

Supplementary materials of Deconvoluting spatial transcriptomics data with single-cell transcriptomes through semi-supervised NMF and least angle regression

December 27, 2024

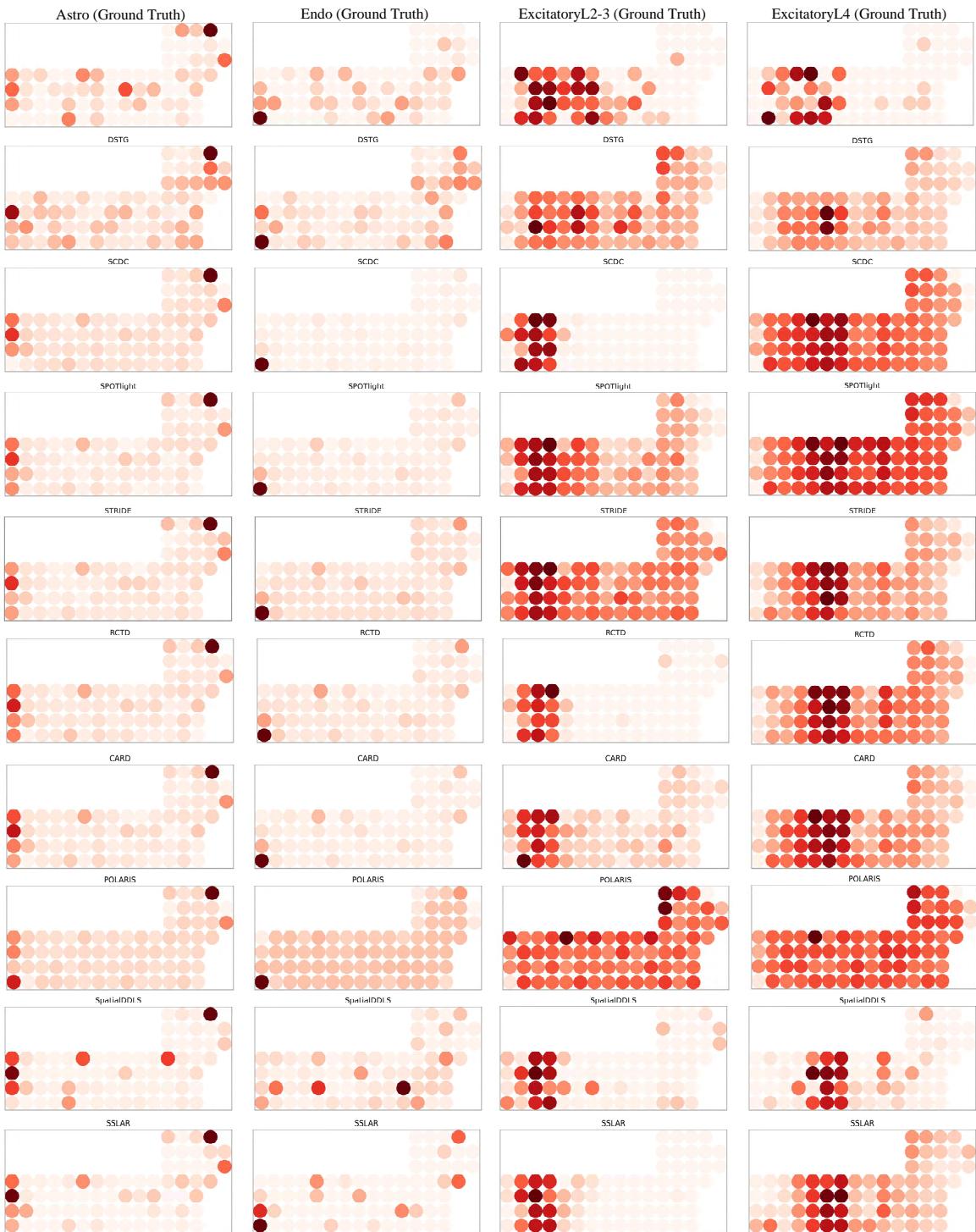


Figure S1: The proportion of four cell types (Astro, Endo, ExcitatoryL2and3, and ExcitatoryL4) in the spots simulated from mouse cortex, containing the ground truth and predictions.

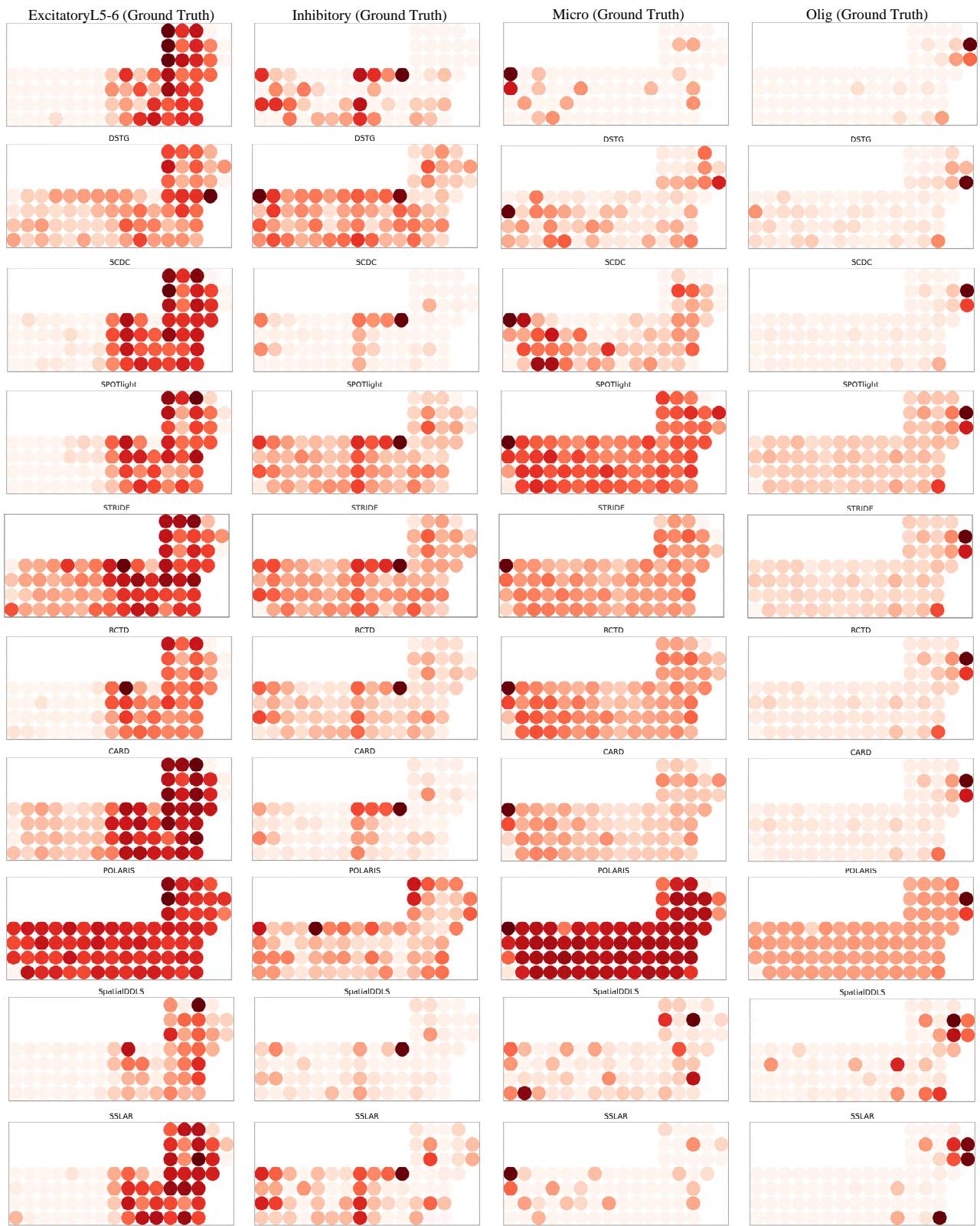


Figure S2: The proportion of four cell types (ExcitatoryL5and6, Inhibitory, Micro, and Olig) in the spots simulated from mouse cortex (SeqFISH+), containing the ground truth and predictions.

