Supplementary Materials for Solubility characteristics of acetaminophen and phenacetin in binary mixtures of aqueous organic solvents: experimental and deep machine learning screening of green dissolution media

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Figure S2. The FTIR-ATR spectra (A) and DSC thermograms (B) measured for phenacetin solid residues and pure reagent. 3

Table S1. The results of data curation for acetaminophen in neat solvents [1,2,11–20,3–10]. Data points were excluded from fitting λh-equation if PE>10%. The optimized values of parameters of the Buchowski-Ksiazczak [21] model applied to acetaminophen solubility in neat solvents are provided in the table in an additional supporting file (see Supplementary Materials S2 in "neat solvents"). 4

Table S2. The results of data curation for phenacetin in neat solvents [19,22–25]. Data points were excluded from fitting λh-equation if PE>10%. The optimized values of parameters of the Buchowski-Ksiazczak [21] model applied to phenacetin solubility in neat solvents are provided in the table in an additional supporting file (see Supplementary Materials S2 in"neat solvents"). 9

Table S3. The data collection of acetaminophen solubility in binary solvent mixtures [1,2,13,14,26,3,4,7–12]. The optimized values of parameters of the Jouyban-Acree model [27] model applied to acetaminophen solubility in binary solvents are provided in the table in an additional supporting file (see Supplementary Materials S2 in "binary solvents"). 15

Table S4. The data collection of phenacetin solubility in binary solvent mixtures [22,23,28]. The optimized values of parameters of the Jouyban-Acree model [27] model applied to phenacetin solubility in binary solvents are provided in the table in an additional supporting file (see Supplementary Materials S2 in "binary solvents"). 19

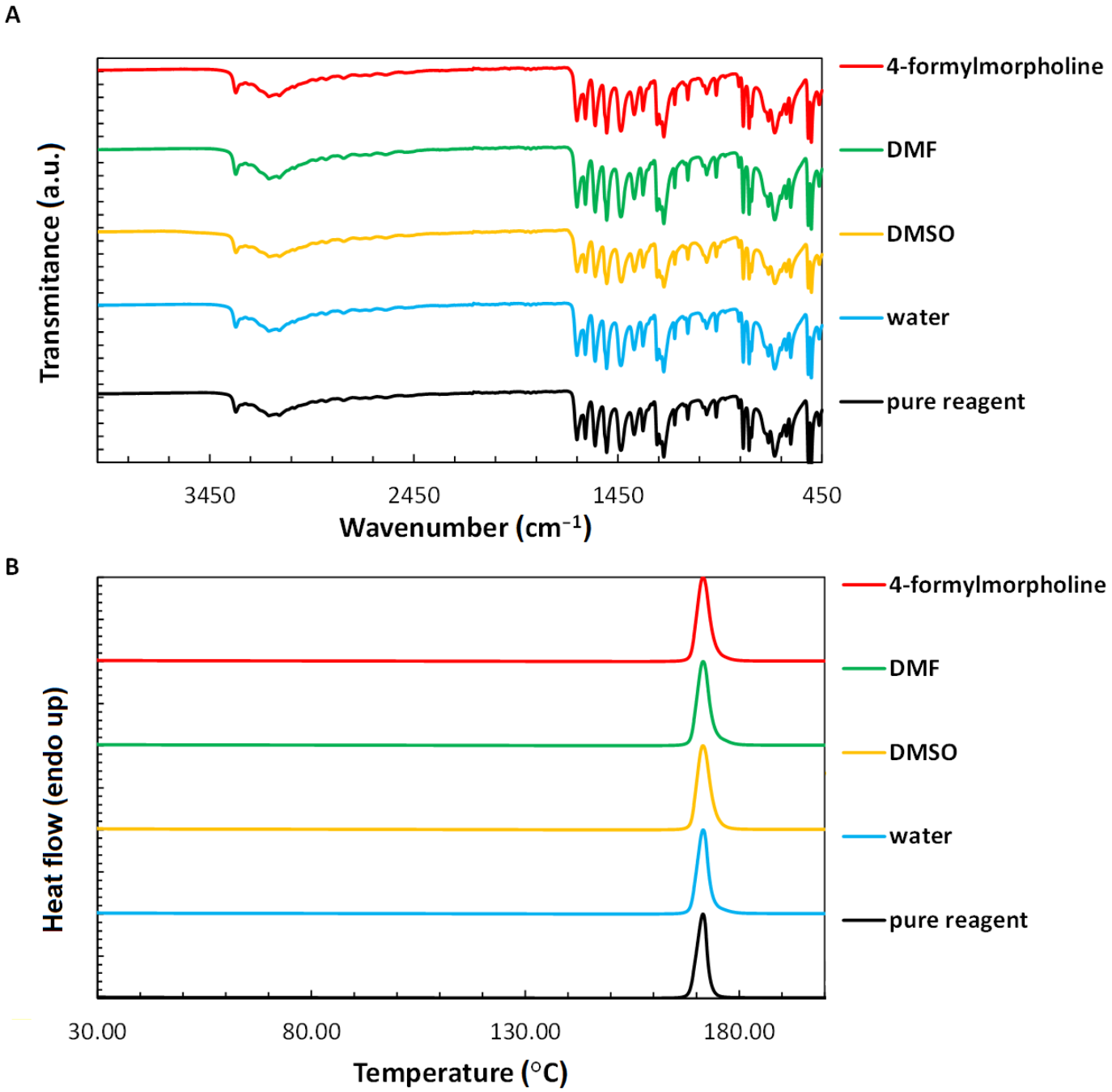


Figure S1. The FTIR-ATR spectra (A) and DSC thermograms (B) measured for acetaminophen solid residues and pure reagent.

