

# Visual Documentation v1.0.4.1



#### User Interface









Number of wells associated









Process pipeline





Wells coordinate





Currently activated descriptor











Available and activated descriptors When inactivated, the descriptors will not be taken into account for any process.

**----**





















When pressed, all the wells will















Current value of the selected well





Save new Info and Name





Contextual menu: Kegg (right click over a well) Locus ID is required for this option



selected well



# Options









🧟 Imp	ort									
Plate	Plate Dimensions									
c	Columns 24									
	lows 16									
	Data Name	Selection	Туре	_	Readout 0					
• •	Plate384	<b>V</b>	Plate name	-	SRP000459					
	Well 384w	<b>V</b>	Well position	-	D24					
	Cat		Descriptor	•	Druggable					
	Catalog Number		Descriptor	-	1					
	Gene Symbol		Descriptor	-	1					

























Note: display distribution option requires the have loaded a distributions based screen

Options

Mac. Syst. Errors Identif.

Display well information

Name

Display Statistics

🗇 Info

Gutter 4

Gradient Color

Ok

Histogram

Plate Design

Graph Design





























#### File format: scalar format



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	N14 $\checkmark ( f_x )$									
	А	В	С	D	E	F	G	Н	l. I	J
1	Plate Name	Well Position	Name	Class	Locus ID	Concentration	Info	Descriptor_0	Descriptor_1	Descriptor_2
2	Plate_0	A01	Cpds0	0	6530	0.00001	0	11.59151912	16.25808835	30.29250145
3	Plate_0	B01	Cpds1	0	5000	0.00001	0	6.573503613	-28.04967165	5.618658662
4	Plate_0	C01	Ctrl	1	3215	0.00001	0	17.62773991	-2.510358691	-36.73953295
5	Plate_0	D01	Cpds	3	1201	0.00001	0	-5.770683885	44.46689606	-10.2195251
6	Plate_0	E01	Cpds	4	1236	0.00001	0	22.58089542	-23.62939835	6.616227627
7	Plate_0	F01	Cpds	0		0.00001	0	7.266432643	37.79076338	4.967932999

SimpleMultivariate.csv - Notepad	- 0 ×
File Edit Format View Help	
Plate Name,Well Position,Name,Class,Locus ID,Concentration,Info,Descriptor_0,Descriptor_1,Descriptor_2	
Plate_0,A01,cpds0,0,6530,0.00001,0,11.59151912,16.25808835,30.29250145 Plate_0,B01,cpds1,0,5000,0.00001,0,6.573503613,-28.04967165,5.618658662 Plate_0,C01,ctrl 1, 3215,0,00001,0,17,62723991,-2,510358691,-36,723953295	
Plate_0, D01, Cpds, 3, 1201, 0. 00001, 0, -5. 770683885, 44. 46689606, -10. 2195251 Plate_0, E01, Cpds, 4, 1236, 0. 00001, 0, 22. 58089542, -23. 62939835, 6. 616227627	
Plate_0,F01,Cpds,0,,0.00001,0,7.266432643,37.79076338,4.967932999 Plate_0,G01,Cpds,0,,0.00001,0,8.677793145,3.751290143,1.836068183	
Plate_0,H01,Cpd5,0,,0.00001,0,-16.428564/9,-26.7681364,-3.993104696 Plate_0,I01,Cpd5,0,,0.00001,0,13.67169738,25.19427538,-6.892587543	
Plate_0,K01,Cpds,0,,0.00001,0,0.86994685,36.63227081,-11.92790985 Plate_0,L01,Cpds,0,,0.00001,0,-7.091733813,-40.36132336,-10.60620189	
Plate_0,M01,cpds,0,,0.00001,0,-10.20479083,-8.052453399,-13.16090941 Plate_0,N01,cpds,0,,0.00001,0,32.01099396,47.48570442,-4.767952859 Plate_0,001,cpds,0,,0.00001,0,-4.246455431,5.263992548,15.16896367	

The first row of the .csv data table should contain the name of every parameter. The order is not important has it can be change during the loading process. However, a column for the plate name, the well position and at least one descriptor (double format) are mandatory.



F	File Home Insert Page Layout Formulas Data Review View Developer Load Test Team									
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	N14	• (*	$f_{x}$							
	А	В	С	D	E	F	G	Н	l.	J
1	Plate Name	Well Position	Name	Class	Locus ID	Concentration	Info	Descriptor_0	Descriptor_1	Descriptor_2
2	Plate_0	A01	Cpds0	0	6530	0.00001	0	11.59151912	16.25808835	30.29250145
3	Plate_0	B01	Cpds1	0	5000	0.00001	0	6.573503613	-28.04967165	5.618658662
4	Plate_0	C01	Ctrl	1	3215	0.00001	0	17.62773991	-2.510358691	-36.73953295
5	Plate_0	D01	Cpds	3	1201	0.00001	0	-5.770683885	44.46689606	-10.2195251
6	Plate_0	E01	Cpds	4	1236	0.00001	0	22.58089542	-23.62939835	6.616227627
7	Plate_0	F01	Cpds	0		0.00001	0	7.266432643	37.79076338	4.967932999

