

Supporting Information

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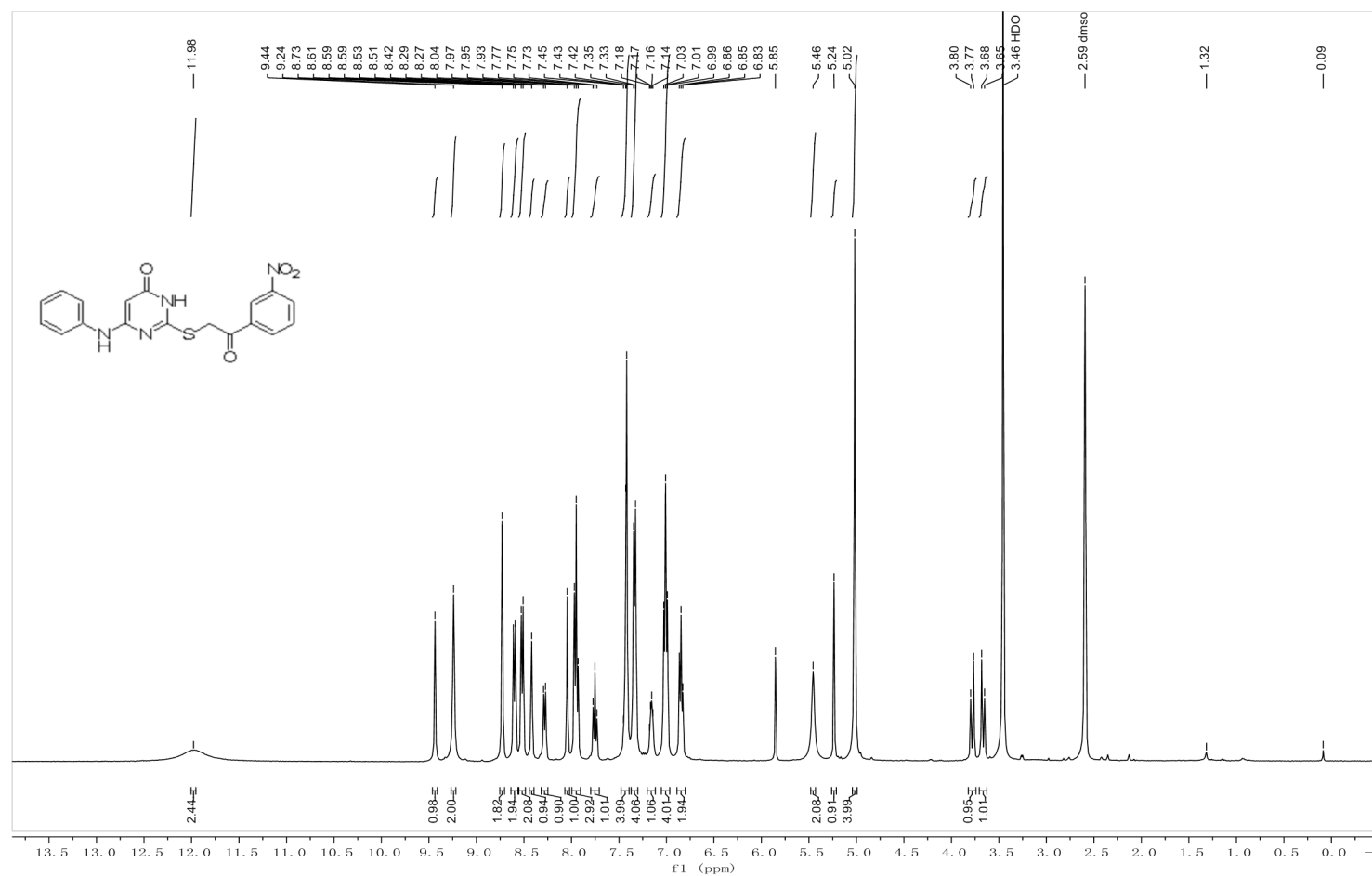


Figure S1. The NMR spectra of **2a**: 2-((2-(3-Nitrophenyl)-2-oxoethyl)thio)-6-(phenylamino)pyrimidin-4(3H)-one.

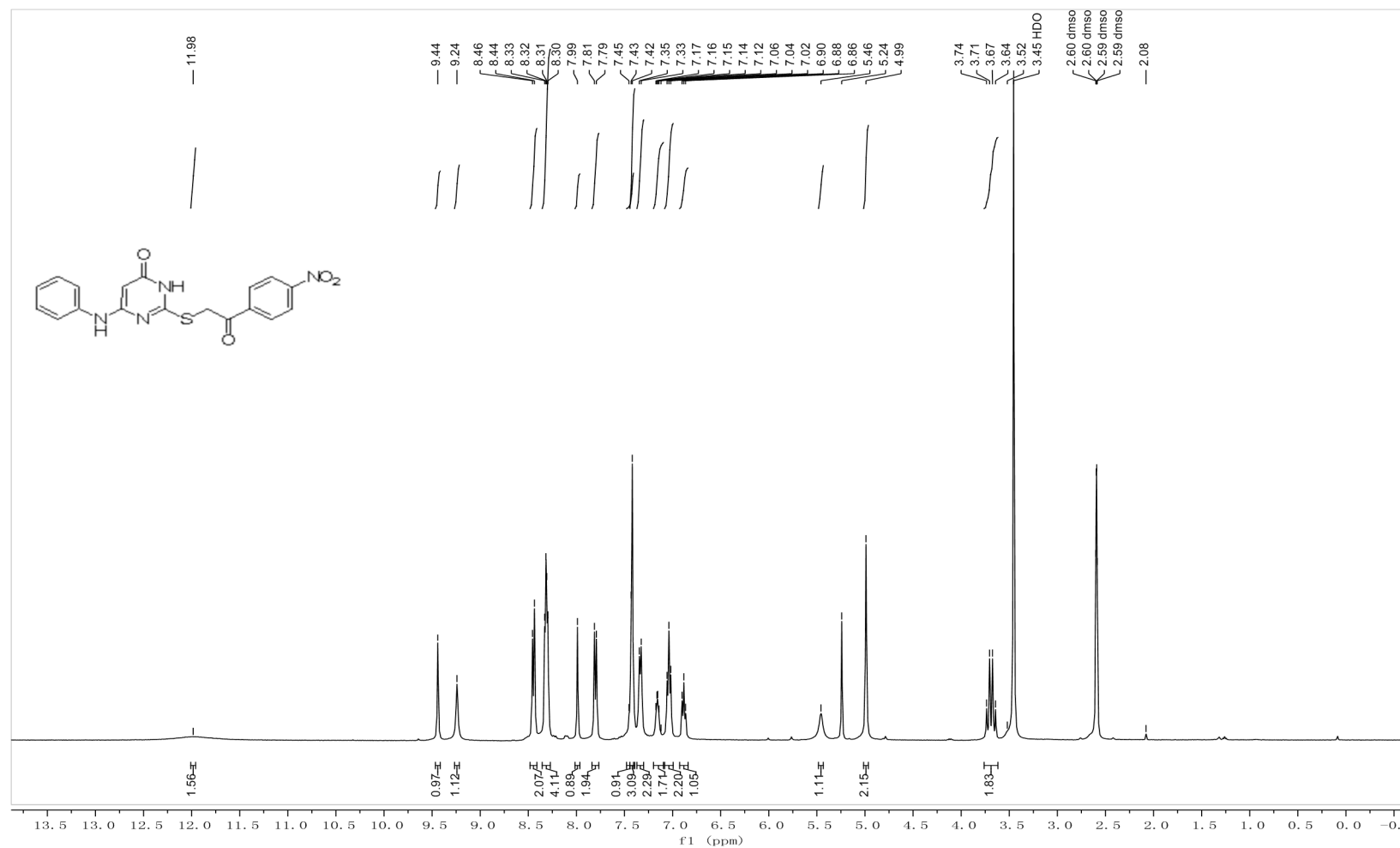


Figure S2. The NMR spectra of **2b**: 2-((2-(4-Nitrophenyl)-2-oxoethyl)thio)-6-(phenylamino)pyrimidin-4(3H)-one.

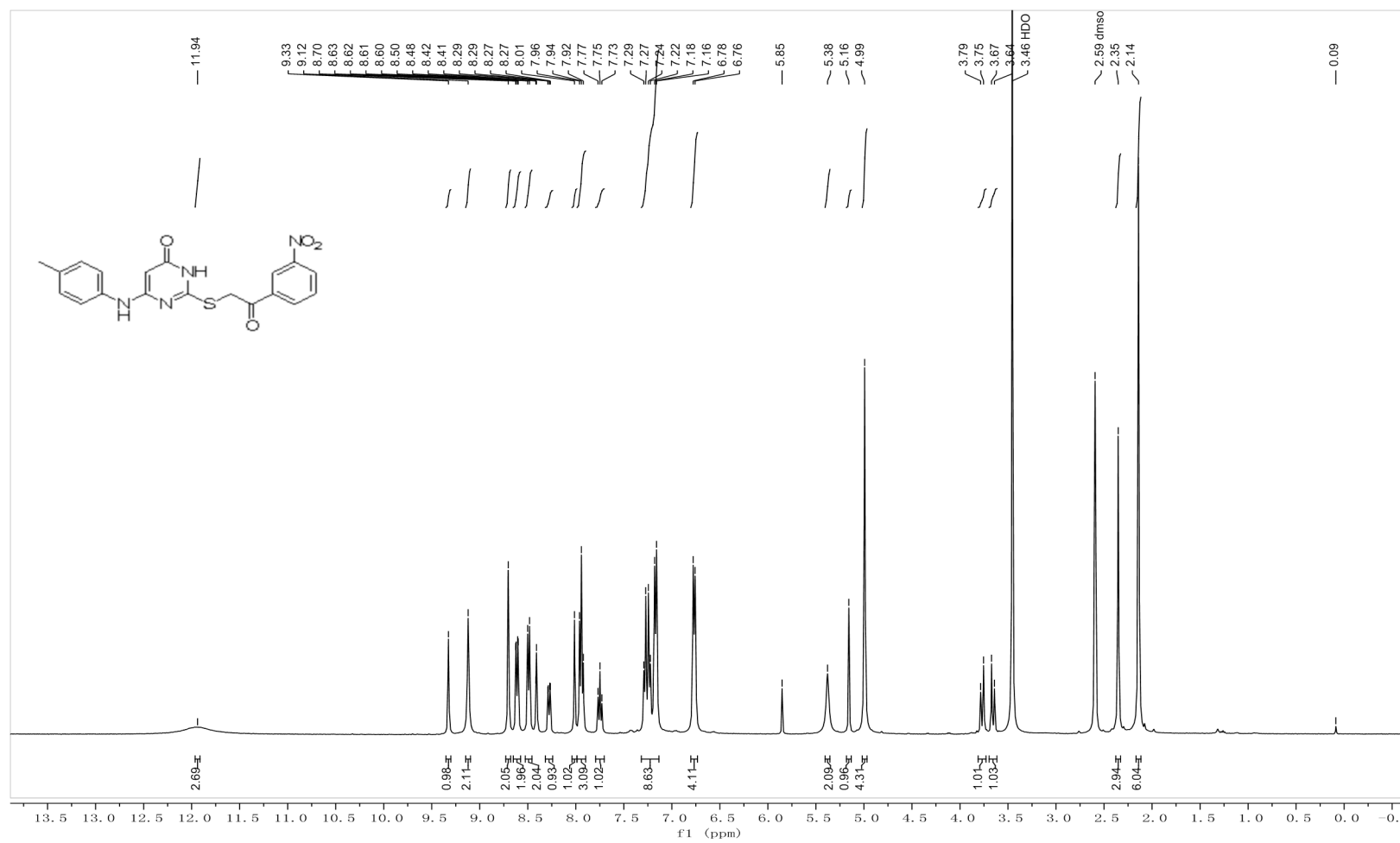


Figure S3. The NMR spectra of **2c**: 2-((2-(3-Nitrophenyl)-2-oxoethyl)thio)-6-(*p*-tolylamino)pyrimidin-4(3*H*)-one.

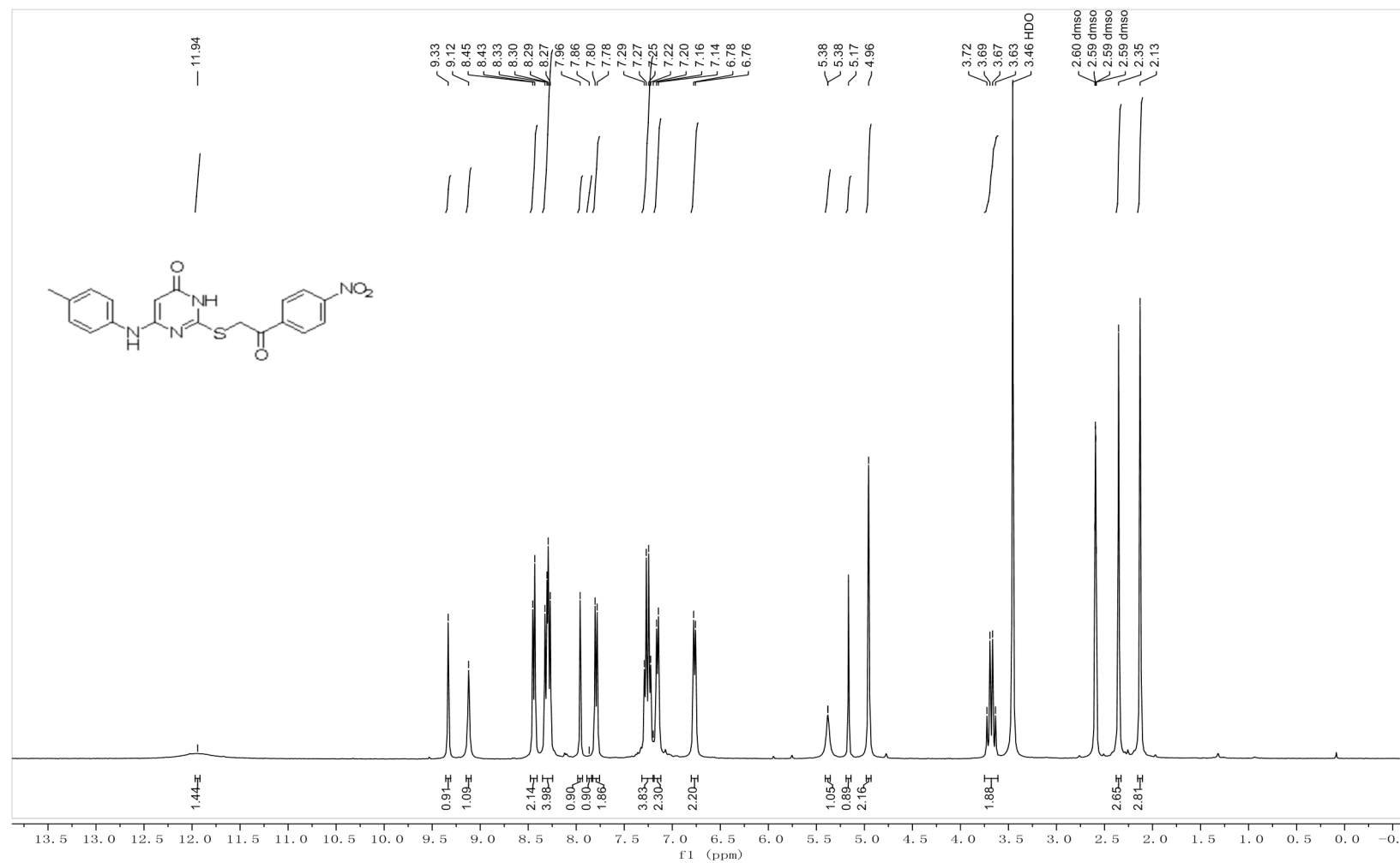


Figure S4. The NMR spectra of **2d**: 2-((2-(4-Nitrophenyl)-2-oxoethyl)thio)-6-(*p*-tolylamino)pyrimidin-4(3*H*)-one.

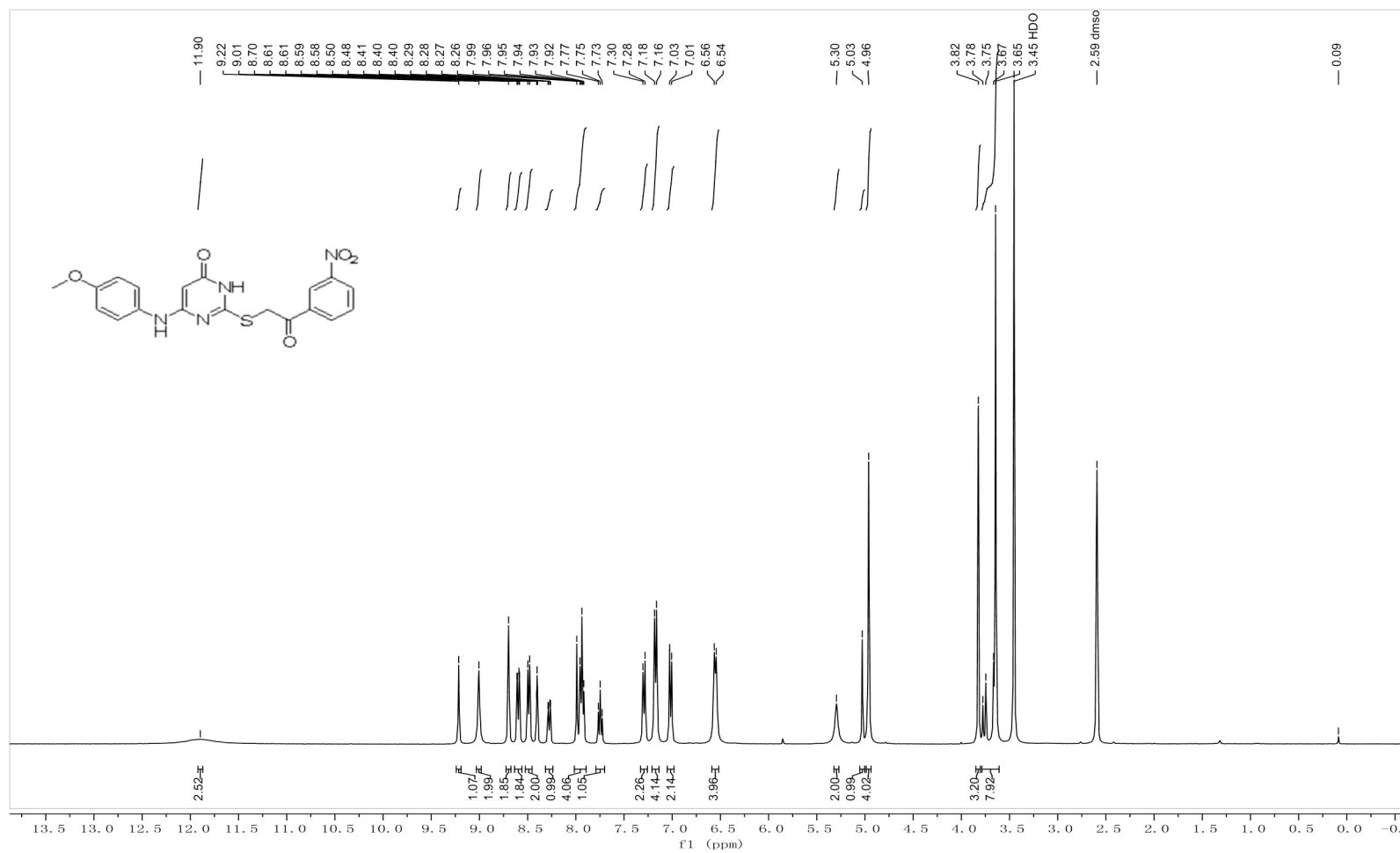


Figure S5. The NMR spectra of **2e**: 6-((4-Methoxyphenyl)amino)-2-((2-(3-nitrophenyl)-2-oxoethyl)thio)pyrimidin-4(3H)-one.

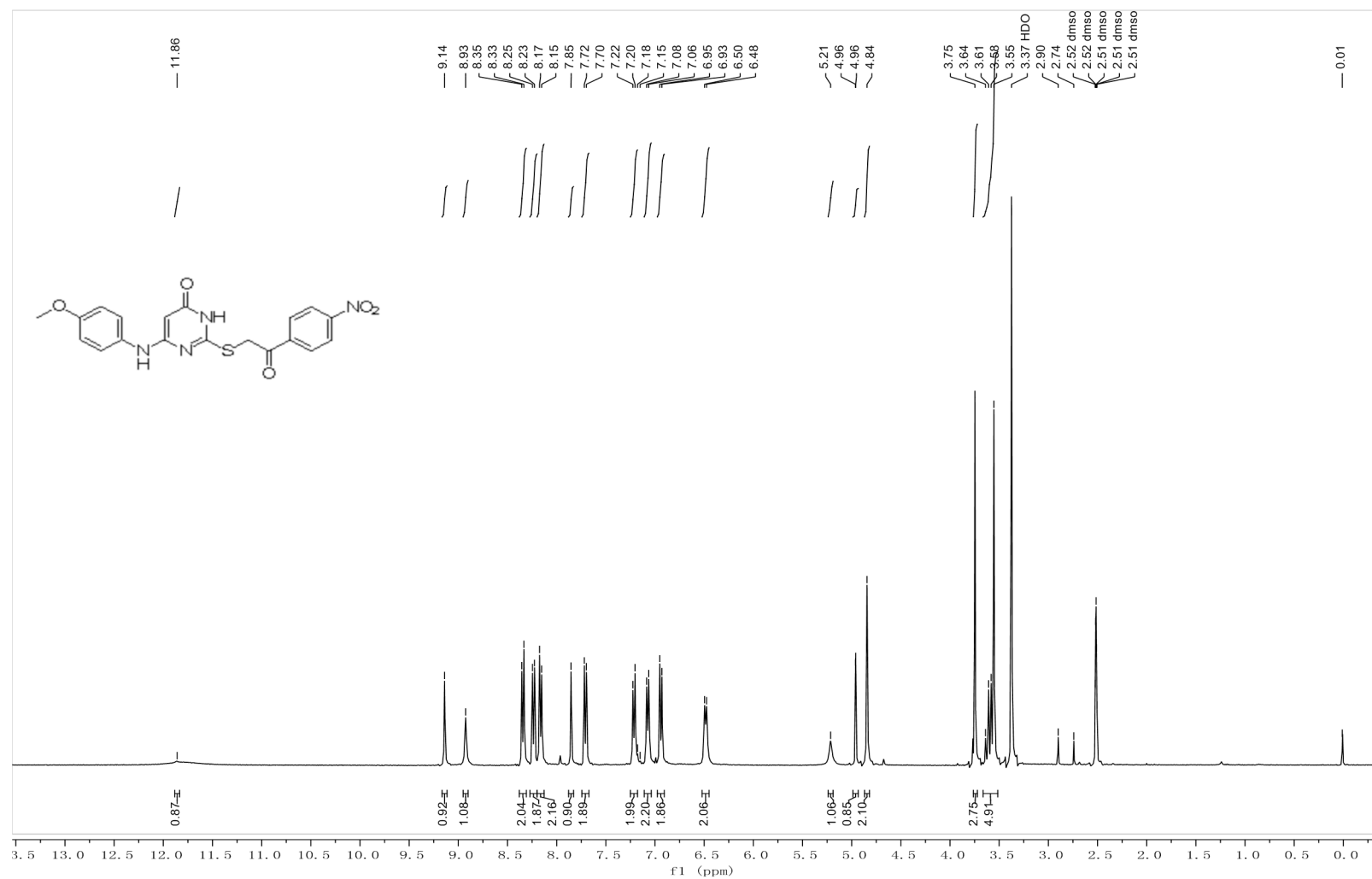


Figure S6. The NMR spectra of **2f**: 6-((4-Methoxyphenyl)amino)-2-((2-(4-nitrophenyl)-2-oxoethyl)thio)pyrimidin-4(3H)-one.

