## Peptide Name
| Peptide name | Peptide Sequence | Unnamed: 2 | Parameters for 11 simulations are reported |
| --- | --- | --- | --- |
| HA | PKYVKQNTLKLAT | NaN | NaN |
| CLIP | VSKMRMATPLLMQA | NaN | NaN |
| YAK | AAYAAAAAAKAAA | NaN | NaN |
| HAY308A | PKAVKQNTLKLAT | NaN | NaN |

## Simulation 1
| Simulation 1: CG\_HA\_COM (starting K=2500) | Unnamed: 1 | Unnamed: 2 | Unnamed: 3 |
| --- | --- | --- | --- |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 1.8 | 1.79 | 800 |
| 1\*\* | 1.9 | 1.88 | 800 |
| 2 | 1.99 | 1.99 | 2500 |
| 3 | 2.06 | 2.07 | 2500 |
| 4\*\* | 2.14 | 2.14 | 2500 |
| 5 | 2.23 | 2.23 | 2500 |
| 6 | 2.31 | 2.29 | 2500 |
| 7 | 2.41 | 2.42 | 2500 |
| 8 | 2.46 | 2.46 | 2500 |
| 9 | 2.61 | 2.59 | 2500 |
| 10\*\* | 2.75 | 2.73 | 2500 |
| 11 | 2.85 | 2.83 | 2500 |
| 12\*\* | 2.95 | 2.93 | 2500 |
| 13 | 3.05 | 3.03 | 2500 |
| 14 | 3.16 | 3.15 | 2500 |
| 15 | 3.31 | 3.3 | 2500 |
| 16\*\* | 3.4 | 3.39 | 2500 |
| 17 | 3.54 | 3.53 | 2500 |
| 18\*\* | 3.7 | 3.69 | 1500 |
| 19\*\* | 3.9 | 3.89 | 800 |

## Simulation 2
| Simulation 2: CG\_HA\_peel-PRO306 (starting K=800) | Unnamed: 1 | Unnamed: 2 | Unnamed: 3 |
| --- | --- | --- | --- |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 2.17 | 2.15 | 800 |
| 1 | 2.32 | 2.3 | 800 |
| 2 | 2.49 | 2.47 | 800 |
| 3 | 2.65 | 2.63 | 800 |
| 4\* | 2.78 | 2.76 | 1500 |
| 5 | 3 | 2.98 | 800 |
| 6 | 3.11 | 3.1 | 800 |
| 7 | 3.23 | 3.21 | 800 |
| 8\*\* | 3.35 | 3.32 | 800 |
| 9\*\* | 3.47 | 3.45 | 800 |
| 10 | 3.62 | 3.61 | 800 |
| 11 | 3.85 | 3.85 | 800 |
| 12 | 3.95 | 3.95 | 800 |

## Simulation 3
| Simulation 3: CG\_HA\_peel-THR318 (starting K=1500) | Unnamed: 1 | Unnamed: 2 | Unnamed: 3 |
| --- | --- | --- | --- |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 1.82 | 1.84 | 1500 |
| 1 | 1.9 | 1.92 | 1500 |
| 2 | 1.96 | 1.97 | 1500 |
| 3\*\* | 2.05 | 2.03 | 800 |
| 4 | 2.15 | 2.13 | 1500 |
| 5 | 2.25 | 2.24 | 1500 |
| 6 | 2.34 | 2.36 | 1500 |
| 7 | 2.41 | 2.43 | 1500 |
| 8 | 2.55 | 2.55 | 1500 |
| 9 | 2.64 | 2.63 | 1500 |
| 10 | 2.79 | 2.77 | 1500 |
| 11 | 2.9 | 2.88 | 1500 |
| 12\*, \*\* | 3.02 | 3 | 2500 |
| 13 | 3.19 | 3.17 | 1500 |
| 14\*\* | 3.29 | 3.27 | 1500 |
| 15 | 3.4 | 3.4 | 1500 |
| 16 | 3.5 | 3.5 | 1500 |
| 17 | 3.6 | 3.6 | 1500 |
| 18 | 3.7 | 3.7 | 1500 |
| 19 | 3.8 | 3.8 | 1500 |

