

Supporting Information

Synthesis and PASS-Assisted Evaluation of New Heterocyclic Compounds Containing Hydroquinoline Scaffold

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¹H-NMR and ¹³C-MR spectra of the Synthesized Compounds

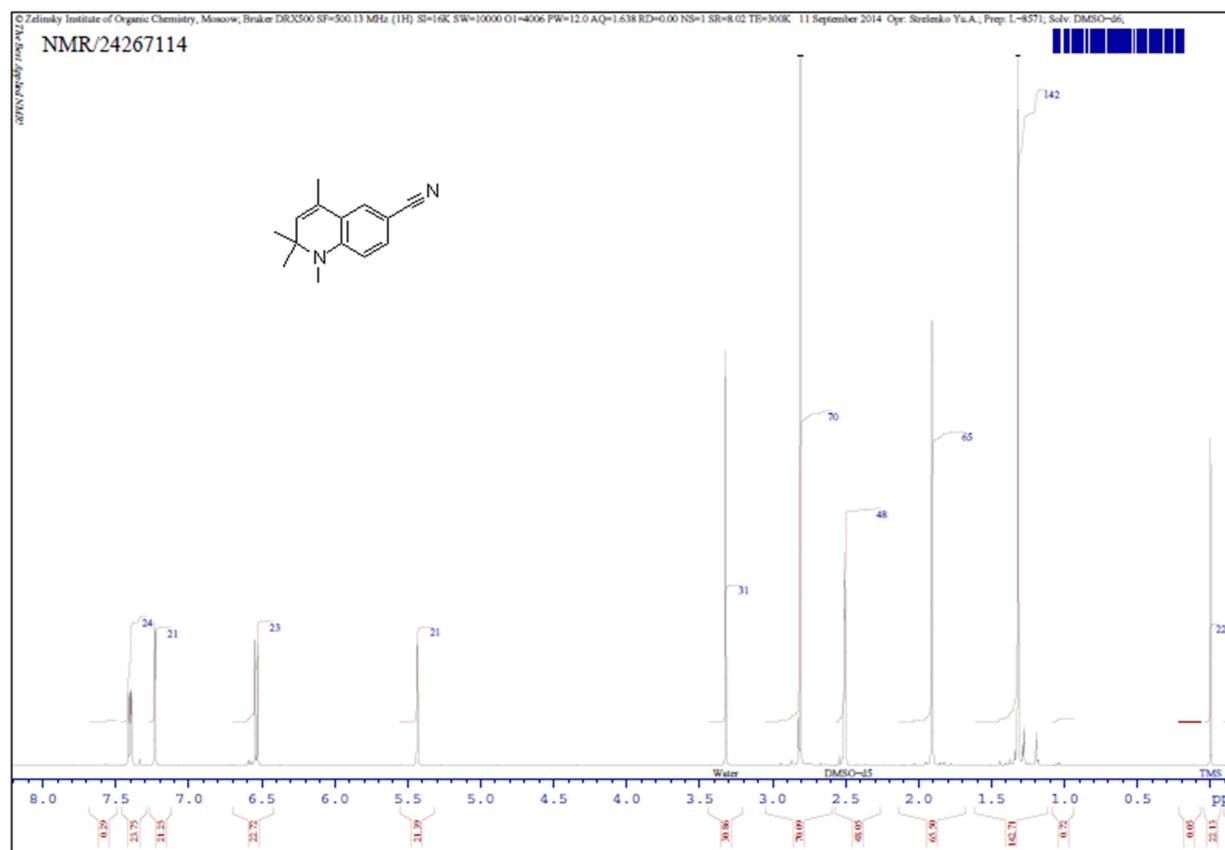


Figure 1. ¹H-NMR spectrum of 1,2,2,4-tetramethyl-1,2-dihydroquinoline-6-carbonitrile 7.

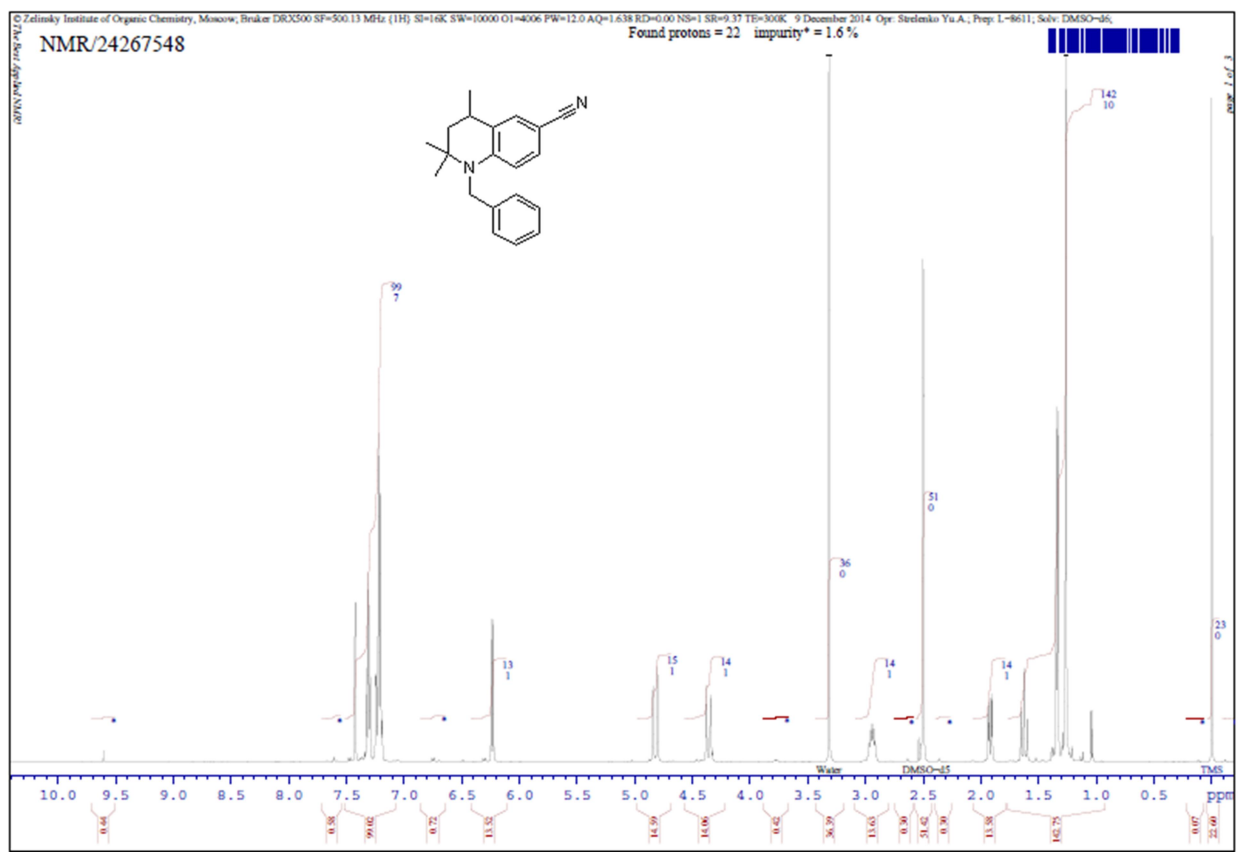


Figure 2. ^1H -NMR spectrum of 1-benzyl-2,2,4-trimethyl-1,2,3,4-tetrahydroquinoline-6-carbonitrile **8**.

