## Supplementary Information

# Collagen Type II – Chitosan interactions as dependent on hydroxylation and acetylation inferred from molecular dynamics simulations

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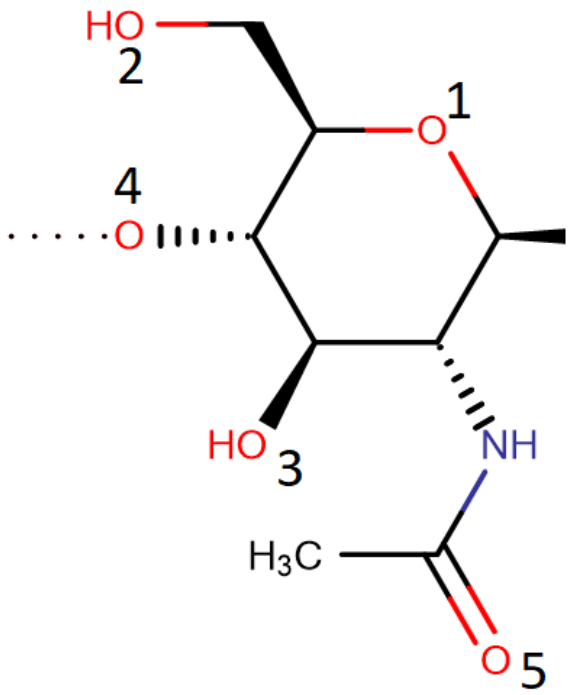


**Figure S1.** The oxygen atoms numbering in units of chitin.

Table S1. The HYP positions presented on the collagen structures used in the study. The first letter links to the chain and the second a position in the primary structure.

| Hydroxylation degree | HYP position in the sequence |
|---|---|
| **0.00** | No HYP residues, only PRO residues present |
| **0.14** | B8-C2-C5-C8-C23-C29<br>A2-B5-B29-C2-C8-C26<br>A5-A23-A26-B2-B5-C8<br>A2-A8-A29-B8-C2-C29<br>A2-A5-A23-B2-B5-B8<br>A8-B2-B5-B29-C2-C5<br>A2-A8-B23-C5-C23-C29<br>A2-A5-A8-A23-C26-C29<br>A26-A29-B2-B29-C2-C5<br>A2-A5-B2-B23-B29-C29 |
| **0.29** | A2-A5-A23-A29-B2-B5-B23-B26-C2-C8-C23-C29<br>A5-A8-A23-A26-A29-B5-B23-C2-C5-C8-C23-C29<br>A5-A23-A26-A29-B2-B23-B29-C2-C5-C23-C26-C29<br>A2-A8-A29-B2-B23-B26-B29-C5-C8-C23-C26-C29<br>A2-A5-A8-A23-A26-A29-B2-B8-B23-B26-B29-C26<br>A2-A5-A23-B5-B8-B23-B26-C5-C8-C23-C26-C29<br>A5-A8-A23-A26-A29-B2-B5-B8-B23-B26-B29-C8<br>A2-A5-A23-A26-A29-B8-B23-B26-B29-C8-C26-C29<br>A2-A5-A23-A26-A29-B2-B26-B29-C2-C5-C8-C29<br>A2-A5-A8-A23-A26-A29-B2-B5-B8-C2-C8-C23 |
| **0.43** | HYP-A2-A5-A8-A23-A26-A29-B2-B5-B8-B23-B26-B29-C2-C5-C8-C23-C26-C29<br>PRO-A1-A4-A7-A14-A19-A22-A25-A28-B1-B4-B7-B14-B19-B22-B25-B28-C1-C4-C7-C14-C19-C22-C25-C28 |