SimpleMultivariate.csv - Notepad	- 0 ×
File Edit Format View Help	
Plate Name.Well Position.Name.Class.Locus ID.Concentration.Info.Descriptor_0.Descriptor_1.Descriptor_2	
Plate_0,A01,Cpds0,0,6530,0.00001,0,11.59151912,16.25808835,30.29250145 Plate_0,B01,Cpds1,0,5000,0.00001,0,6.573503613,-28.04967165,5.618658662	
Plate_0,C01,Ctrl,1,3215,0.00001,0,17.62773991,-2.510358691,-36.73953295 Plate_0,D01,Cpds,3,1201,0.00001,0,-5.770683885,44.46689606,-10.2195251	
Plate_0,E01,Cpds,4,1236,0.00001,0,22.58089542,-23.62939835,6.616227627	
Plate_0,G01,Cpds,0,,0.00001,0,8.677793145,3.751290143,1.836068183	
Plate_0,101,Cpds,0,.00001,0,13.67169738,25.19427538,-6.892587543	
Plate_0,301,Cpds,0,,0.00001,0,-1.746343646,-2.369280269,0.909697036 Plate_0,K01,Cpds,0,,0.00001,0,0.869994685,36.63227081,-11.92790985	
Plate_0,L01,Cpds,0,,0.00001,0,-7.091733813,-40.36132336,-10.60620189  Plate_0,M01,Cpds,0,,0.00001,0,-10.20479083,-8.052453399,-13.16090941	
Plate_0,N01,Cpds,0,,0.00001,0,32.01099396,47.48570442,-4.767952859 Plate_0,001,Cpds,0,,0.00001,0,-4.246455431,5.263992548,15.16896367	

Then, down below, the values are listed: double format for the descriptors and concentration, integer for the locus ID and class (<=10), and string for the others. If a descriptor value is missing or a parameter not formatted in the correct format, the well will be rejected from the screening.



## File format: histogram format



New Volume (E:) > Datab	ases 🕨 TestDAPI 🕨	
rary 🔹 Share with 💌	Burn New folde	r
Name	Туре	Size
퉬 Plate1	File folder	
PlateDay2	File folder	

A general directory containing every plate of the screening has to be created

New Volume (E:)  ► Databa	ases 🕨 TestDAPI 🕨	
rary 🔻 Share with 💌	Burn New folder	r
Name	Туре	Size
Plate1 PlateDay2	File folder File folder	

Every plate is defined by its own sub-directory. The name of the directory will be used as the plate name.



New Volum	e (E:) 🕨 Datab	ases 🕨 T	estDAPI	[ •	
rary 🔻 Sh	are with 🔻	Burn	New	folder	
Name	*	Туре		Size	
📗 Plate1	L	File fold	er		
] Plate	Day2	File fold	er		
	New Volume (E:	) 🕨 Databa	ses ▶ Te	estDAPI 🕨 P	
	ary 🔻 Share	with 🔻	Burn	New folder	
	Name	^			
	1x1.txt				
	1x2.txt				
	1x3.txt				
	2x1.txt				
	2x2.txt				
	2x3.txt				
	2x4.txt				
	13x2.txt				
	14x1.txt				
	14x2.txt				
	15x1.txt				
	16v1 tvt				

A general directory containing every plate of the screening has to be created

Each plate directory should contain a .txt file for every well. The file name is defined as follow:

"MxN.txt"

Where M and N are respectively the column and row position (1 indexed)





For each well, every row describes a descriptor histogram: 1<sup>st</sup> column is the name, then the remaining columns contain the histogram values (tab-separated). <u>Note:</u> consistency between each .txt file is required.



Importing such data can be operated trough the File->Load Histogram Based Screen menu.



## **Importing Data**



File	Edit				
	Load Screen	n	Ctrl+L		
	Import Scre	en	Ctrl+I		nensionalit
	Generate Sp	reen	Ctrl+G		
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<u>چ</u>	Exit		Ctrl+X		

