The 7th International Electronic Conference on Medicinal Chemistry (ECMC 2021)
01–30 NOVEMBER 2021 | ONLINE

Preliminary studies towards influence of simulated digestion on antioxidant activity of selected monoterpenes

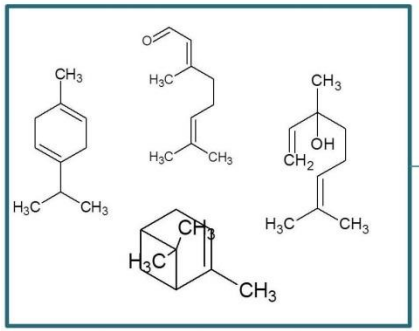
Karolina Wojtunik-Kulesza[1,*], Anna Oniszczuk[1]

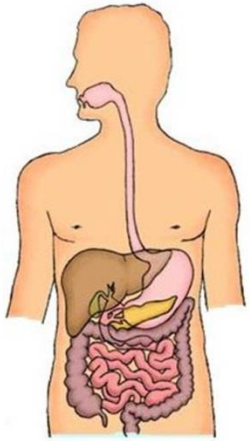
[1] Department of Inorganic Chemistry, Medical University of Lublin, Poland
* Corresponding author: karolina.wojtunik@umlub.pl

Preliminary studies towards influence of simulated digestion on antioxidant activity of selected monoterpenes

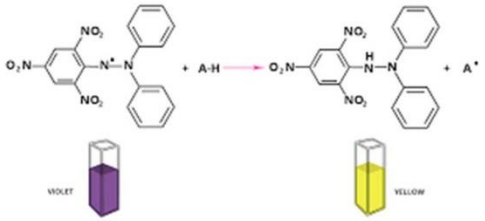
Simulated digestion (*in vitro* conditions)

- Gastric stage
- Duodenal stage





Positive and negative influence on antioxidant activity of selected monoterpenes



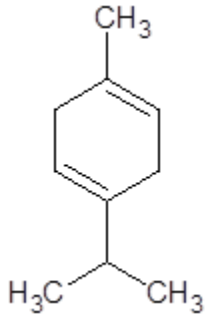
One of the most valuable activity of substances used in pharmacy is antioxidant. One of possible way to protect our cells against oxidative stress is scavenging free radicals through the action of antioxidant. It is known that the level of activity of compounds varies significantly between in vitro and in vivo conditions. Additional significant factor is digestive system along with enzymes and pH in its various parts. In order to approximate the influence of these conditions, simulated digestion was performed.

The basis of the studies was selected monoterpenes which were underwent two steps of simulated digestion: gastric and duodenal. Obtained results revealed both positive and negative influence of the process on antioxidant activity of monoterpenes. Detailed analysis revealed that the changes can be associated with biotransformation of the compounds by the reaction environment and digestive enzymes.

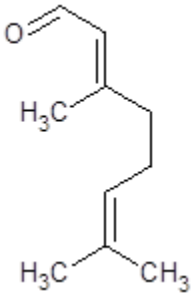
Keywords: antioxadants; monoterpenes; simulated digestion

A few words about monoterpenes…

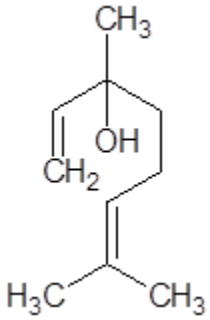
- Natural substances which are one of the main components of essential oils
- Diversified structure of compounds
- Various pro-health and biological activities



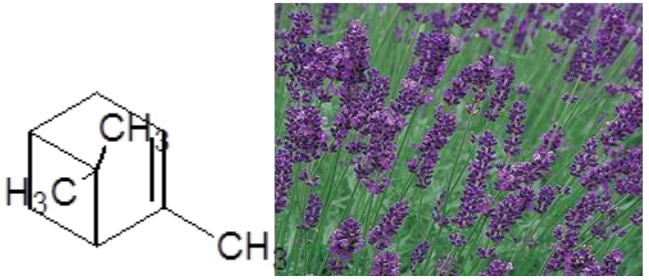
γ-Terpinene



Citral



Linalool

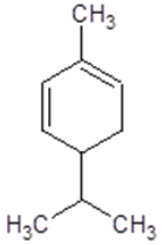


α -Pinene

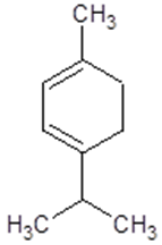
Aim of the study

Determination the influence of simulated digestion (gastic and duodenal stages) on antioxidant activity of selected monoterpenes

