Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Supplementary Information

Collagen Type II – Hyaluronan interactions – effect of proline hydroxylation: molecular dynamics study

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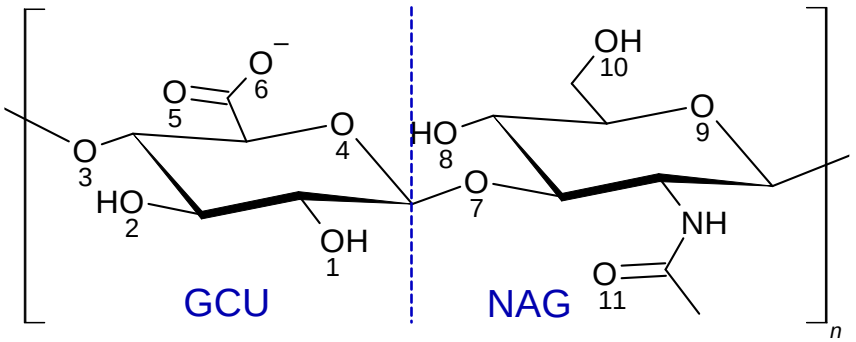

Fig. S1. The oxygen atoms numbering in disaccharide unit of hyaluronan, GCU denotes D-glucuronic acid moiety with ionized carboxyl group, NAG stands for N-acetyl-D-glucosamine.

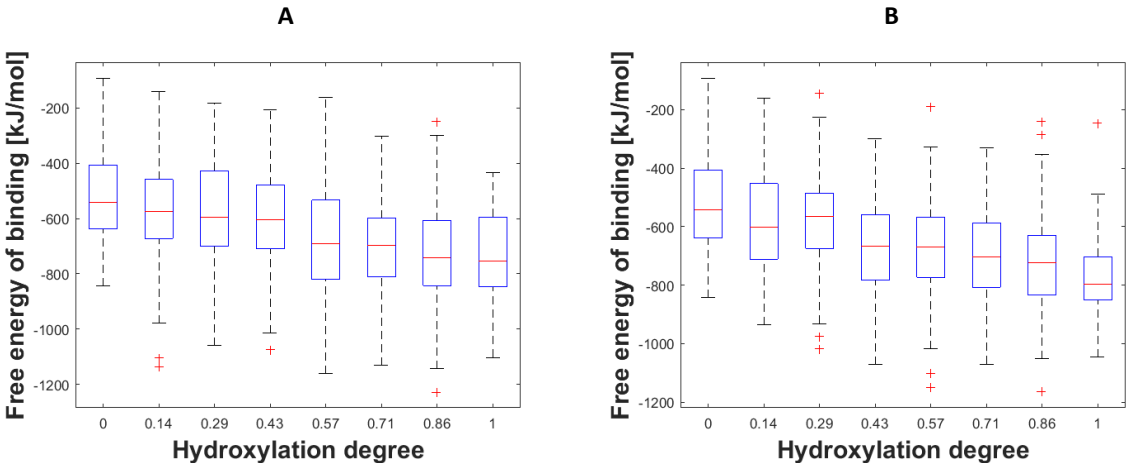

Fig. S2. Boxplot of distribution of free energy of binding for different HD for 3HYP (A) and 4HYP (B).

Table S1. The combinations of collagen sequences corresponding to a particular hydroxylation degree (HD). The first letter denotes chain (A, B or C) and the number to the position in the primary structure.

