Yasuda-Shedlovsky Result

Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

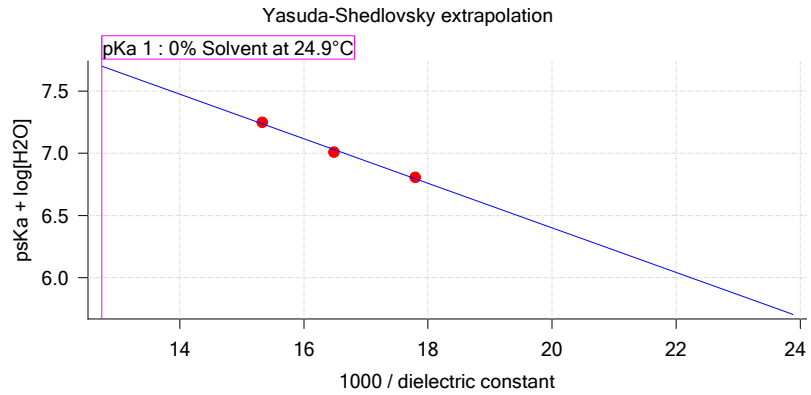
Yasuda-Shedlovsky result

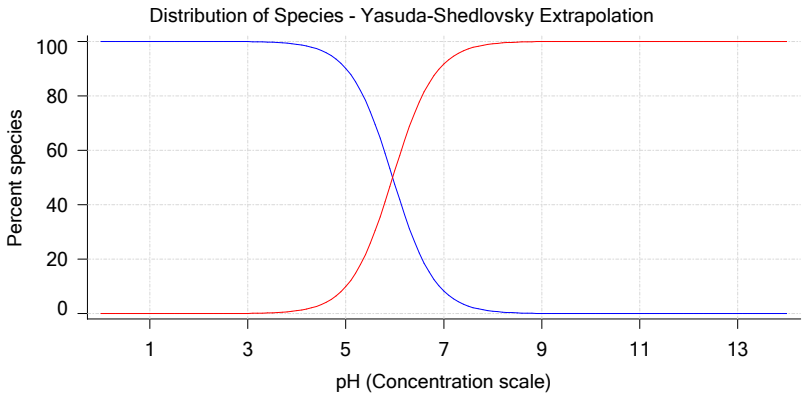
Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.96	±0.06	9.98	-179.0283	0.9934	0.167 M	24.9°C

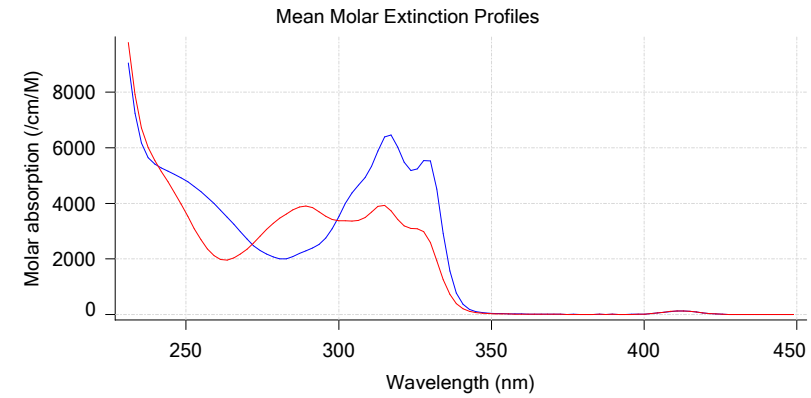
Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
17J-12006 Points 4 to 63	50.38 %	Up	UV-metric pKa	56.2	24.2 M	0.159 M	24.9°C	☑	5.42
17J-12006 Points 65 to 125	40.75 %	Up	UV-metric pKa	60.7	29.6 M	0.167 M	24.9°C	☑	5.54
17J-12006 Points 127 to 192	30.69 %	Up	UV-metric pKa	65.2	35.5 M	0.173 M	24.9°C	☑	5.70

Graphs







UV-metric psKa Titration 1 of 3 17J-12006 Points 4 to 63

Results

pKa 1	**5.42**
RMSD	**0.001 0.004**
Chi squared	**0.0113**
PCA calculated number of pKas	**3**
Average ionic strength	**0.159 M**
Average temperature	**24.9°C**
Analyte concentration range	**85.3 µM to 80.3 µM**
Methanol weight %	**50.4 %**
Dielectric constant	**56.2**
Water concentration	**24.2 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**

Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Results (continued)

pH clipping **1.476 to 12.535**

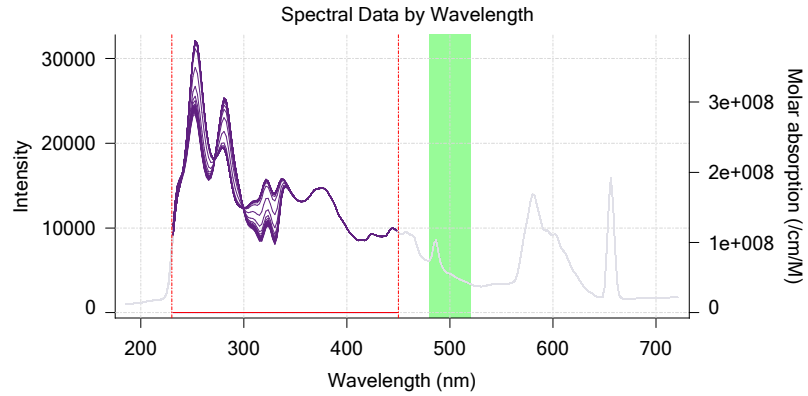
Warnings and errors

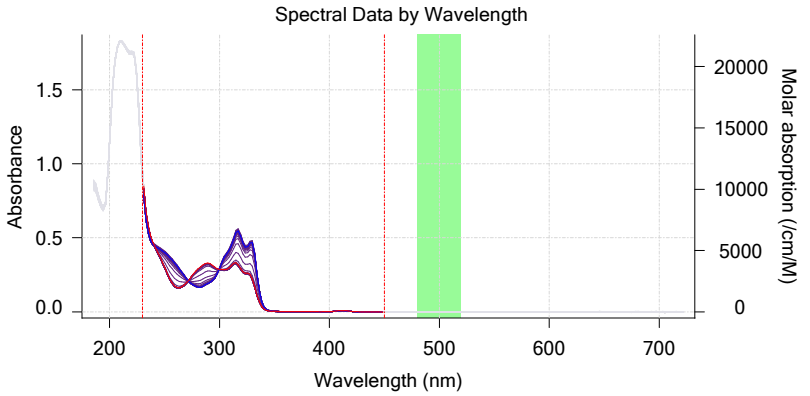
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

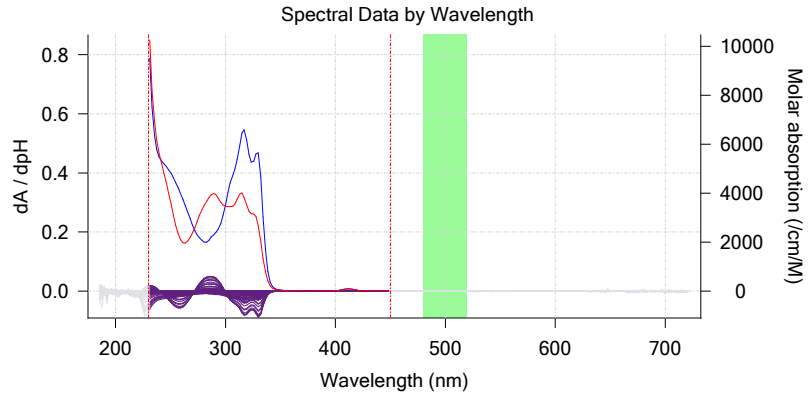
Assay Settings

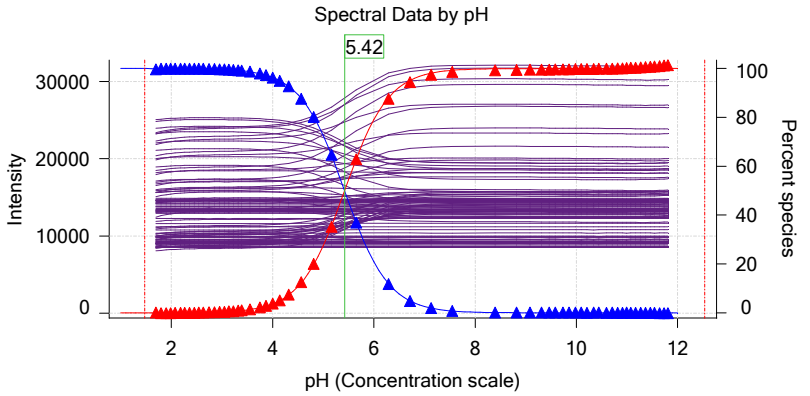
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	No			
Assay Medium				

