Supplementary Information

Synthesis, characterization, electronic and fastness properties of novel hetarylazopyrazolones

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1-Phenyl-3-amino-4-(2-benzothiazolilazo)pyrazol-5-one (1a)

Elemental analysis; %C;56.95 (calc;57.14), %H;3.81 (calc;3.57), %N;25.25 (calc;25.01), %S;9.11(calc;9.52); UV-Vis (DMSO) λ, nm; 390, 432; FTIR (KBr) √, cm^{-1}; 3435 (hyd NH), 3339, 3192 (NH_2), 3063 (Ar CH), 1670 (k C=O), 1638, 1590, 1491 (C=N, C=C).^{1}H NMR (400 MHz, DMSO-d6) δ, ppm; 6.50 (s, 2H, -NH_2), 7.00-7.25 (m, 4H, ph), 7.30 (d, 2H, *J* 8.0 Hz bth), 7.75 (d, 2H, *J* 8.0 Hz bth), 13.75 (s, 1H, hyd -NH-). bth:benzothiazol, hyd:hydrazo, ph:phenyl

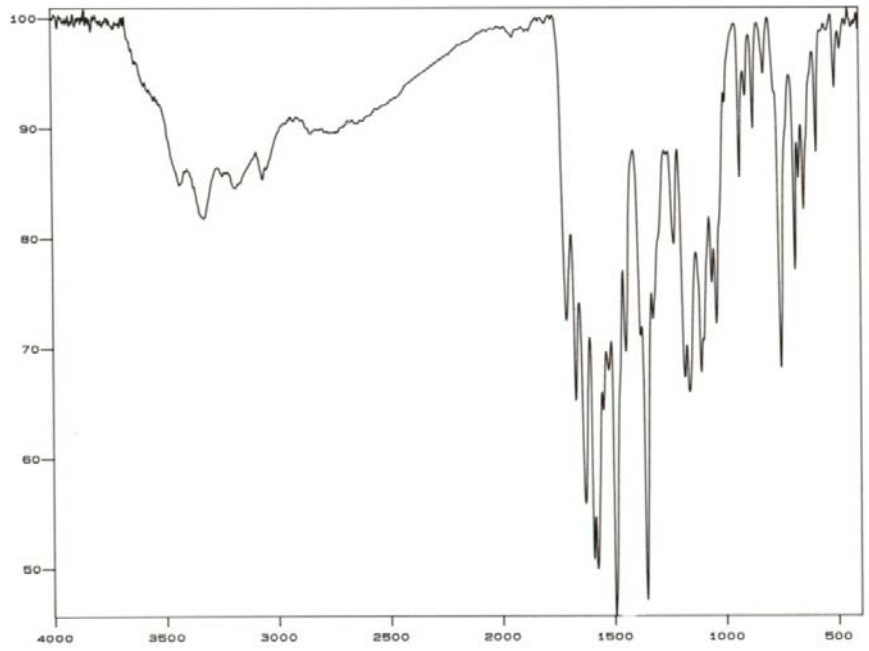


