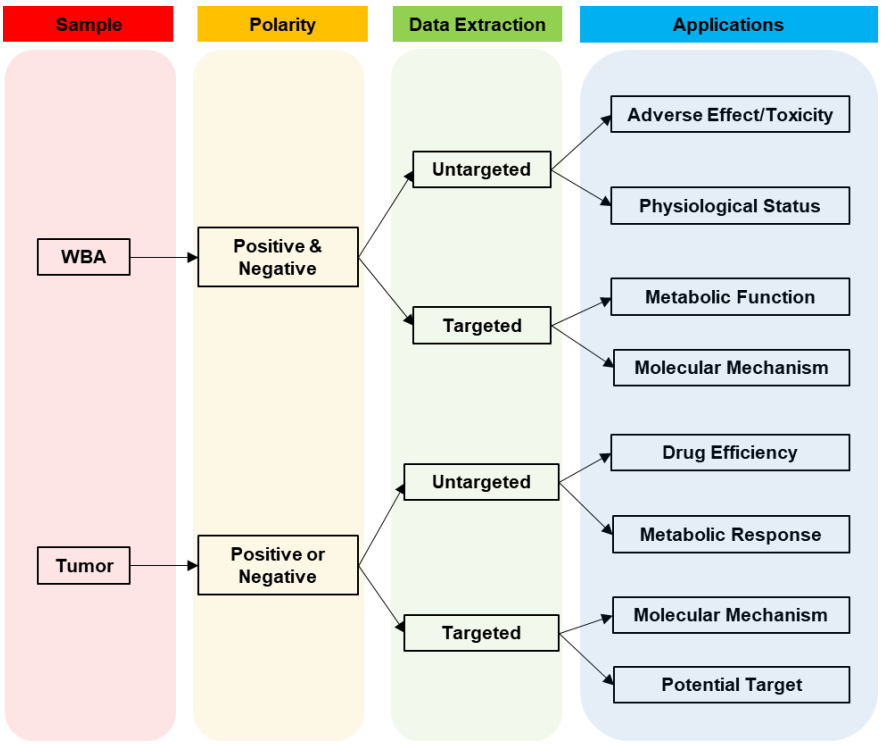
X-dimensional Mass Spectrometry Imaging

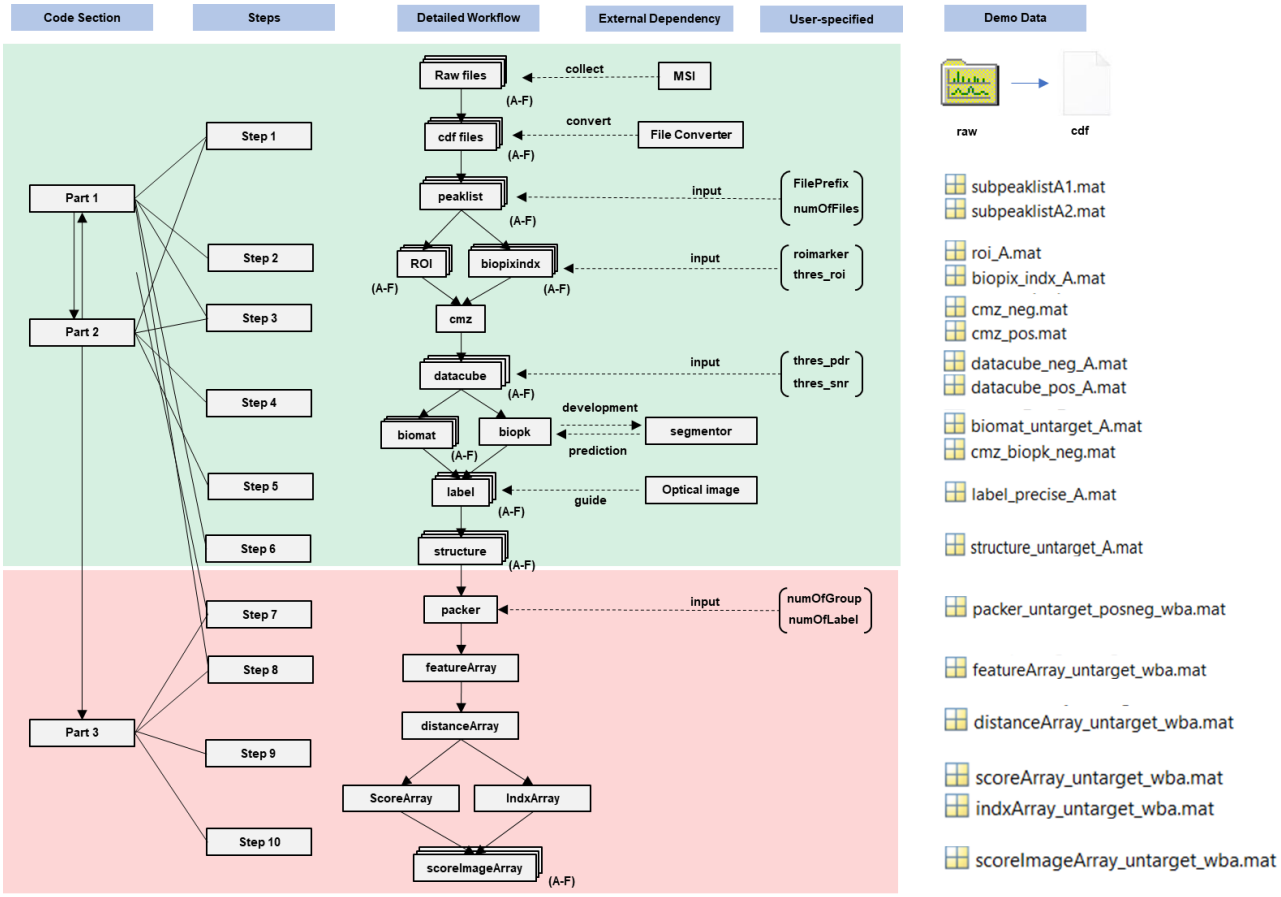
1.Background introduction of the demo data

