

Efficient Synthesis of Novel Triazolo[5,1-b]purines by PIDA-Mediated Oxidative Cyclization of Schiff Bases

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ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Spectra of compounds

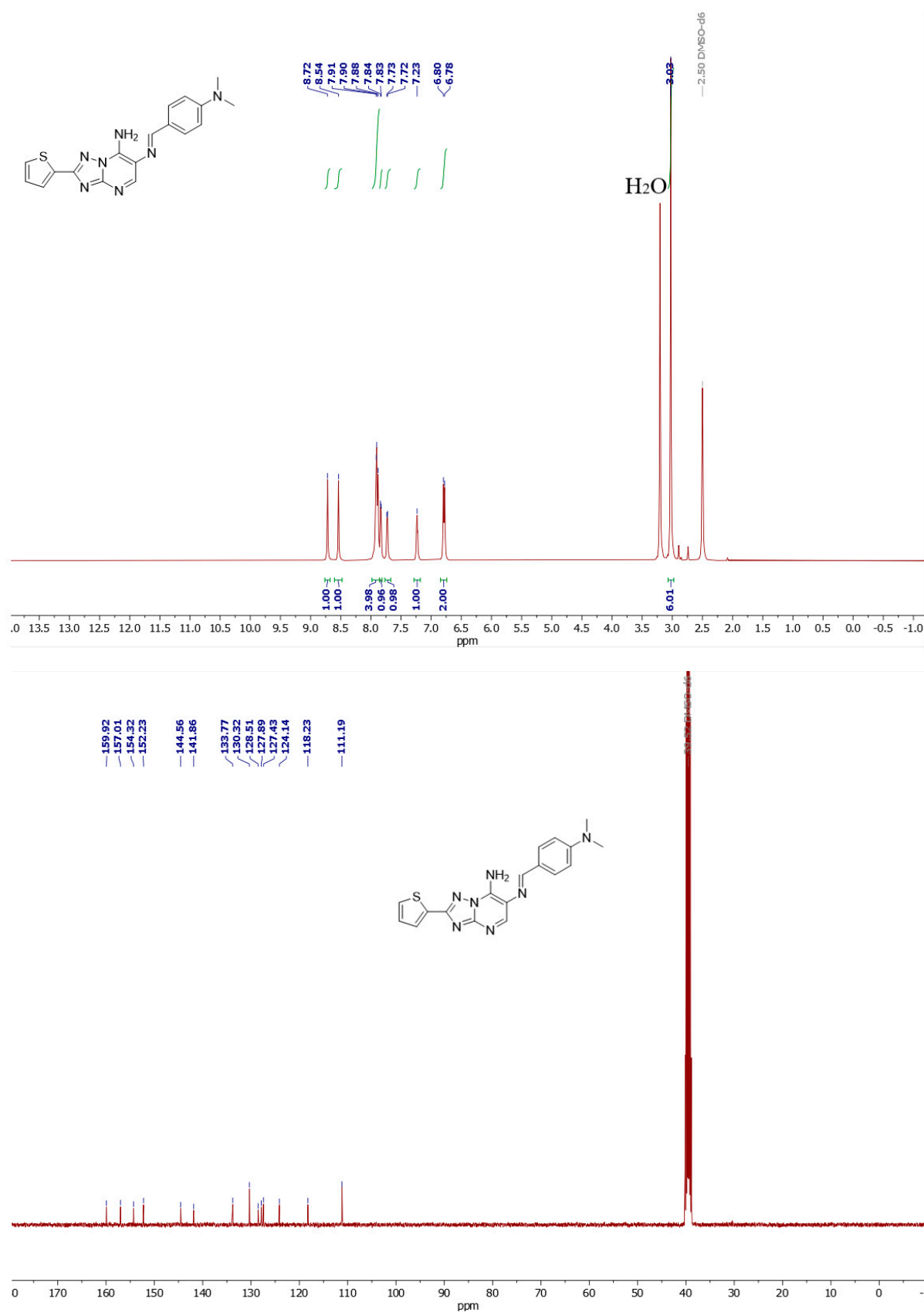


Figure S1. ¹H and ¹³C NMR spectra of ((4-(dimethylamino)benzylidene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (**3a**)

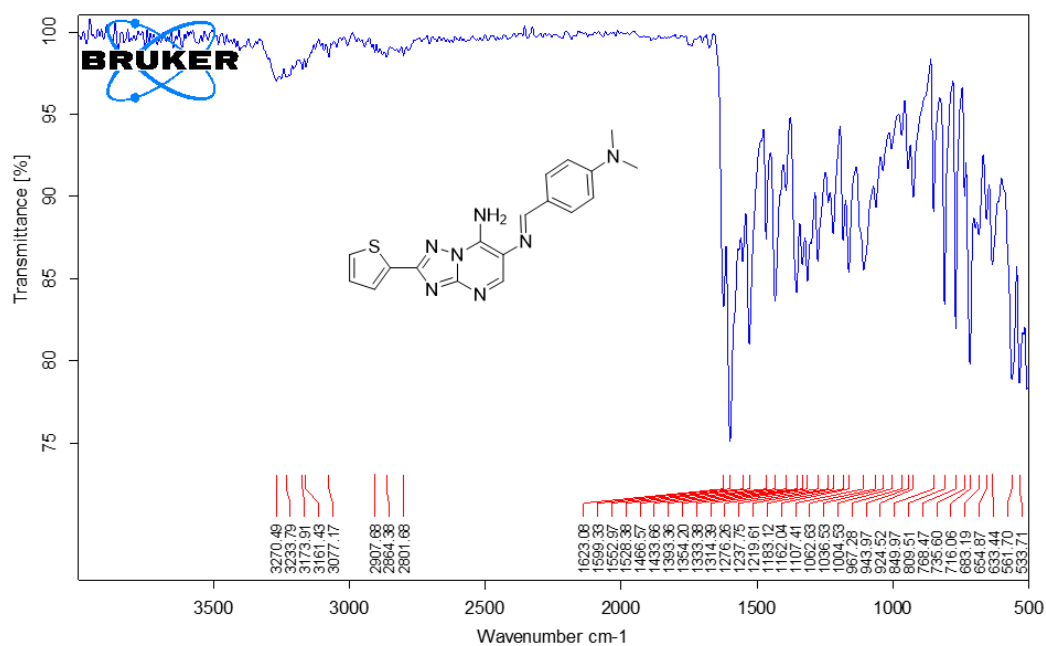
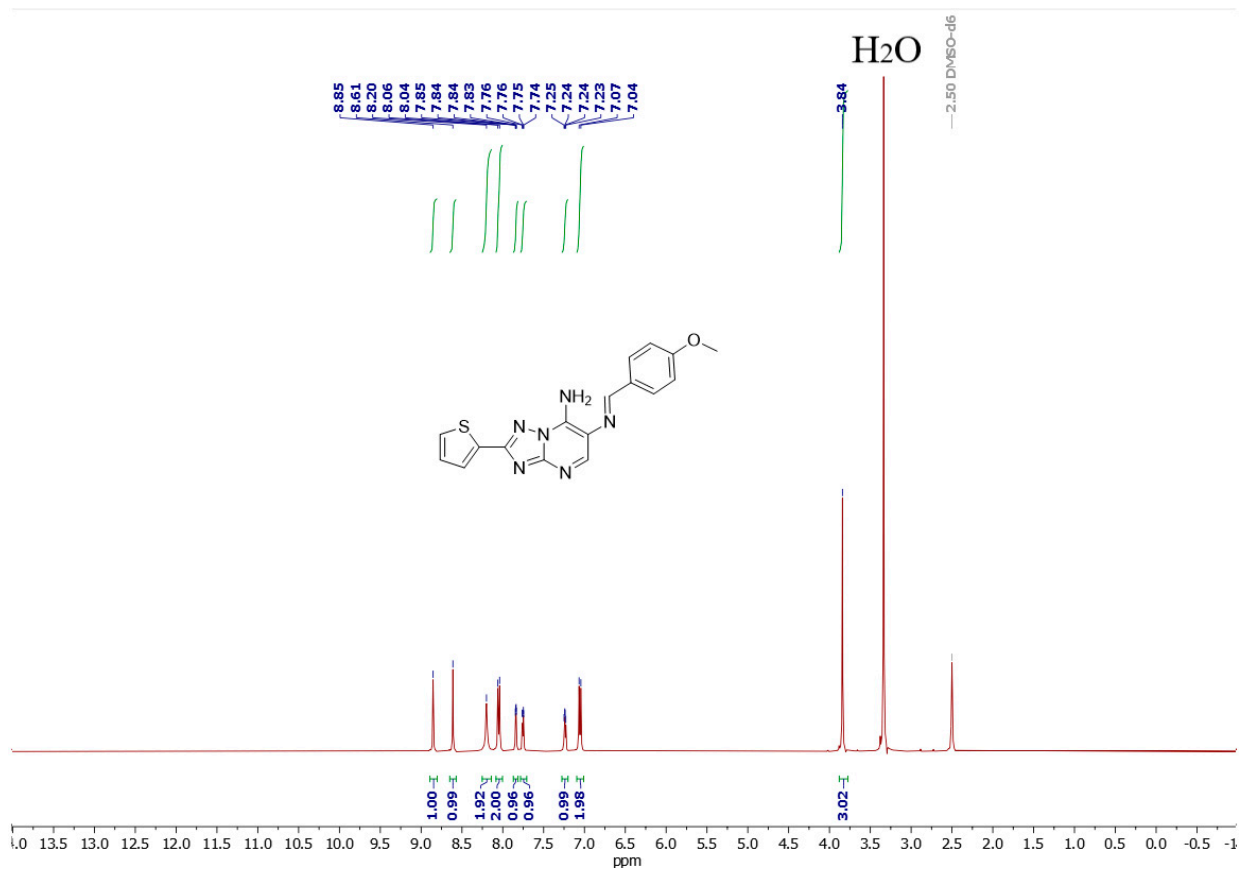


Figure S2. IR spectra of ((4-(dimethylamino)benzylidene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (**3a**)



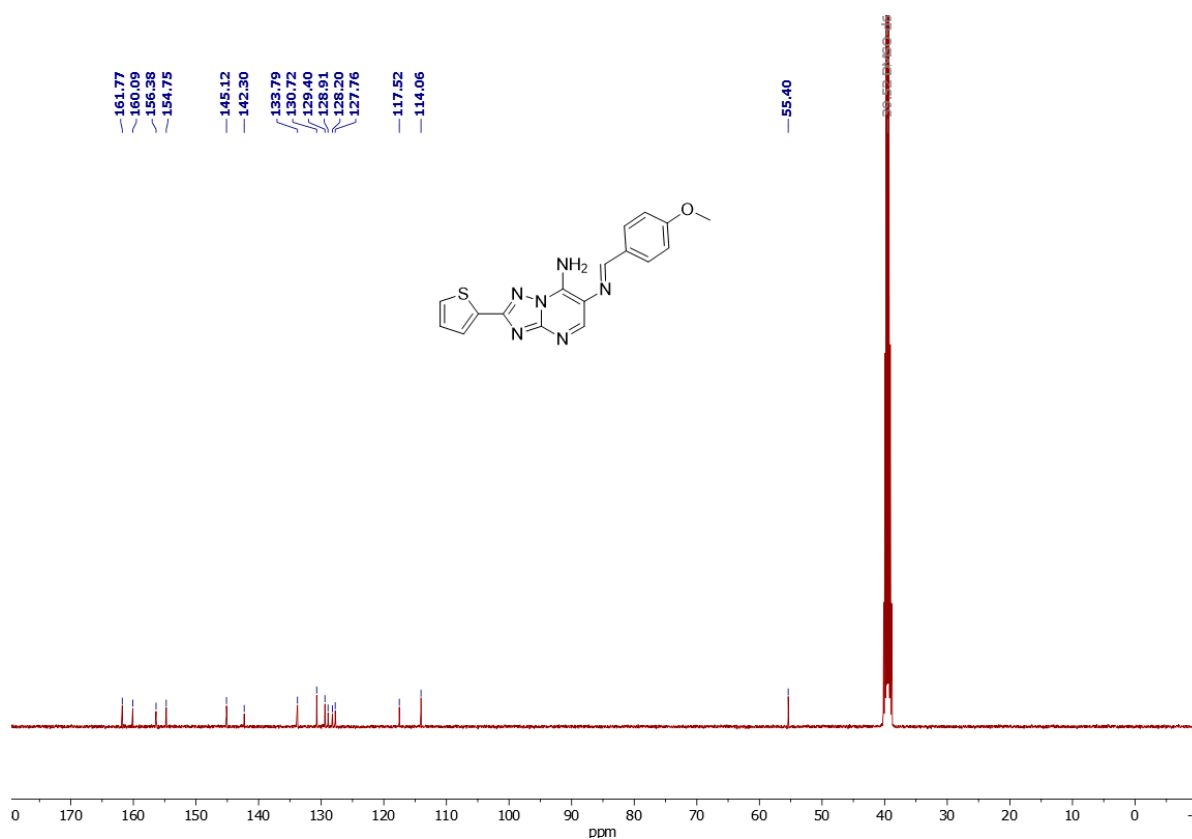


Figure S3. ¹H and ¹³C NMR spectra of ((4-methoxybenzylidene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (**3b**)

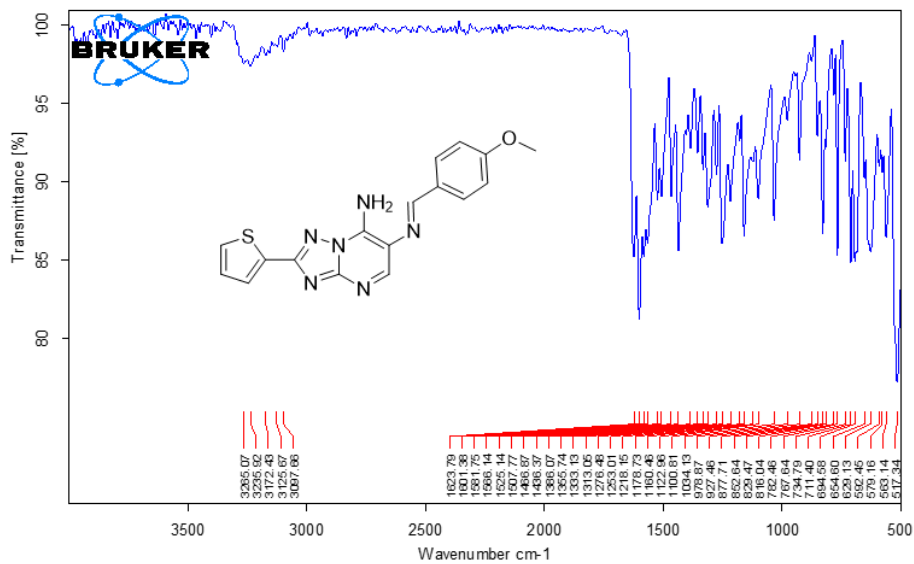


Figure S4. IR spectra of ((4-methoxybenzylidene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (**3b**)

