

Sample name: **M01**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-06011**  
Filename: **C:\Sirius\_T3\17J-06011\_M01\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 1:41:57 PM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

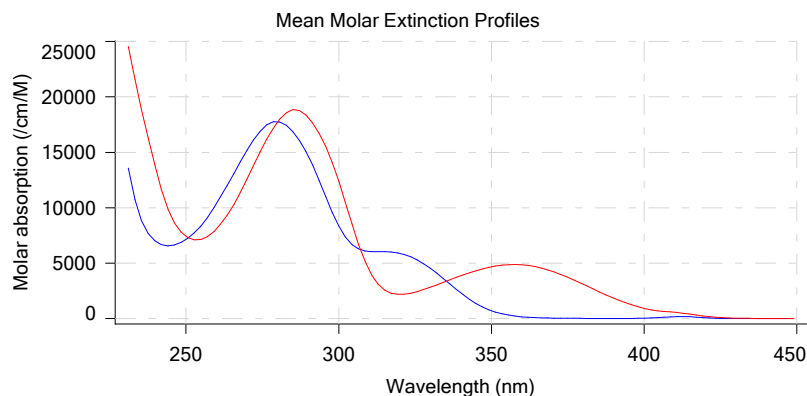
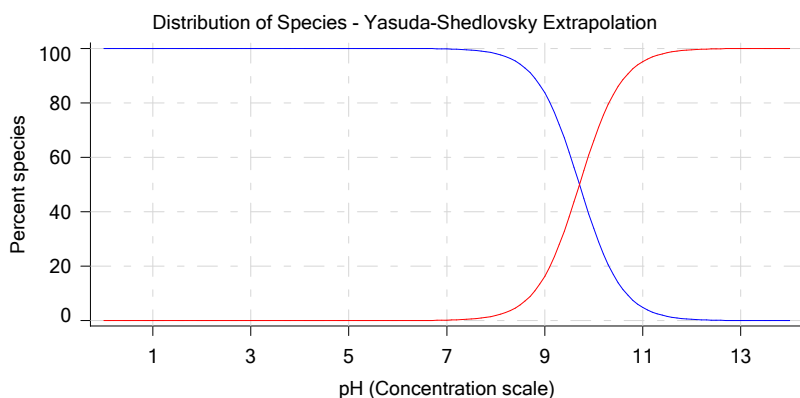
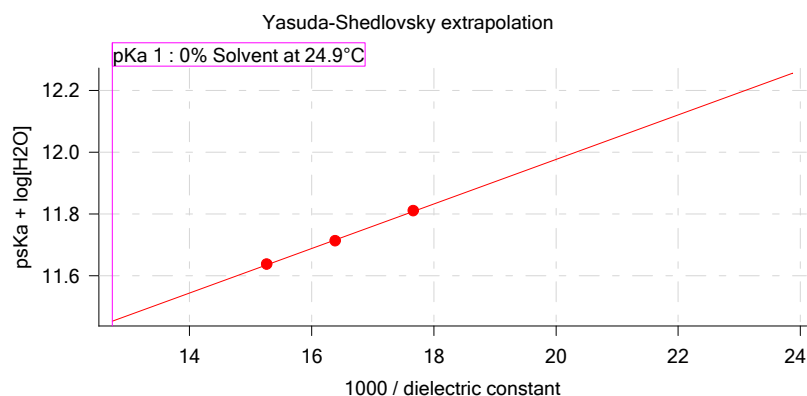
## Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R <sup>2</sup>	Ionic strength	Temperature
Yasuda-Shedlovsky	9.71	±0.01	10.53	72.0847	0.9987	0.165 M	24.9°C

## Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1
17J-06011 Points 4 to 27	49.55 %	Up	UV-metric pKa	56.6	24.7 M	0.157 M	24.9°C	✓ 10.42
17J-06011 Points 29 to 66	39.95 %	Up	UV-metric pKa	61.0	30.0 M	0.166 M	25.0°C	✓ 10.24
17J-06011 Points 68 to 109	30.09 %	Up	UV-metric pKa	65.5	35.8 M	0.172 M	24.9°C	✓ 10.08

## Graphs



## UV-metric psKa Titration 1 of 3 17J-06011 Points 4 to 27

### Results

pKa 1	<b>10.42</b>
RMSD	<b>0.001 0.001</b>
Chi squared	<b>0.0018</b>
PCA calculated number of pKas	<b>1</b>
Average ionic strength	<b>0.157 M</b>
Average temperature	<b>24.9°C</b>
Analyte concentration range	<b>55.5 µM to 52.3 µM</b>
Methanol weight %	<b>49.6 %</b>
Dielectric constant	<b>56.6</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 1.472 to 12.544

