

## Supplemental text S2: Posterior sampling

The Markov Chain Monte Carlo algorithm is a method often used to sample from a posterior distribution, generating a distribution of solutions. To sample conformations, we used the Metropolis-Hasting algorithm.

From the current conformation  $C_n$ , it is randomly perturbed (see figure 2) to generate the structure  $C_{n+1}$ . We then calculate the acceptance ratio  $\alpha = \frac{P(C_{n+1})}{P(C_n)}$ . If  $\alpha > 1$ , then we accept the new proposed conformation, otherwise, we accept  $C_{n+1}$  with probability  $\alpha$ .