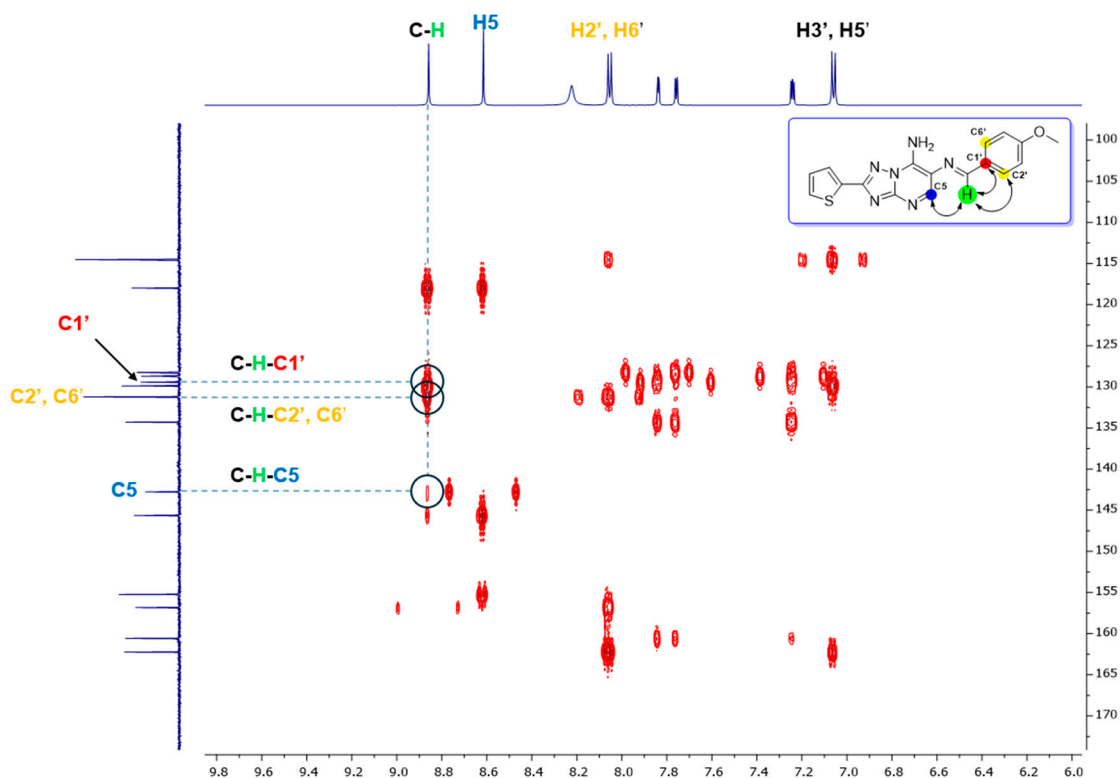
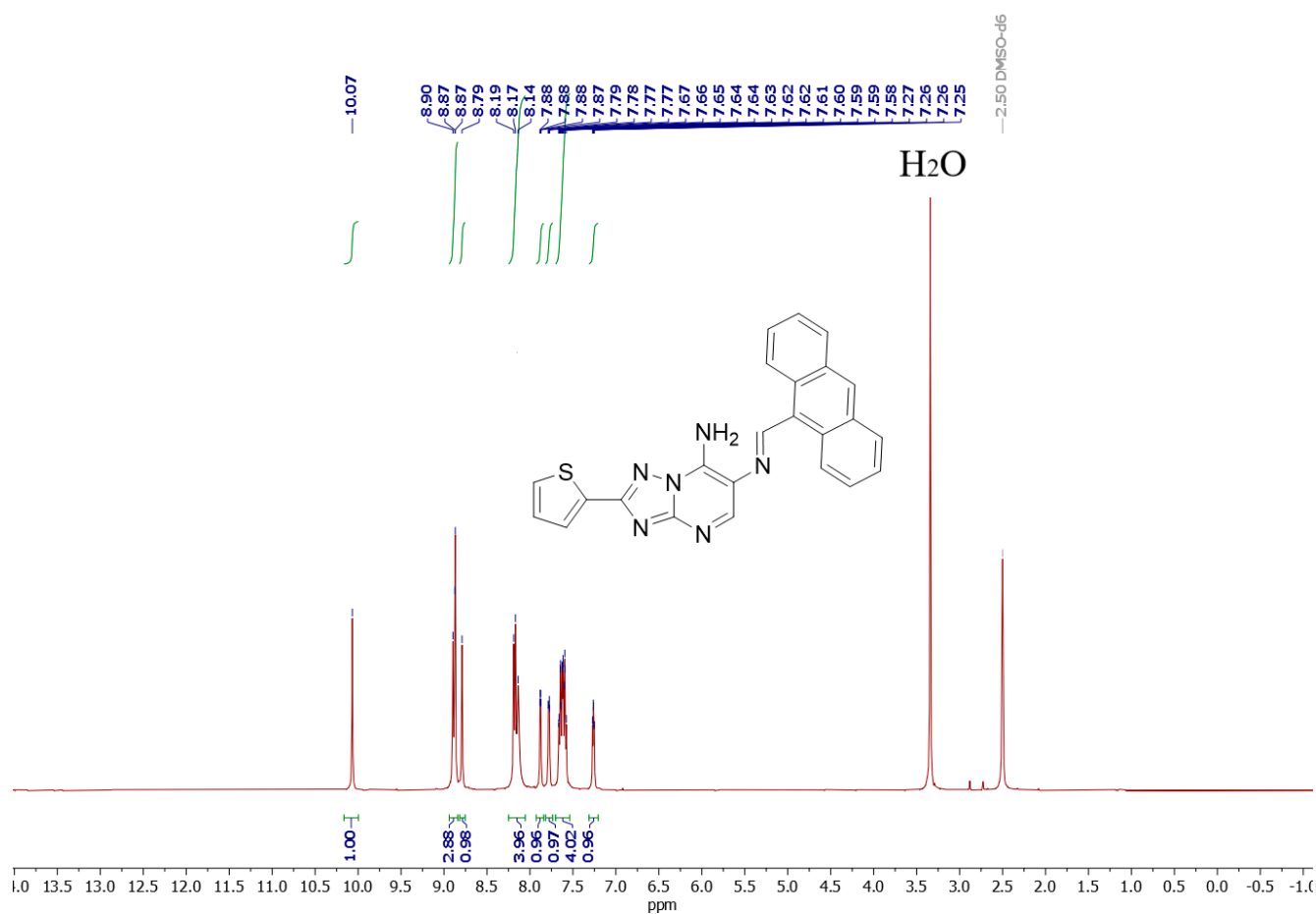


Figure S5. Key interactions in the ^1H - ^{13}C HMBC of the compound ((4-methoxybenzylidene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (**3b**)



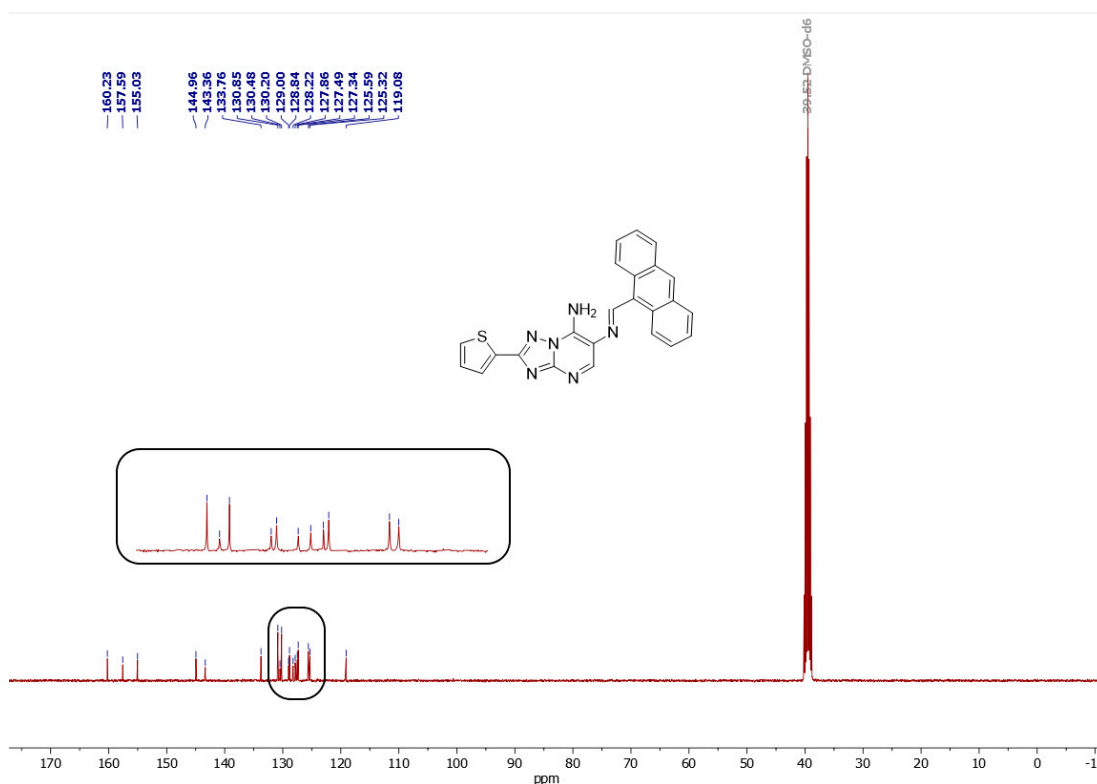


Figure S6. ¹H and ¹³C NMR spectra of ((anthracen-9-ylmethylene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (3c)

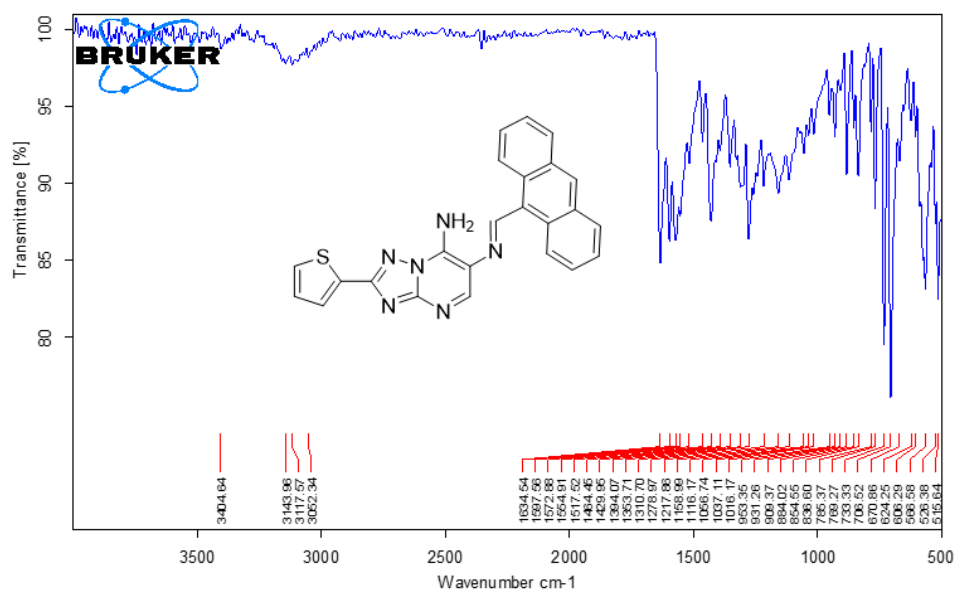


Figure S7. IR spectra of ((anthracen-9-ylmethylene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (3c)