| Hydroxylation degree | HYP position in the sequence |
|---|---|
| **0.57** | A2-A5-A7-A8-A23-A26-A29-B1-B2-B4-B5-B7-B8-B23-B26-B28-B29-C2-C5-C8-C14-C23-C26-C29<br>A2-A5-A8-A22-A23-A26-A29-B2-B4-B5-B8-B22-B23-B26-B28-B29-C2-C5-C8-C14-C23-C26-C28-C29<br>A2-A5-A8-A19-A22-A23-A26-A29-B1-B2-B5-B7-B8-B23-B26-B29-C2-C4-C5-C8-C22-C23-C26-C29<br>A2-A5-A8-A23-A26-A29-B2-B5-B8-B14-B19-B23-B25-B26-B29-C2-C5-C8-C14-C22-C23-C25-C26-C29<br>A2-A4-A5-A7-A8-A22-A23-A26-A29-B2-B5-B8-B23-B26-B29-C2-C5-C7-C8-C23-C25-C26-C28-C29<br>A2-A5-A7-A8-A19-A23-A25-A26-A28-A29-B2-B5-B7-B8-B23-B26-B29-C2-C5-C8-C19-C23-C26-C29<br>A2-A5-A7-A8-A14-A19-A23-A26-A29-B1-B2-B4-B5-B8-B23-B26-B28-B29-C2-C5-C8-C23-C26-C29<br>A1-A2-A5-A7-A8-A23-A25-A26-A29-B2-B5-B8-B23-B25-B26-B28-B29-C2-C5-C8-C14-C23-C26-C29<br>A2-A5-A8-A14-A19-A22-A23-A26-A29-B2-B5-B8-B22-B23-B26-B29-C2-C5-C8-C19-C23-C26-C28-C29<br>A2-A5-A8-A19-A23-A25-A26-A28-A29-B1-B2-B5-B8-B19-B22-B23-B26-B29-C2-C5-C8-C23-C26-C29 |
| **0.71** | A1-A2-A4-A5-A8-A14-A22-A23-A26-A28-A29-B2-B4-B5-B7-B8-B22-B23-B26-B28-B29-C2-C4-C5-C8-C23-C25-C26-C28-C29<br>A2-A5-A7-A8-A14-A22-A23-A25-A26-A28-A29-B2-B5-B7-B8-B22-B23-B25-B26-B29-C1-C2-C5-C7-C8-C14-C22-C23-C26-C29<br>A1-A2-A4-A5-A8-A19-A22-A23-A26-A29-B2-B4-B5-B8-B14-B19-B23-B26-B29-C1-C2-C5-C7-C8-C19-C22-C23-C25-C26-C29<br>A2-A4-A5-A7-A8-A14-A22-A23-A25-A26-A28-A29-B1-B2-B5-B8-B22-B23-B26-B29-C1-C2-C4-C5-C8-C14-C23-C26-C28-C29<br>A1-A2-A5-A8-A14-A22-A23-A26-A29-B1-B2-B4-B5-B8-B14-B19-B23-B26-B28-B29-C2-C4-C5-C7-C8-C14-C22-C23-C26-C29<br>A1-A2-A4-A5-A8-A14-A19-A23-A25-A26-A29-B1-B2-B5-B8-B14-B22-B23-B25-B26-B29-C1-C2-C5-C8-C14-C23-C26-C28-C29<br>A2-A4-A5-A7-A8-A19-A22-A23-A26-A29-B1-B2-B5-B7-B8-B14-B19-B23-B25-B26-B28-B29-C1-C2-C5-C8-C22-C23-C26-C29<br>A2-A4-A5-A7-A8-A19-A22-A23-A26-A29-B1-B2-B4-B5-B8-B23-B25-B26-B29-C1-C2-C4-C5-C7-C8-C19-C22-C23-C26-C29<br>A2-A4-A5-A7-A8-A14-A22-A23-A25-A26-A28-A29-B2-B5-B7-B8-B14-B19-B23-B26-B29-C2-C5-C8-C19-C22-C23-C25-C26-C29<br>A1-A2-A5-A8-A14-A19-A22-A23-A25-A26-A29-B2-B5-B7-B8-B22-B23-B26-B29-C2-C5-C8-C14-C19-C22-C23-C25-C26-C28-C29 |

| Hydroxylation degree | HYP position in the sequence |
|---|---|
| **0.86** | A1-A2-A4-A5-A8-A14-A22-A23-A26-A29-B2-B4-B5-B7-B8-B14-B19-B22-B23-B25-B26-B28-B29-C1-C2-C4-C5-C7-C8-C14-C19-C22-C23-C25-C26-C29<br>A1-A2-A4-A5-A7-A8-A14-A19-A22-A23-A26-A28-A29-B1-B2-B4-B5-B7-B8-B22-B23-B25-B26-B28-B29-C2-C4-C5-C7-C8-C19-C22-C23-C25-C26-C29<br>A1-A2-A5-A7-A8-A14-A19-A22-A23-A25-A26-A29-B1-B2-B4-B5-B7-B8-B14-B19-B23-B26-B28-B29-C2-C4-C5-C7-C8-C19-C22-C23-C25-C26-C28-C29<br>A1-A2-A4-A5-A7-A8-A14-A19-A22-A23-A25-A26-A28-A29-B2-B4-B5-B8-B14-B22-B23-B26-B28-B29-C1-C2-C5-C7-C8-C19-C22-C23-C25-C26-C28-C29<br>A2-A4-A5-A7-A8-A14-A22-A23-A25-A26-A28-A29-B1-B2-B5-B7-B8-B14-B23-B26-B28-B29-C1-C2-C4-C5-C7-C8-C14-C19-C22-C23-C25-C26-C28-C29<br>A2-A4-A5-A7-A8-A19-A23-A25-A26-A28-A29-B1-B2-B4-B5-B7-B8-B14-B19-B23-B25-B26-B28-B29-C1-C2-C4-C5-C7-C8-C14-C19-C23-C26-C28-C29<br>A1-A2-A5-A7-A8-A14-A19-A23-A25-A26-A29-B1-B2-B5-B7-B8-B14-B19-B23-B25-B26-B28-B29-C1-C2-C4-C5-C7-C8-C14-C19-C22-C23-C25-C26-C29<br>A2-A4-A5-A7-A8-A14-A19-A22-A23-A25-A26-A28-A29-B1-B2-B5-B8-B14-B19-B22-B23-B25-B26-B29-C1-C2-C4-C5-C8-C14-C22-C23-C25-C26-C28-C29<br>A2-A4-A5-A7-A8-A19-A22-A23-A25-A26-A28-A29-B1-B2-B4-B5-B8-B14-B19-B23-B25-B26-B28-B29-C2-C4-C5-C7-C8-C14-C22-C23-C25-C26-C28-C29<br>A1-A2-A4-A5-A8-A14-A22-A23-A25-A26-A28-A29-B1-B2-B5-B7-B8-B14-B19-B22-B23-B25-B26-B28-B29-C1-C2-C5-C7-C8-C19-C23-C25-C26-C28-C29 |
| **1.00** | No PRO residues, only HYP residues present |

