

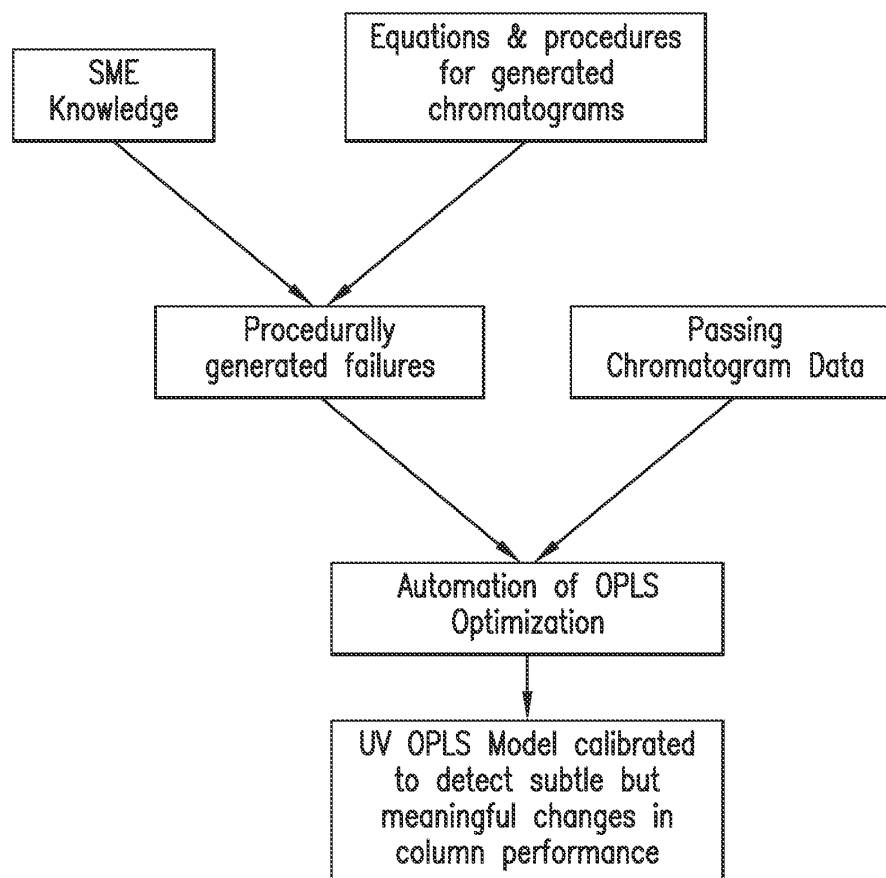


FIG.1A

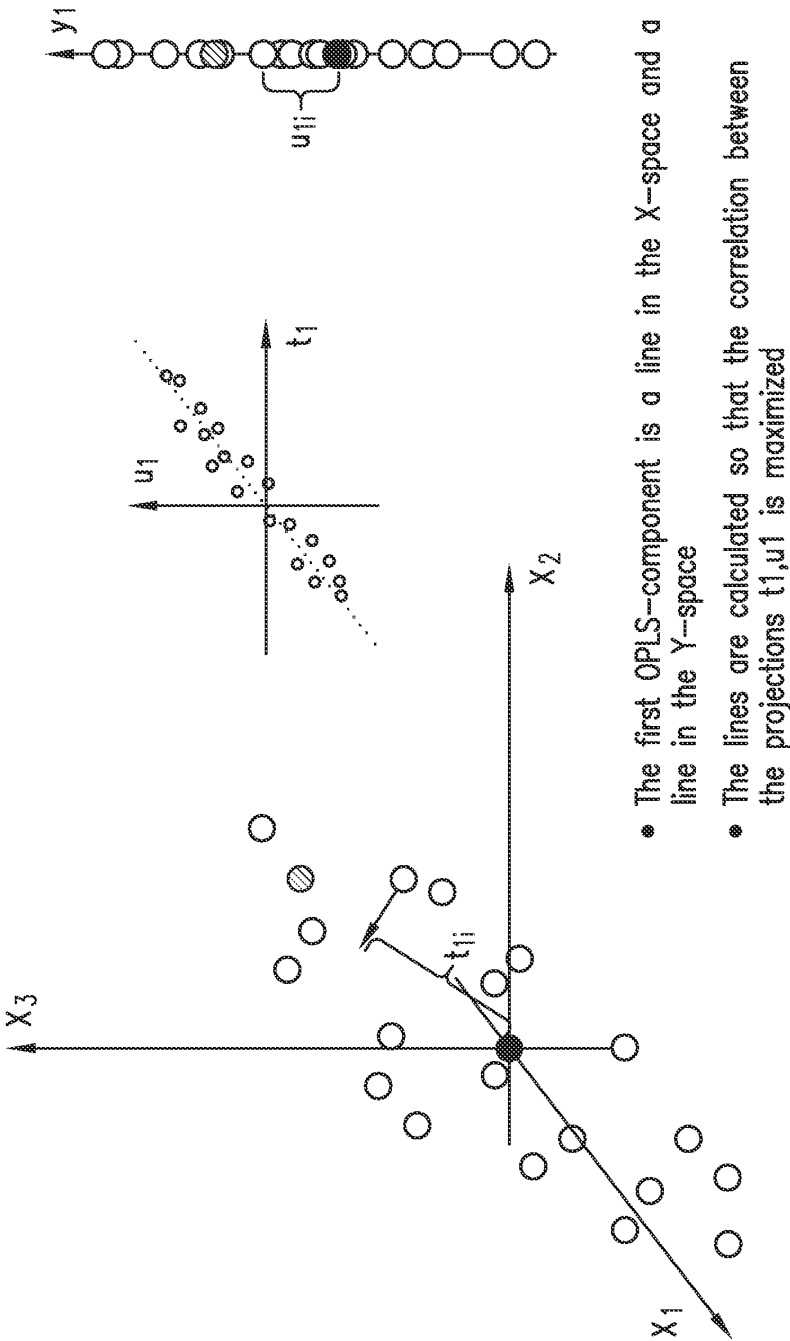
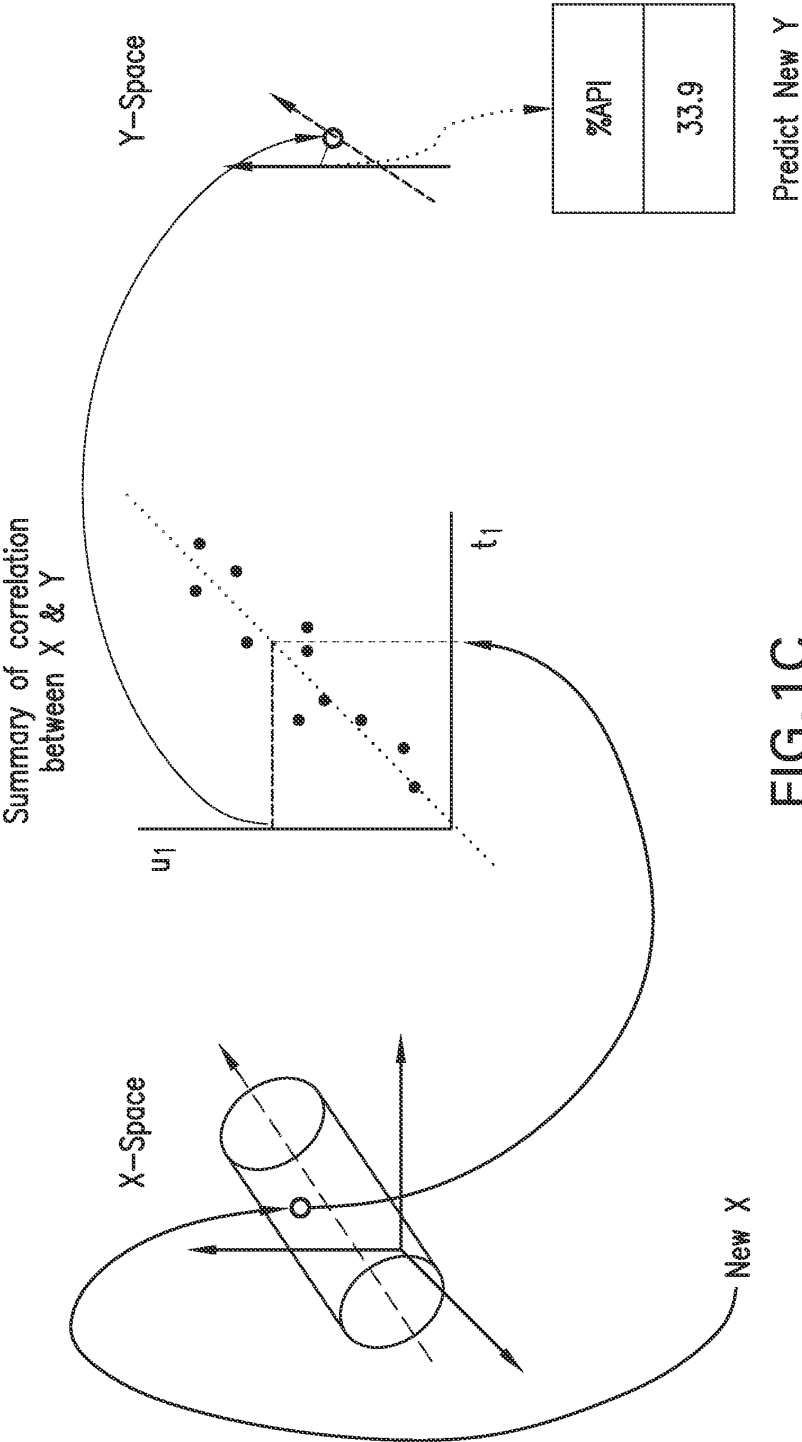


FIG.1B



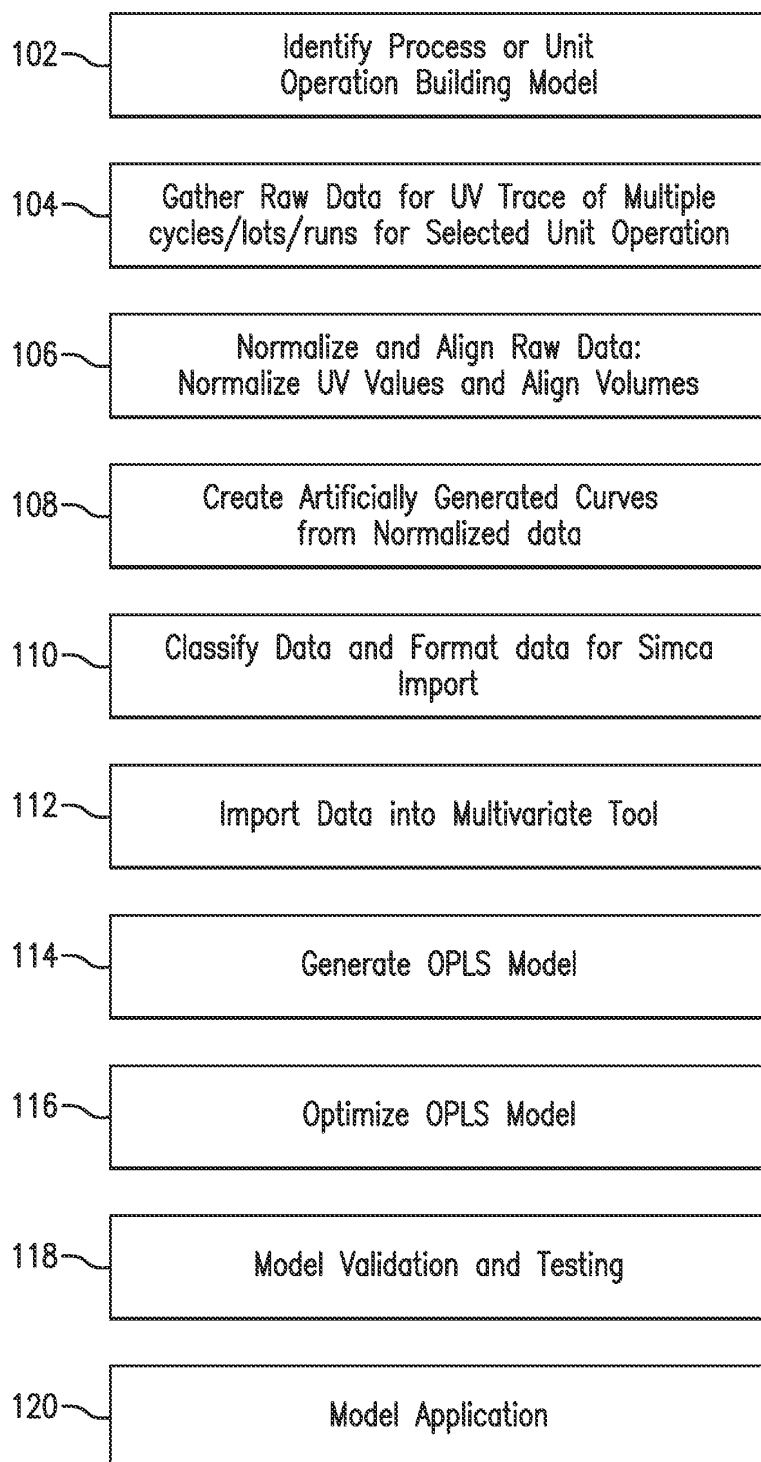


FIG. 1D

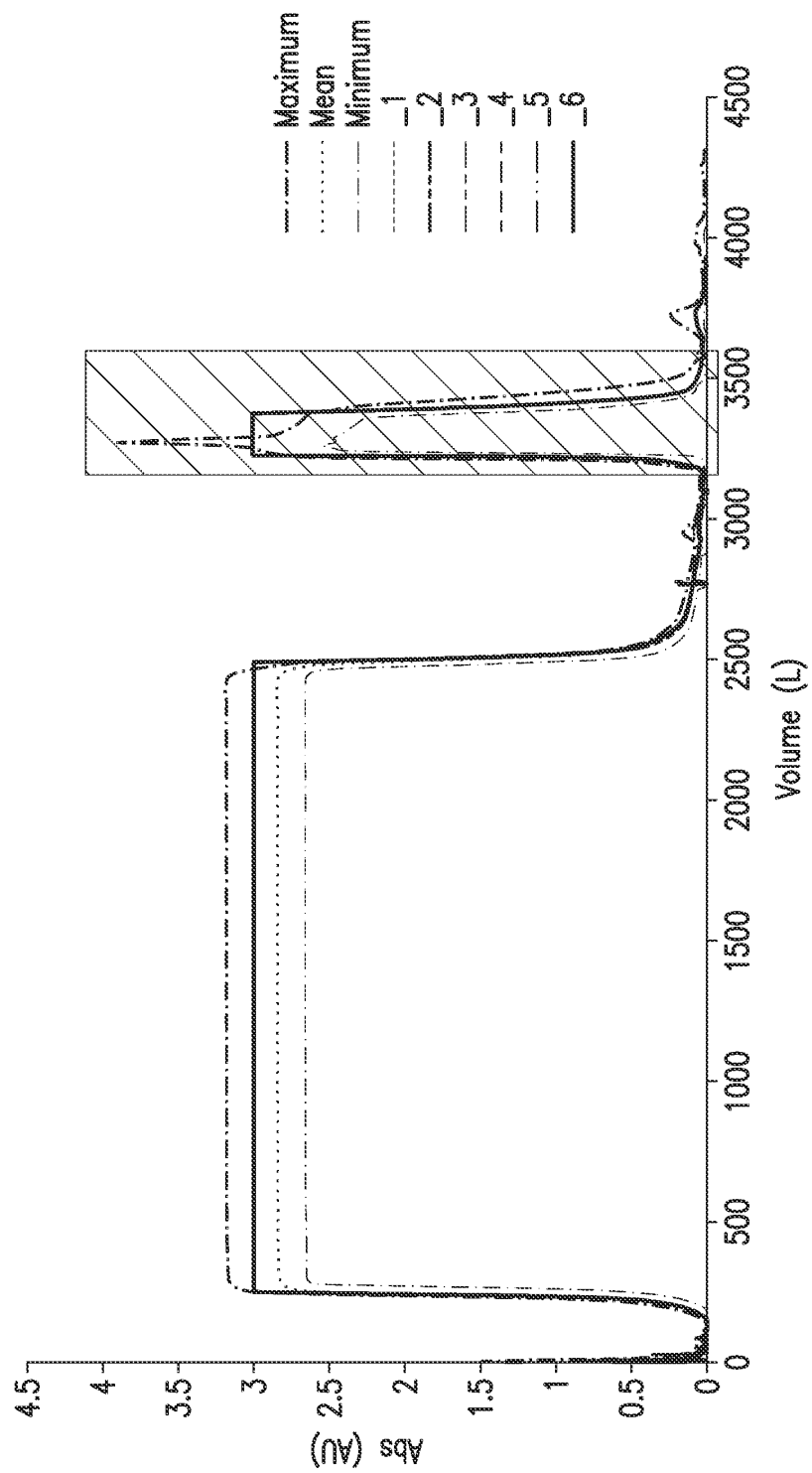


FIG.2

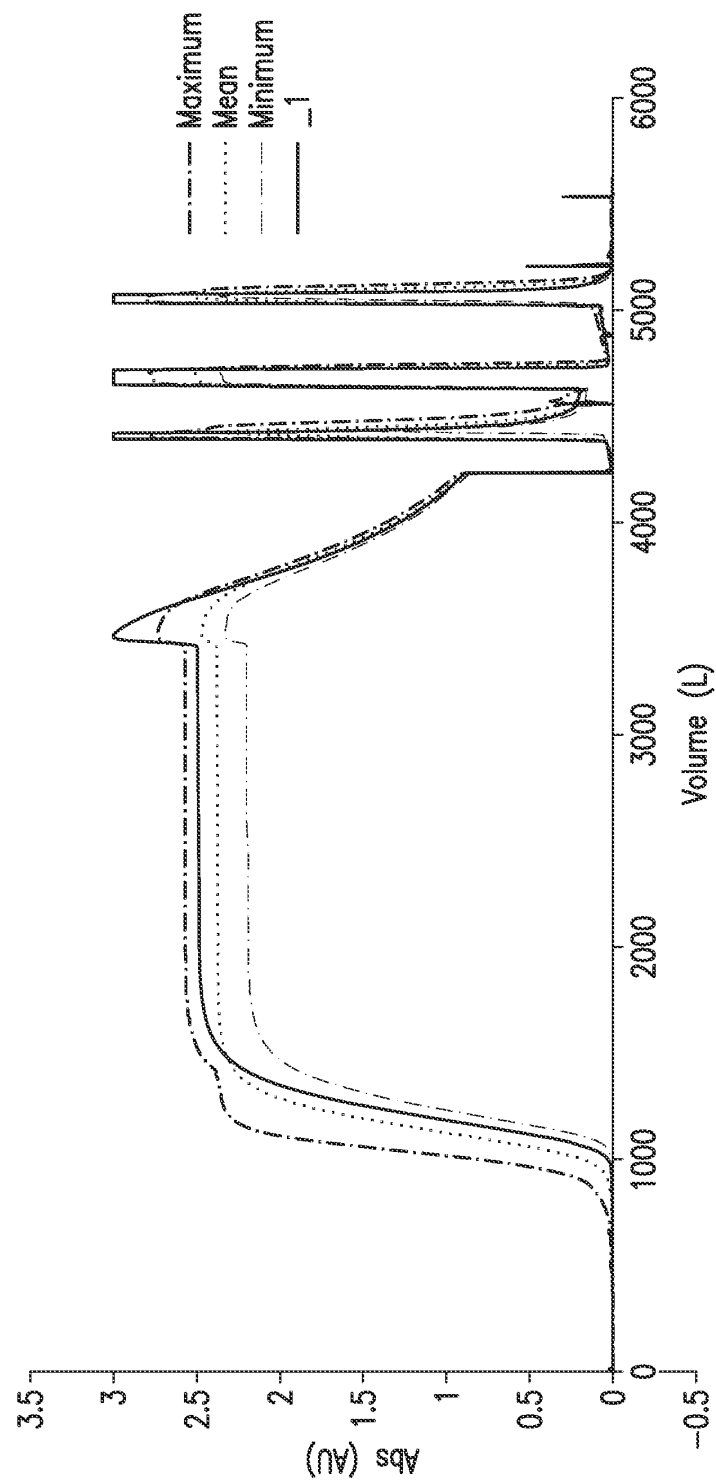


FIG.3

A1	▼	✕	✓	fx	Chrom.1												
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	
1	Chrom.1		Chrom.1														
2	UV1:131		Run Log														
3	I	AU	I	Logbook													
4	0	0	0	0	Method Run 2/14/2020 1:45:41 PM -05:00 Method: PA7 REGN668 ProA Load Elution Revision 1 Result:/ECN54013												
5	0.365351	0.0001	0	0	Batch ID: c3a5cb72-07dc-4545-9d59-f627e566502f												
6	0.730702	8.73E-05	0	0	Base CV, Vc=157.000 {}, Any												
7	1.096053	1.00E-04	0	0	Phase Method Settings												
8	1.461404	8.38E-05	0	0	Base SameAsMain												
9	1.826755	1.11E-05	0	0	End Phase												
10	2.192106	1.00E-04	0	0	Phase User Defined												
11	2.557457	7.18E-04	0	0	Base SameAsMain												
12	2.922808	0.001177	0	0	Press_PIA111_Alarm 4.00 {bar} 0.00 {bar} 4.00 {bar} 0.00 {bar} 0.00 {bar} 0.00 {bar} Enabled												
13	3.288159	7.86E-05	0	0	Press_PIA112_Alarm 3.00 {bar} 0.00 {bar} 3.00 {bar} 0.00 {bar} 0.00 {bar} 0.00 {bar} Enabled												
14	3.65351	5.63E-05	0	0	AirTrapLevelControl Disabled 10.0 {sec}												
15	4.018861	0	0	0	Block Set Up												
16	4.384212	0.0001	0	0	Base SameAsMain												
17	4.749563	1.28E-07	0	0	Message Ensure the column equilibration has been performed ^{ms}												
18	5.114914	6.67E-05	0	0	Message Ensure that the column is in bypass and the MPTV and MPBV are closed ^{ms}												
19	5.480265	0.00E+00	0	0	Message Ensure appropriate filter has been installed ^{ms}												
20	5.845616	7.41E-05	0	0	Message Ensure harvest material is connected to INLET A1/air sensor and primed ^{ms}												
21	6.210967	0.0001	0	0	Message Ensure Buffer 1 (item master number 10416) is connected to inlet A2. ^{ms}												
22	6.576318	0.00E+00	0	0	Message Ensure Buffer 2 (item master number 10487) is connected to inlet B1. ^{ms}												
23	6.941669	0.0001	0	0	Message Ensure Buffer 3 (item master number 10488) is connected to inlet B2. ^{ms}												
24	7.30702	1.14E-05	0	0	Message Ensure Buffer 4 (item master number 10415) is connected to inlet B3. ^{ms}												
25	7.672371	1.93E-05	0	0	Message Ensure the pool vessel is set up and connected to outlet 1. ^{ms}												
26	8.037722	0.0001	0	0	Message Ensure Outlet 2 is connected to drain ^{ms}												
27	8.403073	5.17E-05	0	0	Message Click "Continue" when complete. ^{ms}												
28	8.768424	1.00E-04	0	0	Pause Infinite min 2/14/2020 1:45:41 PM -05:00												
29	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
30	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
31	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
32	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
33	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
34	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
35	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
36	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
37	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
38	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
39	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
40	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
41	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
42	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
43	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
44	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
45	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
46	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
47	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
48	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
49	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
50	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
51	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
52	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
53	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
54	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
55	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
56	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
57	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
58	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
59	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
60	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
61	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
62	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
63	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
64	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
65	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
66	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
67	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
68	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
69	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
70	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
71	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
72	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
73	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
74	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
75	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
76	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
77	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
78	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
79	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
80	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
81	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
82	9.133775	8.08E-06	0	0	Message Ensure the column equilibration has been performed ^{ms} confirmed by REGENERON/alissa.reyes (Manual)*												
83	9																

