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## Automated open-access liquid chromatography high resolution mass spectrometry to support medicinal chemistry projects

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The need of a continuous productivity increase in the pharmaceutical industry motivated the development of new open-access tools on many analytical techniques. On LC, these platforms have been commonly used with low-resolution MS detectors while they have been reported with very limited automation on high-resolution MS spectrometers. Typically, samples with concentration ranges around 0.1 mg/mL are prepared by medicinal chemists for reaction monitoring and for UV purity assessment. Together with the evolution of the instrumentation, new software packages to automatically process HRMS data have appeared. These systems are typically run by specialists and developed for biological samples with compounds in concentrations of µg/mL range. In this work, the development of a fully automated open-access methodology on a UHPLC-DAD/ESI-QTOF system is reported, being applied to medicinal chemistry discovery projects from Janssen R&D. With the first MS conditions applied, accuracies  $<\pm 1$  mDa were not achieved in 20-30% of the cases in ESI+ due to oversaturation. After optimization of MS conditions, a new ESI+ method was implemented. This method has been used by chemists for more than 2,000 compounds from structurally diverse chemical series with a success  $>98\%$  in exact mass determinations. For the other 2% of the samples, specific conditions are used. Upon training, chemists log-in samples and interpret the results by themselves in 90-95% of the cases. To our knowledge, for the first time, full automation has been achieved for an open-access LC-DAD-HRMS platform developed for end-users in a pharmaceutical environment.

### Biography

Alberto Fontana completed his Master of Science in Chemistry from University Autónoma of Madrid. He joined Janssen Research & Development (Spain) in 1998. Since 2001, he works as Scientist in the analytical sciences team. He is focused on analytical LCMS, GCMS and on preparative LC, developing new methodology for Medicinal Chemistry groups, mainly within Neuroscience area. He is currently pursuing his PhD at University of Alcalá de Henares, Madrid. He is the main Author of one publication and Co-author of another five papers. He has presented several posters with his research work on LCMS at different international congresses.

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