

Supplementary Information

Microfibers degradation processes in water under simulated solar irradiation: a small- and wide-angle X-ray scattering study

Astra Piccinini¹, Giulia Lucia¹, Daniele Colarossi², Paolo Principi², Heinz Amenitsch³, Lucia Pittura¹, Francesco Regoli¹, Stefania Gorbi¹ and Francesco Spinozzi¹

¹ Department of Life and Environmental Sciences, Polytechnic University of Marche, Ancona, 60131, Italy

² Department of Industrial Engineering and Mathematical Sciences, Polytechnic University of Marche, Ancona, 60131, Italy

³ Institute for Inorganic Chemistry, Graz University of Technology, Graz, 8010, Austria



Figure S1: Modified caps of the bottles with the top surface made of quartz (left) and bottles ready to be filled with fibers (center and right).

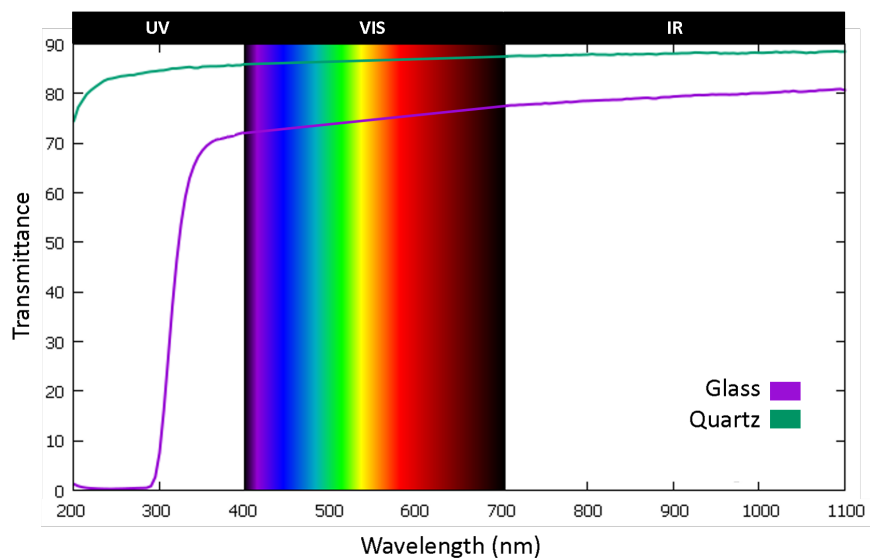


Figure S2: Comparison between glass and quartz transmittance considering the spectrum of the solar radiation.

Mean solar irradiance (kWh/m ²)	1200
5% UV component (kWh/m ²)	60
UV component of solar simulator power (kW/m ²)	0.06
Exposition time per day (h)	24
Total energy per day (kWh/m ²)	1.44
Total exposition time to simulate 1 year of solar exposure (days)	41.67

Table S1: Physical parameters considered for the evaluation of the fibers exposure time under the solar simulator apparatus.

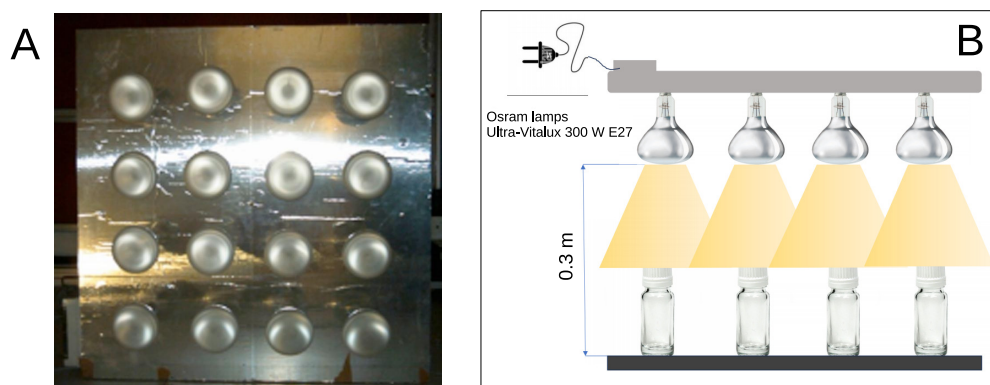


Figure S3: Solar simulator used during the experiment, kindly offered by the Department of Industrial Engineering and Mathematical Sciences at the Polytechnic University of Marche (Ancona, Italy).



Figure S4: SAXS cell used during the SAXS/WAXS experiment at Elettra in December 2021. The solid sample of the fibers was adjusted inside the cell and then irradiated by X-ray.

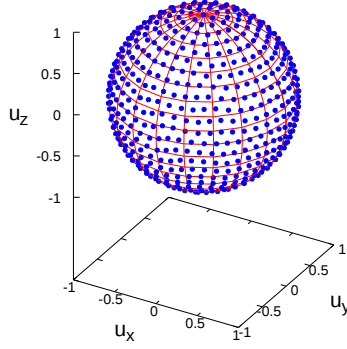


Figure S5: Representation of the $N_u = 801$ points over a surface of a unit sphere chosen for calculating the orientational averages.

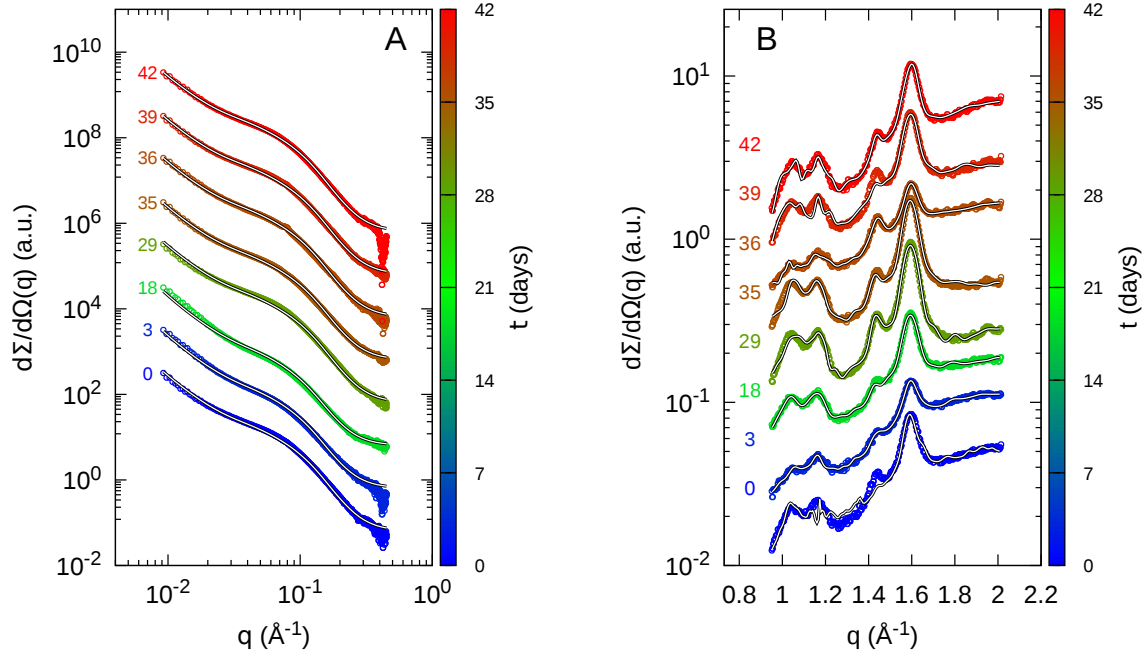


Figure S6: SAXS (panel A) and WAXS (panel B) curves for the MFs of cotton in FW recorded as a function of the irradiation time. The color of the points is selected according to vertical color box representing the the irradiation time. Solid black and white lines are the best fits obtained with GENFIT.

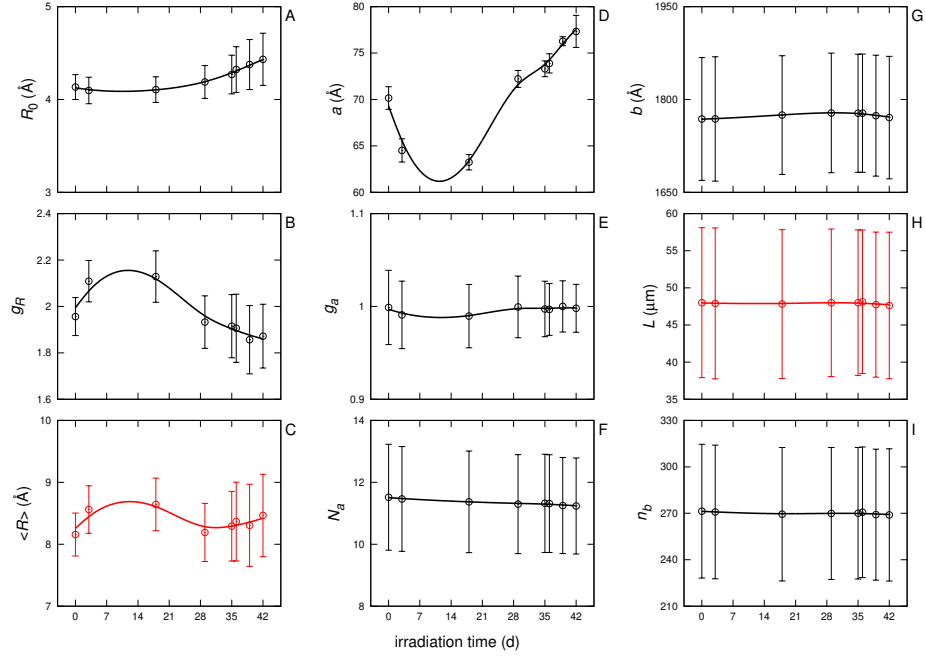


Figure S7: Panels A-I: fitting parameters (black points) and derived parameters (red points) of the SAXS curves for the MFs of cotton in FW reported as a function of the irradiation time. Smooth black or red curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

