ASFit - an all-inclusive tool for analysis of UV-Vis spectra of colored dissolved organic matter (CDOM)

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The study of dissolved organic matter (DOM) in natural waters is hindered by their complex structure and the creation of molecular aggregates. Spectroscopic methods are most commonly used for its characterization due to their simplicity, rapid response, low price and high sensitivity (Li and Hur, 2017). This applies primarily to fluorescence spectroscopy and UV/Vis spectrometry. Advantage of UV/Vis spectrometry is that it is practical for studies of DOM containing chromophores (CDOM) due their ability to absorb light in UV and visible part of electromagnetic spectrum. The absorption spectrum of CDOM has a distinctive shape with an exponential decrease in absorbance with increasing wavelength and often with few slight shoulders, the most obvious one around 270 nm. While absorbance intensity gives information about CDOM concentration, shape of the spectrum might provide insight into its composition. Therefore, study of spectral changes provides useful information in distinguishing sources, determining degree of degradation as well as in studying the interactions of DOM with metals and disinfectants. For this purpose, various approaches for the characterization of the absorption spectra have been proposed over the years. There is over 20 different features (parameters) which were derived from UV/Vis spectra to get insight into the properties and/or signatures of CDOM in natural waters. Only few of these parameters are commonly used (e.g. $S_{275-290}$, $S_{350-400}$, S_R, SUVA, a_{254}) (Helms et al., 2008; Stedmon et al., 2000, Loiselle et al., 2009; Massicotte and Markager, 2016; Yan and Korshin, 2014), whereas others (mainly ratios) are proposed based on "well correlated" relationship with other DOM specific parameter (Li and Hur, 2017). There is still no general agreement among scientists on the justification of all these parameters, partly because many of them are found to be "site specific". Although analysis of UV-Vis spectra is relatively simple, there are numerous "combinations" to treat the raw spectra.

Here we present a new, windows-based "all-inclusive" tool for the basic treatment of spectra, various parameters calculation (data handling methods) and interactive graphical presentation of CDOM UV/Vis spectra (Fig.1), with following main features:

- common spectral slopes (exponential and log-linearized)
- spectral slope curve (moving spectral slope)
- user defined absorbance ratios
- gaussian + exponential decomposition (up to 6 gauss peaks)
- baseline subtraction (4 methods)
- differential spectra
- derivative spectra (1st and 2nd derivative)
- Savitzky-Golay smoothing
- conversion of absorbance to absorption coefficient (normalization)
- saving of baseline corrected spectra and gaussian curves
- export to Excel or copy of data and graphs.

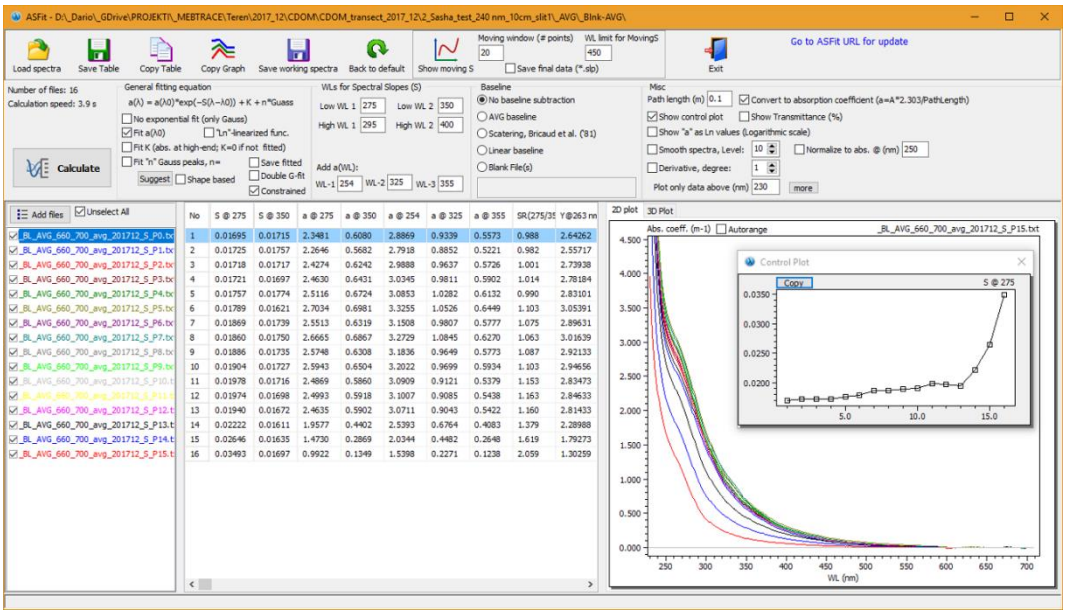

Figure 1. Main window of ASFit showing baseline corrected spectra along the Krka River estuary and the change in the spectral slope ($S_{275-295}$)

Calculation of spectral slopes and gaussian decomposition is performed using Levenberg–Marquardt algorithm with (preferred) or without constrains.

Currently ASFit supports simple XY ASCII data format (space or TAB delimited) and Perkin Elmer WinLab ASCII and binary format (*.asc; *.sp). However, any ASCII format could be included. The support for instrument specific binary file format is an option, but could not be guaranteed as the "reverse engineering" should be performed to read the structure of the file.

ASFit is developed under Embarcadero Delphi XE8 environment. It is freely available for download at: https://sites.google.com/site/daromasoft/home/spectral-slope

Acknowledgement

ASFit is developed within the framework of the MEBTRACE project (IP–2014–09–7530; 2015-2019), financially supported by the Croatian Science Foundation.

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