Evidence of the paracetamol's aromatic ring breaking thanks to a non-thermal plasma

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This study deals with the treatment of drug residue in aqueous media by using non-thermal plasma which may generate many oxidizing species, such as O, OH, O_3, H_2O_2, etc. More precisely, paracetamol solution was treated in a plasma reactor with multiple needle-to-plate structure. The treated solution was analyzed by high resolution mass spectrometry which allowed to determine with certainty several products, such as nitric acid and nitrate ion. But, further experiments, such as the use of labeled paracetamol, were necessary to identify other products like the dicarboxylic acid. The identification of this latter acid showed clearly that the non-thermal plasma enabled to break the paracetamol's aromatic ring.

The advanced oxidation process using non-thermal plasma (NTP) is a promising technique for the treatment of drug residue in aqueous media [1-2]. Indeed, many oxidizing species, such as O, OH, O_3, H_2O_2, etc. are produced by the NTP depending on their experimental conditions.

Our group works on the treatment of paracetamol ($C_8H_9NO_2$) in an aqueous medium by a NTP created in a multiple needle-to-plate reactor [3] and obtained about full degradation of paracetamol under specific conditions [4]. In order to determine the mechanisms of degradation, the treated solution was analyzed by high resolution mass spectrometry (HRMS) using a Q-TOF. Several products, such as nitric acid and nitrate ion, were easily determined with certainty, while others required further experiments as described partly in this communication.

In fact, this communication reports the identification of the dicarboxylic acid in treated solution, and so the evidence of the breaking of the aromatic ring of paracetamol by the NTP, through the investigation of the chemical species, of molecular mass of 199.0481, produced during the treatment. Indeed, the mass peak of high intensity at *m/z* = 198.0413, in negative mode (figure 1), corresponds to the ion having a condensed formula $C_8H_8NO_5^-$. A multitude of skeletal formulas can match the above condensed formula, but by taking into account the structure of paracetamol, only two of them are retained: tetraphenol which is an aromatic compound and dicarboxylic acid which has a broken aromatic ring. The skeletal formulas of these two latter spacies are shown in figure 2. In order to prove that the dicarboxylic acid was produced by plasma, labeled paracetamol with four Deuterium on aromatic ring was used during the degradation by NTP and studies have been made by HRMS and tandem MS technique. The details of these investigations will be presented at the conference.

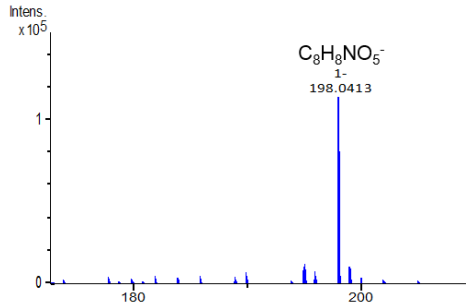

Figure 1. mass spectrum of a paracetamol solution treated by plasma.

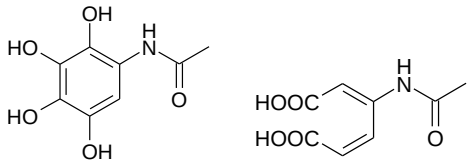

Figure 2. Tetraphenol and dicarboxylic acid skeletal formulas.

References

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