**Table S1.** Lower-ranking binding conformations of **1** to NAE and their corresponding docking scores generated by virtual ligand docking.

|  |  |
| --- | --- |
| **Conformation** | **ICM docking score** |
| **conf2** | –28.35 |
| **conf3** | –25.67 |
| **conf4** | –24.46 |