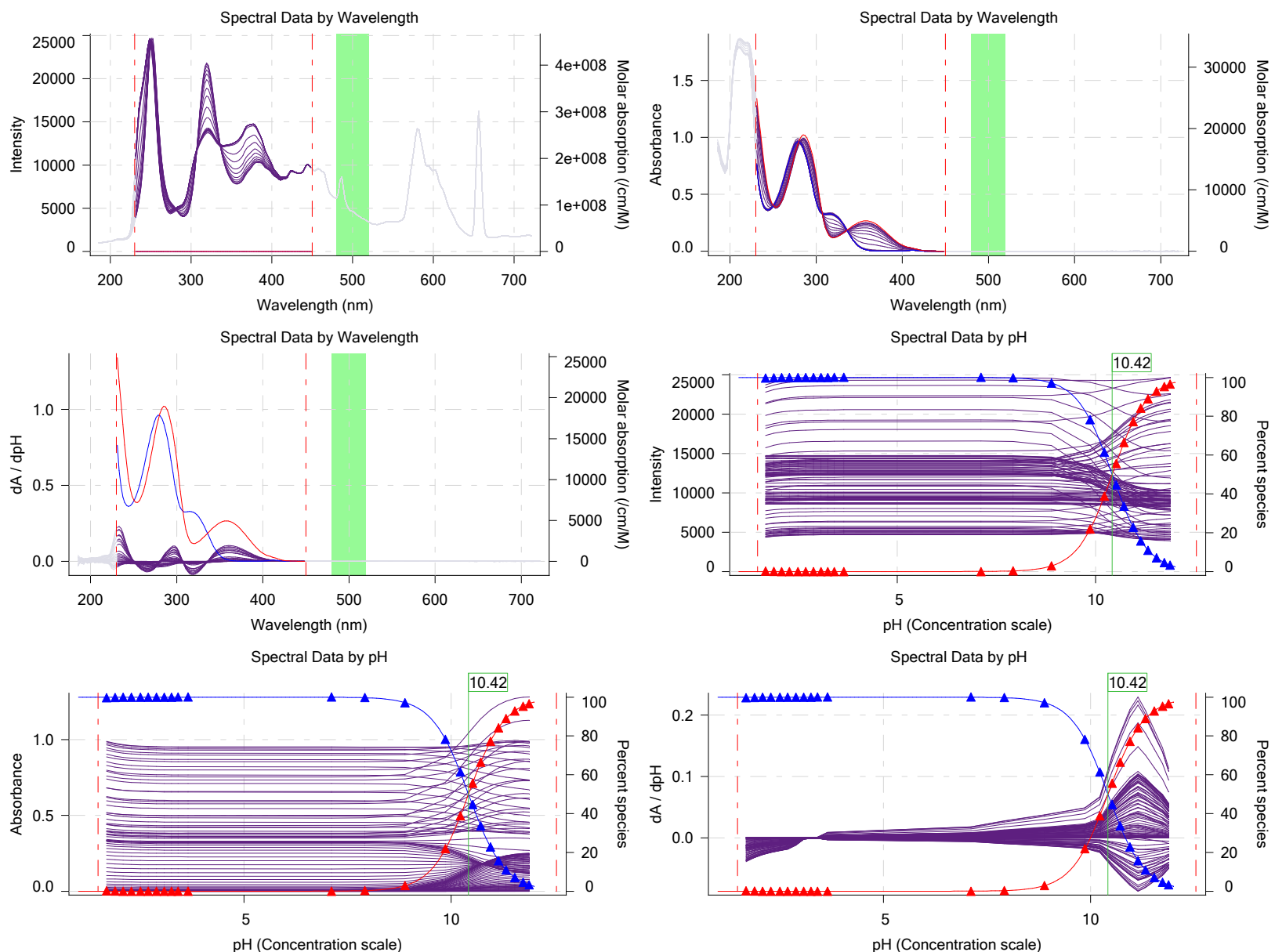
## Warnings and errors

Errors None  
 Warnings None

## 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			

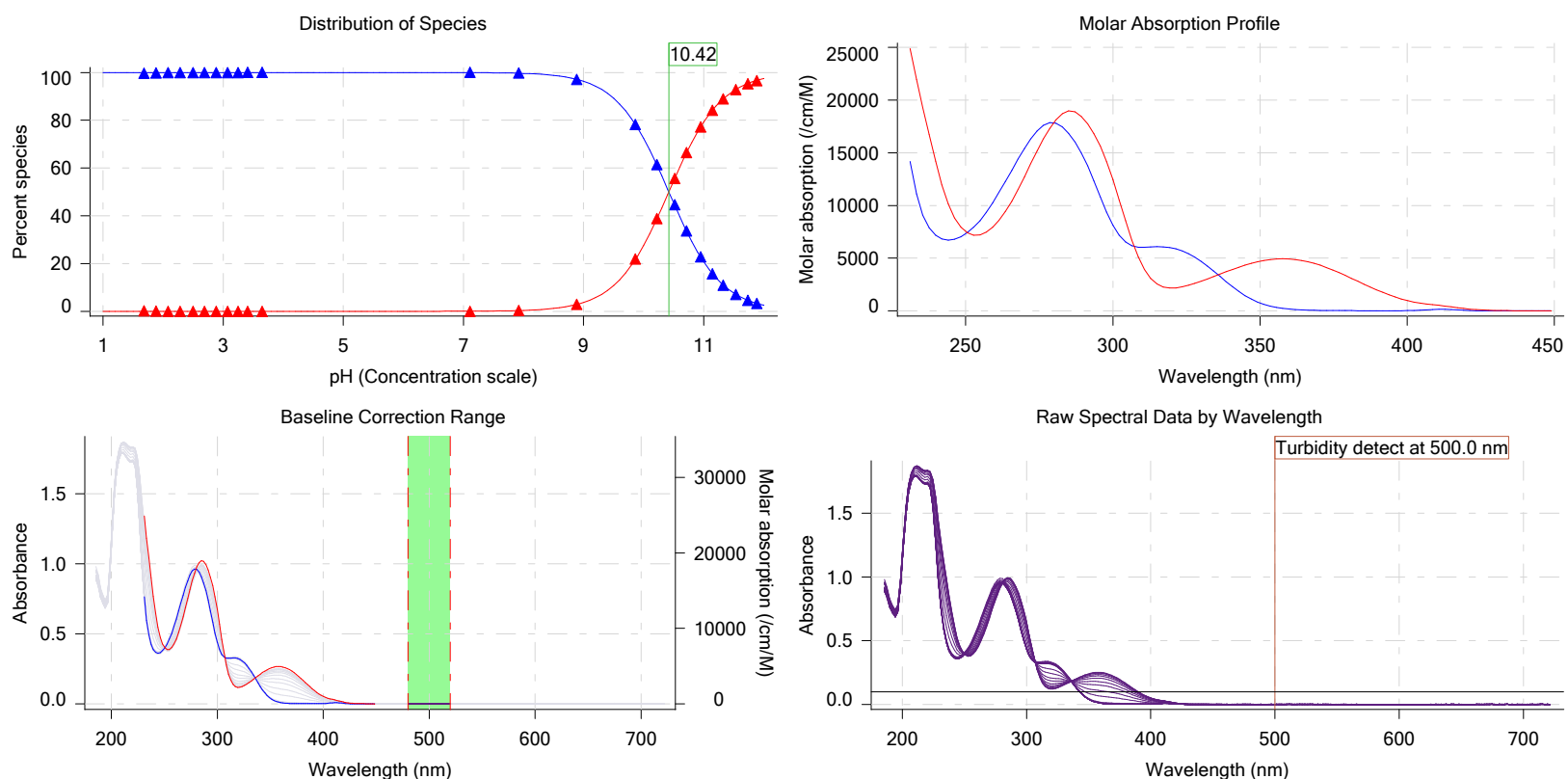
## Graphs



Sample name: **M01**  
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Analyst: **Dorothy Levorse**  
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## Graphs (continued)



