Binding affinities of NAD+ in SIRT3 and Sir2TM complexes estimated using MM-PB(GB)SA

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | NAD+ in SIRT3 and Sir2TM ternary complex | | NAD+ in SIRT3 and Sir2TM in complex with NAM | |
|  | SIRT3/Ac-CS2/ NAD+ | Sir2TM/Ac-p53/ NAD+ | SIRT3/Ac-CS2/NAD+/NAM | Sir2TM/Ac-p53/NAD+/NAM |
| MM-PBSA | -5.35 | -23.19 | -8.10 | -16.15 |
| MM-GBSA | -65.63 | -105.48 | -63.12 | -81.78 |