Supporting information for

Deep Eutectic Solvent Engineering: A Novel Ternary System for Efficient Lignocellulose Extraction

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| Biomass | DESs | | | | Treatment Conditions | | | |
|----------------|------|--|----------------|-------------|----------------------|-------------|----------------------------------|--|
| | Name | HBA:HBD | Molar ratio | PEG (ml) | Temperature (°C) | Time (h) | Treatment effect | |
| Wheat straw | D | D-5 K ₂ CO ₃ :Gly D-10 | 1:5 | / | 160 | | □Satisfactory \$General □Poor | |
| | D-5 | | | 5 | | | ©Satisfactory □General □Poor | |
| | D-10 | | | 10 | | 24 | ©Satisfactory □General □Poor | |
| | D-20 | | | 20 | | | ©Satisfactory □General □Poor | |

Table S1 The details of different DESs and treatment conditions.

Note: Alkaline DESs (PH value:12.5-13)

| Table S2 Parameters of Arrhenius equation fitting curves. | | | | | | | | |
|---|------------------------|--------------------------------|------|--|--|--|--|--|
| Nome | Para | \mathbb{R}^2 | | | | | | |
| Name | η_1 | $E_{\eta} (kJ \cdot mol^{-1})$ | K- | | | | | |
| D | 1.71×10 ⁻¹¹ | 72.21 | 0.99 | | | | | |
| D-5 | 8.40×10 ⁻¹¹ | 65.63 | 0.99 | | | | | |
| D-10 | 2.93×10 ⁻¹⁰ | 60.16 | 0.99 | | | | | |
| D-20 | 2.62×10-9 | 51.54 | 0.99 | | | | | |

Table S2 Parameters of Arrhenius equation fitting curves.

Note: E_{η} is the viscous flow activation energy, which is not only the energy needed to overcome the action of the surrounding molecules when the macromolecule transitions to the hole, but also a measure of the melt viscosity-temperature sensitivity. That is, the larger the E_{η} , the fluidity is also worse, and the viscosity-temperature change is more sensitive.

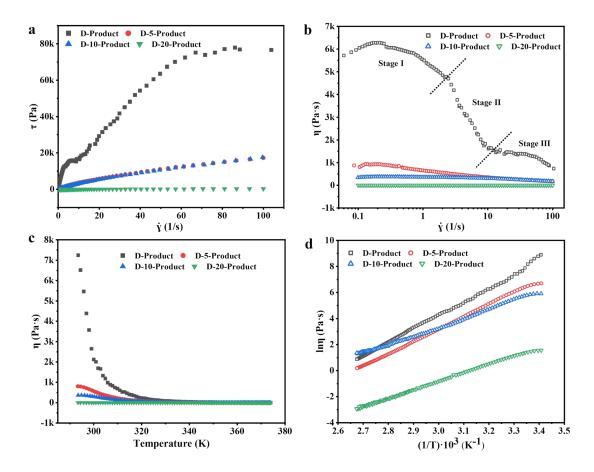


Fig. S1 Rheological properties test of D-product, D-5-product, D-10-product and D-20product: (a) Rheological curve (shear stress-shear rate); (b) Viscosity-shear rate dependence curve; (c) Viscosity-temperature dependence curve; (d) Viscosity-temperature sensitivity fitting curve.

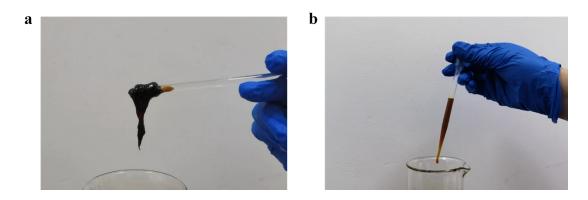


Fig. S2 Fluidity of (a) D-product and (b) D-10-product.

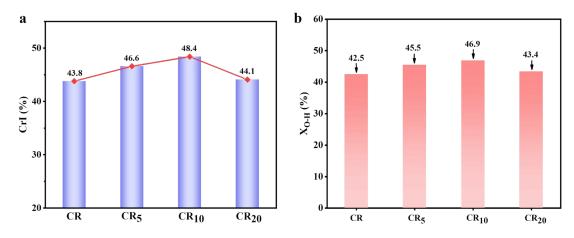


Fig. S3 Calculation results of CR, CR₅, CR₁₀ and CR₂₀: (a) CrI values; (b) X_{O-H} values.