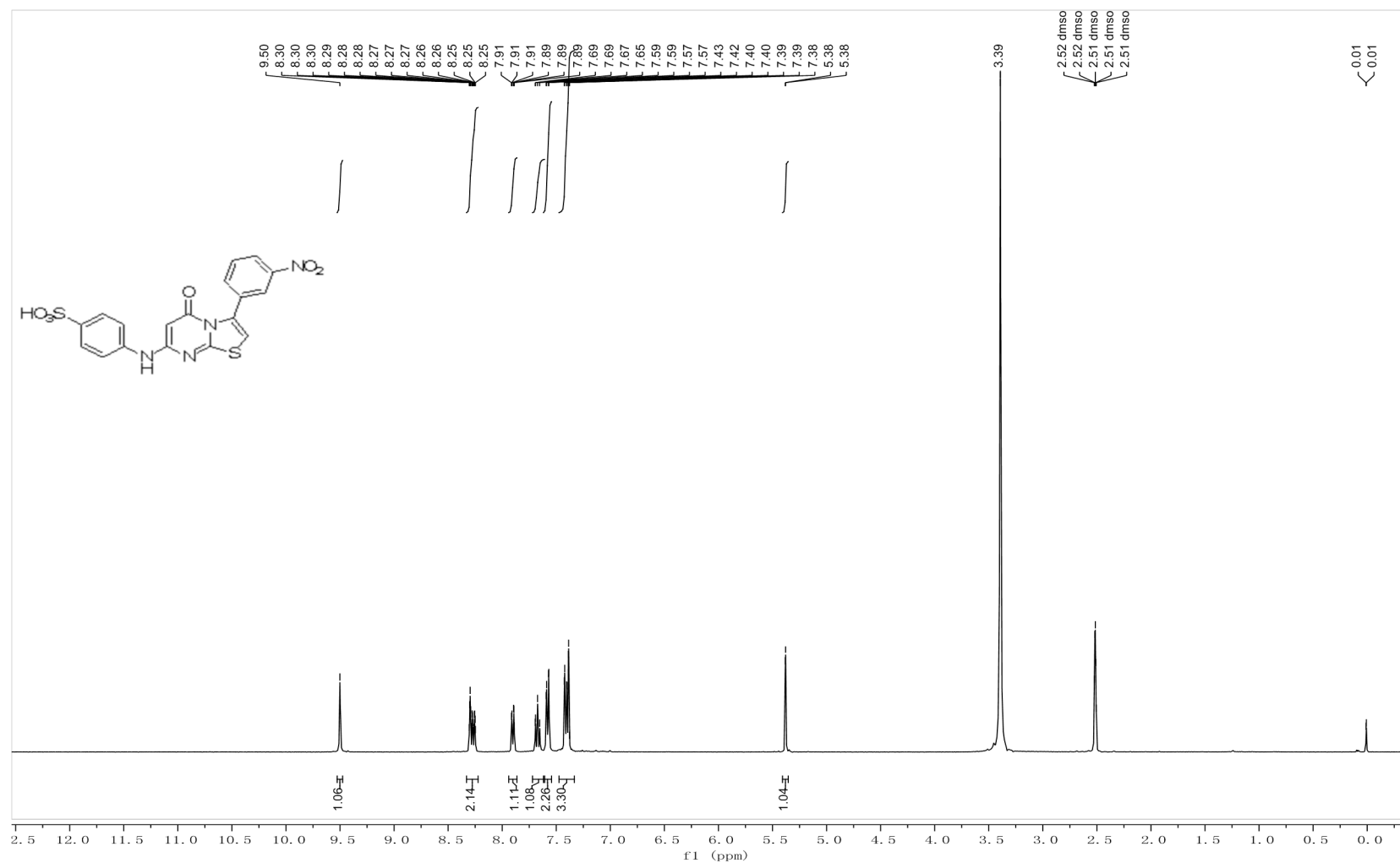


Figure S7. The ¹H-NMR spectra of **3a**: 4-((3-(3-Nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

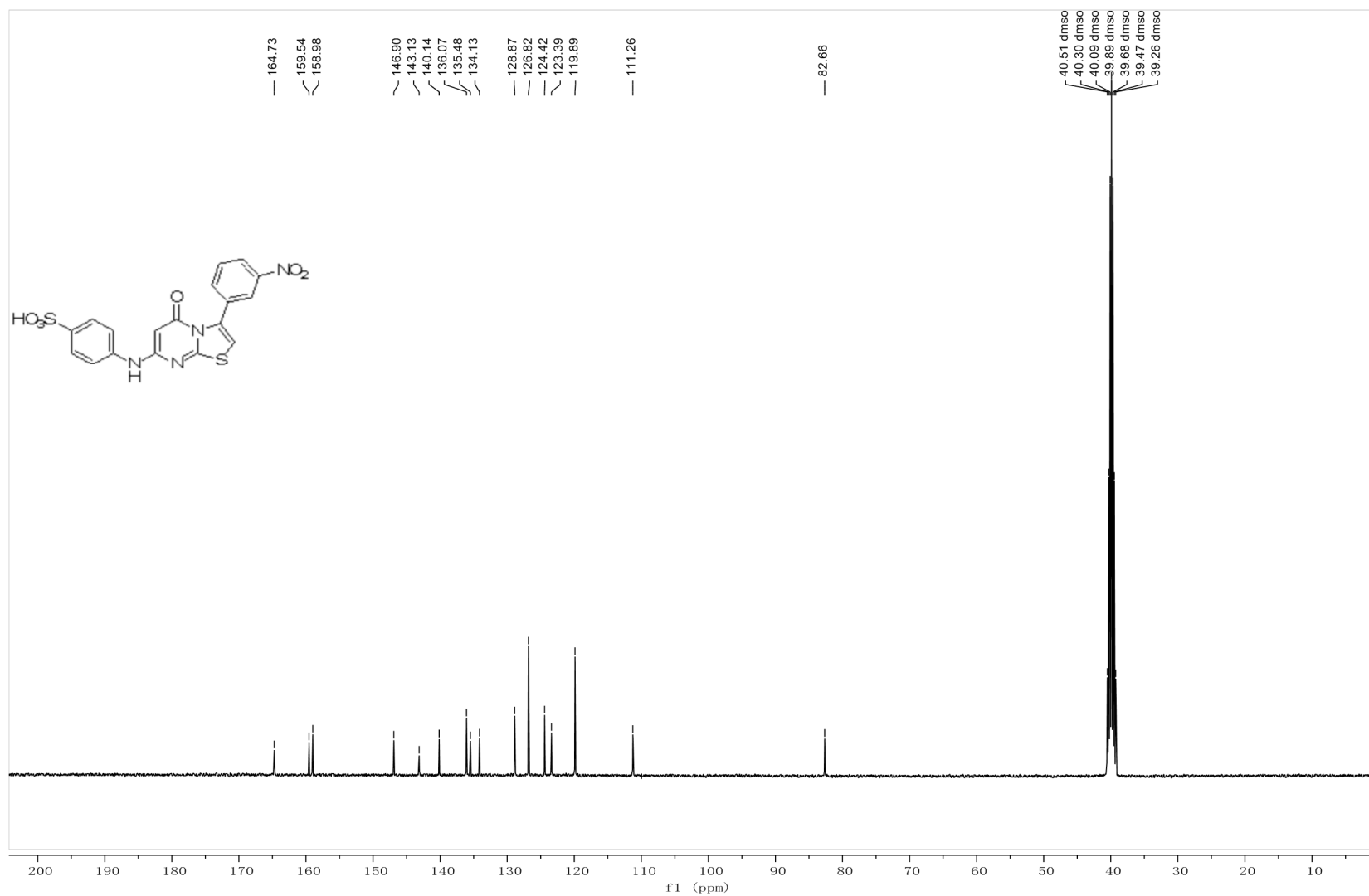


Figure S8. The ¹³C-NMR spectra of **3a**: 4-((3-(3-Nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

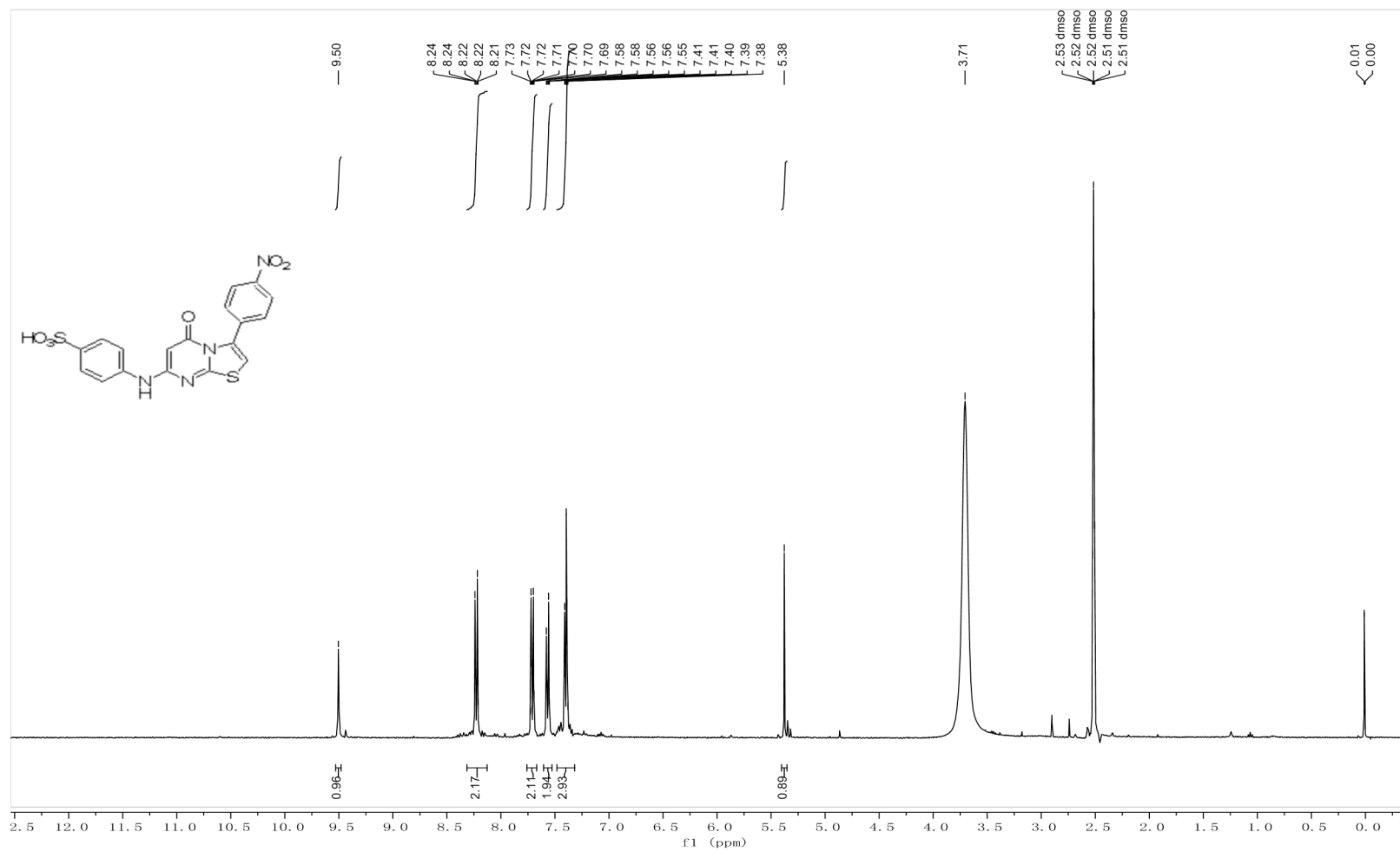


Figure S9. The ¹H-NMR spectra of **3b**: 4-((3-(4-Nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

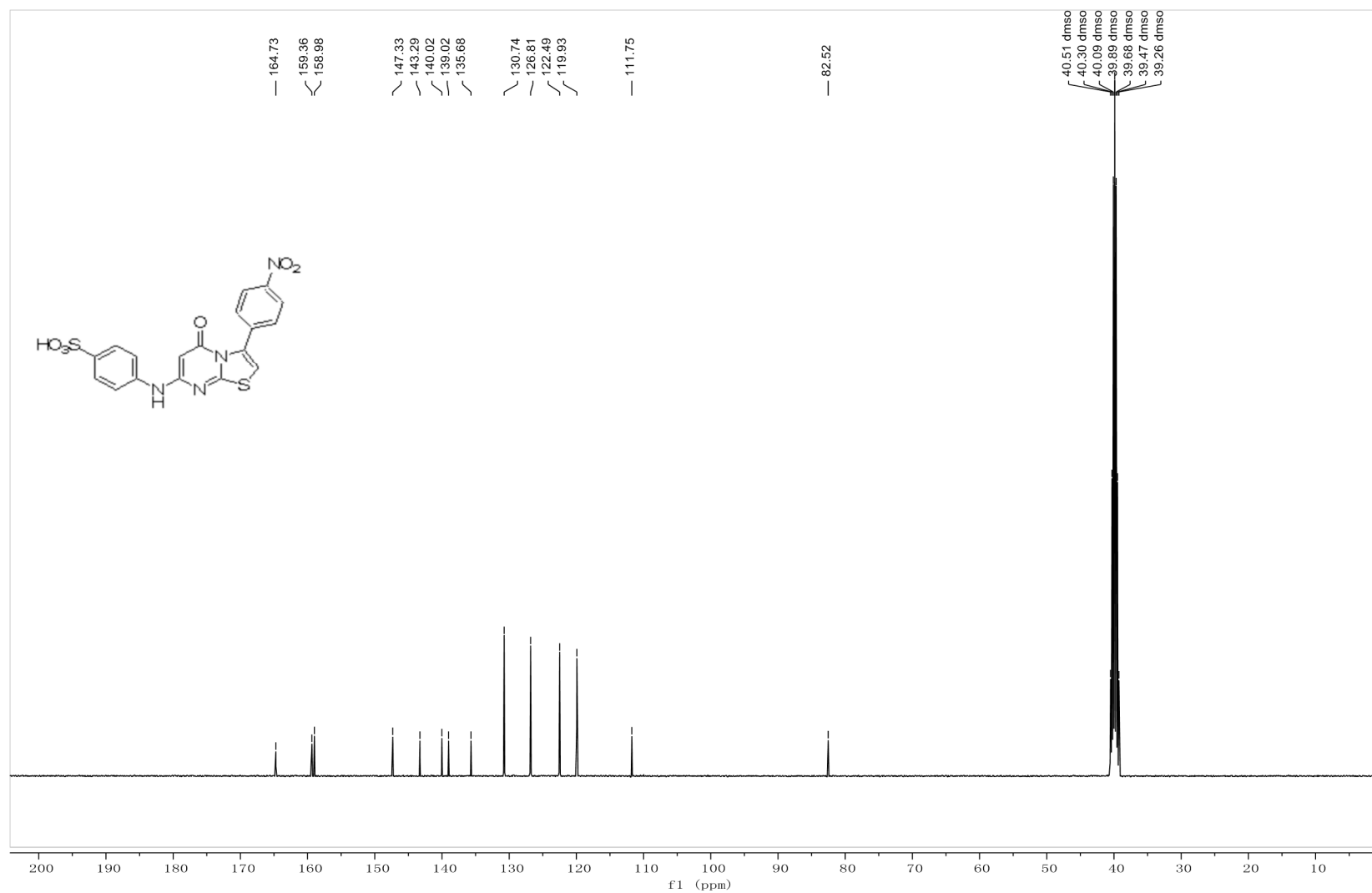


Figure S10. The ¹³C-NMR spectra of **3b**: 4-((3-(4-Nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

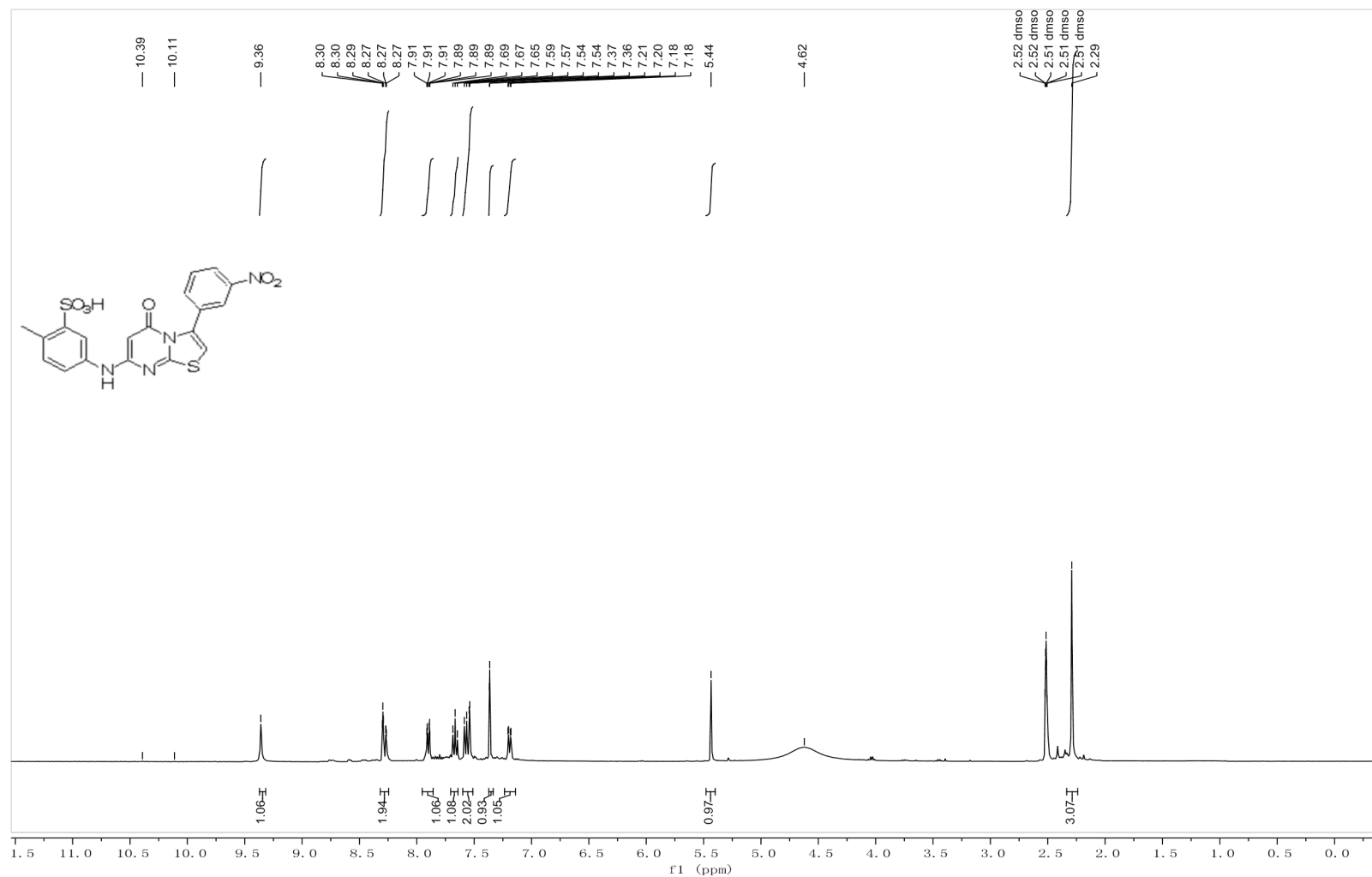


Figure S11. The ¹H-NMR spectra of **3c**: 2-Methyl-5-((3-(3-nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

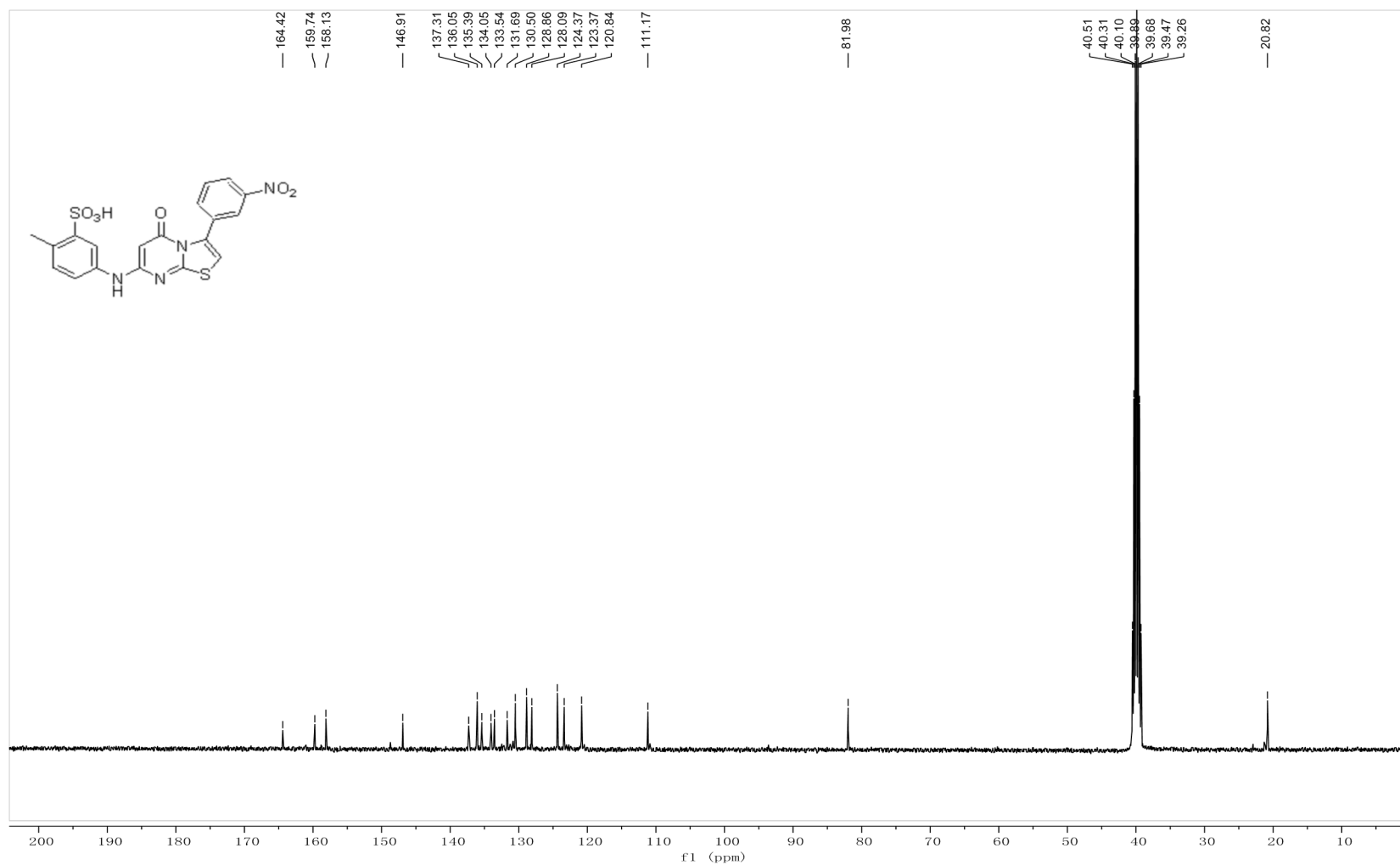


Figure S12. The ¹³C-NMR spectra of **3c**: 2-Methyl-5-((3-(3-nitrophenyl)-5-oxo-5*H*-thiazolo[3,2-*a*]pyrimidin-7-yl)amino)benzenesulfonic acid.

