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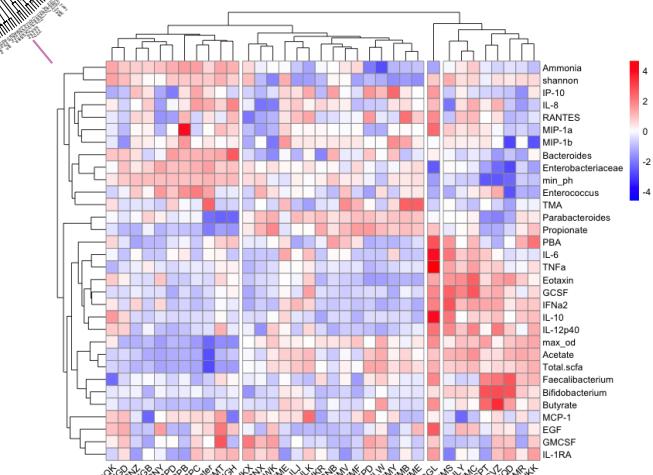
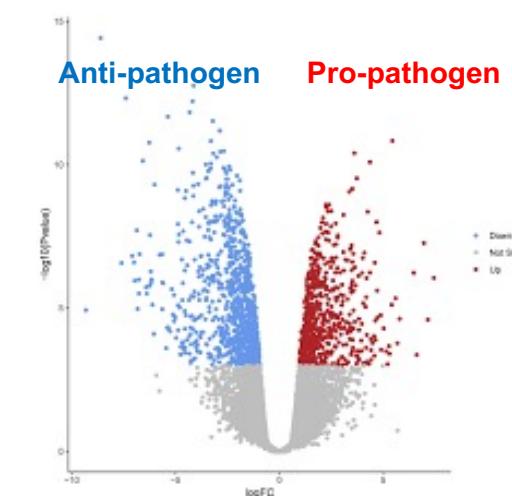
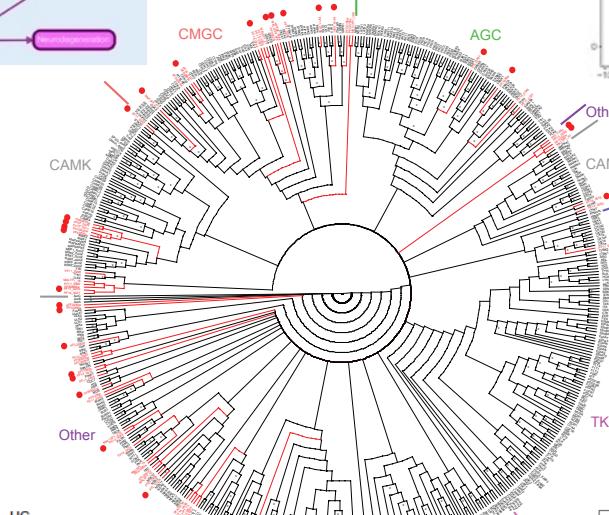
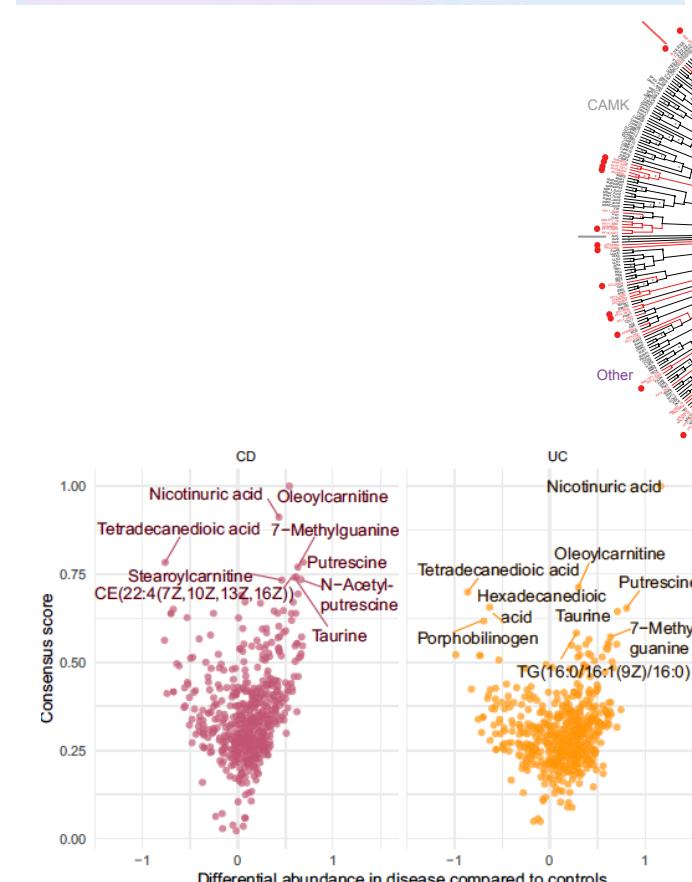
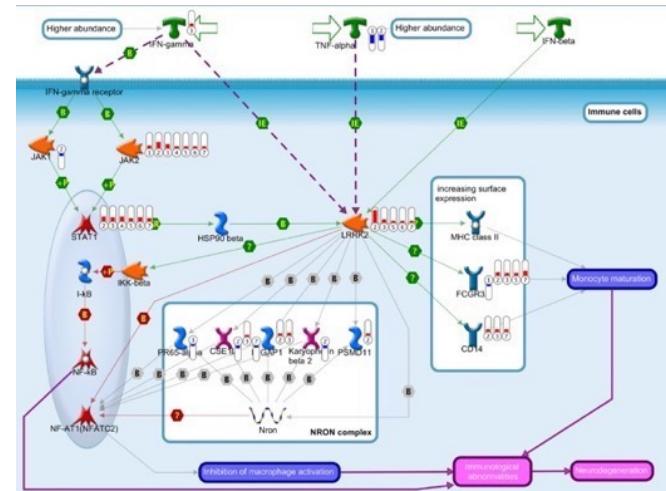
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Former affiliations: GSK , Kaleido Biosciences, Novasenta

