1. Component analysis for NAD+ in SIRT3 complexes with NAM, isoNAM and methyl-NAM:

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | SIRT3/Ac-CS2/NAD+/NAM | | SIRT3/Ac-CS2/ NAD+/isoNAM | | | SIRT3/Ac-CS2/ NAD+/methyl-NAM | | |
|  | Average | Std. Dev. | | Average | Std. Dev. | | Average | Std. Dev. | |
| VDWAALS\_complex | -2292.54 | 22.24 | | -2291.36 | 26.33 | | -2287.53 | 24.00 | |
| EEL\_complex | -18607.05 | 79.63 | | -18848.86 | 94.11 | | -18943.65 | 87.39 | |
| EGB\_complex | -3628.77 | 63.85 | | -3549.13 | 75.36 | | -3359.65 | 72.34 | |
| ESURF\_complex | 97.99 | 1.71 | | 99.39 | 2.24 | | 98.97 | 1.86 | |
| EPB\_complex | -3364.63 | 60.02 | | -3283.26 | 78.97 | | -3091.84 | 72.16 | |
| ENPOLAR\_complex | 2194.97 | 9.05 | | 2201.98 | 11.31 | | 2202.70 | 10.26 | |
| EDISPER\_complex | -1250.40 | 10.93 | | -1260.10 | 13.26 | | -1259.92 | 14.03 | |
| G\_gas\_complex | -3935.93 | 86.17 | | -3968.19 | 98.67 | | -4175.90 | 90.71 | |
| G\_solv\_igb2\_complex | -3530.79 | 63.31 | | -3449.73 | 74.09 | | -3260.67 | 71.63 | |
| G\_solv\_pb\_complex | -2420.06 | 59.71 | | -2341.38 | 79.66 | | -2149.05 | 71.62 | |
| VDWAALS\_receptor | -2209.64 | 21.52 | | -2206.88 | 25.30 | | -2208.16 | 23.54 | |
| EEL\_receptor | -18637.48 | 77.84 | | -18844.00 | 90.31 | | -18874.92 | 85.75 | |
| EGB\_receptor | -3441.90 | 62.07 | | -3406.37 | 72.00 | | -3267.96 | 70.72 | |
| ESURF\_receptor | 101.74 | 1.65 | | 102.88 | 2.25 | | 101.95 | 1.89 | |
| EPB\_receptor | -3177.13 | 58.46 | | -3146.28 | 74.75 | | -3007.49 | 70.02 | |
| ENPOLAR\_receptor | 2182.62 | 8.87 | | 2189.29 | 11.23 | | 2187.94 | 10.38 | |
| EDISPER\_receptor | -1269.82 | 10.65 | | -1280.68 | 13.15 | | -1276.66 | 14.41 | |
| G\_gas\_receptor | -3794.12 | 84.24 | | -3787.60 | 94.57 | | -3933.74 | 89.56 | |
| G\_solv\_igb2\_receptor | -3340.16 | 61.50 | | -3303.49 | 70.67 | | -3166.01 | 70.00 | |
| G\_solv\_pb\_receptor | -2264.33 | 58.56 | | -2237.67 | 75.53 | | -2096.20 | 69.41 | |
| VDWAALS\_ligand | -9.96 | 1.70 | | -10.28 | 1.61 | | -11.14 | 1.20 | |
| EEL\_ligand | -22.14 | 7.69 | | -13.45 | 9.76 | | -8.47 | 9.72 | |
| EGB\_ligand | -152.93 | 3.73 | | -154.30 | 5.87 | | -158.58 | 4.77 | |
| ESURF\_ligand | 5.06 | 0.04 | | 5.14 | 0.04 | | 5.24 | 0.05 | |
| EPB\_ligand | -159.70 | 3.27 | | -161.15 | 5.92 | | -164.54 | 4.47 | |
