Comparison of SIRT3/NAD+/ac-LYS from 4FVT (NAD+ converted from carba-NAD+) and w/ loop substitution on residues 155-178 from 4BVG.

SIRT3/NAD+/ac-LYS w/o loop substitution:

|  |  |
| --- | --- |
| **SIRT3/NAD+/ac-LYS h-opt** | **Prime Energy** |
| Prime Energy Calculation #1 | -10030.5 |
| Prime minimization #2 | -12477.1 |
| Prime minimization #3 | -12484.7 |
| Prime minimization #4 | -12489.0 |
| Prime minimization #5 | -12491.0 |
| Prime minimization #6 | -12491.9 |
| Prime minimization #7 | -12492.1 |
| Prime minimization #8 | -12492.4 |
| Prime minimization #9 | -12492.8 |
| Prime minimization #10 | -12493.4 |
| Prime minimization #11 | -12493.5 |
| Prime minimization #12 | -12493.9 |
| Prime minimization #13 | -12494.0 |
| Prime minimization #14 | -12494.1 |
| Prime minimization #15 | -12494.1 |

SIRT3/NAD+/ac-LYS w/ loop substitution:

|  |  |
| --- | --- |
| **SIRT3/NAD+/ac-LYS h-opt** | **Prime Energy** |
| Prime Energy Calculation #1 | 111376821.0 |
| Prime minimization #2 | -12427.3 |
| Prime minimization #3 | -12428.3 |
| Prime minimization #4 | -12428.3 |

The two energies cannot be prepared directly because the second complex has only one water in the structure while the first complex has two water.

Further calculations are needed for more meaningful comparison.