Descriptions about the software platform
This software platform that is built in-house is for Raman data processing. In particular, the software imports a set of Raman spectra with a user-defined spectral window; enables data de-noising (smoothing) based on the 'Savitzky–Golay' algorithm [1]; and baseline fitting and subtraction based on a polynomial fit [2]. The software supports batch processing.

References cited
[1] https://www.mathworks.com/help/signal/ref/sgolayfilt.html
[2] Mazet, V. et al. Background removal from spectra by designing and minimizing a non-quadratic cost function. *Chemometrics and Intelligent Laboratory Systems* **76**, 121–133 (2005); software was adapted from https://www.mathworks.com/matlabcentral/fileexchange/27429-background-correction

System requirements
- Desktop/laptop that has MATLAB at any versions that provides GUIDE (graphical user interface development environment) module.
- GUIDE has been optimized with respect to a display resolution of 1,920 × 1,200.

Instruction for use

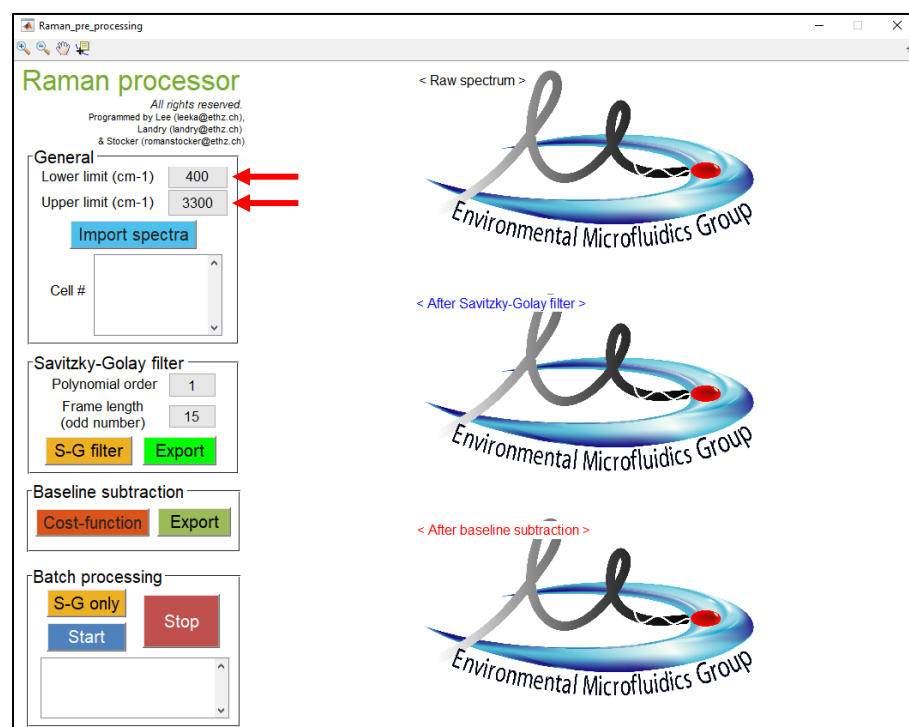1. Right-click on the 'Raman_pre_processing.fig' file. Click 'Open in GUIDE'.
