The structural motif of the low molecular weight organogelator (R)-9-hydroxystearic acid revealed by X-ray synchrotron radiation

Fioretta Asaro\textsuperscript{1*}, Carla Boga\textsuperscript{2}, Patrizia Nitti\textsuperscript{1}, Sara Drioli\textsuperscript{1}, Francesco Princivalle\textsuperscript{3}, Ennio Zangrando\textsuperscript{1}

\textsuperscript{1}Department of Chemical and Pharmaceutical Sciences, University of Trieste, Trieste, Italy
\textsuperscript{2}Department of Industrial Chemistry “Toso Montanari”, University of Bologna, Bologna, Italy
\textsuperscript{3}Department of Mathematics and Geosciences, University of Trieste, Trieste, Italy

\textsuperscript{*}e-mail: fasaro@units.it

(R)-12-hydroxystearic acid ((R)-12-HSA) is one of the most popular low molecular weight organogelators. However, in spite of the many investigations, the supramolecular arrangement inside the helical fibres that constitute the gel skeleton is still unclear [1]. Even, the single crystal X-ray structure is missing because no crystal was obtained, at variance with the racemic mixture, a by far less efficient organogelator, if any. (R)-9-HSA, which bears the OH group halfway the chain, retains the orgagelation ability. The gel obtained at 0.5 % wt in paraffin oil is amorphous (XRD) and displays a CD band, diagnostic of helical aggregates. It can also be crystallized. We obtained the X-ray structure of a single crystal of enantiopure (R)-9-HSA, from extract of seeds of Dimorphoteca sinuata L., at high resolution by means of X-ray synchrotron radiation at Elettra, Trieste. It revealed twisted carboxylic acid dimers, made of two independent molecules, somewhat strained, forming undulated layers. They are packed in head-tail fashion and hydrogen bonded at the mid chain OH groups. The observed arrangement is remarkably different from that found in the crystals of the racemic mixture of 12-HSA [2, 3]. On the basis of recent models that explain the twisting transition occurring in amyloids, the strain stored in the crystalline lattice may be responsible for the twist of organogel fibers.

\textbf{Figure 1.} From left to right: (R)-9-HSA paraffin oil gel, flower of Dimorphoteca sinuata L., layer of (R)-9-HSA dimers.

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