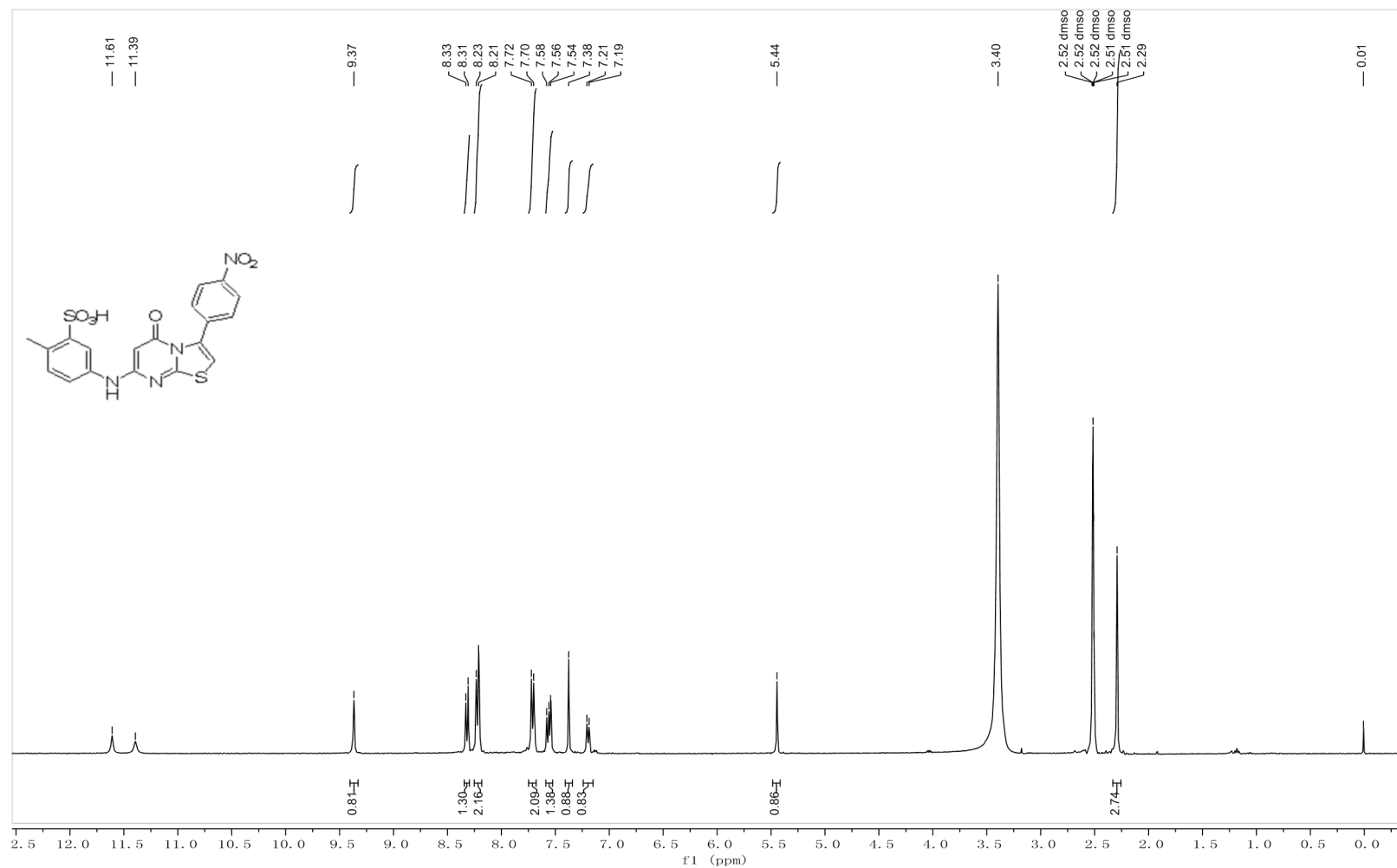


Figure S13. The ¹H-NMR spectra of **3d**: 2-Methyl-5-((3-(4-nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

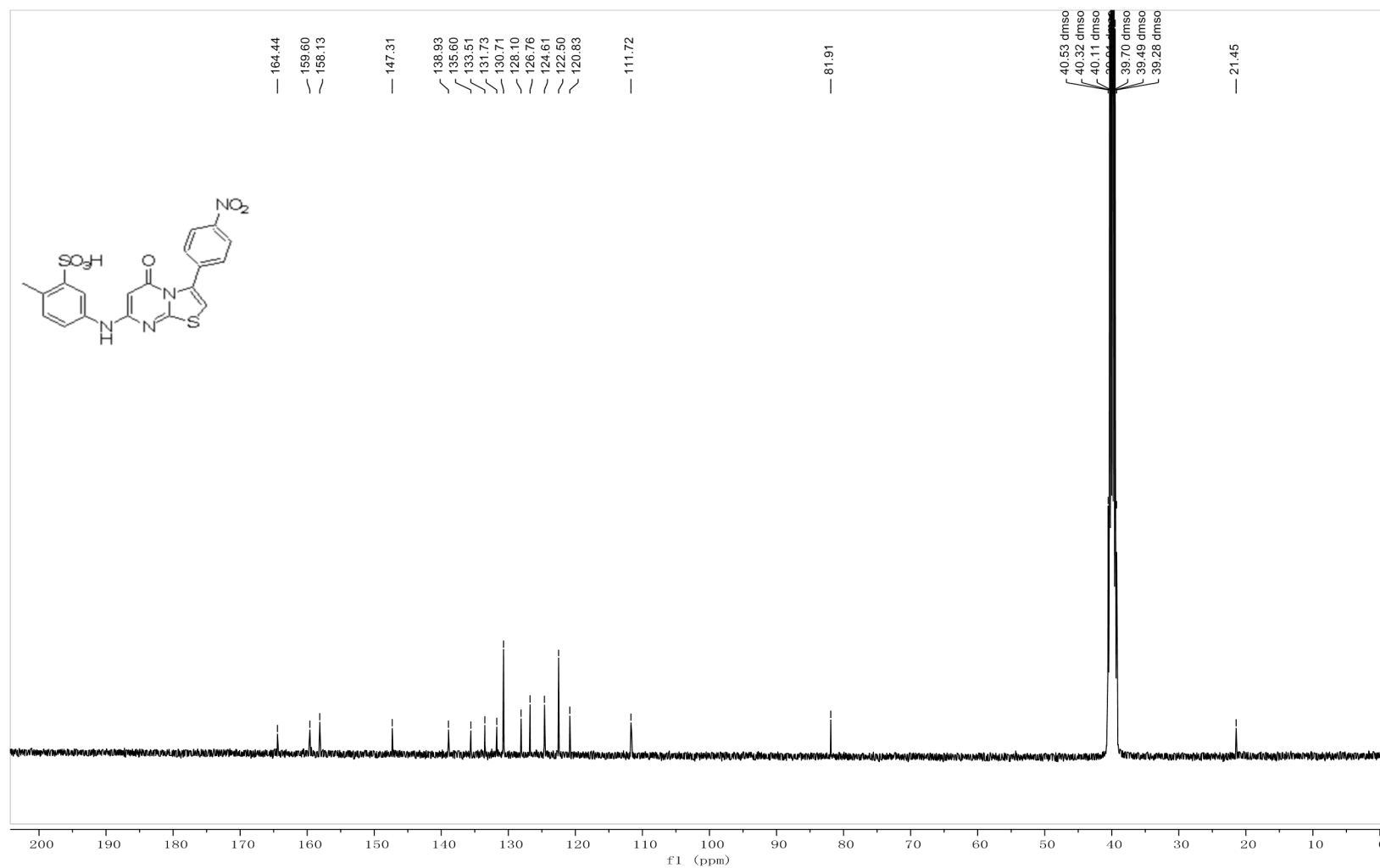


Figure S14. The ¹³C-NMR spectra of **3d**: 2-Methyl-5-((3-(4-nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

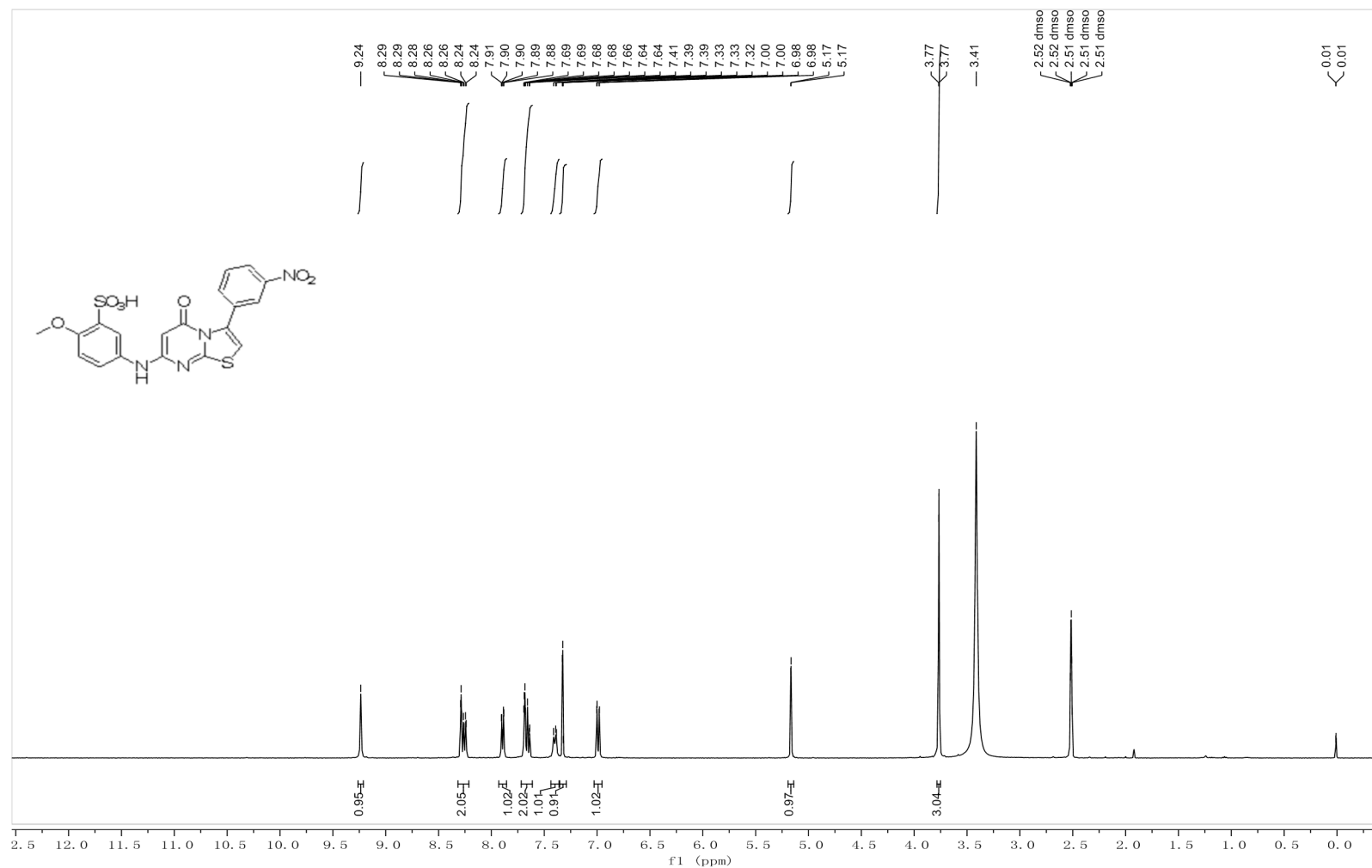


Figure S15. The ¹H-NMR spectra of **3e**: 2-Methoxy-5-((3-(3-nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

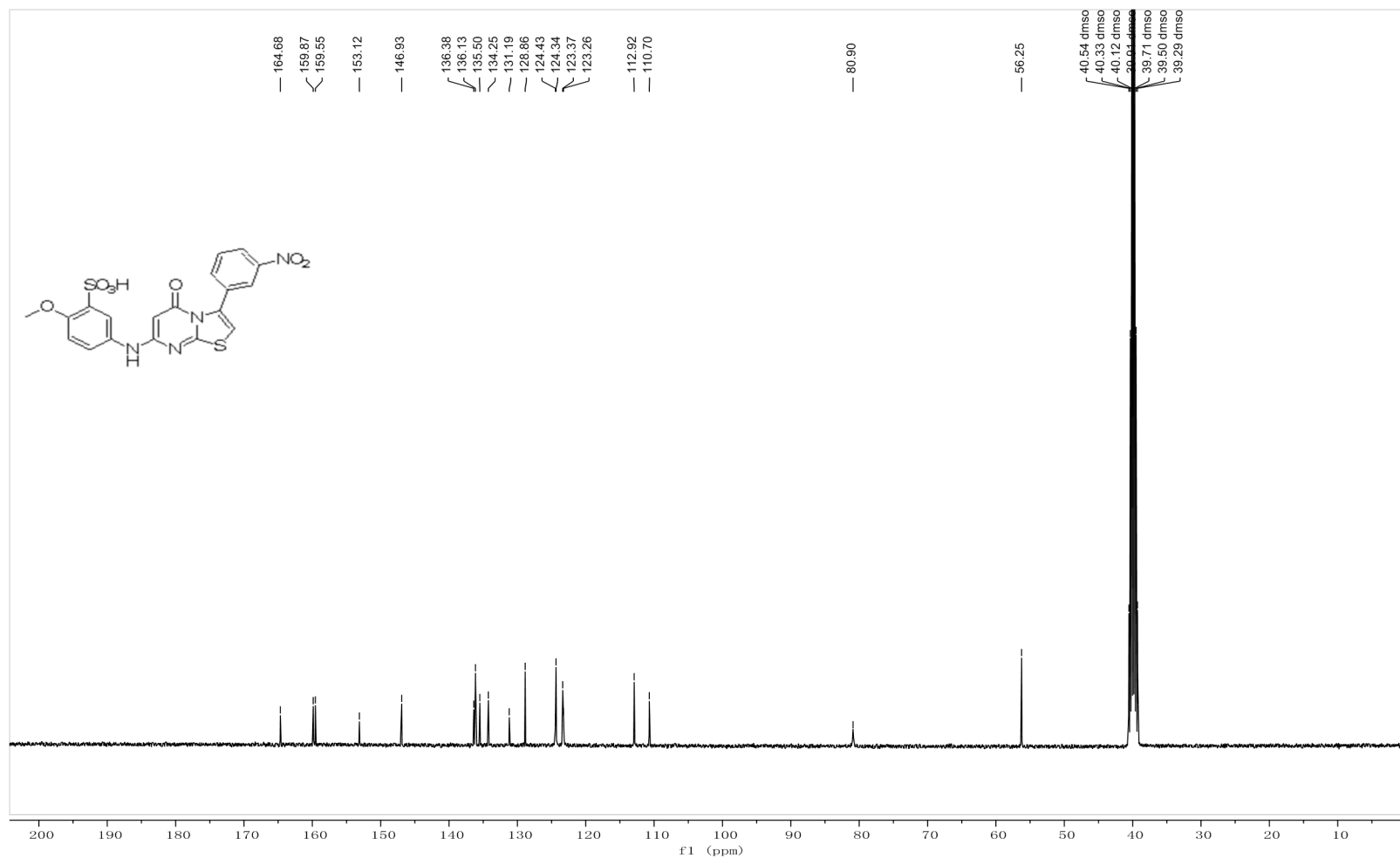


Figure S16. The ¹³C-NMR spectra of **3e**: 2-Methoxy-5-((3-(3-nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

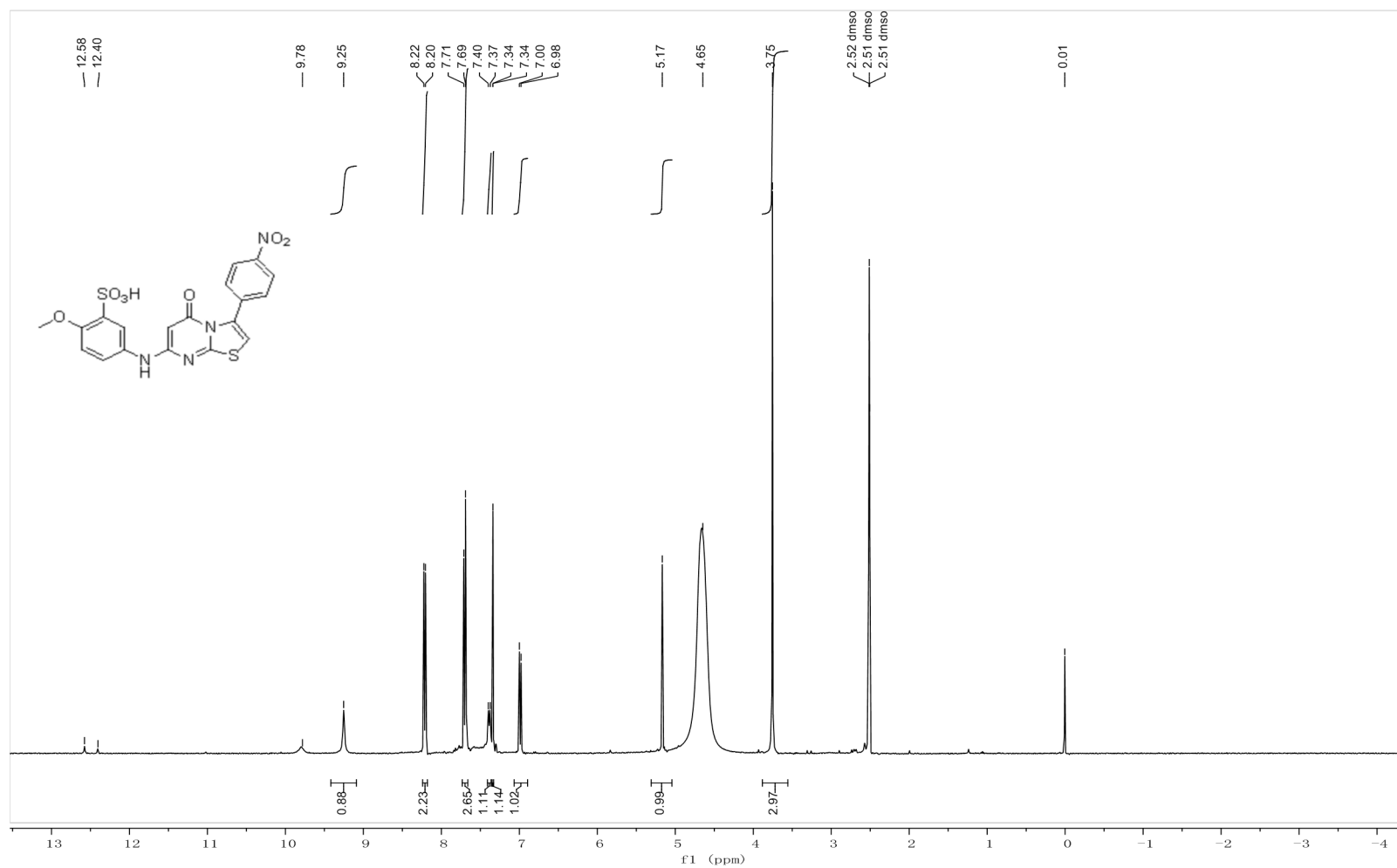


Figure S17. The ¹H-NMR spectra of **3f**: 2-Methoxy-5-((3-(4-nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

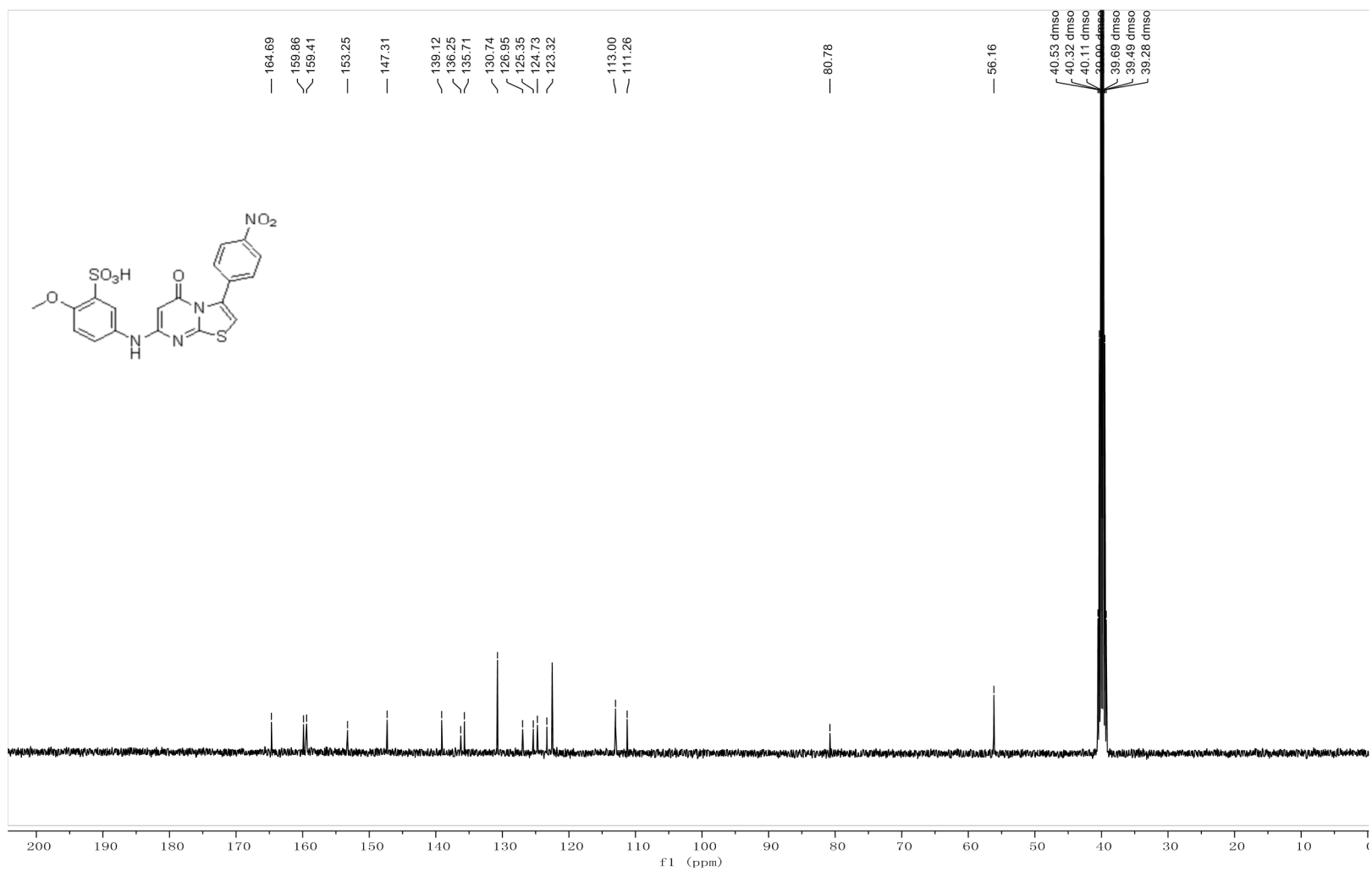


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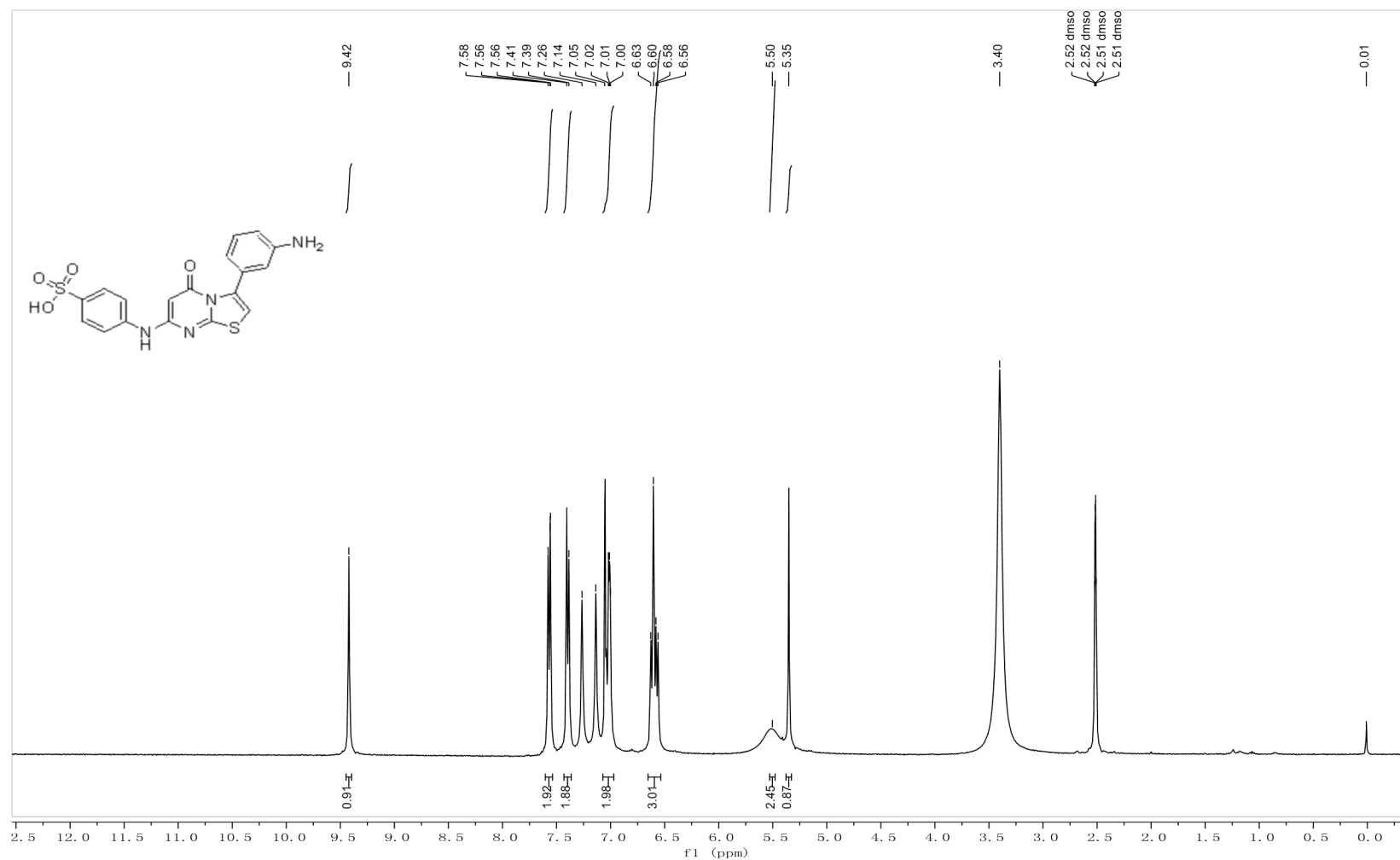


