

Sample name: **M06**
Assay name: **UV-metric psKa**
Assay ID: **17K-10008**
Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric psKa.t3r**

Experiment start time: **11/10/2017 3:50:27 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

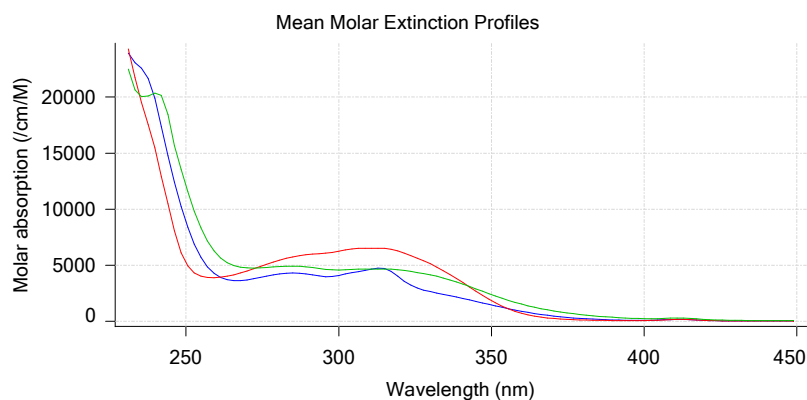
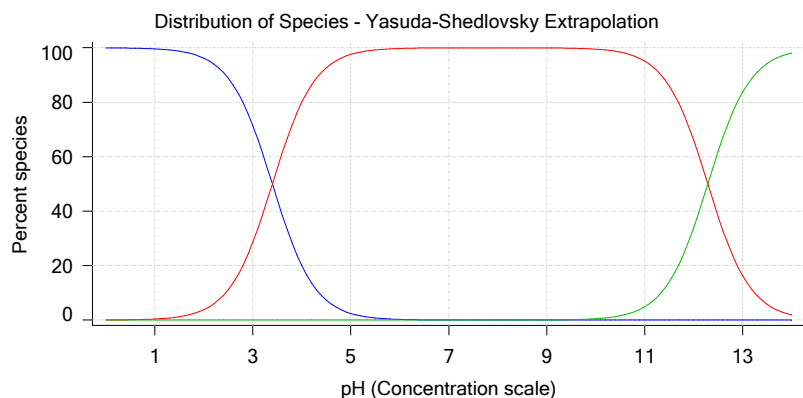
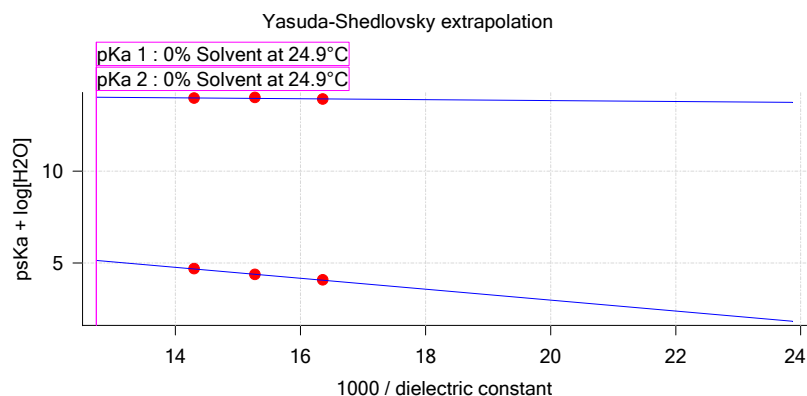
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.40	±0.02	8.92	-296.7781	0.9993	0.163 M	24.9°C
Yasuda-Shedlovsky	12.29	±0.08	14.35	-25.0565	0.4406	0.163 M	24.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1	psKa 2
17K-10008 Points 4 to 33	39.79 %	Up	UV-metric pKa	61.1	30.1 M	0.156 M	24.8°C	✓	2.59 ✓
17K-10008 Points 35 to 73	30.14 %	Up	UV-metric pKa	65.5	35.8 M	0.164 M	24.9°C	✓	2.82 ✓
17K-10008 Points 75 to 119	20.13 %	Up	UV-metric pKa	69.9	42.0 M	0.169 M	24.9°C	✓	3.06 ✓

Graphs



UV-metric psKa Titration 1 of 3 17K-10008 Points 4 to 33

Results

pKa 1	2.59
pKa 2	12.45
RMSD	0.002 0.002 0.002
Chi squared	0.0236
PCA calculated number of pKas	3
Average ionic strength	0.156 M
Average temperature	24.8°C
Analyte concentration range	94.3 µM to 89.1 µM
Methanol weight %	39.8 %
Dielectric constant	61.1
Water concentration	30.1 M

Sample name: **M06**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-10008**
 Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric psKa.t3r**

Experiment start time: **11/10/2017 3:50:27 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Results (continued)

Number of pKas source **Manual (2)**
 Wavelength clipping **244.8 nm to 450.0 nm**
 pH clipping **1.453 to 12.544**

