

Sample name: **D06**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-06003**  
Filename: **C:\Sirius\_T3\17J-06003\_D06\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 2:22:58 AM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

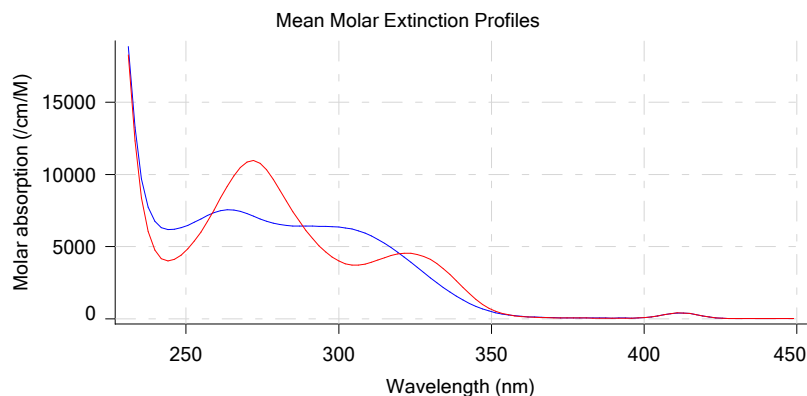
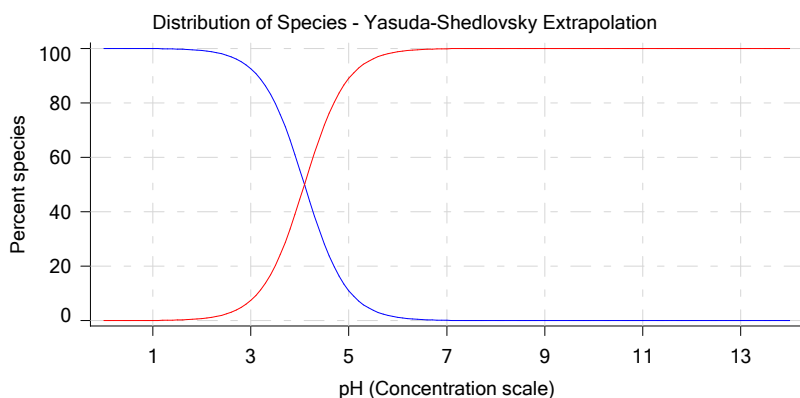
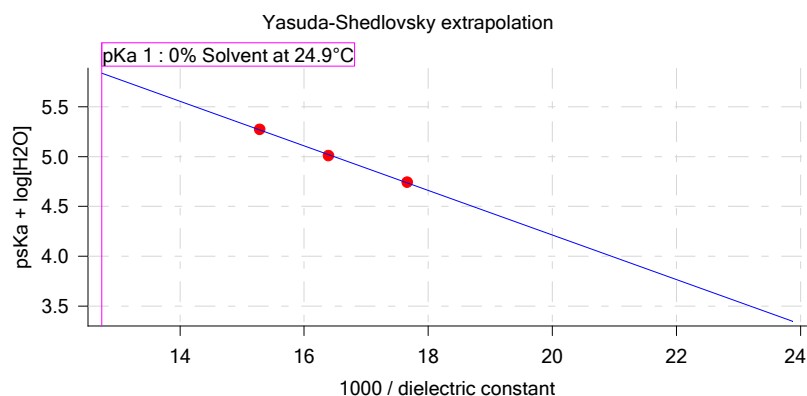
## Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R <sup>2</sup>	Ionic strength	Temperature
Yasuda-Shedlovsky	4.09	±0.03	8.68	-223.5544	0.9990	0.165 M	24.9°C

## Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1
17J-06003 Points 4 to 33	49.53 %	Up	UV-metric pKa	56.6	24.7 M	0.157 M	24.9°C	✓ 3.35
17J-06003 Points 35 to 73	40.03 %	Up	UV-metric pKa	61.0	30.0 M	0.166 M	24.9°C	✓ 3.53
17J-06003 Points 75 to 117	30.27 %	Up	UV-metric pKa	65.4	35.7 M	0.172 M	24.9°C	✓ 3.72

## Graphs



## UV-metric psKa Titration 1 of 3 17J-06003 Points 4 to 33

### Results

pKa 1	<b>3.35</b>
RMSD	<b>0.004 0.002</b>
Chi squared	<b>0.0078</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>29.7 µM to 28.0 µM</b>
Methanol weight %	<b>49.5 %</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 1.481 to 12.537

