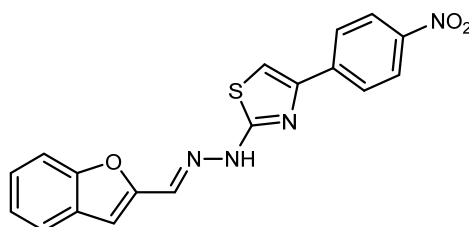


Supplementary Data

This supplementary data is a part of a paper entitled “Design, Synthesis, *In-Silico* Study of Novel Benzofuran Thiazolyl Hydrazones as Anticancer Agents Targeting EGFR Kinase”.



2-(2-(benzofuran-2-ylmethylene)hydrazineyl)-4-(4-nitrophenyl)thiazole (**5a**)

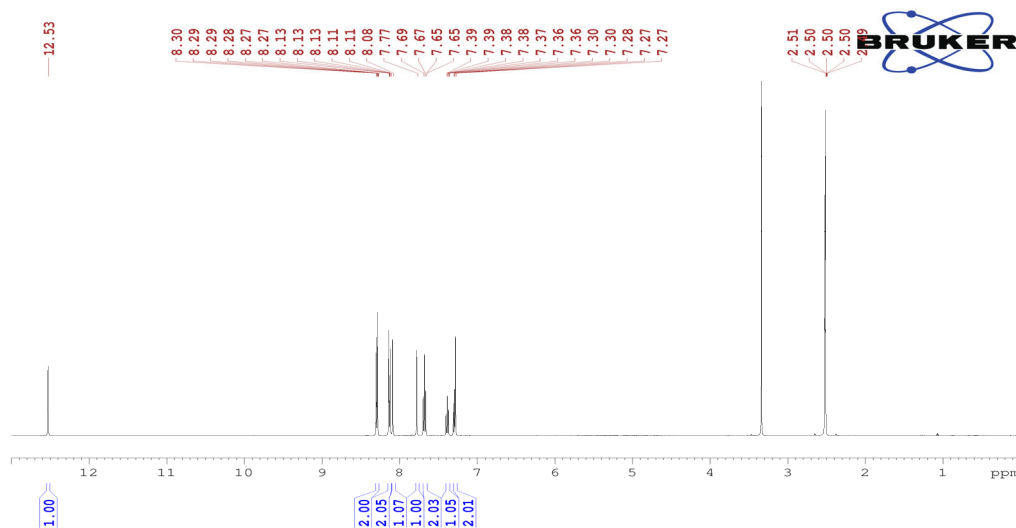


Fig S1. ¹H-NMR spectrum of compound **5a** (DMSO-*d*₆, 500 MHz)

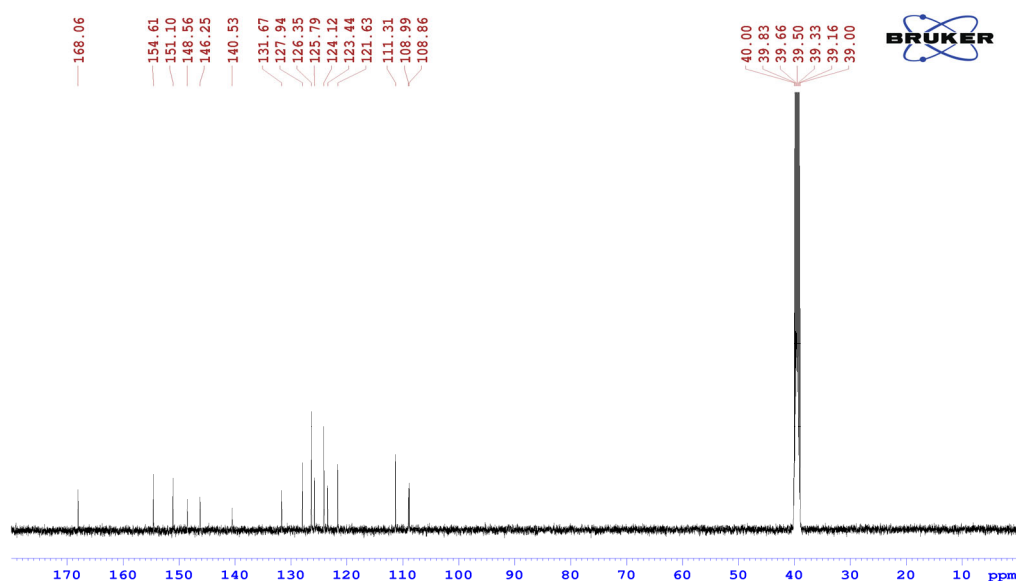


Fig S2. ¹³C-NMR spectrum of compound **5a** (DMSO-*d*₆, 125 MHz)

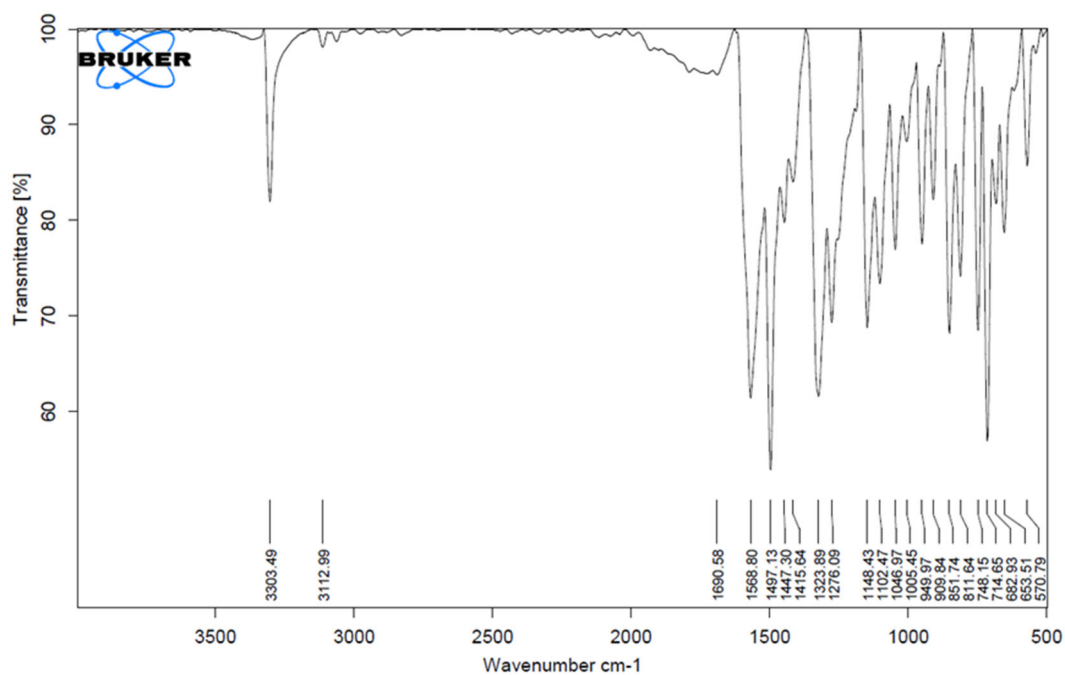


Fig S3. FTIR spectrum of compound 5a

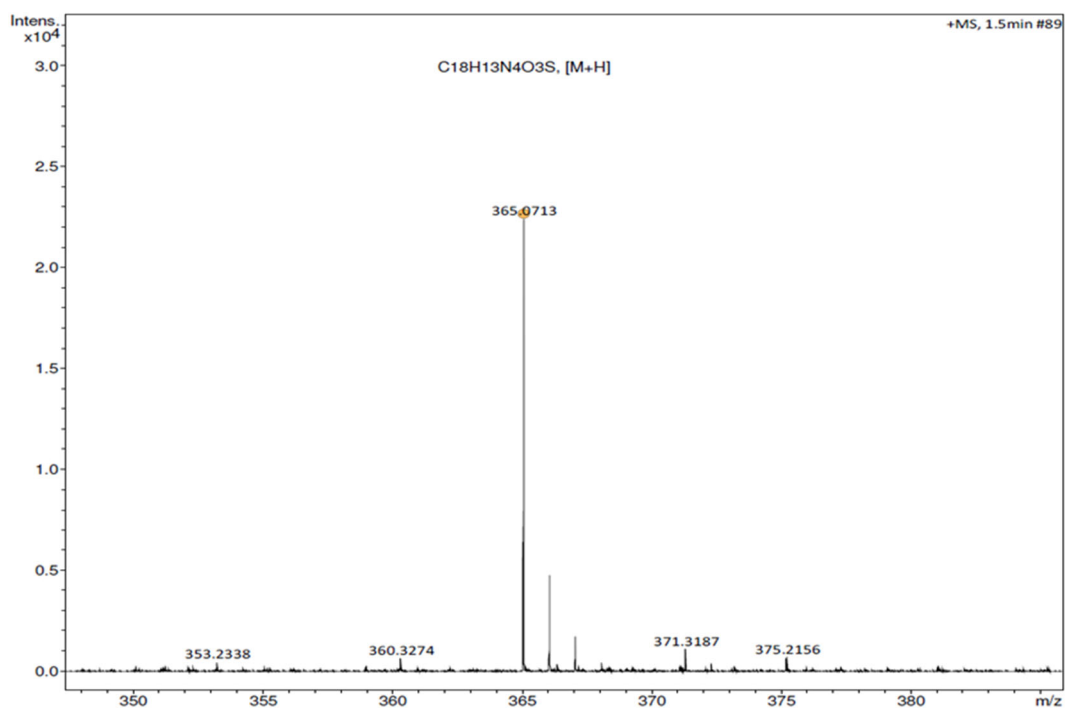
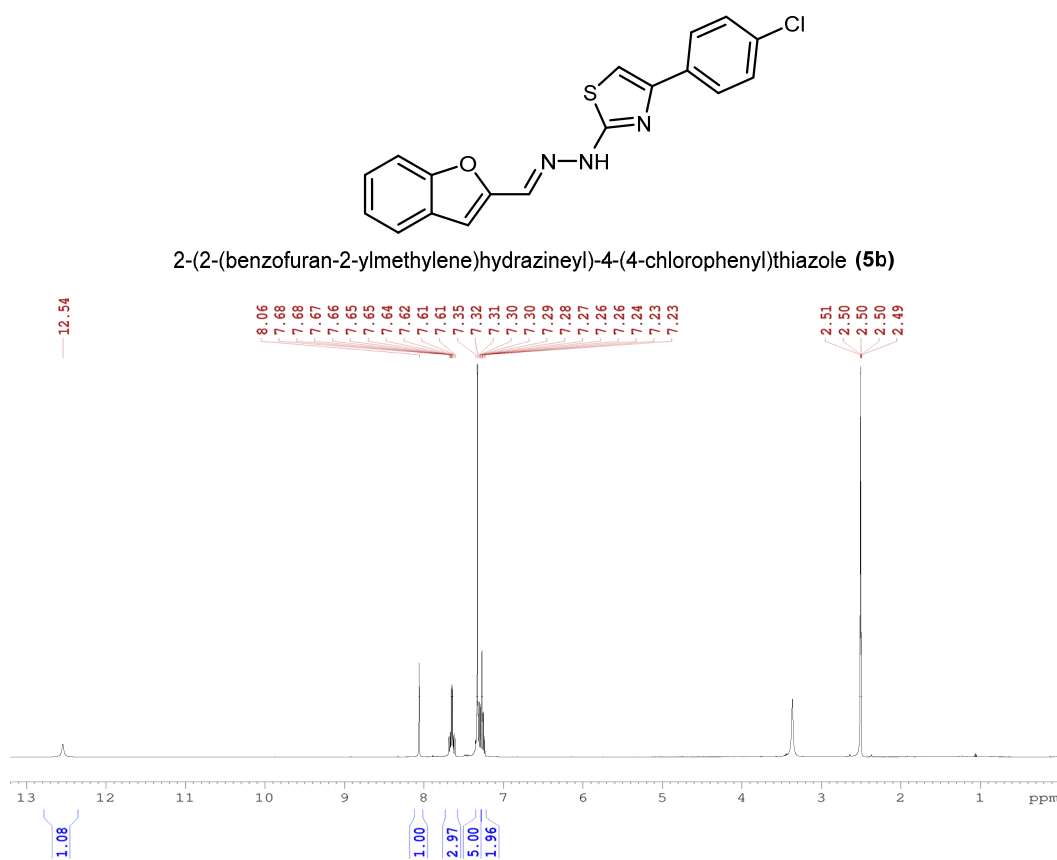
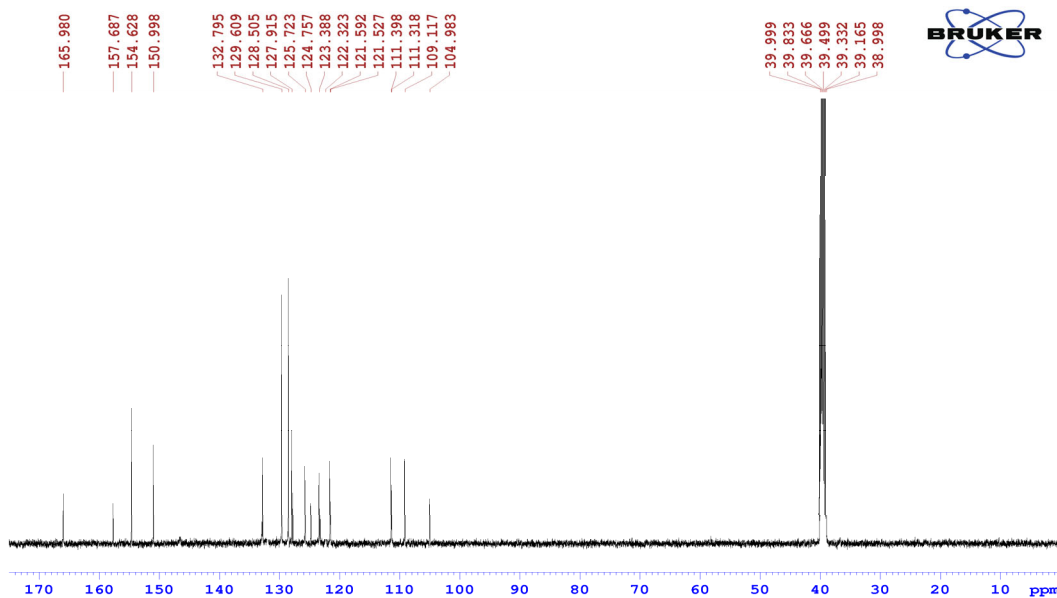