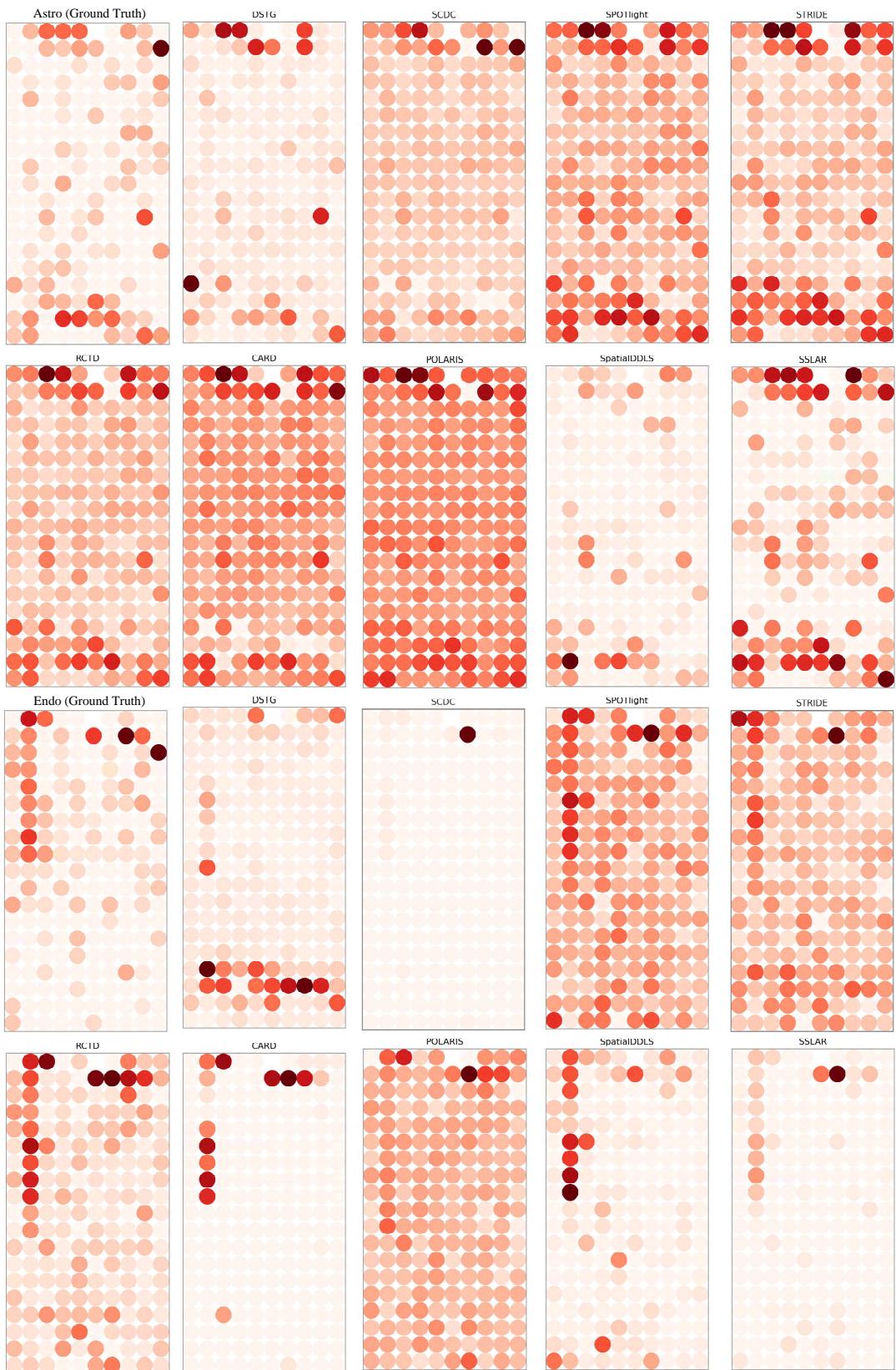


Figure S3: The proportion of two cell types (Astro and Endo) in the spots simulated from mouse visual cortex (STARmap), containing the ground truth and predictions.

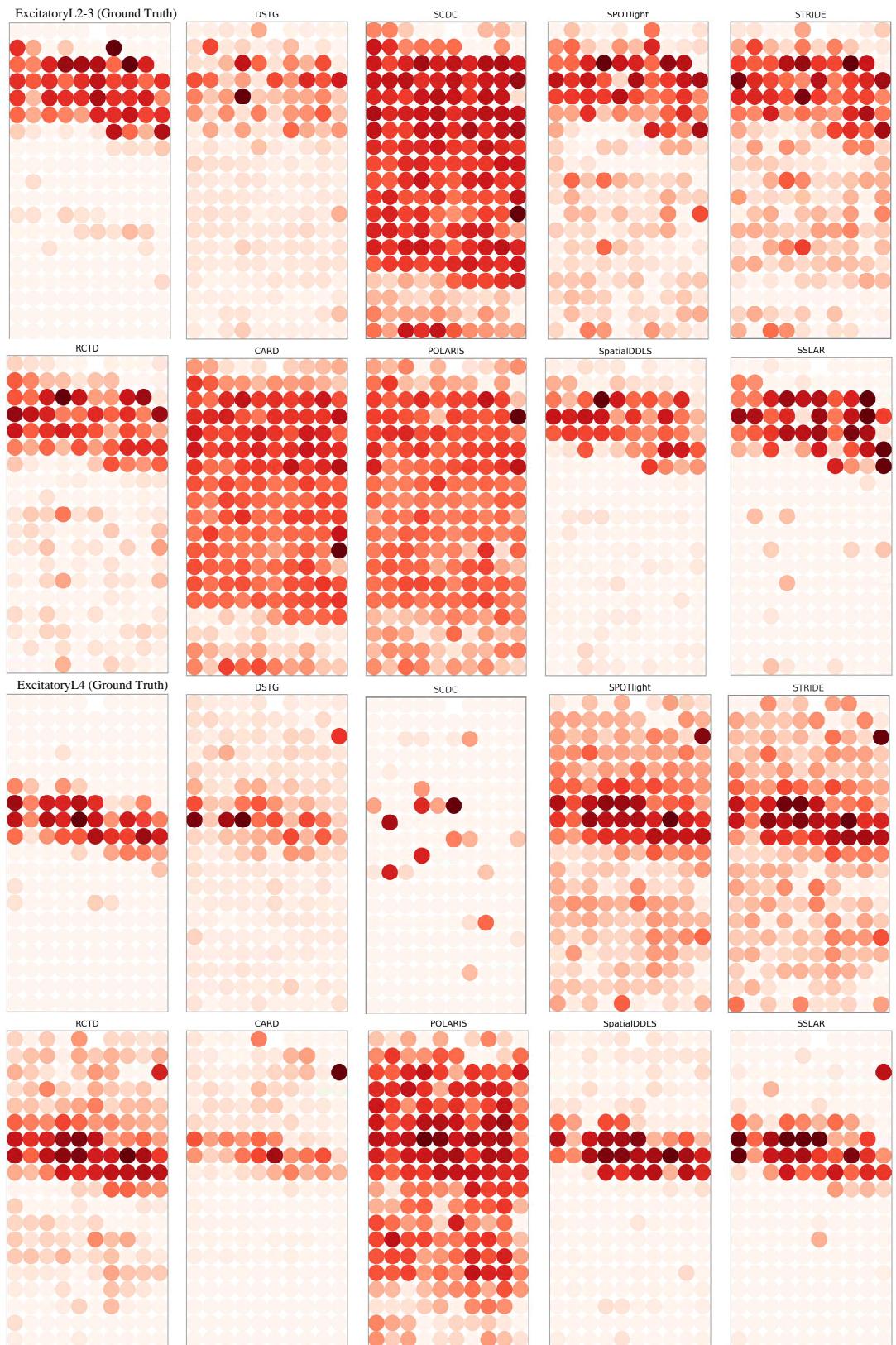


Figure S4: The proportion of two cell types (ExcitatoryL2-3 and ExcitatoryL4) in the spots simulated from mouse visual cortex (STARmap), containing the ground truth and predictions.

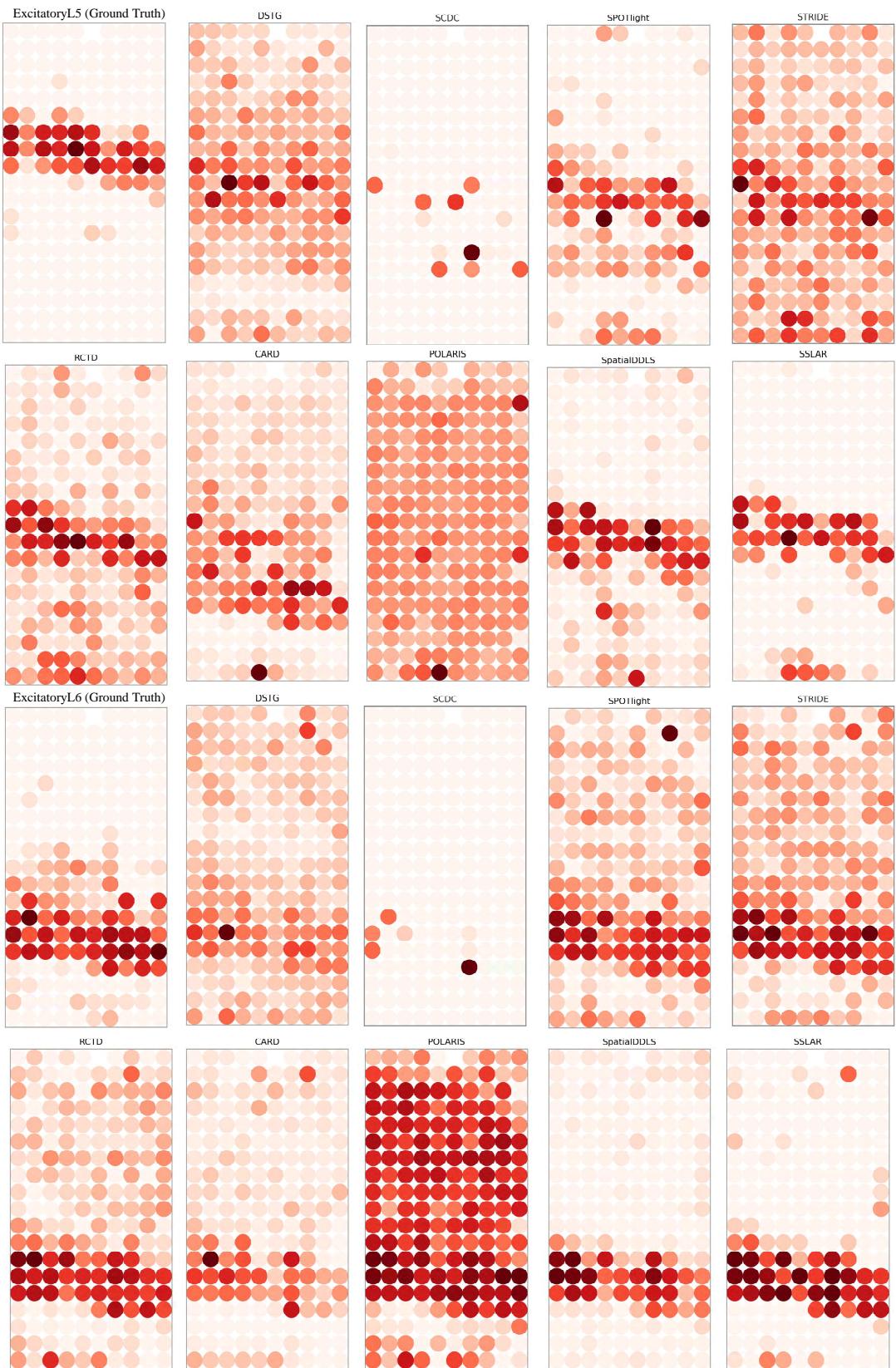


Figure S5: The proportion of two cell types (ExcitatoryL5 and ExcitatoryL6) in the spots simulated from mouse visual cortex (STARmap), containing the ground truth and predictions.

