Developed tools

## 1. mIMT-visHTS (publication□ [here]( ))

mIMT-visHTS is a software for multiplexing time-resolved protein abundance profiles, typically collected by, but not limited to, isobaric mass tagging methods. The only input needed is the file containing the relative protein abundances. The downloadable package includes:

1. A brief tutorial (PDF)
2. The application file (RebuildSuperDataSet)
3. Three .dll files to run the application file
4. 3 TMT-6plex sample datasets (all proteins quantified with 2 or more unique peptides)
5. The mIMT.r for standalone clustering
6. The mIMT-visHTS_packages.r script

Software Snapshot : Proteins in different conditions hold the same kinetics and classified in

cluster 13

# Example 1: proteins that behave the <u>same</u> in all three conditi
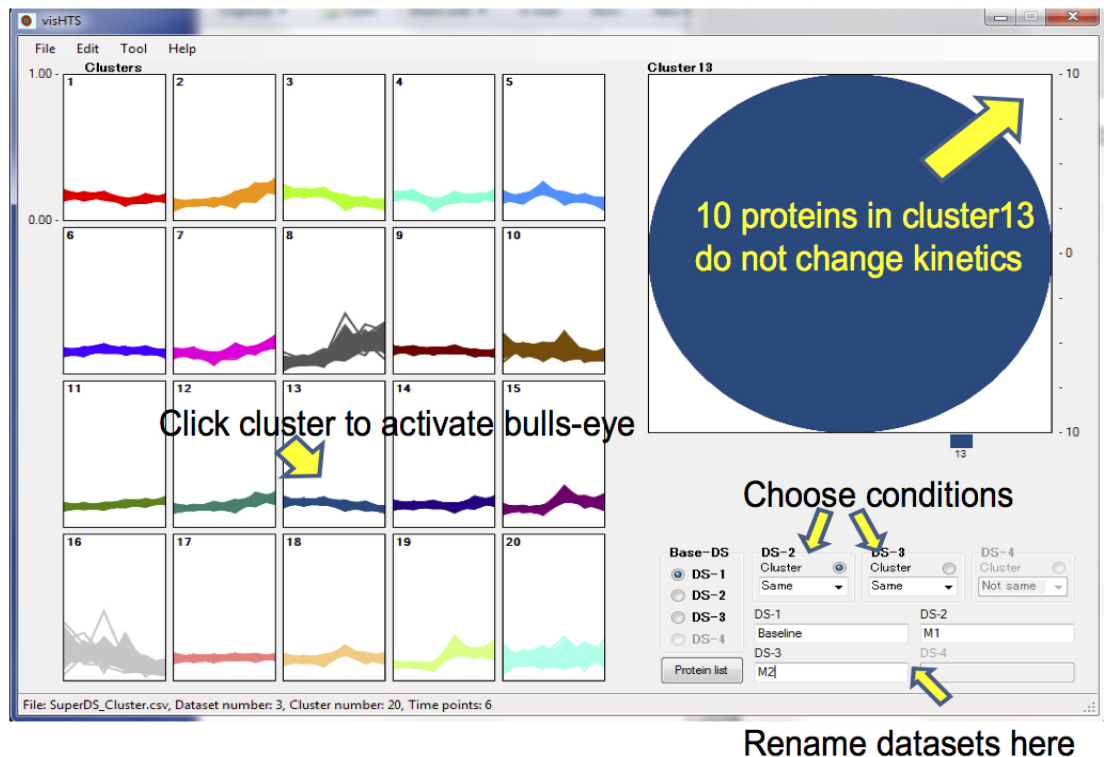
2. A novel tool for analysing extremely small sized ratio datasets: Dodeca Panel (publication☐ [here](#))

The naïve use of expression ratios in high-throughput biological studies can greatly limit analytical outcome especially when sample size is small. In the worst-case scenario, with only one reference and one test state each (often due to the severe lack of study material); such limitations make it difficult to perform statistically meaningful analysis. Workarounds include the single sample Z-test or through network inference. Here, we describe a complementary plot-based approach for analysing such extremely small sized ratio (ESSR) data – a generalisation of the Bland-Altman plot, which we shall refer to as the Dodeca-Panels. Included in this paper is an R implementation of the Dodeca-Panels method.