Figure S19. The ¹H-NMR spectra of **4a**: 4-((3-(3-Aminophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

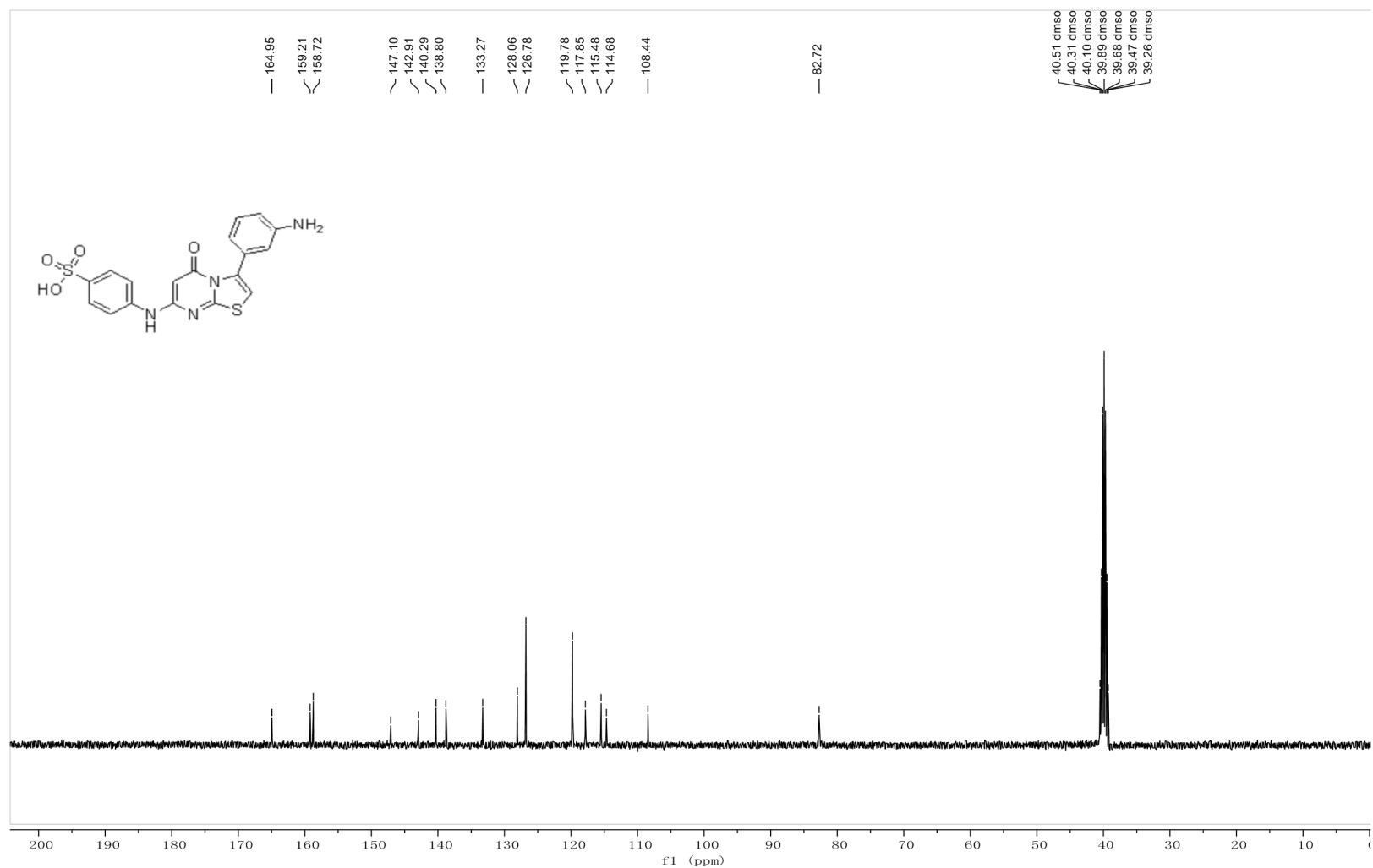


Figure S20. The ¹³C-NMR spectra of **4a**: 4-((3-(3-Aminophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

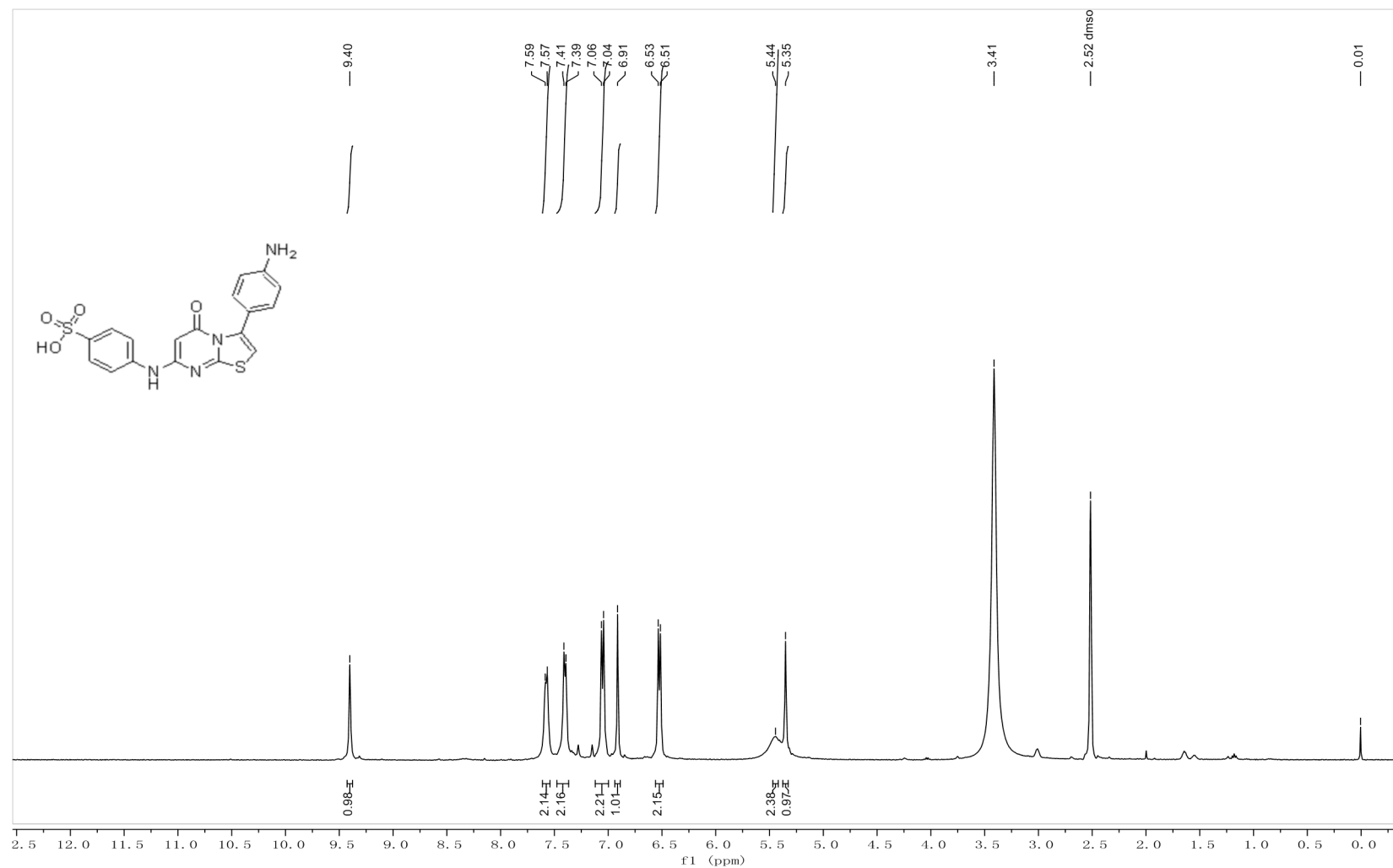


Figure S21. The ¹H-NMR spectra of **4b**: 4-((3-(4-Aminophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

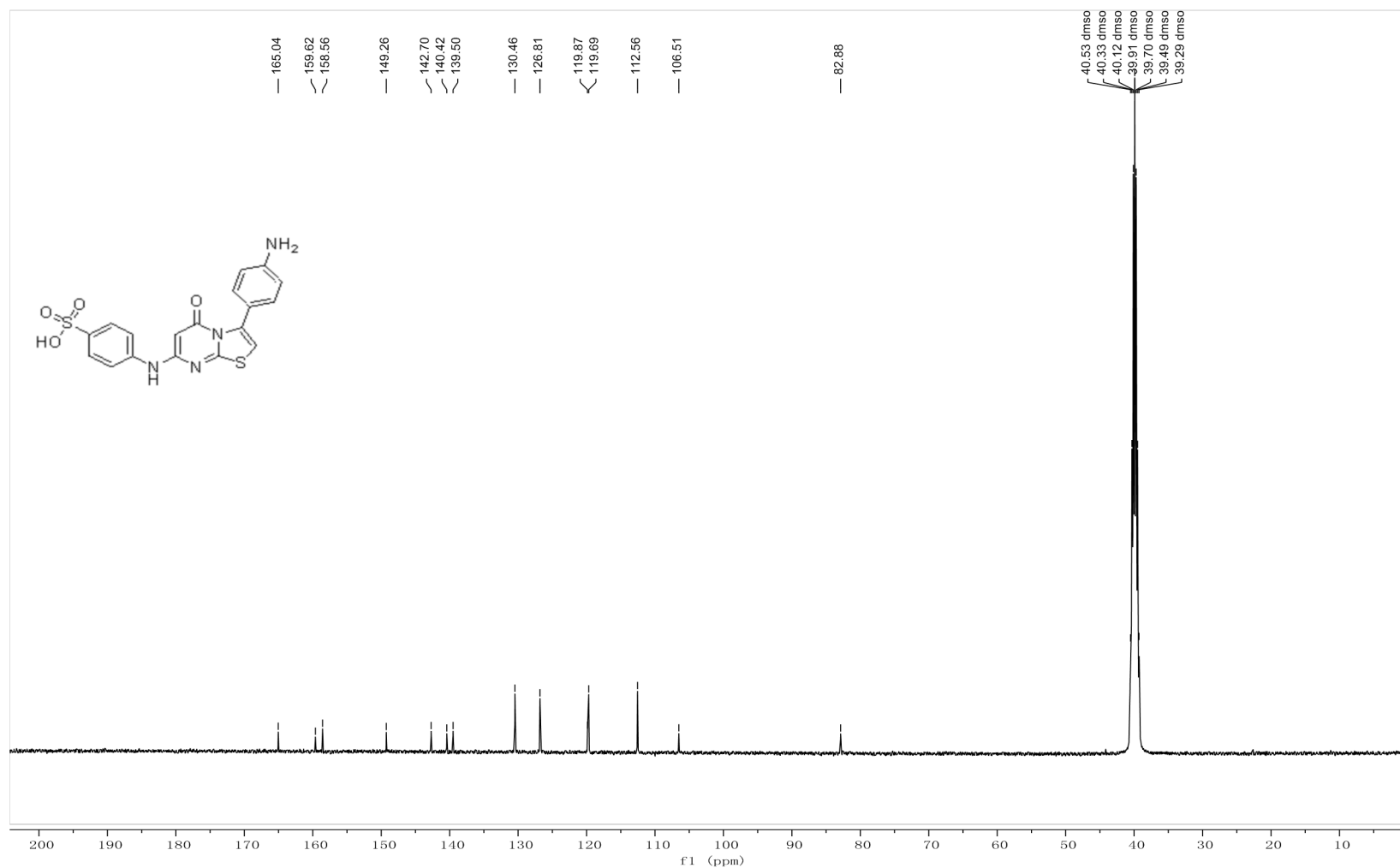


Figure S22. The ¹³C-NMR spectra of **4b**: 4-((3-(4-Aminophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

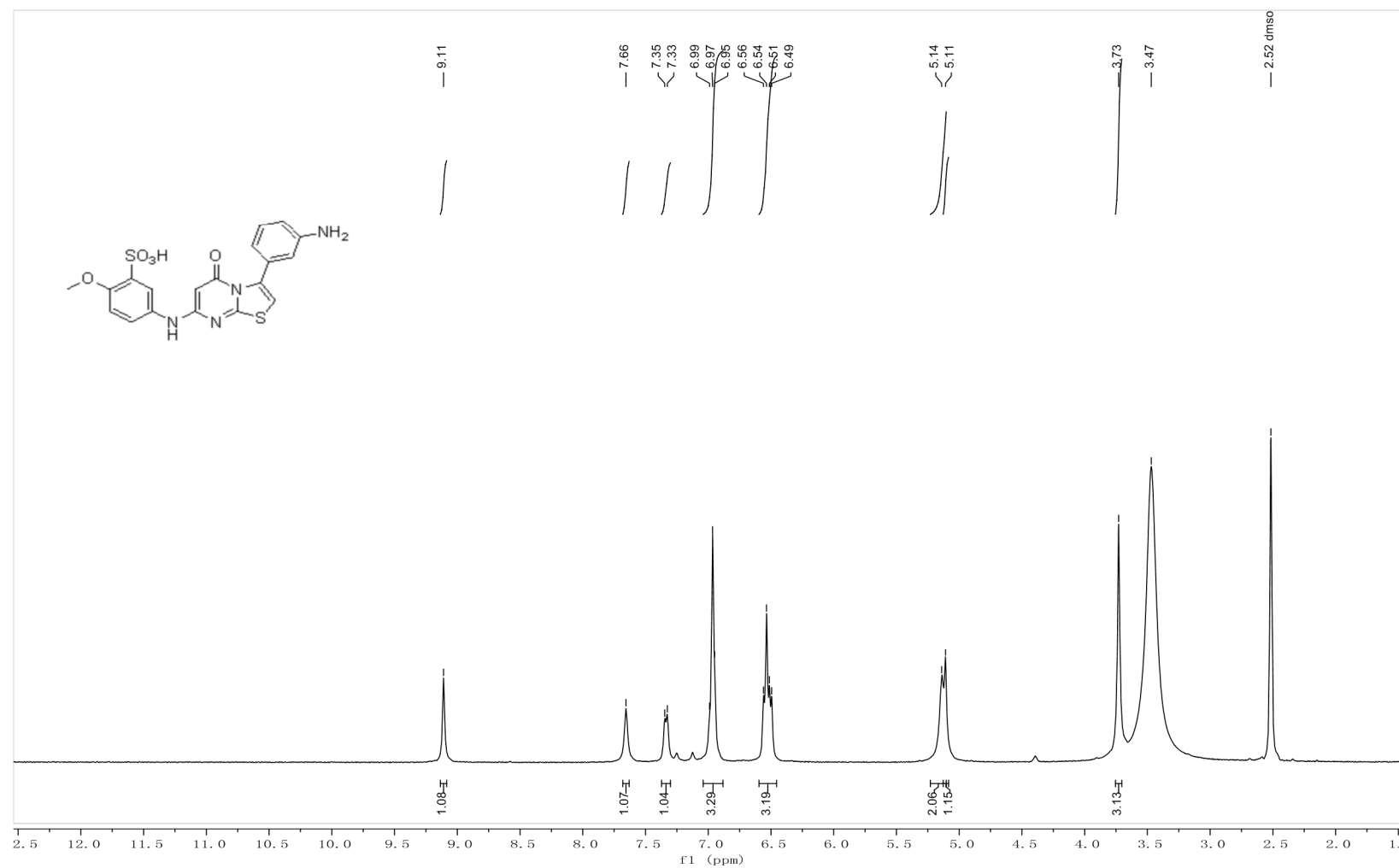


Figure S23. The ¹H-NMR spectra of **4c**: 5-((3-(3-Aminophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)-2-methoxybenzenesulfonic acid.

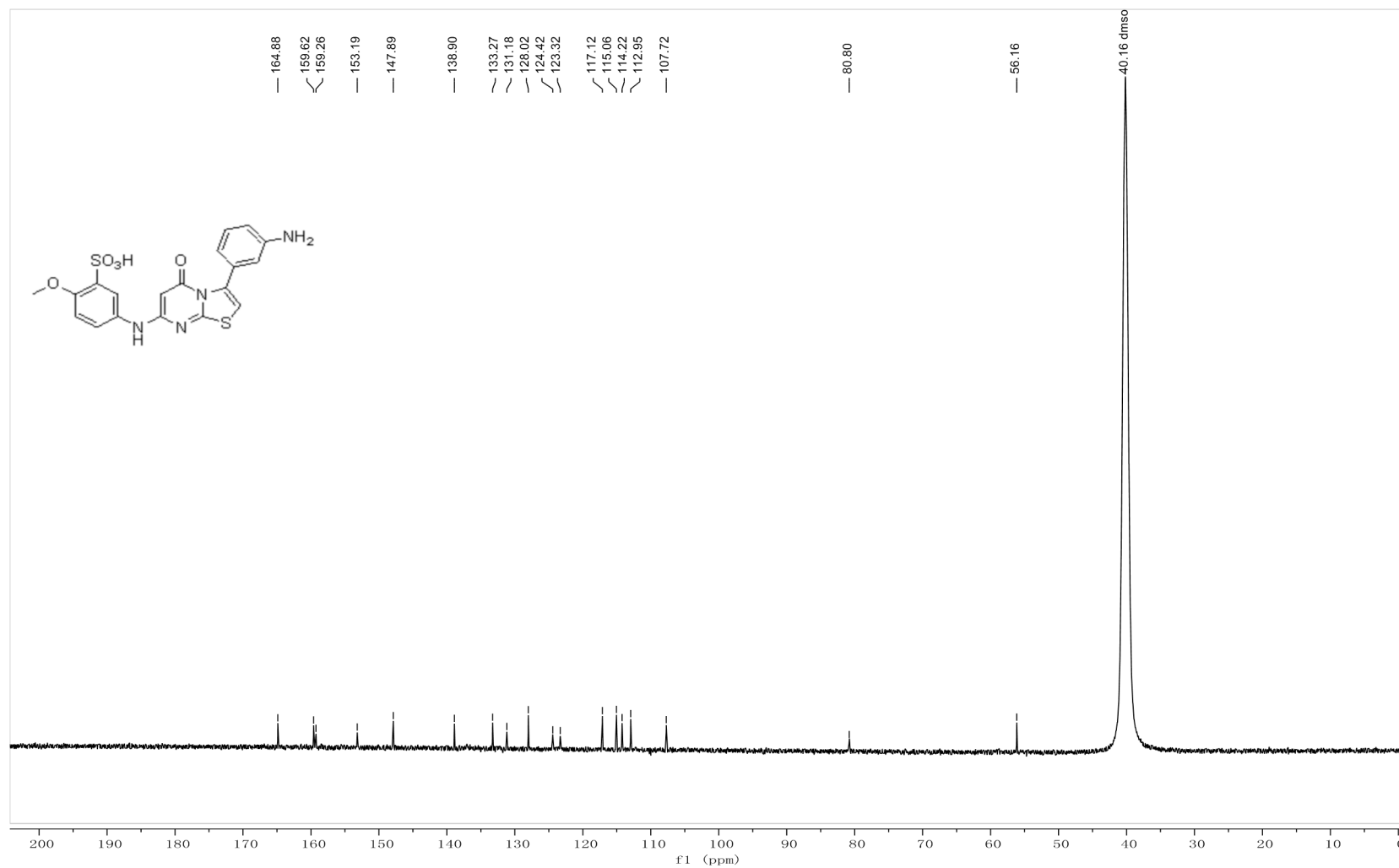


Figure S24. The ^{13}C -NMR spectra of **4c**: 5-((3-(3-Aminophenyl)-5-oxo-5*H*-thiazolo[3,2-*a*]pyrimidin-7-yl)amino)-2-methoxybenzenesulfonic acid.

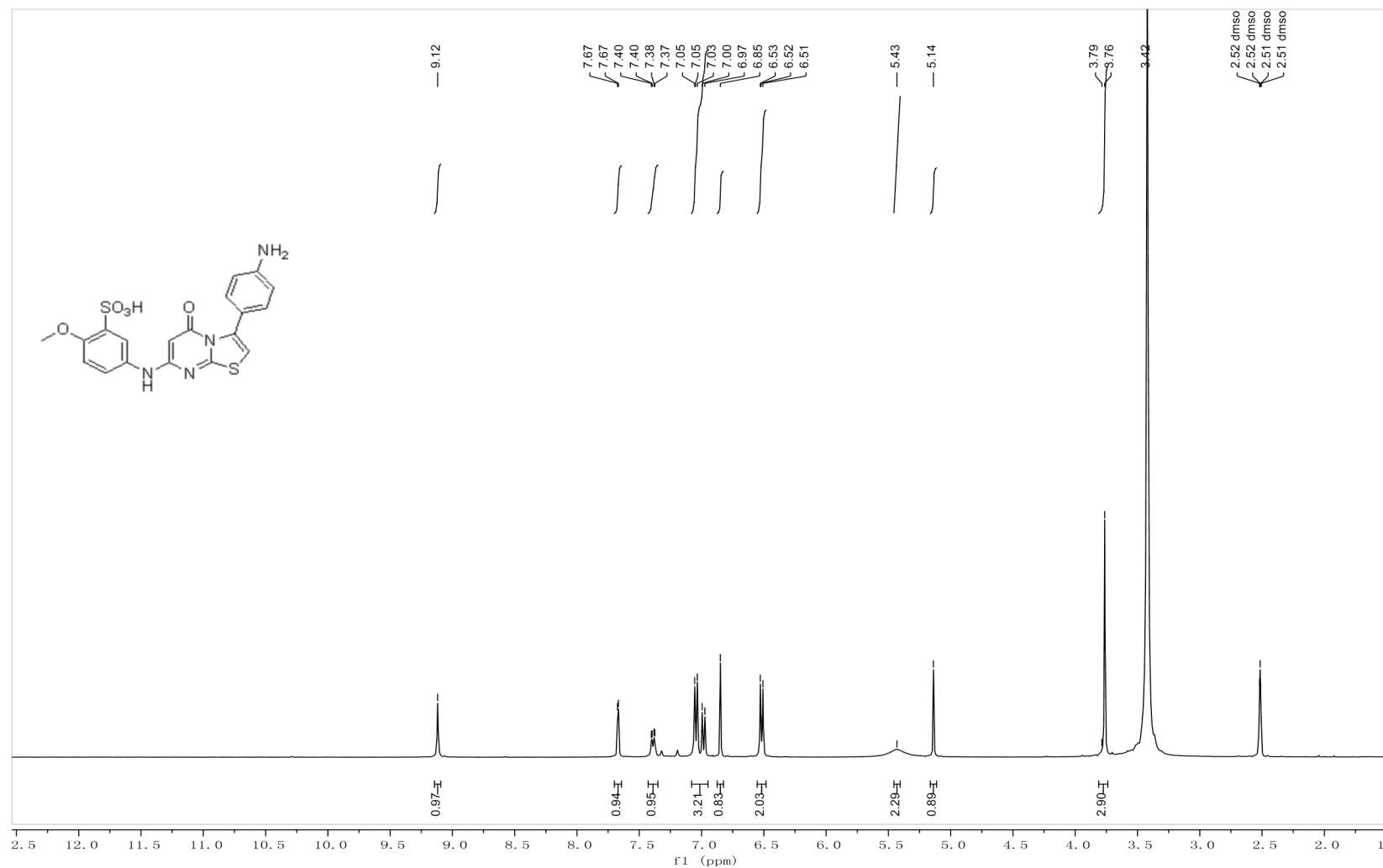


Figure S25. The ¹H-NMR spectra of **4d**: 5-((3-(4-Aminophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)-2-methoxybenzenesulfonic acid.