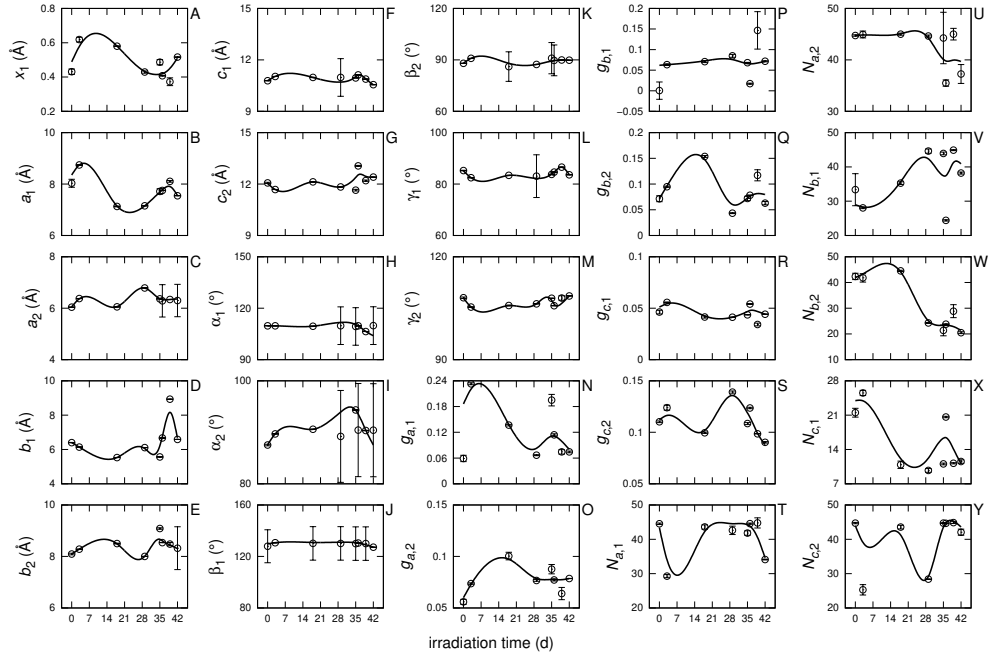


Figure S8: Panels A-Y: fitting parameters of the WAXS curves for the MFs of cotton in FW reported as a function of the irradiation time. Smooth black curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

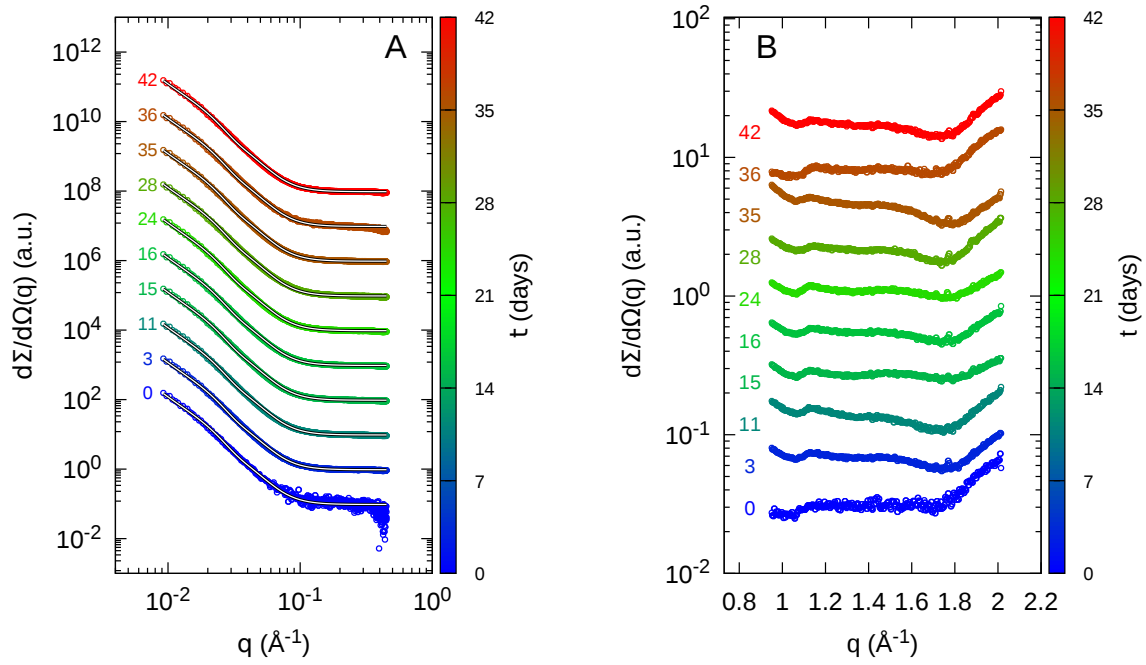


Figure S9: SAXS (panel A) and WAXS (panel B) curves for the MFs of cellulose acetate in ASW recorded as a function of the irradiation time. The color of the points is selected according to vertical color box representing the the irradiation time. Solid black and white lines are the best fits obtained with GENFIT.

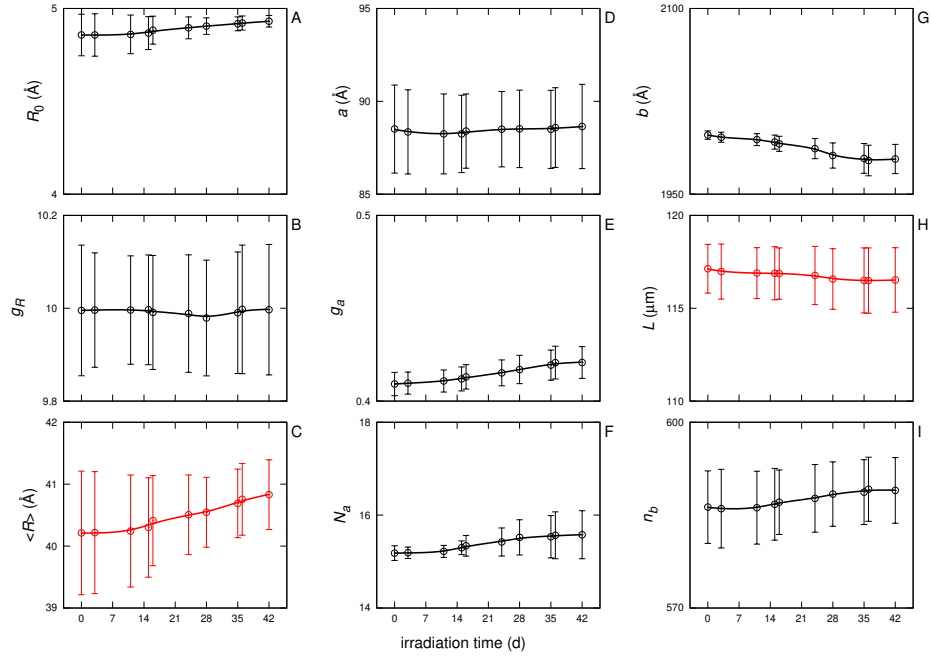


Figure S10: Panels A-I: fitting parameters (black points) and derived parameters (red points) of the SAXS curves for the MFs of cellulose acetate in ASW reported as a function of the irradiation time. Smooth black or red curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

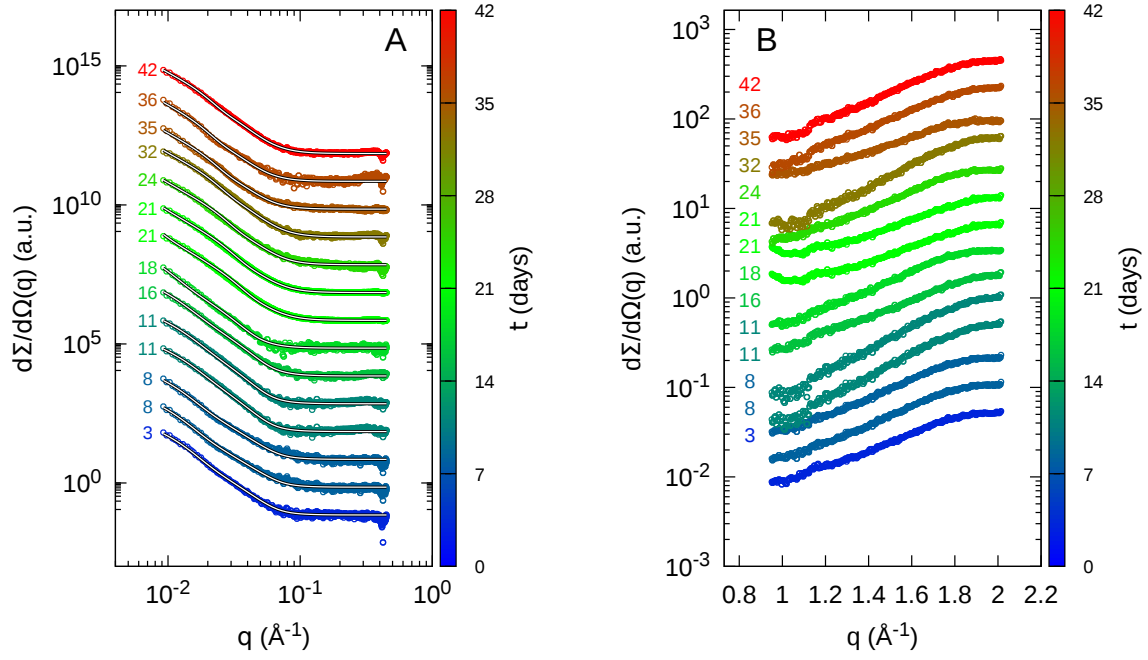


Figure S11: SAXS (panel A) and WAXS (panel B) curves for the MFs of cellulose acetate in FW recorded as a function of the irradiation time. The color of the points is selected according to vertical color box representing the the irradiation time. Solid black and white lines are the best fits obtained with GENFIT.

