Supplementary Information

2D, 3D and Hybrid QSAR Studies of Nostoclide Analogues as Inhibitors of the Photosystem II

Pedro O. M. de Carvalho* and Márcia M. C. Ferreira **

*Instituto de Química, Universidade Estadual de Campinas, 13083-970 Campinas-SP, Brazil

Table S1. 2D QSAR molecular descriptors values

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*Percentage of photosynthesis inhibition; **non effective: PI < 5 %.

*e-mail: marcia@iqm.unicamp.br
Table S2. 3D QSAR molecular descriptors values

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\textsuperscript{a}Percentage of photosynthesis inhibition; \textsuperscript{b}non effective: PI < 5 %.
Table S3. Hybrid QSAR molecular descriptors values

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*Percentage of photosynthesis inhibition; * non effective: PI < 5 %.
Table S4. Measured and predicted percentages of photosynthesis inhibition

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<th>Predicted PI (2D QSAR)</th>
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$^a$Percentage of photosynthesis inhibition; $^b$non effective: PI < 5 %.
Figure S1. Graphs of (a) $R^2 \times Q^2$; (b) $R^2_{(y,\text{rand})} \times R^2$; and (c) $R^2_{(y,\text{rand})} \times Q^2$ of the $y$-randomization test for 2D-QSAR model.

Figure S2. Graphs of (a) $R^2 \times Q^2$; (b) $R^2_{(y,\text{rand})} \times R^2$; and (c) $R^2_{(y,\text{rand})} \times Q^2$ of the $y$-randomization test for 3D-QSAR model.

Figure S3. Graphs of (a) $R^2 \times Q^2$; (b) $R^2_{(y,\text{rand})} \times R^2$; and (c) $R^2_{(y,\text{rand})} \times Q^2$ of the $y$-randomization test for hybrid-QSAR model.