%% jobRDA.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.

% 2019-10-07: HZ - Added relative path to files

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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'}, {'Lac'}, {'PE322'}, {'PE398'} (for 'MEGA')

 % - {'GABA', 'GSH'}, {'GABA', 'Lac'}, {'NAA', 'NAAG'} (for 'HERMES'and 'HERCULES')

 % Specify data scenario

dataScenario = 'invivo'; % OPTIONS: - 'invivo' (default)

 % - 'phantom'

 % - 'PRIAM'

 % - 'MRSI'

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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'

% Which algorithm do you want to align the sub spectra? L2 norm

% optimazation is the default. This is only used for edited MRS!

opts.SubSpecAlignment = 'L2Norm'; % OPTIONS: - 'L2Norm' (default)

 % - 'L1Norm'

 % - 'none'

% Save LCModel-exportable files for each spectrum?

opts.saveLCM = 1; % OPTIONS: - 0 (no, default)

 % - 1 (yes)

% Save jMRUI-exportable files for each spectrum?

opts.savejMRUI = 1; % OPTIONS: - 0 (no, default)

 % - 1 (yes)

% Save processed spectra in NIfTI-MRS format?

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

 % - 1 (yes)

% Save PDF output for all Osprey modules and subjects?

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

 % - 1 (yes)

% Choose the fitting algorithm

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

 % - 'LCModel'

% 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]; % [ppm] Default: [0.5 4]

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 = 0.4; % [ppm] Default: 0.4.

% Add macromolecule and lipid basis functions to the fit?

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

 % - 1 (yes, default)

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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!

% Clear existing files

clear files files\_ref files\_w files\_nii files\_mm

% Data folder in BIDS format

% The filparts(which()) comment is needed to find the data on your machine. If you set

% up the jobFile for your own data you can set a direct path to your data

% folder e.g., data\_folder = /Volumes/MyProject/data/'

data\_folder = 'C:\DOKUMENTE\MRT\SPEKTROSKOPIE\data\_SpectrotACS'; %fileparts(which('exampledata/rda/jobRDA.m'));

% The following lines perform an automated set-up of the jobFile which

% takes advatage of the BIDS foramt. If you are not using BIDS (highly

% recommended) you can look at the definitions below the loop to see how to

% set up direct path links to your data.

subs = dir(data\_folder);

subs(1:2) = [];

subs = subs([subs.isdir]);

subs = subs(contains({subs.name},'sub'));

counter = 1;

for kk = 1:2%:length(subs)

 % Loop over sessions

 sess = dir([subs(kk).folder filesep subs(kk).name]);

 sess(1:2) = [];

 sess = sess([sess.isdir]);

 sess = sess(contains({sess.name},'ses'));

 for ll = 1%:length(sess)

 % Loop over tasks

 task = dir([sess(ll).folder filesep sess(ll).name filesep 'mrs']);

 task(1:2) = [];

 task = task([task.isdir]);

 task = task(contains({task.name},'task'));

 for mm = 1%:length(task)

 % Specify metabolite data

 % (MANDATORY)

 dir\_metabolite = dir([task(mm).folder filesep task(mm).name filesep subs(kk).name '\_' sess(ll).name '\_' task(mm).name '\_run-1\_megapress\_rda']);

 files(counter) = {[dir\_metabolite(end).folder filesep]};

% files(counter) = {[dir\_metabolite(end).folder filesep dir\_metabolite(end).name]};

 % 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.

% dir\_ref = dir([task(mm).folder filesep 'type-ref' filesep subs(kk).name '\_' sess(ll).name '\_type-ref\_run-1\_megapress\_rda' filesep '\*acq-off\*.rda']);

% files\_ref(counter) = {[dir\_ref(end).folder filesep dir\_ref(end).name]};

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

 % (OPTIONAL)

 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

 files\_nii(counter) = {[sess(ll).folder filesep sess(ll).name filesep 'anat' filesep subs(kk).name '\_' sess(ll).name '\_run-01\_T1w.nii.gz']};

 counter = counter + 1;

 end

 end

end

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% Definitions without using BIDS

% You can always supply direct path to each of the files within

% the cell array. For example:

% Specify metabolite data

% (MANDATORY)

% files(counter) = {'/Volumes/MyProject/data/sub-01/mrs/PRESS\_act.rda',...

% '/Volumes/MyProject/data/sub-02/mrs/PRESS\_act.rda'};

% 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(counter) = {'/Volumes/MyProject/data/sub-01/mrs/PRESS\_ref.rda',...

% '/Volumes/MyProject/data/sub-02/mrs/PRESS\_ref.rda'};

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

% (OPTIONAL)

% files\_w = {};

% Specify metabolite-nulled data for quantification

% (OPTIONAL)

% files\_mm = {};

% Specify T1-weighted structural imaging data

% (OPTIONAL)

% Link to single NIfTI (\*.nii.gz or #.nii) files for GE, Siemens and Philips data

% files\_nii = {'/Volumes/MyProject/data/sub-01/anat/T1w.nii.gz',...

% '/Volumes/MyProject/data/sub-02/anat/T1w.nii.gz'};

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%%% 4. SPECIFY STAT FILE %%%

% Supply location of a csv file, which contains possible correlation

% measures and group variables. Each column must start with the name of the

% measure. For the grouping variable use 'group' and numbers between 1 and

% the number of included groups. If no group is supplied the data will be

% treated as one group. (You can always use the direct path)

file\_stat = '';

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%%% 5. 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 (you can always use the direct path)

% (MANDATORY)

outputFolder = fullfile(data\_folder, 'derivatives','RDA');

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