## UV-metric psKa Titration 2 of 3 17J-06011 Points 29 to 66

### Results

pKa 1	<b>10.24</b>
RMSD	<b>0.001 0.001</b>
Chi squared	<b>0.0024</b>
PCA calculated number of pKas	<b>3</b>
Average ionic strength	<b>0.166 M</b>
Average temperature	<b>25.0°C</b>
Analyte concentration range	<b>45.6 µM to 43.1 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>1.507 to 12.531</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**

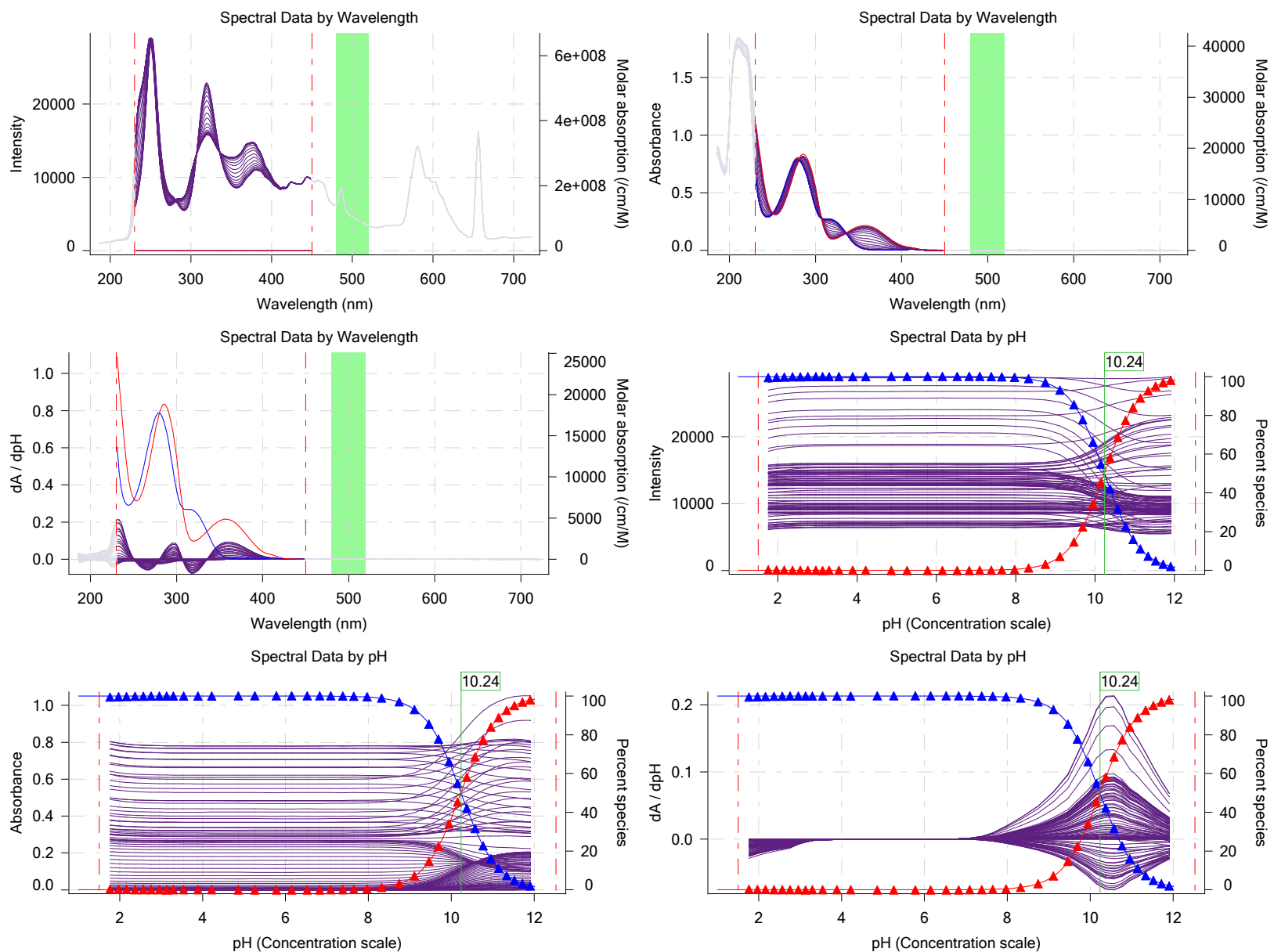
Sample name: **M01**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-06011**  
Filename: **C:\Sirius\_T3\17J-06011\_M01\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 1:41:57 PM**  
Analyst: **Dorothy Levorse**  
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			

