

Synthesis of isoxazol-5-one derivatives catalyzed by amine-functionalized cellulose

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Supplementary Materials (Figures S1-S36)

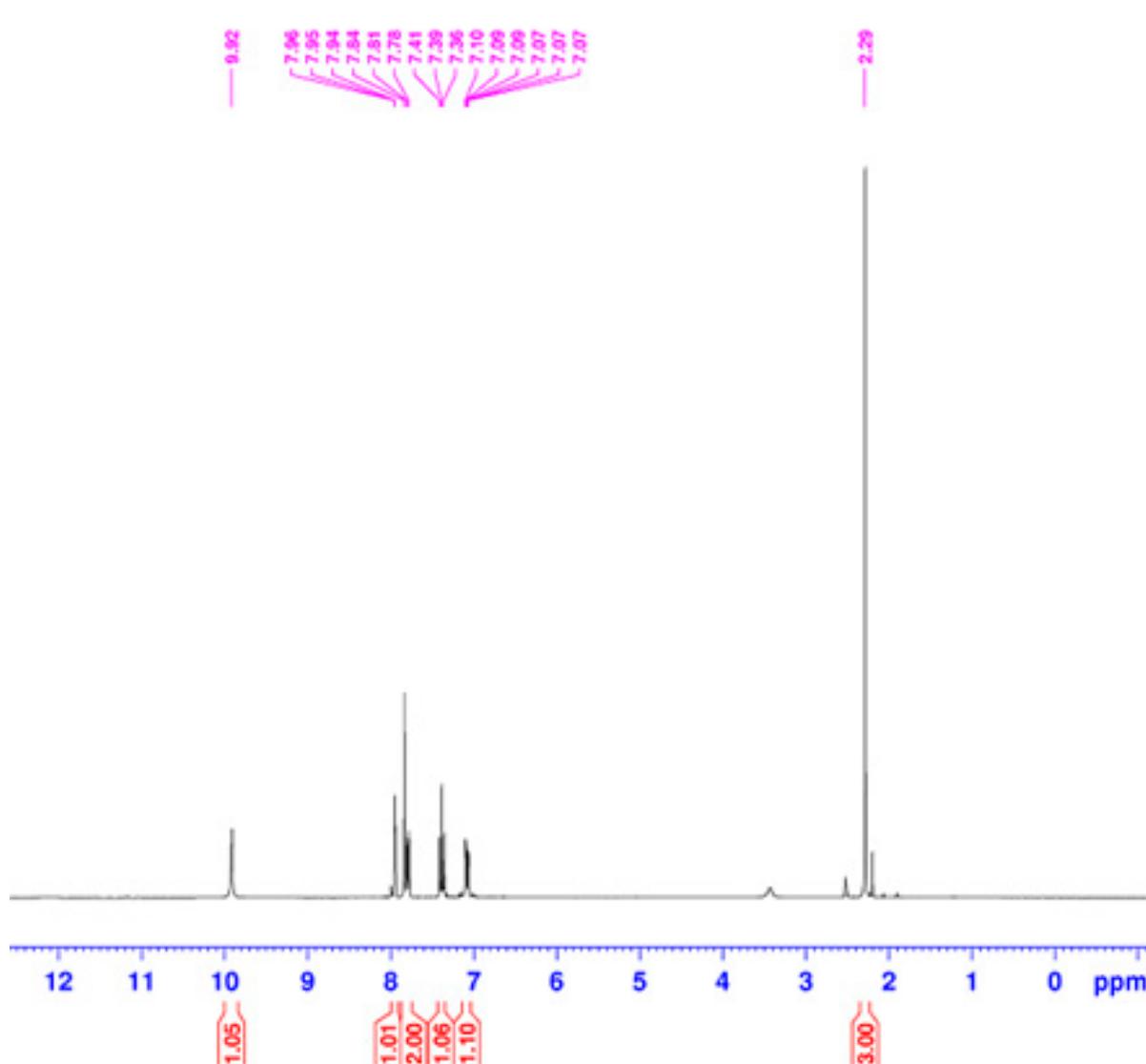


Figure S1. ¹H NMR (300 MHz, DMSO-*d*₆) spectrum of 4-(3-hydroxybenzylidene)-3-methylisoxazol-5(4*H*)-one (**4e**)

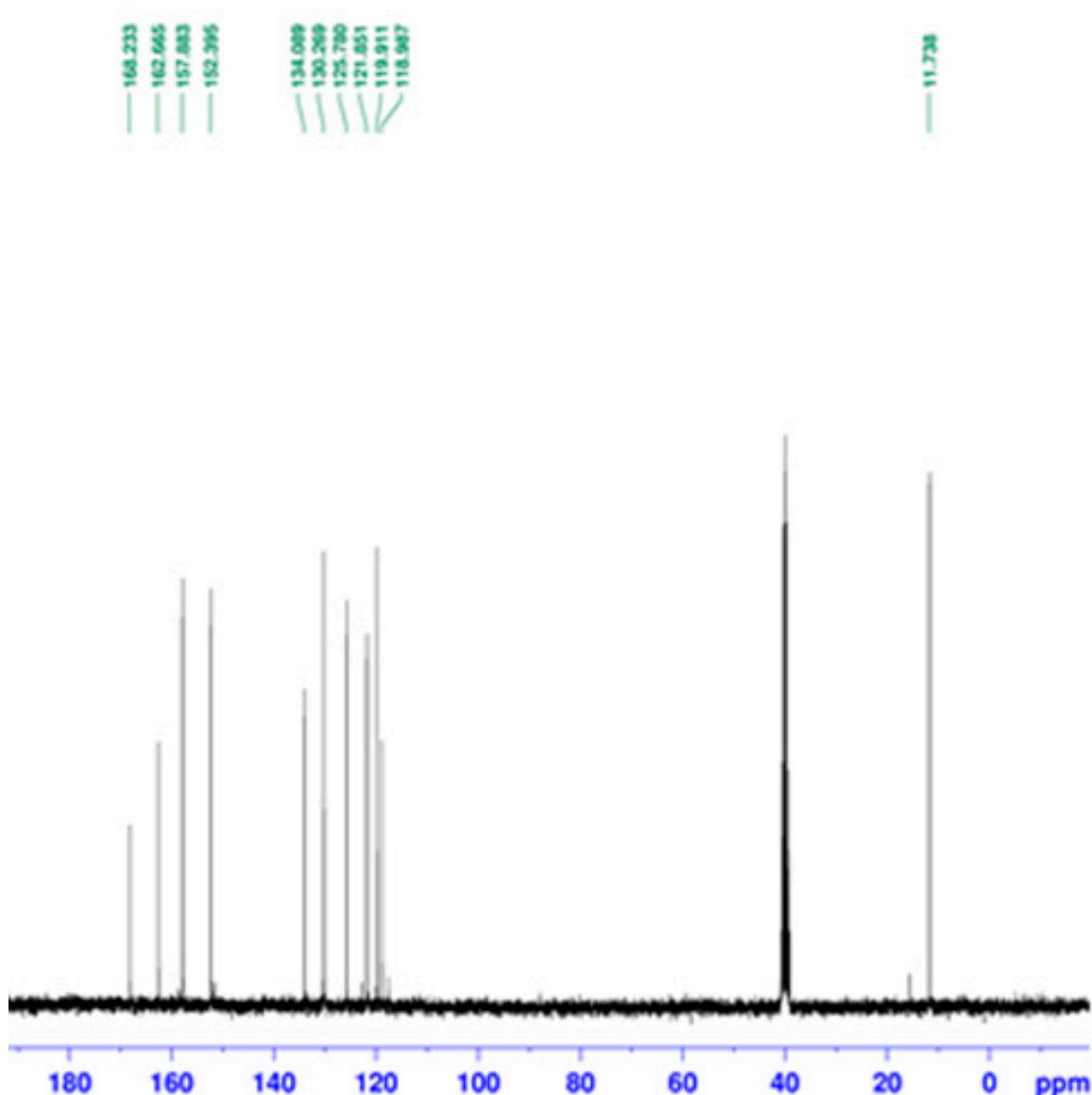


Figure S2. ¹³C NMR (75 MHz, DMSO-*d*₆) spectrum of 4-(3-hydroxybenzylidene)-3-methylisoxazol-5(4*H*)-one (**4e**)

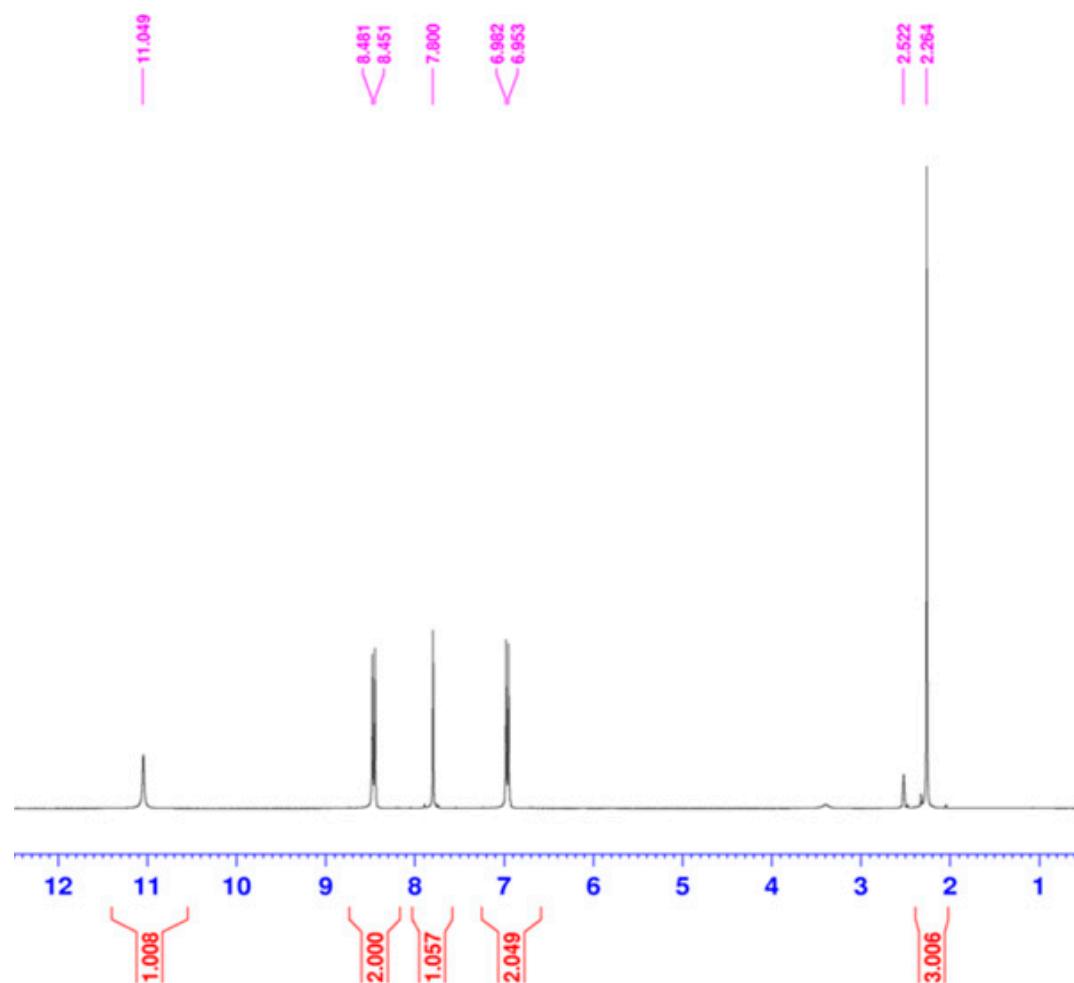


Figure S3. ¹H NMR (300 MHz, DMSO-*d*₆) spectrum of 4-(4-hydroxybenzylidene)-3-methylisoxazol-5(4*H*)-one (**4f**)

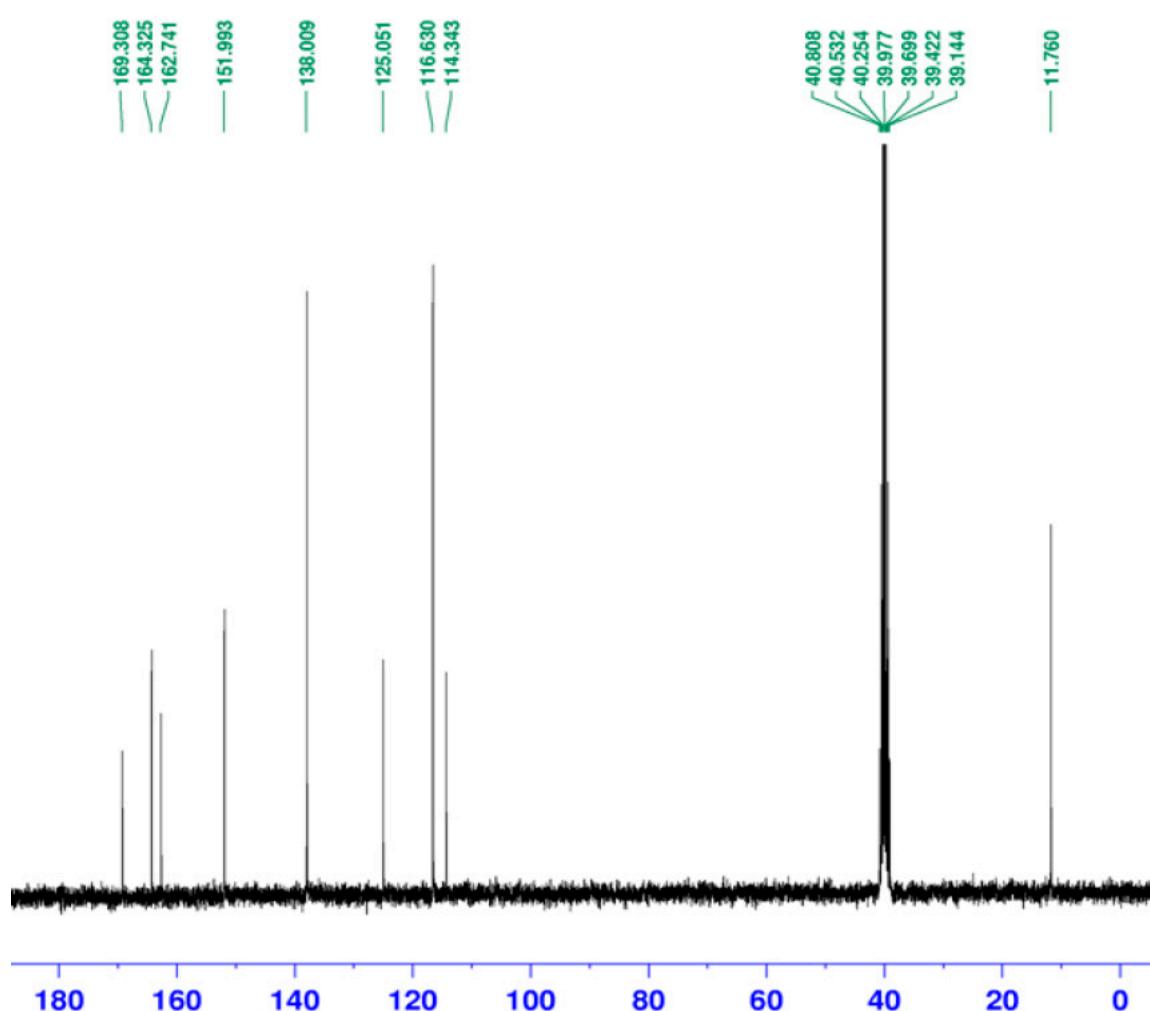


Figure S4. ^{13}C NMR (75 MHz, $\text{DMSO}-d_6$) spectrum of 4-(4-hydroxybenzylidene)-3-methylisoxazol-5(4H)-one (4f)

