

SmartArray

User Manual

BIOADA TEAM¹

October 8, 2021

 $^{^1 {\}tt www.bioada.com}$

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1

Introduction

There are many factors that make data preparation challenging, from understanding where to find the data to extracting it, then properly formatting it and finally loading it to a database management system (DBMS). SmartArray reduces data preparation time, so that you the focus is on using a high quality and enriched data for visualization, statistical analysis and predictive modeling. With Bioada, users have the full control on the data.

SmartArray provides a unique interactive data exploration platform for ad-hoc queries, data visualizations and statistical analysis. Users can explore data interactively and apply statistical models and analytical techniques to find potential biomarkers in the genomic data. Users can focus and emphasize on interactivity and effective integration of techniques from data science.

Genomic datasets are high-dimensional molecular profiles pose challenges to data interpretation and hypothesis generation. SmartArray has a method that discovers significantly enriched pathways and gene ontology terms across datasets. SmartArray enrichment is a versatile method that improves systems-level understanding of cellular entities in health and disease through integration of genomic datasets and pathway and gene ontology annotations.

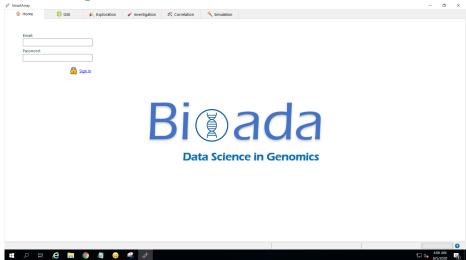
Home

The Home tab is the first screen of SmartArray. Every user is given a set of credentials to login to the application according to their roles.

2.1 Login

To login into the SmartArray application please enter the following details:

- 1. Enter Email and Password in the related fields.
- 2. Click on to Sign-In.



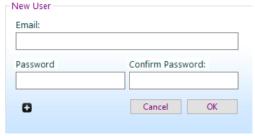
2.2 Add user

Admins have access to add/edit/delete users.

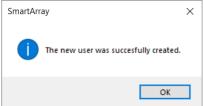
1. Sign-in into the application.

2. HOME 4

2. Click on w "User" icon. A message box appears as below.



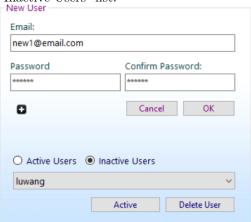
3. Enter the new email, password, and confirm password in the related fields. Once the user is saved the below popup appears



2.3 Edit user

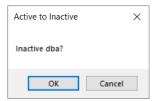
This feature activates, inactivates, or deletes a user.

- Activate User:
 - 1. Sign-in to the application.
 - 2. Click on urger "User" icon.
 - 3. Click on the **⑤** button. All the Inactive users will be displayed under "Inactive Users" list.



4. Select an user to Activate and click on the Active button. A confirmation message appears as shown below.

2. HOME 5



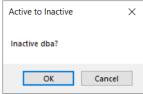
5. Once the user is activated, it will be displayed under active users list.

• Inactivate User:

- 1. Sign-in to the application.
- 2. Click on "User" icon.
- 3. Click on the button. All the active users will be displayed under "Active Users" list.



4. Select an user to inactivate and click on the Inactivate User button.A confirmation message appears as shown below.



5. Once the user is inactivated, it will be displayed under inactive users list.

• Delete User:

- 1. Sign-in to the application.
- 2. Click on w "User" icon.
- 3. Click on the button. All the active users will be displayed under "Active Users" and inactive users on "Inactive Users" related lists.

2. HOME 6

new1@email.com		
Password	Confirm Password:	
****	****	
0	Cancel OK	
Active Users	nactive Users	
Active Users	nactive Users	

4. Select an user to delete and click on the Delete User button. A confirmation message appears as shown below. On click of "OK" the user will be deleted permanently.



3

Data

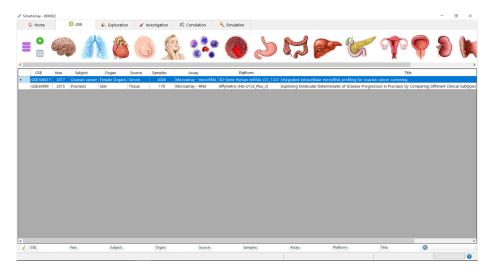
The Data(GSE) tab allows you to load data from database, add new data to database and compare two different databases.



3.1 Load data

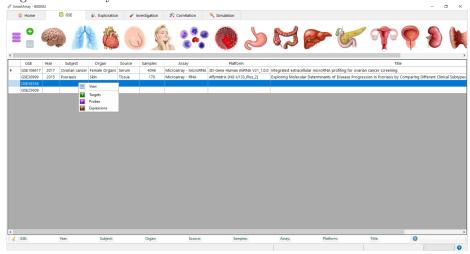
Loads all the existing databases.

