

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07004**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07004_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 4:49:57 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

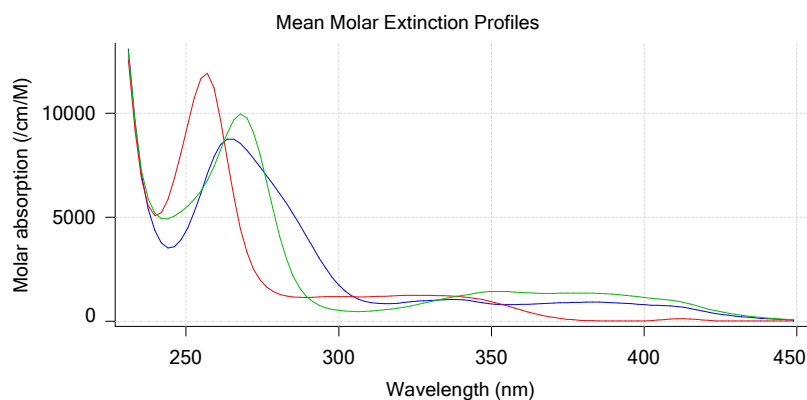
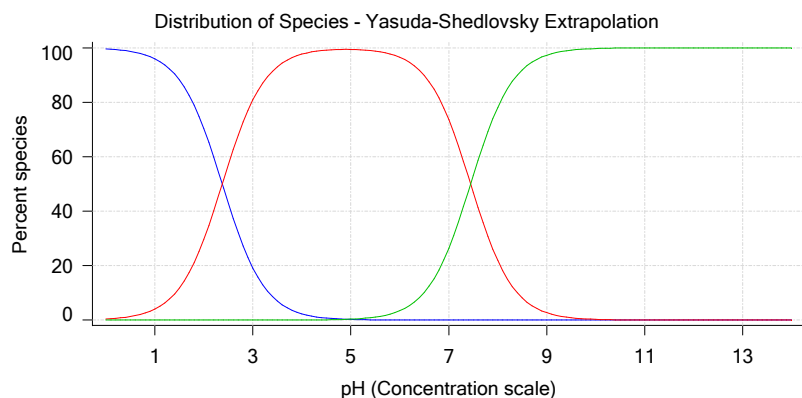
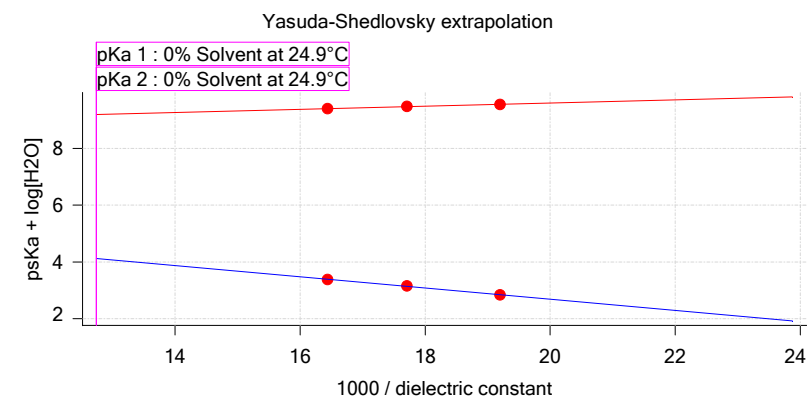
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	2.37	±0.04	6.63	-197.3121	0.9981	0.166 M	24.9°C
Yasuda-Shedlovsky	7.45	±0.03	8.49	55.1823	0.9877	0.166 M	24.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1	psKa 2
17J-07004 Points 4 to 70	59.09 %	Up	UV-metric pKa	52.1	19.6 M	0.157 M	24.9°C	✓ 1.54	✓ 8.25
17J-07004 Points 72 to 141	49.80 %	Up	UV-metric pKa	56.5	24.5 M	0.167 M	24.9°C	✓ 1.76	✓ 8.08
17J-07004 Points 143 to 215	40.38 %	Up	UV-metric pKa	60.8	29.8 M	0.174 M	24.9°C	✓ 1.91	✓ 7.91

Graphs



UV-metric psKa Titration 1 of 3 17J-07004 Points 4 to 70

Results

pKa 1	1.54
pKa 2	8.25
RMSD	0.002 0.004 0.004
Chi squared	0.0210
PCA calculated number of pKas	6
Average ionic strength	0.157 M
Average temperature	24.9°C
Analyte concentration range	80.6 µM to 75.8 µM
Methanol weight %	59.1 %
Dielectric constant	52.1
Water concentration	19.6 M

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Experiment start time: **10/7/2017 4:49:57 AM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.471 to 12.550**

