**Conformational analysis of milk derived tripeptides, IPP, VPP and LPP, and investigation of their anti-COVID-19 potentials by molecular docking and molecular dynamics studies**

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**Contents**

Table S1 ……………………………………………………………………...S2

**Table S1.** The dihedral angles (o) of IPP, LPP, VPP tripeptides, calculated by Fortran

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Atoms | IPP | Atoms | LPP | Atoms | VPP |
| C5-C7-C13-C16 | 169.7 | C5-C7-C10-C12 | -175.9 | C9-C7-C5-C17 | -178.4 |
| C9-C7-C5-C20 | 170.8 | C5-C7-C10-C16 | 58.8 | C13-C7-C5-C17 | 57.7 |
| C9-C7-C13-C16 | -65.6 | C10-C7-C5-C20 | 50.2 | N2-C5-C7-C9 | -55.9 |
| N2-C5-C7-C9 | -65.9 | N2-C5-C7-C10 | 173.5 | N2-C5-C7-C13 | -179.9 |
| N2-C5-C20-N22 | 151.5 | N2-C5-C20-N22 | 98.0 | N2-C5-C17-O18 | -63.2 |
| C5-C20-N22-C23 | -7.8 | C7-C5-C20-N22 | -138.0 | N2-C5-C17-N19 | 116.8 |
| C5-C20-N22-C32 | 172.2 | C5-C20-N22-C23 | -6.2 | C5-C17-N19-C20 | 0.9 |
| N22-C32-C34-N36 | 165.0 | C5-C20-N22-C32 | 173.8 | C5-C17-N19-C29 | -179.1 |
| C29-C32-C34-N36 | -77.5 | C20-N22-C32-C29 | 180.0 | C17-N19-C29-C31 | -57.6 |
| C32-C34-N36-C37 | -2.3 | N22-C32-C34-N36 | 164.5 | N19-C29-C31-N33 | 162.8 |
| C32-C34-N36-C46 | 177.8 | C32-C34-N36-C37 | -2.8 | C29-C31-N33-C34 | -2.5 |
| C34-N36-C37-C40 | -180.0 | C32-C34-N36-C46 | 177.2 | C29-C31-N33-C43 | 177.5 |
| C34-N36-C46-C43 | 180.0 | C34-N36-C46-C43 | 180.0 | C31-N33-C43-C40 | -180.0 |
| C34-N36-C46-C48 | 0 | C34-N36-C46-C48 | 0 | C31-N33-C34-C37 | 180.0 |
| N36-C46-C48-O49 | -99.6 | N36-C46-C48-O49 | -98.3 | N33-C43-C45-O46 | -100.6 |
| N36-C46-C48-O50 | 80.4 | N36-C46-C48-O50 | 81.7 | N33-C43-C45-O47 | 79.4 |