

Classification of mass spectral data to assist in the identification of novel synthetic cannabinoids.

Kristopher C. Evans-Newman, Garion L. Schneider and Nuwan T. Perera

Supplementary Materials

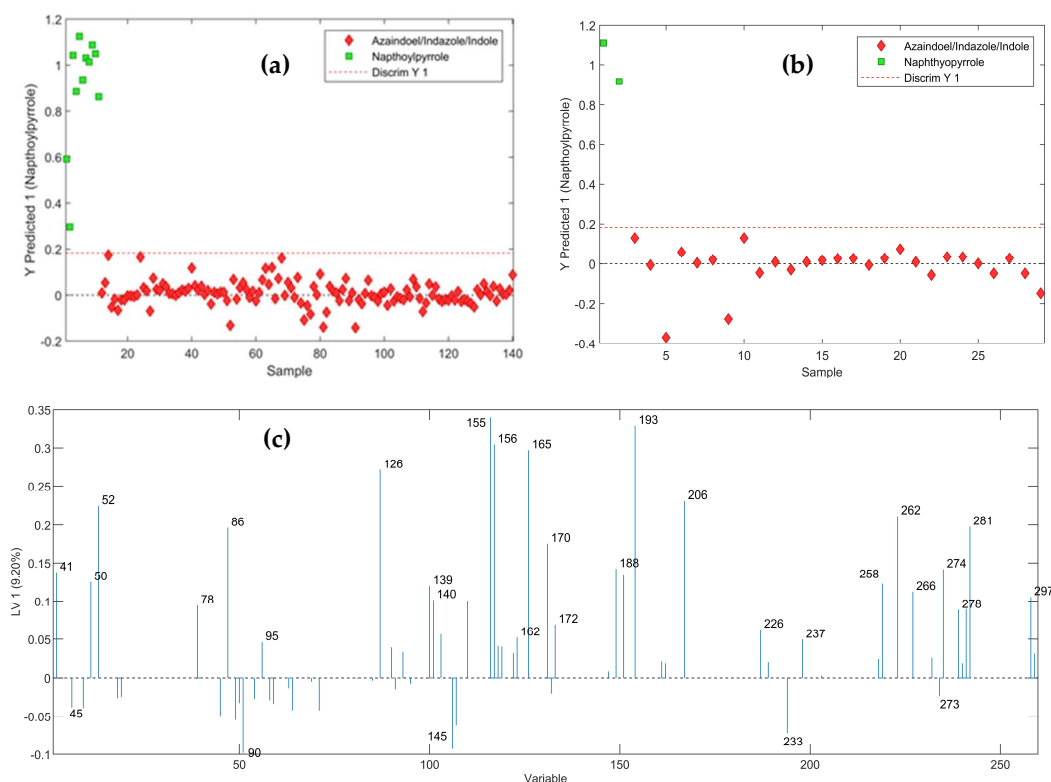


Figure S1. The Results of PLS-DA analysis of cannabinoids with naphthopyrrole core and cannabinoids with indole, azaindole, or indazole core groups: (a) score plot of the training set and (b) prediction set using GA as the variable selection method. (c) LV1 with the weights.