Figure S1. FTIR (KBr) spectrum of compound 1a

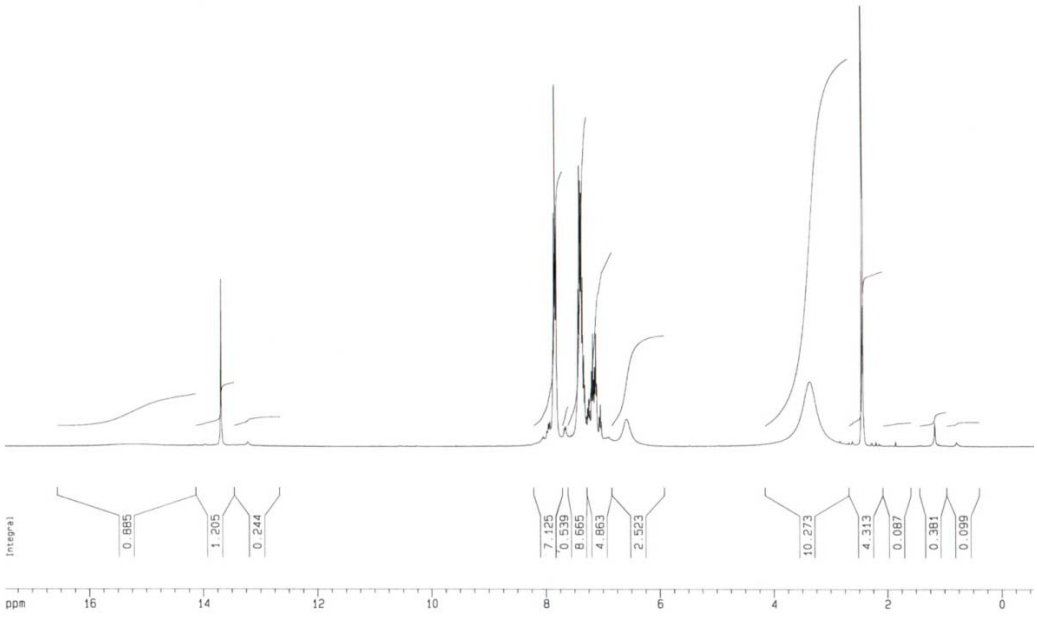


Figure S2. ^{1}H NMR spectrum (400 MHz, DMSO-*d6*) of compound 1a

1-Phenyl-3-amino-4-(6-methoxy-2-benzothiazolilazo)pyrazol-5-one (1b)

Elemental analysis; %C;55.89 (calc;55.73), %H;3.62 (calc;3.82), %N;22.91 (calc;22.95), %S;8.38(calc;8.74); UV-Vis (DMSO) λ, nm; 444; FTIR (KBr) √, cm^{-1}; 3467 (hyd NH), 3290, 3281(NH_2),3184 (Ar CH), 2988, 2933 (Al CH), 1666 (k C=O), 1636, 1595, 1470 (C=N, C=C).^{1}H NMR (400 MHz, DMSO-d6) δ, ppm; 3.60 (s, 3H, bth OCH_3), 6.40 (s, 2H, NH_2), 6.80-7.00 (m, 4H, ph), 7.25 (d, 1H, bth, *J* 8.0 Hz), 7.50 (d, 1H, *J* 8.0 Hz bth), 7.75 (s, 1H, bth), 13.20 (s, 1H, hyd NH). bth:benzothiazol, hyd:hydrazo, ph: phenyl