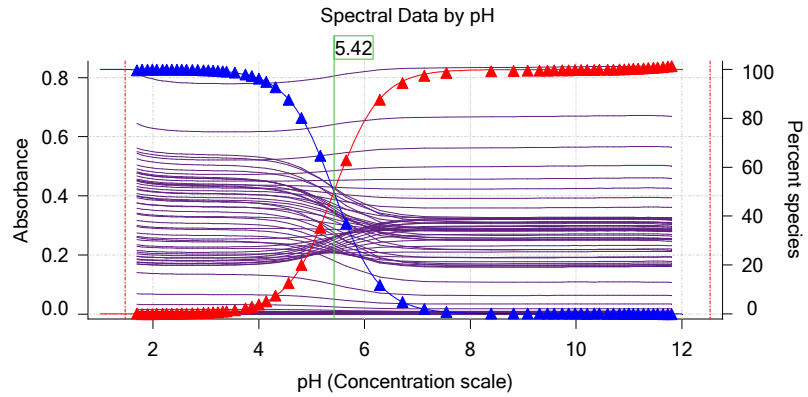
Graphs

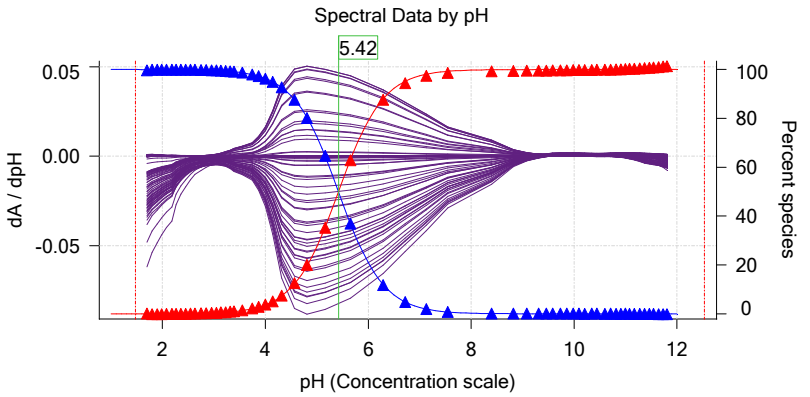








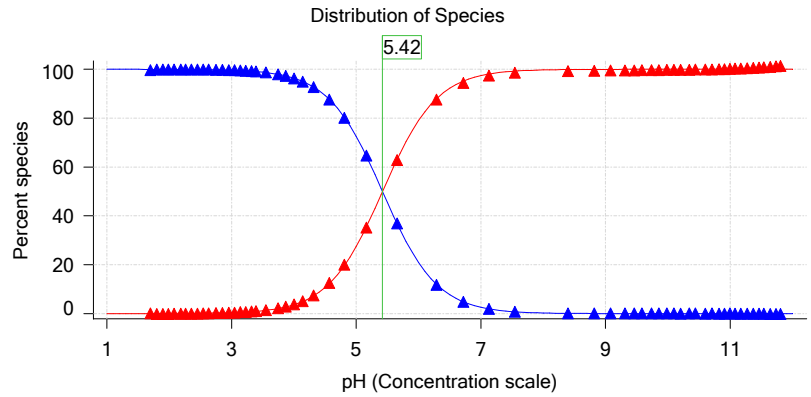


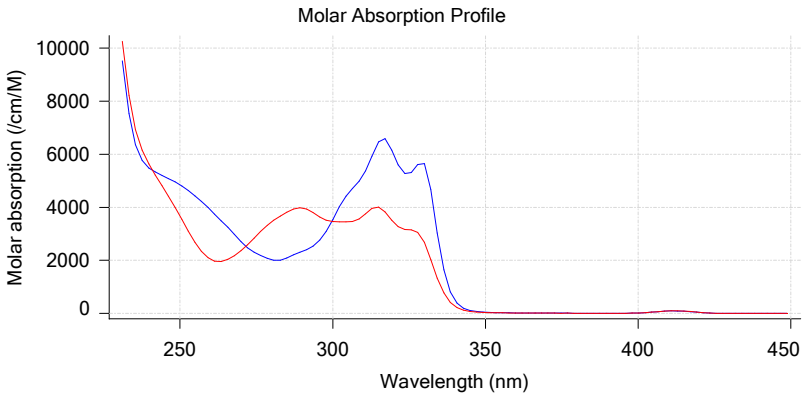


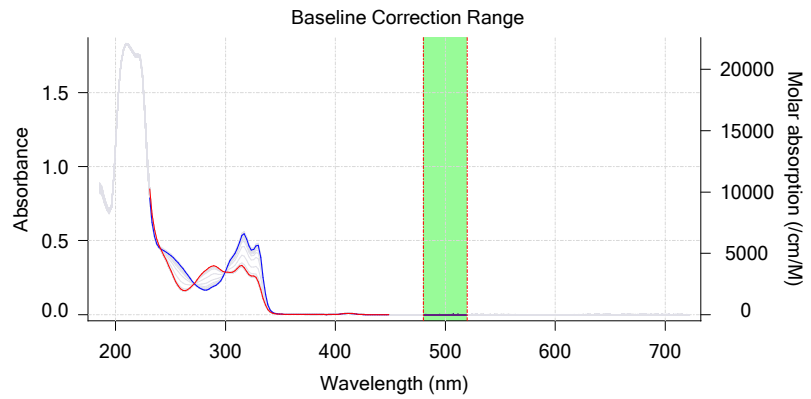
Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

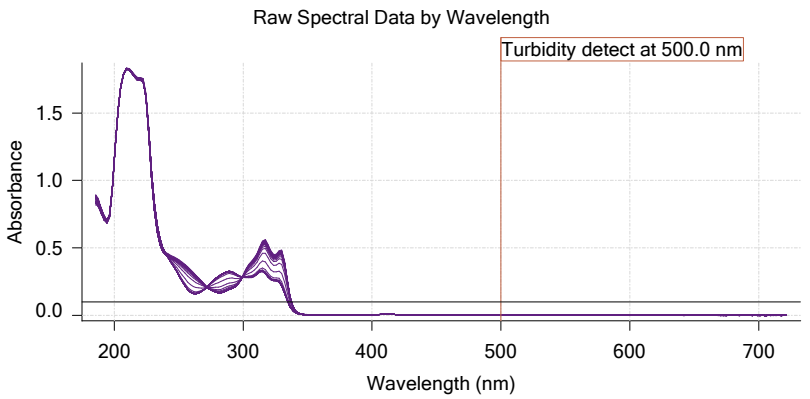
Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









UV-metric psKa Titration 2 of 3 17J-12006 Points 65 to 125

Results

pKa 1	**5.54**
RMSD	**0.001 0.005**
Chi squared	**0.0124**
PCA calculated number of pKas	**4**
Average ionic strength	**0.167 M**
Average temperature	**24.9°C**
Analyte concentration range	**70.0 µM to 66.3 µM**
Methanol weight %	**40.7 %**
Dielectric constant	**60.7**
Water concentration	**29.6 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.499 to 12.519**

Warnings and errors

Errors None
Warnings PCA calculation disagrees with predicted number of pKas

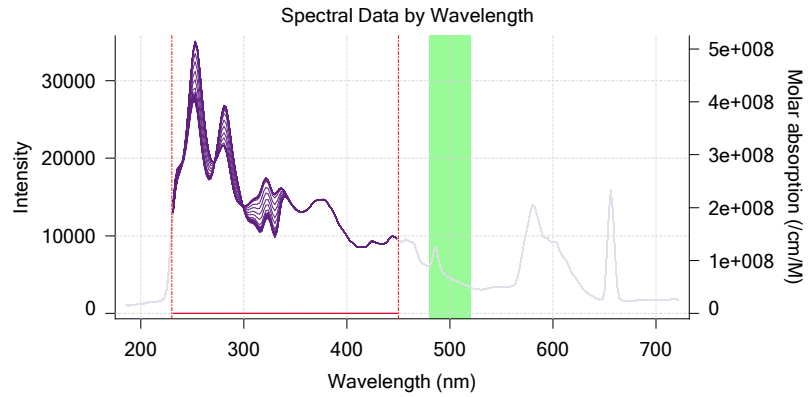
Assay Settings

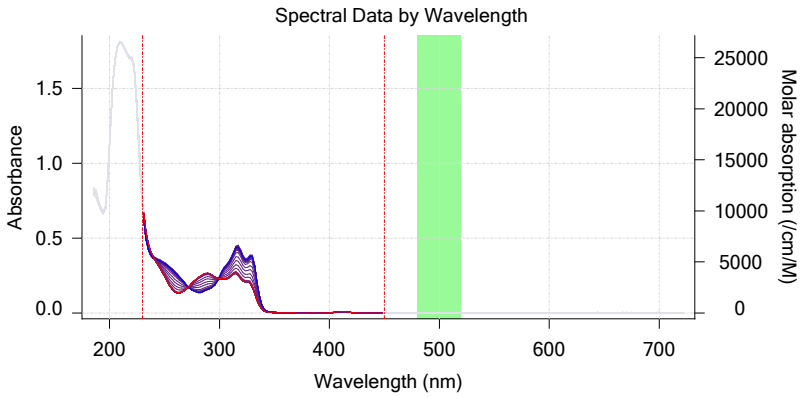
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	No			
Assay Medium				