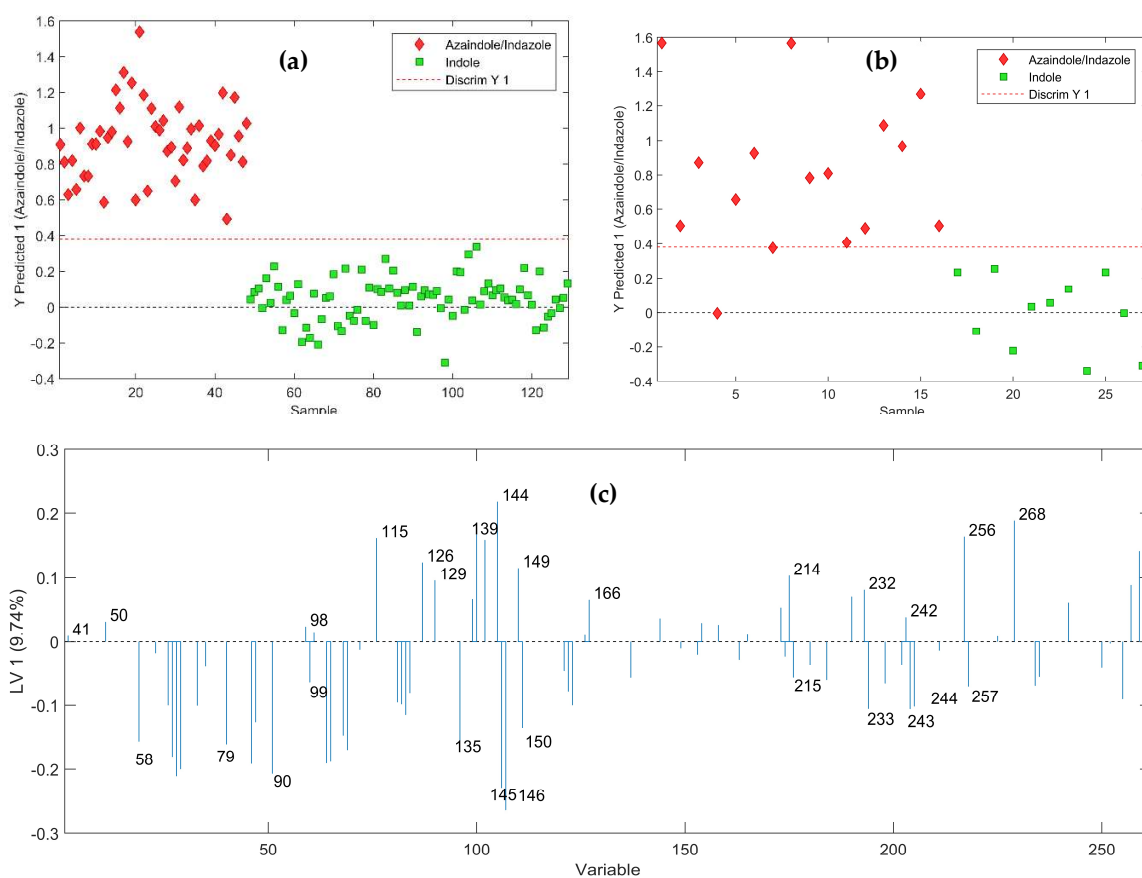


Figure S2. The Results of PLS-DA analysis of indole core containing cannabinoids versus azaindole or indazole core containing cannabinoids: (a) score plot of the training set and (b) prediction set using GA as the variable selection method. (c) LV1 with the weights.

