WP 5.1.1b
Ecological hazard assessement of BP alternatives

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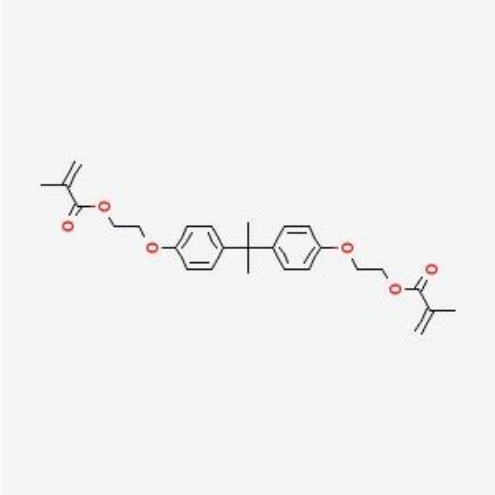
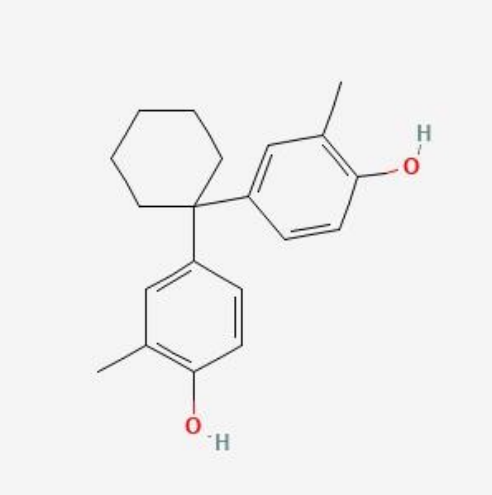
Bisphenol A (BPA) has long been a focal point of environmental concern due to its widespread use in various industrial applications, particularly in the production of plastics, resins, and thermal paper. It is valued for its ability to enhance the strength and flexibility of synthetic products. BPA is a key ingredient in producing polycarbonate plastics, epoxy resins, certain flame retardants, and various other materials. BPA is found in things like plastic containers, metal can linings, packaging for cosmetics and personal care items, cookware, toys, receipts, sports gear, and medical devices. It has even been detected in canned foods, drinks, and cosmetic and personal care products.

76 bisphenols, potential alternatives to BPA

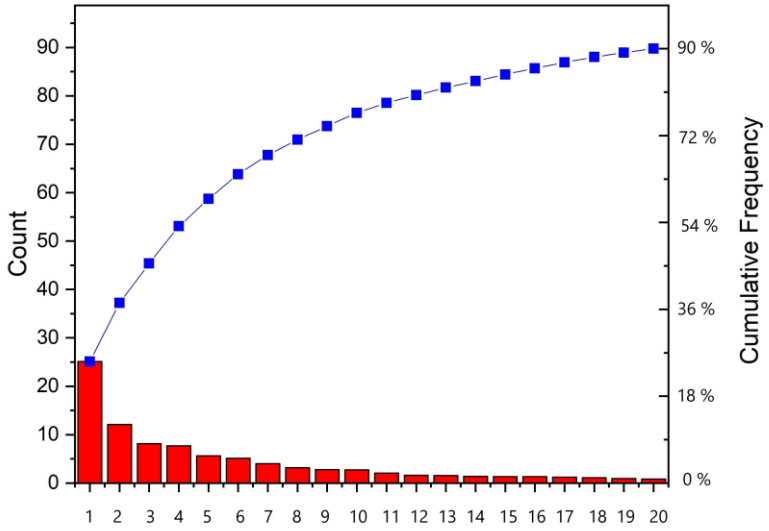
- Data provided by PARC and EChA
- Their structures, encoded in SMILES notations, have been used to calculate 708 descriptors using the alvaDesc version 2.0.10 tool, which calculates 33 different groups of descriptors, classified as 0-dimensional, 1-dimensional, or 2-dimensional ones.

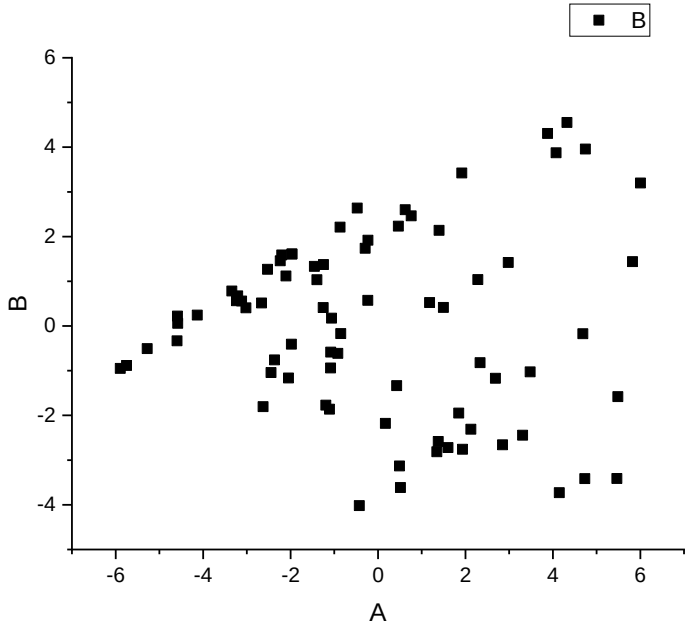




Principal Component Analysis (PCA)

A total of 708 structural descriptors, devoid of ecotoxicological information, were utilized to encode these compounds. Subsequently, principal component analysis (PCA) was applied to compress the data and generate visual representations. Moving to the second phase, we aimed to predict various ecotoxicological properties using thirteen available in silico models.