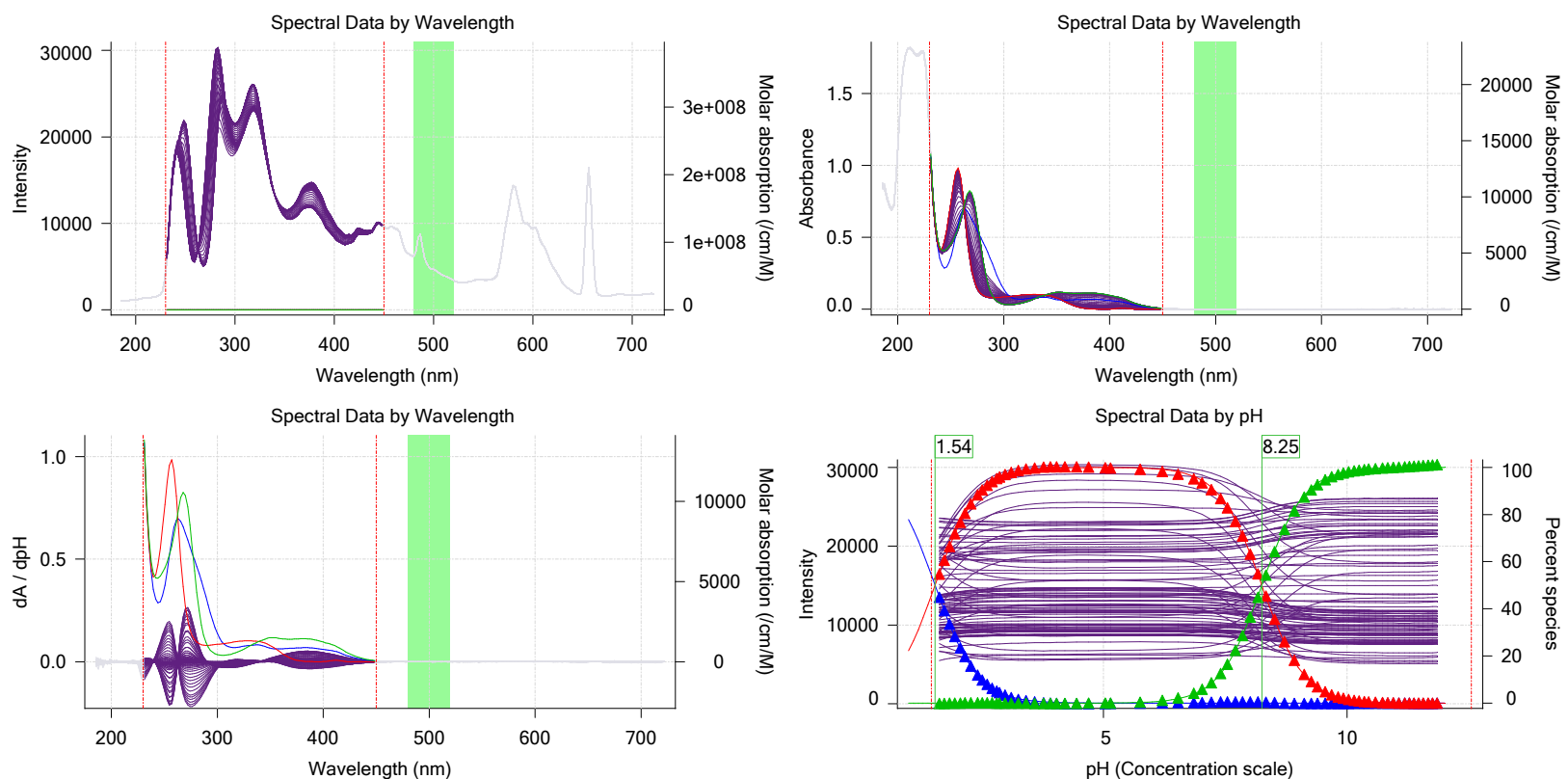
Warnings and errors

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			

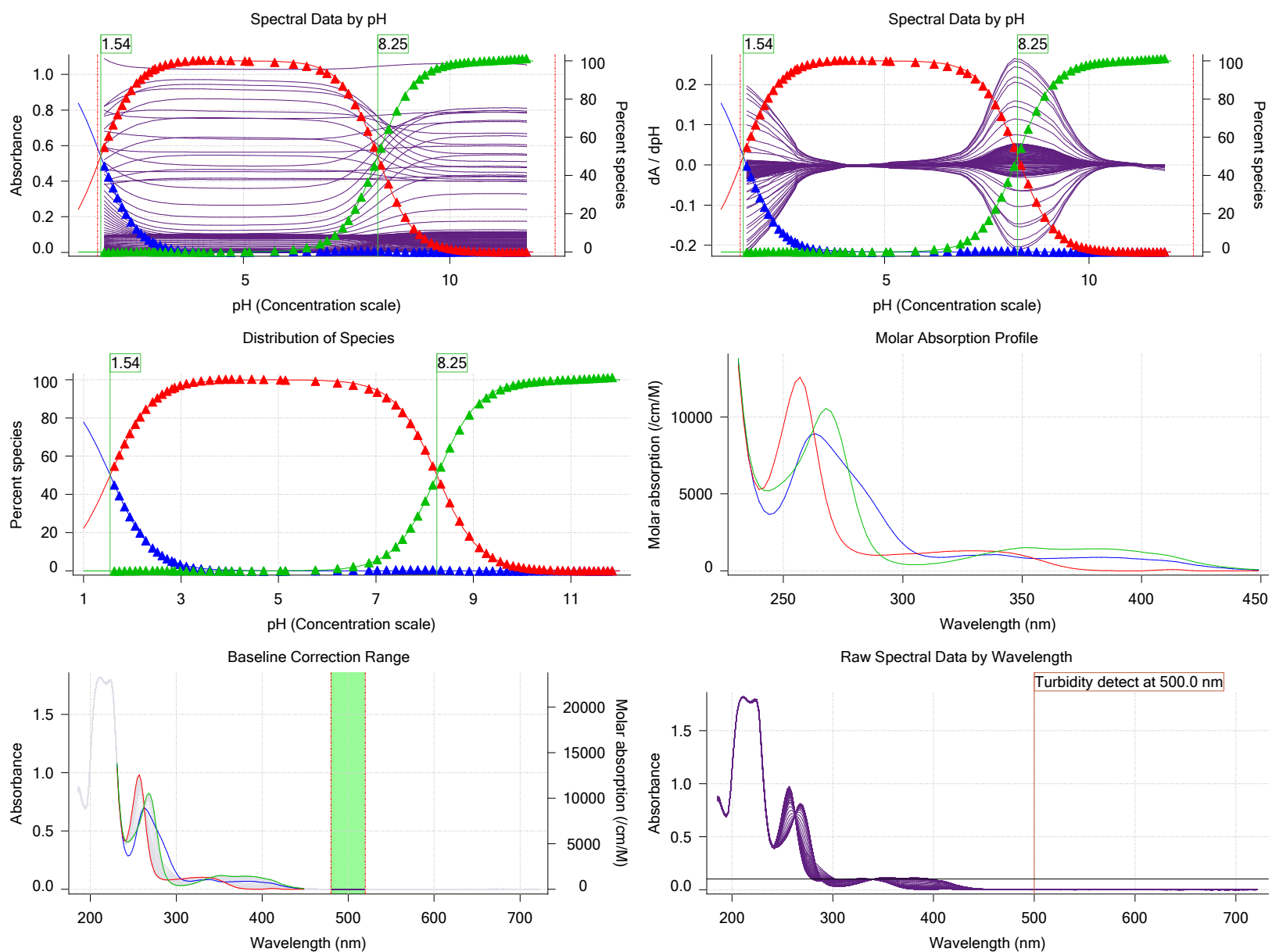
Graphs



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Experiment start time: **10/7/2017 4:49:57 AM**
 Analyst: **Dorothy Levorse**
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Graphs (continued)



UV-metric psKa Titration 2 of 3 17J-07004 Points 72 to 141

Results

pKa 1 **1.76**
 pKa 2 **8.08**
 RMSD **0.004 0.009 0.007**
 Chi squared **0.0521**
 PCA calculated number of pKas **6**
 Average ionic strength **0.167 M**
 Average temperature **24.9°C**
 Analyte concentration range **69.0 µM to 65.3 µM**
 Methanol weight % **49.8 %**
 Dielectric constant **56.5**
 Water concentration **24.5 M**

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Experiment start time: **10/7/2017 4:49:57 AM**
 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 12.523**

