Yasuda-Shedlovsky Result

Sample name: **D06**
Assay name: **UV-metric psKa**
Assay ID: **17J-06004**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 3:28:39 AM**
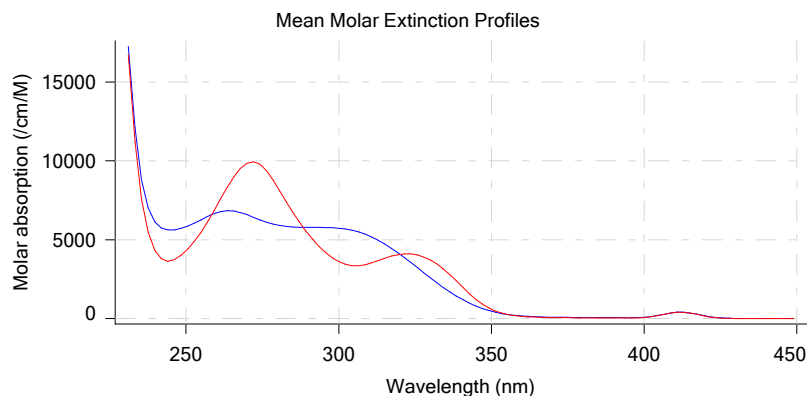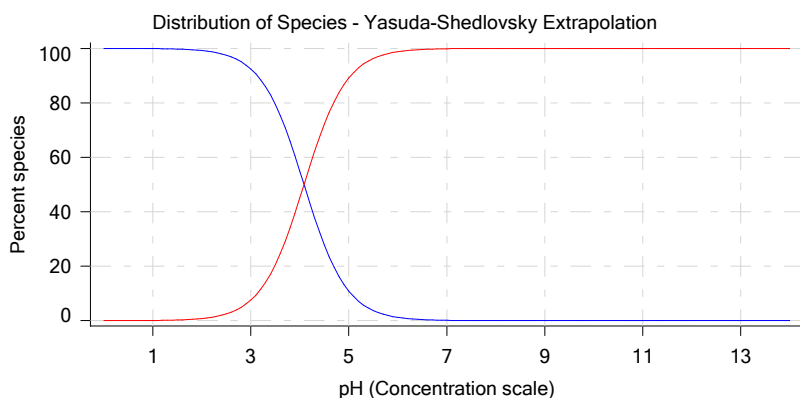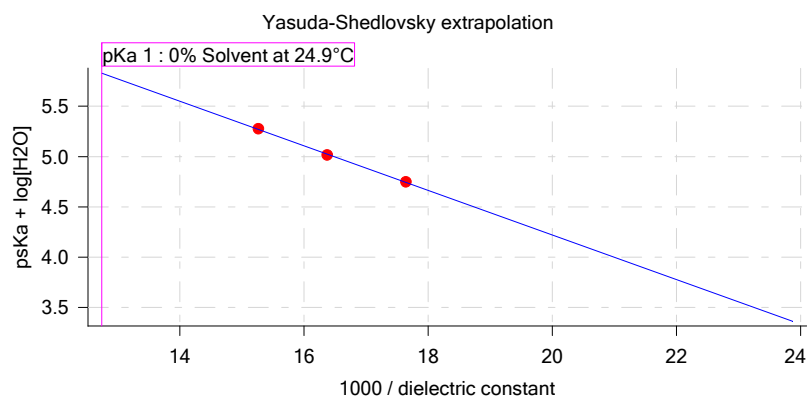Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.09	±0.03	8.65	-221.4318	0.9991	0.165 M	24.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
17J-06004 Points 4 to 40	49.39 %	Up	UV-metric pKa	56.7	24.7 M	0.157 M	24.9°C	☑	3.35
17J-06004 Points 42 to 83	39.86 %	Up	UV-metric pKa	61.1	30.1 M	0.166 M	24.9°C	☑	3.54
17J-06004 Points 85 to 123	30.07 %	Up	UV-metric pKa	65.5	35.8 M	0.173 M	24.9°C	☑	3.72

Graphs

Yasuda-Shedlovsky extrapolation
pKa 1 : 0% Solvent at 24.9°C

Distribution of Species - Yasuda-Shedlovsky Extrapolation

Mean Molar Extinction Profiles

UV-metric psKa   Titration 1 of 3   17J-06004 Points 4 to 40

Results

pKa 1	**3.35**
RMSD	**0.003 0.002**
Chi squared	**0.0082**
PCA calculated number of pKas	**1**
Average ionic strength	**0.157 M**
Average temperature	**24.9°C**
Analyte concentration range	**29.7 µM to 27.9 µM**
Methanol weight %	**49.4 %**
Dielectric constant	**56.7**
Water concentration	**24.7 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**

Sample name: **D06**	Experiment start time: **10/6/2017 3:28:39 AM**
Assay name: **UV-metric psKa**	Analyst: **Dorothy Levorse**
Assay ID: **17J-06004**	Instrument ID: **T311053**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**	

Results (continued)

pH clipping   **1.462 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			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

