

Synthesis of Functionalized 3-Cyanoisoxazoles Using a Dianionic Reagent

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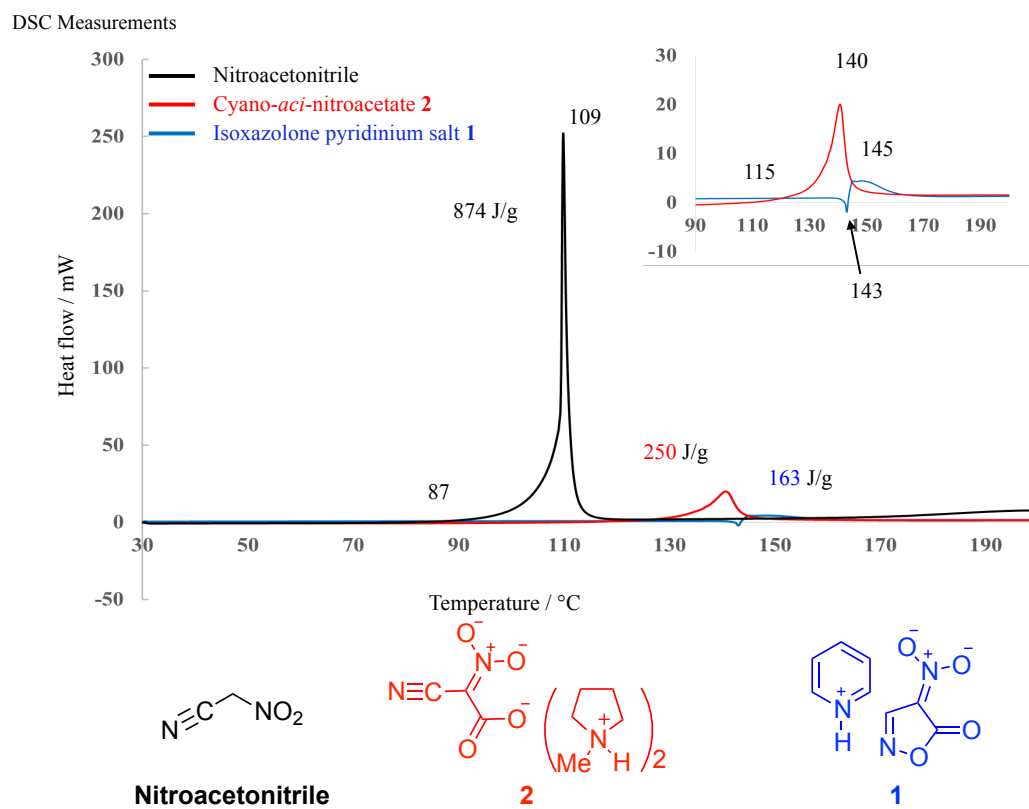
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- S4** Copies of ¹H and ¹³C NMR spectra
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¹H and ¹³C NMR spectra

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Figure S1. DSC measurement



Copies of ^1H and ^{13}C NMR spectra

Figure S2. ^1H NMR of 4-(4-chlorophenyl)-3-cyano-5-ethanoylisoxazole (**7a**)

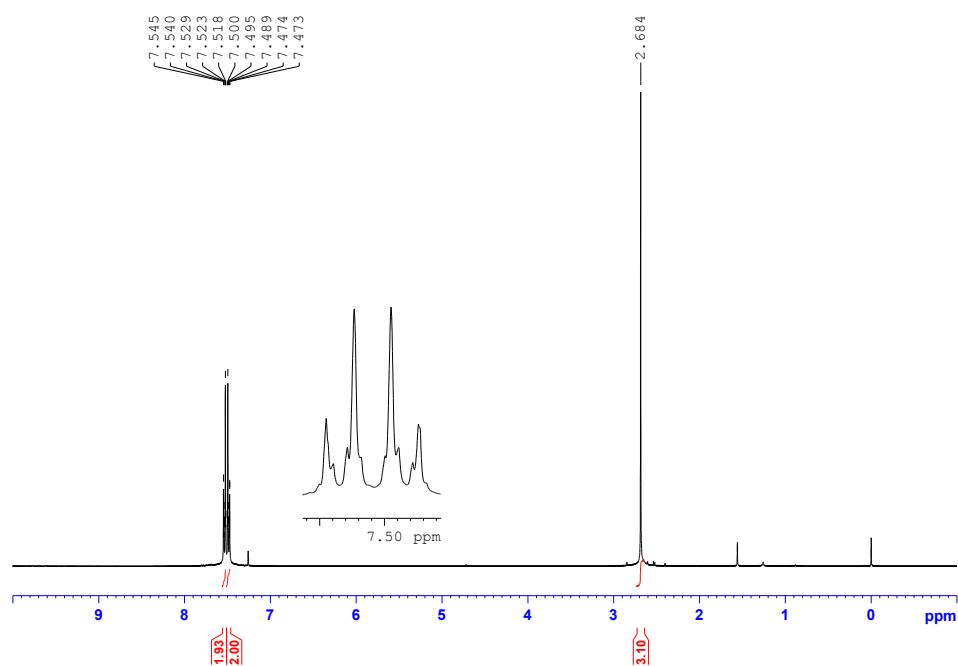


Figure S3. ^{13}C NMR of 4-(4-chlorophenyl)-3-cyano-5-ethanoylisoxazole (**7a**)

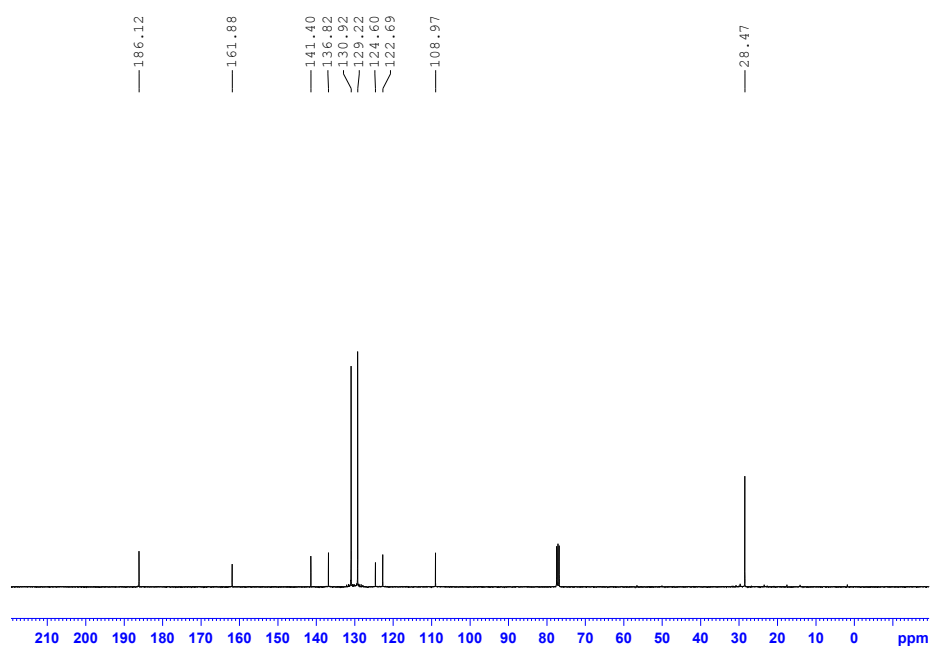


Figure S4. ^1H NMR of 3-cyano-5-ethanoyl-4-(4-methoxyphenyl)isoxazole (**7b**)

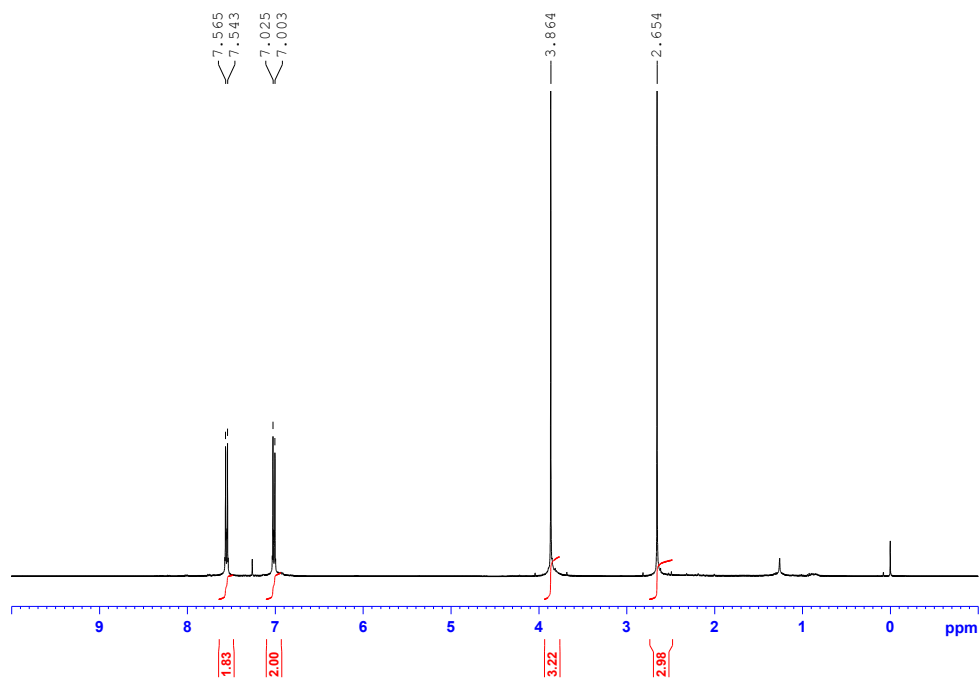


Figure S5. ^{13}C NMR of 3-cyano-5-ethanoyl-4-(4-methoxyphenyl)isoxazole (**7b**)

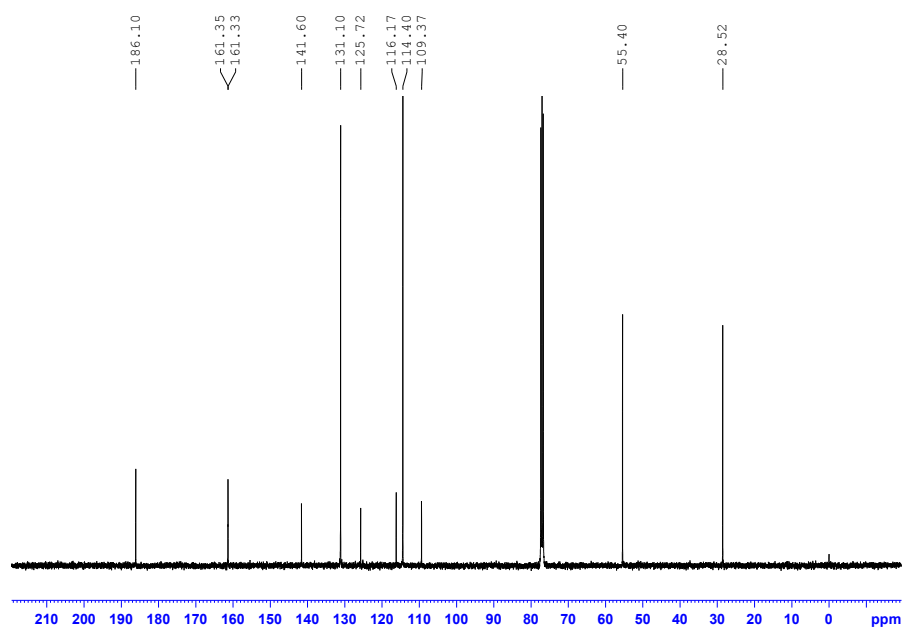


Figure S6. ^1H NMR of 3-cyano-5-ethanoyl-4-(4-methylphenyl)isoxazole (**7c**)

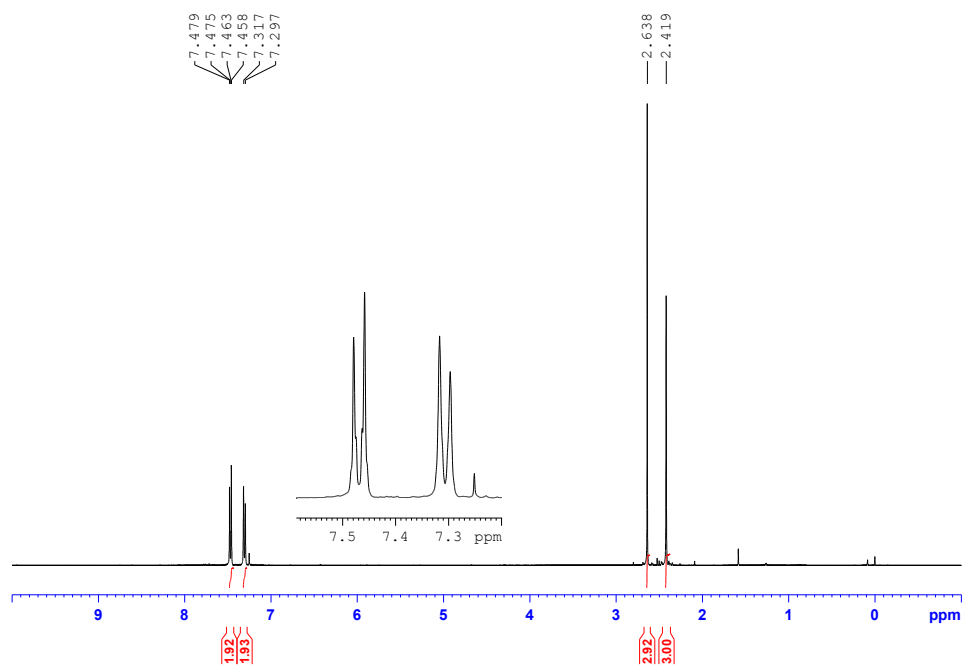


Figure S7. ^{13}C NMR of 3-cyano-5-ethanoyl-4-(4-methylphenyl)isoxazole (**7c**)