Ctrl+X	=	🚣 Import							
		Plate I	Dimensions						
		Cal	24						
		CO		•					
		Ro	ws 16	<b></b>					
			Data Name	Selection	Туре		Readout 0	Readout 1	Readout 2
		•	Plate384	<b>V</b>	Plate name	-	SRP000459	SRP000479	SRP000502
			Well 384w	<b>V</b>	Well position	-	D24	P20	G11
			Cat		Descriptor	-	Druggable	Druggable	Druggable
			Catalog Number		Descriptor	-	1	2	3
			Gene Symbol		Descriptor	•	1	2	3
			Description		Descriptor	•	adrenocortical dy	deleted in esoph	hypothetical pro
			Locus ID		Descriptor	•	65057	115123	57574
			Fluo1		Descriptor	•	0.8228594	0.7233504	0.9090863
			Size		Descriptor	•	0.9823682	0.9870385	0.7240621
			Volume		Descriptor	•	59.26911984	183.9027118	137.0042838
			Ratio 1		Descriptor	•	144.2518279	234.0326818	139.0108669
			Fluo2		Descriptor	•	90.0408859	176.5919403	74.81596763
			Texture		Descriptor	•	104.5234322	231.5573299	195.0901458
			Rand1		Descriptor	•	48.66297765	0.909940097	34.82005831
			Rand2		Descriptor	-	35.75050135	7.755161101	5.351135178
			Rand3		Descriptor	-	36.28191786	22.86227618	40.45101283
			Rand4		Descriptor	•	14.83044153	23.36147298	0.397935311
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Plate dimensions	Plate Co Ro	Dimensions lumns 24 ws 16						
		Data Name	Selection	Туре		Readout 0	Readout 1	Readout 2
	+	Plate384	<b>V</b>	Plate name	-	SRP000459	SRP000479	SRP000502
		Well 384w	<b>V</b>	Well position	-	D24	P20	G11
		Cat		Descriptor	-	Druggable	Druggable	Druggable
		Catalog Number		Descriptor	-	1	2	3
		Gene Symbol		Descriptor	-	1	2	3
		Description		Descriptor	-	adrenocortical dy	deleted in esoph	hypothetical pro
		Locus ID		Descriptor	-	65057	115123	57574
		Fluo1		Descriptor	-	0.8228594	0.7233504	0.9090863
		Size		Descriptor	-	0.9823682	0.9870385	0.7240621
		Volume		Descriptor	-	59.26911984	183.9027118	137.0042838
		Ratio 1		Descriptor	-	144.2518279	234.0326818	139.0108669
		Fluo2		Descriptor	-	90.0408859	176.5919403	74.81596763
		Texture		Descriptor	-	104.5234322	231.5573299	195.0901458
		Rand1		Descriptor	-	48.66297765	0.909940097	34.82005831
		Rand2		Descriptor	-	35.75050135	7.755161101	5.351135178
		Rand3		Descriptor	-	36.28191786	22.86227618	40.45101283
		Rand4		Descriptor	-	14.83044153	23.36147298	0.397935311
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Pl	ate Dimensions						
	Columns 24	-					
	Rows 16	×					
	Data Name	Selection	Туре	Readout 0	Readout 1	Readout 2	
•	Plate384	~	Plate name 🔻	SRP000459	SRP000479	SRP000502	
	Well 384w		Well position 🔻	D24	P20	G11	
	Cat		Descriptor 💌	Druggable	Druggable	Druggable	
	Catalog Number		Descriptor 🔻	1	2	3	
	Gene Symbol		Descriptor 🔻	1	2	3	
	Description		Descriptor 🔻	adrenocortical dy	deleted in esoph	hypothetical pro	
	Locus ID		Descriptor 🔻	65057	115123	57574	
	Fluo1		Descriptor 🔻	0.8228594	0.7233504	0.9090863	 Readouts preview
	Size		Descriptor 🔻	0.9823682	0.9870385	0.7240621	
	Volume		Descriptor 🔻	59.26911984	183.9027118	137.0042838	
	Ratio 1		Descriptor 🔻	144.2518279	234.0326818	139.0108669	
	Fluo2		Descriptor 🔻	90.0408859	176.5919403	74.81596763	
	Texture		Descriptor 💌	104.5234322	231.5573299	195.0901458	
	Rand1		Descriptor 💌	48.66297765	0.909940097	34.82005831	
	Rand2		Descriptor -	35.75050135	7.755161101	5.351135178	
	Rand3		Descriptor -	36.28191786	22.86227618	40.45101283	
	Rand4		Descriptor -	14.83044153	23.36147298	0.397935311	
•			III				
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		- Plate I	Dimensions						
		Cal	umps 24						
		CO		•					
		Ro	ws 16	-					
			Data Name	Selection	Туре		Readout 0	Readout 1	Readout 2
			Plate384	<b>V</b>	Plate name	-	SRP000459	SRP000479	SRP000502
			Well 384w	<b>V</b>	Well position	-	D24	P20	G11
		I	Cat		Descriptor	-	Druggable	Druggable	Druggable
			Catalog Number		Descriptor	•	1	2	3
			Gene Symbol		Descriptor	-	1	2	3
			Description	<b>V</b>	Descriptor	•	adrenocortical dy	deleted in esoph	hypothetical pro
Names that be associated			Locus ID	<b>V</b>	Descriptor	-	65057	115123	57574
with the data			Fluo1	<b>V</b>	Descriptor	-	0.8228594	0.7233504	0.9090863
			Size	<b>V</b>	Descriptor	-	0.9823682	0.9870385	0.7240621
			Volume	<b>V</b>	Descriptor	-	59.26911984	183.9027118	137.0042838
			Ratio 1	<b>V</b>	Descriptor	-	144.2518279	234.0326818	139.0108669
			Fluo2	<b>V</b>	Descriptor	-	90.0408859	176.5919403	74.81596763
			Texture	<b>V</b>	Descriptor	-	104.5234322	231.5573299	195.0901458
			Rand1		Descriptor	-	48.66297765	0.909940097	34.82005831
			Rand2		Descriptor	-	35.75050135	7.755161101	5.351135178
			Rand3	<b>V</b>	Descriptor	•	36.28191786	22.86227618	40.45101283
			Rand4	<b>V</b>	Descriptor	-	14.83044153	23.36147298	0.397935311
		•			III				•
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	Pi	nport ate Dimensions Columns 24 Rows 16					
		Data Name	Selection	Туре	Readout 0	Readout 1	Readout 2
		Plate 384	<b>V</b>	Plate name	▼ SRP000459	SRP000479	SRP000502
		Well 384w	<b>V</b>	Well position	▼ D24	P20	G11
	.0	Cat		Descriptor	▼ Druggable	Druggable	Druggable
		Catalog Number		Descriptor	▼ 1	2	3
		Gene Symbol		Descriptor	▼ 1	2	3
If unchecked,		Description		Descriptor	<ul> <li>adrenocortical dy</li> </ul>	deleted in esoph	hypothetical pro
the corresponding data		Locus ID		Descriptor	▼ 65057	115123	57574
will not be loaded		Fluo 1		Descriptor	• 0.8228594	0.7233504	0.9090863
will not be loaded		Size		Descriptor	<ul> <li>0.9823682</li> </ul>	0.9870385	0.7240621
		Volume	<b>V</b>	Descriptor	<ul> <li>59.26911984</li> </ul>	183.9027118	137.0042838
		Ratio 1		Descriptor	<ul> <li>144.2518279</li> </ul>	234.0326818	139.0108669
		Fluo2		Descriptor	• 90.0408859	176.5919403	74.81596763
		Texture		Descriptor	<ul> <li>104.5234322</li> </ul>	231.5573299	195.0901458
		Rand1		Descriptor	<ul> <li>48.66297765</li> </ul>	0.909940097	34.82005831
		Rand2		Descriptor	▼ 35.75050135	7.755161101	5.351135178
		Rand3		Descriptor	▼ 36.28191786	22.86227618	40.45101283
		Rand4		Descriptor	▼ 14.83044153	23.36147298	0.397935311
	•			III			► Dk