Each column corresponds to the UV values for a certain CV point in the analysis
Ex: 0.1 CVs into the elution block

	G	H	I	J	K	L	M	N	O
1 Lot_cycle	0	0.02	0.04	0.06	0.08	0.1	0.12	0.14	0.16
2 _1	-1.02032	-0.99778	-0.99705	-0.99707	-0.99778	-0.99781	-0.99778	-0.99842	-0.99852
3 _2	-1.01667	-0.99781	-0.99703	-0.99771	-0.99771	-0.99771	-0.99771	-0.99782	-0.99852
4 _3	-1.01593	-0.99778	-0.99698	-0.99778	-0.99778	-0.99778	-0.99778	-0.99852	-0.99852
5 _4	-1.01742	-0.99705	-0.99704	-0.99703	-0.99778	-0.99778	-0.99771	-0.99778	-0.99845
6 _5	-1.01593	-0.99776	-0.99779	-0.99779	-0.99779	-0.99779	-0.99846	-0.99846	-0.99852
7 _6	-1.01525	-0.99785	-0.99711	-0.99711	-0.99778	-0.9978	-0.99785	-0.99785	-0.99859
8 _1	-1.02035	-0.99784	-0.99707	-0.99784	-0.99778	-0.99778	-0.99854	-0.99852	-0.99853
9 _2	-1.01742	-0.99778	-0.99704	-0.99778	-0.99773	-0.99773	-0.99778	-0.99845	-0.99845
10 _3	-1.01742	-0.99704	-0.99704	-0.99704	-0.99704	-0.99771	-0.99775	-0.99771	-0.99775
11 _4	-1.01667	-0.99697	-0.99701	-0.99704	-0.99701	-0.99698	-0.99771	-0.99771	-0.99771
12 _5	-1.01593	-0.99706	-0.99627	-0.99698	-0.99698	-0.99698	-0.99698	-0.99779	-0.99778
13 _6	-1.01667	-0.99704	-0.99704	-0.99704	-0.99779	-0.9978	-0.99771	-0.99775	-0.99852
14									
15									
16									
17									
18	All UV Values Normalized to -1 to 1								
19									
20									
21									
22									
23									
24									
25									
26									
27									
28									
29									
◀ ▶	Raw Data	Norm Data	IX-Adj Data	X Matrix	Sheet1	⊕			

Each row corresponds to the UV values for a certain run/cycle
Ex: _6

Cont.
On FIG.5-2

FIG.5-1

Curve to be fitted by
the mathematical model

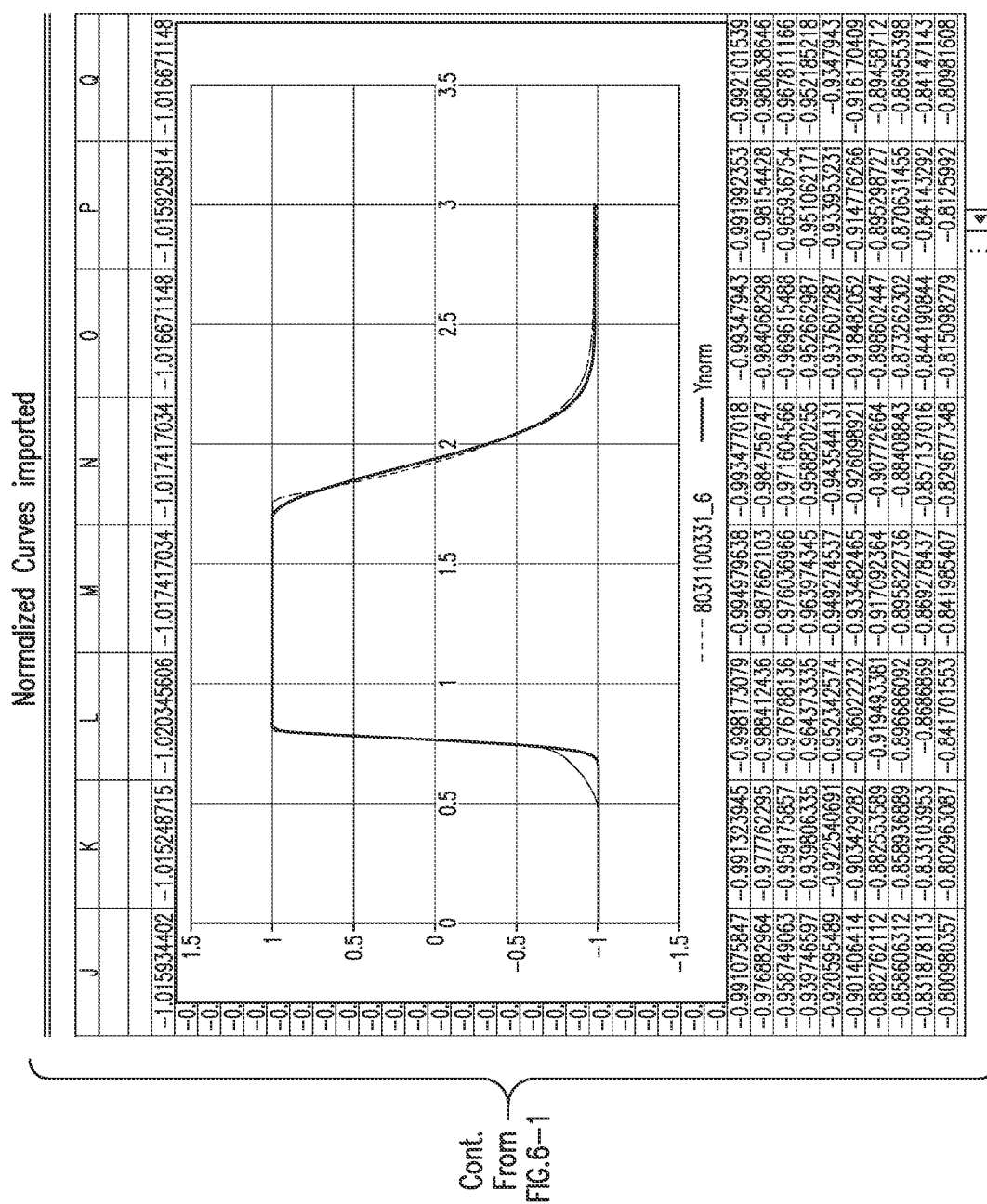
Bi	A	∇	$\times$	$\checkmark$	f_x	F	G	H	I
1									
2	Normalized								
3	0	-1.016671148	-1.020315753	-1.016671148	-1.015926146	-1.017417034			
4	0.02	-0.997042216	-0.997781731	-0.997811502	-0.997782811	-0.997045385			
5	0.04	-0.997042216	-0.99705085	-0.997026311	-0.99697644	-0.997041122			
6	0.06	-0.997042216	-0.997074679	-0.99714439	-0.997782811	-0.997033556			
7	0.08	-0.997788236	-0.997781731	-0.99714439	-0.997782811	-0.997780841			
8	0.1	-0.997799287	-0.997807756	-0.99714439	-0.997782811	-0.997780841			
9	0.12	-0.997714439	-0.997781731	-0.99714439	-0.997782811	-0.997113594			
10	0.14	-0.99775084	-0.998422565	-0.997819696	-0.998521983	-0.997780841			
11	0.16	-0.998521108	-0.998522798	-0.998521108	-0.998521983	-0.998453314			
12	0.18	-0.998578818	-0.998522798	-0.998569313	-0.998521983	-0.998453314			
13	0.2	-0.998521108	-0.998555411	-0.998521108	-0.998521983	-0.998453314			
14	0.22	-0.998521108	-0.998522798	-0.998521108	-0.99761156	-0.998453314			
15	0.24	-0.999260554	-0.999263865	-0.999211367	-0.999261156	-0.99926028			
16	0.26	-0.999260554	-0.999252007	-0.999207976	-0.999261156	-0.99926028			
17	0.28	-0.999260554	-0.999263865	-0.999260554	-0.999210678	-0.99926028			
18	0.3	-0.999260554	-0.999263865	-0.999212187	-0.999241326	-0.99926028			
19	0.32	-0.999260554	-0.999263865	-0.999244777	-0.999261156	-0.99926028			
20	0.34	-0.999193822	-0.99937562	-0.999260554	-0.99933132	-0.999179718			
21	0.36	-0.999980768	-0.99937562	-0.999204806	-0.99933132	-0.99932753			
22	0.38	-1	-0.99937562	-1	-0.99933132	-0.999985401			
23	0.4	-0.999948192	-0.99937562	-0.999986226	-0.99933132	-0.99979335			
24	0.42	-1	-0.99937562	-1	-0.99933132	-1			
25	0.44	-0.999932778	-0.99938215	-0.99993439	-0.99933132	-0.99969329			
26	0.46	-1	-0.99937562	-0.99938665	-0.99933132	-0.99999885			
27	0.48	-0.998521108	-0.999216423	-0.999260554	-0.998521983	-0.998112969			
28	0.5	-0.992101539	-0.994143766	-0.994860769	-0.992003822	-0.989787297			
29	0.52	-0.980638646	-0.983354754	-0.984807744	-0.980533693	-0.975663555			
30	0.54	-0.967811166	-0.970614809	-0.971311004	-0.966940928	-0.959192408			
31	0.56	-0.952185218	-0.957808257	-0.956500222	-0.952173711	-0.941361756			
32	0.58	-0.9347943	-0.945767724	-0.940809895	-0.938682307	-0.924289768			
33	0.6	-0.916170409	-0.931018336	-0.924513848	-0.922575796	-0.906550284			
34	0.62	-0.89458712	-0.914367169	-0.906074415	-0.904114482	-0.888780606			
35	0.64	-0.86955398	-0.894298806	-0.884811172	-0.88284962	-0.866013113			
36	0.66	-0.84147143	-0.871514097	-0.859812987	-0.858330582	-0.840916042			
37	0.68	-0.80981608	-0.845002023	-0.831952272	-0.831057655	-0.811299687			
Generation Manipulation Import $\oplus$									

Cont. On
FIG.6-2

FIG.6-1

Cont. On
FIG. 6-3

26GF



RMSE Value

R	S	T	U	V	W	
	Description	Start:	$\Sigma(p - o)^2$: 0.25146	RMSE:	0.040	
	height of peak liftoff	hm1	0.85			Row
	liftoff location	tm1	0.81			7.68
	liftoff steepness	s1	0.04			1.69
						2.90
		End:				3.87
	Height of peak dropdown	hm2	0.84			4.03
	Dropdown location	tm2	1.69			3.26
	Dropdown steepness	s2	0.21			2.06
						1.0
		Boundaries:				3.88
	Point where eqn1->eqn pminstart		0.81			1.1
	Point where eqn2->eqn pminend		1.69			2.6
						4.85
	ht of 1/3 eqns	uniform h	0.85			6.83
						7.49
		Max:				6.40
	Height of peak max	hm3	0			4.26
	Location of peak max	tm3	0.92			2.20
	Width of peak max	s3	0.01			8.90
						2.79
		Tailing factor:				6.84
	increases tailing	tail	0.01			1.30
						1.93
	Key					2.23
	Parameter should remain constant					2.01
	Parameter should be changed					1.4
						7.70
						3.27
						1.08
						2.79
						5.62
						8.79
						1.07
						0.000
						0.000
						0.004

Cont. From
FIG.6-2

FIG.6-3

Fit model to existing chromatograms and copy to space on the right with "CTL-SHIFT-C"

R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD
	Description	Start:	$\Sigma (p - o)^2$	0.25146	RMSE:	0.04080844	Ynorm	329.1	329.6	331.1	331.6	
	height of peak lfftoff	hm1	0.85			Row		-1	-1	-1	-1	
	lfftoff location	tm1	0.81			7.6821E-90		-1	-1	-1	-1	
	lfftoff steepness	s1	0.04			1.6921E-85		-1	-1	-1	-1	
						2.9026E-81		-1	-1	-1	-1	
		End:				3.8779E-77		-1	-1	-1	-1	
	Height of peak dropdown	hm2	0.84			4.0347E-73		-1	-1	-1	-1	
	Dropdown location	tm2	1.69			3.2694E-69		-1	-1	-1	-1	
	Dropdown steepness	s2	0.21			2.0632E-65		-1	-1	-1	-1	
						1.014E-61		-1	-1	-1	-1	
		Boundaries:				3.8813E-58		-1	-1	-1	-1	
	Point where eqn1->eqn prnstart		0.81			1.157E-54		-1	-1	-1	-1	
	Point where eqn2->eqn prnend		1.69			2.686E-51		-1	-1	-1	-1	
						4.8565E-48		-1	-1	-1	-1	
	ht of 1/3 eqns	uniform h	0.85			6.8394E-45		-1	-1	-1	-1	
		Max:				7.4993E-42		-1	-1	-1	-1	
						6.4048E-39		-1	-1	-1	-1	
	Height of peak max	hm3	0			4.2601E-36		-1	-1	-1	-1	
	Location of peak max	tm3	0.92			2.2068E-33		-1	-1	-1	-1	
	Width of peak max	s3	0.01			8.9028E-31		-1	-1	-1	-1	
						2.7972E-28		-1	-1	-1	-1	
		Tailing factor:				6.8445E-26		-1	-1	-1	-1	
	Increases tailing	tail	0.01			1.3043E-23		-1	-1	-1	-1	
						1.9358E-21		-1	-1	-1	-1	
	Key:					2.2375E-19		-1	-1	-1	-1	
	Parameter should remain constant					2.0141E-17		-1	-1	-1	-1	
	Parameter should be changed					1.412E-15		-1	-1	-1	-1	
						7.7083E-14		-1	-1	-1	-1	
						3.2781E-12		-1	-1	-1	-1	
						1.0855E-10		-1	-1	-1	-1	
						2.7997E-08		-1	-1	-1	-1	
						5.6233E-08		-1	-1	-1	-1	
						8.7963E-07		-1	-1	-1	-1	
						1.0716E-05	-0.99997	-1	-0.99997	-0.99997	-0.99997	
						0.00010167	-0.99976	-0.9999	-0.99976	-0.99976	-0.99976	
						0.00075125	-0.99823	-0.9993	-0.99823	-0.99823	-0.99823	
						0.00432316	-0.99983	-0.9956	-0.99983	-0.99983	-0.99983	

FIG.7

Chart showing generated Curves. Real data is in blue, curves generated in previous step are in Green, the artificial curve generated from the parameters being manipulated is in brown (in figure shown below curves are stacked on top of each other)

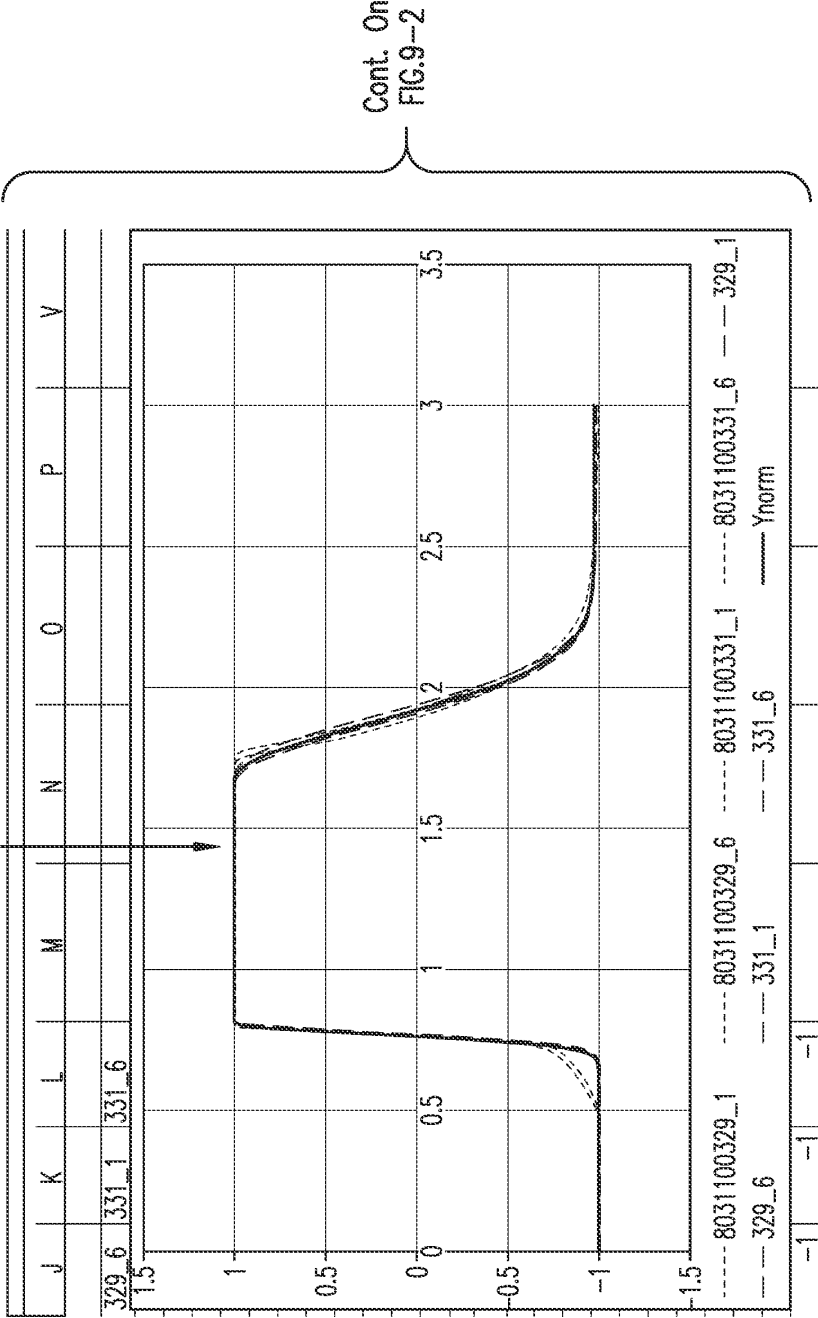


FIG.9-1

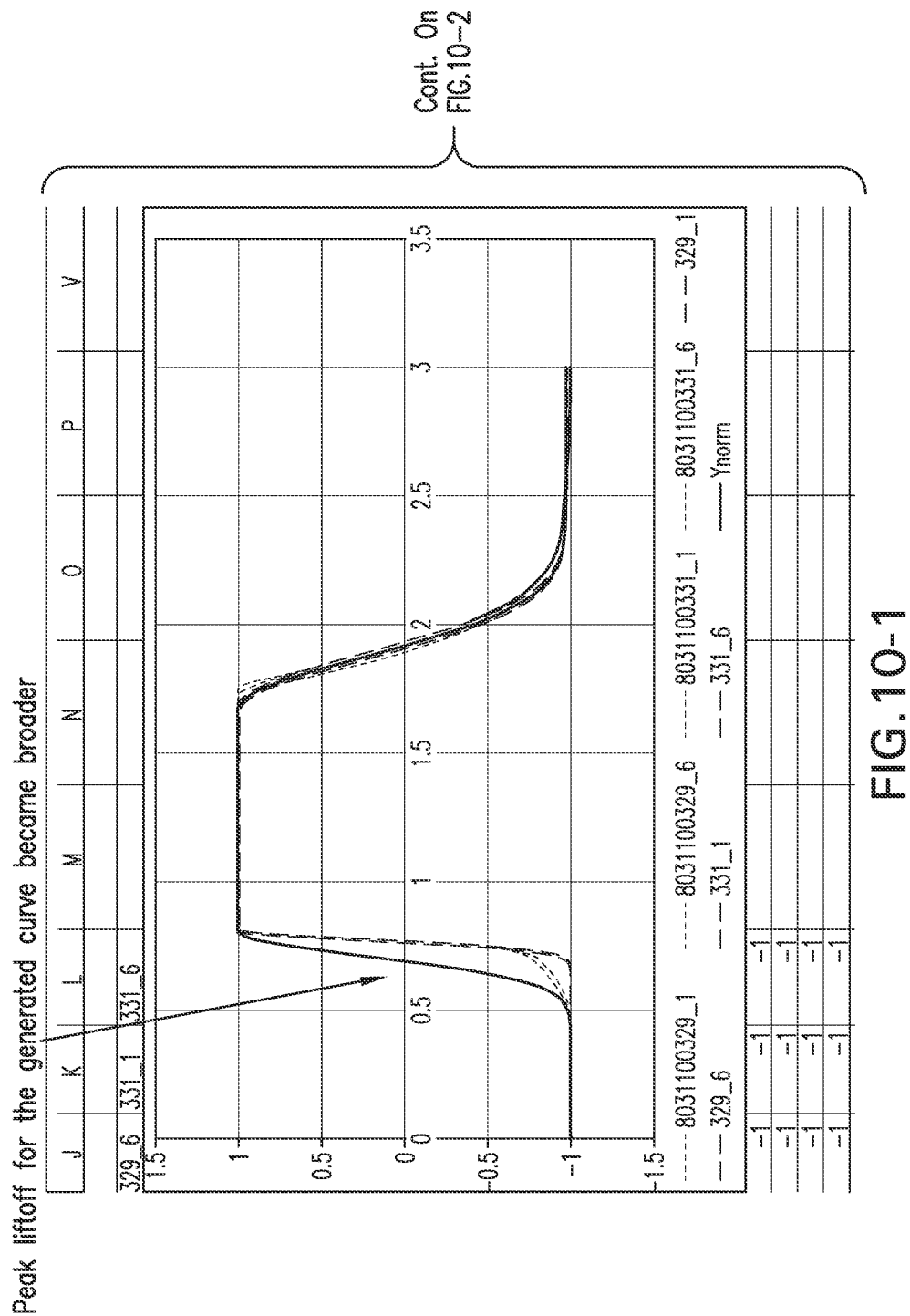
Adjust SD values to generate Chromatograms representative of column deterioration. Parameter values will be equal to the mean plus the number of standard deviations specified

