Abstract

Flavor and fragrance products are integral part of our daily life. Meanwhile, we have to face an increasing concern with chemicals, which are released to the environment during the life of chemical containing products. A challenge is how to produce environmentally friendly "green chemicals" for sustainable development of chemical industries. One possibility is to design chemical products in such a way that the chemicals are readily biodegradable when they are released to the environment. It is known that biodegradability of organic compounds is commonly depending on the intrinsic properties of the chemical molecules and environmental conditions. However, the current knowledge about the influences of chemical structure, molecular size or molecular weight and functional groups on biodegradation potential is still weak. Therefore, the aim of the present work was to find out the influence of oxygen functional groups, which are the most often found functional groups in organic molecules, on the biodegradability of organic chemicals. Through investigation of the experimental biodegradation results of numerous flavor and fragrance molecules containing various oxygen functional groups and a wide range of molecular structures, it was found that different oxygen functional groups and molecular structures have enhancing or inhibiting effects on the biodegradation potential of these molecules. The results of this work suggested that the biodegradability of organic molecules could be improved by a) introducing oxygen functional groups with enhancing effects into molecules; b) replacing structures with polycyclic systems, multi branched chains and cycloaliphatic rings with structures consistent of linear carbon chains, macrocyclic systems or mono aromatic rings; and c) modifying the connection manners of functional groups and carbon skeletons. Additionally, predictions of biodegradability of flavor and fragrance molecules using the Quantitative Structure-Biodegradability Relationship (QSBR) program BIOWIN 4.10 demonstrated that such models are useful tools to support the development of new molecules but cannot replace experimental study for classification and safety assessment of these molecules due to their moderate accuracy. The finding of this work provided supporting information for modifying of existing chemical compounds and designing of the new molecules to develop environment friendly "green chemicals".

Key words: organic compounds, green chemistry, oxygen containing functional group, chemical modification, ready biodegradability.