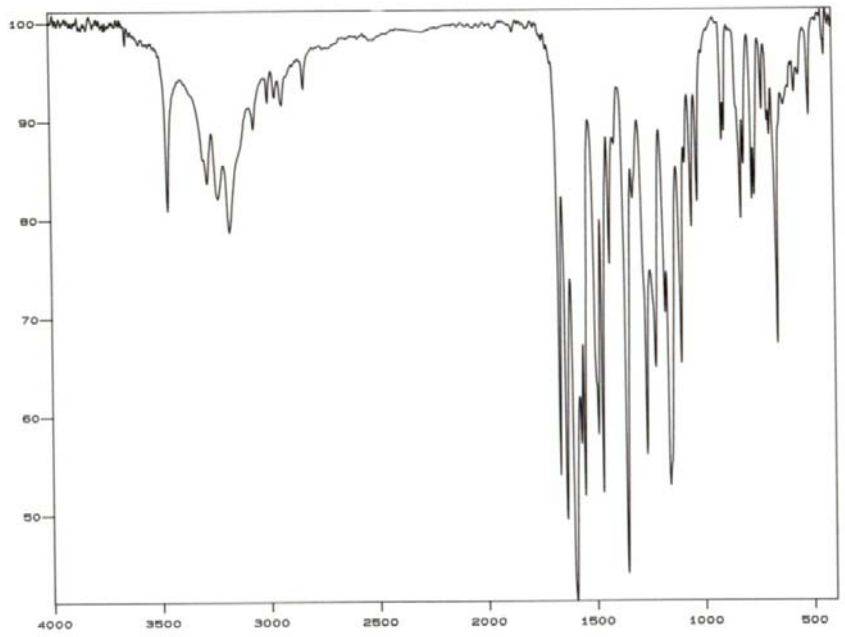


Figure S3. FTIR (KBr) spectrum of compound 1b

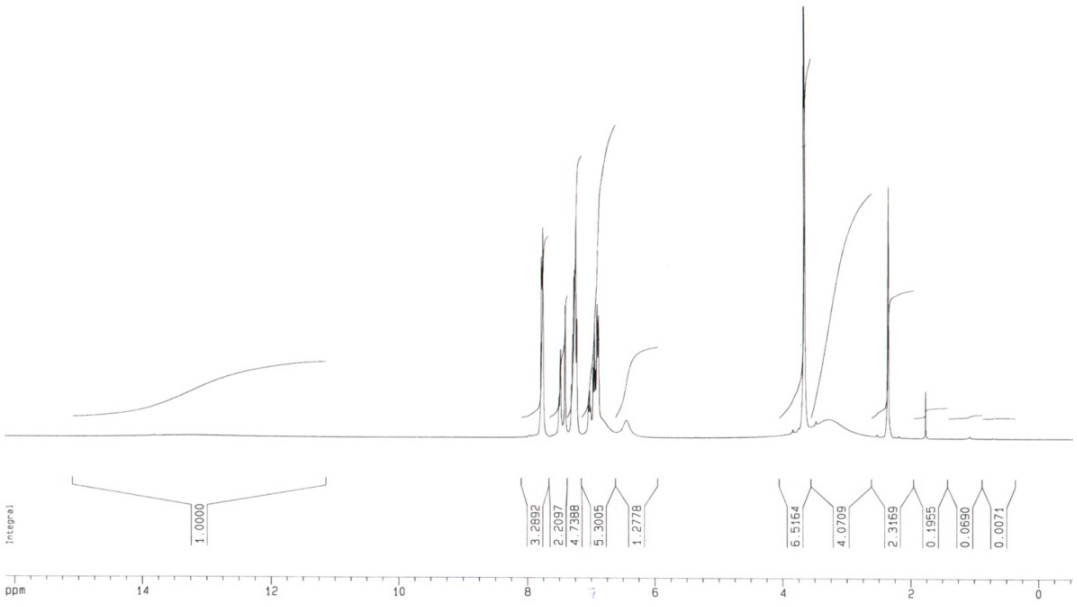


Figure S4. ^{1}H NMR spectrum (400 MHz, DMSO-*d6*) of compound 1b

1-Phenyl-3-amino-4-(6-nitro-2-benzothiazolilazo)pyrazol-5-one (1c)

Elemental analysis; %C;50.13 (calc;50.39), %H;3.07 (calc;2.88), %N;26.05 (calc;25.72), %S;8.21(calc;8.39); UV-Vis (DMSO) λ, nm; 356, 491; FTIR (KBr) √, cm^{-1}; 3423 (hyd NH), 3389, 3265(NH_2),3185, 3070 (Ar CH), 1677 (k C=O), 1585,1553,1503(C=N, C=C); ^{1}H NMR (400 MHz, DMSO-d6) δ, ppm; 6.80 (s, 2H, NH_2), 7.25-7.45 (m, 4H, ph), 7.60 (d, 1H, *J* 8.0 Hz, bth), 7.90 (s, 1H, bth), 8.00 (d, 1H, *J* 8.0 Hz, bth),14.00 (s, 1H, hyd NH). bth:benzothiazol, hyd:hydrazo, ph: phenyl

