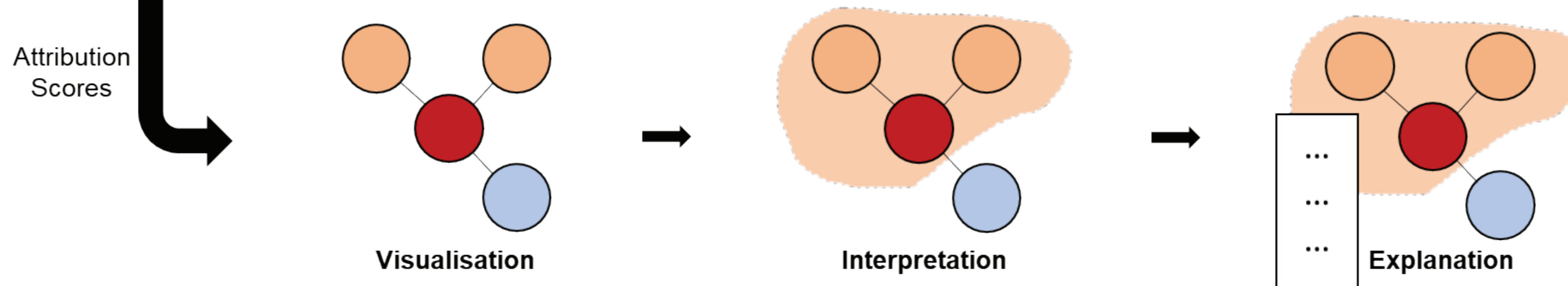
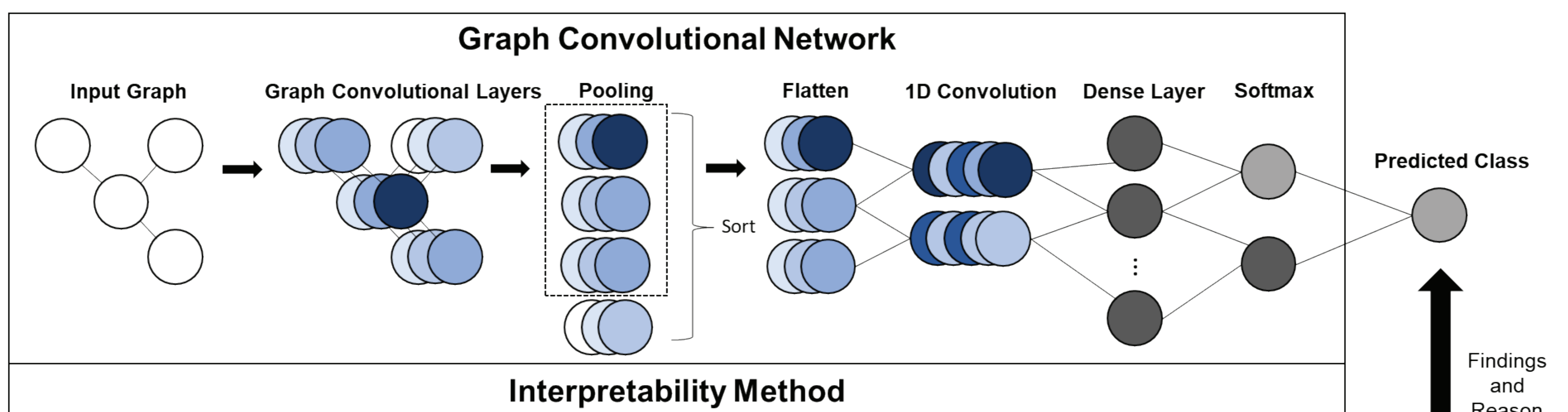


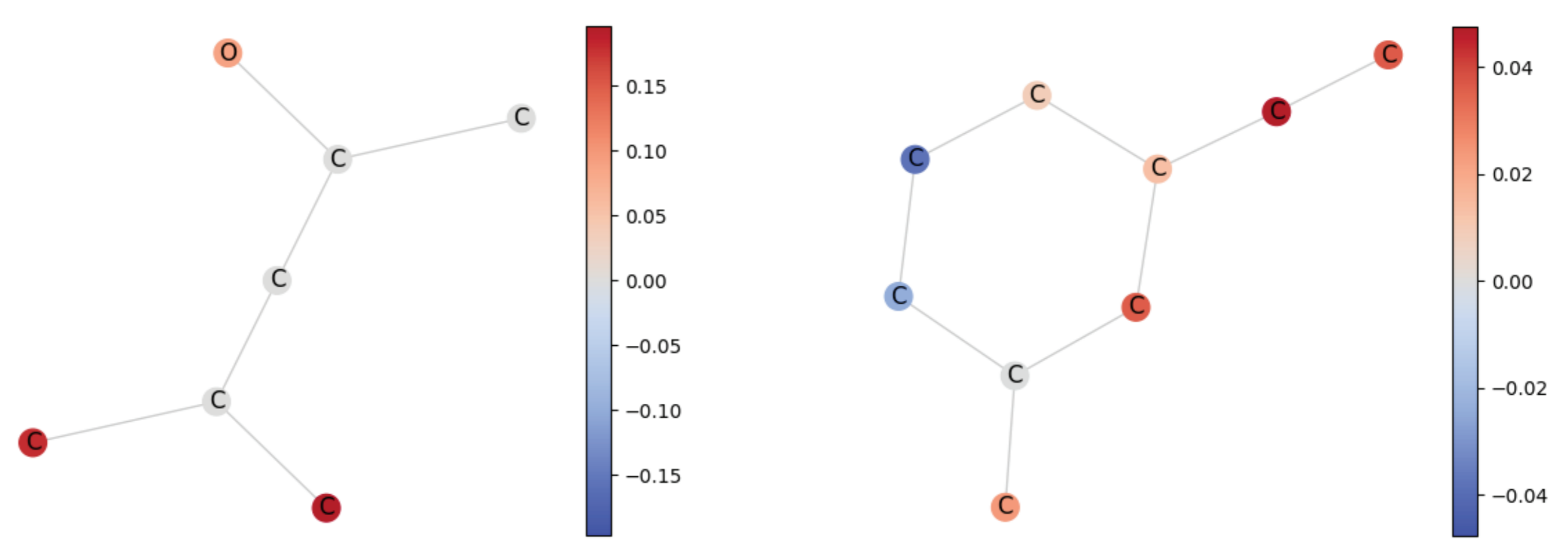
Explainable Graph Classification

Creating an end-to-end process for explainability

Deep learning methods in the recent years have shown growing prevalence in the machine learning community. However, such applications on classifying graphs remains a black box. Understanding how the neural network reacts to the inputs will help researchers zoom into the areas that could generate explanations for the graph's classification.



- **Red** denotes positive contribution
- **Blue** denotes negative contribution



The resulting visualisation heat-maps can be used to generate explanations for the predicted graph classification. In TOX21 dataset, the process enables the identification of atoms in a chemical structure that could potentially cause the chemical compound to be toxic.

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