1. Click on button. It loads the existing databases in the local database server.

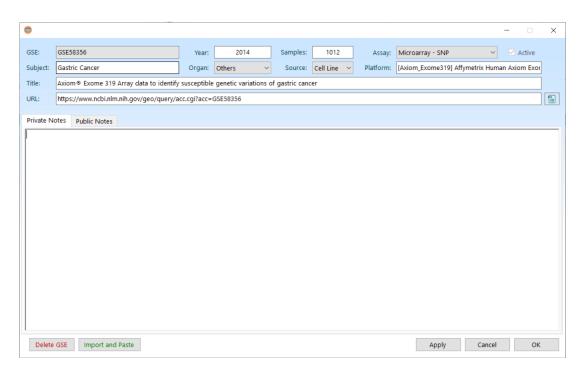


2. The multiple filters(GSE, Year, Subject, Organ, Source, Samples, Assay, Platform, Title) at the bottom of the screen can be used to filter the databases.



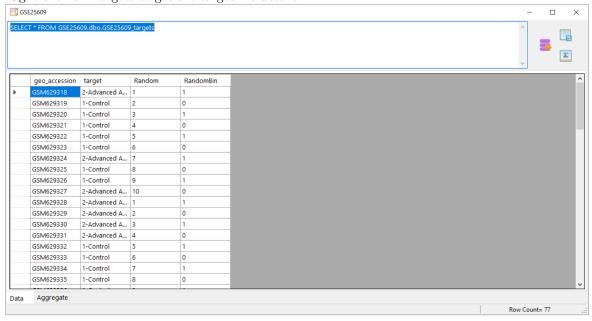


4. Enter the details of the data-set and click on Apply/OK.



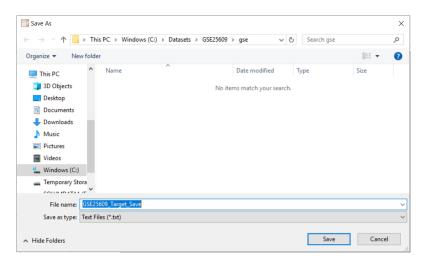
5. Delete GSE button can be used to delete the GSE from the database server.

6. Right click on Targets to get the target file details.



7. Click on to run the query and the results are as shown above.

8. Click on to save the query results.



9. Click on **E** to get the aggregate of the selected column.

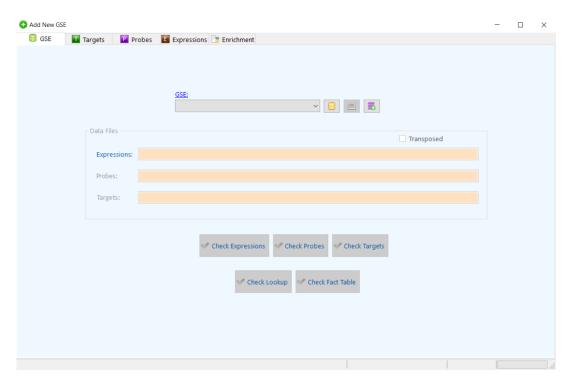


10. Similar results are obtained for Probes and Expressions.

3.2 New Data

Adds a new database to the local database server.

1. Click on •• button. A new window is opened as shown below.

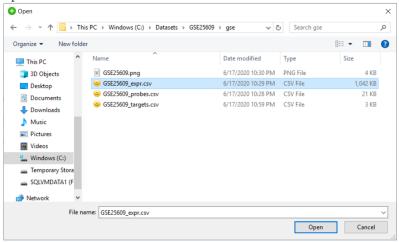


2. <u>Click on . Enter new database</u> name and click OK.

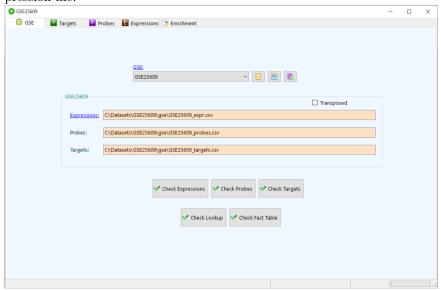


3. The newly added database appears in the GSE list. Select the database and click \sqsubseteq on to connect.

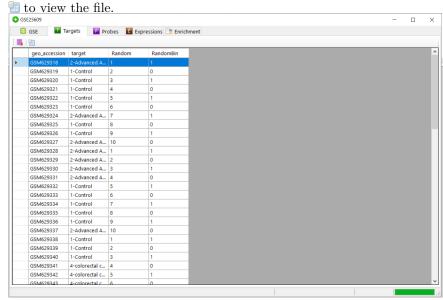
4. Click on the Expressions hyperlink and select the expression file to be uploaded.



