Supporting Information

Measurements and Correlation of Water Activity in Aqueous Solutions Containing Diphenhydramine-Hydrochloride Drug, (D+)-Galactose, (D-)-Fructose, (D+)-Lactose and Sucrose at 298.15 K

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S.1. NRTL equation

The activity coefficient equation of the solvent for NRTL model [40] is as follow for ternary system:

$$\ln \gamma_m^{*,NRTL} = \frac{(\exp(-\alpha_{sm}\tau_{sm})x_s + \exp(-\alpha_{Em}\tau_{Em})(x_a + x_c))(\exp(-\alpha_{sm}\tau_{sm})x_s\tau_{sm} + (\exp(-\alpha_{Em}\tau_{Em})\tau_{Em}(x_a + x_c)}{(x_m + \exp(-\alpha_{sm}\tau_{sm})x_s + \exp(-\alpha_{Em}\tau_{Em})(x_a + x_c))^2}$$
$$+ \frac{\exp(-\alpha_{ms}\tau_{ms})x_s(x_s\tau_{ms} + \exp(-\alpha_{Es}\tau_{Es})(x_a + x_c)(\tau_{ms} - \tau_{Es}))}{(x_s + \exp(-\alpha_{ms}\tau_{ms})x_m + \exp(-\alpha_{Es}\tau_{Es})(x_a + x_c))^2}$$
$$+ \frac{\exp(-\alpha_{mE}\tau_{mE})x_a(x_c\tau_{mE} + \exp(-\alpha_{sE}\tau_{sE})x_s)(\tau_{mE} - \tau_{sE}))}{(x_c + \exp(-\alpha_{sE}\tau_{sE})x_s + \exp(-\alpha_{mE}\tau_{mE})x_m)^2} + \frac{\exp(-\alpha_{mE}\tau_{mE})x_c(x_a\tau_{mE} + \exp(-\alpha_{sE}\tau_{sE})x_s)(\tau_{mE} - \tau_{sE}))}{(x_a + \exp(-\alpha_{sE}\tau_{sE})x_s + \exp(-\alpha_{mE}\tau_{mE})x_m)^2} \quad (S.1)$$

Here, x is mole fraction; subscripts E, m and s denote DPH-HCl, water and saccharide, respectively; α_{mE}, α_{Em}, α_{sE}, α_{Es}, α_{sm} and α_{ms} are nonrandomness factors and in this work its values are set to $\alpha_{mE} = 0.4$, $\alpha_{Em} = 0.4$, $\alpha_{sE} = 0.1$, $\alpha_{Es} = 0.1$, $\alpha_{sm} = 0.4$ and $\alpha_{ms} = 0.4$ for obtaining the better fitting quality. τ_{mE}, τ_{Em}, τ_{sE}, τ_{Es}, τ_{sm} and τ_{ms} are the adjustable parameters of NRTL model.

S.2. NRF-NRTL equation

The activity coefficient equation of the solvent for NRF-NRTL model [41] is as follow for ternary system:

$$
\begin{aligned}
\ln \gamma_m^{*,NRF-NRTL} = {} & \frac{(\exp(-\alpha_{sm}\tau_{sm})x_s + \exp(-\alpha_{Em}\tau_{Em})x_a + \exp(-\alpha_{Em}\tau_{Em})x_c)(\exp(-\alpha_{sm}\tau_{sm})x_s\tau_{sm} + \exp(-\alpha_{Em}\tau_{Em})x_a\tau_{Em} + \exp(-\alpha_{Em}\tau_{Em})x_c\tau_{Em})}{(x_m + \exp(-\alpha_{sm}\tau_{sm})x_s + \exp(-\alpha_{Em}\tau_{Em})x_a + \exp(-\alpha_{Em}\tau_{Em})x_c)^2} \\
& - \frac{(x_a + x_c + x_s)(x_s\tau_{sm} + x_a\tau_{Em} + x_c\tau_{Em})}{(x_a + x_c + x_s + x_m)^2} \\
& + \frac{(\exp(-\alpha_{ms}\tau_{ms})(x_s\tau_{ms} + \exp(-\alpha_{Es}\tau_{Es})x_a\tau_{ms} + \exp(-\alpha_{Es}\tau_{Es})x_c\tau_{ms} - \exp(-\alpha_{Es}\tau_{Es})x_a\tau_{Es} - \exp(-\alpha_{Es}\tau_{Es})x_c\tau_{Es})}{(x_s + \exp(-\alpha_{ms}\tau_{ms})x_m + \exp(-\alpha_{Es}\tau_{Es})x_a + \exp(-\alpha_{Es}\tau_{Es})x_c)^2} \\
& - \frac{x_s(x_a\tau_{ms} + x_c\tau_{ms} + x_s\tau_{ms} - x_a\tau_{Es} - x_c\tau_{Es})}{(x_a + x_c + x_s + x_m)^2} + \frac{(\exp(-\alpha_{mE}\tau_{mE}x_a)(x_c\tau_{mE} + \exp(-\alpha_{sE}\tau_{sE})x_s\tau_{mE} - \exp(-\alpha_{sE}\tau_{sE})x_s\tau_{sE})}{(x_c + \exp(-\alpha_{sE}\tau_{sE})x_s + \exp(-\alpha_{mE}\tau_{mE})x_m)^2} \\
& - \frac{x_a(x_a\tau_{mE} + x_c\tau_{mE} + x_s\tau_{mE} - x_s\tau_{sE})}{(x_a + x_c + x_s + x_m)^2} + \frac{(\exp(-\alpha_{mE}\tau_{mE}x_c)(x_a\tau_{mE} + \exp(-\alpha_{sE}\tau_{sE})x_s\tau_{mE} - \exp(-\alpha_{sE}\tau_{sE})x_s\tau_{sE})}{(x_a + \exp(-\alpha_{sE}\tau_{sE})x_s + \exp(-\alpha_{mE}\tau_{mE})x_m)^2} \\
& - \frac{x_c(x_a\tau_{mE} + x_c\tau_{mE} + x_s\tau_{mE} - x_s\tau_{sE})}{(x_a + x_c + x_s + x_m)^2}
\end{aligned}
\qquad \text{(S.2)}
$$

