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Understanding the mechanisms in plasma-treated alginate biopolymer

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Cold atmospheric plasma (CAP) is attracting significant attention in the biomedical field due to its potential benefits.[1] CAP has been effective in stabilizing biopolymer solutions that create hydrogels and boosting the production of reactive species. These solutions are especially well-suited for indirect treatment of biological targets.[2] Nonetheless, the direct effects of plasma on biopolymer structures and the associated chemical mechanisms are not yet fully understood.

Therefore, in this investigation, reactive molecular dynamics simulations were performed to study the interaction of the alginate molecule (Figure 1) with oxygen atoms, the main component of reactive oxygen species produced by CAP.

The simulation results showed that the interaction of oxygen atoms with alginate tetramer resulted in significant structural changes. These changes include the formation of alcohol, peroxyl, ketone, ester, and aldehyde groups, as well as the opening of sugar rings and even the cleavage of glycosidic bonds within the structure.

This comprehensive understanding illuminates the atomic-level alterations triggered by cold plasma treatment of biopolymers. These insights could impact the utilization of biopolymers or the hydrogels they create in cancer therapy and other biomedical fields.

References

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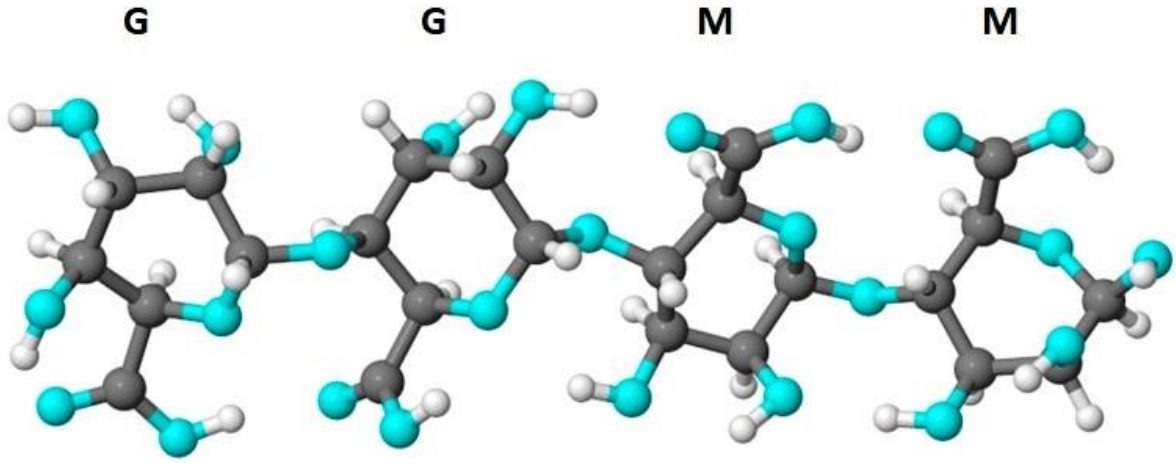

Figure 1. Schematic representation of an alginate tetramer (i.e., guluronic acid (G) and mannuronic acid (M) dimers). Carbon, oxygen, and hydrogen atoms are shown in gray, cyan, and white, respectively.