| ENPOLAR\_ligand | 57.28 | 0.34 | | 57.58 | 0.34 | | 58.28 | 0.35 | |
| EDISPER\_ligand | -65.58 | 0.35 | | -66.06 | 0.43 | | -66.43 | 0.37 | |
| G\_gas\_ligand | -121.45 | 6.48 | | -114.98 | 8.35 | | -113.67 | 7.73 | |
| G\_solv\_igb2\_ligand | -147.87 | 3.71 | | -149.16 | 5.85 | | -153.34 | 4.74 | |
| G\_solv\_pb\_ligand | -168.00 | 3.24 | | -169.64 | 5.92 | | -172.69 | 4.40 | |
| VDWAALS\_diff | -72.94 | 4.35 | | -74.20 | 4.24 | | -68.23 | 4.70 | |
| EEL\_diff | 52.57 | 13.53 | | 8.59 | 16.28 | | -60.26 | 15.39 | |
| EGB\_diff | -33.94 | 12.02 | | 11.54 | 12.75 | | 66.89 | 12.31 | |
| ESURF\_diff | -8.81 | 0.28 | | -8.63 | 0.23 | | -8.22 | 0.30 | |
| EPB\_diff | -27.80 | 12.52 | | 24.18 | 14.07 | | 80.19 | 13.78 | |
| ENPOLAR\_diff | -44.93 | 1.14 | | -44.89 | 0.98 | | -43.52 | 1.45 | |
| EDISPER\_diff | 85.00 | 1.46 | | 86.64 | 1.26 | | 83.17 | 1.77 | |
| G\_gas | -20.37 | 13.27 | | -65.61 | 15.43 | | -128.49 | 15.42 | |
| G\_solv\_igb2 | -42.76 | 12.10 | | 2.91 | 12.68 | | 58.67 | 12.22 | |
| G\_solv\_pb | 12.27 | 12.58 | | 65.93 | 14.02 | | 119.83 | 13.72 | |
| G\_igb2 | -63.12 | 4.37 | | -62.70 | 5.27 | | -69.82 | 5.79 | |
| G\_pb | -8.10 | 5.71 | | 0.33 | 6.52 | | -8.65 | 7.42 | |

1. Component analysis for NAM, isoNAM and methyl-NAM in C pocket in SIRT3 complex systems:

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | SIRT3/Ac-CS2/NAD+/NAM | | | SIRT3/Ac-CS2/ NAD+/isoNAM | | | SIRT3/Ac-CS2/ NAD+/methyl-NAM | | | |
|  | | Average | Std. Dev. | | Average | Std. Dev. | | Average | Std. Dev. |
| VDWAALS\_complex | | -2292.54 | 22.24 | | -2291.36 | 26.33 | | -2287.53 | 24.00 |
| EEL\_complex | | -18607.05 | 79.63 | | -18848.86 | 94.11 | | -18943.65 | 87.39 |
| EGB\_complex | | -3628.77 | 63.85 | | -3549.13 | 75.36 | | -3359.65 | 72.34 |
| ESURF\_complex | | 97.99 | 1.71 | | 99.39 | 2.24 | | 98.97 | 1.86 |
| EPB\_complex | | -3364.63 | 60.02 | | -3283.26 | 78.97 | | -3091.84 | 72.16 |
| ENPOLAR\_complex | | 2194.97 | 9.05 | | 2201.98 | 11.31 | | 2202.70 | 10.26 |
| EDISPER\_complex | | -1250.40 | 10.93 | | -1260.10 | 13.26 | | -1259.92 | 14.03 |
| G\_gas\_complex | | -3935.93 | 86.17 | | -3968.19 | 98.67 | | -4175.90 | 90.71 |
| G\_solv\_igb2\_complex | | -3530.79 | 63.31 | | -3449.73 | 74.09 | | -3260.67 | 71.63 |
| G\_solv\_pb\_complex | | -2420.06 | 59.71 | | -2341.38 | 79.66 | | -2149.05 | 71.62 |