## Simulation 4
| Simulation 4: CG\_ CLIP (using mutated HA sequence) \_COM (starting K=1500) | Unnamed: 1 | Unnamed: 2 | Unnamed: 3 |
| --- | --- | --- | --- |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0\* | 1.96 | 1.95 | 2500 |
| 1\* | 2.09 | 2.11 | 2500 |
| 2 | 2.19 | 2.17 | 1500 |
| 3 | 2.29 | 2.3 | 1500 |
| 4 | 2.39 | 2.38 | 1500 |
| 5\* | 2.54 | 2.53 | 2500 |
| 6 | 2.71 | 2.7 | 1500 |
| 7 | 2.8 | 2.78 | 1500 |
| 8\* | 2.92 | 2.91 | 2500 |
| 9\*, \*\* | 2.98 | 2.98 | 2500 |
| 10 | 3.08 | 3.06 | 1500 |
| 11\*, \*\* | 3.15 | 3.15 | 2500 |
| 12 | 3.25 | 3.25 | 1500 |
| 13\*\* | 3.35 | 3.33 | 1500 |
| 14 | 3.44 | 3.44 | 1500 |
| 15\*\* | 3.5 | 3.5 | 1500 |
| 16\*\* | 3.61 | 3.62 | 1500 |
| 17 | 3.72 | 3.72 | 1500 |
| 18 | 3.84 | 3.84 | 1500 |
| 19 | 3.97 | 3.95 | 1500 |
| 20 | 4.1 | 4.09 | 1500 |
| 21 | 4.2 | 4.18 | 1500 |
| 22 | 4.24 | 4.23 | 1500 |
| 23 | 4.36 | 4.35 | 1500 |
| 24 | 4.46 | 4.46 | 1500 |
| 25 | 4.57 | 4.57 | 1500 |
| 26 | 4.64 | 4.65 | 1500 |
| 27 | 4.73 | 4.74 | 1500 |
| 28 | 4.83 | 4.83 | 1500 |

## Simulation 5
| Simulation 5: CG\_YAK\_COM (starting K=1500) | Unnamed: 1 | Unnamed: 2 | Unnamed: 3 |
| --- | --- | --- | --- |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 1.58 | 1.6 | 800 |
| 1\*\* | 1.77 | 1.75 | 1500 |
| 2 | 1.84 | 1.82 | 1500 |
| 3 | 1.89 | 1.89 | 1500 |
| 4\*\* | 1.96 | 1.95 | 800 |
| 5\*\* | 2.02 | 2.03 | 1500 |
| 6 | 2.1 | 2.1 | 800 |
| 7 | 2.16 | 2.18 | 1500 |
| 8\*\* | 2.25 | 2.26 | 800 |
| 9 | 2.32 | 2.33 | 1500 |
| 10 | 2.37 | 2.37 | 1500 |
| 11\*, \*\* | 2.41 | 2.41 | 2500 |
| 12 | 2.5 | 2.52 | 1500 |
| 13\*, \*\* | 2.57 | 2.55 | 2500 |
| 14\* | 2.65 | 2.64 | 2500 |
| 15\* | 2.71 | 2.69 | 5000 |
| 16\*\* | 2.75 | 2.73 | 5000 |
| 17 | 2.87 | 2.85 | 1500 |
| 18 | 2.95 | 2.93 | 1500 |
| 19\*\* | 3 | 3.02 | 1500 |
| 20 | 3.13 | 3.14 | 1500 |
| 21 | 3.33 | 3.32 | 1500 |
| 22 | 3.38 | 3.38 | 1500 |
| 23 | 3.42 | 3.42 | 1500 |
| 24 | 3.49 | 3.48 | 1500 |
| 25 | 3.62 | 3.62 | 1500 |
| 26\* | 3.7 | 3.7 | 1500 |
| 27 | 3.79 | 3.78 | 1500 |
| 28 | 3.9 | 3.88 | 1500 |
| 29 | 4.01 | 3.99 | 1500 |
| 30\*\* | 4.2 | 4.18 | 800 |