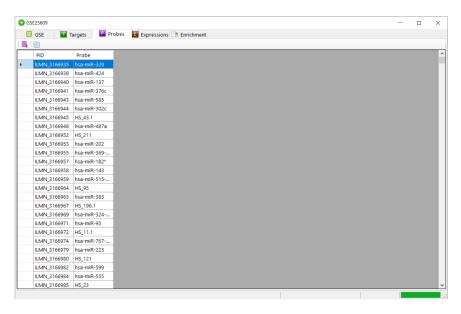
5. The probes and target files are automatically uploaded on selection of expression file.



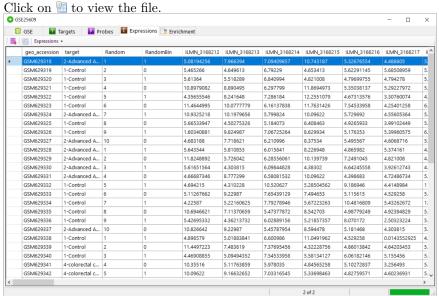
- 6. Click on various Check buttons to ensure all the files are intact.
- 7. Go to Targets tab and click on to upload the data to database.Click on



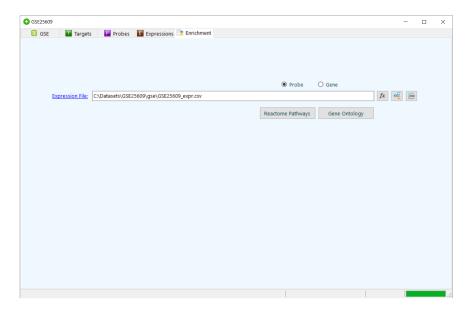
8. Go to Probes tab and click on \blacksquare to upload the data to database. Click on \blacksquare to view the file.



9. Go to Expressions tab and click on to upload the data to database.

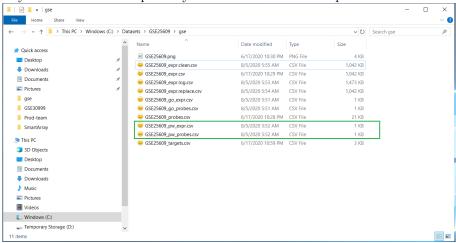


10. Go to Enrichment tab and click on Expression File hyperlink to select the expression file to transform the data.

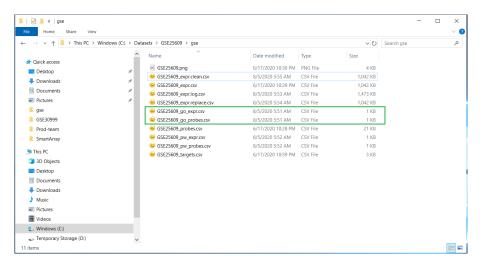


11. Select on the Probe/Gene depending on the data.

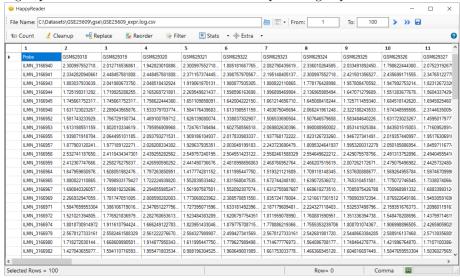
12. Click on Reactome Pathway button to compress the data to higher pathway. This creates a new pathway file with Probe and Sample details.



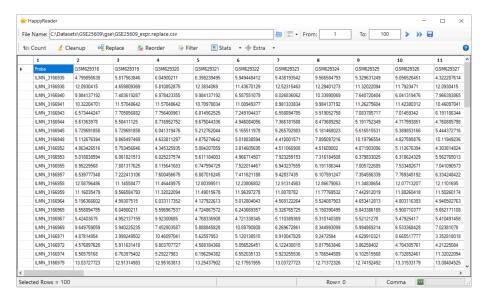
13. Click on Gene Ontology button.



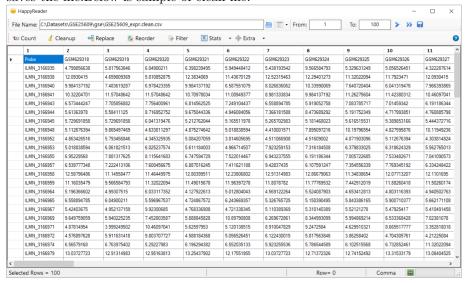
14. Click on fx for Log transformation. This transforms the expression file to log expression and saves the file. Below is sample of log expression file.



15. Click on • to replace any missing value with the average value of corresponding row. This modifies the expression file and saves the file.Below is sample of replaced file.



16. Click on \sqsubseteq to delete any empty row . This changes the expression file and saves the file.Below is sample of clean file.



