Quantitative Assessment of Carbonyl Lone Pair—π Interactions Using a Small Molecule Model

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Abstract: The quantitative assessment of the strength of carbonyl lone pair—pi (CO(lp)—pi) interactions is an important part of understanding the stability and conformational preferences of proteins. Three molecular balances involving a pyridinone arm were synthesized using a modular process; each of these molecular balances was characterized in solution (using ^{1}H NMR spectroscopy) and in the solid state (using X-ray crystallography). These molecular balances form a well-defined CO(lp)—pi interaction between the pyridinone arm and an aromatic shelf in the folded conformation, and the strength of the interaction was assessed using the folded: unfolded conformation ratio revealed by the integration of relevant signals in the ^{1}H NMR spectra. The CO(lp)—pi) interactions appear to be repulsive when the aromatic shelf is electron rich but become attractive when the electron shelf is electron deficient.