

Intersample calculations:

Examples:

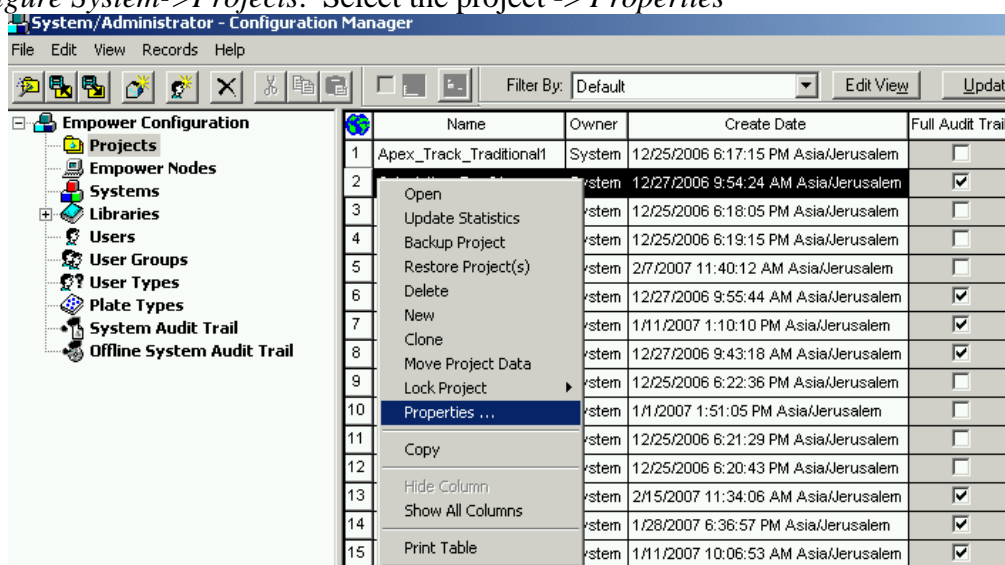
1. Average of Area/Amount of group of standards with the same label.
2. Differences between *Area/Amount* of two different standards
3. Average of duplicate samples' *Area*

Please note the following:

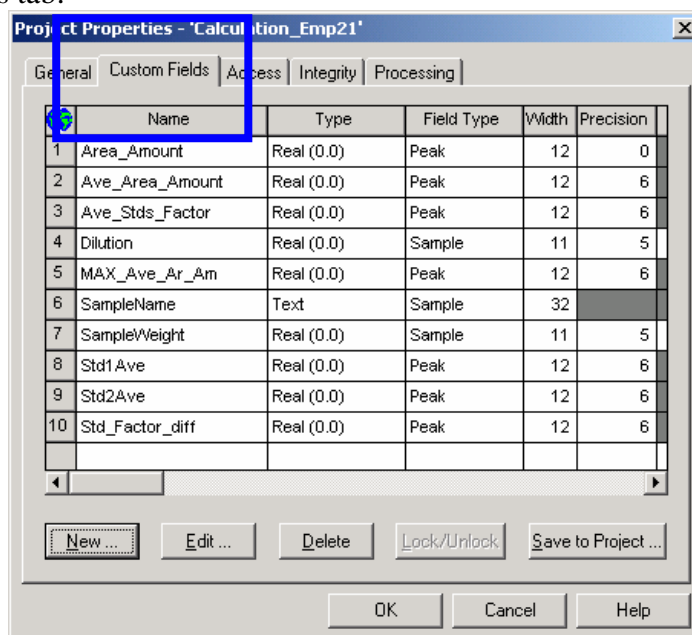
- All the re-processing is done on sample sets: NOT on separate results.
- Calculations are done only after all results are calculated and stored.
- The calculations can be done within or between sample sets.