Graphs

Sample name: **D06**
Assay name: **UV-metric psKa**
Assay ID: **17J-06004**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 3:28:39 AM**
Analyst: **Dorothy Levorse**
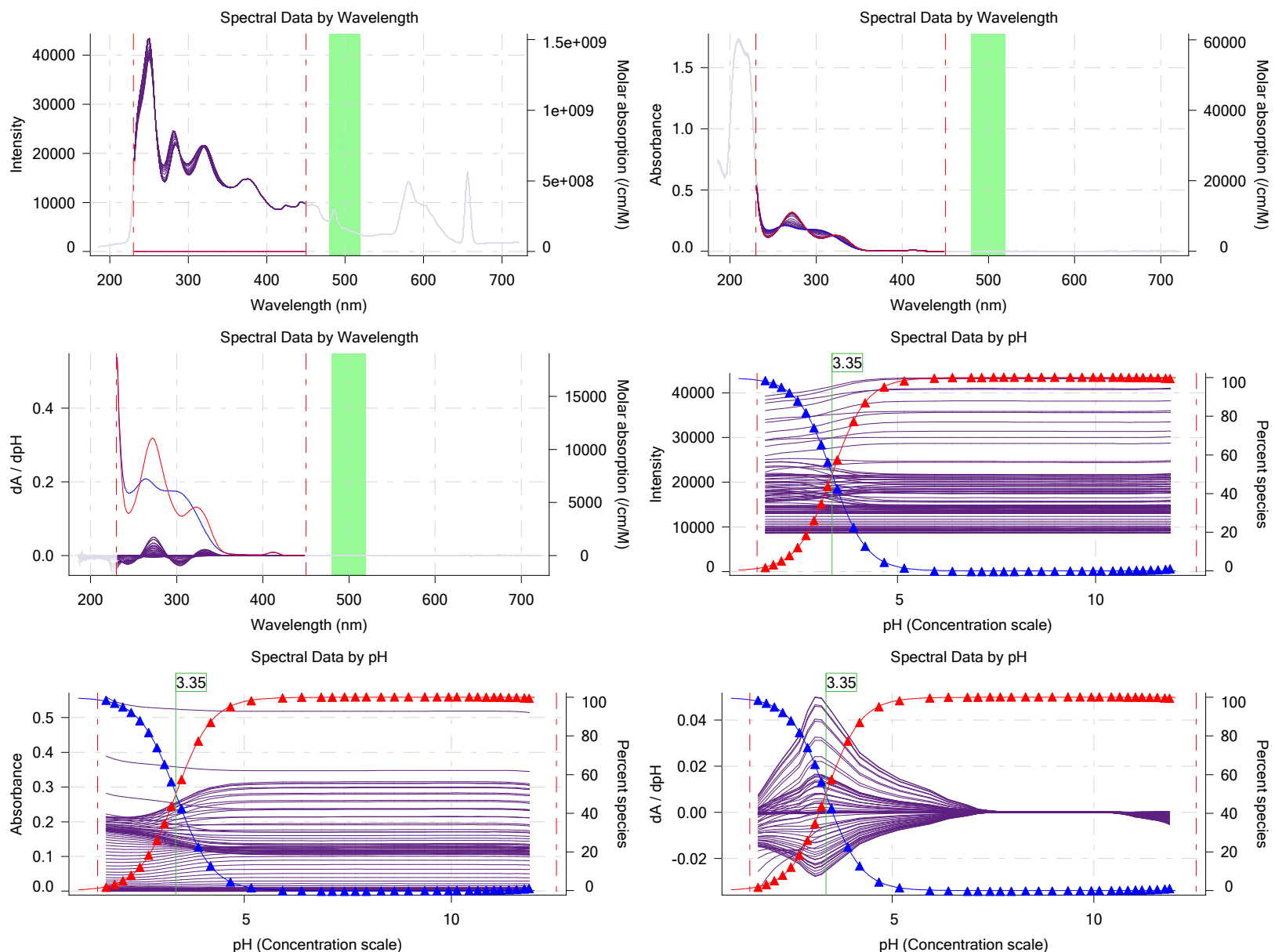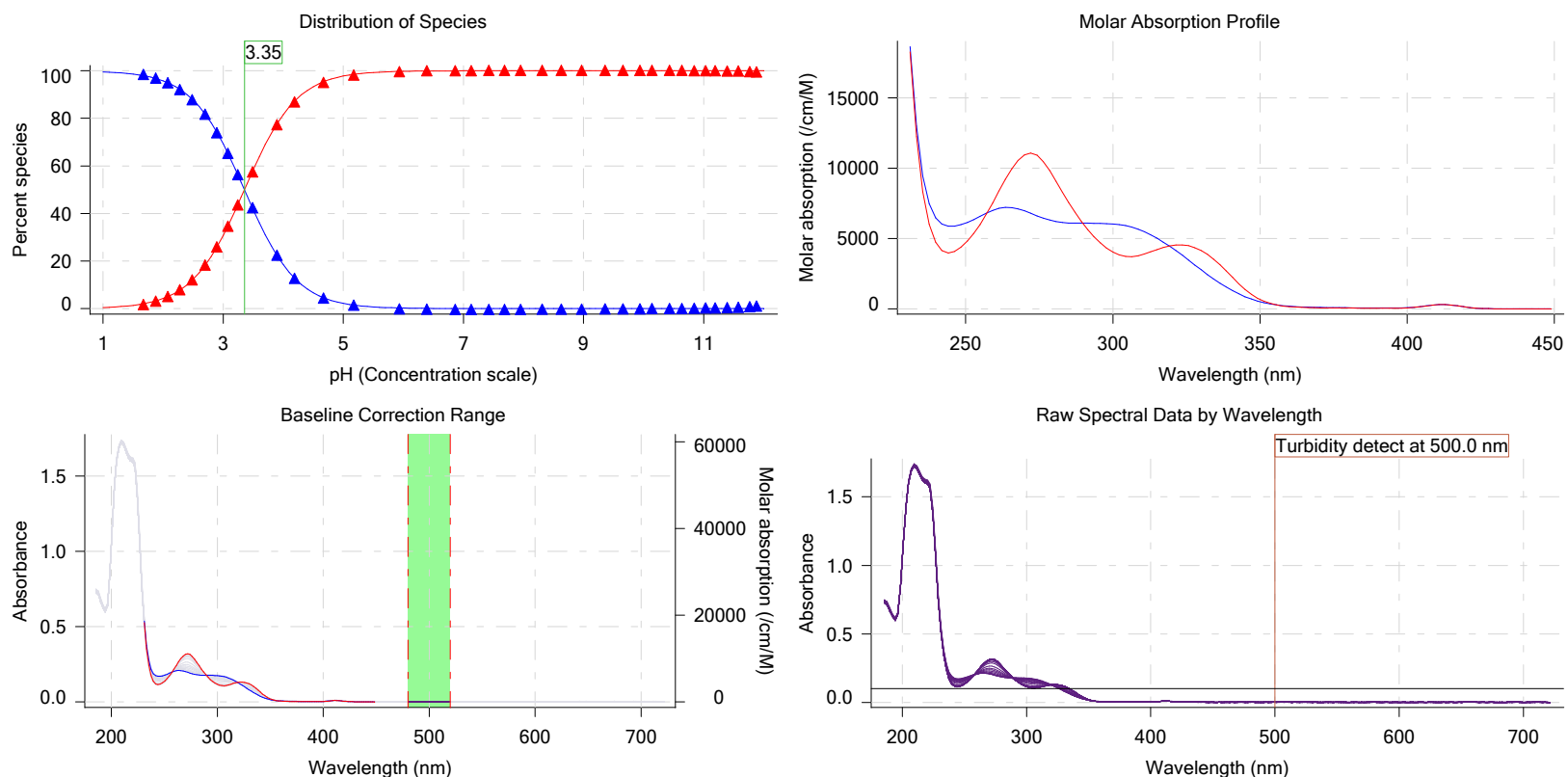Instrument ID: **T311053**

Graphs (continued)

