An efficient computational model to predict protonation at the amide nitrogen and reactivity along the C–N rotational pathway.

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Streszczenie

N-Protonation of amides is critical in numerous biological processes, including amide bonds proteolysis and protein folding as well as in organic synthesis as a method to activate amide bonds towards unconventional reactivity. A computational model enabling prediction of protonation at the amide bond nitrogen atom along the C–N rotational pathway is reported. Notably, this study provides a blueprint for the rational design and application of amides with a controlled degree of rotation in synthetic chemistry and biology.

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