Yasuda-Shedlovsky Result

Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

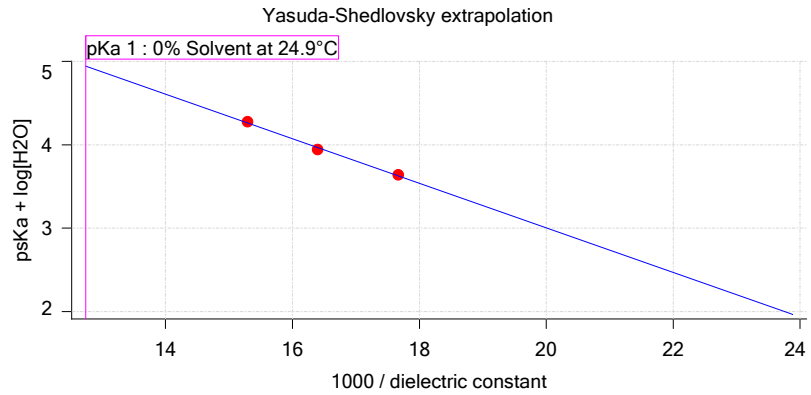
Yasuda-Shedlovsky result

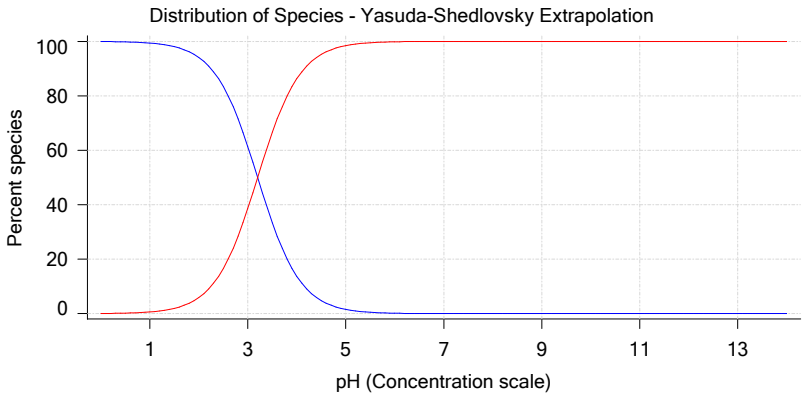
Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.20	±0.07	8.34	-266.9875	0.9952	0.165 M	24.9°C

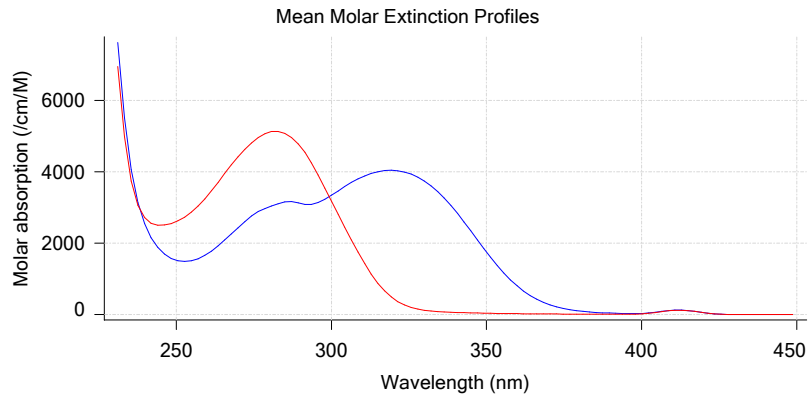
Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
17J-12011 Points 4 to 29	49.56 %	Up	UV-metric pKa	56.6	24.7 M	0.157 M	24.9°C	☑	2.25
17J-12011 Points 31 to 69	40.00 %	Up	UV-metric pKa	61.0	30.0 M	0.166 M	25.0°C	☑	2.46
17J-12011 Points 71 to 113	30.30 %	Up	UV-metric pKa	65.4	35.7 M	0.171 M	25.0°C	☑	2.72