Distribution of Species

Molar Absorption Profile

Baseline Correction Range

Raw Spectral Data by Wavelength

UV-metric psKa   Titration 2 of 3   17J-06004 Points 42 to 83

Results

pKa 1	**3.54**
RMSD	**0.005 0.003**
Chi squared	**0.0090**
PCA calculated number of pKas	**3**
Average ionic strength	**0.166 M**
Average temperature	**24.9°C**
Analyte concentration range	**24.3 µM to 23.0 µM**
Methanol weight %	**39.9 %**
Dielectric constant	**61.1**
Water concentration	**30.1 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.494 to 12.537**

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-06004**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 3:28:39 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

Spectral Data by Wavelength

Spectral Data by Wavelength

Spectral Data by Wavelength

Spectral Data by pH

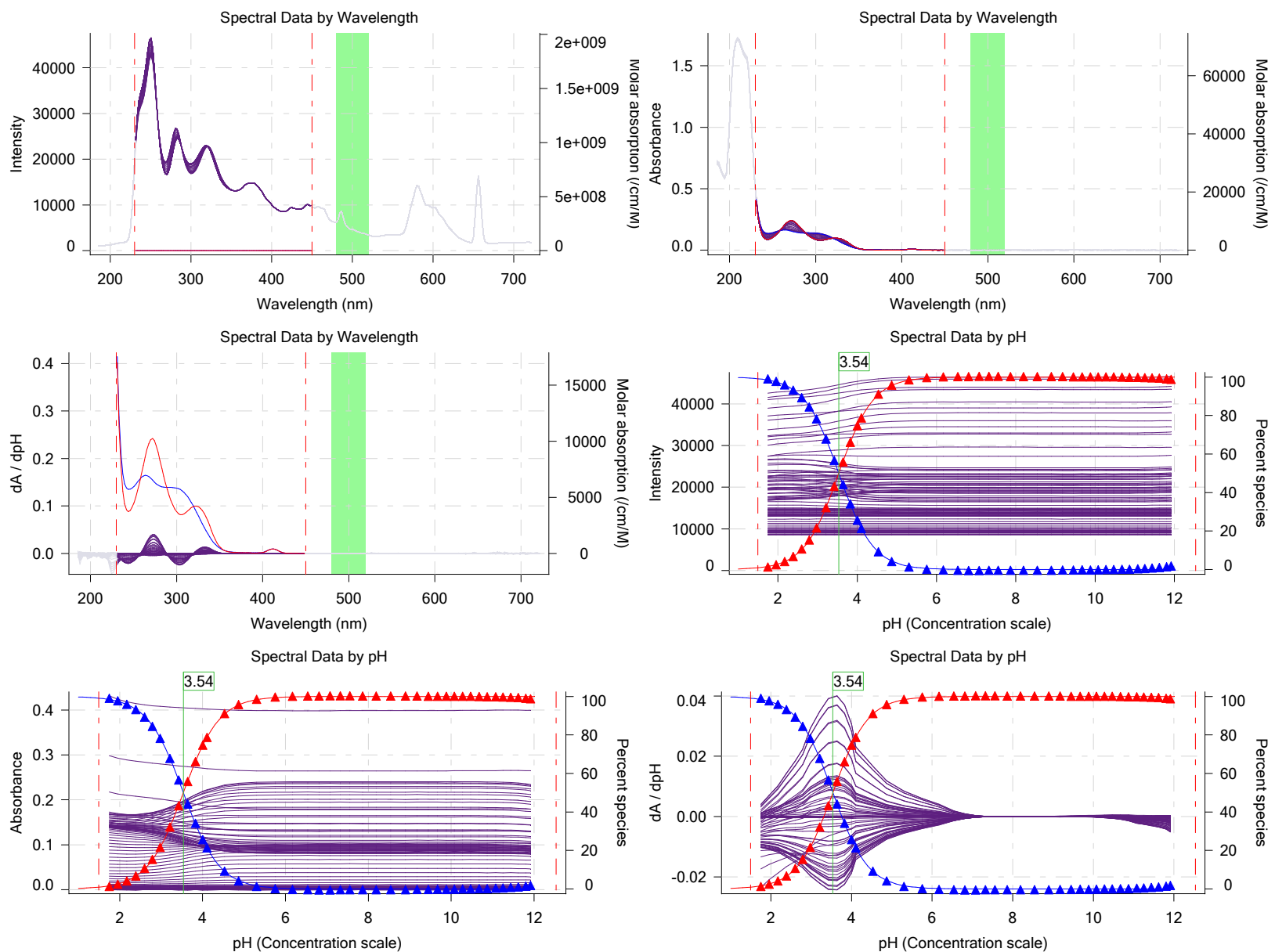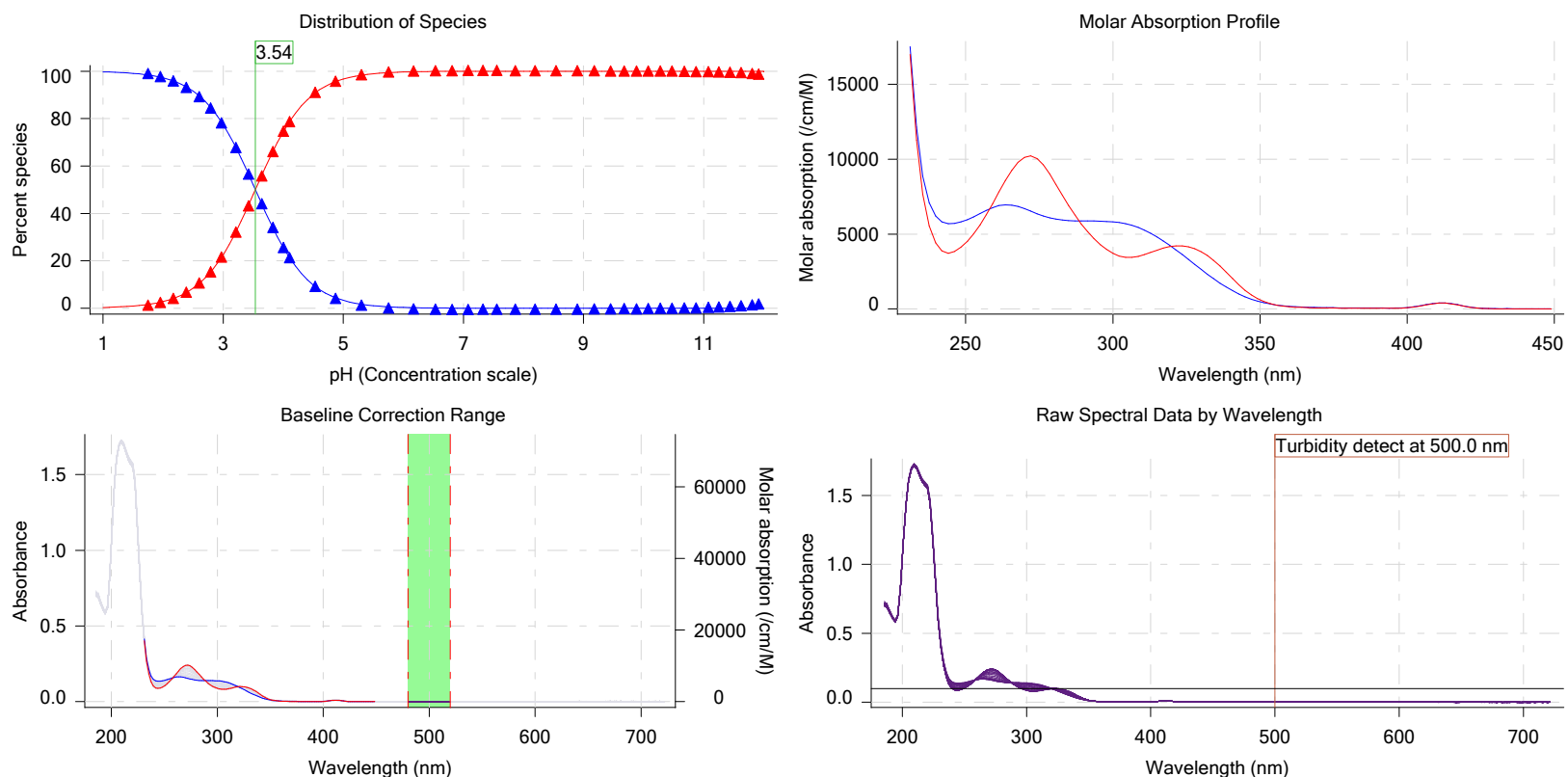Spectral Data by pH

