

Environmental Chemistry

On-line Monitoring of β -Blockers Ozone Degradation via Electro spray Ionization Mass Spectrometry

Cristina Quispe,¹ Fabiane M. Nachtigall,² Maria Francesca R. Fonseca,² Rosana M. Alberici,³ Luis Astudillo,⁴ Jorge Villaseñor,¹ Marcos N. Eberlin,² Leonardo S. Santos⁵

equispe@utalca.cl

¹Laboratory of Physical-Chemistry, Chemistry Institute of Natural Resources, Talca University, P.O. Box 747, Talca, Chile

²ThoMSon Mass Spectrometry Laboratory, Institute of Chemistry, University of Campinas-UNICAMP, Campinas, SP, 13083-970, Brazil

³Laboratory of Organic Synthesis, Talca University, P.O. Box 747, Talca, Chile.

⁴Laboratory of Asymmetric Synthesis, Talca University, P.O. Box 747, Talca, Chile.

The structures of products and the mechanism of ozone degradation of different pharmaceutical compounds (Figure 1) has been studied. As exemplified herein for three common pharmaceuticals, ESI mass spectrometry (and its tandem version) is a powerful technique able to provide detailed information about organic intermediates connecting parent molecules and final mineralization products during advanced oxidation processes. Under the conditions employed, complete ozone degradation of nadolol was achieved after 100 min. The degradation products obtained in aqueous solution were characterized by electro spray ionization mass (and tandem mass) spectrometry (ESI-MS and ESI-MS/MS). In the proposed mechanism, ozone attacks at the aniline amino group giving rise to nitroaromatic compounds and further degradation occurs via a series of oxidative processes. Continuous on-line monitoring by ESI-MS(/MS) with high accuracy mass measurements showed that ozone degradation of atenolol (ATE) and acebutolol (ACE) occurs via mechanisms similar to that of nadolol. Whereas classical off-line approaches such as GC-MS analysis can handle the more volatile and lighter species, the more polar, relatively unstable, or even transient intermediates or products, which may escape detection by other off-line techniques or on-line techniques based on volatile species, may be intercepted and structurally characterized by on-line and real-time ESI-MS and ESI-MS/MS monitoring¹.

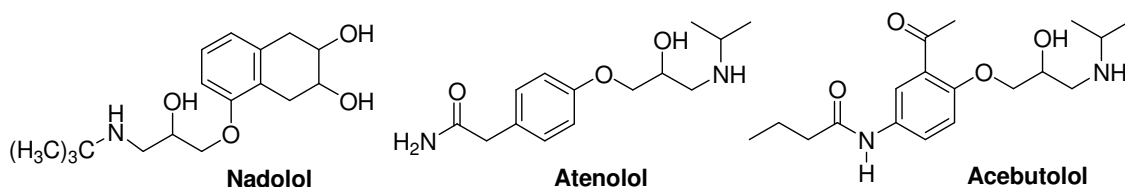


Figure 1. Pharmaceutical compounds to degrade

[1] Santos, L.S. (ed.) In *Reactive Intermediates: MS Investigations in Solution*. Santos, L.S. (ed.), Wiley-VCH **2010**.