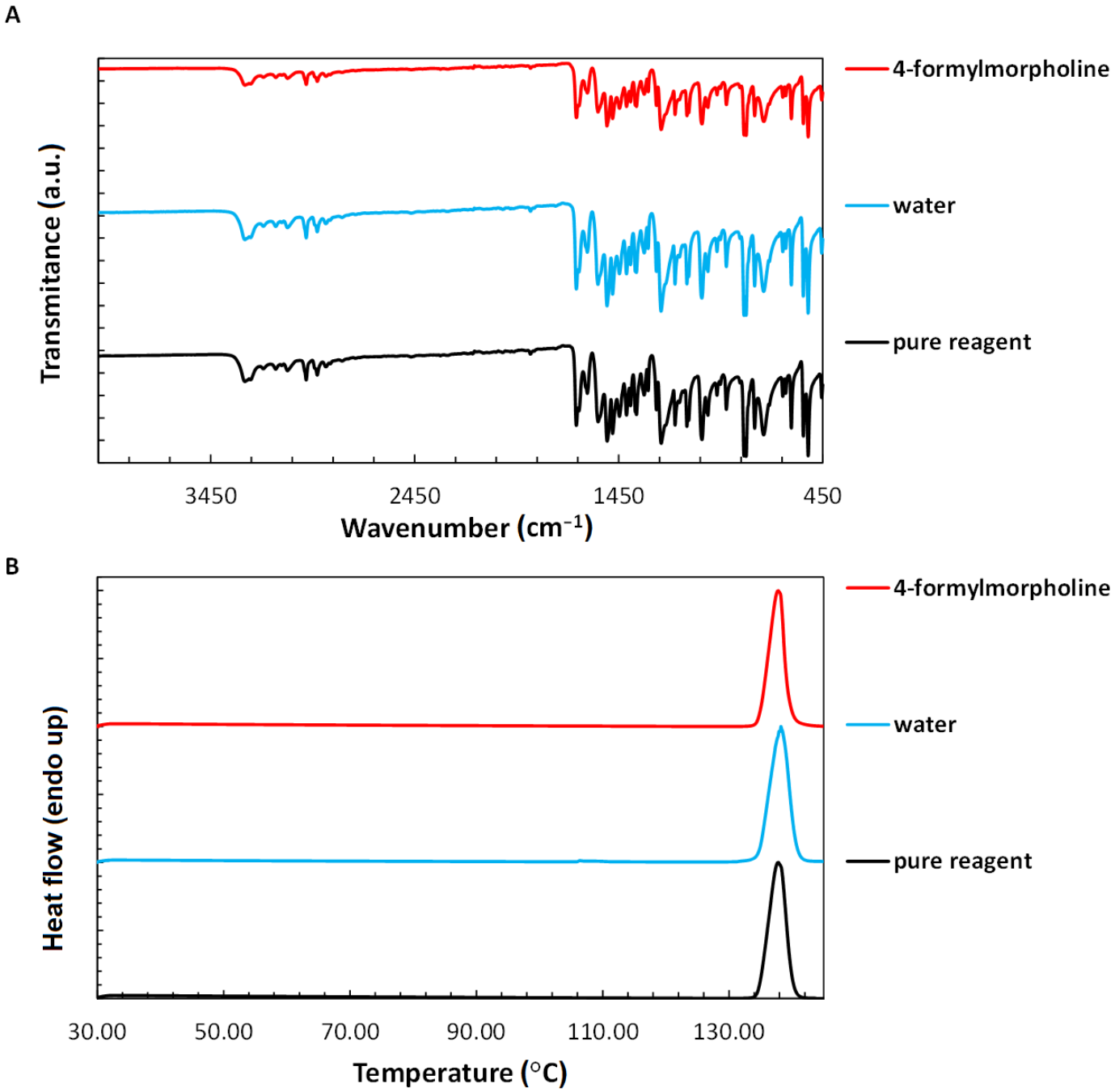
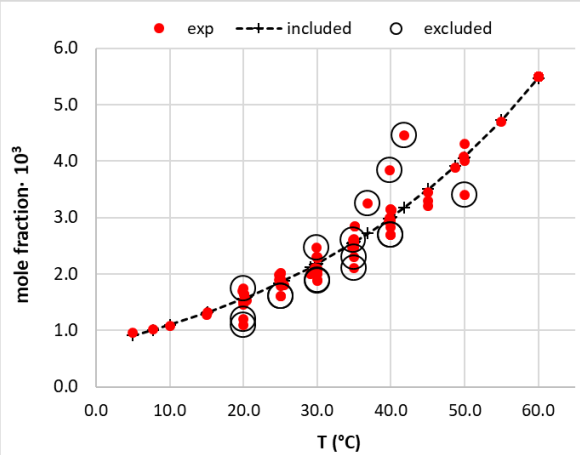
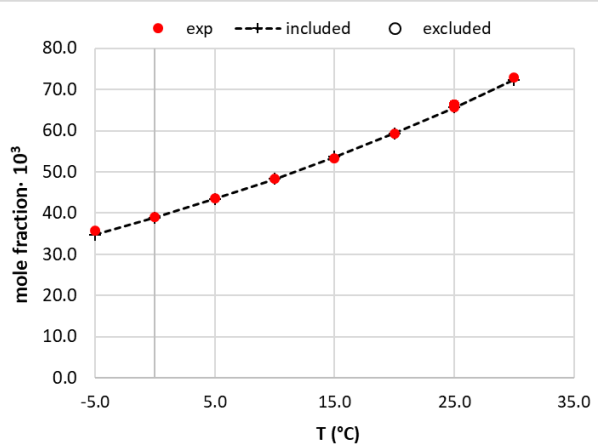
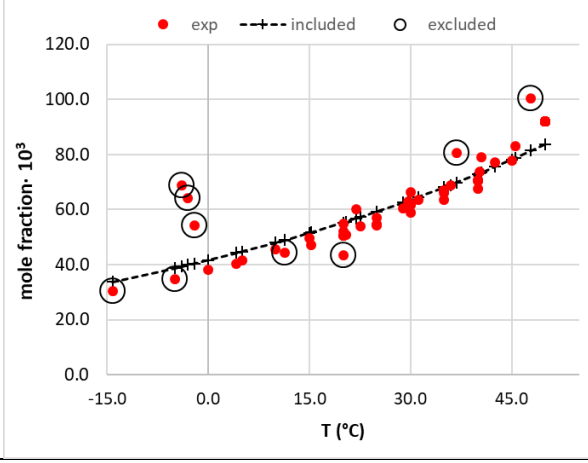
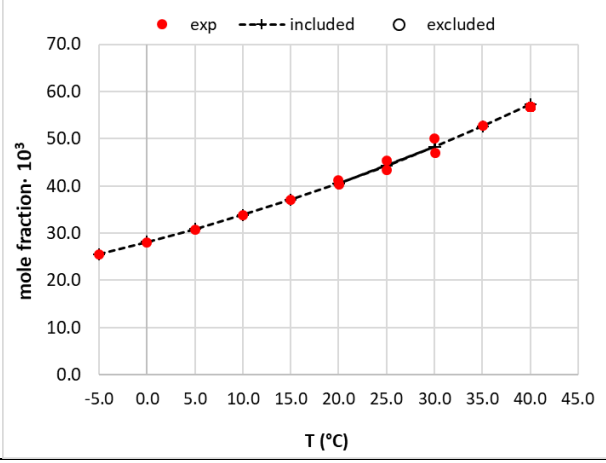
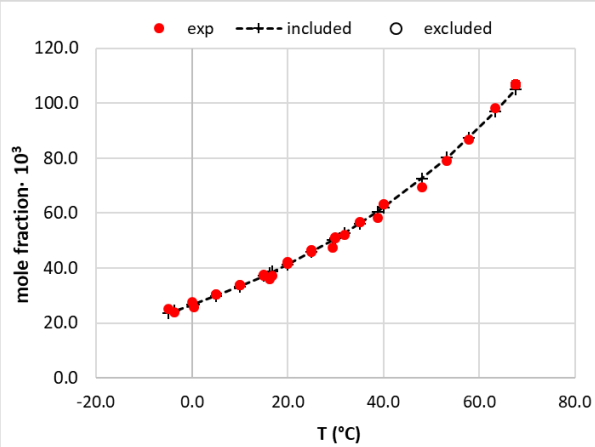
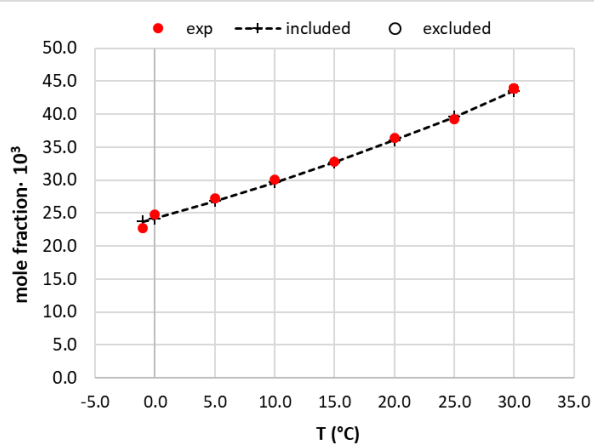
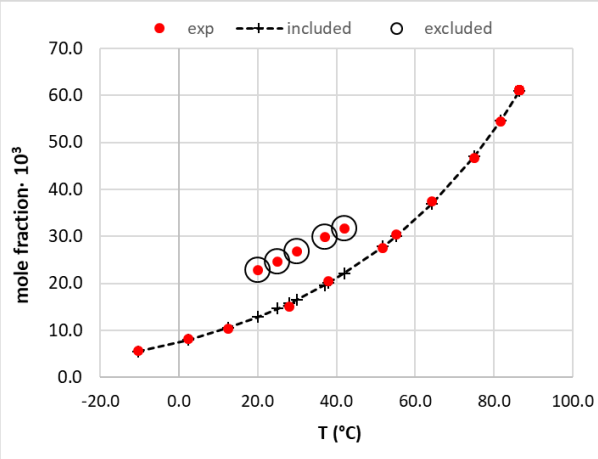
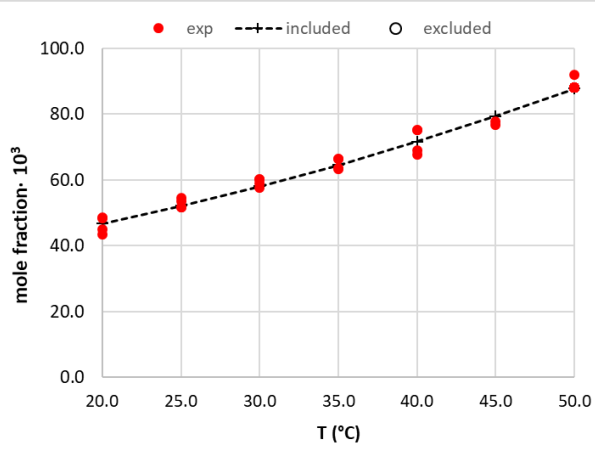
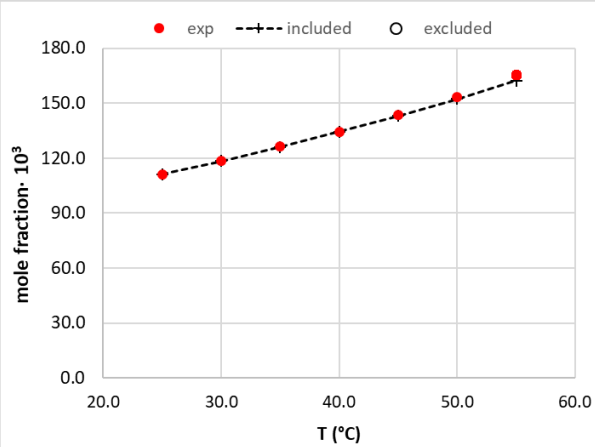
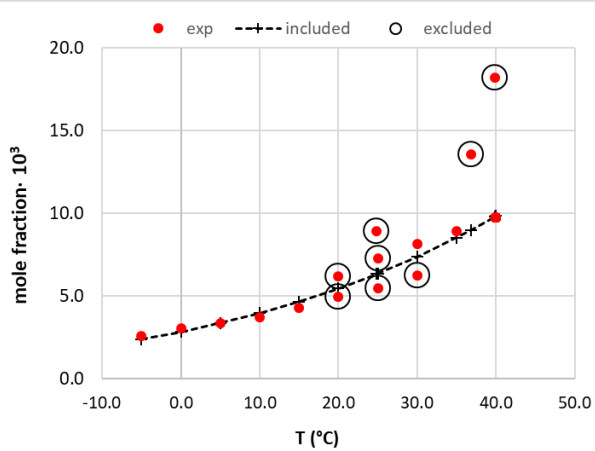
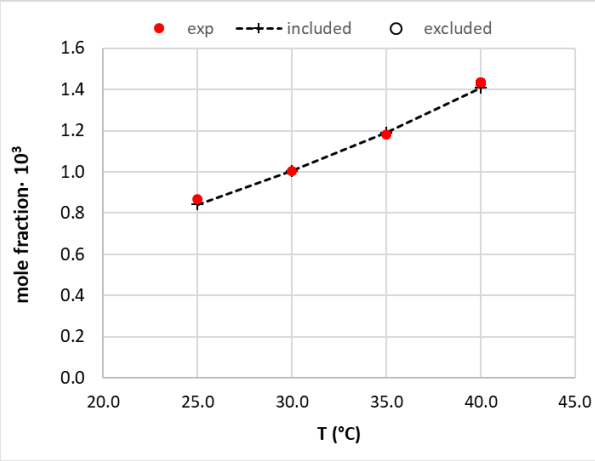
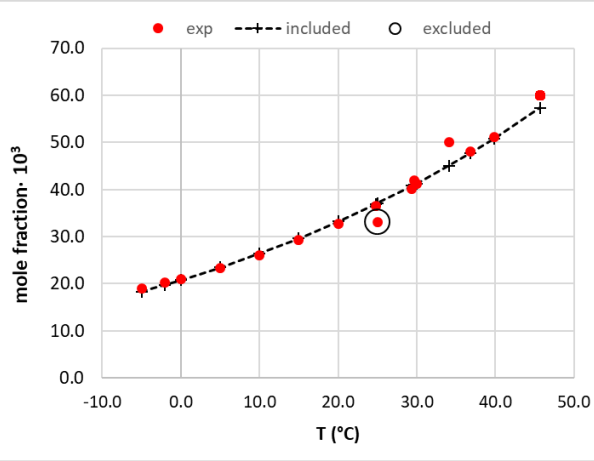


