Multi biomarkers, including plant wax, algal biomarkers, glycerol dialkyl glycerol tetraethers (GDGTs) from bacterial and archaea, were studied in surface sediments of the northern South China Sea (NSCS). The terrestrial plant wax derived from odd \( n \)-alkanes (\( n-C_{27}, n-C_{29}, n-C_{31} \)) and even \( n \)-alkanols (\( n-C_{22}, n-C_{24}, n-C_{26} \)) exhibited high contents at the outer shelf than in the inner shelf regions, implying the transport of Taiwan Island-source sedimentary organic matter (OM) and depositions at the offshore areas were mainly controlled by deep-water contour current, while the low contents of branched GDGTs indicated limiting contribution of soil OM to the sediments. Algal biomarkers (brassicasterol, dinosterol, \( C_{37} \)-alkenones and \( C_{30} \)-diol/keto-ol corresponding to diatoms, dinoflagellates, coccolithophorids and estigmatophytes, respectively) were studied to understand changes in phytoplankton community structure in the region. High diatoms and dinoflagellates community were generally found near the Pearl River Estuary (PRE), southwest off the Taiwan Island and southeast off the Hainan Island, while relatively high biomass of coccolithophorids and estigmatophytes were found at the outer shelf areas, indicating the high competition of the nutrients for the former and low for the latter. High abundance of isoprenoid GDGTs (\( i \)GDGTs), which mainly occurred in the deep water indicated their low-level requirement for nutrients. Based on the correlation, location and \( i \)GDGT [2/3] ratio, two groups were identified, one for the inner shelf sites with lower \( i \)GDGT [2/3] (< 5) and relatively low correlation coefficient (\( R^2 = 0.4-0.8 \)), and the other group for the outer shelf regions showing high \( i \)GDGT [2/3] (> 4) and strong correlation (\( R^2 > 0.9 \)). This result revealed relative single bio-source in the deep water regions, with complexity in the shallow water areas. Bias based on the two organic thermometers (\( U_{37}^{K'37} \) and \( T_{EX86}^{3} \)) was evaluated, and \( C_{37:3} \)-alkenone > 5 ng/g and \( i \)GDGT [2/3] > 4 are proposed as the threshold for the reliable temperature reconstruction. This study highlights the importance of utilizing multi biomarkers to fully understand the controlling factors on the source inputs and distribution characteristics of sedimentary OM, phytoplankton community structure, and feasibility on the application of organic biomarkers-based proxies in paleoceanographic studies.