

Supporting Information

Soluting-In, Soluting-Out, and Washing-Out Effects of Various Additives on Aqueous 1-Butanol Solutions

Nosaibah Ebrahimi, Ameneh Alidoosti, Rahmat Sadeghi*

Department of Chemistry, University of Kurdistan, Sanandaj, Iran

Table S1. The Liquid-liquid demixing data as cloud point temperature (T_{Cp}) against 1-butanol mass fraction (w_b) for ternary systems of 1-butanol in aqueous amino acid solutions at $P = 845$ hPa.

| Amino acid | Glycine | L-Alanine | L-Serine | L-Proline | S-Glutamine |
|---|---------|-----------|----------|-----------|-------------|
| T_{Cp} / K | w_b | | | | |
| 1-Butanol in aqueous 0.2 mol.kg ⁻¹ of amino acid | | | | | |
| 283.1 | 0.0796 | 0.0816 | 0.0784 | 0.0837 | 0.0845 |
| 293.1 | 0.0719 | 0.0723 | 0.0674 | 0.0742 | 0.0753 |
| 303.1 | 0.0646 | 0.0656 | 0.0624 | 0.0680 | 0.0686 |
| 313.1 | 0.0613 | 0.0623 | 0.0605 | 0.0635 | 0.0642 |
| 323.1 | 0.0610 | 0.0619 | 0.0589 | 0.0630 | 0.0636 |
| 333.1 | 0.0619 | 0.0627 | 0.0600 | 0.0634 | 0.0635 |
| 343.1 | 0.0646 | 0.0655 | 0.0630 | 0.0661 | 0.0666 |
| 353.1 | 0.0676 | 0.0685 | 0.0660 | 0.0688 | 0.0694 |
| 1-Butanol in aqueous 0.4 mol.kg ⁻¹ of amino acid | | | | | |
| 283.1 | 0.0709 | 0.0763 | 0.0683 | 0.0768 | |
| 293.1 | 0.0638 | 0.0662 | 0.0602 | 0.0668 | |
| 303.1 | 0.0592 | 0.0613 | 0.0567 | 0.0620 | |
| 313.1 | 0.0579 | 0.0594 | 0.0554 | 0.0599 | |
| 323.1 | 0.0567 | 0.0579 | 0.0549 | 0.0585 | |
| 333.1 | 0.0576 | 0.0590 | 0.0563 | 0.0595 | |
| 343.1 | 0.0614 | 0.0621 | 0.0597 | 0.0625 | |
| 353.1 | 0.0646 | 0.0653 | 0.0637 | 0.0654 | |
| 1-Butanol in aqueous 0.6 mol.kg ⁻¹ of amino acid | | | | | |
| 283.1 | 0.0650 | 0.0660 | 0.0610 | 0.0663 | |
| 293.1 | 0.0578 | 0.0584 | 0.0549 | 0.0590 | |
| 303.1 | 0.0541 | 0.0548 | 0.0514 | 0.0558 | |
| 313.1 | 0.0530 | 0.0540 | 0.0510 | 0.0545 | |
| 323.1 | 0.0524 | 0.0536 | 0.0502 | 0.0544 | |
| 333.1 | 0.0545 | 0.0553 | 0.0524 | 0.0556 | |
| 343.1 | 0.0585 | 0.0590 | 0.0565 | 0.0593 | |
| 353.1 | 0.0621 | 0.0629 | 0.0604 | 0.0633 | |

The standard uncertainty in w_b , m_s , T_{Cp} and P is $5 \cdot 10^{-4}$, $1 \cdot 10^{-1}$ mol.kg⁻¹, $4 \cdot 10^{-1}$ K and 10 hPa, respectively.

m_s : molality of the additive solute (here amino acids)

* Corresponding author. E-mail address: rahsadeghi@yahoo.com and rsadeghi@uok.ac.ir

Table S2. The Liquid-liquid demixing data as cloud point temperature (T_{cp}) against 1-butanol mass fraction (w_b) for ternary systems of 1-butanol in aqueous ionic liquid (IL) solutions at $P = 845$ hPa.

| IL | [C ₄ mim]Br | [C ₈ mim]Br |
|---|------------------------|------------------------|
| T_{cp} / K | w_b | |
| 1-Butanol in aqueous 0.2 mol.kg ⁻¹ of IL | | |
| 283.1 | 0.0923 | 0.2136 |
| 293.1 | 0.0852 | 0.2065 |
| 303.1 | 0.0789 | 0.2065 |
| 313.1 | 0.0769 | 0.2070 |
| 323.1 | 0.0773 | 0.2134 |
| 333.1 | 0.0780 | 0.2341 |
| 343.1 | 0.0851 | 0.2674 |
| 353.1 | 0.1014 | 0.3226 |
| 1-Butanol in aqueous 0.4 mol.kg ⁻¹ of IL | | |
| 283.1 | 0.0946 | 0.3618 |
| 293.1 | 0.0882 | 0.3633 |
| 303.1 | 0.0861 | 0.3706 |
| 313.1 | 0.0838 | 0.3813 |
| 323.1 | 0.0842 | 0.4048 |
| 333.1 | 0.0916 | 0.4395 |
| 343.1 | 0.1104 | 0.5044 |
| 353.1 | 0.1421 | |
| 1-Butanol in aqueous 0.6 mol.kg ⁻¹ of IL | | |
| 283.1 | 0.0963 | 0.4710 |
| 293.1 | 0.0913 | 0.4797 |
| 303.1 | 0.0904 | 0.4929 |
| 313.1 | 0.0967 | 0.5141 |
| 323.1 | 0.1061 | |
| 333.1 | 0.1399 | |
| 343.1 | 0.1917 | |
| 353.1 | 0.3571 | |

The standard uncertainty in w_b , m_s , T_{cp} and P is $5 \cdot 10^{-4}$, $1 \cdot 10^{-1} \text{mol.kg}^{-1}$, $4 \cdot 10^{-1} \text{K}$ and 10 hPa, respectively.

m_s : molality of the additive solute (here IL)

Table S3. The Liquid-liquid demixing data as cloud point temperature (T_{Cp}) against 1-butanol mass fraction (w_b) for ternary systems of 1-butanol in aqueous polymer solutions at $P = 845$ hPa.

| IL | PEG400 | PEG10000 |
|--------------------------------------|--------|----------|
| T_{Cp} / K | w_b | |
| 1-Butanol in aqueous 0.05 w/w of PEG | | |
| 283.1 | 0.0900 | 0.0880 |
| 293.1 | 0.0806 | 0.0814 |
| 303.1 | 0.0785 | 0.0783 |
| 313.1 | 0.0781 | 0.0763 |
| 323.1 | 0.0789 | 0.0758 |
| 333.1 | 0.0799 | 0.0757 |
| 343.1 | 0.0887 | 0.0759 |
| 353.1 | 0.0982 | 0.0730 |
| 1-Butanol in aqueous 0.10 w/w of PEG | | |
| 283.1 | 0.0904 | 0.0892 |
| 293.1 | 0.0817 | 0.0838 |
| 303.1 | 0.0814 | 0.0831 |
| 313.1 | 0.0818 | 0.0827 |
| 323.1 | 0.0874 | 0.0893 |
| 333.1 | 0.0987 | 0.0949 |
| 343.1 | 0.1135 | 0.0947 |
| 353.1 | 0.1415 | 0.0903 |
| 1-Butanol in aqueous 0.15 w/w of PEG | | |
| 283.1 | 0.0908 | 0.0870 |
| 293.1 | 0.0878 | 0.0832 |
| 303.1 | 0.0909 | 0.0895 |
| 313.1 | 0.0958 | 0.0999 |
| 323.1 | 0.1102 | 0.1177 |
| 333.1 | 0.1326 | 0.1206 |
| 343.1 | 0.1634 | 0.1148 |
| 353.1 | 0.2097 | 0.0997 |

