

Supplementary materials

For the paper “**Combining Neural Networks, UMAP, and DBM Clustering to Identify Cell Populations Accurately, Quickly and Easily in Mass and Fluorescence Cytometry**”

1. Datasets Description

To enable an undistracted bioinformatics focus, we evaluate our pipeline using the manual gating and datasets shown in 9 peer-reviewed biology publications. Five of these datasets are collected on conventional cytometers, three on mass cytometers, and one on a spectral cytometer.

The first five datasets listed below are [OMIP protocols](#), which are special peer-reviewed Cytometry Part A publication-type optimized multicolor panels for flow cytometry.

1. [OMIP-044](#)⁽¹⁰⁾
 - a. Standard 28-color protocol for the human dendritic cell compartment on a conventional cytometer.
 - b. [Manual gating](#) uses 14 markers to define 13 cell populations.
 - c. LDA and MLP test with 2-fold cross validation on 1,966,719 x 1,966,718 training x test set cells. We use 2 of their 6 samples which each contain 2.5 million cells
 - i. samples_AllCells A5807 part1_030.fcs
 - ii. samples_FMO1_CD40_033
2. [OMIP-047](#)⁽¹¹⁾
 - a. Standard 16 color protocol that does -dimensional phenotypic characterization of B cells on a conventional cytometer.
 - b. [Manual gating](#) uses 9 markers to define 8 cell populations..
 - c. LDA and MLP test with 5-fold cross validation 5x1, 4x2, 4x2 and 5x1 training x test samples.
We use 6 of their 7 samples omitting **150120_AK156 070309 late chronic_031.fcs**
3. [OMIP-058](#)⁽¹²⁾
 - a. Standard 28 color protocol that characterizes NKT, NK, unconventional. and conventional T Cells on a conventional cytometer.
 - b. [Manual gating](#) uses 17 markers to define 35 cell populations.

- c. LDA and MLP test with 2-fold cross validation of 394,000x3904,000 training x test cells.

We use all 2 of their samples which each contain approximately 1 million cells.

4. [OMIP-069](#) ⁽¹³⁾

- a. Standard 40 color standard protocol for deep immunophenotyping in human peripheral blood on a spectral cytometer.
- b. [Manual gating](#) uses 26 markers to define 46 cell populations.
- c. LDA and MLP test with 3-fold cross validation, 3x1, 2x2 and 3x1 training x test samples.

We use all 4 of their samples that each contain approximately 640,000 cells

5. [OMIP-077](#) ⁽¹⁴⁾

- a. Standard 12 color protocol for defining principal human leukocyte populations on a conventional cytometer.
- b. [Manual gating](#) uses 14 markers to define 14 cell populations
- c. LDA and MLP test with 4-fold cross validation, 3x1, 3x1, 3x1 and 3x1 training x test samples.

We use all 4 of their samples which contain 7, 3, 1.4 and 2.3 million cells

6. [ESHGHI](#) ⁽³⁵⁾

- a. Study of quantitative differences with manual and t-SNE populations from different sites on a mass cytometer
- b. [Manual gating](#) uses 27 markers to define 29 cell populations.
- c. LDA and MLP test with 5-fold cross validation of 392,373x98,093 training x test cells.

We use their 1 sample of a half million cells merged from 10 samples.

7. [GHOSN](#) ⁽¹⁶⁾

- a. Study of macrophages and B cells in the peritoneal cavity of 3 strains of mice each stained with a slightly different reagent cocktail on a conventional cytometer.
- b. [Manual gating](#) uses 9 markers to define 13 cell populations.
- c. LDA and MLP test with 2-fold cross validation, 2x1 and 1x2 training x test samples.

We use 3 of their 4 samples (C57 and BALB/c strain) which each contain 200,000 cells

8. [LEIPOLD](#) ⁽³⁶⁾

- a. Study comparing CyTOF assays from 6 sites on a mass cytometer.
- b. Manual gating uses 15 markers to define 18 cell populations.
- c. LDA and MLP test with 4-fold cross validation, 5x1, 4x2, 4x2, 5x1 training x test samples.

We use all 6 of their samples which range in size from 29,713 to 112,843 cells.

9. PANORAMA ⁽¹⁵⁾

- a. An often-cited dataset collected on the mass cytometer. It is frequently used for testing gating methods. The publication that introduces the X-Shift classifier, which explores this dataset,
- b. Manual gating uses 25 markers to define 24 cell populations.
- c. LDA and MLP test with 5-fold cross validation of 8x2 training x test samples.

We use all 10 of their samples which range in size from 75,513 to 95,087 cells.

2. Performance metrics

- **F1-score** measures population overlap via the harmonic mean of precision and recall⁽⁴⁸⁾. Since FlowCAP⁽¹⁹⁾, most flow informatics publications assess gating accuracy using the F1-score.
- **Jaccard index (JI)** measures population overlap more simply by computing the fraction of cells in both populations⁽⁴⁹⁾. We compute two indices.
 - **JI 100%** looks at all members of populations. This is not used in all testing scenarios.
 - **JI 80% (AKA Central similarity or CS)** looks at the central dense region of combined populations. We remove the 20% of the cells in the union of the populations that are farthest from the union's mean using Mahalanobis distance. This definition is based on a key characteristic of phenotypes: their event measurements show a marked central tendency in all dimensions, indicating that they are "atomic", i.e., not splittable in all tested dimensions.
- **Earth mover's distance (EMD)** compares the mass+distance similarity of populations by computing the cost to move them together, i.e., to join them, as though they were separate piles of earth in high-dimensional space⁽⁵¹⁾. EMD is not an overlap metric. Thus, the populations can come from different samples within the same high-

dimensional coordinates. We use a fast EMD algorithm that we developed previously^(40, 25).

3. Testing Round 1

3.1. Testing MLP and LDA

In our first round of testing with LDA and MLP the

- Data used for both training and predicting has unclassified cells removed and thus contains only members of the *same cell populations*. This is the data preparation pattern practiced by Abdelaal et al ⁽²⁾. We confirmed this by inspecting both the code as well as the datasets for which the LDA publication provides a link (<https://github.com/abdelaal/CyTOF-Linear-Classifer>).

The sample files given for the PANORAMA, AML and BMMC datasets lack unlabelled (unclassified) cells while their dataset-specific code explicitly removes unclassified cells from the sample files of MultiCenter, HMIS-1 and HIMS-2.

- For MultiCenter samples the numeric label is 0.
- For HMIS-1 and HMIS-2 the string label is “Discard”. For these 2 datasets only there is a miscellaneous class labeled “Others”.

The code when run for all 6 datasets gets the same F1-scores shown in their publication. Thus to compare directly with their processing this round prepares each sample in all of our 9 datasets by removing the unlabeled cells for both training and predicting.

We generalize Abdelaal’s multiple dataset-specific scripts into one generic one and then plug in our MLP alongside their LDA. As a quality control check we rerun LDA with these modified scripts on the 6 CyTOF datasets described in their publication in order to reproduce their published results and thus confirm that our changes have not introduced problems. The results of this quality control check are in our [supplementary materials](#).

- Original and modified scripts do 1-to-1 matching using the MATLAB confusion matrix from which all 3 match-strength metrics are then computed (F1-scores, Central similarity and EMD).

3.2. Testing FlowSOM and PhenoGraph

With FlowSOM and PhenoGraph however the

- Data used contains both unclassified and classified cells since we call these algorithms

from FlowJo plugins which operate on a position of the gating hierarchy

- Matching is done many-to-many using our QFMatch. This means either automatically gated populations (FlowSOM and PhenoGraph) or manually gated populations are merged in order to obtain the best F1-score: one or more manually gated populations could match best with one or more automatic gated populations.

3.3. Overall results

The overall accuracy of each classifier in matching 197 known cell populations from 9 different published datasets is

<i>Performance metric</i> Classifier	<i>F1-score</i>		<i>Central Similarity</i>		<i>EMD</i>	
	<i>Median</i>	<i>Mean</i>	<i>Median</i>	<i>Mean</i>	<i>Median</i>	<i>Mean</i>
MLP	0.99	0.95	0.99	0.94	1	0.98
FlowSOM	0.87	0.74	0.86	0.70	0.96	0.87
LDA	0.88	0.81	0.83	0.76	0.96	0.93
PhenoGraph	0.87	0.72	0.84	0.66	0.95	0.87

3.4. Results for datasets

Dataset	MLP			FlowSOM			LDA			Phenograph		
	<i>F1-score</i>	<i>Central similarity</i>	<i>EMD</i>	<i>F1-score</i>	<i>Central similarity</i>	<i>EMD</i>	<i>F1-score</i>	<i>Central similarity</i>	<i>EMD</i>	<i>F1-score</i>	<i>Central similarity</i>	<i>EMD</i>
OMIP-044 ¹⁰ 13 cell populations defined with 14 markers collected by a conventional cytometer	.99 1	1 1	1 1	.97 .88	.98 .86	.98 .94	.93 .85	.90 .81	.98 .94	.92 .81	.92 .78	.96 .93
OMIP-047 ¹¹ 8 cell populations defined with 9 markers collected by a conventional cytometer	1 1	1 1	1 1	.87 .86	.83 .81	.96 .95	.96 .96	.95 .96	.98 .98	.90 .83	.87 .77	.97 .93
OMIP-058 ¹² 35 cell populations defined with 17 markers collected by a conventional cytometer	.99 .97	.99 .97	1 .99	.80 .60	.73 .55	.92 .77	.84 .76	.81 .70	.95 .93	.82 .63	.77 .58	.93 .77
OMIP-069 ¹³ 43 cell populations defined with 26 markers collected by a spectral cytometer	.98 .93	.97 .90	.99 .98	.51 .48	.37 .40	.83 .74	.83 .76	.73 .68	.95 .92	.55 .52	.41 .43	.86 .81
OMIP-077 ¹⁴	.97	.97	.99	.96	.95	.98	.72	.62	.88	.96	.96	.99

14 cell populations defined with 14 markers collected by a conventional cytometer	.89	.85	.96	.92	.92	.99	.62	.57	.87	.86	.86	.94
ESHGHI ³⁵ 29 cell populations defined with 27 parameters collected by a mass cytometer	1 .99	1 .99	1 1	.94 .84	.95 .82	.96 .93	.90 .86	.86 .82	.97 .95	.88 .74	.84 .71	.95 .87
GHOSN ¹⁶ 13 cell populations defined with 9 markers collected by a conventional cytometer	.99 .94	.99 .92	1 .98	.93 .83	.92 .82	.96 .88	.92 .89	.93 .85	.96 .94	.87 .79	.89 .74	.95 .92
LEIPOLD ³⁶ 18 cell populations defined with 15 markers collected by a mass cytometer	.99 .96	.99 .95	1 .99	.87 .72	.86 .70	.95 .86	.86 .78	.80 .73	.96 .93	.84 .68	.80 .64	.93 .81
PANORAMA ¹⁵ 24 cell populations defined with 25 markers collected by a mass cytometer	.97 .88	.89 .75	.99 .94	.56 .53	.41 .44	.88 .78	.88 .79	.83 .74	.95 .91	.56 .59	.37 .48	.89 .85

Columns

Rows

Legend

- F1-score=overlap measured by harmonic mean of percision + recall (AKA *F measure*).
- CS=overlap in central core region.
- EMD=earth mover's distance

Coloring is based on ranking by *F1-Score mean*

<i>Narrow lead over next</i>	1st	2nd	3rd	Last
<i>Wide lead over next</i>	1st	2nd	3rd	Nothing is next

Ties get same ranked color....

Median minus mean size is **emphasized** pos/neg.

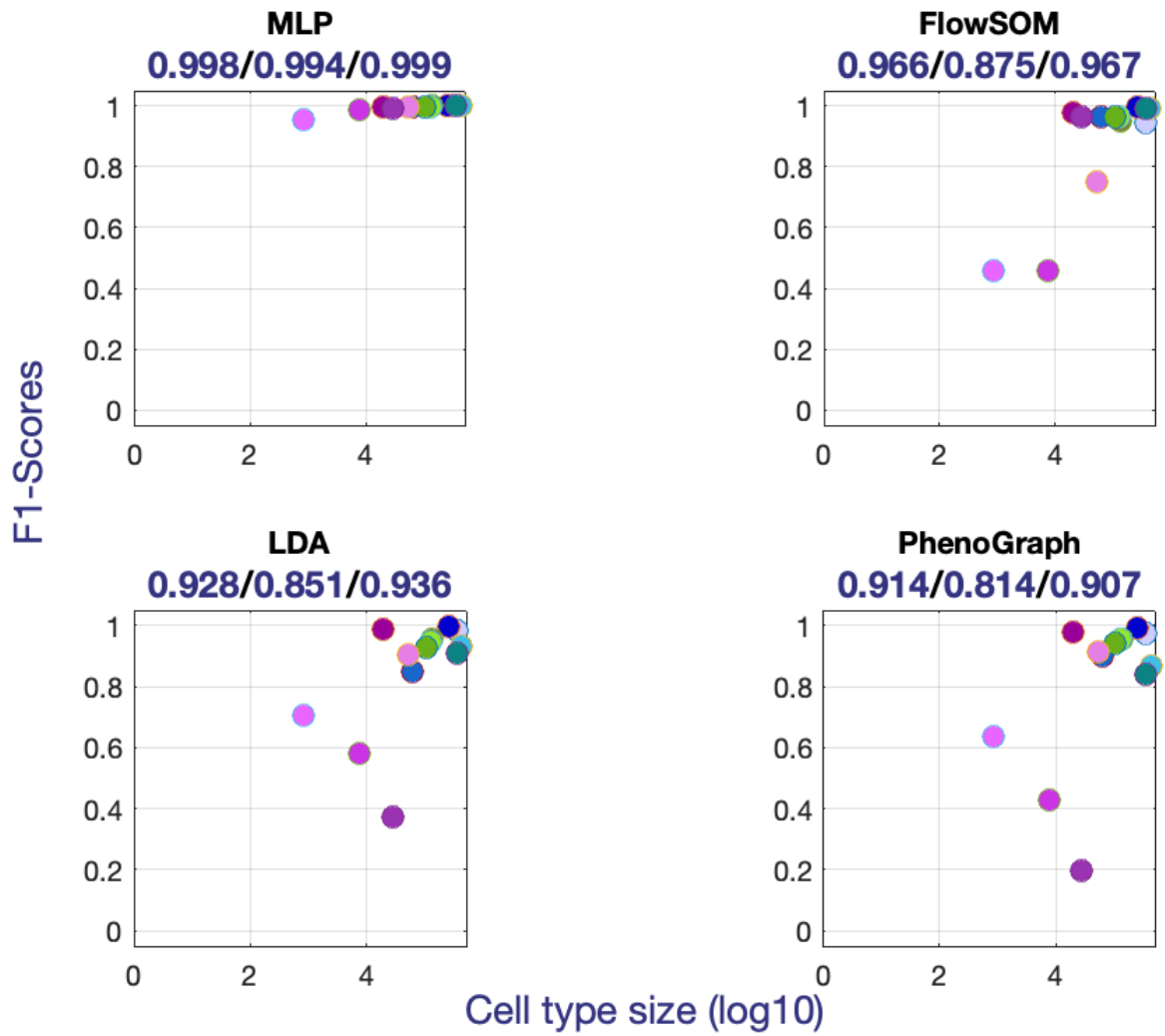
3.5. Results for populations

3.5.1. OMIP-044

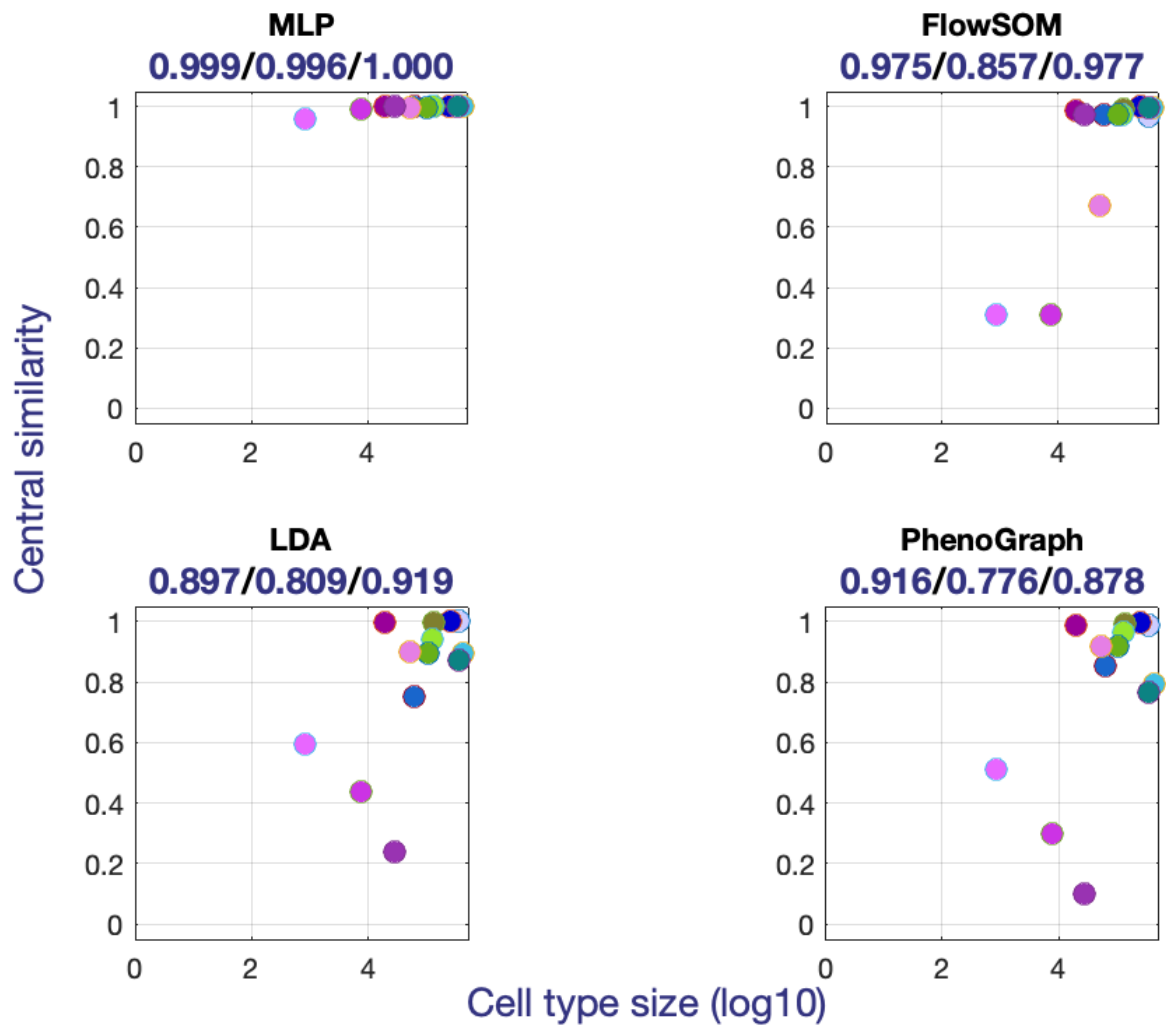
2 samples, 1x1 training x test samples,
13 cell types, 14 markers.

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP 	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
●	CD14+	18%	1	0.944	0.984	0.974	1	0.970	1	0.989	1	0.954	0.984	0.990
●	CD19+	13%	1	0.995	0.997	0.994	1	0.999	1	0.999	1	0.998	0.999	0.998
●	naive CD4+	22%	1	0.990	0.931	0.869	1	0.999	0.896	0.792	1	0.995	0.984	0.970
●	not naive CD4+	18%	1	0.990	0.910	0.840	1	0.999	0.871	0.765	1	0.995	0.977	0.952
●	CD56+ NK	7%	0.999	0.952	0.955	0.954	1	0.994	0.997	0.994	1	0.943	0.941	0.939
●	naive CD8+	6.5%	0.999	0.966	0.948	0.954	0.999	0.975	0.940	0.962	1	0.983	0.988	0.985
●	DN	3.2%	0.998	0.966	0.851	0.900	1	0.975	0.752	0.854	1	0.983	0.873	0.950
●	not naive CD8+	5.4%	0.998	0.966	0.928	0.939	0.997	0.975	0.897	0.916	1	0.983	0.977	0.986
●	CD123+ pDC	1%	0.997	0.978	0.987	0.981	0.999	0.986	0.999	0.989	0.997	0.993	0.993	0.992
●	DN DCs	2.7%	0.996	0.750	0.906	0.914	0.999	0.672	0.900	0.916	0.999	0.825	0.949	0.954
●	DCs-	1.4%	0.993	0.966	0.375	0.197	0.999	0.975	0.238	0.102	0.998	0.983	0.847	0.700
●	CD1c DCs	0.39%	0.988	0.458	0.582	0.426	0.991	0.311	0.438	0.298	0.998	0.788	0.813	0.749
●	CD141+DCs	0.04%	0.955	0.458	0.703	0.637	0.959	0.311	0.595	0.510	0.990	0.788	0.842	0.838
Median			0.998	0.966	0.928	0.914	0.999	0.975	0.897	0.916	1	0.983	0.977	0.954
Mean			0.994	0.875	0.851	0.814	0.996	0.857	0.809	0.776	0.999	0.939	0.936	0.923

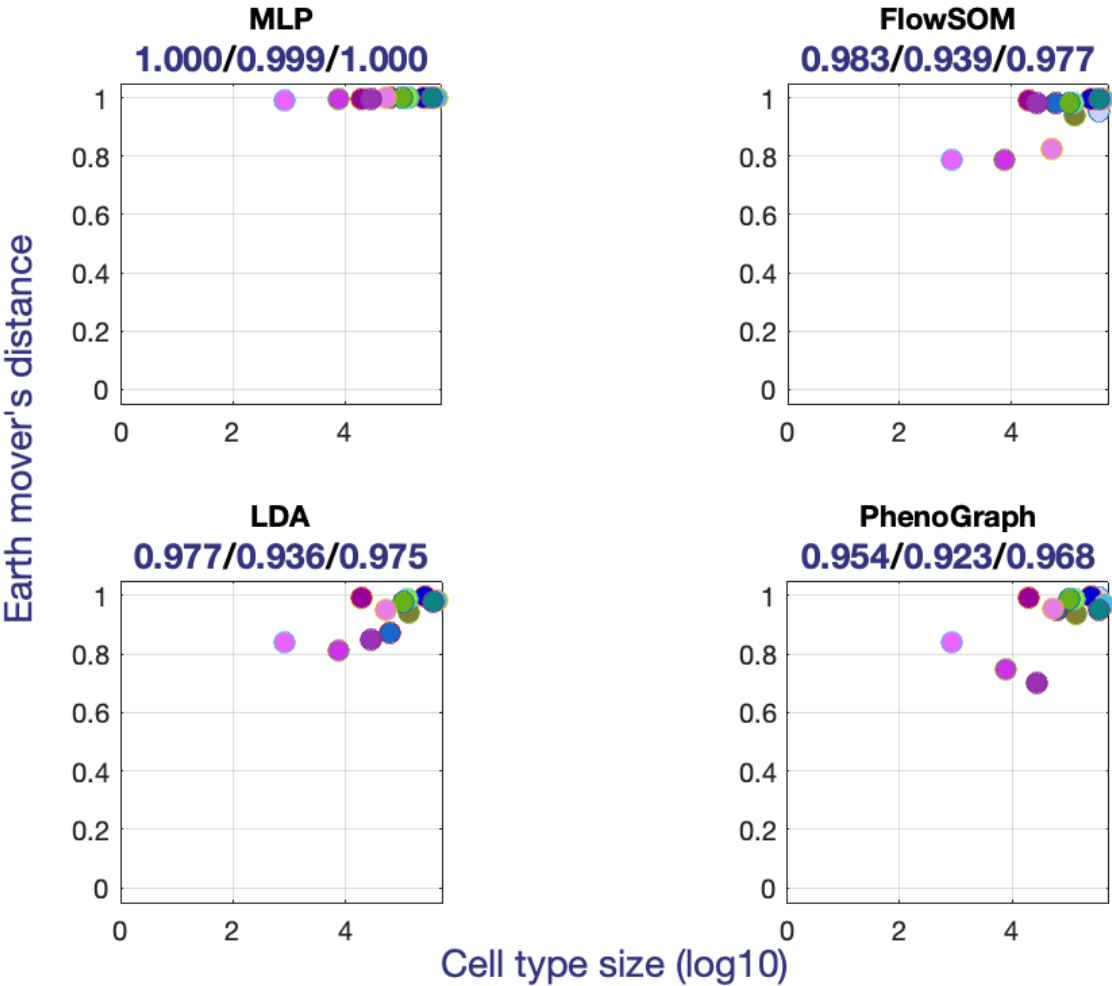
OMIP-044 F1-Scores median/mean/weighted



OMIP-044 Central similarity median/mean/weighted



OMIP-044 Earth mover's distance median/mean/weighted



3.5.1.1. Merged matches

With FlowSOM QFMatch finds 5 of 8 matches where merging multiple manual or FlowSOM gated populations obtains a higher F1-score. The 2nd, 4th and 8th ranked match merges multiple manually gated populations to match 1 FlowSOM gated population. The 1st and 3rd ranked matches merge 2 FlowSOM gated populations to match 1 manually gated population.

MATCH sets: training=all 13 matched!, test=10/13 (3 NEW!)									
Rank		#	Subset (class) name	Mat-ches	Similarity (QFMatch)	% Overlap (F-measure)	Train-ing set?	Freq.	
4	•	6	DCs-	5	98.3%	96.6%	yes	0.8%	1
4	•	10	naive CD8+	5	98.3%	96.6%	yes	6.7%	1
4	•	12	DN	5	98.3%	96.6%	yes	2.7%	5
4	•	13	[not naive CD8+]	5	98.3%	96.6%	yes	5.4%	1
4	•	18	FlowSOM.CD45+ live.Pop3	5	98.3%	96.6%	no	15.3%	3
1	•	4	CD19+	3	99.8%	99.5%	yes	12.9%	2
1	•	16	FlowSOM.CD45+ live.Pop0	3	99.8%	99.5%	no	12.9%	2
1	•	22	FlowSOM.CD45+ live.Pop1	3	99.8%	99.5%	no	0%	
2	•	7	naive CD4+	3	99.5%	99%	yes	23.4%	4
2	•	8	[not naive CD4+]	3	99.5%	99%	yes	17.2%	3
2	•	25	FlowSOM.CD45+ live.Pop8	3	99.5%	99%	no	41%	8
3	•	11	CD123+ pDC	3	99.3%	97.8%	yes	1.2%	2
3	•	20	FlowSOM.CD45+ live.Pop6	3	99.3%	97.8%	no	0.4%	
3	•	21	FlowSOM.CD45+ live.Pop10	3	99.3%	97.8%	no	0.8%	1
8	•	1	CD141+DCs	3	78.8%	45.8%	yes	0%	
8	•	9	CD1c DCs	3	78.8%	45.8%	yes	0.4%	
8	•	17	FlowSOM.CD45+ live.Pop7	3	78.8%	45.8%	no	1.6%	3
5	•	2	CD14+	2	95.4%	94.4%	yes	19%	3
5	•	24	FlowSOM.CD45+ live.Pop11	2	95.4%	94.4%	no	16.9%	3

With PhenoGraph QFMatch finds 8 of 13 matches where merging multiple PhenoGraph gated populations to match 1 manually gated population obtains a higher F1-score: the 1st, 2nd, 3rd, 4th, 6th, 8th, 9th and 10th ranked matches.

Sync QF F1 MATCH sets: training=all 13 matched!, te

Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	Similarity (QFMatch)
6	●	7	naive CD4+	6	86.9%	97%
6	●	16	naive CD4+ (Phenograph2M5N24)	6	86.9%	97%
6	●	22	naive CD4+ (Phenograph2M5N11)	6	86.9%	97%
6	●	23	naive CD4+ (Phenograph2M5N29)	6	86.9%	97%
6	●	34	naive CD4+ (Phenograph2M5N1)	6	86.9%	97%
6	●	37	naive CD4+ (Phenograph2M5N3)	6	86.9%	97%
8	●	8	[not naive CD4+]	6	84%	95.2%
8	●	19	[not naive CD4+] (Phenograph2M5N4)	6	84%	95.2%
8	●	27	[not naive CD4+] (Phenograph2M5N10)	6	84%	95.2%
8	●	30	[not naive CD4+] (Phenograph2M5N22)	6	84%	95.2%
8	●	38	[not naive CD4+] (Phenograph2M5N31)	6	84%	95.2%
8	●	45	[not naive CD4+] (Phenograph2M5N9)	6	84%	95.2%
1	●	4	CD19+	5	99.4%	99.8%
1	●	14	CD19+ (Phenograph2M5N12)	5	99.4%	99.8%
1	●	25	CD19+ (Phenograph2M5N32)	5	99.4%	99.8%
1	●	40	CD19+ (Phenograph2M5N34)	5	99.4%	99.8%
1	●	41	CD19+ (Phenograph2M5N2)	5	99.4%	99.8%
3	●	2	CD14+	5	97.4%	99%
3	●	29	CD14+ (Phenograph2M5N8)	5	97.4%	99%
3	●	36	CD14+ (Phenograph2M5N13)	5	97.4%	99%
3	●	43	CD14+ (Phenograph2M5N5)	5	97.4%	99%
3	●	46	CD14+ (Phenograph2M5N18)	5	97.4%	99%
4	●	13	[not naive CD8+]	4	93.9%	98.6%
4	●	20	[not naive CD8+] (Phenograph2M5N21)	4	93.9%	98.6%
4	●	32	[not naive CD8+] (Phenograph2M5N14)	4	93.9%	98.6%
4	●	33	[not naive CD8+] (Phenograph2M5N16)	4	93.9%	98.6%
2	●	11	CD123+ pDC	3	98.1%	99.2%
2	●	18	CD123+ pDC (Phenograph2M5N20)	3	98.1%	99.2%
2	●	24	CD123+ pDC (Phenograph2M5N25)	3	98.1%	99.2%

Mair, F. and Prlic, M. (2018), **OMIP-044: 28-color immunophenotyping of the human dendritic cell compartment**. Cytometry, 93: 402-405.

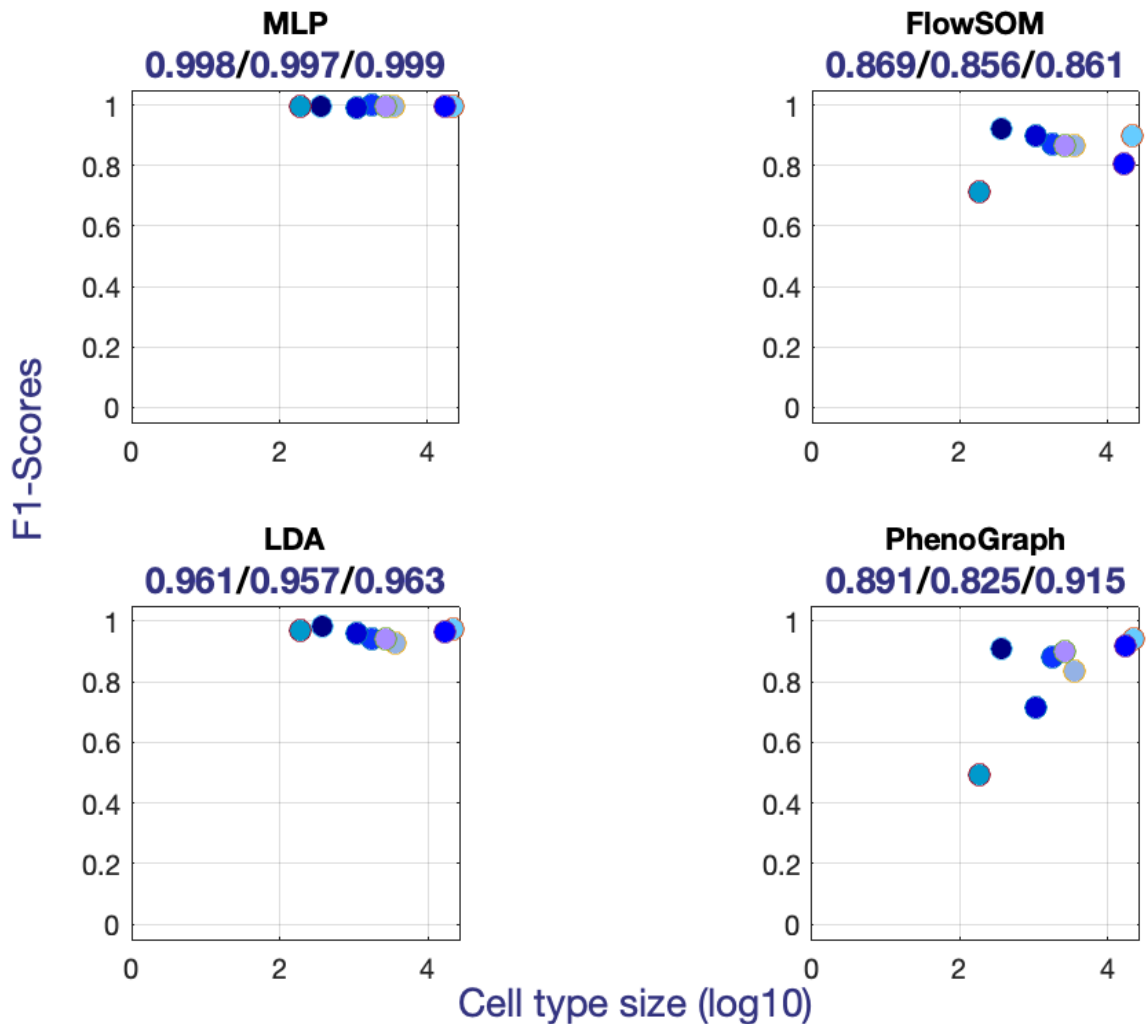
<https://doi.org/10.1002/cyto.a.23331>

3.5.2. OMIP-047

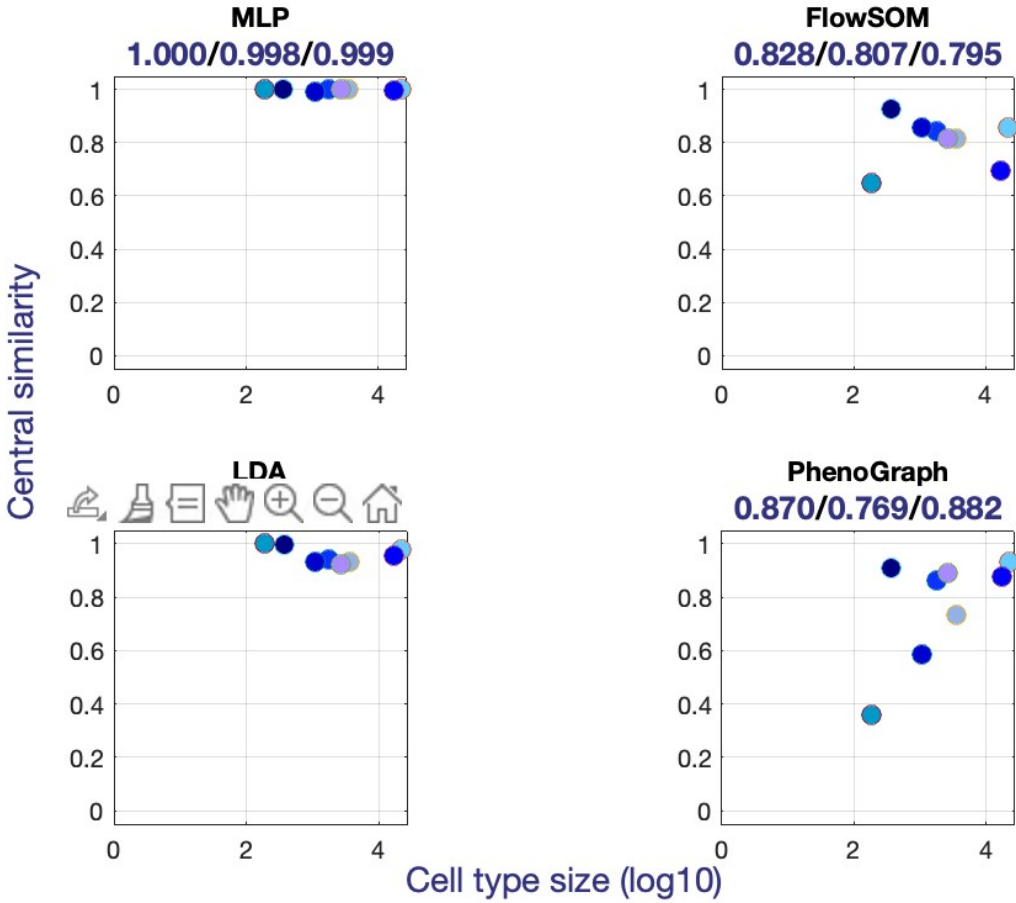
6 samples, 5 fold cross validation 5x1, 4x2, 4x2 and 5x1 training x test samples,
8 cell types, 9 markers

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP 	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
•	IgG1+	3.6%	0.999	0.873	0.939	0.883	1	0.842	0.940	0.865	0.999	0.959	0.963	0.970
•	Naive	45%	0.999	0.899	0.974	0.943	0.999	0.859	0.976	0.930	1	0.952	0.990	0.976
•	IgA_FSC-A Neg_IgA_IgG1_IgG3	7.3%	0.999	0.866	0.929	0.836	1	0.815	0.930	0.734	0.999	0.962	0.978	0.925
•	MZ B cells	35%	0.999	0.807	0.963	0.918	0.998	0.694	0.953	0.875	1	0.922	0.982	0.970
•	IgA_FSC-A_IgA+	5.5%	0.998	0.866	0.942	0.899	0.999	0.815	0.923	0.893	0.999	0.962	0.971	0.971
•	IgG3+	0.75%	0.997	0.923	0.984	0.910	1	0.926	0.998	0.911	0.996	0.974	0.982	0.970
•	PB	0.38%	0.996	0.714	0.968	0.495	1	0.647	1	0.357	0.994	0.889	0.953	0.753
•	Transitional	2.2%	0.993	0.899	0.958	0.716	0.990	0.859	0.933	0.586	0.997	0.952	0.988	0.875
Median			0.998	0.869	0.961	0.891	1	0.828	0.947	0.870	0.999	0.955	0.980	0.970
Mean			0.997	0.856	0.957	0.825	0.998	0.807	0.957	0.769	0.998	0.946	0.976	0.926

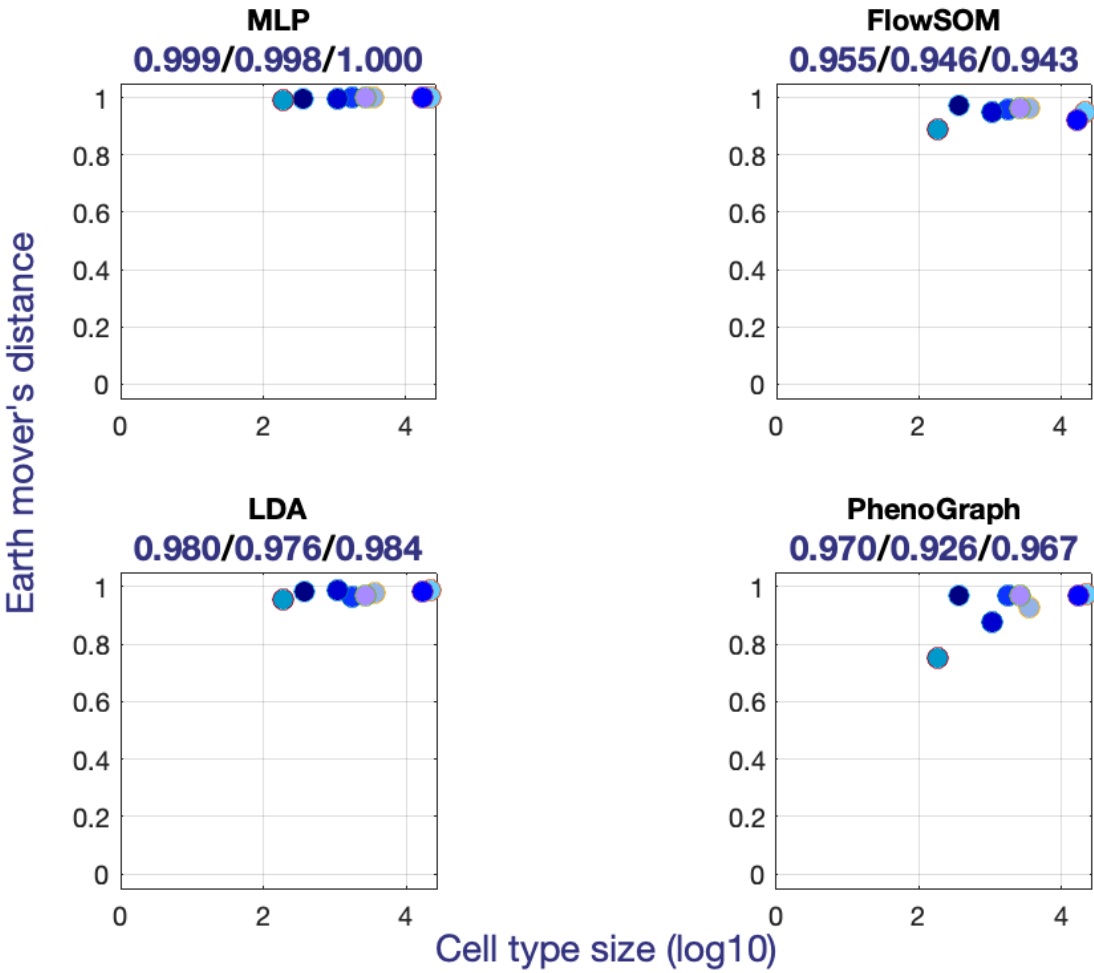
OMIP-047 F1-Scores median/mean/weighted



OMIP-047 Central similarity median/mean/weighted



OMIP-047 Earth mover's distance median/mean/weighted



3.5.2.1. Merged matches

With FlowSOM QFMatch finds 3 of 6 matches where merging multiple manual or FlowSOM gated populations obtains a higher F1-score. The 2nd and 4th ranked match merges 2 manually gated populations to match 1 FlowSOM gated population. The 5th ranked match merges 2 FlowSOM gated populations to match 1 manually gated population.

Rank ²		Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set? ³	Freq.
2	•	IgA, FSC-A Neg IgA IgG1 IgG3	3	86.6%	81.5%	96.2%	yes	8.7%
2	•	IgA, FSC-A IgA+	3	86.6%	81.5%	96.2%	yes	5.5%
2	•	FlowSOM.B cells.Pop3	3	86.6%	81.5%	96.2%	no	14.7%
4	•	Naive	3	89.9%	85.9%	95.2%	yes	45.9%
4	•	Transitional	3	89.9%	85.9%	95.2%	yes	2.1%
4	•	FlowSOM.B cells.Pop7	3	89.9%	85.9%	95.2%	no	52.6%
5	•	MZ B cells	3	80.7%	69.4%	92.2%	yes	33.1%
5	•	FlowSOM.B cells.Pop0	3	80.7%	69.4%	92.2%	no	0.6%
5	•	FlowSOM.B cells.Pop1	3	80.7%	69.4%	92.2%	no	26.5%
1	•	IgG3+	2	92.3%	92.6%	97.4%	yes	0.8%
1	•	FlowSOM.B cells.Pop5	2	92.3%	92.6%	97.4%	no	0.8%
3	•	IgG1+	2	87.3%	84.2%	95.9%	yes	3.6%
3	•	FlowSOM.B cells.Pop6	2	87.3%	84.2%	95.9%	no	3.9%
6	•	PB	2	71.4%	64.7%	88.9%	yes	0.4%
6	•	FlowSOM.B cells.Pop4	2	71.4%	64.7%	88.9%	no	0.5%
7	•	FlowSOM.B cells.Pop2	0	N/A	N/A	N/A	no	0.4%

With PhenoGraph QFMatch finds 3 of 8 matches where merging multiple PhenoGraph gated populations to match 1 manually gated population obtains a higher F1-score: the 1st, 3rd and 8th ranked matches.

           MATCH sets: training=all 8 matched!, test=13 / 14 (1 NEW!)									
Rank ²		#	Subset (class) name	Mat-ches ¹	Similarity (QFMatch)	% Overlap (F-measure)	Train-ing set? ³	Freq.	
1	●	1	Naive	4	97.6%	94.3%	yes	45.9%	2
1	●	17	PhenographWSN93	4	97.6%	94.3%	no	13%	
1	●	18	PhenographWSN95	4	97.6%	94.3%	no	11.4%	
1	●	21	PhenographWSN92	4	97.6%	94.3%	no	15%	
3	●	5	MZ B cells	4	97%	91.8%	yes	33.1%	·
3	●	13	PhenographWSN94	4	97%	91.8%	no	12%	
3	●	15	PhenographWSN91	4	97%	91.8%	no	15%	
3	●	16	PhenographWSN96	4	97%	91.8%	no	7.8%	
6	●	6	IgA, FSC-A Neg IgA IgG1 IgG3	3	92.5%	83.6%	yes	8.7%	
6	●	9	PhenographWSN910	3	92.5%	83.6%	no	3.9%	
6	●	10	PhenographWSN98	3	92.5%	83.6%	no	5.7%	
2	●	7	IgA, FSC-A IgA+	2	97.1%	89.9%	yes	5.5%	
2	●	12	PhenographWSN97	2	97.1%	89.9%	no	6%	

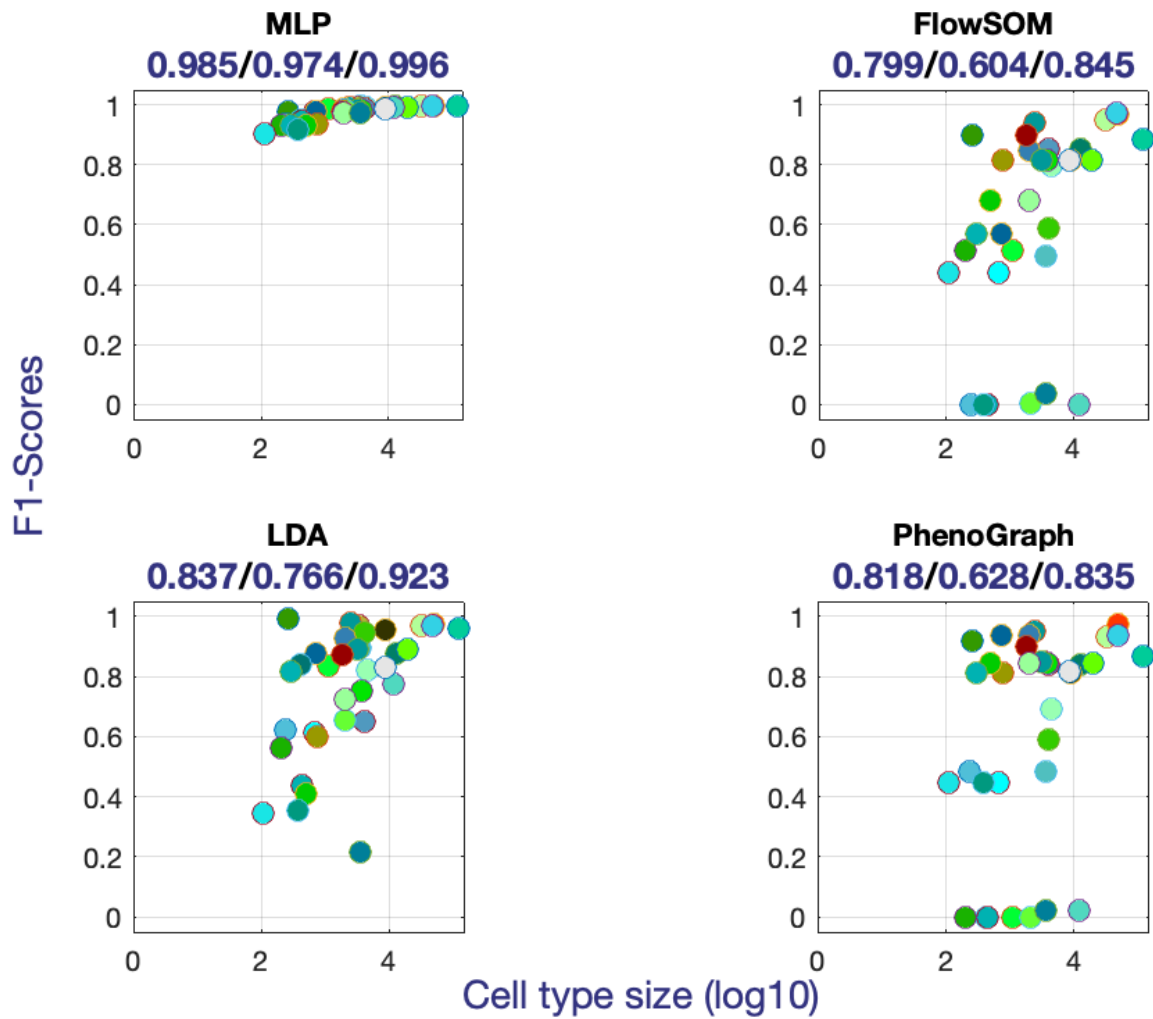
Liechti, T., Günthard, H.F. and Trkola, A. (2018), **OMIP-047: High-Dimensional phenotypic characterization of B cells**. Cytometry, 93: 592-596.
<https://doi.org/10.1002/cyto.a.23488>

3.5.3. OMIP-058

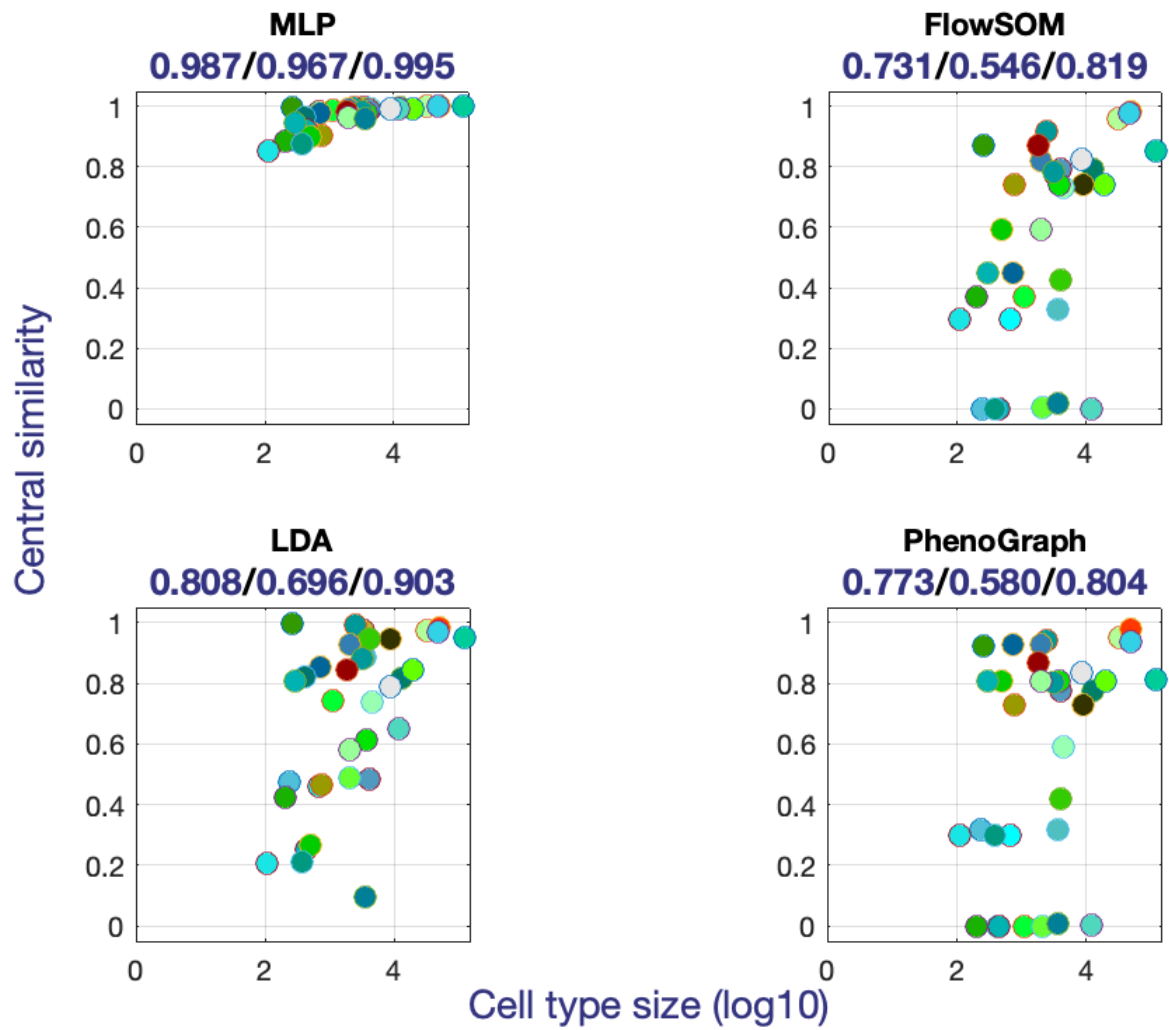
2 samples, 2 fold cross validation of 365k x 356k training x test *cells*,
35 cell types, 17 markers.

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
●	CD4+ TCM T cells CD27+ CD28+	34%	0.999	0.886	0.960	0.867	0.999	0.850	0.951	0.812	1	0.974	0.993	0.952
●	CD8+ TEMRA T cells CD27- CD28-	9%	0.999	0.951	0.967	0.934	1	0.961	0.973	0.952	1	0.974	0.982	0.965
●	HLA-DR+	14%	0.998	0.970	0.973	0.973	0.999	0.981	0.984	0.980	1	0.988	0.978	0.988
●	CD4+ Naive T cells CD27+ CD28+	13%	0.998	0.972	0.970	0.938	0.999	0.979	0.969	0.936	1	0.993	0.995	0.957
●	CD4+ TCM T cells CD27- CD28+	3.5%	0.996	0.854	0.878	0.838	0.996	0.792	0.818	0.773	0.999	0.959	0.985	0.966
●	CD4+ TEM T cells CD27- CD28-	1%	0.995	0.495	0.894	0.483	0.998	0.330	0.885	0.318	0.999	0.923	0.960	0.927
●	Early NK	0.92%	0.994	0.831	0.967	0.847	0.997	0.776	0.973	0.801	0.998	0.944	0.990	0.941
●	CD8+ TEM T cells CD27+ CD28+	5.4%	0.994	0.814	0.891	0.846	0.993	0.741	0.846	0.807	0.999	0.940	0.969	0.949
●	Vd2 high Vg9+ T cells	0.68%	0.994	0.939	0.980	0.949	0.998	0.920	0.991	0.941	0.998	0.985	0.988	0.986
●	Mature NK	2.5%	0.993	0.817	0.954	0.814	0.992	0.741	0.948	0.727	0.999	0.895	0.983	0.886
●	CD4+ TEM T cells CD27+ CD28+	3.3%	0.993	N/A	0.777	0.022	0.991	N/A	0.650	0.003	0.999	N/A	0.955	0.650
●	CD8+ Naive T cells CD27+ CD28+	1.1%	0.991	0.588	0.945	0.591	0.993	0.424	0.945	0.420	0.998	0.881	0.960	0.877
●	CD8+ TEMRA T cells CD27+ CD28-	1.2%	0.990	0.799	0.821	0.692	0.990	0.731	0.738	0.590	0.998	0.955	0.938	0.861
●	CD4+ TEM T cells CD27- CD28+	1.1%	0.989	0.854	0.648	0.838	0.987	0.792	0.483	0.773	0.998	0.959	0.944	0.966
●	NK CD16- CD56-	2.4%	0.988	0.815	0.829	0.818	0.991	0.827	0.788	0.834	0.999	0.877	0.921	0.872
●	CD8+ TEM T cells CD27- CD28+	0.31%	0.987	0.513	0.837	N/A	0.988	0.370	0.743	N/A	0.997	0.818	0.954	N/A
●	Vd2 low Vg9+ T cells CD56-	0.55%	0.987	0.847	0.927	0.934	0.991	0.821	0.925	0.929	0.997	0.941	0.973	0.982
●	CD8+ TCM T cells CD27+ CD28+	1.1%	0.985	0.814	0.751	0.846	0.977	0.741	0.614	0.807	0.998	0.940	0.954	0.949
●	Vd1+ Vg9- T cells CD56-	0.88%	0.982	0.814	0.891	0.848	0.982	0.782	0.880	0.802	0.997	0.920	0.954	0.953
●	CD8+ TEM T cells CD27- CD28-	0.57%	0.981	0.004	0.653	N/A	0.975	0.002	0.489	N/A	0.996	0.401	0.889	N/A
●	CD4+ TEMRA T cells CD27- CD28-	0.18%	0.980	0.439	0.614	0.447	0.984	0.294	0.459	0.300	0.994	0.900	0.767	0.783
●	iNKT cells	0.07%	0.977	0.901	0.994	0.917	0.995	0.873	0.995	0.921	0.985	0.970	0.992	0.909
●	MAIT cells	0.51%	0.976	0.901	0.871	0.898	0.982	0.873	0.844	0.865	0.996	0.970	0.926	0.963
●	Vd2 low Vg9+ T cells CD56+	0.20%	0.976	0.569	0.878	0.934	0.976	0.447	0.855	0.929	0.990	0.868	0.958	0.982
●	CD8+ TEMRA T cells CD27+ CD28+	0.55%	0.973	0.681	0.724	0.846	0.964	0.595	0.583	0.807	0.996	0.936	0.942	0.949
●	CD4+ TSCM T cells CD27+ CD28+	1%	0.972	0.036	0.216	0.022	0.958	0.015	0.097	0.008	0.997	0.486	0.886	0.497
●	Vd1+ Vg9- T cells CD56+	0.12%	0.952	N/A	0.842	N/A	0.965	N/A	0.819	N/A	0.985	N/A	0.938	N/A
●	CD4+ TEMRA T cells CD27+ CD28+	0.12%	0.947	N/A	0.439	N/A	0.922	N/A	0.253	N/A	0.983	N/A	0.804	N/A
●	CD4+ TEM T cells CD27+ CD28-	0.07%	0.938	N/A	0.623	0.483	0.889	N/A	0.473	0.318	0.977	N/A	0.887	0.927
●	Terminal NK	0.21%	0.937	0.817	0.597	0.814	0.905	0.741	0.464	0.727	0.990	0.895	0.911	0.886
●	CD8+ TSCM T cells CD27+ CD28+	0.14%	0.933	0.681	0.409	0.846	0.901	0.595	0.266	0.807	0.989	0.936	0.915	0.949
●	CD8+ TCM T cells CD27- CD28+	0.06%	0.931	0.513	0.563	N/A	0.887	0.370	0.424	N/A	0.982	0.818	0.904	N/A
●	Q2: Vd1+ Vg9+	0.08%	0.930	0.569	0.818	0.813	0.946	0.447	0.808	0.808	0.976	0.868	0.921	0.902
●	CD4+ TSCM T cells CD27- CD28+	0.10%	0.919	N/A	0.356	0.447	0.877	N/A	0.210	0.300	0.981	N/A	0.881	0.783
●	CD4+ TEMRA T cells CD27- CD28+	0.03%	0.905	0.439	0.345	0.447	0.851	0.294	0.207	0.300	0.972	0.900	0.771	0.783
Median			0.985	0.799	0.837	0.818	0.987	0.731	0.808	0.773	0.997	0.920	0.954	0.927
Mean			0.974	0.604	0.766	0.628	0.967	0.546	0.696	0.580	0.993	0.766	0.933	0.770

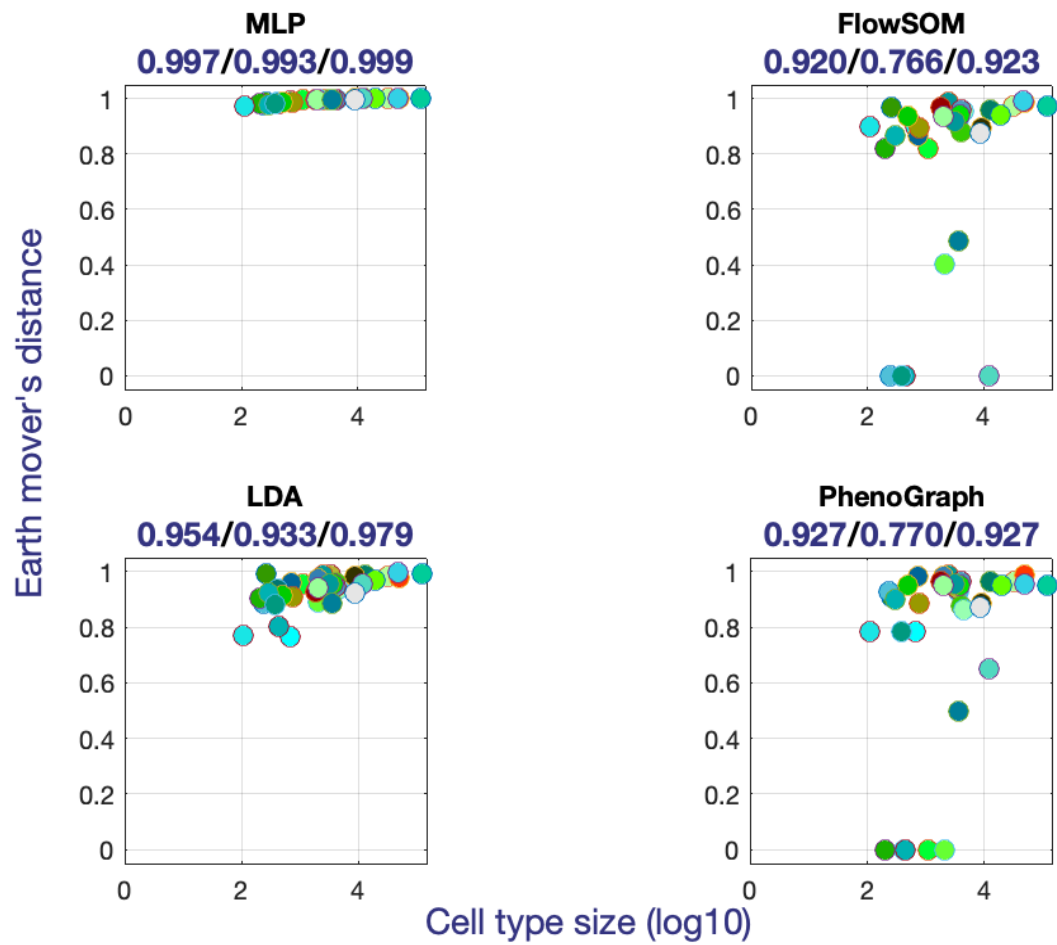
OMIP-058 F1-Scores median/mean/weighted



OMIP-058 Central similarity median/mean/weighted



OMIP-058 Earth mover's distance median/mean/weighted



3.5.3.1. Merged matches

With FlowSOM QFMatch finds 15 of 22 matches where merging multiple FlowSOM gated populations and multiple manually gated populations obtains a higher F1-score.







 MATCH sets: training=30/35 (5 UNMATCHED), test=31/35 (4 NEW)

Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	Similarity (QFMatch)	Train-ing set?	Freq.	
2	●	27	HLA-DR+	4	97%	98.8%	yes	9.9%	3
2	●	47	FlowSOM.Viable cells.Pop0	4	97%	98.8%	no	1.4%	
2	●	63	FlowSOM.Viable cells.Pop13	4	97%	98.8%	no	0.2%	
2	●	66	FlowSOM.Viable cells.Pop5	4	97%	98.8%	no	7.4%	2
14	●	1	Vd1+ Vg9- T cells CD56-	4	81.4%	92%	yes	1.6%	
14	●	37	FlowSOM.Viable cells.Pop3	4	81.4%	92%	no	0.5%	
14	●	38	FlowSOM.Viable cells.Pop30	4	81.4%	92%	no	0.3%	
14	●	65	FlowSOM.Viable cells.Pop29	4	81.4%	92%	no	0.5%	
4	●	12	CD4+ TCM T cells CD27+ CD28+	3	88.6%	97.4%	yes	20.5%	6
4	●	39	FlowSOM.Viable cells.Pop32	3	88.6%	97.4%	no	4.9%	1
4	●	48	FlowSOM.Viable cells.Pop25	3	88.6%	97.4%	no	17.7%	6
5	●	2	CD8+ TEMRA T cells CD27- CD28-	3	95.1%	97.4%	yes	17.8%	5
5	●	46	FlowSOM.Viable cells.Pop4	3	95.1%	97.4%	no	14.6%	5
5	●	61	FlowSOM.Viable cells.Pop11	3	95.1%	97.4%	no	2.7%	1
6	●	15	MAIT cells	3	90.1%	97%	yes	0.6%	
6	●	18	INKT cells	3	90.1%	97%	yes	0.1%	
6	●	60	FlowSOM.Viable cells.Pop9	3	90.1%	97%	no	0.7%	
7	●	4	CD4+ TEM T cells CD27- CD28+	3	85.4%	95.9%	yes	1%	
7	●	29	CD4+ TCM T cells CD27- CD28+	3	85.4%	95.9%	yes	3.6%	1
7	●	55	FlowSOM.Viable cells.Pop24	3	85.4%	95.9%	no	4.2%	1
8	●	3	CD8+ TEMRA T cells CD27+ CD28-	3	79.9%	95.5%	yes	1.9%	
8	●	69	FlowSOM.Viable cells.Pop7	3	79.9%	95.5%	no	1.5%	
8	●	70	FlowSOM.Viable cells.Pop18	3	79.9%	95.5%	no	0.3%	
9	●	13	Early NK	3	83.1%	94.4%	yes	1%	
9	●	36	FlowSOM.Viable cells.Pop8	3	83.1%	94.4%	no	0.2%	
9	●	51	FlowSOM.Viable cells.Pop2	3	83.1%	94.4%	no	0.9%	
11	●	19	CD8+ TCM T cells CD27+ CD28+	3	81.4%	94%	yes	0.6%	
11	●	20	CD8+ TEM T cells CD27+ CD28+	3	81.4%	94%	yes	4%	1
11	●	64	FlowSOM.Viable cells.Pop17	3	81.4%	94%	no	3.5%	1
12	●	6	CD8+ TEMRA T cells CD27+ CD28+	3	68.1%	93.6%	yes	0.6%	
12	●	34	CD8+ TSCM T cells CD27+ CD28+	3	68.1%	93.6%	yes	0.1%	
12	●	40	FlowSOM.Viable cells.Pop26	3	68.1%	93.6%	no	0.5%	
15	●	7	CD4+ TEMRA T cells CD27- CD28-	3	43.9%	90%	yes	0.1%	
15	●	11	CD4+ TEMRA T cells CD27- CD28+	3	43.9%	90%	yes	0%	
15	●	43	FlowSOM.Viable cells.Pop12	3	43.9%	90%	no	0.2%	

With PhenoGraph QFMatch finds 10 of 21 matchers where merging multiple PhenoGraph gated cases and multiple manually gated populations obtains a higher F1-score.

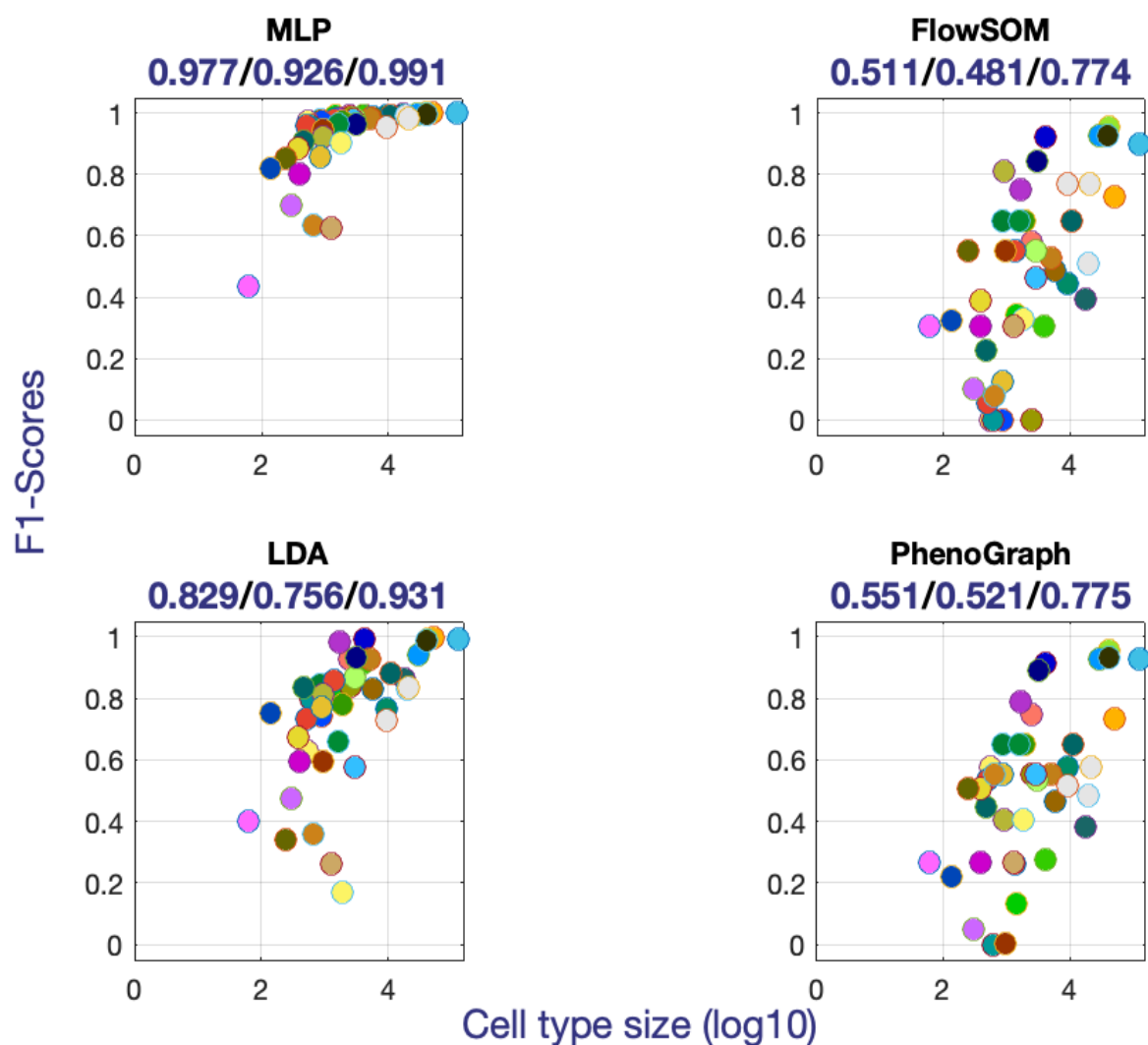
                                      

3.5.4. OMIP-069

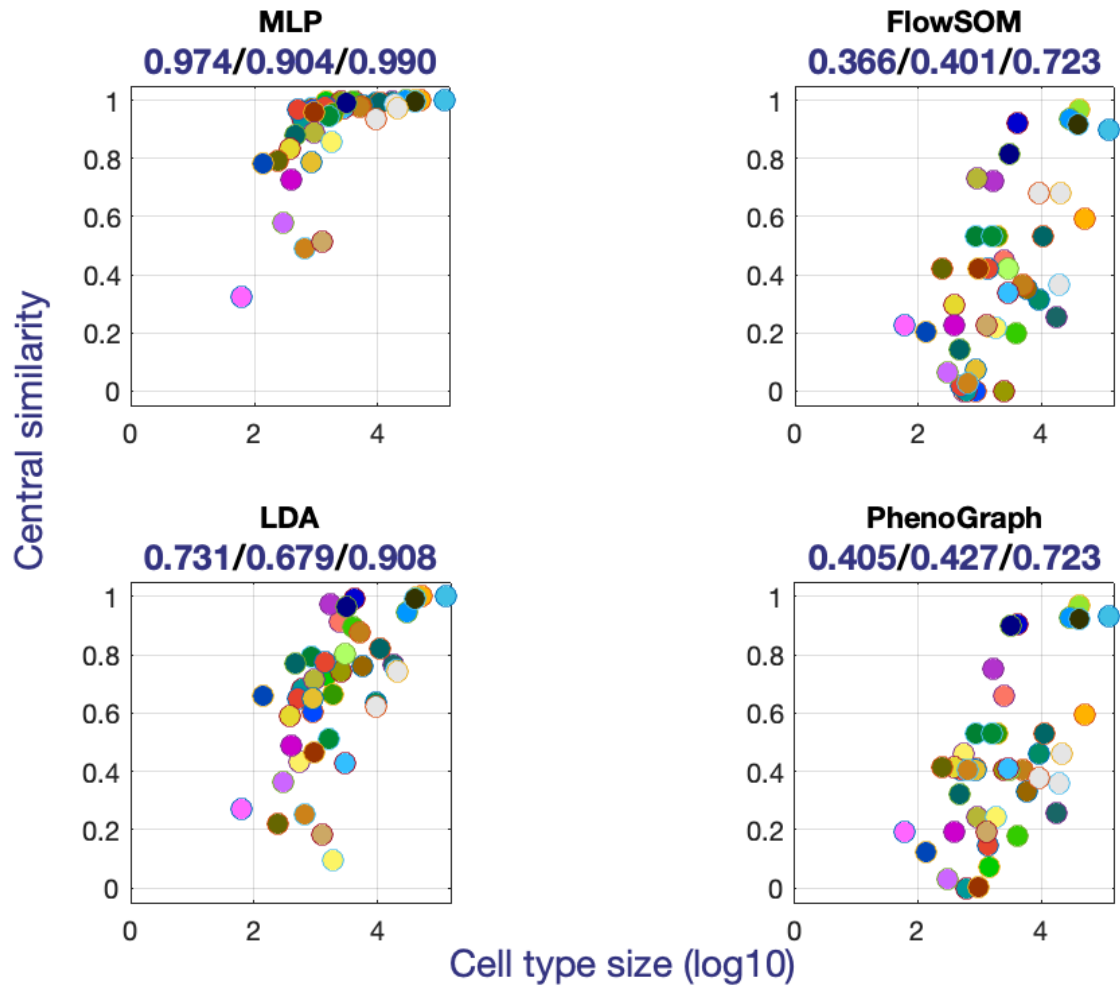
4 samples, 3-fold cross validation, 3x1, 2x2 & 3x1 training x test samples,
43 cell types, 26 markers.