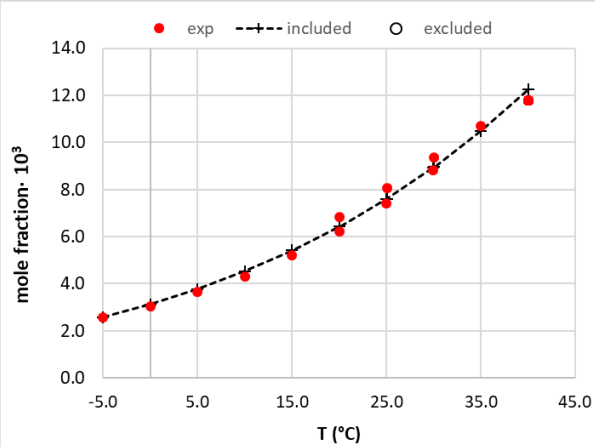
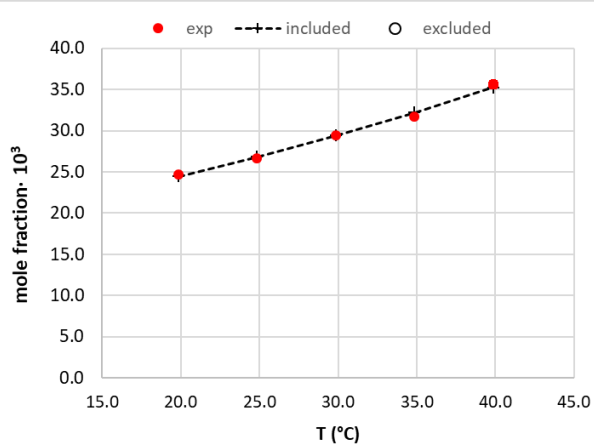
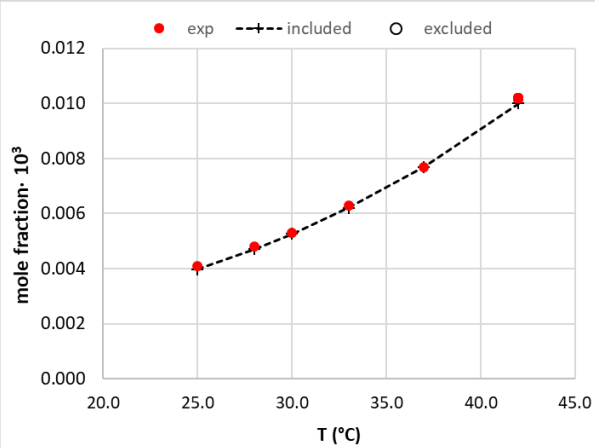
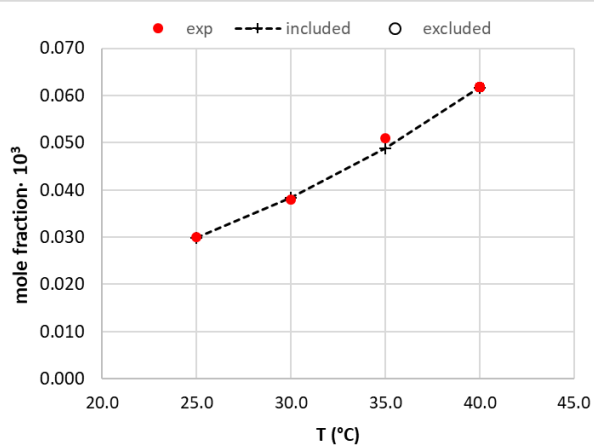
Figure S2. The FTIR-ATR spectra (A) and DSC thermograms (B) measured for phenacetin solid residues and pure reagent.

Table S1. The results of data curation for acetaminophen in neat solvents [1,2,11–20,3–10]. Data points were excluded from fitting λh-equation if PE>10%. The optimized values of parameters of the Buchowski-Ksiazczak [21] model applied to acetaminophen solubility in neat solvents are provided in the table in an additional supporting file (see Supplementary Materials S2 in "neat solvents").

API+solvent	Solubility-temperature characteristics	API+solvent	Solubility-temperature characteristics
A+water [2,3,17–21,4–7,13–16]		A+methanol [6,8]	
A+ethanol [3,5,19]		A+1-propanol [8,14]	

API+solvent	Solubility-temperature characteristics	API+solvent	Solubility-temperature characteristics
A+2-propanol [8,9,15,16]		A+1-butanol [8]	
A+1-octanol [9,10]		A+propylene glycol [3–5]	

API+solvent	Solubility-temperature characteristics	API+solvent	Solubility-temperature characteristics
A+transcutol [5]		A+ethyl acetate [8,11,19]	
A+isopropyl myristate [12]		A+acetone [8,11,16]	

API+solvent	Solubility-temperature characteristics	API+solvent	Solubility-temperature characteristics
A+acetonitrile [2,8]		A+1,4-dioxane [18]	
A+hexane [10]		A+cyclohexane [12]	

