OMEGA: The Gold Standard for Conformer Generation, Now Faster with Bayesian Sampling

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Summary:

- OMEGA is the most widely used and highly cited conformer generation tool, robustly sampling conformational space across drug-like molecules and macrocycles.
- OMEGA with Bayesian sampling algorithm delivers a 2-3x speedup over exhaustive enumeration.
- High accuracy with 80% of ligands reproduced within 1 Å RMSD of the experimental conformation across 6,000 Iridium HT-scored PDB structures.

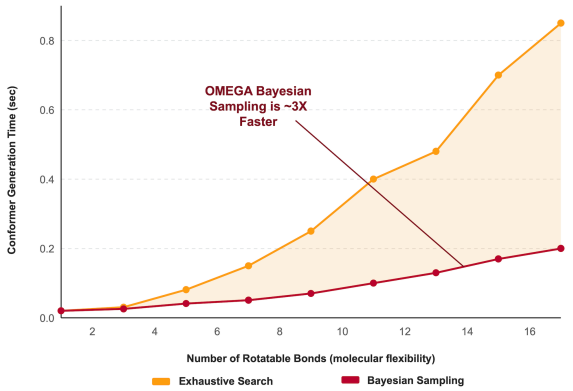
Product Keywords: OMEGA, Orion®

Abstract:

Generating high-quality conformer ensembles at scale is a core requirement for 3D virtual screening, pose prediction, and machine learning workflows. OMEGA is the gold standard for this task, both in speed and accuracy. Its core algorithm has been improved by using Bayesian sampling to intelligently focus on low-energy structures rather than exhaustively enumerating every torsion angle combination.

Benchmarked across 39,000 diverse molecules Bayesian sampling achieves a 3x speedup in FastROCS mode and 2x in Classic mode, with the largest gains seen in molecules with more rotatable bonds.

More importantly, this performance gain preserves the accuracy. Validated against 6,000 PDB crystal structures with Highly Trustworthy Iridium scores, OMEGA with Bayesian sampling reproduces 80% of bioactive conformations within 1 Å RMSD, equivalent to exhaustive sampling. Virtual screening performance, for both ligand- and structure-based methods, also remains unaffected.



Torsion driving with Bayesian sampling is ~2- 3X faster than exhaustive sampling.

For scientists running large-scale conformer generation, OMEGA with Bayesian sampling delivers meaningful speed gains without compromising the quality that has made it the industry standard.

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