Toxicity Evaluation of Particulate Matters using QSAR-driven Model in Underground Subway Stations

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Iron-containing particulate matters (PMs) are the most abundant and frequently encountered air pollutants in underground subway stations, which is known that the toxicity of PMs in the subway stations is attributed to their high iron content but their toxicological data are still limited. This study aims to evaluate the toxicology and health risk of the iron species in PMs at Seoul metro station, Korea, where a quantitative structure activity relationship (QSAR) model utilizing chemical structures to predict properties/activities of chemical substances was developed. The study indicates that it could successfully evaluate the real-time health risk of the iron-containing PMs with QSAR model since it can select the key molecular descriptors systematically and predict the toxicity of iron compounds in PMs computationally. This clearly showed that the toxicity of the iron-rich PMs in subway stations comes from the forms of magnetite (Fe3O4) and maghemite (α-Fe2O3), can be predicted computationally by using a QSAR-toxicology model. Acknowledgements : This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP) (No.2015R1A2A2A11001120).