Synthesis and Properties of Cationic and Neutral Radical Diaza[4]helicenes as Components of Supramolecular Polymers

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Helicenes are screw-shaped molecules formed by *ortho*-fused aromatic rings, whose peculiar shape derives from the steric hindrance of the terminal aryl rings or substituents. This unique structure makes them chiral chromophores, which exist in two enantiomeric configurations, denoted as (*M*) and (*P*) (*Figure 1*). In this work, cationic and neutral radical [4]helicenes are studied based on dimethoxyquinacridine (DMQA) scaffolds of type **I**. [1]

Thanks to Ir-catalyzed direct C(sp^2)-H borylation, regioselective functionalization of the three positions *para* to the formal positive charge of **I** is achieved, enabling the introduction of a variety of functional groups.

The incorporation of amide moieties (**II**) bearing linear alkylamine chains, such as *n*-octylamine, is pursued to investigate the formation of higher-order aggregates (*Figure 2*). Such structural features are well-known in supramolecular chemistry for promoting ordered aggregation. [2,3]

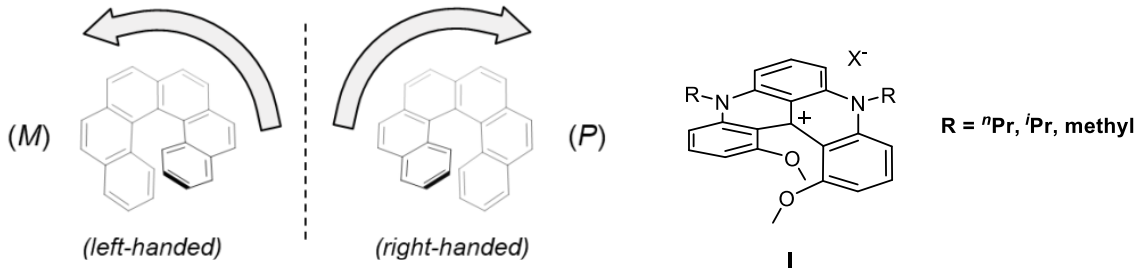
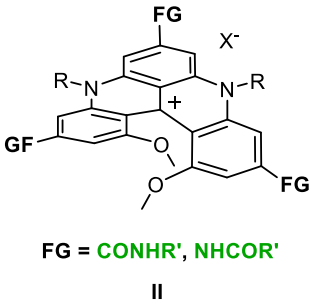


Figure 1



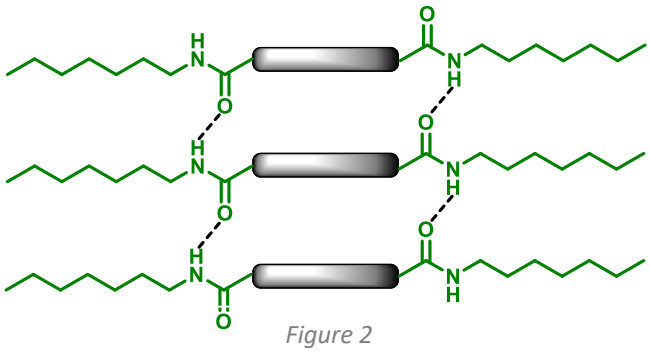


Figure 2

With the introduction of new functional groups, detailed optical and chiroptical studies are conducted. These investigations aim to provide a comprehensive understanding of intrinsic properties and to predict the supramolecular assembly, both in cationic form (with different counterions) and as neutral radicals generated via one-electron reduction, exploring the influence of different side chains on the scaffold.

[1] J. Bosson, N. Bisballe, B. W. Laursen, J. Lacour, *Helicenes* **2022**, 127–165. .
[2] L. Villar, N. V. Orlov, N. S. Kondratyev, U. Uria, J. L. Vicario, A. V. Malkov, *Chem. Eur. J.* **2018**, *24*, 16262-16265.
[3] S. M. C. Schoenmakers, A. J. H. Spiering, S. Herziger, C. Bottcher, R. Haag, A. R. A. Palmans, E. W. Meijer, *ACS Macro Letters* **2022,** *11* (5), 711-715.