

Sample name: **D08**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07006**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07006_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 8:42:52 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

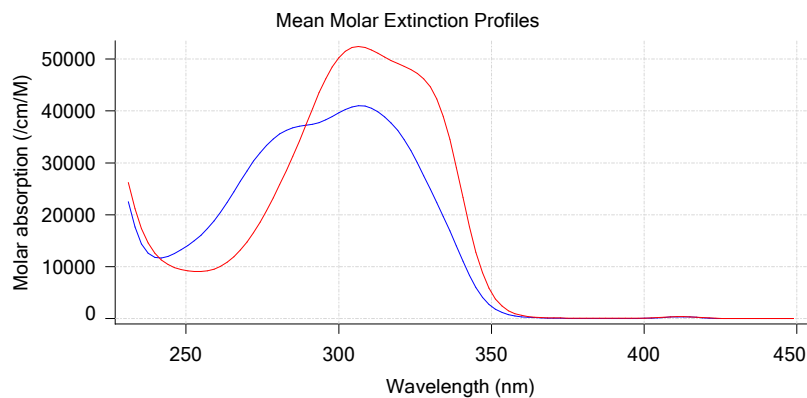
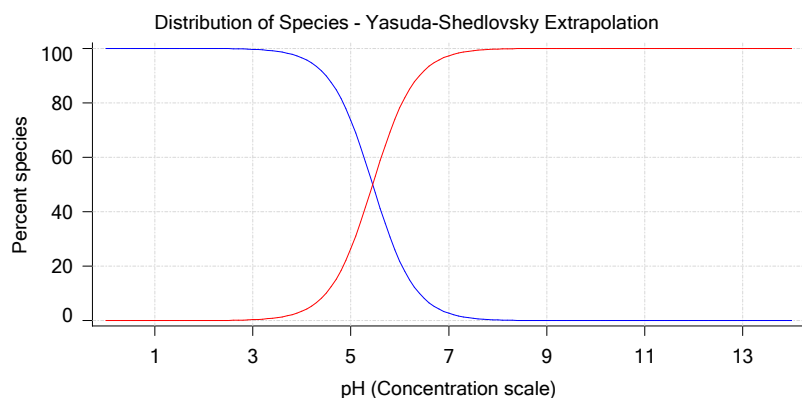
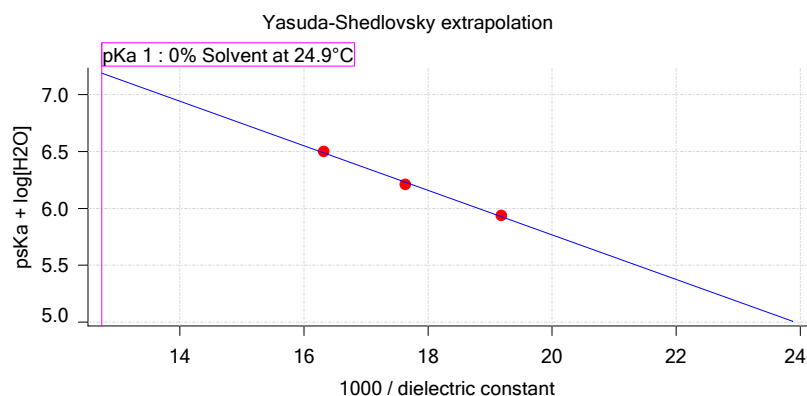
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.45	±0.06	9.68	-195.8810	0.9960	0.167 M	24.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1
17J-07006 Points 4 to 58	58.99 %	Up	UV-metric pKa	52.1	19.6 M	0.158 M	24.9°C	✓ 4.64
17J-07006 Points 60 to 130	49.30 %	Up	UV-metric pKa	56.7	24.8 M	0.168 M	24.9°C	✓ 4.81
17J-07006 Points 132 to 203	39.42 %	Up	UV-metric pKa	61.3	30.3 M	0.176 M	24.9°C	✓ 5.02

Graphs



UV-metric psKa Titration 1 of 3 17J-07006 Points 4 to 58

Results

pKa 1	4.64
RMSD	0.004 0.002
Chi squared	0.0110
PCA calculated number of pKas	3
Average ionic strength	0.158 M
Average temperature	24.9°C
Analyte concentration range	29.3 µM to 27.4 µM
Methanol weight %	59.0 %
Dielectric constant	52.1
Water concentration	19.6 M
Number of pKas source	Predicted
Wavelength clipping	230.0 nm to 450.0 nm

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Results (continued)