Instructions:

Go to *Configure System->Projects*. Select the project -> *Properties*



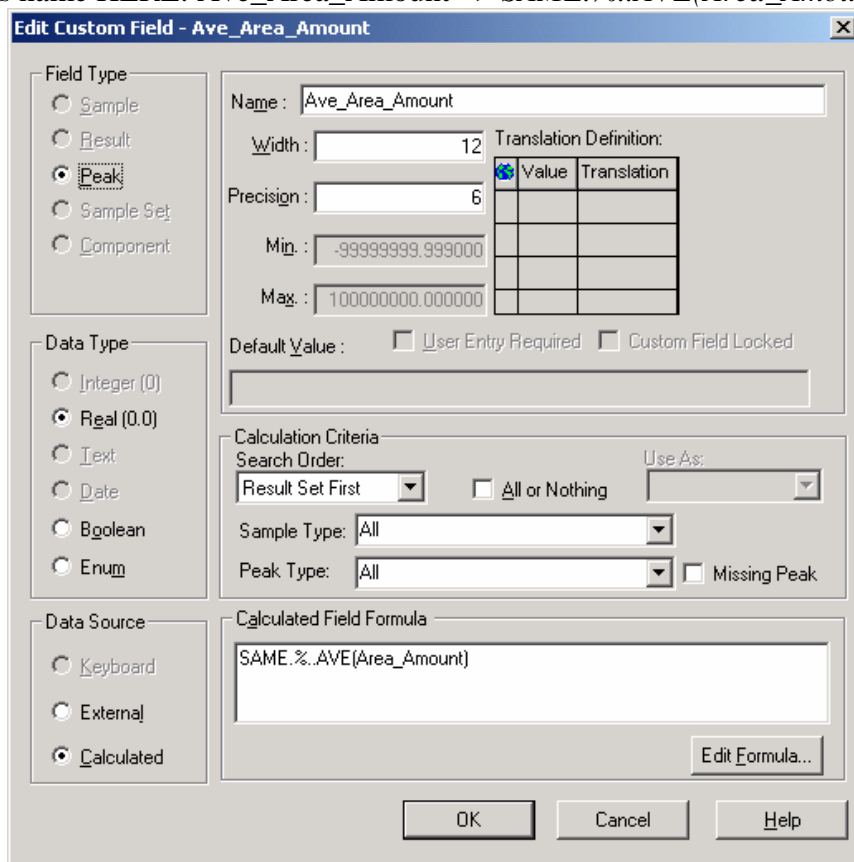
Go to the Custom Fields tab:



Example 1:

Area/Amount is averaged over a group of runs with identical label.