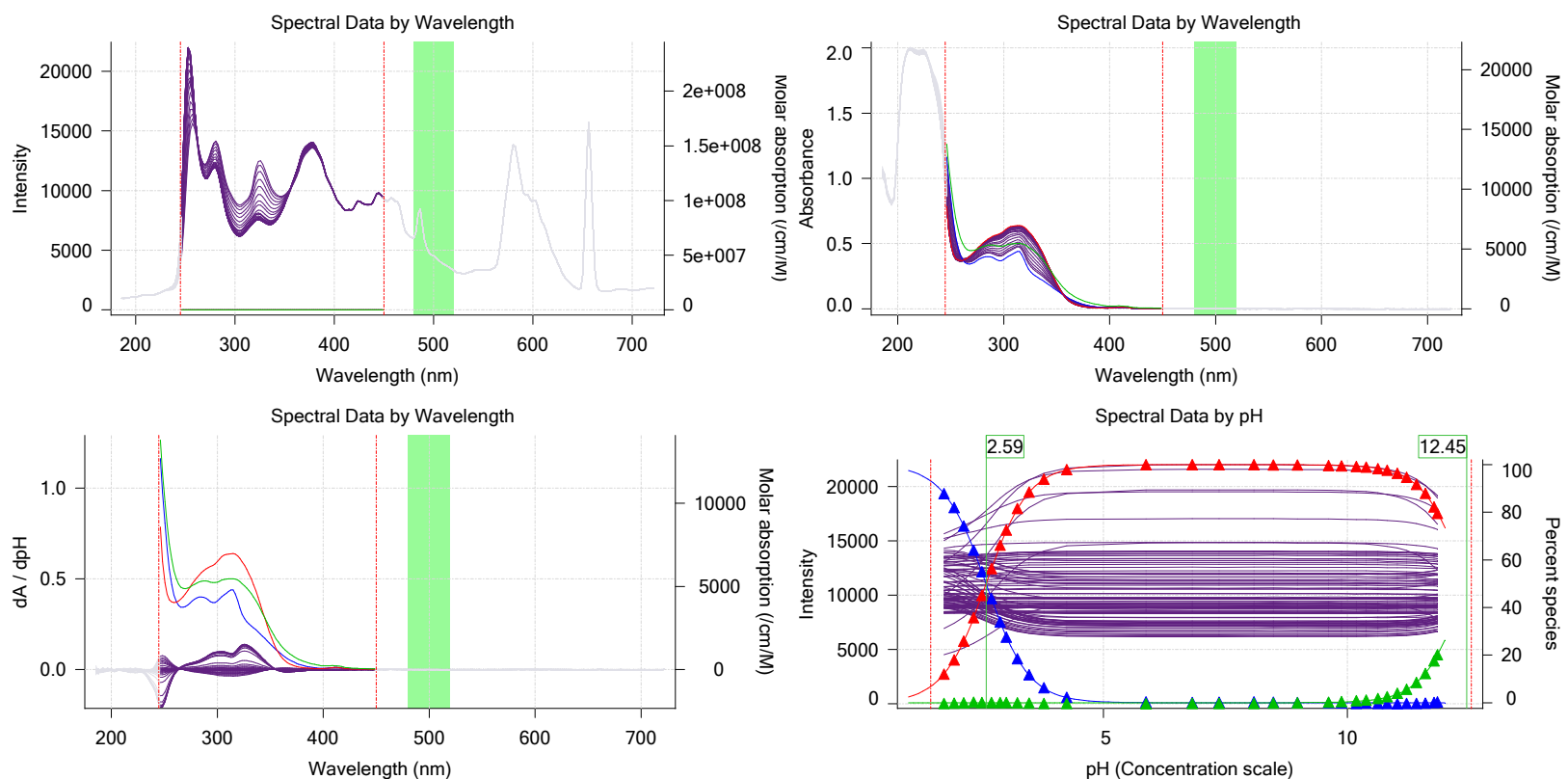
Warnings and errors

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				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

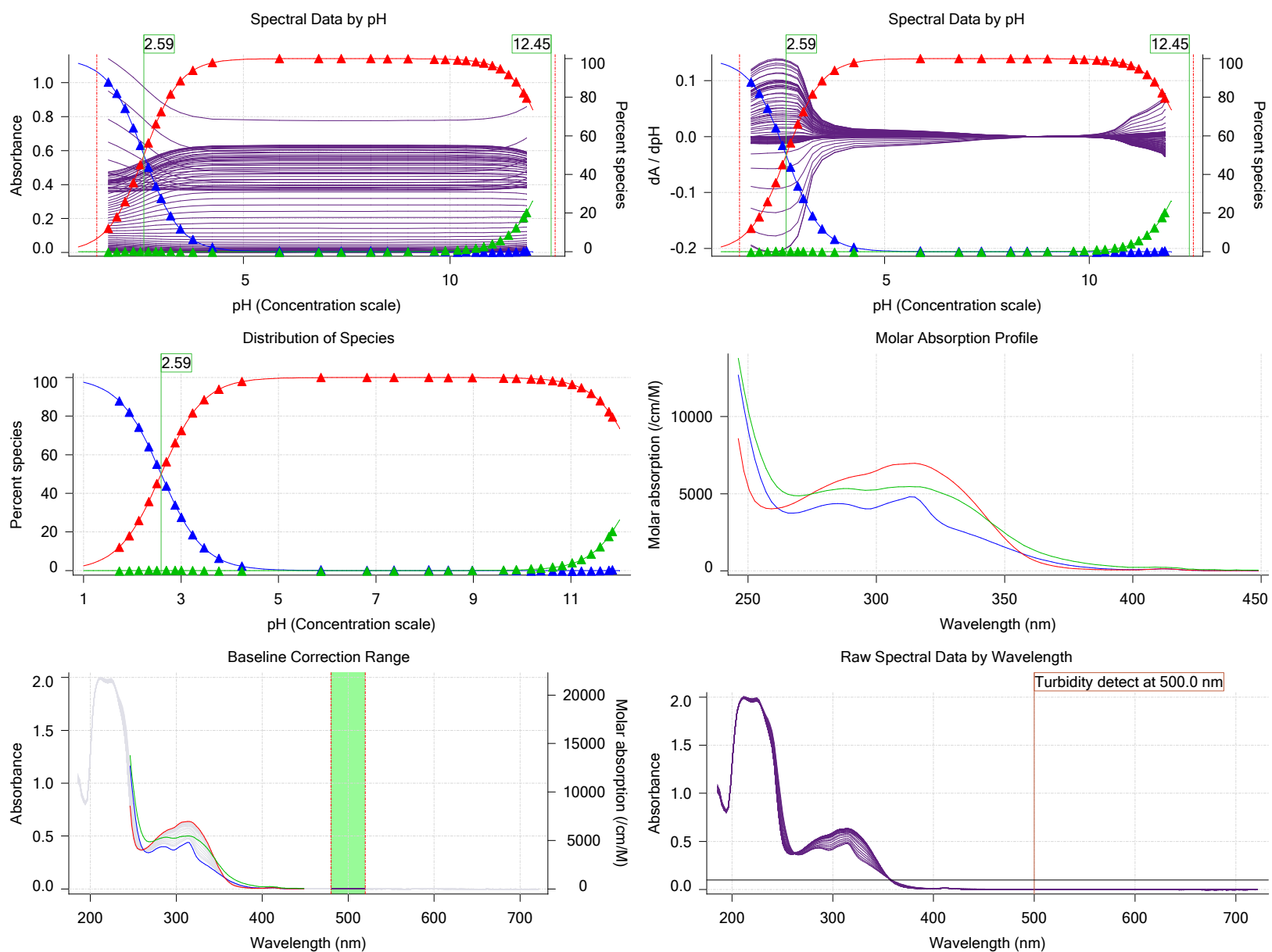
Graphs



Sample name: **M06**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-10008**
 Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric psKa.t3r**

Experiment start time: **11/10/2017 3:50:27 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Graphs (continued)



UV-metric psKa Titration 2 of 3 17K-10008 Points 35 to 73

Results

pKa 1 **2.82**
 pKa 2 **12.45**
 RMSD **0.002 0.001 0.002**
 Chi squared **0.0229**
 PCA calculated number of pKas **3**
 Average ionic strength **0.164 M**
 Average temperature **24.9°C**
 Analyte concentration range **72.7 µM to 68.9 µM**
 Methanol weight % **30.1 %**
 Dielectric constant **65.5**
 Water concentration **35.8 M**

