



Article

The Synthesis, In Vitro Bio-Evaluation, and In Silico Molecular Docking Studies of Pyrazoline–Thiazole Hybrid Analogues as Promising Anti- α -Glucosidase and Anti-Urease Agents

Yousaf Khan ¹, Shoaib Khan ², Rafaqat Hussain ^{3,*}, Aneela Maalik ^{1,*}, Wajid Rehman ³,
Mohamed W. Attwa ⁴, Rafia Masood ¹, HanyW. Darwish ⁴ and Hazem A. Ghabbour ⁵

¹ Department of Chemistry, COMSATS University Islamabad Campus, Islamabad 45550, Pakistan;

yousaf7n@gmail.com (Y.K.); rafia12@yahoo.com (R.M.)

² Department of Chemistry, Abbottabad University of Science and Technology (AUST),
Abbottabad 22500, Pakistan; shoaibkhanswati@gmail.com

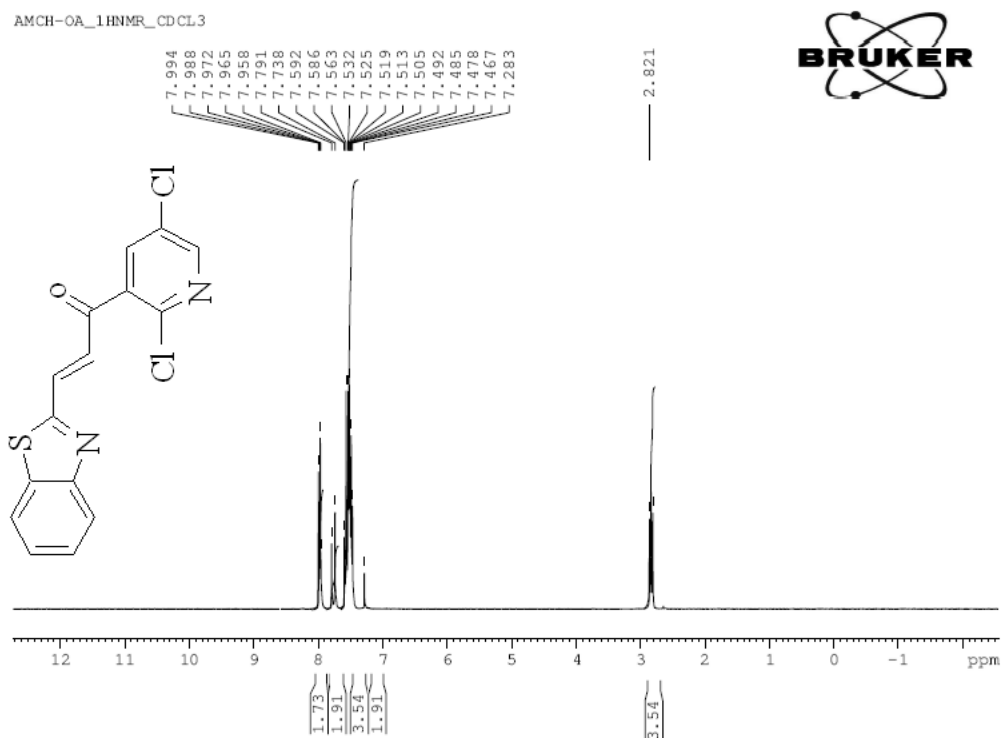
³ Department of Chemistry, Hazara University, Mansehra 21120, Pakistan; sonowaj@yahoo.com

⁴ Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University,
Riyadh 11451, Saudi Arabia; mzeidan@ksu.edu.sa (M.W.A.); hdarwish@ksu.edu.sa (H.W.D.)

⁵ School of Health and Biomedical Sciences, RMIT University, Melbourne 3083, Australia;

hazem.ghabbour@rmit.edu.au

* Correspondence: rafaqathussain0347@gmail.com (R.H.); aneela.maalik@comsats.edu.pk (A.M.)