## Simulation 6
| Simulation 6: CG\_HAY308A\_COM (starting K=1500) | Unnamed: 1 | Unnamed: 2 | Unnamed: 3 |
| --- | --- | --- | --- |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 2.28 | 2.28 | 1500 |
| 1 | 2.48 | 2.48 | 1500 |
| 2 | 2.58 | 2.57 | 1500 |
| 3 | 2.69 | 2.68 | 1500 |
| 4 | 2.79 | 2.8 | 1500 |
| 5 | 2.89 | 2.88 | 1500 |
| 6\* | 3 | 3 | 2500 |
| 7\* | 3.07 | 3.05 | 2500 |
| 8\* | 3.15 | 3.15 | 2500 |
| 9\* | 3.25 | 3.25 | 2500 |
| 10 | 3.35 | 3.33 | 1500 |
| 11\* | 3.51 | 3.53 | 2500 |
| 12\*, \*\* | 3.4 | 3.4 | 2500 |
| 13\* | 3.6 | 3.61 | 2500 |
| 14 | 3.68 | 3.67 | 1500 |
| 15 | 3.8 | 3.8 | 1500 |
| 16 | 3.9 | 3.9 | 1500 |
| 17\* | 4 | 4 | 2500 |
| 18 | 4.12 | 4.11 | 1500 |
| 19 | 4.22 | 4.2 | 1500 |
| 20 | 4.31 | 4.31 | 1500 |
| 21 | 4.46 | 4.46 | 1500 |
| 22 | 4.57 | 4.57 | 1500 |
| 23 | 4.64 | 4.64 | 1500 |
| 24 | 4.75 | 4.75 | 1500 |
| 25 | 4.85 | 4.85 | 1500 |
| 26 | 4.95 | 4.95 | 1500 |
| 27 | 5.07 | 5.07 | 1500 |
| 28 | 5.16 | 5.16 | 1500 |
| 29 | 5.26 | 5.27 | 1500 |
| 30 | 5.34 | 5.35 | 1500 |
| 31 | 5.47 | 5.47 | 1500 |
| 32 | 5.57 | 5.57 | 1500 |
| 33 | 5.69 | 5.7 | 1500 |

## Simulation 7
| Simulation 7: CG\_HA-segment-(PKY|VKQ|NTL|KLAT)\_COM | Unnamed: 1 | Unnamed: 2 | Unnamed: 3 |
| --- | --- | --- | --- |
| PKY (starting K=2500) | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 2.09 | 2.1 | 2500 |
| 1 | 2.19 | 2.19 | 2500 |
| 2 | 2.28 | 2.86 | 2500 |
| 3 | 2.39 | 2.37 | 2500 |
| 4\*\* | 2.6 | 2.58 | 2500 |
| 5 | 2.7 | 2.68 | 2500 |
| 6 | 2.75 | 2.75 | 2500 |
| 7 | 2.86 | 2.85 | 2500 |
| 8 | 2.97 | 2.96 | 2500 |
| 9 | 3.08 | 3.08 | 2500 |
| 10\*\* | 3.2 | 3.2 | 2500 |
| 11 | 3.29 | 3.29 | 2500 |
| VKQ (starting K=2000) | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0\* | 2.08 | 2.06 | 2500 |
| 1\* | 2.1 | 2.12 | 2500 |
| 2 | 2.23 | 2.23 | 2000 |
| 3\*\* | 2.4 | 2.38 | 2000 |
| 4 | 2.51 | 2.51 | 2000 |
| 5 | 2.58 | 2.56 | 2000 |
| 6 | 2.67 | 2.68 | 2000 |
| 7 | 2.75 | 2.73 | 2000 |
| 8 | 2.86 | 2.85 | 2000 |
| 9 | 2.96 | 2.96 | 2000 |
| 10 | 3.12 | 3.11 | 2000 |
| 11 | 3.19 | 3.19 | 2000 |
| 12 | 3.31 | 3.3 | 2000 |
| 13 | 3.41 | 3.41 | 2000 |
| 14 | 3.46 | 3.46 | 2000 |
| 15 | 3.56 | 3.56 | 2000 |
| 16 | 3.64 | 3.64 | 2000 |
| NTL (starting K=2500) | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0\* | 1.7 | 1.72 | 2500 |
| 1 | 1.83 | 1.85 | 2500 |
| 2 | 1.94 | 1.94 | 2500 |
| 3 | 1.98 | 2 | 2500 |
| 4 | 2.04 | 2.06 | 2500 |
| 5 | 2.13 | 2.12 | 2500 |
| 6\* | 2.2 | 2.18 | 2500 |
| KLAT (starting K=2000) | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 1.88 | 1.88 | 2000 |
| 1 | 1.98 | 1.98 | 2000 |
| 2 | 2.08 | 2.09 | 2000 |
| 3 | 2.19 | 2.2 | 2000 |
| 4 | 2.35 | 2.36 | 2000 |
| 5 | 2.46 | 2.46 | 2000 |
| 6 | 2.56 | 2.54 | 2000 |
| 7 | 2.6 | 2.61 | 2000 |
| 8 | 2.7 | 2.71 | 2000 |
| 9\*\* | 2.8 | 2.78 | 2000 |
| 10\*\* | 2.9 | 2.92 | 2000 |
| 11 | 3.03 | 3.02 | 2000 |
| 12 | 3.13 | 3.14 | 2000 |
| 13 | 3.23 | 3.23 | 2000 |
| 14 | 3.33 | 3.33 | 2000 |
| 15 | 3.43 | 3.44 | 2000 |
| 16 | 3.53 | 3.53 | 2000 |
| 17 | 3.62 | 3.61 | 2000 |
| 18 | 3.73 | 3.74 | 2000 |
| 19 | 3.81 | 3.81 | 2000 |
| 20 | 4.04 | 4.03 | 2000 |

