

Environmental Fate of Porphyrin Derivatives from Petroleum

Yana Koleva¹ and Asen Kolev²

¹Department of chemistry, Burgas State University “Prof. Dr. Assen Zlatarov”, Burgas 8010, Bulgaria), e-mail: ykoleva@btu.bg

²“LUKOIL Neftochim Burgas”AD, Burgas, Bulgaria

GOAL OF THE STUDY

Porphyrin derivatives (geoporphyrins or petroporphyrins) are naturally occurring compounds found in petroleum. They are structurally similar to chlorophyll and hemoglobin, and their presence in crude oil provides evidence for the biological origins of petroleum. These compounds, often complexed with metals like nickel and vanadium, are crucial for understanding petroleum's formation and maturation processes. The aim of this work is to calculate and analyze various properties related to the environmental fate of porphyrin derivatives from petroleum, using the CompTox Chemistry Dashboard [1].

MATERIALS AND METHODS

Structure of chlorin (Figure 1).

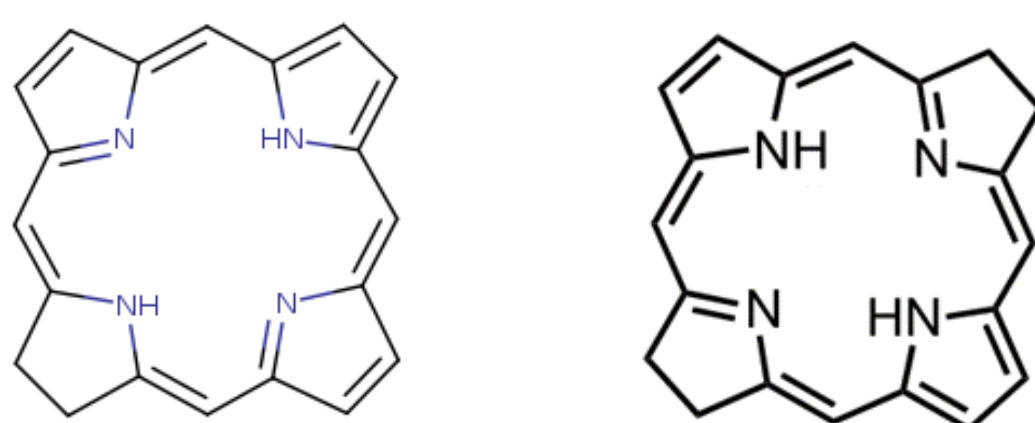


Fig. 1. Structure of chlorin and bacteriochlorin

CompTox Chemistry Dashboard.

The Dashboard is a freely accessible web-based application and data hub providing access to data associated with chemical substances. It accesses data from nine component databases housing generic data types. The Dashboard also integrates data from other platforms (specifically PubChem and PubMed) via web services and visualization widgets. The Dashboard represents a first step in building a comprehensive chemical substance-centric informatics architecture to provide flexible access to data, models and analysis tools in support of EPA's research programs [1].

RESULTS AND DISCUSSION

The results of the bioconcentration factor prediction for porphyrin derivatives from the CompTox Chemistry Dashboard are presented in Table 1.

Table 1. Predicted property (bioconcentration factor) for the porphyrin derivatives in petroleum

Nº	Experimental / Predicted average	Experimental / Predicted median	Experimental / Predicted range
1	- / 12.9	- / 12.9	- / 12.9
2	- / 22.4	- / 22.4	- / 22.4

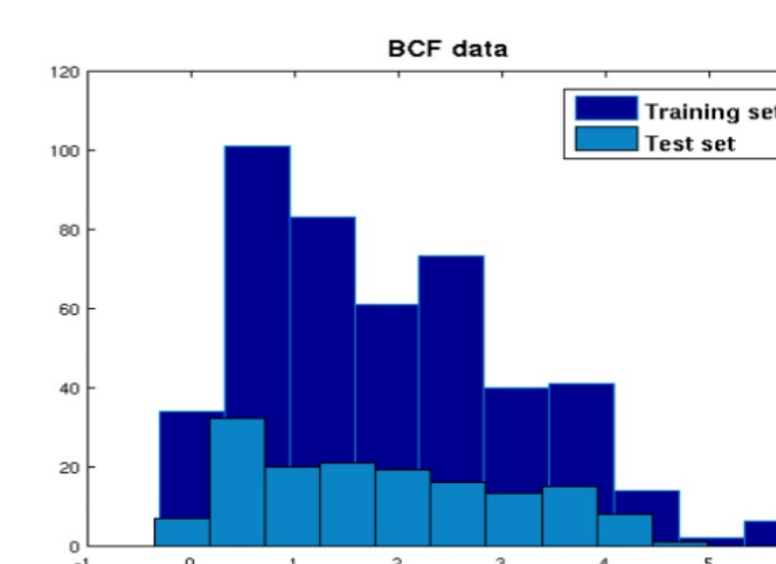


Fig. 1. Training and test set of the BCF data.

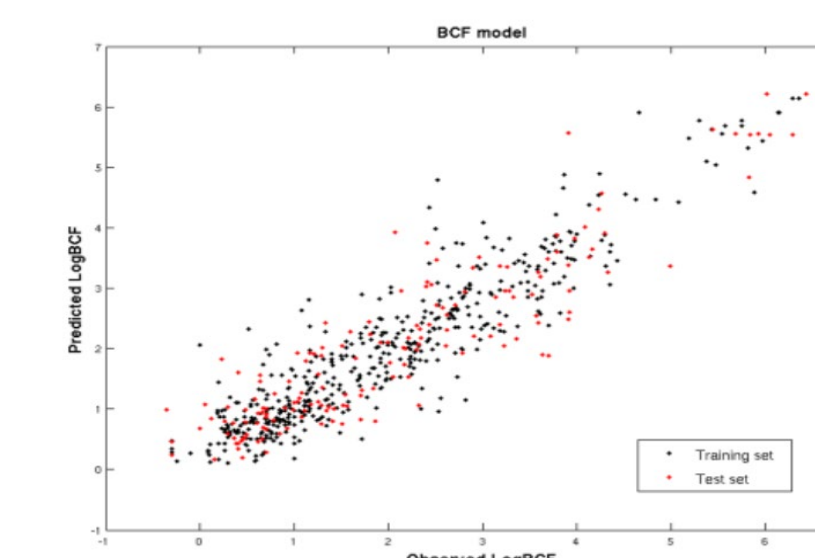


Fig. 2. Predicted BCF model

Table 2. BCF model (weighted KNN model).

5-fold CV (75%)		Training (75%)		Test (25%)	
Q ²	RMSE	R ²	RMSE	RMSE	R ²
0.840	0.550	0.850	0.530	0.640	0.830

CONCLUSIONS

In general, experimental data on the fate of porphyrin derivatives in the environment are limited. Theoretical chemistry has developed alternative methods for this purpose. In the present work, different properties (bioconcentration factor, atmospheric hydroxylation rate etc.) related to environmental fate of the porphyrin derivatives were calculated. Analysis of the calculated data can help in further working with them and gaining knowledge about the possibilities of their application.

ACKNOWLEDGMENT

This study was financially supported by the Burgas State University through the Scientific Research Sector - Project number 511/2025.

REFERENCES

1. A.J. Williams, C.M. Grulke, J. Edwards, A.D. McEachran, K. Mansouri, N.C. Baker, G. Patlewicz, I. Shah, J.F. Wambaugh, R.S. Judson and A.M. Richard. The CompTox Chemistry Dashboard: A community data resource for environmental chemistry. J. Cheminform. **9**, 61 (2017).