Table S2 Distribution of H-bonds between chitosan and collagen amino acid atoms for HD=0 and DD=1. Percentages represent the contributions of H-bonds identified between chitosan and a given amino acid residue.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| **N** | 0% | 33% | 0% | 17% | 7% | 10% | 0% | 0% | 0% | 0% | 44% | 30% | 7% | 20% | 13% | 0% | 13% | 0% |
| **O1** | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% |
| **O2** | 0% | 50% | 0% | 0% | 28% | 10% | 7% | 0% | 0% | 0% | 26% | 37% | 7% | 40% | 20% | 7% | 7% | 7% |
| **O3** | 0% | 0% | 0% | 0% | 14% | 17% | 0% | 0% | 0% | 0% | 26% | 26% | 20% | 7% | 7% | 13% | 7% | 7% |
| **O4** | 0% | 0% | 0% | 0% | 7% | 0% | 0% | 0% | 0% | 0% | 4% | 7% | 0% | 0% | 0% | 0% | 0% | 0% |
| **O5** | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% |

ARG - NE, HH1 and NH2 guanidino group of the side chain, N - nitrogen of the amino group in the main chain, GLU - OE1 and OE2 oxygen atoms from the carboxyl group, N - nitrogen of the amino group in the main chain; HYP - OD1 - oxygen from the hydroxyl group, N - nitrogen of the amino group in the main chain; PRO - N - nitrogen of the amino group in the main chain, O - oxygen in the main chain; GLY - N - nitrogen of the amino group in the main chain, O - oxygen in the main chain; ALA - N - nitrogen of the amino group in the main chain, O - oxygen in the main chain; The numbering of atoms in Chitosan according to Fig. S1

Table S3 Distribution of H-bonds between chitosan and collagen amino acid atoms for HD=0.42 and DD=1. Percentages represent the contributions of H-bonds identified between chitosan and a given amino acid residue. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| **N** | 17% | 0% | 0% | 0% | 19% | 8% | 3% | 19% | 16% | 0% | 42% | 33% | 0% | 44% | 21% | 0% | 5% | 5% |
| **O1** | 0% | 0% | 0% | 17% | 0% | 0% | 0% | 2% | 0% | 0% | 0% | 0% | 6% | 0% | 0% | 0% | 0% | 0% |
| **O2** | 17% | 17% | 17% | 0% | 6% | 19% | 3% | 13% | 11% | 8% | 17% | 44% | 17% | 22% | 5% | 5% | 0% | 26% |
| **O3** | 0% | 17% | 0% | 0% | 17% | 22% | 0% | 16% | 21% | 0% | 33% | 23% | 0% | 11% | 11% | 16% | 0% | 0% |
| **O4** | 0% | 0% | 0% | 0% | 3% | 0% | 0% | 2% | 2% | 0% | 0% | 0% | 0% | 0% | 0% | 5% | 0% | 0% |
| **O5** | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% |

Table S4 Distribution of H-bonds between chitosan and collagen amino acid atoms for HD=1 and DD=1. Percentages represent the contributions of H-bonds identified between chitosan and a given amino acid residue. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| **N** | 9% | 9% | 0% | 0% | 14% | 7% | 4% | 28% | 13% | 0% | 0% | 34% | 6% | 19% | 21% | 5% | 11% | 0% |
| **O1** | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 5% | 0% | 0% |
| **O2** | 9% | 9% | 0% | 9% | 11% | 29% | 4% | 21% | 12% | 0% | 0% | 38% | 25% | 25% | 0% | 0% | 21% | 21% |
| **O3** | 9% | 9% | 18% | 18% | 29% | 4% | 0% | 14% | 8% | 0% | 0% | 28% | 19% | 6% | 16% | 0% | 0% | 0% |
| **O4** | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 2% | 1% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% |
| **O5** | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% |

