

Sample name: **M11**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-04003**  
Filename: **C:\Sirius\_T3\17J-04003\_M11\_UV-metric psKa.t3r**

Experiment start time: **10/4/2017 2:49:42 AM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

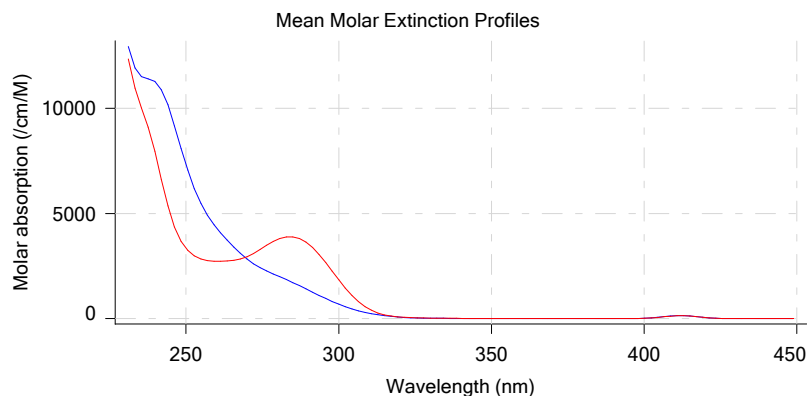
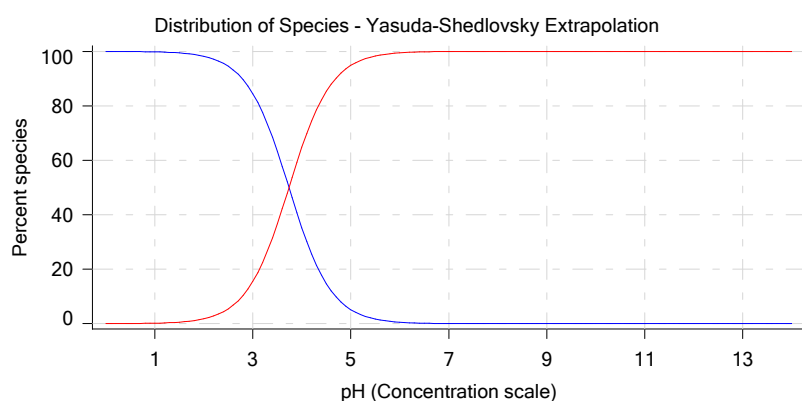
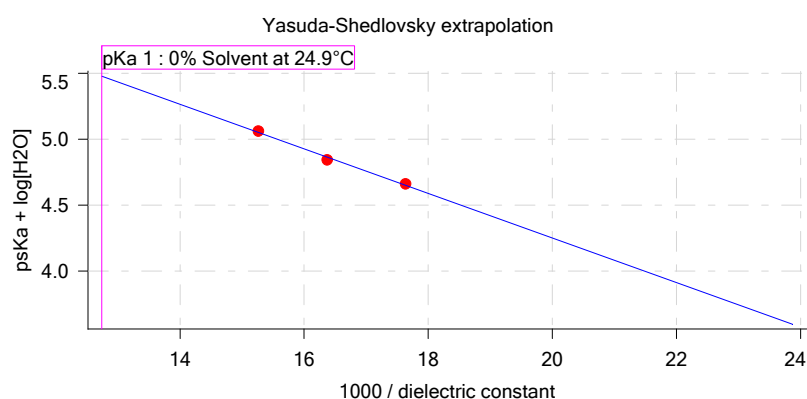
## Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R <sup>2</sup>	Ionic strength	Temperature
Yasuda-Shedlovsky	3.74	±0.06	7.63	-169.0126	0.9924	0.165 M	24.9°C

## Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1
17J-04003 Points 4 to 35	49.36 %	Up	UV-metric pKa	56.7	24.8 M	0.157 M	24.8°C	✓ 3.27
17J-04003 Points 37 to 75	39.84 %	Up	UV-metric pKa	61.1	30.1 M	0.166 M	24.9°C	✓ 3.37
17J-04003 Points 77 to 119	30.06 %	Up	UV-metric pKa	65.5	35.8 M	0.173 M	24.9°C	✓ 3.51

## Graphs



## UV-metric psKa Titration 1 of 3 17J-04003 Points 4 to 35

### Results

pKa 1	<b>3.27</b>
RMSD	<b>0.002 0.005</b>
Chi squared	<b>0.0100</b>
PCA calculated number of pKas	<b>2</b>
Average ionic strength	<b>0.157 M</b>
Average temperature	<b>24.8°C</b>
Analyte concentration range	<b>80.0 µM to 75.2 µM</b>
Methanol weight %	<b>49.4 %</b>
Dielectric constant	<b>56.7</b>
Water concentration	<b>24.8 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 12.549

