Analysis of fluctuation in the heme-binding pocket and heme distortion in hemoglobin and myoglobin

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**Table S1**. The mean values and standard deviation (std) of the pocket volume in each subunit in each trajectory.

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| **System** | **Mean ± std**  **(trajectory1)** | **Mean ± std**  **(trajectory2)** |
| dHb a1 | 466.073 ± 25.613 | 475.049 ± 30.022 |
| dHb a2 | 457.488 ± 33.651 | 471.098 ± 29.834 |
| dHb b1 | 462.927 ± 27.394 | 460.732 ± 34.738 |
| dHb b2 | 456.854 ± 33.004 | 454.707 ± 31.314 |
| oHb a1 | 446.463 ± 25.613 | 438.122 ± 24.688 |
| oHb a2 | 452.951 ± 23.947 | 438.732 ± 29.808 |
| oHb b1 | 477.585 ± 39.005 | 478.244 ± 30.544 |
| oHb b2 | 458.561 ± 29.228 | 474.049 ± 31.654 |
| dMb | 613.049 ± 52.655 | 557.024 ± 43.794 |
| oMb | 502.732 ± 40.792 | 518.293 ± 33.807 |