

Sample name: **D09**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-06009**  
Filename: **C:\Sirius\_T3\17J-06009\_D09\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 10:11:03 AM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

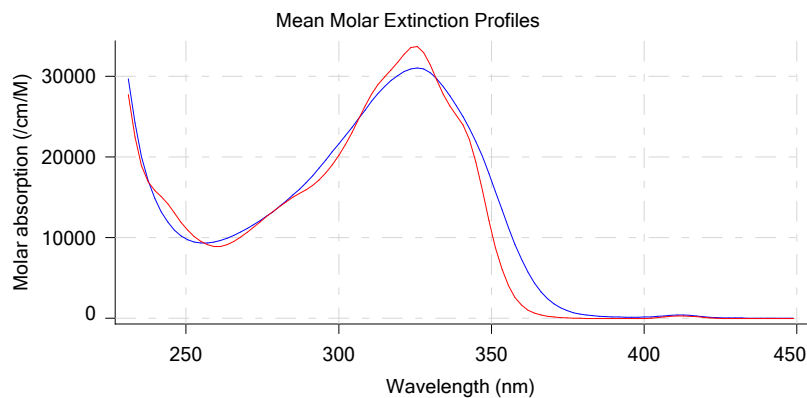
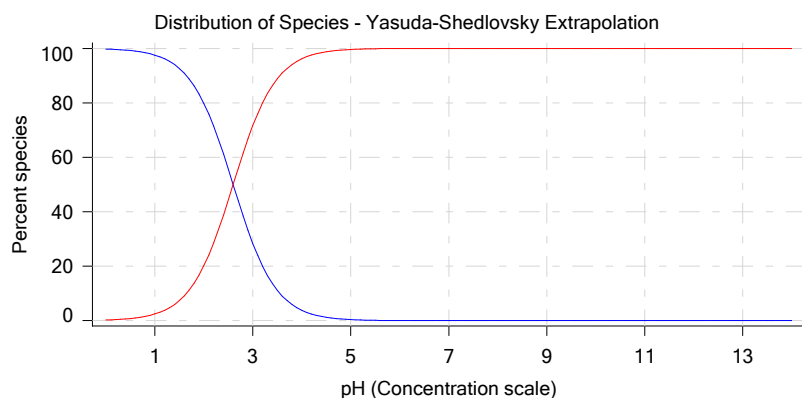
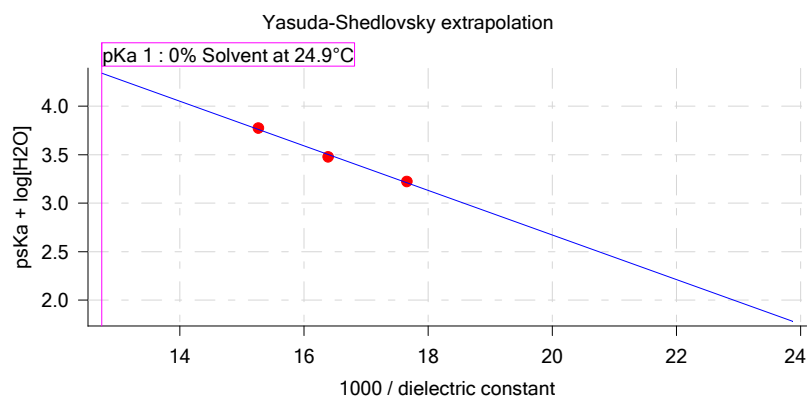
## Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R <sup>2</sup>	Ionic strength	Temperature
Yasuda-Shedlovsky	2.60	±0.07	7.26	-229.6136	0.9935	0.165 M	24.9°C

## Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1
17J-06009 Points 4 to 34	49.49 %	Up	UV-metric pKa	56.6	24.7 M	0.157 M	24.9°C	✓ 1.83
17J-06009 Points 36 to 74	39.96 %	Up	UV-metric pKa	61.0	30.0 M	0.166 M	24.9°C	✓ 2.00
17J-06009 Points 76 to 116	30.08 %	Up	UV-metric pKa	65.5	35.8 M	0.172 M	24.9°C	✓ 2.22

## Graphs



## UV-metric psKa Titration 1 of 3 17J-06009 Points 4 to 34

### Results

pKa 1	<b>1.83</b>
RMSD	<b>0.001 0.002</b>
Chi squared	<b>0.0026</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>29.5 µM to 27.8 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 1.462 to 12.533