Spectral Data by pH

Sample name: **D06**
Assay name: **UV-metric psKa**
Assay ID: **17J-06004**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 3:28:39 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)

Distribution of Species

Molar Absorption Profile

Baseline Correction Range

Raw Spectral Data by Wavelength

Turbidity detect at 500.0 nm

UV-metric psKa   Titration 3 of 3   17J-06004 Points 85 to 123

Results

pKa 1	**3.72**
RMSD	**0.009 0.012**
Chi squared	**0.0164**
PCA calculated number of pKas	**2**
Average ionic strength	**0.173 M**
Average temperature	**24.9°C**
Analyte concentration range	**18.7 µM to 17.7 µM**
Methanol weight %	**30.1 %**
Dielectric constant	**65.5**
Water concentration	**35.8 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.526 to 12.544**

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-06004**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 3:28:39 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

Spectral Data by Wavelength

Spectral Data by Wavelength

Spectral Data by Wavelength

Spectral Data by pH

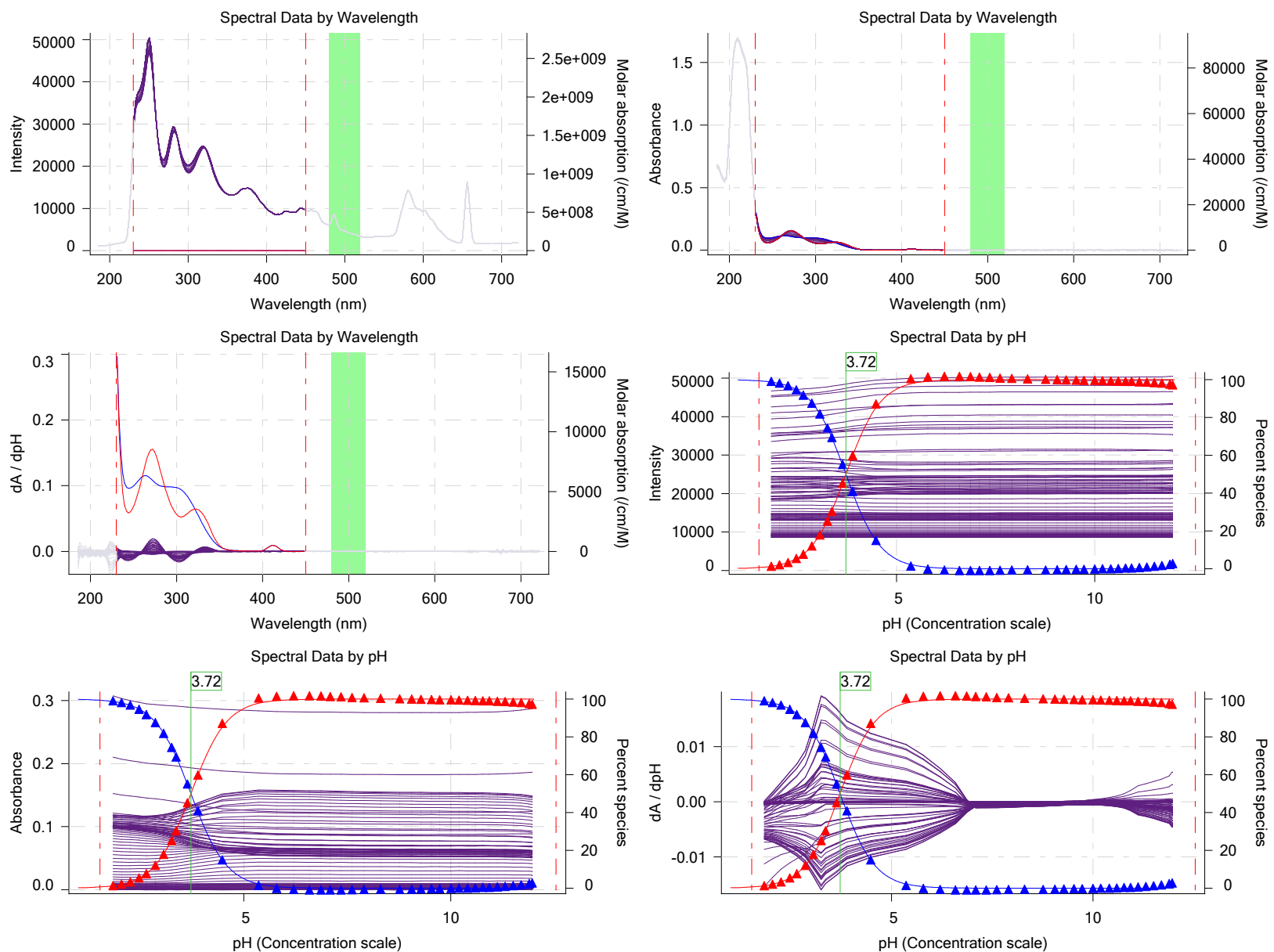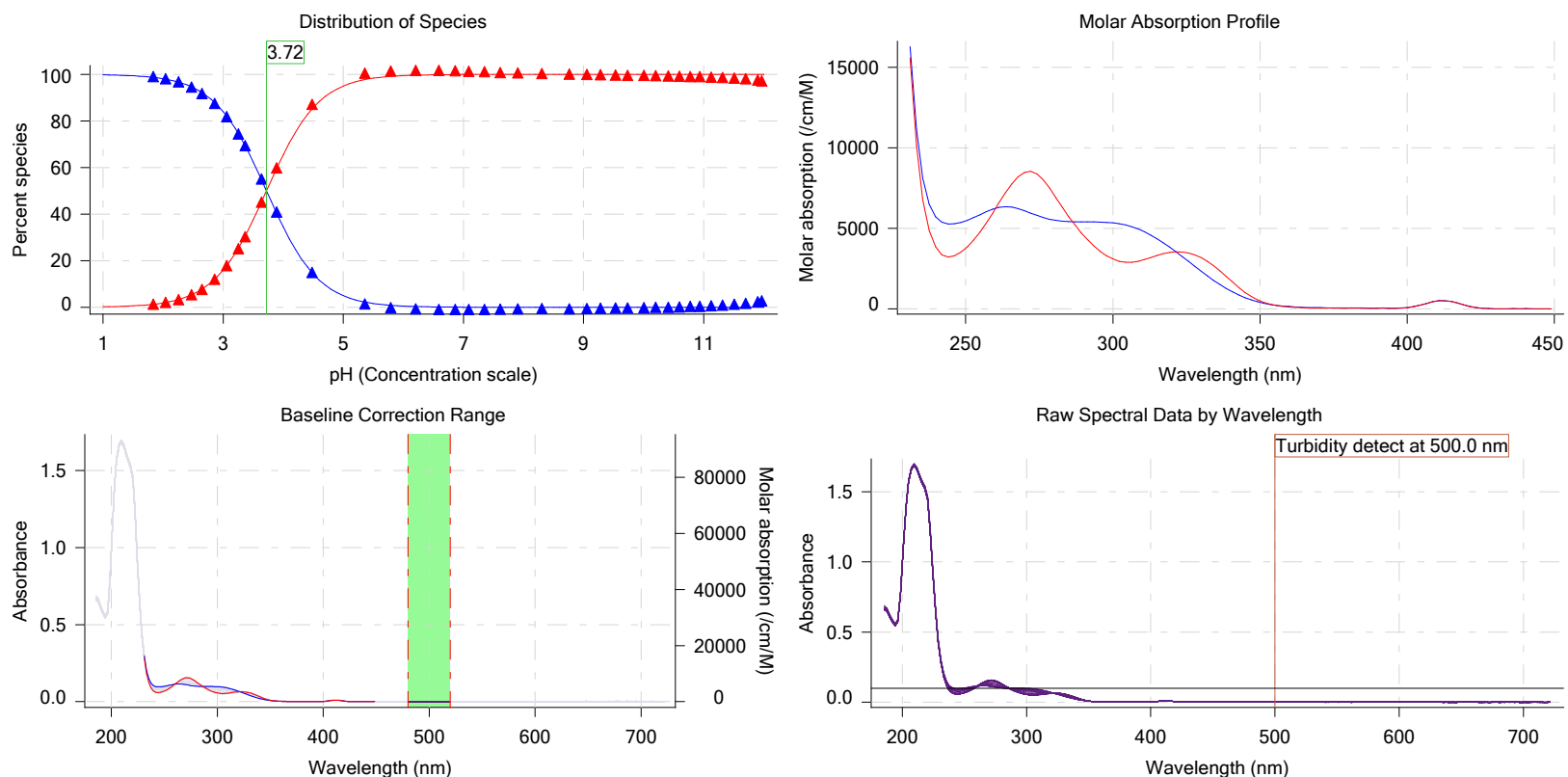Spectral Data by pH