Copy Mean and SD values from generation tab into table

W	X	Y	Z	AA	AB	AC	AD
				Description	Start:		SD
				height of peak	lftoff	hm1	0.85
				lftoff location		tm1	0.8125
				lftoff steepness	s1	0.04	0
				AVG	SD		
	tm1	0.8125	0.00433				
	s1	0.04	0		End:		
	tm2	1.6725	0.01299	Height of peak	dropdown	hm2	0.84
	s2	0.21	0	Dropdown location		tm2	1.6725
	hm3	0	0	Dropdown steepness	s2	0.21	0
	tm3	1.025	0.139555				
	s3	0.31	0.51962		Boundaries:		
	tail	0.01	0	Point where eqn1->eqn	pmstart	0.8125	0
		0.2548	0.05386	Point where eqn2->eqn	pmend	1.6725	0
				ht of 1/3 eqns	unifo	0.85	
					Max:		
				Height of peak max	hm3	0	0
				Location of peak max	tm3	1.025	0
				Width of peak max	s3	0.31	0
					Tailing factor:		
				increases tailing	tail	0.01	0
				Key			
				Parameter should remain constant			

Cont. From FIG.9-1

FIG.9-2



S1 Value was manually changed to 0.1
(SD was 0 so had to manually adjust)

Normalized UV
values for artificial
curve are stored.
Copy values into
columns to the right
to save values.
Name the curve
based on what
parameter was
changed (Ex: s1:0.1)

W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG
				Description	Start:		SD	0.276329	0.27632918	
				height of peak liftoff	hm1	0.85	0		Row	Ynorm
				Liftoff location	tm1	0.8125	0		3.9292E-15	-1
				Liftoff steepness	s1	0.11	0		1.9559E-4	-1
	AVG	SD							9.3545E-14	-1
tm1	0.8125	0.00433							4.2985E-13	-1
s1	0.04	0			End:				1.8978E-12	-1
tm2	1.6725	0.01299			Height of peak dropdown	hm2	0.84	0	8.0501E-12	-1
s2	0.21	0			Dropdown location	tm2	1.6725	0	3.2809E-11	-1
hm3	0	0			Dropdown steepness	s2	0.21	0	1.2847E-10	-1
tm3	1.025	0.13955							4.8333E-10	-1
s3	0.31	0.51962			Boundaries:				1.7471E-09	-1
tail	0.01	0			Point where eqn1->eqn pmstart	0.8125	0		6.0674E-09	-1
	0.2548	0.05386			Point where eqn2->eqn pmend	1.6725	0		2.0246E-08	-1
									6.4906E-08	-1
				ht of 1/3 eqns	unifo	0.85			1.9992E-07	-1
									5.9166E-07	-1
					Max:				1.6823E-06	-1
				Height of peak max	hm3	0	0		4.596E-06	-0.99999
				Location of peak max	tm3	1.025	0		1.2063E-05	-0.99997
				Width of peak max	s3	0.31	0		3.0422E-05	-0.99993
									7.3713E-05	-0.99983
				increases tailing	Tailing factor:				0.0001716	-0.9996
					tail	0.01	0		0.00038382	-0.9991
				Key					0.00082483	-0.99806
				Parameter should remain constant					0.00170306	-0.99599
				Parameter should be changed					0.00337847	-0.99205
									0.00643933	-0.98485
									0.01179203	-0.97225

Cont.
From
FIG.10-1

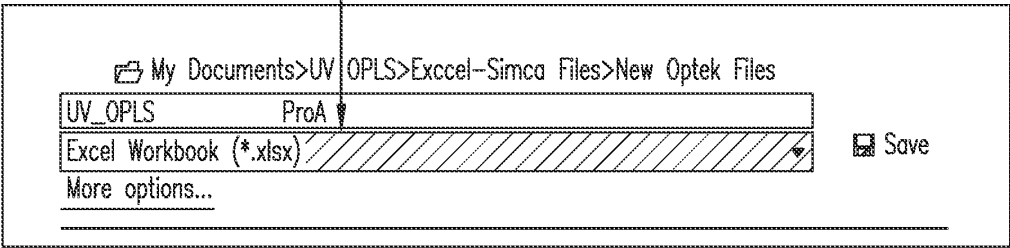
FIG.10-2

[illegible]

FIG. 1-2

Cont. From
FIG. 1-1

1. Save Excel file as regular excel file (not macro enabled)



2. Open Simca and Select "File"

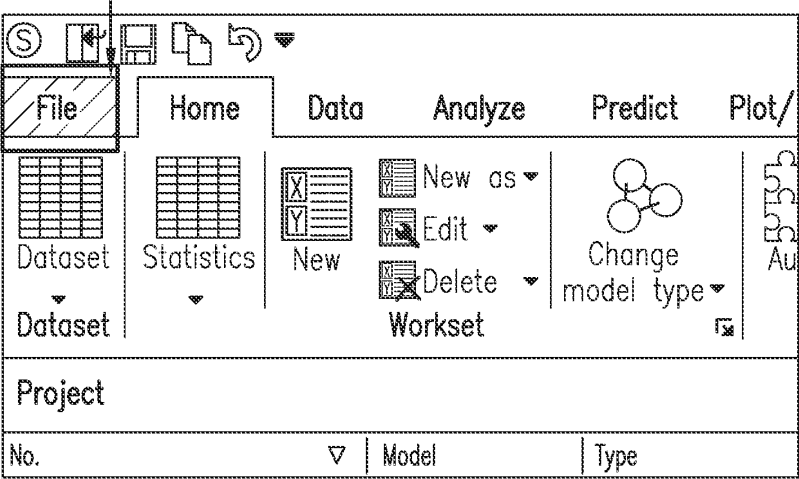
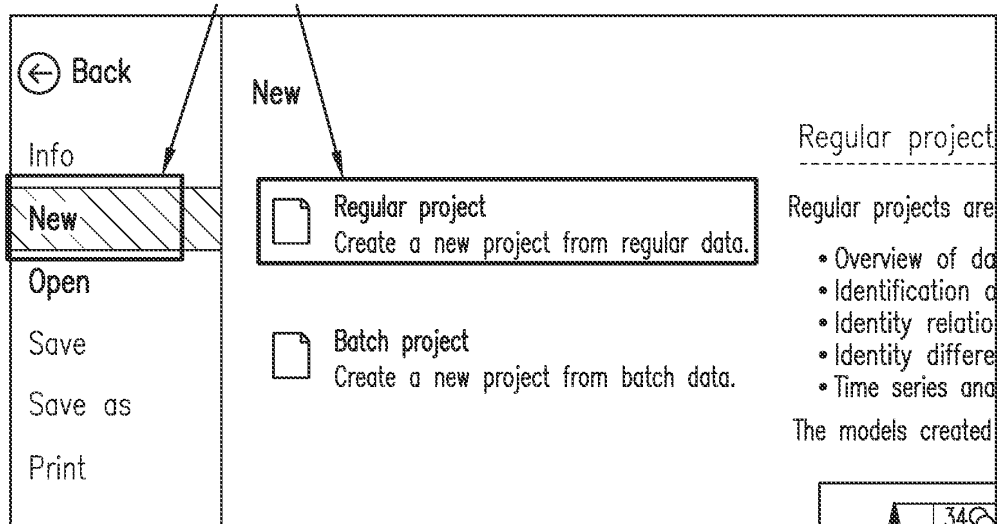


FIG.12A

3. Select "New" then Regular project



4. Select Excel file and Select "Open"

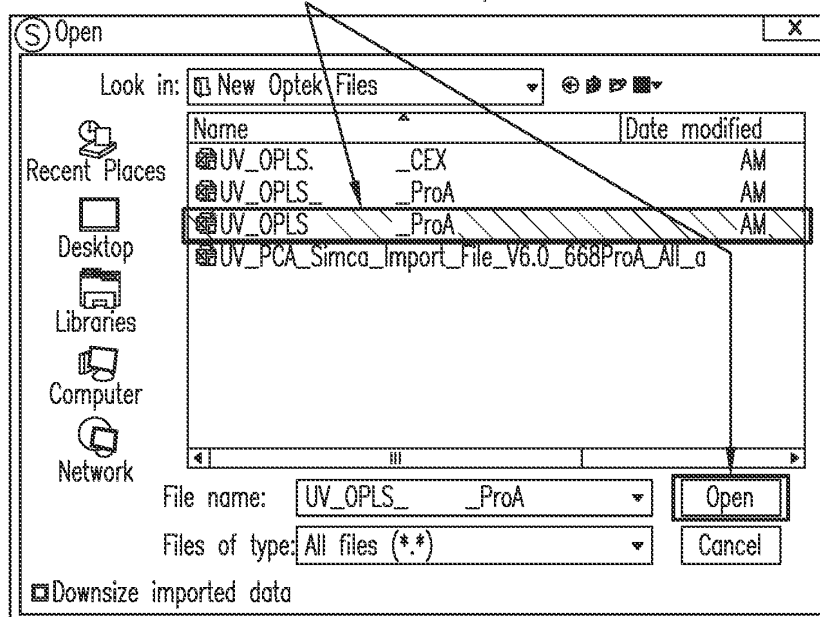


FIG.12B

5. Uncheck all sheets except "X Matrix". Then click Ok

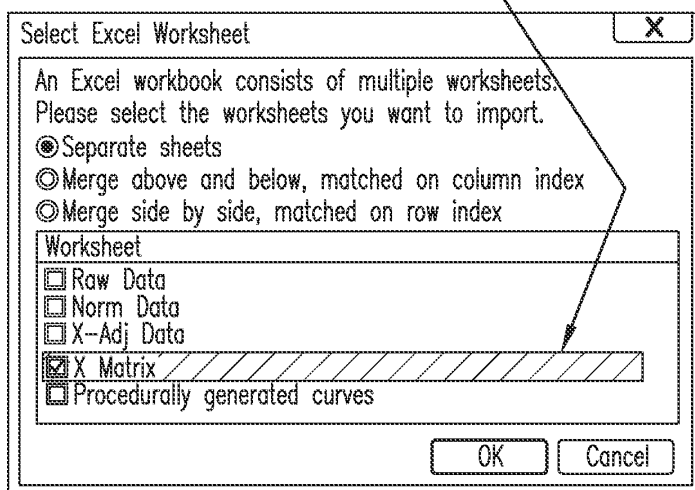


FIG. 13A

SIMCA Import - [X Matrix]

File Home Edit View

Add data Primary variable ID Secondary variable ID Variable IDs Primary observation ID Secondary observation ID Observation IDs Class ID Quantitative Qualitative Data Types

X Matrix

	Primary ID	Qualitative	3	Qualitative	5	6	7
1	Lot_cycle	Process Area	Column Pack	Good/Bad	Bifurcation?	Severe Tailing?	0
2	1 PA7		32	Good			-1.02032
3	2 PA7		32	Good			-1.01667
4	3 PA7		32	Good			-1.01593
5	4 PA7		32	Good			-1.01742
6	5 PA7		32	Good			-1.01593
7	6 PA7		32	Good			-1.01525
8	1 PA7		32	Good			-1.02035
9	2 PA7		32	Good			-1.01742
10	3 PA7		32	Good			-1.01742
11	4 PA7		32	Good			-1.01667
12	5 PA7		32	Good			-1.01593
13	6 PA7		32	Good			-1.01667
14	329_1	PCC	PCC	Good			-1
15	329_6	PCC	PCC	Good			-1
16	331_1	PCC	PCC	Good			-1
17	331_6	PCC	PCC	Good			-1
18	s1:0.1	PCC	PCC	Bad			-1
19	s1:0.12	PCC	PCC	Bad			-1
20	s2:0.5	PCC	PCC	Bad			-1
21	s2:0.4	PCC	PCC	Bad			-1
22	s2:0.35	PCC	PCC	Bad			-1
23	tm1:0.65	PCC	PCC	Bad			-1
24	tm1:0.68	PCC	PCC	Bad			-1
25	tm2:2	PCC	PCC	Bad			-1
26	tm2:1.75, s2:0.35	PCC	PCC	Bad			-1
27	tm1:0.78, s1:0.1	PCC	PCC	Bad			-1

Issues

► Resolve all

Sheet: X Matrix (155 variables, 27 observations, 69 (1.65%) missing)

① No primary var. ID

Cont. On
FIG.13B-2

6. Ensure First Column is Primary ID

FIG.13B-1

[illegible]

FIG. 13B-2

7. Select row 1 and click Primary variable ID. The row should now be colored green

SIMCA Import - [X Matrix]																	
File Home Edit View			Add data			Primary variable ID			Secondary variable ID			Primary observation ID			Secondary observation ID		

9. Ensure all columns containing volume values are selected as X-variables.

		SIMCA Import - [X Matrix]																													
Primary observation ID	Secondary observation ID	Class ID	Data Types														Variable roles														
			Quantitative	Qualitative	Date/Time	X-variable	Y-variable	Exclude	Include	Clear formatting	Apply formatting	Finish Import																			
Observation IDs			42	43	44	45	46	47	48	49	50	51	52	53	54	55	56														
0.7					0.72	0.74	0.76	0.78	0.8	0.82	0.84	0.86	0.88	0.9	0.92	0.94	0.96	0.98													
813134			-0.771643	-0.682579	-0.404407	0.240945	0.920306		1	1	1	1	1	1	1	1	1	1													
804179			-0.7633	-0.682857	-0.432052	0.179919	0.941744		1	1	1	1	1	1	1	1	1	1													
799459			-0.56732	-0.671411	-0.409283	0.219025	0.970041		1	1	1	1	1	1	1	1	1	1													
777148			-0.72855	-0.610504	-0.270594	0.4299			1	1	1	1	1	1	1	1	1	1													
765666			-0.15754	-0.597939	-0.251072	0.453864			1	1	1	1	1	1	1	1	1	1													
762208			-0.19212	-0.624938	-0.320685	0.345817			1	1	1	1	1	1	1	1	1	1													
804741			-0.75396	-0.615453	-0.216251	0.445888			1	1	1	1	1	1	1	1	1	1													
0.80636			-0.76346	-0.652518	-0.318478	0.277313			1	1	1	1	1	1	1	1	1	1													
792687			-0.44492	-0.616817	-0.239288	0.404626			1	1	1	1	1	1	1	1	1	1													
776074			-0.71661	-0.578371	-0.163576	0.491405			1	1	1	1	1	1	1	1	1	1													
774282			-0.722537	-0.584497	-0.202146	0.437634			1	1	1	1	1	1	1	1	1	1													
774555			-0.712532	-0.565237	-0.205214	0.509624			1	1	1	1	1	1	1	1	1	1													
977782			-0.912126	-0.729329	-0.530695	0.213061	0.764094																								
954412			-0.840881	-0.56747	-0.0843333	0.509679	0.939466																								
954412			-0.840881	-0.56747	-0.0843333	0.509679	0.939466																								
954412			-0.840881	-0.56747	-0.0843333	0.509679	0.939466																								
952192			0.303867	0.537772	0.742524	0.897116	0.984436																								
288777			0.485351	0.666355	0.617468	0.927978	0.989179																								
966603			-0.886968	-0.69617	-0.351367	0.0997823	0.480992		0.591903	0.591986	0.592761	0.593086	0.595306	0.600647	0.612118	0.634044	0.671169	1													
961686			-0.862025	-0.613039	-0.154799	0.437735	0.90469																								
961686			-0.862025	-0.613039	-0.154799	0.437735	0.90469																								
961686			-0.862025	-0.613039	-0.154799	0.437735	0.90469																								
457298			0.67054	0.846233	0.960397																										
961686			-0.862025	-0.613039	-0.154799	0.437735	0.90469																								
961686			-0.862025	-0.613039	-0.154799	0.437735	0.90469																								
961686			-0.862025	-0.613039	-0.154799	0.437735	0.90469																								
457298			0.67054	0.846233	0.960397																										

FIG.15A

SIMCA Import - [X Matrix]

File Home Edit View

Add data Primary variable ID Secondary variable ID Primary observation ID Secondary observation ID Class ID Quantitative

X Matrix

Primary ID	Lot_cycle	Primary ID	Secondary ID	Secondary ID	Secondary ID	Secondary ID	Secondary ID
			Process Area	Column Pack	Good/Bad	Bifurcation?	Severe Tailing?
2		1	PA7	32	Good		
3		2	PA7	32	Good		
4		3	PA7	32	Good		
5		4	PA7	32	Good		
6		5	PA7	32	Good		
7		6	PA7	32	Good		
8		1	PA7	32	Good		
9		2	PA7	32	Good		
10		3	PA7	32	Good		
11		4	PA7	32	Good		
12		5	PA7	32	Good		
13		6	PA7	32	Good		
14	329_1		PGC	PGC	Good		
15	329_6		PGC	PGC	Good		
16	331_1		PGC	PGC	Good		
17	331_6		PGC	PGC	Good		
18	s1:0.1		PGC	PGC	Bad		
19	s1:0.12		PGC	PGC	Bad		
20	s2:0.5		PGC	PGC	Bad		
21	s2:0.4		PGC	PGC	Bad		
22	s2:0.35		PGC	PGC	Bad		
23	tm1:0.65		PGC	PGC	Bad		
24	tm1:0.68		PGC	PGC	Bad		
25	tm2:2		PGC	PGC	Bad		
26	tm2:1.75, s2:0.35		PGC	PGC	Bad		
27	tm1:0.78, s1:0.1		PGC	PGC	Bad		

Issues

► Resolve all

Sheet: X Matrix (151 variables, 26 observations)