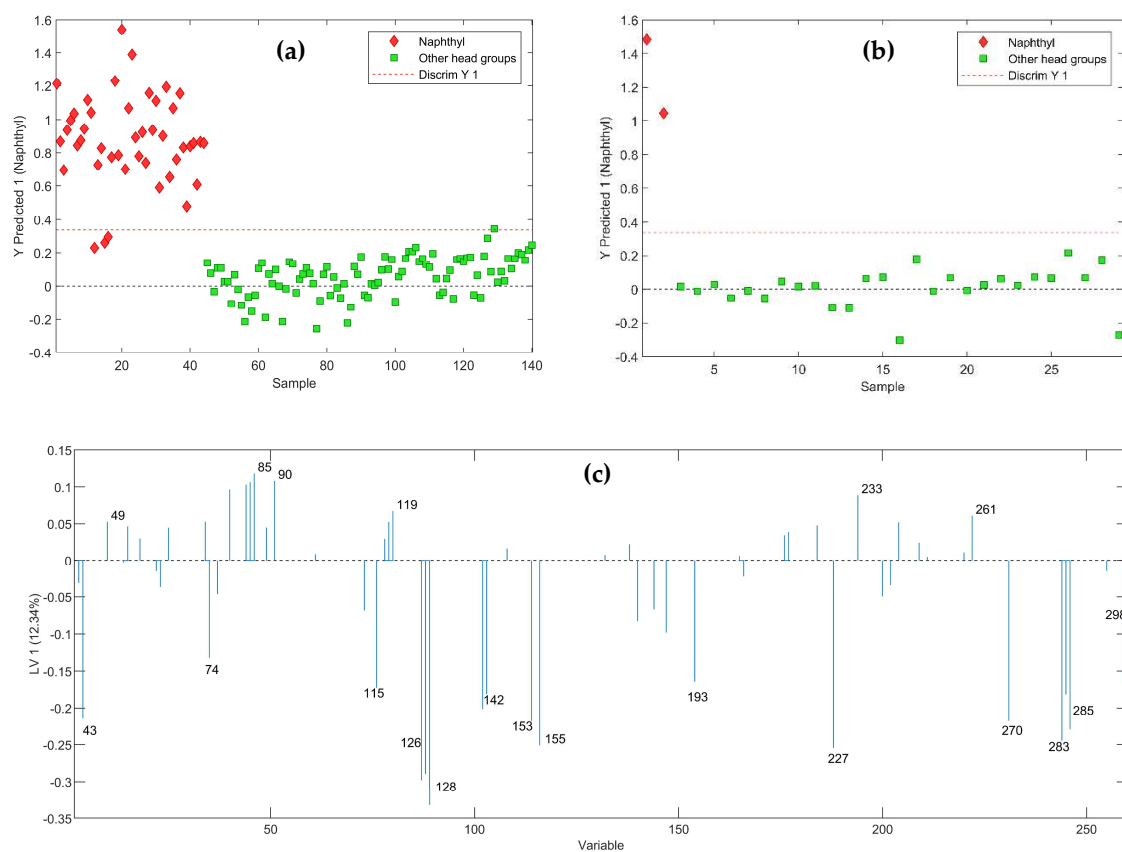


Figure S3. The Results of PLS-DA analysis of cannabinoids containing naphthyl head group versus cannabinoids containing other head groups: (a) score plot of the training set and (b) prediction set using GA as the variable selection method. (c) LV1 with the weights.