The standard uncertainty in w_b , w_s , T_{Cp} and P is $5 \cdot 10^{-3}$, $1 \cdot 10^{-2}$, $4 \cdot 10^{-1}$ K and 10 hPa, respectively.

w_s : mass fraction of the additive solute (here PEG)

Table S4. The Liquid-liquid demixing data as cloud point temperature (T_{cp}) against 1-butanol mass fraction (w_b) for ternary systems of 1-butanol in aqueous 1-/2-propanol solutions at $P = 845$ hPa.

| IL | 1-Propanol | 2-Propanol |
|--|------------|------------|
| T_{cp} / K | w_b | |
| 1-Butanol in aqueous 0.05 w/w of 1-/2-propanol | | |
| 283.1 | 0.0700 | 0.0812 |
| 293.1 | 0.0668 | 0.0751 |
| 303.1 | 0.0642 | 0.0711 |
| 313.1 | 0.0616 | 0.0699 |
| 323.1 | 0.0636 | 0.0706 |
| 333.1 | 0.0676 | 0.0760 |
| 343.1 | 0.0746 | 0.0815 |
| 353.1 | 0.0877 | 0.0925 |
| 1-Butanol in aqueous 0.10 w/w of 1-/2-propanol | | |
| 283.1 | 0.0758 | 0.0820 |
| 293.1 | 0.0720 | 0.0808 |
| 303.1 | 0.0702 | 0.0834 |
| 313.1 | 0.0728 | 0.0875 |
| 323.1 | 0.0789 | 0.0950 |
| 333.1 | 0.0852 | 0.1073 |
| 343.1 | 0.1013 | 0.1221 |
| 353.1 | 0.1232 | 0.1490 |
| 1-Butanol in aqueous 0.15 w/w of 1-/2-propanol | | |
| 283.1 | 0.0836 | 0.1044 |
| 293.1 | 0.0869 | 0.1180 |
| 303.1 | 0.0920 | 0.1295 |
| 313.1 | 0.0991 | 0.1416 |
| 323.1 | 0.1106 | 0.1567 |
| 333.1 | 0.1280 | 0.1725 |
| 343.1 | 0.1520 | 0.1959 |
| 353.1 | 0.1844 | 0.2265 |

The standard uncertainty in w_b , w_s , T_{cp} and P is $5 \cdot 10^{-3}$, $1 \cdot 10^{-2}$, $4 \cdot 10^{-1}$ K and 10 hPa, respectively.

w_s : mass fraction of the additive solute (here 1-/2-propanol)

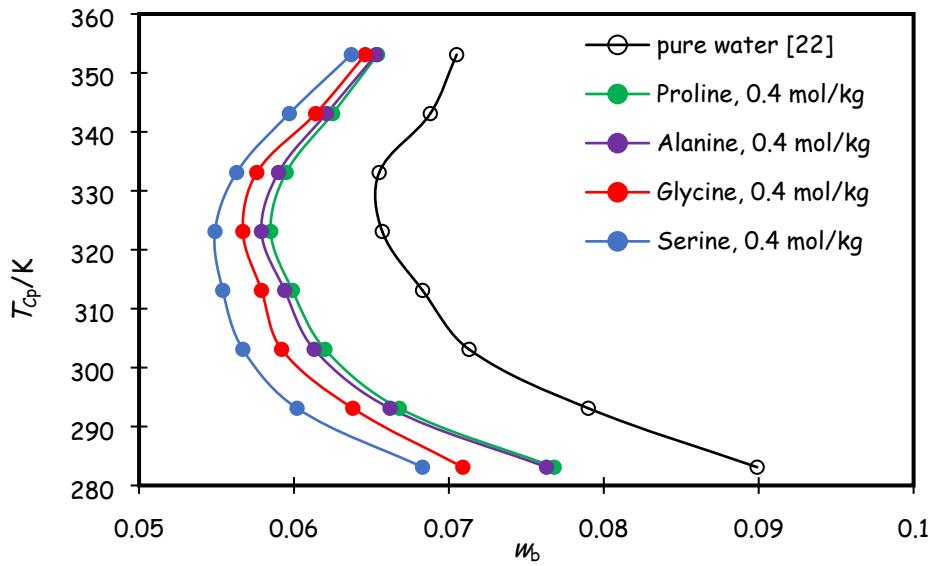


Figure S1. Cloud point temperature, T_{Cp} , against 1-butanol mass fraction, w_b , for the binary system of 1-butanol in water and the ternary systems of 1-butanol in aqueous solutions of 0.4 mol.kg⁻¹ of the amino acids investigated.

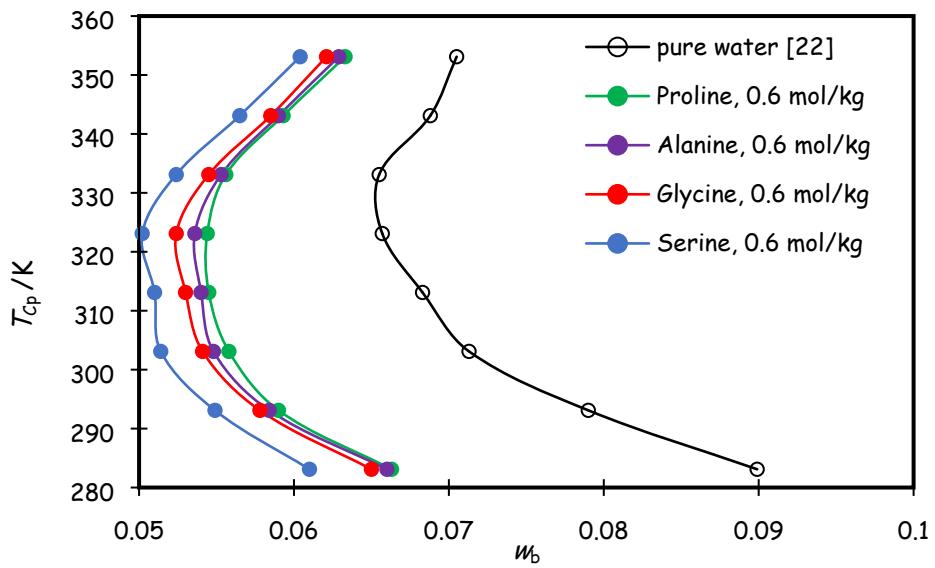


Figure S2. Cloud point temperature, T_{Cp} , against 1-butanol mass fraction, w_b , for the binary system of 1-butanol in water and the ternary systems of 1-butanol in aqueous solutions of 0.6 mol.kg⁻¹ of the amino acids investigated.

