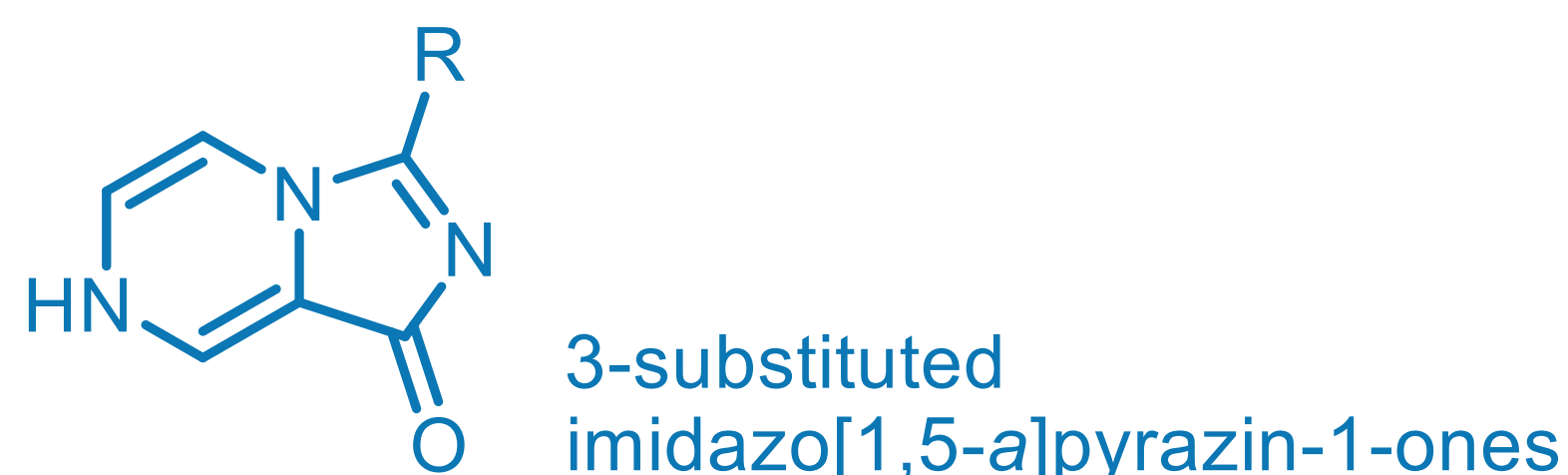


An Unprecedented Pathway to Fused Imidazole Derivatives from Azine Carboxamides: Scope, Limitations, and Mechanistic Insights