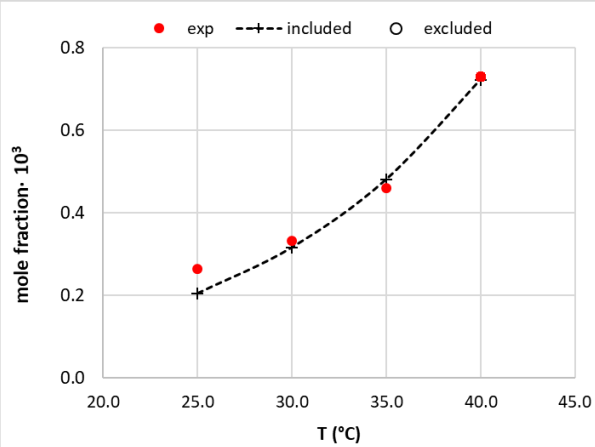
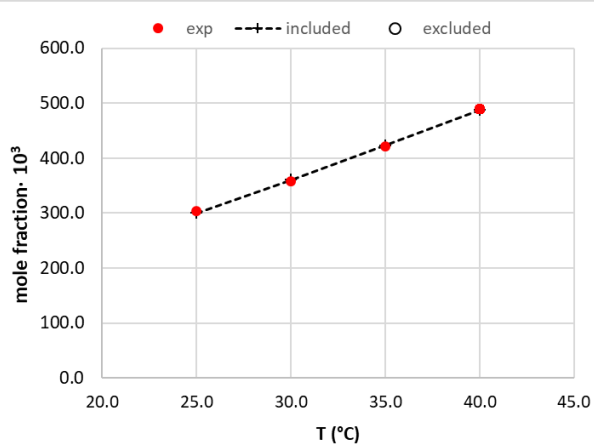
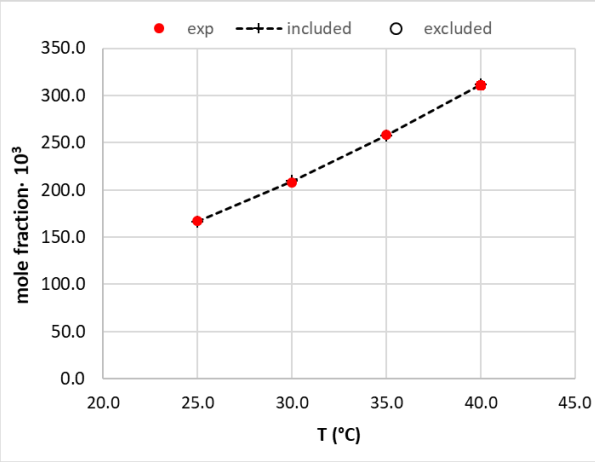
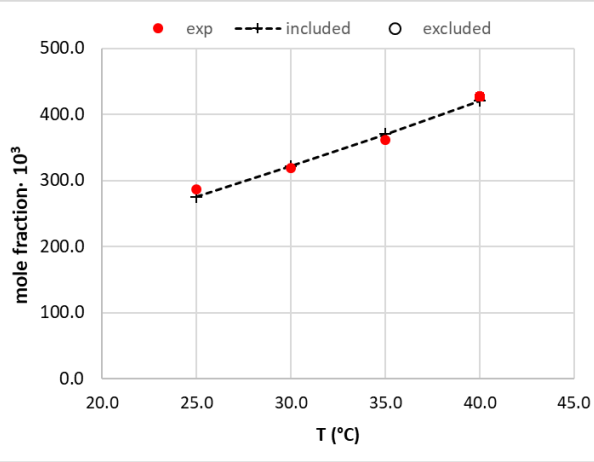
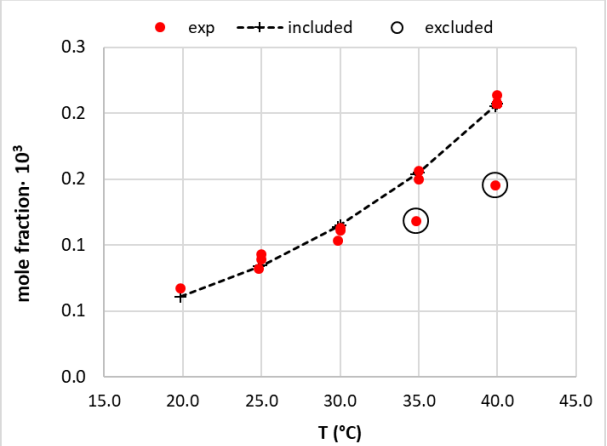
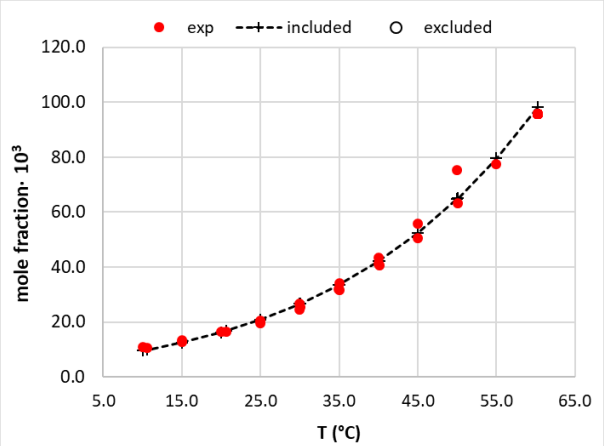
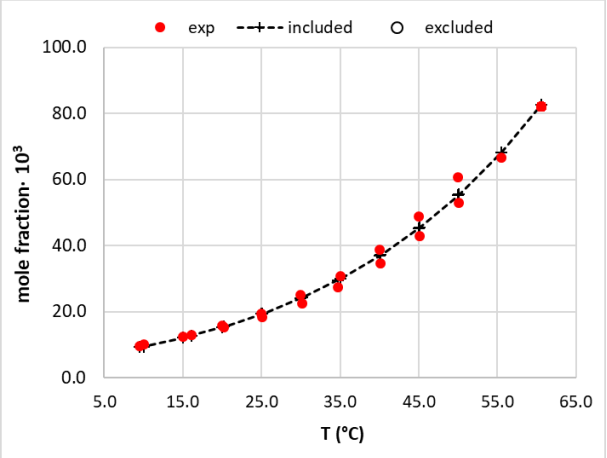
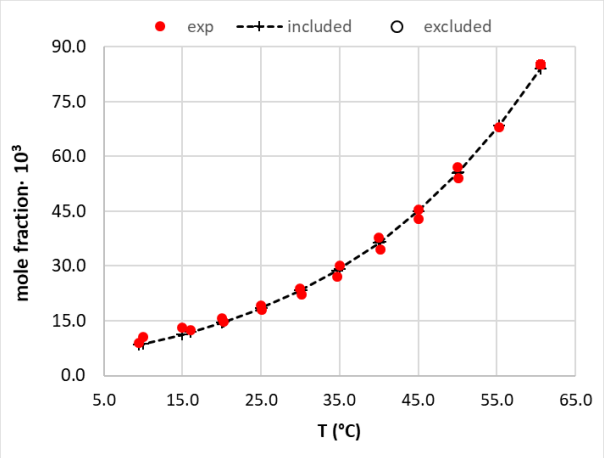
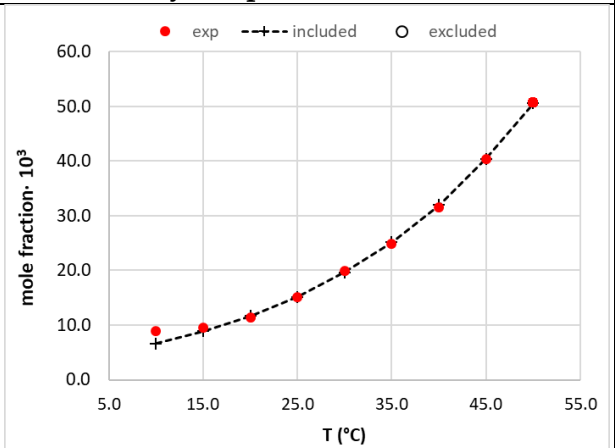
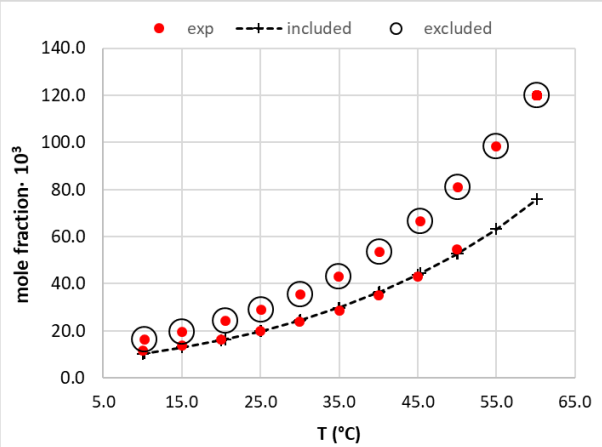
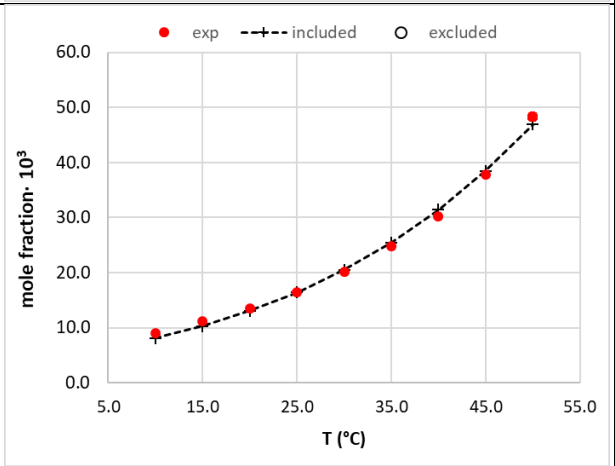
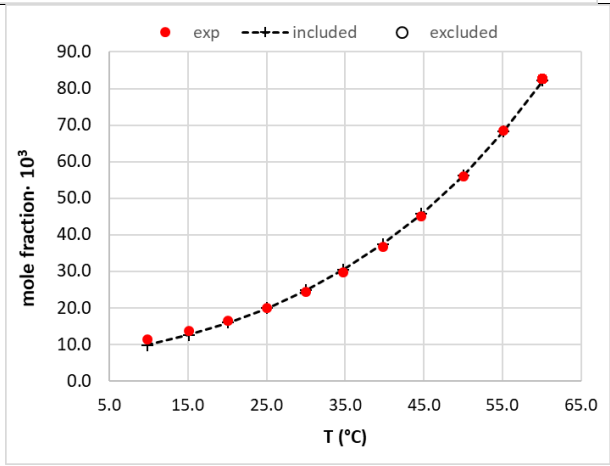
