**PROTEINS’ ENTANGLEMENT**

1. Gauss double integral between two closed curves and in is known as the linking number, given by:
2. Assume that a subchain from index to , and a subchain from index to with the condition , their Gaussian entanglement is defined as:

where the average positions , is position of the atoms, and the bond vectors .

1. The largest absolute value of the mutual entanglement found for all possible pairs (, ) having the lasso structure is:
2. Calculation result for 81 protein structures.

Chart, scatter chart

Description automatically generated

***Figure 1*** *- The correlation between the rupture force of protein and their greatest absolute value of the mutual entanglement .*

***Table 1*** *- Calculation results for 81 protein structures. N is the number of residues of protein used in the computation of . is the rupture force taken from Bio-molecule Stretching Database (BSDB)[1]. is the largest absolute value of the mutual entanglement.*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **No.** | **PDB ID** | **N** | **(pN)** |  |
| 1 | 1A6N | 151 | 147.4 | 0.476 |
| 2 | 1ADW | 123 | 242.0 | 0.740 |
| 3 | 1APS | 98 | 206.8 | 1.622 |
| 4 | 1ARR | 53 | 92.4 | 0.139 |
| 5 | 1AUE | 100 | 110.0 | 0.389 |
| 6 | 1AYI | 87 | 114.4 | 0.314 |
| 7 | 1BA5 | 53 | 77.0 | 0.336 |
| 8 | 1BD8 | 156 | 165.0 | 0.548 |
| 9 | 1BFE | 119 | 127.6 | 0.772 |
| 10 | 1BNI | 110 | 152.9 | 0.596 |
| 11 | 1BRS | 110 | 141.9 | 0.596 |
| 12 | 1C9O | 66 | 137.5 | 0.392 |
| 13 | 1CDC | 99 | 68.2 | 0.555 |
| 14 | 1CSP | 67 | 128.7 | 0.402 |
| 15 | 1CUN | 213 | 169.4 | 0.419 |
| 16 | 1DIV | 149 | 224.4 | 0.836 |
| 17 | 1E0G | 48 | 88.0 | 0.324 |
| 18 | 1E41 | 104 | 89.1 | 0.328 |
| 19 | 1E65 | 128 | 250.8 | 0.924 |
| 20 | 1EAL | 127 | 135.3 | 0.289 |
| 21 | 1EHB | 82 | 118.8 | 0.686 |
| 22 | 1ENH | 54 | 101.2 | 0.370 |
| 23 | 1FEX | 59 | 86.9 | 0.335 |
| 24 | 1FKF | 107 | 165.0 | 0.940 |
| 25 | 1FTG | 168 | 201.3 | 0.932 |
| 26 | 1G6P | 66 | 119.9 | 0.555 |
| 27 | 1GM1 | 86 | 110.0 | 0.633 |
| 28 | 1HRC | 105 | 116.6 | 0.564 |
| 29 | 1IDY | 54 | 78.1 | 0.339 |
| 30 | 1IMQ | 86 | 111.1 | 0.504 |
| 31 | 1JMQ | 46 | 107.8 | 0.295 |
| 32 | 1JO8 | 58 | 141.9 | 0.621 |
| 33 | 1JOO | 149 | 127.6 | 0.825 |
| 34 | 1K0S | 151 | 162.8 | 1.177 |
| 35 | 1K85 | 88 | 188.1 | 0.656 |
| 36 | 1K8M | 93 | 132.0 | 0.656 |
| 37 | 1LOP | 164 | 162.8 | 1.757 |
| 38 | 1MJC | 69 | 158.4 | 0.566 |
| 39 | 1N88 | 96 | 141.9 | 0.795 |
| 40 | 1NPS | 88 | 183.7 | 1.139 |
| 41 | 1NTI | 86 | 116.6 | 0.643 |
| 42 | 1O6X | 81 | 96.8 | 0.818 |
| 43 | 1PBA | 81 | 94.6 | 0.675 |
| 44 | 1PGB | 56 | 313.5 | 0.390 |
| 45 | 1PNJ | 86 | 91.3 | 0.422 |
| 46 | 1POH | 85 | 178.2 | 0.485 |
| 47 | 1PRB | 53 | 118.8 | 0.205 |
| 48 | 1PRS | 173 | 133.1 | 1.243 |
| 49 | 1PSF | 69 | 94.6 | 0.474 |
| 50 | 1QTU | 117 | 234.3 | 1.136 |
| 51 | 1RFA | 79 | 257.4 | 0.917 |
| 52 | 1RIS | 101 | 137.5 | 1.370 |
| 53 | 1SCE | 112 | 89.1 | 0.463 |
| 54 | 1SHG | 62 | 100.1 | 0.513 |
| 55 | 1SPR | 104 | 146.3 | 0.571 |
| 56 | 1SRL | 64 | 85.8 | 0.574 |
| 57 | 1ST7 | 86 | 121.0 | 0.500 |
| 58 | 1TEN | 90 | 181.5 | 0.674 |
| 59 | 1TIT | 98 | 231.0 | 0.606 |
| 60 | 1TTF | 94 | 124.3 | 0.502 |
| 61 | 1UBQ | 76 | 240.9 | 0.802 |
| 62 | 1UZC | 71 | 127.6 | 0.502 |
| 63 | 1W4J | 51 | 117.7 | 0.650 |
| 64 | 1WIT | 93 | 300.3 | 0.717 |
| 65 | 1YCC | 108 | 130.9 | 0.703 |
| 66 | 1YEA | 112 | 114.4 | 0.732 |
| 67 | 1YZA | 106 | 100.1 | 0.240 |
| 68 | 2A3D | 73 | 117.7 | 0.302 |
| 69 | 2A5E | 156 | 150.7 | 0.560 |
| 70 | 2ACY | 98 | 188.1 | 1.362 |
| 71 | 2CI2 | 83 | 172.7 | 0.685 |
| 72 | 2EAL | 148 | 149.6 | 0.977 |
| 73 | 2FDQ | 86 | 118.8 | 0.545 |
| 74 | 2HPR | 87 | 126.5 | 0.484 |
| 75 | 2HQI | 72 | 112.2 | 0.750 |
| 76 | 2LZM | 164 | 148.5 | 0.359 |
| 77 | 2PDD | 43 | 79.2 | 0.282 |
| 78 | 2PTL | 60 | 238.7 | 0.588 |
| 79 | 2RN2 | 155 | 215.6 | 0.999 |
| 80 | 2VIK | 126 | 152.9 | 0.864 |
| 81 | 3CHY | 128 | 192.5 | 0.979 |

1. Sikora, M., Sulkowska, J. I., Witkowski, B. S., and Cieplak, M., *BSDB: the biomolecule stretching database.* Nucleic Acids Res, 2011. **39**(Database issue): p. D443-50.