

Sample name: **D06**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-06002**  
Filename: **C:\Sirius\_T3\17J-06002\_D06\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 1:16:39 AM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

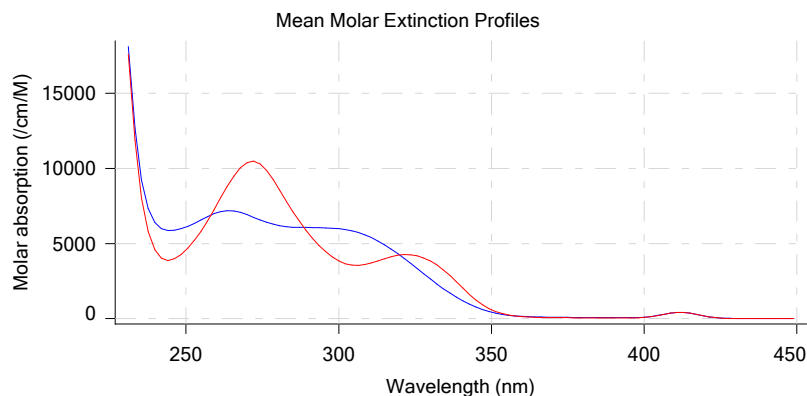
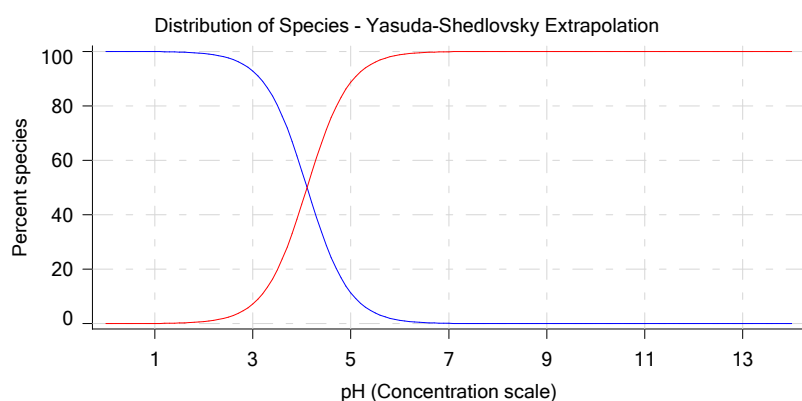
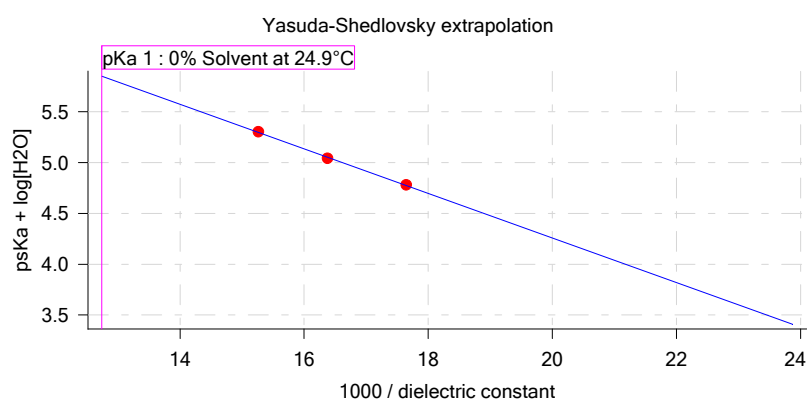
## Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R <sup>2</sup>	Ionic strength	Temperature
Yasuda-Shedlovsky	4.11	±0.03	8.64	-219.1802	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-06002 Points 4 to 36	49.43 %	Up	UV-metric pKa	56.7	24.7 M	0.157 M	24.9°C	✓ 3.38
17J-06002 Points 38 to 75	39.91 %	Up	UV-metric pKa	61.0	30.1 M	0.166 M	24.9°C	✓ 3.56
17J-06002 Points 77 to 119	30.08 %	Up	UV-metric pKa	65.5	35.8 M	0.172 M	24.9°C	✓ 3.75

## Graphs



## UV-metric psKa Titration 1 of 3 17J-06002 Points 4 to 36

### Results

pKa 1	<b>3.38</b>
RMSD	<b>0.003 0.002</b>
Chi squared	<b>0.0096</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 27.9 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 1.476 to 12.541

