Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information

Self-assembling of Boc-*p*-nitro-L-phenylalanyl-*p*-nitro-L-phenylalanine and Boc-L-phenylalanyl-L-tyrosine in solution and into piezoelectric electrospun fibers

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Results and Discussion

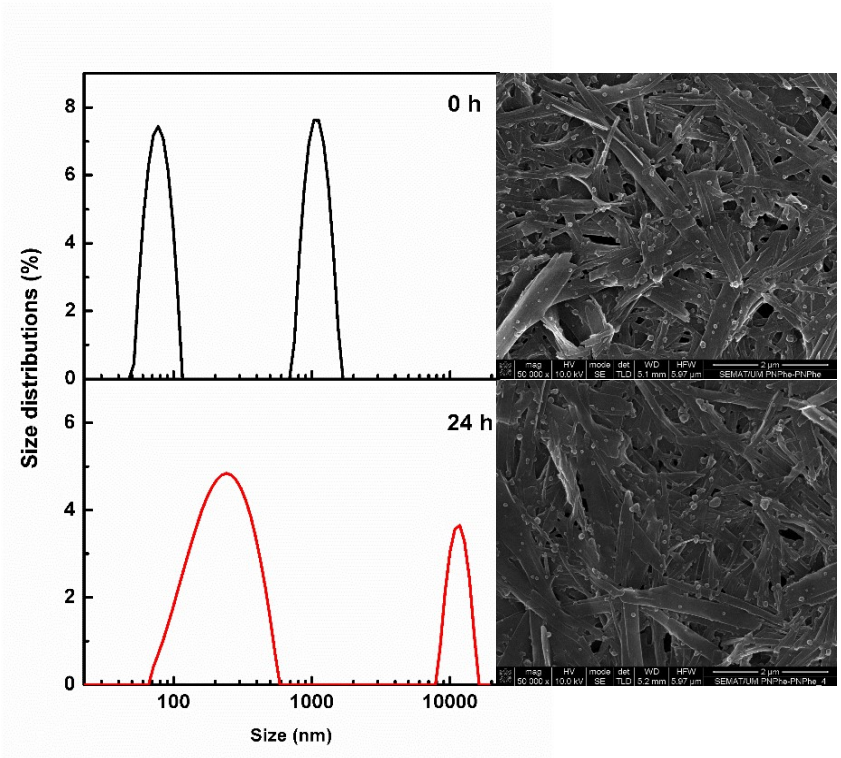

Fig. S1 Intensity weighted particle size distributions of Boc-*p*NPhe*p*NPhe. First measurement (0h) in black line and second measurement (24h) in red.

Raman studies: Raman scattering gives us information about structural features of the crystalline compounds, in particular in the hydrogen bonds.[1] The intermolecular properties of the dipeptide self-assembled structures were characterized by Raman scattering spectroscopy. The studies were performed on single crystal of each of dipeptides Boc-*p*NPhe*p*NPhe and Boc-PheTyr and compared with that of Boc-PhePhe. For Boc-PheTyr structures, the characteristic bands are similar to those

reported for Boc-PhePhe nanotubes.[2, 3] Relatively to Boc-*p*NPhe*p*NPhe dipeptide some differences are found in the region 800-1700 cm^{-1}. The ring breathing band at 1003 cm^{-1} is not present and instead a very intense band at 1345 cm^{-1} corresponding to the NO_2 group vibrations, which is covalent bonded to the phenyl benzene ring, is now the most intense band. This is probably due to the presence of the two NO_2 groups which hinders the 1003 cm^{-1} band and deviates it to the new band appearing at 1104 cm^{-1}. For both Boc-*p*NPhe*p*NPhe Boc-PheTyr the crystalline lattice vibrations bands are similar to that of Boc-PhePhe dipeptide as well the bands correspondent to the aromatic C-H stretches.