HD	Sequences
0.00	No HYP residues, only PRO residues present
0.14	B8-C2-C5-C8-C23-C29 A2-B5-B29-C2-C8-C26 A5-A23-A26-B2-B5-C8 A2-A8-A29-B8-C2-C29 A2-A5-A23-B2-B5-B8 A8-B2-B5-B29-C2-C5 A2-A8-B23-C5-C23-C29 A2-A5-A8-A23-C26-C29 A26-A29-B2-B29-C2-C5 A2-A5-B2-B23-B29-C29
0.29	A2-A5-A23-A29-B2-B5-B23-B26-C2-C8-C23-C29 A5-A8-A23-A26-A29-B5-B23-C2-C5-C8-C23-C29 A5-A23-A26-A29-B2-B23-B29-C2-C5-C23-C26-C29 A2-A8-A29-B2-B23-B26-B29-C5-C8-C23-C26-C29 A2-A5-A8-A23-A26-A29-B2-B8-B23-B26-B29-C26 A2-A5-A23-B5-B8-B23-B26-C5-C8-C23-C26-C29 A5-A8-A23-A26-A29-B2-B5-B8-B23-B26-B29-C8 A2-A5-A23-A26-A29-B8-B23-B26-B29-C8-C26-C29 A2-A5-A23-A26-A29-B2-B26-B29-C2-C5-C8-C29 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 PRO-A1-A4-A7-A14-A19-A22-A25-A28-B1-B4-B7-B14-B19-B22-B25-B28-C1-C4-C7-C14
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 A2-A5-A8-A22-A23-A26-A29-B2-B4-B5-B8-B22-B23-B26-B28-B29-C2-C5-C8-C14-C23-C26-C28-C29 A2-A5-A8-A19-A22-A23-A26-A29-B1-B2-B5-B7-B8-B23-B26-B29-C2-C4-C5-C8-C22-C23-C26-C29 A2-A5-A8-A23-A26-A29-B2-B5-B8-B14-B19-B23-B25-B26-B29-C2-C5-C8-C14-C22-C23-C25-C26-C29 A2-A4-A5-A7-A8-A22-A23-A26-A29-B2-B5-B8-B23-B26-B29-C2-C5-C7-C8-C23-C25-C26-C28-C29 A2-A5-A7-A8-A19-A23-A25-A26-A28-A29-B2-B5-B7-B8-B23-B26-B29-C2-C5-C8-C19-C23-C26-C29 A2-A5-A7-A8-A14-A19-A23-A26-A29-B1-B2-B4-B5-B8-B23-B26-B28-B29-C2-C5-C8-C23-C26-C29 A1-A2-A5-A7-A8-A23-A25-A26-A29-B2-B5-B8-B23-B25-B26-B28-B29-C2-C5-C8-C14-C23-C26-C29 A2-A5-A8-A14-A19-A22-A23-A26-A29-B2-B5-B8-B22-B23-B26-B29-C2-C5-C8-C19-C23-C26-C28-C29 A2-A5-A8-A19-A23-A25-A26-A28-A29-B1-B2-B5-B8-B19-B22-B23-B26-B29-C2-C5-C8-C23-C26-C29

HD	Sequences
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 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 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 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 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 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 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 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 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 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
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 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 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 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 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 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 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 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 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 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

Description for Tables S2-S13

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 – O3 and O4 - oxygen from the side chain hydroxyl group in 3HYP and 4HYP variants respectively, 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; GLN - OE1 - oxygen of the amino group in the side chain, NE2- nitrogen of the amino group in the side chain, N - nitrogen of the amino group in the main chain, O - oxygen in the main chain. The numbering of atoms in HA according to Fig. S1 (GCU – O5 and O6 oxygen from the carboxyl group, O2 and O3 oxygen from the hydroxyl group, O5 - oxygen in the ring; NAG - N - nitrogen at the acetyl group, O7 oxygen from the acetyl group, O5 oxygen in the ring, O4 and O6 hydroxyl groups).

Table S2 Distribution of H-bonds between HA and collagen amino acid atoms for HD=0. Percentages represent a contributions of H-bonds identified between HA and a given amino acid residue The numbering of atoms is presented in "Description for Tables S2-S13" section (atoms O3 and O7 in HA did not form any H-bonds with collagen).

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	PRO	PRO	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	N	O	N	O	N	O	OE1	NE2	O	N
N	0%	0%	0%	0%	2%	3%	0%	0%	7%	0%	7%	0%	0%	7%	0%	3%	0%
O1	3%	1%	1%	2%	10%	5%	2%	0%	26%	0%	34%	7%	22%	3%	7%	7%	0%

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	PRO	PRO	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	N	O	N	O	N	O	OE1	NE2	O	N
O2	1%	3%	4%	0%	3%	7%	0%	0%	17%	1%	18%	2%	13%	7%	3%	17%	0%
O4	0%	0%	1%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
O5	1%	5%	12%	8%	0%	0%	5%	0%	0%	0%	0%	11%	2%	0%	0%	0%	3%
O6	2%	5%	8%	9%	0%	0%	3%	0%	0%	0%	0%	9%	0%	0%	0%	0%	0%
O8	1%	2%	2%	1%	10%	9%	0%	1%	19%	0%	11%	4%	9%	0%	0%	0%	0%
O9	0%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	7%	3%	7%
O10	3%	3%	5%	1%	12%	12%	16%	0%	26%	0%	28%	6%	7%	3%	7%	3%	0%
O11	1%	6%	3%	4%	0%	0%	0%	3%	0%	0%	0%	7%	0%	0%	3%	0%	7%

Table S3 Distribution of H-bonds between HA and collagen amino acid atoms for HD=1 (3HYP). Percentages represent a contributions of H-bonds identified between HA and a given amino acid residue. The numbering of atoms is presented in "Description for Tables S2-S13" section on page 5 (atoms O3 and O7 in HA did not form any H-bonds with collagen).