Table S5 Distribution of H-bonds between chitosan and collagen amino acid atoms for HD=0 and DD=0.125. Percentages represent the contributions of H-bonds identified between chitosan and a given amino acid residue. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| **N** | 0% | 0% | 0% | 0% | 0% | 6% | 0% | 0% | 0% | 0% | 10% | 7% | 0% | 0% | 10% | 0% | 0% | 0% |
| **O1** | 0% | 8% | 4% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 3% | 0% | 0% | 0% | 0% | 0% |
| **O2** | 13% | 0% | 8% | 8% | 28% | 11% | 6% | 0% | 0% | 7% | 53% | 76% | 24% | 32% | 13% | 7% | 17% | 10% |
| **O3** | 0% | 8% | 13% | 4% | 0% | 17% | 6% | 0% | 0% | 7% | 20% | 14% | 9% | 9% | 3% | 13% | 3% | 3% |
| **O4** | 0% | 4% | 0% | 0% | 11% | 0% | 0% | 0% | 0% | 0% | 0% | 3% | 0% | 3% | 0% | 0% | 0% | 0% |
| **O5** | 4% | 25% | 0% | 0% | 0% | 0% | 17% | 0% | 0% | 3% | 0% | 0% | 21% | 0% | 0% | 17% | 0% | 3% |

Table S6 Distribution of H-bonds between chitosan and collagen amino acid atoms for HD=0.42 and DD=0.5. Percentages represent the contributions of H-bonds identified between chitosan and a given amino acid residue. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| **N** | 0% | 0% | 0% | 0% | 12% | 9% | 0% | 9% | 15% | 0% | 25% | 36% | 0% | 21% | 15% | 0% | 8% | 0% |
| **O1** | 0% | 5% | 0% | 0% | 0% | 0% | 0% | 3% | 0% | 0% | 0% | 0% | 5% | 0% | 0% | 0% | 0% | 0% |
| **O2** | 15% | 30% | 10% | 0% | 30% | 0% | 3% | 14% | 18% | 13% | 25% | 31% | 42% | 21% | 8% | 8% | 8% | 31% |

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| **O3** | 0% | 5% | 5% | 0% | 21% | 12% | 3% | 19% | 8% | 13% | 13% | 31% | 11% | 0% | 0% | 0% | 8% | 8% |
| **O4** | 0% | 0% | 0% | 0% | 3% | 3% | 0% | 4% | 3% | 0% | 13% | 3% | 0% | 0% | 0% | 8% | 0% | 0% |
| **O5** | 0% | 15% | 10% | 5% | 0% | 0% | 3% | 9% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% |

Table S7 Distribution of H-bonds between chitosan and collagen amino acid atoms for HD=1 and DD=0.125. Percentages represent the contributions of H-bonds identified between chitosan and a given amino acid residue. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| **N** | 0% | 0% | 0% | 0% | 7% | 7% | 0% | 9% | 1% | 0% | 0% | 9% | 0% | 5% | 5% | 0% | 5% | 0% |
| **O1** | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 2% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% | 0% |
| **O2** | 0% | 9% | 18% | 9% | 7% | 20% | 7% | 24% | 14% | 0% | 0% | 75% | 45% | 23% | 5% | 15% | 10% | 25% |
| **O3** | 0% | 27% | 0% | 0% | 7% | 33% | 0% | 20% | 7% | 0% | 0% | 13% | 14% | 5% | 5% | 0% | 5% | 10% |
| **O4** | 0% | 9% | 0% | 0% | 7% | 0% | 0% | 3% | 1% | 0% | 0% | 3% | 0% | 0% | 0% | 0% | 0% | 0% |
| **O5** | 0% | 18% | 0% | 9% | 0% | 0% | 7% | 17% | 0% | 0% | 0% | 0% | 9% | 0% | 0% | 5% | 0% | 10% |

