Time-Resolved Ultrathin-Layer Chromatography

Original programming scripts written for the Mathworks ® MATLAB platform authored by:

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Description

This collection of programming code is designed for the analysis of video frames extracted from recordings of coloured sample separations in planar chromatography (TLC, thin-layer chromatography; and UTLC, ultrathin-layer chromatography). The tool set enables semi-automatic extraction of colour-filtered chromatograms and calculation of standard chromatographic separation performance metrics (figures of merit). The operation, limitations, and benefits of this time-resolved ultrathin-layer chromatography (TR-UTLC) approach have been thoroughly detailed in related publications:

> Chapter 6 "Time-resolved UTLC" in:
> S.R. Jim, Nanoengineered Glancing Angle Deposition Thin Films for Ultrathin-Layer Chromatography, PhD Thesis, University of Alberta (Edmonton, Canada) (2014)
> http://hdl.handle.net/10402/era.37014

> A.J. Oko, S.R. Jim, M.T. Taschuk, M.J. Brett, Time resolved chromatograms in ultra-thin layer chromatography, J. Chromatogr. A. 1249 (2012) 226–232.
> http://dx.doi.org/10.1016/j.chroma.2012.05.090

This brief guide provides some tips on the installation and use of this software package. Note that some of these scripts are based on code co-written with Anthony J. Oko, MSc (2012), GLAD Research Group.

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This custom programming code should be accepted "As-Is." Although carefully prepared, the author does not state or imply any guarantees or warranties about its functioning. Users are encouraged to use this programming code in academic (non-commercial) research. Minor modifications may be made as required with the assumption that appropriate attribution is provided.

Compatibility and Installation

The enclosed MATLAB *.m files are intended to function with versions of Mathworks ® MATLAB Version 7 and later. The *.m files are text files that may be opened and edited using any text editor (Notepad, Wordpad, Microscoft Word, and others). To install TR-UTLC package, unzip all *.m files into the primary MATLAB directory. The programming scripts should not be renamed as some of the primary scripts call secondary functions.

Included Custom TR-UTLC Scripts

The TR-UTLC programming package consists of the below 13 scripts:
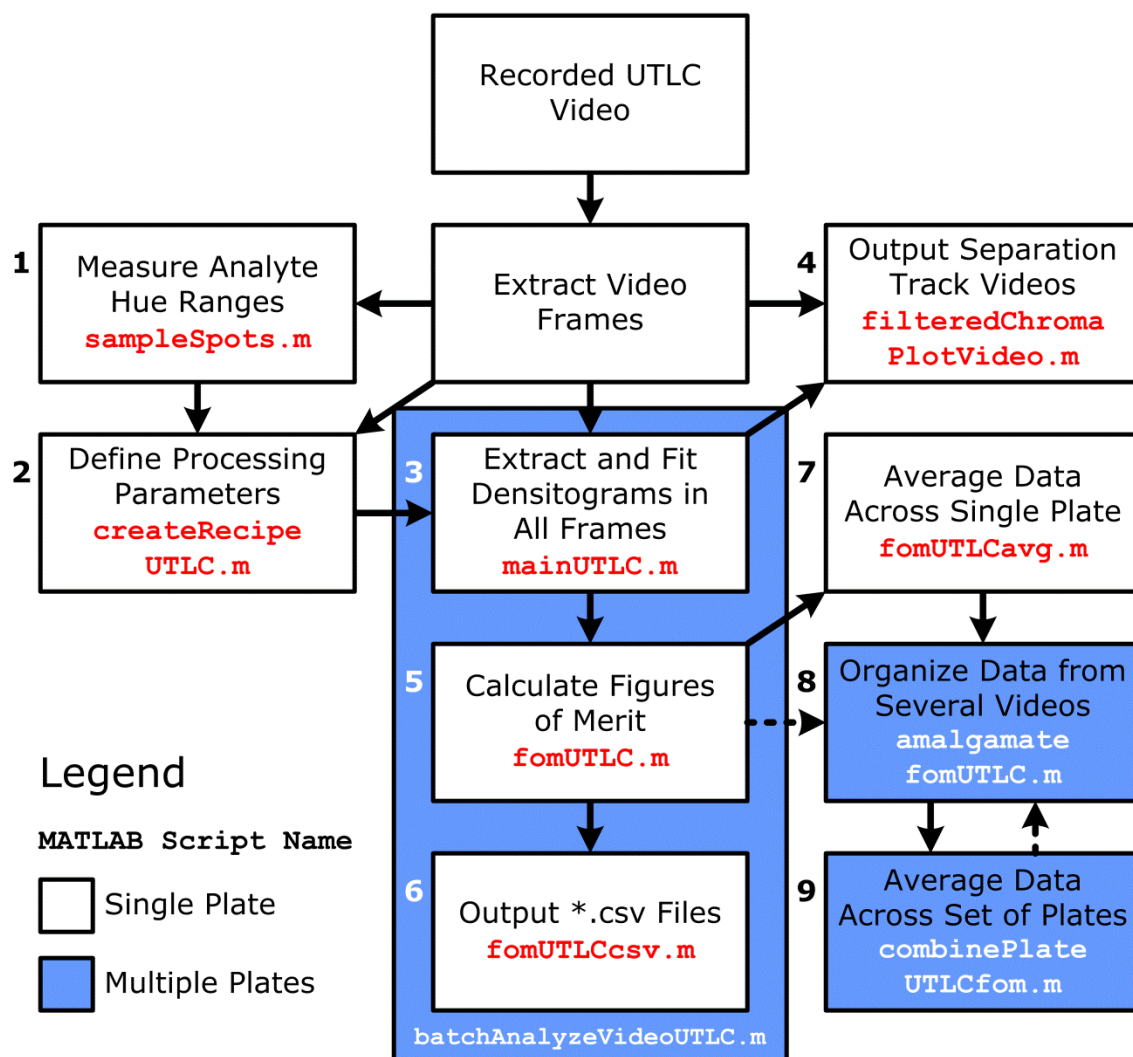
- amalgamatefomUTLC.m
- batchAnalyzeVideoUTLC.m
- combinePlateUTLCfom.m
- createRecipeUTLC.m
- filteredChromaPlotVideo.m
- filteredDensitogram.m
- fomUTLC.m
- fomUTLCavg.m
- fomUTLCcsv.m
- frontFit.m
- iterativeGaussFit.m
- mainUTLC.m
- sampleSpots.m

An additional script (singleImageUTLC.m) is not formally a part of the TR-UTLC system. It adapts the above capabilities for the analysis of individual images (single video frames).

Analysis Procedure

The below block diagram provides the analysis sequence recommended in TR-UTLC analysis. Data is stored in the form of proprietary MATLAB *.mat files. Data files generated by one script are input into the next. Some basic knowledge of MATLAB is assumed as analysis parameters are generally input into the command window (terminal) using text strings and numerical vectors. If further help is required, please refer to the previously-mentioned publications and the thorough comments contained within the source code.

Note: The provided version of batchAnalyzeVideoUTLC.m does not currently generate output files adequate for filteredChromaPlotVideo.m. In order to generate the additional data (raw and fitted colour-filtered densitograms) required by filteredChromaPlotVideo.m, either modify lines 106-110 in batchAnalyzeVideoUTLC.m or manually process each recipe file separately using the mainUTLC.m script to generate this data.

Overview of enhanced time-resolved UTLC process flow. Some MATLAB programming scripts operate on individual data sets (white). Others are used to process or collect several data sets together (blue).

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