

Toxicological Profile of Porphyrin Derivative From Petroleum

Yana Koleva

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

GOAL OF THE STUDY

Porphyrins and chlorins are both tetrapyrrole macrocycles, but chlorins are partially hydrogenated porphyrins, meaning they have one pyrroline ring instead of four pyrrole rings. Porphyrins are the foundational structure, while chlorins are derived from them through hydrogenation. Chlorophylls and their derivatives are the most common pigments used for light absorption, energy transfer, and charge separation in photo synthetic organisms. Their functions change upon different aggregation states and specific pigment–protein interactions. Differences in the aromatic π -system and substituents finely tune Chlorophylls electronic, spectroscopic, and supramolecular characteristics. The goal of the present work is to predict the toxicological properties of porphyrin derivative (chlorin) by the CompTox Chemistry Dashboard.

MATERIALS AND METHODS

Structure of chlorin (Figure 1).

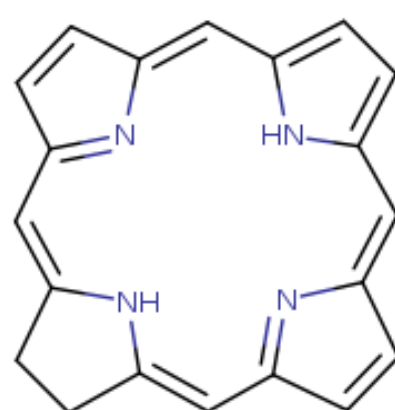


Fig. 1. Structure of chlorin

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].

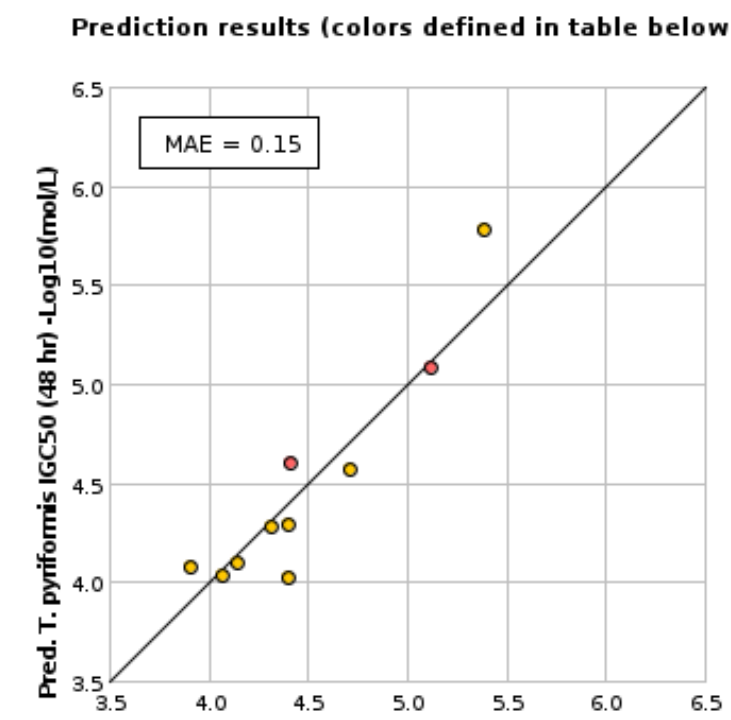
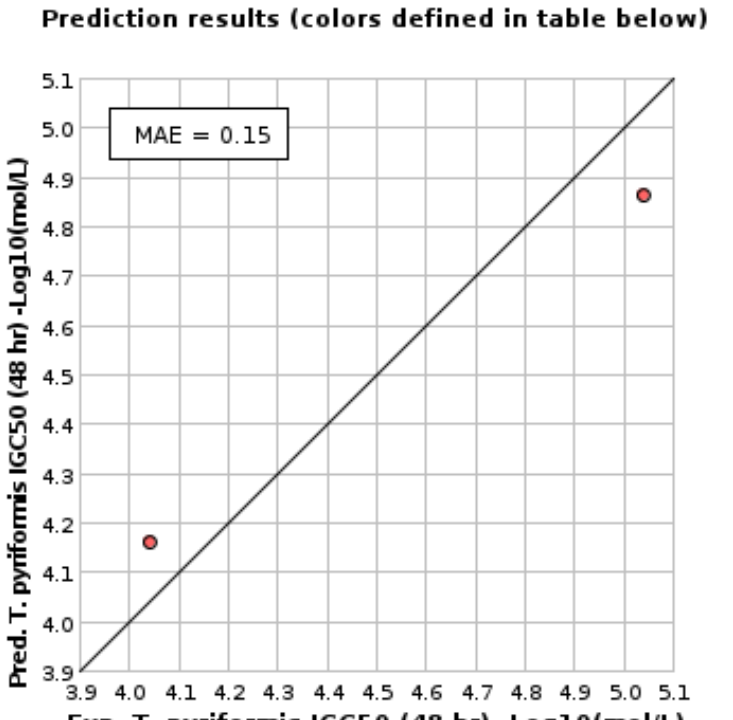
RESULTS AND DISCUSSION

Data of prediction (toxicological endpoints) of chlorin by the CompTox Chemistry Dashboard are presented in Table 1.

Table 1. Predicted results of toxicological endpoints for chlorin

Properties	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 h Fathead minnow LC_{50} , mg/L	0.262	0.180	0.180	-	0.558
48 h Daphnia magna LC_{50} , mg/L	0.909	0.303	0.410	-	6.059
48 h Tetrahymena pyriformis IGC_{50} , mg/L	3.792	-	-	1.315	10.941

Table 2. Predicted toxicological property (48 h *Tetrahymena pyriformis*, IGC_{50}) of chlorin by Consensus method.

Toxicological properties	Predictions for the test chemical and for the most similar chemicals in the training set	MAE*	Predictions for the test chemical and for the most similar chemicals in the external test set	MAE*
48 h Tetrahymena pyriformis IGC_{50} , mg/L		Entire set-0.28 Similarity coefficient ≥ 0.5 (0.15)		Entire set-0.33 Similarity coefficient ≥ 0.5 (0.15)

CONCLUSIONS

Porphyrins are macrocyclic compounds that can be modified in a seemingly infinite number of ways. These derivatizations often have remarkable and unique properties that can be used in a variety of applications. Overall, porphyrins are an interesting, diverse, and versatile class of molecules that is constantly expanding. Due to the wide application of porphyrins, it is necessary to study the possible toxicological potential for human health and the environment. Experimental data are limited, forcing decisions about the potential of a compound now and in the future to be made on the basis of limited data and information. Therefore, alternative *in silico* methods, such as the CompTox Chemistry Dashboard, are used to assess their behavior (potential toxicity).

ACKNOWLEDGMENT

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REFERENCES

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