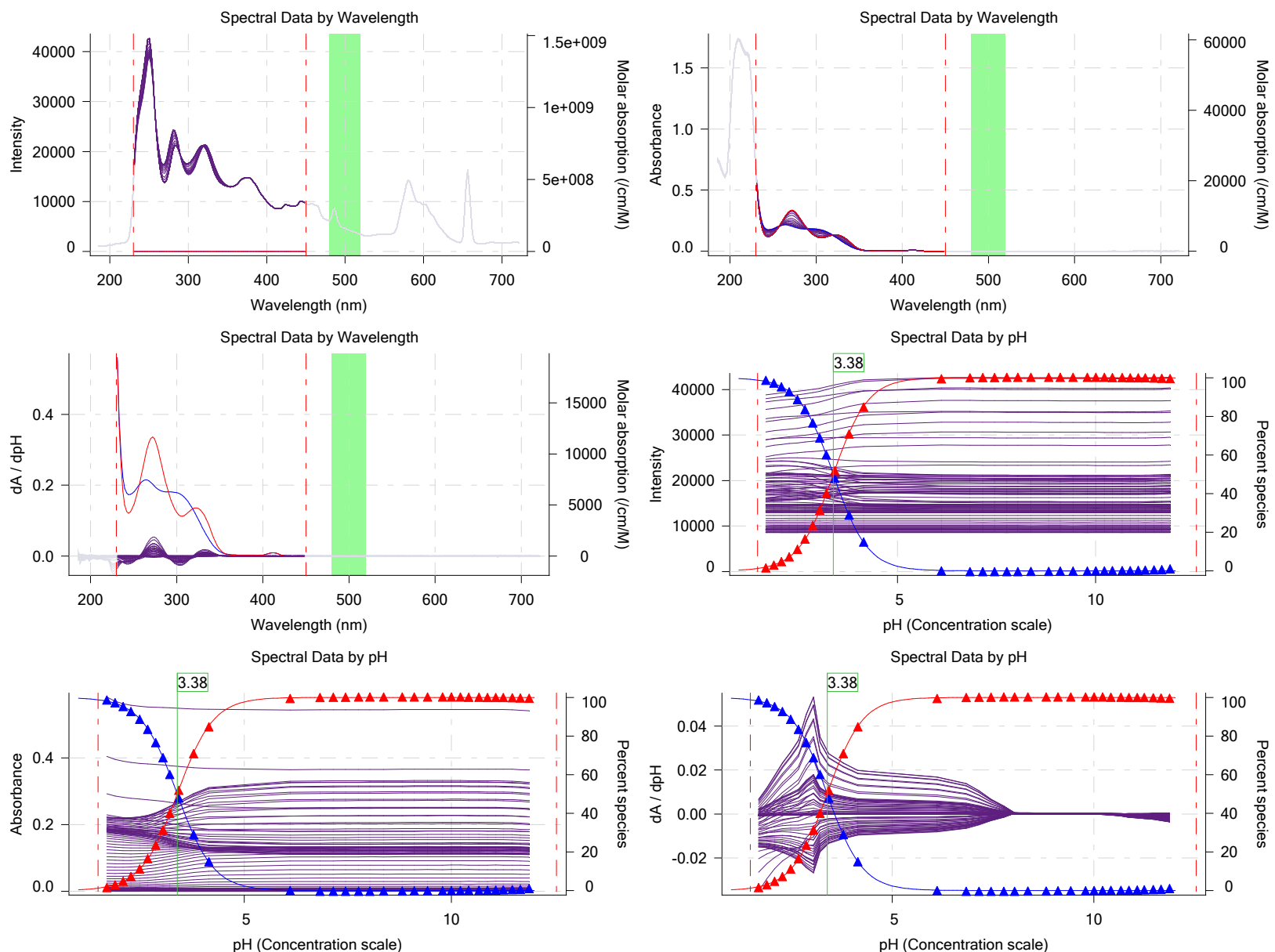
## Warnings and errors

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			

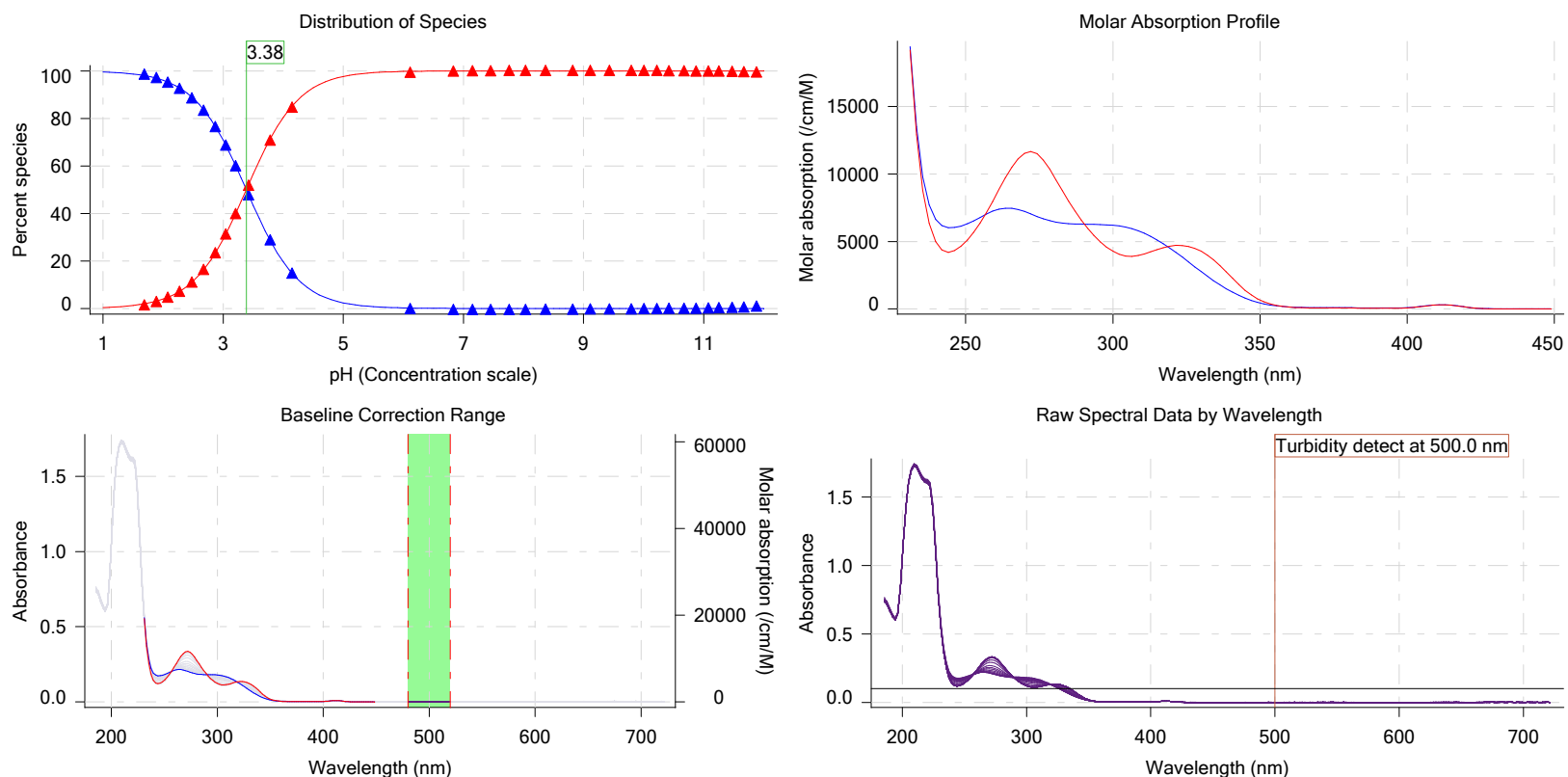
## Graphs



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## Graphs (continued)



## UV-metric psKa Titration 2 of 3 17J-06002 Points 38 to 75

### Results

pKa 1	<b>3.56</b>
RMSD	<b>0.005 0.003</b>
Chi squared	<b>0.0092</b>
PCA calculated number of pKas	<b>1</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>39.9 %</b>
Dielectric constant	<b>61.0</b>
Water concentration	<b>30.1 M</b>
Number of pKas source	<b>Predicted</b>
Wavelength clipping	<b>230.0 nm to 450.0 nm</b>
pH clipping	<b>1.500 to 12.526</b>