Graphs







UV-metric psKa Titration 1 of 3 17J-12011 Points 4 to 29

Results

pKa 1	**2.25**
RMSD	**0.002 0.001**
Chi squared	**0.0007**
PCA calculated number of pKas	**2**
Average ionic strength	**0.157 M**
Average temperature	**24.9°C**
Analyte concentration range	**81.0 µM to 76.2 µM**
Methanol weight %	**49.6 %**
Dielectric constant	**56.6**
Water concentration	**24.7 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**

Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Results (continued)

pH clipping **1.467 to 12.530**

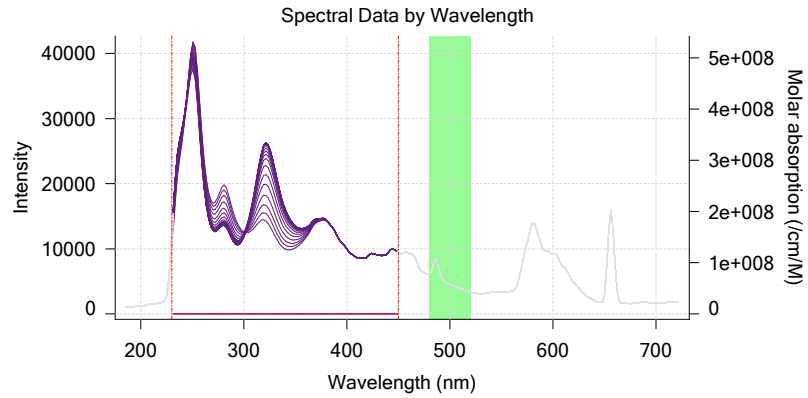
Warnings and errors

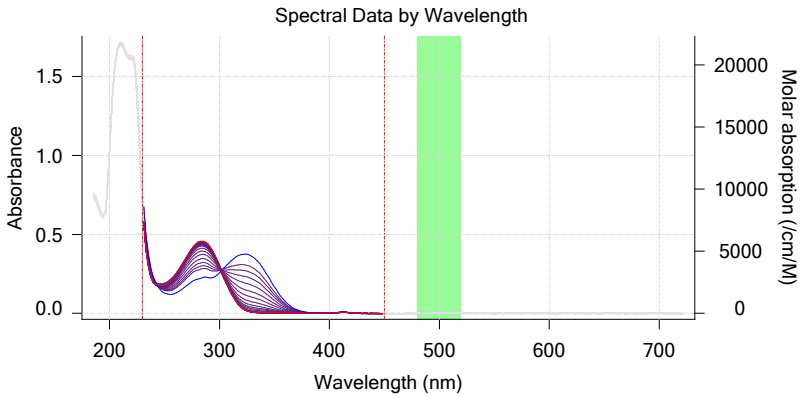
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