Figure 2 The Dodeca-Panels in diagram form (only for explanatory purposes and not base real data). Generally, the centre zone (unmarked) and peripheral zones (marked represents non-responders and responders, respectively (see online version for colo
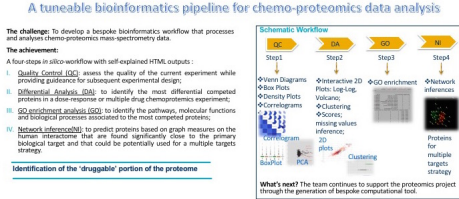

Dodeca Panel Guide

The panels each are correlated with meaning about the data in those regions. Here is a guide clarifying the implications
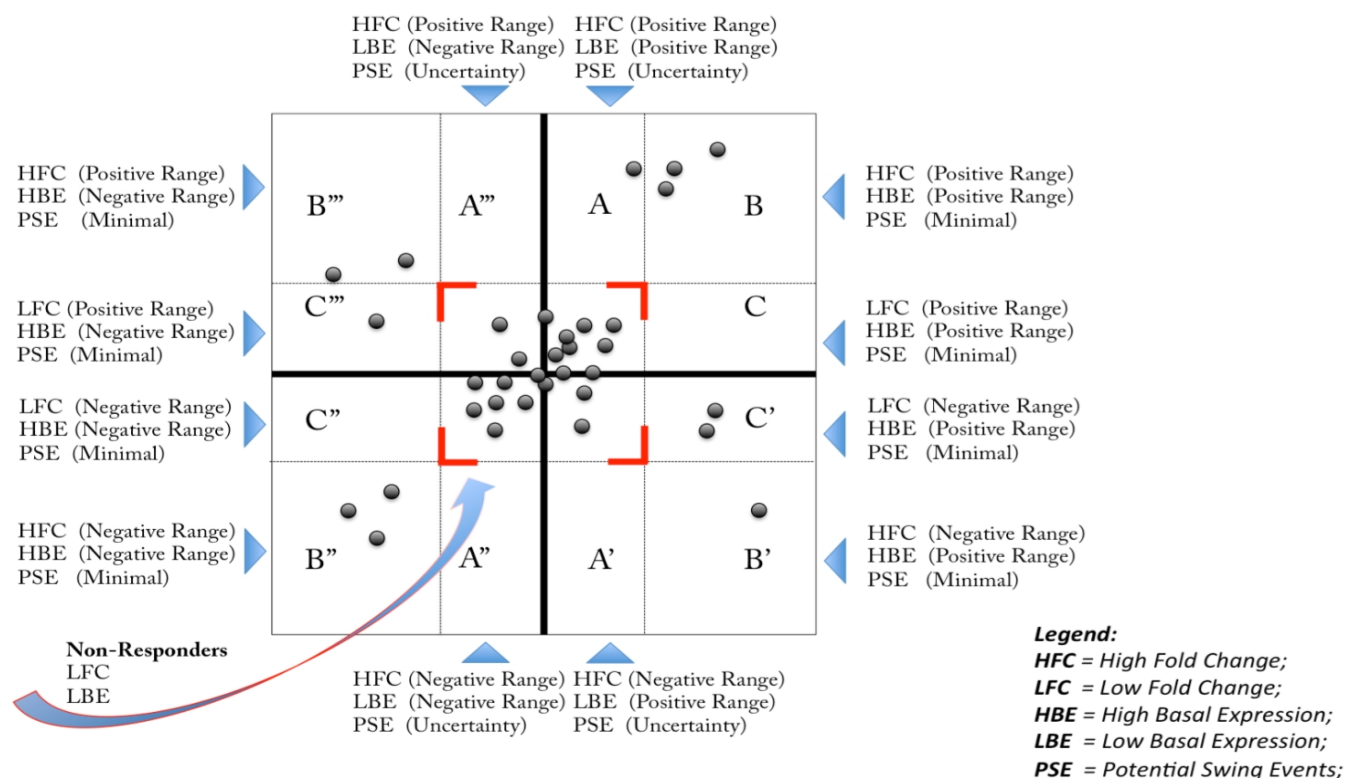
3. DOSCHEDA (publication here)

Mass Spectrometry (MS) based chemoproteomics has recently become a main tool to identify and quantify cellular target protein interactions with ligands/drugs in drug discovery. The complexity associated with these new types of data requires scientists with a limited computational background to perform systematic data quality controls as well as to visualize the results derived from the analysis to enable rapid decision making. To date, there are no readily accessible platforms specifically designed for chemoproteomics data analysis. We developed a Shiny-based web application named DOSCHEDA (Down Stream Chemoproteomics Data Analysis) to assess the quality of chemoproteomics experiments, to filter peptide intensities based on linear correlations between replicates, and to perform statistical analysis based on the experimental design. In order to increase its accessibility, DOSCHEDA is designed to be used with minimal user input and it does not require programming knowledge. Typical inputs can be protein fold changes or peptide intensities obtained from Proteome Discover, MaxQuant or other similar software. DOSCHEDA aggregates results from bioinformatics analyses performed on the input dataset into a dynamic interface, it encompasses interactive graphics and enables customized output reports. DOSCHEDA is implemented entirely in R language. It can be launched by any system with R

installed, including Windows, Mac OS and Linux distributions. DOSCHEDA is hosted on a shiny-server at https://doscheda.shinyapps.io/doscheda and is also available as a Bioconductor package (http://www.bio conductor.org/
).

Typical Workflow:

Chemo-protoemics readings:

- How chemoproteomics can enable drug discovery and development
- Mass Spectrometry-Based Proteomics in Preclinical Drug Discovery