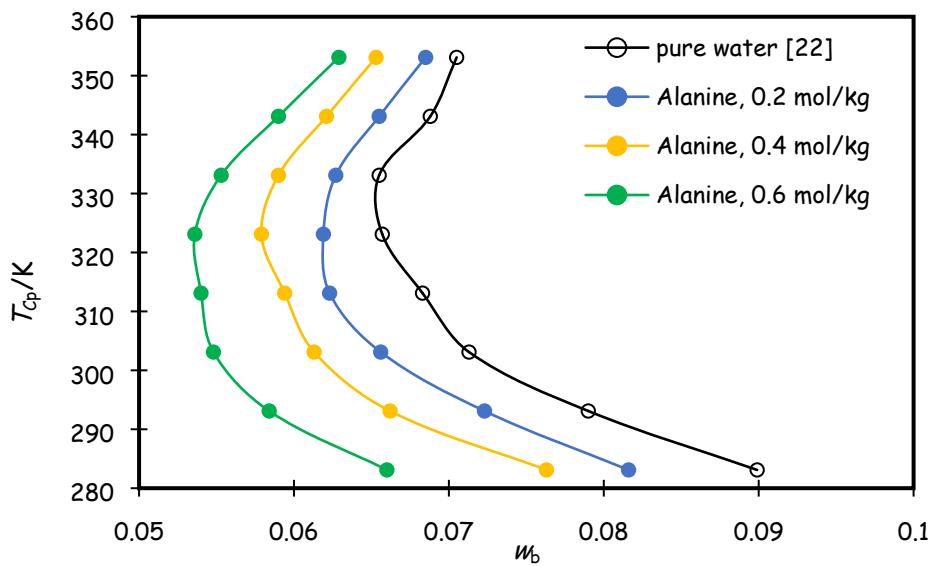


Figure S3. Cloud point temperature, T_{Cp} , against 1-butanol mass fraction, w_b , for the binary system of 1-butanol in water and the ternary systems of 1-butanol in aqueous solutions of 0.2, 0.4, and 0.6 mol. kg^{-1} of the amino acid alanine.

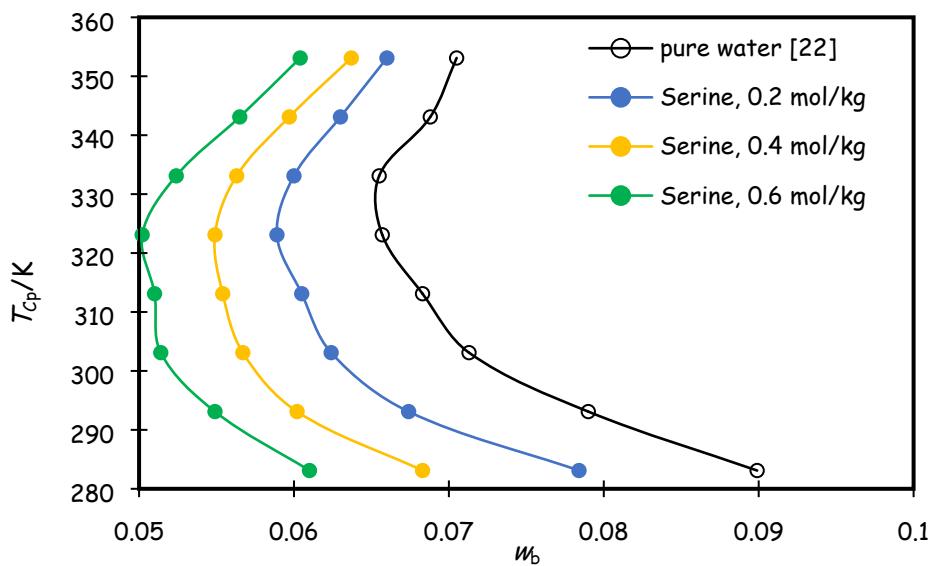


Figure S4. Cloud point temperature, T_{Cp} , against 1-butanol mass fraction, w_b , for the binary system of 1-butanol in water and the ternary systems of 1-butanol in aqueous solutions of 0.2, 0.4, and 0.6 mol. kg^{-1} of the amino acid serine.

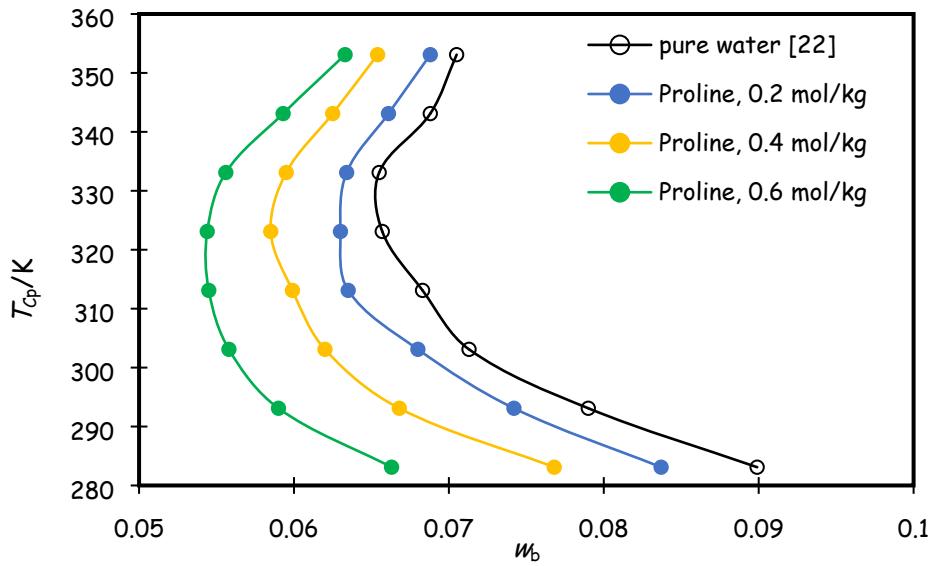


Figure S5. Cloud point temperature, T_{Cp} , against 1-butanol mass fraction, w_b , for the binary system of 1-butanol in water and the ternary systems of 1-butanol in aqueous solutions of 0.2, 0.4, and 0.6 mol.kg⁻¹ of the amino acid proline.

