

Sample name: **M08**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-12007**  
Filename: **C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-12007\_M08\_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 8:30:07 AM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

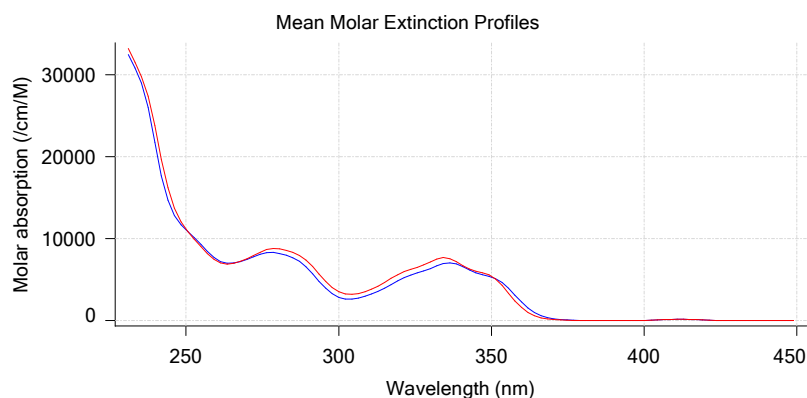
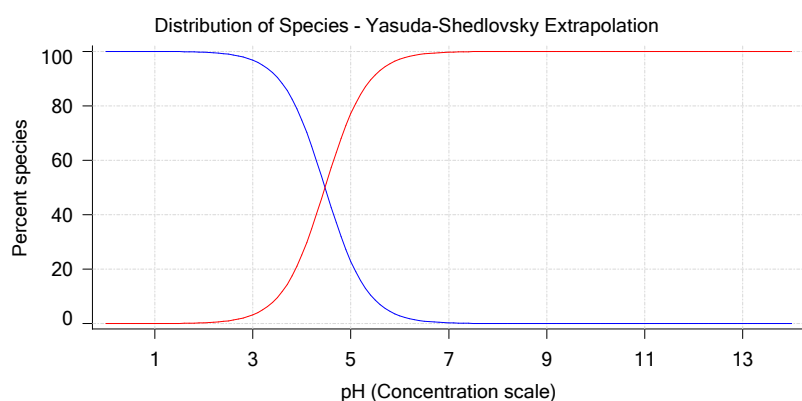
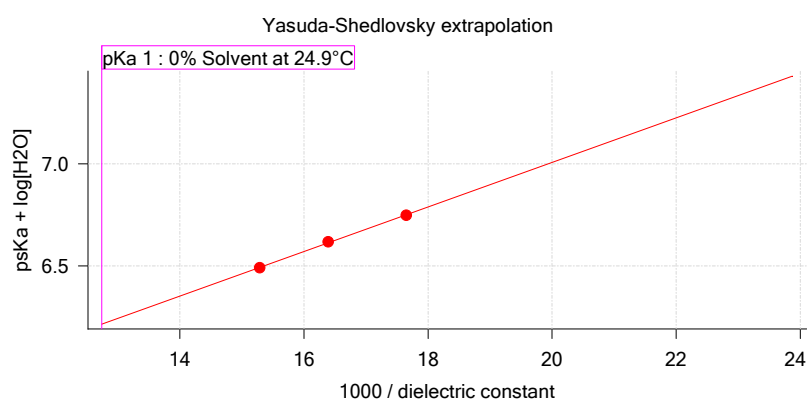
## Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R <sup>2</sup>	Ionic strength	Temperature
Yasuda-Shedlovsky	4.47	±0.01	4.83	109.0096	0.9988	0.165 M	24.9°C

## Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1
17J-12007 Points 4 to 40	49.39 %	Up	UV-metric pKa	56.7	24.7 M	0.157 M	24.9°C	✓ 5.35
17J-12007 Points 42 to 81	39.96 %	Up	UV-metric pKa	61.0	30.0 M	0.165 M	24.9°C	✓ 5.14
17J-12007 Points 83 to 122	30.30 %	Up	UV-metric pKa	65.4	35.7 M	0.172 M	24.9°C	✓ 4.94

## Graphs



## UV-metric psKa Titration 1 of 3 17J-12007 Points 4 to 40

## Results

pKa 1	<b>5.35</b>
RMSD	<b>0.019 0.014</b>
Chi squared	<b>0.0253</b>
PCA calculated number of pKas	<b>3</b>
Average ionic strength	<b>0.157 M</b>
Average temperature	<b>24.9°C</b>
Analyte concentration range	<b>67.2 µM to 63.3 µM</b>
Methanol weight %	<b>49.4 %</b>
Dielectric constant	<b>56.7</b>
Water concentration	<b>24.7 M</b>
Number of pKas source	<b>Predicted</b>
Wavelength clipping	<b>230.0 nm to 450.0 nm</b>

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## Results (continued)