- There were 7 whole-body animal (WBA) cryosections scanned by the air-flow-assisted desorption electrospray ionization mass spectrometry imaging method (AFADESI-MSI) under an ALTERNATIVE switching mode.
- The alternative scan was composed of three channels:
- Channel 1: m/z 50-1000 (negative)
- Channel 2: m/z 50-1000 (positive)
- Channel 3: t-SIM scan specific to drug ion: PTX, 876.3203 [M+Na]+; PTR, 983.4172 [M+H]+; PTS, 1039.4440 [M+H]+
- Tumor cryosections were scanned by AFADESI-MSI SEPARATELY from the WBA sample for the purpose of gaining more detailed metabolic profile information.
- The 7 WBA samples were coded from A to G: (A) healthy control; (B) xenograft tumor (negative treatment); (C) paclitaxel (PTX); (D) paclitaxel derivative 1 (PTR); and (E) low, (F) medium, (G) high dosage of paclitaxel derivative 2 (PTS).

2.General MSI(x) Strategy and its application in preclinical drug research and development.



3.More detailed pipeline for MSI$^{(X)}$ analysis



Step 1: Import CDF Files and save as a peaklist

Step 2: Delineate the Region of Interest and Register Pixel Index

Step 3: Generate the common peaks vector and construct a datacube

Step 4: Reduce the datacube volume size by SNR and PDR criteria

Step 5: Convert a datacube to a biomatrix

Step 6: Spatial Segmentation for WBA /tumor

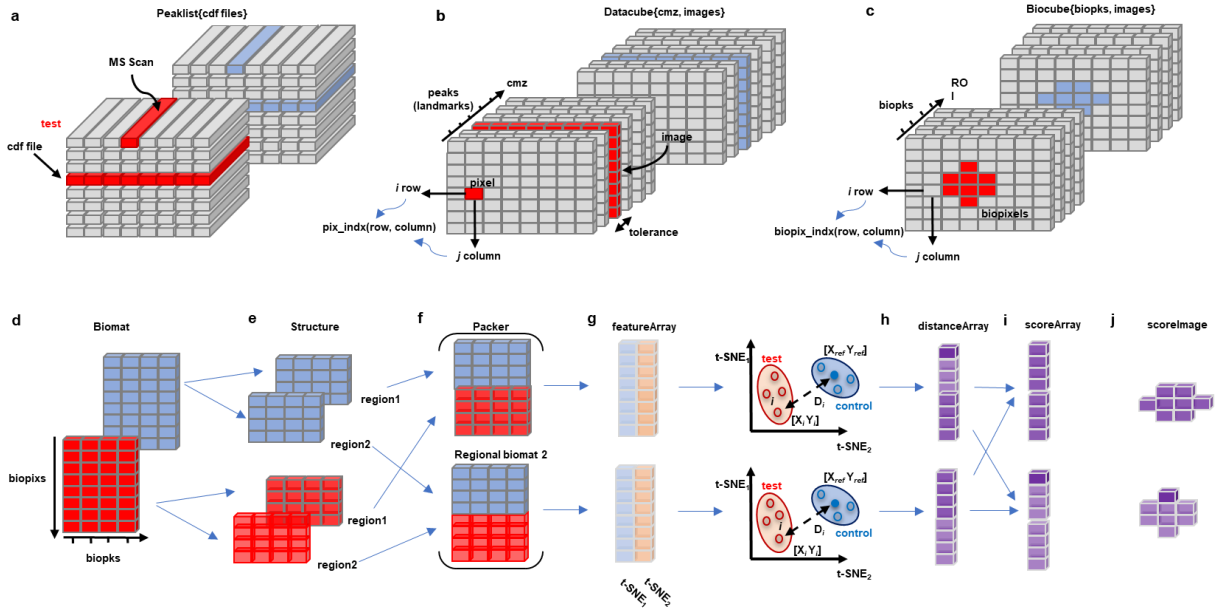
Step 7: Biomatrix splitting and regional biomatrix recombination