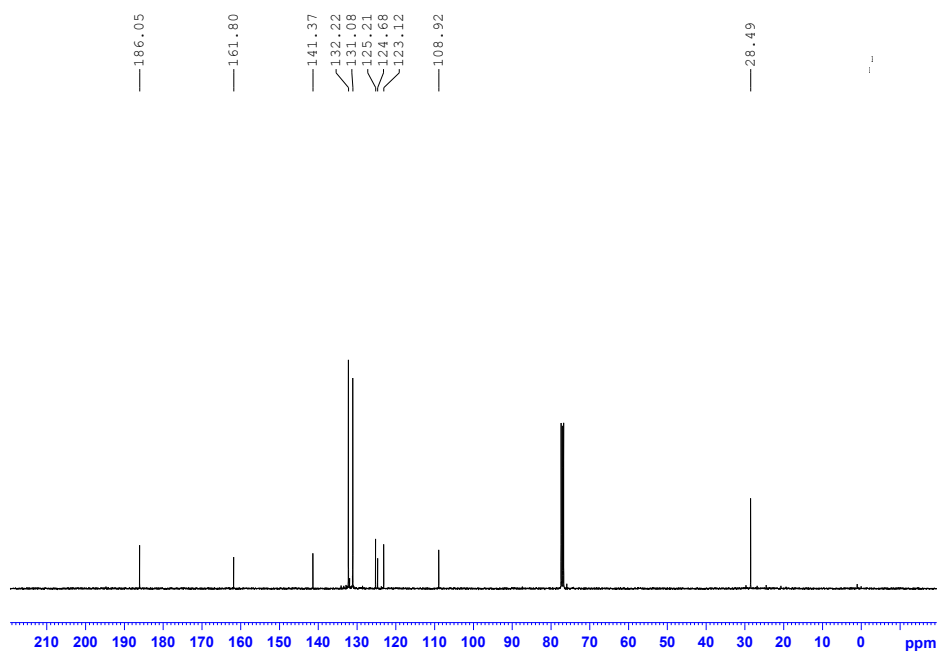


Figure S8. ^1H NMR of 3-cyano-5-ethanoyl-4-phenylisoxazole (**7d**)

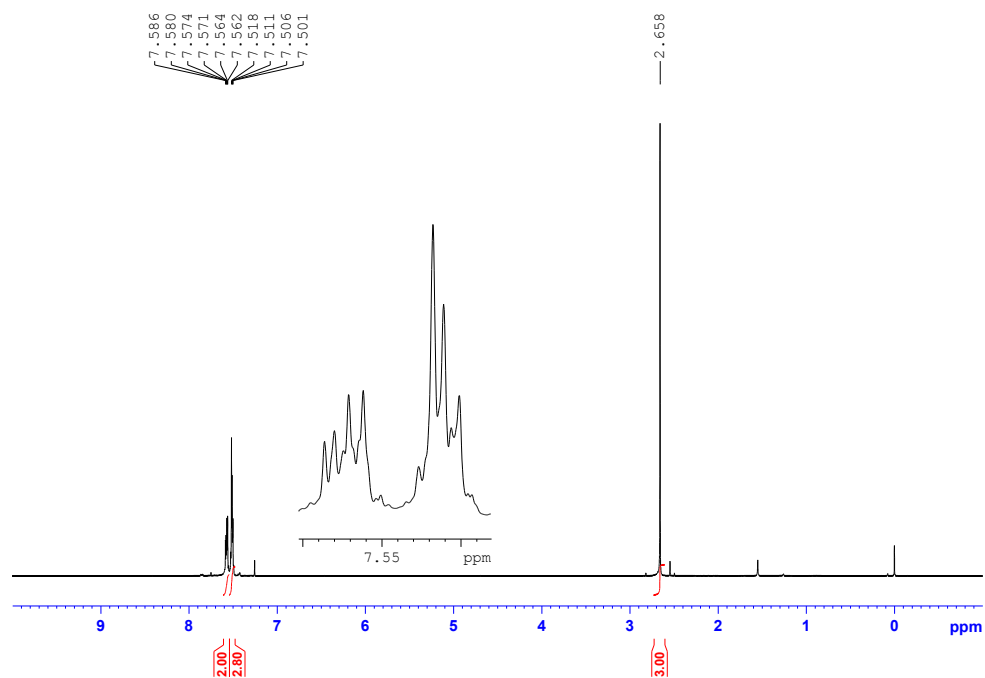


Figure S9. ^{13}C NMR of 3-cyano-5-ethanoyl-4-phenylisoxazole (**7d**)

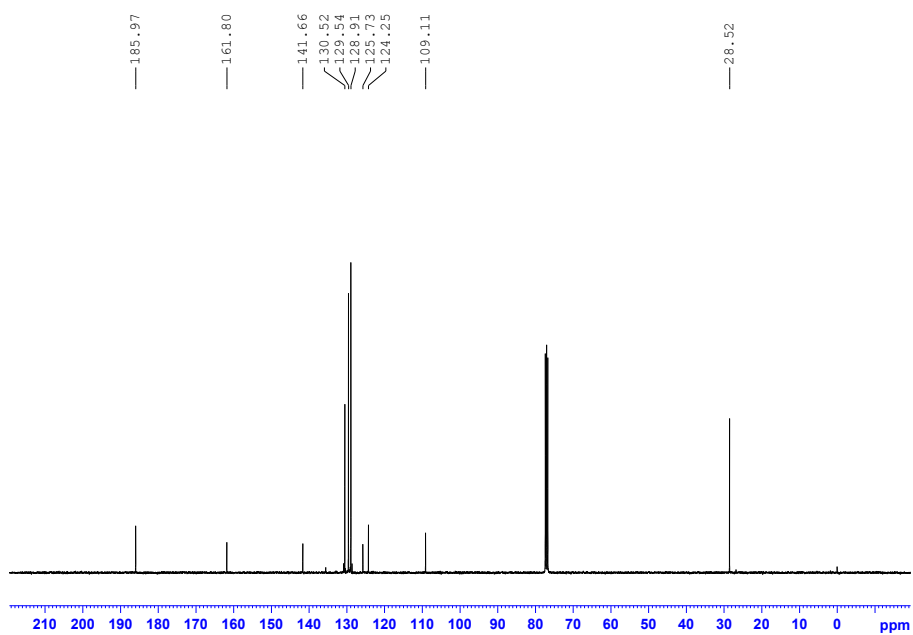


Figure S10. ^1H NMR of 4-(4-bromophenyl)-3-cyano-5-ethanoylisoxazole (**7e**)

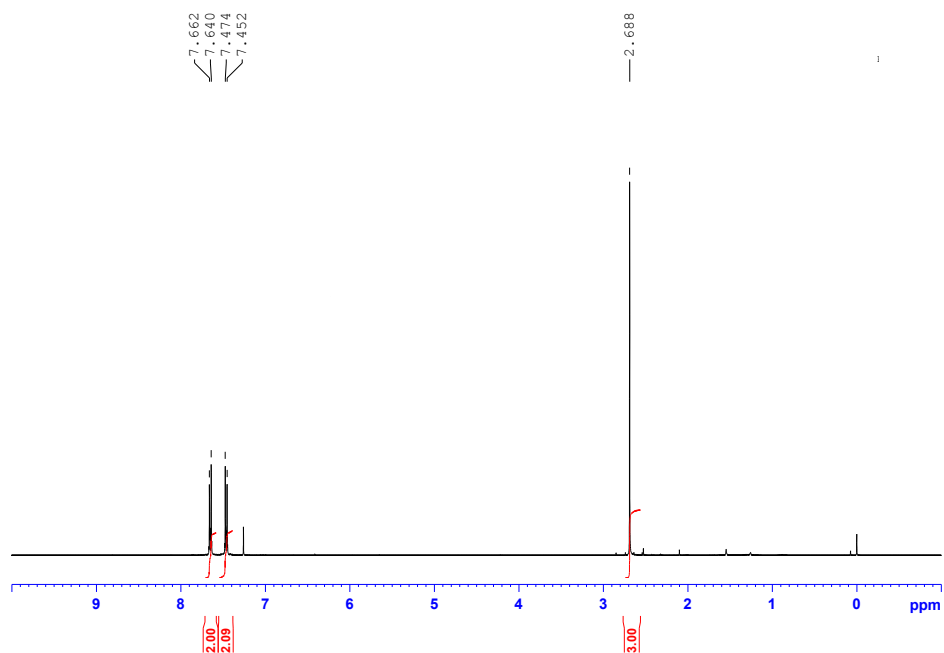


Figure S11. ^{13}C NMR of 4-(4-bromophenyl)-3-cyano-5-ethanoylisoxazole (**7e**)

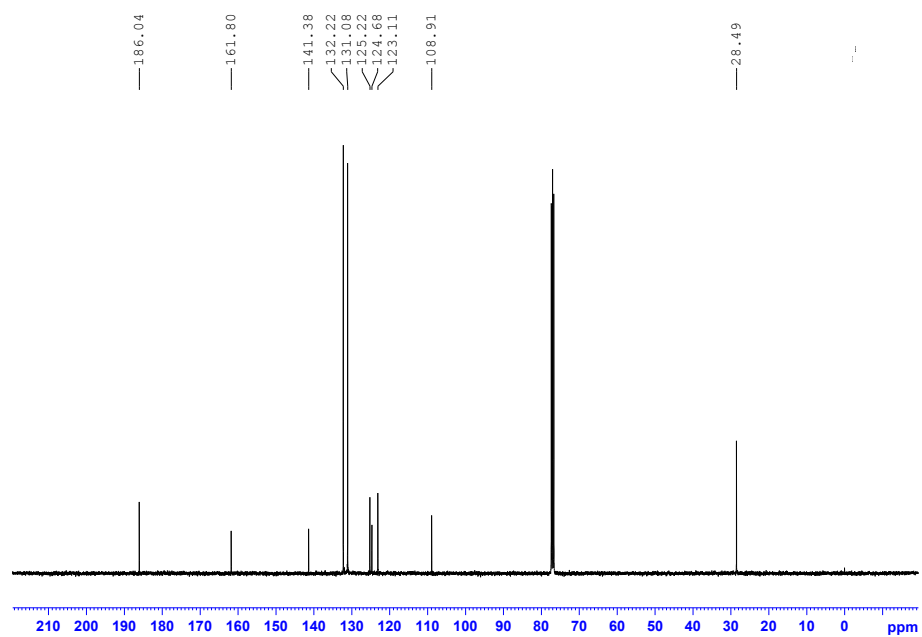


Figure S12. ^1H NMR of 3-cyano-5-ethanoyl-4-(4-nitrophenyl)isoxazole (**7f**)

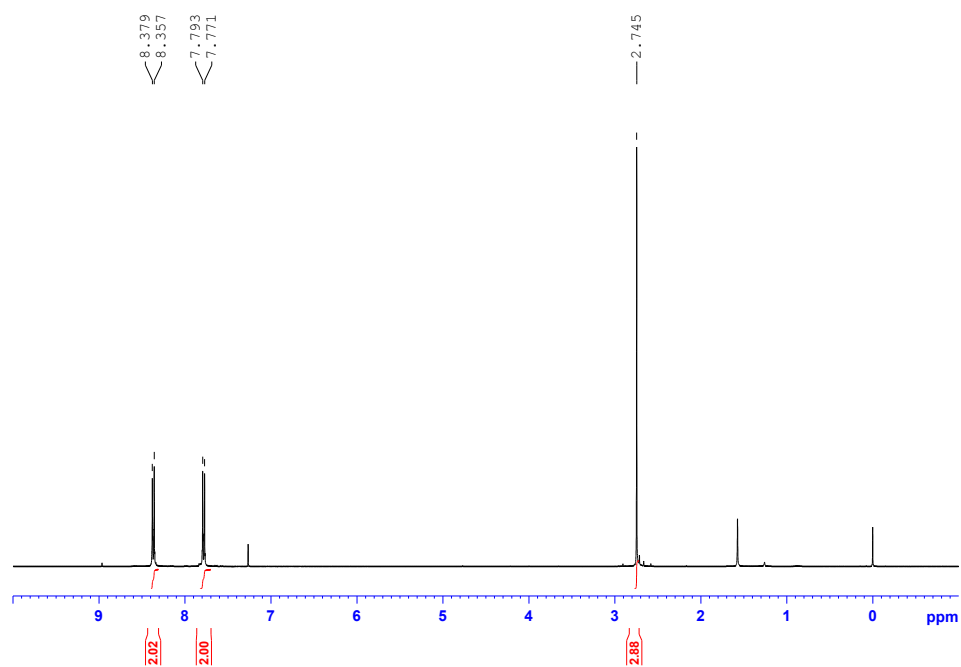


Figure S13. ^{13}C NMR of 3-cyano-5-ethanoyl-4-(4-nitrophenyl)isoxazole (**7f**)

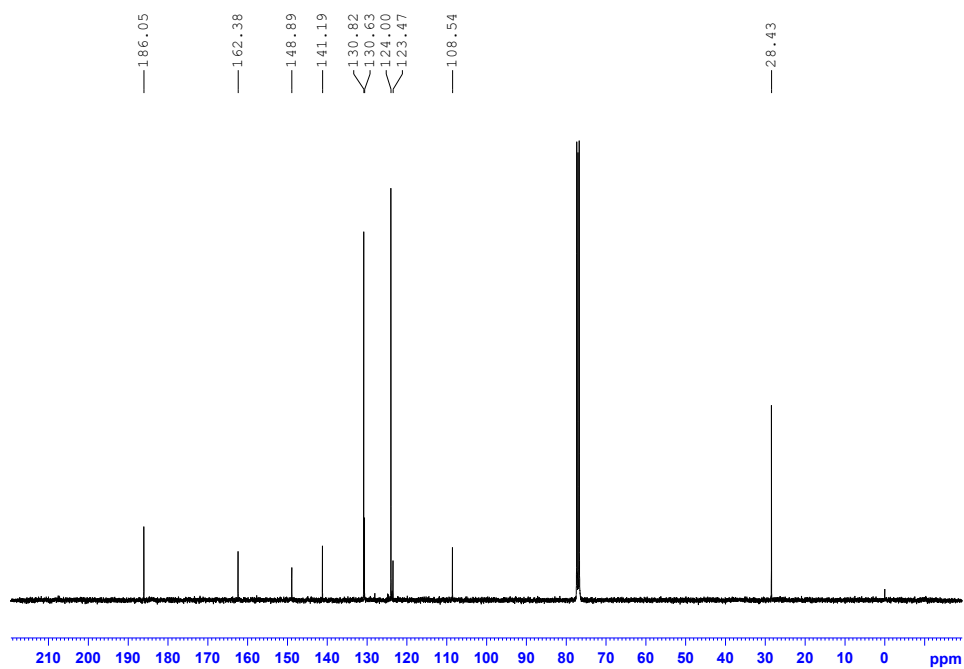


Figure S14. ^1H NMR of 3-cyano-5-(4-methoxybenzoyl)-4-phenylisoxazole (**7g**)