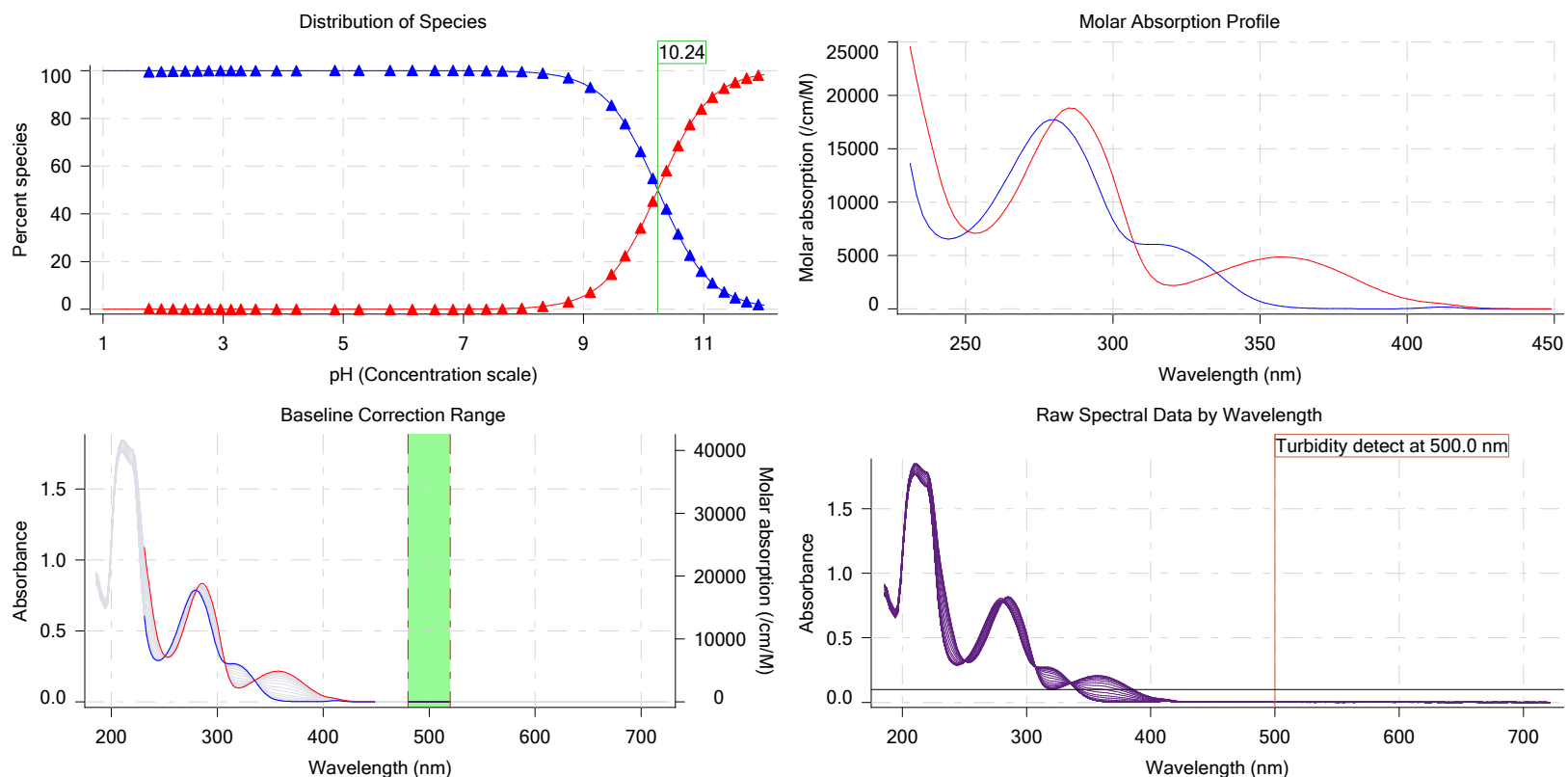
## Graphs



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## Graphs (continued)



## UV-metric psKa Titration 3 of 3 17J-06011 Points 68 to 109

### Results

pKa 1 **10.08**  
 RMSD **0.001 0.001**  
 Chi squared **0.0023**  
 PCA calculated number of pKas **2**  
 Average ionic strength **0.172 M**  
 Average temperature **24.9°C**  
 Analyte concentration range **35.0 µM to 33.2 µM**  
 Methanol weight % **30.1 %**  
 Dielectric constant **65.5**  
 Water concentration **35.8 M**

Number of pKas source **Predicted**  
 Wavelength clipping **230.0 nm to 450.0 nm**  
 pH clipping **1.501 to 12.513**

### 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**

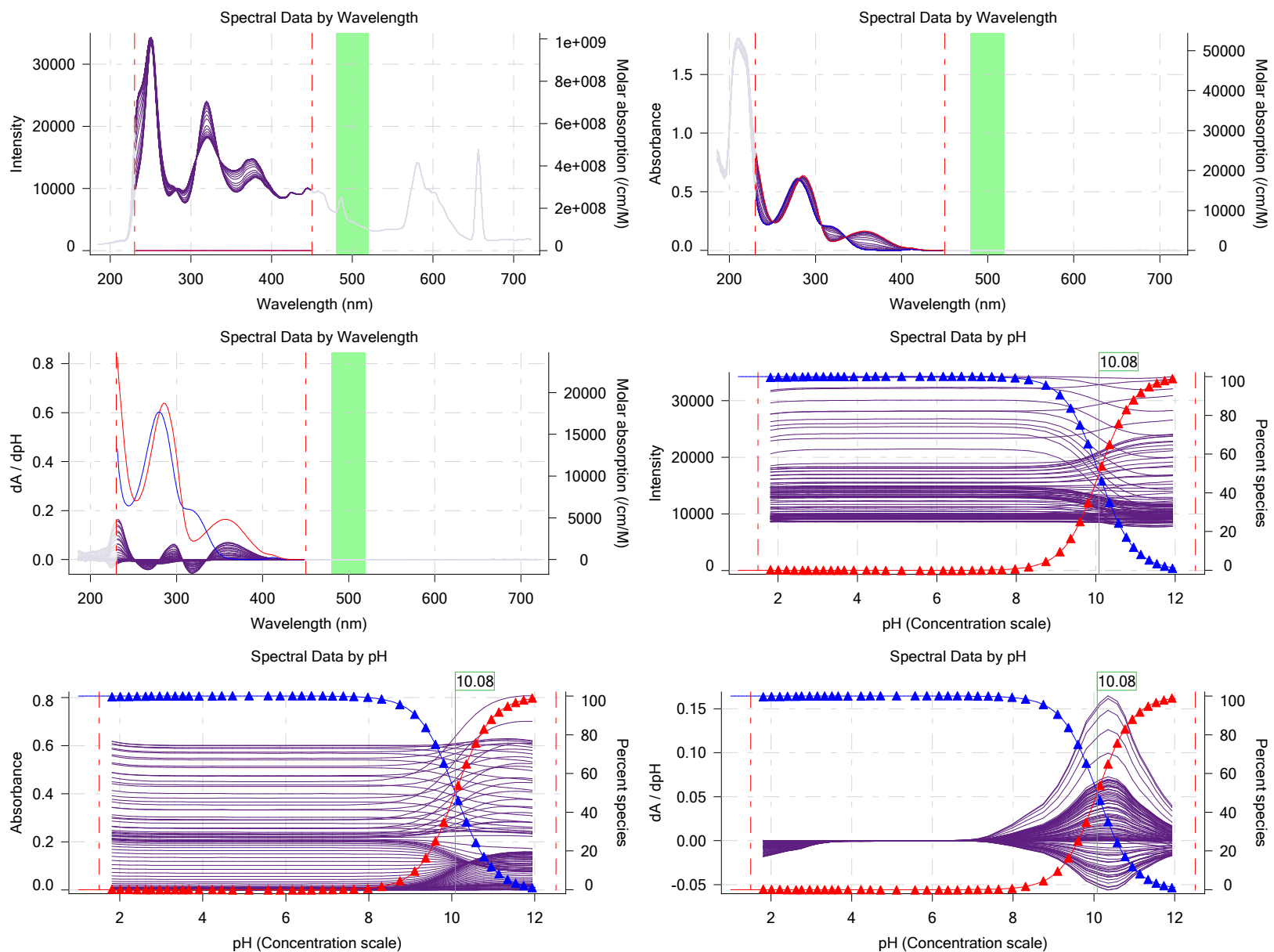
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Experiment start time: **10/6/2017 1:41:57 PM**  
 Analyst: **Dorothy Leverse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