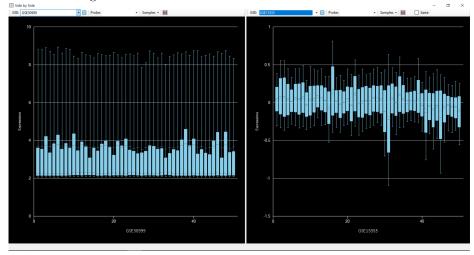
3.3 Compare GSE

Compare two databases of same category.

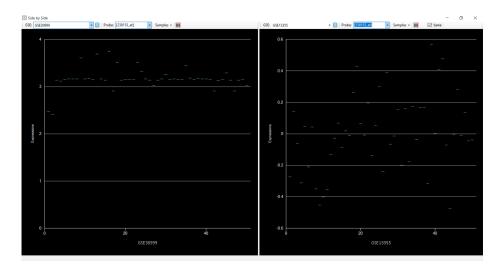
1. Click on .A new compare window opens up.



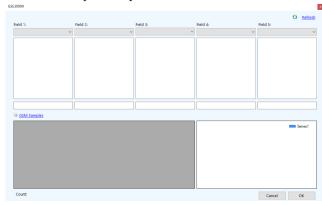
- $2. \,$ Select two databases that similar to same category for comparison.
- 3. Click on \blacksquare to get the distribution of data from both data-sets.



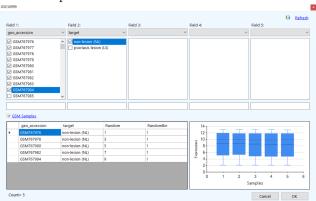
- 4. Click on Same checkbox to compare the same samples on either sides if available.
- 5. Select probes on each side to compare individual probes in the data-sets.



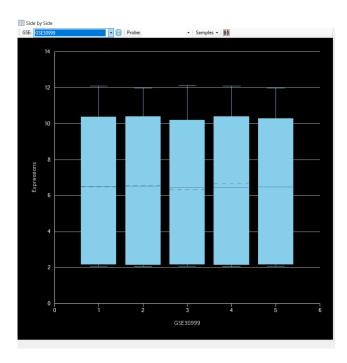
6. Click on Samples drop-down for filters. Click on ${\overline{\bf v}}$ Add Filter.



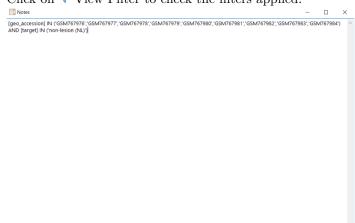
7. Select the filters to apply and the filtered data will be displayed under GSM Samples on click.



8. Click on ${}^{\mbox{\tiny \Box}}$ Refresh link to clear all the filters or click on "OK" to apply the filter.



9. Click on ♥ View Filter to check the filters applied.



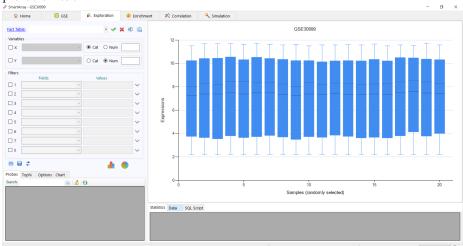
10. Click on ${\color{red} \overline{\lor}}$ Delete Filter to delete the existing filter. ${\color{gray} \times}$



4

Exploration

The exploration tab performs the statistical analysis on the database. Upon double clicking on the database in GSE tab, it redirects to the default page of Exploration tab.



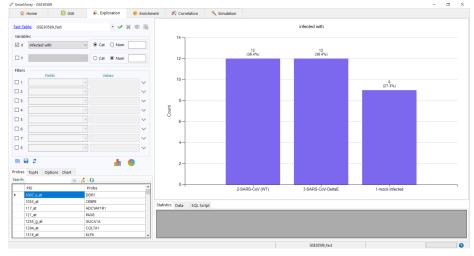
- 1. Click on the Fact Table hyperlink to load the fact tables from the database. Select the corresponding fact table and click on Click on ✓ to load the table. The original fact table cannot be deleted, renamed or exported.
- 2. Click on **x** to delete the fact table.
- 3. Click on to rename the fact table.
- 4. Click on 🖺 to export the fact table.

4.1 Univariate Analysis

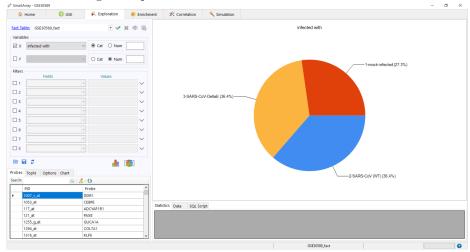
Univariate analysis on a numerical or categorical variant can be performed.

1. Select any variant as X variable to perform univariate analysis. Depending on the variant selected, the type is changed to Cat(Categorical) or Num(Numerical).