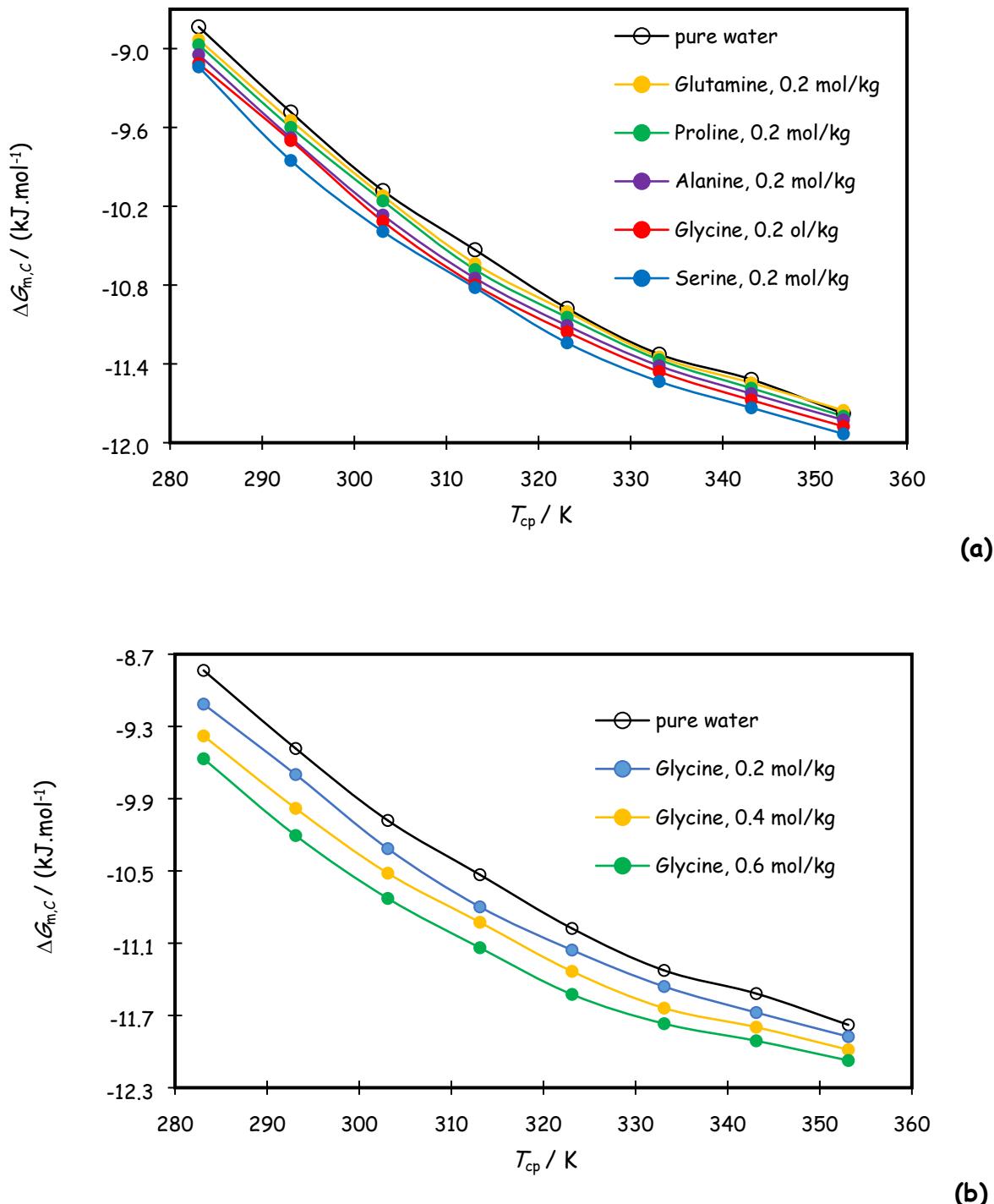


Figure S6. Gibbs free energy of clouding, $\Delta G_{m,C}$, against cloud point temperature, T_{Cp} , for **(a)** 1-butanol in aqueous solutions of $0.2 \text{ mol} \cdot \text{kg}^{-1}$ of the amino acids investigated; and **(b)** 1-butanol in aqueous solutions of 0.2 , 0.4 , and $0.6 \text{ mol} \cdot \text{kg}^{-1}$ of the amino acid glycine.

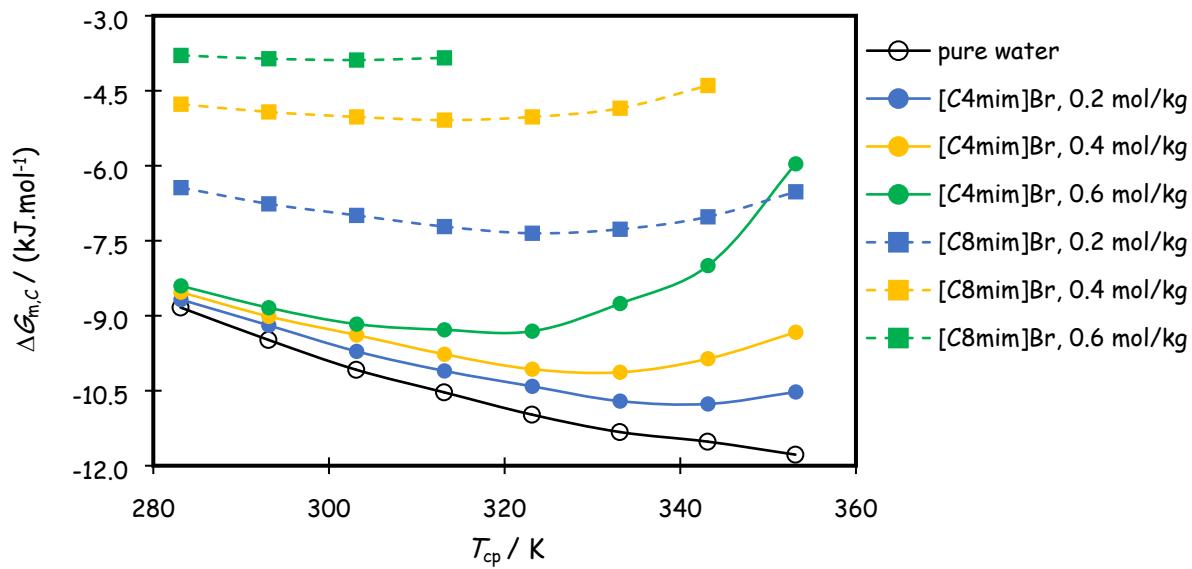


Figure S7. Gibbs free energy of clouding, $\Delta G_{m,C}$, against cloud point temperature, T_{Cp} , for 1-butanol in aqueous solutions of 0.2, 0.4, and 0.6 mol.kg⁻¹ of the ILs investigated.

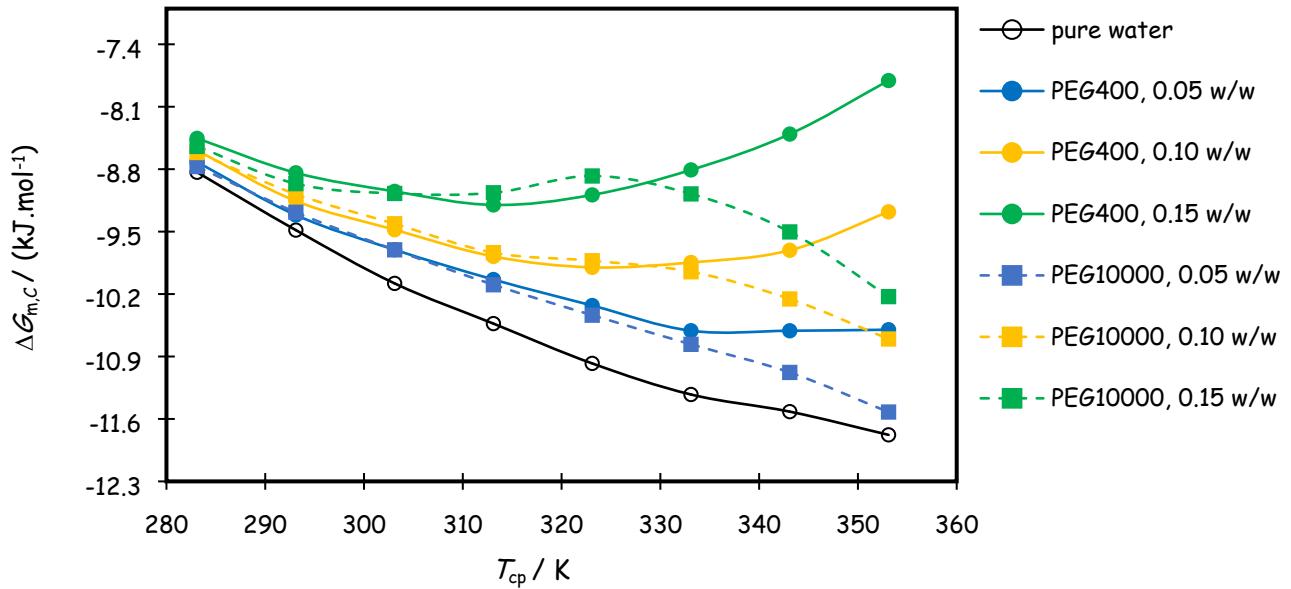


Figure S8. Gibbs free energy of clouding, $\Delta G_{m,C}$, against cloud point temperature, T_{Cp} , for 1-butanol in aqueous solutions of 0.05, 0.10, and 0.15 w/w of the polymers investigated.