Fig S4. HRMS result of compound 5a

Fig S5. ¹H-NMR spectrum of compound **5b** (DMSO-*d*₆, 500 MHz)Fig S6. ¹³C-NMR spectrum of compound **5b** (DMSO-*d*₆, 125 MHz)

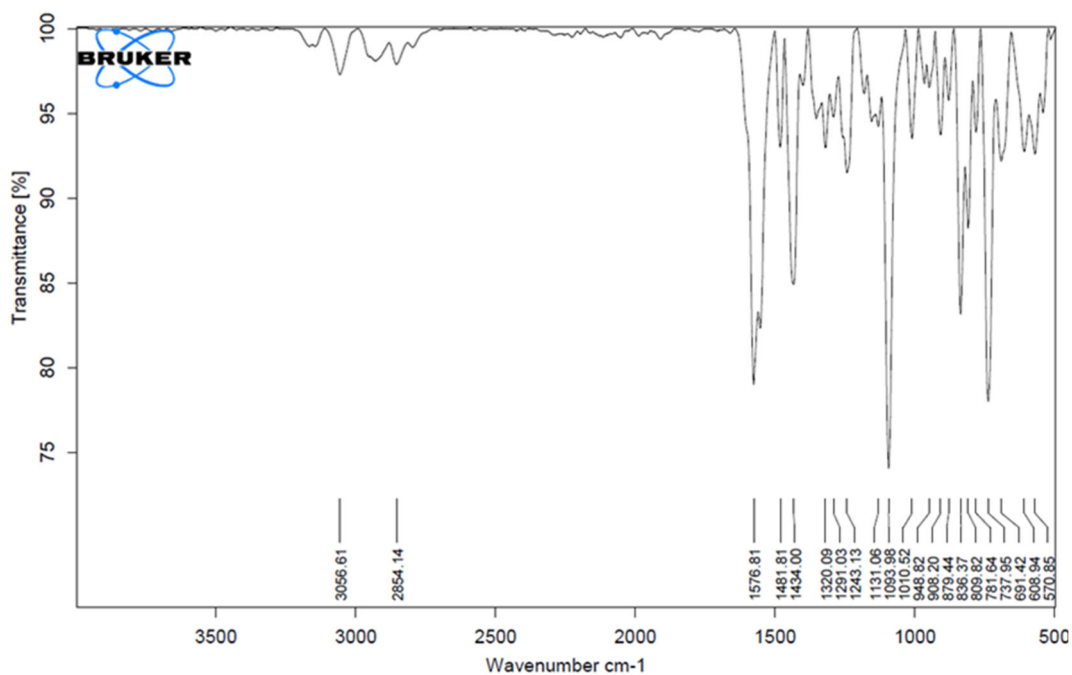


Fig S7. FTIR spectrum of compound 5b

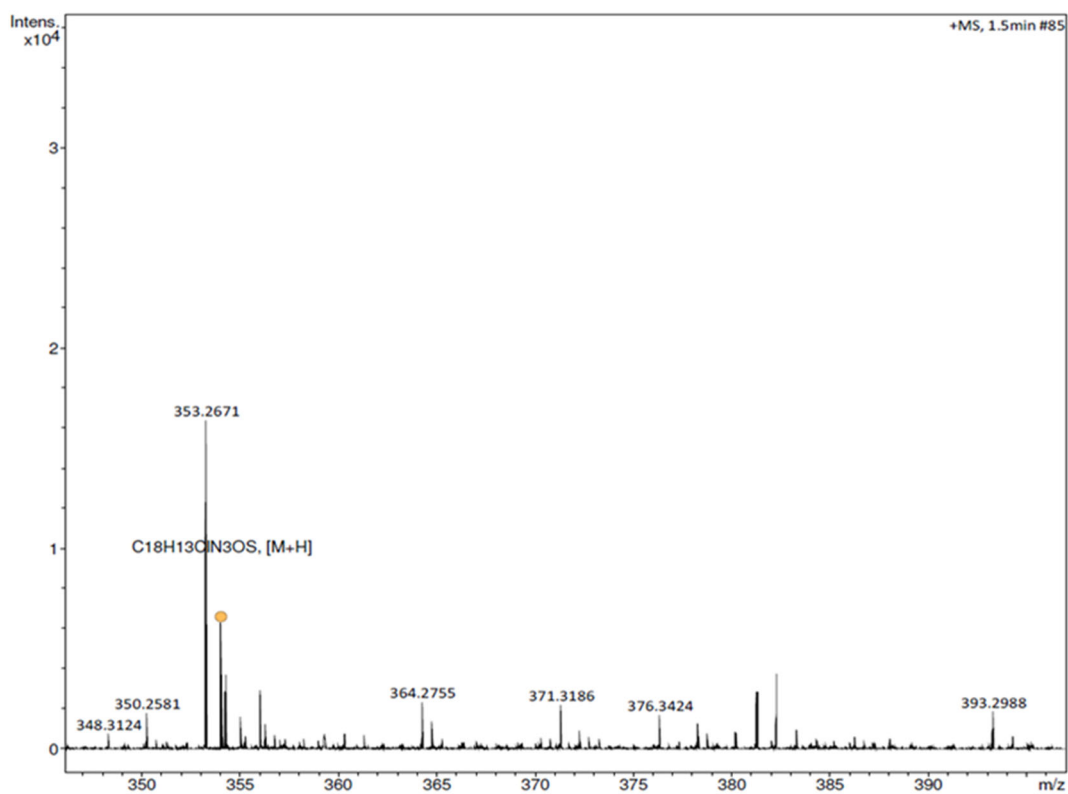
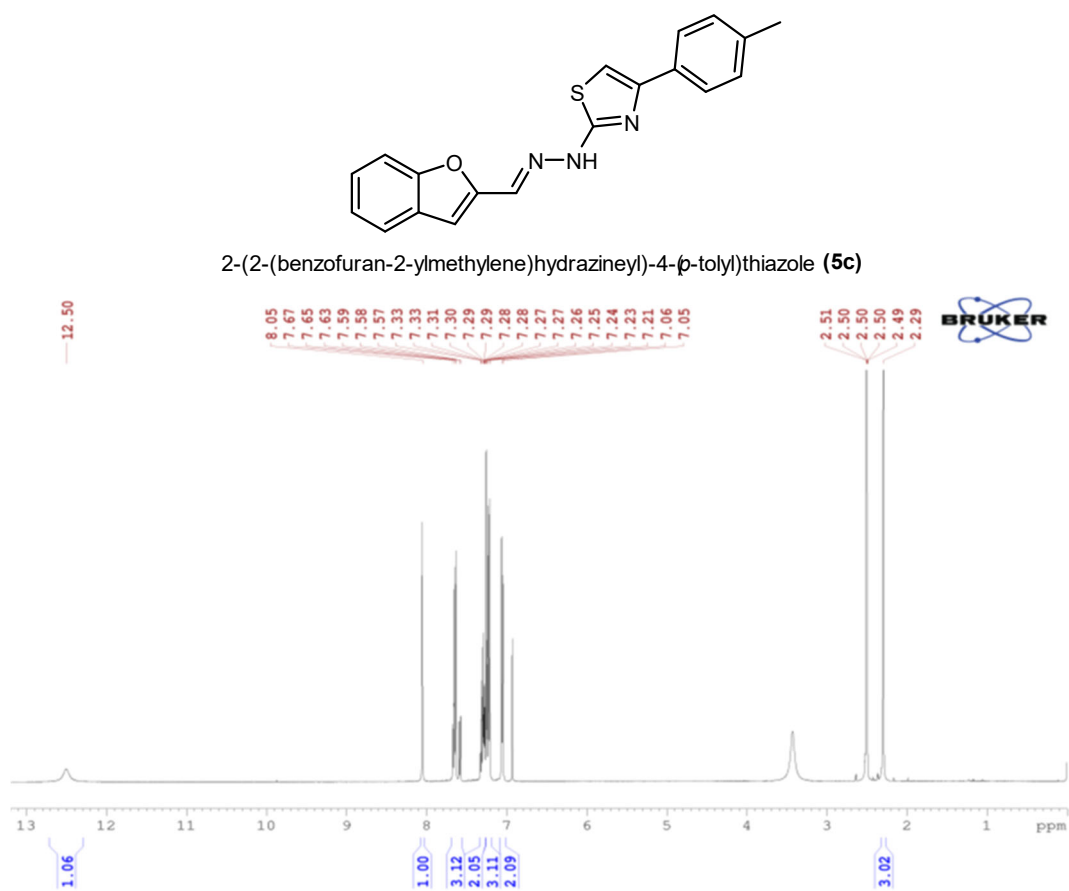
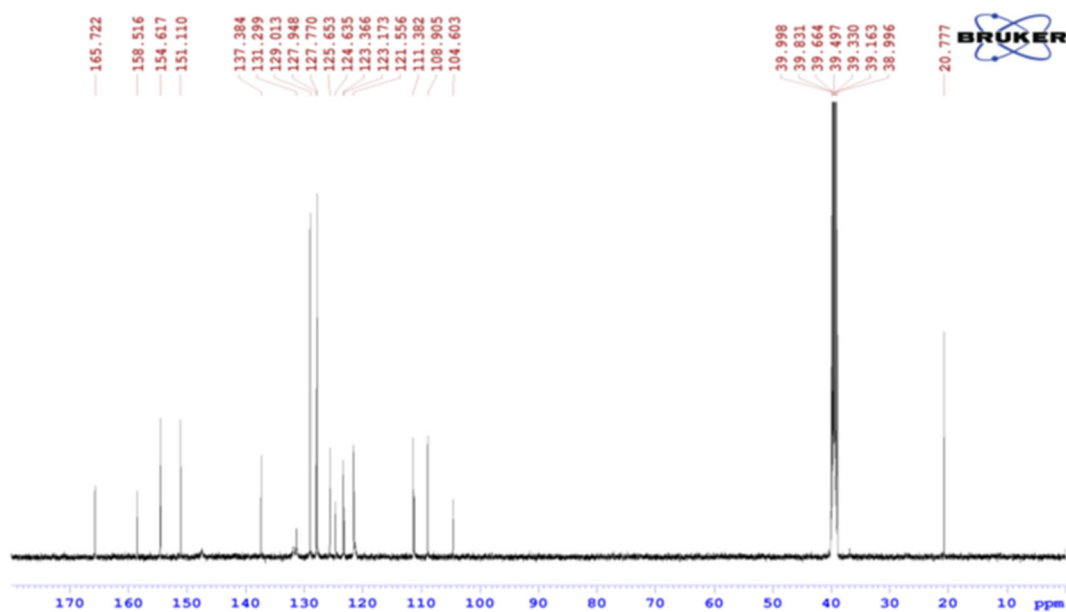