2. Click on to get the distribution of the variant. The data and the SQL Script used can be seen at the bottom of the screen.



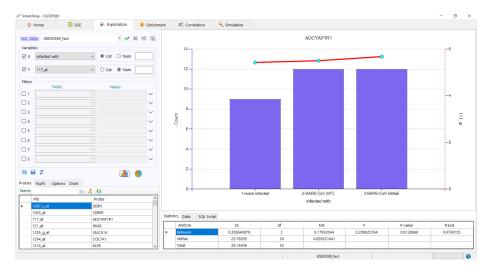
3. Click on 5 to get the pie chart distribution.



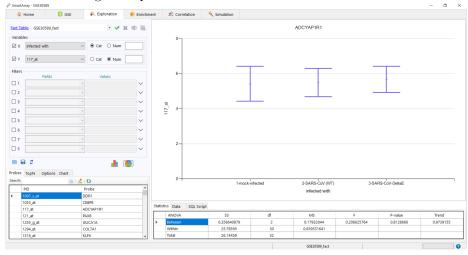
4.2 Bivariate Analysis

Bivariate analysis on a numerical or categorical variant can be performed.

- 1. Select any variant as Y variable to perform bivariate analysis. Depending on the variant selected, the type is changed to Cat(Categorical) or Num(Numerical).
- 2. Click on to get the distribution of the variant. The statistics, data and the SQL Script used can be seen at the bottom of the screen.



3. Click on sto get the pie chart distribution.



4. Keep changing the values in the Y variable to get the correlation of each value with X variant.

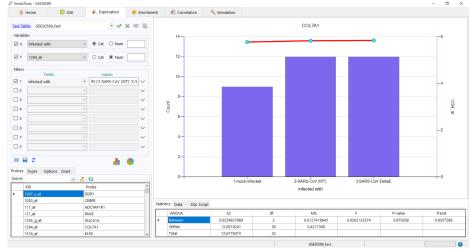
4.3 Visualization

The top $5{,}100$ or 800 subsets can be sliced to form another dataset.

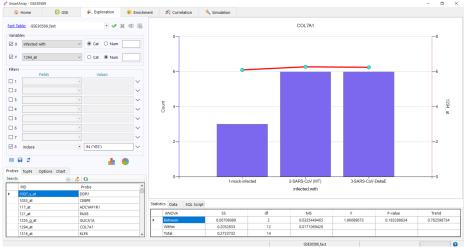
1. Filters: Apply filters for more clear view of the data.7 Filters (Filter 1- 8) can be applied for filter functionality.



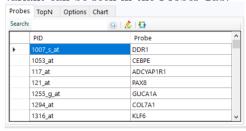
• Select a variable to apply the filter. Click on $\stackrel{1}{\blacksquare}$ or $\stackrel{1}{\bigcirc}$ to see the result.



• Filter No. 8 adds another dimension to the data. Click on do or to see the result.

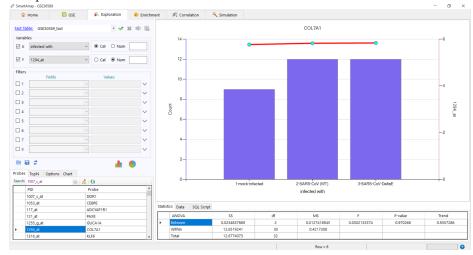


- Click on $\stackrel{>}{\sim}$ to refresh the existing filters.
- Click on 🖥 to save the data.
- Click on boto load the saved filters.
- 2. Probes: The correlation between each value of Y variable with any X variant can be seen in the Probes Tab.

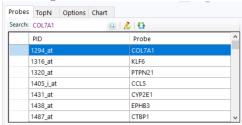


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• Keep clicking on different values to see the distribution changing in box plot.

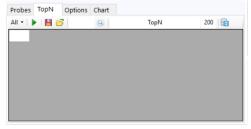


• Enter the probe ID/name to search and click on ⁽²⁾ to search the next matching value.



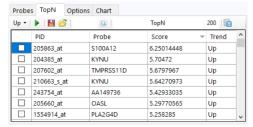


- Click on to refresh the data.
- 3. Top: Allows users to see the correlation between all the values in Y variable with respect to X variable.

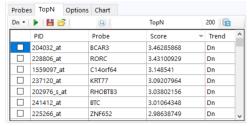


- Click on All dropdown to filter the data to be displayed.
 - (a) All Displays the complete data.

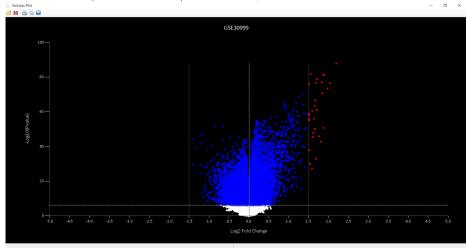
(b) Upregulated - Displays the data that has trend Up.