Step 8: Regional Metabolomic Feature Extraction

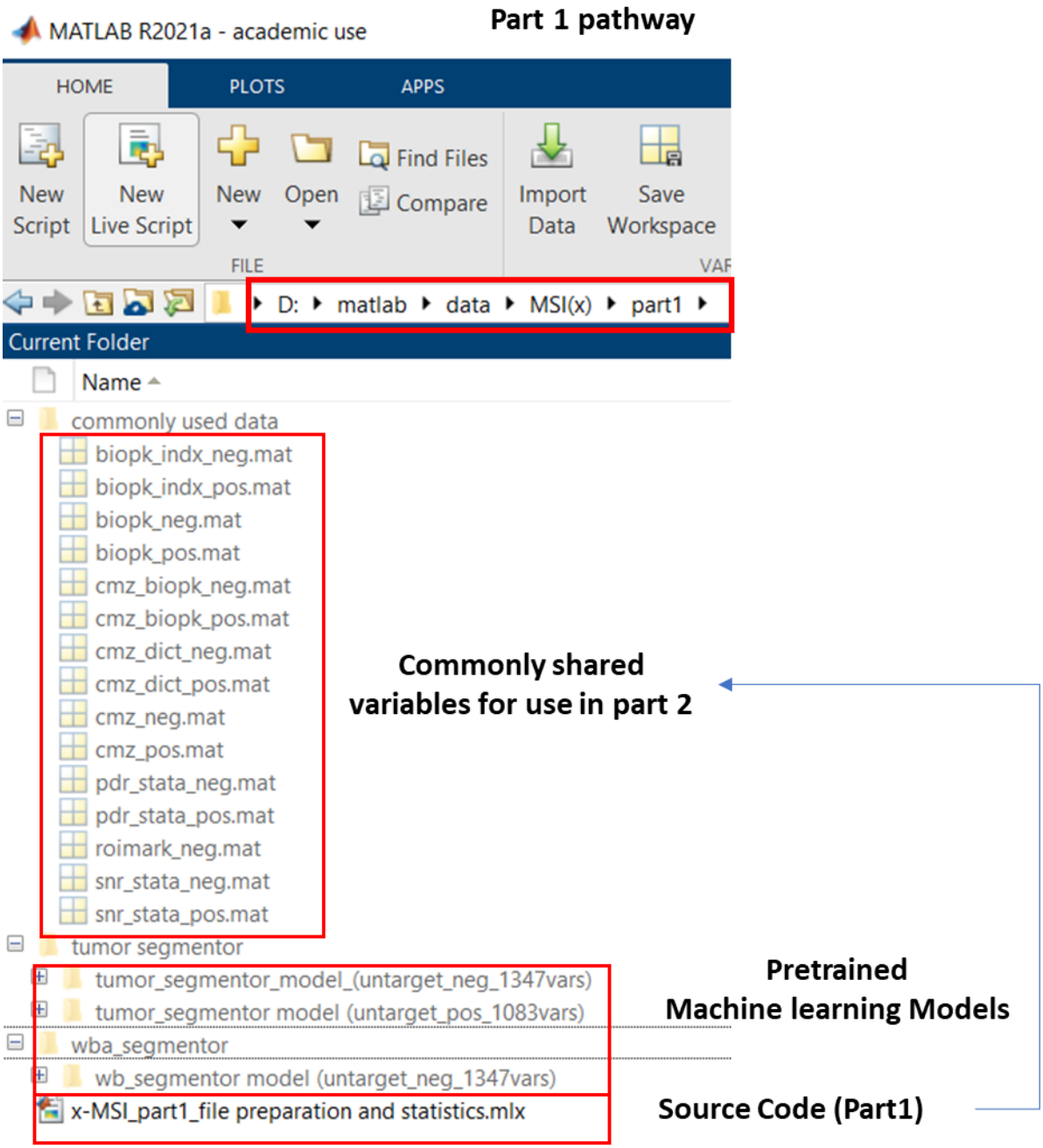
Step 9: Measure the General Perturbation for untargeted metabolomics or each pathway