No issues

Cont. On
FIG.15B-2

10. Check bottom of import window for "Issues section". check that it displays "No issues" Then click finish import

FIG.15B-1

10. Check bottom of import window for "Issues section". check that it displays "No issues" Then click finish import

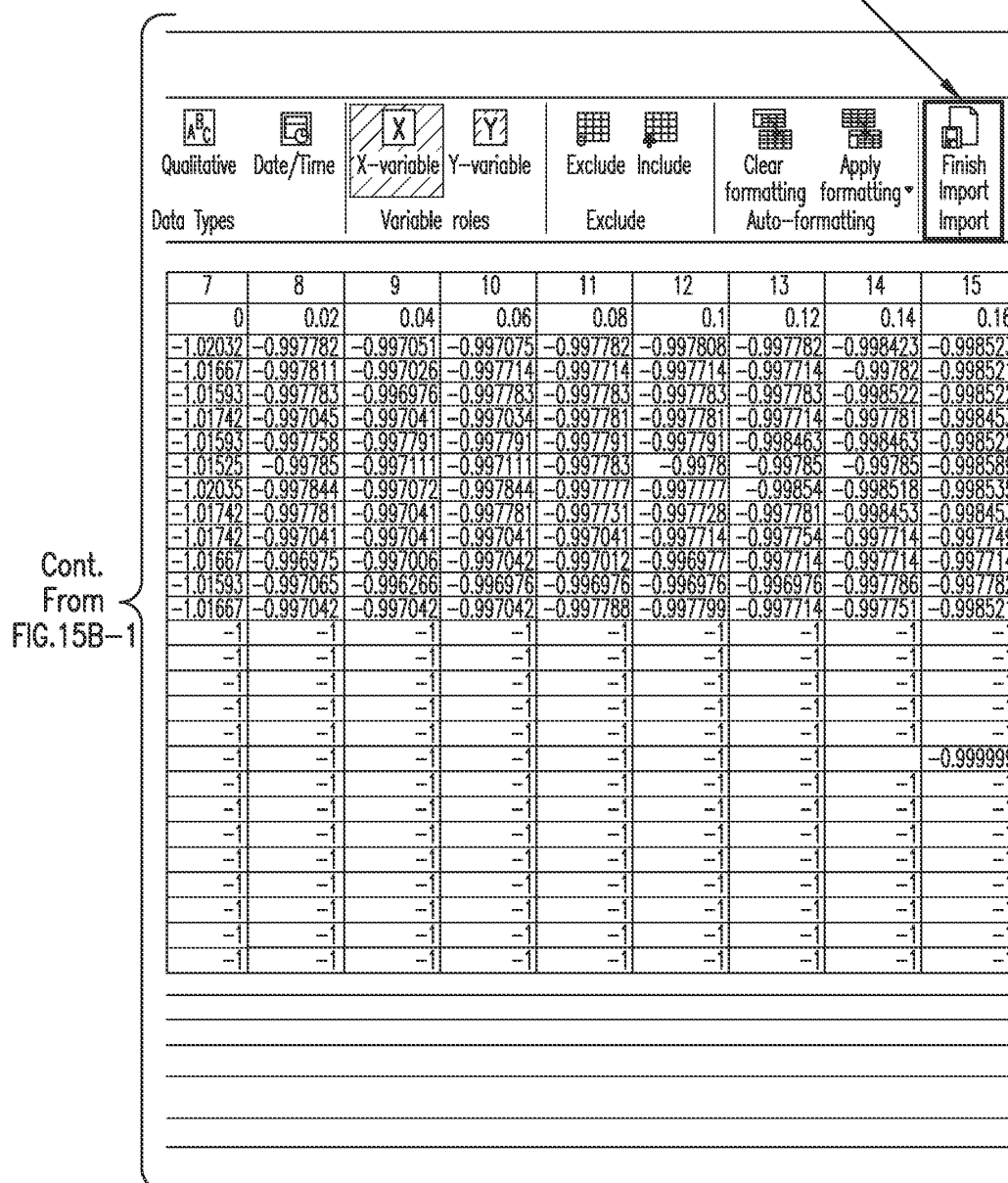


FIG. 15B-2

11. Save and Name new Simca file. Name the file, select the location where the file will be saved, then click save

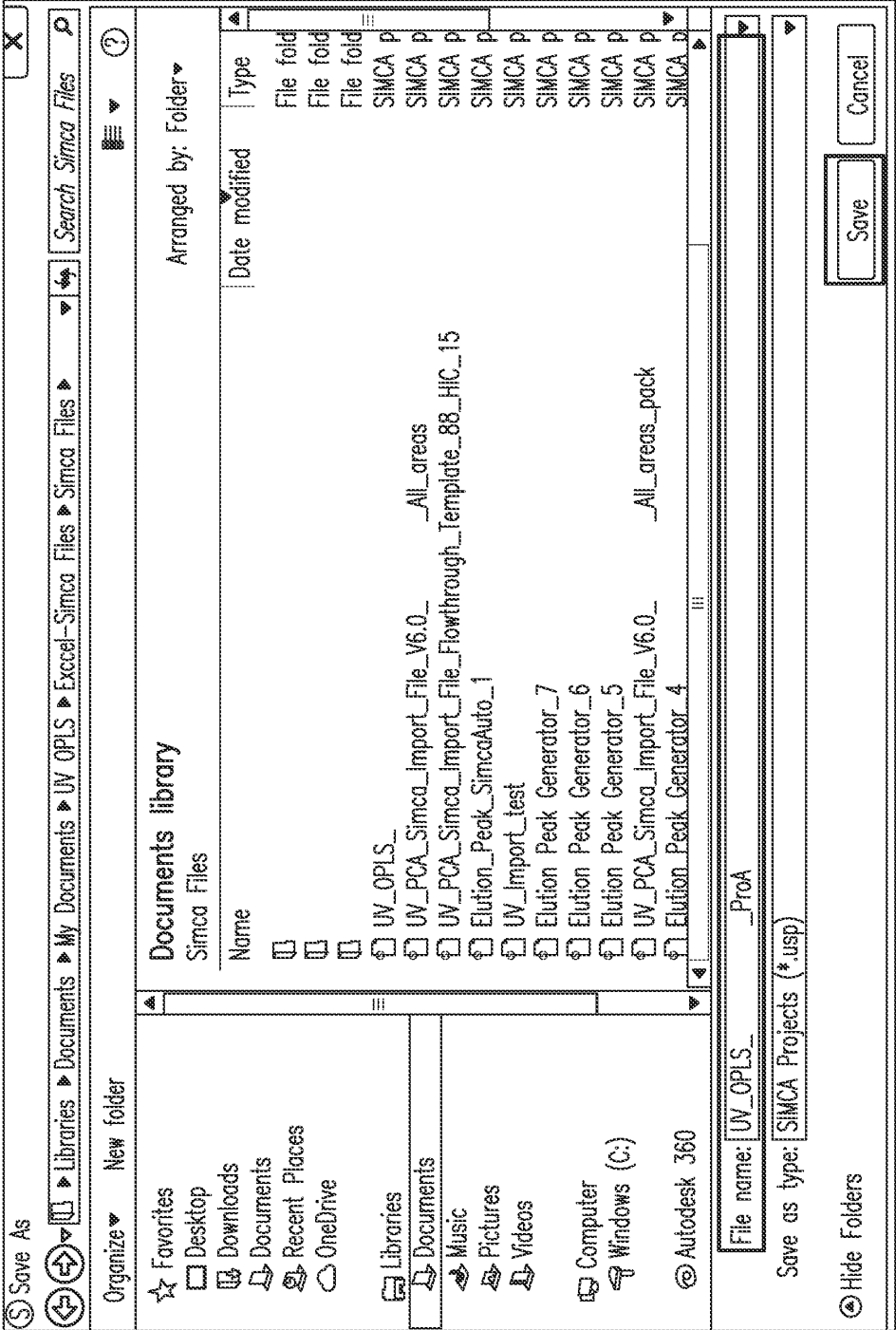
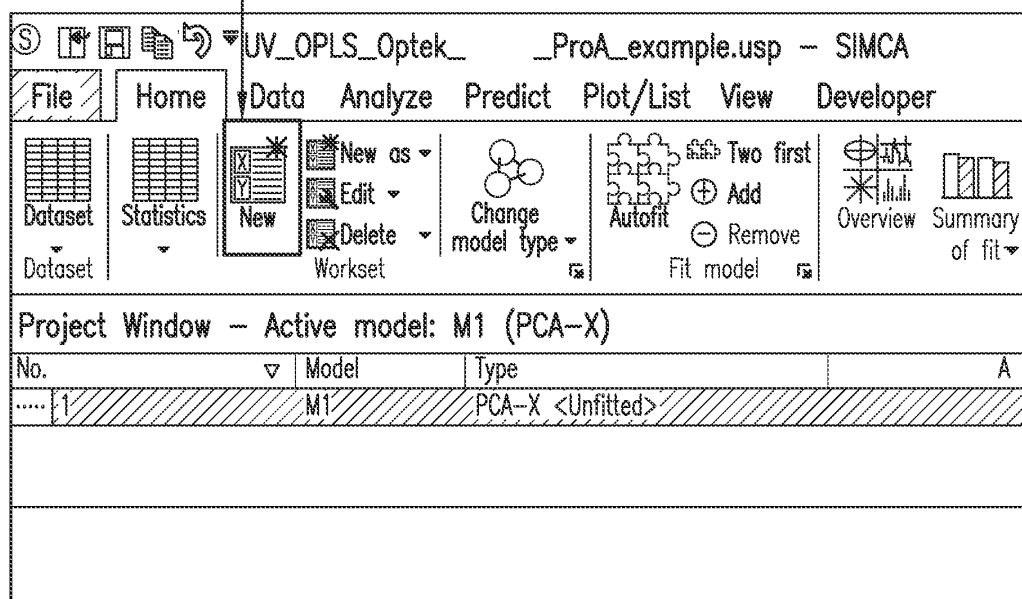


FIG.16

1. Select New



2. Select Observations, Then select the down arrow next to Class from obs ID and select Good/Bad

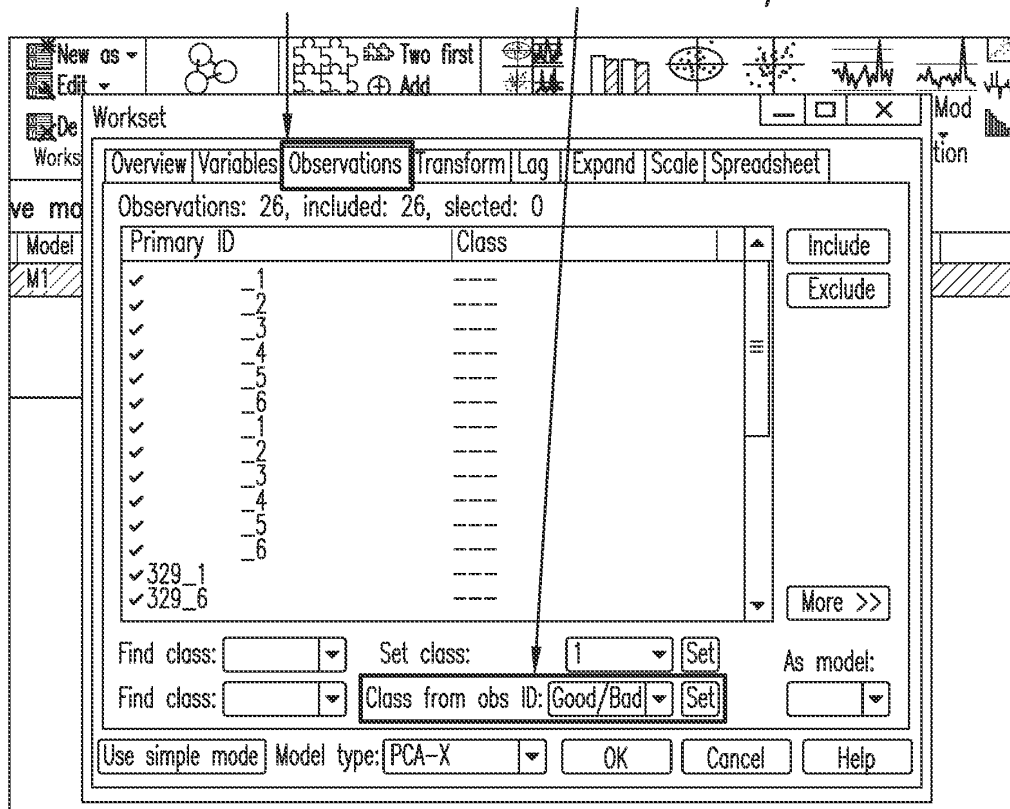
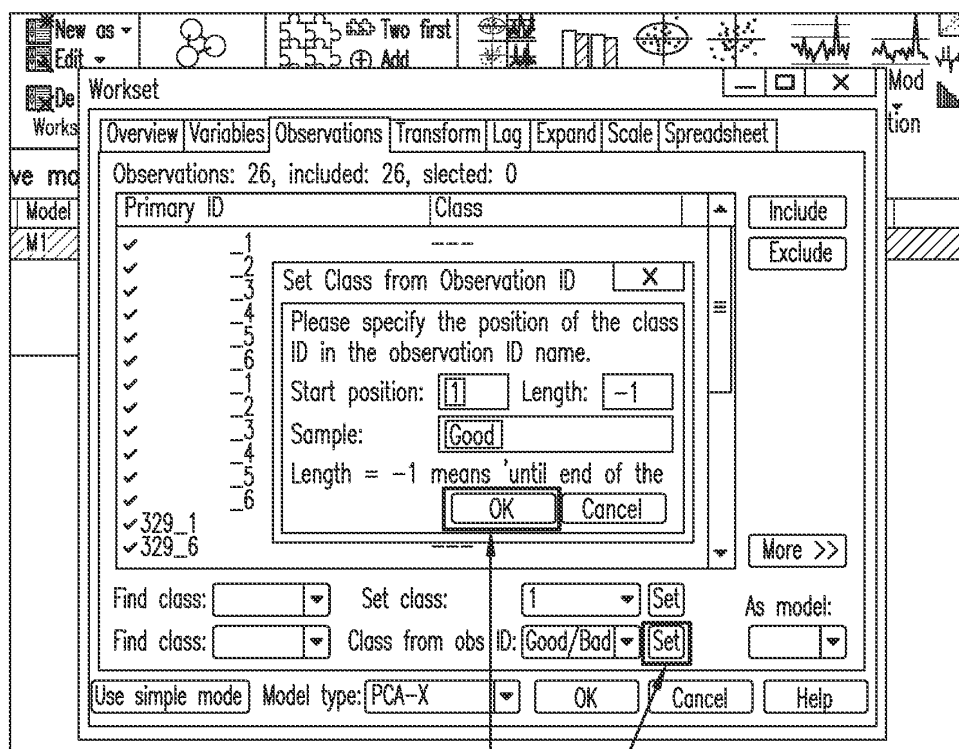
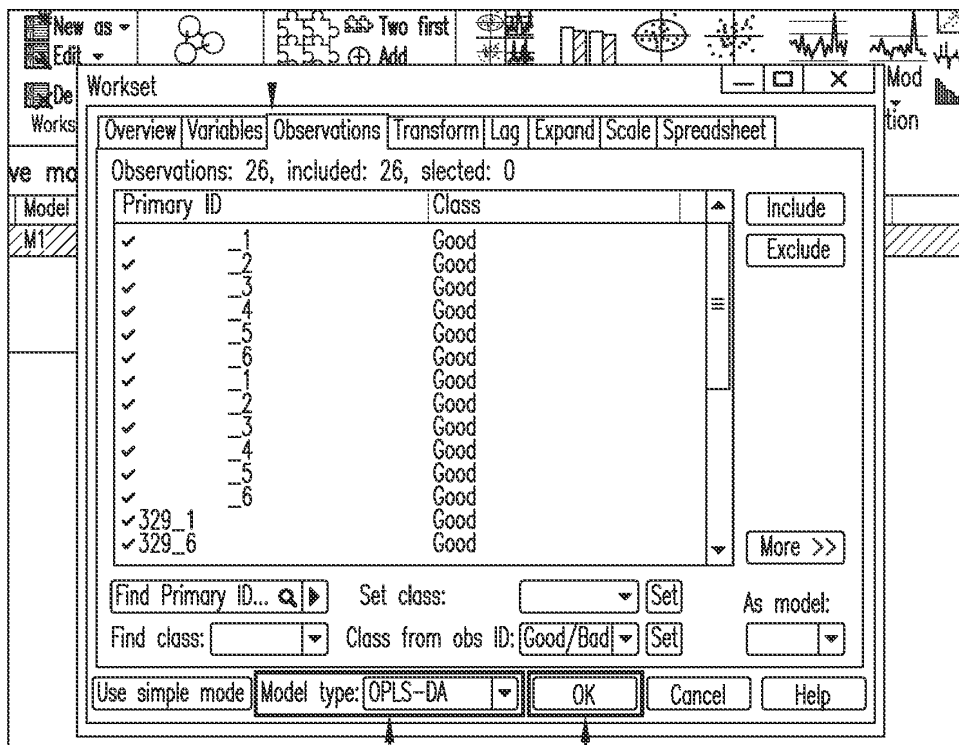


FIG. 17



3. Select "set", then select "Ok" in the pop up window



4. The model type displays as OPLS-DA. Select "Ok"

FIG.18

5. Click Autofit. This fit automatically fit the optimal number of components to the model.
A chart displaying the summary of fit will appear at the bottom

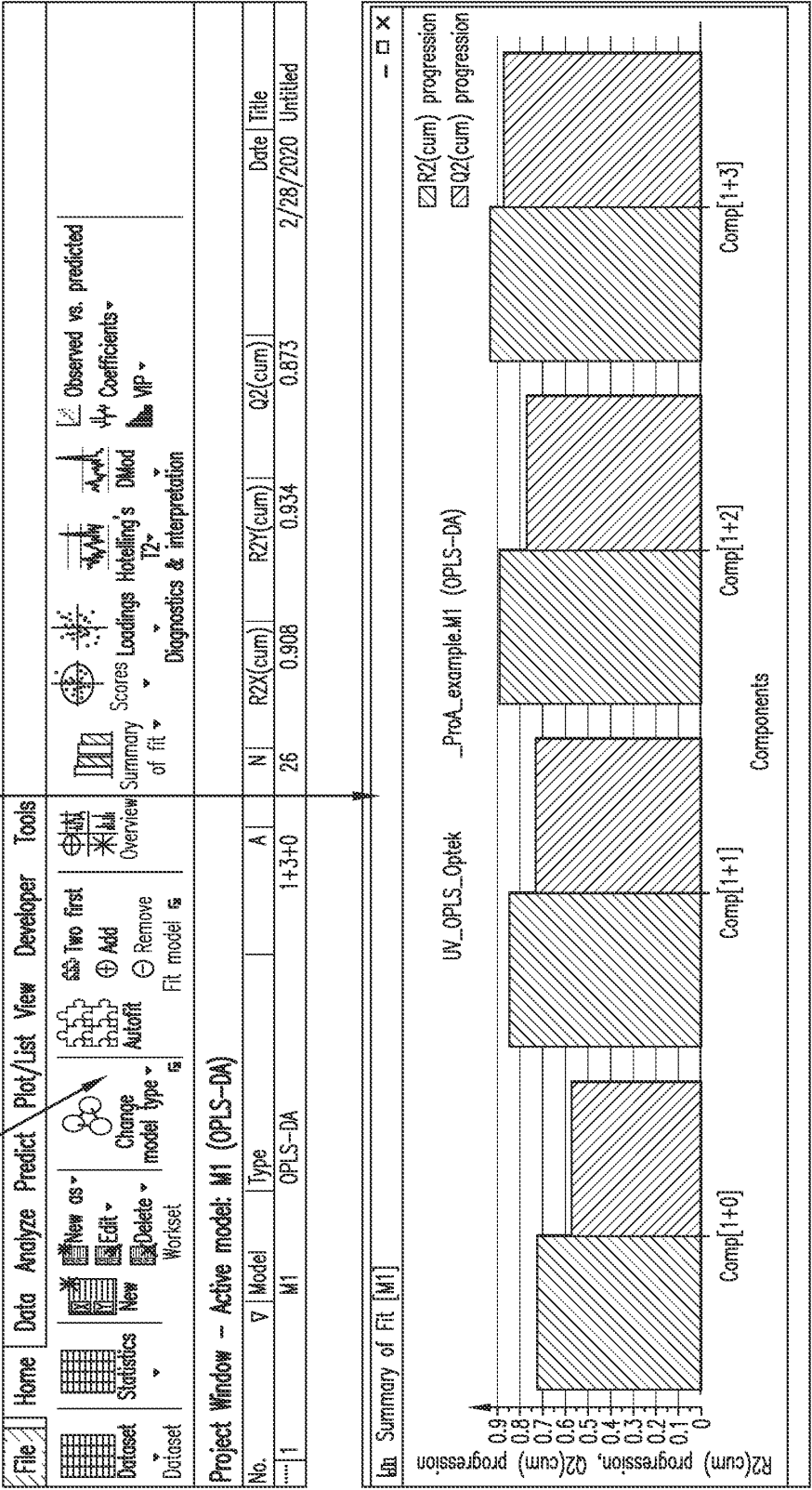


FIG.19

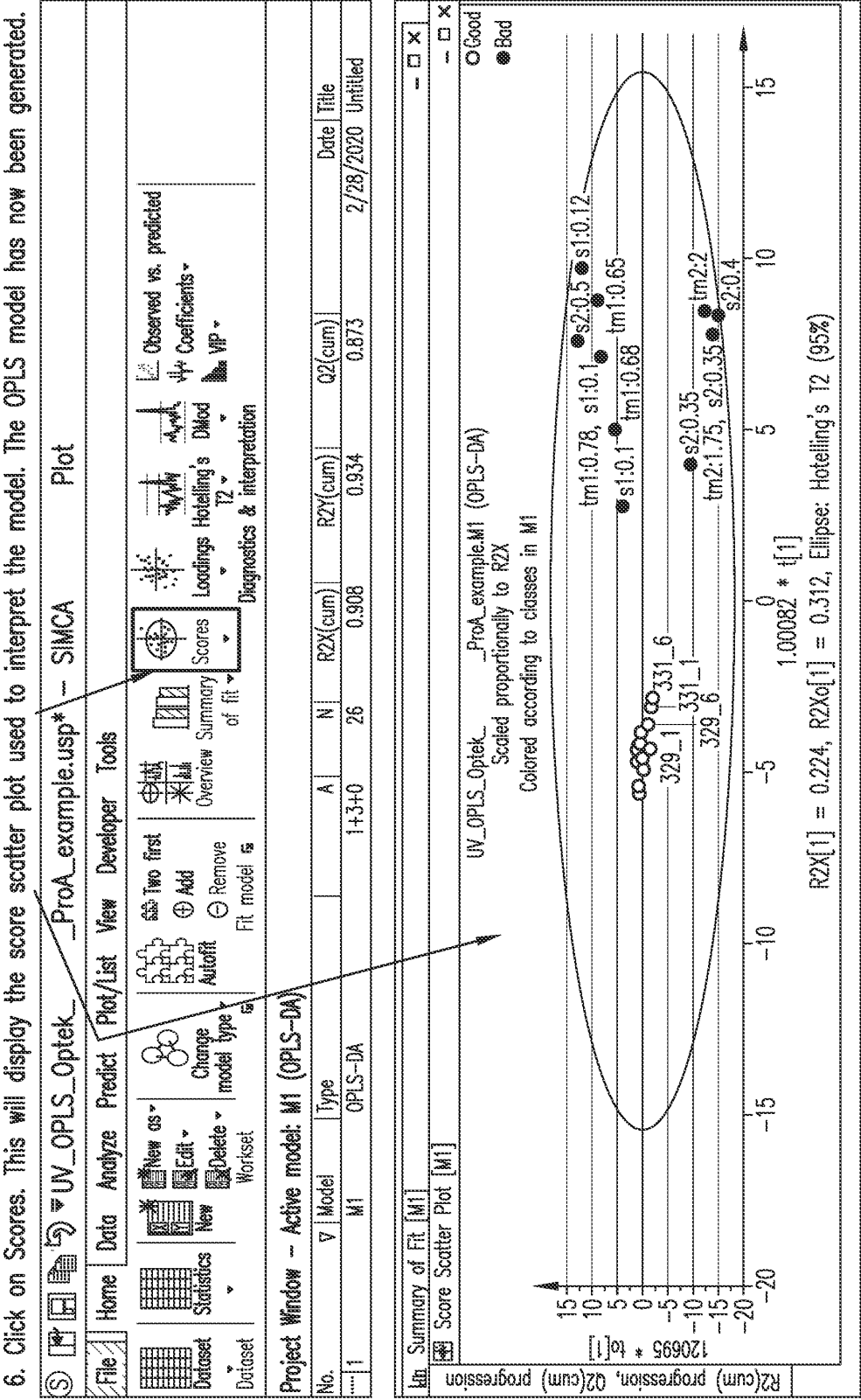
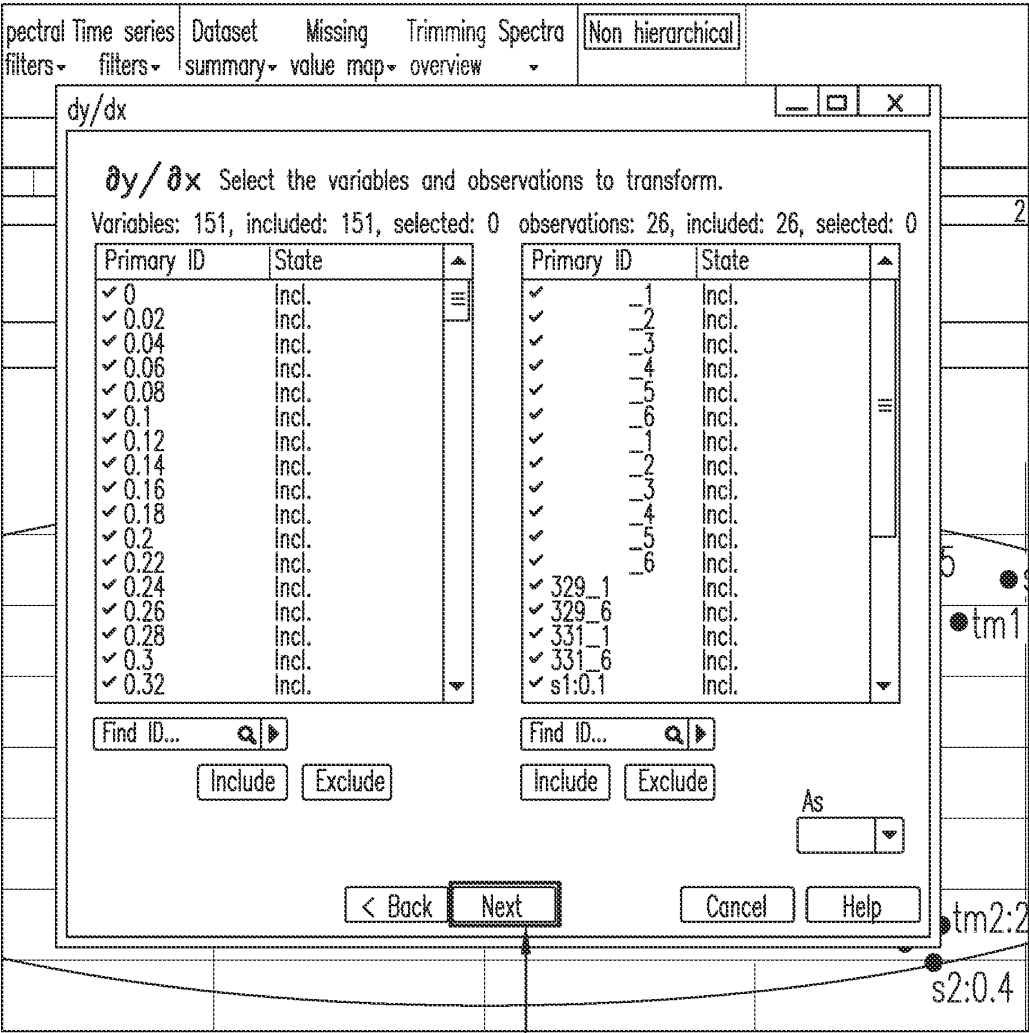
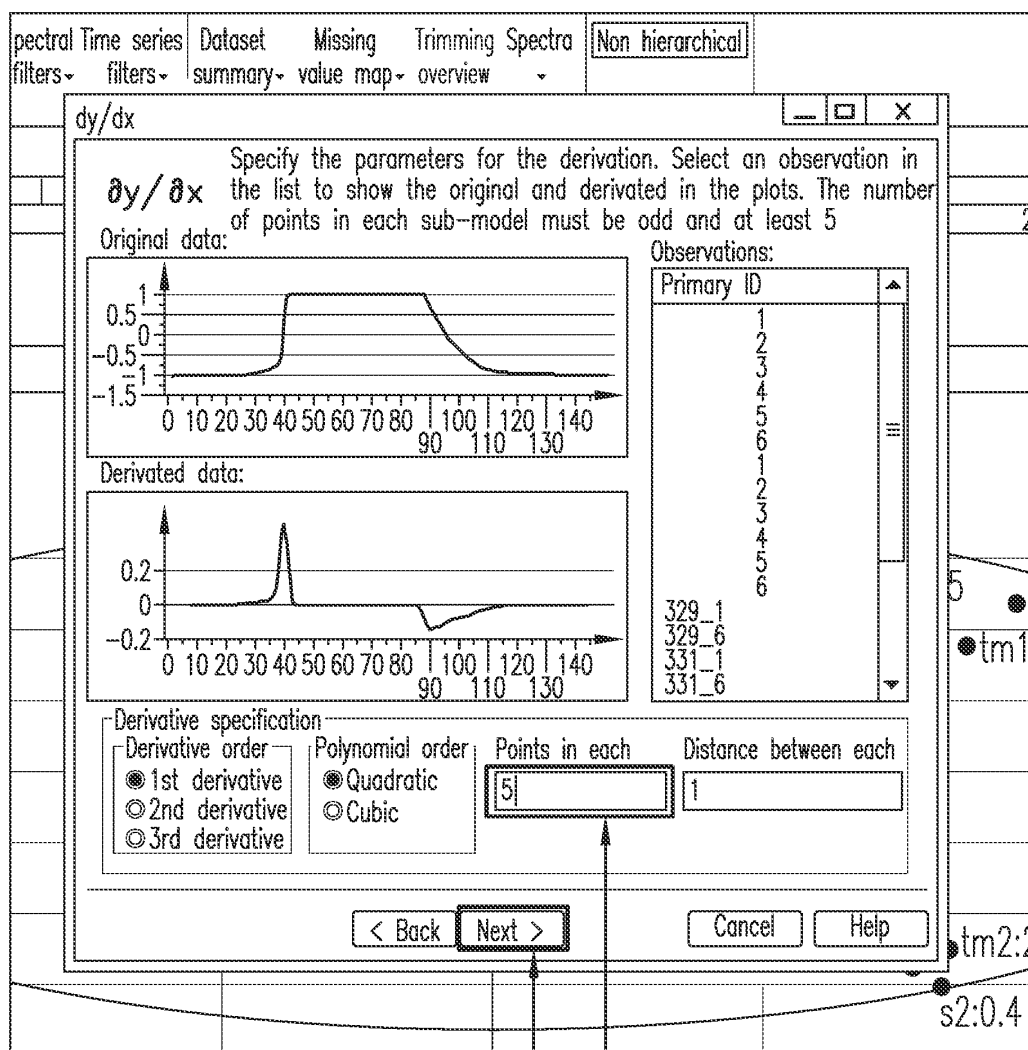