## Simulation 8
| Simulation 8: CG\_HA-segment-(PKYV|KQN|TLK|LAT)\_COM | Unnamed: 1 | Unnamed: 2 | Unnamed: 3 |
| --- | --- | --- | --- |
| PKYV (starting K=1500) | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 2.12 | 2.1 | 800 |
| 1 | 2.26 | 2.25 | 1500 |
| 2\* | 2.35 | 2.34 | 2500 |
| 3 | 2.46 | 2.46 | 1500 |
| 4\*, \*\* | 2.6 | 2.58 | 2500 |
| 5 | 2.66 | 2.65 | 1500 |
| 6 | 2.76 | 2.75 | 1500 |
| 7\*\* | 2.85 | 2.84 | 1500 |
| 8 | 2.93 | 2.93 | 1500 |
| 9 | 2.98 | 2.97 | 1500 |
| 10 | 3.08 | 3.06 | 1500 |
| 11\* | 3.18 | 3.17 | 2500 |
| 12\*\* | 3.24 | 3.24 | 1500 |
| 13 | 3.35 | 3.35 | 1500 |
| 14 | 3.49 | 3.48 | 1500 |
| 15 | 3.56 | 3.56 | 1500 |
| 16 | 3.6 | 3.6 | 1500 |
| KQN (starting K=1000) | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 2.31 | 2.31 | 1500 |
| 1 | 2.45 | 2.43 | 1000 |
| 2 | 2.54 | 2.54 | 1000 |
| 3 | 2.63 | 2.63 | 1000 |
| 4 | 2.69 | 2.68 | 1000 |
| 5 | 2.89 | 2.9 | 1000 |
| 6 | 2.99 | 3 | 1000 |
| 7 | 3.11 | 3.1 | 1000 |
| 8 | 3.18 | 3.18 | 1000 |
| 9 | 3.27 | 3.27 | 1000 |
| 10 | 3.37 | 3.38 | 1000 |
| 11 | 3.48 | 3.49 | 1000 |
| 12 | 3.55 | 3.55 | 1000 |
| 13 | 3.64 | 3.55 | 1000 |
| 14 | 3.75 | 3.74 | 1000 |
| 15 | 3.85 | 3.85 | 1000 |
| TLK (starting K=800) | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 1.45 | 1.46 | 800 |
| 1\* | 1.55 | 1.56 | 2500 |
| 2\* | 1.62 | 1.8 | 1500 |
| 3\* | 1.7 | 1.71 | 2500 |
| 4\* | 1.8 | 1.8 | 1500 |
| 5\* | 1.9 | 1.91 | 1500 |
| 6 | 2.03 | 2.03 | 800 |
| 7\* | 2.14 | 2.15 | 2500 |
| 8\* | 2.28 | 2.29 | 1500 |
| 9\* | 2.36 | 2.36 | 2500 |
| 10\* | 2.5 | 2.51 | 1500 |
| 11 | 2.6 | 2.6 | 800 |
| 12\* | 2.83 | 2.81 | 1500 |
| 13\* | 2.92 | 2.91 | 1500 |
| 14 | 3.15 | 3.15 | 800 |
| 15 | 3.3 | 3.32 | 800 |
| 16 | 3.43 | 3.41 | 800 |
| 17 | 3.55 | 3.54 | 800 |
| 18 | 3.65 | 3.65 | 800 |
| 19 | 3.83 | 3.83 | 800 |
| LAT (starting K=800) | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 1.07 | 1.05 | 800 |
| 1 | 1.13 | 1.15 | 800 |
| 2 | 1.33 | 1.35 | 800 |
| 3 | 1.62 | 1.6 | 800 |
| 4 | 1.73 | 1.73 | 800 |
| 5 | 1.81 | 1.79 | 800 |
| 6 | 1.89 | 1.9 | 800 |
| 7 | 1.99 | 2 | 800 |
| 8 | 2.16 | 2.15 | 800 |
| 9 | 2.32 | 2.3 | 800 |
| 10 | 2.44 | 2.45 | 800 |
| 11 | 2.49 | 2.49 | 800 |
| 12 | 2.61 | 2.63 | 800 |
| 13 | 2.65 | 2.66 | 800 |
| 14 | 2.77 | 2.79 | 800 |
| 15 | 2.89 | 2.9 | 800 |
| 16 | 2.99 | 2.98 | 800 |
| 17 | 3.09 | 3.1 | 800 |
| 18 | 3.21 | 3.2 | 800 |
| 19 | 3.34 | 3.35 | 800 |
| 20 | 3.44 | 3.45 | 800 |
| 21 | 3.55 | 3.56 | 800 |