The custom field's name HERE: Ave_Area_Amount => *SAME.%.AVE(Area_Amount)*



In which the calculation is: **SAME.%.AVE(Area_Amount)**

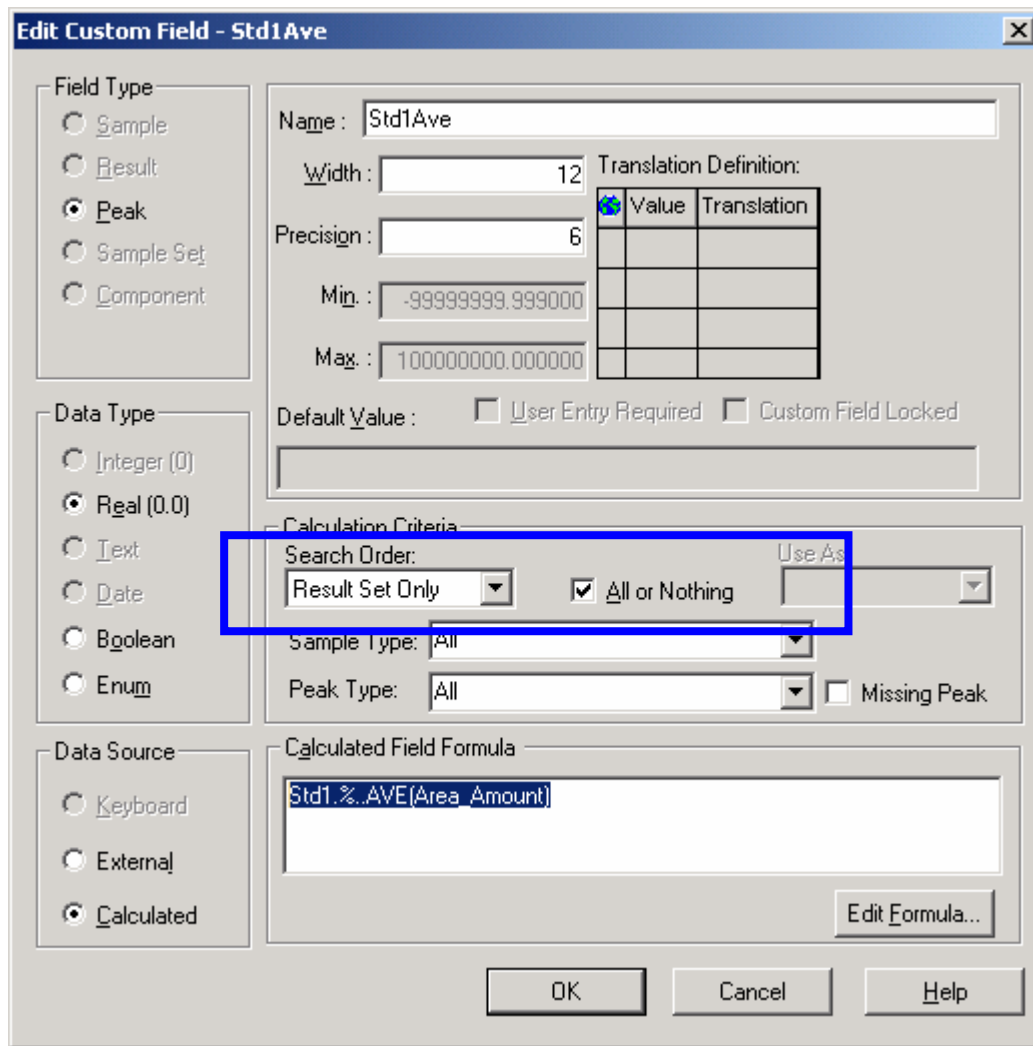


Example 2

Average of Area/Amount field of Std1 and Std2 having label Std1 and Std2 respectively. The difference and Average are calculated as the following:

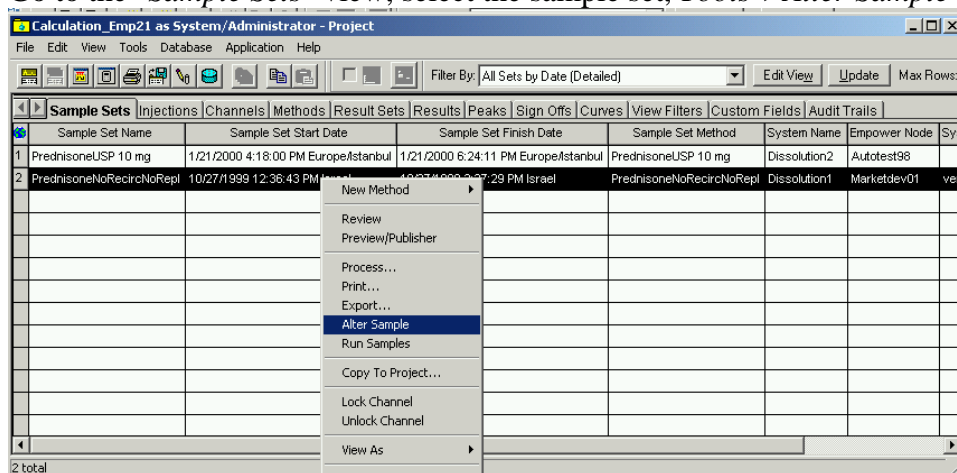
- a. Average for each standard:
 - Std1Ave => *Std1.%.AVE(Area_Amount)*
 - Std2Ave => *Std2.%.AVE(Area_Amount)*
- b. Maximum value of Average Area/Amount series
 - MAX_Ave_Ar_Am = Std%.%.MAX(Ave_Area_Amount)*
- c. Difference between the two average values over the maximal value:
 - ((Std1Ave-Std2Ave)/MAX_Ave_Ar_Am)*100*

The custom field formula is created and the settings of "Search Order" should be "Result Set Only" and "All or Nothing" in THIS SPECIFIC CASE.



