

Sample name: **M06**
Assay name: **UV-metric psKa**
Assay ID: **17K-09021**
Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09021_M06_UV-metric psKa.t3r**

Experiment start time: **11/9/2017 6:51:39 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

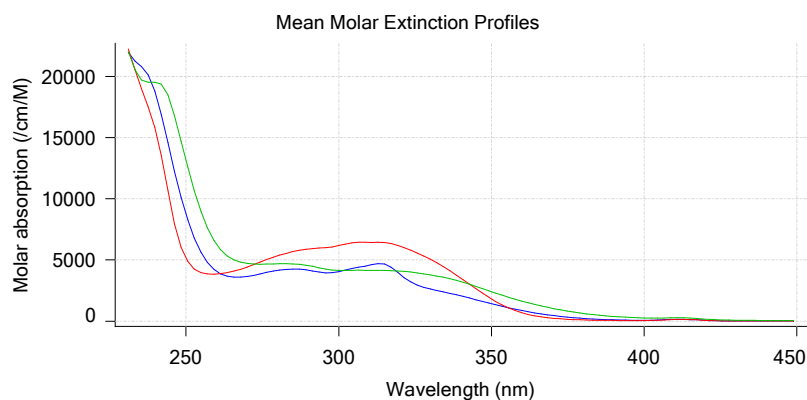
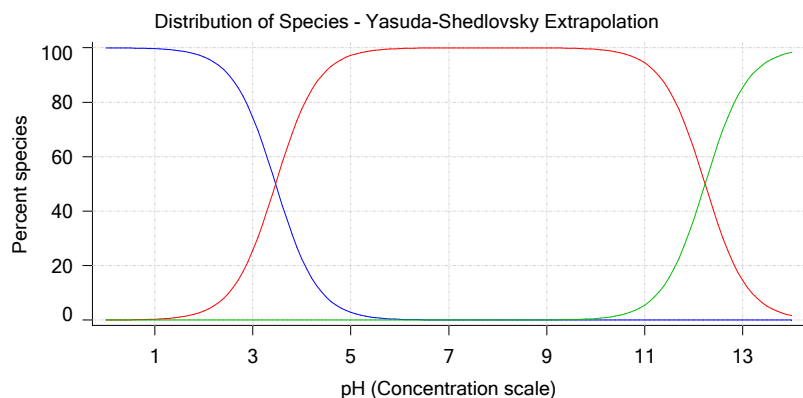
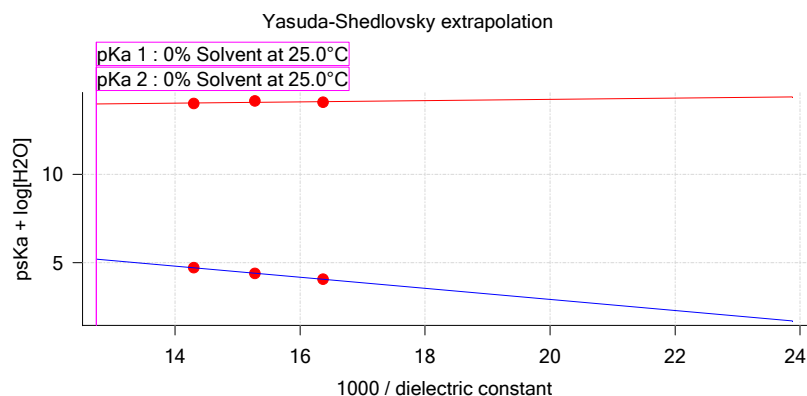
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.46	±0.03	9.21	-314.3541	0.9991	0.163 M	25.0°C
Yasuda-Shedlovsky	12.23	±0.16	13.54	34.5706	0.2587	0.163 M	25.0°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1	psKa 2
17K-09021 Points 4 to 40	39.81 %	Up	UV-metric pKa	61.1	30.1 M	0.156 M	24.9°C	✓	2.59 ✓
17K-09021 Points 42 to 82	30.15 %	Up	UV-metric pKa	65.4	35.8 M	0.164 M	25.0°C	✓	2.84 ✓
17K-09021 Points 84 to 116	20.08 %	Up	UV-metric pKa	69.9	42.0 M	0.169 M	24.9°C	✓	3.10 ✓

Graphs



UV-metric psKa Titration 1 of 3 17K-09021 Points 4 to 40

Results

pKa 1 **2.59**
pKa 2 **12.59**
RMSD **0.005 0.002 0.003**
Chi squared **0.0883**
PCA calculated number of pKas **2**
Average ionic strength **0.156 M**
Average temperature **24.9°C**
Analyte concentration range **94.3 µM to 89.1 µM**
Methanol weight % **39.8 %**
Dielectric constant **61.1**
Water concentration **30.1 M**

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Experiment start time: **11/9/2017 6:51:39 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.469 to 12.528**