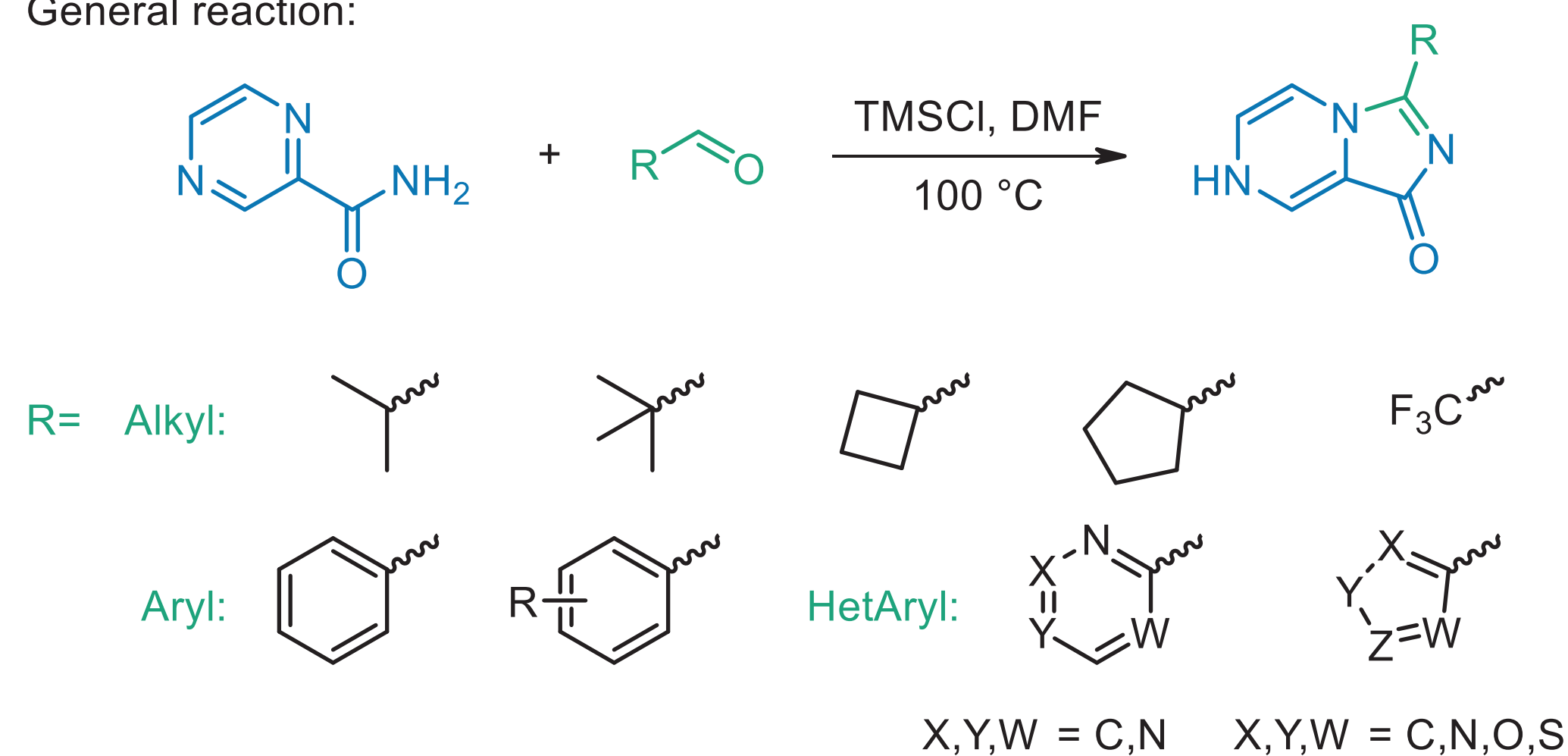
Andriy I. Frolov, Svitlana V. Stetsenko, Galyna P. Grabchuk, Olexandr Isayev, Tetiana Zubatiuk, Olexandr Ye. Pashenko, Dmytro M. Volochnyuk, Serhiy V. Ryabukhin

General synthesis and scope

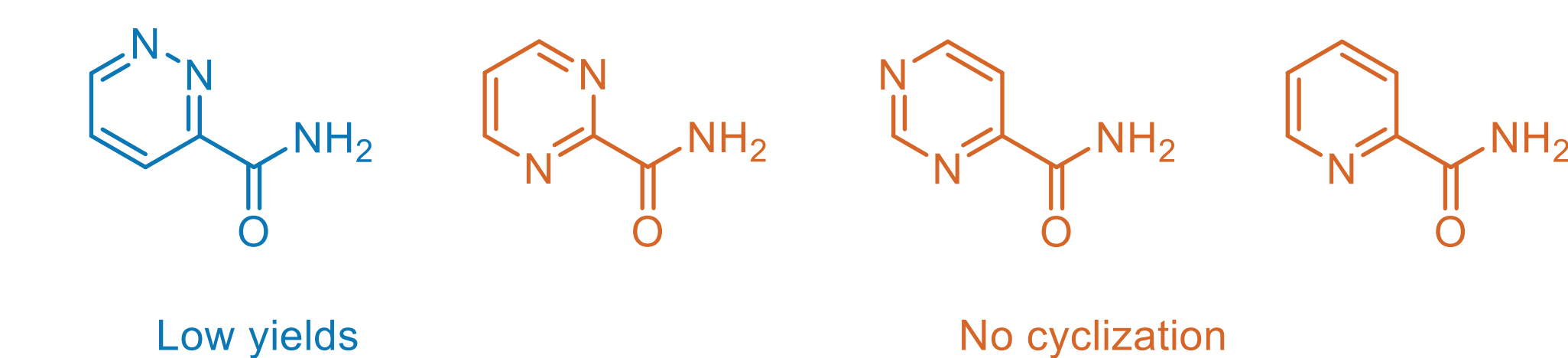
Novel imidazo[1,5-a]pyrazin-1-ones obtained by reacting pyrazine carboxamides with aldehydes using TMSCl-DMF as water scavenging system.