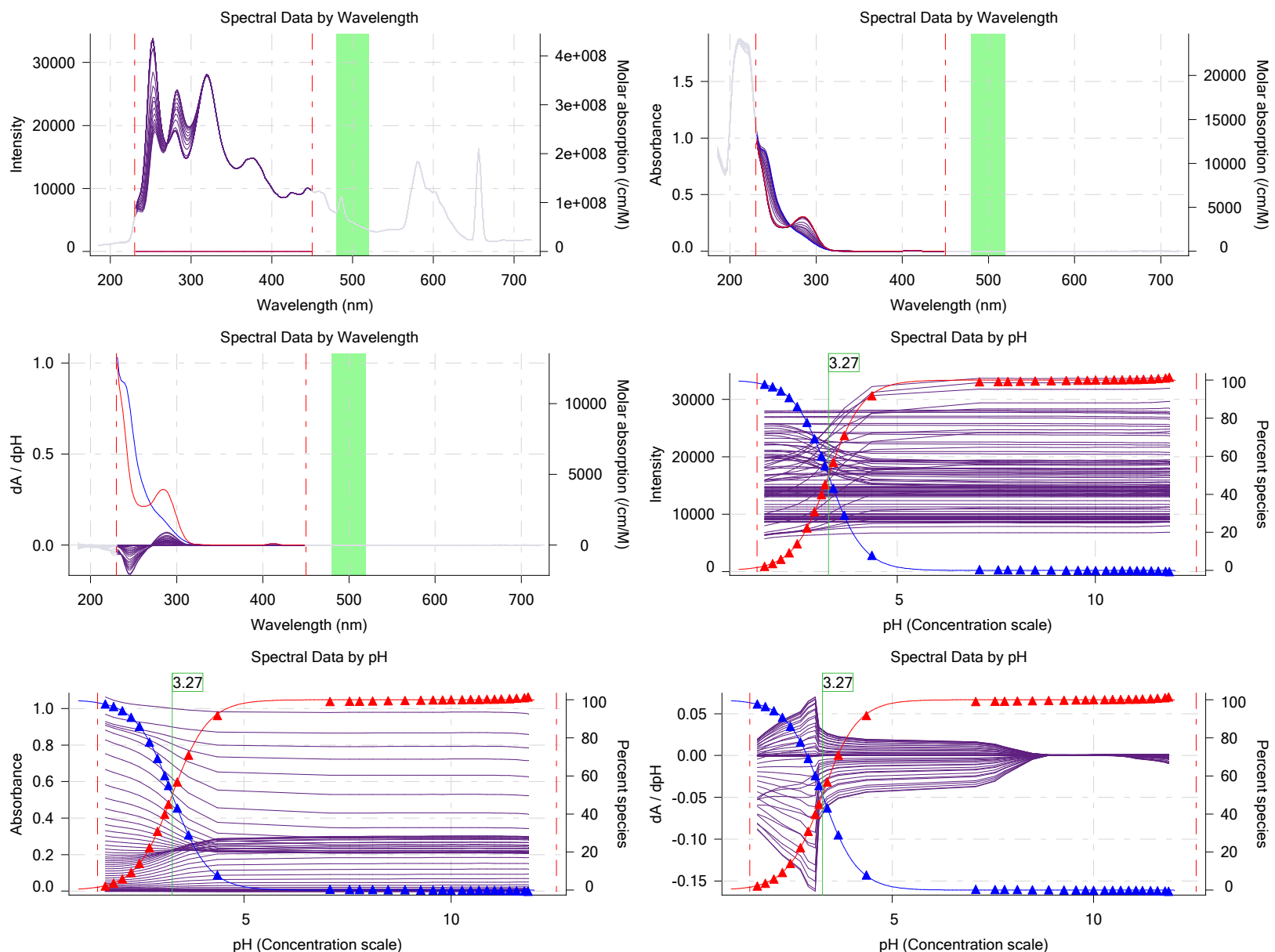
## Warnings and errors

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			

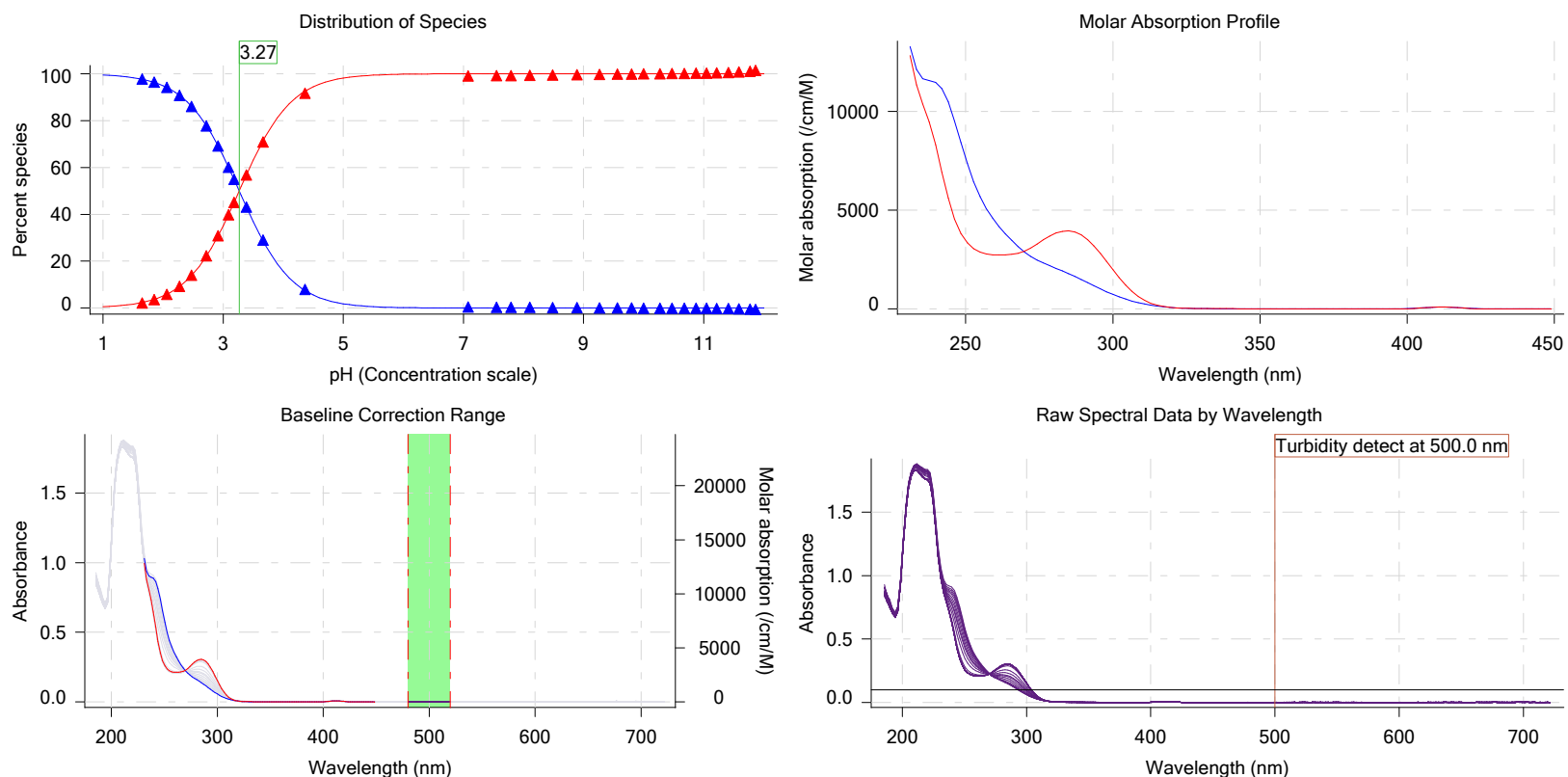
## Graphs



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## Graphs (continued)



## UV-metric psKa Titration 2 of 3 17J-04003 Points 37 to 75

### Results

pKa 1	<b>3.37</b>
RMSD	<b>0.003 0.006</b>
Chi squared	<b>0.0095</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>65.6 µM to 62.1 µM</b>
Methanol weight %	<b>39.8 %</b>
Dielectric constant	<b>61.1</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>1.502 to 12.508</b>