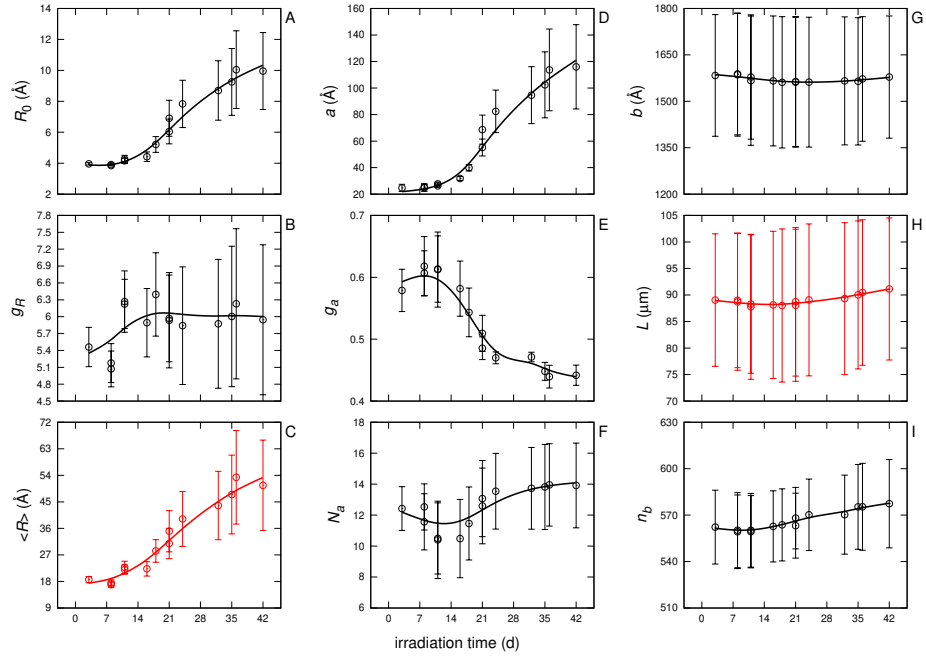


Figure S12: Panels A-I: fitting parameters (black points) and derived parameters (red points) of the SAXS curves for the MFs of cellulose acetate in FW reported as a function of the irradiation time. Smooth black or red curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

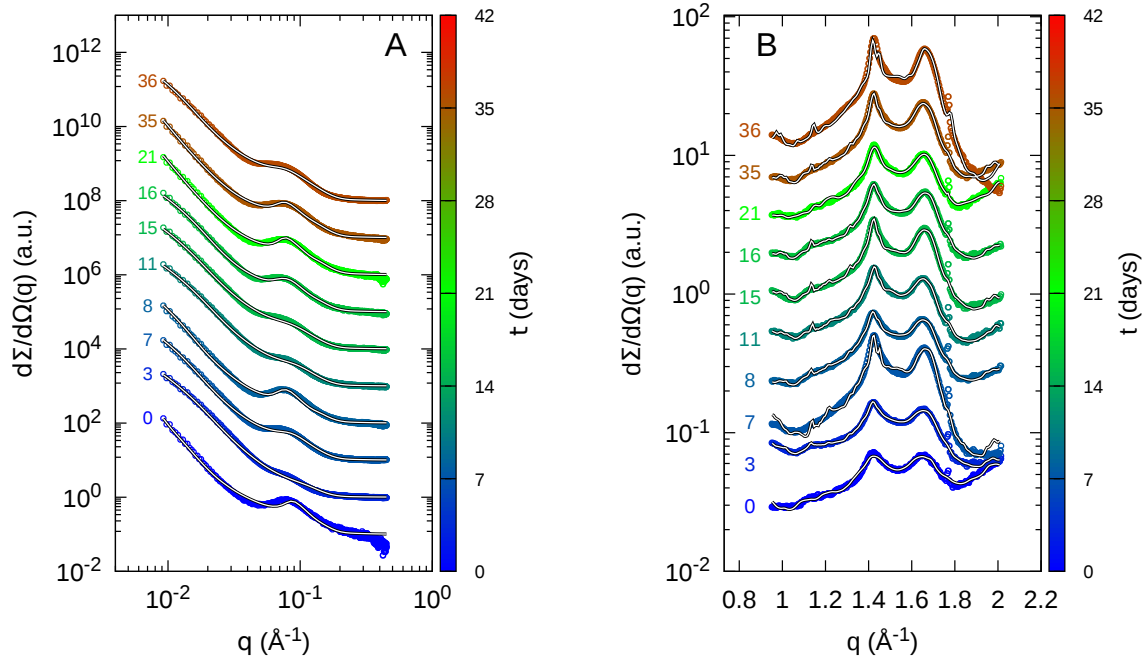


Figure S13: SAXS (panel A) and WAXS (panel B) curves for the MFs of polyamide in ASW recorded as a function of the irradiation time. The color of the points is selected according to vertical color box representing the the irradiation time. Solid black and white lines are the best fits obtained with GENFIT.

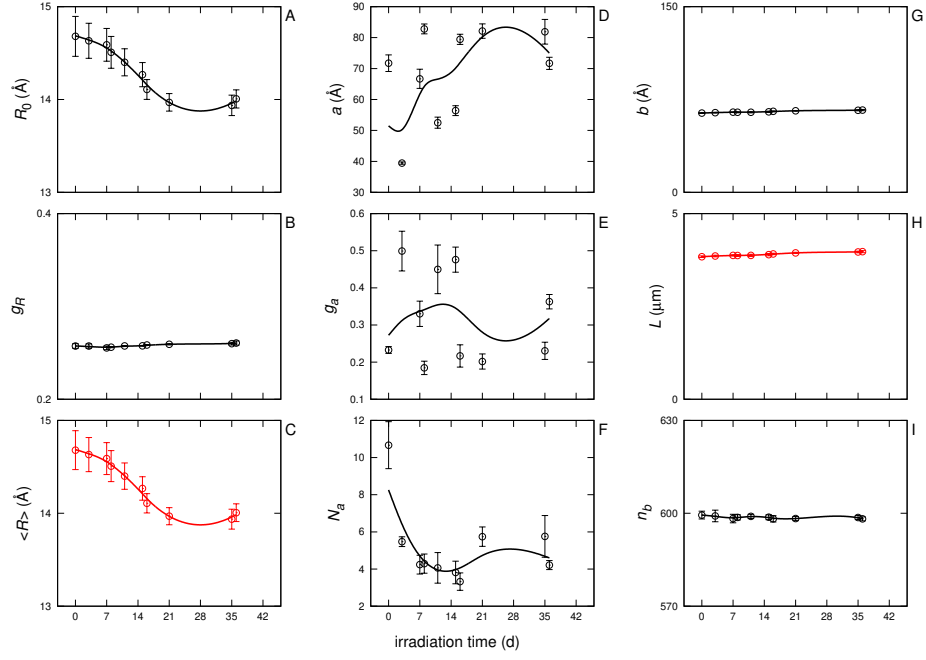


Figure S14: Panels A-I: fitting parameters (black points) and derived parameters (red points) of the SAXS curves for the MFs of polyamide in ASW reported as a function of the irradiation time. Smooth black or red curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

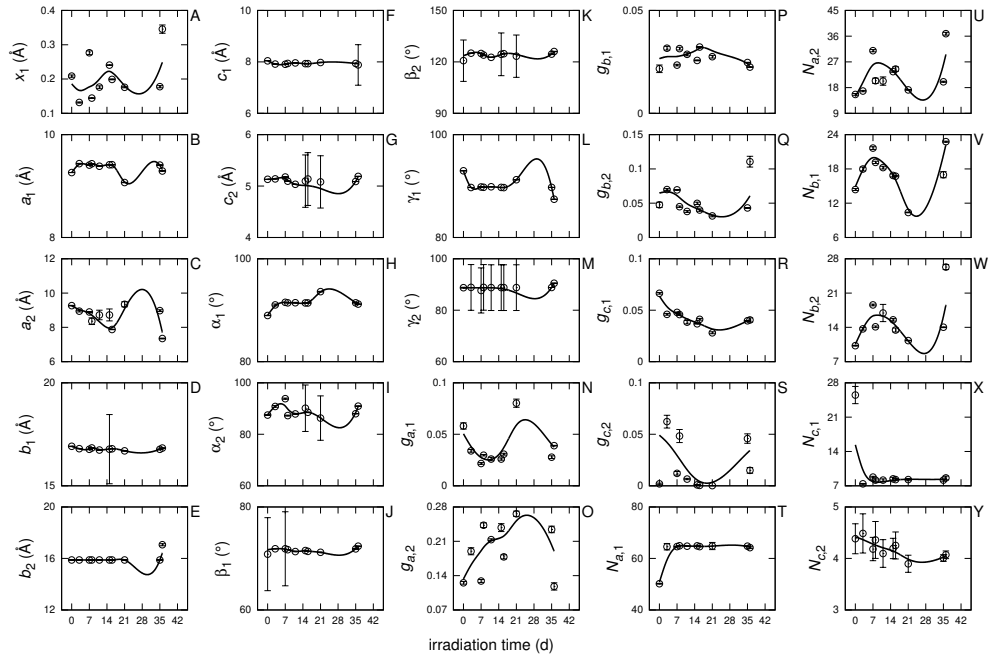


Figure S15: Panels A-Y: fitting parameters of the WAXS curves for the MFs of polyamide in ASW reported as a function of the irradiation time. Smooth black curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

