b**) in $CDCl_3$.*

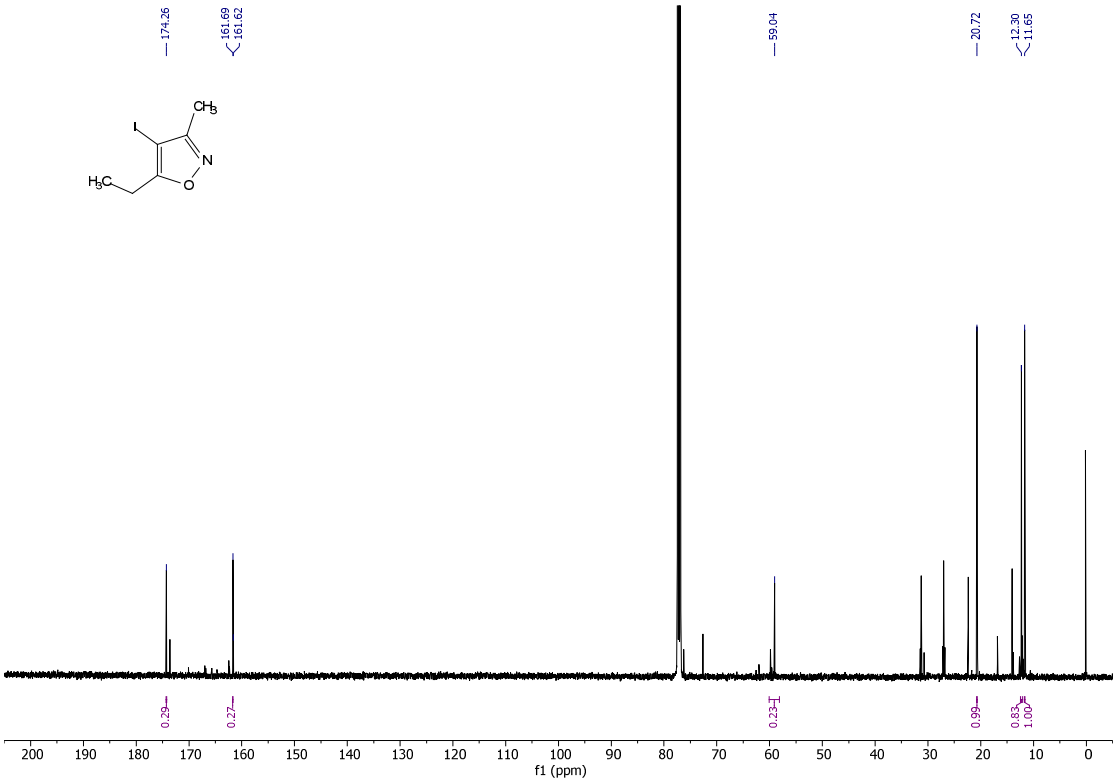


Figure S7B. *^{13}C MMR spectrum of 5-ethyl-4-iodo-3-methylisoxazole (**11b**) in $CDCl_3$.*

