Supplementary Information

Effect of temperature and solvents on thermo-physical properties of pyrimidine substituted thiazolidinone derivatives at three different temperatures

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Supplemental Materials

Content

- Synthetic procedure of AZ_1 and AZ_2
- Spectral analysis of AZ_1 and AZ_2
- IR, ^{1}H NMR, ^{13}C NMR, and Mass spectra of compounds AZ_1 and AZ_2.

Procedure for synthesis of 5-(4-fluorobenzylidene)-2-(furan-2-yl)-3-(pyrimidin-2-yl)thiazolidin-4-one (AZ_1) and 2-(furan-2-yl)-5-(4-methoxybenzylidene)-3-(pyrimidin-2-yl)thiazolidin-4-one (AZ_2).

2-(furan-2-yl)-3-(pyrimidin-2-yl)thiazolidin-4-one was dissolved in ethanol (0.01 mol), and various aromatic aldehydes (0.01 mol) were then added. The catalyst for the reaction was sodium ethoxide. The reaction mixture was refluxed at 50–60 °C for 4–6 hours. The finished reaction mixture was poured onto crushed ice after being allowed to cool at ambient temperature to get the desired compounds **(AZ_1 and AZ_2).** The produced product underwent filtering, distilled water washing, vacuum oven drying, and recrystallization.

5-(4-fluorobenzylidene)-2-(furan-2-yl)-3-(pyrimidin-2-yl)thiazolidin-4-one, AZ_1: Yield 52%, solid, dirty white, m.p. 162-164°C. IR (KBr, νmax, cm-1): 683 (C-S), 1177 (C-F), 1287 (C-O-C), 1334 (-C-N), 1598 (-C=N-), 1687 (C=O), 3066 (C-H). 1H NMR spectrum (500 MHz, DMSO-d6, δ ppm): 6.36 (t, J = 7.53 Hz,1H, C=CH), 6.43 – 6.48 (m, 2H), 6.96 (t, J = 7.51 Hz, 1H, C=CH), 7.19 – 7.26 (m, 2H), 7.47 (d, J = 7.46 Hz, 1H, O-CH), 7.57 – 7.64

(m, 2H), 7.81 (s, 1H, C=CH), 8.42 (d, J = 7.53 Hz, 2H, CH=C-CH). 13C NMR spectrum (125 MHz, DMSO-d6, δ ppm): δ 58.02, 109.38, 110.01, 113.47, 115.70, 115.86, 128.82, 129.88, 129.91, 129.93, 129.94, 134.95, 142.54, 147.89, 153.08, 157.72, 159.80, 161.82, 163.06. LCMS (ESI) m/z: 354.3307 [M+1]+. Anal. calcd. for C18H12FN3O4S: C, 61.18; H, 3.42; N, 11.89%. Found: C, 61.17; H, 3.44; N, 11.87%.

2-(furan-2-yl)-5-(4-methylbenzylidene)-3-(pyrimidin-2-yl)thiazolidin-4-one, AZ_2: Yield 31%, solid, white, m.p. 164-166°C. IR (KBr, νmax, cm-1): 665 (C-S), 1226 (C-O-C), 1279 (-C-N), 1516 (-C=N-), 1726 (C=O), 2927 (C-CH3), 3055 (C-H). 1H NMR spectrum (500 MHz, DMSO-d6, δ ppm): 2.41 (d, J = 0.81 Hz, 3H, C-CH3), 6.36 (t, J = 7.52 Hz, 1H, C=CH), 6.43 – 6.48 (m, 2H), 6.93 – 7.00 (m, 1H), 7.29 – 7.35 (m, 2H), 7.44 – 7.51 (m, 3H), 7.82 (s, 1H, C=CH), 8.42 (d, J = 7.55 Hz, 2H, CH=C-CH). 13C NMR spectrum (125 MHz, DMSO-d6, δ ppm): δ 23.69, 58.54, 109.90, 110.53, 113.99, 128.63, 129.34, 129.62, 131.09, 135.49, 139.41, 143.06, 148.40, 153.60, 158.24, 163.72. HRMS (ESI) m/z: 350.4136[M+1]+. Anal. calcd. for C19H15N3O2S: C, 65.31; H, 4.33; N, 12.03%. Found: C, 65.33; H, 4.31; N, 12.05%.

