Supporting Information

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Efficient synthesis of benzylidene semicarbazones from aromatic aldehydes by urea-hydrogen peroxide (UHP)

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S1: *General Procedure for the Synthesis of 1-benzylidene semicarbazones Derivatives* ***2a-h***

A mixture of the aldehyde (**1a-h**) (1 mmol), ammonium acetate (1mmol) and UHP (1mmol) dissolved in acetonitrile (5ml) and the reaction mixture was refluxed. The completion of the reaction was monitored by thin layer chromatography (TLC) (ethyl acetate/n-hexane 3:7). After the completion of the reaction, the reaction mixture was left to cool to room temperature and resulting precipitate was collected by suction filtration, then was washed with water, and dried under vacuum. The dried yellow or white solids were recrystallized from ethanol to afford the desired product as yellow or white crystals.

1-Benzylidenesemicarbazide (**2a**): white crystal, m. p. : 218-220, Lit.[1]: 222°C. IR (cm^{-1}): 1663, 1614, 1471, 1395, 1262, 1091,703, 590. ^{1}H NMR (ppm): 7.41(br s , 1H) , 7.49 (t,J=7.4$_{Hz}$, 2H) , 7.6 (t,J=7.4$_{Hz}$, 1H) , 7.96 (d, J =7.2$_H$, 2H) , 8.06 (br s , 1H)

*1-(4-Methylbenzylidene) semicarbazide (**2b**):* white crystal, m. p. : 230-234. Lit.[1]:234 °C. IR (cm^{-1}): 2854 ,1629 , 1461 , 1399 , 1268 , 670. ^{1} H NMR(ppm): 1.82 (s , 1H) , 2.35 (s , 3H) , 7.29 (d, J=8Hz , 2H) , 7.41(br s , 1H) , 7.86 (d, J=8.2Hz , 2H) , 8.1(br s , 1H).

*1-(4-Methoxybenzylidene) semicarbazide (**2c**):* white crystal, m. p.:208-211. Lit.[1]:210°C. IR(cm^{-1}): 3362 , 3208 , 2949 ,2846 , 1701 , 1637 , 1469 , 1402 , 1250 , 1169 , 1086 , 1017 , 758. ^{1}H NMR(ppm): 3.81 (s , 3H) , 7.01(d, J=8.8Hz , 2H) ,7.36 (br s , 1H) , 7.98 (d, J=8.8 , 2H) , 8.12 (br s , 1H) , 10.38 (br s , 1H).

*1-(4-chlorobenzylidene) semicarbazide (**2d**):* white crystal, m. p.: 231-233. Lit.[1]: 233 °C. IR(cm^{-1}): 3350 , 3219 , 1662 , 1614 , 1467 , 1397 , 1259 , 1088 , 666. HNMR(ppm): 7.44 (br s , 1H) , 7.56 (d, J=8.5Hz , 2H) , 7.96 (d, J=8.6Hz , 2H) , 7.99 (br s , 1H) , 10.63(s , 1H).

References

[1] Shriner, Ralph L., Hermann, Christine K. F., Morrill,Terence C., Curtin, David Y., Fuson, Reynold C., The Systematic Identification of Organic Compounds, 8th Edition, John Wiley & Sons, NewYork, **2004**.