Plate I	Dimensions						
Col		V					
Ro	ws 16						
	Data Name	Selection	Туре		Readout 0	Readout 1	Readout 2
	Plate384	<b>V</b>	Plate name	-	SRP000459	SRP000479	SRP000502
	Well 384w		Well position	-	D24	P20	G11
	Cat	<b>V</b>	Info	-	Druggable	Druggable	Druggable
	Catalog Number		Descriptor	-	1	2	3
	Gene Symbol		Descriptor	-	1	2	3
	Description		Name	-	adrenocortical dy	deleted in esoph	hypothetical
	-Leeus-ID		- Locus ID	-	65057	115123	57574
	Fluo1		Descriptor	-	0.8228594	0.7233504	0.9090863
	Size	<b>V</b>	Descriptor	-	0.9823682	0.9870385	0.7240621
	Volume		Descriptor	-	59.26911984	183.9027118	137.0042838
	Ratio 1		Descriptor	-	144.2518279	234.0326818	139.0108669
	Fluo2		Descriptor	-	90.0408859	176.5919403	74.81596763
	Texture	<b>v</b>	Descriptor	-	104.5234322	231.5573299	195.0901458
	Rand1		Descriptor	-	48.66297765	0.909940097	34.82005831
	Rand2		Descriptor	-	35.75050135	7.755161101	5.351135178
	Rand3		Descriptor	-	36.28191786	22.86227618	40.45101283
+	Concentration		Descriptor	-	14.83044153	23.36147298	0.397935311
4			Plate name Well position Class Name Locus ID				
			Concentration Info Descriptor				Dk

Data type. Mandatory: Plate Name, well position and at least one descriptor. Note: Locus ID should be defined as an integer.



# Generating artificial univariate screening data



-	s analyzer v1.0.:	3					
File	Edit						
1	Load Screen	Ctrl+L		-			
	Import Screen	Ctrl+I		Dime	nsionality Reduc	tion	Syst
	Generate Scree	n	•		Univariate	Ctrl+G	
	Save Screen		►		Multivariate	Ctrl+Alt+G	
	Add Plates	Ctrl+A					
22	Link Data						
<u>"</u>	Exit	Ctrl+X					













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Descriptor\_0

L\_\_\_\_\_



🙅 Gen	erate Screening		
	Number of Plates Columns Rows	10 24 16	
lue distributions	Row Effect     Shift		
Bias Va	Column Effect		
	Edge Effect		
	Shift 1.0	\$	
	Iteration 8	÷	
	Bowl Effect		
	Shift 1.0	÷	
	Ratio X/Y 1.50	÷	
	Gen	erate	

If an effect **X** is selected, it will be combined to original data by the following way:

Resulting Data = Original Data \* (X + Shift\_X)











The higher **Shift\_X** is, the lower **X** contribution to the generated data























#### If a parameter **X** is checked, its value will vary from, increasing with a step defined in the options window.









# Generating artificial multivariate screening data



1	⊵ нс	S analyzer v1.0.3	3					
	File	Edit						
		Load Screen	Ctrl+L		-			
		Import Screen	Ctrl+I		Dimer	nsionality Reduc	tion	Syste
		Generate Scree	n	•		Univariate	Ctrl+G	
		Save Screen		F		Multivariate	Ctrl+Alt+G	
		Add Plates	Ctrl+A					
	$\frac{2\pi n}{r}$	Link Data						
		Exit	Ctrl+X					

