NATO SPS ASI G5535 CETRARO 2019 “DETECTION, DIAGNOSIS, AND HEALTH CONCERNS OF TOXIC CHEMICAL BIOLOGICAL AGENTS”

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Applications of LC-MS for Detection of some Chemicals and their Metabolites in Water

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CONTEXT

Surface waters are at risk from certain specific chemicals (priority substances) that could cause harm to the aquatic ecosystem (fish, plants, food chain, etc.) or affect human health through exposure to water (e.g. drinking, bathing, seafood, etc.). The Water Framework Directive (WFD) [1] requires the Commission to come forward with a strategy on pollution of surface waters. The European Directive 2000/60/CE stresses the need of adopting measures against water pollution in order to achieve a progressive reduction of contaminants and recuperate water for new uses.

Crossed benefits of wastewater reuse.

OBJECT – APPROACH

The main objective is the application of LC-MS for the identification of polluting chemical compounds and their degradation intermediates in water. In this poster some results are reported about the identification of:

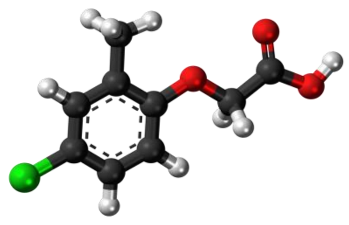
- tetra-hydro-cannabinol (THC) and other metabolites of Cannabis found in real water samples collected from the effluent of a wastewater treatment plant (WWTP) in Vila Nova De Gaia (Portugal),
- levofloxacin and MCPA and their metabolites in water samples undergone heterogeneous photocatalytic degradation using titanium dioxide coatings (TIO_2).

RESULTS

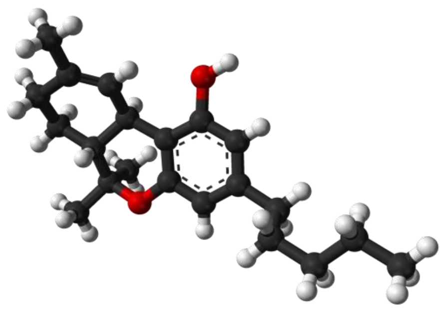
Results of this investigation show as the mass spectrometry is very important for the detection of different polluting chemicals at low concentration. Our and literature findings demonstrate that

- traditional water treatments are not able to remove contaminants from wastewater and consequently recalcitrant pollutant water can entry the water cycle;
- the heterogeneous photo-catalytic system tested in our experiments is able to degrade the chemicals used as model molecules and may find application in the remediation of water contaminated with recalcitrant residues due to poor efficiency of treatment plants normally adopted for the purification of wastewater.

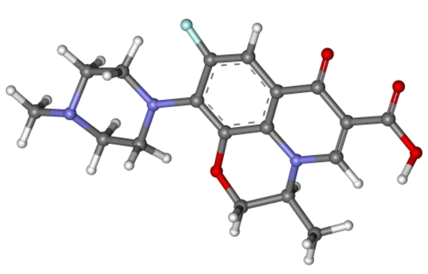
COMPOUNDS STUDIED



(4-Chloro-2-methylphenoxy) acetic acid (MCPA, herbicide)



(−)-(6aR,10aR)-6,6,9-trimethyl- 3-pentyl-6a,7,8,10a-tetrahydro- 6H-benzo[c]chromen-1-ol (Tetrahydrocannabinol, drug)



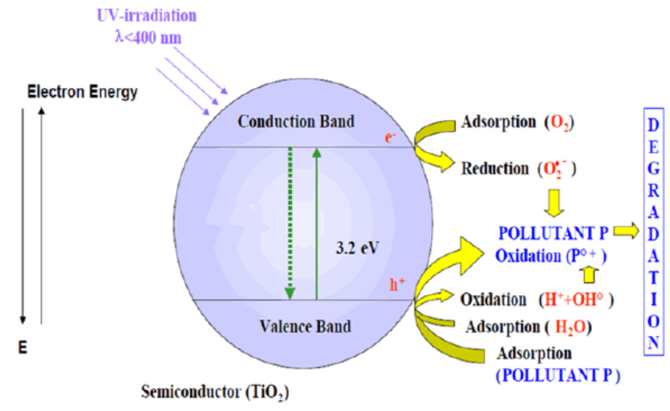
(-)-(S)-9-fluoro-2,3-dihydro-3-methyl-10-(4-methyl-1-piperazinyl)-7-oxo-7H-pyrido[1,2,3-de]-benzoxazine-6-carboxylic acid hemihydrate (Levofloxacin, pharmaceutical)

