

Supporting Information

AZOLO[1,5-a]PYRIMIDINES AND THEIR CONDENSED ANALOGS WITH ANTICOAGULANT ACTIVITY

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Table of contents

Spectra of compounds.....	2
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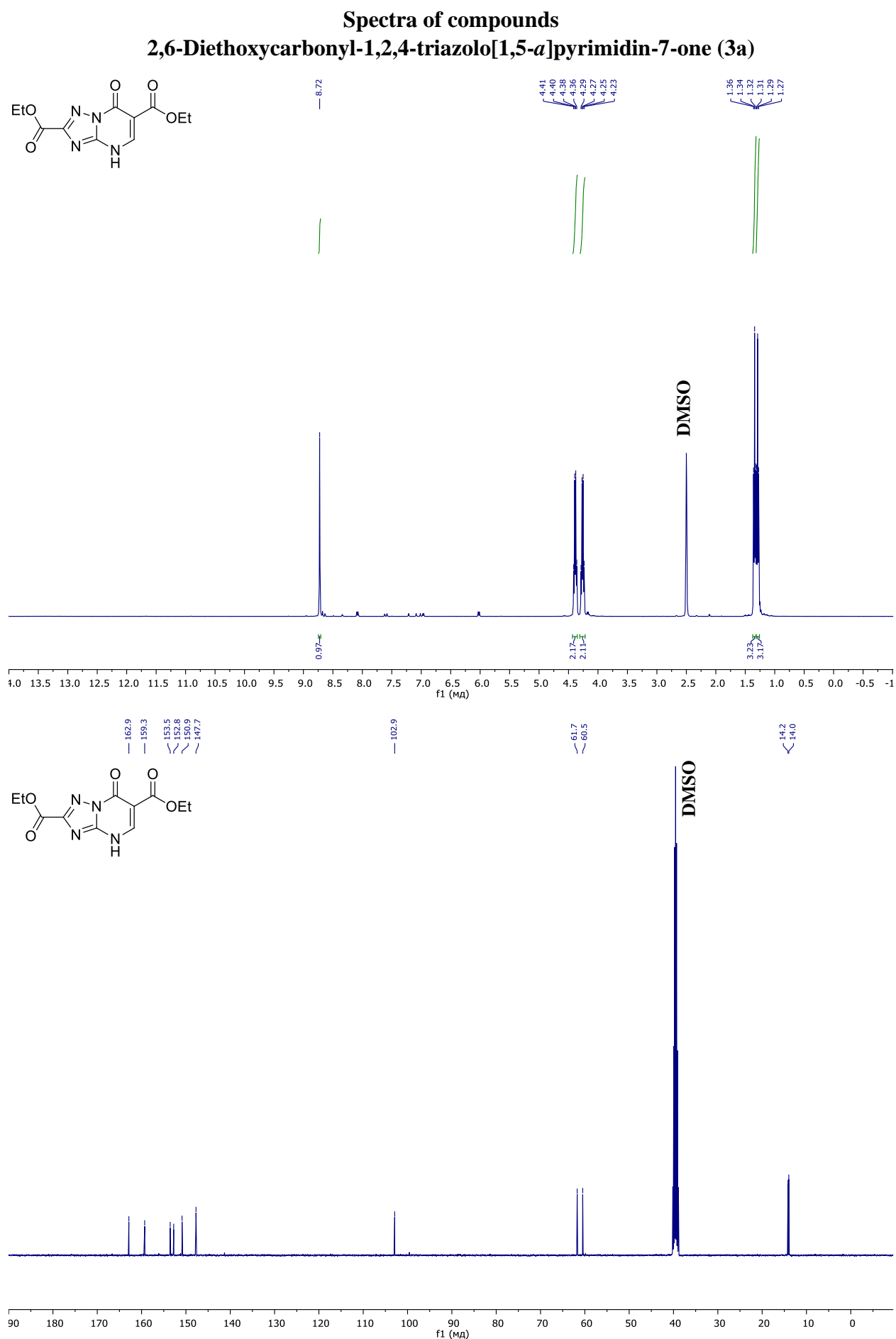


Figure S1. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **3a**

2,6-Diethoxycarbonyl-1,2,4-triazolo[1,5-a]pyrimidin-7-one (3a)

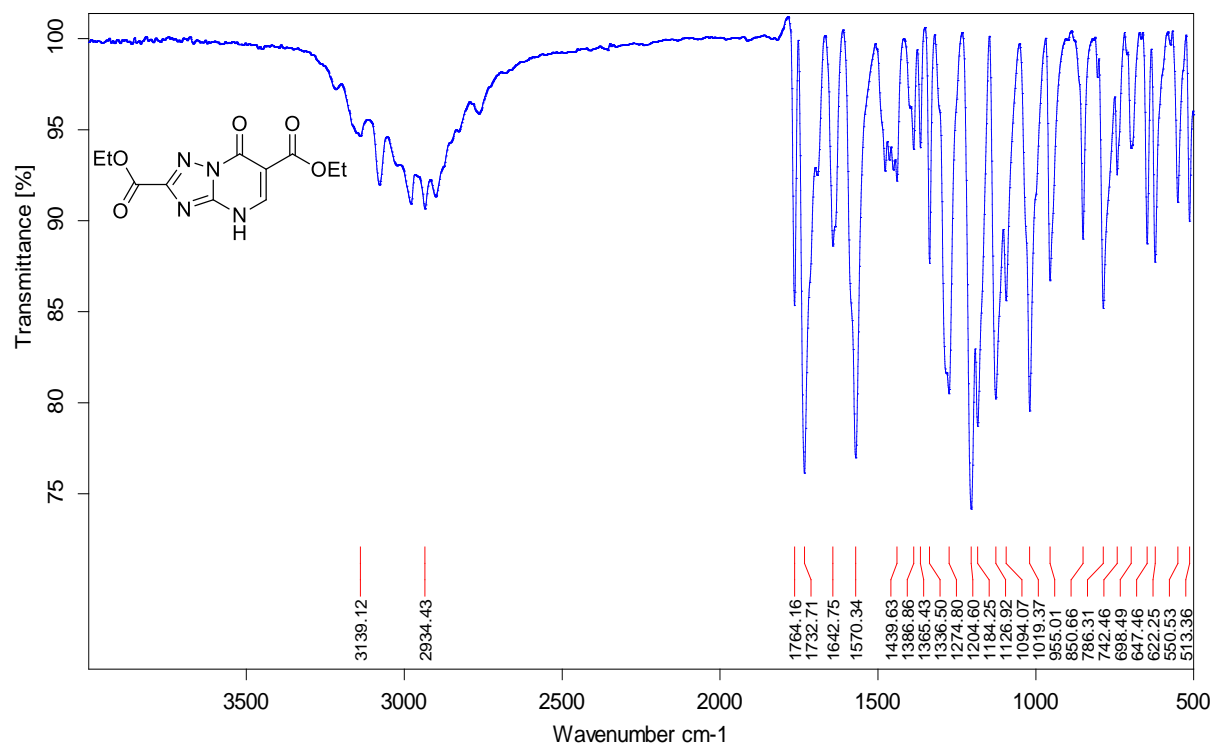


Figure S2. IR spectra of **3a**

2-(Thien-2-yl)-6-ethoxycarbonyl-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one (3f)

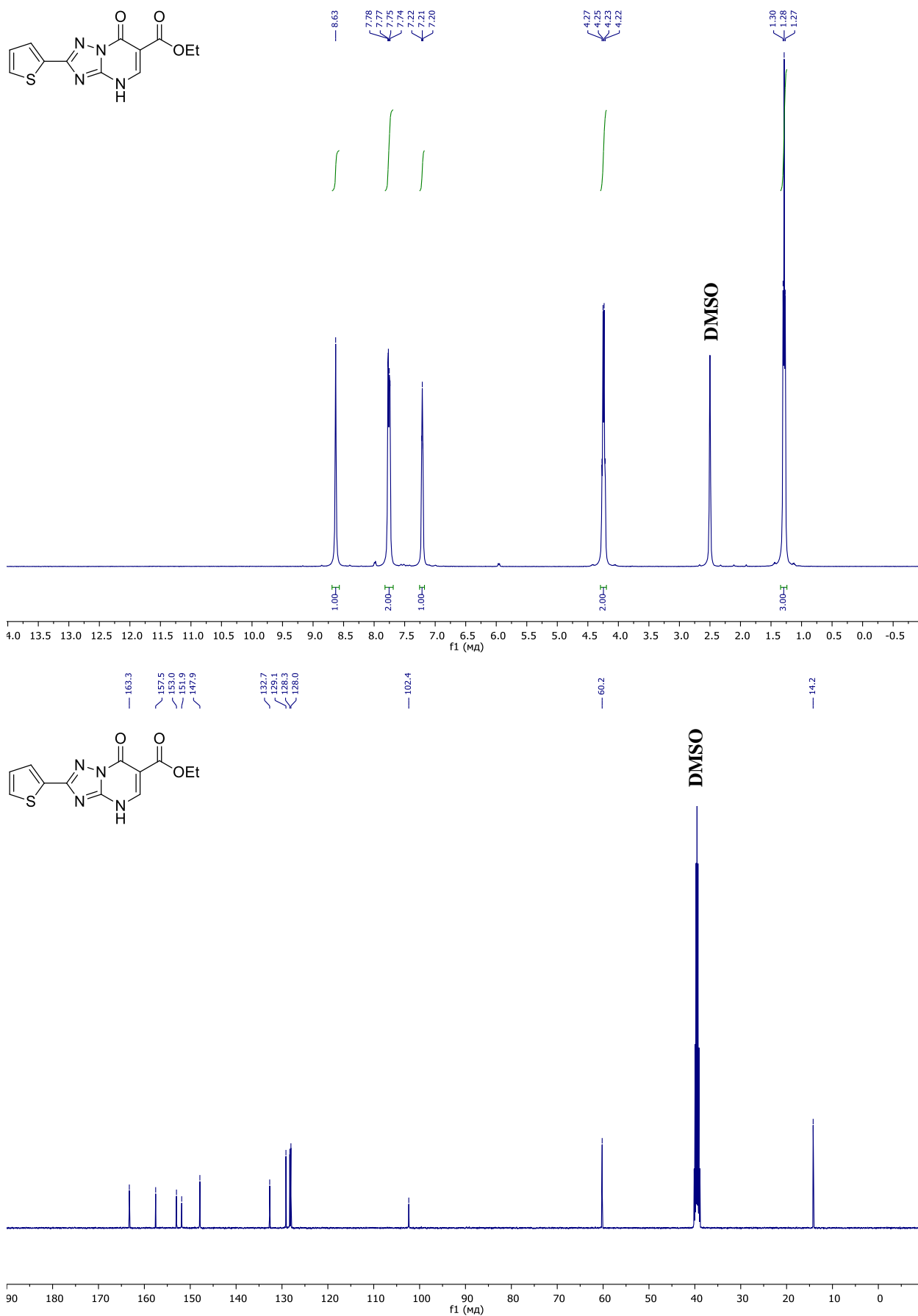


Figure S3. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **3f**

2-(Thien-2-yl)-6-ethoxycarbonyl-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one (3f)

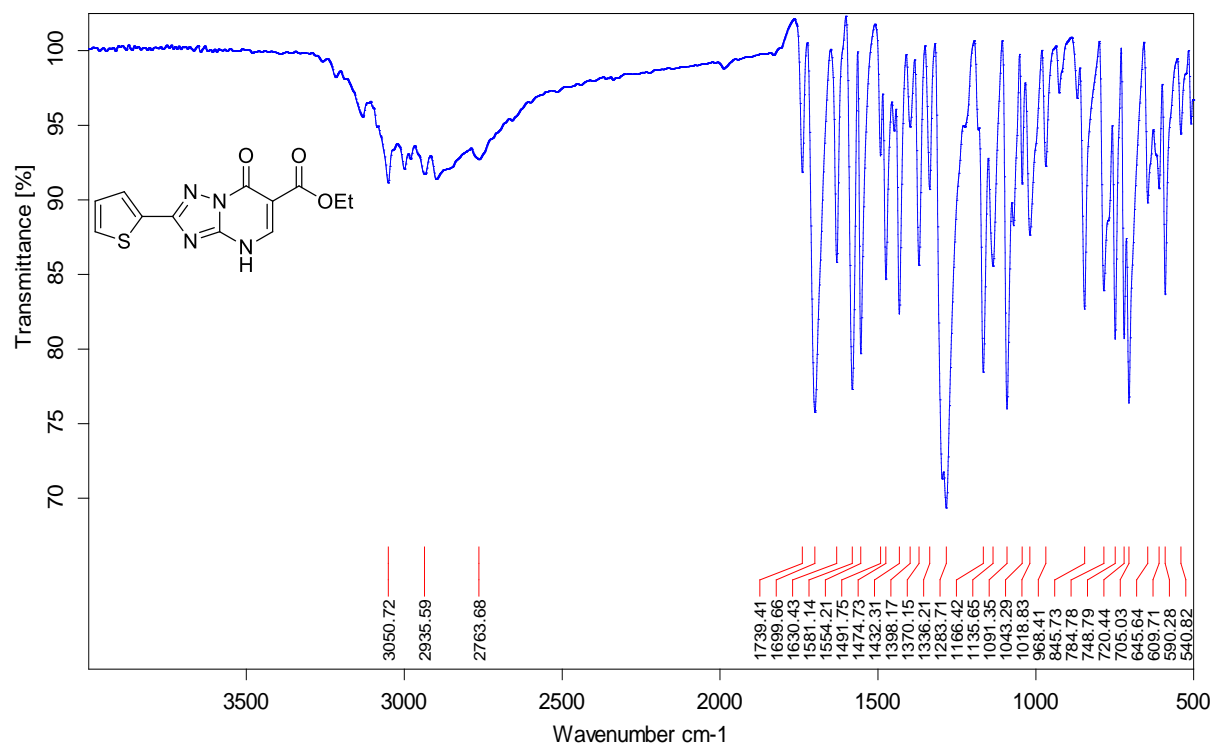


Figure S4. IR spectra of **3f**

2-(Pyridin-3-yl)-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one (3g)

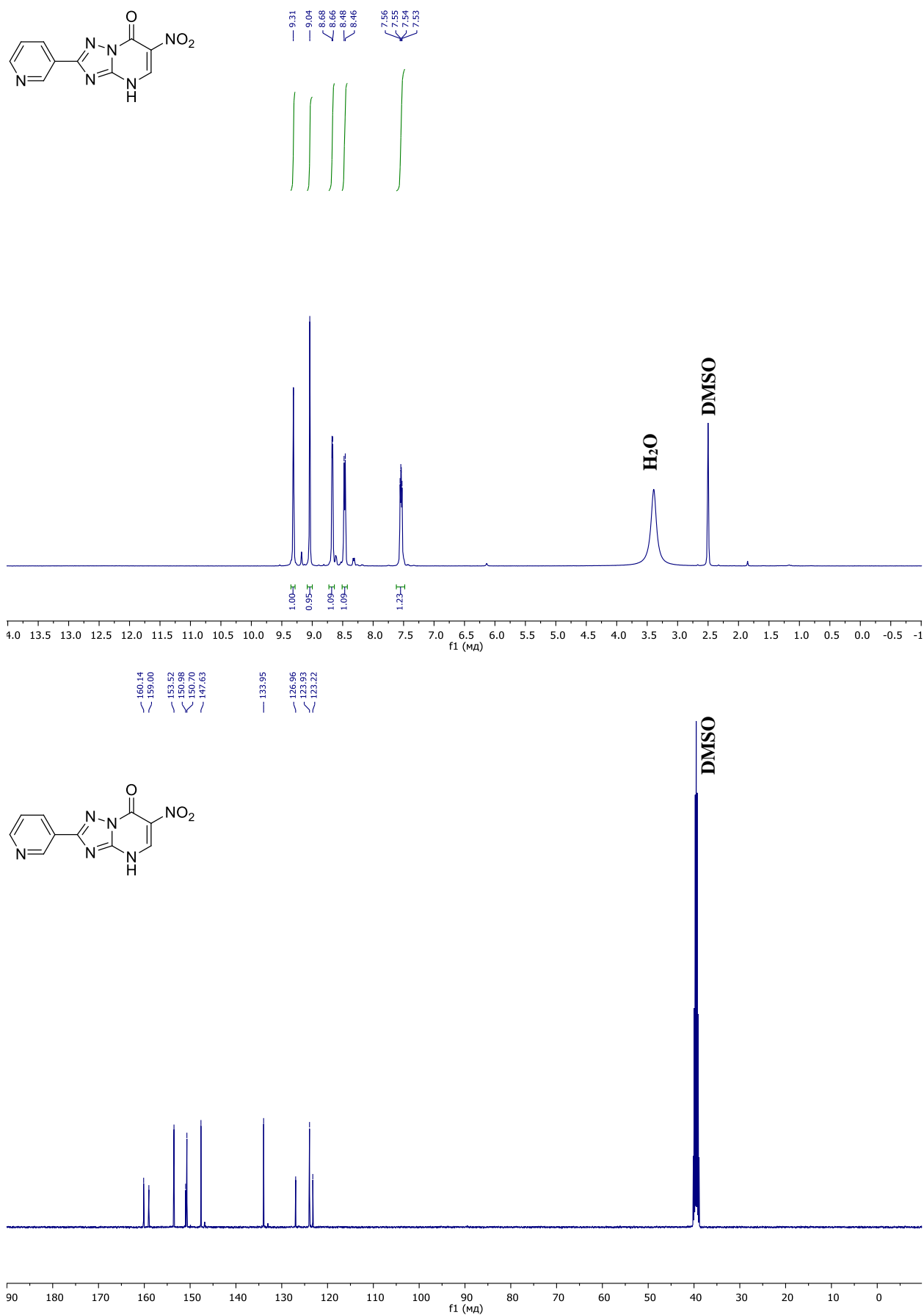


Figure S5. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **3g**

2-(Pyridin-3-yl)-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one (3g)

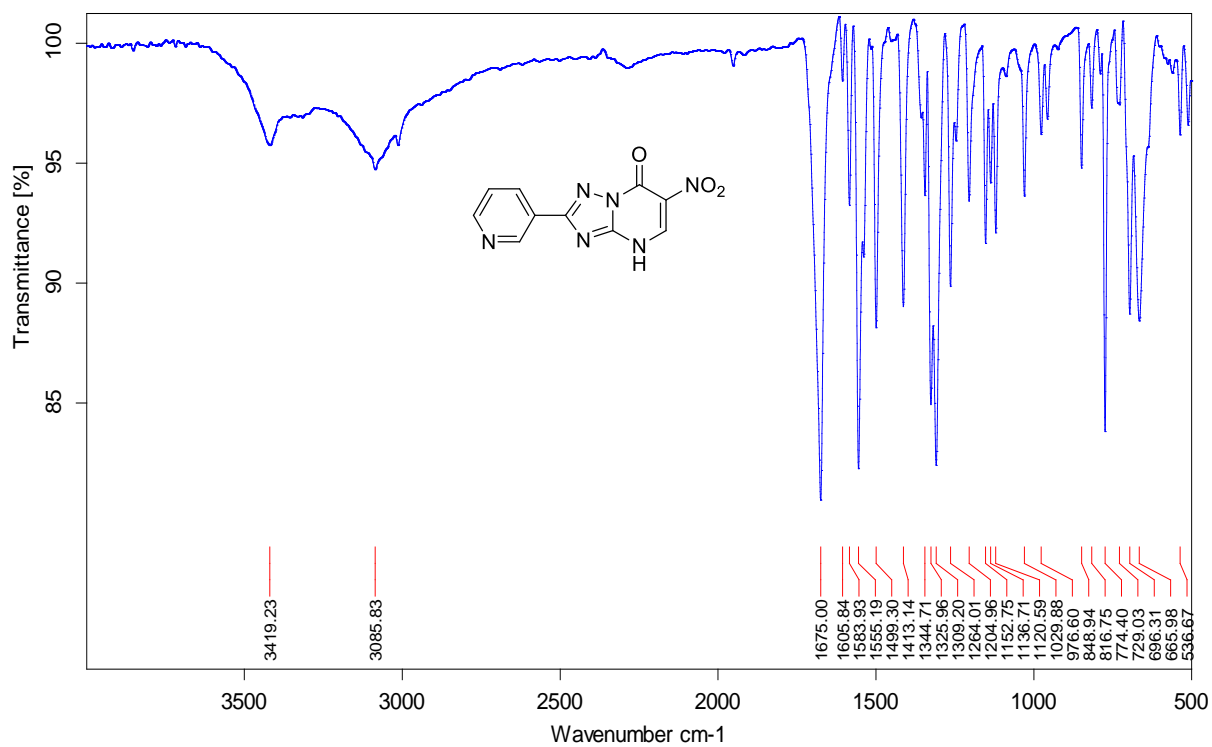


Figure S6. IR spectra of **3g**

2-phenyl-6-nitro-1,2,4-triazolo[1,5-a]pyrimidin-7-one pyridinium (3h)