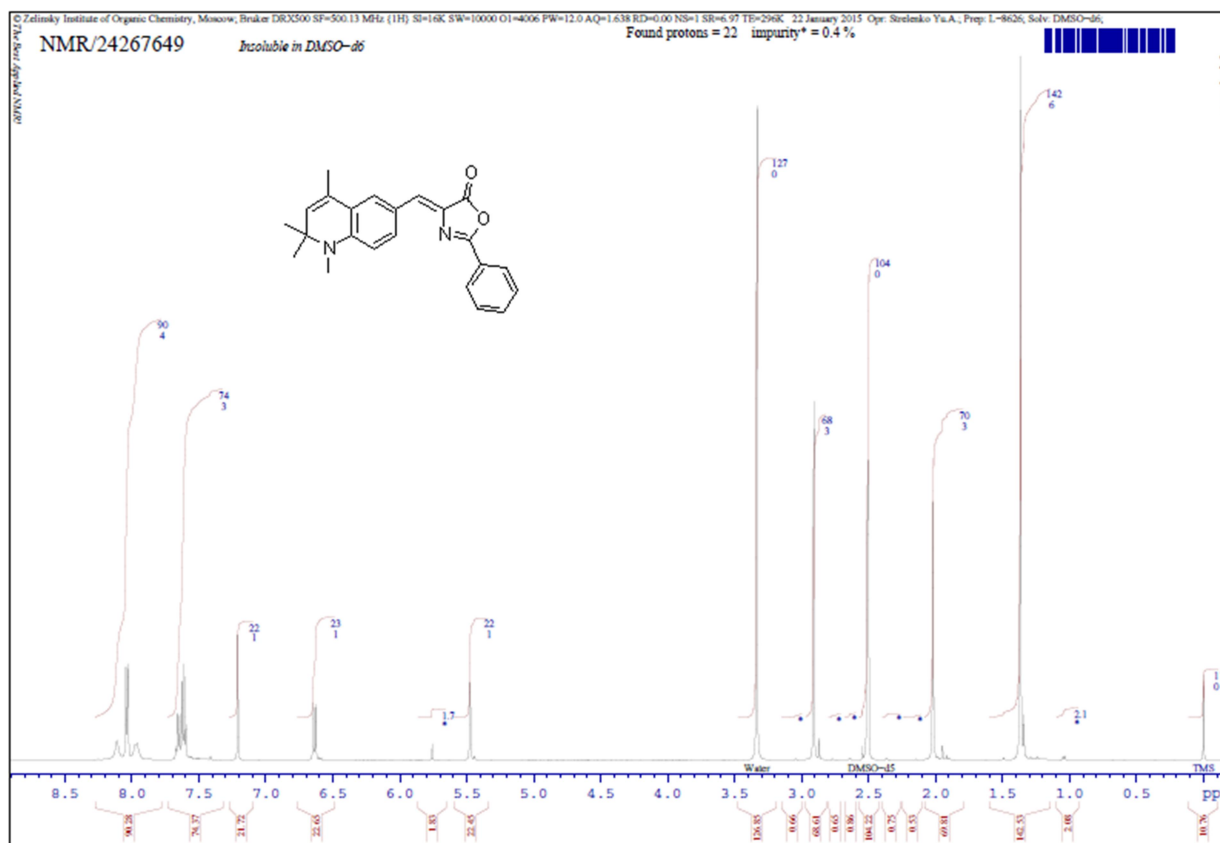


Figure 3. ^1H -NMR spectrum of (Z)-2-phenyl-4-((1,2,2,4-tetramethyl-1,2-dihydroquinolin-6-yl)methylene)oxazol-5(4H)-one **9a**.

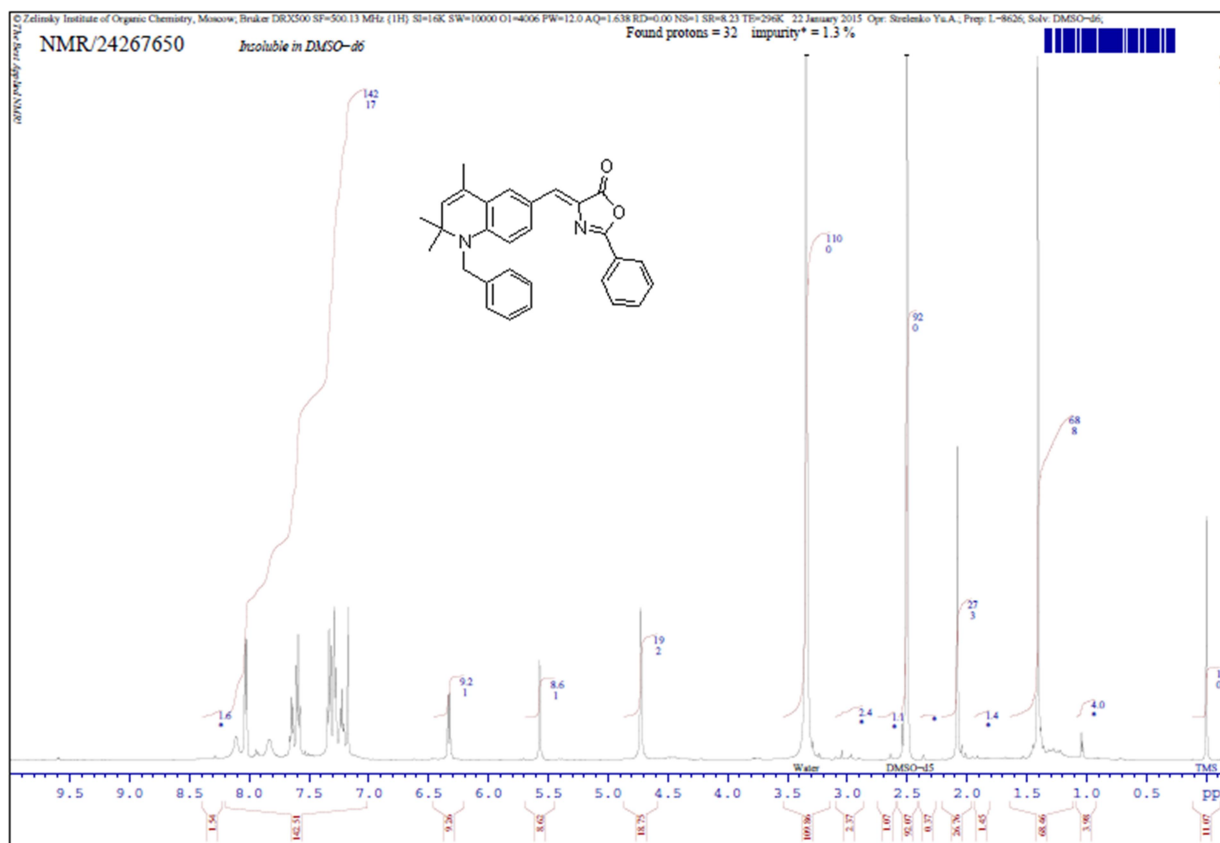


Figure 4. ^1H -NMR spectrum of (Z)-4-((1-benzyl-2,2,4-trimethyl-1,2-dihydroquinolin-6-yl)methylene)-2-phenyloxazol-5(4H)-one **9b**.

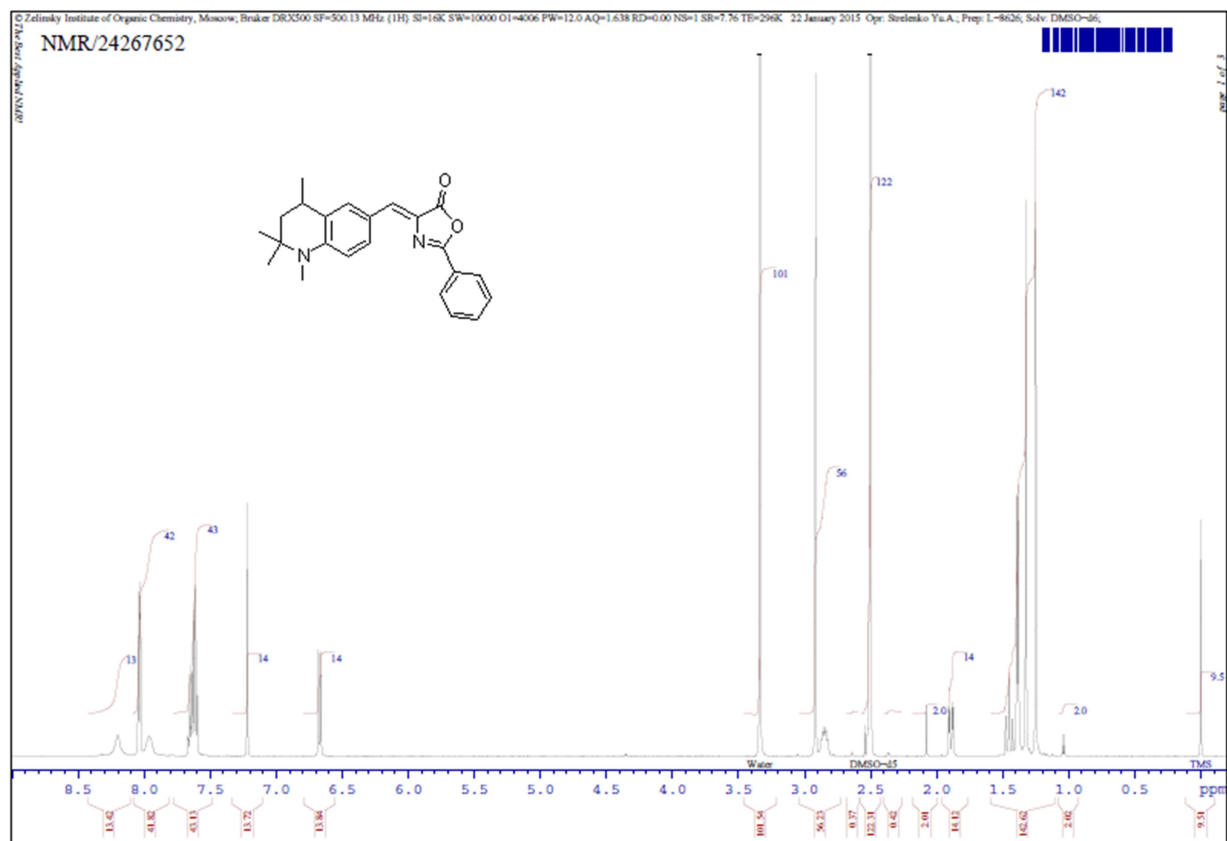


Figure 5. ^1H -NMR spectrum of (Z)-2-phenyl-4-((1,2,2,4-tetramethyl-1,2,3,4-tetrahydroquinolin-6-yl)methylene)oxazol-5(4H)-one **10a**.