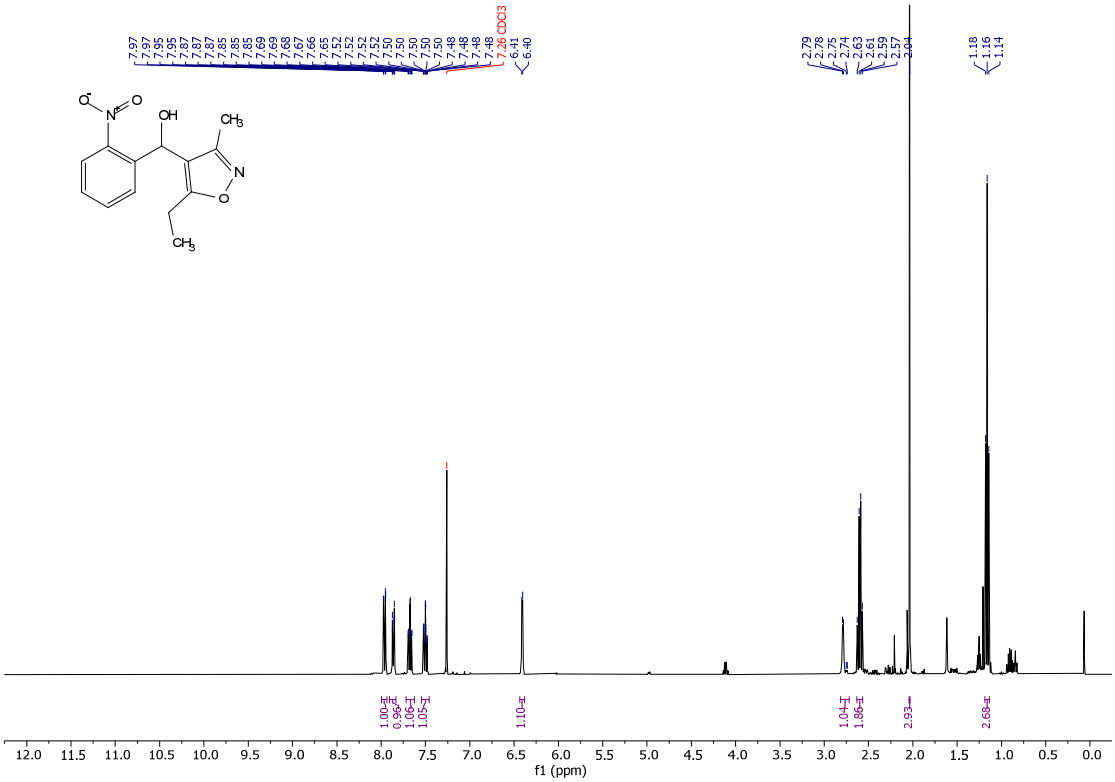


Figure S*8A*. *^{1}H NMR spectrum of (5-ethyl-3-methylisoxazol-4-yl)(2-nitrophenyl)methanol (**12b**) in $CDCl_3$.*