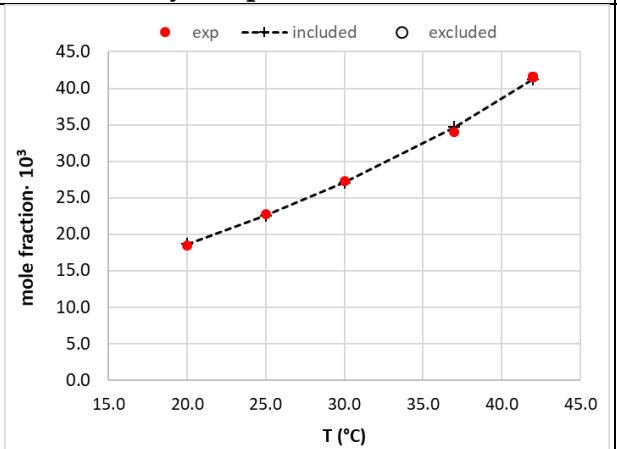
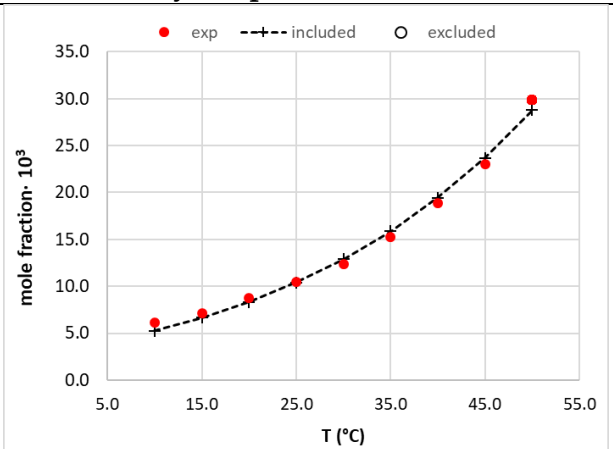
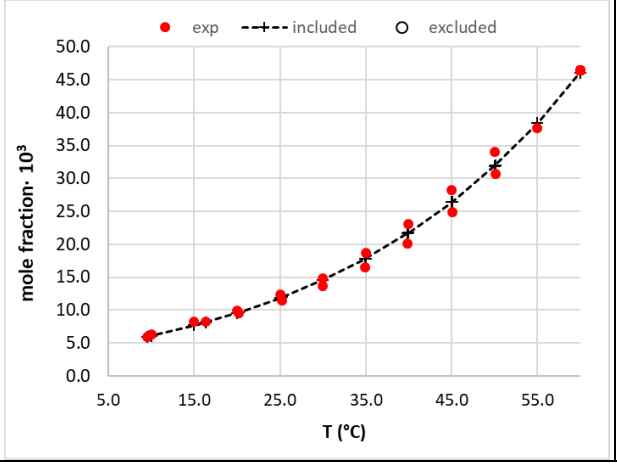
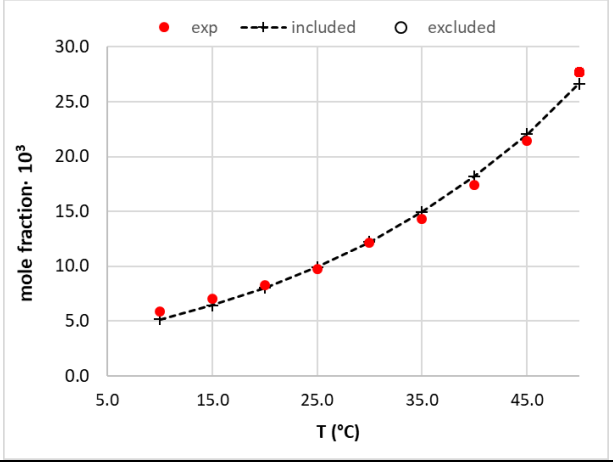
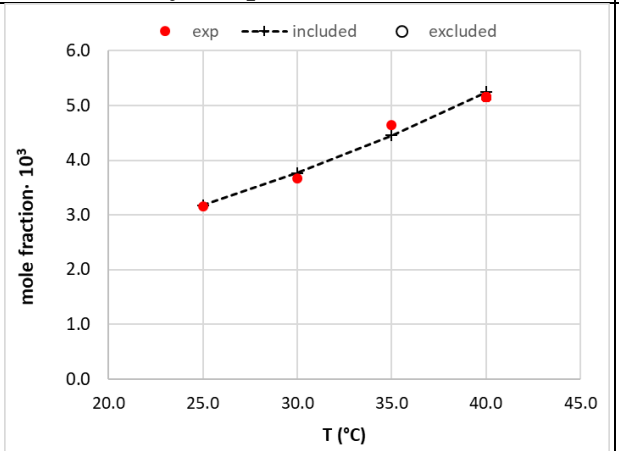
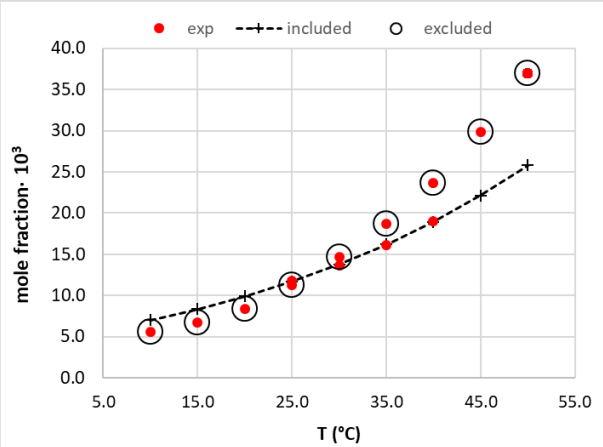
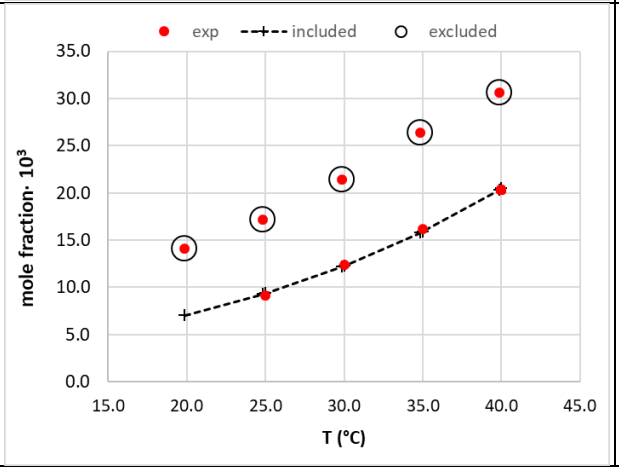
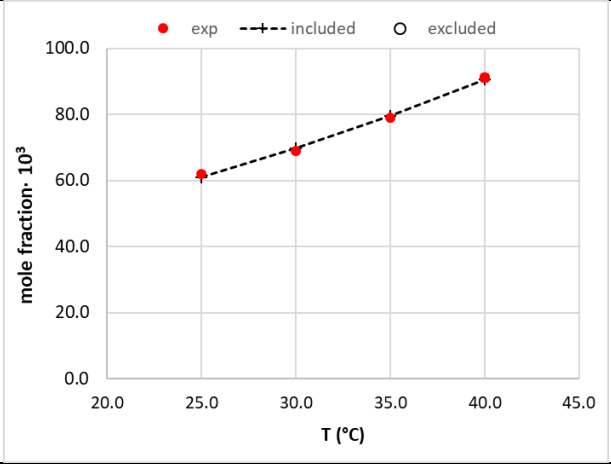
API+solvent	Solubility-temperature characteristics	API+solvent	Solubility-temperature characteristics
A+chloroform [12]		A+DMSO [this work]	
A+4-formylmorpholine [this work]		A+DMF [this work]	

