Short ISOQuant configuration guide

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1 ISOQuant Workflow

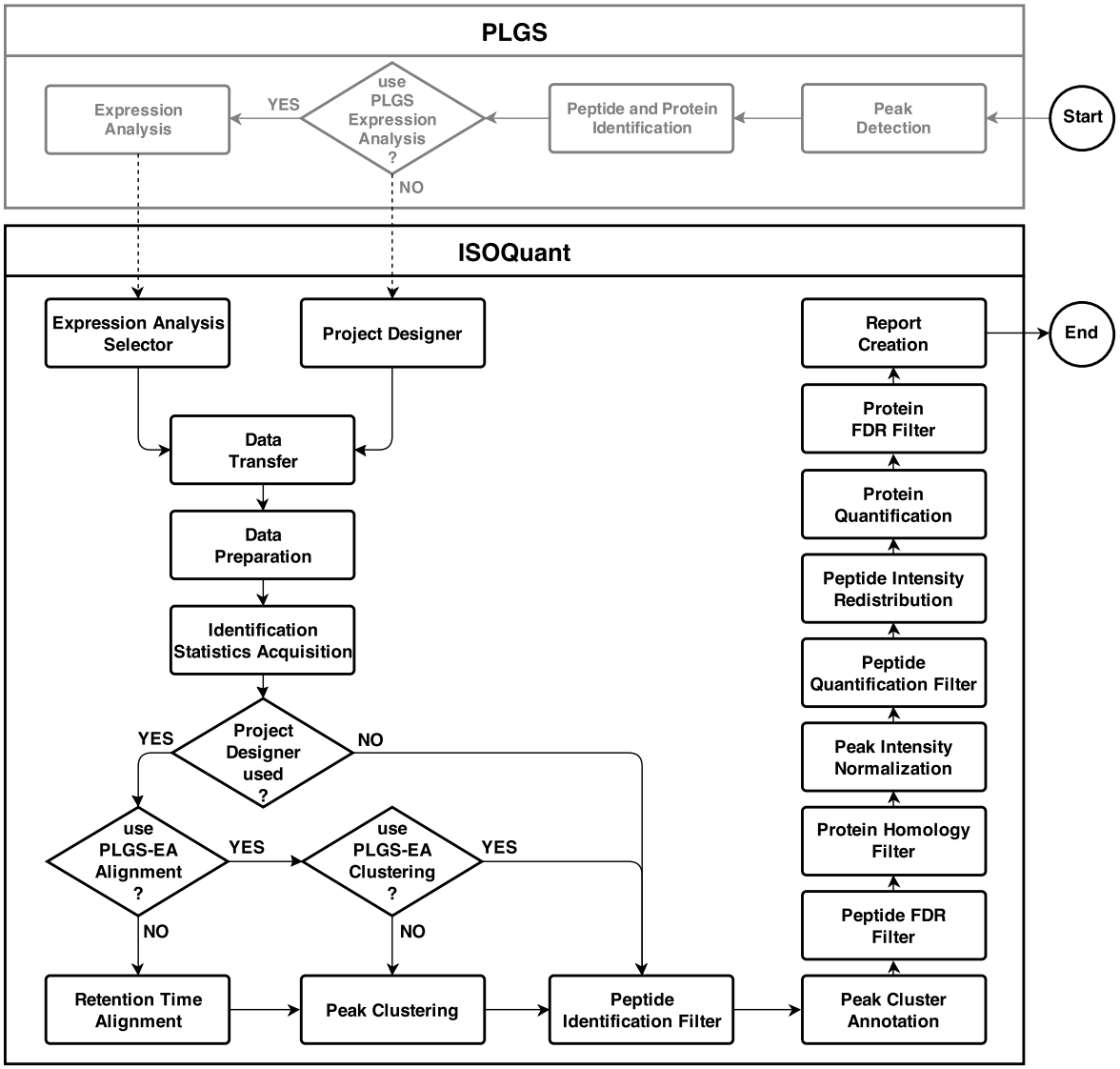

Figure 1: ISOQuant workflow

2 Configuration parameters

Every block of contiguous config parameters is commented with usage and parameter effect notes in the order as the parameters appear in the config file in alphabetic order by their full name. Note: the alphabetic order differs from the chronological processing workflow shown in figure!