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
●	Naive CD4+	29%	1	0.898	0.994	0.926	1	0.897	1	0.932	1	0.953	0.997	0.980
●	Classical monocytes	12%	0.999	0.729	0.996	0.733	1	0.593	1	0.596	1	0.989	0.998	0.990
●	Naive CD8+	9.6%	0.999	0.957	0.994	0.957	1	0.971	0.997	0.970	1	0.992	0.999	0.993
●	Early Effector CD4+	4.1%	0.998	0.393	0.862	0.384	0.999	0.255	0.766	0.257	1	0.763	0.964	0.749
●	B-2 CD27-	6.8%	0.998	0.929	0.941	0.927	1	0.934	0.945	0.928	1	0.976	0.968	0.979
●	Mature NK	9.5%	0.997	0.925	0.988	0.931	0.998	0.919	0.992	0.922	1	0.981	0.996	0.983
●	B-1 IgG	0.97%	0.994	0.925	0.992	0.916	0.997	0.924	0.994	0.906	0.999	0.981	0.997	0.982
●	Early like effector CD4+	2.2%	0.994	0.444	0.765	0.577	0.994	0.315	0.637	0.459	0.999	0.854	0.946	0.864
●	Early Effector CD8+	2.6%	0.994	0.650	0.882	0.648	0.992	0.533	0.819	0.528	0.999	0.828	0.971	0.865
●	Central Memory CD8+	0.34%	0.993	0.342	0.830	0.132	0.998	0.223	0.731	0.071	0.998	0.889	0.966	0.618
●	CCR7- CD45RA+ TCRgD+	0.57%	0.992	0.581	0.926	0.747	0.994	0.449	0.914	0.657	0.997	0.868	0.971	0.938
●	Terminal Effector CD45RA+ CD8+	0.94%	0.991	0.306	0.915	0.275	0.996	0.200	0.894	0.178	0.998	0.844	0.964	0.818
●	Central Memory CD4+ CXCR5-, CXCR3	4.6%	0.991	0.511	0.829	0.483	0.989	0.366	0.749	0.358	0.998	0.899	0.963	0.878
●	Terminal NK	0.59%	0.988	N/A	0.842	0.553	0.995	N/A	0.742	0.405	0.996	N/A	0.977	0.954
●	CD2+ CD8+ NKT	1.3%	0.985	0.484	0.831	0.466	0.983	0.352	0.760	0.332	0.996	0.819	0.948	0.811
●	Intermediate monocytes	1.2%	0.983	0.527	0.926	0.553	0.979	0.367	0.877	0.405	0.995	0.833	0.954	0.954
●	Central Memory CD4+ CXCR5-, CXCR3-	4.9%	0.983	0.769	0.836	0.577	0.974	0.683	0.744	0.459	0.996	0.948	0.951	0.864
●	CD123+ pDCs	0.39%	0.982	0.751	0.984	0.788	0.976	0.723	0.976	0.750	0.996	0.934	0.996	0.965
●	CD4- CD8-	0.69%	0.981	0.550	0.869	0.536	0.985	0.420	0.803	0.405	0.995	0.804	0.945	0.749
●	Terminal Effector	0.20%	0.979	0.650	0.842	0.648	0.974	0.533	0.793	0.528	0.992	0.828	0.960	0.865
●	B-2 CD27+	0.68%	0.978	0.461	0.578	0.551	0.973	0.338	0.428	0.409	0.996	0.810	0.913	0.890
●	CCR7- CD45RA- TCRgD+	0.32%	0.977	0.550	0.858	0.262	0.976	0.420	0.775	0.146	0.993	0.804	0.981	0.826
●	B-1 IgM+	0.21%	0.974	N/A	0.741	0.551	0.970	N/A	0.602	0.409	0.992	N/A	0.951	0.890
●	Intermediate Effector CD8+	0.45%	0.974	0.650	0.778	0.648	0.956	0.533	0.662	0.528	0.993	0.828	0.957	0.865
●	ILCs CD2+ CD4+	0.13%	0.973	N/A	0.629	0.577	0.965	N/A	0.432	0.459	0.994	N/A	0.846	0.864
●	B-1 IgG- IgM-	0.73%	0.966	0.842	0.933	0.892	0.992	0.817	0.964	0.901	0.991	0.957	0.953	0.966
●	Early like effector CD8+	0.38%	0.964	0.650	0.658	0.648	0.944	0.533	0.511	0.528	0.994	0.828	0.923	0.865
●	Terminal Effector CD4+	0.14%	0.962	N/A	0.796	N/A	0.943	N/A	0.683	N/A	0.993	N/A	0.926	N/A
●	CCR7+ TCRgD+	0.12%	0.958	0.055	0.735	0.536	0.967	0.019	0.653	0.405	0.987	0.612	0.900	0.749
●	Central Memory CD4+ CXCR5, CXCR3	2.2%	0.953	0.769	0.730	0.514	0.935	0.683	0.624	0.380	0.993	0.948	0.920	0.840
●	CD2+ CD8-	0.22%	0.945	0.550	0.593	0.005	0.961	0.420	0.466	0.002	0.985	0.804	0.929	0.279
●	Early NK	0.22%	0.924	0.811	0.810	0.403	0.892	0.730	0.717	0.244	0.987	0.963	0.922	0.782
●	CD4+ CD8+ T	0.11%	0.909	0.224	0.833	0.447	0.882	0.142	0.770	0.320	0.971	0.582	0.928	0.805
●	ILCs CD4-	0.43%	0.904	0.328	0.170	0.403	0.857	0.216	0.095	0.244	0.984	0.645	0.835	0.782
●	ILCs CD2- CD4-	0.09%	0.885	0.389	0.675	0.506	0.833	0.297	0.589	0.412	0.972	0.740	0.874	0.799
●	CD11c+ CD16+ DCs	0.20%	0.858	0.124	0.772	0.553	0.787	0.072	0.649	0.405	0.981	0.781	0.948	0.954
●	CD2- NKT cells	0.06%	0.854	0.550	0.340	0.506	0.793	0.420	0.222	0.412	0.947	0.804	0.552	0.799
●	Plasmablasts	0.03%	0.822	0.326	0.753	0.221	0.782	0.201	0.658	0.121	0.961	0.951	0.953	0.867
●	CD1c+ DCs	0.09%	0.802	0.305	0.595	0.268	0.727	0.224	0.489	0.191	0.978	0.631	0.925	0.643
●	CD1c- CD141- DCs	0.07%	0.701	0.100	0.473	0.048	0.579	0.066	0.364	0.031	0.969	0.570	0.812	0.479
●	Non classical monocytes	0.15%	0.635	0.075	0.360	0.553	0.491	0.026	0.254	0.405	0.869	0.499	0.787	0.954
●	CD16- CD14- monocytes	0.30%	0.625	0.305	0.262	0.268	0.512	0.224	0.185	0.191	0.925	0.631	0.667	0.643
●	CD1c- CD141+ DCs	0.01%	0.437	0.305	0.398	0.268	0.324	0.224	0.272	0.191	0.870	0.631	0.878	0.643
Median			0.977	0.511	0.829	0.551	0.974	0.366	0.731	0.405	0.994	0.828	0.951	0.864
Mean			0.926	0.481	0.756	0.521	0.904	0.401	0.679	0.427	0.983	0.744	0.924	0.814

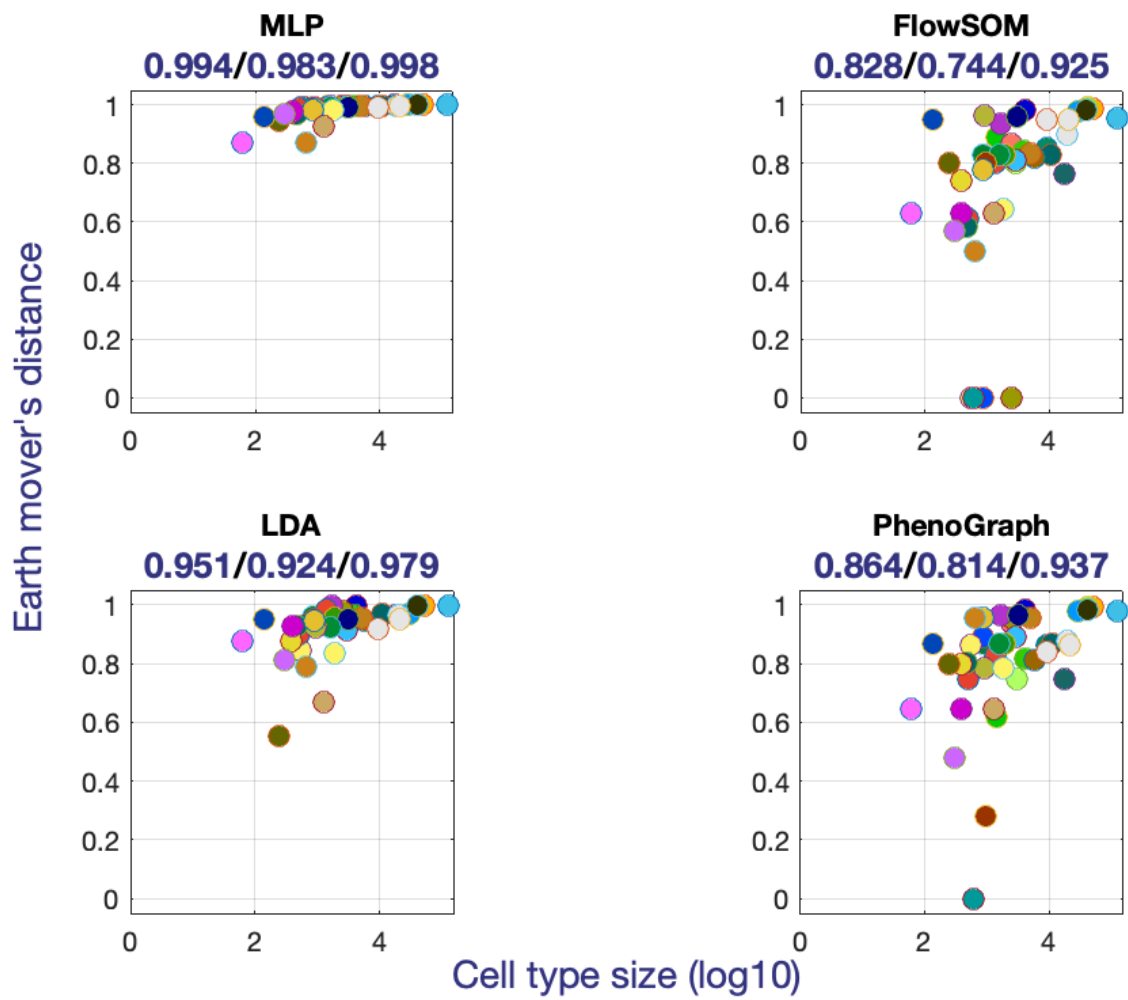
OMIP-069 F1-Scores median/mean/weighted



OMIP-069 Central similarity median/mean/weighted



OMIP-069 Earth mover's distance median/mean/weighted



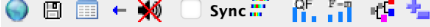
3.5.4.1. Merged matches

With FlowSOM QFMatch finds 7 of 30 matches where merging multiple manual or FlowSOM gated populations obtains a higher F1-score. The 10th, 18th, 21st and 26th ranked matches merge multiple manually gated populations to match 1 FlowSOM gated population. The 2nd, 5th and 12th ranked matches merge multiple FlowSOM gated populations to match 1 manually gated population.

Sync QF F-m ? MATCH sets: training=39/43 (4 UNMATCHED!), test=33/43 (10 NEV

Rank	#	Subset (class) name	Mat-ches	% Overlap (F-measure)	Similarity (QFMatch)	Train-ing set?	Freq.
18	4	Early like effector CD8+	5	65%	82.8%	yes	0.6%
18	8	Early Effector CD8+	5	65%	82.8%	yes	3%
18	14	Intermediate Effector CD8+	5	65%	82.8%	yes	0.5%
18	30	Terminal Effector	5	65%	82.8%	yes	0.2%
18	83	Early like effector CD8+ (FlowSOM....	5	65%	82.8%	no	2.6%
21	1	CCR7- CD45RA- TCRgD+	5	55%	80.4%	yes	0.5%
21	2	CD2+ CD8-	5	55%	80.4%	yes	0.4%
21	19	CD4- CD8-	5	55%	80.4%	yes	1.5%
21	37	CD2- NKT cells	5	55%	80.4%	yes	0.1%
21	65	CCR7- CD45RA- TCRgD+ (FlowSOM...	5	55%	80.4%	no	1.8%
26	11	CD1c+ DCs	4	30.5%	63.1%	yes	0.1%
26	16	CD1c- CD141+ DCs	4	30.5%	63.1%	yes	0%
26	35	CD16- CD14- monocytes	4	30.5%	63.1%	yes	0.4%
26	67	CD1c+ DCs (FlowSOM.CD45+.Pop1)	4	30.5%	63.1%	no	0.4%
2	42	Classical monocytes	3	72.9%	98.9%	yes	7.9%
2	63	Classical monocytes (FlowSOM.CD4...	3	72.9%	98.9%	no	5.7%
2	75	Classical monocytes (FlowSOM.CD4...	3	72.9%	98.9%	no	4.4%
5	12	B-2 CD27-	3	92.9%	97.6%	yes	6.8%
5	48	B-2 CD27- (FlowSOM.CD45+.Pop6)	3	92.9%	97.6%	no	4.4%
5	72	B-2 CD27- (FlowSOM.CD45+.Pop5)	3	92.9%	97.6%	no	1.3%
10	25	Central Memory CD4+ CXCR5, CXC...	3	76.9%	94.8%	yes	6.5%
10	41	Central Memory CD4+ CXCR5-, CXC...	3	76.9%	94.8%	yes	6.5%
10	81	Central Memory CD4+ CXCR5, CXC...	3	76.9%	94.8%	no	9.1%
12	21	Central Memory CD4+ CXCR5-, CXC...	3	51.1%	89.9%	yes	4.7%
12	58	Central Memory CD4+ CXCR5-, CXC...	3	51.1%	89.9%	no	6.1%
12	68	Central Memory CD4+ CXCR5-, CXC...	3	51.1%	89.9%	no	0.6%
1	23	Naive CD8+	2	95.7%	99.2%	yes	13.1%
1	51	Naive CD8+ (FlowSOM.CD45+.Pop30)	2	95.7%	99.2%	no	10.4%

With PhenoGraph there are *10 of 28 matches* where merging multiple manual or PhenoGraph gated populations obtains a higher F1-score. The 9th, 11th, 14th, 15th, 21st, 22nd, 24th and 25th ranked matches merge multiple manually gated populations to match 1 PhenoGraph gated population. The 2nd and 5th ranked matches merge multiple PhenoGraph gated populations to match 1 manually gated population.


 MATCH sets: training=42/43 (1 UNMATCHED!), test=31/38 (7 NEW!)

Rank	#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.
9	13	Non classical monocytes	5	55.3%	40.5%	95.4%	yes	0.1%
9	15	Terminal NK	5	55.3%	40.5%	95.4%	yes	0.1%
9	26	Intermediate monocytes	5	55.3%	40.5%	95.4%	yes	0.8%
9	31	CD11c+ CD16+ DCs	5	55.3%	40.5%	95.4%	yes	0.1%
9	55	PhenographLP7217	5	55.3%	40.5%	95.4%	no	1.9%
14	4	Early like effector CD8+	5	64.8%	52.8%	86.5%	yes	0.6%
14	8	Early Effector CD8+	5	64.8%	52.8%	86.5%	yes	3%
14	14	Intermediate Effector CD8+	5	64.8%	52.8%	86.5%	yes	0.5%
14	30	Terminal Effector	5	64.8%	52.8%	86.5%	yes	0.2%
14	70	PhenographLP7212	5	64.8%	52.8%	86.5%	no	3.5%
5	18	Naive CD4+	4	92.6%	93.2%	98%	yes	28.4%
5	47	PhenographLP7210	4	92.6%	93.2%	98%	no	4.3%
5	66	PhenographLP7218	4	92.6%	93.2%	98%	no	1.5%
5	71	PhenographLP721	4	92.6%	93.2%	98%	no	16.5%
15	10	ILCs CD2+ CD4+	4	57.7%	45.9%	86.4%	yes	0.1%
15	41	Central Memory CD4+ CXCR5-, CXC...	4	57.7%	45.9%	86.4%	yes	6.5%
15	43	Early like effector CD4+	4	57.7%	45.9%	86.4%	yes	1.7%
15	64	PhenographLP726	4	57.7%	45.9%	86.4%	no	4.9%
25	11	CD1c+ DCs	4	26.8%	19.1%	64.3%	yes	0.1%
25	16	CD1c- CD141+ DCs	4	26.8%	19.1%	64.3%	yes	0%
25	35	CD16- CD14- monocytes	4	26.8%	19.1%	64.3%	yes	0.4%
25	45	PhenographLP7224	4	26.8%	19.1%	64.3%	no	0.7%
2	42	Classical monocytes	3	73.3%	59.6%	99%	yes	7.9%
2	73	PhenographLP725	3	73.3%	59.6%	99%	no	5%
2	74	PhenographLP727	3	73.3%	59.6%	99%	no	4.9%
11	6	B-1 IgM+	3	55.1%	40.9%	89%	yes	0.1%
11	7	B-2 CD27+	3	55.1%	40.9%	89%	yes	0.7%
11	67	PhenographLP7219	3	55.1%	40.9%	89%	no	1.4%
21	3	ILCs CD2- CD4-	3	50.6%	41.2%	79.9%	yes	0.1%
21	37	CD2- NKT cells	3	50.6%	41.2%	79.9%	yes	0.1%
21	78	PhenographLP7231	3	50.6%	41.2%	79.9%	no	0.1%
22	5	Early NK	3	40.3%	24.4%	78.2%	yes	0.2%
22	20	ILCs CD4-	3	40.3%	24.4%	78.2%	yes	0.2%
22	81	PhenographLP7223	3	40.3%	24.4%	78.2%	no	0.9%
24	19	CD4- CD8-	3	53.6%	40.5%	74.9%	yes	1.5%
24	29	CCR7+ TCRgD+	3	53.6%	40.5%	74.9%	yes	0.1%
24	51	PhenographLP7222	3	53.6%	40.5%	74.9%	no	0.9%
1	23	Naive CD8+	2	95.7%	97%	99.3%	yes	13.1%
1	44	PhenographLP722	2	95.7%	97%	99.3%	no	10.3%

Park, L.M., Lannigan, J. and Jaimes, M.C. (2020), **OMIP-069: Forty-Color Full Spectrum Flow Cytometry Panel for Deep Immunophenotyping of Major Cell Subsets in Human Peripheral Blood**. Cytometry, 97: 1044-1051.

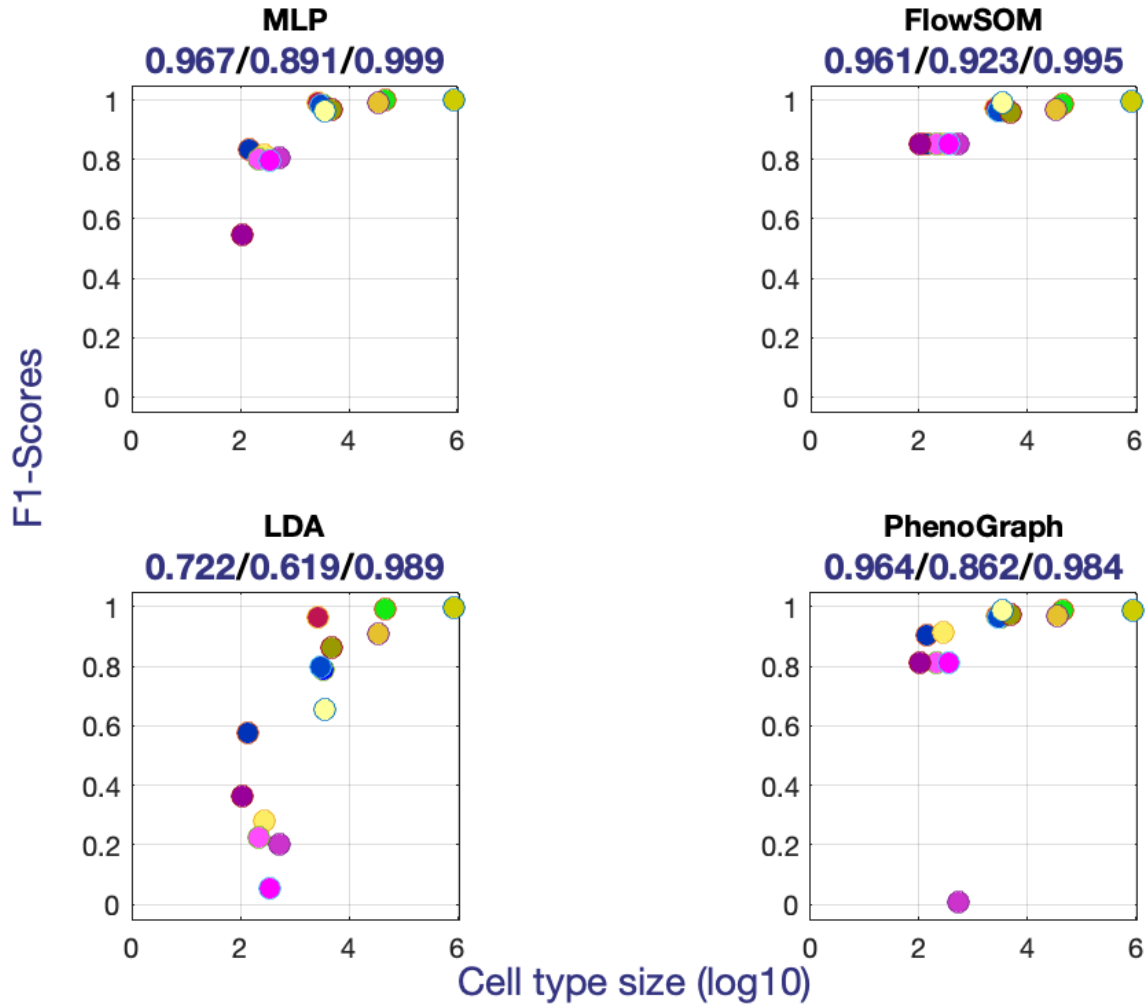
<https://doi.org/10.1002/cyto.a.24213>

3.5.5. OMIP-077

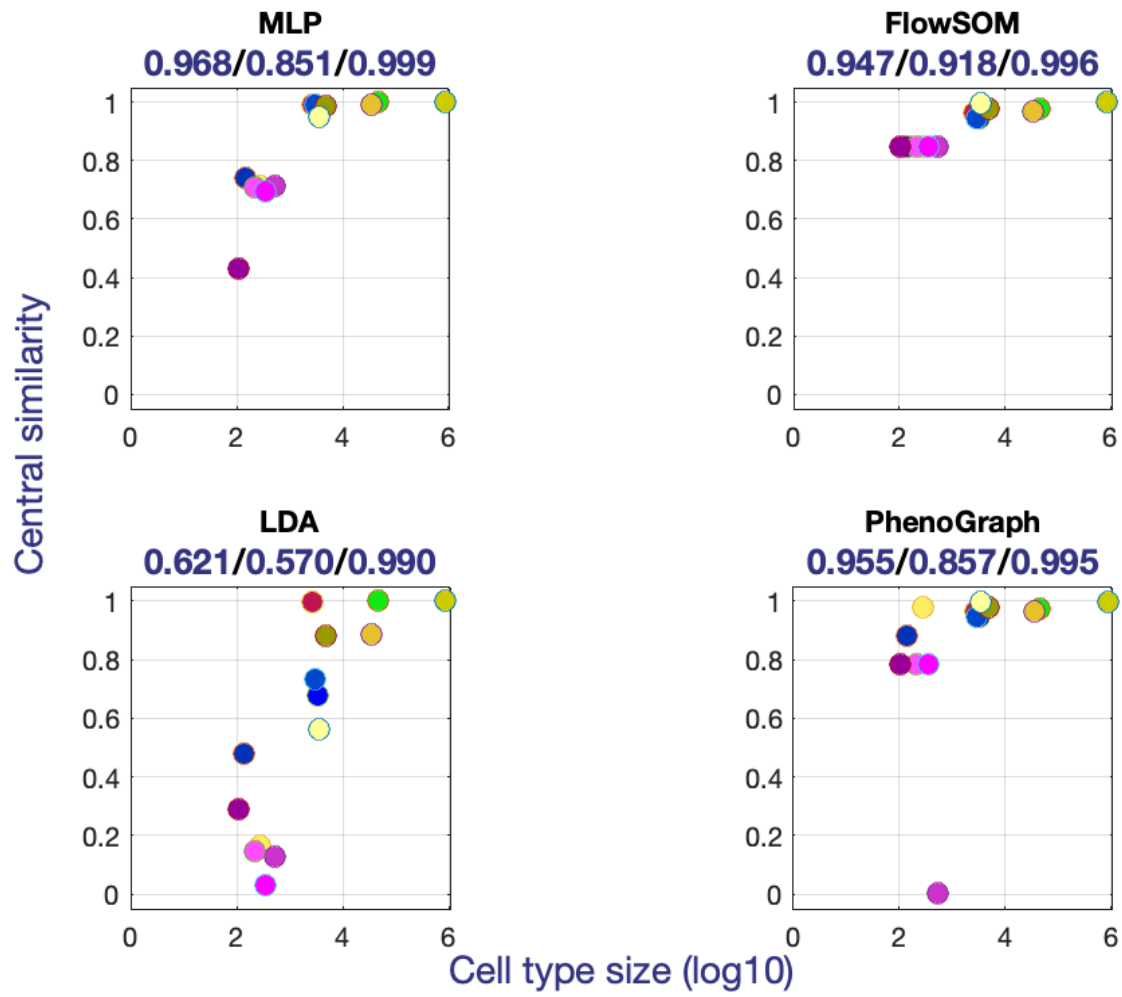
4 samples; 4-fold cross validation of 4 3x1 training X test samples
15 Phenotyping markers, 14 cell types

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP 	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
●	Neutrophils	90%	1	0.997	0.997	0.985	1	0.999	1	0.998	1	0.998	0.998	0.987
●	T cells	4.8%	0.999	0.986	0.990	0.986	1	0.976	1	0.976	1	0.999	0.992	0.999
●	Basophils	0.28%	0.994	0.971	0.964	0.971	0.993	0.962	0.996	0.962	0.997	0.994	0.950	0.994
●	Monocytes	3.6%	0.990	0.970	0.907	0.969	0.994	0.967	0.885	0.966	0.997	0.984	0.952	0.984
●	MZB cells	0.34%	0.982	0.963	0.787	0.964	0.985	0.947	0.678	0.948	0.993	0.997	0.937	0.997
●	Non MZB cells	0.30%	0.981	0.963	0.800	0.964	0.993	0.947	0.731	0.948	0.996	0.997	0.950	0.997
●	NK cells	0.50%	0.969	0.960	0.861	0.975	0.988	0.977	0.882	0.978	0.987	0.979	0.923	0.994
●	Eosinophils	0.36%	0.965	0.990	0.656	0.990	0.952	0.996	0.563	0.996	0.986	0.993	0.842	0.994
●	Plasma cells	0.01%	0.833	0.853	0.579	0.906	0.742	0.847	0.480	0.880	0.946	0.974	0.851	0.953
●	Progenitors	0.03%	0.813	0.853	0.281	0.913	0.715	0.847	0.164	0.980	0.956	0.974	0.734	0.929
●	CD141- mDCs	0.05%	0.806	0.853	0.203	0.006	0.715	0.847	0.130	0.004	0.978	0.974	0.782	0.398
●	CD1c+ mDCs	0.02%	0.802	0.853	0.224	0.812	0.708	0.847	0.147	0.786	0.960	0.974	0.823	0.944
●	CD141+ mDCs	0.04%	0.796	0.853	0.056	0.812	0.693	0.847	0.031	0.786	0.960	0.974	0.732	0.944
●	pDCs	0.01%	0.547	0.853	0.365	0.812	0.429	0.847	0.290	0.786	0.743	0.974	0.663	0.944
Median			0.967	0.961	0.722	0.964	0.968	0.947	0.621	0.955	0.987	0.981	0.887	0.985
Mean			0.891	0.923	0.619	0.862	0.851	0.918	0.570	0.857	0.964	0.985	0.866	0.933

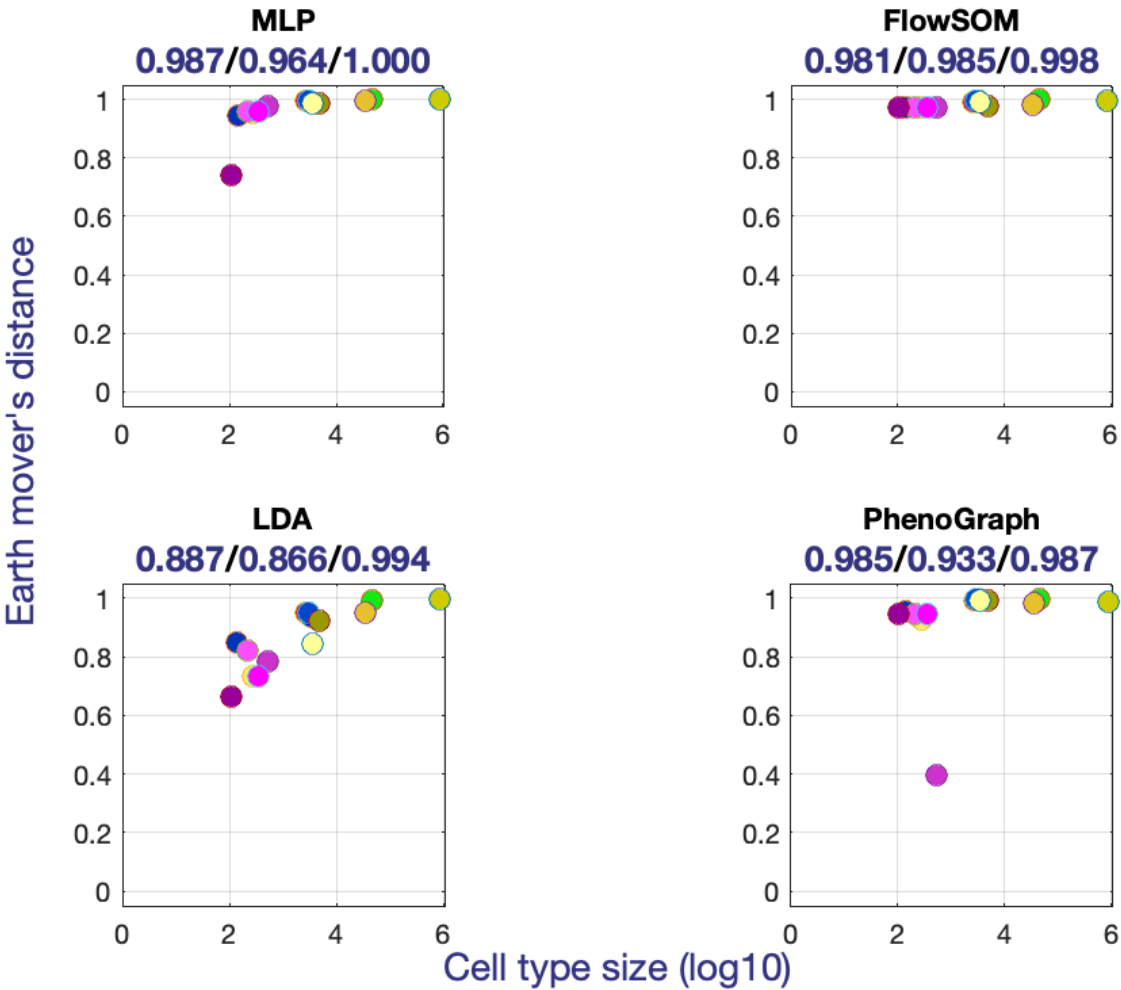
OMIP-077 F1-Scores median/mean/weighted



OMIP-077 Central similarity median/mean/weighted



OMIP-077 Earth mover's distance median/mean/weighted



3.5.5.1. Merged matches

With FlowSOM QFMatch finds 5 of 8 matches where merging multiple manual or FlowSOM gated populations obtains a higher F1-score. The 8th ranked match merges 6 manually gated populations to match 1 FlowSOM gated population. The 3rd ranked match merges 2 manually gated populations to match 1 FlowSOM gated population with .963 F1-score. The 1st, 2nd and 6th ranked matches merge multiple FlowSOM gated populations to match 1 manually gated population.

MATCH sets: training=all 14 matched!, test=12/14 (2 NEW!)								
Rank		Subset (class) name	Matches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Training set?	Freq.
8	•	CD141+ mDCs	7	85.3%	84.7%	97.4%	yes	0%
8	•	CD141- mDCs	7	85.3%	84.7%	97.4%	yes	0%
8	•	Progenitors	7	85.3%	84.7%	97.4%	yes	0.1%
8	•	pDCs	7	85.3%	84.7%	97.4%	yes	0%
8	•	CD1c+ mDCs	7	85.3%	84.7%	97.4%	yes	0%
8	•	Plasma cells	7	85.3%	84.7%	97.4%	yes	0.1%
8	•	CD141+ mDCs (FlowSOM.Leukocyt...	7	85.3%	84.7%	97.4%	no	0.3%
2	●	Neutrophils	4	99.7%	99.9%	99.8%	yes	76.7%
2	•	Neutrophils (FlowSOM.Leukocytes....	4	99.7%	99.9%	99.8%	no	1.8%
2	•	Neutrophils (FlowSOM.Leukocytes....	4	99.7%	99.9%	99.8%	no	0.4%
2	●	Neutrophils (FlowSOM.Leukocytes....	4	99.7%	99.9%	99.8%	no	74.3%
1	•	T cells	3	98.6%	97.6%	99.9%	yes	10.6%
1	•	T cells (FlowSOM.Leukocytes.Pop13)	3	98.6%	97.6%	99.9%	no	9.8%
1	•	T cells (FlowSOM.Leukocytes.Pop11)	3	98.6%	97.6%	99.9%	no	0.5%
3	•	Non MZB cells	3	96.3%	94.7%	99.7%	yes	1.4%
3	•	MZB cells	3	96.3%	94.7%	99.7%	yes	0.5%
3	•	Non MZB cells (FlowSOM.Leukocyt...	3	96.3%	94.7%	99.7%	no	1.9%
6	•	Monocytes	3	97%	96.7%	98.4%	yes	6.9%
6	•	Monocytes (FlowSOM.Leukocytes....	3	97%	96.7%	98.4%	no	6.9%
6	•	Monocytes (FlowSOM.Leukocytes....	3	97%	96.7%	98.4%	no	0.4%
4	•	Basophils	2	97.1%	96.2%	99.4%	yes	0.3%
4	•	Basophils (FlowSOM.Leukocytes.P...	2	97.1%	96.2%	99.4%	no	0.3%

With PhenoGraph QFMatch finds 5 of 11 matches where merging multiple manual or PhenoGraph gated populations obtains a higher F1-score. The 2nd and 9th ranked matches merge multiple manually gated populations to match 1 PhenoGraph gated population. The 1st, 6th and 7th ranked matches merge multiple PhenoGraph gated populations to match 1 manually gated population.

MATCH sets: training=all 14 matched!, test=20/24 (4 NEW!)								
Rank ²		Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set? ³	Freq.
6	●	Neutrophils	8	98.5%	99.8%	98.7%	yes	76.7%
6	●	Neutrophils (PhenographQ1295)	8	98.5%	99.8%	98.7%	no	9.6%
6	●	Neutrophils (PhenographQ1294)	8	98.5%	99.8%	98.7%	no	10.1%
6	●	Neutrophils (PhenographQ1293)	8	98.5%	99.8%	98.7%	no	10.5%
6	●	Neutrophils (PhenographQ1298)	8	98.5%	99.8%	98.7%	no	8.2%
6	●	Neutrophils (PhenographQ1297)	8	98.5%	99.8%	98.7%	no	8.5%
6	●	Neutrophils (PhenographQ1291)	8	98.5%	99.8%	98.7%	no	14.5%
6	●	Neutrophils (PhenographQ1292)	8	98.5%	99.8%	98.7%	no	13.2%
1	●	T cells	4	98.6%	97.6%	99.9%	yes	10.6%
1	●	T cells (PhenographQ12914)	4	98.6%	97.6%	99.9%	no	1.2%
1	●	T cells (PhenographQ1296)	4	98.6%	97.6%	99.9%	no	8.7%
1	●	T cells (PhenographQ12915)	4	98.6%	97.6%	99.9%	no	0.6%
9	●	CD141+ mDCs	4	81.2%	78.6%	94.4%	yes	0%
9	●	pDCs	4	81.2%	78.6%	94.4%	yes	0%
9	●	CD1c+ mDCs	4	81.2%	78.6%	94.4%	yes	0%
9	●	CD141+ mDCs (PhenographQ12920)	4	81.2%	78.6%	94.4%	no	0.1%
2	●	Non MZB cells	3	96.4%	94.8%	99.7%	yes	1.4%
2	●	MZB cells	3	96.4%	94.8%	99.7%	yes	0.5%
2	●	Non MZB cells (PhenographQ12911)	3	96.4%	94.8%	99.7%	no	1.9%
7	●	Monocytes	3	96.9%	96.6%	98.4%	yes	6.9%
7	●	Monocytes (PhenographQ12916)	3	96.9%	96.6%	98.4%	no	0.4%
7	●	Monocytes (PhenographQ1299)	3	96.9%	96.6%	98.4%	no	6.9%
3	●	NK cells	2	97.5%	97.8%	99.4%	yes	2%
3	●	NK cells (PhenographQ12910)	2	97.5%	97.8%	99.4%	no	2%

Boesch, M, Sykora, M, Gasteiger, S, Baty, F, Brutsche, MH, Sopper, S. **OMIP-077: Definition of all principal human leukocyte populations using a broadly applicable 14-color panel.** Cytometry. 2022; 101: 15– 20. <https://doi.org/10.1002/cyto.a.24481>

3.5.6. ESHGHI

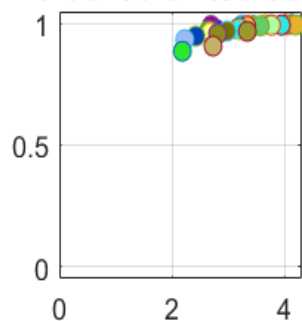
10 samples merged into 1, 5 fold cross validation, 383k training x 96k test cells
29 cell types, 27 markers

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
•	CD4 N	15%	0.997	0.939	0.938	0.907	0.998	0.953	0.949	0.924	0.999	0.962	0.986	0.979
•	CD16hi NK	12%	0.996	0.973	0.974	0.968	0.998	0.985	0.990	0.989	0.999	0.993	0.994	0.993
•	CD8 N	4.8%	0.996	0.812	0.940	0.925	0.997	0.740	0.949	0.939	0.999	0.930	0.970	0.980
•	CD4 CM	6.2%	0.995	0.939	0.849	N/A	0.994	0.953	0.771	N/A	0.999	0.962	0.967	N/A
•	CD14hi Mono	17%	0.995	0.962	0.938	0.957	0.994	0.972	0.936	0.961	0.999	0.985	0.982	0.979
•	gd Tcells	1.9%	0.995	0.829	0.966	0.908	0.996	0.796	0.971	0.917	0.998	0.929	0.984	0.949
•	CD4 EM	9.6%	0.994	0.939	0.875	0.659	0.992	0.953	0.819	0.508	0.999	0.962	0.961	0.876
•	Naive B	2.7%	0.994	0.955	0.960	0.959	0.998	0.974	0.977	0.979	0.998	0.975	0.981	0.983
•	CD8 Temra	6.3%	0.994	0.710	0.866	0.706	0.994	0.608	0.816	0.598	0.999	0.850	0.927	0.838
•	Basophils	2.5%	0.994	0.980	0.963	0.978	0.998	0.995	0.995	0.994	0.998	0.985	0.960	0.991
•	pDCs	0.54%	0.992	0.964	0.944	0.953	0.995	0.986	0.978	0.978	0.995	0.973	0.953	0.960
•	CD8 EM	4%	0.992	0.812	0.827	0.634	0.992	0.740	0.746	0.486	0.999	0.930	0.949	0.835
•	CD8 MAIT	1.9%	0.991	0.907	0.871	0.878	0.991	0.904	0.846	0.847	0.998	0.961	0.925	0.932
•	CD16hi Mono	2.3%	0.990	0.905	0.914	0.869	0.990	0.884	0.893	0.844	0.998	0.973	0.978	0.956
•	Neutrophil	1.7%	0.984	0.965	0.960	0.970	0.988	0.978	0.979	0.980	0.997	0.987	0.976	0.991
•	int Mono	1.6%	0.976	0.962	0.776	0.869	0.967	0.972	0.693	0.844	0.997	0.985	0.971	0.956
•	CD4 Temra	1.7%	0.975	0.939	0.565	0.103	0.960	0.953	0.412	0.058	0.996	0.962	0.906	0.414
•	Trans B	0.67%	0.974	0.864	0.868	0.875	0.971	0.828	0.835	0.836	0.992	0.962	0.966	0.963
•	CD8 CM	0.48%	0.970	0.812	0.632	0.634	0.946	0.740	0.484	0.486	0.992	0.930	0.926	0.835
•	Treg	1%	0.969	0.939	0.694	0	0.958	0.953	0.566	0	0.995	0.962	0.938	0.566
•	HLADRlo Mono	2.4%	0.969	0.962	0.778	0.957	0.955	0.972	0.669	0.961	0.996	0.985	0.964	0.979
•	Mem B	0.64%	0.966	0.864	0.878	0.908	0.968	0.828	0.873	0.941	0.993	0.962	0.973	0.948
•	CD14- CD16-	0.56%	0.965	0.606	0.598	0.530	0.952	0.478	0.467	0.386	0.993	0.878	0.871	0.862
•	Eosinophil	0.52%	0.962	0.942	0.935	0.950	0.975	0.960	0.957	0.961	0.986	0.977	0.979	0.977
•	CD56hi NK	0.70%	0.959	0.973	0.796	0.760	0.936	0.985	0.723	0.687	0.993	0.993	0.976	0.952
•	Plasmablast	0.28%	0.949	0.844	0.839	0.849	0.939	0.808	0.801	0.811	0.987	0.956	0.948	0.959
•	IgD- CD27- B	0.18%	0.935	0.268	0.540	0.908	0.910	0.185	0.432	0.941	0.981	0.641	0.850	0.948
•	Lineage Negative	0.57%	0.908	0.434	0.429	0.445	0.852	0.330	0.296	0.336	0.986	0.746	0.822	0.772
•	CD123-	0.17%	0.887	0.434	0.567	0.445	0.838	0.330	0.455	0.336	0.970	0.746	0.817	0.772
Median			0.984	0.939	0.868	0.875	0.988	0.953	0.819	0.844	0.997	0.962	0.964	0.952
Mean			0.975	0.842	0.817	0.742	0.967	0.819	0.768	0.708	0.994	0.932	0.945	0.867

F1-Scores

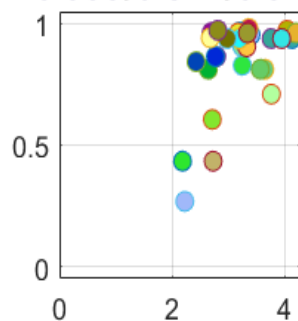
MLP

0.984/0.975/0.991



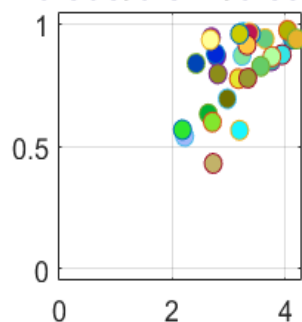
FlowSOM

0.939/0.842/0.912



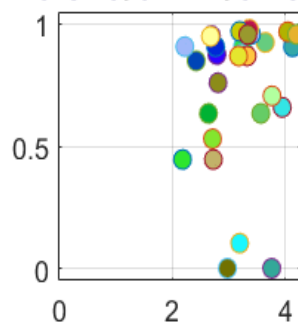
LDA

0.868/0.817/0.897



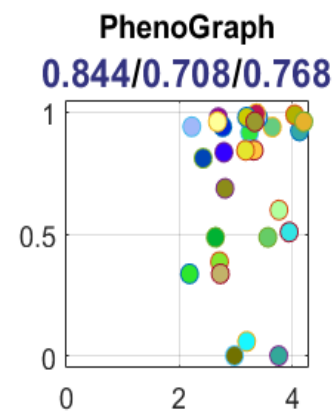
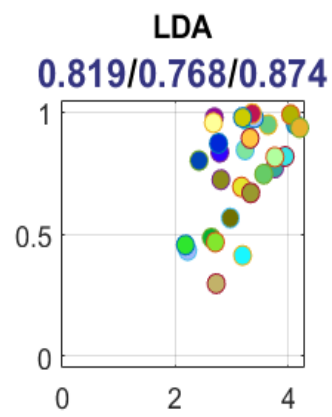
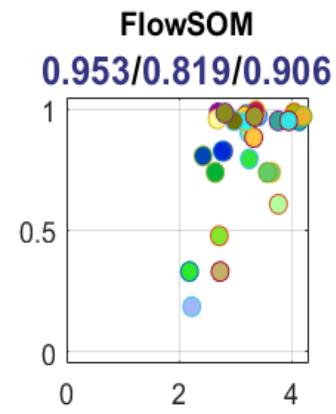
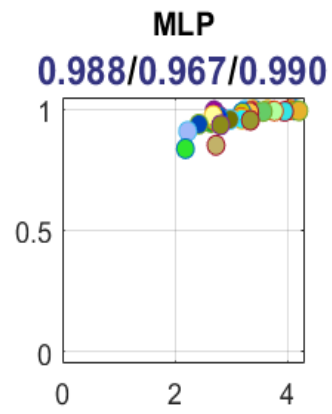
PhenoGraph

0.875/0.742/0.792



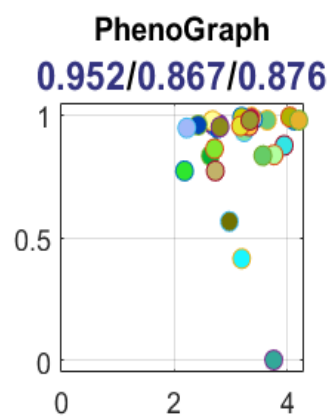
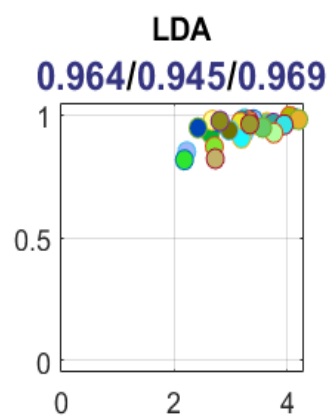
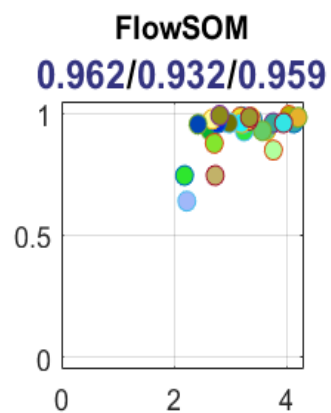
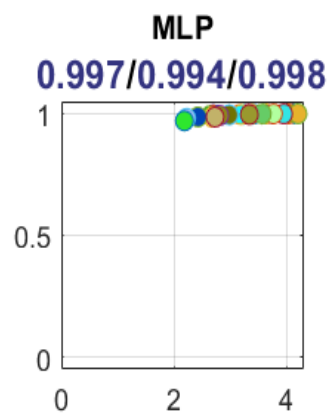
Cell type size (log10)

Central similarity



Cell type size (log10)

Earth mover's distance



Cell type size (log10)

3.5.6.1. Merged matches

With FlowSOM QFMatch finds 7 of 19 matches where merging multiple manual or FlowSOM gated populations obtains a higher F1-score. The 1st, 4th, 9th, 10th, 13th, and 17th ranked matches merge multiple manually gated populations to match 1 FlowSOM gated population. The 14th ranked match merges 2 FlowSOM gated populations to match 1 manually gated population.

MATCH sets: training=all 29 matched!, test=19/29 (10 NEW!)									
Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.
10	●	3	CD4 CM	6	93.9%	95.3%	96.2%	yes	6.2%
10	●	11	Treg	6	93.9%	95.3%	96.2%	yes	1%
10	●	18	CD4 EM	6	93.9%	95.3%	96.2%	yes	9.6%
10	●	20	CD4 N	6	93.9%	95.3%	96.2%	yes	14.6%
10	●	26	CD4 Temra	6	93.9%	95.3%	96.2%	yes	1.7%
10	●	39	CD4 CM (FlowSOM.Residual.Pop10)	6	93.9%	95.3%	96.2%	no	29.2%
4	●	2	HLADRIo Mono	4	96.2%	97.2%	98.5%	yes	2.4%
4	●	13	int Mono	4	96.2%	97.2%	98.5%	yes	1.6%
4	●	19	CD14hi Mono	4	96.2%	97.2%	98.5%	yes	17.3%
4	●	56	HLADRIo Mono (FlowSOM.Residual....	4	96.2%	97.2%	98.5%	no	21%
13	●	16	CD8 EM	4	81.2%	74%	93%	yes	4%
13	●	21	CD8 CM	4	81.2%	74%	93%	yes	0.5%
13	●	24	CD8 N	4	81.2%	74%	93%	yes	4.8%
13	●	57	CD8 EM (FlowSOM.Residual.Pop0)	4	81.2%	74%	93%	no	9.7%
1	●	25	CD56hi NK	3	97.3%	98.5%	99.3%	yes	0.7%
1	●	29	CD16hi NK	3	97.3%	98.5%	99.3%	yes	12%
1	●	32	CD56hi NK (FlowSOM.Residual.Pop3)	3	97.3%	98.5%	99.3%	no	12.6%
9	●	17	Mem B	3	86.4%	82.8%	96.2%	yes	0.6%
9	●	23	Trans B	3	86.4%	82.8%	96.2%	yes	0.7%
9	●	52	Mem B (FlowSOM.Residual.Pop19)	3	86.4%	82.8%	96.2%	no	1.4%
14	●	10	gd Tcells	3	82.9%	79.6%	92.9%	yes	1.9%
14	●	35	gd Tcells (FlowSOM.Residual.Pop2)	3	82.9%	79.6%	92.9%	no	0.8%
14	●	48	gd Tcells (FlowSOM.Residual.Pop7)	3	82.9%	79.6%	92.9%	no	1.1%
17	●	5	Lineage Negative	3	43.4%	33%	74.6%	yes	0.6%
17	●	6	[CD123-]	3	43.4%	33%	74.6%	yes	0.2%
17	●	51	Lineage Negative (FlowSOM.Residua...	3	43.4%	33%	74.6%	no	0.3%
2	●	12	Neutrophil	2	96.5%	97.8%	98.7%	yes	1.7%
2	●	38	Neutrophil (FlowSOM.Residual.Pop18)	2	96.5%	97.8%	98.7%	no	1.7%

With PhenoGraph QFMatch finds 12 of 24 matches where merging multiple manual or PhenoGraph gated populations obtains a higher F1-score. The 7th, 12th, 15th, 20th, and 21st ranked matches merge multiple manual gates to match 1 PhenoGraph gated population. The 1st, 4th, 6th, 8th, 17th, 18th and 19th ranked matches merge multiple PhenoGraph gated populations to match 1 manually gated population.

Rank ²		#	Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.	
17		18	CD4 EM	5	65.9%	50.8%	87.6%	yes	9.6%	4
17		39	CD4 EM (PhenographYJ6F11)	5	65.9%	50.8%	87.6%	no	3.4%	1
17		48	CD4 EM (PhenographYJ6F5)	5	65.9%	50.8%	87.6%	no	5.1%	2
17		57	CD4 EM (PhenographYJ6F17)	5	65.9%	50.8%	87.6%	no	2.2%	1
17		64	CD4 EM (PhenographYJ6F4)	5	65.9%	50.8%	87.6%	no	6.8%	3
1		29	CD16hi NK	3	96.8%	98.9%	99.3%	yes	12%	5
1		44	CD16hi NK (PhenographYJ6F3)	3	96.8%	98.9%	99.3%	no	7.9%	3
1		68	CD16hi NK (PhenographYJ6F10)	3	96.8%	98.9%	99.3%	no	3.5%	1
4		4	Naive B	3	95.9%	97.9%	98.3%	yes	2.7%	1
4		54	Naive B (PhenographYJ6F13)	3	95.9%	97.9%	98.3%	no	2.5%	1
4		70	Naive B (PhenographYJ6F41)	3	95.9%	97.9%	98.3%	no	0.1%	
6		20	CD4 N	3	90.7%	92.4%	97.9%	yes	14.6%	6
6		30	CD4 N (PhenographYJ6F8)	3	90.7%	92.4%	97.9%	no	4.3%	2
6		46	CD4 N (PhenographYJ6F2)	3	90.7%	92.4%	97.9%	no	9.5%	4
7		2	HLADRIo Mono	3	95.7%	96.1%	97.9%	yes	2.4%	1
7		19	CD14hi Mono	3	95.7%	96.1%	97.9%	yes	17.3%	8
7		65	HLADRIo Mono (PhenographYJ6F1)	3	95.7%	96.1%	97.9%	no	18.5%	9
8		28	Eosinophil	3	95%	96.1%	97.7%	yes	0.5%	
8		33	Eosinophil (PhenographYJ6F27)	3	95%	96.1%	97.7%	no	0.5%	
8		38	Eosinophil (PhenographYJ6F49)	3	95%	96.1%	97.7%	no	0%	
12		13	int Mono	3	86.9%	84.4%	95.6%	yes	1.6%	
12		27	CD16hi Mono	3	86.9%	84.4%	95.6%	yes	2.3%	1
12		66	int Mono (PhenographYJ6F9)	3	86.9%	84.4%	95.6%	no	3.9%	1
15		8	IgD- CD27- B	3	90.8%	94.1%	94.8%	yes	0.2%	
15		17	Mem B	3	90.8%	94.1%	94.8%	yes	0.6%	
15		63	IgD- CD27- B (PhenographYJ6F22)	3	90.8%	94.1%	94.8%	no	0.8%	
18		7	[CD14- CD16-]	3	53%	38.6%	86.2%	yes	0.6%	
18		52	[CD14- CD16-] (PhenographYJ6F45)	3	53%	38.6%	86.2%	no	0%	
18		55	[CD14- CD16-] (PhenographYJ6F20)	3	53%	38.6%	86.2%	no	1.3%	
19		14	CD8 Temra	3	70.6%	59.8%	83.8%	yes	6.3%	2
19		45	CD8 Temra (PhenographYJ6F14)	3	70.6%	59.8%	83.8%	no	2.5%	1
19		53	CD8 Temra (PhenographYJ6F12)	3	70.6%	59.8%	83.8%	no	2.8%	1
20		16	CD8 EM	3	63.4%	48.6%	83.5%	yes	4%	1
20		21	CD8 CM	3	63.4%	48.6%	83.5%	yes	0.5%	
20		62	CD8 EM (PhenographYJ6F6)	3	63.4%	48.6%	83.5%	no	5%	2
21		5	Lineage Negative	3	44.5%	33.6%	77.2%	yes	0.6%	
21		6	[CD123-]	3	44.5%	33.6%	77.2%	yes	0.2%	
21		69	Lineage Negative (PhenographYJ6F31)	3	44.5%	33.6%	77.2%	no	0.3%	
2		12	Neutrophil	2	97%	98%	99.1%	yes	1.7%	

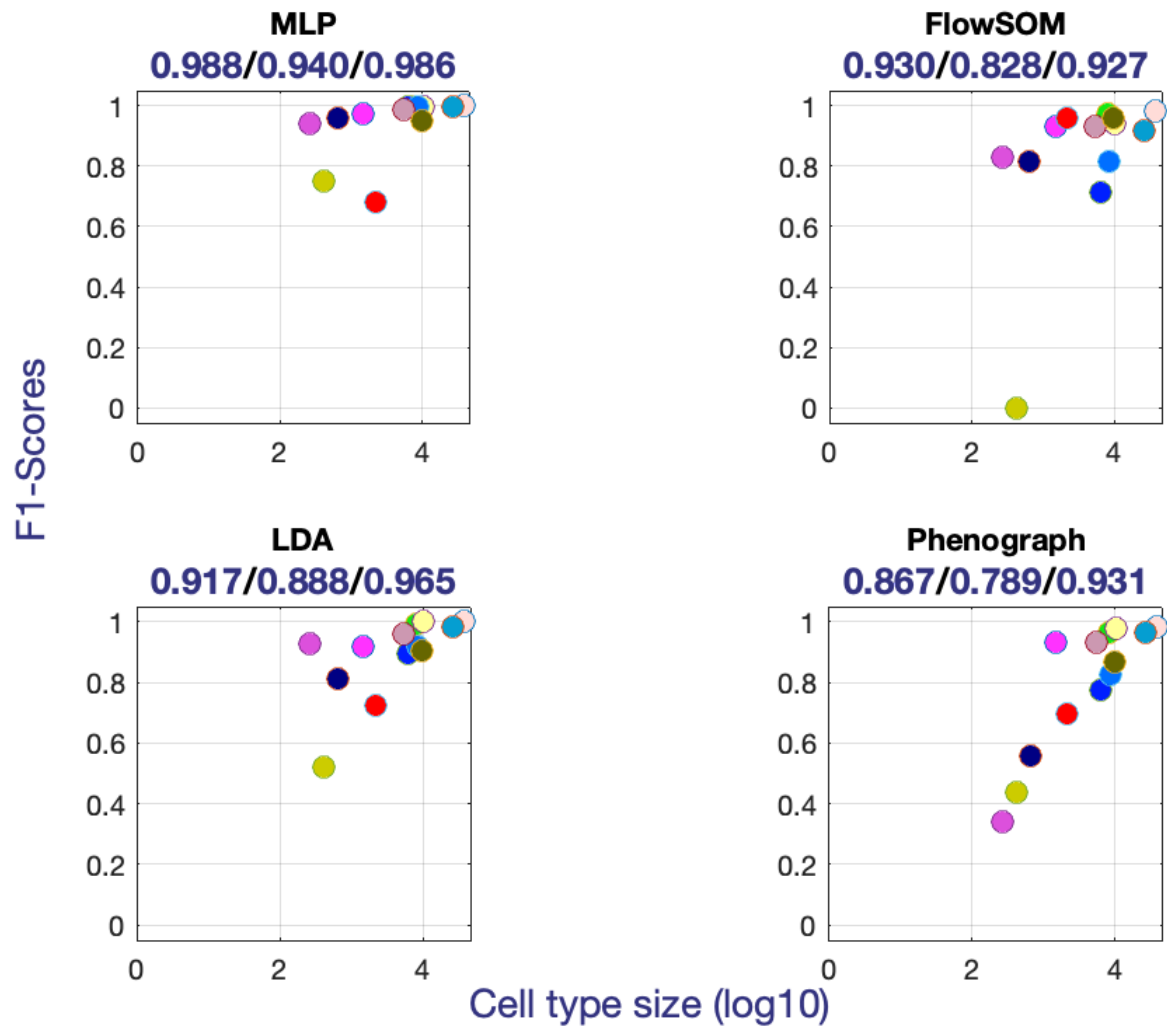
Toghi Eshghi S, Au-Yeung A, Takahashi C, Bolen CR, Nyachienga MN, Lear SP, Green C, Mathews WR and O'Gorman WE (2019) **Quantitative Comparison of Conventional and t-SNE-guided Gating Analyses**. Front. Immunol. 10:1194. doi: 10.3389/fimmu.2019.01194.
<https://www.frontiersin.org/articles/10.3389/fimmu.2019.01194/full>

3.5.7. GHOSN

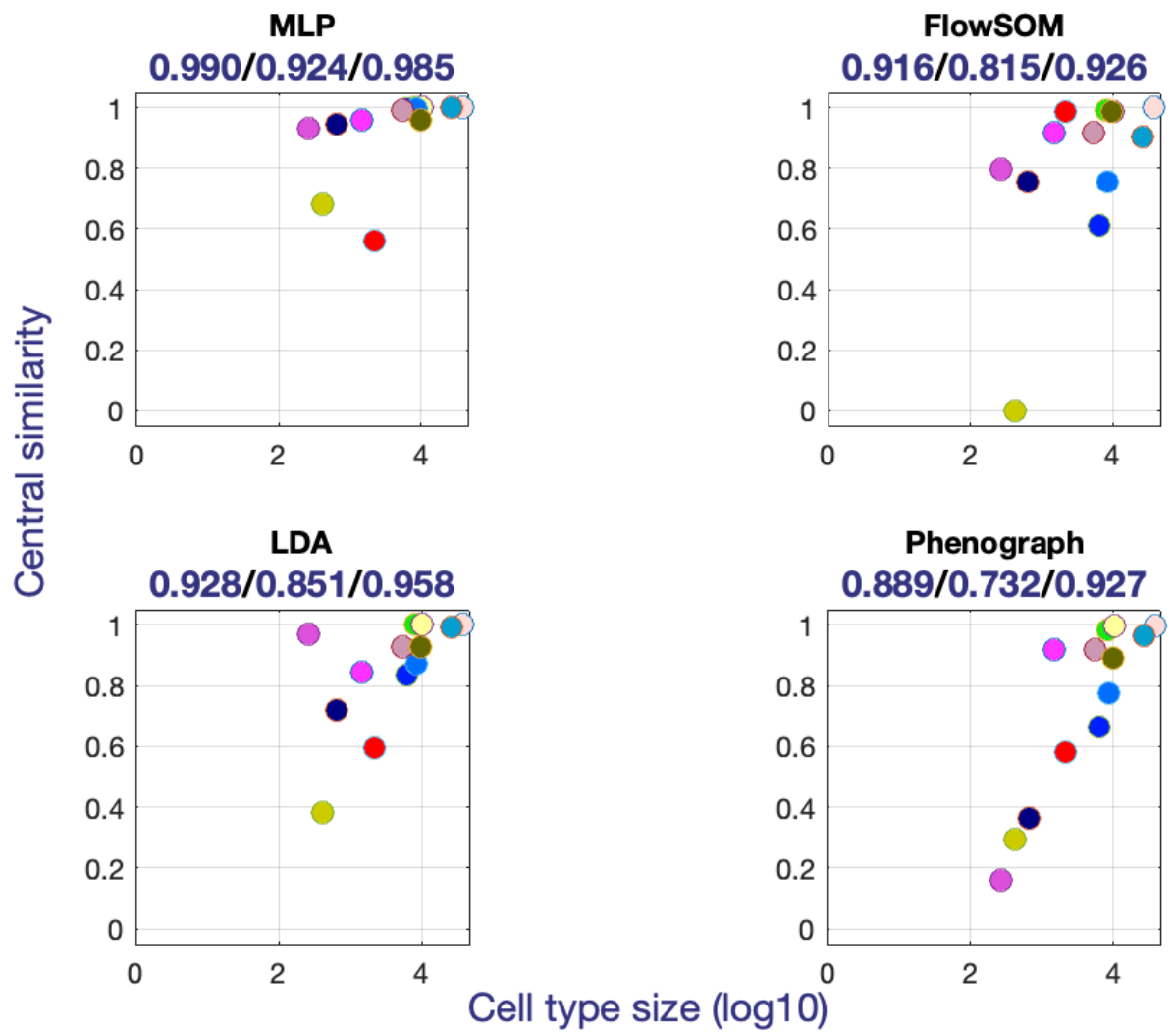
3 samples, 2-fold cross validation 2x1 and 1x2 training x test samples,
13 cell types, 9 markers.

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP 	Flow SOM	LDA	Pheno graph	MLP	Flow SOM	LDA	Pheno graph	MLP	Flow SOM	LDA	Pheno graph
	Large macrophages	32%	1	0.982	1	0.982	1	0.999	1	0.999	1	0.991	1	0.992
	B-1	22%	0.999	0.919	0.981	0.963	1	0.905	0.993	0.965	0.999	0.958	0.990	0.994
	T cells	6.9%	0.996	0.972	0.992	0.963	1	0.990	1	0.982	0.999	0.984	0.997	0.976
	Eosinophils	8.6%	0.996	0.943	1	0.979	1	0.986	1	0.997	0.998	0.961	1	0.993
	B-2 IgM high	5.3%	0.996	0.715	0.893	0.777	0.998	0.610	0.833	0.665	0.999	0.864	0.941	0.951
	B-2 IgM medium	7.2%	0.995	0.814	0.917	0.824	0.997	0.754	0.873	0.773	0.997	0.897	0.957	0.942
	Small macrophages	4.6%	0.988	0.930	0.958	0.932	0.990	0.916	0.928	0.920	0.997	0.976	0.973	0.977
	CD11b+ dendritic	1.3%	0.971	0.930	0.916	0.932	0.960	0.916	0.845	0.920	0.994	0.976	0.959	0.977
	Developing B	0.55%	0.962	0.814	0.812	0.556	0.943	0.754	0.720	0.362	0.969	0.897	0.842	0.771
	NK, NKT	8.3%	0.949	0.959	0.903	0.867	0.958	0.986	0.929	0.889	0.970	0.984	0.929	0.908
	CD11b- dendritic	0.23%	0.943	0.827	0.929	0.342	0.933	0.798	0.968	0.162	0.939	0.969	0.934	0.632
	Neutrophils	0.36%	0.749	N/A	0.519	0.440	0.681	N/A	0.380	0.294	0.932	N/A	0.718	0.836
	ckit+ mast cells	1.8%	0.682	0.959	0.724	0.697	0.558	0.986	0.593	0.582	0.912	0.984	0.954	0.950
Median			0.988	0.930	0.917	0.867	0.990	0.916	0.928	0.889	0.997	0.969	0.957	0.951
Mean			0.940	0.828	0.888	0.789	0.924	0.815	0.851	0.732	0.977	0.880	0.938	0.915

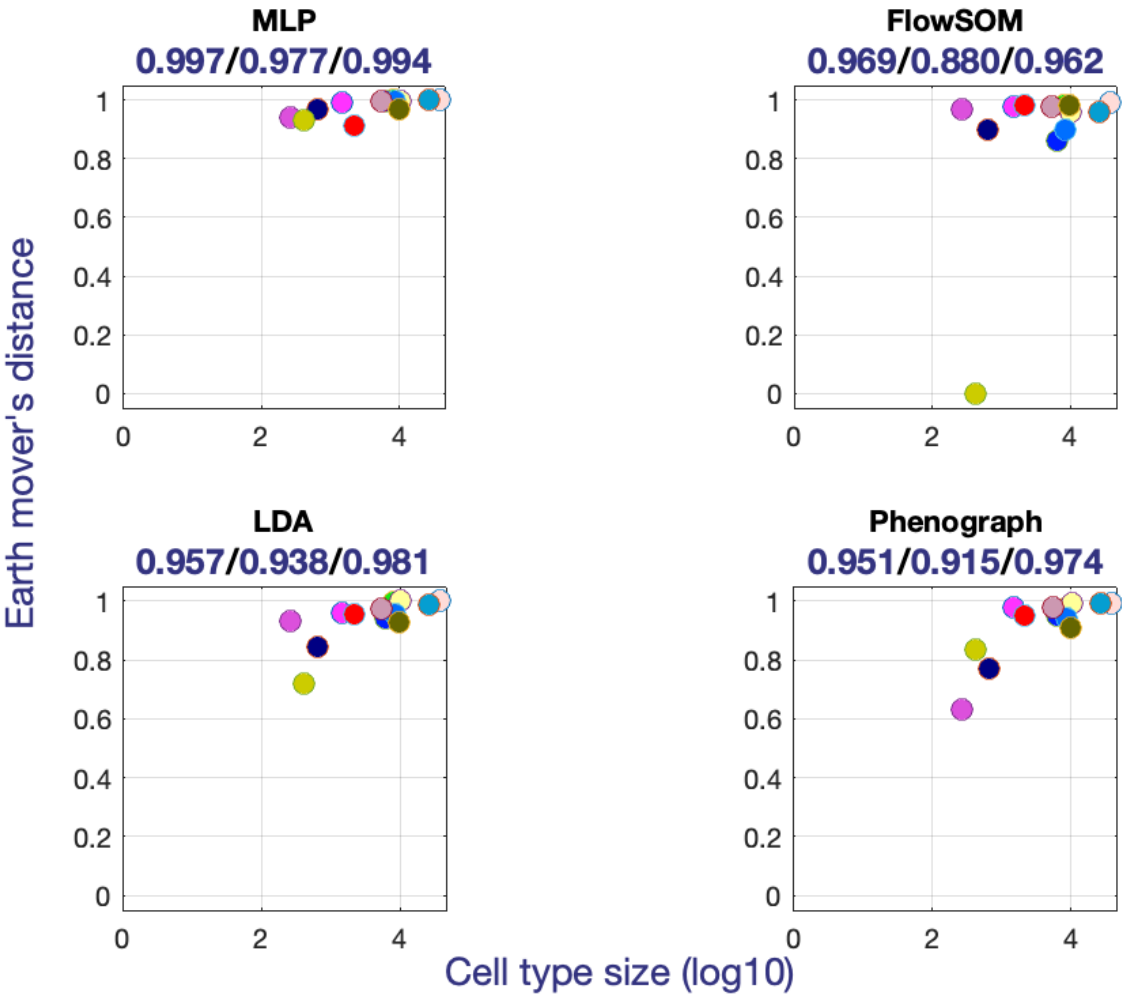
GHOSN F1-Scores median/mean/weighted



GHOSN Central similarity median/mean/weighted



GHOSN Earth mover's distance median/mean/weighted



3.5.7.1. Merged matches

With FlowSOM QFMatch finds 3 of 9 matches where merging 2 manually gated populations for 1 FlowSOM gated populations obtains a higher F1-score. The 3rd, 4th and 8th ranked matches.

Rank ²		#	Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.
3		9	NK, NKT	3	95.9%	98.4%	98.5%	yes	9%
3		11	ckit+ mast cells	3	95.9%	98.4%	98.5%	yes	1.8%
3		18	FlowSOM.Live singlets.Pop10	3	95.9%	98.4%	98.5%	no	10.9%
4		3	Small macrophages	3	93%	91.8%	97.6%	yes	4.5%
4		5	CD11b+ dendritic	3	93%	91.8%	97.6%	yes	1.2%
4		24	FlowSOM.Live singlets.Pop7	3	93%	91.8%	97.6%	no	5.8%
8		7	Developing B	3	81.4%	75%	89.4%	yes	0.5%
8		10	B-2 IgM medium	3	81.4%	75%	89.4%	yes	7%
8		20	FlowSOM.Live singlets.Pop5	3	81.4%	75%	89.4%	no	7.1%
1		1	Large macrophages	2	98.2%	99.9%	99.1%	yes	31.9%
1		15	FlowSOM.Live singlets.Pop0	2	98.2%	99.9%	99.1%	no	31.4%

With PhenoGraph QFMatch finds 5 of 12 matches where merging multiple manual or PhenoGraph gated populations obtains a higher F1-score. The 4th ranked match merges 2 manually gated populations to match 1 PhenoGraph gated population. The 1st, 3rd, 8th and 9th ranked matches merge multiple PhenoGraph gated populations to match 1 manually gated population.

        MATCH sets: training=all 13 matched!, test=21/22 (1 NEW!)									
Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.
1	●	13	B-1	6	96.3%	97.1%	99.3%	yes	22.1%
1	●	14	Phenograph29FL8	6	96.3%	97.1%	99.3%	no	6.9%
1	●	19	Phenograph29FL13	6	96.3%	97.1%	99.3%	no	3.9%
1	●	20	Phenograph29FL21	6	96.3%	97.1%	99.3%	no	0.3%
1	●	28	Phenograph29FL1	6	96.3%	97.1%	99.3%	no	9.9%
1	●	32	Phenograph29FL22	6	96.3%	97.1%	99.3%	no	0.1%
3	●	1	Large macrophages	5	98.2%	99.9%	99.2%	yes	31.9%
3	●	17	Phenograph29FL6	5	98.2%	99.9%	99.2%	no	7.3%
3	●	25	Phenograph29FL4	5	98.2%	99.9%	99.2%	no	7.8%
3	●	27	Phenograph29FL3	5	98.2%	99.9%	99.2%	no	8.6%
3	●	30	Phenograph29FL5	5	98.2%	99.9%	99.2%	no	7.7%
4	●	3	Small macrophages	3	93.2%	92.1%	97.8%	yes	4.5%
4	●	5	CD11b+ dendritic	3	93.2%	92.1%	97.8%	yes	1.2%
4	●	23	Phenograph29FL9	3	93.2%	92.1%	97.8%	no	5.9%
8	●	9	NK, NKT	3	86.7%	88.6%	91.4%	yes	9%
8	●	26	Phenograph29FL11	3	86.7%	88.6%	91.4%	no	4.7%
8	●	34	Phenograph29FL15	3	86.7%	88.6%	91.4%	no	2.3%
9	●	2	B-2 IgM high	3	77.7%	68.1%	91.1%	yes	5.1%
9	●	15	Phenograph29FL16	3	77.7%	68.1%	91.1%	no	2.2%
9	●	18	Phenograph29FL12	3	77.7%	68.1%	91.1%	no	4.5%
2	●	8	Eosinophils	2	97.9%	99.7%	99.3%	yes	9.5%
2	●	33	Phenograph29FL2	2	97.9%	99.7%	99.3%	no	9.3%

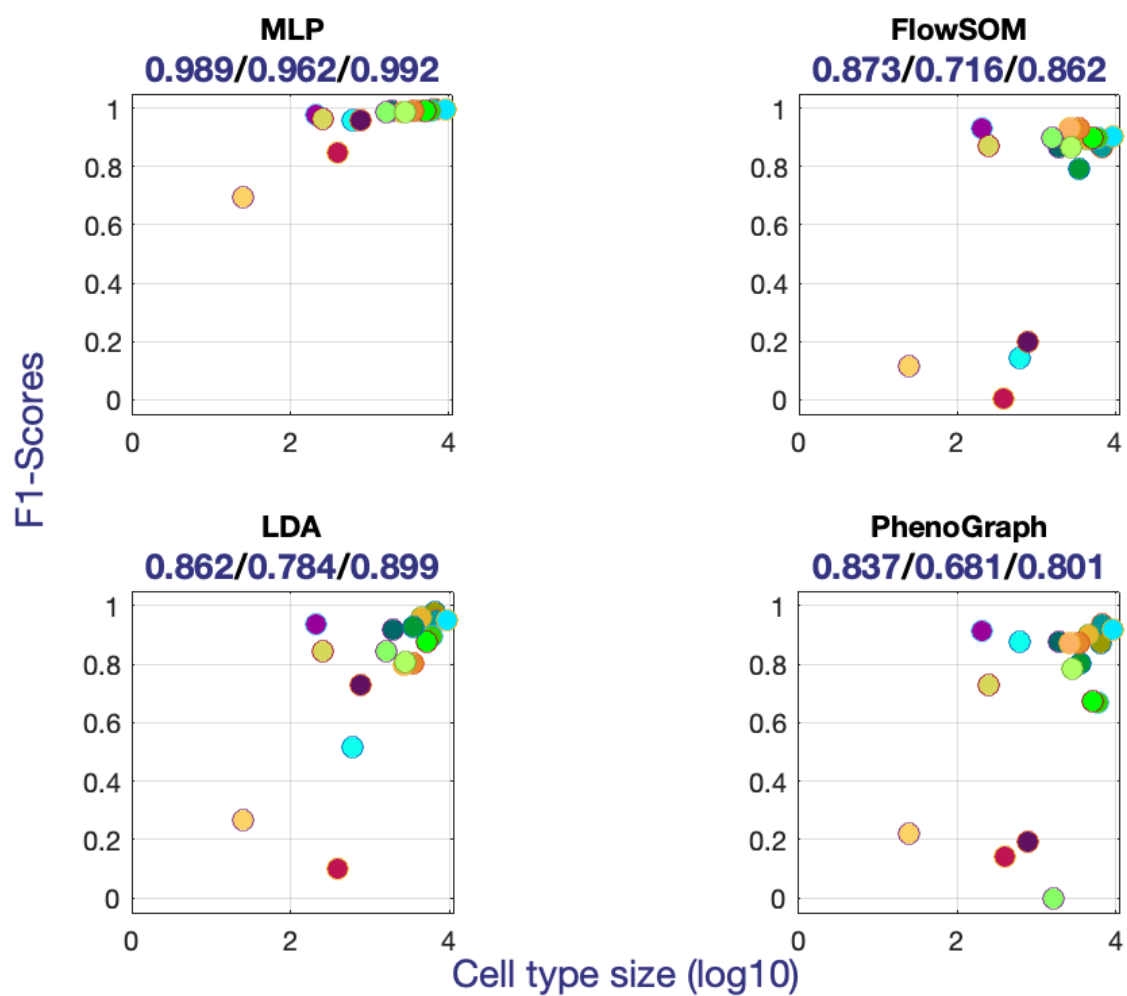
Eliver Eid Bou Ghosn, Alexandra A. Cassado, Gregory R. Govoni, +6, and Leonore A. Herzenberg (2010), **Two physically, functionally, and developmentally distinct peritoneal macrophage subsets**, PNAS Vol. 107|No. 6 2568-2573, January 25, 2010
<https://doi.org/10.1073/pnas.0915000107>

3.5.8. LEIPOLD

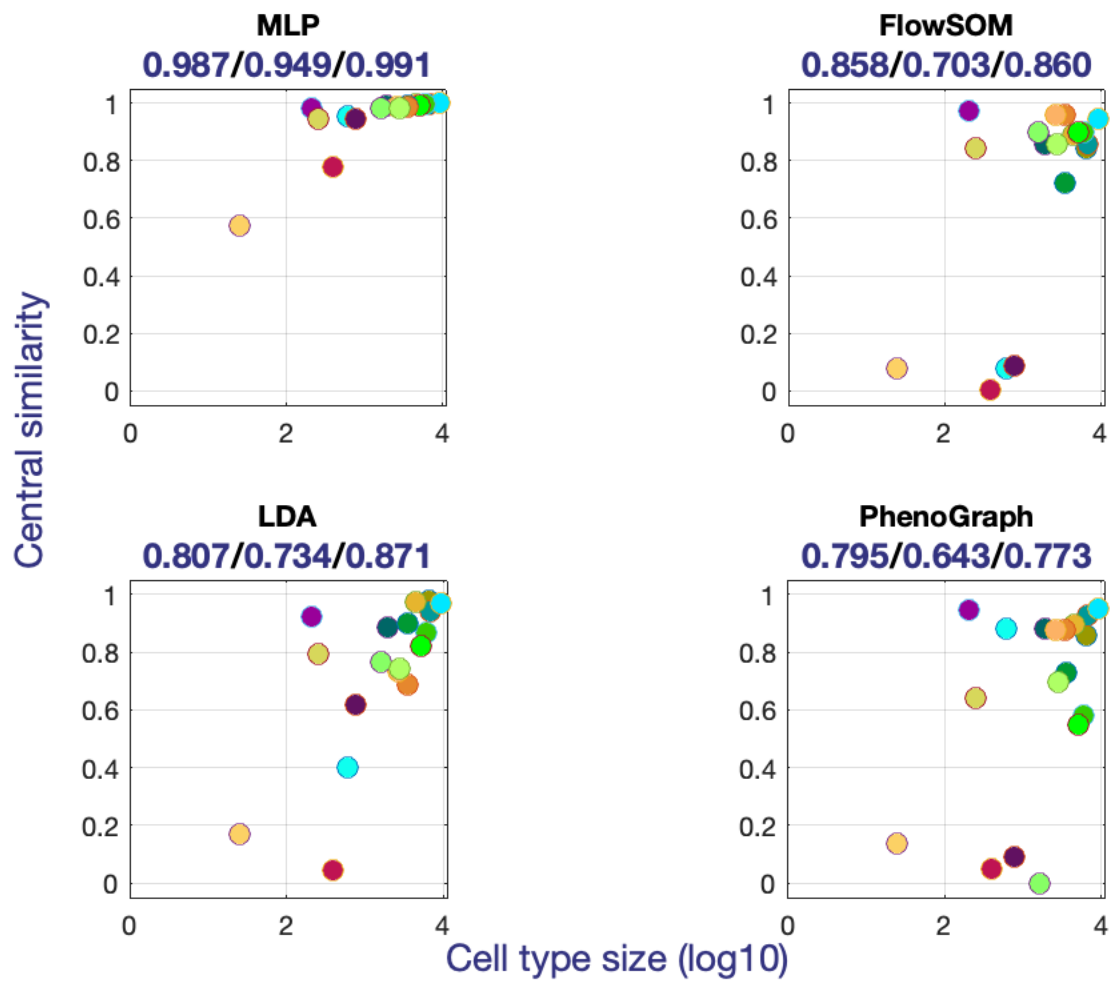
6 samples,4-fold cross validation: 5x1 training by test samples;
18 cell types, 15 markers

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP 	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
	NK cells	12%	0.997	0.873	0.977	0.872	0.997	0.845	0.978	0.858	0.999	0.951	0.992	0.947
	CD4 T cells CD45RA- , CD27+	12%	0.997	0.866	0.950	0.939	0.997	0.858	0.940	0.929	0.999	0.953	0.989	0.991
	CD4 T cells CD45RA+ , CD27+	16%	0.996	0.902	0.951	0.916	0.999	0.944	0.969	0.949	0.999	0.972	0.981	0.975
	CD4 T cells CD45RA- , CD27-	3.4%	0.994	0.866	0.920	0.878	0.993	0.858	0.885	0.880	0.998	0.953	0.975	0.944
	CD16- monocytes	7.9%	0.994	0.894	0.959	0.900	0.997	0.888	0.974	0.896	0.999	0.956	0.971	0.961
	CD8 T cells CD45RA+ , CD27+	11%	0.993	0.898	0.897	0.669	0.994	0.901	0.866	0.582	0.999	0.967	0.952	0.840
	CD8 T cells CD45RA+ , CD27-	9.1%	0.993	0.898	0.878	0.671	0.993	0.901	0.819	0.548	0.998	0.967	0.980	0.902
	CD8 T cells CD45RA- , CD27+	6.3%	0.993	0.794	0.929	0.804	0.992	0.724	0.898	0.731	0.999	0.957	0.980	0.968
	CD38 CD56- B cells	6.2%	0.991	0.931	0.805	0.870	0.988	0.958	0.688	0.876	0.998	0.964	0.941	0.914
	CD38+CD56 B cells	4.7%	0.988	0.931	0.797	0.870	0.985	0.958	0.735	0.876	0.998	0.964	0.955	0.914
	CD8 T cells CD45RA- , CD27-	2.8%	0.986	0.898	0.846	N/A	0.985	0.901	0.767	N/A	0.997	0.967	0.958	N/A
	CD4- CD8-	5%	0.986	0.866	0.806	0.786	0.985	0.858	0.743	0.697	0.997	0.953	0.946	0.915
	pDCs	0.37%	0.980	0.933	0.935	0.915	0.984	0.973	0.922	0.948	0.989	0.948	0.960	0.941
	CD56 bright NK cells	0.44%	0.966	0.873	0.844	0.729	0.946	0.845	0.796	0.642	0.988	0.951	0.943	0.945
	CD4 T cells CD45RA+ , CD27-	1.1%	0.961	0.141	0.518	0.878	0.957	0.076	0.400	0.880	0.990	0.640	0.874	0.944
	mDCs	1.4%	0.959	0.197	0.730	0.194	0.946	0.089	0.619	0.091	0.990	0.572	0.925	0.555
	Basophils	0.69%	0.850	0.005	0.102	0.141	0.777	0.002	0.044	0.048	0.975	0.408	0.734	0.406
	CD16+ monocytes	0.04%	0.697	0.115	0.268	0.220	0.574	0.076	0.171	0.137	0.829	0.428	0.652	0.552
Median			0.989	0.873	0.862	0.837	0.987	0.858	0.807	0.795	0.998	0.953	0.957	0.928
Mean			0.962	0.716	0.784	0.681	0.949	0.703	0.734	0.643	0.986	0.860	0.928	0.812

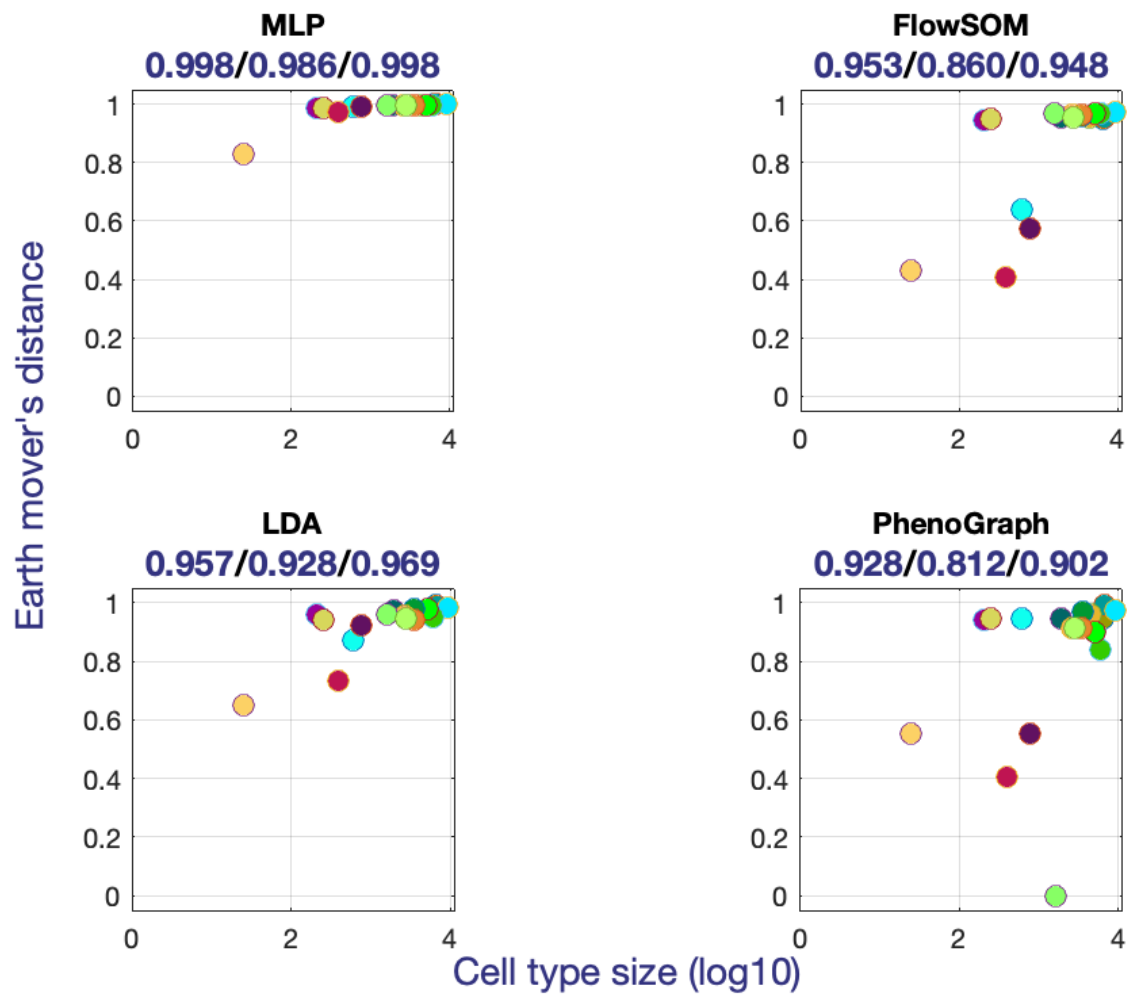
LEIPOLD F1-Scores median/mean/weighted



LEIPOLD Central similarity median/mean/weighted



LEIPOLD Earth mover's distance median/mean/weighted



3.5.8.1. Merged matches

With FlowSOM QFMatch finds 8 of 10 matches where merging multiple manual or FlowSOM gated populations obtains a higher F1-score. The 2nd, 3rd, 6th and 8th ranked matches merge ? manually gated populations to match 1 FlowSOM gated population. The 1st, 5th, 9th and 10th ranked matches merge multiple FlowSOM gated populations to match 1 manually gated population.