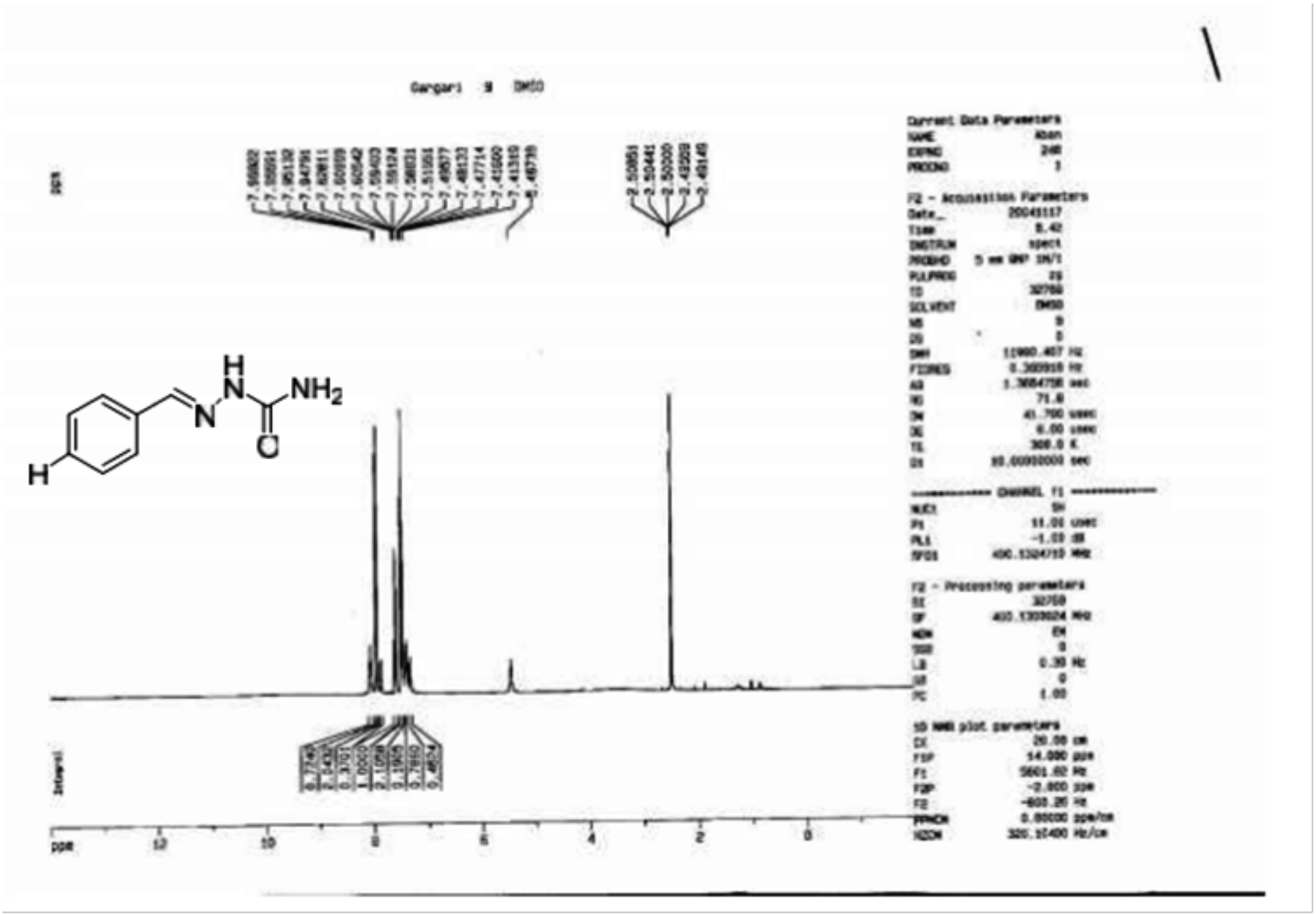

Figure S1 : ^{1}H NMR (DMSO-d_6,, 400 MHz) spectrum of compound **2a**