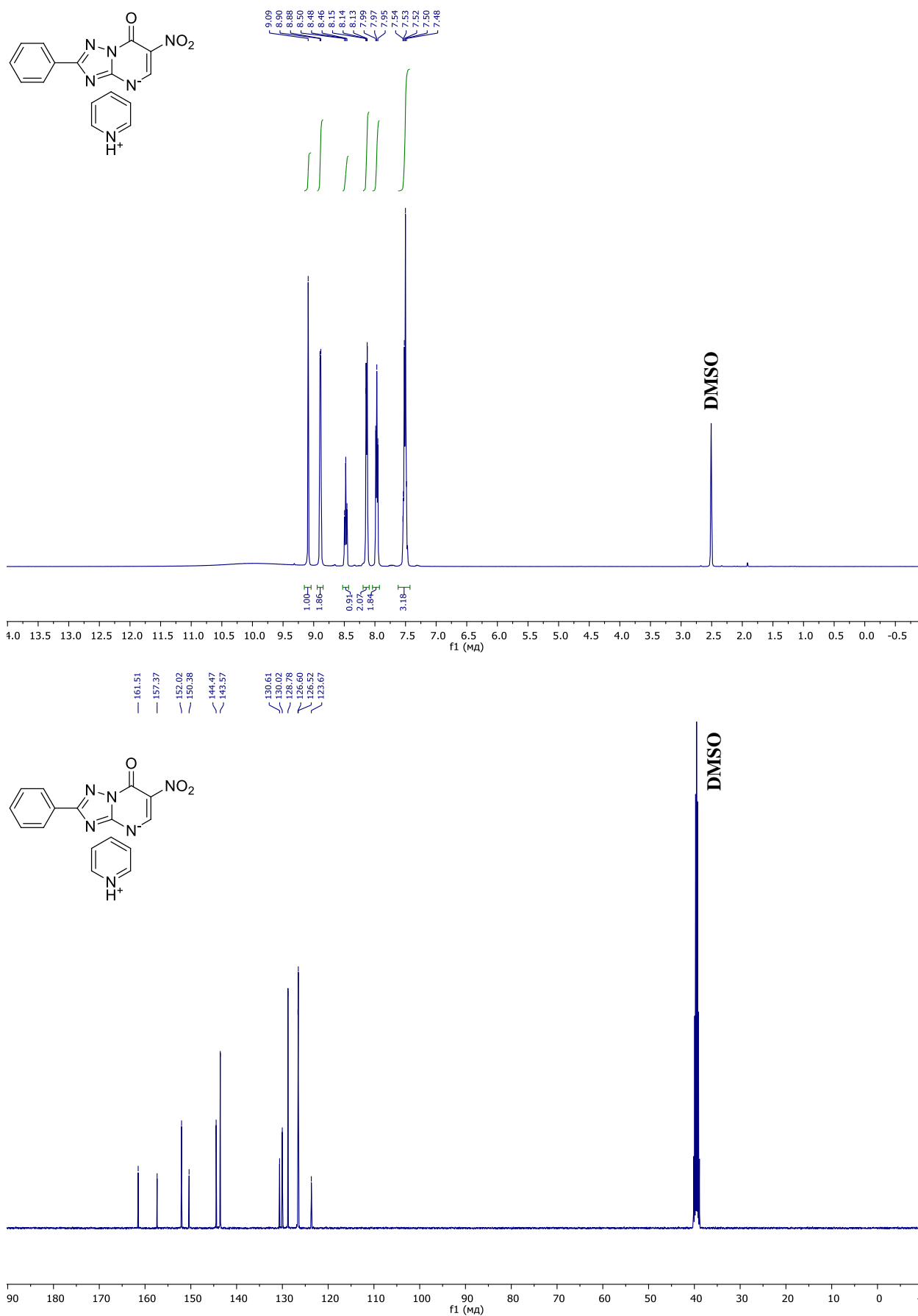


Figure S7. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **3h**

2-phenyl-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one pyridinium (3h)

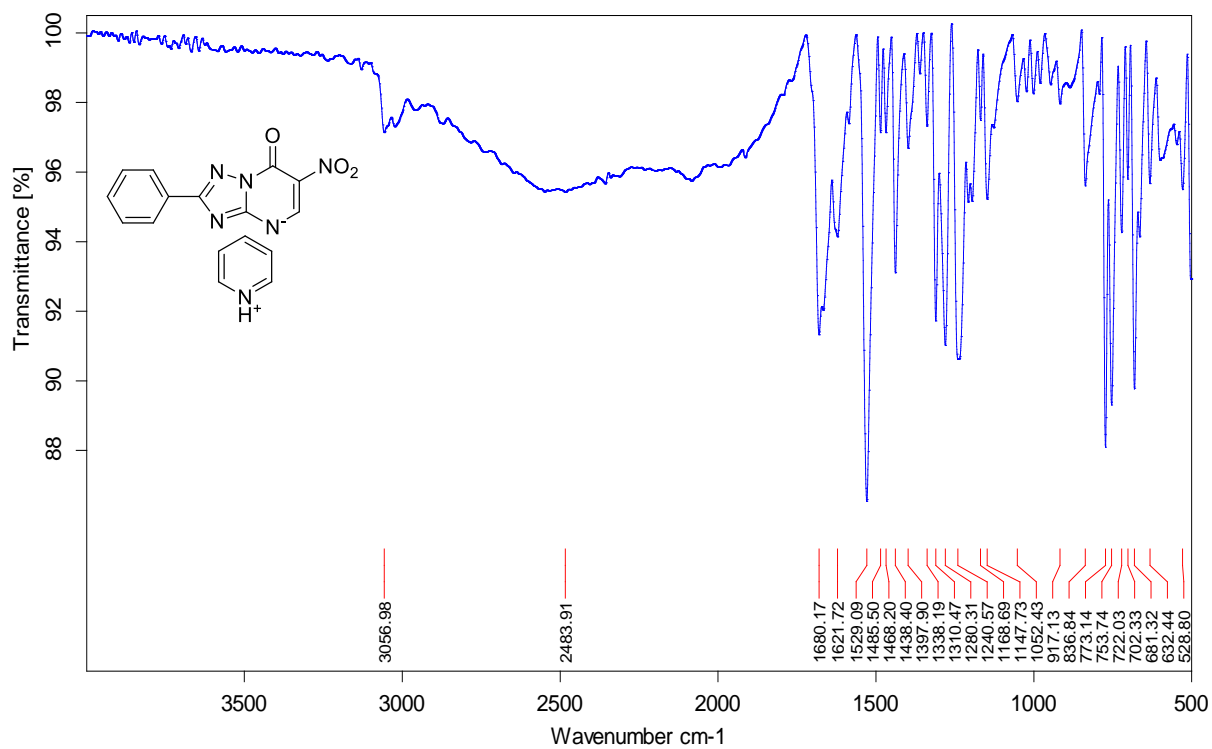


Figure S8. IR spectra of **3h**

2-(fur-2-yl)-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one pyridinium (3i)

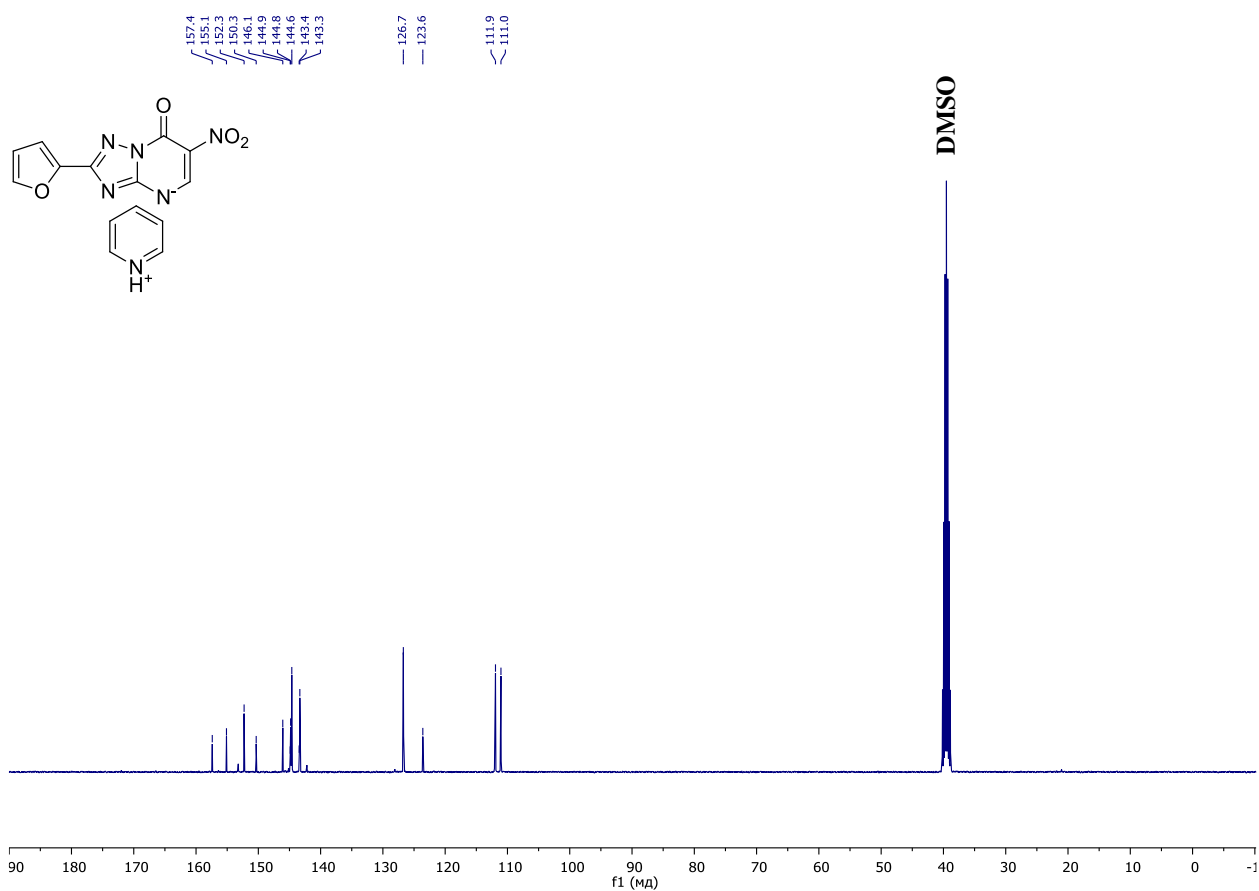
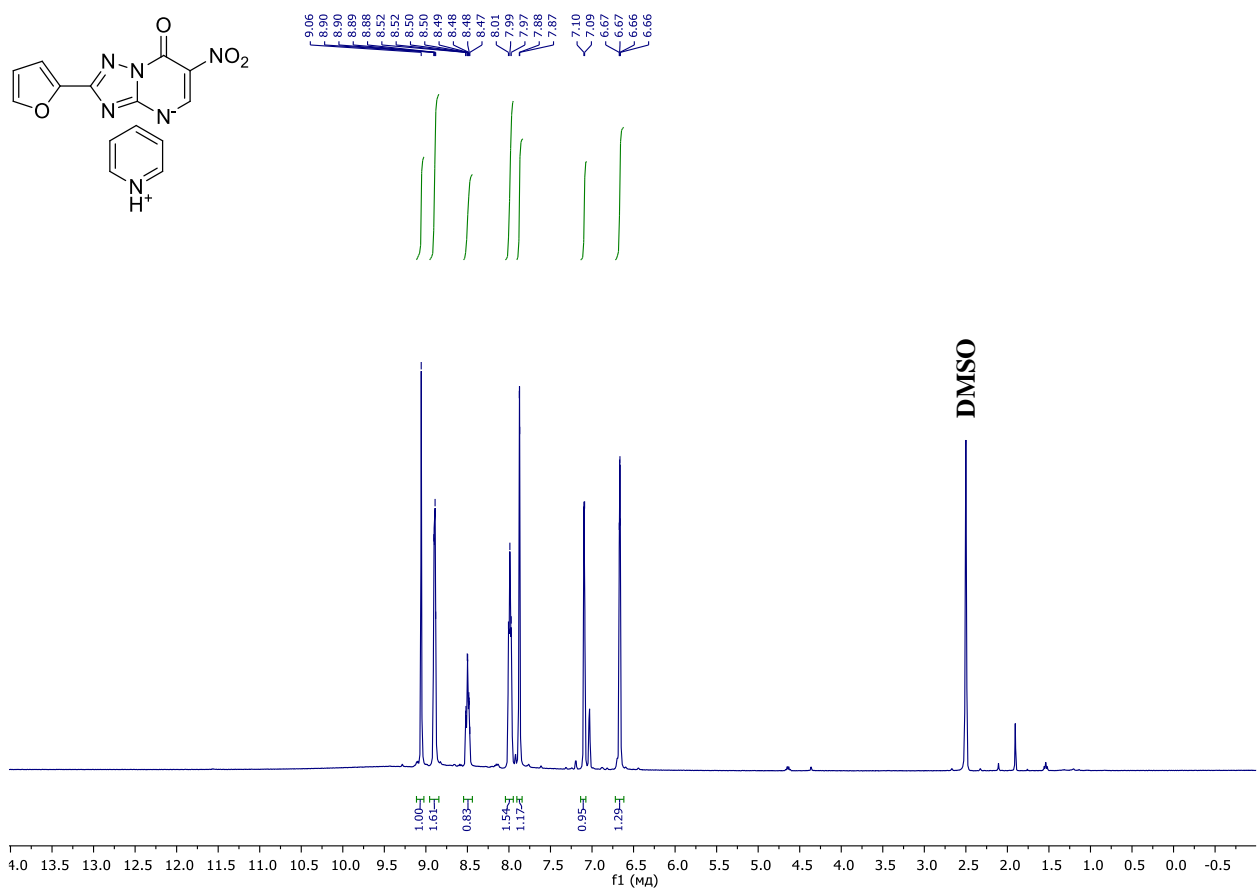


Figure S9. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **3i**

2-(fur-2-yl)-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one pyridinium (3i)

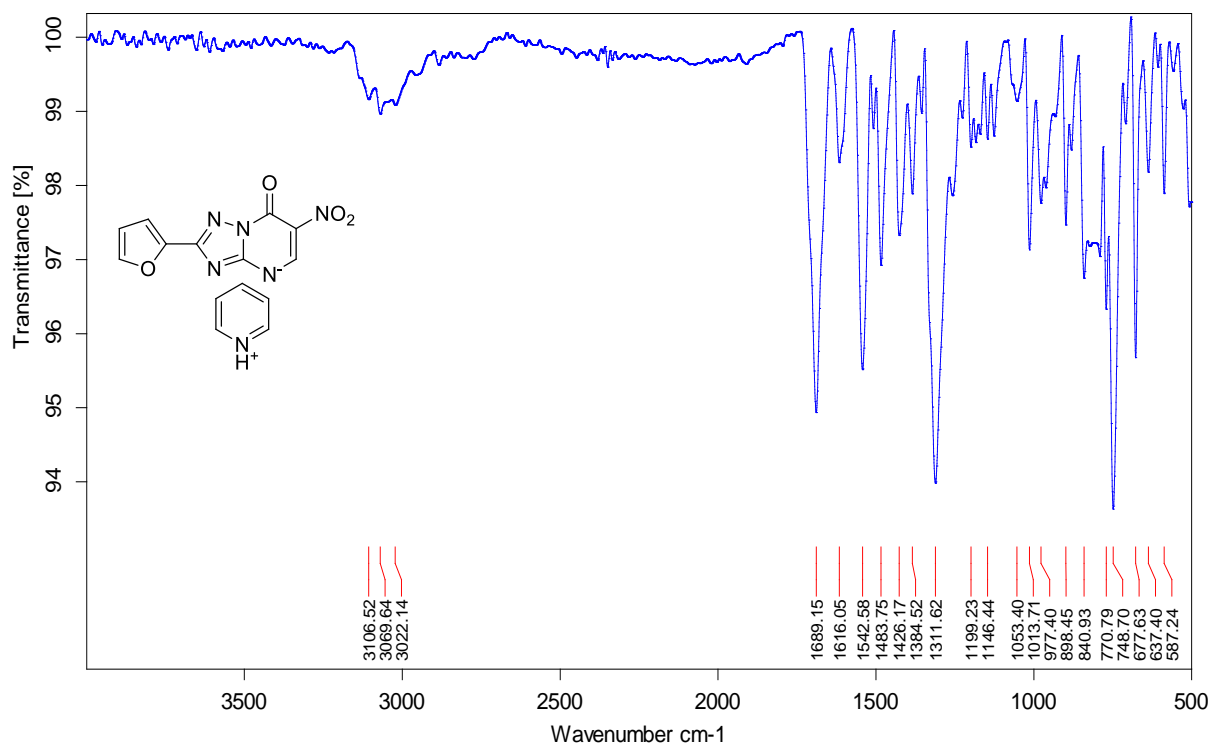


Figure S10. IR spectra of **3i**

2-(thien-2-yl)-6-nitro-1,2,4-triazolo[1,5-a]pyrimidin-7-one pyridinium (3j)

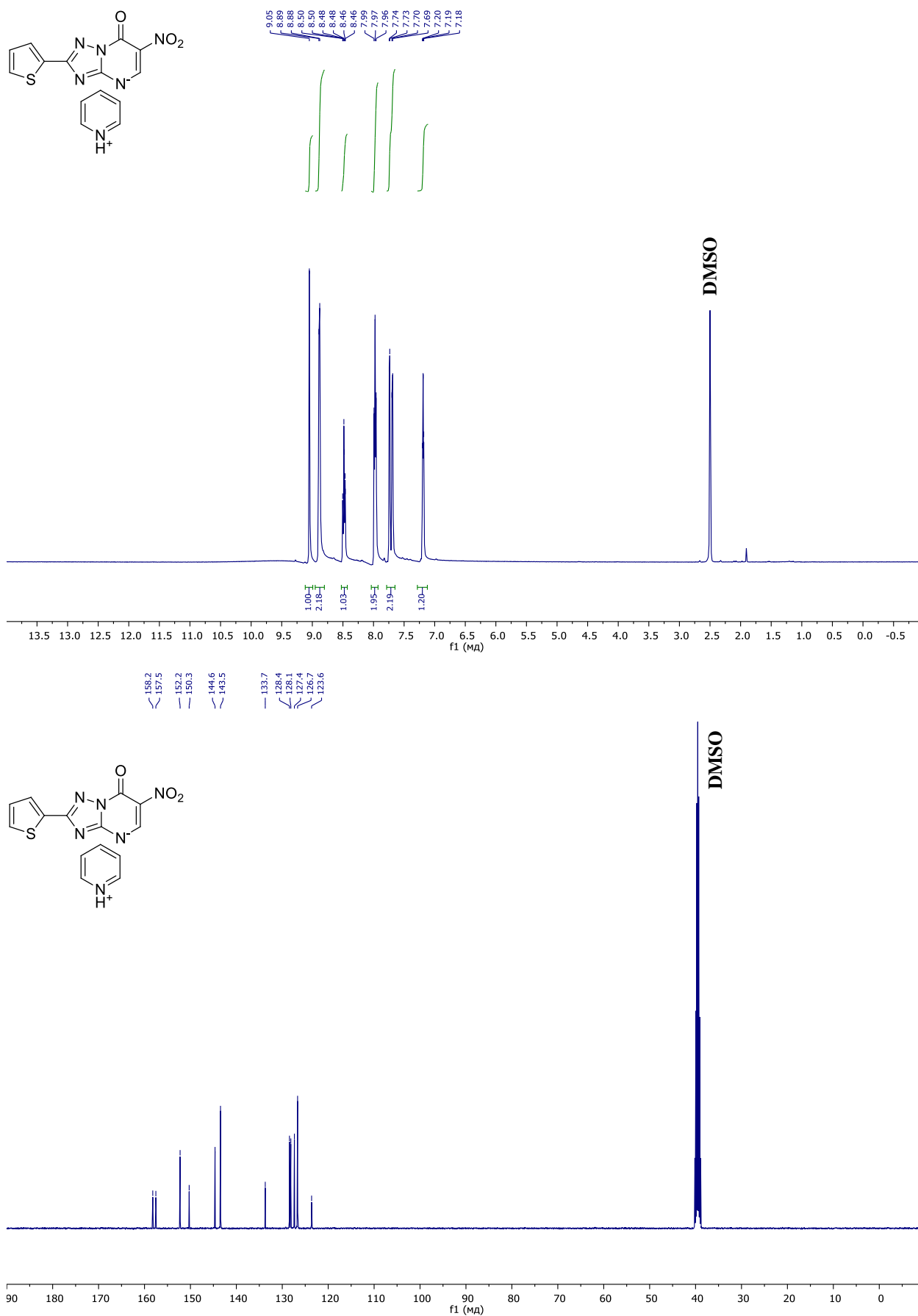


Figure S11. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **3j**

2-(thien-2-yl)-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one pyridinium (3j)