### Warnings and errors

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

### Assay Settings

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

**Assay Medium**

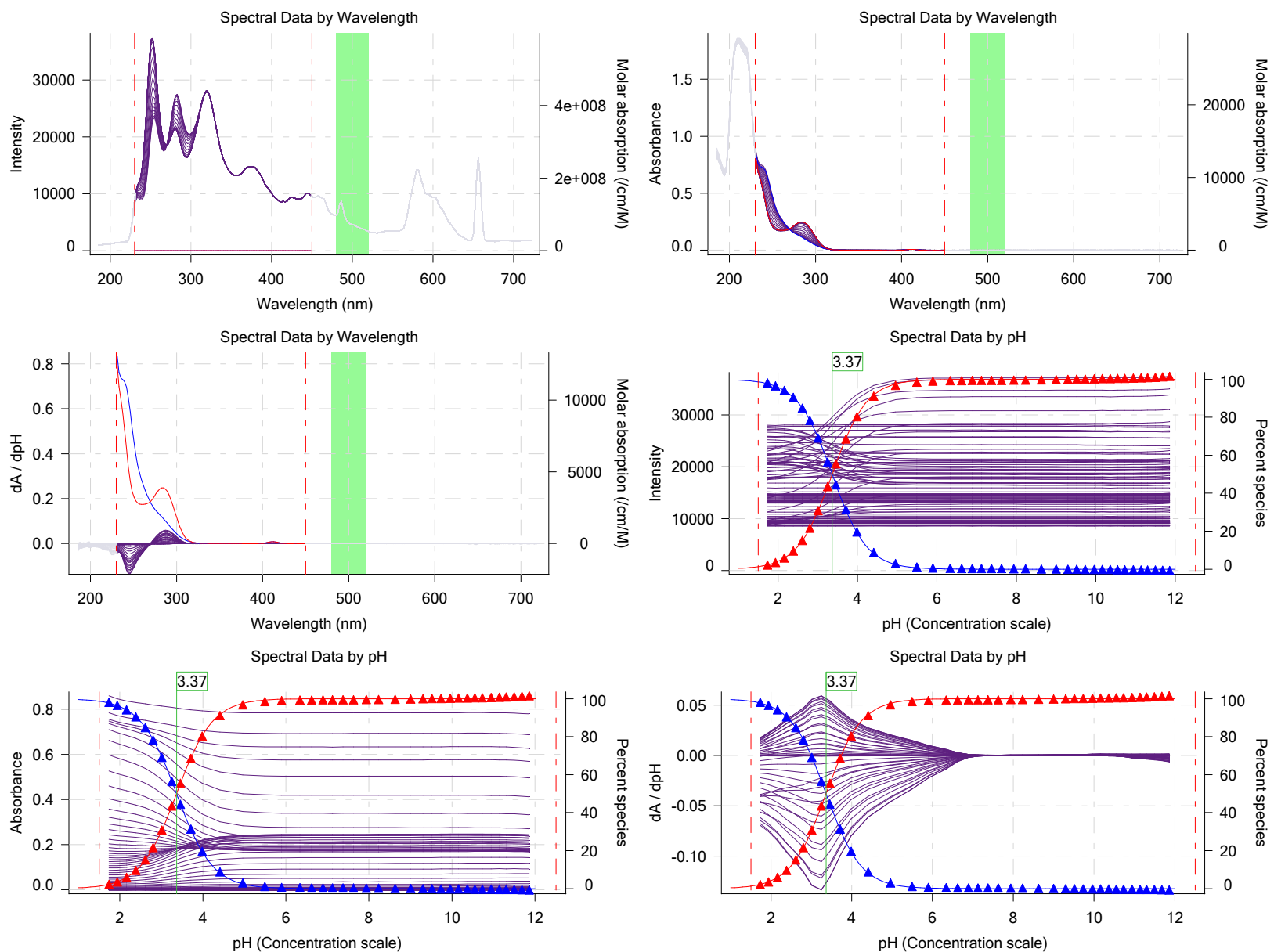
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 Assay ID: **17J-04003**  
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Experiment start time: **10/4/2017 2:49:42 AM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