General reaction:

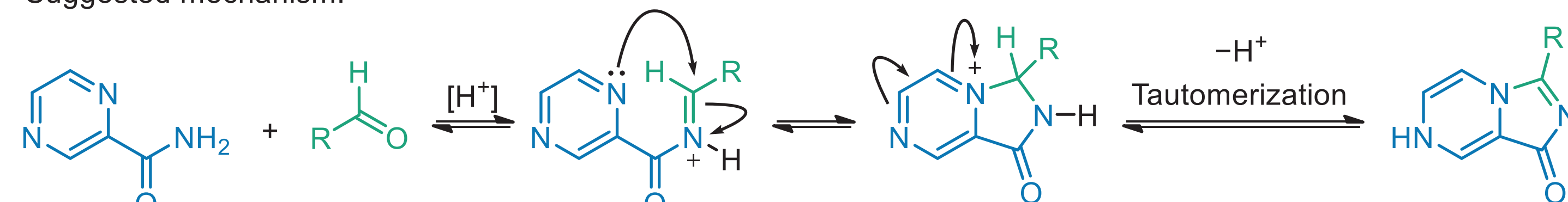


Other 6-membered *N*-heterocycles as a substrate:

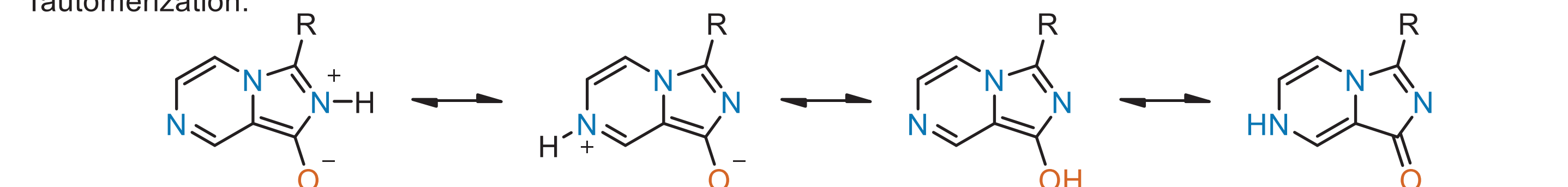