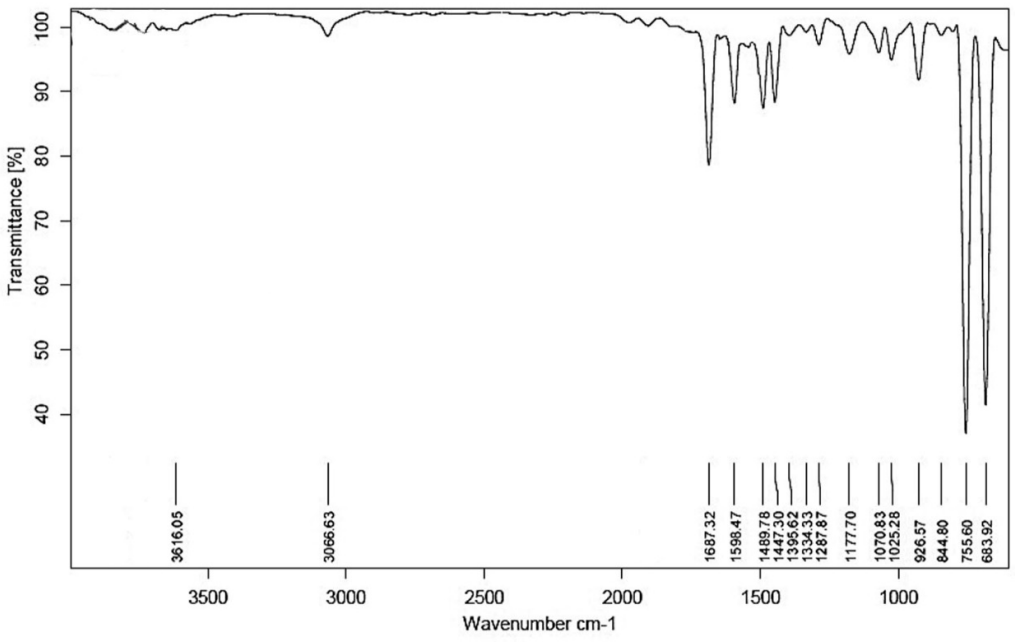

Figure 1: IR spectrum of compound AZ_1

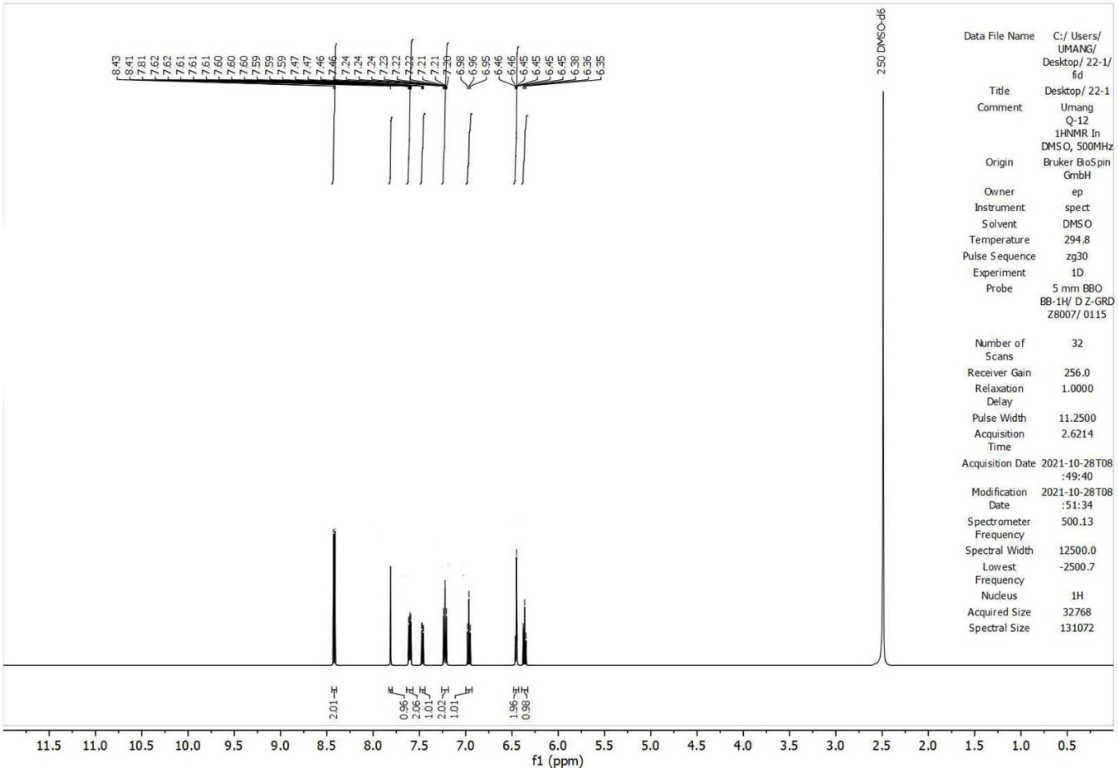

