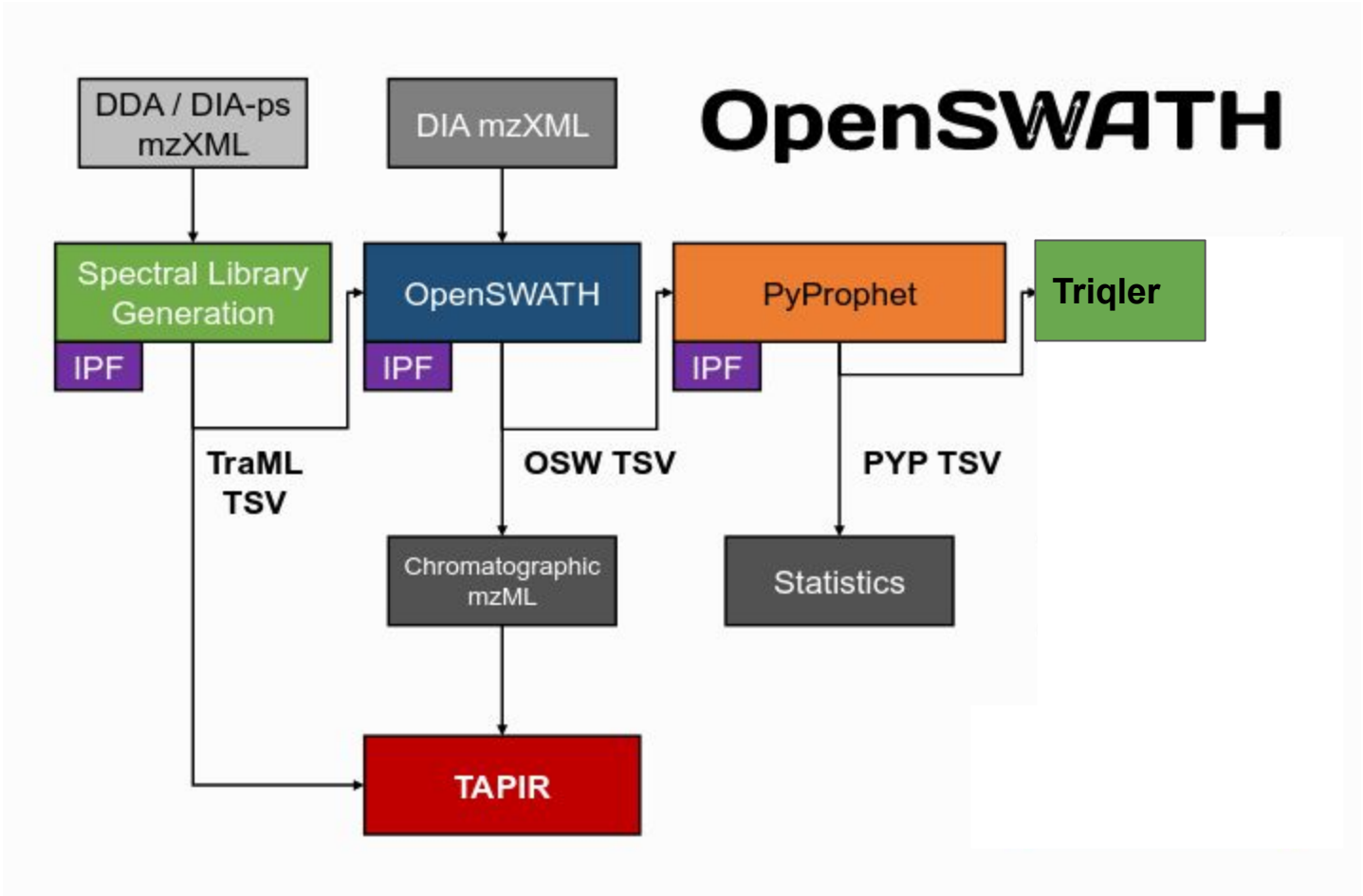
OpenSwath vs Triqler

2021-03-31


DDA / DIA-ps mzXML
DIA mzXML
OpenSWATH
Spectral Library Generation
IPF
OpenSWATH
IPF
PyProphet
IPF
Triqler
TraML TSV
OSW TSV
PYP TSV
Chromatographic mzML
Statistics
TAPIR

Data

Spectral library based on UniProt - SwissProt (from Tenzer repo PXD002952). No proteoforms.

OpenSwath (PyProphet) filtering m_score fdr < 0.01.

Intensity for protein with highest searchScore (-np.log10(m_score)) selected (same as Triqler).

Triqler threshold protein_id_posterior_error_prob < 0.01.