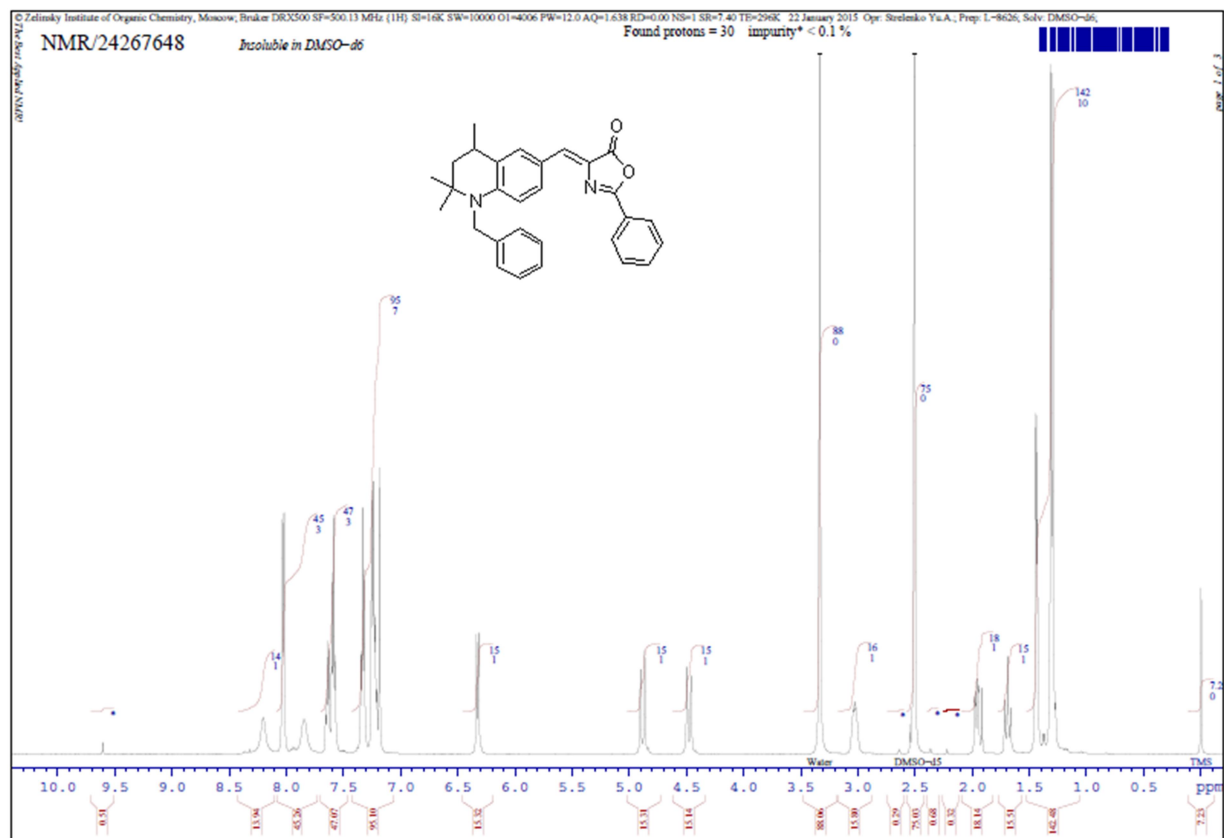


Figure 6. ¹H-NMR spectrum of (Z)-4-((1-benzyl-2,2,4-trimethyl-1,2,3,4-tetrahydroquinolin-6-yl)methylene)-2-phenyloxazol-5(4H)-one **10b**.

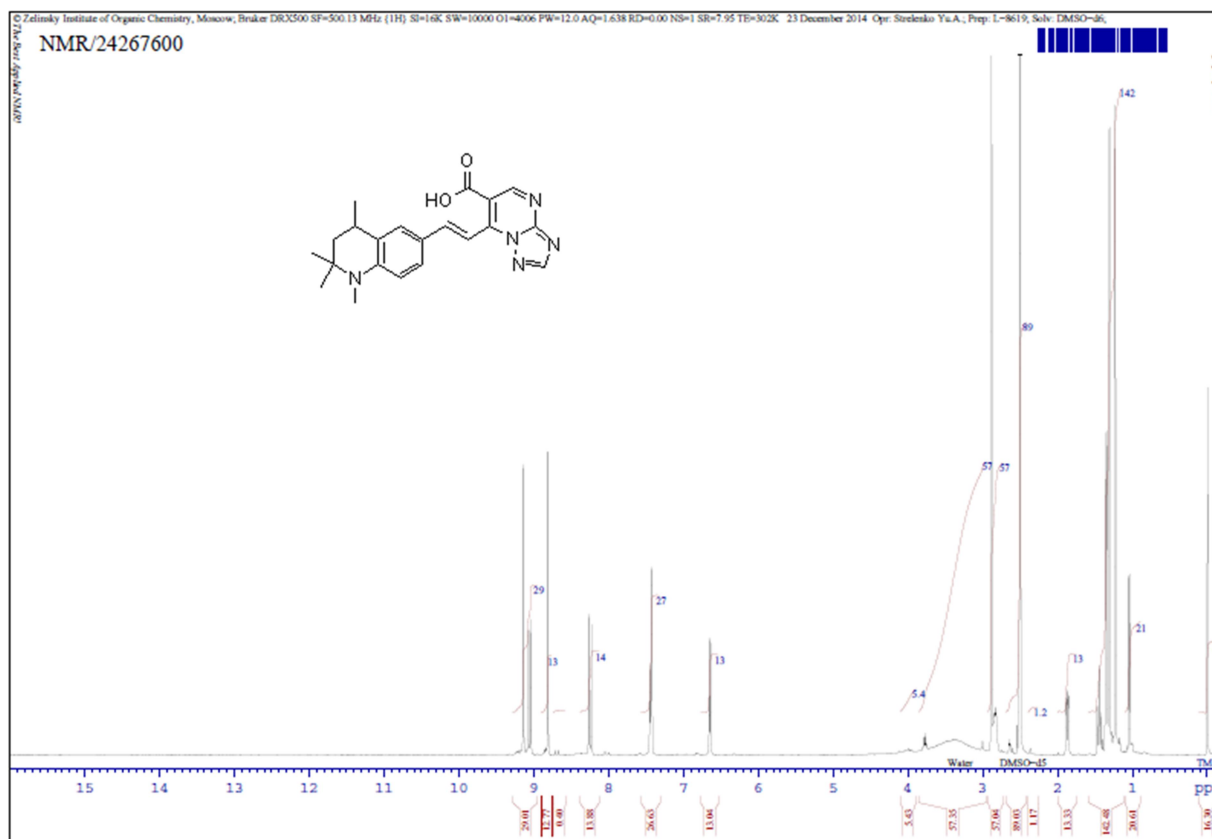


Figure 7. ^1H -NMR spectrum of (E)-7-(2-(1,2,2,4-tetramethyl-1,2,3,4-tetrahydroquinolin-6-yl)vinyl)-[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylic acid **12a**.

