QCQuan report: Test
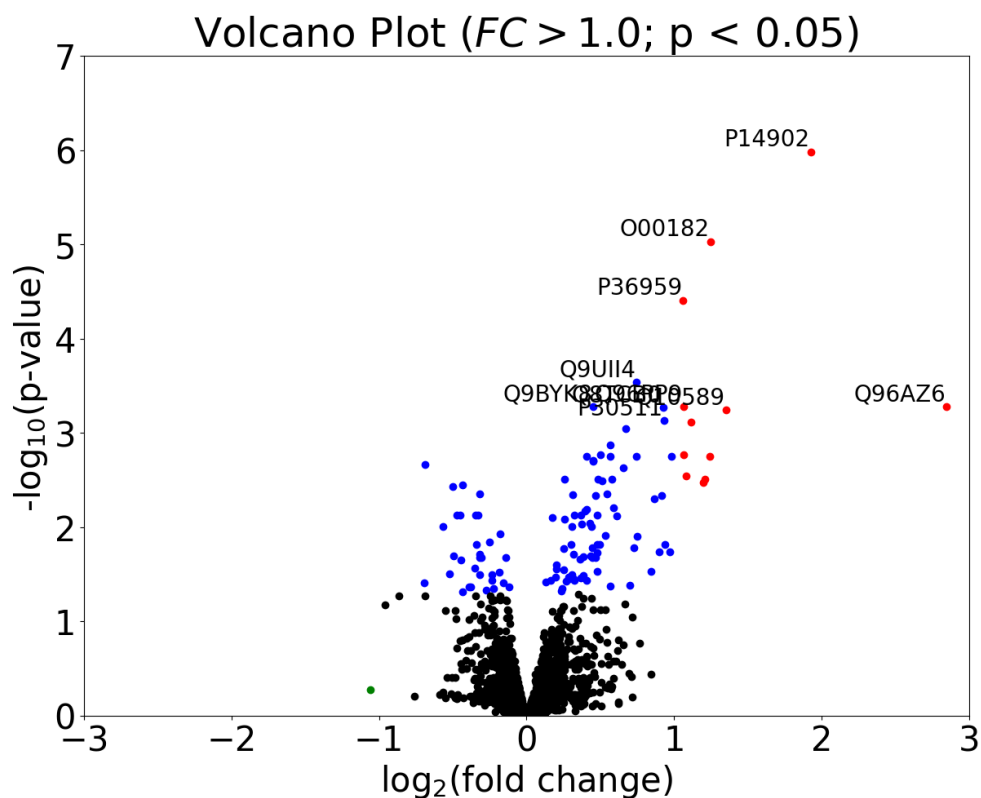
1 Differential Expression Analysis

Reference condition: **Untreated**

1.1 Minimal expression

IFN:

Volcano Plot ($FC > 1.0$; $p < 0.05$)

protein description	log2 fold change (IFN)	adjusted p-value (IFN)	#peptides (IFN)	#peptides (Untreated)
P14902	1.926372	0.000001	28	28
O00182	1.248225	0.000009	16	16
P36959	1.062272	0.000039	12	12
Q9UII4	0.746718	0.000287	16	16
Q96AZ6	2.847470	0.000527	4	4
Q9BYK8	0.453692	0.000527	36	36
Q96PP9	1.065580	0.000527	16	16
Q8TCB0	0.926452	0.000542	8	8
Q10589	1.350176	0.000573	16	16
P30511	0.931567	0.000741	4	4

2 Quality control

2.1 Experimental setup schema

MS run	Untreated	IFN
QEHF2_3821_VG_PSMs	['QEHF2_3821_VG_PSMs_Untreated_127N', 'QEHF2_3821_VG_PSMs_Untreated_127C', 'QEHF2_3821_VG_PSMs_Untreated_128N', 'QEHF2_3821_VG_PSMs_Untreated_128C']	['QEHF2_3821_VG_PS 'QEHF2_3821_VG_PSM 'QEHF2_3821_VG_PSM 'QEHF2_3821_VG_PSM
QEHF2_4114_VG_PSMs	['QEHF2_4114_VG_PSMs_Untreated_127N', 'QEHF2_4114_VG_PSMs_Untreated_127C', 'QEHF2_4114_VG_PSMs_Untreated_128N', 'QEHF2_4114_VG_PSMs_Untreated_128C']	['QEHF2_4114_VG_PS 'QEHF2_4114_VG_PSM 'QEHF2_4114_VG_PSM 'QEHF2_4114_VG_PSM