Spectral Data by pH

Sample name: **D06**
Assay name: **UV-metric psKa**
Assay ID: **17J-06004**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 3:28:39 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)

Distribution of Species

Molar Absorption Profile

Baseline Correction Range

Raw Spectral Data by Wavelength

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
3:37.5	Dark spectrum								
3:39.0	Reference spectrum								
4:06.6	Volume reset due to vial change								
4:50.8	Initial pH = 8.35								
6:03.8	Data point 4	0.34995 mL	0.06990 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.962	-0.01002	0.66011
6:32.7	Data point 5	0.34995 mL	0.06990 mL	0.02521 mL	1.15005 mL	0.02500 mL	2.163	-0.01760	0.70132
6:49.7	Data point 6	0.34995 mL	0.06990 mL	0.04123 mL	1.15005 mL	0.02500 mL	2.358	0.01535	0.59497
7:06.6	Data point 7	0.34995 mL	0.06990 mL	0.05129 mL	1.15005 mL	0.02500 mL	2.556	0.00317	0.22790
7:23.4	Data point 8	0.34995 mL	0.06990 mL	0.05774 mL	1.15005 mL	0.02500 mL	2.761	0.00544	0.59074
7:40.1	Data point 9	0.34995 mL	0.06990 mL	0.06171 mL	1.15005 mL	0.02500 mL	2.972	0.01007	0.84032