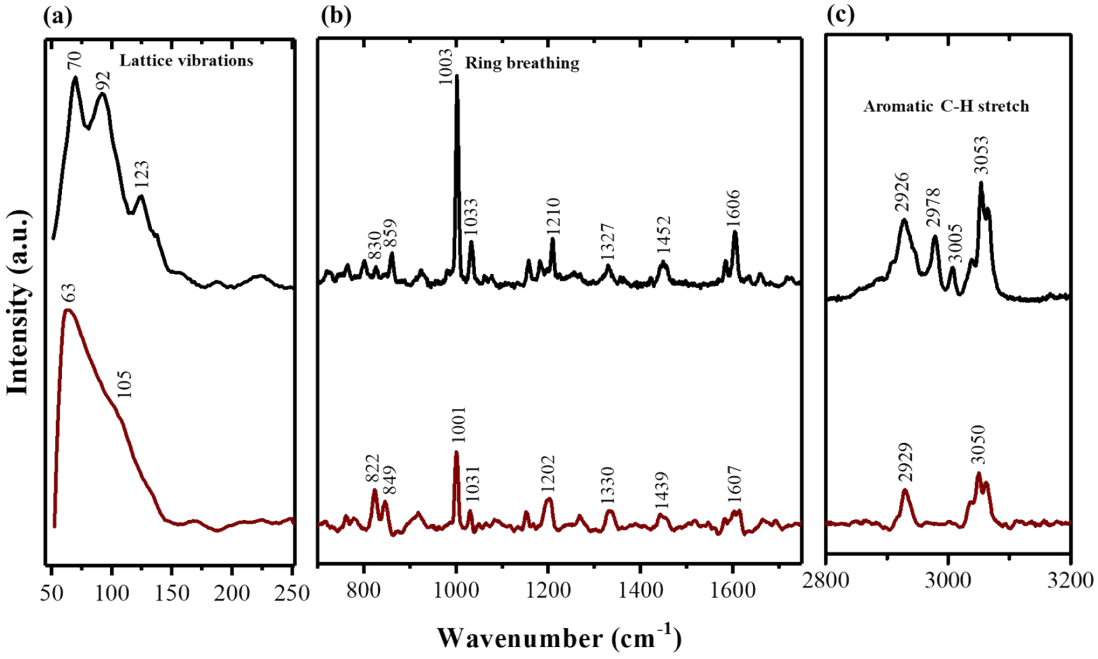

Fig. S2 Raman spectra of Boc-PhePhe (black line) and Boc-PheTyr (red line) segmented into three spectral regions: 40–250 cm^{-1} (**a**), 700–1750 cm^{-1} (**b**) and 2800–3200 cm^{-1} (**c**).