We assessed the eco-toxicological properties of BPA and derivatives using the Ecotox models integrated within the online platform VEGAHUB 2013. We focused on models that included one or more bisphenol derivatives in their training data.

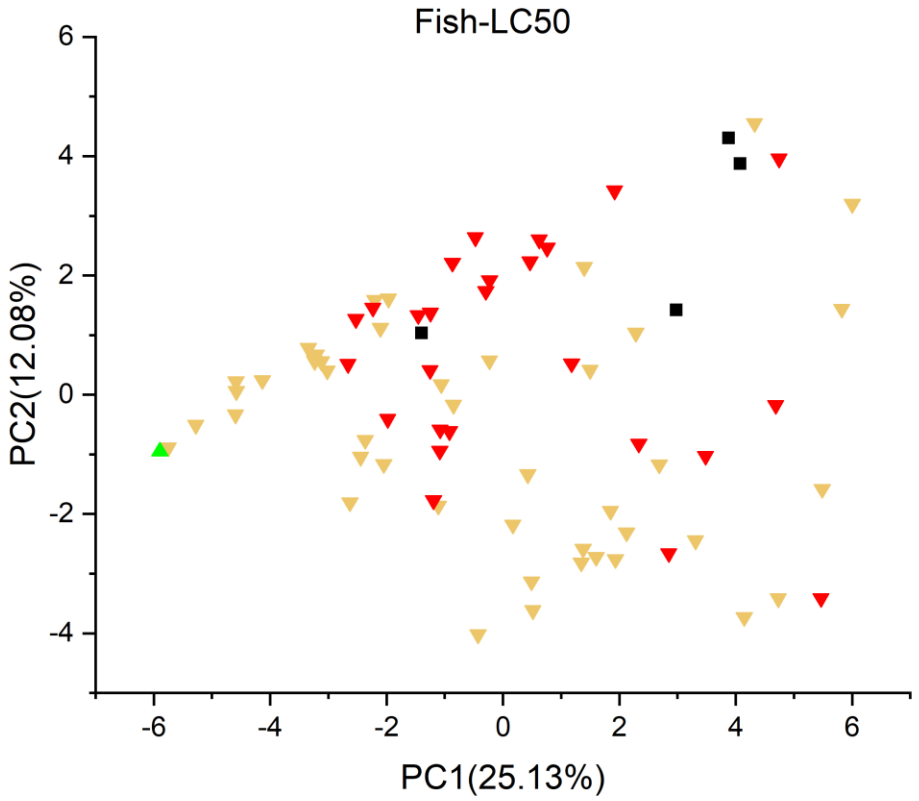
- Thirteen models were considered.
- We colored the scores in PCA plots according to the predictions:

red – compounds of concern

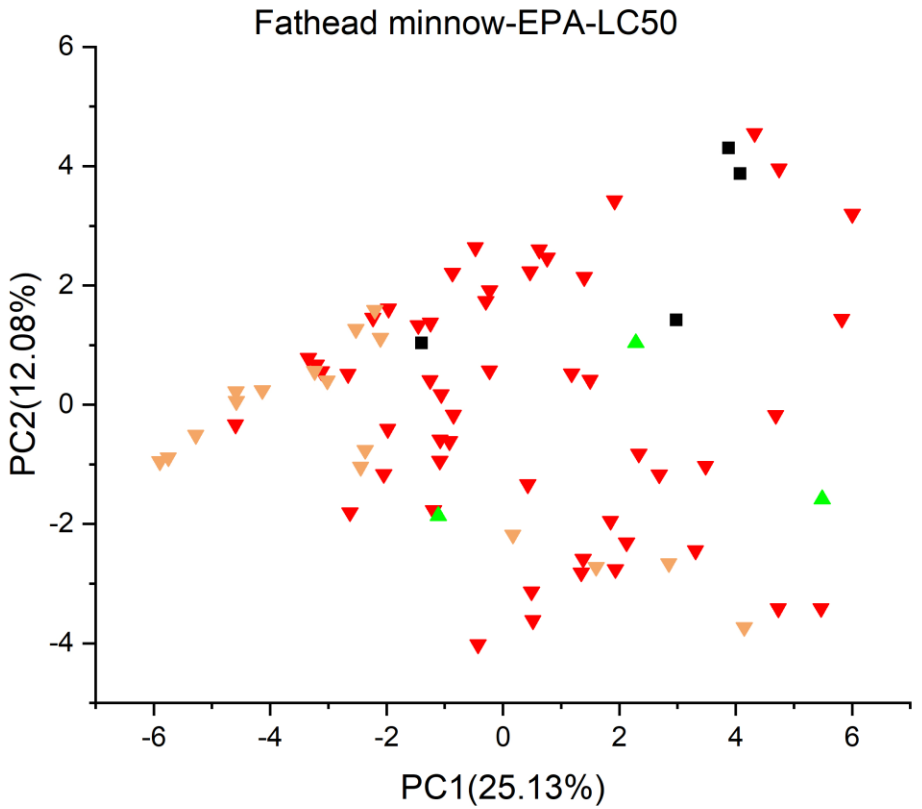
Yellow – some concern

Green – no concern

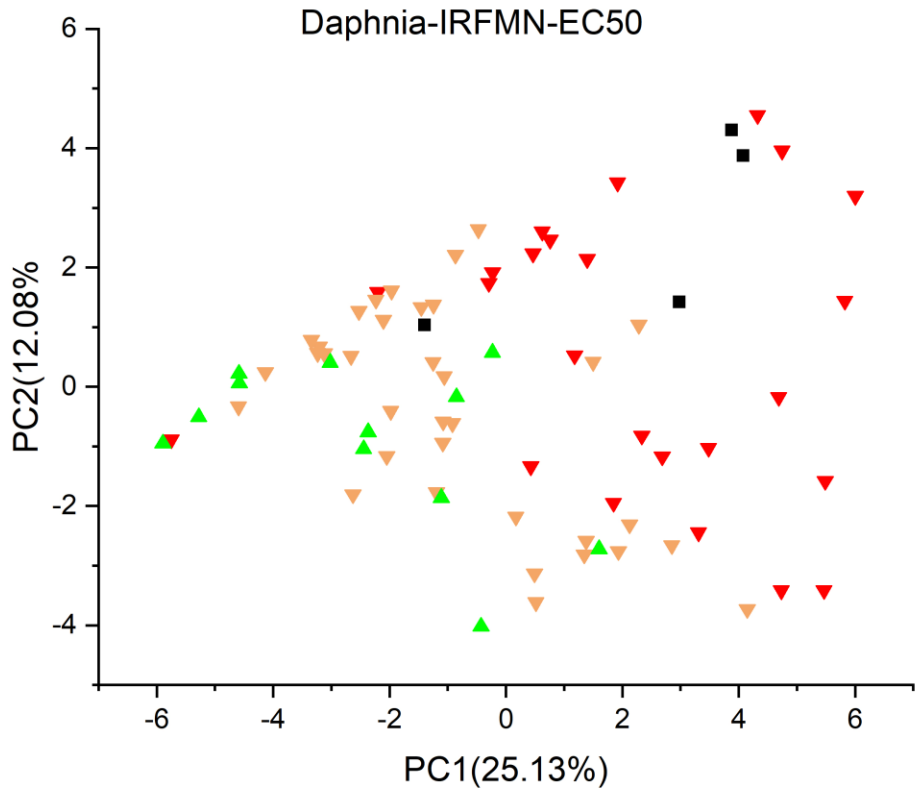
Fish Acute (LC50) Toxicity Model (IRFMN) Version 1.0.1



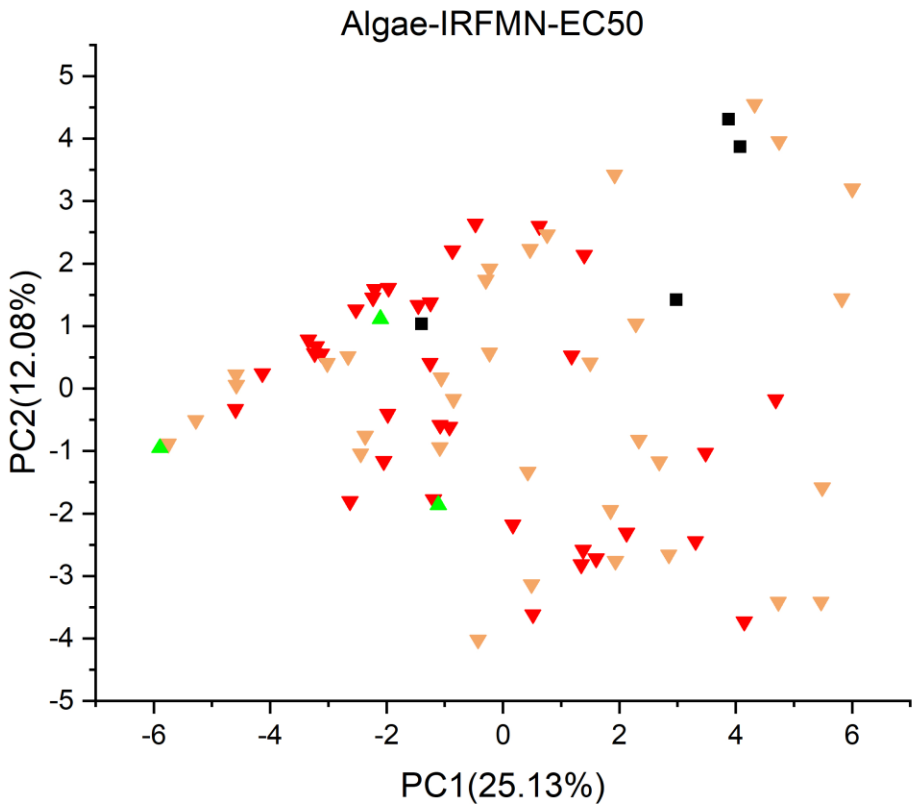
Fathead Minnow LC50 (96 h) (EPA) Version 1.0.7