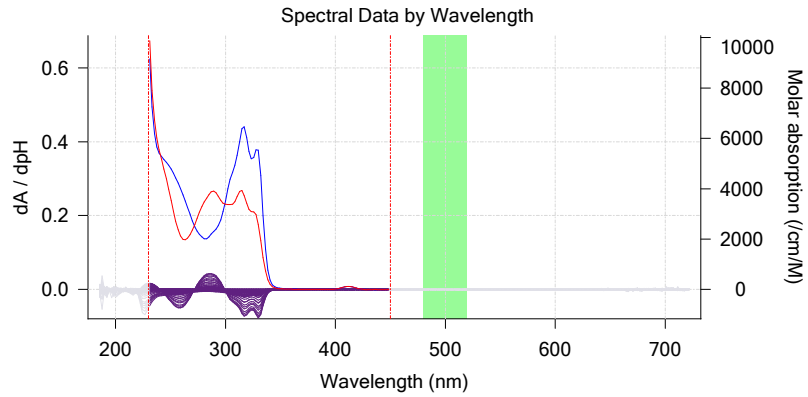
Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

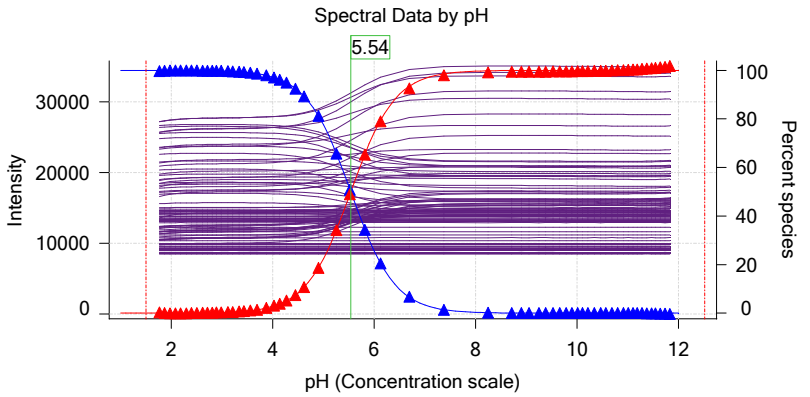
Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

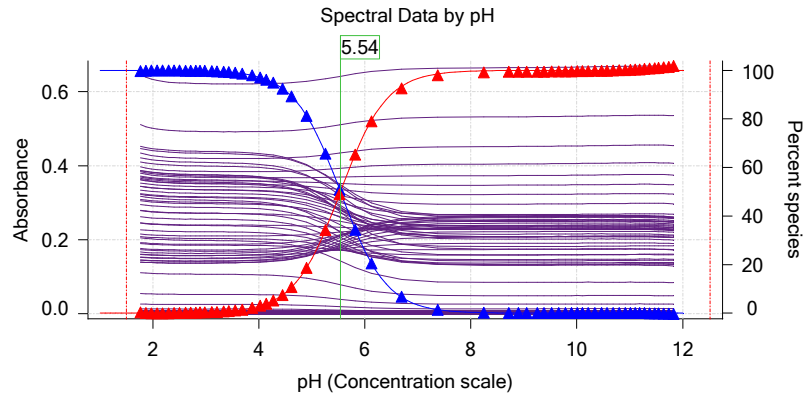
Graphs

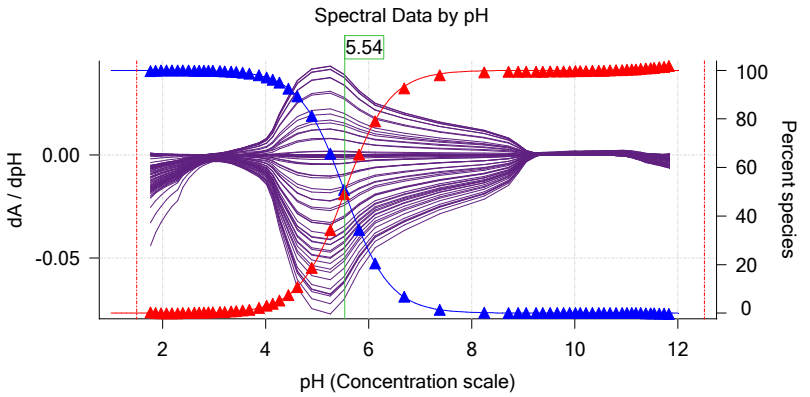


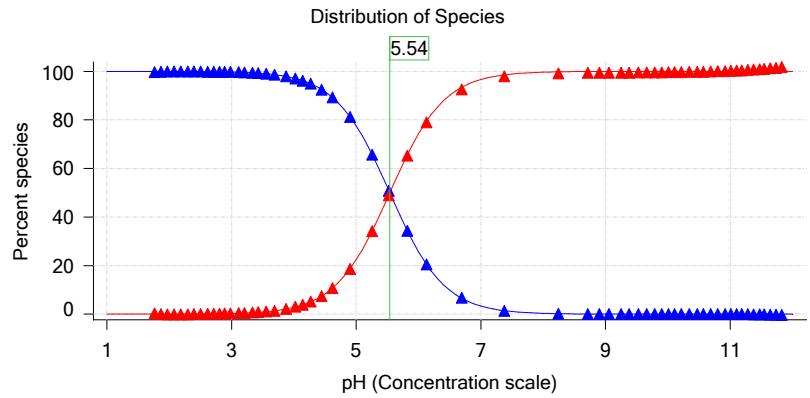


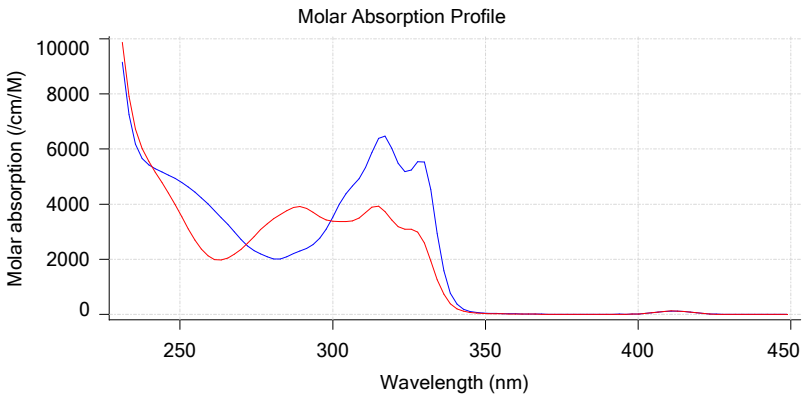








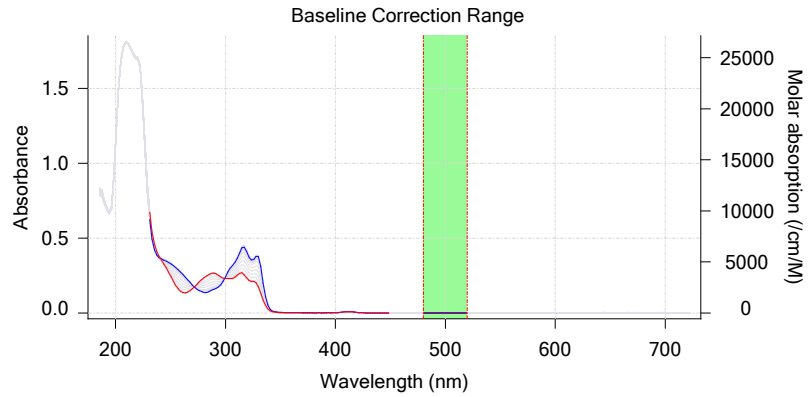


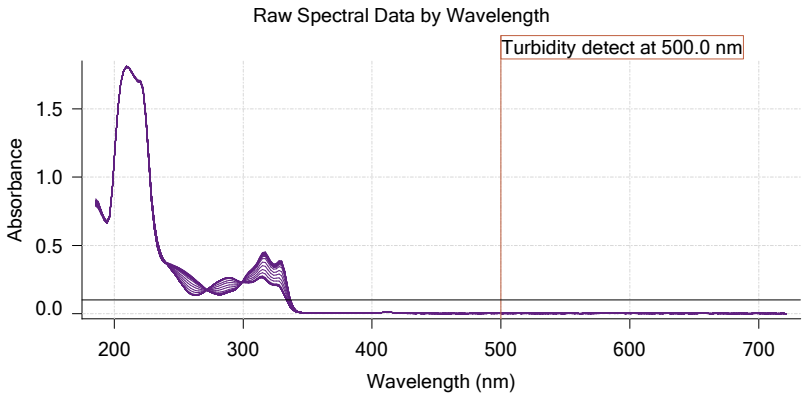


Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)





UV-metric psKa Titration 3 of 3 17J-12006 Points 127 to 192

Results

pKa 1	**5.70**
RMSD	**0.002 0.007**
Chi squared	**0.0173**
PCA calculated number of pKas	**3**
Average ionic strength	**0.173 M**
Average temperature	**24.9°C**
Analyte concentration range	**53.9 µM to 51.1 µM**
Methanol weight %	**30.7 %**
Dielectric constant	**65.2**
Water concentration	**35.5 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.501 to 12.516**

