Identification of Transformation Products of Iohexol Performed in Sunlight Simulator using ESI-QQTOF-MS

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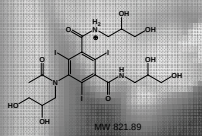
Abstract

Photodegradation of Iohexol under controlled laboratory conditions simulating environmental settings in surface water was studied.
Ionated X-ray media (ICM) are among the most widely used drugs for intravascular administration for imaging of organs or blood vessels during diagnostic tests. Its worldwide consumption is estimated to be about 3.5 million kg per year. They are metabolically stable in the human body and are rapidly eliminated via urine or faeces. Most of these radiographic contrast media, including iohexol, are derivatives of 2,4,6-triiodobenzoic acid possessing polar carboxylic and hydroxylic moieties in their side chains. The potential adverse environmental impact of ICM has been considered since it was discovered that these compounds contribute substantially to organically bound halogens adsorbable on activated carbon (AOX) in hospital wastewater. As a resault of of the high dosages administred and diminished biotransformation in the human body, iohexol is frequently encountered in waste¡water at ug/L levels.

Compound Iohexol (IOX)



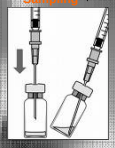
MW 821.89

Sample preparation

Quartz vials

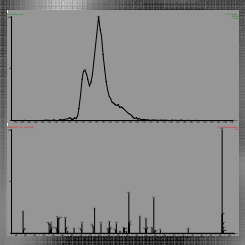
Prepare Solution

Suntest CPS system



Sampling

UPLC-(+)ESI-QqToF-MS



Instrument

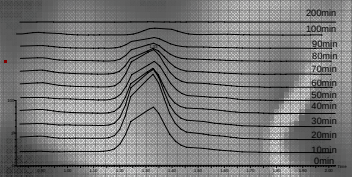
UPLC-(+)ESI-QqToF-MS: Waters Acquity UPLC instrument, equipped with a binary solvent delivery systemand an autosampler. The LC system was coupled to a quadrupole time-of-flight tandem mass spectrometer, QqToF-Micro (Waters Corp., Milford, MA, USA).
Nebulizer gas: 600 L h^{-1}; Desolvation Temp: 350 ° C; Source Temp: 120 ° C; Capillary voltage: 3000 V; Cone voltage: 25 V; Polarity: ES+

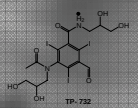
Chromatographic conditions

Column: Waters Waters ACQUITY column UPLC BEH C18 (50 x 2.1 mm, 1.7 μm); flow rate: 400 μL min^{-1}
Mobile phase: A: Acetonitrile; B: 0.04% Formic acid in water
Flow rate: 0.4 mL min^{-1}; Mobile phase; Injection volumn: 10 μL
Gradient:

Time (min)	0.1	3.0	4.0	4.1	5.6	5.7
Mobile phase A (%)	3.0	3.0	25.0	95.0	95.0	3.0

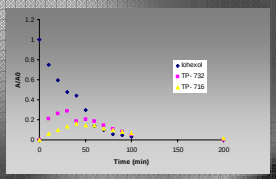
Chromatography and TP Identification



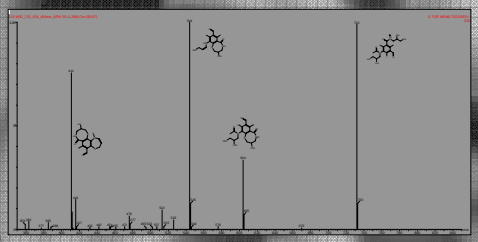


TP- 732

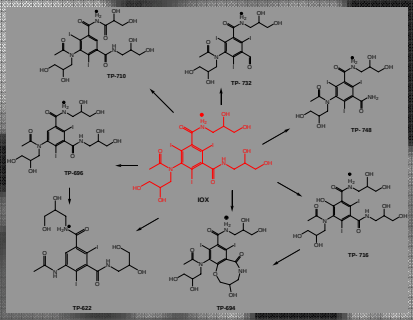
TP- 732 Degradation Kinetics



MS/MS Spectra of Iohexol and TPs



Preliminary Identification of the transformation products of Iohexol



Determination and identification of the iohexol photoproducts in model solutions is of significant interest for its apllication to understanding the fate of iohexol in the environment as it is a significant stakeholder in the Ionated Contrast Media usage. Transformation products present an interesting research path since the Iohexol TPs show further degradation soon after creation which would suggest suitable photodegradation in the environment

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