Yasuda-Shedlovsky Result

Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

Experiment start time: **10/11/2017 5:31:56 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

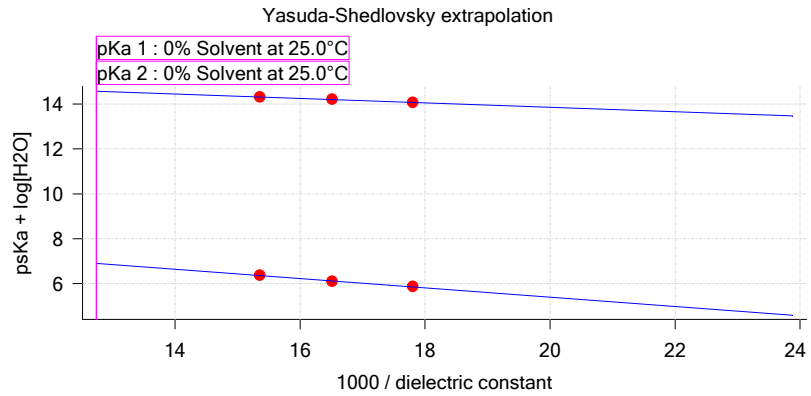
Yasuda-Shedlovsky result

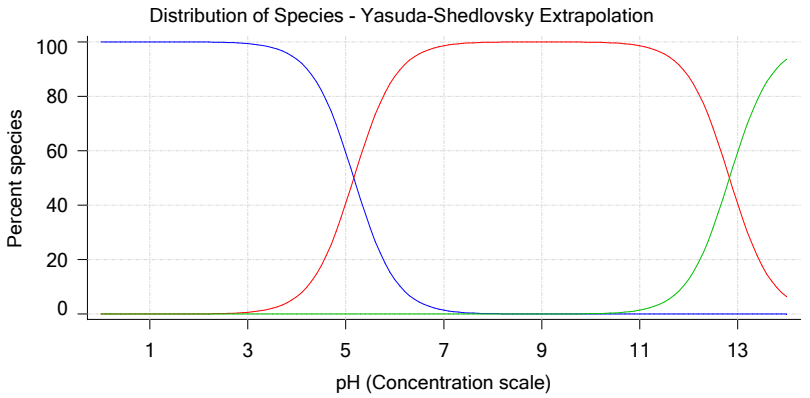
Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.16	±0.07	9.55	-207.1663	0.9931	0.166 M	25.0°C
Yasuda-Shedlovsky	12.83	±0.03	15.84	-99.3936	0.9946	0.166 M	25.0°C

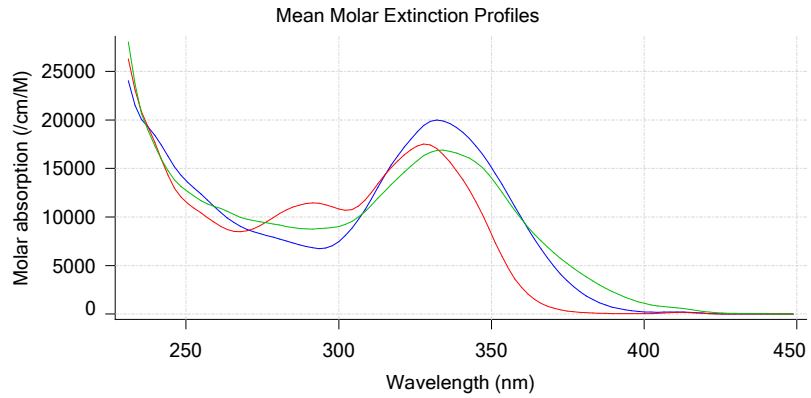
Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1	psKa 2
17J-11014 Points 4 to 65	50.42 %	Up	UV-metric pKa	56.2	24.2 M	0.159 M	24.9°C ☑	4.49 ☑	12.69
17J-11014 Points 67 to 131	40.94 %	Up	UV-metric pKa	60.6	29.5 M	0.167 M	25.0°C ☑	4.63 ☑	12.74
17J-11014 Points 133 to 204	30.92 %	Up	UV-metric pKa	65.1	35.3 M	0.172 M	24.9°C ☑	4.83 ☑	12.76

Graphs







UV-metric psKa Titration 1 of 3 17J-11014 Points 4 to 65

Results

pKa 1	**4.49**
pKa 2	**12.69**
RMSD	**0.002 0.004 0.005**
Chi squared	**0.2213**
PCA calculated number of pKas	**4**
Average ionic strength	**0.159 M**
Average temperature	**24.9°C**
Analyte concentration range	**71.3 µM to 67.1 µM**
Methanol weight %	**50.4 %**
Dielectric constant	**56.2**
Water concentration	**24.2 M**

Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

Experiment start time: **10/11/2017 5:31:56 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
Wavelength clipping **237.3 nm to 450.0 nm**
pH clipping **1.458 to 12.511**

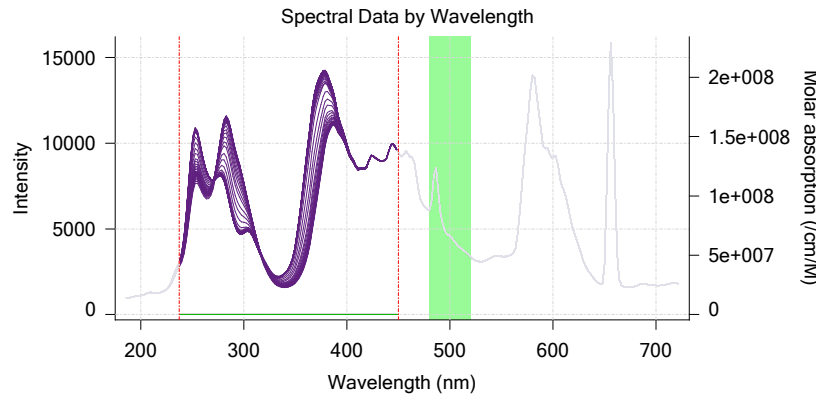
Warnings and errors

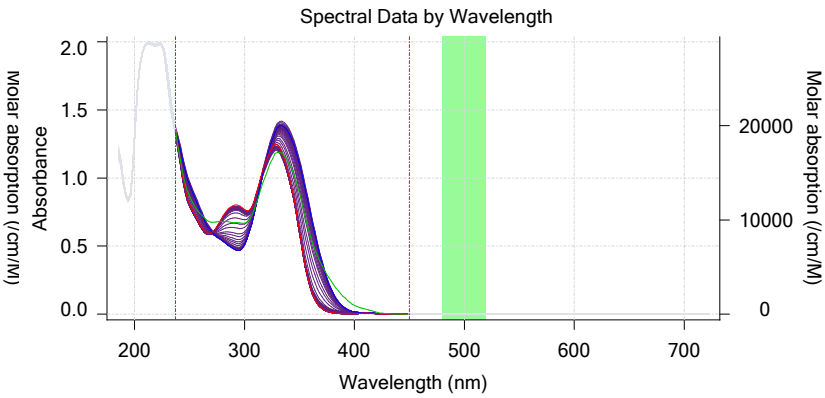
Errors None
Warnings Calculated pKa outside clip range
PCA calculation disagrees with predicted number of pKas

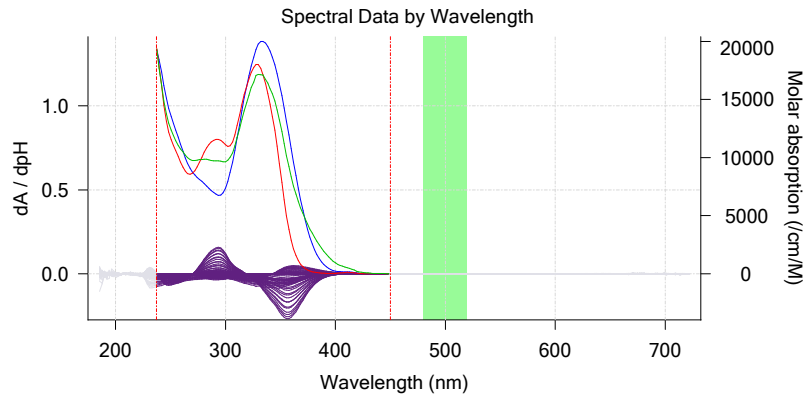
Assay Settings

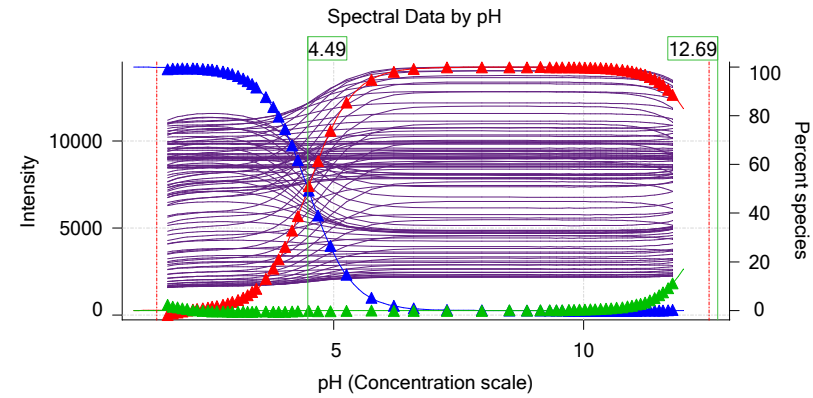
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	No			
Assay Medium				

