**Table 1. Primer sequences for qPCR.**

|  |  |
| --- | --- |
| **Gene** | **Primer sequence** |
| *MMP2* | F: ACGACCGCGACAAGAAGTAT |
| R: ATTTGTTGCCCAGGAAAGTG |
| *Vimentin* | F: ACTACGTCCACCCGCACCTA |
| R: CAGCGAGAAGTCCACCGAGT |
| *Cyclin D1* | F: GTCGCTGGAGCCCGTGA |
| R: GGATGGAGTTGTCGGTGTAGATG |
| *c-Myc* | F: GGCTCCTGGCAAAAGGTCA |
| R: CTGCGTAGTTGTGCTGATGT |
| F, forward; R, reverse. | |

**Table 2. MM/GBSA binding free energy (kcal/mol) of simulation systems.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Energy**  **Component** | **Systems** | | | | |
| **wt-STAT3\_DNA** | **Y2P-STAT3\_DNA** | **6-EDS\_wt-STAT3** | **6-EDS\_wt-STAT3\_DNA** | **6-EDS\_Y2P-STAT3\_DNA** |
| ΔEvdw | -63.86 ± 4.44 | -66.19 ± 14.26 | -40.10 ± 3.30 | -46.14 ± 4.81 | -35.55 ± 7.94 |
| ΔEele | -1035.82 ± 96.01 | -1270.16 ± 111.34 | -18.06 ± 7.89 | -1270.52 ± 76.17 | -890.26 ± 87.68 |
| ΔEGB | 890.92 ± 94.95 | 1119.66 ± 106.10 | 19.23 ± 5.46 | 1219.46 ± 71.51 | 816.27 ± 87.97 |
| ΔESURF | -9.08 ± 0.47 | -8.99 ± 1.92 | -5.04 ± 0.30 | -7.16 ± 0.46 | -5.06 ± 1.23 |
| ΔGGAS | -1099.69 ± 96.42 | -1336.34 ± 103.66 | -59.17 ± 8.84 | -916.66 ± 76.46 | -925.78 ± 92.47 |
| ΔGsolv | 881.83 ± 94.97 | 1110.68 ± 107.01 | 14.19 ± 5.32 | 811.31 ± 71.31 | 811.21 ± 81.27 |
| ΔGbind | -217.85 ± 5.81 | -225.66 ± 9.00 | -44.98 ± 4.63 | -105.36 ± 8.19 | -114.57 ± 10.55 |