### 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			

**Assay Medium**

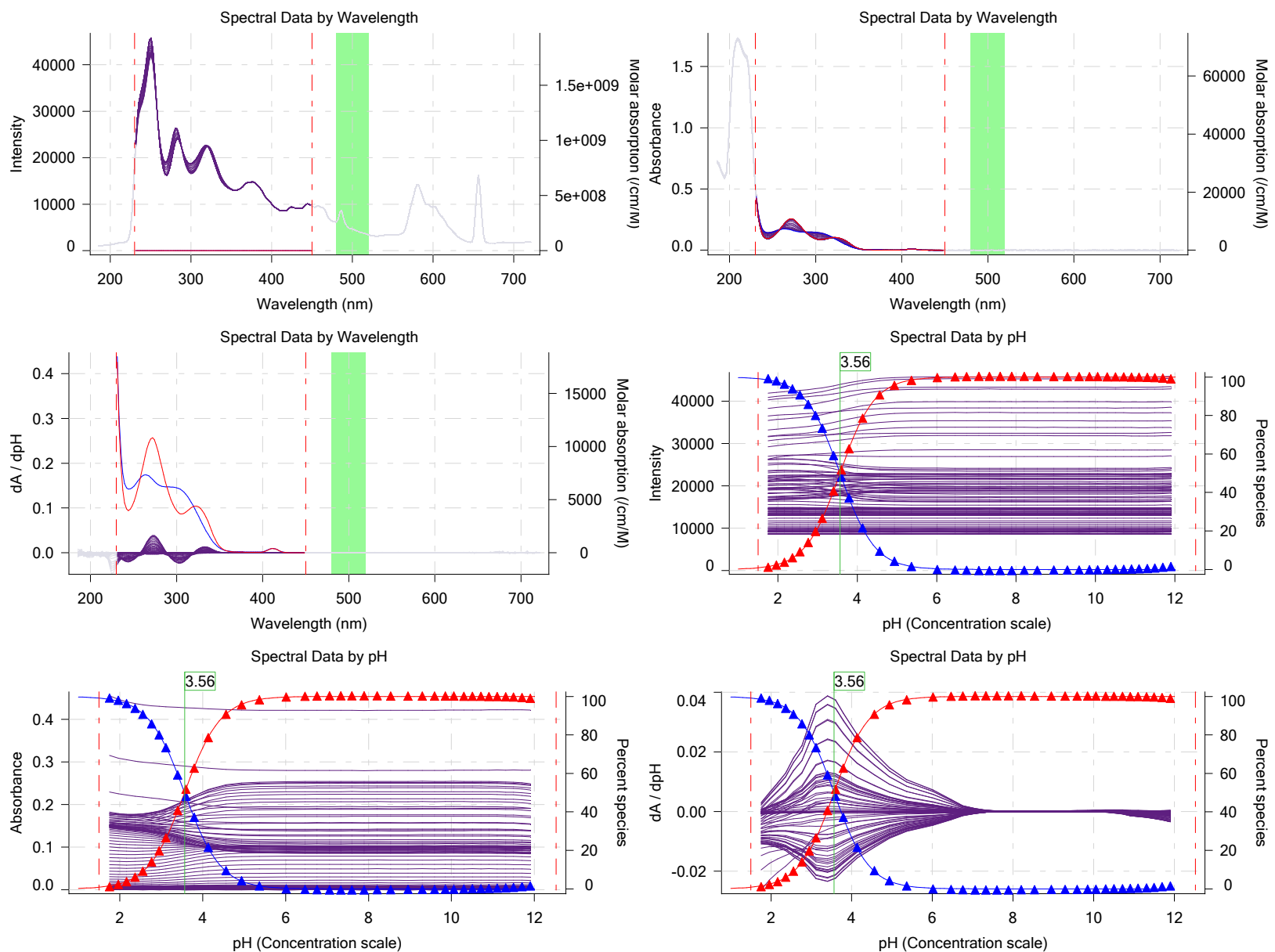
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Experiment start time: **10/6/2017 1:16:39 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