After all custom fields were created go to the sample set that was run.

Go to the "Sample Sets" view, select the sample set, *Tools->Alter Sample*



The following screen is opened, where parameters are filled in and the last line would be "**Summarize Custom Fields**":

SampleName	Vial	Label	Function	Sample Type	Method Set / Report Method	Label Reference	Level	Sample/Weight	Dilution	Ini Vol (uL)	Processing
Prednisone_Tab	6	A3	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	7	A4	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	8	A4	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Pred_Std	100	Std2	Inject Standards	Standard	Prednisone Mth		2	1.00000	1.00000	20.0	Normal
Prednisone_Tab	9	A5	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	10	A5	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	11	A6	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	12	A6	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	13	A7	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	14	A7	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	15	A8	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	16	A8	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Pred_Std	100	Std2	Inject Standards	Standard	Prednisone Mth		2	1.00000	1.00000	20.0	Normal
Prednisone_Tab	17	A9	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	18	A9	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	19	A10	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	20	A10	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	21	A11	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	22	A11	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	23	A12	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Prednisone_Tab	24	A12	Inject Samples	Unknown	Prednisone Mth			1.00000	1.00000	20.0	Don't Process or Report
Pred_Std	100	Std2	Inject Standards	Standard	Prednisone Mth		2	1.00000	1.00000	20.0	Normal
			Quantitate			A*					Normal
			Summarize Custom Fields								Normal

Values of label and standards amounts and all other custom fields' values are filled in. Then *File* > *Save*.

After preparing the processing parameter the sample set is selected, then *Tools* > *Process*, and select the method set and check the "Clear Calibration" click OK. **REMEMBER TO WAIT UNTIL ALL CALCULATIONS ARE OVER AND RESULTS ARE SAVED.**

Calculation_Emp21 - Background Processing and Reporting

Processing

Process

Use acquisition method set (i.e. from the sample set used to acquire data)

Use specified method set: Prednisone Mth Set

Use specified processing method

Clear Calibration How: Calibrate and Quantitate

Reporting

Print: \\MAD\Color Laser

Use acquisition method set (i.e. from the sample set used to acquire data)

Use specified method set

Use specified report method

Exporting

Export

Use acquisition method set (i.e. from the sample set used to acquire data)

Use specified method set

Use specified export method

Default Comments: new info

Comments: new info

OK Cancel Help

Create a report method for a summary of the standards by selecting the standards' results