Fig S8. HRMS result of compound 5b

Fig S9. $^1\text{H-NMR}$ spectrum of compound **5c** ($\text{DMSO-}d_6$, 500 MHz)Fig S10. $^{13}\text{C-NMR}$ spectrum of compound **5c** ($\text{DMSO-}d_6$, 125 MHz)

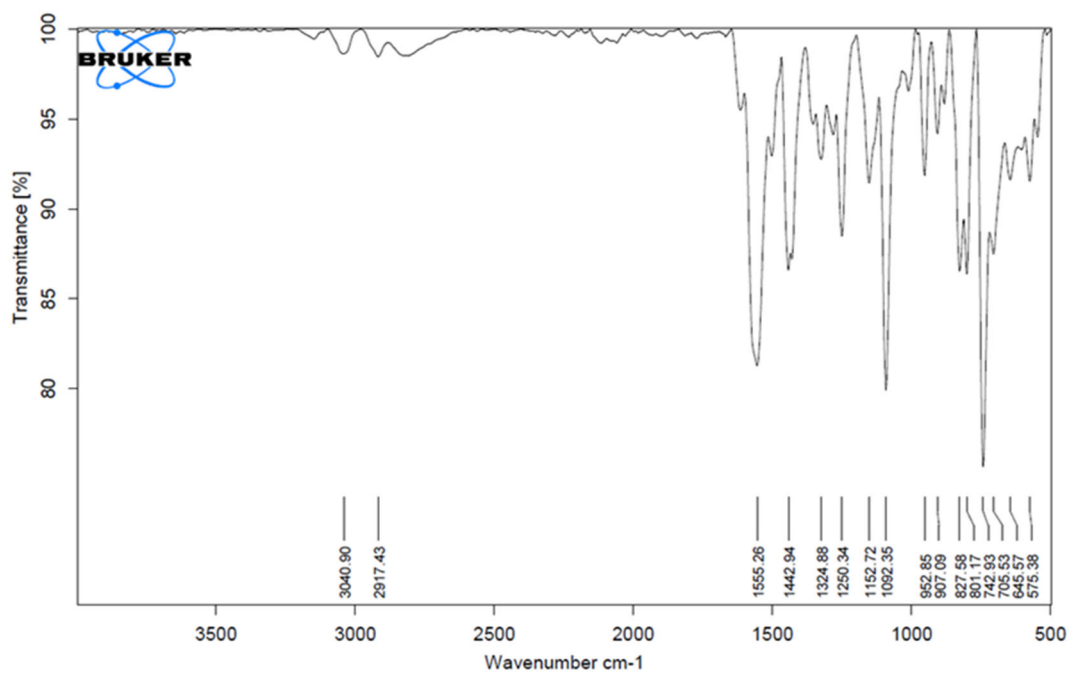


Fig S11. FTIR spectrum of compound 5c

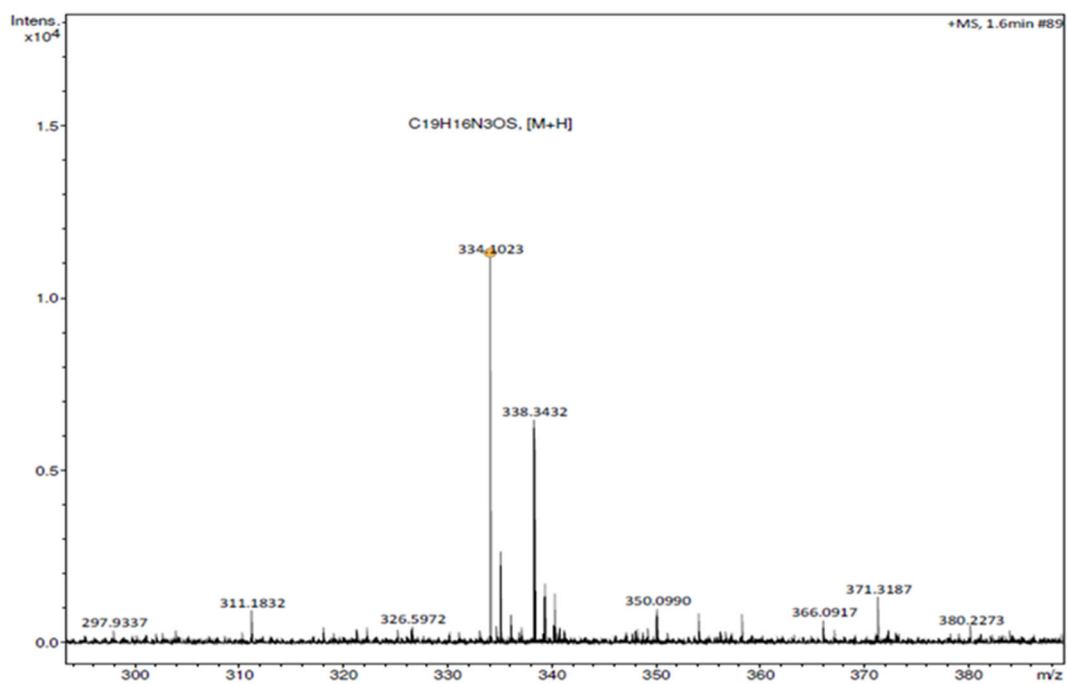
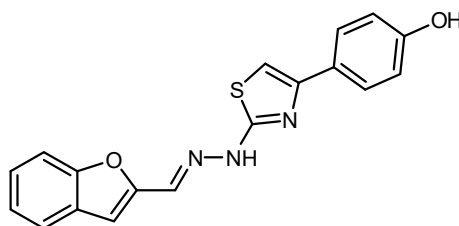
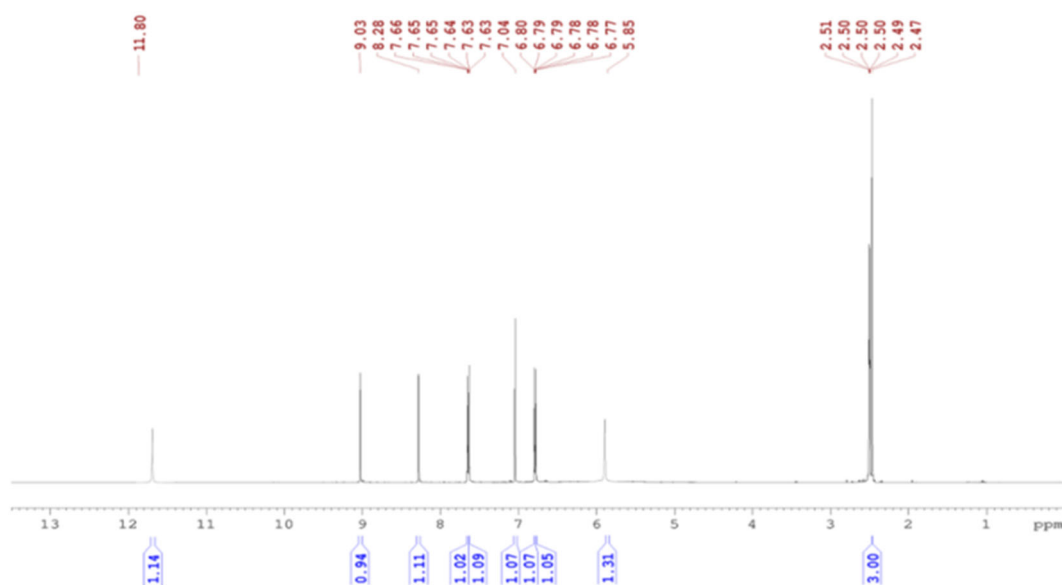
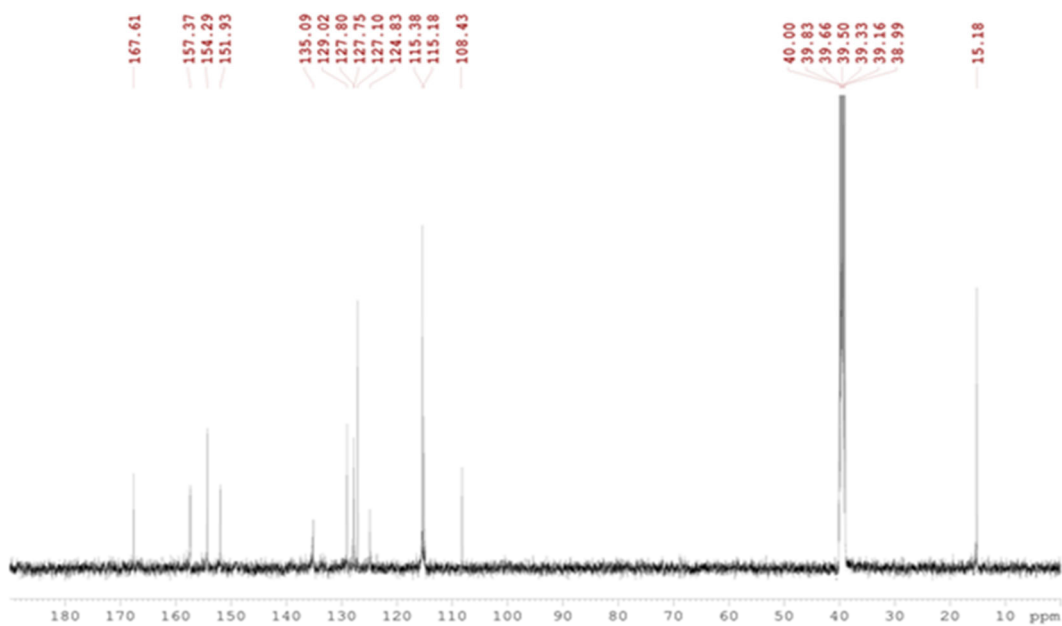


Fig S12. HRMS result of compound 5c



4-(2-(2-(benzofuran-2-ylmethylene)hydrazineyl)thiazol-4-yl)phenol(5d)

Fig S13. $^1\text{H-NMR}$ spectrum of compound 5d (DMSO- d_6 , 500 MHz)Fig S14. $^{13}\text{C-NMR}$ spectrum of compound 5d (DMSO- d_6 , 125 MHz)