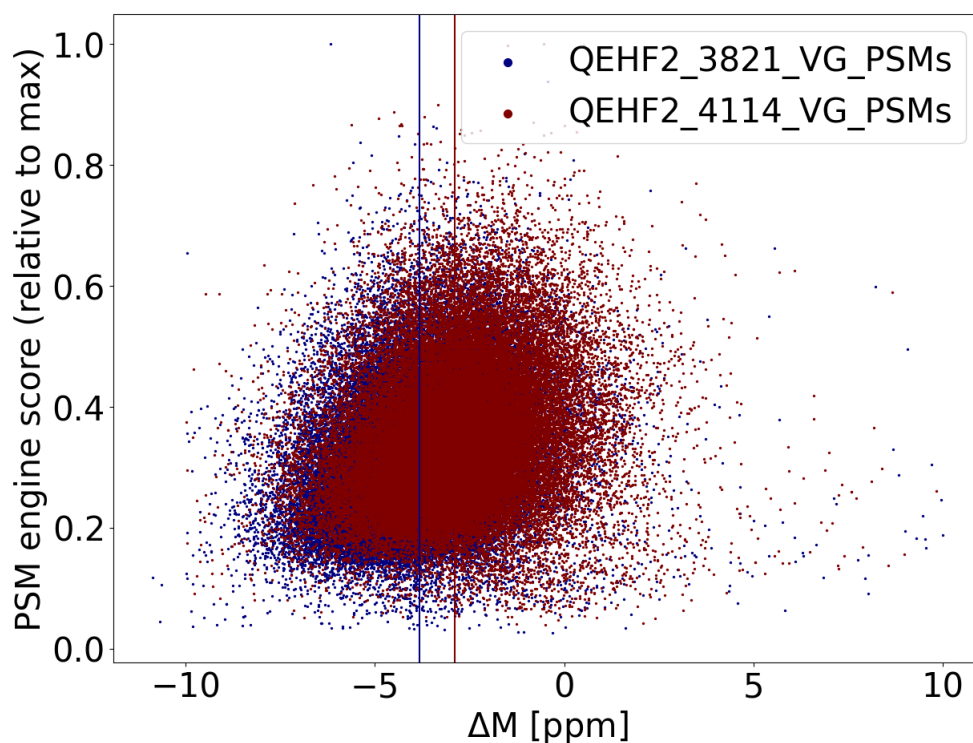## 2.2 Principal components analysis plot
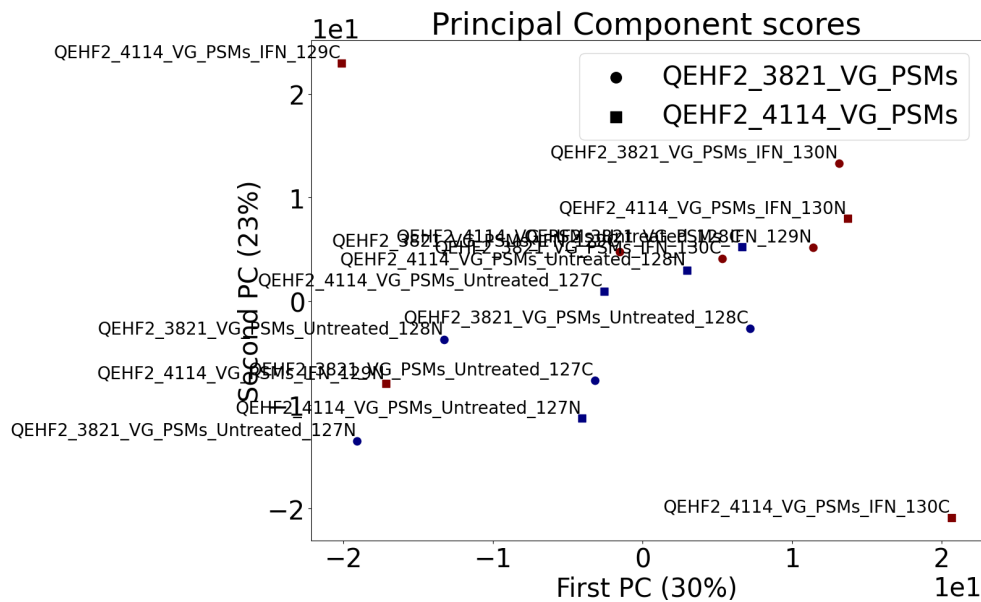
2.3 Hierarchical clustering dendrogram
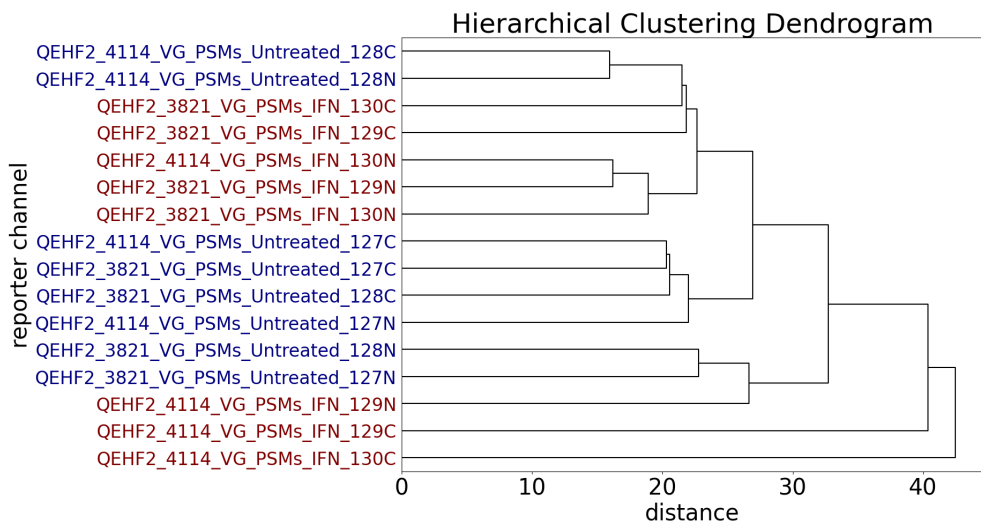
2.3 Miscellaneous