						Dime	nsion 7	A V	Number of Plates 10 0 Columns 24 0 Rows 16 0									
	Name	Column		Selection	Mean0	Stdv0	Mean1	Stdv1	Mean2	Stdv2	Mean3	Stdv3	Mean4	Stdv4	Mean5	Stdv5	Mean6	Stdv
1	Phenotype 0	0	•	V	0	20	0	20	0	20	0	20	0	20	0	20	0	20
	Phenotype 1	1	•	<b>V</b>	50	20	50	20	50	20	50	20	50	20	50	20	50	20
	Phenotype 2	Entire plate	•	V	100	20	100	20	100	20	100	20	100	20	100	20	100	20
1	Phenotype 3	3	•		150	20	150	20	150	20	150	20	150	20	150	20	150	20
	Phenotype 4	4	-		200	20	200	20	200	20	200	20	200	20	200	20	200	20
1	Phenotype 5	5	•		250	20	250	20	250	20	250	20	250	20	250	20	250	20
1	Phenotype 6	6	•		300	20	300	20	300	20	300	20	300	20	300	20	300	20
	Phenotype 7	7	-		350	20	350	20	350	20	350	20	350	20	350	20	350	20
1	Phenotype 8	8	-		400	20	400	20	400	20	400	20	400	20	400	20	400	20
•	Phenotype 9	9	-		450	20	450	20	450	20	450	20	450	20	450	20	450	20





Form	mForMultivariat	teScreen																	
										Plate	Dimension								
										Nu	umber of Plat	es 10	-						
						Dime	nsion 7		×		Columns	24		]					
											000000000		×						
											nows	16							
	Name	Column	_	Selection	Mean0	Stdv0	Mean1	-	Stdv1	Mean2	Stdv2	Mean3	Stdv3	Mean4	Stdv4	Mean5	Stdv5	Mean6	Stdv6
	Phenotype 0	0	-	<b>V</b>	0	20	0		20	0	20	0	20	0	20	0	20	0	20
	Phenotype 1	1	-	<b>V</b>	50	20	50		20	50	20	50	20	50	20	50	20	50	20
	Phenotype 2	Entire plate	•	<b>V</b>	100	20	100	1	20	100	20	100	20	100	20	100	20	100	20
	Phenotype 3	3	•		150	20	150		20	150	20	150	20	150	20	150	20	150	20
	Phenotype 4	4	•		200	20	200		20	200	20	200	20	200	20	200	20	200	20
	Phenotype 5	5	•		250	20	250		20	250	20	250	20	250	20	250	20	250	20
	Phenotype 6	6	•		300	20	300		20	300	20	300	20	300	20	300	20	300	20
	Phenotype 7	7	•		350	20	350		20	350	20	350	20	350	20	350	20	350	20
	Phenotype 8	8	•		400	20	400		20	400	20	400	20	400	20	400	20	400	20
+	Phenotype 9	9	-		450	20	450		20	450	20	450	20	450	20	450	20	450	20
										Gen	erate								

🚣 HCS analyzer v1.0.3 - • × File Edit Plate\_0 Plate Screen View Plug-ins Help Current Pilde 🔎 Dimensionality Reduction 🔥 Systematic Error Identification & Correction 🖾 Normalization 🔟 Cassification & Custering 💷 Report Export Class selection Positive (0) - ### 113.929 Current Descriptor Descriptor\_0 Global Descriptor List Descriptor\_Dis
 Descriptor\_0
 Descriptor\_1
 Descriptor\_2
 Descriptor\_3
 Descriptor\_4
 Descriptor\_5
 Descriptor\_6 Global only selected **4**-----Apply to all plates Display class -8.115 **Q** 

The dimension corresponds to the number of descriptors



SormForMultiv	variateScreen													
			Plate	Dimension										
			N	umber of Plate	es 10	×								
Dimension	2	* *		Columns	24									
				Columna		•								
	Hows 16 v													
Name	Column	_	Selection	Mean()	Stdv0	Mean1	Stdv1							
Phenoty	pe 0 0	-		0	20	0	20							
Phenoty	pe 1 1	-	<b>V</b>	50	20	50	20							
Phenoty	pe 2 Entire plate	· •	<b>V</b>	100	20	100	20							
Phenoty	pe 3 3	•		150	20	150	20							
Phenoty	pe 4 4	-		200	20	200	20							
Phenoty	pe 5 5	-		250	20	250	20							
Phenoty	pe 6 6	-		300	20	300	20							
Phenoty	pe 7 <mark>7</mark>	-		350	20	350	20							
Phenoty	pe 8 8	-		400	20	400	20							
Phenotype	pe 9 9	-		450	20	450	20							
			-											
			Ger	ierate										



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SormForMultivariate	FormForMultivariateScreen												
			Plate	Dimension									
			N	umber of Plate	:s 10	•							
Dimension 2	* *			Columna	2/		1						
				Columns	2-1 								
				Hows	16	Ē							
Name	Column	Sal	ection	МезрО	Stdy0	Mean 1	Stdv1						
Phenotype 0	0	•		0	20	0	20						
Phenotype 1	1		<b>V</b>	50	20	50	20						
Phenotype 2	· Entire plate			100	20	100	20						
Phenotype 3	3			150	20	150	20						
Phenotype 4	4			200	20	200	20						
Phenotype 5	5			250	20	250	20						
Phonetime 6	с с			200	20	200	20						
Phenotype 8	7			250	20	250	20						
Phenotype 7	0			400	20	400	20						
Phenotype 8	0			400	20	400	20						
<ul> <li>Prienotype 9</li> </ul>	9			400	20	400	20						
			Gen	erate									