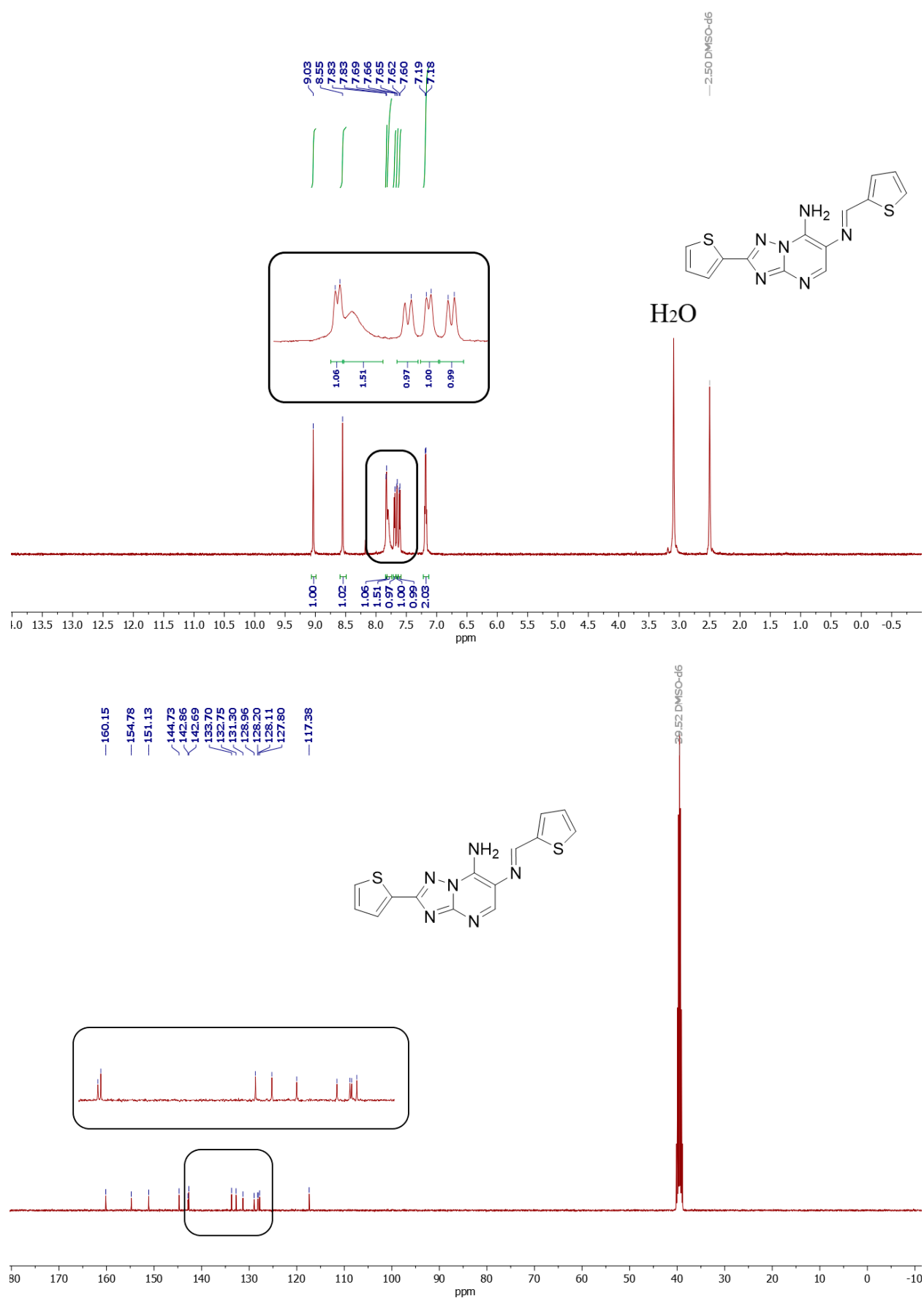


Figure S8. ^1H and ^{13}C NMR spectra of (thiophen-2-yl)-6-((thiophen-3-ylmethylene)amino)-[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (**3d**)

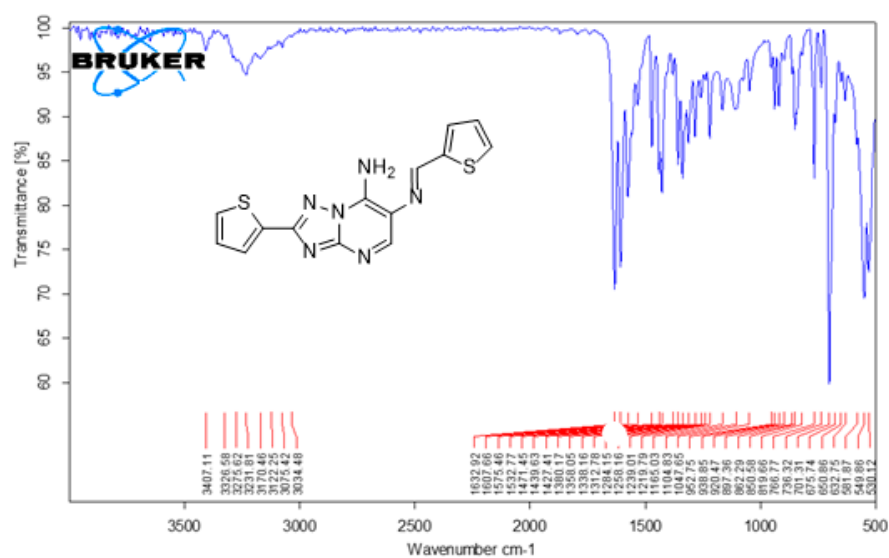
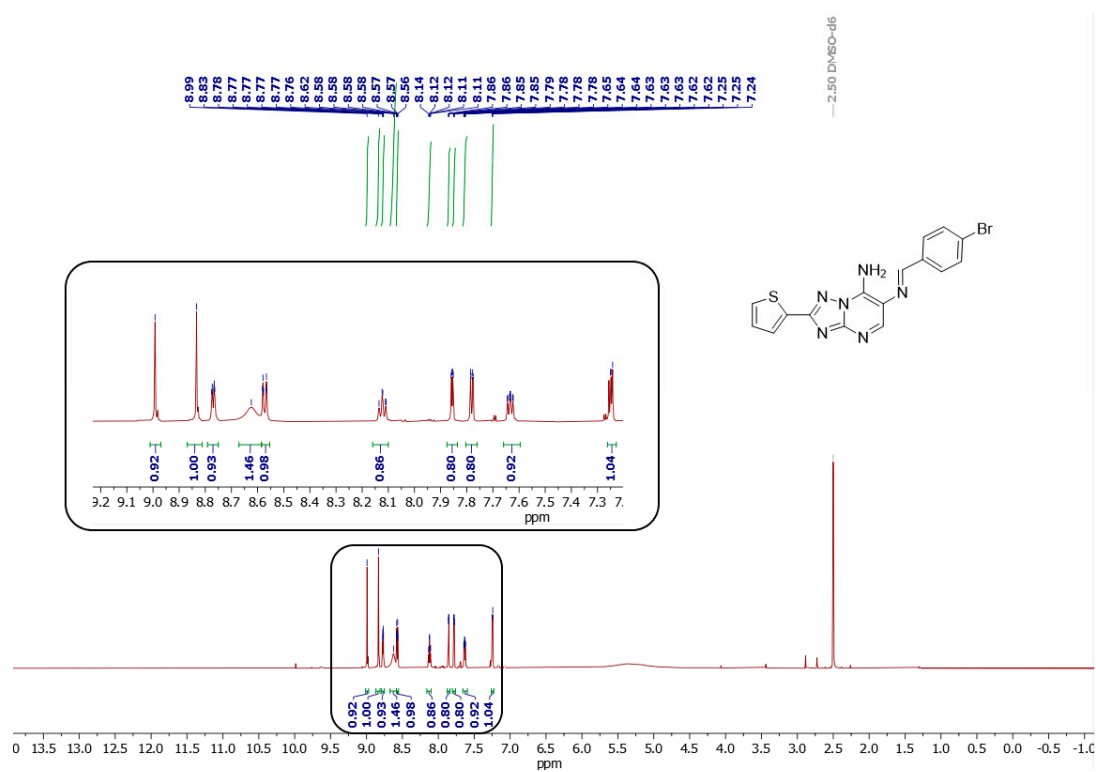


Figure S9. IR spectra of (thiophen-2-yl)-6-((thiophen-3-ylmethylene)amino)-[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (**3d**)



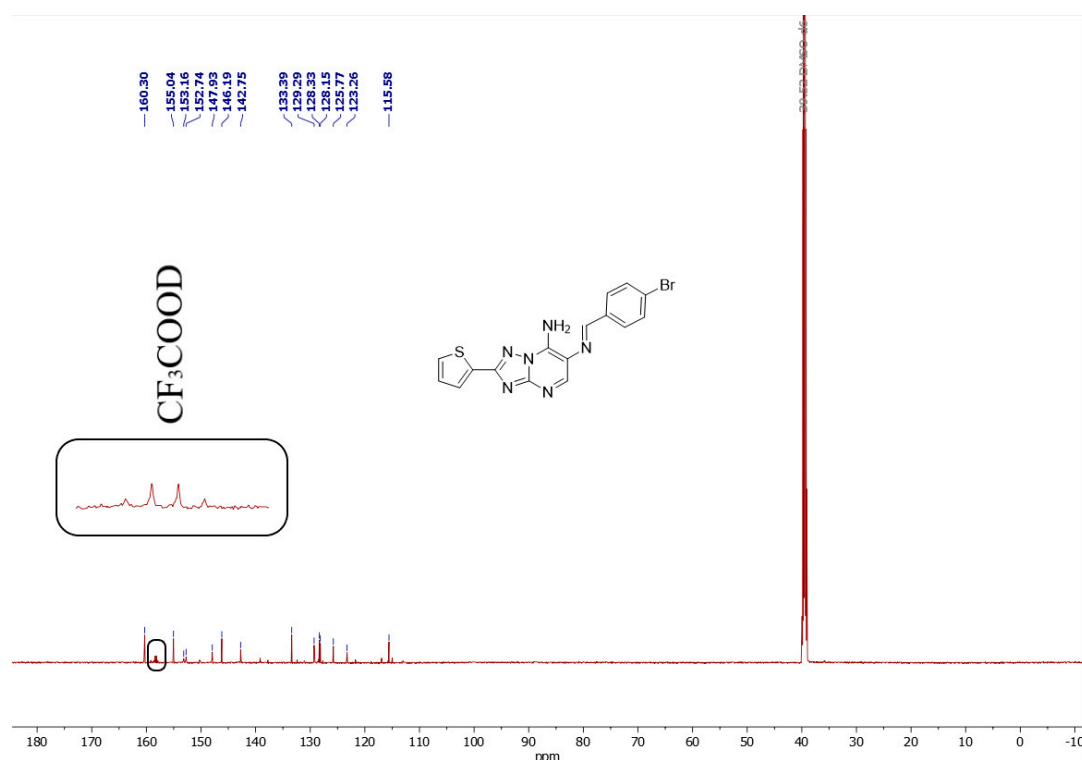


Figure S10. ¹H and ¹³C NMR spectra of 6-((4-bromobenzylidene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (3e)

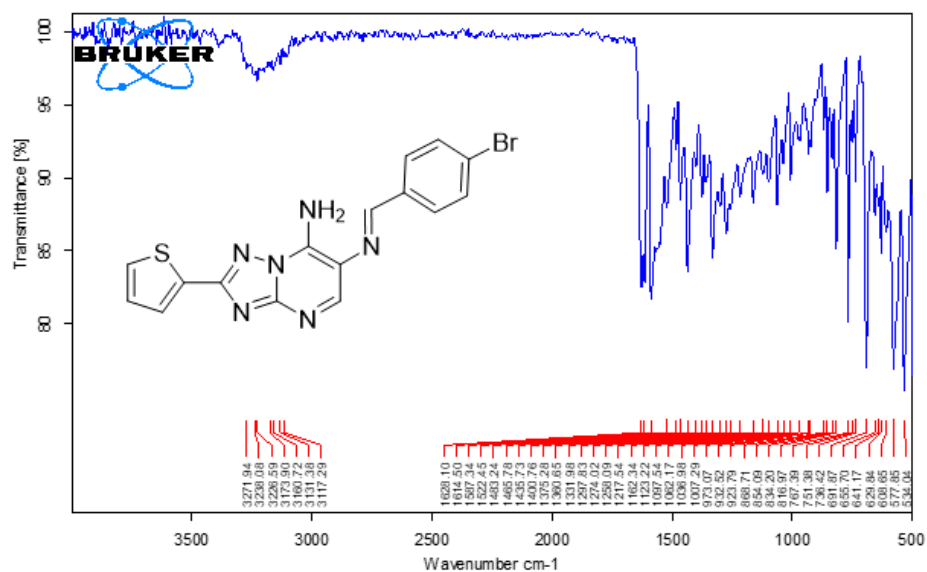


Figure S11. IR spectra of 6-((4-bromobenzylidene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (3e)

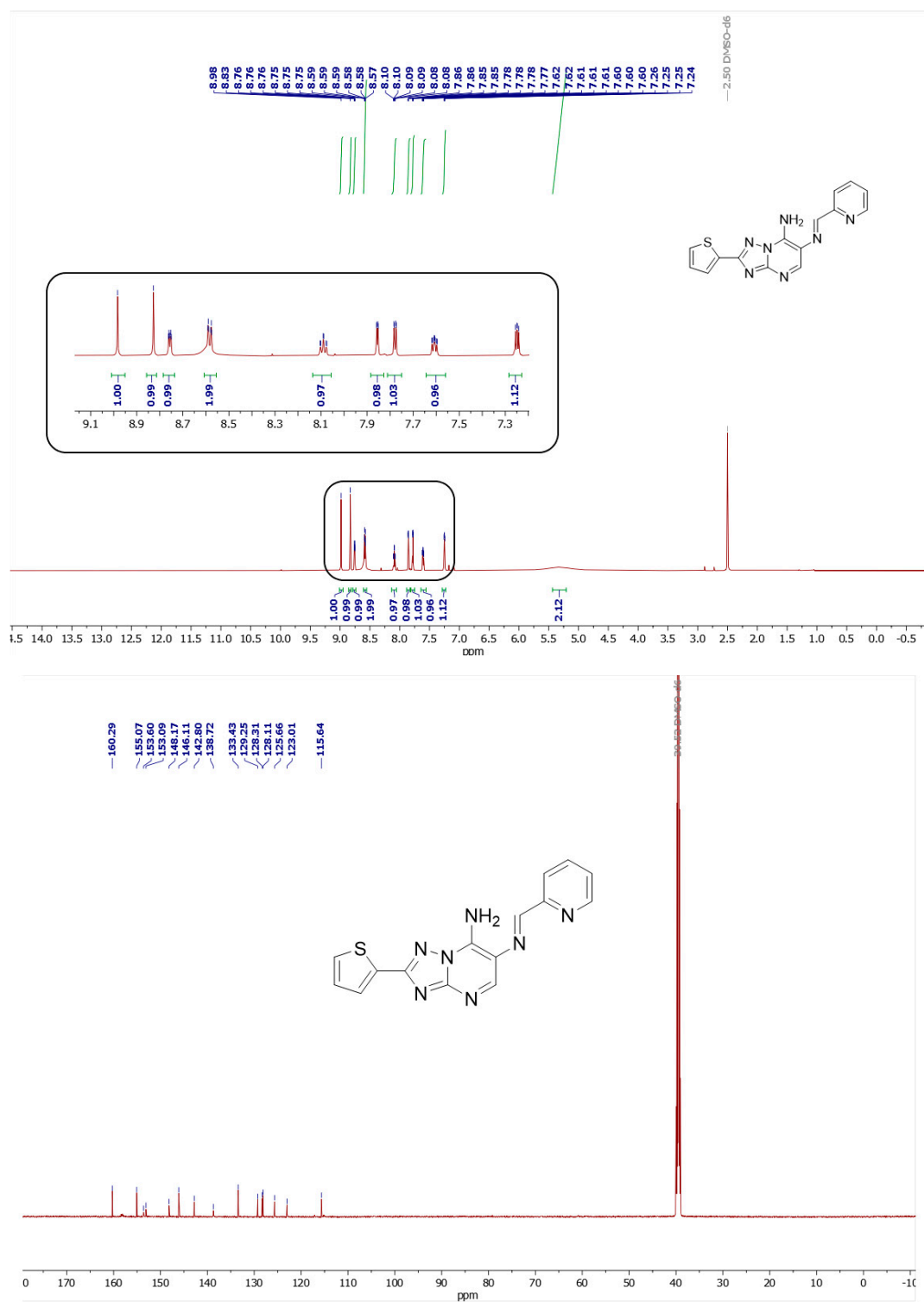


Figure S12. ¹H and ¹³C NMR spectra of 6-((pyridin-2-ylmethylene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (**3f**)