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

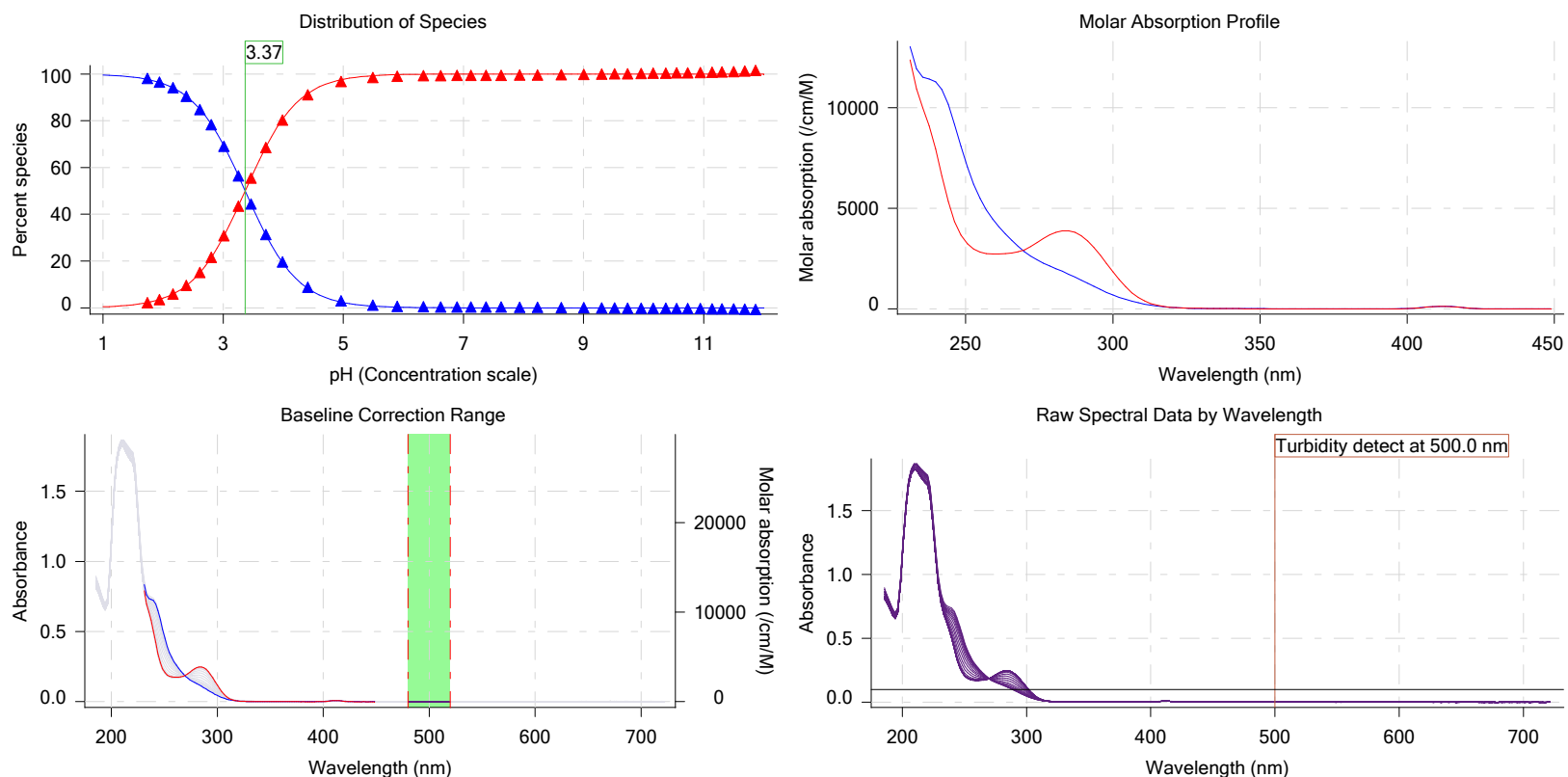
## Graphs



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## Graphs (continued)



## UV-metric psKa Titration 3 of 3 17J-04003 Points 77 to 119

### Results

pKa 1	<b>3.51</b>
RMSD	<b>0.003 0.007</b>
Chi squared	<b>0.0099</b>
PCA calculated number of pKas	<b>2</b>
Average ionic strength	<b>0.173 M</b>
Average temperature	<b>24.9°C</b>
Analyte concentration range	<b>50.5 µM to 47.8 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>1.496 to 12.537</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**

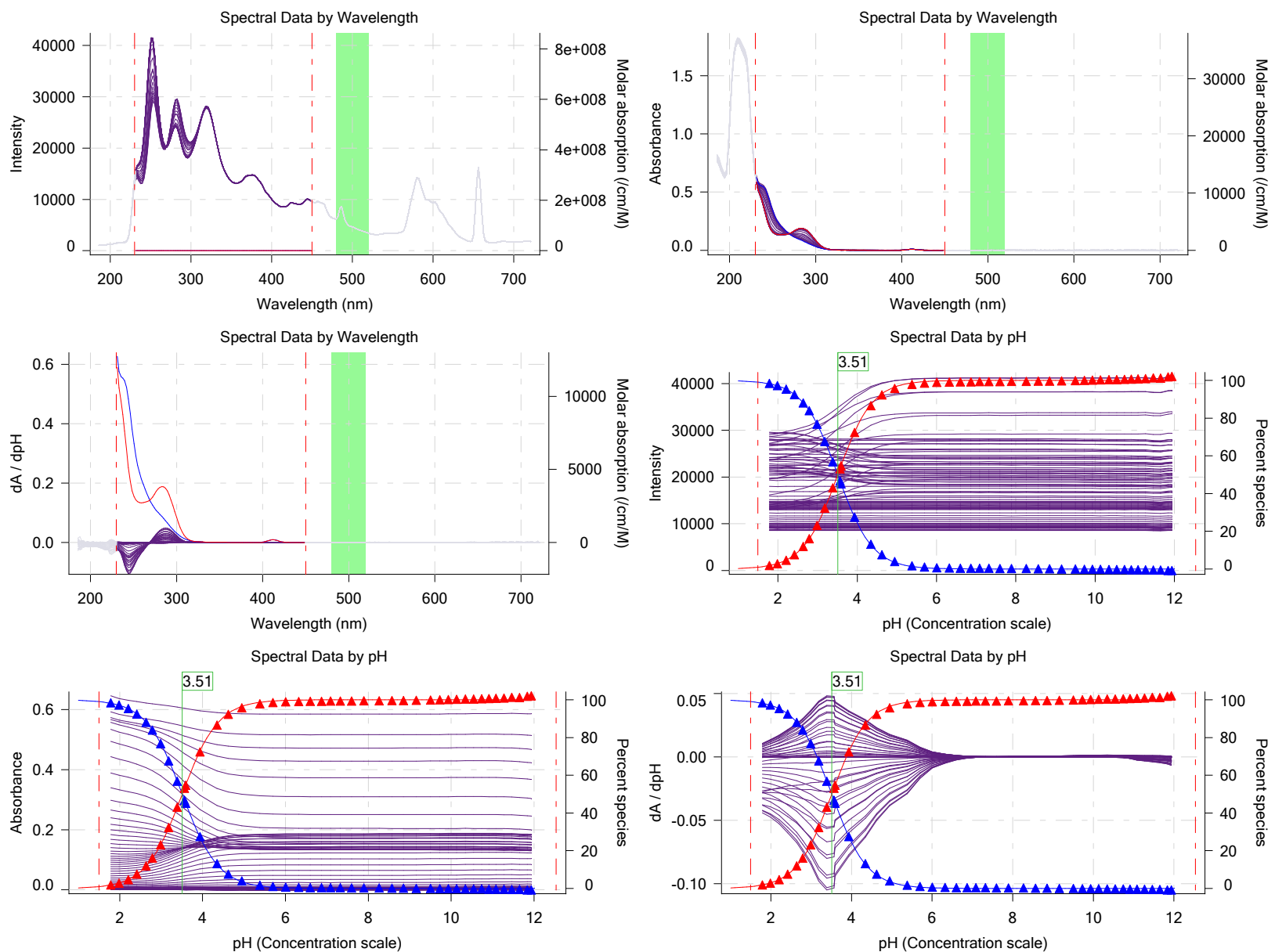
Sample name: **M11**  
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 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