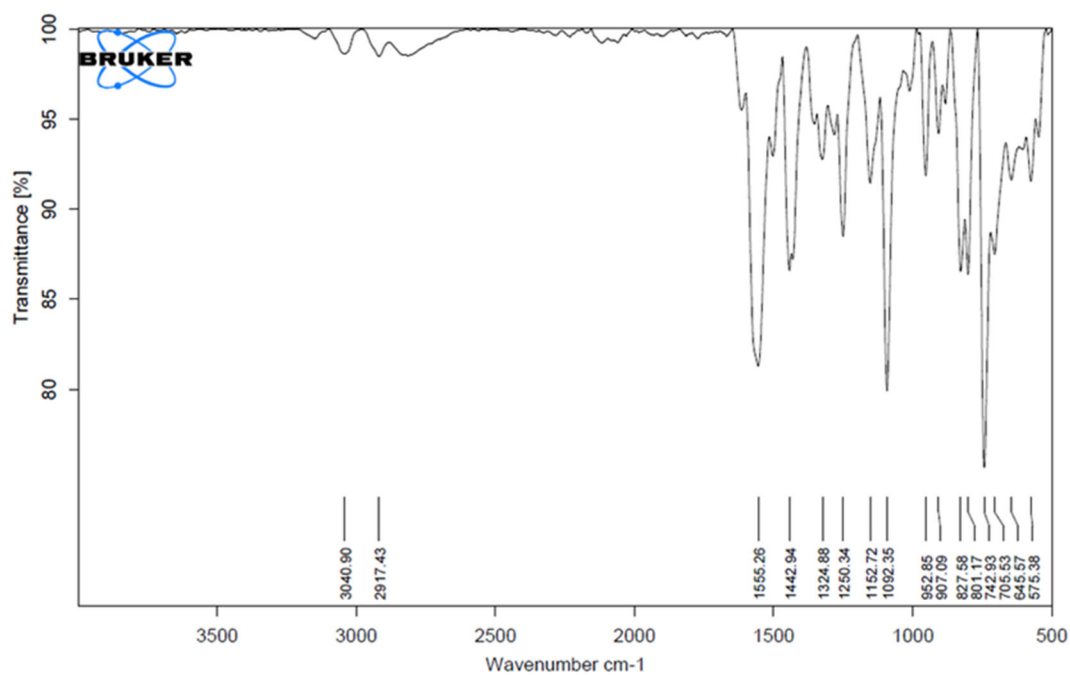


Fig S15. FTIR spectrum of compound 5d

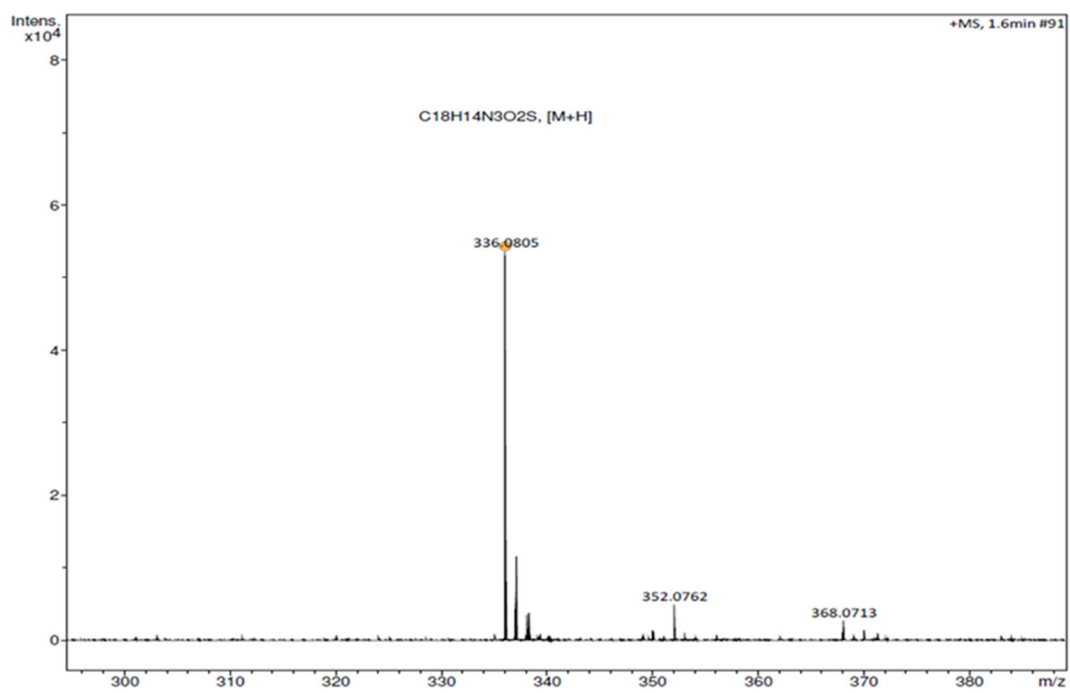
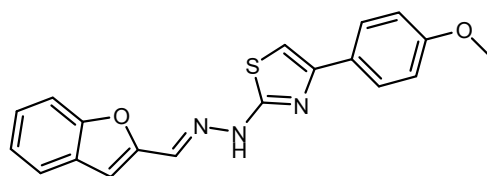
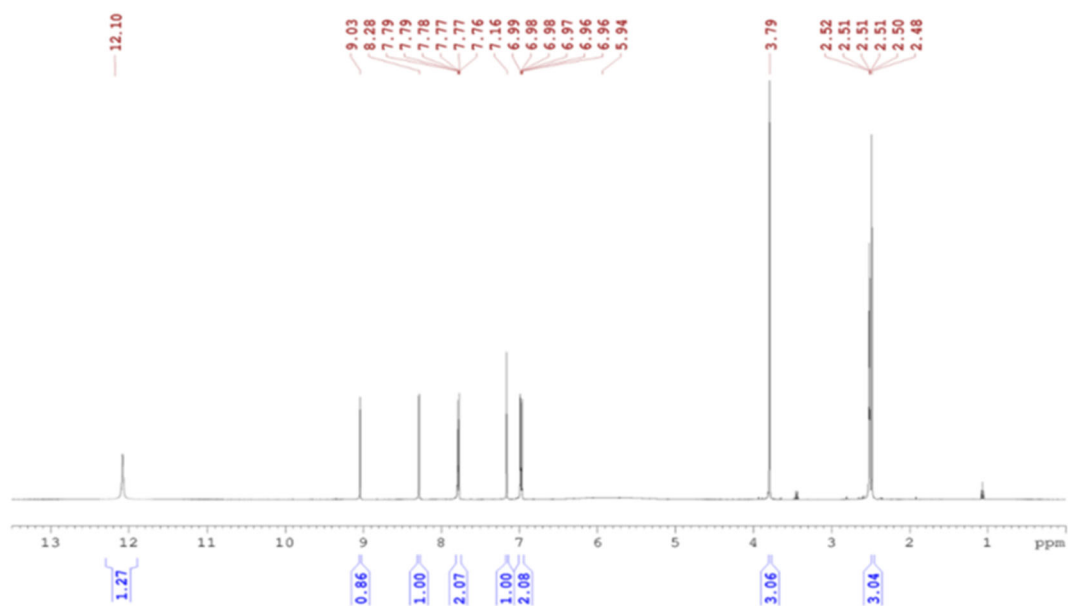
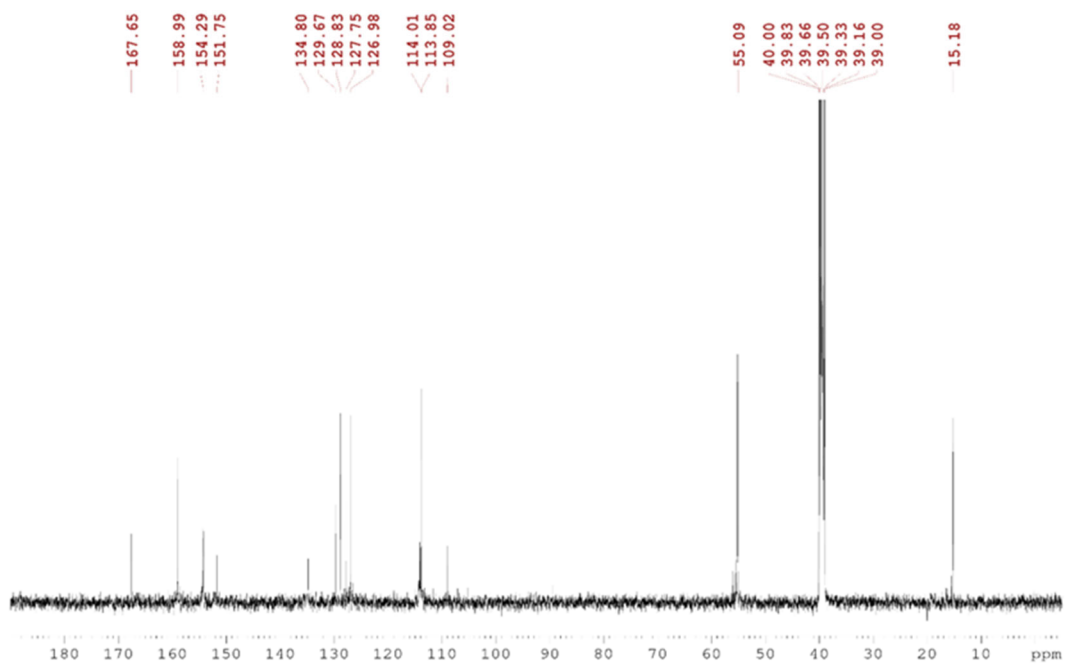


Fig S16. HRMS result of compound 5d

2-(2-(benzofuran-2-ylmethylene)hydrazineyl)-4-(4-methoxyphenyl)thiazole (**5e**)Fig S17. ^1H -NMR spectrum of compound **5e** ($\text{DMSO-}d_6$, 500 MHz)Fig S18. ^{13}C -NMR spectrum of compound **5e** ($\text{DMSO-}d_6$, 125 MHz)