(c) Downregulated - Displays the data that has trend Down(Dn).



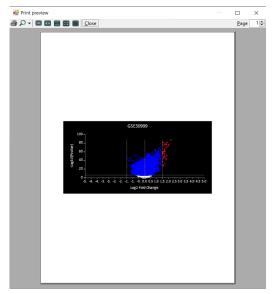
• Click on • to get the Volcano/Manhattan plot.



- (a) Click on of to load the data used for obtaining volcano plot.
- (b) Click on 🖺 to save the data used for obtaining volcano plot.
- (c) Click on \(\bigcirc\) to print the volcano plot.

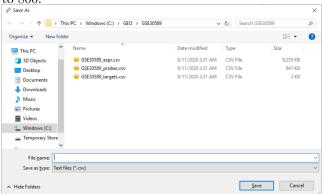
4. EXPLORATION

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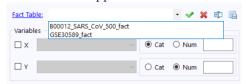


- (d) Click on **b** to copy the volcano plot.
- (e) Click on 🖥 to save the volcano plot.
- Click on (a) to search for Probe ID or Probe name.
- Click on

 to save the top N data where N can be in the range of 5
 to 800.



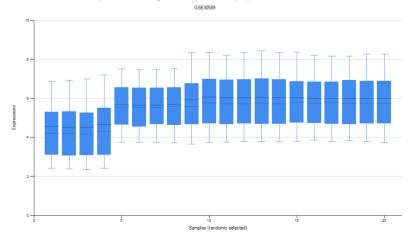
- Click on 🛎 to load the existing subset dataset.
- Click on 🖫 to save the Top N data to database. The textbox can be used to name the table and the number of rows(N) to be saved. The saved dataset appears on the Fact Table list.



- 4. Options tab provides more features for SNPs.
 - Exclude NC (No Call): Excludes NC genotype for the statistical analysis

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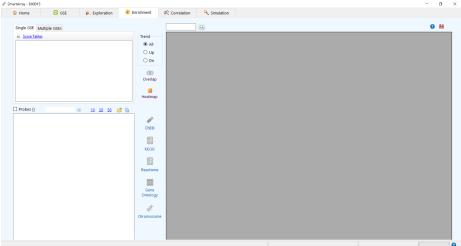
- Encode SNP: Encodes the SNPs
- In-memory Aggregation: This feature allows users to use the inmemory of their local computers to run SmartArray application
- 5. Chart tab provides more features on visualization.
 - Font Size: Increasing or decreasing of font size changes the font displayed on the charts.
 - Click on Density Plot to get the density plot for the data-set.



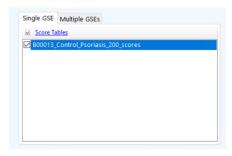
- To copy the density plot, use and edit it in any image editor.
- Click on late to print the density plot.
- Click on 🖥 to save the density plot.
- X-axis Show Range: Shows the range of values in X-axis.
- $\bullet~Y_2~\%$ Format: Shows the plot with y-axis values in terms of percentage.
- Volcano Plot: Check on this item to show the volcano plot after running. Uncheck to not show the plot. Click on 🗓 to show the saved plot
- X-axis Sort by Count: Sorts the data according to the x-axis value count.
- Minimum Y-Axis: Use minimum value of Y-axis instead of 0 as minimum value.
- Log_2FC : It takes the value of $(Log_2(B) Log_2(A))$ if checked and B A if unchecked in X-axis of the volcano plot.
- X-axis Reversed: Reverses the X-axis and displays the plot.
- $-Log_{10}$ (Pvalue): On check considers $-Log_{10}$ (Pvalue) as Y-axis value else takes the score as Y-value in the volcano plot.

Enrichment

Enrichment displays the relation of probes with chemicals, pathways, gene ontology and chromosomes. The chemical details are saved in the database.



Click on Score Tables to load the subset data-sets.



- 1. Click on Overlap to see the probes.
- 2. Click on \blacksquare Heat-map to see the heat-map of all probes.



- $3.\ \,$ Trend Options allows to see the trend of probes.
 - $\bullet\,$ All Displays all the probes of subset.

	1 0	/
Probe	Trend	B00013_Control
AI819863	Up	352.07009887
N4BP1	Up	350.67520141
GZMB	Up	350.61669921
ARSF	Up	350.57559204
UBE2C	Up	350.31600952
SLC7A11	Up	349.76889038
PARD3	Dn	349.17541503
NFKBIZ	Up	348.44610595
ATP12A	Up	346.82611083
INPP5A	Dn	345.92028808
FOXM1	Up	344.40719604
PGM2	Up	344.28781127
TRIM14	Up	343.84820556
ABCC1	Up	343.31509399
PYCARD	Up	343.07269287
UBE2N	Up	342.91378784
FBXO9	Up	342.68978881
SPTSSA	Up	342.10281372

 \bullet <u>Up - Displays probes</u> that are up regulated.