where the nonrandomness factor values are set to $\alpha_{mE} = 0.4$, $\alpha_{Em} = 0.4$, $\alpha_{sE} = 0.1$, $\alpha_{Es} = 0.1$, $\alpha_{sm} = 0.4$ and $\alpha_{ms} = 0.4$ for obtaining the better fitting quality in this work. τ_{mE}, τ_{Em}, τ_{sE}, τ_{Es}, τ_{sm} and τ_{ms} are the adjustable parameters of NRF-NRTL model.

S.3. mNRTL equation

The activity coefficient equation of the solvent for mNRTL model [42] is as follow for ternary system:

$$\ln \gamma_m^{*,mNRTL} = -\frac{\begin{aligned}&x_c(x_a^3\tau_{mE}+\exp(-\alpha_{sE}\tau_{sE})^2(x_s^3\tau_{mE}-x_s^3\tau_{sE}+x_a x_s^2\tau_{mE}-x_a x_s^2\tau_{sE}+x_c x_s^2\tau_{sE})+x_a^2 x_s\tau_{mE}\\&+\exp(-\alpha_{sE}\tau_{sE})(2x_a x_s^2\tau_{mE}+2x_a^2 x_s\tau_{mE}-x_a x_s^2\tau_{sE}-x_a^2 x_s\tau_{sE}-x_c x_s^2\tau_{sE}+x_a x_c x_s\tau_{sE})\\&+\exp(-\alpha_{mE}\tau_{mE})(-x_a x_s^2\tau_{mE}-2x_a^2 x_s\tau_{mE}-x_a^3\tau_{mE}-x_a x_m^2\tau_{mE}+x_a x_s^2\tau_{sE}+x_a^2 x_s\tau_{sE}-x_c x_s^2\tau_{sE}-x_a x_c x_s\tau_{sE}-2x_c x_s x_m\tau_{sE})\\&+\exp(-\alpha_{mE}\tau_{mE})^2(x_a x_m^2\tau_{mE}+x_s x_m^2\tau_{mE}-x_s x_m^2\tau_{sE})-x_a x_c x_s\tau_{sE}+\exp(-\alpha_{sE}\tau_{sE})\exp(-\alpha_{mE}\tau_{mE})(-x_s^3\tau_{mE}\\&+x_s^3\exp(-\alpha_{sE}\tau_{sE})-2x_a x_s^2\tau_{mE}-x_a^2 x_s\tau_{mE}+x_a x_s^2\tau_{sE}+x_c x_s^2\tau_{sE}-x_s x_m^2\tau_{mE}+x_s x_m^2\tau_{sE}+x_a x_c x_s\tau_{sE}+2x_c x_s x_m\tau_{sE})\end{aligned}}{(x_a+x_s+x_m)^2(x_a+\exp(-\alpha_{sE}\tau_{sE})x_s+\exp(-\alpha_{mE}\tau_{mE})x_m)^2}$$