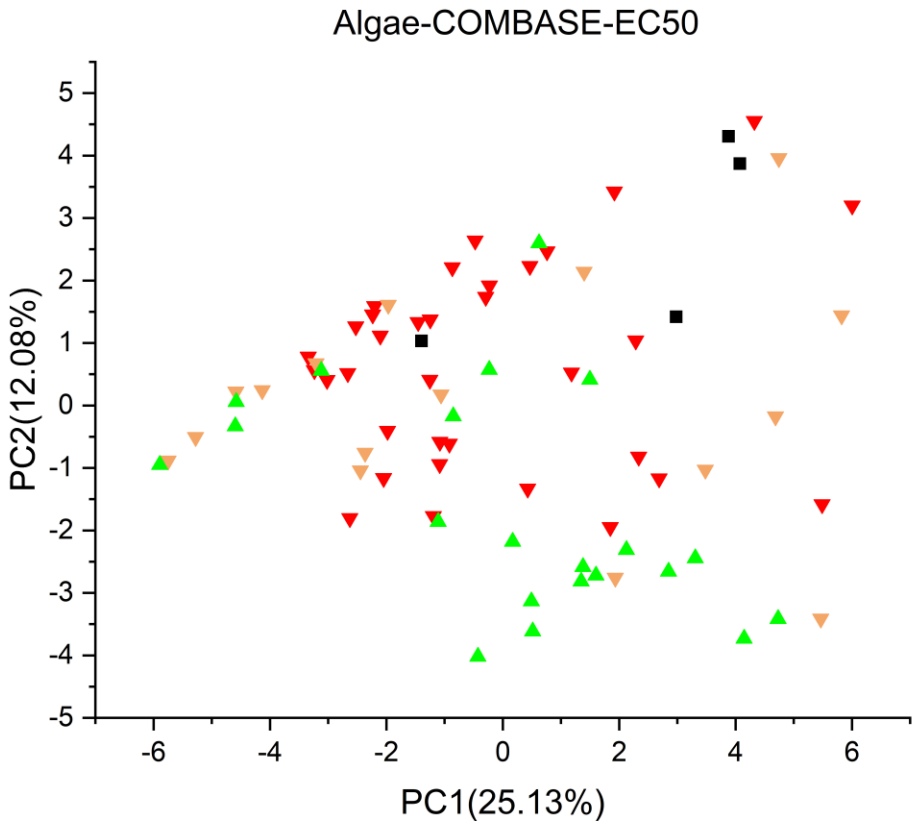
Daphnia Acute (EC50) Toxicity Model (IRFMN) Version 1.0.1



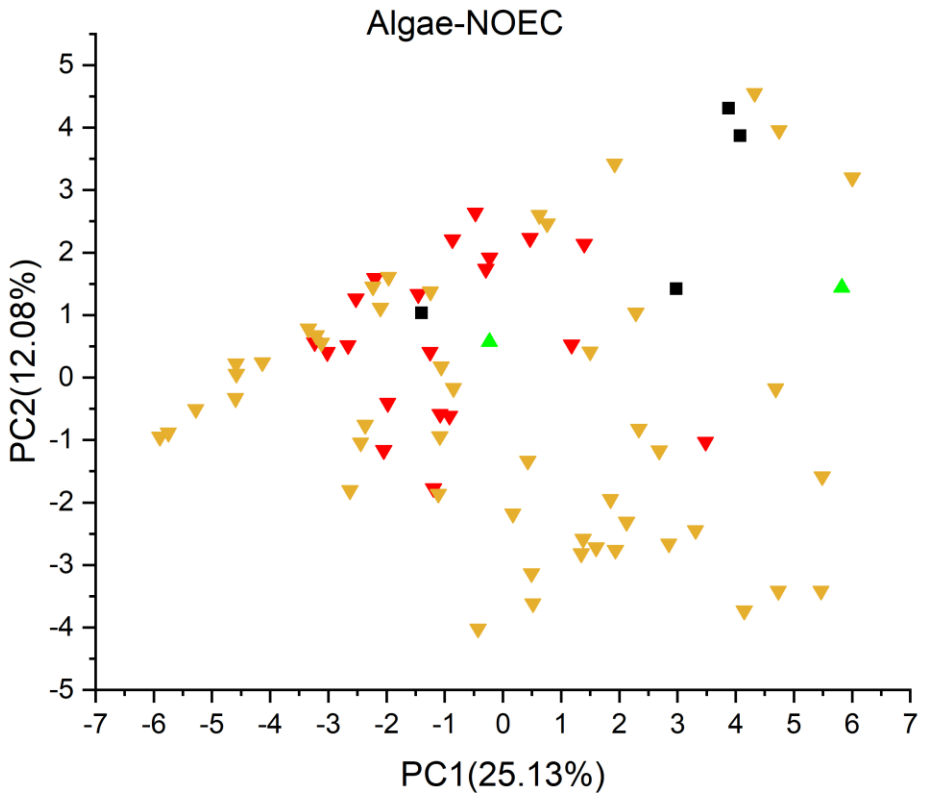
Algae Acute EC50 Toxicity Model (IRFMN) Version 1.0.1