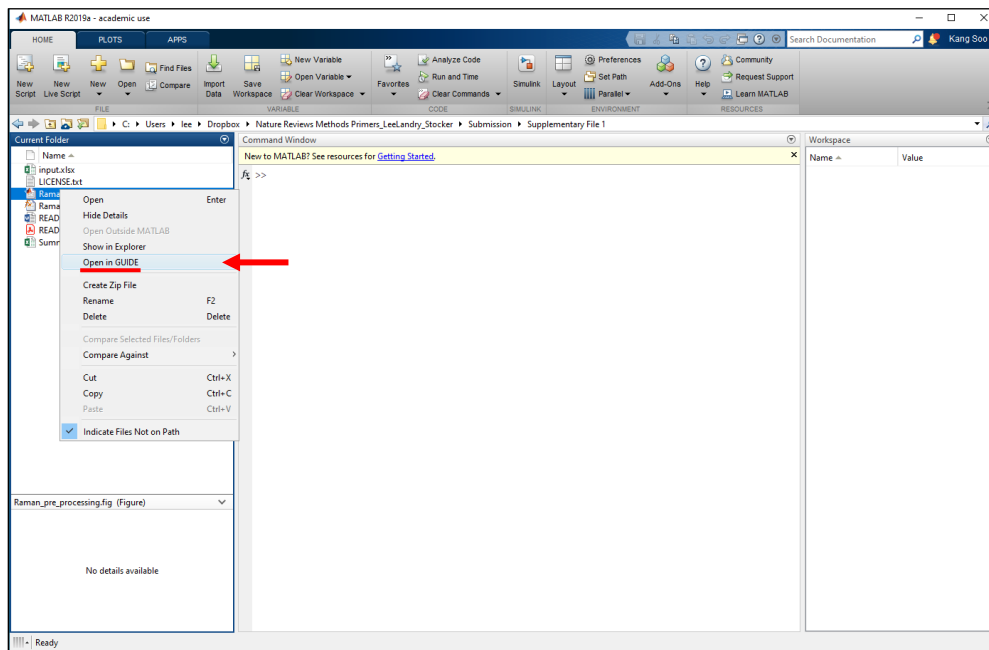
2. Click the green **Run** button to start the GUI platform.
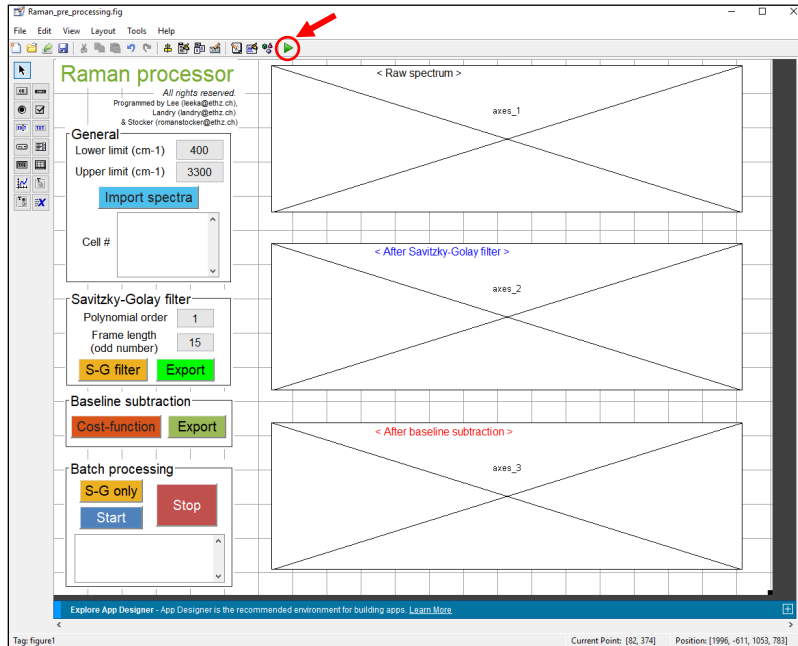
3. Data to be processed should be in a file 'input.xlsx' (an example file included).
   1) 'Column A' should be formatted with 'Raman shift; Cell_1; Cell_2; Cell_3; …'.