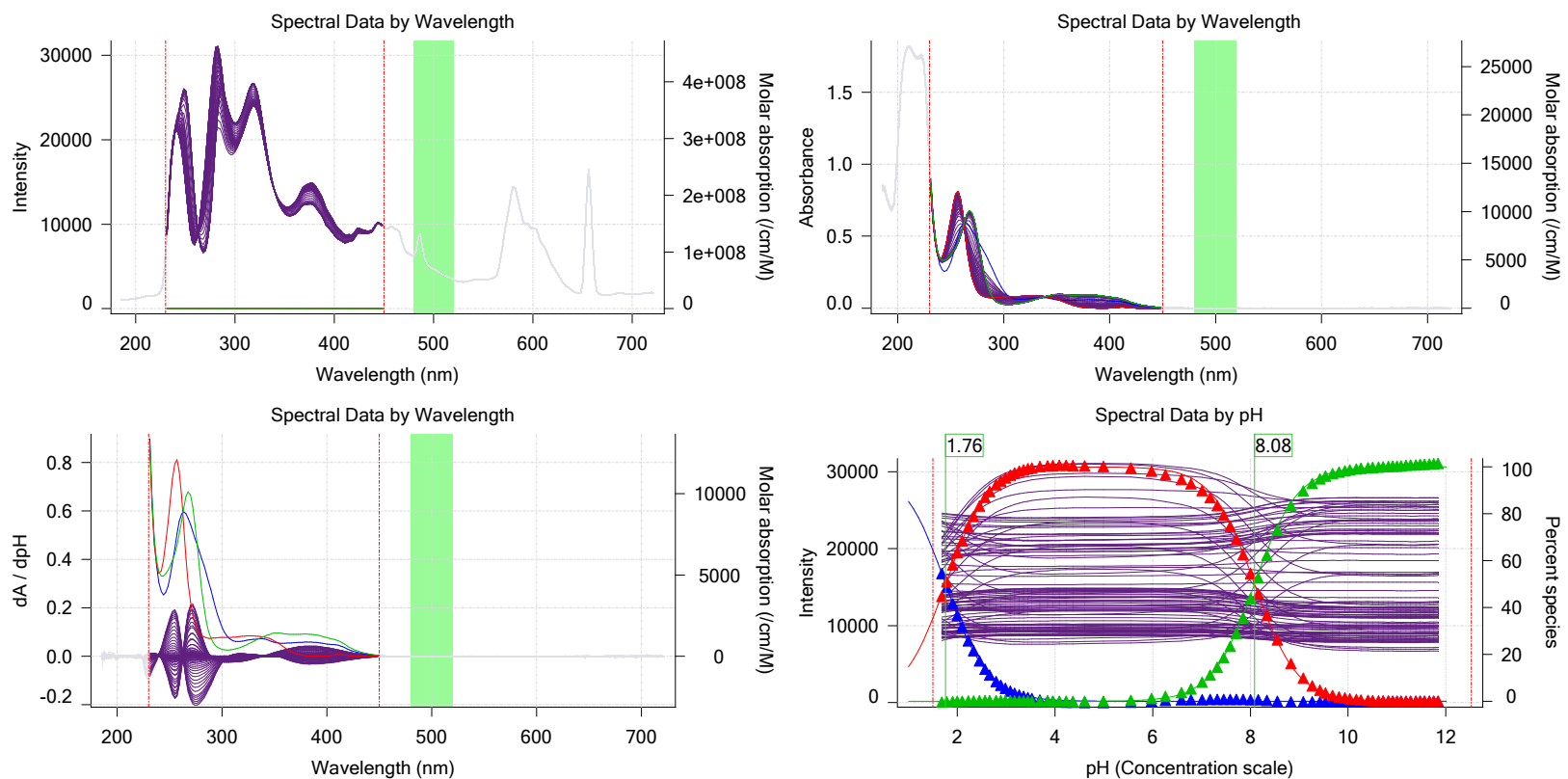
Warnings and errors

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			

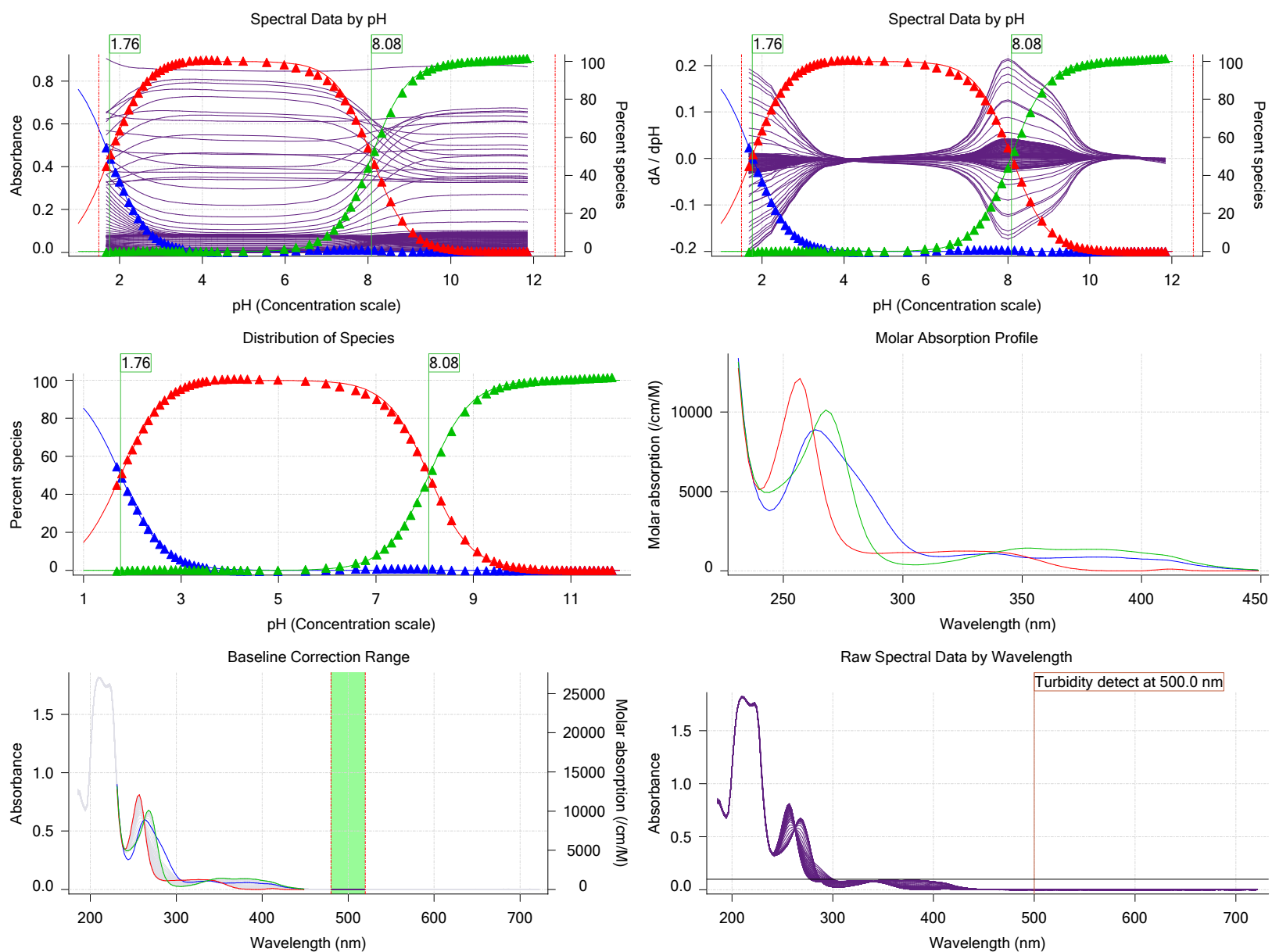
Graphs



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Graphs (continued)



UV-metric psKa Titration 3 of 3 17J-07004 Points 143 to 215

Results

pKa 1 **1.91**
 pKa 2 **7.91**
 RMSD **0.021 0.014 0.025**
 Chi squared **0.1664**
 PCA calculated number of pKas **5**
 Average ionic strength **0.174 M**
 Average temperature **24.9°C**
 Analyte concentration range **57.1 µM to 53.9 µM**
 Methanol weight % **40.4 %**
 Dielectric constant **60.8**
 Water concentration **29.8 M**

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Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.494 to 12.537**

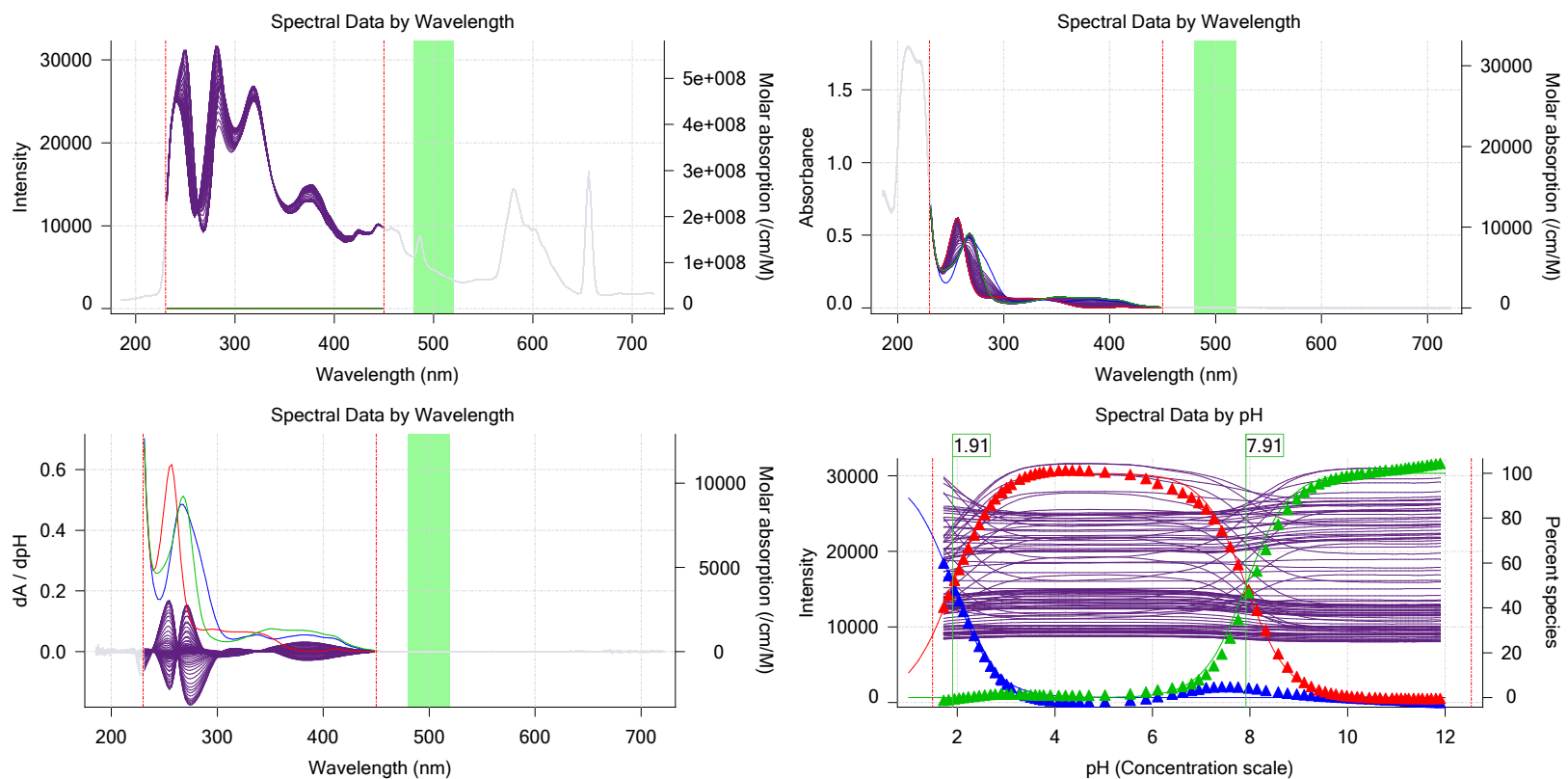
Warnings and errors

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				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

