**Table S17.** Relative energies and Boltzmann populations of stable conformers of (2S, 2’R)-loxoprofen.

|  |  |  |
| --- | --- | --- |
| **Entry No.** | **Δ*E*** **(kcal/mol)** | **Population 1** |
| 1 | 0.00 | 1.000 |
| 2 | 1.39 | 0.096 |
| 3 | 1.41 | 0.092 |
| 4 | 1.58 | 0.069 |
| 5 | 1.86 | 0.043 |
| 6 | 2.61 | 0.012 |
| 7 | 2.67 | 0.011 |
| 8 | 2.67 | 0.011 |

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