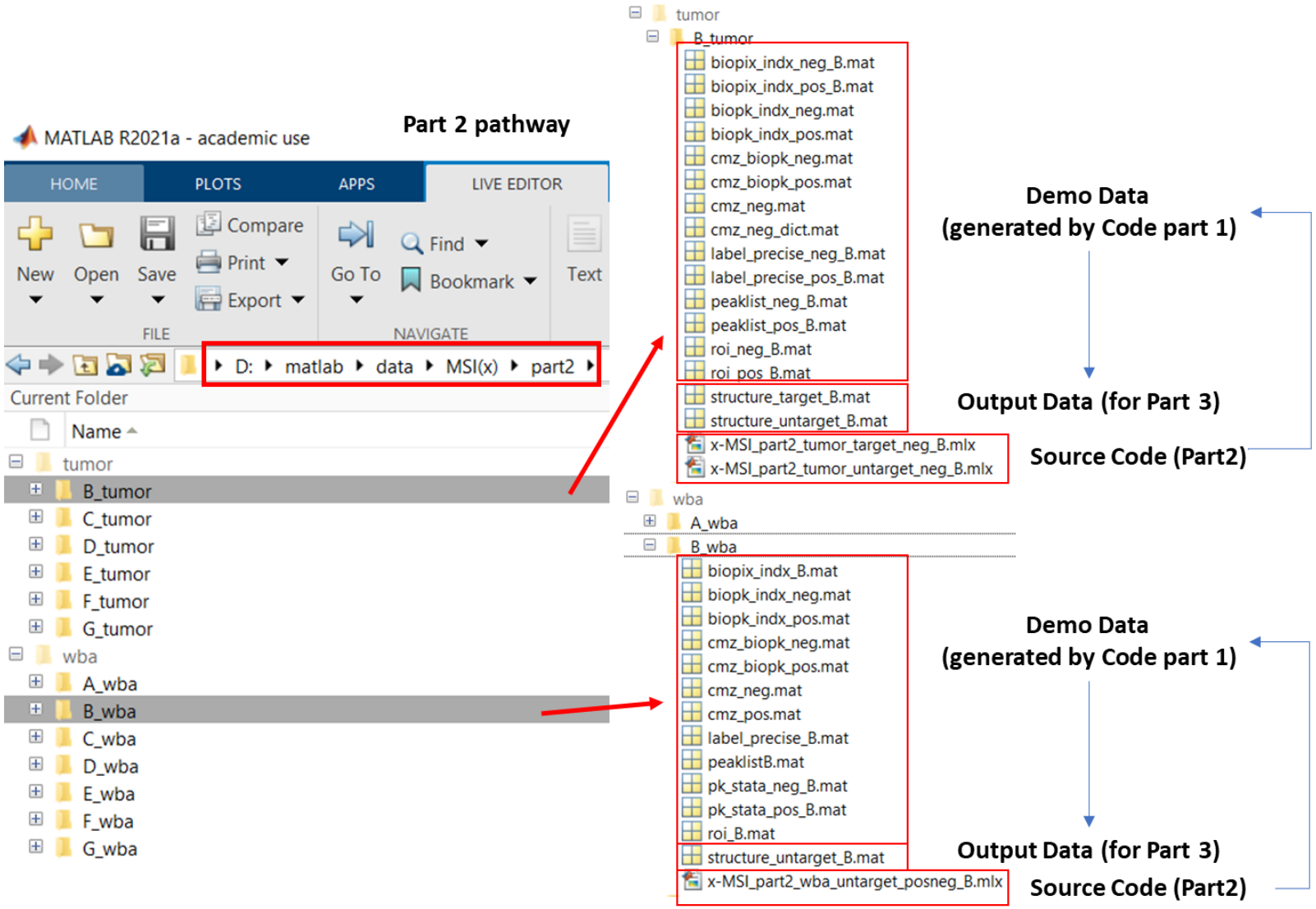
Step 10: Construct Metabolic Perturbation Image for WBA/tumor