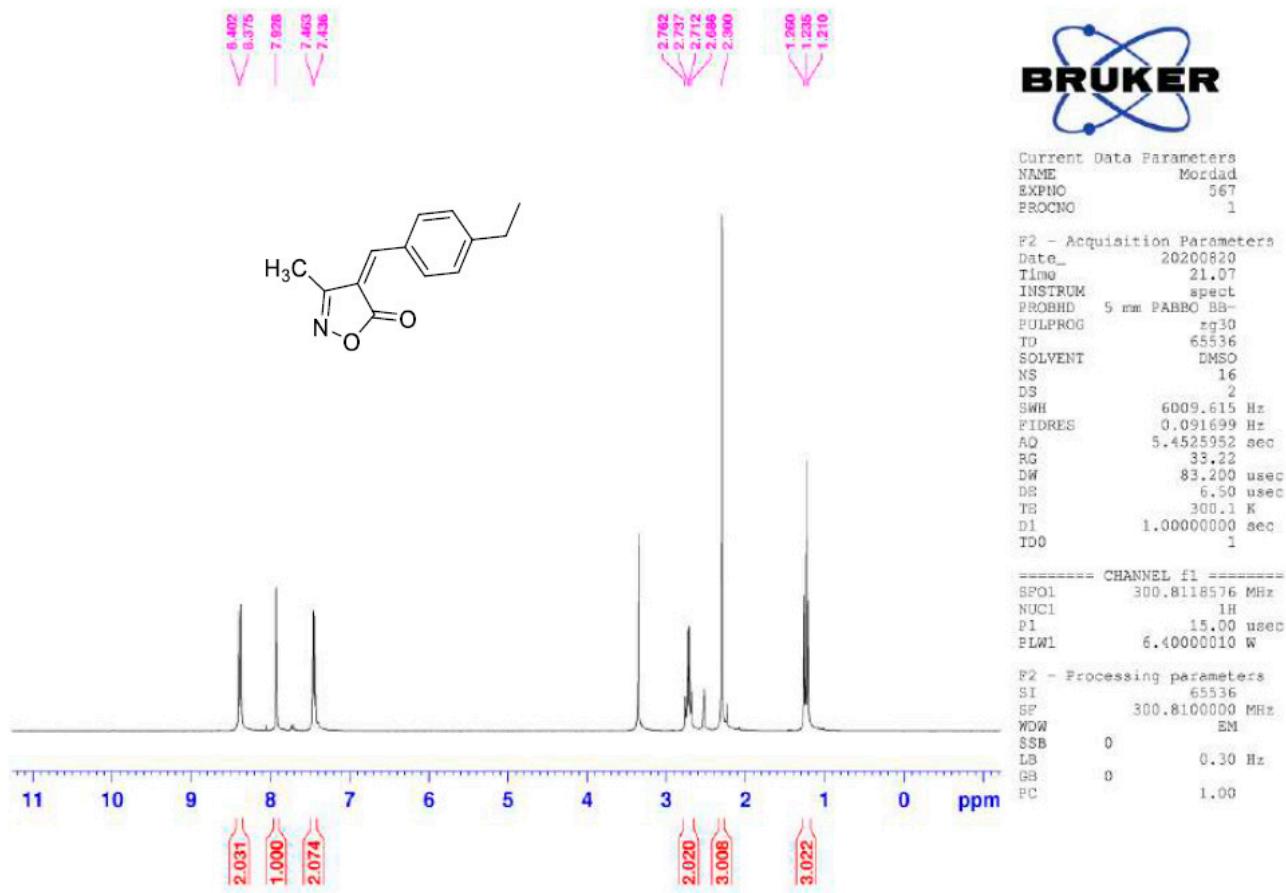


Figure S5. ^1H NMR (300 MHz, DMSO- d_6) spectrum of 4-(4-ethylbenzylidene)-3-methylisoxazol-5(4H)-one (**4h**)

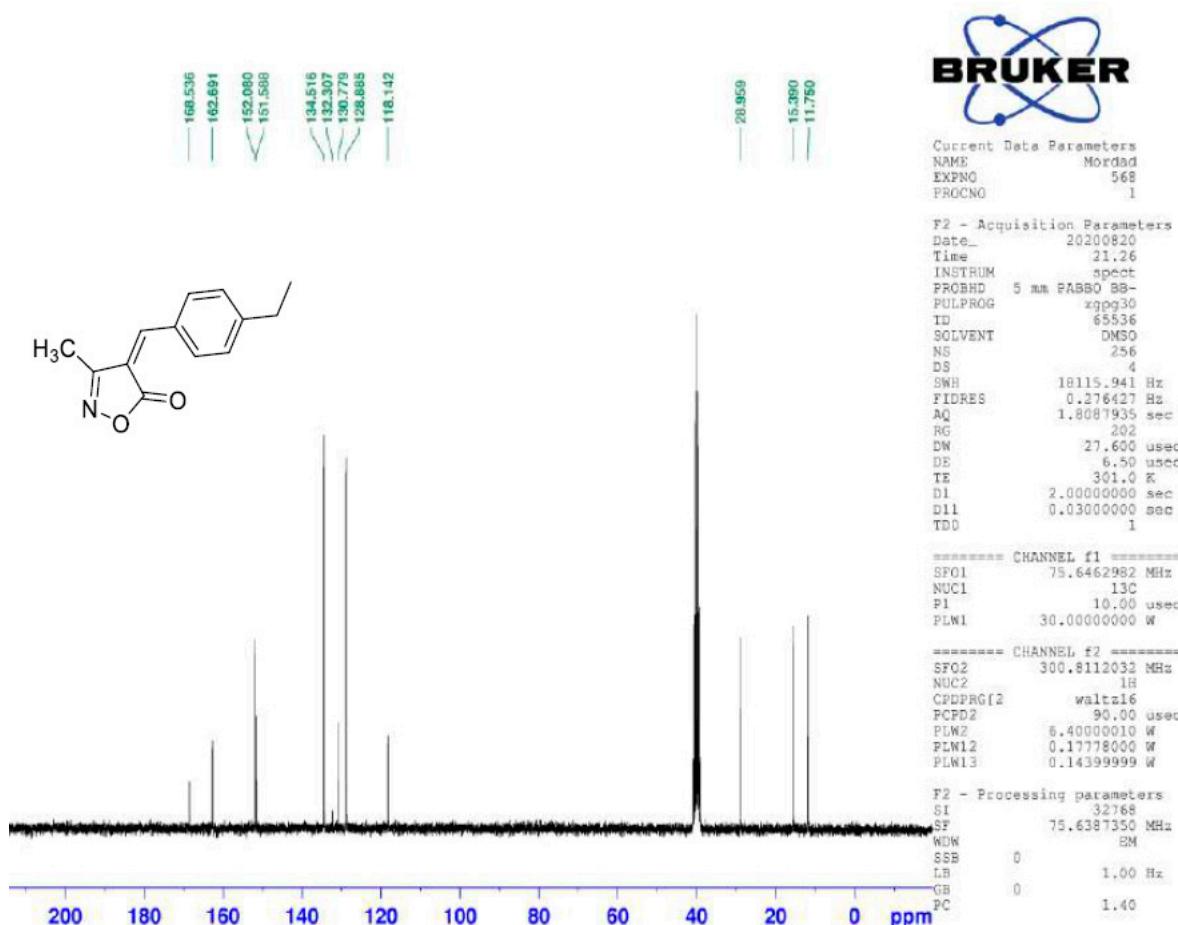


Figure S6. ^{13}C NMR (300 MHz, $\text{DMSO}-d_6$) spectrum of 4-(4-ethylbenzylidene)-3-methylisoxazol-5(4H)-one (**4h**)

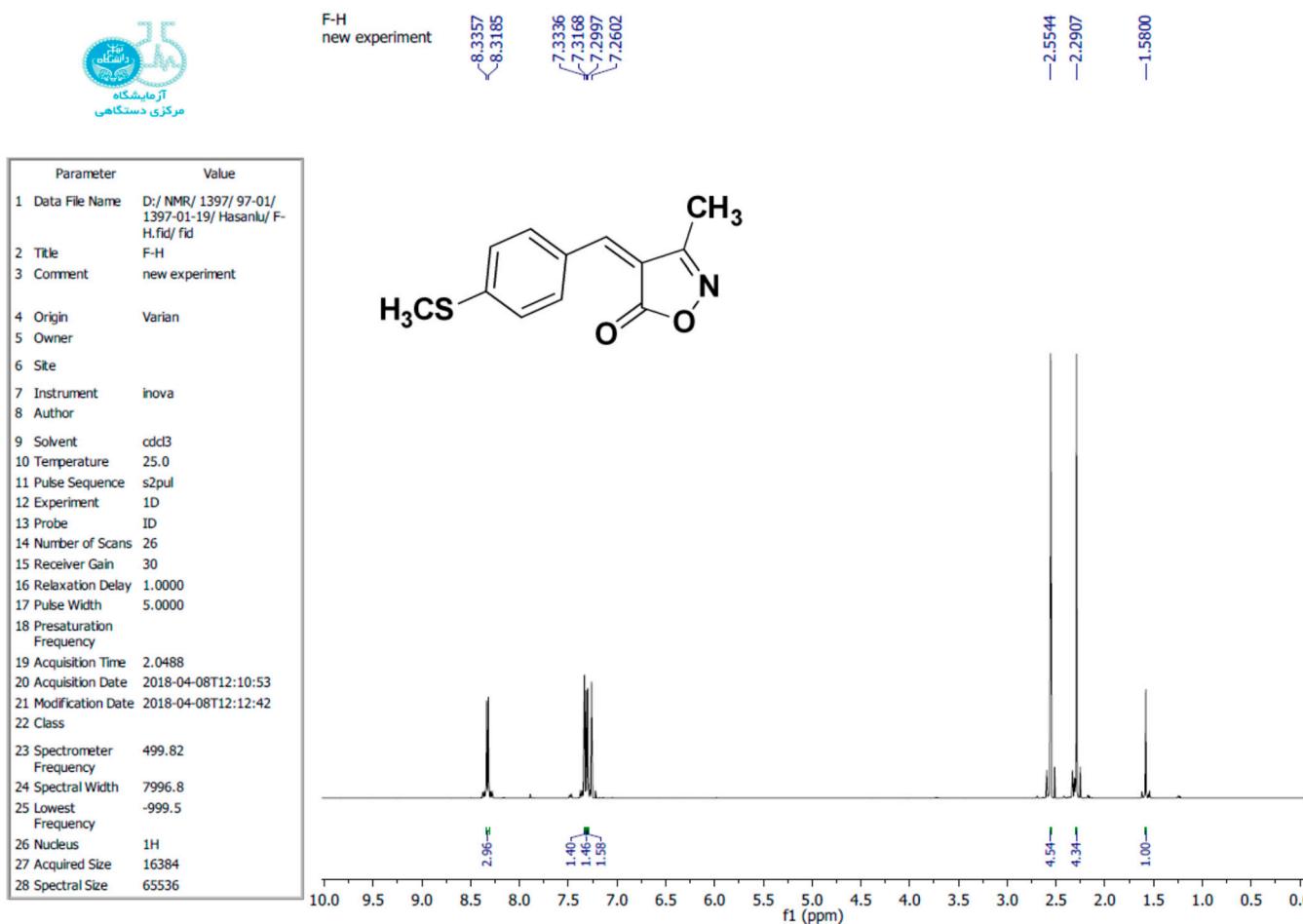


Figure S7. ^1H NMR (500 MHz, CDCl_3) spectrum of 3-methyl-4-(4-(methylthio)benzylidene)isoxazol-5(4*H*)-one (**4i**)

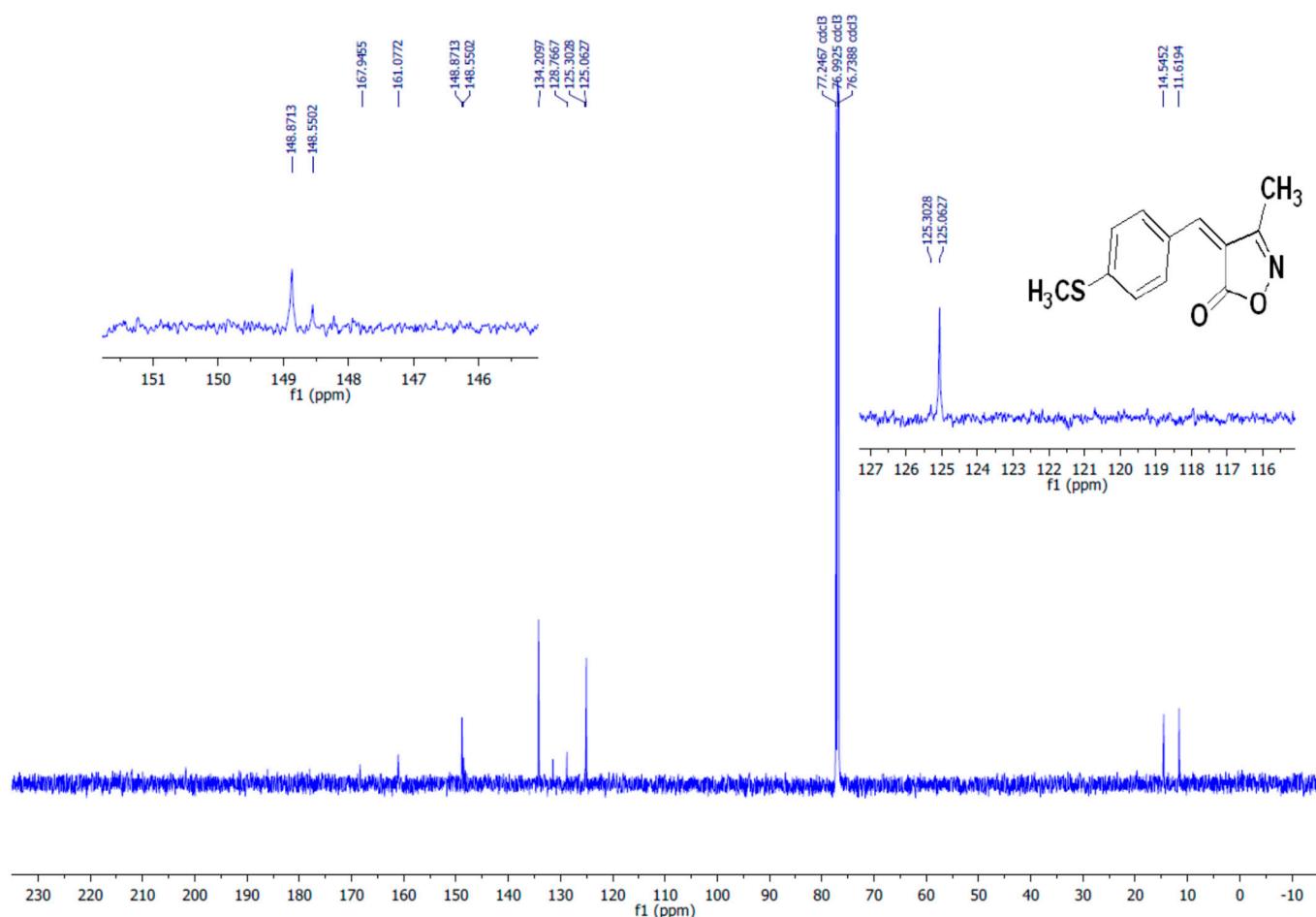


Figure S8. ^{13}C NMR (CDCl_3 , 125 MHz) spectrum of 3-methyl-4-(4-(methylthio)benzylidene)isoxazol-5(4*H*)-one (**4i**)