Figure 2: ^{1}H NMR spectrum of compound AZ_1

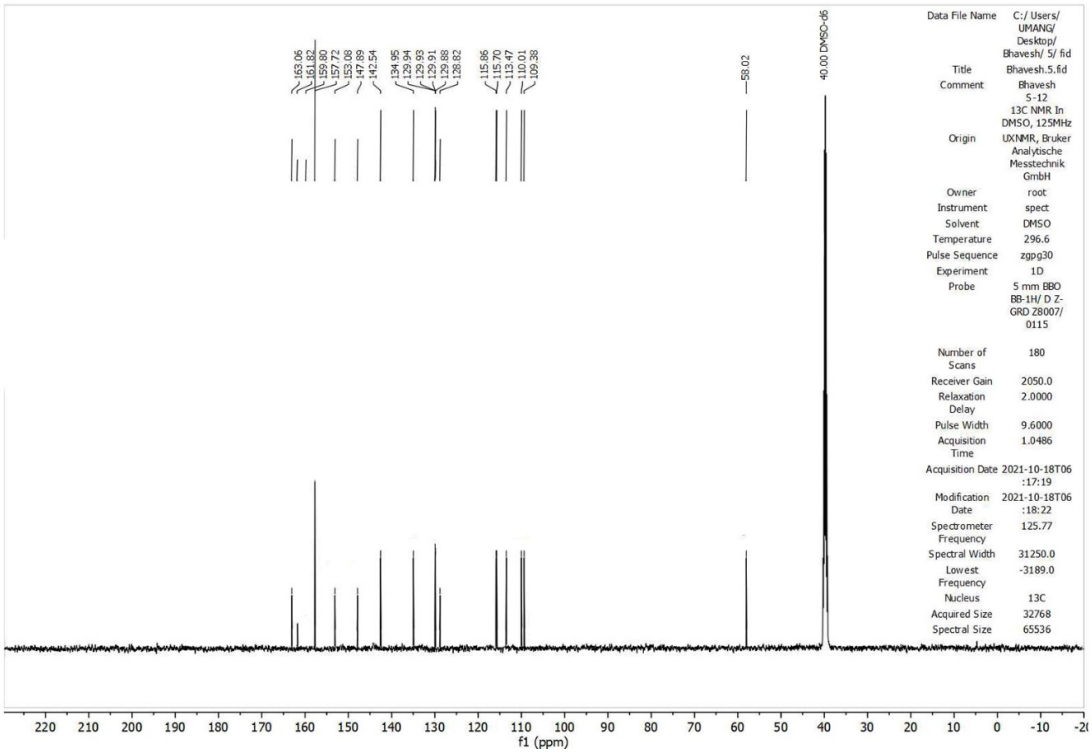

Figure 3: ^{13}C NMR spectrum of compound AZ_1