SampleName	Label	Vial	Injection	Sample Type	Channel	Date Acquired	Date Processed	Processing Method	Processed By	Result #
Prednisone_Tab	A10	19	1	Unknown	2487Channel 1	10/27/1999 3:00:45 PM Israel	2/26/2007 7:21:20 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A9	18	1	Unknown	2487Channel 1	10/27/1999 2:55:24 PM Israel	2/26/2007 7:21:20 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A9	17	1	Unknown	2487Channel 1	10/27/1999 2:50:03 PM Israel	2/26/2007 7:21:19 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Pred_Std	Std2	100	1	Standard	2487Channel 1	10/27/1999 2:44:20 PM Israel	2/26/2007 7:21:14 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	8
Prednisone_Tab	A8	16	1	Unknown	2487Channel 1	10/27/1999 2:38:40 PM Israel	2/26/2007 7:21:19 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A8	15	1	Unknown	2487Channel 1	10/27/1999 2:33:14 PM Israel	2/26/2007 7:21:19 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A7	14	1	Unknown	2487Channel 1	10/27/1999 2:27:50 PM Israel	2/26/2007 7:21:18 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A7	13	1	Unknown	2487Channel 1	10/27/1999 2:22:23 PM Israel	2/26/2007 7:21:18 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A6	12	1	Unknown	2487Channel 1	10/27/1999 2:17:00 PM Israel	2/26/2007 7:21:18 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A6	11	1	Unknown	2487Channel 1	10/27/1999 2:11:39 PM Israel	2/26/2007 7:21:17 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A5	10	1	Unknown	2487Channel 1	10/27/1999 2:06:17 PM Israel	2/26/2007 7:21:17 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A5	9	1	Unknown	2487Channel 1	10/27/1999 2:00:54 PM Israel	2/26/2007 7:21:17 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Pred_Std	Std2	100	1	Standard	2487Channel 1	10/27/1999 1:55:12 PM Israel	2/26/2007 7:21:13 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	8
Prednisone_Tab	A4	8	1	Unknown	2487Channel 1	10/27/1999 1:49:28 PM Israel	2/26/2007 7:21:17 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A4	7	1	Unknown	2487Channel 1	10/27/1999 1:44:01 PM Israel	2/26/2007 7:21:17 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A3	6	1	Unknown	2487Channel 1	10/27/1999 1:38:34 PM Israel	2/26/2007 7:21:16 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A3	5	1	Unknown	2487Channel 1	10/27/1999 1:33:08 PM Israel	2/26/2007 7:21:16 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A2	4	1	Unknown	2487Channel 1	10/27/1999 1:27:44 PM Israel	2/26/2007 7:21:16 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A2	3	1	Unknown	2487Channel 1	10/27/1999 1:22:21 PM Israel	2/26/2007 7:21:15 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A1	2	1	Unknown	2487Channel 1	10/27/1999 1:16:57 PM Israel	2/26/2007 7:21:15 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Prednisone_Tab	A1	1	1	Unknown	2487Channel 1	10/27/1999 1:11:33 PM Israel	2/26/2007 7:21:15 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	7
Pred_Std	Std1	100	6	Standard	2487Channel 1	10/27/1999 1:06:09 PM Israel	2/26/2007 7:21:13 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	8
Pred_Std	Std1	100	5	Standard	2487Channel 1	10/27/1999 1:00:50 PM Israel	2/26/2007 7:21:12 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	8
Pred_Std	Std1	100	4	Standard	2487Channel 1	10/27/1999 12:55:12 PM Israel	2/26/2007 7:21:12 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	8
Pred_Std	Std1	100	3	Standard	2487Channel 1	10/27/1999 12:49:51 PM Israel	2/26/2007 7:21:12 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	8
Pred_Std	Std1	100	2	Standard	2487Channel 1	10/27/1999 12:44:13 PM Israel	2/26/2007 7:21:11 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	8
Pred_Std	Std1	100	1	Standard	2487Channel 1	10/27/1999 12:38:51 PM Israel	2/26/2007 7:21:11 PM Asia/Jerusalem	Prednisone Proc Mth	System/Administrator	8

Then *Tools->Preview/Publisher* and use a method with the following features

A modified *Calibration Points Table*:

Standards Information									
Peak: PrednisoneLabel: Std1									
	SampleName	Label	Date Acquired	Sample Type	Name	Level	X Value	Response	Area_Amount
1	Pred_Std	Std1	10/27/1999 12:38:51 PM Israel	Standard	Prednisone	1	0.020000	945507	47275368
2	Pred_Std	Std1	10/27/1999 12:44:13 PM Israel	Standard	Prednisone	1	0.020000	932645	46632253
3	Pred_Std	Std1	10/27/1999 12:49:51 PM Israel	Standard	Prednisone	1	0.020000	964646	48232299
4	Pred_Std	Std1	10/27/1999 12:55:12 PM Israel	Standard	Prednisone	1	0.020000	990797	49539833
5	Pred_Std	Std1	10/27/1999 1:00:50 PM Israel	Standard	Prednisone	1	0.020000	949814	47490681
6	Pred_Std	Std1	10/27/1999 1:06:09 PM Israel	Standard	Prednisone	1	0.020000	964034	48201704
Mean									47895356
Max									49539833