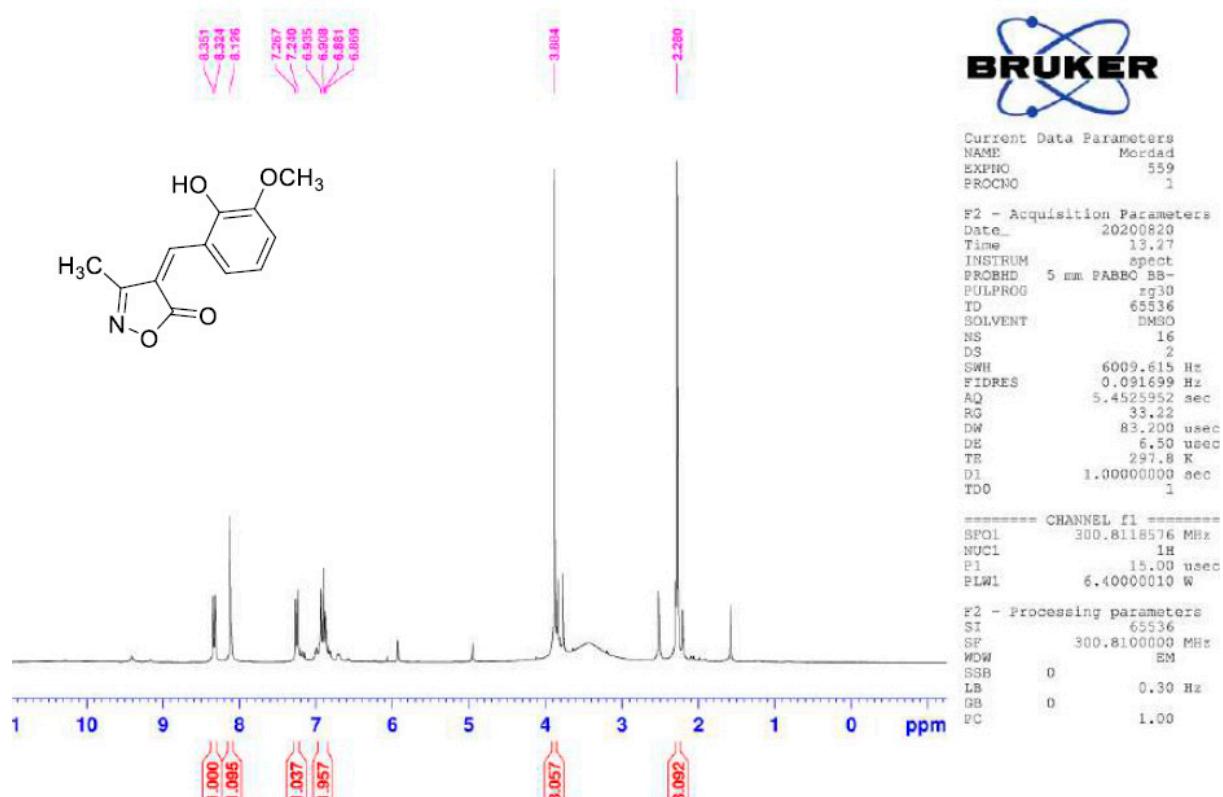


Figure S9. ¹H NMR (300 MHz, CDCl₃) spectrum of 4-(2-Hydroxy-3-methoxybenzylidene)-3-methylisoxazol-5(4H)-one (4j)

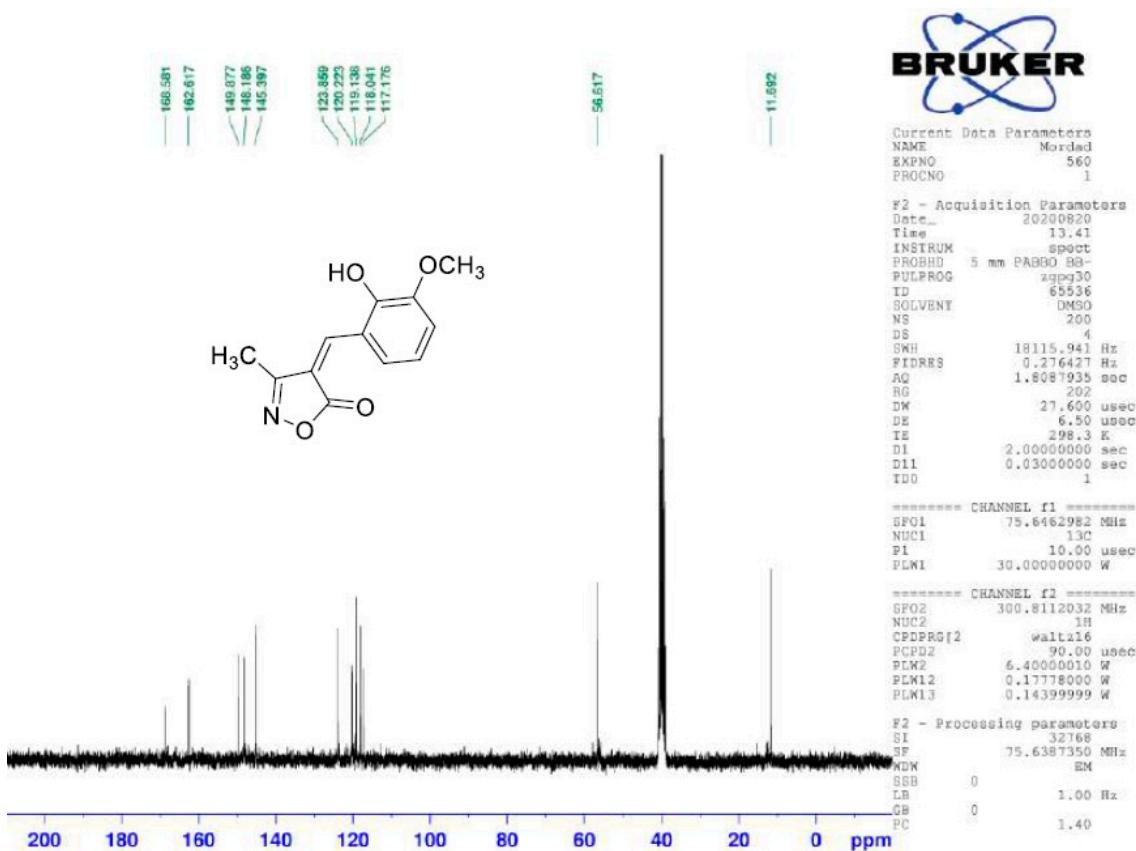


Figure S10. ¹³C NMR (75 MHz, DMSO-d₆) spectrum of 4-(2-Hydroxy-3-methoxybenzylidene)-3-methylisoxazol-5(4H)-one (4j)

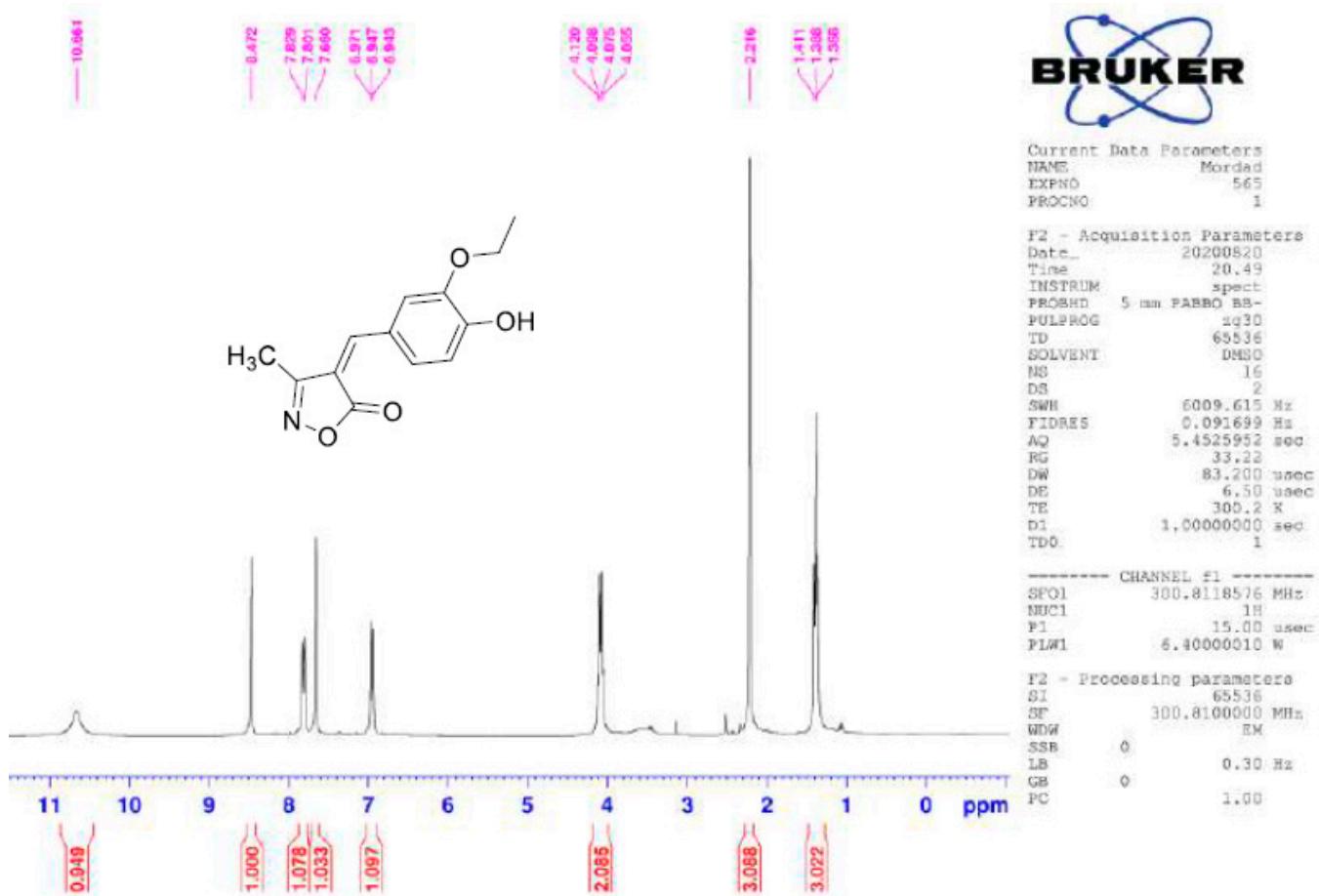


Figure S11. ^1H NMR (300 MHz, DMSO- d_6) spectrum of 4-(3-ethoxy-4-hydroxybenzylidene)-3-methylisoxazol-5(4H)-one (4k)

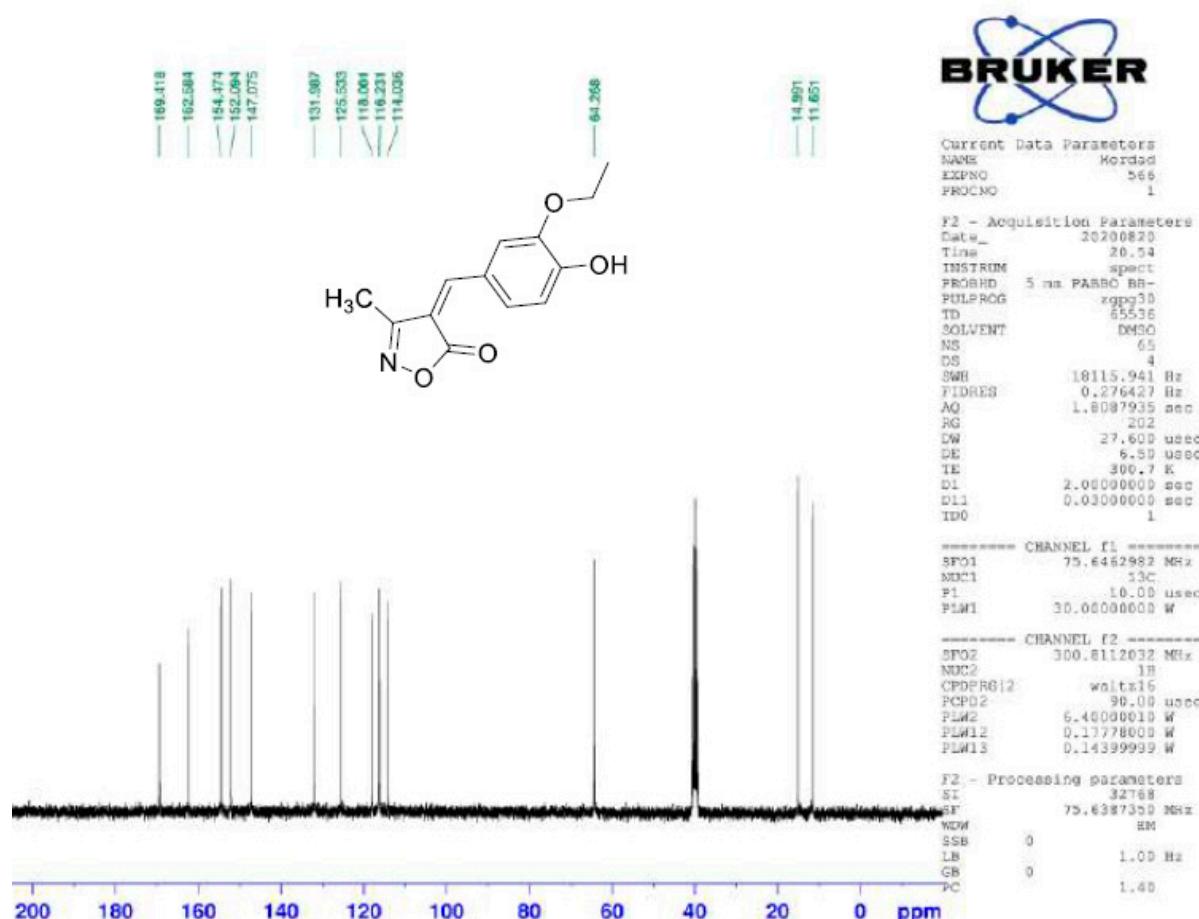


Figure S12. ^{13}C NMR (75 MHz, DMSO-*d*₆) spectrum of 4-(3-ethoxy-4-hydroxybenzylidene)-3-methylisoxazol-5(4H)-one (4k)

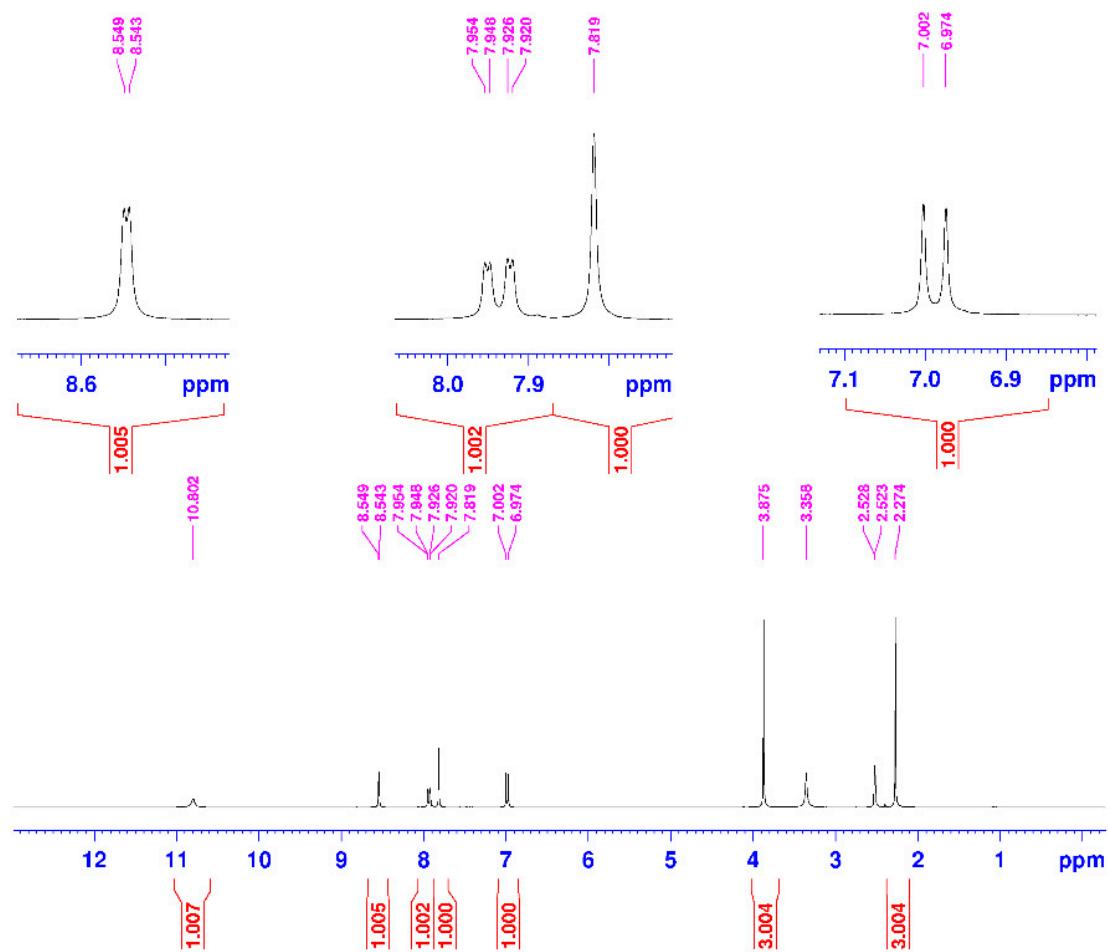


Figure S13. ¹H NMR (500 MHz, DMSO-*d*₆) spectrum of 4-(4-hydroxy-3-methoxybenzylidene)-3-methylisoxazol-5(4*H*)-one (**4l**)