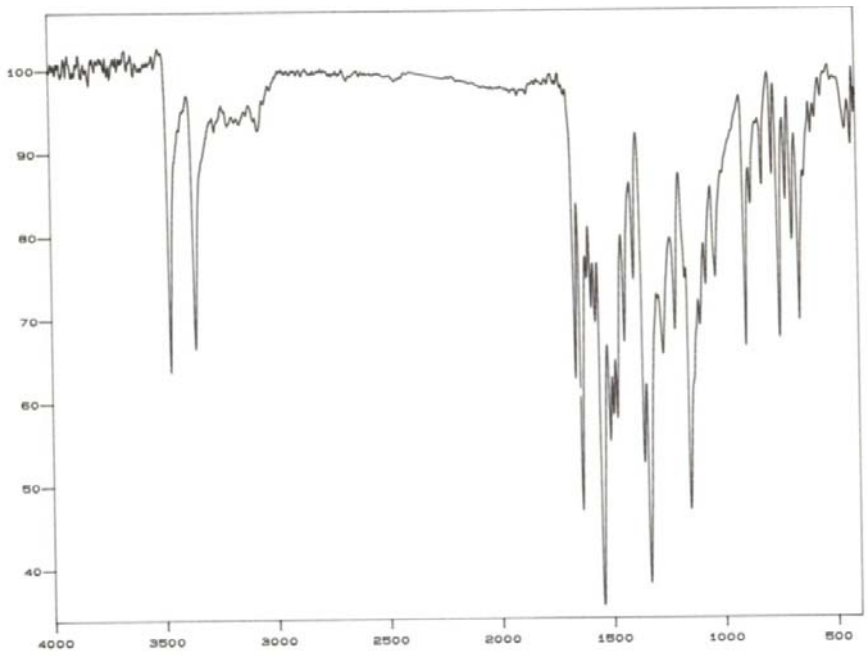


Figure S5. FTIR (KBr) spectrum of compound 1c

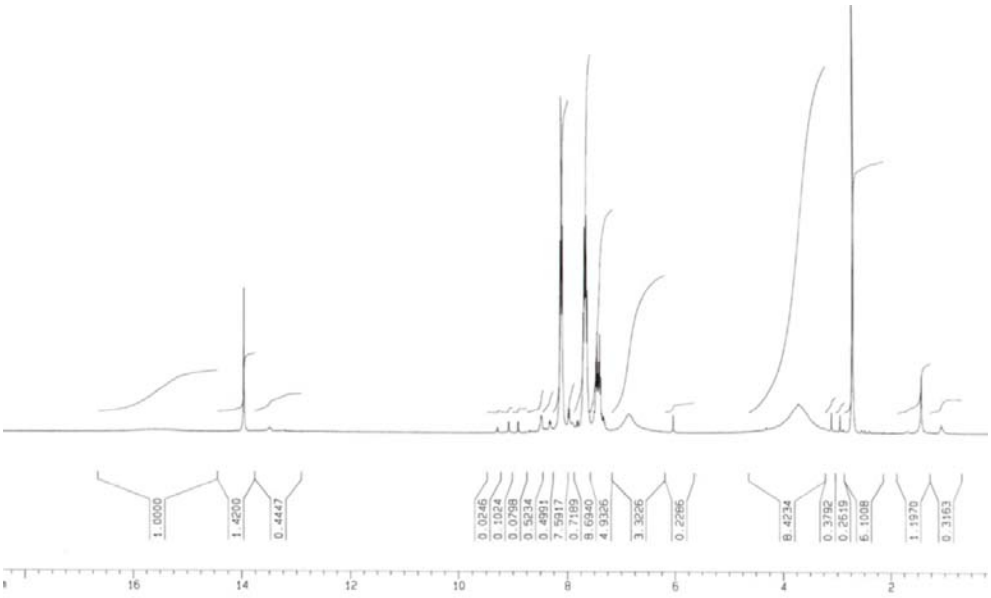


Figure S6. ^{1}H NMR spectrum (400 MHz, DMSO-*d6*) of compound 1c

1-Phenyl-3-acetamido-4-(2-benzothiazolilazo)pyrazol-5-one (2a)