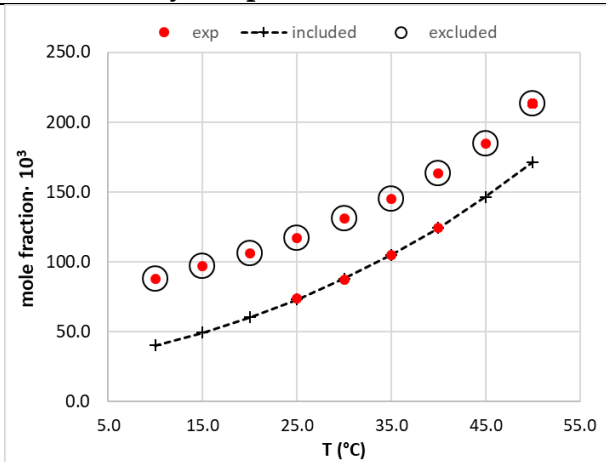
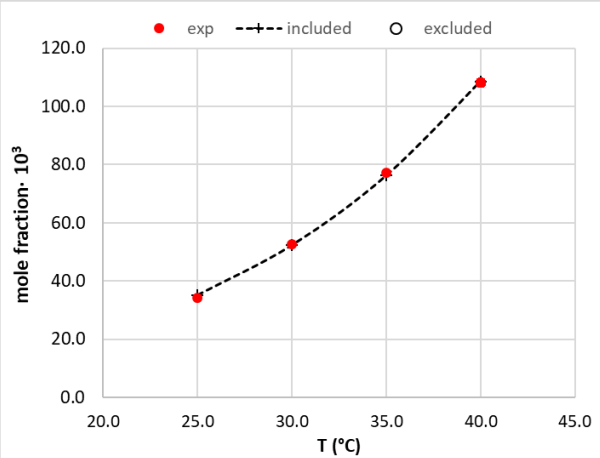
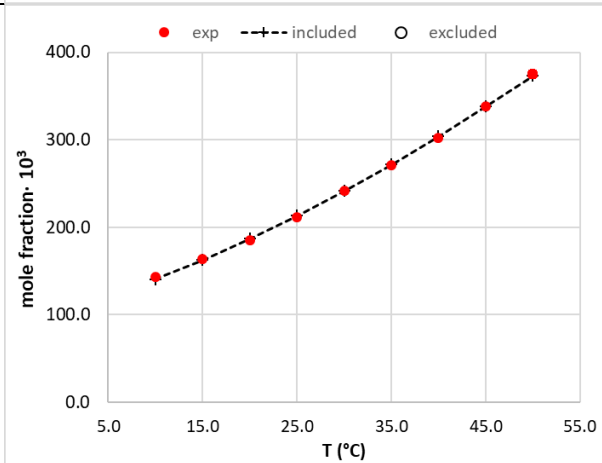
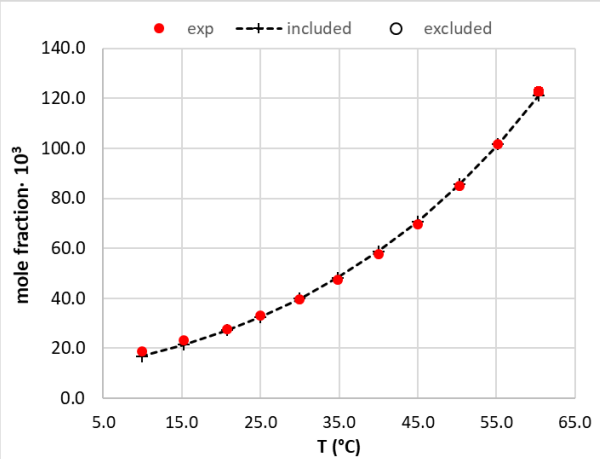
Table S2. The results of data curation for phenacetin in neat solvents [19,22–25]. Data points were excluded from fitting λh-equation if PE>10%. The optimized values of parameters of the Buchowski-Ksiazczak [21] model applied to phenacetin solubility in neat solvents are provided in the table in an additional supporting file (see Supplementary Materials S2 in "neat solvents").

