**Table S12.** Relative energies and Boltzmann populations of stable conformers of leucine.

|  |  |  |
| --- | --- | --- |
| **Entry No.** | **Δ*E*** **(kcal/mol)** | **Population 1** |
| 1 | 0.00 | 1.000 |
| 2 | 0.81 | 0.255 |
| 3 | 1.59 | 0.068 |
| 4 | 1.72 | 0.055 |
| 5 | 2.03 | 0.032 |
| 6 | 2.11 | 0.028 |
| 7 | 2.76 | 0.009 |

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