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

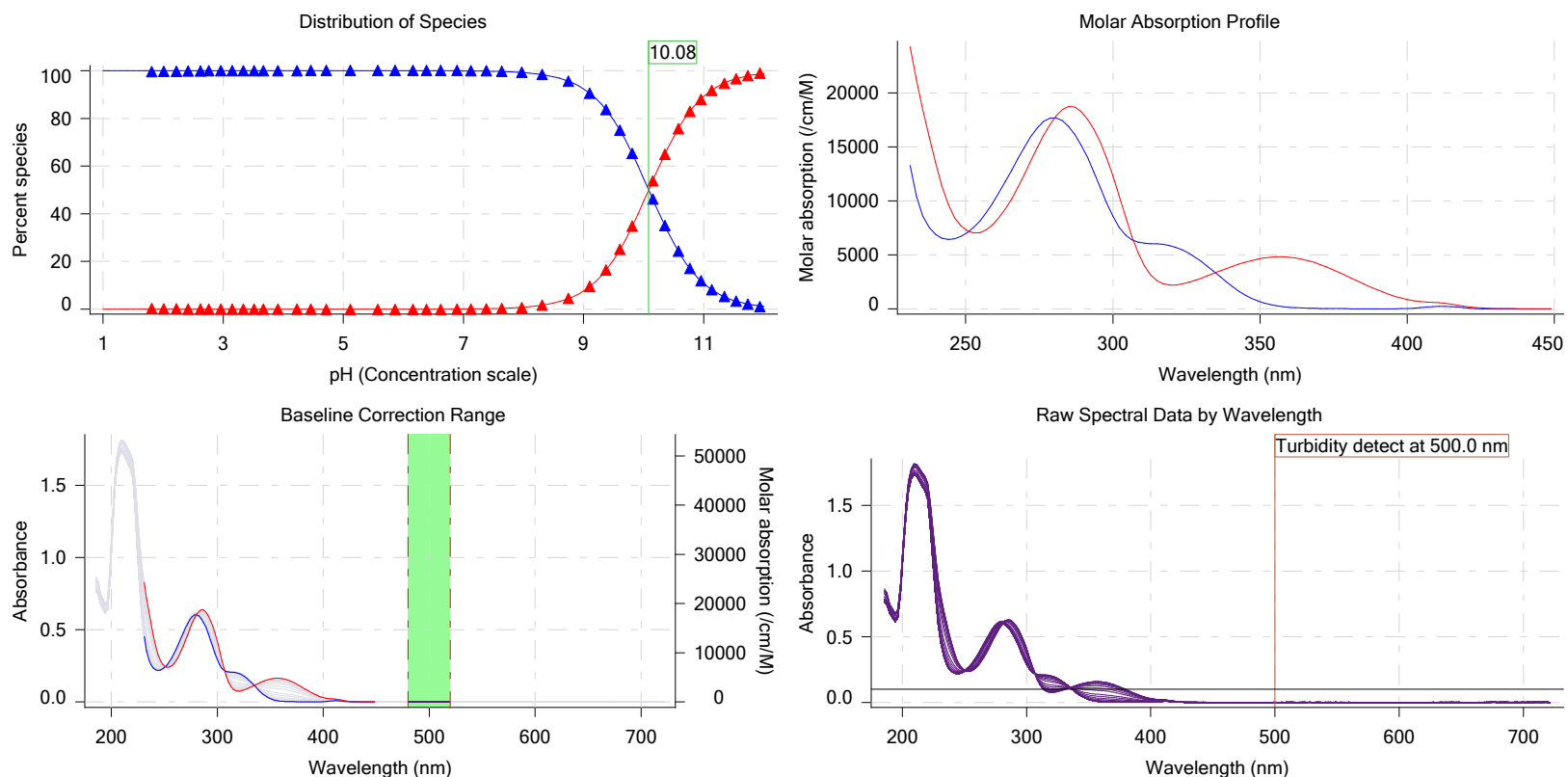
## Graphs



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Experiment start time: **10/6/2017 1:41:57 PM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Graphs (continued)



## Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M01	10/3/2017 3:32:38 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0018 mL	10/5/2017 4:50:42 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.050600 M	10/5/2017 4:50:59 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	217.22	10/3/2017 3:31:54 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	10/3/2017 3:31:42 PM	User entered value
Sample is a	Acid	10/3/2017 3:31:42 PM	User entered value
pKa 1	9.00	10/3/2017 3:31:42 PM	User entered value
logP (neutral XH)	-10.00	10/3/2017 3:31:42 PM	User entered value
logP (X -)	-10.00		Default value

## Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:08.4	Dark spectrum								
3:09.8	Reference spectrum								
3:37.4	Volume reset due to vial change								
4:21.6	Initial pH = 8.41								
5:26.3	Data point 4	0.34995 mL	0.06884 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.972	-0.01591	0.85131
5:55.1	Data point 5	0.34995 mL	0.06884 mL	0.02467 mL	1.15005 mL	0.02500 mL	2.171	0.00014	0.00016
6:12.1	Data point 6	0.34995 mL	0.06884 mL	0.04019 mL	1.15005 mL	0.02500 mL	2.364	0.02355	0.78344
6:28.9	Data point 7	0.34995 mL	0.06884 mL	0.05005 mL	1.15005 mL	0.02500 mL	2.561	0.02259	0.83748
6:45.7	Data point 8	0.34995 mL	0.06884 mL	0.05635 mL	1.15005 mL	0.02500 mL	2.774	0.02184	0.89485
7:02.4	Data point 9	0.34995 mL	0.06884 mL	0.06021 mL	1.15005 mL	0.02500 mL	2.961	0.01275	0.63857