Sample name: **D06**
Assay name: **UV-metric psKa**
Assay ID: **17J-06004**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 3:28:39 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
7:56.7	Data point 10	0.34995 mL	0.06990 mL	0.06416 mL	1.15005 mL	0.02500 mL	3.168	0.00961	0.68126	0.00
8:13.3	Data point 11	0.34995 mL	0.06990 mL	0.06571 mL	1.15005 mL	0.02500 mL	3.349	0.01363	0.89904	0.00
8:29.9	Data point 12	0.34995 mL	0.06990 mL	0.06675 mL	1.15005 mL	0.02500 mL	3.512	0.01328	0.83342	0.00
8:51.6	Data point 13	0.34995 mL	0.06990 mL	0.06816 mL	1.15005 mL	0.02500 mL	3.754	0.02655	0.96412	0.00
9:13.5	Data point 14	0.34995 mL	0.06990 mL	0.06893 mL	1.15005 mL	0.02500 mL	4.154	0.06728	0.98771	0.00
9:35.2	Data point 15	0.34995 mL	0.06990 mL	0.06924 mL	1.15005 mL	0.02500 mL	4.447	0.09889	0.97850	0.00
10:08.3	Data point 16	0.34995 mL	0.06990 mL	0.06952 mL	1.15005 mL	0.02500 mL	4.921	0.09981	0.99271	0.00
11:03.6	Data point 17	0.34995 mL	0.06990 mL	0.06964 mL	1.15005 mL	0.02500 mL	5.421	-0.38634	0.88764	0.02
12:20.4	Data point 18	0.34995 mL	0.06990 mL	0.06971 mL	1.15005 mL	0.02500 mL	6.169	0.10072	0.99243	0.00
13:26.2	Data point 19	0.34995 mL	0.06990 mL	0.06978 mL	1.15005 mL	0.02500 mL	6.621	0.10059	0.99677	0.00
14:26.0	Data point 20	0.34995 mL	0.06990 mL	0.06987 mL	1.15005 mL	0.02500 mL	7.090	0.10032	0.98947	0.00
15:14.6	Data point 21	0.34995 mL	0.06990 mL	0.06997 mL	1.15005 mL	0.02500 mL	7.353	0.09645	0.97071	0.00
15:56.6	Data point 22	0.34995 mL	0.06990 mL	0.07008 mL	1.15005 mL	0.02500 mL	7.644	0.09961	0.99337	0.00
16:40.9	Data point 23	0.34995 mL	0.06990 mL	0.07020 mL	1.15005 mL	0.02500 mL	7.901	0.09937	0.98537	0.00
17:24.4	Data point 24	0.34995 mL	0.06990 mL	0.07030 mL	1.15005 mL	0.02500 mL	8.167	0.09965	0.98557	0.00
18:09.1	Data point 25	0.34995 mL	0.06990 mL	0.07039 mL	1.15005 mL	0.02500 mL	8.520	0.10004	0.98647	0.00
18:52.5	Data point 26	0.34995 mL	0.06990 mL	0.07046 mL	1.15005 mL	0.02500 mL	8.838	0.09832	0.97573	0.00
19:35.8	Data point 27	0.34995 mL	0.06990 mL	0.07053 mL	1.15005 mL	0.02500 mL	9.170	0.09712	0.97677	0.00
20:22.8	Data point 28	0.34995 mL	0.06990 mL	0.07063 mL	1.15005 mL	0.02500 mL	9.560	0.09981	0.97353	0.00
21:00.0	Data point 29	0.34995 mL	0.06990 mL	0.07074 mL	1.15005 mL	0.02500 mL	9.851	0.09973	0.97425	0.00
21:26.8	Data point 30	0.34995 mL	0.06990 mL	0.07086 mL	1.15005 mL	0.02500 mL	10.130	0.09405	0.97979	0.00
21:54.2	Data point 31	0.34995 mL	0.06990 mL	0.07103 mL	1.15005 mL	0.02500 mL	10.329	0.04838	0.94968	0.00
22:10.7	Data point 32	0.34995 mL	0.06990 mL	0.07135 mL	1.15005 mL	0.02500 mL	10.620	0.01618	0.92441	0.00
22:42.4	Data point 33	0.34995 mL	0.06990 mL	0.07208 mL	1.15005 mL	0.02500 mL	10.823	0.00198	0.19664	0.00
22:59.0	Data point 34	0.34995 mL	0.06990 mL	0.07309 mL	1.15005 mL	0.02500 mL	11.025	-0.00022	0.00406	0.00
23:15.6	Data point 35	0.34995 mL	0.06990 mL	0.07469 mL	1.15005 mL	0.02500 mL	11.210	-0.00307	0.59986	0.00
23:32.2	Data point 36	0.34995 mL	0.06990 mL	0.07714 mL	1.15005 mL	0.02500 mL	11.369	-0.00712	0.76479	0.00
23:59.1	Data point 37	0.34995 mL	0.06990 mL	0.08048 mL	1.15005 mL	0.02500 mL	11.563	-0.00934	0.80570	0.00
24:15.8	Data point 38	0.34995 mL	0.06990 mL	0.08608 mL	1.15005 mL	0.02500 mL	11.745	-0.00713	0.69865	0.00
24:32.5	Data point 39	0.34995 mL	0.06990 mL	0.09471 mL	1.15005 mL	0.02500 mL	11.929	-0.00372	0.18700	0.00
24:49.3	Data point 40	0.34995 mL	0.06990 mL	0.10212 mL	1.15005 mL	0.02500 mL	12.041	-0.01052	0.79278	0.00
26:25.6	Reference spectrum									
27:29.7	Data point 42	0.50000 mL	0.16990 mL	0.10214 mL	1.15005 mL	0.02500 mL	1.994	-0.05273	0.94129	0.00
27:57.1	Data point 43	0.50000 mL	0.16990 mL	0.12705 mL	1.15005 mL	0.02500 mL	2.192	0.01329	0.94617	0.00
28:14.1	Data point 44	0.50000 mL	0.16990 mL	0.14320 mL	1.15005 mL	0.02500 mL	2.407	0.01108	0.67226	0.00
28:30.9	Data point 45	0.50000 mL	0.16990 mL	0.15299 mL	1.15005 mL	0.02500 mL	2.618	0.01196	0.73490	0.00
28:47.6	Data point 46	0.50000 mL	0.16990 mL	0.15898 mL	1.15005 mL	0.02500 mL	2.828	-0.00735	0.28553	0.00
29:04.3	Data point 47	0.50000 mL	0.16990 mL	0.16268 mL	1.15005 mL	0.02500 mL	3.016	-0.00125	0.01212	0.00
29:21.1	Data point 48	0.50000 mL	0.16990 mL	0.16508 mL	1.15005 mL	0.02500 mL	3.197	0.01366	0.92035	0.00
29:37.8	Data point 49	0.50000 mL	0.16990 mL	0.16665 mL	1.15005 mL	0.02500 mL	3.433	0.01039	0.83413	0.00
30:09.8	Data point 50	0.50000 mL	0.16990 mL	0.16766 mL	1.15005 mL	0.02500 mL	3.640	0.02151	0.92062	0.00
30:26.4	Data point 51	0.50000 mL	0.16990 mL	0.16823 mL	1.15005 mL	0.02500 mL	3.859	0.01758	0.80049	0.00
30:43.1	Data point 52	0.50000 mL	0.16990 mL	0.16858 mL	1.15005 mL	0.02500 mL	4.042	0.04756	0.98182	0.00
30:59.7	Data point 53	0.50000 mL	0.16990 mL	0.16881 mL	1.15005 mL	0.02500 mL	4.217	0.07166	0.98770	0.00
31:16.2	Data point 54	0.50000 mL	0.16990 mL	0.16896 mL	1.15005 mL	0.02500 mL	4.317	0.08993	0.98570	0.00
31:37.9	Data point 55	0.50000 mL	0.16990 mL	0.16917 mL	1.15005 mL	0.02500 mL	4.740	0.10050	0.99353	0.00
32:20.2	Data point 56	0.50000 mL	0.16990 mL	0.16931 mL	1.15005 mL	0.02500 mL	5.075	0.09822	0.98947	0.00
33:08.5	Data point 57	0.50000 mL	0.16990 mL	0.16938 mL	1.15005 mL	0.02500 mL	5.503	0.09874	0.98740	0.00
34:12.3	Data point 58	0.50000 mL	0.16990 mL	0.16945 mL	1.15005 mL	0.02500 mL	5.949	0.10014	0.99190	0.00
35:08.3	Data point 59	0.50000 mL	0.16990 mL	0.16952 mL	1.15005 mL	0.02500 mL	6.361	0.09840	0.98714	0.00
36:01.1	Data point 60	0.50000 mL	0.16990 mL	0.16961 mL	1.15005 mL	0.02500 mL	6.725	0.10042	0.99710	0.00
36:36.3	Data point 61	0.50000 mL	0.16990 mL	0.16971 mL	1.15005 mL	0.02500 mL	6.998	0.09370	0.97699	0.00
37:11.2	Data point 62	0.50000 mL	0.16990 mL	0.16983 mL	1.15005 mL	0.02500 mL	7.260	0.09507	0.97306	0.00
37:48.1	Data point 63	0.50000 mL	0.16990 mL	0.16994 mL	1.15005 mL	0.02500 mL	7.503	0.09742	0.98245	0.00
38:26.0	Data point 64	0.50000 mL	0.16990 mL	0.17006 mL	1.15005 mL	0.02500 mL	7.735	0.09916	0.97212	0.00
39:07.8	Data point 65	0.50000 mL	0.16990 mL	0.17020 mL	1.15005 mL	0.02500 mL	8.038	0.09609	0.96777	0.00
39:51.8	Data point 66	0.50000 mL	0.16990 mL	0.17032 mL	1.15005 mL	0.02500 mL	8.363	0.09913	0.98814	0.00

