%% GUTMIC\_jobfile\_MEGA\_pilot.m

% This function describes an Osprey job defined in a MATLAB script.

%

% A valid Osprey job contains four distinct classes of items:

% 1. basic information on the MRS sequence used

% 2. several settings for data handling and modeling

% 3. a list of MRS (and, optionally, structural imaging) data files

% to be loaded

% 4. an output folder to store the results and exported files

%

% The list of MRS and structural imaging files is provided in the form of

% cell arrays. They can simply be provided explicitly, or from a more

% complex script that automatically determines file names from a given

% folder structure.

%

% Osprey distinguishes between four sets of data:

% - metabolite (water-suppressed) data

% (MANDATORY)

% Defined in cell array "files"

% - water reference data acquired with the SAME sequence as the

% metabolite data, just without water suppression RF pulses. This

% data is used to determine complex coil combination

% coefficients, and perform eddy current correction.

% (OPTIONAL)

% Defined in cell array "files\_ref"

% - additional water data used for water-scaled quantification,

% usually from short-TE acquisitions due to reduced T2-weighting

% (OPTIONAL)

% Defined in cell array "files\_w"

% - Structural image data used for co-registration and tissue class

% segmentation (usually a T1 MPRAGE). These files need to be

% provided in the NIfTI format (\*.nii) or, for GE data, as a

% folder containing DICOM Files (\*.dcm).

% (OPTIONAL)

% Defined in cell array "files\_nii"

%

% Files in the formats

% - .7 (GE)

% - .SDAT, .DATA/.LIST, .RAW/.SIN/.LAB (Philips)

% - .DAT (Siemens)

% usually contain all of the acquired data in a single file per scan. GE

% systems store water reference data in the same .7 file, so there is no

% need to specify it separately under files\_ref.

%

% Files in the formats

% - .DCM (any)

% - .IMA, .RDA (Siemens)

% may contain separate files for each average. Instead of providing

% individual file names, please specify folders. Metabolite data, water

% reference data, and water data need to be located in separate folders.

%

% In the example script at hand the MATLAB functions strrep and which are

% used to generate a relative path, which allows you to run the examples

% on your machine directly. To set up your own Osprey job supply the

% specific locations as described above.

%

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% HISTORY:

% 2019-07-15: First version of the code.

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%%% 1. SPECIFY SEQUENCE INFORMATION %%%

% Specify sequence type

seqType = 'MEGA'; % OPTIONS: - 'unedited' (default)

% - 'MEGA'

% - 'HERMES'

% - 'HERCULES'

% Specify editing targets

editTarget = {'GABA'}; % OPTIONS: - {'none'} (default if 'unedited')

% - {'GABA'}, {'GSH'} (for 'MEGA')

% - {'GABA, 'GSH}, {'GABA, GSH, EtOH'} (for 'HERMES')

% - {'HERCULES1'}, {'HERCULES2'} (for 'HERCULES')

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%%% 2. SPECIFY DATA HANDLING AND MODELING OPTIONS %%%

% Which spectral registration method should be used? Robust spectral

% registration is default, a frequency restricted spectral registration

% method is also availaible and is linked to the fit range.

opts.SpecReg = 'RobSpecReg'; % OPTIONS: - 'RobSpecReg' (default)

% - 'RestrSpecReg'

% - 'none'

% Save LCModel-exportable files for each spectrum?

opts.saveLCM = 0; % OPTIONS: - 0 (no, default)

% - 1 (yes)

% Save jMRUI-exportable files for each spectrum?

opts.savejMRUI = 0; % OPTIONS: - 0 (no, default)

% - 1 (yes)

% Save processed spectra in vendor-specific format (SDAT/SPAR, RDA, P)?

opts.saveVendor = 0; % OPTIONS: - 0 (no, default)

% - 1 (yes)

% Choose the fitting algorithm

opts.fit.method = 'Osprey'; % OPTIONS: - 'Osprey' (default)

% - 'AQSES' (planned)

% - 'TARQUIN' (planned)

% Select the metabolites to be included in the basis set as a cell array,

% with entries separates by commas.