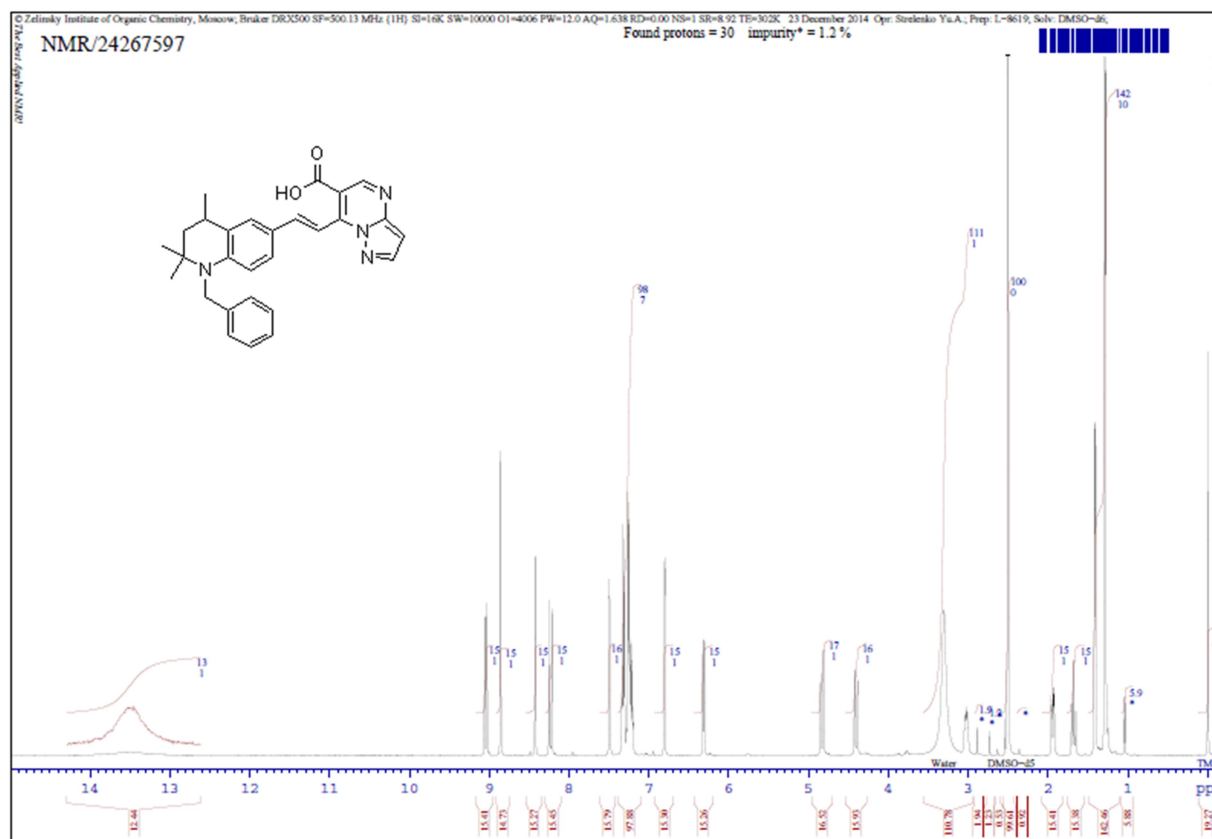


Figure 8. ^1H -NMR spectrum of (E)-7-(2-(1-benzyl-2,2,4-trimethyl-1,2,3,4-tetrahydroquinolin-6-yl)vinyl)pyrazolo[1,5-a]pyrimidine-6-carboxylic acid **12b**.

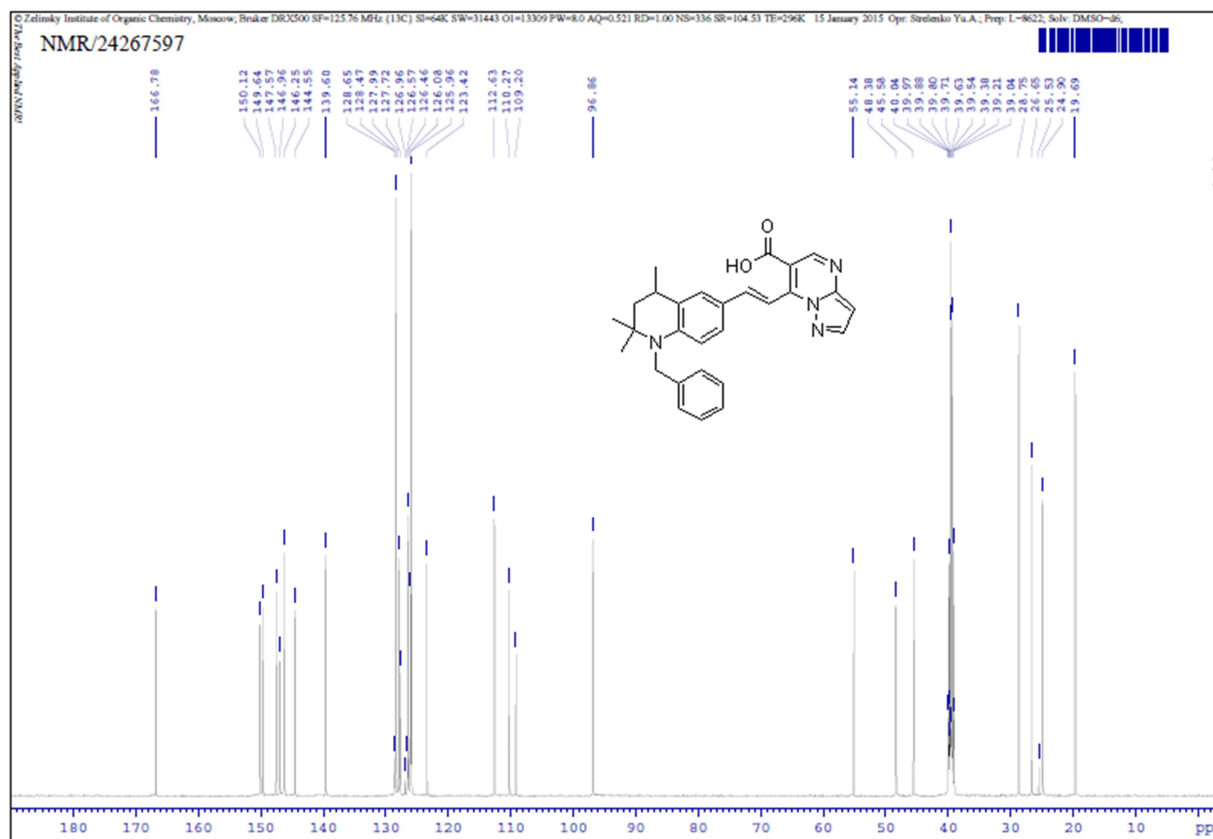


Figure 9. ^{13}C -NMR spectrum of (E)-7-(2-(1-benzyl-2,2,4-trimethyl-1,2,3,4-tetrahydroquinolin-6-yl)vinyl)pyrazolo[1,5-a]pyrimidine-6-carboxylic acid **12b**.

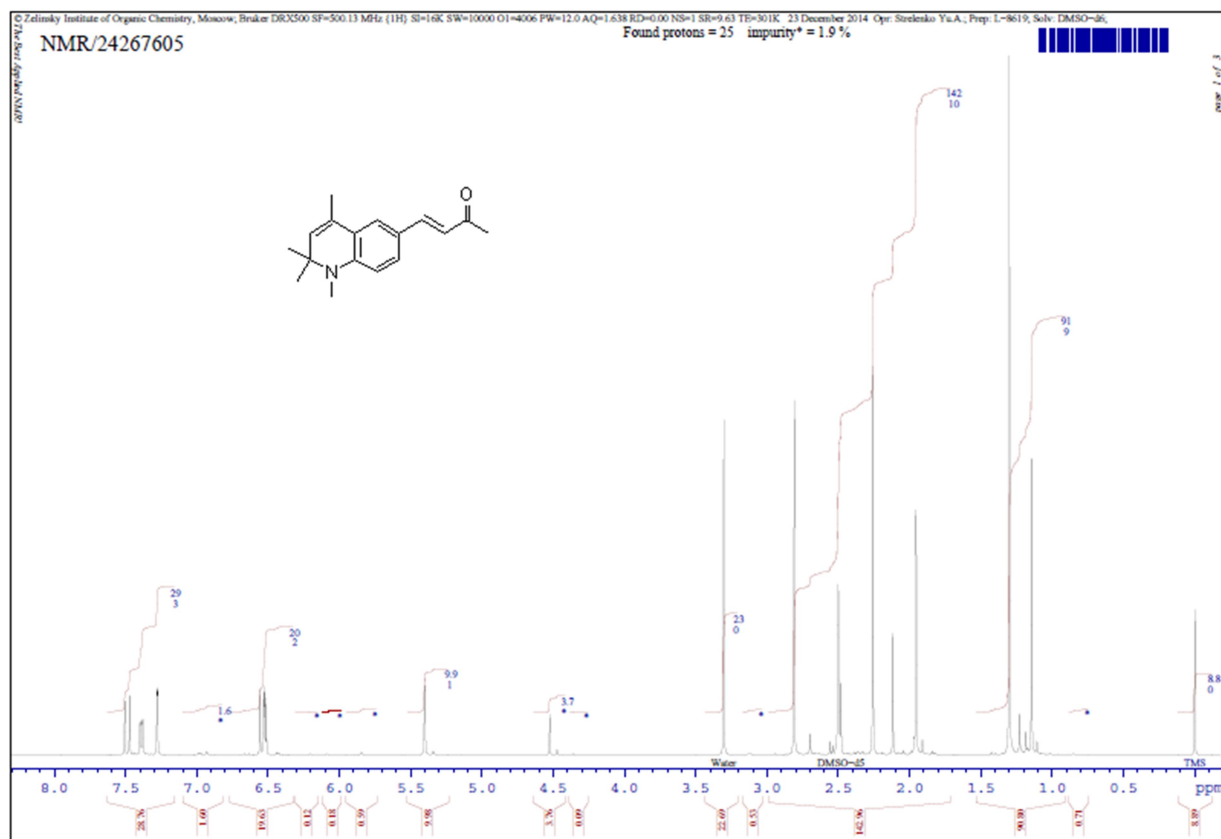


Figure 10. ^1H -NMR spectrum of (E)-4-(1,2,2,4-tetramethyl-1,2-dihydroquinolin-6-yl)but-3-en-2-one **13a**.