Table S8 H-bonds lengths [Å] between chitosan and collagen amino acid atoms for HD=0 and DD=1. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| **N** | - | 1,89 | - | 1,95 | 1,87 | 1,94 | - | - | - | - | 2,00 | 2,01 | 1,87 | 1,93 | 2,105 | - | 1,91 | - |
| **O1** | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| **O2** | - | 2,06 | - | - | 1,70 | 1,75 | 2,04 | - | - | - | 1,84 | 1,78 | 1,98 | 1,74 | 1,80 | 2,19 | 2,1 | 2,04 |
| **O3** | - | - | - | - | 1,68 | 1,81 | - | - | - | - | 1,86 | 1,86 | 2,12 | 1,54 | 1,65 | 2,09 | 1,86 | 2,32 |
| **O4** | - | - | - | - | 1,84 | - | - | - | - | - | 1,69 | 1,64 | - | - | - | - | - | - |
| **O5** | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Table S9 H-bonds lengths [Å] between chitosan and collagen amino acid atoms for HD=0.42 and DD=1. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| N | 2,05 | - | - | - | 1,98 | 1,88 | 2,2 | 2,03 | 2,05 | - | 2,06 | 2,10 | - | 2,06 | 2,0675 | - | 2,26 | 1,9 |
| O1 | - | - | - | 2,1 | - | - | - | 1,95 | - | - | - | - | 2,2 | - | - | - | - | - |
| O2 | 2,3 | 2,11 | 1,76 | - | 1,88 | 1,70 | 2,08 | 1,99 | 1,78 | 2,08 | 1,68 | 1,83 | 2,05 | 1,93 | 1,64 | 2,29 | - | 2,16 |
| O3 | - | 2,21 | - | - | 1,65 | 1,78 | - | 1,79 | 1,84 | - | 1,87 | 1,88 | - | 1,79 | 1,765 | 2,07 | - | - |
| O4 | - | - | - | - | 1,65 | - | - | 2,02 | 1,59 | - | - | - | - | - | - | 1,78 | - | - |
| O5 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Table S10 H-bonds lengths [Å] between chitosan and collagen amino acid atoms for HD=1 and DD=1. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| N | 2,09 | 1,99 | - | - | 1,92 | 2,22 | 2,16 | 2,08 | 2,04 | - | - | 2,03 | 2,07 | 1,96 | 2,16 | 2,18 | 1,89 | - |
| O1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 1,99 | - | - |
| O2 | 2,38 | 1,79 | - | 1,85 | 1,65 | 1,82 | 1,86 | 1,86 | 1,86 | - | - | 1,86 | 2,07 | 1,93 | - | - | 1,72 | 2,16 |
| O3 | 1,91 | 2,11 | 2,18 | 1,86 | 1,74 | 1,64 | - | 1,93 | 1,92 | - | - | 1,80 | 2,03 | 2,11 | 1,72 | - | - | - |
| O4 | - | - | - | - | - | - | - | 1,87 | 2,08 | - | - | - | - | - | - | - | - | - |
| O5 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Table S11 H-bonds lengths [Å] between chitosan and collagen amino acid atoms for HD=0 and DD=0.125. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | N | O | O | N | O | OE1 | NE2 | O | N |
| N | - | - | - | - | - | 2.00 | - | - | - | - | - | 2,16 | 2,12 | - | - | 2,08 | - | - | - |
| O1 | - | 2,16 | 2,27 | - | - | - | - | - | - | - | - | - | - | 2,43 | - | - | - | - | - |
| O2 | 2,02 | - | 1,97 | 2,29 | 1,79 | 1,69 | 2,3 | - | - | - | 2,03 | 1,88 | 1,81 | 2,05 | 1,85 | 1,88 | 2,06 | 1,96 | 2,19 |
| O3 | - | 1,94 | 1,96 | 1,88 | - | 1,79 | 2.00 | - | - | - | 2,01 | 1,76 | 1,82 | 2,07 | 1,95 | 1,95 | 1,90 | 1,66 | 2,22 |

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | N | O | O | N | O | OE1 | NE2 | O | N |
| O4 | - | 1,97 | - | - | 1,71 | - | - | - | - | - | - | - | 2,04 | - | 1,88 | - | - | - | - |
| O5 | 1,99 | 1,94 | - | - | - | - | 2,12 | - | - | - | 1,99 | - | - | 2,07 | - | - | 2,00 | - | 2,29 |

Table S12 H-bonds lengths [Å] between chitosan and collagen amino acid atoms for HD=0.42 and DD=0.5. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| N | - | - | - | - | 1,98 | 2,21 | - | 2,13 | 2,07 | - | 1,95 | 2,02 | - | 2,02 | 1,96 | - | 2,39 | - |
| O1 | - | 2,39 | - | - | - | - | - | 2,11 | - | - | - | - | 1,97 | - | - | - | - | - |
| O2 | 2,18 | 2,01 | 2,01 | - | 1,705 | - | 2,18 | 1,88 | 1,92 | 2,09 | 1,8 | 1,85 | 2,06 | 1,85 | 1,74 | 2,03 | 1,83 | 2,01 |
| O3 | - | 2,38 | 2,04 | - | 1,74 | 1,83 | 2,23 | 1,95 | 1,87 | 1,92 | 1,71 | 1,86 | 2,05 | - | - | - | 1,8 | 2,42 |
| O4 | - | - | - | - | 1,85 | 2,08 | - | 1,94 | 1,81 | - | 1,87 | 1,65 | - | - | - | 2,07 | - | - |
| O5 | - | 1,89 | 1,87 | 1,95 | - | - | 2,02 | 1,80 | - | - | - | - | - | - | - | - | - | - |