API+solvent	Solubility-temperature characteristics	API+solvent	Solubility-temperature characteristics
P+water [12,22,23]		P+methanol [23–25]	
P+ethanol [24,25]		P+1-propanol [24,25]	

API+solvent	Solubility-temperature characteristics	API+solvent	Solubility-temperature characteristics
P+2-propanol [24]		P+1-butanol [24,25]	
P+2-butanol [24]		P+1-pentanol [25]	

API+solvent	Solubility-temperature characteristics	API+solvent	Solubility-temperature characteristics
P+1-octanol [10]		P+ethyl formate [24]	
P+ethyl acetate [24,25]		P+n-propyl acetate [24]	

API+solvent	Solubility-temperature characteristics	API+solvent	Solubility-temperature characteristics
P+isopropyl myristate [12]		P+acetonitrile [23,24]	
P+1,4-dioxane [22,23]		P+4-formylmorpholine [this work]	

API+solvent	Solubility-temperature characteristics	API+solvent	Solubility-temperature characteristics
P+DMF [23,24]		P+DMSO [23]	
P+N,N-dimethylacetamide [24]		P+THF [25]	

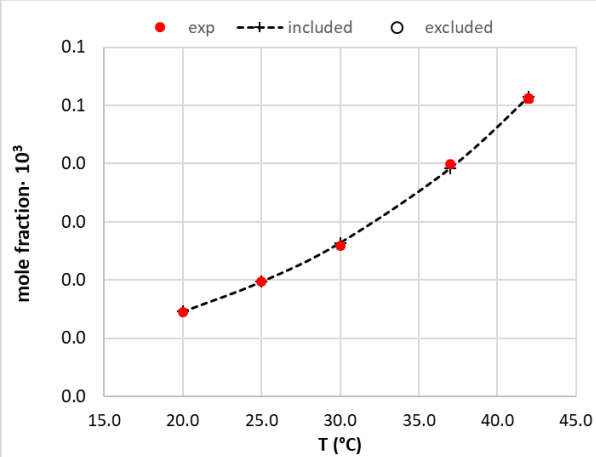
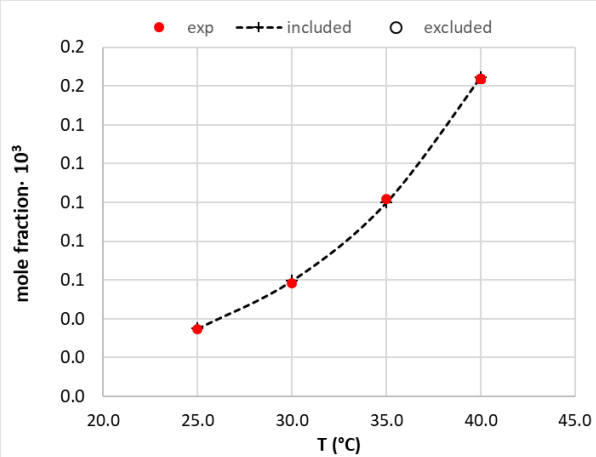
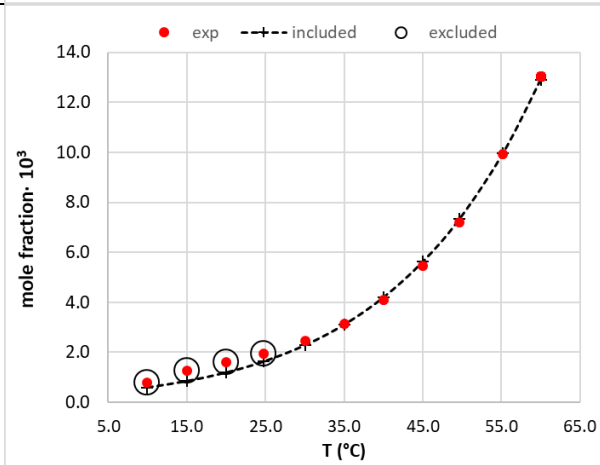
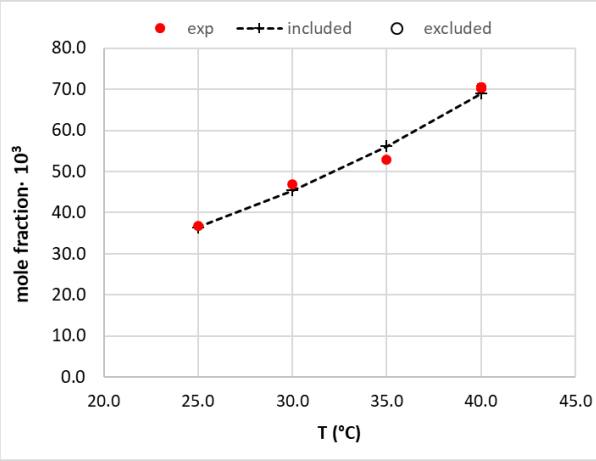
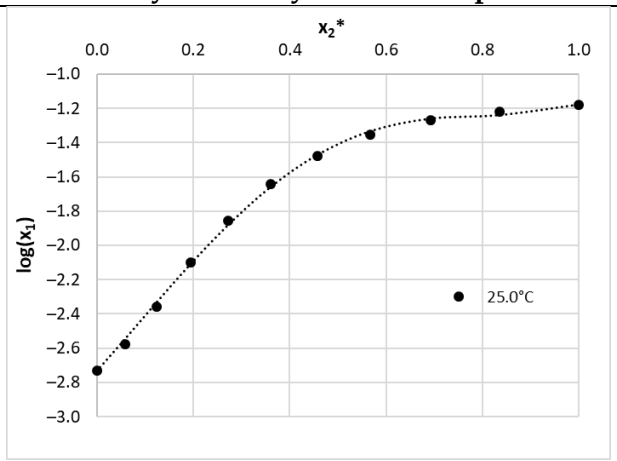
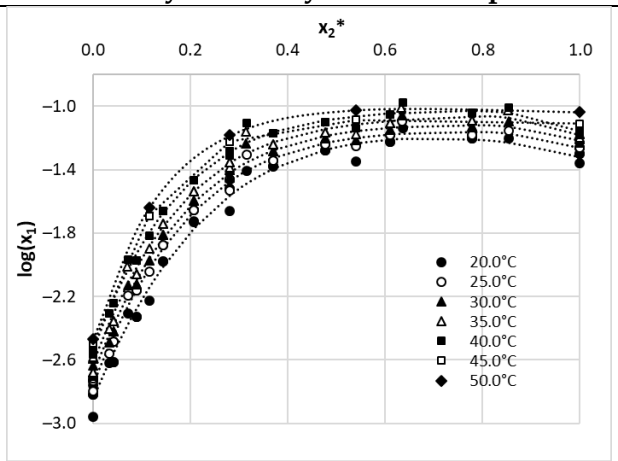
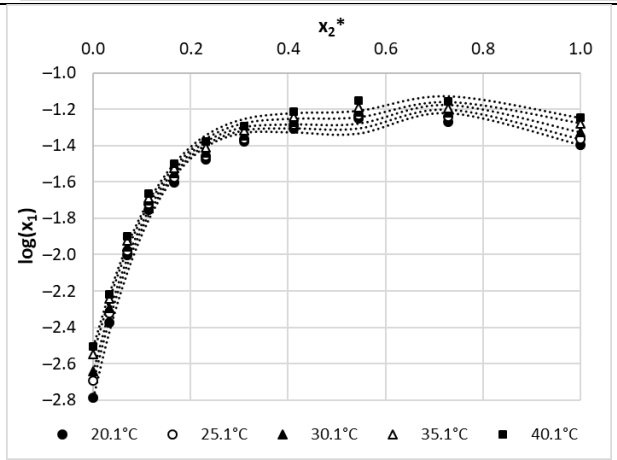
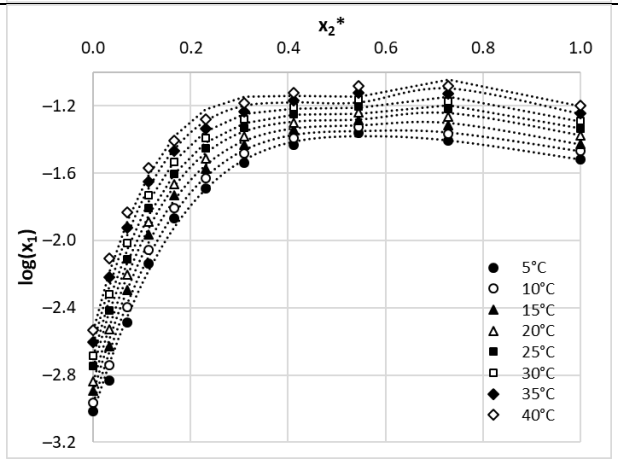
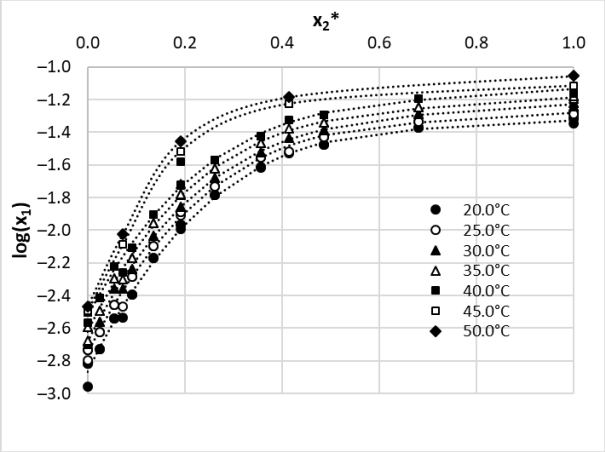
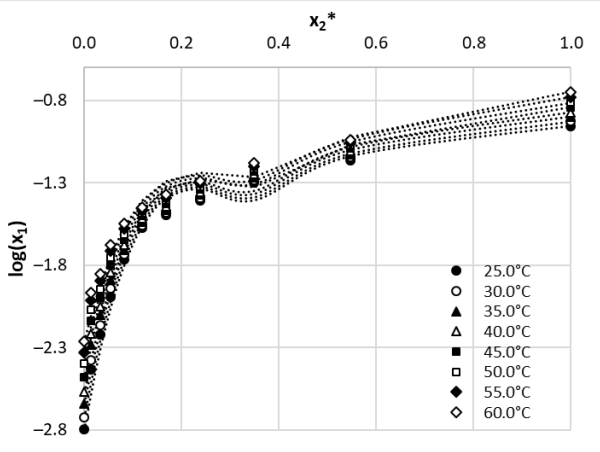
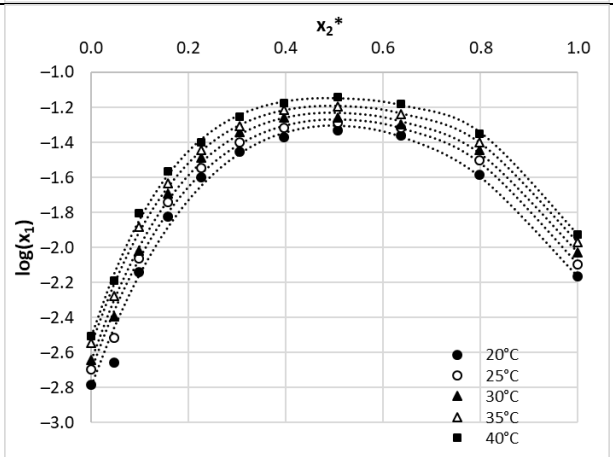
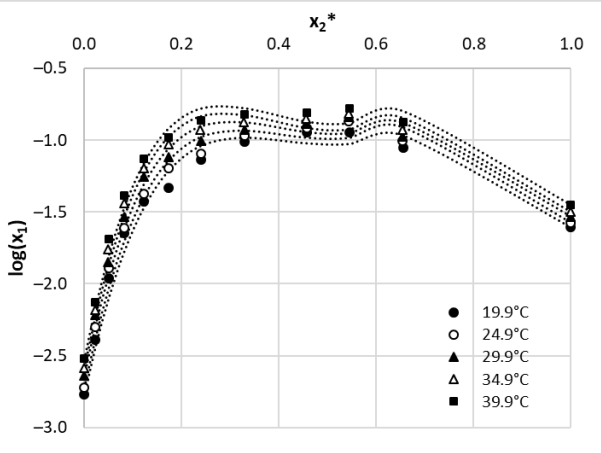
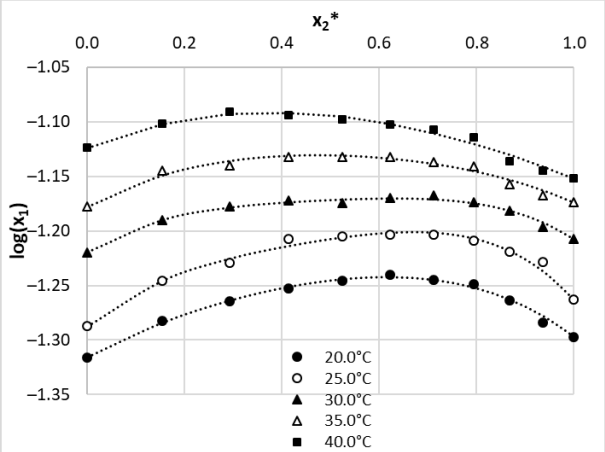
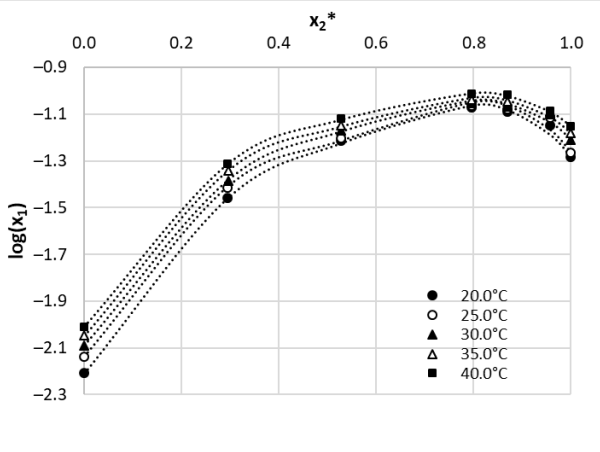
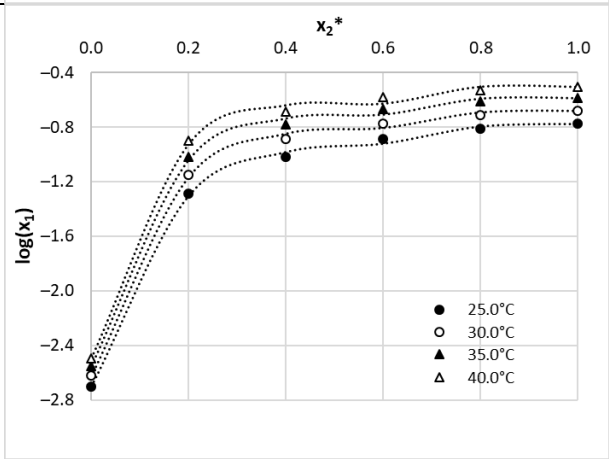
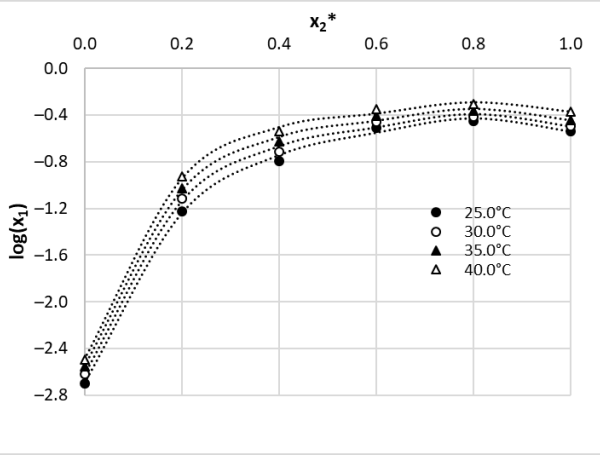
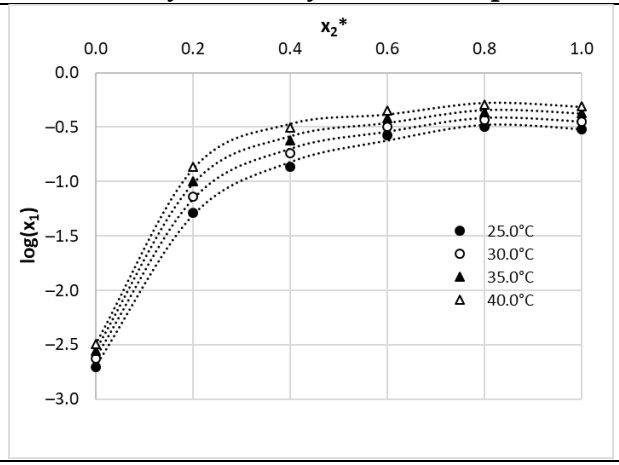
API+solvent	Solubility-temperature characteristics	API+solvent	Solubility-temperature characteristics
P+hexane [10]		P+cyclohexane [12]	
P+benzene [25]		P+chloroform [12]	