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	HYP	HYP	HYP	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	O3	O	N	N	O	N	O	OE1	NE2	O	N
N	0%	0%	0%	0%	0%	0%	0%	4%	2%	0%	0%	10%	0%	0%	7%	0%	0%	0%
O1	0%	2%	4%	2%	12%	9%	21%	14%	10%	0%	0%	28%	5%	14%	7%	7%	13%	0%
O2	2%	2%	6%	4%	6%	6%	6%	12%	4%	0%	0%	14%	14%	8%	7%	0%	0%	7%
O4	0%	1%	0%	0%	0%	0%	0%	0%	0.5%	0%	0%	0%	0%	0%	0%	0%	0%	0%
O5	2%	3%	4%	6%	0%	0%	3%	10%	0%	1%	0%	0%	19%	0%	0%	0%	0%	7%
O6	3%	5%	12%	6%	0%	0%	0%	13%	0%	0%	0%	0%	11%	0%	0%	7%	0%	0%
O8	0%	0%	5%	2%	9%	3%	3%	10%	4%	0%	0%	12%	3%	5%	0%	0%	0%	0%
O9	0%	0%	1%	0%	0%	0%	0%	0%	0.5%	0%	0%	0%	0%	0%	0%	0%	7%	0%
O10	5%	4%	5%	4%	3%	3%	15%	7%	4%	0%	0%	36%	5%	8%	0%	0%	13%	7%
O11	2%	2%	2%	4%	0%	0%	3%	6%	0%	0%	0%	0%	8%	0%	0%	7%	0%	7%

Table S4 Distribution of H-bonds between HA and collagen amino acid atoms for HD=1 (4HYP). Percentages represent a contributions of H-bonds identified between HA and a given amino acid residue. The numbering of atoms is presented in "Description for Tables S2-S13" section on page 5 (atoms O3 and O7 in HA did not form any H-bonds with collagen).

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	HYP	HYP	HYP	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	O4	O	N	N	O	N	O	OE1	NE2	O	N
N	0%	0%	0%	0%	5%	15%	0%	4%	3%	0%	0%	9%	0%	2%	9%	0%	5%	0%
O1	3%	4%	2%	2%	0%	0%	10%	8%	6%	0%	0%	35%	3%	14%	5%	14%	0%	5%
O2	5%	4%	2%	1%	5%	0%	5%	10%	4%	0%	1%	13%	12%	10%	14%	5%	0%	9%
O4	0%	0%	1%	0%	0%	0%	0%	0.5%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	HYP	HYP	HYP	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	O4	O	N	N	O	N	O	OE1	NE2	O	N
O5	1%	8%	10%	9%	0%	0%	5%	17%	0%	0%	0%	0%	10%	0%	0%	5%	0%	5%
O6	3%	7%	8%	3%	0%	0%	0%	15%	0%	0%	0%	0%	5%	0%	0%	5%	0%	0%
O8	0%	1%	0%	1%	10%	10%	0%	7%	4%	0%	0%	15%	5%	3%	0%	0%	0%	0%
O9	0%	1%	1%	0%	0%	0%	0%	0.5%	0%	0%	0%	0%	0%	0%	5%	0%	9%	0%
O10	1%	8%	2%	1%	10%	15%	5%	12%	4%	0%	0%	27%	12%	12%	0%	0%	9%	0%
O11	0%	5%	6%	2%	0%	0%	5%	5%	0%	0%	0%	0%	10%	0%	0%	0%	0%	0%

Table S5 H-bonds lengths [nm] between HA and collagen amino acid atoms for HD=0. The numbering of atoms is presented in "Description for Tables S2-S13" section on page 5 (atoms O3 and O7 in HA did not form any H-bonds with collagen). In the parentheses the standard deviation values were provided.