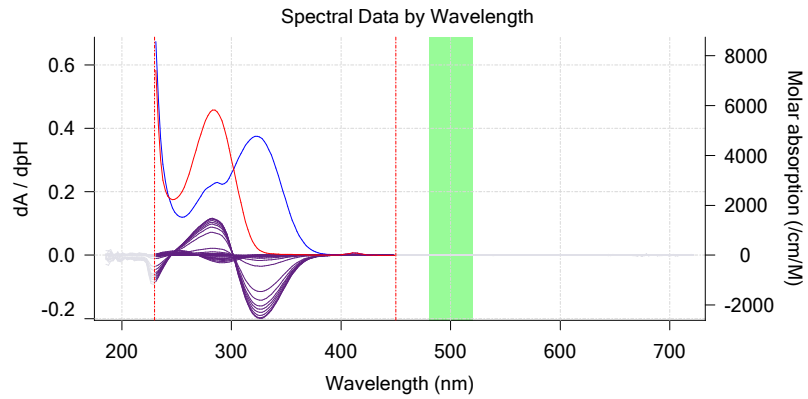
Assay Settings

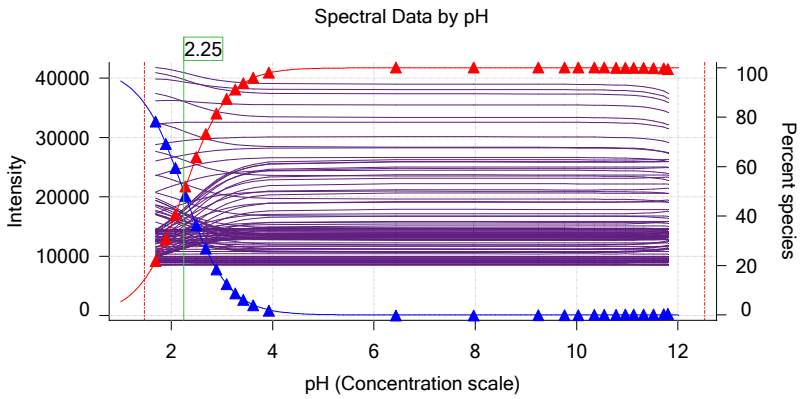
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

