



**Internship subject KREATiS 2026 in collaboration
with IPCMS at Strasbourg University**

Determination of the photoinduced (auto)oxidation potential: determination of chemical structures and mechanistic studies

Internship : Autooxidation

Start date : February 2026

Length : 6 months

Locality : IPCMS, 23 Rue de Loess, Strasbourg, France (<https://www.ipcms.fr/>)

Level of diploma : Master 2 / Bac+5

Context

The photoinduced (aut)oxidation of chemical substances generates biological effects observed in various organisms. The investigation of skin sensitization in humans (also known as contact allergy) induced by chemicals is required by chemical regulations in the broad sense (REACH, cosmetics regulations, pesticides, biocides, medical devices, etc.). Skin sensitization can also be induced by substances that are generated by photochemical processes such as the photoinduced (aut)oxidation of fragrances. The Master 2 internship will be performed in the context of a research collaboration with KREATiS which is a pure in silico R&D company. (<https://www.kreatis.eu/>)

The training will be located in the laboratory of IPCMS at Strasbourg University under the supervision of Pr. Hoffmann; if you are interested, please send him your CV and cover letter.

Supervisor: Norbert Hoffmann norbert.hoffmann@ipcms.unistra.fr (<https://www.ipcms.fr/en/norbert-hoffmann-2/>)

Purpose

Substances belonging to different families such as terpenes, aromatics or ketones will be irradiated with light under various conditions (different light sources, presence or absence of oxygen, different reaction media, ...). The relative rates of the decomposition or autooxidation will be determined for a number of compounds. In cases of photo-instability, the structure of degradation or oxidation products will be determined – mainly by NMR analysis of isolated and purified compounds – which will enable us to discuss reaction mechanisms. These detailed studies will be performed on 2 to 3 compounds belonging to different families.

For the project needs, a training will be given to the intern in order for him/her to have a sufficiently high level of understanding of the subject. Good analytical skills and a B2 level of English are needed.

The meeting with the KREATiS chemists is scheduled at the beginning of the internship.

At the end of the project the intern will have a good understanding of organic photochemical reactions, in particular oxidations and an insight in the domain of skin sensitization caused by such reactions.

References

- (1) J.-F. Rontani, S. T. Belt, Photo- and autooxidation of unsaturated algal lipides in the marine environment: An overview of processes, their potential tracers, and limitations. *Org. Geochem.* **2020**, 139, 103941. [Link](#)
- (2) J. Lin, J. N. Apell, K. McNeill, M. Emberger, V. Ciraulo, S. Gimeno. A streamlined workflow to study direct photodegradation kinetic and transformation products for persistence assessment of a fragrance ingredient in natural waters. *Environ. Sci.: Processes Impacts* **2018**, 21, 1713-1721. [link](#)
- (3) E. Ay, V. Gérard, B. Graff, F. Morlet-Savary, W. Mutilangi, C. Galopin, J. Lalevée. Citral Photodegradation in Solution: Highlighting of a Radical Pathway in Parallel to Cyclization Pathway. *J. Agric. Food Chem.* **2019**, 67, 3752-3760. [Link](#)