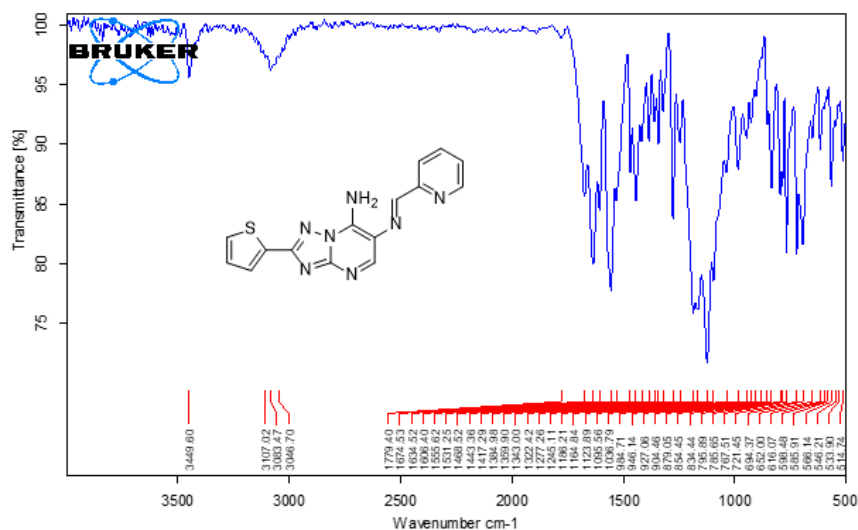
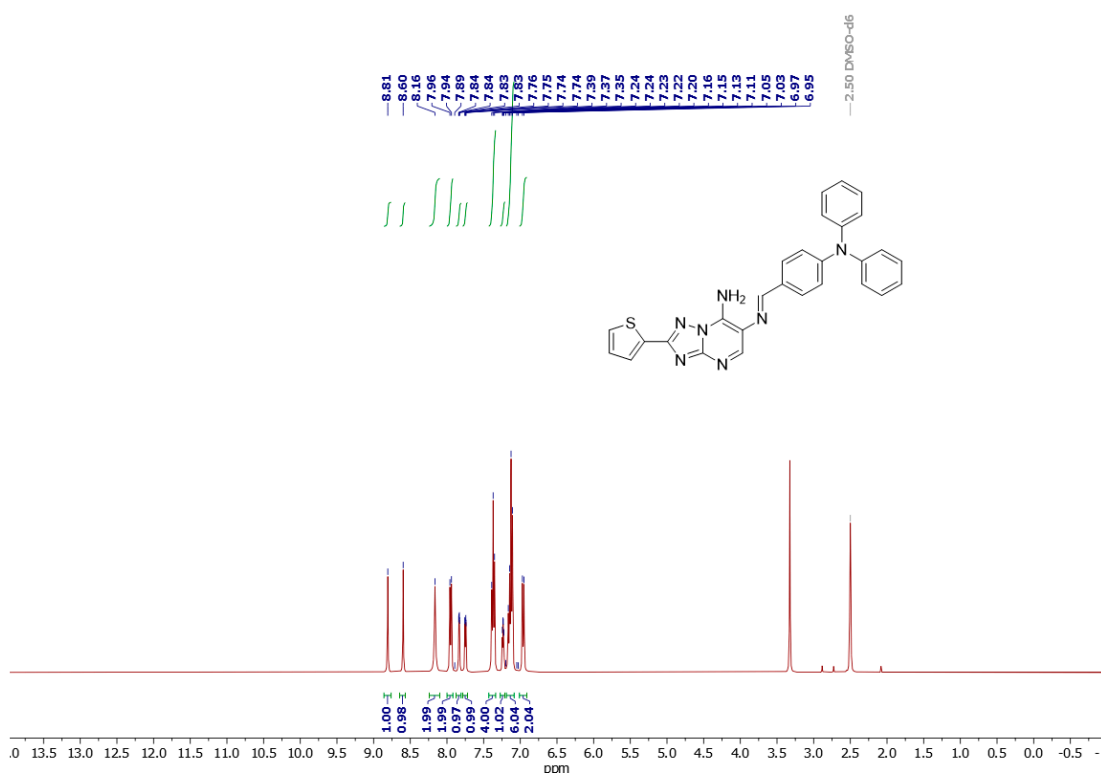


Figure S13. IR spectra of 6-((pyridin-2-ylmethylene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (**3f**)



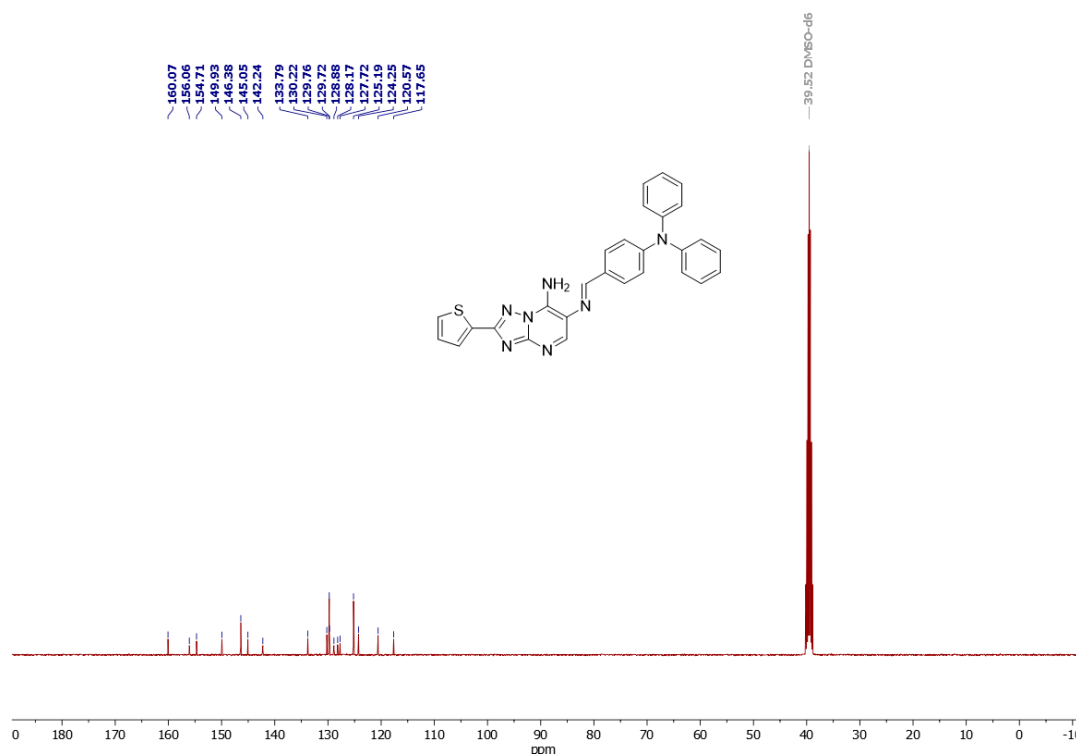


Figure S14. ¹H and ¹³C NMR spectra of ((4-(diphenylamino)benzylidene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (**3e**)

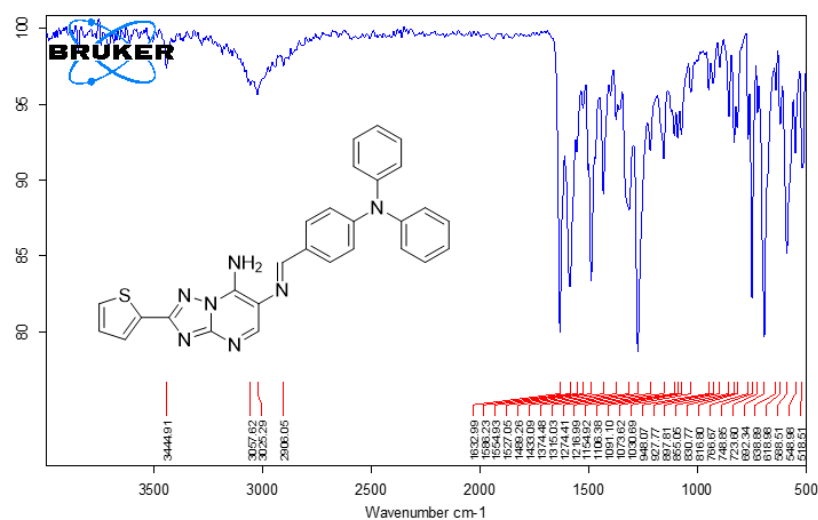


Figure S15. IR spectra of ((4-(diphenylamino)benzylidene)amino)-2-(thiophen-2-yl)-[1,2,4]triazolo[1,5-*a*]pyrimidin-7-amine (**3e**)

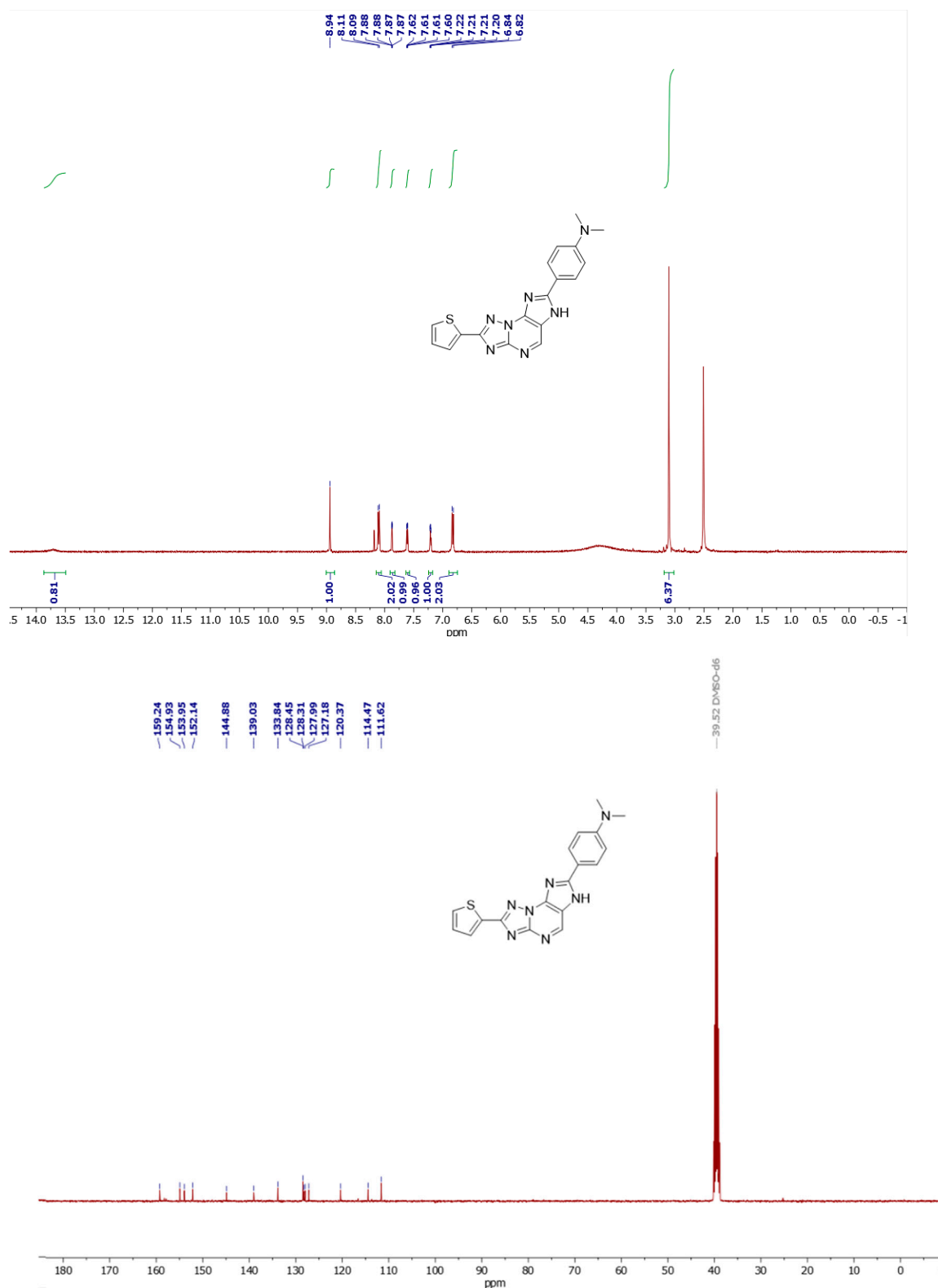


Figure S16. ¹H and ¹³C NMR spectra of *N,N*-dimethyl-4-(2-(thiophen-2-yl)-6*H*-[1,2,4]triazolo[5,1-*b*]purin-7-yl)aniline (**4a**)