Figure

S1. ¹HNMR for the compound **Chalcone** (E)-3-(benzo[d]thiazol-2-yl)-1-(2,5-dichloropyridin-3-yl)prop-2-en-1-one

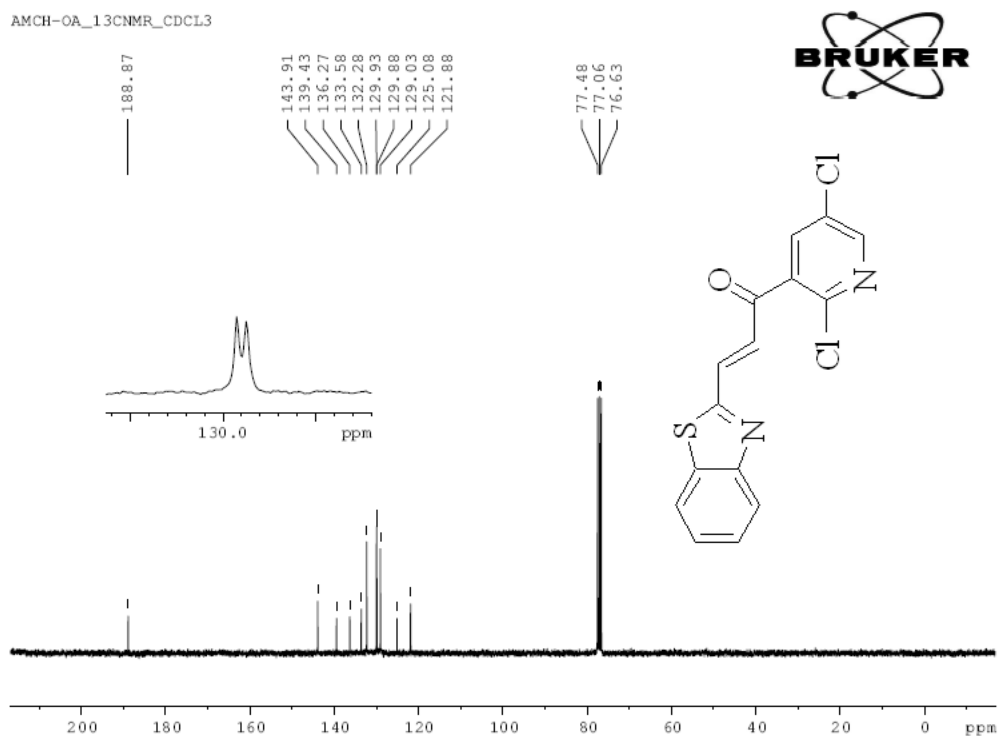


Figure S2. ¹³CNMR Spectra for the compound **Chalcone** (E)-3-(benzo[d]thiazol-2-yl)-1-(2,5-dichloropyridin-3-yl)prop-2-en-1-one

