

ADME Potential of Porphyrin Derivative From Petroleum

Yana Koleva¹, Viktoria Trifonova¹, Asen Kolev² and Yordanka Tasheva³

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

³Burgas State University “Prof. Dr. Assen Zlatarov”, Burgas 8010, Bulgaria

GOAL OF THE STUDY

Chlorins are tetrapyrrole pigments that are partially hydrogenated porphyrins. The parent chlorin is an unstable compound which undergoes air oxidation to porphine. Chlorins are excellent photosensitizing agents. The most abundant chlorin is the photosynthetic pigment chlorophyll. Chlorophylls usually feature magnesium as a central metal atom, replacing the two NH centers in the parent. Microbes produce two reduced variants of chlorin, bacteriochlorins and isobacteriochlorins. Numerous synthetic chlorins with different functional groups and/or ring modifications have been studied. The aim of the present study is to predict the biological effects of porphyrin derivative (chlorin) by applying an *in silico* approach. Dear authors, in the first section you could explain the investigated problem and the goals of the study.

MATERIALS AND METHODS

Structure of chlorin (Figure 1).

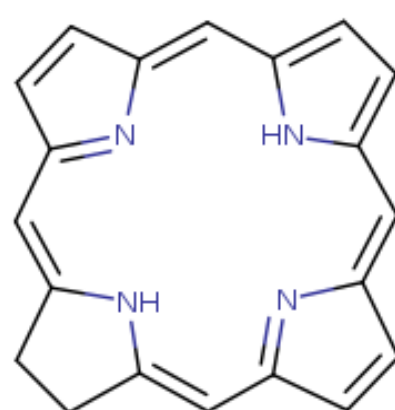


Fig. 1. Structure of chlorin

SwissADME. By means of it, free access to various properties and predictive models necessary in determining physicochemical parameters and for evaluating pharmacokinetics is obtained [1].

RESULTS AND DISCUSSION

Some physicochemical parameters of chlorin are given Table 1.

Table 1. Physicochemical properties of the compound (chlorin).

MW (g/mol)	Num. heavy atoms	Num. arom. heavy atoms	Fraction Csp ³	Num. rotatable bonds	Num. H-bond acceptors	Num. H-bond donors	Molar refractivity	TPSA (Å ²)
312.37	24	5	0.10	0	2	2	109.05	52.54

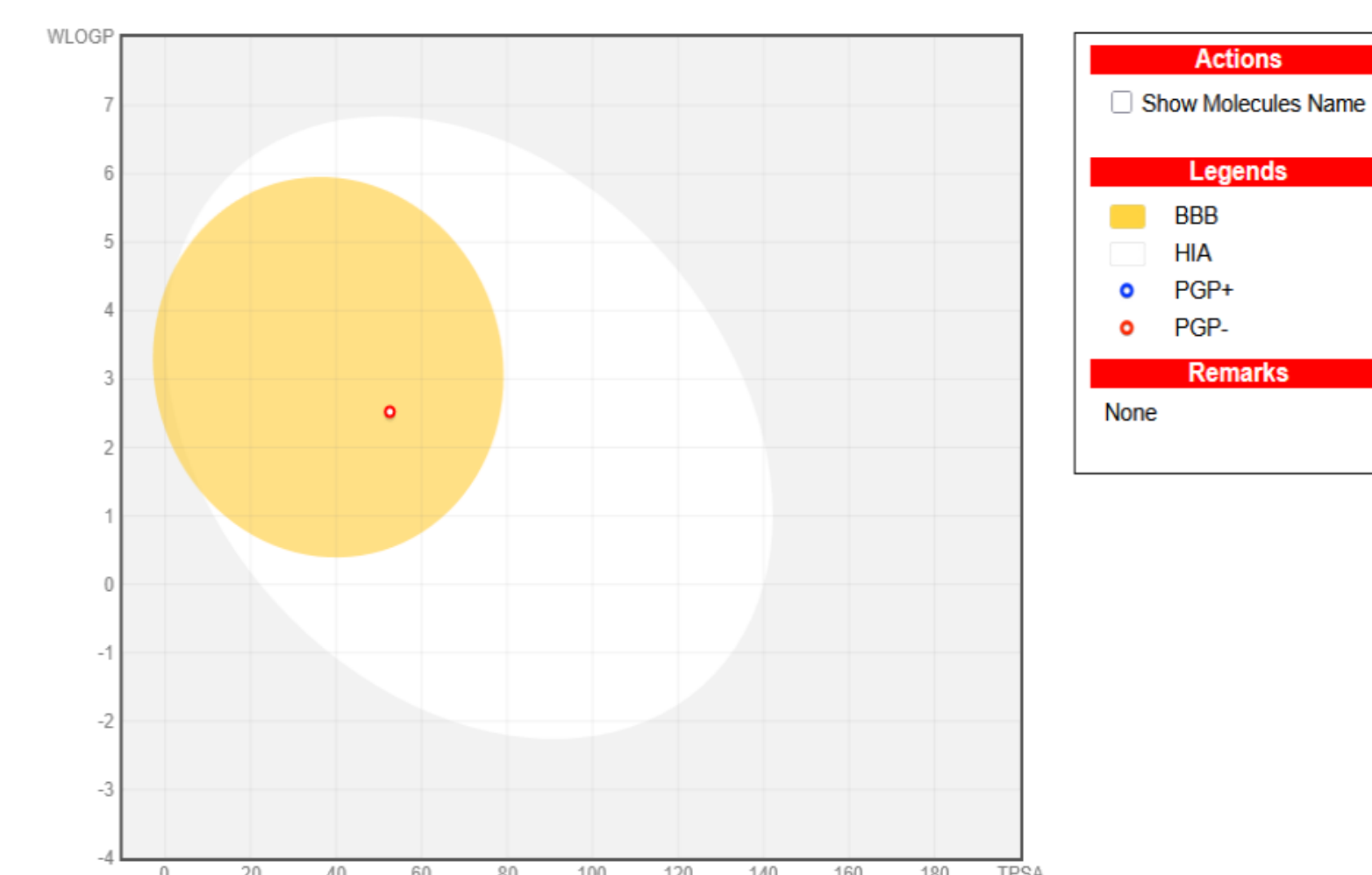


Fig 3. Schematic representation of perceptive evaluation of passive gastrointestinal absorption (HIA) and Brain penetration (BBB) using BOILED-Egg (WLOGP vs TPSA).

CONCLUSIONS

Porphyrins are a large and diverse class of pigments that are present in various plants and animals and play an essential role in the biochemistry of life. Porphyrins are able to resist decay and their tetrapyrrole core structure is usually preserved despite structural modifications during fossilization. The SwissADME tool allows the calculation of medically important physicochemical, pharmacokinetic and other parameters of porphyrin derivatives, which would enable the study of their beneficial effects and applications.

ACKNOWLEDGMENT

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REFERENCES

1. A. Daina, O. Michielin, V. Zoete, SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. [Sci. Rep. 7, 42717 \(2017\).](#)