				Plate	Dimension				
				N	umber of Plat	10	÷		
	Dimension 2	÷			Columns		24	* *	
					Rows		16	·	
	Name	Column		Selection	Mean0	Stdv0	Mean 1	Stdy	1
	Phenotype 0	0	-		0	5	0	5	<u> </u>
•	Phenotype 1	1	-	<b>V</b>	50	20	50	20	
	Phenotype 2	Entire plate	•	<b>V</b>	100	20	200	-20	
	Phenotype 3	3	-		150	20	150	20	
	Phenotype 4	4	•		200	20	200	20	
	Phenotype 5	5	•		250	20	250	20	
	Phenotype 6	6	•		300	20	300	20	
	Phenotype 7	7	•		350	20	350	20	
	Phenotype 8	8	•		400	20	400	20	
	Phenotype 9	9	•		450	20	450	20	
		[	_	Gen					
				Gen	erate				

Each cloud (phenotype) is modeled by a Gaussian distribution defined by its means in every dimension





				Plate	Dimens	sion	_		-			
			-	N	umber o	of Plates	10	)				
	Dimension 2	×			Colur	nns	24	1	1			
					D		10	•	1			
					Row	IS	IE		1			
	Name	Column		Selection	Mean	0	Stdv0	Mean1	Stdv1	1		
	Phenotype 0	0	-	<b>V</b>	0		5	0	5			
•	Phenotype 1	1	•	<b>V</b>	50		20	50	20			
	Phenotype 2	Entire plate	-	<b>V</b>	100		20	200	20			
	Phenotype 3	3	-		150		20	150	20	11		
	Phenotype 4	4	-		200		20	200	20			
	Phenotype 5	5	-		250		20	250	20			
	Phenotype 6	6	-		300		20	300	20			
	Phenotype 7	7	-		350		20	350	20	11		
	Phenotype 8	8	-		400		20	400	20		Í	🧟 Scatter P
	Phenotype 9	9	•		450		20	450	20			Export
			_	-		_				1		
				Gen	erate							

As well as its variances.





### **Dimensionality reduction**







🚣 HCS analyzer v1.0.2		
File Edit SRP000441-HIV Grid-2010-02-20-(2007-1	0-26_15-25-36) - Plate Screen View Help	
Current Plate Dimensionality Reduc	ton 🔥 Systematic error identification & correction 🦾 Normalization 🔛 Classification & Clustering	Current Descriptor
New Dimension C Unsupervised PCA Principal Component Analysis. For more information, go to: http://en.wikipedia.org/wiki/Principal component analysis Reduce Dimensional Component	2 Program Program Pr	Mean Green

#### Desired new dimension











### **Descriptors** management



















## Quality controls







Display the sorted Z-factors of the current plate for each selected descriptor





Display the sorted Z-factors of the selected descriptor for all the active plates













Current Plate							-	Plate Screen View	Plug-ins Help				
	୵୷	Dimensionality Re	eduction		Syster	matic erro	r ider	ntification & correction	Normalization	Classification & Clustering	Report Export		Class selection
ate I	Descriptor	Anderson-Darling test	edge effect	column artifact	row artifact	bowl effect	*	Correction		Rejection			Current Descriptor
P000438 F	luo1	14.308	х				=	B-Score	-	Z-Factor	<b>•</b>		Fluo1
P000438 S	Size	16.773									local.		Descriptor List
P000439 F	luo 1	11.287	х				_			Threshold 0.50	×		🔽 Fluo 1
P000439 S	Size	15.17						B-Score.		Z-Score based rejection.			Size
P000440 F	luo1	7.778	х					For more information, go to: http://en.wikipedia.org/wiki	Information gain in d	Remove plates with a lower Z-fac defined by the thresold.	tor values than		Ratio 1
P000440 S	Size	9.753	Х					ecision trees	· · · · · · · · · · · · · · · · · · ·	For more information, go to:	ctor		
P000441 F	luo1	9.302	Х							http://en.wikipedia.org/wiki/2ha			
P000441 S	Size	10.088	Х										
P000442 F	luo1	16.081	Х										
P000442 S	Size	7.561	Х	Х									
P000442 V	/olume	5.046		х									
P000443 F	luo1	12.05	Х										
P000443 S	Size	6.648	х	Х									
P000443 V	/olume	6.071			)	<							
P000444 F	luo1	16.308	Х										
P000444 S	Size	8.778	Х				-						
	Sys	stematic error identi	ification					Plate by Plate 0	Correction	Reject Plates		analyzer	
		_											
ld sy each	lentif ystem selec	y the pot natic erro ted plate	tentia ors fo es on	al or eacl	h								
	P000438 F P000438 S P000439 F P000439 F P000440 F P000440 F P000440 F P000441 S P000442 F P000442 F P000442 F P000442 F P000443 F P000443 F P000444 F P000444 S P000444 S P000445 S P00045 S P0005 S P005 S P0005 S P005	P000438         Fluo 1           P000438         Size           P000439         Fluo 1           P000400         Size           P000400         Size           P000400         Size           P000400         Size           P000401         Size           P00041         Size           P00042         Fluo 1           P00043         Size           P000441         Size           P000442         Size           P000443         Rico 1           P000443         Size           P000444         Fluo 1           P000443         Size           P000444         Fluo 1           P000444         Size           P000445         Size           P000446         Size           P00045         Size           P00046         Size	P000433         Puo1         14.308           P000438         Size         16.773           P000438         Size         15.773           P000439         Fuo1         11.287           P000430         Size         15.17           P000440         Puo1         7.778           P000440         Puo1         9.753           P000441         Fuo1         9.302           P000441         Size         10.088           P000442         Fuo1         16.081           P000443         Fuo1         12.05           P000443         Fuo1         16.308           P000443         Volume         6.071           P000443         Size         8.778           P000444         Size         8.778           P000445         Size         8.778	P001439         Ruo1         14.308         X           P000438         Size         16.773         1           P000439         Ruo1         11.287         X           P000439         Ruo1         11.287         X           P000439         Size         15.17         1           P000400         Size         9.753         X           P000440         Ruo1         9.783         X           P000441         Ruo1         9.302         X           P000441         Size         7.661         X           P000442         Ruo1         16.081         X           P000443         Ruo1         12.05         X           P000443         Ruo1         12.05         X           P000443         Size         6.648         X           P000444         Size         8.778         X <td>P000438         Fluo 1         14.308         X         Image: Constraint of the second se</td> <td>P000438         Fuo 1         14.308         X         Image: Constraint of the second sec</td> <td>P00438         Puo 1         14.308         X         Image: Constraint of the second seco</td> <th>P00438         Puo 1         14.308         X         Image: Constraint of the second seco</th> <td>P000438         Ruo 1         14.308         X         Image: Constraint of the second sec</td> <td>P000438         Flue 1         14.308         X         Image: Control of the second secon</td> <td>P000438       Ruo 1       14.308       X</td> <td>P000433       No 1       14.308       X       No       No</td> <td>200430       Ruot       14.308       X       Image: Constant of Constan</td>	P000438         Fluo 1         14.308         X         Image: Constraint of the second se	P000438         Fuo 1         14.308         X         Image: Constraint of the second sec	P00438         Puo 1         14.308         X         Image: Constraint of the second seco	P00438         Puo 1         14.308         X         Image: Constraint of the second seco	P000438         Ruo 1         14.308         X         Image: Constraint of the second sec	P000438         Flue 1         14.308         X         Image: Control of the second secon	P000438       Ruo 1       14.308       X	P000433       No 1       14.308       X       No       No	200430       Ruot       14.308       X       Image: Constant of Constan





