Evaluation of the Solubility, Aggregation Behavior, and Spectroscopic Properties of Water-soluble Porphyrins Bearing Oligo(ethylene glycol) Side Chains via Phenyl or Alkyl Linkers

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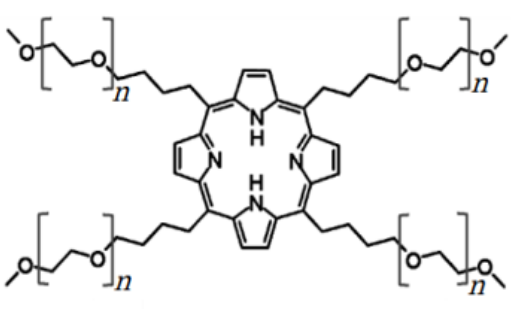
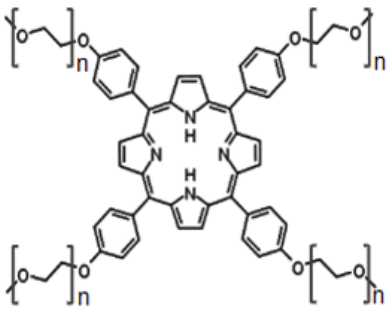
Porphyrin derivatives have been extensively studied as photosensitizers and catalysts, and molecular designs for in vivo applications are also being actively explored. For biomedical use, imparting sufficient water solubility is essential, and one common strategy is to introduce oligo(ethylene glycol) (OEG) chains, which are neutral functional groups, as peripheral substituents. However, OEG-based water-soluble porphyrins reported to date are limited to derivatives in which OEG chains are installed via a phenylene spacer.

In this study, we synthesized a new series of porphyrin derivatives, P-C_4EG*n* (*n* = 3, 5, 7), featuring a tetramethylene (C_4) spacer, and compared their solubility, spectroscopic properties (UV–vis absorption and fluorescence), and aggregation behavior in water and THF with those of the corresponding phenylene-spacer analogues (P-PhEG*n*). At *n* = 3, P-C_4EG3 was soluble in water at 1 mM, whereas P-PhEG3 was insoluble. In addition, for P-PhEG5, the Soret band in water showed a pronounced decrease in absorbance and clear splitting relative to that in THF, suggesting aggregation in water. For P-PhEG7, splitting of the Soret band was also observed, but with little decrease in absorbance. These results indicate OEG-chain-length-dependent spectral behavior. In contrast, P-C_4EG5 and P-C_4EG7 showed little change in their absorption spectra between THF and water, suggesting suppressed aggregation in water for the C_4-spacer series.

Overall, our findings demonstrate that both the spacer structure and the OEG chain length are key factors in controlling the balance between water solubility and aggregation.



P-C_4EG*n*



P-PhEG*n*

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