Sample name: **D06** Experiment start time: **10/6/2017 3:28:39 AM**
Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse**
Assay ID: **17J-06004** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
40:35.0	Data point 67	0.50000 mL	0.16990 mL	0.17041 mL	1.15005 mL	0.02500 mL	8.711	0.09721	0.97972	0.
41:22.0	Data point 68	0.50000 mL	0.16990 mL	0.17051 mL	1.15005 mL	0.02500 mL	9.061	0.09894	0.98151	0.
42:01.2	Data point 69	0.50000 mL	0.16990 mL	0.17060 mL	1.15005 mL	0.02500 mL	9.340	0.09300	0.95805	0.
42:36.0	Data point 70	0.50000 mL	0.16990 mL	0.17072 mL	1.15005 mL	0.02500 mL	9.610	0.09710	0.95471	0.
43:00.2	Data point 71	0.50000 mL	0.16990 mL	0.17086 mL	1.15005 mL	0.02500 mL	9.831	0.06788	0.93957	0.
43:27.0	Data point 72	0.50000 mL	0.16990 mL	0.17105 mL	1.15005 mL	0.02500 mL	10.037	0.04039	0.96037	0.
43:58.9	Data point 73	0.50000 mL	0.16990 mL	0.17133 mL	1.15005 mL	0.02500 mL	10.231	0.01942	0.89124	0.
44:30.7	Data point 74	0.50000 mL	0.16990 mL	0.17178 mL	1.15005 mL	0.02500 mL	10.427	0.01245	0.76689	0.
45:02.6	Data point 75	0.50000 mL	0.16990 mL	0.17246 mL	1.15005 mL	0.02500 mL	10.621	0.00390	0.50418	0.
45:34.6	Data point 76	0.50000 mL	0.16990 mL	0.17357 mL	1.15005 mL	0.02500 mL	10.823	-0.00421	0.40520	0.
46:06.6	Data point 77	0.50000 mL	0.16990 mL	0.17495 mL	1.15005 mL	0.02500 mL	11.015	-0.00568	0.66935	0.
46:23.2	Data point 78	0.50000 mL	0.16990 mL	0.17709 mL	1.15005 mL	0.02500 mL	11.219	-0.00750	0.83112	0.
46:39.8	Data point 79	0.50000 mL	0.16990 mL	0.18053 mL	1.15005 mL	0.02500 mL	11.392	-0.00914	0.93419	0.
46:56.4	Data point 80	0.50000 mL	0.16990 mL	0.18568 mL	1.15005 mL	0.02500 mL	11.573	-0.00818	0.79124	0.
47:13.2	Data point 81	0.50000 mL	0.16990 mL	0.19358 mL	1.15005 mL	0.02500 mL	11.751	-0.00853	0.83329	0.
47:30.2	Data point 82	0.50000 mL	0.16990 mL	0.20569 mL	1.15005 mL	0.02500 mL	11.931	-0.00906	0.74512	0.
47:47.0	Data point 83	0.50000 mL	0.16990 mL	0.21588 mL	1.15005 mL	0.02500 mL	12.037	-0.01132	0.87449	0.
49:32.3	Reference spectrum									
50:55.7	Data point 85	0.83996 mL	0.30303 mL	0.21590 mL	1.15005 mL	0.02500 mL	2.026	-0.00832	0.51240	0.
51:23.3	Data point 86	0.83996 mL	0.30303 mL	0.24186 mL	1.15005 mL	0.02500 mL	2.225	0.01261	0.69647	0.
51:40.4	Data point 87	0.83996 mL	0.30303 mL	0.25896 mL	1.15005 mL	0.02500 mL	2.436	-0.00646	0.24646	0.
51:57.3	Data point 88	0.83996 mL	0.30303 mL	0.26947 mL	1.15005 mL	0.02500 mL	2.647	-0.02990	0.87185	0.
52:29.8	Data point 89	0.83996 mL	0.30303 mL	0.27601 mL	1.15005 mL	0.02500 mL	2.821	0.01090	0.76800	0.
52:46.6	Data point 90	0.83996 mL	0.30303 mL	0.28029 mL	1.15005 mL	0.02500 mL	3.032	-0.01100	0.62366	0.
53:03.1	Data point 91	0.83996 mL	0.30303 mL	0.28295 mL	1.15005 mL	0.02500 mL	3.230	-0.00717	0.42087	0.
53:19.6	Data point 92	0.83996 mL	0.30303 mL	0.28462 mL	1.15005 mL	0.02500 mL	3.421	-0.00349	0.17055	0.
53:36.2	Data point 93	0.83996 mL	0.30303 mL	0.28570 mL	1.15005 mL	0.02500 mL	3.532	0.00684	0.67101	0.
53:57.9	Data point 94	0.83996 mL	0.30303 mL	0.28699 mL	1.15005 mL	0.02500 mL	3.802	0.00148	0.01773	0.
54:19.6	Data point 95	0.83996 mL	0.30303 mL	0.28753 mL	1.15005 mL	0.02500 mL	4.053	0.02391	0.92704	0.
54:41.3	Data point 96	0.83996 mL	0.30303 mL	0.28801 mL	1.15005 mL	0.02500 mL	4.637	0.00668	0.02387	0.
55:08.1	Data point 97	0.83996 mL	0.30303 mL	0.28829 mL	1.15005 mL	0.02500 mL	5.508	0.09897	0.97976	0.
55:46.9	Data point 98	0.83996 mL	0.30303 mL	0.28843 mL	1.15005 mL	0.02500 mL	5.938	0.09832	0.97125	0.
56:20.1	Data point 99	0.83996 mL	0.30303 mL	0.28852 mL	1.15005 mL	0.02500 mL	6.349	-0.07796	0.61956	0.
56:44.3	Data point 100	0.83996 mL	0.30303 mL	0.28862 mL	1.15005 mL	0.02500 mL	6.727	-0.09611	0.93415	0.
57:14.0	Data point 101	0.83996 mL	0.30303 mL	0.28871 mL	1.15005 mL	0.02500 mL	7.001	0.00616	0.01639	0.
57:40.8	Data point 102	0.83996 mL	0.30303 mL	0.28880 mL	1.15005 mL	0.02500 mL	7.224	0.07837	0.90570	0.
58:12.9	Data point 103	0.83996 mL	0.30303 mL	0.28892 mL	1.15005 mL	0.02500 mL	7.483	0.09841	0.98382	0.
58:47.2	Data point 104	0.83996 mL	0.30303 mL	0.28902 mL	1.15005 mL	0.02500 mL	7.743	0.09743	0.97259	0.
59:20.6	Data point 105	0.83996 mL	0.30303 mL	0.28909 mL	1.15005 mL	0.02500 mL	8.034	0.09698	0.97585	0.
59:57.3	Data point 106	0.83996 mL	0.30303 mL	0.28916 mL	1.15005 mL	0.02500 mL	8.430	0.09849	0.98556	0.
1:00:39.0	Data point 107	0.83996 mL	0.30303 mL	0.28923 mL	1.15005 mL	0.02500 mL	8.885	0.09357	0.96255	0.
1:01:13.2	Data point 108	0.83996 mL	0.30303 mL	0.28930 mL	1.15005 mL	0.02500 mL	9.172	0.09802	0.95359	0.
1:01:43.9	Data point 109	0.83996 mL	0.30303 mL	0.28937 mL	1.15005 mL	0.02500 mL	9.394	0.09662	0.95175	0.
1:02:14.3	Data point 110	0.83996 mL	0.30303 mL	0.28949 mL	1.15005 mL	0.02500 mL	9.644	0.08279	0.94349	0.
1:02:36.0	Data point 111	0.83996 mL	0.30303 mL	0.28963 mL	1.15005 mL	0.02500 mL	9.844	0.03597	0.92943	0.
1:02:52.6	Data point 112	0.83996 mL	0.30303 mL	0.28986 mL	1.15005 mL	0.02500 mL	10.113	-0.01142	0.73030	0.
1:03:24.5	Data point 113	0.83996 mL	0.30303 mL	0.29033 mL	1.15005 mL	0.02500 mL	10.305	-0.00191	0.04496	0.
1:03:41.1	Data point 114	0.83996 mL	0.30303 mL	0.29099 mL	1.15005 mL	0.02500 mL	10.513	-0.01796	0.88463	0.
1:03:57.6	Data point 115	0.83996 mL	0.30303 mL	0.29203 mL	1.15005 mL	0.02500 mL	10.699	-0.02607	0.90830	0.
1:04:14.2	Data point 116	0.83996 mL	0.30303 mL	0.29360 mL	1.15005 mL	0.02500 mL	10.878	-0.02429	0.87150	0.
1:04:30.8	Data point 117	0.83996 mL	0.30303 mL	0.29598 mL	1.15005 mL	0.02500 mL	11.034	-0.02424	0.95168	0.
1:04:57.9	Data point 118	0.83996 mL	0.30303 mL	0.29896 mL	1.15005 mL	0.02500 mL	11.223	-0.01624	0.94326	0.
1:05:14.5	Data point 119	0.83996 mL	0.30303 mL	0.30421 mL	1.15005 mL	0.02500 mL	11.411	-0.02434	0.96350	0.
1:05:31.2	Data point 120	0.83996 mL	0.30303 mL	0.31239 mL	1.15005 mL	0.02500 mL	11.601	-0.02206	0.94217	0.
1:05:48.1	Data point 121	0.83996 mL	0.30303 mL	0.32528 mL	1.15005 mL	0.02500 mL	11.786	-0.02248	0.94007	0.
1:06:05.1	Data point 122	0.83996 mL	0.30303 mL	0.34558 mL	1.15005 mL	0.02500 mL	11.977	-0.02692	0.94664	0.
1:06:21.9	Data point 123	0.83996 mL	0.30303 mL	0.35595 mL	1.15005 mL	0.02500 mL	12.044	-0.01783	0.93297	0.