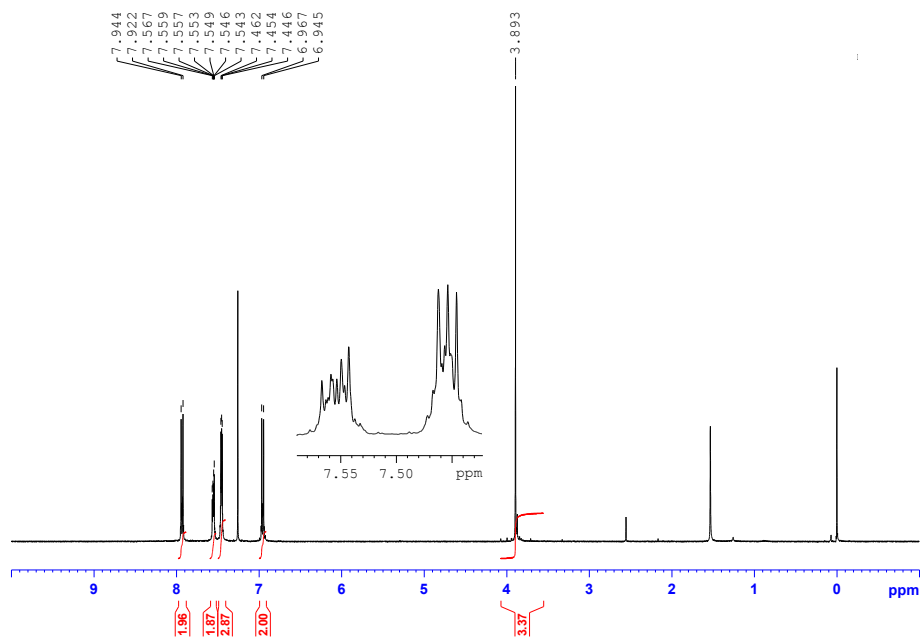


Figure S15. ^{13}C NMR of 3-cyano-5-(4-methoxybenzoyl)-4-phenylisoxazole (**7g**)

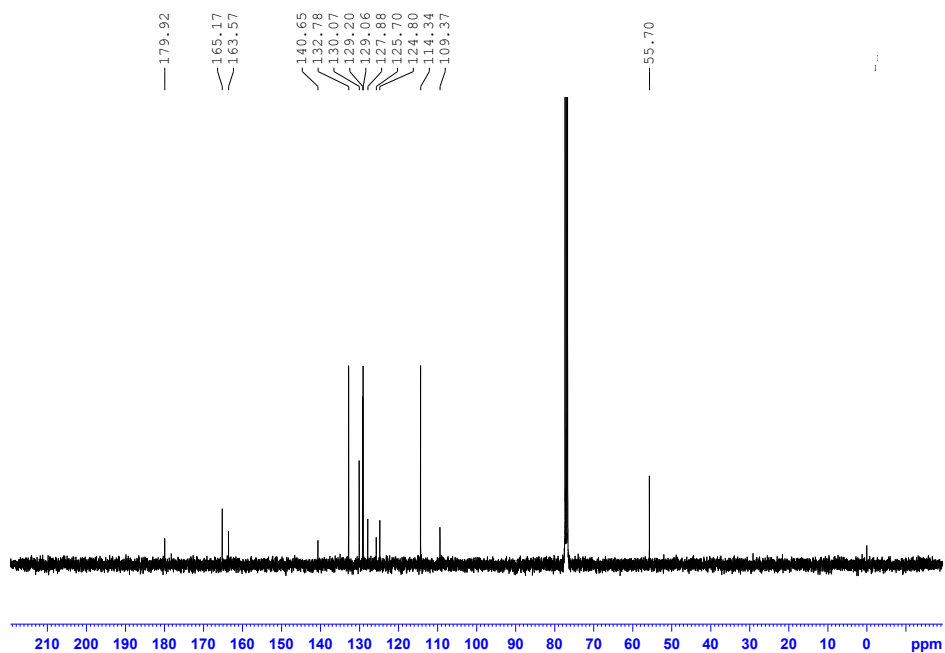


Figure S16. ^1H NMR of 3-cyano-5-(3-methoxybenzoyl)-4-phenylisoxazole (**7h**)

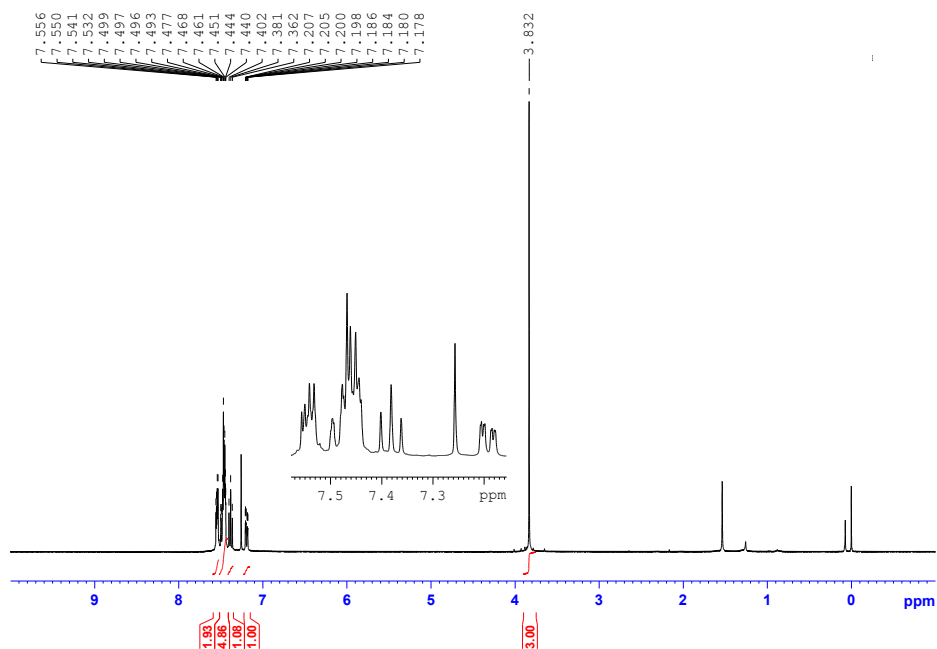


Figure S17. ^{13}C NMR of 3-cyano-5-(3-methoxybenzoyl)-4-phenylisoxazole (**7h**)

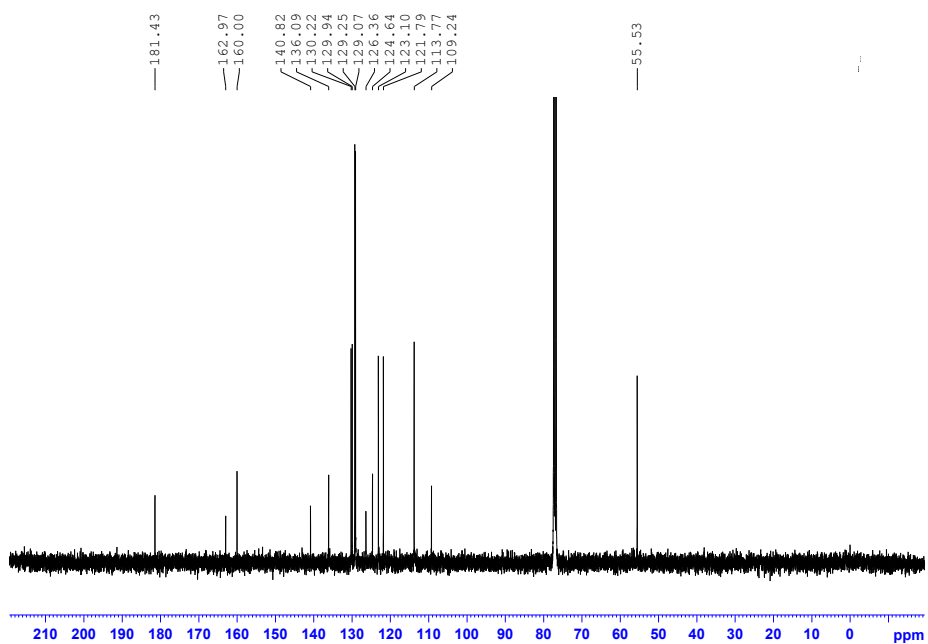


Figure S18. ^1H NMR of 3-cyano-5-(4-methylbenzoyl)-4-phenylisoxazole (**7i**)

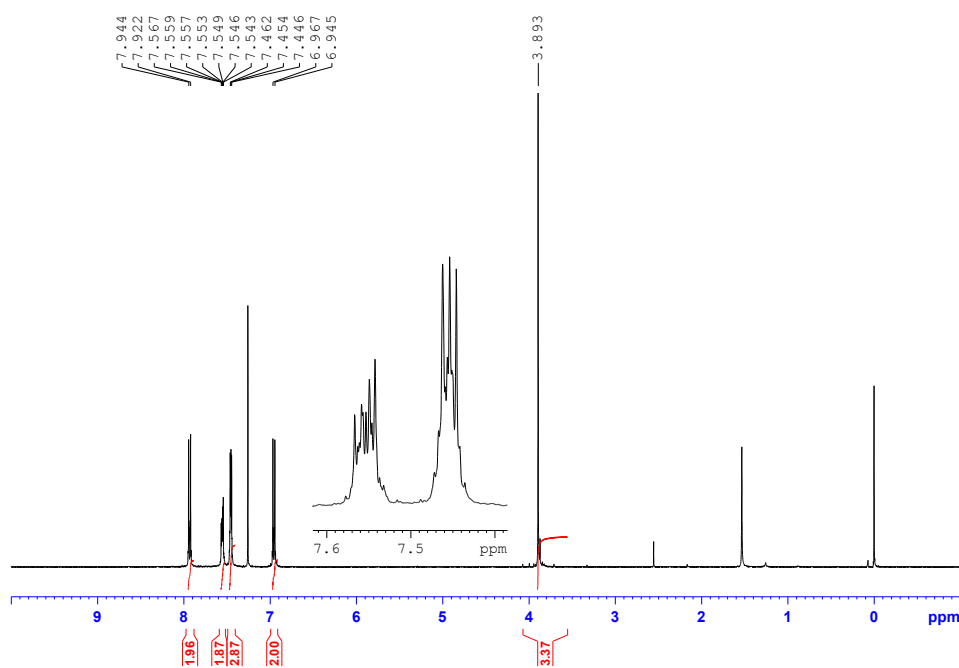


Figure S19. ^{13}C NMR of 3-cyano-5-(4-methylbenzoyl)-4-phenylisoxazole (**7i**)

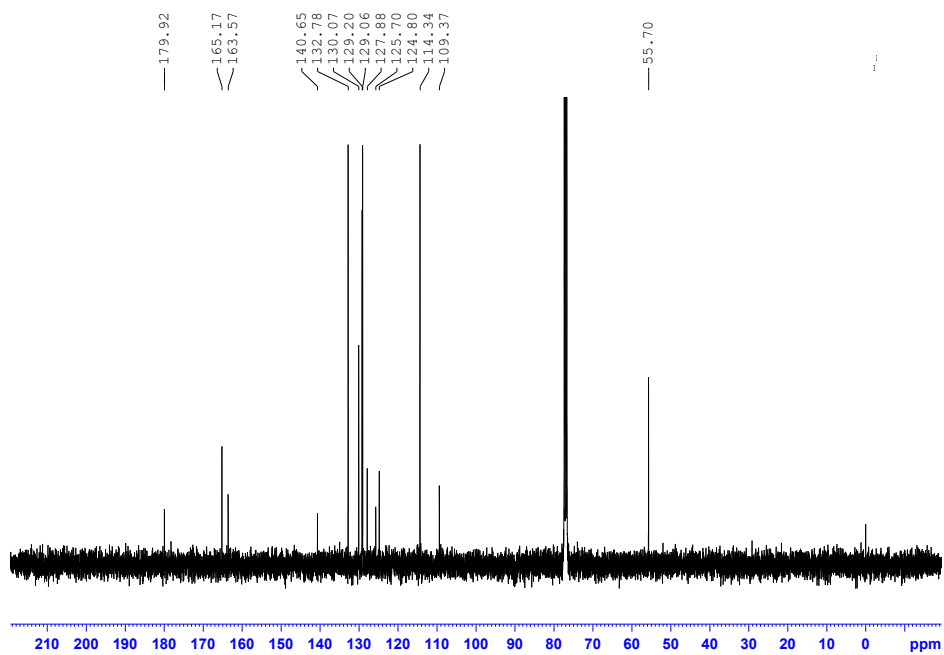


Figure S20. ^1H NMR of 5-benzoyl-3-cyano-4-phenylisoxazole (**7j**)

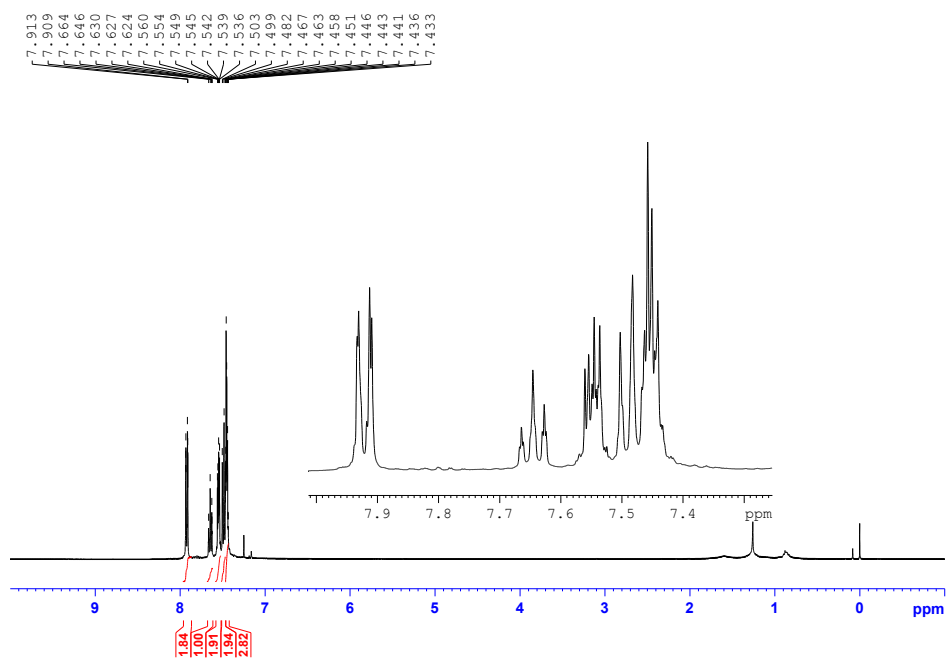


Figure S21. ^{13}C NMR of 5-benzoyl-3-cyano-4-phenylisoxazole (**7j**)