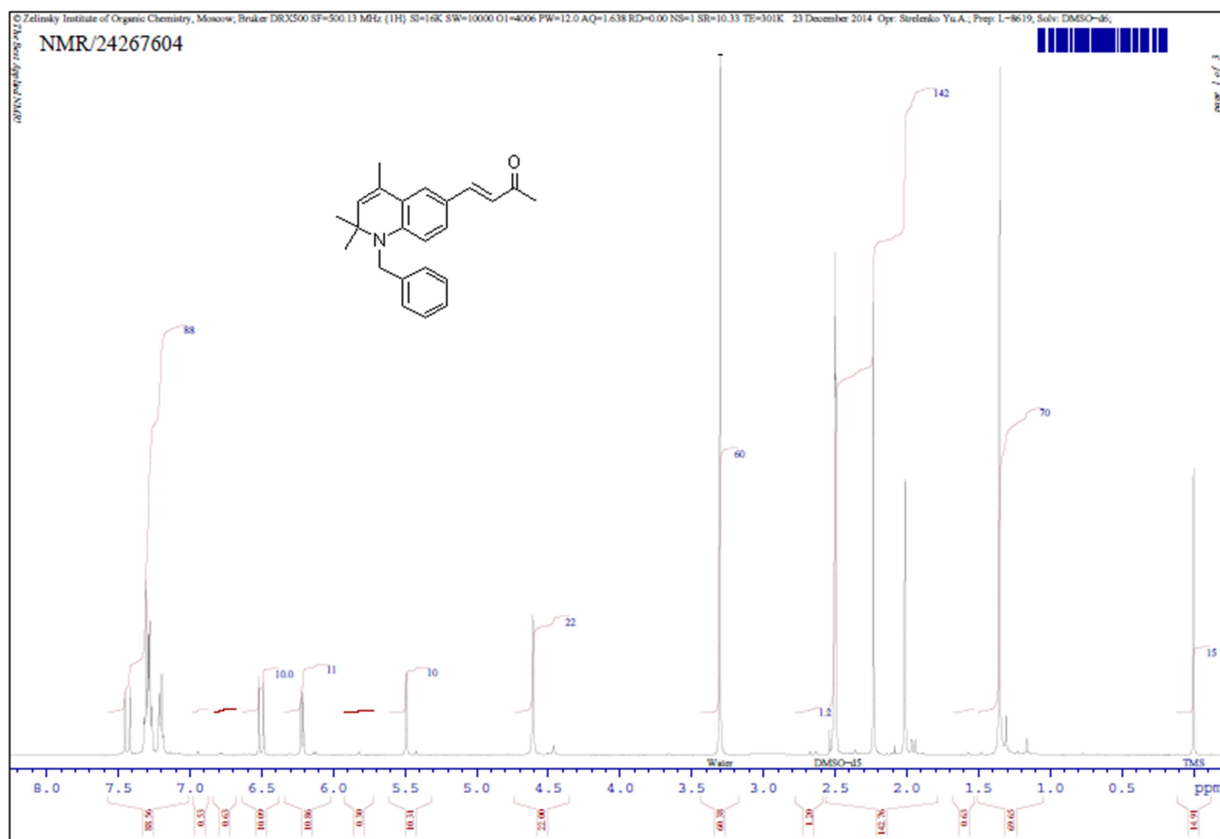


Figure 11. ^1H -NMR spectrum of (E)-4-(1-benzyl-2,2,4-trimethyl-1,2-dihydroquinolin-6-yl)but-3-en-2-one **13b**.

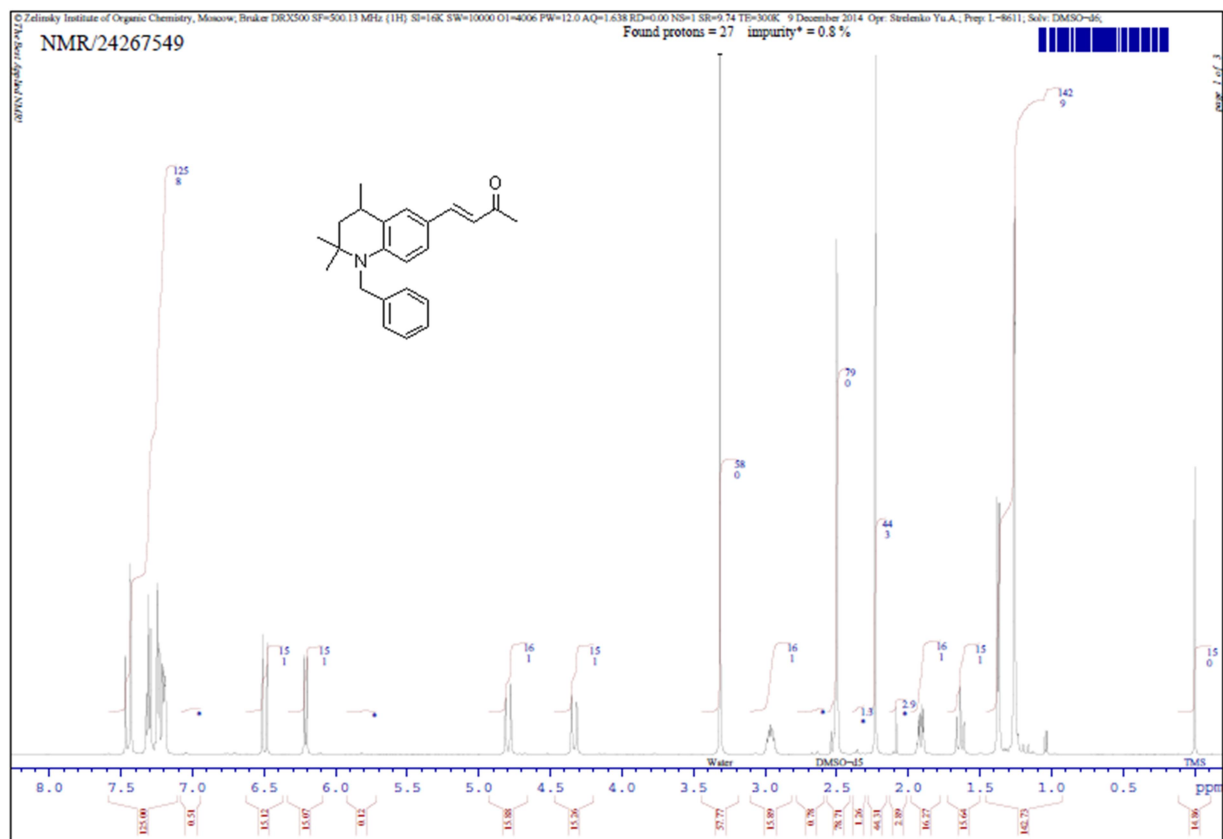


Figure 12. ^1H -NMR spectrum of (E)-4-(1-benzyl-2,2,4-trimethyl-1,2,3,4-tetrahydroquinolin-6-yl)but-3-en-2-one **14**.