Sample name: **M06**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-10008**
 Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric psKa.t3r**

Experiment start time: **11/10/2017 3:50:27 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **243.2 nm to 450.0 nm**
 pH clipping **1.471 to 12.536**

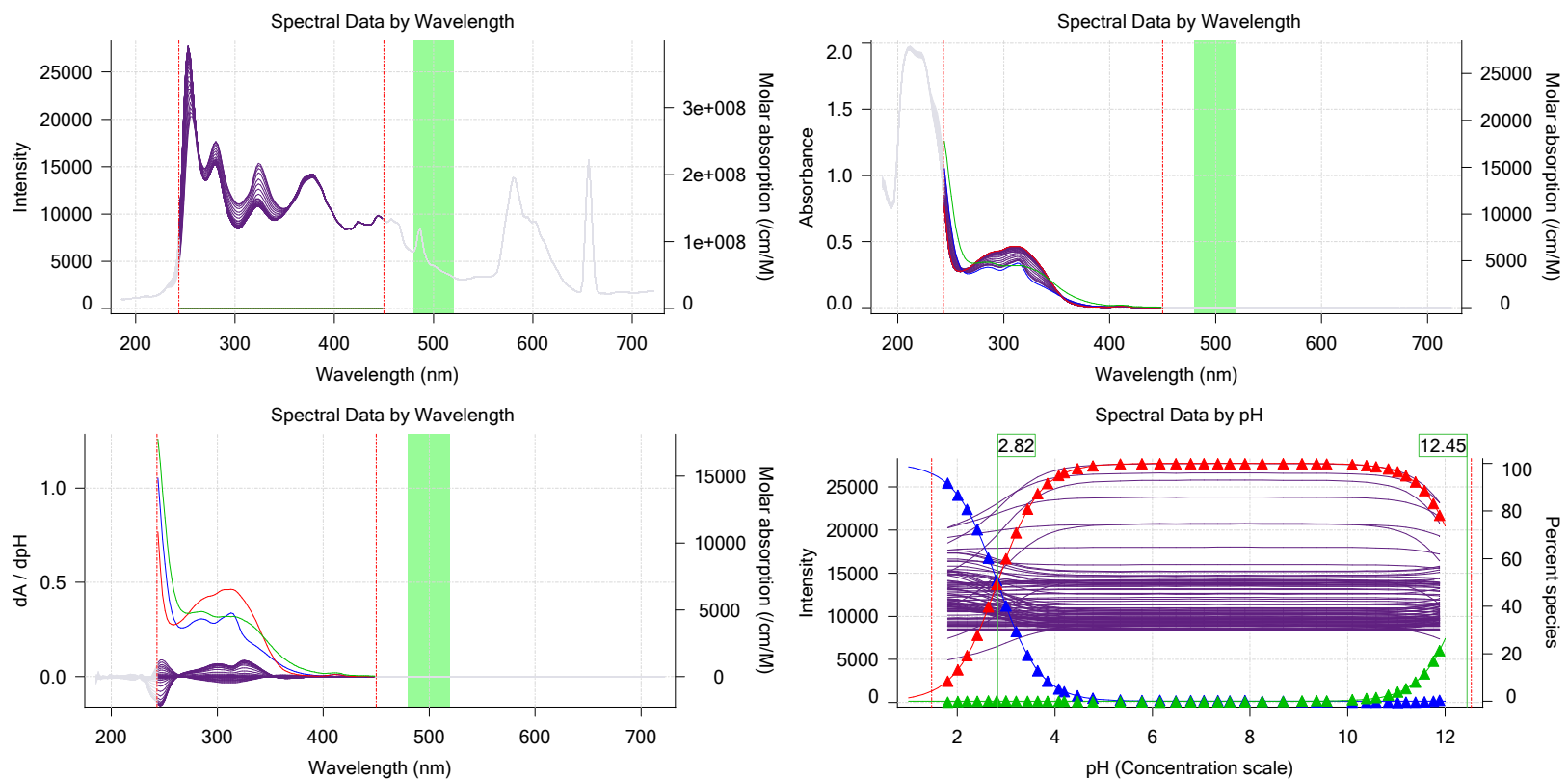
Warnings and errors

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				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