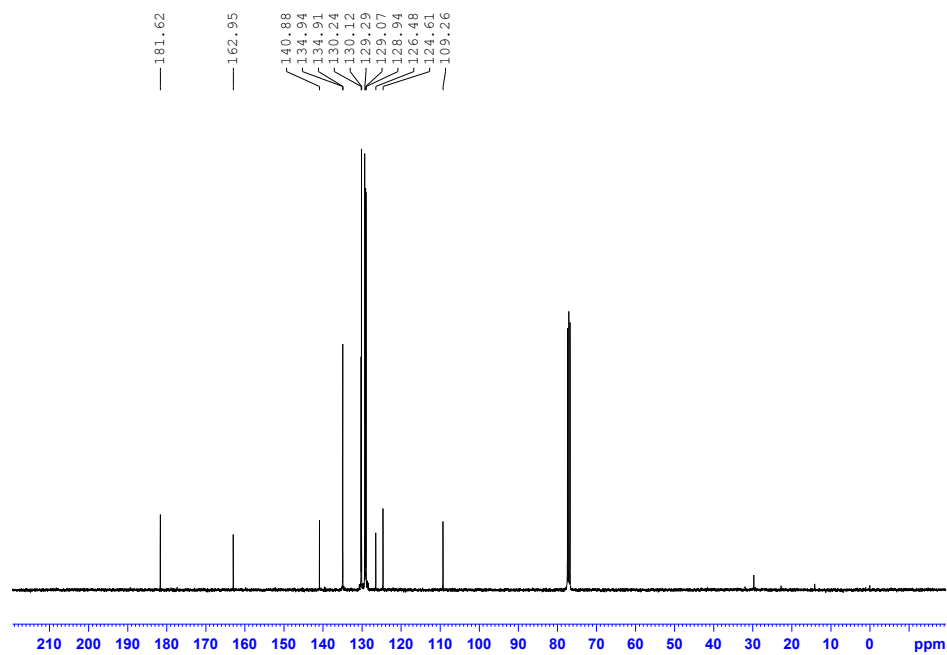


Figure S22. ^1H NMR of 5-(4-chlorobenzoyl)-3-cyano-4-phenylisoxazole (**7k**)

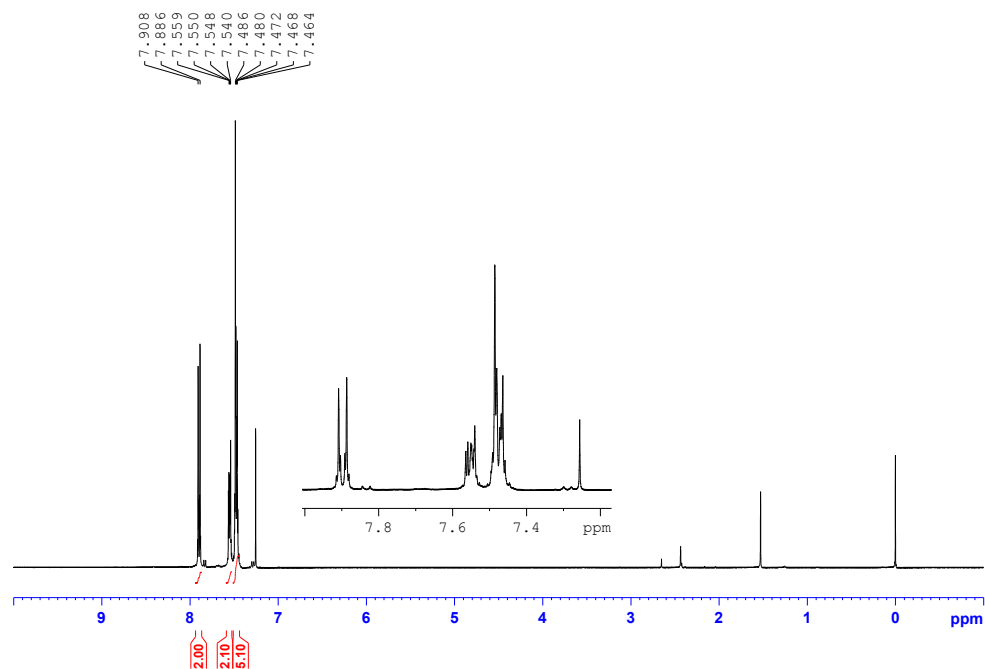


Figure S23. ^{13}C NMR of 5-(4-chlorobenzoyl)-3-cyano-4-phenylisoxazole (**7k**)

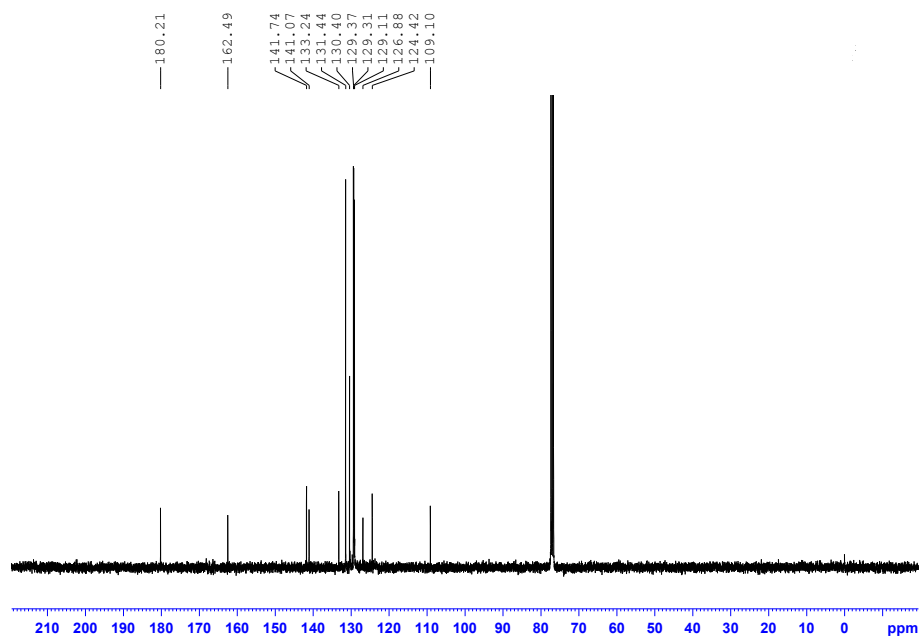


Figure S24. ^1H NMR of 3-cyano-5-(4-nitrobenzoyl)-4-phenylisoxazole (**7l**)

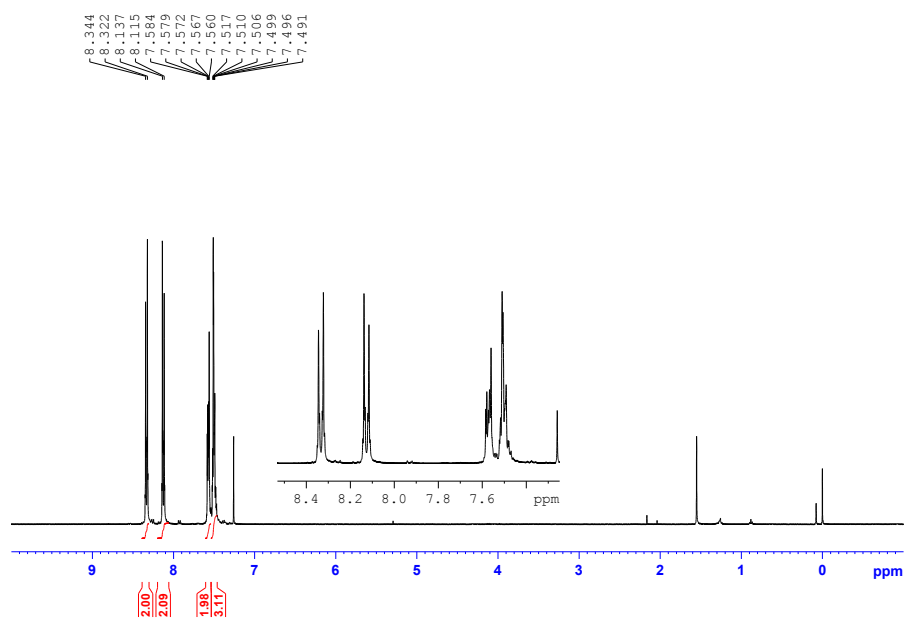


Figure S25. ^{13}C NMR 3-cyano-5-(4-nitrobenzoyl)-4-phenylisoxazole (**7l**)

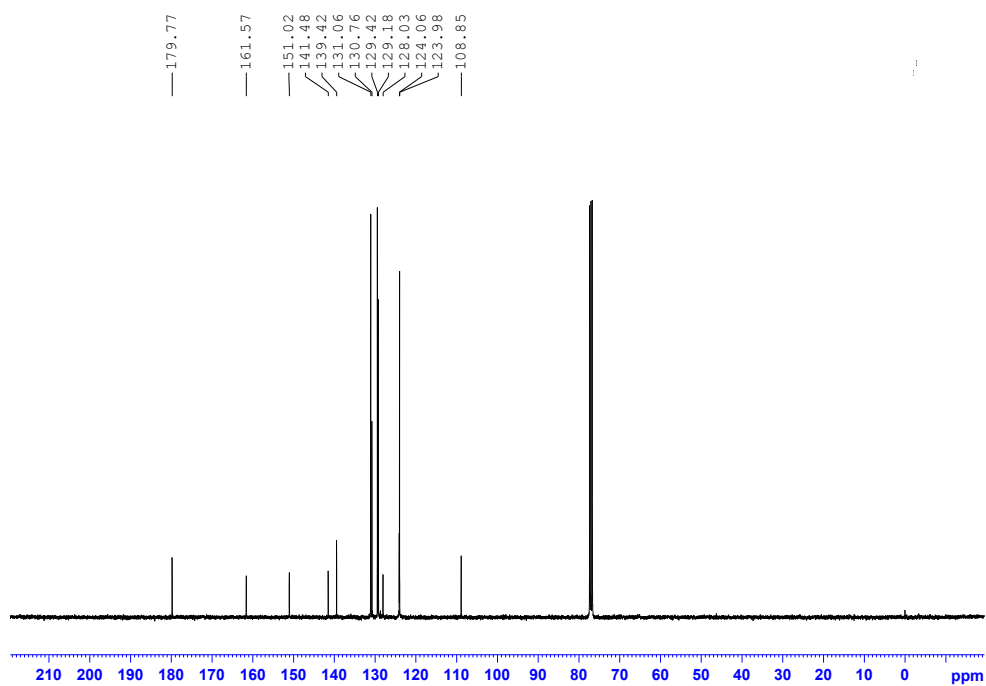


Figure S26. ^1H NMR of 3-cyano-5-(4-methylbenzoyl)-4-(4-methylphenyl)isoxazole (7m)

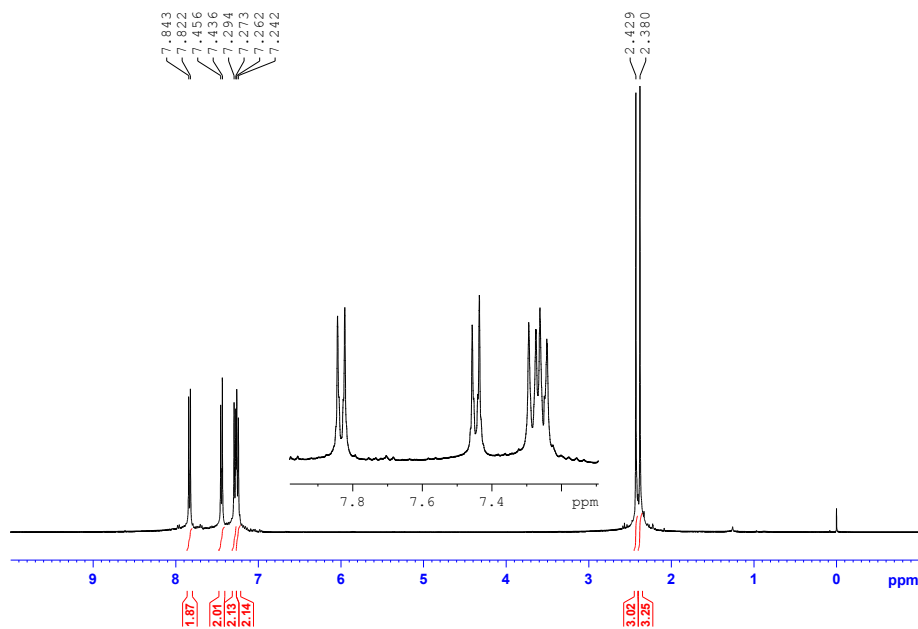


Figure S27. ^{13}C NMR of 3-cyano-5-(4-methylbenzoyl)-4-(4-methylphenyl)isoxazole (7m)

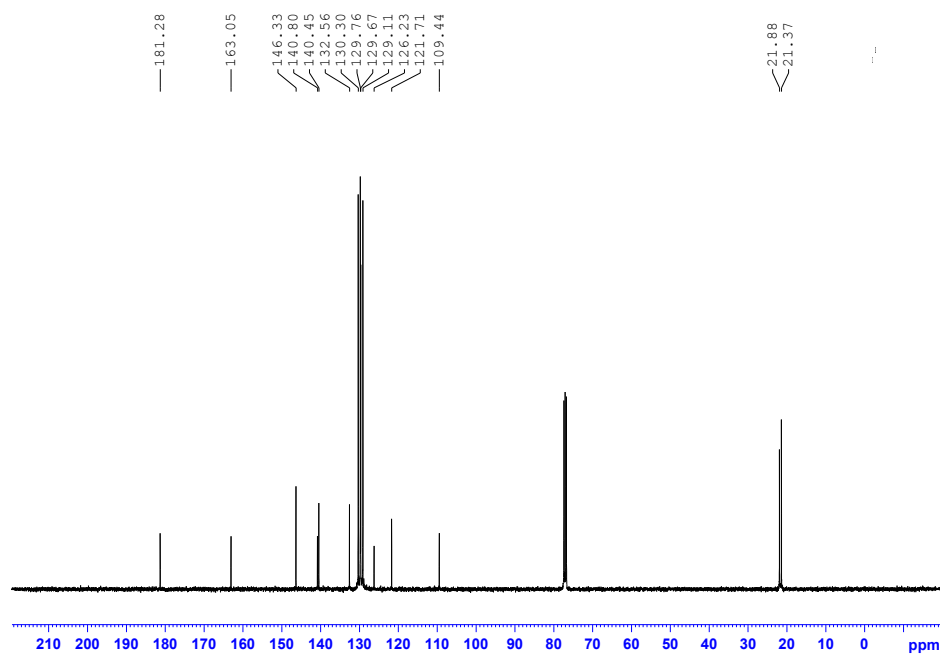


Figure S28. ^1H NMR of 5-benzoyl-3-cyano-4-(5-chloro-2-furyl)isoxazole (**7n**)

