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

Liu, Xue; Nie, Yi; Zhang, Suojiang; Skov, Anne Ladegaard

Publication date:
2018

Document Version
Peer reviewed version

Citation (APA):
Screen the best ionic liquid for keratin dissolution by using COSMO-RS

Xue Liu\textsuperscript{(1)(2)}, Yi Nie\textsuperscript{(2)}, Suojiang Zhang\textsuperscript{(2)*}, Anne Ladegaard Skov\textsuperscript{(1)*}

(1) Danish Polymer Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark;
(2) CAS Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing, China;
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>
<thead>
<tr>
<th>Author</th>
<th>ILs</th>
<th>Temperature °C</th>
<th>Time</th>
<th>Solubility</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yimei Ai</td>
<td>[B(CN)[Na][SO][H2O]]</td>
<td>100</td>
<td>1h</td>
<td>6.6</td>
</tr>
<tr>
<td>Haibo Xie</td>
<td>[B(CN)[Cl],[B(CN)[Br]]</td>
<td>130</td>
<td>10h</td>
<td>ND</td>
</tr>
<tr>
<td>Yu-Xian Wang</td>
<td>[H0][[Emim][NTe][Na][SO]]</td>
<td>130</td>
<td>24h</td>
<td>ND</td>
</tr>
<tr>
<td>Adria Idris</td>
<td>[Bis-(2-ethylhexyl)]</td>
<td>130</td>
<td>10h</td>
<td>45</td>
</tr>
<tr>
<td>Shuangning Zhang</td>
<td>[Bis-(2-ethylhexyl)]</td>
<td>130</td>
<td>10h</td>
<td>ND</td>
</tr>
</tbody>
</table>

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

Xue Liu [1]*, Yi Niu [2], Suijiang Zhang [2*], Anne Ladegaard Skov [1]*

[1] Danish Polymer Center, Department of Chemical and Biotechnological Engineering, Technical University of Denmark, Kgs. Lyngby, Denmark.

Abstract: Electrostatic interactions (EIs), which are often referred to as "artificial receptors", play a crucial role in the recognition and interaction between biomolecules. Keratin, which is rich in cysteine, tyrosine, and phenylalanine, is expected to be more biocompatible and interact more strongly with other proteins than with the same proteins from other sources. The interaction between keratin and water, which can lead to the biocompatibility of keratin, is thus essential for the formation of the secondary structure in the protein-KIL system. An efficient dissolution of keratin is the basis for keratin-receptor interactions. A new class of Lewis-acidic salen complexes was tested for their dissolution ability in water. The Lewis-acidic salen complexes were selected due to their unique properties such as high thermal stability, variable concentration, and good solubility in water. The compounds tested were 1-3. Two papers were compared for their ability to dissolve keratin in water. The results showed that the 1-2 complex was the most effective at dissolving keratin, with over 95% dissolution after 24 hours. The use of 1-2 complex is recommended for further studies on the dissolution of keratin in water.

1. Application of keratin in elastomer materials

Keratin has a unique structure that makes it a suitable material for use in elastomer materials. This unique structure makes it easy to dissolve and form stable bonds with other substances.

2. Structures of keratin and keratin models in this study

Keratin models are used to simulate the structure and properties of keratin. These models are important for understanding the dissolution process and predicting the behavior of keratin in different environments.

3. Predict result

The prediction of keratin models and keratin models is based on the dissolution process and the dissolution process of keratin. The prediction of keratin models is important for understanding the behavior of keratin in different environments.

4. Conclusions and Advances

Three models concerning keratin bonds were designed for describing wool keratin. The computational results are in agreement with both models and up to the eleventh bond. The results show that the three models can describe the dissolution process of keratin and can be used to improve the dissolution process of keratin in water.

Acknowledgments

The authors gratefully acknowledge the National Natural Science Foundation of China (NSFC), National Key Research and Development Program of China (2016YFA0202001), and the Danish Council for Independent Research ( Grundforskning) for financial support.

References