Elemental analysis; %C;57.56 (calc;57.14), %H;3.37 (calc;3.70), %N;22.65 (calc;22.22), %S;7.93(calc;8.46); UV-Vis (DMSO) λ, nm; 477; FTIR (KBr) √, cm^{-1}; 3454 (hyd NH), 3082 (Ar CH), 2938 (Al CH), 1718 (ac C=O), 1664 (k C=O),1592 (ac NH), 1548,1503 (C=N, C=C). ^{1}H NMR (400 MHz, DMSO-d6) δ,ppm; 3.10(s, 3H, ac CH_3), 7.30 (m, 2H, ph), 7.55 (m, 2H, ph), 8.05 (d, 2H, *J* 8.0 Hz, bth), 8.20 (d, 1H, *J* 8.0 Hz, bth), 8.40 (d, 1H, *J* 8.0 Hz bth), 9.25 (s, 1H, ac-NH). bth:benzothiazol, ph: phenyl, ac:acetil

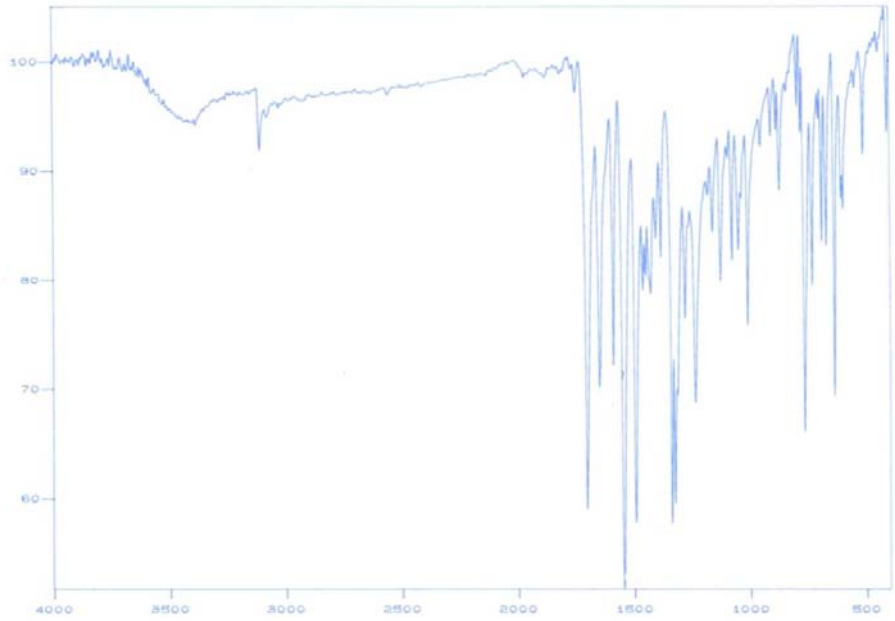


Figure S7. FTIR (KBr) spectrum of compound 2a

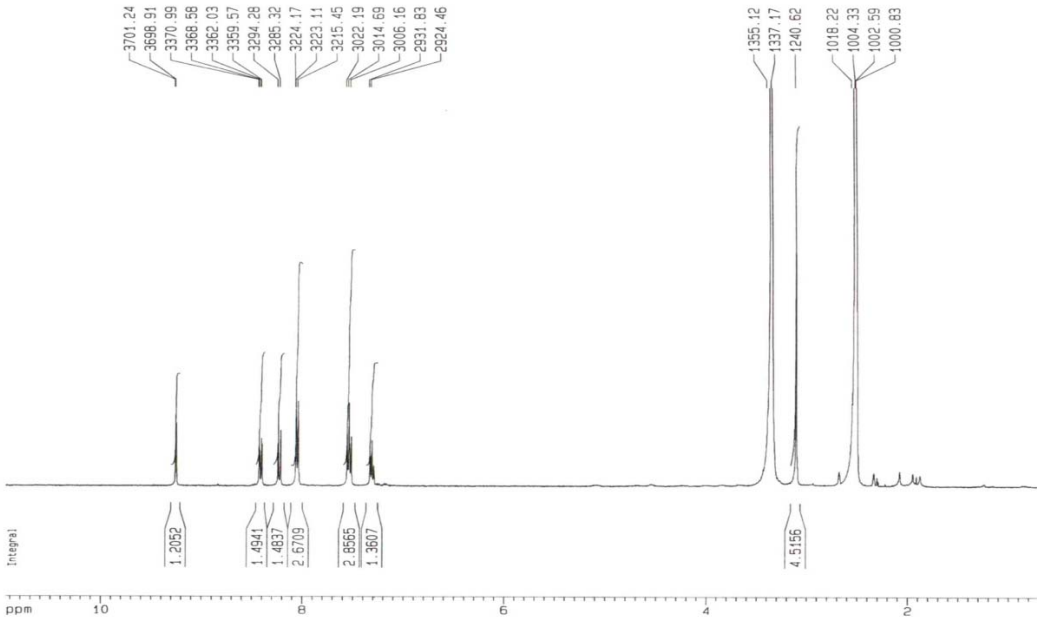


Figure S8. ^{1}H NMR spectrum (400 MHz, DMSO-*d6*) of compound 2a

1-Phenyl-3-acetamido-4-(6-methoxy-2-benzothiazolilazo)pyrazol-5-one (2b)

Elemental analysis; %C;56.23(calc;55.88), %H;3.59 (calc;3.93), %N;23.02 (calc;20.58), %S;7.43(calc;7.84); UV-Vis (DMSO) λ, nm; 335^{s}, 480; FTIR (KBr) √, cm^{-1}; 3469 (hyd NH), 3070, 2998 (Ar CH), 2935, 2844 (Al CH),1703 (ac C=O),1644 (k C=O), 1595 (ac NH), 1533, 1470 (C=N, C=C). ^{1}H NMR (400 MHz, DMSO-d6) δ, ppm; 2.90 (s,3H, ac CH_3), 3.90 (s,3H, bth OCH_3), 7.10 (m, 1H, ph), 7.20 (m, 1H, ph), 7.40(d, 1H, bth), 7.75 (s, 1H, bth), 7.90 (s, 1H, ac-NH), 8.10 (d, 1H, *J* 8.0 Hz, bth). ^{s}Shoulder, bth:benzothiazol, ph: phenyl,ac:acetil