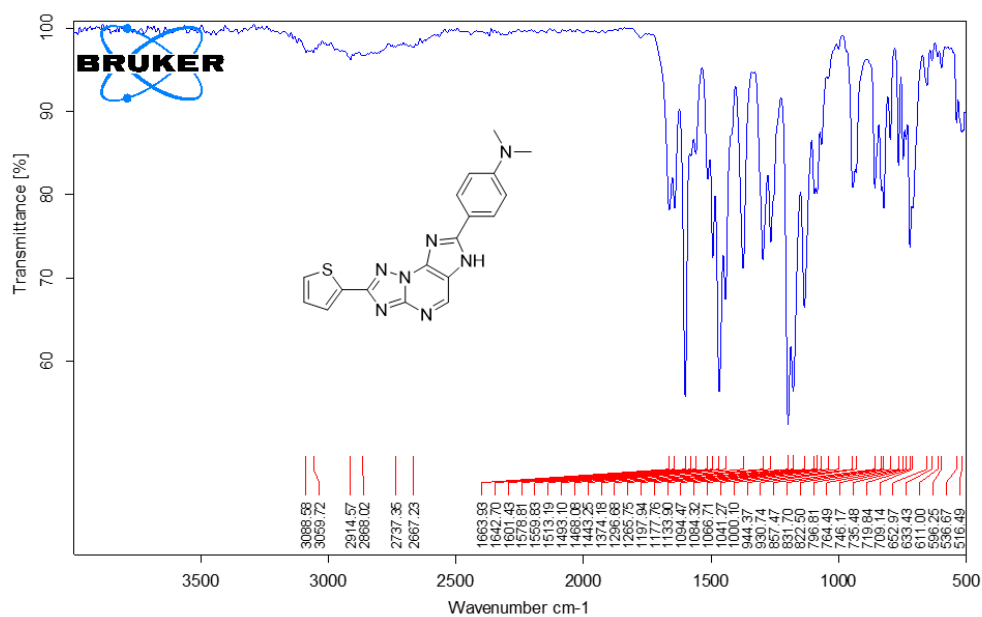


Figure S17. IR spectra of *N,N*-dimethyl-4-(2-(thiophen-2-yl)-6*H*-[1,2,4]triazolo[5,1-*b*]purin-7-yl)aniline (**4a**)

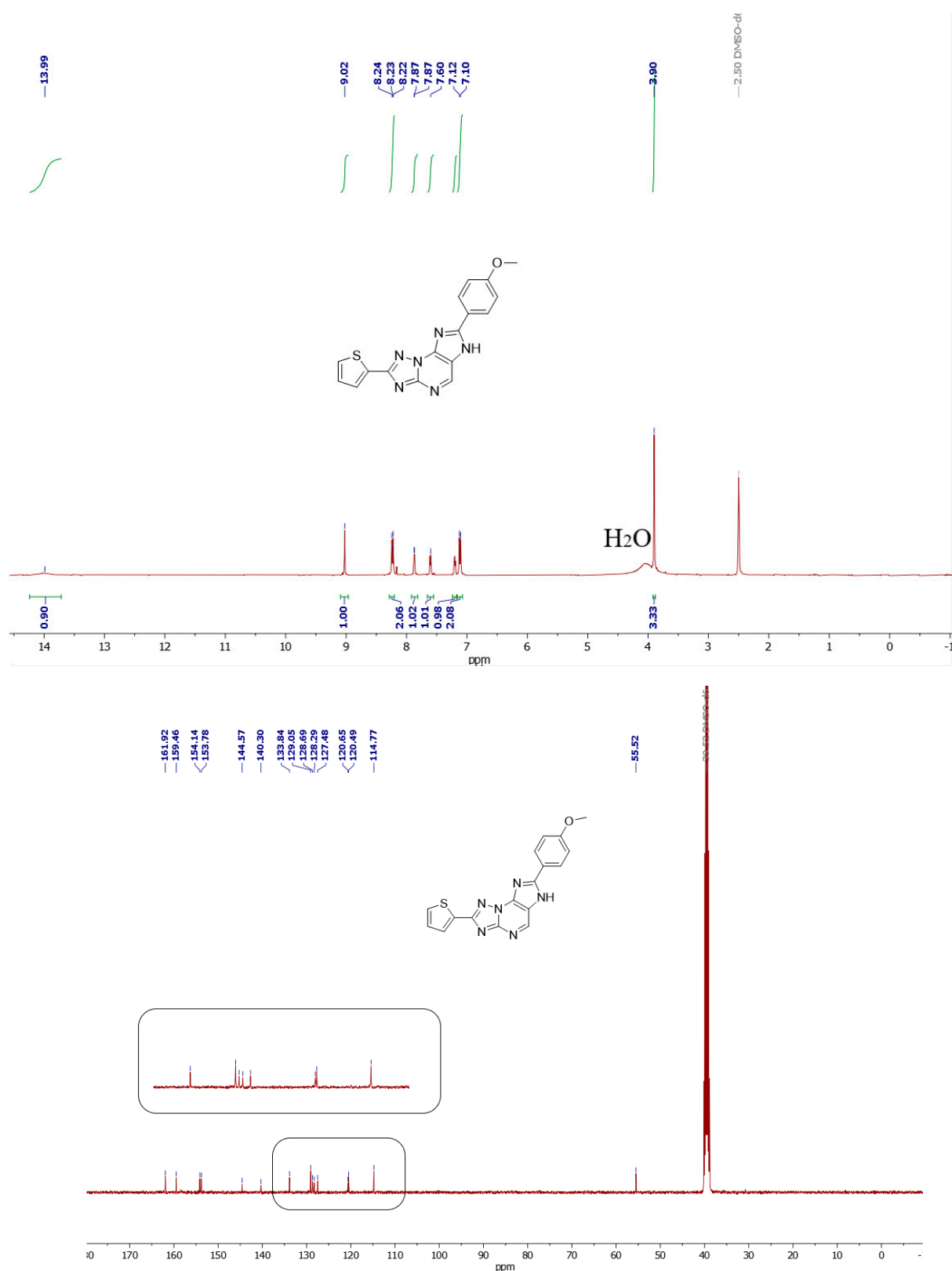


Figure S18. ¹H and ¹³C NMR spectra of 7-(4-methoxyphenyl)-2-(thiophen-2-yl)-6H-[1,2,4]triazolo[5,1-*b*]purine (**4b**)

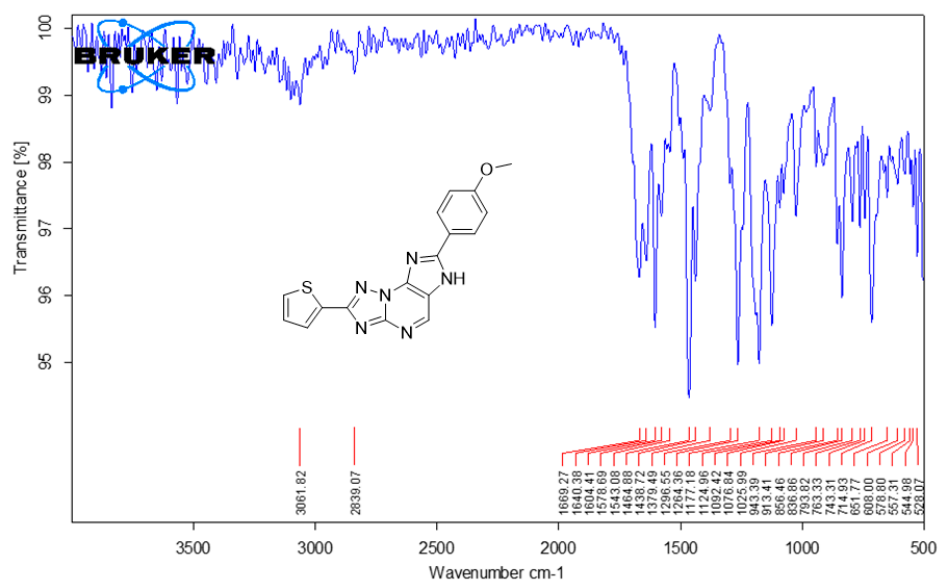
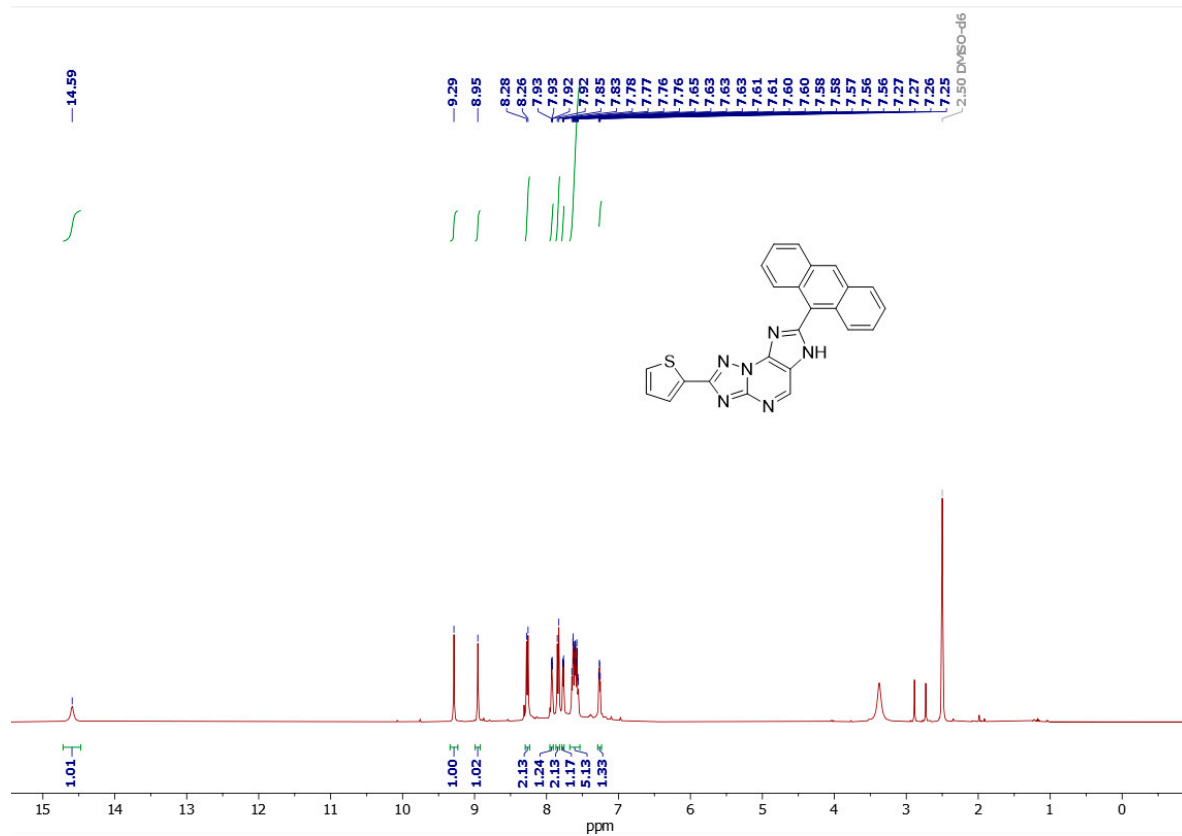


Figure S19. IR spectra of 7-(4-methoxyphenyl)-2-(thiophen-2-yl)-6H-[1,2,4]triazolo[5,1-b]purine (**4b**)



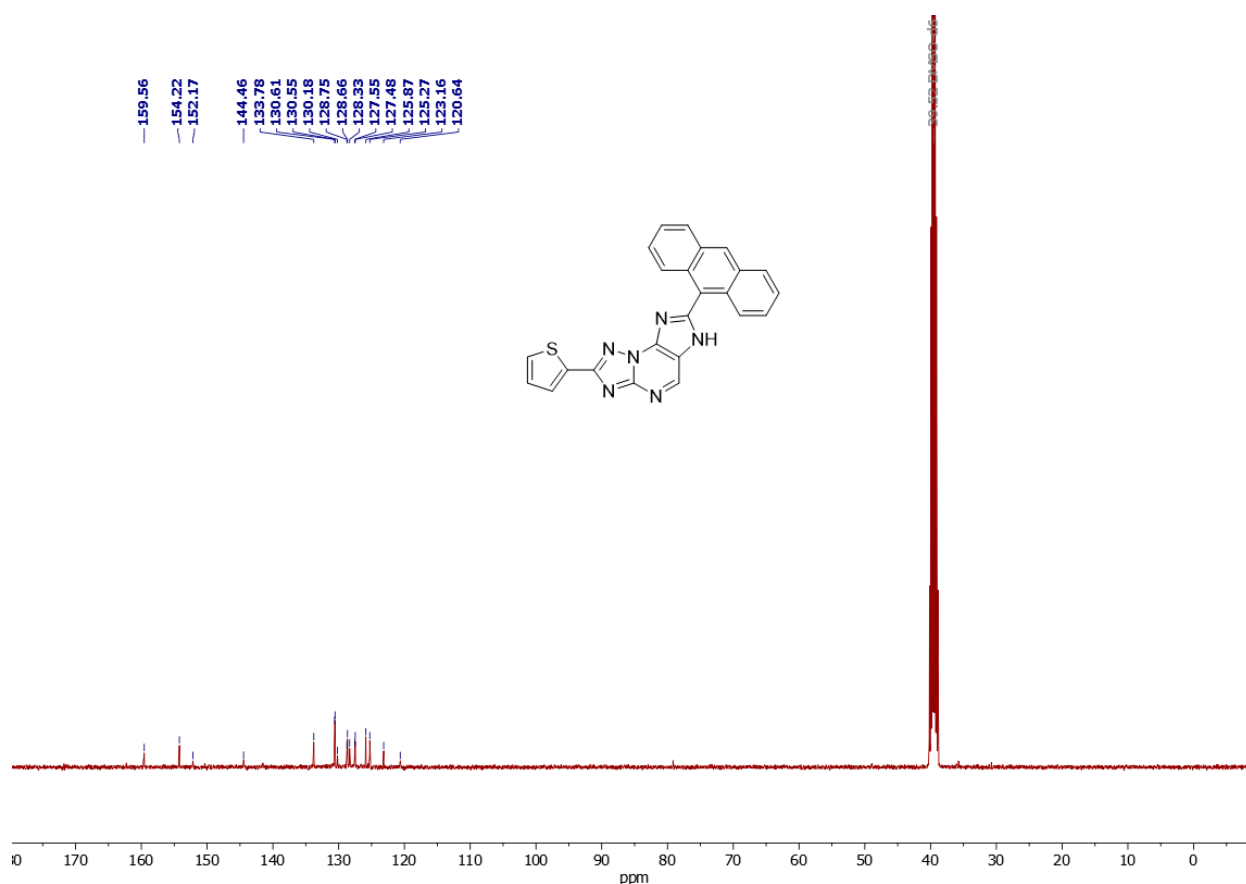


Figure S20. ¹H and ¹³C NMR spectra of 7-(anthracen-9-yl)-2-(thiophen-2-yl)-6H-[1,2,4]triazolo[5,1-b]purine (4c)

