Component analysis of MM-PB(GB)SA results for acetylated peptide, NAD+

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  | Mean |  |  |  |  | Mean |
| AcCS2 Binding: GBSA |  | -47.936 |  | AcCS2 Binding: PBSA |  | -9.314 |
| G\_igb2\_com | G\_igb2\_rec | G\_igb2\_lig | G\_igb2 |  | G\_pb\_com | G\_pb\_rec | G\_pb\_lig | G\_pb |
| -7352.719 | -7302.957 | 5.629 | -55.392 |  | -6255.144 | -6246.318 | 4.734 | -13.561 |
| -7340.571 | -7291.542 | 5.931 | -54.960 |  | -6240.800 | -6231.330 | 5.328 | -14.799 |
| -7338.191 | -7289.537 | 5.096 | -53.750 |  | -6239.618 | -6230.002 | 4.549 | -14.164 |
| -7337.093 | -7289.345 | 7.355 | -55.104 |  | -6236.104 | -6227.899 | 6.454 | -14.660 |
| -7347.851 | -7301.920 | 7.151 | -53.083 |  | -6259.238 | -6252.575 | 5.830 | -12.493 |
| -7353.335 | -7310.329 | 4.288 | -47.294 |  | -6272.321 | -6266.910 | 3.386 | -8.796 |
| -7355.126 | -7310.178 | 4.156 | -49.105 |  | -6279.721 | -6273.275 | 3.694 | -10.140 |
| -7361.573 | -7317.785 | 3.821 | -47.609 |  | -6270.943 | -6264.034 | 2.912 | -9.821 |
| -7377.192 | -7335.217 | 4.469 | -46.444 |  | -6276.062 | -6271.335 | 3.426 | -8.153 |
| -7382.774 | -7338.068 | 4.519 | -49.225 |  | -6291.173 | -6285.223 | 3.711 | -9.662 |
|  |  |  |  |  |  |  |  |  |
|  |  |  | Mean |  |  |  |  | Mean |
| NAD+ Binding: GBSA |  | -65.629 |  | NAD+ Binding: PBSA |  | -5.354 |
| G\_igb2\_com | G\_igb2\_rec | G\_igb2\_lig | G\_igb2 |  | G\_pb\_com | G\_pb\_rec | G\_pb\_lig | G\_pb |
| -7352.719 | -7032.076 | -257.903 | -62.739 |  | -6255.144 | -5980.275 | -279.576 | 4.708 |
| -7340.571 | -7022.438 | -256.775 | -61.358 |  | -6240.800 | -5969.503 | -279.185 | 7.887 |
| -7338.191 | -7023.218 | -256.812 | -58.161 |  | -6239.618 | -5970.158 | -279.054 | 9.594 |
| -7337.093 | -7021.304 | -256.512 | -59.277 |  | -6236.104 | -5966.532 | -278.713 | 9.141 |
| -7347.851 | -7030.499 | -257.049 | -60.303 |  | -6259.238 | -5988.295 | -278.883 | 7.940 |
| -7353.335 | -7026.240 | -259.414 | -67.682 |  | -6272.321 | -5984.674 | -280.995 | -6.651 |
| -7355.126 | -7029.635 | -258.714 | -66.778 |  | -6279.721 | -5992.227 | -280.053 | -7.441 |
| -7361.573 | -7038.676 | -259.127 | -63.770 |  | -6270.943 | -5985.819 | -280.400 | -4.724 |
| -7377.192 | -7054.088 | -259.587 | -63.517 |  | -6276.062 | -5994.005 | -280.837 | -1.220 |
| -7382.774 | -7057.276 | -259.102 | -66.396 |  | -6291.173 | -6003.585 | -280.853 | -6.735 |

\* ∆G is calculated every 200 frames in 2 ns simulation;

Mean value is averaged over the 1000 frames from last 10 ns;

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Free\_SIRT3\_G\_igb2 | Free\_AcCS2\_G\_igb2 | Free\_NADp\_G\_igb2 |  |  | Free\_SIRT3\_G\_pb | Free\_AcCS2\_G\_pb | Free\_NADp\_G\_pb |  |
| -7006.465 | 4.395 | -276.130 |  |  | -5982.357 | 5.685 | -291.932 |  |