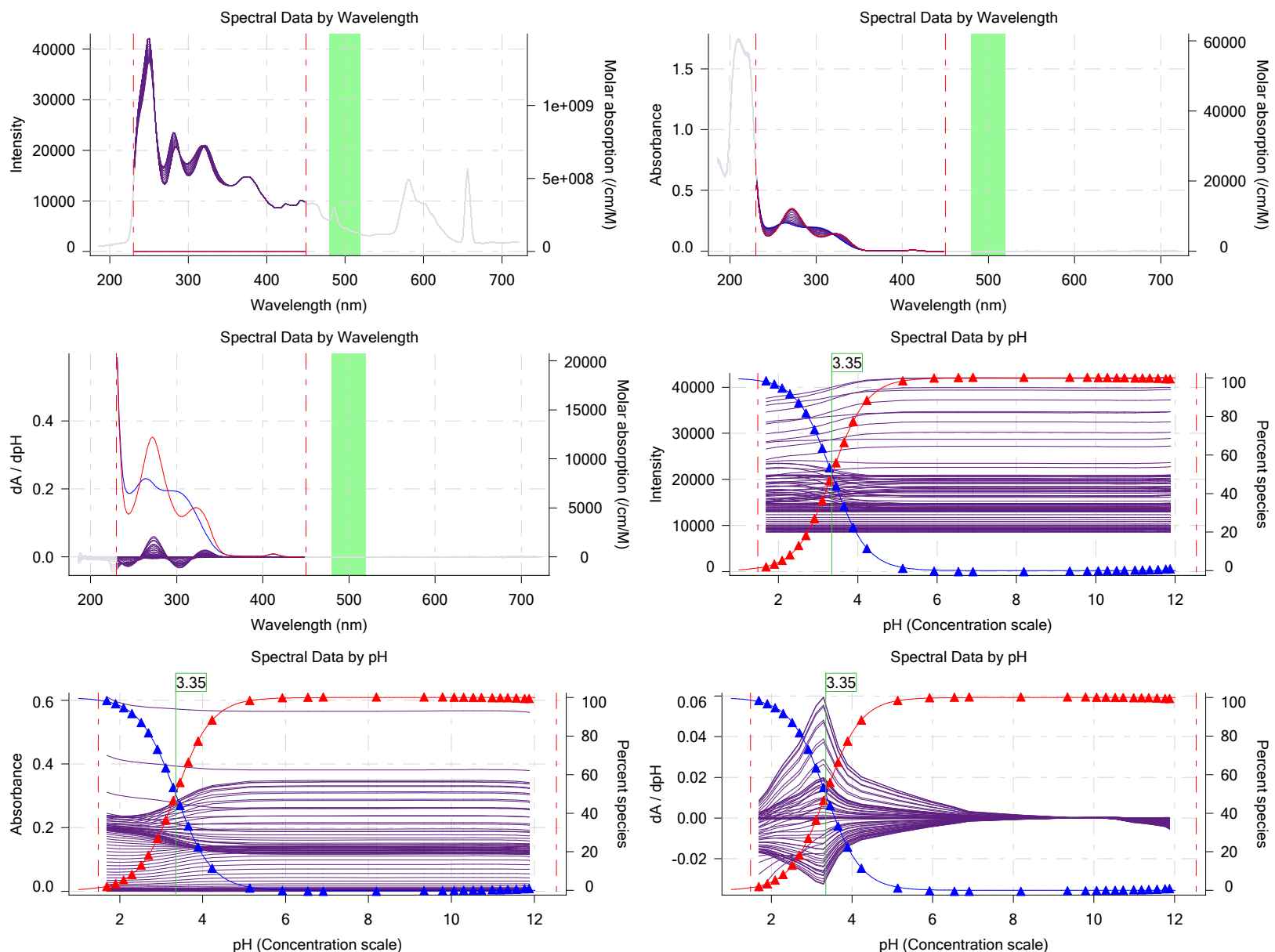
## Warnings and errors

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			

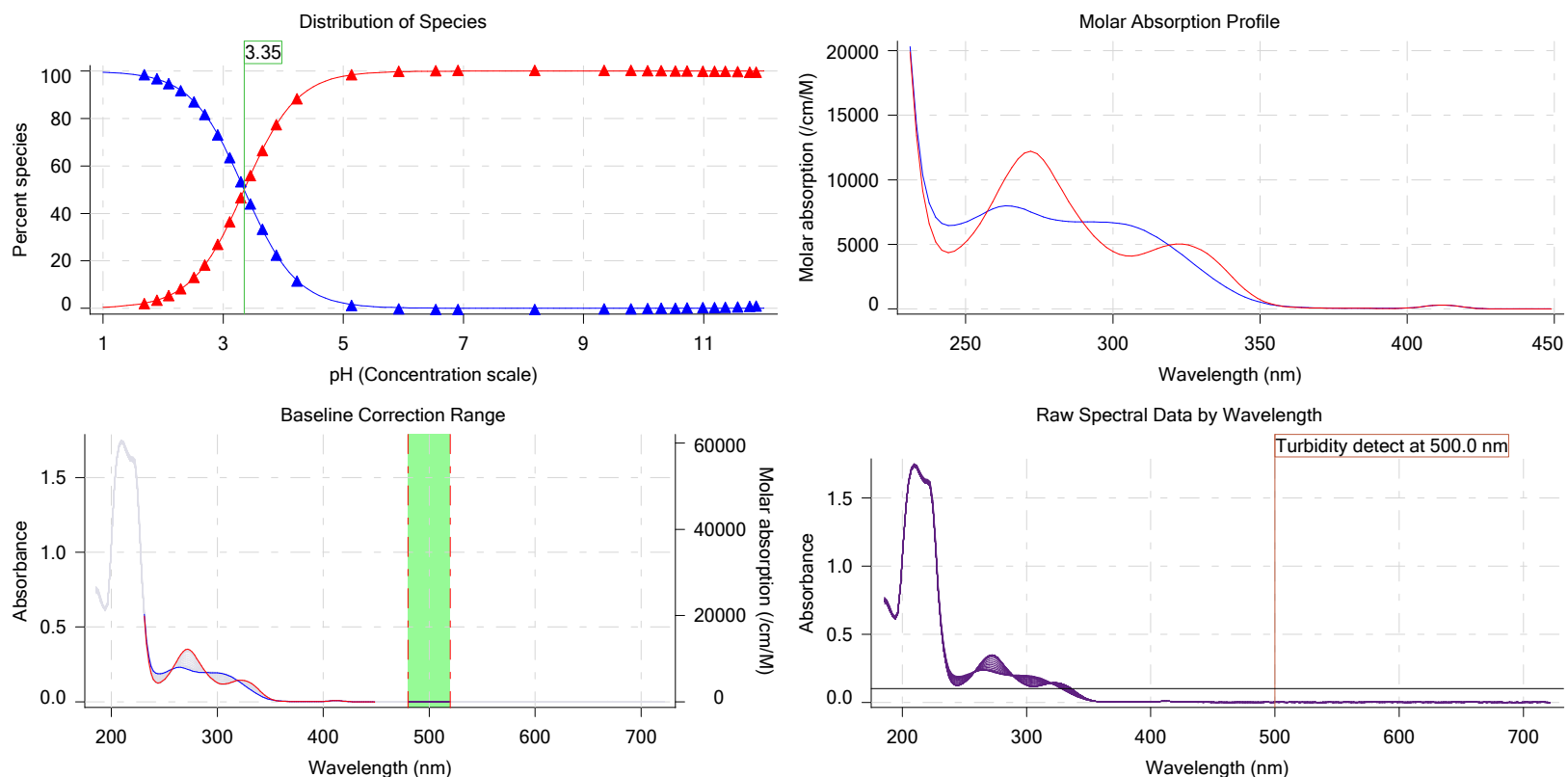
## Graphs



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## Graphs (continued)



## UV-metric psKa Titration 2 of 3 17J-06003 Points 35 to 73

### Results

pKa 1	<b>3.53</b>
RMSD	<b>0.006 0.004</b>
Chi squared	<b>0.0102</b>
PCA calculated number of pKas	<b>2</b>
Average ionic strength	<b>0.166 M</b>
Average temperature	<b>24.9°C</b>
Analyte concentration range	<b>24.4 µM to 23.1 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>1.503 to 12.540</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			
<b>Assay Medium</b>				

