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:

\[
\ln \gamma_{m}^{*,\text{NRTL}} = \frac{(\exp(-\alpha_{mE}^{*}mE)x_{a}^{*}mE + \exp(-\alpha_{sE}^{*}sE)x_{c}^{*}sE)(\tau_{mE} - \tau_{sE}))}{(x_{c} + \exp(-\alpha_{mE}^{*}mE)x_{m})^{2}}
\]

\[
+ \frac{(\exp(-\alpha_{ms}^{*}ms)x_{a}^{*}ms + \exp(-\alpha_{Es}^{*}Es)(x_{a} + x_{c})(\tau_{ms} - \tau_{Es}))}{(x_{s} + \exp(-\alpha_{ms}^{*}ms)x_{m} + \exp(-\alpha_{Es}^{*}Es)(x_{a} + x_{c}))^{2}}
\]

\[
+ \frac{(\exp(-\alpha_{mE}^{*}mE)x_{a}^{*}mE + \exp(-\alpha_{sE}^{*}sE)x_{c}^{*}sE)(\tau_{mE} - \tau_{sE}))}{(x_{c} + \exp(-\alpha_{sE}^{*}sE)x_{s} + \exp(-\alpha_{mE}^{*}mE)x_{m})^{2}}
\]

\[
+ \frac{(\exp(-\alpha_{ms}^{*}ms)x_{a}^{*}ms + \exp(-\alpha_{Es}^{*}Es)(x_{a} + x_{c})(\tau_{ms} - \tau_{Es}))}{(x_{s} + \exp(-\alpha_{ms}^{*}ms)x_{m} + \exp(-\alpha_{Es}^{*}Es)(x_{a} + x_{c}))^{2}}
\]

(S.1)

Here, \(x\) is mole fraction; subscripts \(E\), \(m\) and \(s\) denote DPH-HCl, water and saccharide, respectively; \(\alpha_{mE}, \alpha_{Em}, \alpha_{sE}, \alpha_{Es}, \alpha_{sm}\) and \(\alpha_{ms}\) 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. \(\tau_{mE}, \tau_{Em}, \tau_{sE}, \tau_{Es}, \tau_{sm}\) and \(\tau_{ms}\) 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:
\[
\ln \gamma_m^{NRF-NRTL} = \frac{\left(\exp(-\alpha_{sm}^s\tau_{sm})x_s^s + \exp(-\alpha_{Em}^s\tau_{Em})x_a^s + \exp(-\alpha_{Es}^s\tau_{Es})x_c^s\right)\left(\exp(-\alpha_{sm}^c\tau_{sm})x_s^c + \exp(-\alpha_{Em}^c\tau_{Em})x_a^c + \exp(-\alpha_{Es}^c\tau_{Es})x_c^c\right)}{(x_a^s + x_c^s + x_s^c)^2}
+ \frac{\exp(-\alpha_{Em}^s\tau_{Em})x_a^s + \exp(-\alpha_{Em}^c\tau_{Em})x_c^s}{(x_a^s + x_c^s + x_s^c)^2} (x_a^s + x_c^s + x_s^c)
\]

(S.2)

where the nonrandomness factor values are set to \(\alpha_{mE} = 0.4, \alpha_{Em} = 0.4, \alpha_{Es} = 0.1, \alpha_{Es} = 0.1\), \(\alpha_{sm} = 0.4\) and \(\alpha_{ms} = 0.4\) for obtaining the better fitting quality in this work. \(\tau_{mE}, \tau_{Em}, \tau_{Es}, \tau_{sm}, \tau_{ms}\) 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:

\[
\ln \gamma_m^{NRF-NRTL} = \frac{\exp(-\alpha_{sm}^s\tau_{sm})x_s^s + \exp(-\alpha_{Em}^s\tau_{Em})x_a^s + \exp(-\alpha_{Es}^s\tau_{Es})x_c^s}{(x_a^s + x_c^s + x_s^c)^2}
+ \frac{\exp(-\alpha_{Em}^s\tau_{Em})x_a^s + \exp(-\alpha_{Em}^c\tau_{Em})x_c^s}{(x_a^s + x_c^s + x_s^c)^2} (x_a^s + x_c^s + x_s^c)
\]