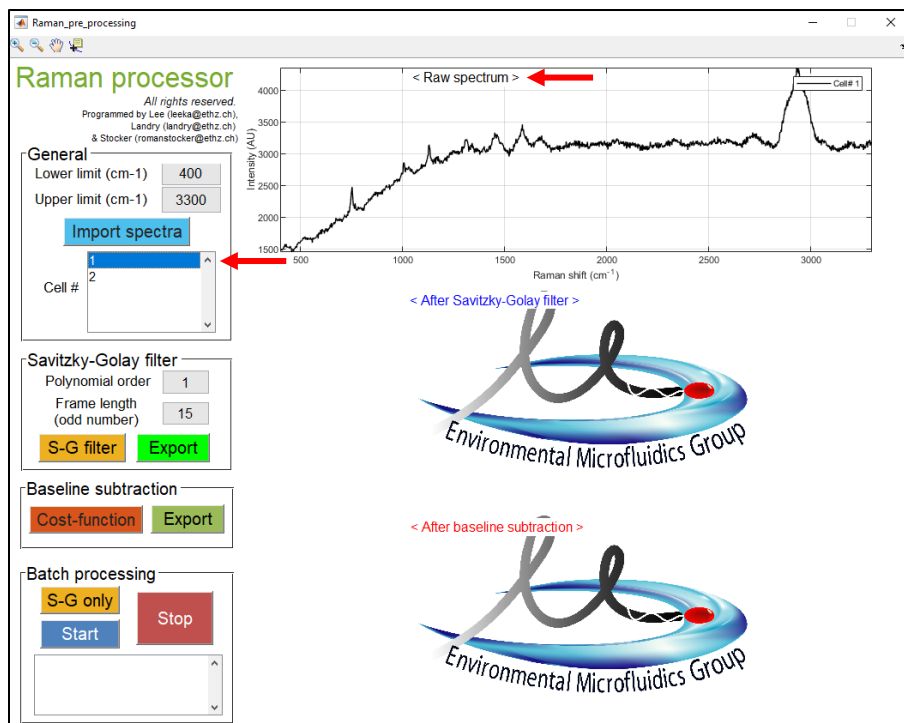   2) 'Row 1' has wavenumbers and corresponding Raman intensities are from 'Row 2'.

4. Select spectral region of interest to be used for the data processing.

5. Click 'Import spectra' to import data in 'input.xlsx'.
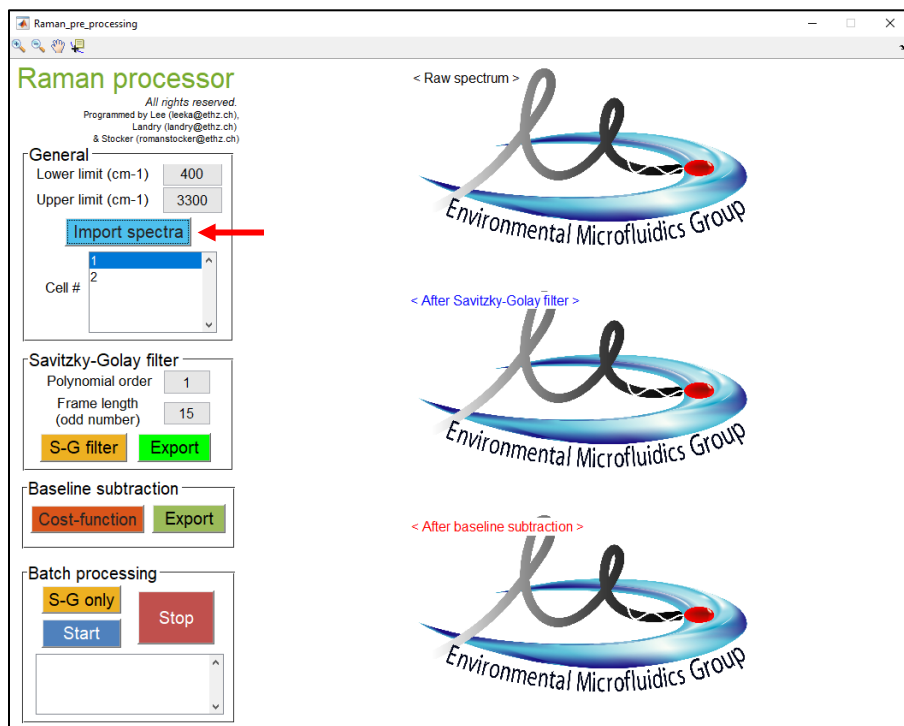
6. Upon clicking each cell number, a corresponding raw spectrum will be displayed on the right top panel (black line).

7. Insert values for 'Polynomial order' and 'Frame length' and click 'S-G filter'. A smoothed spectrum will be displayed on the right middle panel (blue line). If a user wants to finish the data processing and export processed data, click 'Export'. Software will create 'S-G_only_cell_number. xlsx' that contains the processed spectrum and parameters that have been used for the smoothing.