pH clipping 1.477 to 12.526

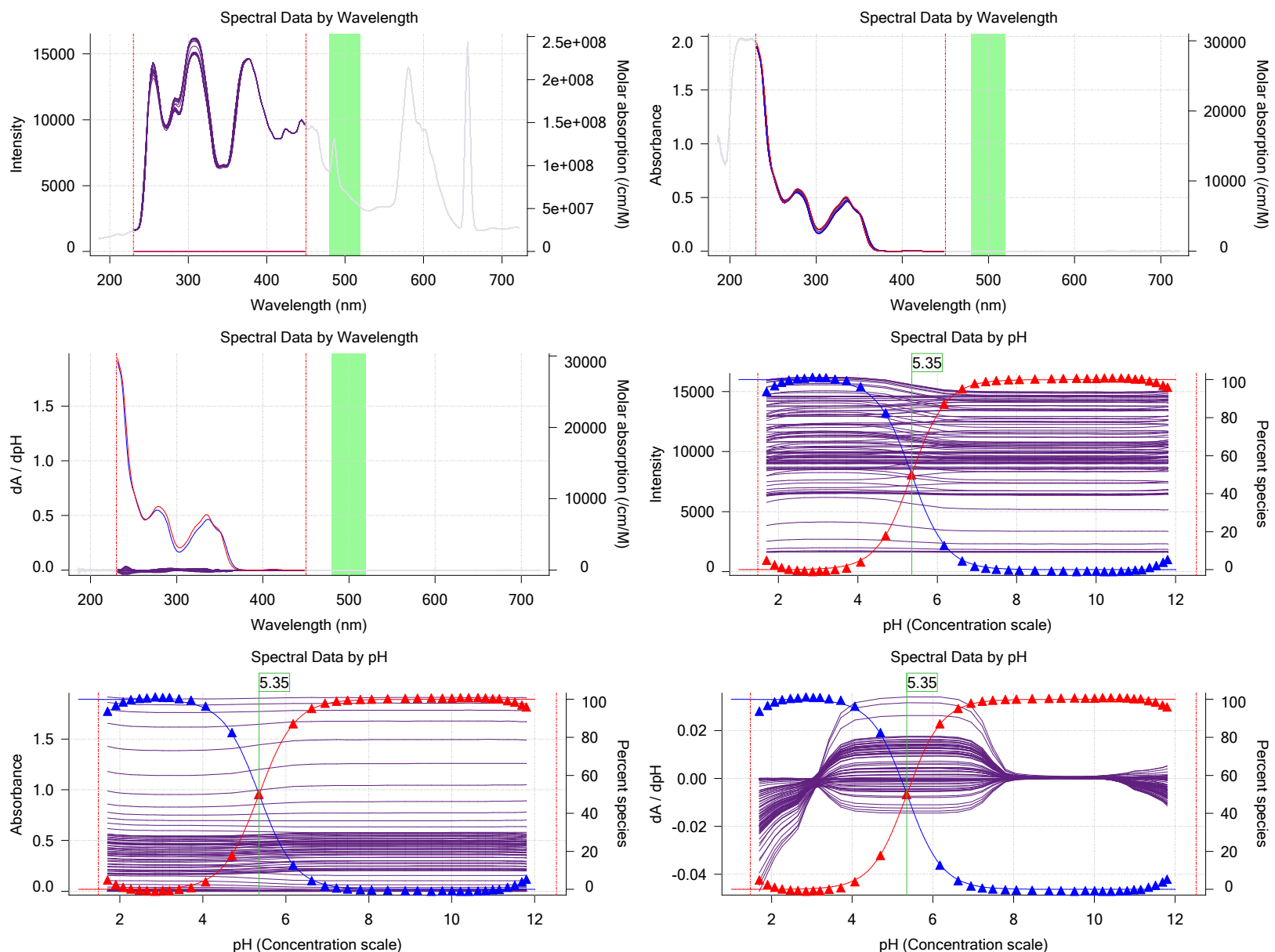
## Warnings and errors

Errors None  
 Warnings PCA calculation disagrees with predicted number of pKas

## Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
<b>Assay Medium</b>				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

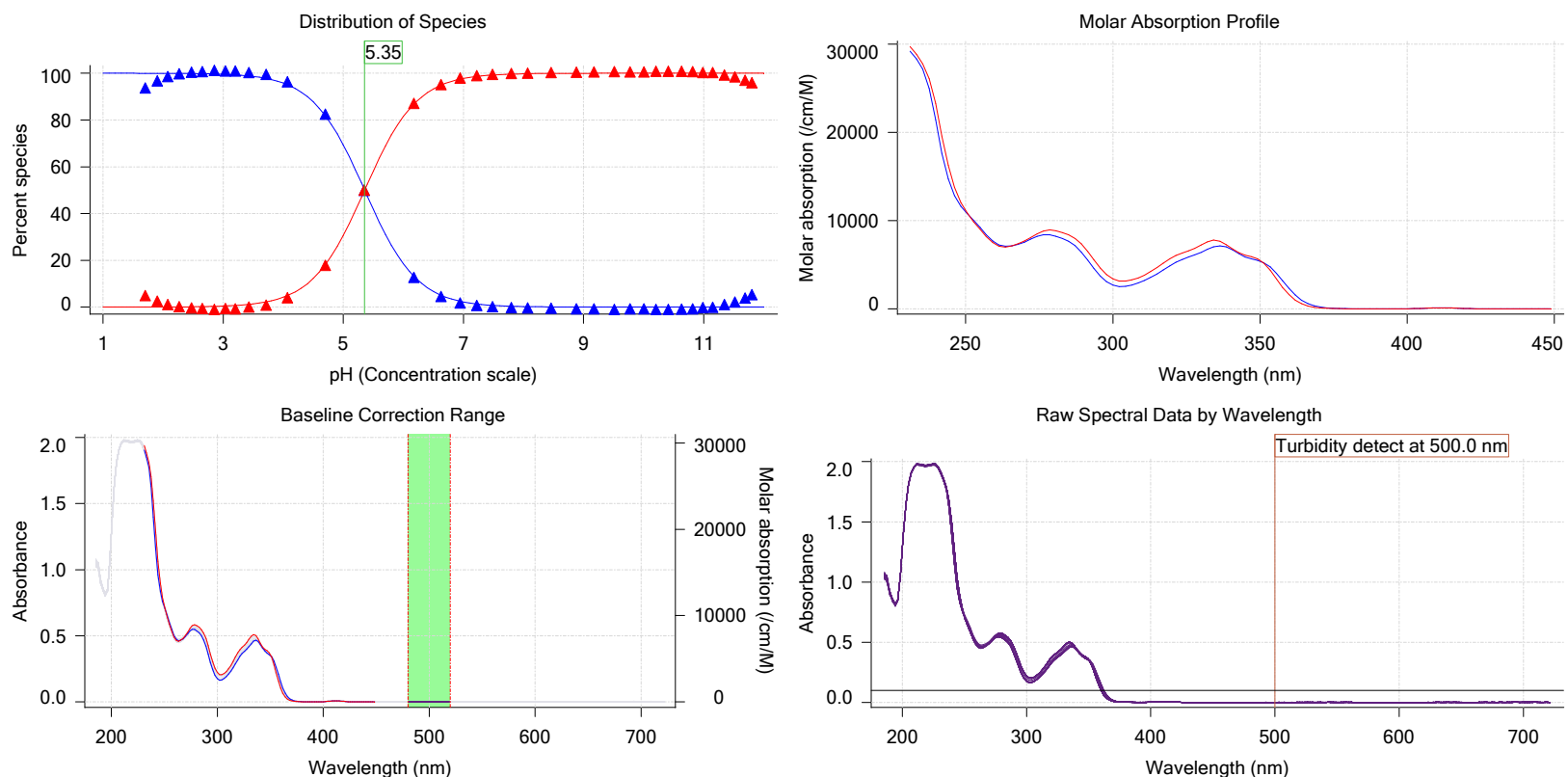
## Graphs



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## Graphs (continued)



## UV-metric psKa Titration 2 of 3 17J-12007 Points 42 to 81

### Results

pKa 1	<b>5.14</b>
RMSD	<b>0.013 0.010</b>
Chi squared	<b>0.0135</b>
PCA calculated number of pKas	<b>3</b>
Average ionic strength	<b>0.165 M</b>
Average temperature	<b>24.9°C</b>
Analyte concentration range	<b>55.2 µM to 52.3 µM</b>
Methanol weight %	<b>40.0 %</b>
Dielectric constant	<b>61.0</b>
Water concentration	<b>30.0 M</b>
Number of pKas source	<b>Predicted</b>
Wavelength clipping	<b>230.0 nm to 450.0 nm</b>
pH clipping	<b>1.505 to 12.517</b>