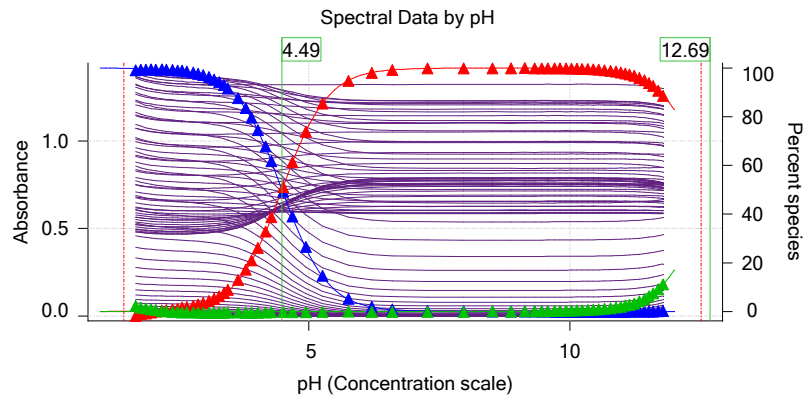
Graphs

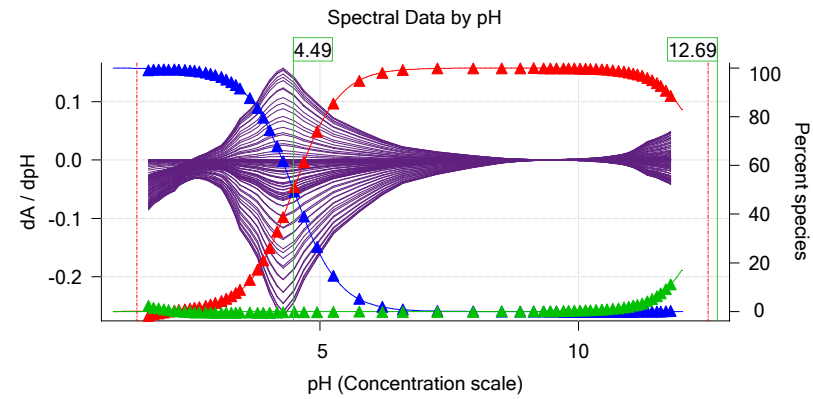








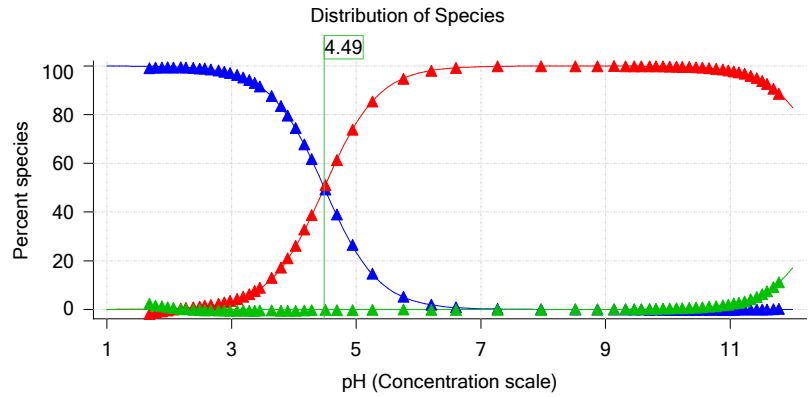


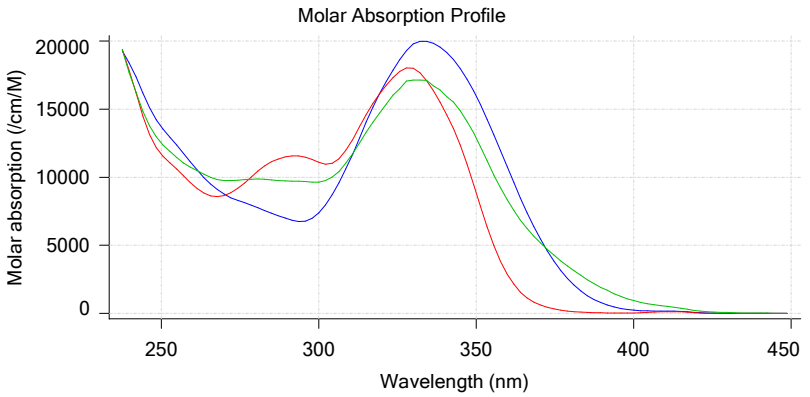


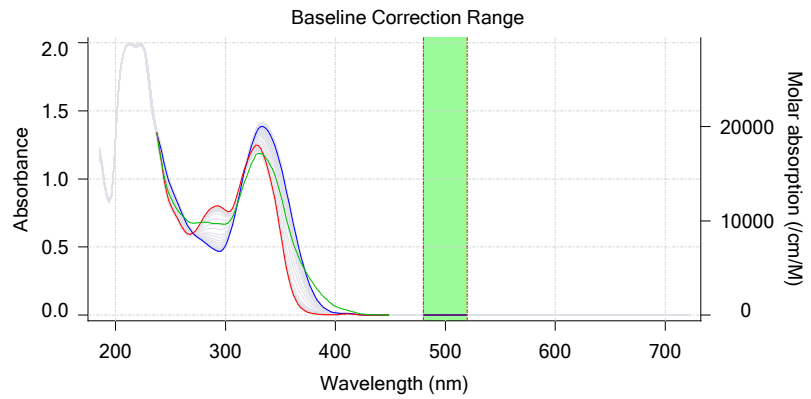
Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

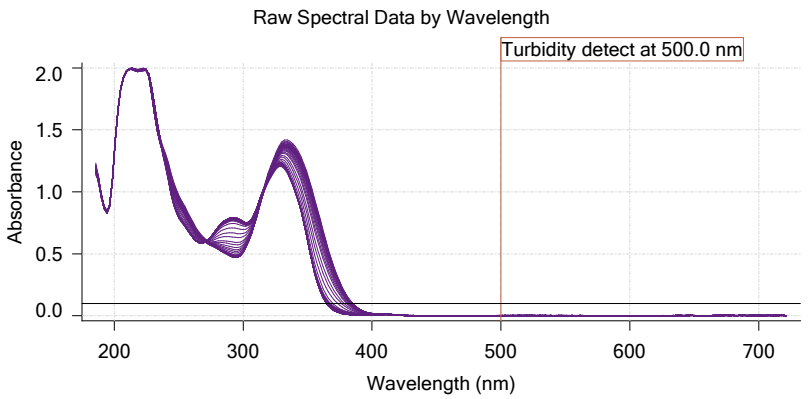
Experiment start time: **10/11/2017 5:31:56 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









UV-metric psKa Titration 2 of 3 17J-11014 Points 67 to 131

Results

pKa 1	**4.63**
pKa 2	**12.74**
RMSD	**0.001 0.003 0.003**
Chi squared	**0.1321**
PCA calculated number of pKas	**4**
Average ionic strength	**0.167 M**
Average temperature	**25.0°C**
Analyte concentration range	**58.7 µM to 55.7 µM**
Methanol weight %	**40.9 %**
Dielectric constant	**60.6**
Water concentration	**29.5 M**
Number of pKas source	**Predicted**
Wavelength clipping	**235.7 nm to 450.0 nm**
pH clipping	**1.484 to 12.503**

Warnings and errors

Errors None
Warnings Calculated pKa outside clip range
PCA calculation disagrees with predicted number of pKas

Assay Settings

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

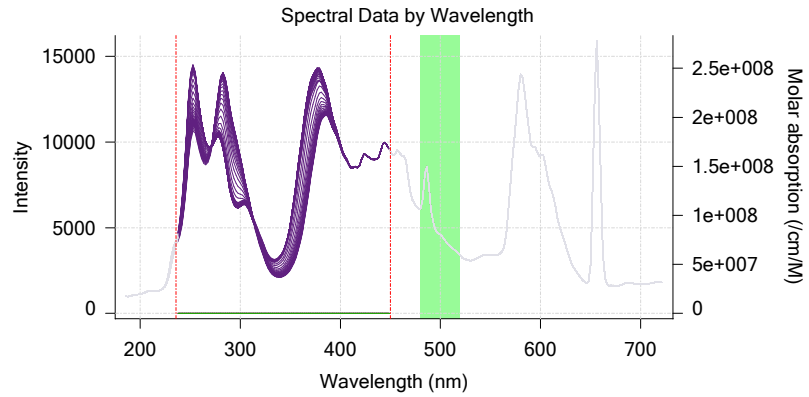
Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

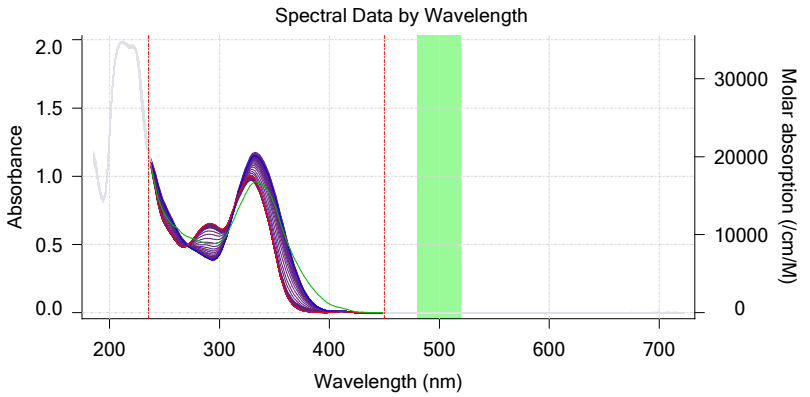
Experiment start time: **10/11/2017 5:31:56 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