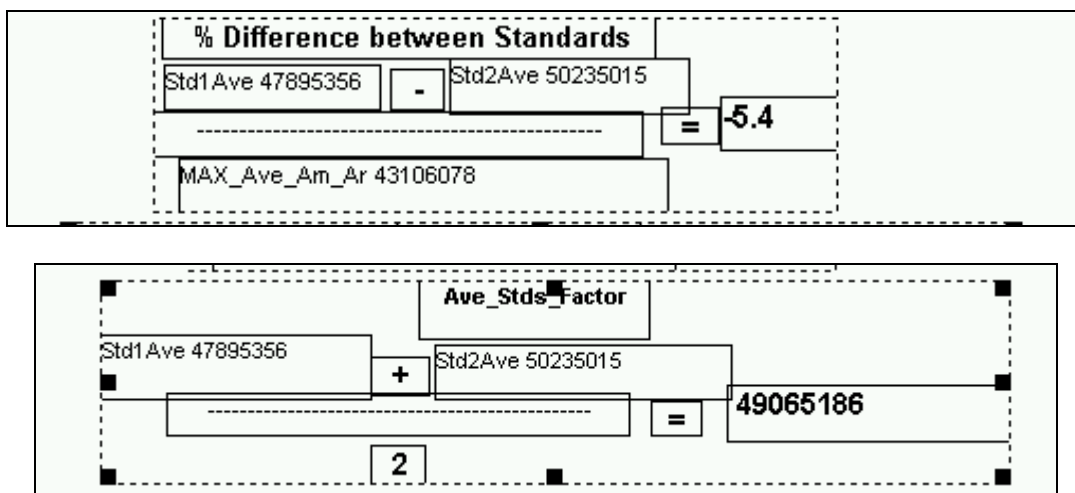
Standards Information									
Peak: PrednisoneLabel: Std2									
	SampleName	Label	Date Acquired	Sample Type	Name	Level	X Value	Response	Area_Amount
1	Pred_Std	Std2	10/27/1999 1:55:12 PM Israel	Standard	Prednisone	2	0.020000	978865	48943228
2	Pred_Std	Std2	10/27/1999 2:44:20 PM Israel	Standard	Prednisone	2	0.020000	1009500	50475015
3	Pred_Std	Std2	10/27/1999 2:22:17 PM Israel	Standard	Prednisone	2	0.020000	1025726	51286802
Mean									50235015
Max									51286802

Where additional information can be added, such as *SampleName*, *Label*, *SampleType*, *Area/Amount*, etc, lines can be grouped by *Labels* and *Area/Amount* can be averaged and maximized in the report as well for troubleshooting.

The intersample calculations results can be summarized in a *Sample results table* after revisions:

Intersample Calculations Results						
Ave_Area_Amount	MAX_Ave_Ar_Am	Std1Ave	Std2Ave	Ave_Stds_Factor	Std_Factor_diff	
1	48675243	43106078	47895356	50235015	49065186	-5.4

Also, the calculations can be visualized using a composite of the separate fields:



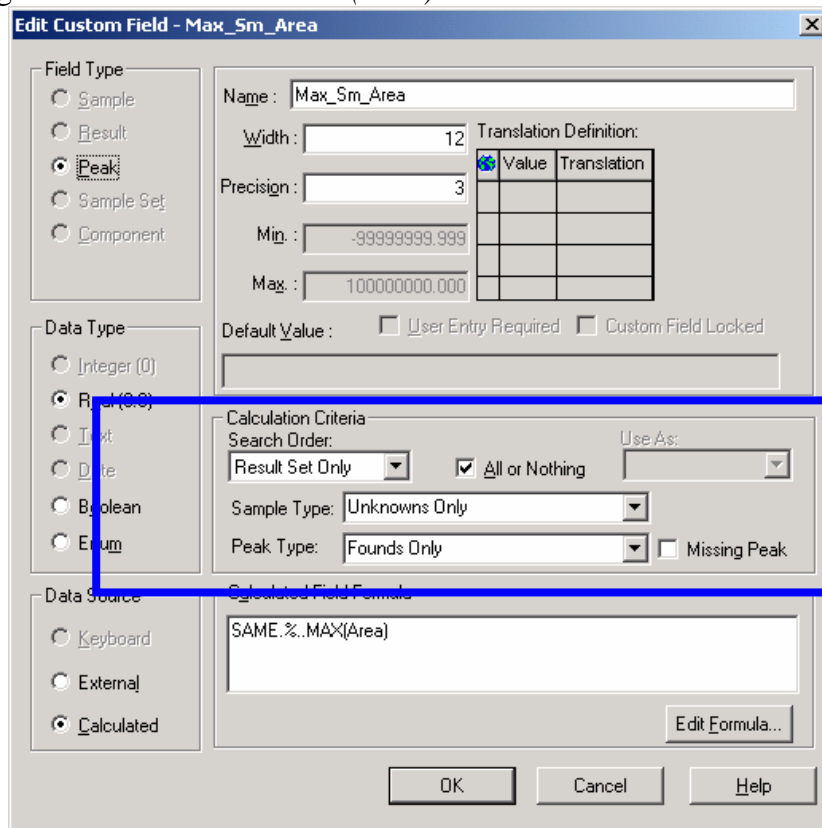
Example 3:

Average of area duplicates of sample: formula is *SAME.%.AVE(Area)*

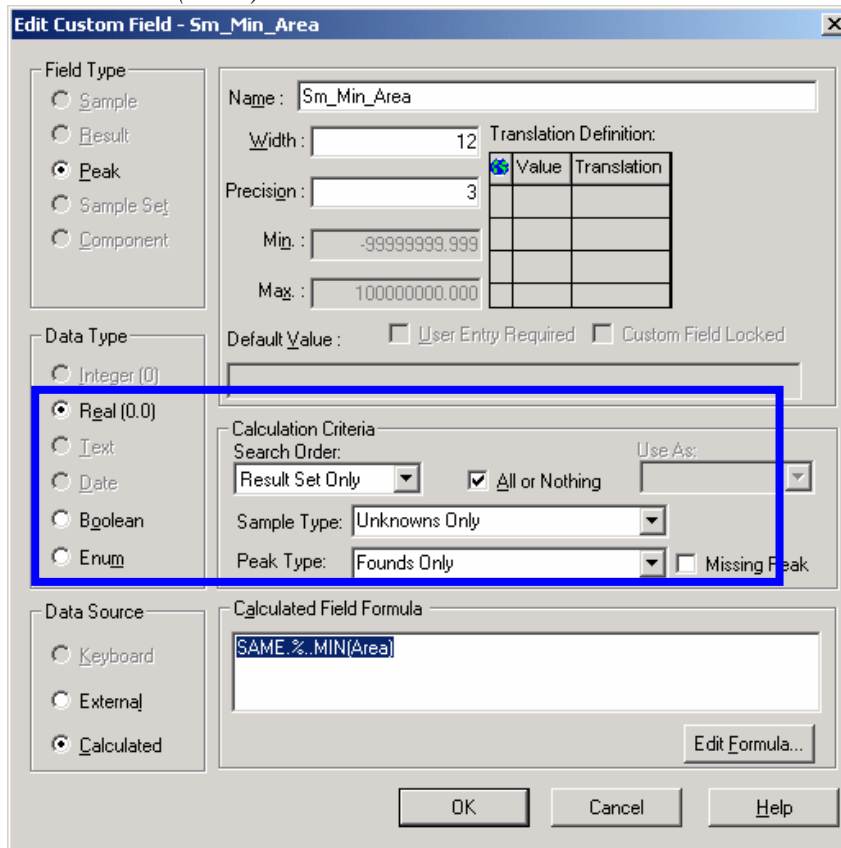
The screenshot shows the 'Edit Custom Field - Ave_Area_Same' dialog box. The 'Field Type' is set to 'Peak'. The 'Data Type' is 'Real (0.0)'. The 'Name' is 'Ave_Area_Same'. The 'Width' is 12 and 'Precision' is 3. The 'Min.' is -99999999.999 and 'Max.' is 100000000.000. The 'Calculated Field Formula' is 'SAME.%.AVE(Area)'. The 'Search Order' is 'Result Set Only' and 'All or Nothing' is checked. The 'Sample Type' is 'All' and 'Peak Type' is 'All'. The 'Missing Peak' checkbox is unchecked. The 'Default Value' field is empty. The 'User Entry Required' and 'Custom Field Locked' checkboxes are unchecked. The 'Translation Definition' table is empty. The 'Edit Formula...' button is visible at the bottom right.

