Phenylalanine-Based Low Molecular Weight Gelators: Synthesis, Supramolecular Characterization and Multicomponent Gelation

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Introduction: L-Phenylalanine (Phe), a neutral and nonpolar essential amino acid, serves as a key building block for supramolecular assemblies. Several low molecular weight gelators (LMWGs) containing Phe have been developed, with potential applications in different areas such as drug delivery, tissue engineering, and oil spill recovery. Similarly, vicinal dialkylamides have also demonstrated LMWG-forming capabilities, being promising materials for future research and development. In this context, the study of potential gelators was carried out with the synthesis of four Phe derivatives using 4,5-bromo-1,2-phenylenediamine (BPD) or (1R,2R)-(−)-1,2-diaminocyclohexane (DAC) as scaffolds.

Methods: N-tert-butoxycarbonyl (Boc)-protected Phe was reacted with BPD or DAC (2:1 molar ratio) to yield **BPD-1** and **DAC-1**, respectively. Subsequent deprotection afforded **BPD-2** and **DAC-2**. Gelation ability of the synthesized compounds was tested in a range of solvents by means of the inverted test-tube method. Minimum gelation concentration (MGC) and sol-gel temperature (Tg) were determined for the resulting gels. Aditionally, gels were characterized morphologically (SEM), rheologically, and by circular dichroism (CD) spectroscopy at low concentrations.

Results: Although not all derivatives prepared could form any gels in common solvents, **BPD-1** was found to produce stable gels in carbon tetrachloride, whereas **DAC-2** generated an unstable gel in tetrahydrofuran. A multicomponent stable gel in carbon tetrachloride (*M1*BDP-1) was also achieved by combining **BPD-1** with a previously reported LMWG with the same scaffold. SEM revealed fibrous three-dimensional network structures composed of fibers in **BPD-1** and *M1*BDP-1 xerogels. Also, CD spectra display signals that suggest chiral supramolecular aggregation in BDP-1 gels.

Conclusion: The results indicate that combining Phe with known LMWG fragments can yield new gelating derivatives, highlighting their potential for functional material design. Further studies should explore gelation in less common solvents and elucidate the assembly mechanism of the multicomponent gels obtained.

Keywords: Gelator; L-Phenylalanine; Supramolecular chirality