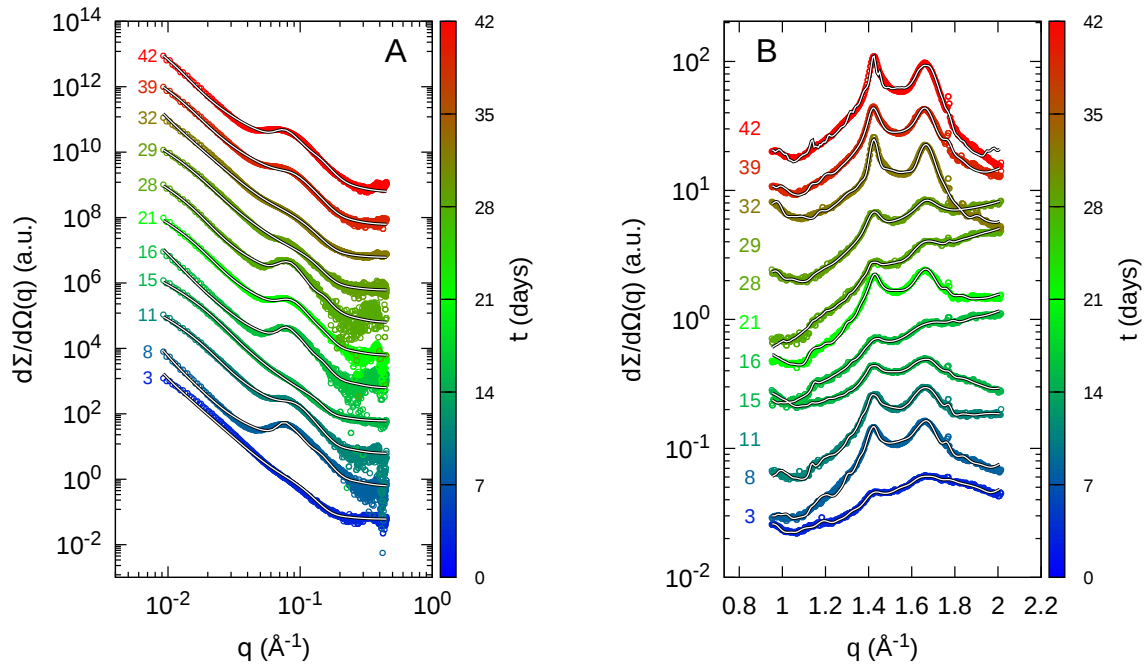


Figure S16: SAXS (panel A) and WAXS (panel B) curves for the MFs of polyamide in FW recorded as a function of the irradiation time. The color of the points is selected according to vertical color box representing the the irradiation time. Solid black and white lines are the best fits obtained with GENFIT.

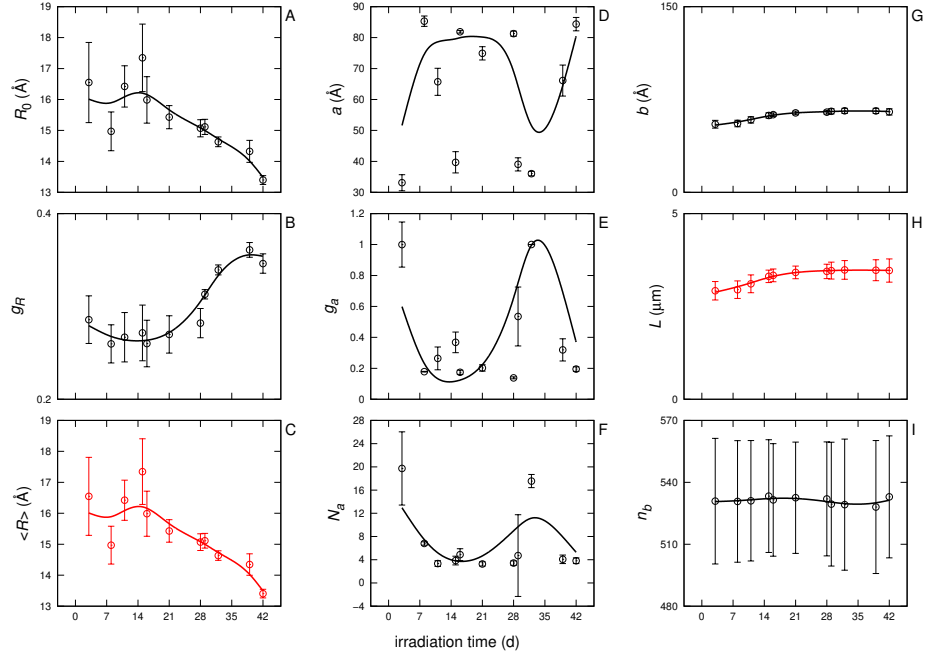


Figure S17: Panels A-I: fitting parameters (black points) and derived parameters (red points) of the SAXS curves for the MFs of polyamide in FW reported as a function of the irradiation time. Smooth black or red curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

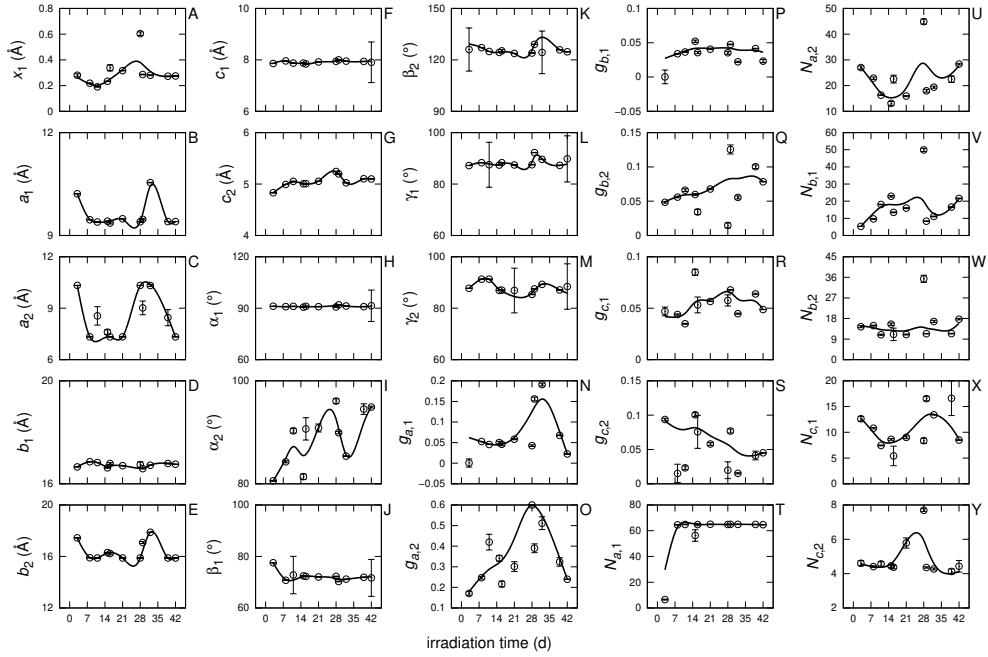


Figure S18: Panels A-Y: fitting parameters of the WAXS curves for the MFs of polyamide in FW reported as a function of the irradiation time. Smooth black curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

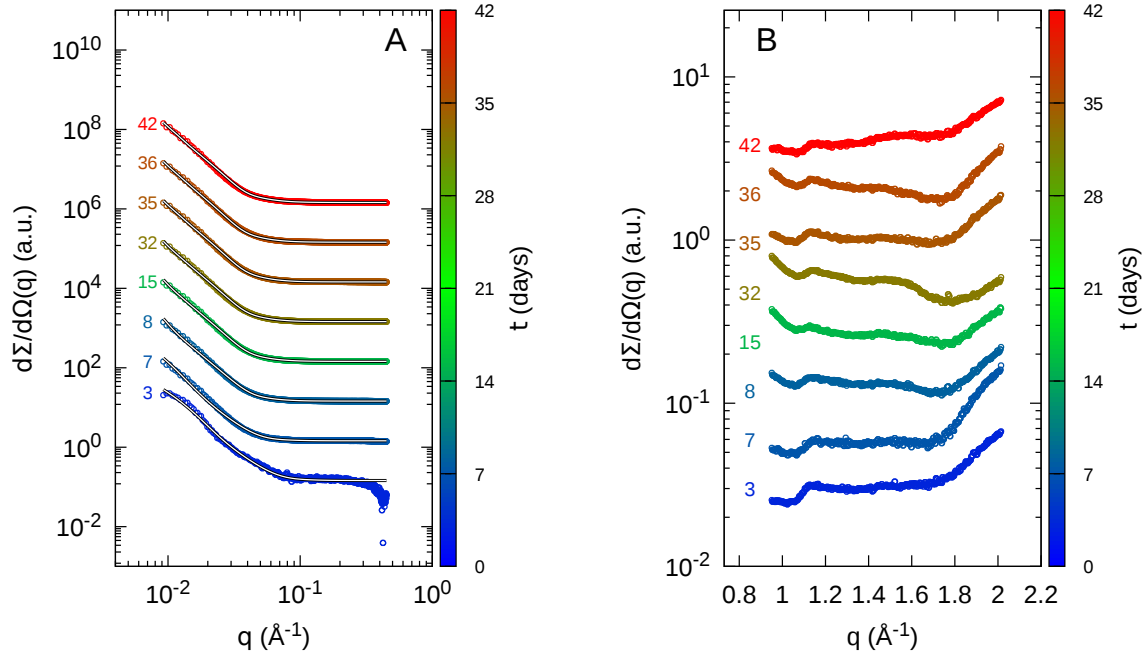


Figure S19: SAXS (panel A) and WAXS (panel B) curves for the MFs of polyester in ASW recorded as a function of the irradiation time. The color of the points is selected according to vertical color box representing the the irradiation time. Solid black and white lines are the best fits obtained with GENFIT.