- **To obtain** accurate masses and molecular formulae,
- **to identify** unknown or unexpected and unusual metabolites,
- **to suggest** degradation pathways

the structural identification of parent molecules and derivatives in very low concentrations represents a great benefit for environmental analytical purposes

PRINCIPLE

Advanced Oxidation Processes (AOPs) are promising ways to perform the mineralization of pollutants. AOPs are characterized by the in situ production of hydroxyl radicals, which are highly reactive species capable of oxidizing organic materials in a non-selective way.

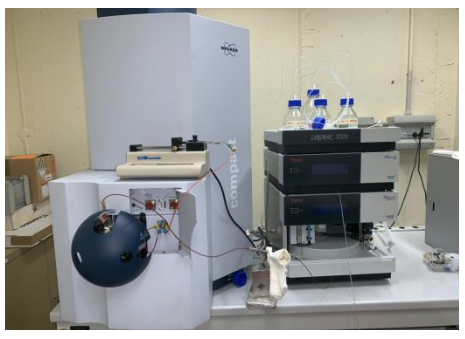


Mechanism of TiO_2 catalytic degradation of organic pollutants.

INSTRUMENTAL

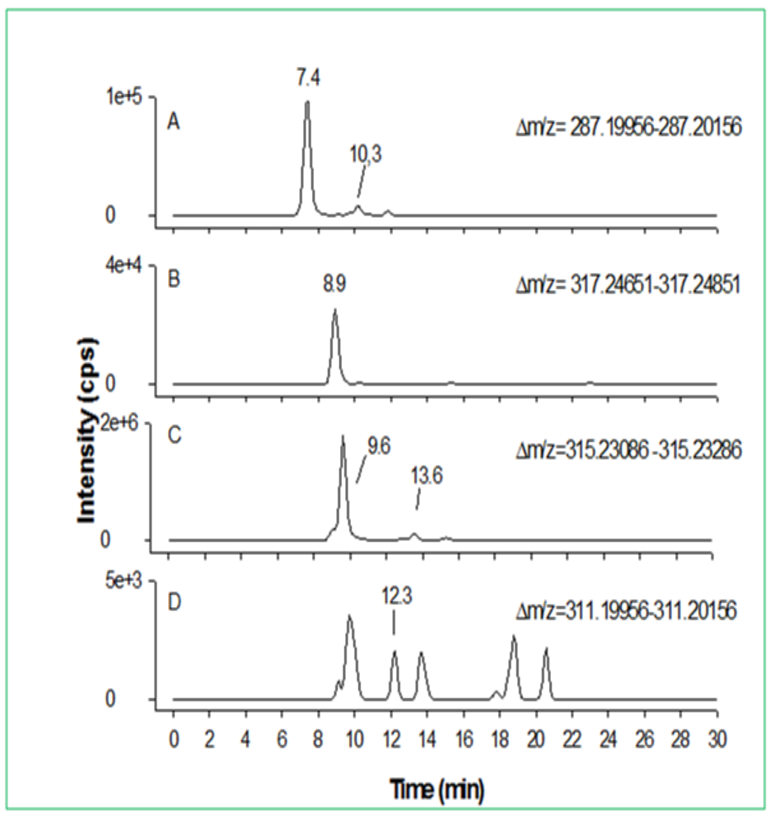
Photodegradation System used for assays on levofloxacin and MCPA