### Warnings and errors

Errors: None  
Warnings: PCA calculation disagrees with predicted number of pKas

### Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			

**Assay Medium**

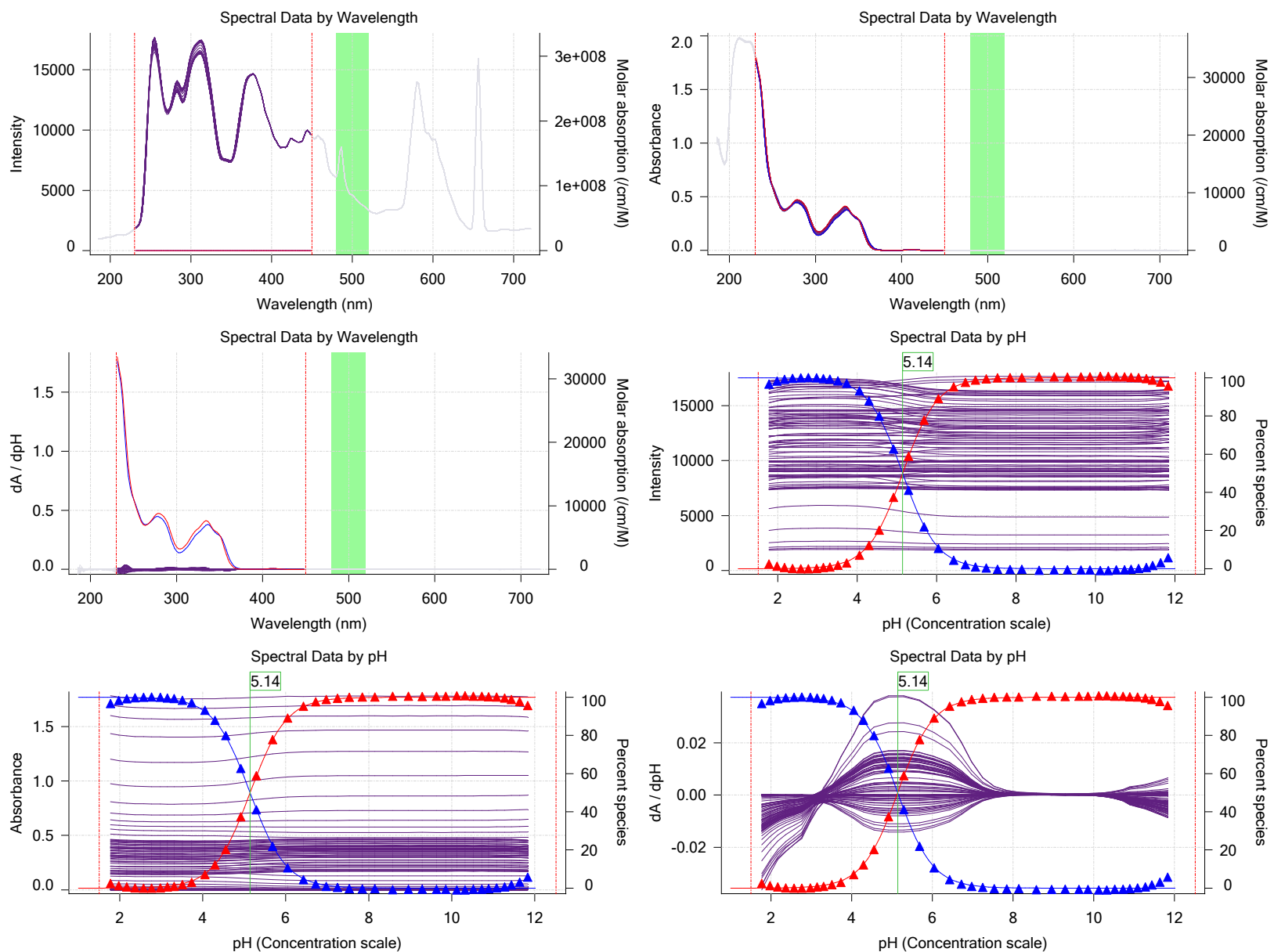
Sample name: **M08**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-12007**  
 Filename: **C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-12007\_M08\_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 8:30:07 AM**  
 Analyst: **Dorothy Leverse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

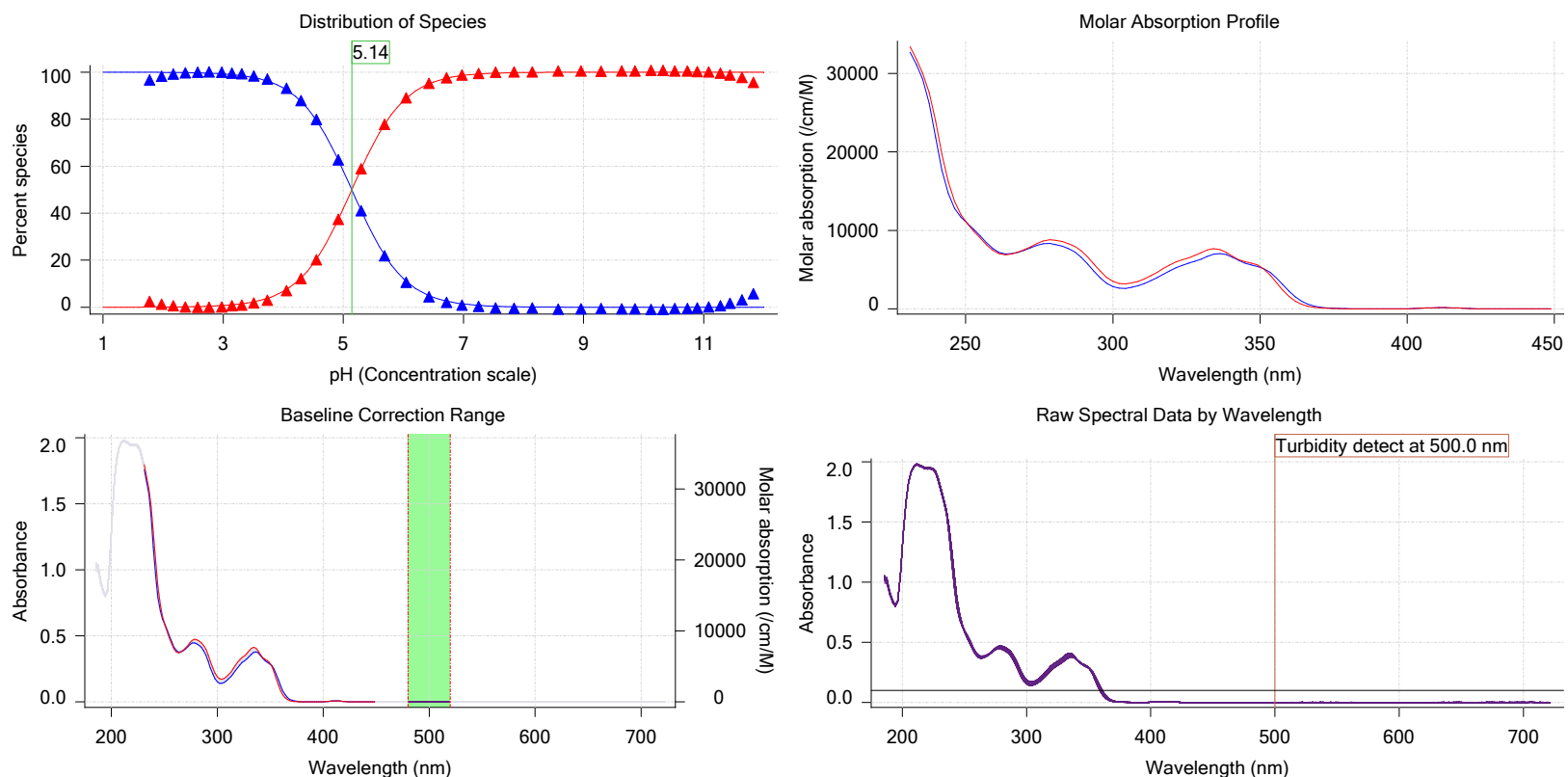
## Graphs



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## Graphs (continued)



