ms_6_samples_analysis

April 2, 2025

1 Mass spec 6 samples analysis

1.0.1 Imports and environment setup

Date of run: 2025-03-02Environment: python 3.12

• Packages required: pandas, numpy, seaborn, matplotlib

2 Data Loading

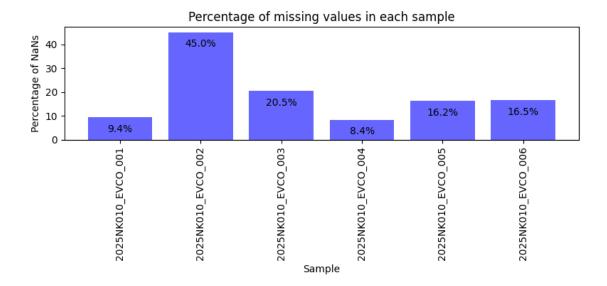
Both the MS and ELISA+metadata matrices were uploaded and some transformations to clean column names are done.

2.1 Samples analysis

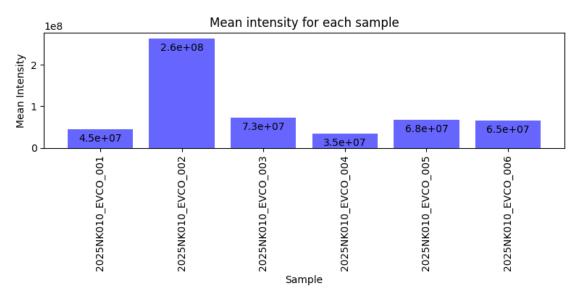
We will analyze in MS the number of missing values and identities distributions.

2025NK010_EVCO_001 667 2025NK010_EVCO_002 3191 2025NK010_EVCO_003 1452 2025NK010_EVCO_004 594 2025NK010_EVCO_005 1152 2025NK010_EVCO_006 1173

dtype: int64

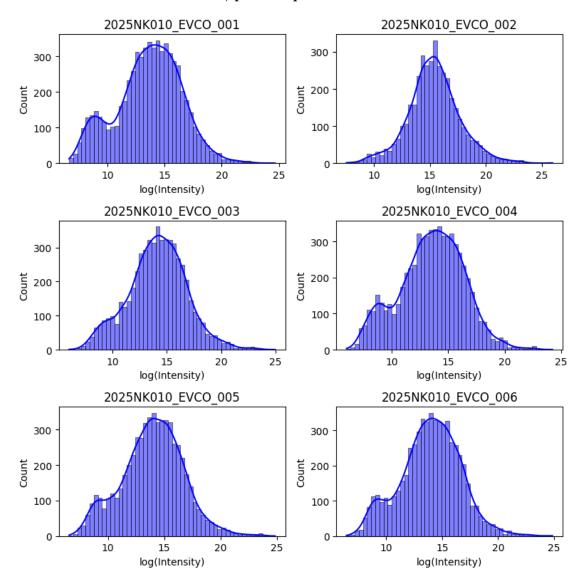


As can be observed, the number of missing values in the sample 2 is much higher than the rest.



The mean of intensities correlate with the percentage of missing values, are these two things related?

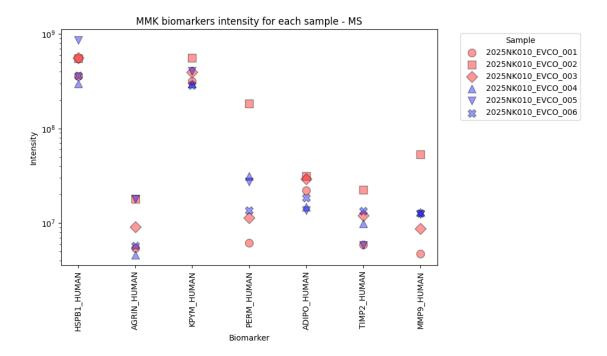
2.1.1 Distributions of intensities, per sample



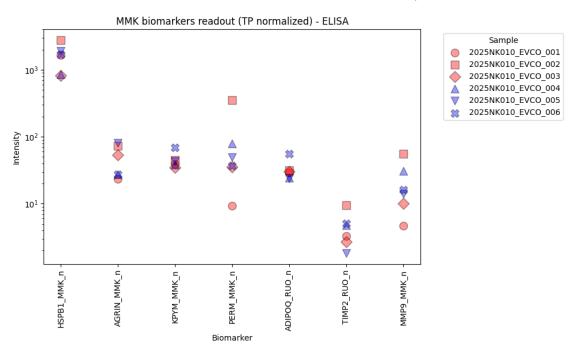
Notably, in the sample 2, the distribution lacks the enriched left tail of low intensity proteins.