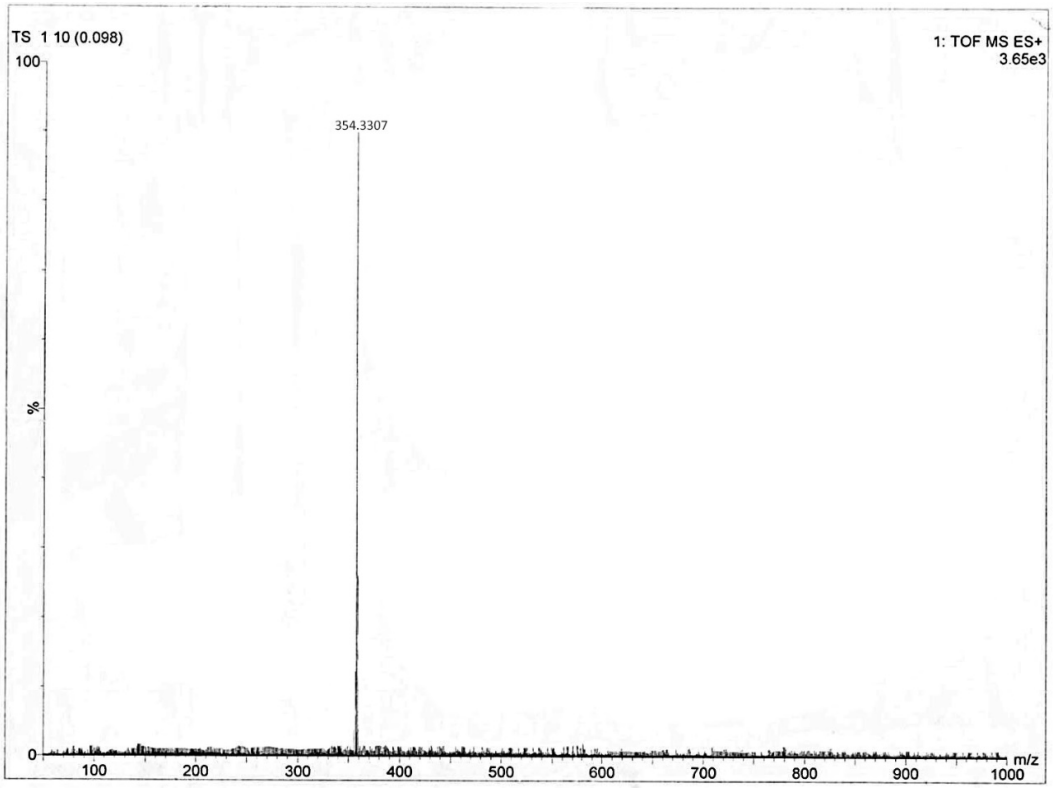

Figure 4: Mass spectrum of compound AZ_1

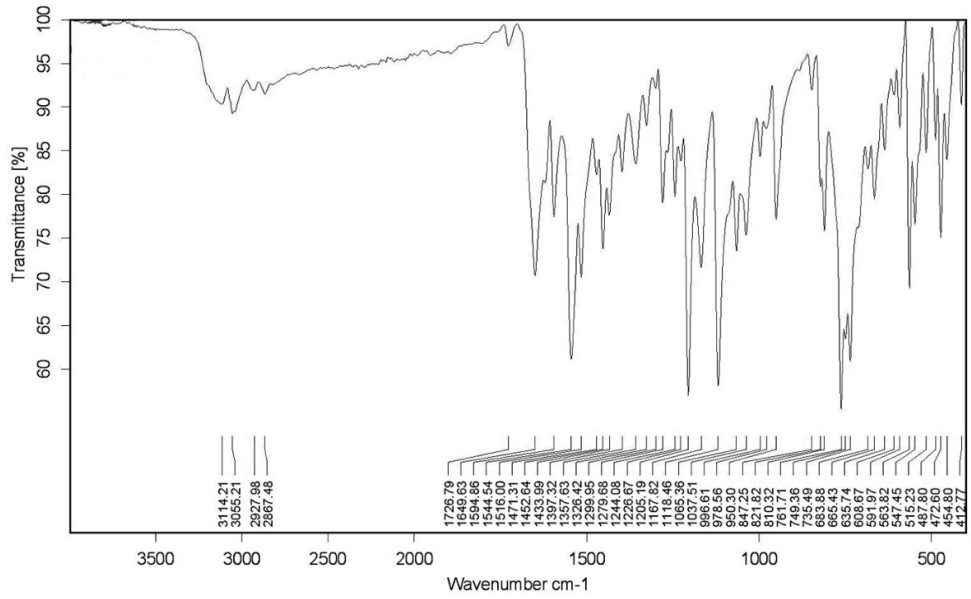

Figure 5: IR spectrum of compound AZ_2