## UV-metric psKa Titration 3 of 3 17J-12007 Points 83 to 122

### Results

pKa 1	<b>4.94</b>
RMSD	<b>0.012 0.009</b>
Chi squared	<b>0.0097</b>
PCA calculated number of pKas	<b>2</b>
Average ionic strength	<b>0.172 M</b>
Average temperature	<b>24.9°C</b>
Analyte concentration range	<b>42.7 µM to 40.5 µM</b>
Methanol weight %	<b>30.3 %</b>
Dielectric constant	<b>65.4</b>
Water concentration	<b>35.7 M</b>
Number of pKas source	<b>Predicted</b>
Wavelength clipping	<b>230.0 nm to 450.0 nm</b>
pH clipping	<b>1.510 to 12.518</b>

### Warnings and errors

Errors: None  
Warnings: PCA calculation disagrees with predicted number of pKas

### Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			

**Assay Medium**

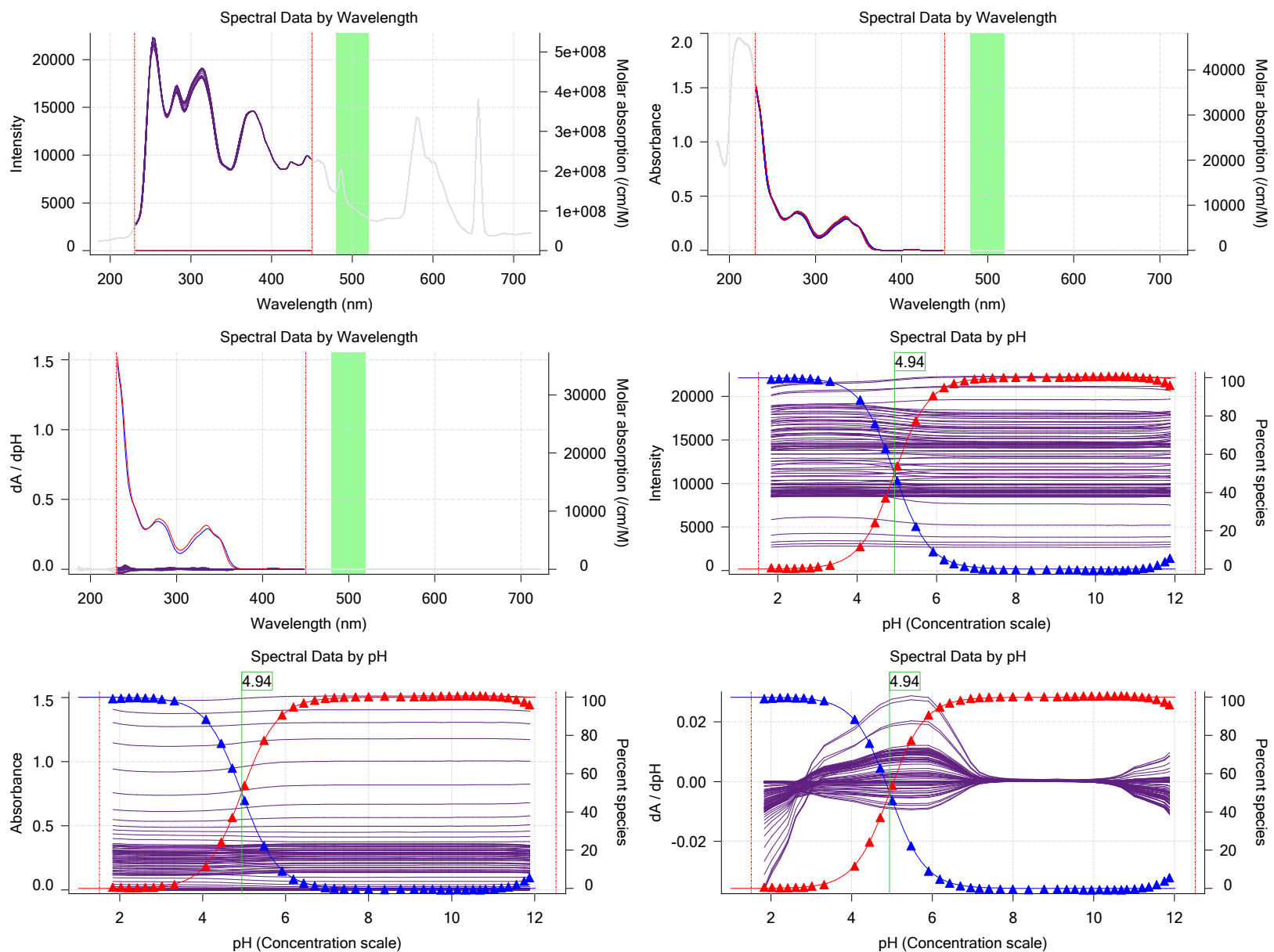
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Experiment start time: **10/12/2017 8:30:07 AM**  
 Analyst: **Dorothy Leverse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