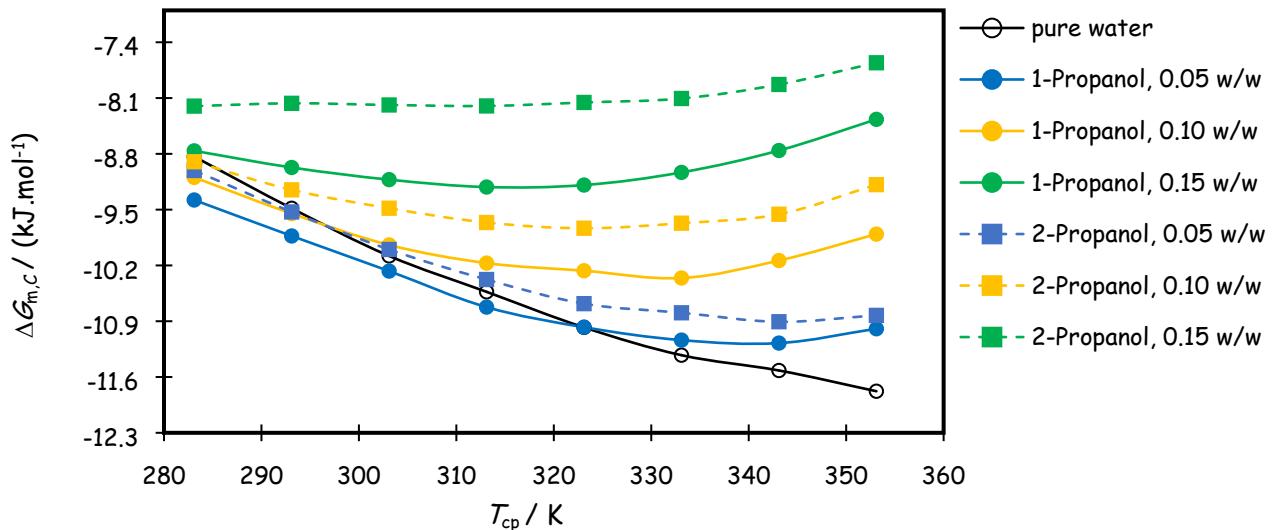


Figure S9. Gibbs free energy of clouding, $\Delta G_{m,C}$, against cloud point temperature, T_{Cp} , for 1-butanol in aqueous solutions of 0.05, 0.10, and 0.15 w/w of 1-/2-propanol.

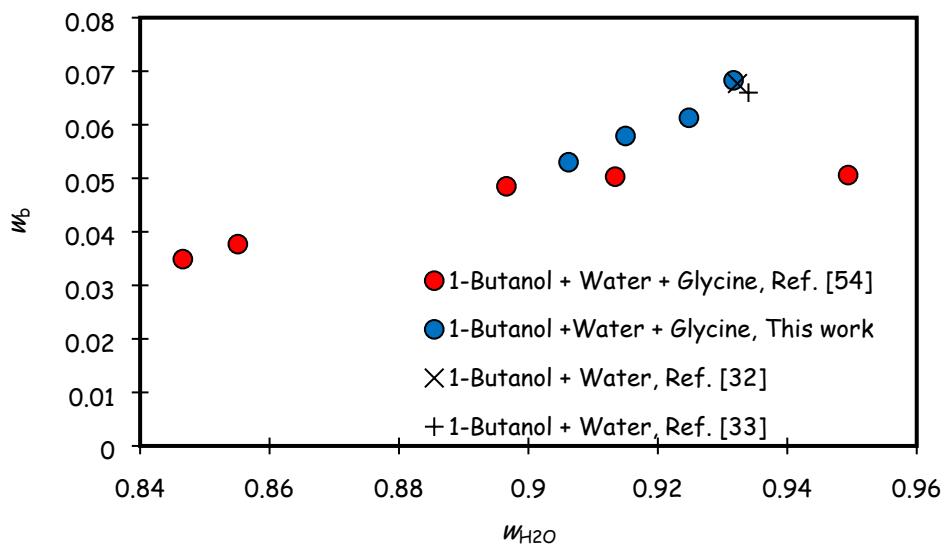


Figure S10. Comparison of liquid-liquid phase diagram data obtained by us and literature,⁵⁴ for ternary mixtures of 1-butanol + water + glycine, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H2O}), at 313.1 K.

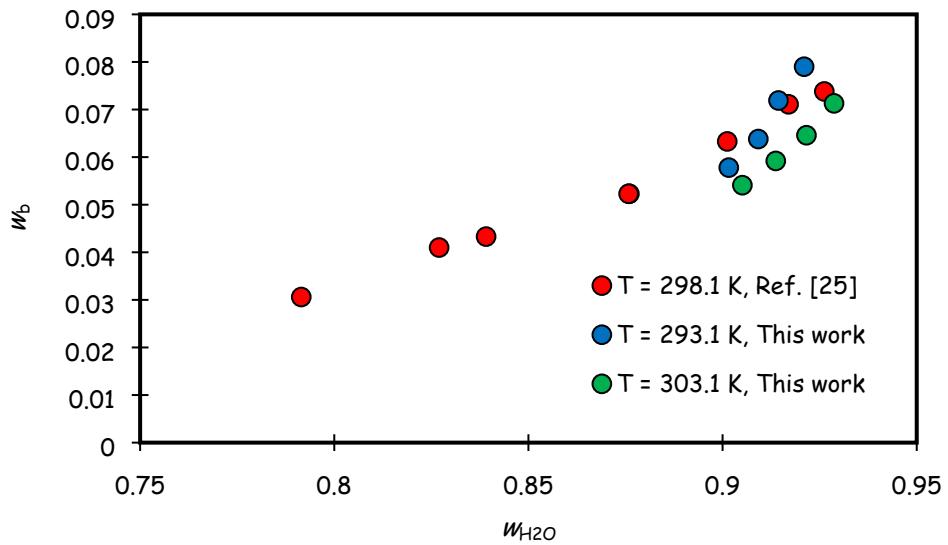


Figure S11. Comparison of liquid-liquid phase diagram data obtained by us at 293.1 and 303.1K, and literature at 298.1 K,²⁵ for ternary mixtures of 1-butanol + water + glycine, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}).