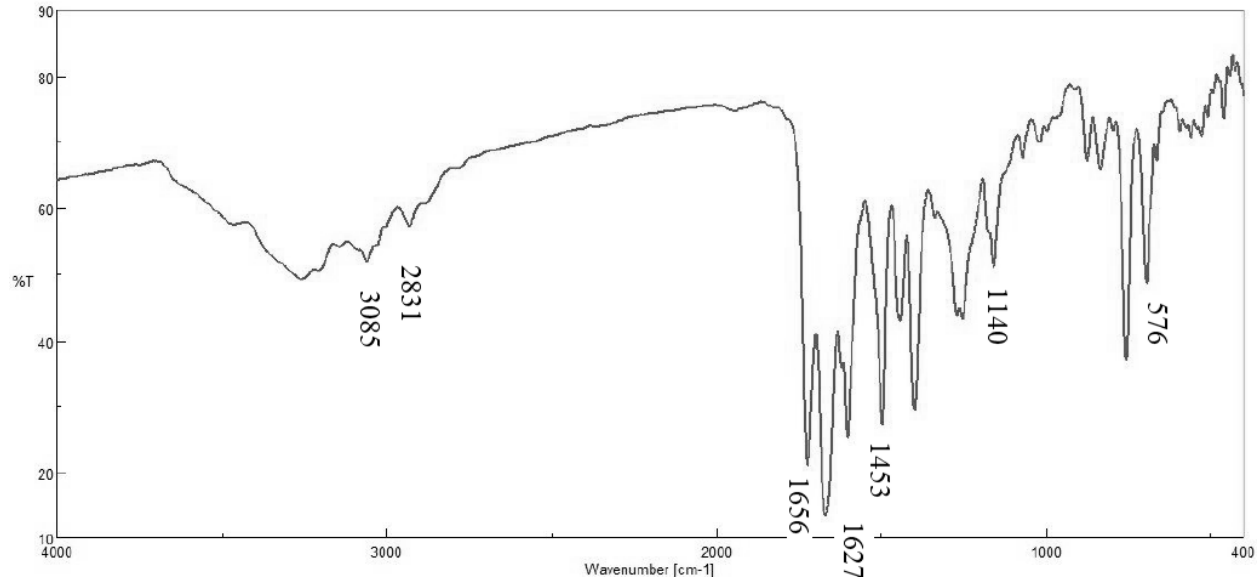


Figure S3. FTIR spectra for the compound **2(R)-2-(3-(2,5-dichloropyridin-3-yl)-1-(4-(2,5-dimethylphenyl)thiazol-2-yl)-4,5-dihydro-1H-pyrazol-5-yl)benzo[d]thiazole**

4A_13CNMR_CDCL3

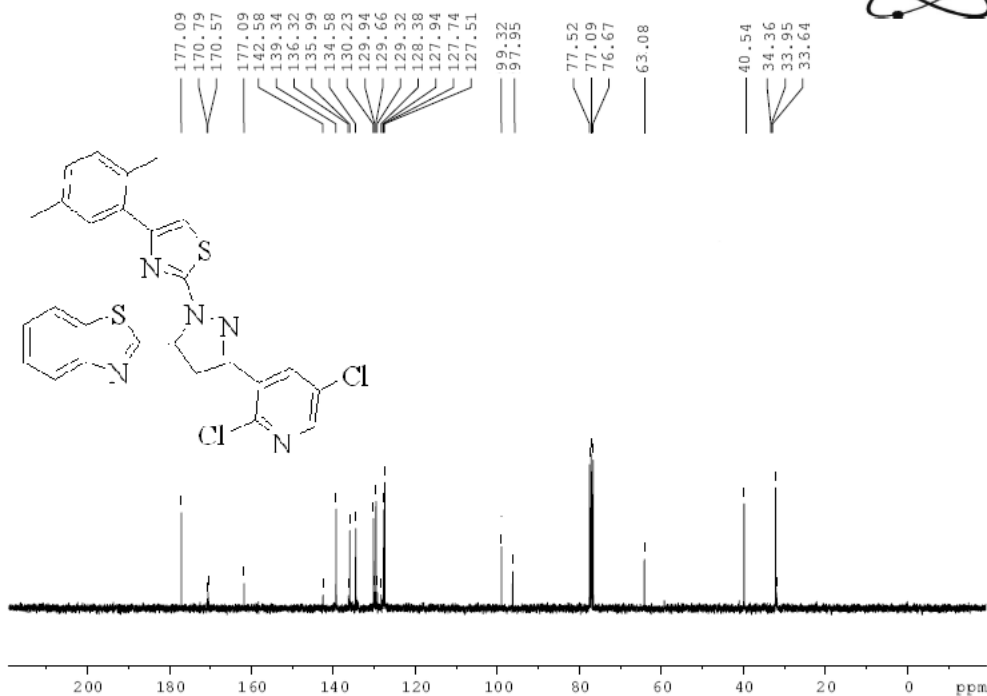


Figure S5. ¹³CNMR for the compound **2** (*R*)-2-(3-(2,5-dichloropyridin-3-yl)-1-(4-(2,5-dimethylphenyl)thiazol-2-yl)-4,5-dihydro-1H-pyrazol-5-yl)benzo[d]thiazole