pH clipping 1.470 to 12.515

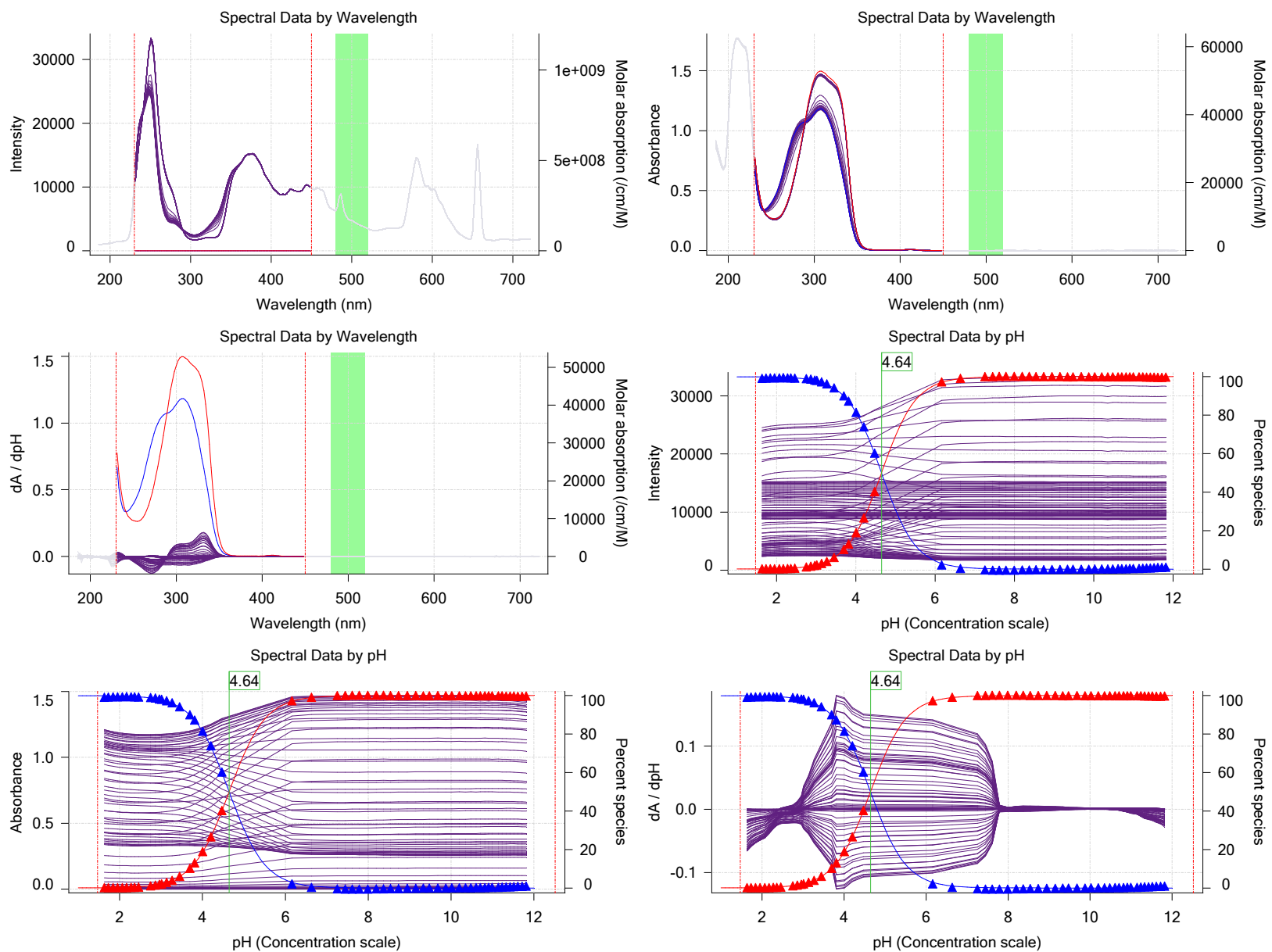
Warnings and errors

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			

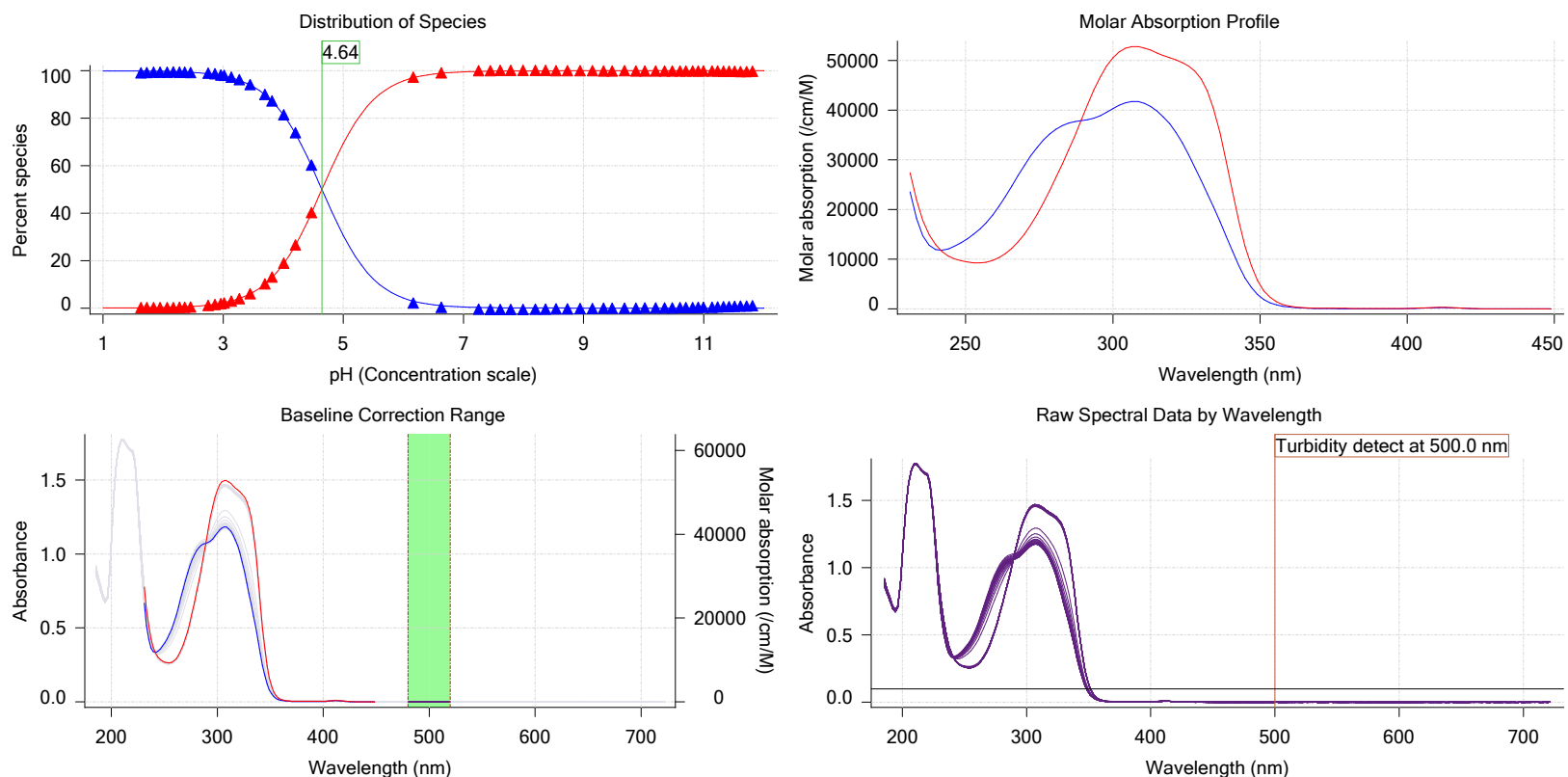
Graphs



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Graphs (continued)



UV-metric psKa Titration 2 of 3 17J-07006 Points 60 to 130

Results

pKa 1	4.81
RMSD	0.003 0.002
Chi squared	0.0039
PCA calculated number of pKas	4
Average ionic strength	0.168 M
Average temperature	24.9°C
Analyte concentration range	24.9 µM to 23.4 µM
Methanol weight %	49.3 %
Dielectric constant	56.7
Water concentration	24.8 M
Number of pKas source	Predicted
Wavelength clipping	230.0 nm to 450.0 nm
pH clipping	1.437 to 12.533

Warnings and errors

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

Assay Settings

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

Assay Medium

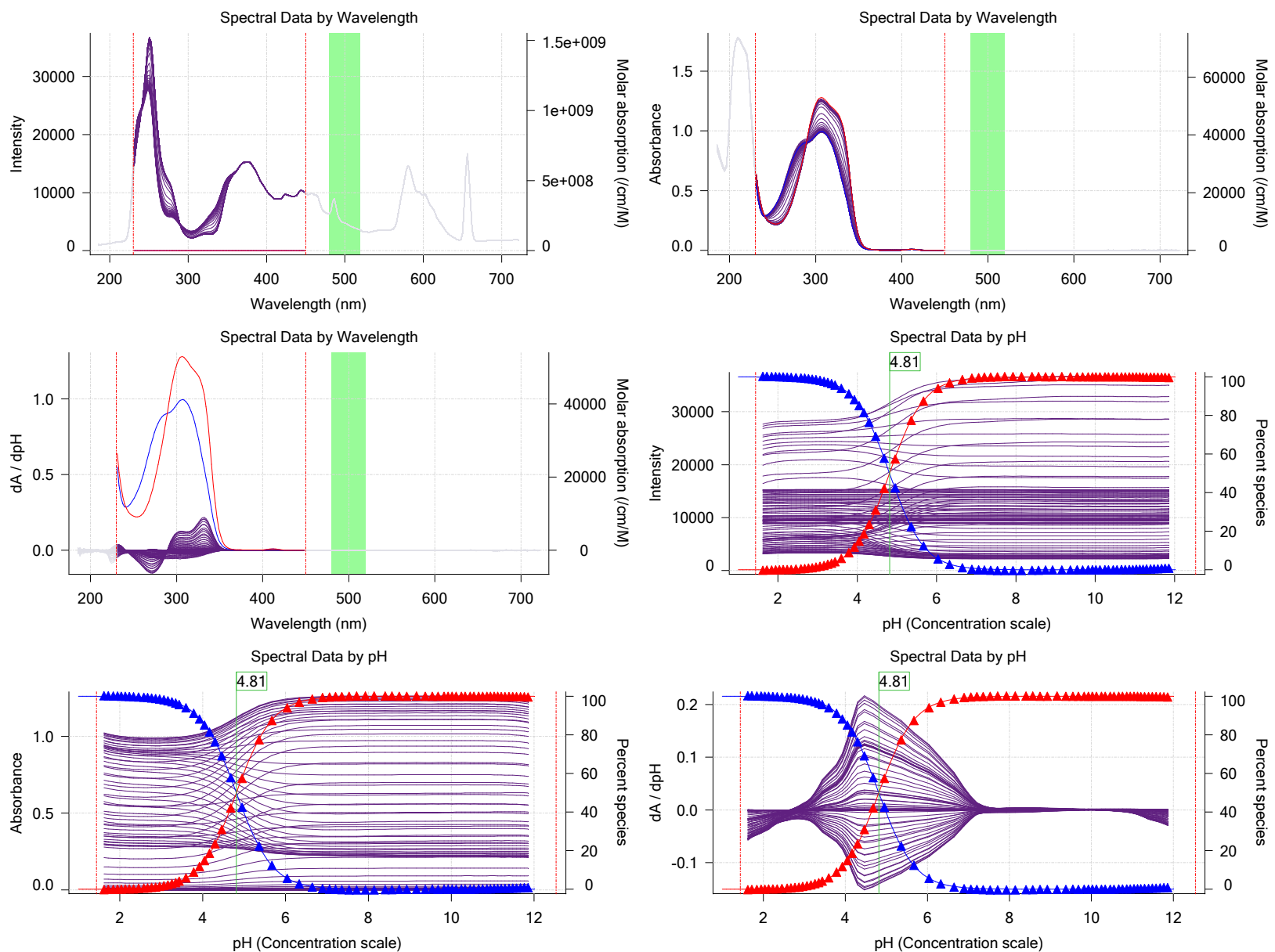
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Experiment start time: **10/7/2017 8:42:52 AM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Assay Settings (continued)

