**S5 Table.** LAO conformers using energy-based search/RG filter

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Generation/ cycle | Total number of conformers in each cycle | Number of conformers within specific  RMSD range to closed structure | | | |
| 1-2 Å | 2-3 Å | 3-4.7 Å | >4.7 Å |
| 1 | 2/0 | 0 | 0 | 0 | 2/0 |
| 2 | 3/0 | 0 | 0 | 0 | 3/0 |
| 3 | 6/2 | 0 | 0 | 1 | 5/1 |
| 4 | 3/1 | 0 | 0 | 1 | 2/0 |
| 5 | 3/2 | 0 | 1 | 1 | 1/0 |
| 6 | 4/3 | 1 | 2 | 0 | 1/0 |
| 7 | 0/0 | 0 | 0 | 0 | 0/0 |
| All cycles | 21/8 | 1 | 3 | 3 | 14/1 |