



## Partition study of caffeic and p-coumaric acids from aqueous two-phase system composed of ethanol + ammonium sulfate + water at 298 K.

Giovana C. A. Netto\*, Fernanda P. Pelaquim, Mariana C. Costa.

### Abstract

Vascular plants synthesize attractive pharmacological compounds of which phenolic acids stand out. Caffeic acid and p-coumaric acids belonged to that category of compounds and they are found in almost every plant. Since their importance and wide range of applications, the aim of this study is to evaluate the partition coefficient (K) and the separation efficiency ( $\eta$ ) of the two acids from an aqueous two-phase system (ATPS) composed of ethanol + ammonium sulfate + water at 298 K. Liquid-liquid equilibrium (LLE) data were obtained by the determination of the binodal curve and the tie-lines, using cloud point and gravimetric methods, respectively. After that, using known concentrations in the biphasic region, the partition coefficient and the separation efficiency were determined. For the caffeic acid, the values obtained were, in order, 14.95 and 90.75%. And, for the p-coumaric acid, the values were 22.20 and 94.47%. Both compounds showed more affinity for the alcoholic phase and can be extracted using the ATPS studied.

### Key words:

Liquid liquid equilibrium, caffeic acid, p-coumaric acid.

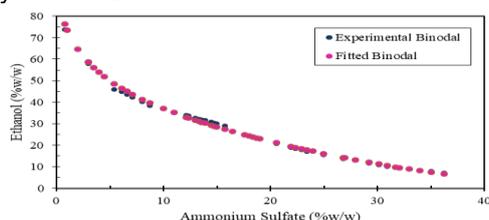
### Introduction

Vascular plants synthesize phenolic compounds that are very important and present a wide range of applications, of which the caffeic acid and the p-coumaric acid stand out. An alternative separation method for phenolic bio compounds is the extraction using ATPS. It was chosen to work with a system formed by ethanol + ammonium sulfate + water at 298 K, since these solvents are nontoxic and easy to recover. The competition between the salt and the alcohol for the water leads to the formation of two phases, what is called salting out. And the partition of the molecule of interest occurs due to the difference of affinity for the phases of the heterogeneous system formed. So, the objective of this work was to study the partitioning of caffeic and p-coumaric acids from the ATPS proposed based on the LLE.

### Results and Discussion

The binodal curve of the ATPS composed of ethanol + ammonium sulfate + water at 298 K is depicted in Image 1. It was determined by the cloud point method and fitted to Merchuck's model, which parameters are showed in Chart 1. As we can see by the high value of the correlation coefficient, the experimental binodal was well fitted to the model used. The tie lines were determined by the gravimetric method and they can be found in Image 2.

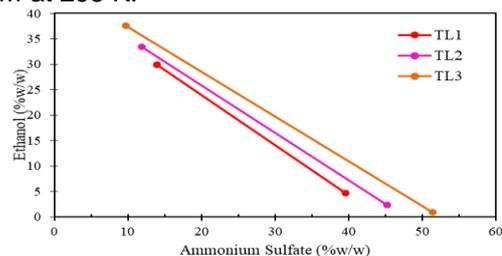
**Image 1.** Binodal curve of ethanol + ammonium sulfate + water system at 298 K.



**Chart 1.** Fitted parameters from Mechuck's equation for the binodal of ethanol+ ammonium sulfate+ water at 298 K.

A	B	C	R <sup>2</sup>
1E+02	-3.09E-01	1.83E-05	0.9953

**Image 2.** Tie-lines of ethanol + ammonium sulfate + water system at 298 K.



Mixtures in the biphasic region were chosen and prepared for the determination of the partition coefficient and the separation efficiency of the phenolic acids using the ATPS proposed. For the caffeic acid, the values were 14.95 and 90.75%, respectively, and for the p-coumaric acid, the same parameters were 22.20 and 94.47%. Both compounds were well extracted using this ATPS and both showed more affinity for the alcoholic phase.

### Conclusions

The ATPS composed by ethanol + ammonium sulfate + water at 298 K was studied for the partitioning of caffeic and p-coumaric acids. The experimental binodal of the system was well fitted to Merchuck's model with  $R^2 = 0.9953$ . And the tie lines were parallel and well anchored to the binodal.

Regarding to the partition, the caffeic acid's partition coefficient obtained was 14.95 and the separation efficient was 90.75%. The same parameters were determined for p-coumaric acid and were 22.20 and 94.47%. Therefore, this ATPS can be used for the extraction of the phenolic acids studied.

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