Supplementary Information: MD Simulations

MD simulations of DNMT1 with four different compounds **1** - **4** were performed to investigate stability and flexibility profiles. To illustrate the dynamic interactions observed, a short supplementary video for each compound has been included. These videos capture the protein-compound complex trajectories.

- **Video S1**: DNMT1 with Compound **1**

- **Video S2**: DNMT1 with Compound **2**

- **Video S3**: DNMT1 with Compound **3**

- **Video S4**: DNMT1 with Compound **4**

Supplementary Materials S5–S9 present the original western blot of the cleaved PARP, B-actin, BCL-XL, and caspase-3 for CCRF-CEM cells treated with compound **4**. In addition, for caspase-3, one image with increased intensity is included to visualize the cleaved caspase-3. The first four wells represent the DMSO, 0.5 × IC_{50}, IC_{50}, and 2 × IC_{50} samples.