

Identification of competitive inhibitors for bovine serum albumin from dynamic combinatorial libraries containing a bienzyme system

Wei He^{a,†}, Zheng Fang^{b,‡}, Zhao Yang^c, Xin Li^a, Haifeng Gan^a, Dong Ji, Zhenjiang Li, and Kai Guo^{a,*}

Supporting information

Part I The effect of BSA in the library

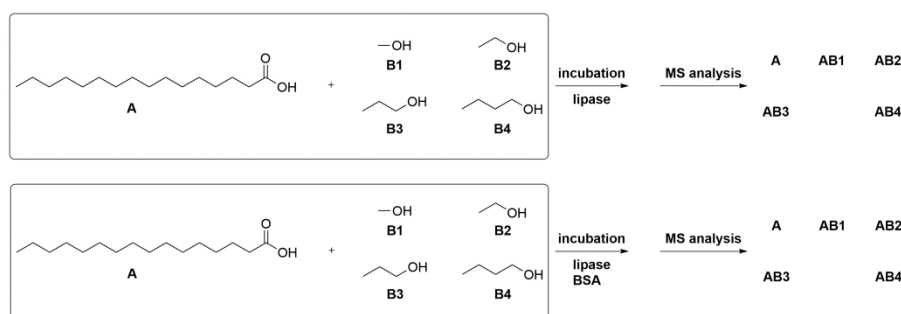


Figure S1 General protocol for the study of the equilibrium

In order to investigate the library composition changes and the equilibrium, a dynamic combinatorial library(1×4) was prepared according to the preparation of DCL 2(Figure S1). Besides, a controlled library was synthesized with the same building blocks and protocol, but without BSA as target, to make a comparison. The gap on the response values (Y-axis) between different results indicated the difference in the concentrations of the same compounds between different libraries. After incubated for 1 day, the MS results (Figure S2) revealed that the content of ethyl palmitate increased when BSA was present. However, the content of other four compounds decreased in the presence of BSA. This phenomenon demonstrates that the library composition changes when BSA is added in the library.

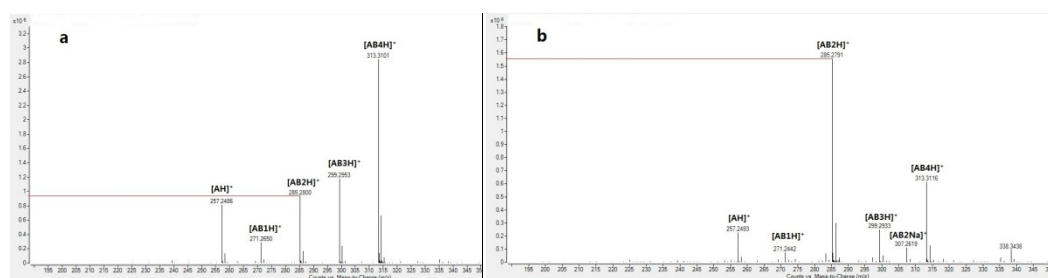


Figure S2 GC analysis of the DCL generated (a) in the absence and (b) in the presence of BSA for 1 day

Part II The study of equilibrium

A similar library was synthesized according to the preparation of DCL 2 in order to observe whether the equilibrium was reached or not. The MS results confirmed that the equilibrium reached when incubated for 48h. The content of ethyl palmitate kept constant with longer reaction time (4 days). Besides, the concentration of other four compounds was the same as that for 2 days. In other words, the equilibrium had been reached when incubated for 2 days.

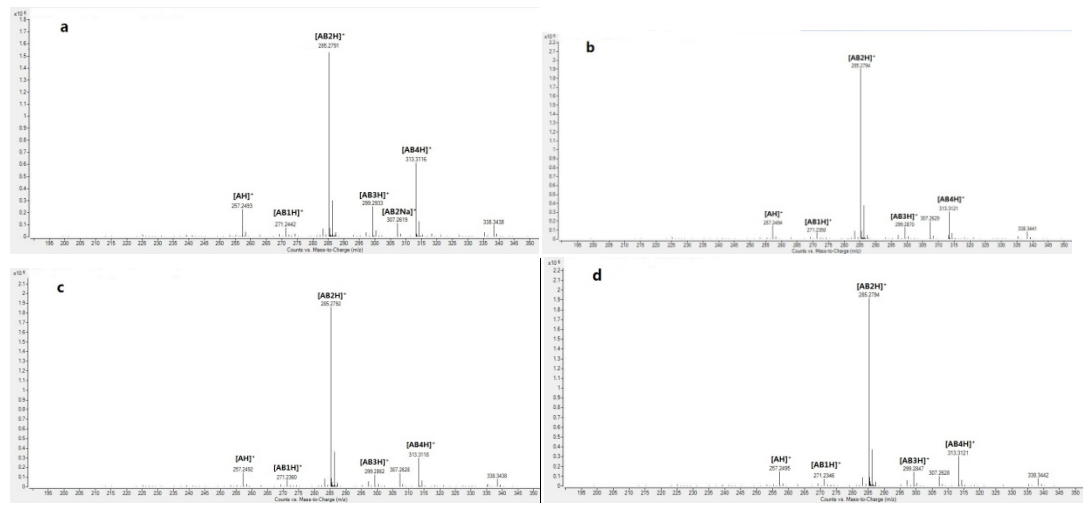


Figure S3 GC analysis of the DCL generated (a) in the presence of BSA for 1 day (b) in the presence of BSA for 2 days (c) in the presence of BSA for 3 days (d) in the presence of BSA for 4 days