Figure S1. Distribution of the RMSD accuracy of the conformer model vs. the non-hydrogen atom count. The % distribution of the RMSD accuracy of the conformer model as a function of the non-hydrogen atom count: (a) before clustering and (b) after clustering.
Figure S2. Distribution of the RMSD accuracy of the conformer model vs. the rotatable bond count. The % distribution of the RMSD accuracy of the conformer model as a function of the rotatable bond count: (a) before clustering and (b) after clustering.
Figure S3. Distribution of the RMSD accuracy of the conformer model vs. the effective rotor count. The % distribution of the RMSD accuracy of the conformer model as a function of the effective rotor count: (a) before clustering and (b) after clustering.
Figure S4. Distribution of the shape-optimized shape-Tanimoto ($ST^{ST-opt}$) accuracy of the conformer model vs. the non-hydrogen atom count. The % distribution of the $ST^{ST-opt}$ accuracy of the conformer model as a function of the non-hydrogen atom count: (a) before clustering and (b) after clustering.
Figure S5. Distribution of the shape-optimized shape-Tanimoto ($ST^{ST-opt}$) accuracy of the conformer model vs. the rotatable bond count. The % distribution of the $ST^{ST-opt}$ accuracy of the conformer model as a function of the rotatable bond count: (a) before clustering and (b) after clustering.
Figure S6. Distribution of the shape-optimized shape-Tanimoto ($S^\text{ST-opt}$) accuracy of the conformer model vs. the effective rotor count. The % distribution of the $S^\text{ST-opt}$ accuracy of the conformer model as a function of the effective rotor count: (a) before clustering and (b) after clustering.
Figure S7. Correlation between the RMSD accuracy and shape-optimized shape-Tanimoto ($ST_{ST-opt}$) accuracy of the conformer models. The % distribution of the conformer models as a function of the $ST_{ST-opt}$ accuracy for a given RMSD accuracy: (a) before cluster and (b) after clustering.