

CPAS Focus on Technology: Preparative LC/MS with Automated Fraction Collection System: Agilent 6120 Single Quadrupole Mass Spectrometer with 1260 HPLC-Fraction Collector

In drug discovery workflow and for compound library generation, small molecules must be purified before structures, activities and pharmacological properties can be determined. Liquid chromatography is ideal for separation of compounds from biological sources and synthetic reactions, and serves as a fractionation tool in library screening. Our fully automated Agilent LC/MS system provides on-line UV (DAD) and low resolution ESI-MS (+/-) detection which enables mass-targeted fraction collection (capacity to 60 x 40 mL collection tubes).

Sample application

- System software controls sample injection, separation and collection (select retention time or mass), while minimizing user time.
- Analytical to preparative level separations (mg to gram scale) for reverse -phase conditions using our currently available columns (Phenomenex semi-prep RP, 10 x 250 mm, 5 μ m; Waters PrepLC 25 mm radial compression module with 25 x 100 mm RP column segments (up to 3)).

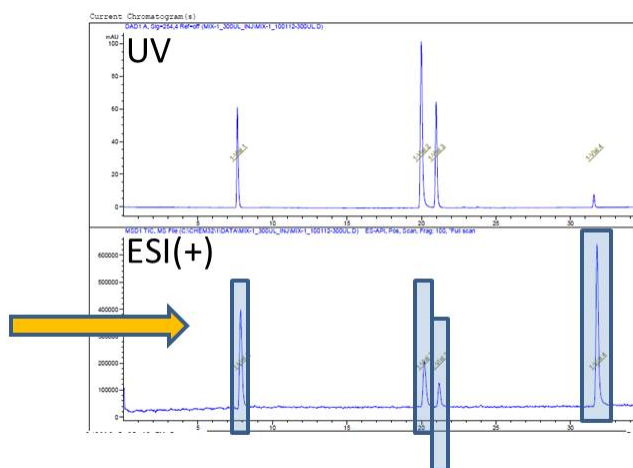


Figure: Agilent 6120 LC/MS (left) and chromatogram (right) of compounds isolated (highlighted in blue) by mass-based collection.

Selected References

- (1) Huber, U. *et al.* "Optimizing mass-based fraction collection for highest purity using Boolean logical -AND-combination with the UV signal", *Agilent Application Note*. **2004**.
- (2) Rolfe, A. *et al.* "S_NAr-Based, Facile Synthesis of a Library of Benzothiazoxepine-1,1'-dioxides." *J. Comb. Chem.* **2010**, 12, 850-854.

For more information on instrument specification and availability, please contact:

Laurent Calcul, Ph.D. - CPAS Director, CAS / calcul@usf.edu

CHEMICAL PURIFICATION, ANALYSIS AND SCREENING CORE FACILITY

UNIVERSITY OF SOUTH FLORIDA ■ DEPARTMENT OF CHEMISTRY

3720 SPECTRUM BLVD. ■ SUITE 318 ■ TAMPA, FLORIDA ■ 33612

P: 813.974.0112 ■ F: 813.974.3203 ■ W: WWW.CHEMISTRY.USF.EDU/RESEARCH/CPAS/