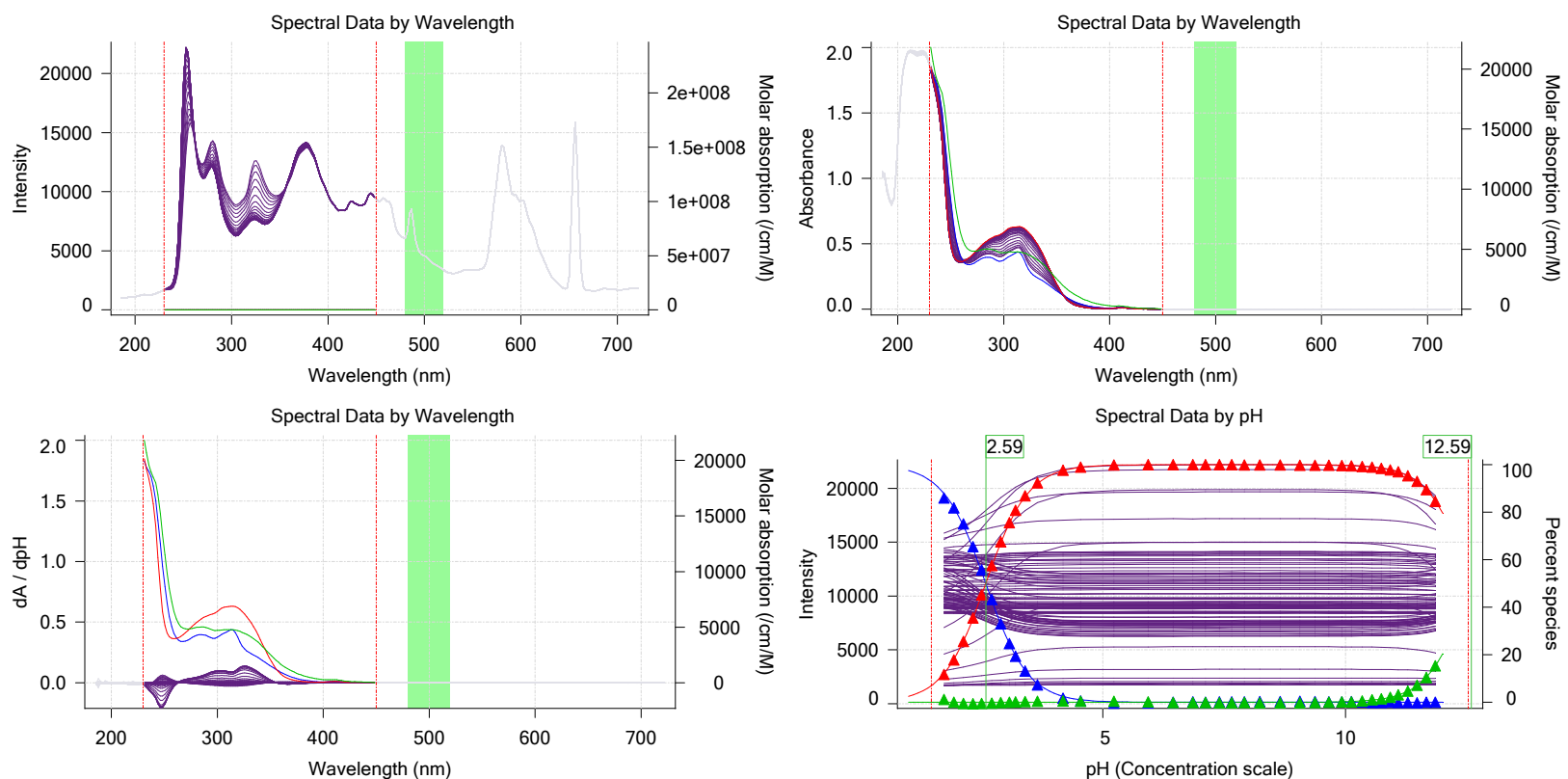
Warnings and errors

Errors **None**
 Warnings **Calculated pKa outside clip range**

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			

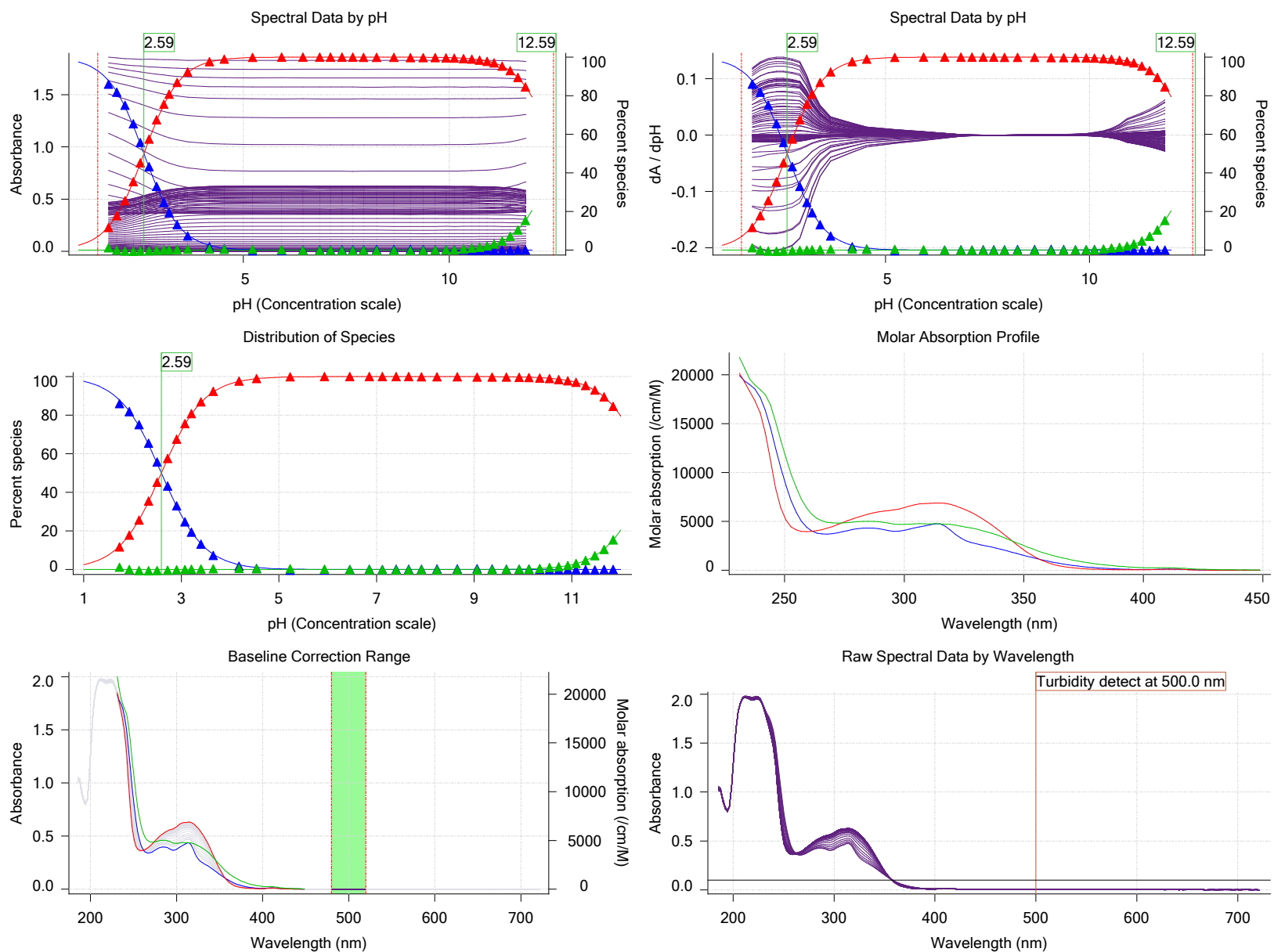
Graphs



Sample name: **M06**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-09021**
 Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09021_M06_UV-metric psKa.t3r**

Experiment start time: **11/9/2017 6:51:39 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Graphs (continued)



UV-metric psKa Titration 2 of 3 17K-09021 Points 42 to 82

Results

pKa 1 **2.84**
 pKa 2 **12.58**
 RMSD **0.003 0.002 0.002**
 Chi squared **0.0635**
 PCA calculated number of pKas **2**
 Average ionic strength **0.164 M**
 Average temperature **25.0°C**
 Analyte concentration range **72.8 µM to 68.9 µM**
 Methanol weight % **30.2 %**
 Dielectric constant **65.4**
 Water concentration **35.8 M**