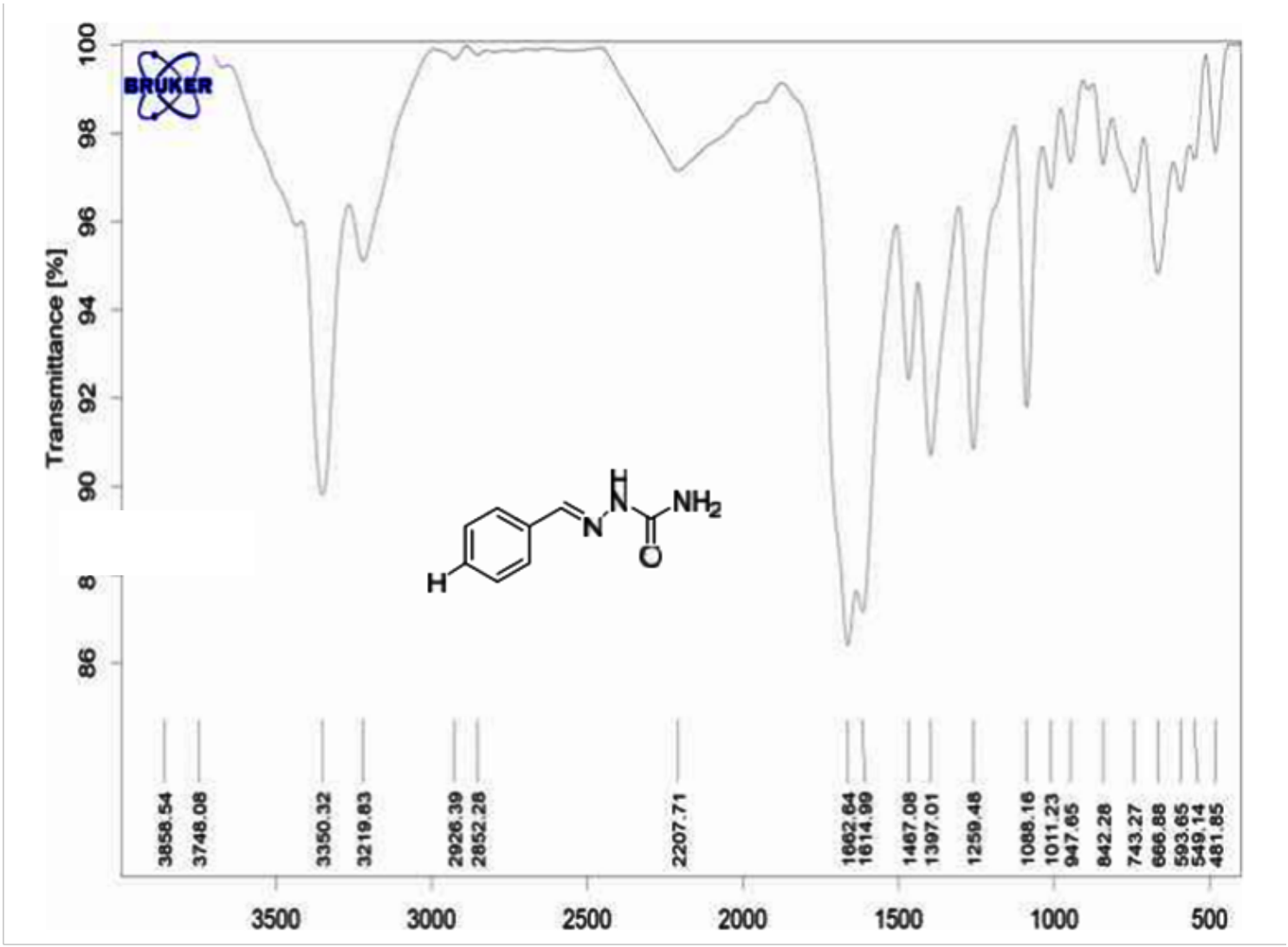

Figure S2 : FT-IR spectrum of compound **2a**

