Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

ELECTRONIC SUPPLEMENTARY INFORMATION

Tubular J-Aggregates of a New Thiacarbocyanine Cy5 Dye for the Far-red Spectral Region – A Spectroscopic and Cryo-Transmission Electron Microscopy Study

Hans v. Berlepsch* and Christoph Böttcher

*Forschungszentrum für Elektronenmikroskopie, Institut für Chemie und Biochemie, Freie Universität Berlin, Fabeckstraße 36a, D-14195 Berlin, Germany
E-Mail: h.v.berlepsch@fzem.fu-berlin.de

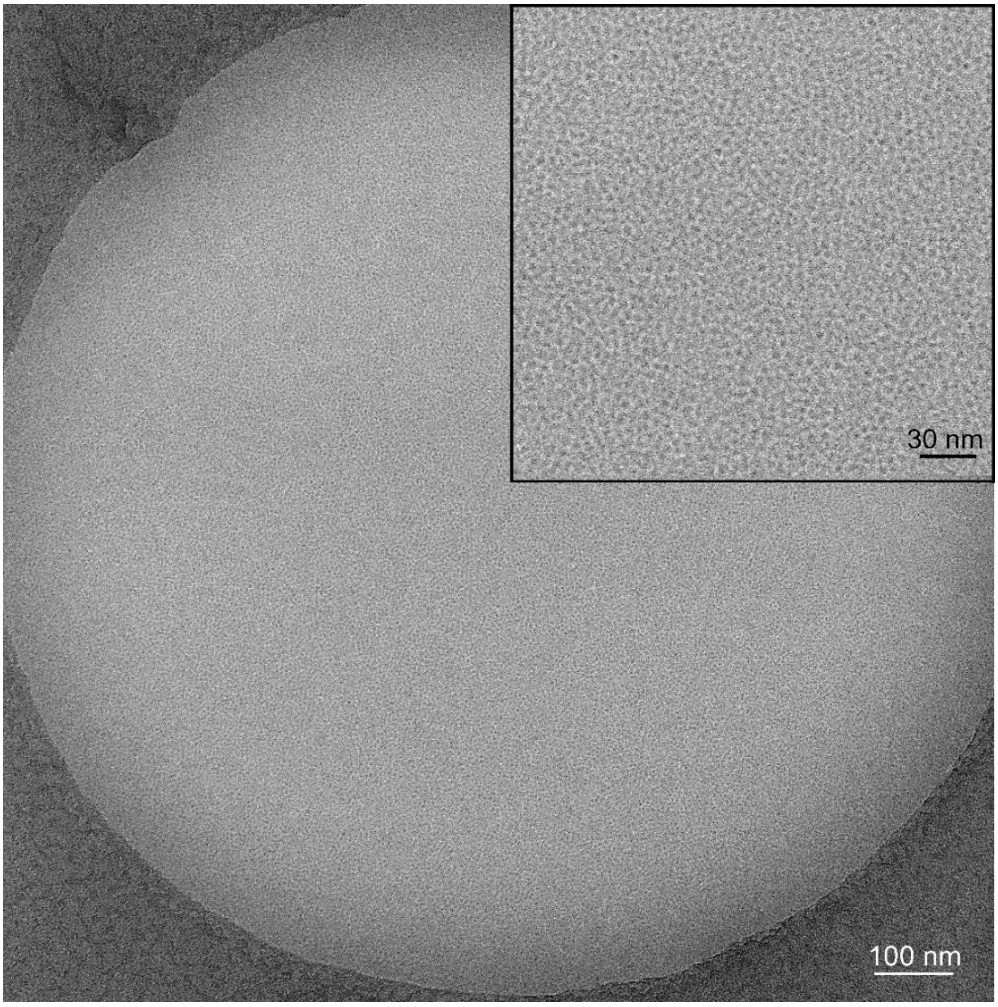

Fig. S1 Cryo-TEM image of a 3-days-old 0.84 mM dye solution in water showing the typical H-aggregate absorption spectrum. Solely monodisperse, spot-like particles of ~ 2.6 nm diameter may be seen. The inset shows the aggregates at larger magnification.

