|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| MM-GBSA (kcal/mol) | NAM | Iso-NAM | Nicotinic Acid (neutral) | Pyridine, 1-oxide | N(1)-methylnicotinamide | Nicotinic Acid, 1-oxide |
| SIRT3 (4FVT), with water | -38.14 |  |  |  |  |  |
| SIRT3 (4FVT), with NAD+ | -28.54 |  |  |  |  |  |
| SIRT3 (4FVT), w/o water | -32.95 | -31.54 | -34.89 | -24.24 | -40.03 | -30.05 |
| SIRT3 (3GLS) | -29.88 | -31.53 | -32.80 | -21.71 | -34.52 | -30.39 |
| SIRT3 (4BVG) | -39.81 | -34.68 | -36.59 | -26.74 | -48.04 | -33.06 |
| SIRT3 (4JSR) | -41.96 | -38.50 | -46.72 | -27.14 | -44.83 | -35.30 |
| SIRT3 (4BN5) | -28.71 | -28.70 | -29.40 | -19.71 | -37.19 | -27.70 |
| SIRT3 (4BVG) with Int | -38.55 | -32.36 | -36.73 | -27.34 | -44.51 | -34.16 |
| IC50 (mM) | 0.03670 | 13.80 | 14.50 | 24.10 | 9.20 | 13.00 |
| pIC50=-log10(IC50) | -4.435 | -1.860 | -1.839 | -1.618 | -2.036 | -1.886 |

Rearrange the table above.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| pIC50 | SIRT3 (4FVT), w/o water | SIRT3 (3GLS) | SIRT3 (4BVG) | SIRT3 (4JSR) | SIRT3 (4BN5) | SIRT3 (4BVG) with Int |  |
| -1.6180 | -24.24 | -21.71 | -26.74 | -27.14 | -19.71 | -27.34 | Pyridine, 1-oxide |
| -1.8386 | -34.89 | -32.80 | -36.59 | -46.72 | -29.40 | -36.73 | Nicotinic Acid (neutral) |
| -1.8601 | -31.54 | -31.53 | -34.68 | -38.50 | -28.70 | -32.36 | Iso-NAM |
| -1.8861 | -30.05 | -30.39 | -33.06 | -35.30 | -27.70 | -34.16 | Nicotinic Acid, 1-oxide |
| -2.0362 | -40.03 | -34.52 | -48.04 | -44.83 | -37.19 | -44.51 | N(1)-methylnicotinamide |

Plotting MM-GBSA vs pIC50