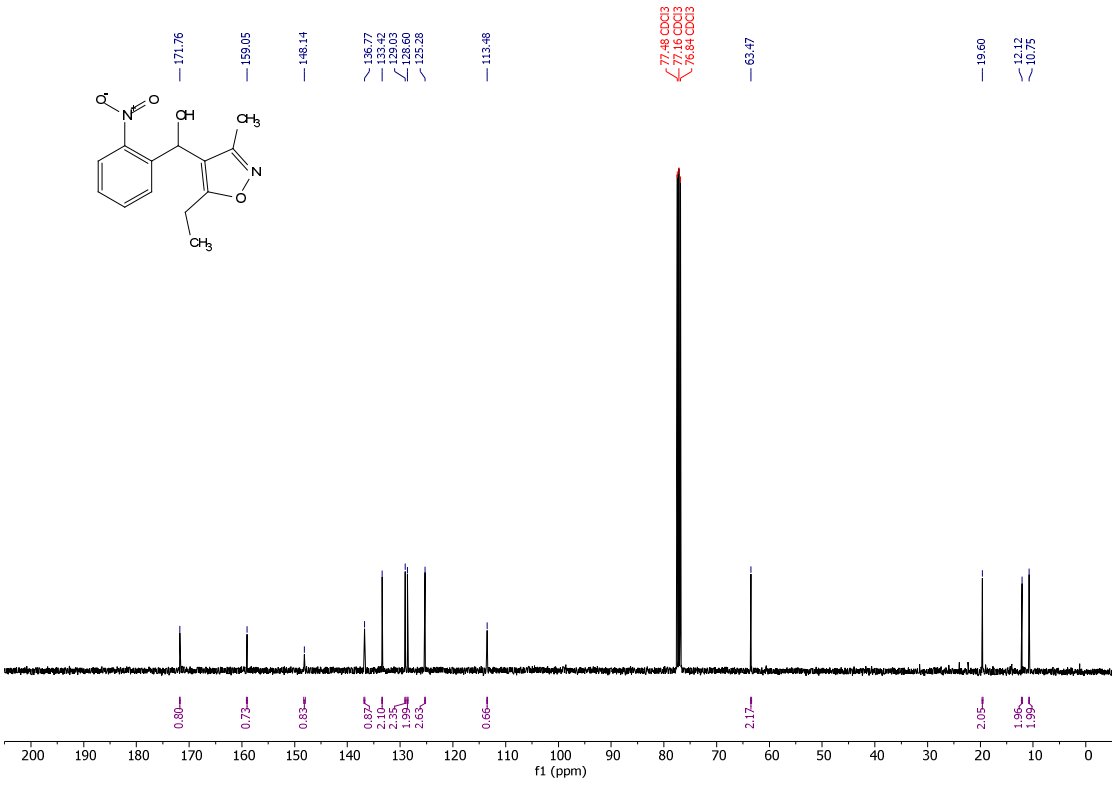


Figure S8B. *^{13}C NMR spectrum of (5-ethyl-3-methylisoxazol-4-yl)(2-nitrophenyl)methanol (**12b**) in $CDCl_3$.*

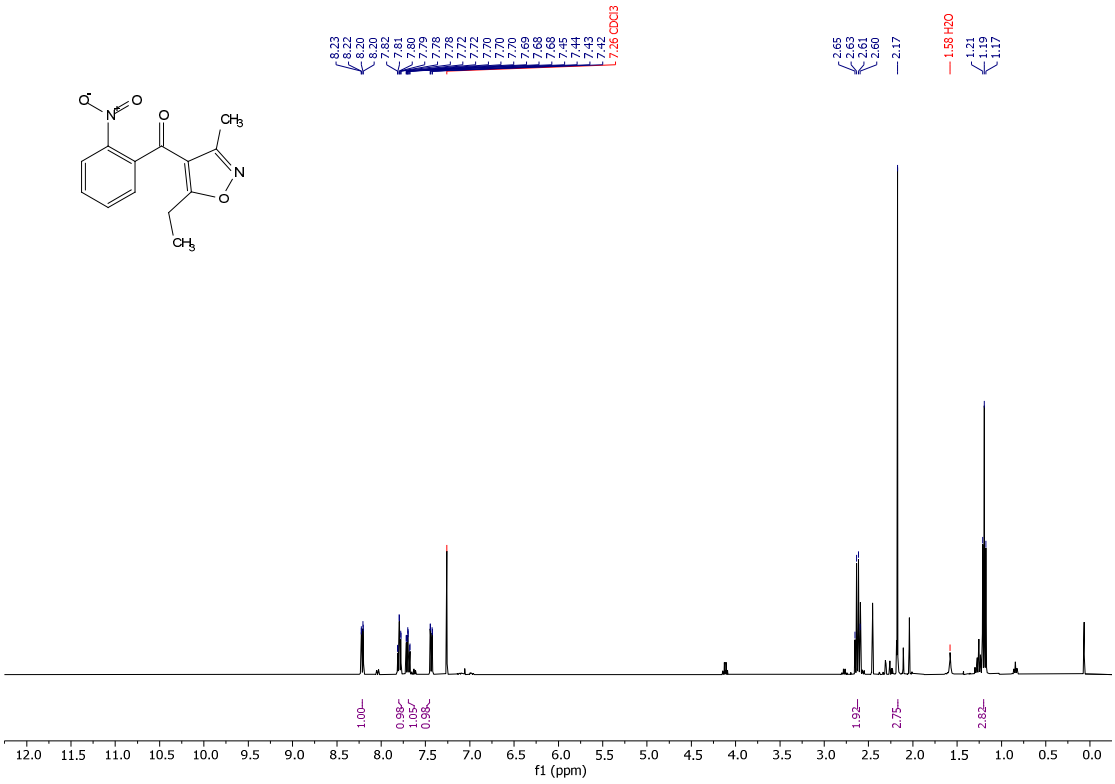


Figure S9A. *¹H NMR spectrum of (5-ethyl-3-methylisoxazol-4-yl)(2-nitrophenyl)methanone (**13b**) in $CDCl_3$.*