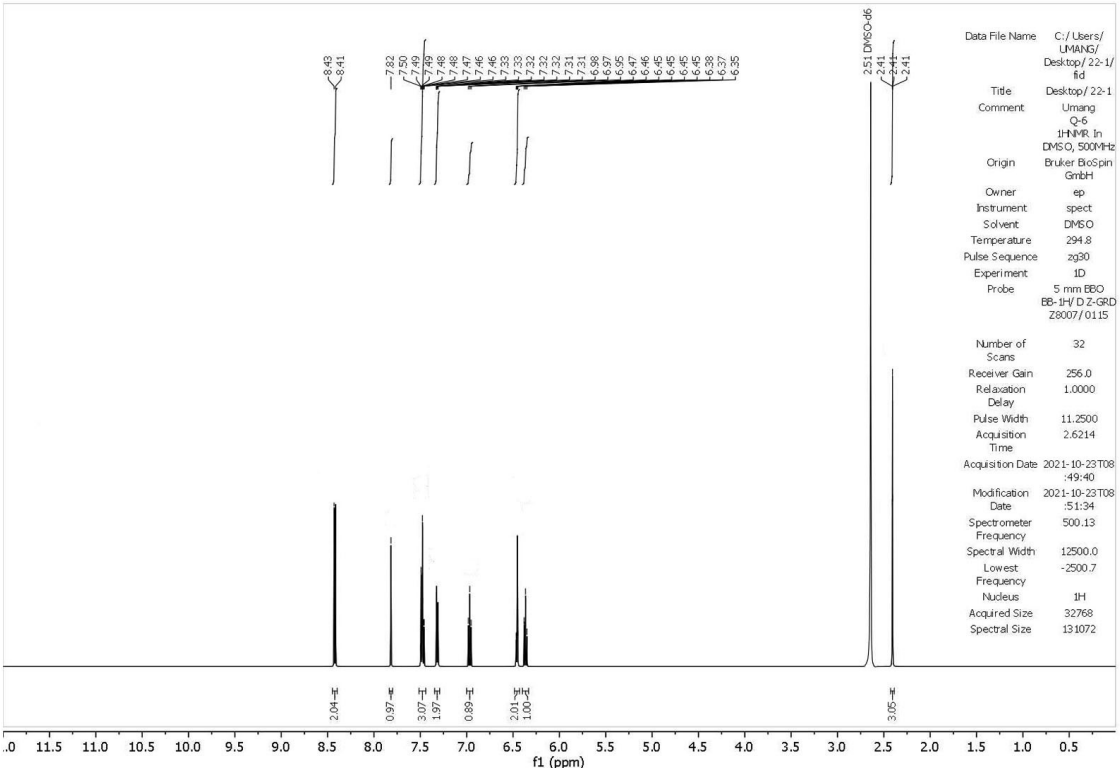

Figure 6: ^{1}H NMR spectrum of compound AZ_2

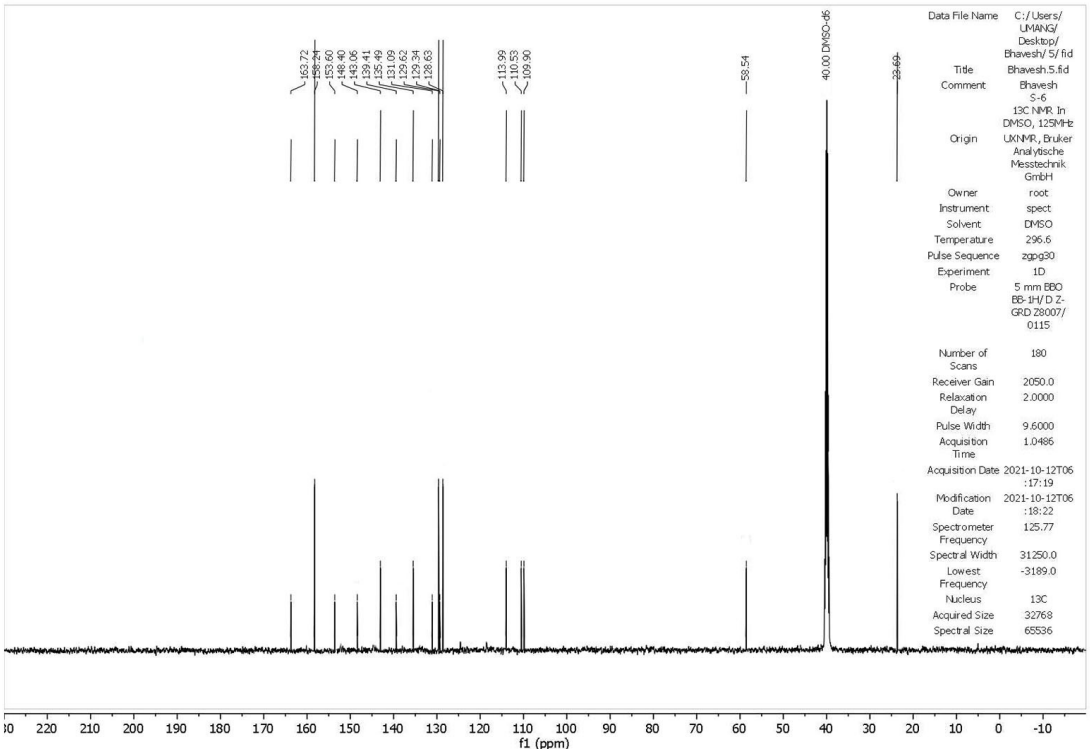