MATCH sets: training=all 18 matched!, test=16/18 (2 NEW!)										
Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.	
2	●	9	CD8 T cells CD45RA- , CD27-	4	89.8%	90.1%	96.7%	yes	2.7%	
2	●	13	CD8 T cells CD45RA+ , CD27-	4	89.8%	90.1%	96.7%	yes	9.8%	
2	●	14	CD8 T cells CD45RA+ , CD27+	4	89.8%	90.1%	96.7%	yes	13.3%	1
2	●	34	CD8 T cells CD45RA- , CD27- (Flow...	4	89.8%	90.1%	96.7%	no	21.6%	2
6	●	12	CD4 T cells CD45RA- , CD27+	4	86.6%	85.8%	95.3%	yes	14.8%	1
6	●	16	CD4 T cells CD45RA- , CD27-	4	86.6%	85.8%	95.3%	yes	4.3%	
6	●	18	CD4- CD8-	4	86.6%	85.8%	95.3%	yes	3.1%	
6	●	23	CD4 T cells CD45RA- , CD27+ (Flow...	4	86.6%	85.8%	95.3%	no	20.5%	1
1	●	15	CD4 T cells CD45RA+ , CD27+	3	90.2%	94.4%	97.2%	yes	16.9%	1
1	●	24	CD4 T cells CD45RA+ , CD27+ (Flo...	3	90.2%	94.4%	97.2%	no	0.9%	
1	●	27	CD4 T cells CD45RA+ , CD27+ (Flo...	3	90.2%	94.4%	97.2%	no	15%	1
3	●	3	CD38 CD56- B cells	3	93.1%	95.8%	96.4%	yes	3.8%	
3	●	4	CD38+CD56 B cells	3	93.1%	95.8%	96.4%	yes	3.8%	
3	●	32	CD38 CD56- B cells (FlowSOM.All c...	3	93.1%	95.8%	96.4%	no	7.3%	
5	●	1	CD16- monocytes	3	89.4%	88.8%	95.6%	yes	6.1%	
5	●	28	CD16- monocytes (FlowSOM.All cell...	3	89.4%	88.8%	95.6%	no	6.2%	
5	●	31	CD16- monocytes (FlowSOM.All cell...	3	89.4%	88.8%	95.6%	no	0.5%	
7	●	6	NK cells	3	87.3%	84.5%	95.1%	yes	11%	
7	●	17	CD56 bright NK cells	3	87.3%	84.5%	95.1%	yes	0.4%	
7	●	36	NK cells (FlowSOM.All cells.Pop3)	3	87.3%	84.5%	95.1%	no	13.5%	1
9	●	8	CD4 T cells CD45RA+ , CD27-	3	14.1%	7.6%	64%	yes	1.1%	
9	●	20	CD4 T cells CD45RA+ , CD27- (Flow...	3	14.1%	7.6%	64%	no	0.1%	
9	●	33	CD4 T cells CD45RA+ , CD27- (Flow...	3	14.1%	7.6%	64%	no	0.8%	
10	●	2	mDCs	3	19.7%	8.9%	57.2%	yes	0.9%	
10	●	22	mDCs (FlowSOM.All cells.Pop2)	3	19.7%	8.9%	57.2%	no	0.3%	
10	●	26	mDCs (FlowSOM.All cells.Pop9)	3	19.7%	8.9%	57.2%	no	2.8%	
4	●	5	CD8 T cells CD45RA- , CD27+	2	79.4%	72.4%	95.7%	yes	6.9%	
4	●	35	CD8 T cells CD45RA- , CD27+ (Flow...	2	79.4%	72.4%	95.7%	no	7.8%	

With PhenoGraph QFMatch finds 8 of 13 matches where merging multiple manual or PhenoGraph gated populations obtains a higher F1-score. The 7th and 10th ranked matches merge 2 manually gated populations to match 1 PhenoGraph gated population. The 1st, 2nd, 4th, 9th, 11th and 13th ranked matches merge multiple PhenoGraph gated populations to match 1 manually gated population.











Sync
 


 MATCH sets: training=17/18 (1 UNMATCHED!), test=23/27 (4 NEW!)

Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.	
2	●	15	CD4 T cells CD45RA+ , CD27+	4	91.6%	94.9%	97.5%	yes	16.9%	1
2	●	19	Phenograph4RFXF16	4	91.6%	94.9%	97.5%	no	1.2%	
2	●	30	Phenograph4RFXF2	4	91.6%	94.9%	97.5%	no	13.5%	1
2	●	39	Phenograph4RFXF19	4	91.6%	94.9%	97.5%	no	0.5%	
9	●	18	CD4- CD8-	4	78.6%	69.7%	91.5%	yes	3.1%	
9	●	22	Phenograph4RFXF23	4	78.6%	69.7%	91.5%	no	0.2%	
9	●	26	Phenograph4RFXF14	4	78.6%	69.7%	91.5%	no	1.3%	
9	●	33	Phenograph4RFXF12	4	78.6%	69.7%	91.5%	no	1.8%	
1	●	12	CD4 T cells CD45RA- , CD27+	3	93.9%	92.9%	99.1%	yes	14.8%	1
1	●	34	Phenograph4RFXF15	3	93.9%	92.9%	99.1%	no	1.2%	
1	●	41	Phenograph4RFXF4	3	93.9%	92.9%	99.1%	no	12.7%	1
4	●	1	CD16- monocytes	3	90%	89.6%	96.1%	yes	6.1%	
4	●	24	Phenograph4RFXF20	3	90%	89.6%	96.1%	no	0.5%	
4	●	37	Phenograph4RFXF8	3	90%	89.6%	96.1%	no	6.1%	
7	●	8	CD4 T cells CD45RA+ , CD27-	3	87.8%	88%	94.4%	yes	1.1%	
7	●	16	CD4 T cells CD45RA- , CD27-	3	87.8%	88%	94.4%	yes	4.3%	
7	●	40	Phenograph4RFXF9	3	87.8%	88%	94.4%	no	5%	
10	●	3	CD38 CD56- B cells	3	87%	87.6%	91.4%	yes	3.8%	
10	●	4	CD38+CD56 B cells	3	87%	87.6%	91.4%	yes	3.8%	
10	●	28	Phenograph4RFXF7	3	87%	87.6%	91.4%	no	6.1%	
11	●	13	CD8 T cells CD45RA+ , CD27-	3	67.1%	54.8%	90.2%	yes	9.8%	
11	●	32	Phenograph4RFXF11	3	67.1%	54.8%	90.2%	no	2.5%	
11	●	44	Phenograph4RFXF1	3	67.1%	54.8%	90.2%	no	13.6%	1
13	●	2	mDCs	3	19.4%	9.1%	55.5%	yes	0.9%	
13	●	21	Phenograph4RFXF24	3	19.4%	9.1%	55.5%	no	0.2%	
13	●	45	Phenograph4RFXF10	3	19.4%	9.1%	55.5%	no	2.8%	
3	●	5	CD8 T cells CD45RA- , CD27+	2	80.4%	73.1%	96.8%	yes	6.9%	
3	●	42	Phenograph4RFXF5	2	80.4%	73.1%	96.8%	no	7.5%	

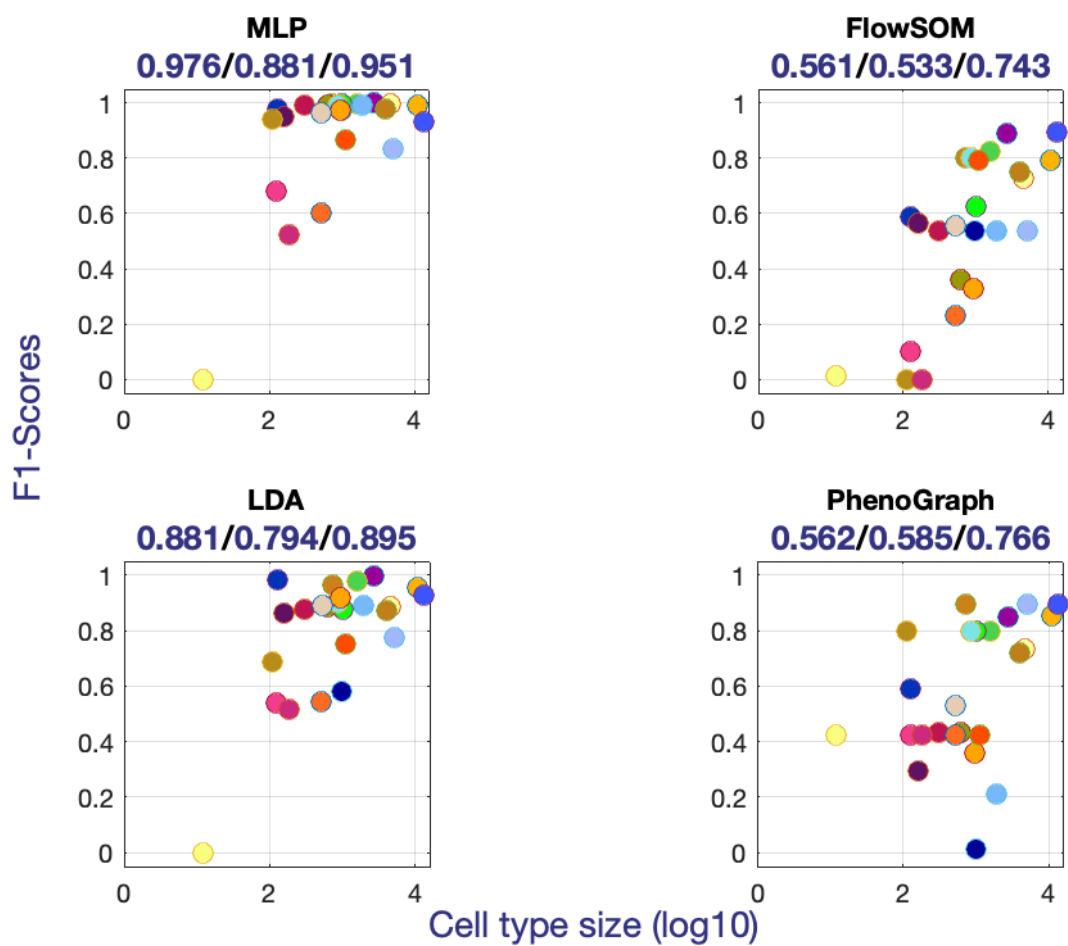
Michael D. Leipold, Gerlinde Obermoser, Craig Fenwick, Katja Kleinstuber, Narges Rashidi, John P. McNevin, Allison N. Nau, Lisa E. Wagar, Virginie Rozot, Mark M. Davis, Stephen DeRosa, Giuseppe Pantaleo, Thomas J. Scriba, Bruce D. Walker, Lars R. Olsen, Holden T. Maecker, (2018) **Comparison of CyTOF assays across sites: Results of a six-center pilot study**, Journal of Immunological Methods, Volume 453, Pages 37-43, ISSN 0022-1759, <https://www.sciencedirect.com/science/article/pii/S0022175917304908>

3.5.9. PANORAMA

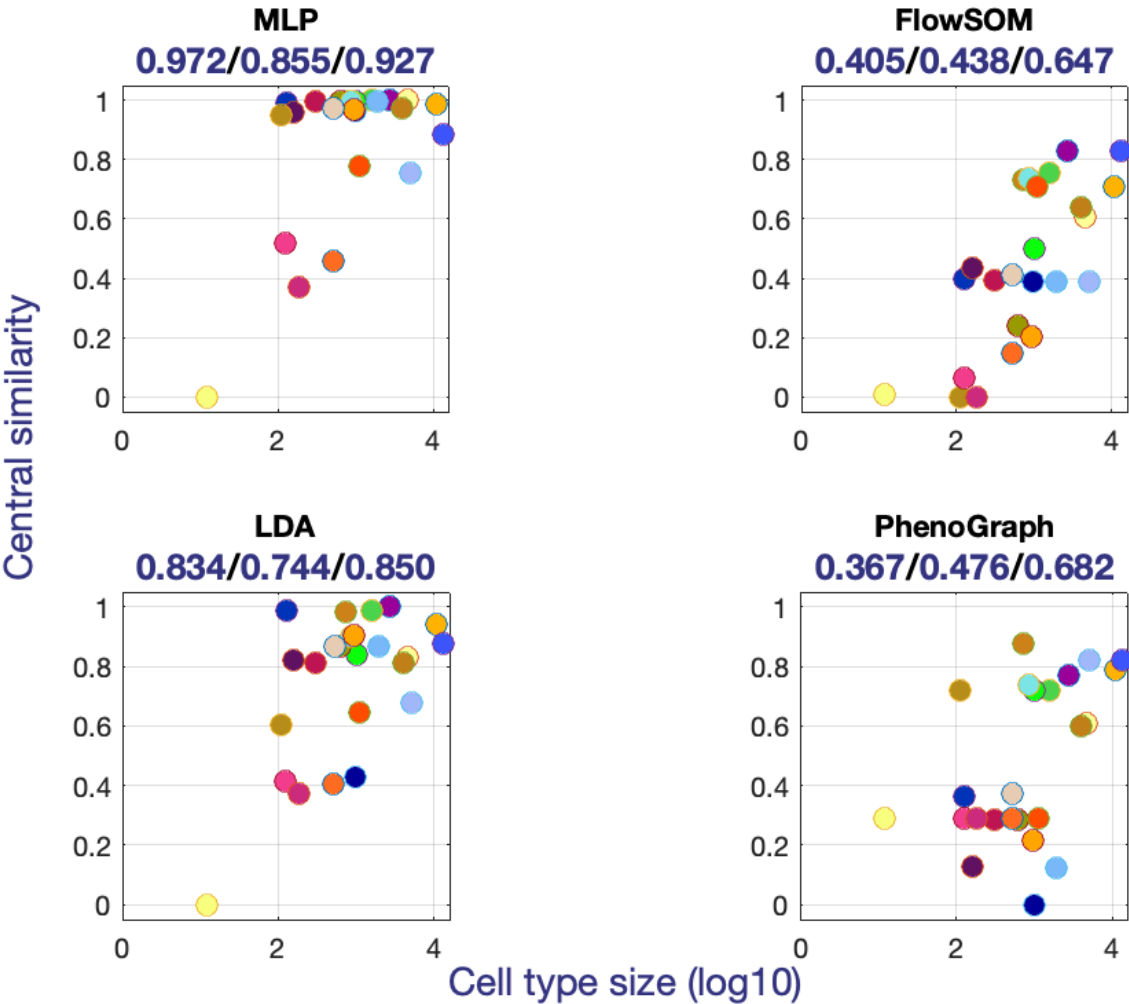
10 samples, 5-fold cross validation: 8x2 training by test samples;
24 cell types, 25 markers

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP 	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
●	pDCs	5.2%	0.999	0.891	0.999	0.851	1	0.832	1	0.771	0.999	0.942	0.999	0.869
●	Eosinophils	8.8%	0.998	0.729	0.887	0.731	0.999	0.605	0.830	0.609	0.999	0.826	0.916	0.833
●	CD8 T cells	3%	0.998	0.825	0.976	0.800	0.999	0.756	0.989	0.718	0.999	0.920	0.988	0.952
●	NKT cells	1.9%	0.996	0.625	0.876	0.800	0.997	0.498	0.838	0.718	0.998	0.904	0.933	0.952
●	Non classical Monocytes	1.4%	0.994	0.800	0.967	0.897	0.997	0.733	0.984	0.877	0.997	0.884	0.985	0.976
●	B cells Frac. D	3.7%	0.994	0.537	0.891	0.212	0.997	0.387	0.868	0.126	0.998	0.825	0.974	0.787
●	NK cells	1.2%	0.993	0.359	0.885	0.432	0.995	0.239	0.869	0.287	0.996	0.874	0.931	0.929
●	Classical Monocytes	21%	0.991	0.793	0.956	0.852	0.989	0.708	0.941	0.790	0.999	0.914	0.991	0.955
●	Basophils	0.57%	0.991	0.539	0.875	0.432	0.995	0.391	0.812	0.287	0.994	0.892	0.947	0.929
●	CD4 T cells	1.6%	0.990	0.800	0.898	0.800	0.996	0.738	0.901	0.738	0.993	0.950	0.947	0.956
●	Plasma Cells	0.24%	0.980	0.586	0.982	0.592	0.990	0.397	0.989	0.362	0.985	0.678	0.986	0.773
●	Intermediate Monocytes	7.7%	0.979	0.752	0.874	0.721	0.972	0.640	0.813	0.601	0.997	0.936	0.965	0.913
●	B cells Frac A-C	1.9%	0.973	0.537	0.581	0.011	0.966	0.387	0.428	0	0.995	0.825	0.890	0.390
●	MEP	1.8%	0.971	0.327	0.920	0.358	0.971	0.205	0.905	0.215	0.994	0.832	0.974	0.806
●	Macrophages	1%	0.965	0.556	0.889	0.531	0.972	0.413	0.868	0.373	0.991	0.908	0.968	0.905
●	mDCs	0.30%	0.952	0.566	0.865	0.293	0.959	0.435	0.821	0.128	0.978	0.827	0.945	0.694
●	gd T cells	0.21%	0.940	N/A	0.686	0.800	0.948	N/A	0.606	0.718	0.971	N/A	0.853	0.952
●	B cells Frac. F	25%	0.933	0.895	0.926	0.895	0.885	0.829	0.875	0.823	0.990	0.984	0.986	0.914
●	GMP	2.1%	0.866	0.793	0.753	0.426	0.778	0.708	0.645	0.291	0.986	0.914	0.904	0.801
●	B cells Frac. E	9.8%	0.833	0.537	0.775	0.895	0.755	0.387	0.680	0.823	0.956	0.825	0.957	0.914
●	CLP	0.24%	0.682	0.103	0.541	0.426	0.520	0.062	0.413	0.291	0.934	0.256	0.820	0.801
●	CMP	1%	0.604	0.232	0.546	0.426	0.460	0.149	0.407	0.291	0.945	0.899	0.914	0.801
●	MPP	0.35%	0.523	0	0.514	0.426	0.371	0	0.375	0.291	0.915	0.379	0.892	0.801
●	HSC	0.02%	0	0.011	0	0.426	0	0.007	0	0.291	0	0.464	0.118	0.801
Median			0.976	0.561	0.881	0.562	0.972	0.405	0.834	0.367	0.993	0.879	0.947	0.887
Mean			0.881	0.533	0.794	0.585	0.855	0.438	0.744	0.476	0.942	0.777	0.908	0.850

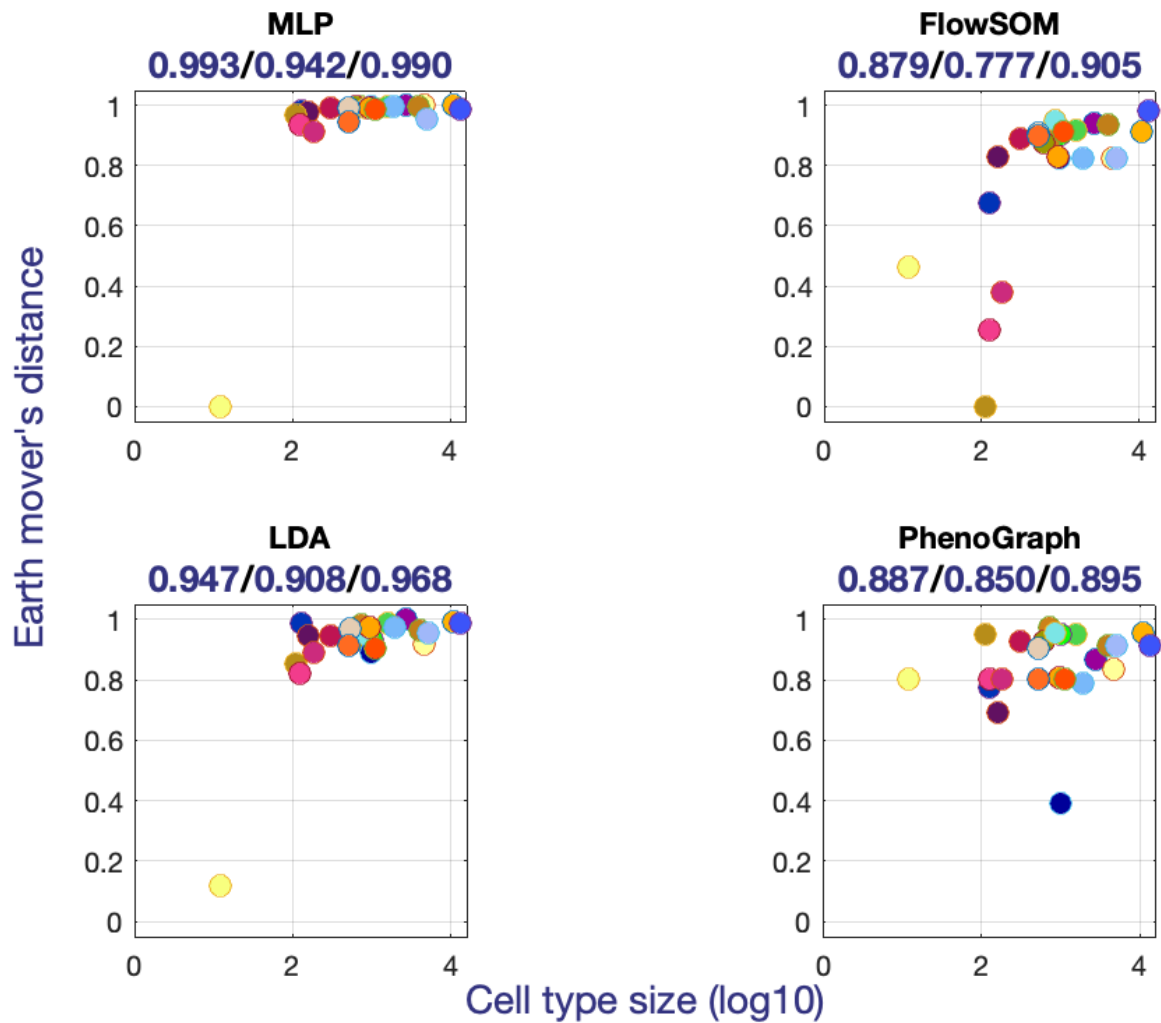
PANORAMA F1-Scores median/mean/weighted



PANORAMA Central similarity median/mean/weighted



PANORAMA Earth mover's distance median/mean/weighted



3.5.9.1. Merged matches

With FlowSOM QFMatch finds 5 of 20 matches where merging multiple manual or FlowSOM gated populations obtains a higher F1-score. The 6th and 16th ranked matches merge multiple manually gated populations to match 1 FlowSOM gated population. The 3rd, 8th and 9th ranked matches merge 2 FlowSOM gated populations to match 1 manually gated population.

MATCH sets: training=23/24 (1 UNMATCHED!), test=23/24 (1 NEW!)										
Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.	
16	•	4	B cells Frac. E	4	53.7%	38.7%	82.5%	yes	6.5%	
16	•	15	B cells Frac. D	4	53.7%	38.7%	82.5%	yes	1.8%	
16	•	24	B cells Frac A-C	4	53.7%	38.7%	82.5%	yes	1%	
16	•	40	FlowSOM.non-Neutrophils.Pop7	4	53.7%	38.7%	82.5%	no	10.8%	
3	•	8	pDCs	3	89.1%	83.2%	94.2%	yes	5.9%	
3	•	33	FlowSOM.non-Neutrophils.Pop4	3	89.1%	83.2%	94.2%	no	1.5%	
3	•	43	FlowSOM.non-Neutrophils.Pop2	3	89.1%	83.2%	94.2%	no	2.4%	
6	•	3	Classical Monocytes	3	79.3%	70.8%	91.4%	yes	28.8%	
6	•	18	GMP	3	79.3%	70.8%	91.4%	yes	2.7%	
6	•	35	FlowSOM.non-Neutrophils.Pop0	3	79.3%	70.8%	91.4%	no	29.5%	
8	•	10	NKT cells	3	62.5%	49.8%	90.4%	yes	2.3%	
8	•	26	FlowSOM.non-Neutrophils.Pop15	3	62.5%	49.8%	90.4%	no	1.6%	
8	•	39	FlowSOM.non-Neutrophils.Pop14	3	62.5%	49.8%	90.4%	no	0.8%	
9	•	9	CMP	3	23.2%	14.9%	89.9%	yes	1%	
9	•	30	FlowSOM.non-Neutrophils.Pop12	3	23.2%	14.9%	89.9%	no	3.6%	
9	•	41	FlowSOM.non-Neutrophils.Pop18	3	23.2%	14.9%	89.9%	no	1.2%	
1	•	13	B cells Frac. F	2	89.5%	82.9%	98.4%	yes	19.7%	
1	•	44	FlowSOM.non-Neutrophils.Pop3	2	89.5%	82.9%	98.4%	no	16.4%	

Samusik, N., Good, Z., Spitzer, M. et al. **Automated mapping of phenotype space with single-cell data**. Nat Methods 13, 493–496 (2016).
<https://doi.org/10.1038/nmeth.3863>

4. Testing Round 2

In the second round of our testing we do the same as in [round 1](#) with LDA and MLP: training and predicting uses data with unclassified cells removed and population matching is 1-to-1. With FlowSOM and PhenoGraph the data usage is the same as in round 1 (on both classified and unclassified cells) but the matching of automated populations is done many-to-1 with manually gated populations using our QFMatch. This means only FlowSOM or PhenoGraph populations are merged in order to obtain the best F1-score and thus one manually gated population can match 1 or more automatic gated populations.

4.1. Overall results

The overall accuracy of each classifier in matching 197 known cell populations from 9 different published datasets is

Performance metric Classifier	F1-Score		Central Similarity		EMD	
	Median	Mean	Median	Mean	Median	Mean
MLP	0.99	0.95	0.99	0.94	1	0.98
FlowSOM	0.61	0.48	0.48	0.44	0.83	0.61
LDA	0.88	0.81	0.83	0.76	0.96	0.93
PhenoGraph	0.76	0.60	0.69	0.55	0.92	0.73

4.2. Results for datasets

The table below shows classifier accuracy for *each* dataset.

Dataset	MLP			FlowSOM			LDA			PhenoGraph		
	<i>F1-Score</i>	<i>Central similarity</i>	<i>EMD</i>	<i>F1-Score</i>	<i>Central similarity</i>	<i>EMD</i>	<i>F1-Score</i>	<i>Central similarity</i>	<i>EMD</i>	<i>F1-Score</i>	<i>Central similarity</i>	<i>EMD</i>

OMIP-044 ¹⁰ 13 cell populations defined with 14 markers collected by a conventional cytometer	1 0.99	1 1	1 1	0.61 0.49	0.51 0.46	0.77 0.70	0.93 0.85	0.90 0.81	0.98 0.94	0.91 0.81	0.92 0.78	0.95 0.92
OMIP-047 ¹¹ 8 cell populations defined with 9 markers collected by a conventional cytometer	1 1	1 1	1 1	0.76 0.60	0.67 0.55	0.90 0.72	0.96 0.96	0.95 0.96	0.98 0.98	0.89 0.83	0.87 0.77	0.97 0.93
OMIP-058 ¹² 35 cell populations defined with 17 markers collected by a conventional cytometer	0.99 0.97	0.99 0.97	1 0.99	0.44 0.42	0.31 0.38	0.87 0.55	0.84 0.76	0.81 0.70	0.95 0.93	0.48 0.44	0.77 0.58	0.86 0.56
OMIP-069 ¹³ 43 cell populations defined with 26 markers collected by a spectral cytometer	0.98 0.93	0.97 0.90	0.99 0.98	0.31 0.35	0.20 0.29	0.78 0.63	0.83 0.76	0.73 0.68	0.95 0.92	0.28 0.34	0.15 0.29	0.75 0.54
OMIP-077 ¹⁴ 14 cell populations defined with 14 markers collected by a conventional cytometer	0.97 0.89	0.97 0.85	0.99 0.96	0.65 0.52	0.55 0.50	0.90 0.59	0.72 0.62	0.62 0.57	0.88 0.87	0.91 0.66	0.92 0.65	0.96 0.73
ESHGHI ³⁵ 29 cell populations defined with 27 parameters collected by a mass cytometer	1 0.99	1 0.99	1 1	0.60 0.49	0.48 0.46	0.76 0.60	0.90 0.86	0.86 0.81	0.97 0.95	0.76 0.61	0.69 0.57	0.93 0.76
GHOSN ¹⁶ 13 cell populations defined with 9 markers collected by a conventional cytometer	0.99 0.94	0.99 0.92	1 0.98	0.81 0.60	0.74 0.59	0.88 0.64	0.92 0.89	0.93 0.85	0.96 0.94	0.81 0.71	0.74 0.65	0.91 0.82
LEIPOLD ³⁶ 18 cell populations defined with 15 markers collected by a mass cytometer	0.99 0.96	0.99 0.95	1 0.99	0.21 0.40	0.11 0.36	0.63 0.50	0.86 0.78	0.80 0.73	0.96 0.93	0.70 0.60	0.61 0.54	0.92 0.76
PANORAMA ¹⁵ 24 cell populations defined with 25 markers collected by a mass cytometer	0.97 0.88	0.97 0.86	0.99 0.94	0.55 0.45	0.40 0.37	0.85 0.69	0.88 0.79	0.83 0.74	0.95 0.91	0.32 0.38	0.19 0.31	0.74 0.58

Legend notes:

- Shading differentiates the rank of the classifier for each dataset: 1st best, 2nd best, 3rd best, 4th.
- The thickness of the table border around a ranking varies based on how much bigger it is than the next lower ranked classifier.
- Mean font size and **boldness** varies based on difference with median $\leq .5$ difference, $> .5$ & $\leq .15$ difference and $> .15$ difference. For example with the scores for FlowSOM with

TOHI ESHGHI dataset we see

- .94 **.84** for F1-score
- .95 **.82** for Central similarity
- .96 ^{.93} for EMD

4.2.1. Effects of many-to-many matching

The difference between this and the prior round's testing for FlowSOM and PhenoGraph is matching automatic populations and manually gated populations 1-to-many instead of many-to-many.

Our QFMatch software provides 4 options for merging

1. Merging subsets in both the training set and in the test set, which allows for *many-to-many matching*.
2. Merging subsets only in the test set which allows for *1-to-many matching*.
3. Merging subsets only in the training set which allows for *many-to-1 matching*.
4. No merging.

The testing results indicate that unsupervised automatically classified populations match better to manually gated populations when many-to-many matching is used.

4.2.1.1. In overall accuracy

Performance metric Classifier	<i>F1-score</i>		<i>Central Similarity</i>		<i>EMD</i>	
	<i>Median</i>	<i>Mean</i>	<i>Median</i>	<i>Mean</i>	<i>Median</i>	<i>Mean</i>
FlowSOM						
Many-to-many	0.87	0.74	0.86	0.70	0.96	0.87
1-to-many	0.61	0.48	0.48	0.44	0.83	0.61
PhenoGraph						
Many-to-many	0.87	0.72	0.84	0.66	0.95	0.87
1-to-many	0.76	0.60	0.69	0.55	0.92	0.73

4.2.1.2. In accuracy per dataset

	FlowSOM	PhenoGraph
--	----------------	-------------------

Dataset	Many-to-many			1-to-many			Many-to-many			1-to-many		
	F1-score	Central similarity	EMD	F1-score	Central similarity	EMD	F1-score	Central similarity	EMD	F1-score	Central similarity	EMD
OMIP-044 ¹⁰ 13 cell populations defined with 14 markers collected by a conventional cytometer	.97 .88 See	.98 .86	.98 .94	0.61 0.49	0.51 0.46	0.77 0.70	.92 .81	.92 .78	.96 .93	0.91 0.81	0.92 0.78	0.95 0.92
OMIP-047 ¹¹ 8 cell populations defined with 9 markers collected by a conventional cytometer	.87 .86 See	.83 .81	.96 .95	0.76 0.60	0.67 0.55	0.90 0.72	.90 .83	.87 .77	.97 .93	0.89 0.83	0.87 0.77	0.97 0.93
OMIP-058 ¹² 35 cell populations defined with 17 markers collected by a conventional cytometer	.80 .60 See	.73 .55	.92 .77	0.44 0.42	0.31 0.38	0.87 0.55	.82 .63	.77 .58	.93 .77	0.48 0.44	0.77 0.58	0.86 0.56
OMIP-069 ¹³ 43 cell populations defined with 26 markers collected by a spectral cytometer	.51 .48 See	.37 .40	.83 .74	0.31 0.35	0.20 0.29	0.78 0.63	.55 .52	.41 .43	.86 .81	0.28 0.34	0.15 0.29	0.75 0.54
OMIP-077 ¹⁴ 14 cell populations defined with 14 markers collected by a conventional cytometer	.96 .92 See	.95 .92	.98 .99	0.65 0.52	0.55 0.50	0.90 0.59	.96 .86	.96 .86	.99 .94	0.91 0.66	0.92 0.65	0.96 0.73
ESHGHI ³⁵ 29 cell populations defined with 27 parameters collected by a mass cytometer	.94 .84 See	.95 .82	.96 .93	0.60 0.49	0.48 0.46	0.76 0.60	.88 .74	.84 .71	.95 .87	0.76 0.61	0.69 0.57	0.93 0.76
GHOSN ¹⁶ 13 cell populations defined with 9 markers collected by a conventional cytometer	.93 .83 See	.92 .82	.96 .88	0.81 0.60	0.74 0.59	0.88 0.64	.87 .79	.89 .74	.95 .92	0.81 0.71	0.74 0.65	0.91 0.82
LEIPOLD ³⁶ 18 cell populations defined with 15 markers collected by a mass cytometer	.87 .72 See	.86 .70	.95 .86	0.21 0.40	0.11 0.36	0.63 0.50	.84 .68	.80 .64	.93 .81	0.70 0.60	0.61 0.54	0.92 0.76
PANORAMA ¹⁵ 24 cell populations defined with 25 markers collected by a mass cytometer	.56 .53 See	.41 .44	.88 .78	0.55 0.45	0.40 0.37	0.85 0.69	.56 .59	.37 .48	.89 .85	0.32 0.38	0.19 0.31	0.74 0.58

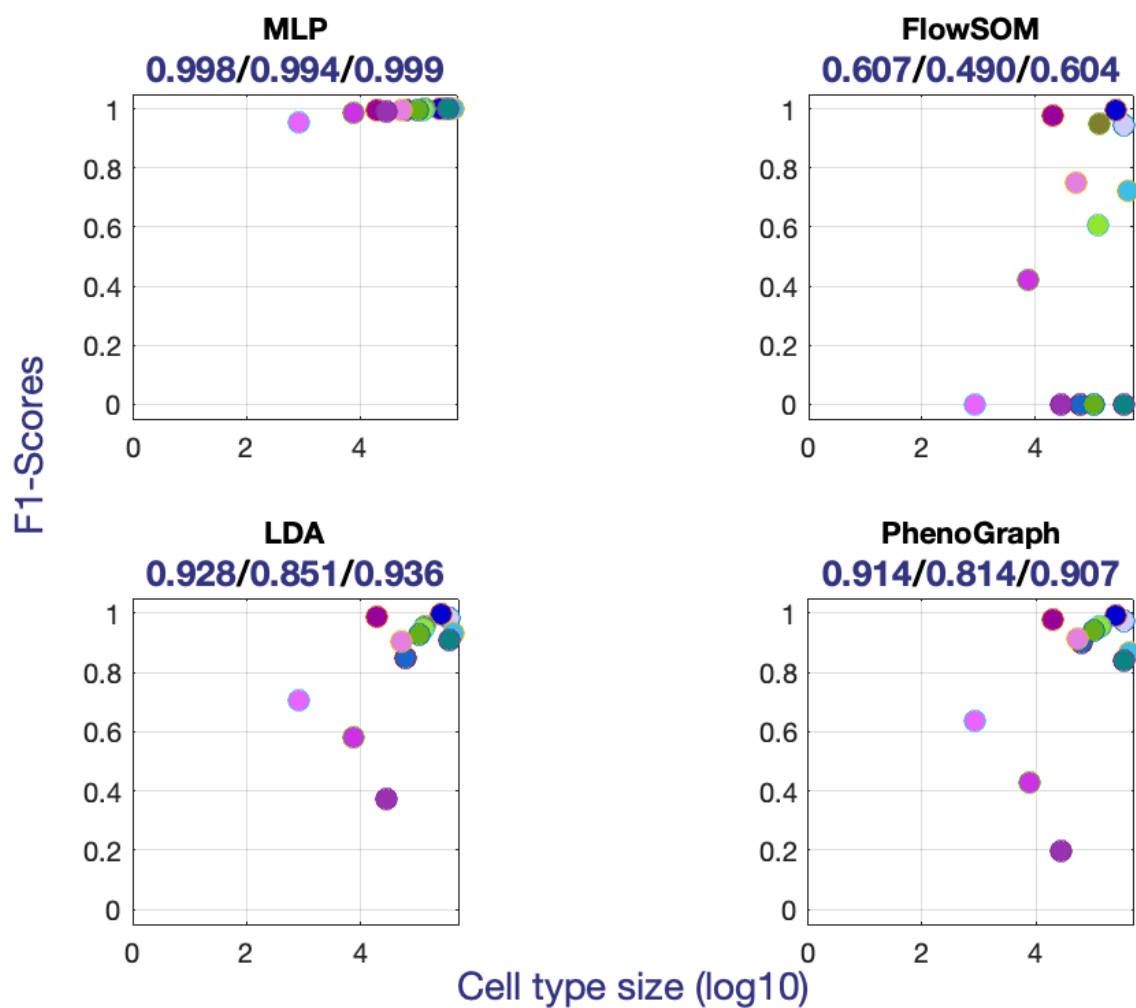
4.3. Results for populations

OMIP-044

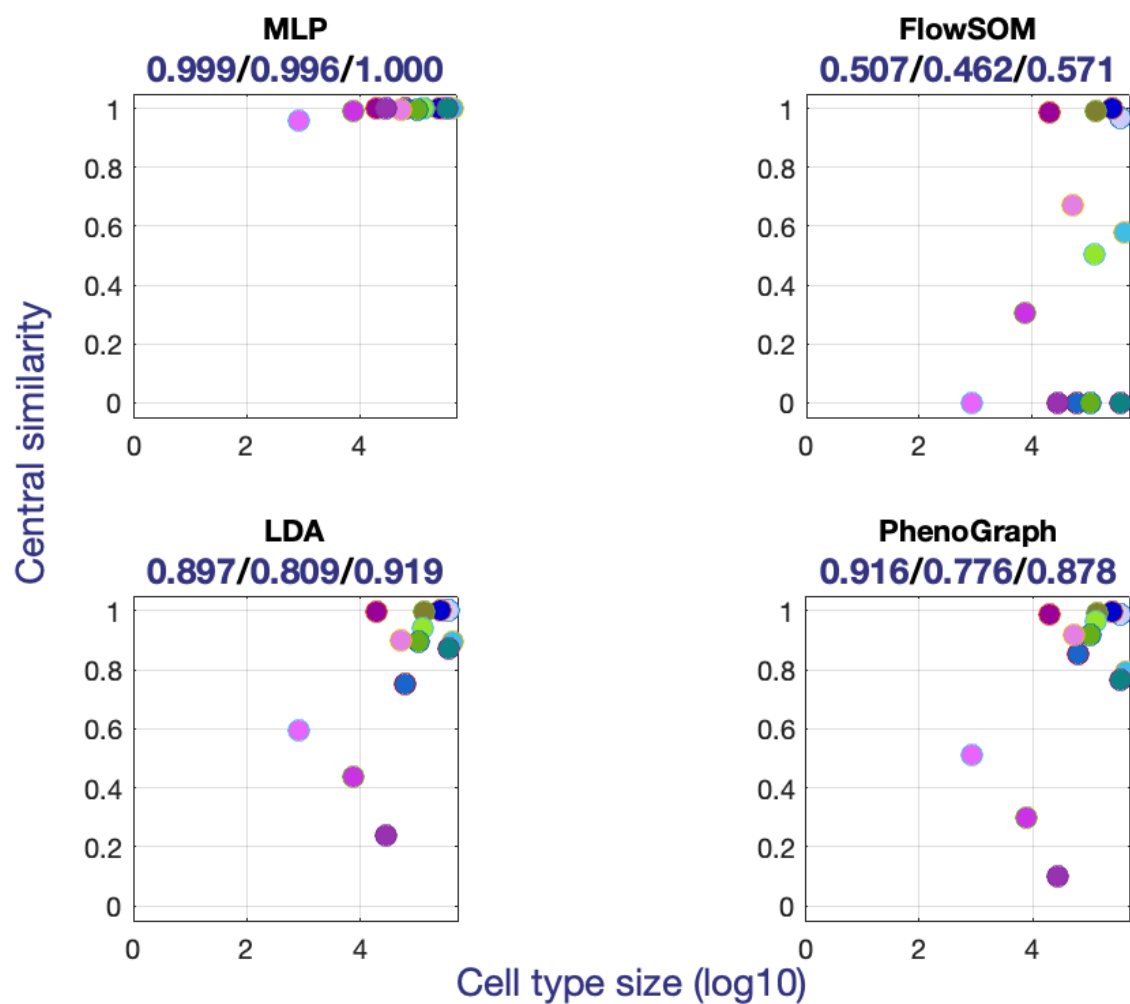
2 samples (~2 million cells each), 2-fold cross validation, 1x1 training x test samples,
13 cell types, 14 markers.

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP 	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
	CD14+	18%	1	0.944	0.984	0.974	1	0.970	1	0.989	1	0.954	0.984	0.990
	CD19+	13%	1	0.995	0.997	0.994	1	0.999	1	0.999	1	0.998	0.999	0.998
	naive CD4+	22%	1	0.722	0.931	0.869	1	0.578	0.896	0.792	1	0.822	0.984	0.970
	not naive CD4+	18%	1	N/A	0.910	0.840	1	N/A	0.871	0.765	1	N/A	0.977	0.952
	CD56+ NK	7%	0.999	0.952	0.955	0.954	1	0.994	0.997	0.994	1	0.943	0.941	0.939
	naive CD8+	6.5%	0.999	0.607	0.948	0.954	0.999	0.507	0.940	0.962	1	0.699	0.988	0.985
	DN	3.2%	0.998	N/A	0.851	0.900	1	N/A	0.752	0.854	1	N/A	0.873	0.950
	not naive CD8+	5.4%	0.998	N/A	0.928	0.939	0.997	N/A	0.897	0.916	1	N/A	0.977	0.986
	CD123+ pDC	1%	0.997	0.978	0.987	0.981	0.999	0.986	0.999	0.989	0.997	0.993	0.993	0.992
	DN DCs	2.7%	0.996	0.750	0.906	0.914	0.999	0.672	0.900	0.916	0.999	0.825	0.949	0.954
	DCs-	1.4%	0.993	0	0.375	0.197	0.999	0	0.238	0.102	0.998	0.402	0.847	0.700
	CD1c DCs	0.39%	0.988	0.423	0.582	0.426	0.991	0.306	0.438	0.298	0.998	0.770	0.813	0.749
	CD141+DCs	0.04%	0.955	N/A	0.703	0.637	0.959	N/A	0.595	0.510	0.990	N/A	0.842	0.838
Median			0.998	0.607	0.928	0.914	0.999	0.507	0.897	0.916	1	0.770	0.977	0.954
Mean			0.994	0.490	0.851	0.814	0.996	0.462	0.809	0.776	0.999	0.570	0.936	0.923

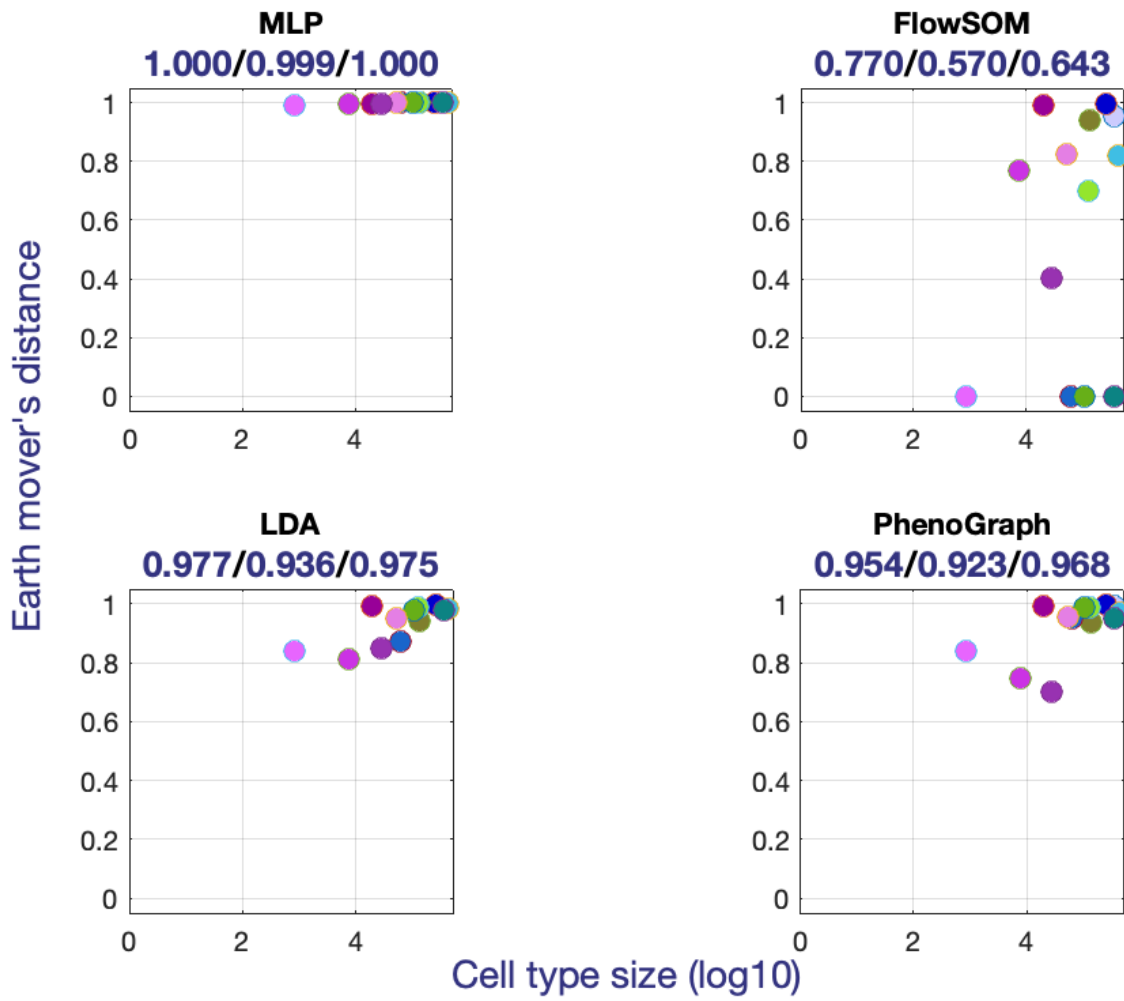
OMIP-044 F1-Scores median/mean/weighted



OMIP-044 Central similarity median/mean/weighted

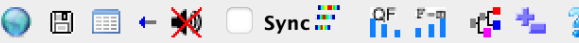


OMIP-044 Earth mover's distance median/mean/weighted



4.3.1.1. Merged matches

With FlowSOM QFMatch finds 2 of 9 matches where merging multiple FlowSOM gated populations to match 1 manually gated population obtains a higher F1-score: the 1st and 2nd, 3rd, 4th, 6th, 8th, 9th and 10th ranked matches.

 MATCH sets: training=9/13 (4 UNMATCHED!), test=11/13 (2 NEW!)									
Rank ²		#	Subset (class) name	Mat-ches ¹	Similarity (QFMatch)	% Overlap (F-measure)	Train-ing set? ³	Freq.	#
1	●	4	CD19+	3	99.8%	99.5%	yes	12.9%	252
1	●	16	FlowSOM.CD45+ live.Pop0	3	99.8%	99.5%	no	12.9%	253
1	●	22	FlowSOM.CD45+ live.Pop1	3	99.8%	99.5%	no	0%	
2	●	11	CD123+ pDC	3	99.3%	97.8%	yes	1.2%	23
2	●	20	FlowSOM.CD45+ live.Pop6	3	99.3%	97.8%	no	0.4%	7
2	●	21	FlowSOM.CD45+ live.Pop10	3	99.3%	97.8%	no	0.8%	16
3	●	2	CD14+	2	95.4%	94.4%	yes	19%	371
3	●	24	FlowSOM.CD45+ live.Pop11	2	95.4%	94.4%	no	16.9%	332

With PhenoGraph QFMatch finds 8 of 13 matches where merging multiple PhenoGraph gated populations to match 1 manually gated population obtains a higher F1-score: the 1st, 2nd, 3rd, 4th, 6th, 8th, 9th and 10th ranked matches.

Sync QF F1 MATCH sets: training=all 13 matched!, te

Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	Similarity (QFMatch)
6	●	7	naive CD4+	6	86.9%	97%
6	●	16	naive CD4+ (Phenograph2M5N24)	6	86.9%	97%
6	●	22	naive CD4+ (Phenograph2M5N11)	6	86.9%	97%
6	●	23	naive CD4+ (Phenograph2M5N29)	6	86.9%	97%
6	●	34	naive CD4+ (Phenograph2M5N1)	6	86.9%	97%
6	●	37	naive CD4+ (Phenograph2M5N3)	6	86.9%	97%
8	●	8	[not naive CD4+]	6	84%	95.2%
8	●	19	[not naive CD4+] (Phenograph2M5N4)	6	84%	95.2%
8	●	27	[not naive CD4+] (Phenograph2M5N10)	6	84%	95.2%
8	●	30	[not naive CD4+] (Phenograph2M5N22)	6	84%	95.2%
8	●	38	[not naive CD4+] (Phenograph2M5N31)	6	84%	95.2%
8	●	45	[not naive CD4+] (Phenograph2M5N9)	6	84%	95.2%
1	●	4	CD19+	5	99.4%	99.8%
1	●	14	CD19+ (Phenograph2M5N12)	5	99.4%	99.8%
1	●	25	CD19+ (Phenograph2M5N32)	5	99.4%	99.8%
1	●	40	CD19+ (Phenograph2M5N34)	5	99.4%	99.8%
1	●	41	CD19+ (Phenograph2M5N2)	5	99.4%	99.8%
3	●	2	CD14+	5	97.4%	99%
3	●	29	CD14+ (Phenograph2M5N8)	5	97.4%	99%
3	●	36	CD14+ (Phenograph2M5N13)	5	97.4%	99%
3	●	43	CD14+ (Phenograph2M5N5)	5	97.4%	99%
3	●	46	CD14+ (Phenograph2M5N18)	5	97.4%	99%
4	●	13	[not naive CD8+]	4	93.9%	98.6%
4	●	20	[not naive CD8+] (Phenograph2M5N21)	4	93.9%	98.6%
4	●	32	[not naive CD8+] (Phenograph2M5N14)	4	93.9%	98.6%
4	●	33	[not naive CD8+] (Phenograph2M5N16)	4	93.9%	98.6%
2	●	11	CD123+ pDC	3	98.1%	99.2%
2	●	18	CD123+ pDC (Phenograph2M5N20)	3	98.1%	99.2%
2	●	24	CD123+ pDC (Phenograph2M5N25)	3	98.1%	99.2%

Mair, F. and Prlic, M. (2018), **OMIP-044: 28-color immunophenotyping of the human dendritic cell compartment**. Cytometry, 93: 402-405.

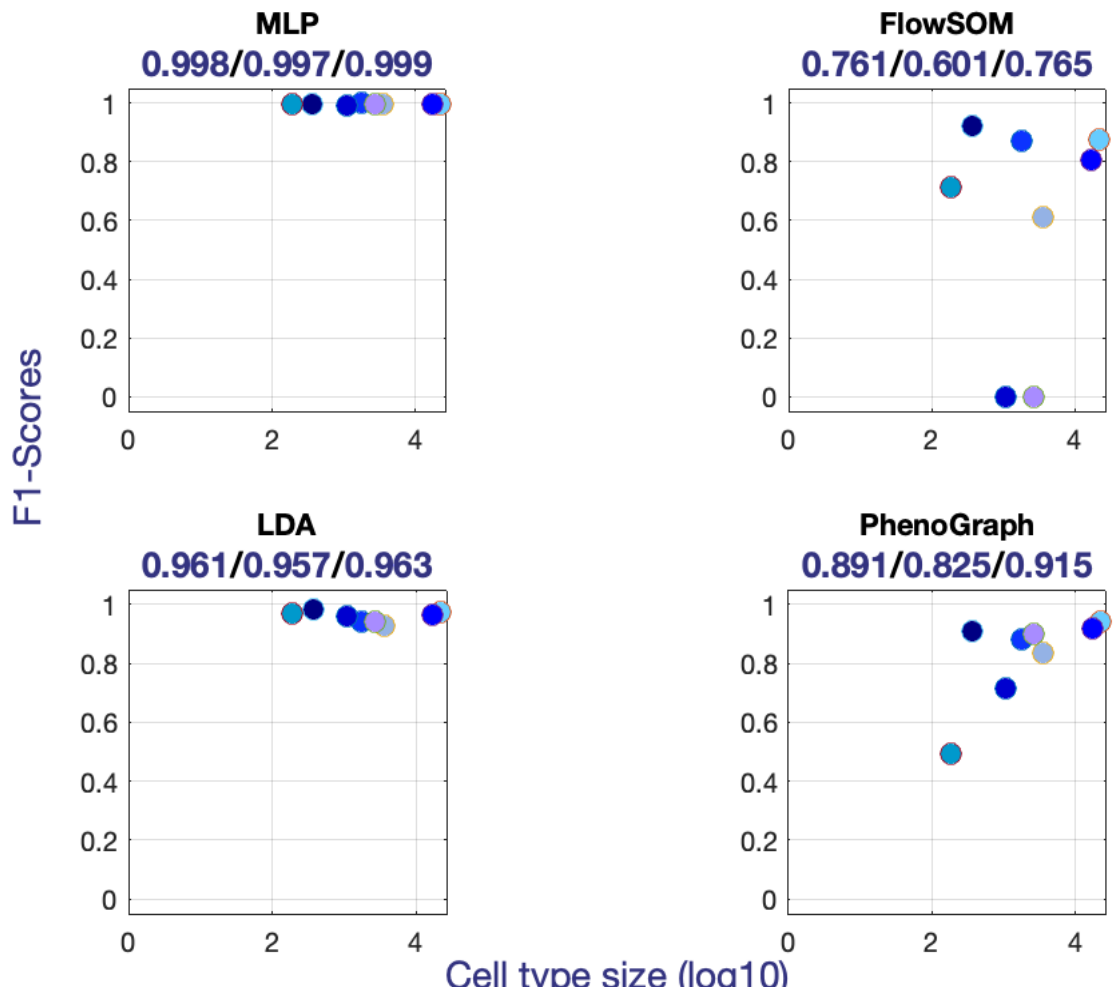
<https://doi.org/10.1002/cyto.a.23331>

4.3.2. OMIP-047

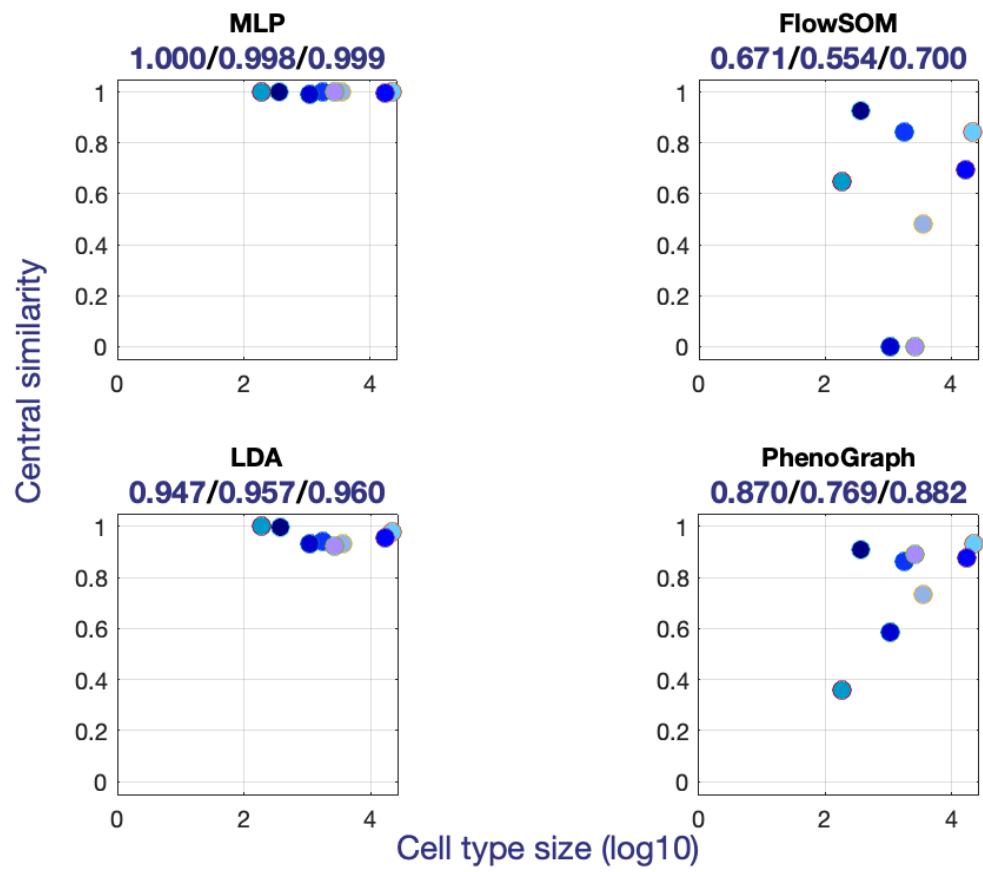
6 samples (~1 million cells each), 5 fold cross validation 5x1, 4x2, 4x2 and 5x1 training x test samples,
8 cell types, 9 markers

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
•	IgG1+	3.6%	0.999	0.873	0.939	0.883	1	0.842	0.940	0.865	0.999	0.959	0.963	0.970
•	Naive	45%	0.999	0.876	0.974	0.943	0.999	0.846	0.976	0.930	1	0.944	0.990	0.976
•	IgA_FSC-A Neg IgA IgG1 IgG3	7.3%	0.999	0.613	0.929	0.836	1	0.482	0.930	0.734	0.999	0.830	0.978	0.925
•	MZ B cells	35%	0.999	0.807	0.963	0.918	0.998	0.694	0.953	0.875	1	0.922	0.982	0.970
•	IgA_FSC-A IgA+	5.5%	0.998	0	0.942	0.899	0.999	0	0.923	0.893	0.999	0.240	0.971	0.971
•	IgG3+	0.75%	0.997	0.923	0.984	0.910	1	0.926	0.998	0.911	0.996	0.974	0.982	0.970
•	PB	0.38%	0.996	0.714	0.968	0.495	1	0.647	1	0.357	0.994	0.889	0.953	0.753
•	Transitional	2.2%	0.993	N/A	0.958	0.716	0.990	N/A	0.933	0.586	0.997	N/A	0.988	0.875
Median			0.998	0.761	0.961	0.891	1	0.671	0.947	0.870	0.999	0.905	0.980	0.970
Mean			0.997	0.601	0.957	0.825	0.998	0.554	0.957	0.769	0.998	0.720	0.976	0.926

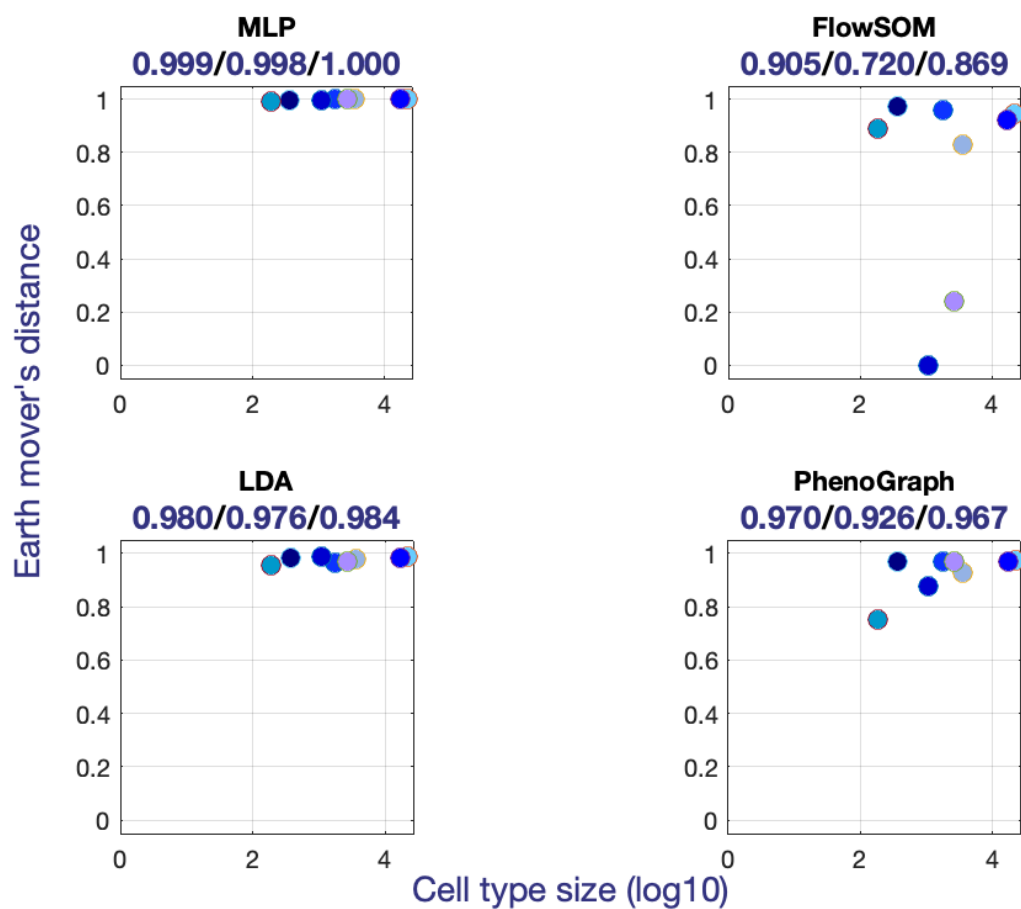
OMIP-047 F1-Scores median/mean/weighted



OMIP-047 Central similarity median/mean/weighted



OMIP-047 Earth mover's distance median/mean/weighted



4.3.2.1. Merged matches

With FlowSOM QFMatch finds 1 of 7 matches where merging 2 FlowSOM gated populations to match 1 manually gated population obtains a higher F1-score.

MATCH sets: training=7/8 (1 UNMATCHED), test=all 8 matched!									
Rank ²		Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set? ³	Freq.	
4	●	MZ B cells	3	80.7%	69.4%	92.2%	yes	33.1%	16
4	●	FlowSOM.B cells.Pop0	3	80.7%	69.4%	92.2%	no	0.6%	
4	●	FlowSOM.B cells.Pop1	3	80.7%	69.4%	92.2%	no	26.5%	14
1	●	IgG3+	2	92.3%	92.6%	97.4%	yes	0.8%	
1	●	FlowSOM.B cells.Pop5	2	92.3%	92.6%	97.4%	no	0.8%	
2	●	IgG1+	2	87.3%	84.2%	95.9%	yes	3.6%	·
2	●	FlowSOM.B cells.Pop6	2	87.3%	84.2%	95.9%	no	3.9%	·
3	●	Naive	2	87.6%	84.6%	94.4%	yes	45.9%	22
3	●	FlowSOM.B cells.Pop7	2	87.6%	84.6%	94.4%	no	52.6%	28
5	●	PB	2	71.4%	64.7%	88.9%	yes	0.4%	
5	●	FlowSOM.B cells.Pop4	2	71.4%	64.7%	88.9%	no	0.5%	
6	●	IgA, FSC-A Neg IgA IgG1 IgG3	2	61.3%	48.2%	83%	yes	8.7%	4
6	●	FlowSOM.B cells.Pop3	2	61.3%	48.2%	83%	no	14.7%	7
7	●	IgA, FSC-A IgA+	2	0%	0%	24%	yes	5.5%	·
7	●	FlowSOM.B cells.Pop2	2	0%	0%	24%	no	0.4%	
8	●	Transitional	0	N/A	N/A	N/A	yes	2.1%	·

With PhenoGraph QFMatch finds 3 of 8 matches where merging multiple PhenoGraph gated populations to match 1 manually gated population obtains a higher F1-score: the 1st, 3rd and 6th ranked matches.







 MATCH sets: training=all 8 matched!, test=13/14 (1 NEW!)

Rank ²	#	Subset (class) name	Mat-ches ¹	Similarity (QFMatch)	% Overlap (F-measure)	Train-ing set? ³	Freq.
1	1	Naive	4	97.6%	94.3%	yes	45.9%
1	17	PhenographWSN93	4	97.6%	94.3%	no	13%
1	18	PhenographWSN95	4	97.6%	94.3%	no	11.4%
1	21	PhenographWSN92	4	97.6%	94.3%	no	15%
3	5	MZ B cells	4	97%	91.8%	yes	33.1%
3	13	PhenographWSN94	4	97%	91.8%	no	12%
3	15	PhenographWSN91	4	97%	91.8%	no	15%
3	16	PhenographWSN96	4	97%	91.8%	no	7.8%
6	6	IgA, FSC-A Neg IgA IgG1 IgG3	3	92.5%	83.6%	yes	8.7%
6	9	PhenographWSN910	3	92.5%	83.6%	no	3.9%
6	10	PhenographWSN98	3	92.5%	83.6%	no	5.7%
2	7	IgA, FSC-A IgA+	2	97.1%	89.9%	yes	5.5%
2	12	PhenographWSN97	2	97.1%	89.9%	no	6%

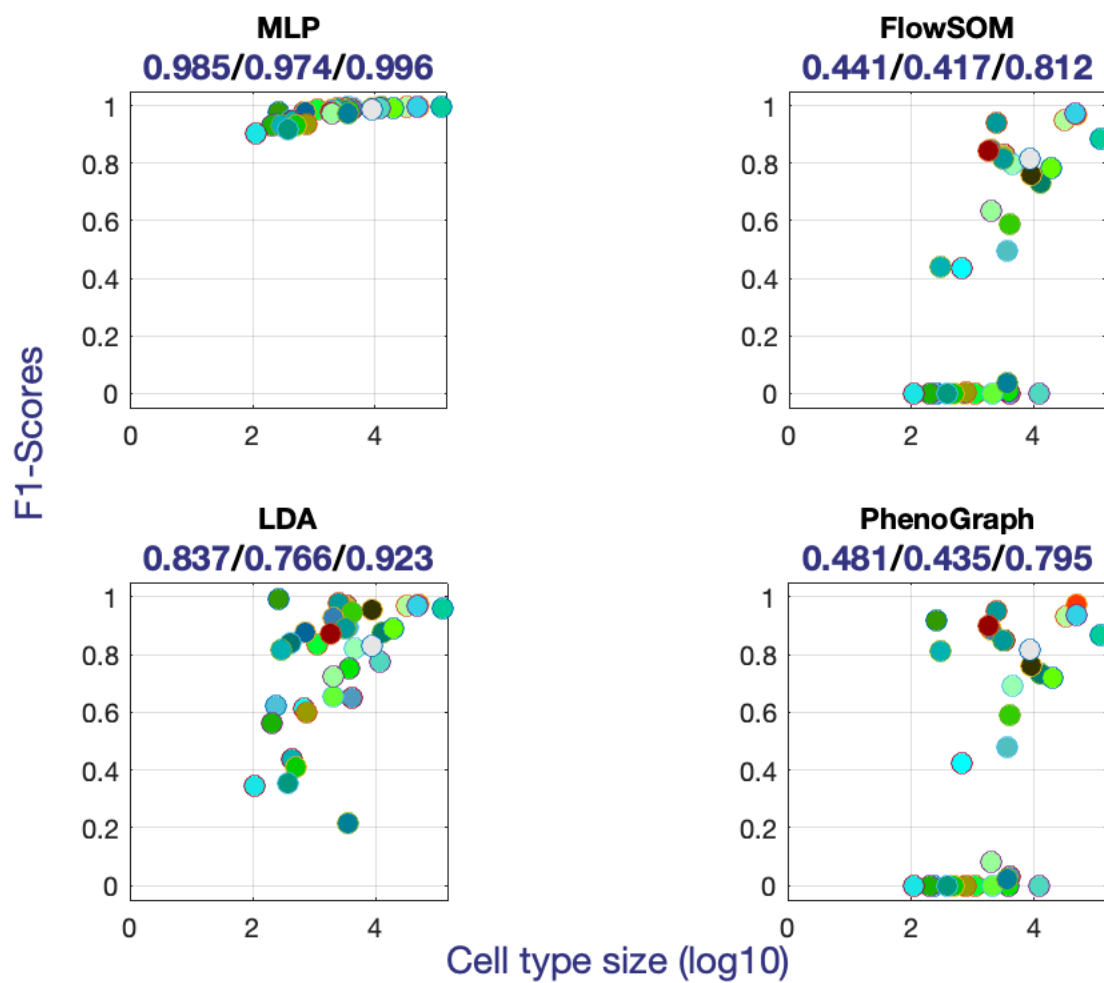
Liechti, T., Günthard, H.F. and Trkola, A. (2018), **OMIP-047: High-Dimensional phenotypic characterization of B cells**. Cytometry, 93: 592-596.
<https://doi.org/10.1002/cyto.a.23488>

4.3.3. OMIP-058

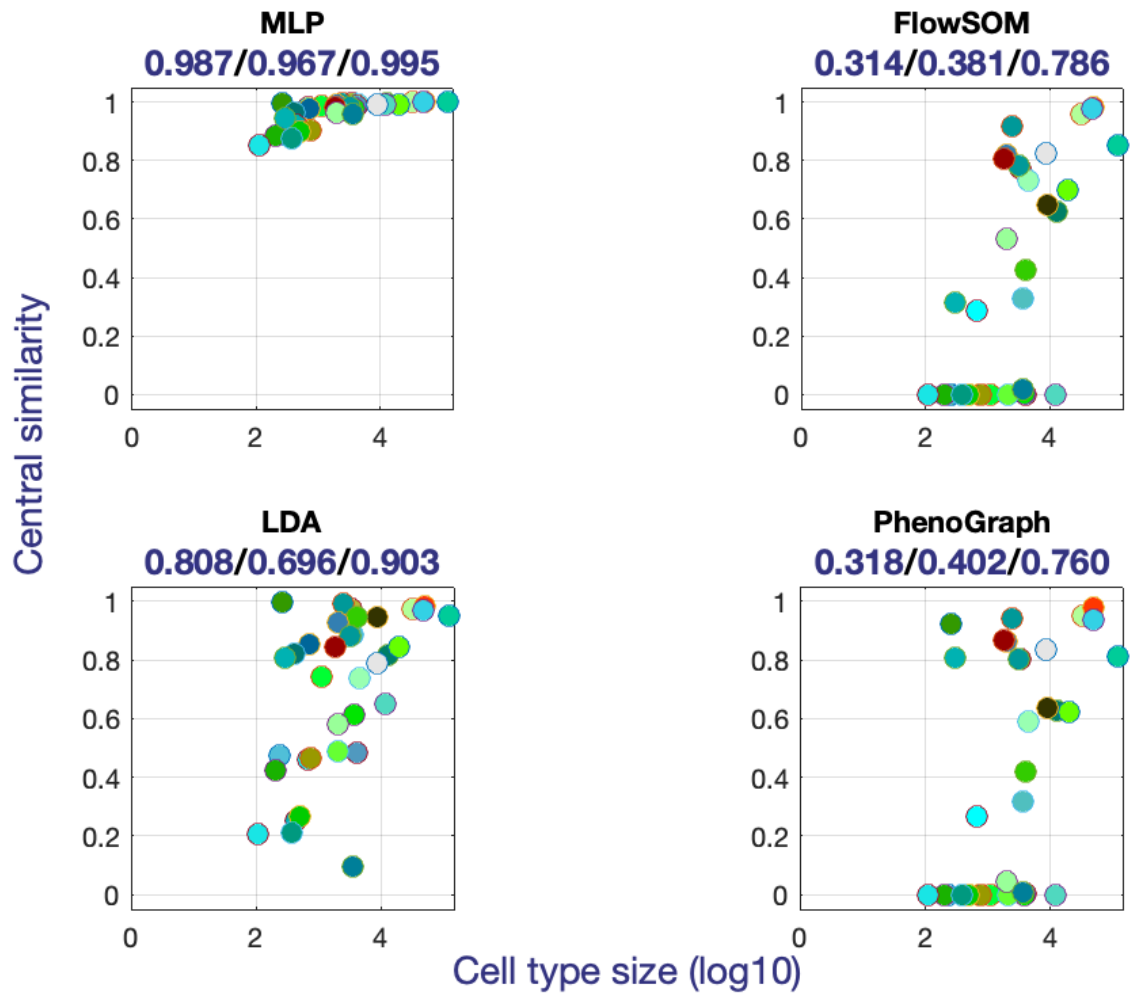
2 samples, 2 fold cross validation of 365k x 356k training x test *cells*,
35 cell types, 17 markers.