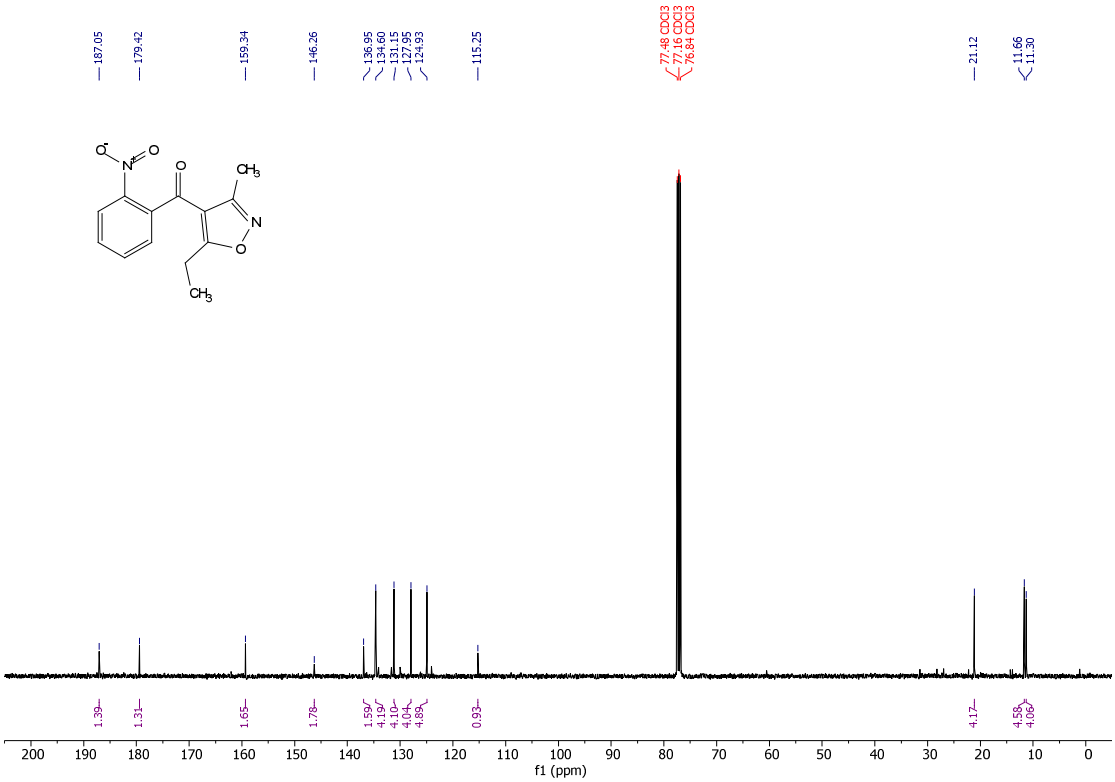


Figure S9B. *¹³C NMR spectrum of (5-ethyl-3-methylisoxazol-4-yl)(2-nitrophenyl)methanone (**13b**) in $CDCl_3$.*