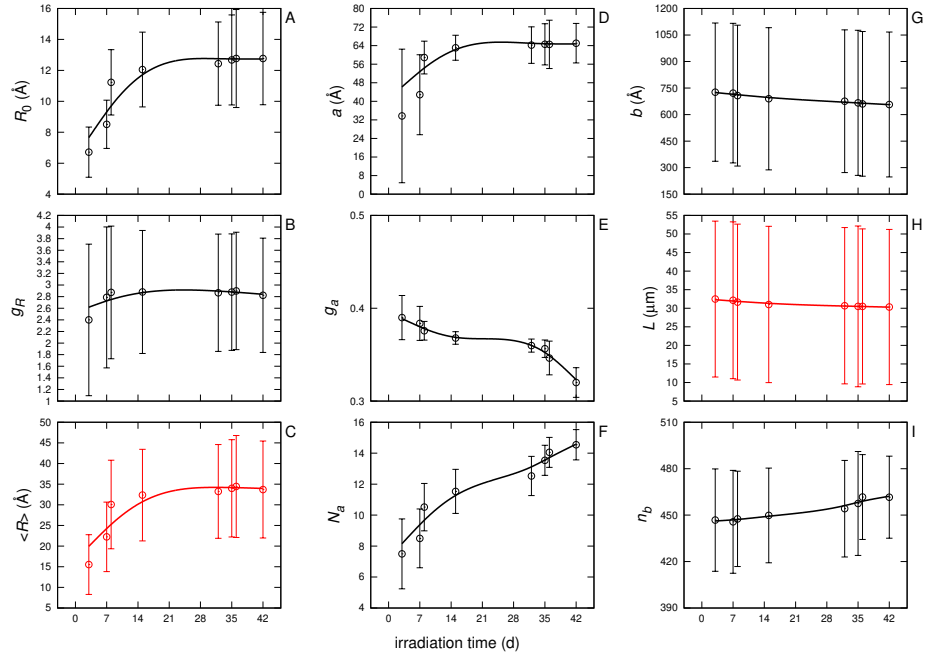


Figure S20: Panels A-I: fitting parameters (black points) and derived parameters (red points) of the SAXS curves for the MFs of polyester in ASW reported as a function of the irradiation time. Smooth black or red curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

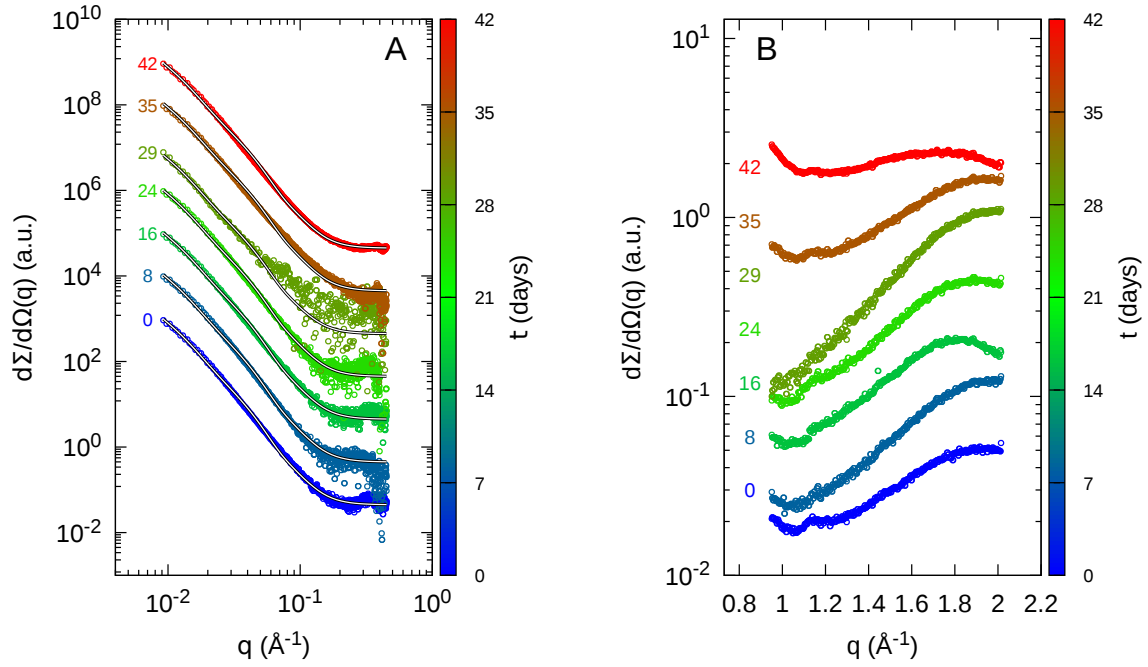


Figure S21: SAXS (panel A) and WAXS (panel B) curves for the MFs of polyester in FW recorded as a function of the irradiation time. The color of the points is selected according to vertical color box representing the the irradiation time. Solid black and white lines are the best fits obtained with GENFIT.

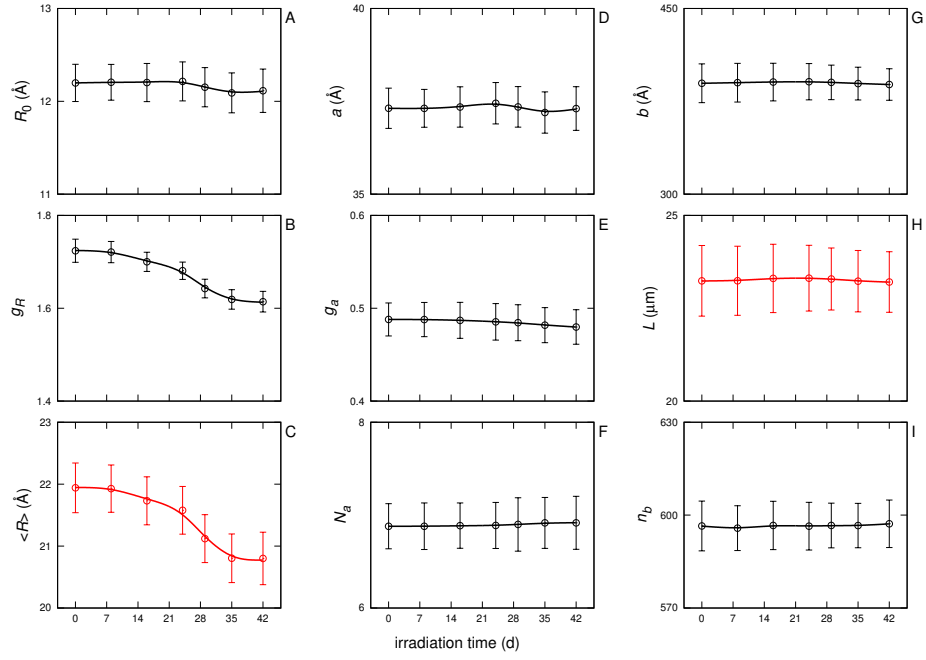


Figure S22: Panels A-I: fitting parameters (black points) and derived parameters (red points) of the SAXS curves for the MFs of polyester in FW reported as a function of the irradiation time. Smooth black or red curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