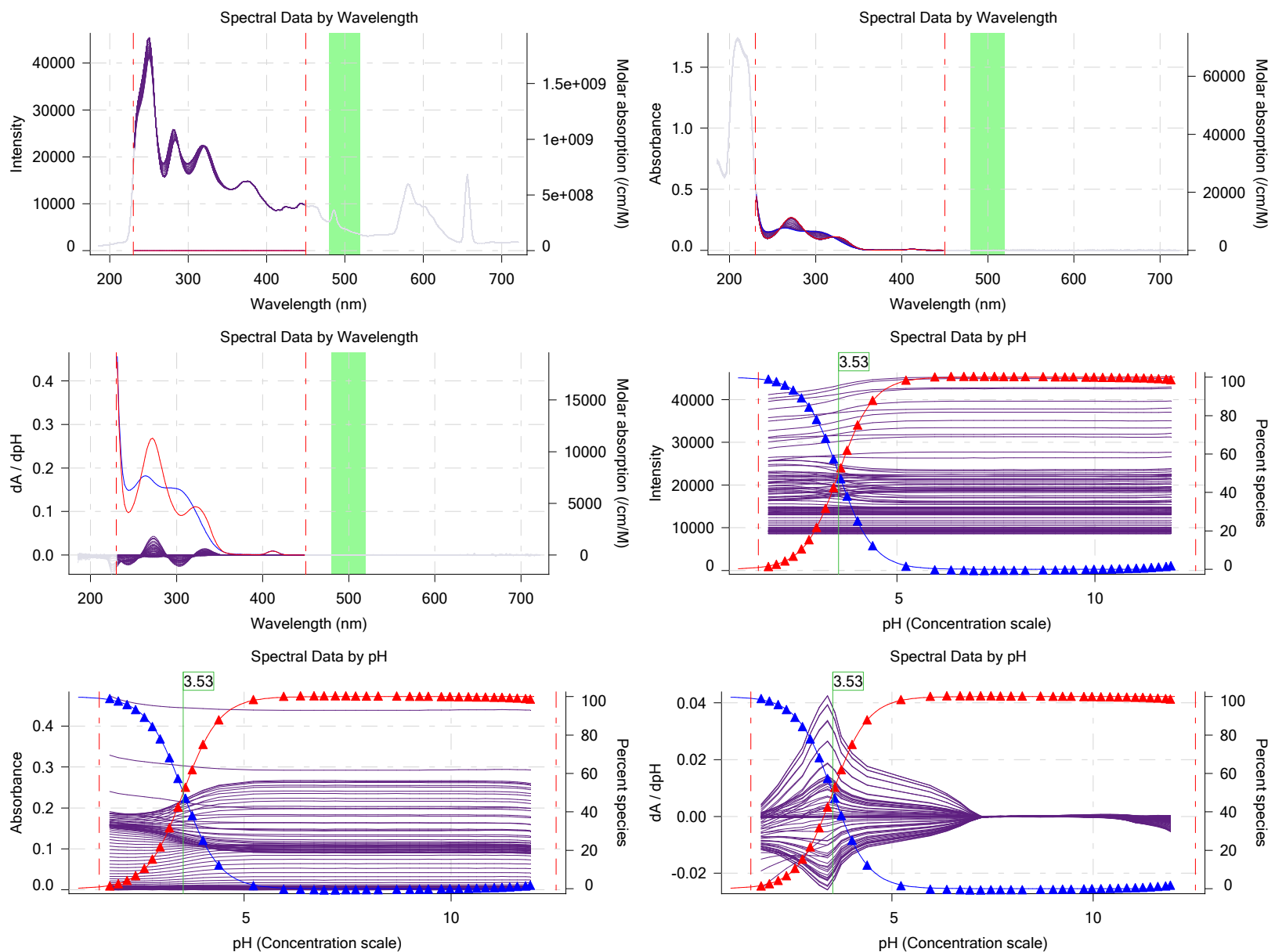
Sample name: **D06**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06003**  
 Filename: **C:\Sirius\_T3\17J-06003\_D06\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 2:22:58 AM**  
 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			

