CORRECTION



Correction: Complex peptide macrocycle optimization: combining NMR restraints with conformational analysis to guide structure-based and ligand-based design

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Correction to: Journal of Computer-Aided Molecular Design (2023) 37:519–535 https://doi.org/10.1007/s10822-023-00524-2

In the original publication, the Fig. 3 was cropped during production and published incorrectly. The corrected Fig. 3 should have appeared as shown below. The original article has been corrected.

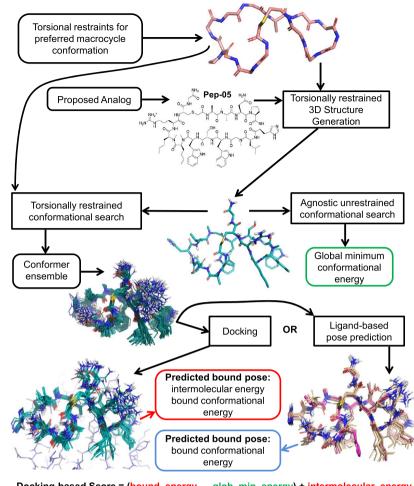
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The original article can be found online at https://doi.org/10.1007/s10822-023-00524-2.

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Fig. 3 Scheme for exploiting a macrocycle conformational preference to predict a bound pose, either using docking (protein structure shown in slate carbons at bottom left) or ligand similarity (exemplar conformer target shown in magenta carbons at bottom right). For the ligand-based score, a constant value of -24.0 kcal/mol was added to the estimated strain energy in order to put the scores from the two protocols on the same rough scale



Docking-based Score = (bound_energy_D - glob_min_energy) + intermolecular_energy Ligand-based Score = (bound_energy_L - glob_min_energy) + constant

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