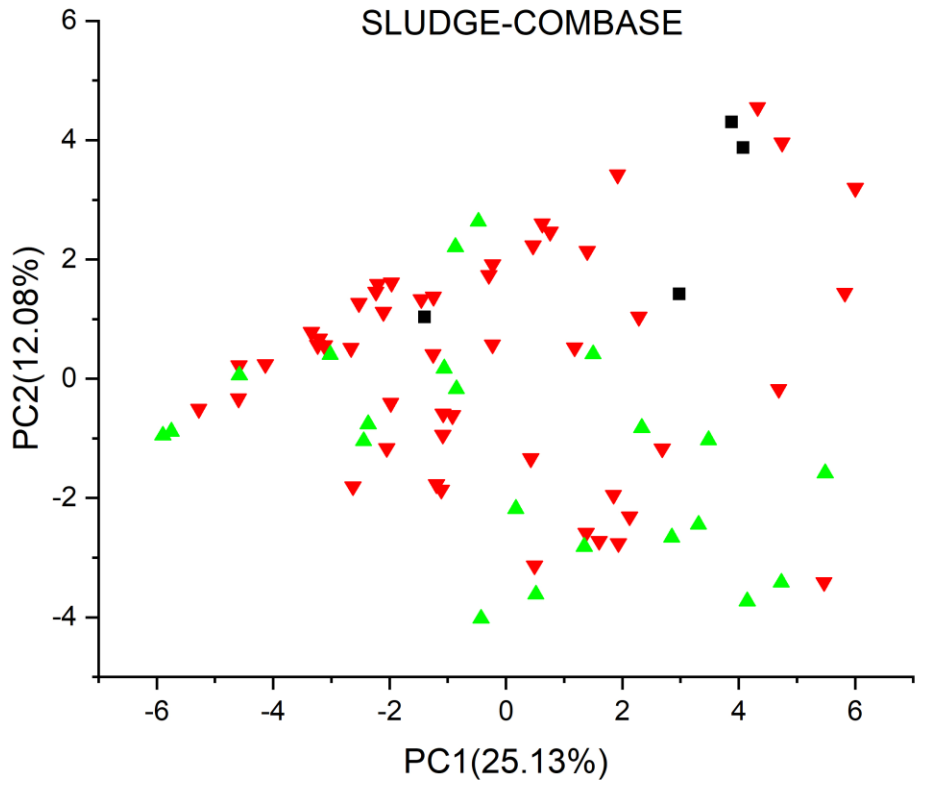
Algae (EC50) Toxicity Model (ProtoQSAR/Combase) Version 1.0.1



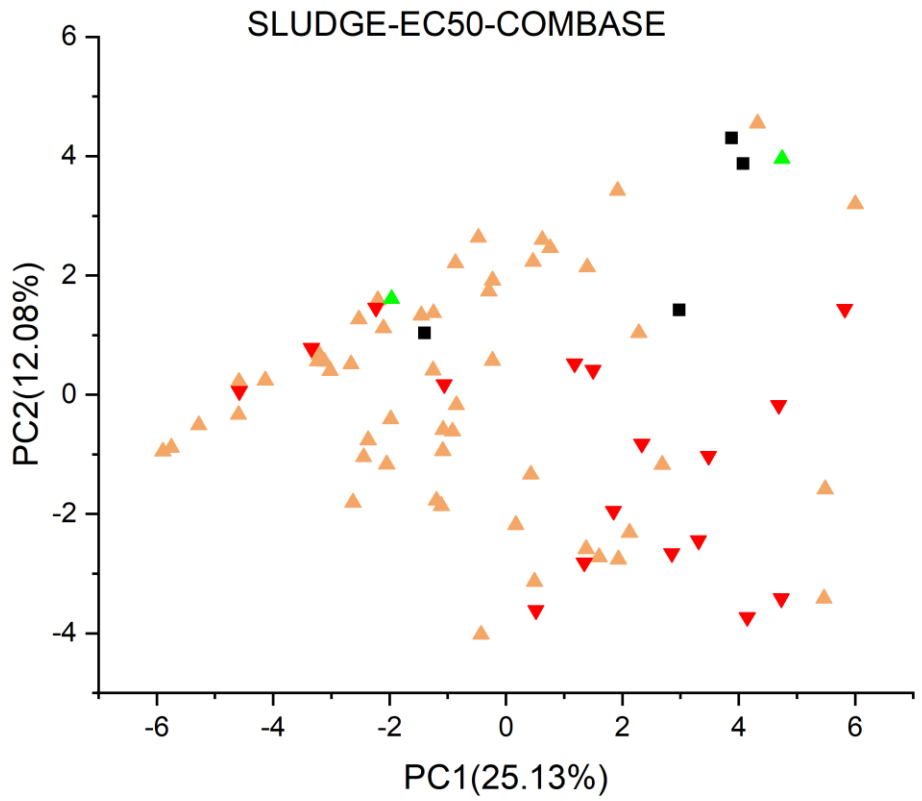
Algae Chronic (NOEC) Toxicity Model (IRFMN) Version 1.0.1