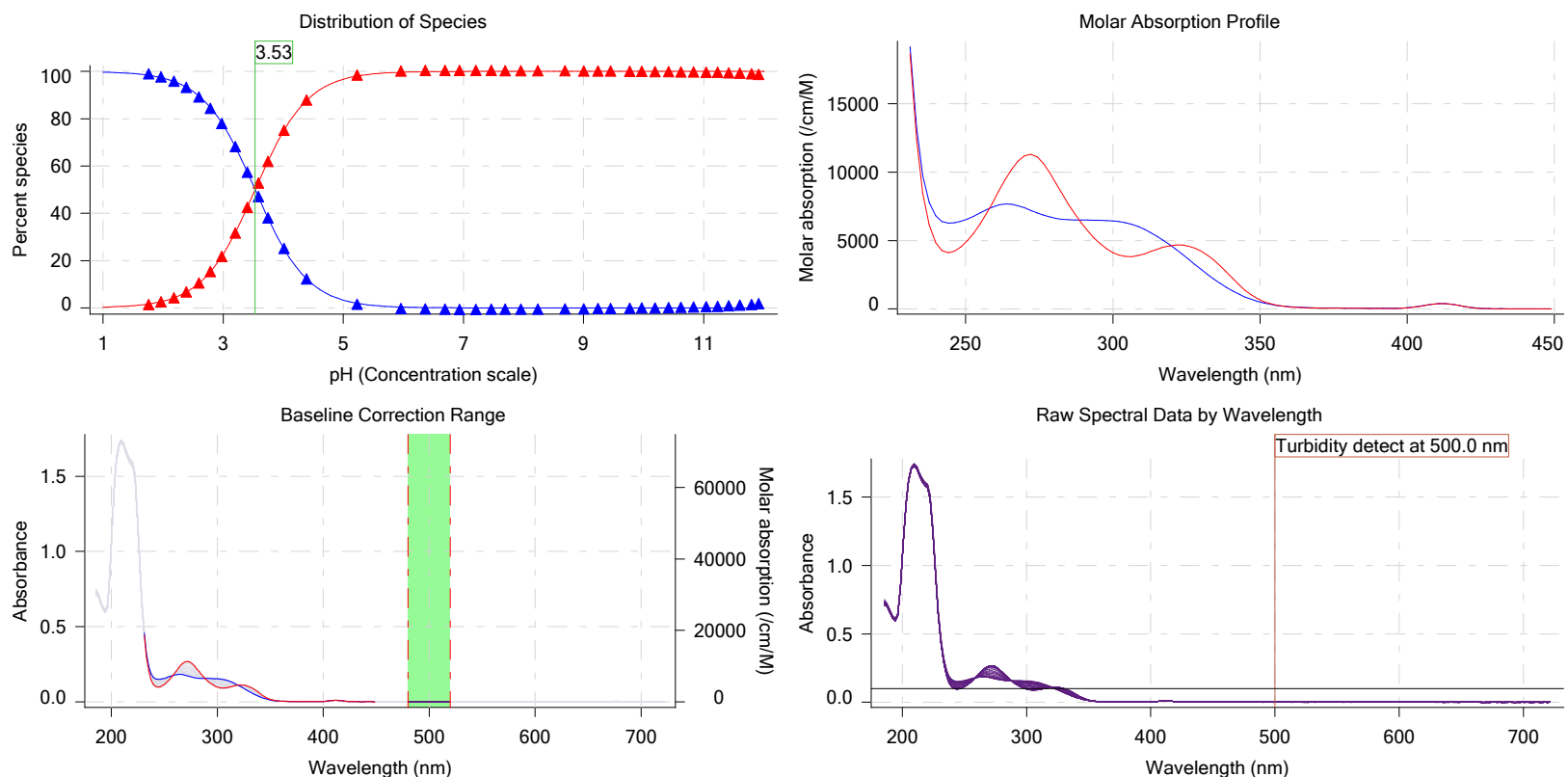
## Graphs



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## Graphs (continued)



## UV-metric psKa Titration 3 of 3 17J-06003 Points 75 to 117

### Results

pKa 1	<b>3.72</b>
RMSD	<b>0.008 0.010</b>
Chi squared	<b>0.0142</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>18.8 µM to 17.8 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>1.504 to 12.540</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**

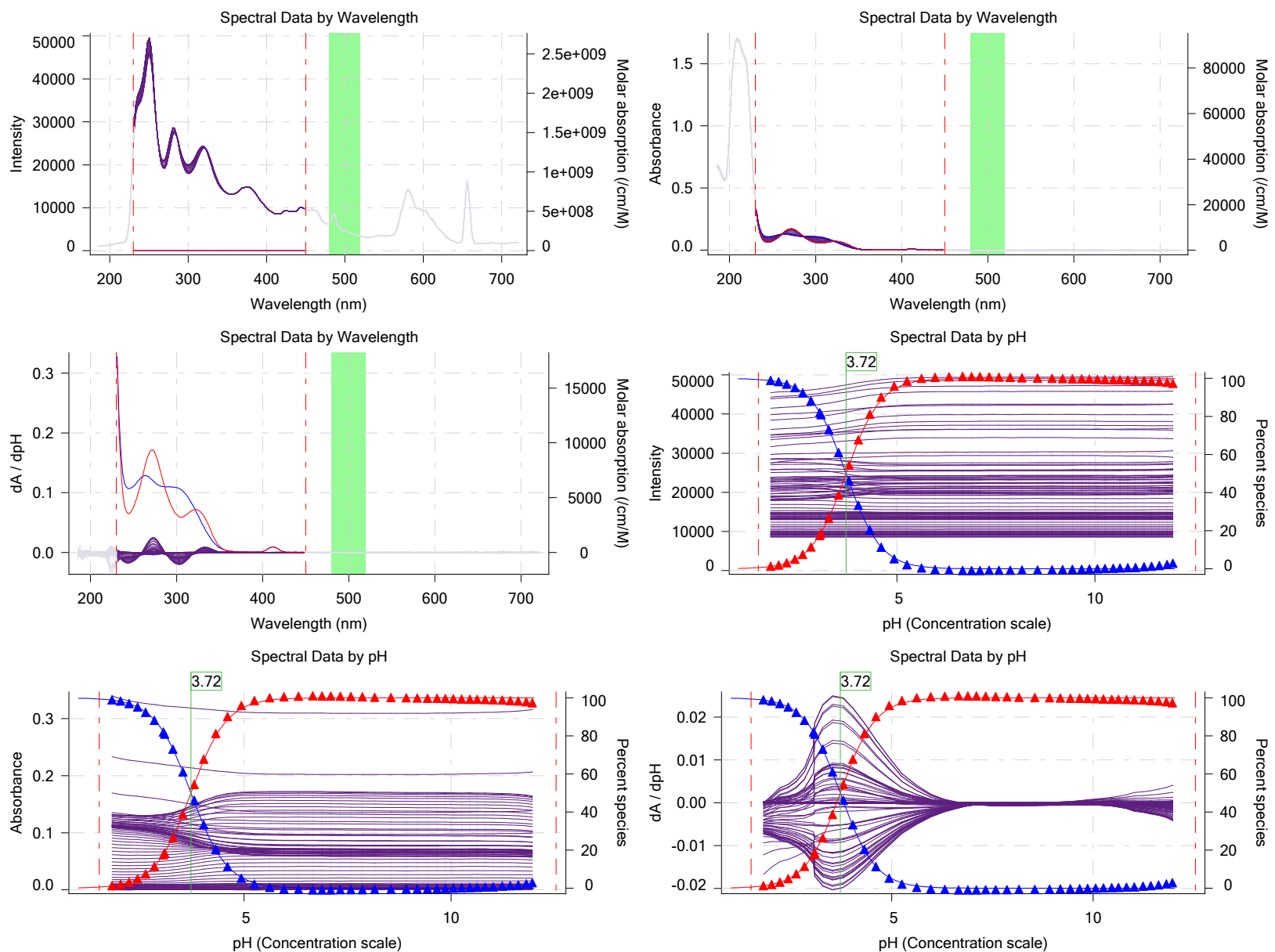
Sample name: **D06**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06003**  
 Filename: **C:\Sirius\_T3\17J-06003\_D06\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 2:22:58 AM**  
 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			