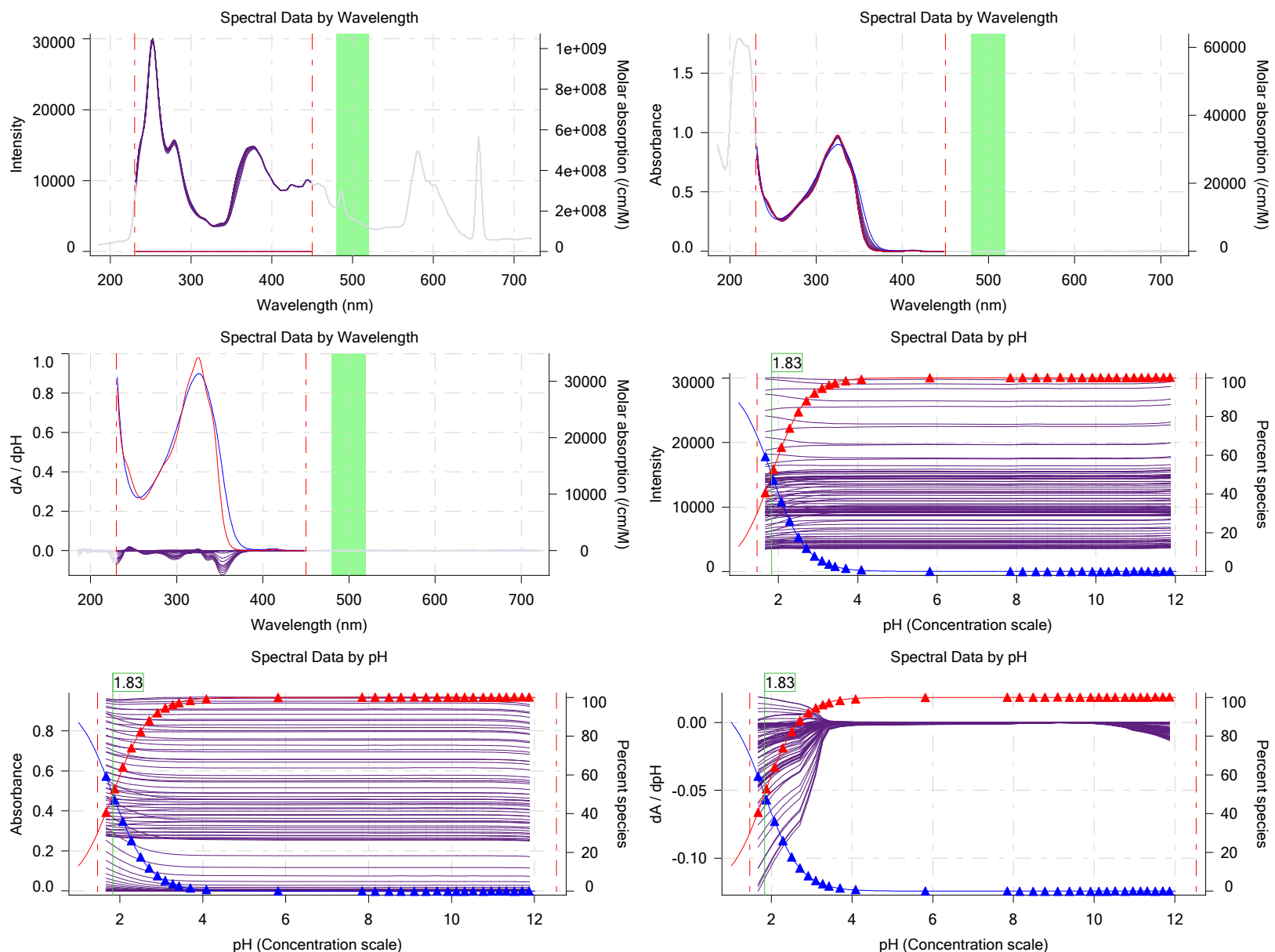
## Warnings and errors

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			

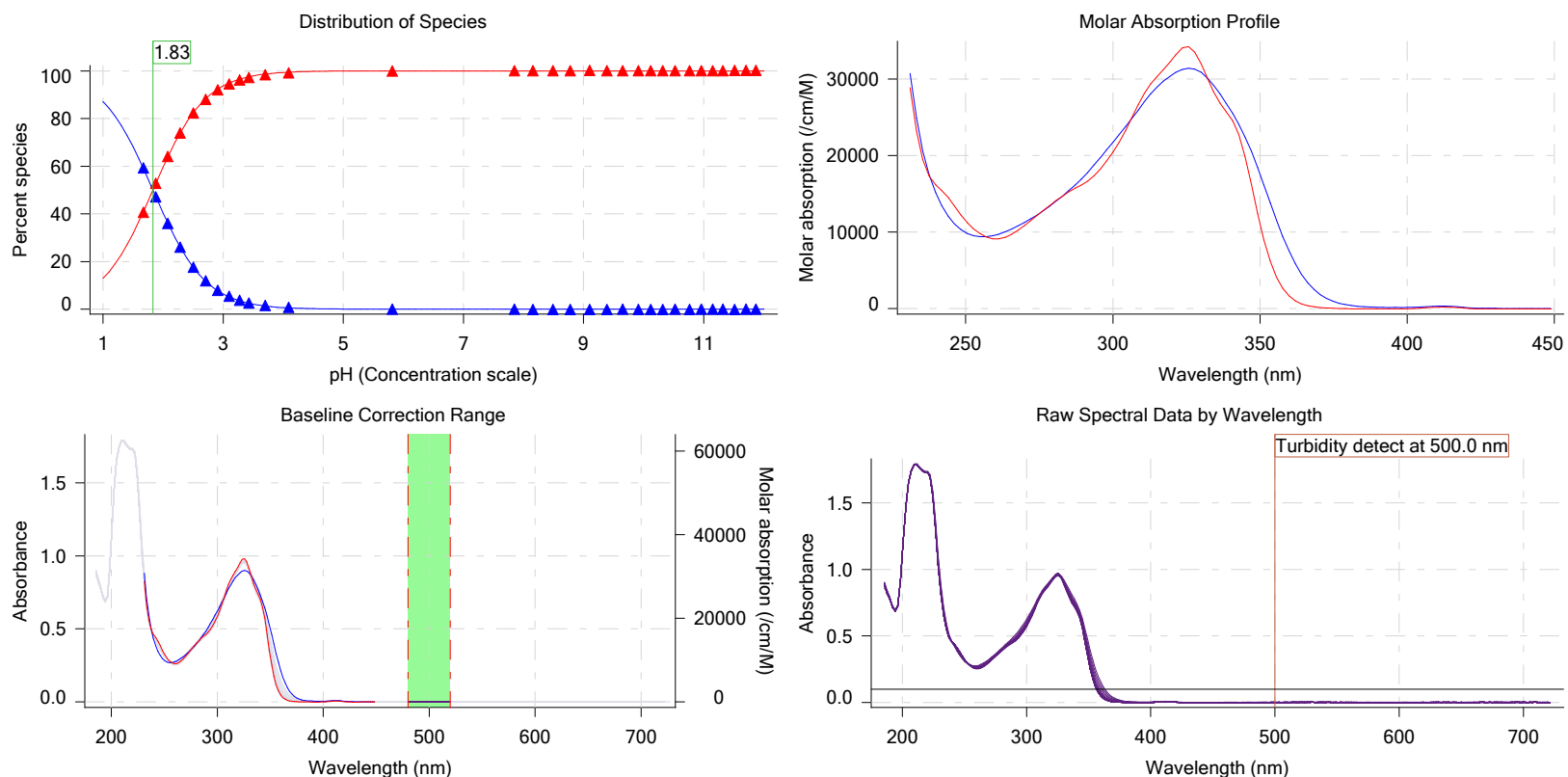
## Graphs



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## Graphs (continued)



## UV-metric psKa Titration 2 of 3 17J-06009 Points 36 to 74

### Results

pKa 1	<b>2.00</b>
RMSD	<b>0.001 0.001</b>
Chi squared	<b>0.0025</b>
PCA calculated number of pKas	<b>4</b>
Average ionic strength	<b>0.166 M</b>
Average temperature	<b>24.9°C</b>
Analyte concentration range	<b>24.2 µM to 22.9 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>1.506 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**