$$+\frac{(\exp(-\alpha_{sm}\tau_{sm})x_s+\exp(-\alpha_{Em}\tau_{Em})(x_a+x_c))(\exp(-\alpha_{sm}\tau_{sm})x_s\tau_{sm}+\exp(-\alpha_{Em}\tau_{Em})(x_a\tau_{Em}+x_c\tau_{Em}))}{(x_m+\exp(-\alpha_{sm}\tau_{sm})(x_a+x_c))^2}$$

$$+\frac{\exp(-\alpha_{ms}\tau_{ms})x_s(x_s\tau_{ms}+\exp(-\alpha_{Es}\tau_{Es})(x_a\tau_{ms}+x_c\tau_{ms}-x_a\tau_{Es}-x_c\tau_{Es})}{(x_s+\exp(-\alpha_{ms}\tau_{ms})x_m+\exp(-\alpha_{Es}\tau_{Es})(x_a+x_c))^2}$$

$$-\frac{\begin{aligned}&x_a(x_c^3\tau_{mE}+\exp(-\alpha_{sE}\tau_{sE})^2(x_s^3\tau_{mE}-x_s^3\tau_{sE}+x_c x_s^2\tau_{mE})+x_c^2 x_s(\tau_{mE}-\tau_{sE})\\&+\exp(-\alpha_{sE}\tau_{sE})(2x_c x_s^2\tau_{mE}+2x_c^2 x_s\tau_{mE}-2x_c x_s^2\tau_{sE})+\exp(-\alpha_{mE}\tau_{mE})(x_c x_s^2\tau_{mE}-2x_c^2 x_s\tau_{mE}-x_c^3\tau_{mE}\\&-x_c x_m^2\tau_{mE}-2x_c x_s x_m\tau_{sE})+\exp(-\alpha_{mE}\tau_{mE})^2(x_c x_m^2\tau_{mE}+x_s x_m^2\tau_{mE}-x_s x_m^2\tau_{sE})+\exp(-\alpha_{sE}\tau_{sE})\exp(-\alpha_{mE}\tau_{mE})(-x_s^3\tau_{mE}\\&+x_s^3\tau_{sE}-2x_c x_s^2\tau_{mE}-x_c^2 x_s\tau_{mE}+2x_c x_s^2\tau_{sE}+x_c^2 x_s\tau_{sE}-x_s x_m^2\tau_{mE}+x_s x_m^2\tau_{sE}+2x_c x_s x_m\tau_{sE})\end{aligned}}{(x_c+x_s+x_m)^2(x_c+\exp(-\alpha_{sE}\tau_{sE})x_s+\exp(-\alpha_{mE}\tau_{mE})x_m)^2}$$

(S.3)

where the nonrandomness factor values are set to $\alpha_{mE} = 0.4$, $\alpha_{Em} = 0.4$, $\alpha_{sE} = 0.4$, $\alpha_{Es} = 0.4$, $\alpha_{sm} = 0.1$ and $\alpha_{ms} = 0.1$ for obtaining the better fitting quality in this work. τ_{mE}, τ_{Em}, τ_{sE}, τ_{Es}, τ_{sm} and τ_{ms} are the adjustable parameters of mNRTL model.

S.4. Wilson equation

The activity coefficient equation of the solvent for Wilson model [43] is as follow for ternary system:

$$\ln\gamma_m^{*,Wilson} = -C\ln(x_m + \exp(-\frac{E_{sm}}{CRT})x_s + \exp(-\frac{E_{Em}}{CRT})(x_a + x_c) - \frac{Cx_m(x_a + x_c + x_s - \exp(-\frac{E_{sm}}{CRT})x_s - \exp(-\frac{E_{Em}}{CRT})(x_a + x_c)}{x_m + \exp(-\frac{E_{sm}}{CRT})x_s + \exp(-\frac{E_{Em}}{CRT})(x_a + x_c)} + \frac{Cx_s(x_s - \exp(-\frac{E_{ms}}{CRT})(x_a + x_c + x_s) + \exp(-\frac{E_{Es}}{CRT})(x_a + x_c)}{x_s + \exp(-\frac{E_{ms}}{CRT})x_m + \exp(-\frac{E_{Es}}{CRT})(x_a + x_c)} + \frac{Cx_a(x_c + \exp(-\frac{E_{sE}}{CRT})x_s - \exp(-\frac{E_{mE}}{CRT})(x_c + x_s)}{(x_c + x_s + x_m)(x_c + \exp(-\frac{E_{sE}}{CRT})x_s + \exp(-\frac{E_{mE}}{CRT})x_m} + \frac{Cx_c(x_a - \exp(-\frac{E_{mE}}{CRT})x_a + x_s(\exp(-\frac{E_{sE}}{CRT}) - \exp(-\frac{E_{mE}}{CRT}))}{(x_a + x_s + x_m)(x_a + \exp(-\frac{E_{sE}}{CRT})x_s + \exp(-\frac{E_{mE}}{CRT})x_m} \quad (S.4)$$

Here, E_{mE}, E_{Em}, E_{sE}, E_{Es}, E_{sm} and E_{ms} are the adjustable parameters of Wilson model; *R* is the universal constant of gases; *C* is the coordination number of the model which was set to 10.