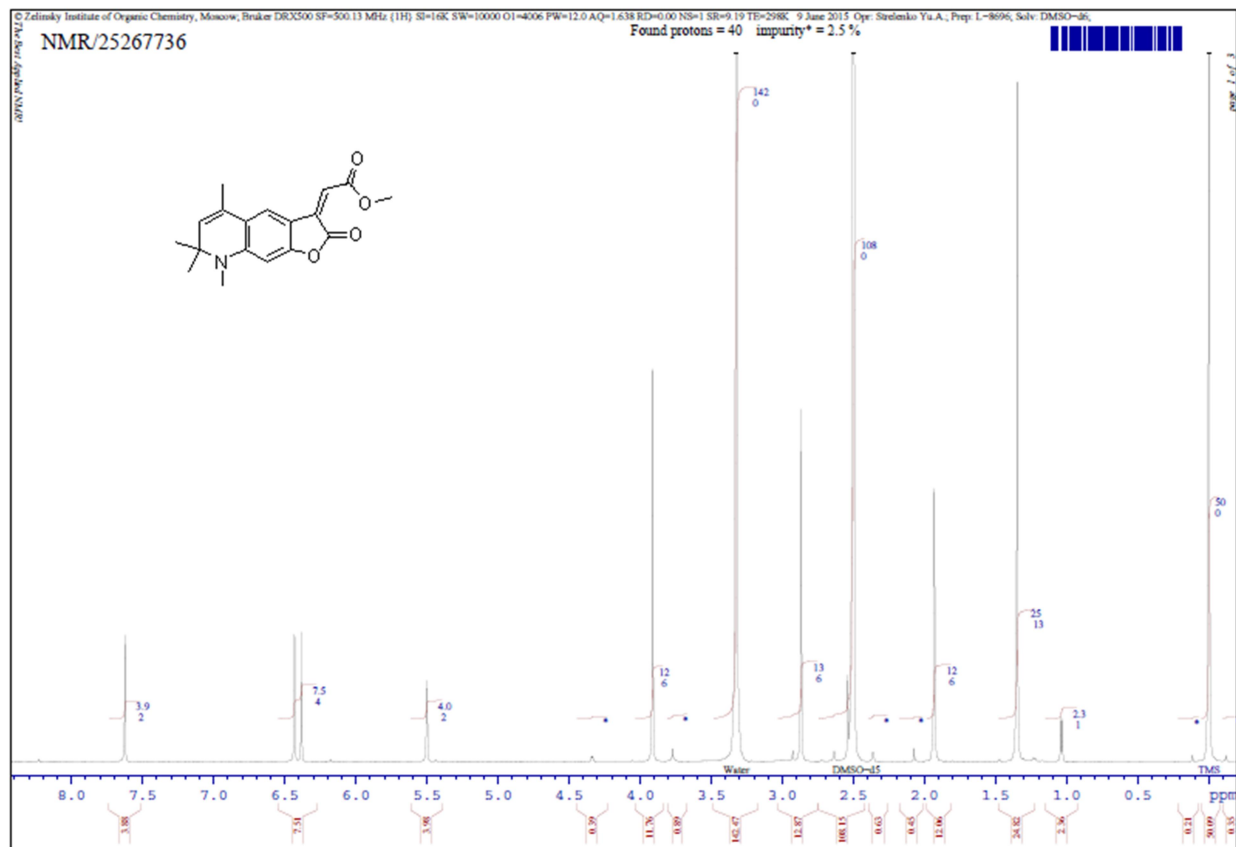


Figure 13. ^1H -NMR spectrum of methyl (Z)-2-(5,7,7,8-tetramethyl-2-oxo-7,8-dihydrofuro[3,2-g]quinolin-3(2H)-ylidene)acetate **16**.

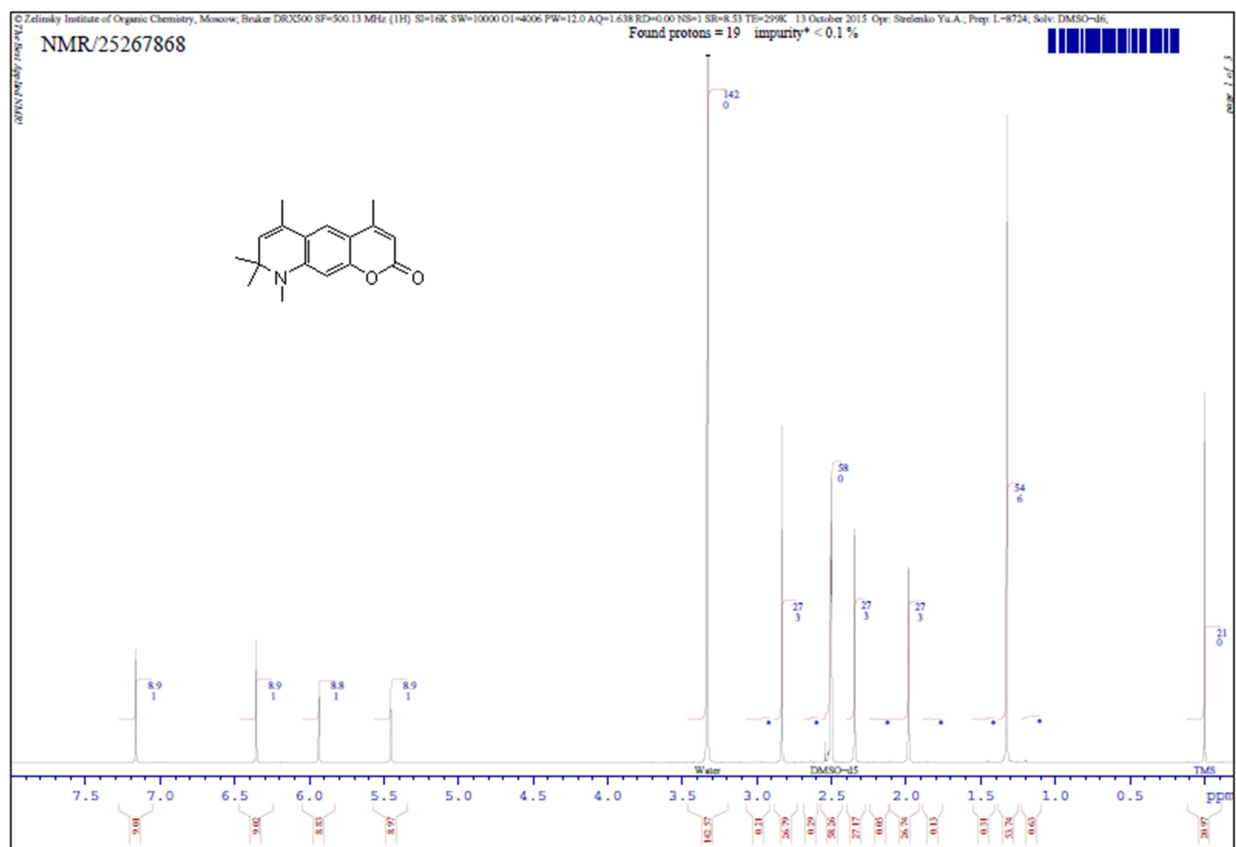


Figure 14. ¹H-NMR spectrum of 4,6,8,8,9-pentamethyl-8,9-dihydro-2H-pyrano[3,2-g]quinolin-2-one **17**.

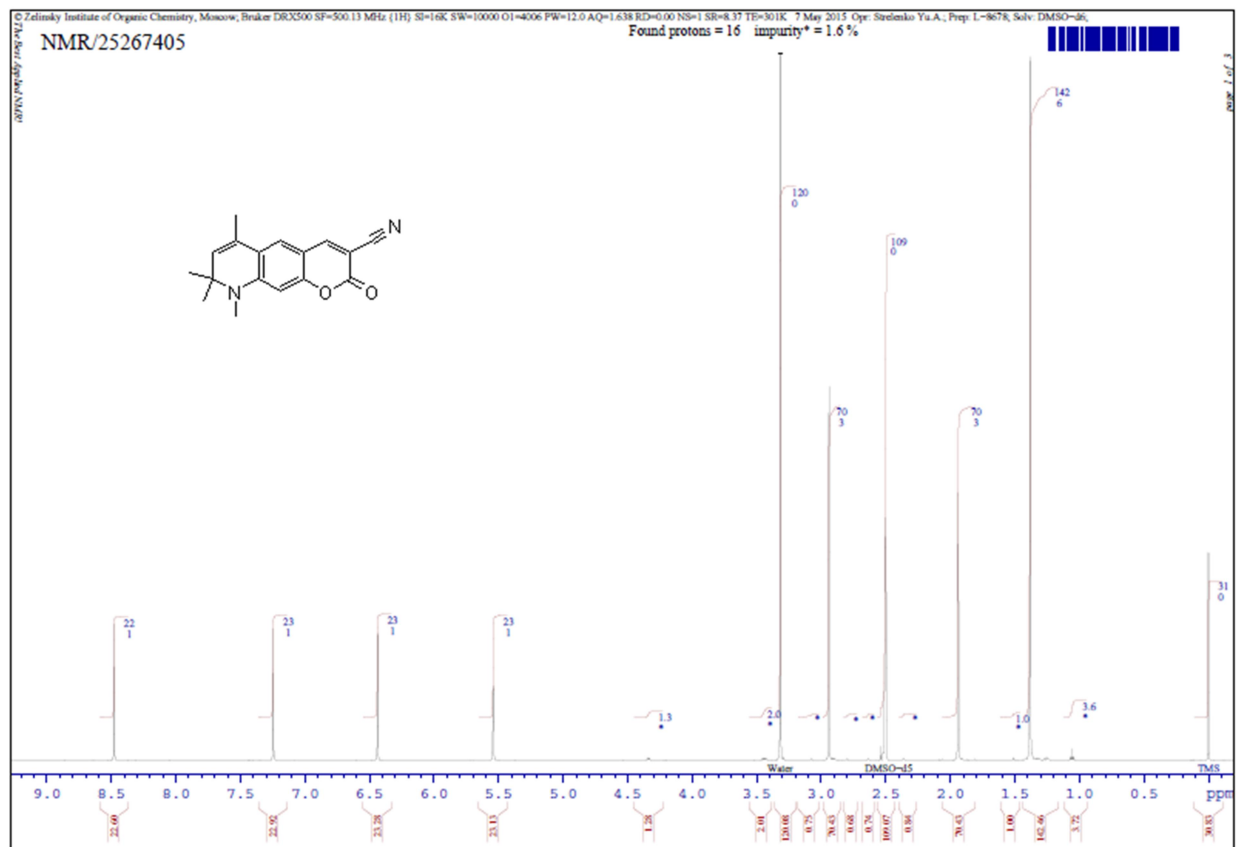


Figure 15. ^1H -NMR Spectrum of 6,8,8,9-tetramethyl-2-oxo-8,9-dihydro-2H-pyrano[3,2-g]quinoline-3-carbonitrile **19a**.