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
●	CD4+ TCM T cells CD27+ CD28+	34%	0.999	0.886	0.960	0.867	0.999	0.850	0.951	0.812	1	0.974	0.993	0.952
●	CD8+ TEMRA T cells CD27- CD28-	9%	0.999	0.951	0.967	0.934	1	0.961	0.973	0.952	1	0.974	0.982	0.965
●	HLA-DR+	14%	0.998	0.970	0.973	0.973	0.999	0.981	0.984	0.980	1	0.988	0.978	0.988
●	CD4+ Naive T cells CD27+ CD28+	13%	0.998	0.972	0.970	0.938	0.999	0.979	0.969	0.936	1	0.993	0.995	0.957
●	CD4+ TCM T cells CD27- CD28+	3.5%	0.996	0.733	0.878	0.732	0.996	0.626	0.818	0.628	0.999	0.949	0.985	0.957
●	CD4+ TEM T cells CD27- CD28-	1%	0.995	0.495	0.894	0.481	0.998	0.330	0.885	0.318	0.999	0.923	0.960	0.920
●	Early NK	0.92%	0.994	0.831	0.967	0.847	0.997	0.776	0.973	0.801	0.998	0.944	0.990	0.941
●	CD8+ TEM T cells CD27+ CD28+	5.4%	0.994	0.785	0.891	0.721	0.993	0.698	0.846	0.622	0.999	0.960	0.969	0.919
●	Vd2 high Vg9+ T cells	0.68%	0.994	0.939	0.980	0.949	0.998	0.920	0.991	0.941	0.998	0.985	0.988	0.986
●	Mature NK	2.5%	0.993	0.760	0.954	0.762	0.992	0.650	0.948	0.638	0.999	0.866	0.983	0.861
●	CD4+ TEM T cells CD27+ CD28+	3.3%	0.993	N/A	0.777	N/A	0.991	N/A	0.650	N/A	0.999	N/A	0.955	N/A
●	CD8+ Naive T cells CD27+ CD28+	1.1%	0.991	0.588	0.945	0.591	0.993	0.424	0.945	0.420	0.998	0.881	0.960	0.877
●	CD8+ TEMRA T cells CD27+ CD28-	1.2%	0.990	0.799	0.821	0.692	0.990	0.731	0.738	0.590	0.998	0.955	0.938	0.861
●	CD4+ TEM T cells CD27- CD28+	1.1%	0.989	N/A	0.648	0.029	0.987	N/A	0.483	0.005	0.998	N/A	0.944	0.553
●	NK CD16- CD56-	2.4%	0.988	0.815	0.829	0.818	0.991	0.827	0.788	0.834	0.999	0.877	0.921	0.872
●	CD8+ TEM T cells CD27- CD28+	0.31%	0.987	N/A	0.837	N/A	0.988	N/A	0.743	N/A	0.997	N/A	0.954	N/A
●	Vd2 low Vg9+ T cells CD56-	0.55%	0.987	0.847	0.927	0.886	0.991	0.821	0.925	0.863	0.997	0.941	0.973	0.952
●	CD8+ TCM T cells CD27+ CD28+	1.1%	0.985	0.009	0.751	N/A	0.977	0.005	0.614	N/A	0.998	0.586	0.954	N/A
●	Vd1+ Vg9- T cells CD56-	0.88%	0.982	0.814	0.891	0.848	0.982	0.782	0.880	0.802	0.997	0.920	0.954	0.953
●	CD8+ TEM T cells CD27- CD28-	0.57%	0.981	N/A	0.653	N/A	0.975	N/A	0.489	N/A	0.996	N/A	0.889	N/A
●	CD4+ TEMRA T cells CD27- CD28-	0.18%	0.980	0.436	0.614	0.424	0.984	0.286	0.459	0.267	0.994	0.931	0.767	0.932
●	iNKT cells	0.07%	0.977	N/A	0.994	0.917	0.995	N/A	0.995	0.921	0.985	N/A	0.992	0.909
●	MAIT cells	0.51%	0.976	0.843	0.871	0.898	0.982	0.808	0.844	0.865	0.996	0.892	0.926	0.963
●	Vd2 low Vg9+ T cells CD56+	0.20%	0.976	N/A	0.878	N/A	0.976	N/A	0.855	N/A	0.990	N/A	0.958	N/A
●	CD8+ TEMRA T cells CD27+ CD28+	0.55%	0.973	0.634	0.724	0.082	0.964	0.534	0.583	0.043	0.996	0.930	0.942	0.693
●	CD4+ TSCM T cells CD27+ CD28+	1%	0.972	0.036	0.216	0.022	0.958	0.015	0.097	0.008	0.997	0.486	0.886	0.497
●	Vd1+ Vg9- T cells CD56+	0.12%	0.952	N/A	0.842	N/A	0.965	N/A	0.819	N/A	0.985	N/A	0.938	N/A
●	CD4+ TEMRA T cells CD27+ CD28+	0.12%	0.947	N/A	0.439	N/A	0.922	N/A	0.253	N/A	0.983	N/A	0.804	N/A
●	CD4+ TEM T cells CD27+ CD28-	0.07%	0.938	N/A	0.623	0	0.889	N/A	0.473	0	0.977	N/A	0.887	0.320
●	Terminal NK	0.21%	0.937	0.005	0.597	N/A	0.905	0.001	0.464	N/A	0.990	0.427	0.911	N/A
●	CD8+ TSCM T cells CD27+ CD28+	0.14%	0.933	N/A	0.409	N/A	0.901	N/A	0.266	N/A	0.989	N/A	0.915	N/A
●	CD8+ TCM T cells CD27- CD28+	0.06%	0.931	N/A	0.563	N/A	0.887	N/A	0.424	N/A	0.982	N/A	0.904	N/A
●	Q2: Vd1+ Vg9+	0.08%	0.930	0.441	0.818	0.813	0.946	0.314	0.808	0.808	0.976	0.720	0.921	0.902
●	CD4+ TSCM T cells CD27- CD28+	0.10%	0.919	N/A	0.356	N/A	0.877	N/A	0.210	N/A	0.981	N/A	0.881	N/A
●	CD4+ TEMRA T cells CD27- CD28+	0.03%	0.905	N/A	0.345	N/A	0.851	N/A	0.207	N/A	0.972	N/A	0.771	N/A
Median			0.985	0.441	0.837	0.481	0.987	0.314	0.808	0.318	0.997	0.866	0.954	0.861
Mean			0.974	0.417	0.766	0.435	0.967	0.381	0.696	0.402	0.993	0.546	0.933	0.564

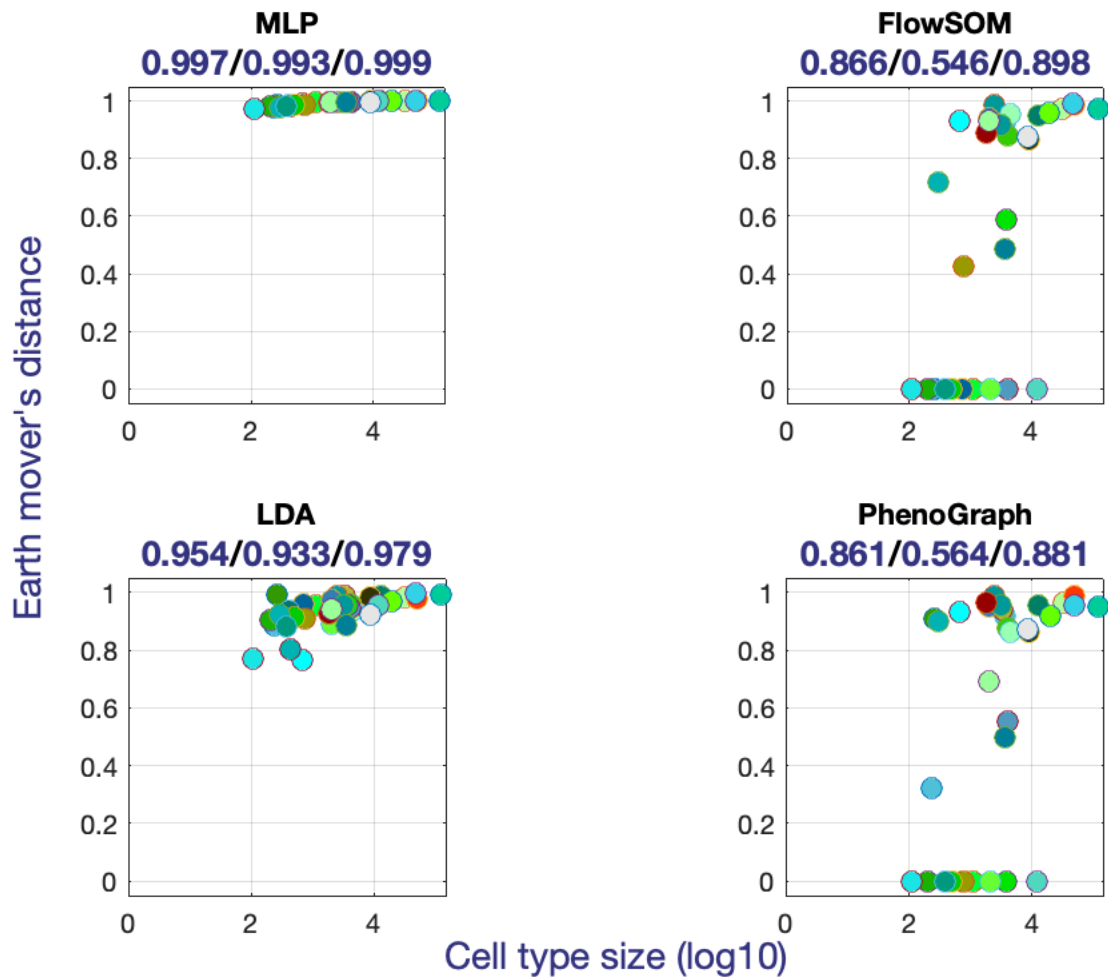
OMIP-058 F1-Scores median/mean/weighted



OMIP-058 Central similarity median/mean/weighted



OMIP-058 Earth mover's distance median/mean/weighted



4.3.3.1. Merged matches

With FlowSOM QFMatch finds 8 of 22 matches where merging multiple FlowSOM gated populations to match 1 manually gated population obtains a higher F1-score: the 2nd, 4th, 5th, 6th, 7th, 9th, 14th and 16th ranked matches.




































Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	Similarity (QFMatch)	Train-ing set?	Freq.
2	●	27	HLA-DR+	4	97%	98.8%	yes	9.9%
2	●	47	HLA-DR+ (FlowSOM.Viable cells.Po...	4	97%	98.8%	no	1.4%
2	●	63	HLA-DR+ (FlowSOM.Viable cells.Po...	4	97%	98.8%	no	0.2%
2	●	66	HLA-DR+ (FlowSOM.Viable cells.Po...	4	97%	98.8%	no	7.4%
6	●	20	CD8+ TEM T cells CD27+ CD28+	4	78.5%	96%	yes	4%
6	●	45	FlowSOM.Viable cells.Pop22	4	78.5%	96%	no	0.7%
6	●	64	CD8+ TCM T cells CD27+ CD28+ (FI...	4	78.5%	96%	no	3.5%
6	●	68	CD8+ TEM T cells CD27- CD28+ (FI...	4	78.5%	96%	no	0.6%
14	●	1	Vd1+ Vg9- T cells CD56-	4	81.4%	92%	yes	1.6%
14	●	37	Vd1+ Vg9- T cells CD56- (FlowSOM....	4	81.4%	92%	no	0.5%
14	●	38	Vd1+ Vg9- T cells CD56- (FlowSOM....	4	81.4%	92%	no	0.3%
14	●	65	Vd1+ Vg9- T cells CD56- (FlowSOM....	4	81.4%	92%	no	0.5%
4	●	12	CD4+ TCM T cells CD27+ CD28+	3	88.6%	97.4%	yes	20.5%
4	●	39	CD4+ TCM T cells CD27+ CD28+ (FI...	3	88.6%	97.4%	no	4.9%
4	●	48	CD4+ TCM T cells CD27+ CD28+ (FI...	3	88.6%	97.4%	no	17.7%
5	●	2	CD8+ TEMRA T cells CD27- CD28-	3	95.1%	97.4%	yes	17.8%
5	●	46	CD8+ TEMRA T cells CD27- CD28- (...)	3	95.1%	97.4%	no	14.6%
5	●	61	CD8+ TEMRA T cells CD27- CD28- (...)	3	95.1%	97.4%	no	2.7%
7	●	3	CD8+ TEMRA T cells CD27+ CD28-	3	79.9%	95.5%	yes	1.9%
7	●	69	CD8+ TEMRA T cells CD27+ CD28- ...	3	79.9%	95.5%	no	1.5%
7	●	70	CD8+ TEMRA T cells CD27+ CD28- ...	3	79.9%	95.5%	no	0.3%
9	●	13	Early NK	3	83.1%	94.4%	yes	1%
9	●	36	Early NK (FlowSOM.Viable cells.Pop8)	3	83.1%	94.4%	no	0.2%
9	●	51	Early NK (FlowSOM.Viable cells.Pop2)	3	83.1%	94.4%	no	0.9%
16	●	22	CD8+ Naive T cells CD27+ CD28+	3	58.8%	88.1%	yes	1.9%
16	●	44	CD8+ Naive T cells CD27+ CD28+ (...)	3	58.8%	88.1%	no	0.2%
16	●	54	CD8+ Naive T cells CD27+ CD28+ (...)	3	58.8%	88.1%	no	3.5%
1	●	21	CD4+ Naive T cells CD27+ CD28+	2	97.2%	99.3%	yes	21.5%
1	●	50	CD4+ Naive T cells CD27+ CD28+ (...)	2	97.2%	99.3%	no	19%

With PhenoGraph QFMatch finds 6 of 16 matches where merging multiple PhenoGraph gated populations to match 1 manually gated population obtains a higher F1-score: 1st, 3rd, 5th, 7th, 8th and 16th ranked matches.

Rank ²		#	Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	Similarity (QFMatch)	Train-ing set?	Freq.	
1		27	HLA-DR+	5	97.3%	98.8%	yes	9.9%	3
1		40	PhenographYO0G4	5	97.3%	98.8%	no	6.9%	2
1		46	PhenographYO0G26	5	97.3%	98.8%	no	0.3%	
1		47	PhenographYO0G16	5	97.3%	98.8%	no	1.8%	
1		58	PhenographYO0G29	5	97.3%	98.8%	no	0.2%	
3		2	CD8+ TEMRA T cells CD27- CD28-	4	93.4%	96.5%	yes	17.8%	5
3		51	PhenographYO0G13	4	93.4%	96.5%	no	2.6%	
3		56	PhenographYO0G3	4	93.4%	96.5%	no	11%	4
3		64	PhenographYO0G11	4	93.4%	96.5%	no	3.2%	1
5		21	CD4+ Naive T cells CD27+ CD28+	4	93.8%	95.7%	yes	21.5%	7
5		41	PhenographYO0G23	4	93.8%	95.7%	no	0.4%	
5		43	PhenographYO0G8	4	93.8%	95.7%	no	3.9%	1
5		60	PhenographYO0G1	4	93.8%	95.7%	no	16.6%	6
7		1	Vd1+ Vg9- T cells CD56-	4	84.8%	95.3%	yes	1.6%	
7		44	PhenographYO0G17	4	84.8%	95.3%	no	1.2%	
7		48	PhenographYO0G28	4	84.8%	95.3%	no	0.2%	
7		54	PhenographYO0G22	4	84.8%	95.3%	no	0.5%	
8		12	CD4+ TCM T cells CD27+ CD28+	3	86.7%	95.2%	yes	20.5%	6
8		49	PhenographYO0G7	3	86.7%	95.2%	no	5.4%	2
8		52	PhenographYO0G2	3	86.7%	95.2%	no	14.9%	5
16		22	CD8+ Naive T cells CD27+ CD28+	3	59.1%	87.7%	yes	1.9%	
16		36	PhenographYO0G30	3	59.1%	87.7%	no	0.2%	
16		63	PhenographYO0G9	3	59.1%	87.7%	no	3.5%	1
2		25	Vd2 high Vg9+ T cells	2	94.9%	98.6%	yes	0.6%	
2		61	PhenographYO0G21	2	94.9%	98.6%	no	0.6%	

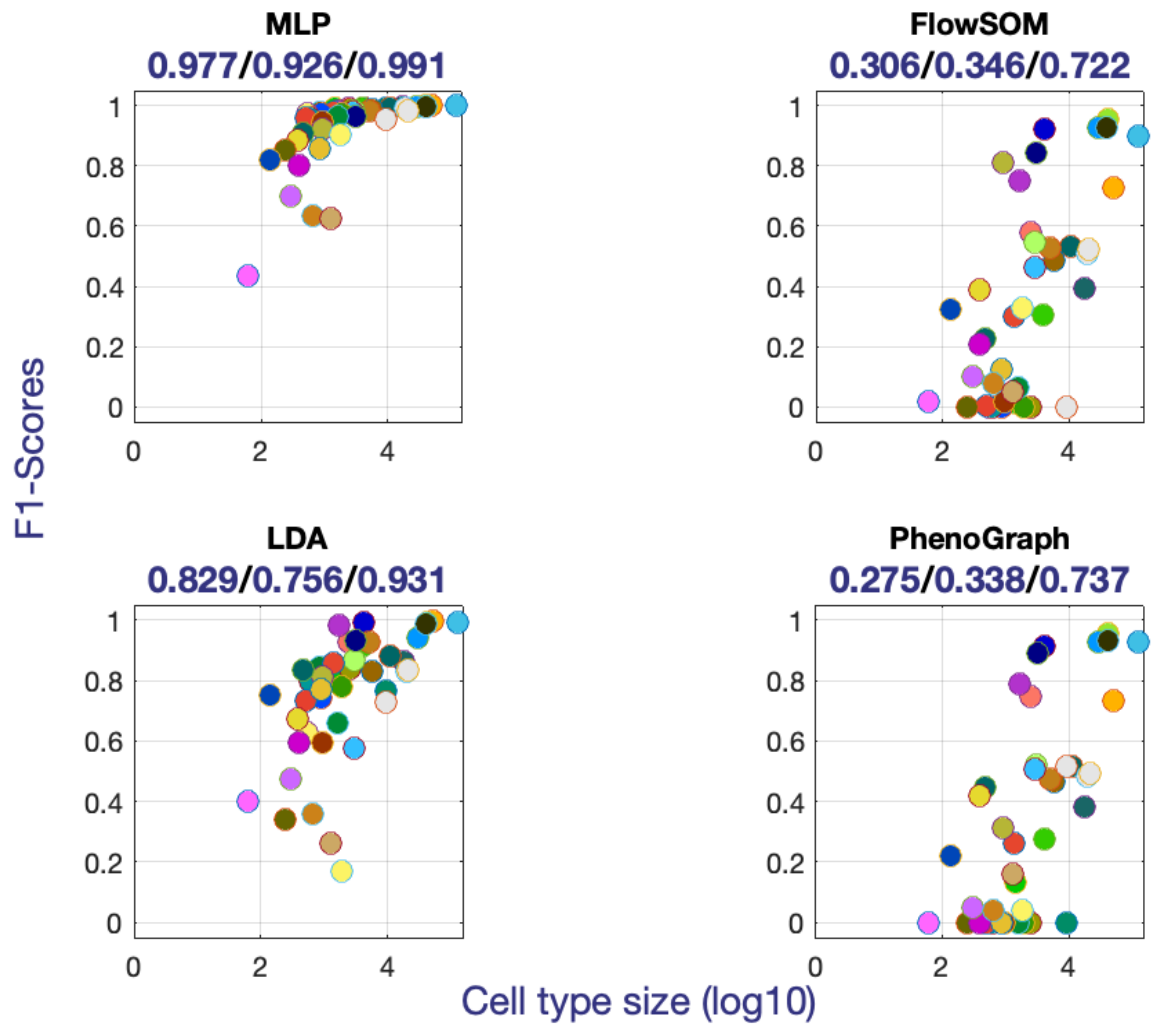
Liechti, T. and Roederer, M. (2019), **OMIP-058: 30-Parameter Flow Cytometry Panel to Characterize iNKT, NK, Unconventional and Conventional T Cells**. Cytometry, 95: 946-951. <https://doi.org/10.1002/cyto.a.23850>

4.3.4. OMIP-069

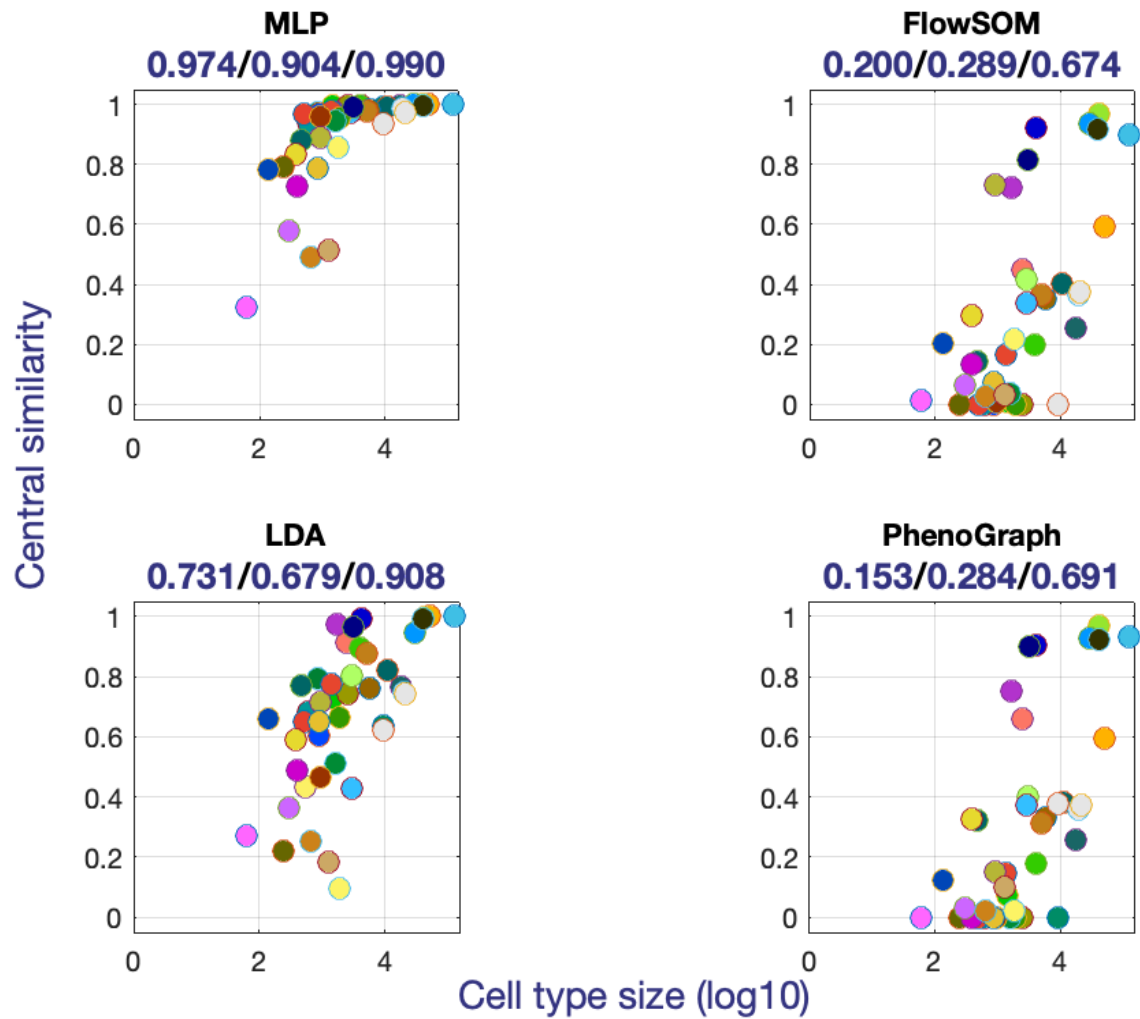
4 samples, 3-fold cross validation, 3x1, 2x2 & 3x1 training x test samples,
43 cell types, 26 markers.

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
●	Naive CD4+	29%	1	0.898	0.994	0.926	1	0.897	1	0.932	1	0.953	0.997	0.980
●	Classical monocytes	12%	0.999	0.729	0.996	0.733	1	0.593	1	0.596	1	0.989	0.998	0.990
●	Naive CD8+	9.6%	0.999	0.957	0.994	0.957	1	0.971	0.997	0.970	1	0.992	0.999	0.993
●	Early Effector CD4+	4.1%	0.998	0.393	0.862	0.384	0.999	0.255	0.766	0.257	1	0.763	0.964	0.749
●	B-2 CD27-	6.8%	0.998	0.929	0.941	0.927	1	0.934	0.945	0.928	1	0.976	0.968	0.979
●	Mature NK	9.5%	0.997	0.925	0.988	0.931	0.998	0.919	0.992	0.922	1	0.981	0.996	0.983
●	B-1 IgG	0.97%	0.994	0.925	0.992	0.916	0.997	0.924	0.994	0.906	0.999	0.981	0.997	0.982
●	Early like effector CD4+	2.2%	0.994	N/A	0.765	N/A	0.994	N/A	0.637	N/A	0.999	N/A	0.946	N/A
●	Early Effector CD8+	2.6%	0.994	0.535	0.882	0.515	0.992	0.404	0.819	0.384	0.999	0.873	0.971	0.831
●	Central Memory CD8+	0.34%	0.993	0.013	0.830	0.132	0.998	0.006	0.731	0.071	0.998	0.556	0.966	0.618
●	CCR7- CD45RA+ TCRgD+	0.57%	0.992	0.581	0.926	0.747	0.994	0.449	0.914	0.657	0.997	0.868	0.971	0.938
●	Terminal Effector CD45RA+ CD8+	0.94%	0.991	0.306	0.915	0.275	0.996	0.200	0.894	0.178	0.998	0.844	0.964	0.818
●	Central Memory CD4+ CXCR5-, CXCR3	4.6%	0.991	0.511	0.829	0.483	0.989	0.366	0.749	0.358	0.998	0.899	0.963	0.878
●	Terminal NK	0.59%	0.988	N/A	0.842	N/A	0.995	N/A	0.742	N/A	0.996	N/A	0.977	N/A
●	CD2+ CD8+ NKT	1.3%	0.985	0.484	0.831	0.466	0.983	0.352	0.760	0.332	0.996	0.819	0.948	0.811
●	Intermediate monocytes	1.2%	0.983	0.527	0.926	0.474	0.979	0.367	0.877	0.312	0.995	0.833	0.954	0.872
●	Central Memory CD4+ CXCR5-, CXCR3-	4.9%	0.983	0.523	0.836	0.495	0.974	0.373	0.744	0.372	0.996	0.948	0.951	0.805
●	CD123+ pDCs	0.39%	0.982	0.751	0.984	0.788	0.976	0.723	0.976	0.750	0.996	0.934	0.996	0.965
●	CD4- CD8-	0.69%	0.981	0.545	0.869	0.523	0.985	0.418	0.803	0.401	0.995	0.835	0.945	0.750
●	Terminal Effector	0.20%	0.979	N/A	0.842	N/A	0.974	N/A	0.793	N/A	0.992	N/A	0.960	N/A
●	B-2 CD27+	0.68%	0.978	0.461	0.578	0.508	0.973	0.338	0.428	0.374	0.996	0.810	0.913	0.880
●	CCR7- CD45RA- TCRgD+	0.32%	0.977	0.300	0.858	0.262	0.976	0.166	0.775	0.146	0.993	0.852	0.981	0.826
●	B-1 IgM+	0.21%	0.974	N/A	0.741	N/A	0.970	N/A	0.602	N/A	0.992	N/A	0.951	N/A
●	Intermediate Effector CD8+	0.45%	0.974	N/A	0.778	N/A	0.956	N/A	0.662	N/A	0.993	N/A	0.957	N/A
●	ILCs CD2+ CD4+	0.13%	0.973	N/A	0.629	N/A	0.965	N/A	0.432	N/A	0.994	N/A	0.846	N/A
●	B-1 IgG- IgM-	0.73%	0.966	0.842	0.933	0.892	0.992	0.817	0.964	0.901	0.991	0.957	0.953	0.966
●	Early like effector CD8+	0.38%	0.964	0.062	0.658	N/A	0.944	0.034	0.511	N/A	0.994	0.517	0.923	N/A
●	Terminal Effector CD4+	0.14%	0.962	N/A	0.796	N/A	0.943	N/A	0.683	N/A	0.993	N/A	0.926	N/A
●	CCR7+ TCRgD+	0.12%	0.958	0.001	0.735	N/A	0.967	< 0.001	0.653	N/A	0.987	0.516	0.900	N/A
●	Central Memory CD4+ CXCR5, CXCR3	2.2%	0.953	N/A	0.730	0.514	0.935	N/A	0.624	0.380	0.993	N/A	0.920	0.840
●	CD2+ CD8-	0.22%	0.945	0.018	0.593	N/A	0.961	0.009	0.466	N/A	0.985	0.498	0.929	N/A
●	Early NK	0.22%	0.924	0.811	0.810	0.314	0.892	0.730	0.717	0.153	0.987	0.963	0.922	0.717
●	CD4+ CD8+ T	0.11%	0.909	0.224	0.833	0.447	0.882	0.142	0.770	0.320	0.971	0.582	0.928	0.805
●	ILCs CD4-	0.43%	0.904	0.328	0.170	0.038	0.857	0.216	0.095	0.022	0.984	0.645	0.835	0.359
●	ILCs CD2- CD4-	0.09%	0.885	0.389	0.675	0.421	0.833	0.297	0.589	0.328	0.972	0.740	0.874	0.624
●	CD11c+ CD16+ DCs	0.20%	0.858	0.124	0.772	N/A	0.787	0.072	0.649	N/A	0.981	0.781	0.948	N/A
●	CD2- NKT cells	0.06%	0.854	N/A	0.340	N/A	0.793	N/A	0.222	N/A	0.947	N/A	0.552	N/A
●	Plasmablasts	0.03%	0.822	0.326	0.753	0.221	0.782	0.201	0.658	0.121	0.961	0.951	0.953	0.867
●	CD1c+ DCs	0.09%	0.802	0.206	0.595	N/A	0.727	0.135	0.489	N/A	0.978	0.876	0.925	N/A
●	CD1c- CD141- DCs	0.07%	0.701	0.100	0.473	0.048	0.579	0.066	0.364	0.031	0.969	0.570	0.812	0.479
●	Non classical monocytes	0.15%	0.635	0.075	0.360	0.041	0.491	0.026	0.254	0.021	0.869	0.499	0.787	0.338
●	CD16- CD14- monocytes	0.30%	0.625	0.049	0.262	0.162	0.512	0.030	0.185	0.102	0.925	0.618	0.667	0.603
●	CD1c- CD141+ DCs	0.01%	0.437	0.017	0.398	N/A	0.324	0.011	0.272	N/A	0.870	0.641	0.878	N/A
Median			0.977	0.306	0.829	0.275	0.974	0.200	0.731	0.153	0.994	0.781	0.951	0.749
Mean			0.926	0.346	0.756	0.338	0.904	0.289	0.679	0.284	0.983	0.629	0.924	0.541

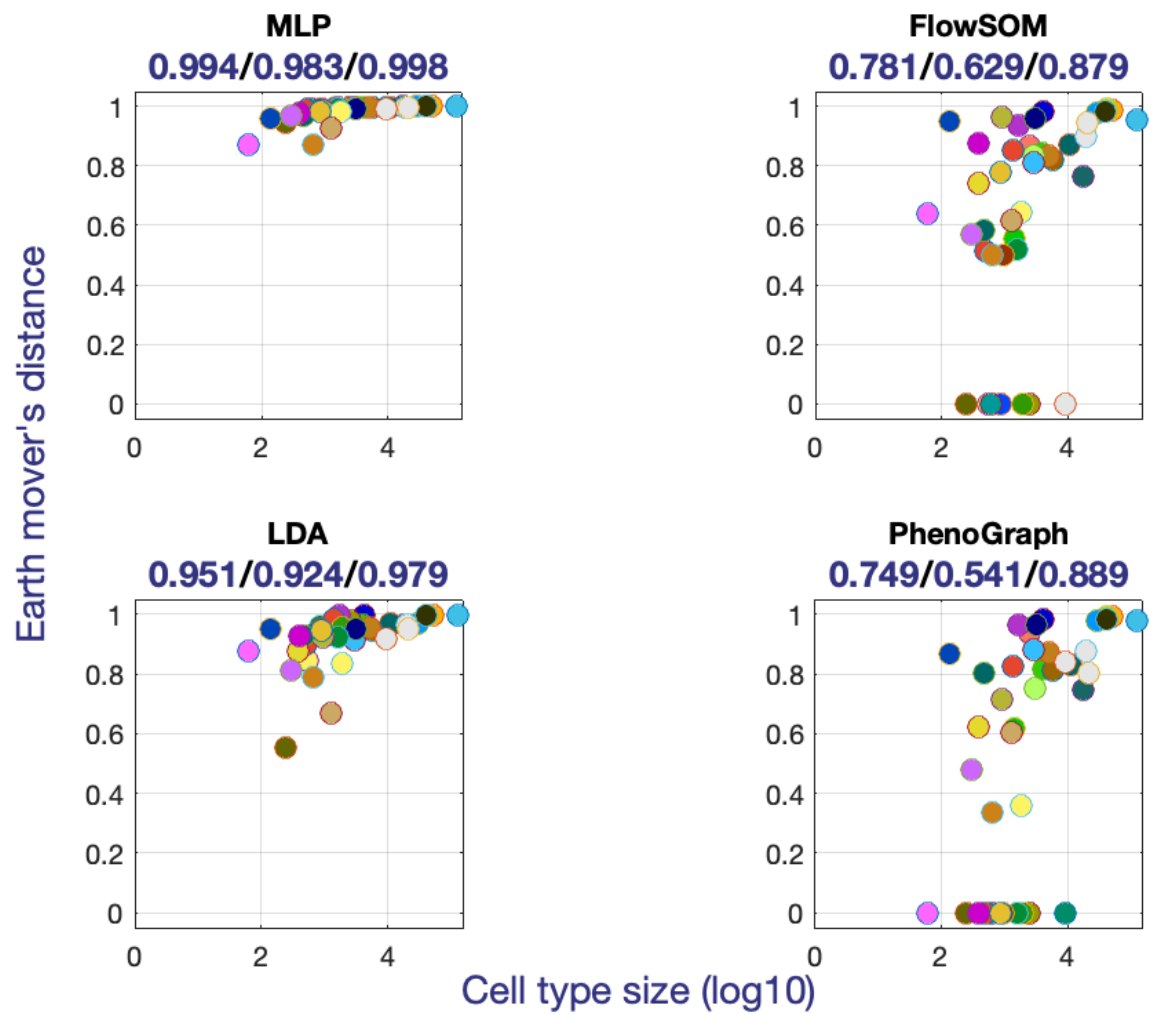
OMIP-069 F1-Scores median/mean/weighted



OMIP-069 Central similarity median/mean/weighted



OMIP-069 Earth mover's distance median/mean/weighted



4.3.4.1. Merged matches

With FlowSOM there QFMatch finds 6 of 34 possible matches where merging multiple FlowSOM gated populations for 1 manually gated population obtains a higher F1-score: the 2nd, 5th, 10th, 12th, 14th and 18th ranked matches.

MATCH sets: training=34/43 (9 UNMATCHED!), test=40/43 (3 NEW!)

Rank	#	Subset (class) name	Matches	Similarity (QFMatch)	% Overlap (F-measure)	Training set?	Freq.
2	42	Classical monocytes	3	98.9%	72.9%	yes	7.9%
2	63	Classical monocytes (FlowSOM.CD4...	3	98.9%	72.9%	no	5.7%
2	75	Classical monocytes (FlowSOM.CD4...	3	98.9%	72.9%	no	4.4%
5	12	B-2 CD27-	3	97.6%	92.9%	yes	6.8%
5	48	B-2 CD27- (FlowSOM.CD45+.Pop6)	3	97.6%	92.9%	no	4.4%
5	72	B-2 CD27- (FlowSOM.CD45+.Pop5)	3	97.6%	92.9%	no	1.3%
10	41	Central Memory CD4+ CXCR5-, CXC...	3	94.8%	52.3%	yes	6.5%
10	59	Early like effector CD4+ (FlowSOM....	3	94.8%	52.3%	no	2.5%
10	81	Central Memory CD4+ CXCR5, CXC...	3	94.8%	52.3%	no	9.1%
12	21	Central Memory CD4+ CXCR5-, CXC...	3	89.9%	51.1%	yes	4.7%
12	58	Central Memory CD4+ CXCR5-, CXC...	3	89.9%	51.1%	no	6.1%
12	68	Central Memory CD4+ CXCR5-, CXC...	3	89.9%	51.1%	no	0.6%
14	8	Early Effector CD8+	3	87.3%	53.5%	yes	3%
14	69	Central Memory CD8+ (FlowSOM.CD...	3	87.3%	53.5%	no	0.8%
14	83	Early like effector CD8+ (FlowSOM....	3	87.3%	53.5%	no	2.6%
18	19	CD4- CD8-	3	83.5%	54.5%	yes	1.5%
18	45	FlowSOM.CD45+.Pop18	3	83.5%	54.5%	no	0.3%
18	56	CCR7+ TCRgD+ (FlowSOM.CD45+....	3	83.5%	54.5%	no	0.9%
1	23	Naive CD8+	2	99.2%	95.7%	yes	13.1%
1	51	Naive CD8+ (FlowSOM.CD45+.Pop30)	2	99.2%	95.7%	no	10.4%

With PhenoGraph there are 4 of 29 matches where merging multiple manual or PhenoGraph gated populations for 1 manually gated population obtains a higher F1-score: the 2nd, 5th, 19th and 26th ranked matches.












 MATCH sets: training=29/43 (14 UNMATCHED!), test=34/38 (4

Rank ²		#	Subset (class) name	Mat-ches ¹	Similarity (QFMatch)	% Overlap (F-measure)	Train-ing set? ³	Freq. ⁴
5	●	18	Naive CD4+	4	98%	92.6%	yes	28.4%
5	●	47	PhenographLP7210	4	98%	92.6%	no	4.3%
5	●	66	PhenographLP7218	4	98%	92.6%	no	1.5%
5	●	71	PhenographLP721	4	98%	92.6%	no	16.5%
2	●	42	Classical monocytes	3	99%	73.3%	yes	7.9%
2	●	73	PhenographLP725	3	99%	73.3%	no	5%
2	●	74	PhenographLP727	3	99%	73.3%	no	4.9%
19	●	41	Central Memory CD4+ CXCR5-, CXC...	3	80.5%	49.5%	yes	6.5%
19	●	50	PhenographLP7232	3	80.5%	49.5%	no	0.1%
19	●	64	PhenographLP726	3	80.5%	49.5%	no	4.9%
26	●	35	CD16- CD14- monocytes	3	60.3%	16.2%	yes	0.4%
26	●	45	PhenographLP7224	3	60.3%	16.2%	no	0.7%
26	●	60	PhenographLP7235	3	60.3%	16.2%	no	0%
1	●	23	Naive CD8+	2	99.3%	95.7%	yes	13.1%
1	●	44	PhenographLP722	2	99.3%	95.7%	no	10.3%

4.3.4.2. The alarming low FlowSOM score.

We run FlowSOM with 44 meta clusters to find 43 cell populations, the 1 extra is for background. But FlowSOM only finds 42 clusters. So we tried running FlowSOM on only the T cells and NKT-like cells which require 9 Phenotyping markers that classify 19 leaf gates starting at the CD3+ TCRgd- branch gate: CCR7, CD2, CD4, CD8, CD27, CD28, CD45RA, CXCR3, CXCR5. We ran FlowSOM on the common parent gate to these populations specifying 20 meta clusters to allow 1 for background. The medians/means of the F1-score shown below are 0.405/0.410. This improves upon the 0.306/0.346 obtained for running FlowSOM on all 46 populations. But this does not inspire trust in the capability of FlowSOM.

Color	Cell type	Frequency %	F1-Score	Central similarity	Earth mover's distance
			Flow SOM Z A↓	Flow SOM	Flow SOM
●	Naive CD8+	18%	0.979	0.996	0.994
●	Naive CD4+	39%	0.950	0.959	0.982
●	CD4- CD8-	2%	0.776	0.651	0.913
●	Central Memory CD4+ CXCR5-, CXCR3	6.3%	0.687	0.533	0.918
●	Early Effector CD8+	4.1%	0.661	0.524	0.850
●	CD4+ CD8+ T	0.13%	0.656	0.499	0.832
●	Early like effector CD4+	2.4%	0.526	0.385	0.879
●	Central Memory CD4+ CXCR5-, CXCR3-	8.8%	0.515	0.354	0.906
●	Early Effector CD4+	5.4%	0.489	0.328	0.788
●	Intermediate Effector CD8+	0.66%	0.405	0.277	0.817
●	Terminal Effector CD45RA+ CD8+	0.61%	0.401	0.273	0.874
●	Early like effector CD8+	0.77%	0.393	0.253	0.741
●	CD2+ CD8+ NKT	2.3%	0.280	0.187	0.745
●	Central Memory CD8+	0.50%	0.071	0.033	0.468
●	Central Memory CD4+ CXCR5, CXCR3	8.8%	0.003	0.001	0.597
●	CD2+ CD8-	0.56%	N/A	N/A	N/A
●	Terminal Effector	0.30%	0	0	0.379
●	CD2- NKT cells	0.13%	N/A	N/A	N/A
●	Terminal Effector CD4+	0.01%	N/A	N/A	N/A
Median			0.405	0.277	0.817
Mean			0.410	0.329	0.668

Park, L.M., Lannigan, J. and Jaimes, M.C. (2020), **OMIP-069: Forty-Color Full Spectrum Flow Cytometry Panel for Deep Immunophenotyping of Major Cell Subsets in Human Peripheral Blood**. Cytometry, 97: 1044-1051.

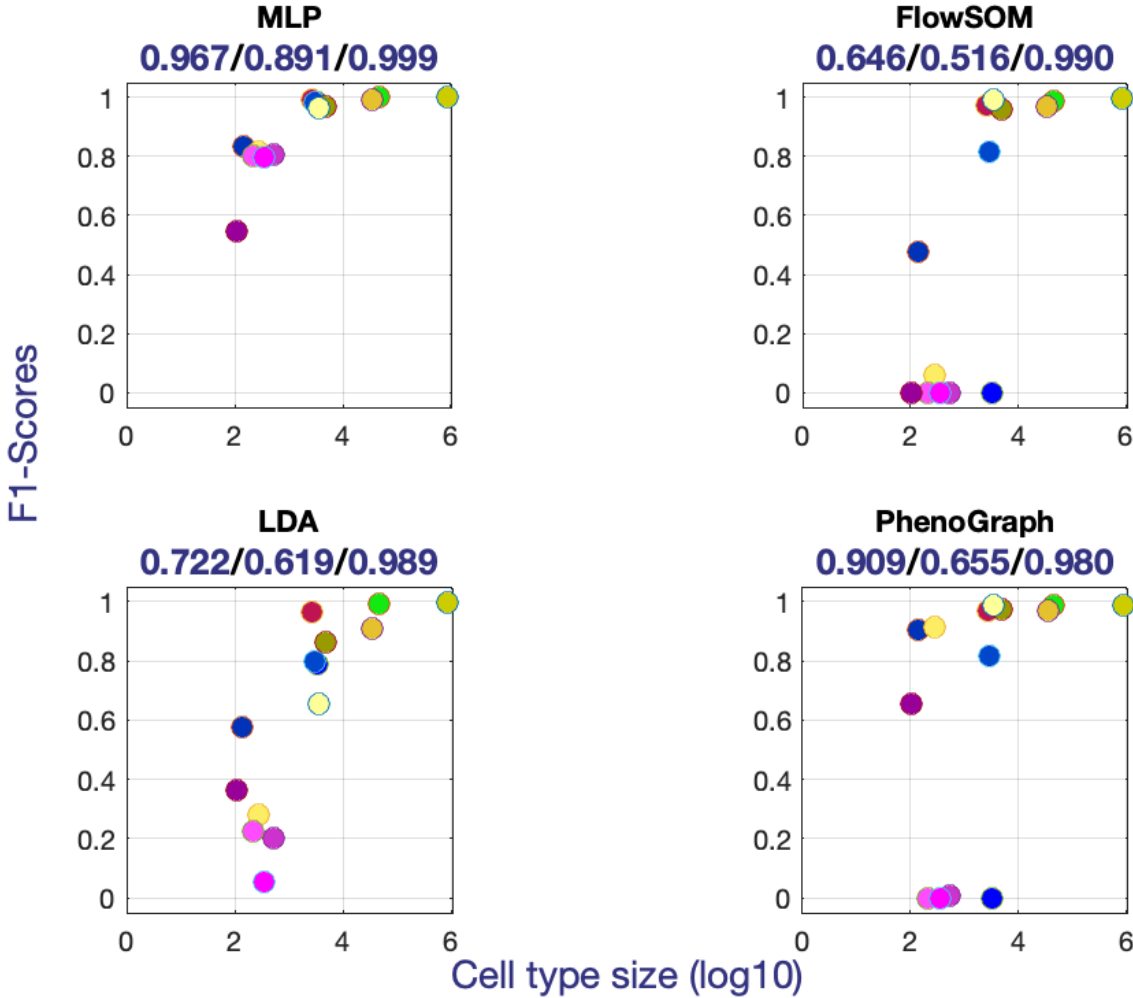
<https://doi.org/10.1002/cyto.a.24213>

4.3.5. OMIP-077

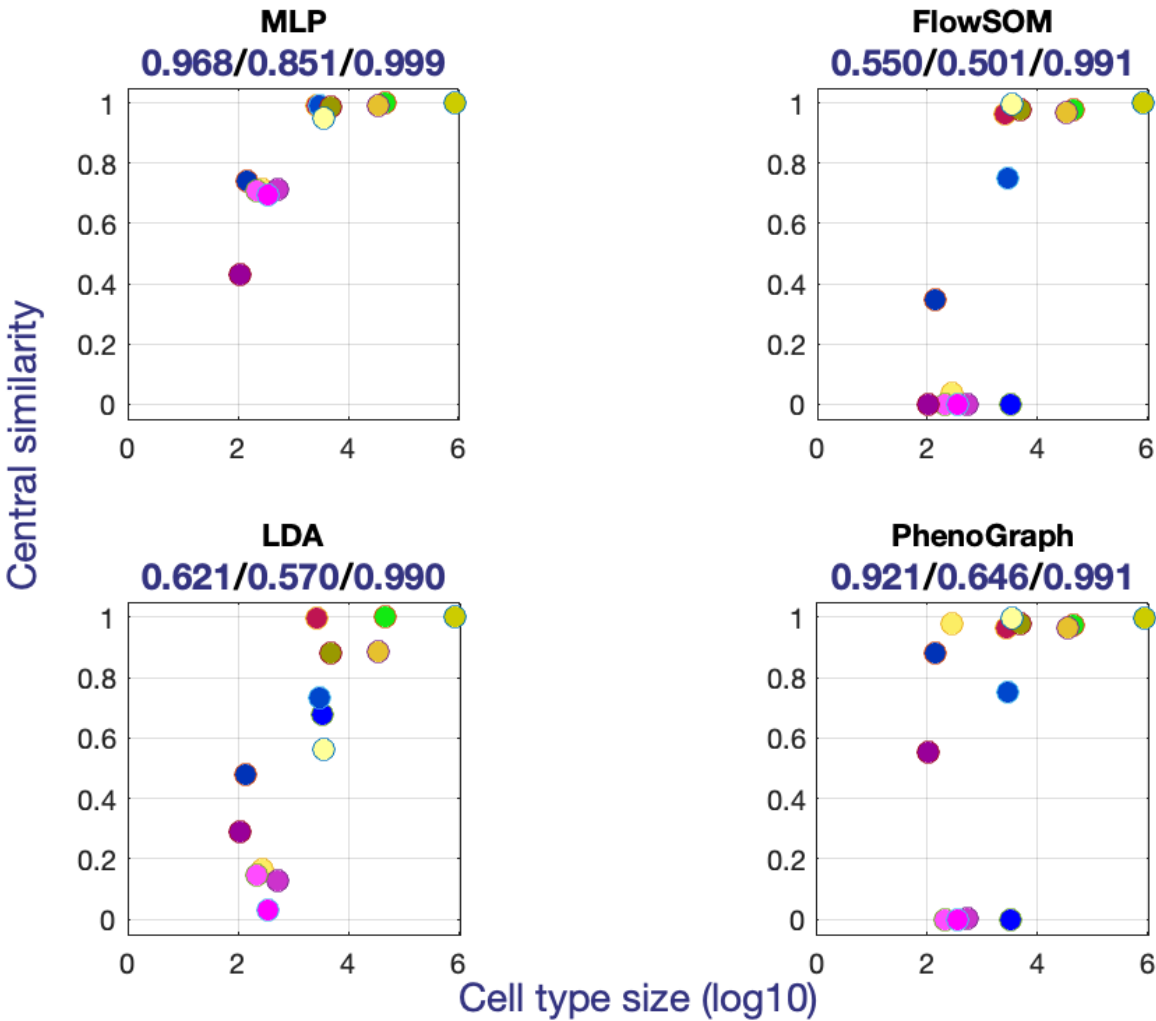
4 samples; 4-fold cross validation of 4 3x1 training X test samples
15 Phenotyping markers, 14 cell types

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP 	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
	Neutrophils	90%	1	0.997	0.997	0.985	1	0.999	1	0.998	1	0.998	0.998	0.987
	T cells	4.8%	0.999	0.986	0.990	0.986	1	0.976	1	0.976	1	0.999	0.992	0.999
	Basophils	0.28%	0.994	0.971	0.964	0.971	0.993	0.962	0.996	0.962	0.997	0.994	0.950	0.994
	Monocytes	3.6%	0.990	0.970	0.907	0.969	0.994	0.967	0.885	0.966	0.997	0.984	0.952	0.984
	MZB cells	0.34%	0.982	N/A	0.787	N/A	0.985	N/A	0.678	N/A	0.993	N/A	0.937	N/A
	Non MZB cells	0.30%	0.981	0.815	0.800	0.814	0.993	0.751	0.731	0.751	0.996	0.964	0.950	0.964
	NK cells	0.50%	0.969	0.960	0.861	0.975	0.988	0.977	0.882	0.978	0.987	0.979	0.923	0.994
	Eosinophils	0.36%	0.965	0.990	0.656	0.990	0.952	0.996	0.563	0.996	0.986	0.993	0.842	0.994
	Plasma cells	0.01%	0.833	0.478	0.579	0.906	0.742	0.349	0.480	0.880	0.946	0.841	0.851	0.953
	Progenitors	0.03%	0.813	0.060	0.281	0.913	0.715	0.034	0.164	0.980	0.956	0.480	0.734	0.929
	CD141- mDCs	0.05%	0.806	N/A	0.203	0.006	0.715	N/A	0.130	0.004	0.978	N/A	0.782	0.398
	CD1c+ mDCs	0.02%	0.802	N/A	0.224	N/A	0.708	N/A	0.147	N/A	0.960	N/A	0.823	N/A
	CD141+ mDCs	0.04%	0.796	N/A	0.056	0	0.693	N/A	0.031	0	0.960	N/A	0.732	0.159
	pDCs	0.01%	0.547	N/A	0.365	0.653	0.429	N/A	0.290	0.551	0.743	N/A	0.663	0.892
Median			0.967	0.646	0.722	0.909	0.968	0.550	0.621	0.921	0.987	0.903	0.887	0.958
Mean			0.891	0.516	0.619	0.655	0.851	0.501	0.570	0.646	0.964	0.588	0.866	0.732

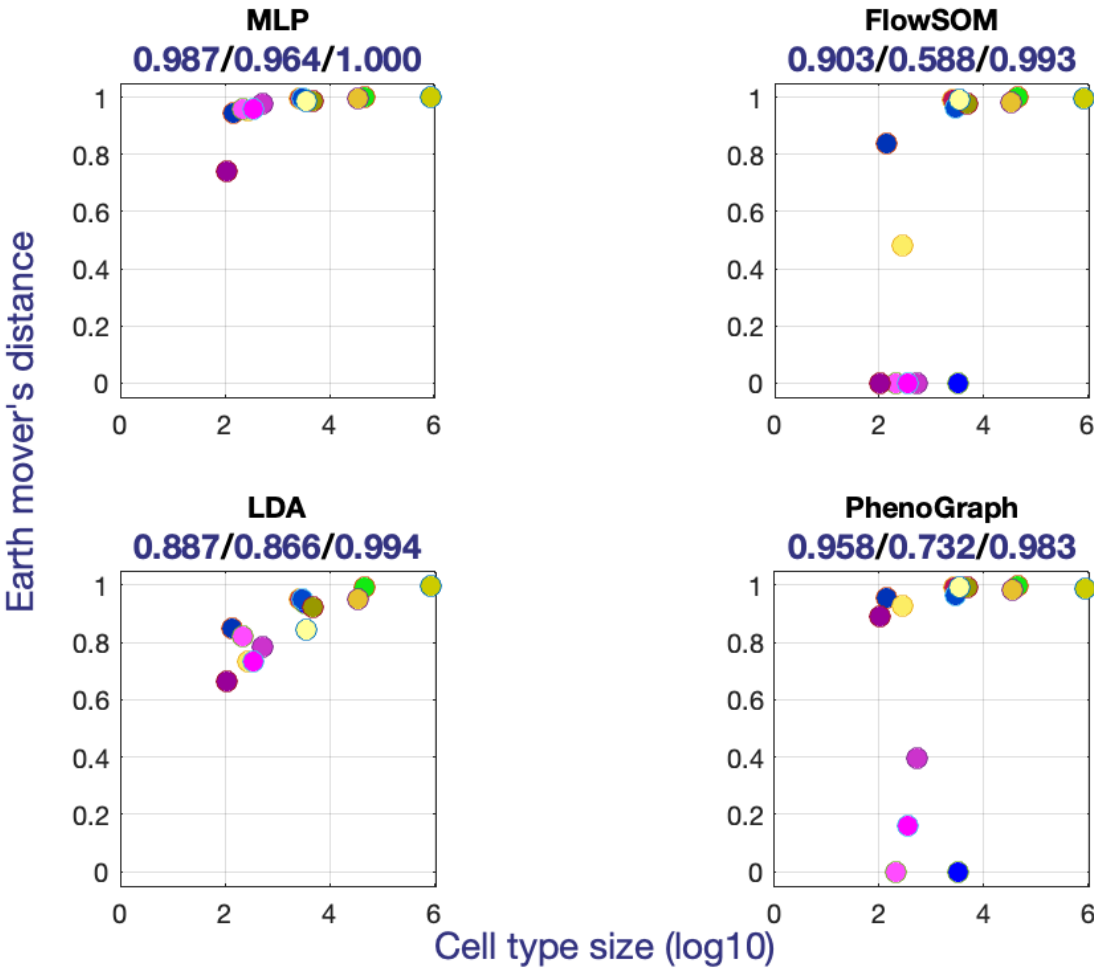
OMIP-077 F1-Scores median/mean/weighted



OMIP-077 Central similarity median/mean/weighted

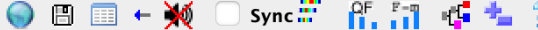


OMIP-077 Earth mover's distance median



4.3.5.1. Merged matches

With FlowSOM QFMatch finds 3 of 9 matches where merging multiple FlowSOM gated populations for 1 manually gated population obtains a higher F1-score: the 1st, 2nd and 5th ranked matches.


 MATCH sets: training=9/14 (5 UNMATCHED!), test=13/14 (1 NEW!)

Rank ²		Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set? ³	Freq.
2	●	Neutrophils	4	99.7%	99.9%	99.8%	yes	76.7%
2	●	Neutrophils (FlowSOM.Leukocytes....	4	99.7%	99.9%	99.8%	no	1.8%
2	●	Neutrophils (FlowSOM.Leukocytes....	4	99.7%	99.9%	99.8%	no	0.4%
2	●	Neutrophils (FlowSOM.Leukocytes....	4	99.7%	99.9%	99.8%	no	74.3%
1	●	T cells	3	98.6%	97.6%	99.9%	yes	10.6%
1	●	T cells (FlowSOM.Leukocytes.Pop13)	3	98.6%	97.6%	99.9%	no	9.8%
1	●	T cells (FlowSOM.Leukocytes.Pop11)	3	98.6%	97.6%	99.9%	no	0.5%
5	●	Monocytes	3	97%	96.7%	98.4%	yes	6.9%
5	●	Monocytes (FlowSOM.Leukocytes....	3	97%	96.7%	98.4%	no	6.9%
5	●	Monocytes (FlowSOM.Leukocytes....	3	97%	96.7%	98.4%	no	0.4%
3	●	Basophils	2	97.1%	96.2%	99.4%	yes	0.3%
3	●	Basophils (FlowSOM.Leukocytes.P...	2	97.1%	96.2%	99.4%	no	0.3%

With PhenoGraph QFMatch finds 3 of 12 matches where merging multiple PhenoGraph gated populations for 1 manually gated population obtains a higher F1-score: the 1st, 5th and 6th ranked matches.

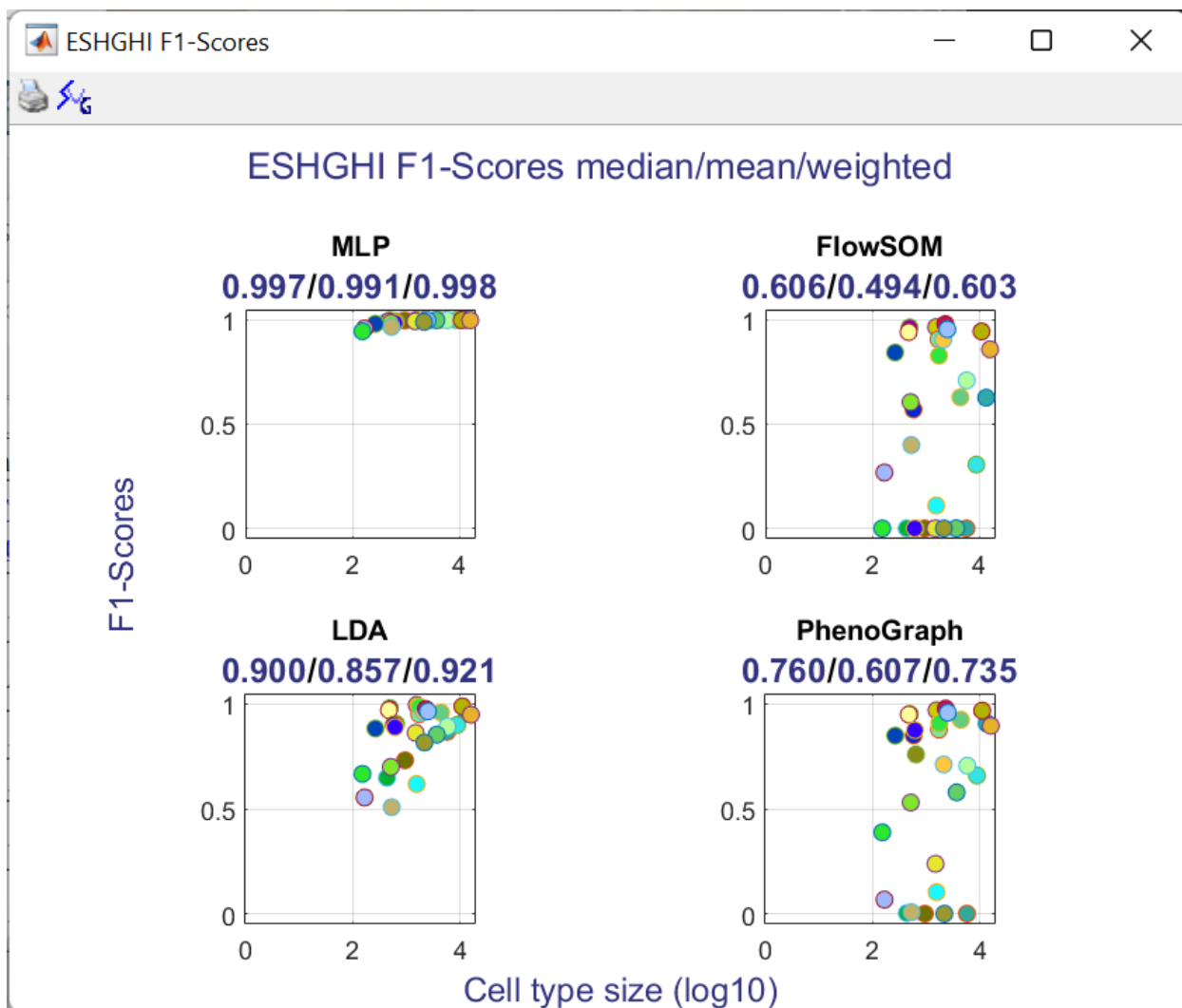
MATCH sets: training=12/14 (2 UNMATCHED!), test=21/24 (3 NEW!)									
Rank ²		Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set? ³	Freq.	
5	●	Neutrophils	8	98.5%	99.8%	98.7%	yes	76.7%	2
5	●	Neutrophils (PhenographQ1295)	8	98.5%	99.8%	98.7%	no	9.6%	:
5	●	Neutrophils (PhenographQ1294)	8	98.5%	99.8%	98.7%	no	10.1%	:
5	●	Neutrophils (PhenographQ1293)	8	98.5%	99.8%	98.7%	no	10.5%	:
5	●	Neutrophils (PhenographQ1298)	8	98.5%	99.8%	98.7%	no	8.2%	:
5	●	Neutrophils (PhenographQ1297)	8	98.5%	99.8%	98.7%	no	8.5%	:
5	●	Neutrophils (PhenographQ1291)	8	98.5%	99.8%	98.7%	no	14.5%	:
5	●	Neutrophils (PhenographQ1292)	8	98.5%	99.8%	98.7%	no	13.2%	:
1	●	T cells	4	98.6%	97.6%	99.9%	yes	10.6%	:
1	●	T cells (PhenographQ12914)	4	98.6%	97.6%	99.9%	no	1.2%	:
1	●	T cells (PhenographQ1296)	4	98.6%	97.6%	99.9%	no	8.7%	:
1	●	T cells (PhenographQ12915)	4	98.6%	97.6%	99.9%	no	0.6%	:
6	●	Monocytes	3	96.9%	96.6%	98.4%	yes	6.9%	:
6	●	Monocytes (PhenographQ12916)	3	96.9%	96.6%	98.4%	no	0.4%	:
6	●	Monocytes (PhenographQ1299)	3	96.9%	96.6%	98.4%	no	6.9%	:
2	●	NK cells	2	97.5%	97.8%	99.4%	yes	2%	:
2	●	NK cells (PhenographQ12910)	2	97.5%	97.8%	99.4%	no	2%	:

Boesch, M, Sykora, M, Gasteiger, S, Baty, F, Brutsche, MH, Sopper, S. **OMIP-077: Definition of all principal human leukocyte populations using a broadly applicable 14-color panel.** Cytometry. 2022; 101: 15– 20. <https://doi.org/10.1002/cyto.a.24481>

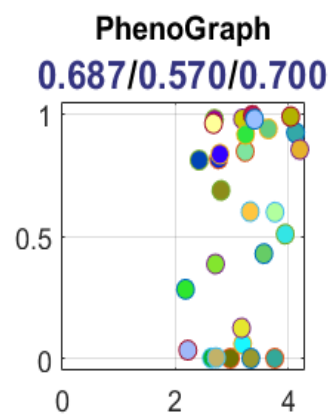
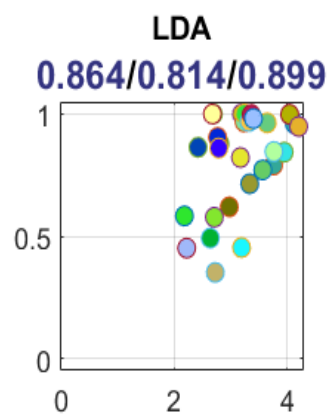
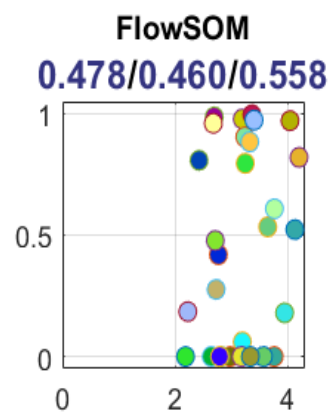
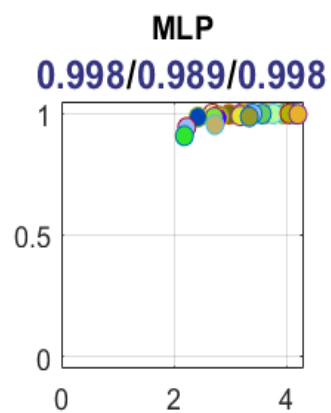
4.3.6. ESHGHI

**10 samples merged into 1, 5 fold cross validation, 383k training x 96k test *cells*
29 cell types, 27 markers**

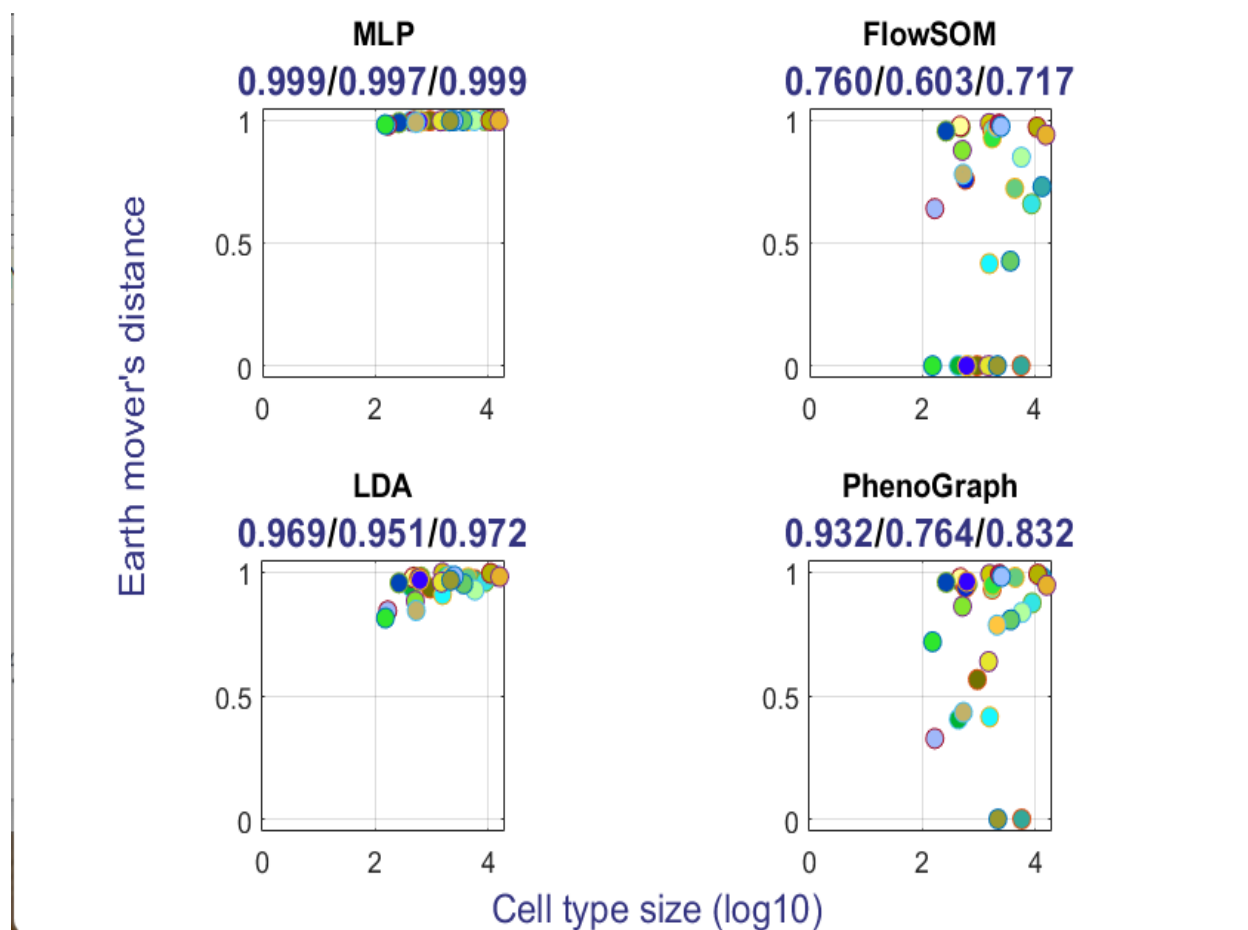
Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			 MLP	 Flow SOM	 LDA	 Pheno Graph	 MLP	 Flow SOM	 LDA	 Pheno Graph	 MLP	 Flow SOM	 LDA	 Pheno Graph
●	CD4 N	15%	1	0.627	0.954	0.907	1	0.523	0.960	0.924	1	0.730	0.987	0.979
●	CD4 CM	6.2%	1	N/A	0.868	N/A	1	N/A	0.791	N/A	1	N/A	0.970	N/A
●	CD8 N	4.8%	0.999	0.629	0.959	0.925	1	0.534	0.964	0.939	1	0.723	0.977	0.980
●	Neutrophil	1.7%	0.999	0.965	0.995	0.970	1	0.978	1	0.980	0.999	0.987	0.998	0.991
●	CD4 EM	9.6%	0.999	0.306	0.900	0.659	0.999	0.180	0.844	0.508	1	0.660	0.963	0.876
●	CD8 Temra	6.3%	0.999	0.710	0.893	0.706	1	0.608	0.846	0.598	1	0.850	0.928	0.838
●	CD16hi NK	12%	0.999	0.945	0.988	0.968	1	0.971	0.999	0.989	1	0.973	0.996	0.993
●	CD8 EM	4%	0.999	0.001	0.854	0.579	0.999	0	0.771	0.428	0.999	0.426	0.953	0.808
●	CD8 MAIT	1.9%	0.999	0.907	0.952	0.878	0.999	0.904	0.968	0.847	0.999	0.961	0.953	0.932
●	gd Tcells	1.9%	0.998	0.829	0.987	0.908	1	0.796	1	0.917	0.999	0.929	0.986	0.949
●	CD14hi Mono	17%	0.998	0.859	0.949	0.896	0.998	0.820	0.949	0.855	1	0.941	0.982	0.948
●	pDCs	0.54%	0.998	0.964	0.980	0.953	1	0.986	1	0.978	0.998	0.973	0.981	0.960
●	CD16hi Mono	2.3%	0.998	0.905	0.963	0.712	0.998	0.884	0.970	0.600	0.999	0.973	0.985	0.786
●	Basophils	2.5%	0.998	0.980	0.976	0.978	0.999	0.995	0.998	0.994	0.999	0.985	0.971	0.991
●	Naive B	2.7%	0.997	0.955	0.965	0.959	1	0.974	0.982	0.979	0.999	0.975	0.984	0.983
●	Treg	1%	0.997	N/A	0.732	0	0.997	N/A	0.620	0	0.998	N/A	0.937	0.566
●	CD4 Temra	1.7%	0.996	0.110	0.618	0.103	0.994	0.060	0.453	0.058	0.999	0.416	0.910	0.414
●	int Mono	1.6%	0.994	N/A	0.862	0.238	0.992	N/A	0.822	0.124	0.998	N/A	0.961	0.638
●	CD56hi NK	0.70%	0.993	N/A	0.905	0.760	0.990	N/A	0.878	0.687	0.997	N/A	0.981	0.952
●	CD8 CM	0.48%	0.992	N/A	0.648	0.003	0.992	N/A	0.492	0.001	0.997	N/A	0.940	0.406
●	Eosinophil	0.52%	0.992	0.942	0.971	0.950	1	0.960	1	0.961	0.996	0.977	0.979	0.977
●	HLADRlo Mono	2.4%	0.991	N/A	0.816	N/A	0.988	N/A	0.714	N/A	0.998	N/A	0.968	N/A
●	Mem B	0.64%	0.986	0.570	0.902	0.851	0.990	0.419	0.904	0.817	0.994	0.760	0.977	0.940
●	Trans B	0.67%	0.986	N/A	0.890	0.875	0.982	N/A	0.861	0.836	0.995	N/A	0.969	0.963
●	CD14- CD16-	0.56%	0.986	0.606	0.700	0.530	0.986	0.478	0.578	0.386	0.993	0.878	0.883	0.862
●	Plasmablast	0.28%	0.981	0.844	0.883	0.849	0.986	0.808	0.864	0.811	0.991	0.956	0.957	0.959
●	Lineage Negative	0.57%	0.966	0.400	0.508	0.007	0.955	0.276	0.352	0.003	0.992	0.781	0.845	0.433
●	IgD- CD27- B	0.18%	0.959	0.268	0.554	0.067	0.943	0.185	0.451	0.033	0.981	0.641	0.844	0.327
●	CD123-	0.17%	0.945	N/A	0.667	0.388	0.909	N/A	0.583	0.283	0.983	N/A	0.815	0.719
Median			0.997	0.606	0.900	0.760	0.998	0.478	0.864	0.687	0.999	0.760	0.969	0.932
Mean			0.991	0.494	0.857	0.607	0.989	0.460	0.814	0.570	0.997	0.603	0.951	0.764



Central similarity



Cell type size (log10)



4.3.6.1. Merged matches

With FlowSOM QFMatch finds 2 of 22 matches where merging multiple FlowSOM gated populations for 1 manually gated population obtains a higher F1-score: the ?, ? and ?th ranked matches.

MATCH sets: training=21/29 (8 UNMATCHED!), test=23/29 (6 NEW!)										
Rank	#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.		
11	10	gd Tcells	3	82.9%	79.6%	92.9%	yes	1.9%		
11	35	gd Tcells (FlowSOM.Residual.Pop2)	3	82.9%	79.6%	92.9%	no	0.8%		
11	48	gd Tcells (FlowSOM.Residual.Pop7)	3	82.9%	79.6%	92.9%	no	1.1%		
14	5	Lineage Negative	3	40%	27.6%	78.1%	yes	0.6%		
14	40	FlowSOM.Residual.Pop14	3	40%	27.6%	78.1%	no	0.1%		
14	51	Lineage Negative (FlowSOM.Residua...	3	40%	27.6%	78.1%	no	0.3%		
1	12	Neutrophil	2	96.5%	97.8%	98.7%	yes	1.7%		
1	38	Neutrophil (FlowSOM.Residual.Pop18)	2	96.5%	97.8%	98.7%	no	1.7%		

With PhenoGraph QFMatch finds 7 of 19 matches where merging multiple PhenoGraph gated populations for 1 manually gated population obtains a higher F1-score: the 1st, 4th, 6th, 7th, 16th, 17th and 18th ranked matches.

MATCH sets: training=27/29 (2 UNMATCHED!), test=36/50 (14 NEW!)										
Rank		#	Subset (class) name	Matches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Training set?	Freq.	
16		18	CD4 EM	5	65.9%	50.8%	87.6%	yes	9.6%	
16		39	CD4 EM (PhenographYJ6F11)	5	65.9%	50.8%	87.6%	no	3.4%	
16		48	CD4 EM (PhenographYJ6F5)	5	65.9%	50.8%	87.6%	no	5.1%	
16		57	CD4 EM (PhenographYJ6F17)	5	65.9%	50.8%	87.6%	no	2.2%	
16		64	CD4 EM (PhenographYJ6F4)	5	65.9%	50.8%	87.6%	no	6.8%	
1		29	CD16hi NK	3	96.8%	98.9%	99.3%	yes	12%	
1		44	CD16hi NK (PhenographYJ6F3)	3	96.8%	98.9%	99.3%	no	7.9%	
1		68	CD16hi NK (PhenographYJ6F10)	3	96.8%	98.9%	99.3%	no	3.5%	
4		4	Naive B	3	95.9%	97.9%	98.3%	yes	2.7%	
4		54	Naive B (PhenographYJ6F13)	3	95.9%	97.9%	98.3%	no	2.5%	
4		70	Naive B (PhenographYJ6F41)	3	95.9%	97.9%	98.3%	no	0.1%	
6		20	CD4 N	3	90.7%	92.4%	97.9%	yes	14.6%	
6		30	CD4 N (PhenographYJ6F8)	3	90.7%	92.4%	97.9%	no	4.3%	
6		46	CD4 N (PhenographYJ6F2)	3	90.7%	92.4%	97.9%	no	9.5%	
7		28	Eosinophil	3	95%	96.1%	97.7%	yes	0.5%	
7		33	Eosinophil (PhenographYJ6F27)	3	95%	96.1%	97.7%	no	0.5%	
7		38	Eosinophil (PhenographYJ6F49)	3	95%	96.1%	97.7%	no	0%	
17		7	[CD14- CD16-]	3	53%	38.6%	86.2%	yes	0.6%	
17		52	[CD14- CD16-] (PhenographYJ6F45)	3	53%	38.6%	86.2%	no	0%	
17		55	[CD14- CD16-] (PhenographYJ6F20)	3	53%	38.6%	86.2%	no	1.3%	
18		14	CD8 Temra	3	70.6%	59.8%	83.8%	yes	6.3%	
18		45	CD8 Temra (PhenographYJ6F14)	3	70.6%	59.8%	83.8%	no	2.5%	
18		53	CD8 Temra (PhenographYJ6F12)	3	70.6%	59.8%	83.8%	no	2.8%	
2		12	Neutrophil	2	97%	98%	99.1%	yes	1.7%	
2		41	Neutrophil (PhenographYJ6F19)	2	97%	98%	99.1%	no	1.7%	

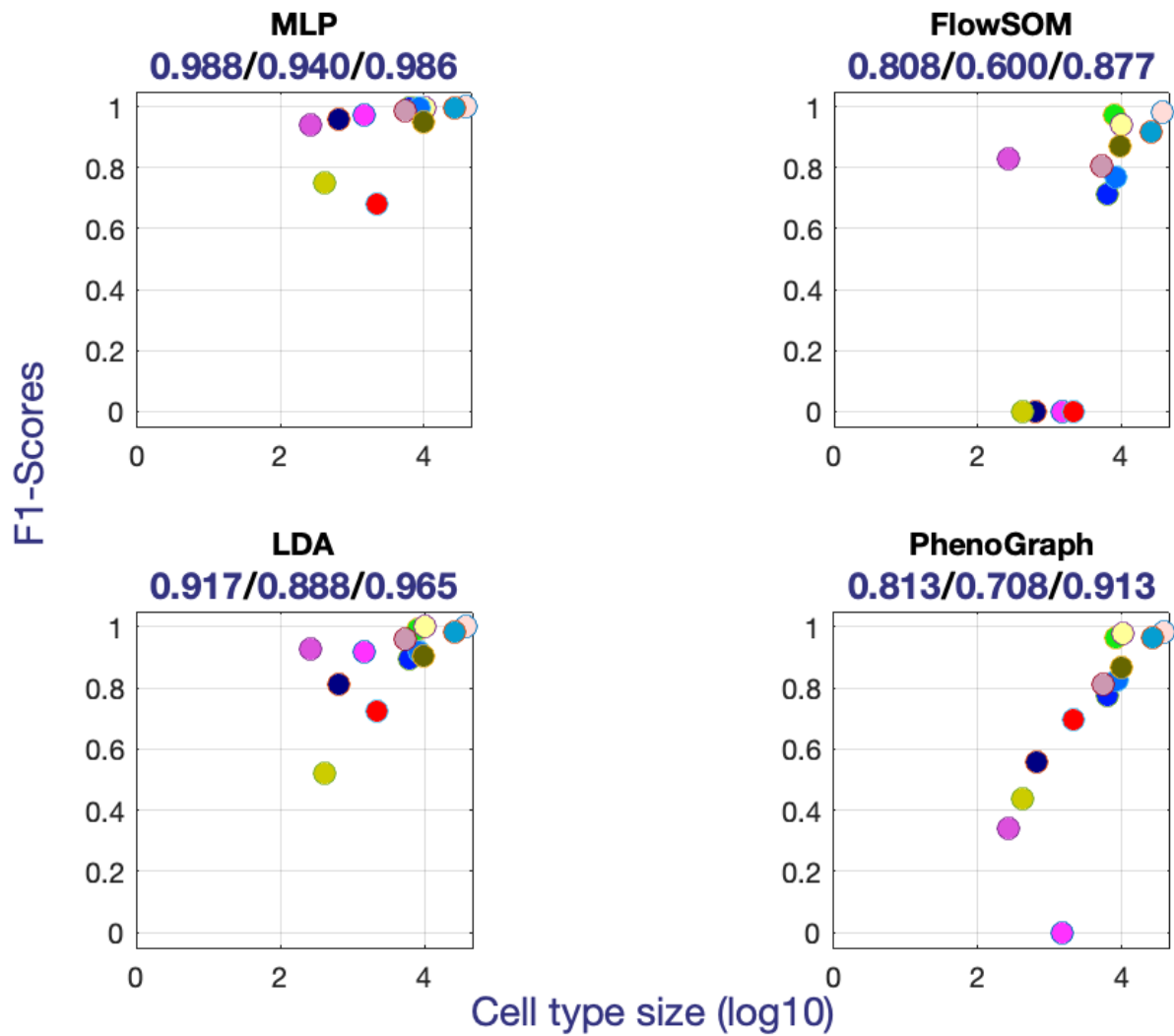
Toghi Eshghi S, Au-Yeung A, Takahashi C, Bolen CR, Nyachienga MN, Lear SP, Green C, Mathews WR and O'Gorman WE (2019) **Quantitative Comparison of Conventional and t-SNE-guided Gating Analyses**. Front. Immunol. 10:1194. doi: 10.3389/fimmu.2019.01194.
<https://www.frontiersin.org/articles/10.3389/fimmu.2019.01194/full>

4.3.7. GHOSN

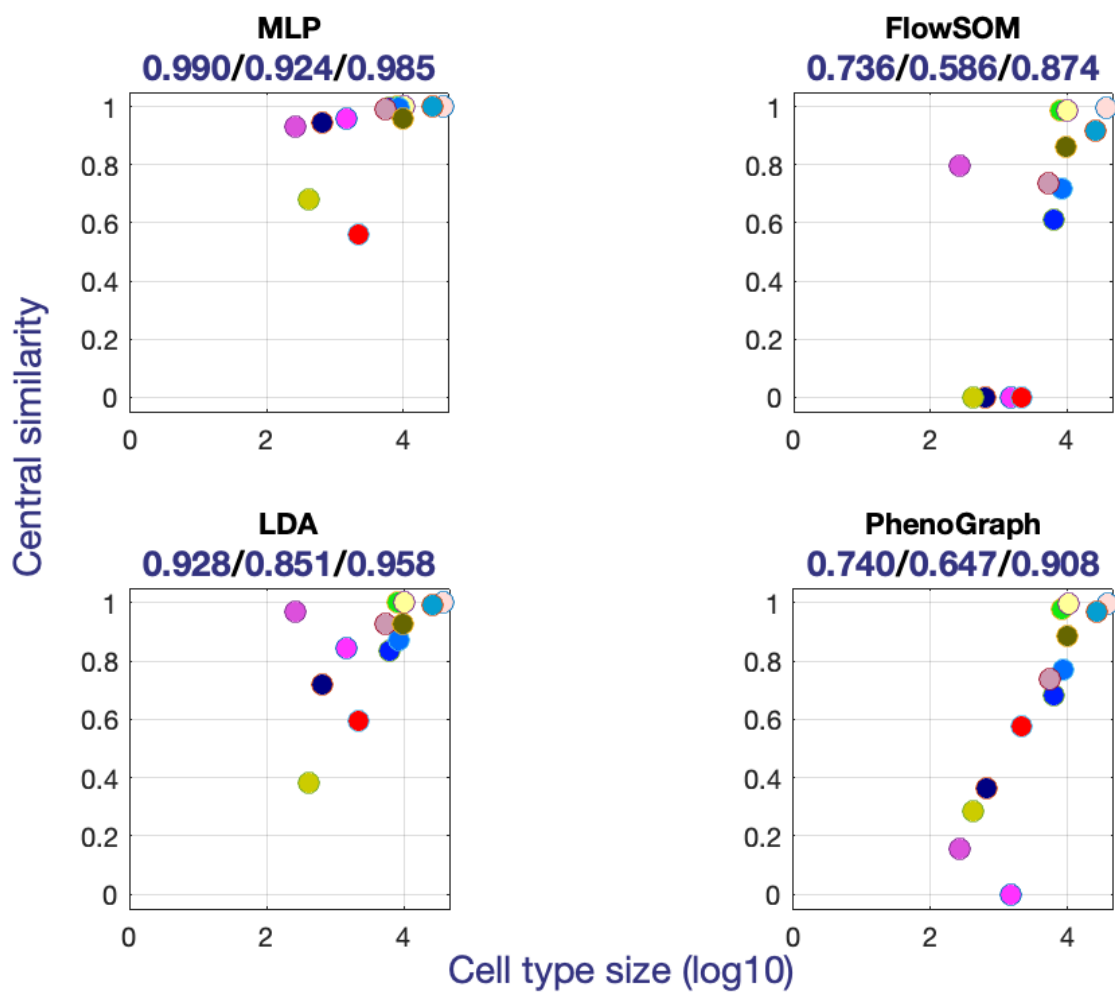
3 samples, 2-fold cross validation 2x1 and 1x2 training x test samples,
13 cell types, 9 markers.