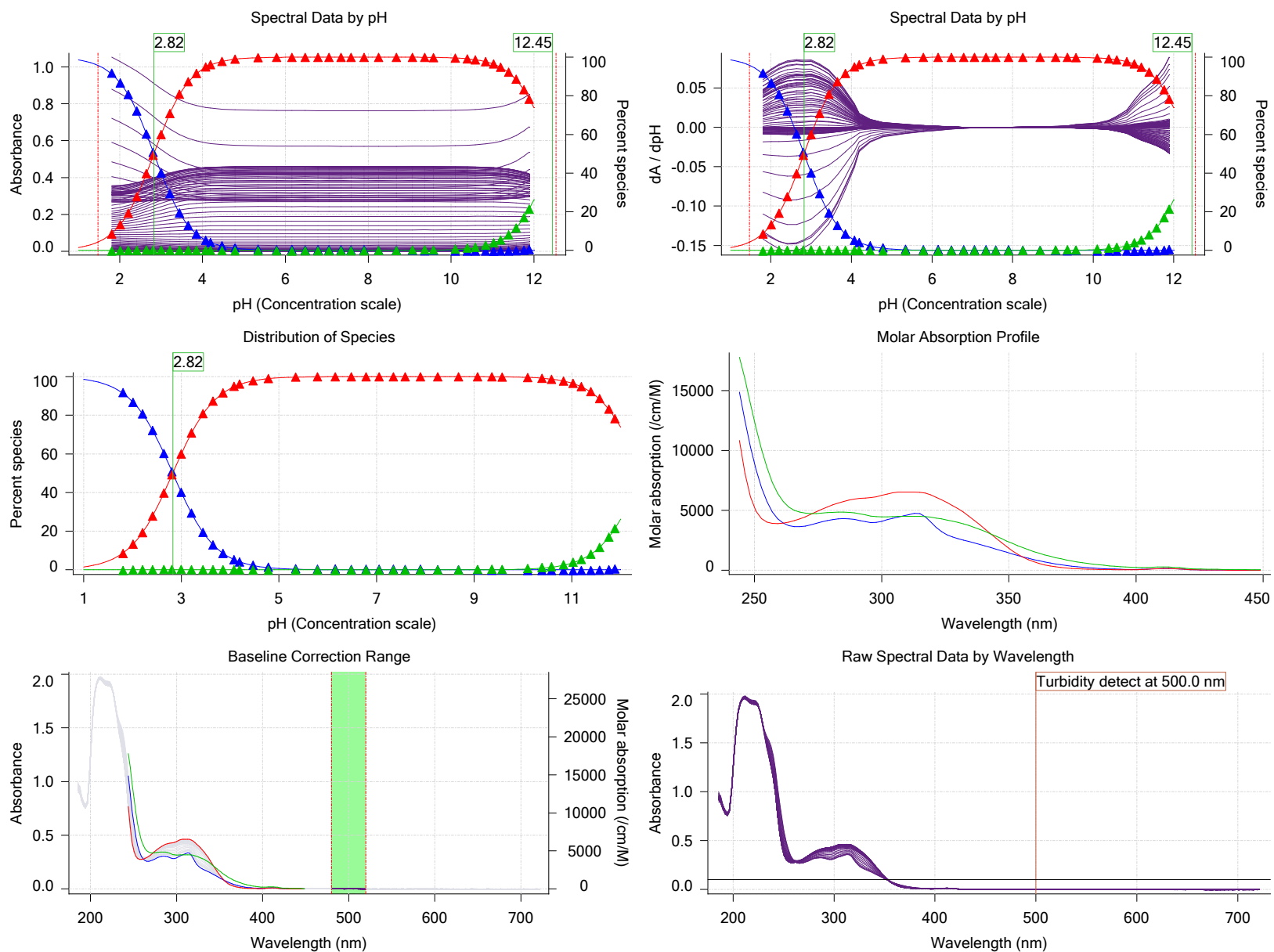
Graphs



Sample name: **M06**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-10008**
 Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric psKa.t3r**

Experiment start time: **11/10/2017 3:50:27 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Graphs (continued)



UV-metric psKa Titration 3 of 3 17K-10008 Points 75 to 119

Results

pKa 1 **3.06**
 pKa 2 **12.35**
 RMSD **0.001 0.002 0.001**
 Chi squared **0.0132**
 PCA calculated number of pKas **2**
 Average ionic strength **0.169 M**
 Average temperature **24.9°C**
 Analyte concentration range **49.6 µM to 47.1 µM**
 Methanol weight % **20.1 %**
 Dielectric constant **69.9**
 Water concentration **42.0 M**

Sample name: **M06**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-10008**
 Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric psKa.t3r**

Experiment start time: **11/10/2017 3:50:27 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 **1.487 to 12.549**