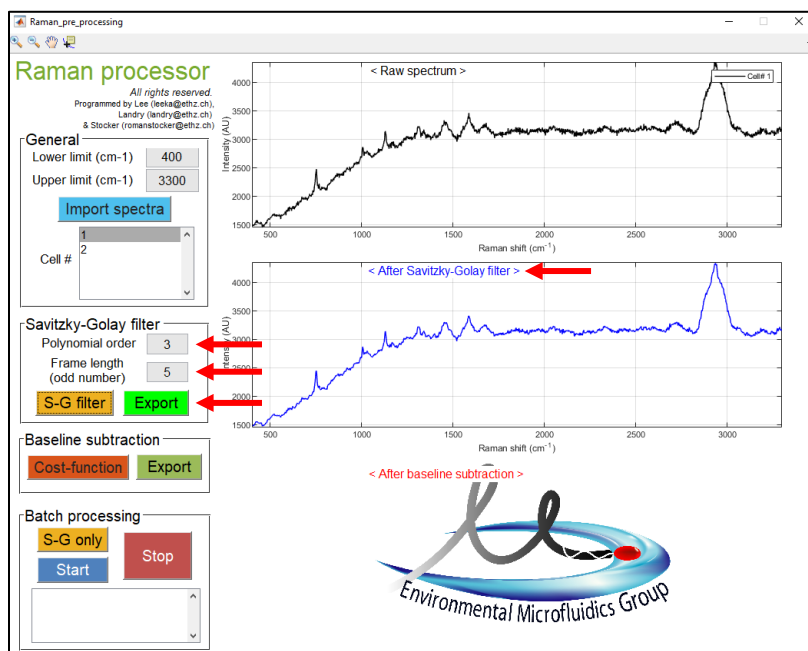
8. Click 'Cost-function'. A new window will pop up. Select values for (i) cost function (ii) threshold value and (iii) polynomial order (between 0–10) for the optimized baseline fitting. Then, click 'OK'.
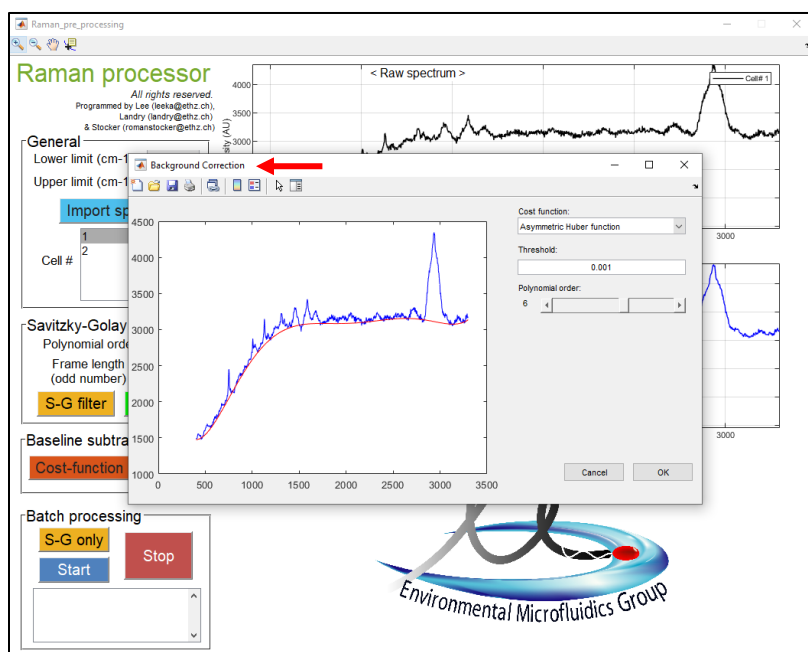
9. The calculated baseline will be displayed on the right middle panel (pink line) and a baseline-subtracted spectrum is displayed on the right bottom panel (red line). Click 'Export' to generate 'Summary_cell_number.xlsx' that contains the spectrum that has been smoothed and then baseline subtracted and the parameters used for the data processing.