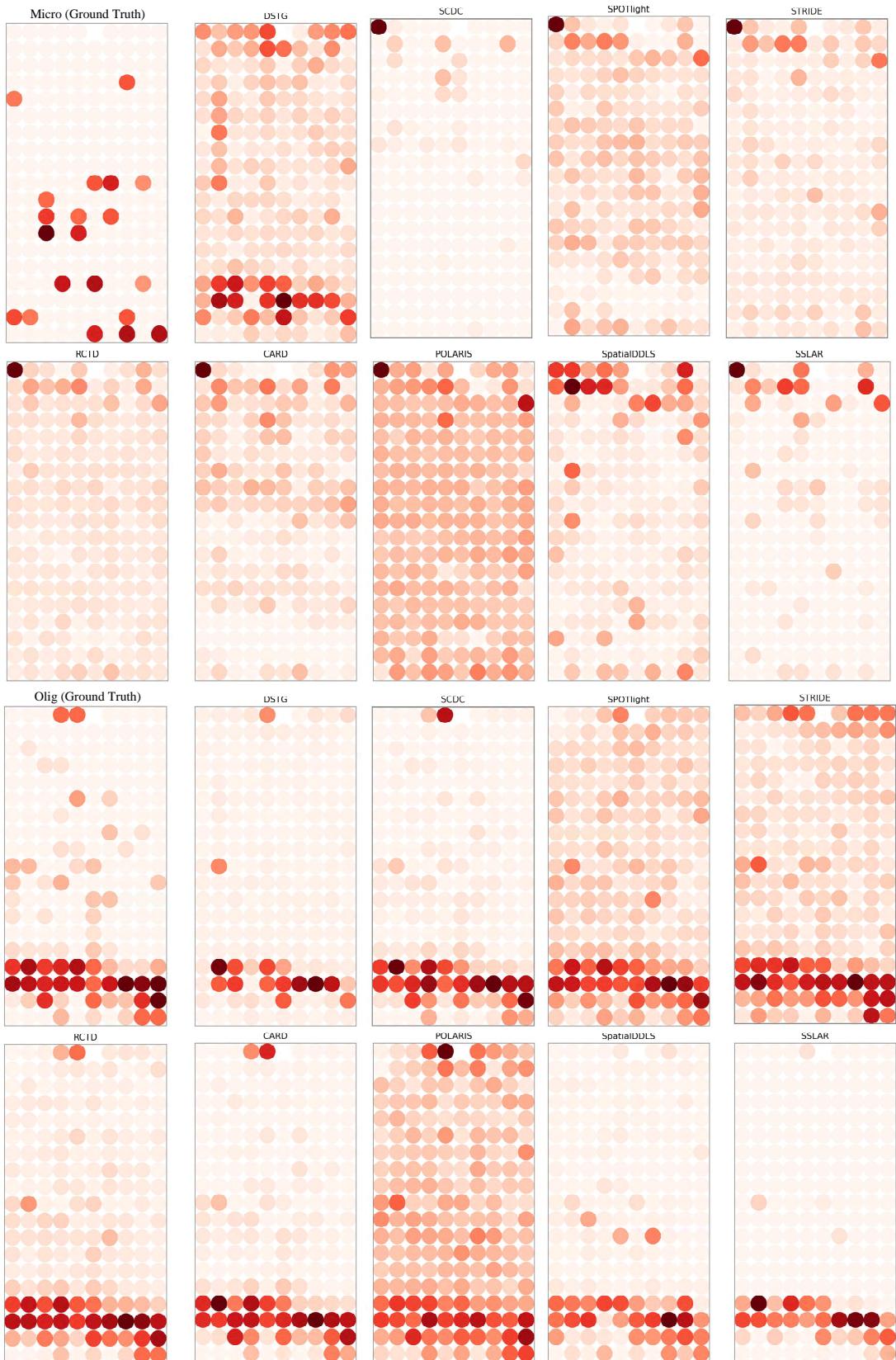


Figure S6: The proportion of two cell types (Micro and Olig) in the spots simulated from mouse visual cortex (STARmap), containing the ground truth and predictions.

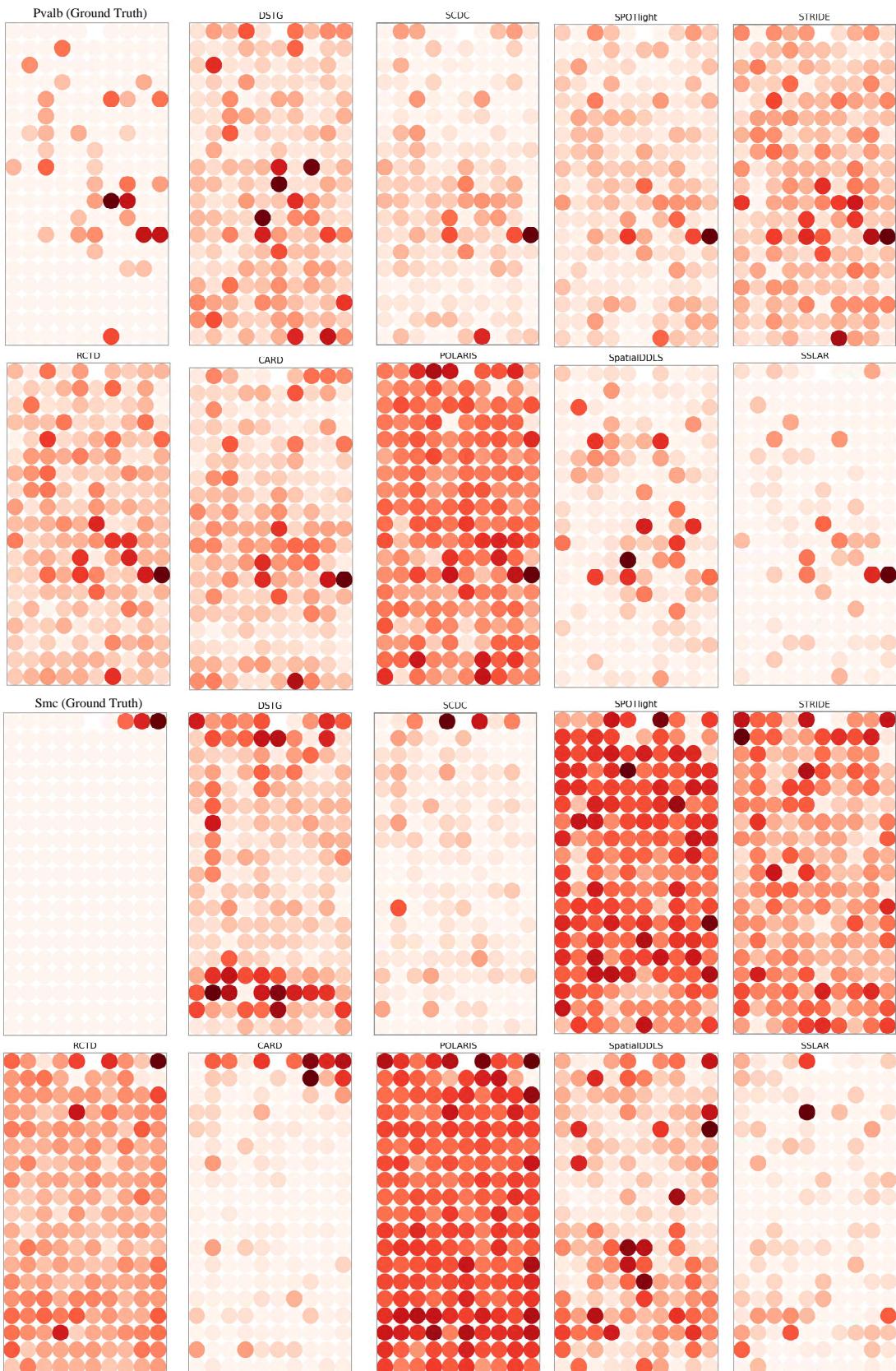


Figure S7: The proportion of two cell types (Pvalb and Smc) in the spots simulated from mouse visual cortex (STARmap), containing the ground truth and predictions.