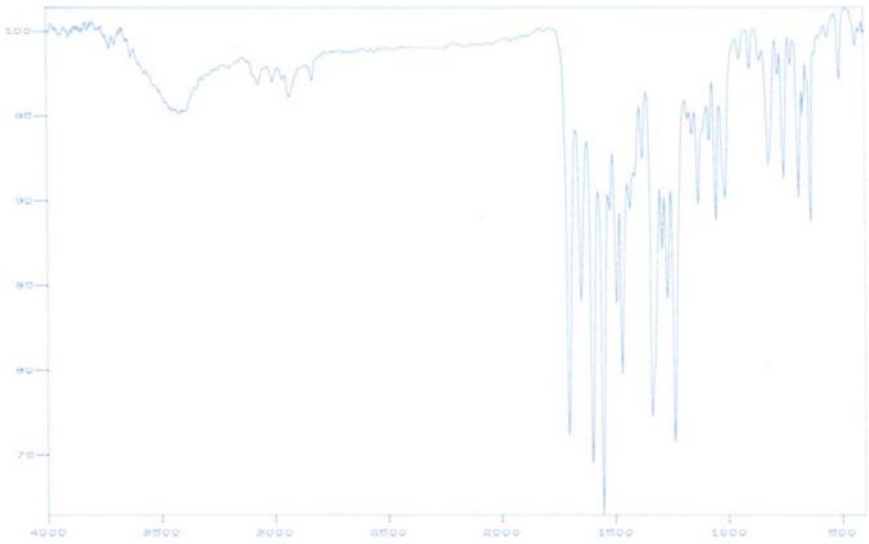


Figure S9. FTIR (KBr) spectrum of compound 2b

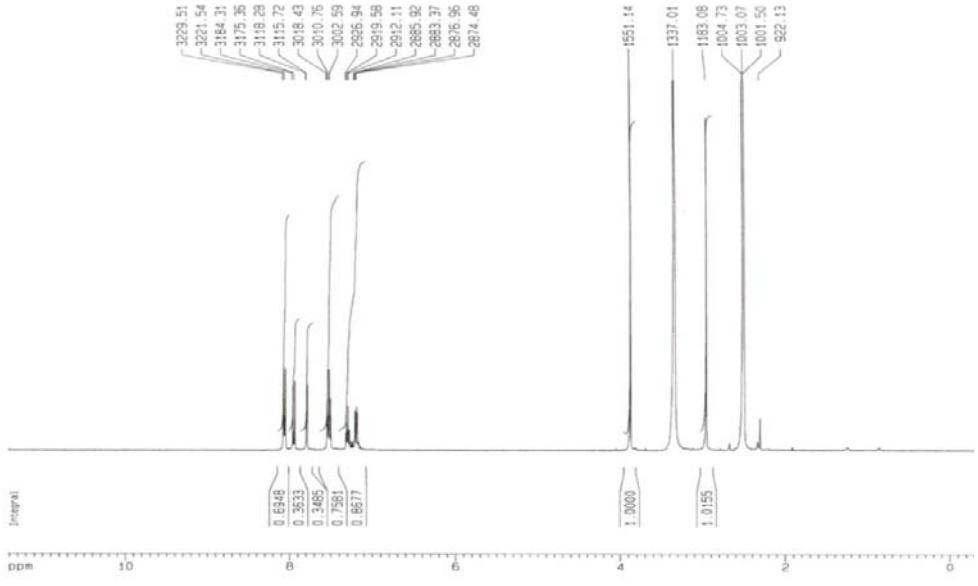


Figure S10. ^{1}H NMR spectrum (400 MHz, DMSO-*d6*) of compound 2b

1-Phenyl-3-acetamido-4-(6-nitro-2-benzothiazolilazo)pyrazol-5-one (2c)

Elemental analysis; %C;53.45 (calc;52.81), %H;3.57 (calc;3.18), %N;20.11(calc;20.53), %S;7.23(calc;7.82); UV-Vis (DMSO) λ, nm; 346, 483; FTIR (KBr) √, cm^{-1}; 3478 (hyd NH), 3070 (Ar CH), 2838 (Al CH),1720 (ac C=O), 1677 (k C=O), 1614 (ac NH), 1580,1503,1470 (C=N, C=C); ^{1}H NMR (400 MHz, DMSO-d6) δ,ppm; 3.10 (s,3H, ac CH_3), 7.25 (m, 2H, ph), 7.50 (m, 2H, ph), 8.05 (s, 1H, bth), 8.20 (d, 1H, *J* 8.0 Hz, bth), 8.40 (d, 1H, *J* 8.0 Hz, bth), 9.25 (s,1H, ac-NH). bth:benzothiazol, ph: phenyl, ac:acetil

