

MAsP App User Manual



05/2022

Outline

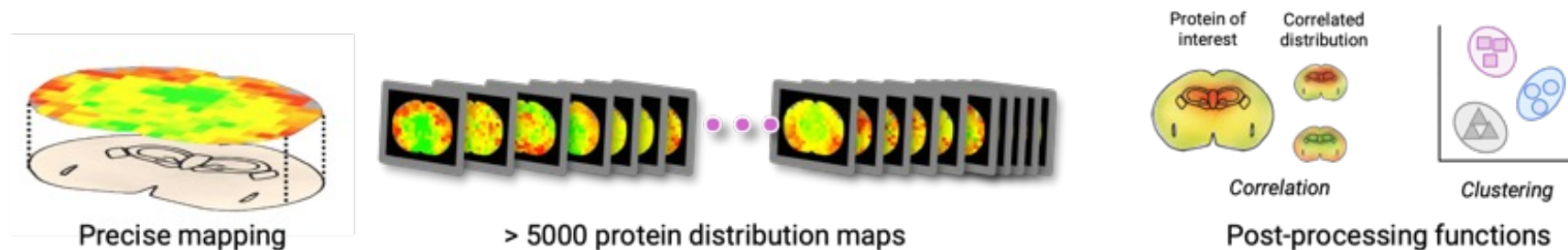
- **Introduction**
- **App setup**
- **Application**

Introduction

MAsP is a R Shiny-based application developed for processing spatial quantitative proteomic data. This app generates customizable protein distribution maps and offers post-processing functions, such as correlation of maps and clustering, identification of region-specific, non-random protein distribution patterns.

Though MAsP has been developed to process the data generated by our novel pipeline of Micro-scaffold Assisted Spatial Proteomics (MASP), it can also be used to process data from other platforms, as long as protein abundance/ratio/Z-score along with coordinate information are provided.

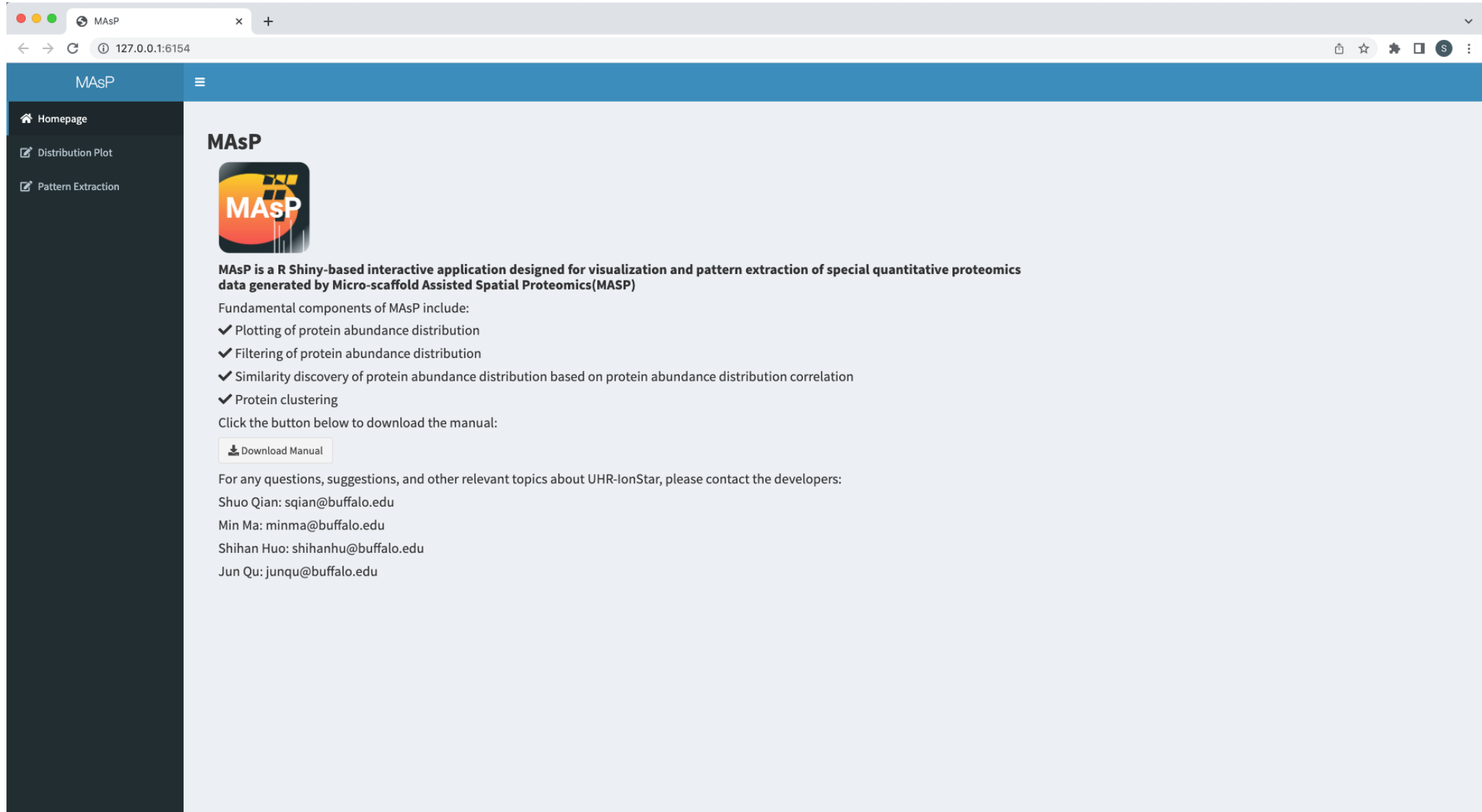
Generation of protein distribution map following accurate protein quantification by UHR-IonStar



<https://github.com/JunQu-Lab/MAsP>

Setup

If the app was installed properly, the web interface would pop up after running the app starting code:



Application

A sample data, which is from our project of measuring mouse cerebral protein distribution using the MASP pipeline, is provided for demonstration. In this project, a total of 5023 proteins were mapped across 208 spatial locations which cover a whole mouse brain slice.