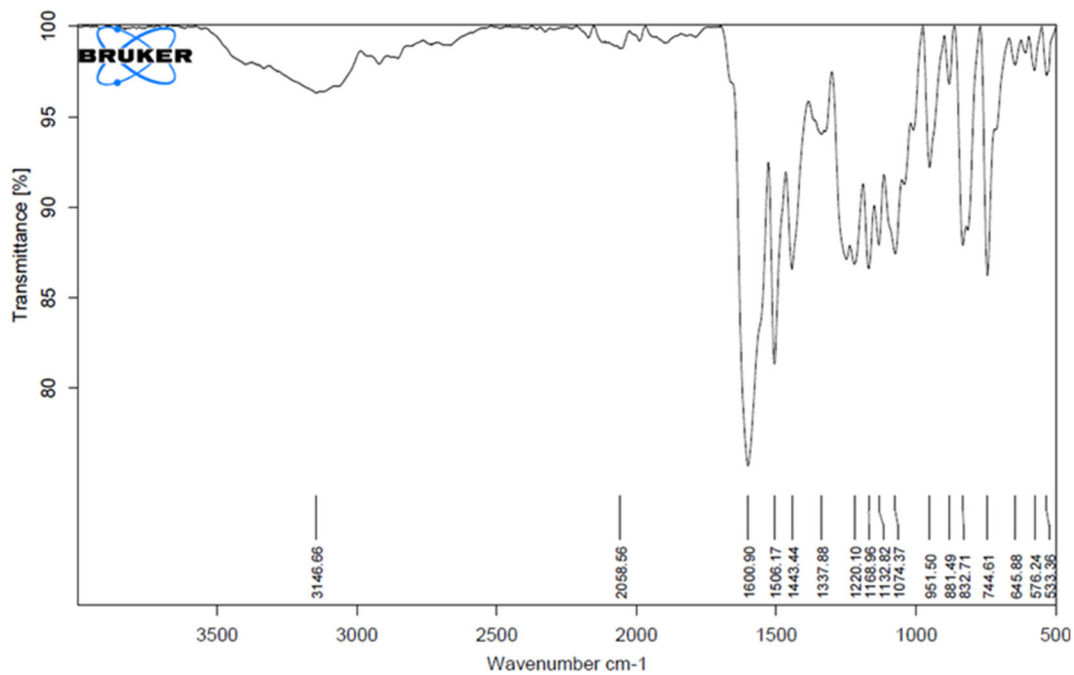


Fig S19. FTIR spectrum of compound 5e

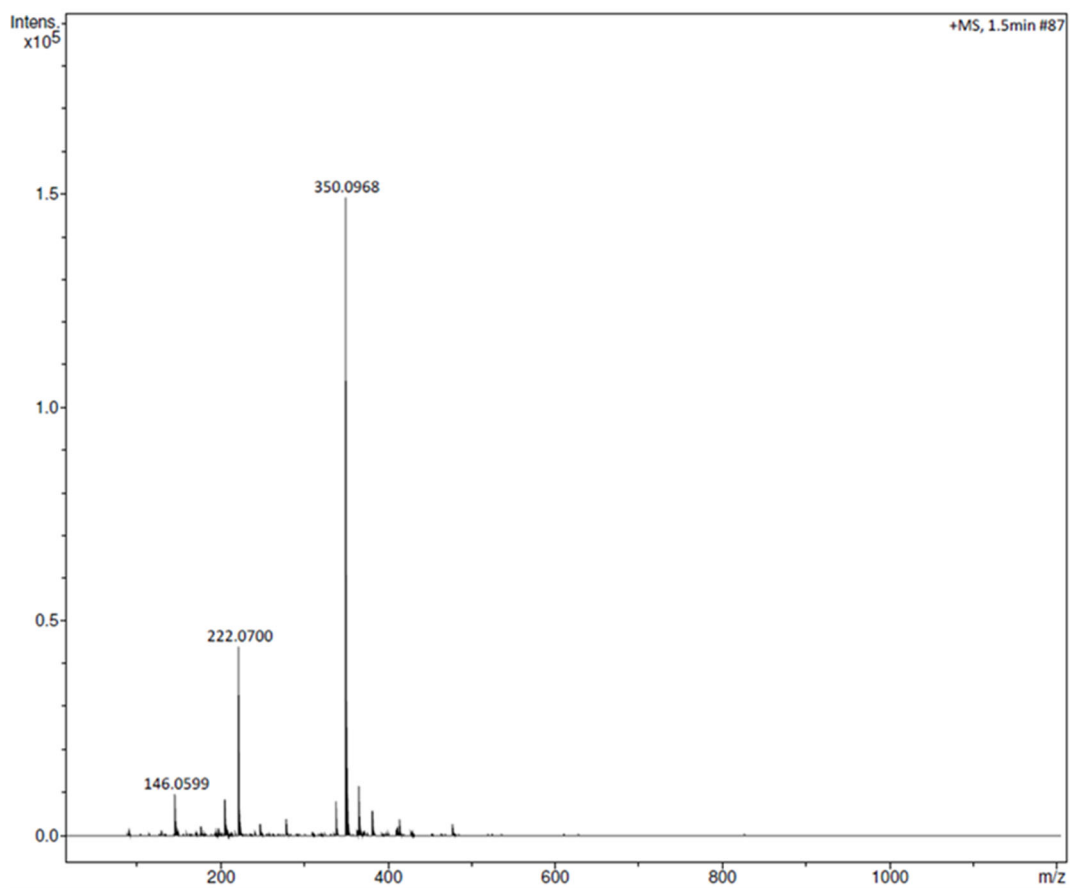
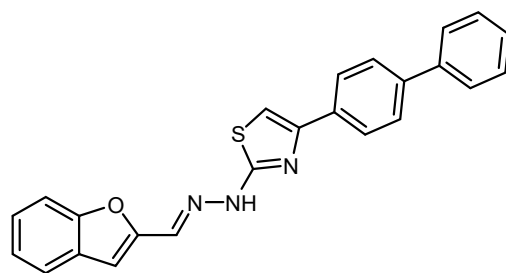
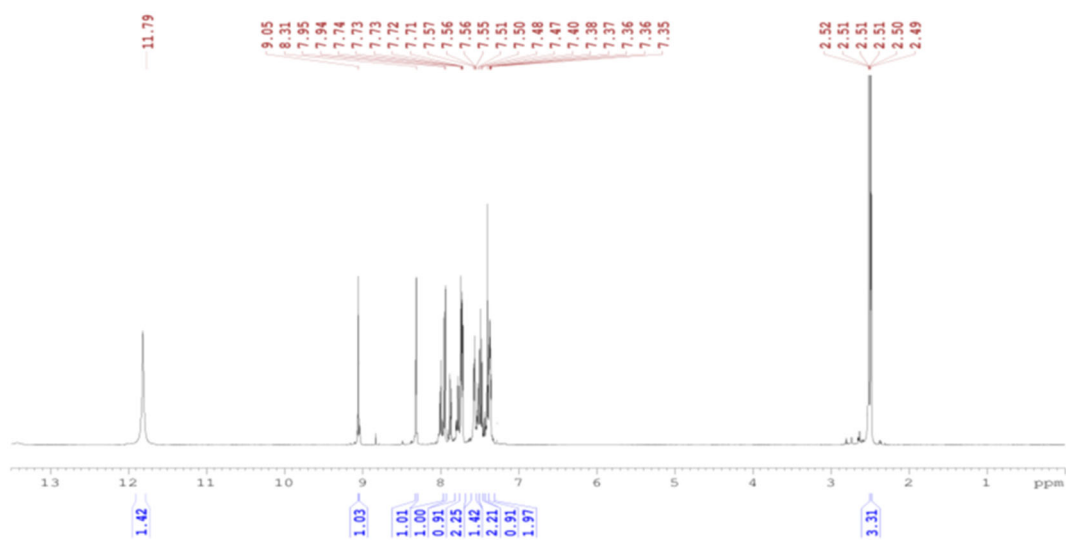
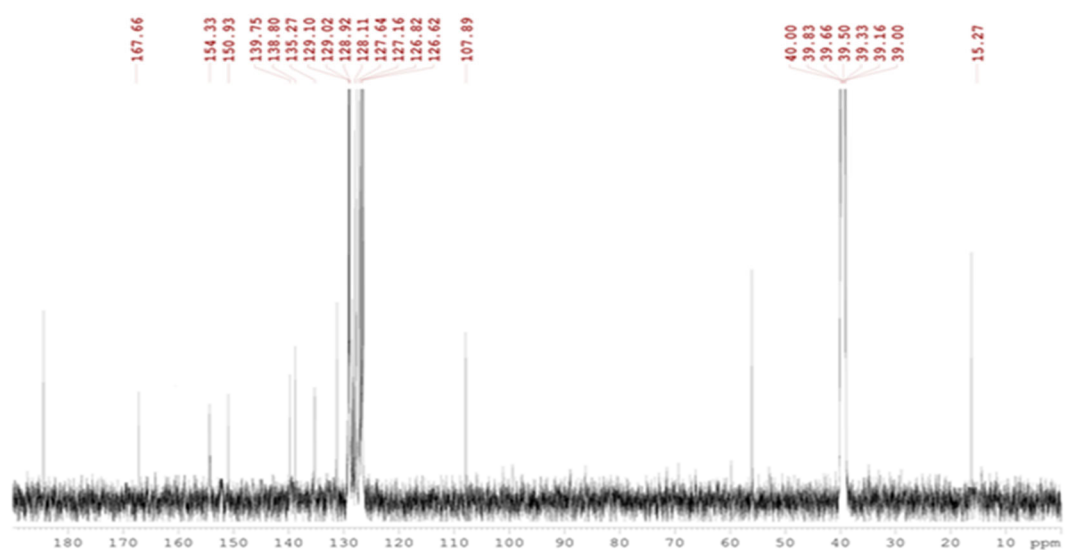


Fig S20. HRMS result of compound 5e

4-([1,1'-biphenyl]-4-yl)-2-(2-(benzofuran-2-ylmethylene)hydrazineyl)thiazole (**5f**)Fig S21. ^1H -NMR spectrum of compound **5f** (DMSO- d_6 , 500 MHz)Fig S22. ^{13}C -NMR spectrum of compound **5f** (DMSO- d_6 , 125 MHz)