5B_1HNMR_CDCL3

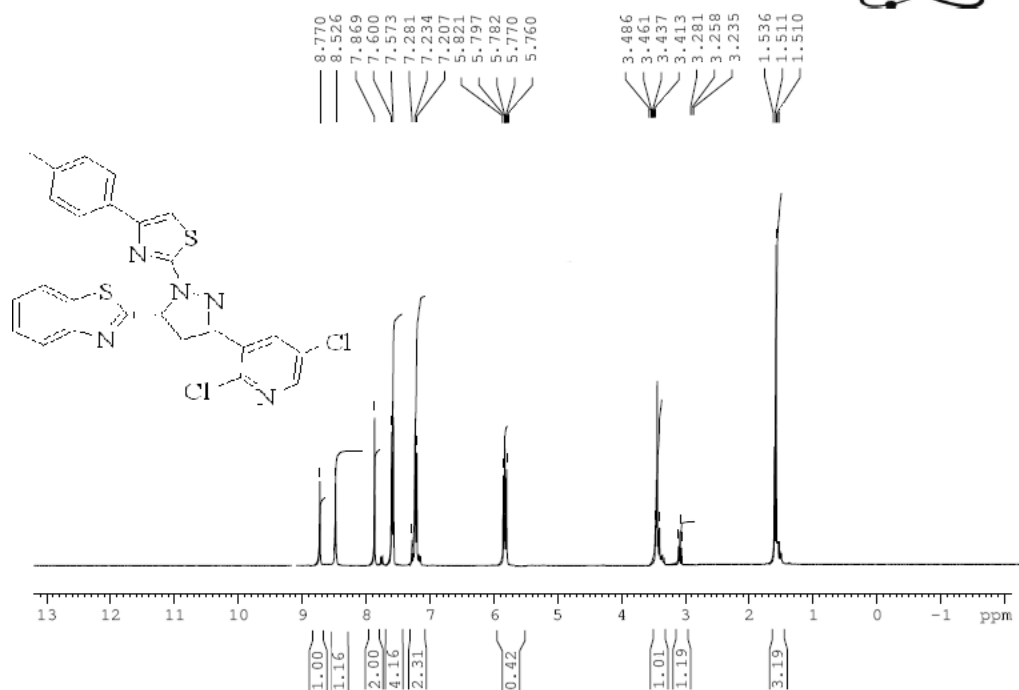
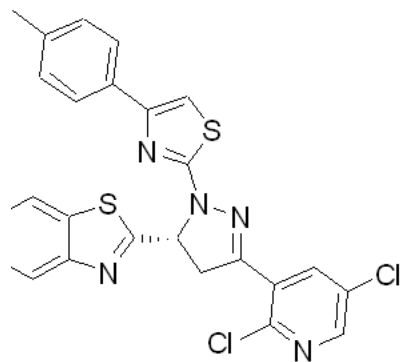


Figure S6. ¹HNMR for the compound **3** (*R*)-2-(3-(2,5-dichloropyridin-3-yl)-1-(4-(*p*-tolyl)thiazol-2-yl)-4,5-dihydro-1H-pyrazol-5-yl)benzo[d]thiazole



IR spectrum showing %T (Y-axis, 20 to 80) versus Wavenumber [cm⁻¹] (X-axis, 4000 to 400). The spectrum displays characteristic absorption bands for polyacetylene, including a broad peak around 3300 cm⁻¹, a sharp peak at 1632 cm⁻¹, and several peaks in the fingerprint region below 1500 cm⁻¹. Labeled peaks include 3286, 3064, 2873, 1687, 1632, 1077, and 598 cm⁻¹.