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

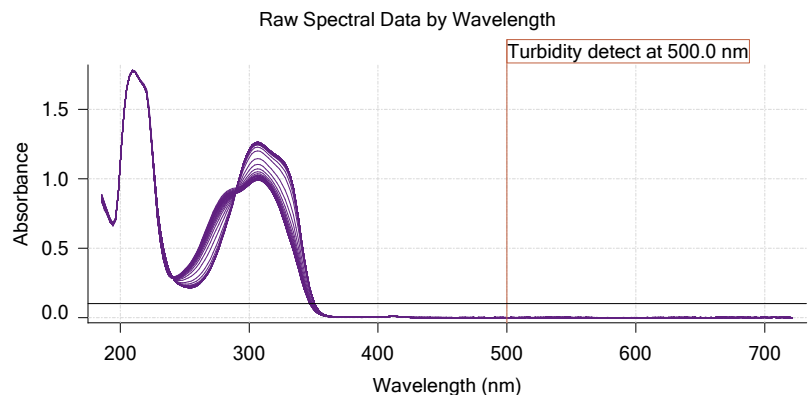
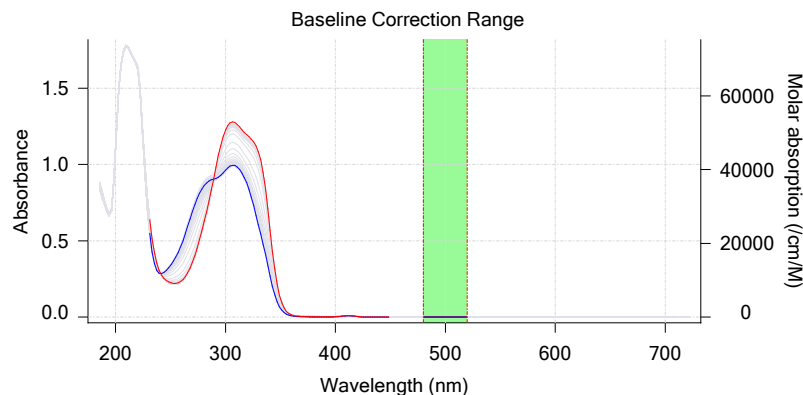
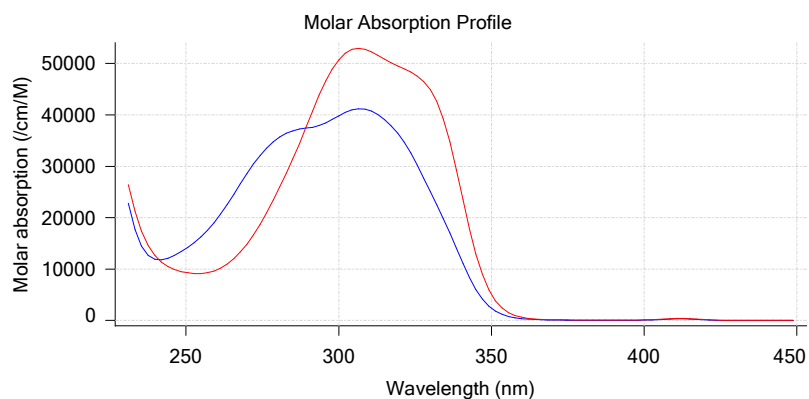
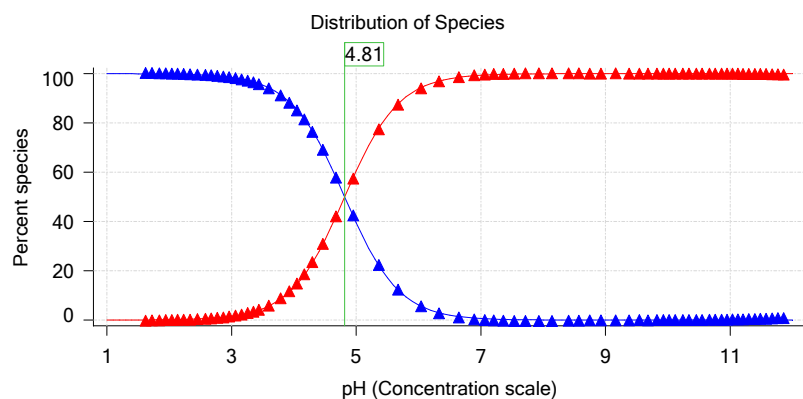
Graphs



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Analyst: **Dorothy Leverse**
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Graphs (continued)



UV-metric psKa Titration 3 of 3 17J-07006 Points 132 to 203

Results

pKa 1	5.02
RMSD	0.005 0.004
Chi squared	0.0141
PCA calculated number of pKas	5
Average ionic strength	0.176 M
Average temperature	24.9°C
Analyte concentration range	20.3 µM to 19.1 µM
Methanol weight %	39.4 %
Dielectric constant	61.3
Water concentration	30.3 M
Number of pKas source	Predicted
Wavelength clipping	230.0 nm to 450.0 nm
pH clipping	1.429 to 12.546

Warnings and errors

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

Assay Settings

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

Assay Medium

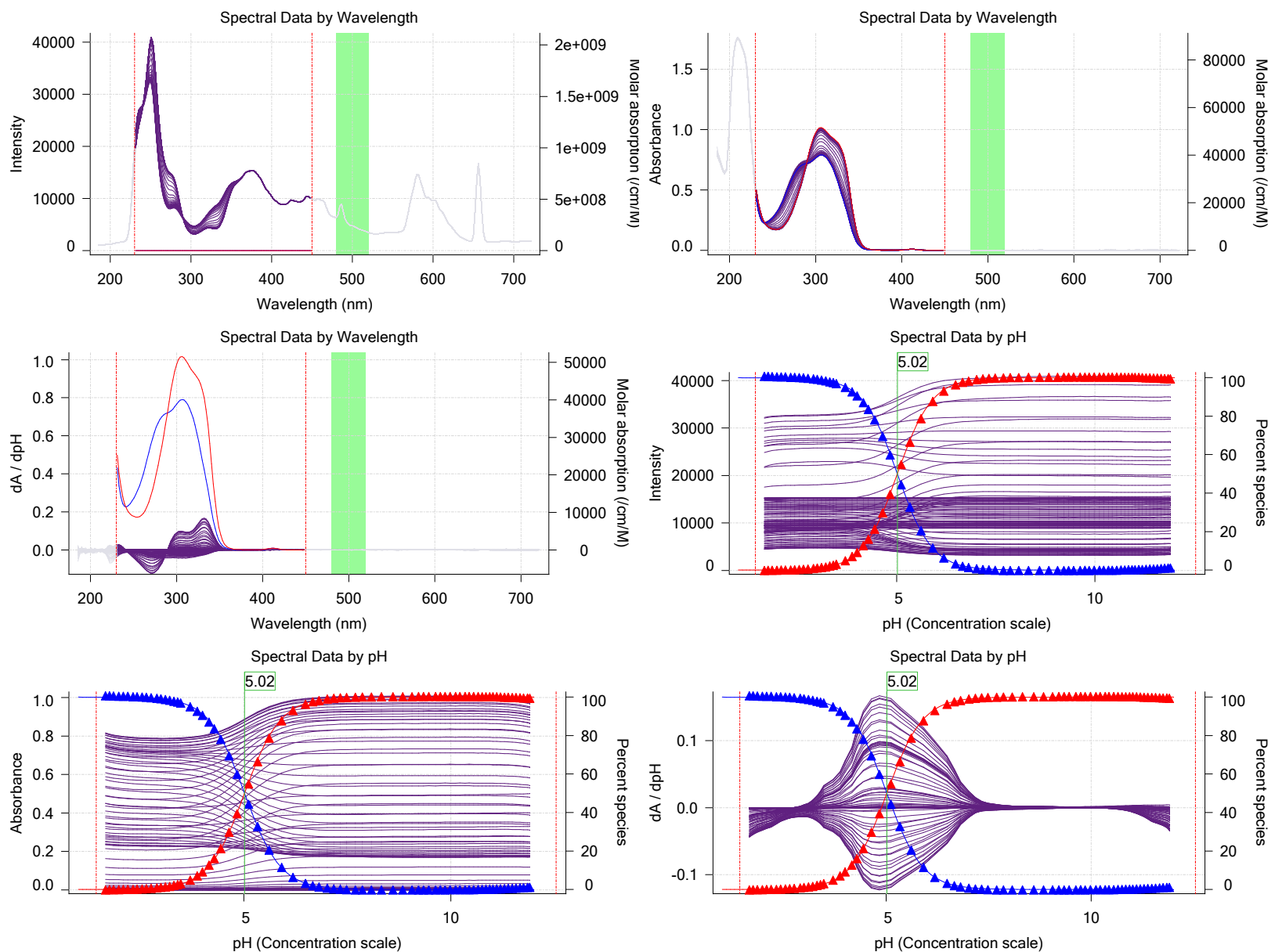
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Experiment start time: **10/7/2017 8:42:52 AM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Assay Settings (continued)