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

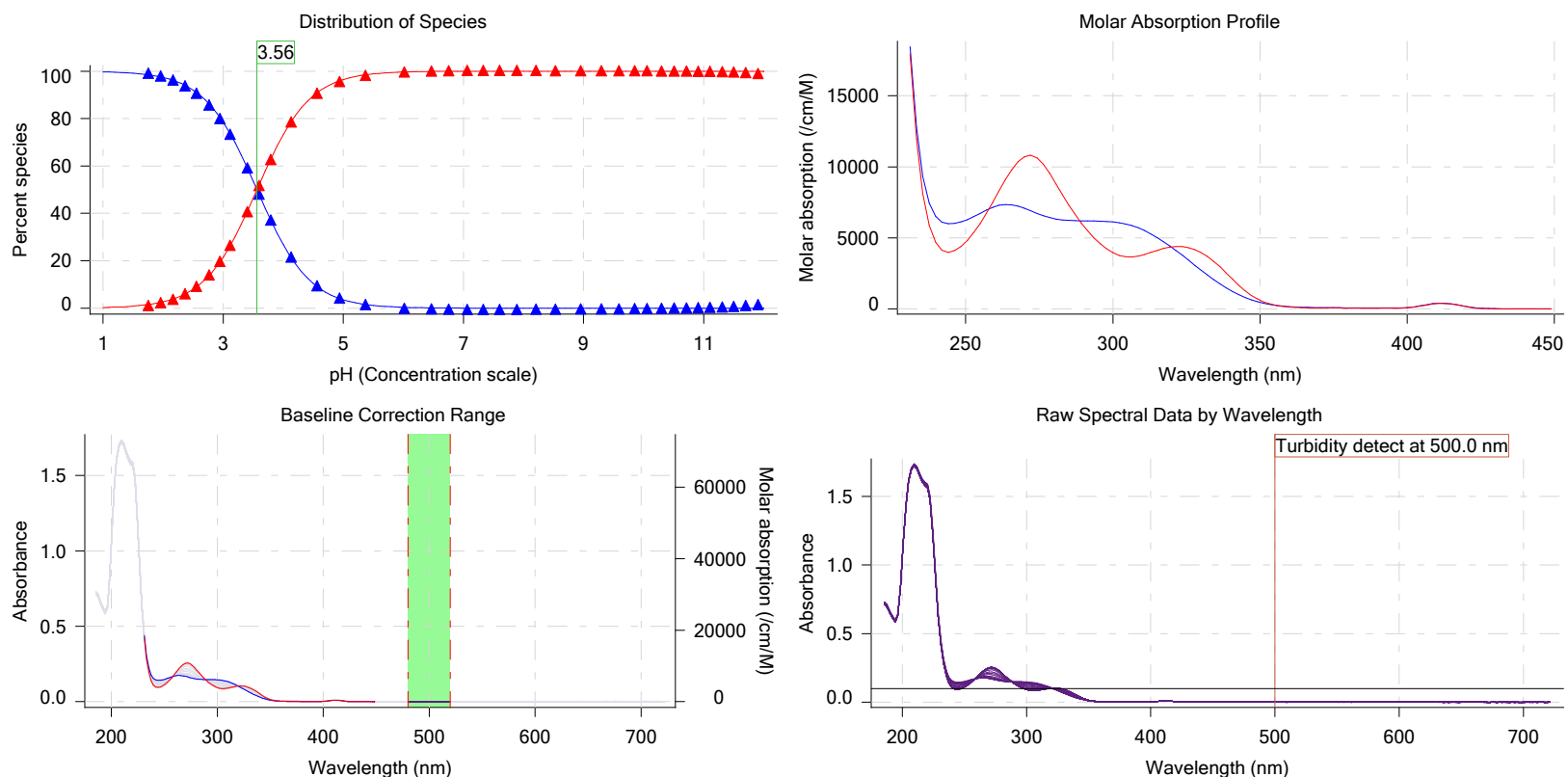
## Graphs



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## Graphs (continued)



## UV-metric psKa Titration 3 of 3 17J-06002 Points 77 to 119

### Results

pKa 1	<b>3.75</b>
RMSD	<b>0.008 0.007</b>
Chi squared	<b>0.0132</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 17.7 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>1.499 to 12.550</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>				

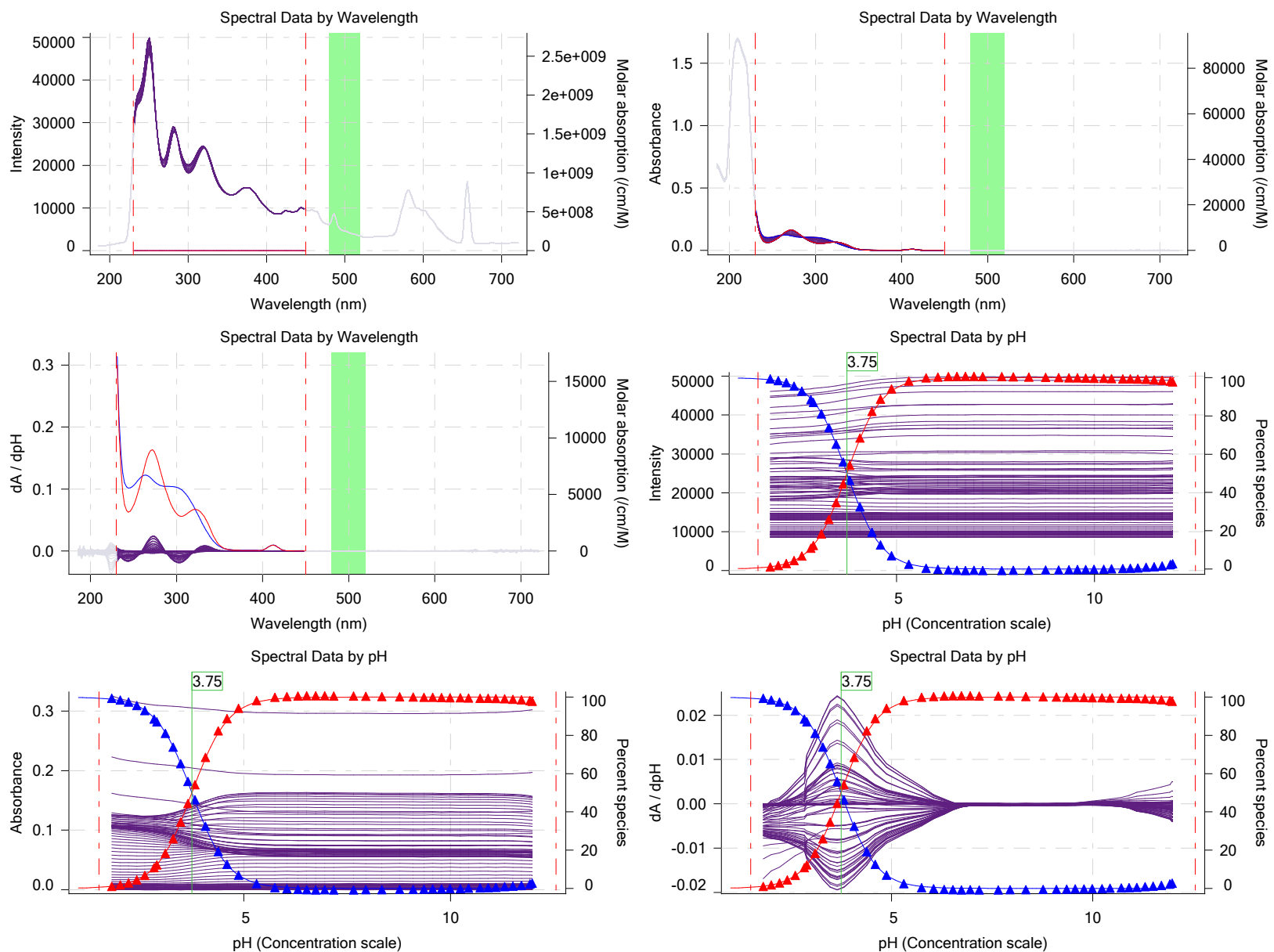
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Experiment start time: **10/6/2017 1:16:39 AM**  
 Analyst: **Dorothy Leverse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