Table S13 H-bonds lengths [Å] between chitosan and collagen amino acid atoms for HD=1 and DD=0.125. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | N | O | N | O | OE1 | NE2 | O | N |
| N | - | - | - | - | 2,19 | 2,3 | - | 2,08 | 2,24 | - | - | - | 2,23 | - | 2,27 | 2,2 | - | 2,1 | - |
| O1 | - | - | - | - | - | - | - | 1,91 | - | - | - | - | - | - | - | - | - | - | - |
| O2 | - | 1,9 | 2 | 1,77 | 1,96 | 1,73 | 2,15 | 1,91 | 1,90 | - | - | 1,92 | 1,86 | 2,01 | 1,77 | 2,2 | 1,99 | 2,05 | 2,1 |
| O3 | - | 2,09 | - | - | 1,67 | 1,78 | - | 1,86 | 1,85 | - | - | - | 1,82 | 2,05 | 2,01 | 1,83 | - | 1,9 | 2,01 |
| O4 | - | 2,26 | - | - | 1,73 | - | - | 1,75 | 1,74 | - | - | - | 1,74 | - | - | - | - | - | - |
| O5 | - | 1,92 | - | 2,19 | - | - | 1,98 | 1,82 | - | - | - | - | - | 2,085 | - | - | 2,11 | - | 2,05 |

Table S14 Energies of H-bonds [kJ/mol] between chitosan and given collagen amino acid residue atom for HD=0 and DD=1. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| **N** | - | 21,1 | - | 12,1 | 18,5 | 15,5 | - | - | - | - | 19,6 | 18,1 | 21,9 | 19,4 | 15,225 | - | 16,5 | - |
| **O1** | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| **O2** | - | 15,1 | - | - | 22,7 | 23,5 | 17,5 | - | - | - | 21,1 | 23,0 | 25 | 21,8 | 18,0 | 8,65 | 19,15 | 25 |
| **O3** | - | - | - | - | 24,6 | 22,3 | - | - | - | - | 20,0 | 20,5 | 16,5 | 24,4 | 21,9 | 21,6 | 24,4 | 9,38 |
| **O4** | - | - | - | - | 21,5 | - | - | - | - | - | 23,8 | 22,7 | - | - | - | - | - | - |
| **O5** | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Table S15 Energies of H-bonds [kJ/mol] between chitosan and given collagen amino acid residue atom for HD=0.42 and DD=1. The numbering of atoms is the same as in Table. S1 and Figure S1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | 16,3 | - | 17,1 | 21,5 |
| **N** | 25 | - | - | - | 17,9 | 22,9 | 9,3 | 18,1 | 14,6 | - | 18,9 | 17,7 | - | 19,0 | - | - | - | - |
| **O1** | - | - | - | 17,8 | - | - | - | 24,4 | - | - | - | - | 17,78 | - | 25 | 11,8 | - | 18,6 |
| **O2** | 15,1 | 15,3 | 22,9 | - | 23,9 | 23 | 22,88 | 20,2 | 20,3 | 7,8 | 21,8 | 21,9 | 22,8 | 21,4 | 21,59 | 18,0 | - | - |
| **O3** | - | 15,6 | - | - | 23,3 | 22,9 | - | 22,8 | 21, 6 | - | 18,8 | 20,2 | - | 18,5 | - | 25 | - | - |
| **O4** | - | - | - | - | 23,8 | - | - | 19,2 | 25 | - | - | - | - | - | - | - | - | - |
| **O5** | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 16,3 | - | 17,1 | 21,5 |

Table S16 Energies of H-bonds [kJ/mol] between chitosan and given collagen amino acid residue atom for HD=1 and DD=1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| **N** | 19,9 | 24,4 | - | - | 17,6 | 13,3 | 12,8 | 15,5 | 16,6 | - | - | 20,2 | 7,3 | 15,2 | 15,7 | 8,6 | 23,1 | - |
| **O1** | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 21,5 | - | - |
| **O2** | 7,18 | 18,6 | - | 21,1 | 23,6 | 22,7 | 13,5 | 22,2 | 20,7 | - | - | 20,3 | 17,6 | 16,8 | - | - | 22,7 | 17,4 |
| **O3** | 25 | 22,0 | 10,8 | 23,44 | 23,3 | 25 | - | 21,5 | 20,1 | - | - | 23,0 | 21,2 | 19,5 | 24,1 | - | - | - |