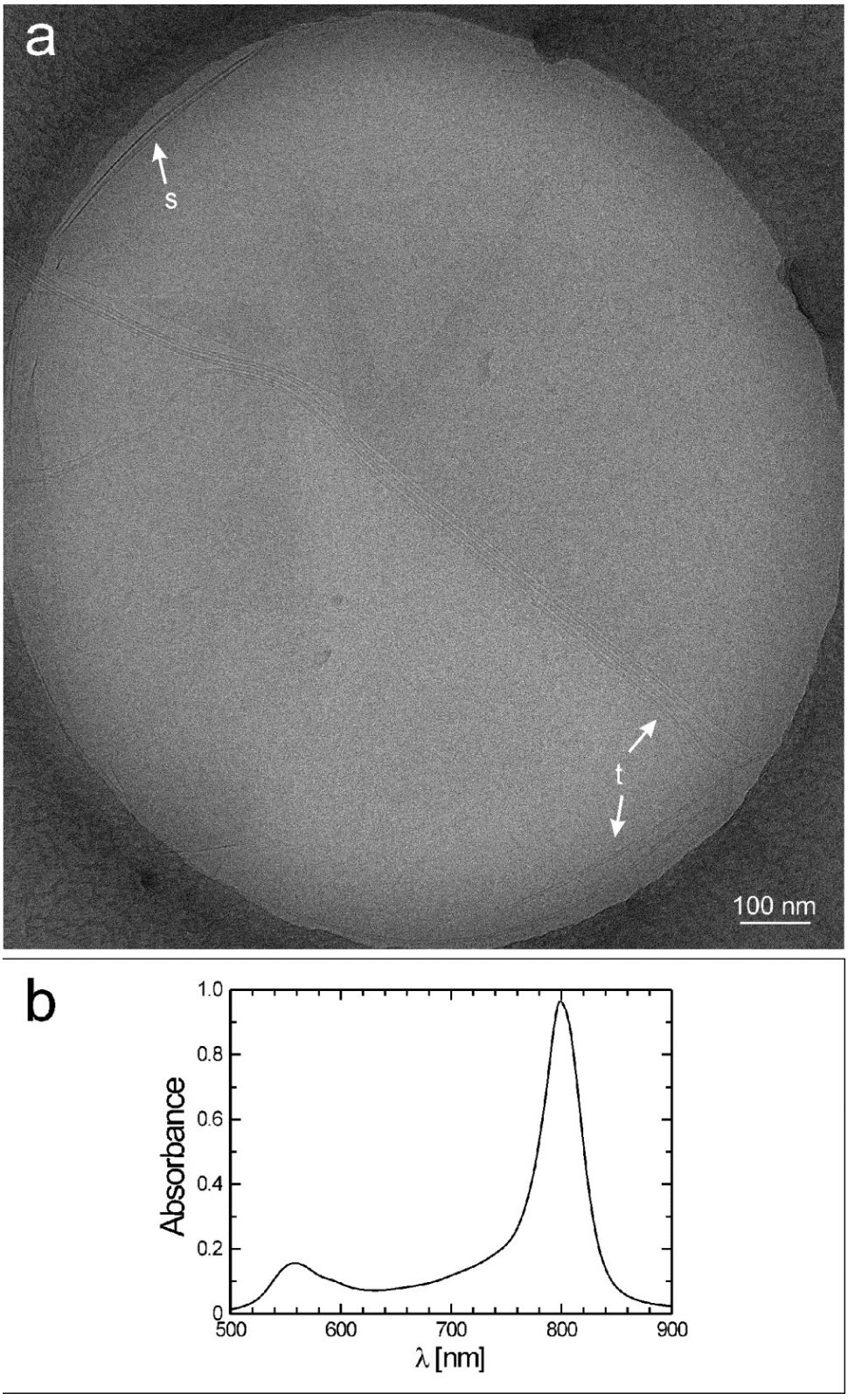

Fig. S2 Cryo-TEM image (a) and absorption spectrum (b) of a 0.55 mM S2284 solution aggregated in water containing 15 mM NaCl one day after preparation. The J-band is still unstructured and broad, indicating the predominance of intermediate J-aggregates. The micrograph reveals sheet-like (s), mono-layered aggregates and nanotubes (t), whereby the aggregates with sheet-like architecture dominate. The sheets often reveal dark lines, which emerge from folds and provide direct quantitative access to their mono-layered cross-section.