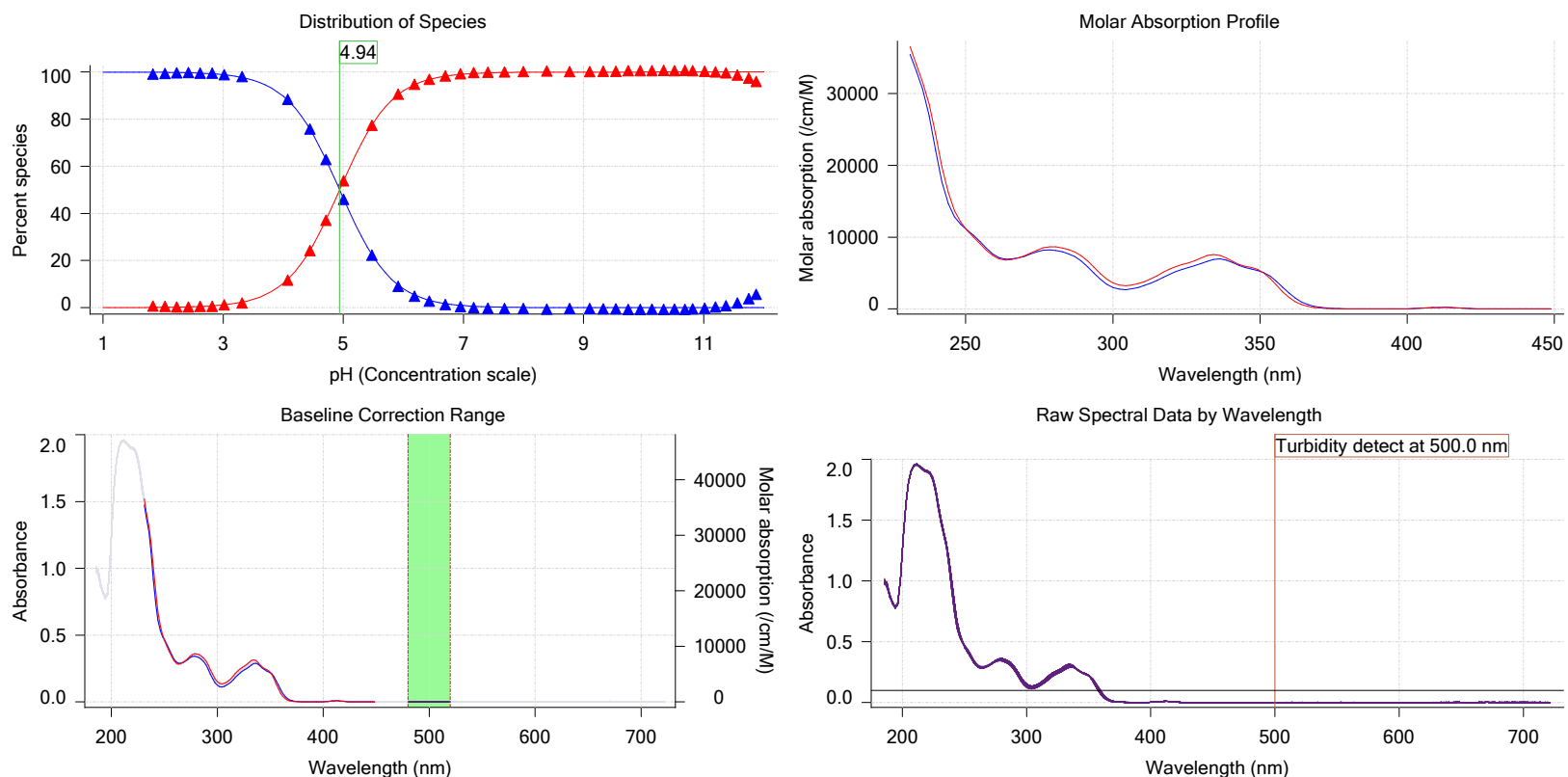
## Graphs



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## Graphs (continued)



## Assay Model

### Settings

	Value	Date/Time changed	Imported from
Sample name	M08	9/18/2017 4:04:04 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0030 mL	9/18/2017 4:04:04 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.035800 M	9/18/2017 4:04:04 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	287.74	9/18/2017 4:04:13 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	9/18/2017 4:04:04 PM	User entered value
Sample is a	Base	9/18/2017 4:04:04 PM	User entered value
pKa 1	5.60	9/18/2017 4:04:04 PM	User entered value
logp (XH +)	-10.00		Default value
logP (neutral X)	-10.00	9/18/2017 4:04:04 PM	User entered value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

## Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:32.6	Dark spectrum								
3:34.0	Reference spectrum								
4:01.6	Volume reset due to vial change								
4:45.9	Initial pH = 7.99								
5:47.5	Data point 4	0.34995 mL	0.06950 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.977	-0.00974	0.60896
6:16.2	Data point 5	0.34995 mL	0.06950 mL	0.02498 mL	1.15005 mL	0.02500 mL	2.177	-0.00914	0.50437