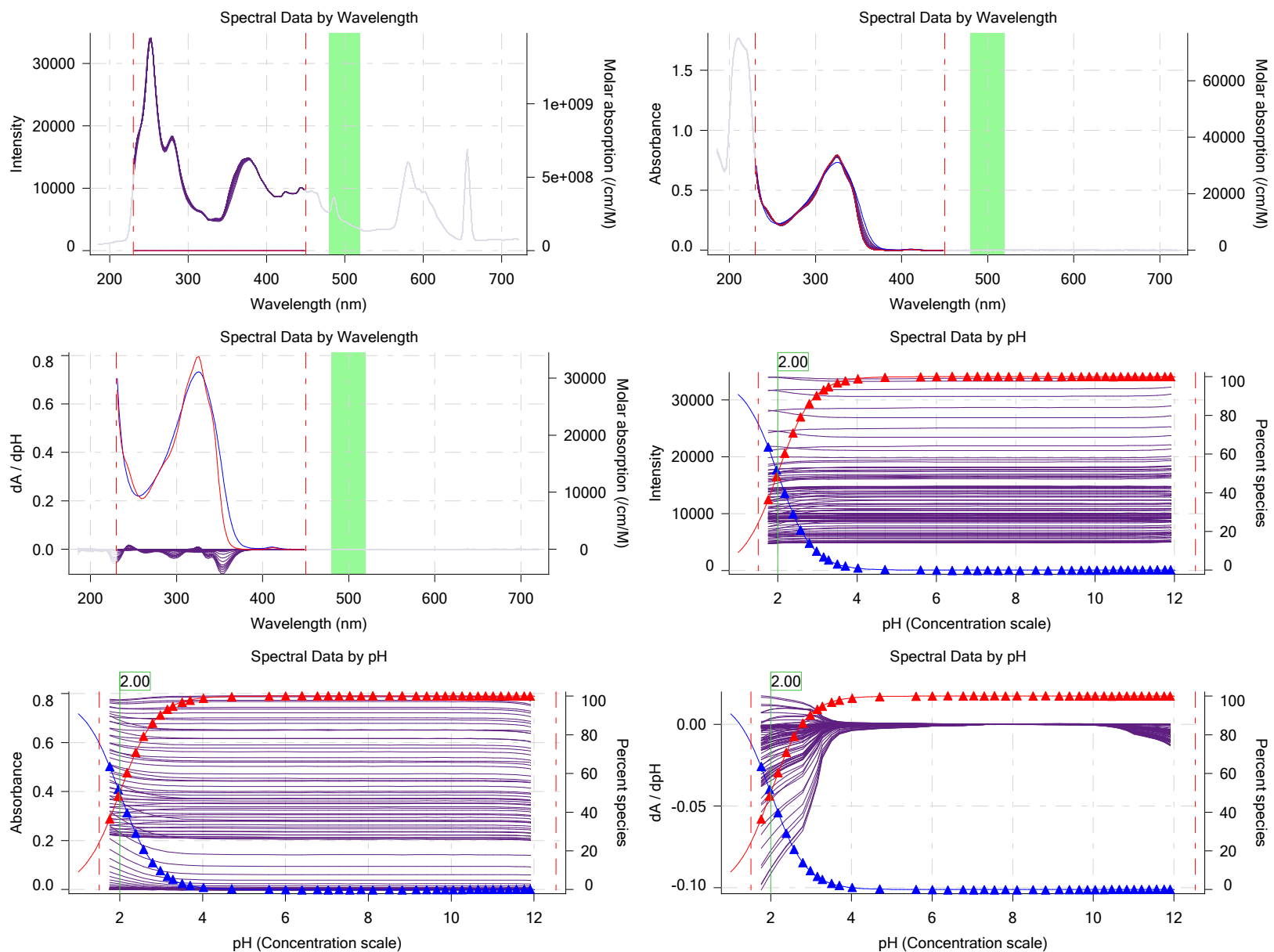
Sample name: **D09**  
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 Assay ID: **17J-06009**  
 Filename: **C:\Sirius\_T3\17J-06009\_D09\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 10:11:03 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			