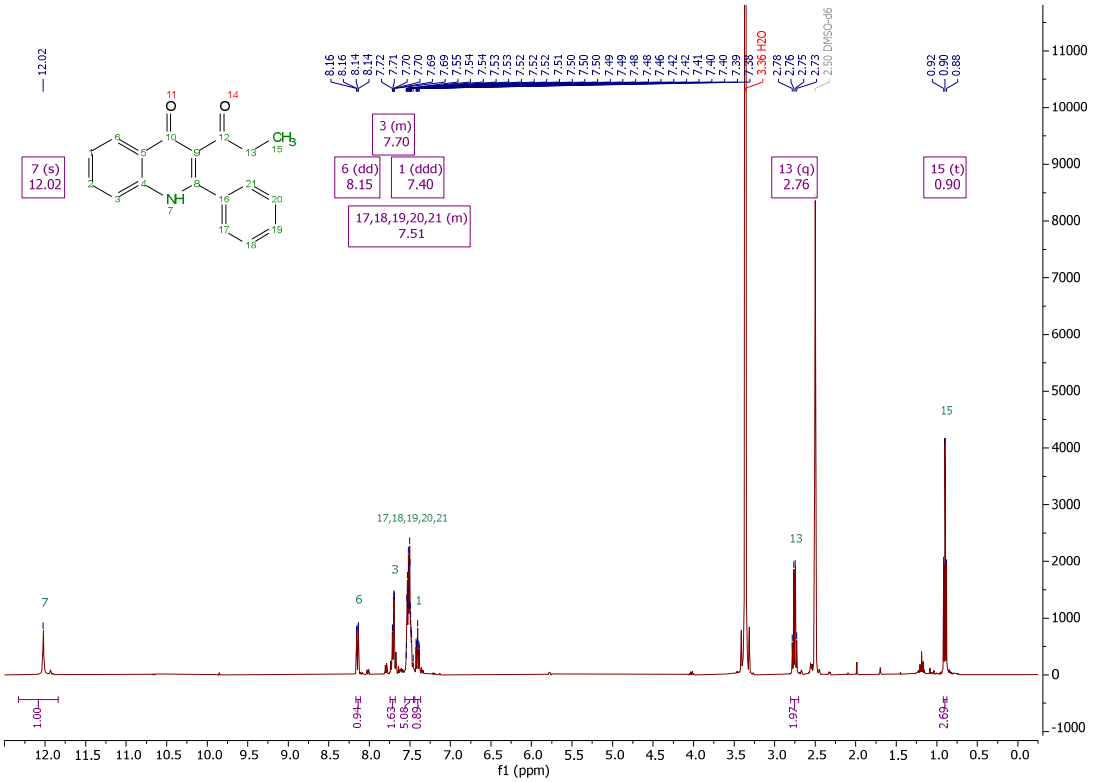


Figure S10A. *^{1}H NMR spectrum of 2-phenyl-3-propionylquinolin-4(1H)-one (**14a**) in DMSO-d_6.*