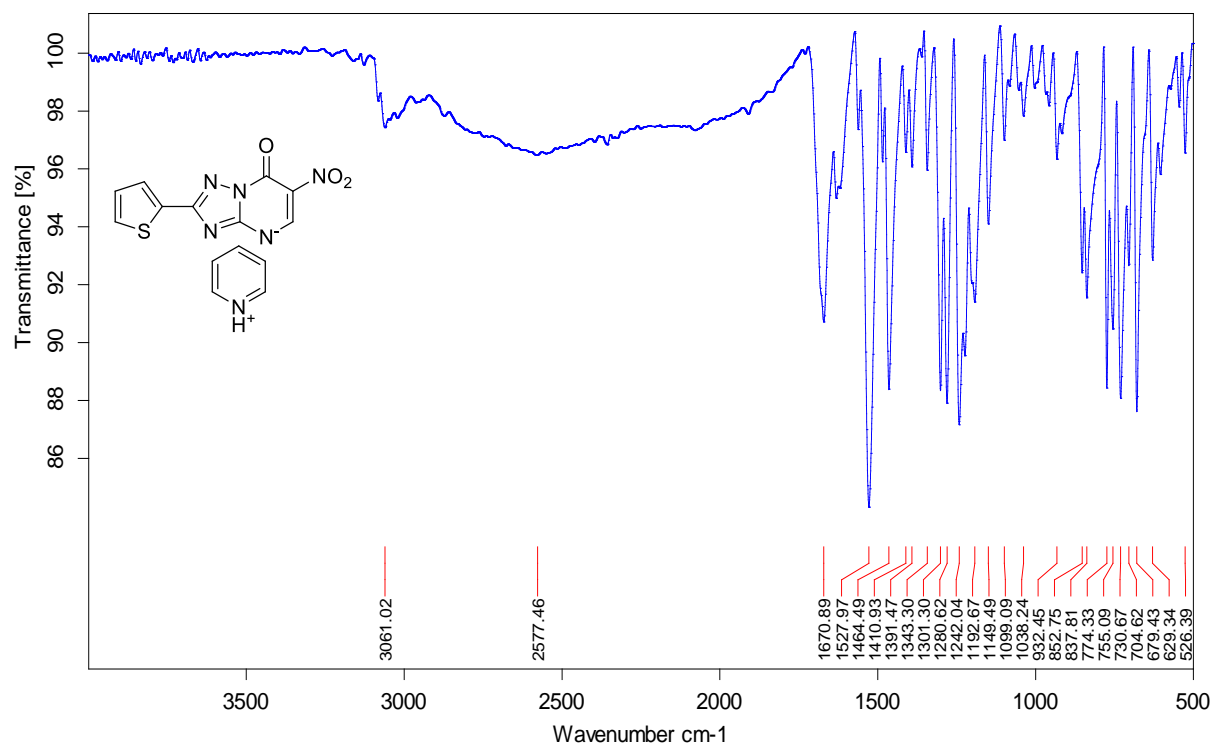


Figure S12. IR spectra of **3j**

2-(5-nitrofur-2-yl)-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one pyridinium (3k)

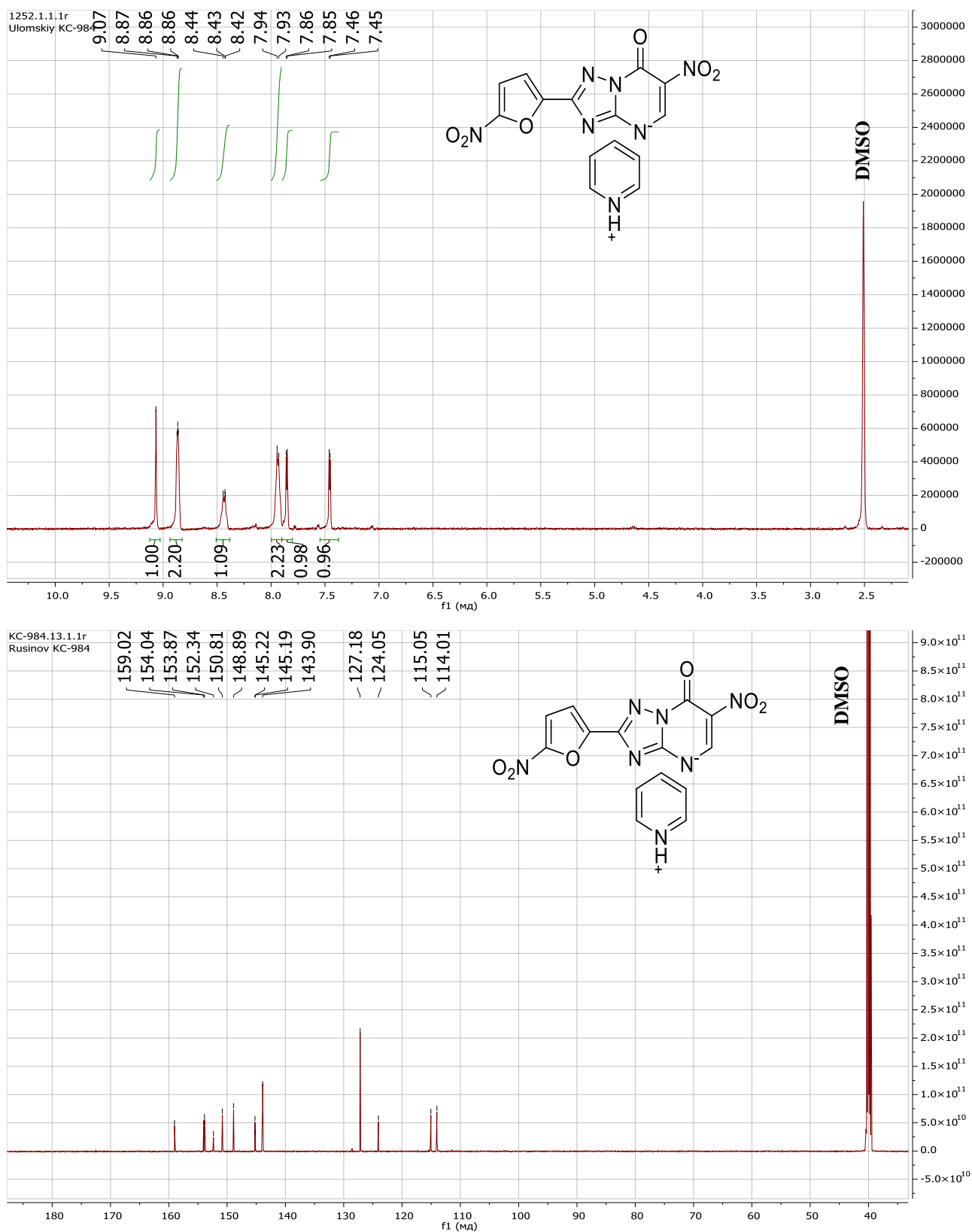


Figure S13. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **3k**

2-(5-nitrofur-2-yl)-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one pyridinium (3k)

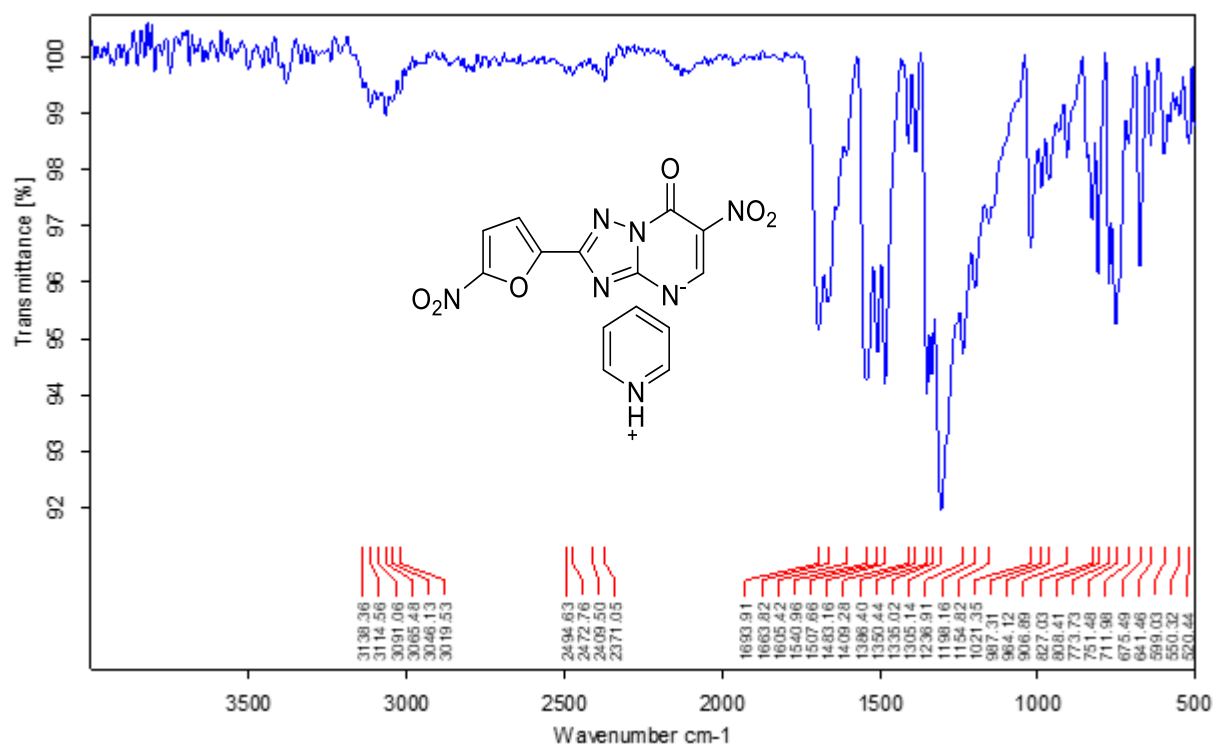


Figure S14. IR spectra of **3k**

2-phenyl-3-cyano-6-nitropyrrazolo[1,5-*a*]pyrimidin-7-one pyridinium (31)

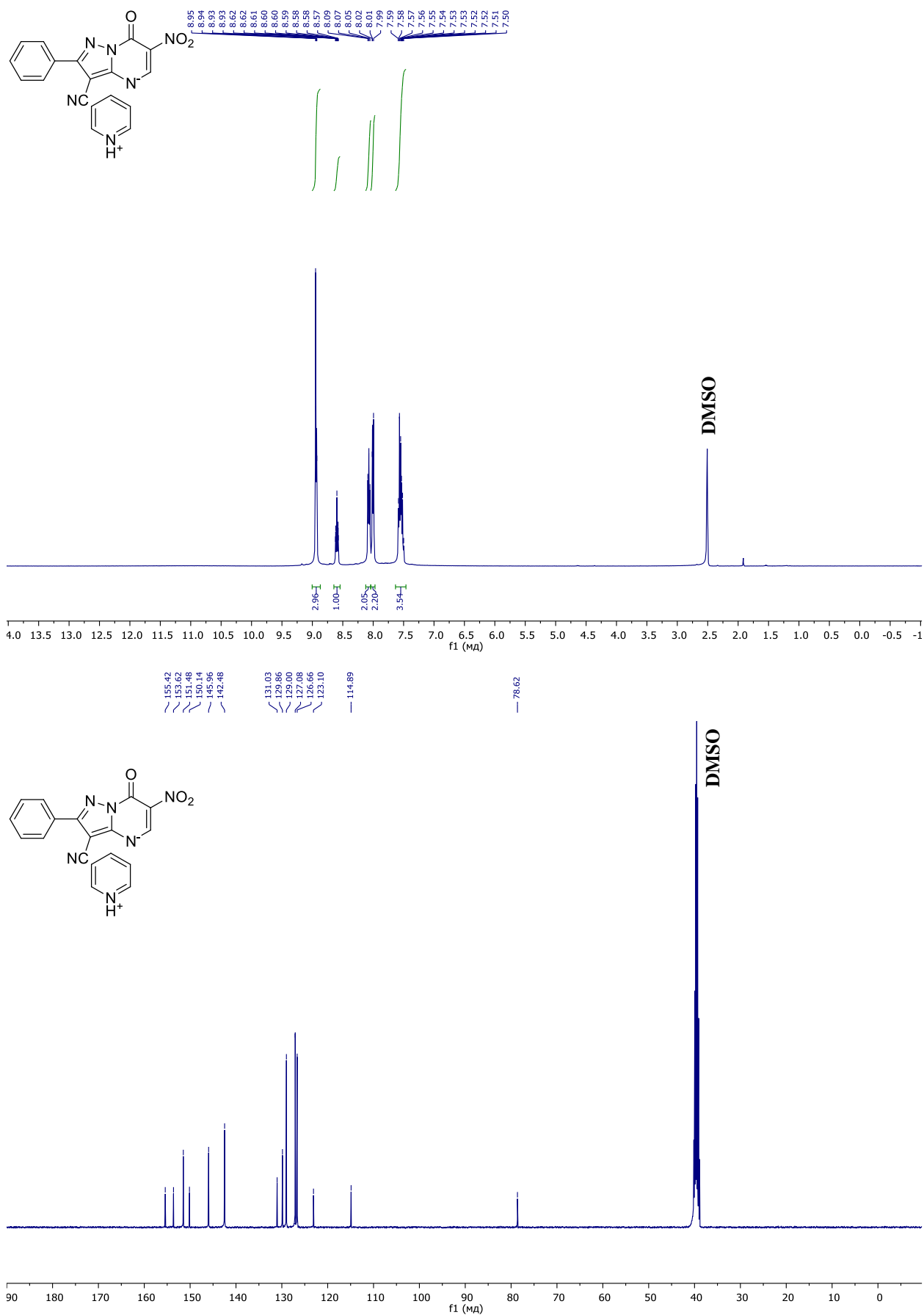


Figure S15. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **31**

2-phenyl-3-cyano-6-nitropyrazolo[1,5-*a*]pyrimidin-7-one pyridinium (3l)

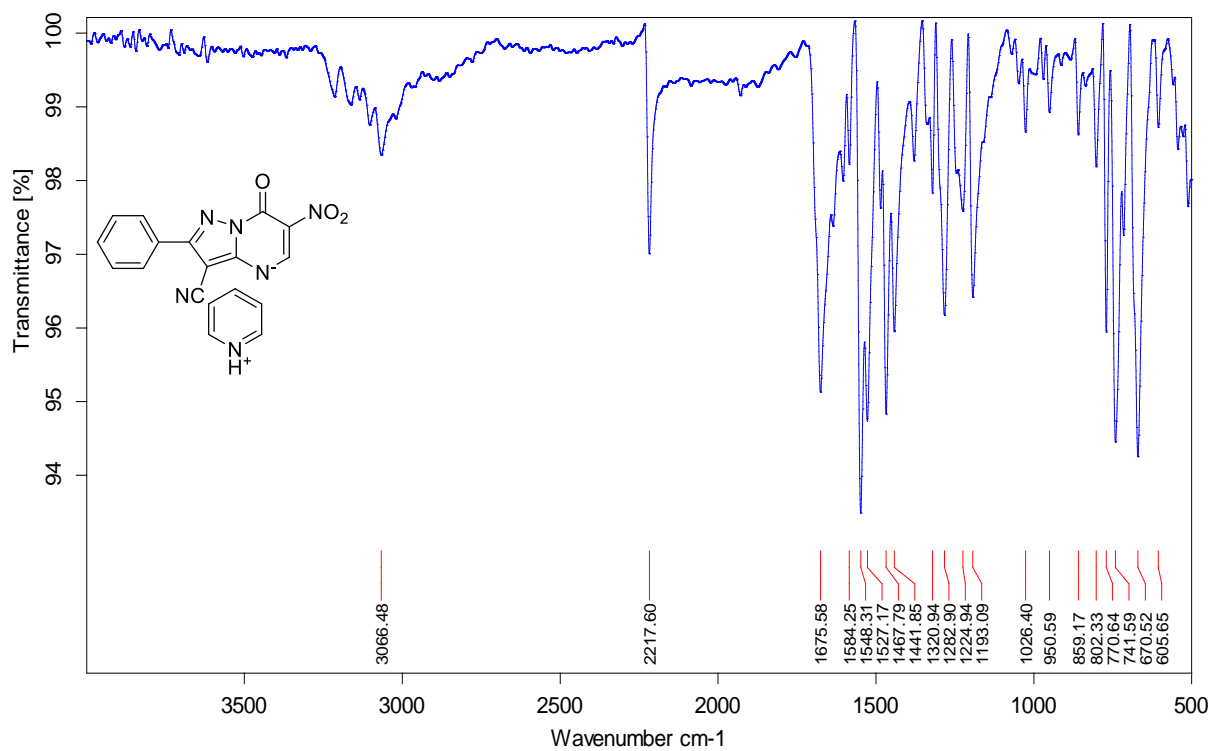


Figure S16. IR spectra of **3l**

2-(5-nitrofur-2-yl)-5-methyl-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one (3m)

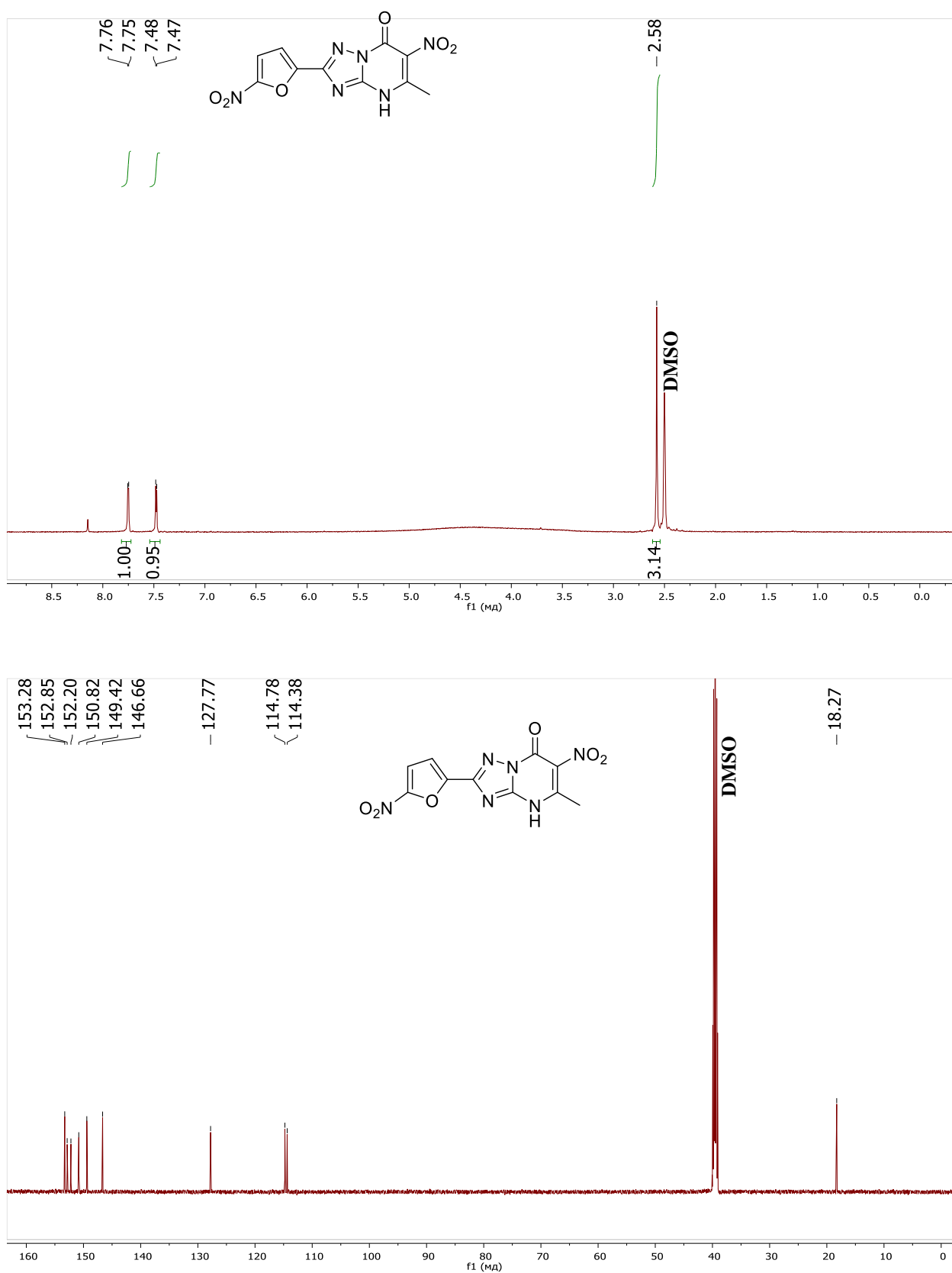


Figure S17. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **3m**

2-(5-nitrofur-2-yl)-5-methyl-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one (3m)