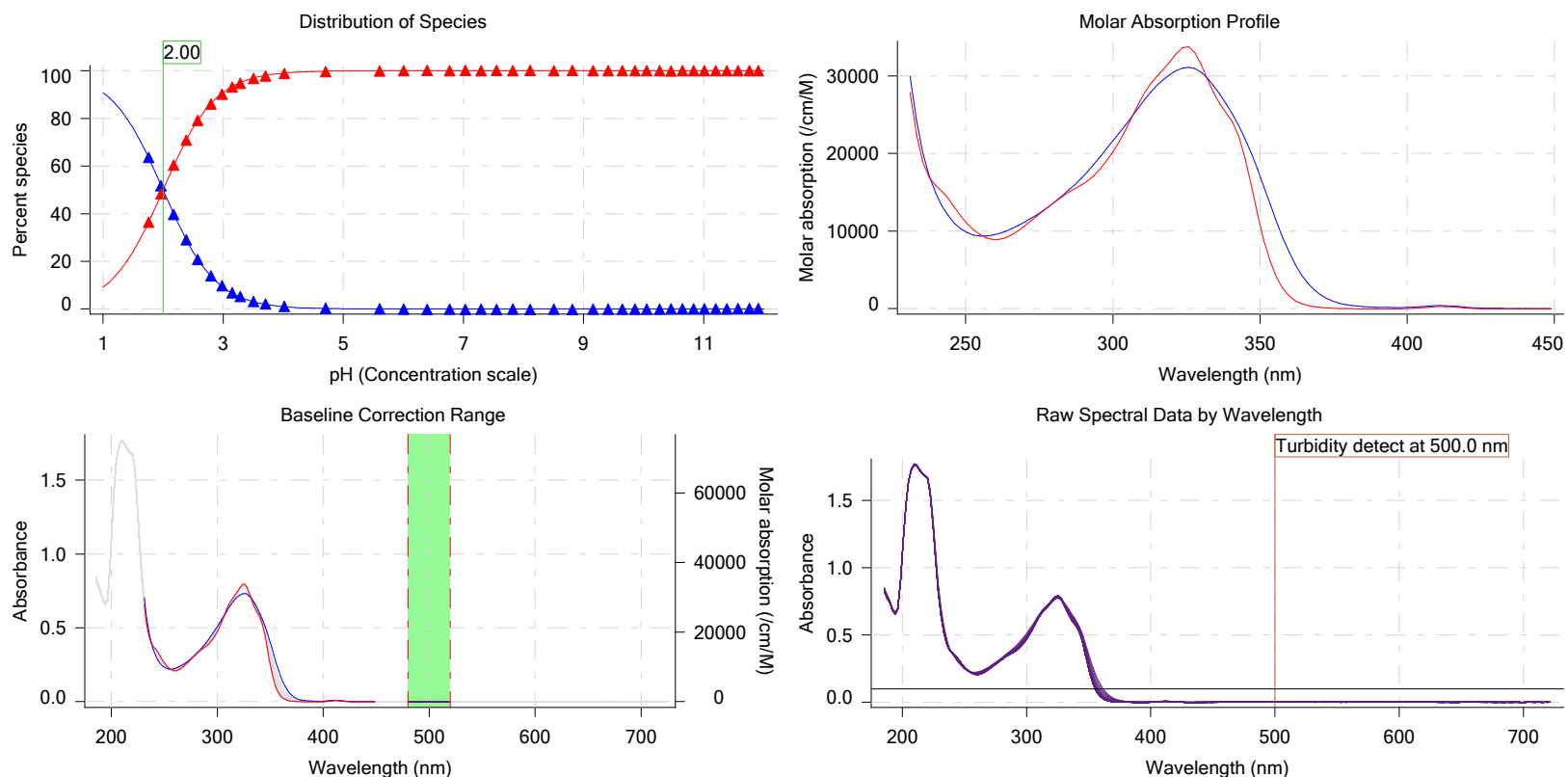
## Graphs



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## Graphs (continued)



## UV-metric psKa Titration 3 of 3 17J-06009 Points 76 to 116

### Results

pKa 1	<b>2.22</b>
RMSD	<b>0.002 0.001</b>
Chi squared	<b>0.0027</b>
PCA calculated number of pKas	<b>3</b>
Average ionic strength	<b>0.172 M</b>
Average temperature	<b>24.9°C</b>
Analyte concentration range	<b>18.6 µM to 17.6 µM</b>
Methanol weight %	<b>30.1 %</b>
Dielectric constant	<b>65.5</b>
Water concentration	<b>35.8 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 12.541</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**

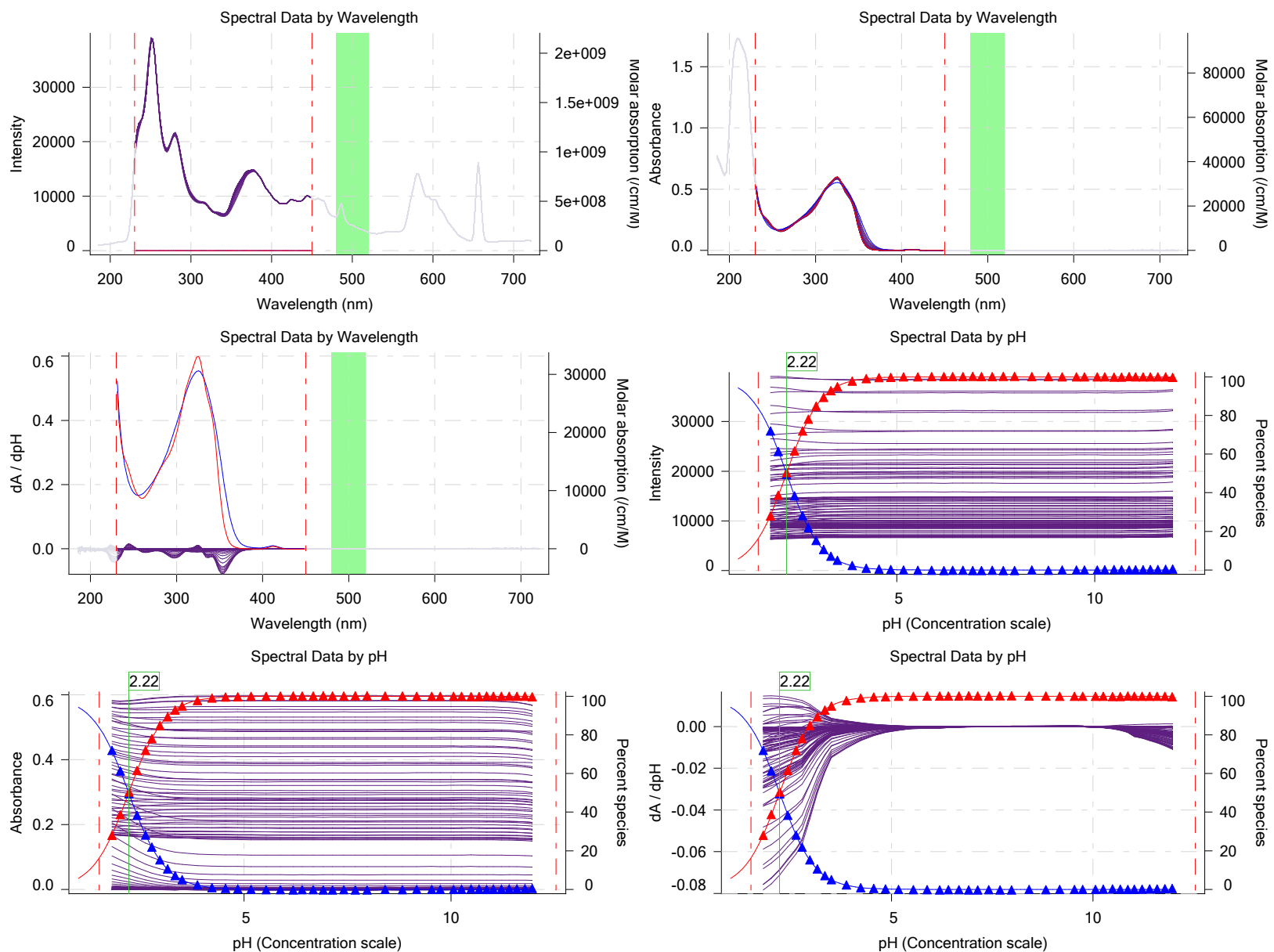
Sample name: **D09**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06009**  
 Filename: **C:\Sirius\_T3\17J-06009\_D09\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 10:11:03 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			

