**Table S15.** Relative energies and Boltzmann populations of stable conformers of aspirin.

|  |  |  |
| --- | --- | --- |
| **Entry No.** | **Δ*E*** **(kcal/mol)** | **Population 1** |
| 1 | 0.00 | 1.000 |
| 2 | 0.00 | 1.000 |
| 3 | 3.00 | 0.006 |
| 4 | 3.00 | 0.006 |

1 Relative population is calculated by the Boltzmann distribution at a temperature of 298 K.