S.5. TNRF-mNRTLequation

The activity coefficient equation of the solvent for TNRF-mNRTL model [44] is as follow for ternary system:

$$
\begin{aligned}
\ln \gamma_m^{*,TNRF-mNRTL} &= \lambda_{Em} x_m Q_1 + \lambda_{sm} x_m Q_1 + x_m (\lambda_{Em} Q_1 - \lambda_{Em} x_m Q_1 - \lambda_{Em} x_m Q_2 - \lambda_{sm} x_s Q_1 \\
&- \lambda_{sm} x_s Q_1 Q_3 - \lambda_{sm} x_s Q_2) + \frac{z_a z_c x_h}{(z_a + z_c)(z_a z_c x_h + x_m + X_s)} [-\lambda_{mE} z_a z_c x_h (-1 + Q_4 z_a z_c x_h + x_m Q_4 \\
&+ x_s Q_4) + \lambda_{mE} z_a z_c x_h (-Q_4 z_a z_c x_h - Q_5 z_a z_c x_h \beta_{mE} + Q_4 - x_m Q_4 - x_m \beta_{mE} Q_5 - x_s Q_4 - x_s Q_3 Q_4 \\
&- x_s \beta_{mE} Q_5) - \lambda_{Es} X_s (Q_6 z_a z_c x_h + X_s Q_6 + X_m Q_6 - 1) - \lambda_{Es} X_s Q_3 (Q_6 z_a z_c x_h + X_s Q_6 + X_m Q_6 - 1) \\
&+ \lambda_{Es} X_s (-Q_6 z_a z_c x_h - Q_7 z_a z_c x_h - X_s Q_6 - X_s Q_3 Q_6 - X_s Q_7 + Q_6 - X_m Q_6 - X_m Q_7)] \\
&- \frac{z_a z_c x_h}{(z_a + z_c)(z_a z_c x_h + x_m + X_s)} [\lambda_{mE} z_a z_c x_h (-1 + Q_4 z_a z_c x_h + x_m Q_4 + x_s Q_4) + \lambda_{Es} X_s (Q_6 z_a z_c x_h \\
&- X_s Q_6 + x_m Q_6 - 1)(z_a z_c x_h - 1 + x_m - X_s - X_s Q_3)] + \frac{x_p}{2 z_a z_c x_h + x_m + X_s} [-2 \lambda_{sE} z_a z_c x_h (Q_4 - 1) \\
&- 2 \lambda_{sE} Q_5 z_a z_c x_h \beta mE - \lambda_{ms} X_s (Q_6 - 1) - \lambda_{ms} X_s (Q_6 - 1) Q_3 - \lambda_{ms} X_s Q_7] \\
&- \frac{x_p}{(2 z_a z_c x_h + x_m + X_s)^2} [2 \lambda_{sE} z_a z_c x_h (Q_4 - 1) + \lambda_{ms} X_s (Q_6 - 1)](1 - x_m - 2 z_a z_c x_h - X_s - X_s z_a z_c x_h)
\end{aligned}
\tag{S.5a}
$$

where

$$
Q_1 = \frac{1}{2 z_a z_c x_h \beta_{Em} + x_m + X_s \beta_{sm}} - 1 \tag{S.5b}
$$

$$
Q_2 = \frac{-2 z_a z_c x_h \beta_{Em} + 1 - x_m - X_s \beta_{sm} - X_s \beta_{sm} \left(\frac{1 - x_m - x_p - x_h}{x_m + x_p + x_h}\right)}{(2 z_a z_c x_h \beta_{Em} + x_m + X_s \beta_{sm})^2} \tag{S.5c}
$$

$$
Q_3 = \frac{1 - x_m - x_p - x_h}{x_m + x_p + x_h} \tag{S.5d}
$$

$$
Q_4 = \frac{\beta_{mE}}{z_a z_c x_h \beta_{mE} + x_m + X_s \beta_{sE}} \tag{S.5e}
$$