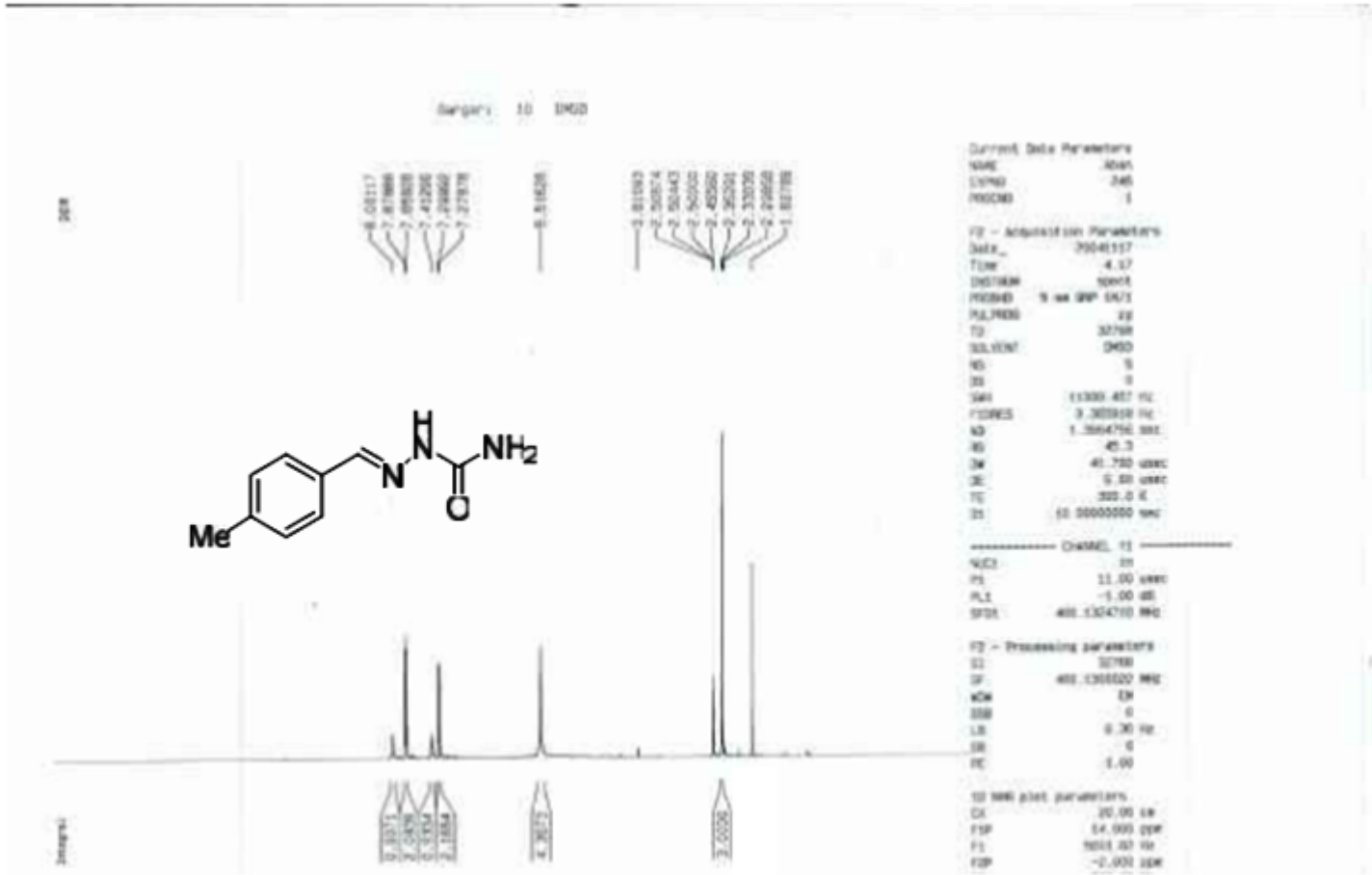

Figure S3 : ^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of compound **2b**