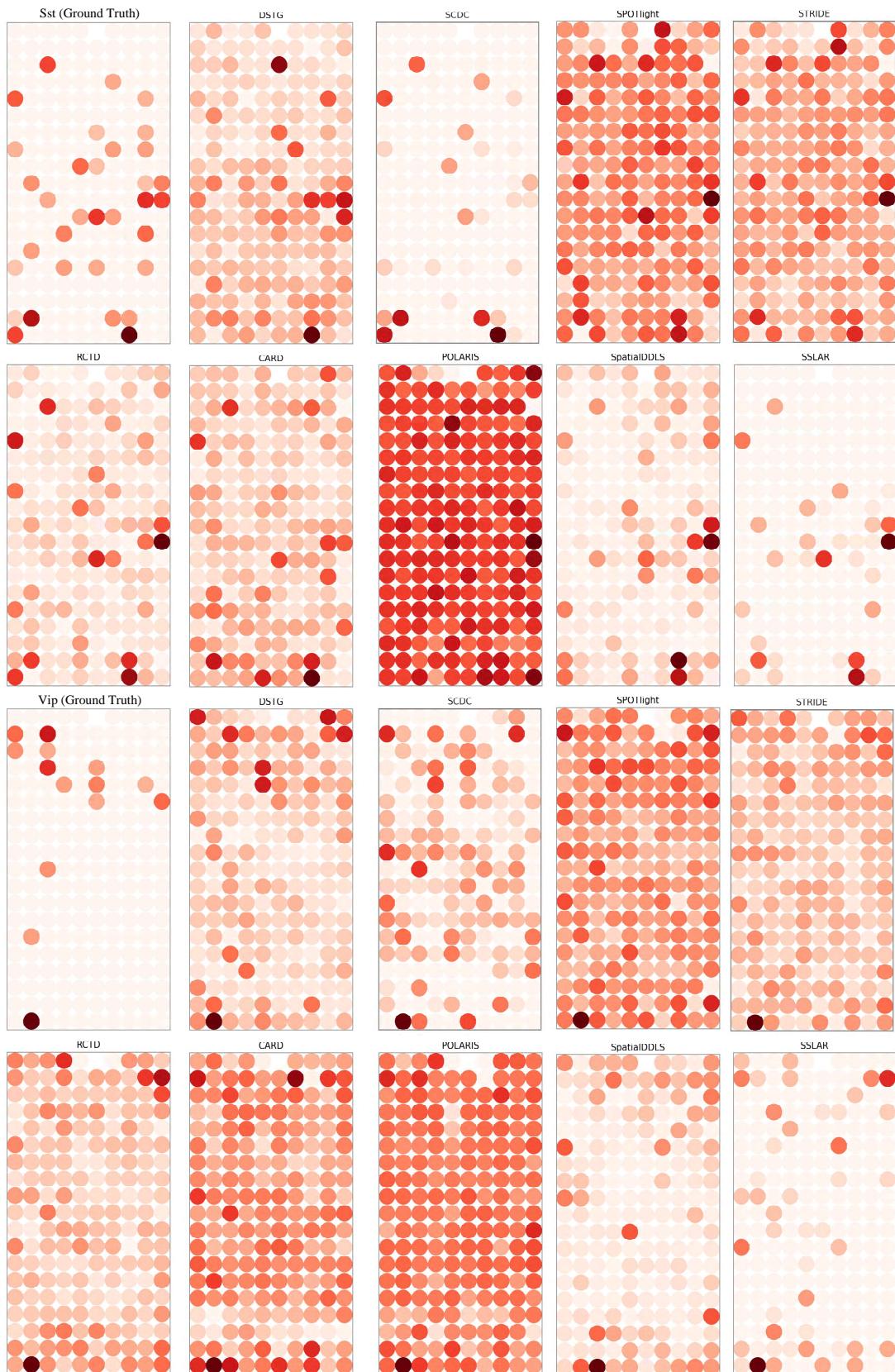


Figure S8: The proportion of two cell types (Sst and Vip) in the spots simulated from mouse visual cortex (STARmap), containing the ground truth and predictions.

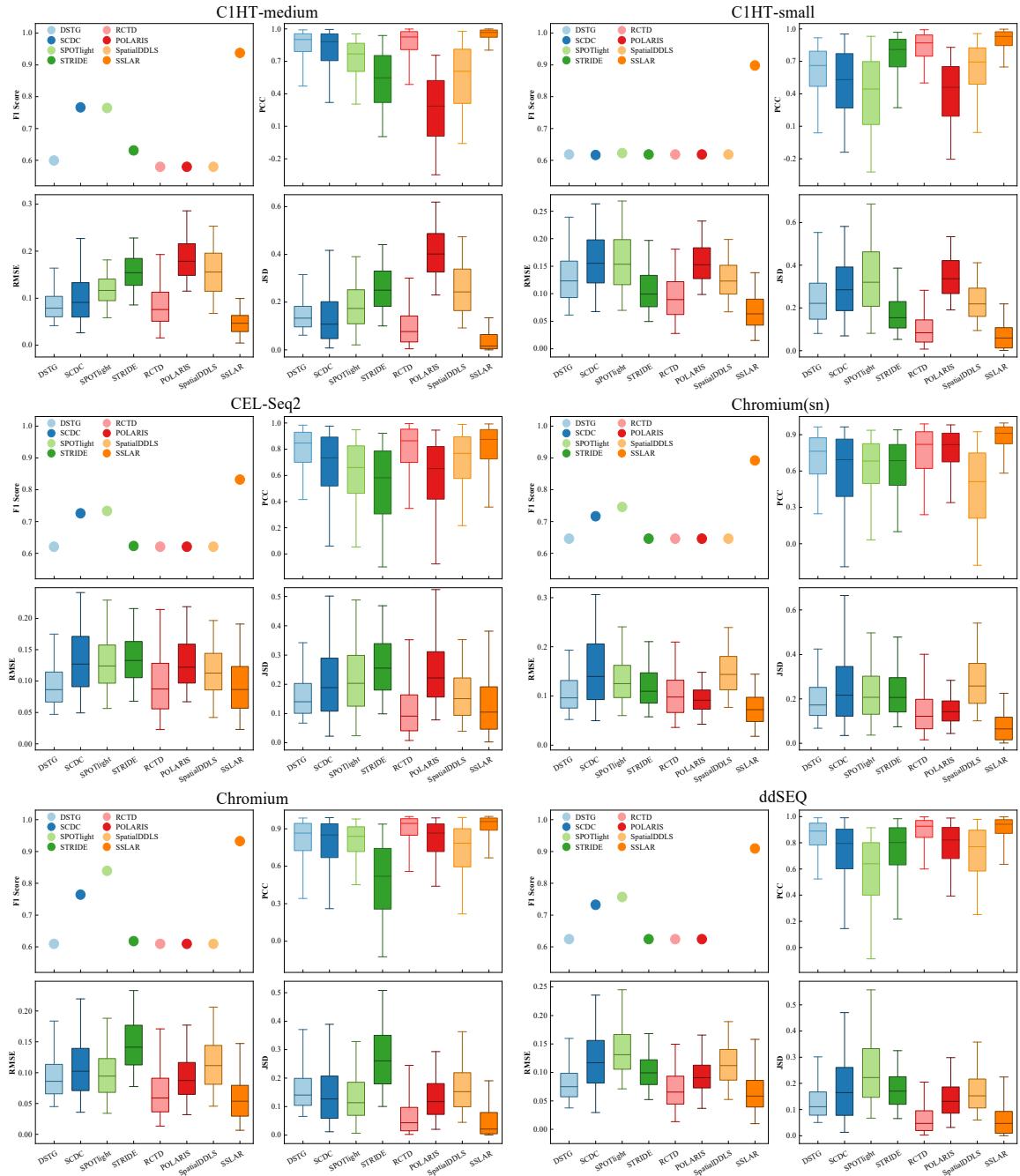


Figure S9: The SSLAR performance on six PBMC datasets from different sequencing platforms (Cel-Seq2, Chromium, Chromium(sn), C1HT-medium, C1HT-Small) on PBMC dataset.