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	PRO	PRO	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	N	O	N	O	N	O	OE1	NE2	O	N
N	-	-	-	-	0.177 (0.009)	0.193 (0.011)	-	-	0.213 (0.020)	-	0.198 (0.014)	-	-	0.209 (0.015)	-	0.179 (0.012)	-
O1	0.223 (0.015)	0.215 (0.006)	0.184 (0.008)	0.201 (0.031)	0.187 (0.031)	0.170 (0.016)	0.205 (0.010)	-	0.181 (0.018)	-	0.196 (0.020)	0.209 (0.014)	0.188 (0.015)	0.161 (0.016)	0.192 (0.020)	0.212 (0.020)	-
O2	0.206 (0.011)	0.212 (0.020)	0.183 (0.011)	-	0.169 (0.016)	0.174 (0.014)	-	-	0.190 (0.021)	0.234 (0.006)	0.192 (0.018)	0.211 (0.018)	0.189 (0.019)	0.186 (0.013)	0.226 (0.015)	0.185 (0.017)	-
O4	-	-	0.213 (0.009)	0.234 (0.021)	-	-	-	-	-	-	-	-	-	-	-	-	-
O5	0.182 (0.007)	0.189 (0.015)	0.191 (0.016)	0.202 (0.013)	-	-	0.213 (0.026)	-	-	-	-	0.205 (0.019)	0.190 (0.009)	-	-	-	0.192 (0.008)
O6	0.185 (0.013)	0.187 (0.019)	0.188 (0.011)	0.192 (0.012)	-	-	0.193 (0.002)	-	-	-	-	0.195 (0.008)	-	-	-	-	-
O8	0.204 (0.008)	0.206 (0.013)	0.199 (0.008)	0.190 (0.017)	0.177 (0.010)	0.182 (0.015)	-	0.204 (0.019)	0.179 (0.020)	-	0.189 (0.016)	0.209 (0.018)	0.186 (0.016)	-	0.210 (0.026)	0.169 (0.014)	0.225 (0.022)
O9	-	0.229 (0.014)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O10	0.203 (0.009)	0.206 (0.020)	0.198 (0.011)	0.222 (0.020)	0.177 (0.012)	0.170 (0.017)	0.198 (0.014)	-	0.186 (0.015)	-	0.187 (0.017)	0.220 (0.007)	0.190 (0.014)	0.183 (0.006)	0.181 (0.008)	0.181 (0.010)	-
O11	0.184 (0.009)	0.201 (0.025)	0.210 (0.017)	0.193 (0.012)	-	-	-	0.210 (0.039)	-	-	-	0.207 (0.016)	-	-	0.212 (0.009)	-	0.213 (0.014)

Table S6 H-bonds lengths [nm] between HA and collagen amino acid atoms for HD=1 (3HYP). The numbering of atoms is presented in "Description for Tables S2-S13" section on page 5 (atoms O3 and O7 in HA did not form any H-bonds with collagen). In the parentheses the standard deviation values were provided.

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	HYP	HYP	HYP	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	O3	O	N	N	O	N	O	OE1	NE2	O	N
N	-	-	-	-	-	-	-	0.202 (0.015)	0.222 (0.014)	-	-	0.200 (0.021)	-	-	0.240 (0.010)	-	-	-
O1	-	0.198 (0.003)	0.200 (0.016)	0.200 (0.014)	0.183 (0.028)	0.162 (0.010)	0.221 (0.016)	0.187 (0.018)	0.193 (0.021)	-	-	0.194 (0.016)	0.206 (0.005)	0.186 (0.018)	0.175 (0.011)	0.226 (0.008)	0.181 (0.007)	-
O2	0.216 (0.015)	0.204 (0.001)	0.198 (0.013)	0.208 (0.014)	0.194 (0.026)	0.171 (0.002)	0.228 (0.014)	0.189 (0.017)	0.189 (0.022)	-	-	0.196 (0.019)	0.222 (0.016)	0.191 (0.005)	0.226 (0.021)	-	-	0.223 (0.021)
O4	-	0.199 (0.005)	-	-	-	-	-	0.187 (0.014)	-	-	-	-	-	-	-	-	-	-
O5	0.198 (0.009)	0.204 (0.011)	0.185 (0.007)	0.205 (0.022)	-	-	0.193 (0.009)	0.179 (0.015)	-	0.182 (0.023)	-	-	0.208 (0.016)	-	-	-	-	0.182 (0.012)
O6	0.196 (0.013)	0.188 (0.014)	0.189 (0.020)	0.192 (0.011)	-	-	-	0.171 (0.015)	-	-	-	-	0.199 (0.016)	-	-	0.199 (0.011)	-	-
O8	-	-	0.207 (0.018)	0.209 (0.024)	0.172 (0.015)	0.158 (0.019)	0.235 (0.016)	0.189 (0.017)	0.189 (0.017)	-	-	0.188 (0.021)	0.230 (0.018)	0.161 (0.006)	-	-	0.211 (0.015)	-
O9	-	-	0.201 (0.003)	-	-	-	-	0.191 (0.015)	-	-	-	-	-	-	-	-	-	-
O10	0.210 (0.021)	0.202 (0.026)	0.200 (0.014)	0.192 (0.010)	0.177 (0.011)	0.161 (0.020)	0.202 (0.011)	0.182 (0.013)	0.195 (0.022)	-	-	0.180 (0.016)	0.210 (0.021)	0.181 (0.014)	-	-	0.184 (0.013)	0.189 (0.007)
O11	0.228 (0.021)	0.218 (0.012)	0.192 (0.012)	0.199 (0.018)	-	-	0.214 (0.021)	0.183 (0.016)	-	-	-	-	0.183 (0.007)	-	-	0.176 (0.006)	-	0.209 (0.004)

Table S7 H-bonds lengths [nm] between HA and collagen amino acid atoms for HD=1 (4HYP). The numbering of atoms is presented in "Description for Tables S2-S13" section on page 5 (atoms O3 and O7 in HA did not form any H-bonds with collagen). In the parentheses the standard deviation values were provided.