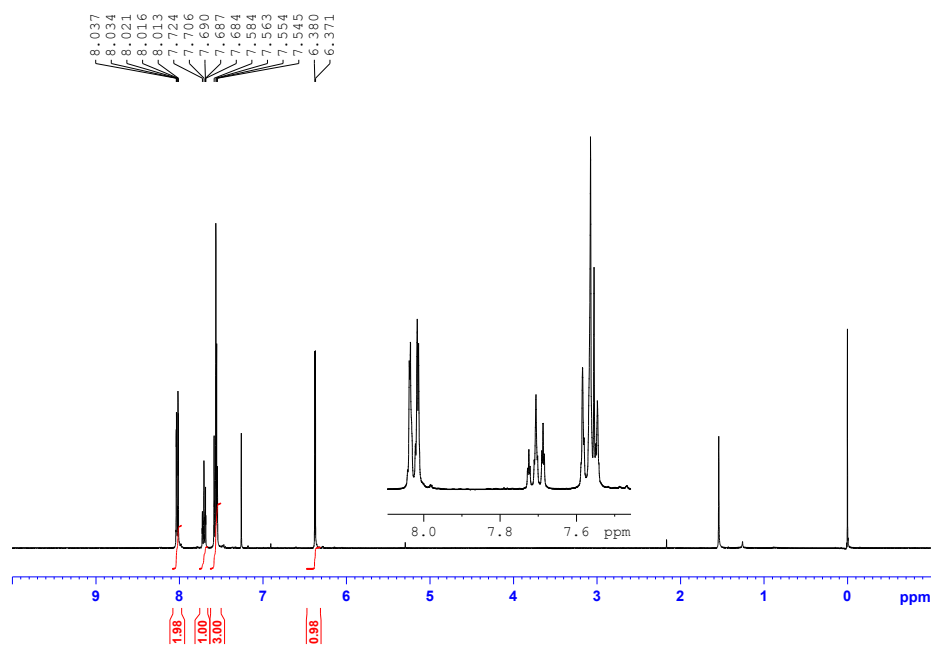


Figure S29. ^{13}C NMR of 5-benzoyl-3-cyano-4-(5-chloro-2-furyl)isoxazole (**7n**)

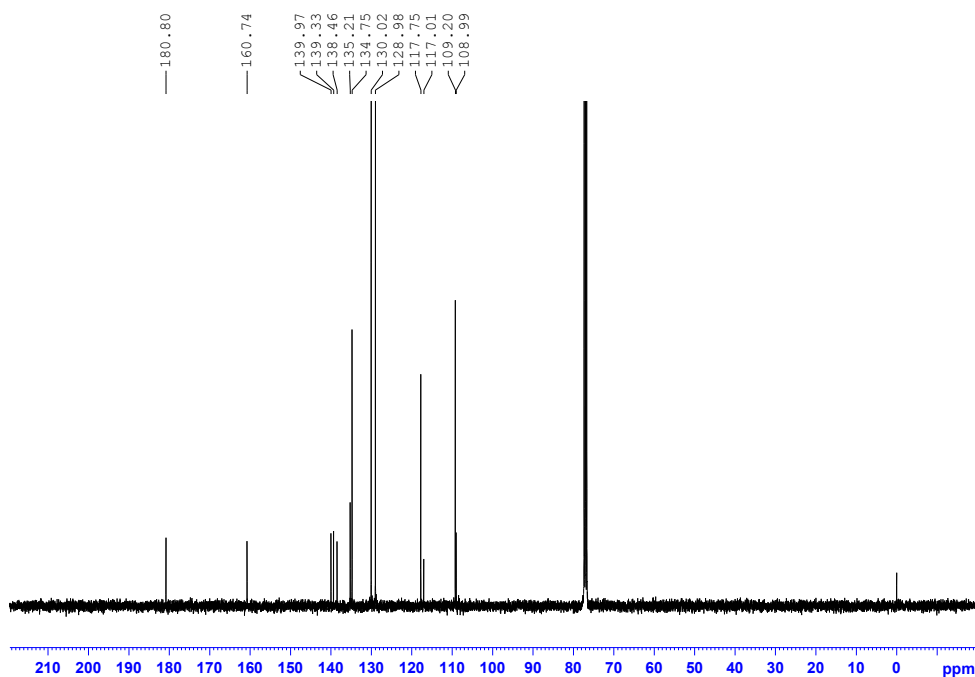


Figure S30. ^1H NMR of 5-benzoyl-3-cyano-4-propylisoxazole (**7o**)

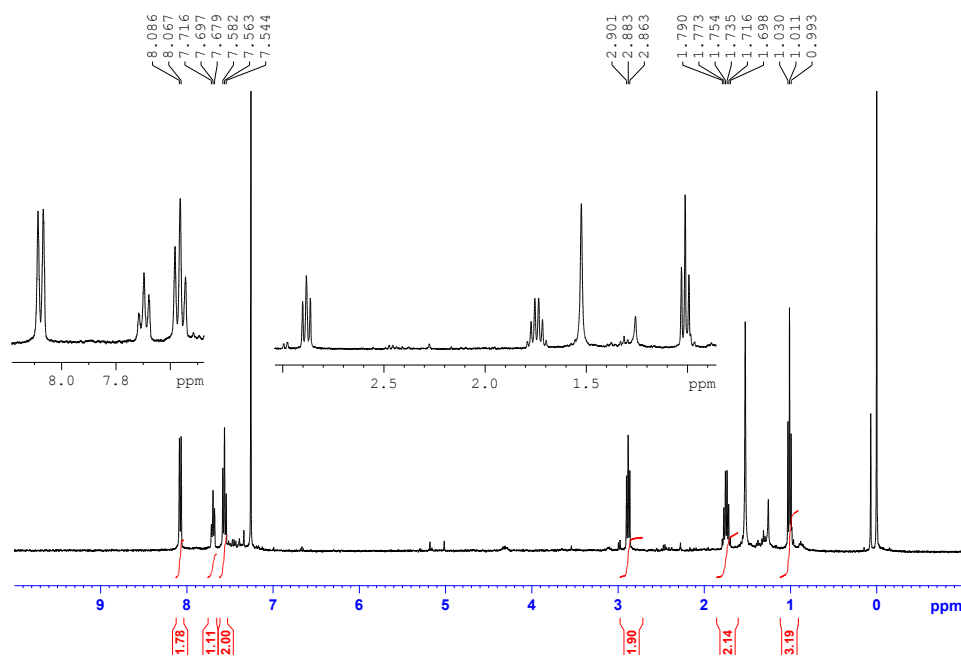


Figure S31. ^{13}C NMR of 5-benzoyl-3-cyano-4-propylisoxazole (**7o**)

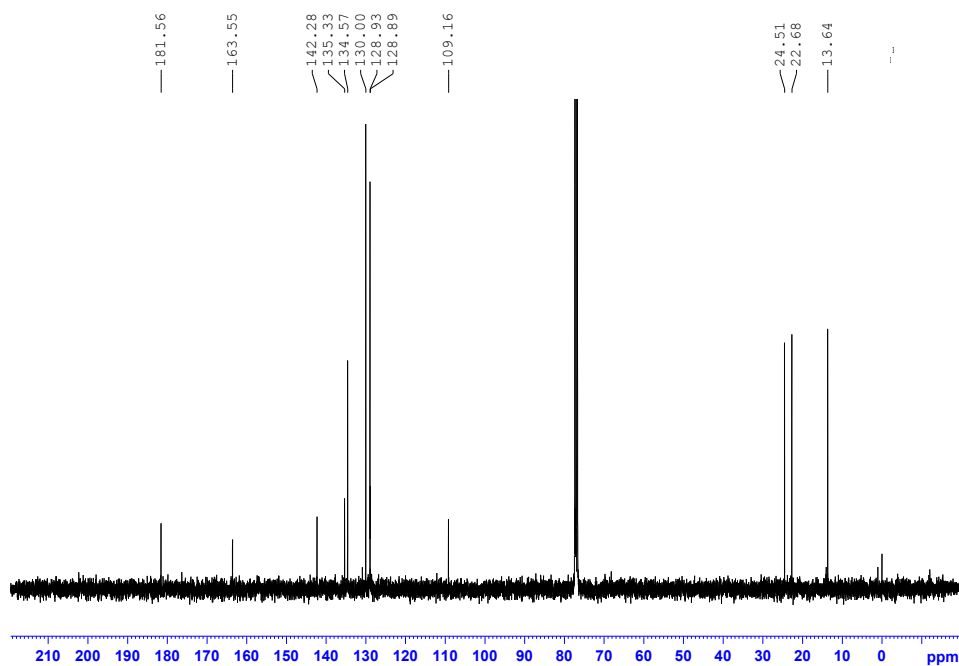


Figure S32. ^1H NMR of 5-benzoyl-3-cyanoisoxazole (**7p**)

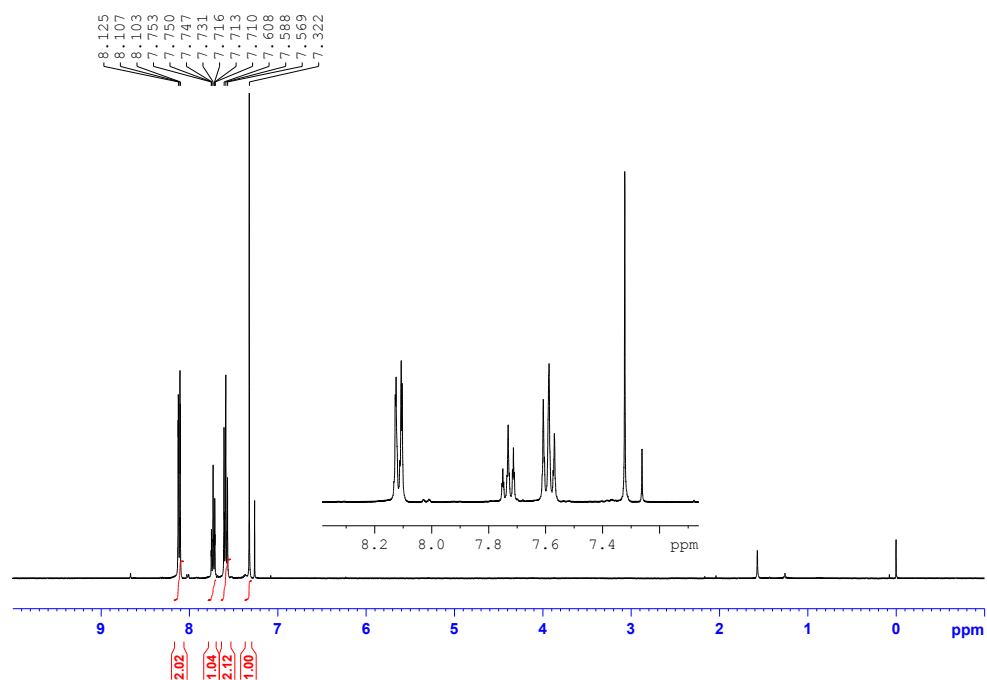


Figure S33. ^{13}C NMR of 5-benzoyl-3-cyanoisoxazole (**7p**)

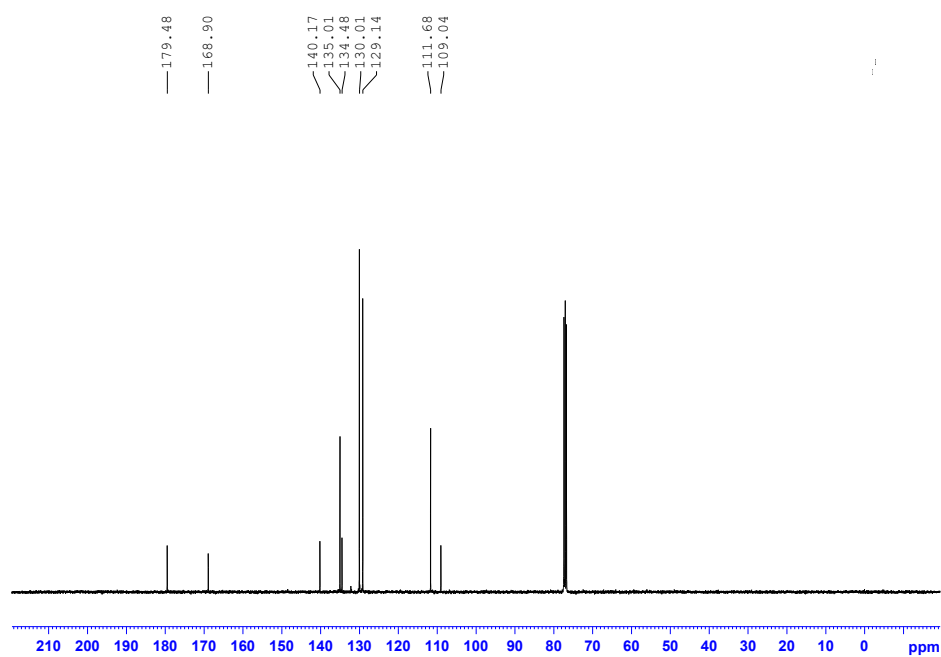


Figure S34. ^1H NMR of 7-oxocyclohexa[*d*]isoxazole-3-carboxamide (**7q**)

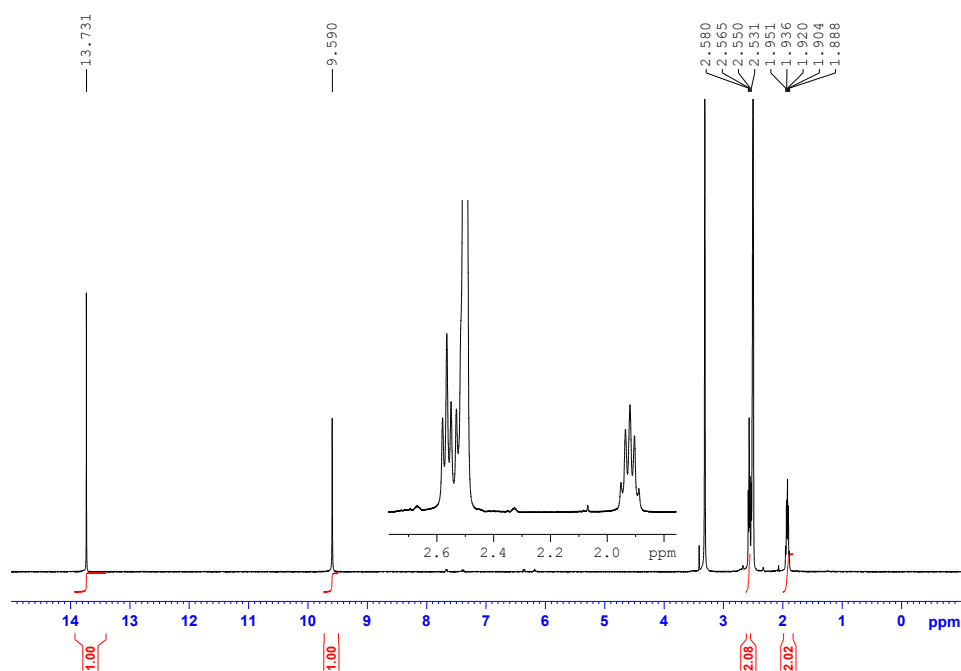


Figure S35. ^{13}C NMR of 7-oxocyclohexa[*d*]isoxazole-3-carboxamide (**7q**)