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**Events (continued)**

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
7:19.0	Data point 10	0.34995 mL	0.06884 mL	0.06270 mL	1.15005 mL	0.02500 mL	3.156	0.00880	0.81719	0.00
7:35.6	Data point 11	0.34995 mL	0.06884 mL	0.06430 mL	1.15005 mL	0.02500 mL	3.343	0.00793	0.69262	0.00
7:52.1	Data point 12	0.34995 mL	0.06884 mL	0.06533 mL	1.15005 mL	0.02500 mL	3.515	0.01542	0.94120	0.00
8:08.6	Data point 13	0.34995 mL	0.06884 mL	0.06602 mL	1.15005 mL	0.02500 mL	3.675	0.02010	0.96605	0.00
8:30.3	Data point 14	0.34995 mL	0.06884 mL	0.06675 mL	1.15005 mL	0.02500 mL	3.913	0.04557	0.99232	0.00
8:57.2	Data point 15	0.34995 mL	0.06884 mL	0.06841 mL	1.15005 mL	0.02500 mL	7.335	0.07729	0.59288	0.00
9:28.4	Data point 16	0.34995 mL	0.06884 mL	0.06881 mL	1.15005 mL	0.02500 mL	8.135	0.09812	0.96775	0.00
10:03.8	Data point 17	0.34995 mL	0.06884 mL	0.06914 mL	1.15005 mL	0.02500 mL	9.092	0.09775	0.94361	0.00
10:44.1	Data point 18	0.34995 mL	0.06884 mL	0.06950 mL	1.15005 mL	0.02500 mL	10.057	0.08956	0.92348	0.00
11:06.4	Data point 19	0.34995 mL	0.06884 mL	0.06985 mL	1.15005 mL	0.02500 mL	10.412	0.02214	0.87876	0.00
11:27.9	Data point 20	0.34995 mL	0.06884 mL	0.07034 mL	1.15005 mL	0.02500 mL	10.705	0.00159	0.13308	0.00
11:60.0	Data point 21	0.34995 mL	0.06884 mL	0.07107 mL	1.15005 mL	0.02500 mL	10.899	-0.00710	0.72780	0.00
12:16.7	Data point 22	0.34995 mL	0.06884 mL	0.07227 mL	1.15005 mL	0.02500 mL	11.130	-0.00909	0.83277	0.00
12:43.7	Data point 23	0.34995 mL	0.06884 mL	0.07427 mL	1.15005 mL	0.02500 mL	11.321	-0.01443	0.90687	0.00
13:00.3	Data point 24	0.34995 mL	0.06884 mL	0.07742 mL	1.15005 mL	0.02500 mL	11.498	-0.00635	0.46422	0.00
13:17.1	Data point 25	0.34995 mL	0.06884 mL	0.08217 mL	1.15005 mL	0.02500 mL	11.707	-0.00337	0.23166	0.00
13:34.0	Data point 26	0.34995 mL	0.06884 mL	0.08998 mL	1.15005 mL	0.02500 mL	11.901	0.00152	0.07513	0.00
13:50.8	Data point 27	0.34995 mL	0.06884 mL	0.09871 mL	1.15005 mL	0.02500 mL	12.044	0.00346	0.21559	0.00
15:27.1	Reference spectrum									
16:31.2	Data point 29	0.50000 mL	0.16839 mL	0.09873 mL	1.15005 mL	0.02500 mL	2.007	-0.04673	0.93138	0.00
16:58.8	Data point 30	0.50000 mL	0.16839 mL	0.12434 mL	1.15005 mL	0.02500 mL	2.209	0.01227	0.85782	0.00
17:15.6	Data point 31	0.50000 mL	0.16839 mL	0.13991 mL	1.15005 mL	0.02500 mL	2.402	0.01134	0.69926	0.00
17:32.3	Data point 32	0.50000 mL	0.16839 mL	0.14984 mL	1.15005 mL	0.02500 mL	2.603	0.00775	0.20041	0.00
17:49.0	Data point 33	0.50000 mL	0.16839 mL	0.15609 mL	1.15005 mL	0.02500 mL	2.797	0.00801	0.31309	0.00
18:05.7	Data point 34	0.50000 mL	0.16839 mL	0.16002 mL	1.15005 mL	0.02500 mL	2.987	-0.00488	0.39553	0.00
18:22.3	Data point 35	0.50000 mL	0.16839 mL	0.16258 mL	1.15005 mL	0.02500 mL	3.183	0.01219	0.86250	0.00
18:39.0	Data point 36	0.50000 mL	0.16839 mL	0.16420 mL	1.15005 mL	0.02500 mL	3.355	0.01201	0.86075	0.00
18:55.6	Data point 37	0.50000 mL	0.16839 mL	0.16529 mL	1.15005 mL	0.02500 mL	3.517	0.02217	0.94307	0.00
19:17.4	Data point 38	0.50000 mL	0.16839 mL	0.16651 mL	1.15005 mL	0.02500 mL	3.762	0.02123	0.89249	0.00
19:39.0	Data point 39	0.50000 mL	0.16839 mL	0.16729 mL	1.15005 mL	0.02500 mL	4.103	0.06156	0.99229	0.00
20:00.7	Data point 40	0.50000 mL	0.16839 mL	0.16764 mL	1.15005 mL	0.02500 mL	4.429	0.10025	0.98057	0.00
20:31.1	Data point 41	0.50000 mL	0.16839 mL	0.16797 mL	1.15005 mL	0.02500 mL	5.065	0.10040	0.99211	0.00
21:17.3	Data point 42	0.50000 mL	0.16839 mL	0.16809 mL	1.15005 mL	0.02500 mL	5.460	0.09779	0.96908	0.00
22:24.5	Data point 43	0.50000 mL	0.16839 mL	0.16818 mL	1.15005 mL	0.02500 mL	5.975	0.09355	0.96316	0.00
23:20.7	Data point 44	0.50000 mL	0.16839 mL	0.16825 mL	1.15005 mL	0.02500 mL	6.340	0.09989	0.98798	0.00
24:06.7	Data point 45	0.50000 mL	0.16839 mL	0.16834 mL	1.15005 mL	0.02500 mL	6.710	0.09962	0.99456	0.00
24:50.2	Data point 46	0.50000 mL	0.16839 mL	0.16844 mL	1.15005 mL	0.02500 mL	7.010	0.09989	0.98151	0.00
25:25.5	Data point 47	0.50000 mL	0.16839 mL	0.16856 mL	1.15005 mL	0.02500 mL	7.277	0.10068	0.98942	0.00
26:02.8	Data point 48	0.50000 mL	0.16839 mL	0.16867 mL	1.15005 mL	0.02500 mL	7.564	0.09596	0.97940	0.00
26:41.9	Data point 49	0.50000 mL	0.16839 mL	0.16879 mL	1.15005 mL	0.02500 mL	7.827	0.09995	0.98600	0.00
27:27.9	Data point 50	0.50000 mL	0.16839 mL	0.16891 mL	1.15005 mL	0.02500 mL	8.146	0.09631	0.97694	0.00
28:06.2	Data point 51	0.50000 mL	0.16839 mL	0.16900 mL	1.15005 mL	0.02500 mL	8.493	0.09834	0.97801	0.00
28:51.4	Data point 52	0.50000 mL	0.16839 mL	0.16907 mL	1.15005 mL	0.02500 mL	8.911	0.09813	0.97478	0.00
29:30.6	Data point 53	0.50000 mL	0.16839 mL	0.16914 mL	1.15005 mL	0.02500 mL	9.277	0.09885	0.97897	0.00
30:06.3	Data point 54	0.50000 mL	0.16839 mL	0.16924 mL	1.15005 mL	0.02500 mL	9.624	0.09624	0.96370	0.00
30:32.4	Data point 55	0.50000 mL	0.16839 mL	0.16936 mL	1.15005 mL	0.02500 mL	9.848	0.10009	0.97755	0.00
30:49.4	Data point 56	0.50000 mL	0.16839 mL	0.16952 mL	1.15005 mL	0.02500 mL	10.104	0.03667	0.94364	0.00
31:21.4	Data point 57	0.50000 mL	0.16839 mL	0.16983 mL	1.15005 mL	0.02500 mL	10.305	0.01803	0.80440	0.00
31:37.9	Data point 58	0.50000 mL	0.16839 mL	0.17025 mL	1.15005 mL	0.02500 mL	10.528	0.00374	0.24063	0.00
31:54.5	Data point 59	0.50000 mL	0.16839 mL	0.17096 mL	1.15005 mL	0.02500 mL	10.723	-0.00391	0.45120	0.00
32:11.1	Data point 60	0.50000 mL	0.16839 mL	0.17206 mL	1.15005 mL	0.02500 mL	10.916	-0.00550	0.69065	0.00
32:27.7	Data point 61	0.50000 mL	0.16839 mL	0.17375 mL	1.15005 mL	0.02500 mL	11.101	-0.00846	0.77571	0.00
32:44.4	Data point 62	0.50000 mL	0.16839 mL	0.17634 mL	1.15005 mL	0.02500 mL	11.284	-0.01169	0.88791	0.00
33:01.2	Data point 63	0.50000 mL	0.16839 mL	0.18032 mL	1.15005 mL	0.02500 mL	11.478	-0.00764	0.70562	0.00
33:18.1	Data point 64	0.50000 mL	0.16839 mL	0.18660 mL	1.15005 mL	0.02500 mL	11.660	-0.00875	0.85169	0.00
33:34.9	Data point 65	0.50000 mL	0.16839 mL	0.19626 mL	1.15005 mL	0.02500 mL	11.846	0.00029	0.00333	0.00
33:51.7	Data point 66	0.50000 mL	0.16839 mL	0.21145 mL	1.15005 mL	0.02500 mL	12.031	0.00704	0.47754	0.00