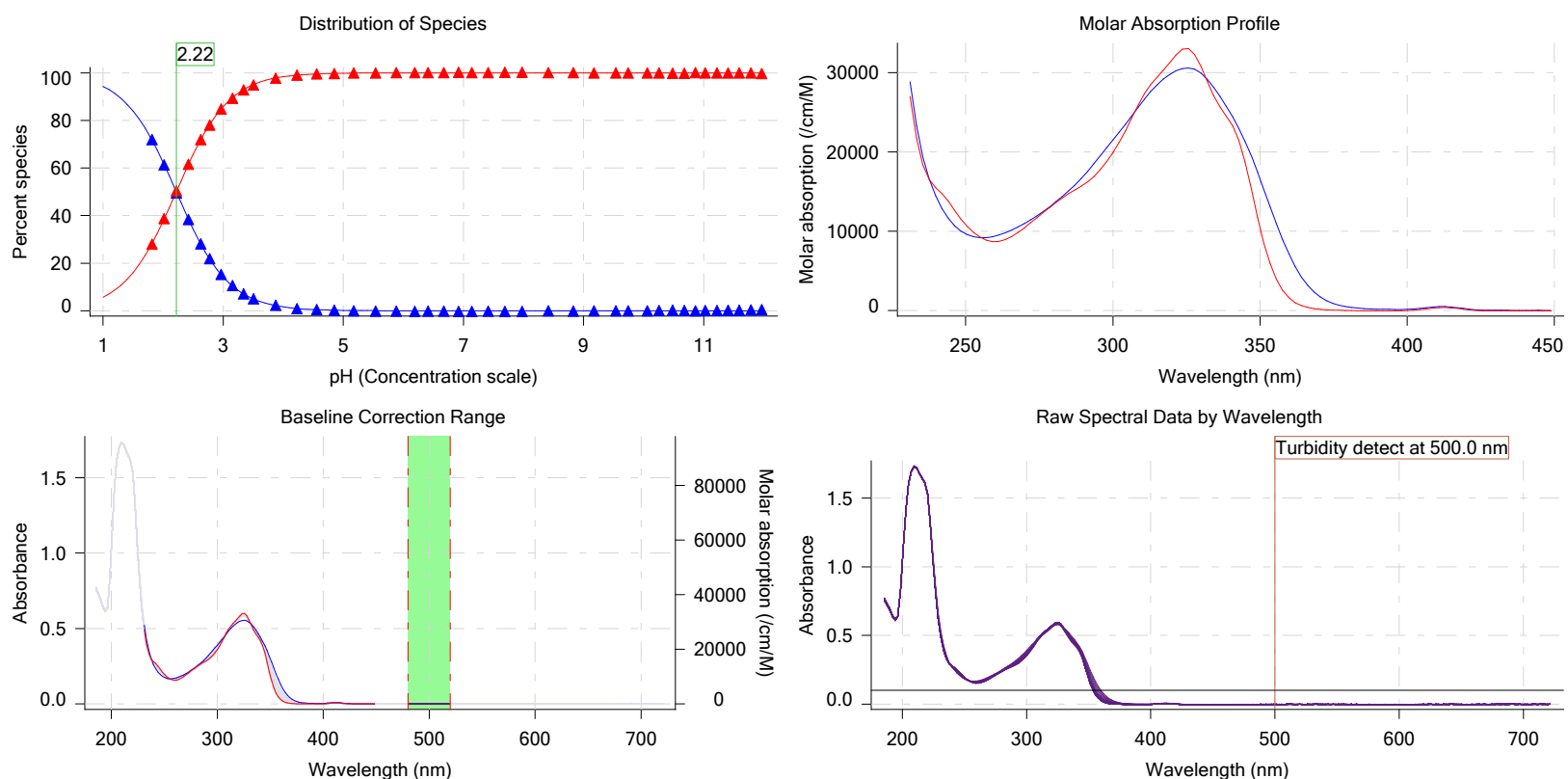
## Graphs



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## Graphs (continued)



## Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	D09	10/2/2017 11:57:35 AM	User entered value
Sample by	Volume		Default value
Sample volume	0.0015 mL	10/5/2017 3:30:01 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.031400 M	10/2/2017 11:59:31 AM	User entered value
Solubility	Unknown		Default value
Molecular weight	391.42	9/29/2017 5:41:30 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	9/29/2017 5:41:11 PM	User entered value
Sample is a	Base	9/29/2017 5:41:11 PM	User entered value
pKa 1	4.74	9/29/2017 5:41:11 PM	User entered value
logp (XH +)	-10.00		Default value
logP (neutral X)	-10.00	9/29/2017 5:41:11 PM	User entered value

## Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:37.9	Dark spectrum								
3:39.3	Reference spectrum								
4:06.9	Volume reset due to vial change								
4:51.1	Initial pH = 8.38								
6:02.7	Data point 4	0.34995 mL	0.06921 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.962	-0.01160	0.72902
6:31.4	Data point 5	0.34995 mL	0.06921 mL	0.02493 mL	1.15005 mL	0.02500 mL	2.162	-0.01226	0.68615
6:48.4	Data point 6	0.34995 mL	0.06921 mL	0.04076 mL	1.15005 mL	0.02500 mL	2.359	0.02042	0.89847
7:05.2	Data point 7	0.34995 mL	0.06921 mL	0.05078 mL	1.15005 mL	0.02500 mL	2.561	0.01145	0.43707
7:21.9	Data point 8	0.34995 mL	0.06921 mL	0.05713 mL	1.15005 mL	0.02500 mL	2.779	0.00636	0.41702
7:38.6	Data point 9	0.34995 mL	0.06921 mL	0.06096 mL	1.15005 mL	0.02500 mL	2.981	0.00308	0.36600