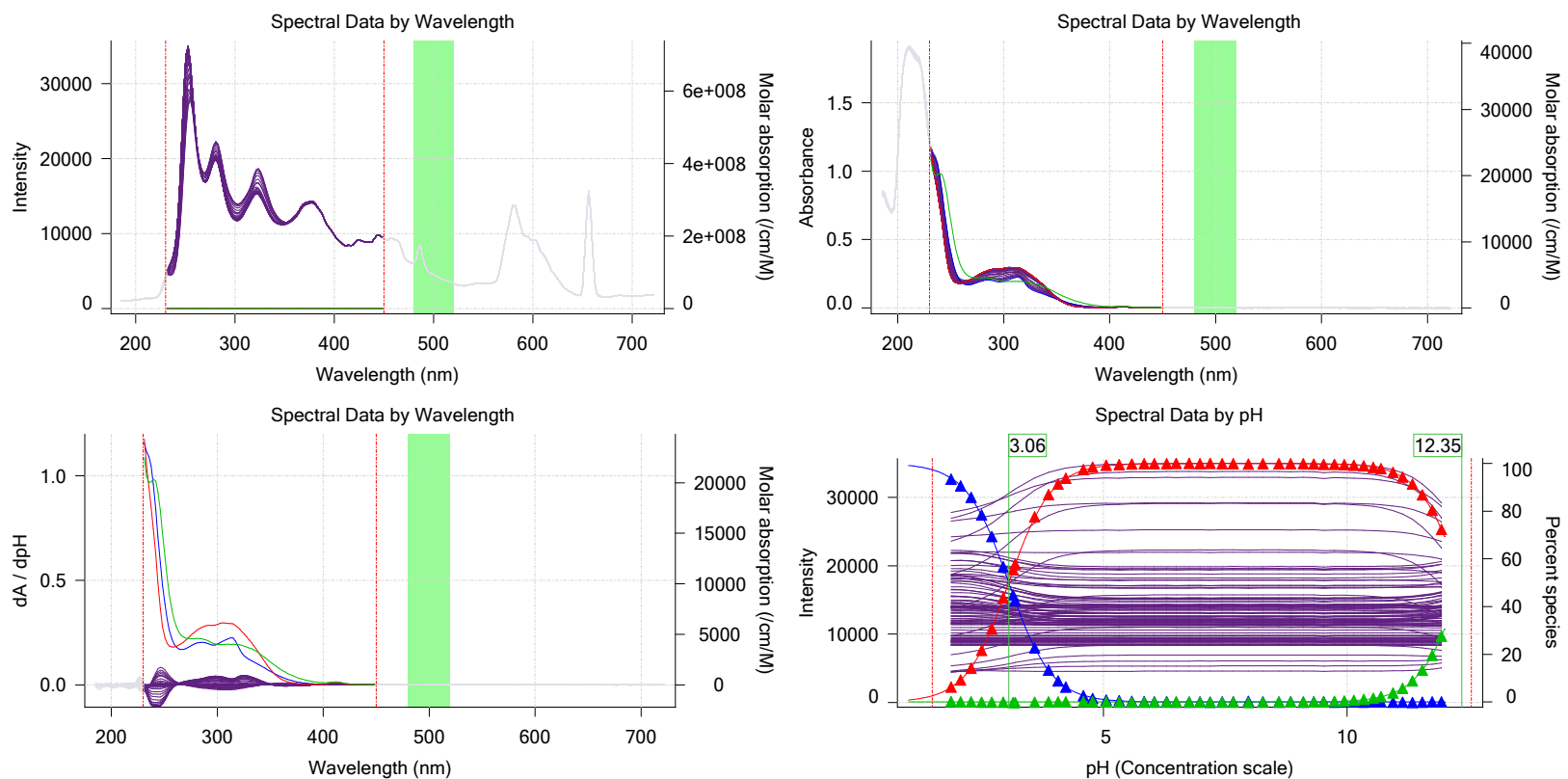
Warnings and errors

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			

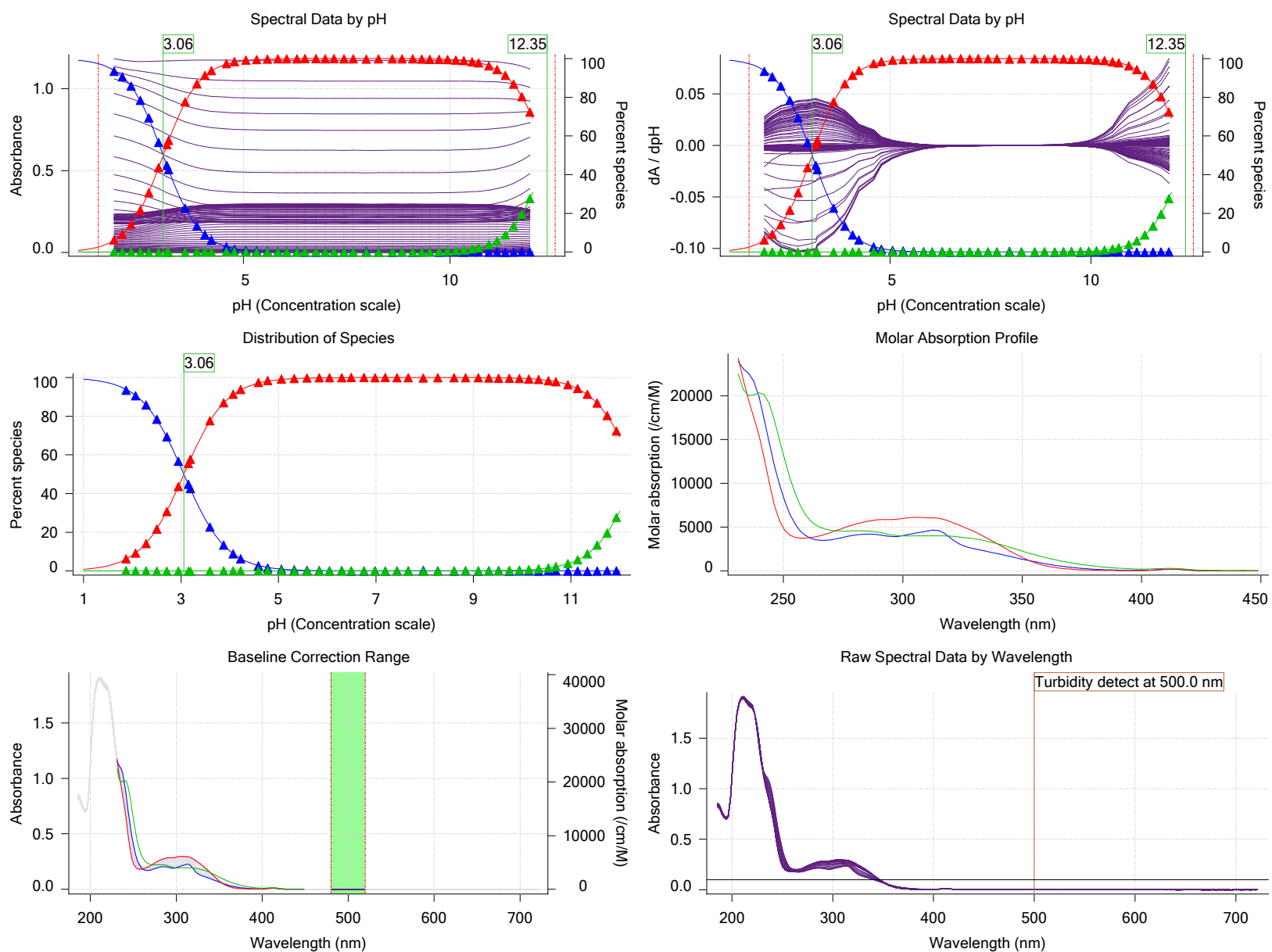
Graphs



Sample name: **M06**
 Assay name: **UV-metric pKa**
 Assay ID: **17K-10008**
 Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric pKa.t3r**

Experiment start time: **11/10/2017 3:50:27 PM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Graphs (continued)



Assay Model

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	0.050000 M	11/9/2017 5:26:58 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

Sample name: **M06**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-10008**
 Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric psKa.t3r**