% With default Osprey basis sets, you can select the following metabolites:

% Ala, Asc, Asp, bHB, bHG, Cit, Cr, CrCH2, EtOH, GABA, GPC, GSH, Glc, Gln,

% Glu, Gly, H2O, Ins, Lac, NAA, NAAG, PCh, PCr, PE, Phenyl, Scyllo, Ser,

% Tau, Tyros, MM09, MM12, MM14, MM17, MM20, Lip09, Lip13, Lip20.

% If you enter 'default', the basis set will include all of the above

% except for Ala, bHB, bHG, Cit, EtOH, Glc, Gly, Phenyl, Ser, and Tyros.

opts.fit.includeMetabs = {'default'}; % OPTIONS: - {'default'}

% - {'full'}

% - {custom}

% Choose the fitting style for difference-edited datasets (MEGA, HERMES, HERCULES)

% (only available for the Osprey fitting method)

opts.fit.style = 'Separate'; % OPTIONS: - 'Concatenated' (default) - will fit DIFF and SUM simultaneously)

% - 'Separate' - will fit DIFF and OFF separately

% Determine fitting range (in ppm) for the metabolite and water spectra

opts.fit.range = [0.5 4.0]; % [ppm] Default: [0.2 4.2]

opts.fit.rangeWater = [2.0 7.4]; % [ppm] Default: [2.0 7.4]

% Determine the baseline knot spacing (in ppm) for the metabolite spectra

opts.fit.bLineKnotSpace = 0.55; % [ppm] Default: 0.4.

% Add macromolecule and lipid basis functions to the fit?

opts.fit.fitMM = 1; % OPTIONS: - 0 (no)

% - 1 (yes, default)

opts.fit.coMM3 = '3to2MMhard';

opts.fit.FWHMcoMM3 = 14;

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%%% 3. SPECIFY MRS DATA AND STRUCTURAL IMAGING FILES %%

% When using single-average Siemens RDA or DICOM files, specify their

% folders instead of single files!

% Specify metabolite data

% (MANDATORY)

files = {'/Volumes/gold/cinn/2020/gbgaba/pilot\_BIDS/sub-001/ses-01/mrs/mega-press/meas\_MID00068\_FID48295\_svs\_edit\_mgs\_univ\_MEGAPRESS.dat'};

% Specify water reference data for eddy-current correction (same sequence as metabolite data!)

% (OPTIONAL)

% Leave empty for GE P-files (.7) - these include water reference data by

% default.

files\_ref = {'/Volumes/gold/cinn/2020/gbgaba/pilot\_BIDS/sub-001/ses-01/mrs/mega-press\_ref/meas\_MID00072\_FID48299\_svs\_edit\_mgs\_univ\_H2O.dat'};

% files\_ref = {};

% Specify water data for quantification (e.g. short-TE water scan)

% (OPTIONAL)

% files\_w = {'/Volumes/research-nfs/gold/cinn/2020/gbgaba/pilot\_BIDS/sub-001/ses-01/mrs/water/meas\_MID00077\_FID48304\_svs\_se\_30\_STR\_H2O.dat'};

files\_w = {};

% Specify metabolite-nulled data for quantification

% (OPTIONAL)

files\_mm = {};

% Specify T1-weighted structural imaging data

% (OPTIONAL)

% Link to single NIfTI (\*.nii) files for Siemens and Philips data

% Link to DICOM (\*.dcm) folders for GE data

files\_nii = {'/Volumes/gold/cinn/2020/gbgaba/pilot\_BIDS/sub-001/ses-01/anat/009\_GBGABA\_pilot1\_t1\_mprage\_DC\_sag\_HCP\_256\_32ch\_20210709153728.nii'};

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%%% 4. SPECIFY OUTPUT FOLDER %%

% The Osprey data container will be saved as a \*.mat file in the output

% folder that you specify below. In addition, any exported files (for use

% with jMRUI, TARQUIN, or LCModel) will be saved in sub-folders.

% Specify output folder

% (MANDATORY)

outputFolder = '/Volumes/gold/cinn/2020/gbgaba/pilot\_BIDS/derivatives/Osprey';

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