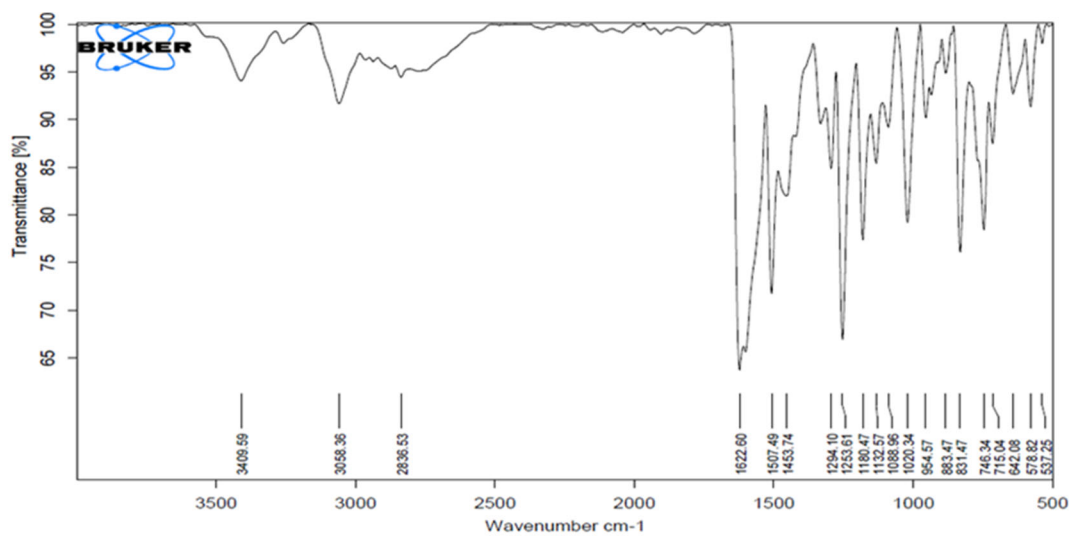


Fig S23. FTIR spectrum of compound 5f

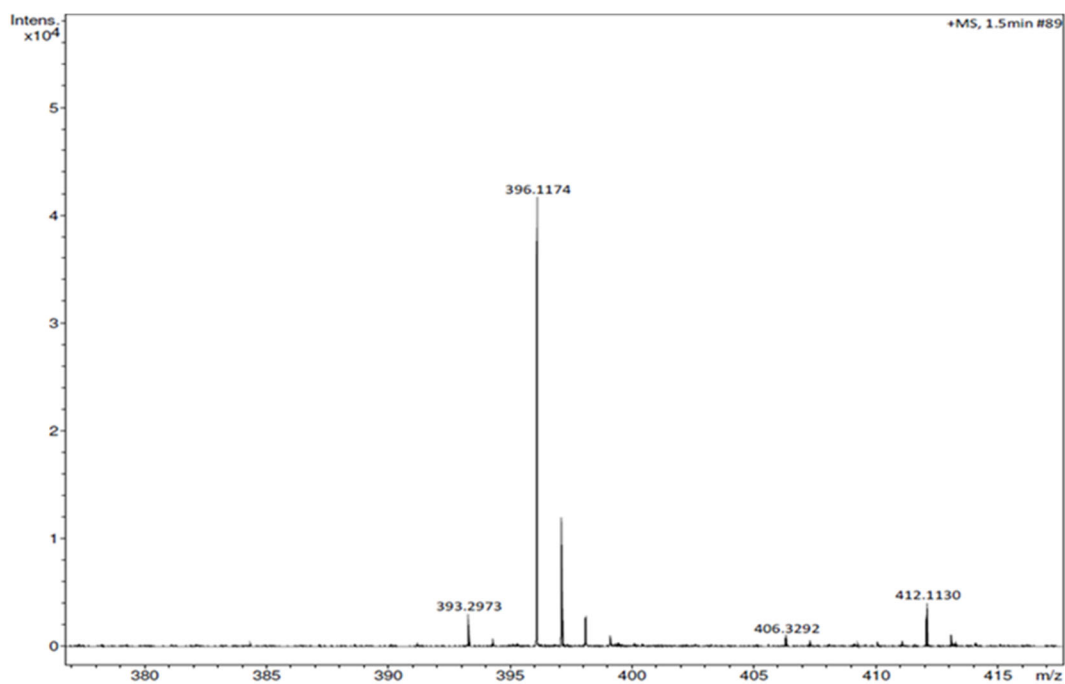
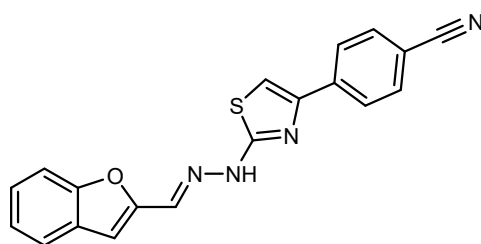
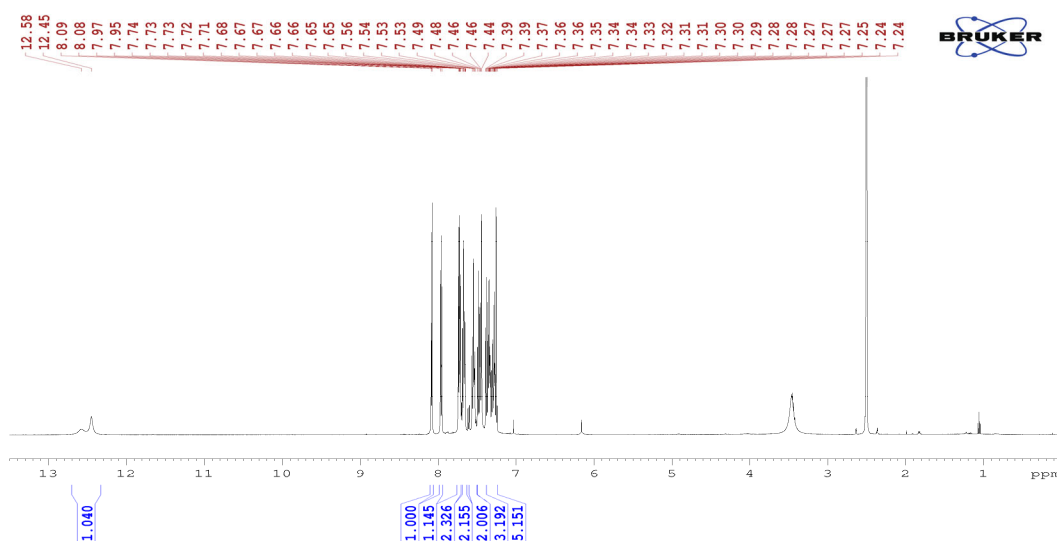
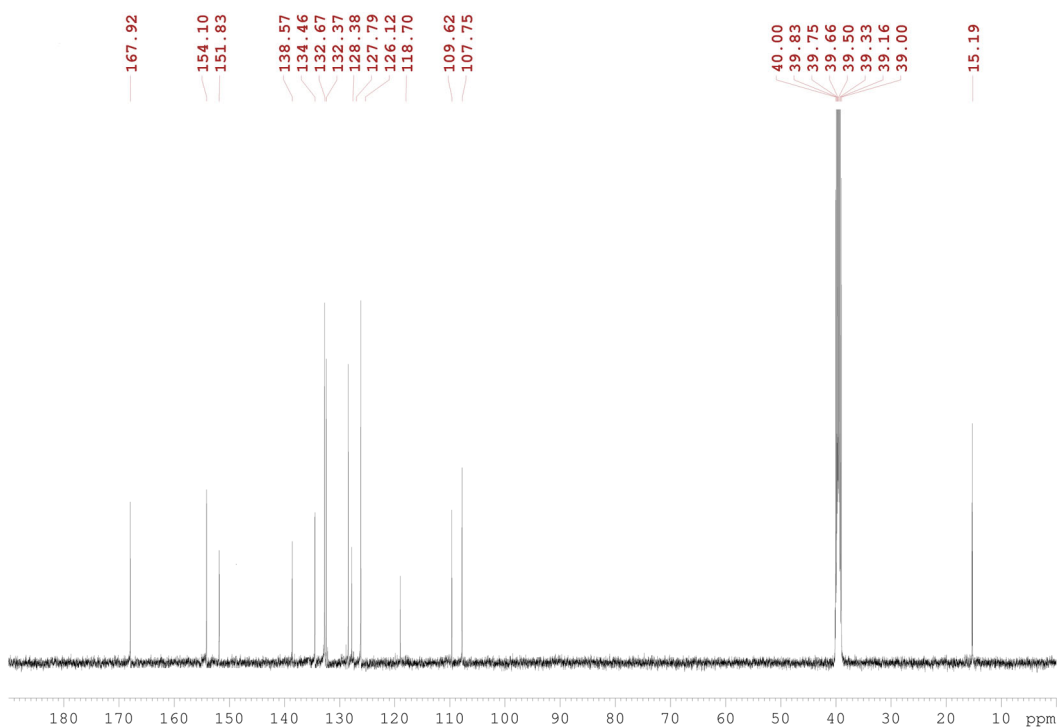


Fig S24. HRMS result of compound 5f

4-(2-(2-(benzofuran-2-ylmethylene)hydrazineyl)thiazol-4-yl)benzonitrile (**5g**)

Fig S25. ^1H -NMR spectrum of compound 5g (DMSO- d_6 , 500 MHz)Fig S26. ^{13}C -NMR spectrum of compound 5g (DMSO- d_6 , 125 MHz)