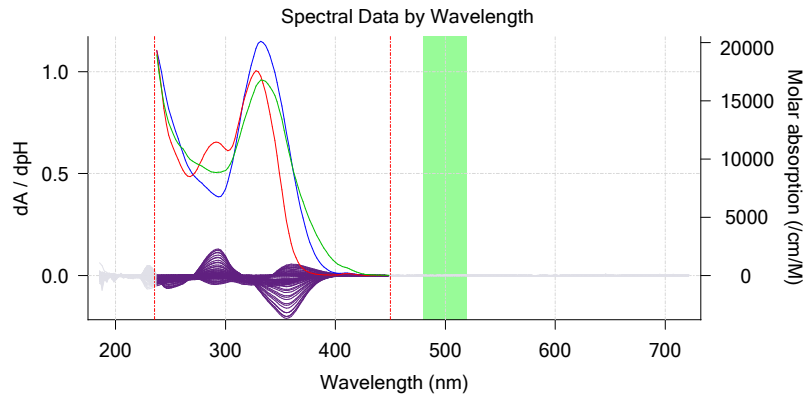
Assay Settings (continued)

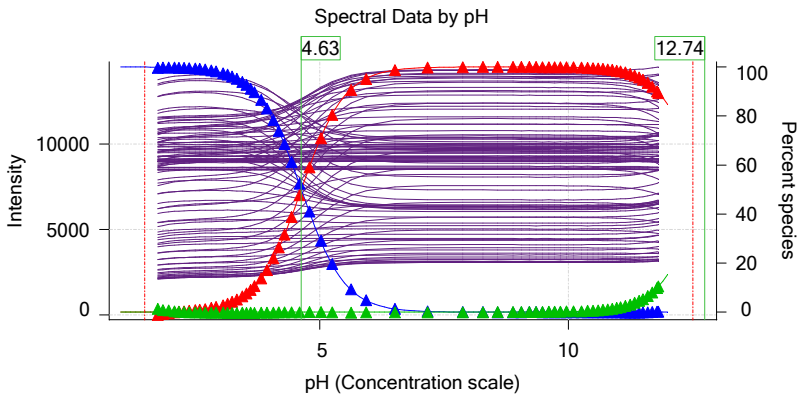
Setting	Value	Original Value	Date/Time changed	Imported from
Assay Medium				

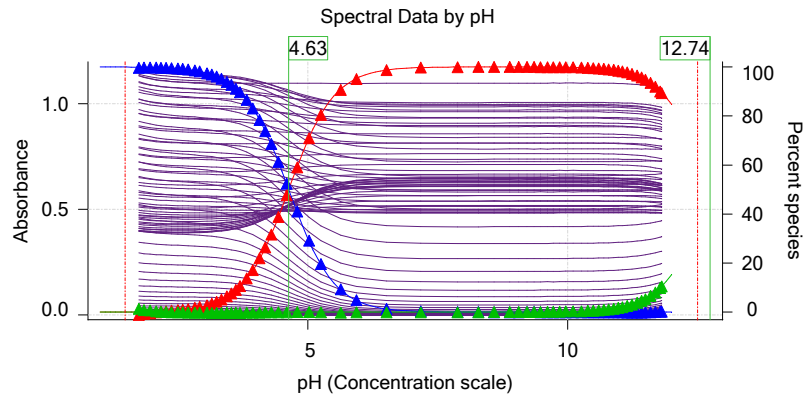
Graphs

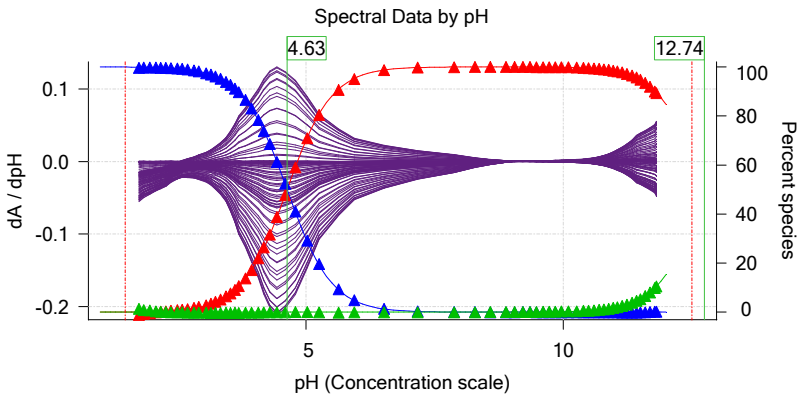








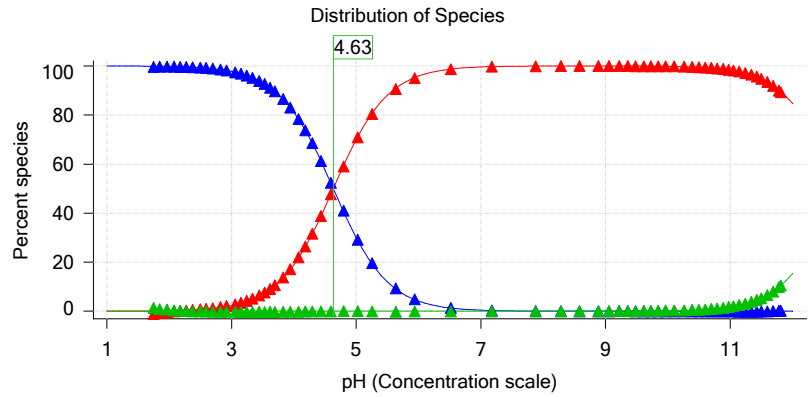


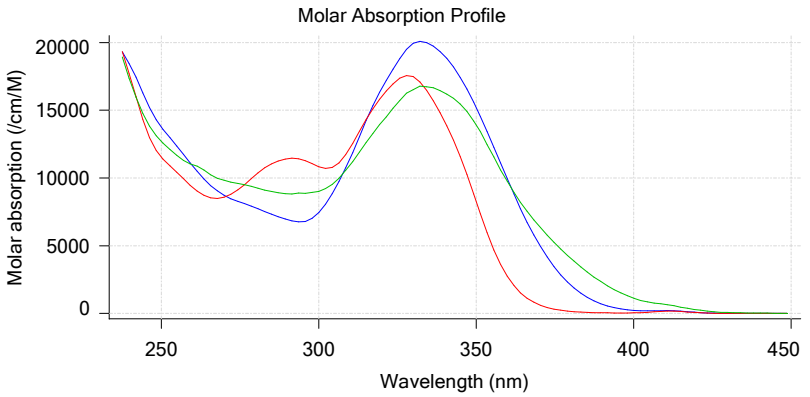


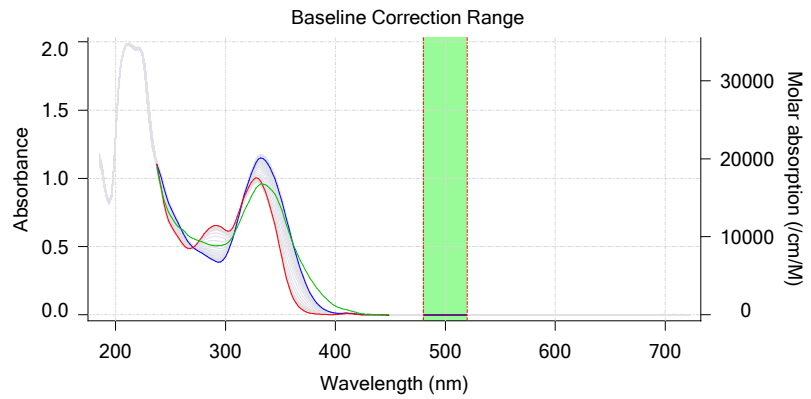
Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

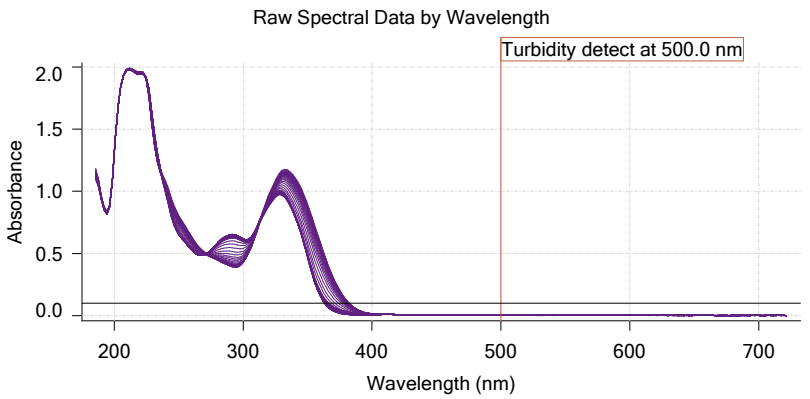
Experiment start time: **10/11/2017 5:31:56 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









UV-metric psKa Titration 3 of 3 17J-11014 Points 133 to 204

Results

pKa 1	**4.83**
pKa 2	**12.76**
RMSD	**0.001 0.002 0.002**
Chi squared	**0.1134**
PCA calculated number of pKas	**4**
Average ionic strength	**0.172 M**
Average temperature	**24.9°C**
Analyte concentration range	**45.3 µM to 43.0 µM**
Methanol weight %	**30.9 %**
Dielectric constant	**65.1**
Water concentration	**35.3 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.480 to 12.501**

Warnings and errors

Errors None
Warnings Calculated pKa outside clip range
PCA calculation disagrees with predicted number of pKas