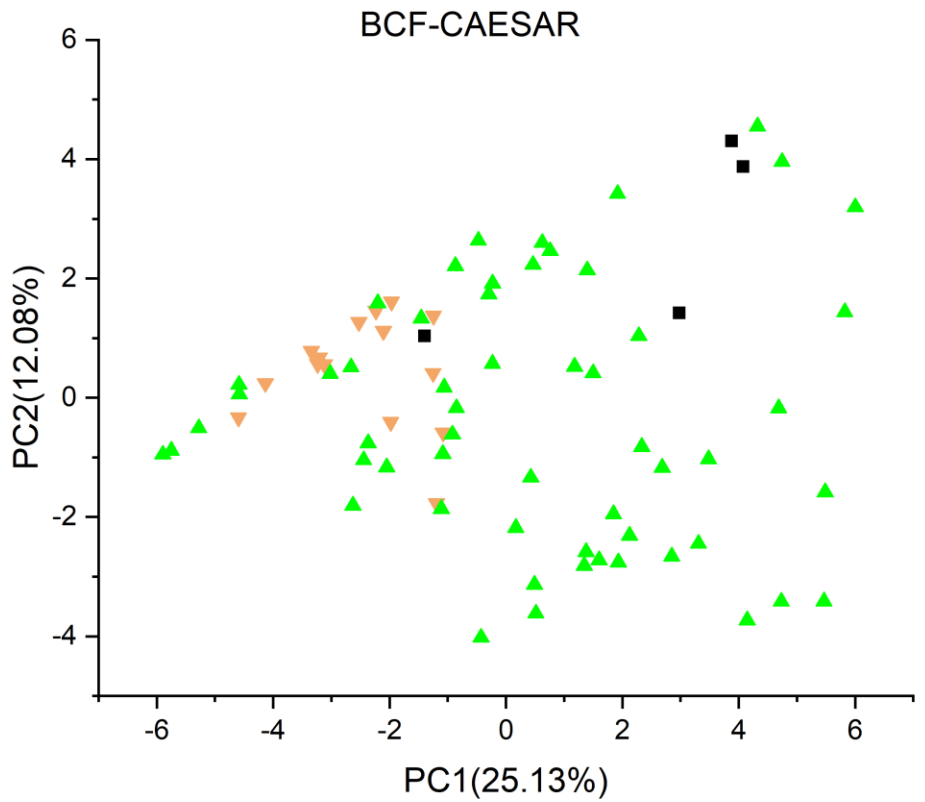
Sludge Classification Toxicity Model for Biocides (ProtoQSAR/COMBASE) Version 1.0.0



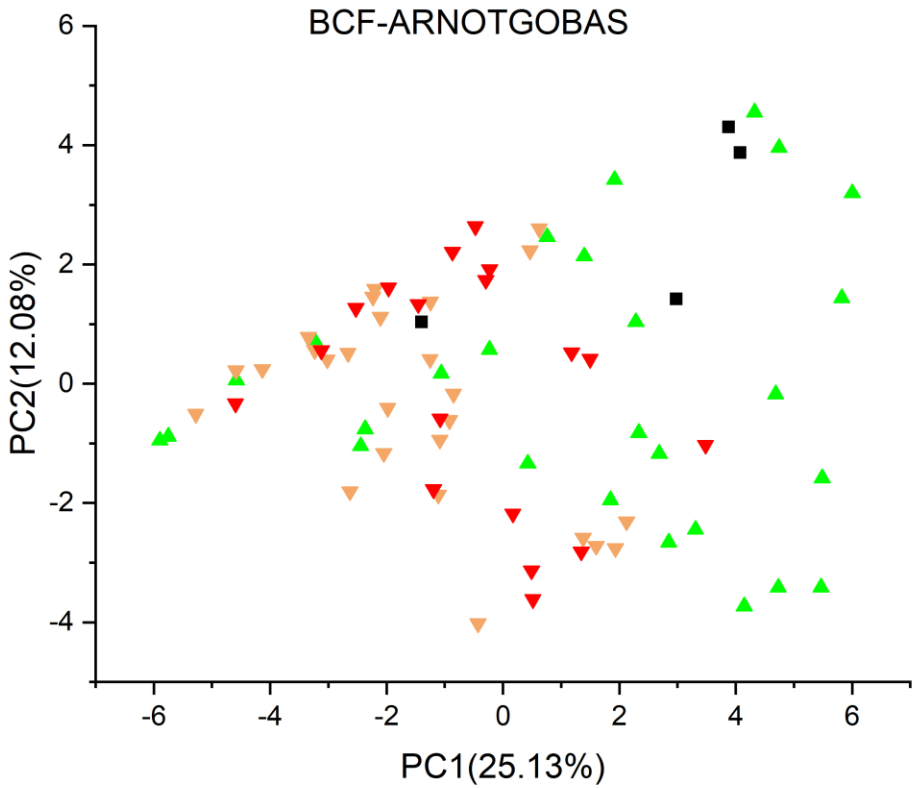
Sludge (EC50) Toxicity Version (ProtoQSAR/COMBASE) 1.0.1