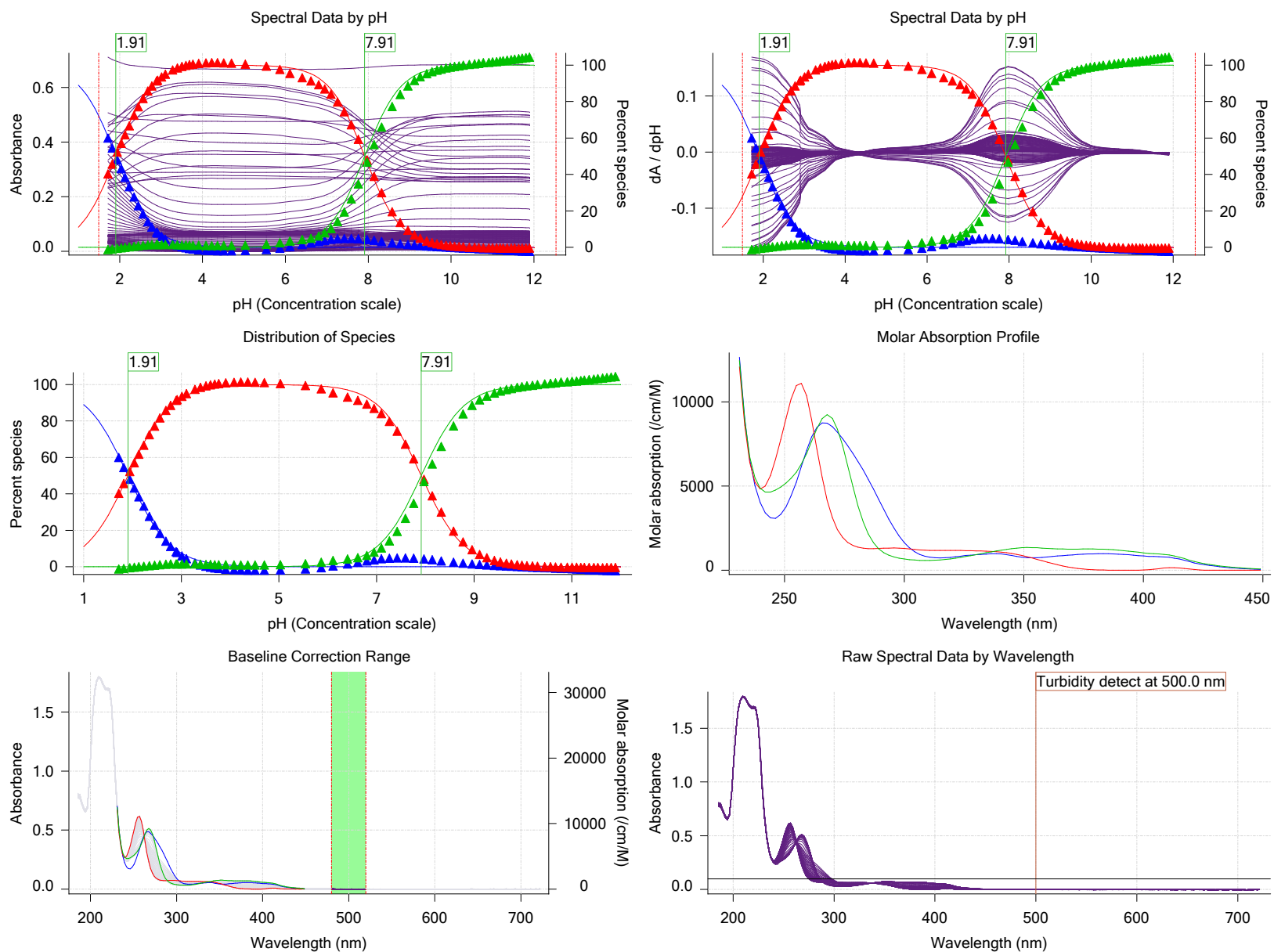
Graphs



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Experiment start time: **10/7/2017 4:49:57 AM**
 Analyst: **Dorothy Levorse**
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Graphs (continued)



Assay Model

Settings

Settings	Value	Date/Time changed	Imported from
Sample name	D07	9/29/2017 6:39:44 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0040 mL	10/6/2017 6:08:56 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.032500 M	10/2/2017 12:59:06 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	396.95	9/29/2017 6:39:58 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	9/29/2017 6:39:44 PM	User entered value
Sample is a	Ampholyte	9/29/2017 6:39:44 PM	User entered value
pKa 1	2.43	9/29/2017 6:39:44 PM	User entered value
Type	Base	9/29/2017 6:39:44 PM	User entered value
pKa 2	7.37	9/29/2017 6:39:44 PM	User entered value
Type	Acid	9/29/2017 6:39:44 PM	User entered value

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Experiment start time: **10/7/2017 4:49:57 AM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logp (XH2 +)	-10.00		Default value
logP (neutral XH)	-10.00	9/29/2017 6:39:44 PM	User entered value
logP (X -)	-10.00		Default value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-square
3:10.4	Dark spectrum								
3:11.8	Reference spectrum								
3:39.6	Volume reset due to vial change								
5:10.4	Initial pH = 8.42								
6:16.1	Data point 4	0.15005 mL	0.07354 mL	0.00000 mL	1.35995 mL	0.02500 mL	1.971	-0.00461	0.23097
6:44.6	Data point 5	0.15005 mL	0.07354 mL	0.01498 mL	1.35995 mL	0.02500 mL	2.075	0.01250	0.67159
7:01.5	Data point 6	0.15005 mL	0.07354 mL	0.02709 mL	1.35995 mL	0.02500 mL	2.184	0.00672	0.62172
7:18.3	Data point 7	0.15005 mL	0.07354 mL	0.03669 mL	1.35995 mL	0.02500 mL	2.291	0.00484	0.30510
7:35.0	Data point 8	0.15005 mL	0.07354 mL	0.04419 mL	1.35995 mL	0.02500 mL	2.402	0.00828	0.73673
7:51.7	Data point 9	0.15005 mL	0.07354 mL	0.05005 mL	1.35995 mL	0.02500 mL	2.498	0.00393	0.30739
8:08.4	Data point 10	0.15005 mL	0.07354 mL	0.05475 mL	1.35995 mL	0.02500 mL	2.616	0.00726	0.82971
8:40.6	Data point 11	0.15005 mL	0.07354 mL	0.05967 mL	1.35995 mL	0.02500 mL	2.752	0.00437	0.59190
9:07.6	Data point 12	0.15005 mL	0.07354 mL	0.06181 mL	1.35995 mL	0.02500 mL	2.850	0.00547	0.55982
9:34.5	Data point 13	0.15005 mL	0.07354 mL	0.06371 mL	1.35995 mL	0.02500 mL	2.946	0.00204	0.36998
9:51.0	Data point 14	0.15005 mL	0.07354 mL	0.06540 mL	1.35995 mL	0.02500 mL	3.047	0.00285	0.23490
10:07.6	Data point 15	0.15005 mL	0.07354 mL	0.06675 mL	1.35995 mL	0.02500 mL	3.142	0.00695	0.83559
10:24.2	Data point 16	0.15005 mL	0.07354 mL	0.06783 mL	1.35995 mL	0.02500 mL	3.196	0.00771	0.80629
10:56.3	Data point 17	0.15005 mL	0.07354 mL	0.06900 mL	1.35995 mL	0.02500 mL	3.310	0.01398	0.91123
11:23.1	Data point 18	0.15005 mL	0.07354 mL	0.06978 mL	1.35995 mL	0.02500 mL	3.439	0.01629	0.96883
11:39.6	Data point 19	0.15005 mL	0.07354 mL	0.07032 mL	1.35995 mL	0.02500 mL	3.578	0.02319	0.97943
12:01.3	Data point 20	0.15005 mL	0.07354 mL	0.07084 mL	1.35995 mL	0.02500 mL	3.736	0.02118	0.96713
12:23.0	Data point 21	0.15005 mL	0.07354 mL	0.07128 mL	1.35995 mL	0.02500 mL	3.912	0.04320	0.98765
12:44.6	Data point 22	0.15005 mL	0.07354 mL	0.07161 mL	1.35995 mL	0.02500 mL	4.094	0.06732	0.98459
13:06.3	Data point 23	0.15005 mL	0.07354 mL	0.07183 mL	1.35995 mL	0.02500 mL	4.231	0.08986	0.98986
13:33.2	Data point 24	0.15005 mL	0.07354 mL	0.07199 mL	1.35995 mL	0.02500 mL	4.354	0.10076	0.99650
14:02.5	Data point 25	0.15005 mL	0.07354 mL	0.07211 mL	1.35995 mL	0.02500 mL	4.522	0.10002	0.99595
14:43.7	Data point 26	0.15005 mL	0.07354 mL	0.07222 mL	1.35995 mL	0.02500 mL	4.758	0.10043	0.99339
15:40.6	Data point 27	0.15005 mL	0.07354 mL	0.07230 mL	1.35995 mL	0.02500 mL	5.000	0.09981	0.98808
16:48.8	Data point 28	0.15005 mL	0.07354 mL	0.07237 mL	1.35995 mL	0.02500 mL	5.340	0.15255	0.99333
18:00.5	Data point 29	0.15005 mL	0.07354 mL	0.07241 mL	1.35995 mL	0.02500 mL	5.443	-0.01290	0.02169
18:52.1	Data point 30	0.15005 mL	0.07354 mL	0.07246 mL	1.35995 mL	0.02500 mL	6.047	0.21263	0.99636
20:03.8	Data point 31	0.15005 mL	0.07354 mL	0.07251 mL	1.35995 mL	0.02500 mL	6.493	0.15081	0.99774
21:15.4	Data point 32	0.15005 mL	0.07354 mL	0.07255 mL	1.35995 mL	0.02500 mL	6.813	0.10462	0.99486
22:32.2	Data point 33	0.15005 mL	0.07354 mL	0.07262 mL	1.35995 mL	0.02500 mL	7.132	0.10027	0.99791
23:23.8	Data point 34	0.15005 mL	0.07354 mL	0.07270 mL	1.35995 mL	0.02500 mL	7.297	0.10030	0.99592
24:11.2	Data point 35	0.15005 mL	0.07354 mL	0.07277 mL	1.35995 mL	0.02500 mL	7.485	0.09965	0.99602
25:02.2	Data point 36	0.15005 mL	0.07354 mL	0.07286 mL	1.35995 mL	0.02500 mL	7.672	0.09948	0.99010
25:48.5	Data point 37	0.15005 mL	0.07354 mL	0.07295 mL	1.35995 mL	0.02500 mL	7.810	0.09719	0.96674
26:22.9	Data point 38	0.15005 mL	0.07354 mL	0.07305 mL	1.35995 mL	0.02500 mL	7.972	0.09728	0.99312
27:04.3	Data point 39	0.15005 mL	0.07354 mL	0.07314 mL	1.35995 mL	0.02500 mL	8.116	0.09924	0.99362
27:44.1	Data point 40	0.15005 mL	0.07354 mL	0.07324 mL	1.35995 mL	0.02500 mL	8.272	0.10092	0.99193
28:27.0	Data point 41	0.15005 mL	0.07354 mL	0.07333 mL	1.35995 mL	0.02500 mL	8.424	0.10018	0.98664
29:08.6	Data point 42	0.15005 mL	0.07354 mL	0.07342 mL	1.35995 mL	0.02500 mL	8.586	0.10016	0.99189
29:52.0	Data point 43	0.15005 mL	0.07354 mL	0.07352 mL	1.35995 mL	0.02500 mL	8.766	0.09910	0.98542
30:38.7	Data point 44	0.15005 mL	0.07354 mL	0.07361 mL	1.35995 mL	0.02500 mL	8.962	0.09737	0.98421
31:25.7	Data point 45	0.15005 mL	0.07354 mL	0.07371 mL	1.35995 mL	0.02500 mL	9.162	0.09797	0.98127
32:13.1	Data point 46	0.15005 mL	0.07354 mL	0.07380 mL	1.35995 mL	0.02500 mL	9.365	0.09990	0.98444
32:52.2	Data point 47	0.15005 mL	0.07354 mL	0.07387 mL	1.35995 mL	0.02500 mL	9.503	0.09648	0.97779
33:27.0	Data point 48	0.15005 mL	0.07354 mL	0.07394 mL	1.35995 mL	0.02500 mL	9.633	0.09874	0.99167
34:01.3	Data point 49	0.15005 mL	0.07354 mL	0.07404 mL	1.35995 mL	0.02500 mL	9.788	0.09841	0.98147