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

Graphs

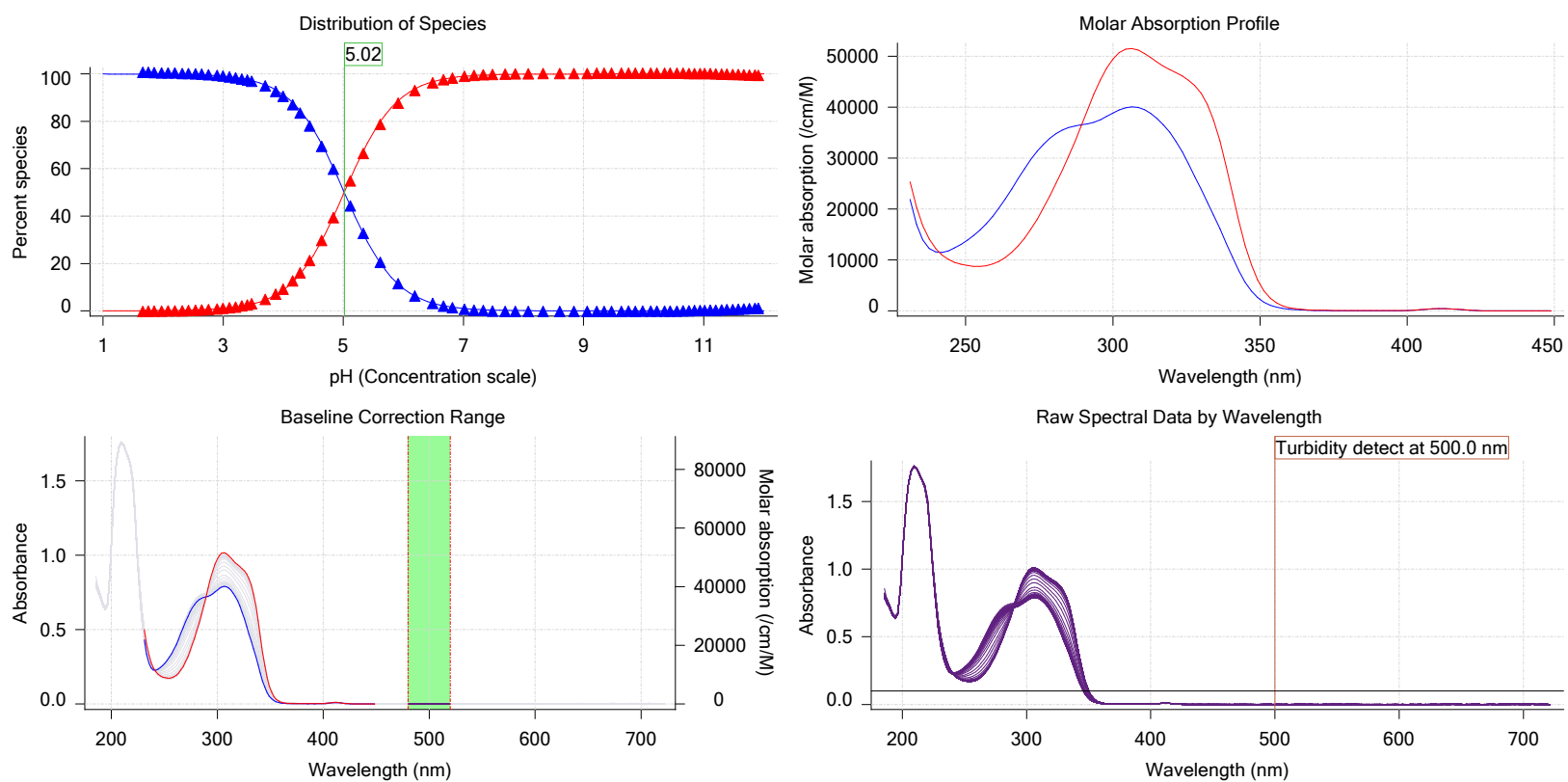


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Instrument ID: **T311053**

Graphs (continued)



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	D08	10/2/2017 12:57:31 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0010 mL	10/6/2017 6:10:30 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.047100 M	10/2/2017 12:59:19 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	420.46	9/29/2017 6:40:43 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	9/29/2017 6:40:34 PM	User entered value
Sample is a	Base	9/29/2017 6:40:34 PM	User entered value
pKa 1	6.16	9/29/2017 6:40:34 PM	User entered value
logp (XH +)	-10.00		Default value
logP (neutral X)	-10.00	9/29/2017 6:40:34 PM	User entered value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-square
3:09.6	Dark spectrum								
3:11.0	Reference spectrum								
3:38.7	Volume reset due to vial change								
8:43.1	Initial pH = 7.97								
9:02.2	Data point 4	0.15005 mL	0.07338 mL	0.00000 mL	1.35995 mL	0.02500 mL	1.970	-0.04515	0.98029
9:30.7	Data point 5	0.15005 mL	0.07338 mL	0.01583 mL	1.35995 mL	0.02500 mL	2.071	0.00844	0.23845
9:47.5	Data point 6	0.15005 mL	0.07338 mL	0.02822 mL	1.35995 mL	0.02500 mL	2.181	-0.00362	0.10685
10:04.5	Data point 7	0.15005 mL	0.07338 mL	0.03782 mL	1.35995 mL	0.02500 mL	2.289	0.00689	0.75600
10:21.2	Data point 8	0.15005 mL	0.07338 mL	0.04532 mL	1.35995 mL	0.02500 mL	2.406	0.00701	0.71076
10:48.4	Data point 9	0.15005 mL	0.07338 mL	0.05151 mL	1.35995 mL	0.02500 mL	2.509	0.00758	0.68741