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 Assay name: **UV-metric pKa**
 Assay ID: **17K-09021**
 Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09021_M06_UV-metric pKa.t3r**

Experiment start time: **11/9/2017 6:51:39 PM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.487 to 12.543**

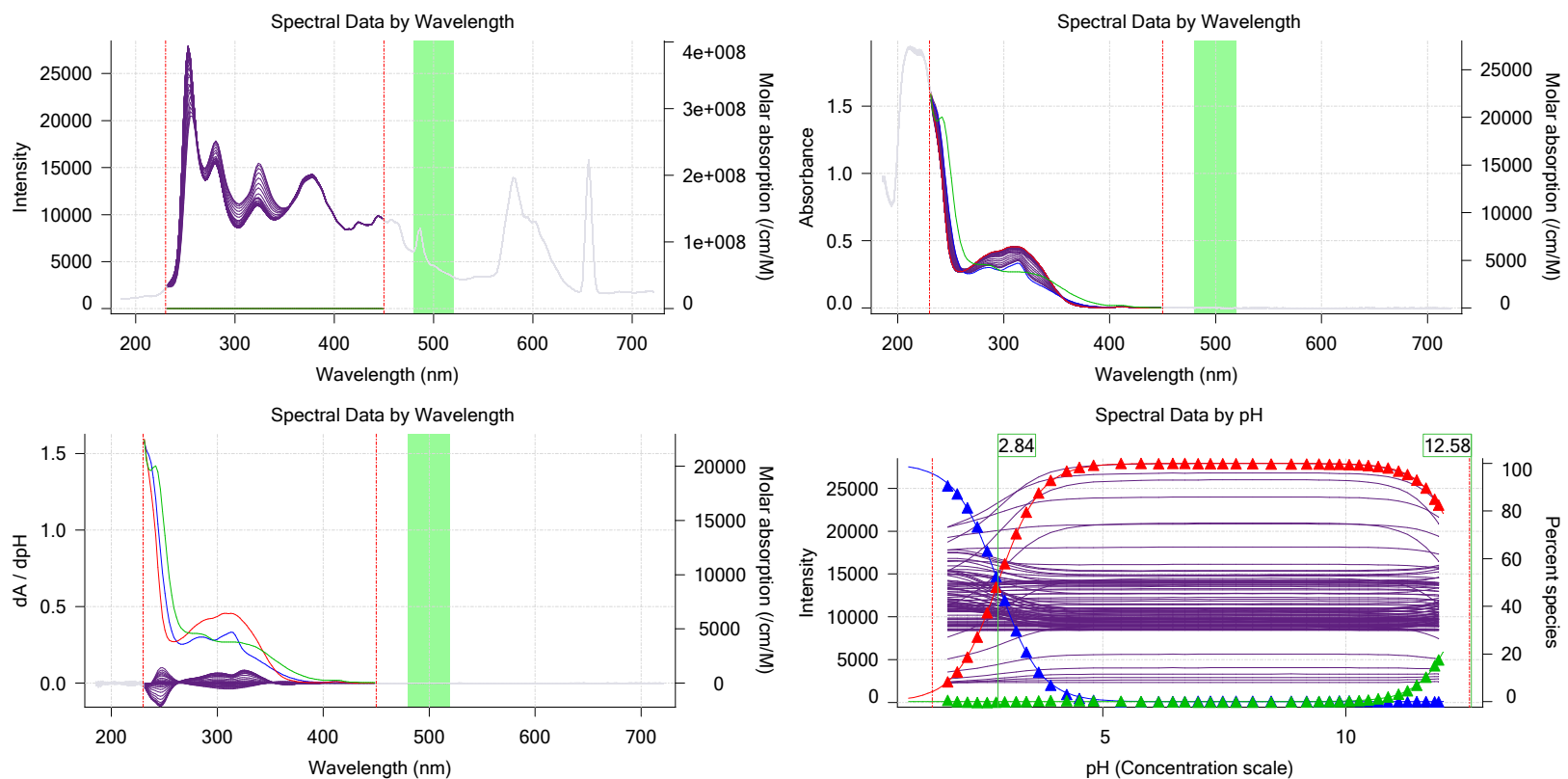
Warnings and errors

Errors **None**
 Warnings **Calculated pKa outside clip range**

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			

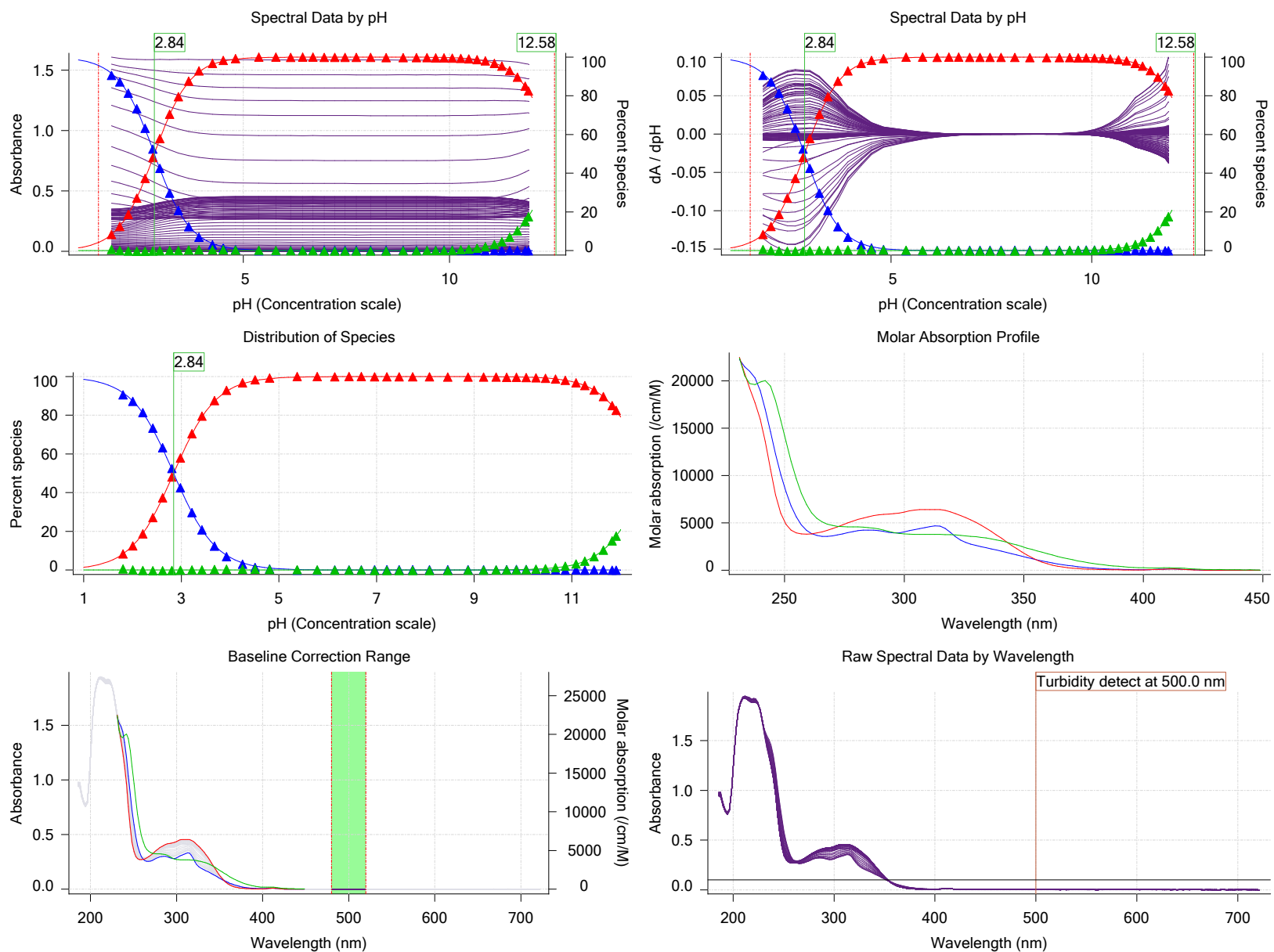
Graphs



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 Assay name: **UV-metric psKa**
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Experiment start time: **11/9/2017 6:51:39 PM**
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Graphs (continued)



UV-metric psKa Titration 3 of 3 17K-09021 Points 84 to 116

Results

pKa 1 **3.10**
 pKa 2 **12.37**
 RMSD **0.001 0.002 0.001**
 Chi squared **0.0102**
 PCA calculated number of pKas **2**
 Average ionic strength **0.169 M**
 Average temperature **24.9°C**
 Analyte concentration range **49.5 µM to 47.1 µM**
 Methanol weight % **20.1 %**
 Dielectric constant **69.9**
 Water concentration **42.0 M**

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Experiment start time: **11/9/2017 6:51:39 PM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.499 to 12.514**