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## Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
6:33.1	Data point 6	0.34995 mL	0.06950 mL	0.03977 mL	1.15005 mL	0.02500 mL	2.353	0.02421	0.83190	0.00
6:49.9	Data point 7	0.34995 mL	0.06950 mL	0.04962 mL	1.15005 mL	0.02500 mL	2.541	0.00917	0.73227	0.00
7:06.6	Data point 8	0.34995 mL	0.06950 mL	0.05611 mL	1.15005 mL	0.02500 mL	2.744	0.00821	0.84755	0.00
7:23.3	Data point 9	0.34995 mL	0.06950 mL	0.06021 mL	1.15005 mL	0.02500 mL	2.927	0.00554	0.62504	0.00
7:39.9	Data point 10	0.34995 mL	0.06950 mL	0.06289 mL	1.15005 mL	0.02500 mL	3.127	0.00608	0.72006	0.00
7:56.5	Data point 11	0.34995 mL	0.06950 mL	0.06458 mL	1.15005 mL	0.02500 mL	3.306	0.00827	0.77810	0.00
8:13.1	Data point 12	0.34995 mL	0.06950 mL	0.06571 mL	1.15005 mL	0.02500 mL	3.471	0.01551	0.88775	0.00
8:55.4	Data point 13	0.34995 mL	0.06950 mL	0.06740 mL	1.15005 mL	0.02500 mL	3.697	0.01953	0.93429	0.00
9:22.2	Data point 14	0.34995 mL	0.06950 mL	0.06806 mL	1.15005 mL	0.02500 mL	3.984	0.04410	0.99252	0.00
9:43.9	Data point 15	0.34995 mL	0.06950 mL	0.06851 mL	1.15005 mL	0.02500 mL	4.334	0.09174	0.97975	0.00
10:10.4	Data point 16	0.34995 mL	0.06950 mL	0.06889 mL	1.15005 mL	0.02500 mL	4.966	0.10038	0.99340	0.00
10:57.8	Data point 17	0.34995 mL	0.06950 mL	0.06912 mL	1.15005 mL	0.02500 mL	5.609	0.10029	0.99033	0.00
11:51.6	Data point 18	0.34995 mL	0.06950 mL	0.06931 mL	1.15005 mL	0.02500 mL	6.430	0.09896	0.99489	0.00
12:54.4	Data point 19	0.34995 mL	0.06950 mL	0.06945 mL	1.15005 mL	0.02500 mL	6.880	0.09871	0.98042	0.00
13:49.6	Data point 20	0.34995 mL	0.06950 mL	0.06957 mL	1.15005 mL	0.02500 mL	7.194	0.09992	0.99035	0.00
14:33.4	Data point 21	0.34995 mL	0.06950 mL	0.06968 mL	1.15005 mL	0.02500 mL	7.473	0.09410	0.98933	0.00
15:19.2	Data point 22	0.34995 mL	0.06950 mL	0.06980 mL	1.15005 mL	0.02500 mL	7.734	0.09911	0.98142	0.00
16:06.3	Data point 23	0.34995 mL	0.06950 mL	0.06994 mL	1.15005 mL	0.02500 mL	8.042	0.09928	0.99433	0.00
16:54.8	Data point 24	0.34995 mL	0.06950 mL	0.07006 mL	1.15005 mL	0.02500 mL	8.315	0.09735	0.98368	0.00
17:43.6	Data point 25	0.34995 mL	0.06950 mL	0.07018 mL	1.15005 mL	0.02500 mL	8.700	0.09932	0.98707	0.00
18:34.0	Data point 26	0.34995 mL	0.06950 mL	0.07027 mL	1.15005 mL	0.02500 mL	9.120	0.10023	0.98171	0.00
19:19.8	Data point 27	0.34995 mL	0.06950 mL	0.07034 mL	1.15005 mL	0.02500 mL	9.415	0.09982	0.98326	0.00
20:01.1	Data point 28	0.34995 mL	0.06950 mL	0.07044 mL	1.15005 mL	0.02500 mL	9.747	0.09799	0.98124	0.00
20:38.0	Data point 29	0.34995 mL	0.06950 mL	0.07056 mL	1.15005 mL	0.02500 mL	10.010	0.09525	0.96007	0.00
21:05.6	Data point 30	0.34995 mL	0.06950 mL	0.07072 mL	1.15005 mL	0.02500 mL	10.239	0.06173	0.97972	0.00
21:32.4	Data point 31	0.34995 mL	0.06950 mL	0.07091 mL	1.15005 mL	0.02500 mL	10.440	0.00858	0.32312	0.00
22:04.5	Data point 32	0.34995 mL	0.06950 mL	0.07126 mL	1.15005 mL	0.02500 mL	10.641	0.01018	0.77178	0.00
22:21.1	Data point 33	0.34995 mL	0.06950 mL	0.07185 mL	1.15005 mL	0.02500 mL	10.863	0.00030	0.00308	0.00
22:37.6	Data point 34	0.34995 mL	0.06950 mL	0.07284 mL	1.15005 mL	0.02500 mL	11.045	-0.00449	0.43776	0.00
22:54.2	Data point 35	0.34995 mL	0.06950 mL	0.07432 mL	1.15005 mL	0.02500 mL	11.216	-0.00380	0.37667	0.00
23:10.8	Data point 36	0.34995 mL	0.06950 mL	0.07651 mL	1.15005 mL	0.02500 mL	11.377	-0.00500	0.55655	0.00
23:37.7	Data point 37	0.34995 mL	0.06950 mL	0.08006 mL	1.15005 mL	0.02500 mL	11.572	-0.00990	0.89357	0.00
23:54.5	Data point 38	0.34995 mL	0.06950 mL	0.08500 mL	1.15005 mL	0.02500 mL	11.745	-0.00458	0.52634	0.00
24:11.3	Data point 39	0.34995 mL	0.06950 mL	0.09238 mL	1.15005 mL	0.02500 mL	11.914	-0.00163	0.10296	0.00
24:33.1	Data point 40	0.34995 mL	0.06950 mL	0.09946 mL	1.15005 mL	0.02500 mL	12.026	-0.00301	0.39342	0.00
26:14.4	Reference spectrum									
27:18.3	Data point 42	0.50000 mL	0.16752 mL	0.09948 mL	1.15005 mL	0.02500 mL	2.005	-0.05171	0.95209	0.00
27:45.7	Data point 43	0.50000 mL	0.16752 mL	0.12422 mL	1.15005 mL	0.02500 mL	2.206	0.00539	0.29011	0.00
28:02.8	Data point 44	0.50000 mL	0.16752 mL	0.13923 mL	1.15005 mL	0.02500 mL	2.397	0.01379	0.49730	0.00
28:19.6	Data point 45	0.50000 mL	0.16752 mL	0.14892 mL	1.15005 mL	0.02500 mL	2.596	-0.00581	0.24227	0.00
28:36.3	Data point 46	0.50000 mL	0.16752 mL	0.15517 mL	1.15005 mL	0.02500 mL	2.802	0.01880	0.91929	0.00
28:53.0	Data point 47	0.50000 mL	0.16752 mL	0.15906 mL	1.15005 mL	0.02500 mL	2.994	0.00758	0.66893	0.00
29:09.6	Data point 48	0.50000 mL	0.16752 mL	0.16155 mL	1.15005 mL	0.02500 mL	3.200	0.01459	0.92117	0.00
29:26.2	Data point 49	0.50000 mL	0.16752 mL	0.16310 mL	1.15005 mL	0.02500 mL	3.371	0.01149	0.84149	0.00
29:42.7	Data point 50	0.50000 mL	0.16752 mL	0.16414 mL	1.15005 mL	0.02500 mL	3.532	0.01125	0.84711	0.00
30:19.8	Data point 51	0.50000 mL	0.16752 mL	0.16550 mL	1.15005 mL	0.02500 mL	3.733	0.02421	0.95772	0.00
30:46.5	Data point 52	0.50000 mL	0.16752 mL	0.16604 mL	1.15005 mL	0.02500 mL	3.957	0.04312	0.99454	0.00
31:08.2	Data point 53	0.50000 mL	0.16752 mL	0.16644 mL	1.15005 mL	0.02500 mL	4.274	0.09518	0.98765	0.00
31:29.9	Data point 54	0.50000 mL	0.16752 mL	0.16670 mL	1.15005 mL	0.02500 mL	4.517	0.09933	0.99277	0.00
32:07.4	Data point 55	0.50000 mL	0.16752 mL	0.16691 mL	1.15005 mL	0.02500 mL	4.771	0.09942	0.98816	0.00
32:44.1	Data point 56	0.50000 mL	0.16752 mL	0.16707 mL	1.15005 mL	0.02500 mL	5.132	0.10038	0.98546	0.00
33:28.9	Data point 57	0.50000 mL	0.16752 mL	0.16719 mL	1.15005 mL	0.02500 mL	5.510	0.10074	0.98949	0.00
34:20.5	Data point 58	0.50000 mL	0.16752 mL	0.16729 mL	1.15005 mL	0.02500 mL	5.898	0.10043	0.99250	0.00
35:11.2	Data point 59	0.50000 mL	0.16752 mL	0.16738 mL	1.15005 mL	0.02500 mL	6.256	0.10003	0.99113	0.00
35:59.8	Data point 60	0.50000 mL	0.16752 mL	0.16747 mL	1.15005 mL	0.02500 mL	6.638	0.10028	0.99177	0.00
36:43.4	Data point 61	0.50000 mL	0.16752 mL	0.16757 mL	1.15005 mL	0.02500 mL	6.931	0.09794	0.99089	0.00
37:25.1	Data point 62	0.50000 mL	0.16752 mL	0.16766 mL	1.15005 mL	0.02500 mL	7.184	0.09644	0.97850	0.00