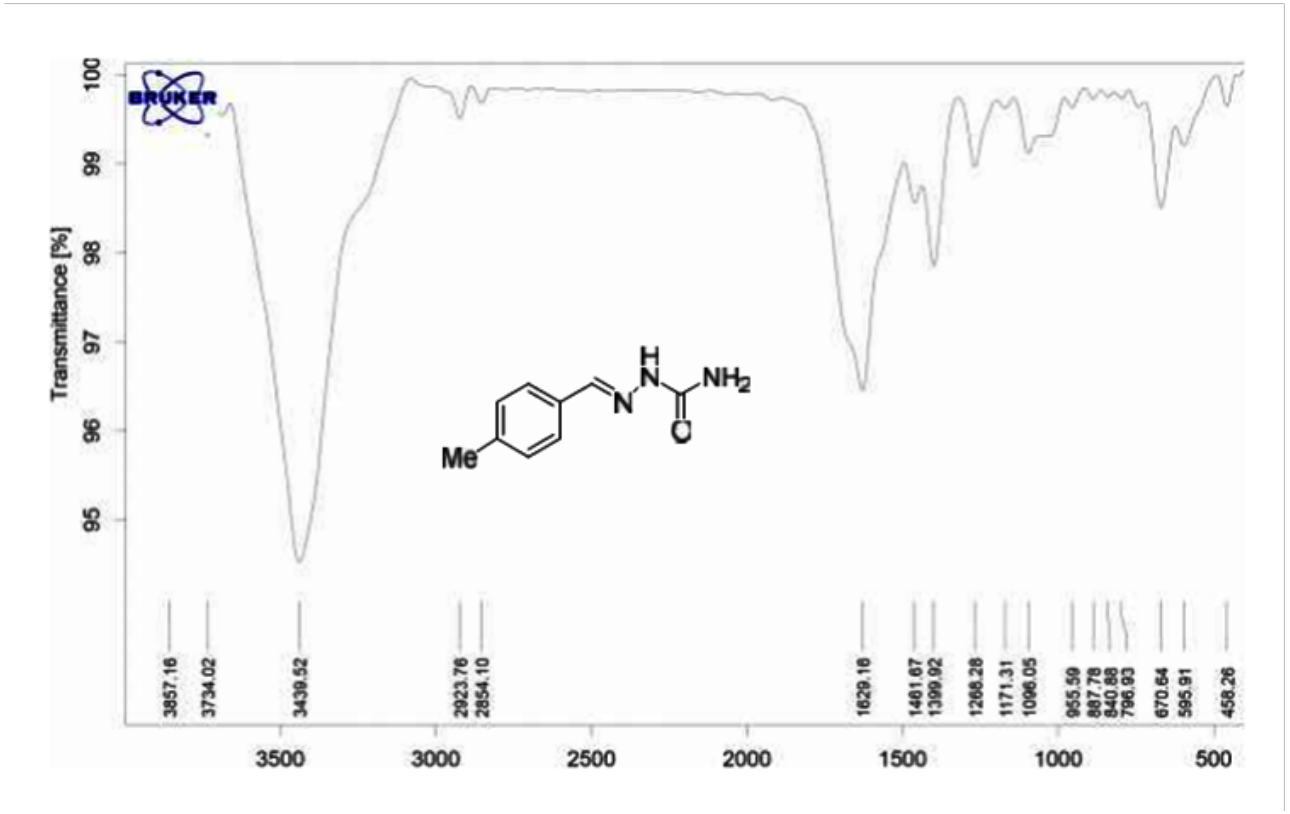

Figure S4 : FT-IR spectrum of compound **2b**