Warnings and errors

Errors None
Warnings PCA calculation disagrees with predicted number of pKas

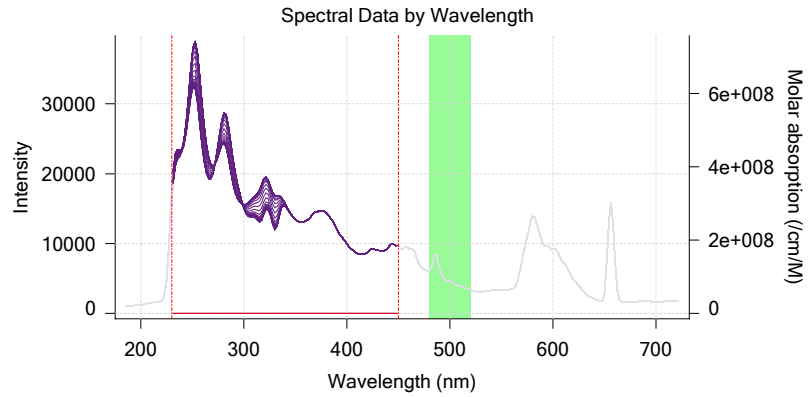
Assay Settings

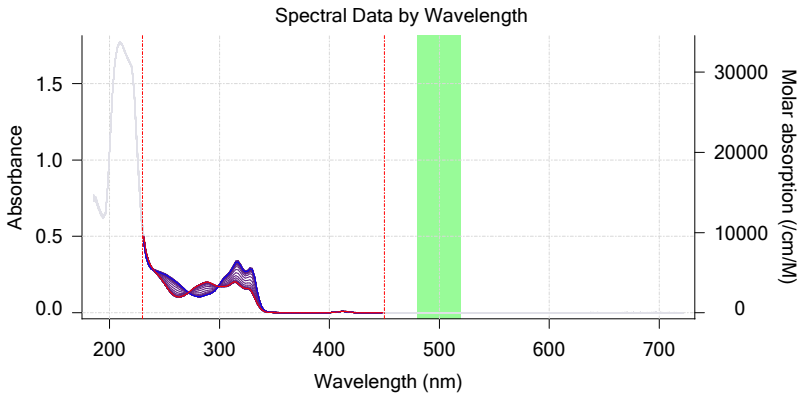
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	No			
Assay Medium				

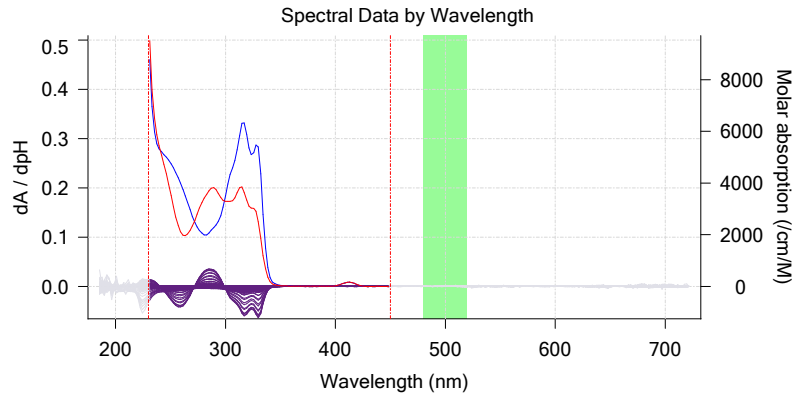
Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

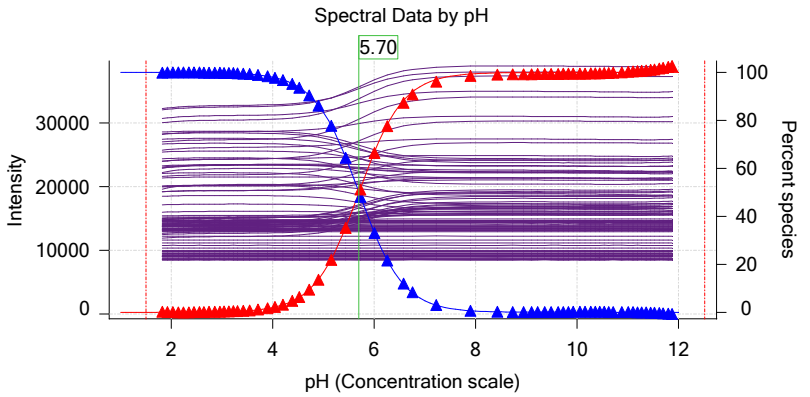
Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