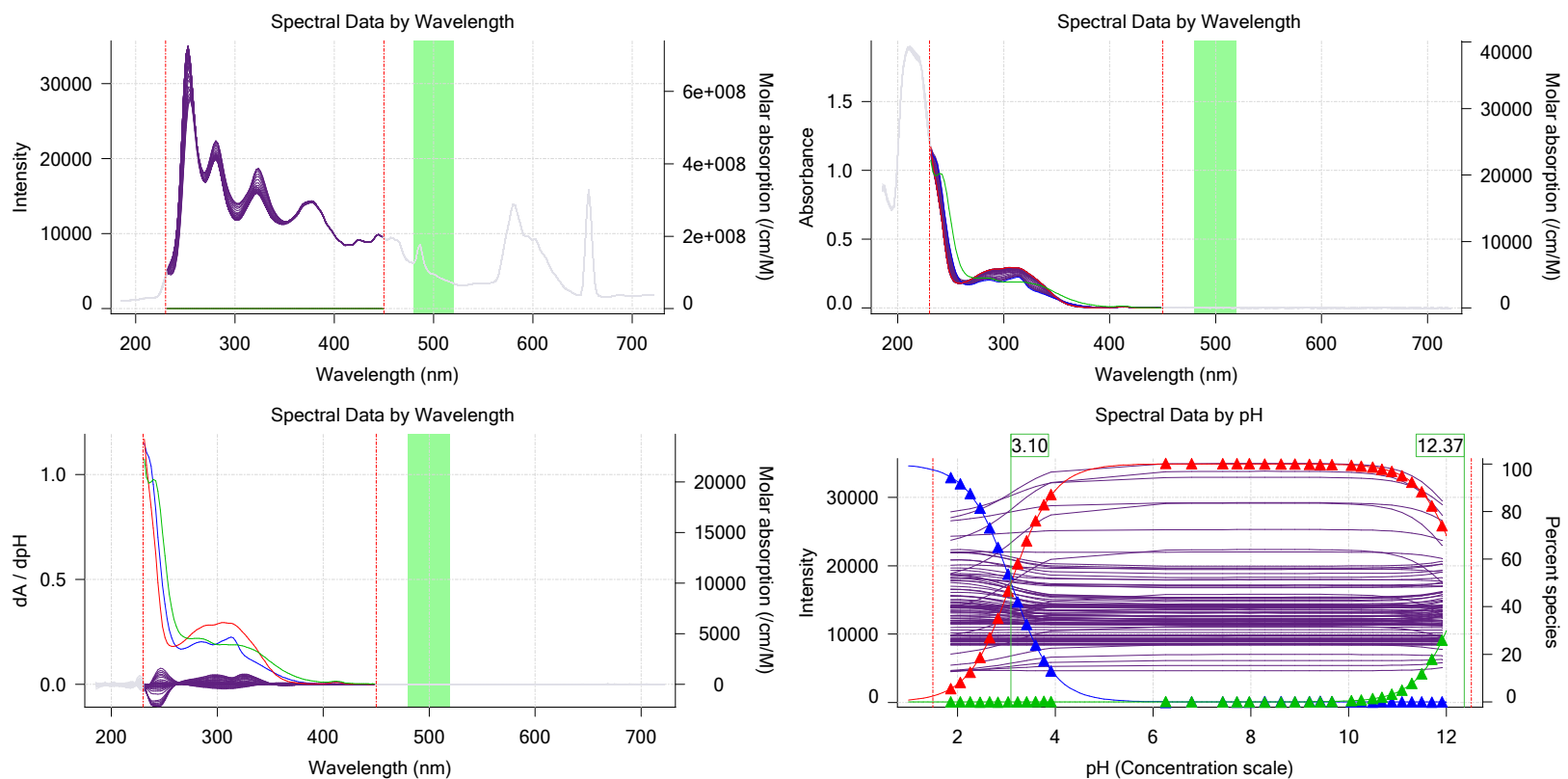
Warnings and errors

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			

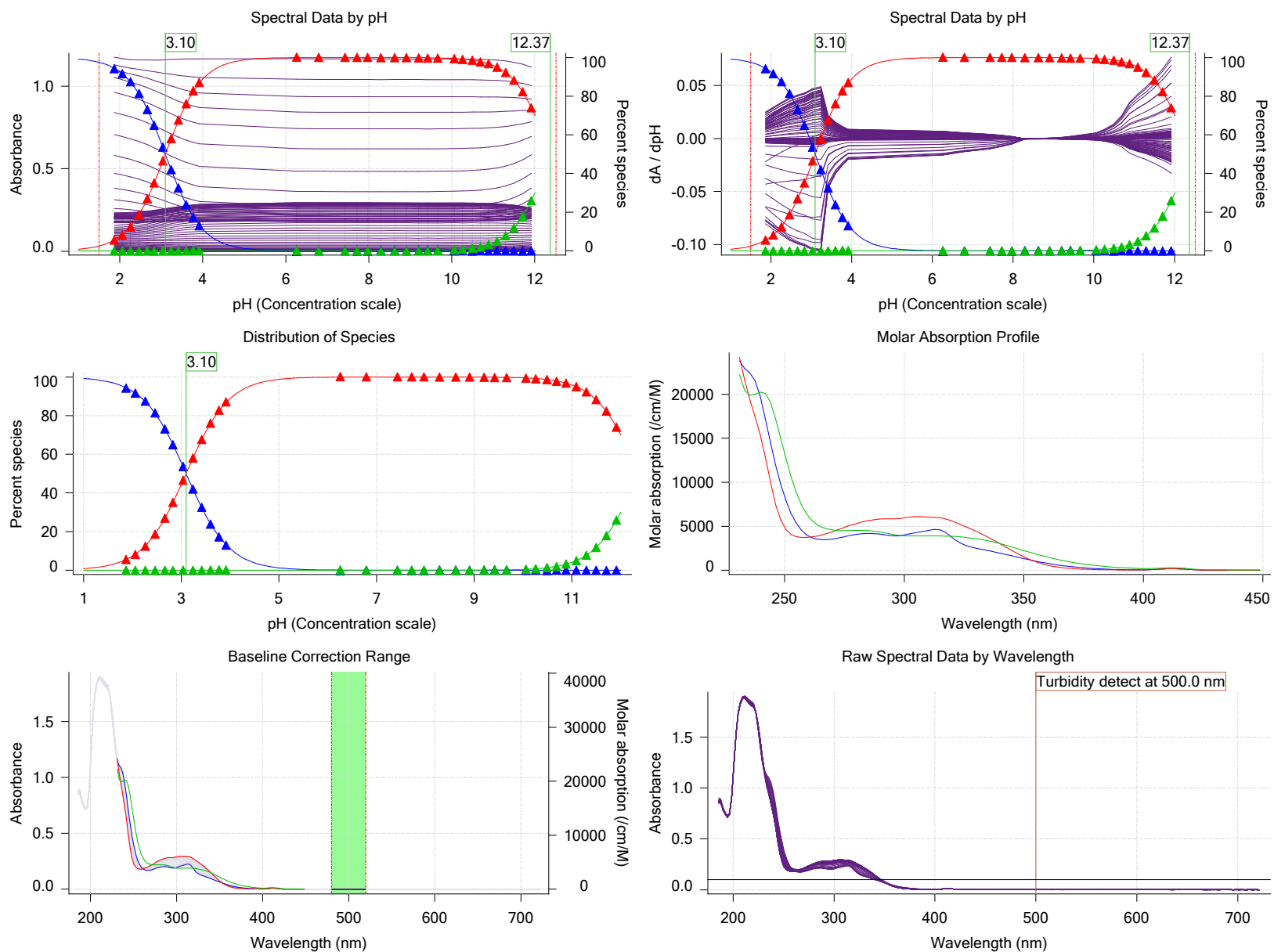
Graphs



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Experiment start time: **11/9/2017 6:51:39 PM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Graphs (continued)



Assay Model

Settings

Settings	Value	Date/Time changed	Imported from
Sample name	M06	11/9/2017 5:26:58 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0030 mL	11/9/2017 5:26:58 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.034400 M	11/10/2017 2:18:04 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	328.16	11/9/2017 5:27:07 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	11/9/2017 5:26:58 PM	User entered value
Sample is a	Ampholyte	11/9/2017 5:26:58 PM	User entered value
pKa 1	3.03	11/9/2017 5:26:58 PM	User entered value
Type	Base	11/9/2017 5:26:58 PM	User entered value
pKa 2	11.74	11/9/2017 5:26:58 PM	User entered value
Type	Acid	11/9/2017 5:26:58 PM	User entered value