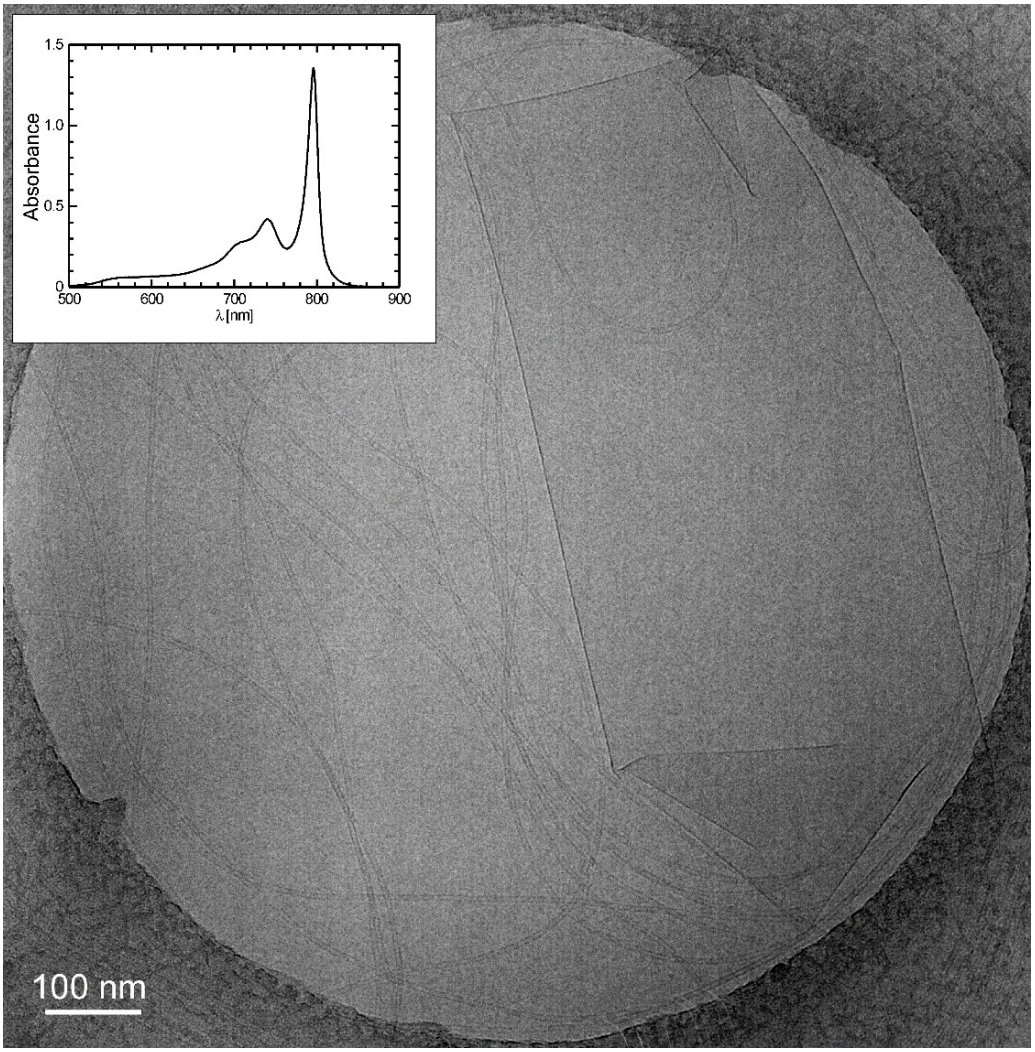

Fig. S3 Cryo-TEM image of a 0.25 mM dye solution aggregated in water containing 30 mM NaCl after storage for 5 months. A number of nanotubes and one large sheet-like aggregate are visible. The inset displays the absorption spectrum of the investigated solution. Typical for that sample preparation is the overwhelming predominance of nanotubes. Only this micrograph of a total of 36 taken from the sample showed a sheet-like aggregate in addition to the nanotubes.

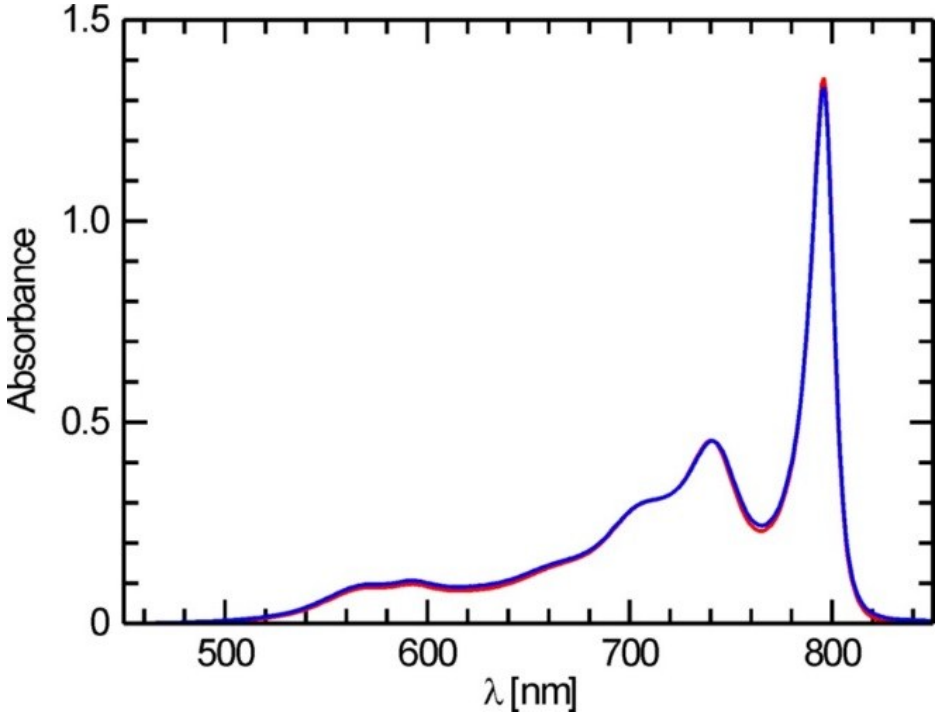

Fig. S4 Long-term stability of tubular J-aggregates. A 0.3 mM dye solution was prepared in 50 mM NaCl. After aggregation the sample was diluted 6-fold up to 50 µM. The absorbance remained stable for at least 3 days. Optical path length: L = 1mm. (blue line): immediately after dilution; (red line): 3 days after dilution.