Assay Events

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Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
34:35.6	Data point 50	0.15005 mL	0.07354 mL	0.07413 mL	1.35995 mL	0.02500 mL	9.920	0.09957	0.98060	0.98060
35:06.5	Data point 51	0.15005 mL	0.07354 mL	0.07425 mL	1.35995 mL	0.02500 mL	10.046	0.09633	0.98503	0.98503
35:29.1	Data point 52	0.15005 mL	0.07354 mL	0.07437 mL	1.35995 mL	0.02500 mL	10.156	0.08319	0.98015	0.98015
35:55.9	Data point 53	0.15005 mL	0.07354 mL	0.07448 mL	1.35995 mL	0.02500 mL	10.258	0.06899	0.98079	0.98079
36:17.5	Data point 54	0.15005 mL	0.07354 mL	0.07465 mL	1.35995 mL	0.02500 mL	10.370	0.04826	0.97545	0.97545
36:44.3	Data point 55	0.15005 mL	0.07354 mL	0.07484 mL	1.35995 mL	0.02500 mL	10.472	0.04406	0.93912	0.93912
37:06.1	Data point 56	0.15005 mL	0.07354 mL	0.07507 mL	1.35995 mL	0.02500 mL	10.576	0.02793	0.93924	0.93924
37:27.7	Data point 57	0.15005 mL	0.07354 mL	0.07535 mL	1.35995 mL	0.02500 mL	10.669	0.01841	0.85323	0.85323
37:49.4	Data point 58	0.15005 mL	0.07354 mL	0.07575 mL	1.35995 mL	0.02500 mL	10.803	0.00722	0.78404	0.78404
38:16.2	Data point 59	0.15005 mL	0.07354 mL	0.07667 mL	1.35995 mL	0.02500 mL	10.946	0.00515	0.59421	0.59421
38:48.0	Data point 60	0.15005 mL	0.07354 mL	0.07742 mL	1.35995 mL	0.02500 mL	11.050	0.00290	0.30303	0.30303
39:14.9	Data point 61	0.15005 mL	0.07354 mL	0.07815 mL	1.35995 mL	0.02500 mL	11.162	0.00118	0.06976	0.06976
39:31.5	Data point 62	0.15005 mL	0.07354 mL	0.07905 mL	1.35995 mL	0.02500 mL	11.275	-0.00210	0.17827	0.17827
39:48.1	Data point 63	0.15005 mL	0.07354 mL	0.08020 mL	1.35995 mL	0.02500 mL	11.394	-0.00212	0.18818	0.18818
40:15.2	Data point 64	0.15005 mL	0.07354 mL	0.08168 mL	1.35995 mL	0.02500 mL	11.490	-0.00188	0.14284	0.14284
40:31.8	Data point 65	0.15005 mL	0.07354 mL	0.08358 mL	1.35995 mL	0.02500 mL	11.585	-0.00168	0.12355	0.12355
40:48.3	Data point 66	0.15005 mL	0.07354 mL	0.08598 mL	1.35995 mL	0.02500 mL	11.679	-0.00183	0.13270	0.13270
41:04.9	Data point 67	0.15005 mL	0.07354 mL	0.08895 mL	1.35995 mL	0.02500 mL	11.770	-0.00225	0.18135	0.18135
41:21.5	Data point 68	0.15005 mL	0.07354 mL	0.09264 mL	1.35995 mL	0.02500 mL	11.871	-0.00596	0.53858	0.53858
41:38.2	Data point 69	0.15005 mL	0.07354 mL	0.09734 mL	1.35995 mL	0.02500 mL	11.959	-0.00702	0.65319	0.65319
41:55.0	Data point 70	0.15005 mL	0.07354 mL	0.10259 mL	1.35995 mL	0.02500 mL	12.050	-0.00348	0.33967	0.33967
43:30.5	Reference spectrum									
44:33.2	Data point 72	0.22001 mL	0.17357 mL	0.10261 mL	1.35995 mL	0.02500 mL	1.999	-0.04242	0.91002	0.91002
45:00.5	Data point 73	0.22001 mL	0.17357 mL	0.11715 mL	1.35995 mL	0.02500 mL	2.099	0.01275	0.95308	0.95308
45:17.6	Data point 74	0.22001 mL	0.17357 mL	0.12977 mL	1.35995 mL	0.02500 mL	2.220	0.01103	0.73785	0.73785
45:39.6	Data point 75	0.22001 mL	0.17357 mL	0.13779 mL	1.35995 mL	0.02500 mL	2.315	0.01386	0.55111	0.55111
46:06.7	Data point 76	0.22001 mL	0.17357 mL	0.14483 mL	1.35995 mL	0.02500 mL	2.415	0.00392	0.37329	0.37329
46:23.5	Data point 77	0.22001 mL	0.17357 mL	0.15106 mL	1.35995 mL	0.02500 mL	2.537	0.01896	0.92903	0.92903
46:50.6	Data point 78	0.22001 mL	0.17357 mL	0.15548 mL	1.35995 mL	0.02500 mL	2.640	0.01501	0.90763	0.90763
47:07.3	Data point 79	0.22001 mL	0.17357 mL	0.15915 mL	1.35995 mL	0.02500 mL	2.759	0.01298	0.90386	0.90386
47:39.3	Data point 80	0.22001 mL	0.17357 mL	0.16244 mL	1.35995 mL	0.02500 mL	2.873	0.01030	0.87606	0.87606
48:06.4	Data point 81	0.22001 mL	0.17357 mL	0.16446 mL	1.35995 mL	0.02500 mL	2.968	0.00425	0.38262	0.38262
48:23.0	Data point 82	0.22001 mL	0.17357 mL	0.16620 mL	1.35995 mL	0.02500 mL	3.100	0.01456	0.90462	0.90462
48:44.9	Data point 83	0.22001 mL	0.17357 mL	0.16726 mL	1.35995 mL	0.02500 mL	3.191	0.01025	0.81801	0.81801
49:11.7	Data point 84	0.22001 mL	0.17357 mL	0.16823 mL	1.35995 mL	0.02500 mL	3.285	0.00900	0.79760	0.79760
49:28.3	Data point 85	0.22001 mL	0.17357 mL	0.16905 mL	1.35995 mL	0.02500 mL	3.384	0.00830	0.62824	0.62824
49:45.0	Data point 86	0.22001 mL	0.17357 mL	0.16971 mL	1.35995 mL	0.02500 mL	3.472	0.01757	0.93175	0.93175
50:01.6	Data point 87	0.22001 mL	0.17357 mL	0.17025 mL	1.35995 mL	0.02500 mL	3.565	0.02023	0.96838	0.96838
50:18.1	Data point 88	0.22001 mL	0.17357 mL	0.17067 mL	1.35995 mL	0.02500 mL	3.653	0.02268	0.96161	0.96161
50:34.7	Data point 89	0.22001 mL	0.17357 mL	0.17103 mL	1.35995 mL	0.02500 mL	3.739	0.03314	0.97278	0.97278
50:51.3	Data point 90	0.22001 mL	0.17357 mL	0.17131 mL	1.35995 mL	0.02500 mL	3.819	0.03322	0.98610	0.98610
51:12.8	Data point 91	0.22001 mL	0.17357 mL	0.17173 mL	1.35995 mL	0.02500 mL	3.983	0.05006	0.97449	0.97449
51:34.7	Data point 92	0.22001 mL	0.17357 mL	0.17204 mL	1.35995 mL	0.02500 mL	4.136	0.04833	0.98168	0.98168
52:06.6	Data point 93	0.22001 mL	0.17357 mL	0.17232 mL	1.35995 mL	0.02500 mL	4.245	0.07472	0.99070	0.99070
52:33.4	Data point 94	0.22001 mL	0.17357 mL	0.17251 mL	1.35995 mL	0.02500 mL	4.377	0.09771	0.98979	0.98979
53:03.2	Data point 95	0.22001 mL	0.17357 mL	0.17265 mL	1.35995 mL	0.02500 mL	4.509	0.09821	0.99038	0.99038
53:39.0	Data point 96	0.22001 mL	0.17357 mL	0.17277 mL	1.35995 mL	0.02500 mL	4.646	0.09810	0.98320	0.98320
54:19.9	Data point 97	0.22001 mL	0.17357 mL	0.17288 mL	1.35995 mL	0.02500 mL	4.887	0.09931	0.99103	0.99103
55:13.7	Data point 98	0.22001 mL	0.17357 mL	0.17295 mL	1.35995 mL	0.02500 mL	5.263	0.10058	0.99094	0.99094
56:25.9	Data point 99	0.22001 mL	0.17357 mL	0.17302 mL	1.35995 mL	0.02500 mL	5.822	0.13605	0.99379	0.99379
57:37.6	Data point 100	0.22001 mL	0.17357 mL	0.17307 mL	1.35995 mL	0.02500 mL	6.237	0.09834	0.97133	0.97133
58:45.3	Data point 101	0.22001 mL	0.17357 mL	0.17312 mL	1.35995 mL	0.02500 mL	6.517	0.09807	0.99281	0.99281
59:51.1	Data point 102	0.22001 mL	0.17357 mL	0.17319 mL	1.35995 mL	0.02500 mL	6.840	0.09427	0.97211	0.97211
1:00:48.0	Data point 103	0.22001 mL	0.17357 mL	0.17326 mL	1.35995 mL	0.02500 mL	7.038	0.09776	0.98880	0.98880
1:01:37.4	Data point 104	0.22001 mL	0.17357 mL	0.17335 mL	1.35995 mL	0.02500 mL	7.262	0.09840	0.98840	0.98840
1:02:18.3	Data point 105	0.22001 mL	0.17357 mL	0.17342 mL	1.35995 mL	0.02500 mL	7.423	0.10059	0.98861	0.98861
1:02:56.1	Data point 106	0.22001 mL	0.17357 mL	0.17350 mL	1.35995 mL	0.02500 mL	7.562	0.09966	0.99203	0.99203