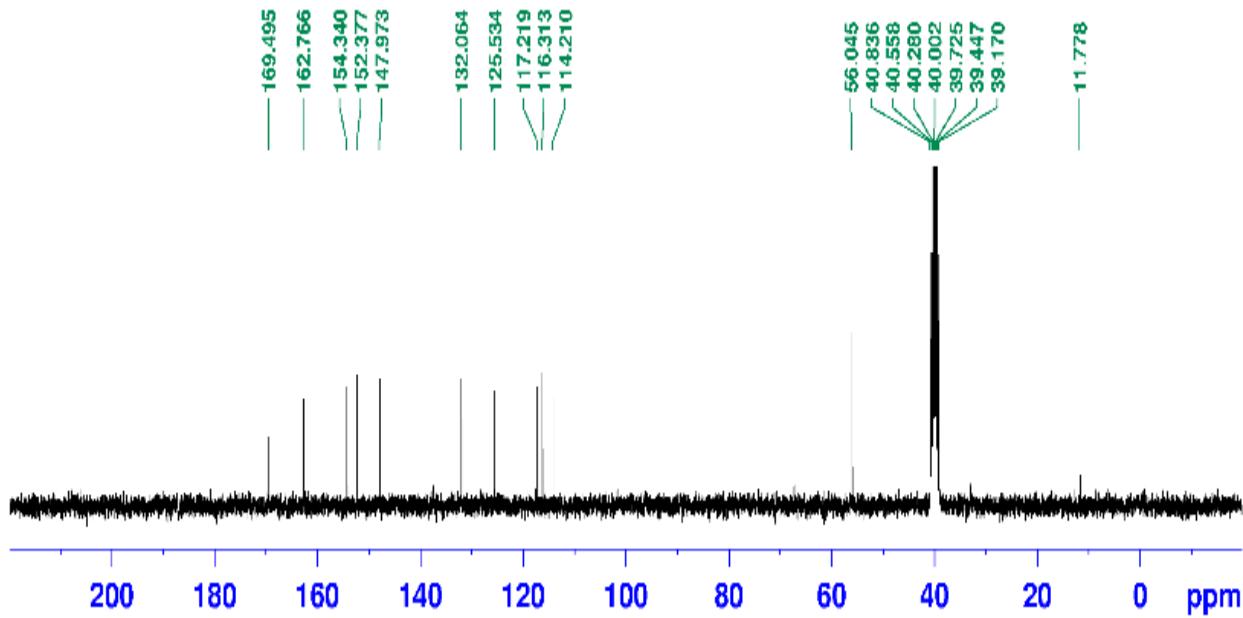


Figure S14. ¹³C NMR (125 MHz, DMSO-*d*₆) spectrum of 4-(4-hydroxy-3-methoxybenzylidene)-3-methylisoxazol-5(4*H*)-one (**4l**)

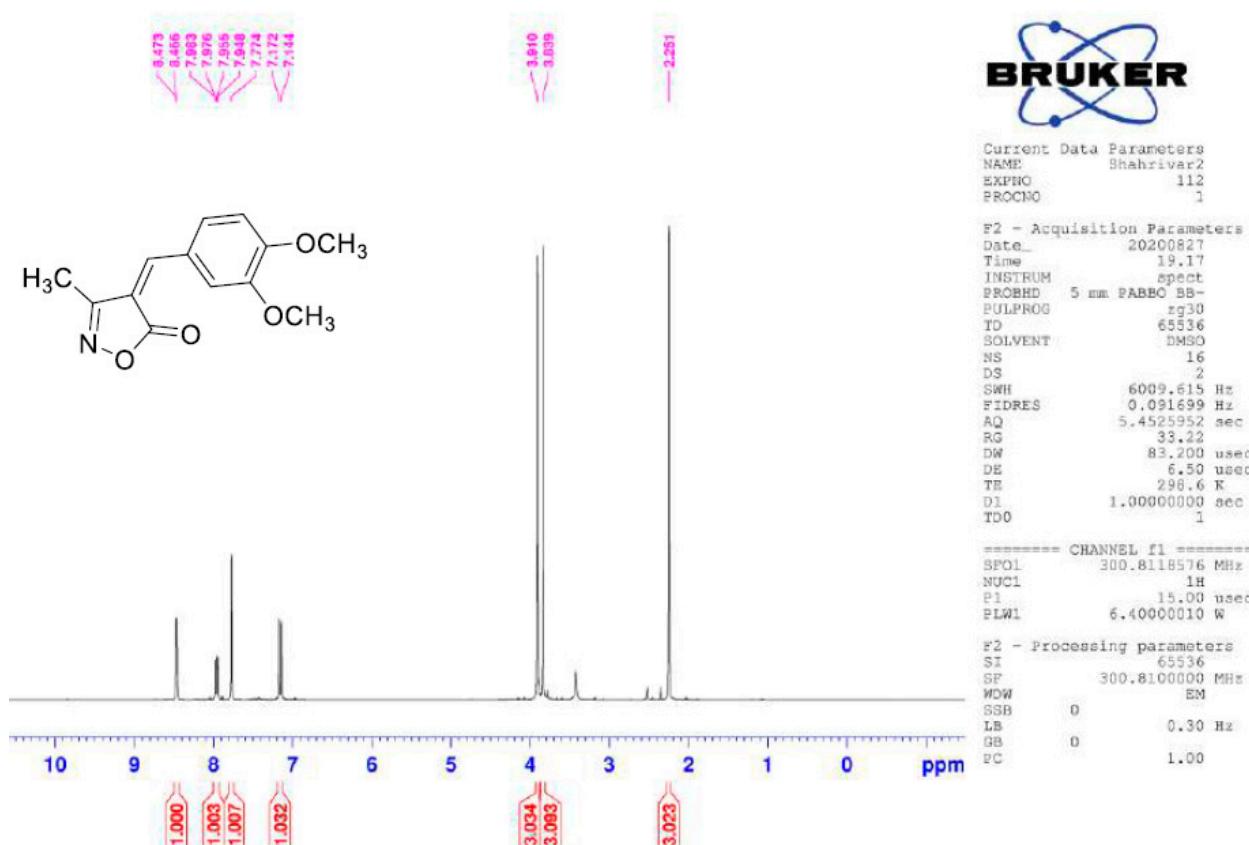


Figure S15. ^1H NMR (300 MHz, $\text{DMSO}-d_6$) spectrum of 4-(3,4-Dimethoxybenzylidene)-3-methylisoxazol-5(4H)-one (**4m**)

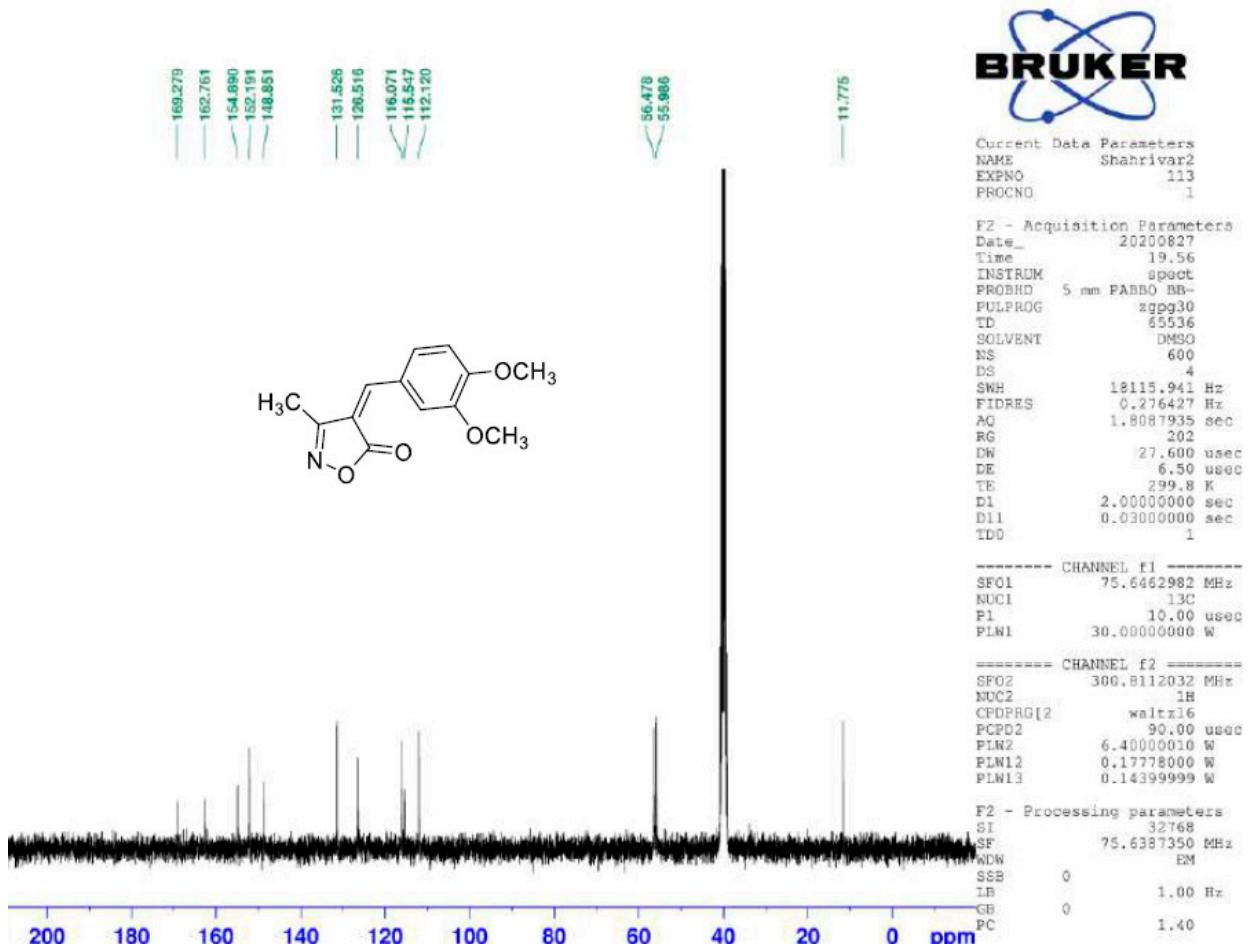


Figure S16. ^{13}C NMR (75 MHz, $\text{DMSO}-d_6$) spectrum of 4-(3,4-Dimethoxybenzylidene)-3-methylisoxazol-5(4*H*)-one (**4m**)

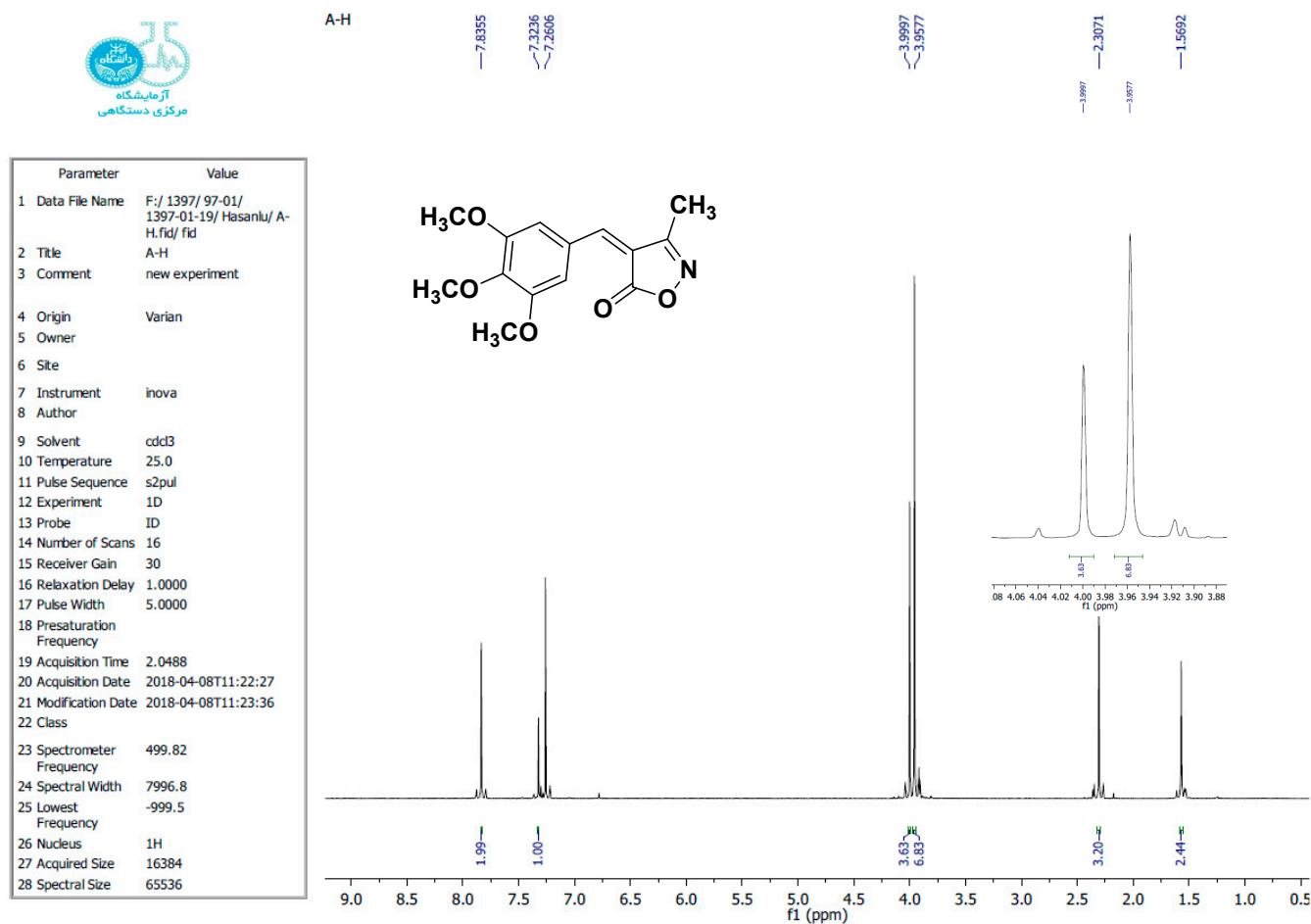


Figure S17. ^1H NMR (500 MHz, CDCl_3) spectrum of 3-methyl-4-(3,4,5-trimethoxybenzylidene)isoxazol-5-(4*H*)-one (**4n**)

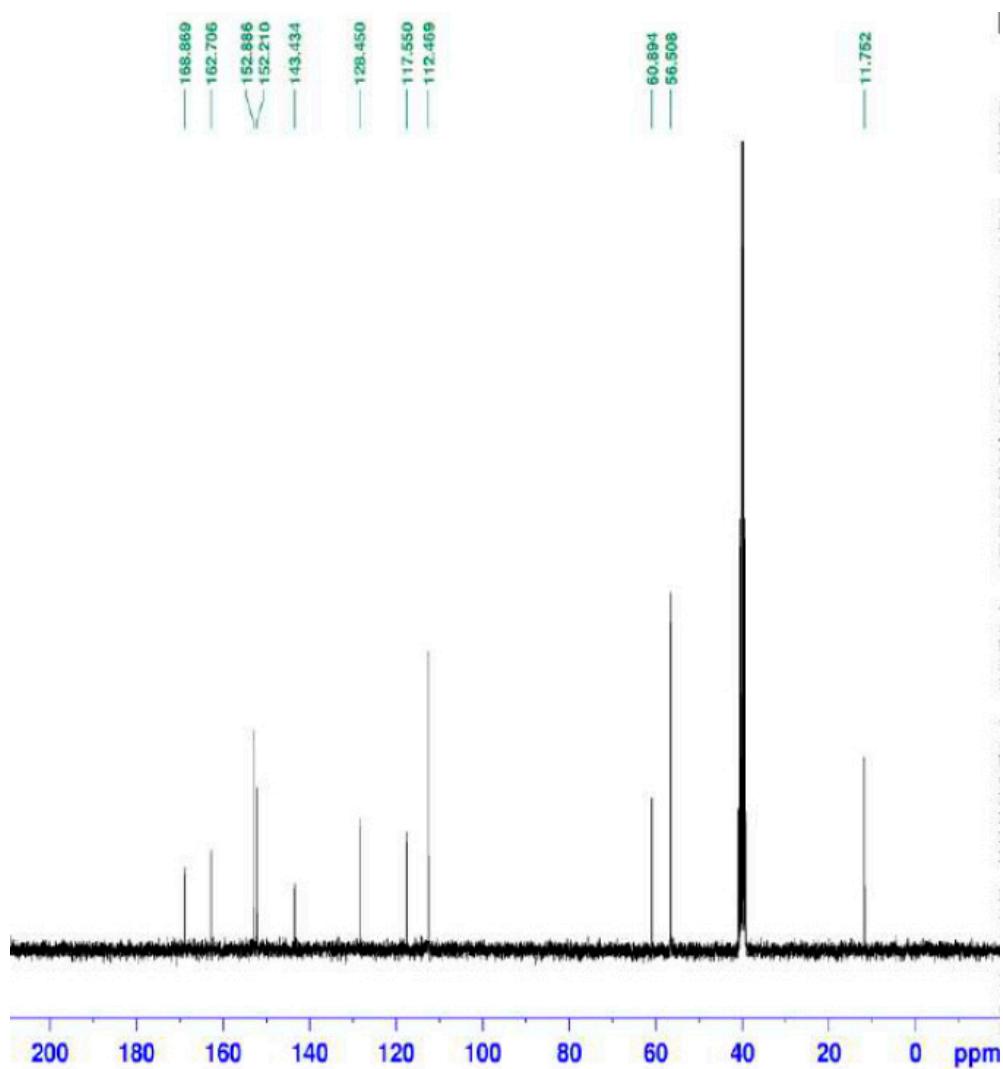


Figure S18. ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) spectrum of 3-methyl-4-(3,4,5-trimethoxybenzylidene)isoxazol-5-(4*H*)-one (**4n**)