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	HYP	HYP	HYP	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	O4	O	N	N	O	N	O	OE1	NE2	O	N
N	-	-	-	-	0.204 (0.012)	0.195 (0.014)	-	0.213 (0.013)	0.210 (0.018)	-	-	0.212 (0.016)	-	0.192 (0.023)	0.221 (0.011)	-	0.241 (0.004)	-
O1	0.212 (0.016)	0.210 (0.023)	0.208 (0.021)	0.203 (0.014)	-	-	0.223 (0.003)	0.188 (0.015)	0.188 (0.021)	0.195 (0.022)	-	0.192 (0.020)	0.216 (0.008)	0.181 (0.019)	0.158 (0.018)	0.197 (0.003)	-	0.194 (0.004)
O2	0.224 (0.013)	0.218 (0.010)	0.224 (0.004)	0.215 (0.015)	0.157 (0.011)	-	0.190 (0.010)	0.192 (0.019)	0.185 (0.019)	0.177 (0.014)	0.214 (0.015)	0.194 (0.013)	0.212 (0.017)	0.181 (0.019)	0.172 (0.007)	0.234 (0.006)	-	0.198 (0.001)
O4	-	-	0.207 (0.003)	-	-	-	-	0.220 (0.023)	-	-	-	-	-	-	-	-	-	-

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	HYP	HYP	HYP	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	O4	O	N	N	O	N	O	OE1	NE2	O	N
O5	0.201 (0.011)	0.195 (0.013)	0.186 (0.011)	0.190 (0.015)	-	-	0.216 (0.012)	0.170 (0.014)	-	-	-	-	0.197 (0.013)	-	-	0.186 (0.011)	-	0.191 (0.012)
O6	0.207 (0.017)	0.195 (0.013)	0.193 (0.020)	0.198 (0.026)	-	-	-	0.171 (0.015)	-	0.203 (0.027)	-	-	0.204 (0.014)	-	-	0.181 (0.008)	-	-
O8	-	0.188 (0.011)	-	0.233 (0.022)	0.172 (0.004)	0.181 (0.006)	-	0.192 (0.016)	0.187 (0.015)	-	-	0.178 (0.015)	0.205 (0.025)	0.185 (0.013)	0.177 (0.015)	-	0.199 (0.004)	-
O9	-	0.227 (0.015)	0.195 (0.018)	-	-	-	-	0.211 (0.014)	-	-	-	-	-	-	-	-	-	-
O10	0.208 (0.009)	0.195 (0.008)	0.189 (0.01)	0.179 (0.009)	0.165 (0.004)	0.175 (0.016)	0.188 (0.012)	0.188 (0.016)	0.183 (0.016)	-	-	0.190 (0.019)	0.214 (0.012)	0.182 (0.020)	-	-	0.171 (0.001)	-
O11	-	0.188 (0.014)	0.202 (0.012)	0.204 (0.006)	-	-	0.230 (0.013)	0.182 (0.018)	-	-	-	-	0.205 (0.013)	-	-	-	-	-

Table S8 Energies of H-bonds [kJ/mol] between HA and given collagen amino acid residue atom for HD=0. The numbering of atoms is presented in "Description for Tables S2-S13" section on page 5 (atoms O3 and O7 in HA did not form any H-bonds with collagen). In the parentheses the standard deviation values were provided.