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**Events (continued)**

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
7:55.2	Data point 10	0.34995 mL	0.06921 mL	0.06336 mL	1.15005 mL	0.02500 mL	3.183	-0.00373	0.26881	0.00
8:11.8	Data point 11	0.34995 mL	0.06921 mL	0.06486 mL	1.15005 mL	0.02500 mL	3.366	0.00623	0.65374	0.00
8:28.3	Data point 12	0.34995 mL	0.06921 mL	0.06585 mL	1.15005 mL	0.02500 mL	3.542	0.01130	0.88495	0.00
8:44.9	Data point 13	0.34995 mL	0.06921 mL	0.06651 mL	1.15005 mL	0.02500 mL	3.695	0.01648	0.87029	0.00
9:11.9	Data point 14	0.34995 mL	0.06921 mL	0.06771 mL	1.15005 mL	0.02500 mL	3.965	0.03988	0.98731	0.00
9:33.5	Data point 15	0.34995 mL	0.06921 mL	0.06818 mL	1.15005 mL	0.02500 mL	4.347	0.08353	0.98868	0.00
10:00.3	Data point 16	0.34995 mL	0.06921 mL	0.06863 mL	1.15005 mL	0.02500 mL	6.054	0.09955	0.99352	0.00
11:04.7	Data point 17	0.34995 mL	0.06921 mL	0.06919 mL	1.15005 mL	0.02500 mL	8.063	0.07896	0.61814	0.00
11:38.6	Data point 18	0.34995 mL	0.06921 mL	0.06945 mL	1.15005 mL	0.02500 mL	8.369	0.09990	0.99461	0.00
12:25.6	Data point 19	0.34995 mL	0.06921 mL	0.06961 mL	1.15005 mL	0.02500 mL	8.701	0.09706	0.98765	0.00
13:13.0	Data point 20	0.34995 mL	0.06921 mL	0.06971 mL	1.15005 mL	0.02500 mL	8.985	0.04908	0.26021	0.00
13:54.3	Data point 21	0.34995 mL	0.06921 mL	0.06980 mL	1.15005 mL	0.02500 mL	9.303	0.09323	0.87444	0.00
14:29.0	Data point 22	0.34995 mL	0.06921 mL	0.06990 mL	1.15005 mL	0.02500 mL	9.588	0.09524	0.93603	0.00
15:03.8	Data point 23	0.34995 mL	0.06921 mL	0.07001 mL	1.15005 mL	0.02500 mL	9.847	0.09843	0.95069	0.00
15:27.4	Data point 24	0.34995 mL	0.06921 mL	0.07016 mL	1.15005 mL	0.02500 mL	10.105	0.06845	0.95141	0.00
15:49.0	Data point 25	0.34995 mL	0.06921 mL	0.07032 mL	1.15005 mL	0.02500 mL	10.311	0.03669	0.87375	0.00
16:10.6	Data point 26	0.34995 mL	0.06921 mL	0.07051 mL	1.15005 mL	0.02500 mL	10.509	0.01373	0.83520	0.00
16:37.0	Data point 27	0.34995 mL	0.06921 mL	0.07093 mL	1.15005 mL	0.02500 mL	10.708	0.00368	0.34936	0.00
16:53.6	Data point 28	0.34995 mL	0.06921 mL	0.07171 mL	1.15005 mL	0.02500 mL	10.950	-0.00162	0.10545	0.00
17:25.3	Data point 29	0.34995 mL	0.06921 mL	0.07317 mL	1.15005 mL	0.02500 mL	11.142	-0.00882	0.78979	0.00
17:42.0	Data point 30	0.34995 mL	0.06921 mL	0.07524 mL	1.15005 mL	0.02500 mL	11.328	-0.00659	0.75416	0.00
17:58.6	Data point 31	0.34995 mL	0.06921 mL	0.07843 mL	1.15005 mL	0.02500 mL	11.496	-0.00774	0.84523	0.00
18:25.7	Data point 32	0.34995 mL	0.06921 mL	0.08307 mL	1.15005 mL	0.02500 mL	11.688	-0.00931	0.75374	0.00
18:42.4	Data point 33	0.34995 mL	0.06921 mL	0.09057 mL	1.15005 mL	0.02500 mL	11.871	-0.00803	0.72698	0.00
18:59.1	Data point 34	0.34995 mL	0.06921 mL	0.10071 mL	1.15005 mL	0.02500 mL	12.033	0.00176	0.16061	0.00
20:35.4	Reference spectrum									
21:39.4	Data point 36	0.50000 mL	0.16832 mL	0.10073 mL	1.15005 mL	0.02500 mL	2.006	-0.04727	0.92750	0.00
22:06.9	Data point 37	0.50000 mL	0.16832 mL	0.12486 mL	1.15005 mL	0.02500 mL	2.204	0.00723	0.63151	0.00
22:23.9	Data point 38	0.50000 mL	0.16832 mL	0.14062 mL	1.15005 mL	0.02500 mL	2.413	0.01564	0.87449	0.00
22:40.7	Data point 39	0.50000 mL	0.16832 mL	0.15031 mL	1.15005 mL	0.02500 mL	2.618	0.01017	0.51891	0.00
22:57.4	Data point 40	0.50000 mL	0.16832 mL	0.15635 mL	1.15005 mL	0.02500 mL	2.807	0.01522	0.63423	0.00
23:14.1	Data point 41	0.50000 mL	0.16832 mL	0.16018 mL	1.15005 mL	0.02500 mL	3.021	0.00146	0.02163	0.00
23:30.7	Data point 42	0.50000 mL	0.16832 mL	0.16254 mL	1.15005 mL	0.02500 mL	3.203	0.01378	0.90878	0.00
23:47.4	Data point 43	0.50000 mL	0.16832 mL	0.16409 mL	1.15005 mL	0.02500 mL	3.375	0.01226	0.91516	0.00
24:04.0	Data point 44	0.50000 mL	0.16832 mL	0.16512 mL	1.15005 mL	0.02500 mL	3.503	0.01544	0.94426	0.00
24:35.9	Data point 45	0.50000 mL	0.16832 mL	0.16613 mL	1.15005 mL	0.02500 mL	3.725	0.02778	0.93811	0.00
25:02.6	Data point 46	0.50000 mL	0.16832 mL	0.16663 mL	1.15005 mL	0.02500 mL	3.920	0.02064	0.90014	0.00
25:19.2	Data point 47	0.50000 mL	0.16832 mL	0.16691 mL	1.15005 mL	0.02500 mL	4.233	0.06294	0.98401	0.00
25:40.8	Data point 48	0.50000 mL	0.16832 mL	0.16719 mL	1.15005 mL	0.02500 mL	4.912	0.09924	0.99069	0.00
26:22.5	Data point 49	0.50000 mL	0.16832 mL	0.16740 mL	1.15005 mL	0.02500 mL	5.801	0.09868	0.96483	0.00
27:20.0	Data point 50	0.50000 mL	0.16832 mL	0.16750 mL	1.15005 mL	0.02500 mL	6.200	0.10006	0.99204	0.00
28:13.7	Data point 51	0.50000 mL	0.16832 mL	0.16759 mL	1.15005 mL	0.02500 mL	6.586	0.09936	0.98955	0.00
28:54.8	Data point 52	0.50000 mL	0.16832 mL	0.16769 mL	1.15005 mL	0.02500 mL	6.959	0.08893	0.79091	0.00
29:22.3	Data point 53	0.50000 mL	0.16832 mL	0.16778 mL	1.15005 mL	0.02500 mL	7.216	0.09688	0.98842	0.00
29:59.6	Data point 54	0.50000 mL	0.16832 mL	0.16790 mL	1.15005 mL	0.02500 mL	7.476	0.10027	0.98417	0.00
30:35.4	Data point 55	0.50000 mL	0.16832 mL	0.16802 mL	1.15005 mL	0.02500 mL	7.731	0.10048	0.98940	0.00
31:17.4	Data point 56	0.50000 mL	0.16832 mL	0.16813 mL	1.15005 mL	0.02500 mL	7.999	0.09949	0.98475	0.00
31:57.5	Data point 57	0.50000 mL	0.16832 mL	0.16823 mL	1.15005 mL	0.02500 mL	8.284	0.09761	0.96567	0.00
32:41.8	Data point 58	0.50000 mL	0.16832 mL	0.16832 mL	1.15005 mL	0.02500 mL	8.674	0.09699	0.97358	0.00
33:25.0	Data point 59	0.50000 mL	0.16832 mL	0.16839 mL	1.15005 mL	0.02500 mL	8.981	0.09786	0.96340	0.00
34:11.5	Data point 60	0.50000 mL	0.16832 mL	0.16849 mL	1.15005 mL	0.02500 mL	9.318	0.09589	0.97202	0.00
34:43.4	Data point 61	0.50000 mL	0.16832 mL	0.16858 mL	1.15005 mL	0.02500 mL	9.569	0.09930	0.97062	0.00
35:20.9	Data point 62	0.50000 mL	0.16832 mL	0.16872 mL	1.15005 mL	0.02500 mL	9.806	0.09458	0.96038	0.00
35:48.2	Data point 63	0.50000 mL	0.16832 mL	0.16889 mL	1.15005 mL	0.02500 mL	10.011	0.05105	0.96657	0.00
36:15.0	Data point 64	0.50000 mL	0.16832 mL	0.16912 mL	1.15005 mL	0.02500 mL	10.205	0.02466	0.80430	0.00
36:31.6	Data point 65	0.50000 mL	0.16832 mL	0.16945 mL	1.15005 mL	0.02500 mL	10.416	0.01005	0.78158	0.00
36:48.3	Data point 66	0.50000 mL	0.16832 mL	0.16999 mL	1.15005 mL	0.02500 mL	10.608	0.00193	0.17348	0.00