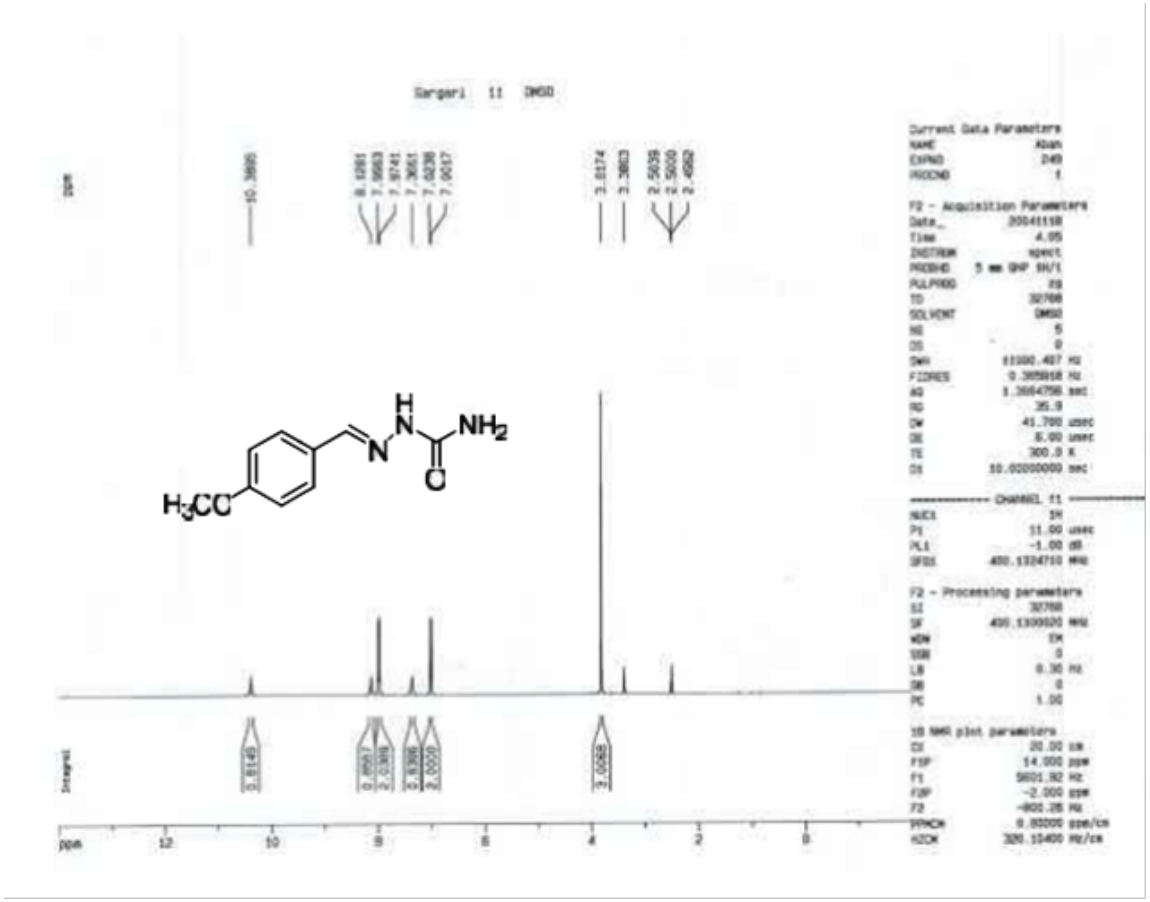

Figure S5 : ^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of compound **2c**