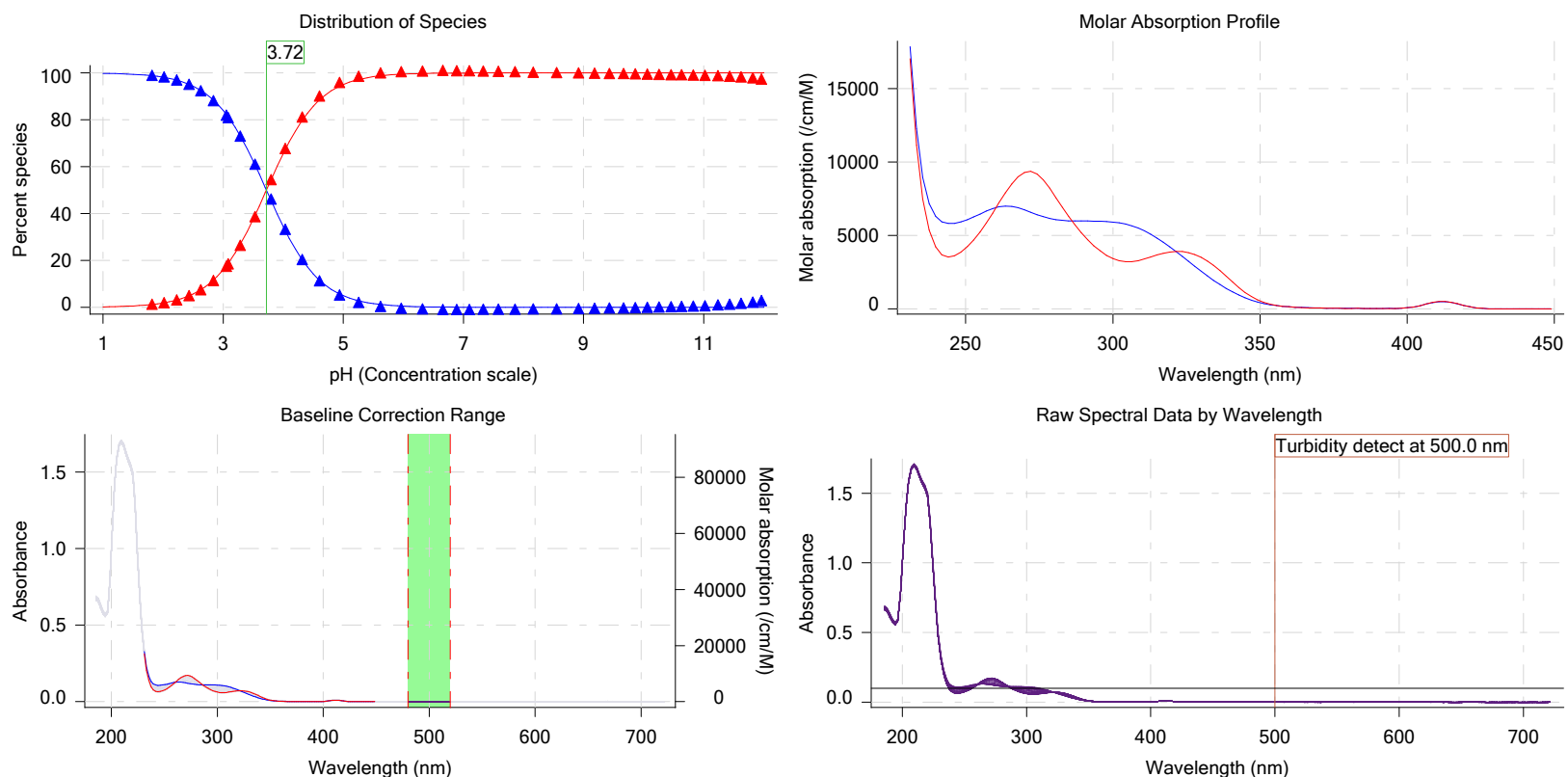
## Graphs



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## Graphs (continued)



## Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	D06	9/29/2017 5:38:58 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0020 mL	10/3/2017 10:11:44 AM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.023700 M	10/2/2017 11:58:50 AM	User entered value
Solubility	Unknown		Default value
Molecular weight	438.09	9/29/2017 5:39:06 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	9/29/2017 5:38:58 PM	User entered value
Sample is a	Base	9/29/2017 5:38:58 PM	User entered value
pKa 1	3.45	9/29/2017 5:38:58 PM	User entered value
logp (XH +)	-10.00		Default value
logP (neutral X)	-10.00	9/29/2017 5:38:58 PM	User entered value

## Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:34.6	Dark spectrum								
3:35.9	Reference spectrum								
4:03.6	Volume reset due to vial change								
4:47.7	Initial pH = 8.37								
6:00.7	Data point 4	0.34995 mL	0.06938 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.981	-0.01249	0.88814
6:29.3	Data point 5	0.34995 mL	0.06938 mL	0.02441 mL	1.15005 mL	0.02500 mL	2.183	-0.01253	0.56039
6:46.2	Data point 6	0.34995 mL	0.06938 mL	0.03960 mL	1.15005 mL	0.02500 mL	2.375	0.01167	0.82881
7:03.0	Data point 7	0.34995 mL	0.06938 mL	0.04929 mL	1.15005 mL	0.02500 mL	2.572	0.00349	0.22056
7:19.7	Data point 8	0.34995 mL	0.06938 mL	0.05548 mL	1.15005 mL	0.02500 mL	2.791	0.00658	0.63700
7:36.4	Data point 9	0.34995 mL	0.06938 mL	0.05920 mL	1.15005 mL	0.02500 mL	2.967	0.01073	0.79933