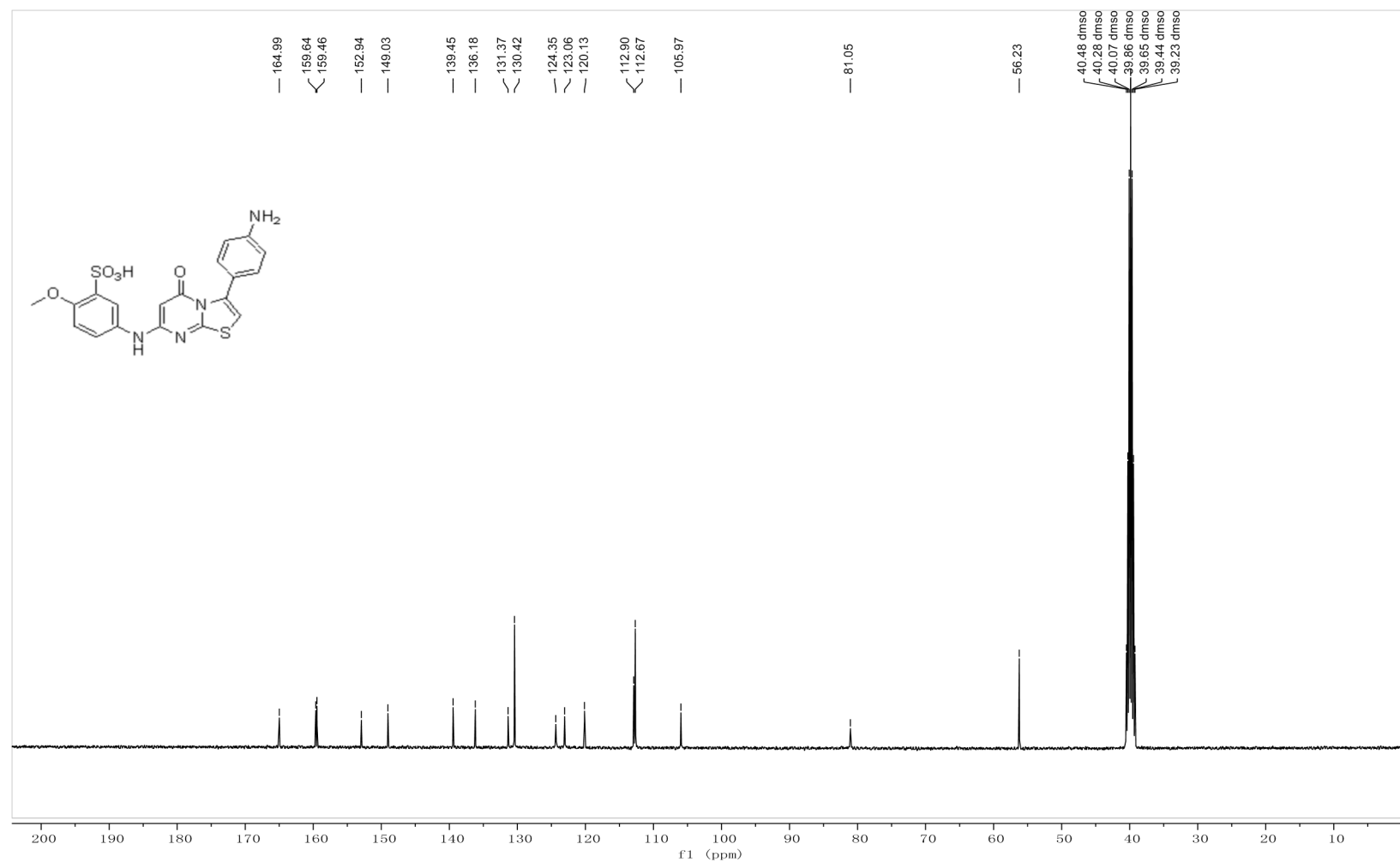


Figure S26. The ¹³C-NMR spectra of **4d**: 5-((3-(4-Aminophenyl)-5-oxo-5*H*-thiazolo[3,2-*a*]pyrimidin-7-yl)amino)-2-methoxybenzenesulfonic acid.

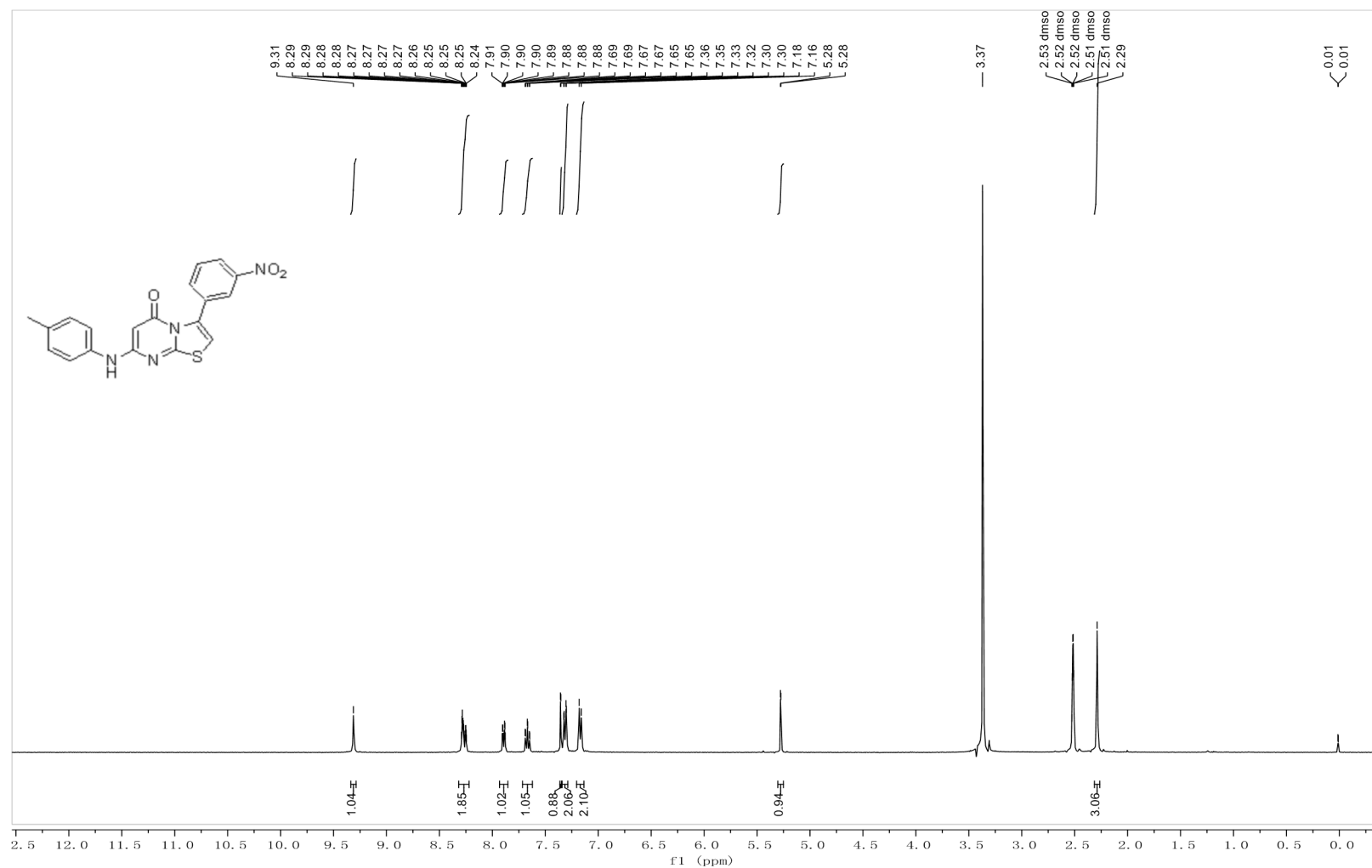


Figure S27. The ¹H-NMR spectra of **5a**: 3-(4-Nitrophenyl)-7-(*p*-tolylamino)-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one.

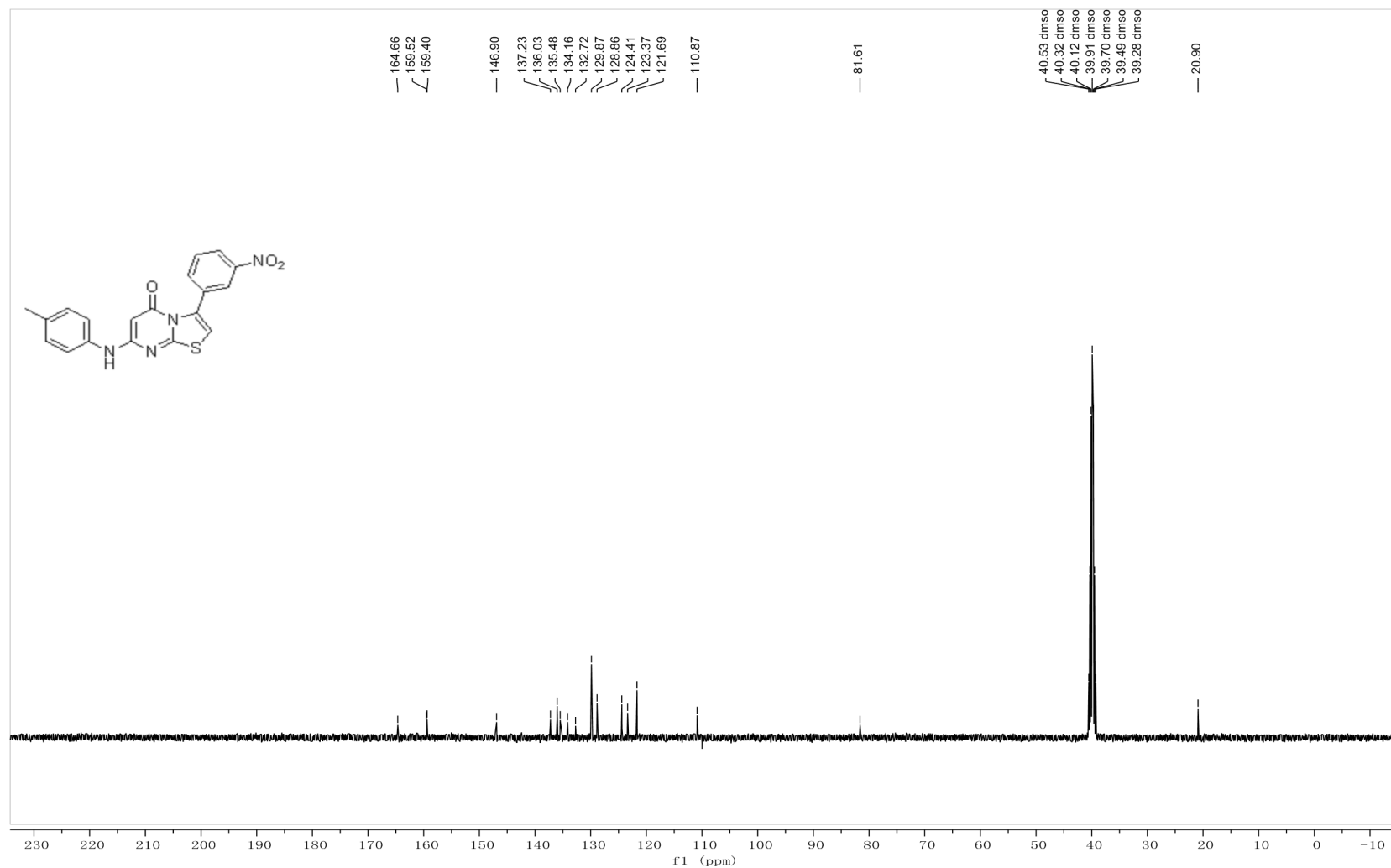


Figure S28. The ¹³C-NMR spectra of **5a**: 3-(4-Nitrophenyl)-7-(*p*-tolylamino)-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one.

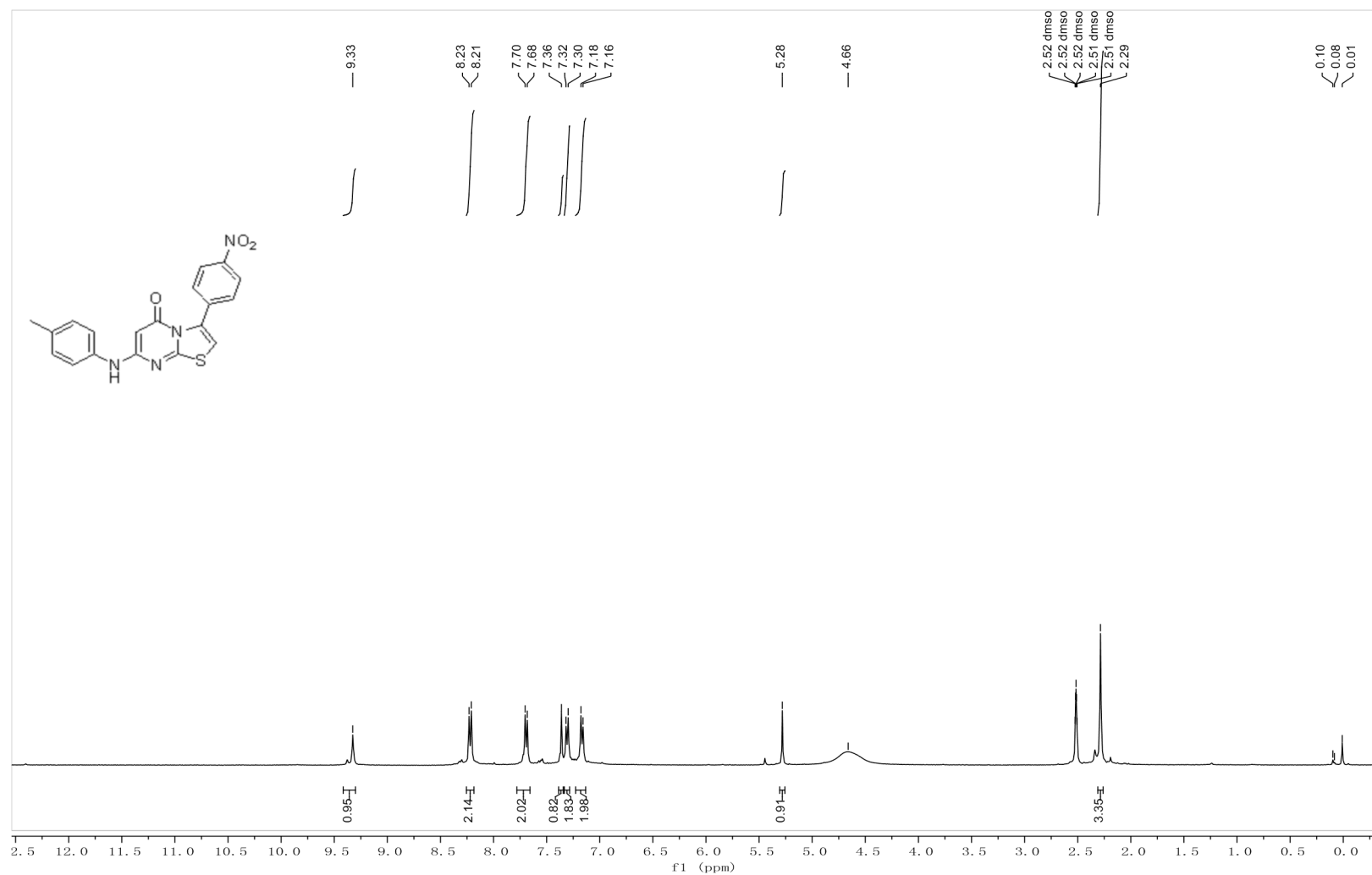


Figure S29. The ¹H-NMR spectra of **5b**: 3-(4-Nitrophenyl)-7-(*p*-tolylamino)-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one.

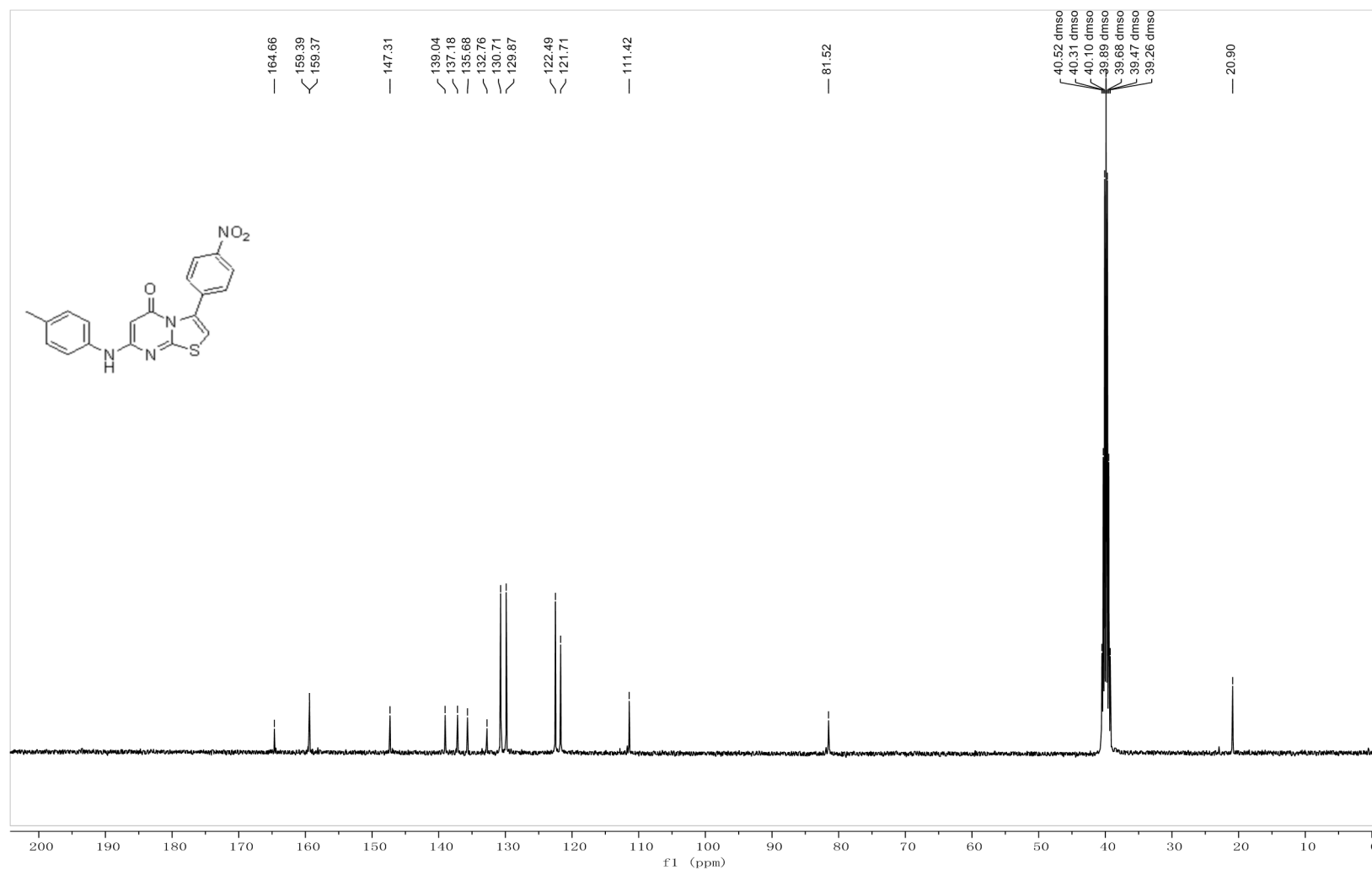


Figure S30. The ¹³C-NMR spectra of **5b**: 3-(4-Nitrophenyl)-7-(*p*-tolylamino)-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one.

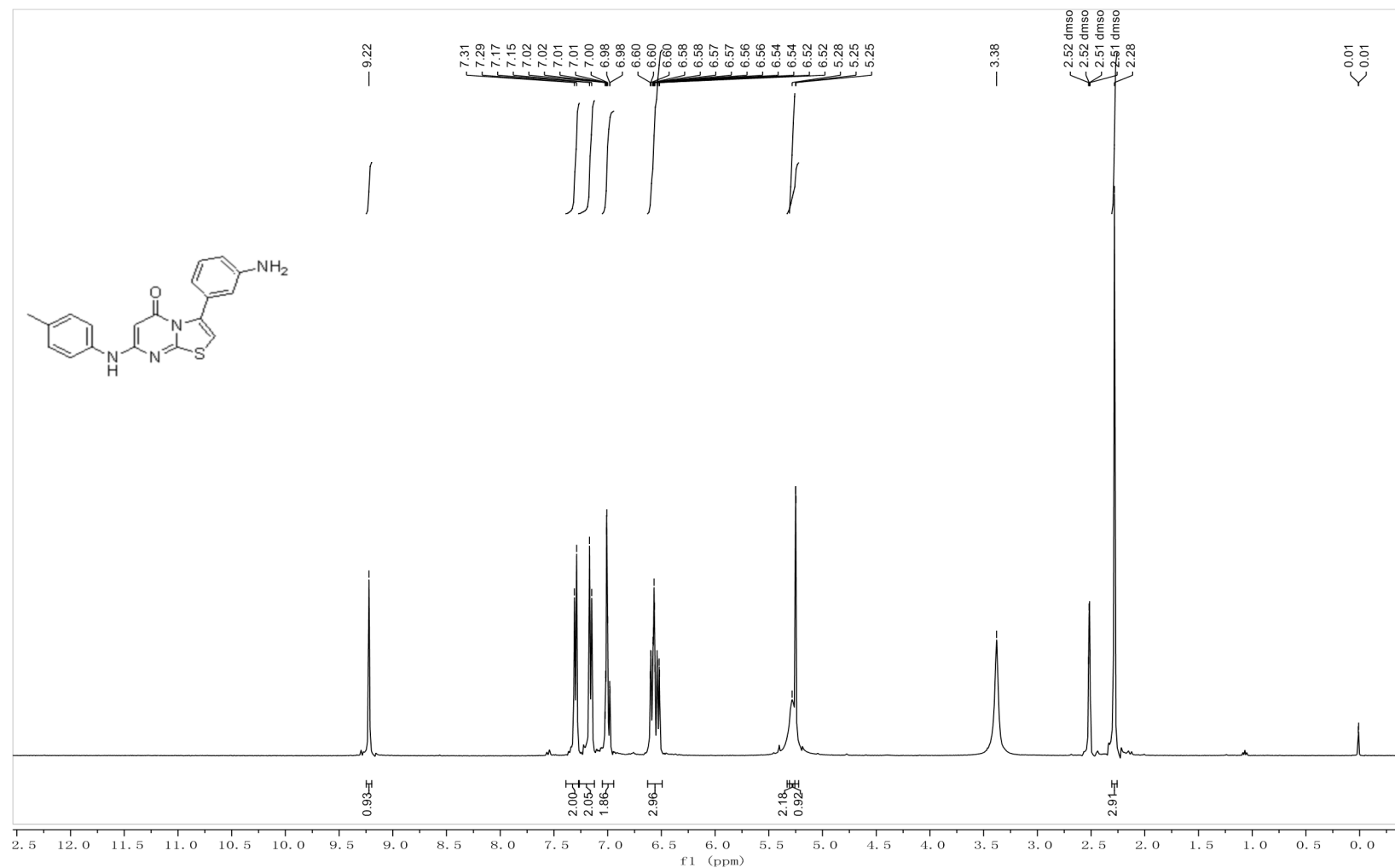


Figure S31. The ¹H-NMR spectra of **6a**: 3-(3-Aminophenyl)-7-(*p*-tolylamino)-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one.