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP 	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
	Large macrophages	32%	1	0.982	1	0.982	1	0.999	1	0.999	1	0.991	1	0.992
	B-1	22%	0.999	0.919	0.981	0.963	1	0.918	0.993	0.971	0.999	0.964	0.990	0.993
	T cells	6.9%	0.996	0.972	0.992	0.963	1	0.988	1	0.978	0.999	0.987	0.997	0.976
	Eosinophils	8.6%	0.996	0.943	1	0.979	1	0.985	1	0.997	0.998	0.953	1	0.993
	B-2 IgM high	5.3%	0.996	0.715	0.893	0.777	0.998	0.612	0.833	0.681	0.999	0.845	0.941	0.911
	B-2 IgM medium	7.2%	0.995	0.769	0.917	0.824	0.997	0.720	0.873	0.772	0.997	0.847	0.957	0.935
	Small macrophages	4.6%	0.988	0.808	0.958	0.813	0.990	0.736	0.928	0.740	0.997	0.880	0.973	0.882
	CD11b+ dendritic	1.3%	0.971	N/A	0.916	N/A	0.960	N/A	0.845	N/A	0.994	N/A	0.959	N/A
	Developing B	0.55%	0.962	N/A	0.812	0.556	0.943	N/A	0.720	0.364	0.969	N/A	0.842	0.689
	NK, NKT	8.3%	0.949	0.871	0.903	0.867	0.958	0.861	0.929	0.886	0.970	0.890	0.929	0.914
	CD11b- dendritic	0.23%	0.943	0.827	0.929	0.342	0.933	0.798	0.968	0.157	0.939	0.958	0.934	0.548
	Neutrophils	0.36%	0.749	N/A	0.519	0.440	0.681	N/A	0.380	0.287	0.932	N/A	0.718	0.838
	ckit+ mast cells	1.8%	0.682	N/A	0.724	0.697	0.558	N/A	0.593	0.578	0.912	N/A	0.954	0.951
Median			0.988	0.808	0.917	0.813	0.990	0.736	0.928	0.740	0.997	0.880	0.957	0.914
Mean			0.940	0.600	0.888	0.708	0.924	0.586	0.851	0.647	0.977	0.640	0.938	0.817

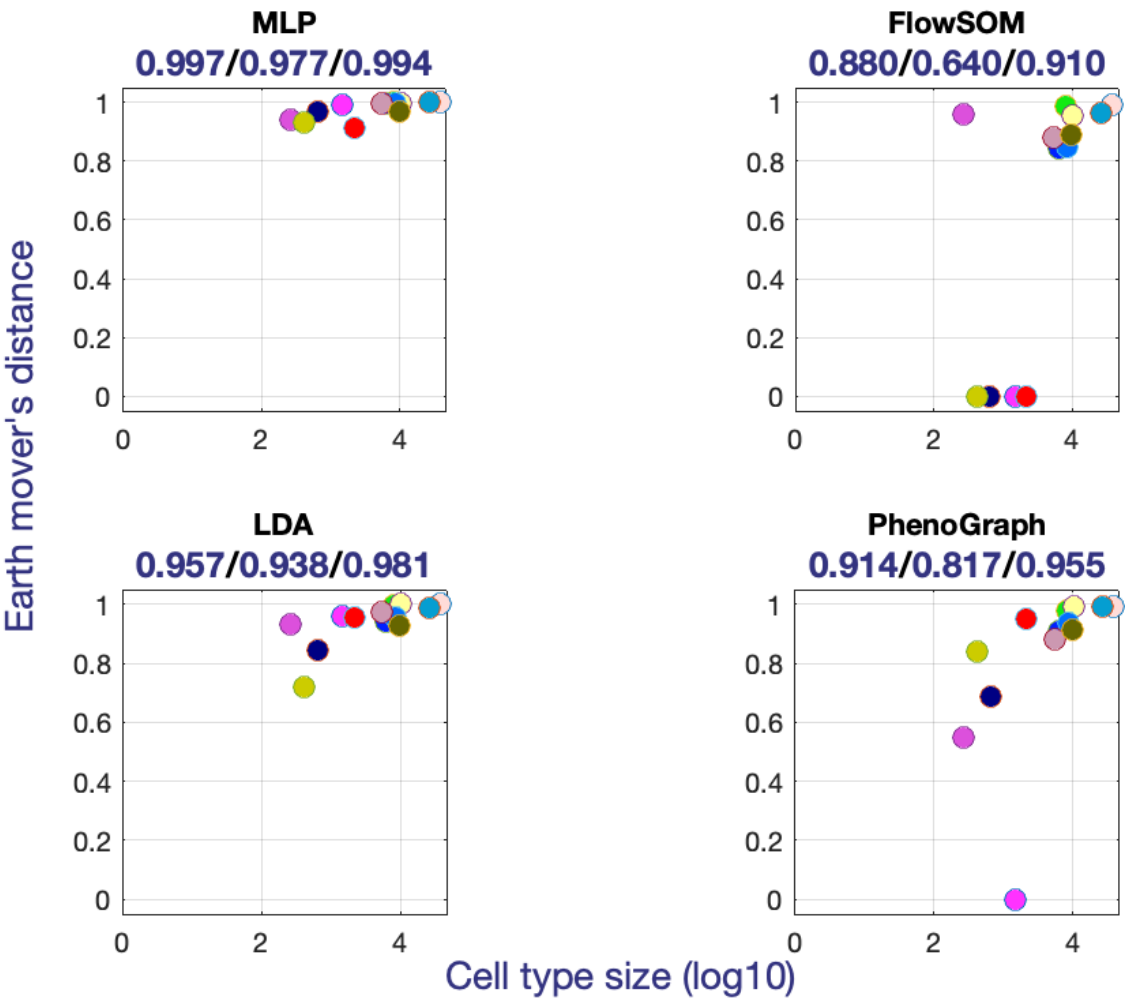
GHOSN F1-Scores median/mean/weighted



GHOSN Central similarity median/mean/weighted



GHOSN Earth mover's distance median/mean/weighted



4.3.7.1. Merged matches

With PhenoGraph QFMatch finds 4 of 12 matches where merging multiple PhenoGraph gated populations for 1 manually gated population obtains a higher F1-score: the 1st, 3rd, 7th and 8th ranked matches.

MATCH sets: training=12/13 (1 UNMATCHED!), test=21/22 (1 NEW!)										
Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.	
1	●	13	B-1	6	96.3%	97.1%	99.3%	yes	22.1%	
1	●	14	Phenograph29FL8	6	96.3%	97.1%	99.3%	no	6.9%	
1	●	19	Phenograph29FL13	6	96.3%	97.1%	99.3%	no	3.9%	
1	●	20	Phenograph29FL21	6	96.3%	97.1%	99.3%	no	0.3%	
1	●	28	Phenograph29FL1	6	96.3%	97.1%	99.3%	no	9.9%	
1	●	32	Phenograph29FL22	6	96.3%	97.1%	99.3%	no	0.1%	
3	●	1	Large macrophages	5	98.2%	99.9%	99.2%	yes	31.9%	
3	●	17	Phenograph29FL6	5	98.2%	99.9%	99.2%	no	7.3%	
3	●	25	Phenograph29FL4	5	98.2%	99.9%	99.2%	no	7.8%	
3	●	27	Phenograph29FL3	5	98.2%	99.9%	99.2%	no	8.6%	
3	●	30	Phenograph29FL5	5	98.2%	99.9%	99.2%	no	7.7%	
7	●	9	NK, NKT	3	86.7%	88.6%	91.4%	yes	9%	
7	●	26	Phenograph29FL11	3	86.7%	88.6%	91.4%	no	4.7%	
7	●	34	Phenograph29FL15	3	86.7%	88.6%	91.4%	no	2.3%	
8	●	2	B-2 IgM high	3	77.7%	68.1%	91.1%	yes	5.1%	
8	●	15	Phenograph29FL16	3	77.7%	68.1%	91.1%	no	2.2%	
8	●	18	Phenograph29FL12	3	77.7%	68.1%	91.1%	no	4.5%	
2	●	8	Eosinophils	2	97.9%	99.7%	99.3%	yes	9.5%	
2	●	33	Phenograph29FL2	2	97.9%	99.7%	99.3%	no	9.3%	

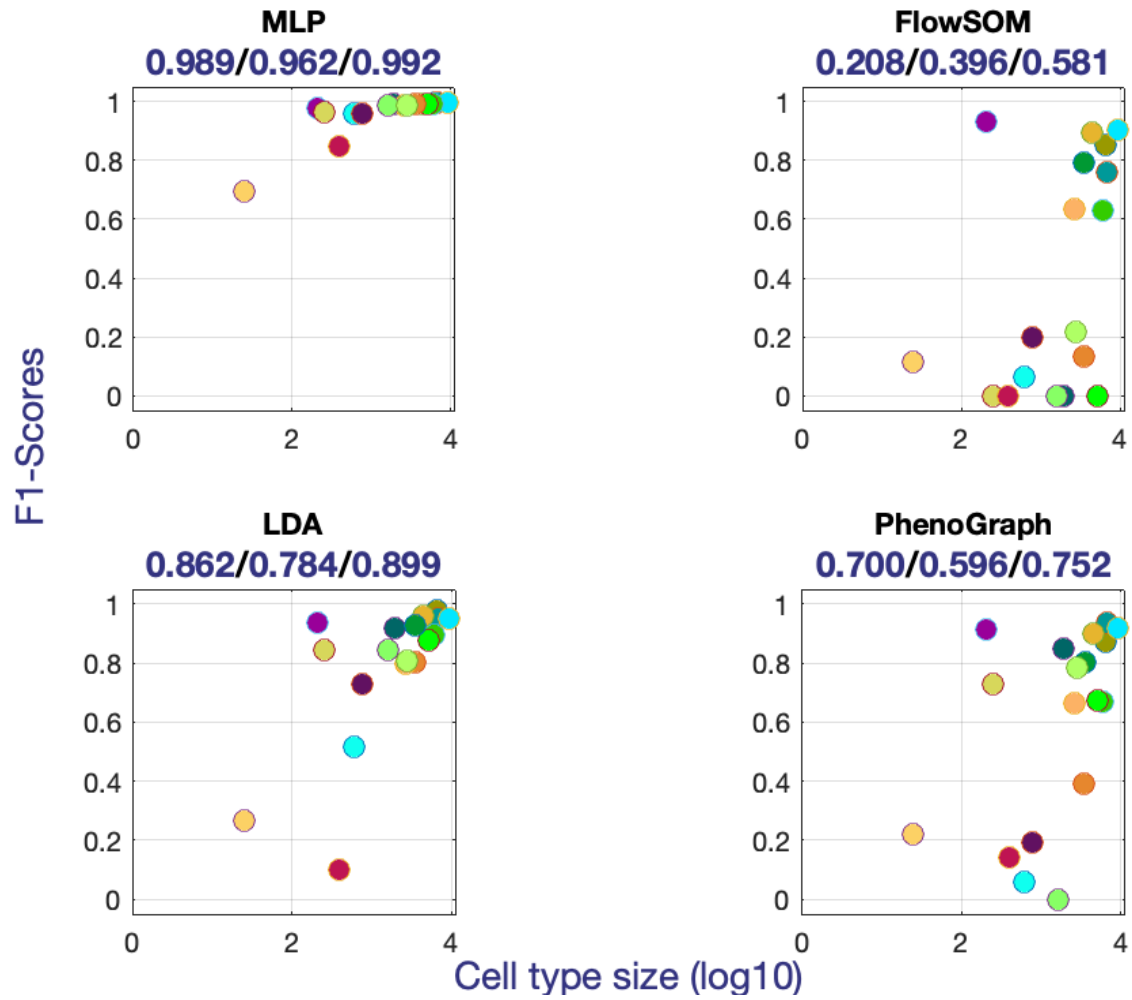
Eliver Eid Bou Ghosn, Alexandra A. Cassado, Gregory R. Govoni, +6, and Leonore A. Herzenberg (2010), **Two physically, functionally, and developmentally distinct peritoneal macrophage subsets**, PNAS Vol. 107|No. 6 2568-2573, January 25, 2010 <https://doi.org/10.1073/pnas.0915000107>

4.3.8. LEIPOLD

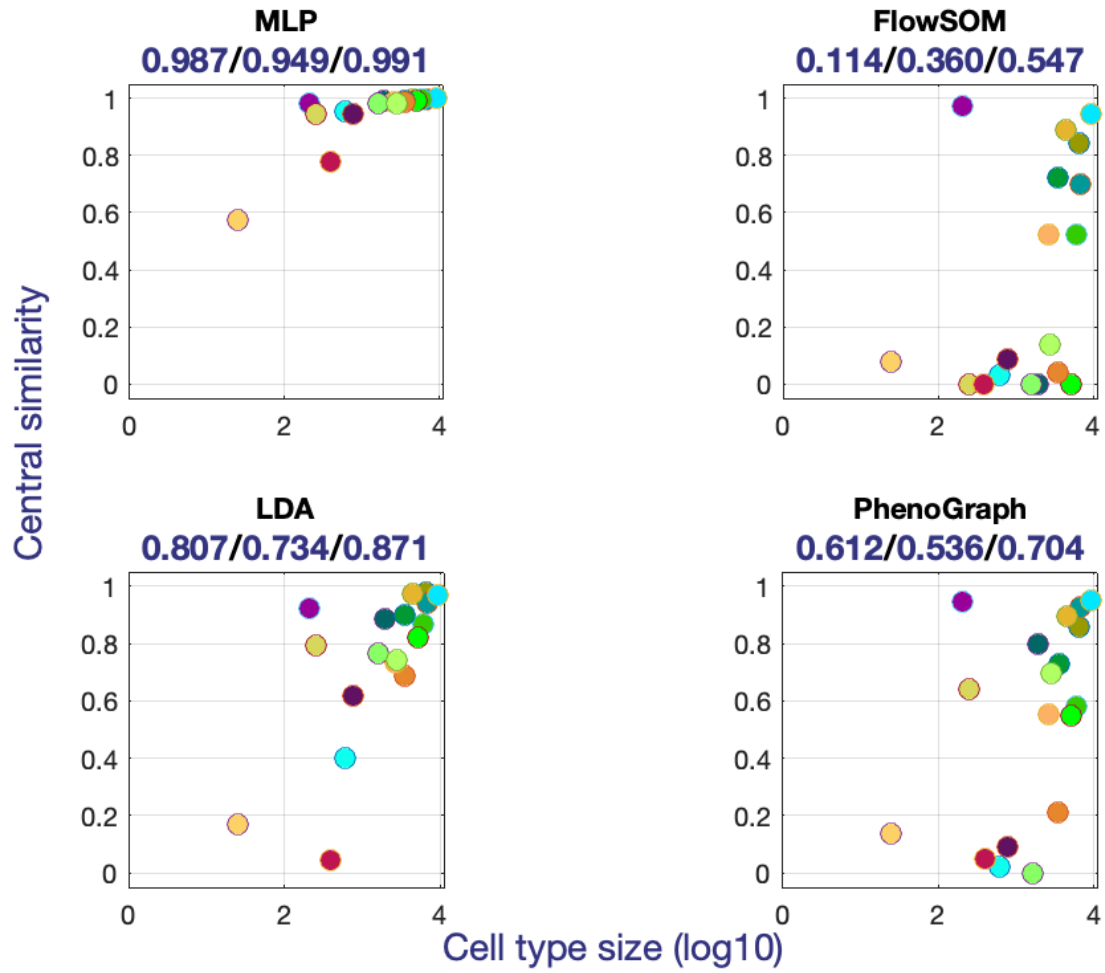
6 samples,4-fold cross validation: 5x1 training by test samples;
18 cell types, 15 markers

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			 MLP	 Flow SOM	LDA	 Pheno Graph	 MLP	 Flow SOM	LDA	 Pheno Graph	 MLP	 Flow SOM	LDA	 Pheno Graph
	NK cells	12%	0.997	0.854	0.977	0.872	0.997	0.843	0.978	0.858	0.999	0.941	0.992	0.947
	CD4 T cells CD45RA- , CD27+	12%	0.997	0.759	0.950	0.939	0.997	0.700	0.940	0.929	0.999	0.863	0.989	0.991
	CD4 T cells CD45RA+ , CD27+	16%	0.996	0.902	0.951	0.916	0.999	0.944	0.969	0.949	0.999	0.972	0.981	0.975
	CD4 T cells CD45RA- , CD27-	3.4%	0.994	N/A	0.920	0.851	0.993	N/A	0.885	0.798	0.998	N/A	0.975	0.946
	CD16- monocytes	7.9%	0.994	0.894	0.959	0.900	0.997	0.888	0.974	0.896	0.999	0.956	0.971	0.961
	CD8 T cells CD45RA+ , CD27+	11%	0.993	0.632	0.897	0.669	0.994	0.521	0.866	0.582	0.999	0.839	0.952	0.840
	CD8 T cells CD45RA+ , CD27-	9.1%	0.993	N/A	0.878	0.671	0.993	N/A	0.819	0.548	0.998	N/A	0.980	0.902
	CD8 T cells CD45RA- , CD27+	6.3%	0.993	0.794	0.929	0.804	0.992	0.724	0.898	0.731	0.999	0.957	0.980	0.968
	CD38 CD56- B cells	6.2%	0.991	0.133	0.805	0.392	0.988	0.040	0.688	0.210	0.998	0.417	0.941	0.668
	CD38+CD56 B cells	4.7%	0.988	0.633	0.797	0.665	0.985	0.521	0.735	0.553	0.998	0.920	0.955	0.917
	CD8 T cells CD45RA- , CD27-	2.8%	0.986	N/A	0.846	N/A	0.985	N/A	0.767	N/A	0.997	N/A	0.958	N/A
	CD4- CD8-	5%	0.986	0.219	0.806	0.786	0.985	0.139	0.743	0.697	0.997	0.539	0.946	0.915
	pDCs	0.37%	0.980	0.933	0.935	0.915	0.984	0.973	0.922	0.948	0.989	0.948	0.960	0.941
	CD56 bright NK cells	0.44%	0.966	N/A	0.844	0.729	0.946	N/A	0.796	0.642	0.988	N/A	0.943	0.945
	CD4 T cells CD45RA+ , CD27-	1.1%	0.961	0.065	0.518	0.059	0.957	0.030	0.400	0.023	0.990	0.695	0.874	0.319
	mDCs	1.4%	0.959	0.197	0.730	0.194	0.946	0.089	0.619	0.091	0.990	0.572	0.925	0.555
	Basophils	0.69%	0.850	N/A	0.102	0.141	0.777	N/A	0.044	0.048	0.975	N/A	0.734	0.406
	CD16+ monocytes	0.04%	0.697	0.115	0.268	0.220	0.574	0.076	0.171	0.137	0.829	0.428	0.652	0.552
Median			0.989	0.208	0.862	0.700	0.987	0.114	0.807	0.612	0.998	0.633	0.957	0.916
Mean			0.962	0.396	0.784	0.596	0.949	0.360	0.734	0.536	0.986	0.558	0.928	0.764

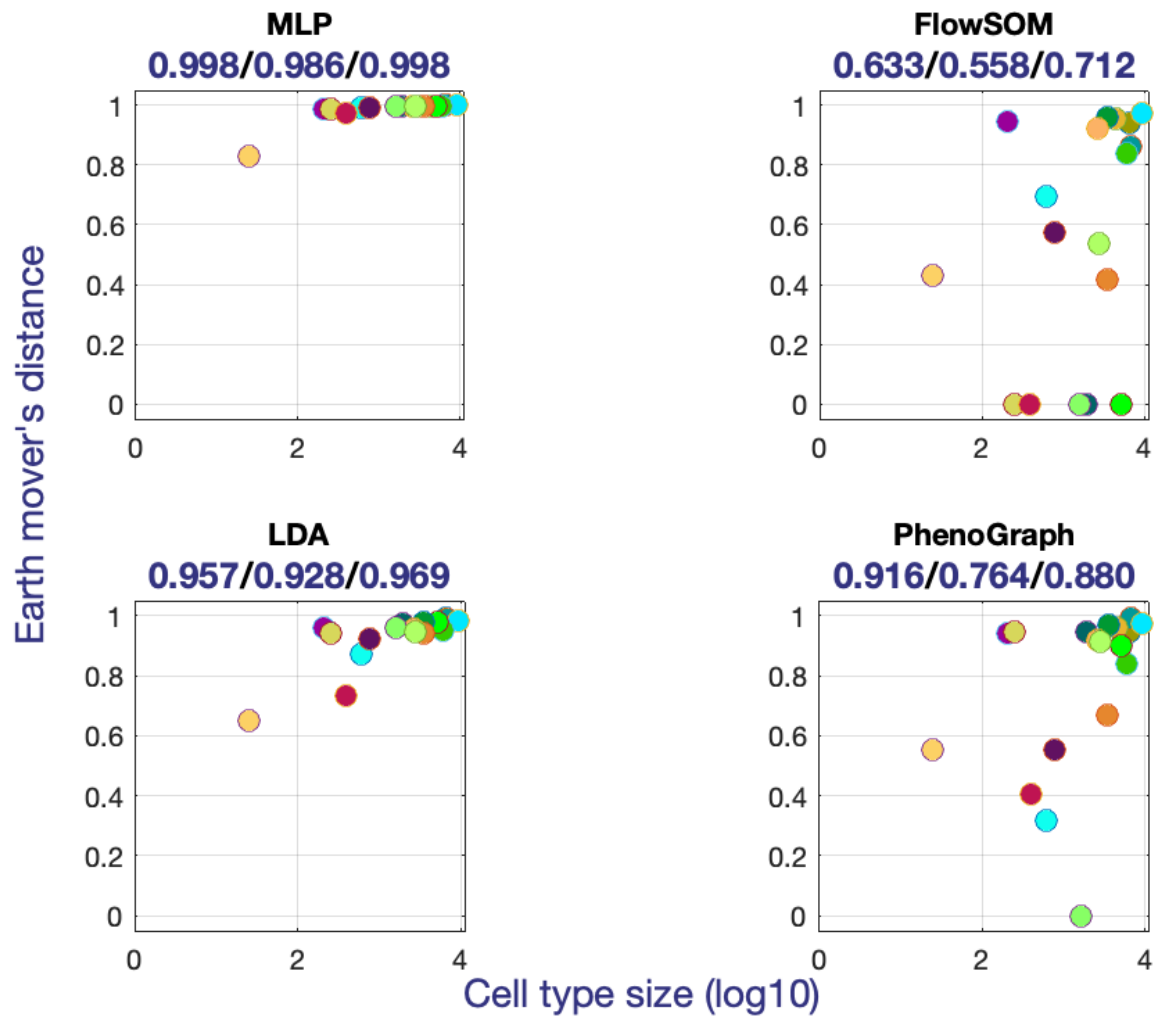
LEIPOLD F1-Scores median/mean/weighted



LEIPOLD Central similarity median/mean/weighted



LEIPOLD Earth mover's distance median/mean/weighted



4.3.8.1. Merged matches

With FlowSOM QFMatch finds 4 of 13 matches where merging 2 FlowSOM gated populations for 1 manually gated population obtains a higher F1-score: the 1st, 3rd, 7th and 10th ranked matches.

MATCH sets: training=13/18 (5 UNMATCHED!), test=17/18 (1 NEW!)										
Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.	
1	●	15	CD4 T cells CD45RA+ , CD27+	3	90.2%	94.4%	97.2%	yes	16.9%	
1	●	24	CD4 T cells CD45RA+ , CD27+ (Flo...	3	90.2%	94.4%	97.2%	no	0.9%	
1	●	27	CD4 T cells CD45RA+ , CD27+ (Flo...	3	90.2%	94.4%	97.2%	no	15%	
3	●	1	CD16- monocytes	3	89.4%	88.8%	95.6%	yes	6.1%	
3	●	28	CD16- monocytes (FlowSOM.All cell...	3	89.4%	88.8%	95.6%	no	6.2%	
3	●	31	CD16- monocytes (FlowSOM.All cell...	3	89.4%	88.8%	95.6%	no	0.5%	
7	●	12	CD4 T cells CD45RA- , CD27+	3	75.9%	70%	86.3%	yes	14.8%	
7	●	23	CD4 T cells CD45RA- , CD27+ (Flow...	3	75.9%	70%	86.3%	no	20.5%	
7	●	29	Basophils (FlowSOM.All cells.Pop12)	3	75.9%	70%	86.3%	no	1.1%	
10	●	2	mDCs	3	19.7%	8.9%	57.2%	yes	0.9%	
10	●	22	mDCs (FlowSOM.All cells.Pop2)	3	19.7%	8.9%	57.2%	no	0.3%	
10	●	26	mDCs (FlowSOM.All cells.Pop9)	3	19.7%	8.9%	57.2%	no	2.8%	
2	●	5	CD8 T cells CD45RA- , CD27+	2	79.4%	72.4%	95.7%	yes	6.9%	
2	●	35	CD8 T cells CD45RA- , CD27+ (Flow...	2	79.4%	72.4%	95.7%	no	7.8%	

With PhenoGraph QFMatch finds 6 of ? matches where merging multiple PhenoGraph gated populations for 1 manually gated population obtains a higher F1-score: the ?, ? and ?th ranked matches.

MATCH sets: training=17/18 (1 UNMATCHED!), test=25/27 (2 NEW!)

Rank ²	#	Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.	
2	15	CD4 T cells CD45RA+ , CD27+	4	91.6%	94.9%	97.5%	yes	16.9%	1
2	19	CD4 T cells CD45RA+ , CD27+ (Phe...	4	91.6%	94.9%	97.5%	no	1.2%	
2	30	CD4 T cells CD45RA+ , CD27+ (Phe...	4	91.6%	94.9%	97.5%	no	13.5%	1
2	39	CD4 T cells CD45RA+ , CD27+ (Phe...	4	91.6%	94.9%	97.5%	no	0.5%	
10	18	CD4- CD8-	4	78.6%	69.7%	91.5%	yes	3.1%	
10	22	CD4- CD8- (Phenograph4RXF23)	4	78.6%	69.7%	91.5%	no	0.2%	
10	26	CD4- CD8- (Phenograph4RXF14)	4	78.6%	69.7%	91.5%	no	1.3%	
10	33	CD4- CD8- (Phenograph4RXF12)	4	78.6%	69.7%	91.5%	no	1.8%	
1	12	CD4 T cells CD45RA- , CD27+	3	93.9%	92.9%	99.1%	yes	14.8%	1
1	34	CD4 T cells CD45RA- , CD27+ (Phen...	3	93.9%	92.9%	99.1%	no	1.2%	
1	41	CD4 T cells CD45RA- , CD27+ (Phen...	3	93.9%	92.9%	99.1%	no	12.7%	1
4	1	CD16- monocytes	3	90%	89.6%	96.1%	yes	6.1%	
4	24	CD16- monocytes (Phenograph4RXF...	3	90%	89.6%	96.1%	no	0.5%	
4	37	CD16- monocytes (Phenograph4RXF8)	3	90%	89.6%	96.1%	no	6.1%	
11	13	CD8 T cells CD45RA+ , CD27-	3	67.1%	54.8%	90.2%	yes	9.8%	
11	32	CD8 T cells CD45RA+ , CD27- (Phen...	3	67.1%	54.8%	90.2%	no	2.5%	
11	44	CD8 T cells CD45RA+ , CD27- (Phen...	3	67.1%	54.8%	90.2%	no	13.6%	1
14	2	mDCs	3	19.4%	9.1%	55.5%	yes	0.9%	
14	21	mDCs (Phenograph4RXF24)	3	19.4%	9.1%	55.5%	no	0.2%	
14	45	mDCs (Phenograph4RXF10)	3	19.4%	9.1%	55.5%	no	2.8%	
3	5	CD8 T cells CD45RA- , CD27+	2	80.4%	73.1%	96.8%	yes	6.9%	
3	42	CD8 T cells CD45RA- , CD27+ (Phen...	2	80.4%	73.1%	96.8%	no	7.5%	

Michael D. Leipold, Gerlinde Obermoser, Craig Fenwick, Katja Kleinstuber, Narges Rashidi, John P. McNevin, Allison N. Nau, Lisa E. Wagar, Virginie Rozot, Mark M. Davis, Stephen DeRosa, Giuseppe Pantaleo, Thomas J. Scriba, Bruce D. Walker, Lars R. Olsen, Holden T. Maecker, (2018) **Comparison of CyTOF assays across sites: Results of a six-center pilot study**, Journal of Immunological Methods, Volume 453, Pages 37-43, ISSN 0022-1759, <https://www.sciencedirect.com/science/article/pii/S0022175917304908>

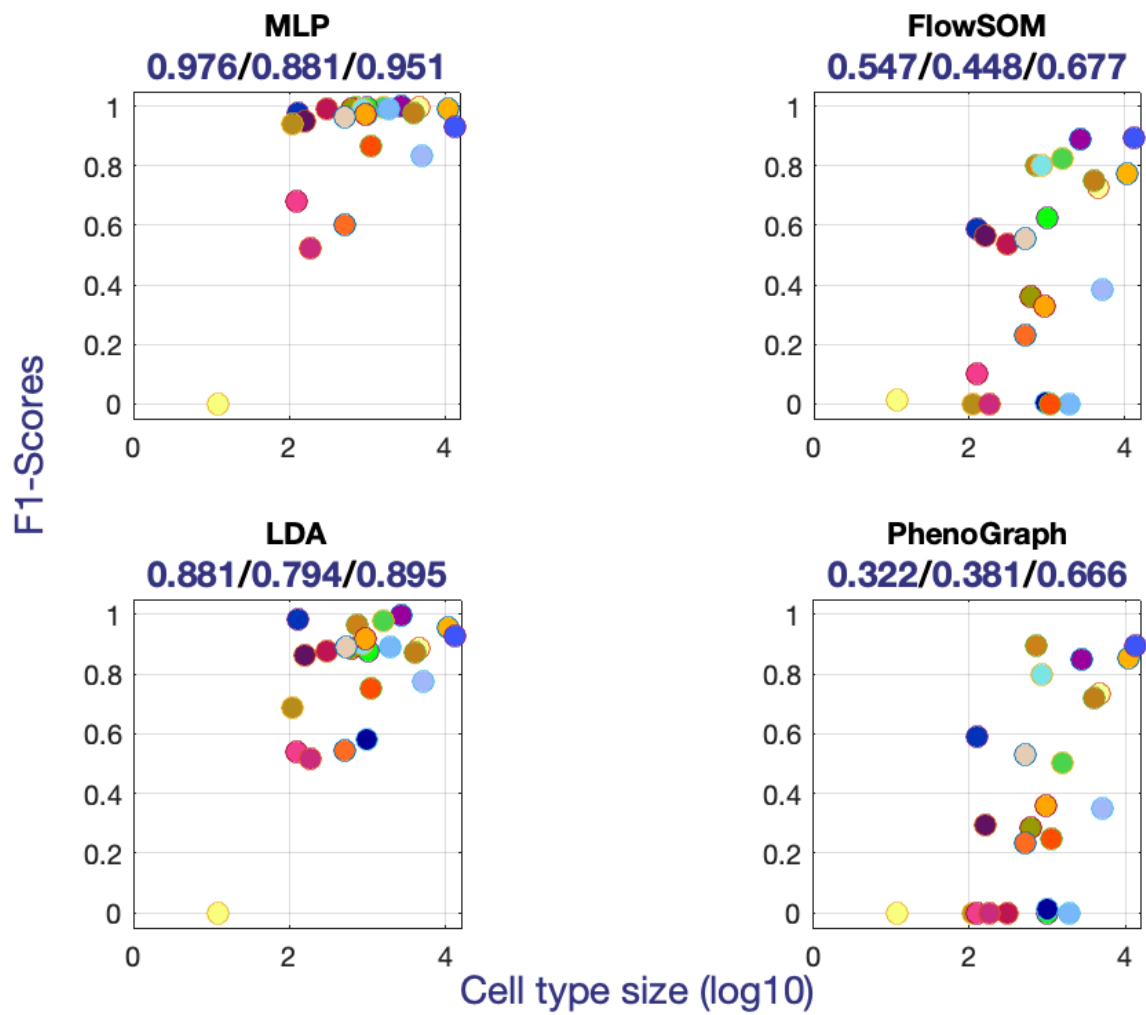
4.3.9. PANORAMA

10 samples, 5-fold cross validation: 8x2 training by test samples;

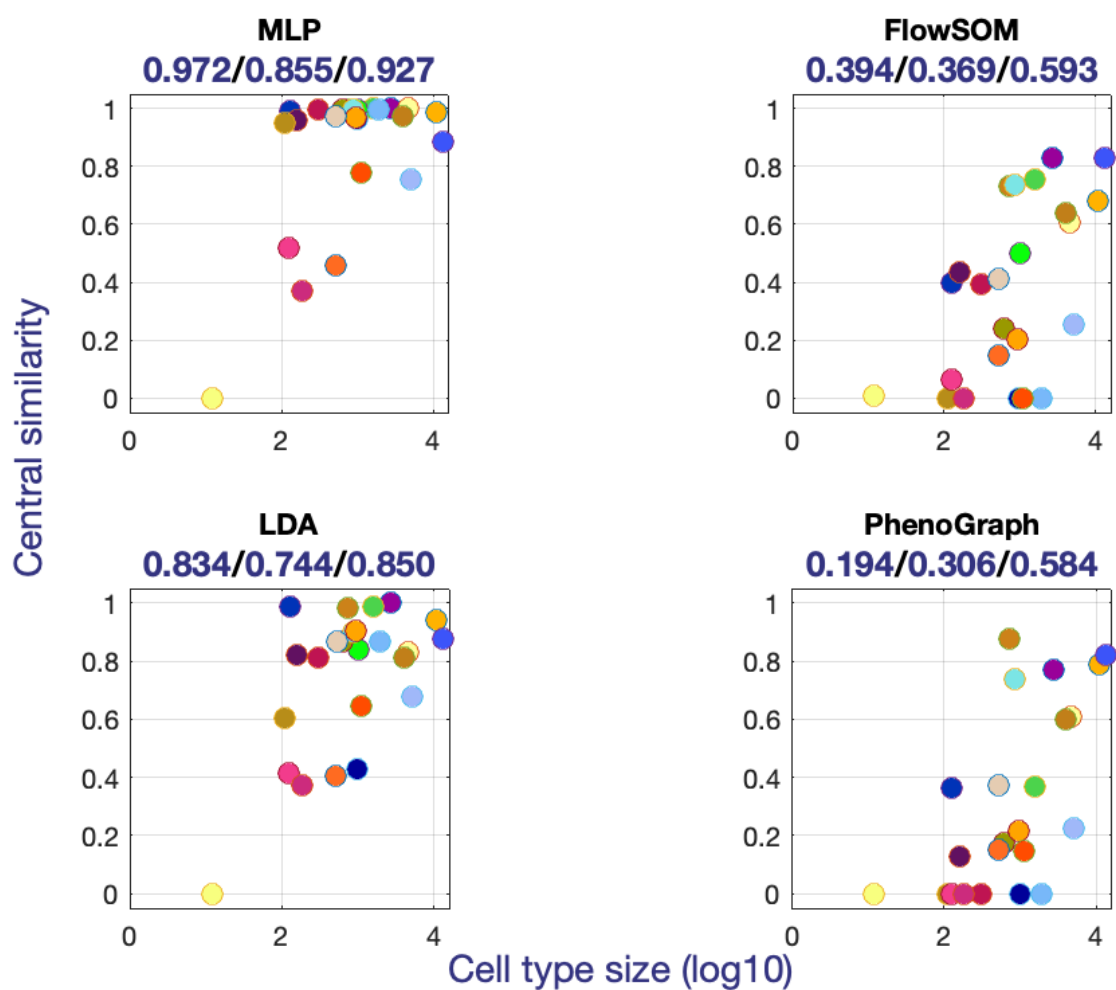
24 cell types, 25 markers

Color	Cell type	Frequency %	F1-Score				Central similarity				Earth mover's distance			
			MLP 	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph	MLP	Flow SOM	LDA	Pheno Graph
	pDCs	5.2%	0.999	0.891	0.999	0.851	1	0.832	1	0.771	0.999	0.942	0.999	0.869
	Eosinophils	8.8%	0.998	0.729	0.887	0.731	0.999	0.605	0.830	0.609	0.999	0.826	0.916	0.833
	CD8 T cells	3%	0.998	0.825	0.976	0.500	0.999	0.756	0.989	0.369	0.999	0.920	0.988	0.702
	NKT cells	1.9%	0.996	0.625	0.876	N/A	0.997	0.498	0.838	N/A	0.998	0.904	0.933	N/A
	Non classical Monocytes	1.4%	0.994	0.800	0.967	0.897	0.997	0.733	0.984	0.877	0.997	0.884	0.985	0.976
	B cells Frac. D	3.7%	0.994	N/A	0.891	N/A	0.997	N/A	0.868	N/A	0.998	N/A	0.974	N/A
	NK cells	1.2%	0.993	0.359	0.885	0.285	0.995	0.239	0.869	0.173	0.996	0.874	0.931	0.898
	Classical Monocytes	21%	0.991	0.773	0.956	0.852	0.989	0.683	0.941	0.790	0.999	0.882	0.991	0.955
	Basophils	0.57%	0.991	0.539	0.875	N/A	0.995	0.391	0.812	N/A	0.994	0.892	0.947	N/A
	CD4 T cells	1.6%	0.990	0.800	0.898	0.800	0.996	0.738	0.901	0.738	0.993	0.950	0.947	0.956
	Plasma Cells	0.24%	0.980	0.586	0.982	0.592	0.990	0.397	0.989	0.362	0.985	0.678	0.986	0.773
	Intermediate Monocytes	7.7%	0.979	0.752	0.874	0.721	0.972	0.640	0.813	0.601	0.997	0.936	0.965	0.913
	B cells Frac A-C	1.9%	0.973	0.001	0.581	0.011	0.966	0	0.428	0	0.995	0.463	0.890	0.390
	MEP	1.8%	0.971	0.327	0.920	0.358	0.971	0.205	0.905	0.215	0.994	0.832	0.974	0.806
	Macrophages	1%	0.965	0.556	0.889	0.531	0.972	0.413	0.868	0.373	0.991	0.908	0.968	0.905
	mDCs	0.30%	0.952	0.566	0.865	0.293	0.959	0.435	0.821	0.128	0.978	0.827	0.945	0.694
	gd T cells	0.21%	0.940	N/A	0.686	N/A	0.948	N/A	0.606	N/A	0.971	N/A	0.853	N/A
	B cells Frac. F	25%	0.933	0.895	0.926	0.894	0.885	0.829	0.875	0.823	0.990	0.984	0.986	0.973
	GMP	2.1%	0.866	N/A	0.753	0.248	0.778	N/A	0.645	0.144	0.986	N/A	0.904	0.682
	B cells Frac. E	9.8%	0.833	0.385	0.775	0.350	0.755	0.254	0.680	0.223	0.956	0.713	0.957	0.665
	CLP	0.24%	0.682	0.103	0.541	N/A	0.520	0.062	0.413	N/A	0.934	0.256	0.820	N/A
	CMP	1%	0.604	0.232	0.546	0.235	0.460	0.149	0.407	0.151	0.945	0.899	0.914	0.893
	MPP	0.35%	0.523	N/A	0.514	N/A	0.371	N/A	0.375	N/A	0.915	N/A	0.892	N/A
	HSC	0.02%	0	0.011	0	N/A	0	0.007	0	N/A	0	0.464	0.118	N/A
Median			0.976	0.547	0.881	0.322	0.972	0.394	0.834	0.194	0.993	0.853	0.947	0.738
Mean			0.881	0.448	0.794	0.381	0.855	0.369	0.744	0.306	0.942	0.668	0.908	0.578

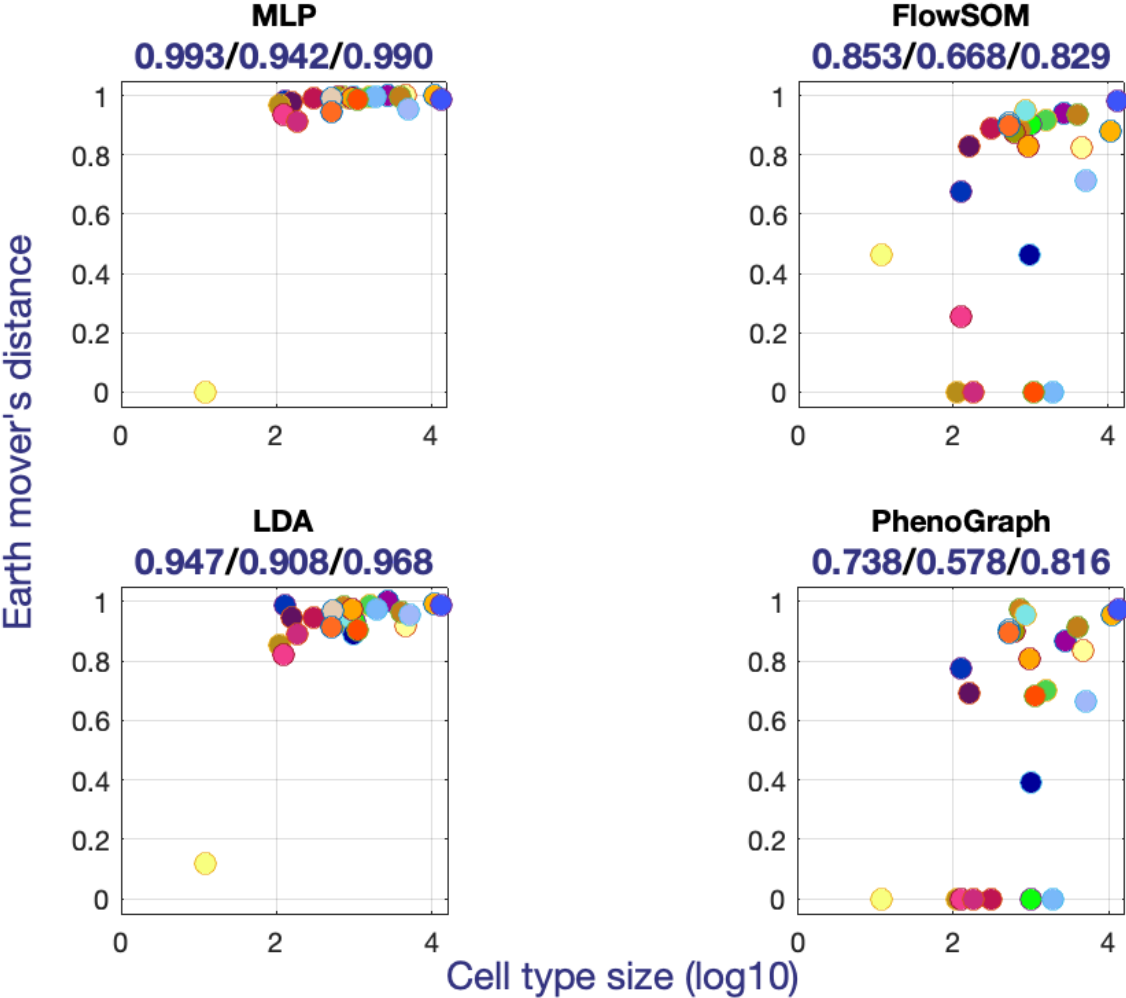
PANORAMA F1-Scores median/mean/weighted



PANORAMA Central similarity median/mean/weighted



PANORAMA Earth mover's distance median/mean/weighted



4.3.9.1. Merged matches

With FlowSOM QFMatch finds 4 of 11 matches where merging multiple FlowSOM gated populations for 1 manually gated population obtains a higher F1-score: the 3rd, 7th, 8th and 11th ranked matches.

MATCH sets: training=20/24 (4 UNMATCHED!), test=all 24 matched!

Rank	#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.
3	8	pDCs	3	89.1%	83.2%	94.2%	yes	5.9%
3	33	pDCs (FlowSOM.non-Neutrophils.Po...	3	89.1%	83.2%	94.2%	no	1.5%
3	43	pDCs (FlowSOM.non-Neutrophils.Po...	3	89.1%	83.2%	94.2%	no	2.4%
7	10	NKT cells	3	62.5%	49.8%	90.4%	yes	2.3%
7	26	NKT cells (FlowSOM.non-Neutrophils...	3	62.5%	49.8%	90.4%	no	1.6%
7	39	NKT cells (FlowSOM.non-Neutrophils...	3	62.5%	49.8%	90.4%	no	0.8%
8	9	CMP	3	23.2%	14.9%	89.9%	yes	1%
8	30	CMP (FlowSOM.non-Neutrophils.Pop...	3	23.2%	14.9%	89.9%	no	3.6%
8	41	CMP (FlowSOM.non-Neutrophils.Pop...	3	23.2%	14.9%	89.9%	no	1.2%
11	3	Classical Monocytes	3	77.3%	68.3%	88.2%	yes	28.8%
11	35	Classical Monocytes (FlowSOM.non-...	3	77.3%	68.3%	88.2%	no	29.5%
11	48	FlowSOM.non-Neutrophils.Pop8	3	77.3%	68.3%	88.2%	no	0.5%
1	13	B cells Frac. F	2	89.5%	82.9%	98.4%	yes	19.7%
1	44	B cells Frac. F (FlowSOM.non-Neutr...	2	89.5%	82.9%	98.4%	no	16.4%

Samusik, N., Good, Z., Spitzer, M. et al. **Automated mapping of phenotype space with single-cell data**. Nat Methods 13, 493–496 (2016).

<https://doi.org/10.1038/nmeth.3863>

5. Testing Round 3

In this third *and final* round of our testing with LDA and MLP the matching is 1-to-1 as in rounds [1](#) and [2](#) but the data usage is now the same as with FlowSOM and PhenoGraph: training and predicting is done on both classified and unclassified cells. Prior rounds prepared all samples to contain only members of the same cell populations for both training and predicting in order to match the processing done in the [LDA publication](#).

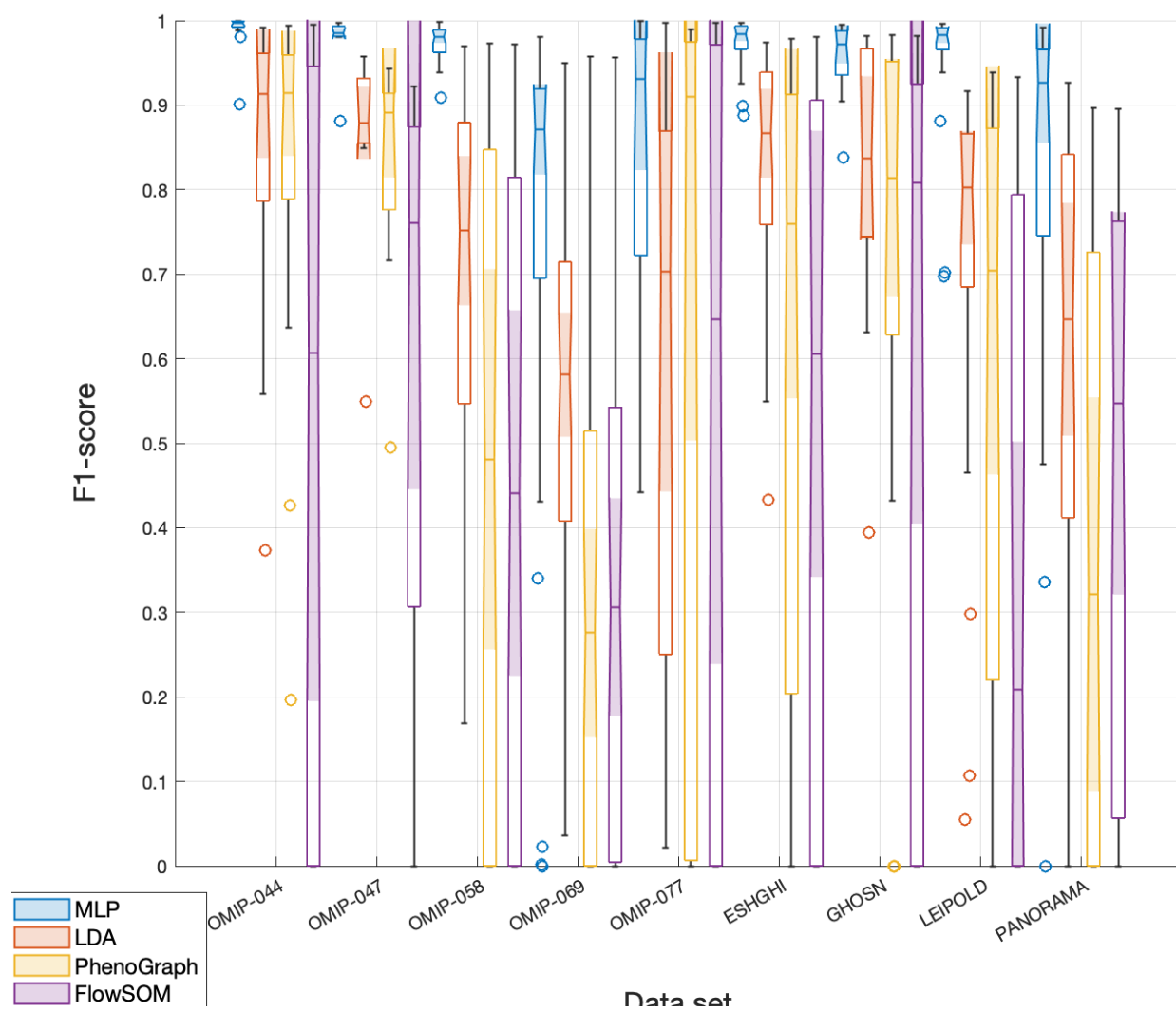
In the third round of our testing with FlowSOM and PhenoGraph the data usage (classified and unclassified) and matching (many-to-1) is exactly as in [round 2](#) cells.

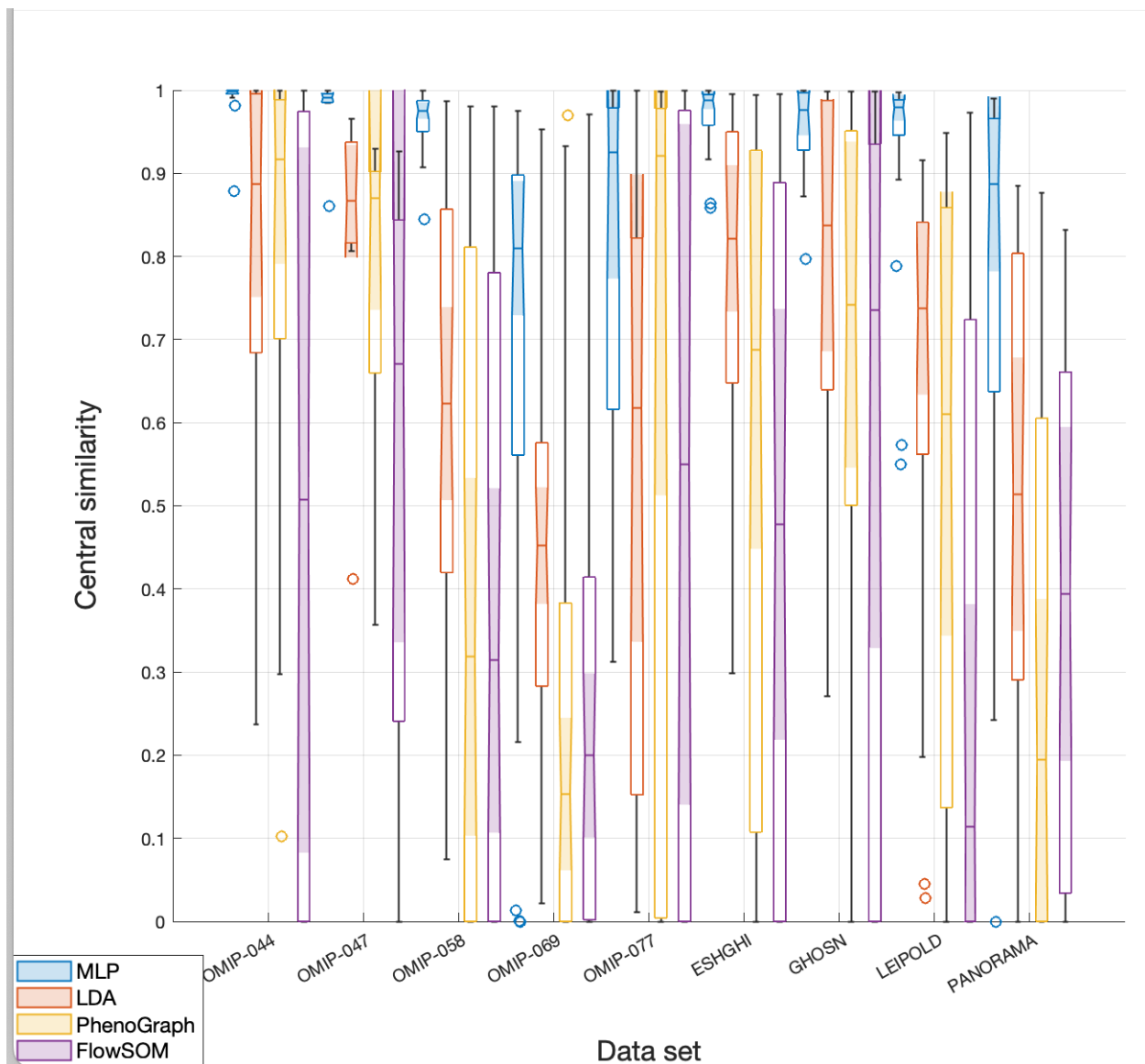
This round of testing also differs from the previous by running both MLP implementations on all of the data: fitcnet and TensorFlow.

5.1. Overall results

Metric Classifier	F1-Score		CS		Earth mover's distance	
	Median	Mean	Median	Mean	Median	Mean
MLP	0.98	0.91	0.98	0.89	0.99	0.97
LDA	0.80	0.72	0.74	0.66	0.94	0.91
PhenoGraph	0.76	0.59	0.69	0.55	0.92	0.73
FlowSOM	0.61	0.48	0.48	0.44	0.85	0.61

5.2. Results for datasets





The overall accuracy of each classifier's matches for 197 known cell populations across 9 datasets is

Classifier		MLP				LDA				PhenoGraph				FlowSOM			
<u>Dataset</u>	# of pop- ulations	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD
<u>OMIP-044</u>	13	1.00 0.99	0.99 0.98	1.00 0.99	1.00 1.00	0.91 0.84	0.84 0.76	0.89 0.80	0.98 0.93	0.91 0.81	0.84 0.74	0.92 0.78	0.95 0.92	0.61 0.49	0.44 0.43	0.51 0.46	0.77 0.56
<u>OMIP-047</u>	8	0.98 0.97	0.97 0.95	0.99 0.98	1.00 0.99	0.88 0.85	0.78 0.76	0.87 0.83	0.97 0.94	0.89 0.83	0.80 0.72	0.87 0.77	0.97 0.93	0.76 0.60	0.62 0.51	0.67 0.55	0.91 0.72
<u>OMIP-058</u>	35	0.98 0.97	0.96 0.95	0.98 0.96	0.99 0.99	0.75 0.70	0.60 0.57	0.62 0.61	0.94 0.91	0.48 0.43	0.32 0.37	0.32 0.40	0.86 0.56	0.44 0.42	0.28 0.35	0.31 0.38	0.87 0.55
<u>OMIP-069</u>	43	0.87 0.76	0.77 0.67	0.81 0.70	0.98 0.95	0.57 0.56	0.41 <i>0.43</i>	0.45 <i>0.46</i>	0.90 0.89	0.28 0.34	0.16 <i>0.26</i>	0.15 <i>0.28</i>	0.75 0.54	0.31 <i>0.34</i>	0.18 0.26	0.20 0.28	0.78 0.62
<u>OMIP-077</u>	14	0.93 0.84	0.87 0.76	0.93 0.79	0.98 0.96	0.70 0.57	0.55 0.49	0.62 0.53	0.90 0.86	0.91 0.65	0.83 0.61	0.92 0.65	0.96 0.73	0.65 0.52	0.50 0.48	0.55 0.50	0.90 0.59
<u>ESHGHI</u>	29	0.98 0.97	0.97 0.95	0.99 0.97	1.00 0.99	0.87 0.82	0.76 0.71	0.82 0.77	0.96 0.95	0.76 0.61	0.61 0.53	0.69 0.56	0.93 0.76	0.61 0.49	0.43 0.42	0.48 0.46	0.76 0.60
<u>GHOSN</u>	13	0.97 0.95	0.95 0.92	0.98 0.95	0.99 0.98	0.84 0.82	0.72 <i>0.73</i>	0.84 0.78	0.95 0.93	0.81 0.70	0.69 0.62	0.74 0.66	0.92 0.79	0.81 0.60	0.68 0.54	0.74 0.59	0.88 0.64
<u>LEIPOLD</u>	18	0.98 0.94	0.97 0.91	0.98 0.92	1.00 0.98	0.80 0.69	0.67 0.57	0.74 0.64	0.94 0.91	0.70 0.60	0.54 0.49	0.61 0.54	0.92 0.77	0.21 0.40	0.12 0.32	0.11 0.36	0.63 0.56
<u>PANORAMA</u>	24	0.93 0.81	0.86 0.74	0.89 0.76	0.99 0.92	0.65 0.62	0.48 <i>0.49</i>	0.51 <i>0.53</i>	0.92 0.87	0.32 0.38	0.19 <i>0.28</i>	0.19 <i>0.31</i>	0.74 0.57	0.55 0.45	0.38 0.35	0.39 0.37	0.85 0.67
Total populations	197																
Medians		0.98	0.96	0.98	0.99	0.80	0.67	0.74	0.94	0.76	0.61	0.69	0.92	0.61	0.43	0.48	0.85
Means		0.91	0.87	0.89	0.97	0.72	0.61	0.66	0.91	0.59	0.52	0.55	0.73	0.48	0.41	0.44	0.61

	Columns	Rows				
Legend	• F1-score=overlap measured by harmonic mean of percision + recall (AKA <i>F measure</i>). • JI 100%=whole population overlap measured by intersection/union (AKA <i>jaccard index</i>). • JI 80%=central core region overlap (AKA <i>central similarity</i>). • EMD=earth mover's distance	Coloring is based on ranking by <i>F1-score mean</i>				
		Narrow lead over next	1st	2nd	3rd	Last
		Wide lead over next	1st	2nd	3rd	Nothing is next
		Ties get same ranked color....				
		Median minus mean size is ^{emph} asized pos/neg.				

5.2.1. Effects of unclassified cells

5.2.1.1. Overall effect

The primary difference between the two sets of data shown in the table below is that in the rows labeled “classified only”, we remove unclassified cells when training and predicting with MLP and LDA.

The testing results indicate that automatically classified populations match better to manually gated populations when unclassified cells are excluded from the computation.

<i>Classification Method</i>	<i>Data Included in Computation</i>	<i>F1-Score</i>		<i>CS</i>		<i>EMD</i>	
		<i>Median</i>	<i>Mean</i>	<i>Median</i>	<i>Mean</i>	<i>Median</i>	<i>Mean</i>
MLP	Classified only	0.99	0.95	0.99	0.94	1	0.98
MLP	All	0.98	0.91	0.98	0.89	0.99	0.97
LDA	Classified only	0.88	0.81	0.83	0.76	0.96	0.93
LDA	All	0.80	0.72	0.74	0.66	0.94	0.91

Differences in overall accuracy

5.2.1.2. Effect per dataset

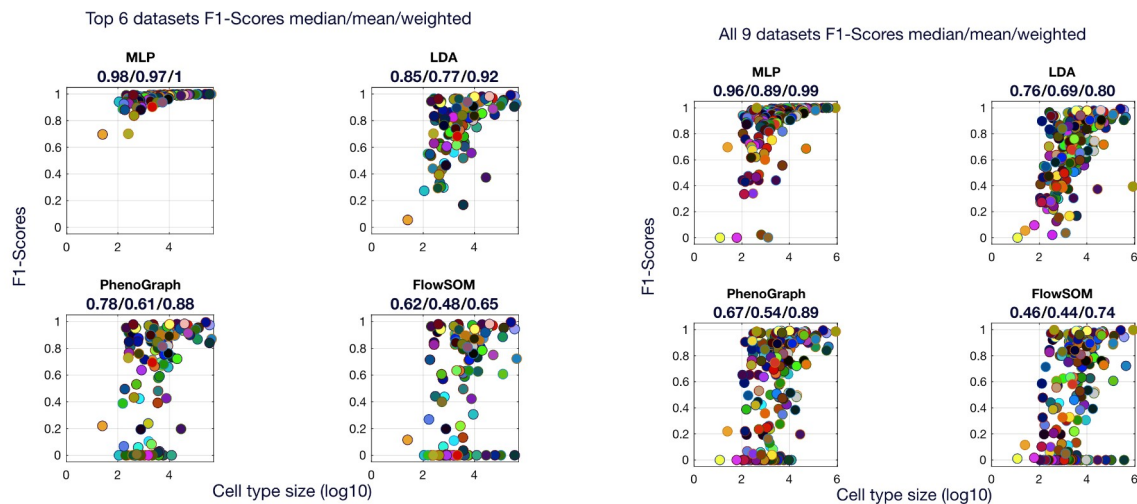
Dataset	MLP						LDA					
	Classified only			Classified+unclassified			Classified only			Classified+unclassified		
	F1-Score	Central similarity	EMD	F1-Score	Central similarity	EMD	F1-Score	Central similarity	EMD	F1-Score	Central similarity	EMD
OMIP-044 ¹⁰	1 0.99	1 /	1 1	1 0.99	1 0.99	1 1	0.93 0.85	0.90 0.81	0.98 0.94	0.91 0.84	0.89 0.80	0.98 0.93
OMIP-047 ¹¹	1 1	1 1	1 1	0.98 0.97	0.99 0.98	1 0.99	0.96 0.96	0.95 0.96	0.98 0.98	0.88 0.85	0.87 0.83	0.97 0.94
OMIP-058 ¹²	0.99 0.97	0.99 0.97	1 0.99	0.98 0.97	0.98 0.96	0.99 0.99	0.84 0.76	0.81 0.70	0.95 0.93	0.75 0.70	0.62 0.61	0.94 0.91
OMIP-069 ¹³	0.98 0.93	0.97 0.90	0.99 0.98	0.87 0.76	0.81 0.70	0.98 0.95	0.83 0.76	0.73 0.68	0.95 0.92	0.58 0.56	0.45 0.46	0.90 0.89
OMIP-077 ¹⁴	0.97 0.89	0.97 0.85	0.99 0.96	0.93 0.84	0.93 0.79	0.98 0.96	0.72 0.62	0.62 0.57	0.88 0.87	0.70 0.57	0.62 0.53	0.90 0.86
ESHGHI ³⁵	1 0.99	1 0.99	1 1	0.98 0.97	0.99 0.97	1 0.99	0.90 0.86	0.86 0.81	0.97 0.95	0.87 0.82	0.82 0.77	0.96 0.95
GHOSN ¹⁶	0.99 0.94	0.99 0.92	1 0.98	0.97 0.95	0.98 0.95	0.99 0.98	0.92 0.89	0.93 0.85	0.96 0.94	0.84 0.82	0.84 0.78	0.95 0.93
LEIPOLD ³⁶	0.99 0.96	0.99 0.95	1 0.99	0.98 0.94	0.98 0.92	1 0.98	0.86 0.78	0.80 0.73	0.96 0.93	0.80 0.69	0.74 0.64	0.94 0.91
PANORAMA ¹⁵	0.97 0.88	0.97 0.86	0.99 0.94	0.93 0.81	0.89 0.76	0.99 0.92	0.88 0.79	0.83 0.74	0.95 0.91	0.65 0.62	0.51 0.53	0.93 0.87

All datasets except OMIP-077 LDA's predictive accuracy improves significantly more than MLP's predictive accuracy improves. Moreover, there are only 3 of 9 (OMIP-047, OMIP-058 and PANORAMA) datasets where MLP's F1-score improves by more than 0.01. In these 3 datasets, we also observe significantly lower central similarity scores telling us that MLP sees the dense central regions of phenotypes in N-dimensional space more clearly for these assays when unclassified cells are removed.

Pursuing improvements in this manner however is non ideal because while removing unclassified cells may be fair and easy for training, predicting on such data requires a prior pre-gating step that makes it difficult to deprecate manual gating. Therefore, we draw our conclusions on test results where unclassified cells are included.

5.2.2. Small population issues

Automatic gating methods often miss smaller populations ⁽²⁰⁾ important to clinical research. In our testing however MLP's F1-score is ≥ 0.70 in 6 datasets. In the other 3 datasets, 11 populations have MLP F1-scores < 0.50 : 1 in [OMIP-077](#) (0.44), 4 in [PANORAMA](#) and 6 in [OMIP-069](#).



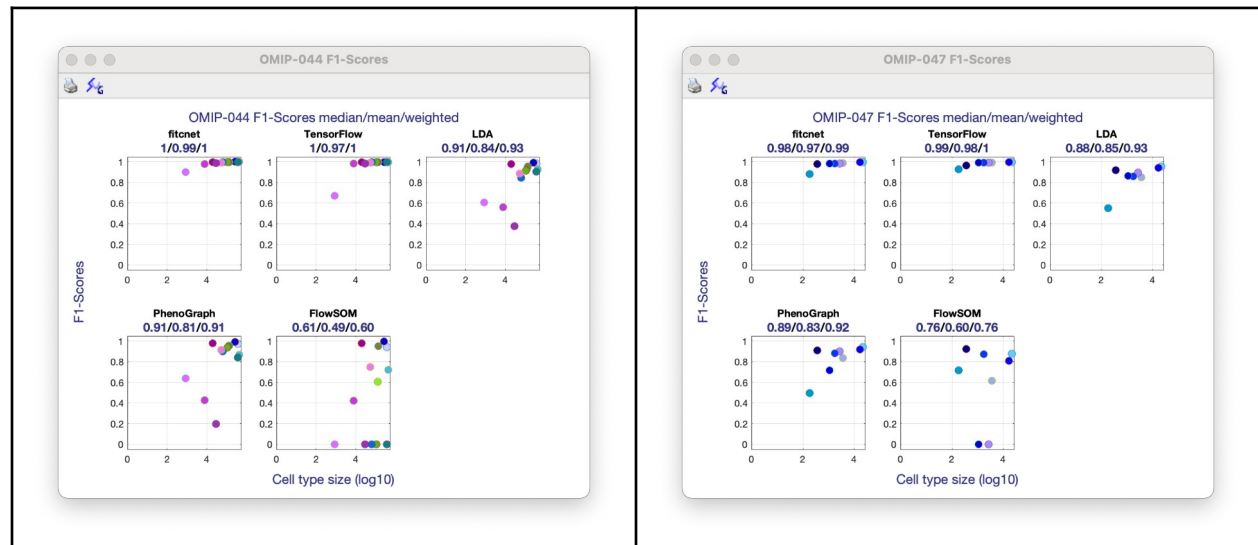
Classifier	Minimum F1-Score				# populations < 0.50 F1-Score				Mean frequency of populations < 0.50 F1-Score			
Dataset	MLP	LDA	PhenoGraph	FlowSOM	MLP	LDA	PhenoGraph	FlowSOM	MLP	LDA	PhenoGraph	FlowSOM
OMIP-044	0.90	0.37	0.20	0	0/13	1/13	2/13	2/13	1.4%	0.63%	0.63%	
OMIP-047	0.88	0.55	0.49	0	0/8	0/8	1/8	1/8			0.43%	5.5%
OMIP-058	0.91	0.17	0	0.01	0/35	7/35	6/35	6/35	0.23%	0.77%	0.67%	
OMIP-069	0	0.04	0.04	< 0.01	6/43	16/43	16/43	18/43	0.11%	0.17%	1.3%	0.55%
OMIP-077	0.44	0.02	0	0.06	1/14	6/14	2/14	2/14	0.01%	0.03%	0.03%	0.08%
GENENTECH	0.89	0.43	0	< 0.01	0/29	1/29	7/29	5/29	0.57%	0.82%	3.2%	
GHOSN	0.84	0.39	0.43	0.71	0/13	1/13	1/13	0/13	0.36%	0.38%		
LEIPOLD	0.70	0.05	0	0.06	0/18	4/18	6/18	5/18	0.79%	1.5%	1.8%	
PANORAMA	0	0	0.01	< 0.01	4/24	8/24	7/24	7/24	0.40%	0.96%	1.9%	1.6%
Total					11/197	44/197	48/197	46/197				

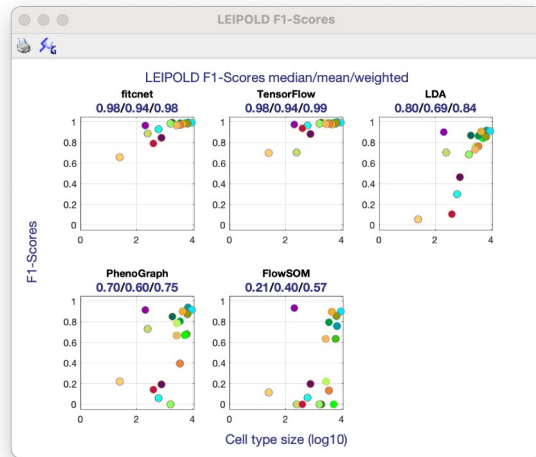
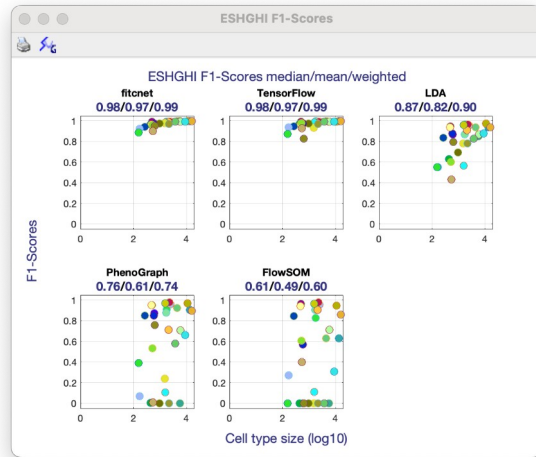
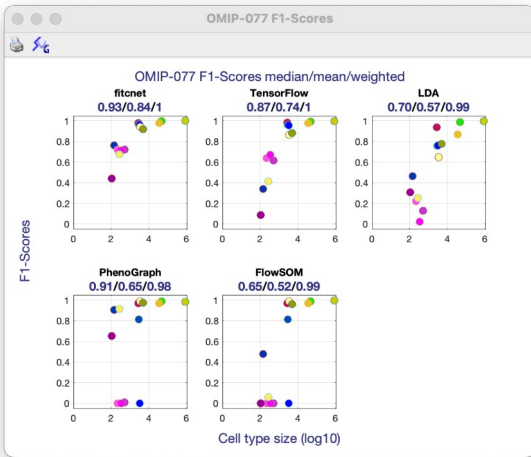
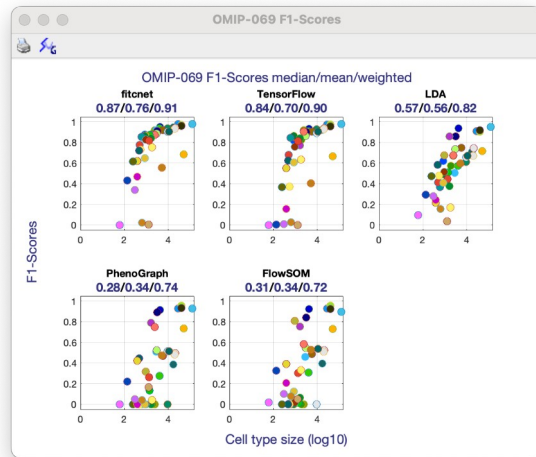
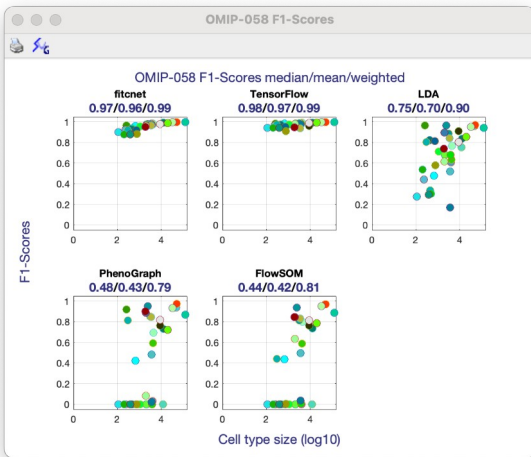
Minimum F1-score, population name and population % frequency				
Classifier Dataset	MLP	LDA	PhenoGraph	FlowSOM
OMIP-044 ¹⁰	0.901 <i>CD141+ DCs 0.04%</i>	.373 <i>DCs.1.4%</i>	.197 <i>DCs.1.4%</i>	0 <i>not naive CD4+.18% and 4 others</i>
OMIP-047 ¹¹	0.881 <i>Transitional 2.2%</i>	.613 <i>IgA, FSC-A IgA, IgG1, IgG3 7.3%</i>	.549 <i>PB 0.38%</i>	0 <i>Transitional 2.2% IgA, FSC-A IgA+ 5.5%</i>
OMIP-058 ¹²	0.902 <i>Terminal NK.1%</i>	0.167 <i>CD4+ TSCM T cells CD27+ CD28+ 1%</i>	0 <i>CD4+ TEMRA T Cells CD27- CD28+ 0.03% and 12 others</i>	0 <i>CD4+ TEMRA T Cells CD27- CD28+.03% and 12 others</i>
OMIP-069 ¹³	0 <i>CD1c- CD141+ DCs 0.01%</i>	0.17 <i>CD16- CD14- monocytes .0.30%</i>	0 <i>B-1 IgM+ 0.21% and 13 others</i>	0 <i>B-1 IgM+ 0.21% and 8 others</i>
OMIP-077 ¹⁴	0.442 <i>pDCs 0.01%</i>	0.022 <i>CD141+ mDCs 0.04%</i>	0 <i>CD141+ mDCs 0.41% and 2 others</i>	0 <i>CD141+ mDCs 0.41% and 4 others</i>
ESHGHI ³⁵	0.895 <i>CD123- 0.17%</i>	0.430 <i>Lineage Negative 0.57%</i>	0 <i>CD123- 0.17% and 3 others</i>	0 <i>CD123- 0.17% and 7 others</i>

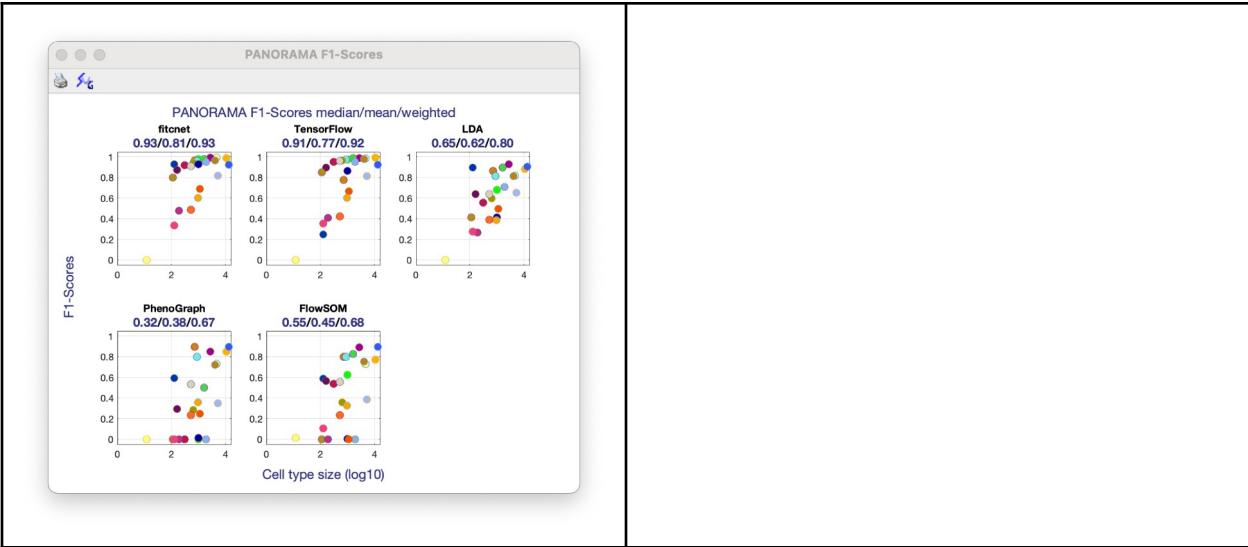
GHOSN ¹⁶	0.854 <i>Neutrophils 0.36%</i>	0.394 <i>Neutrophils 0.36%</i>	0 <i>CD11b+ dendritic 1.3%</i>	0 <i>ckit+ mast cells 1.8% and 3 others</i>
LEIPOLD ³⁶	0.697 <i>CD16+ monocytes 0.04%</i>	0.055 <i>CD16+ monocytes 0.04%</i>	0 <i>CD8 T cells CD45RA- CD27- 2.8%</i>	0 <i>CD16+ monocytes 0.04% and 4 others</i>
PANORAMA ¹⁵	0 <i>HSC 0.02%</i>	0 <i>HSC 0.02%</i>	0 <i>HSC 0.02% and 6 others</i>	0 <i>gd T cells 0.21% and 3 others</i>

MLP is the only classifier having datasets (5 of 9) where the worst F1-score is still decent (>0.85): OMIP-044, OMIP-047, OMIP-058 and ESHGHI. Moreover, for 197 populations overall MLPs F1-Score drops below 0.50 11 times.