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	PRO	PRO	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	N	O	N	O	N	O	OE1	NE2	O	N
N	-	-	-	-	−25.0 (0.0)	−23.0 (2.1)	-	-	−17.7 (5.4)	-	−19.1 (5.0)	-	-	−16.2 (5.3)	-	−21.5 (3.7)	-
O1	−16.8 (6.4)	−15.1 (8.0)	−16.3 (0.9)	−17.5 (8.0)	−18.7 (6.4)	−23.2 (3.1)	−25.0 (0.0)	-	−21.4 (5.0)	-	−19.3 (5.4)	−17.6 (3.1)	−21.8 (4.2)	−22.9 (4.9)	−25.0 (0.0)	−13.0 (5.6)	-
O2	−11.3 (1.6)	−14.3 (7.4)	−21.5 (3.4)	-	−25.0 (0.8)	−24.6 (0.8)	-	-	−21.2 (5.9)	−6.6 (1.1)	−19.9 (4.3)	−15.4 (2.5)	−19.0 (6.6)	−17.0 (5.3)	−17.2 (3.1)	−24.5 (0.7)	-
O4	-	-	−17.6 (2.4)	−8.0 (0.4)	-	-	-	-	-	-	-	-	-	-	-	-	-
O5	−21.6 (4.8)	−19.7 (4.0)	−19.2 (5.1)	−17.4 (3.2)	-	-	−15.2 (8.7)	-	-	-	-	−15.6 (5.8)	−25.0 (0.9)	-	-	-	−24.4 (0.6)
O6	−21.7 (5.7)	−21.7 (4.4)	−19.1 (4.3)	−18.9 (3.0)	-	-	−16.3 (5.1)	-	-	-	-	−23.1 (2.6)	-	-	-	-	-
O8	−21.6 (4.8)	−16.4 (6.2)	−18.5 (2.0)	−21.9 (5.3)	−23.4 (2.0)	−21.3 (3.0)	-	−9.0 (2.5)	−22.7 (4.8)	-	−22.0 (2.4)	−15.7 (0.4)	−21.4 (3.3)	-	−14.4 (2.0)	−25.0 (0.0)	−14.5 (6.5)
O9	-	−6.4 (0.8)	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O10	−21.3 (2.6)	−16.6 (6.4)	−20.1 (3.6)	−12.7 (1.9)	−22.9 (3.3)	−23.8 (2.7)	−22.2 (4.0)	-	−22.2 (3.6)	-	−21.6 (4.3)	−16.4 (3.8)	−20.2 (3.6)	−17.0 (3.8)	−23.1 (1.1)	−25.0 (0.0)	-

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	PRO	PRO	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	N	O	N	O	N	O	OE1	NE2	O	N
O11	−22.0 (1.3)	−18.1 (7.0)	−14.8 (5.5)	−18.2 (2.7)	-	-	-	−12.6 (4.6)	-	-	-	−19.2 (2.9)	-	-	−16.4 (1.8)	-	−19.5 (7.8)

Table S9 Energies of H-bonds [kJ/mol] between HA and given collagen amino acid residue atom for HD=1 (3HYP). The numbering of atoms is presented in "Description for Tables S2-S13" section on page 5 (atoms O3 and O7 in HA did not form any H-bonds with collagen). In the parentheses the standard deviation values were provided.

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	HYP	HYP	HYP	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	O3	O	N	N	O	N	O	OE1	NE2	O	N
N	-	-	-	-	-	-	-	−17.8 (6.5)	−14.2 (7.7)	-	-	−18.3 (6.3)	-	-	−9.8 (1.5)	-	-	-
O1	-	−20.7 (6.1)	−18.9 (4.1)	−20.3 (4.9)	−21.1 (7.3)	−24.8 (0.3)	−13.5 (5.3)	−21.6 (4.8)	−19.6 (4.8)	-	-	−20.9 (4.7)	−23.3 (2.5)	−18.6 (5.3)	−24.4 (0.6)	−15.1 (4.2)	−25.0 (0.0)	-
O2	−17.1 (6.5)	−19.2 (1.0)	−18.5 (4.2)	−15.5 (5.1)	−14.6 (5.7)	−24.7 (0.4)	−14.2 (5.9)	−20.9 (4.2)	−20.4 (5.1)	-	-	−20.9 (4.8)	−14.1 (6.6)	−17.2 (3.4)	−16.5 (1.9)	-	-	−18.6 (1.7)
O4	-	−17.2 (2.9)	-	-	-	-	-	−21.1 (3.0)	-	-	-	-	-	-	-	-	-	-
O5	−19.7 (7.4)	−19.9 (4.4)	−21.3 (2.1)	−18.3 (5.9)	-	-	−21.9 (2.4)	−22.3 (2.9)	-	−22.7 (3.3)	-	-	−19.6 (5.3)	-	-	-	-	−25.0 (0.0)
O6	−23.5 (1.7)	−19.6 (5.4)	−18.7 (5.5)	−20.7 (5.7)	-	-	-	−23.4 (2.4)	-	-	-	-	−20.2 (3.3)	-	-	−25.0 (0.0)	-	-
O8	-	-	−17.0 (6.4)	−18.2 (6.3)	−21.2 (6.0)	−25.0 (0.0)	−12.3 (1.9)	−20.6 (4.8)	−19.9 (4.5)	-	-	−21.7 (5.5)	−8.9 (1.3)	−23.9 (1.5)	-	-	−21.5 (4.9)	-
O9	-	-	−16.0 (1.6)	-	-	-	-	−25.0 (0.0)	-	-	-	-	-	-	-	-	-	-
O10	−17.4 (5.8)	−17.7 (5.6)	−18.4 (6.1)	−19.4 (5.2)	−22.9 (2.4)	−25.0 (0.0)	−19.8 (6.6)	−22.1 (3.9)	−20.1 (6.3)	-	-	−22.4 (3.6)	−15.5 (8.5)	−21.4 (5.0)	-	-	−21.3 (5.2)	−22.3 (2.1)
O11	−13.9 (9.3)	−19.1 (2.8)	−18.6 (4.7)	−17.1 (4.2)	-	-	−22.9 (3.9)	−21.8 (2.7)	-	-	-	-	−19.4 (4.9)	-	-	−25.0 (0.0)	-	−23.5 (1.5)