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

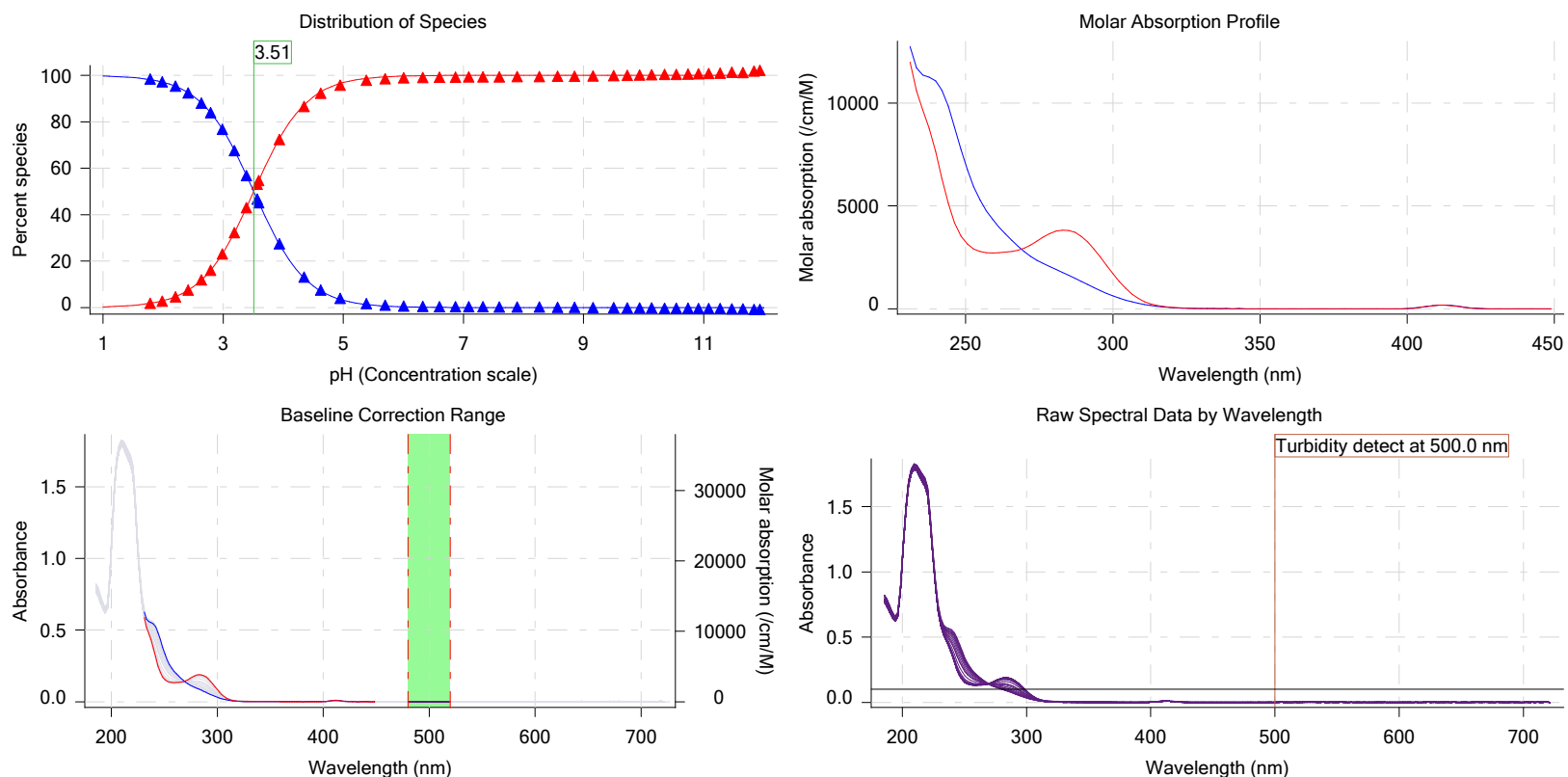
## Graphs



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## Graphs (continued)



## Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M11	10/3/2017 3:43:21 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0020 mL	10/3/2017 3:43:21 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.063900 M	10/3/2017 3:43:21 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	211.22	10/3/2017 3:43:31 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	10/3/2017 3:43:21 PM	User entered value
Sample is a	Base	10/3/2017 3:43:21 PM	User entered value
pKa 1	3.40	10/3/2017 3:43:21 PM	User entered value
logp (XH +)	-10.00		Default value
logP (neutral X)	-10.00	10/3/2017 3:43:21 PM	User entered value

## Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:37.1	Dark spectrum								
3:38.5	Reference spectrum								
4:06.2	Volume reset due to vial change								
4:50.3	Initial pH = 8.34								
6:02.0	Data point 4	0.34995 mL	0.07070 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.962	-0.01552	0.76096
6:30.7	Data point 5	0.34995 mL	0.07070 mL	0.02526 mL	1.15005 mL	0.02500 mL	2.161	-0.00744	0.40929
6:47.7	Data point 6	0.34995 mL	0.07070 mL	0.04193 mL	1.15005 mL	0.02500 mL	2.367	0.01712	0.85621
7:04.6	Data point 7	0.34995 mL	0.07070 mL	0.05226 mL	1.15005 mL	0.02500 mL	2.576	0.00403	0.11874
7:21.3	Data point 8	0.34995 mL	0.07070 mL	0.05873 mL	1.15005 mL	0.02500 mL	2.772	0.00853	0.74838
7:37.9	Data point 9	0.34995 mL	0.07070 mL	0.06284 mL	1.15005 mL	0.02500 mL	3.016	0.00840	0.74257



