

## Twisted *N*-acyl-hydantoins: rotationally inverted urea-imides of relevance in N—C(O) cross-coupling.

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### Streszczenie

We report a combined structural and computational study on the properties of twisted acyclic hydantoins. These compounds feature cyclic urea-imide moiety that is widely found in bioactive compounds and is structurally related to the classic bridged hydantoins proposed by Smissman more than 50 years ago. We demonstrate that C to N-substitution of the imide moiety in the succinimide ring to give hydantoin results in one of the most distorted acyclic amide bonds reported to date. The energetic properties of twisted acyclic hydantoins with respect to structures, resonance energies, barriers to rotation, and proton affinities are discussed. The energetic and structural properties of twisted acyclic hydantoins described provide a benchmark to facilitate the development of twisted amides based on the biorelevant cyclic urea-imide scaffold.

### Adres publiczny

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### Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>