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Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
11:05.2	Data point 10	0.15005 mL	0.07338 mL	0.05607 mL	1.35995 mL	0.02500 mL	2.613	0.01376	0.88647	0.00
11:21.9	Data point 11	0.15005 mL	0.07338 mL	0.05964 mL	1.35995 mL	0.02500 mL	2.697	0.01879	0.89563	0.00
11:43.8	Data point 12	0.15005 mL	0.07338 mL	0.06171 mL	1.35995 mL	0.02500 mL	2.794	0.03688	0.94026	0.00
12:21.4	Data point 13	0.15005 mL	0.07338 mL	0.07352 mL	1.35995 mL	0.02500 mL	3.083	0.01372	0.83028	0.00
12:53.5	Data point 14	0.15005 mL	0.07338 mL	0.07488 mL	1.35995 mL	0.02500 mL	3.191	0.01403	0.94181	0.00
13:10.2	Data point 15	0.15005 mL	0.07338 mL	0.07582 mL	1.35995 mL	0.02500 mL	3.289	0.01621	0.93330	0.00
13:26.8	Data point 16	0.15005 mL	0.07338 mL	0.07658 mL	1.35995 mL	0.02500 mL	3.343	0.01874	0.94657	0.00
13:48.6	Data point 17	0.15005 mL	0.07338 mL	0.07745 mL	1.35995 mL	0.02500 mL	3.463	0.01641	0.93665	0.00
14:10.3	Data point 18	0.15005 mL	0.07338 mL	0.07813 mL	1.35995 mL	0.02500 mL	3.593	0.03448	0.98699	0.00
14:32.0	Data point 19	0.15005 mL	0.07338 mL	0.07874 mL	1.35995 mL	0.02500 mL	3.771	0.08917	0.99469	0.00
14:53.7	Data point 20	0.15005 mL	0.07338 mL	0.07916 mL	1.35995 mL	0.02500 mL	4.015	0.07429	0.98890	0.00
15:15.5	Data point 21	0.15005 mL	0.07338 mL	0.07942 mL	1.35995 mL	0.02500 mL	4.130	0.10060	0.99486	0.00
15:45.2	Data point 22	0.15005 mL	0.07338 mL	0.07961 mL	1.35995 mL	0.02500 mL	4.322	0.10023	0.99335	0.00
16:24.8	Data point 23	0.15005 mL	0.07338 mL	0.07973 mL	1.35995 mL	0.02500 mL	4.514	0.07939	0.76705	0.00
17:15.6	Data point 24	0.15005 mL	0.07338 mL	0.07987 mL	1.35995 mL	0.02500 mL	4.777	0.09874	0.98614	0.00
18:13.4	Data point 25	0.15005 mL	0.07338 mL	0.08006 mL	1.35995 mL	0.02500 mL	6.446	0.32526	0.97802	0.00
19:30.1	Data point 26	0.15005 mL	0.07338 mL	0.08020 mL	1.35995 mL	0.02500 mL	6.911	0.09791	0.97980	0.00
20:23.8	Data point 27	0.15005 mL	0.07338 mL	0.08024 mL	1.35995 mL	0.02500 mL	7.523	0.09742	0.96381	0.00
21:27.4	Data point 28	0.15005 mL	0.07338 mL	0.08036 mL	1.35995 mL	0.02500 mL	7.712	0.09757	0.99076	0.00
22:12.3	Data point 29	0.15005 mL	0.07338 mL	0.08046 mL	1.35995 mL	0.02500 mL	7.877	0.09383	0.95664	0.00
22:57.9	Data point 30	0.15005 mL	0.07338 mL	0.08055 mL	1.35995 mL	0.02500 mL	8.047	0.09820	0.98539	0.00
23:53.3	Data point 31	0.15005 mL	0.07338 mL	0.08067 mL	1.35995 mL	0.02500 mL	8.249	0.09969	0.99259	0.00
24:50.4	Data point 32	0.15005 mL	0.07338 mL	0.08079 mL	1.35995 mL	0.02500 mL	8.450	0.09919	0.98585	0.00
25:35.0	Data point 33	0.15005 mL	0.07338 mL	0.08088 mL	1.35995 mL	0.02500 mL	8.620	0.09937	0.98182	0.00
26:08.1	Data point 34	0.15005 mL	0.07338 mL	0.08095 mL	1.35995 mL	0.02500 mL	8.791	0.09790	0.94302	0.00
26:41.4	Data point 35	0.15005 mL	0.07338 mL	0.08102 mL	1.35995 mL	0.02500 mL	8.980	0.09725	0.94103	0.00
27:14.5	Data point 36	0.15005 mL	0.07338 mL	0.08109 mL	1.35995 mL	0.02500 mL	9.186	0.09181	0.90697	0.00
27:47.6	Data point 37	0.15005 mL	0.07338 mL	0.08116 mL	1.35995 mL	0.02500 mL	9.390	0.08623	0.91636	0.00
28:19.9	Data point 38	0.15005 mL	0.07338 mL	0.08123 mL	1.35995 mL	0.02500 mL	9.571	0.09321	0.88635	0.00
28:51.7	Data point 39	0.15005 mL	0.07338 mL	0.08130 mL	1.35995 mL	0.02500 mL	9.712	0.09216	0.94528	0.00
29:23.0	Data point 40	0.15005 mL	0.07338 mL	0.08140 mL	1.35995 mL	0.02500 mL	9.916	0.09231	0.95220	0.00
29:57.9	Data point 41	0.15005 mL	0.07338 mL	0.08151 mL	1.35995 mL	0.02500 mL	10.103	0.09254	0.92116	0.00
30:29.6	Data point 42	0.15005 mL	0.07338 mL	0.08166 mL	1.35995 mL	0.02500 mL	10.250	0.09330	0.88388	0.00
30:53.8	Data point 43	0.15005 mL	0.07338 mL	0.08184 mL	1.35995 mL	0.02500 mL	10.424	0.09607	0.98010	0.00
31:17.4	Data point 44	0.15005 mL	0.07338 mL	0.08208 mL	1.35995 mL	0.02500 mL	10.572	0.07344	0.98157	0.00
31:39.2	Data point 45	0.15005 mL	0.07338 mL	0.08238 mL	1.35995 mL	0.02500 mL	10.701	0.05108	0.96223	0.00
32:00.9	Data point 46	0.15005 mL	0.07338 mL	0.08278 mL	1.35995 mL	0.02500 mL	10.828	0.02871	0.97421	0.00
32:27.7	Data point 47	0.15005 mL	0.07338 mL	0.08325 mL	1.35995 mL	0.02500 mL	10.924	0.02164	0.97032	0.00
32:44.3	Data point 48	0.15005 mL	0.07338 mL	0.08377 mL	1.35995 mL	0.02500 mL	11.031	-0.00132	0.05719	0.00
33:00.9	Data point 49	0.15005 mL	0.07338 mL	0.08443 mL	1.35995 mL	0.02500 mL	11.124	0.00319	0.38230	0.00
33:17.3	Data point 50	0.15005 mL	0.07338 mL	0.08525 mL	1.35995 mL	0.02500 mL	11.208	0.00286	0.36973	0.00
33:44.3	Data point 51	0.15005 mL	0.07338 mL	0.08723 mL	1.35995 mL	0.02500 mL	11.354	-0.00047	0.01838	0.00
34:06.0	Data point 52	0.15005 mL	0.07338 mL	0.08841 mL	1.35995 mL	0.02500 mL	11.445	-0.00580	0.66541	0.00
34:27.8	Data point 53	0.15005 mL	0.07338 mL	0.08970 mL	1.35995 mL	0.02500 mL	11.537	-0.00342	0.44702	0.00
34:54.8	Data point 54	0.15005 mL	0.07338 mL	0.09170 mL	1.35995 mL	0.02500 mL	11.631	-0.00096	0.03736	0.00
35:11.5	Data point 55	0.15005 mL	0.07338 mL	0.09436 mL	1.35995 mL	0.02500 mL	11.723	-0.00376	0.41745	0.00
35:28.2	Data point 56	0.15005 mL	0.07338 mL	0.09767 mL	1.35995 mL	0.02500 mL	11.818	-0.00498	0.55233	0.00
35:44.8	Data point 57	0.15005 mL	0.07338 mL	0.10181 mL	1.35995 mL	0.02500 mL	11.920	-0.00204	0.05097	0.00
36:01.6	Data point 58	0.15005 mL	0.07338 mL	0.10708 mL	1.35995 mL	0.02500 mL	12.015	-0.00558	0.56866	0.00
37:42.6	Reference spectrum									
38:45.3	Data point 60	0.22001 mL	0.18024 mL	0.10710 mL	1.35995 mL	0.02500 mL	1.937	-0.05243	0.93631	0.00
39:12.7	Data point 61	0.22001 mL	0.18024 mL	0.12411 mL	1.35995 mL	0.02500 mL	2.038	0.00598	0.32984	0.00
39:29.6	Data point 62	0.22001 mL	0.18024 mL	0.13874 mL	1.35995 mL	0.02500 mL	2.156	0.02306	0.93296	0.00
39:56.7	Data point 63	0.22001 mL	0.18024 mL	0.14819 mL	1.35995 mL	0.02500 mL	2.258	0.00994	0.52200	0.00
40:18.5	Data point 64	0.22001 mL	0.18024 mL	0.15513 mL	1.35995 mL	0.02500 mL	2.351	0.01923	0.91933	0.00
40:40.5	Data point 65	0.22001 mL	0.18024 mL	0.16101 mL	1.35995 mL	0.02500 mL	2.443	0.01510	0.96207	0.00
41:07.6	Data point 66	0.22001 mL	0.18024 mL	0.16590 mL	1.35995 mL	0.02500 mL	2.542	0.00406	0.29173	0.00