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**Events (continued)**

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
8:04.7	Data point 10	0.34995 mL	0.07070 mL	0.06512 mL	1.15005 mL	0.02500 mL	3.207	0.00989	0.78647	0.00
8:21.3	Data point 11	0.34995 mL	0.07070 mL	0.06665 mL	1.15005 mL	0.02500 mL	3.379	0.01068	0.92300	0.00
8:37.8	Data point 12	0.34995 mL	0.07070 mL	0.06769 mL	1.15005 mL	0.02500 mL	3.472	0.00617	0.62377	0.00
9:09.6	Data point 13	0.34995 mL	0.07070 mL	0.06879 mL	1.15005 mL	0.02500 mL	3.677	0.02489	0.98105	0.00
9:36.3	Data point 14	0.34995 mL	0.07070 mL	0.06940 mL	1.15005 mL	0.02500 mL	3.948	0.04289	0.98907	0.00
9:57.9	Data point 15	0.34995 mL	0.07070 mL	0.06992 mL	1.15005 mL	0.02500 mL	4.638	0.09928	0.98970	0.00
10:41.5	Data point 16	0.34995 mL	0.07070 mL	0.07030 mL	1.15005 mL	0.02500 mL	7.323	0.07513	0.62195	0.00
11:17.5	Data point 17	0.34995 mL	0.07070 mL	0.07058 mL	1.15005 mL	0.02500 mL	7.793	0.09915	0.99089	0.00
12:01.7	Data point 18	0.34995 mL	0.07070 mL	0.07074 mL	1.15005 mL	0.02500 mL	8.028	0.09906	0.98688	0.00
12:46.9	Data point 19	0.34995 mL	0.07070 mL	0.07086 mL	1.15005 mL	0.02500 mL	8.339	0.09458	0.97245	0.00
13:27.7	Data point 20	0.34995 mL	0.07070 mL	0.07095 mL	1.15005 mL	0.02500 mL	8.713	0.09559	0.98081	0.00
14:17.0	Data point 21	0.34995 mL	0.07070 mL	0.07105 mL	1.15005 mL	0.02500 mL	9.113	0.09913	0.98446	0.00
15:05.7	Data point 22	0.34995 mL	0.07070 mL	0.07114 mL	1.15005 mL	0.02500 mL	9.488	0.09943	0.96276	0.00
15:43.9	Data point 23	0.34995 mL	0.07070 mL	0.07126 mL	1.15005 mL	0.02500 mL	9.782	0.09609	0.97063	0.00
16:11.9	Data point 24	0.34995 mL	0.07070 mL	0.07138 mL	1.15005 mL	0.02500 mL	10.013	0.09888	0.97778	0.00
16:35.1	Data point 25	0.34995 mL	0.07070 mL	0.07152 mL	1.15005 mL	0.02500 mL	10.214	0.06263	0.97844	0.00
16:51.8	Data point 26	0.34995 mL	0.07070 mL	0.07175 mL	1.15005 mL	0.02500 mL	10.480	0.03112	0.97280	0.00
17:23.5	Data point 27	0.34995 mL	0.07070 mL	0.07227 mL	1.15005 mL	0.02500 mL	10.681	-0.00180	0.08789	0.00
17:55.2	Data point 28	0.34995 mL	0.07070 mL	0.07302 mL	1.15005 mL	0.02500 mL	10.879	-0.00414	0.58929	0.00
18:11.7	Data point 29	0.34995 mL	0.07070 mL	0.07411 mL	1.15005 mL	0.02500 mL	11.072	-0.00526	0.68123	0.00
18:28.2	Data point 30	0.34995 mL	0.07070 mL	0.07580 mL	1.15005 mL	0.02500 mL	11.249	-0.00436	0.53772	0.00
18:44.8	Data point 31	0.34995 mL	0.07070 mL	0.07834 mL	1.15005 mL	0.02500 mL	11.413	-0.00916	0.84157	0.00
19:11.6	Data point 32	0.34995 mL	0.07070 mL	0.08173 mL	1.15005 mL	0.02500 mL	11.607	-0.00883	0.80669	0.00
19:28.3	Data point 33	0.34995 mL	0.07070 mL	0.08758 mL	1.15005 mL	0.02500 mL	11.778	-0.00670	0.54060	0.00
19:45.1	Data point 34	0.34995 mL	0.07070 mL	0.09638 mL	1.15005 mL	0.02500 mL	11.959	-0.01256	0.83281	0.00
20:01.8	Data point 35	0.34995 mL	0.07070 mL	0.10181 mL	1.15005 mL	0.02500 mL	12.049	-0.01035	0.80665	0.00
21:38.0	Reference spectrum									
22:42.0	Data point 37	0.50000 mL	0.17072 mL	0.10183 mL	1.15005 mL	0.02500 mL	2.002	-0.05402	0.93897	0.00
23:09.6	Data point 38	0.50000 mL	0.17072 mL	0.12709 mL	1.15005 mL	0.02500 mL	2.200	0.00976	0.73307	0.00
23:26.6	Data point 39	0.50000 mL	0.17072 mL	0.14379 mL	1.15005 mL	0.02500 mL	2.421	0.00753	0.46239	0.00
23:43.4	Data point 40	0.50000 mL	0.17072 mL	0.15388 mL	1.15005 mL	0.02500 mL	2.640	0.00116	0.00480	0.00
24:00.1	Data point 41	0.50000 mL	0.17072 mL	0.15995 mL	1.15005 mL	0.02500 mL	2.865	0.02355	0.75603	0.00
24:16.7	Data point 42	0.50000 mL	0.17072 mL	0.16357 mL	1.15005 mL	0.02500 mL	3.051	0.01871	0.93414	0.00
24:33.2	Data point 43	0.50000 mL	0.17072 mL	0.16592 mL	1.15005 mL	0.02500 mL	3.260	0.00599	0.66029	0.00
24:49.9	Data point 44	0.50000 mL	0.17072 mL	0.16738 mL	1.15005 mL	0.02500 mL	3.496	0.01837	0.93068	0.00
25:21.8	Data point 45	0.50000 mL	0.17072 mL	0.16825 mL	1.15005 mL	0.02500 mL	3.704	0.02730	0.95727	0.00
25:38.3	Data point 46	0.50000 mL	0.17072 mL	0.16879 mL	1.15005 mL	0.02500 mL	3.952	0.03965	0.98467	0.00
25:60.0	Data point 47	0.50000 mL	0.17072 mL	0.16921 mL	1.15005 mL	0.02500 mL	4.223	0.06328	0.97353	0.00
26:21.6	Data point 48	0.50000 mL	0.17072 mL	0.16954 mL	1.15005 mL	0.02500 mL	4.642	0.09903	0.99037	0.00
27:00.7	Data point 49	0.50000 mL	0.17072 mL	0.16978 mL	1.15005 mL	0.02500 mL	5.188	0.09849	0.97484	0.00
27:54.8	Data point 50	0.50000 mL	0.17072 mL	0.16990 mL	1.15005 mL	0.02500 mL	5.714	0.09744	0.97800	0.00
28:58.9	Data point 51	0.50000 mL	0.17072 mL	0.16997 mL	1.15005 mL	0.02500 mL	6.114	0.09830	0.98849	0.00
30:02.1	Data point 52	0.50000 mL	0.17072 mL	0.17006 mL	1.15005 mL	0.02500 mL	6.548	0.10011	0.98546	0.00
30:50.7	Data point 53	0.50000 mL	0.17072 mL	0.17016 mL	1.15005 mL	0.02500 mL	6.831	0.10014	0.98686	0.00
31:27.8	Data point 54	0.50000 mL	0.17072 mL	0.17027 mL	1.15005 mL	0.02500 mL	7.098	0.09839	0.98900	0.00
32:02.4	Data point 55	0.50000 mL	0.17072 mL	0.17039 mL	1.15005 mL	0.02500 mL	7.328	0.09980	0.98643	0.00
32:40.2	Data point 56	0.50000 mL	0.17072 mL	0.17053 mL	1.15005 mL	0.02500 mL	7.576	0.09713	0.97609	0.00
33:16.9	Data point 57	0.50000 mL	0.17072 mL	0.17067 mL	1.15005 mL	0.02500 mL	7.828	0.09832	0.99023	0.00
34:00.6	Data point 58	0.50000 mL	0.17072 mL	0.17081 mL	1.15005 mL	0.02500 mL	8.132	0.09887	0.98749	0.00
34:48.4	Data point 59	0.50000 mL	0.17072 mL	0.17093 mL	1.15005 mL	0.02500 mL	8.424	0.09907	0.98328	0.00
35:39.1	Data point 60	0.50000 mL	0.17072 mL	0.17105 mL	1.15005 mL	0.02500 mL	8.818	0.09479	0.98621	0.00
36:27.1	Data point 61	0.50000 mL	0.17072 mL	0.17117 mL	1.15005 mL	0.02500 mL	9.187	0.09826	0.98213	0.00
37:12.3	Data point 62	0.50000 mL	0.17072 mL	0.17128 mL	1.15005 mL	0.02500 mL	9.480	0.09815	0.97414	0.00
37:40.5	Data point 63	0.50000 mL	0.17072 mL	0.17140 mL	1.15005 mL	0.02500 mL	9.697	0.09408	0.97466	0.00
38:10.8	Data point 64	0.50000 mL	0.17072 mL	0.17157 mL	1.15005 mL	0.02500 mL	9.911	0.08723	0.98105	0.00
38:32.4	Data point 65	0.50000 mL	0.17072 mL	0.17180 mL	1.15005 mL	0.02500 mL	10.135	0.03976	0.96278	0.00
39:04.1	Data point 66	0.50000 mL	0.17072 mL	0.17218 mL	1.15005 mL	0.02500 mL	10.332	0.01881	0.83926	0.00