Test_data																													
Possible Data Loss Some features might be lost if you save this workbook in the comma-delimited (.csv) format. To preserve these features, save it in an Excel file format.																													
A1																													
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	
1	F18	G18	H17	I18	J18	D15	E17	F17	G17	H16	I17	J17	K17	D14	E16	F16	G16	H15	I16	J16	K1	L1	M1	N1	O1	P1	Q1	R1	S1
2	A2A432-CUL	-0.4533756	-0.3914077	-0.8280064	-0.5809166	-0.1080022	0.25472943	-0.4952796	0.00597102	0.01046282	0.4465283	-0.4098917	0.428244	-0.1739879	-0.4185363	-0.0923904	-0.6921239	-0.5973952	-0.7725014	-0.6382064	-0.3779706	0.							
3	A2A5R2-BIG	-0.0101857	-0.5989411	-0.305836	-0.9627762	-0.4021495	-0.8154395	-0.6575348	-0.3492518	-0.5060478	-0.8261696	-0.5211601	-0.3547306	-1.0028458	-0.8070295	-0.2480464	-0.610395	-0.9799441	-1.1960318	-0.9662134	-0.5938528	0.							
4	A2A690-TAN	0.47154902	0.2536572	0.67066305	0.13692287	0.38009486	0.44070315	0.15164883	0.27959073	0.09369164	0.26969022	0.65624274	0.37516003	0.3660381	0.29072087	0.3893622	-0.1334637	-0.3073782	-0.1296734	-0.1937614	0.21585966	0.							
5	A2A699-F17	-0.8165035	0.44247822	-0.4951924	0.32582649	-0.1360378	1.06998803	-0.4404359	-0.2906883	0.45355344	0.06691361	-0.7718634	0.55562281	0.13537296	-0.2864325	0.19132695	0.31332135	-1.0823721	-1.0026131	-0.8694896	0.3221984	0.							
6	A2A8L1-CHD	-0.3980057	0.01633735	0.69047497	-0.2076855	0.44712285	0.10134945	-0.2600314	0.00642857	-0.3620589	0.30244222	0.14783839	0.22855825	1.23259525	-0.0663058	0.08995583	-0.4911835	-0.5206007	1.1791267	-0.0119834	-0.2009432	-0.							
7	A2A8L5-PTPF	-0.8798746	-0.8377991	-0.9291402	-0.4939222	-0.2060549	-0.2401711	-0.8277548	-0.3922302	-0.7941643	-1.0003774	-0.6983382	-0.3702592	-0.7440628	-0.9798286	-0.8984143	-1.0907812	-0.6962364	-0.8056607	-0.8805049	-0.35164	-0.							
8	A2A8Z1-OSB	0.42533034	1.2114993	1.13356516	0.21386803	0.99090169	0.96634337	1.37445075	1.79165975	0.81626181	2.65669199	-0.0921202	2.33496424	0.42175296	-0.9156366	0.34498322	0.79199524	0.31065202	0.19973518	-0.1900414	-0.01515	1.							
9	A2ADY9-DDV	0.08496585	0.14334742	-0.5882256	-0.259049	-0.3045752	0.24558669	-0.0455714	0.23614222	0.04572938	0.00473397	-0.2543356	-0.3376792	-0.8629766	0.0840488	0.35533664	-0.2735461	-0.3930276	-1.183993	-0.6745571	-0.0267913	-0.							
10	A2AG50-MA	-0.8274334	-1.6799517	-0.957491	-1.3405383	-1.643316	-1.5696753	-0.4740339	-0.1601165	-0.8380973	-1.760168	-0.7913093	-1.6828863	-2.2118835	-2.0527453	-0.6085641	-0.5028906	-0.4134714	-0.0262461	-0.1888412	-1.4299108	-0.							
11	A2AGL3-RYR	0.12742992	0.23471471	0.185437	0.27855254	0.77910867	1.03680863	0.9024941	0.72009758	0.49855041	-0.3761685	0.03081497	0.55428372	1.05442045	0.92267334	0.94537342	1.24623342	-0.2805942	-0.8568514	-0.1718825	0.50023723	0.							
12	A2AGT5-CKA	0.27040189	-0.1792427	0.11529663	-0.2928887	-0.1241091	-0.027984	-0.6064098	0.07396746	-0.473934	-0.2696982	0.1348392	-0.486878	-0.2064974	-0.3864364	-0.3006039	-0.0393368	-0.5239066	-0.12052	-0.2201297	-0.0723154	0.							
13	A2AH3C-CAW	-0.3390181	0.30683667	-0.3896506	0.17014	0.12581215	0.22341077	-0.4393962	-0.3344321	0.01342918	-0.4972857	0.09321372	0.25411701	-0.3903724	-0.6339981	0.19209632	-0.2816377	-0.5761784	-0.9247686	-0.8294603	0.27653577	0.							
14	A2AHG0-LZT	0.51306049	2.19313015	1.20410184	0.98915536	0.45305322	1.72524529	0.81825525	0.19172568	-0.1471338	0.39801523	0.11081656	-0.0198522	0.2118901	1.43940834	0.68841075	0.25282337	0.33693422	-0.7727776	1.17836701	1.04505866	0.							
15	A2AIA9-AJM	0.80080679	0.6305806	0.76766784	0.40433778	0.71429554	0.98422719	-0.1200976	-0.117758	0.37180553	-0.1503066	0.48620441	0.4300597	0.33183838	0.51359754	0.41712329	-0.1020331	-0.6477565	-0.2962217	0.05327157	0.50139054	0.							
16	A2AJI0-MA7	-0.125547	-0.1942607	-0.9859952	-0.1648958	-0.5234697	-0.3249669	-0.408867	0.06393306	-0.1877982	-0.4062986	-0.2767703	-0.5504025	-0.7803755	-0.3584751	-0.4837692	-0.4215508	-0.2224467	-0.0915305	0.23495955	-0.2023821	-0.							
17	A2ALK8-PTN	-0.3483146	0.84600008	-0.3789008	-0.2882876	-0.7579164	0.83141084	-1.0197988	-0.8074805	0.6036398	-1.3840645	-0.6438418	-0.3236591	-1.7837665	-0.159455	0.49978345	1.29198828	-1.9942139	-2.8385222	-2.1430988	-1.3877854	-0.							