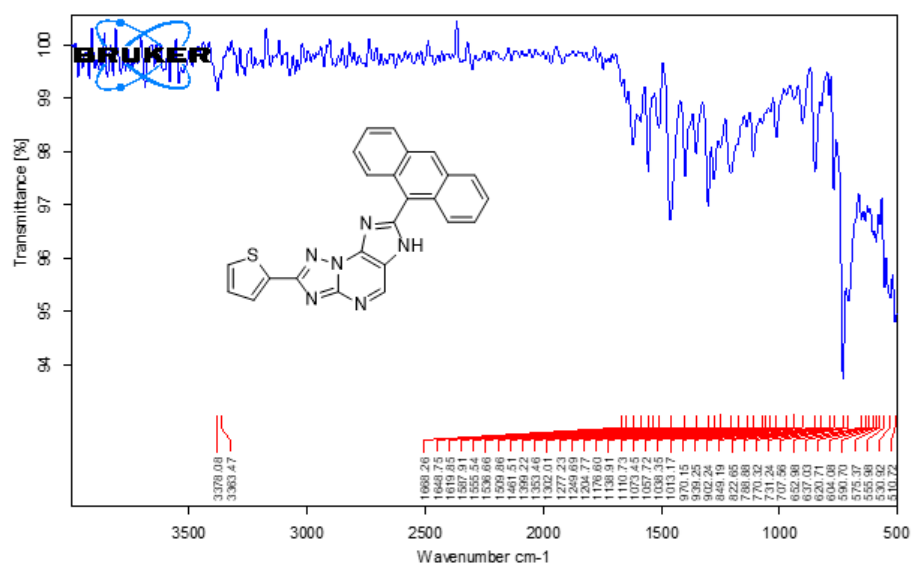


Figure S21. IR spectra of 7-(anthracen-9-yl)-2-(thiophen-2-yl)-6H-[1,2,4]triazolo[5,1-b]purine (4c)

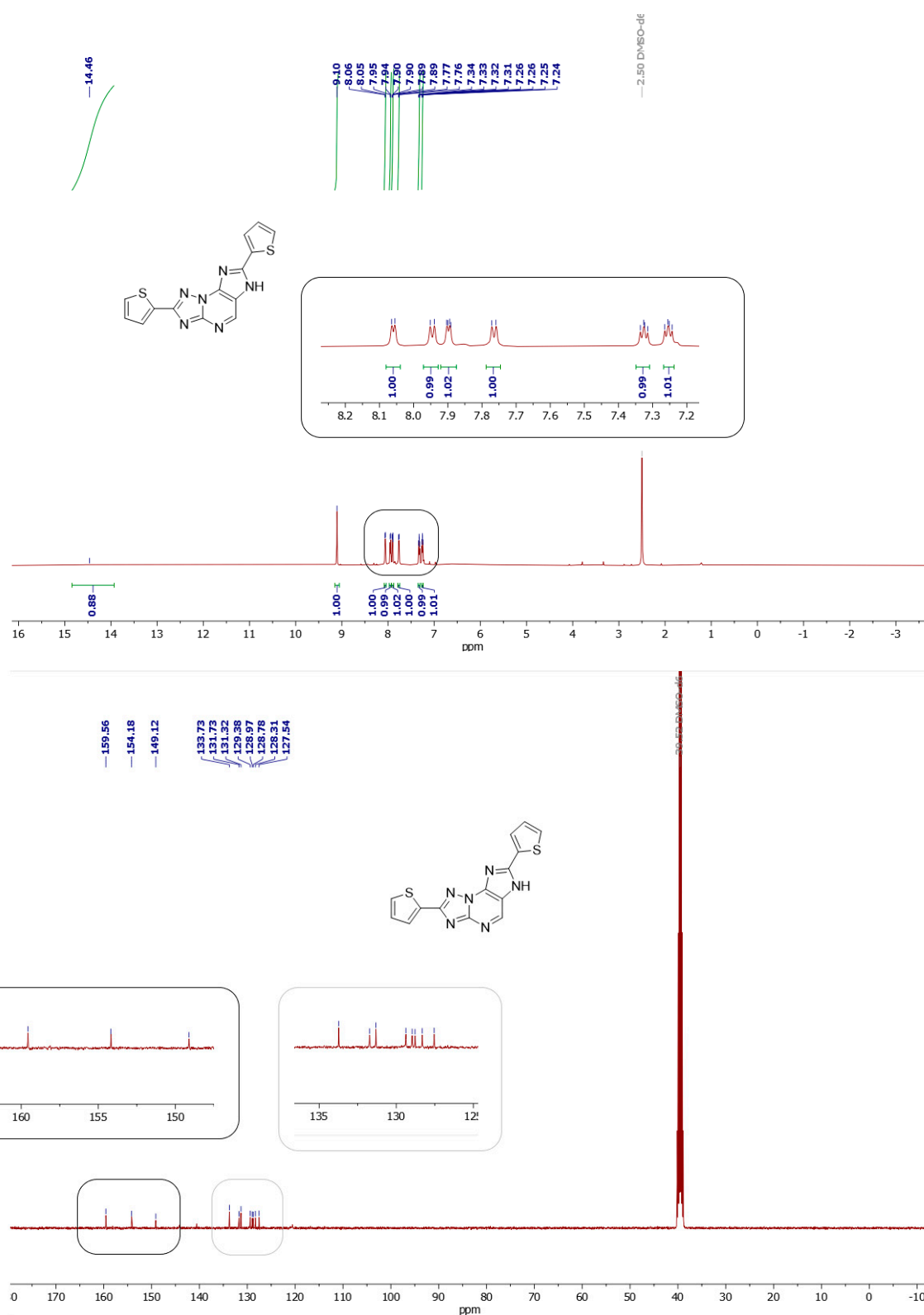


Figure S22. ¹H and ¹³C NMR spectra of 2,7-di(thiophen-2-yl)-6H-[1,2,4]triazolo[5,1-b]purine (4c)

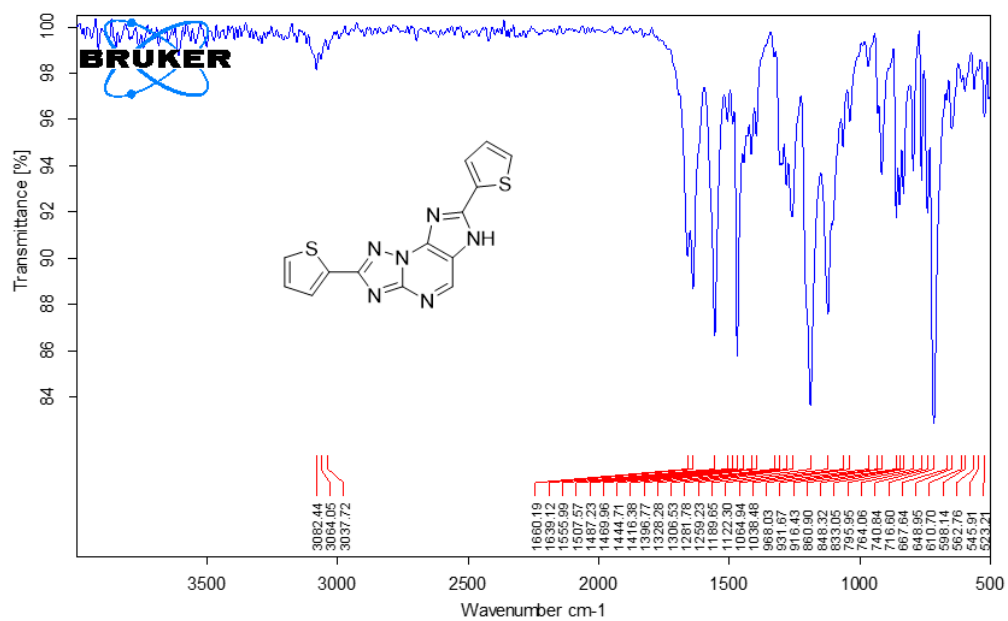
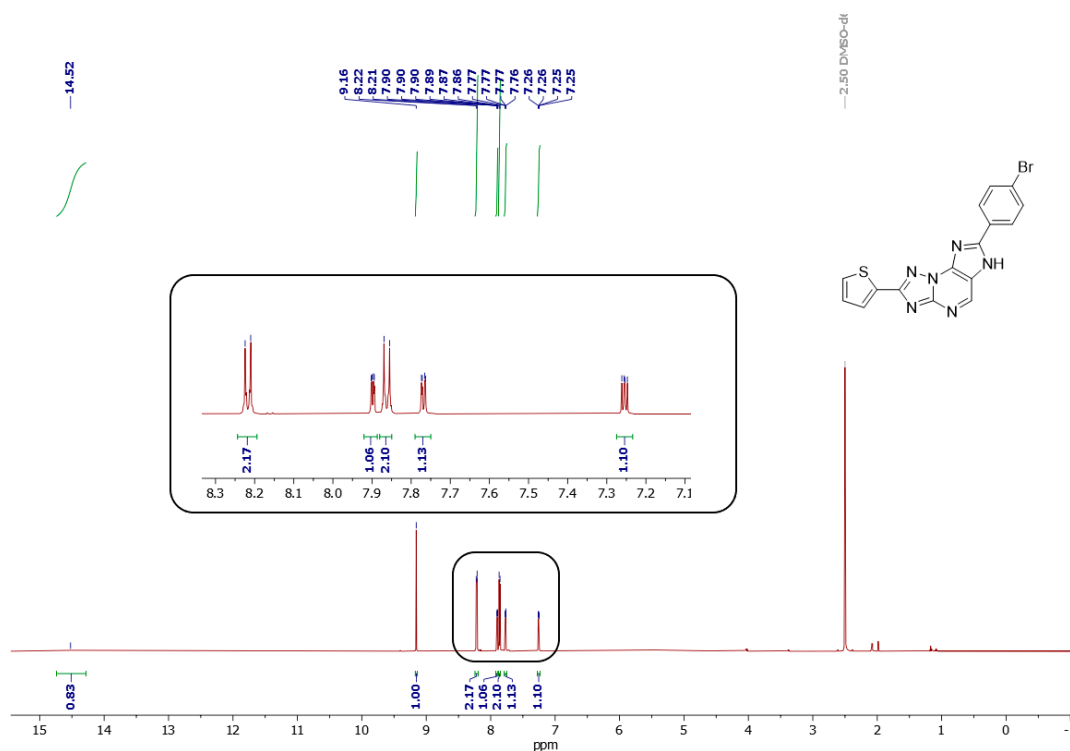


Figure S23. IR spectra of 2,7-di(thiophen-2-yl)-6H-[1,2,4]triazolo[5,1-b]purine (4c)



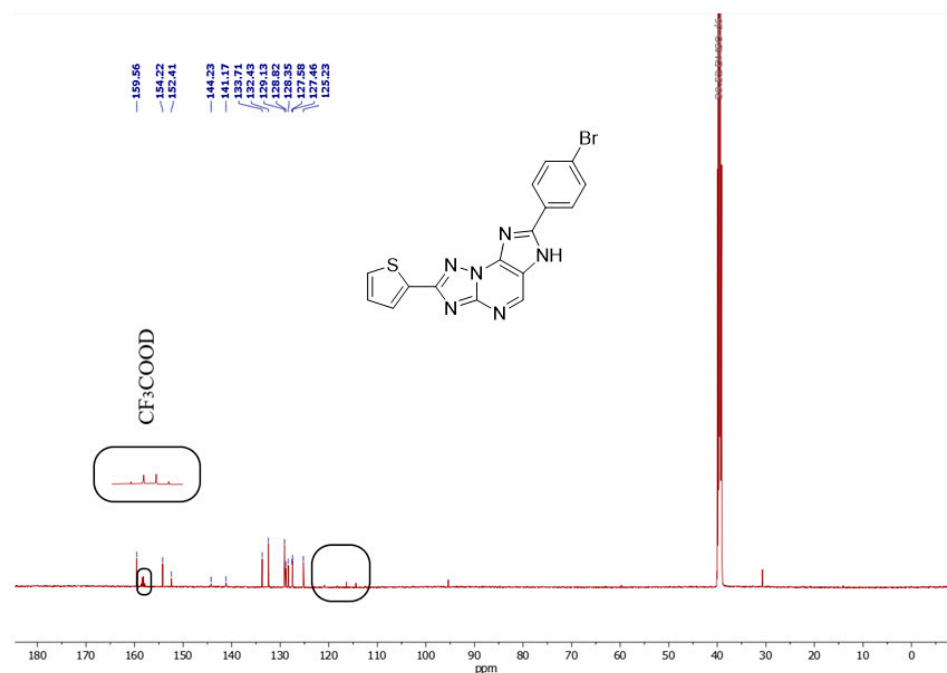


Figure S24. ^1H and ^{13}C NMR spectra of 7-(4-bromophenyl)-2-(thiophen-2-yl)-6H-[1,2,4]triazolo[5,1-*b*]purine (3e)