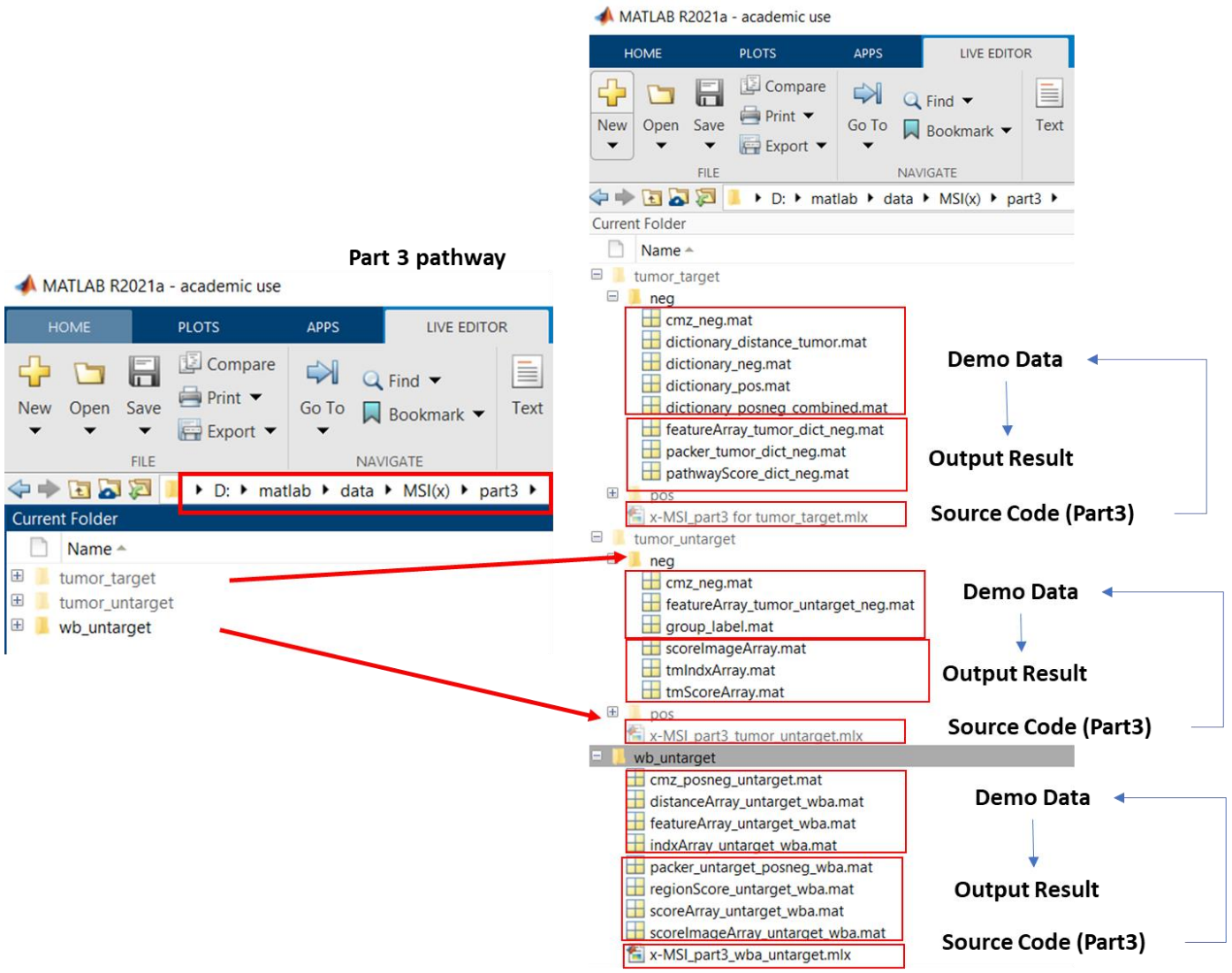
4.Diagram of Data Structure used in MSI$^{(X)}$