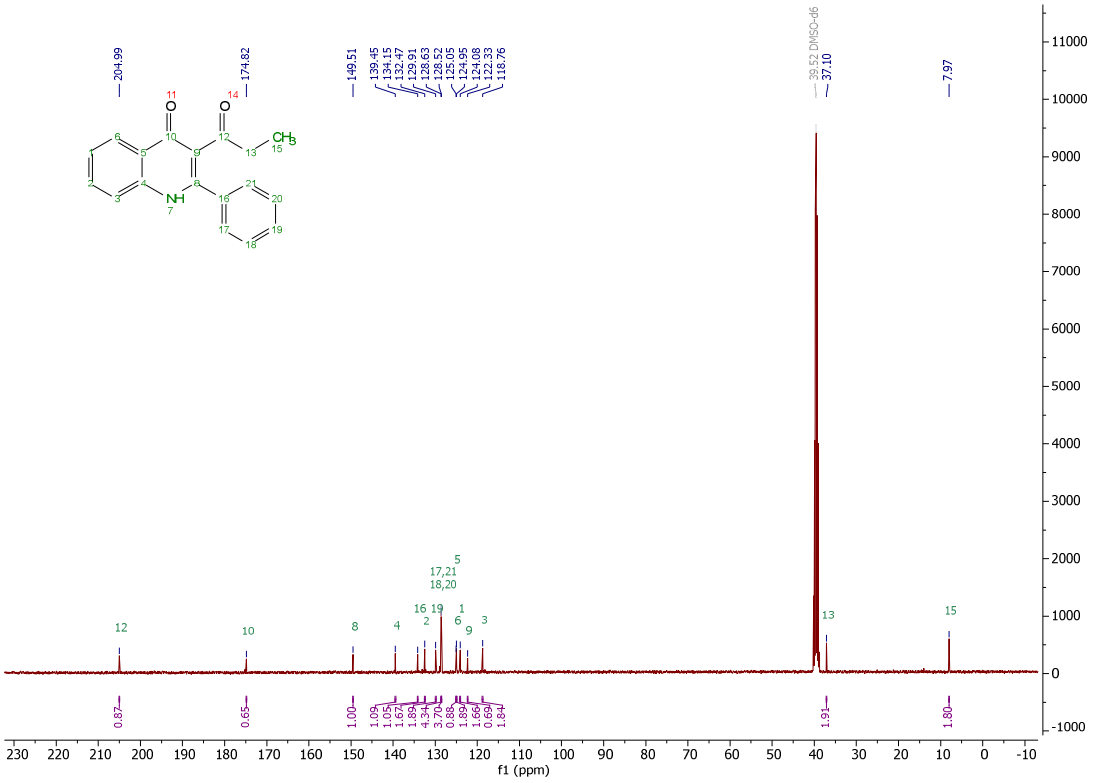


Figure S10B. *^{13}C NMR spectrum of 2-phenyl-3-propionylquinolin-4(1H)-one (**14a**) in DMSO-d_6.*

