

The effects of solvent composition on the Whelk-O1 stationary phase: A molecular dynamics study

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Solvent mixtures of n-hexane and 2-propanol are commonly used in chiral chromatography, and are popular normal phase solvents when using the Whelk-O1 chiral stationary phase. However, the role of solvent composition has not been thoroughly studied. Previous molecular dynamics simulations have examined the selection mechanism of the Whelk-O1 for R/S-styrene oxide, R,R/S,S-stilbene oxide and other chiral analytes.^{1,2} These studies found that selectivity stems from competing docking mechanisms involving the cleft region of the Whelk-O1 selector. Hydrogen bonding and π - π stacking^{1,2} provide the energetic stabilization of the docked complexes.

This study explores the effects of solvent composition upon the selectivity and docking mechanisms of Whelk-O1. Results for styrene oxide will be presented. To this end, molecular dynamics simulations have been carried out studying the Whelk-O1 interface in the presence of styrene oxide while varying the solvent environment of the system. Two solvent environments were used; 90:10 (v/v) n-hexane:2-propanol, and 80:20 (v/v) n-hexane:2-propanol. The interactions between the Whelk-O1 selector and the enantiomers of styrene oxide are analyzed to determine separation factors.

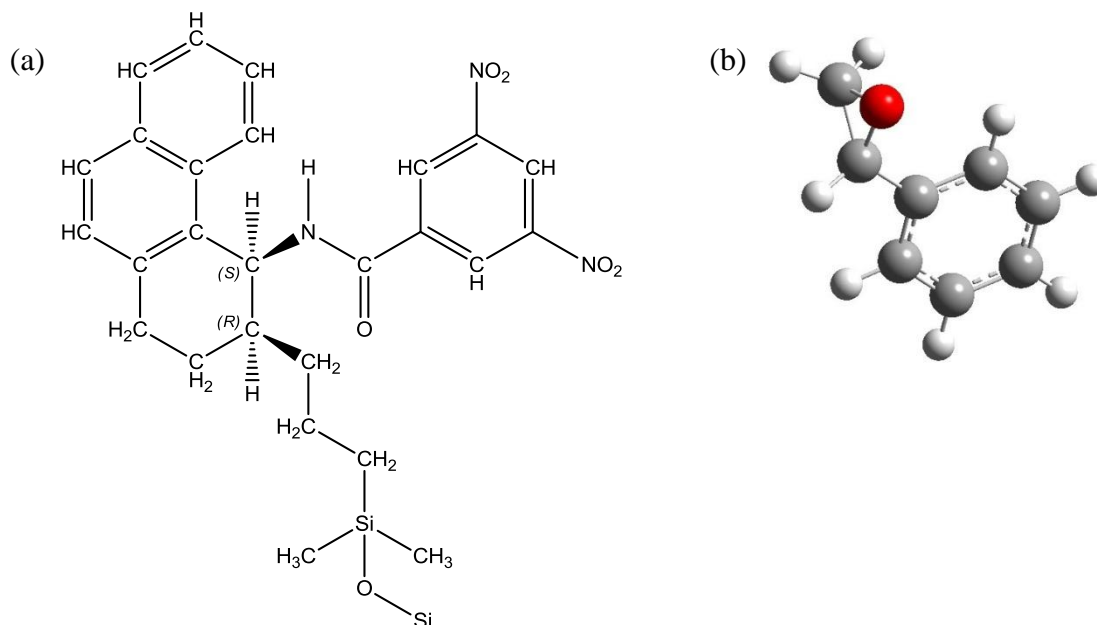


Figure 1: (a) The structure of the Whelk-O1 chiral stationary phase selector.
(b) (R)-styrene oxide

1. Zhao, C.; Cann, N. M. *J. Chromatogr., A* **2007**, 1149, 197-218.
2. Zhao, C.; Cann, N. M. *Anal. Chem.* **2008**, 80, 2426-2438.