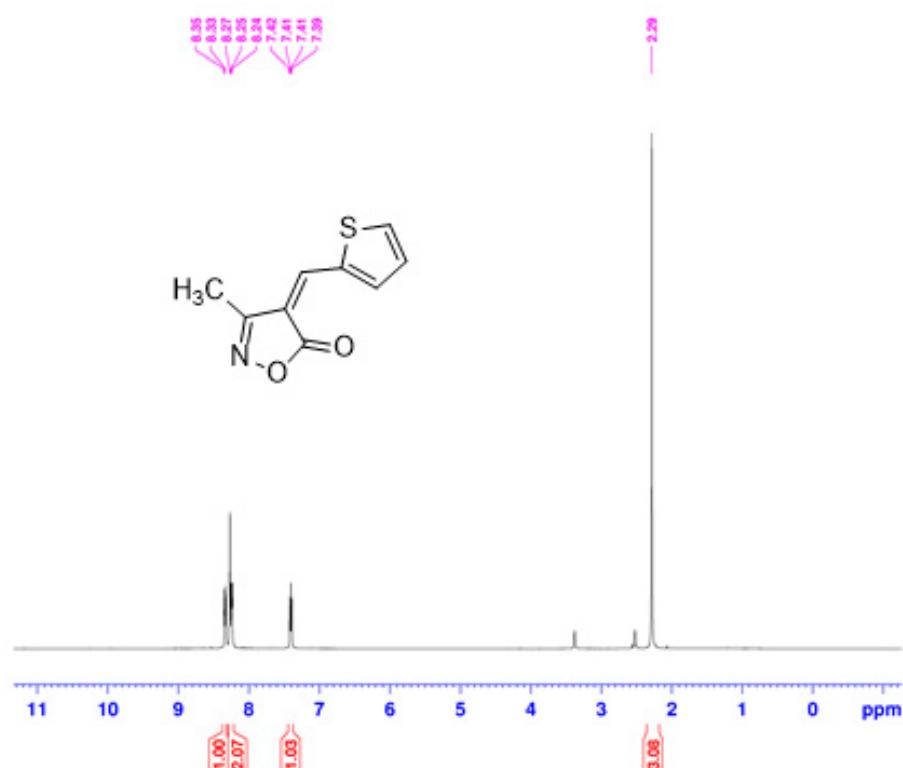


Figure S19. ¹H NMR (300 MHz, CDCl₃) spectrum of 3-methyl-4-(thiophen-2-ylmethylene)isoxazol-5(4*H*)-one (**4o**)

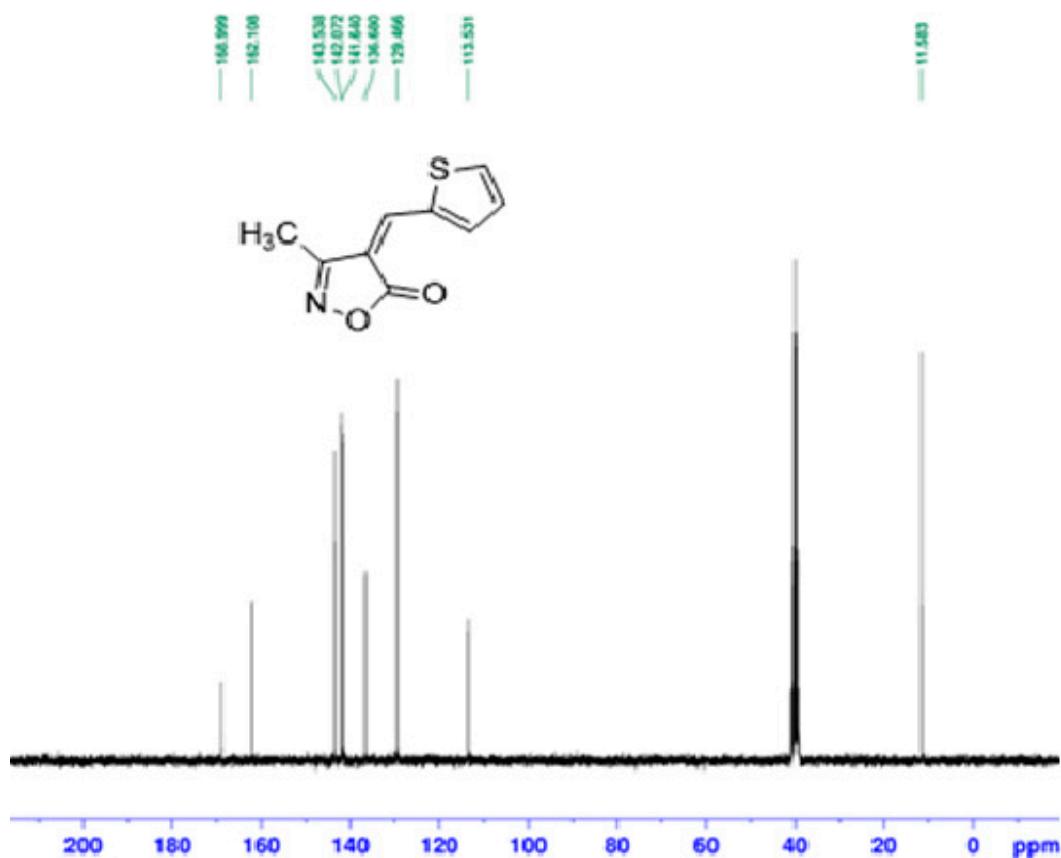


Figure S20. ¹³C NMR (75 MHz, CDCl₃) spectrum of 3-methyl-4-(thiophen-2-ylmethylene)isoxazol-5(4*H*)-one (**4o**)

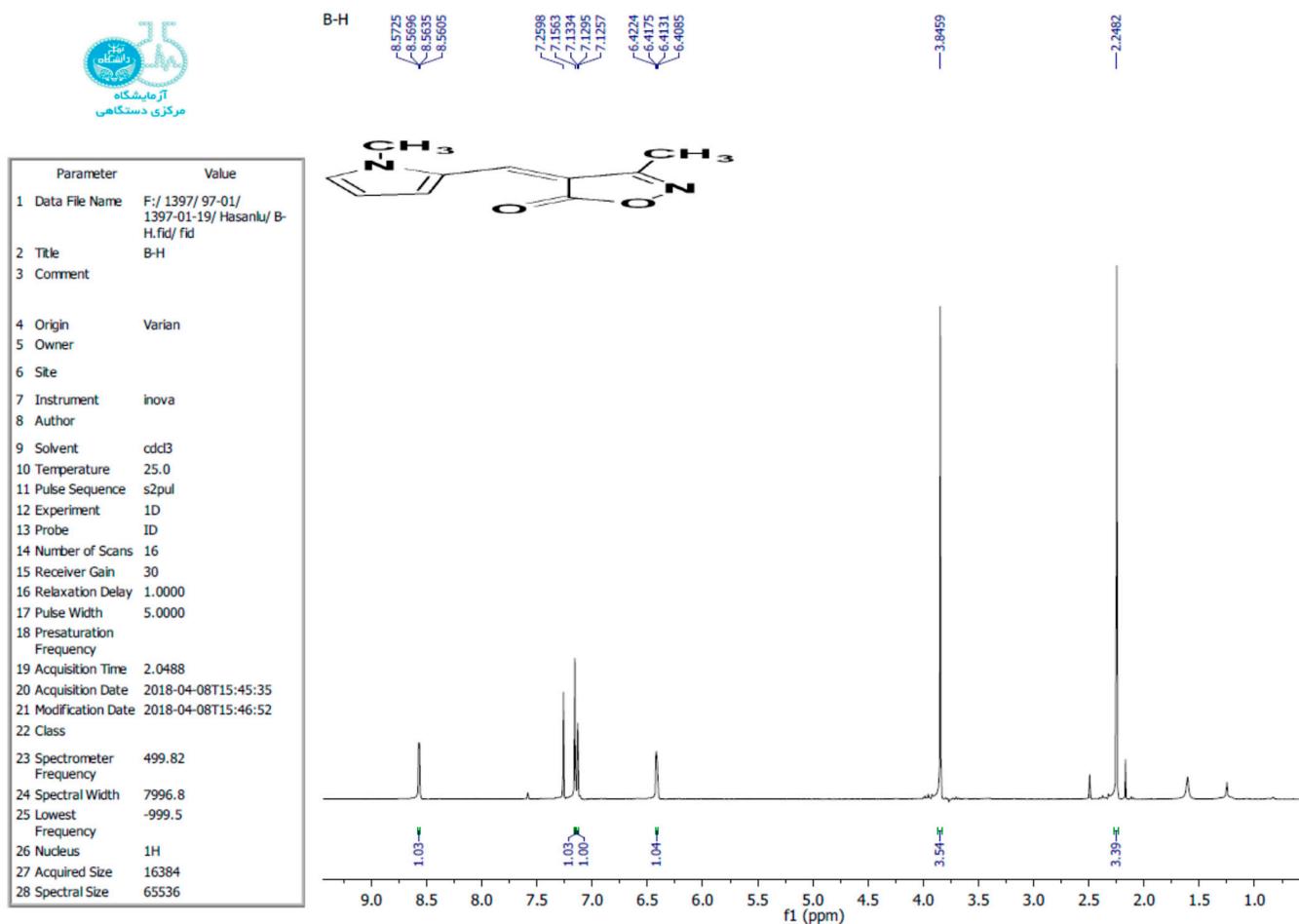


Figure S21. ^1H NMR (500 MHz, CDCl_3) spectrum of 3-methyl-4-((1-methyl-1*H*-pyrrol-2-yl)methylene)isoxazol-5(4*H*)-one (**4p**)

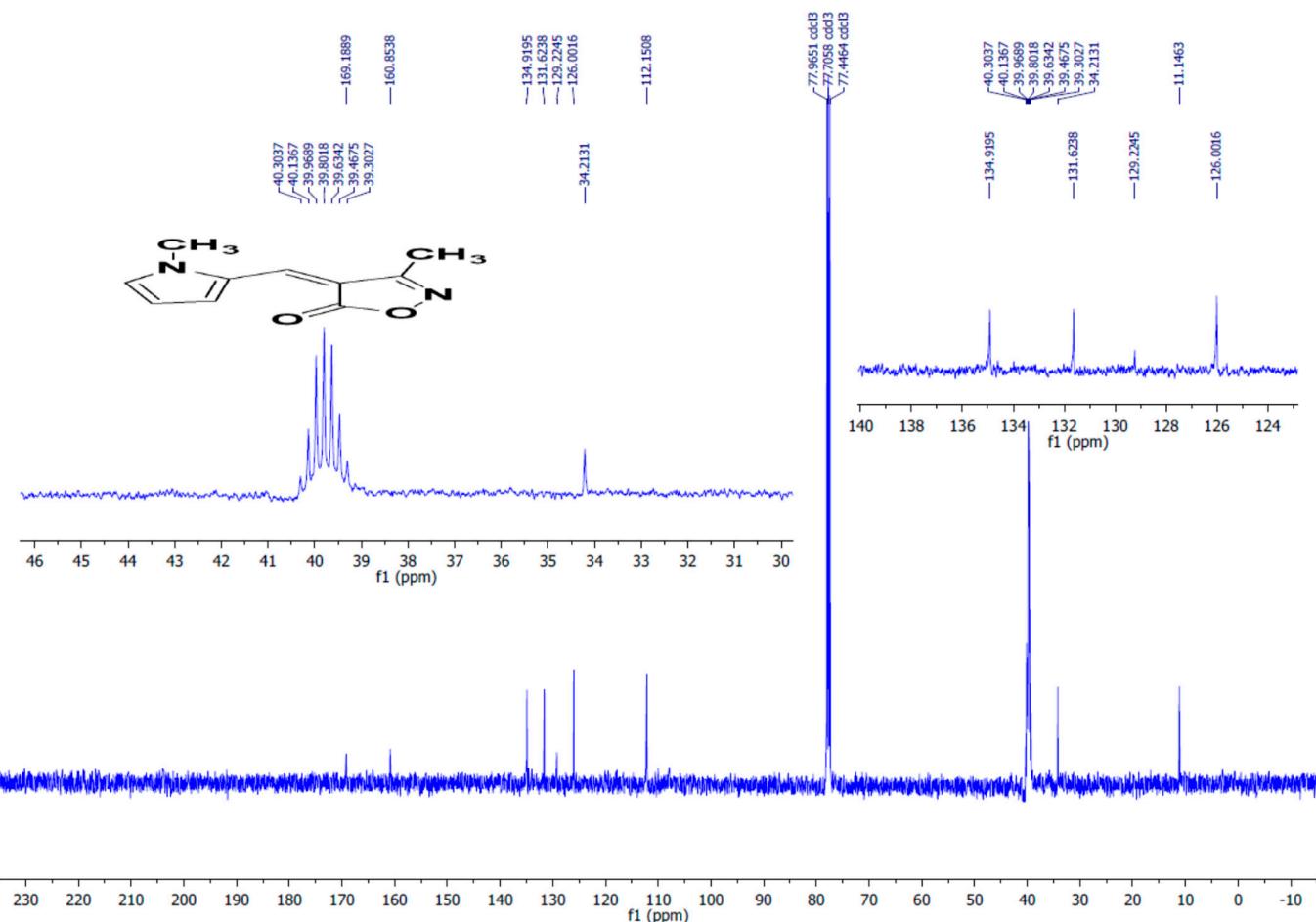


Figure S22. ^{13}C NMR (125 MHz, $\text{CDCl}_3 + \text{DMSO}-d_6$) spectrum of 3-methyl-4-((1-methyl-1*H*-pyrrol-2-yl)methylene)isoxazol-5(4*H*)-one (**4p**)