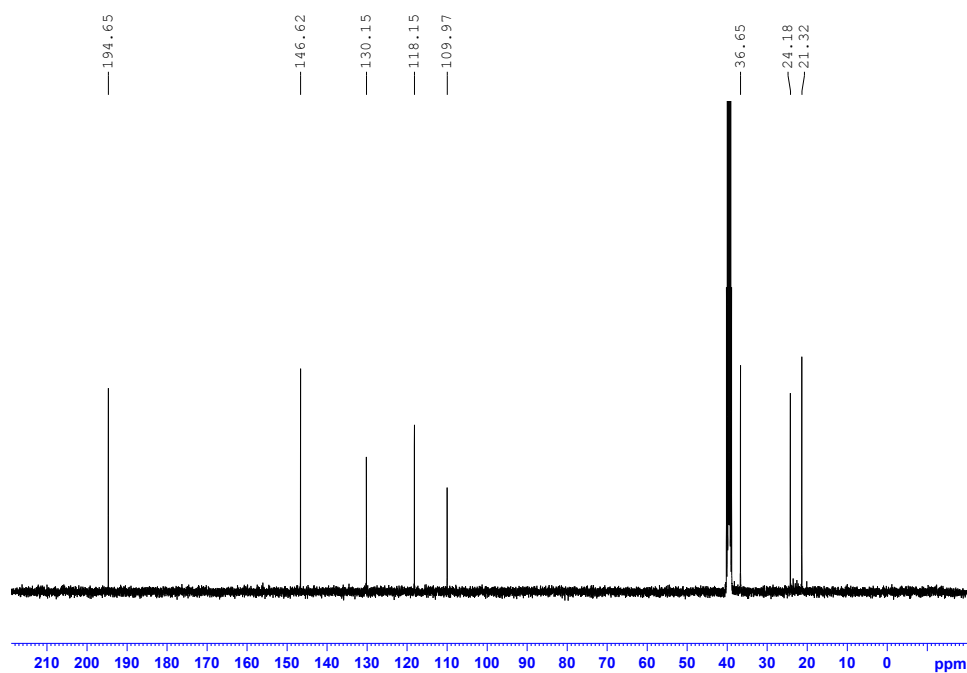


Figure S36. ^1H NMR of 6-oxocyclopenta[*d*]isoxazole-3-carboxamide (**7r**)

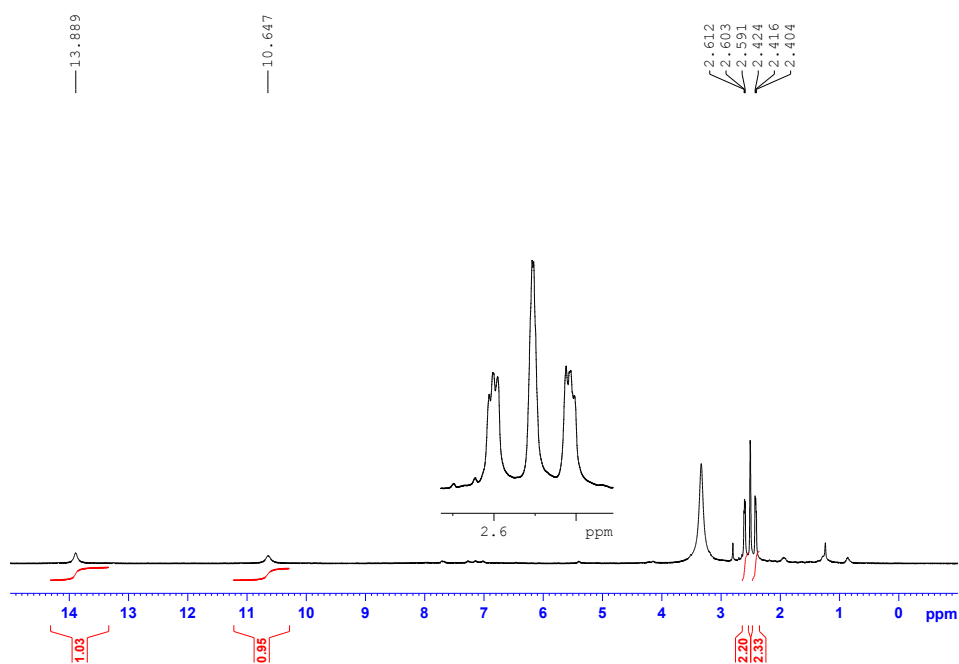


Figure S37. ^{13}C NMR of 6-oxocyclopenta[*d*]isoxazole-3-carboxamide (**7r**)

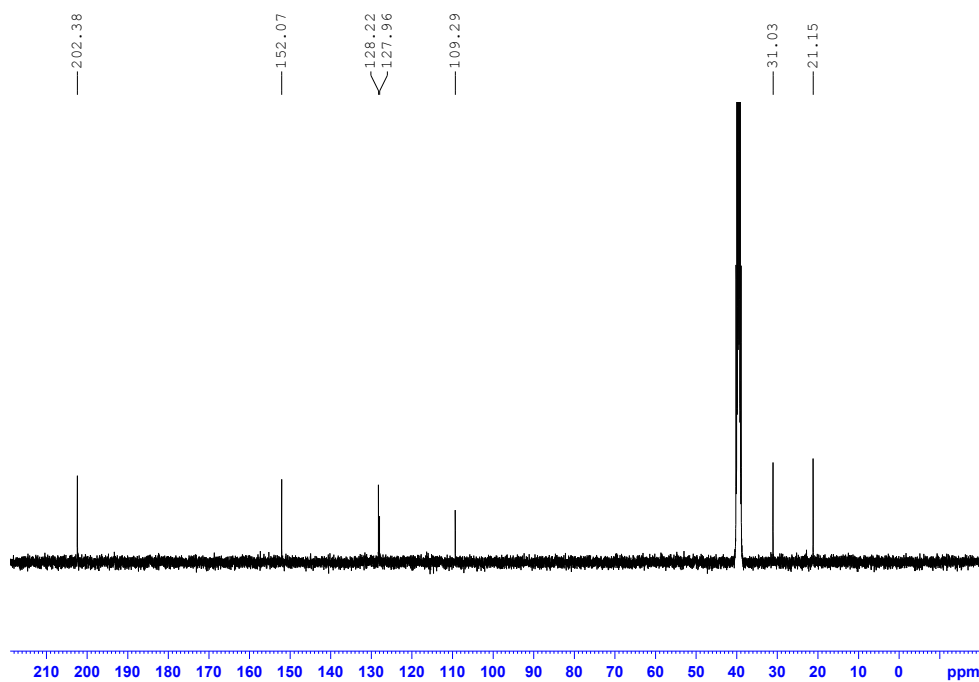


Figure S38. ^1H NMR of methyl 4-(4-chlorophenyl)-5-ethanoylisoxazole-3-carboxylate (10)

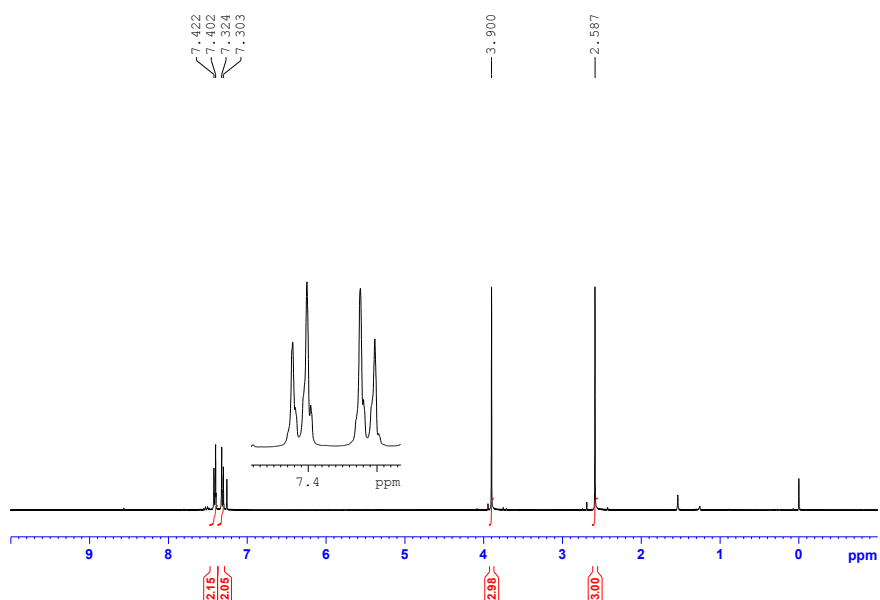


Figure S39. ^{13}C NMR of methyl 4-(4-chlorophenyl)-5-ethanoylisoxazole-3-carboxylate (10)

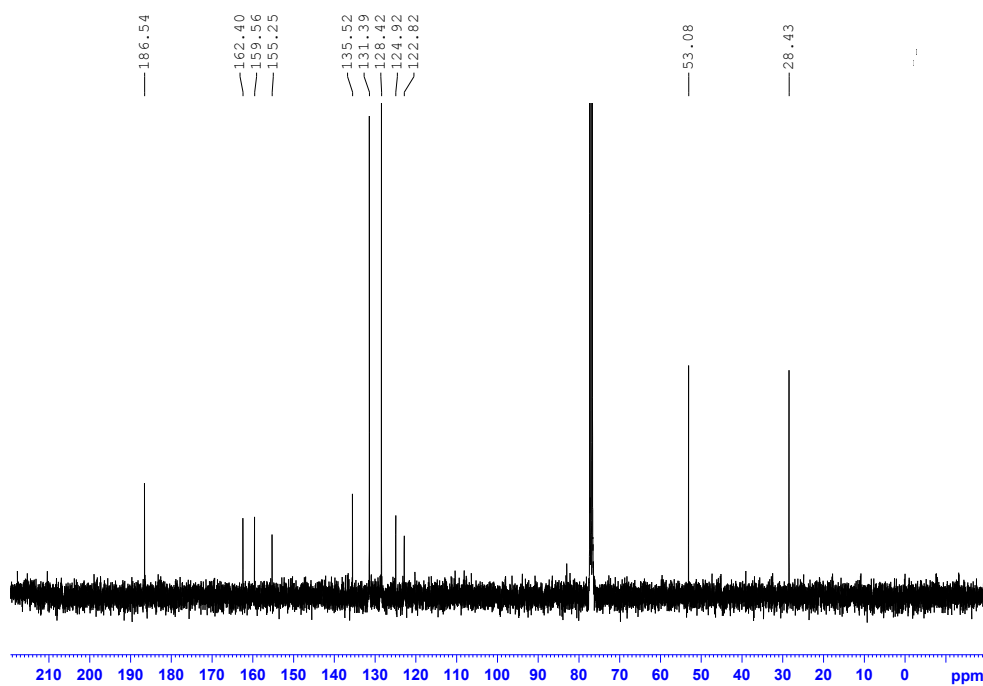


Figure S40. ^1H NMR of ethyl-5-(4-methylbenzoyl)-4-(4-methylphenyl)isoxazole-3-carboxylate (**11**)

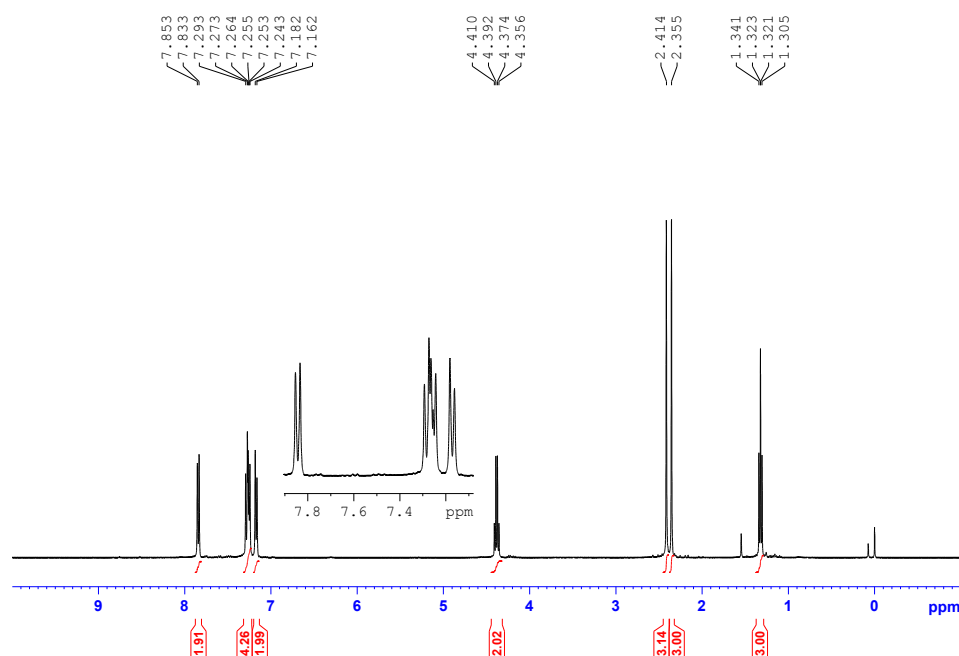


Figure S41. ^{13}C NMR of ethyl-5-(4-methylbenzoyl)-4-(4-methylphenyl)isoxazole-3-carboxylate (**11**)

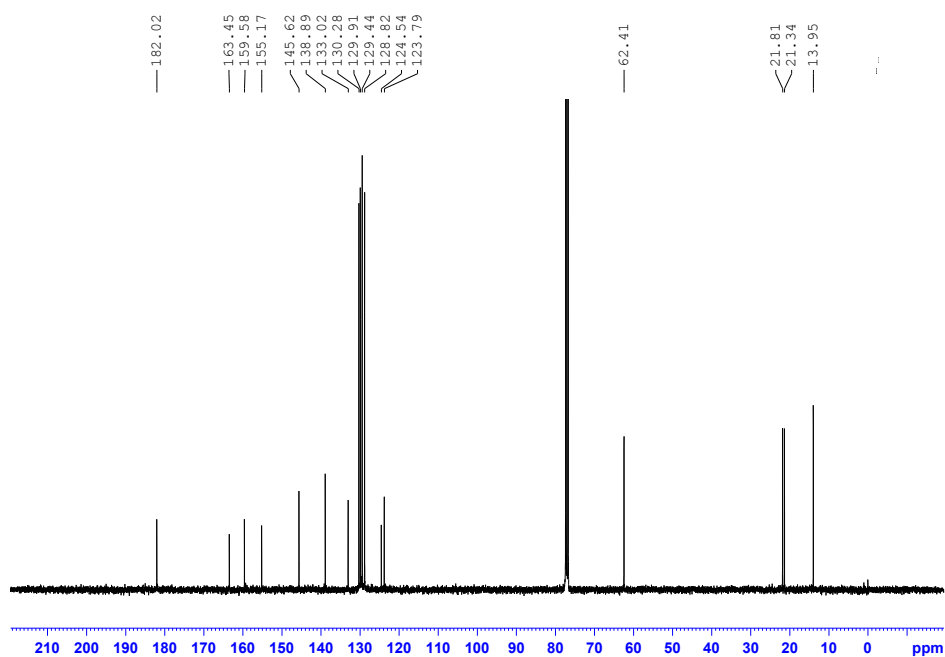


Figure S42. ^1H NMR of
5-(4-methylbenzoyl)-4-(4-methylphenyl)-3-(5-(1-benzyltetrazolyl))isoxazole (**13a**)