(The *q_value* and *posterior_error_prob* columns represent respectively the FDR and PEP for the hypothesis that the protein was correctly identified and has a fold change larger than the specified --fold_change_eval.

The *protein_id_PEP* and *diff_exp_prob_<FC>* columns are simply the separate probabilities that make up the above hypothesis test, i.e. for correct identification and for fold change respectively.

NOTE: Using the q_value or posterior_error_prob for the hypothesis that the protein was correctly identified and has a fold change larger than the specified --fold_change_eval gives 1 significant hit...)

ECOLI A:B 4:1 ratio, log2fc_treshold = 2.0

	005-Pedro_group_2_log2(B)	006-Pedro_group_1_log2(B)	003-Pedro_group_2_log2(B)	004-Pedro_group_1_log2(B)	007-Pedro_group_2_log2(B)	002-Pedro_group_1_log2(B)
005-roup_2_log2(A)	0	108	124	99	119	87
006-roup_1_log2(A)	185	0	175	100	188	101
003-roup_2_log2(A)	129	100	0	106	129	91
004-roup_1_log2(A)	146	89	149	0	165	76
007-roup_2_log2(A)	115	107	119	92	0	87
002-roup_1_log2(A)	205	138	184	112	221	0

	1:002-Pedro_log2(B)	1:004-Pedro_log2(B)	1:006-Pedro_log2(B)	2:003-Pedro_log2(B)	2:005-Pedro_log2(B)	2:007-Pedro_log2(B)
1:002-Pedro_log2(A)	0	12	17	134	228	342
1:004-Pedro_log2(A)	5	0	16	57	93	132
1:006-Pedro_log2(A)	5	9	0	56	76	109
2:003-Pedro_log2(A)	1	1	3	0	1	1
2:005-Pedro_log2(A)	2	2	5	0	0	0

ECOLI A:B 4:1 ratio, log2fc_treshold = 2.0

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2:005-Pedro_log2(A)	2	2	5	0	0	0

YEAST A:B = 2:1 ratio, log2fc_treshold = 1.0

	005-Pedro_group_2_log2(B)	006-Pedro_group_1_log2(B)	003-Pedro_group_2_log2(B)	004-Pedro_group_1_log2(B)	007-Pedro_group_2_log2(B)	002-Pedro_group_1_log2(B)
005-roup_2_log2(A)	0	228	266	242	271	272
006-roup_1_log2(A)	526	0	534	303	479	366
003-roup_2_log2(A)	264	237	0	245	265	282
004-roup_1_log2(A)	509	285	522	0	463	334
007-roup_2_log2(A)	274	227	277	244	0	286
002-roup_1_log2(A)	403	253	403	254	371	0

	1:002-Pedro_log2(B)	1:004-Pedro_log2(B)	1:006-Pedro_log2(B)	2:003-Pedro_log2(B)	2:005-Pedro_log2(B)	2:007-Pedro_log2(B)
1:002-Pedro_log2(A)	0	2	1	348	166	113
1:004-Pedro_log2(A)	6	0	4	756	528	385
1:006-Pedro_log2(A)	9	8	0	830	661	542
2:003-Pedro_log2(A)	15	9	9	0	26	27
2:005-Pedro_log2(A)	13	9	9	32	0	31
2:007-Pedro_log2(A)	8	6	6	40	25	0