- Peptide FDR Filter level, Peak Cluster Annotation restriction and Protein Homology Filter activation

  ```
  process.annotation.peptide.maxFPR=0.01
  process.annotation.peptide.maxSequencesPerEMRTCluster=1
  process.annotation.protein.resolveHomology=true
  ```

- Peak Clustering, minimum neighbor peaks in a cluster, neighborhood radius in ion mobility, mass and rt and clustering performance in CPU cores to utilize

  ```
  process.emrt.clustering.dbscan.minNeighborCount=2
  process.emrt.clustering.distance.unit.drift.bin=2.0
  process.emrt.clustering.distance.unit.mass.ppm=6.0
  process.emrt.clustering.distance.unit.time.min=0.2
  process.emrt.clustering.maxProcesses=8
  ```

- Minimum peaks criteria to use for rt alignment and clustering

  ```
  process.emrt.minIntensity=1000
  process.emrt.minMass=500
  ```

- Retention Time Alignment

  - matching peaks properties

    ```
    process.emrt.rt.alignment.match.maxDeltaDriftTime=2.0
    process.emrt.rt.alignment.match.maxDeltaMass.ppm=10.0
    ```

  - LC-MS runs to align at the same time, good estimation is quarter of available CPU cores

```
process.emrt.rt.alignment.maxProcesses=8
```

- limit peaks for alignment by properties

```
process.emrt.rt.alignment.minIntensity=1000
process.emrt.rt.alignment.minMass=800.0
```

- One of the LC-MS runs is the reference, to which every other run is aligned. The reference could potentially contain some rt bias. If activated, we minimize global rt fluctuations over all runs to the average.

```
process.emrt.rt.alignment.normalizeReferenceTime=false
```

- Peptide Identification Filter properties, only peptides passing filter criteria are used for annotation

```
process.identification.peptide.acceptType.IN_SOURCE=false
process.identification.peptide.acceptType.MISSING_CLEAVAGE=false
process.identification.peptide.acceptType.NEUTRAL_LOSS_H20=false
process.identification.peptide.acceptType.NEUTRAL_LOSS_NH3=false
process.identification.peptide.acceptType.PEP_FRAG_2=false
process.identification.peptide.acceptType.PTM=false
process.identification.peptide.acceptType.VAR_MOD=false
process.identification.peptide.minOverallMaxScore=0.0
process.identification.peptide.minReplicationRate=2.0
process.identification.peptide.minScore=0.0
process.identification.peptide.minSequenceLength=6
```

- Peak Intensity Normalization

```
process.normalization.lowess.bandwidth=0.3
process.normalization.minIntensity=3000
process.normalization.orderSequence=XPIR
```

- Data Preparation, we can completely remove peptides from database flaged by PLGS. Once removed, you can not recover them!

```
process.peptide.deplete.CURATED_0=false
process.peptide.deplete.PEP_FRAG_2=false
```

- Protein Quantification and FDR Filter

```
process.quantification.absolute.standard.entry=ENO1_YEAST
process.quantification.absolute.standard.fmol=50.0
process.quantification.absolute.standard.used=true
process.quantification.maxProteinFPR=0.01
process.quantification.minPeptidesPerProtein=1
```

- Peptide Quantification Filter

```
process.quantification.peptide.acceptType.IN_SOURCE=false
process.quantification.peptide.acceptType.MISSING_CLEAVAGE=false
process.quantification.peptide.acceptType.NEUTRAL_LOSS_H2O=false
process.quantification.peptide.acceptType.NEUTRAL_LOSS_NH3=false
process.quantification.peptide.acceptType.PEP_FRAG_2=false
process.quantification.peptide.acceptType.PTM=false
process.quantification.peptide.acceptType.VAR_MOD=false
process.quantification.peptide.minMaxScorePerCluster=0.0
```

- Protein Quantification, how many peptides to use for quantification

```
process.quantification.topx.degree=3
```

- App and user interface settings

```
setup.config.dir=d:\\isoquant\\app
setup.db.autoLoad=true
setup.db.host=localhost
setup.db.pass=
setup.db.user=root
setup.log.dir=log
setup.log.perSession=true
```

```
setup.plgs.root.autoLoad=false
setup.plgs.root.dir=D:\\plgs\\projects\\root
setup.plgs.root.showEACount=true
setup.plgs.root.showFSSize=false
setup.report.csv.columnSeparator=','
setup.report.csv.decimalPoint='.'
setup.report.csv.textQuote='"'
setup.report.dir=d:\\isoquant\\reports
setup.report.mzidentml.DBNCBITaxID=
setup.report.mzidentml.DBOrganismScientificName=
setup.report.mzidentml.DBversion=
setup.report.mzidentml.researcherFirstName=John
setup.report.mzidentml.researcherLastName=Doe
setup.report.mzidentml.researcherOrganization=Uni-Mainz
setup.report.xls.showAbsQuantFMOL=false
setup.report.xls.showAbsQuantFMOLUG=false
setup.report.xls.showAbsQuantNG=false
setup.report.xls.showAbsQuantPPM=true
setup.report.xls.showAllProteins=false
setup.report.xls.showPLGSQuant=false
setup.report.xls.showRTAlignment=false
setup.ui.captureConsoleMessages=true
setup.ui.iconScaleFactor=1.0
setup.ui.location.left=425
setup.ui.location.top=22
setup.ui.promptForExit=false
setup.ui.size.height=808
setup.ui.size.width=1022
```