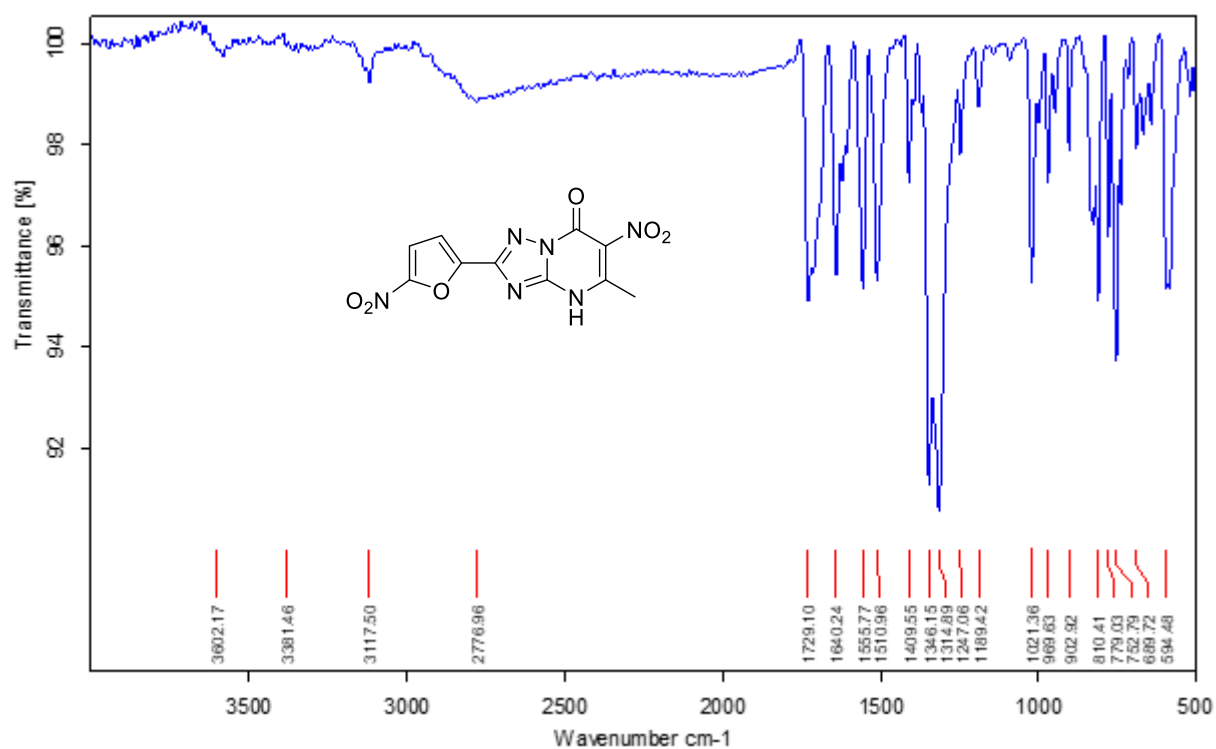


Figure S18. IR spectra of **3m**

2-(fur-2-yl)-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one sodium salt (**3n**)

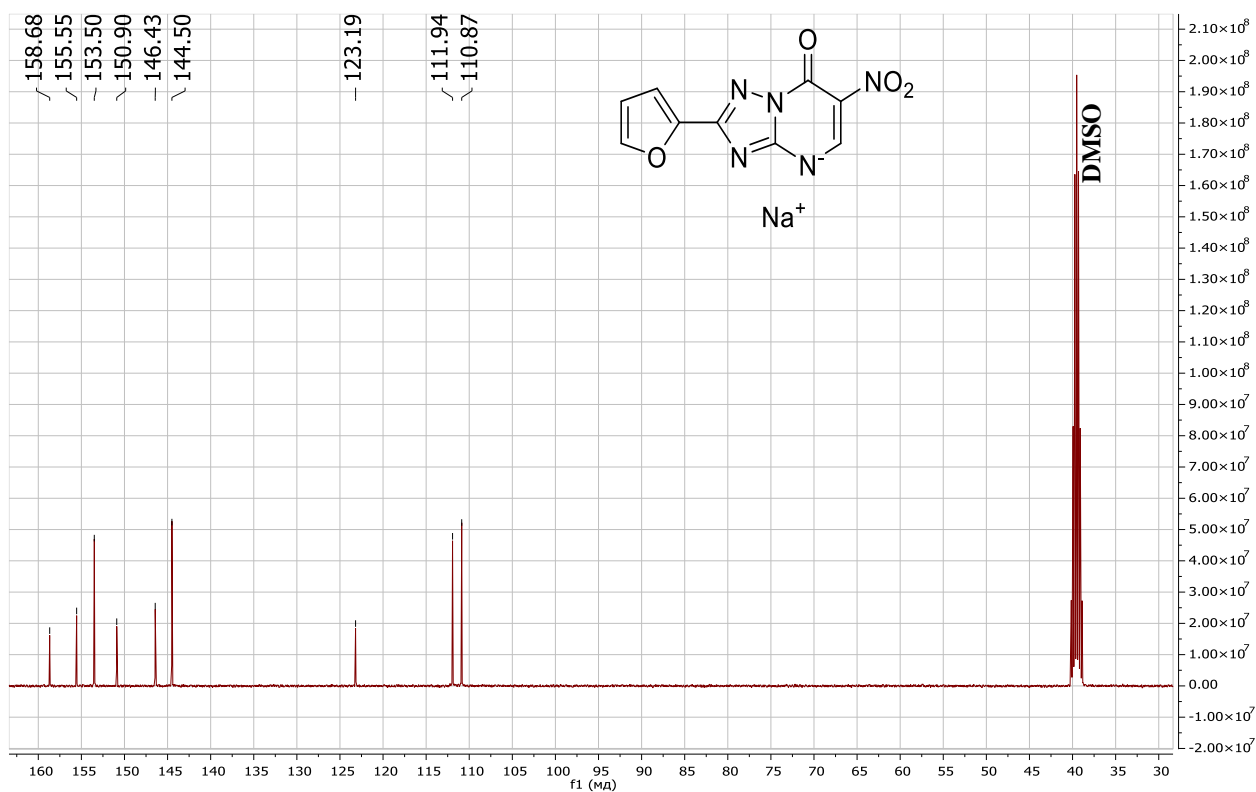
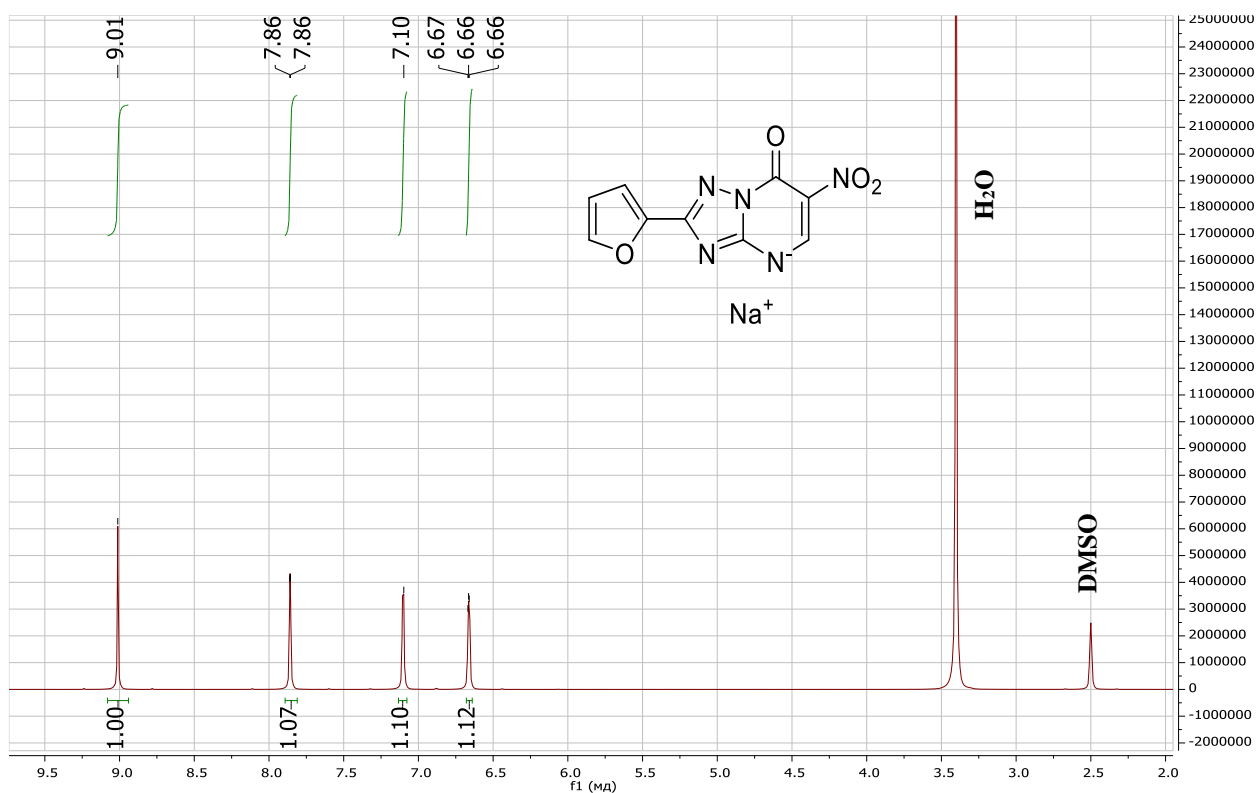


Figure S19. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **3n**

2-(fur-2-yl)-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one sodium salt (**3n**)

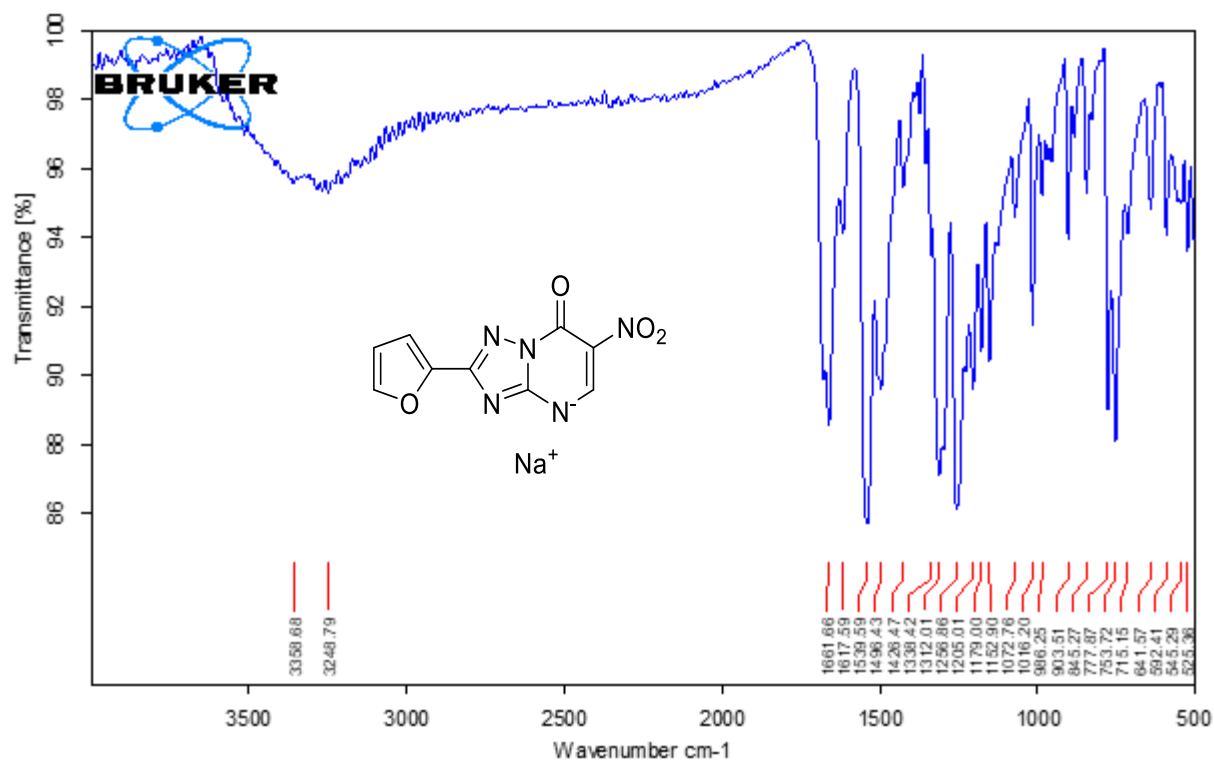


Figure S20. IR spectra of **3n**

2-(fur-2-yl)-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one ammonium salt (3o**)**

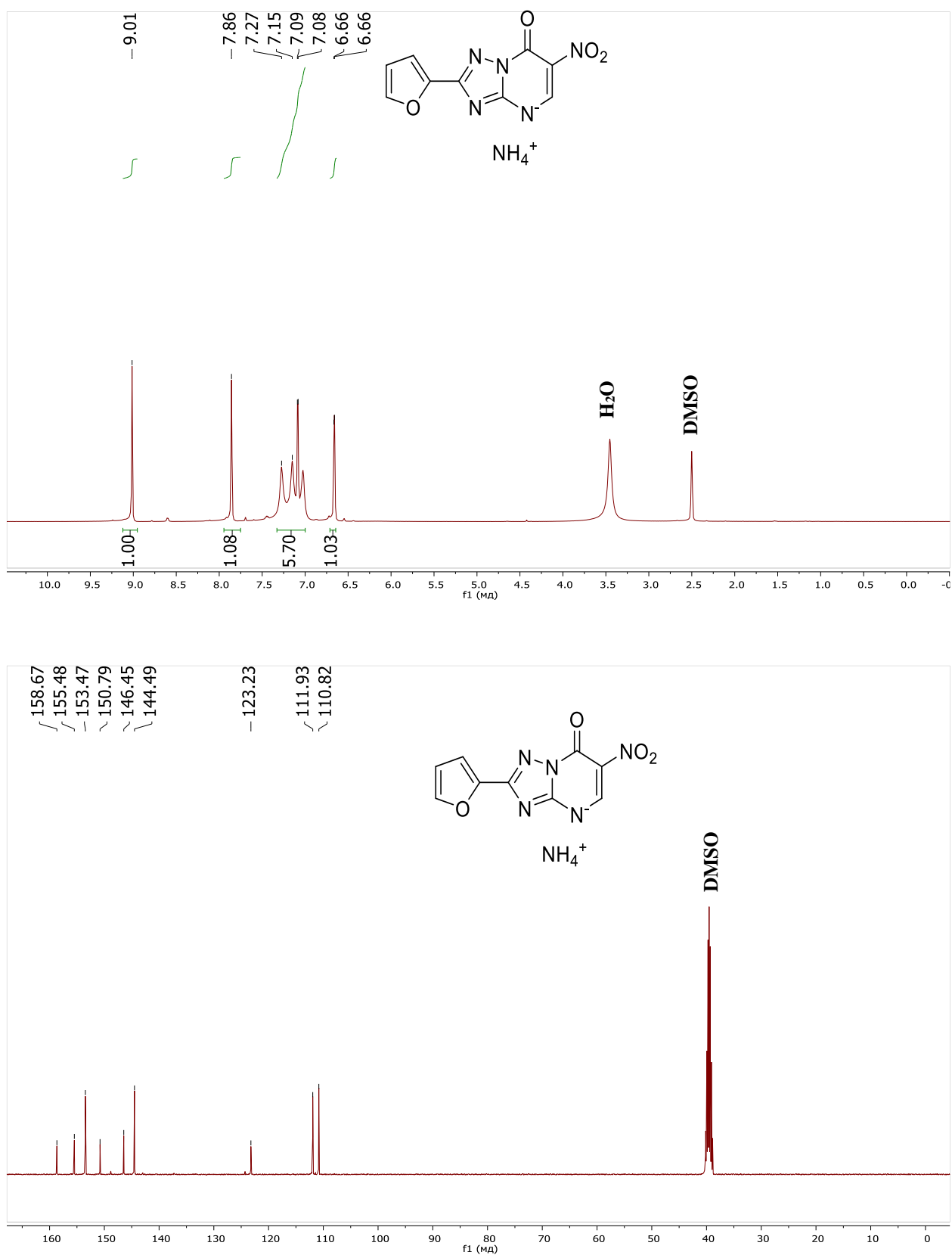


Figure S21. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **3o**

2-(fur-2-yl)-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one ammonium salt (3o)

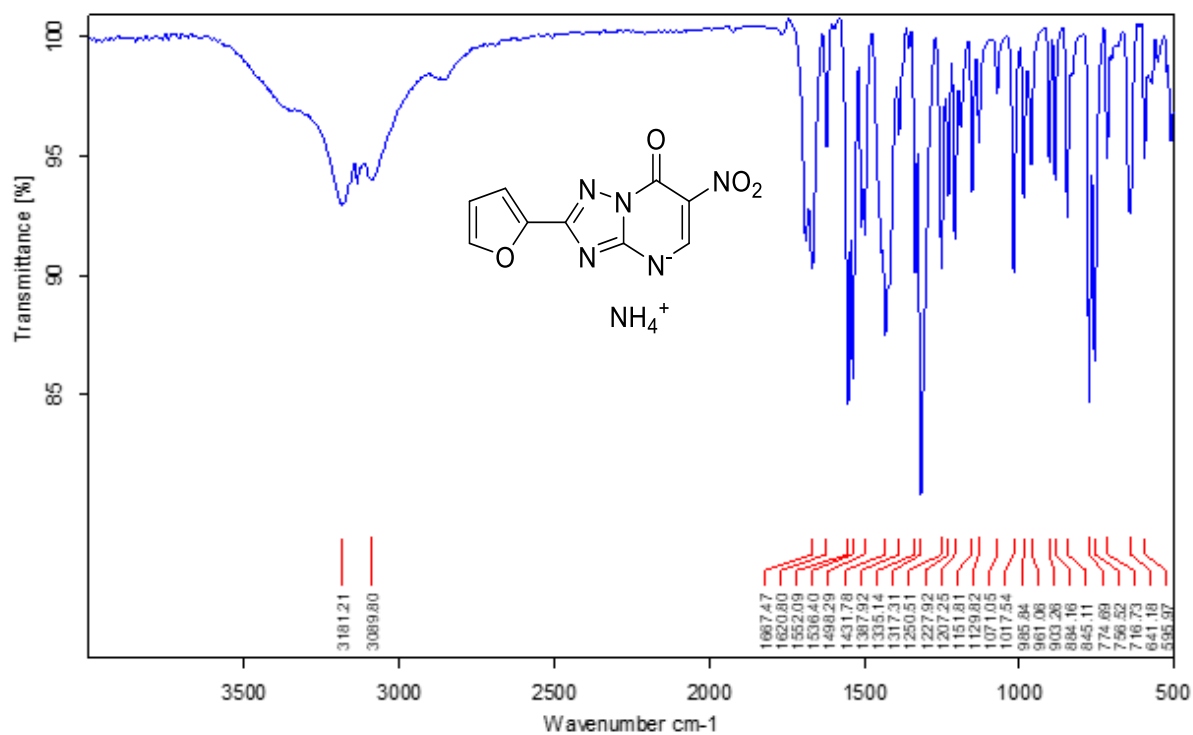


Figure S22. IR spectra of **3o**

2-(fur-2-yl)-6-nitro-1,2,4-triazolo[1,5-a]pyrimidin-7-one morpholinic salt (3p)

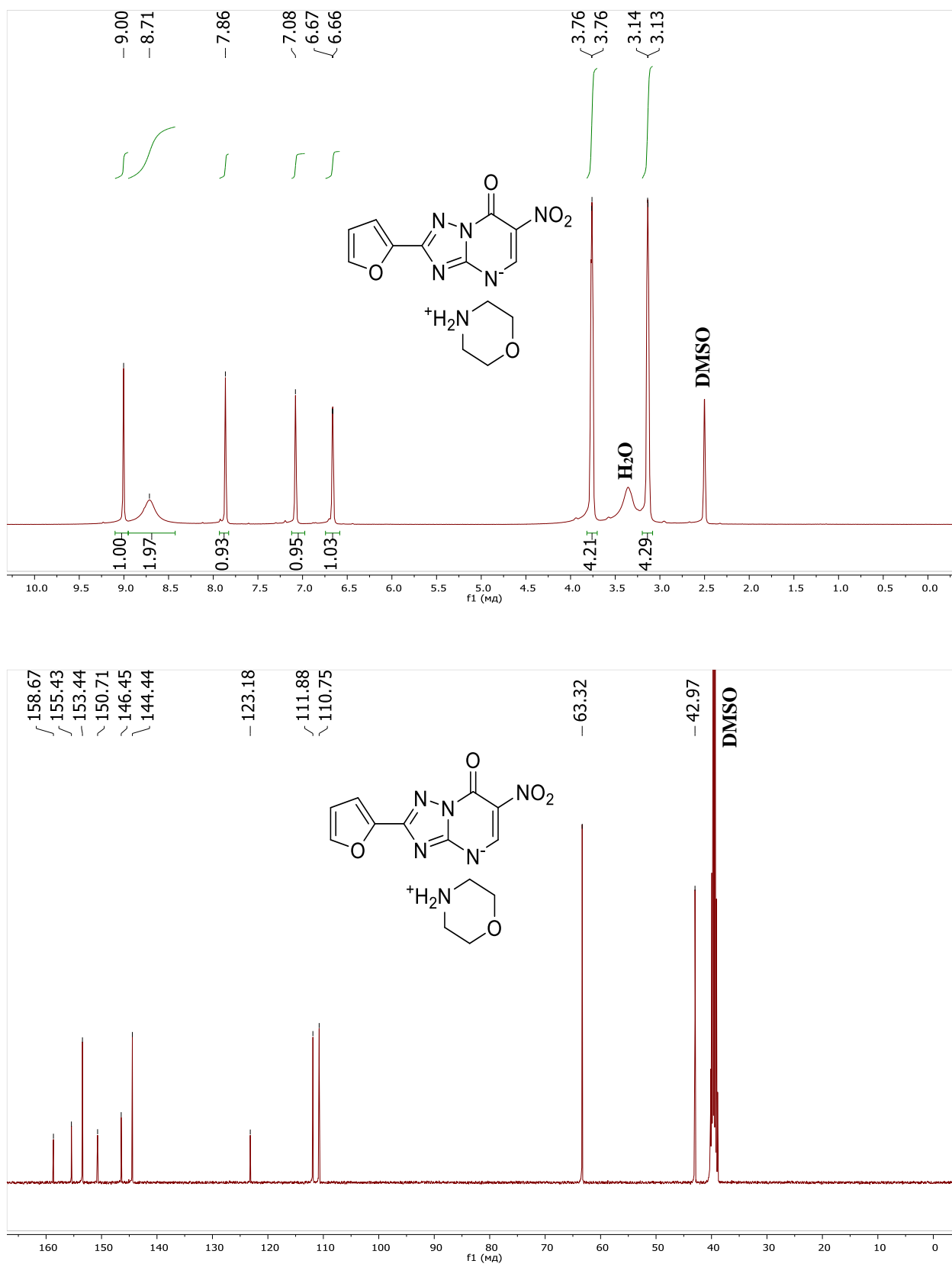


Figure S23. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **3p**

2-(fur-2-yl)-6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidin-7-one morpholinic salt (3p)