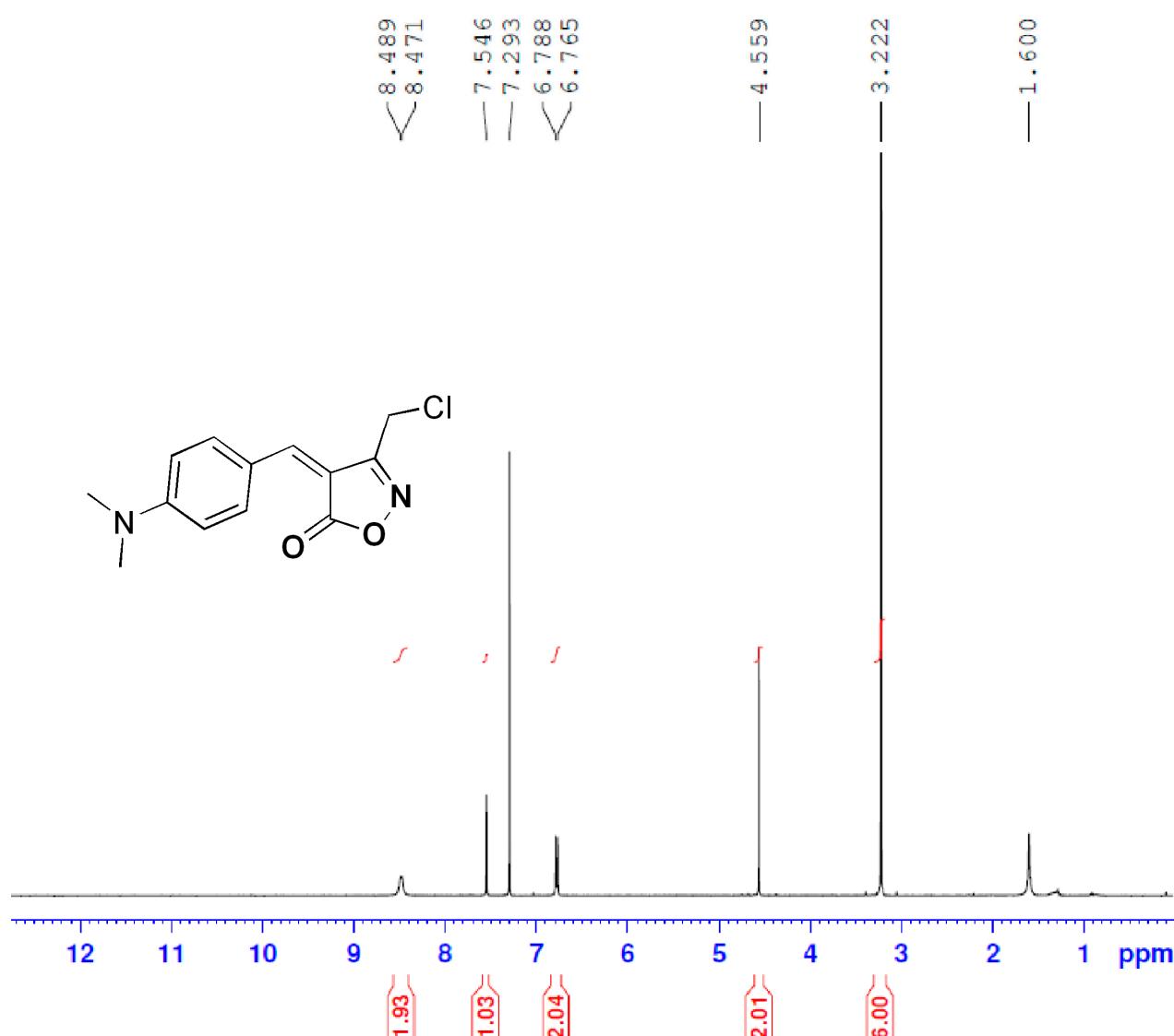


Figure S23. ¹H NMR (400 MHz, CDCl₃) spectrum of 3-(chloromethyl)-4-(dimethylamino)benzylideneisoxazol-5(4*H*)-one (**4v**)

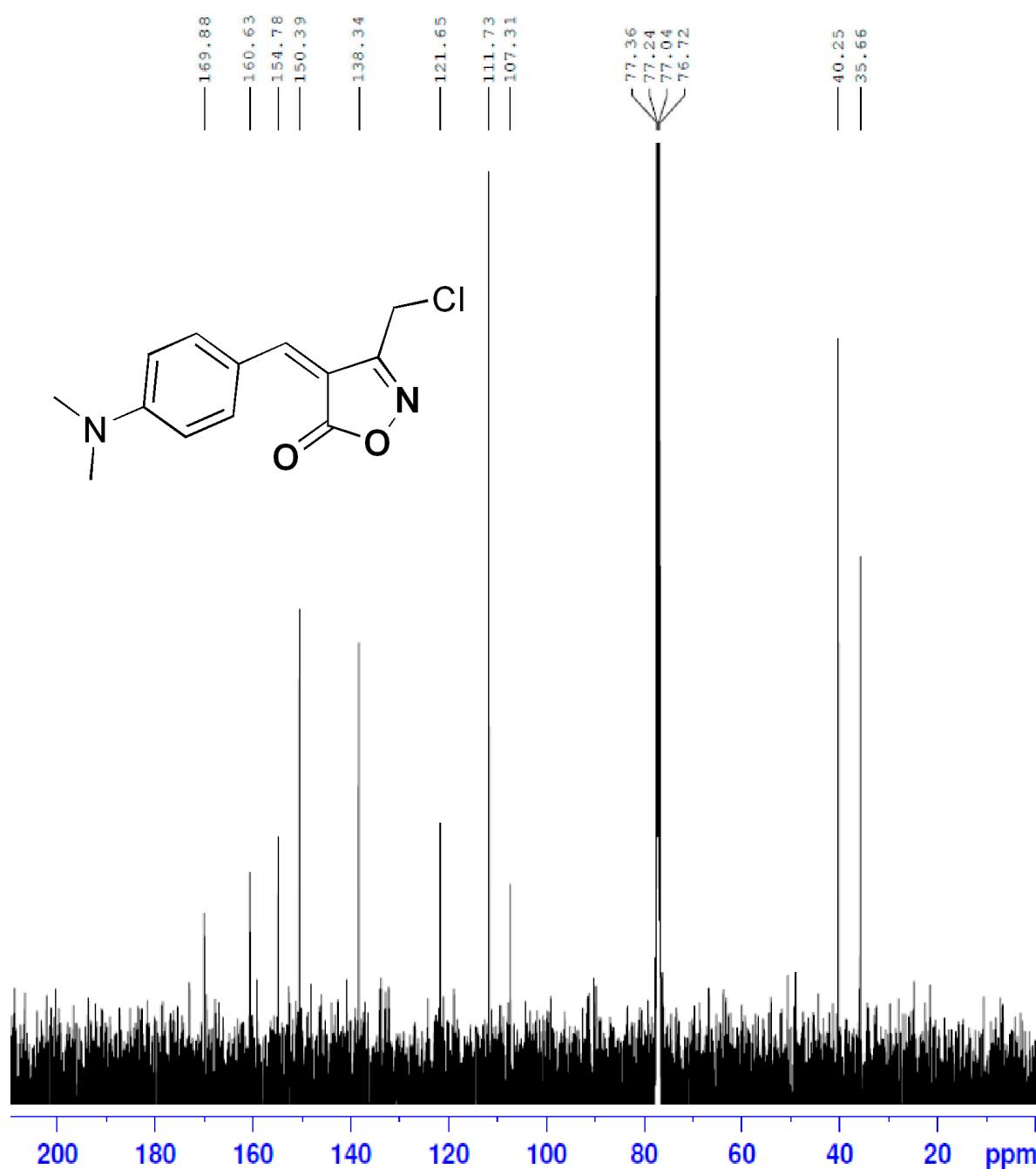


Figure S24. ^{13}C NMR (100 MHz, CDCl_3): spectrum of 3-(chloromethyl)-4-(dimethylamino)benzylideneisoxazol- $(4H)$ -one (**4v**)

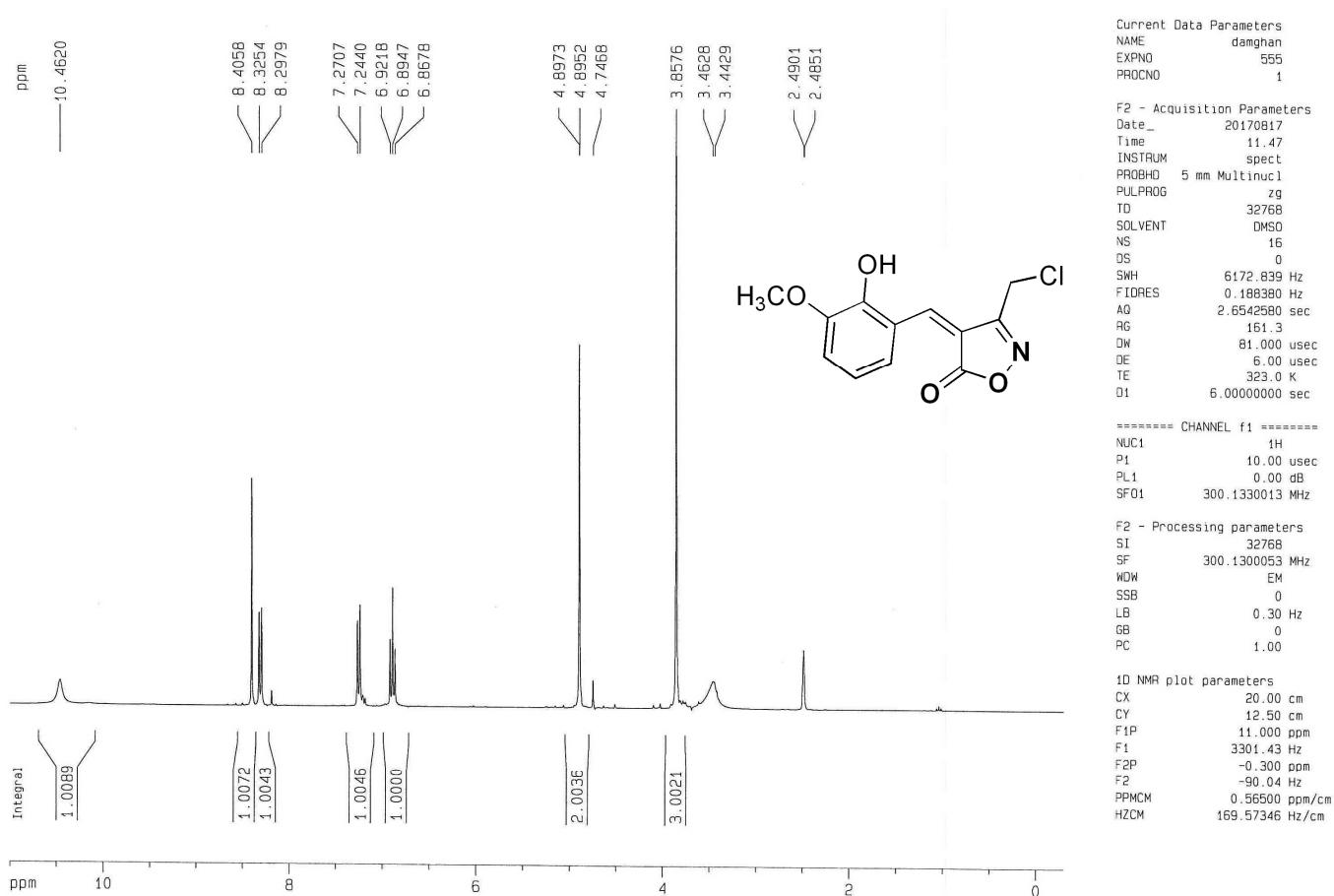


Figure S25. ^1H NMR (300 MHz, $\text{DMSO}-d_6$) spectrum of 3-(chloromethyl)-4-(2-hydroxy-3-methoxybenzylidene)isoxazol-5(4*H*)-one (**4w**)

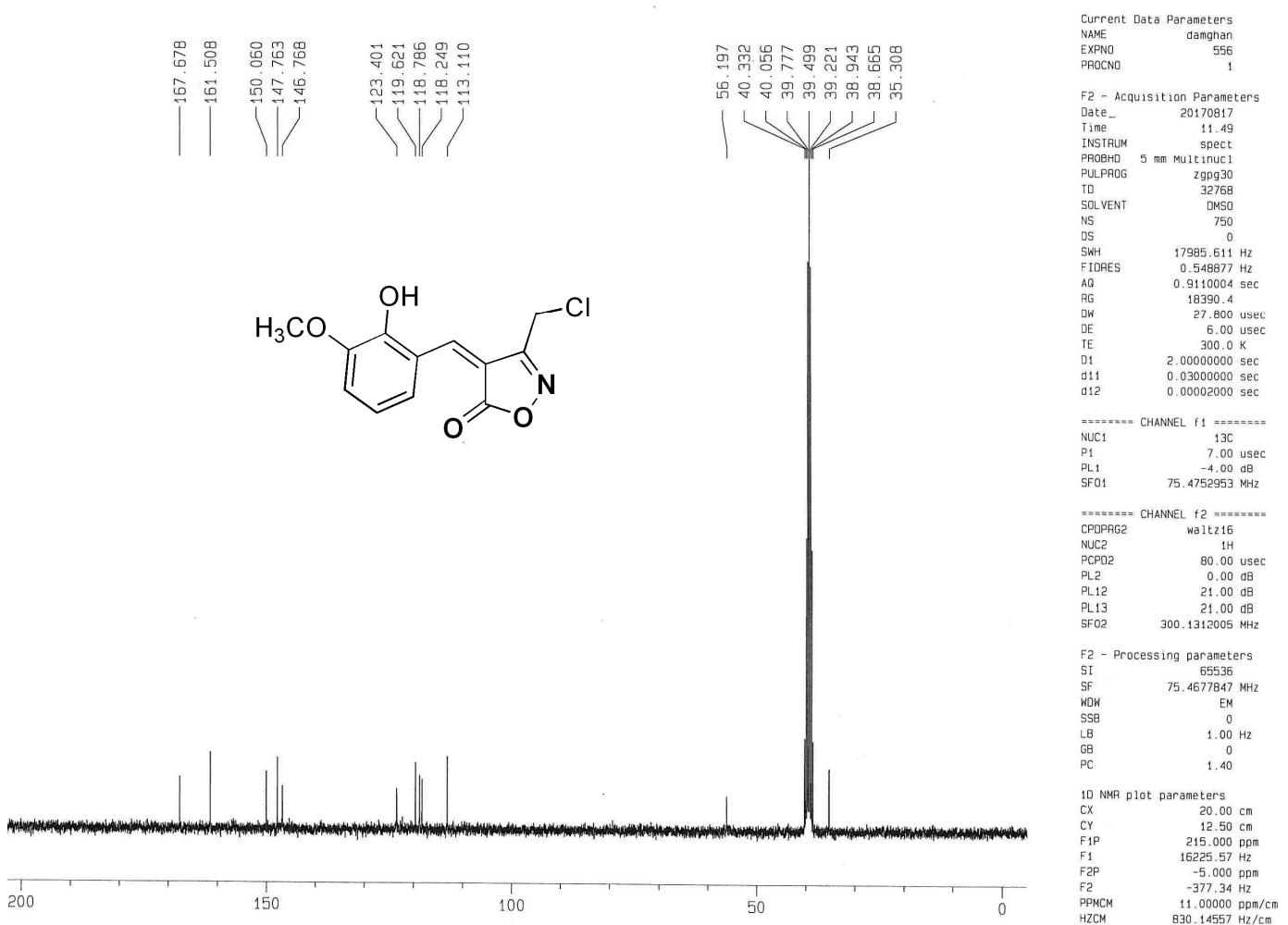


Figure S26. ^{13}C NMR (75 MHz, $\text{DMSO}-d_6$) spectrum of 3-(chloromethyl)-4-(2-hydroxy-3-methoxybenzylidene)isoxazol-5(4*H*)-one (**4w**)

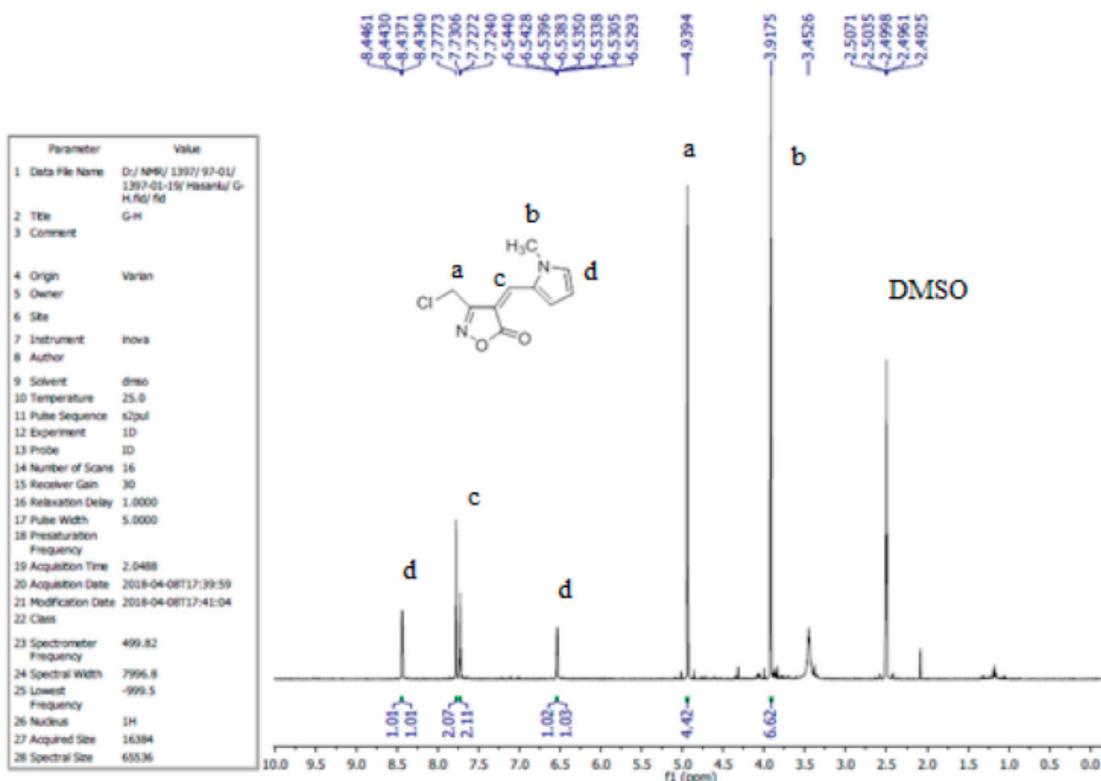


Figure S27. ^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of 3-(chloromethyl)-4-((1-methyl-1*H*-pyrrol-2-yl)methylene)isoxazol-5(4*H*)-one (**4aa**)