Figure S8, FTIR spectra for the compound **7(R)**-2-(2-(5-(benzo[d]thiazol-2-yl)-3-(2,5-dichloropyridin-3-yl)-4,5-dihydro-1H-pyrazol-1-yl)thiazol-4-yl)-5-fluorophenol

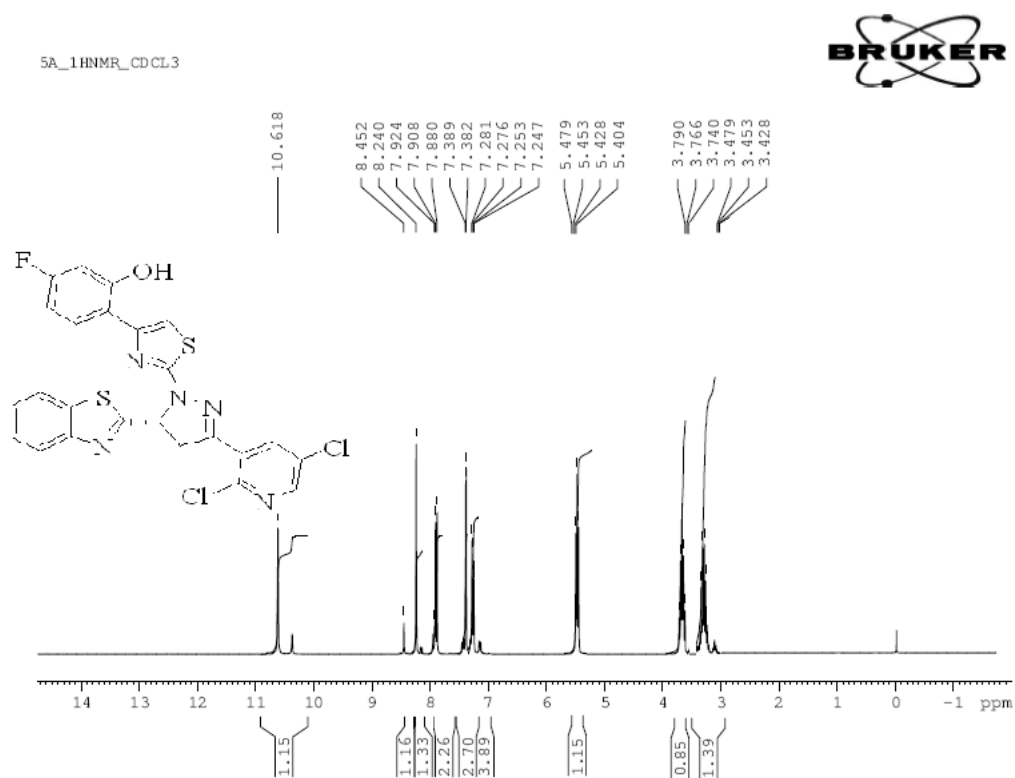


Figure S9. ^1H NMR for the compound **7** (R)-2-(2-(5-(benzo[d]thiazol-2-yl)-3-(2,5-dichloropyridin-3-yl)-4,5-dihydro-1H-pyrazol-1-yl)thiazol-4-yl)-5-fluorophenol