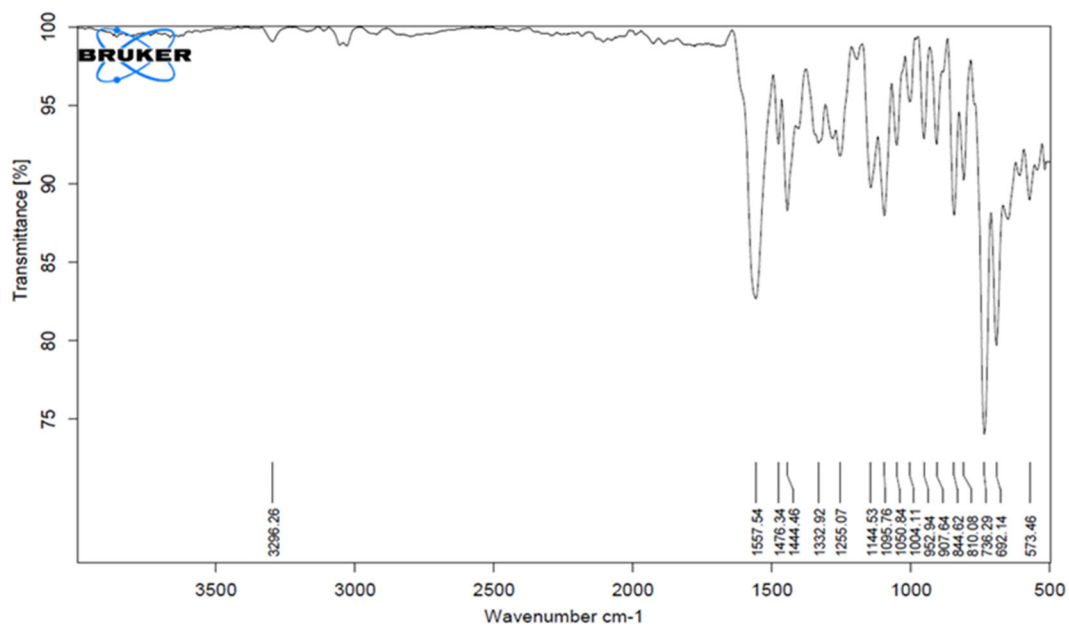


Fig S27. FTIR spectrum of compound 5g

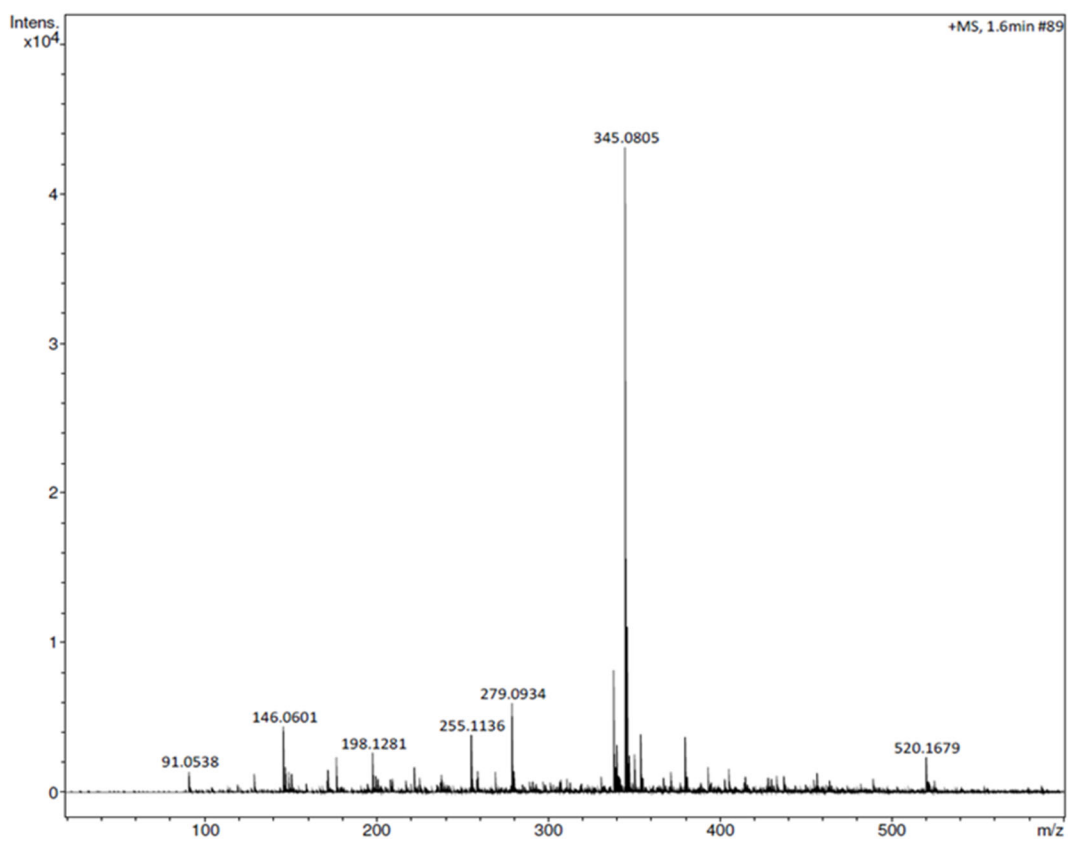
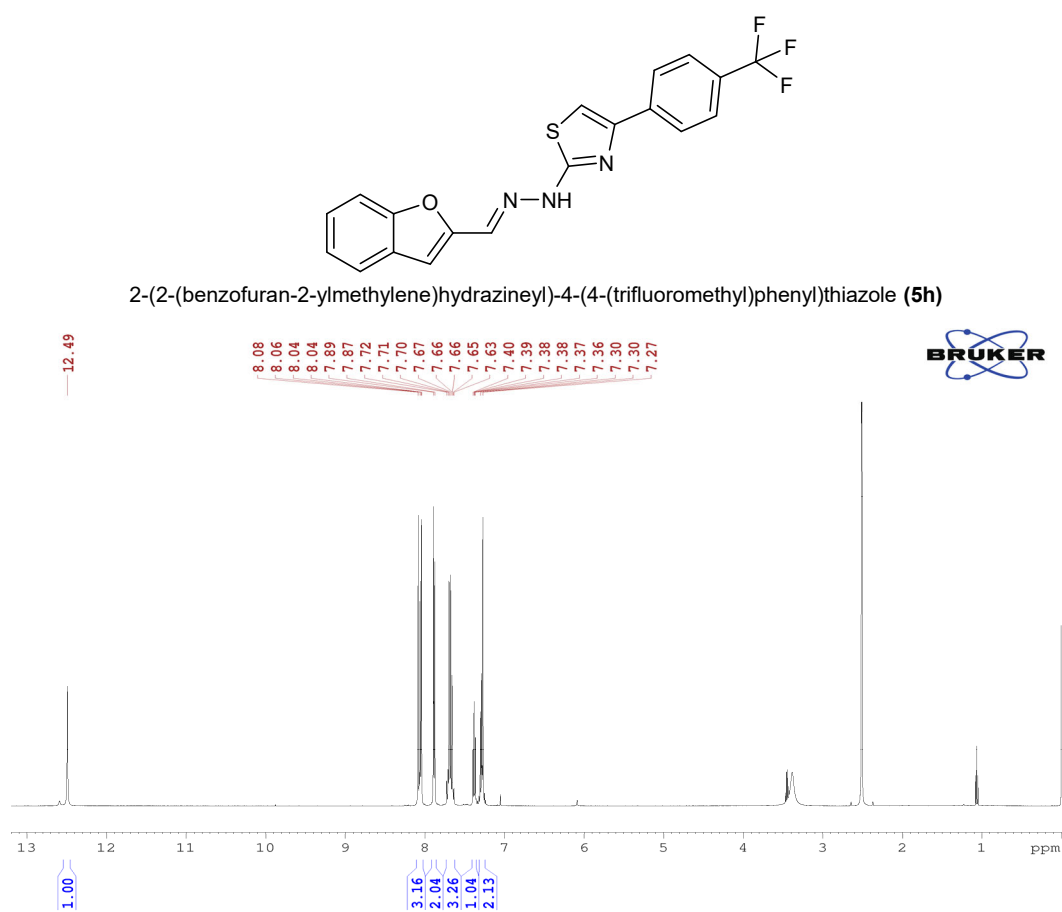
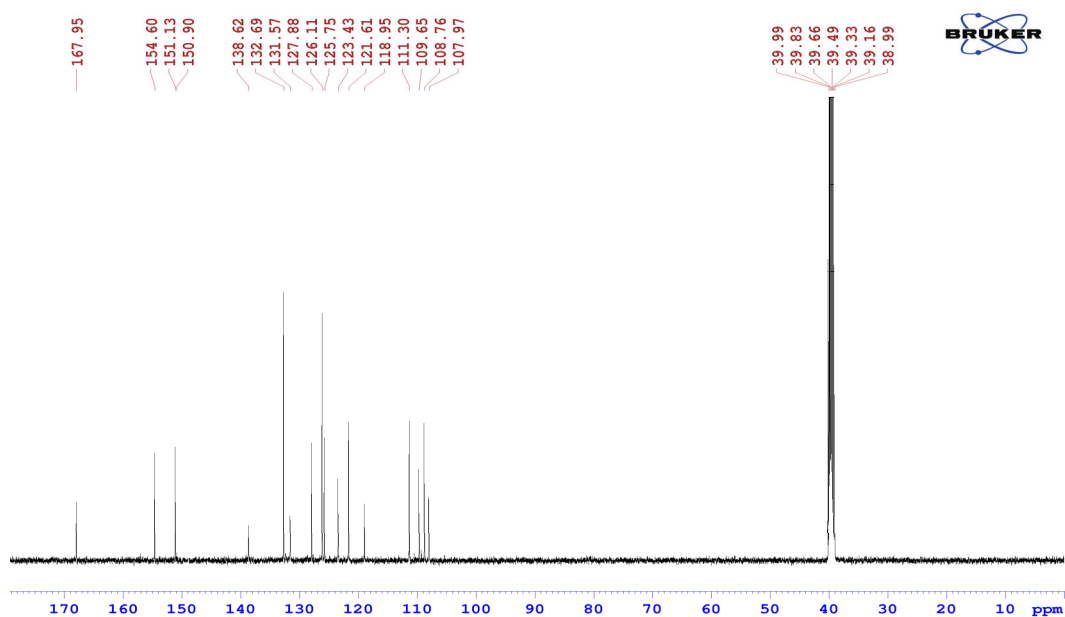


Fig S28. HRMS result of compound 5g

Fig S29. ¹H-NMR spectrum of compound 5h (DMSO-*d*₆, 500 MHz)Fig S30. ¹³C-NMR spectrum of compound 5h (DMSO-*d*₆, 125 MHz)