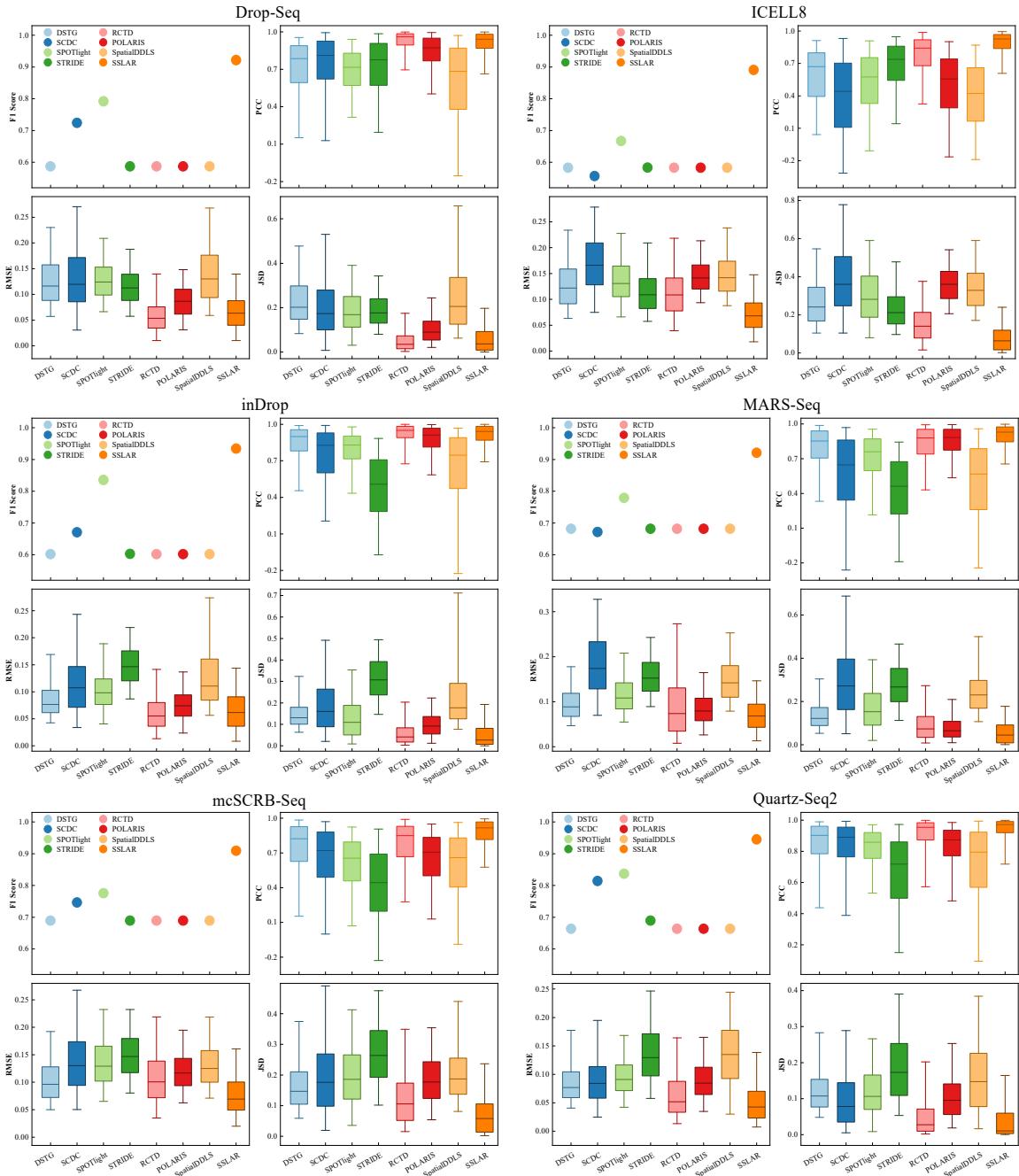


Figure S10: The SSLAR performance on other six PBMC datasets from different sequence platforms (Drop-Seq, iCELL8, inDrop, MARS-Seq, mcSCRB-Seq, Qqartz-Seq2) on PBMC dataset.

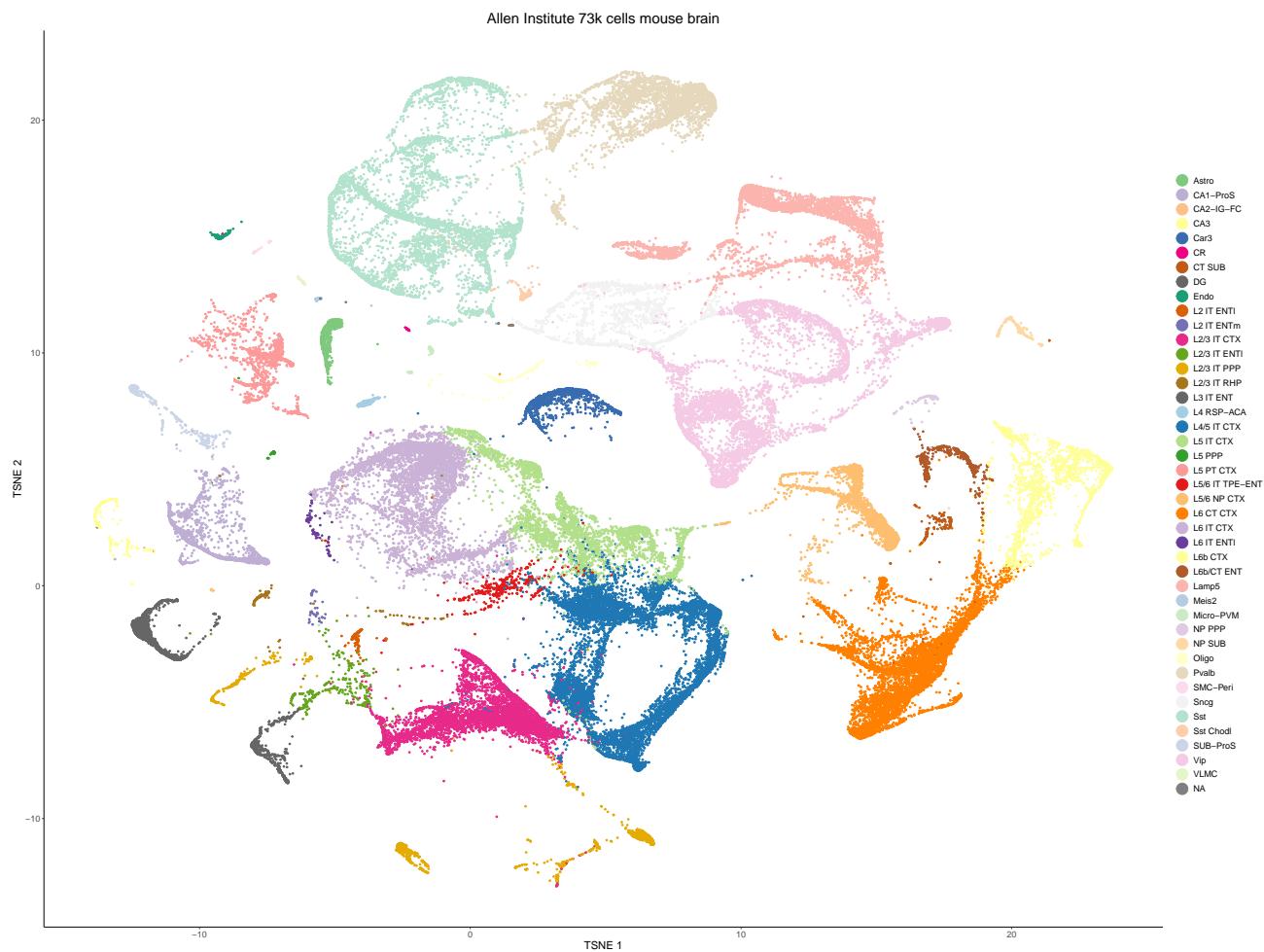


Figure S11: T-SNE projections of 73,363 cells from mouse brain scRNA-seq reference atlas provided by the Allen Institute. Cells are labeled and colored based on known 42 cell type annotations.

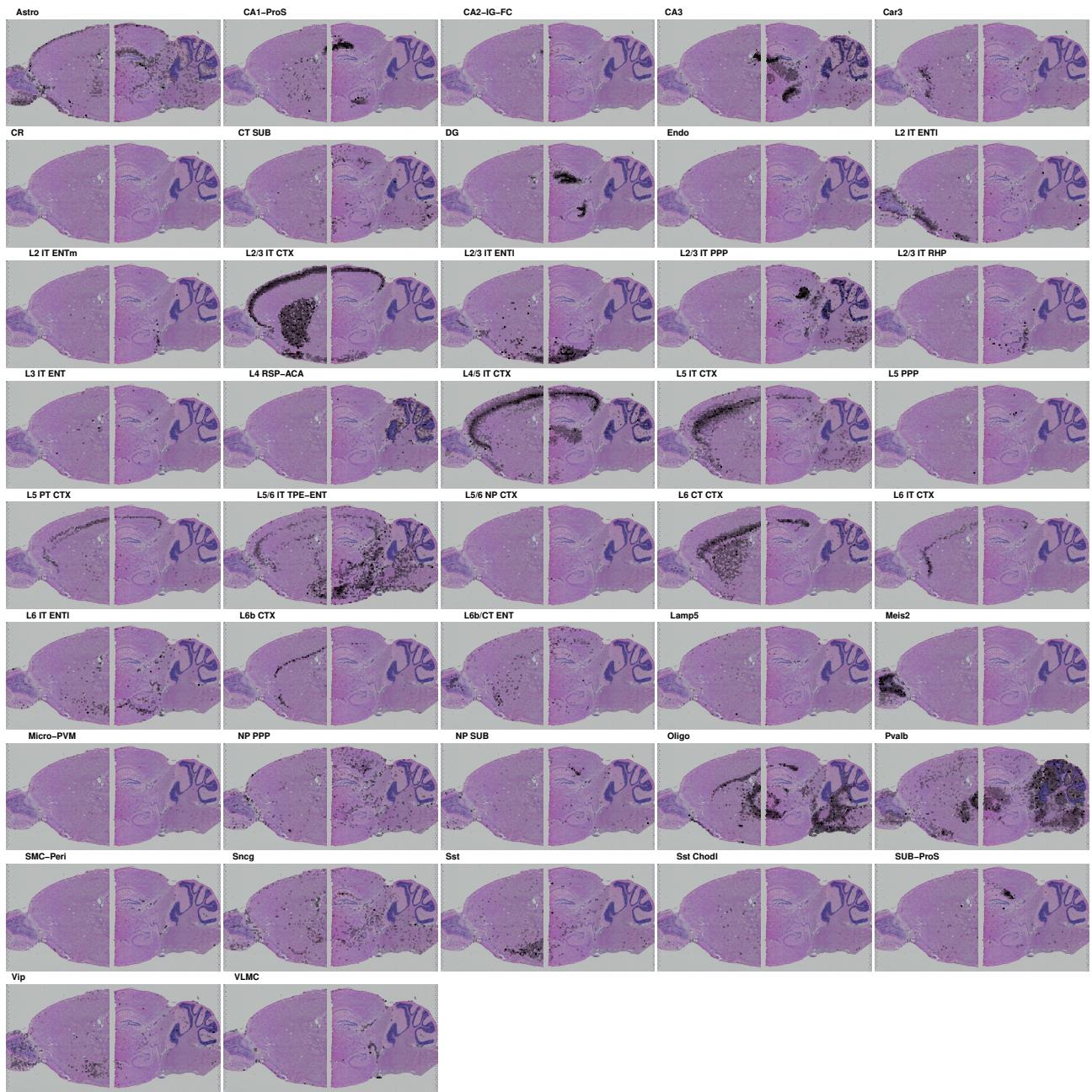


Figure S12: The SSLAR predicted proportions of cell types within each spot on mouse brain.



