

Supplementary materials
Goh et al.

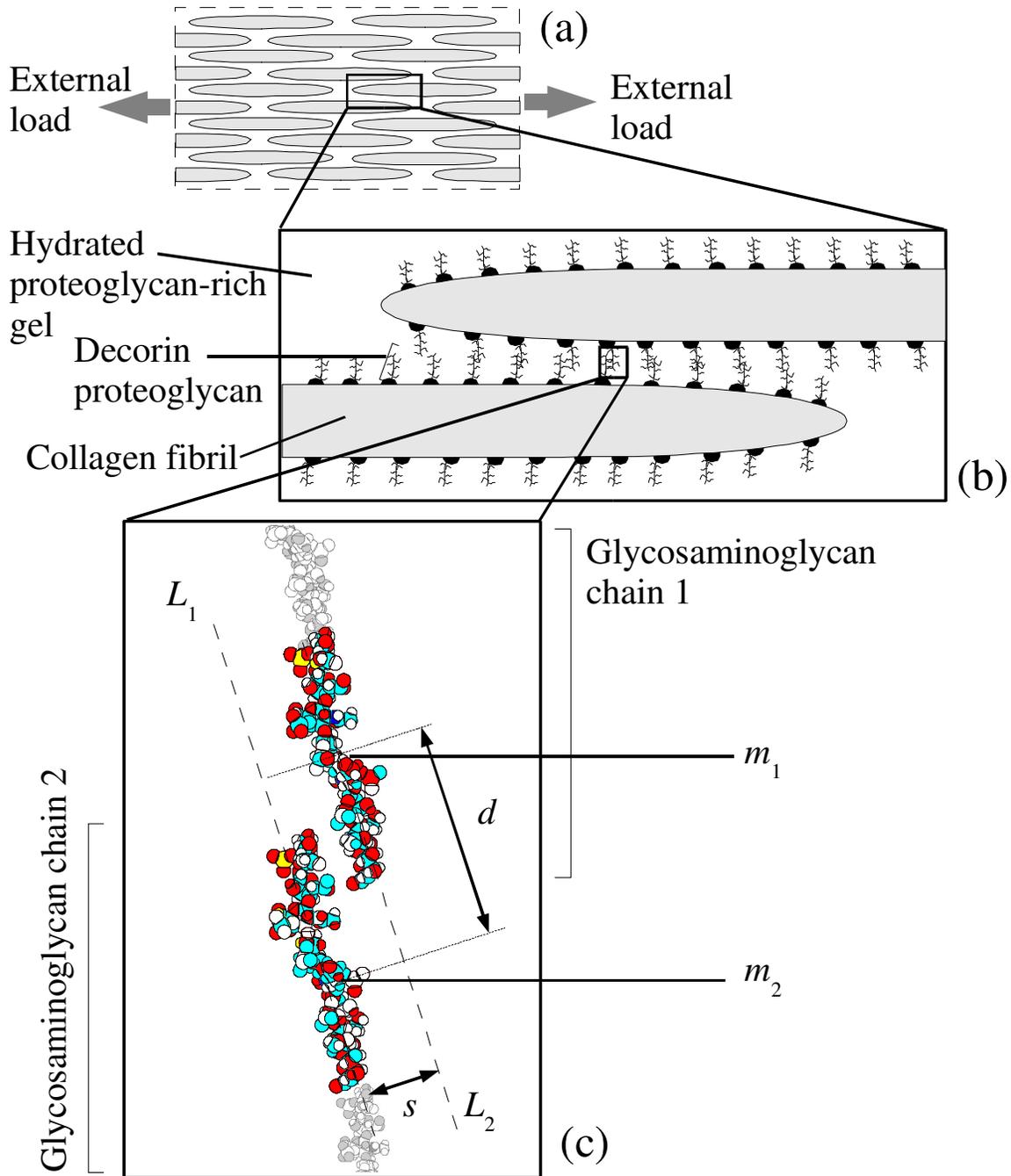


Figure 1 Molecular mechanics study of decorin interactions on adjacent fibrils. A model was developed to evaluate the relationship between VDW energy and cation number density (ρ) under fibril-fibril sliding action. As shown in (c), the model displays the GAG chains (comprising chondroitin-4-sulfate disaccharide repeats) associated with decorin molecules on adjacent fibrils in close proximity. Here, s and d denote the separation and displacement between m_1 and m_2 which are the mid-points within the last four repeats of each GAG chain. L_1 and L_2 are the labels for the axes (long dashes) corresponding to GAG chain 1 and 2, respectively.

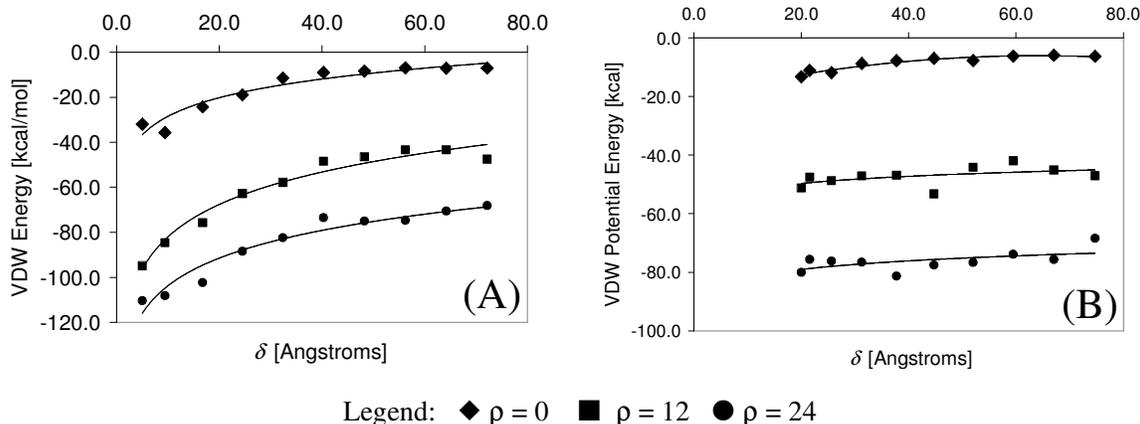


Figure 2 Graphs of Van Der Waals (VDW) potential energy versus sliding distance δ for (a) $s = 5 \text{ \AA}$ and (b) $s = 20 \text{ \AA}$. Here, VDW energy was evaluated from the model (see Figure 1) as a function of δ where $\delta^2 = s^2 + d^2$ (Figure 1). An initial condition was used to describe the GAG-GAG overlapping distance over four chondroitin-4-sulfate disaccharide repeats. Each disaccharide repeat is negatively charged due to the anionic nature of the sulphate and carboxylate groups. Restraints on each chain were implemented to maintain the semi-rigid linear conformation of the chain. Solvent environment was modelled implicitly; the dielectric constant was assigned a value of 80 to correspond to water. The model was implemented using software Hyperchem (Version 7.5, Hypercube, Inc.). Geometry optimisation was investigated using molecular mechanics (AMBER3 force field); the Polak Ribiere (conjugate gradient) algorithm was used to determine the minimum energy value. Atomic partial charges were evaluated successively on the sulphate group and carboxyl group, where the total charge value = -1 for each group, using the single point calculation. Mobile cations (Na^+) were designated in closed proximity to each group to model a hypertonic PG matrix environment. The model predicted that VDW energy increases by about 1.2 times as the number of cations increases two-fold. The value of ρ also influences the rate of decrease in VDW energy with respect to the relative displacement (δ) between the GAGs. The predictions show that VDW energy decreases least rapidly as δ increases when $\rho = 24$. However, VDW energy decreases most rapidly for $\rho = 0$.