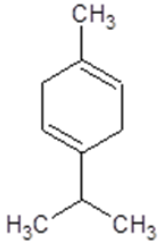
Methodology



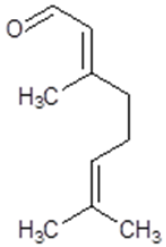
α-phellandrene



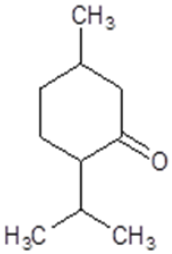
α-terpinene



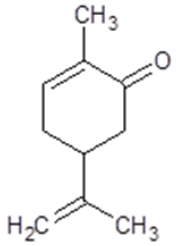
γ-terpinene



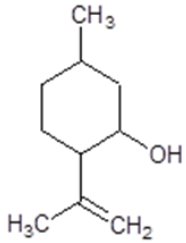
citral



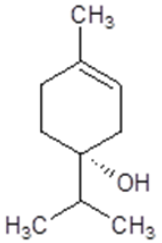
menthone



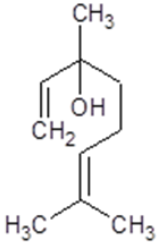
carvone



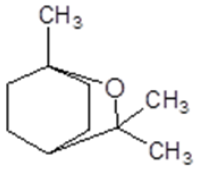
isopulegol



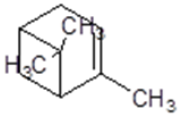
terpinene-4-ol



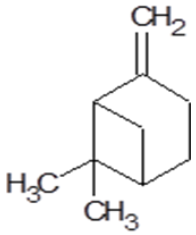
linalool



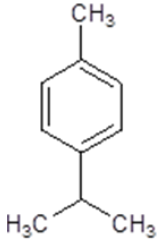
eucalyptol



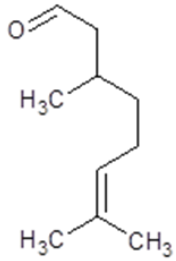
α-pinene



β-pinene



p-cymene



citronellal

Simulated digestion

Gastric stage

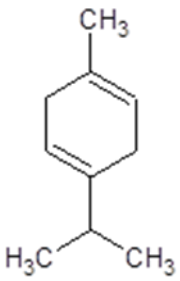
1. Gastric solution + monoterpene
2. Manual stirred for 4 minutes
3. Addition HCl + H_2O to pH 2.2
4. Incubation at 37°C in a shaking water bath
5. Sample drawing from water and oil phases
6. Spectrophotometric measurement with DPPH

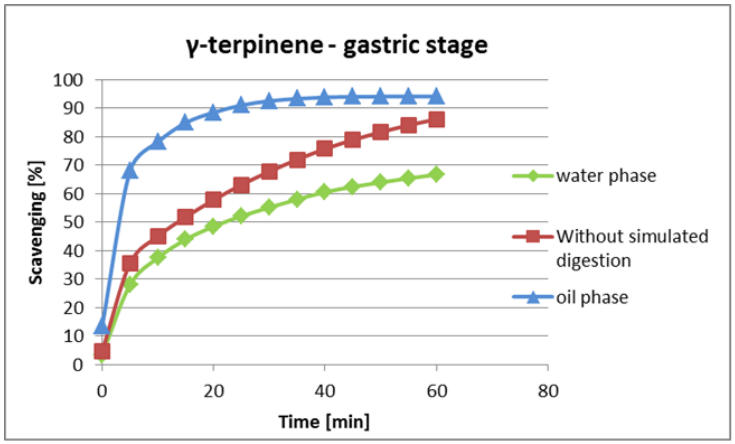
Duodenal stage (after gastric stage)