Figure S13: (a) The predicted proportions of cell types within each spot on the paired PDAC-A inDrops dataset.
(b) The predicted proportions of cell types within each spot on the PDAC-A immune reference dataset.

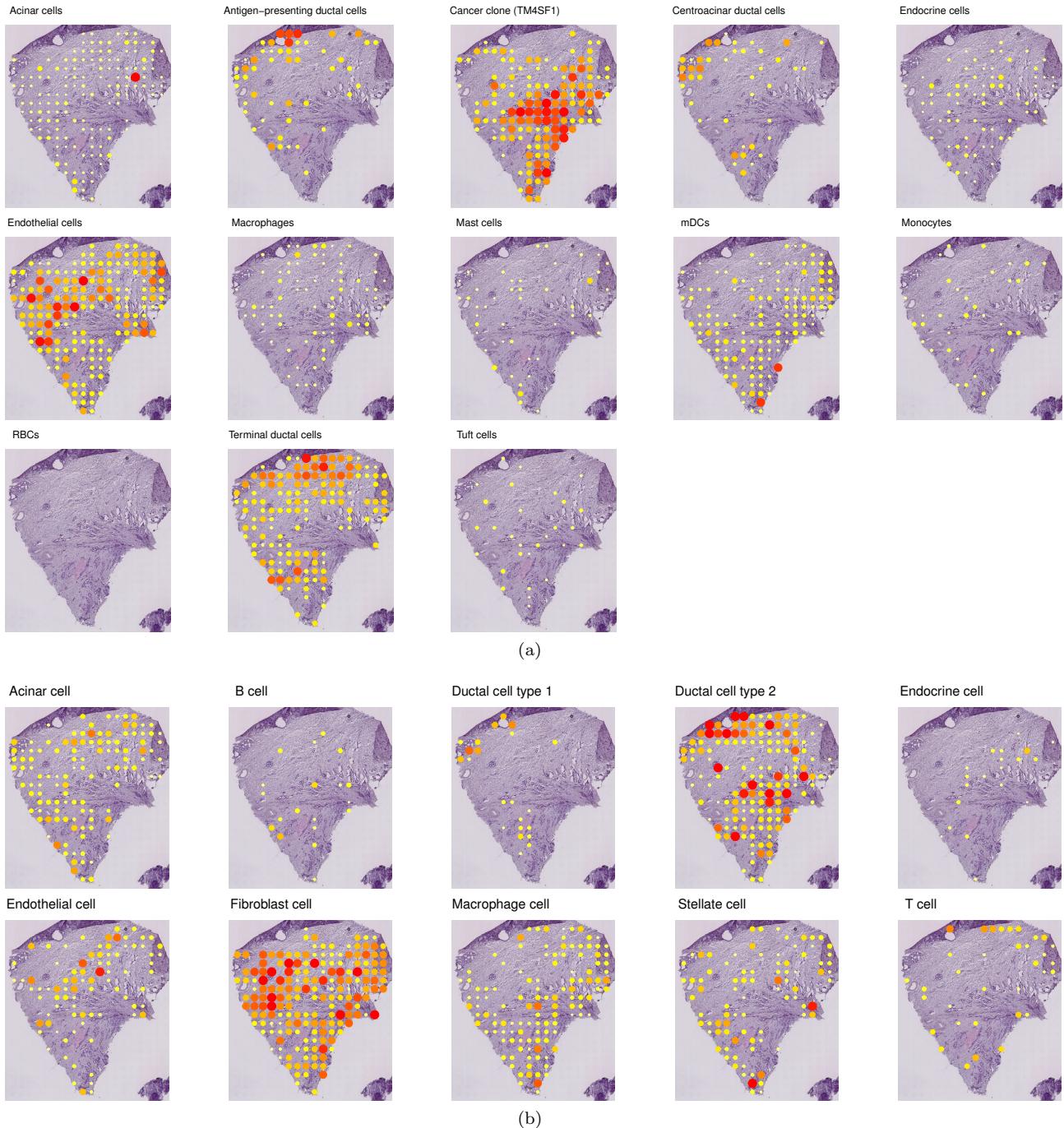


Figure S14: (a) The predicted proportions of cell types within each spot on the paired PDAC-B inDrops dataset.
(b) The predicted proportions of cell types within each spot on the PDAC-B immune reference dataset.

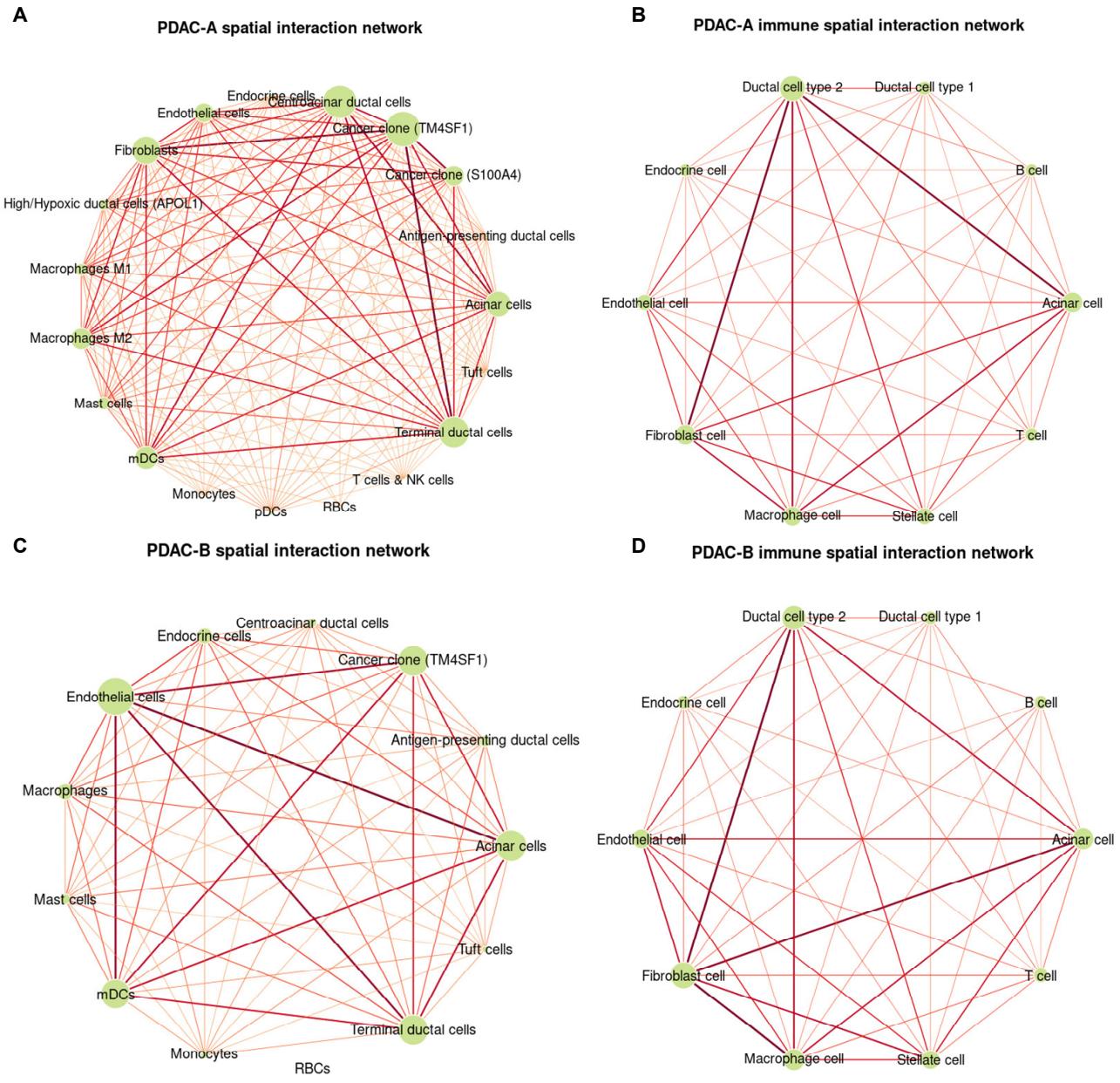


Figure S15: Spatial interaction networks characterizing the degree with which cell types co-localized together. (A) spatial interaction network on PDAC-A cell types. (B) spatial interaction work in PDAC-A immune cell types. (C) spatial interaction network on PDAC-B cell types. (D) spatial interaction work in PDAC-B. An bolder edge denotes more higher frequent of cell type co-localization.