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**Events (continued)**

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
39:25.7	Data point 67	0.50000 mL	0.17072 mL	0.17265 mL	1.15005 mL	0.02500 mL	10.537	0.00496	0.63921	0.00000
39:42.2	Data point 68	0.50000 mL	0.17072 mL	0.17333 mL	1.15005 mL	0.02500 mL	10.717	-0.00375	0.50914	0.00000
39:58.7	Data point 69	0.50000 mL	0.17072 mL	0.17436 mL	1.15005 mL	0.02500 mL	10.897	-0.00768	0.78409	0.00000
40:15.3	Data point 70	0.50000 mL	0.17072 mL	0.17594 mL	1.15005 mL	0.02500 mL	11.106	-0.00771	0.74328	0.00000
40:31.9	Data point 71	0.50000 mL	0.17072 mL	0.17846 mL	1.15005 mL	0.02500 mL	11.300	-0.00825	0.80263	0.00000
40:48.6	Data point 72	0.50000 mL	0.17072 mL	0.18241 mL	1.15005 mL	0.02500 mL	11.461	-0.00886	0.87987	0.00000
41:15.4	Data point 73	0.50000 mL	0.17072 mL	0.18810 mL	1.15005 mL	0.02500 mL	11.652	-0.01038	0.81008	0.00000
41:32.2	Data point 74	0.50000 mL	0.17072 mL	0.19711 mL	1.15005 mL	0.02500 mL	11.834	-0.01051	0.86403	0.00000
41:49.1	Data point 75	0.50000 mL	0.17072 mL	0.21108 mL	1.15005 mL	0.02500 mL	12.008	-0.01149	0.82200	0.00000
43:34.0	Reference spectrum									
44:57.2	Data point 77	0.83996 mL	0.30139 mL	0.21110 mL	1.15005 mL	0.02500 mL	1.996	-0.02675	0.95295	0.00000
45:24.9	Data point 78	0.83996 mL	0.30139 mL	0.23975 mL	1.15005 mL	0.02500 mL	2.193	0.01200	0.88982	0.00000
45:41.9	Data point 79	0.83996 mL	0.30139 mL	0.25912 mL	1.15005 mL	0.02500 mL	2.409	0.00135	0.02184	0.00000
45:58.8	Data point 80	0.83996 mL	0.30139 mL	0.27103 mL	1.15005 mL	0.02500 mL	2.614	-0.02866	0.55743	0.00000
46:15.4	Data point 81	0.83996 mL	0.30139 mL	0.27843 mL	1.15005 mL	0.02500 mL	2.834	-0.01857	0.85625	0.00000
46:47.8	Data point 82	0.83996 mL	0.30139 mL	0.28290 mL	1.15005 mL	0.02500 mL	2.985	-0.00065	0.01114	0.00000
47:14.7	Data point 83	0.83996 mL	0.30139 mL	0.28542 mL	1.15005 mL	0.02500 mL	3.179	0.01128	0.86331	0.00000
47:46.4	Data point 84	0.83996 mL	0.30139 mL	0.28742 mL	1.15005 mL	0.02500 mL	3.376	0.01009	0.72254	0.00000
48:03.1	Data point 85	0.83996 mL	0.30139 mL	0.28869 mL	1.15005 mL	0.02500 mL	3.576	-0.00929	0.47889	0.00000
48:19.7	Data point 86	0.83996 mL	0.30139 mL	0.28951 mL	1.15005 mL	0.02500 mL	3.752	-0.00197	0.05498	0.00000
48:36.2	Data point 87	0.83996 mL	0.30139 mL	0.29005 mL	1.15005 mL	0.02500 mL	3.779	0.01130	0.83870	0.00000
48:57.8	Data point 88	0.83996 mL	0.30139 mL	0.29104 mL	1.15005 mL	0.02500 mL	4.120	-0.01047	0.19819	0.00000
49:19.4	Data point 89	0.83996 mL	0.30139 mL	0.29151 mL	1.15005 mL	0.02500 mL	4.527	0.01086	0.10640	0.00000
49:46.1	Data point 90	0.83996 mL	0.30139 mL	0.29174 mL	1.15005 mL	0.02500 mL	4.802	0.09836	0.98886	0.00000
50:23.3	Data point 91	0.83996 mL	0.30139 mL	0.29186 mL	1.15005 mL	0.02500 mL	5.122	0.09821	0.98574	0.00000
51:03.9	Data point 92	0.83996 mL	0.30139 mL	0.29196 mL	1.15005 mL	0.02500 mL	5.555	0.09795	0.97601	0.00000
51:48.0	Data point 93	0.83996 mL	0.30139 mL	0.29203 mL	1.15005 mL	0.02500 mL	5.866	0.09973	0.98896	0.00000
52:31.6	Data point 94	0.83996 mL	0.30139 mL	0.29210 mL	1.15005 mL	0.02500 mL	6.172	0.09562	0.96921	0.00000
53:11.7	Data point 95	0.83996 mL	0.30139 mL	0.29219 mL	1.15005 mL	0.02500 mL	6.485	-0.06450	0.90072	0.00000
53:38.5	Data point 96	0.83996 mL	0.30139 mL	0.29229 mL	1.15005 mL	0.02500 mL	6.761	0.04841	0.79561	0.00000
54:05.2	Data point 97	0.83996 mL	0.30139 mL	0.29240 mL	1.15005 mL	0.02500 mL	7.027	0.05449	0.81591	0.00000
54:31.8	Data point 98	0.83996 mL	0.30139 mL	0.29252 mL	1.15005 mL	0.02500 mL	7.245	0.08133	0.90058	0.00000
55:03.6	Data point 99	0.83996 mL	0.30139 mL	0.29264 mL	1.15005 mL	0.02500 mL	7.476	0.09940	0.97288	0.00000
55:37.8	Data point 100	0.83996 mL	0.30139 mL	0.29276 mL	1.15005 mL	0.02500 mL	7.750	0.09988	0.98779	0.00000
56:12.6	Data point 101	0.83996 mL	0.30139 mL	0.29285 mL	1.15005 mL	0.02500 mL	8.042	0.09886	0.97621	0.00000
56:53.2	Data point 102	0.83996 mL	0.30139 mL	0.29294 mL	1.15005 mL	0.02500 mL	8.410	0.09932	0.97174	0.00000
57:33.4	Data point 103	0.83996 mL	0.30139 mL	0.29302 mL	1.15005 mL	0.02500 mL	8.711	0.09828	0.95625	0.00000
58:13.7	Data point 104	0.83996 mL	0.30139 mL	0.29309 mL	1.15005 mL	0.02500 mL	8.990	0.09884	0.98223	0.00000
58:51.8	Data point 105	0.83996 mL	0.30139 mL	0.29318 mL	1.15005 mL	0.02500 mL	9.293	0.09586	0.95829	0.00000
59:19.8	Data point 106	0.83996 mL	0.30139 mL	0.29330 mL	1.15005 mL	0.02500 mL	9.636	0.07212	0.98742	0.00000
59:41.4	Data point 107	0.83996 mL	0.30139 mL	0.29341 mL	1.15005 mL	0.02500 mL	9.859	0.05365	0.94664	0.00000
1:00:08.1	Data point 108	0.83996 mL	0.30139 mL	0.29358 mL	1.15005 mL	0.02500 mL	10.063	0.02700	0.91091	0.00000
1:00:34.9	Data point 109	0.83996 mL	0.30139 mL	0.29386 mL	1.15005 mL	0.02500 mL	10.260	0.00865	0.72158	0.00000
1:01:01.5	Data point 110	0.83996 mL	0.30139 mL	0.29431 mL	1.15005 mL	0.02500 mL	10.473	-0.00765	0.67483	0.00000
1:01:33.3	Data point 111	0.83996 mL	0.30139 mL	0.29518 mL	1.15005 mL	0.02500 mL	10.667	-0.00938	0.80569	0.00000
1:01:49.8	Data point 112	0.83996 mL	0.30139 mL	0.29659 mL	1.15005 mL	0.02500 mL	10.862	-0.02187	0.92384	0.00000
1:02:06.4	Data point 113	0.83996 mL	0.30139 mL	0.29878 mL	1.15005 mL	0.02500 mL	11.033	-0.02721	0.90841	0.00000
1:02:22.9	Data point 114	0.83996 mL	0.30139 mL	0.30202 mL	1.15005 mL	0.02500 mL	11.200	-0.02255	0.91159	0.00000
1:02:49.9	Data point 115	0.83996 mL	0.30139 mL	0.30633 mL	1.15005 mL	0.02500 mL	11.390	-0.01493	0.92431	0.00000
1:03:06.6	Data point 116	0.83996 mL	0.30139 mL	0.31371 mL	1.15005 mL	0.02500 mL	11.578	-0.02231	0.82856	0.00000
1:03:23.3	Data point 117	0.83996 mL	0.30139 mL	0.32526 mL	1.15005 mL	0.02500 mL	11.760	-0.02361	0.91056	0.00000
1:03:40.3	Data point 118	0.83996 mL	0.30139 mL	0.34318 mL	1.15005 mL	0.02500 mL	11.945	-0.02271	0.91378	0.00000
1:03:57.1	Data point 119	0.83996 mL	0.30139 mL	0.35635 mL	1.15005 mL	0.02500 mL	12.037	-0.01843	0.94089	0.00000
1:05:56.5	Assay volumes	1.08996 mL	0.44697 mL	0.35635 mL	1.15005 mL	0.02500 mL				