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

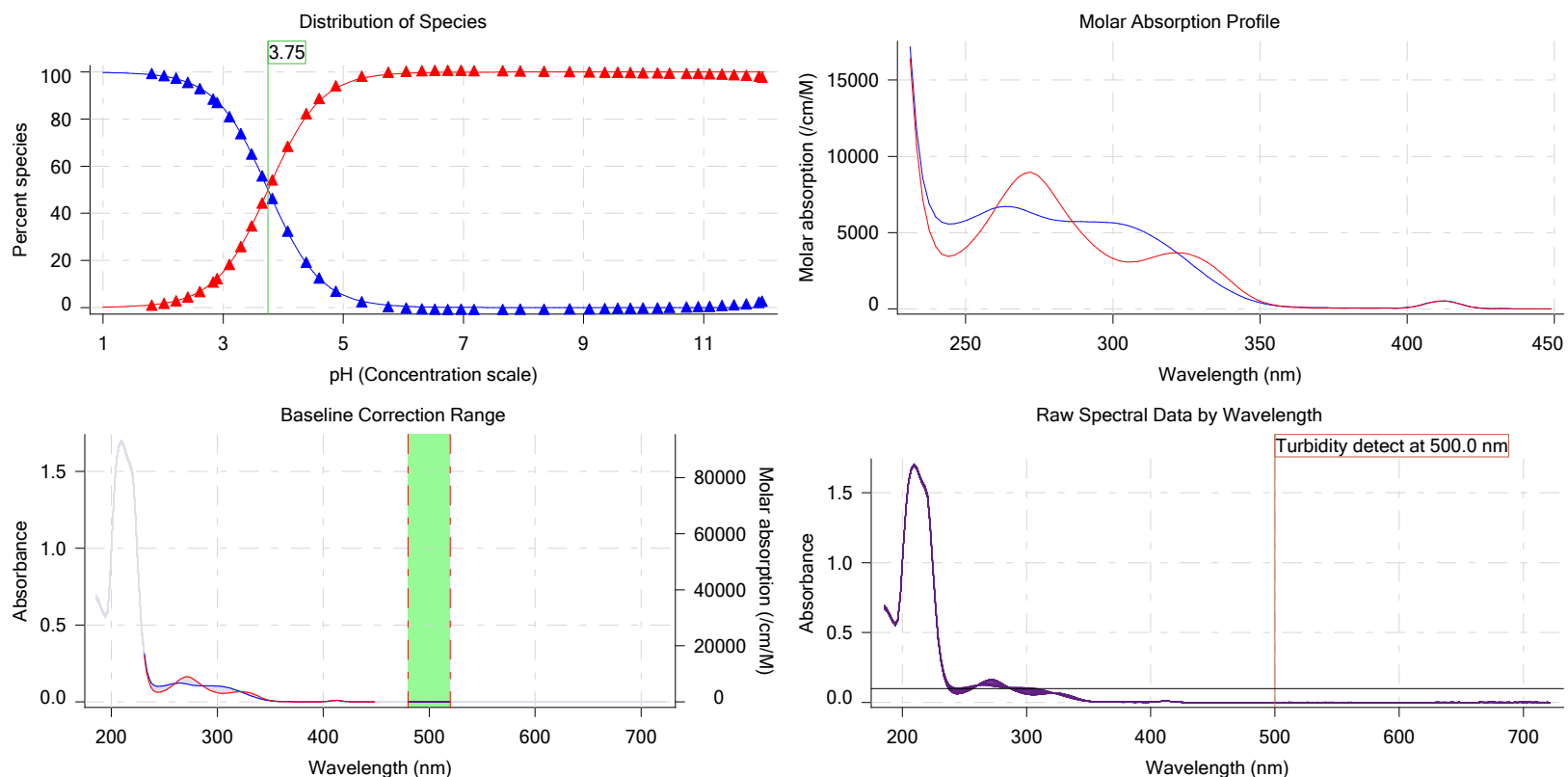
## Graphs



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## Graphs (continued)



## Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	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
3:34.2	Dark spectrum								
3:35.7	Reference spectrum								
4:03.3	Volume reset due to vial change								
4:47.5	Initial pH = 8.35								
6:00.1	Data point 4	0.34995 mL	0.06990 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.976	-0.01295	0.84530
6:28.9	Data point 5	0.34995 mL	0.06990 mL	0.02514 mL	1.15005 mL	0.02500 mL	2.175	-0.00282	0.13350
6:46.0	Data point 6	0.34995 mL	0.06990 mL	0.04059 mL	1.15005 mL	0.02500 mL	2.362	0.02196	0.88625
7:02.9	Data point 7	0.34995 mL	0.06990 mL	0.05052 mL	1.15005 mL	0.02500 mL	2.551	0.00224	0.02718
7:19.6	Data point 8	0.34995 mL	0.06990 mL	0.05703 mL	1.15005 mL	0.02500 mL	2.755	0.00508	0.57817
7:36.3	Data point 9	0.34995 mL	0.06990 mL	0.06110 mL	1.15005 mL	0.02500 mL	2.947	0.00822	0.77567