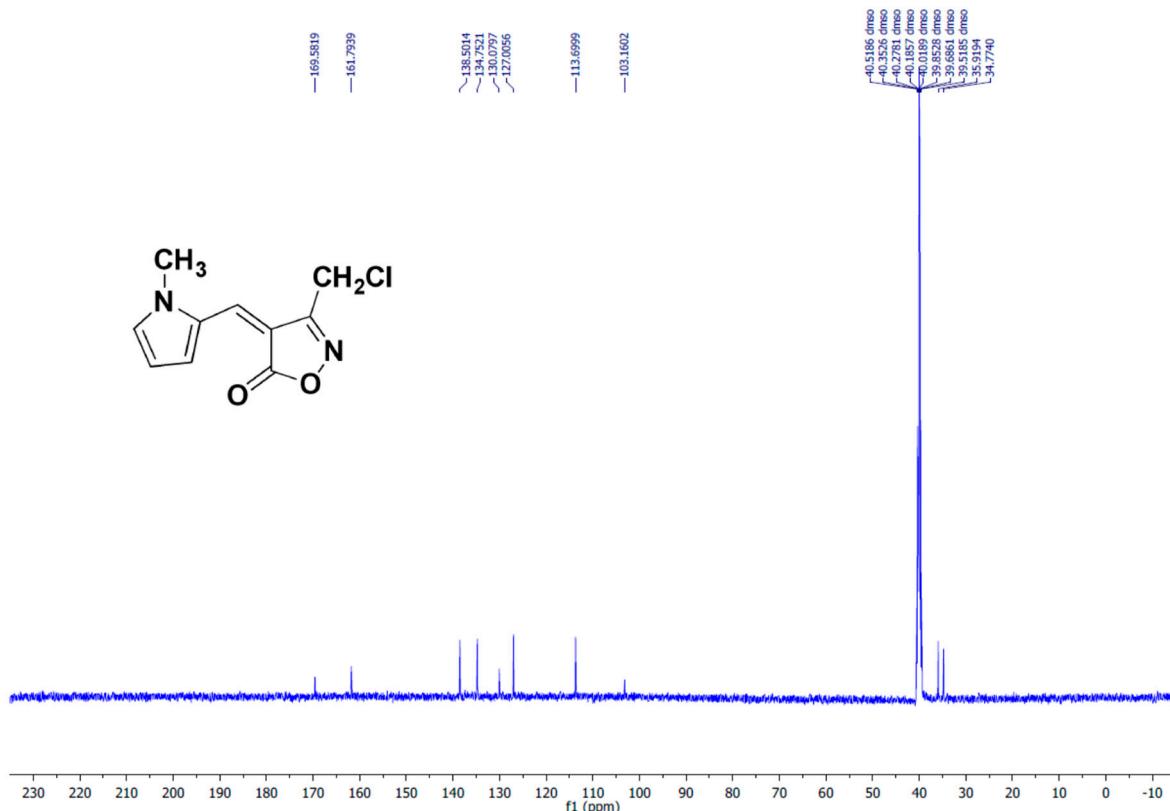


Figure S28. ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) spectrum of 3-(chloromethyl)-4-((1-methyl-1*H*-pyrrol-2-yl)methylene)isoxazol-5(4*H*)-one (**4aa**)

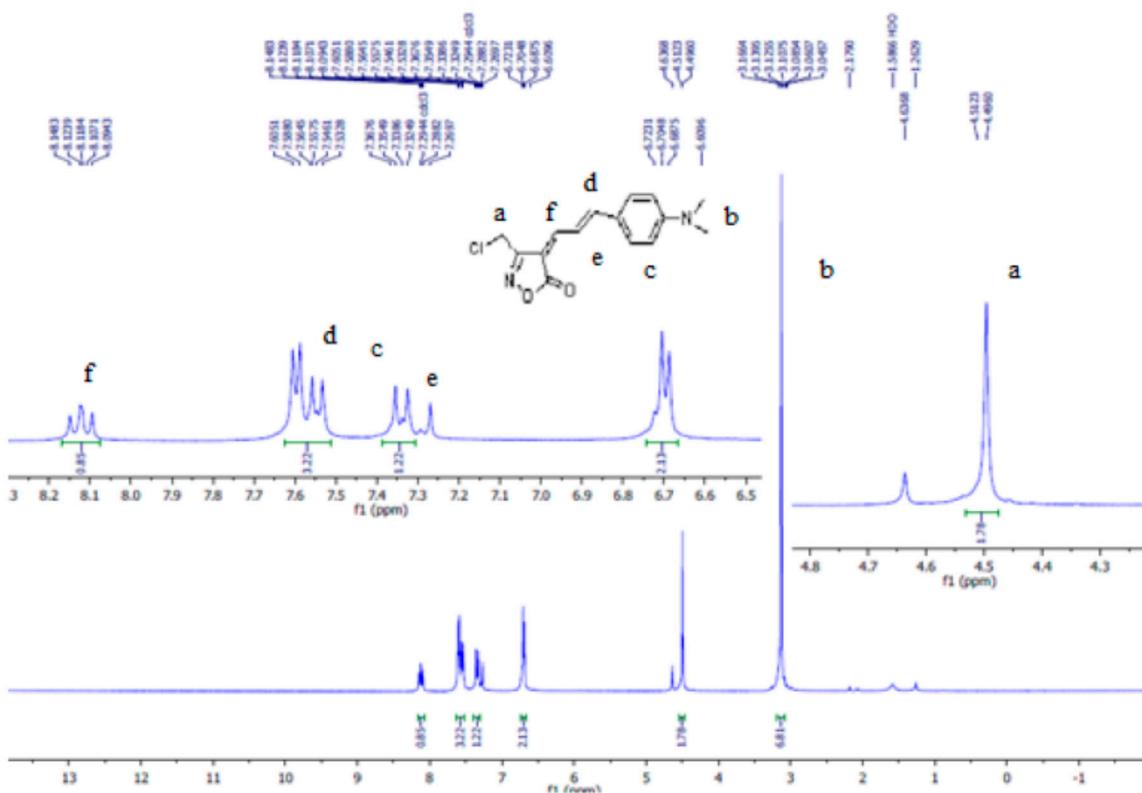


Figure S29. ¹H NMR (500 MHz, CDCl₃) spectrum of 3-(chloromethyl)-4-(3-(dimethylamino)phenylallylidene)isoxazol-5(4H)-one (**4ab**)

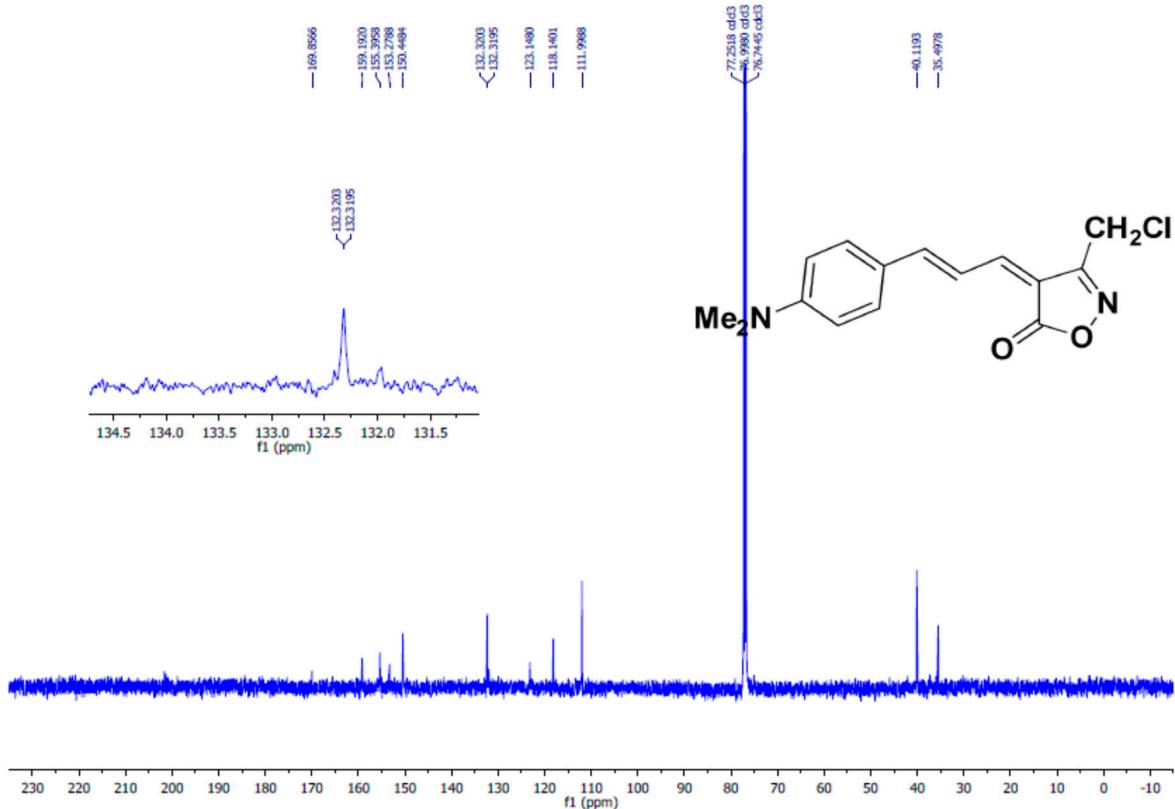


Figure S30. ¹³C NMR (125 MHz, CDCl₃) spectrum of 3-(chloromethyl)-4-(3-(dimethylamino)phenylallylidene)isoxazol-5(4H)-one (**4ab**)

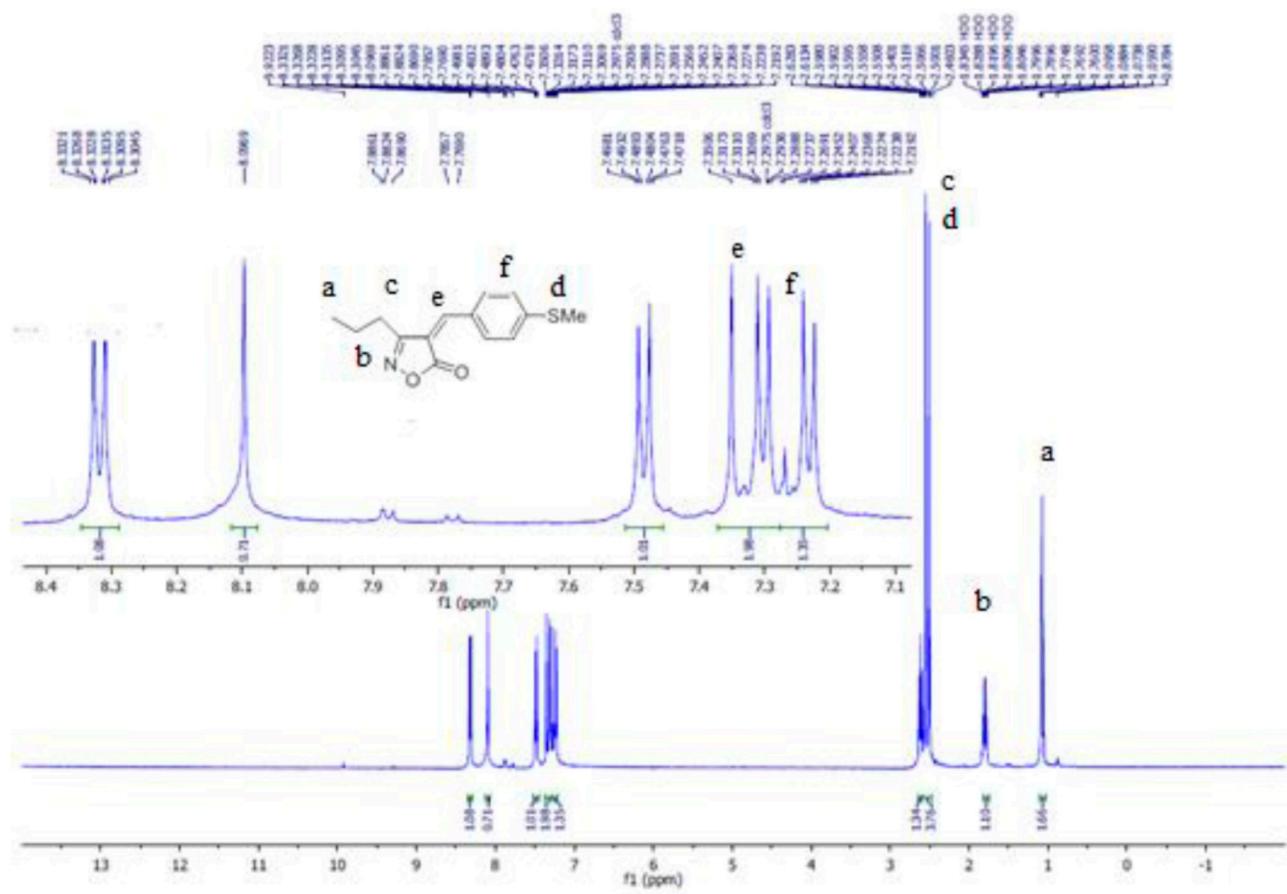


Figure S31. ¹H NMR (500 MHz, CDCl₃) spectrum of 4-(4-(methylthio)benzylidene)-3-propylisoxazol-5(4H)-one (**4ac**)

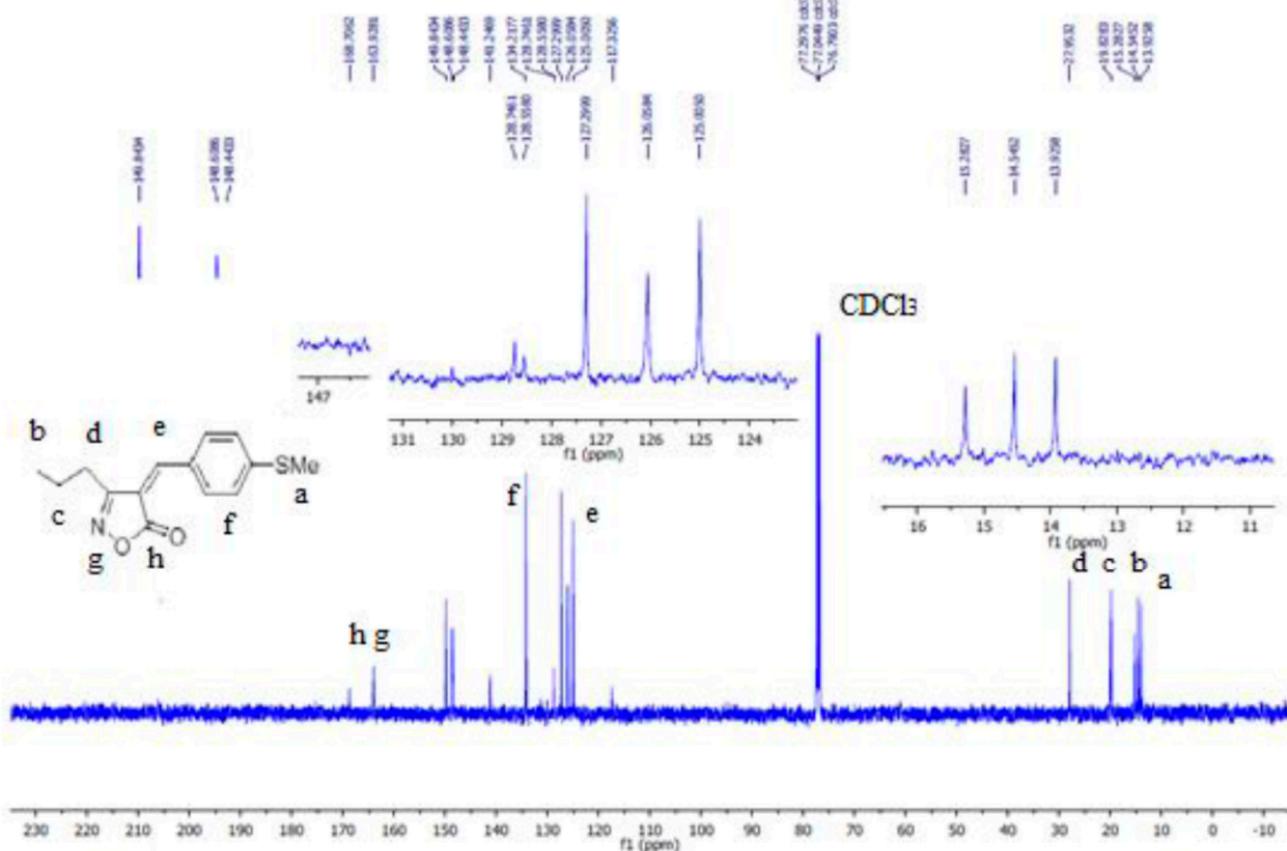


Figure S32. ¹³C NMR (125 MHz, CDCl₃) spectrum of 4-(4-(methylthio)benzylidene)-3-propylisoxazol-5(4H)-one (**4ac**)