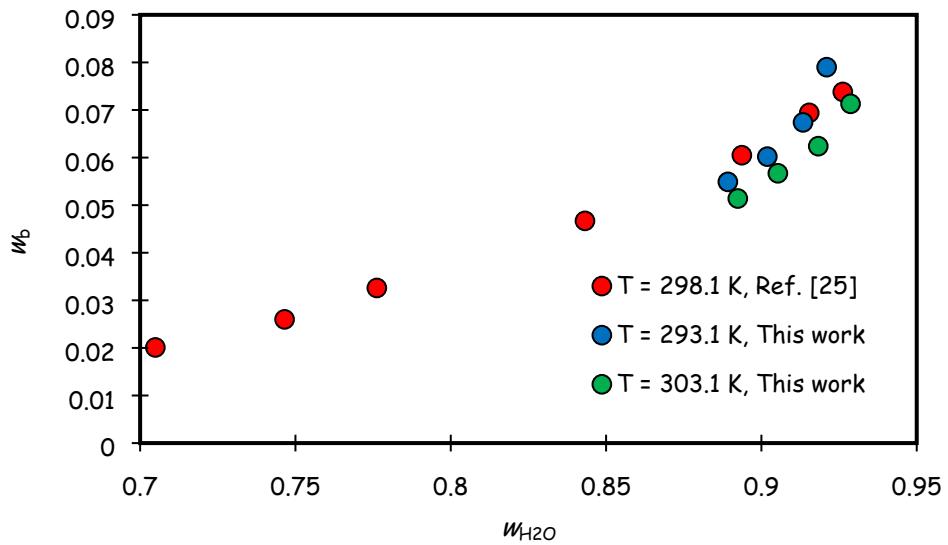


Figure S12. Comparison of liquid-liquid phase diagram data obtained by us at 293.1 and 303.1K, and literature at 298.1 K,²⁵ for ternary mixtures of 1-butanol + water + L-serine, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}).

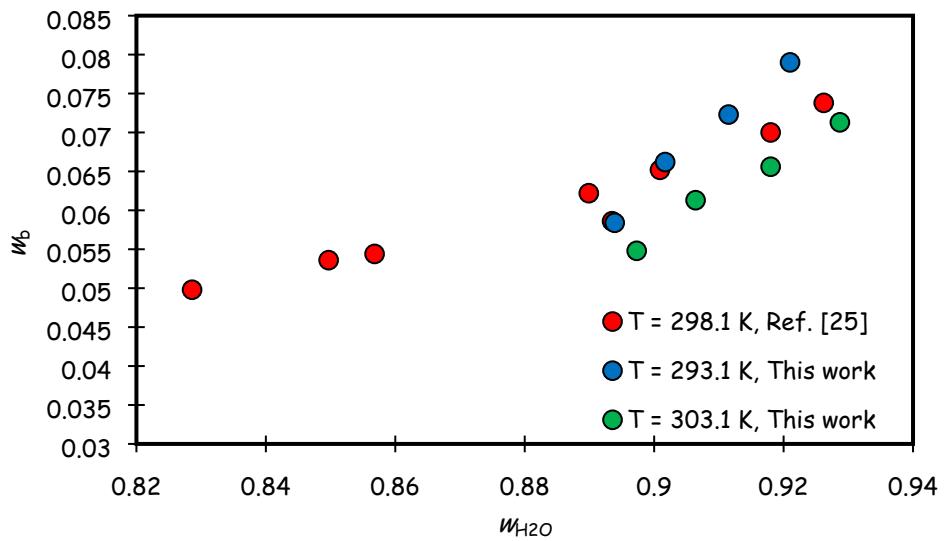


Figure S13. Comparison of liquid-liquid phase diagram data obtained by us at 293.1 and 303.1 K, and literature at 298.1 K,²⁵ for ternary mixtures of 1-butanol + water + L-alanine, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}).

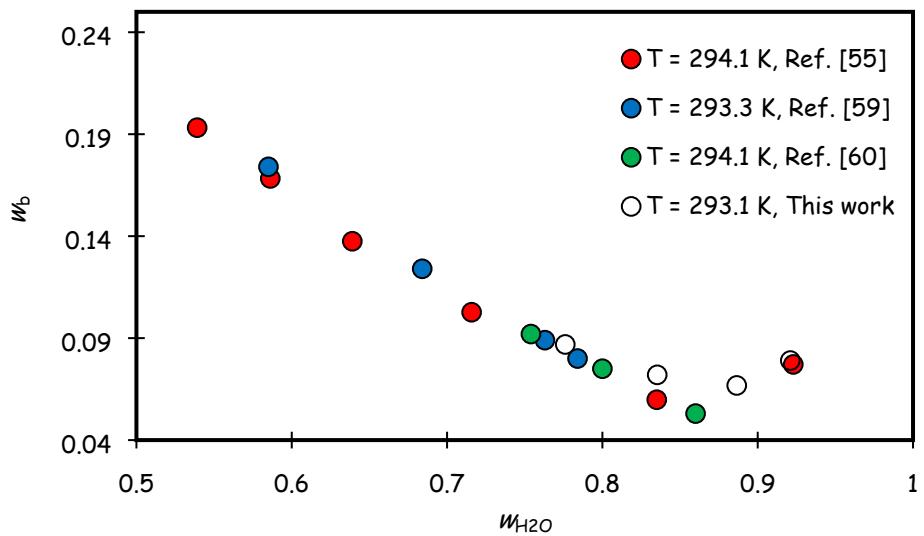


Figure S14. Comparison of liquid-liquid phase diagram data obtained by us at 293.1, and literature at 293.3 and 294.1 K,^{55,59,60} for ternary mixtures of 1-butanol + water + 1-propanol, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}).

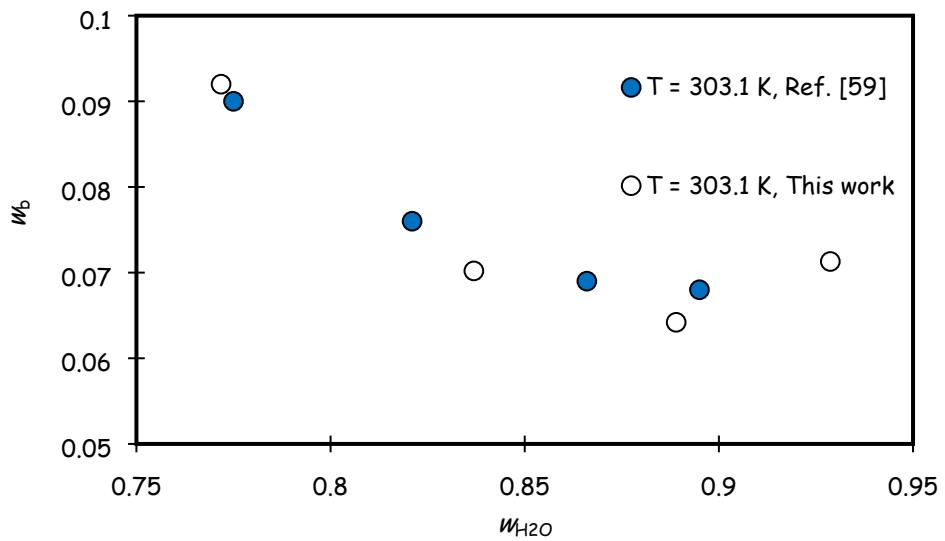


Figure S15. Comparison of liquid-liquid phase diagram data obtained by us and literature,⁵⁹ for ternary mixtures of 1-butanol + water + 1-propanol, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}), at 303.1 K.