## Simulation 9
| Simulation 9: CG\_HA-segment-(PK|YV|KQ)\_COM | Unnamed: 1 | Unnamed: 2 | Unnamed: 3 |
| --- | --- | --- | --- |
| PK (starting K=800) | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 2.31 | 2.31 | 800 |
| 1 | 2.38 | 2.38 | 800 |
| 2 | 2.45 | 2.45 | 800 |
| 3 | 2.5 | 2.5 | 800 |
| 4\*\* | 2.65 | 2.65 | 800 |
| 5 | 2.82 | 2.81 | 800 |
| 6 | 2.98 | 2.97 | 800 |
| 7 | 3.04 | 3.02 | 800 |
| 8 | 3.09 | 3.07 | 800 |
| 9 | 3.18 | 3.17 | 800 |
| 10 | 3.21 | 3.2 | 800 |
| 11 | 3.32 | 3.31 | 800 |
| YV (starting K=1500) | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0\* | 1.85 | 1.83 | 2500 |
| 1 | 1.95 | 1.93 | 1500 |
| 2\* | 2.05 | 2.06 | 2500 |
| 3\*, \*\* | 2.15 | 2.15 | 2500 |
| 4 | 2.27 | 2.27 | 1500 |
| 5 | 2.32 | 2.32 | 1500 |
| 6 | 2.37 | 2.37 | 1500 |
| 7 | 2.46 | 2.46 | 1500 |
| 8 | 2.52 | 2.53 | 1500 |
| 9 | 2.57 | 2.55 | 1500 |
| 10 | 2.61 | 2.61 | 1500 |
| 11 | 2.66 | 2.66 | 1500 |
| 12 | 2.72 | 2.72 | 1500 |
| 13 | 2.76 | 2.75 | 1500 |
| 14 | 2.82 | 2.81 | 1500 |
| 15 | 2.89 | 2.87 | 1500 |
| 16 | 2.92 | 2.92 | 1500 |
| 17 | 2.96 | 2.96 | 1500 |
| 18 | 3.01 | 3 | 1500 |
| 19 | 3.06 | 3.07 | 1500 |
| KQ | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 2.01 | 2 | 800 |
| 1 | 2.15 | 2.12 | 800 |
| 2 | 2.19 | 2.18 | 800 |
| 3 | 2.24 | 2.24 | 800 |
| 4 | 2.31 | 2.3 | 800 |
| 5\*, \*\* | 2.46 | 2.44 | 1500 |
| 6 | 2.62 | 2.62 | 800 |
| 7 | 2.72 | 2.71 | 800 |
| 8 | 2.76 | 2.76 | 800 |
| 9 | 2.89 | 2.89 | 800 |
| 10 | 2.92 | 2.93 | 800 |
| 11 | 3.01 | 3.01 | 800 |
| 12 | 3.26 | 3.26 | 800 |
| 13 | 3.45 | 3.45 | 800 |
| 14 | 3.52 | 3.5 | 800 |
| 15 | 3.54 | 3.54 | 800 |
| 16 | 3.66 | 3.65 | 800 |

