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Molecular Modeling of Geometries, Charge Distributions, and Binding Energies of Small, Druglike Molecules Containing Nitrogen Heterocycles and Exocyclic Amino Groups in the Gas Phase and Aqueous Solution. [J. Chem. Theory Comput. 4,, 1718–1732 (2008)]. By Brian R. White, Carston R. Wagner, Donald G. Truhlar, and Elizabeth A. Amin\*.

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