18	A2ALS5-RPG	-0.436414	-0.9627772	-0.9102123	-0.9444139	-1.4209326	-0.9915674	-0.4935089	-0.6614148	-0.3243923	-0.9118878	-0.8383722	-0.3109017	-1.5035315	-1.1584919	-0.4847147	-0.8611009	-0.3180402	-0.7803069	-0.6249851	-0.7304262	-0.							
19	A2ALU4-SHR	-0.0320936	-0.0356081	-0.3553784	-0.2777873	-0.3445877	0.35736471	-0.5282242	-0.5412045	-0.608003	-0.8189291	-0.5787483	-0.5154283	-0.8049788	0.01370095	-0.1898037	-0.2595407	-0.7645142	-0.6364044	-0.41491	-0.0861644	0.							
20	A2AN08-UBF	0.1418052	-0.2318961	-0.3162838	-0.378862	-0.0153886	0.13412884	-0.239334	-0.0167334	-0.1290574	-0.2384871	-0.1927836	0.15896215	0.12669128	-0.1531537	0.05650099	-0.0682877	-0.6152136	-1.018889	-0.7910204	-0.2451375	-0.							
21	A2AP18-PLC	-0.6523929	-0.0614059	-0.3305677	-0.1765394	-0.1114889	0.20218554	-0.3038631	-0.3293907	-0.0176726	-0.2790602	-0.40214109	0.24531358	0.21170394	-0.8168908	0.33884375	0.6958583	-0.2506907	0.10461996	-0.5392713	0.20072478	0.							
22	A2APV2-FMN	-0.4367807	-0.6063695	-1.1270734	-0.6100119	-0.0656844	0.45899896	-0.5360165	-0.3667335	-0.2623335	-0.6832909	-1.391706	-0.4178888	0.36583334	-0.418458	0.05420085	-0.4572955	-0.7099386	-1.4928001	-0.8549284	-0.4898104	-0.							
23	A2APX8-SCN	-0.0209326	-0.3500276	-0.3403281	-0.6528332	-0.5473597	-0.4629105	-0.0980958	-0.4404623	-0.8667982	-0.4458023	-0.0429105	-0.1895969	-0.6675794	-0.219106	-0.5488117	-0.7548748	-0.9340011	-0.7727008	-0.4883343	0.								
24	A2APY7-NDU	-0.1595432	-0.2732988	-0.0158383	-0.6250616	-0.4737261	-0.3848981	-0.5856294	-0.1818634	-0.5286997	-0.667854	-0.4740973	-0.2436936	-0.6398572	-0.510178	0.13514041	-0.1899355	-0.9384246	-0.9859832	-0.7187487	-0.4827352	-0.							
25	A2AQ07-TBB	-0.4665744	-0.4961811	-0.6153497	-0.4825619	-0.6355866	0.08027896	-0.4385008	-0.2612154	-0.3379665	-0.8092679	-0.4837196	-0.2689785	-0.5717299	-0.9019707	-0.1766365	-0.1115733	-0.5748529	-0.8501994	-0.8714257	-0.2103442	0.							
26	A2AQ25-SKT	0.18114854	-0.0119007	0.29913039	-0.0934951	0.2583472	-0.2631244	-0.2844983	0.05470496	0.26569404	0.97169856	0.45466451	0.52312877	0.59985447	0.31893521	-0.0133285	-0.3859806	0.03190591	0.24849021	0.34293502	-0.3452559	0.							
27	A2AR02-PPIC	-1.3590572	0.04399765	-0.9663793	0.20003996	0.20852567	0.60246898	-0.3263986	-0.1729824	0.0772368	-0.6499572	-0.2462912	0.18074442	-0.9969919	0.58178106	0.56340141	-0.6670349	0.05237114	-0.210437	0.10515321	0.03293003	0.							
28	A2ARP1-VIP1	-1.6304192	-0.4662457	-0.0737781	-0.1215988	-2.2612295	-0.2710803	-2.2984292	-0.9346043	-0.1478031	-2.5466691	-0.424518	-3.245975	-1.4257862	0.33691718	-0.249609	-0.804763	-0.5364088	-0.6433275	-0.386578	-0.								
29	A2AS05-ANR	-0.4208124	0.35119499	-0.8381971	0.92981074	-0.5815166	0.69370008	-0.8431786	-0.388572	-0.5018557	-0.84033489	0.4003989	1.29437293	-0.6748802	-0.7902652	-1.4918264	-1.4267833	0.58006652	0.2629403	1.90472798	2.44778183	1.							
30	A2AS15-SCN2	-0.5814749	-0.4706571	-0.9890138	-0.5426829	-0.9716316	-0.5357558	-0.4509887	-0.2554979	-0.4307602	-0.8404834	-0.9038639	-0.0735018	-1.2737385	-1.1386402	-0.0994633	-0.3299992	-0.4650787	-0.6016666	-0.9019772	-0.2550283	-0.							
31	A2ASQ1-AGF	0.05569967	-0.0874576	-0.2288092	-0.4567548	-0.3850296	-0.054454	-0.3282004	-0.2339612	-0.4890114	-0.383433	-0.1774743	-0.4145646	-0.3842238	0.15680539	0.01855029	-0.481203	-0.4261835	-0.5027757	-0.6316422	-0.1813763	-0.							
32	A2ASZ8-SCM	-0.790191	-0.909479	-1.2274966	-1.197244	-0.8696912	-0.63832	-1.3909555	-1.0595511	-0.7882132	-1.4286228	-1.2924023	-1.1412628	-1.0404337	-0.8801439	-0.8245625	-0.7902745	-1.4947185	-1.5429016	-1.2428713	-1.0127928	-0.							
33	A2AT13-REN	-1.2857477	-0.7725916	-1.5100452	-0.9168556	-0.3261709	-0.3952242	-0.7046067	-0.4146988	-0.4787951	-1.1206562	-0.8477766	-0.2644354	-0.6251456	-0.7425068	-0.2267405	-0.7062043	-0.5501903	-0.0609725	-0.7823447	-0.6941994	-0.							
34	A2AWA9-RB	-0.1686118	-0.3410686	-0.2920774	-0.505323	-0.1731382	0.12798254	-0.4590896	-0.0696649	0.01011152	-0.0490444	-0.3372763	0.13259537	-0.7126896	-0.5604882	0.18431981	0.23044262	-0.7283895	-0.4699977	-0.39247	-0.3488327	0.				</			