2.3.1 MS1 calibration plot

2.3.2 MS1 Intensity histogram

(No MS1 Intensity information available)

2.3.3 Other QC info

peptides(*) means non-redundant, possibly modified peptides

- Total number of peptides(*) found = 34158
- Total number of unique (after protein grouping) peptides(*) found = 31723
- Number of peptides(*) found in all MS runs = 16419
- Number of peptides(*) not found in all MS runs = 17739
- Number of proteins in the minimal expression result = 4928
- Number of PSMs detected and effectively used (i.e. after cleaning and removing PSM Engine redundancy):

	detected	used
QEHF2_3821_VG_PSMs	56867	45068
QEHF2_4114_VG_PSMs	50160	39293

- Percentage of PSMs with too high Isolation interference (>30.0%):

QEHF2_3821_VG_PSMs	**QEHF2_4114_VG_PSMs**
20.4224	21.3904

- Injection time information:

	max	num	max num below
QEHF2_3821_VG_PSMs	110	6231	38837
QEHF2_4114_VG_PSMs	110	7519	31774

- DeltaM [ppm] statistics:

	max	mean	std
QEHF2_3821_VG_PSMs	9.53	-3.80334	1.57187
QEHF2_4114_VG_PSMs	9.82	-2.8783	1.76881

- MS2 intensity statistics:
  - QEHF2_3821_VG_PSMs

	max	mean	std
QEHF2_3821_VG_PSMs_IFN_129N	4892.0	372.169929	298.927023
QEHF2_3821_VG_PSMs_IFN_129C	4627.5	351.893872	276.193856
QEHF2_3821_VG_PSMs_IFN_130N	4121.1	368.277904	294.891101
QEHF2_3821_VG_PSMs_IFN_130C	5675.6	321.620365	265.142201
QEHF2_3821_VG_PSMs_Untreated_127N	3464.0	317.535763	251.717542
QEHF2_3821_VG_PSMs_Untreated_127C	4784.6	377.509936	309.444871
QEHF2_3821_VG_PSMs_Untreated_128N	4652.6	341.934543	277.595271
QEHF2_3821_VG_PSMs_Untreated_128C	4764.4	427.261306	327.249858