Experiment start time: **11/10/2017 3:50:27 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
5:02.9	Dark spectrum								
5:04.3	Reference spectrum								
5:32.0	Volume reset due to vial change								
6:16.0	Initial pH = 8.12								
7:27.9	Data point 4	0.55997 mL	0.06265 mL	0.00000 mL	0.94003 mL	0.02500 mL	1.953	-0.01829	0.71728
7:56.5	Data point 5	0.55997 mL	0.06265 mL	0.02300 mL	0.94003 mL	0.02500 mL	2.153	0.01411	0.56277
8:13.3	Data point 6	0.55997 mL	0.06265 mL	0.03676 mL	0.94003 mL	0.02500 mL	2.348	0.01089	0.61014
8:30.2	Data point 7	0.55997 mL	0.06265 mL	0.04546 mL	0.94003 mL	0.02500 mL	2.547	0.01429	0.40476
8:46.9	Data point 8	0.55997 mL	0.06265 mL	0.05099 mL	0.94003 mL	0.02500 mL	2.713	0.00741	0.75812
9:13.9	Data point 9	0.55997 mL	0.06265 mL	0.05440 mL	0.94003 mL	0.02500 mL	2.906	0.01029	0.78547
9:30.5	Data point 10	0.55997 mL	0.06265 mL	0.05684 mL	0.94003 mL	0.02500 mL	3.085	0.00867	0.72170
9:47.1	Data point 11	0.55997 mL	0.06265 mL	0.05847 mL	0.94003 mL	0.02500 mL	3.215	-0.00437	0.34470
10:18.9	Data point 12	0.55997 mL	0.06265 mL	0.05995 mL	0.94003 mL	0.02500 mL	3.441	0.02080	0.94143
10:50.8	Data point 13	0.55997 mL	0.06265 mL	0.06065 mL	0.94003 mL	0.02500 mL	3.677	0.02251	0.94507
11:07.4	Data point 14	0.55997 mL	0.06265 mL	0.06108 mL	0.94003 mL	0.02500 mL	3.982	0.05815	0.98942
11:28.9	Data point 15	0.55997 mL	0.06265 mL	0.06150 mL	0.94003 mL	0.02500 mL	4.452	0.09795	0.98625
12:02.6	Data point 16	0.55997 mL	0.06265 mL	0.06178 mL	0.94003 mL	0.02500 mL	6.074	0.09789	0.93889
12:55.7	Data point 17	0.55997 mL	0.06265 mL	0.06197 mL	0.94003 mL	0.02500 mL	7.020	0.09396	0.97046
13:29.2	Data point 18	0.55997 mL	0.06265 mL	0.06216 mL	0.94003 mL	0.02500 mL	7.570	0.09918	0.97880
14:09.6	Data point 19	0.55997 mL	0.06265 mL	0.06239 mL	0.94003 mL	0.02500 mL	8.283	0.09875	0.98274
14:55.7	Data point 20	0.55997 mL	0.06265 mL	0.06254 mL	0.94003 mL	0.02500 mL	8.685	0.09144	0.95597
15:46.3	Data point 21	0.55997 mL	0.06265 mL	0.06265 mL	0.94003 mL	0.02500 mL	9.180	0.09771	0.95424
16:34.4	Data point 22	0.55997 mL	0.06265 mL	0.06279 mL	0.94003 mL	0.02500 mL	9.818	0.09924	0.98117
17:02.6	Data point 23	0.55997 mL	0.06265 mL	0.06296 mL	0.94003 mL	0.02500 mL	10.082	0.09338	0.98172
17:24.1	Data point 24	0.55997 mL	0.06265 mL	0.06324 mL	0.94003 mL	0.02500 mL	10.382	0.04501	0.94740
17:56.0	Data point 25	0.55997 mL	0.06265 mL	0.06373 mL	0.94003 mL	0.02500 mL	10.584	0.01920	0.90307
18:28.0	Data point 26	0.55997 mL	0.06265 mL	0.06449 mL	0.94003 mL	0.02500 mL	10.824	0.01057	0.82707
18:59.7	Data point 27	0.55997 mL	0.06265 mL	0.06564 mL	0.94003 mL	0.02500 mL	11.017	0.00601	0.71667
19:26.5	Data point 28	0.55997 mL	0.06265 mL	0.06787 mL	0.94003 mL	0.02500 mL	11.222	0.00249	0.26172
19:53.5	Data point 29	0.55997 mL	0.06265 mL	0.07018 mL	0.94003 mL	0.02500 mL	11.412	0.00296	0.30782
20:10.2	Data point 30	0.55997 mL	0.06265 mL	0.07397 mL	0.94003 mL	0.02500 mL	11.614	0.00408	0.41190
20:26.9	Data point 31	0.55997 mL	0.06265 mL	0.07996 mL	0.94003 mL	0.02500 mL	11.795	0.00308	0.36264
20:43.7	Data point 32	0.55997 mL	0.06265 mL	0.08911 mL	0.94003 mL	0.02500 mL	11.976	0.00407	0.59997
21:00.4	Data point 33	0.55997 mL	0.06265 mL	0.09358 mL	0.94003 mL	0.02500 mL	12.044	0.00386	0.36621
22:43.8	Reference spectrum								
23:48.5	Data point 35	0.83996 mL	0.16077 mL	0.09358 mL	0.94003 mL	0.02500 mL	1.971	-0.09226	0.97064
24:17.2	Data point 36	0.83996 mL	0.16077 mL	0.11917 mL	0.94003 mL	0.02500 mL	2.172	-0.00854	0.79442
24:34.0	Data point 37	0.83996 mL	0.16077 mL	0.13427 mL	0.94003 mL	0.02500 mL	2.362	-0.00229	0.07892
24:50.9	Data point 38	0.83996 mL	0.16077 mL	0.14396 mL	0.94003 mL	0.02500 mL	2.566	0.00497	0.36263
25:07.6	Data point 39	0.83996 mL	0.16077 mL	0.15012 mL	0.94003 mL	0.02500 mL	2.795	-0.00638	0.17392
25:24.4	Data point 40	0.83996 mL	0.16077 mL	0.15369 mL	0.94003 mL	0.02500 mL	2.961	0.00165	0.02408
25:51.1	Data point 41	0.83996 mL	0.16077 mL	0.15569 mL	0.94003 mL	0.02500 mL	3.152	0.00573	0.52245
26:23.1	Data point 42	0.83996 mL	0.16077 mL	0.15713 mL	0.94003 mL	0.02500 mL	3.362	0.01563	0.89987
26:39.8	Data point 43	0.83996 mL	0.16077 mL	0.15811 mL	0.94003 mL	0.02500 mL	3.595	0.01179	0.80508
27:11.5	Data point 44	0.83996 mL	0.16077 mL	0.15882 mL	0.94003 mL	0.02500 mL	3.804	0.03765	0.97754
27:43.2	Data point 45	0.83996 mL	0.16077 mL	0.15924 mL	0.94003 mL	0.02500 mL	4.007	0.05772	0.97741
27:59.8	Data point 46	0.83996 mL	0.16077 mL	0.15948 mL	0.94003 mL	0.02500 mL	4.231	0.07541	0.98952
28:16.4	Data point 47	0.83996 mL	0.16077 mL	0.15962 mL	0.94003 mL	0.02500 mL	4.345	0.09700	0.97017
28:38.0	Data point 48	0.83996 mL	0.16077 mL	0.15978 mL	0.94003 mL	0.02500 mL	4.621	0.09888	0.99052
29:14.5	Data point 49	0.83996 mL	0.16077 mL	0.15990 mL	0.94003 mL	0.02500 mL	4.935	0.10047	0.98327