For potassium carbonate, the main functional group is the vibration absorption peak of carbonate ion. The peaks at 1456 and 1377 cm⁻¹ correspond to the out-of-plane asymmetric stretching vibration of CO_3^{2-} . The peaks at 879 and 707 cm⁻¹ correspond to the out-of-plane asymmetric and in-plane symmetric bending vibration of CO₃²⁻, respectively.¹ For glycerol, the peak at 3288 cm⁻¹ corresponds to the stretching vibration of O-H. The peaks at 2929 and 2875 cm⁻¹ correspond to the asymmetric and symmetric stretching vibrations of -CH₂, respectively. After forming a binary DES system with K₂CO₃, the absorption frequency of the O-H stretching vibration shifts to the low wave number direction and the peak shape is broadened. This indicates the formation of intermolecular associative hydrogen bonding, where the oxygen atom of the CO_3^{2-} attracts the hydrogen proton in glycerol.² The same phenomenon can also be observed in the ternary system formed by introducing PEG-200. In addition, the relative intensity of the asymmetric stretching vibrational peak of -CH₂ is weakened, while the relative intensity of the symmetric stretching vibrational peak is enhanced. This may also be attributed to the presence of hydrogen bonding, which in turn affects the stretching vibration of -CH₂.

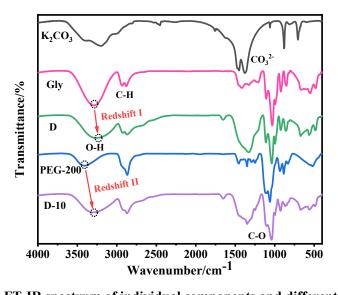


Fig.S4 FT-IR spectrum of individual components and different DESs.

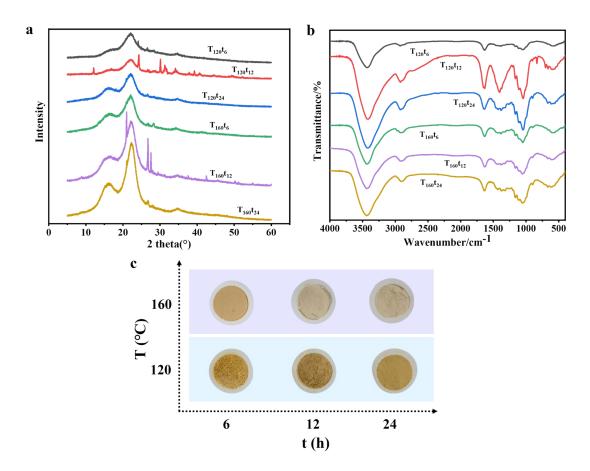


Fig. S5 Comparing tests: (a) XRD characterization; (b) FT-IR characterization; (c) Treatment effects of D-10 at different reaction temperatures and times.

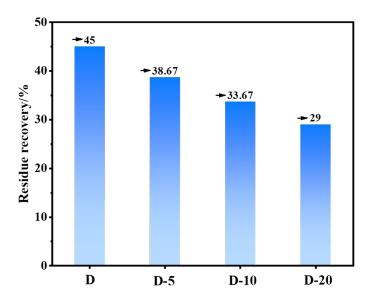


Fig. S6 Residue recovery of D, D-5, D-10 and D-20.

| | DESs | Treatment Conditions | | | Removal (%) | | Residue | | |
|-------------|---|-------------------------|------------|---|-------------|--------|-----------------|------------------------|------------|
| Biomass | (HBA/HBD) | Temperatur e (°C) | e Other Xy | | Xylan | Lignin | recovery (%) | Cellulose yield (%) | References |
| Wheat straw | K ₂ CO ₃ /Gly/PEG -200 | 160 | 24 | / | 81.93 | 96.37 | 33.67 | 73.65 | This work |
| Wheat straw | ChCl/LC | 120 | 6 | / | / | 60.1 | / | 64.9 | 34 |
| Wheat straw | ChCl/LC | 100 | 16 | / | / | / | 44.9 | / | 19 |
| Corn stalk | ChCl/LC | 100 | 16 | / | / | / | 32.2 | / | 19 |
| Corn stover | ChCl/OA/EG | 130 | 1 | High pressure | / | 75.27 | / | / | 20 |
| Bamboo | ChCl/Xylitol | 120 | 3 | 1 wt% H ₂ SO ₄ | 92.79 | 80.75 | 41.5 | / | 22 |
| Bamboo | ChCl/LC | 120 | 3 | Dewaxing | 74.81 | 94.39 | 49.18 | 91.06 | 24 |
| Eucommia | | | | | | | | | |
| ulmoides | ChCl/OA/EG | 100 | 3 | / | 79.7 | 65.6 | / | 84.0 | 37 |
| seed shells | | | | | | | | | |

Table S3 Performances of traditional and our designed ternary DESs treatment on LCB.

1 Hosein. Ghaedi, Payam. Kalhor, M. Zhao, *Frontiers of Environmental Science & Engineering*, 2022, 16, 7, 92.

2 P. C. Meng, J. Li, W. Liu, G. L. Yang, LWT - Food Science and Technology, 2023, 186, 115232.