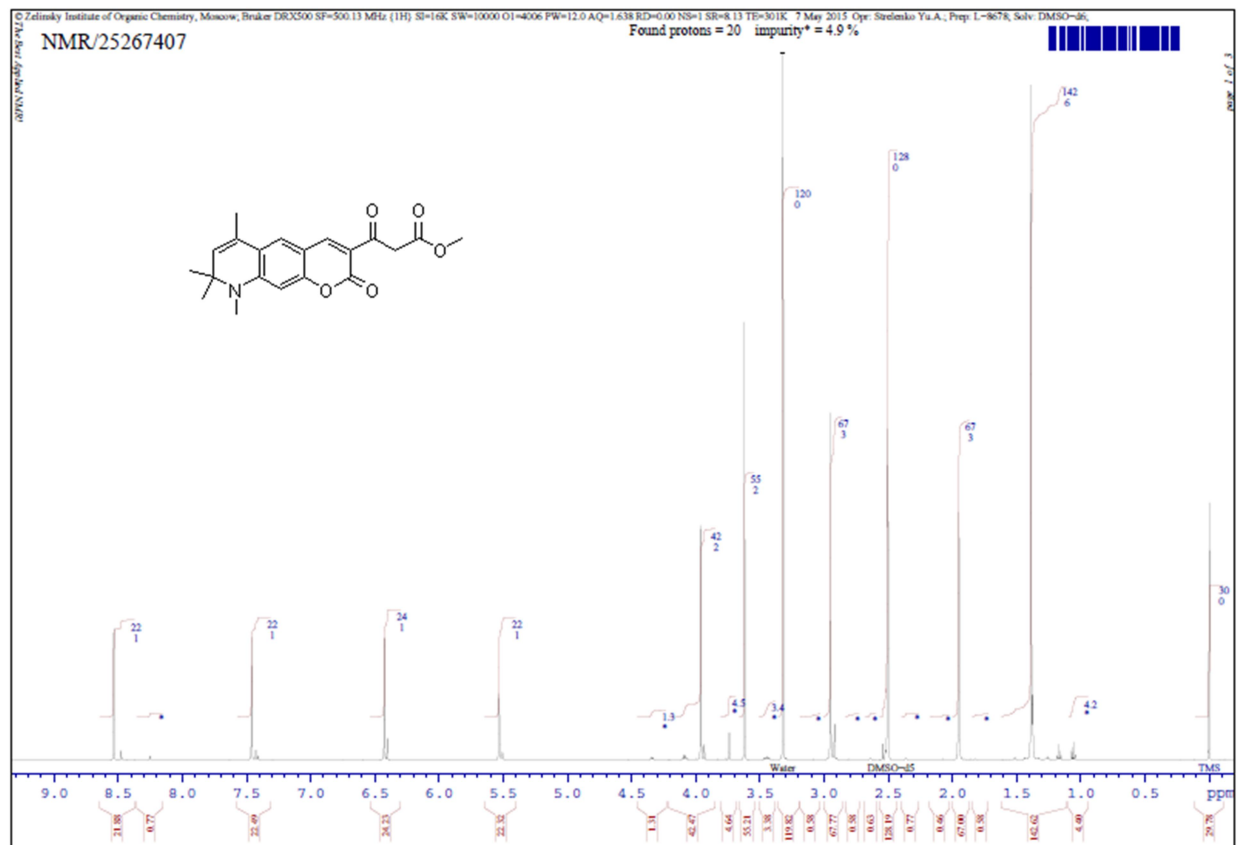


Figure 16. ^1H -NMR spectrum of methyl 3-oxo-3-(6,8,8,9-tetramethyl-2-oxo-8,9-dihydro-2H-pyrano[3,2-g]quinolin-3-yl)propanoate **19b**.

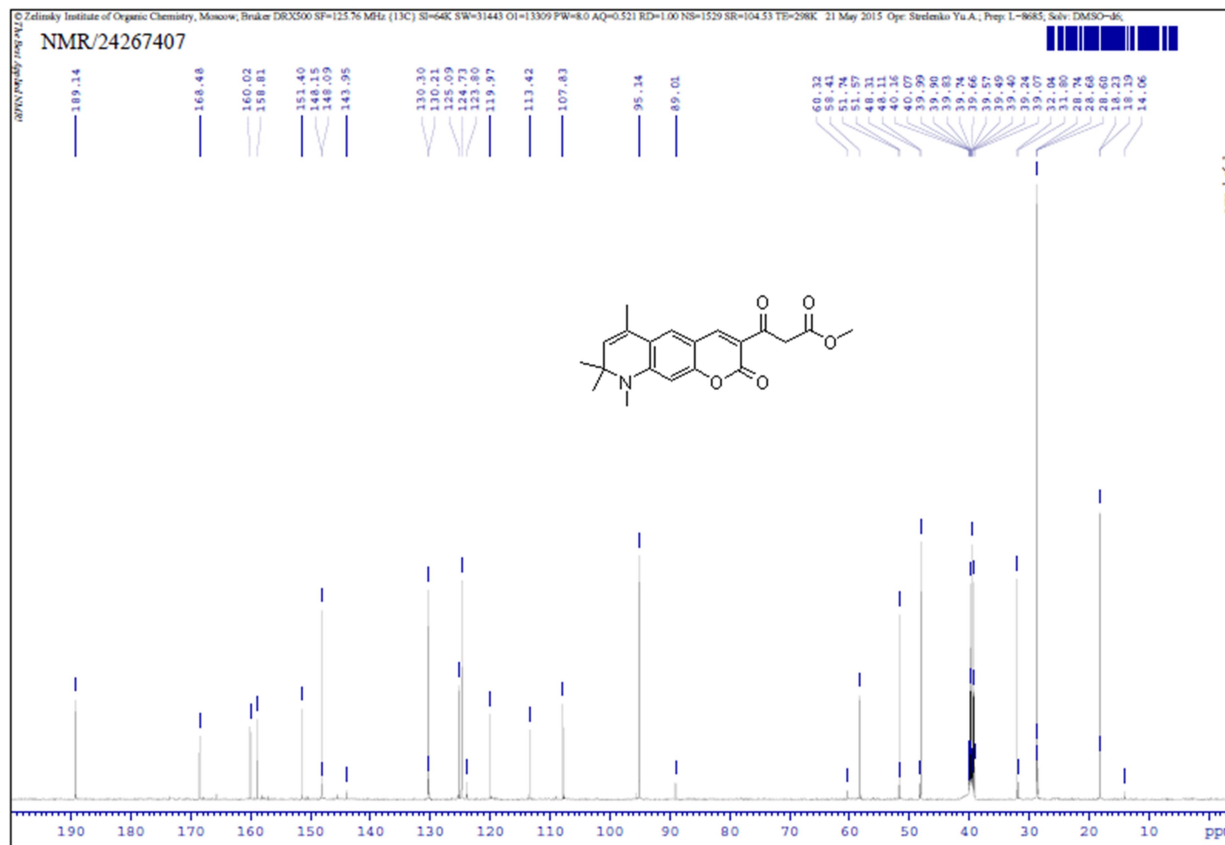


Figure 17. ^{13}C -NMR Spectrum of methyl 3-oxo-3-(6,8,8,9-tetramethyl-2-oxo-8,9-dihydro-2H-pyrano[3,2-g]quinolin-3-yl)propanoate **19b**