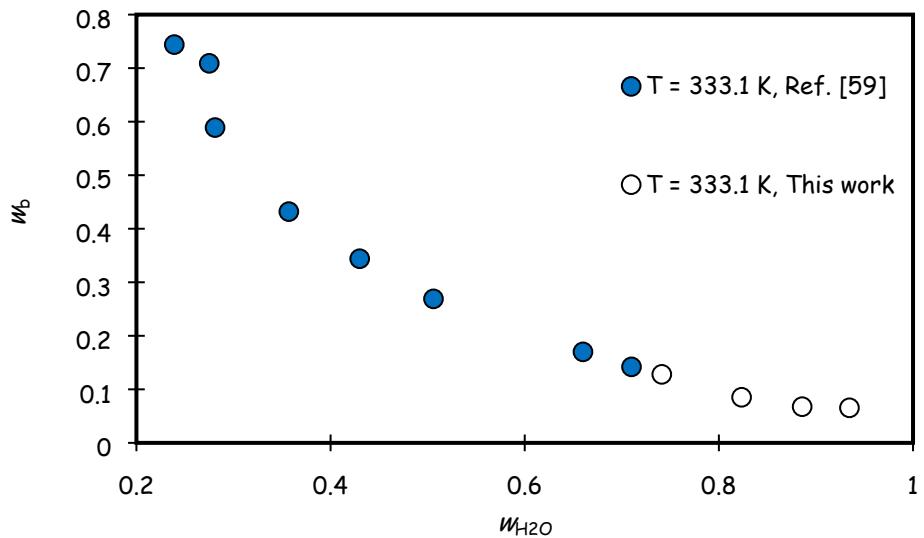


Figure S16. Comparison of liquid-liquid phase diagram data obtained by us and literature,⁵⁹ for ternary mixtures of 1-butanol + water + 1-propanol, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}), at 333.1 K.

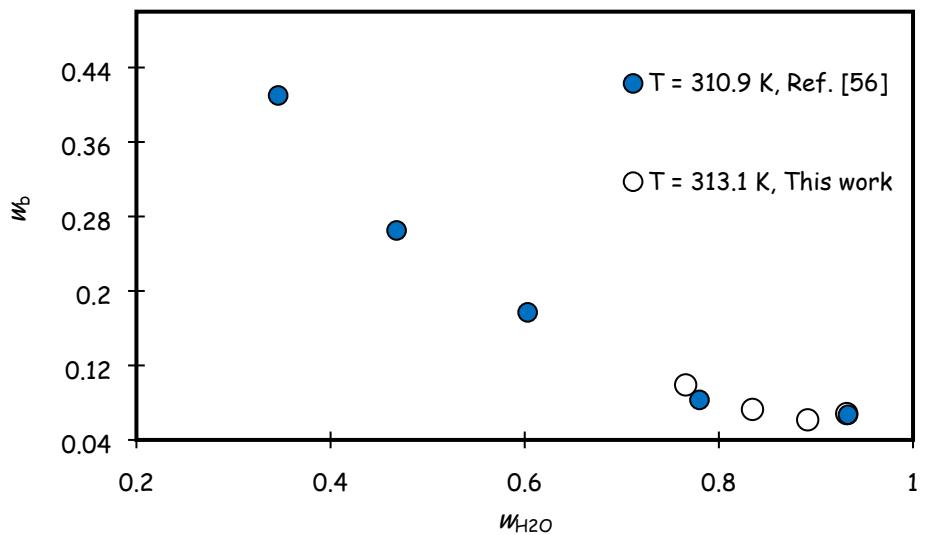


Figure S17. Comparison of liquid-liquid phase diagram data obtained by us at 313.1, and literature at 310.9 K,⁵⁶ for ternary mixtures of 1-butanol + water + 1-propanol, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}).

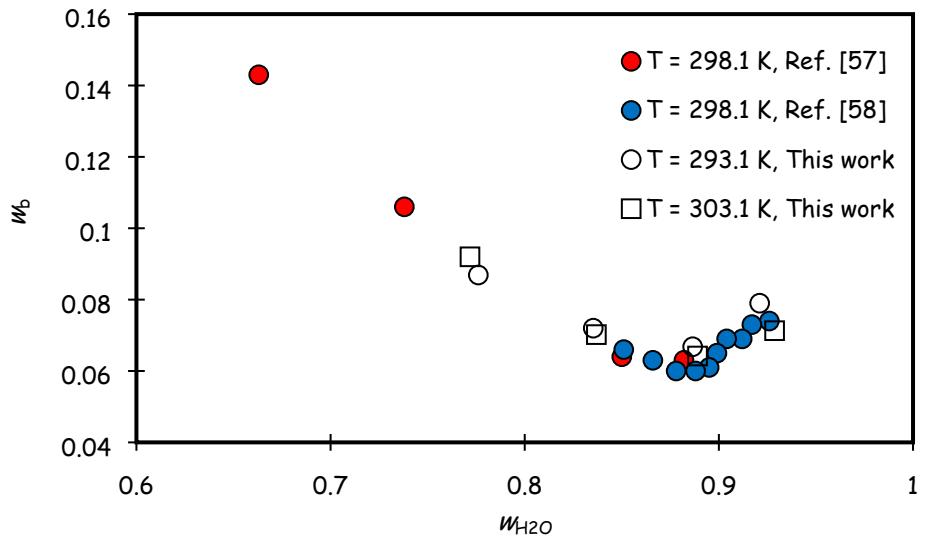


Figure S18. Comparison of liquid-liquid phase diagram data obtained by us at 293.1 and 303.1 K, and literature at 298.1 K,^{57,58} for ternary mixtures of 1-butanol + water + 1-propanol, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}).

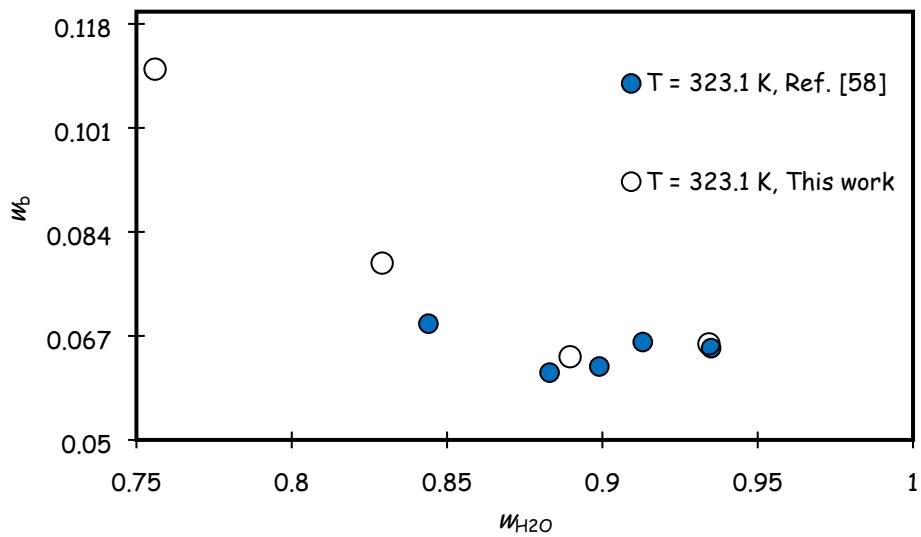


Figure S19. Comparison of liquid-liquid phase diagram data obtained by us and literature,⁵⁸ for ternary mixtures of 1-butanol + water + 1-propanol, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}), at 323.1 K.

