

IDENTIFICATION OF TRANSFORMATION PRODUCTS BY LIQUID CHROMATOGRAPHY-ADVANCED MASS SPECTROMETRY TECHNIQUES

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In the last years, the occurrence of pharmaceuticals in the aquatic environment has become a growing public concern because of their continuous release and their inherent biological activity that can lead to cause adverse effects on aquatic organisms. Once introduced into the environment, they are subject to transportation, distribution and transformation processes. While some drugs constitute fairly inert molecules that persist in the environment and are difficult to degrade, others can be degraded to transformation products. Degradation processes of pharmaceuticals in natural and engineered systems can aid to attenuate the environmental burden with these xenobiotics; however as a result of the transformation a generation of a complex mixture of parent compounds and transformation products can be found in the environment.

The characterization of transformation products of environmentally relevant pharmaceuticals is still in its infancy. It is only thanks to the availability of sophisticated mass spectrometric instrumentation in many laboratories that breakdown pathways of pharmaceuticals in the natural environment has been started to be elucidated. Besides triple-quadrupole and ion trap analyzers, hybrid instrument such a quadrupole-time of flight, hybrid quadrupole-linear ion trap or LTQ-Orbitrap® are now employed to greatly aid in the identification process. Combinations of different platforms that provide complementary structural information have been proven to be particularly powerful. In this work, examples of the successful identification of transformation products using such approach are presented.

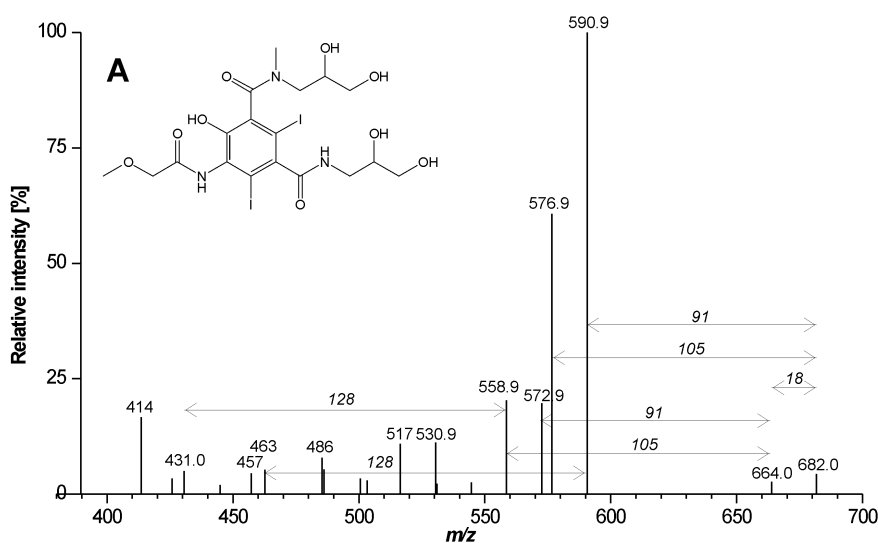


Figure 1 (+)ESI-QqToF-product ion spectrum of a photo transformation product of the X-ray contrast agent iopromide.