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Experiment start time: **11/9/2017 6:51:39 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logp (XH2 +)	-10.00		Default value
logP (neutral XH)	-10.00	11/9/2017 5:26:58 PM	User entered value
logP (X -)	-10.00		Default value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:27.0	Dark spectrum								
3:28.5	Reference spectrum								
3:56.2	Volume reset due to vial change								
4:40.3	Initial pH = 8.17								
5:49.0	Data point 4	0.55997 mL	0.06216 mL	0.00000 mL	0.94003 mL	0.02500 mL	1.969	-0.01701	0.78851
6:17.5	Data point 5	0.55997 mL	0.06216 mL	0.02246 mL	0.94003 mL	0.02500 mL	2.167	0.00062	0.00118
6:34.3	Data point 6	0.55997 mL	0.06216 mL	0.03608 mL	0.94003 mL	0.02500 mL	2.361	0.03094	0.81226
6:51.0	Data point 7	0.55997 mL	0.06216 mL	0.04480 mL	0.94003 mL	0.02500 mL	2.560	0.01172	0.73440
7:07.6	Data point 8	0.55997 mL	0.06216 mL	0.05040 mL	0.94003 mL	0.02500 mL	2.733	0.01305	0.89789
7:24.3	Data point 9	0.55997 mL	0.06216 mL	0.05416 mL	0.94003 mL	0.02500 mL	2.943	0.01039	0.71592
7:40.8	Data point 10	0.55997 mL	0.06216 mL	0.05651 mL	0.94003 mL	0.02500 mL	3.127	0.01528	0.93344
7:57.5	Data point 11	0.55997 mL	0.06216 mL	0.05804 mL	0.94003 mL	0.02500 mL	3.299	0.01381	0.95142
8:14.0	Data point 12	0.55997 mL	0.06216 mL	0.05910 mL	0.94003 mL	0.02500 mL	3.429	0.01844	0.92319
8:40.8	Data point 13	0.55997 mL	0.06216 mL	0.05988 mL	0.94003 mL	0.02500 mL	3.623	0.01995	0.94685
8:57.3	Data point 14	0.55997 mL	0.06216 mL	0.06037 mL	0.94003 mL	0.02500 mL	3.877	0.04973	0.96872
9:18.9	Data point 15	0.55997 mL	0.06216 mL	0.06089 mL	0.94003 mL	0.02500 mL	4.403	0.09991	0.97879
9:53.7	Data point 16	0.55997 mL	0.06216 mL	0.06112 mL	0.94003 mL	0.02500 mL	4.760	0.09911	0.98584
10:39.5	Data point 17	0.55997 mL	0.06216 mL	0.06124 mL	0.94003 mL	0.02500 mL	5.445	0.11523	0.97215
11:56.1	Data point 18	0.55997 mL	0.06216 mL	0.06131 mL	0.94003 mL	0.02500 mL	6.147	0.09876	0.98759
12:54.7	Data point 19	0.55997 mL	0.06216 mL	0.06138 mL	0.94003 mL	0.02500 mL	6.663	0.09923	0.98360
13:51.5	Data point 20	0.55997 mL	0.06216 mL	0.06148 mL	0.94003 mL	0.02500 mL	7.063	0.09921	0.98105
14:36.2	Data point 21	0.55997 mL	0.06216 mL	0.06157 mL	0.94003 mL	0.02500 mL	7.327	0.09783	0.97970
15:20.4	Data point 22	0.55997 mL	0.06216 mL	0.06169 mL	0.94003 mL	0.02500 mL	7.606	0.09670	0.97853
16:02.9	Data point 23	0.55997 mL	0.06216 mL	0.06181 mL	0.94003 mL	0.02500 mL	7.863	0.09575	0.95989
16:48.6	Data point 24	0.55997 mL	0.06216 mL	0.06192 mL	0.94003 mL	0.02500 mL	8.124	0.09856	0.96051
17:30.8	Data point 25	0.55997 mL	0.06216 mL	0.06202 mL	0.94003 mL	0.02500 mL	8.440	0.09853	0.97965
18:19.2	Data point 26	0.55997 mL	0.06216 mL	0.06211 mL	0.94003 mL	0.02500 mL	8.858	0.09723	0.96642
19:07.7	Data point 27	0.55997 mL	0.06216 mL	0.06221 mL	0.94003 mL	0.02500 mL	9.260	0.09800	0.98156
19:47.5	Data point 28	0.55997 mL	0.06216 mL	0.06230 mL	0.94003 mL	0.02500 mL	9.569	0.09685	0.96098
20:19.7	Data point 29	0.55997 mL	0.06216 mL	0.06242 mL	0.94003 mL	0.02500 mL	9.857	0.09864	0.95599
20:45.9	Data point 30	0.55997 mL	0.06216 mL	0.06258 mL	0.94003 mL	0.02500 mL	10.118	0.08872	0.96256
21:12.5	Data point 31	0.55997 mL	0.06216 mL	0.06279 mL	0.94003 mL	0.02500 mL	10.317	0.04585	0.94318
21:29.0	Data point 32	0.55997 mL	0.06216 mL	0.06312 mL	0.94003 mL	0.02500 mL	10.538	0.02074	0.90384
21:45.6	Data point 33	0.55997 mL	0.06216 mL	0.06366 mL	0.94003 mL	0.02500 mL	10.737	0.01349	0.90289
22:02.2	Data point 34	0.55997 mL	0.06216 mL	0.06451 mL	0.94003 mL	0.02500 mL	10.928	0.00742	0.72741
22:18.8	Data point 35	0.55997 mL	0.06216 mL	0.06580 mL	0.94003 mL	0.02500 mL	11.112	0.00779	0.72087
22:35.4	Data point 36	0.55997 mL	0.06216 mL	0.06776 mL	0.94003 mL	0.02500 mL	11.276	0.00123	0.03772
23:02.3	Data point 37	0.55997 mL	0.06216 mL	0.07065 mL	0.94003 mL	0.02500 mL	11.472	-0.00496	0.57262
23:19.0	Data point 38	0.55997 mL	0.06216 mL	0.07514 mL	0.94003 mL	0.02500 mL	11.661	-0.00022	0.00285
23:35.7	Data point 39	0.55997 mL	0.06216 mL	0.08213 mL	0.94003 mL	0.02500 mL	11.846	0.00562	0.57400
23:52.6	Data point 40	0.55997 mL	0.06216 mL	0.09299 mL	0.94003 mL	0.02500 mL	12.028	0.00411	0.51486
25:35.7	Reference spectrum								
26:40.5	Data point 42	0.83996 mL	0.16000 mL	0.09299 mL	0.94003 mL	0.02500 mL	1.987	-0.08045	0.94159
27:09.2	Data point 43	0.83996 mL	0.16000 mL	0.11783 mL	0.94003 mL	0.02500 mL	2.184	0.00690	0.71358
27:26.1	Data point 44	0.83996 mL	0.16000 mL	0.13293 mL	0.94003 mL	0.02500 mL	2.387	0.00863	0.63503
27:43.0	Data point 45	0.83996 mL	0.16000 mL	0.14240 mL	0.94003 mL	0.02500 mL	2.591	-0.00163	0.03819
27:59.8	Data point 46	0.83996 mL	0.16000 mL	0.14831 mL	0.94003 mL	0.02500 mL	2.790	-0.00739	0.31569
28:16.6	Data point 47	0.83996 mL	0.16000 mL	0.15212 mL	0.94003 mL	0.02500 mL	2.978	-0.00252	0.03087
28:33.3	Data point 48	0.83996 mL	0.16000 mL	0.15459 mL	0.94003 mL	0.02500 mL	3.151	0.01020	0.75473
28:49.8	Data point 49	0.83996 mL	0.16000 mL	0.15626 mL	0.94003 mL	0.02500 mL	3.386	0.01029	0.79354