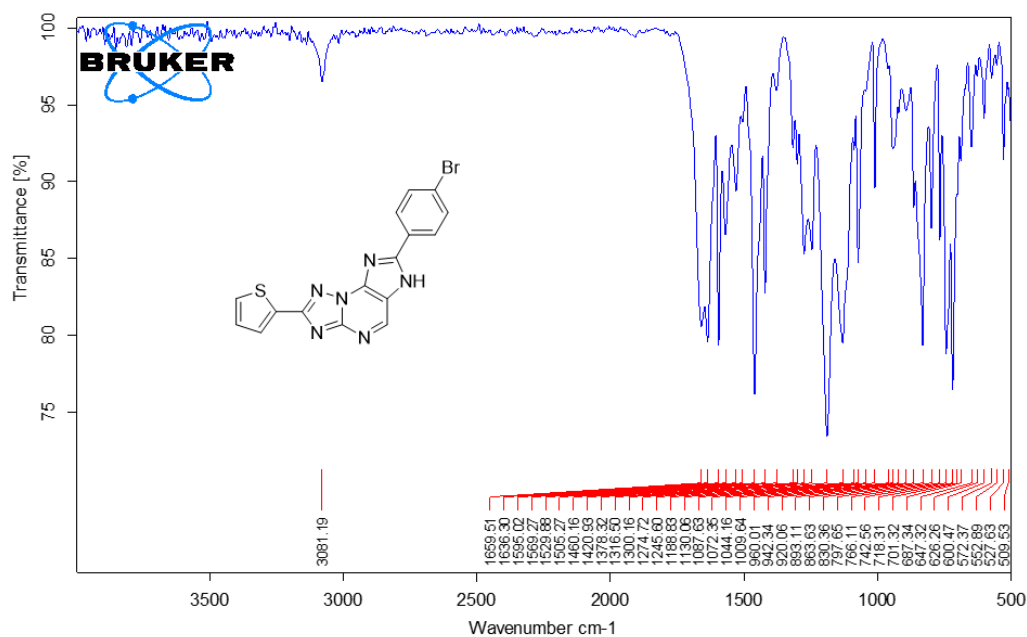


Figure S25. IR spectra of 7-(4-bromophenyl)-2-(thiophen-2-yl)-6H-[1,2,4]triazolo[5,1-*b*]purine (4e)

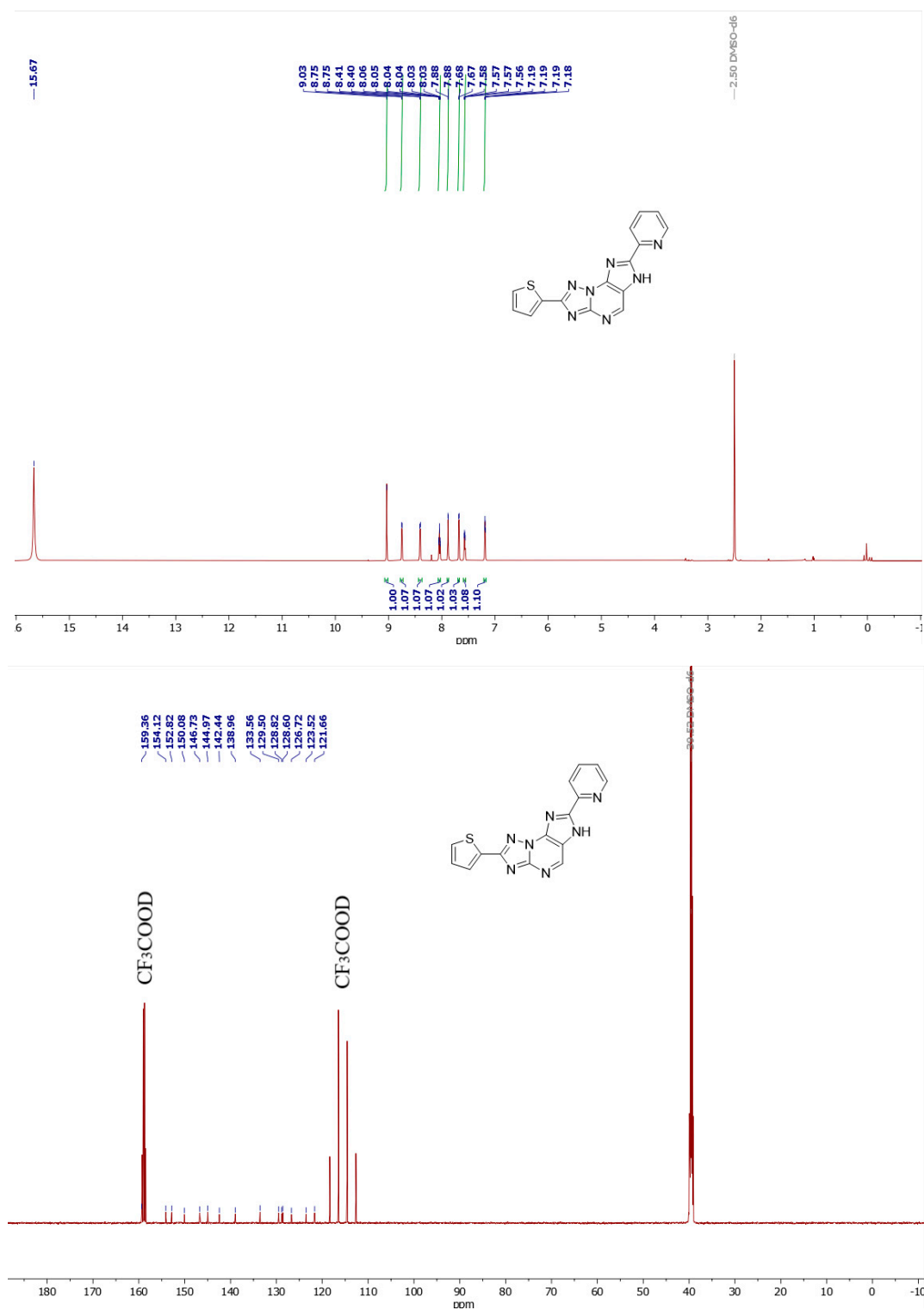


Figure S26. ¹H and ¹³C NMR spectra of 7-(pyridin-2-yl)-2-(thiophen-2-yl)-6H-[1,2,4]triazolo[5,1-*b*]purine (**4f**)

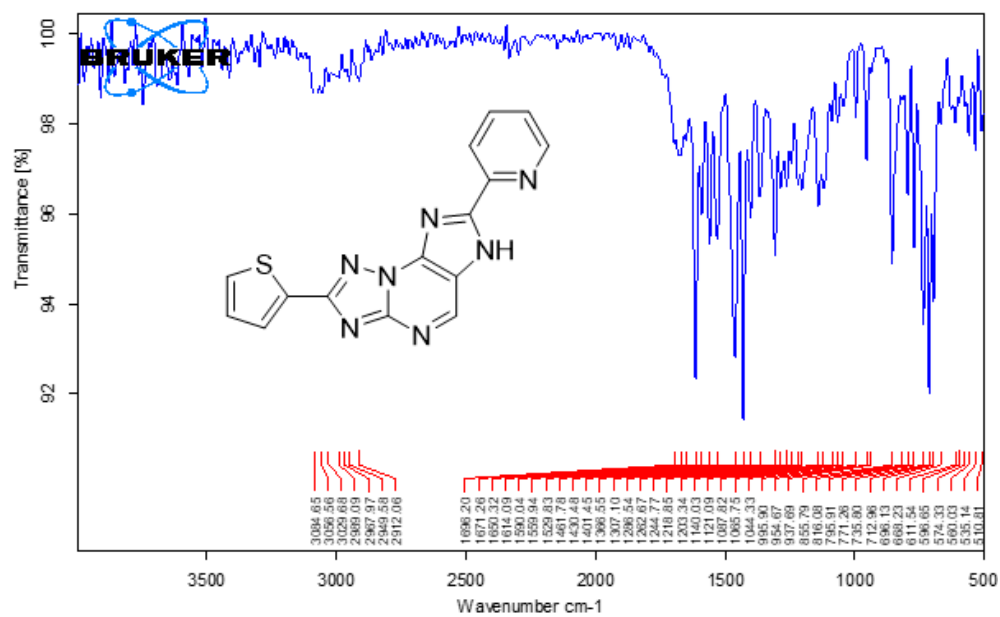
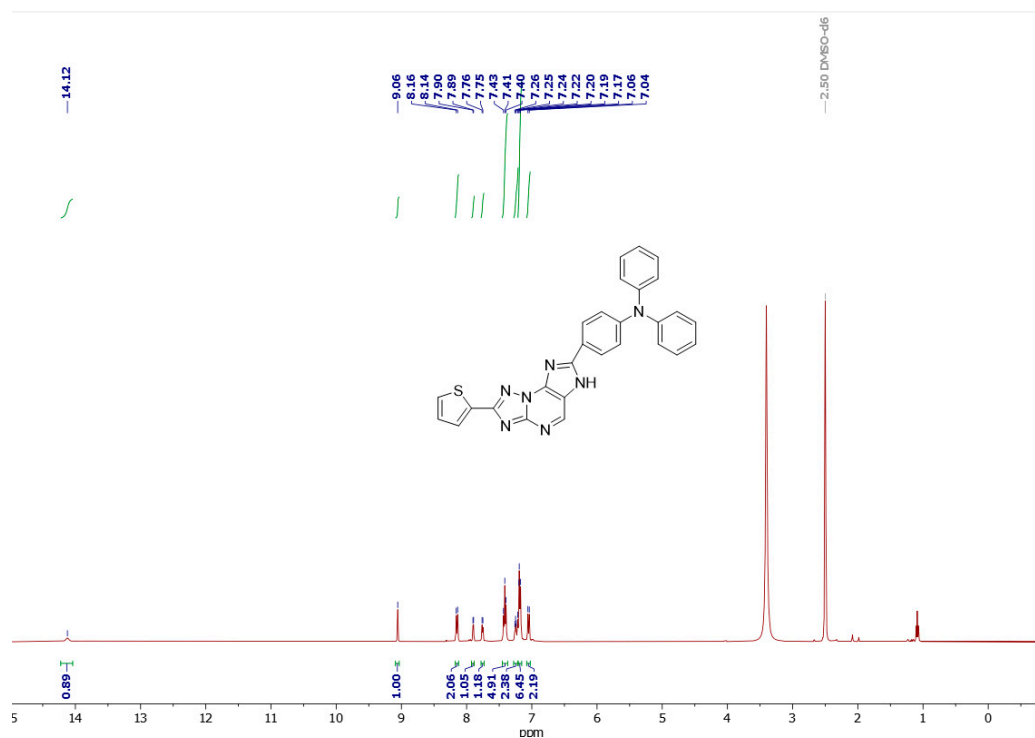


Figure S27. IR spectra of 7-(pyridin-2-yl)-2-(thiophen-2-yl)-6H-[1,2,4]triazolo[5,1-b]purine (4f)



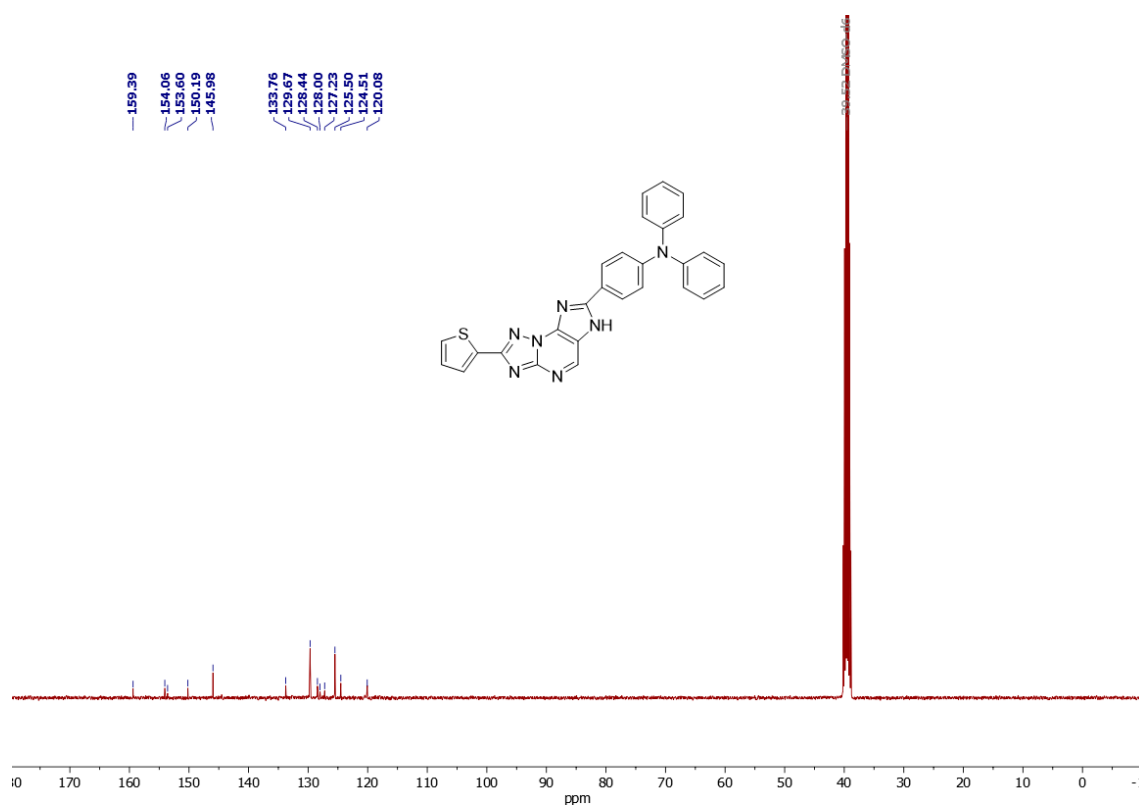


Figure S28. ¹H and ¹³C NMR spectra of *N,N*-diphenyl-4-(2-(thiophen-2-yl)-6*H*-[1,2,4]triazolo[5,1-*b*]purin-7-yl)aniline (**4g**)