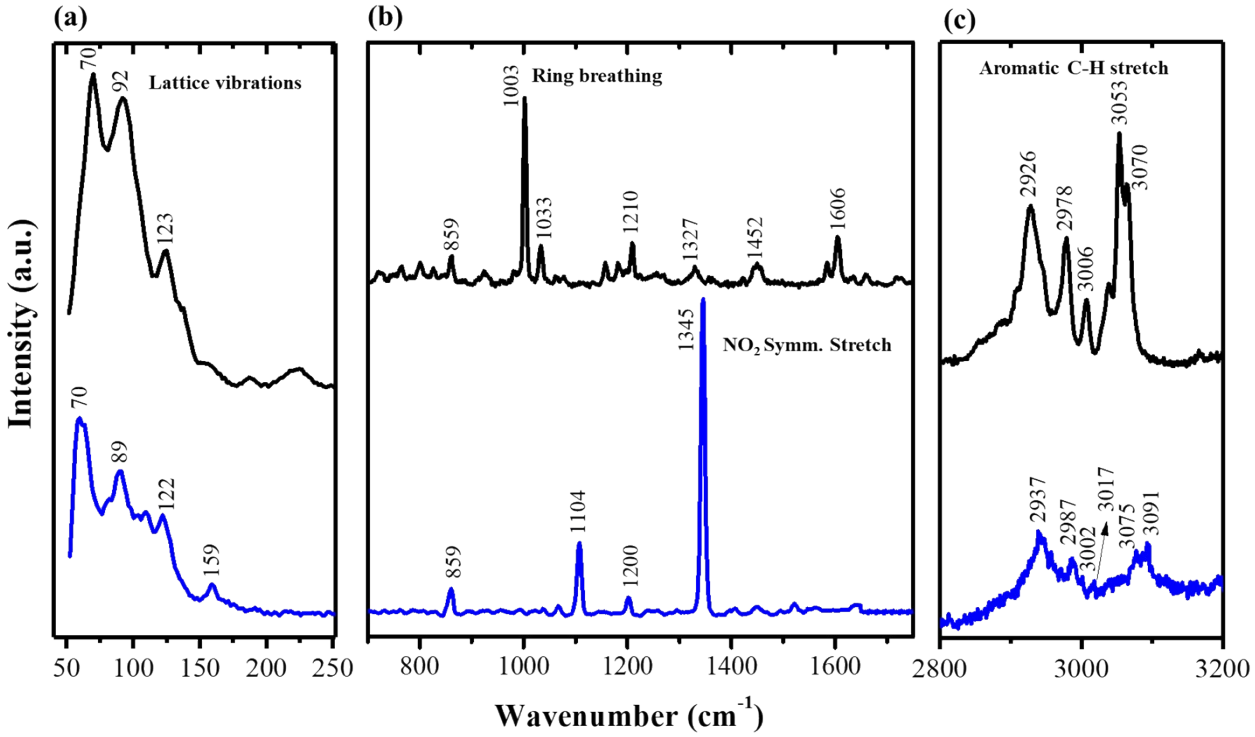

Fig. S3 Raman spectra of Boc-PhePhe (black line) and Boc-*p*NPhe*p*NPhe (blue line) segmented into three spectral regions: 40–250 cm^{-1} (**a**), 700–1750 cm^{-1} (**b**) and 2800–3200 cm^{-1} (**c**).

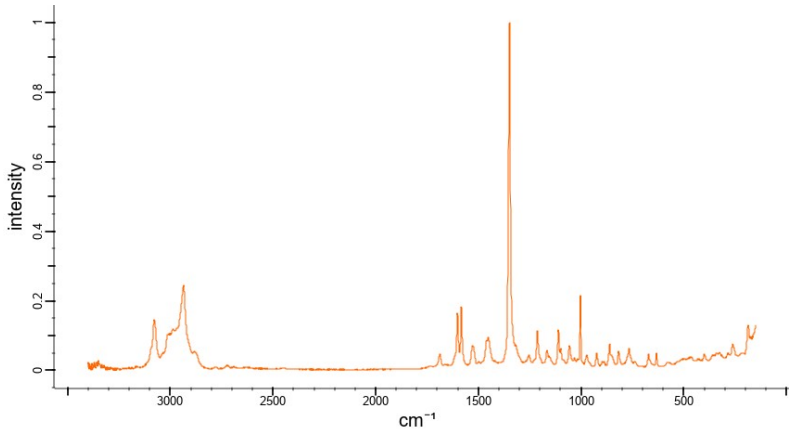

Fig. S4 Raman spectra of Boc-*p*NPhe (found in https://spectrabase.com/spectrum/H84GmThKMH0).