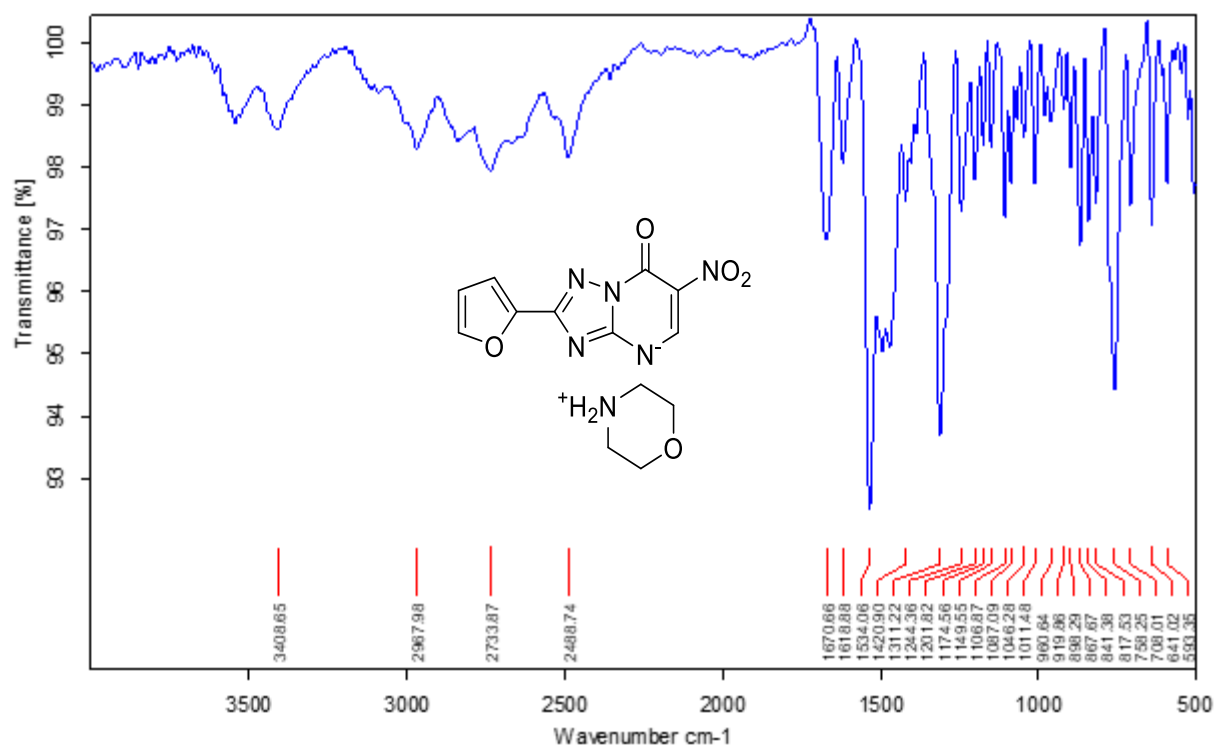


Figure S24. IR spectra of **3p**

2-(fur-2-yl)-6-nitro-1,2,4-triazolo[1,5-a]pyrimidin-7-one *L*-argininium salt (3q)

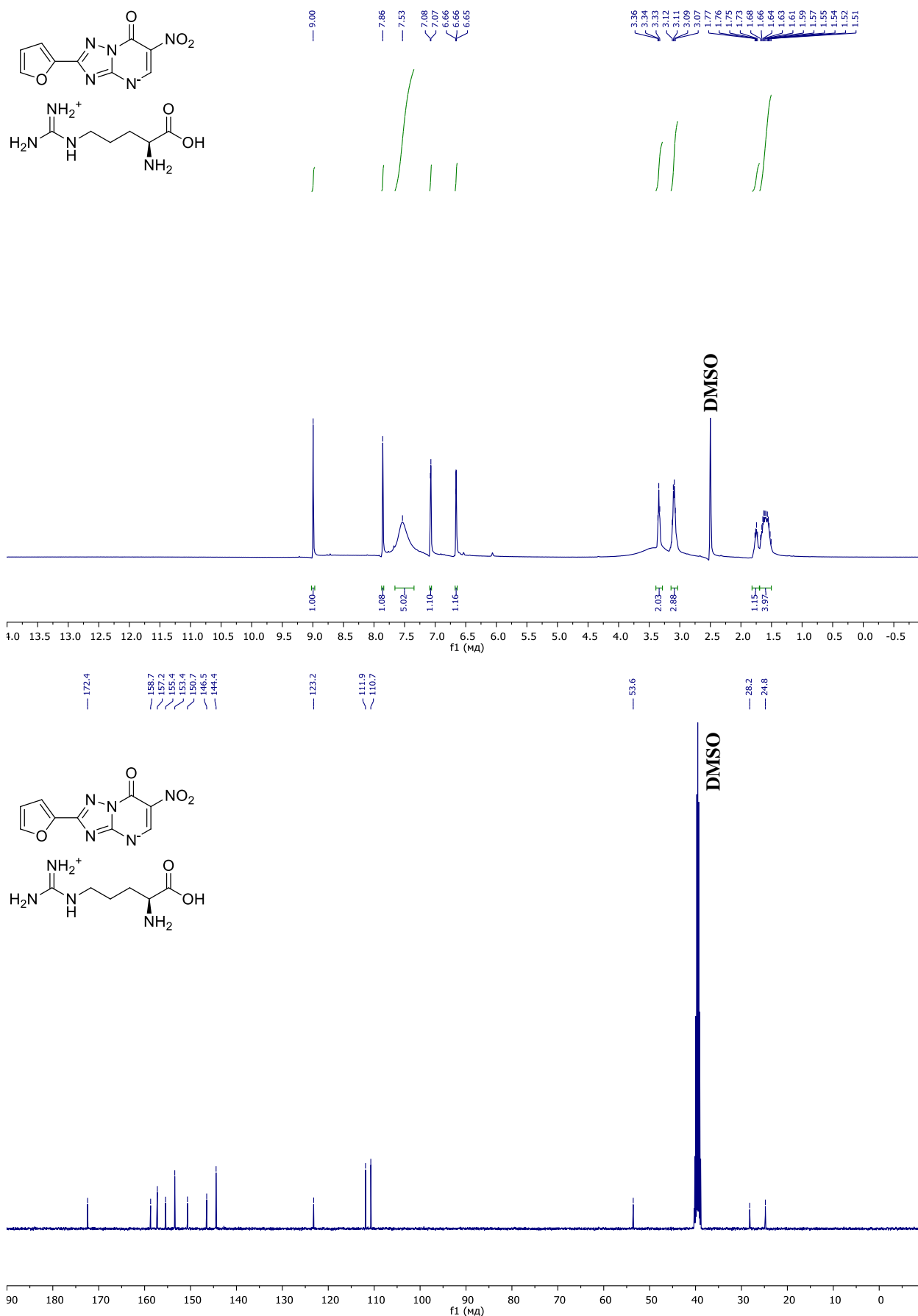


Figure S25. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **3q**

2-(fur-2-yl)-6-nitro-1,2,4-triazolo[1,5-a]pyrimidin-7-one *L*-argininium salt (3q)

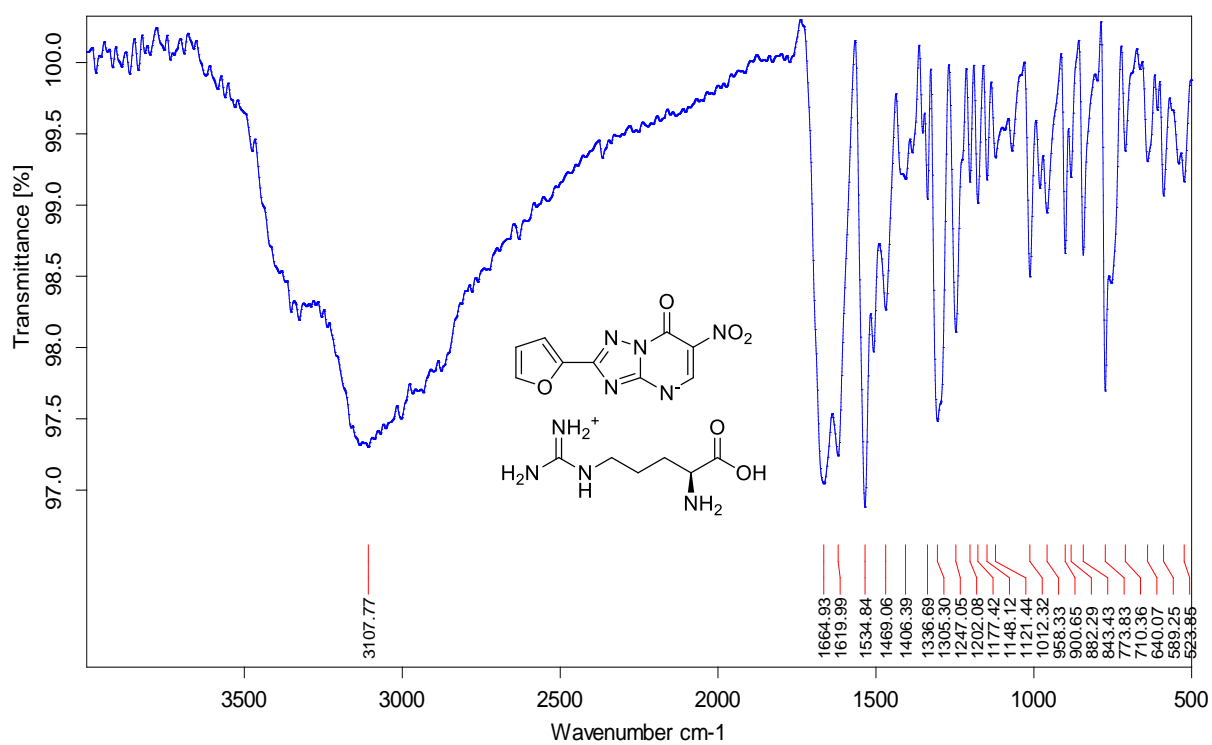


Figure S26. IR spectra of **3q**

3-(4-Hydroxyphenylethyl)-[1,3,4]thiadiazolo[3,2-*a*]purin-8-one (6a)

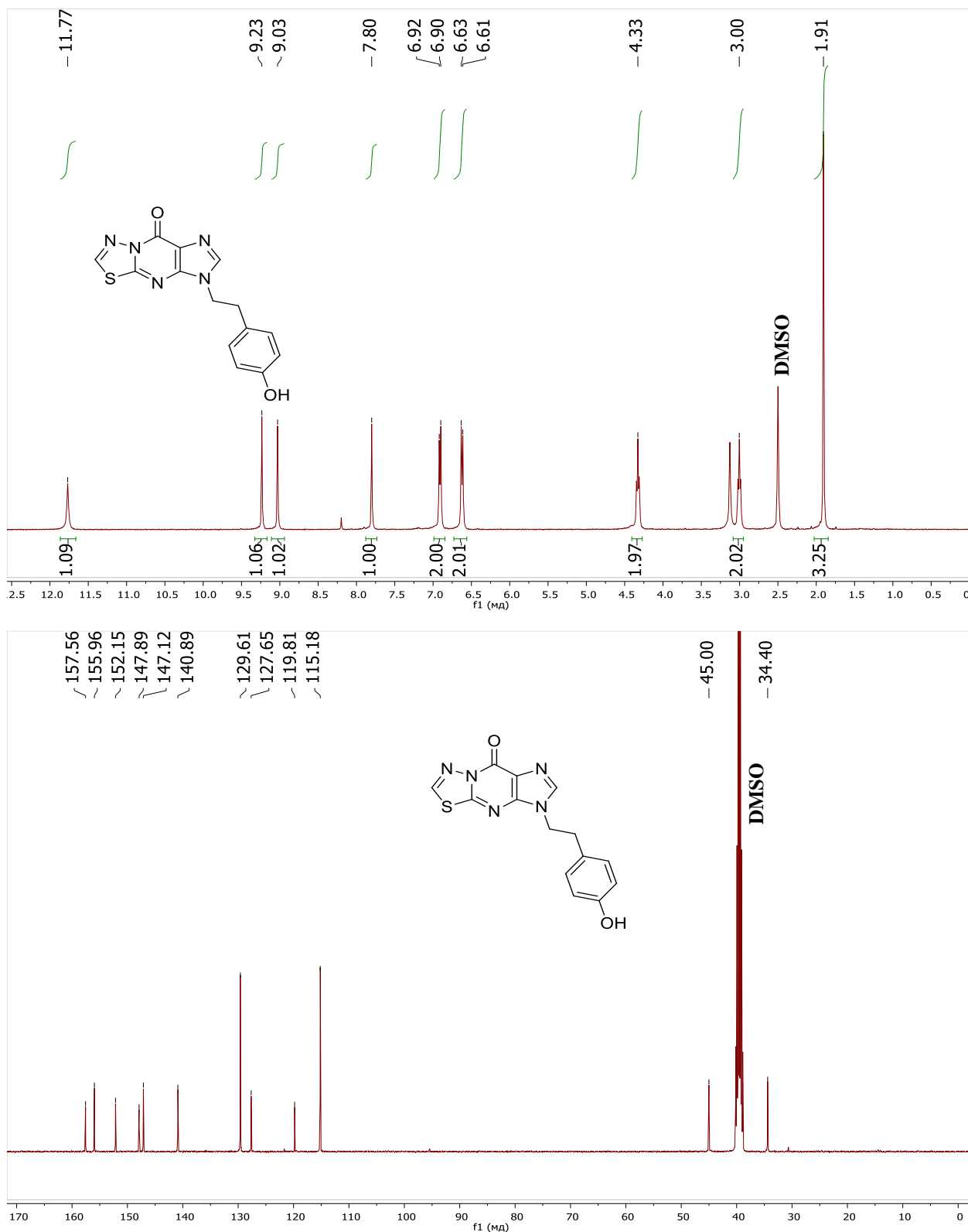


Figure S27. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **6b**

3-(4-Hydroxyphenylethyl)-[1,3,4]thiadiazolo[3,2-*a*]purin-8-one (6a)

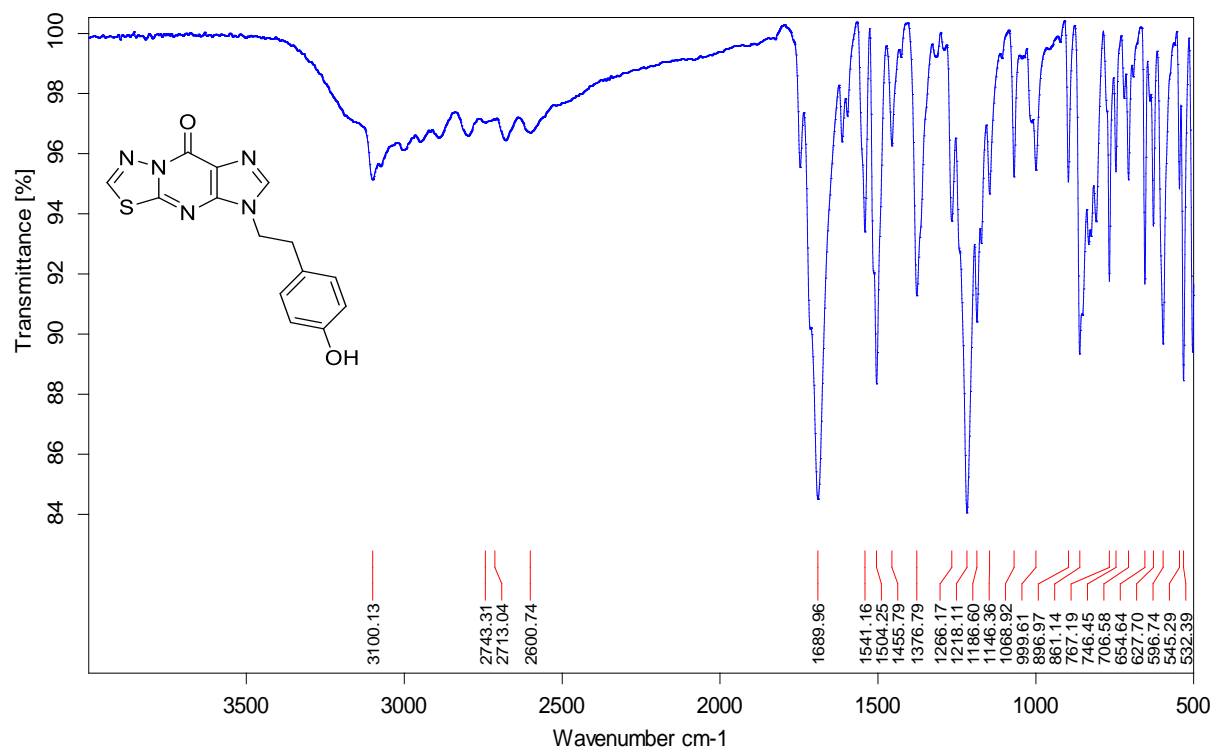


Figure S28. IR spectra of **6a**

3-(Cyclopropyl)-[1,3,4]thiadiazolo[3,2-*a*]purin-8-one (6b)

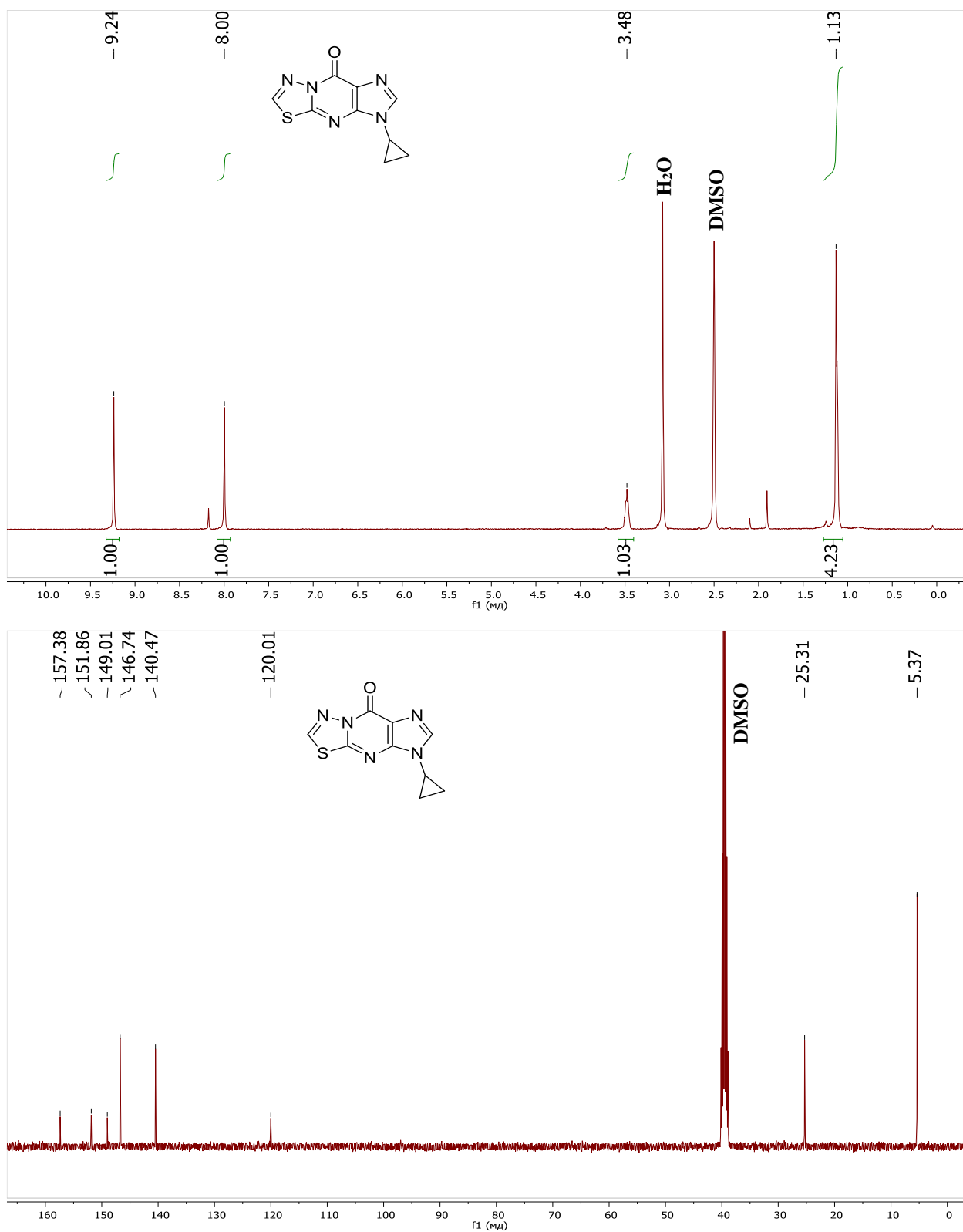


Figure S29. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **6b**

3-(Cyclopropyl)-[1,3,4]thiadiazolo[3,2-*a*]purin-8-one (6b)

