ULST Timisoara
Multidisciplinary Conference on Sustainable Development
30-31 May 2024

Fast and slow reaction kinetics of 2,2-diphenyl-1-pycryl-hydrazyl with antioxidant compounds in *Castanea sativa* Mill. hydrophilic extracts

Agnes Cupin [1], Răzvan L. Drăghici [2], Mădălin-Rareș Bozeșan-Drehe [1], Nicoleta G. Hădărugă [2,3], Daniel I. Hădărugă [1,2,*]

[1]*Department of Applied Chemistry, Organic and Natural Compounds Engineering, Polytechnic University of Timișoara, Vasile Pârvan Bd. 6, 300223-Timișoara, Romania*
[2]*Doctoral School "Engineering of Vegetable and Animal Resources", University of Life Sciences "King Mihai I" from Timișoara, Calea Aradului 119, 300645-Timișoara, Romania*
[3]*Department of Food Science, University of Life Sciences "King Mihai I" from Timișoara, Calea Aradului 119, 300645-Timișoara, Romania*
**daniel.hadaruga@upt.ro*

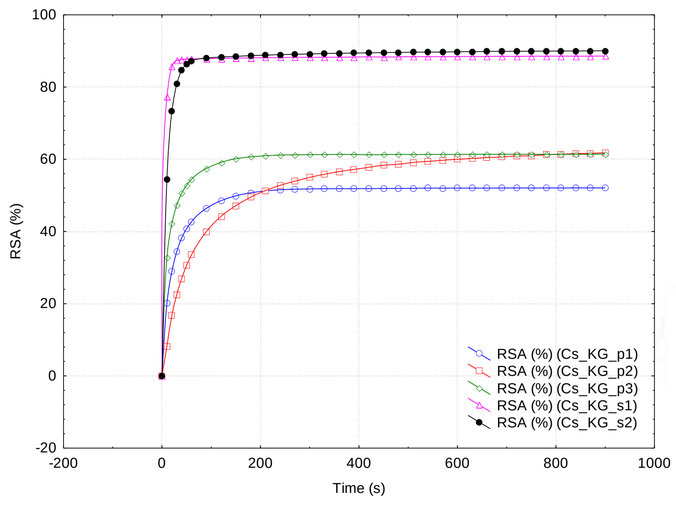
INTRODUCTION

Castanea sativa Mill. (Fagaceae) is the well-known **sweet chestnut** having edible seeds. Both pulp and shell of the chestnut fruit contain antioxidant polyphenols, but their composition differ. Among moisture, starch, sugars, proteins, fats, organic acids, vitamins and minerals, chestnut pulp is a good source of polyphenols (other than vitamins and pro-vitamins – tocopherols, ascorbic acid and carotenoids) such as gallic and ellagic acids. On the other hand, chestnut shell (pericarp and integument – outer and inner shells) contain a wide range of antioxidant compound classes, including phenolic acids and derivatives (ellagic acid, caffeic acid derivatives), flavonoids and derivatives (catechin, epicatechin, epigallocatechin, apigenin-7-*O*-rutinoside, luteolin-7-*O*-rutinoside, oligomeric proanthocyanidins, as well as various ellagitannins). Consequently, the ***antioxidant activity*** of both chestnut **pulp** and **shell** parts is important.

The **goal** of the study was to evaluate the reaction kinetics of the radical 2,2-diphenyl-1-pycryl-hydrazyl (DPPH·) with the overall mixture of antioxidants from the chestnut pulp and shell hydrophilic extracts, using **"fast"** (0-30 s) and **"slow"** (up to 180 s) reaction concepts.

MATERIALS AND METHOD

The ethanolic extracts were obtained from pulp and shell of the edible chestnut (*"KG"* variety, Figure 1 - middle) by Soxhlet method. The DPPH· reaction was monitored for 15 min at 517 nm in the presence of extracts after dilution with ethanol (1:1:4 volume ratio). The radical scavenging activity, $RSA = 100*(1-Abs_t/Abs_0)$, was significant (Figure 1 - left), especially for the shell extracts (89-90%). *RSA* values of 52-62% were obtained for the pulp extracts.



Castanea sativa Mill. var. *"KG"*

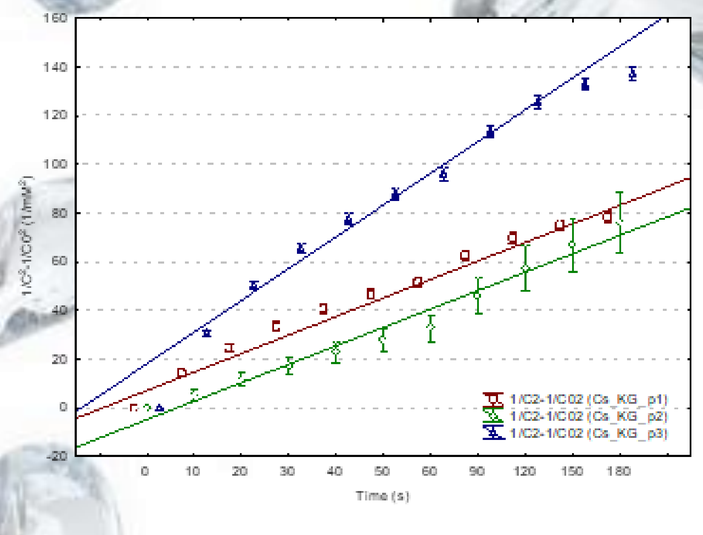


Figure 1. *RSA vs. Time* variation (left) and third-order kinetic model (right) for the reaction of DPPH· with the antioxidant compounds in *Castanea sativa* Mill. var *"KG"* extracts (middle)

RESULTS AND DISCUSSION

According to the statistical parameters, the best kinetic results were obtained for the third order reaction model, with the reaction rate of k_3 = 1.28(±0.80) [1/mM^2/s] for the fast reaction, and k_3 = 0.50(±0.15) [1/mM^2/s] for the slow reaction in the pulp extracts (Figure 1 – right).

The half-life values were $t_{1/2(3)}$ = 38.5(±23.8) [s] and $t_{1/2(3)}$ = 79.2(±20.7) [s], respectively.

On the other hand, the kinetic behavior of the shell extracts was completely different. Only the fast reaction could be modelled with good statistical results, with the same third-order reaction model but significantly higher rate constant in comparison with the pulp samples (k_3 = 46.9(±27.4) [1/mM^2/s], $t_{1/2(3)}$ = 1.2(±0.7) [s]).

CONCLUSION

The kinetic results for the fast and slow reaction proved that the edible chestnut shells have higher antioxidant activity and complex antioxidant compound mixture, with possible applications of the chestnut waste (e.g., in food or cosmetic fields).

REFERENCES:
[1] De Vasconcelos *et al.*, *J. Agric. Food Chem.* **2007**, *55*, 3508-3516.
[2] Pinto *et al.*, *J. CO_2 Util.* **2020**, *40*, 101194.
[3] Hădărugă, D.I.; Hădărugă, N.G., Chemistry, Functionality, and Applications of Flavonols. In: Jafari, S.M.; Rashidinejad, A.; Simal-Gandara, J. (eds.), *Handbook of Food Bioactive Ingredients. Properties and Applications*, Springer Nature Switzerland AG, Cham, **2023**, pp. 1-63, https://doi.org/10.1007/978-3-030-81404-5_5-1.