

## Accepted Manuscript

Title: Peptide retention time prediction in hydrophilic interaction liquid chromatography. Comparison of separation selectivity between bare silica and bonded stationary phases

Authors: Victor Spicer, Oleg V. Krokhin



PII: S0021-9673(17)31844-7  
DOI: <https://doi.org/10.1016/j.chroma.2017.12.046>  
Reference: CHROMA 359102

To appear in: *Journal of Chromatography A*

Received date: 31-10-2017  
Revised date: 14-12-2017  
Accepted date: 16-12-2017

Please cite this article as: Spicer V, Krokhin OV, Peptide retention time prediction in hydrophilic interaction liquid chromatography. Comparison of separation selectivity between bare silica and bonded stationary phases, *Journal of Chromatography A* (2010), <https://doi.org/10.1016/j.chroma.2017.12.046>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

**Peptide retention time prediction in hydrophilic interaction liquid chromatography.  
Comparison of separation selectivity between bare silica and bonded stationary phases**

Victor Spicer<sup>1</sup>, Oleg V. Krokhin<sup>1,2\*</sup>

<sup>1</sup>Manitoba Centre for Proteomics and Systems Biology, 799 JBRC, 715 McDermot Avenue, Winnipeg, R3E 3P4, Canada

<sup>2</sup>Department of Internal Medicine, University of Manitoba, 799 JBRC, 715 McDermot Avenue, Winnipeg, R3E 3P4, Canada

\*Corresponding author:

Oleg Krokhin

Tel: (204) 789 3283, Fax: (204) 480 1362, E-mail: krokhino@cc.umanitoba.ca

Manitoba Centre for Proteomics and Systems Biology 799 JBRC, 715 McDermot Avenue, Winnipeg, R3E 3P4, Canada

**Highlights**

- Peptide retention prediction algorithms have been developed for four different HILIC phases
- Large retention datasets (36-40 thousands peptides each) helped discovery of fine details of retention mechanism
- High prediction accuracy ( $R^2$ -value 0.973-0.98) was demonstrated
- Major retention features of peptide HILIC are opposite to RPLC
- Sequence-specific effects in HILIC are less pronounced compared to RPLC, resulting in higher prediction accuracy

**Abstract**

Peptide separation selectivity of four different HILIC sorbents was compared through the development of sequence-specific retention prediction algorithms for the datasets of 36 to 40 thousands peptides each. Hydrophilicity of these sorbents at pH 4.5 (peptide retention under acetonitrile:water gradients) increases in the following order: Luna HILIC < XBridge Amide < Atlantis Silica ~ Luna HILIC Silica. Bare silica phases are characterized by higher retention coefficients for basic residues (Arg, Lys, His), while interactions with neutral HILIC phases is driven by interaction with the charged residues (Asp, Glu, Arg, Lys, His). Such difference is caused

Download English Version:

<https://daneshyari.com/en/article/7609006>

Download Persian Version:

<https://daneshyari.com/article/7609006>

[Daneshyari.com](https://daneshyari.com)