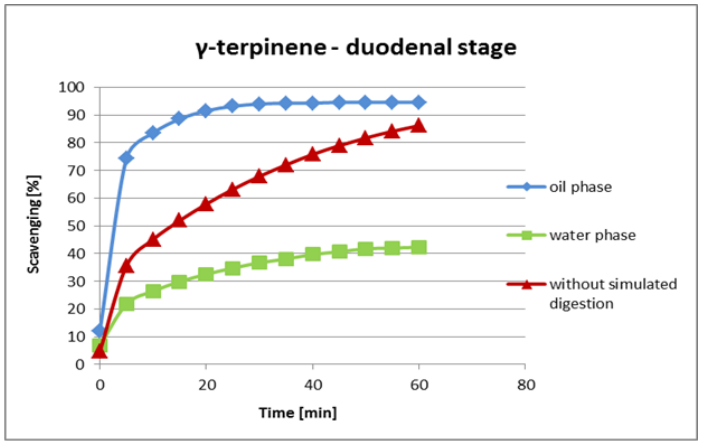
1. ‚gastric sample' + sodium bicarbonate to increase pH to 5.5
2. Addition duodenal solution
3. Addition sodium bicarbonate to pH 6.7
4. Incubation at 37°C in a shaking water bath
5. Sample drawing from water and oil phases
6. Spectrophotometric measurement with DPPH

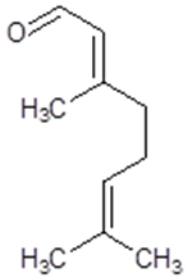
Studies results

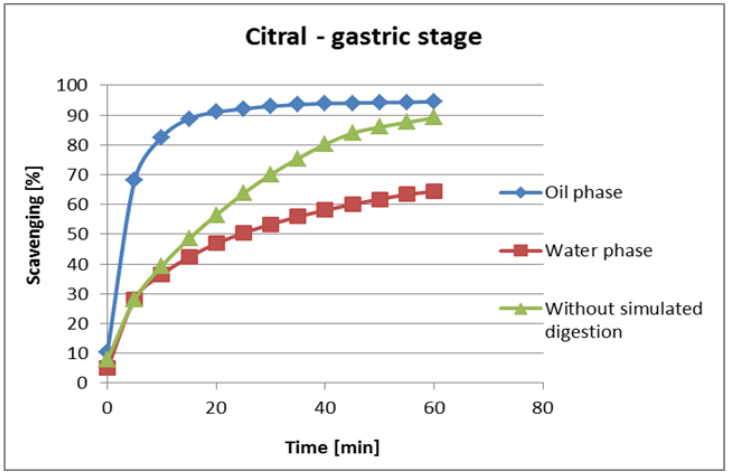
- Positive influence of digestion – oil phase