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| O4 | - | - | - | - | - | - | - | 24,2 | 21,9 | - | - | - | - | - | - | - | - | - |
| O5 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Table S17 Energies of H-bonds [kJ/mol] between chitosan and given collagen amino acid residue atom for HD=0 and DD=0.125.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| N | - | - | - | - | - | 18,6 | - | - | - | - | 18,22 | 16,6 | - | - | 16,9 | - | - | - |
| O1 | - | 12,3 | 11,8 | - | - | - | - | - | - | - | - | - | 7,9 | - | - | - | - | - |
| O2 | 17,5 | - | 19,9 | 10,6 | 24,2 | 25 | 14,8 | - | - | 15,9 | 20,2 | 22,4 | 21,1 | 22,9 | 18,4 | 22,1 | 21,6 | 16,5 |
| O3 | - | 22,5 | 19,0 | 17,2 | - | 23,7 | 23,8 | - | - | 15,7 | 22,7 | 22,4 | 20,3 | 22,6 | 10,6 | 21,2 | 24,4 | 15,2 |
| O4 | - | 21,1 | - | - | 23,4 | - | - | - | - | - | - | 13,5 | - | 21,1 | - | - | - | - |
| O5 | 25 | 19,8 | - | - | - | - | 18,6 | - | - | 15,83 | - | - | 20,3 | - | - | 18,1 | - | 13,6 |

Table S18 Energies of H-bonds [kJ/mol] between chitosan and given collagen amino acid residue atom for HD=0.42 and DD=0.5.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| N | - | - | - | - | 14,7 | 10,9 | - | 13,6 | 14,8 | - | 16,4 | 16,3 | - | 17,1 | 18,4 | - | 8,97 | - |
| O1 | - | 9,7 | - | - | - | - | - | 16,2 | - | - | - | - | 14,2 | - | - | - | - | - |
| O2 | 17,3 | 15,1 | 19,2 | - | 24,0 | - | 16,9 | 20,1 | 19,4 | 7,6 | 21,9 | 23,3 | 17,4 | 23,4 | 24,4 | 25 | 25 | 18,3 |
| O3 | - | 9,2 | 17 | - | 23,4 | 21,8 | 18,6 | 20,6 | 21,2 | 14,5 | 18,7 | 21,8 | 20,5 | - | - | - | 21,9 | 7,4 |
| O4 | - | - | - | - | 22,9 | 17,2 | - | 23,6 | 20,1 | - | 21,9 | 21,9 | - | - | - | 17,8 | - | - |
| O5 | - | 21,0 | 20,0 | 19,6 | - | - | 20,7 | 23,1 | - | - | - | - | - | - | - | - | - | - |

Table S19 Energies of H-bonds [kJ/mol] between chitosan and given collagen amino acid residue atom for HD=1 and DD=0.125.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | O1 | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| N | - | - | - | - | 10,5 | 7,3 | - | 17,9 | 14,5 | 12,8 | - | - | 13,8 | - | 11,7 | 6,9 | - | 25 | - |
| O1 | - | - | - | - | - | - | - | 16,7 | 13,1 | - | - | - | - | - | - | - | - | - | - |
| O2 | - | 22,3 | 21,9 | 25 | 14,5 | 23,7 | 15,4 | 21,1 | 22,1 | 19,5 | - | - | 21,2 | 22,0 | 22,5 | 10,8 | 19,2 | 12,765 | 15,9 |
| O3 | - | 14,6 | - | - | 25 | 23,0 | - | 21,8 | 22,0 | 21,5 | - | - | 21,5 | 18,5 | 12,5 | 16,6 | - | 25 | 23,3 |
| O4 | - | 12,0 | - | - | 23,5 | - | - | 24,3 | 23,6 | 24,7 | - | - | 25 | - | - | - | - | - | - |
| O5 | - | 24,2 | - | 10,8 | - | - | 18,2 | 21,5 | 21,8 | - | - | - | - | 19,9 | - | - | 15,1 | - | 23,3 |

Table S20 The H-bonds acceptor-donor frequency analysis. Values in cells represent how often chitosan in a given interaction plays the role of acceptor for HD=0 and DD=1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| N | - | 100% | - | 100% | 0% | 0% | - | - | - | - | 0% | 0% | 100% | 0% | 0% | - | 0% | - |
| O1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| O2 | - | 100% | - | - | 0% | 0% | 100% | - | - | - | 0% | 0% | 100% | 0% | 0% | 100% | 0% | 100% |
| O3 | - | - | - | - | 0% | 0% | - | - | - | - | 0% | 0% | 100% | 0% | 0% | 100% | 0% | 100% |
| O4 | - | - | - | - | 0% | - | - | - | - | - | 0% | 0% | - | - | - | - | - | - |
| O5 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Table S21 The H-bonds acceptor-donor frequency analysis. Values in cells represent how often chitosan in a given interaction plays the role of acceptor for HD=0.42 and DD=1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| N | 100% | - | - | - | 0% | 0% | 100% | 0% | 0% | - | 0% | 0% | - | 0% | 0% | - | 0% | 100% |
| O1 | - | - | - | 100% | - | - | - | 100% | - | - | - | - | 100% | - | - | - | - | - |
| O2 | 100% | 100% | 100% | - | 0% | 0% | 100% | 75% | 0% | 100% | 0% | 0% | 100% | 0% | 0% | 100% | - | 100% |