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## Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
37:05.0	Data point 67	0.50000 mL	0.16832 mL	0.17084 mL	1.15005 mL	0.02500 mL	10.795	-0.00435	0.60011	0.00000
37:21.7	Data point 68	0.50000 mL	0.16832 mL	0.17213 mL	1.15005 mL	0.02500 mL	10.975	-0.00691	0.71185	0.00000
37:38.3	Data point 69	0.50000 mL	0.16832 mL	0.17408 mL	1.15005 mL	0.02500 mL	11.153	-0.01058	0.88161	0.00000
37:55.0	Data point 70	0.50000 mL	0.16832 mL	0.17702 mL	1.15005 mL	0.02500 mL	11.340	-0.01252	0.87270	0.00000
38:11.7	Data point 71	0.50000 mL	0.16832 mL	0.18154 mL	1.15005 mL	0.02500 mL	11.522	-0.01245	0.86822	0.00000
38:28.3	Data point 72	0.50000 mL	0.16832 mL	0.18850 mL	1.15005 mL	0.02500 mL	11.705	-0.00730	0.80850	0.00000
38:45.2	Data point 73	0.50000 mL	0.16832 mL	0.19929 mL	1.15005 mL	0.02500 mL	11.887	-0.01215	0.86269	0.00000
39:02.1	Data point 74	0.50000 mL	0.16832 mL	0.21242 mL	1.15005 mL	0.02500 mL	12.031	-0.00511	0.67286	0.00000
40:47.4	Reference spectrum									
42:10.8	Data point 76	0.83996 mL	0.30115 mL	0.21244 mL	1.15005 mL	0.02500 mL	2.004	-0.02368	0.92786	0.00000
42:38.5	Data point 77	0.83996 mL	0.30115 mL	0.24001 mL	1.15005 mL	0.02500 mL	2.198	0.00557	0.42656	0.00000
42:55.4	Data point 78	0.83996 mL	0.30115 mL	0.25816 mL	1.15005 mL	0.02500 mL	2.403	-0.01811	0.62950	0.00000
43:12.2	Data point 79	0.83996 mL	0.30115 mL	0.26950 mL	1.15005 mL	0.02500 mL	2.599	-0.01759	0.71452	0.00000
43:28.9	Data point 80	0.83996 mL	0.30115 mL	0.27676 mL	1.15005 mL	0.02500 mL	2.801	0.00921	0.24904	0.00000
44:01.3	Data point 81	0.83996 mL	0.30115 mL	0.28126 mL	1.15005 mL	0.02500 mL	2.947	0.00283	0.14048	0.00000
44:28.3	Data point 82	0.83996 mL	0.30115 mL	0.28403 mL	1.15005 mL	0.02500 mL	3.138	0.00445	0.48530	0.00000
44:44.9	Data point 83	0.83996 mL	0.30115 mL	0.28610 mL	1.15005 mL	0.02500 mL	3.325	-0.01183	0.62179	0.00000
45:01.6	Data point 84	0.83996 mL	0.30115 mL	0.28744 mL	1.15005 mL	0.02500 mL	3.509	-0.00478	0.30125	0.00000
45:18.2	Data point 85	0.83996 mL	0.30115 mL	0.28831 mL	1.15005 mL	0.02500 mL	3.672	-0.00038	0.00282	0.00000
45:50.1	Data point 86	0.83996 mL	0.30115 mL	0.28993 mL	1.15005 mL	0.02500 mL	4.039	0.00565	0.23934	0.00000
46:12.0	Data point 87	0.83996 mL	0.30115 mL	0.29041 mL	1.15005 mL	0.02500 mL	4.389	0.02545	0.69884	0.00000
46:33.5	Data point 88	0.83996 mL	0.30115 mL	0.29066 mL	1.15005 mL	0.02500 mL	4.713	0.09898	0.98875	0.00000
47:03.7	Data point 89	0.83996 mL	0.30115 mL	0.29080 mL	1.15005 mL	0.02500 mL	5.005	0.09675	0.91887	0.00000
47:37.8	Data point 90	0.83996 mL	0.30115 mL	0.29090 mL	1.15005 mL	0.02500 mL	5.322	0.10047	0.98503	0.00000
48:16.1	Data point 91	0.83996 mL	0.30115 mL	0.29097 mL	1.15005 mL	0.02500 mL	5.686	0.09935	0.97488	0.00000
48:55.7	Data point 92	0.83996 mL	0.30115 mL	0.29104 mL	1.15005 mL	0.02500 mL	6.025	0.09877	0.99208	0.00000
49:36.9	Data point 93	0.83996 mL	0.30115 mL	0.29113 mL	1.15005 mL	0.02500 mL	6.333	-0.01223	0.10658	0.00000
49:58.5	Data point 94	0.83996 mL	0.30115 mL	0.29120 mL	1.15005 mL	0.02500 mL	6.551	0.08906	0.92172	0.00000
50:20.1	Data point 95	0.83996 mL	0.30115 mL	0.29130 mL	1.15005 mL	0.02500 mL	6.812	0.01892	0.21970	0.00000
50:41.7	Data point 96	0.83996 mL	0.30115 mL	0.29139 mL	1.15005 mL	0.02500 mL	7.053	0.04458	0.59365	0.00000
51:08.3	Data point 97	0.83996 mL	0.30115 mL	0.29149 mL	1.15005 mL	0.02500 mL	7.274	0.09512	0.92522	0.00000
51:40.0	Data point 98	0.83996 mL	0.30115 mL	0.29160 mL	1.15005 mL	0.02500 mL	7.542	0.09547	0.97282	0.00000
52:21.0	Data point 99	0.83996 mL	0.30115 mL	0.29172 mL	1.15005 mL	0.02500 mL	7.820	0.10010	0.99217	0.00000
52:59.3	Data point 100	0.83996 mL	0.30115 mL	0.29182 mL	1.15005 mL	0.02500 mL	8.103	0.09696	0.98281	0.00000
53:43.0	Data point 101	0.83996 mL	0.30115 mL	0.29191 mL	1.15005 mL	0.02500 mL	8.535	0.09927	0.97687	0.00000
