

Quantitative Detection of Pyrene in Edible Oil via Plasmonic TLC-SERS Combined with Machine Learning Analysis

Jiahui Tian ¹, Xianhe Jiao ¹, Jiaqi Guo ², Qian Yu ¹, Shuqin Zhang ³, Guizhou Gu ^{1,*}, Kundan Sivashanmugan ^{4,*} and Xianming Kong ¹

¹ School of Petrochemical Engineering, Liaoning Petrochemical University, Fushun 113001, China; tianjiahui@stu.lnpu.edu.cn (J.T.); lnpu@lnpu.edu.cn (X.J.); qyu@lnpu.edu.cn (Q.Y.); xmkong@lnpu.edu.cn (X.K.)

² Jiangsu Co-Innovation Center for Efficient Processing, Utilization of Forest Resources and Joint International Research Lab of Lignocellulosic Functional Materials, Nanjing Forestry University, Nanjing 210037, China; jiaqi.guo@njfu.edu.cn

³ Fushun Ecological Environment Monitoring Center of Liaoning Province, Fushun 113001, China; 0413zhangshuq@sina.com

⁴ Center for Fluorescence Spectroscopy, Department of Biochemistry and Molecular Biology, University of Maryland School of Medicine, 721 West Lombard St., Baltimore, MD 21201, USA

* Correspondence: guguizhou2013@163.com (G.G.); skundan@som.umaryland.edu (K.S.)

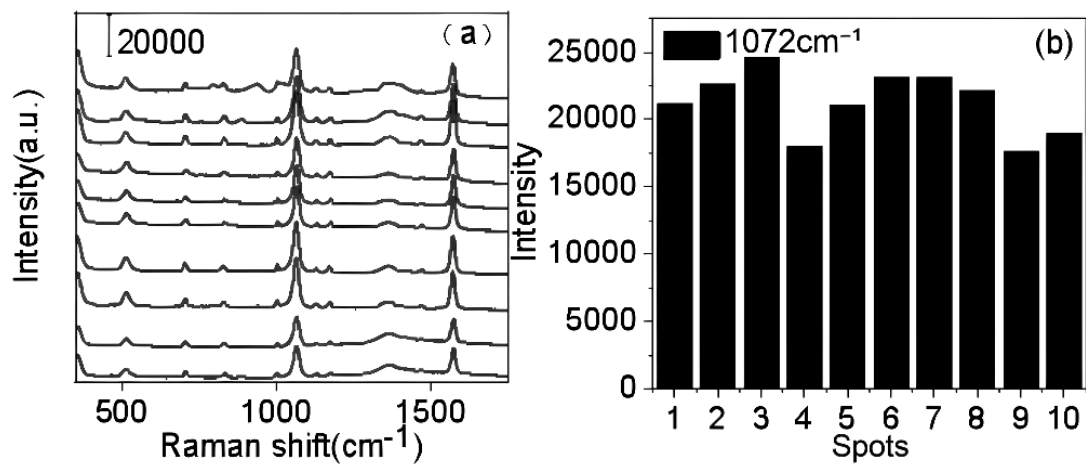


Figure S1. 4-MBA Raman spectra at 10 different positions of diatomite/Ag TLC channel (a) and Raman intensity histograms (b)

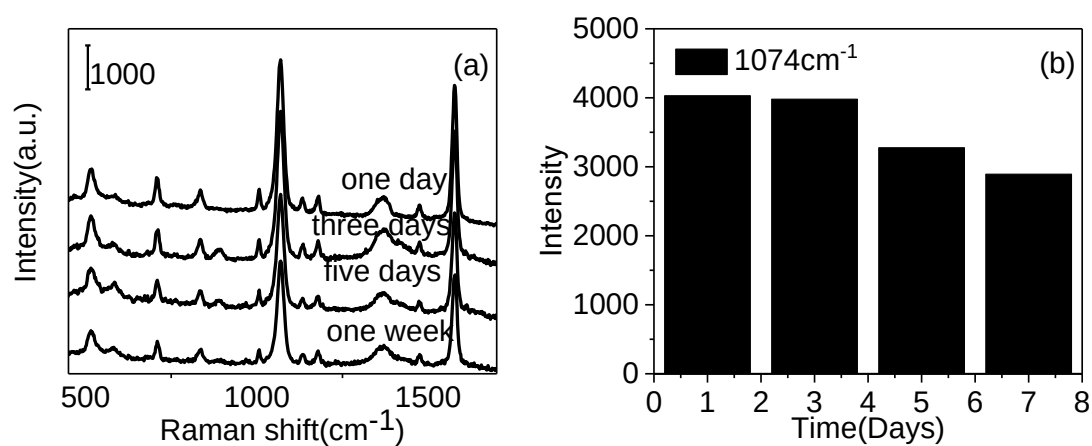


Figure S2. 4-MBA Raman spectra at 10 different positions of diatomite/Ag TLC channel (a) and Raman intensity histograms (b)

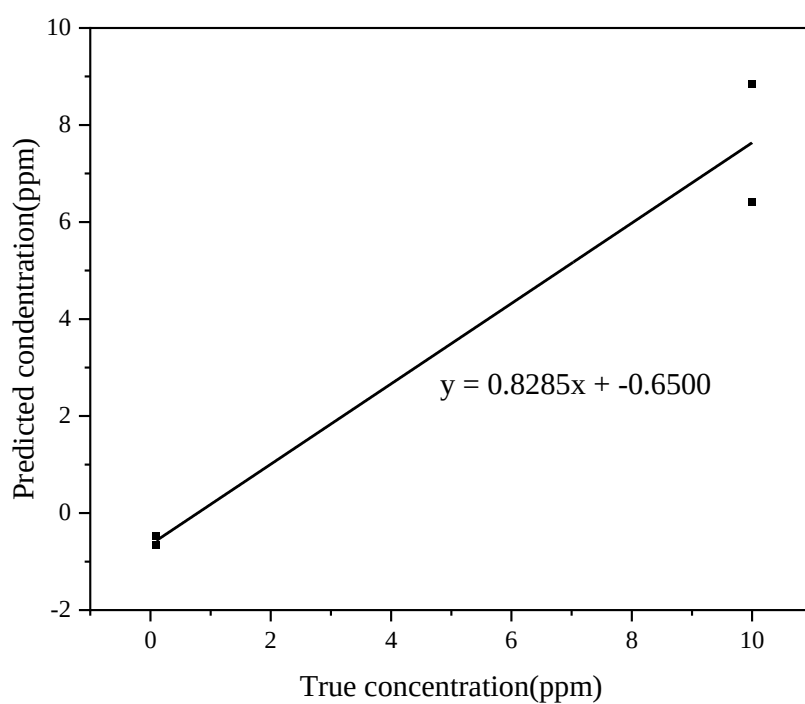


Figure S3. Relationship between real and predicted concentrations of pyrene analysis by PLSR model.