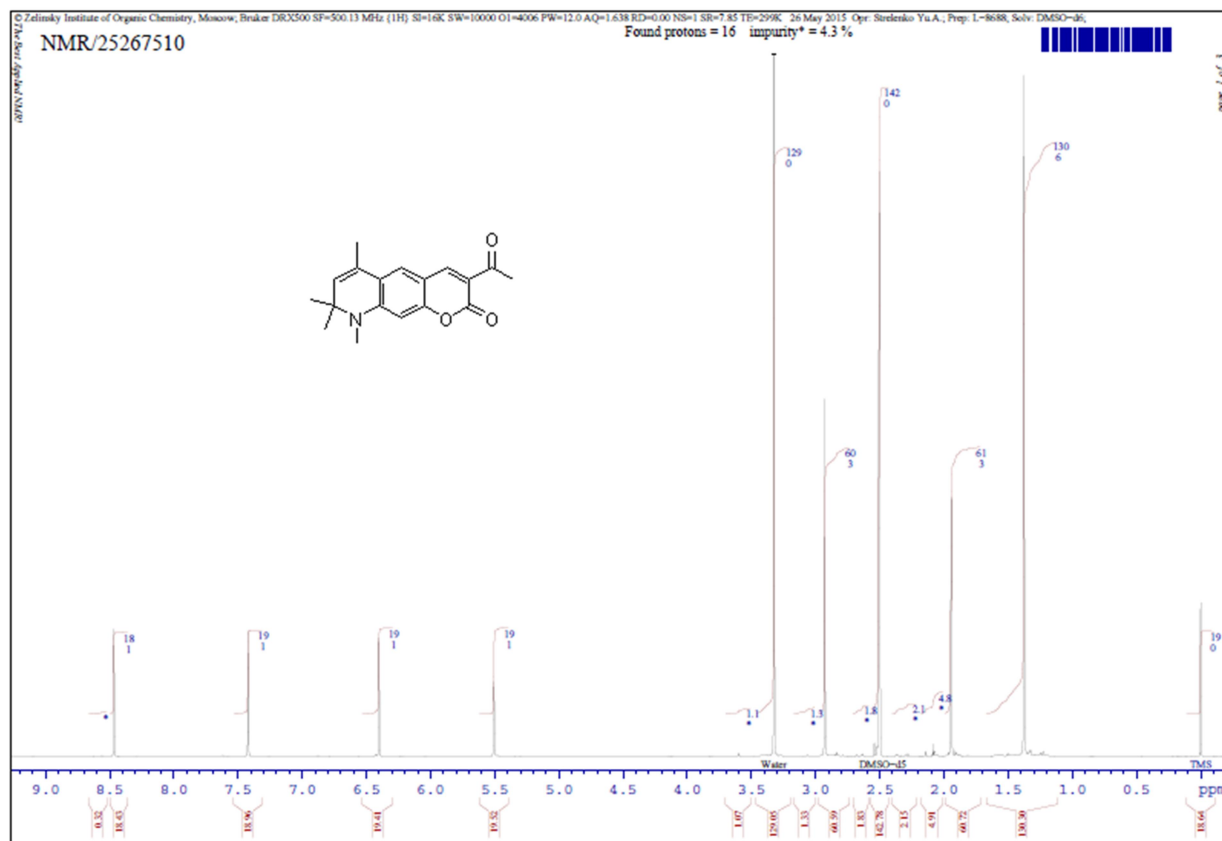


Figure 18. ^1H -NMR Spectrum of 3-acetyl-6,8,8,9-tetramethyl-8,9-dihydro-2H-pyrano[3,2-g]quinolin-2-one **19c**.

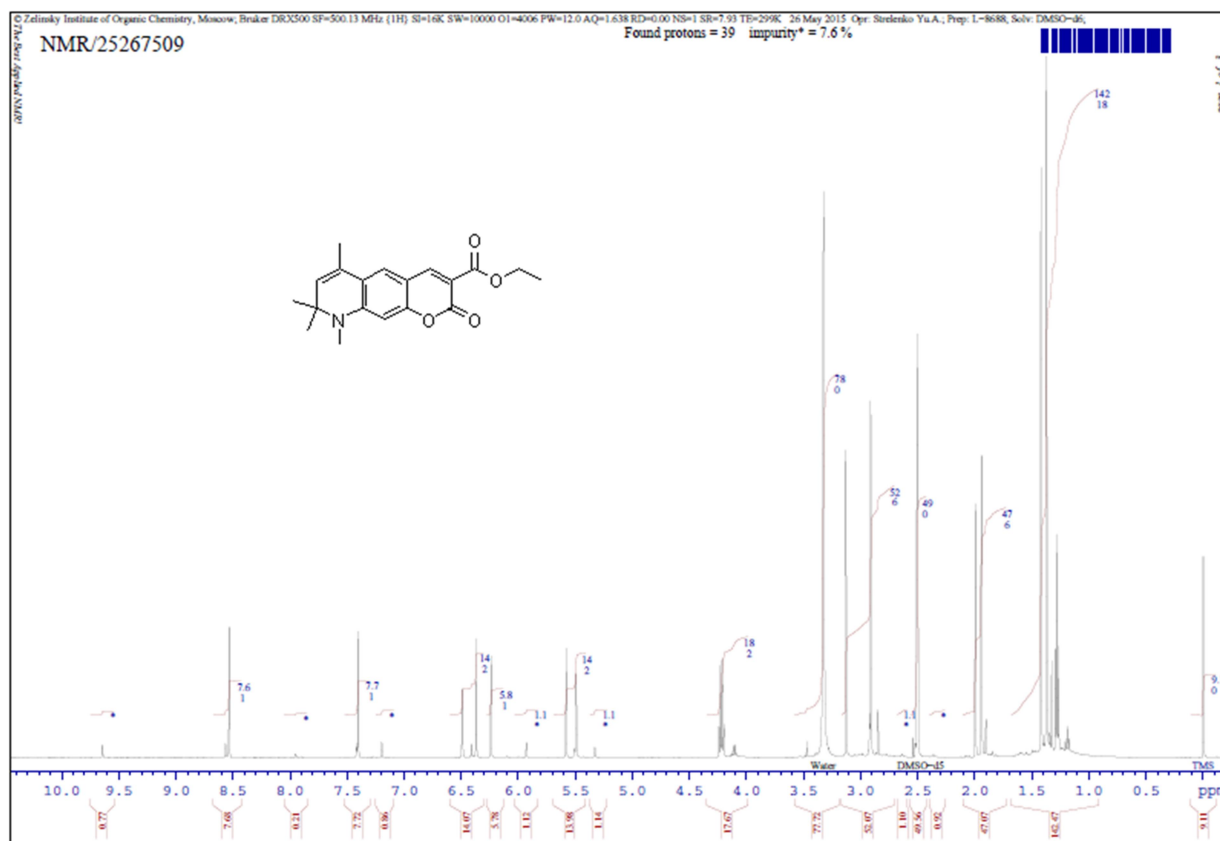


Figure 19. ^1H -NMR Spectrum of ethyl 6,8,8,9-tetramethyl-2-oxo-8,9-dihydro-2H-pyrano[3,2-g]quinoline-3-carboxylate **19d**.

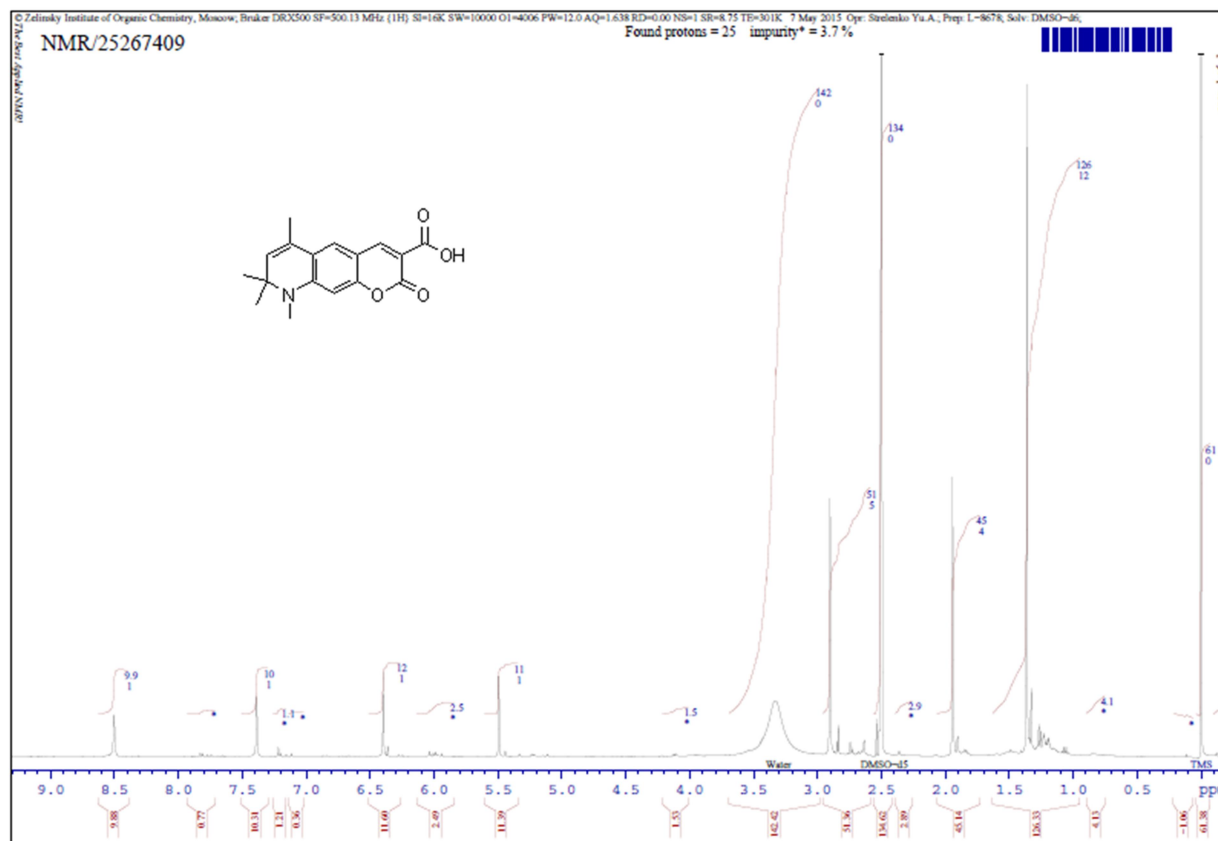


Figure 20. ^1H -NMR Spectrum of 6,8,8,9-tetramethyl-2-oxo-8,9-dihydro-2H-pyrano[3,2-g]quinoline-3-carboxylic acid **21**.