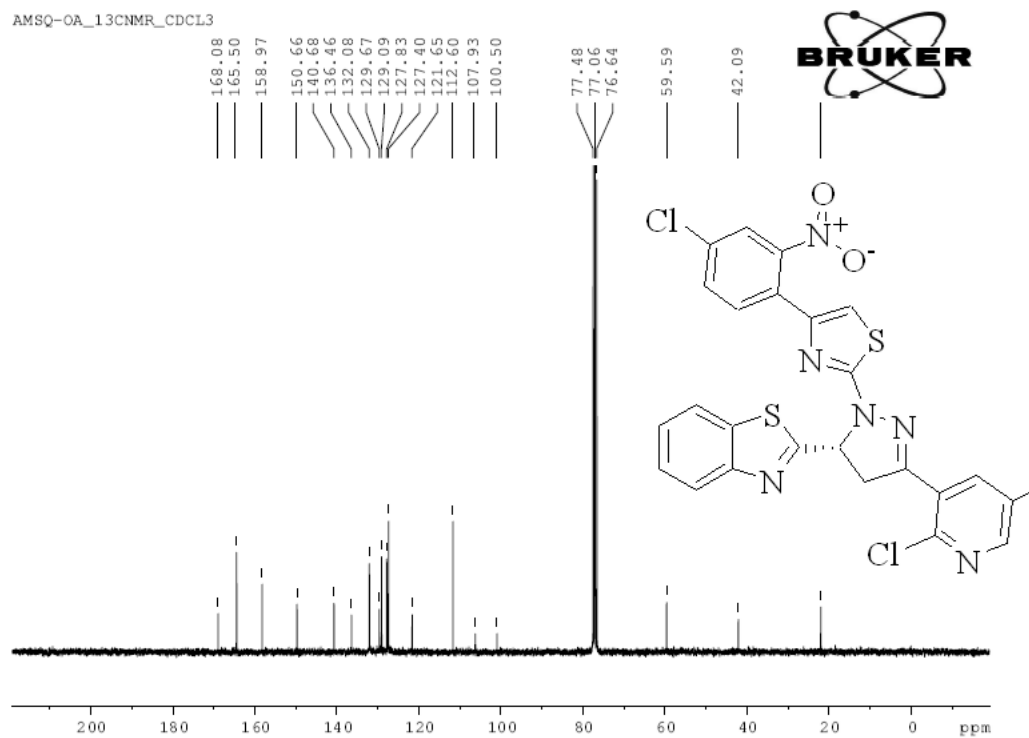


Figure S10. ^{13}C NMR for the compound **9** (*R*)-2-(1-(4-(4-chloro-2-nitrophenyl)thiazol-2-yl)-3-(2,5-dichloropyridin-3-yl)-4,5-dihydro-1H-pyrazol-5-yl)benzo[d]thiazole