Below the F1-Score by Size X/Y plots of all classifiers compared side by side illustrate the strength of MLP with small populations. Even in the two worst cases ([PANORAMA](#) and [OMIP-069](#)), the plots indicate that MLP is much less affected by population size than are LDA, FlowSOM and PhenoGraph. Even in the two worst cases (PANORAMA and OMIP-069), the plots below indicate that overall MLP is much less affected by population size than are LDA, FlowSOM and PhenoGraph.







5.2.3. Jaccard Index on whole population versus central region

Dataset	# of pop- ulations	Classifier MLP		LDA		PhenoGraph		FlowSOM	
		Jl	Jl	Jl	Jl	Jl	Jl	Jl	Jl
		100%	80%	100%	80%	100%	80%	100%	80%
OMIP-044	13	0.99	1	0.84	0.89	0.84	0.92	0.44	0.51
		0.98	0.99	0.76	0.80	0.74	0.78	0.43	0.46
OMIP-047	8	0.97	0.99	0.78	0.87	0.80	0.87	0.62	0.67
		0.95	0.98	0.76	0.83	0.72	0.77	0.51	0.55
OMIP-058	35	0.96	0.98	0.60	0.62	0.32	0.32	0.28	0.31
		0.95	0.96	0.57	0.61	0.37	0.40	0.35	0.38
OMIP-069	43	0.77	0.81	0.41	0.45	0.16	0.15	0.18	0.20
		0.67	0.70	0.43	0.46	0.26	0.28	0.26	0.28
OMIP-077	14	0.87	0.93	0.55	0.62	0.83	0.92	0.50	0.55
		0.76	0.79	0.49	0.53	0.61	0.65	0.48	0.50
ESHGHI	29	0.97	0.99	0.76	0.82	0.61	0.69	0.43	0.48
		0.95	0.97	0.71	0.77	0.53	0.56	0.42	0.46
GHOSN	13	0.95	0.98	0.72	0.84	0.69	0.74	0.68	0.74
		0.92	0.95	0.73	0.78	0.62	0.66	0.54	0.59
LEIPOLD	18	0.97	0.98	0.67	0.74	0.54	0.61	0.12	0.11
		0.91	0.92	0.57	0.64	0.49	0.54	0.32	0.36

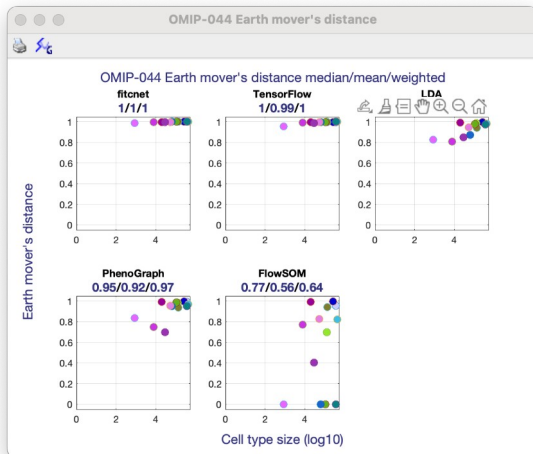
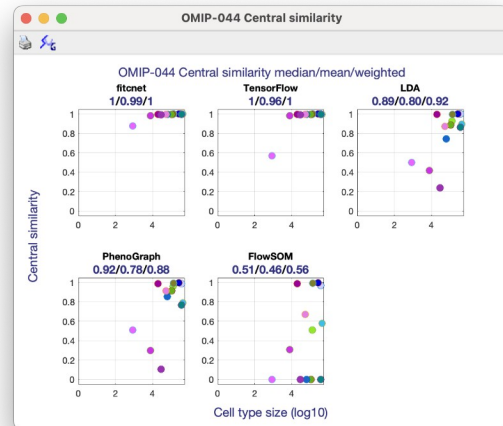
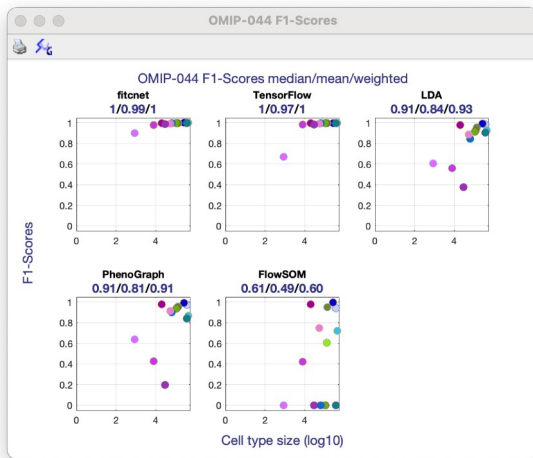
	Columns	Rows				
Legend	- F1-score=overlap measured by harmonic mean of percision + recall (AKA <i>F measure</i>). - JI 100%=whole population overlap measured by intersection/union (AKA <i>jaccard index</i>). - JI 80%=central core region overlap (AKA <i>central similarity</i>).	Coloring is based on ranking by <i>F1-score mean</i>				
		<i>Narrow lead over next</i>	1st	2nd	3rd	Last
		<i>Wide lead over next</i>	1st	2nd	3rd	Nothing is next
		Ties get same ranked color....				
		Median minus mean size is ^{emph} asized pos/neg.				

5.3. Results for populations

Legend	Columns				Rows			
	- F1-score=overlap measured by harmonic mean of percision + recall (AKA <i>F measure</i>). - JI 100%=whole population overlap measured by intersection/union (AKA <i>jaccard index</i>). - JI 80%=central core region overlap (AKA <i>central similarity</i>). - EMD=earth mover's distance				Coloring is based on ranking by <i>F1-score mean</i>			
					<i>Narrow lead over next</i>			
					1st	2nd	3rd	Last
					<i>Wide lead over next</i>			
					1st	2nd	3rd	Nothing is next
					Ties get same ranked color....			
					Median minus mean size is emphasized pos/neg.			

5.3.1. OMIP-044

Population	Classifier	fitnet				TensorFlow				LDA				PhenoGraph				FlowSOM			
	Freq- uency	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD
• CD14+	19%	1	1	1	1	1	1	1	1	0.98	0.97	1	0.98	0.97	0.95	0.99	0.99	0.94	0.89	0.97	0.95
• CD19+	13%	1	1	1	1	1	1	1	1	0.99	0.98	1	1	0.99	0.99	1	1	0.99	0.99	1	1
• naive CD4+	23%	1	1	1	1	1	1	1	1	0.93	0.87	0.89	0.98	0.87	0.77	0.79	0.97	0.72	0.56	0.57	0.82
• [not naive CD4+]	17%	1	1	1	1	1	1	1	1	0.91	0.83	0.86	0.98	0.84	0.72	0.76	0.95				
• naive CD8+	6.7%	1	1	1	1	1	1	1	1	0.94	0.89	0.93	0.99	0.95	0.91	0.96	0.99	0.61	0.44	0.51	0.70
• CD56+ NK	7.4%	1	1	1	1	1	1	1	1	0.95	0.91	1	0.94	0.95	0.91	0.99	0.94	0.95	0.91	0.99	0.94
• [not naive CD8+]	5.4%	1	0.99	1	1	1	1	1	1	0.91	0.84	0.89	0.98	0.94	0.89	0.92	0.99				
• DN	2.7%	1	0.99	1	1	1	0.99	1	1	0.85	0.73	0.75	0.87	0.90	0.82	0.85	0.95				
• CD123+ pDC	1.2%	1	0.99	1	1	1	0.99	1	1	0.98	0.96	1	0.99	0.98	0.96	0.99	0.99	0.98	0.96	0.99	0.99
• DN DCs	2.7%	0.99	0.99	1	1	0.99	0.99	1	1	0.89	0.80	0.87	0.94	0.91	0.84	0.92	0.95	0.75	0.60	0.67	0.82
• DCs-	0.84%	0.99	0.98	0.99	1	0.99	0.97	0.99	0.99	0.37	0.23	0.24	0.85	0.20	0.11	0.10	0.70				
• CD1c DCs	0.42%	0.98	0.96	0.98	1	0.98	0.97	0.99	0.99	0.56	0.39	0.42	0.81	0.43	0.27	0.30	0.75	0.42	0.27	0.31	0.77
• CD141+DCs	0.05%	0.90	0.82	0.88	0.99	0.67	0.54	0.56	0.96	0.61	0.44	0.50	0.83	0.64	0.47	0.51	0.84				
Medians		1	0.99	1	1	1	1	1	1	0.91	0.84	0.89	0.98	0.91	0.84	0.92	0.95	0.61	0.44	0.51	0.77
Means		0.99	0.98	0.99	1	0.97	0.96	0.96	0.99	0.84	0.76	0.80	0.93	0.81	0.74	0.78	0.92	0.49	0.43	0.46	0.56



Merged matches

With FlowSOM QFMatch finds 2 of 9 matches where merging multiple FlowSOM gated populations to match 1 manually gated population obtains a higher F1-score: the 1st and 2nd, 3rd, 4th, 6th, 8th, 9th and 10th ranked matches.

         MATCH sets: training=9/13 (4 UNMATCHED!), test=11/13 (2 NEW!)									
Rank ²		#	Subset (class) name	Mat-ches ¹	Similarity (QFMatch)	% Overlap (F-measure)	Train-ing set? ³	Freq.	#
1	●	4	CD19+	3	99.8%	99.5%	yes	12.9%	252
1	●	16	FlowSOM.CD45+ live.Pop0	3	99.8%	99.5%	no	12.9%	253
1	●	22	FlowSOM.CD45+ live.Pop1	3	99.8%	99.5%	no	0%	
2	●	11	CD123+ pDC	3	99.3%	97.8%	yes	1.2%	23,
2	●	20	FlowSOM.CD45+ live.Pop6	3	99.3%	97.8%	no	0.4%	7,
2	●	21	FlowSOM.CD45+ live.Pop10	3	99.3%	97.8%	no	0.8%	16,
3	●	2	CD14+	2	95.4%	94.4%	yes	19%	371
3	●	24	FlowSOM.CD45+ live.Pop11	2	95.4%	94.4%	no	16.9%	332

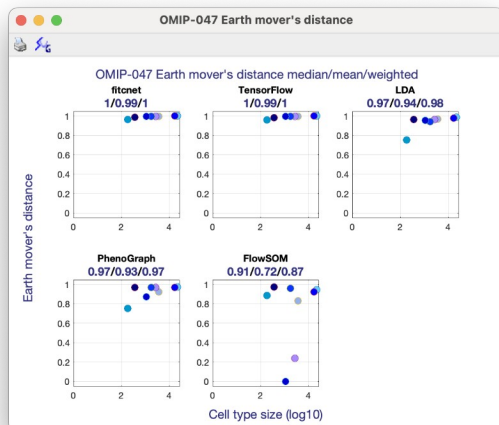
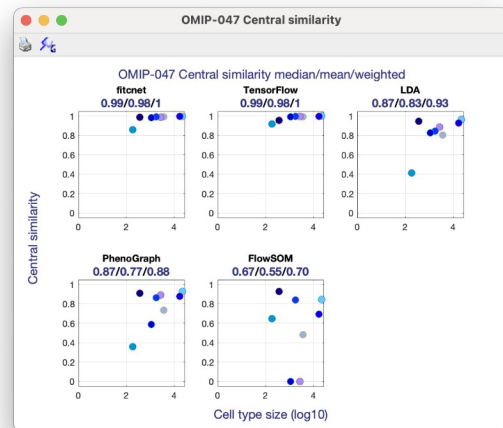
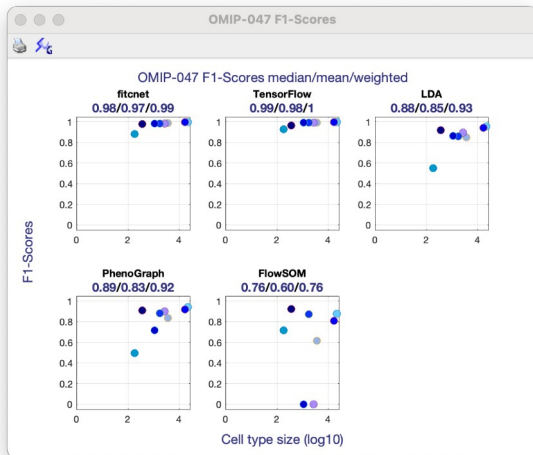
 MATCH sets: training=**all 13 matched!**, te

Mair, F. and Prlic, M. (2018), **OMIP-044: 28-color immunophenotyping**

<https://doi.org/10.1002/cyto.a.23331>

5.3.2. OMIP-047

Classifier		fitcnet				TensorFlow				LDA				PhenoGraph				FlowSOM			
Population	Freq- uency	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD
• Naive	46%	1	1	1	1	1	1	1	1	0.96	0.92	0.97	0.99	0.94	0.89	0.93	0.98	0.88	0.78	0.85	0.94
• MZ B cells	33%	1	0.99	1	1	1	1	1	1	0.94	0.89	0.93	0.98	0.92	0.85	0.88	0.97	0.81	0.68	0.69	0.92
• IgA, FSC-A Neg IgA IgG1 IgG3	8.7%	0.99	0.98	0.99	1	0.99	0.99	0.99	1	0.85	0.74	0.81	0.97	0.84	0.72	0.73	0.93	0.61	0.44	0.48	0.83
• IgA, FSC-A IgA+	5.5%	0.99	0.97	0.99	1	0.99	0.99	1	1	0.90	0.81	0.89	0.97	0.90	0.82	0.89	0.97				
• IgG1+	3.6%	0.98	0.97	0.99	1	0.99	0.99	0.99	1	0.86	0.75	0.84	0.94	0.88	0.79	0.87	0.97	0.87	0.77	0.84	0.96
• Transitional	2.1%	0.98	0.97	0.98	1	0.99	0.99	0.99	1	0.86	0.76	0.83	0.95	0.72	0.56	0.59	0.87				
• IgG3+	0.75%	0.98	0.96	0.99	0.99	0.96	0.93	0.96	0.98	0.92	0.85	0.95	0.96	0.91	0.84	0.91	0.97	0.92	0.86	0.93	0.97
• PB	0.43%	0.88	0.79	0.86	0.97	0.93	0.87	0.92	0.96	0.55	0.38	0.41	0.75	0.49	0.33	0.36	0.75	0.71	0.56	0.65	0.89
Medians		0.98	0.97	0.99	1	0.99	0.99	0.99	1	0.88	0.78	0.87	0.97	0.89	0.80	0.87	0.97	0.76	0.62	0.67	0.91
Means		0.97	0.95	0.98	0.99	0.98	0.97	0.98	0.99	0.85	0.76	0.83	0.94	0.83	0.72	0.77	0.93	0.60	0.51	0.55	0.72



Merged matches

With FlowSOM QFMatch finds 1 of 7 matches where merging 2 FlowSOM gated populations to match 1 manually gated population obtains a higher F1-score.

MATCH sets: training=7/8 (1 UNMATCHED), test=all 8 matched!									
Rank ²		Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set? ³	Freq.	
4	●	MZ B cells	3	80.7%	69.4%	92.2%	yes	33.1%	16
4	●	FlowSOM.B cells.Pop0	3	80.7%	69.4%	92.2%	no	0.6%	
4	●	FlowSOM.B cells.Pop1	3	80.7%	69.4%	92.2%	no	26.5%	14
1	●	IgG3+	2	92.3%	92.6%	97.4%	yes	0.8%	
1	●	FlowSOM.B cells.Pop5	2	92.3%	92.6%	97.4%	no	0.8%	
2	●	IgG1+	2	87.3%	84.2%	95.9%	yes	3.6%	
2	●	FlowSOM.B cells.Pop6	2	87.3%	84.2%	95.9%	no	3.9%	
3	●	Naive	2	87.6%	84.6%	94.4%	yes	45.9%	22
3	●	FlowSOM.B cells.Pop7	2	87.6%	84.6%	94.4%	no	52.6%	26
5	●	PB	2	71.4%	64.7%	88.9%	yes	0.4%	
5	●	FlowSOM.B cells.Pop4	2	71.4%	64.7%	88.9%	no	0.5%	
6	●	IgA, FSC-A Neg IgA IgG1 IgG3	2	61.3%	48.2%	83%	yes	8.7%	4
6	●	FlowSOM.B cells.Pop3	2	61.3%	48.2%	83%	no	14.7%	7
7	●	IgA, FSC-A IgA+	2	0%	0%	24%	yes	5.5%	2
7	●	FlowSOM.B cells.Pop2	2	0%	0%	24%	no	0.4%	
8	●	Transitional	0	N/A	N/A	N/A	yes	2.1%	

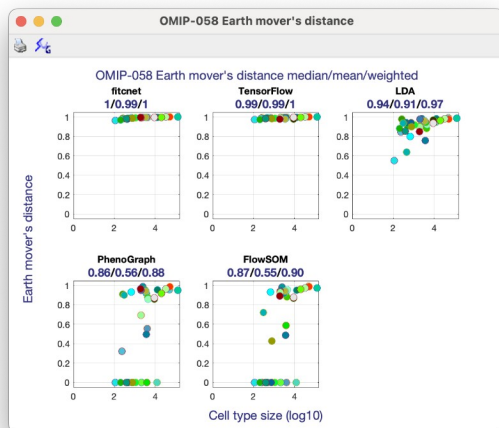
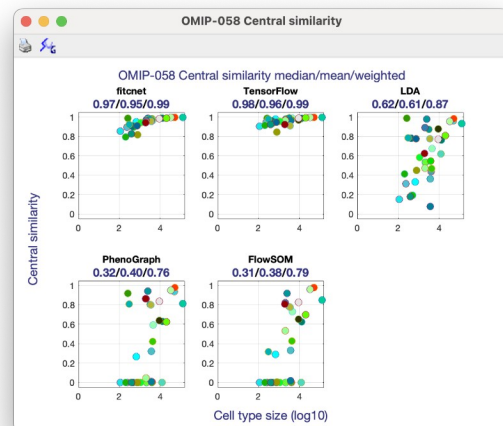
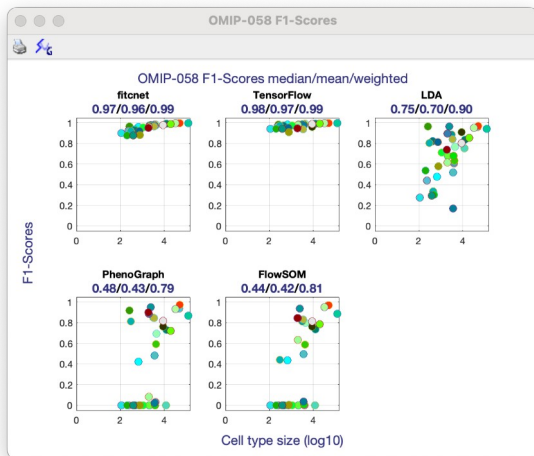
With PhenoGraph QFMatch finds 3 of 8 matches where merging multiple PhenoGraph gated populations to match 1 manually gated population obtains a higher F1-score: the 1st, 3rd and 6th ranked matches.

         MATCH sets: training=all 8 matched!, test=13/14 (1 NEW!)									
Rank ²		#	Subset (class) name	Mat-ches ¹	Similarity (QFMatch)	% Overlap (F-measure)	Train-ing set? ³	Freq.	
1	●	1	Naive	4	97.6%	94.3%	yes	45.9%	2
1	●	17	PhenographWSN93	4	97.6%	94.3%	no	13%	
1	●	18	PhenographWSN95	4	97.6%	94.3%	no	11.4%	
1	●	21	PhenographWSN92	4	97.6%	94.3%	no	15%	
3	●	5	MZ B cells	4	97%	91.8%	yes	33.1%	1
3	●	13	PhenographWSN94	4	97%	91.8%	no	12%	
3	●	15	PhenographWSN91	4	97%	91.8%	no	15%	
3	●	16	PhenographWSN96	4	97%	91.8%	no	7.8%	
6	●	6	IgA, FSC-A Neg IgA IgG1 IgG3	3	92.5%	83.6%	yes	8.7%	
6	●	9	PhenographWSN910	3	92.5%	83.6%	no	3.9%	
6	●	10	PhenographWSN98	3	92.5%	83.6%	no	5.7%	
2	●	7	IgA, FSC-A IgA+	2	97.1%	89.9%	yes	5.5%	
2	●	12	PhenographWSN97	2	97.1%	89.9%	no	6%	

Liechti, T., Günthard, H.F. and Trkola, A. (2018), **OMIP-047: High-Dimensional phenotypic characterization of B cells**. Cytometry, 93: 592-596.
<https://doi.org/10.1002/cyto.a.23488>

OMIP-058

Classifier		fitnet				TensorFlow				LDA				PhenoGraph				FlowSOM			
Population	Freq- uency	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD
CD4+ TCM T cells CD27+ CD28+	34%	1	1	1	1	1	1	1	1	0.94	0.89	0.93	0.99	0.87	0.77	0.81	0.95	0.89	0.79	0.85	0.97
CD4+ Naive T cells CD27+ CD28+	13%	1	0.99	1	1	1	1	1	1	0.96	0.92	0.96	0.99	0.94	0.88	0.94	0.96	0.97	0.94	0.98	0.99
HLA-DR+	14%	1	0.99	1	1	1	1	1	1	0.97	0.94	0.98	0.98	0.97	0.95	0.98	0.99	0.97	0.94	0.98	0.99
CD8+ TEMRA T cells CD27- CD28-	9%	1	0.99	1	1	1	1	1	1	0.95	0.91	0.96	0.98	0.93	0.88	0.95	0.97	0.95	0.91	0.96	0.97
CD4+ TEM T cells CD27+ CD28+	3.3%	0.99	0.98	0.99	1	0.99	0.98	0.98	1	0.75	0.60	0.62	0.95								
CD4+ TCM T cells CD27- CD28+	3.5%	0.99	0.98	0.99	1	0.99	0.99	0.99	1	0.84	0.72	0.76	0.98	0.73	0.57	0.63	0.96	0.73	0.57	0.63	0.95
CD8+ TEM T cells CD27+ CD28+	5.4%	0.99	0.98	0.99	1	0.99	0.98	0.99	1	0.85	0.75	0.81	0.96	0.72	0.56	0.62	0.92	0.78	0.65	0.70	0.96
CD4+ TEM T cells CD27- CD28-	1%	0.98	0.97	0.99	1	0.98	0.97	0.98	1	0.52	0.35	0.36	0.92	0.48	0.32	0.32	0.92	0.49	0.33	0.33	0.92
CD4+ TEM T cells CD27- CD28+	1.1%	0.98	0.97	0.98	1	0.98	0.97	0.97	1	0.61	0.44	0.44	0.94	0.03	0.01	<0.01	0.55				
CD8+ Naive T cells CD27+ CD28+	1.1%	0.98	0.96	0.98	1	0.99	0.98	0.99	1	0.64	0.47	0.47	0.88	0.59	0.42	0.42	0.88	0.59	0.42	0.42	0.88
Vd2 high Vg9+ T cells	0.68%	0.98	0.96	0.99	1	0.98	0.96	0.98	0.99	0.96	0.93	0.98	0.98	0.95	0.90	0.94	0.99	0.94	0.89	0.92	0.99
Mature NK	2.5%	0.98	0.96	0.98	1	0.96	0.92	0.97	0.98	0.91	0.83	0.88	0.97	0.76	0.62	0.64	0.86	0.76	0.61	0.65	0.87
CD8+ TEMRA T cells CD27+ CD28-	1.2%	0.98	0.96	0.97	1	0.99	0.98	0.99	1	0.77	0.62	0.67	0.92	0.69	0.53	0.59	0.86	0.80	0.67	0.73	0.95
NK CD16- CD56-	2.4%	0.98	0.96	0.99	1	0.99	0.97	0.99	1	0.80	0.67	0.77	0.94	0.82	0.69	0.83	0.87	0.81	0.69	0.83	0.88
CD8+ TEM T cells CD27- CD28-	0.57%	0.98	0.95	0.97	1	0.98	0.97	0.98	1	0.68	0.52	0.53	0.91								
CD8+ TCM T cells CD27+ CD28+	1.1%	0.98	0.95	0.97	1	0.98	0.97	0.98	1	0.68	0.52	0.55	0.95					0.01	<0.01	0.01	0.59
Vd1+ Vg9- T cells CD56-	0.88%	0.97	0.95	0.98	1	0.99	0.98	0.99	1	0.89	0.80	0.87	0.96	0.85	0.74	0.80	0.95	0.81	0.69	0.78	0.92
CD4+ TSCM T cells CD27+ CD28+	1%	0.97	0.94	0.96	1	0.97	0.95	0.96	0.99	0.17	0.09	0.07	0.76	0.02	0.01	0.01	0.50	0.04	0.02	0.02	0.49
iNKT cells	0.07%	0.97	0.93	0.99	0.99	0.98	0.96	0.99	0.99	0.97	0.93	0.99	0.98	0.92	0.85	0.92	0.91				
Early NK	0.92%	0.96	0.93	0.96	1	0.94	0.88	0.91	0.98	0.84	0.72	0.78	0.96	0.85	0.73	0.80	0.94	0.83	0.71	0.78	0.94
Vd2 low Vg9+ T cells CD56-	0.55%	0.96	0.93	0.96	0.99	0.97	0.94	0.97	0.99	0.90	0.81	0.89	0.98	0.89	0.80	0.86	0.95	0.85	0.74	0.82	0.94
CD4+ TEMRA T cells CD27- CD28-	0.18%	0.96	0.93	0.95	0.99	0.98	0.96	0.98	0.99	0.48	0.31	0.33	0.80	0.42	0.27	0.27	0.93	0.44	0.28	0.28	0.93
CD8+ TEMRA T cells CD27+ CD28+	0.55%	0.96	0.92	0.95	1	0.98	0.95	0.97	0.99	0.62	0.45	0.47	0.90	0.08	0.04	0.04	0.69	0.63	0.46	0.53	0.93
CD8+ TEM T cells CD27- CD28+	0.31%	0.95	0.91	0.94	0.99	0.97	0.95	0.96	0.99	0.71	0.55	0.57	0.92								
MAIT cells	0.51%	0.95	0.91	0.94	1	0.95	0.90	0.93	0.98	0.74	0.59	0.62	0.85	0.90	0.82	0.87	0.96	0.84	0.73	0.81	0.89
CD4+ TEMRA T cells CD27+ CD28+	0.12%	0.94	0.88	0.91	0.99	0.97	0.95	0.96	0.99	0.33	0.20	0.19	0.64								
CD8+ TSCM T cells CD27+ CD28+	0.14%	0.93	0.86	0.89	0.99	0.96	0.92	0.94	0.99	0.30	0.18	0.19	0.91								
CD4+ TEM T cells CD27+ CD28-	0.07%	0.92	0.86	0.90	0.98	0.97	0.93	0.95	0.99	0.44	0.28	0.31	0.85								
Vd1+ Vg9- T cells CD56+	0.12%	0.92	0.86	0.91	0.98	0.97	0.94	0.96	0.99	0.82	0.70	0.78	0.94								
Vd2 low Vg9+ T cells CD56+	0.20%	0.92	0.85	0.91	0.99	0.95	0.91	0.95	0.99	0.81	0.68	0.77	0.94								
Q2: Vd1+ Vg9+	0.08%	0.92	0.85	0.93	0.98	0.97	0.95	0.98	0.99	0.80	0.67	0.78	0.94	0.81	0.68	0.81	0.90	0.44	0.28	0.31	0.72
CD4+ TEMRA T cells CD27- CD28+	0.03%	0.90	0.82	0.85	0.97	0.94	0.89	0.91	0.98	0.27	0.16	0.15	0.55								
Terminal NK	0.21%	0.88	0.79	0.82	0.99	0.91	0.83	0.84	0.98	0.57	0.41	0.45	0.90					0.01	<0.01	<0.01	0.43
CD8+ TCM T cells CD27- CD28+	0.06%	0.88	0.78	0.80	0.97	0.94	0.89	0.91	0.98	0.54	0.37	0.41	0.88								
CD4+ TSCM T cells CD27- CD28+	0.10%	0.88	0.78	0.83	0.98	0.94	0.89	0.92	0.98	0.28	0.17	0.18	0.86								
Medians		0.97	0.94	0.97	1	0.98	0.96	0.98	0.99	0.75	0.60	0.62	0.94	0.48	0.32	0.32	0.86	0.44	0.28	0.31	0.87
Means		0.96	0.92	0.95	0.99	0.97	0.95	0.96	0.99	0.70	0.57	0.61	0.91	0.43	0.37	0.40	0.56	0.42	0.35	0.38	0.55



Merged matches

With FlowSOM QFMatch finds 8 of 22 matches where merging multiple FlowSOM gated populations to match 1 manually gated population obtains a higher F1-score: the 2nd, 4th, 5th, 6th, 7th, 9th, 14th and 16th ranked matches.






































Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	Similarity (QFMatch)	Train-ing set?	Freq.
2	●	27	HLA-DR+	4	97%	98.8%	yes	9.9%
2	●	47	HLA-DR+ (FlowSOM.Viable cells.Po...	4	97%	98.8%	no	1.4%
2	●	63	HLA-DR+ (FlowSOM.Viable cells.Po...	4	97%	98.8%	no	0.2%
2	●	66	HLA-DR+ (FlowSOM.Viable cells.Po...	4	97%	98.8%	no	7.4%
6	●	20	CD8+ TEM T cells CD27+ CD28+	4	78.5%	96%	yes	4%
6	●	45	FlowSOM.Viable cells.Pop22	4	78.5%	96%	no	0.7%
6	●	64	CD8+ TCM T cells CD27+ CD28+ (FI...	4	78.5%	96%	no	3.5%
6	●	68	CD8+ TEM T cells CD27- CD28+ (FI...	4	78.5%	96%	no	0.6%
14	●	1	Vd1+ Vg9- T cells CD56-	4	81.4%	92%	yes	1.6%
14	●	37	Vd1+ Vg9- T cells CD56- (FlowSOM....	4	81.4%	92%	no	0.5%
14	●	38	Vd1+ Vg9- T cells CD56- (FlowSOM....	4	81.4%	92%	no	0.3%
14	●	65	Vd1+ Vg9- T cells CD56- (FlowSOM....	4	81.4%	92%	no	0.5%
4	●	12	CD4+ TCM T cells CD27+ CD28+	3	88.6%	97.4%	yes	20.5%
4	●	39	CD4+ TCM T cells CD27+ CD28+ (FI...	3	88.6%	97.4%	no	4.9%
4	●	48	CD4+ TCM T cells CD27+ CD28+ (FI...	3	88.6%	97.4%	no	17.7%
5	●	2	CD8+ TEMRA T cells CD27- CD28-	3	95.1%	97.4%	yes	17.8%
5	●	46	CD8+ TEMRA T cells CD27- CD28- (...)	3	95.1%	97.4%	no	14.6%
5	●	61	CD8+ TEMRA T cells CD27- CD28- (...)	3	95.1%	97.4%	no	2.7%
7	●	3	CD8+ TEMRA T cells CD27+ CD28-	3	79.9%	95.5%	yes	1.9%
7	●	69	CD8+ TEMRA T cells CD27+ CD28- ...	3	79.9%	95.5%	no	1.5%
7	●	70	CD8+ TEMRA T cells CD27+ CD28- ...	3	79.9%	95.5%	no	0.3%
9	●	13	Early NK	3	83.1%	94.4%	yes	1%
9	●	36	Early NK (FlowSOM.Viable cells.Pop8)	3	83.1%	94.4%	no	0.2%
9	●	51	Early NK (FlowSOM.Viable cells.Pop2)	3	83.1%	94.4%	no	0.9%
16	●	22	CD8+ Naive T cells CD27+ CD28+	3	58.8%	88.1%	yes	1.9%
16	●	44	CD8+ Naive T cells CD27+ CD28+ (...)	3	58.8%	88.1%	no	0.2%
16	●	54	CD8+ Naive T cells CD27+ CD28+ (...)	3	58.8%	88.1%	no	3.5%
1	●	21	CD4+ Naive T cells CD27+ CD28+	2	97.2%	99.3%	yes	21.5%
1	●	50	CD4+ Naive T cells CD27+ CD28+ (...)	2	97.2%	99.3%	no	19%

With PhenoGraph QFMatch finds 6 of 16 matches where merging multiple PhenoGraph gated populations to match 1 manually gated population obtains a higher F1-score: 1st, 3rd, 5th, 7th, 8th and 16th ranked matches.







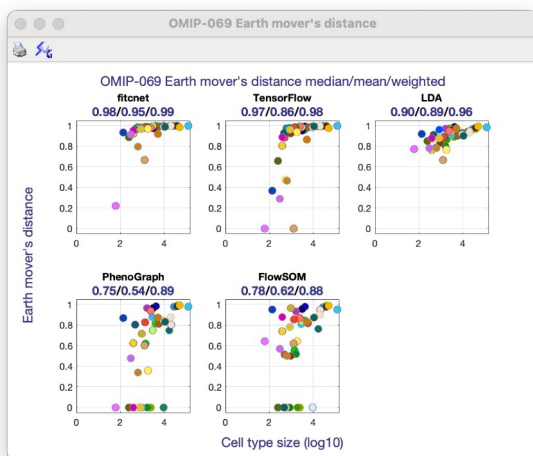
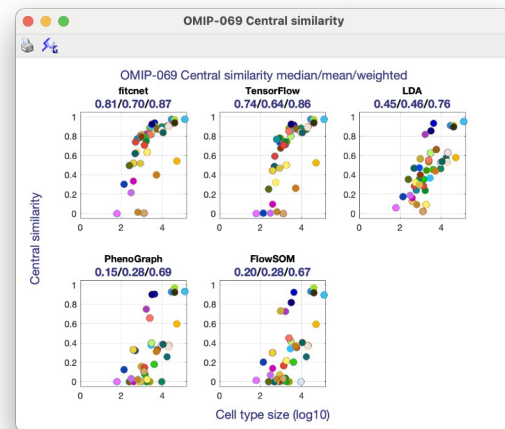
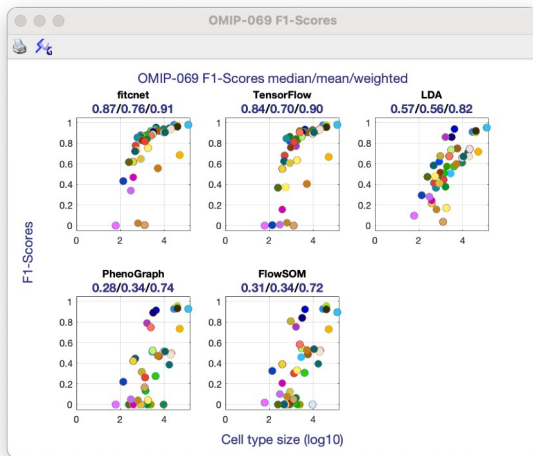

 MATCH sets: training=23/35 (12 UNMATCHED!), test=34/35 (1 NEW!)

Rank ²	#	Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	Similarity (QFMatch)	Train-ing set?	Freq.	
1	27	HLA-DR+	5	97.3%	98.8%	yes	9.9%	3
1	40	PhenographYO0G4	5	97.3%	98.8%	no	6.9%	2
1	46	PhenographYO0G26	5	97.3%	98.8%	no	0.3%	
1	47	PhenographYO0G16	5	97.3%	98.8%	no	1.8%	
1	58	PhenographYO0G29	5	97.3%	98.8%	no	0.2%	
3	2	CD8+ TEMRA T cells CD27- CD28-	4	93.4%	96.5%	yes	17.8%	5
3	51	PhenographYO0G13	4	93.4%	96.5%	no	2.6%	
3	56	PhenographYO0G3	4	93.4%	96.5%	no	11%	4
3	64	PhenographYO0G11	4	93.4%	96.5%	no	3.2%	1
5	21	CD4+ Naive T cells CD27+ CD28+	4	93.8%	95.7%	yes	21.5%	7
5	41	PhenographYO0G23	4	93.8%	95.7%	no	0.4%	
5	43	PhenographYO0G8	4	93.8%	95.7%	no	3.9%	1
5	60	PhenographYO0G1	4	93.8%	95.7%	no	16.6%	6
7	1	Vd1+ Vg9- T cells CD56-	4	84.8%	95.3%	yes	1.6%	
7	44	PhenographYO0G17	4	84.8%	95.3%	no	1.2%	
7	48	PhenographYO0G28	4	84.8%	95.3%	no	0.2%	
7	54	PhenographYO0G22	4	84.8%	95.3%	no	0.5%	
8	12	CD4+ TCM T cells CD27+ CD28+	3	86.7%	95.2%	yes	20.5%	6
8	49	PhenographYO0G7	3	86.7%	95.2%	no	5.4%	2
8	52	PhenographYO0G2	3	86.7%	95.2%	no	14.9%	5
16	22	CD8+ Naive T cells CD27+ CD28+	3	59.1%	87.7%	yes	1.9%	
16	36	PhenographYO0G30	3	59.1%	87.7%	no	0.2%	
16	63	PhenographYO0G9	3	59.1%	87.7%	no	3.5%	1
2	25	Vd2 high Vg9+ T cells	2	94.9%	98.6%	yes	0.6%	
2	61	PhenographYO0G21	2	94.9%	98.6%	no	0.6%	

Liechti, T. and Roederer, M. (2019), **OMIP-058: 30-Parameter Flow Cytometry Panel to Characterize iNKT, NK, Unconventional and Conventional T Cells**. Cytometry, 95: 946-951. <https://doi.org/10.1002/cyto.a.23850>

5.3.4. OMIP-069

Classifier	Population	Frequency	fitcnet				TensorFlow				LDA				PhenoGraph				FlowSOM			
			F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD
• Naive CD4+	29%		0.98	0.96	0.98	1	0.98	0.96	0.97	1	0.95	0.90	0.95	0.99	0.93	0.86	0.93	0.98	0.90	0.81	0.90	0.95
• B-2 CD27-	6.8%		0.98	0.96	0.97	1	0.98	0.95	0.97	1	0.91	0.84	0.91	0.97	0.93	0.86	0.93	0.98	0.93	0.87	0.93	0.98
• Naive CD8+	9.6%		0.97	0.94	0.97	1	0.97	0.95	0.97	1	0.90	0.83	0.91	0.96	0.96	0.92	0.97	0.99	0.96	0.92	0.97	0.99
• Mature NK	9.5%		0.96	0.92	0.94	1	0.96	0.92	0.94	0.99	0.92	0.85	0.90	0.98	0.93	0.87	0.92	0.98	0.92	0.86	0.92	0.98
• B-1 IgG	0.97%		0.95	0.91	0.94	0.99	0.93	0.87	0.92	0.99	0.94	0.88	0.93	0.99	0.92	0.84	0.91	0.98	0.92	0.86	0.92	0.98
• Early Effector CD4+	4.1%		0.95	0.90	0.91	1	0.93	0.86	0.87	0.99	0.71	0.55	0.56	0.94	0.38	0.24	0.26	0.75	0.39	0.24	0.25	0.76
• Central Memory CD4+ CXCR5-, CXCR3-	4.9%		0.94	0.89	0.91	1	0.94	0.88	0.89	0.99	0.74	0.59	0.63	0.95	0.50	0.33	0.37	0.80	0.52	0.35	0.37	0.95
• Terminal Effector CD45RA+ CD8+	0.94%		0.94	0.88	0.91	0.99	0.91	0.83	0.89	0.96	0.56	0.41	0.45	0.89	0.28	0.16	0.18	0.82	0.31	0.18	0.20	0.84
• Early like effector CD4+	2.2%		0.94	0.88	0.89	1	0.93	0.87	0.88	0.99	0.61	0.44	0.46	0.93								
• Central Memory CD4+ CXCR5-, CXCR3	4.6%		0.93	0.88	0.90	1	0.93	0.87	0.89	1	0.67	0.50	0.53	0.93	0.48	0.32	0.36	0.88	0.51	0.34	0.37	0.90
• CD2+ CD8+ NKT	1.3%		0.92	0.85	0.87	0.99	0.91	0.83	0.87	0.98	0.75	0.60	0.66	0.90	0.47	0.30	0.33	0.81	0.48	0.32	0.35	0.82
• Terminal NK	0.59%		0.92	0.85	0.89	0.99	0.92	0.85	0.88	0.99	0.67	0.51	0.53	0.97								
• B-2 CD27+	0.68%		0.92	0.85	0.90	0.99	0.89	0.81	0.85	0.98	0.51	0.34	0.37	0.91	0.51	0.34	0.37	0.88	0.46	0.30	0.34	0.81
• B-1 IgG- IgM-	0.73%		0.91	0.83	0.92	0.97	0.90	0.82	0.92	0.95	0.86	0.75	0.85	0.95	0.89	0.80	0.90	0.97	0.84	0.73	0.82	0.96
• Central Memory CD4+ CXCR5, CXCR3	2.2%		0.91	0.83	0.86	0.99	0.89	0.81	0.84	0.98	0.66	0.49	0.53	0.92	0.51	0.35	0.38	0.84				
• Early Effector CD8+	2.6%		0.91	0.83	0.84	0.99	0.90	0.82	0.84	0.99	0.67	0.50	0.54	0.90	0.51	0.35	0.38	0.83	0.53	0.36	0.40	0.87
• Intermediate Effector CD8+	0.45%		0.89	0.80	0.81	0.98	0.83	0.71	0.74	0.96	0.57	0.40	0.45	0.86								
• CD4- CD8-	0.69%		0.88	0.79	0.82	0.99	0.87	0.76	0.80	0.98	0.74	0.57	0.62	0.94	0.52	0.35	0.40	0.75	0.55	0.37	0.42	0.84
• CD123+ pDCs	0.39%		0.88	0.78	0.82	0.99	0.77	0.63	0.71	0.97	0.86	0.75	0.82	0.97	0.79	0.65	0.75	0.96	0.75	0.60	0.72	0.93
• B-1 IgM+	0.21%		0.88	0.78	0.81	0.98	0.82	0.69	0.73	0.98	0.62	0.45	0.47	0.96								
• CCR7- CD45RA+ TCRgD+	0.57%		0.87	0.78	0.81	0.98	0.90	0.83	0.85	0.99	0.68	0.51	0.55	0.95	0.75	0.60	0.66	0.94	0.57	0.41	0.45	0.87
• Central Memory CD8+	0.34%		0.87	0.77	0.79	0.99	0.83	0.71	0.73	0.98	0.51	0.34	0.35	0.89	0.13	0.07	0.07	0.62	0.01	0.01	0.01	0.56
• Early NK	0.22%		0.87	0.77	0.81	0.98	0.85	0.74	0.78	0.97	0.67	0.51	0.56	0.87	0.31	0.19	0.15	0.72	0.81	0.68	0.73	0.96
• Terminal Effector	0.20%		0.86	0.76	0.79	0.98	0.86	0.76	0.78	0.98	0.49	0.34	0.36	0.87								
• Terminal Effector CD4+	0.14%		0.85	0.74	0.77	0.98	0.85	0.74	0.77	0.97	0.37	0.22	0.24	0.79								
• Early like effector CD8+	0.38%		0.84	0.73	0.75	0.99	0.84	0.72	0.74	0.99	0.37	0.23	0.24	0.80					0.06	0.03	0.03	0.52
• CD2+ CD8-	0.22%		0.83	0.71	0.79	0.97	0.76	0.61	0.68	0.92	0.51	0.35	0.40	0.83					0.02	0.01	0.01	0.50
• CCR7- CD45RA- TCRgD+	0.32%		0.82	0.69	0.71	0.98	0.81	0.69	0.71	0.98	0.44	0.28	0.28	0.89	0.26	0.15	0.15	0.83	0.30	0.18	0.17	0.85
• CCR7+ TCRgD+	0.12%		0.77	0.63	0.74	0.97	0.68	0.53	0.59	0.88	0.41	0.26	0.28	0.87					< 0.01	< 0.01	< 0.01	0.52
• ILCs CD4-	0.43%		0.75	0.60	0.63	0.97	0.64	0.47	0.50	0.94	0.17	0.09	0.09	0.77	0.04	0.02	0.02	0.36	0.33	0.20	0.22	0.64
• ILCs CD2+ CD4+	0.13%		0.73	0.57	0.63	0.96	0.37	0.30	0.32	0.47	0.48	0.31	0.32	0.87								
• CD4+ CD8+ T	0.11%		0.72	0.56	0.62	0.96	0.62	0.45	0.49	0.93	0.57	0.41	0.47	0.91	0.45	0.28	0.32	0.80				
• Classical monocytes	12%		0.69	0.52	0.54	0.98	0.67	0.50	0.52	0.97	0.72	0.56	0.57	0.99	0.73	0.57	0.60	0.99	0.73	0.56	0.59	0.99
• CD11c+ CD16+ DCs	0.20%		0.65	0.48	0.52	0.96	0.60	0.44	0.47	0.96	0.41	0.26	0.30	0.88					0.12	0.07	0.07	0.78
• ILCs CD2- CD4-	0.09%		0.62	0.45	0.52	0.92	0.55	0.38	0.45	0.80	0.22	0.12	0.13	0.76	0.42	0.27	0.33	0.62	0.39	0.24	0.30	0.74
• CD2- NKT cells	0.06%		0.62	0.45	0.50	0.89	0.37	0.22	0.25	0.66	0.47	0.31	0.35	0.85								
• Intermediate monocytes	1.2%		0.56	0.39	0.40	0.92	0.40	0.25	0.26	0.86	0.60	0.43	0.44	0.97	0.47	0.31	0.31	0.87	0.53	0.36	0.37	0.83
• CD1c+ DCs	0.09%		0.47	0.30	0.34	0.95	0.16	0.09	0.09	0.88	0.24	0.14	0.16	0.88					0.21	0.12	0.14	0.88
• Plasmablasts	0.03%		0.43	0.28	0.30	0.93	< 0.01	< 0.01	< 0.01	0.37	0.28	0.17	0.17	0.92	0.22	0.12	0.12	0.87	0.33	0.19	0.20	0.95
• CD1c- CD141- DCs	0.07%		0.34	0.21	0.22	0.92	0.01	< 0.01	< 0.01	0.28	0.28	0.16	0.18	0.78	0.05	0.02	0.03	0.48	0.10	0.05	0.07	0.56
• Non classical monocytes	0.15%		0.02	0.01	0.01	0.80	0.03	0.01	0.02	0.47	0.16	0.08	0.09	0.78	0.04	0.02	0.02	0.34	0.08	0.04	0.03	0.50
• CD16- CD14- monocytes	0.30%		< 0.01	< 0.01	< 0.01	0.67					0.04	0.02	0.02	0.67	0.16	0.09	0.10	0.60	0.05	0.03	0.03	0.62
• CD1c- CD141+ DCs	0.01%										0.10	0.05	0.06	0.77					0.02	0.01	0.01	0.64
Medians			0.87	0.77	0.81	0.98	0.84	0.72	0.74	0.97	0.57	0.41	0.45	0.90	0.28	0.16	0.15	0.75	0.31	0.18	0.20	0.78
Means			0.76	0.67	0.70	0.95	0.70	0.61	0.64	0.86	0.56	0.43	0.46	0.89	0.34	0.26	0.28	0.54	0.34	0.26	0.28	0.62



Merged matches

With FlowSOM there QFMatch finds 6 of 34 possible matches where merging multiple FlowSOM gated populations for 1 manually gated population obtains a higher F1-score: the 2nd, 5th, 10th, 12th, 14th and 18th ranked matches.

Sync QF F1 MATCH sets: training=34/43 (9 UNMATCHED), test=40/43 (3 NEW)

Rank	#	Subset (class) name	Mat-ches	Similarity (QFMatch)	% Overlap (F-measure)	Train-ing set?	Freq.
2	42	Classical monocytes	3	98.9%	72.9%	yes	7.9%
2	63	Classical monocytes (FlowSOM.CD4...	3	98.9%	72.9%	no	5.7%
2	75	Classical monocytes (FlowSOM.CD4...	3	98.9%	72.9%	no	4.4%
5	12	B-2 CD27-	3	97.6%	92.9%	yes	6.8%
5	48	B-2 CD27- (FlowSOM.CD45+.Pop6)	3	97.6%	92.9%	no	4.4%
5	72	B-2 CD27- (FlowSOM.CD45+.Pop5)	3	97.6%	92.9%	no	1.3%
10	41	Central Memory CD4+ CXCR5-, CXC...	3	94.8%	52.3%	yes	6.5%
10	59	Early like effector CD4+ (FlowSOM....	3	94.8%	52.3%	no	2.5%
10	81	Central Memory CD4+ CXCR5, CXC...	3	94.8%	52.3%	no	9.1%
12	21	Central Memory CD4+ CXCR5-, CXC...	3	89.9%	51.1%	yes	4.7%
12	58	Central Memory CD4+ CXCR5-, CXC...	3	89.9%	51.1%	no	6.1%
12	68	Central Memory CD4+ CXCR5-, CXC...	3	89.9%	51.1%	no	0.6%
14	8	Early Effector CD8+	3	87.3%	53.5%	yes	3%
14	69	Central Memory CD8+ (FlowSOM.CD...	3	87.3%	53.5%	no	0.8%
14	83	Early like effector CD8+ (FlowSOM....	3	87.3%	53.5%	no	2.6%
18	19	CD4- CD8-	3	83.5%	54.5%	yes	1.5%
18	45	FlowSOM.CD45+.Pop18	3	83.5%	54.5%	no	0.3%
18	56	CCR7+ TCRgD+ (FlowSOM.CD45+....	3	83.5%	54.5%	no	0.9%
1	23	Naive CD8+	2	99.2%	95.7%	yes	13.1%
1	51	Naive CD8+ (FlowSOM.CD45+.Pop30)	2	99.2%	95.7%	no	10.4%

With PhenoGraph there are 4 of 29 matches where merging multiple manual or PhenoGraph gated populations for 1 manually gated population obtains a higher F1-score: the 2nd, 5th, 19th and 26th ranked matches.

Sync QF F1 MATCH sets: training=29/43 (14 UNMATCHED), test=34/38 (4

Rank	#	Subset (class) name	Mat-ches	Similarity (QFMatch)	% Overlap (F-measure)	Train-ing set?	Freq.
5	18	Naive CD4+	4	98%	92.6%	yes	28.4%
5	47	PhenographLP7210	4	98%	92.6%	no	4.3%
5	66	PhenographLP7218	4	98%	92.6%	no	1.5%
5	71	PhenographLP721	4	98%	92.6%	no	16.5%
2	42	Classical monocytes	3	99%	73.3%	yes	7.9%
2	73	PhenographLP725	3	99%	73.3%	no	5%
2	74	PhenographLP727	3	99%	73.3%	no	4.9%
19	41	Central Memory CD4+ CXCR5-, CXC...	3	80.5%	49.5%	yes	6.5%
19	50	PhenographLP7232	3	80.5%	49.5%	no	0.1%
19	64	PhenographLP726	3	80.5%	49.5%	no	4.9%
26	35	CD16- CD14- monocytes	3	60.3%	16.2%	yes	0.4%
26	45	PhenographLP7224	3	60.3%	16.2%	no	0.7%
26	60	PhenographLP7235	3	60.3%	16.2%	no	0%
1	23	Naive CD8+	2	99.3%	95.7%	yes	13.1%
1	44	PhenographLP722	2	99.3%	95.7%	no	10.3%

5.3.4.1. Lowest MLP scores ?

Our [population level results](#) in this dataset stand out because

1. This is where MLP's scores lowest.
2. Nevertheless the gap between MLP scores and those of LDA, FlowSOM and PhenoGraph is the biggest

Concerning item 1 above, the matches that are atypically poor for MLP occur on cell populations whose manual gate sequence contains drawings that are also atypical by not enclosing the density features that probability coloring and contours highlight in the X/Y plots reflecting prior biology knowledge *beyond* the data's structure. If we ignore such regions (e.g. monocytes) and instead focus on a region like that containing the 19 leaf gates under the parent gates "T cells" and "NKT-like cells" then we find that MLP achieves more typical high scores.

Color	Cell type	Frequency %	F1-Score		Central similarity		Earth mover's distance	
			fitc net	LDA	fitc net	LDA	fitc net	LDA
●	Naive CD4+	46%	0.995	0.979	0.999	0.997	0.997	0.991
●	Naive CD8+	15%	0.994	0.945	0.999	0.978	0.999	0.966
●	Early like effector CD4+	3.4%	0.980	0.676	0.981	0.563	0.997	0.886
●	Early Effector CD4+	6.4%	0.979	0.796	0.979	0.725	0.995	0.939
●	Central Memory CD4+ CXCR5-, CXCR3	7.1%	0.964	0.761	0.962	0.682	0.996	0.915
●	Central Memory CD4+ CXCR5-, CXCR3-	7.6%	0.954	0.785	0.939	0.709	0.992	0.910
●	Early Effector CD8+	4%	0.945	0.811	0.920	0.736	0.989	0.940
●	Intermediate Effector CD8+	0.70%	0.943	0.719	0.924	0.620	0.987	0.887
●	Central Memory CD8+	0.53%	0.943	0.638	0.915	0.485	0.989	0.855
●	Terminal Effector CD4+	0.22%	0.933	0.412	0.918	0.281	0.974	0.677
●	CD4- CD8-	1.1%	0.930	0.710	0.885	0.560	0.985	0.844
●	Terminal Effector	0.31%	0.909	0.571	0.866	0.458	0.981	0.823
●	Early like effector CD8+	0.59%	0.902	0.616	0.853	0.493	0.986	0.878
●	Terminal Effector CD45RA+ CD8+	1.5%	0.885	0.677	0.814	0.572	0.981	0.876
●	Central Memory CD4+ CXCR5-, CXCR3	3.4%	0.863	0.724	0.809	0.617	0.973	0.892
●	CD4+ CD8+ T	0.17%	0.844	0.700	0.797	0.562	0.960	0.809
●	CD2- NKT cells	0.09%	0.154	0.254	0.097	0.158	0.775	0.772
●	CD2+ CD8+ NKT	2.1%	0.053	0.120	0.025	0.067	0.761	0.684
●	CD2+ CD8-	0.34%	0.029	0.050	0.015	0.030	0.490	0.490
Median			0.933	0.700	0.915	0.563	0.986	0.878
Mean			0.800	0.629	0.774	0.542	0.937	0.844

Concerning item 2, MLP's significantly greater accuracy also occurs with the PANORAMA and OMIP-058 datasets. We suspect there must be more tuning with each of these classifiers' configuration parameters than those settings which FlowJo's support team recommended with PhenoGraph and FlowSOM plugins or that which the LDA publication's supplementary code illustrated. The OMIP-069 publication itself discusses the use of FlowSOM on their data. There may be better tunings of FlowSOM, LDA or PhenoGraph that are more accurate for this

spectral cytometry dataset as well as for the others, but this means that they do not meet 1 the Herzenberg Lab's bioinformatics goals of being easy to use for the biologist as well as accurate and quick.

Exploring this further for OMIP-069 we pointed FlowSOM at the same data region upon which we narrowed MLP's attention for the same reasons. This region contains 19 populations so we set FlowSOM to find 20 meta clusters to allow 1 for background and then ran it producing the results discussed in our [supplementary document](#). The medians/means of the F1-score was 0.405/0.410 which improves upon the 0.306/0.346 obtained for running FlowSOM on all 46 populations. But this does not inspire trust in the capability of FlowSOM.

If QFMatch is run to find the best many-to-many F1-score between FlowSOM gated populations and manually gated populations, however, the median/mean goes from 0.31/0.35 to 0.511 /0.481. [QFMatch finds](#) 7 of 30 matches where merging multiple manual or FlowSOM gated populations obtains a higher F1-score. The 10th, 18th, 21st and 26th ranked matches merge multiple manually gated populations to match 1 FlowSOM gated population. The 2nd, 5th and 12th ranked matches merge multiple FlowSOM gated populations to match 1 manually gated population.

5.3.4.2. Low FlowSOM scores

We run FlowSOM with 44 meta clusters to find 43 cell populations, the 1 extra is for background. But FlowSOM only finds 42 clusters. So we tried running FlowSOM on only the T cells and NKT-like cells which require 9 phenotyping markers that classify 19 leaf gates starting at the CD3+ TCRgd- branch gate: CCR7, CD2, CD4, CD8, CD27, CD28, CD45RA, CXCR3, CXCR5. We ran FlowSOM on the common parent gate to these populations specifying 20 meta clusters to allow 1 for background. The medians/means of the F1-score shown below are 0.405/0.410. This improves upon the 0.306/0.346 obtained for running FlowSOM on all 46 populations. *The same populations found by FlowSOM when starting at the "CD45+" branch closest to all 43 cell populations get lower scores than when FlowSOM starts at the lower CD3+ TCRgd- branch: for example, Naive CD8+ gets 0.90 F1-score on the CD45+ branch run and 0.98 on the run for the branch with only NKT and T leaves. I am wary of methods that rely on reading T leaves!*

Color	Cell type	Frequency %	F1-Score	Central similarity	Earth mover's distance
			Flow SOM 	Flow SOM	Flow SOM
●	Naive CD8+	18%	0.979	0.996	0.994
●	Naive CD4+	39%	0.950	0.959	0.982
●	CD4- CD8-	2%	0.776	0.651	0.913
●	Central Memory CD4+ CXCR5-, CXCR3	6.3%	0.687	0.533	0.918
●	Early Effector CD8+	4.1%	0.661	0.524	0.850
●	CD4+ CD8+ T	0.13%	0.656	0.499	0.832
●	Early like effector CD4+	2.4%	0.526	0.385	0.879
●	Central Memory CD4+ CXCR5-, CXCR3-	8.8%	0.515	0.354	0.906
●	Early Effector CD4+	5.4%	0.489	0.328	0.788
●	Intermediate Effector CD8+	0.66%	0.405	0.277	0.817
●	Terminal Effector CD45RA+ CD8+	0.61%	0.401	0.273	0.874
●	Early like effector CD8+	0.77%	0.393	0.253	0.741
●	CD2+ CD8+ NKT	2.3%	0.280	0.187	0.745
●	Central Memory CD8+	0.50%	0.071	0.033	0.468
●	Central Memory CD4+ CXCR5, CXCR3	8.8%	0.003	0.001	0.597
●	CD2+ CD8-	0.56%	N/A	N/A	N/A
●	Terminal Effector	0.30%	0	0	0.379
●	CD2- NKT cells	0.13%	N/A	N/A	N/A
●	Terminal Effector CD4+	0.01%	N/A	N/A	N/A
Median			0.405	0.277	0.817
Mean			0.410	0.329	0.668

5.3.4.3. Improving PhenoGraph accuracy

Running PhenoGraph on the more narrow region of the gating tree at the **CD3+ TCRgd-** branch also improves the F1-score median/mean from 0.275/0.338 to 0.414/0.375. Individual populations like CD4- CD8- improves from 0.52 to 0.76.

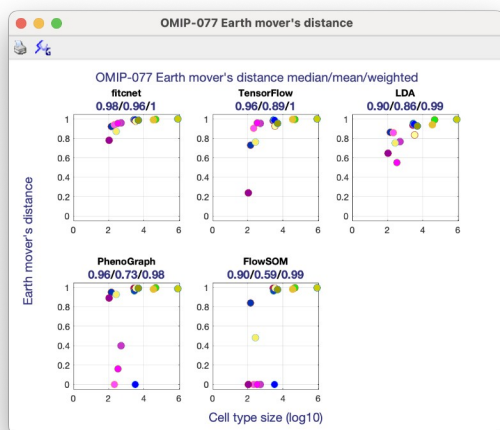
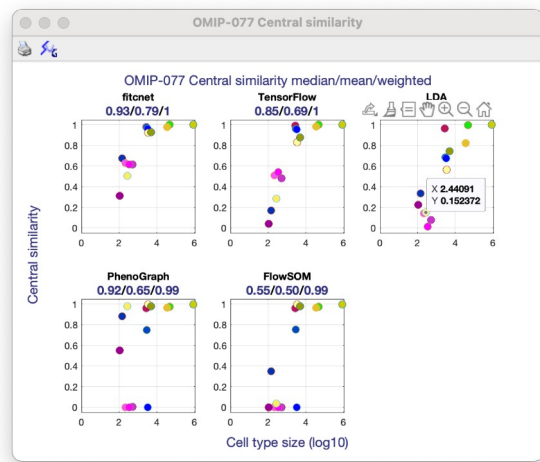
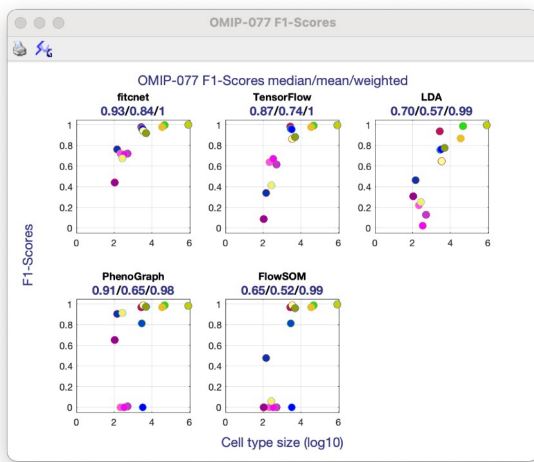
OMIP-069-NKT-T scores for 1 classifier					
See underlying data file					
Color	Cell type	Frequency %	F1-Score	Central similarity	Earth mover's distance
			Pheno Graph	Pheno Graph	Pheno Graph
●	Naive CD8+	18%	0.97	0.99	0.99
●	Naive CD4+	39%	0.92	0.92	0.97
●	CD4- CD8-	2%	0.76	0.65	0.93
●	Central Memory CD4+ CXCR5, CXCR3	8.8%	0.68	0.56	0.95
●	Early like effector CD4+	2.4%	0.61	0.46	0.92
●	Early Effector CD8+	4.1%	0.56	0.43	0.85
●	Central Memory CD4+ CXCR5-, CXCR3	6.3%	0.52	0.39	0.86
●	CD4+ CD8+ T	0.13%	0.47	0.28	0.81
●	CD2+ CD8+ NKT	2.3%	0.44	0.31	0.81
●	CD2- NKT cells	0.13%	0.41	0.30	0.69
●	Early Effector CD4+	5.4%	0.40	0.26	0.80
●	Terminal Effector CD45RA+ CD8+	0.61%	0.26	0.16	0.76
●	Central Memory CD4+ CXCR5-, CXCR3-	8.8%	0.09	0.05	0.65
●	Intermediate Effector CD8+	0.66%	0.01		0.31
●	Central Memory CD8+	0.50%	0.01	0.01	0.47
●	CD2+ CD8-	0.56%	0.01	0.01	0.37
●	Early like effector CD8+	0.77%			
●	Terminal Effector	0.30%			
●	Terminal Effector CD4+	0.01%			0.46
19 cell populations		Median	0.414	0.283	0.805
		Mean	0.375	0.303	0.664

Park, L.M., Lannigan, J. and Jaimes, M.C. (2020), **OMIP-069: Forty-Color Full Spectrum Flow Cytometry Panel for Deep Immunophenotyping of Major Cell Subsets in Human Peripheral Blood**. Cytometry, 97: 1044-1051.
<https://doi.org/10.1002/cyto.a.24213>

5.3.5. OMIP-077

Population	Classifier	Frequency	fitcnet				TensorFlow				LDA				PhenoGraph				FlowSOM			
			F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD
• Neutrophils		77%	1	1	1	1	1	1	1	1	1	0.99	1	1	0.99	0.97	1	0.99	1	0.99	1	1
• T cells		11%	1	1	1	1	0.99	0.98	1	1	0.99	0.98	1	0.99	0.99	0.97	0.98	1	0.99	0.97	0.98	1
• Monocytes		6.9%	0.98	0.96	0.98	0.99	0.98	0.96	0.99	1	0.87	0.77	0.82	0.94	0.97	0.94	0.97	0.98	0.97	0.94	0.97	0.98
• Basophils		0.34%	0.98	0.96	0.98	0.99	0.98	0.97	0.99	0.98	0.94	0.88	0.97	0.94	0.97	0.94	0.96	0.99	0.97	0.94	0.96	0.99
• Non MZB cells		1.4%	0.97	0.93	0.97	0.99	0.96	0.92	0.96	0.99	0.76	0.61	0.68	0.96	0.81	0.69	0.75	0.96	0.82	0.69	0.75	0.96
• MZB cells		0.52%	0.96	0.92	0.96	0.99	0.96	0.92	0.96	0.99	0.76	0.62	0.67	0.95								
• Eosinophils		1.3%	0.94	0.89	0.92	0.98	0.86	0.76	0.83	0.93	0.65	0.50	0.56	0.84	0.99	0.98	1	0.99	0.99	0.98	1	0.99
• NK cells		2%	0.92	0.85	0.93	0.99	0.88	0.79	0.88	0.96	0.78	0.64	0.74	0.93	0.97	0.95	0.98	0.99	0.96	0.92	0.98	0.98
• Plasma cells		0.09%	0.76	0.62	0.68	0.93	0.34	0.20	0.17	0.73	0.46	0.30	0.33	0.86	0.91	0.83	0.88	0.95	0.48	0.31	0.35	0.84
• CD1c+ mDCs		0.03%	0.72	0.56	0.63	0.94	0.64	0.47	0.51	0.90	0.22	0.13	0.14	0.86								
• CD141- mDCs		0.04%	0.72	0.56	0.62	0.96	0.62	0.46	0.48	0.96	0.13	0.07	0.08	0.77	0.01	< 0.01	< 0.01	0.40				
• CD141+ mDCs		0.01%	0.71	0.55	0.61	0.95	0.67	0.51	0.54	0.96	0.02	0.01	0.01	0.55								
• Progenitors		0.07%	0.68	0.51	0.50	0.87	0.41	0.26	0.28	0.76	0.25	0.15	0.15	0.75	0.91	0.84	0.98	0.93	0.06	0.03	0.03	0.48
• pDCs		0.04%	0.44	0.28	0.31	0.78	0.08	0.05	0.04	0.24	0.30	0.19	0.23	0.65	0.65	0.48	0.55	0.89				
Medians			0.93	0.87	0.93	0.98	0.87	0.77	0.85	0.96	0.70	0.55	0.62	0.90	0.91	0.83	0.92	0.96	0.65	0.50	0.55	0.90
Means			0.84	0.76	0.79	0.96	0.74	0.66	0.69	0.89	0.57	0.49	0.53	0.86	0.65	0.61	0.65	0.73	0.52	0.48	0.50	0.59

Columns		Rows	
Legend	• F1-score=overlap measured by harmonic mean of precision + recall (AKA <i>F measure</i>).	Coloring is based on ranking by <i>F1-score mean</i>	
	• JI 100%=whole population overlap measured by intersection/union (AKA <i>jaccard index</i>).	Narrow lead over next	
	• JI 80%=central core region overlap (AKA <i>central similarity</i>).	Wide lead over next	
	• JI 80% minus JI 100% size has <i>low</i> to high <i>emphasis</i> .	Ties get same ranked color....	
		Median minus mean size is <i>emphasized</i> pos/neg.	



Merged matches

With FlowSOM QFMatch finds 3 of 9 matches where merging multiple FlowSOM gated populations for 1 manually gated population obtains a higher F1-score: the 1st, 2nd and 5th ranked matches.

MATCH sets: training=9/14 (5 UNMATCHED!), test=13/14 (1 NEW!)

Rank	Subset (class) name	Matches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Training set?	Freq.
2	Neutrophils	4	99.7%	99.9%	99.8%	yes	76.7%
2	Neutrophils (FlowSOM.Leukocytes....	4	99.7%	99.9%	99.8%	no	1.8%
2	Neutrophils (FlowSOM.Leukocytes....	4	99.7%	99.9%	99.8%	no	0.4%
2	Neutrophils (FlowSOM.Leukocytes....	4	99.7%	99.9%	99.8%	no	74.3%
1	T cells	3	98.6%	97.6%	99.9%	yes	10.6%
1	T cells (FlowSOM.Leukocytes.Pop13)	3	98.6%	97.6%	99.9%	no	9.8%
1	T cells (FlowSOM.Leukocytes.Pop11)	3	98.6%	97.6%	99.9%	no	0.5%
5	Monocytes	3	97%	96.7%	98.4%	yes	6.9%
5	Monocytes (FlowSOM.Leukocytes....	3	97%	96.7%	98.4%	no	6.9%
5	Monocytes (FlowSOM.Leukocytes....	3	97%	96.7%	98.4%	no	0.4%
3	Basophils	2	97.1%	96.2%	99.4%	yes	0.3%
3	Basophils (FlowSOM.Leukocytes.P...	2	97.1%	96.2%	99.4%	no	0.3%

With PhenoGraph QFMatch finds 3 of 12 matches where merging multiple PhenoGraph gated populations for 1 manually gated population obtains a higher F1-score: the 1st, 5th and 6th ranked matches.

MATCH sets: training=12/14 (2 UNMATCHED!), test=21/24 (3 NEW!)

Rank	Subset (class) name	Matches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Training set?	Freq.
5	Neutrophils	8	98.5%	99.8%	98.7%	yes	76.7%
5	Neutrophils (PhenographQ1295)	8	98.5%	99.8%	98.7%	no	9.6%
5	Neutrophils (PhenographQ1294)	8	98.5%	99.8%	98.7%	no	10.1%
5	Neutrophils (PhenographQ1293)	8	98.5%	99.8%	98.7%	no	10.5%
5	Neutrophils (PhenographQ1298)	8	98.5%	99.8%	98.7%	no	8.2%
5	Neutrophils (PhenographQ1297)	8	98.5%	99.8%	98.7%	no	8.5%
5	Neutrophils (PhenographQ1291)	8	98.5%	99.8%	98.7%	no	14.5%
5	Neutrophils (PhenographQ1292)	8	98.5%	99.8%	98.7%	no	13.2%
1	T cells	4	98.6%	97.6%	99.9%	yes	10.6%
1	T cells (PhenographQ12914)	4	98.6%	97.6%	99.9%	no	1.2%
1	T cells (PhenographQ1296)	4	98.6%	97.6%	99.9%	no	8.7%
1	T cells (PhenographQ12915)	4	98.6%	97.6%	99.9%	no	0.6%
6	Monocytes	3	96.9%	96.6%	98.4%	yes	6.9%
6	Monocytes (PhenographQ12916)	3	96.9%	96.6%	98.4%	no	0.4%
6	Monocytes (PhenographQ1299)	3	96.9%	96.6%	98.4%	no	6.9%
2	NK cells	2	97.5%	97.8%	99.4%	yes	2%
2	NK cells (PhenographQ12910)	2	97.5%	97.8%	99.4%	no	2%

Boesch, M, Sykora, M, Gasteiger, S, Baty, F, Brutsche, MH, Sopper, S. **OMIP-077: Definition of all principal human leukocyte populations using a broadly applicable 14-color panel.** Cytometry. 2022; 101: 15– 20. <https://doi.org/10.1002/cyto.a.24481>

5.3.5.1. Special notes

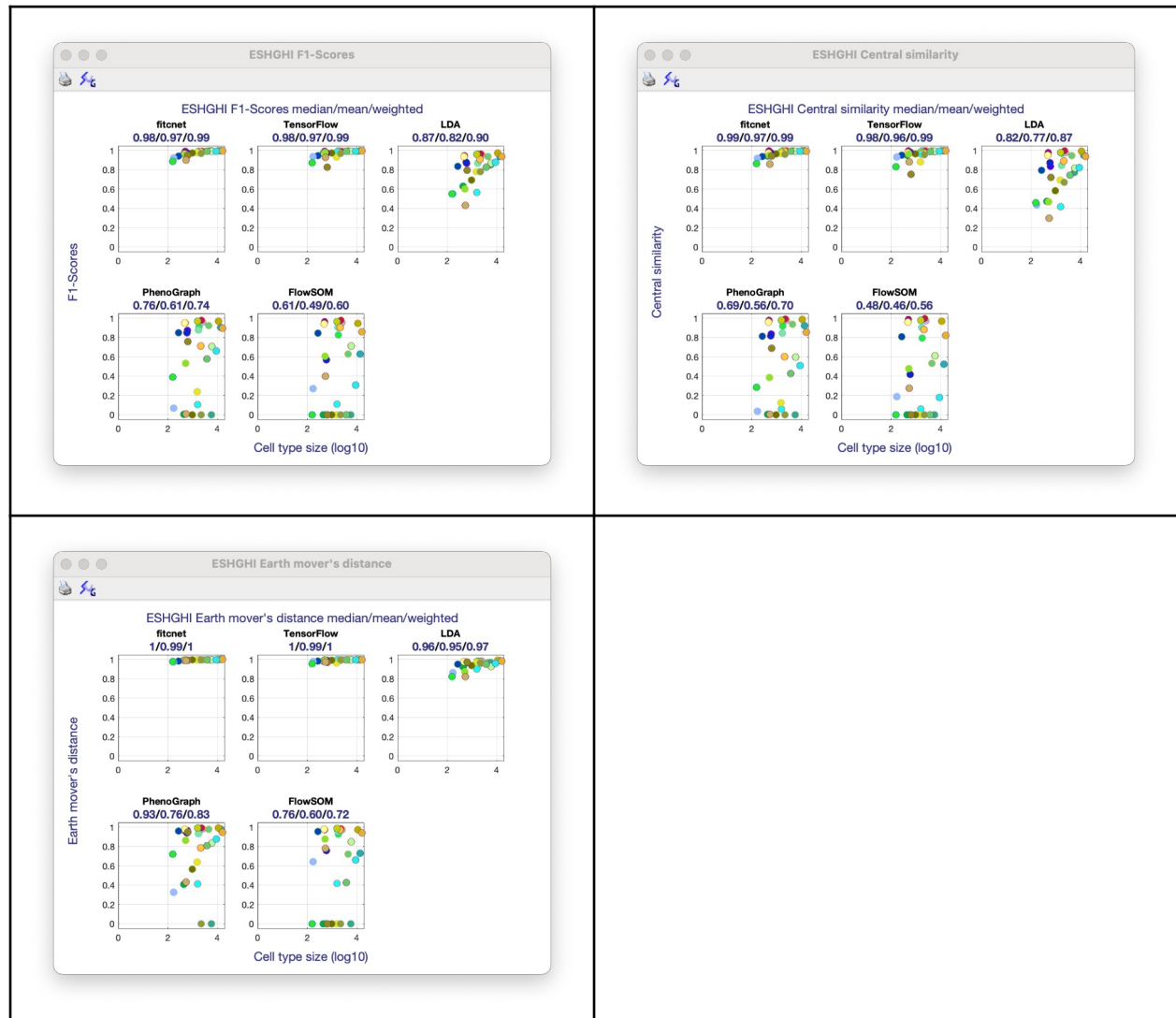
Our [population level results](#) in this dataset stand out because

1. PhenoGraph ranks 2nd ahead of LDA.
2. FlowSOM does surprisingly poorly when QFMatch does not merge manually gated populations to get a better F1-score. However when QFMatch is run to allow such merging the mean/median F1-scores go from 0.65/0.51 to **0.96/0.92** as shown in our [supplementary document](#). When examining [the details](#) of this we see:
 - a. One FlowSOM gated population matches with a 0.853 F1-score to **6** manually gated population. This 1-to-many match is not very helpful since the F1-Score is less than 0.9, the number of manual gates is greater than 3. However the population frequency is very low so 1 FlowSOM gate is representing 6 very small manually gated populations.
 - b. Another FlowSOM gated population matches with a .963 F1-score to 2 manually gated populations. This is a helpful 1-to-many match since the F1-Score is high, the population frequency is small and only 2 manually gated populations merge for the match.

Individual PhenoGraph gated populations also match 1-to-many manually gated populations for OMIP-077 improving its overall median/mean scoring. This is generally true for all datasets when QFMatch is allowed to merge multiple manually gated populations to get a better F1-score.

