



2012 Winter Quarterly Meeting

Featuring Dr. Paul Boswell,
Research Assistant Professor, University of Minnesota

Extremely Accurate Prediction of Gas and Liquid Chromatographic Retention on Virtually Any Instrument

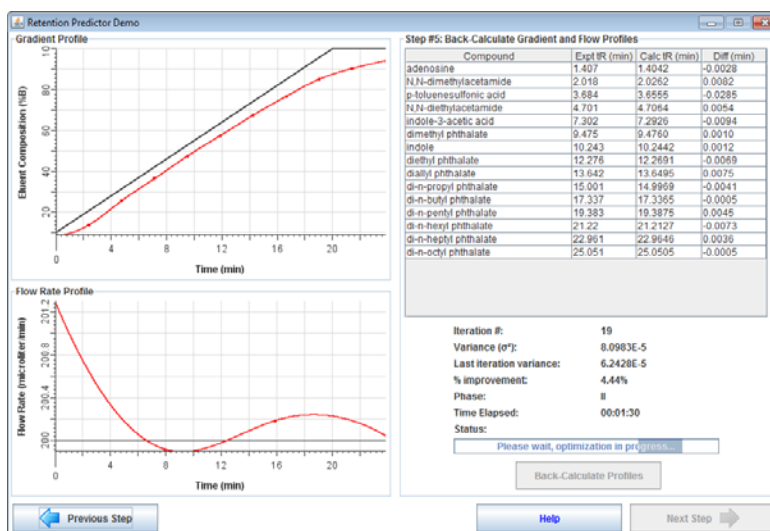
Wednesday, January 25th, 2012

Appetizers: 6:30 pm

Talk: 7:00-8:00 pm

Abstract

GC and HPLC retention information, if properly harnessed, could be extremely useful for the purpose of compound identification. Yet in the vast majority of analyses, the information is ignored because it remains largely irreproducible between laboratories. Much of this error is the result of small differences in the temperature and gas flow rate profiles (in GC) or the solvent gradient and flow rate profiles (in HPLC) *actually produced* by the instruments. We recently showed a simple methodology to very precisely account for these differences. We spike our sample with a set of "instrument calibration compounds" for which we know their retention behavior precisely. Then we run the sample, and based on the experimental retention times of the instrument calibration compounds, we back-calculate what the profiles *must have been* to produce those retention times. When we then use those back-calculated profiles to calculate the retention of other compounds, the predictions are of *unprecedented* accuracy. In GC, we can predict the retention of a set of chemically diverse compounds to ± 1.1 s in a 40 min temperature ramp. In HPLC, we can predict to ± 2.8 s in a 20 min solvent gradient. Unlike retention indexing, the accuracy remains high with different temperature programs/gradients, flow rates, column dimensions, and even with different make/models of HPLC/GC instruments. We developed a website and online software (below) to demonstrate the new methodology at www.retentionprediction.org.





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In this talk we will discuss how the new methodology works, how it can be used to catalogue retention information in your own lab, and what you can expect from it in the coming years as we begin to build a public database of retention information.

Biography

Dr. Paul Boswell is a Research Assistant Professor in the Department of Horticultural Science at the University of Minnesota. He is researching new ways to improve methodology for compound identification by GC- and LC-MS. After earning a BS in Chemistry and Biochemistry from Bethel University, he obtained a Ph.D. in Analytical Chemistry in the lab of Philippe Bühlmann at the University of Minnesota, where he developed new electrochemical sensors based on highly fluorinated materials. After a year at a small chemical instrumentation company in Pennsylvania, he returned to the University of Minnesota as a postdoctoral researcher in Jerry Cohen and Adrian Hegeman's labs working on methods development for metabolomics before entering his present position.

Location:

***Please note the new address.*

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