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 Instrument ID: **T311053**

**Events (continued)**

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
35:36.7	Reference spectrum									
37:00.0	Data point 68	0.83996 mL	0.30106 mL	0.21148 mL	1.15005 mL	0.02500 mL	2.001	-0.02164	0.93209	0.00
37:27.6	Data point 69	0.83996 mL	0.30106 mL	0.23953 mL	1.15005 mL	0.02500 mL	2.197	0.01392	0.80804	0.00
37:44.5	Data point 70	0.83996 mL	0.30106 mL	0.25778 mL	1.15005 mL	0.02500 mL	2.399	0.00142	0.02334	0.00
38:01.4	Data point 71	0.83996 mL	0.30106 mL	0.26914 mL	1.15005 mL	0.02500 mL	2.591	-0.03085	0.81264	0.00
38:18.1	Data point 72	0.83996 mL	0.30106 mL	0.27660 mL	1.15005 mL	0.02500 mL	2.795	0.00893	0.46134	0.00
38:50.5	Data point 73	0.83996 mL	0.30106 mL	0.28116 mL	1.15005 mL	0.02500 mL	2.936	0.00850	0.71603	0.00
39:12.3	Data point 74	0.83996 mL	0.30106 mL	0.28417 mL	1.15005 mL	0.02500 mL	3.132	-0.00198	0.09760	0.00
39:28.8	Data point 75	0.83996 mL	0.30106 mL	0.28626 mL	1.15005 mL	0.02500 mL	3.318	0.00034	0.00210	0.00
39:45.4	Data point 76	0.83996 mL	0.30106 mL	0.28763 mL	1.15005 mL	0.02500 mL	3.500	-0.00597	0.37909	0.00
40:02.1	Data point 77	0.83996 mL	0.30106 mL	0.28852 mL	1.15005 mL	0.02500 mL	3.679	-0.00611	0.27962	0.00
40:18.5	Data point 78	0.83996 mL	0.30106 mL	0.28911 mL	1.15005 mL	0.02500 mL	3.832	0.00801	0.50694	0.00
40:45.5	Data point 79	0.83996 mL	0.30106 mL	0.29017 mL	1.15005 mL	0.02500 mL	4.070	0.02095	0.91753	0.00
41:07.2	Data point 80	0.83996 mL	0.30106 mL	0.29062 mL	1.15005 mL	0.02500 mL	4.388	0.03686	0.88659	0.00
41:38.9	Data point 81	0.83996 mL	0.30106 mL	0.29087 mL	1.15005 mL	0.02500 mL	4.616	0.09701	0.98203	0.00
42:08.3	Data point 82	0.83996 mL	0.30106 mL	0.29102 mL	1.15005 mL	0.02500 mL	4.871	0.09623	0.97405	0.00
42:46.6	Data point 83	0.83996 mL	0.30106 mL	0.29113 mL	1.15005 mL	0.02500 mL	5.267	0.09755	0.98389	0.00
43:32.3	Data point 84	0.83996 mL	0.30106 mL	0.29123 mL	1.15005 mL	0.02500 mL	5.722	0.09901	0.98062	0.00
44:14.9	Data point 85	0.83996 mL	0.30106 mL	0.29130 mL	1.15005 mL	0.02500 mL	6.008	0.09466	0.95352	0.00
44:53.7	Data point 86	0.83996 mL	0.30106 mL	0.29139 mL	1.15005 mL	0.02500 mL	6.302	0.05321	0.84264	0.00
45:15.4	Data point 87	0.83996 mL	0.30106 mL	0.29146 mL	1.15005 mL	0.02500 mL	6.524	0.09037	0.92263	0.00
45:37.5	Data point 88	0.83996 mL	0.30106 mL	0.29156 mL	1.15005 mL	0.02500 mL	6.759	0.03959	0.61242	0.00
46:04.3	Data point 89	0.83996 mL	0.30106 mL	0.29168 mL	1.15005 mL	0.02500 mL	7.028	0.08918	0.88867	0.00
46:32.1	Data point 90	0.83996 mL	0.30106 mL	0.29179 mL	1.15005 mL	0.02500 mL	7.256	0.09400	0.96321	0.00
47:04.8	Data point 91	0.83996 mL	0.30106 mL	0.29191 mL	1.15005 mL	0.02500 mL	7.514	0.09245	0.94466	0.00
47:40.8	Data point 92	0.83996 mL	0.30106 mL	0.29203 mL	1.15005 mL	0.02500 mL	7.769	0.09560	0.98464	0.00
48:18.8	Data point 93	0.83996 mL	0.30106 mL	0.29214 mL	1.15005 mL	0.02500 mL	8.100	0.09510	0.97545	0.00
48:59.6	Data point 94	0.83996 mL	0.30106 mL	0.29224 mL	1.15005 mL	0.02500 mL	8.434	0.09533	0.97414	0.00
49:42.8	Data point 95	0.83996 mL	0.30106 mL	0.29233 mL	1.15005 mL	0.02500 mL	8.869	0.09962	0.97513	0.00
50:17.5	Data point 96	0.83996 mL	0.30106 mL	0.29243 mL	1.15005 mL	0.02500 mL	9.220	0.09878	0.98074	0.00
50:51.7	Data point 97	0.83996 mL	0.30106 mL	0.29255 mL	1.15005 mL	0.02500 mL	9.485	0.09672	0.97130	0.00
51:14.9	Data point 98	0.83996 mL	0.30106 mL	0.29269 mL	1.15005 mL	0.02500 mL	9.717	0.05488	0.97433	0.00
51:41.7	Data point 99	0.83996 mL	0.30106 mL	0.29287 mL	1.15005 mL	0.02500 mL	9.918	0.03324	0.91770	0.00
51:58.3	Data point 100	0.83996 mL	0.30106 mL	0.29316 mL	1.15005 mL	0.02500 mL	10.260	-0.01592	0.81629	0.00
52:25.1	Data point 101	0.83996 mL	0.30106 mL	0.29372 mL	1.15005 mL	0.02500 mL	10.458	-0.00711	0.59535	0.00
52:41.7	Data point 102	0.83996 mL	0.30106 mL	0.29464 mL	1.15005 mL	0.02500 mL	10.681	-0.02209	0.89909	0.00
52:58.3	Data point 103	0.83996 mL	0.30106 mL	0.29617 mL	1.15005 mL	0.02500 mL	10.873	-0.02986	0.94004	0.00