Test_data

Home Insert Draw Page Layout Formulas Data Review View

Paste

Calibri (Body) 12

General

Conditional Formatting Format as Table Cell Styles

Insert Delete Format

AutoSum Fill Sort & Filter Find & Select

Possible Data Loss Some features might be lost if you save this workbook in the comma-delimited (.csv) format. To preserve these features, save it in an Excel file format. Save As...

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1		F18	G18	H17	I18	J18	D15	E17	F17	G17	H16	I17	J17	K17	D14	E16	F16	G16	H15	I16	J16	K16
2	A2A432:CU	-0.4533756	-0.3914077	-0.8280064	-0.5809166	-0.1080022	0.25472943	-0.4952796	0.00597102	0.01046282	0.4465283	-0.4098917	0.428244	-0.1739879	-0.4185363	-0.0923904	-0.6921239	-0.5973952	-0.7725014	-0.6382064	-0.3779706	0
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7	A2A8L5:PTPF	-0.8798746	-0.8377991	-0.9291402	-0.4939222	-0.2060549	-0.2401711	-0.8277548	-0.3922302	-0.7941643	-1.0003774	-0.6983382	-0.3702592	-0.7440628	-0.9798286	-0.8984143	-1.0907812	-0.6962364	-0.8056607	-0.8805049	-0.35164	1
8	A2A8Z1:OSB	0.42533034	1.2114993	1.13356516	0.21386803	0.99090169	0.96634337	1.37445075	1.79165975	0.81626181	2.65669199	-0.0921202	2.33496424	0.42175296	-0.9156366	0.34498322	0.79199524	0.31065202	0.19973518	-0.1900414	-0.01515	1

Locations

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Calibri (Body) 12

General

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	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
1		18	17	16	15	14	13	12	11	10	9	8	7	6	5	4	3	2	1		
2	A					B10	B9	A6	A5	A4	A3	A2	A1								
3	B					B8	B7	B6	B5	B4	B3	B2	B1								
4	C				C13	C12	C11	C10	C9	C8	C7	C6	C5	C4	C3	C2	C1				
5	D		D15	D14	D13	D12	D11	D10	D9	D8	D7	D6	D5	D4	D3	D2	D1				
6	E		E17	E16	E15	E14	E13	E12	E11	E10	E9	E8	E7	E6	E5	E4	E3	E2	E1		
7	F	F18	F17	F16	F15	F14	F13	F12	F11	F10	F9	F8	F7	F6	F5	F4	F3	F2	F1		
8	G	G18	G17	G16	G15	G14	G13	G12	G11	G10	G9	G8	G7	G6	G5	G4	G3	G2	G1		
9	H	H17	H16	H15	H14	H13	H12	H11	H10	H9	H8	H7	H6	H5	H4	H3	H2	H1	H0		
10	I	I18	I17	I16	I15	I14	I13	I12	I11	I10	I9	I8	I7	I6	I5	I4	I3	I2	I1		
11	J	J18	J17	J16	J15	J14	J13	J12	J11	J10	J9	J8	J7	J6	J5	J4	J3	J2	J1		
12	K		K17	K16	K15	K14	K13	K12	K11	K10	K9	K8	K7	K6	K5	K4	K3	K2	K1		
13	L			L16	L15	L14	L13	L12	L11	L10	L9	L8	L7	L6	L5	L4	L3	L2			
14	M			M15	M14	M13	M12	M11	M10	M9	M8	M7	M6	M5	M4	M3	M2				
15	N					N11	N10	N9	N8	N7	N6	N5	N4	N3	N2	N1					

Ready Calculate

Input datasets

- Spatial protein abundances
 - Row name: protein names
 - Column name: location
- Protein location information

Generation of Distribution Maps

Functions:

- **Location preview:** MAsP automatically generate a location plot read from the location file, helping the user to visualize and confirm different tissue locations.
- **Generation of single protein distribution map:** MAsP creates an abundance/Z-score distribution map for any protein selected by the user. Several parameters, such as data scaling, colors of map, value boundaries, can be personalized by the user.
- **Batch mode for multiple protein distribution maps:** The user can choose batch mode if the user wishes to create multiple protein distribution maps, one for each unique protein. All the distribution maps will be automatically saved in the directory that the user selects.

MA sP

Homepage

Distribution Map

Pattern Discovery/Extraction

Distribution Map

Location Preview

This preview plot is generated after inputting the location information file.

1				A6	A5	A4		A3	A2	A1											
2				B10	B9	B8	B7	B6	B5	B4	B3	B2	B1								
3				C13	C12	C11	C10	C9	C8	C7	C6	C5	C4	C3	C2	C1					
4				D15	D14	D13	D12	D11	D10	D9	D8	D7	D6	D5	D4	D3	D2	D1			
5				E17	E16	E15	E14	E13	E12	E11	E10	E9	E8	E7	E6	E5	E4	E3	E2	E1	
6				F18	F17	F16	F15	F14	F13	F12	F11	F10	F9	F8	F7	F6	F5	F4	F3	F2	F1
7				G18	G17	G16	G15	G14	G13	G12	G11	G10	G9	G8	G7	G6	G5	G4	G3	G2	G1
8				H17	H16	H15	H14	H13	H12	H11	H10	H9	H8	H7	H6	H5	H4	H3	H2	H1	H0
9				I18	I17	I16	I15	I14	I13	I12	I11	I10	I9	I8	I7	I6	I5	I4	I3	I2	I1
10				J18	J17	J16	J15	J14	J13	J12	J11	J10	J9	J8	J7	J6	J5	J4	J3	J2	J1
11				K17	K16	K15	K14	K13	K12	K11	K10	K9	K8	K7	K6	K5	K4	K3	K2	K1	
12				L16	L15	L14	L13	L12	L11	L10	L9	L8	L7	L6	L5	L4	L3	L2			
13				M15	M14	M13	M12	M11	M10	M9	M8	M7	M6	M5	M4	M3	M2				
14				N11	N10	N9	N8	N7	N6	N5	N4	N3	N2	N1							
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18			

Apply a tissue shape template

The values exceeding the range would be set to the upper or lower bound.