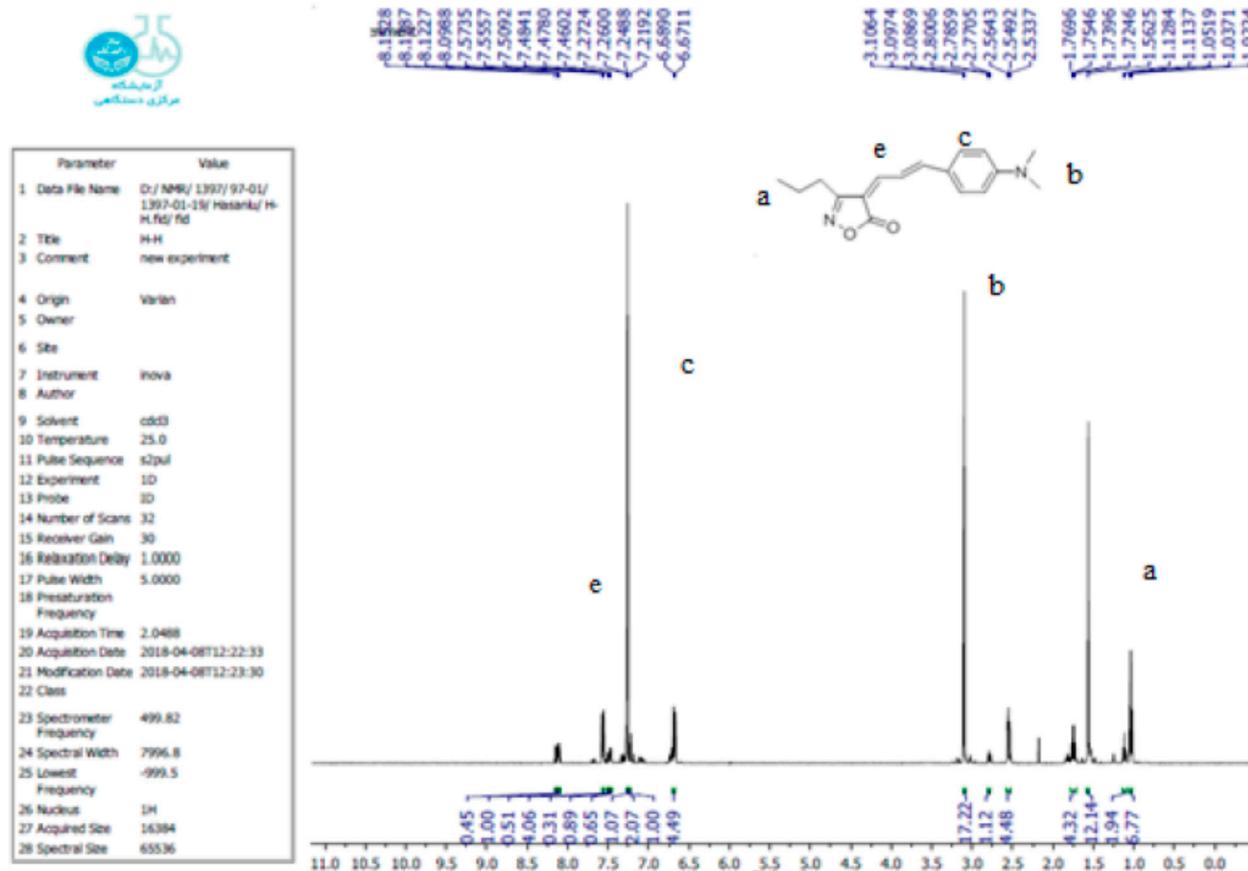


Figure S33. ^1H NMR (500 MHz, CDCl_3) spectrum of (4-(dimethylamino)phenyl)allylidene)-3-propylisoxazol-5(4*H*)-one (**4ad**)

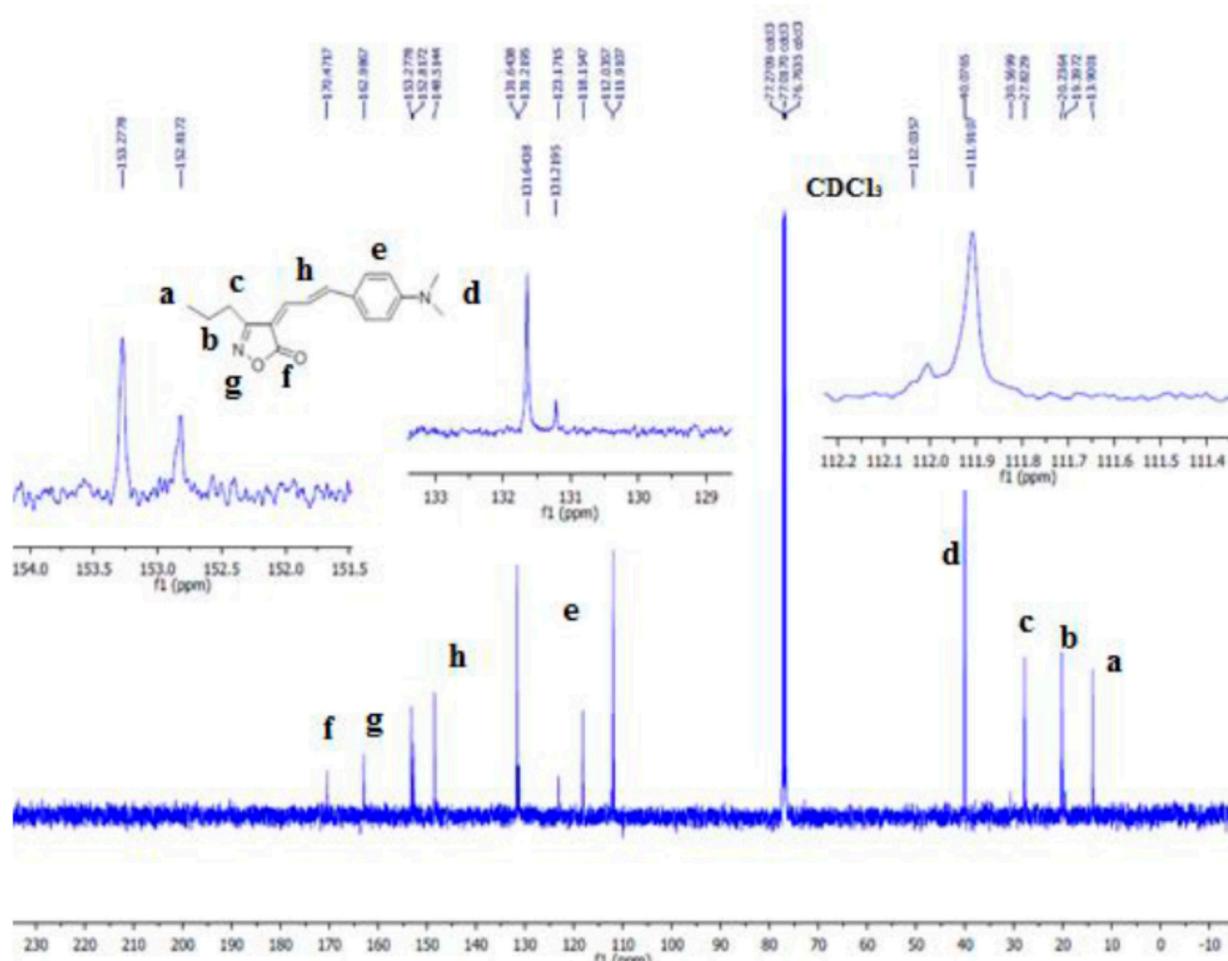


Figure S34. ^{13}C NMR (125 MHz, CDCl₃) spectrum of (4-(dimethylamino)phenylallylidene)-3-propylisoxazol-5(4H)-one (**4ad**)

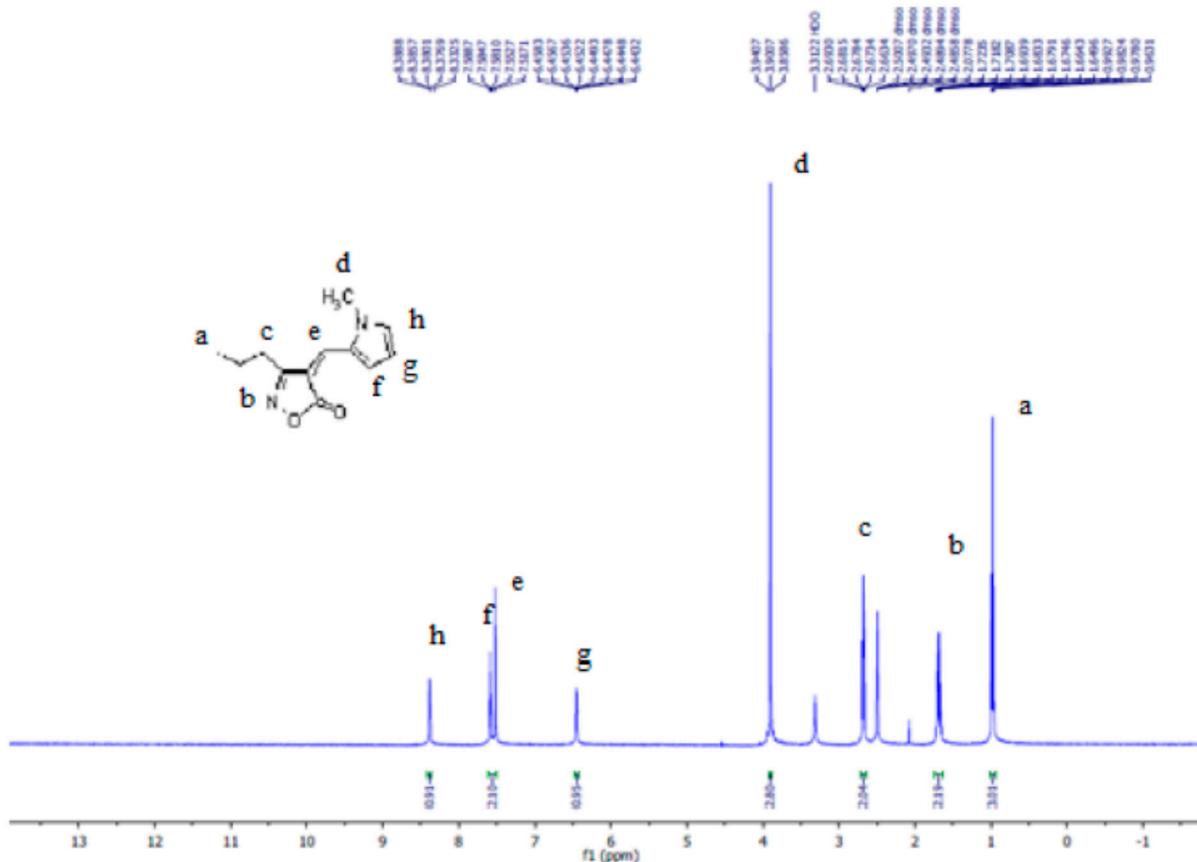


Figure S35. ^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of 4-((1-methyl-1*H*-pyrrol-2-yl)methylene)-3-propylisoxazol-5(4*H*)-one (**4ae**)

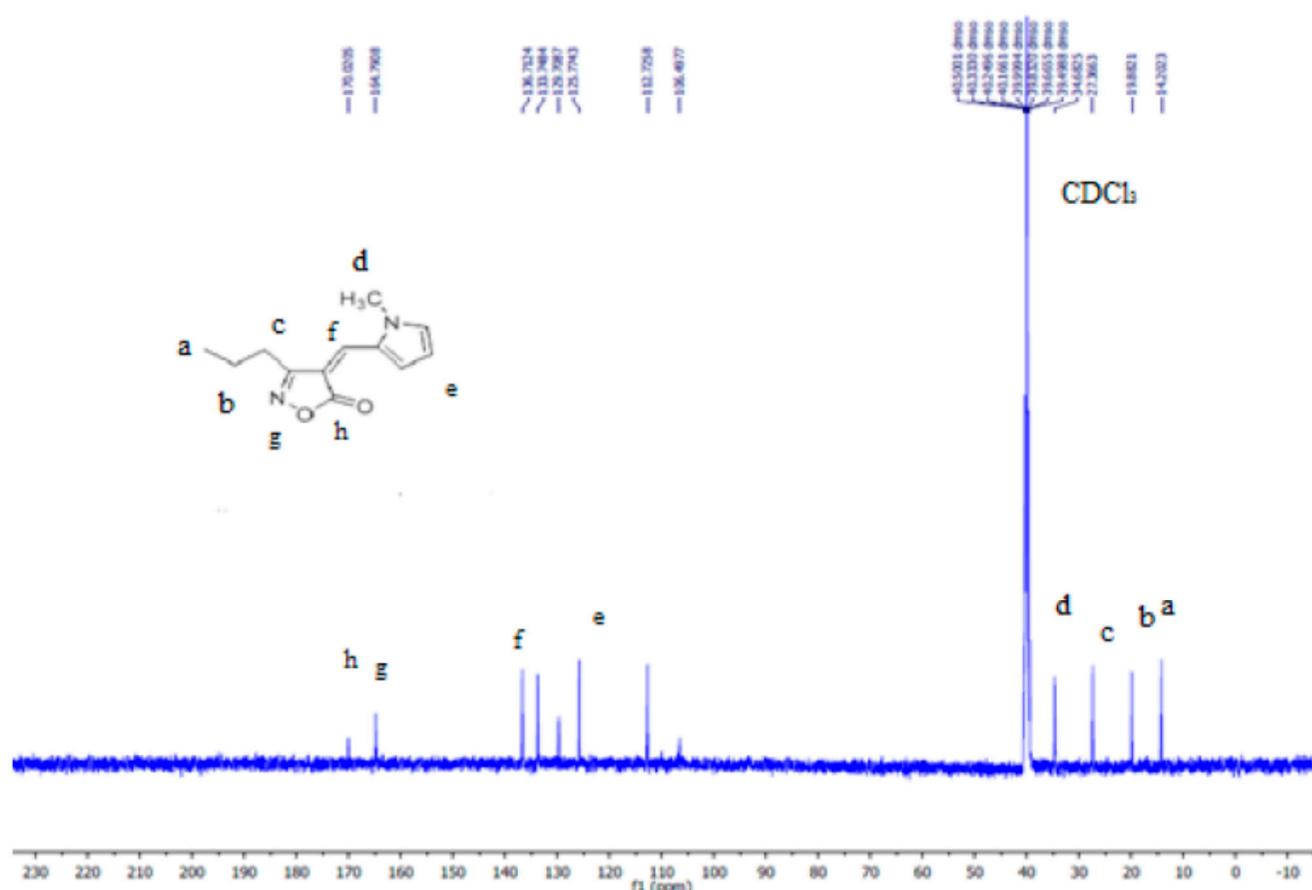


Figure S36. ^{13}C NMR (125 MHz, DMSO- d_6) spectrum of 4-((1-methyl-1*H*-pyrrol-2-yl)methylene)-3-propylisoxazol-5(4*H*)-one (**4ae**)