Screen the best ionic liquids for keratin dissolution by using COSMO-RS

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Screen the best ionic liquid for keratin dissolution by using COSMO-RS

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Application of PDMS in tissue engineering

- Most PDMS used in tissue engineering applications are nonpolar, inert and highly hydrophobic, which lead to the low biocompatibility and interaction responses between implantations and cells.

Keratin molecules have many inter- and intra-molecular strong bonds and also have no regular repeating units, which lead to it difficult to be dissolved by traditional solvent.

Keratin has the special amino acid sequence for cell adhesion, which can increase susceptibility to bio-decomposition.

Keratin can improve the mechanical properties of composites.
Keratin dissolution in ionic liquids

Ionic liquid (IL) is a salt in which the ions are poorly coordinated, which results in these solvents being liquid below 100°C, or even at room temperature.

Properties of ILs:
- High chemical stability and thermal stability
- Wider liquid state, Non-volatile
- Low vapor pressure
- Tunable structure and properties
- Wide electrochemical windows
- High electrical conductivity

Advantages of ILs in dissolving keratin:
- Higher solubility
- It can be recycled with high recovery rate
- Less damage to keratin structure
- Tunable structure and properties

It is nevertheless a challenge to identify the best ILs for keratin dissolution;
Experimental measurement of all these systems is not practically feasible;
A rapid and a priori screening method to predict the keratin solubility capacity for ILs is needed.

Study of keratin dissolution in ionic liquids:

<table>
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Screen the best ionic liquid for keratin dissolution by using COSMO-RS

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Abstract

electronic interactions, which are often referred to as “artificial receptors” are now receiving much attention, such as ion-sensors, battery-active materials, and liquid metal sensors. Molecular dynamics (MD) simulations have shown that ionic liquids (ILs) are a promising class of materials that can be used as solvent-free catalysts. This work investigates the solvent-free catalysis performance of ILs, with the help of the COSMO-RS model, for keratin dissolution. The interaction between proteins and ILs is studied, which can be described as ion-dipole interactions. The results show that the interaction energy is significantly influenced by the ILs and the keratin structure. The ILs with higher interaction energy are more suitable for keratin dissolution. The ILs with lower interaction energy have a higher chance of forming a precipitation complex, which can inhibit keratin dissolution.

1. Application of keratin in elastomer materials

2. Structures of keratin and keratin models in this study

3. Predict result

4. Conclusions and Advances

Acknowledgments and References

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