

Supporting Information

A facile strategy applied to simultaneous qualitative-detection on multiple components of mixture samples: a joint study of infrared spectroscopy and multi-label algorithms on PBX explosives

Minqi Wang^a, Xuan He^b, Qing Xiong^a, Runyu Jing^a, Yuxiang Zhang^a, Zhining Wen^a, Qifan Kuang^a, Xuemei Pu^{a,*}, Menglong Li^{a,*} and Tao Xu^{b*}

^a *xmpuscu@scu.edu.cn* College of Chemistry, Sichuan University, Chengdu, People's Republic of China. Fax: +86-028-85412290; Tel.: +86-028-85412290; E-mail:

^b *Institute of Chemical Materials, Chinese Academy of Engineering Physics, Mianyang, People's Republic of China.*

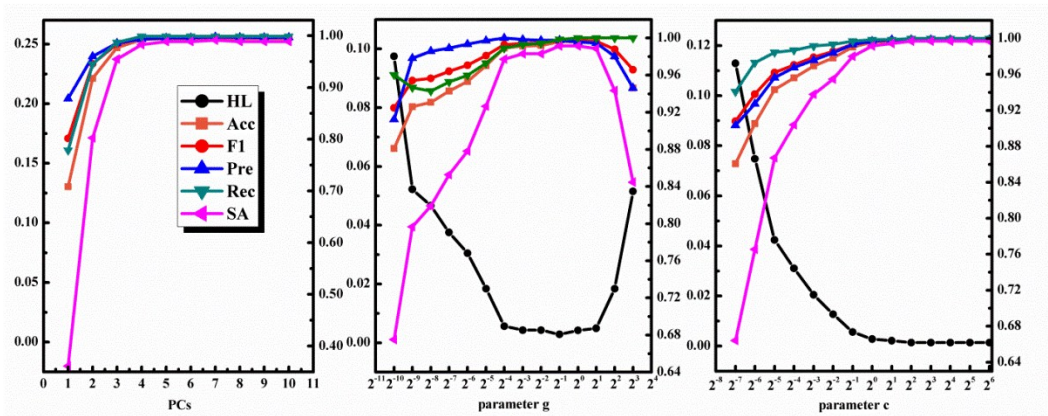


Fig.S1 The tuning procedure of PCs, kernel scale factor g , and regularization constant c for the Rank CVMz model. HL, Acc, F1, Pre, Rec and SA denoted Hamming loss, Accuracy, F1, Precision, Recall and subset accuracy, respectively. As mentioned above, an excellent model should achieve a smaller value for hamming loss, and larger values for the other five measures (accuracy, precision, recall, F1 and subset accuracy). Herein, the indicative Subset accuracy measure is taken as a criterion to tune these parameters. Consequently, we obtained the optimized model with PCs of 7, g of 0.5 and C of 4.