Sample name: **M11**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-04003**  
 Filename: **C:\Sirius\_T3\17J-04003\_M11\_UV-metric psKa.t3r**

Experiment start time: **10/4/2017 2:49:42 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>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>				

Sample name: **M11**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17J-04003**  
 Filename: **C:\Sirius\_T3\17J-04003\_M11\_UV-metric psKa.t3r**

Experiment start time: **10/4/2017 2:49:42 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	0.150	10/4/2017 2:49:42 AM	C:\Sirius_T3\17J-03018_Blank standardisation.t3r
Four-Plus S	0.9943	10/4/2017 2:49:42 AM	C:\Sirius_T3\17J-03018_Blank standardisation.t3r
Four-Plus jH	0.6	10/4/2017 2:49:42 AM	C:\Sirius_T3\17J-03018_Blank standardisation.t3r
Four-Plus jOH	-0.8	10/4/2017 2:49:42 AM	C:\Sirius_T3\17J-03018_Blank standardisation.t3r
Base concentration factor	1.011	10/4/2017 2:49:42 AM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	1.007	10/4/2017 2:49:42 AM	C:\Sirius_T3\17J-03018_Blank standardisation.t3r

## Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T311053		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1100253	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	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	9/29/2017 9:58:40 AM
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



## Assay Settings

Sample name: **M11**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-04003**  
Filename: **C:\Sirius\_T3\17J-04003\_M11\_UV-metric psKa.t3r**

Experiment start time: **10/4/2017 2:49:42 AM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

## Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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
Titrator		T3TM1100153	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 10:21:54 AM
E0 calibration	-8.25 mV		10/4/2017 2:50:06 AM
Filling solution	3M KCl	KCL095	10/2/2017 9:26:59 AM
Liquids			
Wash 1	50% IPA:50% Water		10/3/2017 9:05:00 AM
Wash 2	0.5% Triton X-100 in H2O		10/3/2017 9:05:01 AM
Buffer position 1	pH7 Wash		10/3/2017 9:05:03 AM
Buffer position 2	pH 7		10/3/2017 9:05:05 AM
Storage position			10/3/2017 9:05:10 AM
Wash water	7.7e+003 mL	10-3-17	10/3/2017 9:04:49 AM
Waste	2.3e+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	313:32:06		11/23/2010 12:22:28 PM
Calibrated on	9/26/2017 9:22:07 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		



## Assay Settings

Sample name: **M11**  
Assay name: **UV-metric psKa**  
Assay ID: **17J-04003**  
Filename: **C:\Sirius\_T3\17J-04003\_M11\_UV-metric psKa.t3r**

Experiment start time: **10/4/2017 2:49:42 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 E1