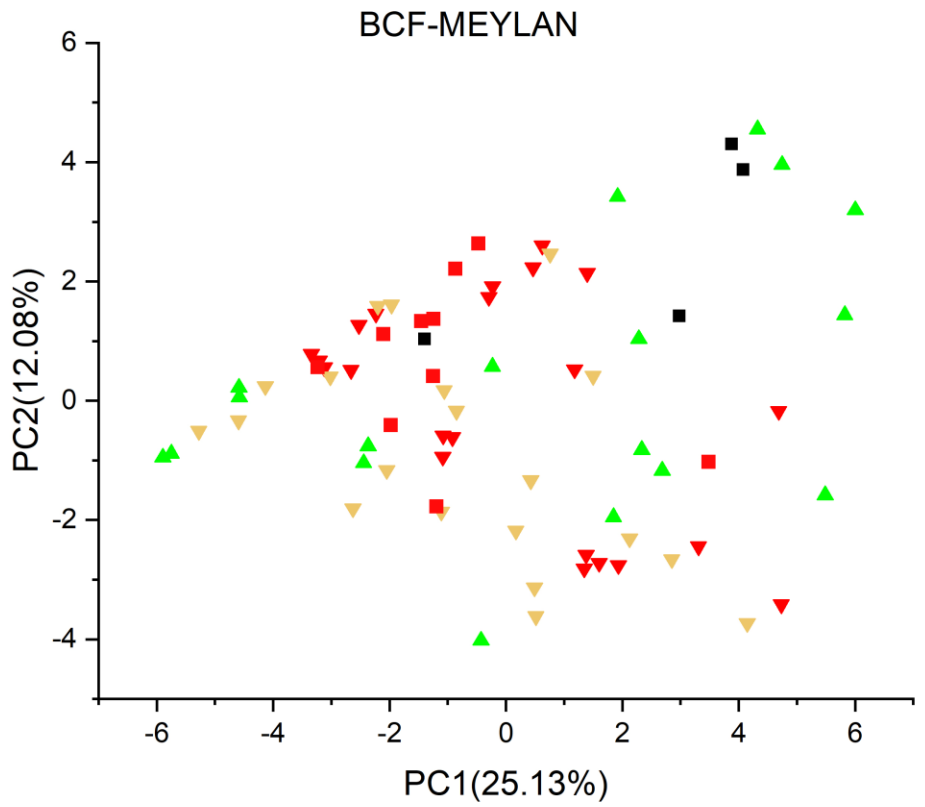
Bioconcentration Factors (BCF) Model (CAESAR) Version 2.1.15



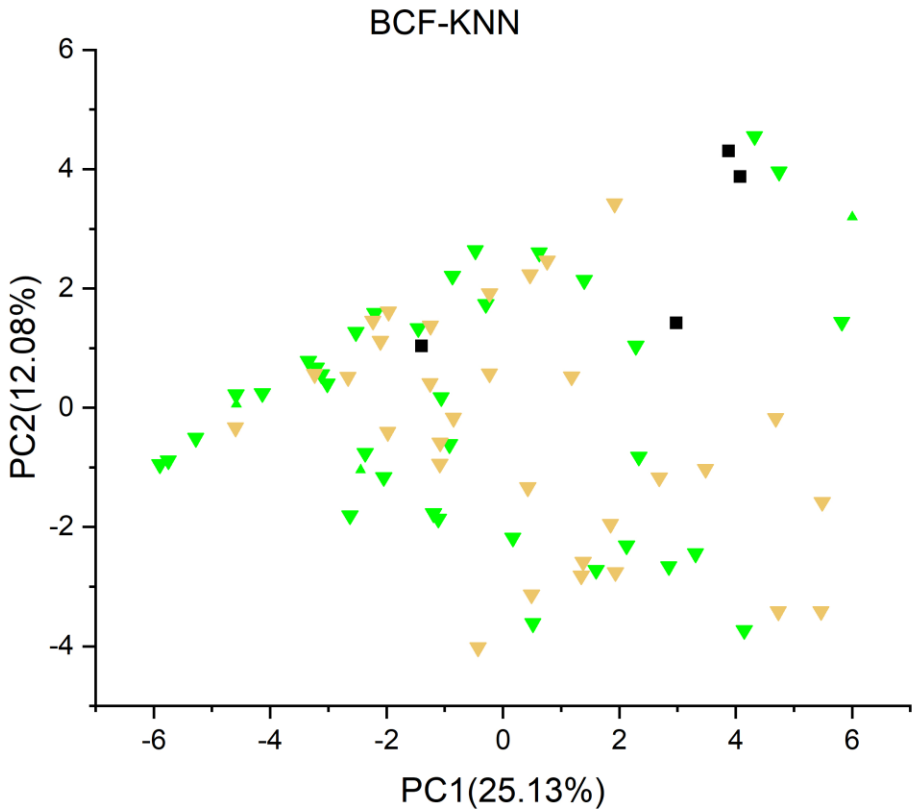
Bioconcentration Factors (BCF) Model (Arnot-Gobas) Version 1.0.1



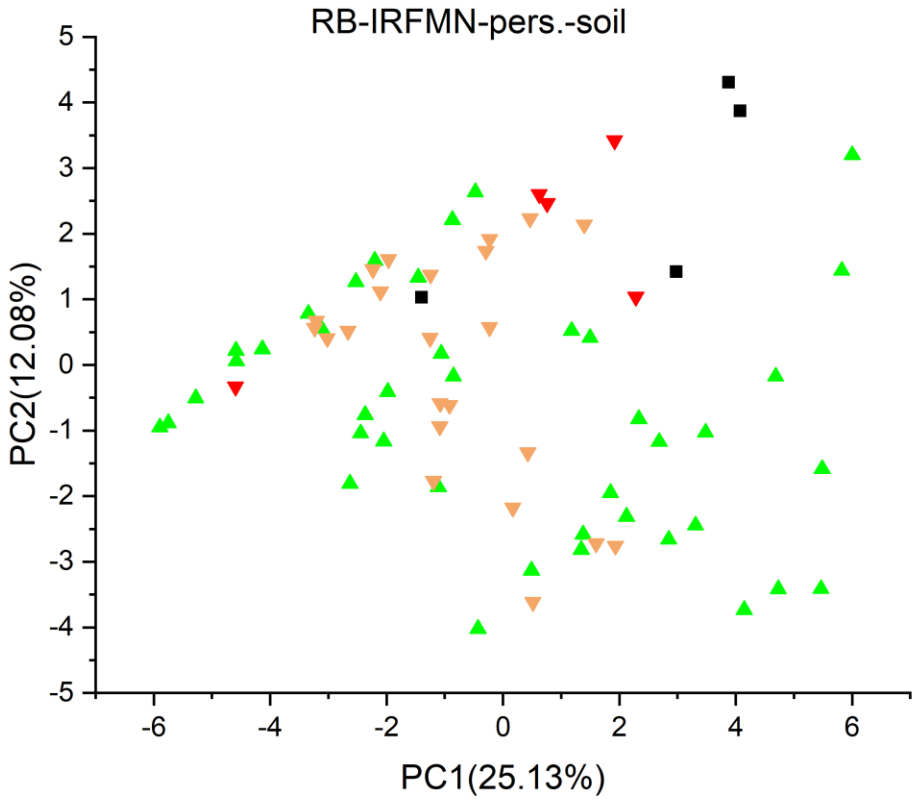
Bioconcentration Factors (BCF) Model (Meylan) Version 1.0.4