Assay Events

Sample name: **M06** Experiment start time: **11/10/2017 3:50:27 PM**
Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse**
Assay ID: **17K-10008** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric psKa.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH Slope
30:00.7	Data point 50	0.83996 mL	0.16077 mL	0.16000 mL	0.94003 mL	0.02500 mL	5.495	0.09665	0.96373	0.96373
31:10.4	Data point 51	0.83996 mL	0.16077 mL	0.16007 mL	0.94003 mL	0.02500 mL	5.941	0.09683	0.98615	0.98615
31:59.0	Data point 52	0.83996 mL	0.16077 mL	0.16014 mL	0.94003 mL	0.02500 mL	6.308	0.09948	0.98721	0.98721
32:44.7	Data point 53	0.83996 mL	0.16077 mL	0.16023 mL	0.94003 mL	0.02500 mL	6.634	0.09682	0.97422	0.97422
33:16.4	Data point 54	0.83996 mL	0.16077 mL	0.16035 mL	0.94003 mL	0.02500 mL	6.938	0.08985	0.94787	0.94787
33:53.2	Data point 55	0.83996 mL	0.16077 mL	0.16049 mL	0.94003 mL	0.02500 mL	7.208	0.09628	0.98266	0.98266
34:29.9	Data point 56	0.83996 mL	0.16077 mL	0.16065 mL	0.94003 mL	0.02500 mL	7.498	0.09909	0.98418	0.98418
35:08.1	Data point 57	0.83996 mL	0.16077 mL	0.16077 mL	0.94003 mL	0.02500 mL	7.739	0.09864	0.98887	0.98887
35:53.4	Data point 58	0.83996 mL	0.16077 mL	0.16089 mL	0.94003 mL	0.02500 mL	8.054	0.09917	0.99066	0.99066
36:46.0	Data point 59	0.83996 mL	0.16077 mL	0.16101 mL	0.94003 mL	0.02500 mL	8.407	0.09812	0.98379	0.98379
37:41.5	Data point 60	0.83996 mL	0.16077 mL	0.16112 mL	0.94003 mL	0.02500 mL	8.836	0.09990	0.97998	0.97998
38:30.8	Data point 61	0.83996 mL	0.16077 mL	0.16126 mL	0.94003 mL	0.02500 mL	9.223	0.09669	0.98430	0.98430
39:09.6	Data point 62	0.83996 mL	0.16077 mL	0.16141 mL	0.94003 mL	0.02500 mL	9.517	0.09568	0.97957	0.97957
39:42.8	Data point 63	0.83996 mL	0.16077 mL	0.16157 mL	0.94003 mL	0.02500 mL	9.729	0.09412	0.96891	0.96891
40:11.4	Data point 64	0.83996 mL	0.16077 mL	0.16232 mL	0.94003 mL	0.02500 mL	10.254	0.02289	0.98704	0.98704
40:33.1	Data point 65	0.83996 mL	0.16077 mL	0.16308 mL	0.94003 mL	0.02500 mL	10.544	0.00921	0.74393	0.74393
41:05.0	Data point 66	0.83996 mL	0.16077 mL	0.16397 mL	0.94003 mL	0.02500 mL	10.740	0.00407	0.44623	0.44623
41:21.6	Data point 67	0.83996 mL	0.16077 mL	0.16522 mL	0.94003 mL	0.02500 mL	10.988	-0.00355	0.36716	0.36716
41:48.4	Data point 68	0.83996 mL	0.16077 mL	0.16724 mL	0.94003 mL	0.02500 mL	11.179	-0.00175	0.12316	0.12316
42:05.0	Data point 69	0.83996 mL	0.16077 mL	0.17058 mL	0.94003 mL	0.02500 mL	11.349	-0.00237	0.21196	0.21196
42:31.9	Data point 70	0.83996 mL	0.16077 mL	0.17568 mL	0.94003 mL	0.02500 mL	11.546	-0.00184	0.11125	0.11125
42:48.7	Data point 71	0.83996 mL	0.16077 mL	0.18347 mL	0.94003 mL	0.02500 mL	11.726	-0.00122	0.05397	0.05397
43:05.5	Data point 72	0.83996 mL	0.16077 mL	0.19532 mL	0.94003 mL	0.02500 mL	11.912	-0.00185	0.17139	0.17139
43:22.4	Data point 73	0.83996 mL	0.16077 mL	0.20708 mL	0.94003 mL	0.02500 mL	12.036	0.00282	0.16576	0.16576
45:13.9	Reference spectrum									
47:30.1	Data point 75	1.54998 mL	0.29991 mL	0.20710 mL	0.94003 mL	0.02500 mL	1.987	0.05400	0.77278	0.77278
48:02.8	Data point 76	1.54998 mL	0.29991 mL	0.23690 mL	0.94003 mL	0.02500 mL	2.180	-0.03982	0.95235	0.95235
48:19.7	Data point 77	1.54998 mL	0.29991 mL	0.25682 mL	0.94003 mL	0.02500 mL	2.392	-0.07873	0.82375	0.82375
48:38.1	Data point 78	1.54998 mL	0.29991 mL	0.26896 mL	0.94003 mL	0.02500 mL	2.611	-0.09301	0.86415	0.86415
48:56.8	Data point 79	1.54998 mL	0.29991 mL	0.27636 mL	0.94003 mL	0.02500 mL	2.817	-0.08897	0.89803	0.89803
49:14.4	Data point 80	1.54998 mL	0.29991 mL	0.28097 mL	0.94003 mL	0.02500 mL	3.053	-0.08975	0.89198	0.89198
49:54.7	Data point 81	1.54998 mL	0.29991 mL	0.28337 mL	0.94003 mL	0.02500 mL	3.256	0.00227	0.21564	0.21564
50:11.3	Data point 82	1.54998 mL	0.29991 mL	0.28502 mL	0.94003 mL	0.02500 mL	3.296	-0.01911	0.78659	0.78659
50:43.5	Data point 83	1.54998 mL	0.29991 mL	0.28747 mL	0.94003 mL	0.02500 mL	3.699	-0.08792	0.86315	0.86315
51:06.6	Data point 84	1.54998 mL	0.29991 mL	0.28808 mL	0.94003 mL	0.02500 mL	3.981	-0.09213	0.86883	0.86883
51:24.7	Data point 85	1.54998 mL	0.29991 mL	0.28841 mL	0.94003 mL	0.02500 mL	4.177	-0.08156	0.86198	0.86198
51:41.7	Data point 86	1.54998 mL	0.29991 mL	0.28862 mL	0.94003 mL	0.02500 mL	4.333	-0.06283	0.77226	0.77226
52:03.3	Data point 87	1.54998 mL	0.29991 mL	0.28885 mL	0.94003 mL	0.02500 mL	4.696	-0.08620	0.81427	0.81427
52:27.1	Data point 88	1.54998 mL	0.29991 mL	0.28897 mL	0.94003 mL	0.02500 mL	4.889	0.04276	0.68720	0.68720
52:48.7	Data point 89	1.54998 mL	0.29991 mL	0.28906 mL	0.94003 mL	0.02500 mL	5.169	0.08215	0.93519	0.93519
53:15.5	Data point 90	1.54998 mL	0.29991 mL	0.28913 mL	0.94003 mL	0.02500 mL	5.432	0.08905	0.86960	0.86960
53:43.1	Data point 91	1.54998 mL	0.29991 mL	0.28920 mL	0.94003 mL	0.02500 mL	5.693	-0.01269	0.05419	0.05419
54:04.6	Data point 92	1.54998 mL	0.29991 mL	0.28928 mL	0.94003 mL	0.02500 mL	5.946	-0.07771	0.61108	0.61108
54:27.5	Data point 93	1.54998 mL	0.29991 mL	0.28935 mL	0.94003 mL	0.02500 mL	6.157	-0.06243	0.51142	0.51142
54:51.5	Data point 94	1.54998 mL	0.29991 mL	0.28944 mL	0.94003 mL	0.02500 mL	6.407	-0.09465	0.93407	0.93407
55:21.0	Data point 95	1.54998 mL	0.29991 mL	0.28953 mL	0.94003 mL	0.02500 mL	6.602	-0.09472	0.93244	0.93244
55:46.7	Data point 96	1.54998 mL	0.29991 mL	0.28965 mL	0.94003 mL	0.02500 mL	6.869	-0.10011	0.97986	0.97986
56:23.4	Data point 97	1.54998 mL	0.29991 mL	0.28977 mL	0.94003 mL	0.02500 mL	7.091	-0.03841	0.94363	0.94363
56:54.9	Data point 98	1.54998 mL	0.29991 mL	0.28989 mL	0.94003 mL	0.02500 mL	7.302	0.06350	0.74601	0.74601
57:26.5	Data point 99	1.54998 mL	0.29991 mL	0.29001 mL	0.94003 mL	0.02500 mL	7.547	0.09550	0.89360	0.89360
57:53.7	Data point 100	1.54998 mL	0.29991 mL	0.29010 mL	0.94003 mL	0.02500 mL	7.775	0.08894	0.90328	0.90328
58:27.8	Data point 101	1.54998 mL	0.29991 mL	0.29019 mL	0.94003 mL	0.02500 mL	8.085	0.09654	0.95825	0.95825
59:01.1	Data point 102	1.54998 mL	0.29991 mL	0.29026 mL	0.94003 mL	0.02500 mL	8.385	0.09264	0.94159	0.94159
59:39.6	Data point 103	1.54998 mL	0.29991 mL	0.29033 mL	0.94003 mL	0.02500 mL	8.715	0.08610	0.90983	0.90983
1:00:10.7	Data point 104	1.54998 mL	0.29991 mL	0.29041 mL	0.94003 mL	0.02500 mL	8.956	0.09298	0.95507	0.95507
1:00:42.0	Data point 105	1.54998 mL	0.29991 mL	0.29050 mL	0.94003 mL	0.02500 mL	9.215	0.08078	0.94376	0.94376
1:01:08.5	Data point 106	1.54998 mL	0.29991 mL	0.29062 mL	0.94003 mL	0.02500 mL	9.434	0.03645	0.91622	0.91622