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07004**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07004_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 4:49:57 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
1:03:31.4	Data point 107	0.22001 mL	0.17357 mL	0.17357 mL	1.35995 mL	0.02500 mL	7.695	0.10003	0.98356	0.98356
1:04:03.6	Data point 108	0.22001 mL	0.17357 mL	0.17364 mL	1.35995 mL	0.02500 mL	7.825	0.10017	0.99453	0.99453
1:04:37.2	Data point 109	0.22001 mL	0.17357 mL	0.17371 mL	1.35995 mL	0.02500 mL	7.952	0.09944	0.98974	0.98974
1:05:11.1	Data point 110	0.22001 mL	0.17357 mL	0.17378 mL	1.35995 mL	0.02500 mL	8.086	0.10080	0.99571	0.99571
1:05:44.4	Data point 111	0.22001 mL	0.17357 mL	0.17385 mL	1.35995 mL	0.02500 mL	8.237	0.10077	0.99337	0.99337
1:06:21.7	Data point 112	0.22001 mL	0.17357 mL	0.17392 mL	1.35995 mL	0.02500 mL	8.390	0.09676	0.99240	0.99240
1:06:60.0	Data point 113	0.22001 mL	0.17357 mL	0.17399 mL	1.35995 mL	0.02500 mL	8.565	0.09780	0.99041	0.99041
1:07:40.1	Data point 114	0.22001 mL	0.17357 mL	0.17406 mL	1.35995 mL	0.02500 mL	8.780	0.09863	0.98329	0.98329
1:08:20.9	Data point 115	0.22001 mL	0.17357 mL	0.17413 mL	1.35995 mL	0.02500 mL	9.055	0.09362	0.95831	0.95831
1:09:05.7	Data point 116	0.22001 mL	0.17357 mL	0.17420 mL	1.35995 mL	0.02500 mL	9.300	0.09828	0.98128	0.98128
1:09:45.5	Data point 117	0.22001 mL	0.17357 mL	0.17427 mL	1.35995 mL	0.02500 mL	9.483	0.09456	0.97127	0.97127
1:10:21.3	Data point 118	0.22001 mL	0.17357 mL	0.17434 mL	1.35995 mL	0.02500 mL	9.638	0.09572	0.97687	0.97687
1:10:54.6	Data point 119	0.22001 mL	0.17357 mL	0.17441 mL	1.35995 mL	0.02500 mL	9.754	0.09919	0.98128	0.98128
1:11:23.8	Data point 120	0.22001 mL	0.17357 mL	0.17451 mL	1.35995 mL	0.02500 mL	9.896	0.09564	0.96543	0.96543
1:11:51.4	Data point 121	0.22001 mL	0.17357 mL	0.17460 mL	1.35995 mL	0.02500 mL	10.028	0.07617	0.97419	0.97419
1:12:12.9	Data point 122	0.22001 mL	0.17357 mL	0.17469 mL	1.35995 mL	0.02500 mL	10.145	0.06889	0.95671	0.95671
1:12:29.5	Data point 123	0.22001 mL	0.17357 mL	0.17479 mL	1.35995 mL	0.02500 mL	10.246	0.04675	0.96388	0.96388
1:12:46.2	Data point 124	0.22001 mL	0.17357 mL	0.17493 mL	1.35995 mL	0.02500 mL	10.374	0.03127	0.97579	0.97579
1:13:08.0	Data point 125	0.22001 mL	0.17357 mL	0.17512 mL	1.35995 mL	0.02500 mL	10.471	0.02270	0.92505	0.92505
1:13:24.5	Data point 126	0.22001 mL	0.17357 mL	0.17535 mL	1.35995 mL	0.02500 mL	10.611	0.00710	0.58930	0.58930
1:13:51.3	Data point 127	0.22001 mL	0.17357 mL	0.17571 mL	1.35995 mL	0.02500 mL	10.706	0.00434	0.57881	0.57881
1:14:07.8	Data point 128	0.22001 mL	0.17357 mL	0.17611 mL	1.35995 mL	0.02500 mL	10.823	0.00120	0.10770	0.10770
1:14:34.6	Data point 129	0.22001 mL	0.17357 mL	0.17662 mL	1.35995 mL	0.02500 mL	10.914	-0.00202	0.17683	0.17683
1:14:51.3	Data point 130	0.22001 mL	0.17357 mL	0.17726 mL	1.35995 mL	0.02500 mL	11.019	-0.00067	0.04360	0.04360
1:15:08.0	Data point 131	0.22001 mL	0.17357 mL	0.17806 mL	1.35995 mL	0.02500 mL	11.109	-0.00305	0.46181	0.46181
1:15:24.7	Data point 132	0.22001 mL	0.17357 mL	0.17905 mL	1.35995 mL	0.02500 mL	11.196	-0.00478	0.52244	0.52244
1:15:41.4	Data point 133	0.22001 mL	0.17357 mL	0.18024 mL	1.35995 mL	0.02500 mL	11.280	-0.00422	0.53639	0.53639
1:16:08.3	Data point 134	0.22001 mL	0.17357 mL	0.18210 mL	1.35995 mL	0.02500 mL	11.375	-0.00623	0.78350	0.78350
1:16:35.2	Data point 135	0.22001 mL	0.17357 mL	0.18391 mL	1.35995 mL	0.02500 mL	11.471	-0.00609	0.57615	0.57615
1:16:51.8	Data point 136	0.22001 mL	0.17357 mL	0.18620 mL	1.35995 mL	0.02500 mL	11.573	-0.00486	0.47651	0.47651
1:17:08.5	Data point 137	0.22001 mL	0.17357 mL	0.18906 mL	1.35995 mL	0.02500 mL	11.662	-0.00870	0.75230	0.75230
1:17:25.1	Data point 138	0.22001 mL	0.17357 mL	0.19262 mL	1.35995 mL	0.02500 mL	11.751	-0.00567	0.56134	0.56134
1:17:41.9	Data point 139	0.22001 mL	0.17357 mL	0.19701 mL	1.35995 mL	0.02500 mL	11.846	-0.00670	0.68052	0.68052
1:17:58.7	Data point 140	0.22001 mL	0.17357 mL	0.20252 mL	1.35995 mL	0.02500 mL	11.933	-0.00651	0.69858	0.69858
1:18:15.5	Data point 141	0.22001 mL	0.17357 mL	0.20934 mL	1.35995 mL	0.02500 mL	12.023	-0.00662	0.62301	0.62301
1:19:57.7	Reference spectrum									
1:21:18.1	Data point 143	0.39005 mL	0.28937 mL	0.20936 mL	1.35995 mL	0.02500 mL	1.994	-0.06312	0.95809	0.95809
1:21:45.5	Data point 144	0.39005 mL	0.28937 mL	0.22601 mL	1.35995 mL	0.02500 mL	2.094	0.00265	0.22562	0.22562
1:22:02.4	Data point 145	0.39005 mL	0.28937 mL	0.24017 mL	1.35995 mL	0.02500 mL	2.214	0.00910	0.51039	0.51039
1:22:24.4	Data point 146	0.39005 mL	0.28937 mL	0.24887 mL	1.35995 mL	0.02500 mL	2.305	-0.00065	0.00526	0.00526
1:22:46.3	Data point 147	0.39005 mL	0.28937 mL	0.25595 mL	1.35995 mL	0.02500 mL	2.396	0.00272	0.10301	0.10301
1:23:13.3	Data point 148	0.39005 mL	0.28937 mL	0.26199 mL	1.35995 mL	0.02500 mL	2.495	0.01152	0.85129	0.85129
1:23:30.0	Data point 149	0.39005 mL	0.28937 mL	0.26759 mL	1.35995 mL	0.02500 mL	2.610	0.00769	0.82578	0.82578
1:23:46.7	Data point 150	0.39005 mL	0.28937 mL	0.27190 mL	1.35995 mL	0.02500 mL	2.714	0.00806	0.78455	0.78455
1:24:03.3	Data point 151	0.39005 mL	0.28937 mL	0.27528 mL	1.35995 mL	0.02500 mL	2.822	0.00497	0.48302	0.48302
1:24:19.9	Data point 152	0.39005 mL	0.28937 mL	0.27792 mL	1.35995 mL	0.02500 mL	2.940	0.01203	0.86286	0.86286
1:24:46.8	Data point 153	0.39005 mL	0.28937 mL	0.27994 mL	1.35995 mL	0.02500 mL	3.037	0.00616	0.55426	0.55426
1:25:19.1	Data point 154	0.39005 mL	0.28937 mL	0.28154 mL	1.35995 mL	0.02500 mL	3.150	0.00338	0.23438	0.23438
1:25:35.7	Data point 155	0.39005 mL	0.28937 mL	0.28279 mL	1.35995 mL	0.02500 mL	3.170	0.00763	0.70403	0.70403
1:26:02.5	Data point 156	0.39005 mL	0.28937 mL	0.28417 mL	1.35995 mL	0.02500 mL	3.265	0.00478	0.40737	0.40737
1:26:29.4	Data point 157	0.39005 mL	0.28937 mL	0.28504 mL	1.35995 mL	0.02500 mL	3.357	0.00860	0.84689	0.84689
1:26:46.0	Data point 158	0.39005 mL	0.28937 mL	0.28582 mL	1.35995 mL	0.02500 mL	3.528	0.00556	0.49429	0.49429
1:27:07.8	Data point 159	0.39005 mL	0.28937 mL	0.28634 mL	1.35995 mL	0.02500 mL	3.643	0.01601	0.93818	0.93818
1:27:24.4	Data point 160	0.39005 mL	0.28937 mL	0.28674 mL	1.35995 mL	0.02500 mL	3.752	0.01762	0.94213	0.94213
1:27:40.9	Data point 161	0.39005 mL	0.28937 mL	0.28704 mL	1.35995 mL	0.02500 mL	3.846	0.02248	0.96187	0.96187
1:27:57.4	Data point 162	0.39005 mL	0.28937 mL	0.28728 mL	1.35995 mL	0.02500 mL	3.931	0.02934	0.94979	0.94979
1:28:13.9	Data point 163	0.39005 mL	0.28937 mL	0.28747 mL	1.35995 mL	0.02500 mL	4.013	0.04482	0.98703	0.98703