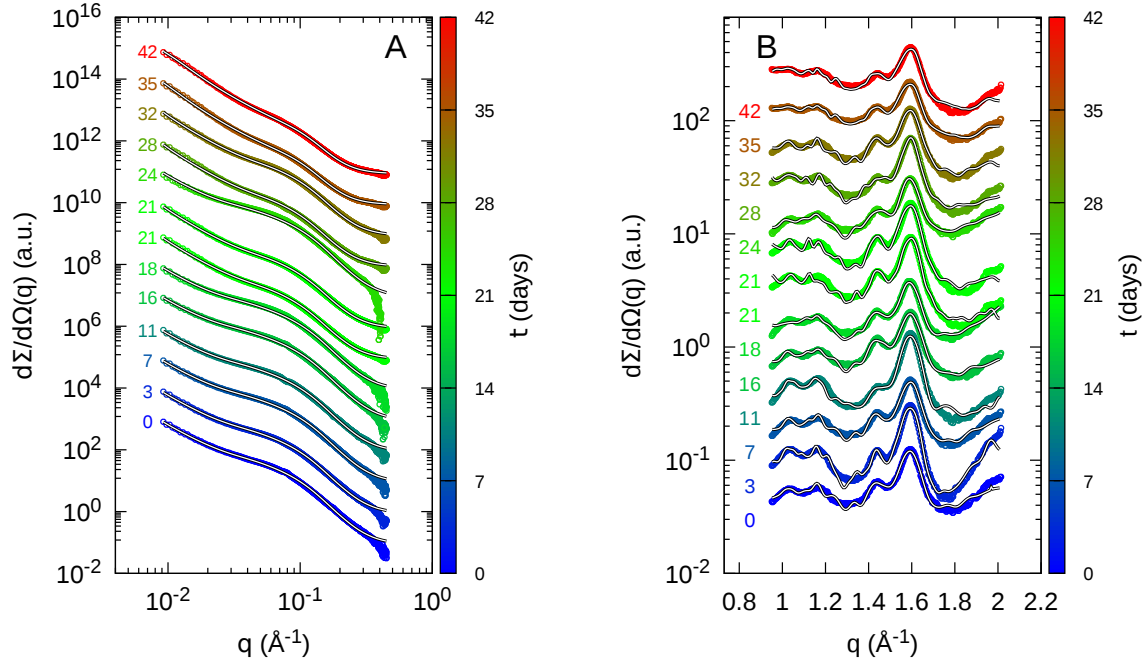


Figure S23: SAXS (panel A) and WAXS (panel B) curves for the MFs of linen in ASW recorded as a function of the irradiation time. The color of the points is selected according to vertical color box representing the the irradiation time. Solid black and white lines are the best fits obtained with GENFIT.

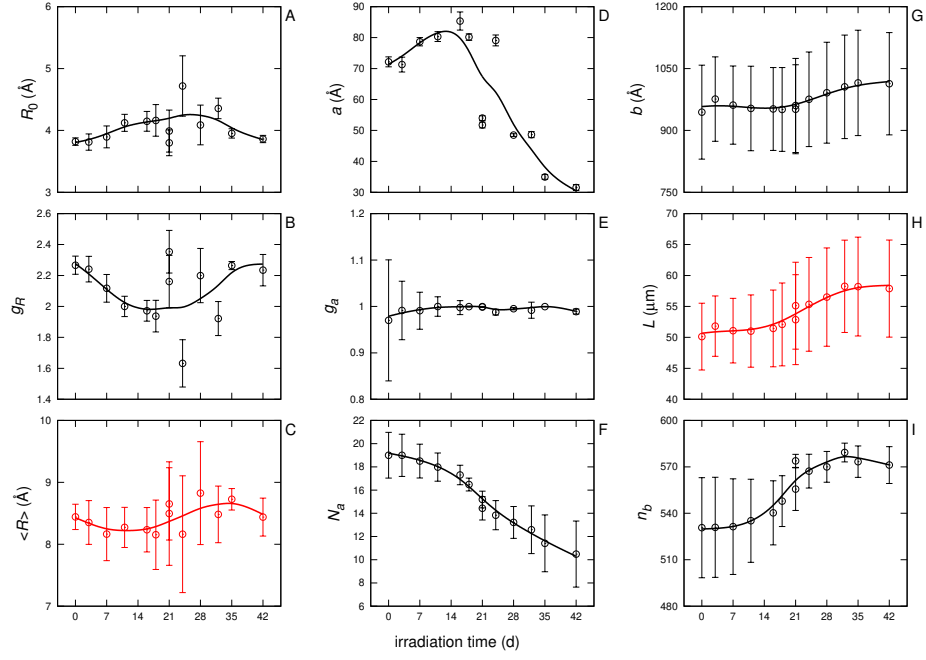


Figure S24: Panels A-I: fitting parameters (black points) and derived parameters (red points) of the SAXS curves for the MFs of linen in ASW reported as a function of the irradiation time. Smooth black or red curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

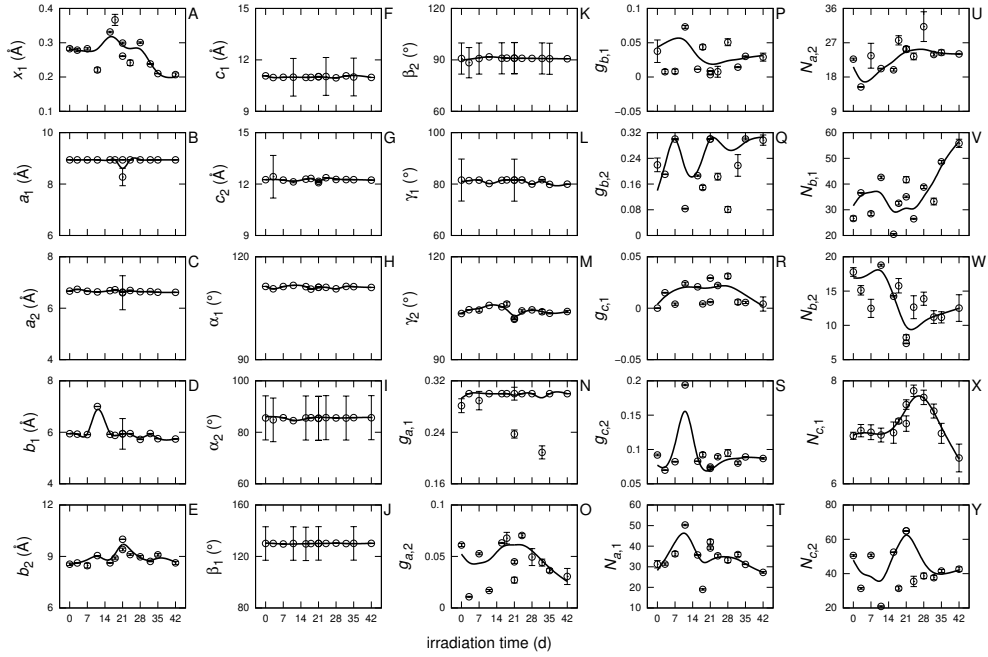


Figure S25: Panels A-Y: fitting parameters of the WAXS curves for the MFs of linen in ASW reported as a function of the irradiation time. Smooth black curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

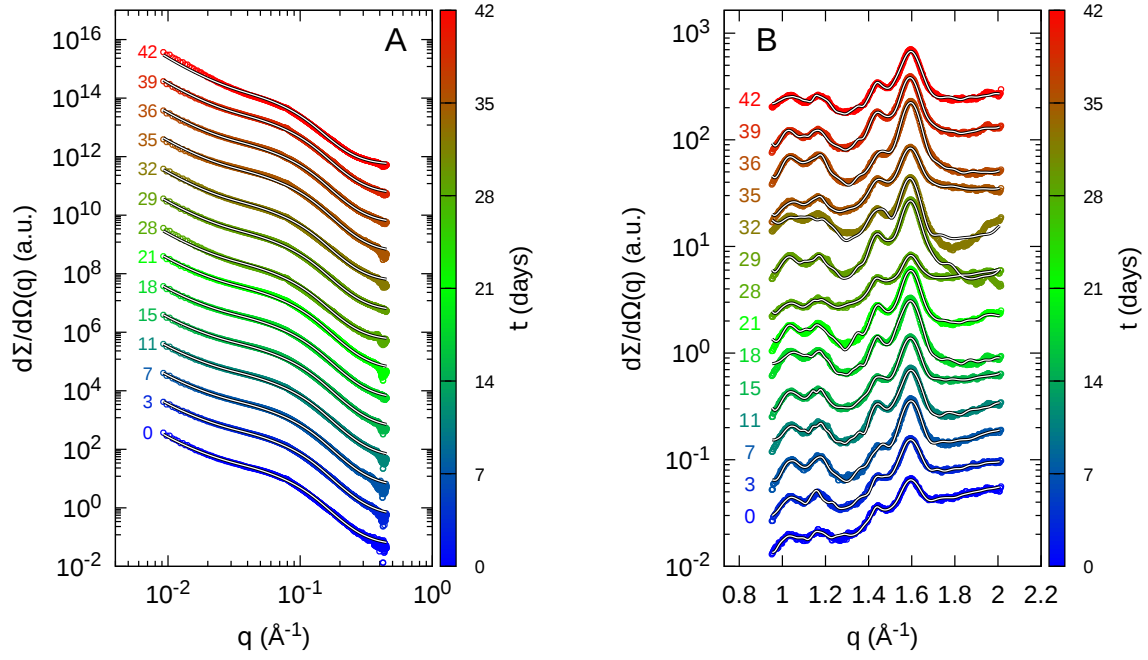


Figure S26: SAXS (panel A) and WAXS (panel B) curves for the MFs of linen in FW recorded as a function of the irradiation time. The color of the points is selected according to vertical color box representing the the irradiation time. Solid black and white lines are the best fits obtained with GENFIT.