Table S10 Energies of H-bonds [kJ/mol] between HA and given collagen amino acid residue atom for HD=1 (4HYP). The numbering of atoms is presented in "Description for Tables S2-S13" section on page 5 (atoms O3 and O7 in HA did not form any H-bonds with collagen). In the parentheses the standard deviation values were provided.

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	HYP	HYP	HYP	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	O4	O	N	N	O	N	O	OE1	NE2	O	N
N	-	-	-	-	−19.6 (1.5)	−21.8 (3.0)	-	−16.5 (3.2)	−18.1 (5.6)	-	-	−18.8 (4.2)	-	−21.5 (1.0)	−11.3 (6.2)	-	−7.5 (0.5)	-
O1	−16.2 (8.4)	−18.2 (7.5)	−10.3 (4.8)	−13.7 (6.9)	-	-	−14.2 (0.7)	−21.0 (4.0)	−20.8 (5.4)	−25.0 (1.7)	-	−20.7 (5.2)	−14.5 (0.0)	−22.7 (4.0)	−25.0 (0.0)	−21.4 (4.5)	-	−21.9 (1.0)

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	HYP	HYP	HYP	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	O4	O	N	N	O	N	O	OE1	NE2	O	N
O2	−13.3 (4.6)	−17.4 (5.3)	−11.5 (3.2)	−22.6 (2.9)	−25.0 (0.0)	-	−25.0 (0.0)	−19.6 (5.6)	−20.4 (4.1)	−21.5 (1.0)	−17.6 (4.2)	−21.4 (4.6)	−18.6 (6.7)	−23.5 (1.9)	−24.5 (0.9)	−8.6 (0.8)	-	−20.0 (4.0)
O4	-	-	−15.1 (1.2)	-	-	-	-	−10.0 (3.2)	-	-	-	-	-	-	-	-	-	-
O5	−21.5 (2.3)	−19.0 (3.4)	−19.7 (3.2)	−19.7 (3.5)	-	-	−15.8 (0.0)	−24.0 (2.3)	-	-	-	-	−22.1 (2.5)	-	-	−25.0 (0.0)	-	−25.0 (0.0)
O6	−16.0 (7.0)	−20.2 (5.4)	−17.4 (6.2)	−13.9 (4.5)	-	-	-	−23.8 (2.6)	-	−14.5 (3.8)	-	-	−20.8 (0.6)	-	-	−25.0 (0.0)	-	-
O8	-	−19.6 (4.7)	-	−8.1 (1.2)	−25.0 (0.0)	−21.0 (3.5)	-	−21.2 (4.1)	−20.6 (3.4)	-	-	−22.2 (4.3)	−20.3 (1.9)	−25.0 (0.0)	−25.0 (0.0)	-	−18.5 (2.1)	-
O9	-	−14.2 (3.4)	−7.7 (0.6)	-	-	-	-	−12.2 (2.9)	-	-	-	-	-	-	-	-	-	-
O10	−19.9 (2.6)	−19.7 (4.3)	−18.2 (5.8)	−25.0 (0.0)	−22.5 (3.6)	−22.8 (2.0)	−25.0 (0.0)	−21.5 (3.4)	−20.9 (4.2)	-	-	−21.4 (3.5)	−18.4 (5.0)	−21.4 (6.3)	-	-	−24.7 (0.4)	-
O11	-	−20.3 (4.4)	−16.7 (4.4)	−15.6 (0.0)	-	-	−15.0 (0.0)	−23.1 (2.3)	-	-	-	-	−17.5 (8.1)	-	-	-	-	-

Table S11 The H-bonds acceptor-donor frequency analysis. Values in cells represent how often HA in a given interaction plays the role of acceptor for HD=0. The numbering of atoms is presented in "Description for Tables S2-S13" section on page 5.

