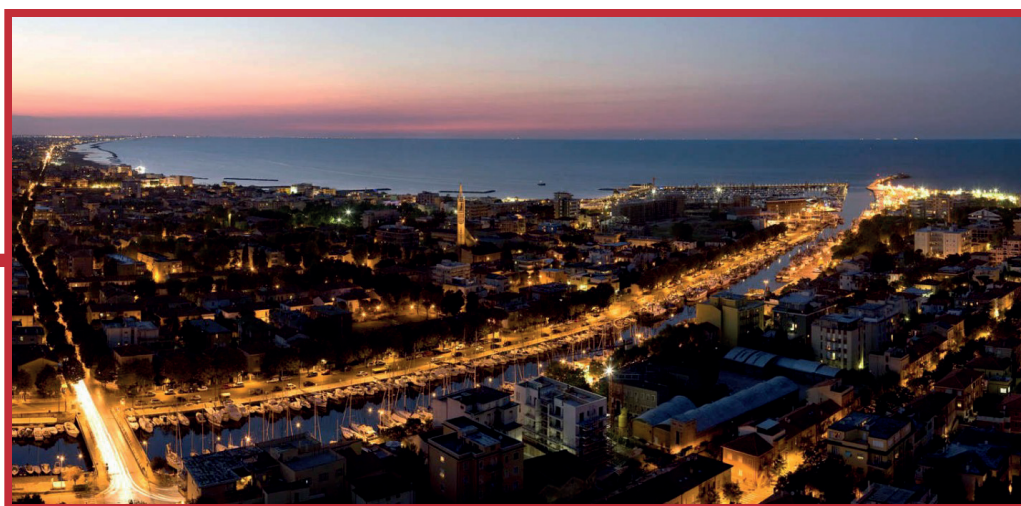


MERCK

Young Chemists' Symposium

2 0 1 9



Book of abstracts

Rimini (Italy)

November 25th-27th, 2019



Società Chimica Italiana
Gruppo Giovani

Proceedings of the
Merck Young Chemists' Symposium
XIX edition

Edited by: G. Annunziato, M. Atzori, F. Bella, C. Bonfio, S. Cinti, M. Da Pian, V. Lazazzara, E. Lenci, E. Paone, F. Ponte, L. Rivoira, M. Schlich, and L. Triggiani

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ISBN: 978-88-94952-15-5



On the effect of mobile phase composition on thermodynamic properties of zwitterionic teicoplanin-based 2- μm superficially porous particles

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The effect of the mobile phase composition on thermodynamic properties of novel zwitterionic macrocyclic glycopeptide chiral stationary phase (CSP) has been evaluated.

The CSP used has been made on latest-generation 2- μm superficially porous particles (SPPs), functionalized with teicoplanin by means of a proprietary bonding protocol that allows to obtain its zwitterionic version.

The investigation of thermodynamic behavior has been performed by calculating adsorption isotherms in both hydrophilic interaction liquid chromatography (HILIC) and reversed phase (RP) modes [1,2]. The study of absolute and excess adsorption isotherms allowed to gain information on surface heterogeneity in terms of adsorption energy distribution, types of adsorption sites, preferential adsorption of one of the component of the binary mobile phase and to investigate if the mobile phase composition has an effect on both the binding constants of enantiomers and the enantioselectivity of the CSP.

On the one hand, excess adsorption isotherms have been calculated by means of the minor disturbance method [3]. The excess of both methanol (RP) and acetonitrile (HILIC) over water was determined from linear perturbations on a series of equilibrium concentrations, when a steady-state equilibrium between mobile and stationary phase has been reached. On the other hand, adsorption isotherms of Z-D,L-Methionine enantiomers have been studied by using the so-called Inverse Method (IM). Results have revealed that the adsorption mechanism in both RP and HILIC mode can be described by means of a competitive Bilangmuir isotherm, which accounts for the presence of two different adsorption sites: one selective, responsible for the chiral recognition mechanism, and one nonselective, in which the two enantiomers identically behave.

[1] S. Felletti, C. De Luca, O.H. Ismail, L. Pasti, V. Costa, F. Gasparrini, A. Cavazzini, and M. Catani, *J. Chrom. A* **1579** (2018) 41-48.

[2] M. Catani, S. Felletti, O.H. Ismail, F. Gasparrini, L. Pasti, N. Marchetti, C. De Luca, V. Costa, and A. Cavazzini, *Anal. Bioanal. Chem.* **410** (2018) 2457-2465.

[3] G. Guiochon, A. Felinger, D.G. Shirazi, A.M. Katti, *Fundamentals of Preparative and Nonlinear Chromatography*, 2nd ed, Academic Press, Elsevier (2006).