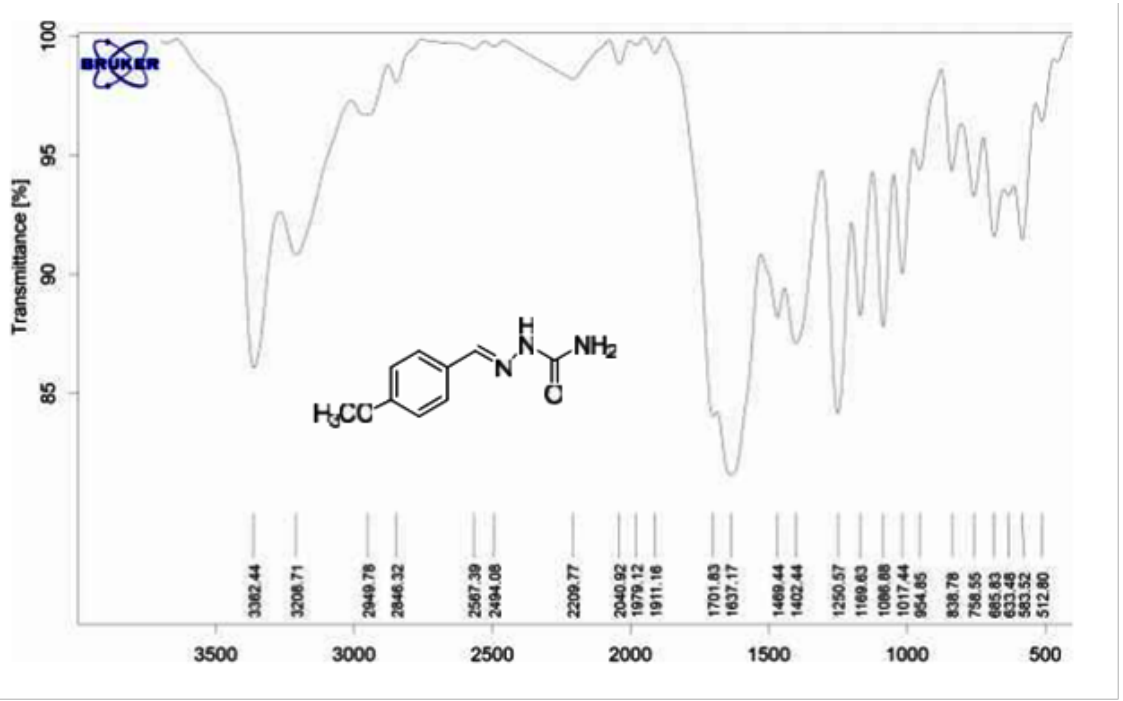

Figure S6 : FT-IR spectrum of compound **2c**

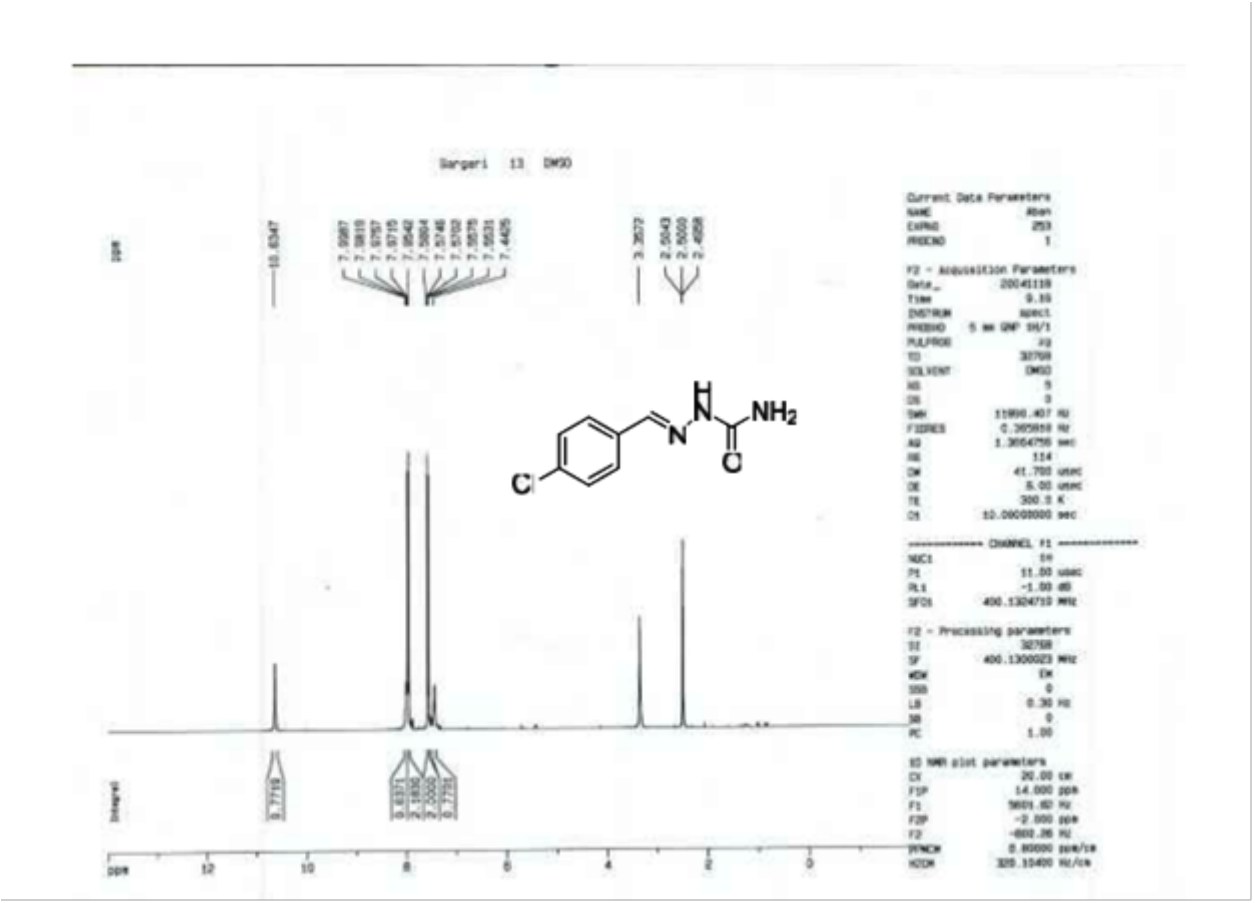