Table S1: F1 score, PCC, RMSE, and JSD of DSTG, SCDC, SPOTlight, STRIDE, RCTD, POLARIS, SpatialDDLS, and SSLAR on synthetic PBMCM (Smart-seq2) dataset with 5 different sequencing depths

	depth	DSTG	SCDC	SPOTlight	STRIDE	RCTD	POLARIS	SpatialDDLS	SSLAR
F1 score	1,000	0.602±0.0054	0.6219±0.0068	0.7585±0.0175	0.6419±0.0153	0.602±0.0054	0.602±0.0054	0.8815±0.0028	
	5,000	0.5987±0.0048	0.7436±0.0045	0.7797±0.0089	0.6145±0.0159	0.5987±0.0048	0.5987±0.0048	0.9163±0.002	
	10,000	0.599+0.0026	0.7624±0.0042	0.7675±0.0046	0.6253±0.0133	0.599±0.0026	0.599±0.0026	0.9244±0.0033	
	20,000	0.5982+0.005	0.764±0.0049	0.7641±0.0026	0.6316±0.0133	0.5982±0.005	0.5982±0.005	0.9343±0.005	
	30,000	0.5983+0.0037	0.7628±0.0041	0.768±0.0026	0.6205±0.0023	0.5983±0.0037	0.5983±0.0037	0.9392±0.0049	
	Ave.	0.5992	0.7309	0.7676	0.6268	0.5992	0.5992	0.9191	
PCC	1,000	0.8899+0.0083	0.7639±0.0097	0.5986±0.1041	0.4749±0.0604	0.9395±0.0044	0.9451±0.0043	0.6191±0.0536	0.9352±0.0039
	5,000	0.8945+0.0323	0.8446±0.0099	0.7736±0.0151	0.2297±0.3313	0.964±0.0029	0.9329±0.0046	0.704±0.0442	0.9602±0.0026
	10,000	0.9034+0.0068	0.8767±0.007	0.7736±0.0064	0.4069±0.3033	0.9668±0.002	0.9306±0.0049	0.7086±0.0456	0.9667±0.0024
	20,000	0.8952+0.0346	0.8834±0.006	0.7719±0.005	0.5354±0.0616	0.9661±0.0012	0.9215±0.0055	0.7192±0.0356	0.9714±0.0025
	30,000	0.9036+0.0171	0.8845±0.0108	0.7736±0.0065	0.285±0.3449	0.9635±0.0025	0.9042±0.0055	0.7248±0.0281	0.9743±0.0022
	Ave.	0.8973	0.8506	0.7383	0.3864	0.96	0.9269	0.6951	0.9616
RMSE	1,000	0.0818+0.0025	0.1802±0.0041	0.1486±0.0198	0.1657±0.0087	0.0642±0.0014	0.0597±0.0016	0.1467±0.0097	0.0677±0.001
	5,000	0.0809+0.0134	0.1188±0.0022	0.1147±0.0027	0.1864±0.0363	0.0508±0.0015	0.0665±0.0016	0.1295±0.009	0.0525±0.0012
	10,000	0.0769+0.0015	0.0997±0.0023	0.116±0.0021	0.1654±0.0325	0.0491±0.0013	0.0675±0.0015	0.1273±0.0098	0.0482±0.0014
	20,000	0.0801+0.0147	0.092±0.0025	0.116±0.0017	0.1557±0.0059	0.0506±0.0011	0.0721±0.003	0.1278±0.0063	0.0445±0.0017
	30,000	0.0774+0.0061	0.0916±0.0038	0.1157±0.0011	0.1819±0.0316	0.0521±0.0014	0.0805±0.0016	0.125±0.0068	0.0424±0.0017
	Ave.	0.0794	0.1165	0.1222	0.171	0.0534	0.0693	0.1313	0.0512
JSD	1,000	0.1326+0.0059	0.2823±0.0126	0.231±0.0421	0.2941±0.0207	0.0587±0.0027	0.051±0.0022	0.2354±0.0173	0.0619±0.0024
	5,000	0.134+0.0234	0.1667±0.0046	0.162±0.0094	0.3832±0.128	0.0321±0.002	0.0569±0.0028	0.1879±0.0171	0.0285±0.0024
	10,000	0.1282+0.0034	0.1282±0.0046	0.17±0.0043	0.3071±0.1147	0.0268±0.0015	0.0569±0.0031	0.1857±0.0139	0.0193±0.002
	20,000	0.1359+0.0286	0.1143±0.0054	0.172±0.0043	0.2671±0.0196	0.0261±0.0021	0.0634±0.005	0.1736±0.0125	0.0145±0.0024
	30,000	0.129+0.0151	0.1087±0.0056	0.1722±0.0035	0.3571±0.1247	0.0259±0.0017	0.0792±0.0054	0.1673±0.0124	0.0118±0.0017
	Ave.	0.1319	0.16	0.1814	0.3217	0.0339	0.0615	0.19	0.0272

Table S2: F1 score and PCC of DSTG, SCDC, SPOTlight, STRIDE, RCTD, POLARIS, SpatialDDLS, and SSLAR on 13 synthetic datasets. PBMC 1-13 denote Cel-Seq2, Chromium, Chromium(sn), C1HT-Small, C1HT-medium, ddSeq, Drop-Seq, ICELL8, inDrop, MARS-Seq, mcSCRB-Seq, and Qqartz-Seq2.

	Dataset	DSTG	SCDC	SPOTlight	STRIDE	RCTD	POLARIS	SpatialDDLS	SSLAR
F1	PBMC1	0.5797±0.0034	0.6088±0.0048	0.6227±0.0038	0.5798±0.0033	0.5797±0.0034	0.5797±0.0034	0.5797±0.0034	0.8128±0.0072
	PBMC2	0.6184±0.0042	0.6167±0.005	0.6229±0.0071	0.6184±0.0042	0.6184±0.0042	0.6184±0.0042	0.6184±0.0042	0.8981±0.0042
	PBMC3	0.6208±0.0028	0.7259±0.0034	0.7333±0.0087	0.6231±0.0048	0.6208±0.0028	0.6208±0.0028	0.6208±0.0028	0.8319±0.0053
	PBMC4	0.6098±0.0043	0.7642±0.004	0.8391±0.0045	0.618±0.0078	0.6098±0.0043	0.6098±0.0043	0.6098±0.0043	0.9325±0.0044
	PBMC5	0.6462±0.004	0.7165±0.0035	0.7458±0.0038	0.6462±0.004	0.6462±0.004	0.6462±0.004	0.6462±0.004	0.8917±0.0033
	PBMC6	0.6244±0.0034	0.7324±0.0055	0.7569±0.011	0.6244±0.0034	0.6244±0.0034	0.6244±0.0034	0.6244±0.0034	0.9095±0.0035
	PBMC7	0.5872±0.0051	0.7241±0.0044	0.7918±0.0056	0.5873±0.0051	0.5872±0.0051	0.5872±0.0051	0.5872±0.0051	0.9217±0.0043
	PBMC8	0.5832±0.0058	0.5669±0.0042	0.667±0.0066	0.5835±0.0058	0.5832±0.0058	0.5832±0.0058	0.5832±0.0058	0.8908±0.0046
	PBMC9	0.6021±0.005	0.6711±0.0046	0.8355±0.0041	0.603±0.0043	0.6021±0.005	0.6021±0.005	0.6021±0.005	0.9342±0.0021
	PBMC10	0.6819±0.0029	0.6719±0.0041	0.7792±0.0045	0.6819±0.0029	0.6819±0.0029	0.6819±0.0029	0.6819±0.0029	0.921±0.001
	PBMC11	0.6893±0.0042	0.7463±0.0041	0.7757±0.0044	0.6893±0.0042	0.6893±0.0042	0.6893±0.0042	0.6893±0.0042	0.9093±0.0034
	PBMC12	0.6637±0.0049	0.8142±0.0039	0.8337±0.0052	0.6895±0.0051	0.6637±0.0049	0.6637±0.0049	0.6637±0.0049	0.945±0.0022
	PBMC13	0.5994±0.0046	0.7662±0.0058	0.7644±0.0062	0.631±0.0108	0.5994±0.0046	0.5994±0.0046	0.5994±0.0046	0.9373±0.0024
PCC	Ave.	0.6235	0.7012	0.7516	0.6289	0.6235	0.6235	0.6235	0.9028
	PBMC1	0.9082±0.0239	0.5135±0.0216	0.4779±0.0105	0.9072±0.0105	0.9236±0.0061	0.2817±0.0077	0.5813±0.025	0.9102±0.0067
	PBMC2	0.8276±0.0789	0.5596±0.0131	0.4364±0.0172	0.786±0.0159	0.8761±0.0043	0.4552±0.0124	0.7027±0.0262	0.9337±0.0033
	PBMC3	0.8281±0.0177	0.7519±0.0109	0.643±0.0126	0.6266±0.0305	0.8721±0.0063	0.6625±0.0148	0.7582±0.0181	0.8844±0.0083
	PBMC4	0.8715±0.0093	0.8522±0.0068	0.8476±0.0046	0.5373±0.0493	0.9437±0.0026	0.863±0.0052	0.7808±0.0086	0.9619±0.0019
	PBMC5	0.7213±0.1059	0.6635±0.0132	0.6896±0.0101	0.625±0.0675	0.8036±0.0097	0.8106±0.0084	0.5173±0.0181	0.9113±0.0043
	PBMC6	0.8887±0.0082	0.7962±0.0067	0.7095±0.0255	0.8657±0.0242	0.9248±0.0033	0.8198±0.008	0.7701±0.0136	0.9396±0.0024
	PBMC7	0.8891±0.0382	0.814±0.006	0.7262±0.0074	0.807±0.0247	0.9609±0.0017	0.8799±0.0073	0.7013±0.0214	0.9478±0.0033
	PBMC8	0.7744±0.08	0.427±0.0124	0.5606±0.0111	0.7062±0.0355	0.8234±0.0099	0.5576±0.0101	0.3992±0.0583	0.9172±0.0057
	PBMC9	0.8757±0.0523	0.8166±0.0128	0.8256±0.0064	0.4599±0.0714	0.9497±0.0036	0.9074±0.0078	0.7659±0.0265	0.9408±0.0022
	PBMC10	0.8238±0.067	0.6387±0.009	0.7559±0.0101	0.693±0.0737	0.8804±0.0031	0.8816±0.0036	0.548±0.0448	0.9302±0.0032
	PBMC11	0.7185±0.1438	0.7239±0.0146	0.6607±0.0075	0.4919±0.038	0.8494±0.0046	0.7152±0.0144	0.6783±0.0313	0.9231±0.0037
	PBMC12	0.8799±0.0801	0.8855±0.0055	0.8609±0.005	0.743±0.0324	0.9539±0.0029	0.8739±0.0064	0.7777±0.0114	0.9695±0.002
	PBMC13	0.8819±0.0523	0.8873±0.0054	0.7734±0.0043	0.5592±0.0314	0.966±0.0017	0.9161±0.0037	0.688±0.0335	0.9724±0.002
	Ave.	0.8376	0.7177	0.6898	0.6775	0.9021	0.7403	0.6668	0.9340

Table S3: RMSE and JSD of DSTG, SCDC, SPOTlight, STRIDE, RCTD, POLARIS, SpatialDDLS, and SSLAR on 13 synthetic datasets. PBMC 1-13 denote Cel-Seq2, Chromium, Chromium(sn), C1HT-Small, C1HT-medium, Drop-Seq, ddSeq, ICELL8, inDrop, MARSSeq, mcSCRB-Seq, and Qqartz-S6eq2.