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 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
41:34.5	Data point 67	0.22001 mL	0.18024 mL	0.17023 mL	1.35995 mL	0.02500 mL	2.644	0.00638	0.62430	0.00040
41:51.2	Data point 68	0.22001 mL	0.18024 mL	0.17392 mL	1.35995 mL	0.02500 mL	2.761	0.01194	0.79448	0.00066
42:23.4	Data point 69	0.22001 mL	0.18024 mL	0.17745 mL	1.35995 mL	0.02500 mL	2.886	-0.00018	0.00125	0.00026
42:45.2	Data point 70	0.22001 mL	0.18024 mL	0.17919 mL	1.35995 mL	0.02500 mL	2.978	0.00293	0.22129	0.00031
43:12.2	Data point 71	0.22001 mL	0.18024 mL	0.18060 mL	1.35995 mL	0.02500 mL	3.074	0.01250	0.85426	0.00067
43:39.1	Data point 72	0.22001 mL	0.18024 mL	0.18175 mL	1.35995 mL	0.02500 mL	3.168	0.01178	0.86078	0.00063
44:05.9	Data point 73	0.22001 mL	0.18024 mL	0.18274 mL	1.35995 mL	0.02500 mL	3.261	0.00855	0.91549	0.00044
44:22.5	Data point 74	0.22001 mL	0.18024 mL	0.18361 mL	1.35995 mL	0.02500 mL	3.361	0.00996	0.86204	0.00053
44:39.0	Data point 75	0.22001 mL	0.18024 mL	0.18431 mL	1.35995 mL	0.02500 mL	3.457	0.01188	0.77730	0.00067
44:55.4	Data point 76	0.22001 mL	0.18024 mL	0.18488 mL	1.35995 mL	0.02500 mL	3.553	0.01685	0.96803	0.00085
45:12.0	Data point 77	0.22001 mL	0.18024 mL	0.18532 mL	1.35995 mL	0.02500 mL	3.645	0.02114	0.97846	0.00106
45:28.5	Data point 78	0.22001 mL	0.18024 mL	0.18568 mL	1.35995 mL	0.02500 mL	3.730	0.01901	0.90547	0.00099
45:50.2	Data point 79	0.22001 mL	0.18024 mL	0.18622 mL	1.35995 mL	0.02500 mL	3.890	0.03460	0.97814	0.00173
46:17.1	Data point 80	0.22001 mL	0.18024 mL	0.18678 mL	1.35995 mL	0.02500 mL	4.074	0.03826	0.95573	0.00193
46:38.7	Data point 81	0.22001 mL	0.18024 mL	0.18702 mL	1.35995 mL	0.02500 mL	4.213	0.06107	0.99226	0.00303
47:05.5	Data point 82	0.22001 mL	0.18024 mL	0.18721 mL	1.35995 mL	0.02500 mL	4.332	0.10033	0.98160	0.00500
47:27.2	Data point 83	0.22001 mL	0.18024 mL	0.18732 mL	1.35995 mL	0.02500 mL	4.450	0.09343	0.91662	0.00481
47:54.7	Data point 84	0.22001 mL	0.18024 mL	0.18742 mL	1.35995 mL	0.02500 mL	4.579	0.09876	0.98401	0.00491
48:29.9	Data point 85	0.22001 mL	0.18024 mL	0.18751 mL	1.35995 mL	0.02500 mL	4.742	0.09926	0.99269	0.00492
49:11.1	Data point 86	0.22001 mL	0.18024 mL	0.18761 mL	1.35995 mL	0.02500 mL	4.954	0.10099	0.99590	0.00499
50:00.7	Data point 87	0.22001 mL	0.18024 mL	0.18768 mL	1.35995 mL	0.02500 mL	5.228	0.09587	0.98211	0.00477
50:59.0	Data point 88	0.22001 mL	0.18024 mL	0.18775 mL	1.35995 mL	0.02500 mL	5.631	0.09902	0.98894	0.00491
51:56.2	Data point 89	0.22001 mL	0.18024 mL	0.18779 mL	1.35995 mL	0.02500 mL	5.935	0.10020	0.99203	0.00496
52:48.8	Data point 90	0.22001 mL	0.18024 mL	0.18784 mL	1.35995 mL	0.02500 mL	6.299	0.09044	0.83264	0.00489
53:48.5	Data point 91	0.22001 mL	0.18024 mL	0.18789 mL	1.35995 mL	0.02500 mL	6.585	0.10059	0.98933	0.00499
54:52.3	Data point 92	0.22001 mL	0.18024 mL	0.18796 mL	1.35995 mL	0.02500 mL	6.899	0.09775	0.98455	0.00486
55:43.0	Data point 93	0.22001 mL	0.18024 mL	0.18803 mL	1.35995 mL	0.02500 mL	7.141	0.09874	0.98717	0.00491
56:26.7	Data point 94	0.22001 mL	0.18024 mL	0.18810 mL	1.35995 mL	0.02500 mL	7.306	0.09863	0.98612	0.00490
57:05.9	Data point 95	0.22001 mL	0.18024 mL	0.18817 mL	1.35995 mL	0.02500 mL	7.449	0.09992	0.99440	0.00494
57:40.3	Data point 96	0.22001 mL	0.18024 mL	0.18824 mL	1.35995 mL	0.02500 mL	7.603	0.10052	0.99277	0.00498
58:15.9	Data point 97	0.22001 mL	0.18024 mL	0.18831 mL	1.35995 mL	0.02500 mL	7.773	0.10010	0.98296	0.00498
58:54.6	Data point 98	0.22001 mL	0.18024 mL	0.18838 mL	1.35995 mL	0.02500 mL	7.953	0.09670	0.98145	0.00482
59:31.5	Data point 99	0.22001 mL	0.18024 mL	0.18845 mL	1.35995 mL	0.02500 mL	8.162	0.09806	0.96957	0.00491
1:00:10.1	Data point 100	0.22001 mL	0.18024 mL	0.18852 mL	1.35995 mL	0.02500 mL	8.371	0.09839	0.99125	0.00488
1:00:50.3	Data point 101	0.22001 mL	0.18024 mL	0.18859 mL	1.35995 mL	0.02500 mL	8.634	0.09751	0.99439	0.00483
1:01:28.6	Data point 102	0.22001 mL	0.18024 mL	0.18864 mL	1.35995 mL	0.02500 mL	8.796	0.10014	0.99270	0.00496
1:02:03.2	Data point 103	0.22001 mL	0.18024 mL	0.18869 mL	1.35995 mL	0.02500 mL	8.970	0.09626	0.97018	0.00482
1:02:38.4	Data point 104	0.22001 mL	0.18024 mL	0.18874 mL	1.35995 mL	0.02500 mL	9.146	0.09967	0.98520	0.00495
1:03:19.1	Data point 105	0.22001 mL	0.18024 mL	0.18881 mL	1.35995 mL	0.02500 mL	9.379	0.09564	0.97203	0.00479
1:03:57.7	Data point 106	0.22001 mL	0.18024 mL	0.18888 mL	1.35995 mL	0.02500 mL	9.592	0.09483	0.97536	0.00474
1:04:33.0	Data point 107	0.22001 mL	0.18024 mL	0.18895 mL	1.35995 mL	0.02500 mL	9.757	0.09934	0.97314	0.00497
1:05:05.2	Data point 108	0.22001 mL	0.18024 mL	0.18902 mL	1.35995 mL	0.02500 mL	9.892	0.09965	0.97193	0.00499
1:05:28.4	Data point 109	0.22001 mL	0.18024 mL	0.18911 mL	1.35995 mL	0.02500 mL	10.034	0.09615	0.97337	0.00481
1:05:50.0	Data point 110	0.22001 mL	0.18024 mL	0.18921 mL	1.35995 mL	0.02500 mL	10.135	0.06645	0.97541	0.00332
1:06:06.6	Data point 111	0.22001 mL	0.18024 mL	0.18930 mL	1.35995 mL	0.02500 mL	10.228	0.04907	0.98940	0.00244
1:06:23.1	Data point 112	0.22001 mL	0.18024 mL	0.18942 mL	1.35995 mL	0.02500 mL	10.324	0.02691	0.96301	0.00135
1:06:39.7	Data point 113	0.22001 mL	0.18024 mL	0.18958 mL	1.35995 mL	0.02500 mL	10.447	0.02261	0.89890	0.00118
1:07:06.2	Data point 114	0.22001 mL	0.18024 mL	0.18982 mL	1.35995 mL	0.02500 mL	10.539	0.01003	0.76414	0.00057
1:07:22.9	Data point 115	0.22001 mL	0.18024 mL	0.19007 mL	1.35995 mL	0.02500 mL	10.655	0.00820	0.70150	0.00048
1:07:44.5	Data point 116	0.22001 mL	0.18024 mL	0.19040 mL	1.35995 mL	0.02500 mL	10.747	0.00453	0.44896	0.00033
1:08:01.1	Data point 117	0.22001 mL	0.18024 mL	0.19085 mL	1.35995 mL	0.02500 mL	10.863	-0.00129	0.05066	0.00028
1:08:27.7	Data point 118	0.22001 mL	0.18024 mL	0.19144 mL	1.35995 mL	0.02500 mL	10.955	-0.00276	0.32506	0.00024
1:08:44.3	Data point 119	0.22001 mL	0.18024 mL	0.19215 mL	1.35995 mL	0.02500 mL	11.055	-0.00354	0.36497	0.00029
1:09:00.9	Data point 120	0.22001 mL	0.18024 mL	0.19304 mL	1.35995 mL	0.02500 mL	11.143	-0.00194	0.17355	0.00023
1:09:17.4	Data point 121	0.22001 mL	0.18024 mL	0.19412 mL	1.35995 mL	0.02500 mL	11.228	-0.00498	0.53616	0.00034
1:09:34.1	Data point 122	0.22001 mL	0.18024 mL	0.19544 mL	1.35995 mL	0.02500 mL	11.314	-0.00703	0.75619	0.00040
1:09:50.6	Data point 123	0.22001 mL	0.18024 mL	0.19704 mL	1.35995 mL	0.02500 mL	11.395	-0.00597	0.66423	0.00036



