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

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Abstract

Dielectric elastomers (DEs), which are often referred to as "artificial muscles", possess many excellent properties, such as large strains, high-energy densities, and fast responses[1]. Polydimethylsiloxane (PDMS) elastomers are one of the most used materials for DEs[2]. Unfortunately, most PDMS used in tissue engineering applications are nonpolar, inert and highly hydrophobic, which lead to the low bio-compatibility and interaction responses between implantations and cells. Keratin, which is polar, hydrophilic, biodegradable and thermostable, is expected to enhance interaction responses between implantations and cells[3]. The bio-functions of silicone/keratin composites for tissue engineering could be achieved due to the special amino acid sequence in keratin. Moreover, keratin can improve the mechanical properties of composites, which probably results from the formation of a common spatial network between keratin and silicone elastomer[4]. But, wool keratin is difficult to dissolve in conventional solvents, due to the tight packing of the secondary structures in the polypeptide[5]. So efficient dissolution of keratin is the basis for the elastomer-keratin composite. As a new class of designer solvents, ionic liquids (ILs) can dissolve a large number of biopolymers, due to their unique properties like high thermal stability, tunable properties, and good dissolving ability[5,6,7]. But it is nevertheless a challenge to identify the best ILs for keratin dissolution. Experimental measurement of all these systems is not practically feasible, hence a rapid and a priori screening method to predict the keratin solubility capacity for ILs is needed. In this work, we designed three models containing disulfide bonds for describing wool keratin, and 462 ILs formed from 21 cations and 22 anions were selected for evaluation of their ability to dissolve wool keratin by COSMO-RS. It lays a foundation for the research of keratin elastomer composites later.

1. Application of keratin in elastomer materials

- Structure of keratin
  - Keratin has a complex structure, and there is a large number of inter- and intra-molecular strong hydrogen bonds and disulfide bonds.
  - Keratin molecules have no regular repeating units.
  - Keratin elastomer composites

2. Structures of ILs and keratin models in this study

- Structure of cations
- Structure of anions
- Structure of keratin models

3. Predict result

- Prediction of p-potentials
- ©profile of keratin models and cations
- ©profile of keratin models and anions
- Logarithmic activity coefficient(ln Y)
- Ipy of model 2 in 462 ILs
- Ipy of model 3 in 462 ILs

4. Conclusions and Advances

- Three models containing disulfide bonds were designed for describing wool keratin;
- 462 ILs formed from 21 cations and 22 anions were selected for evaluation of their ability to dissolve wool keratin by COSMO-RS;
- H-bond interactions between the three models and ILs have a high influence on the solubility of keratin;
- In the process of keratin dissolution, the solubility of keratin in ILs is affected by cation and anion, but the anion plays a leading role;
- Ionic liquid with Ac, Dec, HCOO, Cl, DEP, DMP, DBP, BEN or Br has excellent solubility of keratin.

Acknowledgments and References

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References