Data Upload

Upload quantitative file (.csv):
Browse... Test_data.csv
Upload complete

Upload location information (.csv):
Browse... Locations.csv
Upload complete

Upload tissue shape template (.png):
Browse... Brain_cover.png
Upload complete

Input the name of protein you would like to illustrate:
P04370:MBP_MOUSE

☒ Convert data to Z-score

☒ Add tissue shape template

☐ Make the plot with transparent background while downloading

☒ Plot with legend

Choose the range of map color display:
☒ No limit
☐ Inter-quantile range
☐ Customized

Input the upper bound for protein values (if customized):
2

Input the lower bound for protein values (if customized):
-2

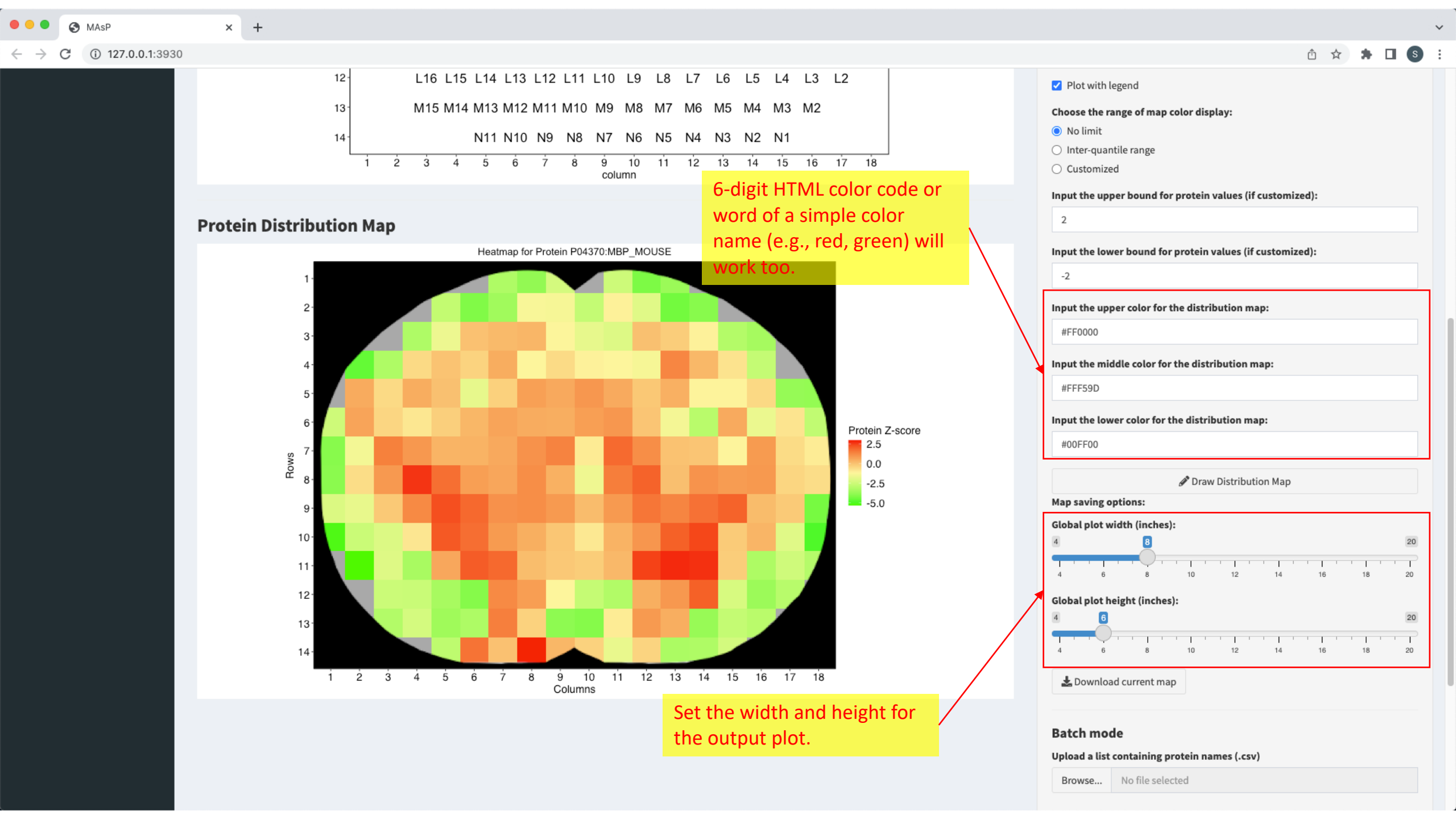
Input the upper color for the distribution map:

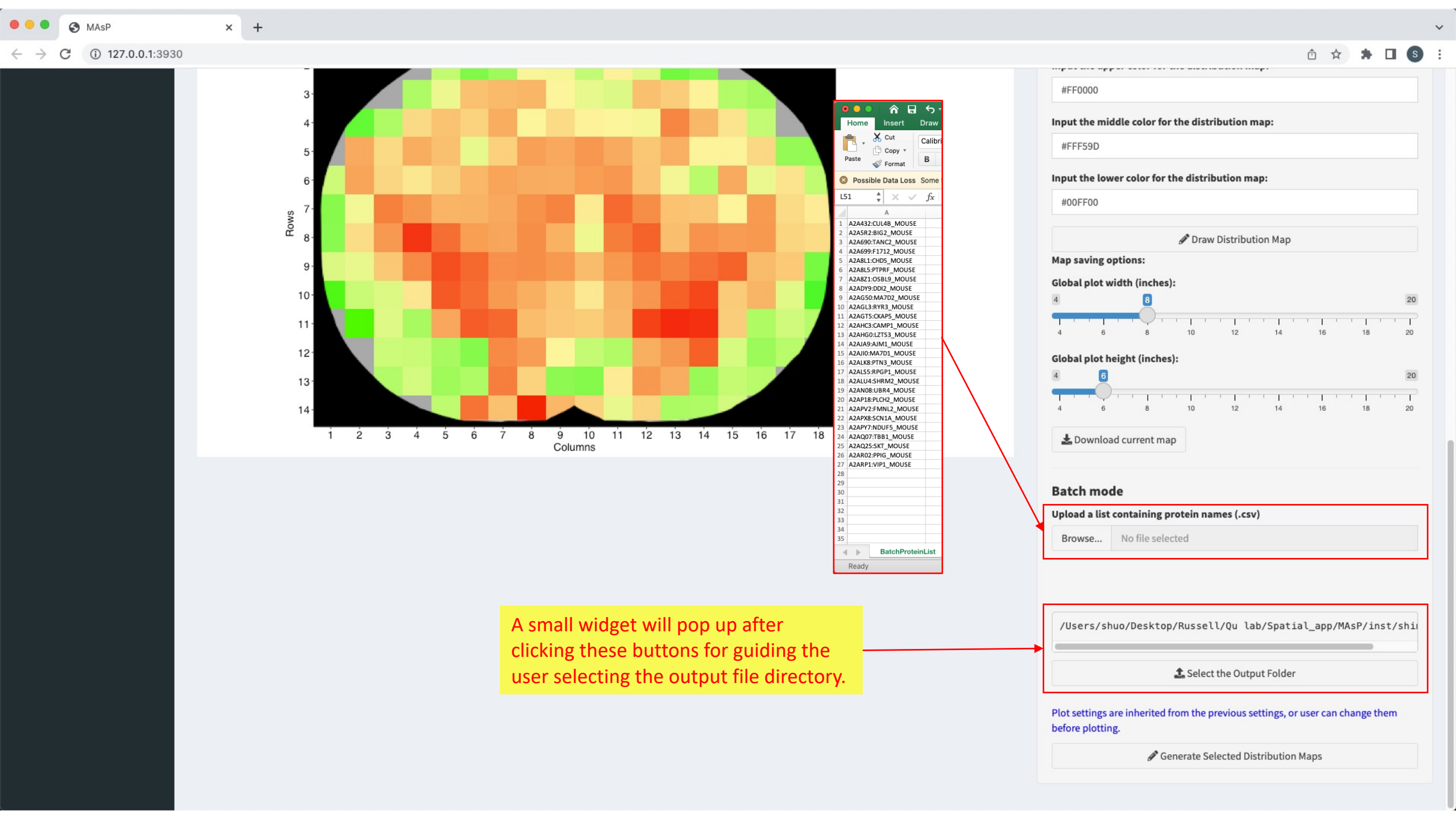
Protein Distribution Map

Heatmap for Protein P04370:MBP_MOUSE

1

2

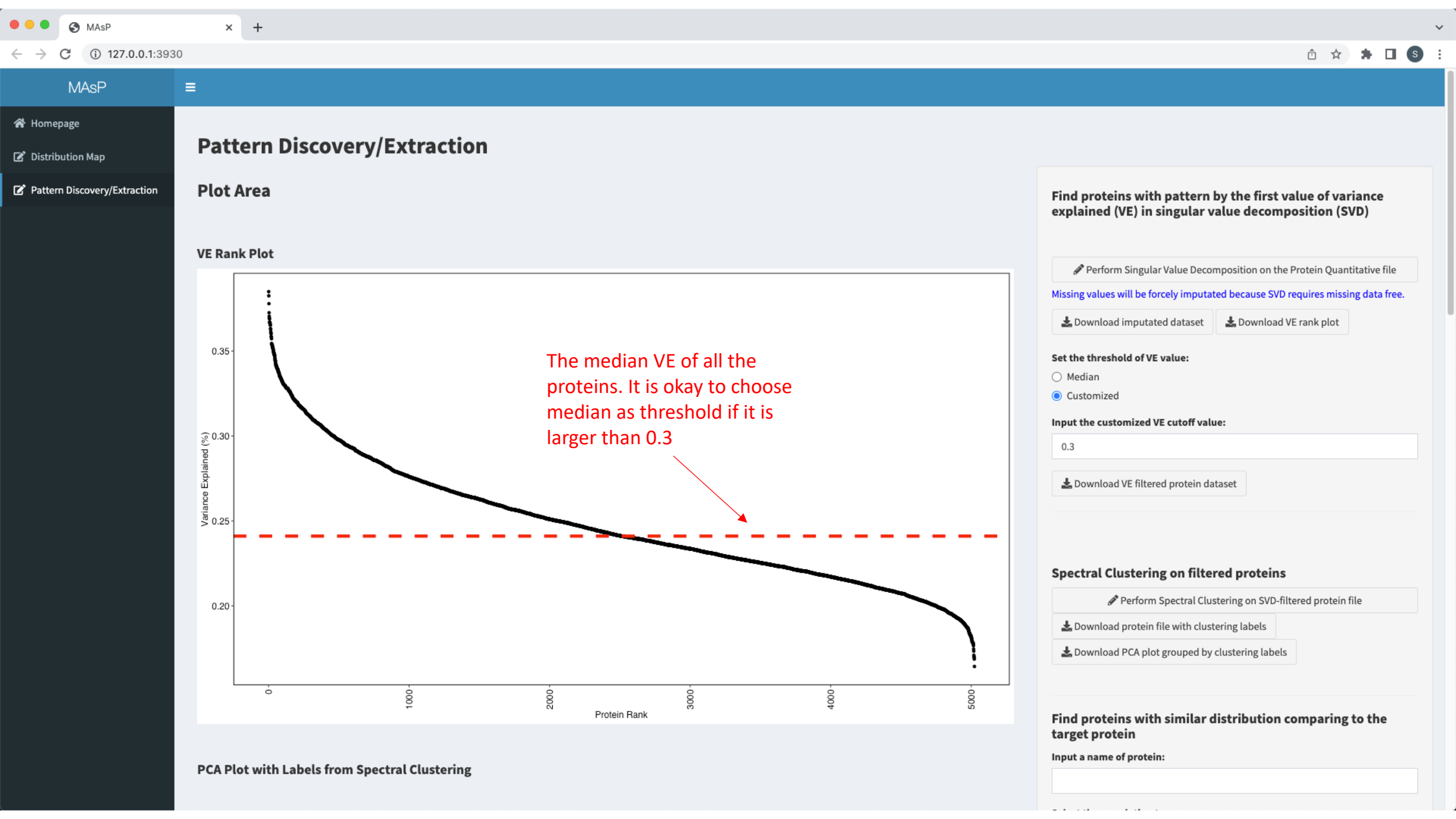




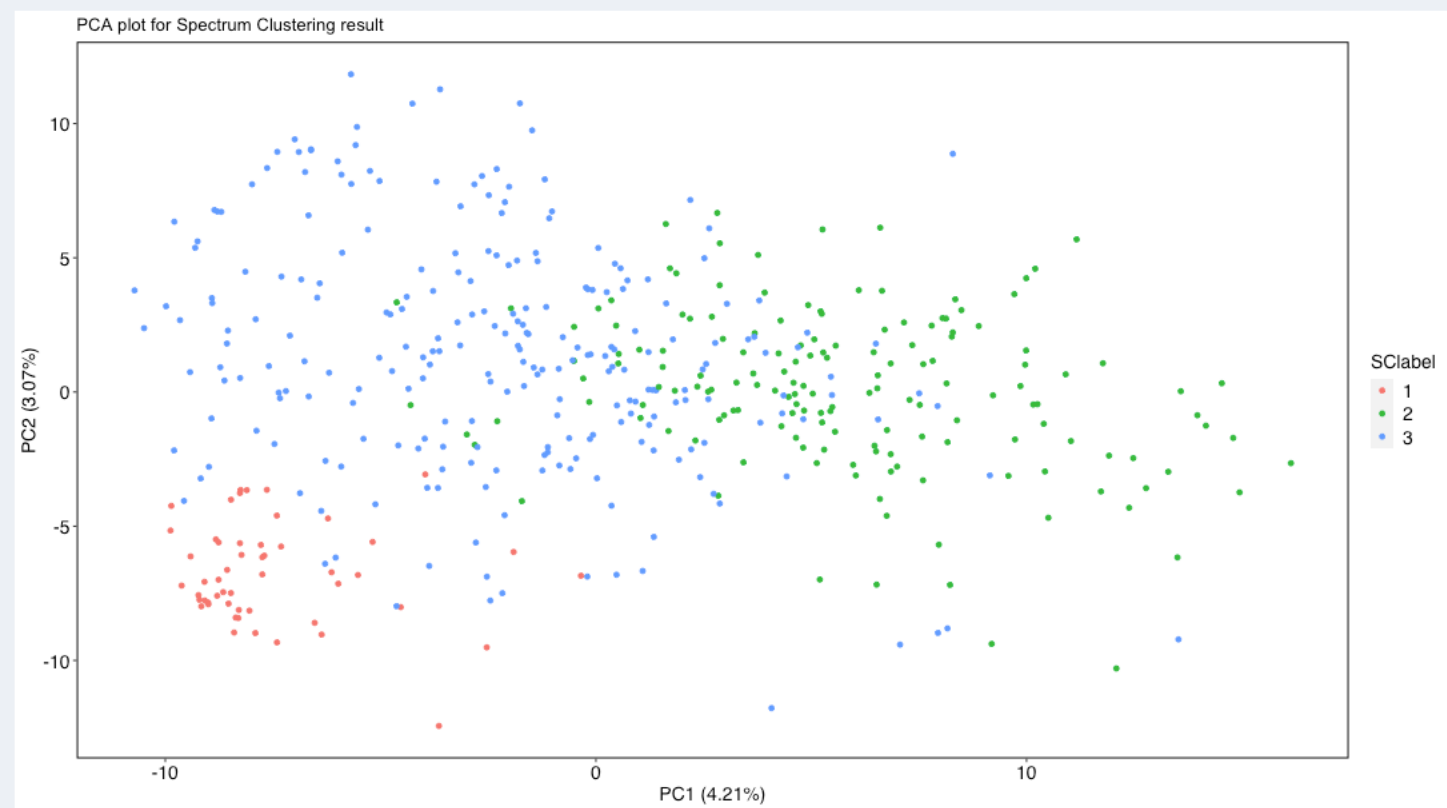
Pattern discovery/extraction

Functions:

- **Data filtering:** To identify proteins with non-random, region-specific distribution patterns, MAsP uses the first value of variance explained (VE) in singular value decomposition (SVD) as a filter to remove protein distribution maps with low VE values (*i.e.* random distributions without a recognizable pattern), which is necessary for further pattern extraction and clustering. The user can set a customized filter threshold and we recommended 0.25-0.35.
- **Clustering of protein distribution maps based on pattern similarity:** For the protein distribution maps surviving the above step, the maps with similar regional distribution patterns can