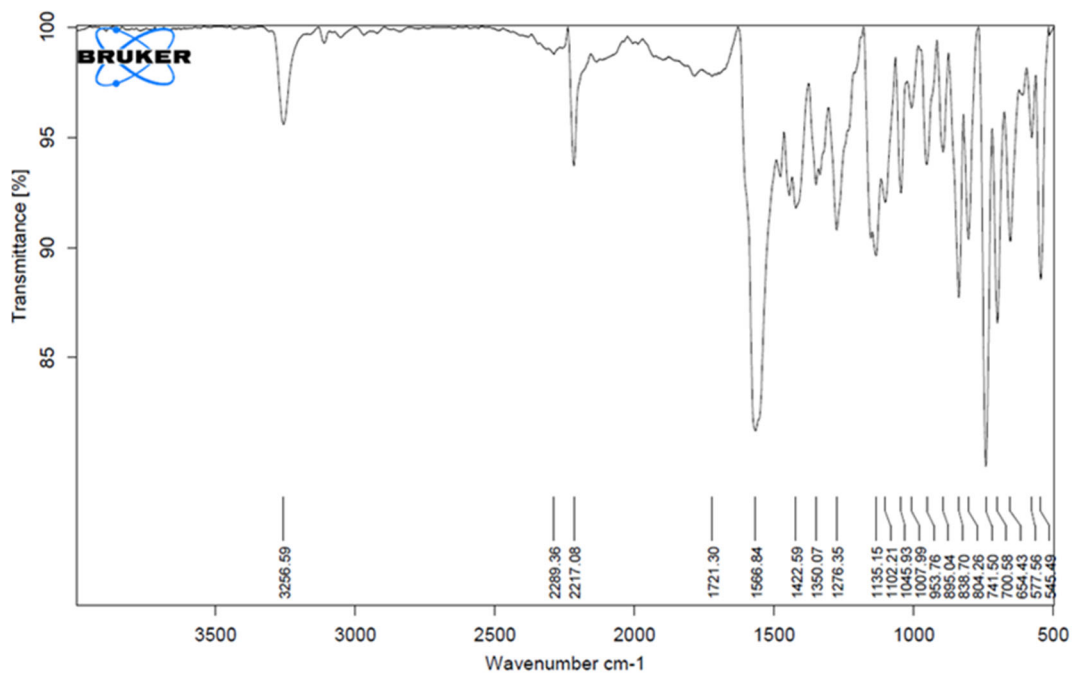


Fig S31. FTIR spectrum of compound 5h

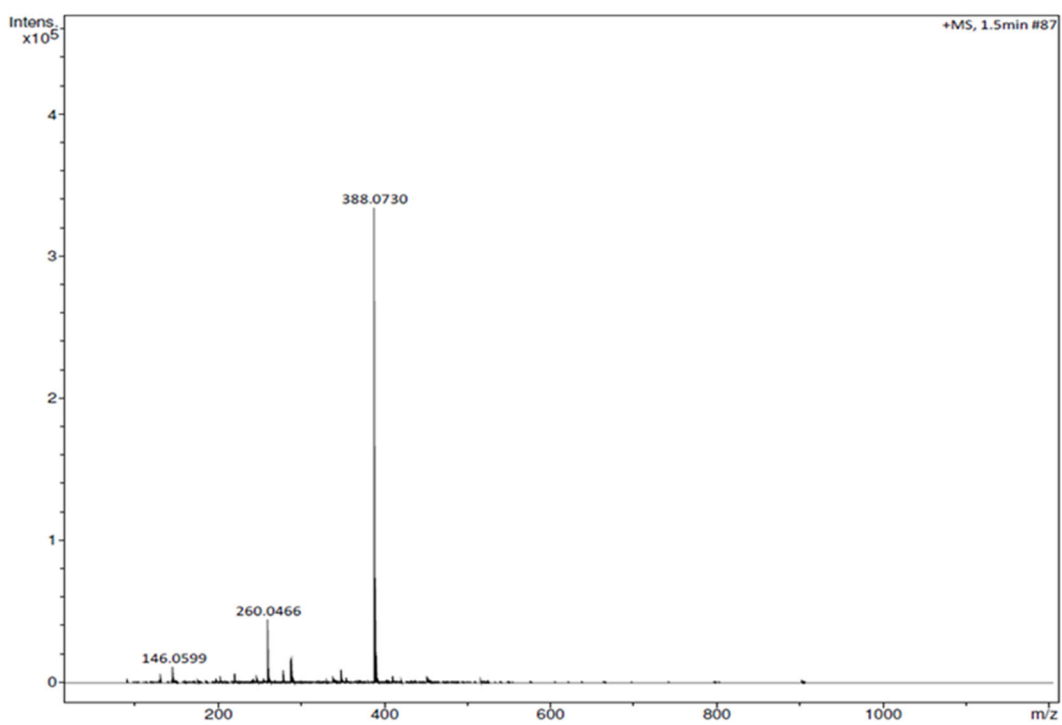


Fig S32. HRMS result of compound 5h

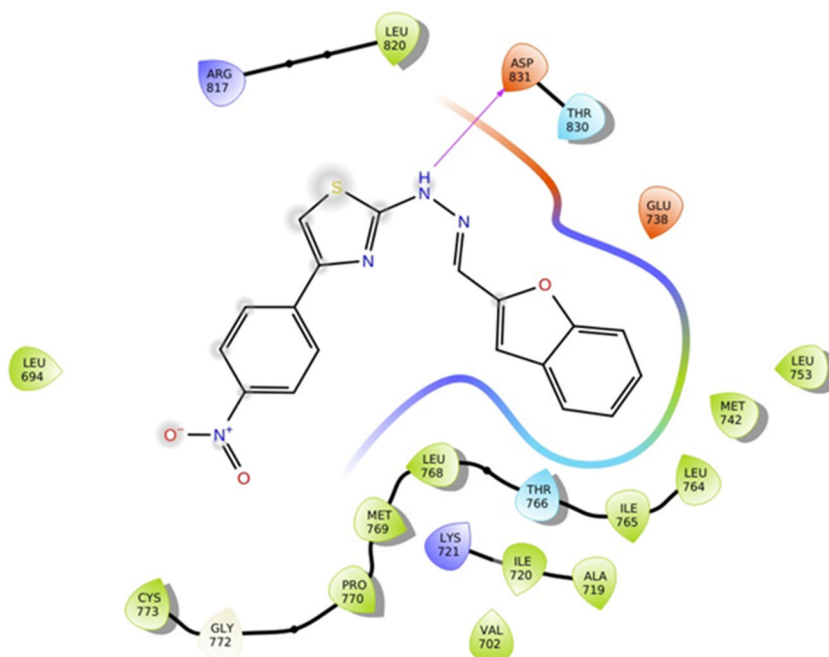


Fig S33. 2D molecular interaction of compound 5a against EGFR

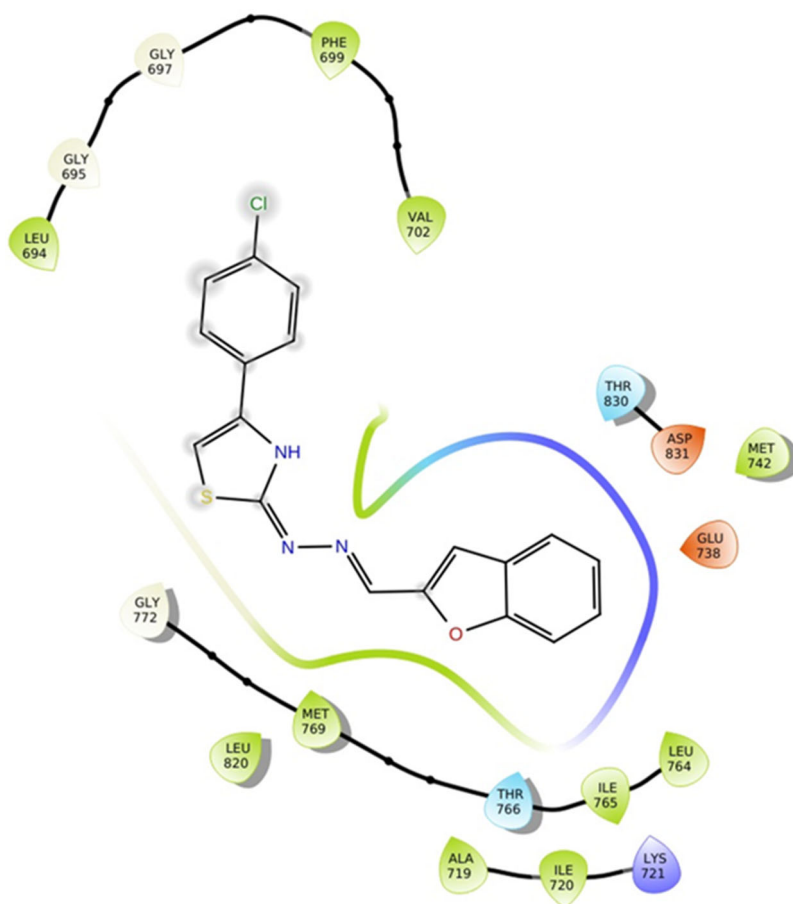


Fig S34. 2D molecular interaction of compound 5b against EGFR

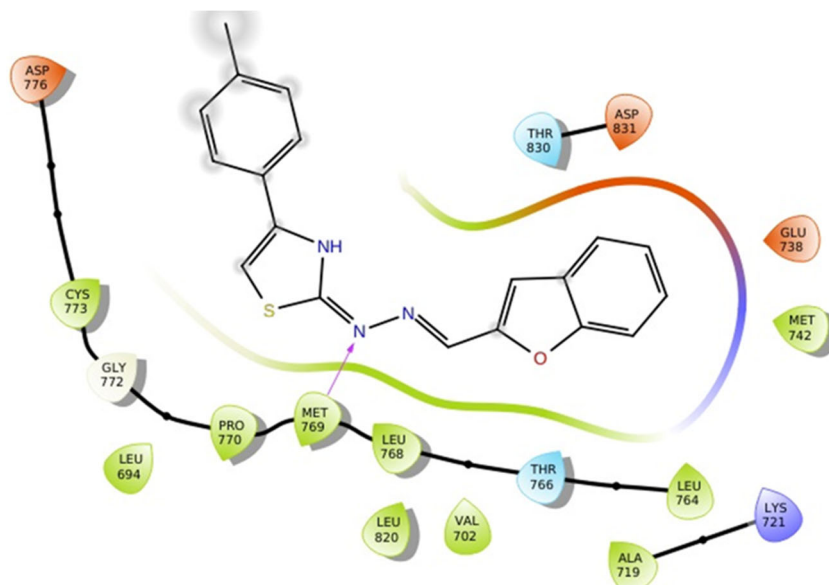


Fig S35. 2D molecular interaction of compound 5c against EGFR

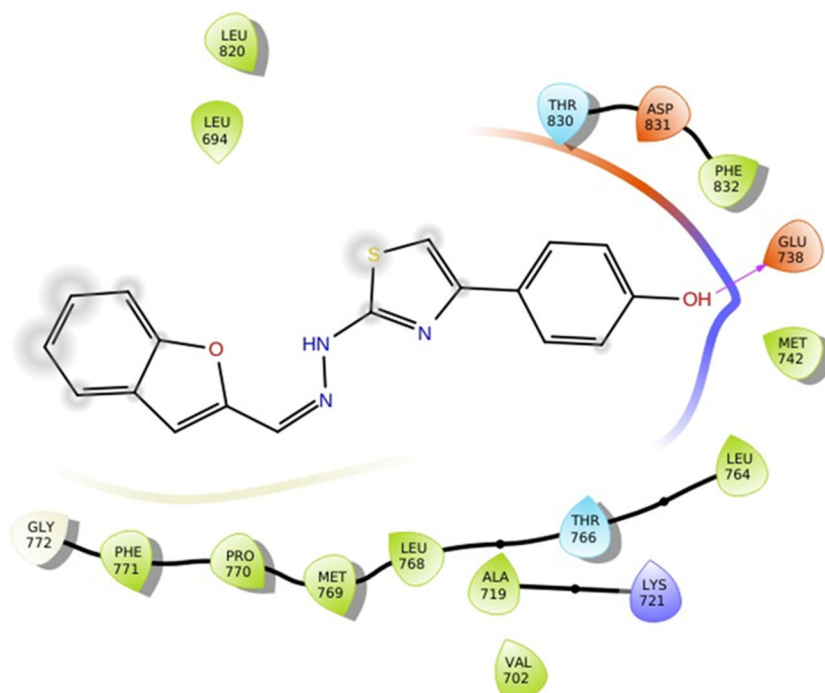


Fig S36. 2D molecular interaction of compound 5d against EGFR

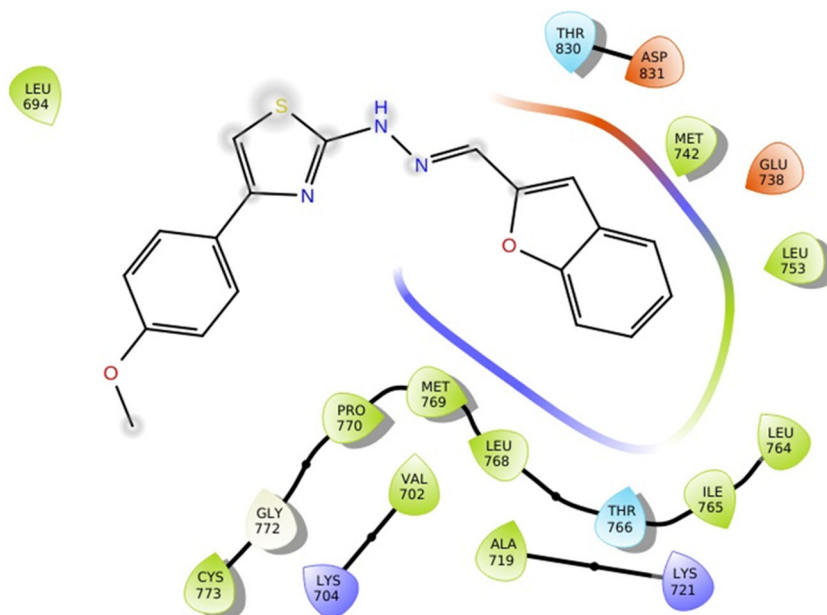


Fig S37. 2D molecular interaction of compound 5e against EGFR

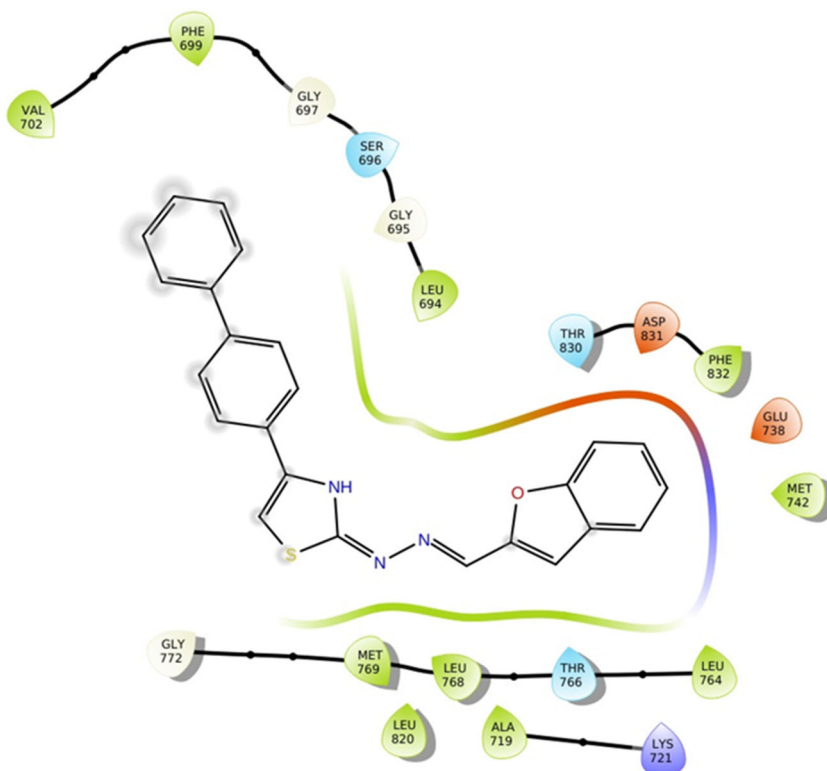


Fig S38. 2D molecular interaction of compound 5f against EGFR

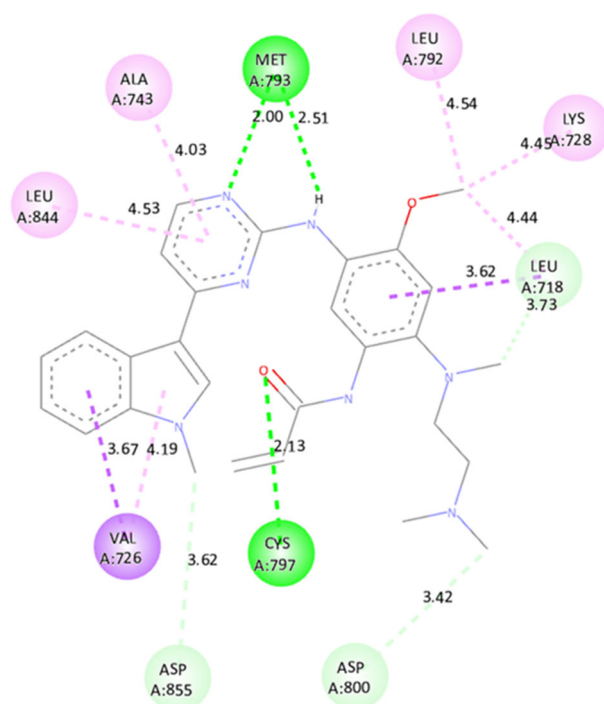


Fig S39. 2D molecular interaction of compound 5i (osimertinib) against EGFR