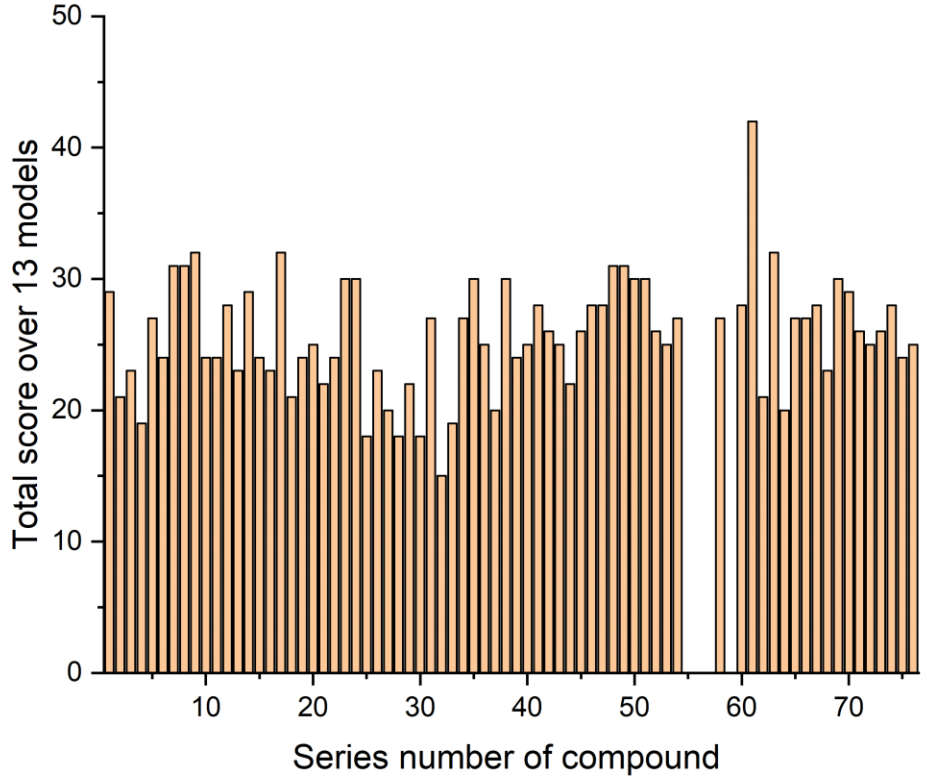
Bioconcentration Factors (BCF) Model (kNN/Read-Across) Version 1.1.1



Persistence (Soil) Quantitative Model (IRFMN) Version 1.0.1

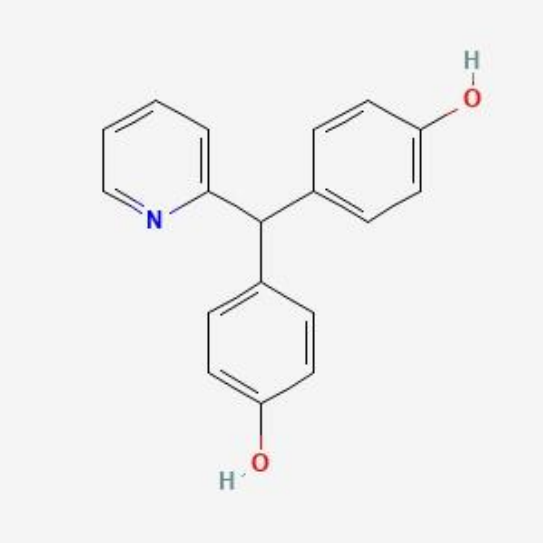


Cumulative hazard predicted by the in silico ecotoxicological model (sums over predictions: 3 for high concern, 2 for medium concern, 1 for no concern)



Conclusions

- Notably, the highest score of 42 was achieved by p,p'-(2 pyridylmethylene) bisphenol (DDPM).
- Additionally, 14 other compounds reached a score over 30: allyl bisphenol A (DAB), tetramethylbisphenol A (TMBPA), BAPP, bisphenol A bisallyl ether, BPG, BPPH, 4,40-methylenebis(2,6- dimethylphenyl cyanate), BPAP, BPM, BPP, BP-TMC, BPZ, DMT-Cl, and BisP-IOTD. These compounds were predicted to exhibit higher toxicity at the selected endpoints, potentially indicating a greater environmental concern.



Thank you for your attention!

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