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Experiment start time: **11/9/2017 6:51:39 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
29:21.5	Data point 50	0.83996 mL	0.16000 mL	0.15729 mL	0.94003 mL	0.02500 mL	3.595	0.03045	0.97930	0.00
29:38.1	Data point 51	0.83996 mL	0.16000 mL	0.15790 mL	0.94003 mL	0.02500 mL	3.848	0.03131	0.96163	0.00
29:59.7	Data point 52	0.83996 mL	0.16000 mL	0.15832 mL	0.94003 mL	0.02500 mL	4.095	0.05734	0.98223	0.00
30:21.4	Data point 53	0.83996 mL	0.16000 mL	0.15863 mL	0.94003 mL	0.02500 mL	4.423	0.08999	0.98916	0.00
30:43.0	Data point 54	0.83996 mL	0.16000 mL	0.15880 mL	0.94003 mL	0.02500 mL	4.680	0.10015	0.97978	0.00
31:13.6	Data point 55	0.83996 mL	0.16000 mL	0.15889 mL	0.94003 mL	0.02500 mL	4.977	0.09620	0.95852	0.00
32:06.2	Data point 56	0.83996 mL	0.16000 mL	0.15898 mL	0.94003 mL	0.02500 mL	5.539	0.09880	0.98475	0.00
32:58.5	Data point 57	0.83996 mL	0.16000 mL	0.15906 mL	0.94003 mL	0.02500 mL	5.950	0.07794	0.68858	0.00
33:38.6	Data point 58	0.83996 mL	0.16000 mL	0.15912 mL	0.94003 mL	0.02500 mL	6.309	0.09725	0.98103	0.00
34:24.2	Data point 59	0.83996 mL	0.16000 mL	0.15922 mL	0.94003 mL	0.02500 mL	6.601	0.09986	0.97315	0.00
34:48.6	Data point 60	0.83996 mL	0.16000 mL	0.15931 mL	0.94003 mL	0.02500 mL	6.849	0.09517	0.98344	0.00
35:23.4	Data point 61	0.83996 mL	0.16000 mL	0.15943 mL	0.94003 mL	0.02500 mL	7.122	0.09747	0.97405	0.00
36:00.8	Data point 62	0.83996 mL	0.16000 mL	0.15955 mL	0.94003 mL	0.02500 mL	7.374	0.09609	0.98785	0.00
36:38.6	Data point 63	0.83996 mL	0.16000 mL	0.15967 mL	0.94003 mL	0.02500 mL	7.623	0.09920	0.97638	0.00
37:16.9	Data point 64	0.83996 mL	0.16000 mL	0.15978 mL	0.94003 mL	0.02500 mL	7.897	0.09748	0.96911	0.00
38:03.7	Data point 65	0.83996 mL	0.16000 mL	0.15990 mL	0.94003 mL	0.02500 mL	8.240	0.09431	0.97450	0.00
38:50.1	Data point 66	0.83996 mL	0.16000 mL	0.16000 mL	0.94003 mL	0.02500 mL	8.617	0.09734	0.97057	0.00
39:36.3	Data point 67	0.83996 mL	0.16000 mL	0.16009 mL	0.94003 mL	0.02500 mL	9.032	0.09833	0.95747	0.00
40:17.0	Data point 68	0.83996 mL	0.16000 mL	0.16018 mL	0.94003 mL	0.02500 mL	9.349	0.10016	0.99282	0.00
40:52.7	Data point 69	0.83996 mL	0.16000 mL	0.16030 mL	0.94003 mL	0.02500 mL	9.603	0.09466	0.96433	0.00
41:18.3	Data point 70	0.83996 mL	0.16000 mL	0.16044 mL	0.94003 mL	0.02500 mL	9.816	0.08162	0.97469	0.00
41:40.0	Data point 71	0.83996 mL	0.16000 mL	0.16063 mL	0.94003 mL	0.02500 mL	10.016	0.05400	0.97618	0.00
42:11.8	Data point 72	0.83996 mL	0.16000 mL	0.16094 mL	0.94003 mL	0.02500 mL	10.218	0.02846	0.89831	0.00
42:43.8	Data point 73	0.83996 mL	0.16000 mL	0.16143 mL	0.94003 mL	0.02500 mL	10.420	0.01282	0.83505	0.00
43:15.6	Data point 74	0.83996 mL	0.16000 mL	0.16218 mL	0.94003 mL	0.02500 mL	10.615	0.00409	0.54642	0.00
43:37.5	Data point 75	0.83996 mL	0.16000 mL	0.16340 mL	0.94003 mL	0.02500 mL	10.817	0.00439	0.25964	0.00
44:09.4	Data point 76	0.83996 mL	0.16000 mL	0.16501 mL	0.94003 mL	0.02500 mL	11.016	-0.00381	0.49753	0.00
44:26.1	Data point 77	0.83996 mL	0.16000 mL	0.16738 mL	0.94003 mL	0.02500 mL	11.234	-0.00185	0.10627	0.00