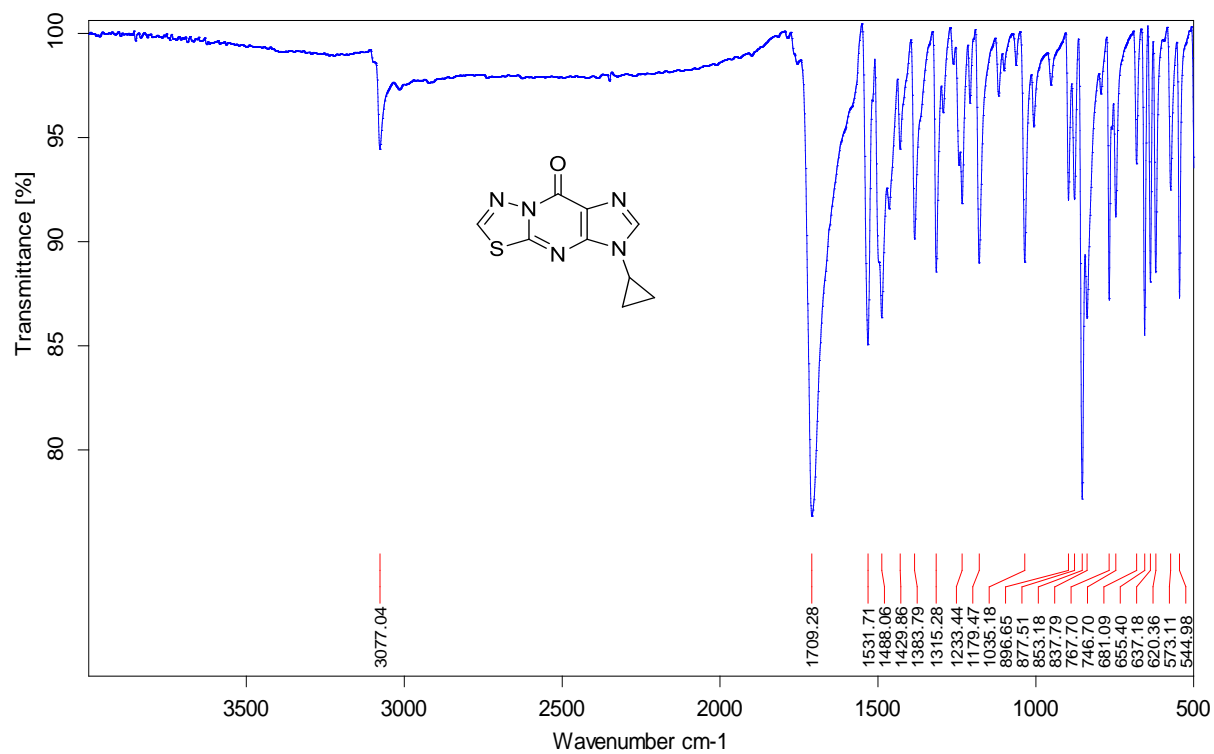


Figure S30. IR spectra of **6b**

5-[4-(diethoxymethoxy)butyl]thiadiazolo[3,2-*a*]purin-8-one (6c)

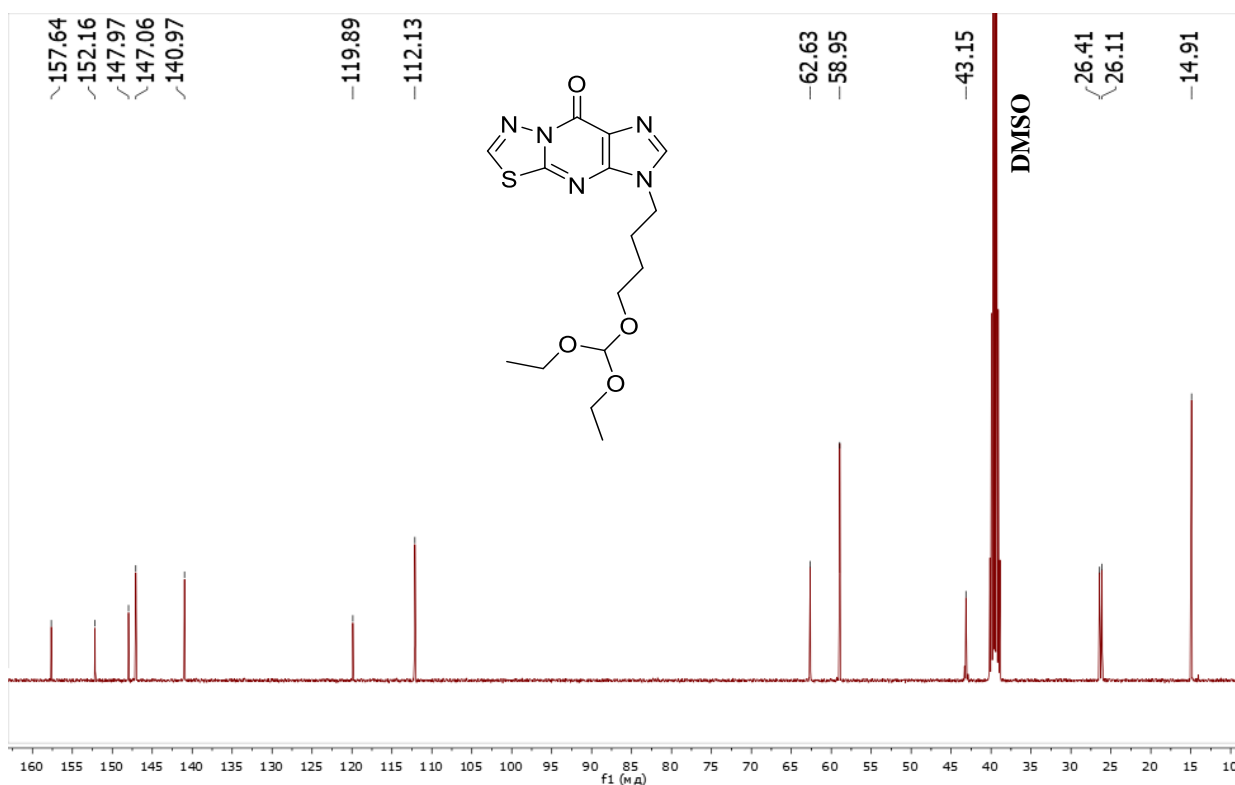
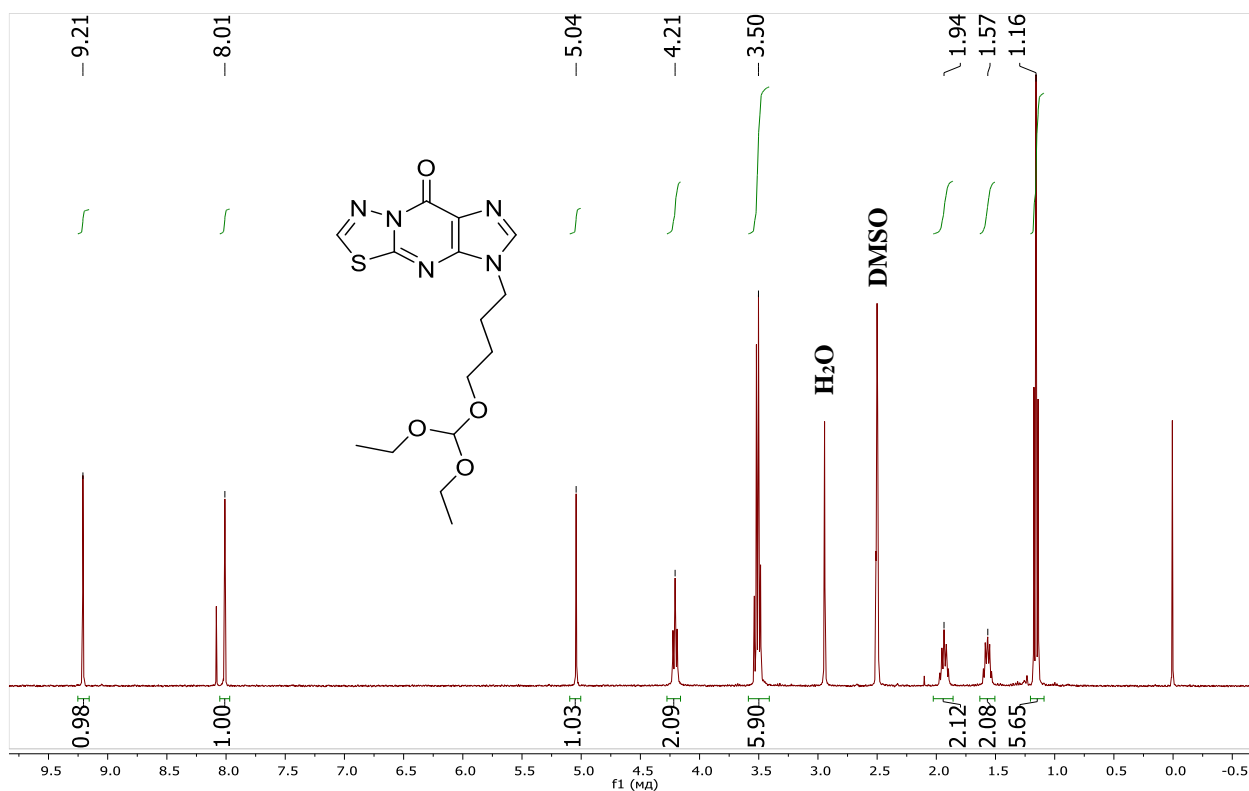


Figure S31. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **6c**

5-[4-(diethoxymethoxy)butyl]thiadiazolo[3,2-*a*]purin-8-one (6c)

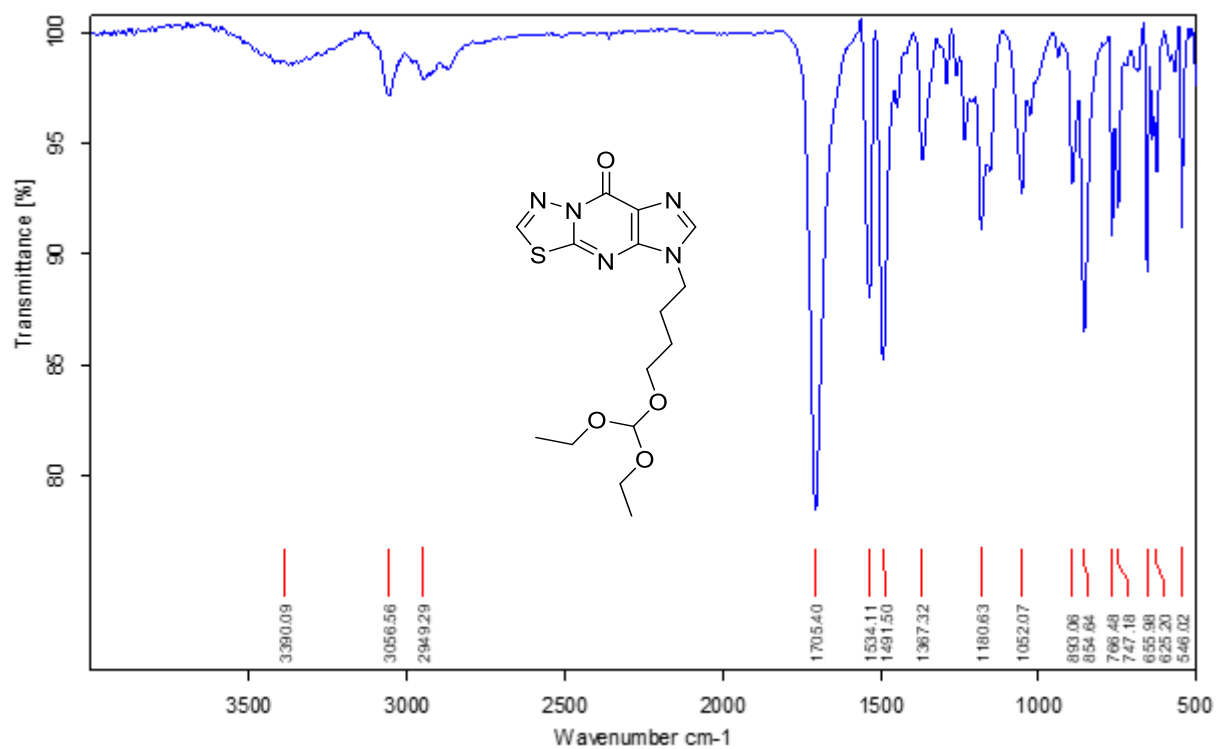


Figure S32. IR spectra of **6c**

3-nitrobenz[4,5]imidazo[1,2-*a*]pyrimidin-4(1*H*)-one sodium salt (9**)**

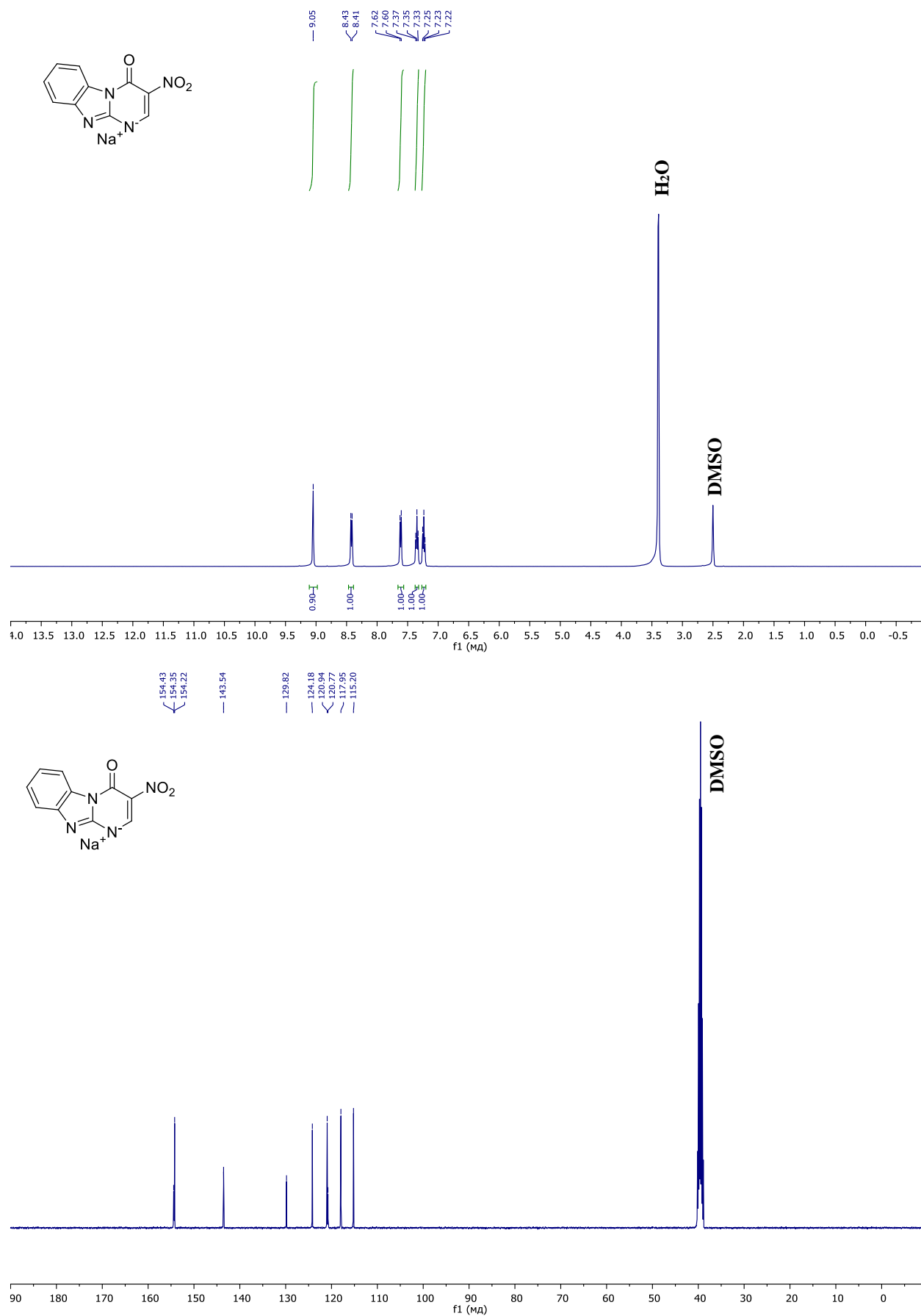


Figure S33. ¹H NMR (400 MHz, DMSO-*d*₆) and ¹³C NMR (100 MHz, DMSO-*d*₆) spectra of **9**

3-nitrobenz[4,5]imidazo[1,2-*a*]pyrimidin-4(1*H*)-one sodium salt (9)

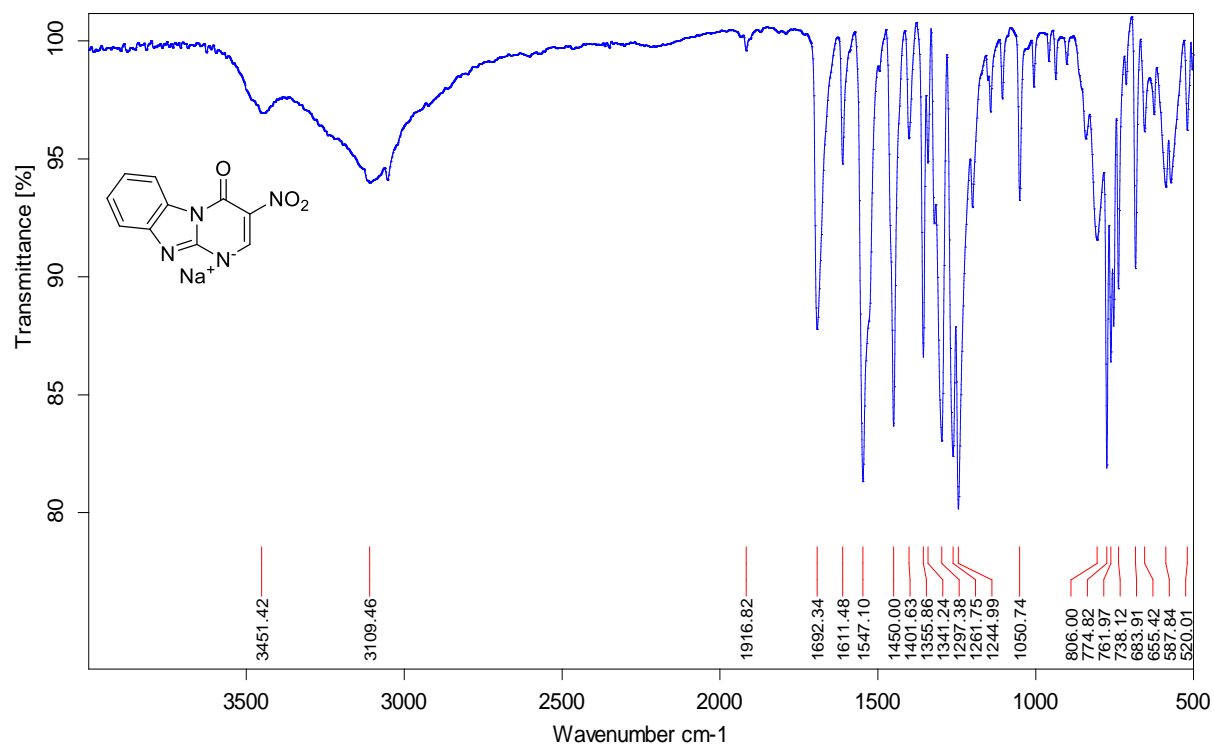


Figure S34. IR spectra of **9**

2-(*p*-Tolyl)-4-(2,3,4-trimethoxyphenyl)-2*H*-benz[4,5]imidazo[1,2-*a*][1,2,3]triazolo[4,5-*e*]pyrimidine (13a)