be grouped by the spectral clustering algorithm, which is a density-based clustering algorithm that are typically used for image processing. A PCA plot and a dataset with clustering labels will be generated.
- **Identification of protein maps correlating with the map of a protein of interest:** Proteins with correlated distribution patterns could imply co-localization of these proteins, which may provide highly valuable information on spatially organized biological processes. Using this approach, we devised a Protein Correlation module to identify proteins that are potentially co-localized with the target protein of interest selected by the user. Two options are provided



PCA Plot with Labels from Spectral Clustering



Input a name of protein:

P04370:MBP_MOUSE

Select the correlation type:

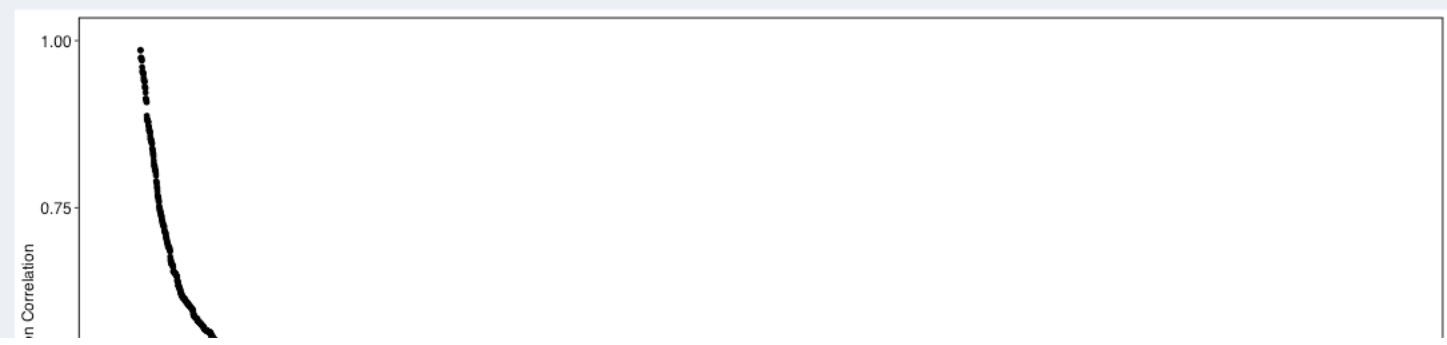
- ☒ Pearson Correlation
☐ Cosine Similarity