Figure 7: ^{13}C NMR spectrum of compound AZ_2

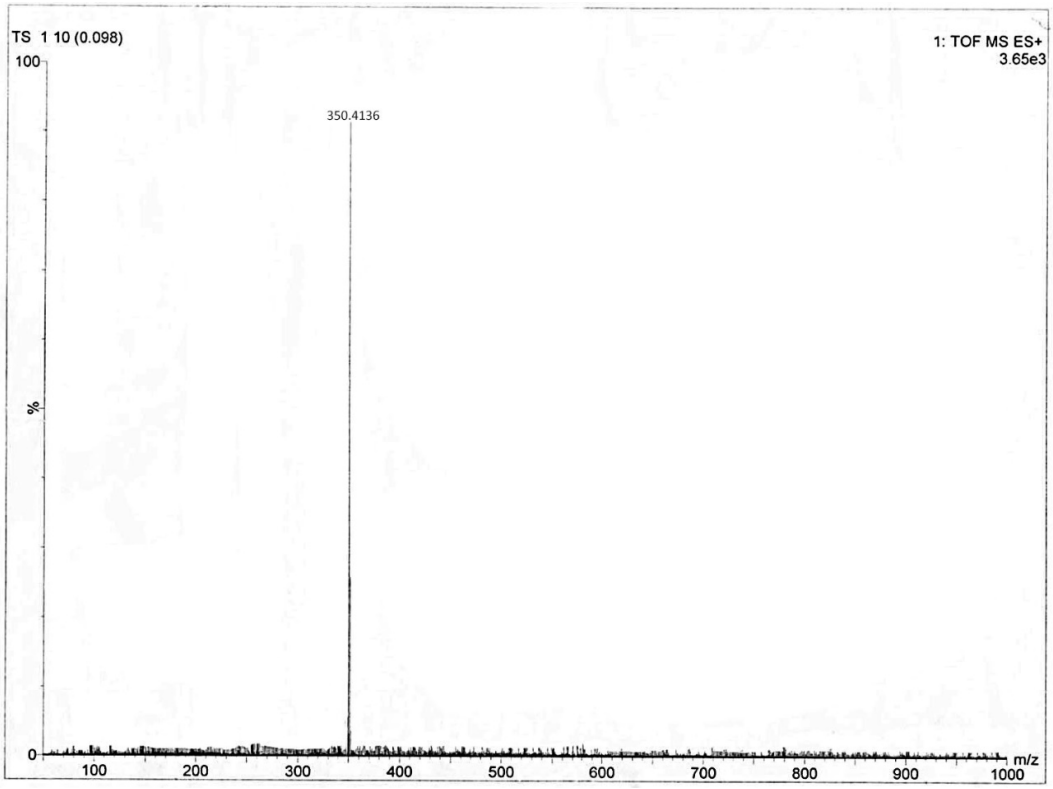

Figure 8: Mass spectrum of compound AZ_2