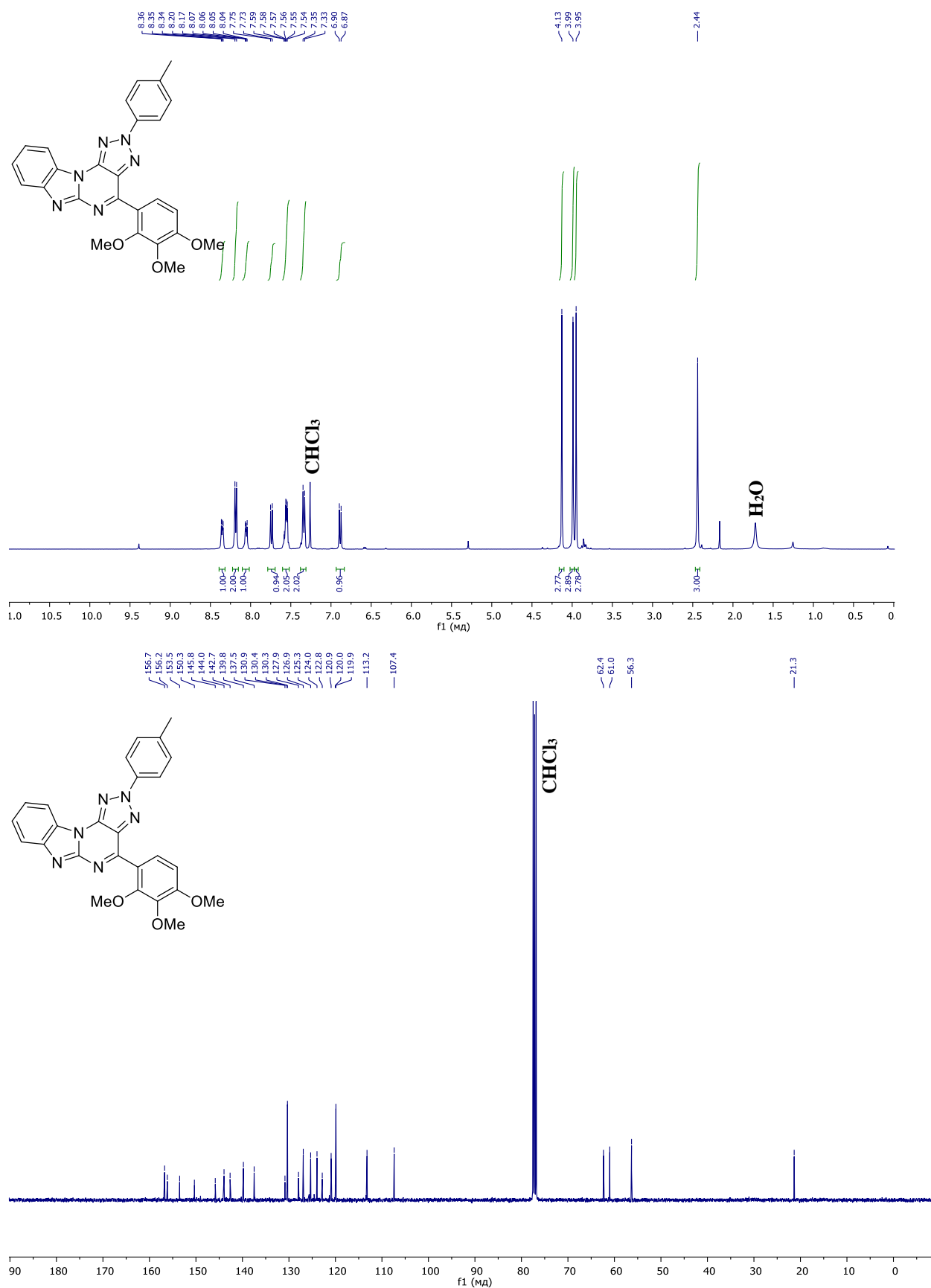


Figure S35. ¹H NMR (400 MHz, CDCl₃) and ¹³C NMR (100 MHz, CDCl₃) spectra of **13a**

2-(*p*-Tolyl)-4-(2,3,4-trimethoxyphenyl)-2*H*-benz[4,5]imidazo[1,2-*a*][1,2,3]triazolo[4,5-*e*]pyrimidine (13a)

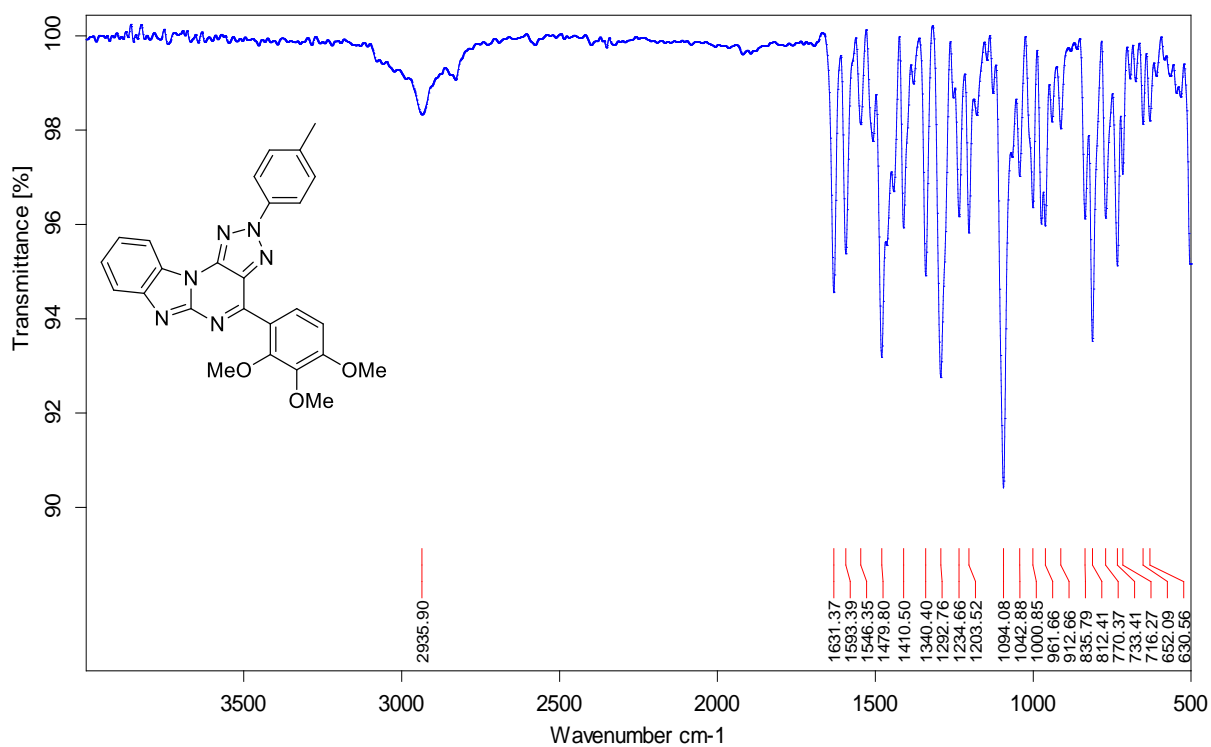


Figure S36. IR spectra of **13a**

2-(*p*-Tolyl)-4-(3,4-trimethoxyphenyl)-2*H*-benz[4,5]imidazo[1,2-*a*][1,2,3]triazolo[4,5-*e*]pyrimidine (13b)

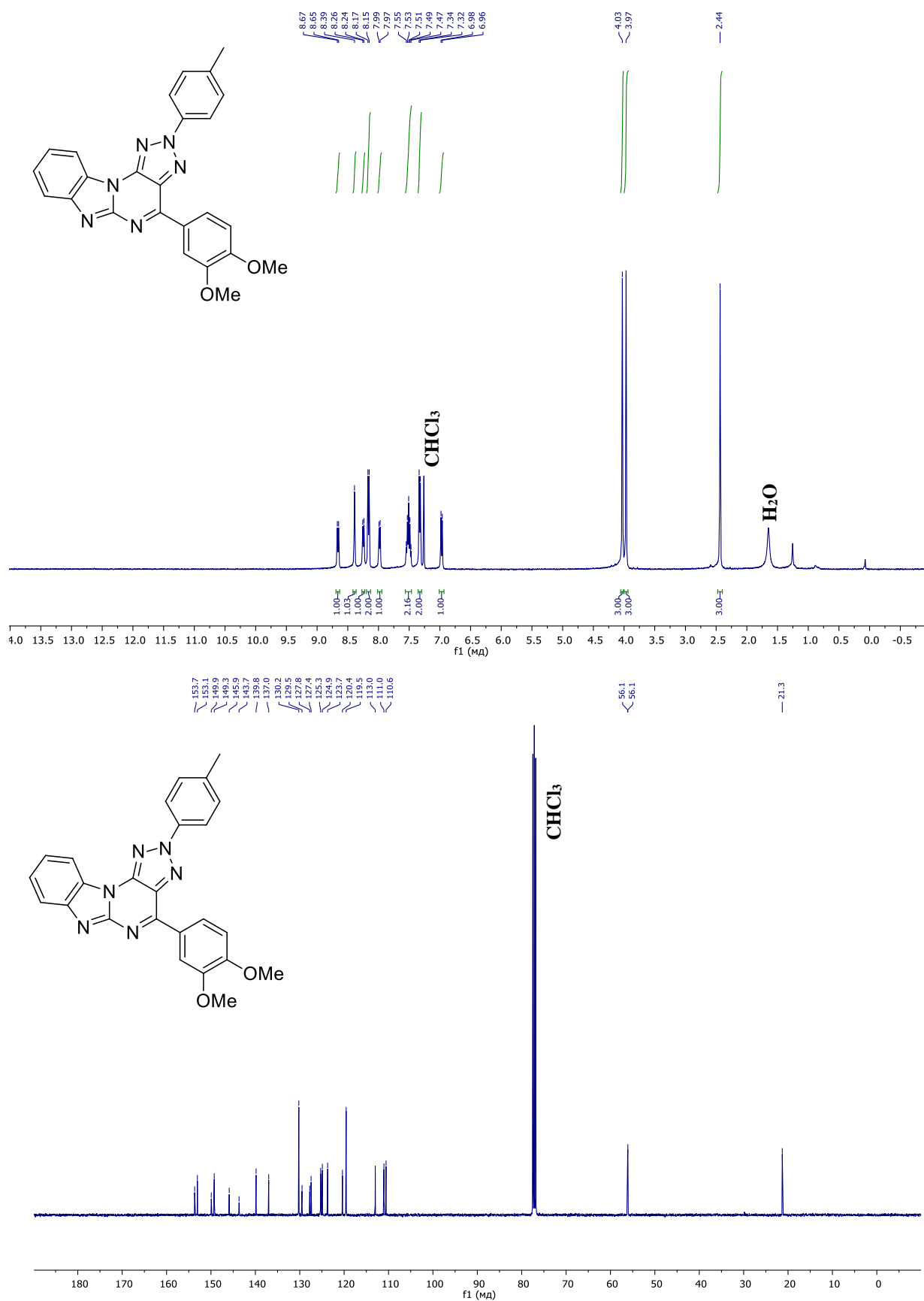


Figure S37. ¹H NMR (400 MHz, CDCl₃) and ¹³C NMR (100 MHz, CDCl₃) spectra of **13b**

2-(*p*-Tolyl)-4-(3,4-trimethoxyphenyl)-2*H*-benz[4,5]imidazo[1,2-*a*][1,2,3]triazolo[4,5-*e*]pyrimidine (13b)

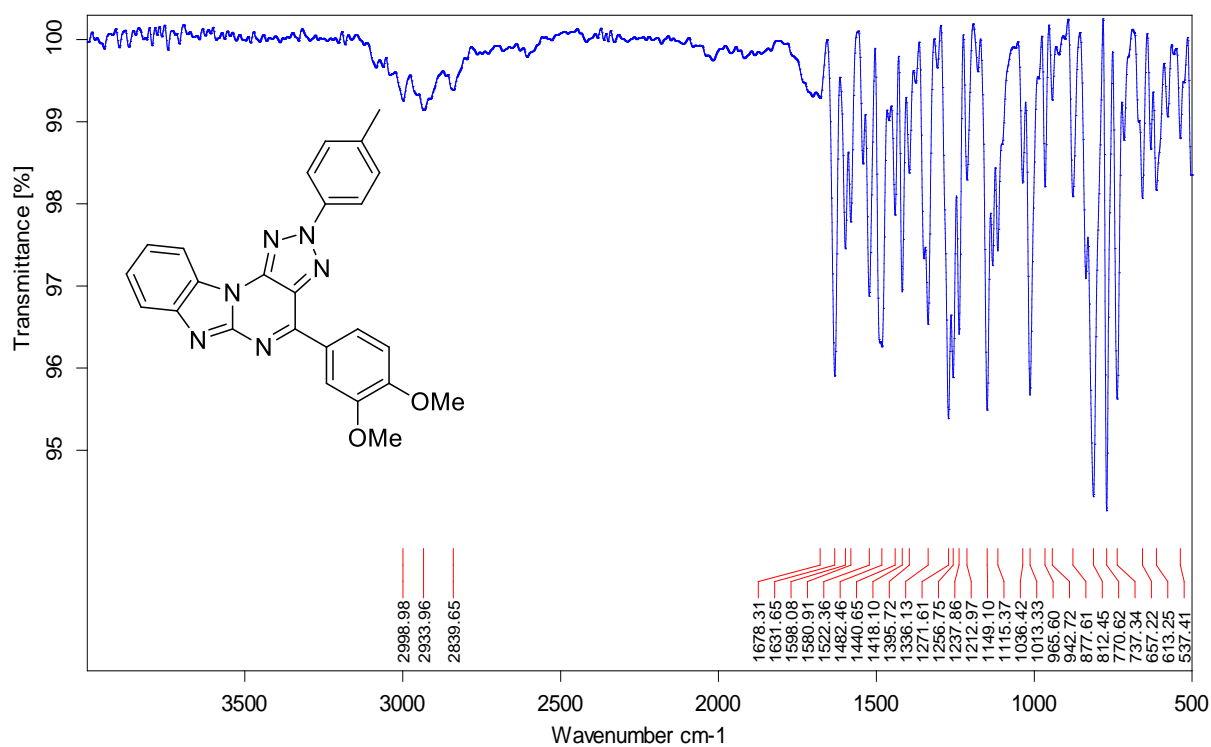


Figure S38. IR spectra of **13b**

2-(*p*-Tolyl)-4-(thien-2-yl)-2*H*-benz[4,5]imidazo[1,2-*a*][1,2,3]triazolo[4,5-*e*]pyrimidine (13c)

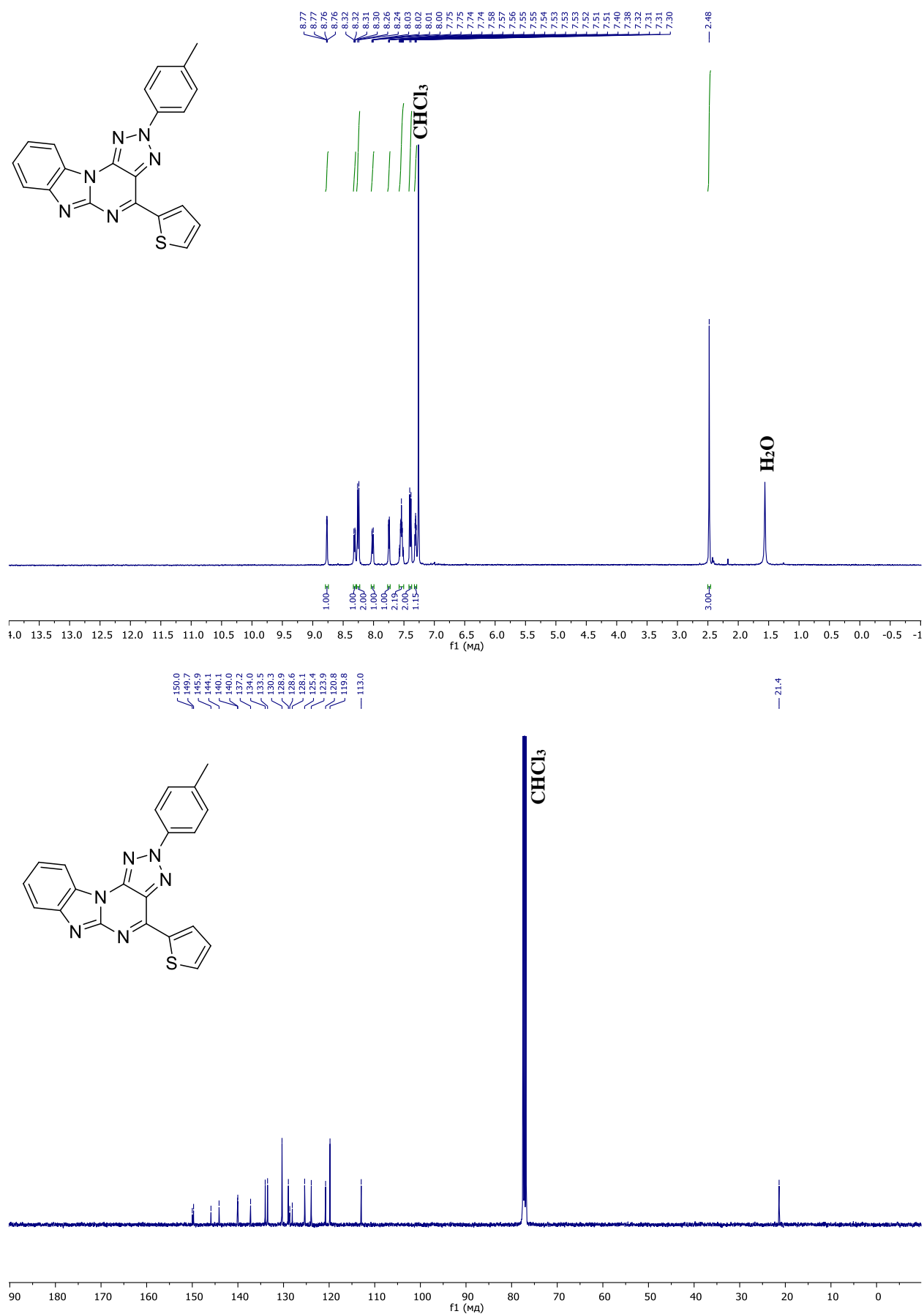


Figure S39. ¹H NMR (400 MHz, CDCl₃) and ¹³C NMR (100 MHz, CDCl₃) spectra of **13c**

2-(*p*-Tolyl)-4-(thien-2-yl)-2*H*-benz[4,5]imidazo[1,2-*a*][1,2,3]triazolo[4,5-*e*]pyrimidine (13c)

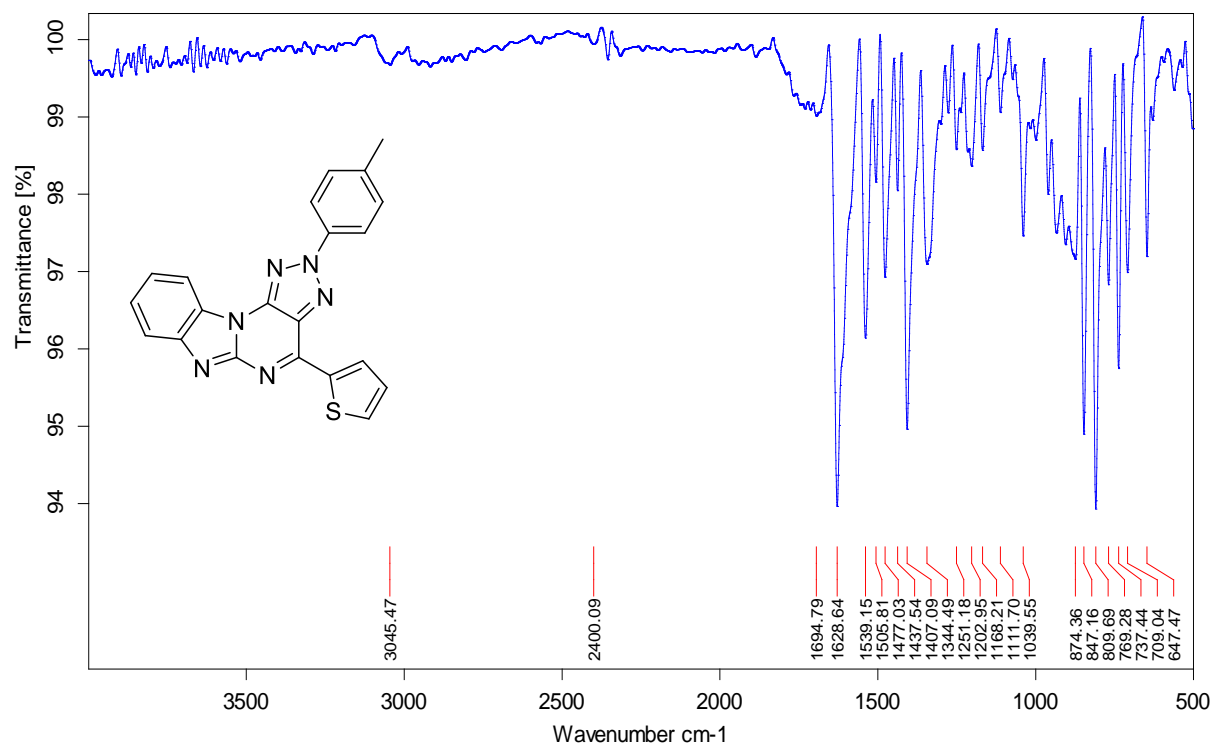


Figure S40. IR spectra of **13c**

2-(*p*-Tolyl)-4-(1-Methyl-1*H*-pyrrol-2-yl)-2*H*-benz[4,5]imidazo[1,2-*a*][1,2,3]triazolo[4,5-*e*]pyrimidine (13d)