2.2 What happens for the interest biomarkers?

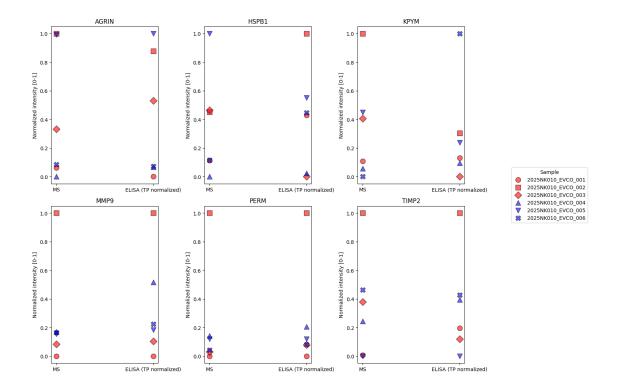
Let's analyze the distributions of intensities for the MMK interest biomarkers over the samples, in MS.



And now let's do the same with the ELISA results we have obtained (normalized by total protein).



Now, let's do the same but comparing the MS and ELISA for each biomarker individually. Since they are expressed in different scales/units, we need to normalize their intensities to compare them.



2.3 Fold changes

A fold change greater than 1 indicates that the biomarker is upregulated in cancer, meaning it shows higher intensity in cancer samples. Conversely, a fold change less than 1 suggests down-regulation in cancer, i.e., the biomarker is less abundant in cancer compared to benign samples. Fold change values are always positive since they represent ratios. However, to make interpretation more intuitive, log2-transformed fold changes are often used: in this scale, positive values indicate upregulation, negative values indicate downregulation, and zero means no change.

2.3.1 Interest biomarkers fold change (MS vs ELISA)

	Biomarker	MS_FoldChange	ELISA_FoldChange	Same	sign	${\tt fold}$	change?
0	AGRIN	-0.201	-0.156				Yes
1	HSPB1	0.047	-0.238				No
2	KPYM	-0.351	0.331				No
3	MMP9	-0.815	-0.203				Yes
4	PERM	-1.475	-1.256				Yes
5	TIMP2	-0.470	-0.401				Yes

2.3.2 Highest cancer upregulated fold changes

	Biomarker	Mean_Benign	Mean_Cancer	Log2_Fold_Change
2407	LIMK2_HUMAN	2627.990	14900000.000	12.469
1752	PTN3_HUMAN	1885.490	1716277.185	9.830
1192	IGF1R_HUMAN	1799.070	676608.960	8.555
3704	KAZRN_HUMAN	3269.570	541000.000	7.370
4463	ARH40_HUMAN	5774.810	717947.410	6.958
169	S35U4_HUMAN	6688.690	639869.000	6.580
2502	RAB38_HUMAN	3403.990	312997.000	6.523
448	CAH12_HUMAN	1287.460	111642.000	6.438
2196	PCP4_HUMAN	2394.330	168667.000	6.138
4687	YIPF5_HUMAN	5885.195	388639.675	6.045
6382	WAC2C_HUMAN	3687.120	188964.000	5.679
4100	RASL3_HUMAN	3155.290	153518.927	5.605
5400	SHRPN_HUMAN	122101.900	4733998.200	5.277
6102	CDC23_HUMAN	15123.300	338560.333	4.485
5823	NDUBB_HUMAN	8373.830	155451.200	4.214
3885	RHG27_HUMAN	22251.900	406093.233	4.190
6439	WIF1_HUMAN	492427.000	8010000.000	4.024
1924	S10A3_HUMAN	161866.000	2460000.000	3.926
4783	IP3KC_HUMAN	4488.950	53377.237	3.572
3491	KIZ_HUMAN	234115.000	2670000.000	3.512

2.3.3 Highest benign upregulated fold changes

	Biomarker	${\tt Mean_Benign}$	Mean_Cancer	Log2_Fold_Change
3001	SEC20_HUMAN	303020.000	8159.930	-5.215
2076	PACR_HUMAN	23700000.000	623467.500	-5.248
3056	SG2A2_HUMAN	222576666.667	5700000.000	-5.287
4253	BPIB2_HUMAN	18776038.000	478888.667	-5.293
3782	ANM9_HUMAN	364311.795	8798.290	-5.372
4868	DIRA2_HUMAN	81695.800	1914.510	-5.415
2326	SCNNB_HUMAN	1030000.000	22421.400	-5.522
2117	GPDM_HUMAN	250142.000	3705.535	-6.077
1507	H12_HUMAN	5109038.000	67950.200	-6.232
4984	SG3A1_HUMAN	59045316.333	671252.500	-6.459
4443	DMXL2_HUMAN	353762.000	3024.990	-6.870
6292	SIK3_HUMAN	1230316.000	8246.617	-7.221
6461	AUP1_HUMAN	507758.500	3387.385	-7.228
2847	TAP2_HUMAN	5600000.000	35118.433	-7.317
4692	OSBP2_HUMAN	4872829.600	16459.210	-8.210
1963	CBS_HUMAN	850742.500	2441.550	-8.445
1386	KCRU_HUMAN	1680000.000	4485.350	-8.549
2419	ATX1_HUMAN	3460000.000	9231.020	-8.550
5883	IF2B1_HUMAN	1730000.000	1514.790	-10.157
2997	NFAC3_HUMAN	2320000.000	1818.630	-10.317

All the presented biomarkers have no NaNs, measurements were obtained for all the displayed proteins.