| VDWAALS\_receptor | | -2271.60 | 22.11 | | -2271.30 | 25.59 | | -2268.34 | 23.86 |
| EEL\_receptor | | -18638.66 | 79.45 | | -18756.56 | 94.44 | | -18714.69 | 88.52 |
| EGB\_receptor | | -3639.47 | 63.75 | | -3551.26 | 75.50 | | -3534.87 | 73.32 |
| ESURF\_receptor | | 99.15 | 1.70 | | 100.41 | 2.16 | | 99.53 | 1.87 |
| EPB\_receptor | | -3384.01 | 59.90 | | -3293.48 | 78.59 | | -3272.94 | 72.66 |
| ENPOLAR\_receptor | | 2193.97 | 9.05 | | 2199.94 | 11.04 | | 2198.02 | 10.41 |
| EDISPER\_receptor | | -1259.60 | 10.88 | | -1268.60 | 12.89 | | -1268.87 | 14.07 |
| G\_gas\_receptor | | -3830.47 | 85.72 | | -3920.32 | 98.27 | | -3925.26 | 90.74 |
| G\_solv\_igb2\_receptor | | -3540.32 | 63.22 | | -3450.85 | 74.28 | | -3435.35 | 72.63 |
| G\_solv\_pb\_receptor | | -2449.64 | 59.59 | | -2362.13 | 79.21 | | -2343.78 | 72.08 |
| VDWAALS\_ligand | | -0.59 | 0.24 | | -0.60 | 0.26 | | -0.77 | 0.33 |
| EEL\_ligand | | 55.71 | 0.83 | | -80.72 | 1.00 | | 9.66 | 1.16 |
| EGB\_ligand | | -16.82 | 0.51 | | -15.97 | 0.55 | | -65.68 | 0.93 |
| ESURF\_ligand | | 1.73 | 0.01 | | 1.73 | 0.01 | | 1.90 | 0.01 |
| EPB\_ligand | | -14.59 | 0.47 | | -13.72 | 0.51 | | -62.86 | 0.88 |
| ENPOLAR\_ligand | | 15.47 | 0.10 | | 15.53 | 0.12 | | 17.87 | 0.12 |
| EDISPER\_ligand | | -16.01 | 0.12 | | -15.97 | 0.13 | | -18.20 | 0.16 |
| G\_gas\_ligand | | -61.02 | 2.53 | | -16.83 | 2.68 | | 6.40 | 3.03 |
| G\_solv\_igb2\_ligand | | -15.09 | 0.51 | | -14.24 | 0.55 | | -63.79 | 0.93 |
| G\_solv\_pb\_ligand | | -15.12 | 0.50 | | -14.17 | 0.53 | | -63.20 | 0.87 |
| VDWAALS\_diff | | -20.34 | 1.90 | | -19.46 | 2.32 | | -18.42 | 1.91 |
| EEL\_diff | | -24.10 | 2.84 | | -11.58 | 3.69 | | -238.62 | 9.64 |
| EGB\_diff | | 27.51 | 1.64 | | 18.10 | 2.02 | | 240.91 | 9.04 |
| ESURF\_diff | | -2.89 | 0.08 | | -2.75 | 0.16 | | -2.45 | 0.13 |
| EPB\_diff | | 33.96 | 2.84 | | 23.94 | 2.93 | | 243.96 | 11.17 |
| ENPOLAR\_diff | | -14.47 | 0.25 | | -13.49 | 0.59 | | -13.19 | 0.60 |
| EDISPER\_diff | | 25.20 | 0.59 | | 24.47 | 0.93 | | 27.15 | 0.85 |
| G\_gas | | -44.44 | 2.59 | | -31.04 | 3.67 | | -257.04 | 10.04 |
| G\_solv\_igb2 | | 24.62 | 1.63 | | 15.35 | 2.01 | | 238.46 | 9.00 |
| G\_solv\_pb | | 44.70 | 3.20 | | 34.92 | 3.33 | | 257.93 | 11.38 |
| G\_igb2 | | -19.82 | 1.89 | | -15.68 | 2.48 | | -18.58 | 2.14 |
| G\_pb | | 0.26 | 3.26 | | 3.89 | 4.18 | | 0.89 | 4.23 |