**Supplemental data:**

*In silico* prediction of chemical aquatic toxicity for marine crustaceans via machine learning

Lin Liu, Hongbin Yang, Yingchun Cai, Qianqian Cao, Lixia Sun, Zhuang Wang, Weihua Li, Guixia Liu, Philip W. Lee and Yun Tang*

Content:

- **Table S1**: The CAS numbers of chemicals and their acute concentration values on the original saltwater crustacean datasets.
- **Table S2**: The detailed descriptors used in model building.
- **Table S3**: The performance of all descriptor-based classification local models.
- **Table S4**: The top ten fingerprint-based local models.
- **Table S5**: The performance of all descriptor-based classification global models.
- **Table S6**: The top ten fingerprint-based global models.
- **Table S7**: The detailed description of ID and OD chemicals in the test set.