Figure S7 : ^{1}H NMR (DMSO-*d6*, 400 MHz) spectrum of compound **2d**

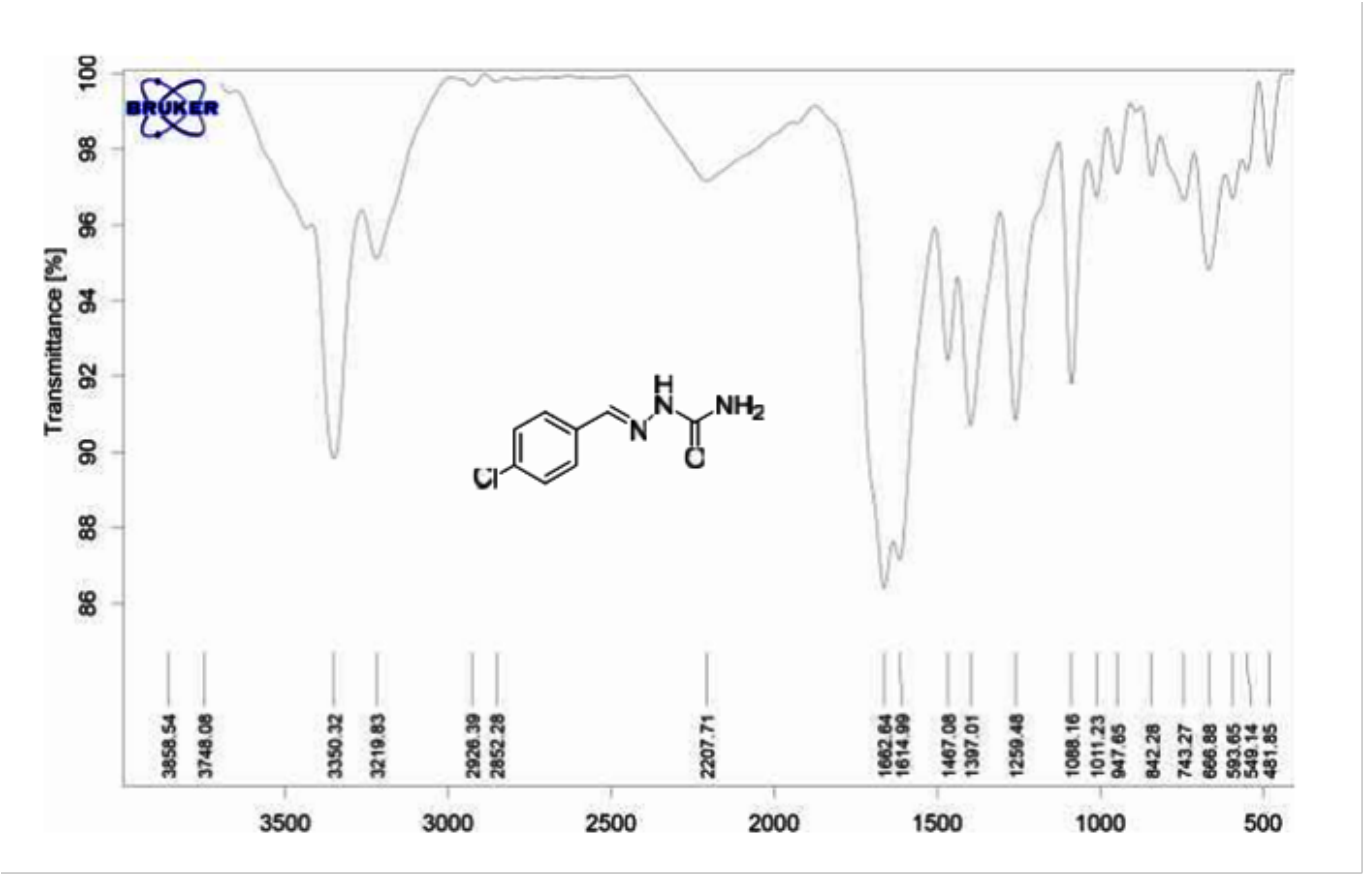

Figure S8 : FT-IR spectrum of compound **2d**