**Table S3** The Binding Sites of Cepharanthine at the Target Protein.

|  |  |  |  |
| --- | --- | --- | --- |
| **Target Protein** | **Type of Interactions** | **Receptor Residue** | **Distance** |
| 1mq4  (AURKA) | Hydrophabic Interactions | LYS-143 | 3.44 |
| PHE-144 | 3.84 |
| PHE-144 | 3.69 |
| GLU-260 | 3.77 |
| Hydrogen Bonds | LYS-143 | 3.3 |
| LYS-162 | 3.63 |
| LYS-258 | 3.92 |
| TRP-277 | 3.45 |
| Salt Bridges | GLU-260 | 5.49 |
| 1fin  (CCNA2) | Hydrophabic Interactions | ILE-182 | 3.58 |
| ILE-182 | 3.73 |
| GLN-313 | 3.73 |
| THR-316 | 3.61 |
| Hydrogen Bonds | ASN-173 | 3.31 |
| Salt Bridges | GLU-268 | 4.83 |
| 1w98  (CCNE1) | Hydrophabic Interactions | GLN-240 | 3.75 |
| Hydrogen Bonds | ASN-236 | 3.07 |
| 4y72  (CDK1) | Hydrophabic Interactions | VAL-227 | 3.35 |
| VAL-227 | 3.83 |
| ILE-269 | 3.47 |
| ILE-269 | 3.33 |
| TYR-270 | 3.8 |
| LYS-274 | 3.98 |
| Hydrogen Bonds | TYR-270 | 3.49 |
| 1ia8  (CHEK1) | Hydrophabic Interactions | GLU-33 | 3.74 |
| ALA-34 | 3.63 |
| Hydrogen Bonds | TYR-71 | 3.04 |
| TYR-86 | 4.03 |
| Salt Bridges | ASP-139 | 5.38 |
| GLU-140 | 5.08 |
| 1q4o  (PLK1) | Hydrophabic Interactions | LYS-420 | 3.88 |
| ASP-438 | 3.56 |
| LYS-474 | 3.23 |
| Hydrogen Bonds | ARG-456 | 2.87 |
| ARG-456 | 3.84 |
| Salt Bridges | ASP-438 | 4.86 |