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Ok

Systematic errors identification parameters can be changed by the options window

Double click on a row display the corresponding readouts


Plate by plate, and descriptor by descriptor, correction procedure can be performed using the dedicated function









after

before





### Normalization





Various approaches for data normalization of the screening data are available (controls based or not)

·-----





before

after

# Clustering and classification





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Some clustering methods allow automated evaluation of the optimum number of clusters. <u>Note:</u> if more than 10 classes are detected, the clustering is not operated.



Clustering (here: 3 classes have identified)





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If the classification operated is tree based (C4.5) a tree diagram is affected for each plate.





### **Hierarchical Tree visualization**







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be time consuming for large number of data







## Pathways analysis



C	Columns 24	* *									
F	Rows 16	*									
	Data Name	Selection	Туре		Readout 0	Readout 1	Readout 2	*			
	Plate384	<b>V</b>	Plate name	-	SRP000459	SRP000479	SRP000502				
	Well 384w	<b>V</b>	Well position	•	D24	P20	G11				
	Cat		Descriptor	-	Druggable	Druggable	Druggable				
	Catalog Number		Descriptor	-	1	2	3				
	Gene Symbol		Descriptor	-	1	2	3	=			
	Description		Descriptor	-	adrenocortical dy	deleted in esoph	hypothetical pro				
I	Locus ID	$\checkmark$	Locus ID	-	65057	115123	57574			-	
	Fluo 1		Descriptor	-	0.8228594	0.7233504	0.9090863		T		
	Size	<b>V</b>	Descriptor	-	0.9823682	0.9870385	0.7240621				
	Volume	<b>V</b>	Descriptor	-	59.26911984	183.9027118	137.0042838				
	Ratio 1	<b>v</b>	Descriptor	-	144.2518279	234.0326818	139.0108669				
	Fluo2		Descriptor	-	90.0408859	176.5919403	74.81596763				
_	Testure		Descriptor	-	104 6004000	221 6672200	105 0001450	Ŧ			