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	PRO	PRO	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	N	O	N	O	N	O	OE1	NE2	O	N
N	-	-	-	-	0%	0%	-	-	0%	-	0%	-	-	0%	-	0%	-
O1	100%	100%	100%	100%	0%	0%	100%	-	0%	-	0%	100%	0%	0%	100%	0%	-
O2	100%	100%	100%	-	0%	0%	-	-	0%	100%	0%	100%	0%	0%	100%	0%	-
O4	-	-	100%	100%	-	-	-	-	-	-	-	-	-	-	-	-	-
O5		100%	100%	100%	-	-	100%	-	-	-	-	100%	0%	-	-	-	100%
O6	100%	100%	100%	100%	-	-	100%	-	-	-	-	100%	-	-	-	-	-
O8	100%	100%	100%	100%	0%	0%	-	100%	0%	-	0%	100%	0%	-	100%	0%	100%
O9	-	100%	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O10	100%	100%	100%	100%	0%	0%	100%	-	0%	-	0%	100%	0%	0%	100%	0%	-
O11	100%	100%	100%	100%	-	-	-	100%	-	-	-	100%	-	-	100%	-	100%

Table S12 The H-bonds acceptor-donor frequency analysis. Values in cells represent how often HA in a given interaction plays the role of acceptor for HD=1 (3HYP). The numbering of atoms is presented in "Description for Tables S2-S13" section on page 5.

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	HYP	HYP	HYP	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	O3	O	N	N	O	N	O	OE1	NE2	O	N
N	-	-	-	-	-	-	-	0%	0%	-	-	0%	-	-	0%	-	-	-
O1	-	100%	100%	100%	0%	0%	100%	49%	0%	-	-	0%	100%	0%	0%	100%	0%	-
O2	100%	100%	100%	100%	0%	0%	100%	54%	0%	-	-	0%	100%	0%	0%	-	-	100%
O4	-	100%	-	-	-	-	-	100%	-	-	-	-	-	-	-	-	-	-
O5		100%	100%	100%	-	-	100%	100%	-	100%	-	-	100%	-	-	-	-	100%
O6	100%	100%	100%	100%	-	-	-	100%	-	-	-	-	100%	-	-	100%	-	-
O8	-	-	100%	100%	0%	0%	100%	52%	0%	-	-	0%	100%	0%	-	-	0%	-
O9	-	-	100%	-	-	-	-	100%	-	-	-	-	-	-	-	-	-	-
O10	100%	100%	100%	100%	0%	0%	100%	50%	0%	-	-	0%	100%	0%	-	-	0%	100%
O11	100%	100%	100%	100%	-	-	100%	100%	-	-	-	-	100%	-	-	100%	-	100%

Table S13 The H-bonds acceptor-donor frequency analysis. Values in cells represent how often HA in a given interaction plays the role of acceptor for HD=1 (4HYP). The numbering of atoms is presented in "Description for Tables S2-S13" section on page 5.

	ARG	ARG	ARG	ARG	GLU	GLU	GLU	HYP	HYP	HYP	GLY	GLY	ALA	ALA	GLN	GLN	GLN	GLN
	N	NH1	NH2	NE	OE1	OE2	N	O4	O	N	N	O	N	O	OE1	NE2	O	N
N	-	-	-	-	0%	0%	-	0%	0%	-	-	0%	-	0%	0%	-	0%	-
O1	100%	100%	100%	100%	-	-	100%	63%	0%	100%	-	0%	100%	0%	0%	100%	-	100%
O2	100%	100%	100%	100%	0%	-	100%	57%	0%	100%	100%	0%	100%	0%	0%	100%	-	100%
O4	-	-	100%	-	-	-	-	100%	-	-	-	-	-	-	-	-	-	-
O5		100%	100%	100%	-	-	100%	100%	-	-	-	-	100%	-	-	100%	-	100%
O6	100%	100%	100%	100%	-	-	-	100%	-	100%	-	-	100%	-	-	100%	-	-
O8	-	100%	-	100%	0%	0%	-	37%	0%	-	-	0%	100%	0%	0%	-	0%	-
O9	-	100%	100%	-	-	-	-	100%	-	-	-	-	-	-	-	-	-	-
O10	100%	100%	100%	100%	0%	0%	100%	60%	0%	-	-	0%	100%	0%	-	-	0%	-
O11	-	100%	100%	100%	-	-	100%	100%	-	-	-	-	100%	-	-	-	-	-