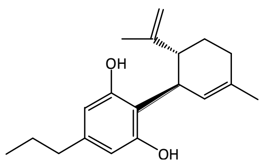
HPLC System



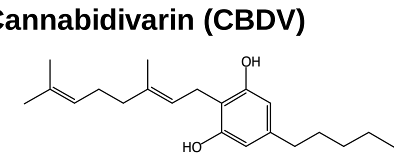
LC system coupled with micrOTOF-Q-II-Mass Spectrometer

COMPOUNDS IDENTIFIED

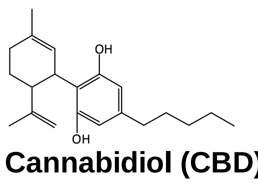




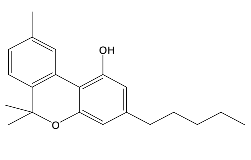
Cannabidivarin (CBDV)



Cannabigerol (CBG)

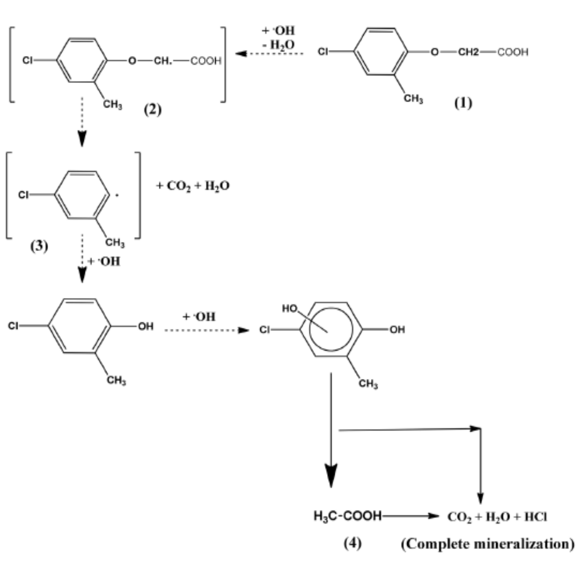


Cannabidiol (CBD)

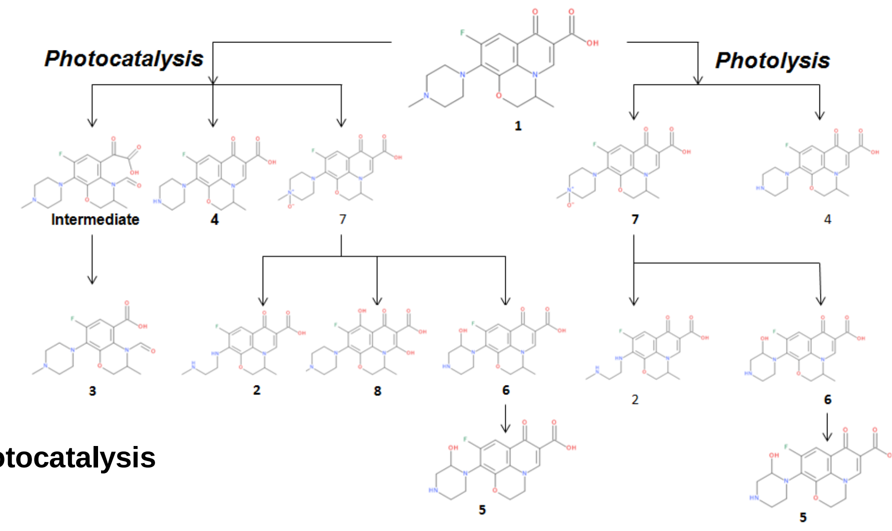


Cannabinol (CBN)

Extracted ion chromatograms using LC-ESI- MS acquired in ESI+ mode of a sample of *Cannabis sativa* L. extract.
The ion monitored are displayed in each trace and peak numbers correspond to (A) CBDV, (B) CBG, (C) CBD at 9.6 min and THC at 13.6 min, (D) CBN. For each cannabinoid the molecular structure is reported



Proposed pathway of MCPA photocatalysis



Proposed patway of Levofloxacin photocatalysis

[1] 130 Directive 2000/60/EC (OJ L 327, 22.12.2000, p. 1). For more information on the Water Framework Directive, please refer to europa.eu.int/comm./environment/water.