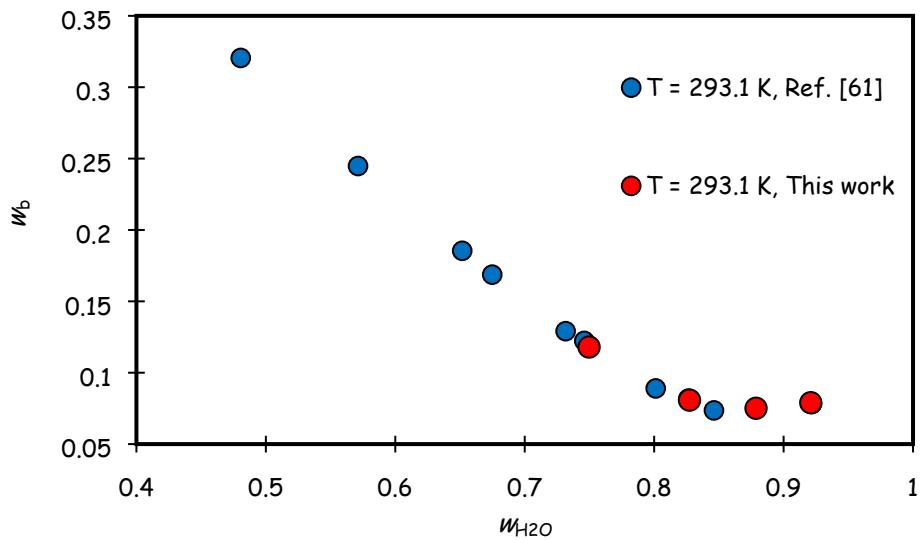


Figure S20. Comparison of liquid-liquid phase diagram data obtained by us and literature,⁶¹ for ternary mixtures of 1-butanol + water + 2-propanol, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}), at 293.1 K.

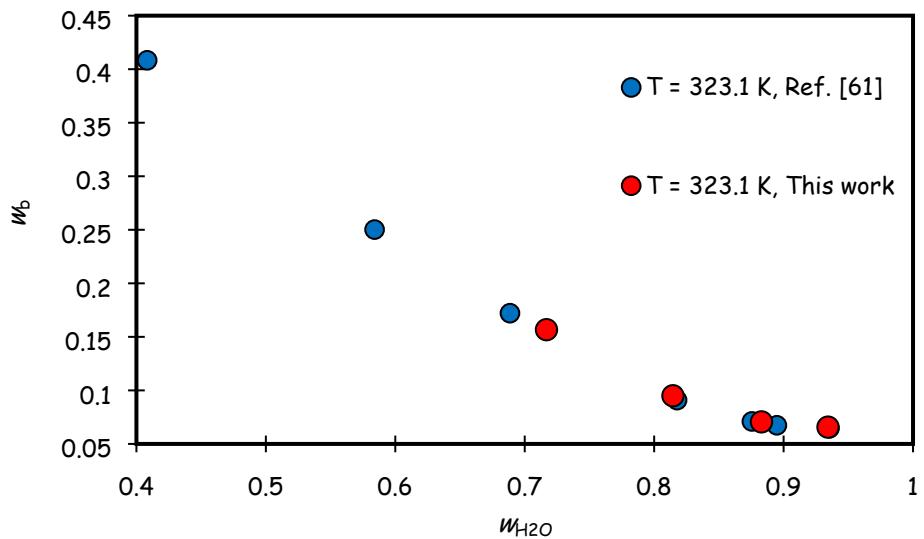


Figure S21. Comparison of liquid-liquid phase diagram data obtained by us and literature,⁶¹ for ternary mixtures of 1-butanol + water + 2-propanol, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}), at 323.1 K.

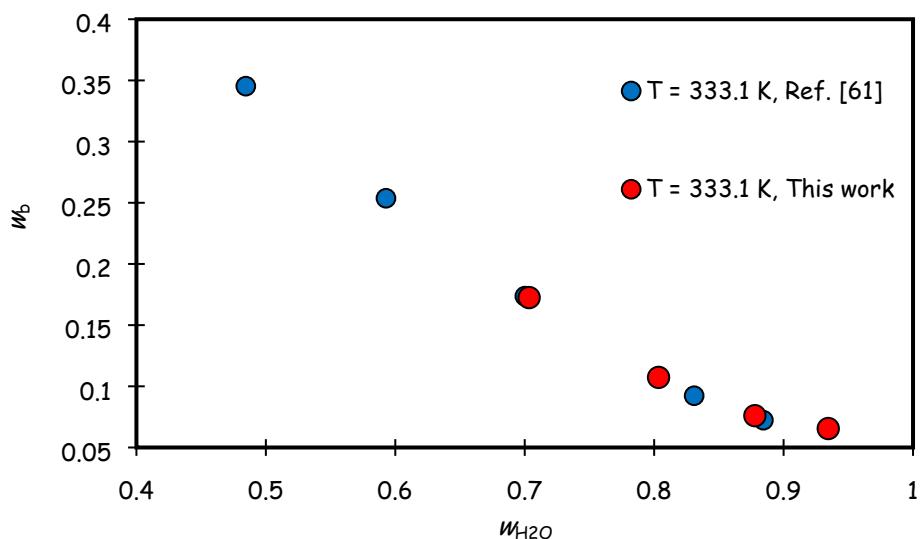


Figure S22. Comparison of liquid-liquid phase diagram data obtained by us and literature,⁶¹ for ternary mixtures of 1-butanol + water + 2-propanol, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}), at 333.1 K.

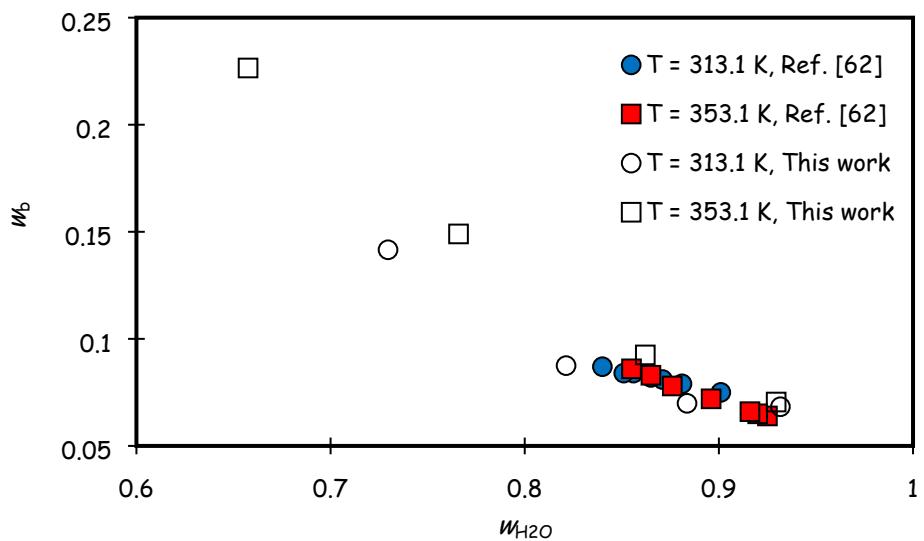


Figure S23. Comparison of liquid-liquid phase diagram data obtained by us and literature,⁶² for ternary mixtures of 1-butanol + water + 2-propanol, as 1-butanol mass fraction (w_b) against water mass fraction (w_{H_2O}), at 313.1 and 353.1 K.