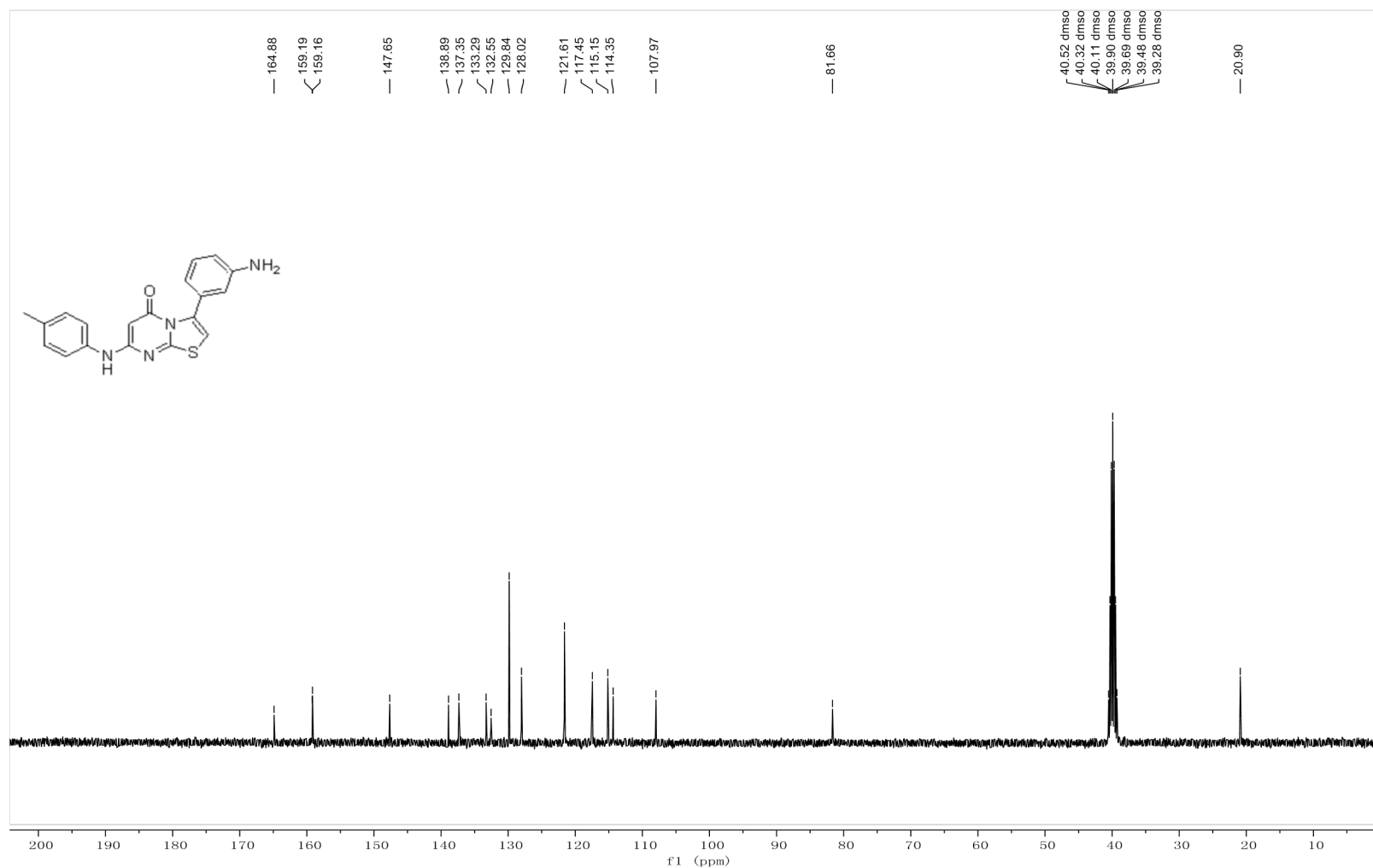


Figure S32. The ¹³C-NMR spectra of **6a**: 3-(3-Aminophenyl)-7-(*p*-tolylamino)-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one.

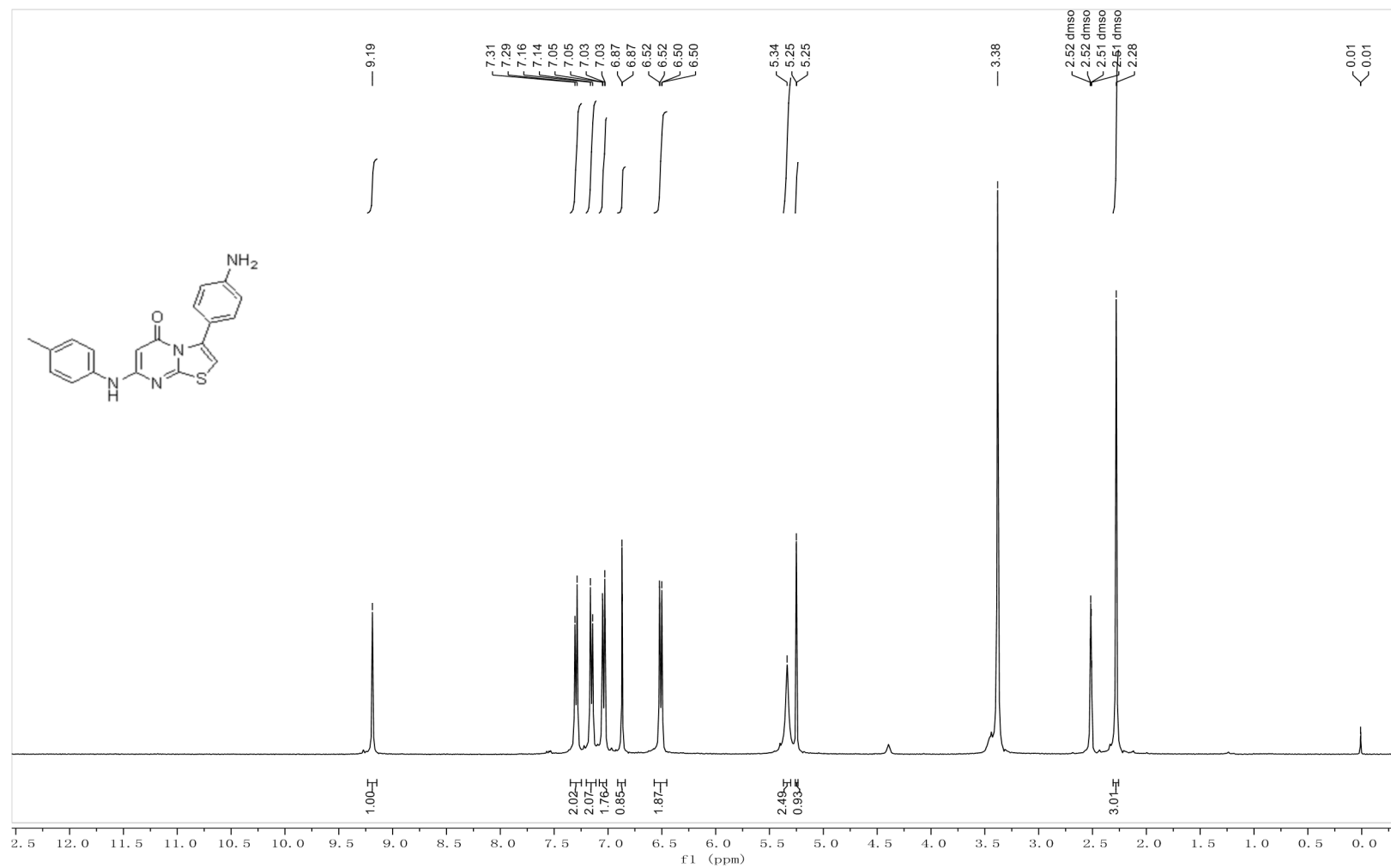


Figure S33. The ^1H -NMR spectra of **6b**: 3-(4-Aminophenyl)-7-(*p*-tolylamino)-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one.

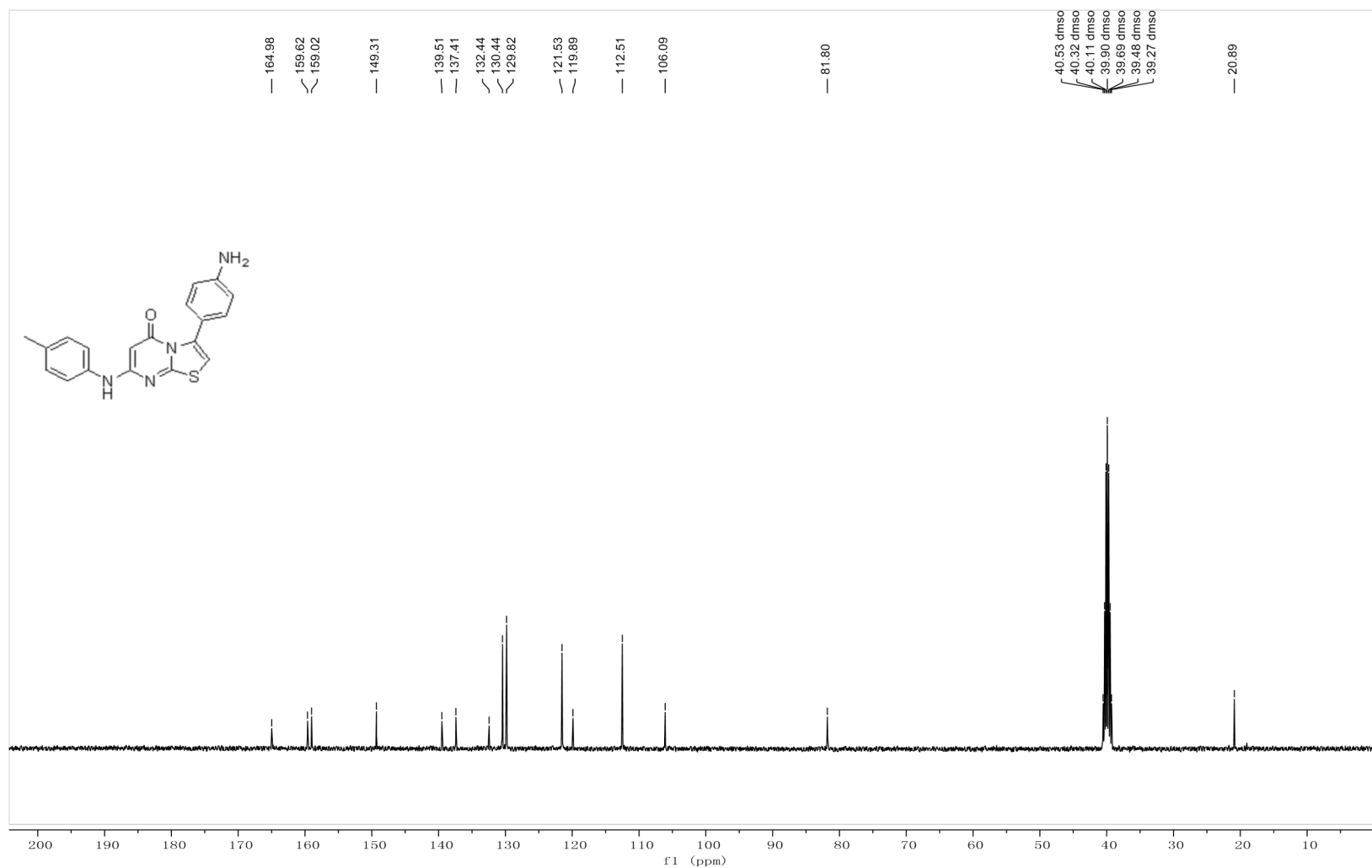


Figure S34. The ¹³C-NMR spectra of **6b**: 3-(4-Aminophenyl)-7-(*p*-tolylamino)-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one.

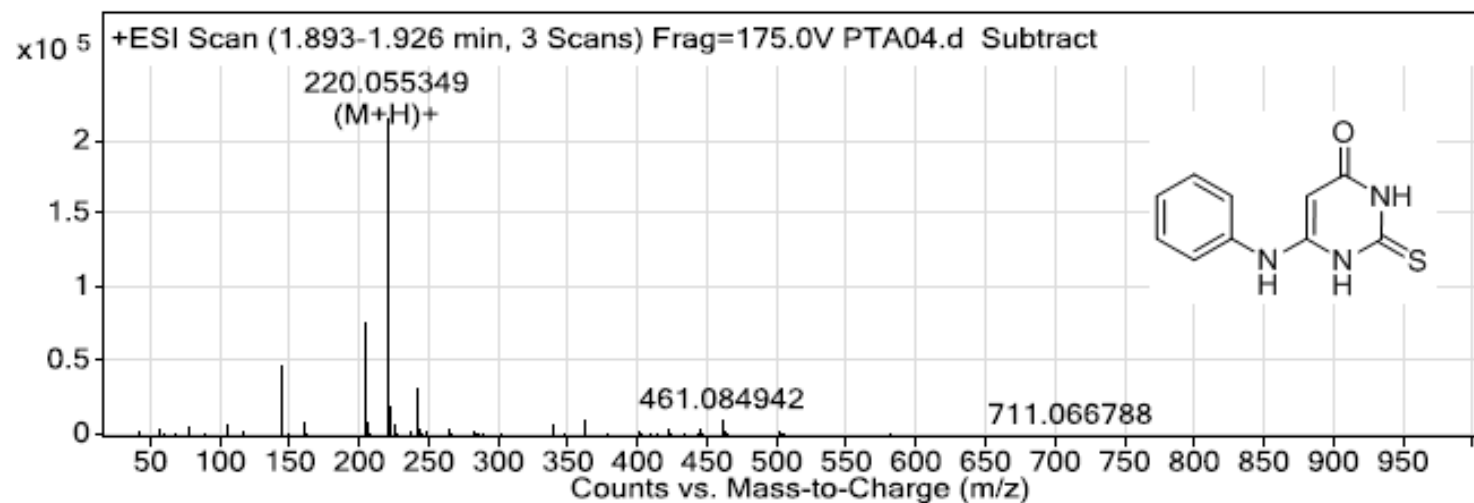


Figure S35. The HRMS spectra of **1a**: 6-(Phenylamino)-2-thioxo-2,3-dihydropyrimidin-4(1H)-one.

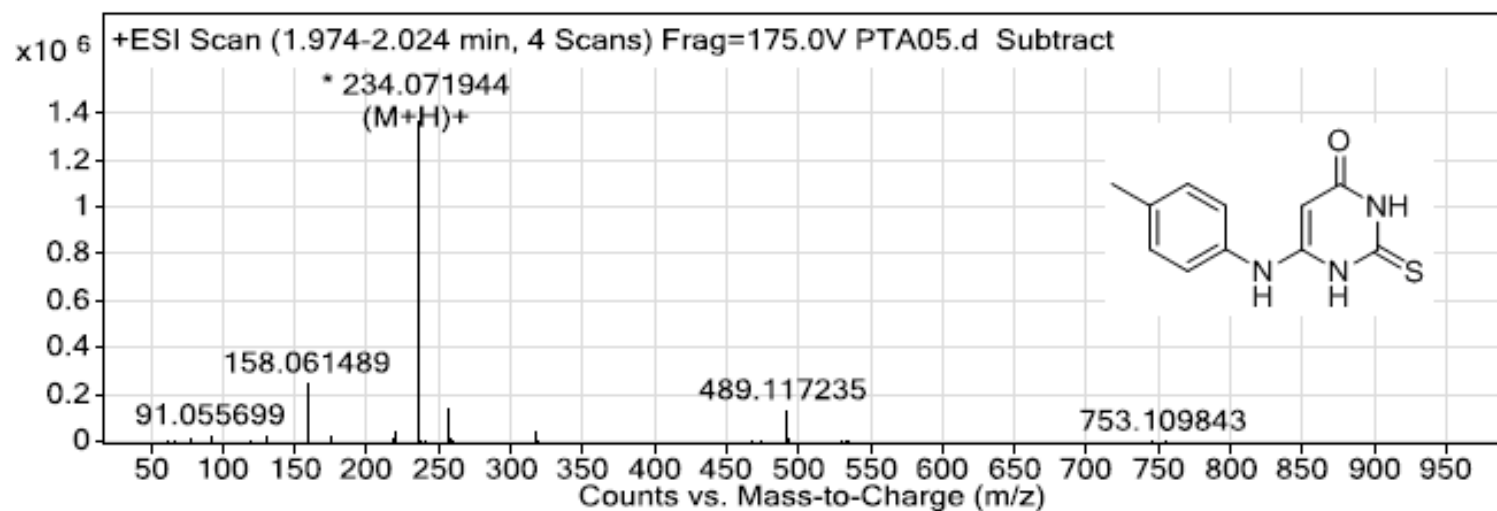


Figure S36. The HRMS spectra of **1b**: 2-Thioxo-6-(p-tolylamino)-2,3-dihydropyrimidin-4(1H)-one.

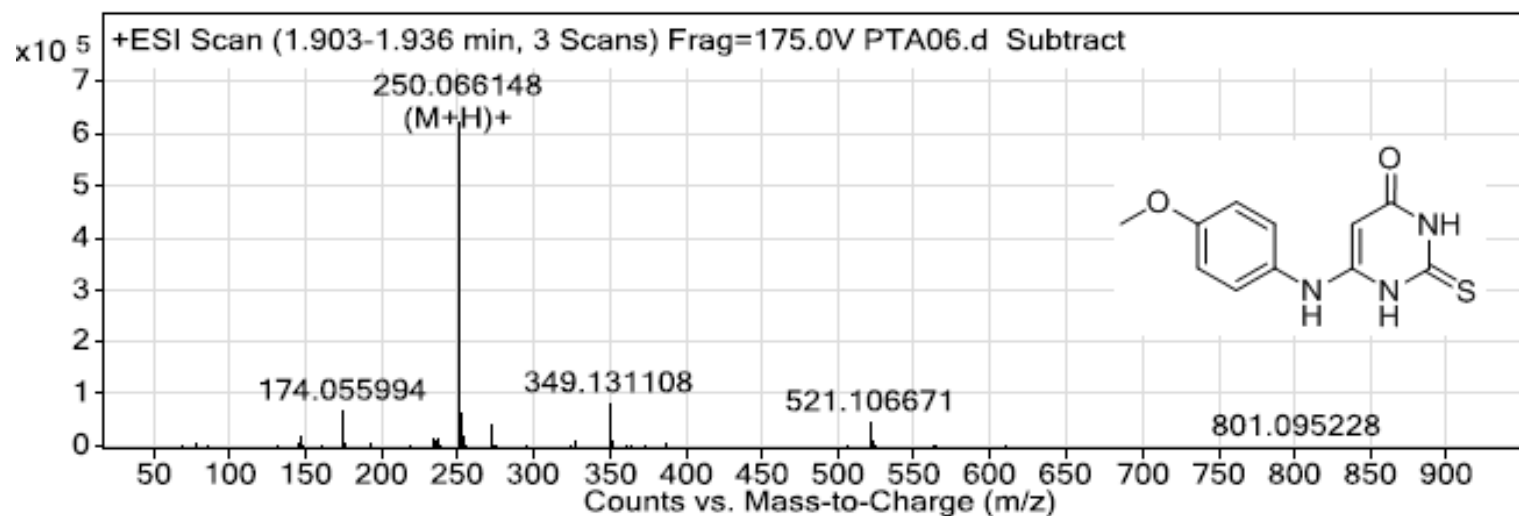


Figure S37. The HRMS spectra of **1c**: 6-((4-Methoxyphenyl)amino)-2-thioxo-2,3-dihydropyrimidin-4(1H)-one.

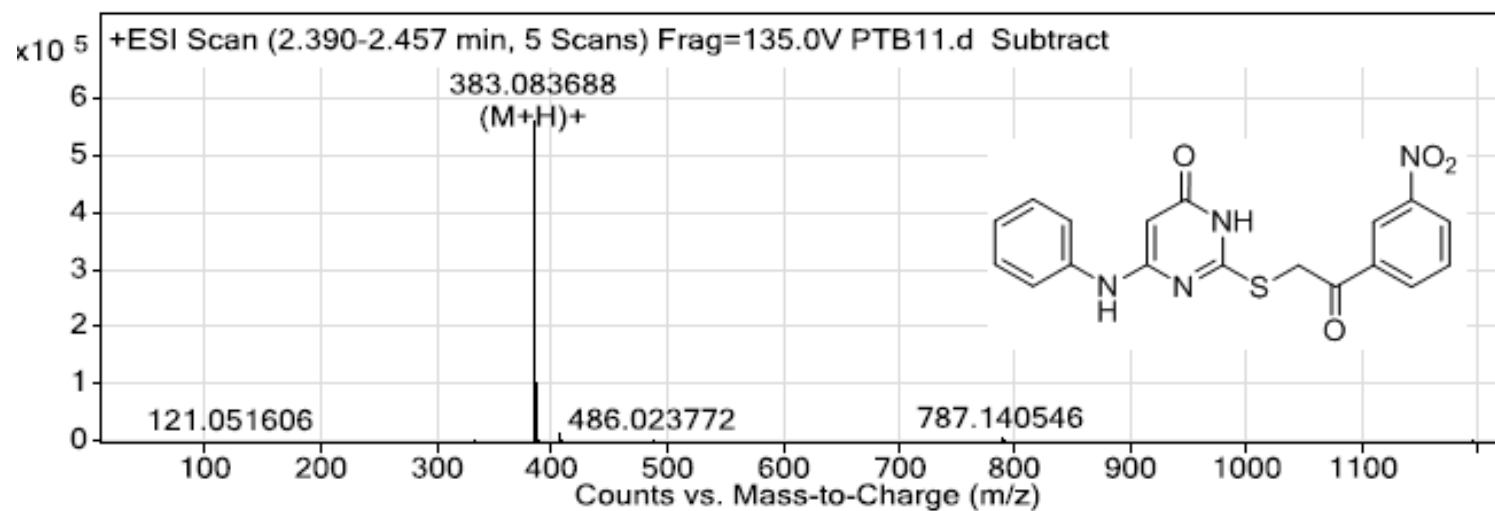


Figure S38. The HRMS spectra of **2a**: 2-((2-(3-Nitrophenyl)-2-oxoethyl)thio)-6-(phenylamino)pyrimidin-4(3H)-one.