Assay Settings

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

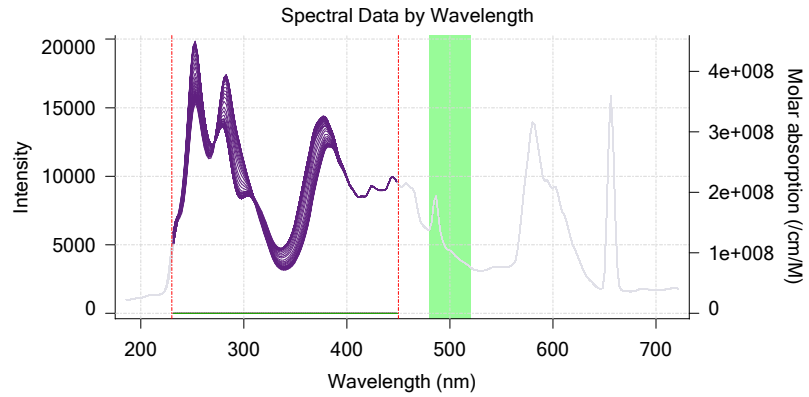
Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

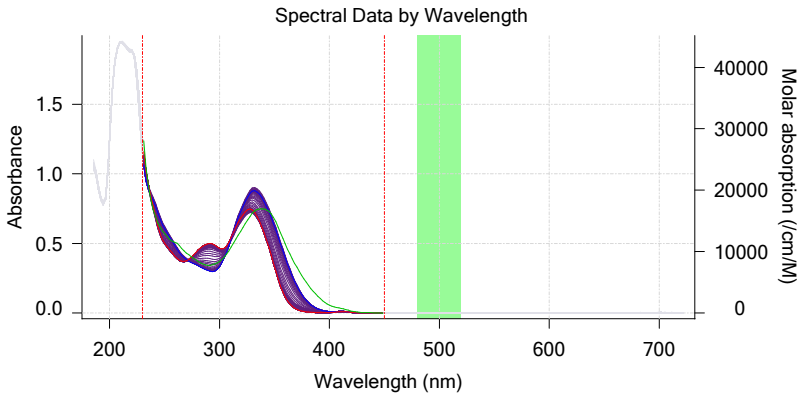
Experiment start time: **10/11/2017 5:31:56 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

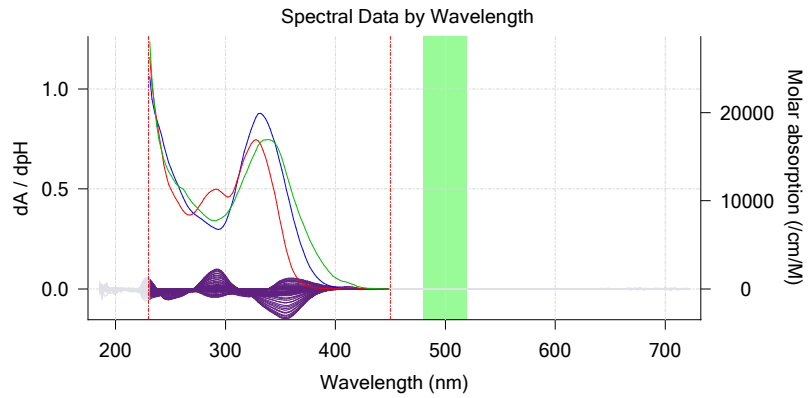
Assay Settings (continued)

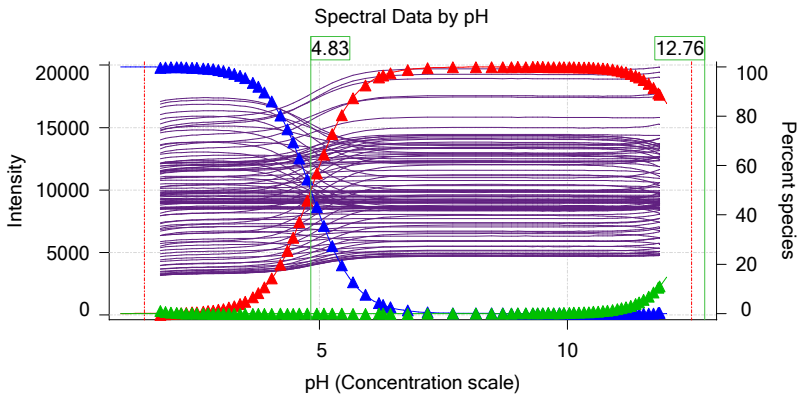
Setting	Value	Original Value	Date/Time changed	Imported from
Assay Medium				

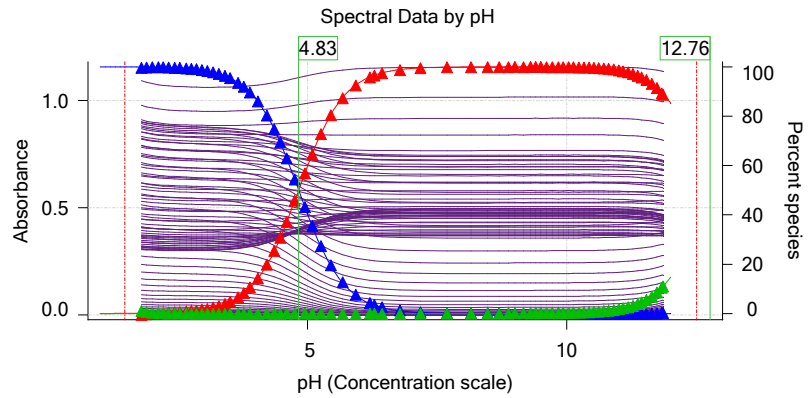
Graphs

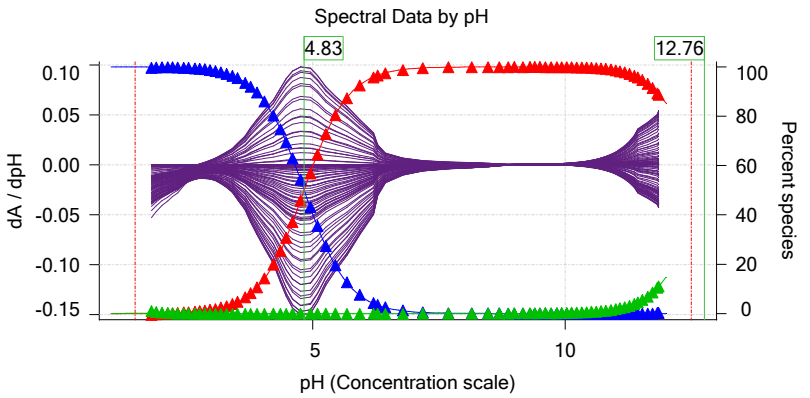








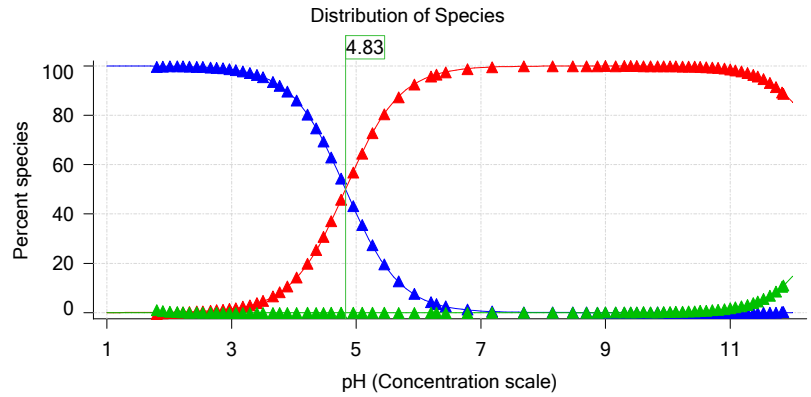


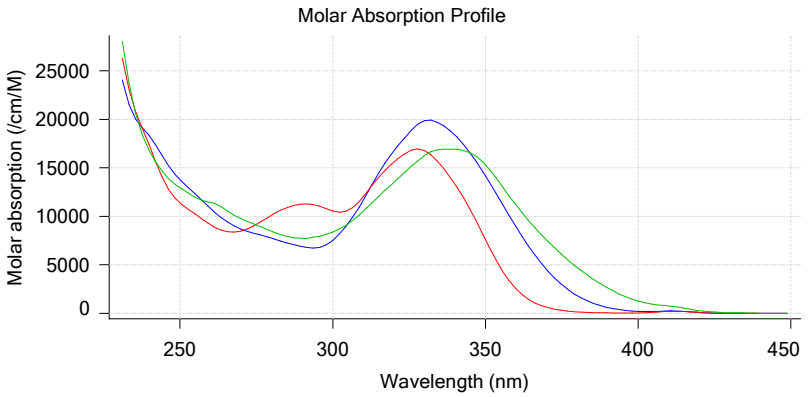


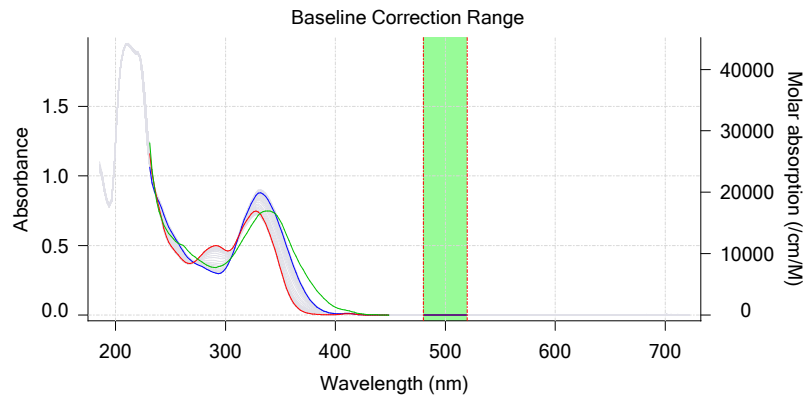
Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