YEAST A:B = 2:1 ratio, log2fc_treshold = 1.0

	005-Pedro_group_2_log2(B)	006-Pedro_group_1_log2(B)	003-Pedro_group_2_log2(B)	004-Pedro_group_1_log2(B)	007-Pedro_group_2_log2(B)	002-Pedro_group_1_log2(B)
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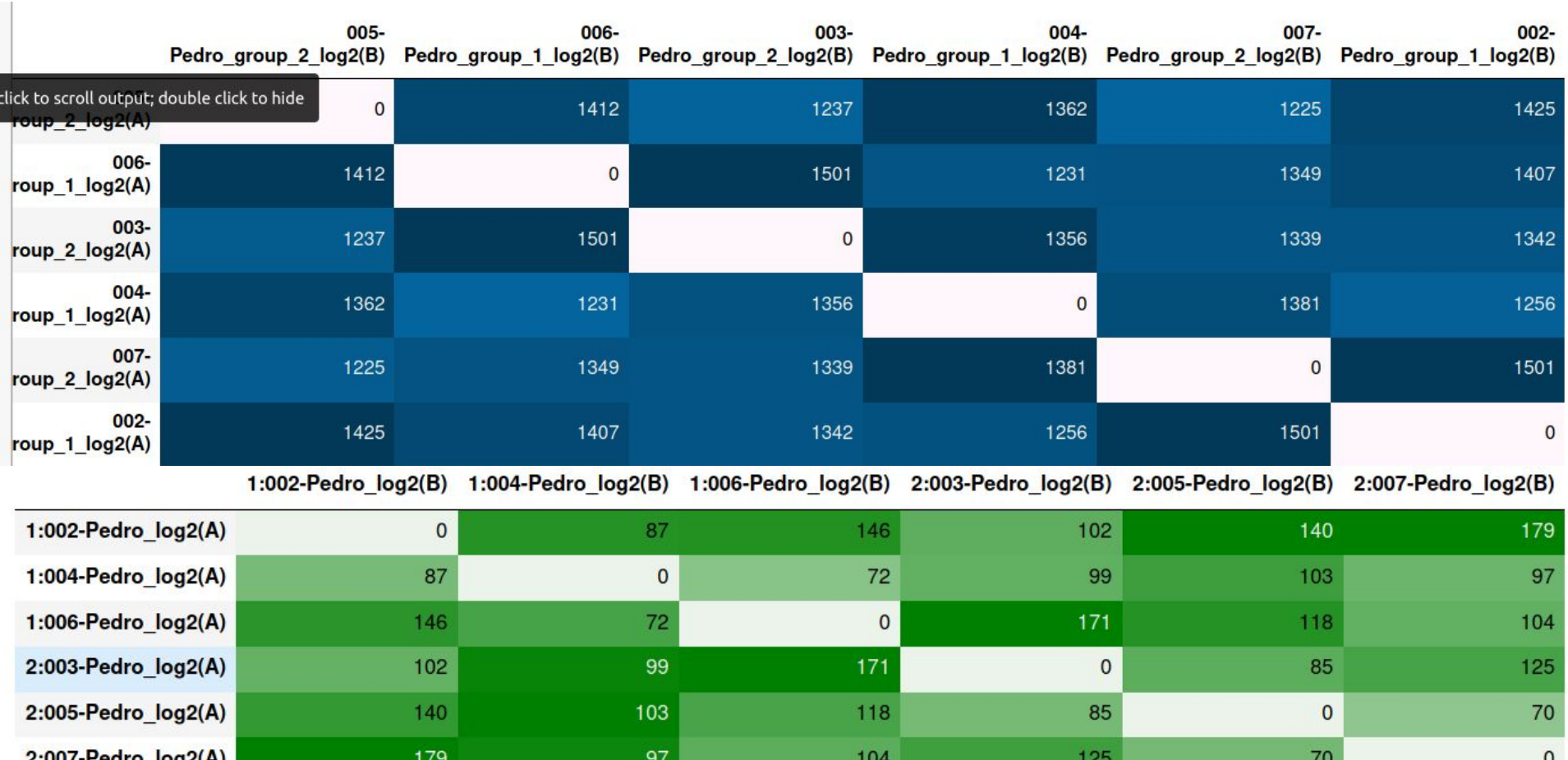
2:005-Pedro_log2(A)	13	9	9	32	0	31
2:007-Pedro_log2(A)	8	6	6	40	25	0

HUMAN A:B = 1:1 ratio, log2fc_treshold = 0.5



	005-Pedro_group_2_log2(B)	006-Pedro_group_1_log2(B)	003-Pedro_group_2_log2(B)	004-Pedro_group_1_log2(B)	007-Pedro_group_2_log2(B)	002-Pedro_group_1_log2(B)
click to scroll output; double click to hide roup_2_log2(A)	0	1412	1237	1362	1225	1425
006-roup_1_log2(A)	1412	0	1501	1231	1349	1407
003-roup_2_log2(A)	1237	1501	0	1356	1339	1342
004-roup_1_log2(A)	1362	1231	1356	0	1381	1256
007-roup_2_log2(A)	1225	1349	1339	1381	0	1501
002-roup_1_log2(A)	1425	1407	1342	1256	1501	0

	1:002-Pedro_log2(B)	1:004-Pedro_log2(B)	1:006-Pedro_log2(B)	2:003-Pedro_log2(B)	2:005-Pedro_log2(B)	2:007-Pedro_log2(B)
1:002-Pedro_log2(A)	0	87	146	102	140	179
1:004-Pedro_log2(A)	87	0	72	99	103	97
1:006-Pedro_log2(A)	146	72	0	171	118	104
2:003-Pedro_log2(A)	102	99	171	0	85	125
2:005-Pedro_log2(A)	140	103	118	85	0	70
2:007-Pedro_log2(A)	179	97	104	125	70	0

HUMAN A:B = 1:1 ratio, log2fc_treshold = 0.5

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004-roup_1_log2(A)	1362	1231	1356	0	1381	1256
007-roup_2_log2(A)	1225	1349	1339	1381	0	1501
002-roup_1_log2(A)	1425	1407	1342	1256	1501	0

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