Correction to "Benchmark of Generic Shapes for Macrocycles"

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Erratum

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In the initial submission, the files "ConforTime.zip" and "Data sets.zip" and the script "timer.sh" to calculate the time computation for Moloc have not been uploaded. We have now provided them as supplementary files.

■ ASSOCIATED CONTENT

ⓢ Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.jcim.1c00522.

Sampling time (ZIP)
Full datasets of results from Moloc, experimental-torsion DG with additional "basic knowledge" alone and in combination with Merck molecular force field/UFF, Conformator, and CCDC software (ZIP)
Script "timer.sh" to calculate the time computation for Moloc (ZIP)