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## Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH Slope
38:05.9	Data point 63	0.50000 mL	0.16752 mL	0.16778 mL	1.15005 mL	0.02500 mL	7.458	0.09853	0.98756	0.98756
38:45.5	Data point 64	0.50000 mL	0.16752 mL	0.16790 mL	1.15005 mL	0.02500 mL	7.741	0.09872	0.99122	0.99122
39:31.6	Data point 65	0.50000 mL	0.16752 mL	0.16802 mL	1.15005 mL	0.02500 mL	8.051	0.10043	0.99272	0.99272
40:14.0	Data point 66	0.50000 mL	0.16752 mL	0.16811 mL	1.15005 mL	0.02500 mL	8.350	0.10051	0.99018	0.99018
41:00.9	Data point 67	0.50000 mL	0.16752 mL	0.16820 mL	1.15005 mL	0.02500 mL	8.779	0.09564	0.94964	0.94964
41:46.2	Data point 68	0.50000 mL	0.16752 mL	0.16827 mL	1.15005 mL	0.02500 mL	9.160	0.09702	0.94871	0.94871
42:26.8	Data point 69	0.50000 mL	0.16752 mL	0.16834 mL	1.15005 mL	0.02500 mL	9.491	0.09616	0.97233	0.97233
42:57.5	Data point 70	0.50000 mL	0.16752 mL	0.16844 mL	1.15005 mL	0.02500 mL	9.831	0.09949	0.98899	0.98899
43:26.8	Data point 71	0.50000 mL	0.16752 mL	0.16858 mL	1.15005 mL	0.02500 mL	10.055	0.05723	0.95111	0.95111
43:43.4	Data point 72	0.50000 mL	0.16752 mL	0.16879 mL	1.15005 mL	0.02500 mL	10.318	0.02228	0.94122	0.94122
44:15.2	Data point 73	0.50000 mL	0.16752 mL	0.16926 mL	1.15005 mL	0.02500 mL	10.519	0.00778	0.56822	0.56822
44:47.2	Data point 74	0.50000 mL	0.16752 mL	0.16992 mL	1.15005 mL	0.02500 mL	10.715	-0.00398	0.31978	0.31978
45:03.8	Data point 75	0.50000 mL	0.16752 mL	0.17088 mL	1.15005 mL	0.02500 mL	10.922	-0.00433	0.40062	0.40062
45:20.4	Data point 76	0.50000 mL	0.16752 mL	0.17241 mL	1.15005 mL	0.02500 mL	11.085	-0.00711	0.63968	0.63968
45:52.4	Data point 77	0.50000 mL	0.16752 mL	0.17521 mL	1.15005 mL	0.02500 mL	11.277	-0.00969	0.78162	0.78162
46:19.2	Data point 78	0.50000 mL	0.16752 mL	0.17898 mL	1.15005 mL	0.02500 mL	11.468	-0.01032	0.90550	0.90550
46:36.0	Data point 79	0.50000 mL	0.16752 mL	0.18431 mL	1.15005 mL	0.02500 mL	11.629	-0.00927	0.87301	0.87301
47:08.3	Data point 80	0.50000 mL	0.16752 mL	0.19396 mL	1.15005 mL	0.02500 mL	11.826	-0.00860	0.90611	0.90611
47:35.5	Data point 81	0.50000 mL	0.16752 mL	0.20884 mL	1.15005 mL	0.02500 mL	12.017	-0.00861	0.78230	0.78230
49:20.3	Reference spectrum									
50:43.6	Data point 83	0.83996 mL	0.28667 mL	0.20887 mL	1.15005 mL	0.02500 mL	2.010	-0.03102	0.95396	0.95396
51:11.2	Data point 84	0.83996 mL	0.28667 mL	0.23638 mL	1.15005 mL	0.02500 mL	2.206	0.00086	0.01098	0.01098
51:28.1	Data point 85	0.83996 mL	0.28667 mL	0.25362 mL	1.15005 mL	0.02500 mL	2.401	-0.01382	0.65994	0.65994
51:44.8	Data point 86	0.83996 mL	0.28667 mL	0.26475 mL	1.15005 mL	0.02500 mL	2.594	0.01229	0.54767	0.54767
52:01.6	Data point 87	0.83996 mL	0.28667 mL	0.27185 mL	1.15005 mL	0.02500 mL	2.789	-0.01384	0.75962	0.75962
52:18.3	Data point 88	0.83996 mL	0.28667 mL	0.27646 mL	1.15005 mL	0.02500 mL	2.990	-0.00611	0.37595	0.37595
52:34.9	Data point 89	0.83996 mL	0.28667 mL	0.27935 mL	1.15005 mL	0.02500 mL	3.188	-0.00491	0.41196	0.41196
53:07.3	Data point 90	0.83996 mL	0.28667 mL	0.28119 mL	1.15005 mL	0.02500 mL	3.489	0.00417	0.38585	0.38585
53:34.4	Data point 91	0.83996 mL	0.28667 mL	0.28544 mL	1.15005 mL	0.02500 mL	4.247	-0.06878	0.73295	0.73295
53:57.6	Data point 92	0.83996 mL	0.28667 mL	0.28577 mL	1.15005 mL	0.02500 mL	4.615	0.04083	0.92144	0.92144
54:24.4	Data point 93	0.83996 mL	0.28667 mL	0.28596 mL	1.15005 mL	0.02500 mL	4.878	0.09100	0.97504	0.97504
54:57.7	Data point 94	0.83996 mL	0.28667 mL	0.28608 mL	1.15005 mL	0.02500 mL	5.173	0.10020	0.98128	0.98128
55:29.4	Data point 95	0.83996 mL	0.28667 mL	0.28617 mL	1.15005 mL	0.02500 mL	5.641	0.09882	0.98891	0.98891
56:06.1	Data point 96	0.83996 mL	0.28667 mL	0.28626 mL	1.15005 mL	0.02500 mL	6.075	0.04946	0.28506	0.28506
56:27.5	Data point 97	0.83996 mL	0.28667 mL	0.28634 mL	1.15005 mL	0.02500 mL	6.349	0.01850	0.51003	0.51003
56:44.1	Data point 98	0.83996 mL	0.28667 mL	0.28641 mL	1.15005 mL	0.02500 mL	6.595	-0.04396	0.81816	0.81816
57:10.9	Data point 99	0.83996 mL	0.28667 mL	0.28650 mL	1.15005 mL	0.02500 mL	6.860	0.00660	0.11299	0.11299
57:37.6	Data point 100	0.83996 mL	0.28667 mL	0.28662 mL	1.15005 mL	0.02500 mL	7.111	0.05213	0.87545	0.87545
58:04.3	Data point 101	0.83996 mL	0.28667 mL	0.28671 mL	1.15005 mL	0.02500 mL	7.332	0.08389	0.86552	0.86552
58:31.6	Data point 102	0.83996 mL	0.28667 mL	0.28681 mL	1.15005 mL	0.02500 mL	7.565	0.09350	0.93779	0.93779
59:04.9	Data point 103	0.83996 mL	0.28667 mL	0.28690 mL	1.15005 mL	0.02500 mL	7.841	0.09680	0.97474	0.97474
59:45.7	Data point 104	0.83996 mL	0.28667 mL	0.28699 mL	1.15005 mL	0.02500 mL	8.154	0.09599	0.96613	0.96613
1:00:27.9	Data point 105	0.83996 mL	0.28667 mL	0.28709 mL	1.15005 mL	0.02500 mL	8.543	0.09144	0.95818	0.95818
1:01:14.1	Data point 106	0.83996 mL	0.28667 mL	0.28718 mL	1.15005 mL	0.02500 mL	8.926	0.09863	0.95717	0.95717
1:01:53.0	Data point 107	0.83996 mL	0.28667 mL	0.28728 mL	1.15005 mL	0.02500 mL	9.254	0.09772	0.94341	0.94341
1:02:22.7	Data point 108	0.83996 mL	0.28667 mL	0.28737 mL	1.15005 mL	0.02500 mL	9.482	0.09700	0.97120	0.97120
1:02:47.3	Data point 109	0.83996 mL	0.28667 mL	0.28749 mL	1.15005 mL	0.02500 mL	9.691	0.07359	0.97477	0.97477
1:03:13.9	Data point 110	0.83996 mL	0.28667 mL	0.28768 mL	1.15005 mL	0.02500 mL	9.898	0.03650	0.91460	0.91460
1:03:45.8	Data point 111	0.83996 mL	0.28667 mL	0.28796 mL	1.15005 mL	0.02500 mL	10.096	0.01218	0.34428	0.34428
1:04:17.8	Data point 112	0.83996 mL	0.28667 mL	0.28838 mL	1.15005 mL	0.02500 mL	10.292	0.00853	0.52708	0.52708
1:04:34.4	Data point 113	0.83996 mL	0.28667 mL	0.28895 mL	1.15005 mL	0.02500 mL	10.486	-0.01347	0.88275	0.88275
1:04:51.1	Data point 114	0.83996 mL	0.28667 mL	0.28982 mL	1.15005 mL	0.02500 mL	10.664	-0.01683	0.93432	0.93432
1:05:07.8	Data point 115	0.83996 mL	0.28667 mL	0.29111 mL	1.15005 mL	0.02500 mL	10.836	-0.02001	0.91540	0.91540
1:05:24.4	Data point 116	0.83996 mL	0.28667 mL	0.29302 mL	1.15005 mL	0.02500 mL	10.968	-0.01821	0.93113	0.93113
1:05:51.2	Data point 117	0.83996 mL	0.28667 mL	0.29567 mL	1.15005 mL	0.02500 mL	11.164	-0.01535	0.93498	0.93498
1:06:08.0	Data point 118	0.83996 mL	0.28667 mL	0.29967 mL	1.15005 mL	0.02500 mL	11.346	-0.02336	0.94126	0.94126
1:06:24.8	Data point 119	0.83996 mL	0.28667 mL	0.30574 mL	1.15005 mL	0.02500 mL	11.516	-0.02063	0.93921	0.93921