53:15.0	Data point 104	0.83996 mL	0.30106 mL	0.29852 mL	1.15005 mL	0.02500 mL	11.053	-0.02434	0.92329	0.00
53:31.7	Data point 105	0.83996 mL	0.30106 mL	0.30207 mL	1.15005 mL	0.02500 mL	11.233	-0.02412	0.93948	0.00
53:48.3	Data point 106	0.83996 mL	0.30106 mL	0.30745 mL	1.15005 mL	0.02500 mL	11.437	-0.02397	0.90885	0.00
54:05.1	Data point 107	0.83996 mL	0.30106 mL	0.31618 mL	1.15005 mL	0.02500 mL	11.630	-0.02624	0.92666	0.00
54:22.0	Data point 108	0.83996 mL	0.30106 mL	0.33001 mL	1.15005 mL	0.02500 mL	11.819	-0.02515	0.92939	0.00
54:39.1	Data point 109	0.83996 mL	0.30106 mL	0.35205 mL	1.15005 mL	0.02500 mL	12.013	-0.02385	0.91284	0.00
56:38.4	Assay volumes	1.08996 mL	0.44177 mL	0.35205 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			

Sample name: **M01**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06011**  
 Filename: **C:\Sirius\_T3\17J-06011\_M01\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 1:41:57 PM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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>Titrant Pre-Dose</b>				
Titrant 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			
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			

Sample name: **M01**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06011**  
 Filename: **C:\Sirius\_T3\17J-06011\_M01\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 1:41:57 PM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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	0.125	10/6/2017 1:41:57 PM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus S	0.9949	10/6/2017 1:41:57 PM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jH	0.8	10/6/2017 1:41:57 PM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jOH	-1.3	10/6/2017 1:41:57 PM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Base concentration factor	1.011	10/6/2017 1:41:57 PM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	1.003	10/6/2017 1:41:57 PM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.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)	8-18-17	9/26/2017 9:05:04 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	9/8/2017 9:21:27 AM
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
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)		
Titrant	Phosphate Buffer		9/12/2017 12:32:29 PM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	9-14-17	9/14/2017 10:30:38 AM
Titration		T3TM1100153	3/31/2009 6:24:17 AM



## Assay Settings

Sample name: **M01**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-06011**  
Filename: **C:\Sirius\_T3\17J-06011\_M01\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 1:41:57 PM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

## Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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	-8.89 mV		10/6/2017 1:42:21 PM
Filling solution	3M KCl	KCL095	10/4/2017 3:50:10 PM
Liquids			
Wash 1	50% IPA:50% Water		10/5/2017 9:59:12 AM
Wash 2	0.5% Triton X-100 in H2O		10/5/2017 9:59:14 AM
Buffer position 1	pH7 Wash		10/5/2017 9:59:17 AM
Buffer position 2	pH 7		10/5/2017 9:59:19 AM
Storage position			10/5/2017 9:58:45 AM
Wash water	3.7e+003 mL	10-3-17	10/3/2017 9:04:49 AM
Waste	6.3e+003 mL		10/3/2017 9:04:54 AM
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	366:44:47		11/23/2010 12:22:28 PM
Calibrated on	10/5/2017 10:23:25 AM		
Integration time	11		
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)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
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		



## Assay Settings

Sample name:	<b>M01</b>	Experiment start time:	<b>10/6/2017 1:41:57 PM</b>
Assay name:	<b>UV-metric psKa</b>	Analyst:	<b>Dorothy Levorse</b>
Assay ID:	<b>17J-06011</b>	Instrument ID:	<b>T311053</b>
Filename:	<b>C:\Sirius_T3\17J-06011_M01_UV-metric psKa.t3r</b>		

### Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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	H1