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07004**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07004_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 4:49:57 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
1:28:35.5	Data point 164	0.39005 mL	0.28937 mL	0.28770 mL	1.35995 mL	0.02500 mL	4.154	0.04876	0.96883	0.0024
1:28:57.2	Data point 165	0.39005 mL	0.28937 mL	0.28791 mL	1.35995 mL	0.02500 mL	4.322	0.07526	0.98803	0.0037
1:29:18.8	Data point 166	0.39005 mL	0.28937 mL	0.28805 mL	1.35995 mL	0.02500 mL	4.460	0.09854	0.98587	0.0049
1:29:42.5	Data point 167	0.39005 mL	0.28937 mL	0.28815 mL	1.35995 mL	0.02500 mL	4.599	0.10010	0.98508	0.0049
1:30:10.5	Data point 168	0.39005 mL	0.28937 mL	0.28822 mL	1.35995 mL	0.02500 mL	4.747	0.09795	0.98469	0.0048
1:30:47.7	Data point 169	0.39005 mL	0.28937 mL	0.28829 mL	1.35995 mL	0.02500 mL	4.933	0.09985	0.99201	0.0049
1:31:33.5	Data point 170	0.39005 mL	0.28937 mL	0.28836 mL	1.35995 mL	0.02500 mL	5.261	0.09777	0.96998	0.0049
1:32:36.9	Data point 171	0.39005 mL	0.28937 mL	0.28843 mL	1.35995 mL	0.02500 mL	5.768	0.09838	0.98911	0.0048
1:33:38.5	Data point 172	0.39005 mL	0.28937 mL	0.28848 mL	1.35995 mL	0.02500 mL	6.088	0.09353	0.93697	0.0047
1:34:31.8	Data point 173	0.39005 mL	0.28937 mL	0.28852 mL	1.35995 mL	0.02500 mL	6.326	0.09986	0.99080	0.0049
1:35:20.4	Data point 174	0.39005 mL	0.28937 mL	0.28859 mL	1.35995 mL	0.02500 mL	6.618	0.09939	0.98154	0.0049
1:36:06.1	Data point 175	0.39005 mL	0.28937 mL	0.28866 mL	1.35995 mL	0.02500 mL	6.829	0.09960	0.98314	0.0049
1:36:42.8	Data point 176	0.39005 mL	0.28937 mL	0.28874 mL	1.35995 mL	0.02500 mL	7.012	0.09671	0.96719	0.0048
1:37:13.0	Data point 177	0.39005 mL	0.28937 mL	0.28880 mL	1.35995 mL	0.02500 mL	7.159	0.10048	0.98846	0.0049
1:37:46.1	Data point 178	0.39005 mL	0.28937 mL	0.28888 mL	1.35995 mL	0.02500 mL	7.306	0.09850	0.97756	0.0049
1:38:20.9	Data point 179	0.39005 mL	0.28937 mL	0.28897 mL	1.35995 mL	0.02500 mL	7.465	0.09693	0.97329	0.0048
1:38:54.2	Data point 180	0.39005 mL	0.28937 mL	0.28906 mL	1.35995 mL	0.02500 mL	7.624	0.09869	0.97717	0.0049
1:39:33.6	Data point 181	0.39005 mL	0.28937 mL	0.28916 mL	1.35995 mL	0.02500 mL	7.793	0.10034	0.98344	0.0050
1:40:13.1	Data point 182	0.39005 mL	0.28937 mL	0.28925 mL	1.35995 mL	0.02500 mL	7.958	0.09494	0.98647	0.0047
1:40:52.9	Data point 183	0.39005 mL	0.28937 mL	0.28935 mL	1.35995 mL	0.02500 mL	8.166	0.09911	0.98938	0.0049
1:41:32.7	Data point 184	0.39005 mL	0.28937 mL	0.28942 mL	1.35995 mL	0.02500 mL	8.336	0.09802	0.98182	0.0048
1:42:12.6	Data point 185	0.39005 mL	0.28937 mL	0.28949 mL	1.35995 mL	0.02500 mL	8.515	0.09447	0.97854	0.0047
1:42:58.3	Data point 186	0.39005 mL	0.28937 mL	0.28958 mL	1.35995 mL	0.02500 mL	8.767	0.09714	0.96760	0.0048
1:43:40.1	Data point 187	0.39005 mL	0.28937 mL	0.28965 mL	1.35995 mL	0.02500 mL	8.957	0.09927	0.98638	0.0049
1:44:19.9	Data point 188	0.39005 mL	0.28937 mL	0.28972 mL	1.35995 mL	0.02500 mL	9.141	0.09629	0.98501	0.0047
1:44:59.6	Data point 189	0.39005 mL	0.28937 mL	0.28979 mL	1.35995 mL	0.02500 mL	9.295	0.09739	0.97467	0.0048
1:45:36.4	Data point 190	0.39005 mL	0.28937 mL	0.28986 mL	1.35995 mL	0.02500 mL	9.437	0.09638	0.98029	0.0048
1:46:12.8	Data point 191	0.39005 mL	0.28937 mL	0.28996 mL	1.35995 mL	0.02500 mL	9.593	0.09639	0.99262	0.0047
1:46:43.6	Data point 192	0.39005 mL	0.28937 mL	0.29005 mL	1.35995 mL	0.02500 mL	9.716	0.09522	0.96958	0.0047
1:47:11.5	Data point 193	0.39005 mL	0.28937 mL	0.29017 mL	1.35995 mL	0.02500 mL	9.834	0.09342	0.94401	0.0047
1:47:33.1	Data point 194	0.39005 mL	0.28937 mL	0.29029 mL	1.35995 mL	0.02500 mL	9.938	0.07033	0.95551	0.0035
1:47:59.9	Data point 195	0.39005 mL	0.28937 mL	0.29043 mL	1.35995 mL	0.02500 mL	10.054	0.05834	0.97284	0.0029
1:48:21.6	Data point 196	0.39005 mL	0.28937 mL	0.29059 mL	1.35995 mL	0.02500 mL	10.151	0.03635	0.91530	0.0018
1:48:48.4	Data point 197	0.39005 mL	0.28937 mL	0.29080 mL	1.35995 mL	0.02500 mL	10.253	0.02853	0.95678	0.0014
1:49:10.2	Data point 198	0.39005 mL	0.28937 mL	0.29109 mL	1.35995 mL	0.02500 mL	10.364	0.01617	0.89631	0.0008
1:49:37.0	Data point 199	0.39005 mL	0.28937 mL	0.29151 mL	1.35995 mL	0.02500 mL	10.462	0.01458	0.89293	0.0007
1:50:03.8	Data point 200	0.39005 mL	0.28937 mL	0.29233 mL	1.35995 mL	0.02500 mL	10.609	0.00199	0.26441	0.0001
1:50:25.5	Data point 201	0.39005 mL	0.28937 mL	0.29297 mL	1.35995 mL	0.02500 mL	10.729	-0.00219	0.23986	0.0002
1:50:57.5	Data point 202	0.39005 mL	0.28937 mL	0.29372 mL	1.35995 mL	0.02500 mL	10.831	0.00119	0.07419	0.0002
1:51:24.3	Data point 203	0.39005 mL	0.28937 mL	0.29445 mL	1.35995 mL	0.02500 mL	10.940	-0.00472	0.52191	0.0003
1:51:40.9	Data point 204	0.39005 mL	0.28937 mL	0.29537 mL	1.35995 mL	0.02500 mL	11.069	-0.00896	0.83044	0.0004
1:52:07.7	Data point 205	0.39005 mL	0.28937 mL	0.29652 mL	1.35995 mL	0.02500 mL	11.163	-0.00718	0.76075	0.0004
1:52:24.3	Data point 206	0.39005 mL	0.28937 mL	0.29802 mL	1.35995 mL	0.02500 mL	11.255	-0.00889	0.80874	0.0004
1:52:40.9	Data point 207	0.39005 mL	0.28937 mL	0.29991 mL	1.35995 mL	0.02500 mL	11.341	-0.00676	0.75978	0.0003
1:52:57.6	Data point 208	0.39005 mL	0.28937 mL	0.30219 mL	1.35995 mL	0.02500 mL	11.410	-0.00817	0.67238	0.0004
1:53:24.5	Data point 209	0.39005 mL	0.28937 mL	0.30489 mL	1.35995 mL	0.02500 mL	11.505	-0.00665	0.75082	0.0003
1:53:41.2	Data point 210	0.39005 mL	0.28937 mL	0.30826 mL	1.35995 mL	0.02500 mL	11.601	-0.00874	0.83035	0.0004
1:53:57.9	Data point 211	0.39005 mL	0.28937 mL	0.31246 mL	1.35995 mL	0.02500 mL	11.683	-0.00902	0.74631	0.0005
1:54:25.0	Data point 212	0.39005 mL	0.28937 mL	0.31755 mL	1.35995 mL	0.02500 mL	11.778	-0.00633	0.67234	0.0003
1:54:41.7	Data point 213	0.39005 mL	0.28937 mL	0.32394 mL	1.35995 mL	0.02500 mL	11.863	-0.00822	0.82961	0.0004
1:54:58.4	Data point 214	0.39005 mL	0.28937 mL	0.33184 mL	1.35995 mL	0.02500 mL	11.950	-0.01164	0.73166	0.0006
1:55:15.3	Data point 215	0.39005 mL	0.28937 mL	0.34156 mL	1.35995 mL	0.02500 mL	12.037	-0.00884	0.77753	0.0005
1:57:14.5	Assay volumes	0.64005 mL	0.42192 mL	0.34156 mL	1.35995 mL	0.02500 mL				