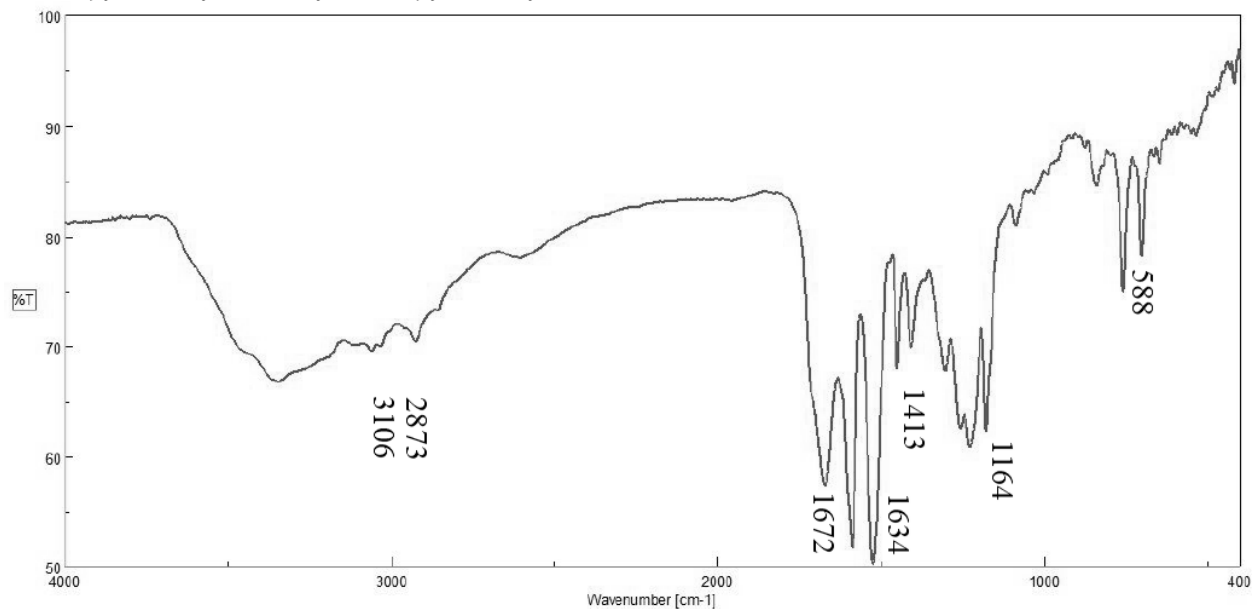


Figure S11. FTIR spectra for the compound **11** (*R*)-2-(3-(2,5-dichloropyridin-3-yl)-1-(4-(2-fluorophenyl)thiazol-2-yl)-4,5-dihydro-1H-pyrazol-5-yl)benzo[d]thiazole

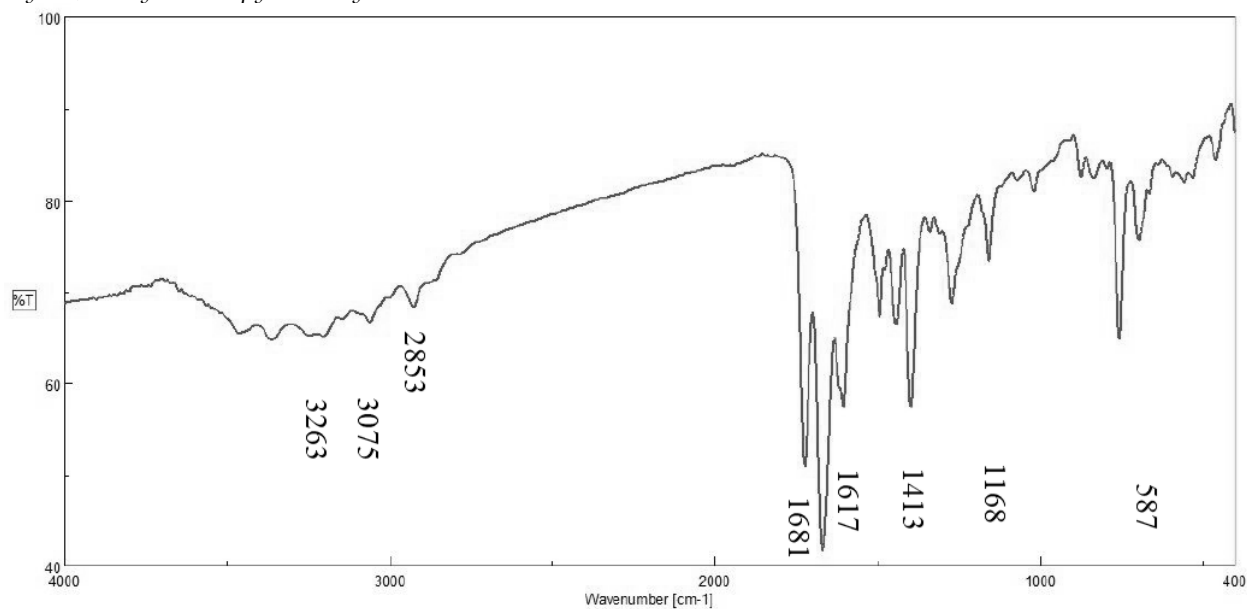


Figure S12. FTIR spectra for the compound **14** (*R*)-2-(2-(5-(benzo[d]thiazol-2-yl)-3-(2,5-dichloropyridin-3-yl)-4,5-dihydro-1H-pyrazol-1-yl)thiazol-4-yl)-3,5-dichlorophenol