Computational Approaches to Drug Target Discovery and Validation



Outline

1. Overview of drug research and development
2. Integrative biomedical databases
3. Human centric data (genetics, clinical trials, drug and tool compounds)
4. Multi-omics evidence databases
5. Protein characterization and interactions databases
6. Comparative genomics and model organism databases
7. Cancer relevant databases
8. Concluding remarks & discussion

Integrative vs Specialized Biomedical Databases and Interfaces

- **Integrative biomedical databases – consolidate multiple specialized databases:**

- NCBI*: <https://www.ncbi.nlm.nih.gov/> (gene viewer)
- Open Targets*: <https://www.opentargets.org/>
- ENSEMBL: <https://useast.ensembl.org/index.html>

- **Specialty resources:**

- Human Genetics – GWAS Catalogue*: <https://www.ebi.ac.uk/gwas/>
- Mouse phenotypes – Mouse Phenome Database (Jackson Lab): <https://phenome.jax.org/>
- RNA expression – GTEx*: <https://gtexportal.org/home/> ; Single Expression Atlas: <https://www.ebi.ac.uk/gxa/sc/release-notes.html>
- Protein Atlas – protein expression*: <https://www.proteinatlas.org/>
- Pathways – Reactome*: <https://reactome.org/> ; WikiPathways: <https://www.wikipathways.org/> ; IntAct: <https://www.ebi.ac.uk/intact/home>
- Protein annotations – UniProt*: <https://www.uniprot.org/>
- Protein-protein interactions – String*: <https://string-db.org/>
- Metabolomics – The Human Metabolome Database*: <https://hmdb.ca/>

- **Clinical trials and tool compounds:**

- Clinical trials -- ClinicalTrials.gov*: <https://clinicaltrials.gov/>
- Drugs and targets – DrugBank*: <https://go.drugbank.com/>
- Bioactive molecules and interactions: ChEMBL*: <https://www.ebi.ac.uk/chembl/>

- **Cancer:**

- The Cancer Genome Atlas Program (TCGA)
- Integrative data-sources for cancer functional genomics – Xenabrowser*: <https://xenabrowser.net/>
- Cancer dependency map -- DepMap*: <https://depmap.org/portal/>
- Cancer cell lines – Cancer Cell Line Encyclopedia (CCLE) *: <https://sites.broadinstitute.org/ccle/>

* Demos covered in this workshop
Please bring your laptop and bookmark these links in your browser (i.e., Chrome) before the workshop