Assay Events

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07006**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07006_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 8:42:52 AM**
Analyst: **Dorothy Leverse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH Slope
1:10:12.3	Data point 124	0.22001 mL	0.18024 mL	0.19866 mL	1.35995 mL	0.02500 mL	11.485	-0.00463	0.61939	0.00000
1:10:39.3	Data point 125	0.22001 mL	0.18024 mL	0.20101 mL	1.35995 mL	0.02500 mL	11.580	-0.00541	0.65198	0.00000
1:10:55.9	Data point 126	0.22001 mL	0.18024 mL	0.20400 mL	1.35995 mL	0.02500 mL	11.669	-0.00431	0.49191	0.00000
1:11:12.6	Data point 127	0.22001 mL	0.18024 mL	0.20769 mL	1.35995 mL	0.02500 mL	11.760	-0.00446	0.46482	0.00000
1:11:29.4	Data point 128	0.22001 mL	0.18024 mL	0.21223 mL	1.35995 mL	0.02500 mL	11.854	-0.00412	0.42072	0.00000
1:11:46.1	Data point 129	0.22001 mL	0.18024 mL	0.21794 mL	1.35995 mL	0.02500 mL	11.945	-0.00680	0.70814	0.00000
1:12:03.0	Data point 130	0.22001 mL	0.18024 mL	0.22502 mL	1.35995 mL	0.02500 mL	12.033	-0.00583	0.60186	0.00000
1:13:45.3	Reference spectrum									
1:15:05.9	Data point 132	0.39005 mL	0.31761 mL	0.22505 mL	1.35995 mL	0.02500 mL	1.929	-0.07070	0.93164	0.00000
1:15:28.2	Data point 133	0.39005 mL	0.31761 mL	0.24269 mL	1.35995 mL	0.02500 mL	2.021	0.00316	0.28474	0.00000
1:15:55.5	Data point 134	0.39005 mL	0.31761 mL	0.25713 mL	1.35995 mL	0.02500 mL	2.119	-0.00351	0.15384	0.00000
1:16:28.1	Data point 135	0.39005 mL	0.31761 mL	0.27067 mL	1.35995 mL	0.02500 mL	2.241	0.01981	0.92763	0.00000
1:16:55.3	Data point 136	0.39005 mL	0.31761 mL	0.27973 mL	1.35995 mL	0.02500 mL	2.347	0.01308	0.92960	0.00000
1:17:12.2	Data point 137	0.39005 mL	0.31761 mL	0.28763 mL	1.35995 mL	0.02500 mL	2.454	0.01234	0.83444	0.00000
1:17:29.1	Data point 138	0.39005 mL	0.31761 mL	0.29384 mL	1.35995 mL	0.02500 mL	2.580	0.00769	0.68470	0.00000
1:17:51.1	Data point 139	0.39005 mL	0.31761 mL	0.29810 mL	1.35995 mL	0.02500 mL	2.679	0.01056	0.77859	0.00000
1:18:07.6	Data point 140	0.39005 mL	0.31761 mL	0.30179 mL	1.35995 mL	0.02500 mL	2.796	0.00589	0.56744	0.00000
1:18:34.6	Data point 141	0.39005 mL	0.31761 mL	0.30506 mL	1.35995 mL	0.02500 mL	2.899	0.00166	0.07851	0.00000
1:18:51.2	Data point 142	0.39005 mL	0.31761 mL	0.30729 mL	1.35995 mL	0.02500 mL	3.010	-0.00430	0.43413	0.00000
1:19:07.8	Data point 143	0.39005 mL	0.31761 mL	0.30903 mL	1.35995 mL	0.02500 mL	3.151	-0.00092	0.02473	0.00000
1:19:34.7	Data point 144	0.39005 mL	0.31761 mL	0.31021 mL	1.35995 mL	0.02500 mL	3.245	0.00797	0.67498	0.00000
1:19:51.3	Data point 145	0.39005 mL	0.31761 mL	0.31120 mL	1.35995 mL	0.02500 mL	3.353	0.00482	0.47676	0.00000
1:20:07.9	Data point 146	0.39005 mL	0.31761 mL	0.31197 mL	1.35995 mL	0.02500 mL	3.455	0.00811	0.65002	0.00000
1:20:24.5	Data point 147	0.39005 mL	0.31761 mL	0.31258 mL	1.35995 mL	0.02500 mL	3.555	0.01015	0.75587	0.00000
1:20:41.1	Data point 148	0.39005 mL	0.31761 mL	0.31305 mL	1.35995 mL	0.02500 mL	3.645	0.00870	0.63312	0.00000
1:20:57.7	Data point 149	0.39005 mL	0.31761 mL	0.31345 mL	1.35995 mL	0.02500 mL	3.719	0.01693	0.95196	0.00000
1:21:24.6	Data point 150	0.39005 mL	0.31761 mL	0.31442 mL	1.35995 mL	0.02500 mL	3.942	0.02497	0.94516	0.00000
1:21:46.3	Data point 151	0.39005 mL	0.31761 mL	0.31479 mL	1.35995 mL	0.02500 mL	4.115	0.03603	0.96427	0.00000
1:22:08.0	Data point 152	0.39005 mL	0.31761 mL	0.31505 mL	1.35995 mL	0.02500 mL	4.237	0.05816	0.98223	0.00000
1:22:29.6	Data point 153	0.39005 mL	0.31761 mL	0.31524 mL	1.35995 mL	0.02500 mL	4.395	0.08320	0.98251	0.00000
1:22:51.2	Data point 154	0.39005 mL	0.31761 mL	0.31536 mL	1.35995 mL	0.02500 mL	4.517	0.10037	0.98987	0.00000
1:23:20.0	Data point 155	0.39005 mL	0.31761 mL	0.31545 mL	1.35995 mL	0.02500 mL	4.673	0.09975	0.98849	0.00000
1:23:54.4	Data point 156	0.39005 mL	0.31761 mL	0.31555 mL	1.35995 mL	0.02500 mL	4.872	0.09725	0.96956	0.00000
1:24:33.6	Data point 157	0.39005 mL	0.31761 mL	0.31562 mL	1.35995 mL	0.02500 mL	5.061	0.09858	0.98743	0.00000
1:25:16.3	Data point 158	0.39005 mL	0.31761 mL	0.31569 mL	1.35995 mL	0.02500 mL	5.339	0.09511	0.97701	0.00000
1:25:60.0	Data point 159	0.39005 mL	0.31761 mL	0.31573 mL	1.35995 mL	0.02500 mL	5.556	0.09646	0.96685	0.00000
1:26:50.1	Data point 160	0.39005 mL	0.31761 mL	0.31578 mL	1.35995 mL	0.02500 mL	5.832	0.09900	0.99180	0.00000
1:27:41.8	Data point 161	0.39005 mL	0.31761 mL	0.31583 mL	1.35995 mL	0.02500 mL	6.126	0.09937	0.98669	0.00000
1:28:32.4	Data point 162	0.39005 mL	0.31761 mL	0.31588 mL	1.35995 mL	0.02500 mL	6.400	0.09937	0.99473	0.00000
1:29:19.0	Data point 163	0.39005 mL	0.31761 mL	0.31594 mL	1.35995 mL	0.02500 mL	6.696	0.09912	0.98511	0.00000
1:29:56.0	Data point 164	0.39005 mL	0.31761 mL	0.31599 mL	1.35995 mL	0.02500 mL	6.871	0.09773	0.97490	0.00000
1:30:28.1	Data point 165	0.39005 mL	0.31761 mL	0.31604 mL	1.35995 mL	0.02500 mL	7.022	0.09892	0.99338	0.00000
1:31:06.4	Data point 166	0.39005 mL	0.31761 mL	0.31611 mL	1.35995 mL	0.02500 mL	7.218	0.10020	0.98713	0.00000
1:31:41.6	Data point 167	0.39005 mL	0.31761 mL	0.31618 mL	1.35995 mL	0.02500 mL	7.375	0.09990	0.98240	0.00000
1:32:14.9	Data point 168	0.39005 mL	0.31761 mL	0.31625 mL	1.35995 mL	0.02500 mL	7.528	0.10013	0.98482	0.00000
1:32:49.5	Data point 169	0.39005 mL	0.31761 mL	0.31632 mL	1.35995 mL	0.02500 mL	7.681	0.10014	0.98007	0.00000
1:33:24.8	Data point 170	0.39005 mL	0.31761 mL	0.31639 mL	1.35995 mL	0.02500 mL	7.888	0.09617	0.97565	0.00000
1:33:57.0	Data point 171	0.39005 mL	0.31761 mL	0.31644 mL	1.35995 mL	0.02500 mL	8.053	0.09792	0.98162	0.00000
1:34:30.1	Data point 172	0.39005 mL	0.31761 mL	0.31649 mL	1.35995 mL	0.02500 mL	8.268	0.09734	0.95560	0.00000
1:35:04.3	Data point 173	0.39005 mL	0.31761 mL	0.31653 mL	1.35995 mL	0.02500 mL	8.512	0.09766	0.98226	0.00000
1:35:41.1	Data point 174	0.39005 mL	0.31761 mL	0.31658 mL	1.35995 mL	0.02500 mL	8.787	0.09884	0.96430	0.00000
1:36:18.7	Data point 175	0.39005 mL	0.31761 mL	0.31663 mL	1.35995 mL	0.02500 mL	9.018	0.09160	0.94795	0.00000
1:36:52.1	Data point 176	0.39005 mL	0.31761 mL	0.31667 mL	1.35995 mL	0.02500 mL	9.238	0.09492	0.95536	0.00000
1:37:25.7	Data point 177	0.39005 mL	0.31761 mL	0.31672 mL	1.35995 mL	0.02500 mL	9.392	0.09798	0.97294	0.00000
1:37:55.4	Data point 178	0.39005 mL	0.31761 mL	0.31677 mL	1.35995 mL	0.02500 mL	9.516	0.09975	0.97893	0.00000
1:38:22.0	Data point 179	0.39005 mL	0.31761 mL	0.31684 mL	1.35995 mL	0.02500 mL	9.640	0.09194	0.95665	0.00000
1:38:52.2	Data point 180	0.39005 mL	0.31761 mL	0.31691 mL	1.35995 mL	0.02500 mL	9.800	0.09553	0.98261	0.00000