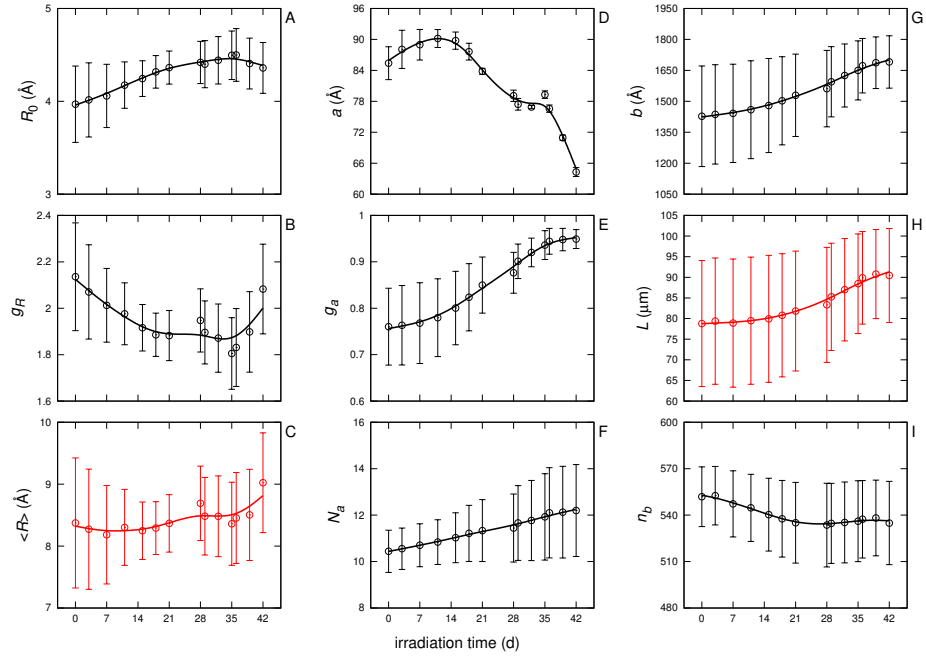


Figure S27: Panels A-I: fitting parameters (black points) and derived parameters (red points) of the SAXS curves for the MFs of linen in FW reported as a function of the irradiation time. Smooth black or red curves among the points have been obtained with cubic splines weighted with uncertainties of the parameters.

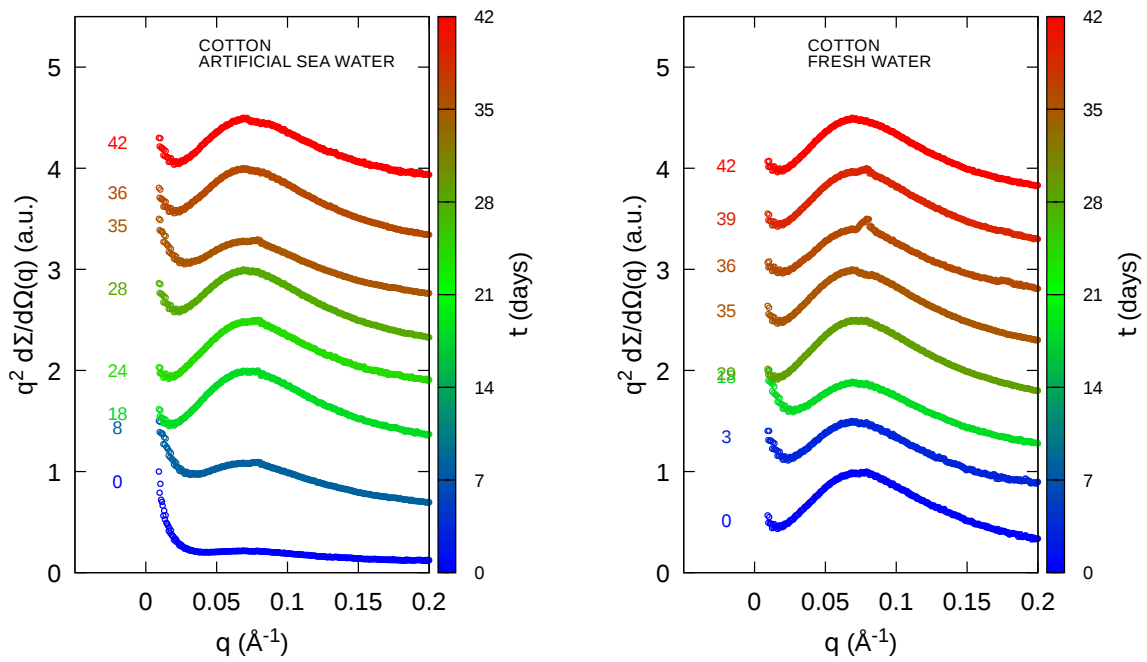


Figure S28: Kratky plots of the SAXS curves of cotton in ASW and FW recorded as a function of the irradiation time.

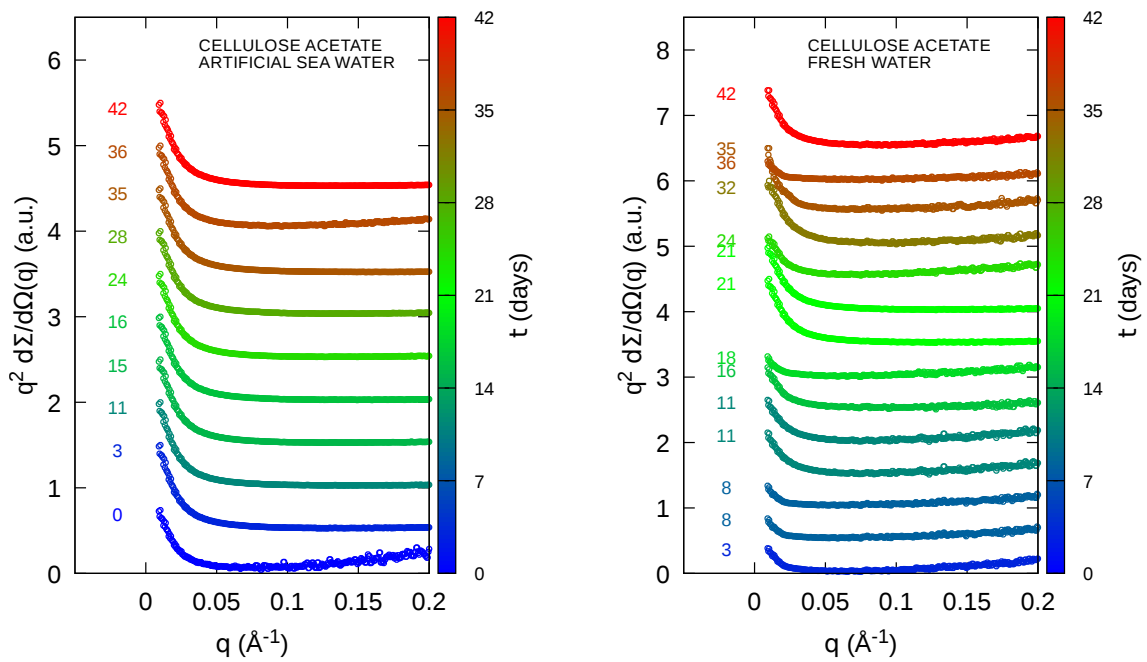


Figure S29: Kratky plots of the SAXS curves of cellulose acetate in ASW and FW recorded as a function of the irradiation time.

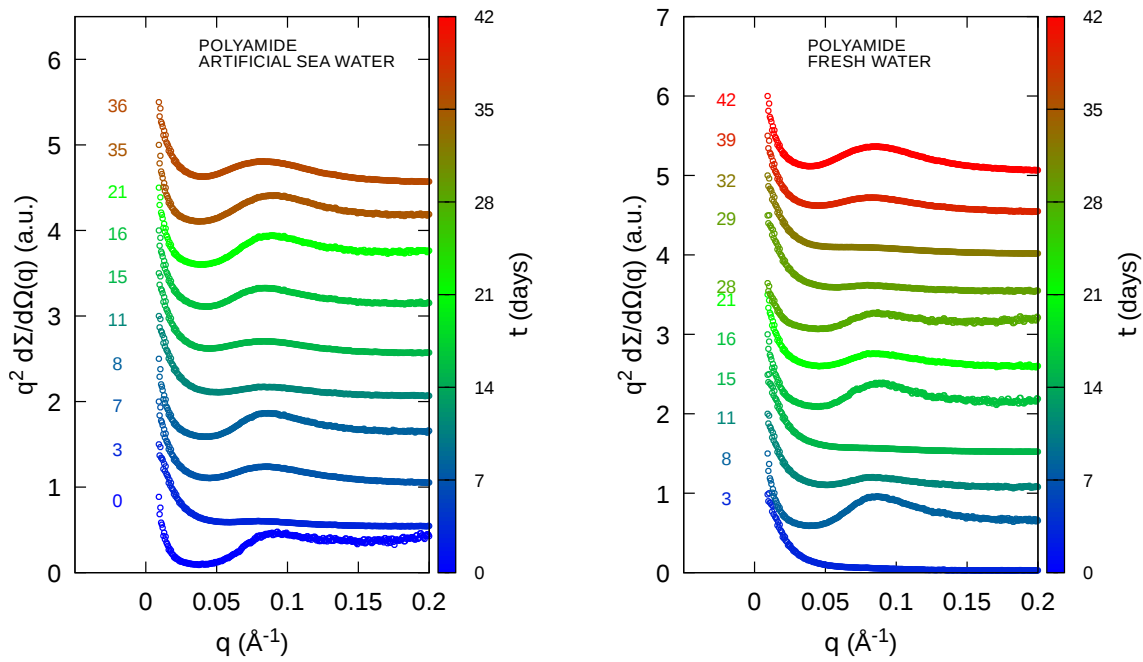


Figure S30: Kratky plots of the SAXS curves of polyamide in ASW and FW recorded as a function of the irradiation time.