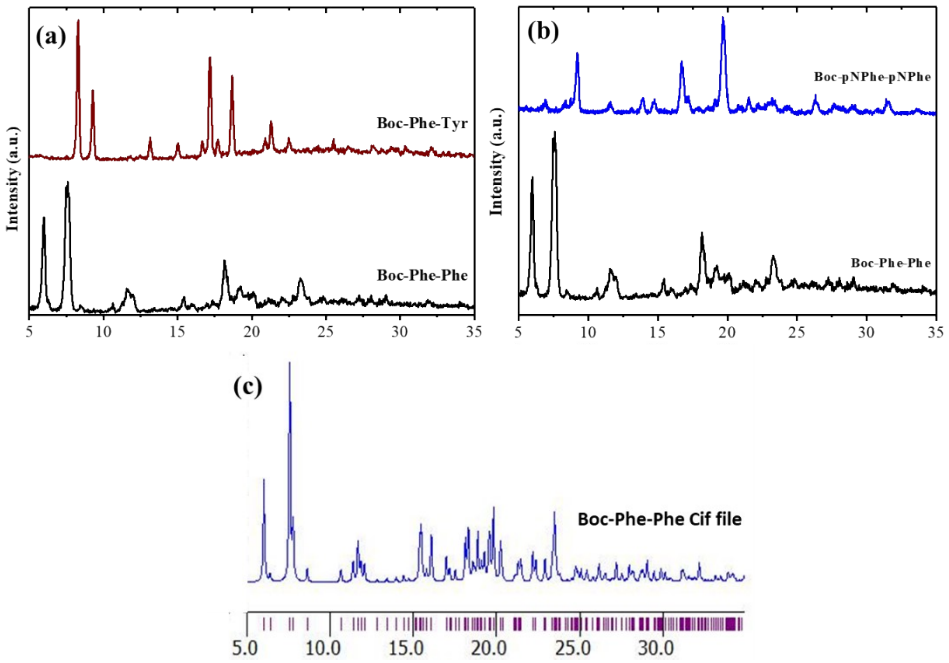

Fig. S5 XRD spectra of Boc-PheTyr (a), Boc-*p*NPhe*p*NPhe (b) nanostructures and Cif file[4] of Boc-PhePhe (c).

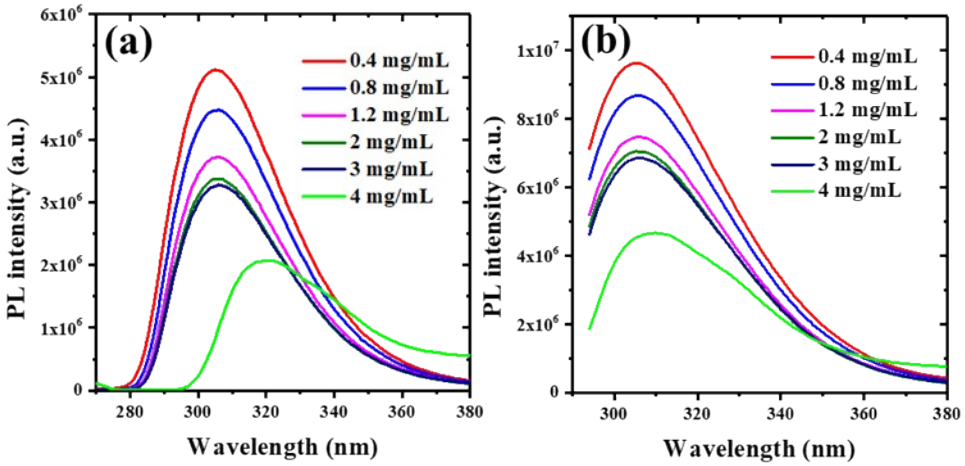

Fig. S6 PL spectra of the Boc-PheTyr MTp at several concentrations in water. The excitation wavelengths are 260 nm (**a**) and 286 nm (**b**).

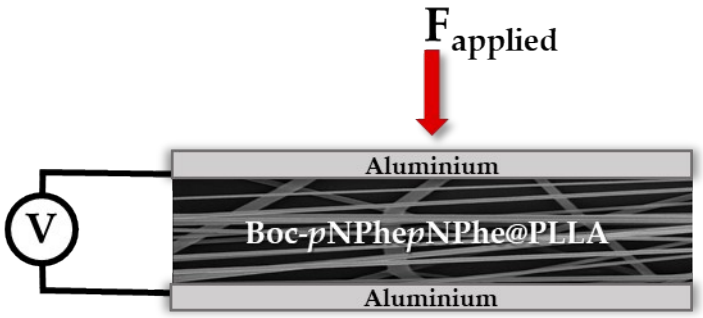

Fig. S7 Schematic piezoelectric setup with Boc-pNPhepNPhe@PLLA fibers arrays. The electrospun fibers were directly deposited on high purity aluminium foil, which served as electrodes. The fiber mat was sandwiched between the electrodes and put on an horizontal stage where the forces were applied vertically. Thin cupper wires were glued to the electrodes and connected to a low band pass filter.

References

1. Z. Gan, X. Wu, X. Zhu and J. Shen, *Angewandte Chemie International Edition*, 2013, **52**, 2055-2059.
2. R. M. F. Baptista, E. de Matos Gomes, M. M. M. Raposo, S. P. G. Costa, P. E. Lopes, B. Almeida and M. S. Belsley, *Nanoscale Advances*, 2019, **1**, 4339-4346.
3. G. Singh, A. M. Bittner, S. Loscher, N. Malinowski and K. Kern, *Adv Mater*, 2008, **20**, 2332-2336.
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