Probe	Trend	B00013_Contro
PI3	Up	1924.9759521
S100A7A	Up	1596.9289550
DEFB4A	Up	1554.3420410
AKR1B10	Up	1270.1479492
S100A12	Up	1151.4560546
TCN1	Up	1060.0539550
KYNU	Up	1053.6300048
IL36G	Up	1046.6469726
SPRR2C	Up	862.453125
SERPINB4	Up	834.02960205
C10orf99	Up	805.28082275
SERPINB3	Up	801.14093017
SPRR2D	Up	780.85211181
ADAMDEC1	Up	750.51721191
HPSE	Up	732.58959960
ZC3H12A	Up	674.53540039
PDZK1IP1	Up	673.92468261
S100A9	Up	628.39172363

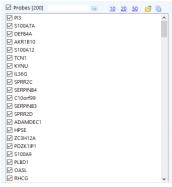
 $\bullet\,$ Down - Displays probes that are down regulated.



4. Text box a can be used to search for probes.

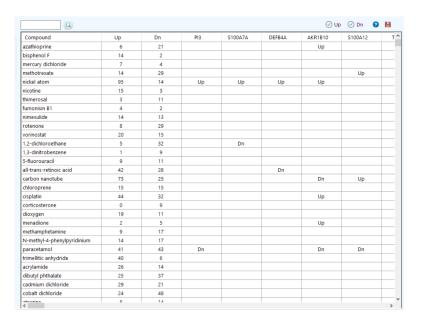
5.1 Chemical Interaction

Multiple chemical interactions can be seen in Enrichment tab. Click on numbers or the checkbox to select the probes.



1. Click on • ChEBI to see the Gene-Compound interactions in probes.

5. ENRICHMENT 31

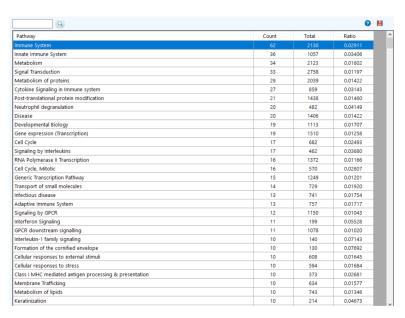


- Click on Up to see the up regulated probes.
- Click on Dn to see the down regulated probes.
- Click on ② to see the ChEBI qualifiers.
- Click on to save the results.
- 2. Click on \blacksquare to see the KEGG pathway enrichment.

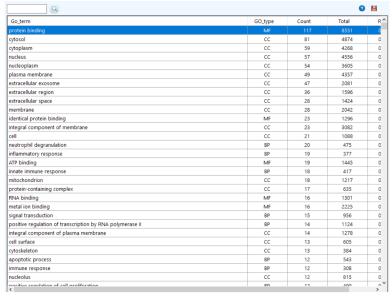


3. Click on 🗄 to see the reactome pathway enrichment.

5. ENRICHMENT 32

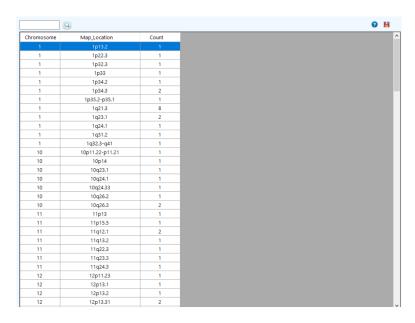


4. Click on to see the gene ontology pathway enrichment.

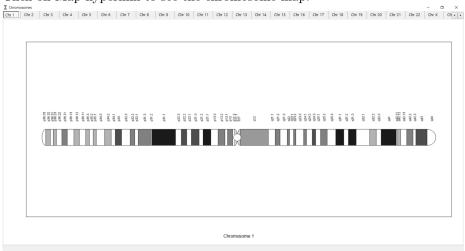


5. Click on of to see the chromosomes frequency.

5. ENRICHMENT 33

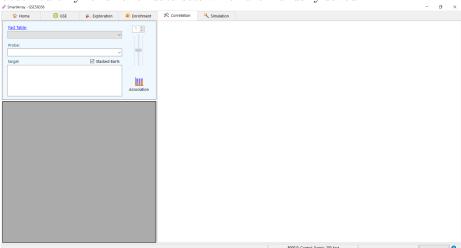


6. Click on Map hyperlink to see the chromosome map.

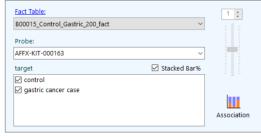


Correlation

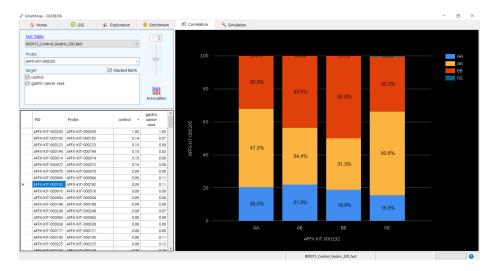
This tab gives the correlation between probes in a data-set. Correlation can be observed only for smaller data-sets which are manually saved.