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| O3 | - | 100% | - | - | 0% | 0% | - | 50% | 0% | - | 0% | 0% | - | 0% | 0% | 100% | - | - |
| O4 | - | - | - | - | 0% | - | - | 100% | 0% | - | - | - | - | - | - | 100% | - | - |
| O5 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Table S22 The H-bonds acceptor-donor frequency analysis. Values in cells represent how often chitosan in a given interaction plays the role of acceptor for HD=1 and DD=1.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| N | 100% | 100% | - | - | 0% | 0% | 100% | 4% | 0% | - | - | 0% | 100% | 0% | 0% | 100% | 0% | - |
| O1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 100% | - | - |
| O2 | 100% | 100% | - | 100% | 0% | 0% | 100% | 57% | 0% | - | - | 0% | 100% | 0% | - | - | 0% | 100% |
| O3 | 100% | 100% | 100% | 100% | 0% | 0% | - | 50% | 0% | - | - | 0% | 100% | 0% | 0% | - | - | - |
| O4 | - | - | - | - | - | - | - | 50% | 0% | - | - | - | - | - | - | - | - | - |
| O5 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

Table S23 The H-bonds acceptor-donor frequency analysis. Values in cells represent how often chitosan in a given interaction plays the role of acceptor for HD=0 and DD=0.125.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| N | - | - | - | - | 0% | 0% | - | - | - | - | 0% | 0% | - | 0% | 0% | - | 0% | - |
| O1 | - | 100% | 100% | - | - | - | - | - | - | - | - | - | 100% | - | - | - | - | - |
| O2 | 100% | - | 100% | 100% | 0% | 0% | 100% | - | - | 100% | 0% | 0% | 100% | 0% | 0% | 100% | 0% | 100% |
| O3 | - | 100% | 100% | 100% | 0% | 0% | 100% | - | - | 100% | 0% | 0% | 100% | 0% | 0% | 100% | 0% | 100% |
| O4 | - | 100% | - | - | 0% | - | - | - | - | - | 0% | 0% | - | - | - | - | - | - |
| O5 | 100% | 100% | - | - | - | - | 100% | - | - | 100% | - | - | 100% | - | - | 100% | - | 100% |

Table S24 The H-bonds acceptor-donor frequency analysis. Values in cells represent how often chitosan in a given interaction plays the role of acceptor for HD=0.42 and DD=0.5.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| **N** | - | - | - | - | 0% | 0% | - | 0% | 0% | - | 0% | 0% | - | 0% | 0% | - | 0% | - |
| **O1** | - | 100% | - | - | - | - | - | 100% | - | - | - | - | 100% | - | - | - | - | - |
| **O2** | 100% | 100% | 100% | - | 0% | - | 100% | 36% | 0% | 100% | 0% | 0% | 100% | 0% | 0% | 100% | 0% | 100% |
| **O3** | - | 100% | 100% | - | 0% | 0% | 100% | 47% | 0% | 100% | 0% | 0% | 100% | - | - | - | 0% | 100% |
| **O4** | - | - | - | - | 0% | 0% | - | 67% | 0% | - | 0% | 0% | - | - | - | 100% | - | - |
| **O5** | - | 100% | 100% | 100% | - | - | 100% | 100% | - | - | - | - | - | - | - | - | - | - |

Table S25 The H-bonds acceptor-donor frequency analysis. Values in cells represent how often chitosan in a given interaction plays the role of acceptor for HD=1 and DD=0.125.

| | ARG | ARG | ARG | ARG | GLU | GLU | GLU | HYP | HYP | PRO | PRO | GLY | ALA | ALA | GLN | GLN | GLN | GLN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | N | NH1 | NH2 | NE | OE1 | OE2 | N | OD1 | O | N | O | O | N | O | OE1 | NE2 | O | N |
| **N** | - | - | - | - | 0% | 0% | - | 0% | 0% | - | - | 0% | - | 0% | 0% | - | 0% | - |
| **O1** | - | - | - | - | - | - | - | 100% | - | - | - | - | - | - | - | - | - | - |
| **O2** | - | 100% | 100% | 100% | 0% | 0% | 100% | 65% | 0% | - | - | 0% | 100% | 0% | 0% | 100% | 0% | 100% |
| **O3** | - | 100% | - | - | 0% | 0% | - | 82% | 0% | - | - | 0% | 100% | 0% | 0% | - | 0% | 100% |
| **O4** | - | 100% | - | - | 0% | - | - | 75% | 0% | - | - | 0% | - | - | - | - | - | - |
| **O5** | - | 100% | - | 100% | - | - | 100% | 100% | - | - | - | - | 100% | - | - | 100% | - | 100% |