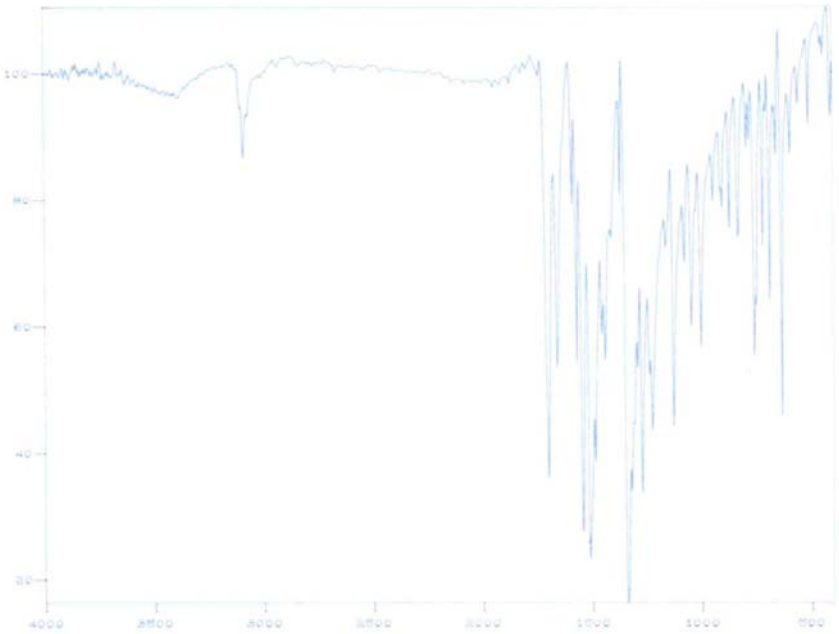


Figure S11. FTIR (KBr) spectrum of compound 2c

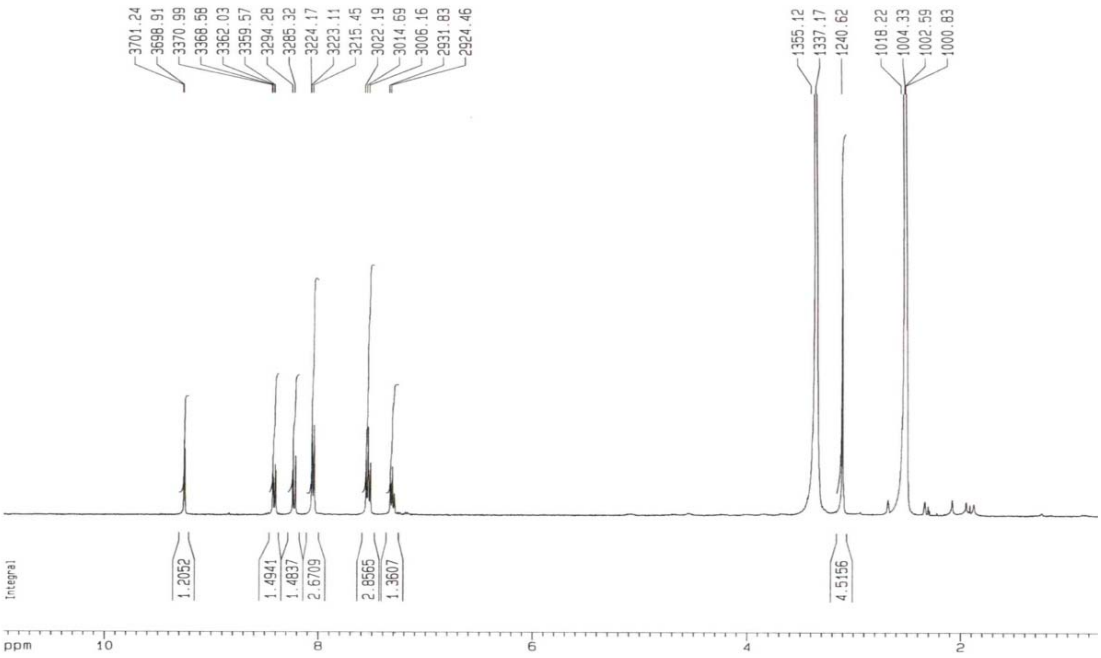


Figure S12. ^{1}H NMR spectrum (400 MHz, DMSO-*d6*) of compound 2c