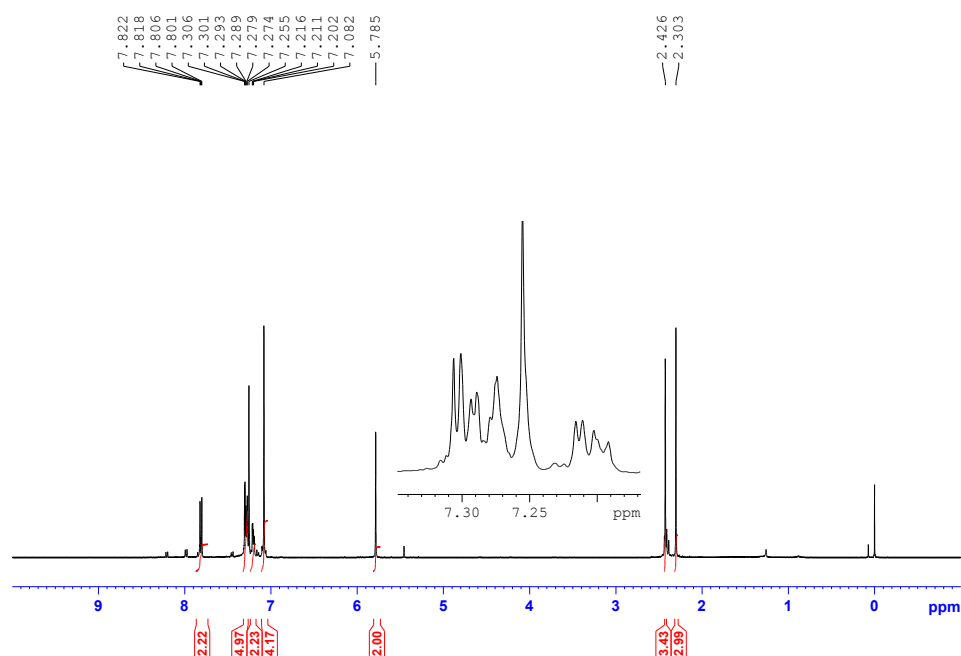


Figure S43. ^{13}C NMR of
5-(4-methylbenzoyl)-4-(4-methylphenyl)-3-(5-(1-benzyltetrazolyl))isoxazole (**13a**)

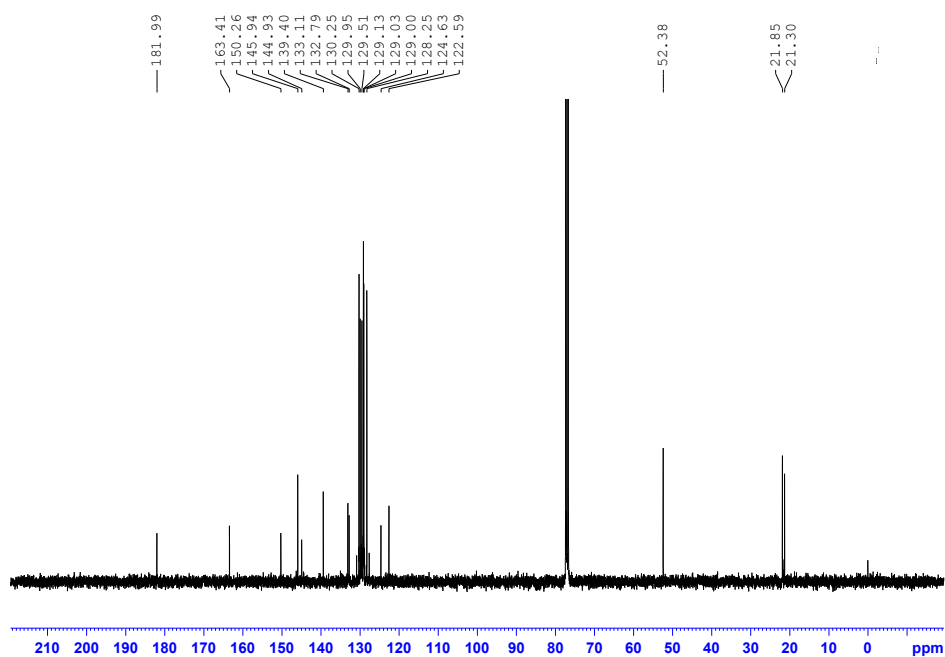


Figure S44. ^1H NMR of
5-(4-methylbenzoyl)-4-(4-methylphenyl)-3-(5-tetrazolyl)isoxazole (**13b**)

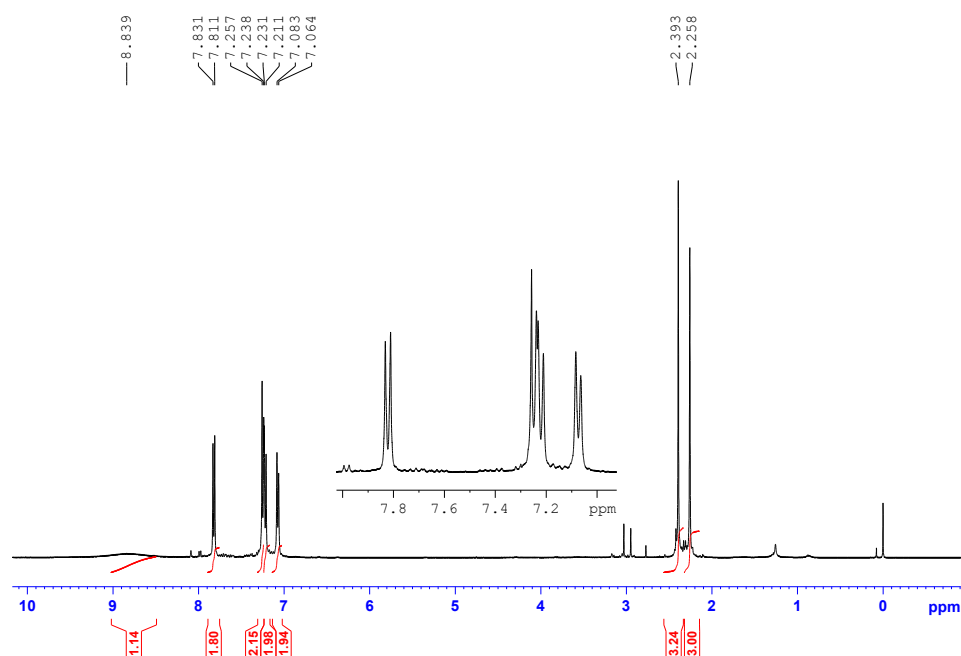


Figure S45. ^{13}C NMR of
5-(4-methylbenzoyl)-4-(4-methylphenyl)-3-(5-tetrazolyl)isoxazole (**13b**)

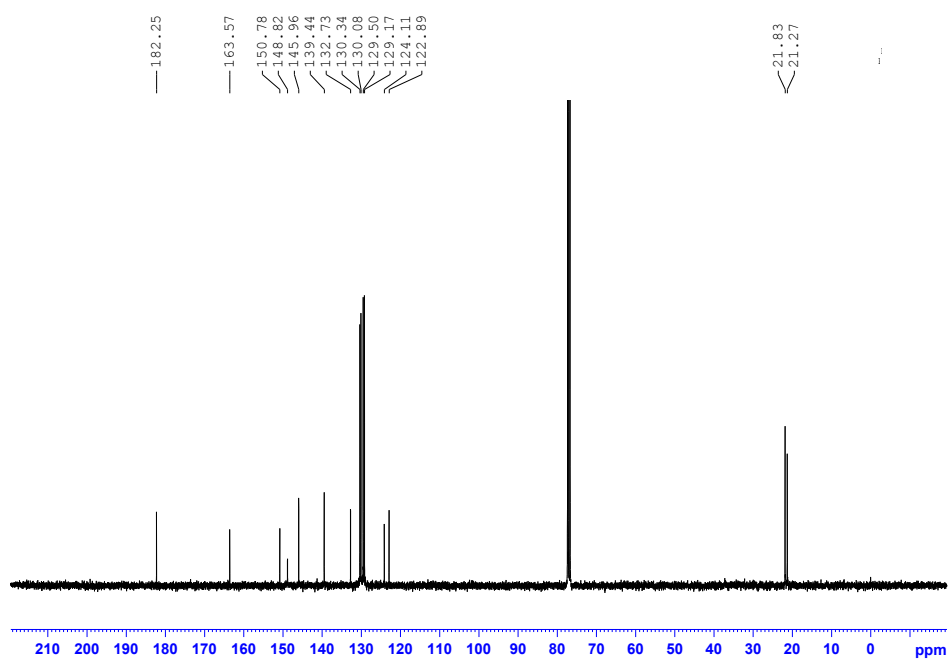


Figure S46. ^1H NMR of
3-cyano-5-[(1-(hydroxyimino)ethyl)]-4-(4-methoxy-phenyl)isoxazole

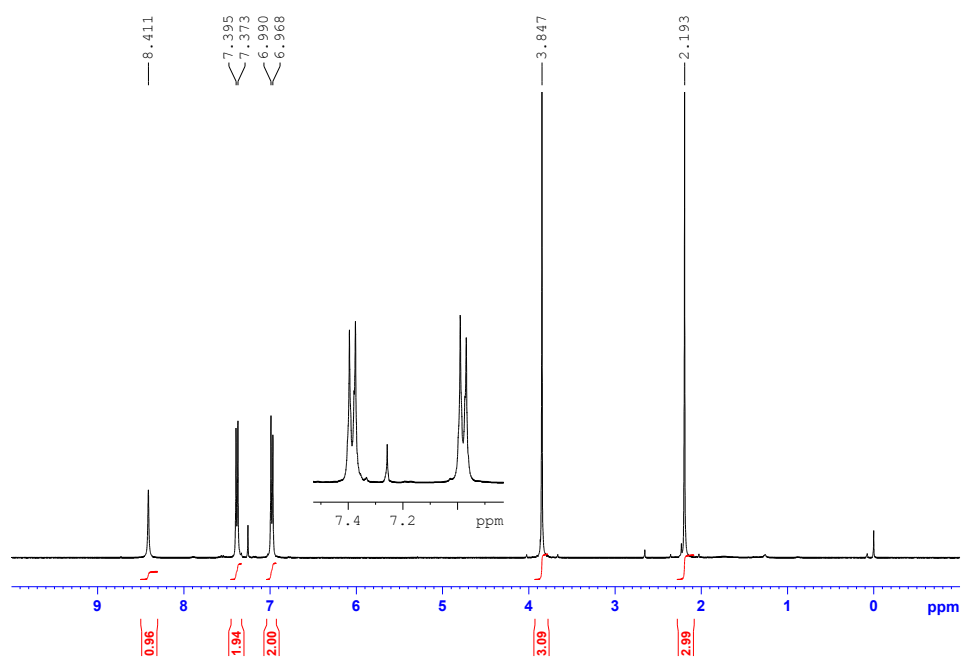


Figure S47. ^{13}C NMR of
3-cyano-5-[(1-(hydroxyimino)ethyl)]-4-(4-methoxy-phenyl)isoxazole

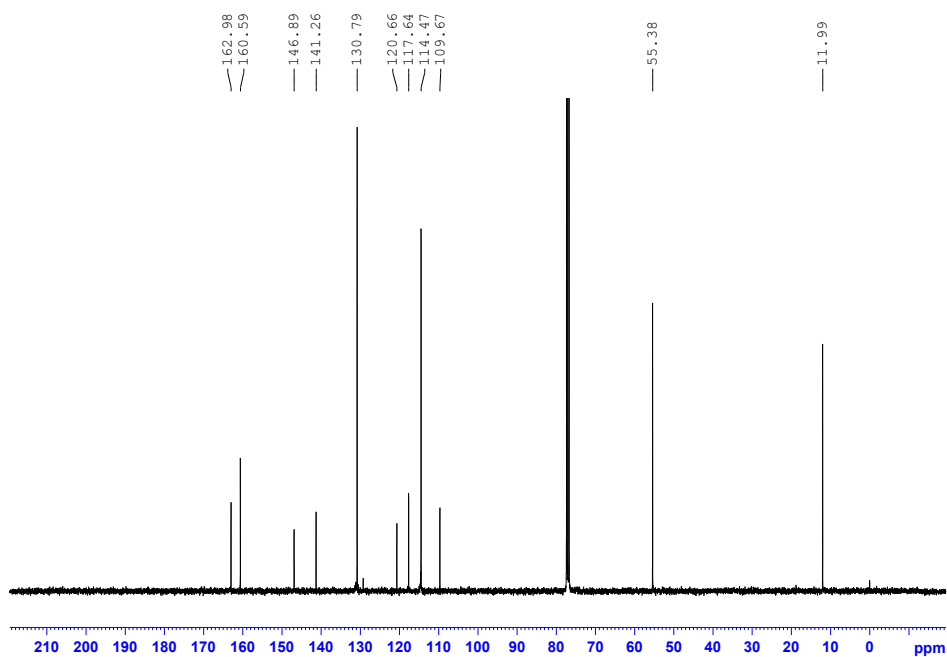


Figure S48. ^1H NMR of
3-cyano-5-[(1-ethanoyloxyimino)ethyl]-4-(4-methoxy-phenyl)isoxazole (**14**)