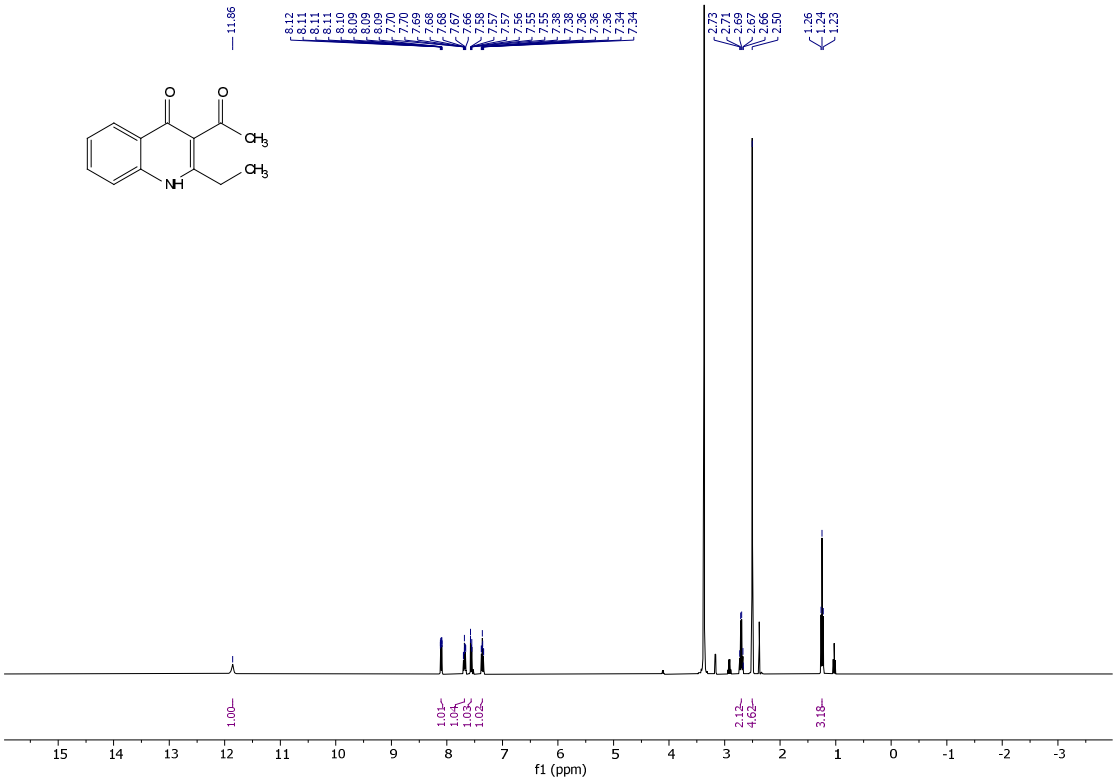


Figure S*11A*. *[1]H NMR spectrum of 3-acetyl-2-ethylquinolin-4(1H)-one (**14b**) in DMSO-d6.*

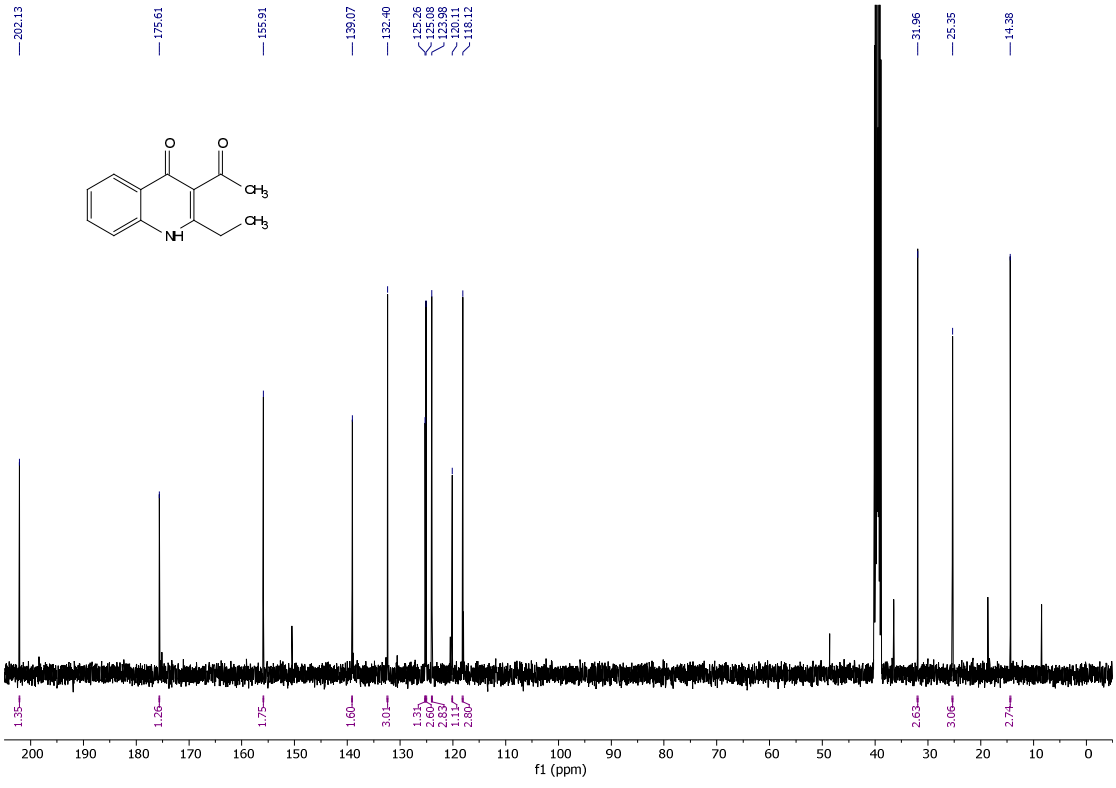


Figure S11B. *[13]C NMR spectrum of 3-acetyl-2-ethylquinolin-4(1H)-one (**14b**) in DMSO-d6.*