% Difference between areas of duplicates of samples:

Larger area is: *SAME.%.MAX(Area)*



Smaller area is: *SAME.%.MIN(Area)*



The % difference between the two values: $((Max_Sm_Area - Sm_Min_Area) / Ave_Area_Same) * 100$

The results can be summarized in a summary report:

Results of Samples Label: A1														
	SampleName	Label	Name	Date Acquired	Vial	Inj	RT	Area	Dilution	Amount	Ave_Area_Same	Diff_Samples %	Sm_Min_Area	Max_Sm_Area
1	Prednisone_Tab	A1	Prednisone	10/27/1999 1:11:33 PM Israel	1	1	1.791	891840	1.00000	0.018	865414	6.107	838988	891840
2	Prednisone_Tab	A1	Prednisone	10/27/1999 1:16:57 PM Israel	2	1	1.795	838988	1.00000	0.017	865414	6.107	838988	891840
Mean								865414						
Results of Samples Label: A2														
	SampleName	Label	Name	Date Acquired	Vial	Inj	RT	Area	Dilution	Amount	Ave_Area_Same	Diff_Samples %	Sm_Min_Area	Max_Sm_Area
1	Prednisone_Tab	A2	Prednisone	10/27/1999 1:22:21 PM Israel	3	1	1.795	902486	1.00000	0.019	863023	9.145	823559	902486
2	Prednisone_Tab	A2	Prednisone	10/27/1999 1:27:44 PM Israel	4	1	1.795	823559	1.00000	0.017	863023	9.145	823559	902486
Mean								863023						
Results of Samples Label: A3														
	SampleName	Label	Name	Date Acquired	Vial	Inj	RT	Area	Dilution	Amount	Ave_Area_Same	Diff_Samples %	Sm_Min_Area	Max_Sm_Area
1	Prednisone_Tab	A3	Prednisone	10/27/1999 1:33:08 PM Israel	5	1	1.791	789674	1.00000	0.016	869471	18.355	789674	949269
2	Prednisone_Tab	A3	Prednisone	10/27/1999 1:38:34 PM Israel	6	1	1.796	949269	1.00000	0.020	869471	18.355	789674	949269
Mean								869471						
Results of Samples Label: A4														
	SampleName	Label	Name	Date Acquired	Vial	Inj	RT	Area	Dilution	Amount	Ave_Area_Same	Diff_Samples %	Sm_Min_Area	Max_Sm_Area
1	Prednisone_Tab	A4	Prednisone	10/27/1999 1:44:01 PM Israel	7	1	1.794	831719	1.00000	0.017	821516	2.484	811313	831719
2	Prednisone_Tab	A4	Prednisone	10/27/1999 1:49:28 PM Israel	8	1	1.794	811313	1.00000	0.017	821516	2.484	811313	831719