Mechanistic investigations

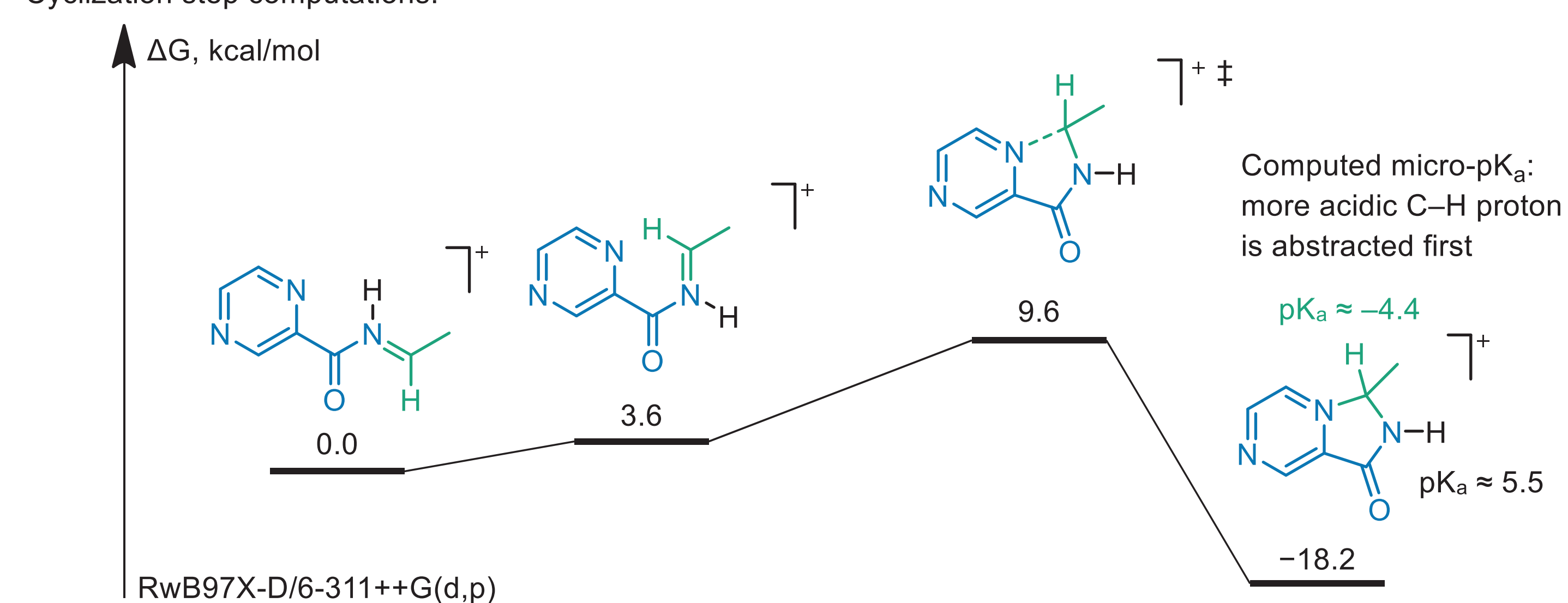
Suggested mechanism:



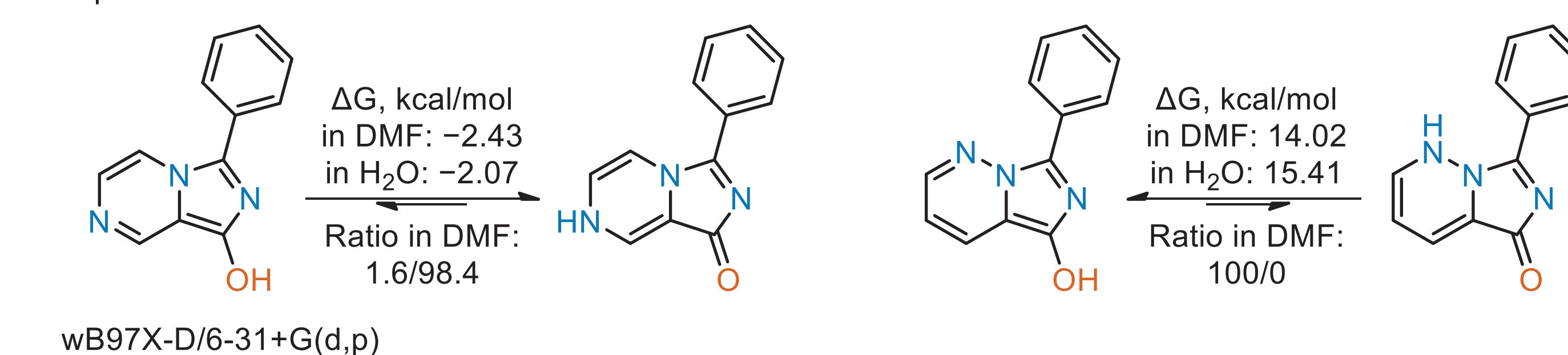
Tautomerization:



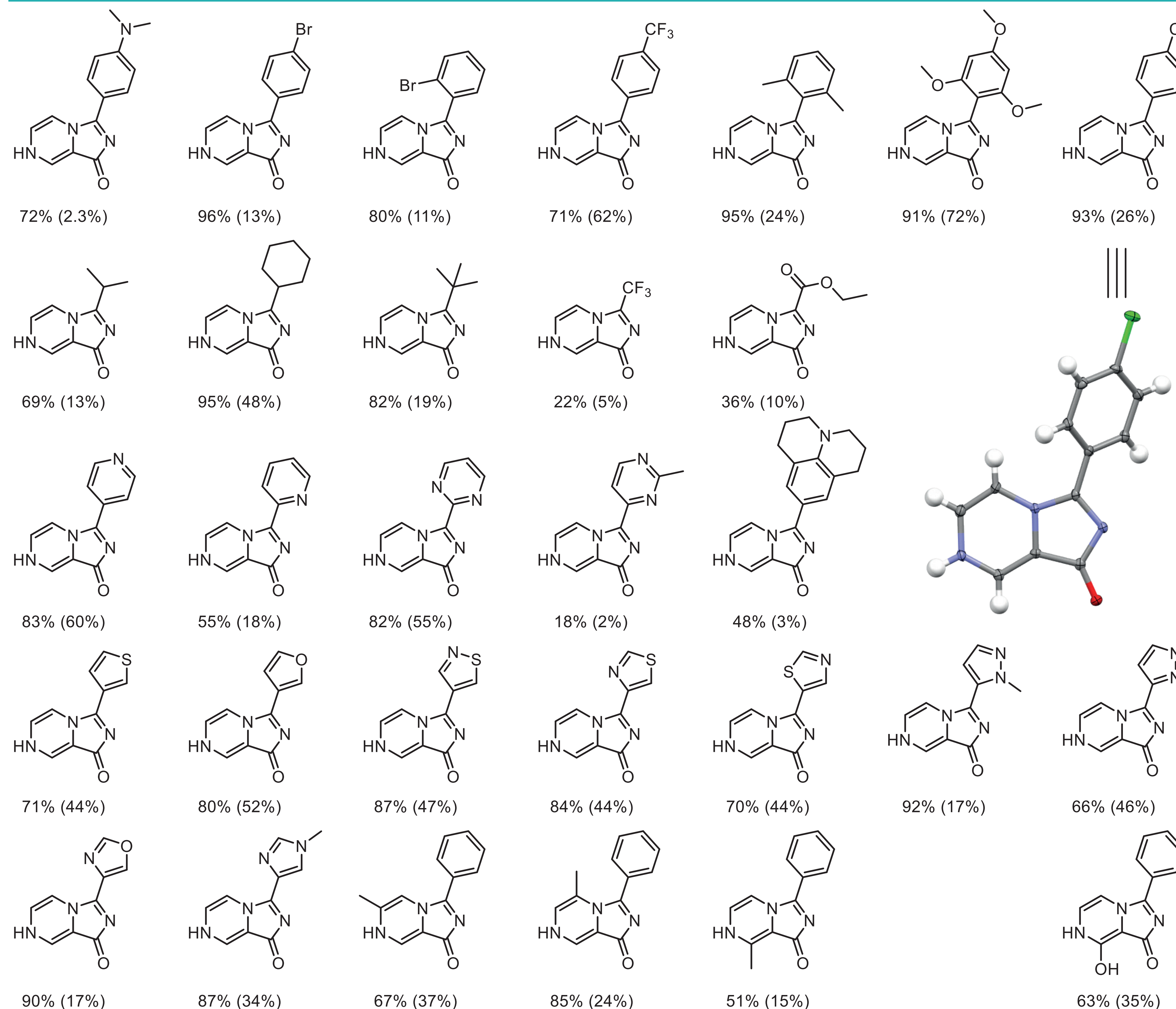
Cyclization step computations:



Computed tautomer ratios:

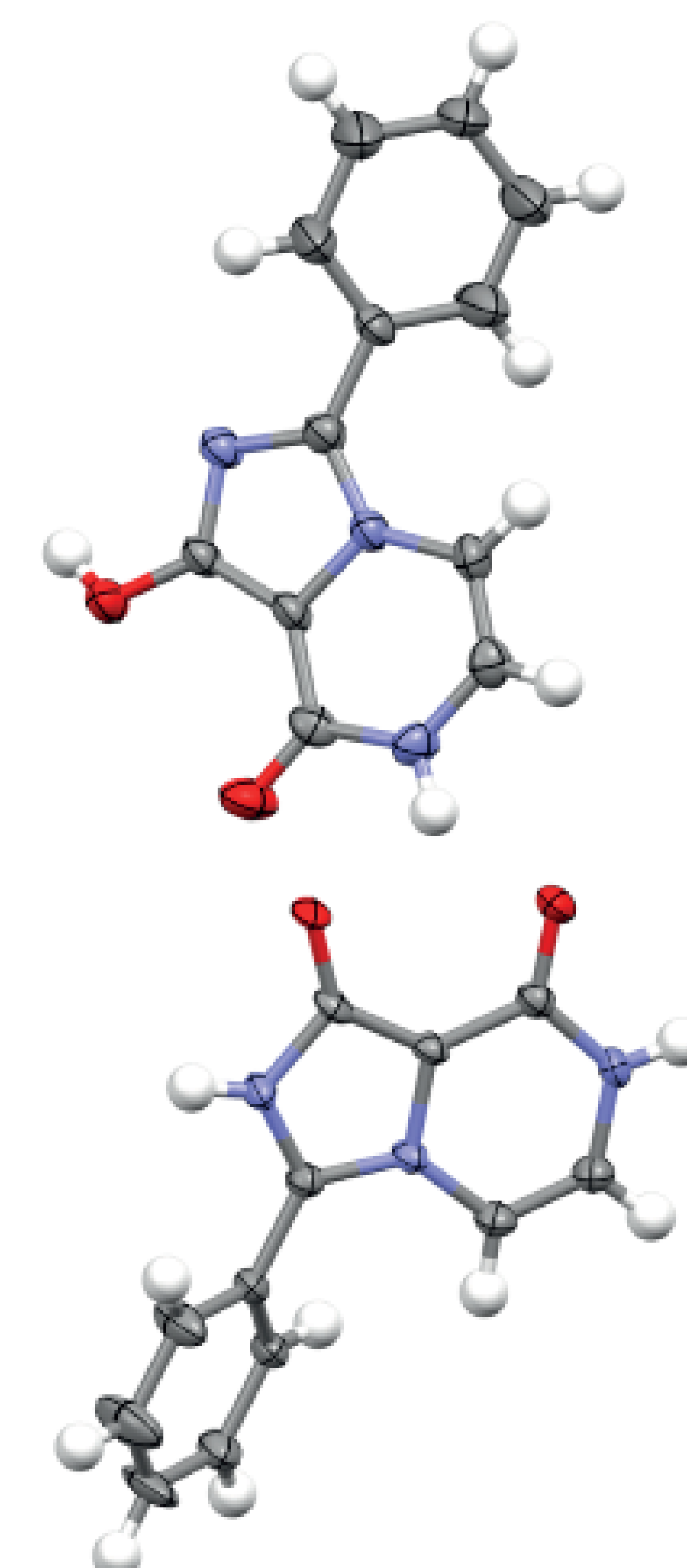


Synthesized examples



Percentages under structures mean: LCMS yield (isolated yield after flash chromatography)

Accommodates wide variety of aldehydes regardless of electronic properties or steric bulk



Contact

Sergey V. Ryabukhin, Prof. Dr. Sci.; Dmytro M. Volochnyuk, Prof. Dr. Sci.
s.v.ryabukhin@gmail.com, d.volochnyuk@gmail.com.