FIG.20



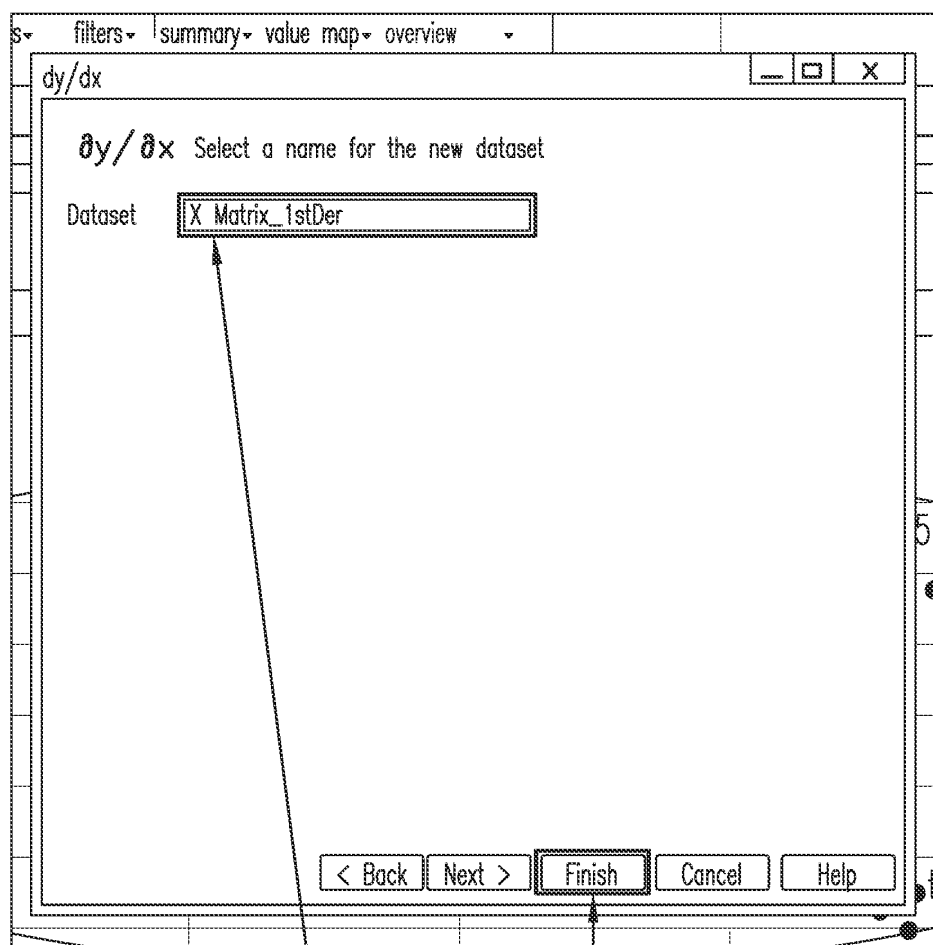
2. Click next on the pop-up menu

FIG.22A



3. The following window will show the data for each run and what the derivative looks like. Change the value for Points in each to 5 to reduce the level of smoothing. Then Click Next

FIG.22B



4. Name the new dataset, then click Finish

FIG.23A

5. Simca will display the new dataset. Click on Home, then New to create a new model with the dataset

File

Home

Data

Analyze

Predict

Plot/List

View

Developer

Tools

Dataset

Statistics

New as

Edit

Delete

Workset

Change model type

Autofit

Two first

Add

Remove

Fit model

Overview

Summary of fit

Scores

Loadings

Hotelling's T²

Diagnostics & Interpretation

Project Window - Active model: M1 (OPLS-DA)

No.	Model	Type	A	N	R2X(cum)
1	M1	OPLS-DA	1+3+0	26	0.908

Score Scatter Plot [M1]

Dataset - X Matrix_1stDer

1	2	3	4	5	6	7	8	9	10	11
Primary ID	Process Area	Column Pack	Good/Bad	Bifurcation?	Severe Tailing?	1stDer0	1stDer0.0	1stDer0.0	1stDer0.0	1stDer0.0
Original ID						10	0.02	0.04	0.06	0.08
1	PA7	32	Good					00457751	2847e-05	00219482
2	PA7	32	Good					00380105	4063e-05	00137627
3	PA7	32	Good					00362867	6332e-05	00161266
4	PA7	32	Good					00392843	00221062	00209224
5	PA7	32	Good					00362539	5651e-06	00134397
6	PA7	32	Good					00356697	1847e-05	00216681
7	PA7	32	Good					00451382	0595e-05	00028699
8	PA7	32	Good					00393717	4781e-05	00142676
9	PA7	32	Good					00407518	00134492	00209832
10	PA7	32	Good					00392512	9634e-07	00135213
11	PA7	32	Good					00379879	2448e-05	00141966
12	PA7	32	Good					00377659	00226009	00210148
1329_1	PGC	PGC	Good					0	0	0
16329_6	PGC	PGC	Good					0	0	0
17331_1	PGC	PGC	Good					0	0	0
18331_6	PGC	PGC	Good					0	0	0
19s1:0.1	PGC	PGC	Bad					0	0	0

FIG.23B

6. Select the derived dataset and unselect the initial dataset

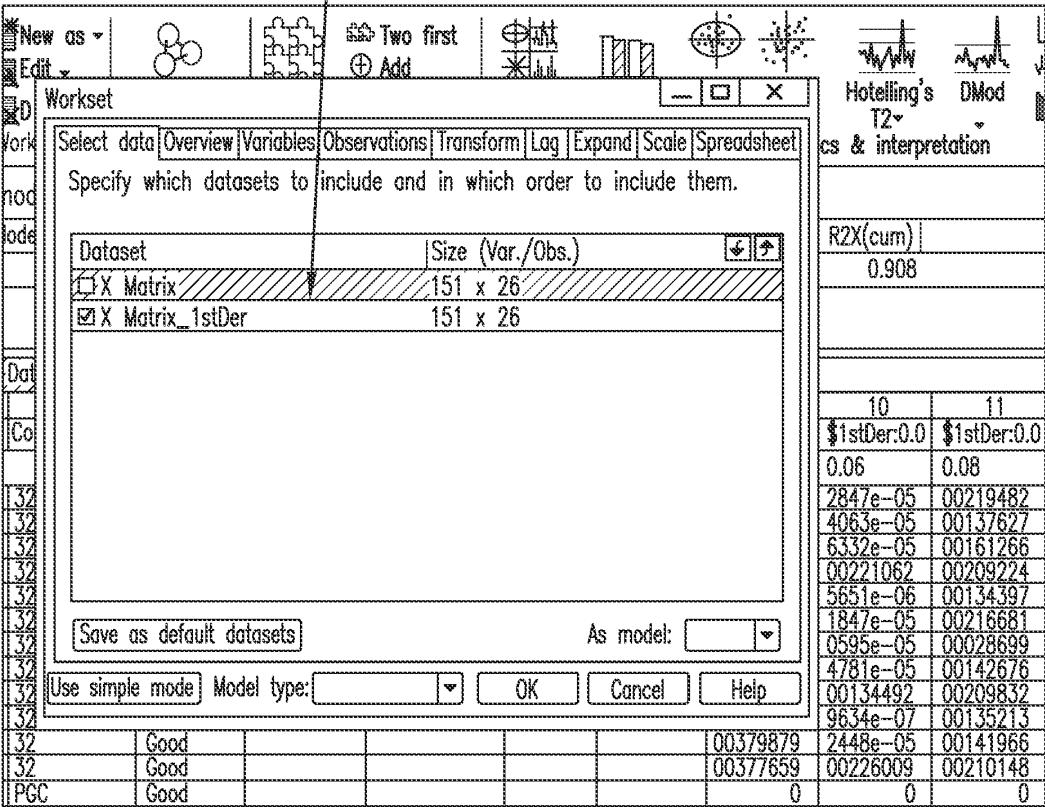
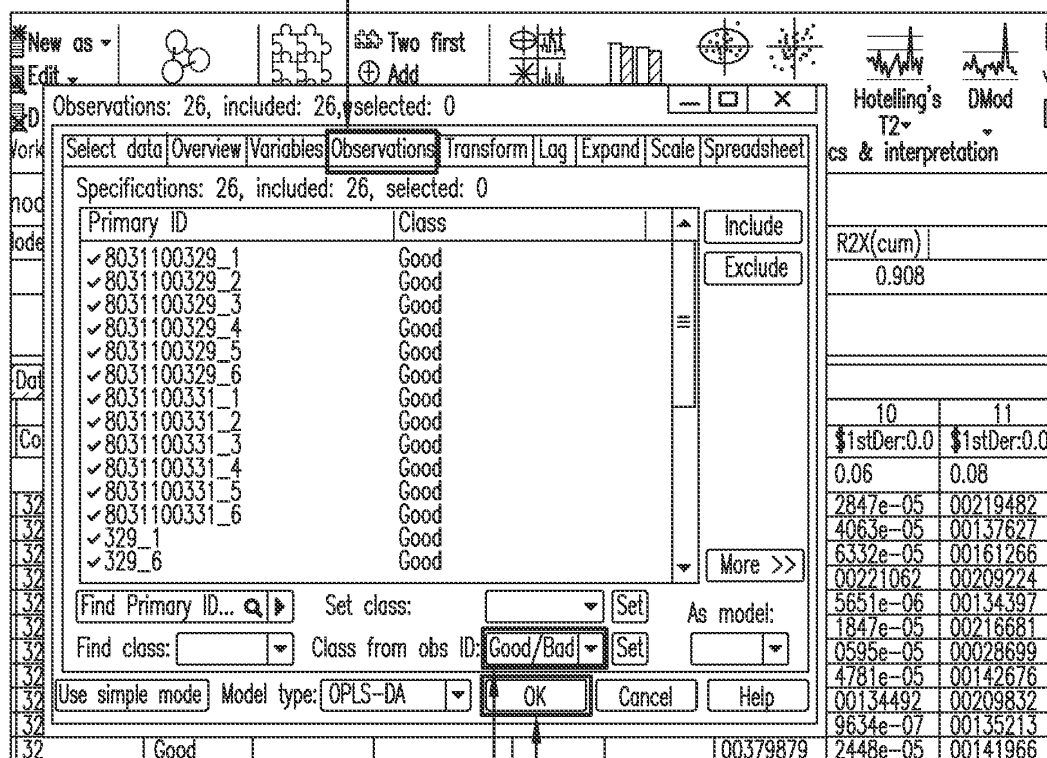


FIG.24A

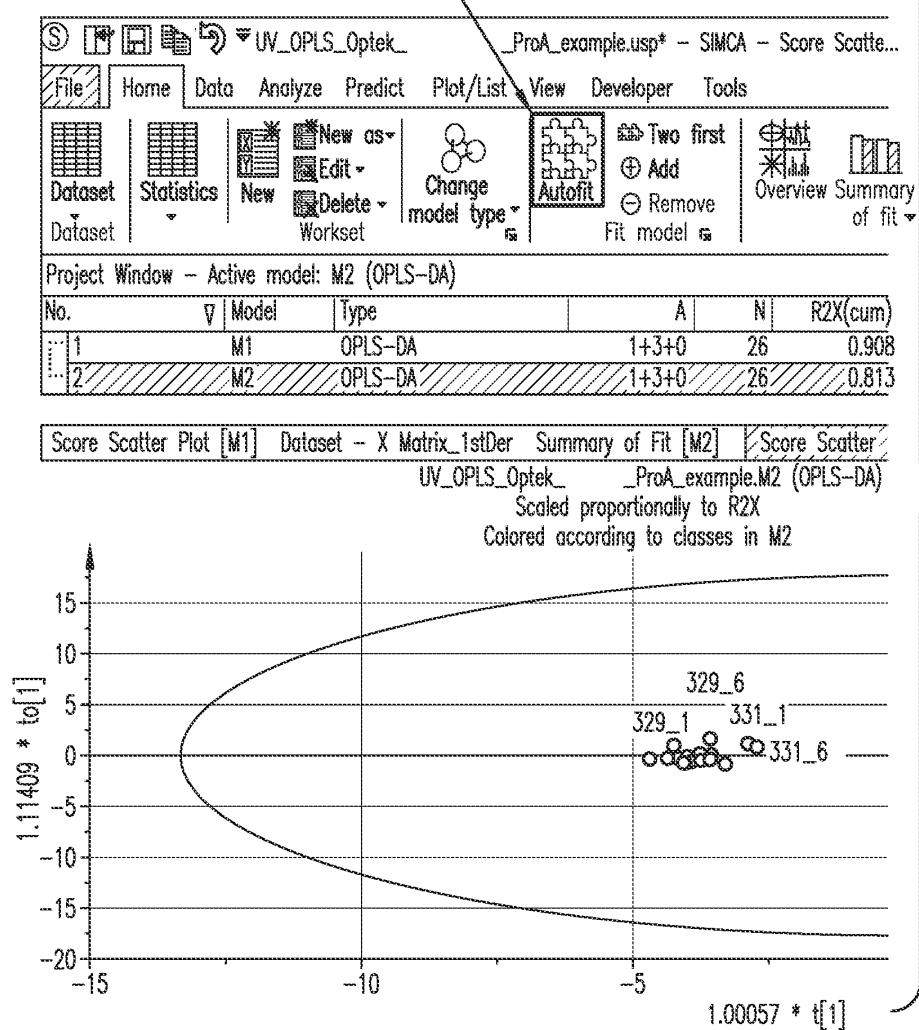
7. Go to the observations tab.