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**Events (continued)**

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
7:53.0	Data point 10	0.34995 mL	0.06938 mL	0.06167 mL	1.15005 mL	0.02500 mL	3.184	0.01154	0.88907	0.00
8:09.7	Data point 11	0.34995 mL	0.06938 mL	0.06317 mL	1.15005 mL	0.02500 mL	3.377	0.01664	0.95153	0.00
8:26.4	Data point 12	0.34995 mL	0.06938 mL	0.06413 mL	1.15005 mL	0.02500 mL	3.560	0.01668	0.92854	0.00
8:43.0	Data point 13	0.34995 mL	0.06938 mL	0.06477 mL	1.15005 mL	0.02500 mL	3.722	0.02227	0.96568	0.00
9:15.0	Data point 14	0.34995 mL	0.06938 mL	0.06536 mL	1.15005 mL	0.02500 mL	3.916	0.02532	0.98176	0.00
9:36.8	Data point 15	0.34995 mL	0.06938 mL	0.06571 mL	1.15005 mL	0.02500 mL	4.147	0.07082	0.99241	0.00
9:58.3	Data point 16	0.34995 mL	0.06938 mL	0.06602 mL	1.15005 mL	0.02500 mL	4.486	0.09753	0.99353	0.00
10:34.6	Data point 17	0.34995 mL	0.06938 mL	0.06635 mL	1.15005 mL	0.02500 mL	5.383	0.10180	0.97831	0.00
11:51.4	Data point 18	0.34995 mL	0.06938 mL	0.06667 mL	1.15005 mL	0.02500 mL	6.161	0.09973	0.98637	0.00
13:07.2	Data point 19	0.34995 mL	0.06938 mL	0.06686 mL	1.15005 mL	0.02500 mL	6.770	0.04117	0.19616	0.00
13:50.0	Data point 20	0.34995 mL	0.06938 mL	0.06700 mL	1.15005 mL	0.02500 mL	7.134	0.09919	0.98835	0.00
14:43.0	Data point 21	0.34995 mL	0.06938 mL	0.06752 mL	1.15005 mL	0.02500 mL	8.402	0.09854	0.98501	0.00
15:36.4	Data point 22	0.34995 mL	0.06938 mL	0.06794 mL	1.15005 mL	0.02500 mL	9.543	0.09830	0.96711	0.00
16:14.7	Data point 23	0.34995 mL	0.06938 mL	0.06820 mL	1.15005 mL	0.02500 mL	9.986	0.09208	0.95270	0.00
16:37.8	Data point 24	0.34995 mL	0.06938 mL	0.06844 mL	1.15005 mL	0.02500 mL	10.261	0.04801	0.97672	0.00
16:59.4	Data point 25	0.34995 mL	0.06938 mL	0.06874 mL	1.15005 mL	0.02500 mL	10.484	0.01823	0.94847	0.00
17:16.0	Data point 26	0.34995 mL	0.06938 mL	0.06919 mL	1.15005 mL	0.02500 mL	10.716	0.00801	0.78329	0.00
17:48.1	Data point 27	0.34995 mL	0.06938 mL	0.06999 mL	1.15005 mL	0.02500 mL	10.908	-0.00456	0.47816	0.00
18:04.7	Data point 28	0.34995 mL	0.06938 mL	0.07121 mL	1.15005 mL	0.02500 mL	11.168	-0.00686	0.68564	0.00
18:31.6	Data point 29	0.34995 mL	0.06938 mL	0.07335 mL	1.15005 mL	0.02500 mL	11.360	-0.00865	0.82358	0.00
18:48.4	Data point 30	0.34995 mL	0.06938 mL	0.07679 mL	1.15005 mL	0.02500 mL	11.535	-0.01130	0.85034	0.00
19:05.1	Data point 31	0.34995 mL	0.06938 mL	0.08198 mL	1.15005 mL	0.02500 mL	11.739	-0.00808	0.86103	0.00
19:21.8	Data point 32	0.34995 mL	0.06938 mL	0.09043 mL	1.15005 mL	0.02500 mL	11.931	-0.00848	0.67730	0.00
19:38.6	Data point 33	0.34995 mL	0.06938 mL	0.09767 mL	1.15005 mL	0.02500 mL	12.037	-0.01044	0.80119	0.00
21:14.8	Reference spectrum									
22:18.7	Data point 35	0.50000 mL	0.16705 mL	0.09770 mL	1.15005 mL	0.02500 mL	2.003	-0.05079	0.93484	0.00
22:46.3	Data point 36	0.50000 mL	0.16705 mL	0.12293 mL	1.15005 mL	0.02500 mL	2.203	0.01287	0.91144	0.00
23:03.2	Data point 37	0.50000 mL	0.16705 mL	0.13859 mL	1.15005 mL	0.02500 mL	2.414	0.01037	0.65098	0.00
23:20.0	Data point 38	0.50000 mL	0.16705 mL	0.14819 mL	1.15005 mL	0.02500 mL	2.616	0.01363	0.60910	0.00
23:36.6	Data point 39	0.50000 mL	0.16705 mL	0.15421 mL	1.15005 mL	0.02500 mL	2.826	-0.00903	0.34930	0.00
23:53.3	Data point 40	0.50000 mL	0.16705 mL	0.15793 mL	1.15005 mL	0.02500 mL	3.013	-0.00206	0.04632	0.00
24:09.9	Data point 41	0.50000 mL	0.16705 mL	0.16035 mL	1.15005 mL	0.02500 mL	3.200	0.01501	0.89255	0.00
24:26.5	Data point 42	0.50000 mL	0.16705 mL	0.16190 mL	1.15005 mL	0.02500 mL	3.422	0.01644	0.94733	0.00
24:43.1	Data point 43	0.50000 mL	0.16705 mL	0.16284 mL	1.15005 mL	0.02500 mL	3.624	0.02437	0.97227	0.00
24:59.8	Data point 44	0.50000 mL	0.16705 mL	0.16343 mL	1.15005 mL	0.02500 mL	3.805	0.02905	0.97096	0.00
25:16.5	Data point 45	0.50000 mL	0.16705 mL	0.16381 mL	1.15005 mL	0.02500 mL	3.965	0.04928	0.99342	0.00
25:38.3	Data point 46	0.50000 mL	0.16705 mL	0.16420 mL	1.15005 mL	0.02500 mL	4.228	0.07452	0.98378	0.00
25:60.0	Data point 47	0.50000 mL	0.16705 mL	0.16449 mL	1.15005 mL	0.02500 mL	4.600	0.09855	0.98115	0.00
26:37.3	Data point 48	0.50000 mL	0.16705 mL	0.16475 mL	1.15005 mL	0.02500 mL	5.431	0.10026	0.98377	0.00
27:38.1	Data point 49	0.50000 mL	0.16705 mL	0.16489 mL	1.15005 mL	0.02500 mL	6.153	0.09994	0.98916	0.00
28:38.5	Data point 50	0.50000 mL	0.16705 mL	0.16501 mL	1.15005 mL	0.02500 mL	6.558	0.10011	0.98813	0.00
29:31.9	Data point 51	0.50000 mL	0.16705 mL	0.16512 mL	1.15005 mL	0.02500 mL	6.881	0.10044	0.99505	0.00
30:14.8	Data point 52	0.50000 mL	0.16705 mL	0.16524 mL	1.15005 mL	0.02500 mL	7.122	0.09788	0.96644	0.00
30:50.5	Data point 53	0.50000 mL	0.16705 mL	0.16538 mL	1.15005 mL	0.02500 mL	7.389	0.09901	0.95854	0.00
31:31.1	Data point 54	0.50000 mL	0.16705 mL	0.16552 mL	1.15005 mL	0.02500 mL	7.642	0.09787	0.96604	0.00
32:11.0	Data point 55	0.50000 mL	0.16705 mL	0.16566 mL	1.15005 mL	0.02500 mL	7.873	0.09270	0.96286	0.00
32:51.7	Data point 56	0.50000 mL	0.16705 mL	0.16583 mL	1.15005 mL	0.02500 mL	8.132	0.08120	0.77608	0.00
33:35.1	Data point 57	0.50000 mL	0.16705 mL	0.16595 mL	1.15005 mL	0.02500 mL	8.413	0.09728	0.97695	0.00
34:23.7	Data point 58	0.50000 mL	0.16705 mL	0.16609 mL	1.15005 mL	0.02500 mL	8.858	0.09553	0.97978	0.00
35:08.8	Data point 59	0.50000 mL	0.16705 mL	0.16618 mL	1.15005 mL	0.02500 mL	9.166	0.09567	0.96601	0.00
35:43.4	Data point 60	0.50000 mL	0.16705 mL	0.16630 mL	1.15005 mL	0.02500 mL	9.403	0.09848	0.97386	0.00
36:25.9	Data point 61	0.50000 mL	0.16705 mL	0.16653 mL	1.15005 mL	0.02500 mL	9.613	0.07771	0.94709	0.00
36:52.8	Data point 62	0.50000 mL	0.16705 mL	0.16684 mL	1.15005 mL	0.02500 mL	9.924	0.05173	0.85529	0.00
37:19.6	Data point 63	0.50000 mL	0.16705 mL	0.16707 mL	1.15005 mL	0.02500 mL	10.125	0.02066	0.73755	0.00
37:41.3	Data point 64	0.50000 mL	0.16705 mL	0.16738 mL	1.15005 mL	0.02500 mL	10.344	0.02074	0.91541	0.00
37:57.9	Data point 65	0.50000 mL	0.16705 mL	0.16785 mL	1.15005 mL	0.02500 mL	10.567	0.00543	0.57576	0.00
38:14.5	Data point 66	0.50000 mL	0.16705 mL	0.16863 mL	1.15005 mL	0.02500 mL	10.768	-0.00188	0.15760	0.00