(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. \( \tau_{mE} \), \( \tau_{Em} \), \( \tau_{sE} \), \( \tau_{Es} \),

\( \tau_{sm} \) and \( \tau_{ms} \) 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:

\[
\ln \gamma_m^{*_{W_1}} = -C \ln(x_m + \exp(-\frac{E_{sm}}{CRT})x_s + \exp(-\frac{E_{Em}}{CRT})(x_a + x_c)) - \\
Cx_m(x_a + x_c + x_s - \exp(-\frac{E_{sm}}{CRT})x_s - \exp(-\frac{E_{Em}}{CRT})(x_a + x_c) + \\
x_m + \exp(-\frac{E_{sm}}{CRT})x_s + \exp(-\frac{E_{Em}}{CRT})(x_a + x_c) + \\
Cx_s(x_s - \exp(-\frac{E_{ms}}{CRT})x_s - \exp(-\frac{E_{Es}}{CRT})(x_a + x_c) + \\
x_s + \exp(-\frac{E_{ms}}{CRT})x_m + \exp(-\frac{E_{Es}}{CRT})(x_a + x_c) + \\
Cx_a(x_a + \exp(-\frac{E_{sa}}{CRT})x_s - \exp(-\frac{E_{Es}}{CRT})(x_c + x_s) + \\
(x_c + x_s + x_m)(x_c + \exp(-\frac{E_{sa}}{CRT})x_s + \exp(-\frac{E_{Es}}{CRT})x_m + \\
Cx_c(x_a - \exp(-\frac{E_{mc}}{CRT})(x_a + x_s)(\exp(-\frac{E_{sa}}{CRT}) + \exp(-\frac{E_{Es}}{CRT})) + \\
(x_a + x_s + x_m)(x_a + \exp(-\frac{E_{ms}}{CRT})x_s + \exp(-\frac{E_{Em}}{CRT})x_m)
\]

(S.4)

Here, \(E_{sa}, E_{sm}, E_{sa}, E_{ms}, E_{Es}, E_{ms}\) 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-mNRTL equation

The activity coefficient equation of the solvent for TNRF-mNRTL model \(^{44}\) is as follow for ternary system:
\[
\ln \gamma_{m}^{*,\text{TNRF} - \text{mNRTL}} = \lambda_{Em}^{x} m^{Q_{1}} + \lambda_{sm}^{x} m^{Q_{1}} + x_{m}^{(\lambda_{Em}^{x} Q_{1} - \lambda_{Em}^{x} Q_{1} - \lambda_{Em}^{x} Q_{1} - \lambda_{sm}^{x} Q_{1})}
- \lambda_{sm}^{x} Q_{-1}^{3} - \lambda_{sm}^{x} Q_{-3}^{3} + \frac{z_{a}^{n_{c}^{x} h_{h}}}{(z_{a}^{n_{c}^{x} h_{h}} + x_{m}^{Q_{m}} + X_{s}^{Q_{m}})}[-\lambda_{mE}^{x} z_{1}^{x} z_{1}^{x} (1 + Q_{4}^{a} z_{1}^{x} z_{1}^{x} + x_{m}^{Q_{m}} + X_{s}^{Q_{m}}) + \lambda_{Es}^{x} Q_{-1}^{3} (Q_{6}^{a} z_{1}^{x} z_{1}^{x} + X_{s}^{Q_{m}} + X_{m}^{Q_{m}} - 1) - \frac{z_{a}^{n_{c}^{x} h_{h}}}{(z_{a}^{n_{c}^{x} h_{h}} + x_{m}^{Q_{m}} + X_{s}^{Q_{m}})}[\lambda_{mE}^{x} z_{1}^{x} z_{1}^{x} (1 + Q_{4}^{a} z_{1}^{x} z_{1}^{x} + x_{m}^{Q_{m}} + X_{s}^{Q_{m}}) + \lambda_{Es}^{x} Q_{-1}^{3} (Q_{6}^{a} z_{1}^{x} z_{1}^{x} + X_{s}^{Q_{m}} + X_{m}^{Q_{m}} - 1) - \frac{z_{a}^{n_{c}^{x} h_{h}}}{(z_{a}^{n_{c}^{x} h_{h}} + x_{m}^{Q_{m}} + X_{s}^{Q_{m}})}[\lambda_{mE}^{x} z_{1}^{x} z_{1}^{x} (1 + Q_{4}^{a} z_{1}^{x} z_{1}^{x} + x_{m}^{Q_{m}} + X_{s}^{Q_{m}}) + \lambda_{Es}^{x} Q_{-1}^{3} (Q_{6}^{a} z_{1}^{x} z_{1}^{x} + X_{s}^{Q_{m}} + X_{m}^{Q_{m}} - 1)]
\]