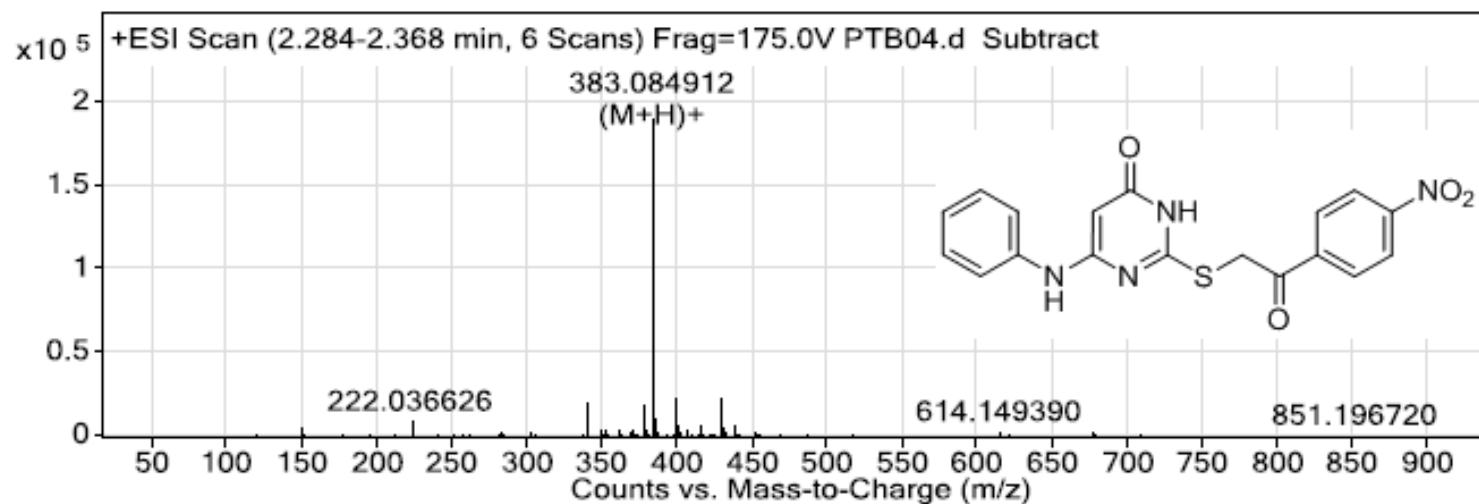


Figure S39. The HRMS spectra of **2b**: 2-((2-(4-Nitrophenyl)-2-oxoethyl)thio)-6-(phenylamino)pyrimidin-4(3*H*)-one.

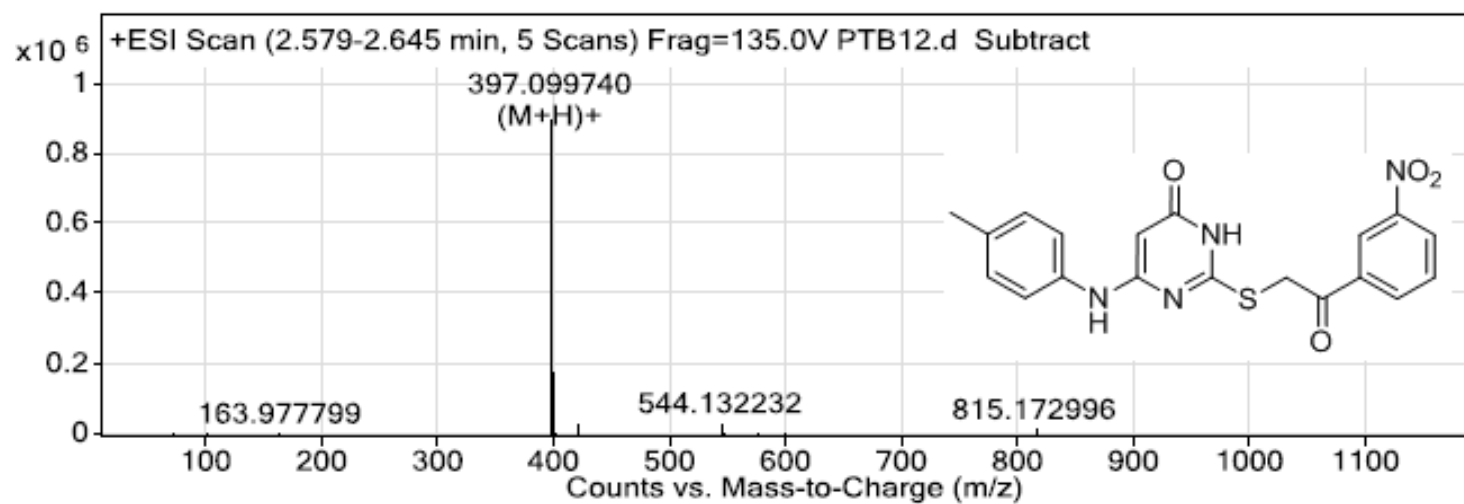


Figure S40. The HRMS spectra of **2c**: 2-((2-(3-Nitrophenyl)-2-oxoethyl)thio)-6-(*p*-tolylamino)pyrimidin-4(3*H*)-one.

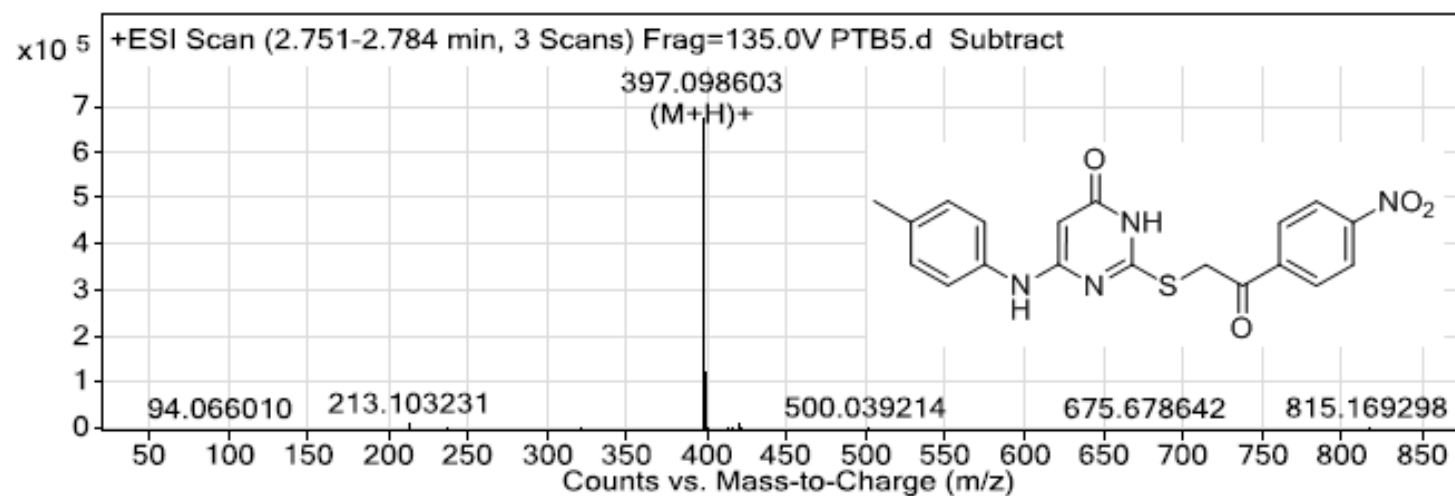


Figure 41S. The HRMS spectra of **2d**: 2-((2-(4-Nitrophenyl)-2-oxoethyl)thio)-6-(*p*-tolylamino)pyrimidin-4(3*H*)-one.

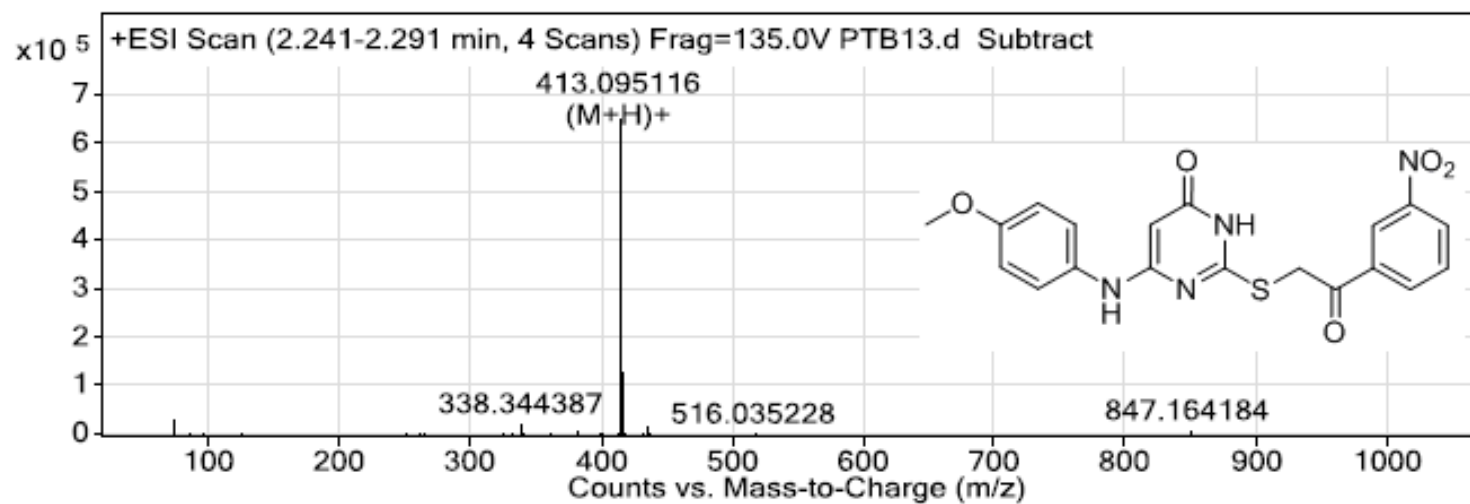


Figure S42. The HRMS spectra of **2e**: 6-((4-Methoxyphenyl)amino)-2-((2-(3-nitrophenyl)-2-oxoethyl)thio)pyrimidin-4(3*H*)-one.

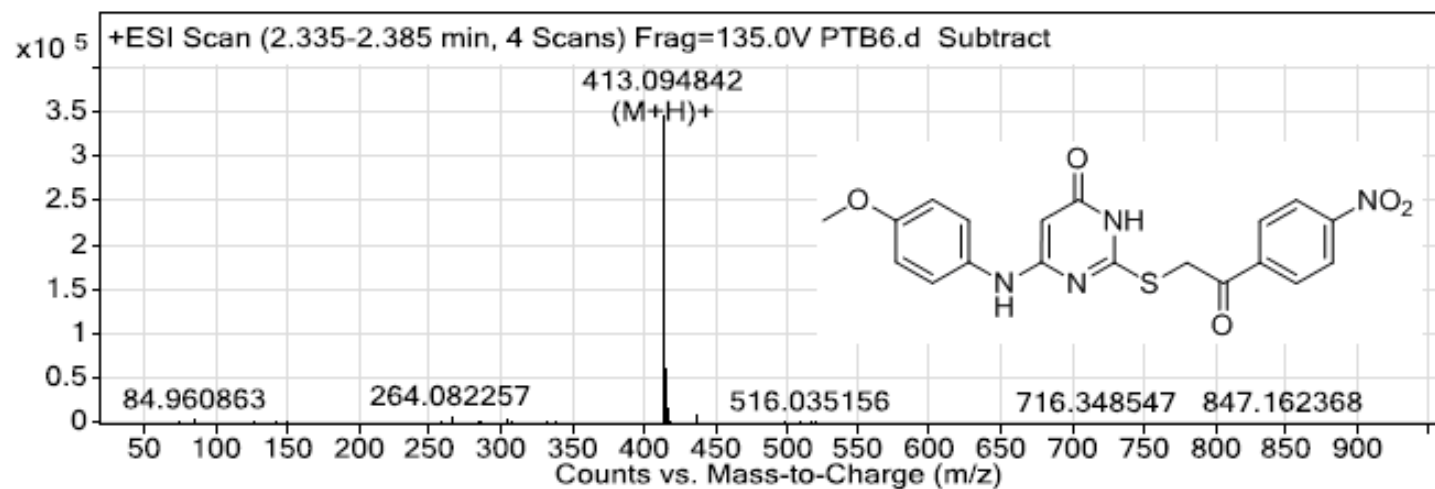


Figure S43. The HRMS spectra of **2f**: 6-((4-Methoxyphenyl)amino)-2-((2-(4-nitrophenyl)-2-oxoethyl)thio)pyrimidin-4(3H)-one.

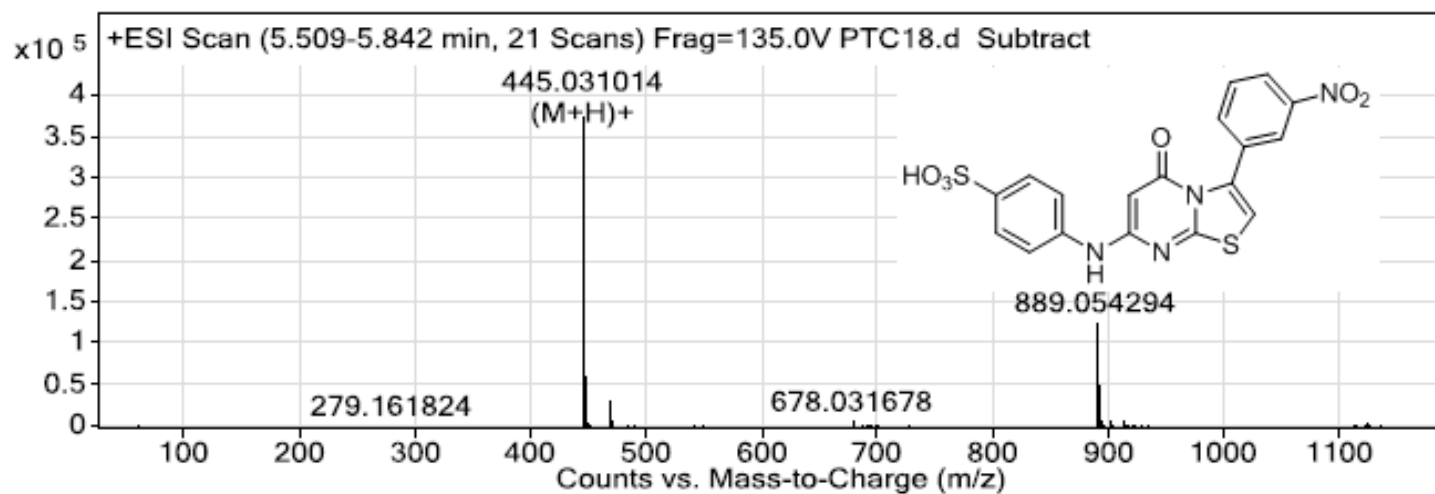


Figure S44. The HRMS spectra of **3a**: 4-((3-(3-Nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

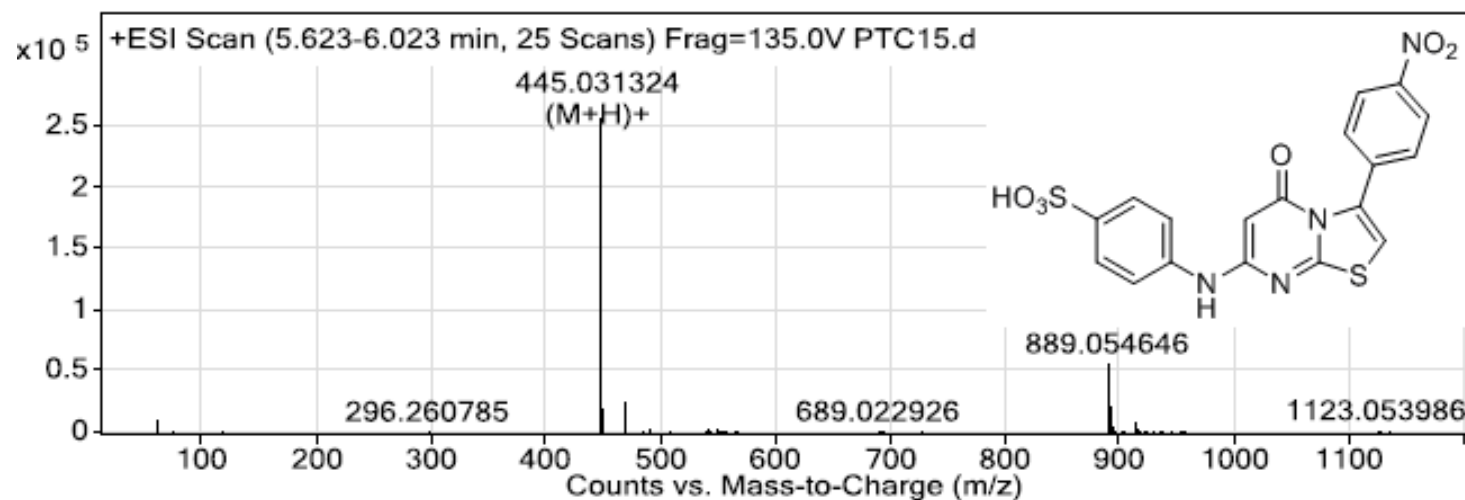


Figure S45. The HRMS spectra of **3b**: 4-((3-(4-Nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

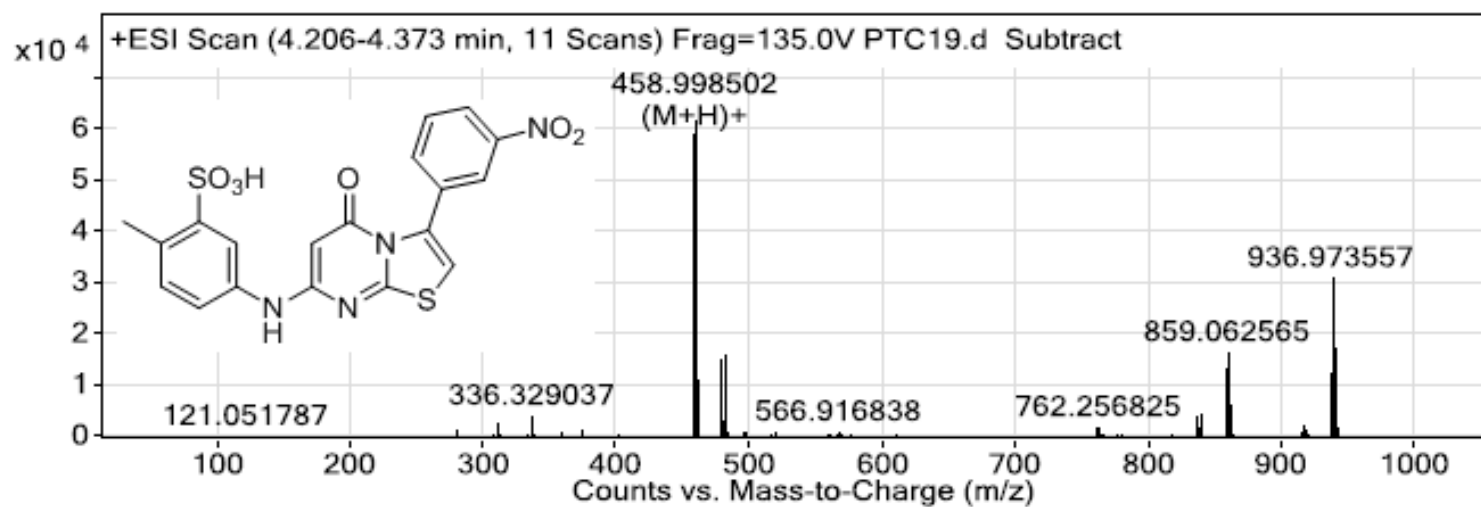


Figure S46. The HRMS spectra of **3c**: 2-Methyl-5-((3-(3-nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

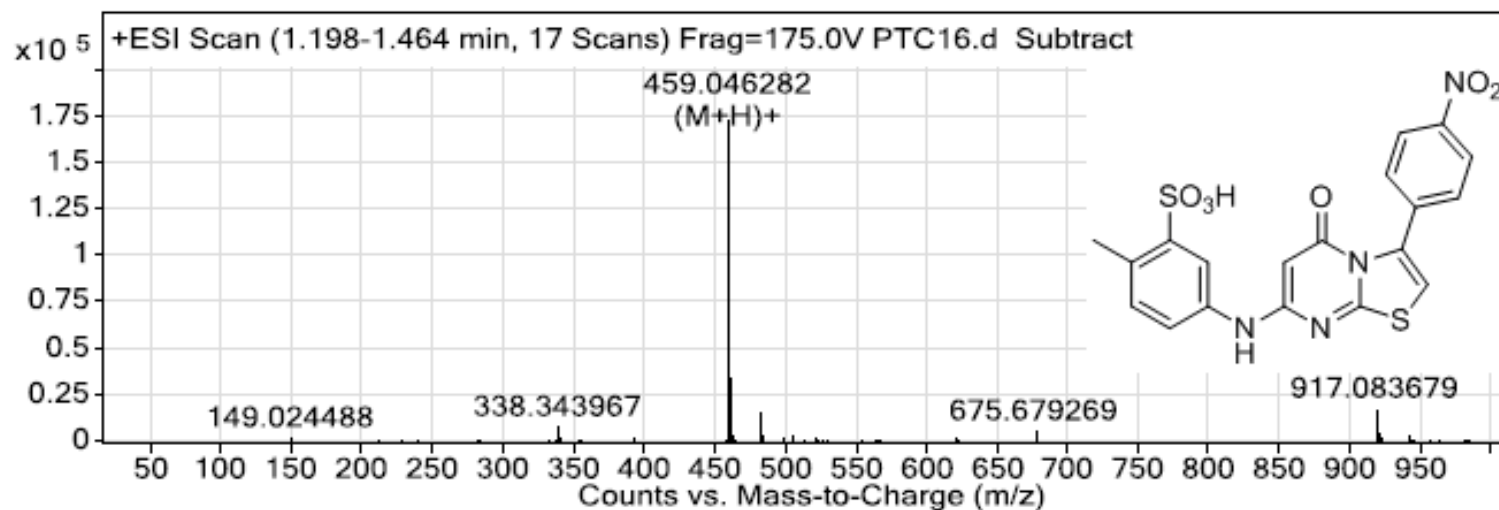


Figure S46. The HRMS spectra of **3d**: 2-Methyl-5-((3-(4-nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

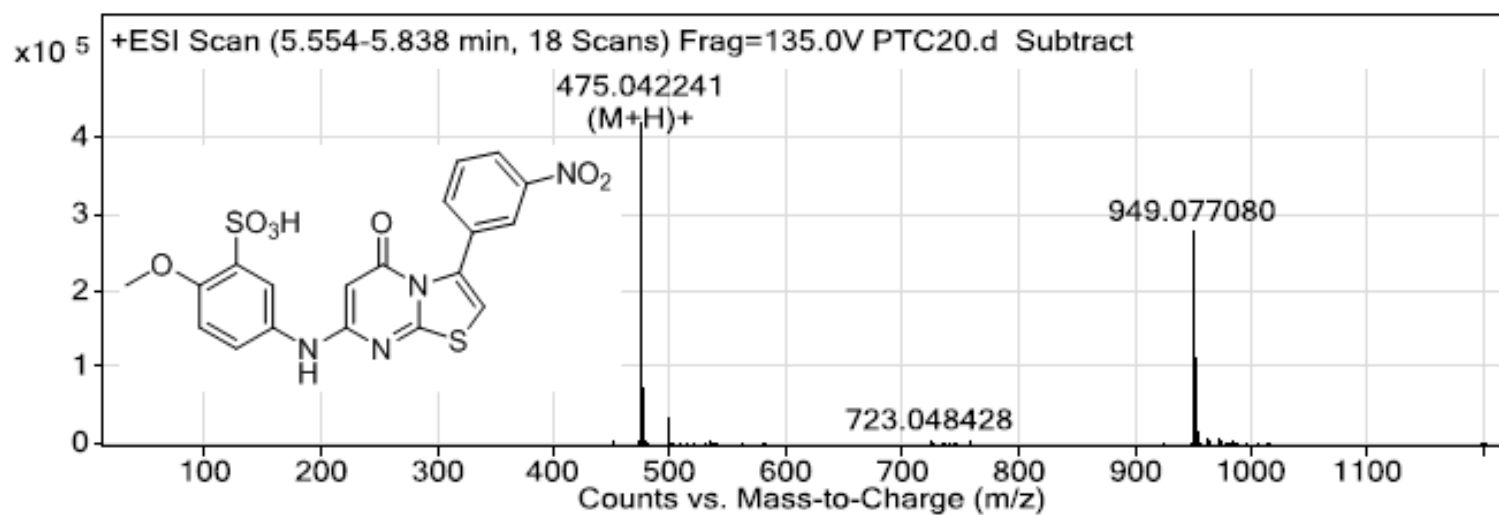


Figure S47. The HRMS spectra of **3e**: 2-Methoxy-5-((3-(3-nitrophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

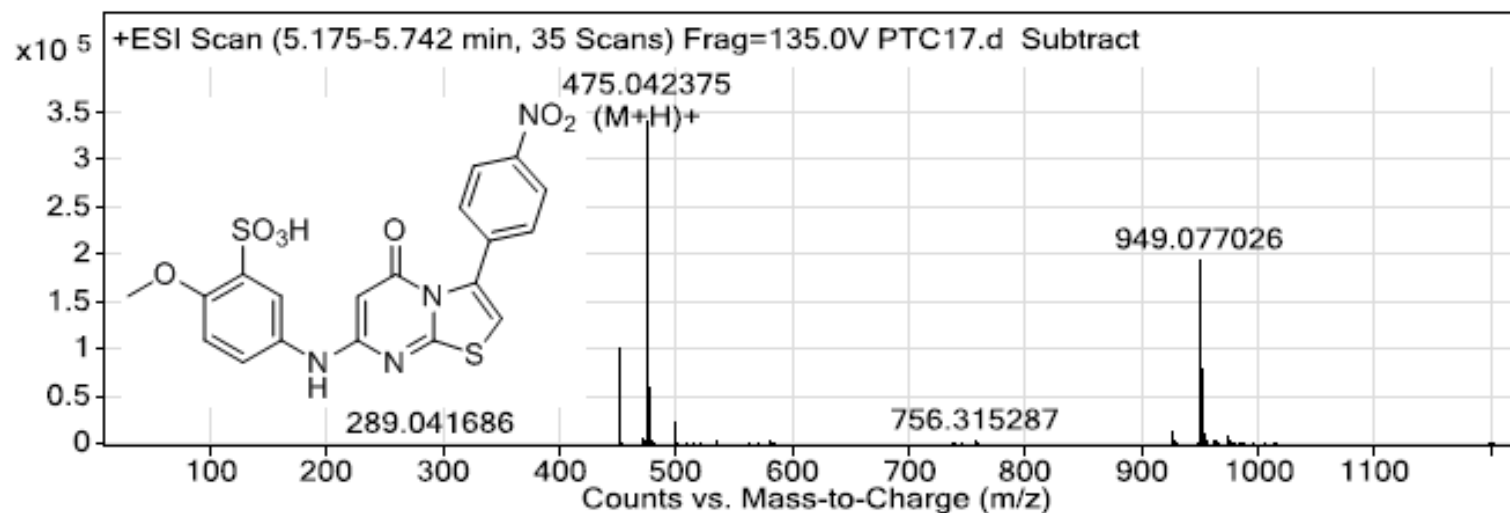


Figure S48. The HRMS spectra of **3f**: 2-Methoxy-5-((3-(4-nitrophenyl)-5-oxo-5*H*-thiazolo[3,2-*a*]pyrimidin-7-yl)amino)benzenesulfonic acid.