44:42.7	Data point 78	0.83996 mL	0.16000 mL	0.17128 mL	0.94003 mL	0.02500 mL	11.411	-0.00660	0.70234	0.00
44:59.4	Data point 79	0.83996 mL	0.16000 mL	0.17716 mL	0.94003 mL	0.02500 mL	11.602	-0.00791	0.78309	0.00
45:16.1	Data point 80	0.83996 mL	0.16000 mL	0.18636 mL	0.94003 mL	0.02500 mL	11.787	-0.00168	0.06425	0.00
45:32.9	Data point 81	0.83996 mL	0.16000 mL	0.20071 mL	0.94003 mL	0.02500 mL	11.966	0.00013	0.00050	0.00
45:49.6	Data point 82	0.83996 mL	0.16000 mL	0.20872 mL	0.94003 mL	0.02500 mL	12.043	0.00223	0.16425	0.00
47:40.9	Reference spectrum									
49:57.2	Data point 84	1.54998 mL	0.30419 mL	0.20875 mL	0.94003 mL	0.02500 mL	1.999	0.08262	0.91980	0.00
50:24.7	Data point 85	1.54998 mL	0.30419 mL	0.23709 mL	0.94003 mL	0.02500 mL	2.187	-0.01124	0.72063	0.00
50:41.7	Data point 86	1.54998 mL	0.30419 mL	0.25689 mL	0.94003 mL	0.02500 mL	2.388	-0.07712	0.81614	0.00
50:58.4	Data point 87	1.54998 mL	0.30419 mL	0.26969 mL	0.94003 mL	0.02500 mL	2.591	-0.09009	0.89312	0.00
51:15.7	Data point 88	1.54998 mL	0.30419 mL	0.27777 mL	0.94003 mL	0.02500 mL	2.788	-0.07888	0.77323	0.00
51:49.2	Data point 89	1.54998 mL	0.30419 mL	0.28288 mL	0.94003 mL	0.02500 mL	2.954	-0.00180	0.06530	0.00
52:11.1	Data point 90	1.54998 mL	0.30419 mL	0.28662 mL	0.94003 mL	0.02500 mL	3.161	-0.07282	0.87582	0.00
52:27.7	Data point 91	1.54998 mL	0.30419 mL	0.28880 mL	0.94003 mL	0.02500 mL	3.361	-0.08553	0.87138	0.00
52:44.7	Data point 92	1.54998 mL	0.30419 mL	0.29019 mL	0.94003 mL	0.02500 mL	3.539	-0.07316	0.80585	0.00
53:01.3	Data point 93	1.54998 mL	0.30419 mL	0.29111 mL	0.94003 mL	0.02500 mL	3.721	-0.08663	0.85560	0.00
53:18.3	Data point 94	1.54998 mL	0.30419 mL	0.29172 mL	0.94003 mL	0.02500 mL	3.894	-0.08777	0.84900	0.00
53:35.4	Data point 95	1.54998 mL	0.30419 mL	0.29214 mL	0.94003 mL	0.02500 mL	4.037	-0.05961	0.78359	0.00
54:02.4	Data point 96	1.54998 mL	0.30419 mL	0.29386 mL	0.94003 mL	0.02500 mL	6.379	-0.09773	0.96141	0.00
54:47.6	Data point 97	1.54998 mL	0.30419 mL	0.29431 mL	0.94003 mL	0.02500 mL	6.911	-0.09412	0.95381	0.00
55:37.0	Data point 98	1.54998 mL	0.30419 mL	0.29464 mL	0.94003 mL	0.02500 mL	7.547	-0.10043	0.99192	0.00
56:28.3	Data point 99	1.54998 mL	0.30419 mL	0.29485 mL	0.94003 mL	0.02500 mL	7.836	-0.06576	0.90083	0.00
57:00.2	Data point 100	1.54998 mL	0.30419 mL	0.29497 mL	0.94003 mL	0.02500 mL	8.086	0.08638	0.85205	0.00
57:29.9	Data point 101	1.54998 mL	0.30419 mL	0.29504 mL	0.94003 mL	0.02500 mL	8.406	0.09779	0.94862	0.00
58:03.7	Data point 102	1.54998 mL	0.30419 mL	0.29511 mL	0.94003 mL	0.02500 mL	8.739	0.09299	0.91652	0.00
58:35.9	Data point 103	1.54998 mL	0.30419 mL	0.29518 mL	0.94003 mL	0.02500 mL	9.022	0.09907	0.96346	0.00
59:00.4	Data point 104	1.54998 mL	0.30419 mL	0.29527 mL	0.94003 mL	0.02500 mL	9.319	0.01309	0.30820	0.00
59:22.0	Data point 105	1.54998 mL	0.30419 mL	0.29539 mL	0.94003 mL	0.02500 mL	9.536	-0.00309	0.06453	0.00
59:43.5	Data point 106	1.54998 mL	0.30419 mL	0.29556 mL	0.94003 mL	0.02500 mL	9.779	-0.05981	0.85474	0.00