5.3.6. ESHGHI

Classifier		fitcnet				TensorFlow				LDA				PhenoGraph				FlowSOM			
Population	Freq- uency	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD
• CD4 N	15%	1	0.99	1	1	1	0.99	1	1	0.94	0.88	0.95	0.99	0.91	0.83	0.92	0.98	0.63	0.46	0.52	0.73
• CD16hi NK	12%	1	0.99	1	1	0.99	0.99	1	1	0.97	0.95	0.99	0.99	0.97	0.94	0.99	0.99	0.94	0.90	0.97	0.97
• CD8 N	4.8%	1	0.99	1	1	1	0.99	1	1	0.94	0.88	0.95	0.97	0.92	0.86	0.94	0.98	0.63	0.46	0.53	0.72
• CD14hi Mono	17%	1	0.99	0.99	1	1	0.99	1	1	0.94	0.88	0.94	0.98	0.90	0.81	0.85	0.95	0.86	0.75	0.82	0.94
• CD4 CM	6.2%	0.99	0.99	0.99	1	0.99	0.99	0.99	1	0.85	0.74	0.77	0.97								
• gd Tcells	1.9%	0.99	0.99	1	1	1	0.99	1	1	0.97	0.93	0.97	0.99	0.91	0.83	0.92	0.95	0.83	0.71	0.80	0.93
• CD8 Temra	6.3%	0.99	0.99	0.99	1	0.99	0.99	0.99	1	0.87	0.76	0.82	0.93	0.71	0.55	0.60	0.84	0.71	0.55	0.61	0.85
• CD4 EM	9.6%	0.99	0.99	0.99	1	0.99	0.99	0.99	1	0.88	0.78	0.82	0.96	0.66	0.49	0.51	0.88	0.31	0.18	0.18	0.66
• Naive B	2.7%	0.99	0.99	1	1	0.99	0.99	1	1	0.96	0.92	0.98	0.98	0.96	0.92	0.98	0.98	0.95	0.91	0.97	0.98
• Basophils	2.5%	0.99	0.99	1	1	0.99	0.99	1	1	0.96	0.93	1	0.96	0.98	0.96	0.99	0.99	0.98	0.96	1	0.99
• CD8 EM	4%	0.99	0.98	0.99	1	0.99	0.98	0.99	1	0.83	0.70	0.75	0.95	0.57	0.41	0.43	0.81				
• pDCs	0.54%	0.99	0.98	1	1	0.99	0.98	1	1	0.95	0.90	0.98	0.95	0.95	0.91	0.98	0.96	0.96	0.93	0.99	0.97
• CD8 MAIT	1.9%	0.99	0.98	0.99	1	0.99	0.98	0.99	1	0.87	0.76	0.85	0.92	0.88	0.78	0.85	0.93	0.91	0.83	0.90	0.96
• CD16hi Mono	2.3%	0.99	0.98	0.99	1	0.98	0.96	0.98	0.99	0.91	0.84	0.89	0.98	0.71	0.55	0.60	0.79	0.91	0.83	0.88	0.97
• Neutrophil	1.7%	0.98	0.97	0.99	1	0.98	0.96	0.98	0.99	0.96	0.93	0.98	0.98	0.97	0.94	0.98	0.99	0.97	0.93	0.98	0.99
• CD4 Temra	1.7%	0.98	0.96	0.97	1	0.98	0.96	0.96	1	0.56	0.39	0.42	0.90	0.10	0.05	0.06	0.41	0.11	0.06	0.06	0.42
• int Mono	1.6%	0.98	0.96	0.97	1	0.93	0.87	0.88	0.97	0.78	0.64	0.70	0.97	0.24	0.13	0.12	0.64				
• Trans B	0.67%	0.97	0.95	0.97	0.99	0.97	0.95	0.98	0.99	0.87	0.76	0.83	0.97	0.87	0.78	0.84	0.96				
• Treg	1%	0.97	0.95	0.96	1	0.97	0.95	0.96	0.99	0.69	0.53	0.57	0.94								
• HLADRIo Mono	2.4%	0.97	0.94	0.96	1	0.97	0.94	0.96	1	0.78	0.64	0.67	0.96								
• Mem B	0.64%	0.97	0.94	0.97	0.99	0.97	0.95	0.98	0.99	0.88	0.78	0.87	0.97	0.85	0.74	0.82	0.94	0.56	0.40	0.42	0.76
• CD8 CM	0.48%	0.97	0.93	0.94	0.99	0.97	0.94	0.95	0.99	0.63	0.46	0.47	0.92	< 0.01	< 0.01	< 0.01	0.41				
• Eosinophil	0.52%	0.96	0.93	0.97	0.99	0.97	0.94	0.98	0.98	0.94	0.88	0.95	0.98	0.95	0.90	0.96	0.98	0.94	0.89	0.96	0.98
• [CD14- CD16-]	0.56%	0.96	0.92	0.95	0.99	0.98	0.96	0.97	0.99	0.60	0.43	0.47	0.87	0.53	0.36	0.39	0.86	0.61	0.43	0.48	0.88
• CD56hi NK	0.70%	0.95	0.91	0.94	0.99	0.83	0.71	0.76	0.97	0.79	0.66	0.72	0.97	0.76	0.61	0.69	0.95				
• Plasmablast	0.28%	0.94	0.89	0.94	0.99	0.95	0.90	0.95	0.98	0.83	0.72	0.80	0.95	0.85	0.74	0.81	0.96	0.84	0.73	0.81	0.96
• IgD- CD27- B	0.18%	0.93	0.86	0.92	0.98	0.94	0.88	0.93	0.98	0.55	0.38	0.44	0.86	0.07	0.03	0.03	0.33	0.27	0.15	0.18	0.64
• Lineage Negative	0.57%	0.90	0.82	0.86	0.99	0.93	0.87	0.88	0.97	0.43	0.28	0.30	0.82	0.01	< 0.01	< 0.01	0.43	0.40	0.25	0.28	0.78
• [CD123-]	0.17%	0.89	0.80	0.86	0.98	0.87	0.78	0.83	0.96	0.55	0.38	0.46	0.82	0.39	0.24	0.28	0.72				
Medians		0.98	0.97	0.99	1	0.98	0.96	0.98	1	0.87	0.76	0.82	0.96	0.76	0.61	0.69	0.93	0.61	0.43	0.48	0.76
Means		0.97	0.95	0.97	0.99	0.97	0.94	0.96	0.99	0.82	0.71	0.77	0.95	0.61	0.53	0.56	0.76	0.49	0.42	0.46	0.60



5.3.6.1. Merged matches

With FlowSOM QFMatch finds 2 of 22 matches where merging multiple FlowSOM gated populations for 1 manually gated population obtains a higher F1-score: the 11th and 14th ranked matches.

MATCH sets: training=21/29 (8 UNMATCHED!), test=23/29 (6 NEW!)										
Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.	
11	●	10	gd Tcells	3	82.9%	79.6%	92.9%	yes	1.9%	
11	●	35	gd Tcells (FlowSOM.Residual.Pop2)	3	82.9%	79.6%	92.9%	no	0.8%	
11	●	48	gd Tcells (FlowSOM.Residual.Pop7)	3	82.9%	79.6%	92.9%	no	1.1%	
14	●	5	Lineage Negative	3	40%	27.6%	78.1%	yes	0.6%	
14	●	40	FlowSOM.Residual.Pop14	3	40%	27.6%	78.1%	no	0.1%	
14	●	51	Lineage Negative (FlowSOM.Residua...	3	40%	27.6%	78.1%	no	0.3%	
1	●	12	Neutrophil	2	96.5%	97.8%	98.7%	yes	1.7%	
1	●	38	Neutrophil (FlowSOM.Residual.Pop18)	2	96.5%	97.8%	98.7%	no	1.7%	

With PhenoGraph QFMatch finds 7 of 19 matches where merging multiple PhenoGraph gated populations for 1 manually gated population obtains a higher F1-score: the 1st, 4th, 6th, 7th, 16th, 17th and 18th ranked matches.

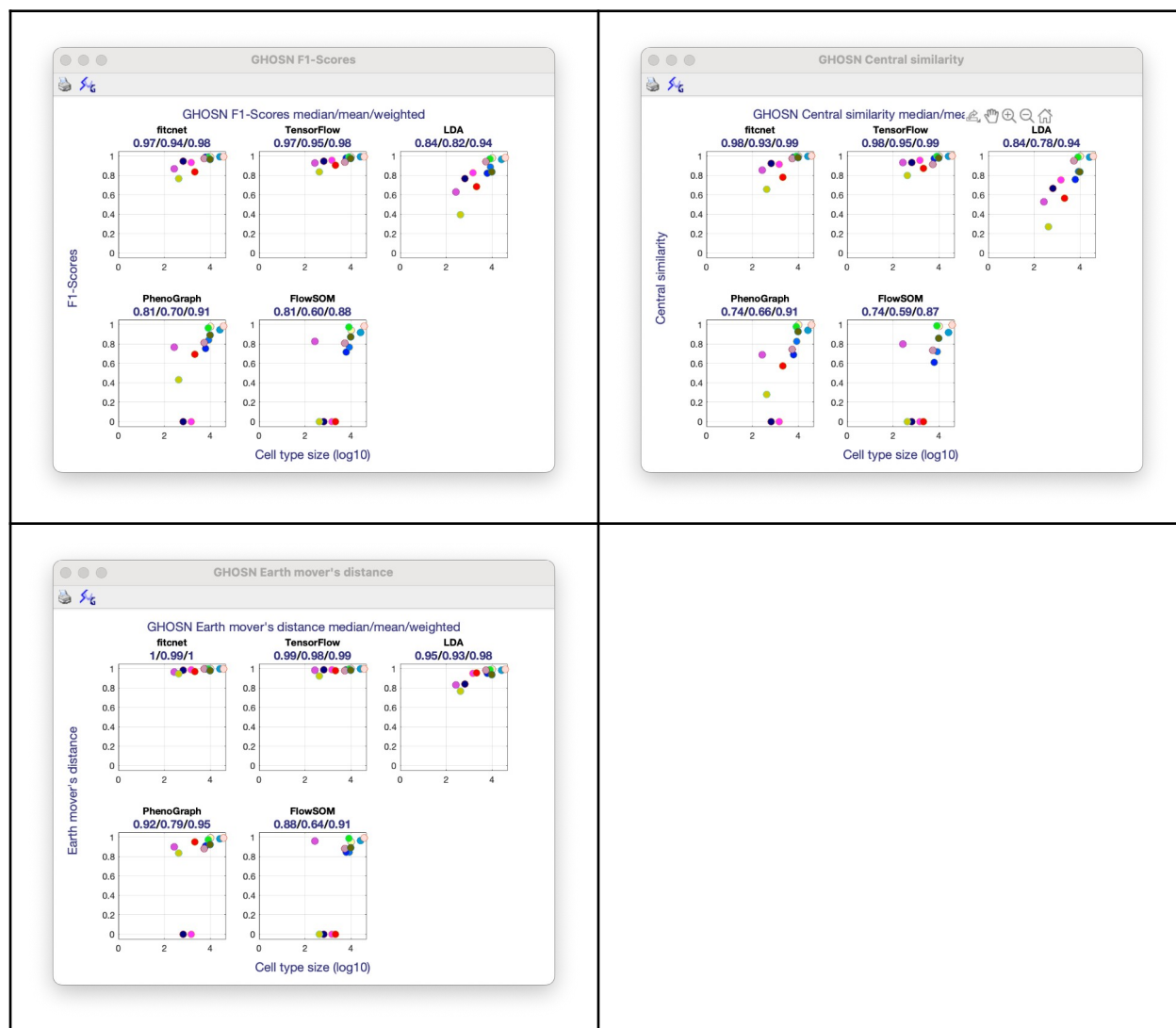
Sync
 QF
 F-M
 MATCH sets: training=27/29 (2 UNMATCHED!), test=36/50 (14 NEW!)

Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.
16		18	CD4 EM	5	65.9%	50.8%	87.6%	yes	9.6%
16		39	CD4 EM (PhenographYJ6F11)	5	65.9%	50.8%	87.6%	no	3.4%
16		48	CD4 EM (PhenographYJ6F5)	5	65.9%	50.8%	87.6%	no	5.1%
16		57	CD4 EM (PhenographYJ6F17)	5	65.9%	50.8%	87.6%	no	2.2%
16		64	CD4 EM (PhenographYJ6F4)	5	65.9%	50.8%	87.6%	no	6.8%
1		29	CD16hi NK	3	96.8%	98.9%	99.3%	yes	12%
1		44	CD16hi NK (PhenographYJ6F3)	3	96.8%	98.9%	99.3%	no	7.9%
1		68	CD16hi NK (PhenographYJ6F10)	3	96.8%	98.9%	99.3%	no	3.5%
4		4	Naive B	3	95.9%	97.9%	98.3%	yes	2.7%
4		54	Naive B (PhenographYJ6F13)	3	95.9%	97.9%	98.3%	no	2.5%
4		70	Naive B (PhenographYJ6F41)	3	95.9%	97.9%	98.3%	no	0.1%
6		20	CD4 N	3	90.7%	92.4%	97.9%	yes	14.6%
6		30	CD4 N (PhenographYJ6F8)	3	90.7%	92.4%	97.9%	no	4.3%
6		46	CD4 N (PhenographYJ6F2)	3	90.7%	92.4%	97.9%	no	9.5%
7		28	Eosinophil	3	95%	96.1%	97.7%	yes	0.5%
7		33	Eosinophil (PhenographYJ6F27)	3	95%	96.1%	97.7%	no	0.5%
7		38	Eosinophil (PhenographYJ6F49)	3	95%	96.1%	97.7%	no	0%
17		7	[CD14- CD16-]	3	53%	38.6%	86.2%	yes	0.6%
17		52	[CD14- CD16-] (PhenographYJ6F45)	3	53%	38.6%	86.2%	no	0%
17		55	[CD14- CD16-] (PhenographYJ6F20)	3	53%	38.6%	86.2%	no	1.3%
18		14	CD8 Temra	3	70.6%	59.8%	83.8%	yes	6.3%
18		45	CD8 Temra (PhenographYJ6F14)	3	70.6%	59.8%	83.8%	no	2.5%
18		53	CD8 Temra (PhenographYJ6F12)	3	70.6%	59.8%	83.8%	no	2.8%
2		12	Neutrophil	2	97%	98%	99.1%	yes	1.7%
2		41	Neutrophil (PhenographYJ6F19)	2	97%	98%	99.1%	no	1.7%

Toghi Eshghi S, Au-Yeung A, Takahashi C, Bolen CR, Nyachienga MN, Lear SP, Green C, Mathews WR and O'Gorman WE (2019) **Quantitative Comparison of Conventional and t-SNE-guided Gating Analyses**. Front. Immunol. 10:1194. doi: 10.3389/fimmu.2019.01194.
<https://www.frontiersin.org/articles/10.3389/fimmu.2019.01194/full>

5.3.7. GHOSN

Classifier		fitcnet				TensorFlow				LDA				PhenoGraph				FlowSOM			
Population	Freq- uency	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD
• B-1	22%	0.99	0.99	1	1	0.99	0.99	1	1	0.97	0.93	0.99	0.98	0.95	0.90	0.94	0.99	0.92	0.85	0.92	0.96
• Large macrophages	32%	0.99	0.99	1	1	0.99	0.98	1	1	0.98	0.97	1	0.99	0.98	0.97	1	0.99	0.98	0.96	1	0.99
• B-2 IgM medium	7.2%	0.99	0.98	0.99	1	0.99	0.98	0.99	1	0.89	0.79	0.84	0.95	0.84	0.73	0.83	0.93	0.77	0.62	0.72	0.85
• Eosinophils	8.6%	0.99	0.98	1	1	0.99	0.97	1	1	0.98	0.96	1	0.99	0.98	0.96	1	0.99	0.94	0.89	0.99	0.95
• B-2 IgM high	5.3%	0.99	0.97	0.99	1	0.98	0.96	0.98	0.99	0.82	0.70	0.76	0.95	0.75	0.60	0.69	0.91	0.71	0.56	0.61	0.84
• T cells	6.9%	0.98	0.97	1	1	0.99	0.97	1	0.99	0.97	0.94	0.99	0.99	0.96	0.93	0.98	0.98	0.97	0.95	0.99	0.99
• Small macrophages	4.6%	0.97	0.95	0.98	1	0.94	0.88	0.91	0.98	0.94	0.89	0.95	0.99	0.81	0.69	0.74	0.88	0.81	0.68	0.74	0.88
• NK, NKT	8.3%	0.97	0.93	0.98	0.98	0.97	0.95	0.98	0.98	0.84	0.72	0.84	0.94	0.89	0.80	0.93	0.92	0.87	0.77	0.86	0.89
• Developing B	0.55%	0.95	0.90	0.92	0.98	0.95	0.90	0.93	0.99	0.77	0.62	0.66	0.84								
• CD11b+ dendritic	1.3%	0.93	0.87	0.91	0.99	0.95	0.91	0.96	0.99	0.83	0.70	0.75	0.95								
• CD11b- dendritic	0.23%	0.87	0.77	0.85	0.96	0.93	0.87	0.93	0.98	0.63	0.46	0.53	0.83	0.77	0.62	0.69	0.90	0.83	0.71	0.80	0.96
• ckit+ mast cells	1.8%	0.84	0.72	0.78	0.97	0.90	0.82	0.87	0.98	0.68	0.52	0.56	0.96	0.69	0.53	0.56	0.95				
• Neutrophils	0.36%	0.77	0.62	0.66	0.94	0.84	0.72	0.80	0.92	0.39	0.25	0.27	0.77	0.43	0.28	0.28	0.83				
Medians		0.97	0.95	0.98	1	0.97	0.95	0.98	0.99	0.84	0.72	0.84	0.95	0.81	0.69	0.74	0.92	0.81	0.68	0.74	0.88
Means		0.94	0.90	0.93	0.99	0.95	0.92	0.95	0.98	0.82	0.73	0.78	0.93	0.70	0.62	0.66	0.79	0.60	0.54	0.59	0.64



5.3.7.1. Merged matches

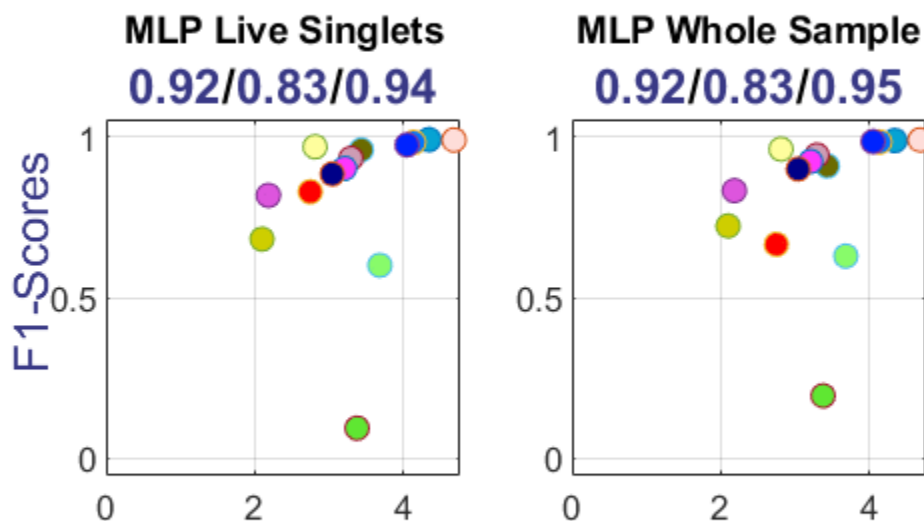
With PhenoGraph QFMatch finds 4 of 12 matches where merging multiple PhenoGraph gated populations for 1 manually gated population obtains a higher F1-score: the 1st, 3rd, 7th and 8th ranked matches.

MATCH sets: training=12/13 (1 UNMATCHED), test=21/22 (1 NEW)									
Rank	#	Subset (class) name	Matches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Training set?	Freq.	
1	13	B-1	6	96.3%	97.1%	99.3%	yes	22.1%	
1	14	Phenograph29FL8	6	96.3%	97.1%	99.3%	no	6.9%	
1	19	Phenograph29FL13	6	96.3%	97.1%	99.3%	no	3.9%	
1	20	Phenograph29FL21	6	96.3%	97.1%	99.3%	no	0.3%	
1	28	Phenograph29FL1	6	96.3%	97.1%	99.3%	no	9.9%	
1	32	Phenograph29FL22	6	96.3%	97.1%	99.3%	no	0.1%	
3	1	Large macrophages	5	98.2%	99.9%	99.2%	yes	31.9%	
3	17	Phenograph29FL6	5	98.2%	99.9%	99.2%	no	7.3%	
3	25	Phenograph29FL4	5	98.2%	99.9%	99.2%	no	7.8%	
3	27	Phenograph29FL3	5	98.2%	99.9%	99.2%	no	8.6%	
3	30	Phenograph29FL5	5	98.2%	99.9%	99.2%	no	7.7%	
7	9	NK, NKT	3	86.7%	88.6%	91.4%	yes	9%	
7	26	Phenograph29FL11	3	86.7%	88.6%	91.4%	no	4.7%	
7	34	Phenograph29FL15	3	86.7%	88.6%	91.4%	no	2.3%	
8	2	B-2 IgM high	3	77.7%	68.1%	91.1%	yes	5.1%	
8	15	Phenograph29FL16	3	77.7%	68.1%	91.1%	no	2.2%	
8	18	Phenograph29FL12	3	77.7%	68.1%	91.1%	no	4.5%	
2	8	Eosinophils	2	97.9%	99.7%	99.3%	yes	9.5%	
2	33	Phenograph29FL2	2	97.9%	99.7%	99.3%	no	9.3%	

5.3.7.2. Whole sample gating

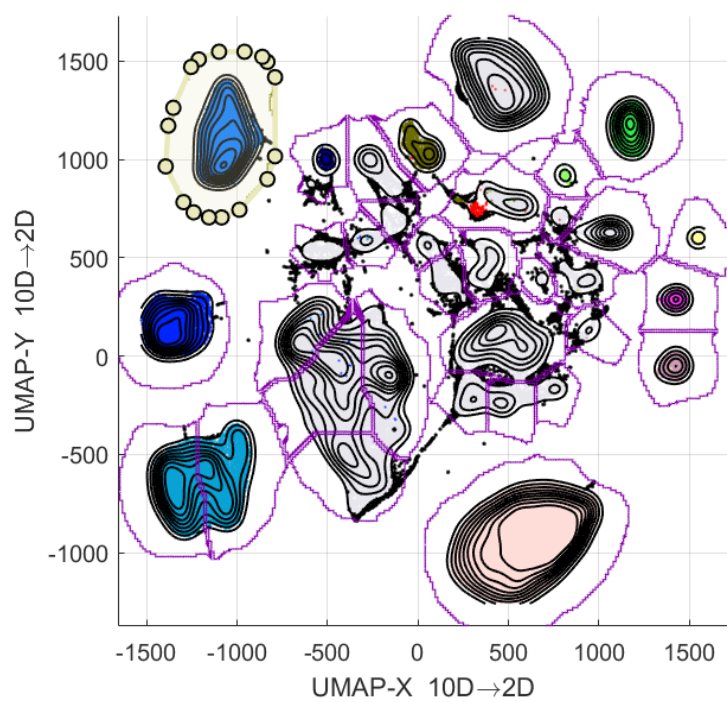
MLP runs as effectively on the whole sample as it does starting at the live singlets branch gate. For example if using the BALB/c mouse strain sample we train MLP on all live singlets versus all cells and then predict on the C57 mouse strain (all_3-2.fcs) we get the following F1-Scores

C57 F1-Scores median/mean/weighted

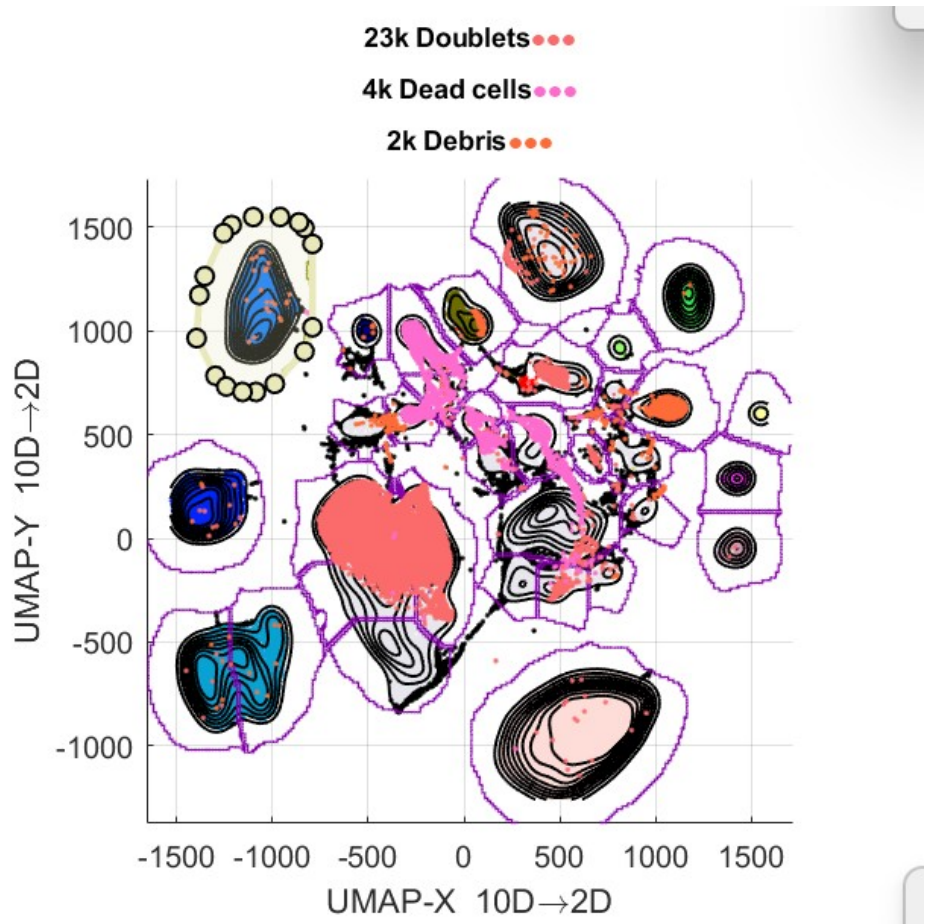


Cell type size (log10)

Supervising UMAP with predictions on the whole C57 sample produces this view



Highlighting manual gates for doublets, dead cells and debris locates most of them in the uncolored clusters



Overlap matrix

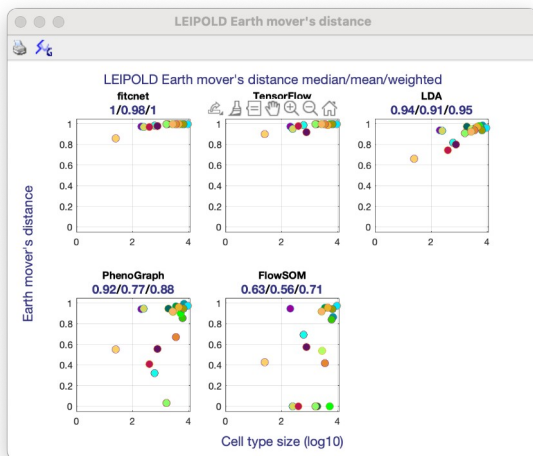
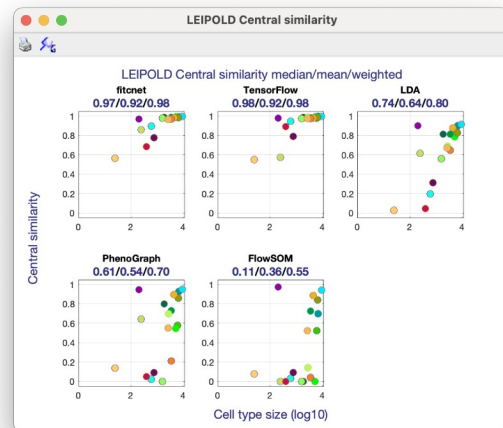
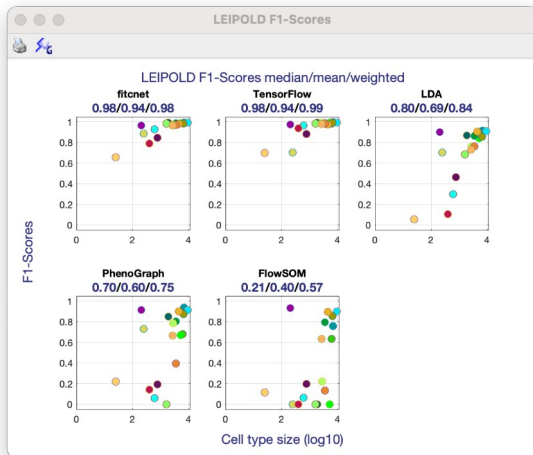
Test set ↓	Training set →		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	Not matched
		events	Doublets	NK, NKT	T cells	CD11b- dendritic	ckit+ mast cells	Small macrophages	Large macrophages	CD11b+ dendritic	Eosinophils	Dead	B-1	B-2 IgM high	B-2 IgM medium	Developing B	Debris	Neutrophils	
1	CD11b+ dendritic	1,500	26,496	9,753	7,513	270	2,552	6,098	40,728	1,489	10,144	5,375	27,815	6,282	8,467	616	34,659	420	114
2	NK, NKT	9,817	6	9,576		2	32												201
3	B-1	28,026	3									2	27,707		13	7			294
4	Eosinophils	10,184	4								10,077	1							102
5	Neutrophils	387																370	17
6	Large macrophages	37,485							37,293			1							191
7	B-2 IgM high	6,351	6									2		6,198	1				144
8	Developing B	628													3	576			49
9	ckit+ mast cells	2,534	1	35			2,370												128
10	CD11b- dendritic	285		1		246													38
11	B-2 IgM medium	8,495											4		8,359	3			129
12	T cells	7,623			7,443		32					1							147
13	Small macrophages	6,081	1					5,912		2								3	163
	Not matched		26,475	141	70	22	118	186	3,435	101	67	5,368	104	84	91	30	34,659	47	

Eliver Eid Bou Ghosn, Alexandra A. Cassado, Gregory R. Govoni, +6, and Leonore A. Herzenberg (2010), **Two physically, functionally, and developmentally distinct**

peritoneal macrophage subsets, PNAS Vol. 107|No. 6 2568-2573, January 25, 2010
<https://doi.org/10.1073/pnas.0915000107>

5.3.8. LEIPOLD

Classifier	Population	Frequency	fitcnet				TensorFlow				LDA				PhenoGraph				FlowSOM			
			F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD
• CD4 T cells CD45RA ⁻ , CD27 ⁺		12%	0.99	0.99	0.99	1	1	0.99	1	1	0.92	0.85	0.90	0.98	0.94	0.88	0.93	0.99	0.76	0.61	0.70	0.86
• CD4 T cells CD45RA ⁺ , CD27 ⁺		16%	0.99	0.99	1	1	0.99	0.99	1	1	0.91	0.83	0.92	0.96	0.92	0.85	0.95	0.97	0.90	0.82	0.94	0.97
• CD4 T cells CD45RA ⁻ , CD27 ⁻		3.4%	0.99	0.98	0.99	1	0.99	0.98	0.99	1	0.87	0.76	0.81	0.97	0.85	0.74	0.80	0.95				
• CD8 T cells CD45RA ⁺ , CD27 ⁺		11%	0.99	0.98	0.99	1	0.98	0.97	0.98	1	0.86	0.76	0.84	0.96	0.68	0.52	0.57	0.85	0.63	0.46	0.52	0.84
• CD8 T cells CD45RA ⁺ , CD27 ⁻		9.1%	0.99	0.98	0.99	1	0.99	0.98	0.99	1	0.84	0.72	0.78	0.98	0.67	0.51	0.55	0.90				
• CD8 T cells CD45RA ⁻ , CD27 ⁺		6.3%	0.99	0.98	0.99	1	0.99	0.98	0.98	1	0.86	0.76	0.81	0.96	0.80	0.67	0.73	0.97	0.79	0.66	0.72	0.96
• CD8 T cells CD45RA ⁻ , CD27 ⁻		2.8%	0.99	0.97	0.98	1	0.98	0.97	0.97	1	0.68	0.52	0.56	0.91								
• NK cells		12%	0.98	0.97	0.98	1	0.99	0.98	0.99	1	0.86	0.75	0.83	0.94	0.87	0.77	0.86	0.95	0.85	0.74	0.84	0.94
• CD16 ⁺ monocytes		7.9%	0.98	0.96	0.99	1	0.98	0.95	0.98	0.99	0.90	0.82	0.88	0.97	0.90	0.82	0.90	0.96	0.89	0.81	0.89	0.96
• CD4 ⁺ CD8 ⁻		5%	0.98	0.95	0.97	1	0.99	0.98	0.99	1	0.76	0.61	0.69	0.95	0.79	0.65	0.70	0.92	0.22	0.12	0.14	0.54
• CD38 CD56 ⁺ B cells		6.2%	0.97	0.94	0.97	1	0.98	0.96	0.98	1	0.76	0.62	0.65	0.94	0.39	0.24	0.21	0.67	0.13	0.07	0.04	0.42
• CD38+CD56 B cells		4.7%	0.97	0.93	0.96	1	0.98	0.96	0.97	1	0.73	0.57	0.67	0.92	0.66	0.50	0.55	0.92	0.63	0.46	0.52	0.92
• pDCs		0.37%	0.97	0.93	0.97	0.98	0.97	0.95	0.98	0.98	0.90	0.82	0.90	0.94	0.92	0.84	0.95	0.94	0.93	0.87	0.97	0.95
• CD4 T cells CD45RA ⁺ , CD27 ⁻		1.1%	0.93	0.87	0.90	0.99	0.97	0.93	0.95	0.99	0.30	0.18	0.20	0.82	0.06	0.03	0.02	0.32	0.06	0.03	0.03	0.69
• CD56 bright NK cells		0.44%	0.89	0.80	0.86	0.97	0.70	0.54	0.56	0.95	0.70	0.54	0.62	0.93	0.73	0.56	0.64	0.95				
• mDCs		1.4%	0.85	0.73	0.78	0.98	0.88	0.79	0.79	0.92	0.47	0.30	0.31	0.80	0.19	0.11	0.09	0.55	0.20	0.11	0.09	0.56
• Basophils		0.69%	0.79	0.65	0.68	0.97	0.94	0.88	0.89	0.98	0.11	0.06	0.05	0.75	0.14	0.08	0.05	0.41				
• CD16 ⁺ monocytes		0.04%	0.65	0.49	0.56	0.86	0.70	0.54	0.55	0.90	0.05	0.03	0.03	0.66	0.22	0.12	0.14	0.55	0.12	0.06	0.08	0.43
Medians			0.98	0.96	0.97	1	0.98	0.97	0.98	1	0.80	0.67	0.74	0.94	0.70	0.54	0.61	0.92	0.21	0.12	0.11	0.63
Means			0.94	0.89	0.92	0.98	0.94	0.91	0.92	0.98	0.69	0.57	0.64	0.91	0.60	0.49	0.54	0.77	0.40	0.32	0.36	0.56



Merged matches

With FlowSOM QFMatch finds 4 of 13 matches where merging 2 FlowSOM gated populations for 1 manually gated population obtains a higher F1-score: the 1st, 3rd, 7th and 10th ranked matches.

MATCH sets: training=13/18 (5 UNMATCHED!), test=17/18 (1 NEW!)									
Rank		#	Subset (class) name	Mat-ches	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.
1		15	CD4 T cells CD45RA+ , CD27+	3	90.2%	94.4%	97.2%	yes	16.9%
1		24	CD4 T cells CD45RA+ , CD27+ (Flo...	3	90.2%	94.4%	97.2%	no	0.9%
1		27	CD4 T cells CD45RA+ , CD27+ (Flo...	3	90.2%	94.4%	97.2%	no	15%
3		1	CD16- monocytes	3	89.4%	88.8%	95.6%	yes	6.1%
3		28	CD16- monocytes (FlowSOM.All cell...	3	89.4%	88.8%	95.6%	no	6.2%
3		31	CD16- monocytes (FlowSOM.All cell...	3	89.4%	88.8%	95.6%	no	0.5%
7		12	CD4 T cells CD45RA- , CD27+	3	75.9%	70%	86.3%	yes	14.8%
7		23	CD4 T cells CD45RA- , CD27+ (Flow...	3	75.9%	70%	86.3%	no	20.5%
7		29	Basophils (FlowSOM.All cells.Pop12)	3	75.9%	70%	86.3%	no	1.1%
10		2	mDCs	3	19.7%	8.9%	57.2%	yes	0.9%
10		22	mDCs (FlowSOM.All cells.Pop2)	3	19.7%	8.9%	57.2%	no	0.3%
10		26	mDCs (FlowSOM.All cells.Pop9)	3	19.7%	8.9%	57.2%	no	2.8%
2		5	CD8 T cells CD45RA- , CD27+	2	79.4%	72.4%	95.7%	yes	6.9%
2		35	CD8 T cells CD45RA- , CD27+ (Flow...	2	79.4%	72.4%	95.7%	no	7.8%

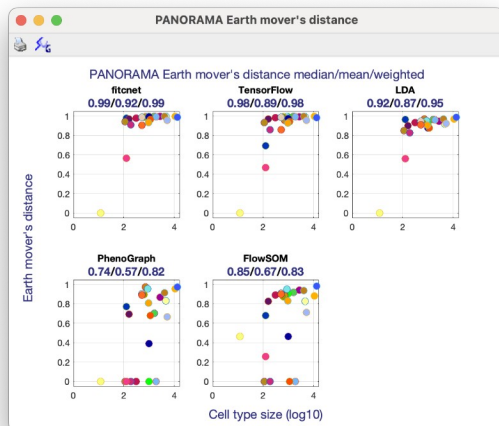
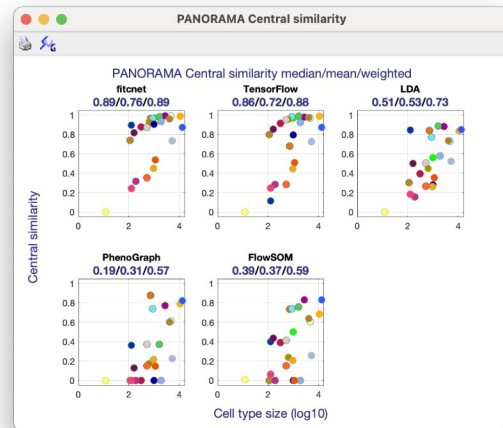
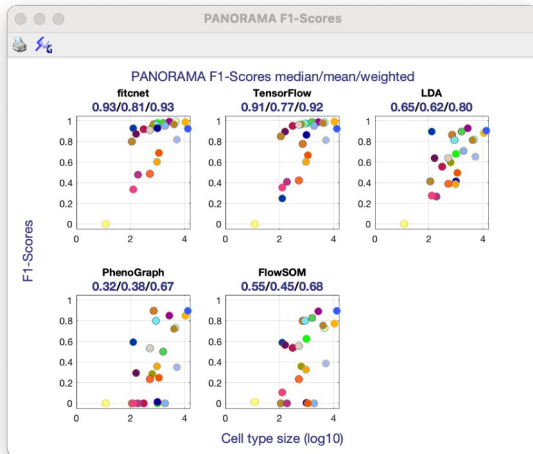
With PhenoGraph QFMatch finds 6 of ? matches where merging multiple PhenoGraph gated populations for 1 manually gated population obtains a higher F1-score: the ?, ? and ?th ranked matches.

Sync MATCH sets: training=17/18 (1 UNMATCHED!), test=25/27 (2 NEW!)										
Rank ²		#	Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.	
2	●	15	CD4 T cells CD45RA+ , CD27+	4	91.6%	94.9%	97.5%	yes	16.9%	1
2	●	19	CD4 T cells CD45RA+ , CD27+ (Phe...	4	91.6%	94.9%	97.5%	no	1.2%	
2	●	30	CD4 T cells CD45RA+ , CD27+ (Phe...	4	91.6%	94.9%	97.5%	no	13.5%	1
2	●	39	CD4 T cells CD45RA+ , CD27+ (Phe...	4	91.6%	94.9%	97.5%	no	0.5%	
10	●	18	CD4- CD8-	4	78.6%	69.7%	91.5%	yes	3.1%	
10	●	22	CD4- CD8- (Phenograph4RXF23)	4	78.6%	69.7%	91.5%	no	0.2%	
10	●	26	CD4- CD8- (Phenograph4RXF14)	4	78.6%	69.7%	91.5%	no	1.3%	
10	●	33	CD4- CD8- (Phenograph4RXF12)	4	78.6%	69.7%	91.5%	no	1.8%	
1	●	12	CD4 T cells CD45RA- , CD27+	3	93.9%	92.9%	99.1%	yes	14.8%	1
1	●	34	CD4 T cells CD45RA- , CD27+ (Phen...	3	93.9%	92.9%	99.1%	no	1.2%	
1	●	41	CD4 T cells CD45RA- , CD27+ (Phen...	3	93.9%	92.9%	99.1%	no	12.7%	1
4	●	1	CD16- monocytes	3	90%	89.6%	96.1%	yes	6.1%	
4	●	24	CD16- monocytes (Phenograph4RXF...	3	90%	89.6%	96.1%	no	0.5%	
4	●	37	CD16- monocytes (Phenograph4RXF8)	3	90%	89.6%	96.1%	no	6.1%	
11	●	13	CD8 T cells CD45RA+ , CD27-	3	67.1%	54.8%	90.2%	yes	9.8%	
11	●	32	CD8 T cells CD45RA+ , CD27- (Phen...	3	67.1%	54.8%	90.2%	no	2.5%	
11	●	44	CD8 T cells CD45RA+ , CD27- (Phen...	3	67.1%	54.8%	90.2%	no	13.6%	1
14	●	2	mDCs	3	19.4%	9.1%	55.5%	yes	0.9%	
14	●	21	mDCs (Phenograph4RXF24)	3	19.4%	9.1%	55.5%	no	0.2%	
14	●	45	mDCs (Phenograph4RXF10)	3	19.4%	9.1%	55.5%	no	2.8%	
3	●	5	CD8 T cells CD45RA- , CD27+	2	80.4%	73.1%	96.8%	yes	6.9%	
3	●	42	CD8 T cells CD45RA- , CD27+ (Phen...	2	80.4%	73.1%	96.8%	no	7.5%	

Michael D. Leipold, Gerlinde Obermoser, Craig Fenwick, Katja Kleinstuber, Narges Rashidi, John P. McNevin, Allison N. Nau, Lisa E. Wagar, Virginie Rozot, Mark M. Davis, Stephen DeRosa, Giuseppe Pantaleo, Thomas J. Scriba, Bruce D. Walker, Lars R. Olsen, Holden T. Maecker, (2018) **Comparison of CyTOF assays across sites: Results of a six-center pilot study**, Journal of Immunological Methods, Volume 453, Pages 37-43, ISSN 0022-1759, <https://www.sciencedirect.com/science/article/pii/S0022175917304908>

5.3.9. PANORAMA

Population	Classifier	fitcnet				TensorFlow				LDA				PhenoGraph				FlowSOM			
	Frequency	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD
• Eosinophils	8.8%	0.99	0.98	0.99	1	0.98	0.97	0.97	0.99	0.82	0.69	0.73	0.92	0.73	0.57	0.61	0.83	0.73	0.56	0.61	0.83
• pDCs	5.2%	0.99	0.98	0.99	1	0.99	0.97	0.98	0.99	0.93	0.86	0.88	0.95	0.85	0.74	0.77	0.87	0.89	0.80	0.83	0.94
• Classical Monocytes	21%	0.99	0.98	0.99	1	0.99	0.98	0.99	1	0.88	0.79	0.83	0.97	0.85	0.74	0.79	0.95	0.77	0.63	0.68	0.88
• CD8 T cells	3%	0.98	0.96	0.98	1	0.99	0.97	0.99	1	0.90	0.81	0.88	0.97	0.50	0.33	0.37	0.70	0.83	0.70	0.76	0.92
• NKT cells	1.9%	0.98	0.96	0.97	1	0.98	0.95	0.97	0.99	0.68	0.51	0.56	0.92					0.62	0.45	0.50	0.90
• Intermediate Monocytes	7.7%	0.97	0.94	0.96	1	0.98	0.96	0.97	1	0.81	0.68	0.73	0.97	0.72	0.56	0.60	0.91	0.75	0.60	0.64	0.94
• Non classical Monocytes	1.4%	0.96	0.93	0.96	0.99	0.78	0.64	0.68	0.96	0.86	0.76	0.84	0.97	0.90	0.81	0.88	0.98	0.80	0.67	0.73	0.88
• CD4 T cells	1.6%	0.96	0.92	0.97	0.99	0.97	0.95	0.98	0.99	0.81	0.68	0.77	0.95	0.80	0.67	0.74	0.96	0.80	0.67	0.74	0.95
• B cells Frac. D	3.7%	0.95	0.90	0.93	0.99	0.95	0.91	0.92	0.99	0.71	0.55	0.57	0.96								
• NK cells	1.2%	0.94	0.89	0.93	0.99	0.97	0.93	0.96	0.99	0.59	0.42	0.45	0.93	0.28	0.17	0.17	0.90	0.36	0.22	0.24	0.87
• B cells Frac A-C	1.9%	0.93	0.87	0.91	0.99	0.86	0.76	0.79	0.97	0.41	0.26	0.28	0.88								
• Plasma Cells	0.24%	0.93	0.86	0.90	0.98	0.25	0.14	0.11	0.69	0.90	0.81	0.85	0.97	0.59	0.42	0.36	0.77	0.59	0.41	0.40	0.68
• B cells Frac. F	25%	0.92	0.86	0.87	0.99	0.92	0.86	0.87	0.98	0.91	0.83	0.85	0.99	0.89	0.81	0.82	0.97	0.90	0.81	0.83	0.98
• Basophils	0.57%	0.92	0.85	0.88	0.98	0.95	0.90	0.91	0.98	0.55	0.38	0.39	0.93					0.54	0.37	0.39	0.89
• Macrophages	1%	0.91	0.84	0.88	0.99	0.96	0.93	0.95	0.99	0.64	0.47	0.50	0.94	0.53	0.36	0.37	0.91	0.56	0.38	0.41	0.91
• mDCs	0.30%	0.87	0.77	0.82	0.97	0.90	0.81	0.85	0.97	0.64	0.47	0.50	0.90	0.28	0.17	0.13	0.69	0.56	0.39	0.44	0.83
• B cells Frac. E	9.8%	0.82	0.69	0.74	0.95	0.81	0.69	0.73	0.95	0.65	0.49	0.52	0.92	0.35	0.21	0.22	0.67	0.38	0.24	0.25	0.71
• gd T cells	0.21%	0.80	0.67	0.74	0.94	0.85	0.74	0.80	0.93	0.41	0.26	0.30	0.85								
• GMP	2.1%	0.69	0.53	0.54	0.97	0.66	0.50	0.51	0.94	0.50	0.33	0.35	0.88	0.25	0.14	0.14	0.68				
• MEP	1.8%	0.60	0.43	0.45	0.93	0.60	0.43	0.45	0.93	0.39	0.24	0.26	0.91	0.36	0.22	0.22	0.81	0.33	0.20	0.21	0.83
• CMP	1%	0.49	0.32	0.35	0.90	0.42	0.27	0.28	0.86	0.39	0.24	0.27	0.91	0.24	0.13	0.15	0.89	0.23	0.13	0.15	0.90
• MPP	0.35%	0.47	0.31	0.32	0.91	0.41	0.26	0.28	0.86	0.26	0.15	0.16	0.83								
• CLP	0.24%	0.34	0.20	0.24	0.56	0.35	0.21	0.25	0.47	0.27	0.16	0.18	0.56					0.10	0.05	0.06	0.26
• HSC	0.02%																	0.01	0.01	0.01	0.46
Medians		0.93	0.86	0.89	0.99	0.91	0.84	0.86	0.98	0.65	0.48	0.51	0.92	0.32	0.19	0.19	0.74	0.55	0.38	0.39	0.85
Means		0.81	0.74	0.76	0.92	0.77	0.70	0.72	0.89	0.62	0.49	0.53	0.87	0.38	0.28	0.31	0.57	0.45	0.35	0.37	0.67



Merged matches

With FlowSOM QFMatch finds 4 of 11 matches where merging multiple FlowSOM gated populations for 1 manually gated population obtains a higher F1-score: the 3rd, 7th, 8th and 11th ranked matches.

MATCH sets: training=20/24 (4 UNMATCHED!), test=all 24 matched!									
Rank ²		#	Subset (class) name	Mat-ches ¹	% Overlap (F-measure)	% Inlier Concordance	Similarity (QFMatch)	Train-ing set?	Freq.
3	●	8	pDCs	3	89.1%	83.2%	94.2%	yes	5.9%
3	●	33	pDCs (FlowSOM.non-Neutrophils.Pop...)	3	89.1%	83.2%	94.2%	no	1.5%
3	●	43	pDCs (FlowSOM.non-Neutrophils.Pop...)	3	89.1%	83.2%	94.2%	no	2.4%
7	●	10	NKT cells	3	62.5%	49.8%	90.4%	yes	2.3%
7	●	26	NKT cells (FlowSOM.non-Neutrophils...)	3	62.5%	49.8%	90.4%	no	1.6%
7	●	39	NKT cells (FlowSOM.non-Neutrophils...)	3	62.5%	49.8%	90.4%	no	0.8%
8	●	9	CMP	3	23.2%	14.9%	89.9%	yes	1%
8	●	30	CMP (FlowSOM.non-Neutrophils.Pop...)	3	23.2%	14.9%	89.9%	no	3.6%
8	●	41	CMP (FlowSOM.non-Neutrophils.Pop...)	3	23.2%	14.9%	89.9%	no	1.2%
11	●	3	Classical Monocytes	3	77.3%	68.3%	88.2%	yes	28.8%
11	●	35	Classical Monocytes (FlowSOM.non-...)	3	77.3%	68.3%	88.2%	no	29.5%
11	●	48	FlowSOM.non-Neutrophils.Pop8	3	77.3%	68.3%	88.2%	no	0.5%
1	●	13	B cells Frac. F	2	89.5%	82.9%	98.4%	yes	19.7%
1	●	44	B cells Frac. F (FlowSOM.non-Neutr...)	2	89.5%	82.9%	98.4%	no	16.4%

5.3.10. Special notes on PANORAMA

This is MLP's 2nd lowest scoring result. When training a model using auto-tuned fitcnet however the mean F1-score is 0.05 higher which is not reported in the table.

When adopting MLP for real research practices we recommend trying all 3 types of training (fitcnet, fitcnet-optimized and TensorFlow) for each assay.

The small HSC population was never found with any MLP configuration and only FlowSOM finds a little of it.

Samusik, N., Good, Z., Spitzer, M. et al. **Automated mapping of phenotype space with single-cell data**. Nat Methods 13, 493–496 (2016).

<https://doi.org/10.1038/nmeth.3863>

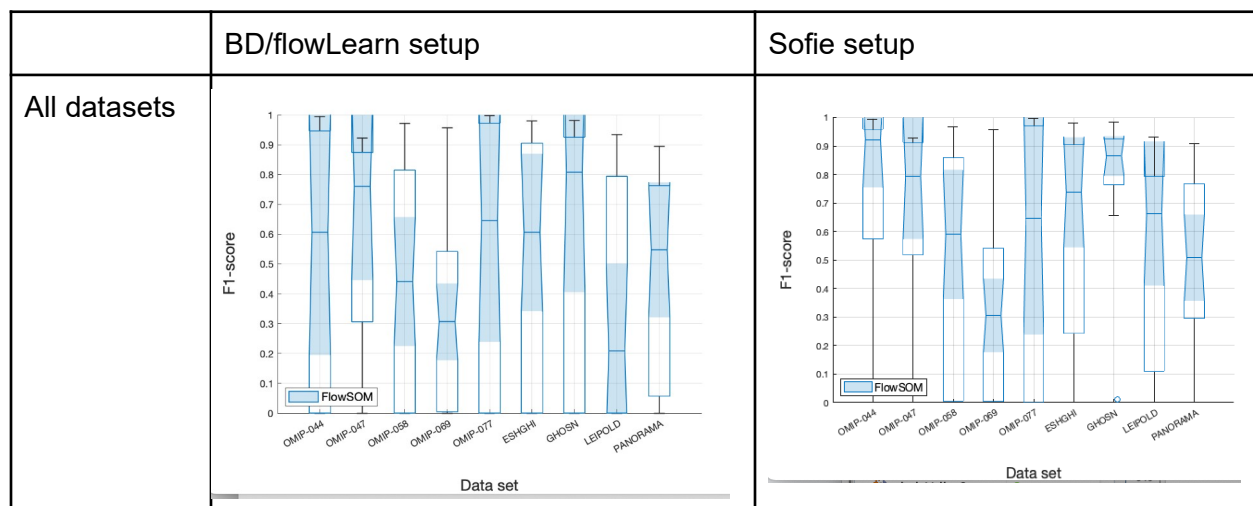
6. Testing Round 4 (final)

6.1. Why another round?

Round 6 differs because

- We rank by F1-score median instead of F1-score mean.
- FlowSOM's results change. The steps for setting up FlowSOM as recommended by BD's FlowJo support team and adhered to by flowLearn were not optimal.

After what we thought (hoped) were our final edits to our manuscript we had a 2.5 hour zoom session with FlowSOM's inventor Sofie Van Gassen who explained that optimal results can not be expected with the guidance given by BD's FlowJo support and followed by the flowLearn publication when they compare with FlowSOM. Setting meta clusters to the # of expected populations + 1 and keeping the grid 10 x 10 is not optimal. The # of meta clusters and clusters given to FlowSOM do need testing and tuning per assay but a better yet rough starting point for meta clusters is 150% of the expected populations rounded down and the W and H of the SOM grid is the square root of 5 times the meta clusters rounded down. The minimum grid size is 10 x 10. All other hyperparameters in the FlowJo plugin configuration screen are unaltered from their default values.



	Summary of median/mean per dataset <table><tr><th colspan="2">Classifier</th><th colspan="2">FlowSOM</th></tr><tr><th>Dataset</th><th># of pop-ulations</th><th>F1-score</th><th>CS</th></tr><tr><td>OMIP-044</td><td>13</td><td>0.61 0.49</td><td>0.51 0.46</td></tr><tr><td>OMIP-047</td><td>8</td><td>0.76 0.60</td><td>0.67 0.55</td></tr><tr><td>OMIP-058</td><td>35</td><td>0.44 0.42</td><td>0.31 0.38</td></tr><tr><td>OMIP-069</td><td>43</td><td>0.31 <i>0.34</i></td><td>0.20 0.28</td></tr><tr><td>OMIP-077</td><td>14</td><td>0.65 0.52</td><td>0.55 0.50</td></tr><tr><td>ESHGHI</td><td>29</td><td>0.61 0.49</td><td>0.48 0.46</td></tr><tr><td>GHOSN</td><td>13</td><td>0.81 0.60</td><td>0.74 0.59</td></tr><tr><td>LEIPOLD</td><td>18</td><td>0.21 0.40</td><td>0.11 0.36</td></tr><tr><td>PANORAMA</td><td>24</td><td>0.55 0.45</td><td>0.39 0.37</td></tr><tr><td>Total populations</td><td>197</td><td colspan="2"></td></tr><tr><td></td><td>Medians</td><td>0.61</td><td>0.48</td></tr><tr><td></td><td>Means</td><td>0.48</td><td>0.44</td></tr></table>	Classifier		FlowSOM		Dataset	# of pop-ulations	F1-score	CS	OMIP-044	13	0.61 0.49	0.51 0.46	OMIP-047	8	0.76 0.60	0.67 0.55	OMIP-058	35	0.44 0.42	0.31 0.38	OMIP-069	43	0.31 <i>0.34</i>	0.20 0.28	OMIP-077	14	0.65 0.52	0.55 0.50	ESHGHI	29	0.61 0.49	0.48 0.46	GHOSN	13	0.81 0.60	0.74 0.59	LEIPOLD	18	0.21 0.40	0.11 0.36	PANORAMA	24	0.55 0.45	0.39 0.37	Total populations	197				Medians	0.61	0.48		Means	0.48	0.44	Summary of median/mean per dataset <table><tr><th colspan="2">Classifier</th><th colspan="2">FlowSOM</th></tr><tr><th>Dataset</th><th># of pop-ulations</th><th>F1-score</th><th>CS</th></tr><tr><td>OMIP-044</td><td>13</td><td>0.92 0.72</td><td>0.91 0.69</td></tr><tr><td>OMIP-047</td><td>8</td><td>0.79 0.67</td><td>0.75 0.62</td></tr><tr><td>OMIP-058</td><td>35</td><td>0.59 0.47</td><td>0.42 <i>0.44</i></td></tr><tr><td>OMIP-069</td><td>43</td><td>0.31 <i>0.34</i></td><td>0.20 0.28</td></tr><tr><td>OMIP-077</td><td>14</td><td>0.65 0.52</td><td>0.55 0.50</td></tr><tr><td>ESHGHI</td><td>29</td><td>0.74 0.61</td><td>0.63 0.56</td></tr><tr><td>GHOSN</td><td>13</td><td>0.86 0.79</td><td>0.81 0.76</td></tr><tr><td>LEIPOLD</td><td>18</td><td>0.66 0.52</td><td>0.56 0.46</td></tr><tr><td>PANORAMA</td><td>24</td><td>0.51 0.49</td><td>0.37 <i>0.40</i></td></tr><tr><td>Total populations</td><td>197</td><td colspan="2"></td></tr><tr><td></td><td>Medians</td><td>0.66</td><td>0.56</td></tr><tr><td></td><td>Means</td><td>0.56</td><td>0.53</td></tr></table>	Classifier		FlowSOM		Dataset	# of pop-ulations	F1-score	CS	OMIP-044	13	0.92 0.72	0.91 0.69	OMIP-047	8	0.79 0.67	0.75 0.62	OMIP-058	35	0.59 0.47	0.42 <i>0.44</i>	OMIP-069	43	0.31 <i>0.34</i>	0.20 0.28	OMIP-077	14	0.65 0.52	0.55 0.50	ESHGHI	29	0.74 0.61	0.63 0.56	GHOSN	13	0.86 0.79	0.81 0.76	LEIPOLD	18	0.66 0.52	0.56 0.46	PANORAMA	24	0.51 0.49	0.37 <i>0.40</i>	Total populations	197				Medians	0.66	0.56		Means	0.56	0.53																
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OMIP-047
12 meta clusters
10 x 10 grid

Color	Cell type	Frequ ency %	F1
•	IgA .FSC-A IgA+	5.5%	
•	IgG3+	0.75%	
•	Naive	46%	
•	IgG1+	3.6%	
•	MZ B cells	33%	
•	PB	0.43%	
•	IgA .FSC-A Neg IgA IgG1 IgG3	8.7%	
•	Transitional	2.1%	
8 cell populations		Median	
		Mean	

Color	Cell type	Frequ ency %	F1
•	Naive	46%	
•	IgG3+	0.75%	
•	MZ B cells	33%	
•	IgG1+	3.6%	
•	PB	0.43%	
•	IgA .FSC-A Neg IgA IgG1 IgG3	8.7%	
•	Transitional	2.1%	
•	IgA .FSC-A IgA+	5.5%	
8 cell populations		Median	
		Mean	

OMIP-058
45 meta clusters
(52 needed, but
max is 45)
15 x 15

Color	Cell type	Frequ ency %	F1
•	CD4+ TEM T cells CD27+ CD28-	0.07%	
•	CD4+ TEM T cells CD27- CD28+	1%	
•	CD4+ TEMRA T cells CD27+ CD28+	0.07%	
•	CD4+ TEMRA T cells CD27- CD28+	0.02%	
•	CD4+ TSCM T cells CD27- CD28+	0.08%	
•	CD8+ TCM T cells CD27- CD28+	0.05%	
•	CD8+ TEM T cells CD27- CD28+	0.20%	
•	CD8+ TEM T cells CD27- CD28-	0.74%	
•	CD8+ TSCM T cells CD27+ CD28+	0.12%	
•	iNKT cells	0.13%	
•	Vd1+ Vg9- T cells CD56+	0.12%	
•	Vd2 low Vg9+ T cells CD56+	0.09%	
•	CD4+ Naive T cells CD27+ CD28+	21%	
•	HLA-DR+	9.9%	
•	CD8+ TEMRA T cells CD27- CD28-	18%	
•	Vd2 high Vg9+ T cells	0.56%	
•	CD4+ TCM T cells CD27+ CD28+	21%	
•	Vd2 low Vg9+ T cells CD56-	0.89%	
•	MAIT cells	0.63%	
•	Early NK	1%	
•	NK CD16- CD56-	2.8%	
•	Vd1+ Vg9- T cells CD56-	1.6%	
•	CD8+ TEMRA T cells CD27+ CD28-	1.9%	
•	CD8+ TEM T cells CD27+ CD28+	4%	
•	Mature NK	2.3%	
•	CD4+ TCM T cells CD27- CD28+	3.6%	
•	CD8+ TEMRA T cells CD27+ CD28+	0.62%	
•	CD8+ Naive T cells CD27+ CD28+	1.9%	
•	CD4+ TEM T cells CD27- CD28-	2.1%	
•	Q2: Vd1+ Vg9+	0.14%	
•	CD4+ TEMRA T cells CD27- CD28-	0.10%	
•	CD4+ TSCM T cells CD27+ CD28+	0.79%	
•	CD4+ TEM T cells CD27+ CD28+	1.8%	
•	CD8+ TCM T cells CD27+ CD28+	0.60%	
•	Terminal NK	0.35%	
35 cell populations		Median	
		Mean	

Color	Cell type	Frequ ency %	F1
•	CD4+ TEM T cells CD27+ CD28+	1.8%	
•	CD4+ TEM T cells CD27- CD28+	1%	
•	CD4+ TEMRA T cells CD27+ CD28+	0.07%	
•	CD4+ TEMRA T cells CD27- CD28+	0.02%	
•	CD4+ TSCM T cells CD27- CD28+	0.08%	
•	HLA-DR+	9.9%	
•	iNKT cells	0.13%	
•	CD4+ Naive T cells CD27+ CD28+	21%	
•	CD8+ TEMRA T cells CD27- CD28-	18%	
•	Vd2 high Vg9+ T cells	0.56%	
•	MAIT cells	0.63%	
•	Mature NK	2.3%	
•	CD4+ TCM T cells CD27+ CD28+	21%	
•	Vd2 low Vg9+ T cells CD56-	0.89%	
•	Early NK	1%	
•	Vd1+ Vg9- T cells CD56-	1.6%	
•	NK CD16- CD56-	2.8%	
•	Q2: Vd1+ Vg9+	0.14%	
•	CD8+ TEM T cells CD27+ CD28+	4%	
•	CD4+ TCM T cells CD27- CD28+	3.6%	
•	CD8+ TEM T cells CD27- CD28+	0.20%	
•	CD8+ TEMRA T cells CD27+ CD28-	1.9%	
•	CD8+ Naive T cells CD27+ CD28+	1.9%	
•	CD8+ TEMRA T cells CD27+ CD28+	0.62%	
•	CD4+ TEM T cells CD27- CD28-	2.1%	
•	CD4+ TEMRA T cells CD27- CD28-	0.10%	
•	Terminal NK	0.35%	
•	CD8+ TCM T cells CD27+ CD28+	0.60%	
•	CD8+ TEM T cells CD27- CD28-	0.74%	
•	CD4+ TSCM T cells CD27+ CD28+	0.79%	
•	CD8+ TSCM T cells CD27+ CD28+	0.12%	
•	Vd2 low Vg9+ T cells CD56+	0.09%	
•	Vd1+ Vg9- T cells CD56+	0.12%	
•	CD4+ TEM T cells CD27+ CD28-	0.07%	
•	CD8+ TCM T cells CD27- CD28+	0.05%	
35 cell populations		Median	
		Mean	

OMIP-069

NOT run on parent branch of all 43 populations since 45 meta clusters is maximum

Run on parent branch of 19 populations under NKT and T cells
28 meta clusters
11 x 11 grid

Color	Cell type	Frequency %	F1-Score		Central similarity
			Flow 2 SOM	Flow 3 SOM	
●	Naive CD8+	18%	0.979	0.996	
●	Naive CD4+	39%	0.950	0.959	
●	CD4- CD8-	2%	0.776	0.651	
●	Central Memory CD4+ CXCR5-, CXCR3	6.3%	0.687	0.533	
●	Early Effector CD8+	4.1%	0.661	0.524	
●	CD4+ CD8+ T	0.13%	0.656	0.499	
●	Early like effector CD4+	2.4%	0.526	0.385	
●	Central Memory CD4+ CXCR5-, CXCR3-	8.8%	0.515	0.354	
●	Early Effector CD4+	5.4%	0.489	0.328	
●	Intermediate Effector CD8+	0.66%	0.405	0.277	
●	Terminal Effector CD45RA+ CD8+	0.61%	0.401	0.273	
●	Early like effector CD8+	0.77%	0.393	0.253	
●	CD2+ CD8+ NKT	2.3%	0.280	0.187	
●	Central Memory CD8-	0.50%	0.071	0.033	
●	Central Memory CD4+ CXCR5, CXCR3	8.8%	0.003	0.001	
●	CD2+ CD8-	0.56%	N/A	N/A	N
●	Terminal Effector	0.30%	0	0	
●	CD2- NKT cells	0.13%	N/A	N/A	N
●	Terminal Effector CD4+	0.01%	N/A	N/A	N
Median			0.405	0.277	
Mean			0.410	0.329	

Color	Cell type	Frequency %
●	Naive CD8+	18%
●	Naive CD4+	39%
●	CD4- CD8-	2%
●	Central Memory CD4+ CXCR5-, CXCR3	6.3%
●	CD4+ CD8+ T	0.13%
●	Early Effector CD8+	4.1%
●	Central Memory CD4+ CXCR5, CXCR3	8.8%
●	Early Effector CD4+	5.4%
●	Early like effector CD4+	2.4%
●	Terminal Effector CD45RA+ CD8+	0.61%
●	CD2+ CD8+ NKT	2.3%
●	Central Memory CD8+	0.50%
●	Central Memory CD4+ CXCR5-, CXCR3-	8.8%
●	Intermediate Effector CD8+	0.66%
●	CD2+ CD8-	0.56%
●	CD2- NKT cells	0.13%
●	Early like effector CD8+	0.77%
●	Terminal Effector	0.30%
●	Terminal Effector CD4+	0.01%
19 cell populations		Median
		Mean

OMIP-077

21 meta clusters
10 x 10 grid

Color	Cell type	Frequency %	F1
●	CD141+ mDCs	0.01%	S
●	CD141- mDCs	0.04%	
●	CD1c+ mDCs	0.03%	
●	MZB cells	0.52%	
●	pDCs	0.04%	
●	Neutrophils	77%	
●	Eosinophils	1.3%	
●	T cells	11%	
●	Basophils	0.34%	
●	Monocytes	6.9%	
●	NK cells	2%	
●	Non MZB cells	1.4%	
●	Plasma cells	0.09%	
●	Progenitors	0.07%	
14 cell populations		Median	
		Mean	

Color	Cell type	Frequency %	F1
●	CD141- mDCs	0.04%	S
●	CD1c+ mDCs	0.03%	
●	MZB cells	0.52%	
●	Neutrophils	77%	
●	Eosinophils	1.3%	
●	T cells	11%	
●	Basophils	0.34%	
●	Monocytes	6.9%	
●	NK cells	2%	
●	Non MZB cells	1.4%	
●	Plasma cells	0.09%	
●	Progenitors	0.07%	
●	CD141+ mDCs	0.01%	
●	pDCs	0.04%	
14 cell populations		Median	
		Mean	

ESHGHI

43 meta clusters
14 x 14 grid

(40 meta clusters
did not work!)

Color	Cell type	Frequency %
	CD56hi NK	0.70%
	int Mono	1.6%
	Basophils	2.5%
	Neutrophil	1.7%
	pDCs	0.54%
	Naive B	2.7%
	CD16hi NK	12%
	Eosinophil	0.52%
	CD8 MAIT	1.9%
	CD16hi Mono	2.3%
	CD14hi Mono	17%
	Plasmablast	0.28%
	gd Tcells	1.9%
	CD8 Temra	6.3%
	CD8 N	4.8%
	CD4 N	15%
	CD14- CD16-	0.56%
	Mem B	0.64%
	Lineage Negative	0.57%
	CD4 EM	9.6%
	IgD- CD27- B	0.18%
	CD4 Temra	1.7%
	Treg	1%
	Trans B	0.67%
	CD8 CM	0.48%
	CD123-	0.17%
	CD8 EM	4%
	HLADRlo Mono	2.4%
	CD4 CM	6.2%
29 cell populations		Median Mean

Color	Cell type	Frequency %	F _S
	Basophils	2.5%	
	CD16hi NK	12%	
	pDCs	0.54%	
	Naive B	2.7%	
	Neutrophil	1.7%	
	Eosinophil	0.52%	
	CD4 N	15%	
	CD16hi Mono	2.3%	
	CD14hi Mono	17%	
	gd Tcells	1.9%	
	CD8 MAIT	1.9%	
	Plasmablast	0.28%	
	CD8 N	4.8%	
	CD56hi NK	0.70%	
	int Mono	1.6%	
	CD8 Temra	6.3%	
	CD8 EM	4%	
	CD4 EM	9.6%	
	Mem B	0.64%	
	CD14- CD16-	0.56%	
	CD123-	0.17%	
	IgD- CD27- B	0.18%	
	Treg	1%	
	Lineage Negative	0.57%	
	CD4 Temra	1.7%	
	CD4 CM	6.2%	
	CD8 CM	0.48%	
	Trans B	0.67%	
	HLADRlo Mono	2.4%	
29 cell populations		Median Mean	

GHOSN

19 meta clusters
10 x 10 grid

Color	Cell type	Frequency %	F1-Score Flow SOM	Central similarity Flow SOM	Earth mover's distance Flow SOM
	ckit+ mast cells	1.8%			
	Neutrophils	0.38%			
	Large macrophages	32%	0.99	1	0.99
	T cells	6.8%	0.97	0.99	0.99
	Eosinophils	9.5%	0.94	0.99	0.95
	B-1	22%	0.92	0.92	0.96
	NK_NKT	9%	0.87	0.86	0.89
	CD11b- dendritic	0.22%	0.83	0.80	0.96
	Small macrophages	4.5%	0.81	0.74	0.88
	B-2 IgM medium	7%	0.77	0.72	0.85
	B-2 IgM high	5.1%	0.71	0.61	0.84
	CD11b+ dendritic	1.2%	<0.01		0.22
	Developing B	0.54%			0.01
13 cell populations		Median	0.808	0.736	0.880
		Mean	0.601	0.586	0.657

Color	Cell type	Frequency %	F1-Score Flow SOM	Central similarity Flow SOM	Earth mover's distance Flow SOM
	Large macrophages	32%	0.99	1	0.99
	T cells	6.8%	0.97	0.99	0.99
	Eosinophils	9.5%	0.94	0.99	0.95
	Small macrophages	4.5%	0.92	0.91	0.97
	B-1	22%	0.90	0.89	0.97
	NK_NKT	9%	0.89	0.92	0.91
	CD11b+ dendritic	1.2%	0.86	0.81	0.98
	Developing B	0.54%	0.83	0.75	0.92
	CD11b- dendritic	0.22%	0.83	0.80	0.96
	B-2 IgM medium	7%	0.79	0.74	0.88
	B-2 IgM high	5.1%	0.67	0.56	0.87
	ckit+ mast cells	1.8%	0.66	0.54	0.93
	Neutrophils	0.38%	0.01	0.01	0.30
13 cell populations		Median	0.865	0.810	0.953
		Mean	0.790	0.762	0.895

LEIPOLD

27 meta clusters

11 x 11 grid

Color	Cell type	Frequency %	F1-Score
			$\frac{F1}{SQ}$
	Basophils	0.64%	
	CD4 T cells CD45RA- , CD27-	4.3%	
	CD56 bright NK cells	0.45%	
	CD8 T cells CD45RA+ , CD27-	9.8%	
	CD8 T cells CD45RA- , CD27-	2.7%	
	pDCs	0.30%	
	CD4 T cells CD45RA+ , CD27+	17%	
	CD16- monocytes	6.1%	
	NK cells	11%	
	CD8 T cells CD45RA- , CD27+	6.9%	
	CD4 T cells CD45RA- , CD27+	15%	
	CD38+CD56 B cells	3.8%	
	CD8 T cells CD45RA+ , CD27+	13%	
	CD4- CD8-	3.1%	
	mDCs	0.89%	
	CD38 CD56- B cells	3.8%	
	CD16+ monocytes	0.09%	
	CD4 T cells CD45RA+ , CD27-	1.1%	
18 cell populations		Median	
		Mean	

PANORAMA

36 meta clusters

13 X 13 grid

Color	Cell type	Frequency %	F1-Score
			$\frac{F1}{SQ}$
	B cells Frac. D	1.8%	
	gd T cells	0.21%	
	GMP	2.7%	
	B cells Frac. F	20%	
	pDCs	5.9%	
	CD8 T cells	2.1%	
	Non classical Monocytes	1.7%	
	CD4 T cells	1.3%	
	Classical Monocytes	29%	
	Intermediate Monocytes	11%	
	Eosinophils	9.1%	
	NKT cells	2.3%	
	Plasma Cells	0.26%	
	mDCs	0.28%	
	Macrophages	0.67%	
	Basophils	0.40%	
	B cells Frac. E	6.5%	
	NK cells	0.76%	
	MEP	1.3%	
	CMP	1%	
	CLP	0.39%	
	HSC	0.04%	
	B cells Frac A-C	1%	
	MPP	0.60%	
24 cell populations		Median	
		Mean	

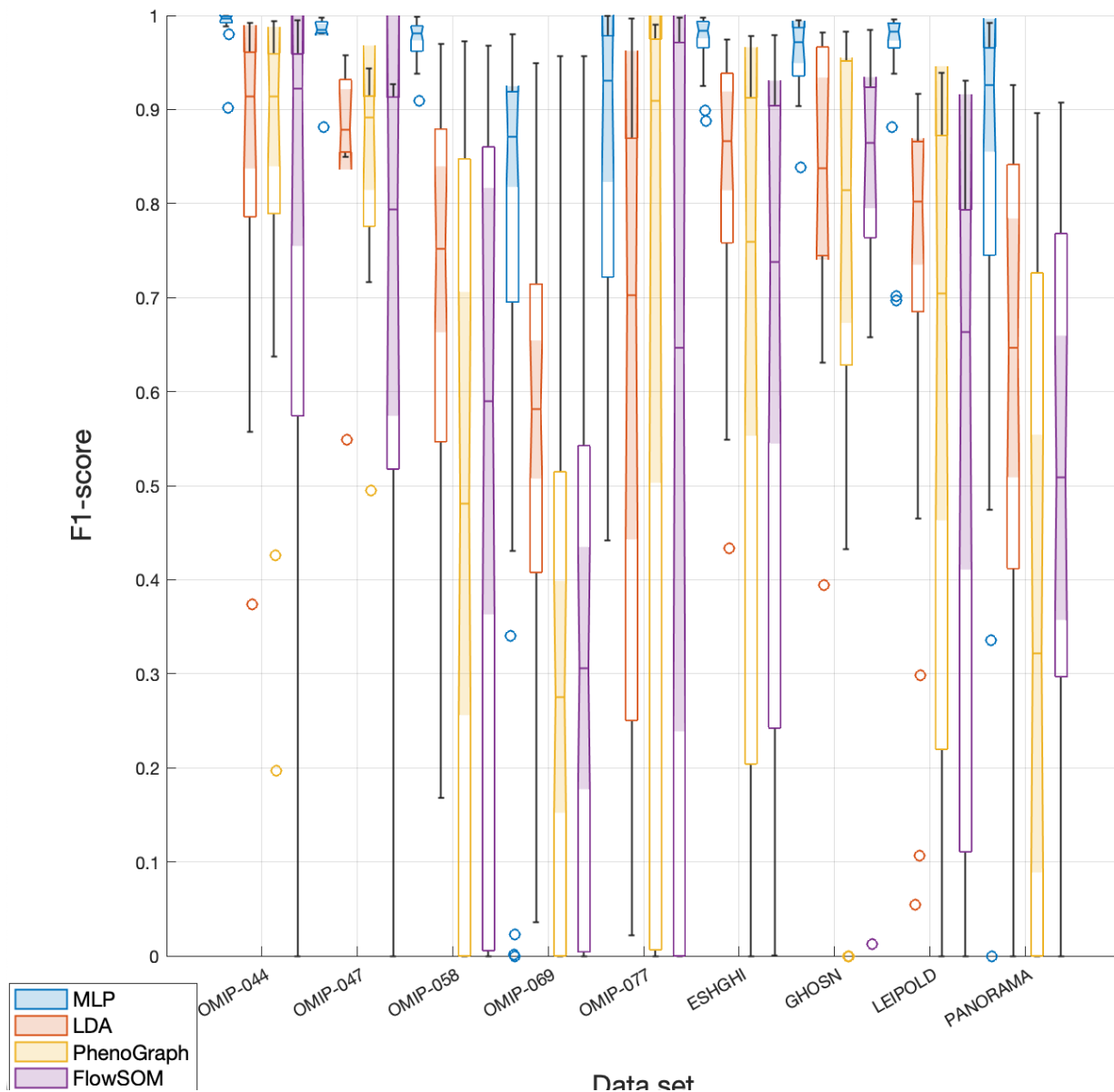
Color	Cell type	Frequency %	F1-Score
			$\frac{F1}{SQ}$
	pDCs	0.30%	
	NK cells	11%	
	CD16- monocytes	6.1%	
	CD4 T cells CD45RA+ , CD27+	17%	
	CD4 T cells CD45RA- , CD27+	15%	
	CD56 bright NK cells	0.45%	
	CD8 T cells CD45RA- , CD27+	6.9%	
	CD8 T cells CD45RA+ , CD27-	9.8%	
	CD4- CD8-	3.1%	
	CD8 T cells CD45RA+ , CD27+	13%	
	CD38+CD56 B cells	3.8%	
	mDCs	0.89%	
	CD38 CD56- B cells	3.8%	
	CD8 T cells CD45RA- , CD27-	2.7%	
	Basophils	0.64%	
	CD16+ monocytes	0.09%	
	CD4 T cells CD45RA+ , CD27-	1.1%	
	CD4 T cells CD45RA- , CD27-	4.3%	
18 cell populations		Median	
		Mean	

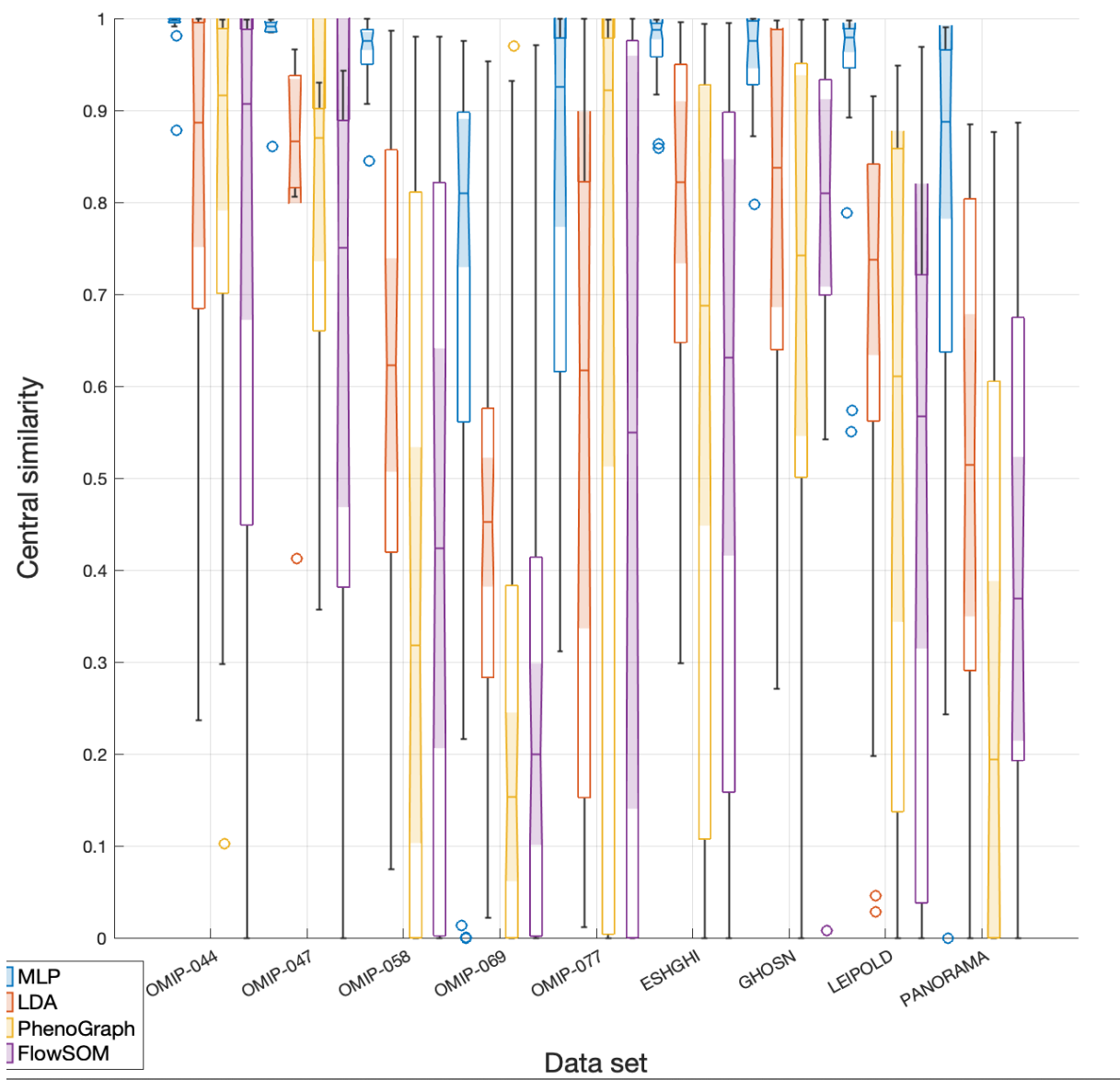
OMIP-058 can only improve partially. It has 35 populations thus instead of 52 meta clusters we can only change it to 45 meta clusters.