## Simulation 10
| Simulation 10: CG\_HAY308A\_segment-(PKA|VKQ)\_COM | Unnamed: 1 | Unnamed: 2 | Unnamed: 3 |
| --- | --- | --- | --- |
| PKA (starting K=1000) | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 2.34 | 2.35 | 1000 |
| 1 | 2.44 | 2.44 | 1000 |
| 2 | 2.54 | 2.55 | 1000 |
| 3 | 2.65 | 2.65 | 1000 |
| 4\* | 2.82 | 2.81 | 1500 |
| 5\*, \*\* | 2.9 | 2.9 | 1500 |
| 6 | 3.05 | 3.03 | 1000 |
| 7 | 3.16 | 3.16 | 1000 |
| 8 | 3.27 | 3.26 | 1000 |
| 9 | 3.37 | 3.37 | 1000 |
| VKQ (starting K=1500) | NaN | NaN | NaN |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 1.83 | 1.85 | 1500 |
| 1 | 1.89 | 1.9 | 1500 |
| 2 | 2.01 | 1.99 | 1500 |
| 3 | 2.12 | 2.14 | 1500 |
| 4 | 2.21 | 2.2 | 1500 |
| 5 | 2.31 | 2.28 | 1500 |
| 6 | 2.41 | 2.38 | 1500 |
| 7 | 2.51 | 2.49 | 1500 |
| 8 | 2.61 | 2.6 | 1500 |
| 9 | 2.71 | 2.7 | 1500 |
| 10 | 2.83 | 2.85 | 1500 |
| 11 | 3.09 | 3.07 | 1500 |
| 12 | 3.17 | 3.17 | 1500 |
| 13 | 3.28 | 3.27 | 1500 |
| 14 | 3.36 | 3.36 | 1500 |
| 15 | 3.59 | 3.58 | 1500 |
| 16 | 3.61 | 3.61 | 1500 |

## Simulation 11
| Simulation 11: CG\_CLIP (using 3QXA crystal structure) \_COM (starting K=1500) | Unnamed: 1 | Unnamed: 2 | Unnamed: 3 |
| --- | --- | --- | --- |
| Window ID | Set Position (nm) | Simulated Position (nm) | K (kJ/(mol\*nm)) |
| 0 | 2.18 | 2.2 | 1500 |
| 1\* | 2.23 | 2.23 | 5000 |
| 2 | 2.35 | 2.34 | 1500 |
| 3\*\* | 2.42 | 2.41 | 1500 |
| 4\*\* | 2.52 | 2.51 | 1500 |
| 5\*, \*\* | 2.58 | 2.58 | 8000 |
| 6\*\* | 2.7 | 2.72 | 1500 |
| 7\* | 2.8 | 2.78 | 2500 |
| 8 | 2.9 | 2.91 | 2500 |
| 9\*\* | 3 | 2.98 | 1500 |
| 10\* | 3.09 | 3.07 | 2500 |
| 11 | 3.15 | 3.14 | 5000 |
| 12 | 3.22 | 3.21 | 1500 |
| 13\* | 3.3 | 3.32 | 5000 |
| 14\*, \*\* | 3.41 | 3.41 | 5000 |
| 15 | 3.51 | 3.5 | 1500 |
| 16\*\* | 3.6 | 3.6 | 1500 |
| 17 | 3.72 | 3.71 | 1500 |