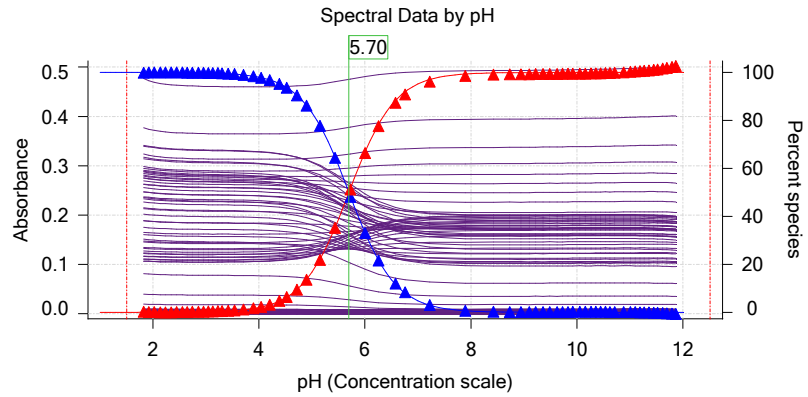
Graphs

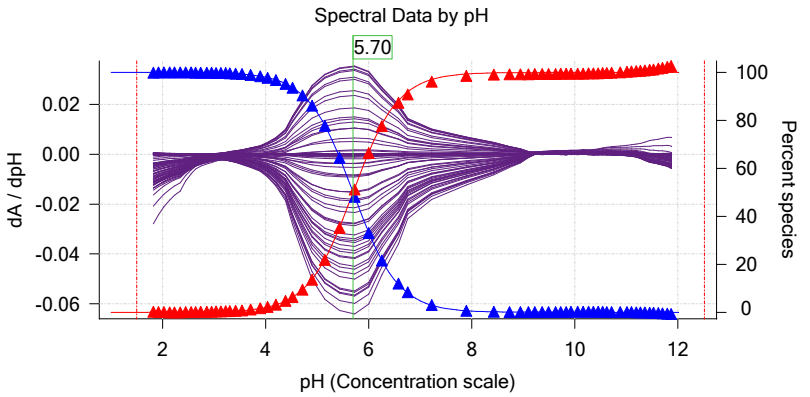


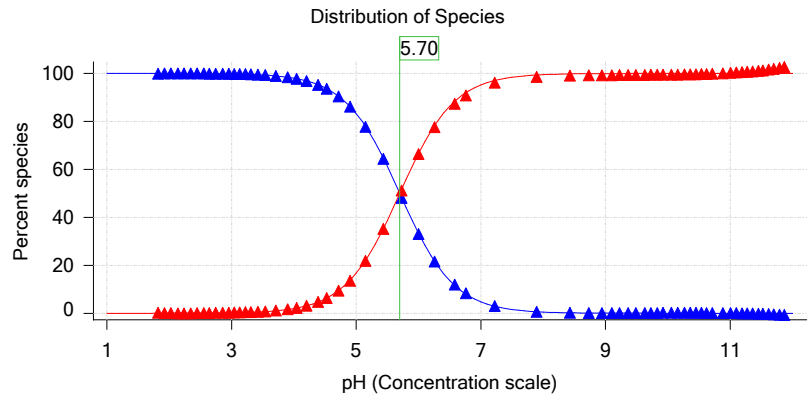


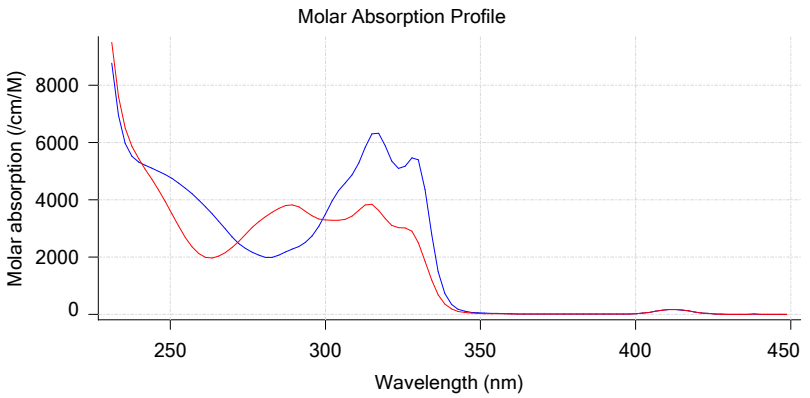








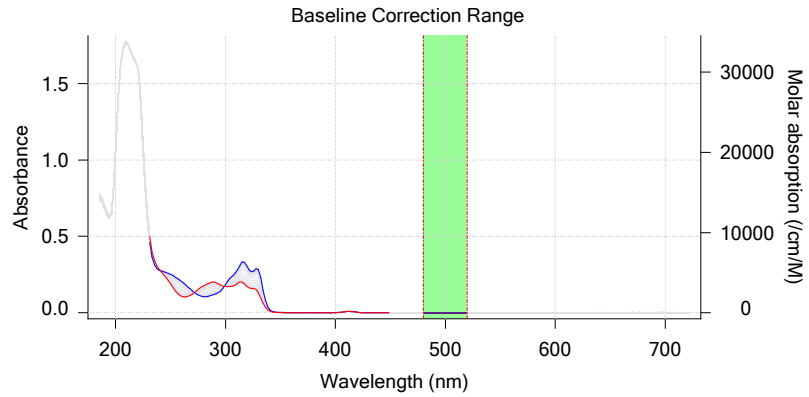


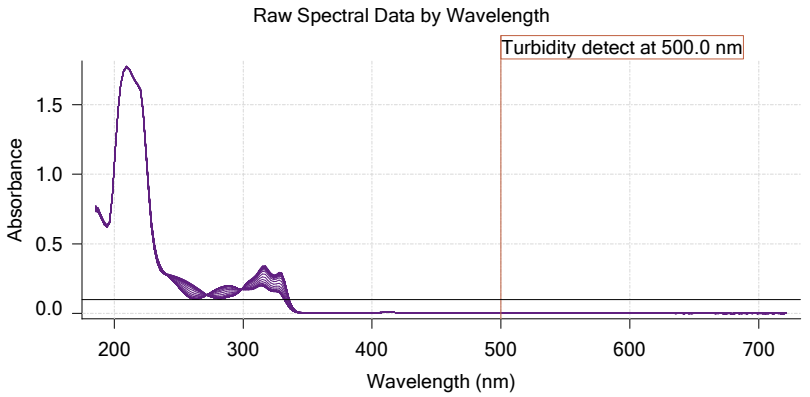


Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)





Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M07	10/11/2017 4:12:48 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0025 mL	10/11/2017 4:11:34 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.053600 M	10/11/2017 4:13:02 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	328.16	9/18/2017 4:02:12 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	10/11/2017 4:13:13 PM	User entered value
Sample is a	Base	10/11/2017 4:13:17 PM	User entered value
pKa 1	5.70	10/11/2017 4:13:26 PM	User entered value
logp (XH +)	-10.00		Default value
logP (neutral X)	-10.00	9/18/2017 4:02:02 PM	User entered value

Events

Time	Event	Water	Acid	Base	Methanol	pH	dpH/dt	pH R-squared	pH SD
3:33.0	Dark spectrum								
3:34.4	Reference spectrum								
4:02.0	Volume reset due to vial change								
7:50.1	Initial pH = 5.69								
8:31.0	Data point 4	0.34995 mL	0.06785 mL	0.00000 mL	1.15005 mL	1.976	-0.02005	0.94403	0.0010
8:59.4	Data point 5	0.34995 mL	0.06785 mL	0.01449 mL	1.15005 mL	2.077	-0.00541	0.09897	0.0008
9:26.7	Data point 6	0.34995 mL	0.06785 mL	0.02505 mL	1.15005 mL	2.176	0.00216	0.27344	0.0002
9:43.6	Data point 7	0.34995 mL	0.06785 mL	0.03325 mL	1.15005 mL	2.265	0.00790	0.76179	0.0004
10:00.4	Data point 8	0.34995 mL	0.06785 mL	0.03993 mL	1.15005 mL	2.355	0.00573	0.62925	0.0003
10:17.2	Data point 9	0.34995 mL	0.06785 mL	0.04539 mL	1.15005 mL	2.462	-0.00405	0.31626	0.0003
10:33.9	Data point 10	0.34995 mL	0.06785 mL	0.04972 mL	1.15005 mL	2.542	0.00416	0.40077	0.0003
10:55.6	Data point 11	0.34995 mL	0.06785 mL	0.05270 mL	1.15005 mL	2.635	0.00857	0.77004	0.0004
11:22.6	Data point 12	0.34995 mL	0.06785 mL	0.05567 mL	1.15005 mL	2.732	0.00150	0.10561	0.0002
11:39.2	Data point 13	0.34995 mL	0.06785 mL	0.05800 mL	1.15005 mL	2.822	0.00482	0.49566	0.0003
11:55.8	Data point 14	0.34995 mL	0.06785 mL	0.05988 mL	1.15005 mL	2.911	0.00448	0.64911	0.0002
12:12.4	Data point 15	0.34995 mL	0.06785 mL	0.06141 mL	1.15005 mL	3.024	0.00485	0.64078	0.0003
12:29.0	Data point 16	0.34995 mL	0.06785 mL	0.06258 mL	1.15005 mL	3.127	0.00817	0.83243	0.0004
12:45.5	Data point 17	0.34995 mL	0.06785 mL	0.06352 mL	1.15005 mL	3.232	0.01204	0.94947	0.0006
13:02.0	Data point 18	0.34995 mL	0.06785 mL	0.06425 mL	1.15005 mL	3.324	0.01558	0.92717	0.0008
13:18.5	Data point 19	0.34995 mL	0.06785 mL	0.06484 mL	1.15005 mL	3.412	0.01645	0.95658	0.0008
13:35.1	Data point 20	0.34995 mL	0.06785 mL	0.06533 mL	1.15005 mL	3.502	0.01811	0.97716	0.0009
13:51.7	Data point 21	0.34995 mL	0.06785 mL	0.06573 mL	1.15005 mL	3.593	0.02415	0.95559	0.0012
14:08.2	Data point 22	0.34995 mL	0.06785 mL	0.06604 mL	1.15005 mL	3.665	0.02895	0.98744	0.0014
14:29.9	Data point 23	0.34995 mL	0.06785 mL	0.06651 mL	1.15005 mL	3.825	0.03755	0.99024	0.0018

Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
15:01.7	Data point 24	0.34995 mL	0.06785 mL	0.06743 mL	1.15005 mL	4.019	0.04281	0.97404	0.00214	10.0 s
15:23.3	Data point 25	0.34995 mL	0.06785 mL	0.06764 mL	1.15005 mL	4.141	0.08228	0.97233	0.00411	10.0 s
15:50.0	Data point 26	0.34995 mL	0.06785 mL	0.06783 mL	1.15005 mL	4.273	0.10056	0.98825	0.00499	12.5 s
16:19.2	Data point 27	0.34995 mL	0.06785 mL	0.06794 mL	1.15005 mL	4.411	0.09477	0.90367	0.00492	14.0 s
16:50.0	Data point 28	0.34995 mL	0.06785 mL	0.06804 mL	1.15005 mL	4.585	0.09848	0.96992	0.00493	22.5 s
17:29.3	Data point 29	0.34995 mL	0.06785 mL	0.06813 mL	1.15005 mL	4.834	0.09850	0.98731	0.00489	39.0 s
18:25.0	Data point 30	0.34995 mL	0.06785 mL	0.06820 mL	1.15005 mL	5.076	0.10055	0.99406	0.00498	48.0 s
19:29.9	Data point 31	0.34995 mL	0.06785 mL	0.06827 mL	1.15005 mL	5.427	0.08396	0.79301	0.00465	49.5 s
20:35.9	Data point 32	0.34995 mL	0.06785 mL	0.06834 mL	1.15005 mL	5.915	0.09646	0.96687	0.00484	52.0 s
21:44.6	Data point 33	0.34995 mL	0.06785 mL	0.06841 mL	1.15005 mL	6.547	0.16250	0.99501	0.00804	Timed out at 59.5 s
22:56.0	Data point 34	0.34995 mL	0.06785 mL	0.06846 mL	1.15005 mL	6.972	0.10759	0.99439	0.00532	Timed out at 59.5 s
24:07.7	Data point 35	0.34995 mL	0.06785 mL	0.06851 mL	1.15005 mL	7.383	0.09990	0.99360	0.00494	59.0 s
25:18.4	Data point 36	0.34995 mL	0.06785 mL	0.06856 mL	1.15005 mL	7.797	0.09286	0.93609	0.00474	50.5 s
26:25.4	Data point 37	0.34995 mL	0.06785 mL	0.06863 mL	1.15005 mL	8.643	0.09097	0.93006	0.00466	44.0 s
27:26.1	Data point 38	0.34995 mL	0.06785 mL	0.06870 mL	1.15005 mL	9.063	0.09854	0.96496	0.00495	31.5 s
28:14.5	Data point 39	0.34995 mL	0.06785 mL	0.06877 mL	1.15005 mL	9.326	0.07302	0.71688	0.00426	19.5 s
28:50.7	Data point 40	0.34995 mL	0.06785 mL	0.06884 mL	1.15005 mL	9.553	0.09819	0.97051	0.00492	21.5 s
29:28.9	Data point 41	0.34995 mL	0.06785 mL	0.06891 mL	1.15005 mL	9.702	0.09928	0.97400	0.00496	16.5 s
30:02.0	Data point 42	0.34995 mL	0.06785 mL	0.06898 mL	1.15005 mL	9.825	0.09896	0.99027	0.00491	14.0 s
30:32.8	Data point 43	0.34995 mL	0.06785 mL	0.06907 mL	1.15005 mL	9.975	0.09437	0.97442	0.00472	11.0 s
31:00.5	Data point 44	0.34995 mL	0.06785 mL	0.06917 mL	1.15005 mL	10.095	0.09268	0.97685	0.00463	10.0 s
31:22.1	Data point 45	0.34995 mL	0.06785 mL	0.06928 mL	1.15005 mL	10.220	0.06602	0.98233	0.00329	10.0 s
31:48.8	Data point 46	0.34995 mL	0.06785 mL	0.06943 mL	1.15005 mL	10.334	0.04233	0.94487	0.00215	10.0 s
32:10.5	Data point 47	0.34995 mL	0.06785 mL	0.06959 mL	1.15005 mL	10.444	0.03117	0.97206	0.00156	10.0 s
32:32.1	Data point 48	0.34995 mL	0.06785 mL	0.06978 mL	1.15005 mL	10.578	0.02074	0.94808	0.00105	10.0 s
32:53.8	Data point 49	0.34995 mL	0.06785 mL	0.07001 mL	1.15005 mL	10.677	0.01104	0.84098	0.00059	10.0 s
33:10.4	Data point 50	0.34995 mL	0.06785 mL	0.07030 mL	1.15005 mL	10.833	0.00686	0.86102	0.00036	10.0 s

Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
33:32.0	Data point 51	0.34995 mL	0.06785 mL	0.07072 mL	1.15005 mL	10.942	0.00090	0.08593	0.00015	10.0 s
33:48.4	Data point 52	0.34995 mL	0.06785 mL	0.07124 mL	1.15005 mL	11.053	-0.00449	0.45584	0.00033	10.0 s
34:05.0	Data point 53	0.34995 mL	0.06785 mL	0.07190 mL	1.15005 mL	11.143	-0.00140	0.16210	0.00017	10.0 s
34:21.7	Data point 54	0.34995 mL	0.06785 mL	0.07270 mL	1.15005 mL	11.229	-0.00520	0.65238	0.00032	10.0 s
34:38.4	Data point 55	0.34995 mL	0.06785 mL	0.07368 mL	1.15005 mL	11.311	-0.00623	0.75370	0.00035	10.0 s
35:05.4	Data point 56	0.34995 mL	0.06785 mL	0.07514 mL	1.15005 mL	11.404	-0.00591	0.71459	0.00035	10.0 s
35:32.3	Data point 57	0.34995 mL	0.06785 mL	0.07742 mL	1.15005 mL	11.505	-0.00452	0.58313	0.00029	10.0 s
35:59.1	Data point 58	0.34995 mL	0.06785 mL	0.07942 mL	1.15005 mL	11.599	-0.00740	0.68557	0.00044	10.0 s
36:15.7	Data point 59	0.34995 mL	0.06785 mL	0.08170 mL	1.15005 mL	11.691	-0.00542	0.47103	0.00039	10.0 s
36:32.4	Data point 60	0.34995 mL	0.06785 mL	0.08452 mL	1.15005 mL	11.771	-0.00310	0.32569	0.00027	10.0 s
36:59.3	Data point 61	0.34995 mL	0.06785 mL	0.08911 mL	1.15005 mL	11.870	-0.00793	0.66513	0.00048	10.0 s
37:26.3	Data point 62	0.34995 mL	0.06785 mL	0.09419 mL	1.15005 mL	11.962	-0.00816	0.66475	0.00049	10.0 s
37:48.1	Data point 63	0.34995 mL	0.06785 mL	0.09925 mL	1.15005 mL	12.035	-0.00473	0.38766	0.00037	10.0 s
39:29.5	Reference spectrum									
40:33.3	Data point 65	0.50000 mL	0.16251 mL	0.09927 mL	1.15005 mL	1.999	-0.05445	0.91099	0.00281	10.0 s
41:00.5	Data point 66	0.50000 mL	0.16251 mL	0.11258 mL	1.15005 mL	2.099	0.00694	0.38799	0.00055	10.0 s
41:17.2	Data point 67	0.50000 mL	0.16251 mL	0.12321 mL	1.15005 mL	2.205	0.02043	0.79514	0.00113	10.0 s
41:33.9	Data point 68	0.50000 mL	0.16251 mL	0.13154 mL	1.15005 mL	2.311	0.00329	0.05690	0.00068	10.0 s
41:50.6	Data point 69	0.50000 mL	0.16251 mL	0.13805 mL	1.15005 mL	2.415	0.01528	0.77111	0.00086	10.0 s
42:07.3	Data point 70	0.50000 mL	0.16251 mL	0.14318 mL	1.15005 mL	2.528	0.01374	0.88560	0.00072	10.0 s
42:24.0	Data point 71	0.50000 mL	0.16251 mL	0.14713 mL	1.15005 mL	2.628	0.01445	0.89726	0.00075	10.0 s
42:40.7	Data point 72	0.50000 mL	0.16251 mL	0.15028 mL	1.15005 mL	2.735	0.01168	0.82651	0.00063	10.0 s
42:57.4	Data point 73	0.50000 mL	0.16251 mL	0.15275 mL	1.15005 mL	2.847	0.01291	0.90682	0.00067	10.0 s
43:14.2	Data point 74	0.50000 mL	0.16251 mL	0.15468 mL	1.15005 mL	2.944	0.01235	0.92662	0.00063	10.0 s
43:30.8	Data point 75	0.50000 mL	0.16251 mL	0.15621 mL	1.15005 mL	3.037	0.01311	0.91877	0.00068	10.0 s
43:47.5	Data point 76	0.50000 mL	0.16251 mL	0.15746 mL	1.15005 mL	3.120	0.01436	0.87065	0.00076	10.0 s
44:14.3	Data point 77	0.50000 mL	0.16251 mL	0.15842 mL	1.15005 mL	3.211	0.01143	0.85103	0.00061	10.0 s
44:30.9	Data point 78	0.50000 mL	0.16251 mL	0.15924 mL	1.15005 mL	3.343	0.01435	0.93006	0.00073	10.0 s
44:57.7	Data point 79	0.50000 mL	0.16251 mL	0.15981 mL	1.15005 mL	3.437	0.01330	0.83790	0.00072	10.0 s

Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
45:14.3	Data point 80	0.50000 mL	0.16251 mL	0.16030 mL	1.15005 mL	3.561	0.02604	0.93601	0.00133	10.0 s
45:41.2	Data point 81	0.50000 mL	0.16251 mL	0.16068 mL	1.15005 mL	3.657	0.01883	0.92087	0.00097	10.0 s
45:57.7	Data point 82	0.50000 mL	0.16251 mL	0.16098 mL	1.15005 mL	3.781	0.03435	0.97586	0.00172	10.0 s
46:19.3	Data point 83	0.50000 mL	0.16251 mL	0.16129 mL	1.15005 mL	3.914	0.03835	0.97574	0.00192	10.0 s
46:41.0	Data point 84	0.50000 mL	0.16251 mL	0.16157 mL	1.15005 mL	4.098	0.07002	0.98005	0.00349	10.0 s
47:02.7	Data point 85	0.50000 mL	0.16251 mL	0.16176 mL	1.15005 mL	4.246	0.07969	0.98693	0.00396	10.0 s
47:24.3	Data point 86	0.50000 mL	0.16251 mL	0.16190 mL	1.15005 mL	4.364	0.09773	0.98297	0.00486	12.0 s
47:47.9	Data point 87	0.50000 mL	0.16251 mL	0.16199 mL	1.15005 mL	4.493	0.09830	0.97524	0.00491	18.5 s
48:23.1	Data point 88	0.50000 mL	0.16251 mL	0.16209 mL	1.15005 mL	4.668	0.09980	0.99125	0.00495	24.0 s
48:58.9	Data point 89	0.50000 mL	0.16251 mL	0.16216 mL	1.15005 mL	4.841	0.09806	0.98918	0.00487	29.0 s
49:44.6	Data point 90	0.50000 mL	0.16251 mL	0.16223 mL	1.15005 mL	5.121	0.09552	0.95420	0.00483	34.5 s
50:36.0	Data point 91	0.50000 mL	0.16251 mL	0.16230 mL	1.15005 mL	5.474	0.10058	0.99436	0.00498	41.5 s
51:29.1	Data point 92	0.50000 mL	0.16251 mL	0.16235 mL	1.15005 mL	5.741	0.09883	0.95655	0.00499	39.5 s
52:20.4	Data point 93	0.50000 mL	0.16251 mL	0.16239 mL	1.15005 mL	6.036	0.09811	0.99172	0.00486	47.5 s
53:19.6	Data point 94	0.50000 mL	0.16251 mL	0.16244 mL	1.15005 mL	6.343	0.10007	0.99499	0.00495	51.5 s
54:22.7	Data point 95	0.50000 mL	0.16251 mL	0.16251 mL	1.15005 mL	6.905	0.09836	0.98297	0.00490	54.0 s
55:33.5	Data point 96	0.50000 mL	0.16251 mL	0.16258 mL	1.15005 mL	7.589	0.09858	0.97894	0.00492	55.5 s
56:45.7	Data point 97	0.50000 mL	0.16251 mL	0.16265 mL	1.15005 mL	8.453	0.07907	0.83578	0.00427	41.5 s
57:43.8	Data point 98	0.50000 mL	0.16251 mL	0.16272 mL	1.15005 mL	8.921	0.09543	0.94859	0.00483	32.0 s
58:27.4	Data point 99	0.50000 mL	0.16251 mL	0.16277 mL	1.15005 mL	9.105	0.09595	0.97351	0.00480	23.5 s
59:02.5	Data point 100	0.50000 mL	0.16251 mL	0.16282 mL	1.15005 mL	9.260	0.09637	0.97179	0.00483	20.5 s
59:39.7	Data point 101	0.50000 mL	0.16251 mL	0.16289 mL	1.15005 mL	9.456	0.09748	0.98700	0.00484	18.0 s
1:00:14.5	Data point 102	0.50000 mL	0.16251 mL	0.16296 mL	1.15005 mL	9.584	0.10013	0.98134	0.00499	13.5 s
1:00:49.9	Data point 103	0.50000 mL	0.16251 mL	0.16305 mL	1.15005 mL	9.728	0.09475	0.96389	0.00476	12.5 s
1:01:19.3	Data point 104	0.50000 mL	0.16251 mL	0.16317 mL	1.15005 mL	9.864	0.09994	0.98646	0.00496	11.5 s
1:01:47.6	Data point 105	0.50000 mL	0.16251 mL	0.16329 mL	1.15005 mL	9.988	0.07459	0.98956	0.00370	10.0 s
1:02:14.3	Data point 106	0.50000 mL	0.16251 mL	0.16343 mL	1.15005 mL	10.103	0.05300	0.96969	0.00266	10.0 s
1:02:41.1	Data point 107	0.50000 mL	0.16251 mL	0.16359 mL	1.15005 mL	10.212	0.03560	0.92231	0.00183	10.0 s

Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dtime
1:03:02.7	Data point 108	0.50000 mL	0.16251 mL	0.16378 mL	1.15005 mL	10.309	0.02665	0.94983	0.00135	10.0 s
1:03:24.3	Data point 109	0.50000 mL	0.16251 mL	0.16399 mL	1.15005 mL	10.416	0.01858	0.91191	0.00096	10.0 s
1:03:46.1	Data point 110	0.50000 mL	0.16251 mL	0.16432 mL	1.15005 mL	10.543	0.00906	0.71583	0.00053	10.0 s
1:04:07.8	Data point 111	0.50000 mL	0.16251 mL	0.16479 mL	1.15005 mL	10.669	0.00387	0.44036	0.00029	10.0 s
1:04:29.5	Data point 112	0.50000 mL	0.16251 mL	0.16550 mL	1.15005 mL	10.767	-0.00053	0.00774	0.00030	10.0 s
1:04:51.2	Data point 113	0.50000 mL	0.16251 mL	0.16623 mL	1.15005 mL	10.885	-0.00582	0.70799	0.00034	10.0 s
1:05:23.2	Data point 114	0.50000 mL	0.16251 mL	0.16717 mL	1.15005 mL	10.999	-0.00305	0.23034	0.00031	10.0 s
1:05:55.2	Data point 115	0.50000 mL	0.16251 mL	0.16820 mL	1.15005 mL	11.114	-0.00359	0.36695	0.00029	10.0 s
1:06:21.9	Data point 116	0.50000 mL	0.16251 mL	0.16919 mL	1.15005 mL	11.209	-0.00891	0.80635	0.00049	10.0 s
1:06:38.5	Data point 117	0.50000 mL	0.16251 mL	0.17046 mL	1.15005 mL	11.299	-0.00842	0.86560	0.00045	10.0 s
1:06:55.1	Data point 118	0.50000 mL	0.16251 mL	0.17204 mL	1.15005 mL	11.382	-0.00960	0.76837	0.00054	10.0 s
1:07:22.0	Data point 119	0.50000 mL	0.16251 mL	0.17446 mL	1.15005 mL	11.475	-0.00724	0.51657	0.00050	10.0 s
1:07:48.9	Data point 120	0.50000 mL	0.16251 mL	0.17747 mL	1.15005 mL	11.571	-0.00775	0.64609	0.00048	10.0 s
1:08:16.0	Data point 121	0.50000 mL	0.16251 mL	0.18079 mL	1.15005 mL	11.665	-0.00866	0.76633	0.00049	10.0 s
1:08:32.6	Data point 122	0.50000 mL	0.16251 mL	0.18443 mL	1.15005 mL	11.736	-0.00613	0.67310	0.00037	10.0 s
1:08:59.6	Data point 123	0.50000 mL	0.16251 mL	0.18972 mL	1.15005 mL	11.832	-0.00603	0.68737	0.00036	10.0 s
1:09:26.8	Data point 124	0.50000 mL	0.16251 mL	0.19675 mL	1.15005 mL	11.927	-0.00536	0.69822	0.00032	10.0 s
1:09:54.0	Data point 125	0.50000 mL	0.16251 mL	0.20543 mL	1.15005 mL	12.019	-0.00268	0.26932	0.00025	10.0 s
1:11:38.7	Reference spectrum									
1:13:01.9	Data point 127	0.83996 mL	0.28918 mL	0.20546 mL	1.15005 mL	2.001	-0.02888	0.94963	0.00146	10.0 s
1:13:29.3	Data point 128	0.83996 mL	0.28918 mL	0.22079 mL	1.15005 mL	2.101	0.00818	0.38893	0.00065	10.0 s
1:13:46.2	Data point 129	0.83996 mL	0.28918 mL	0.23276 mL	1.15005 mL	2.204	0.00459	0.36893	0.00037	10.0 s
1:14:03.1	Data point 130	0.83996 mL	0.28918 mL	0.24262 mL	1.15005 mL	2.315	0.02411	0.89587	0.00126	10.0 s
1:14:20.0	Data point 131	0.83996 mL	0.28918 mL	0.24993 mL	1.15005 mL	2.413	0.00105	0.01497	0.00042	10.0 s
1:14:36.8	Data point 132	0.83996 mL	0.28918 mL	0.25593 mL	1.15005 mL	2.519	0.00927	0.78968	0.00051	10.0 s
1:14:53.6	Data point 133	0.83996 mL	0.28918 mL	0.26056 mL	1.15005 mL	2.624	0.00776	0.63687	0.00048	10.0 s
1:15:10.4	Data point 134	0.83996 mL	0.28918 mL	0.26421 mL	1.15005 mL	2.730	0.00114	0.02875	0.00033	10.0 s
1:15:27.1	Data point 135	0.83996 mL	0.28918 mL	0.26710 mL	1.15005 mL	2.819	0.00344	0.28752	0.00032	10.0 s
1:15:43.7	Data point 136	0.83996 mL	0.28918 mL	0.26945 mL	1.15005 mL	2.918	0.00013	0.00047	0.00029	10.0 s

Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:16:00.3	Data point 137	0.83996 mL	0.28918 mL	0.27133 mL	1.15005 mL	3.032	0.00335	0.26964	0.00032	10.0 s
1:16:16.9	Data point 138	0.83996 mL	0.28918 mL	0.27277 mL	1.15005 mL	3.129	0.00621	0.53123	0.00042	10.0 s
1:16:33.4	Data point 139	0.83996 mL	0.28918 mL	0.27392 mL	1.15005 mL	3.216	0.00806	0.69241	0.00048	10.0 s
1:16:49.9	Data point 140	0.83996 mL	0.28918 mL	0.27486 mL	1.15005 mL	3.305	0.00598	0.55949	0.00039	10.0 s
1:17:06.5	Data point 141	0.83996 mL	0.28918 mL	0.27564 mL	1.15005 mL	3.397	0.00634	0.68263	0.00038	10.0 s
1:17:23.0	Data point 142	0.83996 mL	0.28918 mL	0.27625 mL	1.15005 mL	3.481	0.00922	0.68359	0.00055	10.0 s
1:17:44.7	Data point 143	0.83996 mL	0.28918 mL	0.27693 mL	1.15005 mL	3.593	0.01156	0.82755	0.00063	10.0 s
1:18:06.5	Data point 144	0.83996 mL	0.28918 mL	0.27742 mL	1.15005 mL	3.715	0.01369	0.89255	0.00072	10.0 s
1:18:28.1	Data point 145	0.83996 mL	0.28918 mL	0.27789 mL	1.15005 mL	3.881	0.01595	0.80571	0.00088	10.0 s
1:18:49.8	Data point 146	0.83996 mL	0.28918 mL	0.27825 mL	1.15005 mL	4.070	0.03525	0.96078	0.00178	10.0 s
1:19:11.5	Data point 147	0.83996 mL	0.28918 mL	0.27846 mL	1.15005 mL	4.213	0.04960	0.98422	0.00247	10.0 s
1:19:33.2	Data point 148	0.83996 mL	0.28918 mL	0.27862 mL	1.15005 mL	4.373	0.07352	0.98886	0.00365	10.0 s
1:19:54.8	Data point 149	0.83996 mL	0.28918 mL	0.27874 mL	1.15005 mL	4.556	0.09934	0.97705	0.00496	11.0 s
1:20:17.5	Data point 150	0.83996 mL	0.28918 mL	0.27881 mL	1.15005 mL	4.695	0.09673	0.98778	0.00480	17.0 s
1:20:51.2	Data point 151	0.83996 mL	0.28918 mL	0.27888 mL	1.15005 mL	4.888	0.09915	0.99209	0.00491	21.5 s
1:21:24.4	Data point 152	0.83996 mL	0.28918 mL	0.27893 mL	1.15005 mL	5.069	0.09767	0.98738	0.00485	25.0 s
1:22:01.0	Data point 153	0.83996 mL	0.28918 mL	0.27897 mL	1.15005 mL	5.318	0.09998	0.97788	0.00499	31.5 s
1:22:44.2	Data point 154	0.83996 mL	0.28918 mL	0.27902 mL	1.15005 mL	5.604	0.09928	0.99498	0.00491	32.5 s
1:23:28.4	Data point 155	0.83996 mL	0.28918 mL	0.27907 mL	1.15005 mL	5.893	0.09979	0.98873	0.00495	33.0 s
1:24:13.0	Data point 156	0.83996 mL	0.28918 mL	0.27912 mL	1.15005 mL	6.167	0.10018	0.98788	0.00498	31.0 s
1:24:50.4	Data point 157	0.83996 mL	0.28918 mL	0.27916 mL	1.15005 mL	6.422	0.09885	0.98815	0.00491	33.0 s
1:25:35.1	Data point 158	0.83996 mL	0.28918 mL	0.27921 mL	1.15005 mL	6.742	0.10032	0.99521	0.00496	32.5 s
1:26:14.3	Data point 159	0.83996 mL	0.28918 mL	0.27923 mL	1.15005 mL	6.922	0.10014	0.99325	0.00496	36.5 s
1:27:02.2	Data point 160	0.83996 mL	0.28918 mL	0.27928 mL	1.15005 mL	7.386	0.10020	0.98459	0.00498	44.0 s
1:27:58.0	Data point 161	0.83996 mL	0.28918 mL	0.27933 mL	1.15005 mL	8.056	0.08919	0.91796	0.00459	40.0 s
1:28:49.6	Data point 162	0.83996 mL	0.28918 mL	0.27937 mL	1.15005 mL	8.586	0.09390	0.92582	0.00482	29.5 s
1:29:30.7	Data point 163	0.83996 mL	0.28918 mL	0.27942 mL	1.15005 mL	8.891	0.09854	0.95146	0.00499	22.0 s
1:30:04.4	Data point 164	0.83996 mL	0.28918 mL	0.27947 mL	1.15005 mL	9.102	0.09668	0.98334	0.00481	19.0 s
1:30:34.9	Data point 165	0.83996 mL	0.28918 mL	0.27952 mL	1.15005 mL	9.259	0.09813	0.97059	0.00492	16.0 s
1:31:02.4	Data point 166	0.83996 mL	0.28918 mL	0.27956 mL	1.15005 mL	9.382	0.09600	0.97891	0.00479	14.0 s
1:31:33.1	Data point 167	0.83996 mL	0.28918 mL	0.27963 mL	1.15005 mL	9.520	0.09373	0.92865	0.00480	10.0 s
1:31:59.8	Data point 168	0.83996 mL	0.28918 mL	0.27970 mL	1.15005 mL	9.644	0.08349	0.97193	0.00418	10.0 s
1:32:21.4	Data point 169	0.83996 mL	0.28918 mL	0.27980 mL	1.15005 mL	9.784	0.04758	0.96580	0.00239	10.0 s
1:32:48.0	Data point 170	0.83996 mL	0.28918 mL	0.27989 mL	1.15005 mL	9.882	0.04704	0.96694	0.00236	10.0 s
1:33:14.7	Data point 171	0.83996 mL	0.28918 mL	0.28001 mL	1.15005 mL	9.986	0.02581	0.89591	0.00135	10.0 s
1:33:36.3	Data point 172	0.83996 mL	0.28918 mL	0.28013 mL	1.15005 mL	10.079	0.01575	0.77079	0.00088	10.0 s
1:33:52.8	Data point 173	0.83996 mL	0.28918 mL	0.28029 mL	1.15005 mL	10.209	0.00324	0.35699	0.00027	10.0 s
1:34:14.5	Data point 174	0.83996 mL	0.28918 mL	0.28050 mL	1.15005 mL	10.313	-0.00076	0.02200	0.00025	10.0 s
1:34:31.1	Data point 175	0.83996 mL	0.28918 mL	0.28076 mL	1.15005 mL	10.420	-0.00491	0.35136	0.00041	10.0 s
1:34:47.7	Data point 176	0.83996 mL	0.28918 mL	0.28109 mL	1.15005 mL	10.514	-0.00584	0.49809	0.00041	10.0 s
1:35:04.4	Data point 177	0.83996 mL	0.28918 mL	0.28149 mL	1.15005 mL	10.602	-0.00986	0.81608	0.00054	10.0 s
1:35:21.0	Data point 178	0.83996 mL	0.28918 mL	0.28198 mL	1.15005 mL	10.690	-0.00655	0.55536	0.00043	10.0 s
1:35:37.5	Data point 179	0.83996 mL	0.28918 mL	0.28260 mL	1.15005 mL	10.773	-0.01239	0.69315	0.00073	10.0 s
1:36:04.4	Data point 180	0.83996 mL	0.28918 mL	0.28354 mL	1.15005 mL	10.865	-0.01113	0.80449	0.00061	10.0 s
1:36:46.9	Data point 181	0.83996 mL	0.28918 mL	0.28469 mL	1.15005 mL	11.033	-0.01153	0.79541	0.00064	10.0 s
1:37:13.8	Data point 182	0.83996 mL	0.28918 mL	0.28869 mL	1.15005 mL	11.159	-0.01107	0.87018	0.00059	10.0 s
1:37:40.7	Data point 183	0.83996 mL	0.28918 mL	0.29024 mL	1.15005 mL	11.251	-0.01123	0.87445	0.00059	10.0 s
1:37:57.4	Data point 184	0.83996 mL	0.28918 mL	0.29238 mL	1.15005 mL	11.340	-0.01419	0.92621	0.00073	10.0 s
1:38:14.1	Data point 185	0.83996 mL	0.28918 mL	0.29501 mL	1.15005 mL	11.421	-0.01276	0.86557	0.00068	10.0 s
1:38:35.9	Data point 186	0.83996 mL	0.28918 mL	0.29882 mL	1.15005 mL	11.510	-0.01166	0.87899	0.00061	10.0 s
1:39:03.0	Data point 187	0.83996 mL	0.28918 mL	0.30299 mL	1.15005 mL	11.602	-0.00825	0.73344	0.00048	10.0 s
1:39:19.7	Data point 188	0.83996 mL	0.28918 mL	0.30781 mL	1.15005 mL	11.674	-0.01153	0.80253	0.00064	10.0 s
1:39:46.7	Data point 189	0.83996 mL	0.28918 mL	0.31406 mL	1.15005 mL	11.766	-0.00675	0.61894	0.00042	10.0 s
1:40:03.4	Data point 190	0.83996 mL	0.28918 mL	0.32112 mL	1.15005 mL	11.847	-0.01157	0.79726	0.00064	10.0 s
1:40:30.7	Data point 191	0.83996 mL	0.28918 mL	0.33184 mL	1.15005 mL	11.941	-0.00792	0.73205	0.00046	10.0 s
1:40:52.8	Data point 192	0.83996 mL	0.28918 mL	0.34221 mL	1.15005 mL	12.016	-0.00639	0.56993	0.00042	10.0 s
1:42:52.1	Assay volumes	1.08996 mL	0.42620 mL	0.34221 mL	1.15005 mL					

Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

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	1.15 mL			
Cosolvent added	Automatic			
ISA water volume	0.35 mL			
Water added	Automatic			
Buffer in use	No			
After medium addition, stir for	5 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	30 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	0.15 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Titration 3				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			

Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Add additional water	0.34 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Data Point Stability				
Stir during data point collection	Yes			
For point collection, stir at	15%			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00500 dpH/dt			
Stability timeout after	60 seconds			
Experiment cleanup				
Adjust pH to cleanup	To start pH			
And then stir for	60 seconds			
For cleaning, stir at	20%			
Then add water volume	0.25 mL			
And then stir for	30 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.109	10/12/2017 6:46:11 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus S	1.0007	10/12/2017 6:46:11 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jH	0.3	10/12/2017 6:46:11 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jOH	-0.2	10/12/2017 6:46:11 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Base concentration factor	1.011	10/12/2017 6:46:12 AM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	0.995	10/12/2017 6:46:11 AM	C:\Sirius_T3\17J-11005_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)	10-10-2017	10/10/2017 10:48:53 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
Syringe volume	0.5 mL		

Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Firmware version	1.2.1(r2)		
Titrant	Phosphate Buffer		10/10/2017 9:57:33 AM
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	-8.33 mV		10/12/2017 6:46:35 AM
Filling solution	3M KCl	KCL095	10/10/2017 9:58:43 AM
Liquids			
Wash 1	50% IPA:50% Water		10/11/2017 8:31:15 AM
Wash 2	0.5% Trition X-100 in H20		10/11/2017 8:31:17 AM
Buffer position 1	pH7 Wash		10/11/2017 8:31:21 AM
Buffer position 2	pH 7		10/11/2017 8:31:23 AM
Storage position			10/11/2017 8:31:26 AM
Wash water	4.5e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	5.6e+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	419:28:33		11/23/2010 12:22:28 PM
Calibrated on	10/11/2017 8:30:19 AM		
Integration time	10		
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%		

Sample name: **M07**
Assay name: **UV-metric psKa**
Assay ID: **17J-12006**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12006_M07_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 6:46:12 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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 C1