  - QEHF2_4114_VG_PSMs

	max	mean	std
QEHF2_4114_VG_PSMs_IFN_129N	5082.0	243.380171	207.942294
QEHF2_4114_VG_PSMs_IFN_129C	3799.6	242.924792	207.954209
QEHF2_4114_VG_PSMs_IFN_130N	4018.6	236.017569	204.176522
QEHF2_4114_VG_PSMs_IFN_130C	2927.8	224.651112	179.703780
QEHF2_4114_VG_PSMs_Untreated_127N	4898.1	235.473661	193.931393
QEHF2_4114_VG_PSMs_Untreated_127C	3456.8	226.352696	186.853533
QEHF2_4114_VG_PSMs_Untreated_128N	4543.0	253.046798	201.418506
QEHF2_4114_VG_PSMs_Untreated_128C	4012.5	264.926095	206.254875

3 Log

- QCQuan version = 0.10.2
- date = 2024-01-17 14:02:06
- job duration = 182s

INFO:root:Starting processing of MSRun 'QEHF2_3821_VG_PSMs' of job 'Test' at 2024-01-17 14:03:02
WARNING:root:Column 'Intensity' was not found. Not gathering MS1 intensity QC info.
WARNING:root:Some PSMs have been removed from the workflow due to missing values: see removedData['missing'].
WARNING:root:Not all necessary columns found (see below); Adding 'Protein Descriptions' column with all empty strings.
Missing: Protein Descriptions
WARNING:root:Column 'Intensity' was not found. Not gathering MS1 intensity QC info.
WARNING:root:No PTM aggregation done.
INFO:root:Finished processing of MSRun 'QEHF2_3821_VG_PSMs' of job 'Test' at 2024-01-17 14:03:48

INFO:root:Starting processing of MSRun 'QEHF2_4114_VG_PSMs' of job 'Test' at 2024-01-17 14:03:48
WARNING:root:Column 'Intensity' was not found. Not gathering MS1 intensity QC info.
WARNING:root:Some PSMs have been removed from the workflow due to missing values: see removedData['missing'].
WARNING:root:Not all necessary columns found (see below); Adding 'Protein Descriptions' column with all empty strings.
Missing: Protein Descriptions
WARNING:root:Column 'Intensity' was not found. Not gathering MS1 intensity QC info.
WARNING:root:No PTM aggregation done.
INFO:root:Finished processing of MSRun 'QEHF2_4114_VG_PSMs' of job 'Test' at 2024-01-17 14:04:27
INFO:root:Starting analysis of job: Test at 2024-01-17 14:04:27
WARNING:root:Entry 'MS1Intensities_PSMs_all' was not found for MSRun QEHF2_3821_VG_PSMs. Not gathering ANY MS1 intensity QC info.
WARNING:root:Entry 'MS1Intensities_PSMs_all' was not found for MSRun QEHF2_4114_VG_PSMs. Not gathering ANY MS1 intensity QC info.
INFO:root:Finished analysis of job: Test at 2024-01-17 14:05:56
INFO:root:Starting visualization and report generation of job: Test at 2024-01-17 14:05:56
WARNING:matplotlib.axes._axes:'c' argument looks like a single numeric RGB or RGBA sequence, which should be avoided as value-mapping will have precedence in case its length matches with 'x' & 'y'. Please use a 2-D array with a single row if you really want to specify the same RGB or RGBA value for all points.
WARNING:matplotlib.axes._axes:'c' argument looks like a single numeric RGB or RGBA sequence, which should be avoided as value-mapping will have precedence in case its length matches with 'x' & 'y'. Please use a 2-D array with a single row if you really want to specify the same RGB or RGBA value for all points.
WARNING:root:QC entry 'MS1Intensities_PSMs_all' was not found. Not producing MS1IntensityHist.