

Supporting Information S2. The original numerical values for the 12 physicochemical properties of dinucleotide, where the physicochemical property “A-philicity” [22] is denoted by P(1); “base stacking” [23] by P(2); “B-DNA twist” [24] by P(3); “bendability” [25] by P(4); “DNA bending stiffness” [26] by P(5); “DNA denaturation” [27] by P(6); “duplex disrupt energy” [28] by P(7); “duplex free energy” [29] by P(8); “propeller twist” [30] by P(9); “protein deformation” [31] by P(10); “protein-DNA twist” [31] by P(11); and “Z-DNA” [32] by P(12). Their values were taken from the papers cited above, respectively.

| Dinucleotide | Physicochemical properties ^a | | | | | | | | | | | |
|--------------|---|--------|------|-------|------|--------|------|------|--------|-------|-------|-------|
| | P(1) | P(2) | P(3) | P(4) | P(5) | P(6) | P(7) | P(8) | P(9) | P(10) | P(11) | P(12) |
| AA | 0.97 | -5.37 | 35.5 | -0.27 | 35 | 66.51 | 1.9 | -1.2 | -18.66 | 12.1 | 35.1 | 3.9 |
| AC | 0.13 | -10.51 | 33.1 | -0.21 | 60 | 108.8 | 1.3 | -1.5 | -13.1 | 9.8 | 31.5 | 4.6 |
| AG | 0.33 | -6.78 | 30.6 | -0.08 | 60 | 85.12 | 1.6 | -1.5 | -14.0 | 6.3 | 31.9 | 3.4 |
| AT | 0.58 | -6.57 | 43.2 | -0.28 | 20 | 72.29 | 0.9 | -0.9 | -15.01 | 2.1 | 29.3 | 5.9 |
| CA | 1.04 | -6.57 | 37.7 | -0.01 | 60 | 64.92 | 1.9 | -1.7 | -9.45 | 6.1 | 37.3 | 1.3 |
| CC | 0.19 | -8.26 | 35.3 | -0.03 | 130 | 99.31 | 3.1 | -2.3 | -8.11 | 2.9 | 32.9 | 2.4 |
| CG | 0.52 | -9.69 | 31.3 | -0.03 | 85 | 88.84 | 3.6 | -2.8 | -10.03 | 4.5 | 36.1 | 0.7 |
| CT | 0.33 | -6.78 | 30.6 | -0.18 | 60 | 85.12 | 1.6 | -1.5 | -14 | 1.6 | 31.9 | 3.4 |
| GA | 0.98 | -9.81 | 39.6 | 0.03 | 60 | 80.03 | 1.6 | -1.5 | -13.48 | 2.3 | 36.3 | 3.4 |
| GC | 0.73 | -14.6 | 38.4 | 0.02 | 85 | 135.83 | 3.1 | -2.3 | -11.08 | 4 | 33.6 | 4.0 |
| GG | 0.19 | -8.26 | 35.3 | -0.06 | 130 | 99.31 | 3.1 | -2.3 | -8.11 | 6.1 | 32.9 | 2.4 |
| GT | 0.13 | -10.51 | 33.1 | -0.18 | 60 | 108.8 | 1.3 | -1.5 | -13.1 | 2.1 | 31.5 | 4.6 |
| TA | 0.73 | -3.82 | 31.6 | 0.18 | 20 | 50.11 | 1.5 | -0.9 | -11.85 | 2.3 | 37.8 | 2.5 |
| TC | 0.98 | -9.81 | 39.6 | -0.11 | 60 | 80.03 | 1.6 | -1.5 | -13.48 | 4.5 | 36.3 | 3.4 |
| TG | 1.04 | -6.57 | 37.7 | 0.13 | 60 | 64.92 | 1.9 | -1.7 | -9.45 | 9.8 | 37.3 | 1.3 |
| TT | 0.97 | -5.37 | 35.5 | -0.28 | 35 | 66.51 | 1.9 | -1.2 | -18.66 | 2.8 | 35.1 | 3.9 |