54:24.8	Data point 102	0.83996 mL	0.30115 mL	0.29198 mL	1.15005 mL	0.02500 mL	8.947	0.09428	0.96400	0.00000
54:58.4	Data point 103	0.83996 mL	0.30115 mL	0.29205 mL	1.15005 mL	0.02500 mL	9.291	0.09347	0.94185	0.00000
55:30.1	Data point 104	0.83996 mL	0.30115 mL	0.29217 mL	1.15005 mL	0.02500 mL	9.651	0.08008	0.93780	0.00000
55:51.8	Data point 105	0.83996 mL	0.30115 mL	0.29231 mL	1.15005 mL	0.02500 mL	9.853	0.04397	0.94702	0.00000
56:08.3	Data point 106	0.83996 mL	0.30115 mL	0.29255 mL	1.15005 mL	0.02500 mL	10.170	-0.01449	0.82496	0.00000
56:35.1	Data point 107	0.83996 mL	0.30115 mL	0.29299 mL	1.15005 mL	0.02500 mL	10.361	-0.00610	0.61058	0.00000
56:51.7	Data point 108	0.83996 mL	0.30115 mL	0.29374 mL	1.15005 mL	0.02500 mL	10.588	-0.02364	0.92302	0.00000
57:08.2	Data point 109	0.83996 mL	0.30115 mL	0.29499 mL	1.15005 mL	0.02500 mL	10.781	-0.02540	0.91894	0.00000
57:24.8	Data point 110	0.83996 mL	0.30115 mL	0.29690 mL	1.15005 mL	0.02500 mL	10.964	-0.02207	0.92014	0.00000
57:41.5	Data point 111	0.83996 mL	0.30115 mL	0.29979 mL	1.15005 mL	0.02500 mL	11.126	-0.02656	0.93680	0.00000
58:08.3	Data point 112	0.83996 mL	0.30115 mL	0.30355 mL	1.15005 mL	0.02500 mL	11.315	-0.02194	0.96132	0.00000
58:25.0	Data point 113	0.83996 mL	0.30115 mL	0.31009 mL	1.15005 mL	0.02500 mL	11.497	-0.02644	0.92141	0.00000
58:41.8	Data point 114	0.83996 mL	0.30115 mL	0.32013 mL	1.15005 mL	0.02500 mL	11.682	-0.02435	0.92692	0.00000
58:58.7	Data point 115	0.83996 mL	0.30115 mL	0.33591 mL	1.15005 mL	0.02500 mL	11.871	-0.02707	0.91447	0.00000
59:15.7	Data point 116	0.83996 mL	0.30115 mL	0.35788 mL	1.15005 mL	0.02500 mL	12.041	-0.02682	0.91973	0.00000
1:01:15.4	Assay volumes	1.08996 mL	0.44732 mL	0.35788 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			

Sample name: **D09**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06009**  
 Filename: **C:\Sirius\_T3\17J-06009\_D09\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 10:11:03 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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			
Additional cosolvent volume	0.00 mL			

Sample name: **D09**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06009**  
 Filename: **C:\Sirius\_T3\17J-06009\_D09\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 10:11:03 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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 10:11:03 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus S	0.9949	10/6/2017 10:11:03 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jH	0.8	10/6/2017 10:11:03 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jOH	-1.3	10/6/2017 10:11:03 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Base concentration factor	1.011	10/6/2017 10:11:03 AM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	1.003	10/6/2017 10:11:03 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
Syringe volume	0.5 mL		

Sample name: **D09**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06009**  
 Filename: **C:\Sirius\_T3\17J-06009\_D09\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 10:11:03 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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	-9.30 mV		10/6/2017 10:11:27 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	4e+003 mL	10-3-17	10/3/2017 8:04:49 AM
Waste	6e+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		
E0 calibration preparation stir speed	30%		



Sample name: **D09**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-06009**  
Filename: **C:\Sirius\_T3\17J-06009\_D09\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 10:11:03 AM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

### Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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 F5