

## **Mass spectrometry-based metabolomics combined with quantitative analysis of the microalgal diatom (*Chaetoceros calcitrans*)**

### **ABSTRACT**

Although many metabolomics studies of higher land plant species have been conducted, similar studies of lower nonland plant species, which include microalgae, are still developing. The present study represents an attempt to characterize the metabolic profile of a microalgal diatom *Chaetoceros calcitrans*, by applying high-resolution mass spectrometry detection, via QExactive™ Plus Orbitrap mass spectrometry. The results showed that 54 metabolites of various classes were tentatively identified. Experimentally, the chloroform and acetone extracts were clearly distinguished from other solvent extracts in chemometric regression analysis using PLS, showing the differences in the *C. calcitrans* metabolome between the groups. In addition, specific metabolites were evaluated, which supported the finding of antioxidant and anti-inflammatory activities. This study also provides data on the quantitative analysis of four carotenoids based on the identification results. Therefore, these findings could serve as a reliable tool for identifying and quantifying the metabolome that could reflect the metabolic activities of *C. calcitrans*.

**Keyword:** Microalgal diatom; Metabolic profiles; Algalomics; Chemical markers; UHPLC-MS