5. Pathway of source codes and correspondent demo Data




Part 2 pathway
MATLAB R2021a - academic use
HOME
PLOTS
APPS
LIVE EDITOR
New
Open
Save
Compare
Print
Export
FILE
Go To
Find
Bookmark
NAVIGATE
Text
D: ▸ matlab ▸ data ▸ MSI(x) ▸ part2 ▸
Current Folder
Name
tumor
B_tumor
C_tumor
D_tumor
E_tumor
F_tumor
G_tumor
wba
A_wba
B_wba
C_wba
D_wba
E_wba
F_wba
G_wba
tumor
B_tumor
biopix_indx_neg_B.mat
biopix_indx_pos_B.mat
biopk_indx_neg.mat
biopk_indx_pos.mat
cmz_biopk_neg.mat
cmz_biopk_pos.mat
cmz_neg.mat
cmz_neg_dict.mat
label_precise_neg_B.mat
label_precise_pos_B.mat
peaklist_neg_B.mat
peaklist_pos_B.mat
roi_neg_B.mat
roi_pos_B.mat
structure_target_B.mat
structure_untarget_B.mat
x-MSI_part2_tumor_target_neg_B.mlx
x-MSI_part2_tumor_untarget_neg_B.mlx
Demo Data
(generated by Code part 1)
Output Data (for Part 3)
Source Code (Part2)
wba
A_wba
B_wba
biopix_indx_B.mat
biopk_indx_neg.mat
biopk_indx_pos.mat
cmz_biopk_neg.mat
cmz_biopk_pos.mat
cmz_neg.mat
cmz_pos.mat
label_precise_B.mat
peaklistB.mat
pk_stata_neg_B.mat
pk_stata_pos_B.mat
roi_B.mat
structure_untarget_B.mat
x-MSI_part2_wba_untarget_posneg_B.mlx
Demo Data
(generated by Code part 1)
Output Data (for Part 3)
Source Code (Part2)


Part 3 pathway
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HOME
PLOTS
APPS
LIVE EDITOR
New
Open
Save
Compare
Print
Export
FILE
Go To
Find
Bookmark
NAVIGATE
Text
D: ▸ matlab ▸ data ▸ MSI(x) ▸ part3 ▸
Current Folder
Name
tumor_target
tumor_untarget
wb_untarget
neg
cmz_neg.mat
dictionary_distance_tumor.mat
dictionary_neg.mat
dictionary_pos.mat
dictionary_posneg_combined.mat
featureArray_tumor_dict_neg.mat
packer_tumor_dict_neg.mat
pathwayScore_dict_neg.mat
pos
x-MSI_part3 for tumor_target.mlx
Demo Data
Output Result
Source Code (Part3)
featureArray_tumor_untarget_neg.mat
group_label.mat
scoreImageArray.mat
tmIndxArray.mat
tmScoreArray.mat
x-MSI_part3_tumor_untarget.mlx
cmz_posneg_untarget.mat
distanceArray_untarget_wba.mat
featureArray_untarget_wba.mat
indxArray_untarget_wba.mat
packer_untarget_posneg_wba.mat
regionScore_untarget_wba.mat
scoreArray_untarget_wba.mat
scoreImageArray_untarget_wba.mat
x-MSI_part3_wba_untarget.mlx