Table S3. The data collection of acetaminophen solubility in binary solvent mixtures [1,2,13,14,26,3,4,7–12]. The optimized values of parameters of the Jouyban-Acree model [27] model applied to acetaminophen solubility in binary solvents are provided in the table in an additional supporting file (see Supplementary Materials S2 in "binary solvents").

API+solvent	Solubility vs. binary solvent composition	API+solvent	Solubility vs. binary solvent composition
A+methanol+water [6]		A+ethanol+water [3,5,19,21,26]	
A+ acetaminophen+propanol [14] (*)		A+ isopropanol+water [15] (*)	

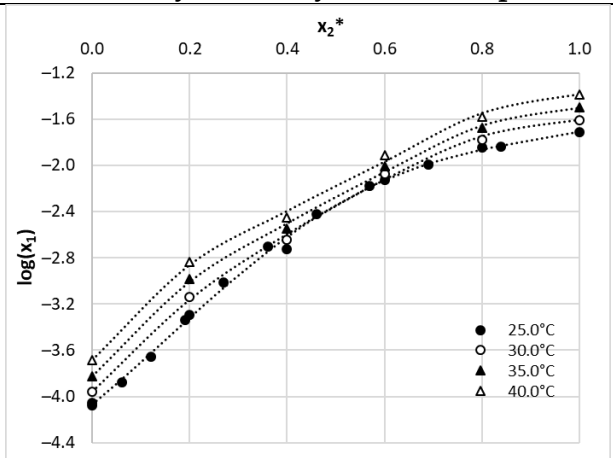
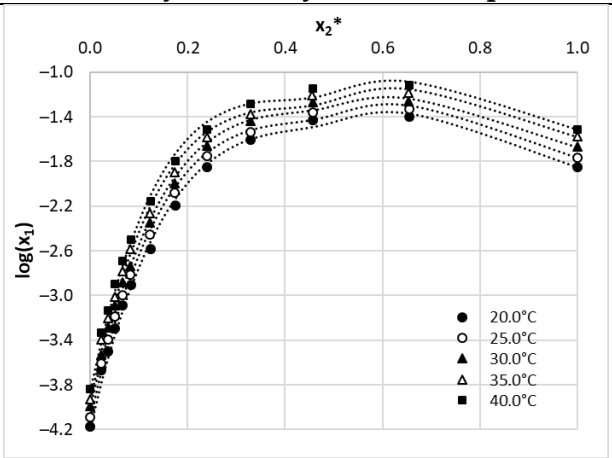
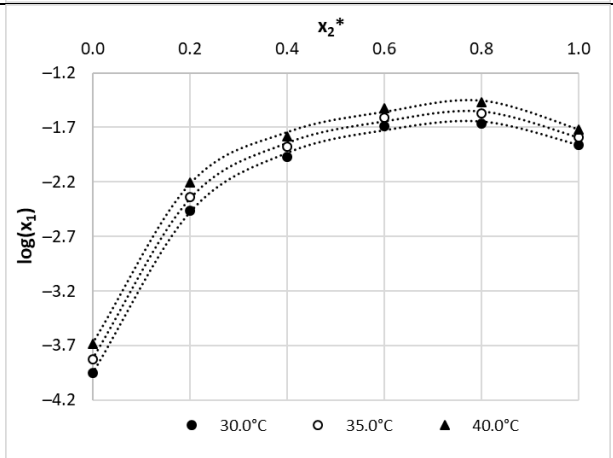
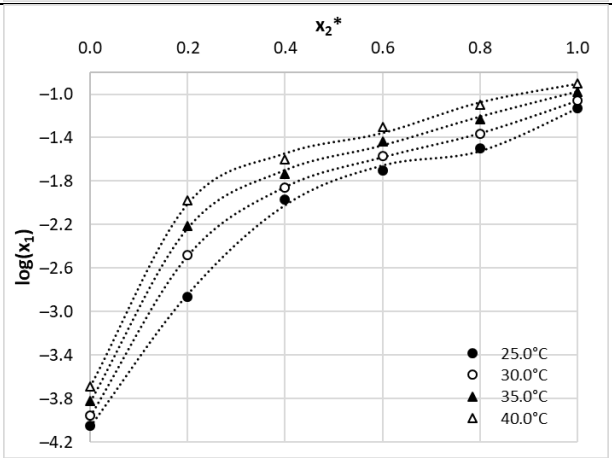
API+solvent	Solubility vs. binary solvent composition	API+solvent	Solubility vs. binary solvent composition
A+propylene glycol+water [4][3][5]		A+transcutol+water [7](*)	
A+acetonitrile+water [2]		A+1,4-dioxane+water [18] (*)	

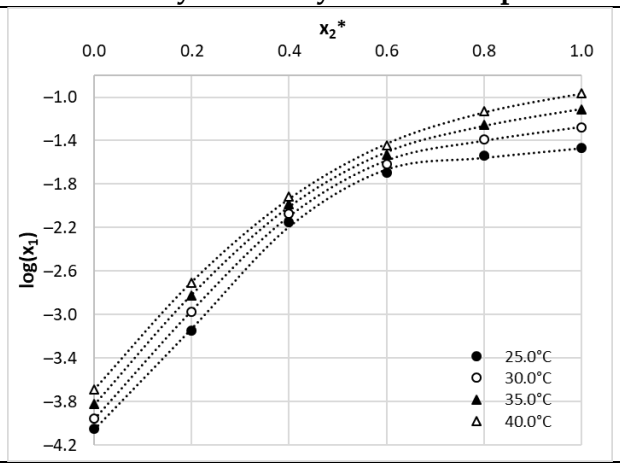
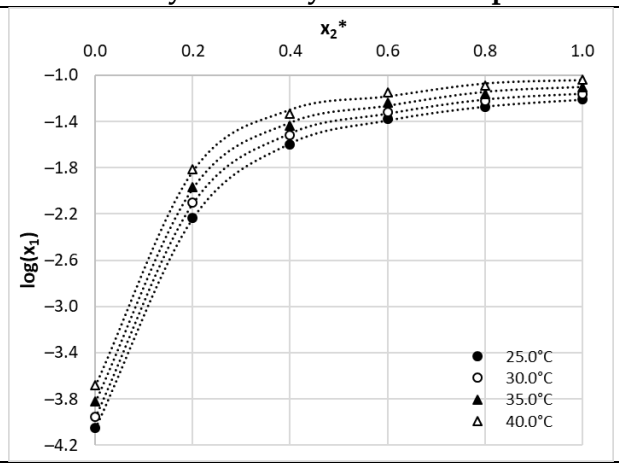
API+solvent	Solubility vs. binary solvent composition	API+solvent	Solubility vs. binary solvent composition
A+ethanol+propylene glycol [20]		A+ethanol+ethyl acetate [19]	
A+4-formylmorpholine +water [this work]		A+DMF+water [this work]	

API+solvent	Solubility vs. binary solvent composition	API+solvent	Solubility vs. binary solvent composition
A+DMSO+water [this work]			

(*)these system challenged the JA model leading to inaccurate back-computed solubility values in regions of high concentration of organic solvent.

Table S4. The data collection of phenacetin solubility in binary solvent mixtures [22,23,28]. The optimized values of parameters of the Jouyban-Acree model [27] model applied to phenacetin solubility in binary solvents are provided in the table in an additional supporting file (see Supplementary Materials S2 in "binary solvents").

API+solvent	Solubility vs. binary solvent composition	API+solvent	Solubility vs. binary solvent composition
P+methanol+water [23,27]		P+1,4-dioxane+water [22,23] (*)	
P+acetonitrile+water [23]		P+DMF+water [23] (*)	

API+solvent	Solubility vs. binary solvent composition	API+solvent	Solubility vs. binary solvent composition
P+DMSO+water [23]		P+4-formylmorpholine+ water [this work]	

(*)these system challenged the JA model leading to inaccurate back-computed solubility values in regions of high concentration of organic solvent.

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