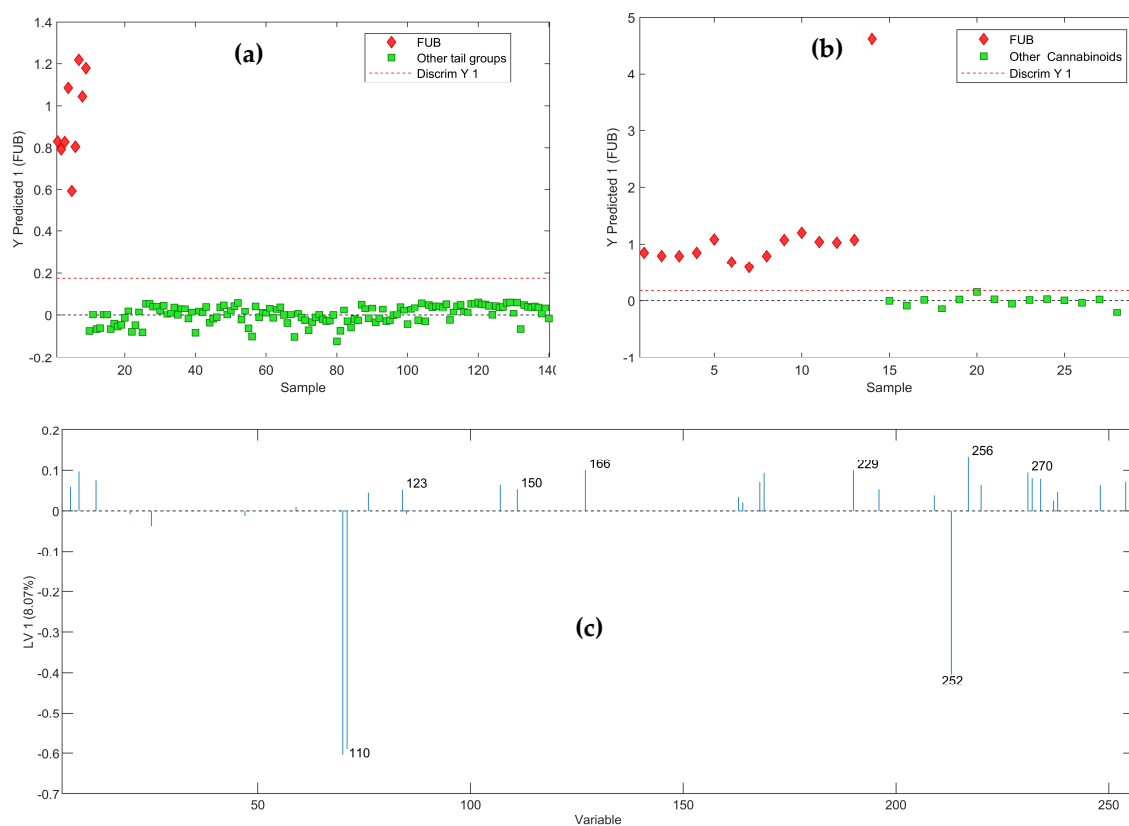


Figure S4. The Results of PLS-DA analysis of cannabinoids containing FUB tail group versus cannabinoids containing other head groups: (a) score plot of the training set and (b) prediction set with using GA as the variable selection method. (c) LV1 with the weights.

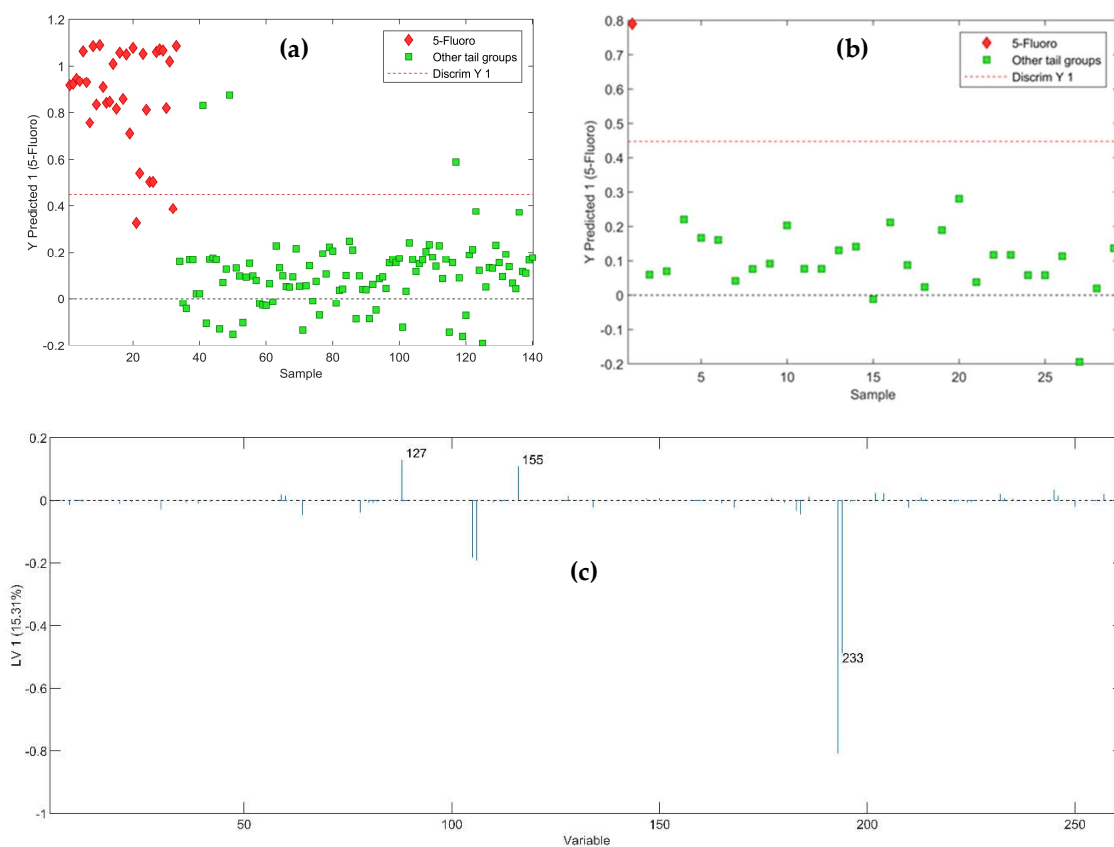


Figure S5. The Results of PLS-DA analysis of cannabinoids containing 5-Fluoro tail group versus cannabinoids containing other tail groups: (a) score plot of the training set and (b) prediction set using GA as the variable selection method. (c) LV1 with the weights.