Sample name: **D08**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07006**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07006_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 8:42:52 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
1:39:15.4	Data point 181	0.39005 mL	0.31761 mL	0.31698 mL	1.35995 mL	0.02500 mL	9.918	0.08276	0.94810	0.0041
1:39:37.1	Data point 182	0.39005 mL	0.31761 mL	0.31705 mL	1.35995 mL	0.02500 mL	10.026	0.06128	0.96875	0.0030
1:39:58.6	Data point 183	0.39005 mL	0.31761 mL	0.31717 mL	1.35995 mL	0.02500 mL	10.149	0.03482	0.96390	0.0017
1:40:15.1	Data point 184	0.39005 mL	0.31761 mL	0.31733 mL	1.35995 mL	0.02500 mL	10.281	0.01580	0.83644	0.0008
1:40:36.8	Data point 185	0.39005 mL	0.31761 mL	0.31755 mL	1.35995 mL	0.02500 mL	10.385	0.01502	0.87508	0.0007
1:40:53.3	Data point 186	0.39005 mL	0.31761 mL	0.31780 mL	1.35995 mL	0.02500 mL	10.509	0.00050	0.00965	0.0002
1:41:19.9	Data point 187	0.39005 mL	0.31761 mL	0.31818 mL	1.35995 mL	0.02500 mL	10.601	0.00361	0.24790	0.0003
1:41:36.6	Data point 188	0.39005 mL	0.31761 mL	0.31863 mL	1.35995 mL	0.02500 mL	10.713	-0.00668	0.56888	0.0004
1:41:53.3	Data point 189	0.39005 mL	0.31761 mL	0.31919 mL	1.35995 mL	0.02500 mL	10.816	-0.00639	0.70853	0.0003
1:42:09.8	Data point 190	0.39005 mL	0.31761 mL	0.31990 mL	1.35995 mL	0.02500 mL	10.913	-0.00840	0.78022	0.0004
1:42:26.4	Data point 191	0.39005 mL	0.31761 mL	0.32079 mL	1.35995 mL	0.02500 mL	11.004	-0.00995	0.82256	0.0005
1:42:43.0	Data point 192	0.39005 mL	0.31761 mL	0.32190 mL	1.35995 mL	0.02500 mL	11.094	-0.01020	0.86528	0.0005
1:42:59.6	Data point 193	0.39005 mL	0.31761 mL	0.32324 mL	1.35995 mL	0.02500 mL	11.169	-0.00997	0.87872	0.0005
1:43:26.6	Data point 194	0.39005 mL	0.31761 mL	0.32519 mL	1.35995 mL	0.02500 mL	11.260	-0.00825	0.73165	0.0004
1:43:48.4	Data point 195	0.39005 mL	0.31761 mL	0.32674 mL	1.35995 mL	0.02500 mL	11.350	-0.00832	0.74868	0.0004
1:44:15.3	Data point 196	0.39005 mL	0.31761 mL	0.32907 mL	1.35995 mL	0.02500 mL	11.445	-0.00615	0.65026	0.0003
1:44:32.0	Data point 197	0.39005 mL	0.31761 mL	0.33210 mL	1.35995 mL	0.02500 mL	11.535	-0.00983	0.83929	0.0005
1:44:48.6	Data point 198	0.39005 mL	0.31761 mL	0.33587 mL	1.35995 mL	0.02500 mL	11.628	-0.00955	0.82036	0.0005
1:45:05.3	Data point 199	0.39005 mL	0.31761 mL	0.34052 mL	1.35995 mL	0.02500 mL	11.721	-0.00810	0.76135	0.0004
1:45:22.1	Data point 200	0.39005 mL	0.31761 mL	0.34636 mL	1.35995 mL	0.02500 mL	11.812	-0.00727	0.80402	0.0004
1:45:38.8	Data point 201	0.39005 mL	0.31761 mL	0.35362 mL	1.35995 mL	0.02500 mL	11.899	-0.01135	0.83996	0.0006
1:45:55.6	Data point 202	0.39005 mL	0.31761 mL	0.36258 mL	1.35995 mL	0.02500 mL	11.990	-0.00949	0.78051	0.0005
1:46:12.2	Data point 203	0.39005 mL	0.31761 mL	0.36898 mL	1.35995 mL	0.02500 mL	12.046	-0.00558	0.61981	0.0003
1:48:11.6	Assay volumes	0.64005 mL	0.45200 mL	0.36898 mL	1.35995 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	0.100			
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%			
Titrant Pre-Dose				
Titrant 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			
Buffer in use	Yes			
Buffer type	Phosphate Buffer			

Sample name: **D08**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07006**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07006_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 8:42:52 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			
After medium addition, stir for	5 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	60 seconds			
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			
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 8:42:52 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus S	0.9927	10/7/2017 8:42:52 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus jH	0.5	10/7/2017 8:42:52 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus jOH	-0.7	10/7/2017 8:42:52 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Base concentration factor	1.011	10/7/2017 8:42:52 AM	C:\Sirius_T3\KOH17122.t3r
Acid concentration factor	1.003	10/7/2017 8:42:52 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r

Sample name: **D08** Experiment start time: **10/7/2017 8:42:52 AM**
 Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse**
 Assay ID: **17J-07006** Instrument ID: **T311053**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07006_D08_UV-metric psKa.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)		
Titration	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)		
Titration	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)		
Titration	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
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titration	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)		
Titration	Octanol	9-14-17	9/14/2017 10:30:38 AM
Titration		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 8:43:16 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	8.5e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	1.5e+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		



Assay Settings

Sample name: **D08** Experiment start time: **10/7/2017 8:42:52 AM**
Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse**
Assay ID: **17J-07006** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07006_D08_UV-metric psKa.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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		
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 G1