Sample name: **M06**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-09021**
 Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09021_M06_UV-metric psKa.t3r**

Experiment start time: **11/9/2017 6:51:39 PM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
59:59.9	Data point 107	1.54998 mL	0.30419 mL	0.29584 mL	0.94003 mL	0.02500 mL	10.172	-0.08901	0.87585	0.0047
1:00:27.8	Data point 108	1.54998 mL	0.30419 mL	0.29645 mL	0.94003 mL	0.02500 mL	10.374	-0.03253	0.92023	0.0016
1:00:44.4	Data point 109	1.54998 mL	0.30419 mL	0.29744 mL	0.94003 mL	0.02500 mL	10.607	-0.09416	0.88669	0.0049
1:01:16.3	Data point 110	1.54998 mL	0.30419 mL	0.29911 mL	0.94003 mL	0.02500 mL	10.798	-0.02117	0.96872	0.0010
1:01:32.9	Data point 111	1.54998 mL	0.30419 mL	0.30160 mL	0.94003 mL	0.02500 mL	10.996	-0.09396	0.88293	0.0049
1:01:49.5	Data point 112	1.54998 mL	0.30419 mL	0.30555 mL	0.94003 mL	0.02500 mL	11.202	-0.09213	0.86354	0.0048
1:02:06.3	Data point 113	1.54998 mL	0.30419 mL	0.31190 mL	0.94003 mL	0.02500 mL	11.405	-0.08893	0.83779	0.0047
1:02:23.1	Data point 114	1.54998 mL	0.30419 mL	0.32211 mL	0.94003 mL	0.02500 mL	11.603	-0.07838	0.91589	0.0040
1:02:40.0	Data point 115	1.54998 mL	0.30419 mL	0.33841 mL	0.94003 mL	0.02500 mL	11.810	-0.08038	0.91472	0.0041
1:02:57.2	Data point 116	1.54998 mL	0.30419 mL	0.36533 mL	0.94003 mL	0.02500 mL	12.014	-0.07995	0.92157	0.0041
1:04:27.9	Assay volumes	1.54998 mL	0.46630 mL	0.36533 mL	0.94003 mL	0.02500 mL				

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Leverse			
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	0.94 mL			
Cosolvent added	Automatic			
ISA water volume	0.56 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			

Sample name: **M06** Experiment start time: **11/9/2017 6:51:39 PM**
 Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse**
 Assay ID: **17K-09021** Instrument ID: **T311053**
 Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09021_M06_UV-metric psKa.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.28 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	0.71 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	0.109	11/9/2017 6:51:39 PM	C:\Sirius_T3\HCl17K09.t3r
Four-Plus S	1.0008	11/9/2017 6:51:39 PM	C:\Sirius_T3\HCl17K09.t3r
Four-Plus jH	0.6	11/9/2017 6:51:39 PM	C:\Sirius_T3\HCl17K09.t3r
Four-Plus jOH	-1.2	11/9/2017 6:51:39 PM	C:\Sirius_T3\HCl17K09.t3r
Base concentration factor	1.008	11/9/2017 6:51:39 PM	C:\Sirius_T3\KOH17K09.t3r
Acid concentration factor	0.998	11/9/2017 6:51:39 PM	C:\Sirius_T3\HCl17K09.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)	10-10-2017	11/8/2017 11:33:30 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM

Sample name: **M06**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-09021**
 Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09021_M06_UV-metric psKa.t3r**

Experiment start time: **11/9/2017 6:51:39 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	11-8-17	11/8/2017 11:32:21 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)	10-30-17	10/30/2017 8:01:46 AM
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	11/1/2017 10:56:16 AM
Port B	Cyclohexane		10/19/2017 2:11:05 PM
Port C	MeCN (50%, 0.15 M KCl)	10-30-17	10/30/2017 8:02:00 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		11/8/2017 11:32:27 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	10/13/2017 7:46:59 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	-7.35 mV		11/9/2017 6:52:03 PM
Filling solution	3M KCl	KCL095	11/8/2017 11:31:02 AM
Liquids			
Wash 1	50% IPA:50% Water		11/9/2017 8:31:16 AM
Wash 2	0.5% Triton X-100 in H2O		11/9/2017 8:31:19 AM
Buffer position 1	pH7 Wash		11/9/2017 8:31:22 AM
Buffer position 2	pH 7		11/9/2017 8:31:24 AM
Storage position			11/9/2017 8:31:29 AM
Wash water	3.3e+003 mL	10-13-17	10/13/2017 8:58:01 AM
Waste	7.1e+003 mL		10/13/2017 8:58:05 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	512:14:04		11/23/2010 11:22:28 AM
Calibrated on	11/8/2017 1:14:37 PM		
Integration time	10		
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		



Assay Settings

Sample name: **M06** Experiment start time: **11/9/2017 6:51:39 PM**
Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse**
Assay ID: **17K-09021** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09021_M06_UV-metric psKa.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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%		
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 B1