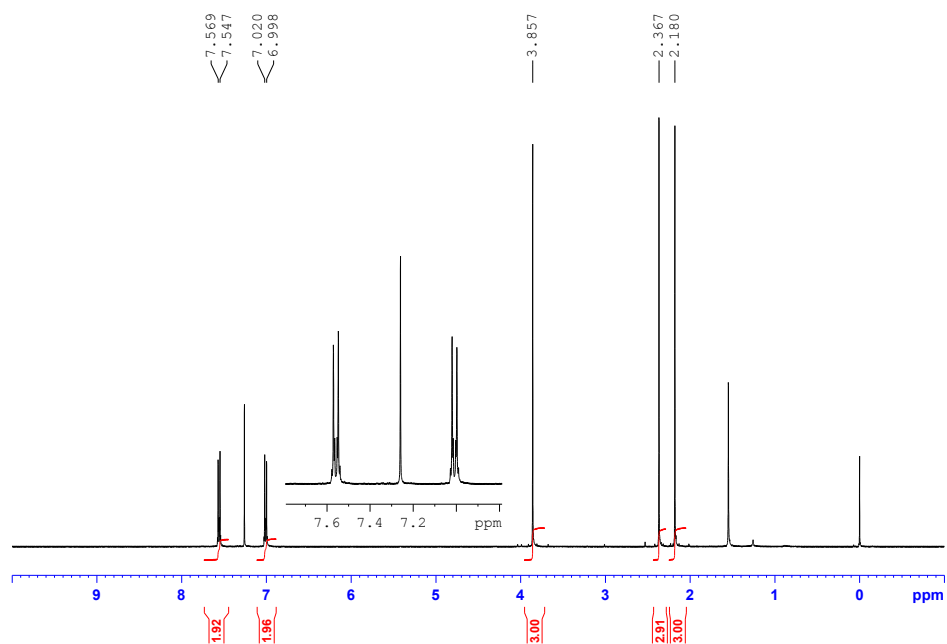


Figure S49. ^{13}C NMR of
3-cyano-5-[(1-ethanoyloxyimino)ethyl]-4-(4-methoxy-phenyl)isoxazole (**14**)

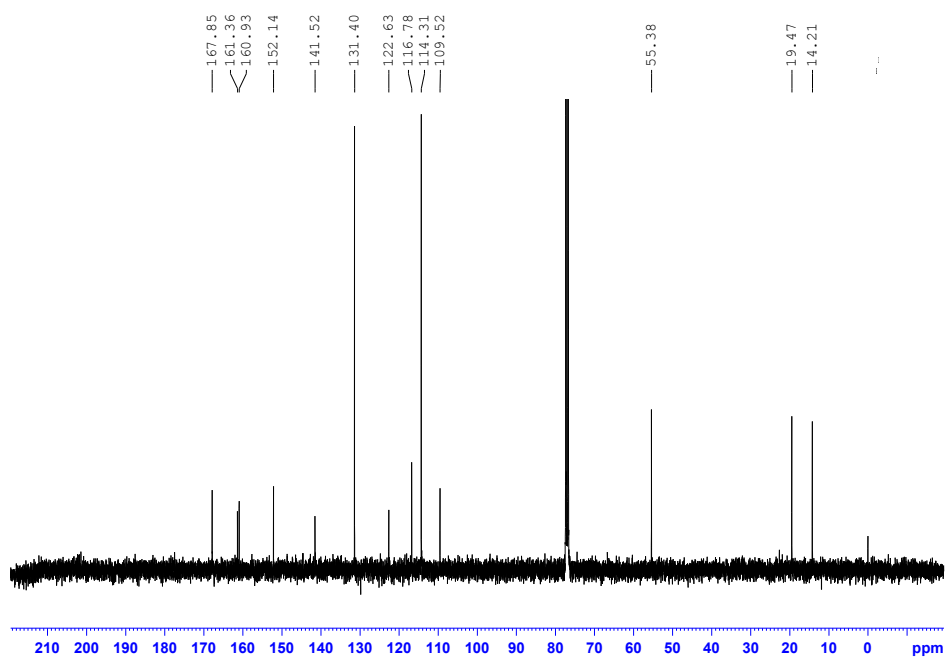


Figure S50. ^1H NMR of 1-cyano-7-methoxy-4-methylisoxazolo[5,4-*c*]quinoline (**15**)

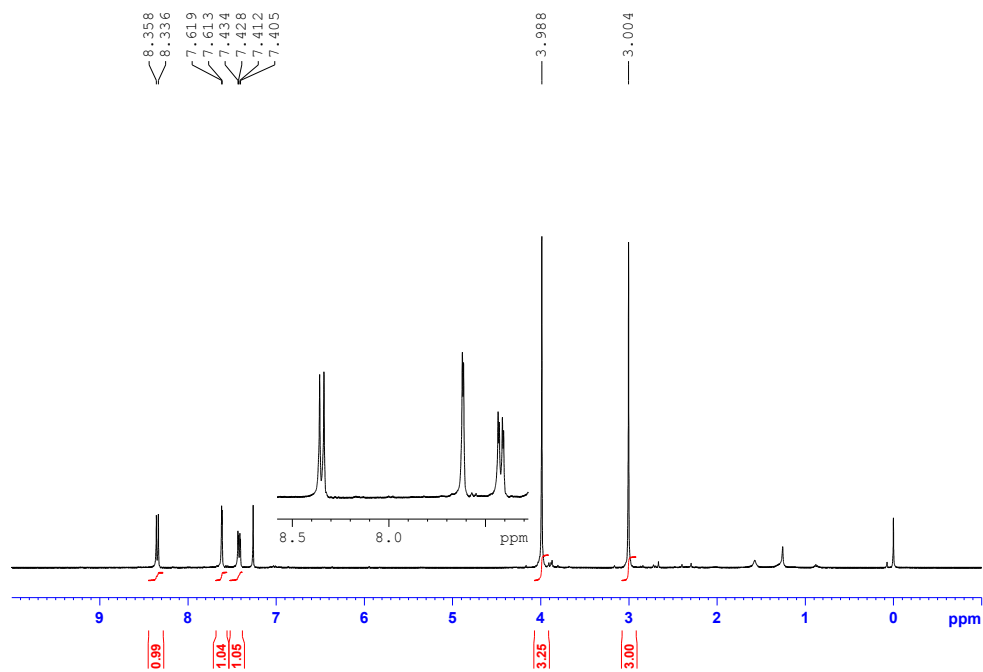


Figure S51. ^{13}C NMR of 1-cyano-7-methoxy-4-methylisoxazolo[5,4-*c*]quinoline (**15**)

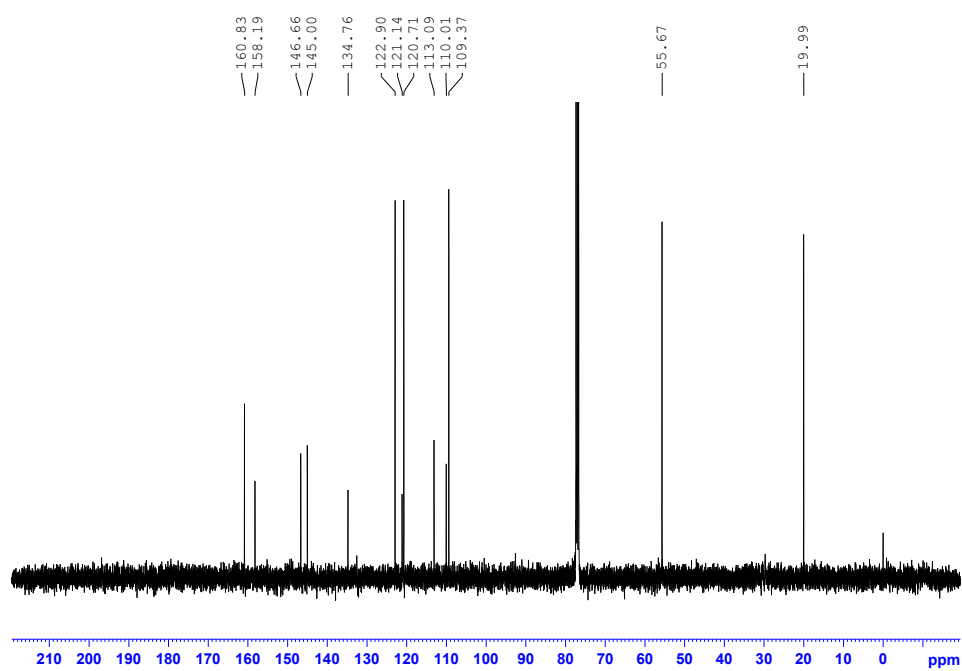


Figure S52. ^1H NMR of 2,4-dinitrophenylhydrazone of isoxazole **7a**

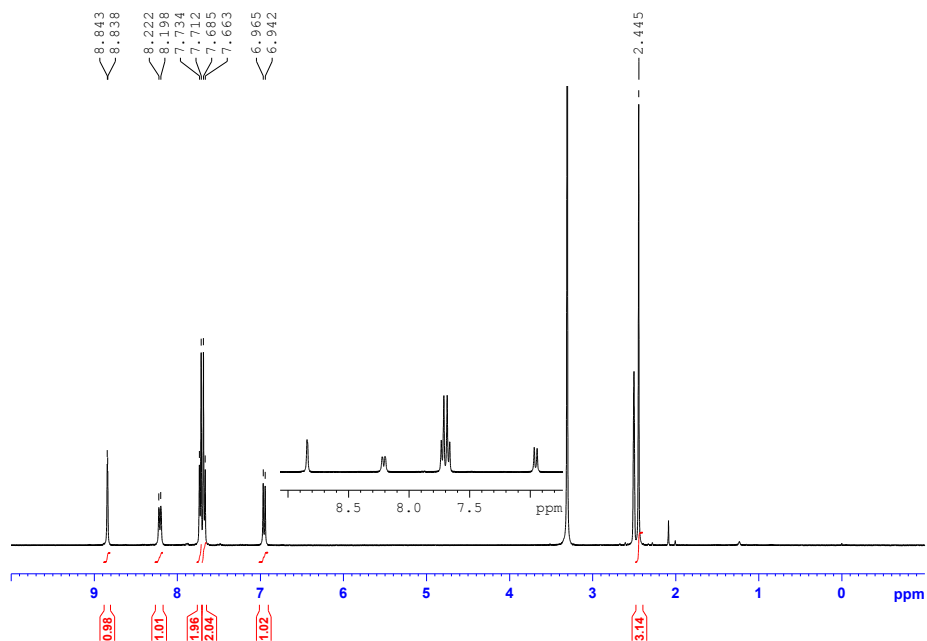
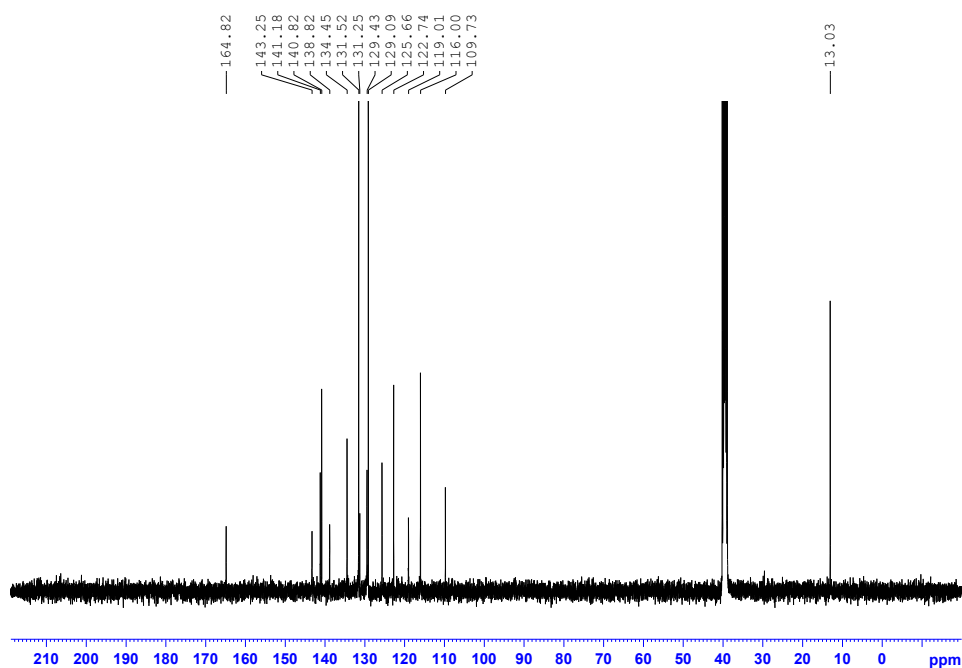


Figure S53. ^{13}C NMR of 2,4-dinitrophenylhydrazone of isoxazole **7a**



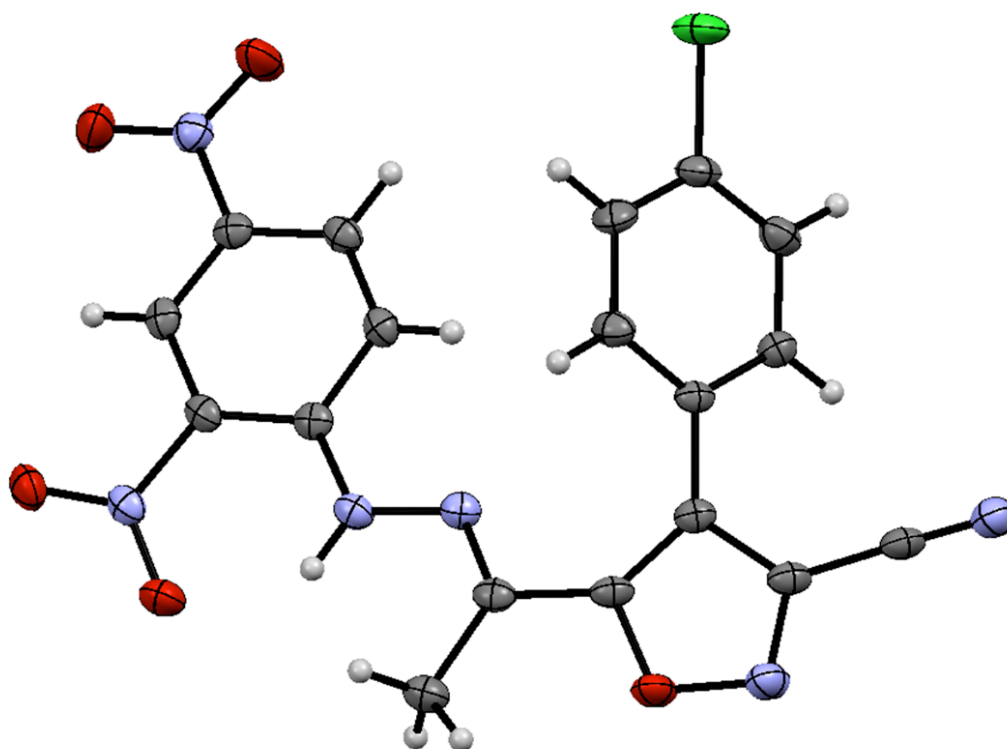


Figure S54. The structure of **7a** was determined by X-ray structural analysis using the 2,4-dinitrophenylhydrazone. Thermal ellipsoids are drawn at the 50% probability level. CCDC 1542549 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.