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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:
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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.

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

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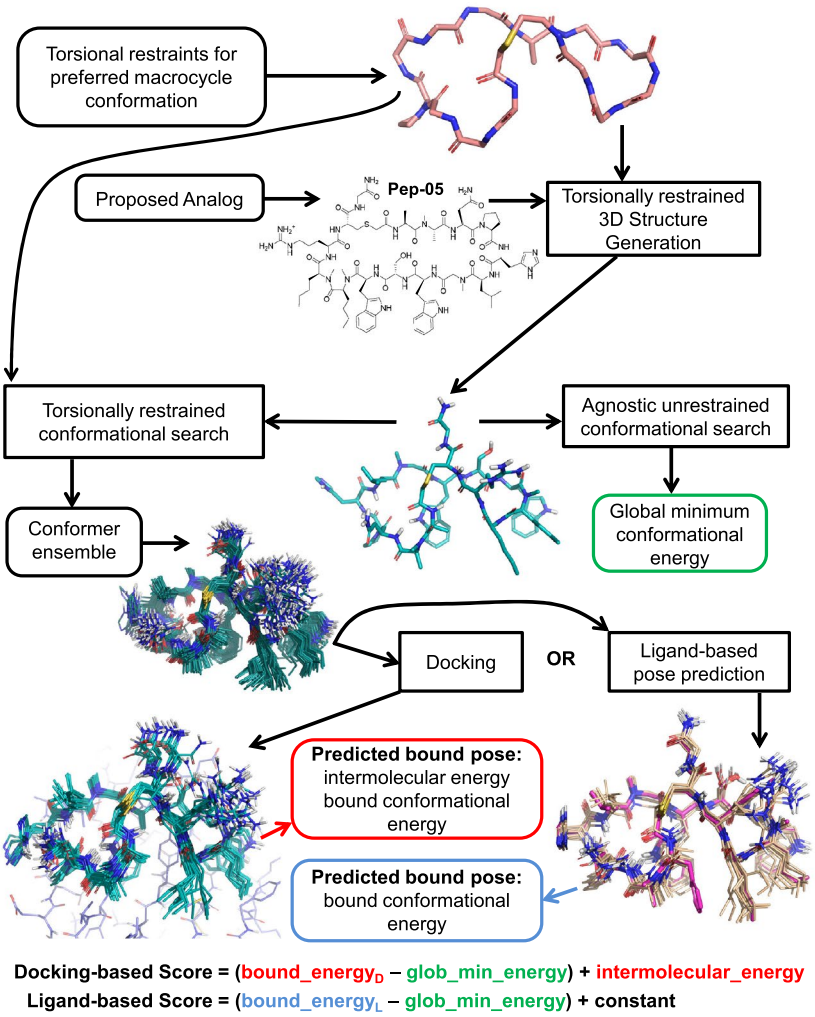

Fig. 3 Scheme for exploiting a macrocycle conformational preference to predict a bound pose, either using docking (protein structure shown in slate carbons at bottom left) or ligand similarity (exemplar conformer target shown in magenta carbons at bottom right). For the ligand-based score, a constant 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