Set Class from obs ID to Good/Bad. Then click Ok

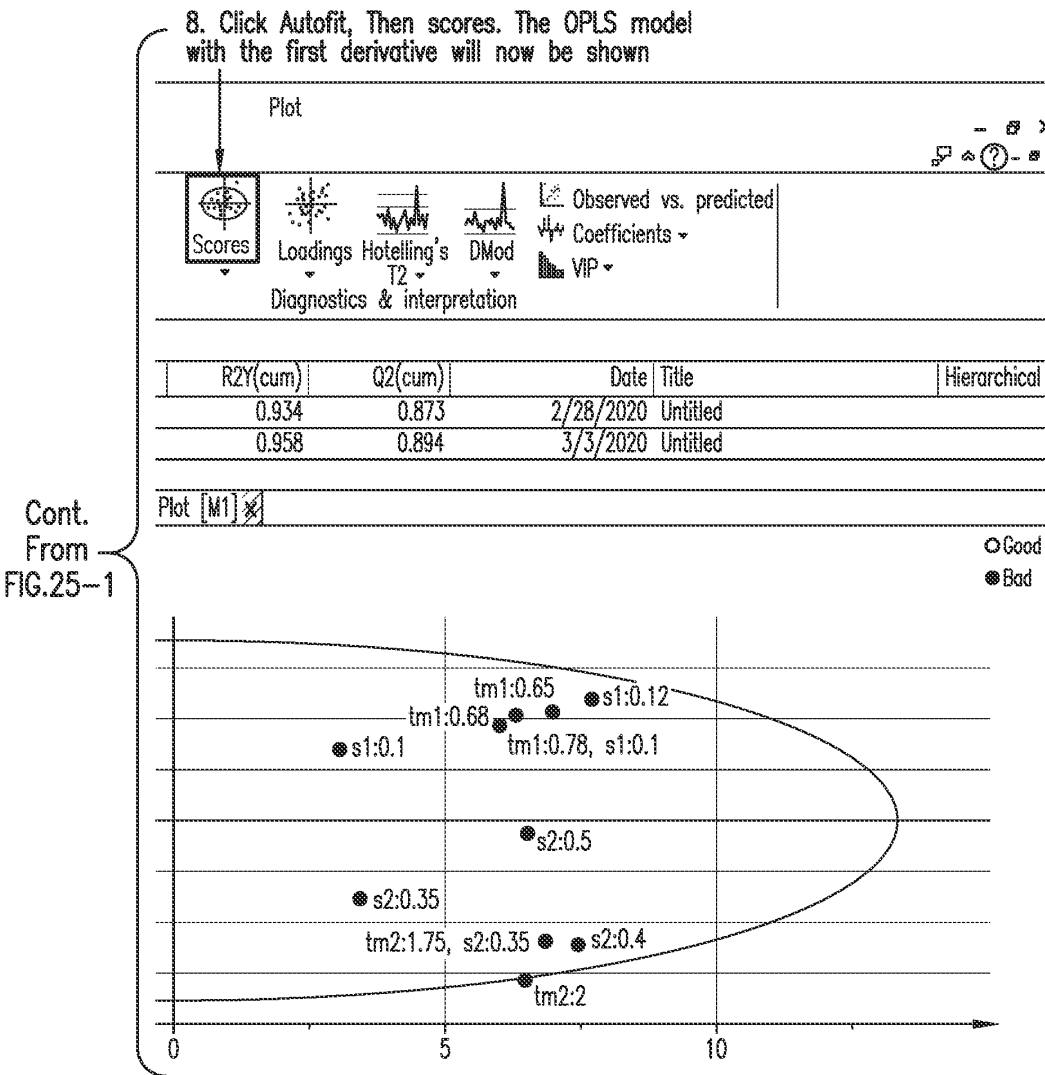
FIG.24B

8. Click Autofit, Then scores. The OPLS model with the first derivative will now be shown



Cont. On
FIG.25-2

FIG.25-1



Cont.
From
FIG.25-1

FIG.25-2

1. Navigate to the Data tab, Then click Import dataset

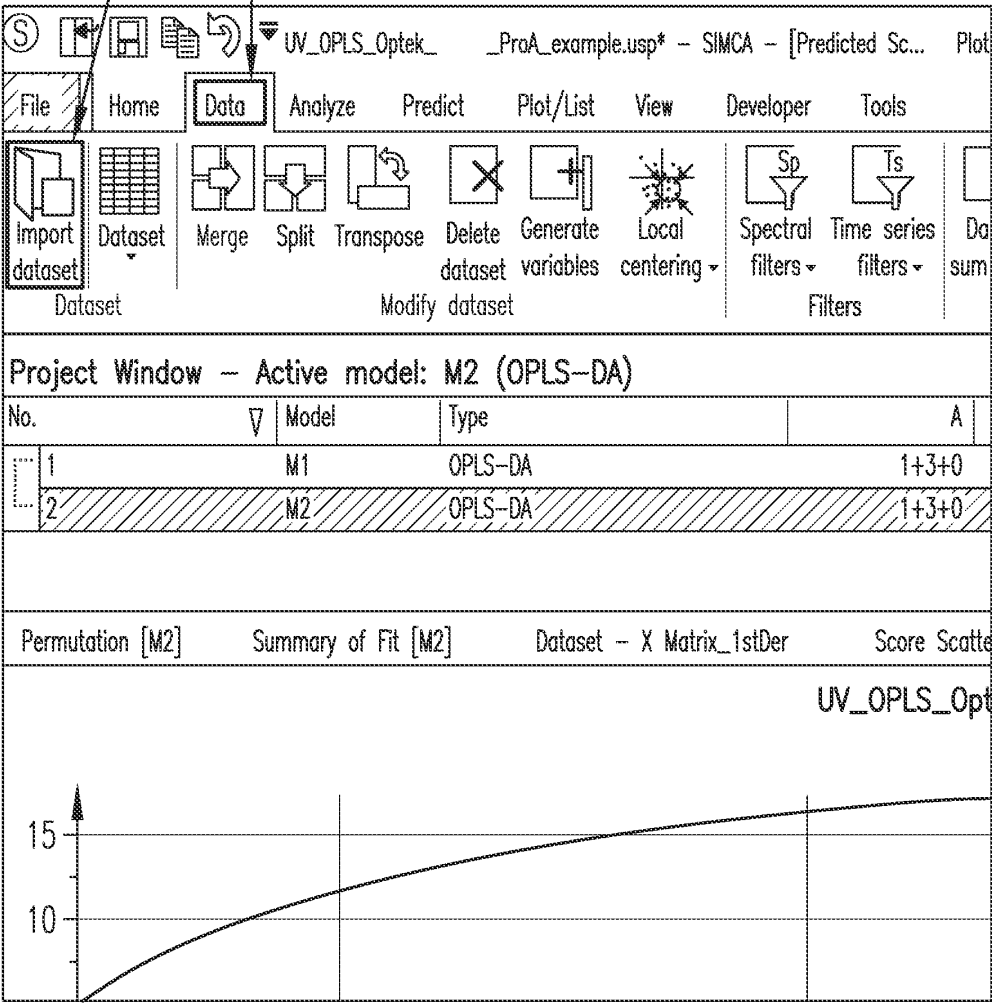


FIG.26A

2. Select the file with the new data to be predicted by the model and click open

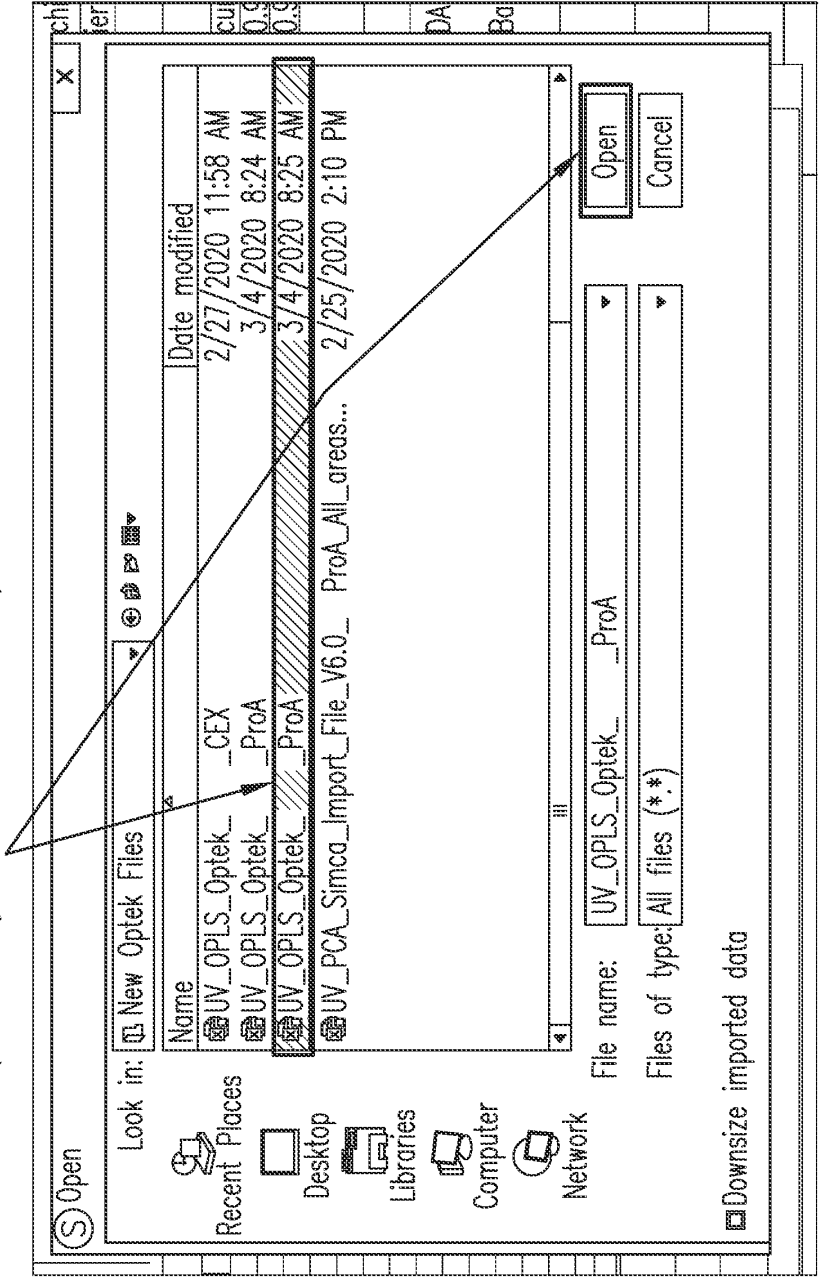


FIG.26B

The screenshot shows the 'Select Excel Worksheet' dialog box. The 'Observation ID...' tab is selected, displaying icons for Quantitative, Qualitative, and Date/Time data types. Below these are three radio button options: 'Separate sheets' (selected), 'Merge above and below, matched on column index', and 'Merge side by side, matched on row index'. A list of worksheets is provided, with 'X Matrix' highlighted. The 'OK' and 'Cancel' buttons are at the bottom right.

3. Select the sheet containing the data and click ok

FIG. 27A

4. Follow the same method detailed before to format the import. Rename the dataset to be unique (Double click) and exclude data already in the other dataset by selecting the rows of data and clicking exclude. Click Finish and import when done.

SimCA Import -- [X Matrix_335]

File Home Edit View

Add data

Primary variable ID observation ID

Secondary variable ID observation ID

Class ID

Quantitative Qualitative Date/Time

Variable roles

X X Y Y

X-variable Y-variable

Exclude Include

Clear formatting Auto-formatting

Apply formatting

Finish Import

X Matrix_335 x1

Primary ID	Secondary ID	Process Area	Column Pack	Good/Bad	Bifurcation?	Severe Tailing?	0	0.02	0.04	0.06	0.08	0.1	0.12	0.14	0.16
2	8031100329_1	PA7	32	Good			-1.02032	-0.99782	-0.997051	-0.997075	-0.99782	-0.997808	-0.99782	-0.998423	-0.998523
3	8031100329_2	PA7	32	Good			-1.01667	-0.997811	-0.997026	-0.997714	-0.997714	-0.997714	-0.997714	-0.99782	-0.998521
4	8031100329_3	PA7	32	Good			-1.01593	-0.99783	-0.996976	-0.99783	-0.99783	-0.99783	-0.99783	-0.998522	-0.998522
5	8031100329_4	PA7	32	Good			-1.01742	-0.997045	-0.997041	-0.997034	-0.99781	-0.99781	-0.997714	-0.997714	-0.998453
6	8031100329_5	PA7	32	Good			-1.01593	-0.997758	-0.99779	-0.99779	-0.99779	-0.99779	-0.99779	-0.998463	-0.998522
7	8031100329_6	PA7	32	Good			-1.01525	-0.99785	-0.997111	-0.997111	-0.99783	-0.9978	-0.99785	-0.99785	-0.998589
8	8031100331_1	PA7	32	Good			-1.02035	-0.997844	-0.997072	-0.997844	-0.99777	-0.99777	-0.99777	-0.99854	-0.99855
9	8031100331_2	PA7	32	Good			-1.01742	-0.997781	-0.997041	-0.997041	-0.997731	-0.997728	-0.997781	-0.998453	-0.998453
10	8031100331_3	PA7	32	Good			-1.01742	-0.997041	-0.997041	-0.997041	-0.997041	-0.99714	-0.99714	-0.99714	-0.997749
11	8031100331_4	PA7	32	Good			-1.01667	-0.996975	-0.997006	-0.997042	-0.997012	-0.996977	-0.99714	-0.99714	-0.997714
12	8031100331_5	PA7	32	Good			-1.01593	-0.997065	-0.996766	-0.996976	-0.996976	-0.996976	-0.996976	-0.99786	-0.99782
13	8031100331_6	PA7	32	Good			-1.01667	-0.997042	-0.997042	-0.997042	-0.997788	-0.997799	-0.997714	-0.997714	-0.998521
14	8031100335_1	PA7	32				1.02172	0.997025	0.996368	0.997066	0.997066	0.997066	0.997066	0.997797	0.997763
15	8031100335_2	PA7	32				-1.0181	-0.99781	-0.996772	-0.99704	-0.996973	-0.99704	-0.99713	-0.99775	-0.997713
16	8031100335_3	PA7	32				-1.01742	-0.997041	-0.996301	-0.996352	-0.997022	-0.997041	-0.997041	-0.99781	-0.997781
17	8031100335_4	PA7	32				-1.01739	-0.997303	-0.997015	-0.997015	-0.997015	-0.997755	-0.997755	-0.997755	-0.997755
18	8031100335_5	PA7	32				-1.0181	-0.996973	-0.9963	-0.9963	-0.996973	-0.996973	-0.996973	-0.997713	-0.997713
19	8031100335_6	PA7	32				-1.01593	-0.997168	-0.997023	-0.997023	-0.996976	-0.997019	-0.99782	-0.99785	-0.997836

Issues

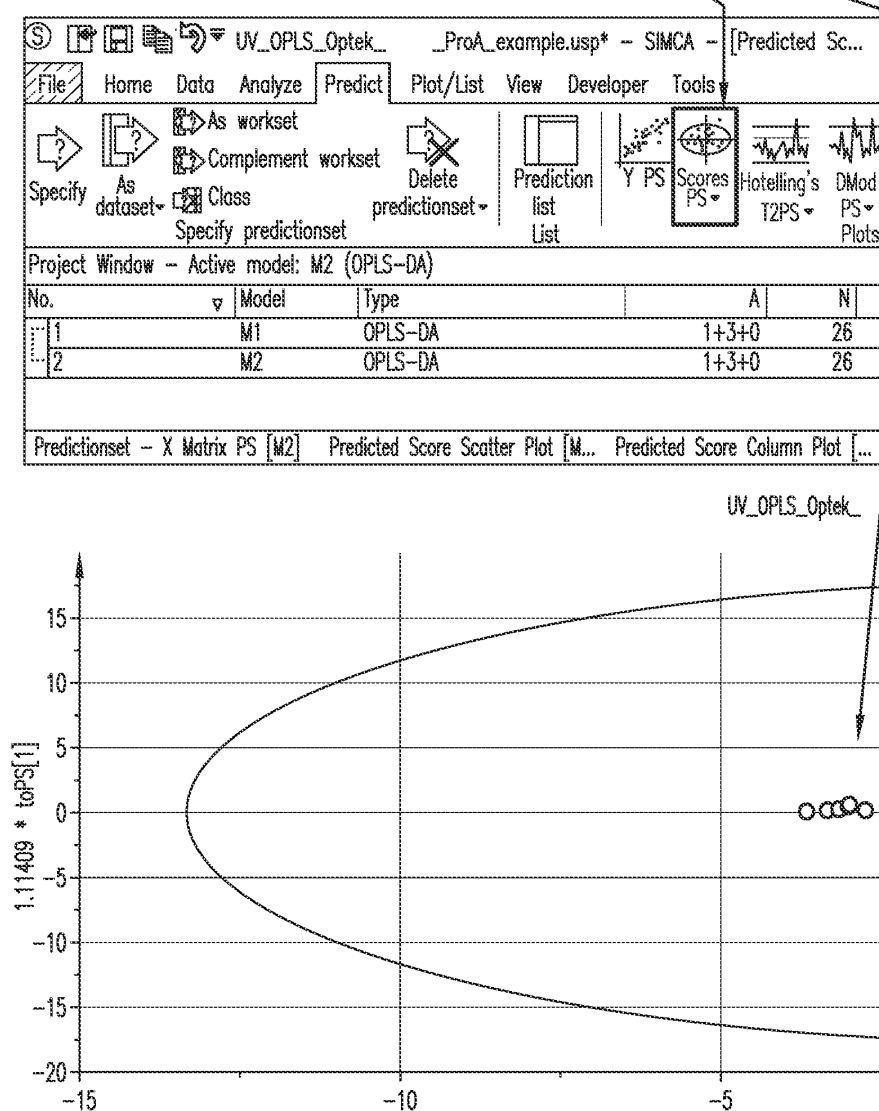
Resolve all

Sheet: X Matrix_335 (151 variables, 6 observations)

No issues

FIG.27B

6. Click on Score PS. A Score Plot showing the predicted scores will appear in the window at the bottom



Cont. On
FIG.29-2

FIG.29-1

Cont.
From
FIG.29-1

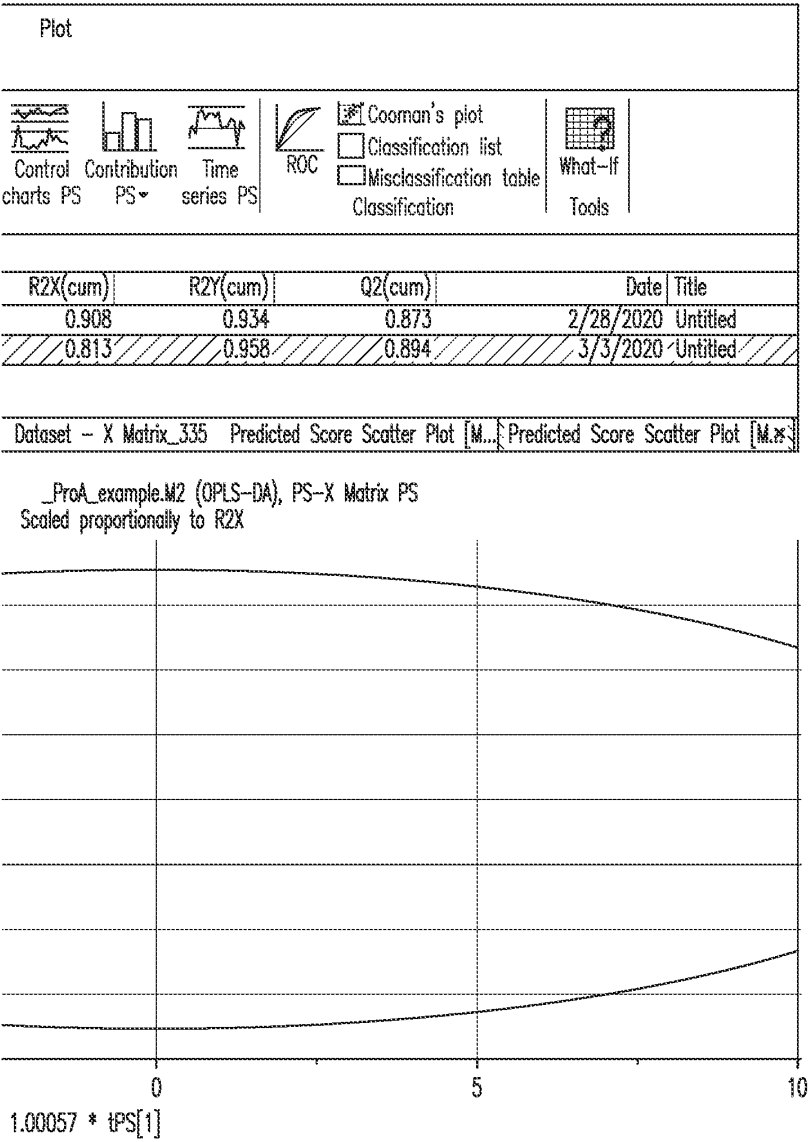


FIG.29-2

7. To add the points from the model to the score plot to compare where the predicted points are, click specify, change the source to the original dataset, select the data observations you want to compare with, hit the right arrow, then click ok.

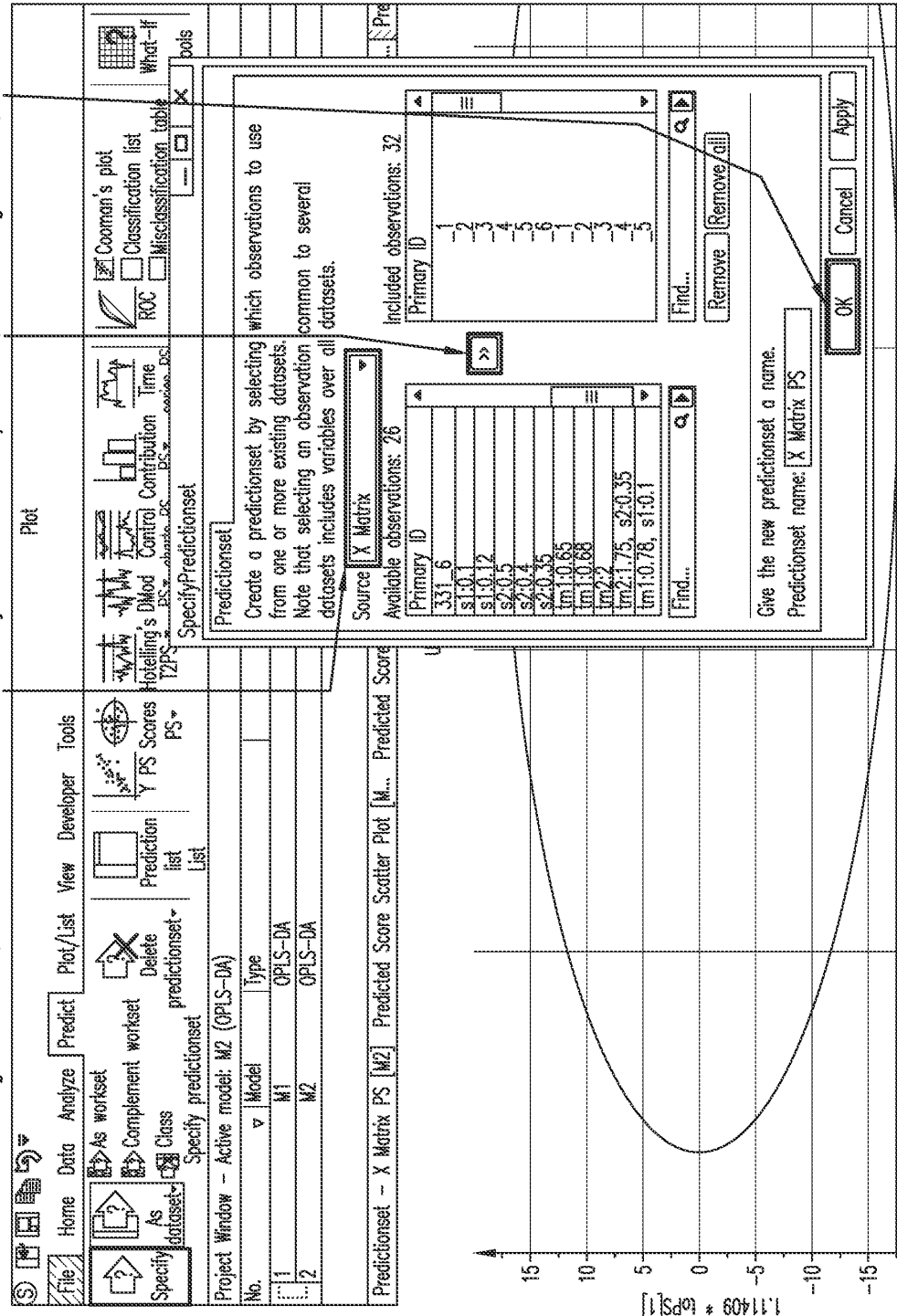
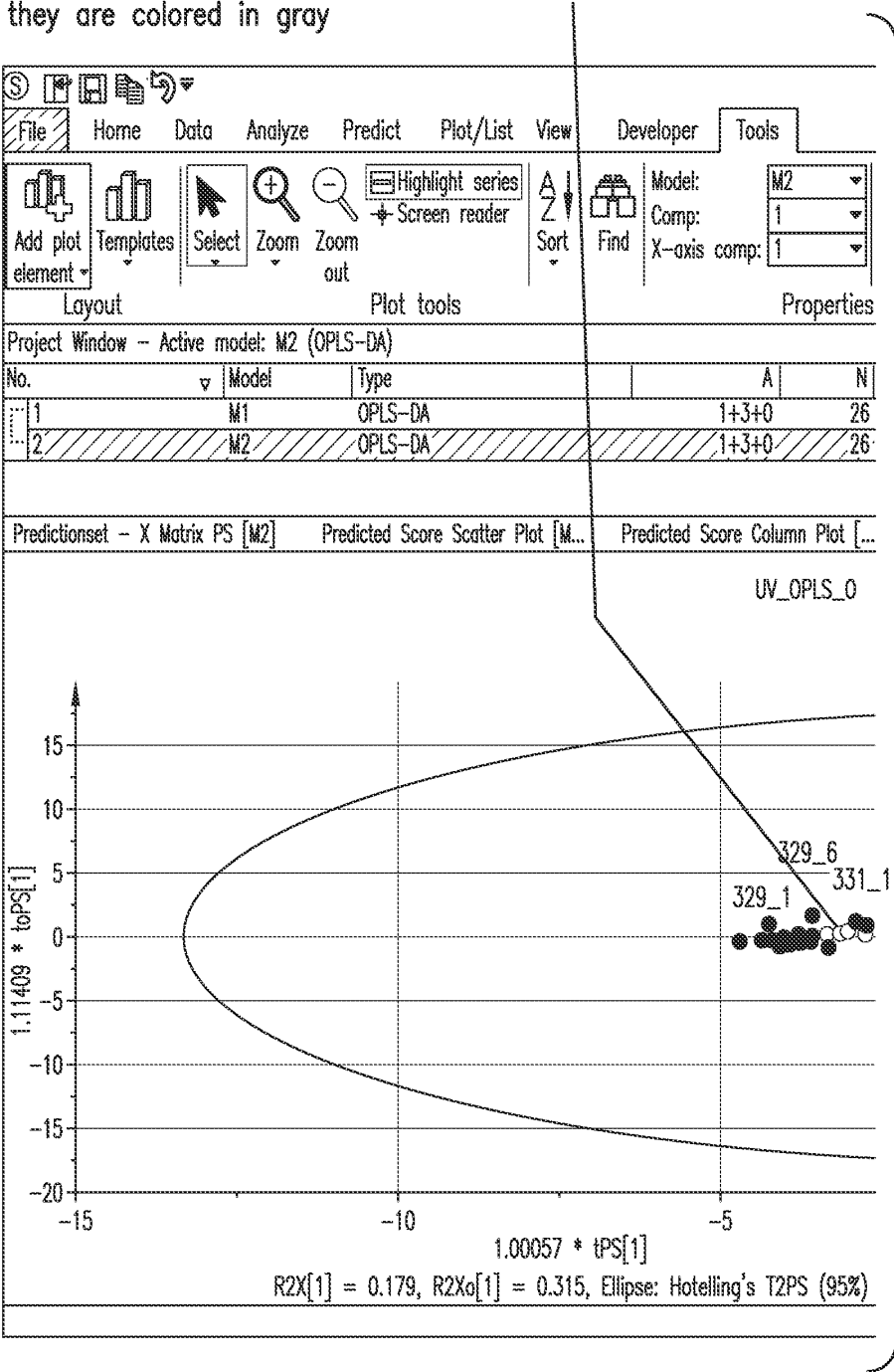


