Deep belief network기반 PCB 바이오농축인자 예측 QSAR 모델

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A quantitative structure-property relationship (QSPR) study for predicting bio-concentration factors (log BCF) of polychlorinated biphenyls (PCBs) is investigated in this current work. QSPR model can serve as an alternative method of reducing experimental steps in determination of log BCF. This research proposes a deep belief network (DBN) method to developed new QSPR model to predict the physiochemical properties of PCBs. The prediction accuracy of proposed method was investigated and compared the results from OECD QSAR toolbox. The predictive ability of the DBN based QSPR model is clearly superior and can effectively capture the predictive features of the PCBs without highly reliable experimental BCF. Acknowledgments:This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government(MSIT). (No. 2017R1E1A1A03070713).