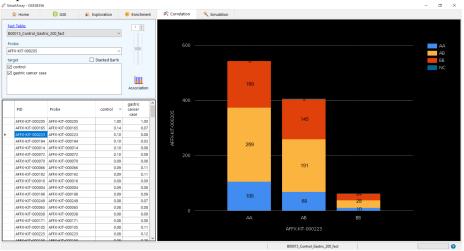
1. Click on Fact Table hyperlink to load the saved data-sets.



2. Select a probe/SNP and click on E- Correlation in case of probes or Association in case of SNPs.



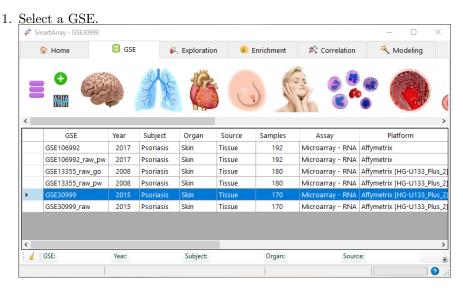
3. Unchecking of Stacked Bar% gives the plot with the count of SNPs instead of percent.



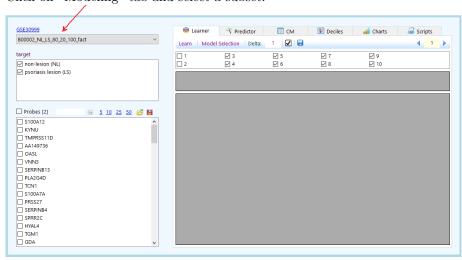
4. The zoom option is enabled for probes and can be used to change the offset of Y-axis.

7

Modelling

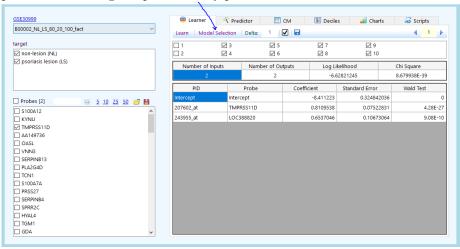


2. Click on "Modeling" tab and select a subset.

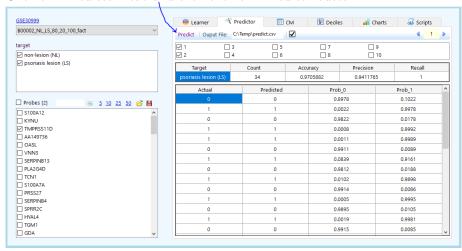


7. MODELLING 37

3. Click on "Model Selection" button. SmarrtArray automatically chooses probes with the highest predictability power.

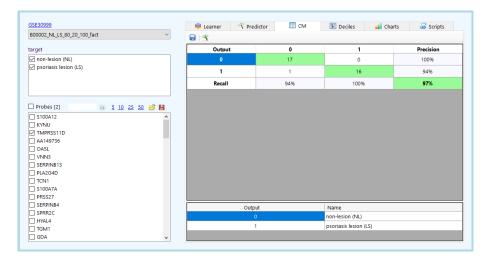


4. Click on "Predictor" tab and then click on "Predict" button.

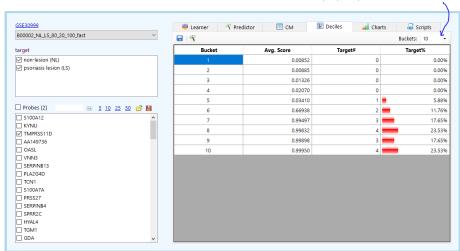


5. Click on "CM" tab (Confusion Matrix).

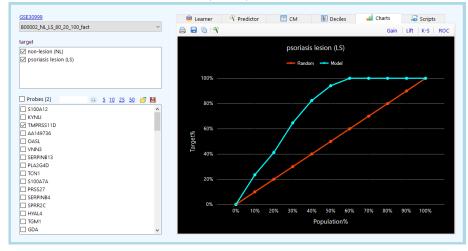
7. MODELLING 38



6. Click on "Deciles" tab. The number of buckets can be 2, 5, 10, 20 and 100.



7. Click on "Charts" tab to view Lift, Gain, K-S and ROC charts.



7. MODELLING 39

8. Click on "Scripts" tab to view the predictive model scripts in SQL, Python, Java, C# and VB.

