Supporting Information

Synthesis of Iminoisoindolinones via a Cascade of Three-Component
Ugi Reaction, Palladium Catalyzed Isocyanide Insertion,
Hydroxylation and an Unexpected Rearrangement Reaction

Zhi-Lin Ren, Ping He, Wen-Ting Lu, Mei Sun and Ming-Wu Ding*

Key Laboratory of Pesticide & Chemical Biology of Ministry of Education, Hubei International Scientific and
Technological Cooperation Base of Pesticide and Green Synthesis, Central China Normal University, Wuhan,
430079, P. R. China
e-mail: mwding@mail.ccnu.edu.cn

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1. Crystal data and structure refinement for 6q

Crystal data and structure refinement for 6q.

Identification code  6q
Empirical formula  C_{23}H_{28}ClN_{3}O_{2}
Formula weight  413.93
Temperature  297(2) K
Wavelength  0.71073 Å
Crystal system  Monoclinic
Space group  Cc
Unit cell dimensions  
\[a = 27.492(6) \text{ Å, } \alpha = 90^\circ, b = 10.710(2) \text{ Å, } \beta = 131.125(6)^\circ, c = 20.869(5) \text{ Å, } \gamma = 90^\circ.\]
Volume  4628.8(18) Å³
Z  8
Density (calculated)  1.188 Mg/m³
Absorption coefficient  0.187 mm⁻¹
F(000)  1760
Crystal size  0.200 x 0.200 x 0.100 mm³
Theta range for data collection  1.967 to 26.288°.
Index ranges  -34<=h<=34, -13<=k<=13, -25<=l<=25
Reflections collected  17217
Independent reflections  8235 [R(int) = 0.0490]
Completeness to theta = 25.242°  100.0 %
Absorption correction  None
Refinement method  Full-matrix least-squares on F²
Data / restraints / parameters  8235 / 2 / 537
Goodness-of-fit on F²  0.979
Final R indices [I>2sigma(I)]  R1 = 0.0445, wR2 = 0.1150
R indices (all data)  R1 = 0.0605, wR2 = 0.1269
Absolute structure parameter  0.05(4)
Extinction coefficient  n/a
Largest diff. peak and hole  0.512 and -0.196 e.Å⁻³
2. Copies of $^1$H and $^{13}$C NMR spectrum of compounds 4 and 6