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07004**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07004_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 4:49:57 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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	0.100			
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%			
Titration Pre-Dose				
Titration pre-dose	None			
Assay Medium				
Cosolvent in use	Yes			
Cosolvent type	Methanol			
Cosolvent volume	1.35 mL			
Cosolvent added	Automatic			
ISA water volume	0.15 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				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.07 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Titration 3				
Titrate from	Low to high pH			

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07004**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07004_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 4:49:57 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Additional cosolvent volume	0.00 mL			
Add additional water	0.17 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	0.161	10/7/2017 4:49:57 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus S	0.9927	10/7/2017 4:49:57 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus jH	0.5	10/7/2017 4:49:57 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus jOH	-0.7	10/7/2017 4:49:57 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Base concentration factor	1.011	10/7/2017 4:49:57 AM	C:\Sirius_T3\KOH17122.t3r
Acid concentration factor	1.003	10/7/2017 4:49:57 AM	C:\Sirius_T3\17J-06018_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 and 172875	10/6/2017 2:55:40 PM
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	10/5/2017 5:02:03 PM
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
Dispenser 3	Buffer		8/3/2010 6:05:16 AM

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07004**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07004_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 4:49:57 AM**
 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	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	-7.88 mV		10/7/2017 4:50:21 AM
Filling solution	3M KCl	KCL095	10/4/2017 3:50:10 PM
Liquids			
Wash 1	50% IPA:50% Water		10/6/2017 2:50:08 PM
Wash 2	0.5% Triton X-100 in H2O		10/6/2017 2:50:11 PM
Buffer position 1	pH7 Wash		10/6/2017 2:50:17 PM
Buffer position 2	pH 7		10/6/2017 2:50:19 PM
Storage position			10/6/2017 2:50:25 PM
Wash water	8.8e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	1.2e+003 mL		10/6/2017 3:04:33 PM
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	391:10:29		11/23/2010 12:22:28 PM
Calibrated on	10/5/2017 10:23:25 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		
E0 calibration stir duration	5 s		



Assay Settings

Sample name: **D07** Experiment start time: **10/7/2017 4:49:57 AM**
Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse**
Assay ID: **17J-07004** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07004_D07_UV-metric psKa.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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 F3