FIG.30

8. The predicted scores plot will now show the points from the regular scores plot. The data is colored based on good/bad categorization. Since the new predicted runs were not classified as good or bad, they are colored in gray



Cont. On
FIG.31-2

FIG.31-1

Cont.
From
FIG.31-1

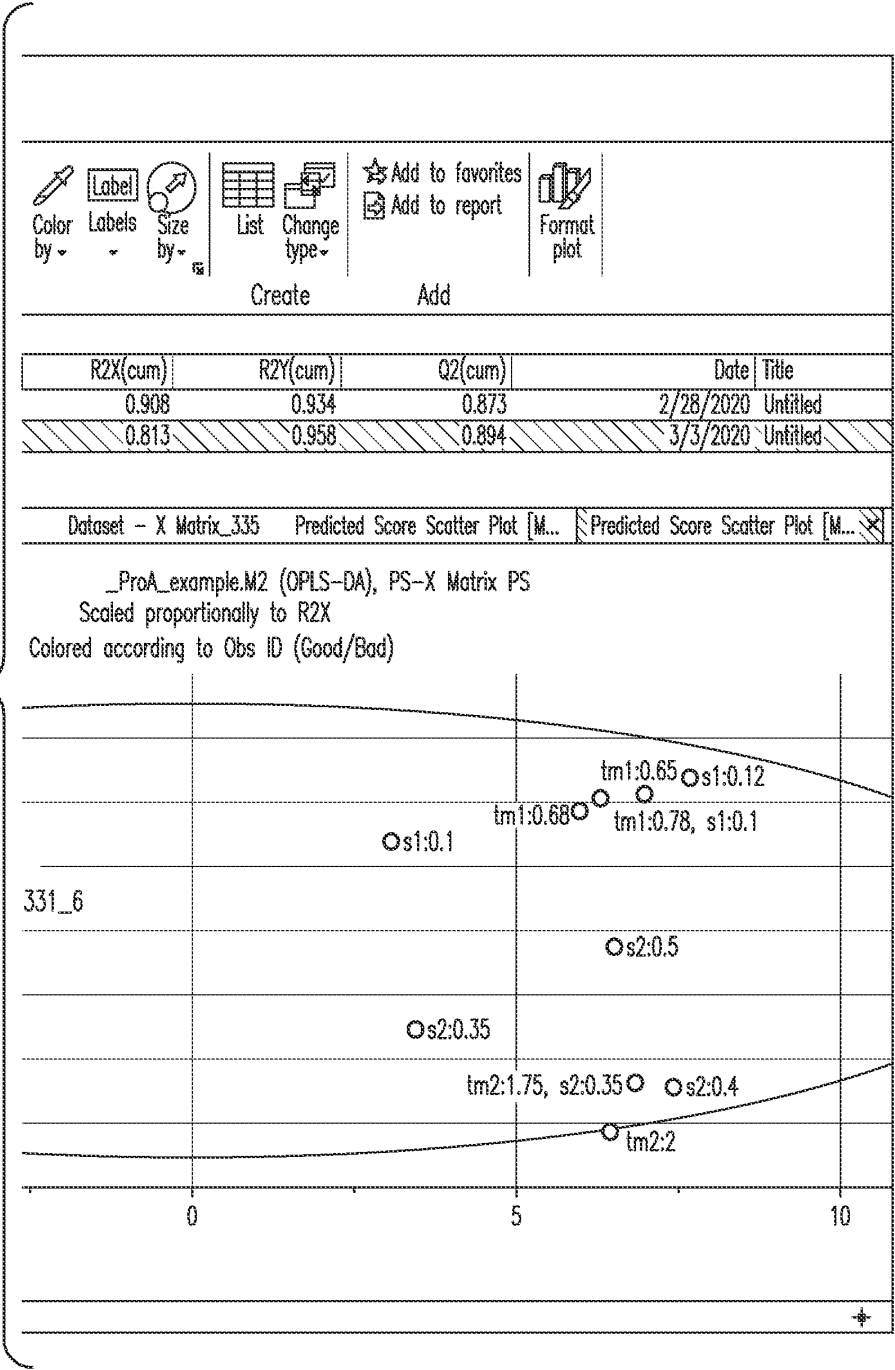
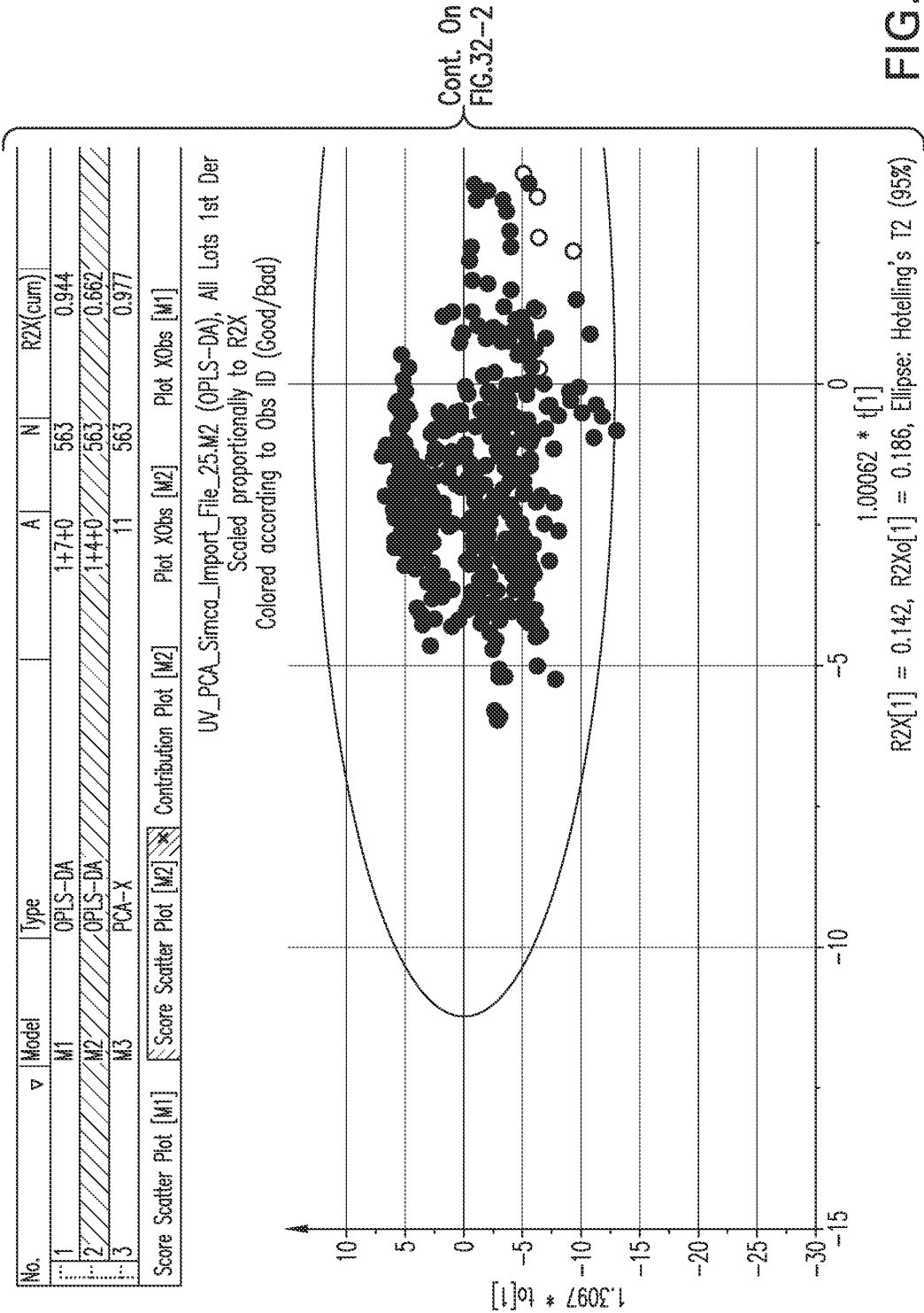
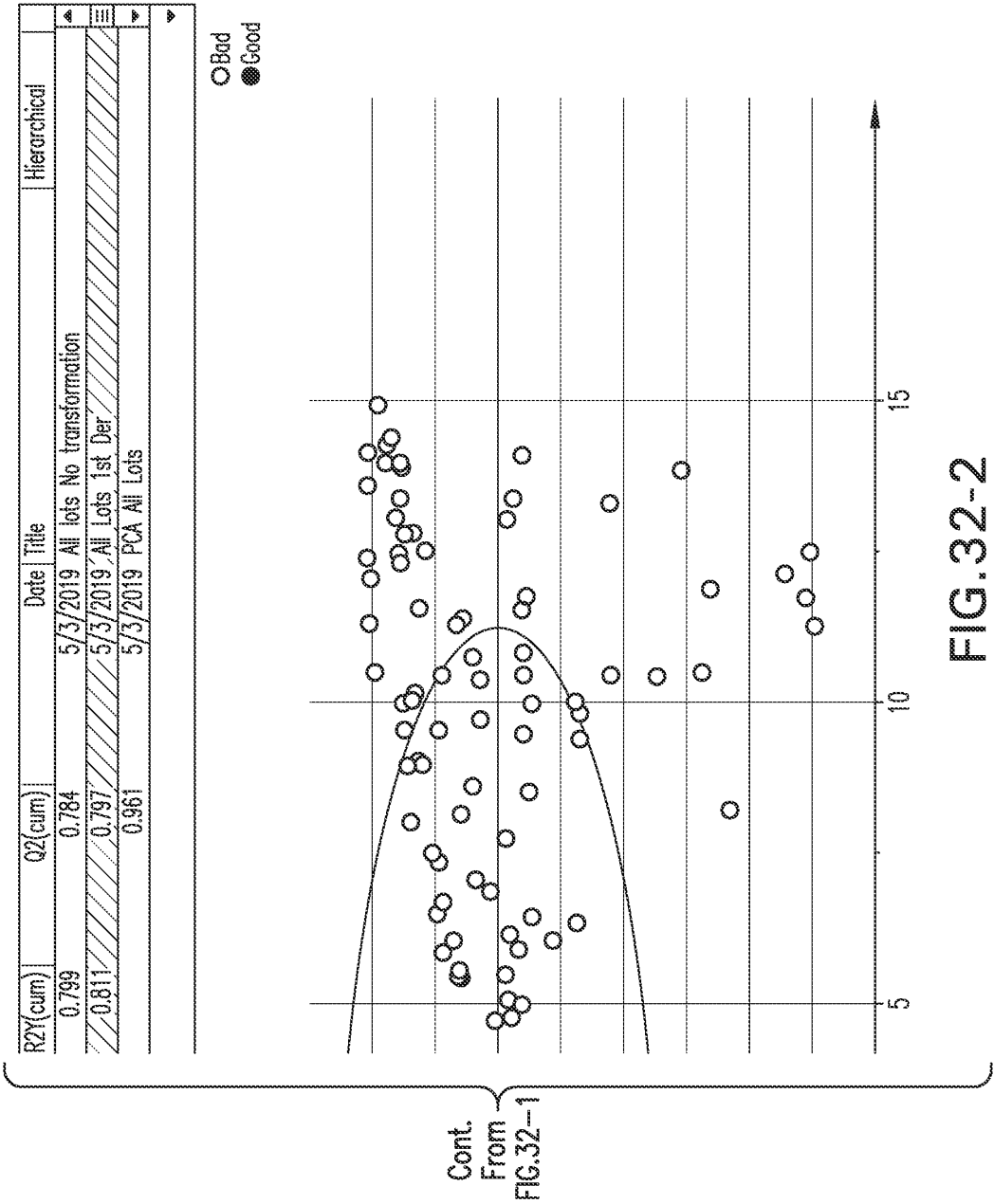


FIG.31-2





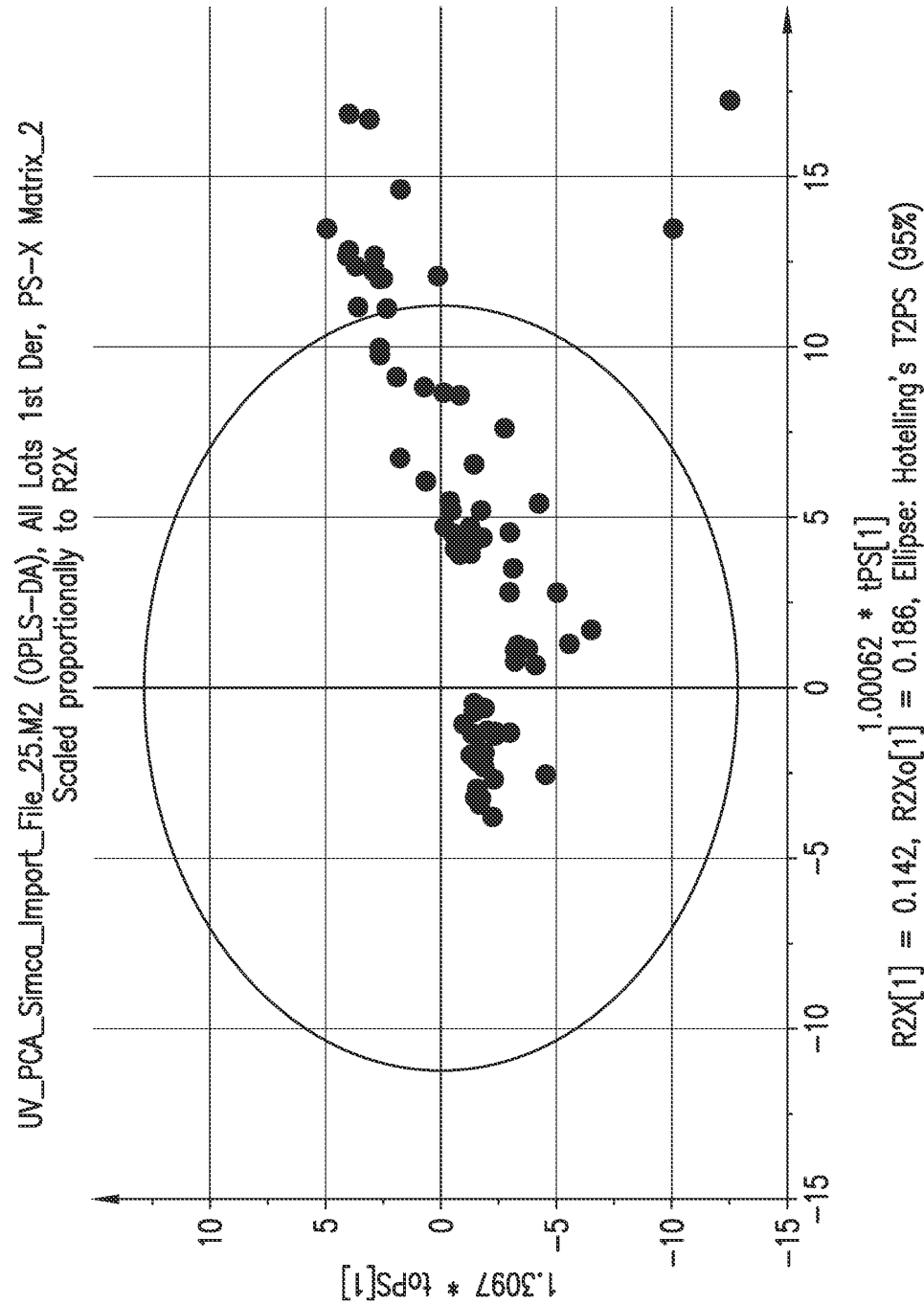


FIG.33

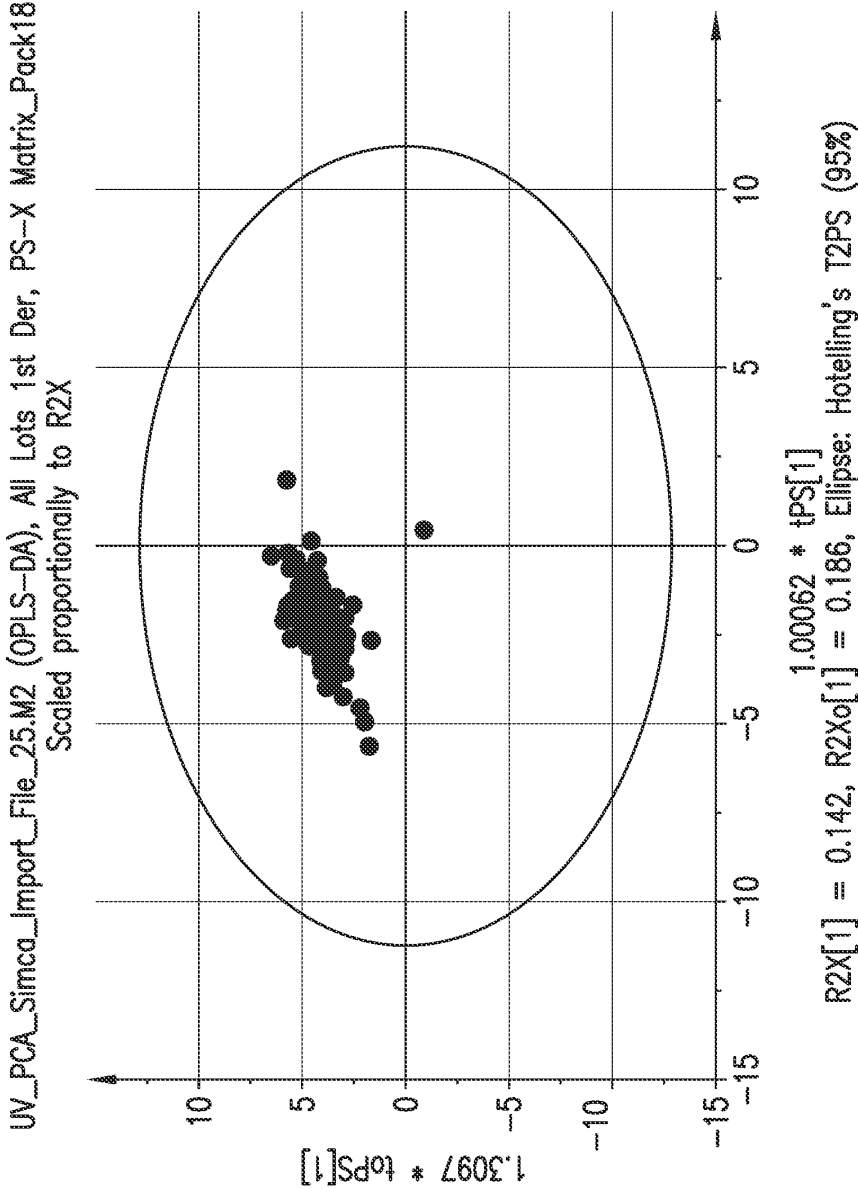


FIG.34

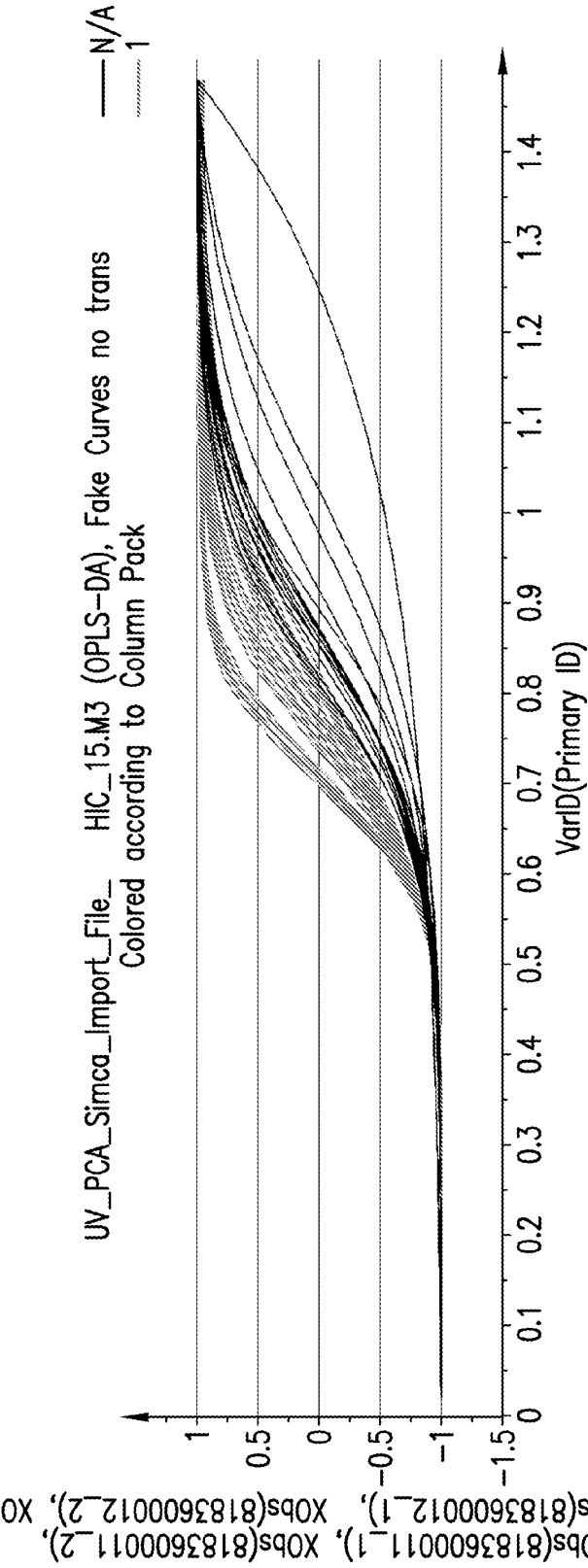
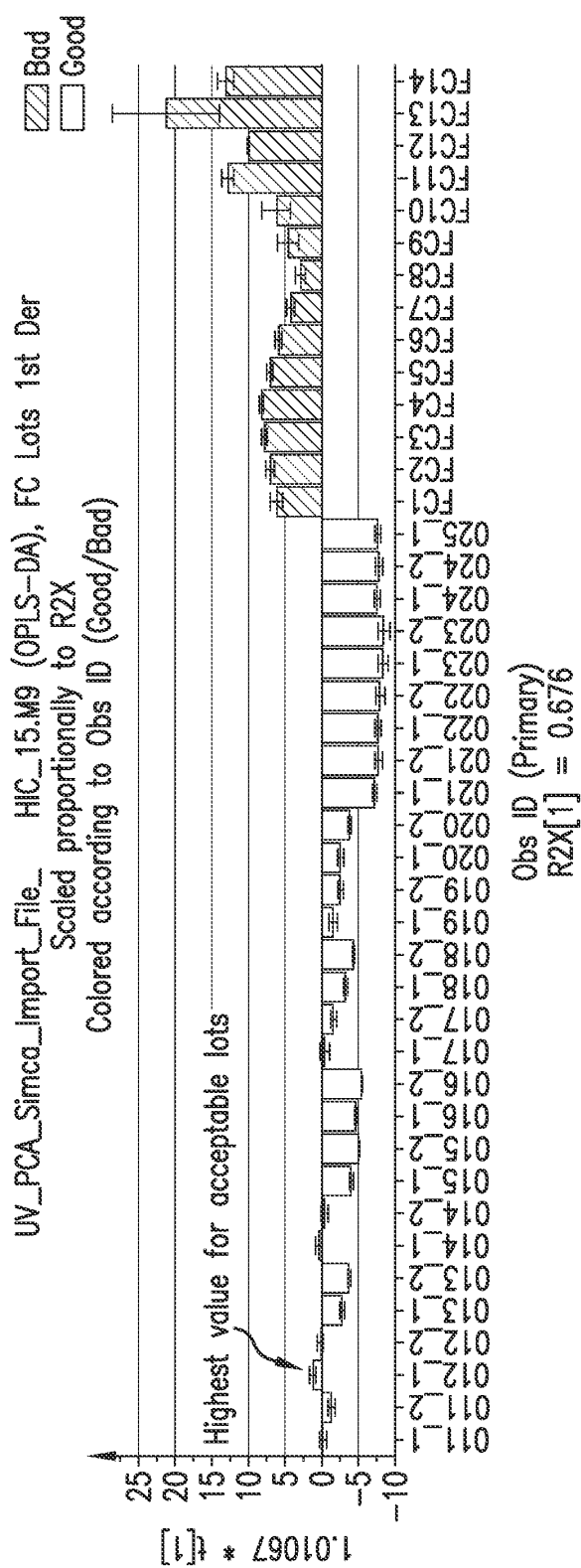


