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Molecular Mechanics of Coiled Coils Loaded in the Shear Geometry

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This library contains the circular dichroism (CD) spectra as well as the data from CD thermal denaturation experiments and atomic force microscope (AFM)-based single-molecule force spectroscopy (SMFS). Please find additional information in the supplementary material of the article.

1. CD spectra

To obtain information about the secondary structure of the coiled coils (CCs), CD spectra were collected for all CCs as well as for the corresponding PEG-CC conjugates. Phosphate-buffered saline (PBS) pH 7.4 was used for all measurements. The data for the CCs was measured with a Jasco J-710 CD spectrometer, using a quartz cuvette with 1 mm path length (Hellma Analytics). The data for the PEG-CC conjugates was measured with a Chirascan CD spectrometer (Applied Photophysics), again using a quartz cuvette with 1 mm path length. All measurements were performed in a wavelength range from 180 to 260 nm with 1 nm step size. The data (e.g. A4B4) is saved in .txt format in the zipped folder <02_CD_Spectra>.

2. CD thermal denaturation

The thermodynamic stability of the CCs and the corresponding PEG-CC conjugates was assessed using thermal denaturation (TD) experiments over a temperature range from 4.5 to 90 °C. All data was measured with a Chirascan CD spectrometer, using a quartz cuvette with 1 mm path length. This data is organized in subfolders with the format <CC> or <PEG-CC> (e.g. A4B4, PEG-A4B4). For each CC or CC-PEG conjugate, three independent TD repeats were performed (TD_1 to TD_3). The .txt files include the CD signal (in mdeg) for the wavelength range of 200 to 250 nm, at each measured temperature. The TD data for all CCs can be found in the zipped folder <03_CD_ThermalDenaturation>.

The melting temperatures were determined using Global3 analysis software (Applied Photophysics). Details of the fitting process as well as the resulting melting temperatures can be found in the supplementary material of the article.

3. AFM-based SMFS

The mechanical stability of the CCs was investigated using AFM-SMFS (again using PBS pH 7.4). Measurements were performed at six different retract speeds (50, 200, 400, 1000, 2500 and 5000 nm s^{-1}) to obtain information about the dynamic mechanical range of each CC. Three independent experiments (with different cantilevers and surfaces) were performed for each CC (labelled as CL1 to CL3).

The zipped folders with the numbers 04 to 12 and the name <nr_SMFS_CC_proc_CL> (e.g. 04_SMFS_proc_CL1) contain force-extension curves (processed; proc) that were selected for further analysis.

The data was processed using the JPKSPM data processing software (Version 6.1.41, JPK instruments), applying the following steps:
- post-calibration data of the cantilever were inserted
- baseline correction of the retract part of the curves was performed
- contact point with the surface was defined (correction of x-offset)
- correction for cantilever bending
- force-extension curves displaying single rupture events were fitted with the wormlike chain model

Each zipped folder with processed data contains subfolders with the selected force-extension curves saved in .txt format. In addition, each folder contains the fit results (i.e. the determined rupture forces and loading rates). The fit results are named <speed_chainfits> and saved in .tsv format (e.g. 50nms_chainfits.tsv). The .tsv file can be opened with a text editor, e.g. notepad. Data sets that showed a low number of single-molecule rupture events, which did not allow for the determination of the most probable rupture force, are not included.

A Gaussian fit was used to obtain the most probable values from the distributions of the rupture forces and loading rates. Fits were performed in IGORPro (Version 7.0.8.1, Wavemetrics Inc.). The resulting most probable values (most probable rupture force [pN] and most probable loading rate [pN s^{-1}]) are listed in the supplementary material of the manuscript.

The zipped folders with the numbers 13 to 66 and the name <nr_SMFS_CC_raw_CL_speed> (e.g. 13_SMFS_A4B4_raw_CL1_50nms) contain all measured force-extension curves (raw), collected in the independent experiments CL1 to CL3. The force-extension curves are again saved in .txt format. Here, a separate zipped folder is included for each retract speed.