6. Structure of the Functional Metabolite Ion Library

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	'metabolite'	'exact m/z'	'adduct ion'	'choline m...	'urea cycle'	'immunosu...	'krebs cycle...	'one-carbon'	'acetylation'	'methylatio...	'dehydroge...	'deaminati...	'amines'	'lipid polar...	'polyamines'
2	'Trimethyla...	60.0804	'[M+H]+'	0	0	0	0	0	0	0	0	0	1	0	0
3	'urea'	61.0404	'[M+H]+'	0	1	0	0	0	0	0	0	0	0	0	0
4	'ethanolam...	62.0601	'[M+H]+'	0	0	0	0	0	0	0	0	0	0	1	0
5	'dimethyla...	68.0470	'[M+Na]+'	0	0	0	0	0	0	1	0	0	0	0	0
6	'Glycoxylic ...	75.0077	'[M+H]+'	0	0	0	0	0	0	0	0	0	0	0	0
7	'trimethyla...	76.0757	'[M+H]+'	0	0	0	0	0	0	0	0	0	1	0	0
8	'Hydroxyur...	77.0346	'[M+H]+'	0	0	0	0	0	0	0	0	0	0	0	0
9	'Cysteamine'	78.0372	'[M+H]+'	0	0	0	0	0	0	0	0	0	0	0	0
10	'urea'	83.0216	'[M+Na]+'	0	1	0	0	0	0	0	0	0	0	0	0
11	'dimethyla...	84.0210	'[M+K]+'	0	0	0	0	0	0	1	0	0	0	0	0
12	'ethanolam...	84.0420	'[M+Na]+'	0	0	0	0	0	0	0	0	0	0	1	0
13	'Pyruvate'	89.0233	'[M+H]+'	0	0	0	1	0	0	0	0	0	0	0	0
14	'putrescine'	89.1073	'[M+H]+'	0	0	0	0	0	0	0	0	0	0	0	1
15	'alanine/sa...	90.0550	'[M+H]+'	0	0	0	0	0	0	0	0	0	0	0	0
16	'glyceralde...	91.0390	'[M+H]+'	0	0	0	0	0	0	0	0	0	0	0	0
17	'Glycoxylic ...	96.9896	'[M+Na]+'	0	0	0	0	0	0	0	0	0	0	0	0
18	'Glycine'	98.0212	'[M+Na]+'	0	0	0	0	1	0	0	0	0	0	0	0
19	'trimethyla...	98.0576	'[M+Na]+'	0	0	0	0	0	0	0	0	0	1	0	0
20	'urea'	98.9955	'[M+K]+'	0	1	0	0	0	0	0	0	0	0	0	0
21	'Hydroxyur...	99.0165	'[M+Na]+'	0	0	0	0	0	0	0	0	0	0	0	0
22	'ethanolam...	100.0159	'[M+K]+'	0	0	0	0	0	0	0	0	0	0	1	0
23	'Cysteamine'	100.0191	'[M+Na]+'	0	0	0	0	0	0	0	0	0	0	0	0
24	'N,N-dimet...	100.0763	'[M+H-H2...	0	0	0	0	0	0	1	0	0	0	0	0
25	'2-Hydroxy...	101.0603	'[M+H-H2...	0	0	0	0	0	0	0	0	0	0	0	0

7. Nomenclature of variables

Folder/Pathway	Variable name	Description
D:\MATLAB\Data\MSI(x)\Part1	biopk_indx_neg	indexes of selected 1347 among the 3552 negative ions
	biopk_indx_pos	indexes of selected 1083 among the 5370 positive ions;
	cmz_biopk_neg	selected 1347 negative ions
	cmz_biopk_pos	selected 1083 positive ions
	cmz_dict_neg	498 negative ions included in the dictionary
	cmz_dict_pos	1317 positive ions included in the dictionary
	cmz_neg	3552 negative ions from average mass spectrum of WBA sample
	cmz_pos	5370 positive ions from average mass spectrum of WBA sample
	pdr_stata_neg	Summary of Positive detection rate (PDR) of 3552 negative ions among 7 WBA groups
	pdr_stata_pos	Summary of Positive detection rate (PDR) of 5370 positive ions among 7 WBA groups
	roimark_neg	Negative marker ions for ROI delineation
	snr_stata_neg	Summary of signal-to-noise ratio (SNR) of 3552 negative ions among 7 WBA groups
	snr_stata_pos	Summary of signal-to-noise ratio (SNR) of 5370 positive ions among 7 WBA groups
	dictionary_pos	dictionary that only includes 1317 positive ions and their corresponding pathway, function, species, and biotransformation
	dictionary_neg	dictionary that only includes 498 negative ions and their corresponding pathway, function, species, and biotransformation
	dictionary_posneg	dictionary that includes all 1815 ions and their corresponding pathway, function, species, and biotransformation
D:\MATLAB\Data\MSI(x)\Part2\tumor\B_tumor	peaklist_neg_B	all negative MS scans acquired from the group B tumor sample
	peaklist_pos_B	all positive MS scans acquired from the group B tumor sample
	roi_pos_B	Region of interest (ROI) delineated by the sum of positive marker ion intensities
	roi_neg_B	See above
	biopix_indx_neg_B	Row and column index of pixels within the delineated ROI of group B tumor
	biopix_indx_pos_B	See above

	label_precise_neg_B	Physiological region of pixels predicted by a pretrain machine learning model
	label_precise_pos_B	See above
D:\MATLAB\Data\MSI(x)\Part2\tumor\C_tumor	subpeaklist1_pos_C	First half of positive MS scans acquired from the group C tumor sample
	subpeaklist2_pos_C	Second hald of positive MS scans acquired from the group C tumor sample
	peaklist_neg_C	-----
	roi_neg_C	-----
	roi_pos_C	-----
	label_precise_pos_C	-----
	label_precise_neg_C	-----
	biopix_indx_pos_C	-----
	biopix_indx_neg_C	-----