\[
Q_{1} = \frac{1}{2z_{a}^{n_{c}^{x} h_{h}}^{2} + x_{m}^{2} + X_{s}^{2}} - 1 \quad \text{(S.5b)}
\]

\[
Q_{2} = \frac{-2z_{a}^{n_{c}^{x} h_{h}}^{2} + x_{m}^{2} - X_{s}^{2}}{(2z_{a}^{n_{c}^{x} h_{h}}^{2} + x_{m}^{2} + X_{s}^{2})^{2}} \quad \text{(S.5c)}
\]

\[
Q_{3} = \frac{1-x_{m}^{4-1} - x_{p}^{1-1}}{x_{m}^{1-1} + x_{p}^{1-1}} \quad \text{(S.5d)}
\]

\[
Q_{4} = \frac{\beta_{mE}^{x}}{z_{a}^{n_{c}^{x} h_{h}}^{2} + x_{m}^{2} + X_{s}^{2}} \quad \text{(S.5e)}
\]

where
where $x_h = 1 - x_m - x_p$; and $\lambda_{mE}$, $\lambda_{Em}$, $\lambda_{Es}$, $\lambda_{sE}$, $\lambda_{sm}$ and $\lambda_{ms}$ 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 $\nu_c$ and $\nu_a$ 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:

\[
\ln a_m^{NRTL} = \frac{(\tau_{mE} m_E + \tau_{ms} m_s)}{m_E + m_s} \exp(-\alpha(\frac{\tau_{mE} m_E + \tau_{ms} m_s}{m_E + m_s})) \\
+ \frac{(\tau_{Em} m_E + \tau_{sm} m_s)}{m_E + m_s} \exp(-\alpha(\frac{\tau_{Em} m_E + \tau_{sm} m_s}{m_E + m_s})) \\
+ \left(\frac{1000}{M_m} - (h_E m_E + h_s m_s)\right)\left(\frac{1000}{M_m} - (h_E m_E + h_s m_s)\right)^2 \exp(-\alpha(\frac{\tau_{Em} m_E + \tau_{sm} m_s}{m_E + m_s})) \\
+ \frac{(\tau_{Em} m_E + \tau_{sm} m_s)}{m_E + m_s} \exp(-\alpha(\frac{\tau_{Em} m_E + \tau_{sm} m_s}{m_E + m_s})) \\
+ \left(\frac{1000}{M_m} - (h_E m_E + h_s m_s)\right)\left(\frac{1000}{M_m} - (h_E m_E + h_s m_s)\right)^2 \exp(-\alpha(\frac{\tau_{Em} m_E + \tau_{sm} m_s}{m_E + m_s})) \\
+ \frac{(\tau_{Em} m_E + \tau_{sm} m_s)}{m_E + m_s} \exp(-\alpha(\frac{\tau_{Em} m_E + \tau_{sm} m_s}{m_E + m_s})) \\
+ \ln\left(\frac{1000}{M_m} + m_E + m_s\right)
\]

(S.6)

where \( \alpha \) is nonrandomness factors and in this work its value is equal to 0.3 as original work. \( \tau_{mE} \), \( \tau_{Em} \), \( \tau_{sm} \), \( h_E \) and \( h_s \) are the adjustable parameters of this model.