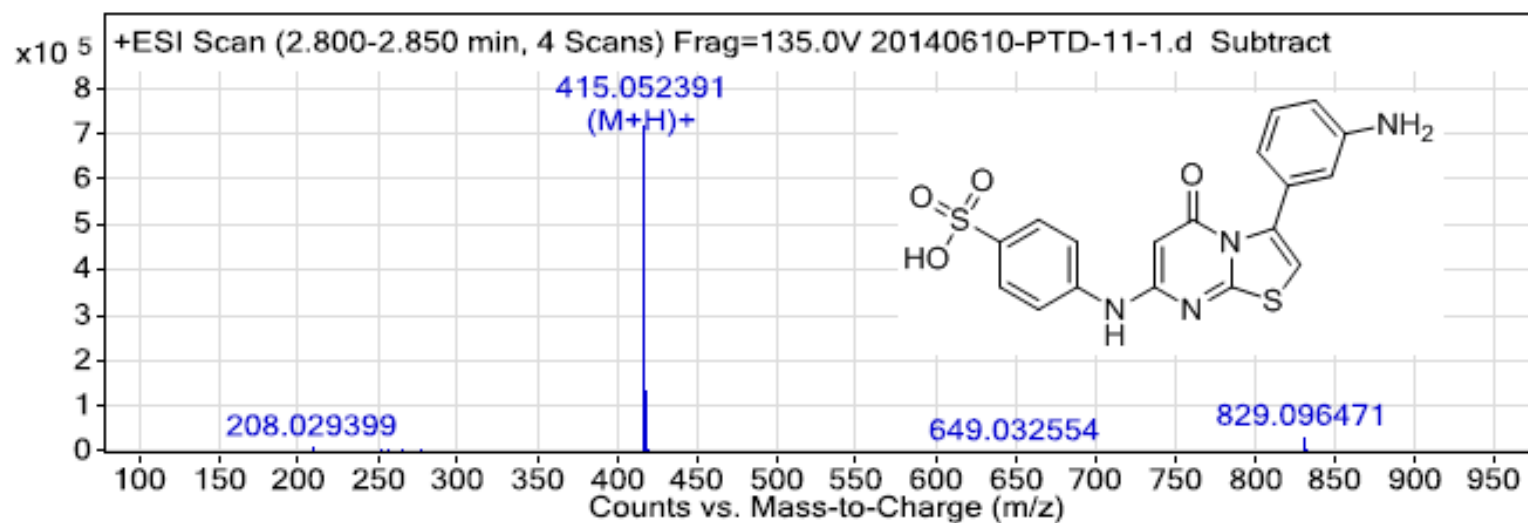


Figure S49. The HRMS spectra of **4a**: 4-((3-(3-Aminophenyl)-5-oxo-5*H*-thiazolo[3,2-*a*]pyrimidin-7-yl)amino)benzenesulfonic acid.

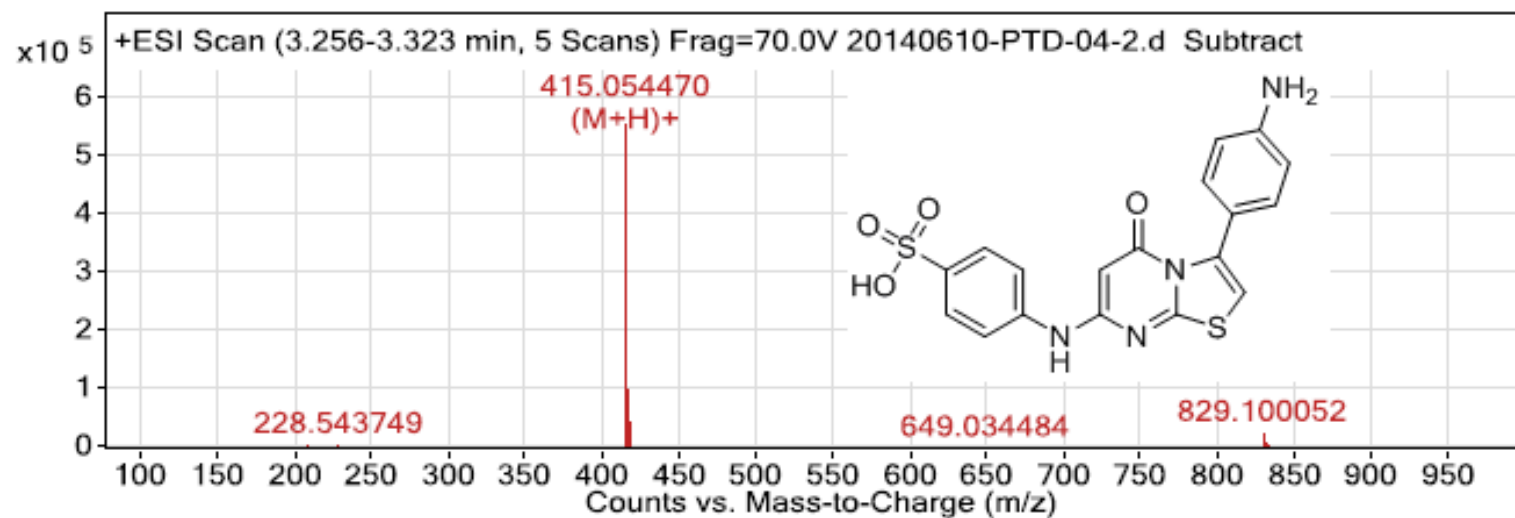


Figure S50. The HRMS spectra of **4b**: 4-((3-(4-Aminophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)benzenesulfonic acid.

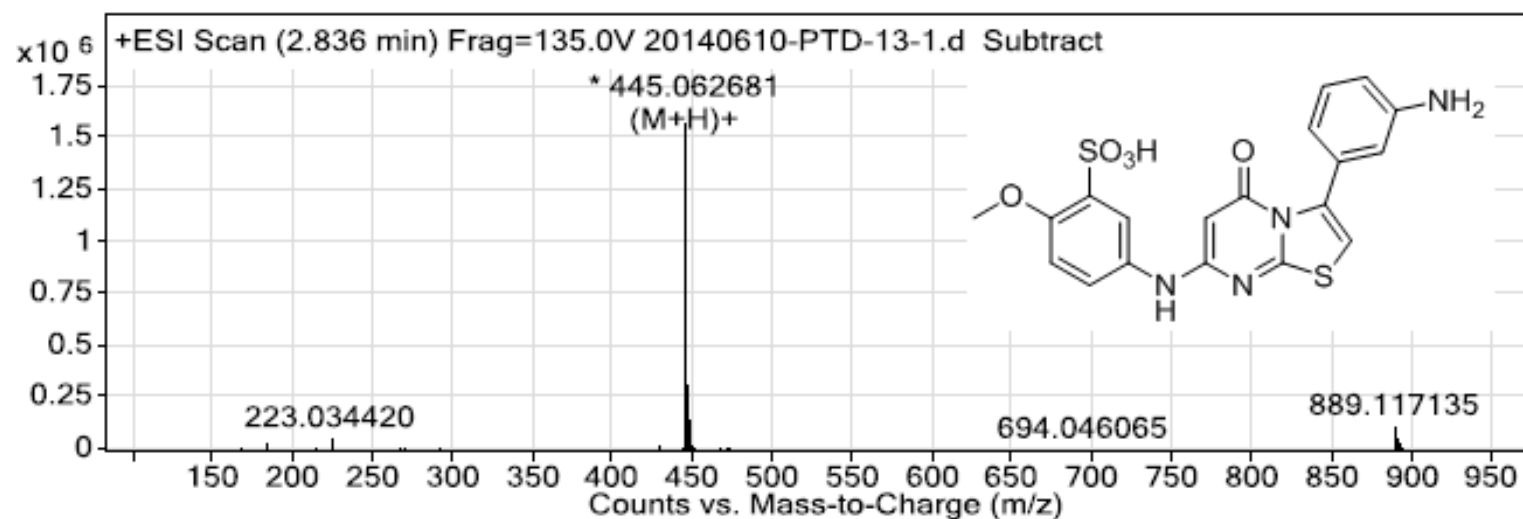


Figure S51. The HRMS spectra of **4c**: 5-((3-(3-Aminophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)-2-methoxybenzenesulfonic acid.

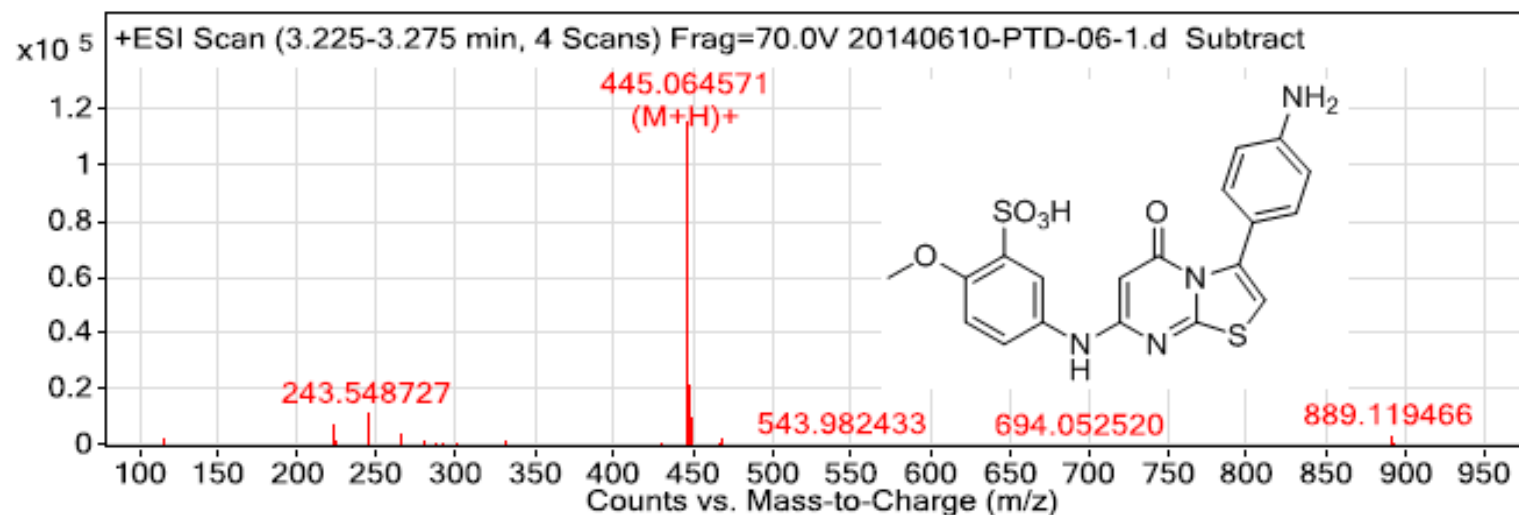


Figure S52. The HRMS spectra of **4d**: 5-((3-(4-Aminophenyl)-5-oxo-5H-thiazolo[3,2-a]pyrimidin-7-yl)amino)-2-methoxybenzenesulfonic acid.

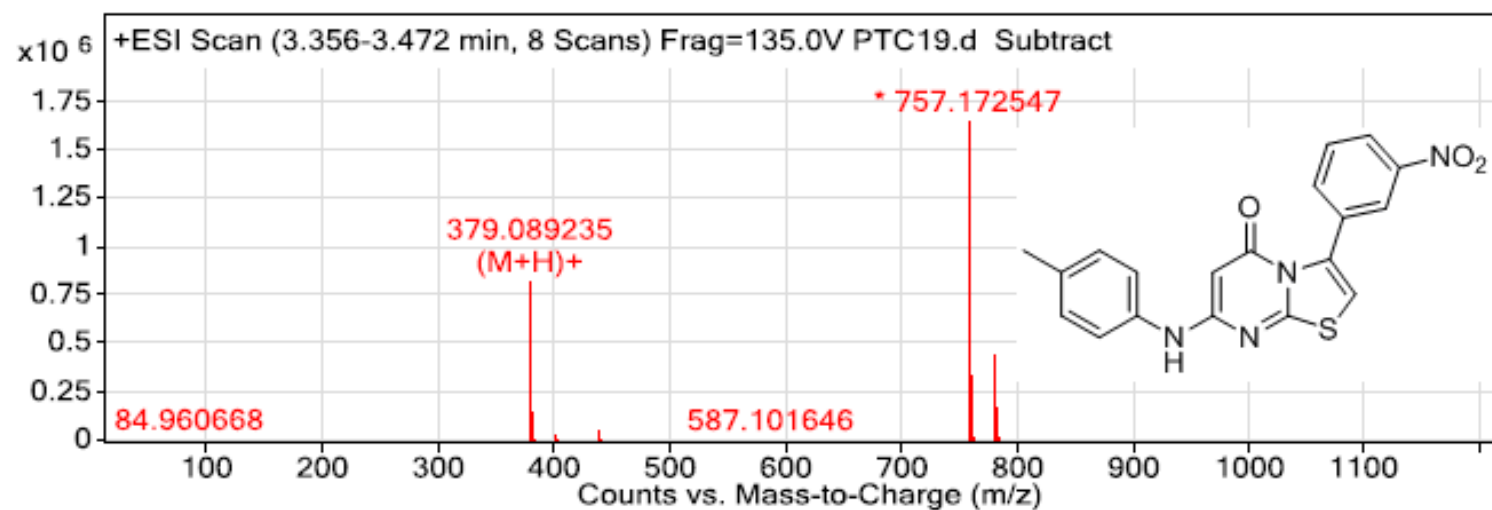


Figure S53. The HRMS spectra of **5a**: 3-(4-Nitrophenyl)-7-(p-tolylamino)-5H-thiazolo[3,2-a]pyrimidin-5-one.

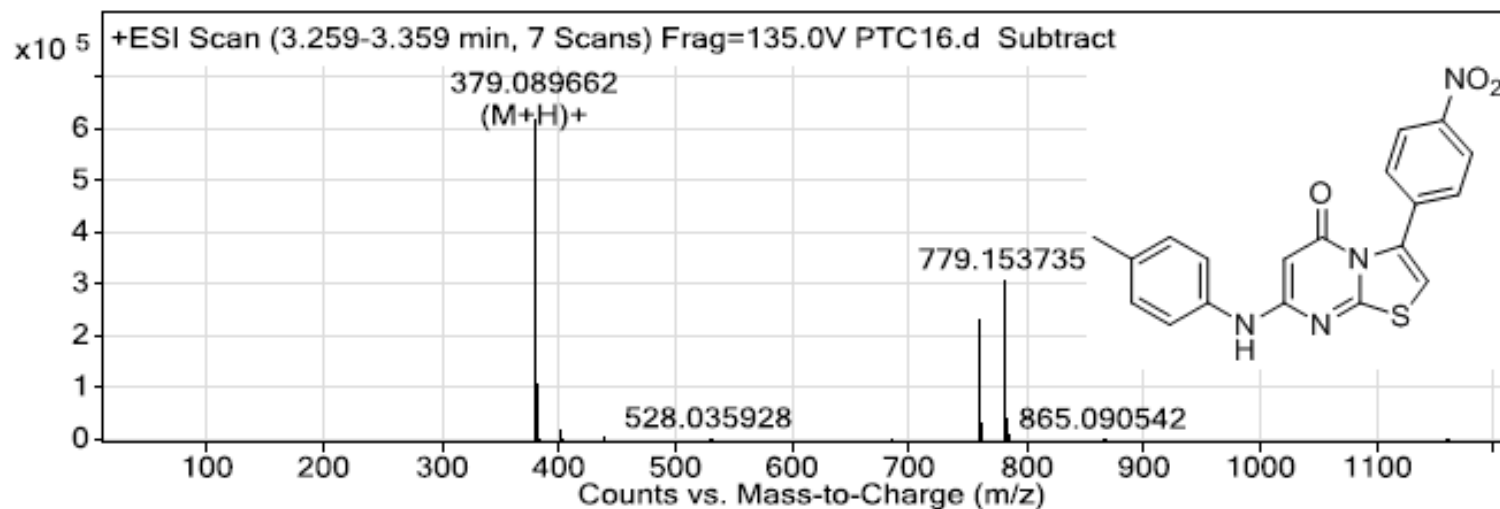


Figure S54. The HRMS spectra of **5b**: 3-(4-Nitrophenyl)-7-(*p*-tolylamino)-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one.

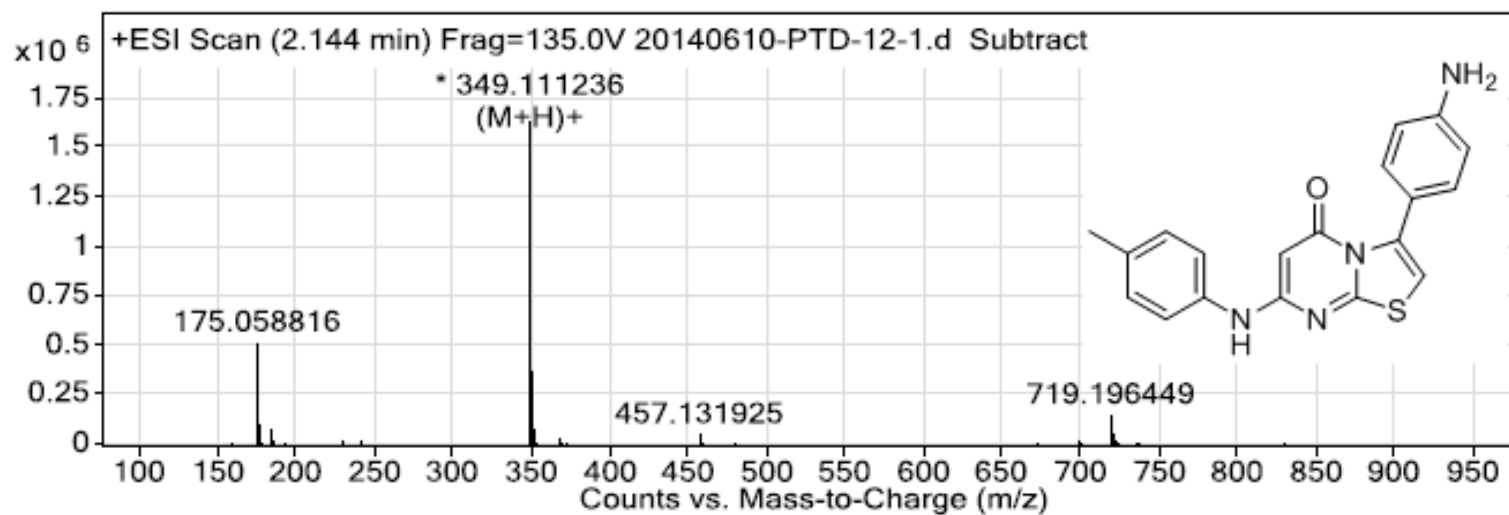


Figure S55. The HRMS spectra of **6a**: 3-(3-Aminophenyl)-7-(*p*-tolylamino)-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one.

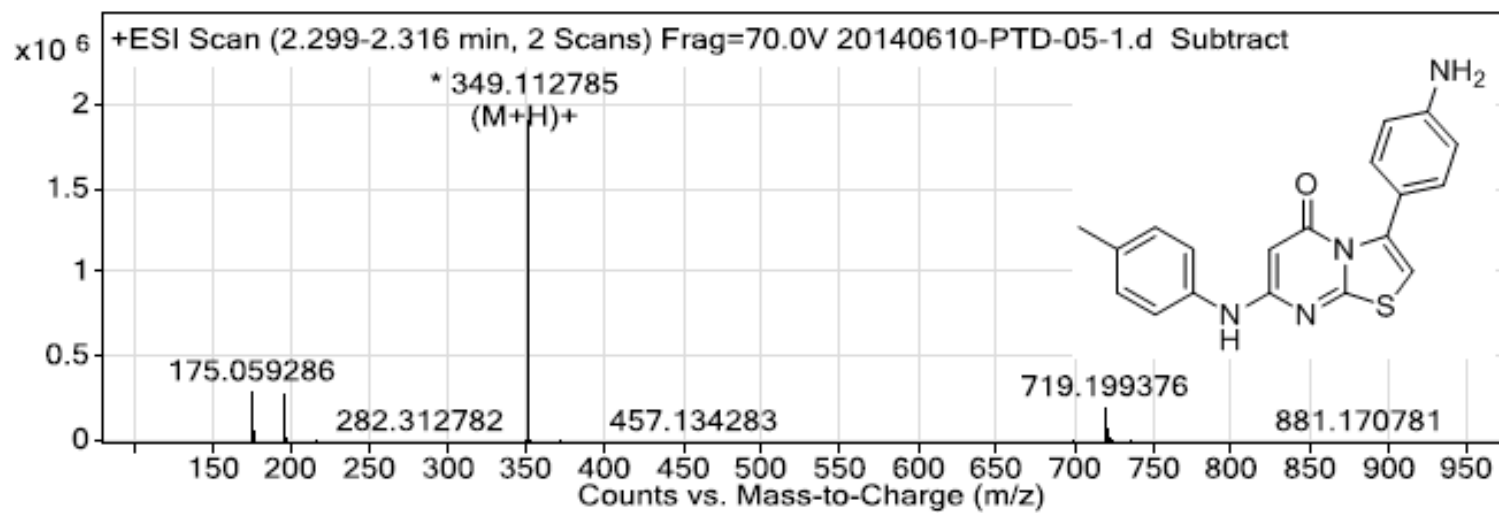


Figure S56. The HRMS spectra of **6b**: 3-(4-Aminophenyl)-7-(*p*-tolylamino)-5*H*-thiazolo[3,2-*a*]pyrimidin-5-one.