FIG.35



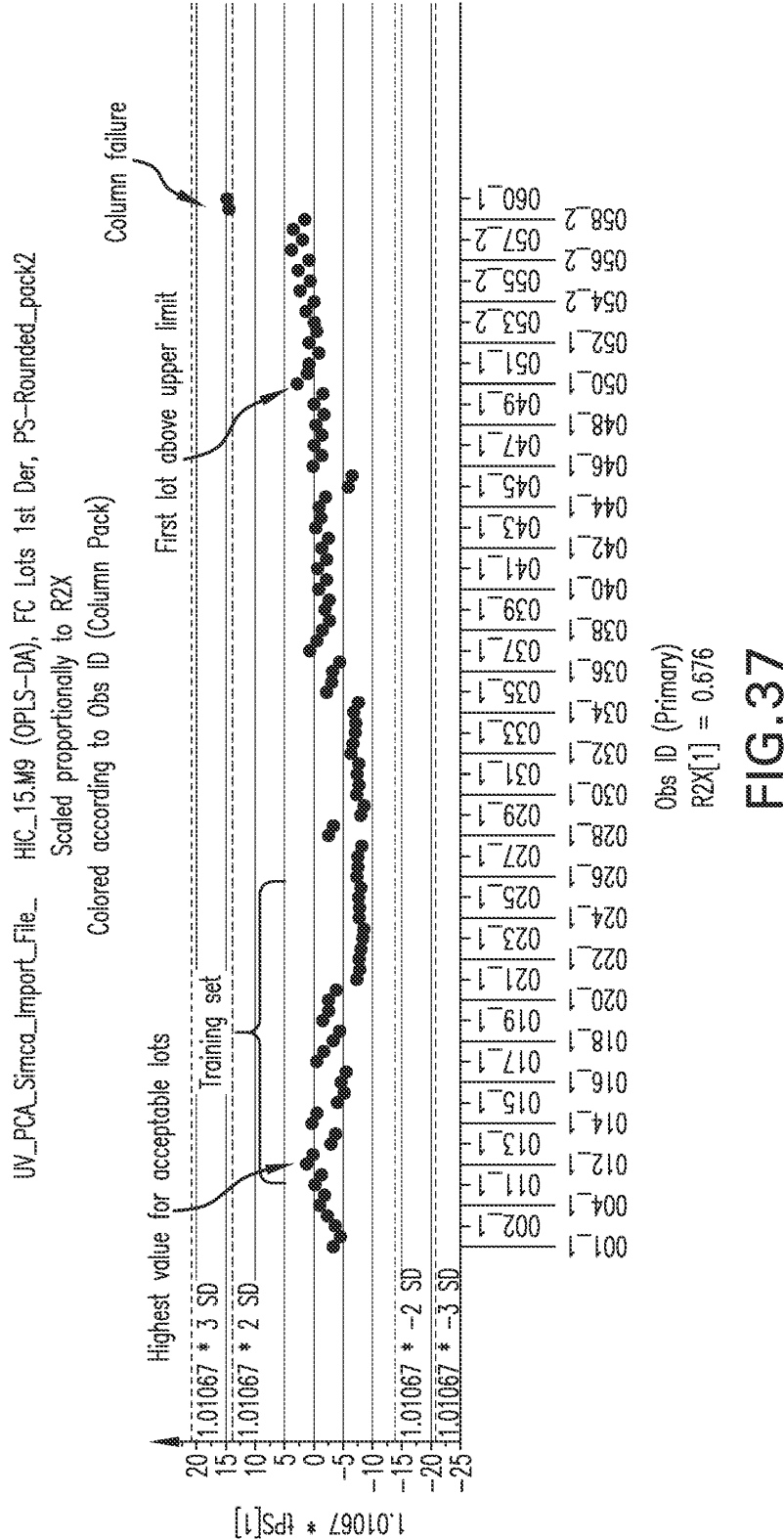
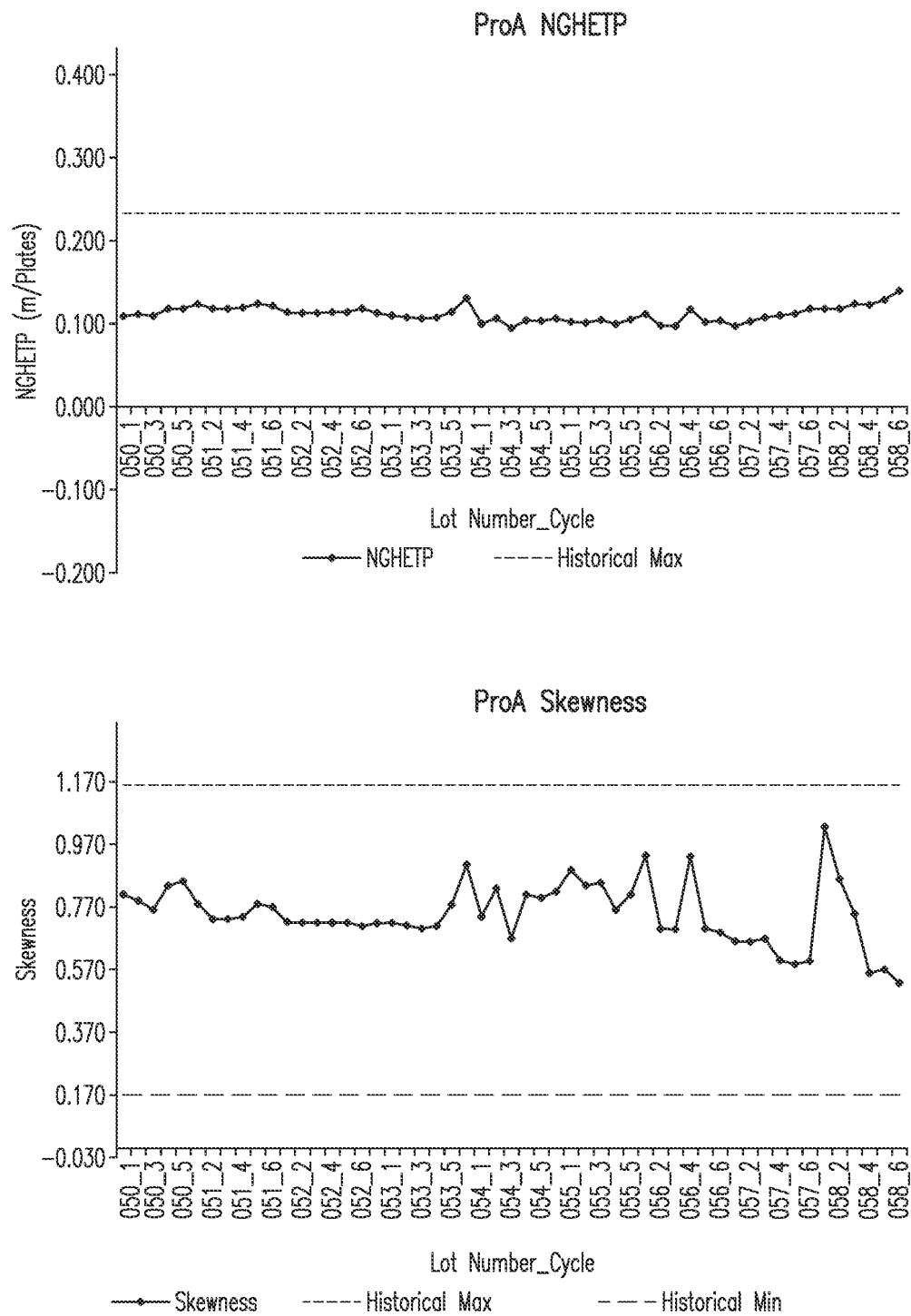
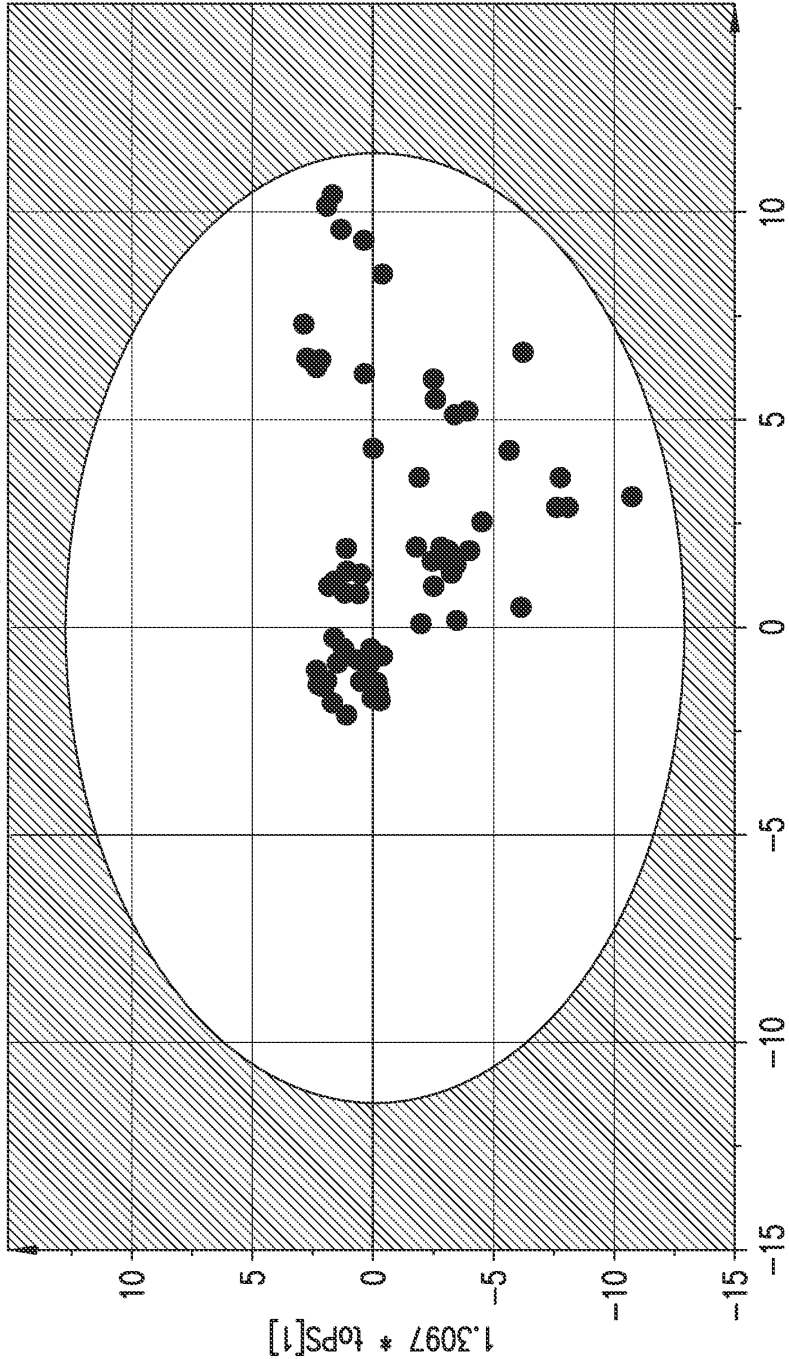


FIG.37

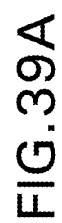


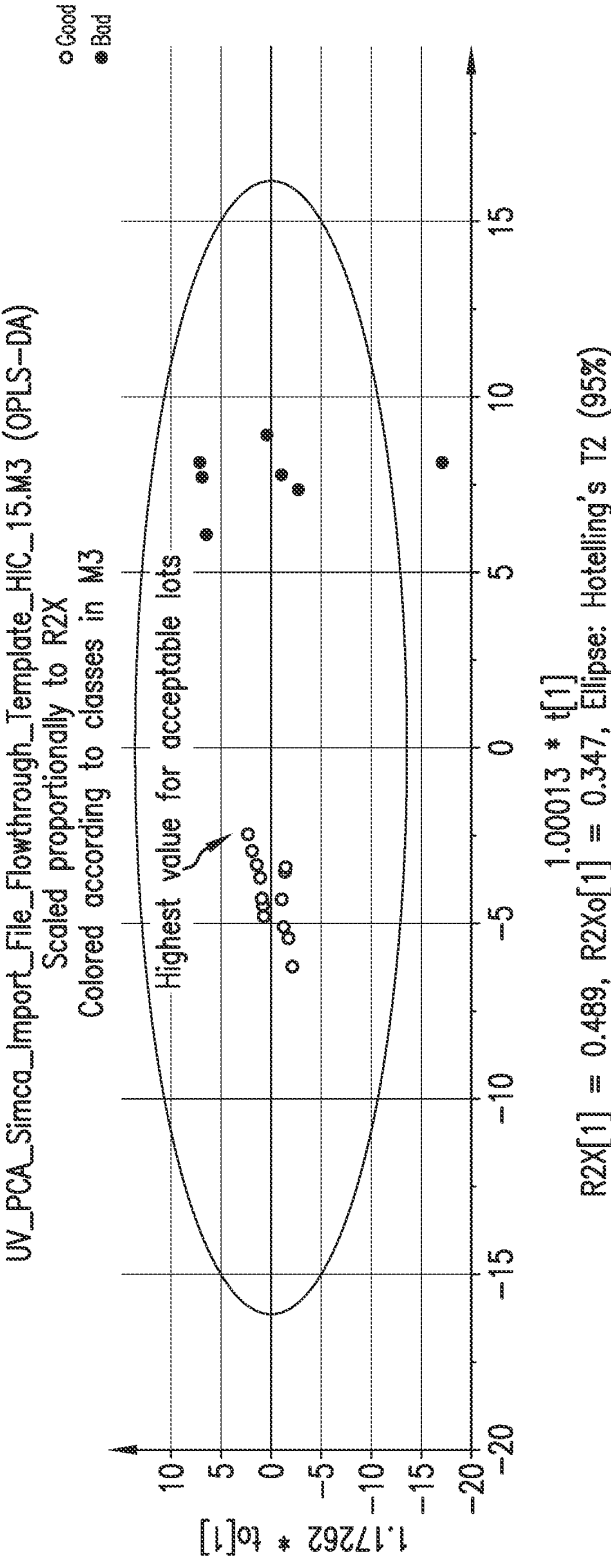
UV_PCA_Simca_Import_File_25.M2 (OPLS-DA), All Lots 1st Der, PS-X Matrix_Pack 11
Scaled proportionally to R2X



$R2X[1] = 0.142$, $R2Xo[1] = 0.186$, Ellipse: Hotelling's T2PS (95%)

FIG.38B





UV_PCA_Simca_Import_File_Flowthrough_Template_88_HIC_15.M3 (OPLS-DA), PS-Rounded_pack21
Scaled proportionally to R2X
Colored according to Obs ID (Column Pack)

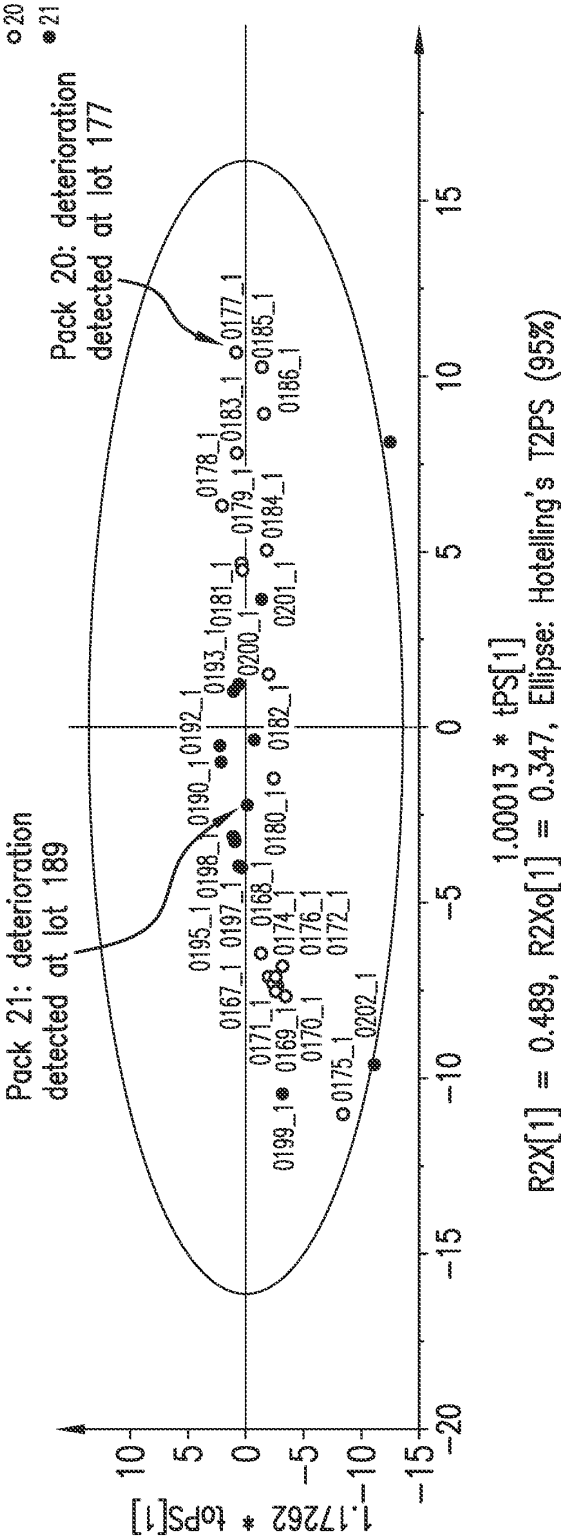


FIG.40

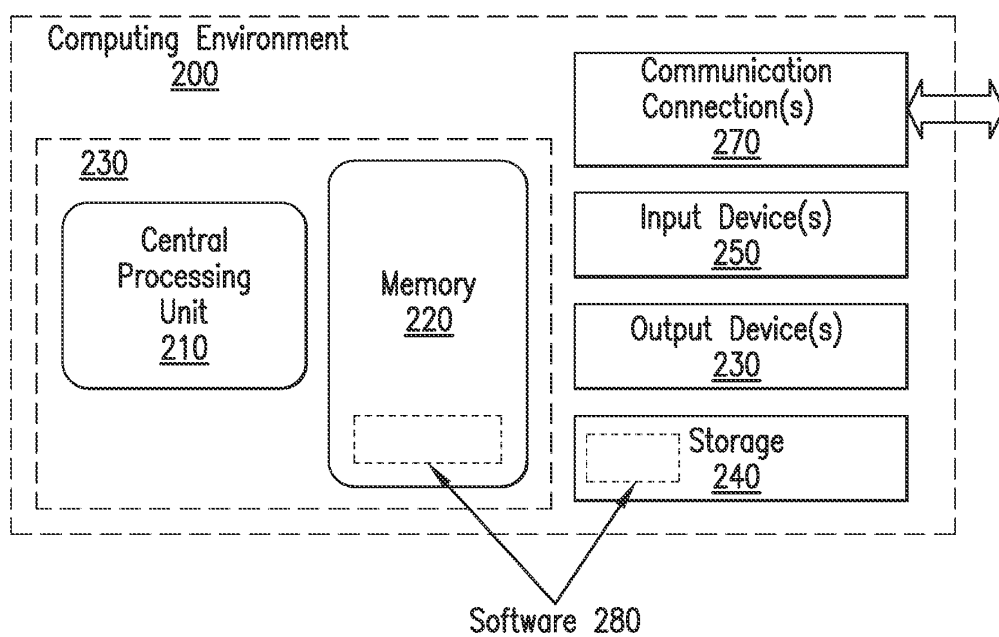


FIG.41