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**Events (continued)**

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
7:52.9	Data point 10	0.34995 mL	0.06990 mL	0.06369 mL	1.15005 mL	0.02500 mL	3.138	0.00892	0.68388	0.00
8:09.6	Data point 11	0.34995 mL	0.06990 mL	0.06536 mL	1.15005 mL	0.02500 mL	3.312	0.00318	0.22811	0.00
8:26.1	Data point 12	0.34995 mL	0.06990 mL	0.06649 mL	1.15005 mL	0.02500 mL	3.475	0.00908	0.79084	0.00
8:47.8	Data point 13	0.34995 mL	0.06990 mL	0.06794 mL	1.15005 mL	0.02500 mL	3.690	0.00789	0.36203	0.00
9:09.7	Data point 14	0.34995 mL	0.06990 mL	0.06881 mL	1.15005 mL	0.02500 mL	4.043	0.05576	0.97199	0.00
9:31.4	Data point 15	0.34995 mL	0.06990 mL	0.06921 mL	1.15005 mL	0.02500 mL	4.405	0.06328	0.91540	0.00
9:58.2	Data point 16	0.34995 mL	0.06990 mL	0.06959 mL	1.15005 mL	0.02500 mL	6.348	0.08342	0.85683	0.00
10:54.4	Data point 17	0.34995 mL	0.06990 mL	0.06980 mL	1.15005 mL	0.02500 mL	7.060	0.09757	0.97654	0.00
11:39.9	Data point 18	0.34995 mL	0.06990 mL	0.06994 mL	1.15005 mL	0.02500 mL	7.376	0.09678	0.96799	0.00
12:24.2	Data point 19	0.34995 mL	0.06990 mL	0.07008 mL	1.15005 mL	0.02500 mL	7.672	0.09783	0.98728	0.00
13:12.3	Data point 20	0.34995 mL	0.06990 mL	0.07023 mL	1.15005 mL	0.02500 mL	7.981	0.09850	0.97823	0.00
13:54.1	Data point 21	0.34995 mL	0.06990 mL	0.07032 mL	1.15005 mL	0.02500 mL	8.250	0.10024	0.97844	0.00
14:38.0	Data point 22	0.34995 mL	0.06990 mL	0.07041 mL	1.15005 mL	0.02500 mL	8.577	0.09765	0.98069	0.00
15:25.4	Data point 23	0.34995 mL	0.06990 mL	0.07051 mL	1.15005 mL	0.02500 mL	9.025	0.09271	0.96312	0.00
16:10.5	Data point 24	0.34995 mL	0.06990 mL	0.07058 mL	1.15005 mL	0.02500 mL	9.312	0.09508	0.96930	0.00
16:49.9	Data point 25	0.34995 mL	0.06990 mL	0.07067 mL	1.15005 mL	0.02500 mL	9.628	0.09878	0.96264	0.00
17:21.0	Data point 26	0.34995 mL	0.06990 mL	0.07079 mL	1.15005 mL	0.02500 mL	9.988	0.09506	0.98429	0.00
17:45.2	Data point 27	0.34995 mL	0.06990 mL	0.07091 mL	1.15005 mL	0.02500 mL	10.197	0.08642	0.96583	0.00
18:12.0	Data point 28	0.34995 mL	0.06990 mL	0.07110 mL	1.15005 mL	0.02500 mL	10.411	0.03860	0.96965	0.00
18:38.9	Data point 29	0.34995 mL	0.06990 mL	0.07143 mL	1.15005 mL	0.02500 mL	10.610	0.01677	0.91877	0.00
18:55.5	Data point 30	0.34995 mL	0.06990 mL	0.07204 mL	1.15005 mL	0.02500 mL	10.856	0.00829	0.85401	0.00
19:27.6	Data point 31	0.34995 mL	0.06990 mL	0.07319 mL	1.15005 mL	0.02500 mL	11.055	-0.00289	0.43736	0.00
19:44.3	Data point 32	0.34995 mL	0.06990 mL	0.07488 mL	1.15005 mL	0.02500 mL	11.256	-0.00373	0.50550	0.00
20:01.0	Data point 33	0.34995 mL	0.06990 mL	0.07759 mL	1.15005 mL	0.02500 mL	11.430	-0.00474	0.47601	0.00
20:17.7	Data point 34	0.34995 mL	0.06990 mL	0.08166 mL	1.15005 mL	0.02500 mL	11.647	-0.00619	0.62436	0.00
20:34.4	Data point 35	0.34995 mL	0.06990 mL	0.08843 mL	1.15005 mL	0.02500 mL	11.838	-0.00896	0.86396	0.00
20:51.2	Data point 36	0.34995 mL	0.06990 mL	0.09922 mL	1.15005 mL	0.02500 mL	12.041	-0.00381	0.44803	0.00
22:27.4	Reference spectrum									
23:31.4	Data point 38	0.50000 mL	0.16940 mL	0.09925 mL	1.15005 mL	0.02500 mL	2.000	-0.05546	0.92871	0.00
23:59.0	Data point 39	0.50000 mL	0.16940 mL	0.12498 mL	1.15005 mL	0.02500 mL	2.201	0.01133	0.89801	0.00
24:15.9	Data point 40	0.50000 mL	0.16940 mL	0.14080 mL	1.15005 mL	0.02500 mL	2.399	0.00731	0.65862	0.00
24:32.8	Data point 41	0.50000 mL	0.16940 mL	0.15082 mL	1.15005 mL	0.02500 mL	2.599	0.00947	0.69905	0.00
24:49.5	Data point 42	0.50000 mL	0.16940 mL	0.15713 mL	1.15005 mL	0.02500 mL	2.786	0.01725	0.77892	0.00
25:06.2	Data point 43	0.50000 mL	0.16940 mL	0.16117 mL	1.15005 mL	0.02500 mL	2.992	0.00765	0.50726	0.00
25:22.8	Data point 44	0.50000 mL	0.16940 mL	0.16369 mL	1.15005 mL	0.02500 mL	3.172	0.01050	0.86444	0.00
25:39.4	Data point 45	0.50000 mL	0.16940 mL	0.16536 mL	1.15005 mL	0.02500 mL	3.338	0.01668	0.87764	0.00
26:01.2	Data point 46	0.50000 mL	0.16940 mL	0.16724 mL	1.15005 mL	0.02500 mL	3.620	0.02112	0.97384	0.00
26:33.3	Data point 47	0.50000 mL	0.16940 mL	0.16797 mL	1.15005 mL	0.02500 mL	3.816	0.03373	0.98148	0.00
27:00.1	Data point 48	0.50000 mL	0.16940 mL	0.16834 mL	1.15005 mL	0.02500 mL	4.010	0.02840	0.92819	0.00
27:16.8	Data point 49	0.50000 mL	0.16940 mL	0.16858 mL	1.15005 mL	0.02500 mL	4.345	0.09241	0.98897	0.00
27:38.5	Data point 50	0.50000 mL	0.16940 mL	0.16879 mL	1.15005 mL	0.02500 mL	4.771	0.09513	0.98404	0.00
28:22.3	Data point 51	0.50000 mL	0.16940 mL	0.16893 mL	1.15005 mL	0.02500 mL	5.143	0.09605	0.98402	0.00
29:20.1	Data point 52	0.50000 mL	0.16940 mL	0.16900 mL	1.15005 mL	0.02500 mL	5.567	0.09889	0.98960	0.00
30:22.3	Data point 53	0.50000 mL	0.16940 mL	0.16907 mL	1.15005 mL	0.02500 mL	6.210	0.09886	0.98557	0.00
31:23.9	Data point 54	0.50000 mL	0.16940 mL	0.16914 mL	1.15005 mL	0.02500 mL	6.654	0.09684	0.98104	0.00
32:19.7	Data point 55	0.50000 mL	0.16940 mL	0.16921 mL	1.15005 mL	0.02500 mL	6.942	0.10001	0.98607	0.00
32:57.5	Data point 56	0.50000 mL	0.16940 mL	0.16931 mL	1.15005 mL	0.02500 mL	7.245	0.09669	0.97317	0.00
33:37.0	Data point 57	0.50000 mL	0.16940 mL	0.16943 mL	1.15005 mL	0.02500 mL	7.512	0.09836	0.96842	0.00
34:13.3	Data point 58	0.50000 mL	0.16940 mL	0.16954 mL	1.15005 mL	0.02500 mL	7.777	0.09689	0.96653	0.00
34:56.3	Data point 59	0.50000 mL	0.16940 mL	0.16966 mL	1.15005 mL	0.02500 mL	8.066	0.09932	0.96922	0.00
35:34.9	Data point 60	0.50000 mL	0.16940 mL	0.16975 mL	1.15005 mL	0.02500 mL	8.377	0.09536	0.98462	0.00
36:12.6	Data point 61	0.50000 mL	0.16940 mL	0.16983 mL	1.15005 mL	0.02500 mL	8.701	0.09864	0.98766	0.00
37:00.5	Data point 62	0.50000 mL	0.16940 mL	0.16992 mL	1.15005 mL	0.02500 mL	9.116	0.09912	0.97626	0.00
37:38.1	Data point 63	0.50000 mL	0.16940 mL	0.17001 mL	1.15005 mL	0.02500 mL	9.456	0.09018	0.88682	0.00
38:06.8	Data point 64	0.50000 mL	0.16940 mL	0.17013 mL	1.15005 mL	0.02500 mL	9.748	0.09505	0.96553	0.00
38:30.0	Data point 65	0.50000 mL	0.16940 mL	0.17030 mL	1.15005 mL	0.02500 mL	10.007	0.05853	0.94505	0.00
38:56.8	Data point 66	0.50000 mL	0.16940 mL	0.17053 mL	1.15005 mL	0.02500 mL	10.208	0.02603	0.80893	0.00