OMIP-069 can't improve since it has 43 populations and the upper limit of meta clusters is 45. As discussed in section [4.3.4.2](#) of this document however we did run FlowSOM on the 19 populations further down the gating hierarchy.

6.2. Results for datasets

6.2.1. Figures and tables





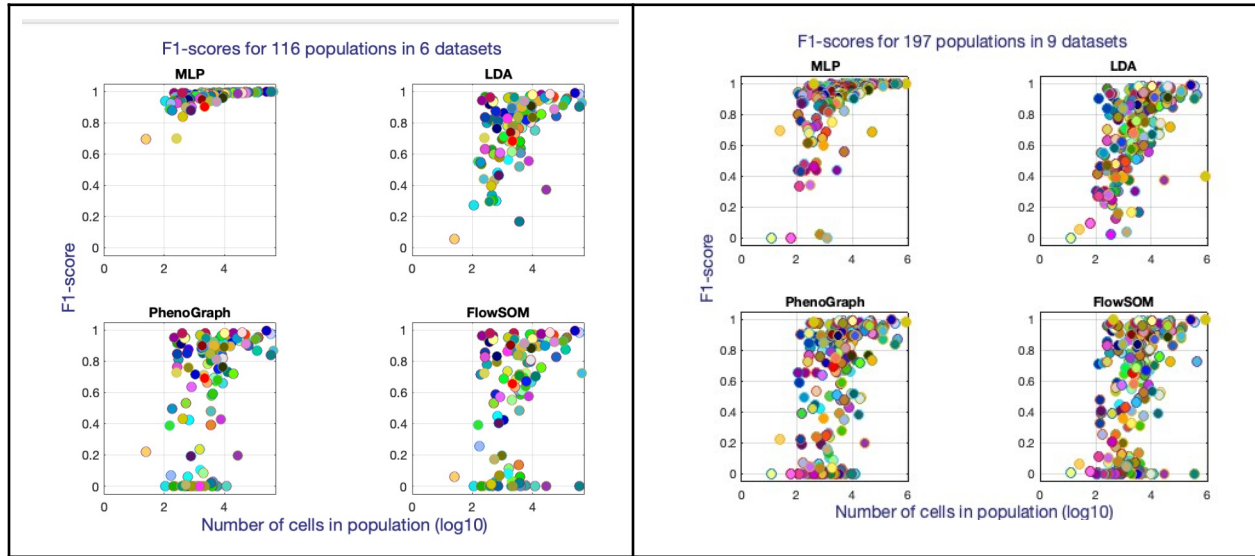
Classifier		MLP		LDA		PhenoGraph		FlowSOM	
Dataset	# of pop-ulations	F1-score	CS	F1-score	CS	F1-score	CS	F1-score	CS
OMIP-044	13	1.00 0.99	1.00 0.99	0.91 0.84	0.89 0.80	0.91 0.81	0.92 0.78	0.92 0.72	0.91 0.69
OMIP-047	8	0.98 0.97	0.99 0.98	0.88 0.85	0.87 0.83	0.89 0.83	0.87 0.77	0.79 0.67	0.75 0.62
OMIP-058	35	0.98 0.97	0.98 0.96	0.75 0.70	0.62 0.61	0.48 0.43	0.32 0.40	0.59 0.47	0.42 <i>0.44</i>
OMIP-069	43	0.87 0.76	0.81 0.70	0.57 0.56	0.45 <i>0.46</i>	0.28 0.34	0.15 0.28	0.31 <i>0.34</i>	0.20 0.28
OMIP-077	14	0.93 0.84	0.93 0.79	0.70 0.57	0.62 0.53	0.91 0.65	0.92 0.65	0.65 0.52	0.55 0.50
ESHGHI	29	0.98 0.97	0.99 0.97	0.87 0.82	0.82 0.77	0.76 0.61	0.69 0.56	0.74 0.61	0.63 0.56
GHOSN	13	0.97 0.95	0.98 0.95	0.84 0.82	0.84 0.78	0.81 0.70	0.74 0.66	0.86 0.79	0.81 0.76
LEIPOLD	18	0.98 0.94	0.98 0.92	0.80 0.69	0.74 0.64	0.70 0.60	0.61 0.54	0.66 0.52	0.56 0.46
PANORAMA	24	0.93 0.81	0.89 0.76	0.65 0.62	0.51 <i>0.53</i>	0.32 0.38	0.19 <i>0.31</i>	0.51 <i>0.49</i>	0.37 <i>0.40</i>
Total populations		197							
Medians		0.98	0.98	0.80	0.74	0.76	0.69	0.66	0.56
Means		0.91	0.89	0.72	0.66	0.59	0.55	0.56	0.53

Columns		Rows				
Legend	- F1-score=overlap measured by harmonic mean of percision + recall (AKA <i>F measure</i>). - CS=overlap in central core region.	Coloring is based on ranking by <i>F1-score median</i>				
		<i>Narrow lead over next</i>	1st	2nd	3rd	Last
		<i>Wide lead over next</i>	1st	2nd	3rd	Nothing is next
		<i>Ties get same ranked color....</i>				
		Median minus mean size is ^{cmph} asized pos/neg.				

Classifier		MLP				LDA				PhenoGraph				FlowSOM			
Dataset	# of pop-ulations	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD
OMIP-044	13	1.00 0.99	0.99 0.98	1.00 0.99	1.00 1.00	0.91 0.84	0.84 0.76	0.89 0.80	0.98 0.93	0.91 0.81	0.84 0.74	0.92 0.78	0.95 0.92	0.92 0.72	0.86 0.66	0.91 0.69	0.94 0.82
OMIP-047	8	0.98 0.97	0.97 0.95	0.99 0.98	1.00 0.99	0.88 0.85	0.78 0.76	0.87 0.83	0.97 0.94	0.89 0.83	0.80 0.72	0.87 0.77	0.97 0.93	0.79 0.67	0.67 0.56	0.75 0.62	0.92 0.81
OMIP-058	35	0.98 0.97	0.96 0.95	0.98 0.96	0.99 0.99	0.75 0.70	0.60 0.57	0.62 0.61	0.94 0.91	0.48 0.43	0.32 0.37	0.32 0.40	0.86 0.56	0.59 0.47	0.42 0.40	0.42 0.44	0.89 0.68
OMIP-069	43	0.87 0.76	0.77 0.67	0.81 0.70	0.98 0.95	0.57 0.56	0.41 0.43	0.45 0.46	0.90 0.89	0.28 0.34	0.16 0.26	0.15 0.28	0.75 0.54	0.31 0.34	0.18 0.26	0.20 0.28	0.78 0.62
OMIP-077	14	0.93 0.84	0.87 0.76	0.93 0.79	0.98 0.96	0.70 0.57	0.55 0.49	0.62 0.53	0.90 0.86	0.91 0.65	0.83 0.61	0.92 0.65	0.96 0.73	0.65 0.52	0.50 0.49	0.55 0.50	0.90 0.62
ESHGHI	29	0.98 0.97	0.97 0.95	0.99 0.97	1.00 0.99	0.87 0.82	0.76 0.71	0.82 0.77	0.96 0.95	0.76 0.61	0.61 0.53	0.69 0.56	0.93 0.76	0.74 0.61	0.57 0.53	0.63 0.56	0.89 0.81
GHOSN	13	0.97 0.95	0.95 0.92	0.98 0.95	0.99 0.98	0.84 0.82	0.72 0.73	0.84 0.78	0.95 0.93	0.81 0.70	0.69 0.62	0.74 0.66	0.92 0.79	0.86 0.79	0.76 0.70	0.81 0.76	0.95 0.90
LEIPOLD	18	0.98 0.94	0.97 0.91	0.98 0.92	1.00 0.98	0.80 0.69	0.67 0.57	0.74 0.64	0.94 0.91	0.70 0.60	0.54 0.49	0.61 0.54	0.92 0.77	0.66 0.52	0.50 0.42	0.56 0.46	0.89 0.76
PANORAMA	24	0.93 0.81	0.86 0.74	0.89 0.76	0.99 0.92	0.65 0.62	0.48 0.49	0.51 0.53	0.92 0.87	0.32 0.38	0.19 0.28	0.19 0.31	0.74 0.57	0.51 0.49	0.34 0.38	0.37 0.40	0.87 0.80
Total populations		197															
Medians		0.98	0.96	0.98	0.99	0.80	0.67	0.74	0.94	0.76	0.61	0.69	0.92	0.66	0.50	0.56	0.89
Means		0.91	0.87	0.89	0.97	0.72	0.61	0.66	0.91	0.59	0.52	0.55	0.73	0.56	0.49	0.53	0.76

	Columns	Rows				
Legend	• F1-score=overlap measured by harmonic mean of percision + recall (AKA <i>F measure</i>). • JI 100%=whole population overlap measured by intersection/union (AKA <i>jaccard index</i>). • JI 80%=central core region overlap (AKA <i>central similarity</i>). • EMD=earth mover's distance	Coloring is based on ranking by <i>F1-score median</i>				
		<i>Narrow lead over next</i>	1st	2nd	3rd	Last
		<i>Wide lead over next</i>	1st	2nd	3rd	Nothing is next
		<i>Ties get same ranked color...</i>				
		Median minus mean size is ^{emph} asized pos/neg.				

6.2.2. Small population issues



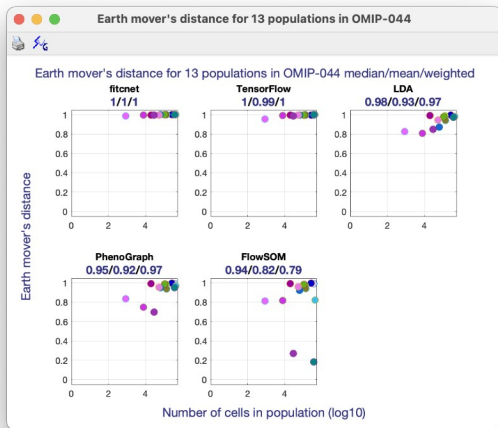
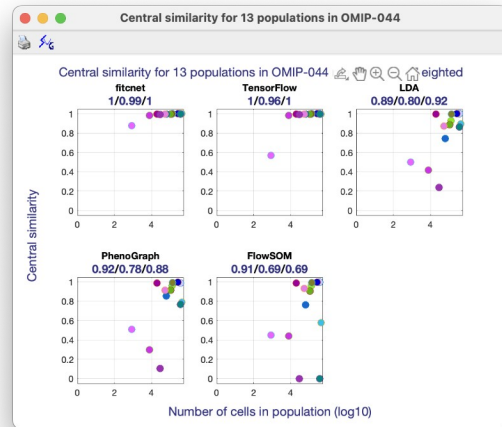
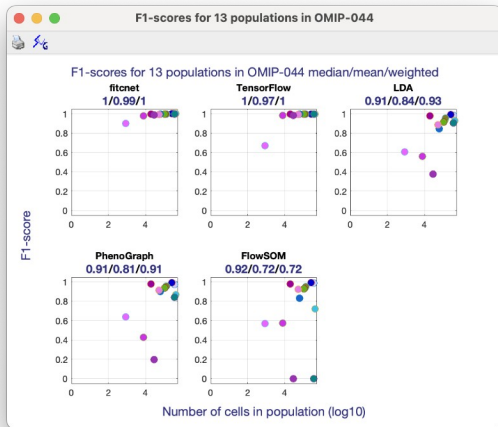
Classifier	Minimum F1-Score				# populations < 0.50 F1-Score				Mean frequency of populations < 0.50 F1-Score			
	MLP	LDA	PhenoGraph	FlowSOM	MLP	LDA	PhenoGraph	FlowSOM	MLP	LDA	PhenoGraph	FlowSOM
Dataset												
OMIP-044	0.90	0.37	0.20	0	0/13	1/13	2/13	2/13	1.4%	0.63%	9%	
OMIP-047	0.88	0.55	0.49	0	0/8	0/8	1/8	2/8			0.43%	3.8%
OMIP-058	0.91	0.17	0	0	0/35	7/35	6/35	11/35	0.23%	0.77%	0.46%	
OMIP-069	0	0.04	0.04	< 0.01	6/43	16/43	16/43	18/43	0.11%	0.17%	1.3%	0.55%
OMIP-077	0.44	0.02	0	0	1/14	6/14	2/14	4/14	0.01%	0.03%	0.03%	0.05%
GENENTECH	0.89	0.43	0	< 0.01	0/29	1/29	7/29	9/29	0.57%	0.82%	1.5%	
GHOSN	0.84	0.39	0.43	0.01	0/13	1/13	1/13	1/13	0.36%	0.38%	0.38%	
LEIPOLD	0.70	0.05	0	0	0/18	4/18	6/18	7/18	0.79%	1.5%	1.9%	
PANORAMA	0	0	0.01	0	4/24	8/24	7/24	12/24	0.40%	0.96%	1.9%	1.4%
Total					11/197	44/197	48/197	66/197				

6.3. Results for populations

6.3.1. OMIP-044

Classifier	Population	Frequency	MLP				LDA				PhenoGraph				FlowSOM			
			F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD
• CD14+	19%	1.00	1.00	1.00	1.00	0.98	0.97	1.00	0.98	0.97	0.95	0.99	0.99	0.99	0.99	0.97	1.00	0.99
• CD19+	13%	1.00	1.00	1.00	1.00	0.99	0.98	1.00	1.00	0.99	0.99	1.00	1.00	0.99	0.99	1.00	1.00	1.00
• naive CD4+	23%	1.00	1.00	1.00	1.00	0.93	0.87	0.89	0.98	0.87	0.77	0.79	0.97	0.72	0.56	0.57	0.82	0.82
• [not naive CD4+]	17%	1.00	1.00	1.00	1.00	0.91	0.83	0.86	0.98	0.84	0.72	0.76	0.95					
• naive CD8+	6.7%	1.00	1.00	1.00	1.00	0.94	0.89	0.93	0.99	0.95	0.91	0.96	0.99	0.94	0.89	0.96	0.97	0.97
• CD56+ NK	7.4%	1.00	1.00	1.00	1.00	0.95	0.91	1.00	0.94	0.95	0.91	0.99	0.94	0.95	0.91	0.99	0.94	0.94
• [not naive CD8+]	5.4%	1.00	0.99	1.00	1.00	0.91	0.84	0.89	0.98	0.94	0.89	0.92	0.99	0.93	0.86	0.91	0.98	0.98
• DN	2.7%	1.00	0.99	1.00	1.00	0.85	0.73	0.75	0.87	0.90	0.82	0.85	0.95	0.83	0.71	0.76	0.92	0.92
• CD123+ pDC	1.2%	1.00	0.99	1.00	1.00	0.98	0.96	1.00	0.99	0.98	0.96	0.99	0.99	0.98	0.96	0.99	0.99	0.99
• DN DCs	2.7%	0.99	0.99	1.00	1.00	0.89	0.80	0.87	0.94	0.91	0.84	0.92	0.95	0.92	0.86	0.93	0.96	0.96
• DCs-	0.84%	0.99	0.98	0.99	1.00	0.37	0.23	0.24	0.85	0.20	0.11	0.10	0.70					
• CD1c DCs	0.42%	0.98	0.96	0.98	1.00	0.56	0.39	0.42	0.81	0.43	0.27	0.30	0.75	0.57	0.40	0.44	0.82	0.82
• CD141+DCs	0.05%	0.90	0.82	0.88	0.99	0.61	0.44	0.50	0.83	0.64	0.47	0.51	0.84	0.56	0.40	0.45	0.81	0.81
Medians			1.00	0.99	1.00	1.00	0.91	0.84	0.89	0.98	0.91	0.84	0.92	0.95	0.92	0.86	0.91	0.94
Means			0.99	0.98	0.99	1.00	0.84	0.76	0.80	0.93	0.81	0.74	0.78	0.92	0.72	0.66	0.69	0.82

Columns		Rows			
Legend	• F1-score=overlap measured by harmonic mean of precision + recall (AKA <i>F measure</i>).	Coloring is based on ranking by <i>F1-score median</i>			
	• JI 100%=whole population overlap measured by intersection/union (AKA <i>jaccard index</i>).	Narrow lead over next	1st	2nd	3rd
	• JI 80%=central core region overlap (AKA <i>central similarity</i>).	Wide lead over next	1st	2nd	3rd
	• JI 80% minus JI 100% size has <i>low</i> to high <i>emphasis</i> .				Nothing is next
• EMD=earth mover's distance		Ties get same ranked color....			
		Median minus mean size is <i>emphasized</i> pos/neg.			



6.3.2. OMIP-047

	Population	Classifier	MLP				LDA				PhenoGraph				FlowSOM			
		Freq- uency	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD
	• Naive	46%	1.00	1.00	1.00	1.00	0.96	0.92	0.97	0.99	0.94	0.89	0.93	0.98	0.93	0.86	0.92	0.97
	• MZ B cells	33%	1.00	0.99	1.00	1.00	0.94	0.89	0.93	0.98	0.92	0.85	0.88	0.97	0.90	0.82	0.85	0.96
• IgA, FSC-A Neg IgA IgG1 IgG3	8.7%	0.99	0.98	0.99	1.00	0.85	0.74	0.81	0.97	0.84	0.72	0.73	0.93	0.61	0.44	0.50	0.83	
• IgA, FSC-A IgA+	5.5%	0.99	0.97	0.99	1.00	0.90	0.81	0.89	0.97	0.90	0.82	0.89	0.97					
• IgG1+	3.6%	0.98	0.97	0.99	1.00	0.86	0.75	0.84	0.94	0.88	0.79	0.87	0.97	0.87	0.77	0.86	0.96	
• Transitional	2.1%	0.98	0.97	0.98	1.00	0.86	0.76	0.83	0.95	0.72	0.56	0.59	0.87	0.42	0.27	0.27	0.77	
• IgG3+	0.75%	0.98	0.96	0.99	0.99	0.92	0.85	0.95	0.96	0.91	0.84	0.91	0.97	0.92	0.86	0.94	0.98	
• PB	0.43%	0.88	0.79	0.86	0.97	0.55	0.38	0.41	0.75	0.49	0.33	0.36	0.75	0.71	0.56	0.66	0.88	
	Medians	0.98	0.97	0.99	1.00	0.88	0.78	0.87	0.97	0.89	0.80	0.87	0.97	0.79	0.67	0.75	0.92	
	Means	0.97	0.95	0.98	0.99	0.85	0.76	0.83	0.94	0.83	0.72	0.77	0.93	0.67	0.56	0.62	0.81	

Columns

Rows

• F1-score=overlap measured by harmonic mean of percision + recall (AKA *F measure*).

• JI 100%=whole population overlap measured by intersection/union (AKA *jaccard index*).

• JI 80%=central core region overlap (AKA *central similarity*).

• JI 80% minus JI 100% size has *low* to high *emphasis*.

• EMD=earth mover's distance

Coloring is based on ranking by *F1-score median*

Narrow lead over next

Wide lead over next

Ties get same ranked color....

Median minus mean size is *emphasized* pos/neg.

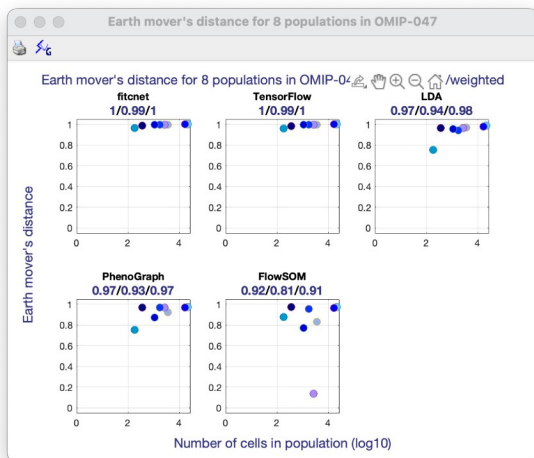
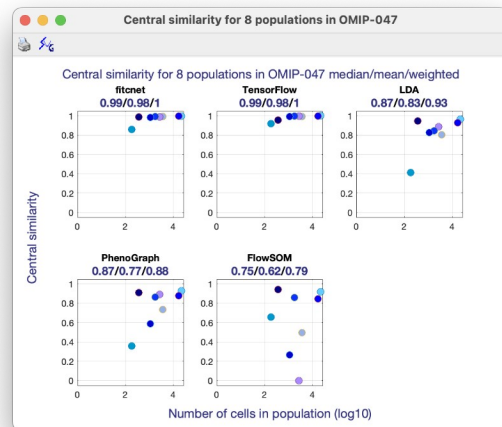
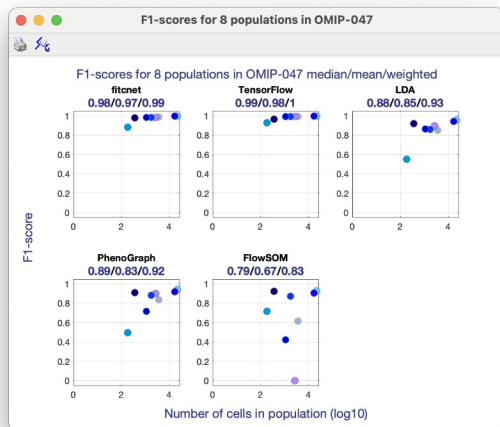
1st

2nd

3rd

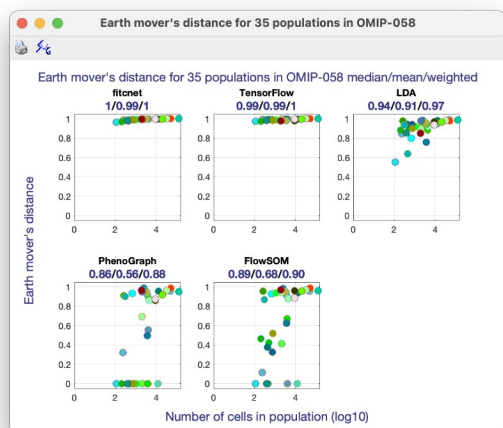
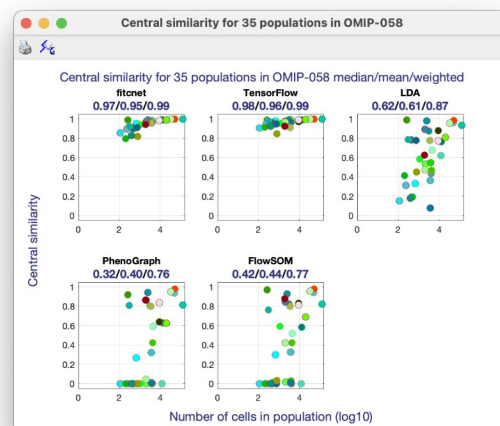
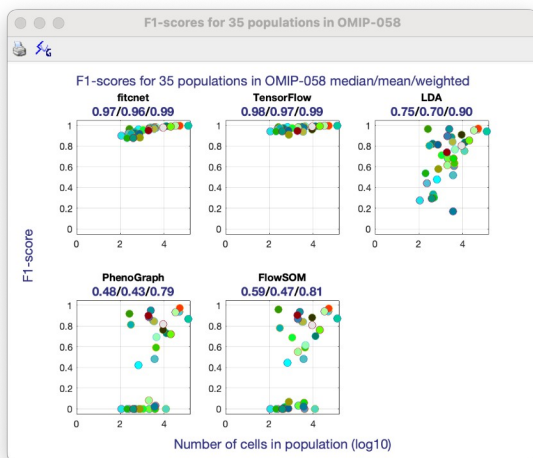
Last

Nothing is next



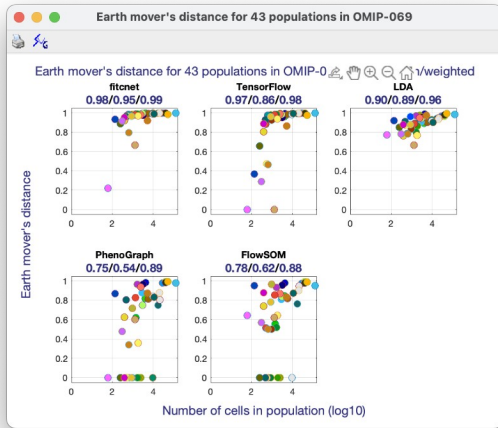
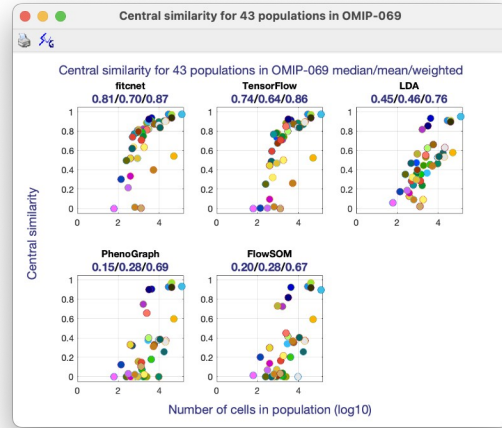
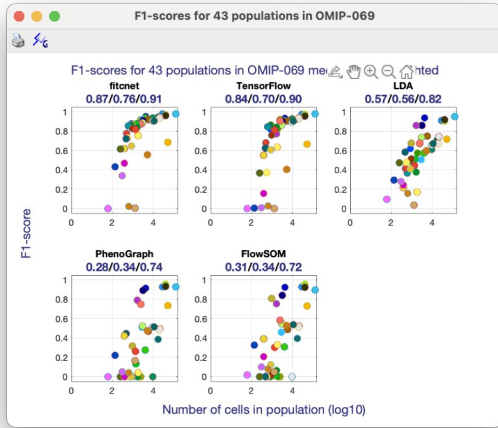
6.3.3. OMIP-058

Classifier	Population	Frequency	MLP				LDA				PhenoGraph				FlowSOM			
			F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD
• CD4+ Naive T cells CD27+ CD28+		13%	1.00	1.00	1.00	1.00	0.96	0.92	0.96	0.99	0.94	0.88	0.94	0.96	0.94	0.89	0.94	0.96
• CD4+ TCM T cells CD27+ CD28+		34%	1.00	1.00	1.00	1.00	0.94	0.89	0.93	0.99	0.87	0.77	0.81	0.95	0.87	0.78	0.82	0.96
• HLA-DR+		14%	1.00	1.00	1.00	1.00	0.97	0.94	0.98	0.98	0.97	0.95	0.98	0.99	0.97	0.94	0.98	0.99
• CD8+ TEMRA T cells CD27- CD28-		9%	1.00	1.00	1.00	1.00	0.95	0.91	0.96	0.98	0.93	0.88	0.95	0.97	0.94	0.89	0.96	0.97
• CD4+ TCM T cells CD27- CD28+		3.5%	0.99	0.99	0.99	1.00	0.84	0.72	0.76	0.98	0.73	0.57	0.63	0.96	0.70	0.54	0.57	0.94
• CD8+ Naive T cells CD27+ CD28+		1.1%	0.99	0.98	0.99	1.00	0.64	0.47	0.47	0.88	0.59	0.42	0.42	0.88	0.59	0.42	0.42	0.88
• CD8+ TEM T cells CD27+ CD28+		5.4%	0.99	0.98	0.99	1.00	0.85	0.75	0.81	0.96	0.72	0.56	0.62	0.92	0.76	0.61	0.69	0.95
• Vd1+ Vg9- T cells CD56-		0.88%	0.99	0.98	0.99	1.00	0.89	0.80	0.87	0.96	0.85	0.74	0.80	0.95	0.84	0.73	0.82	0.95
• CD8+ TEMRA T cells CD27+ CD28-		1.2%	0.99	0.98	0.99	1.00	0.77	0.62	0.67	0.92	0.69	0.53	0.59	0.86	0.61	0.44	0.52	0.88
• CD4+ TEM T cells CD27+ CD28+		3.3%	0.99	0.98	0.98	1.00	0.75	0.60	0.62	0.95								
• NK CD16- CD56-		2.4%	0.99	0.97	0.99	1.00	0.80	0.67	0.77	0.94	0.82	0.69	0.83	0.87	0.81	0.68	0.82	0.89
• CD8+ TCM T cells CD27+ CD28+		1.1%	0.98	0.97	0.98	1.00	0.68	0.52	0.55	0.95					0.06	0.03	0.03	0.67
• CD4+ TEM T cells CD27- CD28-		1%	0.98	0.97	0.98	1.00	0.52	0.35	0.36	0.92	0.48	0.32	0.32	0.92	0.48	0.32	0.32	0.91
• CD8+ TEM T cells CD27- CD28-		0.57%	0.98	0.97	0.98	1.00	0.68	0.52	0.53	0.91					0.03	0.02	0.02	0.41
• CD4+ TEM T cells CD27- CD28+		1.1%	0.98	0.97	0.97	1.00	0.61	0.44	0.44	0.94	0.03	0.01	< 0.01	0.55				
• iNKT cells		0.07%	0.98	0.96	0.99	0.99	0.97	0.93	0.99	0.98	0.92	0.85	0.92	0.91	0.96	0.92	0.97	0.96
• CD4+ TEMRA T cells CD27- CD28-		0.18%	0.98	0.96	0.98	0.99	0.48	0.31	0.33	0.80	0.42	0.27	0.27	0.93	0.45	0.28	0.30	0.93
• Vd2 high Vg9+ T cells		0.68%	0.98	0.96	0.98	0.99	0.96	0.93	0.98	0.98	0.95	0.90	0.94	0.99	0.94	0.88	0.93	0.99
• CD8+ TEMRA T cells CD27+ CD28+		0.55%	0.98	0.95	0.97	0.99	0.62	0.45	0.47	0.90	0.08	0.04	0.04	0.69	0.55	0.38	0.42	0.94
• CD4+ TSCM T cells CD27+ CD28+		1%	0.97	0.95	0.96	0.99	0.17	0.09	0.07	0.76	0.02	0.01	0.01	0.50	0.02	0.01	0.01	0.63
• CD4+ TEMRA T cells CD27+ CD28+		0.12%	0.97	0.95	0.96	0.99	0.33	0.20	0.19	0.64								
• CD8+ TEM T cells CD27- CD28+		0.31%	0.97	0.95	0.96	0.99	0.71	0.55	0.57	0.92					0.69	0.53	0.59	0.94
• Q2: Vd1+ Vg9+		0.08%	0.97	0.95	0.98	0.99	0.80	0.67	0.78	0.94	0.81	0.68	0.81	0.90	0.78	0.64	0.76	0.87
• Vd2 low Vg9+ T cells CD56-		0.55%	0.97	0.94	0.97	0.99	0.90	0.81	0.89	0.98	0.89	0.80	0.86	0.95	0.87	0.76	0.85	0.94
• Vd1+ Vg9- T cells CD56+		0.12%	0.97	0.94	0.96	0.99	0.82	0.70	0.78	0.94								
• CD4+ TEM T cells CD27+ CD28-		0.07%	0.97	0.93	0.95	0.99	0.44	0.28	0.31	0.85								
• Mature NK		2.5%	0.96	0.92	0.97	0.98	0.91	0.83	0.88	0.97	0.76	0.62	0.64	0.86	0.88	0.79	0.83	0.96
• CD8+ TSCM T cells CD27+ CD28+		0.14%	0.96	0.92	0.94	0.99	0.30	0.18	0.19	0.91					0.02	0.01	0.01	0.42
• Vd2 low Vg9+ T cells CD56+		0.20%	0.95	0.91	0.95	0.99	0.81	0.68	0.77	0.94								
• MAIT cells		0.51%	0.95	0.90	0.93	0.98	0.74	0.59	0.62	0.85	0.90	0.82	0.87	0.96	0.90	0.82	0.88	0.97
• CD4+ TEMRA T cells CD27- CD28+		0.03%	0.94	0.89	0.91	0.98	0.27	0.16	0.15	0.55								
• CD8+ TCM T cells CD27- CD28+		0.06%	0.94	0.89	0.91	0.98	0.54	0.37	0.41	0.88								
• CD4+ TSCM T cells CD27- CD28+		0.10%	0.94	0.89	0.92	0.98	0.28	0.17	0.18	0.86								
• Early NK		0.92%	0.94	0.88	0.91	0.98	0.84	0.72	0.78	0.96	0.85	0.73	0.80	0.94	0.84	0.73	0.80	0.95
• Terminal NK		0.21%	0.91	0.83	0.84	0.98	0.57	0.41	0.45	0.90					0.07	0.03	0.03	0.52



6.3.4. OMIP-069

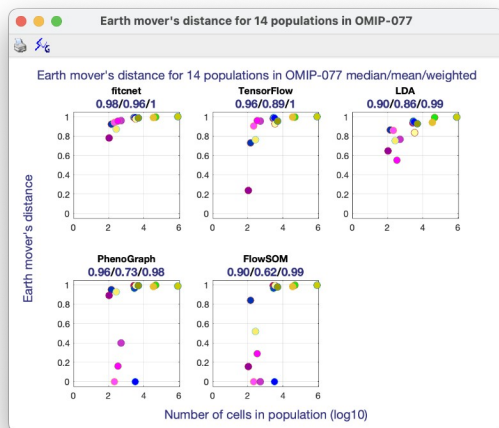
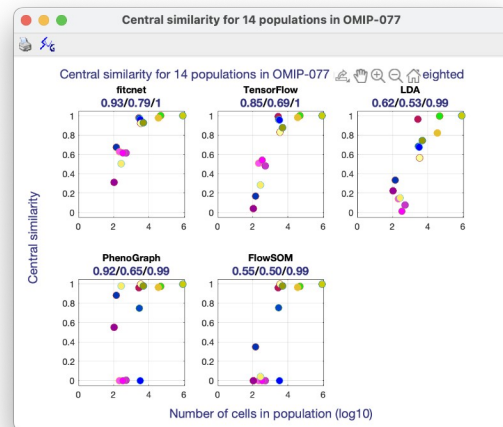
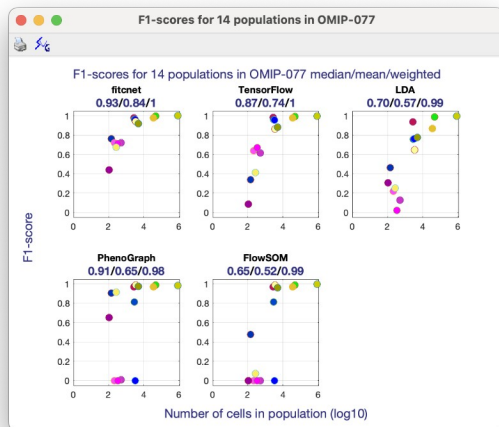
	Classifier	Population	Frequency	MLP				LDA				PhenoGraph				FlowSOM			
				F1-score	J1 100%	J1 80%	EMD	F1-score	J1 100%	J1 80%	EMD	F1-score	J1 100%	J1 80%	EMD	F1-score	J1 100%	J1 80%	EMD
* Naive CD4+		29%	0.98	0.96	0.98	1.00	0.95	0.90	0.95	0.99	0.93	0.86	0.93	0.98	0.90	0.81	0.90	0.95	
		6.8%	0.98	0.96	0.97	1.00	0.91	0.84	0.91	0.97	0.93	0.86	0.93	0.98	0.93	0.87	0.93	0.98	
		9.6%	0.97	0.94	0.97	1.00	0.90	0.83	0.91	0.96	0.96	0.92	0.97	0.99	0.96	0.92	0.97	0.99	
		9.5%	0.96	0.92	0.94	1.00	0.92	0.85	0.90	0.98	0.93	0.87	0.92	0.98	0.92	0.86	0.92	0.98	
		0.97%	0.95	0.91	0.94	0.99	0.94	0.88	0.93	0.99	0.92	0.84	0.91	0.98	0.92	0.86	0.92	0.98	
		4.1%	0.95	0.90	0.91	1.00	0.71	0.55	0.56	0.94	0.38	0.24	0.26	0.75	0.39	0.24	0.25	0.76	
		4.9%	0.94	0.89	0.91	1.00	0.74	0.59	0.63	0.95	0.50	0.33	0.37	0.80	0.52	0.35	0.37	0.95	
		0.94%	0.94	0.88	0.91	0.99	0.56	0.41	0.45	0.89	0.28	0.16	0.18	0.82	0.31	0.18	0.20	0.84	
		2.2%	0.94	0.88	0.89	1.00	0.61	0.44	0.46	0.93									
		4.6%	0.93	0.88	0.90	1.00	0.67	0.50	0.53	0.93	0.48	0.32	0.36	0.88	0.51	0.34	0.37	0.90	
* CD2+ CD8+ NKT		1.3%	0.92	0.85	0.87	0.99	0.75	0.60	0.66	0.90	0.47	0.30	0.33	0.81	0.48	0.32	0.35	0.82	
		0.59%	0.92	0.85	0.89	0.99	0.67	0.51	0.53	0.97									
		0.68%	0.92	0.85	0.90	0.99	0.51	0.34	0.37	0.91	0.51	0.34	0.37	0.88	0.46	0.30	0.34	0.81	
		0.73%	0.91	0.83	0.92	0.97	0.86	0.75	0.85	0.95	0.89	0.80	0.90	0.97	0.84	0.73	0.82	0.96	
		2.2%	0.91	0.83	0.86	0.99	0.66	0.49	0.53	0.92	0.51	0.35	0.38	0.84					
		2.6%	0.91	0.83	0.84	0.99	0.67	0.50	0.54	0.90	0.51	0.35	0.38	0.83	0.53	0.36	0.40	0.87	
		0.45%	0.89	0.80	0.81	0.98	0.57	0.40	0.45	0.86									
		0.69%	0.88	0.79	0.82	0.99	0.74	0.57	0.62	0.94	0.52	0.35	0.40	0.75	0.55	0.37	0.42	0.84	
		0.39%	0.88	0.78	0.82	0.99	0.86	0.75	0.82	0.97	0.79	0.65	0.75	0.96	0.75	0.60	0.72	0.93	
		0.21%	0.88	0.78	0.81	0.98	0.62	0.45	0.47	0.96									
* CCR7- CD45RA+ TCRgD+		0.57%	0.87	0.78	0.81	0.98	0.68	0.51	0.55	0.95	0.75	0.60	0.66	0.94	0.57	0.41	0.45	0.87	
		0.34%	0.87	0.77	0.79	0.99	0.51	0.34	0.35	0.89	0.13	0.07	0.07	0.62	0.01	0.01	0.01	0.56	
		0.22%	0.87	0.77	0.81	0.98	0.67	0.51	0.56	0.87	0.31	0.19	0.15	0.72	0.81	0.68	0.73	0.96	
		0.20%	0.86	0.76	0.79	0.98	0.49	0.34	0.36	0.87									
		0.14%	0.85	0.74	0.77	0.98	0.37	0.22	0.24	0.79									
		0.38%	0.84	0.73	0.75	0.99	0.37	0.23	0.24	0.80					0.06	0.03	0.03	0.52	
		0.22%	0.83	0.71	0.79	0.97	0.51	0.35	0.40	0.83					0.02	0.01	0.01	0.50	
		0.32%	0.82	0.69	0.71	0.98	0.44	0.28	0.28	0.89	0.26	0.15	0.15	0.83	0.30	0.18	0.17	0.85	
		0.12%	0.77	0.63	0.74	0.97	0.41	0.26	0.28	0.87					<0.01	<0.01	<0.01	0.52	
		0.43%	0.75	0.60	0.63	0.97	0.17	0.09	0.09	0.77	0.04	0.02	0.02	0.36	0.33	0.20	0.22	0.64	
* ILCs CD2+ CD4+		0.13%	0.73	0.57	0.63	0.96	0.48	0.31	0.32	0.87									
		0.11%	0.72	0.56	0.62	0.96	0.57	0.41	0.47	0.91	0.45	0.28	0.32	0.80					
		12%	0.69	0.52	0.54	0.98	0.72	0.56	0.57	0.99	0.73	0.57	0.60	0.99	0.73	0.56	0.59	0.99	
		0.20%	0.65	0.48	0.52	0.96	0.41	0.26	0.30	0.88					0.12	0.07	0.07	0.78	
		0.09%	0.62	0.45	0.52	0.92	0.22	0.12	0.13	0.76	0.42	0.27	0.33	0.62	0.39	0.24	0.30	0.74	
		0.06%	0.62	0.45	0.50	0.89	0.47	0.31	0.35	0.85									
		1.2%	0.56	0.39	0.40	0.92	0.60	0.43	0.44	0.97	0.47	0.31	0.31	0.87	0.53	0.36	0.37	0.83	
		0.09%	0.47	0.30	0.34	0.95	0.24	0.14	0.16	0.88					0.21	0.12	0.14	0.88	
		0.03%	0.43	0.28	0.30	0.93	0.28	0.17	0.17	0.92	0.22	0.12	0.12	0.87	0.33	0.19	0.20	0.95	
		0.07%	0.34	0.21	0.22	0.92	0.28	0.16	0.18	0.78	0.05	0.02	0.03	0.48	0.10	0.05	0.07	0.56	
* Non classical monocytes		0.15%	0.02	0.01	0.01	0.80	0.16	0.08	0.09	0.78	0.04	0.02	0.02	0.34	0.08	0.04	0.03	0.50	
		0.30%	<0.01	<0.01	<0.01	0.67	0.04	0.02	0.02	0.67	0.16	0.09	0.10	0.60	0.05	0.03	0.03	0.62	
		0.01%					0.10	0.05	0.06	0.77					0.02	0.01	0.01	0.64	



6.3.5. OMIP-077

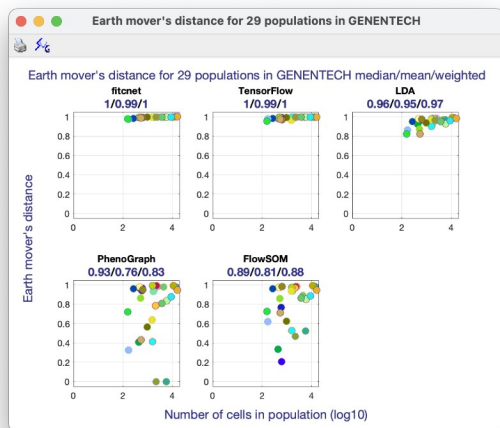
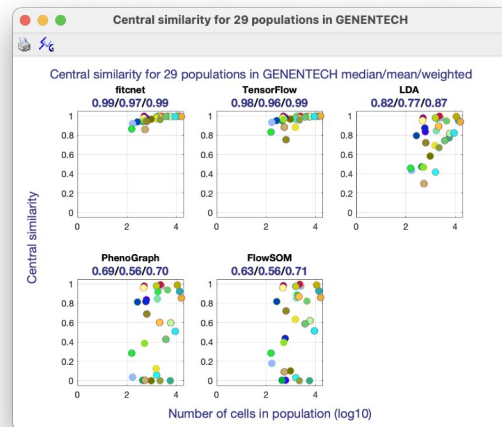
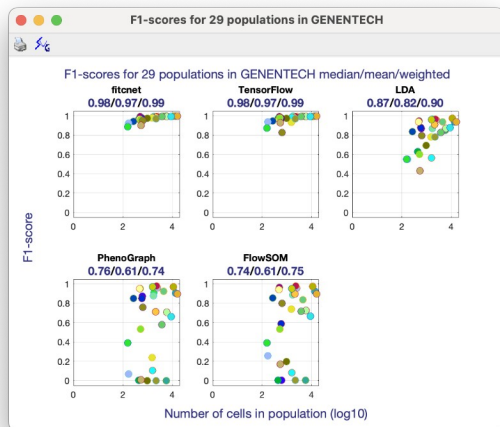
Classifier		MLP				LDA				PhenoGraph				FlowSOM			
Population	Frequency	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD
● Neutrophils	77%	1.00	1.00	1.00	1.00	1.00	0.99	1.00	1.00	0.99	0.97	1.00	0.99	1.00	0.99	1.00	1.00
● T cells	11%	1.00	1.00	1.00	1.00	0.99	0.98	1.00	0.99	0.99	0.97	0.98	1.00	0.99	0.97	0.98	1.00
● Monocytes	6.9%	0.98	0.96	0.98	0.99	0.87	0.77	0.82	0.94	0.97	0.94	0.97	0.98	0.97	0.94	0.97	0.98
● Basophils	0.34%	0.98	0.96	0.98	0.99	0.94	0.88	0.97	0.94	0.97	0.94	0.96	0.99	0.97	0.94	0.96	0.99
● Non MZB cells	1.4%	0.97	0.93	0.97	0.99	0.76	0.61	0.68	0.96	0.81	0.69	0.75	0.96	0.82	0.69	0.75	0.96
● MZB cells	0.52%	0.96	0.92	0.96	0.99	0.76	0.62	0.67	0.95								
● Eosinophils	1.3%	0.94	0.89	0.92	0.98	0.65	0.50	0.56	0.84	0.99	0.98	1.00	0.99	0.99	0.98	1.00	0.99
● NK cells	2%	0.92	0.85	0.93	0.99	0.78	0.64	0.74	0.93	0.97	0.95	0.98	0.99	0.96	0.92	0.98	0.98
● Plasma cells	0.09%	0.76	0.62	0.68	0.93	0.46	0.30	0.33	0.86	0.91	0.83	0.88	0.95	0.48	0.31	0.35	0.84
● CD1c+ mDCs	0.03%	0.72	0.56	0.63	0.94	0.22	0.13	0.14	0.86								
● CD141- mDCs	0.04%	0.72	0.56	0.62	0.96	0.13	0.07	0.08	0.77	0.01	< 0.01	< 0.01	0.40				
● CD141+ mDCs	0.01%	0.71	0.55	0.61	0.95	0.02	0.01	0.01	0.55								
● Progenitors	0.07%	0.68	0.51	0.50	0.87	0.25	0.15	0.15	0.75	0.91	0.84	0.98	0.93	0.07	0.04	0.04	0.52
● pDCs	0.04%	0.44	0.28	0.31	0.78	0.30	0.19	0.23	0.65	0.65	0.48	0.55	0.89				
Medians		0.93	0.87	0.93	0.98	0.70	0.55	0.62	0.90	0.91	0.83	0.92	0.96	0.65	0.50	0.55	0.90
Means		0.84	0.76	0.79	0.96	0.57	0.49	0.53	0.86	0.65	0.61	0.65	0.73	0.52	0.49	0.50	0.62

Columns		Rows	
Legend	• F1-score=overlap measured by harmonic mean of percision + recall (AKA <i>F measure</i>).	Coloring is based on ranking by <i>F1-score median</i>	
	• JI 100%=whole population overlap measured by intersection/union (AKA <i>jaccard index</i>).	Narrow lead over next	1st 2nd 3rd Last
	• JI 80%=central core region overlap (AKA <i>central similarity</i>).	Wide lead over next	1st 2nd 3rd Nothing is next
	• JI 80% minus JI 100% size has <i>low to high emphasis</i> .	Ties get same ranked color....	
		Median minus mean size is <i>emphasized</i> pos/neg.	



6.3.6. ESHGHI

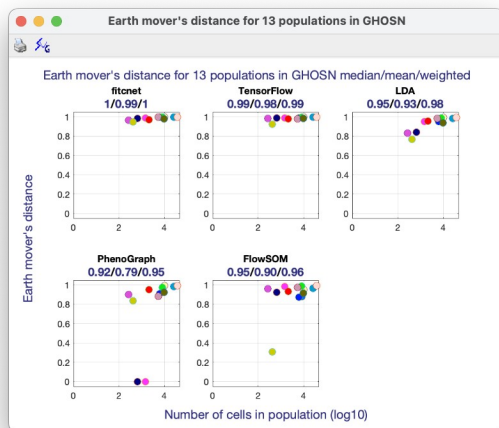
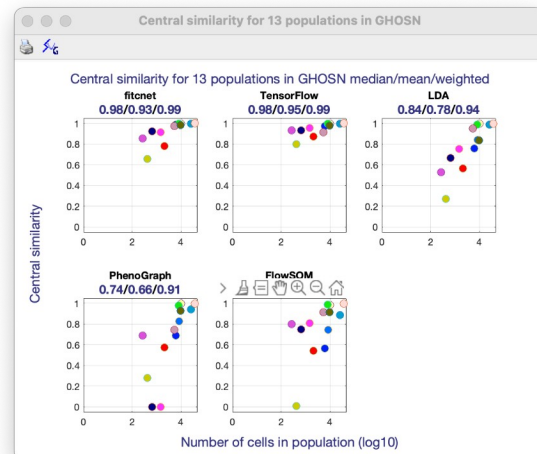
Classifier		MLP				LDA				PhenoGraph				FlowSOM			
Population	Freq- uency	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD	F1- score	JI 100%	JI 80%	EMD
• CD4 N	15%	1.00	0.99	1.00	1.00	0.94	0.88	0.95	0.99	0.91	0.83	0.92	0.98	0.92	0.86	0.93	0.98
• CD16hi NK	12%	1.00	0.99	1.00	1.00	0.97	0.95	0.99	0.99	0.97	0.94	0.99	0.99	0.97	0.95	0.99	0.99
• CD8 N	4.8%	1.00	0.99	1.00	1.00	0.94	0.88	0.95	0.97	0.92	0.86	0.94	0.98	0.84	0.72	0.82	0.89
• CD14hi Mono	17%	1.00	0.99	0.99	1.00	0.94	0.88	0.94	0.98	0.90	0.81	0.85	0.95	0.90	0.81	0.86	0.95
• CD4 CM	6.2%	0.99	0.99	0.99	1.00	0.85	0.74	0.77	0.97								
• gd Tcells	1.9%	0.99	0.99	1.00	1.00	0.97	0.93	0.97	0.99	0.91	0.83	0.92	0.95	0.90	0.81	0.89	0.97
• CD8 Temra	6.3%	0.99	0.99	0.99	1.00	0.87	0.76	0.82	0.93	0.71	0.55	0.60	0.84	0.72	0.56	0.62	0.85
• CD4 EM	9.6%	0.99	0.99	0.99	1.00	0.88	0.78	0.82	0.96	0.66	0.49	0.51	0.88	0.67	0.50	0.52	0.89
• Naive B	2.7%	0.99	0.99	1.00	1.00	0.96	0.92	0.98	0.98	0.96	0.92	0.98	0.98	0.96	0.92	0.98	0.99
• Basophils	2.5%	0.99	0.99	1.00	1.00	0.96	0.93	1.00	0.96	0.98	0.96	0.99	0.99	0.98	0.96	1.00	0.98
• CD8 EM	4%	0.99	0.98	0.99	1.00	0.83	0.70	0.75	0.95	0.57	0.41	0.43	0.81	0.72	0.56	0.59	0.86
• pDCs	0.54%	0.99	0.98	1.00	1.00	0.95	0.90	0.98	0.95	0.95	0.91	0.98	0.96	0.96	0.93	0.99	0.98
• CD8 MAIT	1.9%	0.99	0.98	0.99	1.00	0.87	0.76	0.85	0.92	0.88	0.78	0.85	0.93	0.89	0.79	0.85	0.94
• CD16hi Mono	2.3%	0.99	0.98	0.99	1.00	0.91	0.84	0.89	0.98	0.71	0.55	0.60	0.79	0.90	0.81	0.87	0.97
• Neutrophil	1.7%	0.98	0.97	0.99	1.00	0.96	0.93	0.98	0.98	0.97	0.94	0.98	0.99	0.95	0.91	0.97	0.97
• CD4 Temra	1.7%	0.98	0.96	0.97	1.00	0.56	0.39	0.42	0.90	0.10	0.05	0.06	0.41	0.08	0.04	0.03	0.53
• int Mono	1.6%	0.98	0.96	0.97	1.00	0.78	0.64	0.70	0.97	0.24	0.13	0.12	0.64	0.74	0.57	0.63	0.94
• Trans B	0.67%	0.97	0.95	0.97	0.99	0.87	0.76	0.83	0.97	0.87	0.78	0.84	0.96	< 0.01	< 0.01	< 0.01	0.21
• Treg	1%	0.97	0.95	0.96	1.00	0.69	0.53	0.57	0.94					0.20	0.11	0.10	0.63
• HLADRlo Mono	2.4%	0.97	0.94	0.96	1.00	0.78	0.64	0.67	0.96								
• Mem B	0.64%	0.97	0.94	0.97	0.99	0.88	0.78	0.87	0.97	0.85	0.74	0.82	0.94	0.59	0.42	0.43	0.77
• CD8 CM	0.48%	0.97	0.93	0.94	0.99	0.63	0.46	0.47	0.92	< 0.01	< 0.01	< 0.01	0.41	< 0.01	< 0.01	< 0.01	0.34
• Eosinophil	0.52%	0.96	0.93	0.97	0.99	0.94	0.88	0.95	0.98	0.95	0.90	0.96	0.98	0.94	0.89	0.96	0.97
• [CD14- CD16-]	0.56%	0.96	0.92	0.95	0.99	0.60	0.43	0.47	0.87	0.53	0.36	0.39	0.86	0.53	0.36	0.40	0.86
• CD56hi NK	0.70%	0.95	0.91	0.94	0.99	0.79	0.66	0.72	0.97	0.76	0.61	0.69	0.95	0.80	0.66	0.72	0.98
• Plasmablast	0.28%	0.94	0.89	0.94	0.99	0.83	0.72	0.80	0.95	0.85	0.74	0.81	0.96	0.86	0.75	0.82	0.96
• IgD- CD27- B	0.18%	0.93	0.86	0.92	0.98	0.55	0.38	0.44	0.86	0.07	0.03	0.03	0.33	0.26	0.15	0.18	0.62
• Lineage Negative	0.57%	0.90	0.82	0.86	0.99	0.43	0.28	0.30	0.82	0.01	< 0.01	< 0.01	0.43	0.17	0.09	0.09	0.71
• [CD123-]	0.17%	0.89	0.80	0.86	0.98	0.55	0.38	0.46	0.82	0.39	0.24	0.28	0.72	0.39	0.24	0.28	0.73
Medians		0.98	0.97	0.99	1.00	0.87	0.76	0.82	0.96	0.76	0.61	0.69	0.93	0.74	0.57	0.63	0.89
Means		0.97	0.95	0.97	0.99	0.82	0.71	0.77	0.95	0.61	0.53	0.56	0.76	0.61	0.53	0.56	0.81



6.3.7. GHOSN

Population	Classifier	Frequency	MLP				LDA				PhenoGraph				FlowSOM			
			F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD
• B-1		22%	0.99	0.99	1.00	1.00	0.97	0.93	0.99	0.98	0.95	0.90	0.94	0.99	0.90	0.82	0.89	0.97
• Large macrophages		32%	0.99	0.98	1.00	1.00	0.98	0.97	1.00	0.99	0.98	0.97	1.00	0.99	0.99	0.97	1.00	0.99
• B-2 IgM medium		7.2%	0.99	0.98	0.99	1.00	0.89	0.79	0.84	0.95	0.84	0.73	0.83	0.93	0.79	0.66	0.74	0.88
• T cells		6.9%	0.99	0.97	1.00	0.99	0.97	0.94	0.99	0.99	0.96	0.93	0.98	0.98	0.97	0.95	0.99	0.99
• Eosinophils		8.6%	0.99	0.97	1.00	1.00	0.98	0.96	1.00	0.99	0.98	0.96	1.00	0.99	0.94	0.89	0.99	0.95
• B-2 IgM high		5.3%	0.98	0.96	0.98	0.99	0.82	0.70	0.76	0.95	0.75	0.60	0.69	0.91	0.67	0.51	0.56	0.87
• NK, NKT		8.3%	0.97	0.95	0.98	0.98	0.84	0.72	0.84	0.94	0.89	0.80	0.93	0.92	0.89	0.80	0.92	0.91
• CD11b+ dendritic		1.3%	0.95	0.91	0.96	0.99	0.83	0.70	0.75	0.95					0.86	0.76	0.81	0.98
• Developing B		0.55%	0.95	0.90	0.93	0.99	0.77	0.62	0.66	0.84					0.83	0.71	0.75	0.92
• Small macrophages		4.6%	0.94	0.88	0.91	0.98	0.94	0.89	0.95	0.99	0.81	0.69	0.74	0.88	0.92	0.85	0.91	0.97
• CD11b- dendritic		0.23%	0.93	0.87	0.93	0.98	0.63	0.46	0.53	0.83	0.77	0.62	0.69	0.90	0.83	0.71	0.80	0.96
• ckit+ mast cells		1.8%	0.90	0.82	0.87	0.98	0.68	0.52	0.56	0.96	0.69	0.53	0.56	0.95	0.66	0.49	0.54	0.93
• Neutrophils		0.36%	0.84	0.72	0.80	0.92	0.39	0.25	0.27	0.77	0.43	0.28	0.28	0.83	0.01	0.01	0.01	0.30
Medians			0.97	0.95	0.98	0.99	0.84	0.72	0.84	0.95	0.81	0.69	0.74	0.92	0.86	0.76	0.81	0.95
Means			0.95	0.92	0.95	0.98	0.82	0.73	0.78	0.93	0.70	0.62	0.66	0.79	0.79	0.70	0.76	0.90

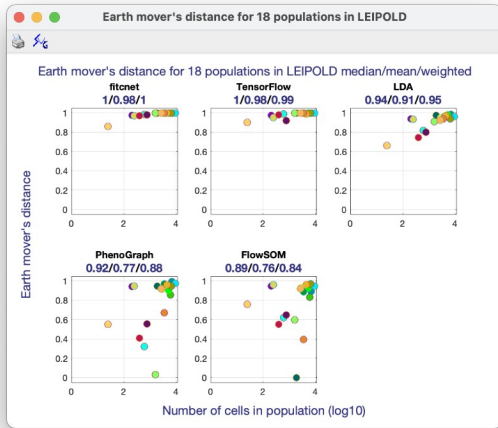
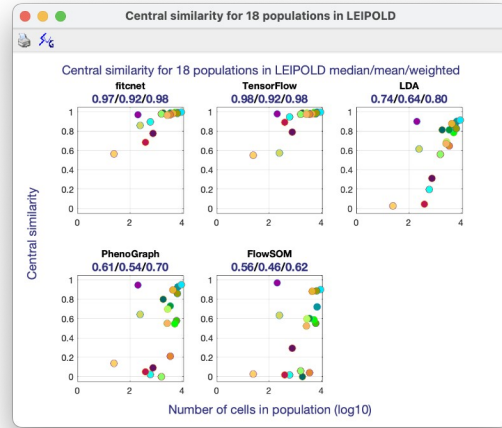
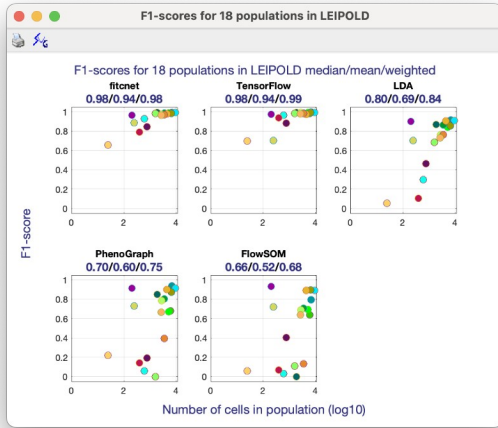
	Columns	Rows				
Legend	- F1-score=overlap measured by harmonic mean of percision + recall (AKA <i>F measure</i>). - JI 100%=whole population overlap measured by intersection/union (AKA <i>jaccard index</i>). - JI 80%=central core region overlap (AKA <i>central similarity</i>). - JI 80% minus JI 100% size has low to high emphasis. - EMD=earth mover's distance	Coloring is based on ranking by <i>F1-score median</i>				
		<i>Narrow lead over next</i>	1st	2nd	3rd	Last
		<i>Wide lead over next</i>	1st	2nd	3rd	Nothing is next
		Ties get same ranked color...				
		Median minus mean size is emph sized pos/neg.				



6.3.8. LEIPOLD

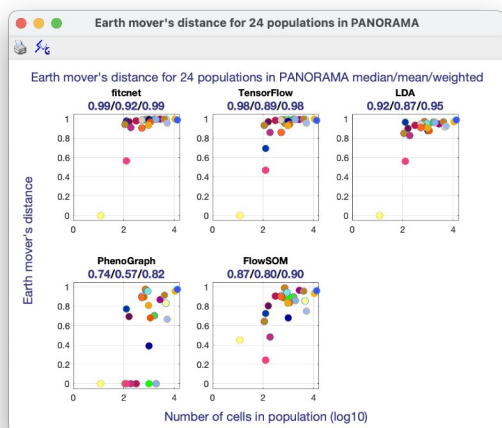
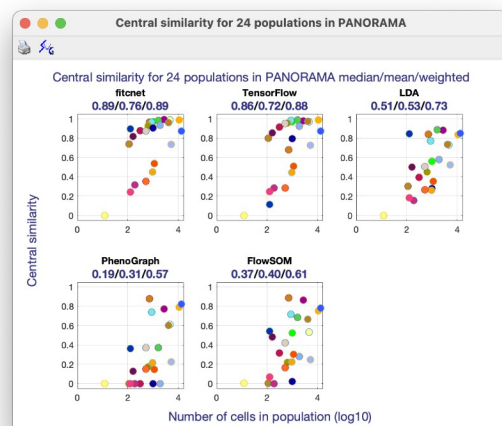
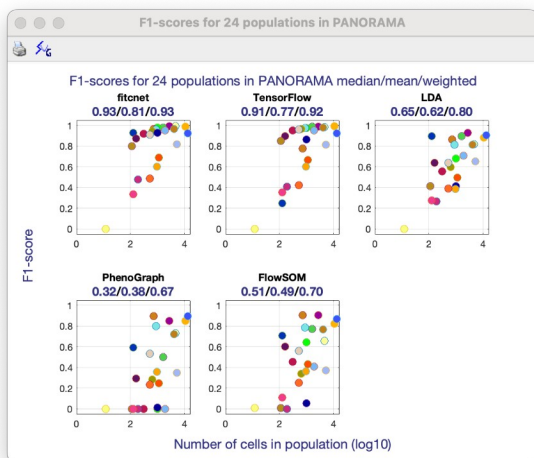
Classifier		MLP					LDA				PhenoGraph				FlowSOM				
Population		Frequency	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	
●	CD4 T cells CD45RA- , CD27+	12%	1.00	0.99	1.00	1.00	0.92	0.85	0.90	0.98	0.94	0.88	0.93	0.99	0.79	0.66	0.72	0.89	
●	CD4 T cells CD45RA+ , CD27+	16%	0.99	0.99	1.00	1.00	0.91	0.83	0.92	0.96	0.92	0.85	0.95	0.97	0.89	0.80	0.90	0.95	
●	CD8 T cells CD45RA+ , CD27-	9.1%	0.99	0.98	0.99	1.00	0.84	0.72	0.78	0.98	0.67	0.51	0.55	0.90	0.69	0.53	0.59	0.92	
●	CD4 T cells CD45RA- , CD27-	3.4%	0.99	0.98	0.99	1.00	0.87	0.76	0.81	0.97	0.85	0.74	0.80	0.95					
●	● NK cells	12%	0.99	0.98	0.99	1.00	0.86	0.75	0.83	0.94	0.87	0.77	0.86	0.95	0.90	0.82	0.89	0.97	
●	● CD4- CD8-	5%	0.99	0.98	0.99	1.00	0.76	0.61	0.69	0.95	0.79	0.65	0.70	0.92	0.69	0.52	0.60	0.93	
●	CD8 T cells CD45RA- , CD27+	6.3%	0.99	0.98	0.98	1.00	0.86	0.76	0.81	0.96	0.80	0.67	0.73	0.97	0.71	0.55	0.60	0.89	
●	CD8 T cells CD45RA- , CD27-	2.8%	0.98	0.97	0.97	1.00	0.68	0.52	0.56	0.91					0.11	0.06	0.06	0.59	
●	CD8 T cells CD45RA+ , CD27+	11%	0.98	0.97	0.98	1.00	0.86	0.76	0.84	0.96	0.68	0.52	0.57	0.85	0.64	0.47	0.55	0.83	
●	● CD38 CD56- B cells	6.2%	0.98	0.96	0.98	1.00	0.76	0.62	0.65	0.94	0.39	0.24	0.21	0.67	0.13	0.07	0.04	0.39	
●	● CD38+CD56 B cells	4.7%	0.98	0.96	0.97	1.00	0.73	0.57	0.67	0.92	0.66	0.50	0.55	0.92	0.64	0.47	0.52	0.92	
●	● CD16- monocytes	7.9%	0.98	0.95	0.98	0.99	0.90	0.82	0.88	0.97	0.90	0.82	0.90	0.96	0.89	0.80	0.88	0.96	
●	● pDCs	0.37%	0.97	0.95	0.98	0.98	0.90	0.82	0.90	0.94	0.92	0.84	0.95	0.94	0.93	0.87	0.97	0.95	
●	CD4 T cells CD45RA+ , CD27-	1.1%	0.97	0.93	0.95	0.99	0.30	0.18	0.20	0.82	0.06	0.03	0.02	0.32	0.03	0.02	0.02	0.62	
●	● Basophils	0.69%	0.94	0.88	0.89	0.98	0.11	0.06	0.05	0.75	0.14	0.08	0.05	0.41	0.07	0.04	0.02	0.55	
●	● mDCs	1.4%	0.88	0.79	0.79	0.92	0.47	0.30	0.31	0.80	0.19	0.11	0.09	0.55	0.40	0.25	0.28	0.65	
●	● CD56 bright NK cells	0.44%	0.70	0.54	0.56	0.95	0.70	0.54	0.62	0.93	0.73	0.56	0.64	0.95	0.72	0.56	0.63	0.96	
●	● CD16+ monocytes	0.04%	0.70	0.54	0.55	0.90	0.05	0.03	0.03	0.66	0.22	0.12	0.14	0.55	0.06	0.03	0.03	0.76	
			Medians	0.98	0.97	0.98	1.00	0.80	0.67	0.74	0.94	0.70	0.54	0.61	0.92	0.66	0.50	0.56	0.89
			Means	0.94	0.91	0.92	0.98	0.69	0.57	0.64	0.91	0.60	0.49	0.54	0.77	0.52	0.42	0.46	0.76

	Columns	Rows										
Legend	- F1-score=overlap measured by harmonic mean of percision & recall (AKA <i>F measure</i>). - JI 100%=whole population overlap measured by intersection/union (AKA <i>jaccard index</i>). - JI 80%=central core region overlap (AKA <i>central similarity</i>). - JI 80% minus JI 100% size has low to high emphasis. - EMD=earth mover's distance	Coloring is based on ranking by F1-score median <table> <tr> <td>Narrow lead over next</td><td>1st</td><td>2nd</td><td>3rd</td><td>Last</td></tr> <tr> <td>Wide lead over next</td><td>1st</td><td>2nd</td><td>3rd</td><td>Nothing is next</td></tr> </table> Ties get same ranked color.... Median minus mean size is emph sized pos/neg.	Narrow lead over next	1st	2nd	3rd	Last	Wide lead over next	1st	2nd	3rd	Nothing is next
Narrow lead over next	1st	2nd	3rd	Last								
Wide lead over next	1st	2nd	3rd	Nothing is next								



6.3.9. PANORAMA

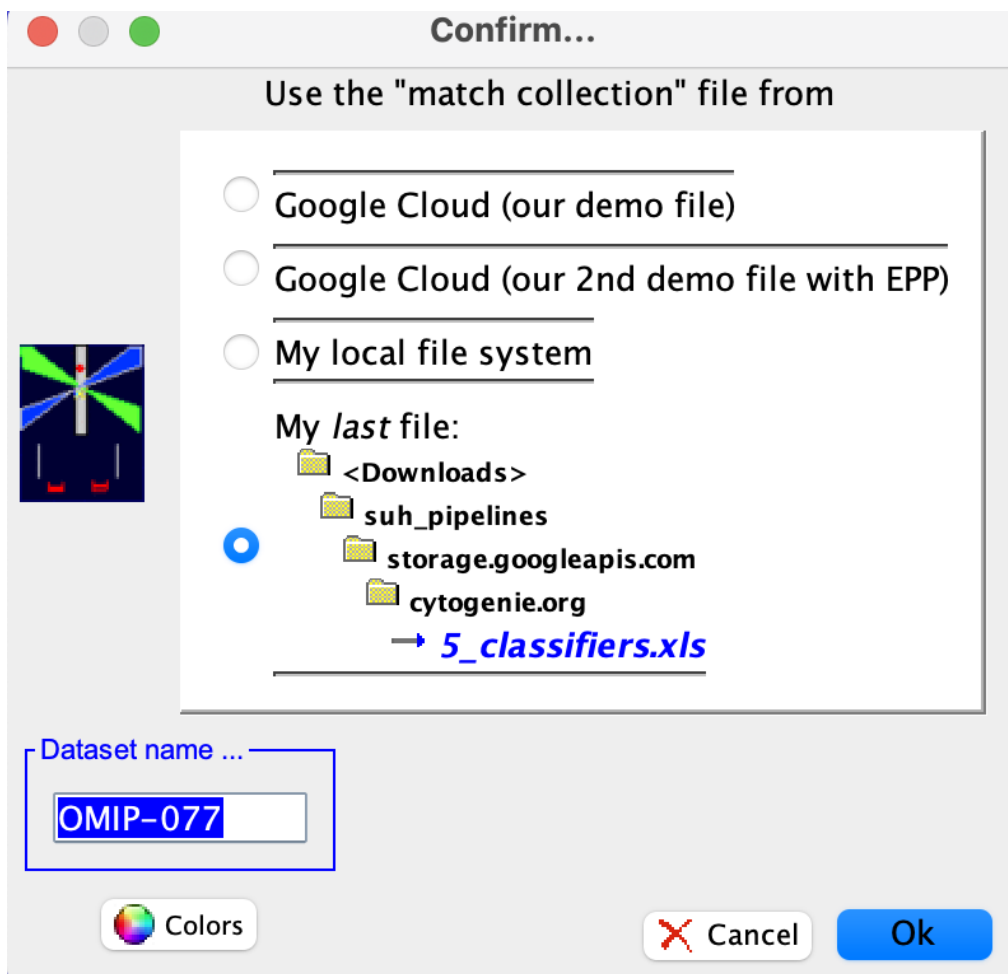
Population	Classifier	Frequency	MLP				LDA				PhenoGraph				FlowSOM			
			F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD	F1-score	JI 100%	JI 80%	EMD
• Eosinophils		8.8%	0.99	0.98	0.99	1.00	0.82	0.69	0.73	0.92	0.73	0.57	0.61	0.83	0.66	0.49	0.53	0.85
• pDCs		5.2%	0.99	0.98	0.99	1.00	0.93	0.86	0.88	0.95	0.85	0.74	0.77	0.87	0.91	0.83	0.86	0.96
• Classical Monocytes		21%	0.99	0.98	0.99	1.00	0.88	0.79	0.83	0.97	0.85	0.74	0.79	0.95	0.82	0.70	0.75	0.93
• CD8 T cells		3%	0.98	0.96	0.98	1.00	0.90	0.81	0.88	0.97	0.50	0.33	0.37	0.70	0.77	0.63	0.68	0.89
• NKT cells		1.9%	0.98	0.96	0.97	1.00	0.68	0.51	0.56	0.92					0.64	0.48	0.52	0.90
• Intermediate Monocytes		7.7%	0.97	0.94	0.96	1.00	0.81	0.68	0.73	0.97	0.72	0.56	0.60	0.91	0.77	0.62	0.67	0.96
• Non classical Monocytes		1.4%	0.96	0.93	0.96	0.99	0.86	0.76	0.84	0.97	0.90	0.81	0.88	0.98	0.91	0.83	0.89	0.99
• CD4 T cells		1.6%	0.96	0.92	0.97	0.99	0.81	0.68	0.77	0.95	0.80	0.67	0.74	0.96	0.79	0.65	0.72	0.94
• B cells Frac. D		3.7%	0.95	0.90	0.93	0.99	0.71	0.55	0.57	0.96					0.41	0.26	0.28	0.86
• NK cells		1.2%	0.94	0.89	0.93	0.99	0.59	0.42	0.45	0.93	0.28	0.17	0.17	0.90	0.34	0.20	0.22	0.89
• B cells Frac A-C		1.9%	0.93	0.87	0.91	0.99	0.41	0.26	0.28	0.88					0.05	0.03	0.02	0.68
• Plasma Cells		0.24%	0.93	0.86	0.90	0.98	0.90	0.81	0.85	0.97	0.59	0.42	0.36	0.77	0.71	0.55	0.54	0.72
• B cells Frac. F		25%	0.92	0.86	0.87	0.99	0.91	0.83	0.85	0.99	0.89	0.81	0.82	0.97	0.87	0.76	0.78	0.96
• Basophils		0.57%	0.92	0.85	0.88	0.98	0.55	0.38	0.39	0.93					0.46	0.30	0.31	0.90
• Macrophages		1%	0.91	0.84	0.88	0.99	0.64	0.47	0.50	0.94	0.53	0.36	0.37	0.91	0.56	0.39	0.42	0.91
• mDCs		0.30%	0.87	0.77	0.82	0.97	0.64	0.47	0.50	0.90	0.28	0.17	0.13	0.69	0.60	0.43	0.48	0.81
• B cells Frac. E		9.8%	0.82	0.69	0.74	0.95	0.65	0.49	0.52	0.92	0.35	0.21	0.22	0.67	0.37	0.23	0.25	0.75
• gd T cells		0.21%	0.80	0.67	0.74	0.94	0.41	0.26	0.30	0.85					0.01	< 0.01	0.01	0.64
• GMP		2.1%	0.69	0.53	0.54	0.97	0.50	0.33	0.35	0.88	0.25	0.14	0.14	0.68	0.43	0.28	0.30	0.84
• MEP		1.8%	0.60	0.43	0.45	0.93	0.39	0.24	0.26	0.91	0.36	0.22	0.22	0.81	0.36	0.22	0.23	0.83
• CMP		1%	0.49	0.32	0.35	0.90	0.39	0.24	0.27	0.91	0.24	0.13	0.15	0.89	0.25	0.15	0.17	0.90
• MPP		0.35%	0.47	0.31	0.32	0.91	0.26	0.15	0.16	0.83								
• CLP		0.24%	0.34	0.20	0.24	0.56	0.27	0.16	0.18	0.56					0.11	0.06	0.07	0.24
• HSC		0.02%													0.01	< 0.01	< 0.01	0.45
Medians			0.93	0.86	0.89	0.99	0.65	0.48	0.51	0.92	0.32	0.19	0.19	0.74	0.51	0.34	0.37	0.87
Means			0.81	0.74	0.76	0.92	0.62	0.49	0.53	0.87	0.38	0.28	0.31	0.57	0.49	0.38	0.40	0.80



6.4. Reproducing tables and figures

To view the tables and figures *interactively* for this final round of testing

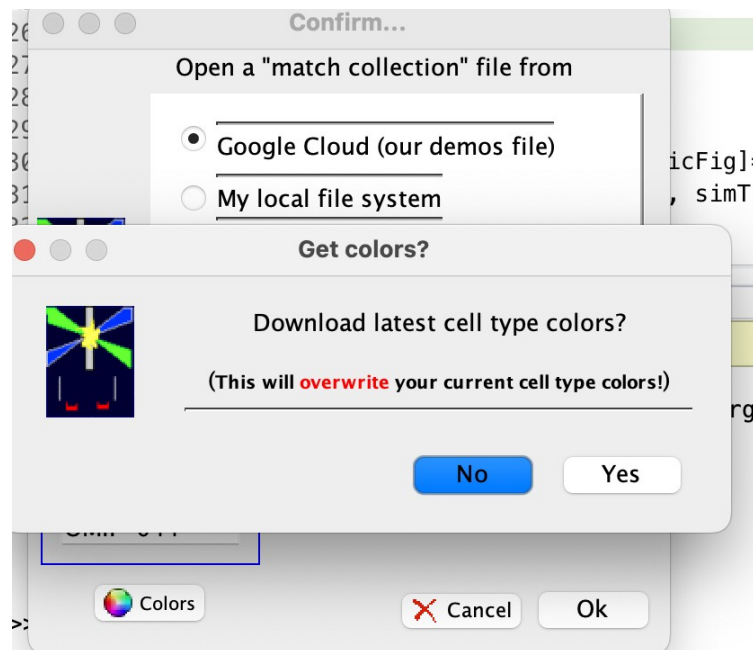
- Open MATLAB R2021a or later
- Type the command `fjb` to start FlowJoBridge
- Type the command `ClassificationTable.See('dataset name')` where 'dataset name' is 'OMIP-044' or whatever name appears in this document above the tables
- The first time you do this select the first option "Google Cloud (our demos file)". After that select the last option "My *last* choice"
- Click OK on this dialog box



The first time you run this command download our xls file and colors from the Google cloud.

To get the xls file select the first item in this dialog.

To get the colors click the color button at the bottom left of the dialog and answer yes to the question.



For all of this testing and validation we assist our reviewers and readers in reproducing our findings by make everything publicly accessible from our Google Cloud storage:

- All the software we developed.
- All the data sets with which we test it.
- FlowJo workspaces that capture publication recommended manual gating *so you don't have to redraw them*.
- Documents describing step by step how to get the above stuff and use our FlowJoBridge GUI to get the same results with each gating method and each dataset

Reproducing our findings requires skill similar to those needed to install and use a text editor. No skill in programming/scripting, mathematics or statistics are needed. Easy reproducibility of the findings of flow informatics by non technical biologists is critical for the progress of immunology. For example, we might have compared MLP directly with flowDensity if it did not cost both significant programming expertise with their R libraries as well as significant manual gating expertise with each gate in each of the publications we evaluate. But we expect flowDensity to be the best at replicating manual gating on a specific assay by specific assay basis if given enough expert programming, testing and re-programming as edge samples for equivalent gating come in. So instead our primary goal is to do as flowDensity did in 2015 without the training expense but with their near perfect replication of expert manual gates. Our

secondary goal is to exceed all methods by being as easy and robust to use as a text editor so that biologists can focus on biology. No need for each and every new biological assay to cost either manual gating or a mini software development project.

One only needs our FlowJo bridge to reproduce our findings with this publication's FlowJo workspaces. Having FlowJo is only necessary to create new workspaces to run with our bridge.