	Dataset	DSTG	SCDC	SPOTlight	STRIDE	RCTD	POLARIS	SpatialDDLS	SSLAR
RMSE	PBMC1	0.0874±0.0105	0.1715±0.0017	0.1678±0.0016	0.0856±0.0034	0.0789±0.0022	0.1807±0.0017	0.1555±0.0046	0.0842±0.0024
	PBMC2	0.0919±0.0162	0.1526±0.0018	0.1549±0.0021	0.1033±0.0027	0.0884±0.0014	0.1534±0.002	0.1201±0.0042	0.0634±0.0014
	PBMC3	0.092±0.0043	0.1245±0.0017	0.1376±0.0053	0.1274±0.0045	0.0852±0.0017	0.1215±0.0021	0.1141±0.0034	0.0822±0.0024
	PBMC4	0.0839±0.0024	0.101±0.0017	0.0914±0.0016	0.1406±0.0041	0.0588±0.0012	0.0878±0.001	0.1107±0.0025	0.05±0.0017
	PBMC5	0.1057±0.0163	0.1416±0.0028	0.1248±0.0016	0.1233±0.0101	0.0996±0.0014	0.0931±0.0013	0.1454±0.0024	0.072±0.001
	PBMC6	0.0753±0.0021	0.112±0.0024	0.1212±0.0035	0.0816±0.0071	0.0654±0.0015	0.0916±9e-04	0.1078±0.0034	0.0603±9e-04
	PBMC7	0.0843±0.0122	0.1236±0.0023	0.1238±0.0016	0.1112±0.0043	0.0523±0.0012	0.0858±0.0026	0.1284±0.0037	0.0602±0.0018
	PBMC8	0.0986±0.0139	0.1666±0.0019	0.1312±0.0017	0.1114±0.0056	0.1088±0.0015	0.1404±0.0017	0.1438±0.0043	0.0684±0.0017
	PBMC9	0.0849±0.0116	0.107±0.0029	0.0994±0.0016	0.1506±0.0056	0.0563±0.0012	0.0746±0.0021	0.1122±0.0052	0.0628±0.0013
	PBMC10	0.0949±0.0132	0.1766±0.0021	0.1114±0.0019	0.1221±0.0095	0.0858±0.0017	0.0802±0.0015	0.1438±0.0044	0.0666±9e-04
	PBMC11	0.1105±0.0221	0.1296±0.002	0.1288±0.0018	0.144±0.0048	0.1002±0.0014	0.1149±0.0022	0.1239±0.0058	0.0683±0.0011
	PBMC12	0.0812±0.0196	0.0852±9e-04	0.0904±0.002	0.1253±0.0049	0.0527±0.0015	0.0847±0.0025	0.1366±0.004	0.0444±0.0012
	PBMC13	0.0852±0.019	0.091±0.0021	0.1159±0.0018	0.1496±0.0044	0.0505±0.0013	0.0739±0.0012	0.1326±0.0067	0.0442±0.0013
JSD	Ave.	0.0904	0.1294	0.1230	0.1212	0.0756	0.1064	0.1288	0.0636
	PBMC1	0.1501±0.0251	0.3051±0.0069	0.329±0.0045	0.1266±0.0058	0.078±0.0027	0.4082±0.004	0.2468±0.0088	0.0996±0.0057
	PBMC2	0.1526±0.0373	0.2769±0.0047	0.3267±0.0085	0.1699±0.008	0.0822±0.0024	0.3382±0.0052	0.214±0.0102	0.0567±0.0025
	PBMC3	0.1517±0.0091	0.1795±0.007	0.2199±0.0099	0.2419±0.0156	0.0862±0.0046	0.2149±0.0057	0.157±0.0109	0.0944±0.005
	PBMC4	0.1345±0.0064	0.1226±0.004	0.1079±0.004	0.2603±0.0132	0.0423±0.0016	0.1135±0.0031	0.1466±0.0046	0.0193±0.0025
	PBMC5	0.1959±0.0419	0.2239±0.0046	0.2038±0.0043	0.2506±0.0335	0.1291±0.006	0.1445±0.0032	0.266±0.0083	0.0669±0.0024
	PBMC6	0.1151±0.006	0.1518±0.0061	0.1955±0.0099	0.1129±0.0206	0.0478±0.0025	0.1334±0.0042	0.1472±0.0077	0.0487±0.0032
	PBMC7	0.1353±0.0261	0.1769±0.0031	0.1733±0.0044	0.185±0.0139	0.0329±0.0013	0.0951±0.0054	0.2019±0.0074	0.0309±0.0044
	PBMC8	0.1847±0.0368	0.3664±0.0059	0.2834±0.0047	0.2163±0.0116	0.1402±0.0039	0.3547±0.0048	0.3342±0.0137	0.0656±0.0032
	PBMC9	0.1444±0.0206	0.1624±0.0068	0.1117±0.004	0.3206±0.0224	0.0424±0.0023	0.0945±0.0044	0.1826±0.0103	0.0282±0.0026
	PBMC10	0.1393±0.0286	0.2759±0.0082	0.1566±0.0043	0.1933±0.0218	0.0726±0.0026	0.0653±0.003	0.2341±0.0136	0.0413±0.0028
	PBMC11	0.1749±0.0453	0.1758±0.0046	0.1855±0.0032	0.2583±0.0115	0.1024±0.0025	0.174±0.0048	0.183±0.0089	0.0528±0.0025
	PBMC12	0.112±0.0373	0.0794±0.0034	0.1038±0.0048	0.1683±0.0144	0.0276±0.0015	0.0932±0.0034	0.1512±0.0045	0.0113±0.0011
	PBMC13	0.1422±0.0351	0.1112±0.0052	0.1731±0.0054	0.2557±0.0114	0.0258±0.0015	0.0664±0.0022	0.1823±0.0131	0.0136±0.0012
	Ave.	0.1487	0.2006	0.1977	0.2123	0.0700	0.1766	0.2036	0.0484

Table S4: Key Resource Table

RESOURCE	SOURCE	IDENTIFIER OR LINK
Deposited data (sc/sn-RNAseq)		
PBMC	Gene Expression Omnibus	GSE133549
HNSCC	Gene Expression Omnibus	GSE103322
melanoma	Gene Expression Omnibus	GSE72056
pancreas	Gene Expression Omnibus	GSE85241
kidney tumor	Github	https://github.com/xuebaliang/scziDesk/tree/master/dataset/Young
mouse primary visual cortex	Allen Institute for Brain Science	https://portal.brain-map.org/atlas-es-and-data/rnaseq/mouse-v1-and-alma-smart-seq
mouse brain	Gene Expression Omnibus	GSE185862
PDAC-A	Gene Expression Omnibus	GSM3036909, GSM3036910, GSM3405527, GSM3405528, GSM3405529, GSM3405530
PDAC-B	Gene Expression Omnibus	GSM3405531, GSM3405532, GSM3405533
pancreatic immune	Genome Sequence Archive	PRJCA001063
Deposited data (spatial transcriptomics)		
mouse cortex	Github	https://github.com/CaiGroup/seqFISH-PLUS
mouse visual cortex	STARmap	https://starmapresources.net/data
mouse brain posterior	10X Genomics	https://www.10xgenomics.com/resources/datasets
mouse brain anterior	10X Genomics	https://www.10xgenomics.com/resources/datasets
PDAC-A	Gene Expression Omnibus	GSM3036911
PDAC-B	Gene Expression Omnibus	GSM3405534
Software and algorithms		
Seurat	R Satija, et al.	https://github.com/satijalab/seurat
STRIDE	D Sun, et al.	https://github.com/wanglabtongji/STRIDE
DSTG	Q Song, et al.	https://github.com/Su-informatics-lab/DSTG
RCTD	D M. Cable, et al.	https://github.com/dmcable/RCTD
SpatialDDLS	D Mananes, et al.	https://github.com/diegommcc/SpatialDDLS
SCDC	M Dong, et al.	https://github.com/meichendong/SCDC/
SPOTlight	M Elosua, et al.	https://github.com/MarcElosua/SPOTlight
POLARIS	J Chen, et al.	https://zenodo.org/records/7302022
CARD	Y Ma, et al.	https://github.com/YMa-lab/CARD
SSLAR	This paper	https://github.com/plhhnu/SSLAR