Sample name: **M08**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-12007**  
 Filename: **C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-12007\_M08\_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 8:30:07 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
1:06:52.0	Data point 120	0.83996 mL	0.28667 mL	0.31609 mL	1.15005 mL	0.02500 mL	11.708	-0.01536	0.86229	0.0008
1:07:19.4	Data point 121	0.83996 mL	0.28667 mL	0.33274 mL	1.15005 mL	0.02500 mL	11.896	-0.01676	0.91130	0.0008
1:07:41.4	Data point 122	0.83996 mL	0.28667 mL	0.34828 mL	1.15005 mL	0.02500 mL	12.018	-0.01851	0.92904	0.0009
1:09:41.0	Assay volumes	1.08996 mL	0.42653 mL	0.34828 mL	1.15005 mL	0.02500 mL				

## Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
<b>General Settings</b>				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
<b>Standard Experiment Settings</b>				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
<b>Advanced General Settings</b>				
Detect turbidity using	Spectrometer			
Monitor at a wavelength of	500.0 nm			
Absorbance threshold of	0.100			
Collect turbidity sensor data	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	15%			
<b>Titration Pre-Dose</b>				
Titration pre-dose	None			
<b>Assay Medium</b>				
Cosolvent in use	Yes			
Cosolvent type	Methanol			
Cosolvent volume	1.15 mL			
Cosolvent added	Automatic			
ISA water volume	0.35 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	15%			
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			
After medium addition, stir for	5 seconds			
<b>Sample Sonication</b>				
Sonicate	No			
<b>Sample Dissolution</b>				
Perform a dissolution stage	No			
<b>Carbonate purge</b>				
Perform a carbonate purge	No			
<b>Temperature Control</b>				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
<b>Titration 1</b>				
Titrate from	Low to high pH			
Adjust to start pH	Yes			

Sample name: **M08**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-12007**  
 Filename: **C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-12007\_M08\_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 8:30:07 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
After pH adjust stir for	10 seconds			
<b>Titration 2</b>				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.15 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
<b>Titration 3</b>				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.34 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
<b>Data Point Stability</b>				
Stir during data point collection	Yes			
For point collection, stir at	15%			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00500 dpH/dt			
Stability timeout after	60 seconds			
<b>Experiment cleanup</b>				
Adjust pH to cleanup	To start pH			
And then stir for	60 seconds			
For cleaning, stir at	20%			
Then add water volume	0.25 mL			
And then stir for	30 seconds			

## Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.109	10/12/2017 8:30:07 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus S	1.0007	10/12/2017 8:30:07 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jH	0.3	10/12/2017 8:30:07 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jOH	-0.2	10/12/2017 8:30:07 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Base concentration factor	1.011	10/12/2017 8:30:07 AM	C:\Sirius_T3\KOH17122.t3r
Acid concentration factor	0.995	10/12/2017 8:30:07 AM	C:\Sirius_T3\17J-11005_Blank standardisation.t3r

## Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T311053		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1100253	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	10-10-2017	10/10/2017 10:48:53 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	166940 and 172875	10/6/2017 2:55:40 PM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9-22-17	9/22/2017 4:02:42 PM

Sample name: **M08**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-12007**  
Filename: **C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-12007\_M08\_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 8:30:07 AM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

## Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	9-26-17	10/5/2017 5:02:03 PM
Port B	Cyclohexane		9/19/2017 2:15:02 PM
Port C	MeCN (50%, 0.15 M KCl)	10-2-17	10/2/2017 11:28:55 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titration	Phosphate Buffer		10/10/2017 9:57:33 AM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titration	Octanol	9-14-17	9/14/2017 10:30:38 AM
Titration		T3TM1100153	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 10:21:54 AM
E0 calibration	-8.34 mV		10/12/2017 8:30:31 AM
Filling solution	3M KCl	KCL095	10/10/2017 9:58:43 AM
Liquids			
Wash 1	50% IPA:50% Water		10/11/2017 8:31:15 AM
Wash 2	0.5% Triton X-100 in H2O		10/11/2017 8:31:17 AM
Buffer position 1	pH7 Wash		10/11/2017 8:31:21 AM
Buffer position 2	pH 7		10/11/2017 8:31:23 AM
Storage position			10/11/2017 8:31:26 AM
Wash water	4.3e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	5.7e+003 mL		10/6/2017 3:04:33 PM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	419:28:33		11/23/2010 12:22:28 PM
Calibrated on	10/11/2017 8:30:19 AM		
Integration time	10		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		



## Assay Settings

Sample name: **M08**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-12007**  
Filename: **C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-12007\_M08\_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 8:30:07 AM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

### Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

### Refinement Settings

Setting	Value	Default value
Turbidity detection method	Spectrometer	Spectrometer
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00
Exclude turbid points	Yes	Yes
Low intensity warning threshold	100	100
Minimum absorbance change threshold	0.100	0.100
Eigenvector autocorrelation threshold	0.80	0.80
Maximum RMSD severe warning	0.250	0.250
Maximum RMSD warning	0.050	0.050

### Tray Information

Title  
Location D1