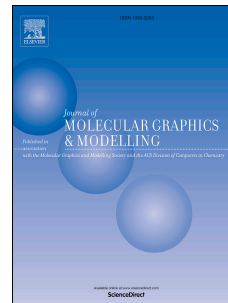


Accepted Manuscript

Computer simulation for the study of the liquid chromatographic separation of explosive molecules

Chuan-Wen Liu, Bing-Cheng Kuo, Min-Hsien Liu, Yu-Ren Huang, Cheng-Lung Chen



PII: S1093-3263(18)30306-1

DOI: [10.1016/j.jmglm.2018.09.009](https://doi.org/10.1016/j.jmglm.2018.09.009)

Reference: JMG 7233

To appear in: *Journal of Molecular Graphics and Modelling*

Received Date: 29 April 2018

Revised Date: 17 August 2018

Accepted Date: 18 September 2018

Please cite this article as: C.-W. Liu, B.-C. Kuo, M.-H. Liu, Y.-R. Huang, C.-L. Chen, Computer simulation for the study of the liquid chromatographic separation of explosive molecules, *Journal of Molecular Graphics and Modelling* (2018), doi: <https://doi.org/10.1016/j.jmglm.2018.09.009>.

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.

Computer Simulation for the Study of the Liquid Chromatographic Separation of Explosive Molecules

Chuan-Wen Liu^a, Bing-Cheng Kuo^b, Min-Hsien Liu^a, Yu-Ren Huang^c,
Cheng-Lung Chen^{b,*}

^a Department of Chemical and Materials Engineering, Chung-Cheng Institute of Technology, National Defense University, Taoyuan 335, Taiwan, ROC

^b Department of Chemistry, National Sun Yat-sen University, Kaohsiung 804, Taiwan, ROC

^c Department of Applied Science, Naval Academy, Zuoying District, Kaohsiung City 813, Taiwan, ROC

* Corresponding author: Prof. Cheng-Lung Chen, School of Department of Chemistry National Sun Yat-sen University, Kaohsiung 804, Taiwan

Abstract

The application of high performance liquid chromatography (HPLC) to separate explosive chemicals was investigated by molecular dynamics (MD) simulations. The explosive ingredients including NG, RDX, HMX and TNT were assigned as solutes, while methanol (CH₃OH) and acetonitrile (CH₃CN) were assigned as solvents in the solution system. The polymeric-molecular siloxanes (Si-C8) and poly-1,2-methylenedioxy-4-propenyl benzene (PISAF) compounds were treated as stationary phase in the simulation. The simulation results showed that the different species of explosive ingredients were separated successfully in the solutions by each of the constructed stationary phase of Si-C8 and PISAF after a total simulation time of 12.0 ps approximately, which were consistent with the experimental analysis of HPLC spectra. The origin for the separation was found due to the electrostatic interactions between polymer and explosives.

Keyword : molecular simulation, liquid chromatography, explosives.

Download English Version:

<https://daneshyari.com/en/article/11002484>

Download Persian Version:

<https://daneshyari.com/article/11002484>

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