Sample name: **M06**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-10008**
 Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric psKa.t3r**

Experiment start time: **11/10/2017 3:50:27 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
1:01:30.2	Data point 107	1.54998 mL	0.29991 mL	0.29076 mL	0.94003 mL	0.02500 mL	9.631	-0.01983	0.62070	0.0012
1:01:46.7	Data point 108	1.54998 mL	0.29991 mL	0.29095 mL	0.94003 mL	0.02500 mL	9.854	-0.07763	0.84862	0.0041
1:02:03.2	Data point 109	1.54998 mL	0.29991 mL	0.29128 mL	0.94003 mL	0.02500 mL	10.061	-0.09153	0.93962	0.0046
1:02:19.7	Data point 110	1.54998 mL	0.29991 mL	0.29177 mL	0.94003 mL	0.02500 mL	10.256	-0.08632	0.88626	0.0045
1:02:36.2	Data point 111	1.54998 mL	0.29991 mL	0.29252 mL	0.94003 mL	0.02500 mL	10.455	-0.08031	0.87304	0.0042
1:02:52.8	Data point 112	1.54998 mL	0.29991 mL	0.29370 mL	0.94003 mL	0.02500 mL	10.654	-0.07991	0.89750	0.0041
1:03:09.3	Data point 113	1.54998 mL	0.29991 mL	0.29548 mL	0.94003 mL	0.02500 mL	10.810	-0.07669	0.86785	0.0040
1:03:41.2	Data point 114	1.54998 mL	0.29991 mL	0.29824 mL	0.94003 mL	0.02500 mL	11.057	-0.03955	0.91750	0.0020
1:03:57.8	Data point 115	1.54998 mL	0.29991 mL	0.30261 mL	0.94003 mL	0.02500 mL	11.256	-0.08008	0.90891	0.0041
1:04:14.5	Data point 116	1.54998 mL	0.29991 mL	0.30960 mL	0.94003 mL	0.02500 mL	11.458	-0.08963	0.91138	0.0046
1:04:31.9	Data point 117	1.54998 mL	0.29991 mL	0.32074 mL	0.94003 mL	0.02500 mL	11.659	-0.07796	0.90028	0.0040
1:04:48.9	Data point 118	1.54998 mL	0.29991 mL	0.33855 mL	0.94003 mL	0.02500 mL	11.860	-0.08667	0.92691	0.0044
1:05:06.2	Data point 119	1.54998 mL	0.29991 mL	0.36555 mL	0.94003 mL	0.02500 mL	12.049	-0.07840	0.91858	0.0040
1:06:37.0	Assay volumes	1.54998 mL	0.46364 mL	0.36555 mL	0.94003 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	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				

Sample name: **M06**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-10008**
 Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric psKa.t3r**

Experiment start time: **11/10/2017 3:50:27 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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				
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	0.081	11/10/2017 3:50:27 PM	C:\Sirius_T3\HCl17K10.t3r
Four-Plus S	1.0039	11/10/2017 3:50:27 PM	C:\Sirius_T3\HCl17K10.t3r
Four-Plus jH	1.1	11/10/2017 3:50:27 PM	C:\Sirius_T3\HCl17K10.t3r
Four-Plus jOH	-0.5	11/10/2017 3:50:27 PM	C:\Sirius_T3\HCl17K10.t3r
Base concentration factor	1.008	11/10/2017 3:50:27 PM	C:\Sirius_T3\KOH17K09.t3r
Acid concentration factor	0.999	11/10/2017 3:50:27 PM	C:\Sirius_T3\HCl17K10.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		

Sample name: **M06**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-10008**
 Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric psKa.t3r**

Experiment start time: **11/10/2017 3:50:27 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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
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
Titration		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	-6.26 mV		11/10/2017 3:39:12 PM
Filling solution	3M KCl	KCL095	11/10/2017 10:16:10 AM
Liquids			
Wash 1	50% IPA:50% Water		11/10/2017 10:14:45 AM
Wash 2	0.5% Triton X-100 in H2O		11/10/2017 10:14:49 AM
Buffer position 1	pH7 Wash		11/10/2017 10:14:51 AM
Buffer position 2	pH 7		11/10/2017 10:14:54 AM
Storage position			11/10/2017 10:15:25 AM
Wash water	9.7e+003 mL	11-10-17	11/10/2017 10:14:37 AM
Waste	7.7e+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	518:34:28		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		



Assay Settings

Sample name: **M06** Experiment start time: **11/10/2017 3:50:27 PM**
Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse**
Assay ID: **17K-10008** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20171110_exp17_pKa\17K-10008_M06_UV-metric psKa.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
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 A1