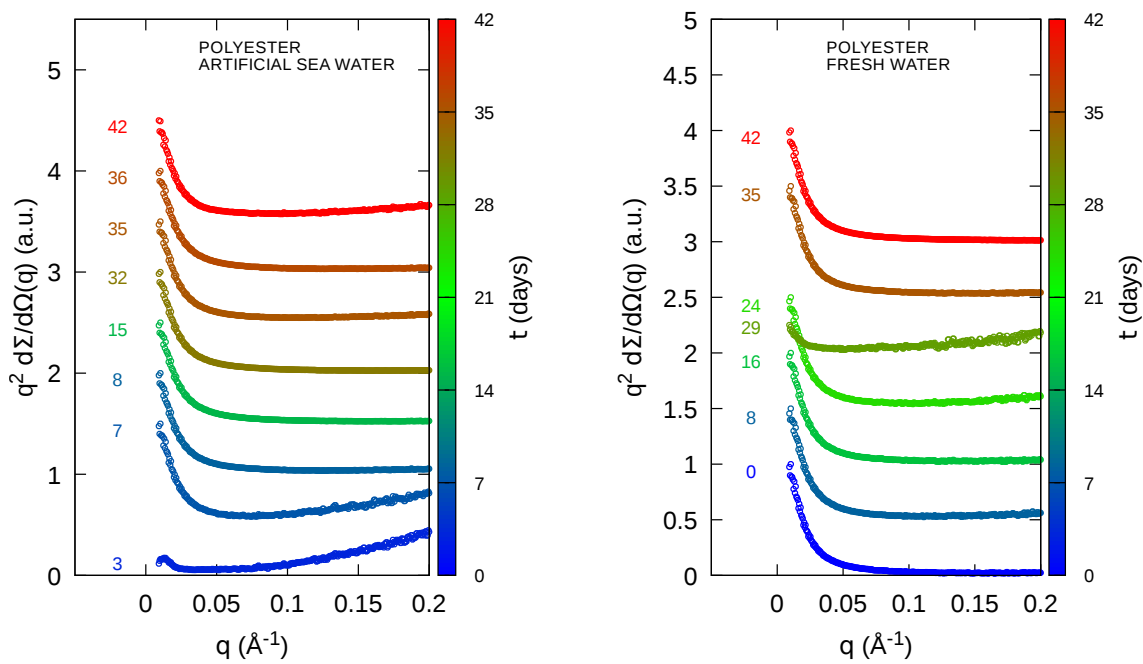


Figure S31: Kratky plots of the SAXS curves of polyester in ASW and FW recorded as a function of the irradiation time.

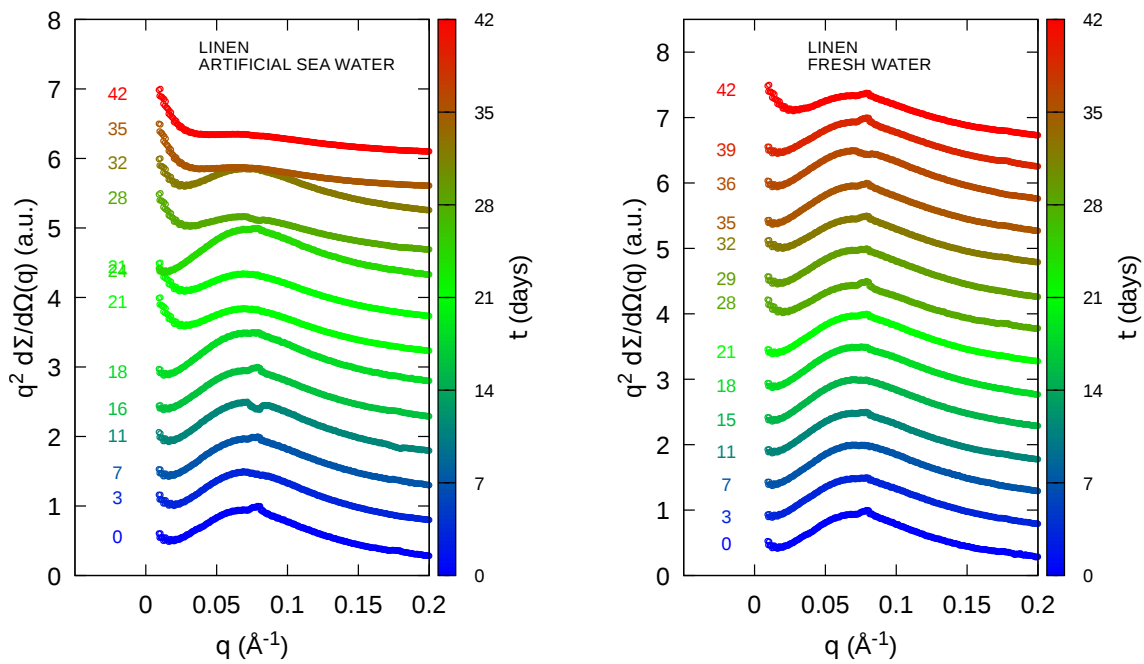


Figure S32: Kratky plots of the SAXS curves of linen in ASW and FW recorded as a function of the irradiation time.

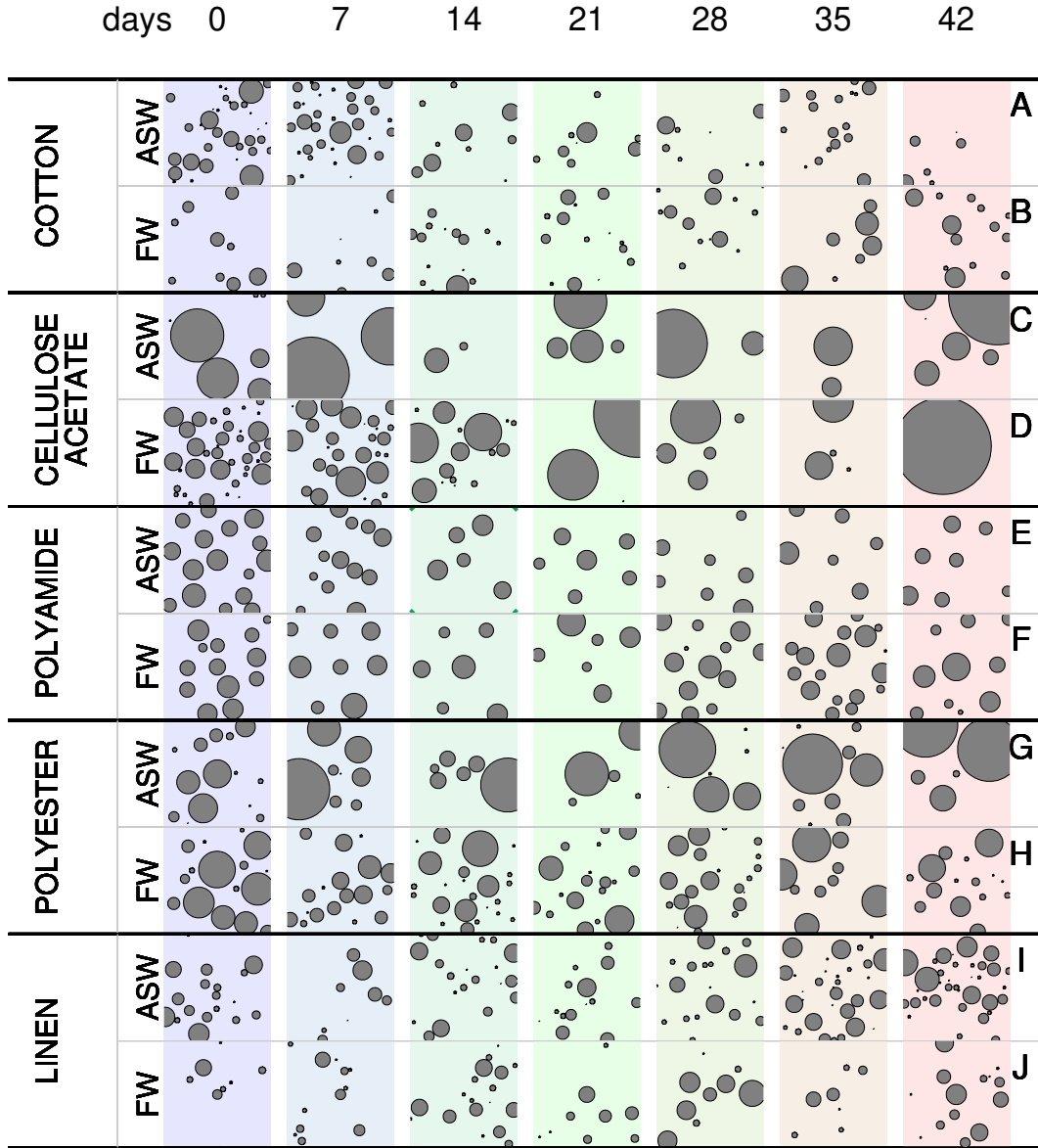


Figure S33: Representation of the internal structure of the macrofibrils derived by the SAXS fitting parameters for the five investigated MFs in ASW (panels A, C, E, G and I) and in FW (panels B, D, F, H, J). The small gray circles inside the large circles, representing the microfibrils, have been traced with a radius R sampled by the Gaussian distribution $p(R)$ (Eq. 7) by using the fitting parameters R_0 and g_R . The positions of their centres have been sampled from a distorted hexagonal lattice, according to the paracrystal theory, by using the fitting parameters a , g_a and N_a . The side of each squared image is 100 Å.