$$Q_5 = \frac{-z_a z_c x_h \beta_{mE} + 1 - x_m - X_s \beta_{sE} - X_s \beta_{sE} (\frac{1 - x_m - x_p - x_h}{x_m + x_p + x_h})}{(z_a z_c x_h \beta_{Em} + x_m + X_s \beta_{sm})^2} \quad \text{(S.5f)}$$

$$Q_6 = \frac{1}{2 z_a z_c x_h \beta_{Es} + x_m \beta_{ms} + X_s} \quad \text{(S.5g)}$$

$$Q_7 = \frac{-2 z_a z_c x_h \beta_{Es} + \beta_{ms} - x_m \beta_{ms} - X_s - X_s (\frac{1 - x_m - x_p - x_h}{x_m + x_p + x_h})}{(2 z_a z_c x_h \beta_{Es} + x_m \beta_{ms} + X_s)^2} \quad \text{(S.5h)}$$

$$\beta_{Es} = \exp(-\frac{\lambda_{Es}}{Z}) \qquad \beta_{ms} = \exp(-\frac{\lambda_{ms}}{Z}) \quad \text{(S.5i)}$$

$$\beta_{Em} = \exp(-\frac{\lambda_{Em}}{Z}) \qquad \beta_{sm} = \exp(-\frac{\lambda_{sm}}{Z}) \quad \text{(S.5j)}$$

$$\beta_{mE} = \exp(-\frac{\lambda_{mE}}{Z}) \qquad \beta_{sE} = \exp(-\frac{\lambda_{sE}}{Z}) \quad \text{(S.5k)}$$

$$X_m = x_m \quad \text{(S.5l)}$$

$$X_s = \frac{x_p}{x_p + x_m + 2 z_a z_c x_h} \quad \text{(S.5m)}$$

where $x_h = 1 - x_m - x_p$; and λ_{mE}, λ_{Em}, λ_{sE}, λ_{Es} , λ_{sm} and λ_{ms} are the adjustable parameters of TNRF-mNRTL model; Z is the nonrandom factor which was set to 8 for obtaining the better quality of fitting in this work; z_a and z_c are the charge number of anion and cation of DPH-HCl, respectively. $\nu = \nu_c + \nu_a$, where ν_c and ν_a are the stoichiometric coefficients of cation and anion of DPH-HCl, respectively; Subscript p stands for saccharide.

S.6. liquid modified NRTL model proposed by Xu et al. [45]

The activity equation of the solvent for liquid modified NRTL model proposed by Xu et al. [45] is as follow for ternary system:

$$\ln a_m^{NRTL} = \frac{(\tau_{mE}m_E+\tau_{ms}m_s)\exp(-\alpha(\frac{\tau_{mE}m_E+\tau_{ms}m_s}{m_E+m_s}))}{m_E+m_s+(\frac{1000}{M_m}-(h_E m_E+h_s m_s))\exp(-\alpha(\frac{\tau_{mE}m_E+\tau_{ms}m_s}{m_E+m_s}))}$$

$$+\frac{(\tau_{Em}m_E+\tau_{sm}m_s)\exp(-\alpha(\frac{\tau_{Em}m_E+\tau_{sm}m_s}{m_E+m_s}))}{\frac{1000}{M_m}-(h_E m_E+h_s m_s)+(m_E+m_s)\exp(-\alpha(\frac{\tau_{Em}m_E+\tau_{sm}m_s}{m_E+m_s}))}$$

$$+(\frac{1000}{M_m}-(h_E m_E+h_s m_s))(\frac{-(\tau_{mE}m_E+\tau_{ms}m_s)\exp(-\alpha(\frac{\tau_{mE}m_E+\tau_{ms}m_s}{m_E+m_s}))^2}{(m_E+m_s+(\frac{1000}{M_m}-(h_E m_E+h_s m_s))\exp(-\alpha(\frac{\tau_{mE}m_E+\tau_{ms}m_s}{m_E+m_s})))^2}$$

$$-\frac{(\tau_{Em}m_E+\tau_{sm}m_s)\exp(-\alpha(\frac{\tau_{Em}m_E+\tau_{sm}m_s}{m_E+m_s}))}{(\frac{1000}{M_m}-(h_E m_E+h_s m_s)+(m_E+m_s)\exp(-\alpha(\frac{\tau_{mE}m_E+\tau_{ms}m_s}{m_E+m_s})))^2})+\ln(\frac{\frac{1000}{M_m}}{\frac{1000}{M_m}+m_E+m_s}) \quad \text{(S.6)}$$

where α is nonrandomness factors and in this work its value is equal to 0.3 as original work. τ_{mE}, τ_{Em}, τ_{sE}, τ_{Es}, τ_{sm}, τ_{ms}, h_E and h_s are the adjustable parameters of this model.