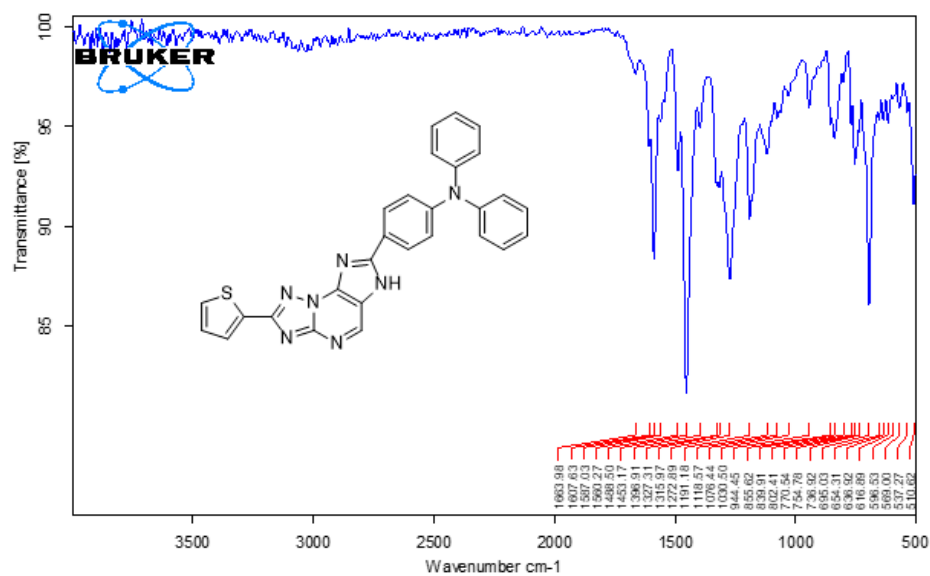


Figure S29. IR spectra of *N,N*-diphenyl-4-(2-(thiophen-2-yl)-6*H*-[1,2,4]triazolo[5,1-*b*]purin-7-yl)aniline (**4g**)

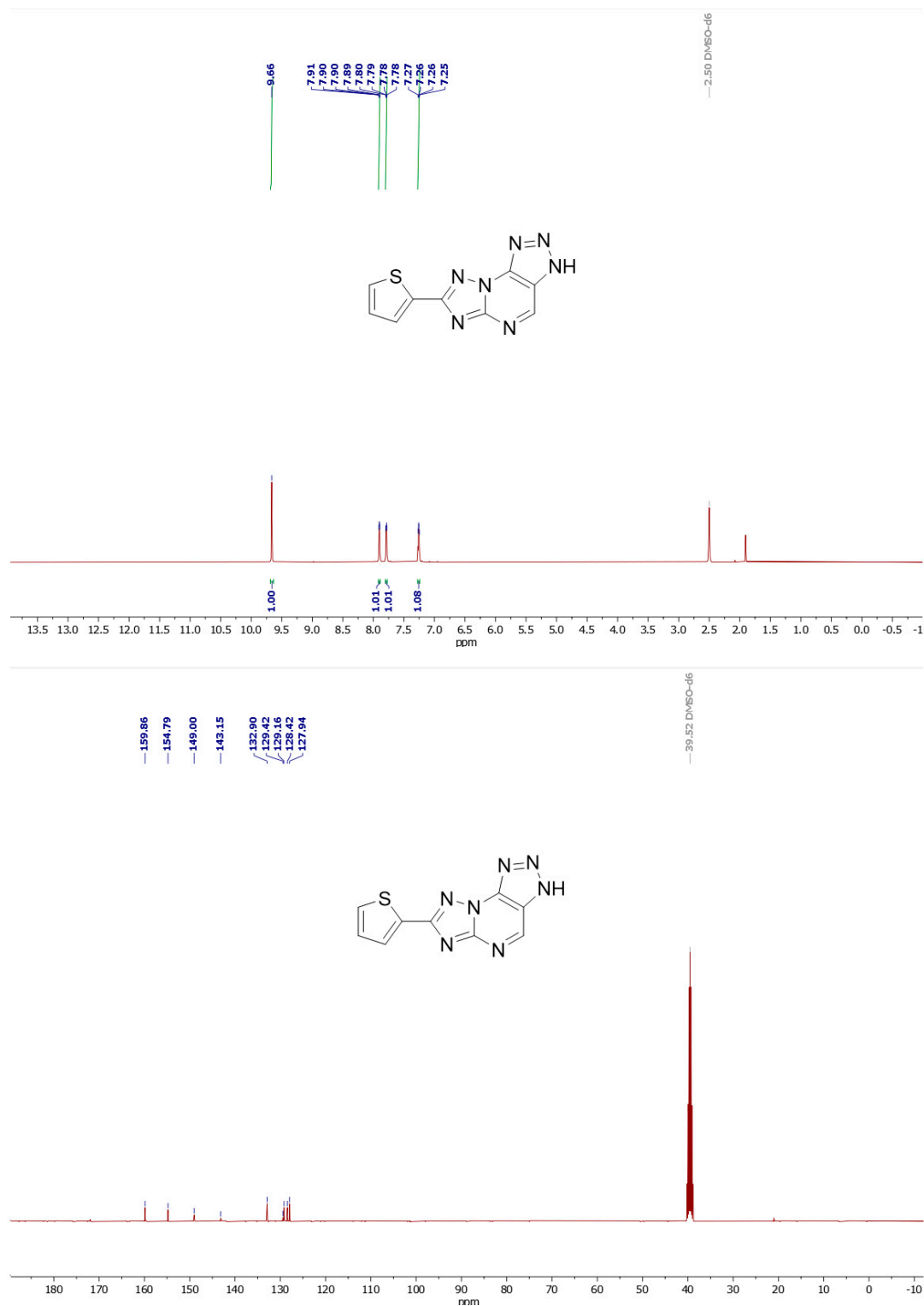


Figure S30. ¹H and ¹³C NMR spectra of 7-(thiophen-2-yl)-3H-[1,2,3]triazolo[4,5-e][1,2,4]triazolo[1,5-a]pyrimidine (5)

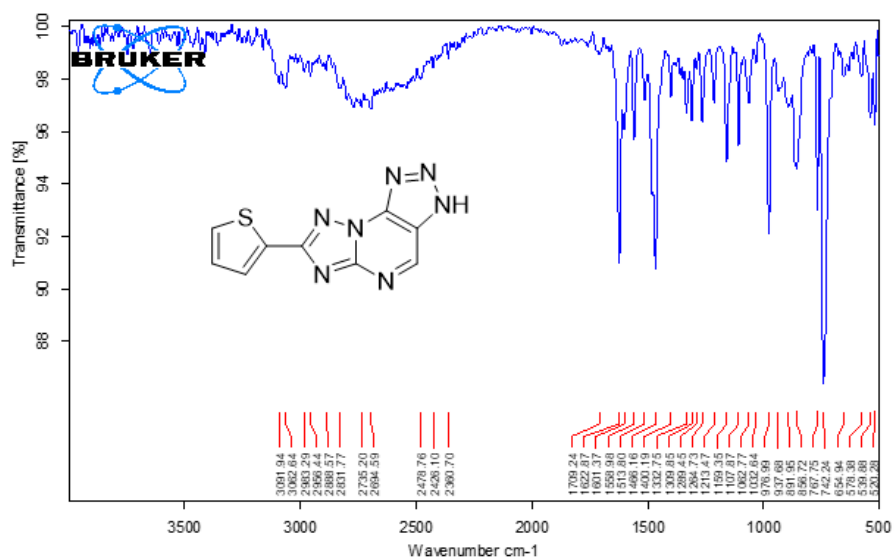
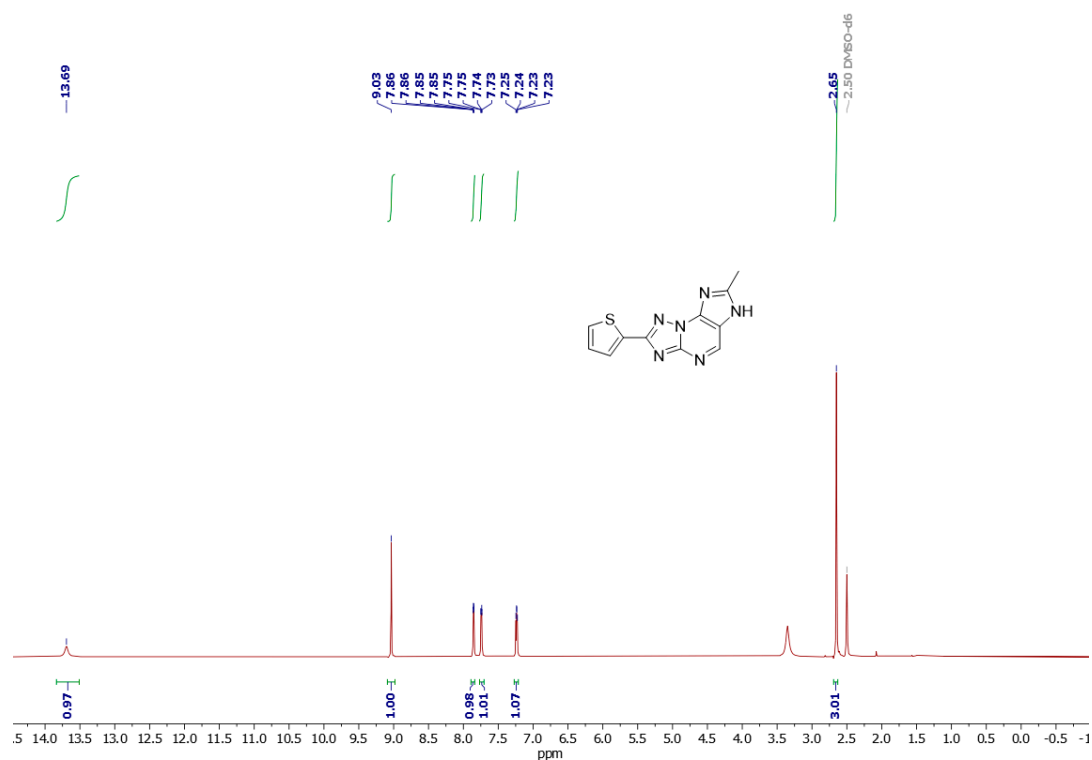


Figure S31. IR spectra of 7-(thiophen-2-yl)-3H-[1,2,3]triazolo[4,5-e][1,2,4]triazolo[1,5-a]pyrimidine (**5**)



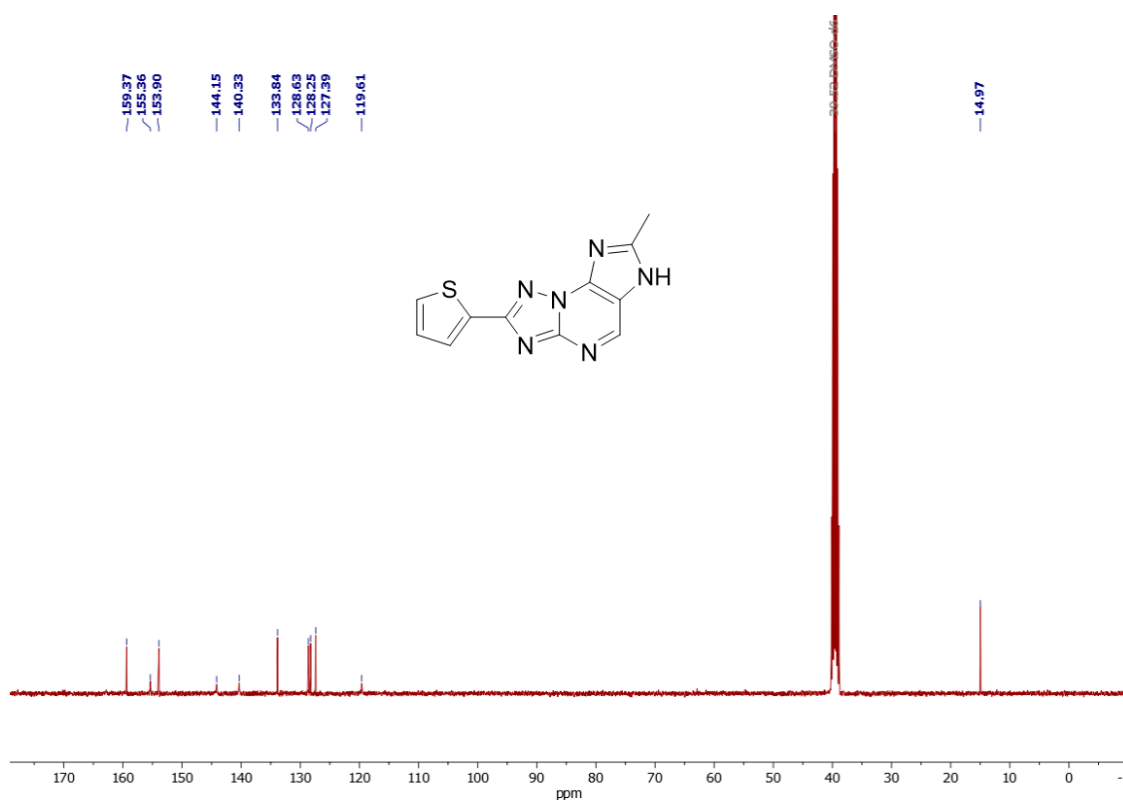


Figure S32. ¹H and ¹³C NMR spectra of 7-methyl-2-(thiophen-2-yl)-6H-[1,2,4]triazolo[5,1-b]purine (6)

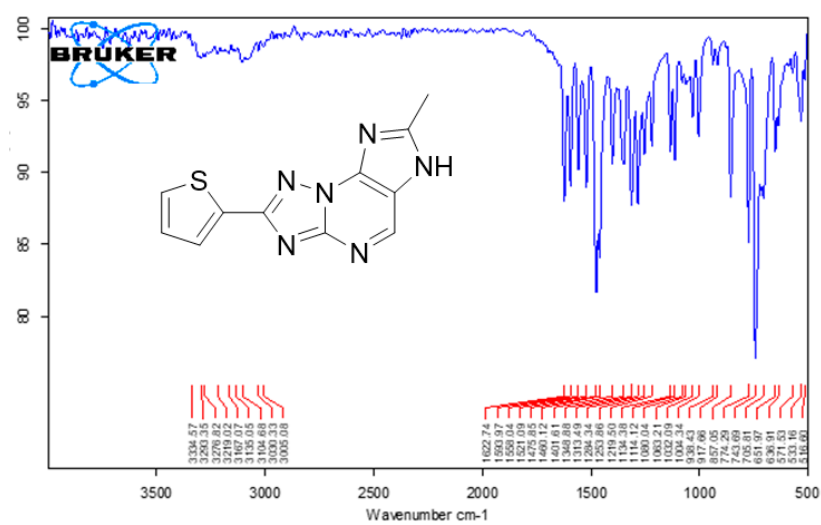


Figure S33. IR spectra of 7-methyl-2-(thiophen-2-yl)-6H-[1,2,4]triazolo[5,1-b]purine (6)