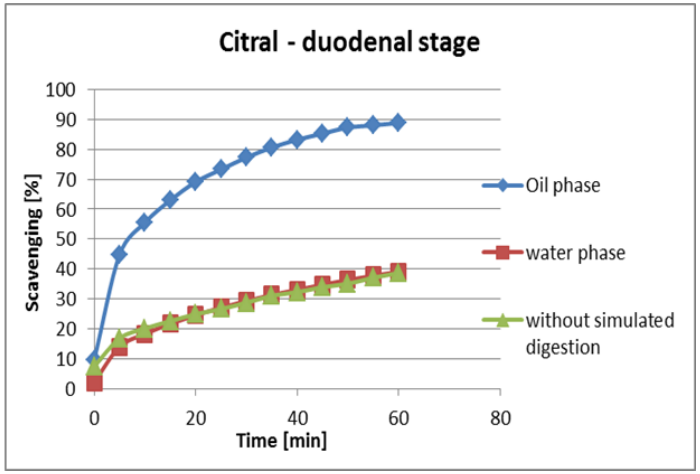




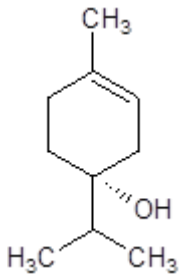


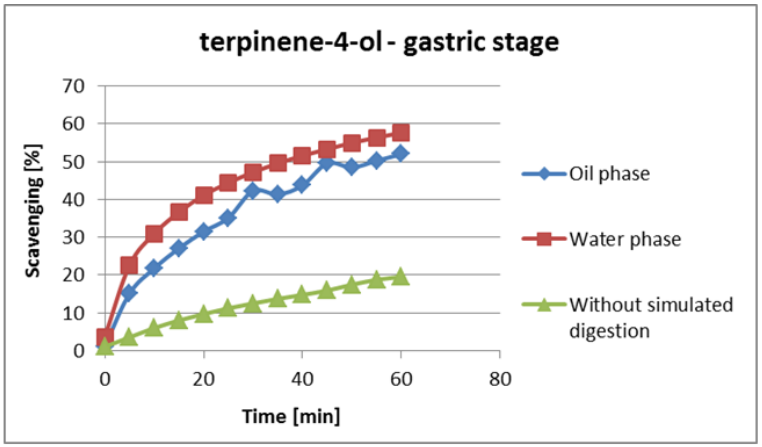


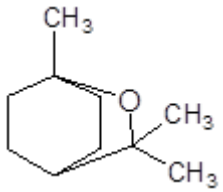


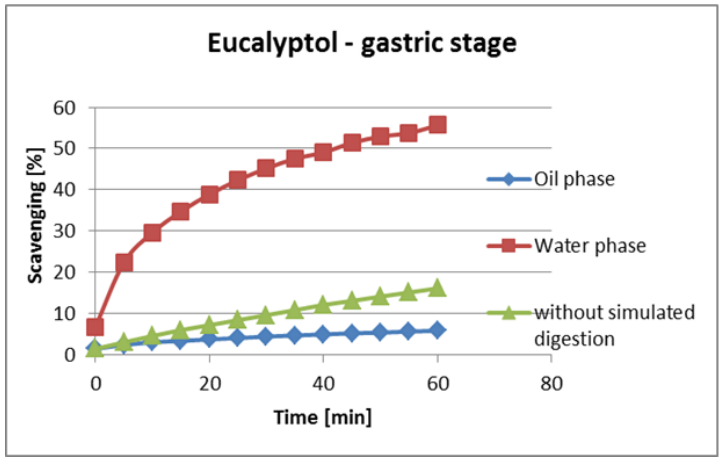


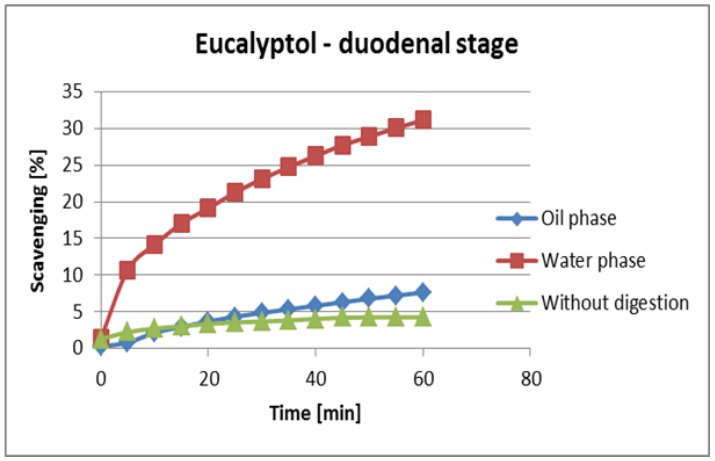
- Positive influence of digestion – water phase











Conclusions

- In most cases, simulated digestion caused increase in free radical activity of monoterpenes
- Both oil phase and water phase in gastric and duodenal stages revealed monoterpenes able to scavenge free radicals
- There is not example of negative influence of both oil and water phase on antioxidant activity of monoterpenes
- Differences in antioxidant activity were conditioned by monoterpenes' structure and their solubility in water-oil phase
- Antioxidant activity of monoterpenes can be significantly higher in our organism in comparison to *in vitro* conditions

Thank you for your attention !