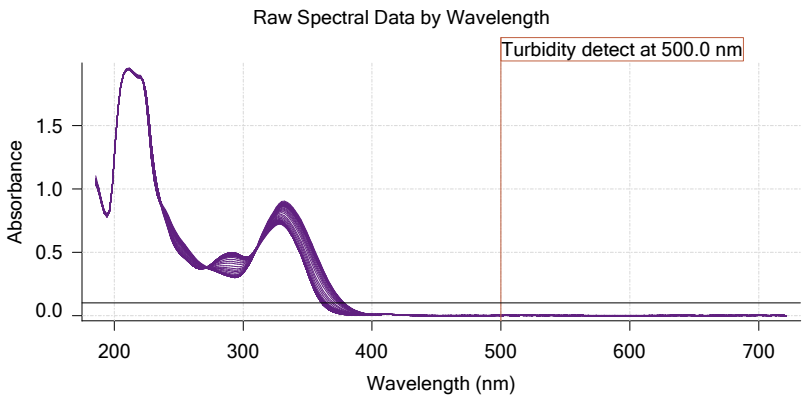
Experiment start time: **10/11/2017 5:31:56 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M12	10/3/2017 3:44:45 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0030 mL	10/3/2017 3:44:45 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.037300 M	10/3/2017 3:44:45 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	292.16	10/3/2017 3:44:53 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	10/3/2017 3:44:45 PM	User entered value
Sample is a	Base	10/3/2017 3:44:45 PM	User entered value
pKa 1	3.40	10/3/2017 3:44:45 PM	User entered value
pKa 2	5.60	10/3/2017 3:44:45 PM	User entered value
logP (XH2 2+)	-10.00		Default value
logp (XH +)	-10.00		Default value
logP (neutral X)	-10.00	10/3/2017 3:44:45 PM	User entered value

Events

Time	Event	Water	Acid	Base	Methanol	pH	dpH/dt	pH R-squared	pH SD
4:10.7	Dark spectrum								
4:12.2	Reference spectrum								
4:39.8	Volume reset due to vial change								
8:27.6	Initial pH = 4.62								
9:08.5	Data point 4	0.34995 mL	0.06679 mL	0.00000 mL	1.15005 mL	1.958	-0.02061	0.85638	0.0011
9:36.9	Data point 5	0.34995 mL	0.06679 mL	0.01437 mL	1.15005 mL	2.058	-0.00751	0.43967	0.0005
9:53.7	Data point 6	0.34995 mL	0.06679 mL	0.02498 mL	1.15005 mL	2.159	0.01103	0.79180	0.0006
10:10.4	Data point 7	0.34995 mL	0.06679 mL	0.03330 mL	1.15005 mL	2.253	0.01377	0.87102	0.0007

Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

Experiment start time: **10/11/2017 5:31:56 PM**
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
10:27.2	Data point 8	0.34995 mL	0.06679 mL	0.04008 mL	1.15005 mL	2.348	-0.00140	0.06513	0.00027	10.0 s
10:43.8	Data point 9	0.34995 mL	0.06679 mL	0.04563 mL	1.15005 mL	2.463	0.00272	0.19537	0.00030	10.0 s
11:00.4	Data point 10	0.34995 mL	0.06679 mL	0.04993 mL	1.15005 mL	2.548	0.00026	0.00238	0.00026	10.0 s
11:17.1	Data point 11	0.34995 mL	0.06679 mL	0.05348 mL	1.15005 mL	2.665	0.00114	0.06246	0.00022	10.0 s
11:44.1	Data point 12	0.34995 mL	0.06679 mL	0.05616 mL	1.15005 mL	2.763	0.00945	0.76145	0.00053	10.0 s
12:00.6	Data point 13	0.34995 mL	0.06679 mL	0.05833 mL	1.15005 mL	2.848	0.00555	0.69061	0.00033	10.0 s
12:22.1	Data point 14	0.34995 mL	0.06679 mL	0.05992 mL	1.15005 mL	2.943	0.00787	0.74958	0.00045	10.0 s
12:38.7	Data point 15	0.34995 mL	0.06679 mL	0.06136 mL	1.15005 mL	3.065	0.01215	0.82635	0.00066	10.0 s
13:00.5	Data point 16	0.34995 mL	0.06679 mL	0.06225 mL	1.15005 mL	3.157	0.00779	0.81928	0.00043	10.0 s
13:27.2	Data point 17	0.34995 mL	0.06679 mL	0.06305 mL	1.15005 mL	3.250	0.00959	0.83208	0.00052	10.0 s
13:43.7	Data point 18	0.34995 mL	0.06679 mL	0.06376 mL	1.15005 mL	3.364	0.01534	0.89496	0.00080	10.0 s
14:00.3	Data point 19	0.34995 mL	0.06679 mL	0.06430 mL	1.15005 mL	3.462	0.01836	0.95039	0.00093	10.0 s
14:16.8	Data point 20	0.34995 mL	0.06679 mL	0.06475 mL	1.15005 mL	3.557	0.02502	0.96470	0.00126	10.0 s
14:33.4	Data point 21	0.34995 mL	0.06679 mL	0.06510 mL	1.15005 mL	3.645	0.03039	0.98019	0.00152	10.0 s
14:50.0	Data point 22	0.34995 mL	0.06679 mL	0.06538 mL	1.15005 mL	3.724	0.03659	0.98510	0.00182	10.0 s
15:11.5	Data point 23	0.34995 mL	0.06679 mL	0.06583 mL	1.15005 mL	3.917	0.05070	0.97011	0.00254	10.0 s
15:33.2	Data point 24	0.34995 mL	0.06679 mL	0.06613 mL	1.15005 mL	4.064	0.07456	0.97698	0.00372	10.0 s
15:54.9	Data point 25	0.34995 mL	0.06679 mL	0.06635 mL	1.15005 mL	4.171	0.09155	0.99495	0.00453	10.0 s
16:21.6	Data point 26	0.34995 mL	0.06679 mL	0.06656 mL	1.15005 mL	4.297	0.09988	0.99117	0.00495	13.5 s
16:51.8	Data point 27	0.34995 mL	0.06679 mL	0.06679 mL	1.15005 mL	4.439	0.09985	0.99506	0.00494	19.0 s
17:32.5	Data point 28	0.34995 mL	0.06679 mL	0.06710 mL	1.15005 mL	4.554	0.09604	0.95916	0.00484	14.5 s
18:03.8	Data point 29	0.34995 mL	0.06679 mL	0.06731 mL	1.15005 mL	4.773	0.09812	0.98147	0.00489	26.0 s
18:46.5	Data point 30	0.34995 mL	0.06679 mL	0.06738 mL	1.15005 mL	4.955	0.10035	0.99417	0.00497	31.5 s
19:34.8	Data point 31	0.34995 mL	0.06679 mL	0.06747 mL	1.15005 mL	5.207	0.09776	0.98311	0.00486	43.5 s
20:35.1	Data point 32	0.34995 mL	0.06679 mL	0.06754 mL	1.15005 mL	5.525	0.09943	0.99299	0.00492	53.0 s
21:44.8	Data point 33	0.34995 mL	0.06679 mL	0.06762 mL	1.15005 mL	6.020	0.13305	0.97740	0.00664	Timed out at 59.5 s
22:56.4	Data point 34	0.34995 mL	0.06679 mL	0.06766 mL	1.15005 mL	6.463	0.16293	0.99741	0.00805	Timed out at 59.5 s

Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

Experiment start time: **10/11/2017 5:31:56 PM**
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
24:08.1	Data point 35	0.34995 mL	0.06679 mL	0.06771 mL	1.15005 mL	6.857	0.13768	0.99658	0.00680	Timed out at 59.5 s
25:24.7	Data point 36	0.34995 mL	0.06679 mL	0.06778 mL	1.15005 mL	7.523	0.14423	0.99127	0.00715	Timed out at 59.5 s
26:41.5	Data point 37	0.34995 mL	0.06679 mL	0.06785 mL	1.15005 mL	8.214	0.09750	0.94493	0.00495	49.0 s
27:47.2	Data point 38	0.34995 mL	0.06679 mL	0.06792 mL	1.15005 mL	8.763	0.08962	0.92550	0.00460	37.0 s
28:40.8	Data point 39	0.34995 mL	0.06679 mL	0.06799 mL	1.15005 mL	9.116	0.09810	0.97641	0.00490	29.0 s
29:26.3	Data point 40	0.34995 mL	0.06679 mL	0.06806 mL	1.15005 mL	9.379	0.09698	0.97849	0.00484	24.0 s
30:07.1	Data point 41	0.34995 mL	0.06679 mL	0.06813 mL	1.15005 mL	9.566	0.09846	0.98624	0.00489	20.0 s
30:43.9	Data point 42	0.34995 mL	0.06679 mL	0.06820 mL	1.15005 mL	9.700	0.09712	0.96561	0.00488	14.5 s
31:15.0	Data point 43	0.34995 mL	0.06679 mL	0.06827 mL	1.15005 mL	9.816	0.09664	0.97191	0.00484	13.5 s
31:45.3	Data point 44	0.34995 mL	0.06679 mL	0.06837 mL	1.15005 mL	9.949	0.09982	0.97687	0.00499	12.0 s
32:08.9	Data point 45	0.34995 mL	0.06679 mL	0.06846 mL	1.15005 mL	10.052	0.09983	0.98026	0.00498	10.0 s
32:30.4	Data point 46	0.34995 mL	0.06679 mL	0.06856 mL	1.15005 mL	10.162	0.08681	0.96574	0.00436	10.0 s
32:57.2	Data point 47	0.34995 mL	0.06679 mL	0.06867 mL	1.15005 mL	10.269	0.05613	0.96822	0.00282	10.0 s
33:18.9	Data point 48	0.34995 mL	0.06679 mL	0.06881 mL	1.15005 mL	10.374	0.04923	0.97523	0.00246	10.0 s
33:40.5	Data point 49	0.34995 mL	0.06679 mL	0.06898 mL	1.15005 mL	10.470	0.03422	0.95947	0.00172	10.0 s
33:57.0	Data point 50	0.34995 mL	0.06679 mL	0.06914 mL	1.15005 mL	10.578	0.02134	0.90738	0.00111	10.0 s
34:13.6	Data point 51	0.34995 mL	0.06679 mL	0.06936 mL	1.15005 mL	10.686	0.01080	0.77963	0.00060	10.0 s
34:30.1	Data point 52	0.34995 mL	0.06679 mL	0.06964 mL	1.15005 mL	10.790	0.01116	0.91716	0.00057	10.0 s
34:46.6	Data point 53	0.34995 mL	0.06679 mL	0.06999 mL	1.15005 mL	10.898	0.00536	0.50282	0.00037	10.0 s
35:03.1	Data point 54	0.34995 mL	0.06679 mL	0.07044 mL	1.15005 mL	11.012	0.00327	0.44209	0.00024	10.0 s
35:19.6	Data point 55	0.34995 mL	0.06679 mL	0.07103 mL	1.15005 mL	11.115	0.00076	0.04103	0.00019	10.0 s
35:36.2	Data point 56	0.34995 mL	0.06679 mL	0.07178 mL	1.15005 mL	11.205	0.00143	0.12441	0.00020	10.0 s
35:52.8	Data point 57	0.34995 mL	0.06679 mL	0.07270 mL	1.15005 mL	11.291	-0.00182	0.17697	0.00021	10.0 s
36:09.4	Data point 58	0.34995 mL	0.06679 mL	0.07382 mL	1.15005 mL	11.373	-0.00305	0.55352	0.00020	10.0 s
36:36.2	Data point 59	0.34995 mL	0.06679 mL	0.07549 mL	1.15005 mL	11.466	-0.00270	0.41061	0.00021	10.0 s
37:03.2	Data point 60	0.34995 mL	0.06679 mL	0.07787 mL	1.15005 mL	11.562	-0.00360	0.51552	0.00025	10.0 s
37:29.9	Data point 61	0.34995 mL	0.06679 mL	0.08001 mL	1.15005 mL	11.658	-0.00469	0.53880	0.00032	10.0 s

Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

Experiment start time: **10/11/2017 5:31:56 PM**
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
37:46.5	Data point 62	0.34995 mL	0.06679 mL	0.08262 mL	1.15005 mL	11.746	-0.00103	0.05891	0.00021	10.0 s
38:03.3	Data point 63	0.34995 mL	0.06679 mL	0.08582 mL	1.15005 mL	11.823	0.00079	0.04545	0.00018	10.0 s
38:30.3	Data point 64	0.34995 mL	0.06679 mL	0.09048 mL	1.15005 mL	11.920	-0.00193	0.19582	0.00021	10.0 s
38:57.5	Data point 65	0.34995 mL	0.06679 mL	0.09664 mL	1.15005 mL	12.011	0.00138	0.11564	0.00020	10.0 s
40:33.3	Reference spectrum									
41:37.0	Data point 67	0.50000 mL	0.15741 mL	0.09666 mL	1.15005 mL	1.984	-0.05925	0.92666	0.00304	10.0 s
42:04.3	Data point 68	0.50000 mL	0.15741 mL	0.10988 mL	1.15005 mL	2.082	0.00358	0.13224	0.00049	10.0 s
42:21.2	Data point 69	0.50000 mL	0.15741 mL	0.12105 mL	1.15005 mL	2.197	0.01874	0.59829	0.00120	10.0 s
42:37.9	Data point 70	0.50000 mL	0.15741 mL	0.12963 mL	1.15005 mL	2.313	0.00335	0.04368	0.00079	10.0 s
42:59.8	Data point 71	0.50000 mL	0.15741 mL	0.13464 mL	1.15005 mL	2.407	0.01325	0.90450	0.00069	10.0 s
43:26.7	Data point 72	0.50000 mL	0.15741 mL	0.13914 mL	1.15005 mL	2.507	0.01286	0.87351	0.00068	10.0 s
43:53.8	Data point 73	0.50000 mL	0.15741 mL	0.14306 mL	1.15005 mL	2.609	0.00865	0.86302	0.00046	10.0 s
44:10.4	Data point 74	0.50000 mL	0.15741 mL	0.14638 mL	1.15005 mL	2.730	0.01381	0.84713	0.00074	10.0 s
44:37.2	Data point 75	0.50000 mL	0.15741 mL	0.14871 mL	1.15005 mL	2.822	0.00786	0.80929	0.00043	10.0 s
44:53.9	Data point 76	0.50000 mL	0.15741 mL	0.15075 mL	1.15005 mL	2.929	0.01220	0.90713	0.00063	10.0 s
45:10.5	Data point 77	0.50000 mL	0.15741 mL	0.15235 mL	1.15005 mL	3.055	0.01580	0.89135	0.00083	10.0 s
45:37.4	Data point 78	0.50000 mL	0.15741 mL	0.15336 mL	1.15005 mL	3.149	0.01814	0.93680	0.00093	10.0 s
45:54.0	Data point 79	0.50000 mL	0.15741 mL	0.15433 mL	1.15005 mL	3.288	0.01321	0.86057	0.00070	10.0 s
46:15.6	Data point 80	0.50000 mL	0.15741 mL	0.15492 mL	1.15005 mL	3.380	0.01604	0.96826	0.00080	10.0 s
46:37.2	Data point 81	0.50000 mL	0.15741 mL	0.15541 mL	1.15005 mL	3.471	0.02014	0.93375	0.00103	10.0 s
47:04.2	Data point 82	0.50000 mL	0.15741 mL	0.15588 mL	1.15005 mL	3.565	0.01677	0.92212	0.00086	10.0 s
47:20.8	Data point 83	0.50000 mL	0.15741 mL	0.15626 mL	1.15005 mL	3.672	0.02859	0.96956	0.00143	10.0 s
47:37.4	Data point 84	0.50000 mL	0.15741 mL	0.15654 mL	1.15005 mL	3.759	0.03506	0.98231	0.00174	10.0 s
47:54.0	Data point 85	0.50000 mL	0.15741 mL	0.15677 mL	1.15005 mL	3.844	0.03652	0.96528	0.00184	10.0 s
48:10.6	Data point 86	0.50000 mL	0.15741 mL	0.15696 mL	1.15005 mL	3.920	0.04714	0.98584	0.00234	10.0 s
48:32.3	Data point 87	0.50000 mL	0.15741 mL	0.15720 mL	1.15005 mL	4.054	0.05588	0.98753	0.00278	10.0 s
48:53.9	Data point 88	0.50000 mL	0.15741 mL	0.15739 mL	1.15005 mL	4.167	0.07414	0.99665	0.00366	10.0 s
49:15.6	Data point 89	0.50000 mL	0.15741 mL	0.15755 mL	1.15005 mL	4.299	0.09889	0.98657	0.00491	10.0 s
49:37.3	Data point 90	0.50000 mL	0.15741 mL	0.15767 mL	1.15005 mL	4.407	0.10061	0.99318	0.00499	11.5 s

Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

Experiment start time: **10/11/2017 5:31:56 PM**
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
50:00.5	Data point 91	0.50000 mL	0.15741 mL	0.15776 mL	1.15005 mL	4.520	0.09756	0.98213	0.00486	12.5 s
50:29.6	Data point 92	0.50000 mL	0.15741 mL	0.15786 mL	1.15005 mL	4.659	0.09953	0.96637	0.00500	15.5 s
51:01.8	Data point 93	0.50000 mL	0.15741 mL	0.15795 mL	1.15005 mL	4.818	0.10081	0.99136	0.00500	19.5 s
51:37.9	Data point 94	0.50000 mL	0.15741 mL	0.15804 mL	1.15005 mL	5.019	0.09825	0.98646	0.00488	26.5 s
52:26.1	Data point 95	0.50000 mL	0.15741 mL	0.15814 mL	1.15005 mL	5.249	0.10046	0.98612	0.00499	31.5 s
53:14.5	Data point 96	0.50000 mL	0.15741 mL	0.15821 mL	1.15005 mL	5.475	0.09871	0.96815	0.00495	32.0 s
54:03.2	Data point 97	0.50000 mL	0.15741 mL	0.15828 mL	1.15005 mL	5.855	0.09887	0.98512	0.00491	47.0 s
55:01.8	Data point 98	0.50000 mL	0.15741 mL	0.15832 mL	1.15005 mL	6.157	0.10057	0.99257	0.00498	52.0 s
56:05.4	Data point 99	0.50000 mL	0.15741 mL	0.15840 mL	1.15005 mL	6.734	0.09961	0.99016	0.00494	52.0 s
57:14.2	Data point 100	0.50000 mL	0.15741 mL	0.15847 mL	1.15005 mL	7.386	0.09533	0.97305	0.00477	59.0 s
58:29.8	Data point 101	0.50000 mL	0.15741 mL	0.15854 mL	1.15005 mL	8.091	0.09725	0.96315	0.00489	48.5 s
59:34.9	Data point 102	0.50000 mL	0.15741 mL	0.15861 mL	1.15005 mL	8.492	0.09711	0.93091	0.00497	36.5 s
1:00:28.2	Data point 103	0.50000 mL	0.15741 mL	0.15868 mL	1.15005 mL	8.789	0.07960	0.70096	0.00469	34.0 s
1:01:23.9	Data point 104	0.50000 mL	0.15741 mL	0.15877 mL	1.15005 mL	9.093	0.09401	0.93387	0.00480	26.5 s
1:02:07.0	Data point 105	0.50000 mL	0.15741 mL	0.15884 mL	1.15005 mL	9.261	0.09051	0.83639	0.00488	21.5 s
1:02:45.2	Data point 106	0.50000 mL	0.15741 mL	0.15891 mL	1.15005 mL	9.423	0.09569	0.97559	0.00478	19.5 s
1:03:21.4	Data point 107	0.50000 mL	0.15741 mL	0.15898 mL	1.15005 mL	9.560	0.09939	0.97818	0.00496	16.5 s
1:03:59.7	Data point 108	0.50000 mL	0.15741 mL	0.15910 mL	1.15005 mL	9.683	0.10033	0.98212	0.00500	12.5 s
1:04:33.9	Data point 109	0.50000 mL	0.15741 mL	0.15927 mL	1.15005 mL	9.815	0.09460	0.98316	0.00471	11.5 s
1:05:02.0	Data point 110	0.50000 mL	0.15741 mL	0.15938 mL	1.15005 mL	9.929	0.09291	0.96791	0.00466	10.0 s
1:05:23.7	Data point 111	0.50000 mL	0.15741 mL	0.15950 mL	1.15005 mL	10.047	0.07931	0.96996	0.00397	10.0 s
1:05:50.4	Data point 112	0.50000 mL	0.15741 mL	0.15964 mL	1.15005 mL	10.164	0.04847	0.98159	0.00242	10.0 s
1:06:11.9	Data point 113	0.50000 mL	0.15741 mL	0.15983 mL	1.15005 mL	10.304	0.03228	0.96029	0.00162	10.0 s
1:06:33.5	Data point 114	0.50000 mL	0.15741 mL	0.16009 mL	1.15005 mL	10.464	0.01539	0.90610	0.00080	10.0 s
1:06:55.1	Data point 115	0.50000 mL	0.15741 mL	0.16042 mL	1.15005 mL	10.592	0.00776	0.79797	0.00043	10.0 s
1:07:16.8	Data point 116	0.50000 mL	0.15741 mL	0.16077 mL	1.15005 mL	10.694	0.00639	0.75121	0.00036	10.0 s
1:07:33.2	Data point 117	0.50000 mL	0.15741 mL	0.16117 mL	1.15005 mL	10.797	0.00060	0.01368	0.00025	10.0 s
1:07:49.9	Data point 118	0.50000 mL	0.15741 mL	0.16167 mL	1.15005 mL	10.894	-0.00053	0.01894	0.00019	10.0 s

Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

Experiment start time: **10/11/2017 5:31:56 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	pH	dpH/dt	pH R-squared	pH SD	dpH/time
1:08:06.6	Data point 119	0.50000 mL	0.15741 mL	0.16228 mL	1.15005 mL	10.990	-0.00336	0.47444	0.00024	10.0 s
1:08:23.3	Data point 120	0.50000 mL	0.15741 mL	0.16305 mL	1.15005 mL	11.083	-0.00375	0.47086	0.00027	10.0 s
1:08:39.9	Data point 121	0.50000 mL	0.15741 mL	0.16399 mL	1.15005 mL	11.170	-0.00533	0.75131	0.00030	10.0 s
1:08:56.4	Data point 122	0.50000 mL	0.15741 mL	0.16515 mL	1.15005 mL	11.250	-0.00548	0.68104	0.00033	10.0 s
1:09:23.3	Data point 123	0.50000 mL	0.15741 mL	0.16693 mL	1.15005 mL	11.343	-0.00508	0.52133	0.00035	10.0 s
1:09:50.3	Data point 124	0.50000 mL	0.15741 mL	0.16928 mL	1.15005 mL	11.438	-0.00707	0.81328	0.00039	10.0 s
1:10:17.2	Data point 125	0.50000 mL	0.15741 mL	0.17161 mL	1.15005 mL	11.532	-0.00432	0.50207	0.00030	10.0 s
1:10:33.7	Data point 126	0.50000 mL	0.15741 mL	0.17425 mL	1.15005 mL	11.619	-0.00193	0.17949	0.00022	10.0 s
1:10:50.4	Data point 127	0.50000 mL	0.15741 mL	0.17749 mL	1.15005 mL	11.694	-0.00478	0.58682	0.00031	10.0 s
1:11:17.3	Data point 128	0.50000 mL	0.15741 mL	0.18213 mL	1.15005 mL	11.790	-0.00530	0.64616	0.00033	10.0 s
1:11:44.5	Data point 129	0.50000 mL	0.15741 mL	0.18831 mL	1.15005 mL	11.882	-0.00366	0.51598	0.00025	10.0 s
1:12:11.7	Data point 130	0.50000 mL	0.15741 mL	0.19551 mL	1.15005 mL	11.974	-0.00286	0.28361	0.00027	10.0 s
1:12:28.4	Data point 131	0.50000 mL	0.15741 mL	0.19826 mL	1.15005 mL	12.003	-0.00532	0.60244	0.00034	10.0 s
1:14:13.0	Reference spectrum									
1:15:36.2	Data point 133	0.83996 mL	0.27954 mL	0.19828 mL	1.15005 mL	1.980	-0.05713	0.98577	0.00284	10.0 s
1:16:03.6	Data point 134	0.83996 mL	0.27954 mL	0.21355 mL	1.15005 mL	2.079	0.00240	0.06127	0.00048	10.0 s
1:16:20.5	Data point 135	0.83996 mL	0.27954 mL	0.22615 mL	1.15005 mL	2.190	-0.00199	0.06407	0.00039	10.0 s
1:16:37.2	Data point 136	0.83996 mL	0.27954 mL	0.23638 mL	1.15005 mL	2.306	0.02878	0.87682	0.00152	10.0 s
1:16:59.1	Data point 137	0.83996 mL	0.27954 mL	0.24203 mL	1.15005 mL	2.398	0.00607	0.47603	0.00043	10.0 s
1:17:26.1	Data point 138	0.83996 mL	0.27954 mL	0.24770 mL	1.15005 mL	2.500	0.01670	0.95489	0.00084	10.0 s
1:17:42.8	Data point 139	0.83996 mL	0.27954 mL	0.25252 mL	1.15005 mL	2.618	0.00541	0.49761	0.00038	10.0 s
1:18:09.9	Data point 140	0.83996 mL	0.27954 mL	0.25621 mL	1.15005 mL	2.715	0.00844	0.69643	0.00050	10.0 s
1:18:26.5	Data point 141	0.83996 mL	0.27954 mL	0.25920 mL	1.15005 mL	2.841	0.00417	0.39174	0.00033	10.0 s
1:18:53.5	Data point 142	0.83996 mL	0.27954 mL	0.26110 mL	1.15005 mL	2.939	0.01077	0.71541	0.00063	10.0 s
1:19:20.2	Data point 143	0.83996 mL	0.27954 mL	0.26293 mL	1.15005 mL	3.038	0.01309	0.81058	0.00072	10.0 s
1:19:36.8	Data point 144	0.83996 mL	0.27954 mL	0.26435 mL	1.15005 mL	3.141	0.00876	0.76956	0.00049	10.0 s
1:19:53.4	Data point 145	0.83996 mL	0.27954 mL	0.26548 mL	1.15005 mL	3.246	0.00885	0.79190	0.00049	10.0 s
1:20:09.9	Data point 146	0.83996 mL	0.27954 mL	0.26637 mL	1.15005 mL	3.355	0.01111	0.85204	0.00059	10.0 s
1:20:26.5	Data point 147	0.83996 mL	0.27954 mL	0.26705 mL	1.15005 mL	3.467	0.00792	0.58455	0.00051	10.0 s

Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

Experiment start time: **10/11/2017 5:31:56 PM**
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
1:20:43.1	Data point 148	0.83996 mL	0.27954 mL	0.26759 mL	1.15005 mL	3.583	0.01443	0.84501	0.00077	10.0 s
1:21:09.8	Data point 149	0.83996 mL	0.27954 mL	0.26799 mL	1.15005 mL	3.681	0.02073	0.96001	0.00104	10.0 s
1:21:26.3	Data point 150	0.83996 mL	0.27954 mL	0.26832 mL	1.15005 mL	3.836	0.02171	0.91122	0.00112	10.0 s
1:21:48.0	Data point 151	0.83996 mL	0.27954 mL	0.26856 mL	1.15005 mL	3.944	0.03448	0.96106	0.00174	10.0 s
1:22:04.4	Data point 152	0.83996 mL	0.27954 mL	0.26874 mL	1.15005 mL	4.066	0.04100	0.97169	0.00205	10.0 s
1:22:26.2	Data point 153	0.83996 mL	0.27954 mL	0.26893 mL	1.15005 mL	4.215	0.04911	0.97782	0.00245	10.0 s
1:22:47.9	Data point 154	0.83996 mL	0.27954 mL	0.26910 mL	1.15005 mL	4.391	0.06778	0.99200	0.00336	10.0 s
1:23:09.4	Data point 155	0.83996 mL	0.27954 mL	0.26921 mL	1.15005 mL	4.530	0.09214	0.98940	0.00457	10.0 s
1:23:36.0	Data point 156	0.83996 mL	0.27954 mL	0.26931 mL	1.15005 mL	4.645	0.09865	0.98461	0.00490	10.5 s
1:24:03.3	Data point 157	0.83996 mL	0.27954 mL	0.26938 mL	1.15005 mL	4.771	0.10027	0.98458	0.00499	14.0 s
1:24:34.0	Data point 158	0.83996 mL	0.27954 mL	0.26945 mL	1.15005 mL	4.927	0.09949	0.99151	0.00493	18.0 s
1:25:08.7	Data point 159	0.83996 mL	0.27954 mL	0.26952 mL	1.15005 mL	5.123	0.09860	0.98592	0.00490	21.0 s
1:25:41.1	Data point 160	0.83996 mL	0.27954 mL	0.26957 mL	1.15005 mL	5.264	0.09620	0.97983	0.00479	22.5 s
1:26:15.3	Data point 161	0.83996 mL	0.27954 mL	0.26961 mL	1.15005 mL	5.431	0.10011	0.99398	0.00496	25.0 s
1:26:52.0	Data point 162	0.83996 mL	0.27954 mL	0.26966 mL	1.15005 mL	5.621	0.10038	0.98171	0.00500	26.0 s
1:27:29.6	Data point 163	0.83996 mL	0.27954 mL	0.26971 mL	1.15005 mL	5.847	0.10071	0.99632	0.00498	30.0 s
1:28:11.3	Data point 164	0.83996 mL	0.27954 mL	0.26976 mL	1.15005 mL	6.101	0.09871	0.99126	0.00489	32.5 s
1:28:55.4	Data point 165	0.83996 mL	0.27954 mL	0.26980 mL	1.15005 mL	6.369	0.09902	0.98826	0.00492	32.0 s
1:29:34.0	Data point 166	0.83996 mL	0.27954 mL	0.26983 mL	1.15005 mL	6.455	0.09820	0.98659	0.00488	18.5 s
1:29:59.0	Data point 167	0.83996 mL	0.27954 mL	0.26985 mL	1.15005 mL	6.603	0.09890	0.98951	0.00490	29.5 s
1:30:40.2	Data point 168	0.83996 mL	0.27954 mL	0.26990 mL	1.15005 mL	6.950	0.09824	0.98291	0.00489	36.5 s
1:31:28.1	Data point 169	0.83996 mL	0.27954 mL	0.26994 mL	1.15005 mL	7.343	0.09903	0.97035	0.00496	37.0 s
1:32:16.8	Data point 170	0.83996 mL	0.27954 mL	0.26999 mL	1.15005 mL	7.851	0.09450	0.93391	0.00482	36.0 s
1:33:04.5	Data point 171	0.83996 mL	0.27954 mL	0.27004 mL	1.15005 mL	8.313	0.08732	0.89046	0.00457	30.0 s
1:33:46.1	Data point 172	0.83996 mL	0.27954 mL	0.27009 mL	1.15005 mL	8.634	0.09732	0.96336	0.00489	23.5 s
1:34:21.3	Data point 173	0.83996 mL	0.27954 mL	0.27013 mL	1.15005 mL	8.854	0.09556	0.97504	0.00478	19.5 s
1:34:52.4	Data point 174	0.83996 mL	0.27954 mL	0.27018 mL	1.15005 mL	9.031	0.09301	0.90532	0.00483	17.5 s
1:35:21.4	Data point 175	0.83996 mL	0.27954 mL	0.27023 mL	1.15005 mL	9.156	0.09205	0.97180	0.00461	14.0 s
1:35:52.2	Data point 176	0.83996 mL	0.27954 mL	0.27030 mL	1.15005 mL	9.321	0.08796	0.80852	0.00483	10.0 s
1:36:18.9	Data point 177	0.83996 mL	0.27954 mL	0.27037 mL	1.15005 mL	9.460	0.09943	0.96283	0.00500	10.5 s
1:36:46.1	Data point 178	0.83996 mL	0.27954 mL	0.27044 mL	1.15005 mL	9.559	0.06621	0.96283	0.00333	10.0 s
1:37:07.8	Data point 179	0.83996 mL	0.27954 mL	0.27051 mL	1.15005 mL	9.657	0.06945	0.97101	0.00348	10.0 s
1:37:34.6	Data point 180	0.83996 mL	0.27954 mL	0.27060 mL	1.15005 mL	9.768	0.04967	0.93667	0.00253	10.0 s
1:38:01.2	Data point 181	0.83996 mL	0.27954 mL	0.27072 mL	1.15005 mL	9.878	0.03288	0.94322	0.00167	10.0 s
1:38:22.8	Data point 182	0.83996 mL	0.27954 mL	0.27086 mL	1.15005 mL	9.993	0.02142	0.92144	0.00110	10.0 s
1:38:49.6	Data point 183	0.83996 mL	0.27954 mL	0.27105 mL	1.15005 mL	10.086	0.01737	0.85820	0.00093	10.0 s
1:39:11.2	Data point 184	0.83996 mL	0.27954 mL	0.27124 mL	1.15005 mL	10.191	0.00828	0.65791	0.00050	10.0 s
1:39:37.9	Data point 185	0.83996 mL	0.27954 mL	0.27150 mL	1.15005 mL	10.282	0.00655	0.59948	0.00042	10.0 s
1:39:59.6	Data point 186	0.83996 mL	0.27954 mL	0.27182 mL	1.15005 mL	10.388	-0.00075	0.01811	0.00028	10.0 s
1:40:31.5	Data point 187	0.83996 mL	0.27954 mL	0.27232 mL	1.15005 mL	10.488	0.00133	0.05079	0.00029	10.0 s
1:41:03.4	Data point 188	0.83996 mL	0.27954 mL	0.27286 mL	1.15005 mL	10.583	-0.00034	0.00982	0.00017	10.0 s
1:41:30.2	Data point 189	0.83996 mL	0.27954 mL	0.27342 mL	1.15005 mL	10.674	-0.00102	0.05048	0.00022	10.0 s
1:42:02.1	Data point 190	0.83996 mL	0.27954 mL	0.27427 mL	1.15005 mL	10.770	-0.00328	0.29122	0.00030	10.0 s
1:42:33.9	Data point 191	0.83996 mL	0.27954 mL	0.27512 mL	1.15005 mL	10.868	-0.00507	0.41179	0.00039	10.0 s
1:43:00.6	Data point 192	0.83996 mL	0.27954 mL	0.27599 mL	1.15005 mL	10.959	-0.00678	0.60168	0.00043	10.0 s
1:43:17.1	Data point 193	0.83996 mL	0.27954 mL	0.27707 mL	1.15005 mL	11.059	-0.00832	0.77640	0.00047	10.0 s
1:43:33.7	Data point 194	0.83996 mL	0.27954 mL	0.27843 mL	1.15005 mL	11.154	-0.00988	0.80264	0.00054	10.0 s
1:43:50.3	Data point 195	0.83996 mL	0.27954 mL	0.28013 mL	1.15005 mL	11.237	-0.00901	0.79163	0.00050	10.0 s
1:44:17.2	Data point 196	0.83996 mL	0.27954 mL	0.28279 mL	1.15005 mL	11.331	-0.00630	0.51564	0.00043	10.0 s
1:44:44.1	Data point 197	0.83996 mL	0.27954 mL	0.28584 mL	1.15005 mL	11.427	-0.00714	0.67877	0.00043	10.0 s
1:45:11.1	Data point 198	0.83996 mL	0.27954 mL	0.28923 mL	1.15005 mL	11.520	-0.00614	0.55576	0.00041	10.0 s
1:45:43.5	Data point 199	0.83996 mL	0.27954 mL	0.29316 mL	1.15005 mL	11.593	-0.00911	0.75680	0.00052	10.0 s
1:46:05.3	Data point 200	0.83996 mL	0.27954 mL	0.29880 mL	1.15005 mL	11.684	-0.00807	0.69880	0.00048	10.0 s
1:46:32.4	Data point 201	0.83996 mL	0.27954 mL	0.30649 mL	1.15005 mL	11.785	-0.00734	0.62077	0.00046	10.0 s
1:46:59.5	Data point 202	0.83996 mL	0.27954 mL	0.31599 mL	1.15005 mL	11.883	-0.00847	0.74340	0.00049	10.0 s
1:47:26.6	Data point 203	0.83996 mL	0.27954 mL	0.32723 mL	1.15005 mL	11.979	-0.00379	0.37547	0.00031	10.0 s
1:47:43.3	Data point 204	0.83996 mL	0.27954 mL	0.33121 mL	1.15005 mL	12.001	-0.00521	0.53217	0.00035	10.0 s

Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

Experiment start time: **10/11/2017 5:31:56 PM**
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	Ten
1:49:42.4	Assay volumes	1.08996 mL	0.41228 mL	0.33121 mL	1.15005 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	1.15 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			

Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**
Experiment start time: **10/11/2017 5:31:56 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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	0.34 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	10/11/2017 5:31:56 PM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus S	1.0007	10/11/2017 5:31:56 PM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jH	0.3	10/11/2017 5:31:56 PM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jOH	-0.2	10/11/2017 5:31:56 PM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Base concentration factor	1.011	10/11/2017 5:31:56 PM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	0.995	10/11/2017 5:31:56 PM	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		

Sample name: **M12**
Assay name: **UV-metric psKa**
Assay ID: **17J-11014**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

Experiment start time: **10/11/2017 5:31:56 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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)		
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	-8.44 mV		10/11/2017 5:32:40 PM
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	5.6e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	4.5e+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	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%		

Sample name: **M12**
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Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-11014_M12_UV-metric psKa.t3r**

Experiment start time: **10/11/2017 5:31:56 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	Spectrometer	Spectrometer
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00
Exclude turbid points	Yes	Yes
Low intensity warning threshold	100	100
Minimum absorbance change threshold	0.100	0.100
Eigenvector autocorrelation threshold	0.80	0.80
Maximum RMSD severe warning	0.250	0.250
Maximum RMSD warning	0.050	0.050

Tray Information

Title
Location A1