

Toxicity Assessment of LOHC Materials with Animal Experiments and Calculation

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Liquid Organic Hydrogen Carrier (LOHC) is an efficient energy carrier that stores hydrogen through chemical bonds. LOHC materials were paid attention to as energy storage technologies of the future substitute for fossil fuel, the main fuel in many fields such as vehicles, ships, and households. Thermophysical and chemical properties of various LOHCs have been studied, although the importance of environmental effect, properties of LOHCs related to toxicity have been investigated rarely. Moreover, most of the toxic properties were obtained from QSAR (Structure-Activity Relationship) calculation. In this study, we carried out the toxicity assessment by comparing the LOHC substances and conventional fossil fuel such as diesel and gasoline by animal experiments. In addition, the toxicity of the lean and rich form of LOHCs was predicted using the QSAR method. LOHC materials were classified according to grade under OECD guideline. As a result, toxicity prediction using QSAR could be evaluated by comparison with experimental data. We expect that this is the basis for the safety evaluation as a comparative group for the structure-toxicity relationship of the developing substance.