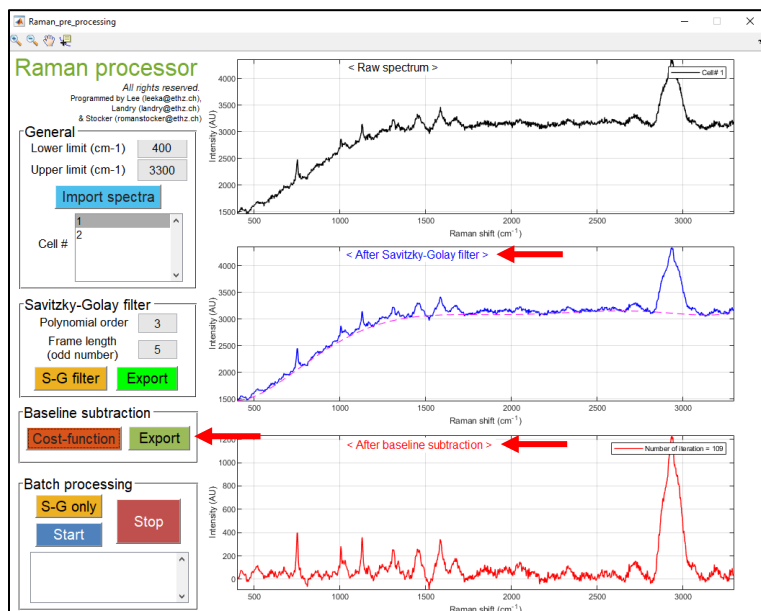

10. For batch processing, click 'S-G only' (if smoothing is only needed) or 'Start' (if smoothing and baseline subtraction are needed). The software will process the data imported at the beginning (step 5) and generate 'Summary.xlsx' that contains a processed dataset and the parameters used for the data processing. Click 'Stop' to stop the batch processing in the middle of the processing. In this case, the software generates 'Summary.xlsx' that contains a dataset until the processor stopped.
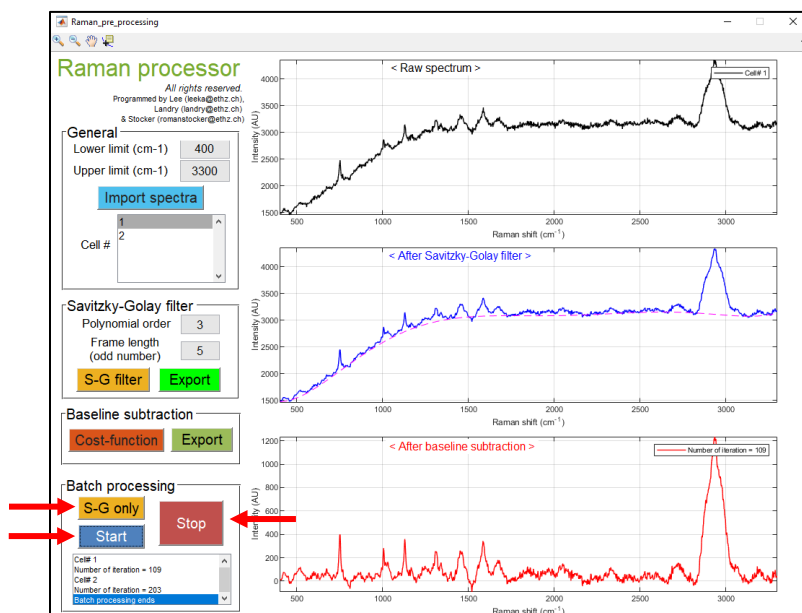
Note: an example of "Summary.xlsx" that is generated after the batch processing:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	S-G_polynomial order	3														
2	S-G_Framelength	5														
3	Baseline_polynomial order	6														
4	Baseline_threshold	0.001														
5	Baseline_function	ah														
6	Raman shift (cm-1)	403.264	405.487	407.712	409.935	412.159	414.382	416.604	418.823	421.045	423.265	425.485	427.705	429.922	432.14	434.358
7	cell# 1	18.6563744	12.54745	9.147146	12.55668	15.83358	26.40752	47.22223	55.05059	70.54877	77.60477	73.99015	70.96279	71.89621	63.67518	47.81512
8	cell# 2	4.07848792	3.851557	0.04302	4.76743	6.310463	21.61518	18.68168	20.51021	18.04333	23.82434	16.5389	10.84426	12.19791	16.99961	19.10668
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