Solubility of Puerarin in Water, Ethanol, and Acetone from (288.2 to 328.2) K

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The solubility of puerarin in water, ethanol, and acetone solutions was measured over the temperature range of (288.2 to 328.2) K. The solubility of puerarin in water increases with increasing temperature, whereas the solubility of puerarin in ethanol and acetone decreases with increasing temperature. The solubility data were correlated with the Apelblat equation.

Introduction

Puerarin, a naturally occurring isoflavone *C*-glycoside, was isolated from *Pueraria lobota*,[1] one of the most popular Chinese herbal medicines that is traditionally used to reduce febrile symptoms and is also used as an anti-inebriation agent.[2] The chemical name of this compound is 8-*β*-D-glucopyransyl-7-hydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one. Figure 1 shows the chemical structure of puerarin. The biomedical effects of puerarin, which have been experimentally or clinically demonstrated,[3,4] include the improvement of blood circulation, prevention of cardiovascular diseases, control of alcoholism,[5] and treatment for arrhythmia.[6]

For pharmaceutical use, puerarin is usually extracted from the powdered Radix puerariae using solvents such as water, alcohols, or mixtures of those, followed by purification and crystallization from the solution.[1] Another way to obtain this compound is to synthesize it.[7] Therefore, it is important to have thermodynamic data for the solubility of puerarin in different solvents.

In the present study, the solubility of puerarin in water, ethanol, and acetone over the temperature range of (288.2 to 328.2) K was measured, where the concentrations were determined by ultraviolet spectrophotometry (UV).

Experimental Section

Reagents and Apparatus. Puerarin ($C_{21}H_{20}O_9$, [3681-99-0]) of pharmaceutical purity grade was kindly provided Zhejiang Chemical Reagent Plant (China). All samples of puerarin used without further purification were dried in vacuum at (105 to 110) °C for 2 h. Other reagents used such as ethanol and acetone were of analytical purity grade, and redistilled deionized water was used throughout.

The absorbance measurements of samples were carried out on a Spectrnblab 52 spectrophotometer (Lengguang Instrument Factory, Shanghai, China).

Sample Preparation. An excess amount of puerarin was added to the solvents in a specially designed sealed dual-wall flask. Between the outer and inner walls of the flask, water at constant temperature was circulated. The temperature of the circulating water was controlled by a thermostat within ±0.1 K. The solution was constantly stirred using a magnetic stirrer. After attaining equilibrium, the stirrer was turned off to let the solution settle for 2 h.[8] Then the upper portion was taken, filtered, and poured into a 50-mL volumetric flask. To prepare the solutions for UV analysis, they were diluted to 50 mL with redistilled water.

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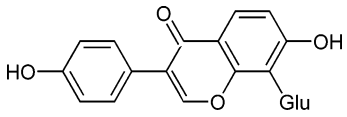

Figure 1. Molecular structure of puerarin.

Table 1. Solubility *c* of Puerarin in Water (1), Ethanol (2), and Acetone (3)

T/K	10^2c_1	$10^2(c_1 - c_1^{calcd})$	10^2c_2	$10^2(c_2 - c_2^{calcd})$	10^2c_3	$10^2(c_3 - c_3^{calcd})$
			mol·L^{-1}			
288.2	0.81	0.01	29.54	0.02	3.25	−0.03
293.2	0.95	0.02	26.01	−0.16	3.00	−0.03
298.2	1.10	0.01	23.02	−0.23	2.80	−0.01
303.2	1.26	−0.02	20.81	0.11	2.70	0.09
308.2	1.42	−0.08	18.60	0.14	2.50	0.07
313.2	1.71	−0.04	16.60	0.11	2.32	0.05
318.2	2.02	−0.03	14.22	−0.54	2.11	−0.01
323.2	2.43	0.03	12.98	−0.26	2.01	0.03
328.2	2.84	0.03	12.00	0.10	1.88	0.01

Sample Analysis. To determine the puerarin concentration in the solution, the absorbance of the standard and sample was measured at 310 nm because the maximum absorption wavelength of puerarin is $\lambda_{max} = 308$ nm. The calibration curve for the estimation of puerarin was prepared by using the standard solutions in the appropriate concentration range.

Results and Discussion

The solubility data of puerarin in pure water, ethanol, and acetone at different temperatures are presented in Table 1. The solubility of puerarin in ethanol is higher than in water and acetone. The solubility in pure water is the lowest.

The experimental data show that the solubility of puerarin in water increases with increasing temperature; however, its solubility in ethanol and in acetone decreases with increasing temperature. The reason for this phenomenon needs to be studied further.

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Table 2. Parameters of Equation 1 for Puerarin in the Solvents

solvent	*A*	*B*	*C*	10^3rmsd
water	−124.5	2967	19.32	0.36
ethanol	38.3	2.72	−6.99	7.39
acetone	6.23	1250	−0.270	4.54

The temperature dependence of puerarin solubility in pure solvents can be described by the modified Apelblat equation[9−11]

$$\ln(c/\mathrm{mol\cdot L^{-1}}) = A + \frac{B}{T/\mathrm{K}} + C\ln(T/\mathrm{K}) \qquad (1)$$

where c is the solubility of puerarin, T is the absolute temperature, and A, B, and C are parameters. The different values between the experimental solubility and the calculated solubility of puerarin are also given in Table 1. The values of parameters A, B, and C and the root-mean-square deviations (rmsd's) are listed in Table 2. The rmsd is defined as

$$\mathrm{rmsd} = \sqrt{\frac{\sum_{i=1}^{N}(c_i^{\mathrm{calcd}} - c_i)^2}{N}} \qquad (2)$$

where N is the number of experimental points, c_i^{calcd} represents the solubility calculated, and c_i represents the experimental solubility values.

From the data listed in Table 2, it can be seen that the calculated solubilities show good agreement with the experimental values, which indicates that the modified Apelblat equation is fit to correlate the solubility data of puerarin in the three solvents.

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