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## Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
39:13.4	Data point 67	0.50000 mL	0.16940 mL	0.17088 mL	1.15005 mL	0.02500 mL	10.451	0.01277	0.85260	0.00000
39:45.3	Data point 68	0.50000 mL	0.16940 mL	0.17154 mL	1.15005 mL	0.02500 mL	10.655	0.00267	0.17440	0.00000
40:01.9	Data point 69	0.50000 mL	0.16940 mL	0.17248 mL	1.15005 mL	0.02500 mL	10.859	-0.00152	0.11231	0.00000
40:18.4	Data point 70	0.50000 mL	0.16940 mL	0.17397 mL	1.15005 mL	0.02500 mL	11.051	-0.00506	0.65948	0.00000
40:35.1	Data point 71	0.50000 mL	0.16940 mL	0.17629 mL	1.15005 mL	0.02500 mL	11.243	-0.00712	0.70590	0.00000
40:51.7	Data point 72	0.50000 mL	0.16940 mL	0.17991 mL	1.15005 mL	0.02500 mL	11.447	-0.01046	0.82403	0.00000
41:08.4	Data point 73	0.50000 mL	0.16940 mL	0.18575 mL	1.15005 mL	0.02500 mL	11.633	-0.00868	0.76906	0.00000
41:25.2	Data point 74	0.50000 mL	0.16940 mL	0.19483 mL	1.15005 mL	0.02500 mL	11.830	-0.00959	0.72093	0.00000
41:42.1	Data point 75	0.50000 mL	0.16940 mL	0.20948 mL	1.15005 mL	0.02500 mL	12.026	-0.01447	0.87439	0.00000
43:26.9	Reference spectrum									
44:50.4	Data point 77	0.83996 mL	0.30096 mL	0.20950 mL	1.15005 mL	0.02500 mL	1.999	-0.04690	0.95850	0.00000
45:18.1	Data point 78	0.83996 mL	0.30096 mL	0.23890 mL	1.15005 mL	0.02500 mL	2.199	0.01108	0.67744	0.00000
45:35.0	Data point 79	0.83996 mL	0.30096 mL	0.25708 mL	1.15005 mL	0.02500 mL	2.396	-0.00809	0.40436	0.00000
45:51.9	Data point 80	0.83996 mL	0.30096 mL	0.26856 mL	1.15005 mL	0.02500 mL	2.589	-0.03024	0.79603	0.00000
46:08.6	Data point 81	0.83996 mL	0.30096 mL	0.27606 mL	1.15005 mL	0.02500 mL	2.784	0.00137	0.02546	0.00000
46:41.0	Data point 82	0.83996 mL	0.30096 mL	0.28076 mL	1.15005 mL	0.02500 mL	3.006	0.00075	0.06291	0.00000
46:57.7	Data point 83	0.83996 mL	0.30096 mL	0.28358 mL	1.15005 mL	0.02500 mL	3.069	0.00540	0.44183	0.00000
47:19.5	Data point 84	0.83996 mL	0.30096 mL	0.28591 mL	1.15005 mL	0.02500 mL	3.272	0.00411	0.39159	0.00000
47:36.1	Data point 85	0.83996 mL	0.30096 mL	0.28744 mL	1.15005 mL	0.02500 mL	3.461	-0.00997	0.58196	0.00000
47:52.6	Data point 86	0.83996 mL	0.30096 mL	0.28843 mL	1.15005 mL	0.02500 mL	3.641	0.00771	0.45576	0.00000
48:09.2	Data point 87	0.83996 mL	0.30096 mL	0.28909 mL	1.15005 mL	0.02500 mL	3.814	0.00927	0.65054	0.00000
48:25.7	Data point 88	0.83996 mL	0.30096 mL	0.28953 mL	1.15005 mL	0.02500 mL	3.981	0.01164	0.83598	0.00000
48:47.3	Data point 89	0.83996 mL	0.30096 mL	0.28996 mL	1.15005 mL	0.02500 mL	4.235	0.03252	0.97014	0.00000
49:09.1	Data point 90	0.83996 mL	0.30096 mL	0.29026 mL	1.15005 mL	0.02500 mL	4.540	0.06265	0.98887	0.00000
49:30.8	Data point 91	0.83996 mL	0.30096 mL	0.29043 mL	1.15005 mL	0.02500 mL	4.753	0.09855	0.95591	0.00000
50:01.5	Data point 92	0.83996 mL	0.30096 mL	0.29055 mL	1.15005 mL	0.02500 mL	5.027	0.09905	0.98530	0.00000
50:42.8	Data point 93	0.83996 mL	0.30096 mL	0.29066 mL	1.15005 mL	0.02500 mL	5.458	0.09550	0.93531	0.00000
51:33.7	Data point 94	0.83996 mL	0.30096 mL	0.29076 mL	1.15005 mL	0.02500 mL	5.895	0.09920	0.99730	0.00000
52:15.4	Data point 95	0.83996 mL	0.30096 mL	0.29085 mL	1.15005 mL	0.02500 mL	6.189	0.09977	0.98635	0.00000
52:56.1	Data point 96	0.83996 mL	0.30096 mL	0.29095 mL	1.15005 mL	0.02500 mL	6.449	0.08287	0.76228	0.00000
53:17.9	Data point 97	0.83996 mL	0.30096 mL	0.29104 mL	1.15005 mL	0.02500 mL	6.663	0.09028	0.91087	0.00000
53:45.2	Data point 98	0.83996 mL	0.30096 mL	0.29116 mL	1.15005 mL	0.02500 mL	6.876	0.09154	0.92911	0.00000
54:18.5	Data point 99	0.83996 mL	0.30096 mL	0.29135 mL	1.15005 mL	0.02500 mL	7.094	0.09908	0.96214	0.00000
54:51.9	Data point 100	0.83996 mL	0.30096 mL	0.29153 mL	1.15005 mL	0.02500 mL	7.311	0.09558	0.96521	0.00000
55:31.4	Data point 101	0.83996 mL	0.30096 mL	0.29205 mL	1.15005 mL	0.02500 mL	7.785	0.08698	0.94893	0.00000
56:10.6	Data point 102	0.83996 mL	0.30096 mL	0.29217 mL	1.15005 mL	0.02500 mL	8.075	0.09470	0.96615	0.00000