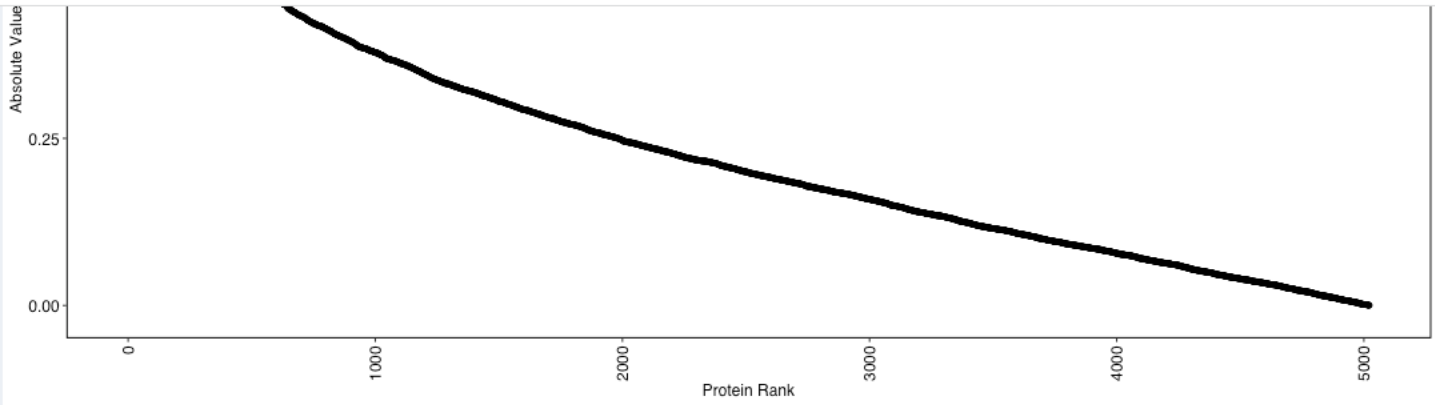
Find correlations

Download correlation rank data

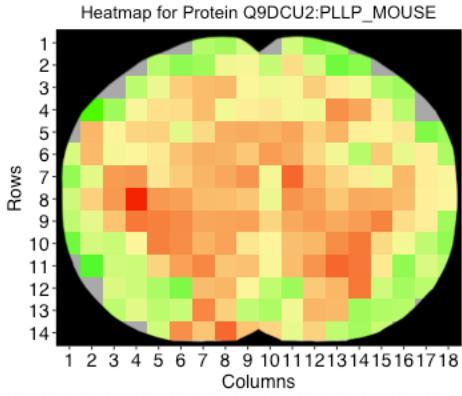
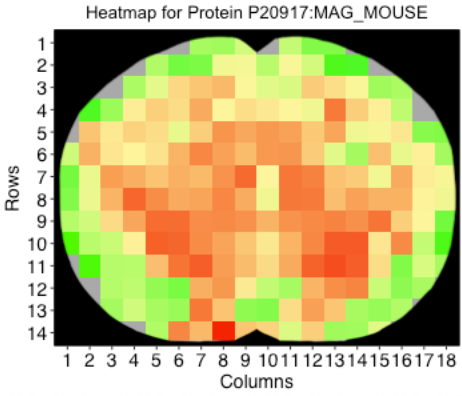
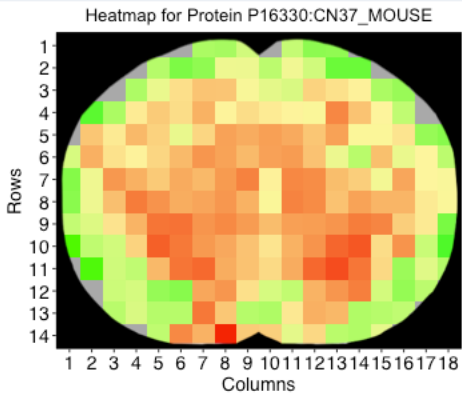
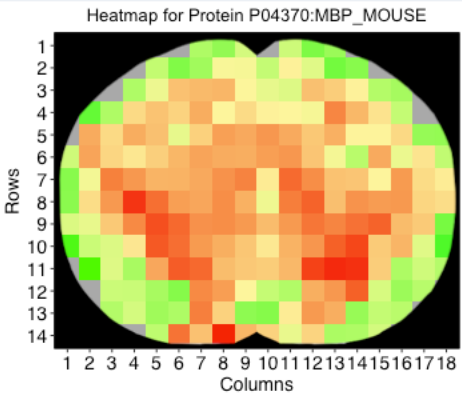
Download correlation rank plot

Correlation Rank Plot





TOP3 Correlated Proteins



Thank you for using MAsP!

For any questions, suggestions and other relevant topics about MAsP, please contact the developers:

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Shihan Huo: shihanhu@buffalo.edu

Jun Qu: junqu@buffalo.edu

Relevant articles:

- Shen, Xiaomeng, et al. "IonStar enables high-precision, low-missing-data proteomics quantification in large biological cohorts." *Proceedings of the National Academy of Sciences* 115.21 (2018): E4767-E4776.
- Wang, Xue, et al. "Ultra-High-Resolution IonStar Strategy Enhancing Accuracy and Precision of MS1-Based Proteomics and an Extensive Comparison with State-of-the-Art SWATH-MS in Large-Cohort Quantification." *Analytical chemistry* 93.11 (2021): 4884-4893.
- Fonville, Judith M., et al. "Robust data processing and normalization strategy for MALDI mass spectrometric imaging." *Analytical chemistry* 84.3 (2012): 1310-1319.