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 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
38:31.2	Data point 67	0.50000 mL	0.16705 mL	0.16983 mL	1.15005 mL	0.02500 mL	10.979	-0.00609	0.62871	0.00000
38:47.9	Data point 68	0.50000 mL	0.16705 mL	0.17178 mL	1.15005 mL	0.02500 mL	11.185	-0.00756	0.74811	0.00000
39:04.6	Data point 69	0.50000 mL	0.16705 mL	0.17491 mL	1.15005 mL	0.02500 mL	11.371	-0.00945	0.82903	0.00000
39:21.3	Data point 70	0.50000 mL	0.16705 mL	0.17975 mL	1.15005 mL	0.02500 mL	11.555	-0.00926	0.73289	0.00000
39:38.1	Data point 71	0.50000 mL	0.16705 mL	0.18725 mL	1.15005 mL	0.02500 mL	11.734	-0.00798	0.73172	0.00000
39:54.9	Data point 72	0.50000 mL	0.16705 mL	0.19882 mL	1.15005 mL	0.02500 mL	11.924	-0.01110	0.88241	0.00000
40:11.7	Data point 73	0.50000 mL	0.16705 mL	0.20945 mL	1.15005 mL	0.02500 mL	12.040	-0.01095	0.86013	0.00000
41:56.7	Reference spectrum									
43:20.1	Data point 75	0.83996 mL	0.28916 mL	0.20948 mL	1.15005 mL	0.02500 mL	2.004	-0.02431	0.93368	0.00000
43:47.6	Data point 76	0.83996 mL	0.28916 mL	0.23742 mL	1.15005 mL	0.02500 mL	2.202	0.00620	0.41194	0.00000
44:04.5	Data point 77	0.83996 mL	0.28916 mL	0.25539 mL	1.15005 mL	0.02500 mL	2.405	-0.01003	0.55530	0.00000
44:21.3	Data point 78	0.83996 mL	0.28916 mL	0.26665 mL	1.15005 mL	0.02500 mL	2.609	-0.02086	0.76544	0.00000
44:38.0	Data point 79	0.83996 mL	0.28916 mL	0.27373 mL	1.15005 mL	0.02500 mL	2.800	0.00880	0.24244	0.00000
44:54.7	Data point 80	0.83996 mL	0.28916 mL	0.27822 mL	1.15005 mL	0.02500 mL	3.008	-0.01064	0.74355	0.00000
45:27.0	Data point 81	0.83996 mL	0.28916 mL	0.28100 mL	1.15005 mL	0.02500 mL	3.226	-0.00315	0.40221	0.00000
45:43.5	Data point 82	0.83996 mL	0.28916 mL	0.28269 mL	1.15005 mL	0.02500 mL	3.256	0.00440	0.36848	0.00000
46:15.7	Data point 83	0.83996 mL	0.28916 mL	0.28471 mL	1.15005 mL	0.02500 mL	3.453	0.00466	0.46582	0.00000
46:42.6	Data point 84	0.83996 mL	0.28916 mL	0.28561 mL	1.15005 mL	0.02500 mL	3.695	0.01261	0.86298	0.00000
46:59.2	Data point 85	0.83996 mL	0.28916 mL	0.28617 mL	1.15005 mL	0.02500 mL	3.962	-0.00347	0.11877	0.00000
47:20.8	Data point 86	0.83996 mL	0.28916 mL	0.28657 mL	1.15005 mL	0.02500 mL	4.193	0.02154	0.80647	0.00000
47:42.6	Data point 87	0.83996 mL	0.28916 mL	0.28685 mL	1.15005 mL	0.02500 mL	4.478	0.05846	0.97640	0.00000
48:04.3	Data point 88	0.83996 mL	0.28916 mL	0.28702 mL	1.15005 mL	0.02500 mL	4.762	0.09955	0.97840	0.00000
48:38.6	Data point 89	0.83996 mL	0.28916 mL	0.28713 mL	1.15005 mL	0.02500 mL	5.090	0.09982	0.97844	0.00000
49:13.4	Data point 90	0.83996 mL	0.28916 mL	0.28721 mL	1.15005 mL	0.02500 mL	5.406	0.09793	0.97129	0.00000
49:54.6	Data point 91	0.83996 mL	0.28916 mL	0.28728 mL	1.15005 mL	0.02500 mL	5.770	0.09682	0.97962	0.00000
50:35.1	Data point 92	0.83996 mL	0.28916 mL	0.28735 mL	1.15005 mL	0.02500 mL	6.111	0.10040	0.98527	0.00000
51:13.7	Data point 93	0.83996 mL	0.28916 mL	0.28744 mL	1.15005 mL	0.02500 mL	6.459	-0.09104	0.86486	0.00000
51:36.8	Data point 94	0.83996 mL	0.28916 mL	0.28756 mL	1.15005 mL	0.02500 mL	6.798	-0.08804	0.94071	0.00000
52:09.2	Data point 95	0.83996 mL	0.28916 mL	0.28768 mL	1.15005 mL	0.02500 mL	7.024	0.06972	0.92653	0.00000
52:35.9	Data point 96	0.83996 mL	0.28916 mL	0.28779 mL	1.15005 mL	0.02500 mL	7.234	0.07228	0.93274	0.00000
53:07.8	Data point 97	0.83996 mL	0.28916 mL	0.28791 mL	1.15005 mL	0.02500 mL	7.461	0.09796	0.95209	0.00000
53:41.2	Data point 98	0.83996 mL	0.28916 mL	0.28803 mL	1.15005 mL	0.02500 mL	7.711	0.09680	0.95770	0.00000
54:22.4	Data point 99	0.83996 mL	0.28916 mL	0.28815 mL	1.15005 mL	0.02500 mL	7.987	0.09811	0.98617	0.00000
55:02.2	Data point 100	0.83996 mL	0.28916 mL	0.28824 mL	1.15005 mL	0.02500 mL	8.285	0.09495	0.97195	0.00000
55:45.2	Data point 101	0.83996 mL	0.28916 mL	0.28834 mL	1.15005 mL	0.02500 mL	8.674	0.09809	0.97115	0.00000
56:31.6	Data point 102	0.83996 mL	0.28916 mL	0.28843 mL	1.15005 mL	0.02500 mL	9.037	0.09466	0.97462	0.00000
57:07.4	Data point 103	0.83996 mL	0.28916 mL	0.28852 mL	1.15005 mL	0.02500 mL	9.300	0.09795	0.96385	0.00000
57:33.6	Data point 104	0.83996 mL	0.28916 mL	0.28864 mL	1.15005 mL	0.02500 mL	9.547	0.07142	0.92319	0.00000
57:55.3	Data point 105	0.83996 mL	0.28916 mL	0.28880 mL	1.15005 mL	0.02500 mL	9.778	0.03069	0.84642	0.00000
58:22.1	Data point 106	0.83996 mL	0.28916 mL	0.28904 mL	1.15005 mL	0.02500 mL	9.974	0.02306	0.88036	0.00000
58:54.1	Data point 107	0.83996 mL	0.28916 mL	0.28939 mL	1.15005 mL	0.02500 mL	10.169	0.00844	0.64351	0.00000
59:20.9	Data point 108	0.83996 mL	0.28916 mL	0.28989 mL	1.15005 mL	0.02500 mL	10.361	-0.00507	0.45673	0.00000
59:37.5	Data point 109	0.83996 mL	0.28916 mL	0.29062 mL	1.15005 mL	0.02500 mL	10.564	-0.01881	0.85998	0.00000
59:54.1	Data point 110	0.83996 mL	0.28916 mL	0.29177 mL	1.15005 mL	0.02500 mL	10.733	-0.01832	0.84759	0.00000
1:00:15.8	Data point 111	0.83996 mL	0.28916 mL	0.29391 mL	1.15005 mL	0.02500 mL	10.929	-0.01790	0.91238	0.00000
1:00:42.8	Data point 112	0.83996 mL	0.28916 mL	0.29605 mL	1.15005 mL	0.02500 mL	11.121	-0.01153	0.81972	0.00000
1:01:19.9	Data point 113	0.83996 mL	0.28916 mL	0.30151 mL	1.15005 mL	0.02500 mL	11.333	-0.01409	0.88999	0.00000
1:01:46.9	Data point 114	0.83996 mL	0.28916 mL	0.30790 mL	1.15005 mL	0.02500 mL	11.523	-0.01340	0.84840	0.00000
1:02:03.8	Data point 115	0.83996 mL	0.28916 mL	0.31851 mL	1.15005 mL	0.02500 mL	11.711	-0.02495	0.87784	0.00000
1:02:20.9	Data point 116	0.83996 mL	0.28916 mL	0.33525 mL	1.15005 mL	0.02500 mL	11.900	-0.02159	0.93148	0.00000
1:02:38.0	Data point 117	0.83996 mL	0.28916 mL	0.35414 mL	1.15005 mL	0.02500 mL	12.040	-0.02303	0.91232	0.00000
1:04:37.7	Assay volumes	1.08996 mL	0.43424 mL	0.35414 mL	1.15005 mL	0.02500 mL				

## Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
<b>General Settings</b>				

Sample name: **D06**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06003**  
 Filename: **C:\Sirius\_T3\17J-06003\_D06\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 2:22:58 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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			
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			

Sample name: **D06**  
 Assay name: **UV-metric pKa**  
 Assay ID: **17J-06003**  
 Filename: **C:\Sirius\_T3\17J-06003\_D06\_UV-metric pKa.t3r**

Experiment start time: **10/6/2017 2:22:58 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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	0.125	10/6/2017 2:22:57 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus S	0.9949	10/6/2017 2:22:57 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jH	0.8	10/6/2017 2:22:57 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jOH	-1.3	10/6/2017 2:22:57 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Base concentration factor	1.011	10/6/2017 2:22:58 AM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	1.003	10/6/2017 2:22:57 AM	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 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	8-18-17	9/26/2017 8:05:04 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	166940	9/8/2017 8:21:27 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9-22-17	9/22/2017 3:02:42 PM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	9-26-17	10/5/2017 4:02:03 PM
Port B	Cyclohexane		9/19/2017 1:15:02 PM
Port C	MeCN (50%, 0.15 M KCl)	10-2-17	10/2/2017 10:28:55 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM

Sample name: **D06**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06003**  
 Filename: **C:\Sirius\_T3\17J-06003\_D06\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 2:22:58 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Phosphate Buffer		9/12/2017 11:32:29 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	9-14-17	9/14/2017 9:30:38 AM
Titrator		T3TM1100153	3/31/2009 5:24:17 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 9:21:54 AM
E0 calibration	-8.99 mV		10/6/2017 2:23:22 AM
Filling solution	3M KCl	KCL095	10/4/2017 2:50:10 PM
Liquids			
Wash 1	50% IPA:50% Water		10/5/2017 8:59:12 AM
Wash 2	0.5% Triton X-100 in H2O		10/5/2017 8:59:14 AM
Buffer position 1	pH7 Wash		10/5/2017 8:59:17 AM
Buffer position 2	pH 7		10/5/2017 8:59:19 AM
Storage position			10/5/2017 8:58:45 AM
Wash water	4.9e+003 mL	10-3-17	10/3/2017 8:04:49 AM
Waste	5.1e+003 mL		10/3/2017 8:04:54 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		072390	11/23/2010 11:22:28 AM
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 11:22:28 AM
Calibrated on	10/5/2017 9:23:25 AM		
Integration time	11		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 9:34:13 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		



## Assay Settings

Sample name: **D06**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-06003**  
Filename: **C:\Sirius\_T3\17J-06003\_D06\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 2:22:58 AM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

### Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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 C3