Folder/Pathway	Variable name	Description
D:\MATLAB\Data\MSI(x)\Part2\tumor\D_tumor	peaklist_neg_D	-----
	peaklist_pos_D	-----
	roi_pos_D	-----
	roi_neg_D	-----
	biopix_indx_neg_D	-----
	biopix_indx_pos_D	-----
	label_precise_neg_D	-----
	label_precise_pos_D	-----
D:\MATLAB\Data\MSI(x)\Part2\tumor\E_tumor	subpeaklist1_pos_E	-----
	subpeaklist2_pos_E	-----
	peaklist_neg_E	-----
	roi_neg_E	-----
	roi_pos_E	-----
	label_precise_pos_E	-----
	label_precise_neg_E	-----
	biopix_indx_pos_E	-----
	biopix_indx_neg_E	-----
D:\MATLAB\Data\MSI(x)\Part2\tumor\F_tumor	peaklist_neg_F	-----
	peaklist_pos_F	-----
	roi_pos_F	-----
	roi_neg_F	-----
	biopix_indx_neg_F	-----
	biopix_indx_pos_F	-----
	label_precise_neg_F	-----
	label_precise_pos_F	-----
D:\MATLAB\Data\MSI(x)\Part2\tumor\G_tumor	peaklist_pos_G	-----
	peaklist_neg_G	-----
	roi_neg_G	-----
	roi_pos_G	-----
	label_precise_pos_G	-----
	label_precise_neg_G	-----
	biopix_indx_pos_G	-----

	biopix_indx_neg_G	-----

Folder/Pathway	Variable name	Description
D:\MATLAB\Data\MSI(x)\Part2\wba\A_wba	subpeaklistA1	-----
	subpeaklistA2	-----
	roi_A	-----
	biopix_indx_A	-----
	label_precise_A	-----
D:\MATLAB\Data\MSI(x)\Part2\tumor\B_wba	peaklist_B	-----
	label_precise_B	-----
	roi_B	-----
	biopix_indx_B	-----
D:\MATLAB\Data\MSI(x)\Part2\tumor\C_wba	peaklist_C	-----
	roi_C	-----
	biopix_indx_C	-----
	label_precise_C	-----
D:\MATLAB\Data\MSI(x)\Part2\tumor\D_wba	subpeaklist_D1	-----
	subpeaklist_D2	-----
	roi_D	-----
	label_precise_D	-----
	biopix_indx_D	-----
D:\MATLAB\Data\MSI(x)\Part2\tumor\E_wba	peaklist_C	-----
	roi_C	-----
	biopix_indx_C	-----
	label_precise_C	-----
D:\MATLAB\Data\MSI(x)\Part2\tumor\F_wba	subpeaklist_D1	-----
	subpeaklist_D2	-----
	roi_D	-----
	label_precise_D	-----
	biopix_indx_D	-----
D:\MATLAB\Data\MSI(x)\Part2\tumor\G_wba	subpeaklist_D1	-----
	subpeaklist_D2	-----
	roi_D	-----
	label_precise_D	-----
	biopix_indx_D	-----

Folder/Pathway	Variable name	Description
D:\MATLAB\Data\MSI(x)\Part3\tumor_target\neg	featureArray_tumor_dict_neg	Metabolomics features extracted by t-SNE
	pathwayScore_dict_neg	Metabolic perturbation score for each search item in the dictionary (library)
	packer_tumor_dict_neg	Organized container that includes all regional biomatrices from the structureA to structureG generated by the code part 2
D:\MATLAB\Data\MSI(x)\Part3\tumor_target\pos	featureArray_tumor_dict_pos	
	pathwayScore_dict_pos	
	packer_tumor_dict_pos	
D:\MATLAB\Data\MSI(x)\Part3\tumor_untarget\neg	featureArray_tumor_untarget_neg	
	packer_tumor_untarget_neg	
	scoreImageArray_tumor_untarget	Metabolic perturbation image of tumor
D:\MATLAB\Data\MSI(x)\Part3\tumor_untarget\pos	featureArray_tumor_untarget_pos	
	packer_tumor_untarget_pos	
D:\MATLAB\Data\MSI(x)\Part3\wba_untarget	packer_wba_untarget_posneg	
	featureArray_wba_untarget	
	scoreImageArray_wba_untarget	Metabolic perturbation image of whole-body animal (wba)