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Spectroscopic data analysis of dissolved organic matter in R - staRdom

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The analysis of dissolved organic matter (DOM) in aquatic ecosystems is commonly done with calculation of spectroscopic indexes and parallel factor decomposition (PARAFAC) based on fluorescence excitation emission matrices (EEMs) and absorbance spectra. At the same time environmental researchers usually use the open source software R to analyze their data. However, until now there are no comprehensive R packages which would enable researchers to do all analysis steps of DOM spectroscopic data in the R environment.
We developed an R package (staRdom) that covers all steps necessary from standardization of raw fluorescence and absorbance data to typical spectroscopic index calculation and PARAFAC analysis of EEMs. In detail, staRdom supports reading the data, data correction and smoothing methods, index calculation, model fitting and validation as well as a suite of visualization options to compare the results. To achieve that, staRdom links the packages eemR (reading EEM data, data correction, peak picking, Massicotte, 2017) and multiway (PARAFAC model fitting, Helwig,
2017) and adds further data correction methods, analysis of absorption data, model validation and visualization of the results. Furthermore, it applies the same approaches to EEM standardization and PARAFAC model establishment and validation as are used in the widespread toolboxes DOMFluor (Stedmon & Bro 2008, Limnol. Ocean.: Meth. 6) and drEEM (Murphy et al. 2013, Analytical Meth. 5). However, it runs in the free R environment and is much faster due to efficient parallel processing.
Here, we present an early version of the staRdom package, which will be available later in 2018.