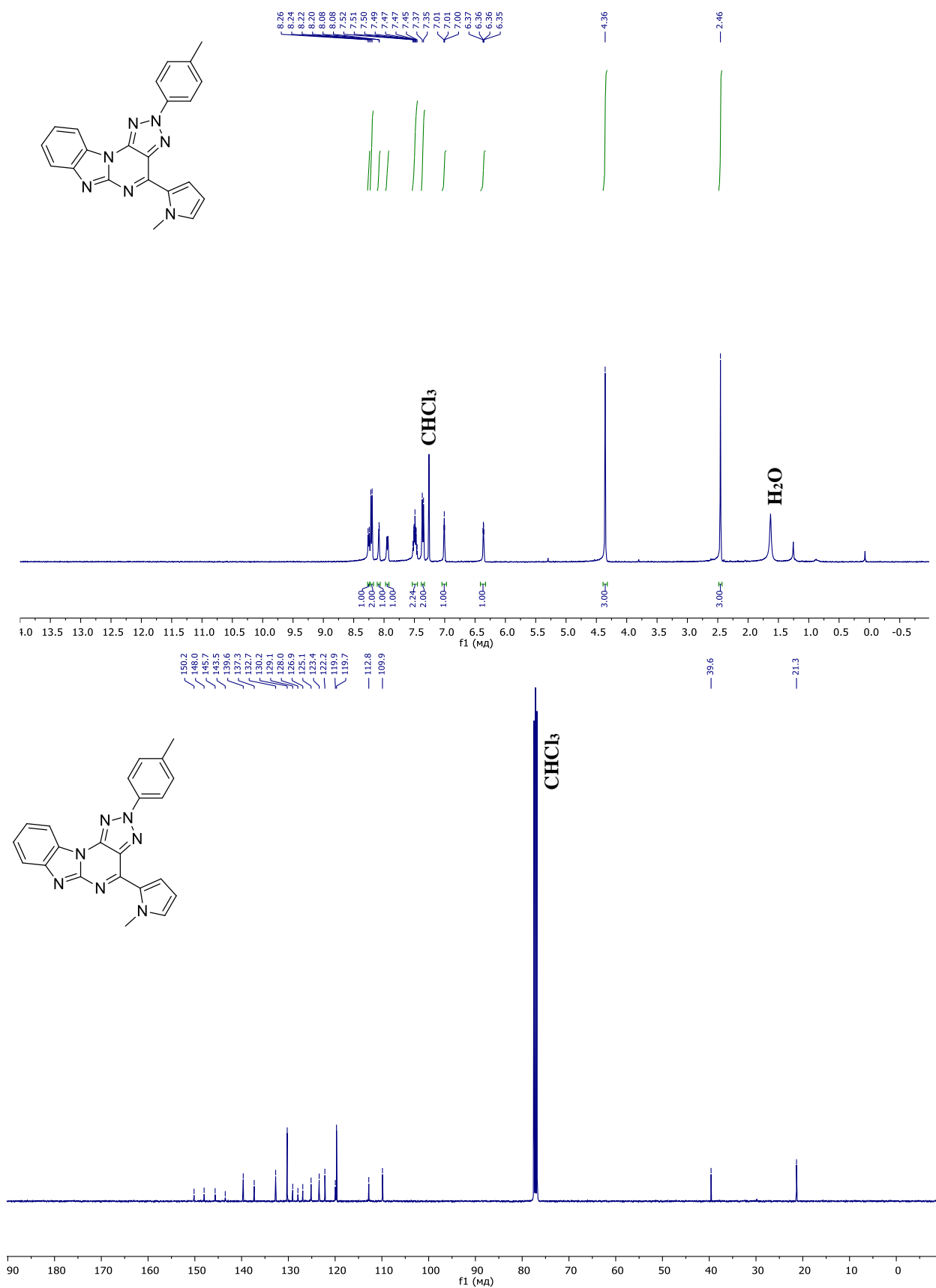


Figure S41. ¹H NMR (400 MHz, CDCl₃) and ¹³C NMR (100 MHz, CDCl₃) spectra of **13d**

2-(*p*-Tolyl)-4-(1-Methyl-1*H*-pyrrol-2-yl)-2*H*-benz[4,5]imidazo[1,2-*a*][1,2,3]triazolo[4,5-*e*]pyrimidine (13d)

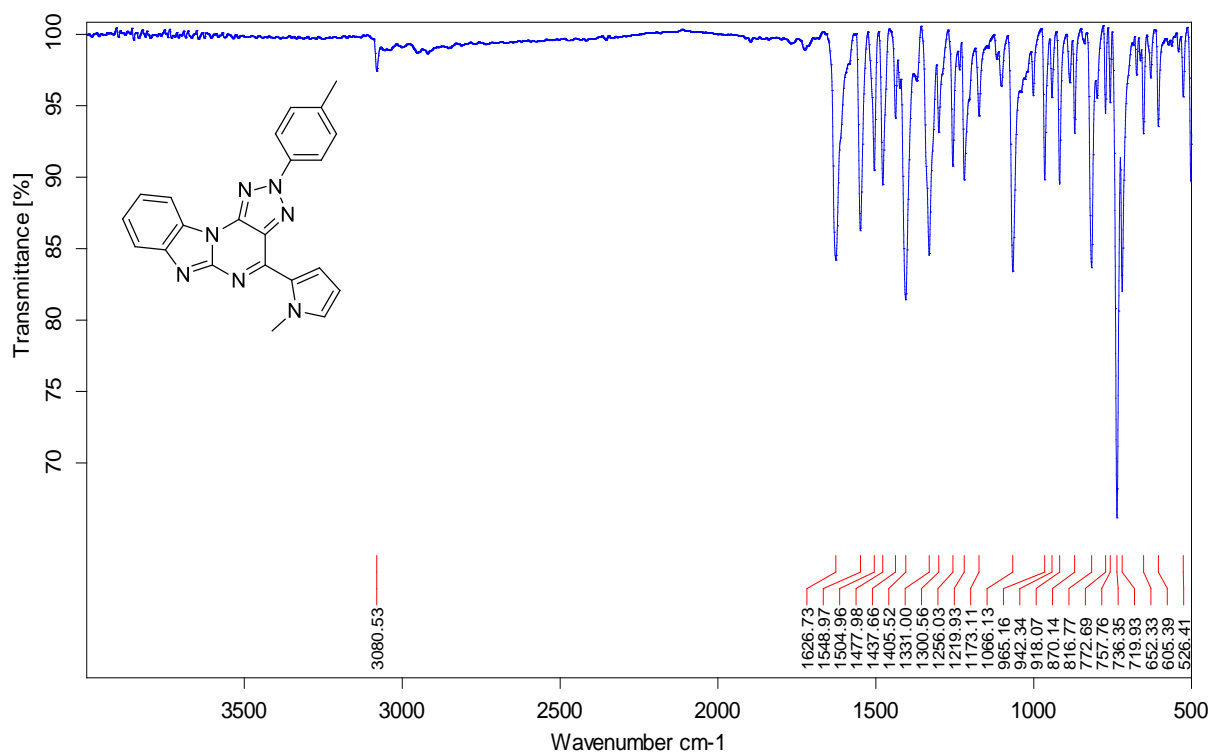


Figure S42. IR spectra of **13d**

2-(*p*-Tolyl)-4-(1-naphthalene-2-ol)-2*H*-benz[4,5]imidazo[1,2-*a*][1,2,3]triazolo[4,5-*e*]pyrimidine (13e)

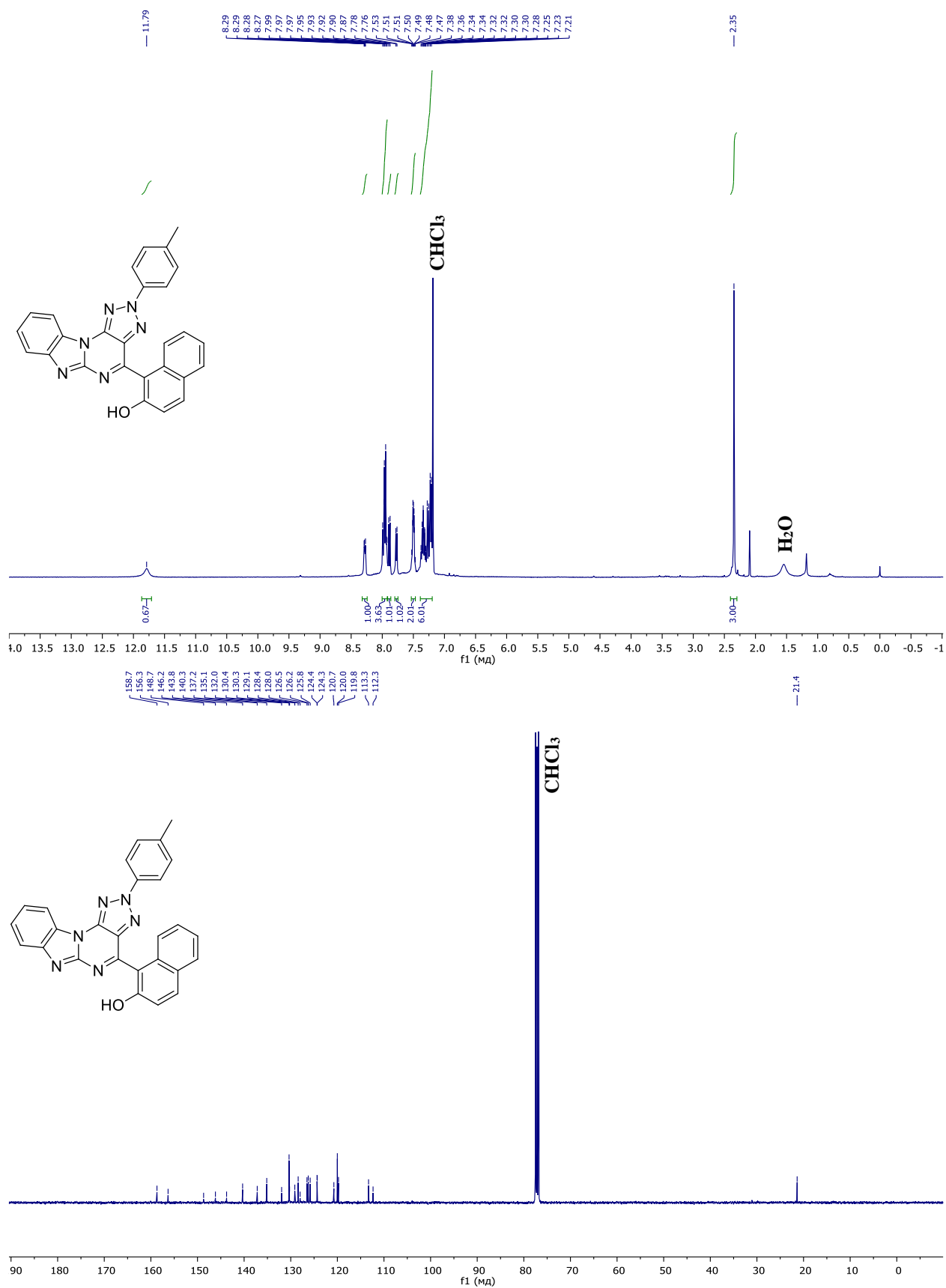


Figure S43. ¹H NMR (400 MHz, CDCl₃) and ¹³C NMR (100 MHz, CDCl₃) spectra of **13e**

2-(*p*-Tolyl)-4-(1-naphthalene-2-ol)-2*H*-benz[4,5]imidazo[1,2-*a*][1,2,3]triazolo[4,5-*e*]pyrimidine (13e)

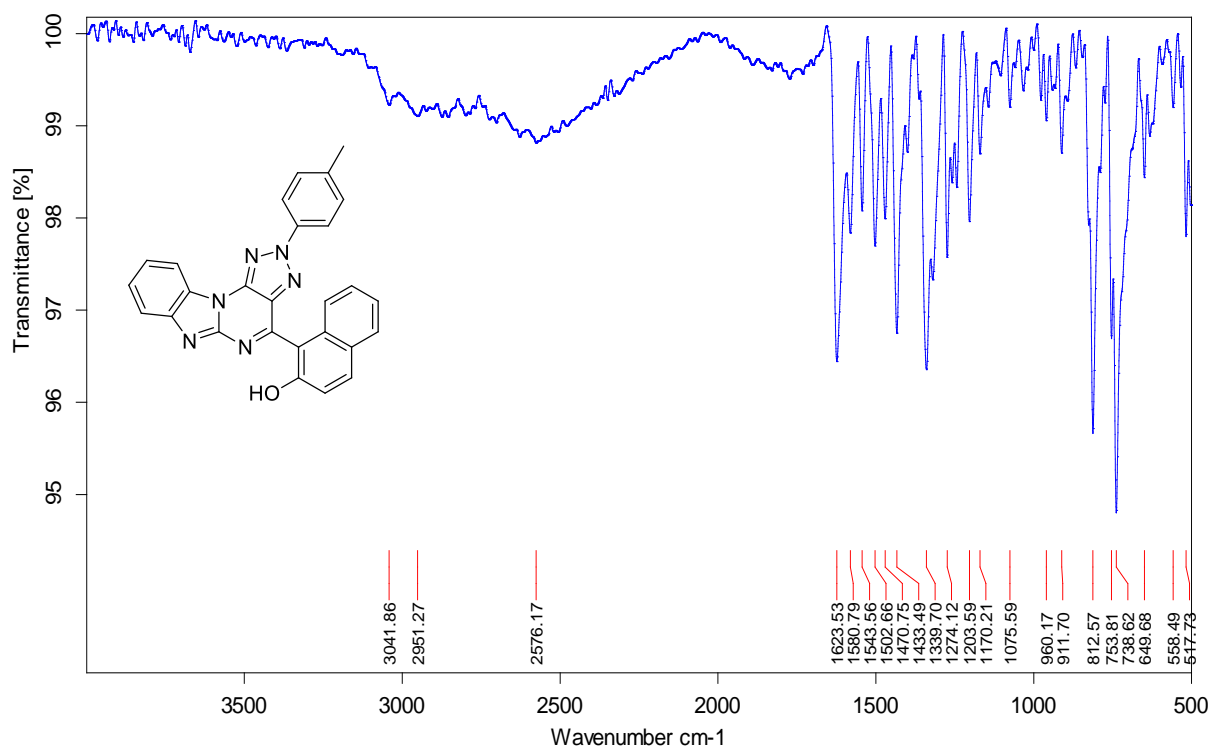


Figure S44. IR spectra of **13e**

8,9-Difluor-2-(*p*-Tolyl)-4-(2,3,4-trimethoxyphenyl)-2*H*-benz[4,5]imidazo[1,2-*a*][1,2,3]triazolo[4,5-*e*]pyrimidine (14a)

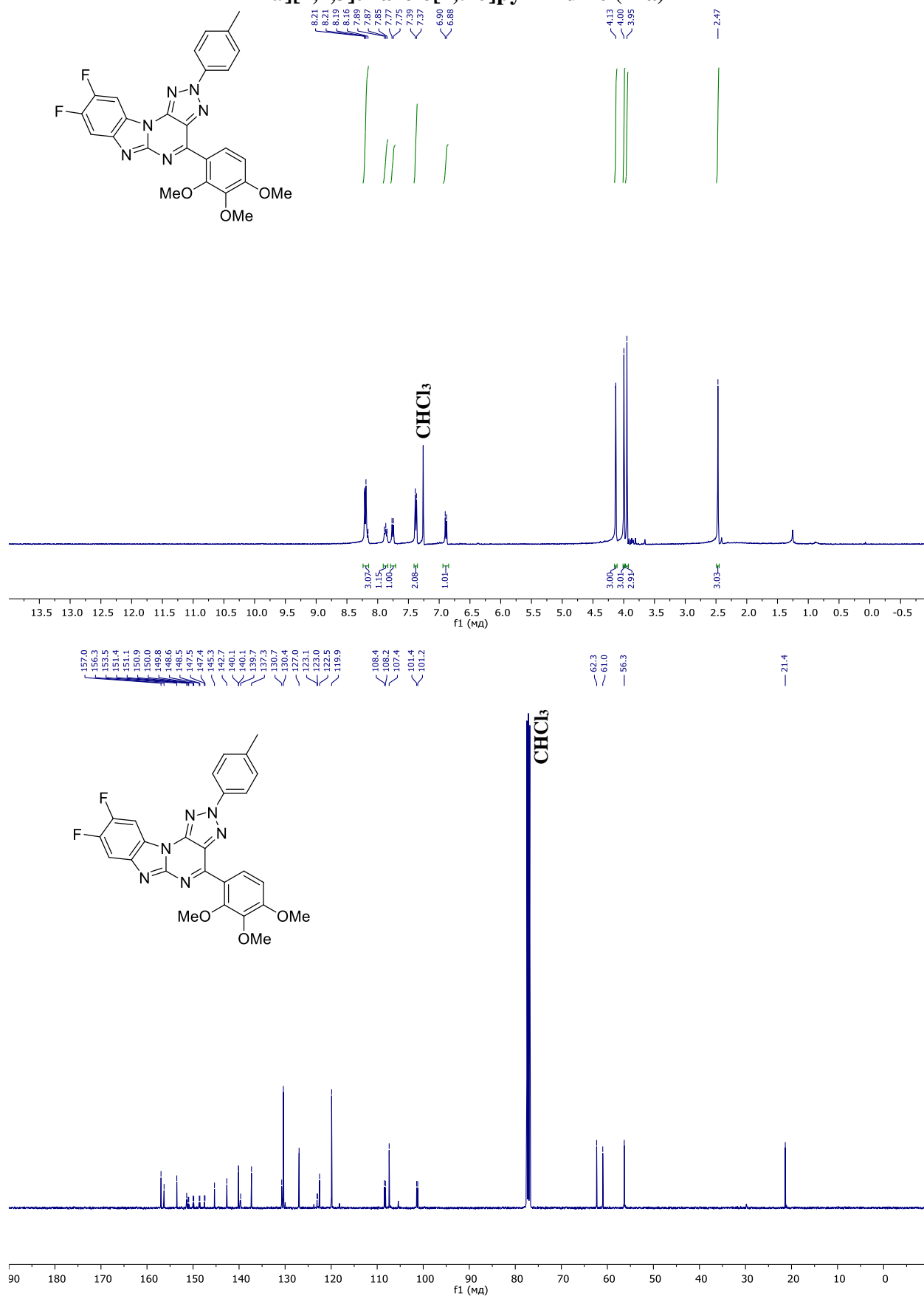


Figure S45. ¹H NMR (400 MHz, CDCl₃) and ¹³C NMR (100 MHz, CDCl₃) spectra of **14a**

8,9-Difluor-2-(*p*-Tolyl)-4-(2,3,4-trimethoxyphenyl)-2*H*-benz[4,5]imidazo[1,2-*a*][1,2,3]triazolo[4,5-*e*]pyrimidine (14a)

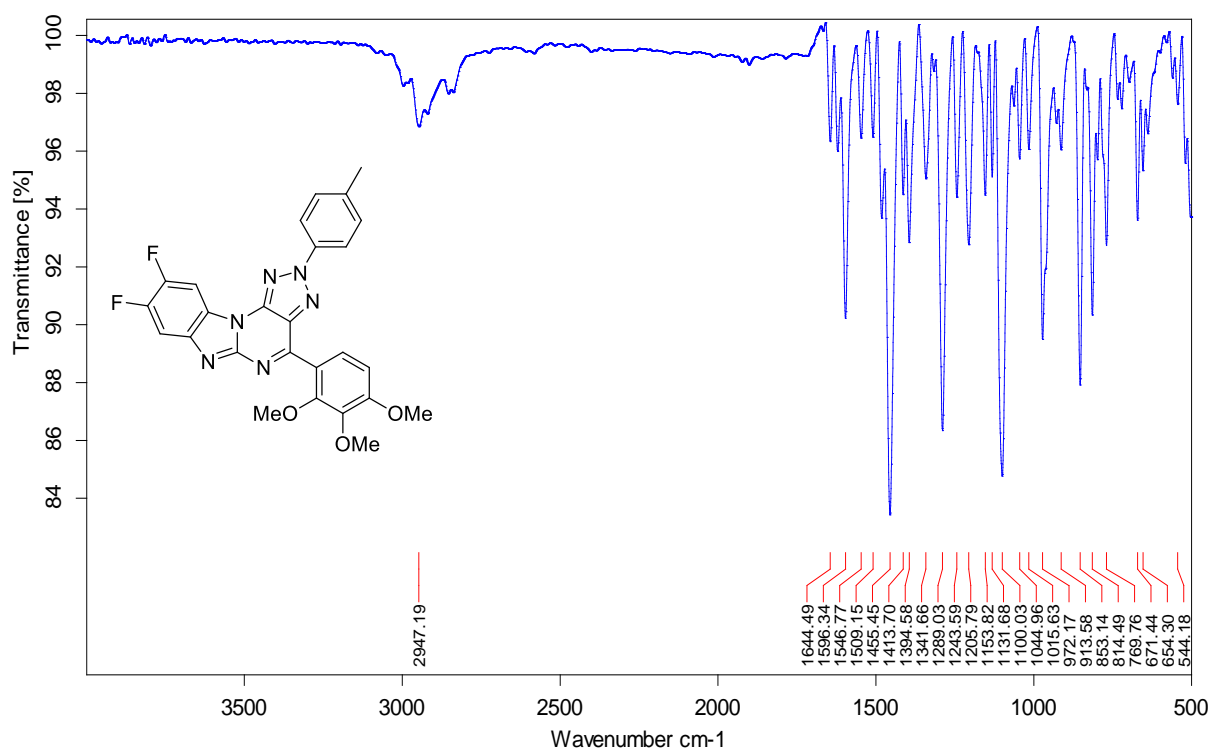


Figure S46. IR spectra of **14a**