Sample name: **D06**
Assay name: **UV-metric psKa**
Assay ID: **17J-06004**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 3:28:39 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD	dpH time
1:08:21.4	Assay volumes	1.08996 mL	0.44922 mL	0.35595 mL	1.15005 mL	0.02500 mL					

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				
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			
Advanced General Settings				
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%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
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			
Sample Sonication				
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	No			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	10 seconds			
Titration 2				

Sample name: **D06**
Assay name: **UV-metric psKa**
Assay ID: **17J-06004**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 3:28:39 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	0.15 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Titration 3				
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			
Data Point Stability				
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			
Experiment cleanup				
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 3:28:39 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus S	0.9949	10/6/2017 3:28:39 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jH	0.8	10/6/2017 3:28:39 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jOH	-1.3	10/6/2017 3:28:39 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Base concentration factor	1.011	10/6/2017 3:28:39 AM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	1.003	10/6/2017 3:28:39 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		

Sample name: **D06**
Assay name: **UV-metric psKa**
Assay ID: **17J-06004**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 3:28:39 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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		
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	-9.37 mV		10/6/2017 3:29:03 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% Trition X-100 in H20		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	4.8e+003 mL	10-3-17	10/3/2017 8:04:49 AM
Waste	5.3e+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		

Sample name: **D06**
Assay name: **UV-metric psKa**
Assay ID: **17J-06004**
Filename: **C:\Sirius_T3\17J-06004_D06_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 3:28:39 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
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   C5