Depolarizing effects in hydrogen bond energy in 310-helices revealed by quantum chemical analysis

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**Table S1**. The H-bond energies in the WH3-10, ST3-10, MH3-10, and MM calculations and the H-bond distance of each H-bond pair.

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|  | WH3-10 | ST3-10 | MH3-10 | MM | Distance |
| 2-1 | -5.253 | -5.253 | -5.763 | -5.136 | 2.023 |
| 3-1† | -4.530 | -4.998 | -5.575 | -5.149 | 2.069 |
| 3-2† | -4.759 | -5.103 | -5.447 | -4.638 | 2.071 |
| 4-1 | -5.080 | -5.128 | -5.747 | -5.307 | 2.033 |
| 4-2 | -4.063 | -4.822 | -5.213 | -4.533 | 2.139 |
| 4-3 | -5.233 | -5.231 | -5.630 | -4.846 | 2.029 |
| 5-1 | -5.158 | -5.144 | -5.755 | -5.341 | 2.016 |
| 5-2 | -4.527 | -4.980 | -5.399 | -4.697 | 2.096 |
| 5-3 | -4.510 | -4.973 | -5.420 | -4.809 | 2.081 |
| 5-4 | -5.356 | -5.234 | -5.619 | -4.843 | 2.017 |
| 6-1 | -5.293 | -5.172 | -5.788 | -5.380 | 2.004 |
| 6-2 | -4.593 | -5.016 | -5.426 | -4.744 | 2.079 |
| 6-3 | -5.054 | -5.109 | -5.586 | -4.948 | 2.042 |
| 6-4 | -4.602 | -4.974 | -5.414 | -4.820 | 2.070 |
| 6-5 | -5.471 | -5.246 | -5.635 | -4.859 | 2.009 |
| 7-1 | -5.365 | -5.180 | -5.801 | -5.405 | 1.996 |
| 7-2 | -4.708 | -5.056 | -5.465 | -4.783 | 2.063 |
| 7-3 | -5.127 | -5.125 | -5.59 | -4.970 | 2.029 |
| 7-4 | -5.179 | -5.111 | -5.582 | -4.961 | 2.031 |
| 7-5 | -4.711 | -4.990 | -5.428 | -4.838 | 2.061 |
| 7-6 | -5.547 | -5.252 | -5.642 | -4.869 | 2.001 |

† The H-bond pairs in the N- and C-termini are adjacent to each other in 3\_10H-3, e.g. the N-terminal H-bond pair of 3\_10H-3, 3-1 is adjacent to the C-terminal H-bond pair, 3-2 and vice versa.