Supporting Information (Information of X-Ray Crystallography)

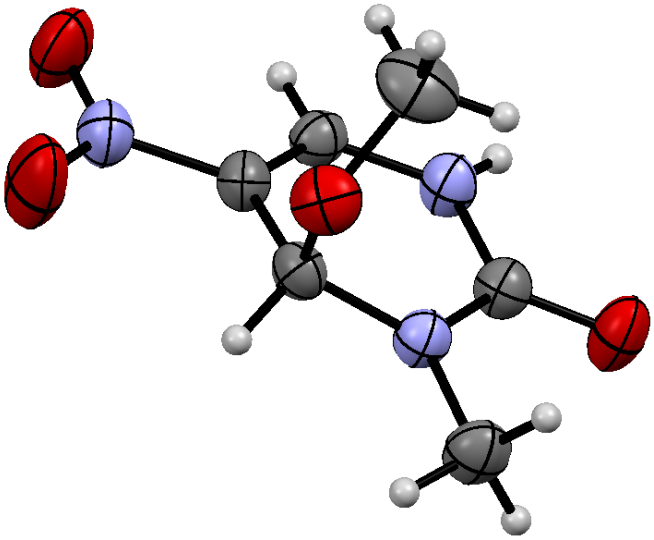

Figure 1. ORTEP showing the 4-methoxy-3-methyl-5-nitro-3,4-dihydropyrimidin-2(*1H*)-one (Color labels: gray, carbon; white, hydrogen; violet, nitrogen; red, oxygen). Thermal ellipsoids are drawn at the 50% probability level.

X-ray Structure Determination. The crystal data for 4-methoxy-3-methyl-5-nitro-3,4-dihydropyrimidin-2(*1H*)-one was collected and integrated with graphite monochromated Mo-Kα (λ = 0.71069 Å) radiation at 296 K. The structure was solved by direct methods[S1] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[S2] on F^2 was based on 2628 observed reflections and 136 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R_1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0461$$

$$wR_2 = [\Sigma \, (\, w \, (Fo^2 - Fc^2)^2 \,) / \, \Sigma \, w(Fo^2)^2]^{1/2} = 0.1579$$

The standard deviation of an observation of unit weight[S3] was 1.02. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.16 and -0.26 e /Å^3, respectively. Neutral atom scattering factors were taken from Cromer and Waber[S4]. Anomalous dispersion effects were included in Fcalc[S5]; the values for Δf' and Δf'' were those of Creagh and McAuley[S6]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[S7]. All calculations were performed using the CrystalStructure[S8] crystallographic software package except for refinement, which was performed using SHELXL-97[S9]. Crystal data for **XX**: $C_6H_9N_3O_4$, M_r = 187.15, monoclinic space group $P2_1/c$, a = 6.373(2) Å, b = 10.922(3) Å, c = 12.348(3) Å, β = 103.50(3) °, V = 835.8(4) Å^3 , Z = 4, ρ_{calcd} = 1.487 g·cm^{-3} , μ = 1.259 cm^{-1} , F(000) = 392, R_1 = 0.0461, wR_2 = 0.1579, 1924 independent reflections [2θ≤50°] and 150 parameters.

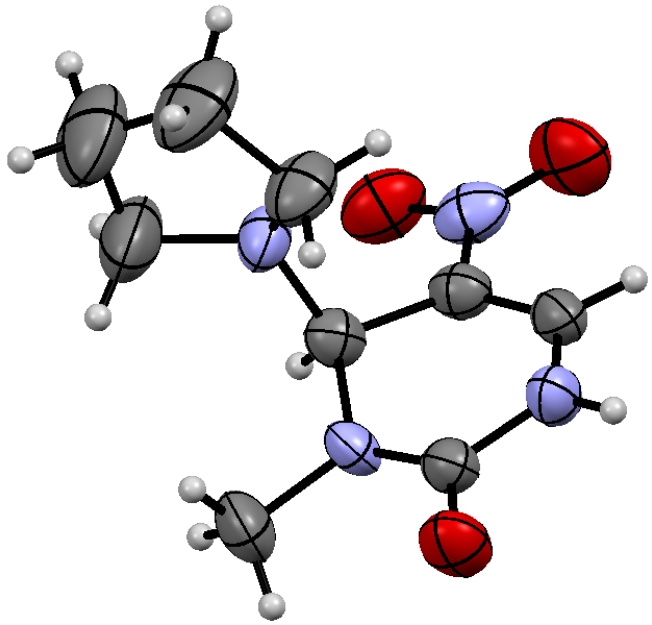

Figure 2. ORTEP showing the 3-methyl-5-nitro-4-(pyrrolidin-1-yl)-3,4-dihydropyrimidin-2(1*H*)-one (Color labels: gray, carbon; white, hydrogen; violet, nitrogen; red, oxygen). Thermal ellipsoids are drawn at the 50% probability level.

X-ray Structure Determination. The crystal data for 3-methyl-5-nitro-4-(pyrrolidin-1-yl)-3,4-dihydropyrimidin-2(1*H*)-one was collected and integrated with graphite monochromated Mo-Kα (λ = 0.71069 Å) radiation at 296 K. The structure was solved by direct methods[S1] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[S2] on F^2 was based on 2480 observed reflections and 153 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R_1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0584$$

$$wR_2 = [\Sigma \, (\, w \, (Fo^2 - Fc^2)^2 \,) / \, \Sigma \, w(Fo^2)^2]^{1/2} = 0.1966$$

The standard deviation of an observation of unit weight[S3] was 1.02. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.19 and -0.22 e /Å^3, respectively. Neutral atom scattering factors were taken from Cromer and Waber[S4]. Anomalous dispersion effects were included in Fcalc[S5]; the values for Δf' and Δf'' were those of Creagh and McAuley[S6]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[S7]. All calculations were performed using the CrystalStructure[S8] crystallographic software package except for refinement, which was performed using SHELXL-97[S9]. Crystal data for **XX**: $C_9H_{14}N_4O_3$, M_r = 226.23, monoclinic space group $P2_1/c$, a = 12.149(3) Å, b = 7.991(5) Å, c = 11.119(4) Å, β = 93.86(2) °, V = 1077.0(8) Å^3 , Z = 4, ρ_{calcd} = 1.395 g·cm^{-3} , μ = 1.069 cm^{-1} , F(000) = 480, R_1 = 0.0584, wR_2 = 0.1966, 2480 independent reflections [2θ≤50°] and 153 parameters.

References

[S1] SIR2008: M.C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G. L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori, D. Siliqi, R. Spagna (2007)

[S2] Least Squares function minimized: (SHELXL97)

$Sw(F_o^2-F_c^2)^2$ where w = Least Squares weights.

[S3] Standard deviation of an observation of unit weight:

$[Sw(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations

N_v = number of variables

[S4] Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

[S5] Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

[S6] Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

[S7] Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

[S8] CrystalStructure 4.0: Crystal Structure Analysis Package, Rigaku Corporation (2000-2010). Tokyo 196-8666, Japan.

[S9] SHELX97: Sheldrick, G.M. (2008). Acta Cryst. A64, 112–122.