

#####

Title: SMOOSY processor

Date of Update: 13/Mar/2020

Version: 1.1

Author: Kengo Ito, Ph.D

Affiliation: RIKEN Center for Sustainable Resource Science (CSRS), Environmental Metabolic Analysis  
Research team (EMAR)

URL: <http://dmar.riken.jp/NMRinformatics/>

License: GPL-3

Reference: Ito, K., Tsuboi, Y. and Kikuchi, J. "Spatial molecular-dynamically ordered NMR spectroscopy of intact bodies and heterogeneous systems" *Commun. Chem.*, **3**(1), 1-8 (2020).

#####

## Available OS

---

### 1. For windows 10

- 1-1. Expand "SMOOSY\_processor.zip"
- 1-2. Put "win10" directory somewhere
- 1-3. Execute "SMOOSY\_processor.exe" (win10 -> dist -> SMOOSY\_processor.exe)

### 2. For linux

- 2-1. Expand "SMOOSY\_processor.zip"
- 2-2. Put "linux" directory somewhere
- 2-3. Execute "SMOOSY\_processor" (linux -> dist -> SMOOSY\_processor)

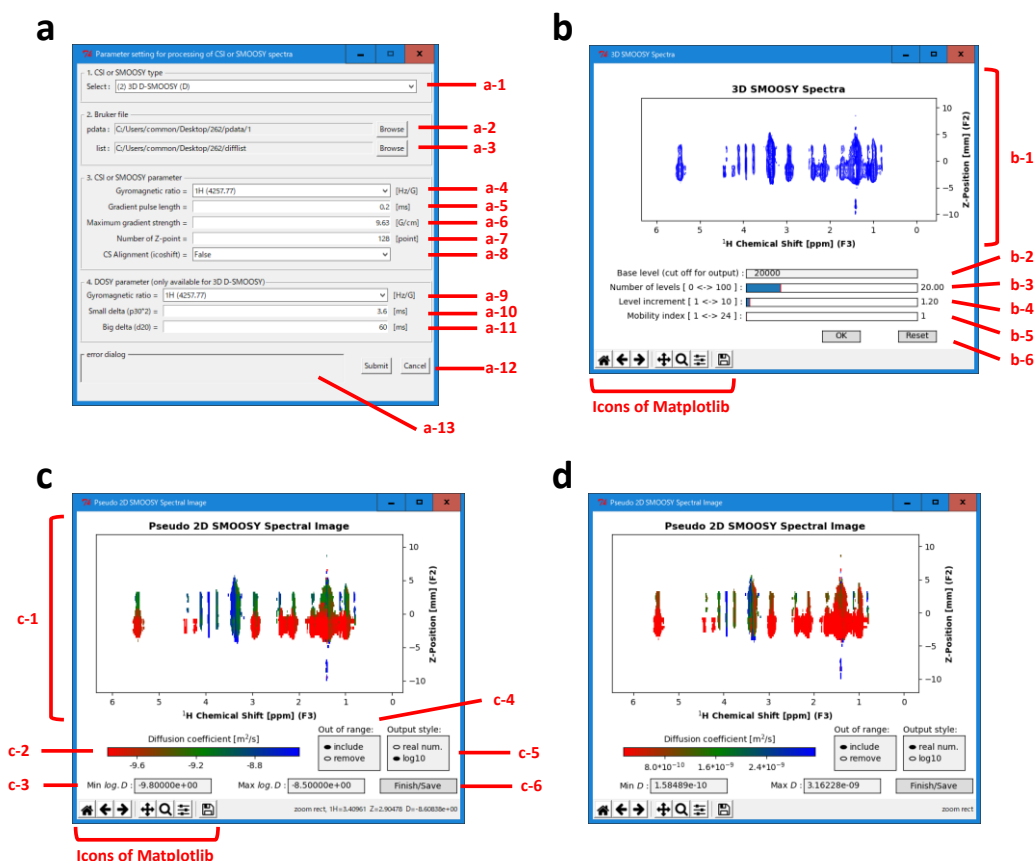
## Test data

---

Bruker data of 3D D-SMOOSY which was used in manuscript is in "test" directory.

(test -> bruker\_data -> 3D\_D-SMOOSY -> 262)

# Method of operation



Details of SMOOSY processor developed for pseudo-3D SMOOSY to pseudo-2D SMOOSY spectral image. **a** The first main window shows the parameter settings for processing the spectra. **a-1** 2D CSI and pseudo-3D SMOOSY (*D*-SMOOSY,  $T_1$ -SMOOSY,  $T_2$ -SMOOSY, REST<sub>1</sub>-SMOOSY, and REST<sub>2</sub>-SMOOSY) can be chosen as the process. **a-2**, **a-3** The Bruker pdata file and list file (difflist: for *D*-SMOOSY, vdlst: for  $T_1$ -SMOOSY,  $T_2$ -SMOOSY, REST<sub>1</sub>-SMOOSY, and REST<sub>2</sub>-SMOOSY) are required. The axes for the chemical shift and spatial *z*-profile should be Fourier transformed, but the diffusion or relaxation dimension (diffusion or relaxation) should not be processed when this input. **a-4** <sup>1</sup>H and <sup>13</sup>C are available to select as the gyromagnetic ratio for observed nucleus. **a-5**, **a-6** The gradient pulse length ( $\delta$  of CSI) and the maximum gradient strength ( $k$  of CSI) depend on the experiment and instrument. **a-7** The size of fid for the spatial *z*-profile is set according to the experiment. **a-8** Chemical shift alignment using icoshift is also available. **b** The plot window for the selected pseudo-3D SMOOSY with the selected parameter setting. **b-1** The spectra of chemical shift versus spatial *z*-position are plotted in the upper part of the screen. The contour plot parameters (base level, number of levels, level increment, and diffusion or relaxation index of the third dimension) are set by scores (from **b-2** to **b-5**). **b-2** Lower limit value of signal intensity is displayed in contour line. The noise signals can be cut off in the section. **b-6** Processing of the diffusion or relaxation dimension starts when the “OK” button is clicked; the “Reset” button returns to the initial state. Matplotlib icons provide the plot functions for zooming, saving the figure, etc. **c** The plot window showing the processed SMOOSY spectra. **c-1** The spectral image of chemical shift versus spatial *z*-position is plotted in the upper part of the screen according to the. **c-2** The signals are colored by diffusion coefficient for *D*-SMOOSY or the relaxation time for  $T_1$ -SMOOSY,  $T_2$ -SMOOSY, REST<sub>1</sub>-SMOOSY, and REST<sub>2</sub>-SMOOSY. The range of diffusion or relaxation is controlled by section **c-3**. How signals that are out of diffusion or relaxation range are plotted can be selected in section **c-4**. **c-5** Diffusion coefficients for *D*-SMOOSY and relaxation time for  $T_1$ -SMOOSY,  $T_2$ -SMOOSY, REST<sub>1</sub>-SMOOSY, and REST<sub>2</sub>-SMOOSY can be scaled by logarithm. **d** SMOOSY can be also scaled by integer, but may not show significant spatial differences compared to logarithm scale. **c-6** The 2D matrix data of the processed spectra can be exported to the “pdata/No.” directory by clicking the “Finish/Save” button. Copyright © 2020, Springer Nature