56:55.7	Data point 103	0.83996 mL	0.30096 mL	0.29229 mL	1.15005 mL	0.02500 mL	8.463	0.09694	0.93765	0.00000
57:40.7	Data point 104	0.83996 mL	0.30096 mL	0.29240 mL	1.15005 mL	0.02500 mL	8.886	0.09671	0.93948	0.00000
58:20.5	Data point 105	0.83996 mL	0.30096 mL	0.29252 mL	1.15005 mL	0.02500 mL	9.214	0.09738	0.98838	0.00000
58:55.7	Data point 106	0.83996 mL	0.30096 mL	0.29264 mL	1.15005 mL	0.02500 mL	9.469	0.09976	0.97010	0.00000
59:19.9	Data point 107	0.83996 mL	0.30096 mL	0.29278 mL	1.15005 mL	0.02500 mL	9.681	0.08385	0.97139	0.00000
59:46.7	Data point 108	0.83996 mL	0.30096 mL	0.29297 mL	1.15005 mL	0.02500 mL	9.891	0.04779	0.95922	0.00000
1:00:08.4	Data point 109	0.83996 mL	0.30096 mL	0.29323 mL	1.15005 mL	0.02500 mL	10.097	0.01394	0.82458	0.00000
1:00:25.0	Data point 110	0.83996 mL	0.30096 mL	0.29365 mL	1.15005 mL	0.02500 mL	10.339	-0.00917	0.59627	0.00000
1:00:51.7	Data point 111	0.83996 mL	0.30096 mL	0.29433 mL	1.15005 mL	0.02500 mL	10.538	-0.00380	0.27116	0.00000
1:01:08.3	Data point 112	0.83996 mL	0.30096 mL	0.29544 mL	1.15005 mL	0.02500 mL	10.815	-0.02374	0.91869	0.00000
1:01:35.3	Data point 113	0.83996 mL	0.30096 mL	0.29727 mL	1.15005 mL	0.02500 mL	11.006	-0.01167	0.81643	0.00000
1:01:51.9	Data point 114	0.83996 mL	0.30096 mL	0.30045 mL	1.15005 mL	0.02500 mL	11.195	-0.02326	0.95582	0.00000
1:02:08.6	Data point 115	0.83996 mL	0.30096 mL	0.30539 mL	1.15005 mL	0.02500 mL	11.398	-0.02332	0.92408	0.00000
1:02:25.3	Data point 116	0.83996 mL	0.30096 mL	0.31333 mL	1.15005 mL	0.02500 mL	11.595	-0.01995	0.92881	0.00000
1:02:42.1	Data point 117	0.83996 mL	0.30096 mL	0.32606 mL	1.15005 mL	0.02500 mL	11.796	-0.02025	0.89331	0.00000
1:02:59.2	Data point 118	0.83996 mL	0.30096 mL	0.34682 mL	1.15005 mL	0.02500 mL	11.996	-0.02312	0.93625	0.00000
1:03:16.0	Data point 119	0.83996 mL	0.30096 mL	0.35470 mL	1.15005 mL	0.02500 mL	12.050	-0.01180	0.90732	0.00000
1:05:15.6	Assay volumes	1.08996 mL	0.44555 mL	0.35470 mL	1.15005 mL	0.02500 mL				

Sample name: **D06**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06002**  
 Filename: **C:\Sirius\_T3\17J-06002\_D06\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 1:16:39 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## 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			
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>				

Sample name: **D06**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06002**  
 Filename: **C:\Sirius\_T3\17J-06002\_D06\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 1:16:39 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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	0.125	10/6/2017 1:16:39 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus S	0.9949	10/6/2017 1:16:39 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jH	0.8	10/6/2017 1:16:39 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jOH	-1.3	10/6/2017 1:16:39 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Base concentration factor	1.011	10/6/2017 1:16:39 AM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	1.003	10/6/2017 1:16:39 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

Sample name: **D06**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-06002**  
 Filename: **C:\Sirius\_T3\17J-06002\_D06\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 1:16:39 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
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	-7.82 mV		10/6/2017 1:17:03 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	5.1e+003 mL	10-3-17	10/3/2017 8:04:49 AM
Waste	5e+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		



## Assay Settings

Sample name: **D06**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-06002**  
Filename: **C:\Sirius\_T3\17J-06002\_D06\_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 1:16:39 AM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

### Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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 C1