**Assignment: Report Online**

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Course: BB2899 Project in Molecular Science

**Title:**

Discovery of drug repurposing therapeutic options in liver, kidney and hepatocyte using genomic metabolic modelling

**Main point:**

1 Exploration of differential expression and gene set enrichment using DrugMatrix1 and GEMs model2,3

2 Findings obtained from simulation of metabolism and metabolic pathways

3 Alternative drug repurposing options in different tissues and potential diseases

**Abstract:**

1 Background introduction and research purpose

2 Main findings

3 Conclusion

**Introduction:**

1 Introduction of drug repurposing strategy3

2 Development and application of systemic medicine3 and genomic metabolic modelling2,3

3 Database for modelling research (DrugMatrix1)

4 Research space in this field

5 Overview of the project (Research procedure along with results)

**Materials and Methods:**

1 Introduction of database (DrugMatrix1) and data type (Affymetrix4,5 array and Codelink6 array)

2 Construction of the analysis pipeline

2.1 Retrieve microarray data from GEO

2.2 Summarize and create meta-data table (Sample ID, tissue, compounds, dose)

2.3 Construct the preprocessing pipeline

2.3.1 Read microarray data

2.3.2 Perform background corrections

2.3.3 Perform normalization (Quantile)

2.3.4 Perform PM intensities corrections

2.3.5 Perform summarization (MAD)

2.4 Construct the analysis pipeline

2.4.1 Perform differential expression analysis

2.4.2 Perform gene set enrichment analysis

2.4.3 Establish metabolic network and perform network analysis7

2.4.4 Stimulate metabolic modelling and validate

3 Make comparison with other methods

**Results:**

1 Results from Data QA and QC analysis in the preprocessing step (Summary, MA plots, etc.)

2 Results from Gene differential expression analysis

3 Findings from Gene set enrichment analysis

4 Gene Network findings

5 Metabolites network findings

6 Findings from metabolic modelling simulation

**Discussion:**

1 Discussion about the key findings when performing DF, GSE, network and GEM analysis

2 Limitations of our genomic metabolic modelling

3 Potential therapeutic strategies

**References:**

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7 Lee, S. *et al.* Network analyses identify liver-specific targets for treating liver diseases. *Molecular systems biology* **13**, 938, doi:10.15252/msb.20177703 (2017).