Locus IDs have to be associated to each well

Note: this operation requires internet connection





### Export









Par	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	65m III - UI - I - IOn -	• n • A' s' A	= = = =	₩ 1000- 100	General \$ - % % #1	A States	States States Form	rt - te - hot -	Σ·97 Ξ·#4 -2·
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_	A1	+ (		& Plate	Name					
		- F	0	Ε		ű.	- H	1	1	- E.
4	Well Position	Class	FILIOS	Real_Size	Volume					
	A01		0.02992	0.71625	-19.8856					
	903	0	0.4584	0.92963	-50 1/586					
44	001	0	0.55554	0.87538	-17.865					
2	001	0	0.29907	0.919/1	-17 2936					
0	EDS	0	0.65164	0.78729	-19 1757					
1	MUL	0	0.59716	0.84612	-18 6867					
	601		0.54701	0.6222	-18.8055					
	HUI	0	0.53988	9.73788	-19 1102					
10	101	0	0.46348	0.01562	-17:0875					
	103	0	0.53052	0.97329	-18.6184					
	101	0	0.47085	0.02304	-11.7094					
	101	0	0.709	0.89047	-31 6002					
렩	NR02	0	0.71505	0.73737	-18 7137					
15	NUS	0	0.5127	0.81529	-20.4122					
20	001		0.50041	0.87228	-19.9777					
10	POS	0	0.60875	0.75476	-21.4674					
28	MUZ .	2	0.22836	0.03756	89.9178					
14	002		0.81693	0.88011	58.6175					
10	0.02	2	0.62752	0.09015	102.984					
	002		0.91943	0.95808	111.054					
44	602	2	0.89058	0.89667	97.7506					
10	MUZ	2	0.87903	0.91354	114.419					
런	002	2	0.91955	0.93167	24,6581					
1.0	HULL		0.07826	0.92157	87 4028					
20	102	2	0.01228	0.91891	24,6648					
런	102	2	0.91486	0.97501	104,476					
10	100	2	0.00555	0.87667	24.6329					
19	100		0.90923	0.80376	344,295					
20	101/2	2	0.61945	0.91278	101,439					
	199.1		0.90068	0.03940	BY 9132					
24	002	2	0.68206	0.47963	20.7410					
-	104		110000	0.004103	0.0072					
	PU0	1	0.00410	0.99619	-0.90901					
32	003	1	0.96458	0.99133	-9.16148					
20	005	1	0.9467	0.98269	5.12075					
2			0.96933	0.973	e.e1502					
20	000	1	0.99751	0.07405	2.70436					
-	104		0.99342	0.97485	0.55692					

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1 Plate		Descripto	Anderson	edi	re effect	col	umn a	t row	artifact	bowl e	ffect	
2 SRP000	459	Fluo1	16.822					x				
a SRP000	459	Size	22.629									
4 SRP000	459	Volume	5.541	х		х						
5 SRP000	479	Fluo1	15.678									
6 SRP000	479	Size	21.654									
7 58P000	479	Volume	8.163	х		×						
8 58P000	502	Fluo1	7.892	х								
9 58200	469	Fluo1	12.218	х								
10 SRP000	469	Size	10.458									
11 SRP000	469	Volume	8.597	к		х						
12 SRP000	463	Fluo1	22.149	к				х				
13 SRP000	463	Size	23.277									
14 SRP000	463	Volume	5.477							x		
15 SRP000	474	Fluo1	19.735									
16 SRP000	474	Size	14.659	х								
17 SRP000	474	Volume	11.893									
18 SRP000	480	Fluo1	14.431	х								
19 SRP000	480	5120	26.226									
20 SRP000	480	Volume	6.139	х		х						
21 SRP000	466	Fluo1	21.266	к				х				
22 SRP000	466	Size	14.299	к								
23 SRPOOR	439	Fluci	11.287	к								
24 SRP000	439	Size	15.17									
25 SRP000	465	Fluo1	27.311									
26 SRP000	465	Size	17.041	X								
27 SRP000	465	Volume	9.126									
28 SRP000	484	Fluo1	11.423	х								
19 SRP000	484	Size	25.69									
58 P000	484	Volume	6.227			х				×		
31 SRP000	438	Fluo1	14.308	х								
12 SRP000	438	Size	16.773									
13 SRP000	483	Fluo1	5.205	к		х						
34 SRP000	483	Size	18.773									
15 SRP000	483	Volume	6.532									
16 SRP000	453	Fluo1	17.171	X				х				
37 SRP000	499	Fluo1	6.245	X				x				
B SRPOOL	499	Size	22,451									
C C F H	Syster	naticError	Report 2	1			114					



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e Edit Plate_0					
Current Plate		Plate Screen View Plug-ins Help			
Screening Information	Dimensionality Reduction	ror Identification & Correction	tion & Clustering	Report Export	Class selection
And a stream of a solition of		Fid Screen     Plate Format			Current Descriptor
late dimensions: 24 x 16	<b>^</b>				Descriptor_1 •
umber of plates: 10 (/ 10)	Plate Na SRP0004	me Column Row Class Name 8744 1 1 4 CD1			Descriptor List
le 1 : Plate_0 384 active wells / 1 classer in 2 : Plate 1	54/004		40 480 °C		V Descriptor_1
384 active wells / 1 classe e 3 : Plate_2	ss.	assilication			
384 active wells / 1 classe te 4 : Plate_3 384 active wells / 1 classe	8. 	Classification Tree usity Control			
86 5 Plate_4 384 active wells / 1 classe	50. E	✓Correlation Matrix and Ranking ✓Systematic Errors Table			
late 6 : Plate_5 384 active wells / 1 classe late 7 : Plate 6	s.	Z-Factors RNA screening			
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late 9 : Plate_8 384 active wells / 1 classe	95	Veka Att He			
late 10 : Plate_9 384 active wells / 1 classe	s.			1	
umber of active descriptors: 2 (/ 2)					
escriptor 1 : Descriptor_0	-	Export		analyzer	
<b>Q</b>	🕌 « Databases 🕨 export	• 49 Search export			
Organize	✓ Include in library ▼	Share with ★ Burn >> 🔠 ★			
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	Correlation_Matrix.emf	- EMF-File	10.KB		
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**HCS** Analyzer



### **Core Development**





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Look, develop, modify, debug, test



#### **Plugins Development**





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Add information about your plugin (menu, etc.)



Develop your plugin and do not forget to share it

