

## Supplemental data :

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

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#### **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.