

## Computational Rationalization of the Ring Transformation of 3-hydroxy-4-(1,2-dihydroxyethyl)- $\beta$ -lactams

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The reactivity of 3-hydroxy-4-(1,2-dihydroxyethyl)- $\beta$ -lactams with regard to the oxidant sodium periodate was evaluated, unexpectedly resulting in the exclusive formation of new 2-hydroxy-1,4-oxazin-3-ones through a C3C4 bond cleavage of the intermediate 4-formyl-3-hydroxy- $\beta$ -lactams followed by a ring expansion. This peculiar transformation stands in sharp contrast with the known NaIO<sub>4</sub>-mediated oxidation of 3-alkoxy- and 3-phenoxy-4-(1,2-dihydroxyethyl)- $\beta$ -lactams, which exclusively leads to the corresponding 4-formyl- $\beta$ -lactams without a subsequent ring enlargement. In addition, this new class of functionalized oxazin-3-ones was further evaluated for its potential use as building blocks in the synthesis of a variety of differently substituted oxazin-3-ones, morpholin-3-ones and pyrazinones. Furthermore, additional insights into the mechanism and the factors governing this new ring-expansion reaction were provided by means of density functional theory calculations.

### References

1. K. Mollet, H. Goossens, N. Piens, S. Catak, M. Waroquier, K. W. Tornroos, V. Van Speybroeck, M. D'Hooghe and N. De Kimpe, *Chemistry – Eur. J.* **19**, 3383 (2013).