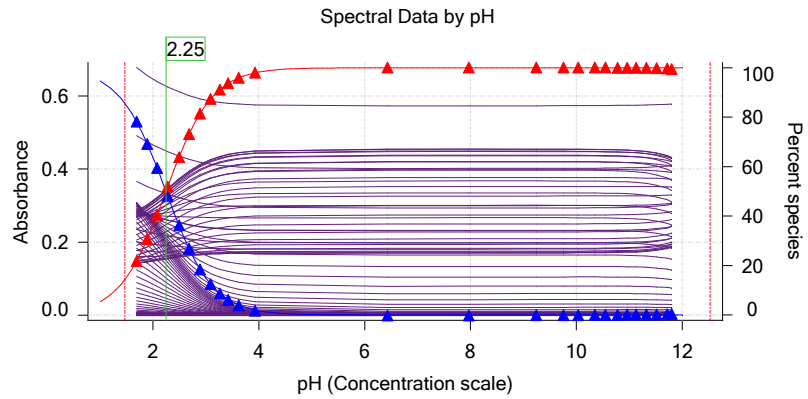
Graphs

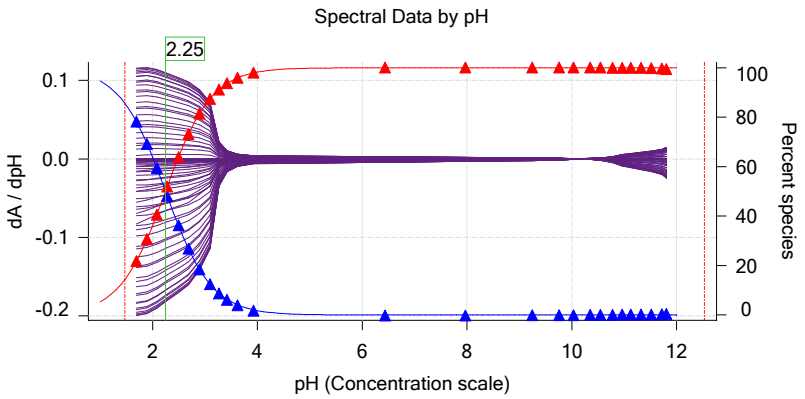








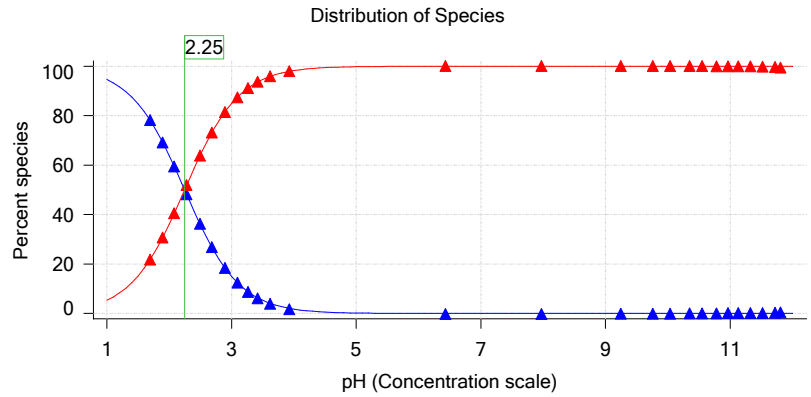


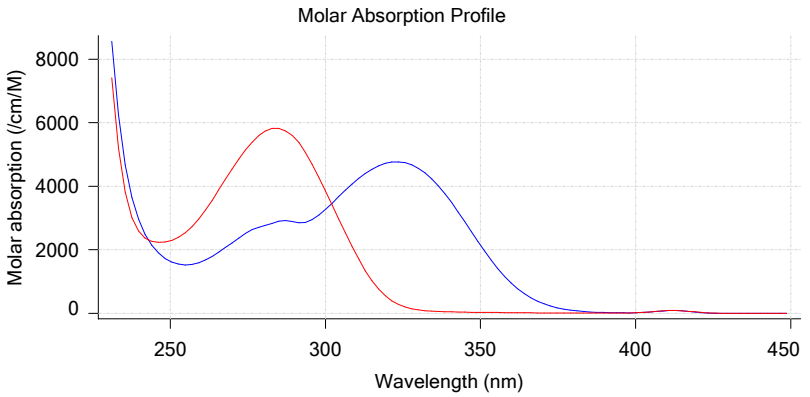


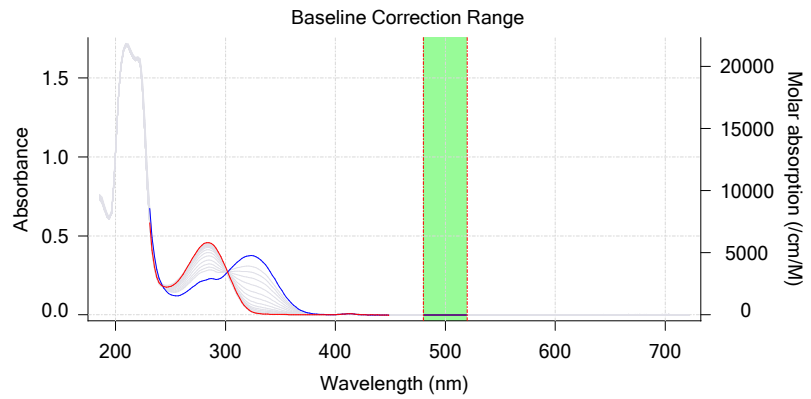
Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

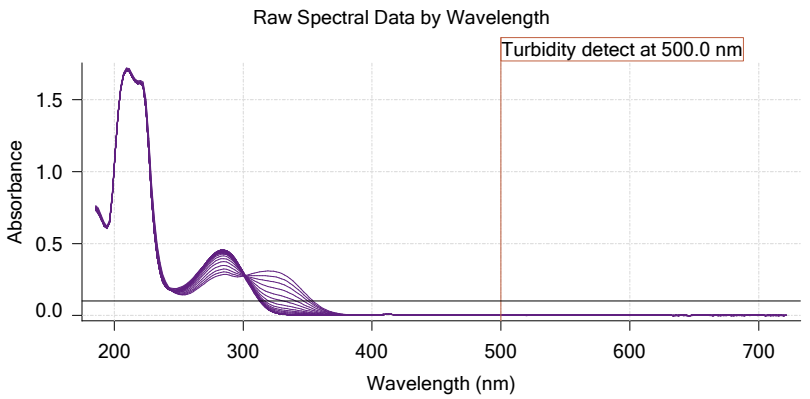
Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









UV-metric psKa Titration 2 of 3 17J-12011 Points 31 to 69

Results

pKa 1	**2.46**
RMSD	**0.005 0.008**
Chi squared	**0.0096**
PCA calculated number of pKas	**2**
Average ionic strength	**0.166 M**
Average temperature	**25.0°C**
Analyte concentration range	**66.5 µM to 62.9 µM**
Methanol weight %	**40.0 %**
Dielectric constant	**61.0**
Water concentration	**30.0 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.512 to 12.506**

Warnings and errors

Errors None
Warnings PCA calculation disagrees with predicted number of pKas

Assay Settings

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

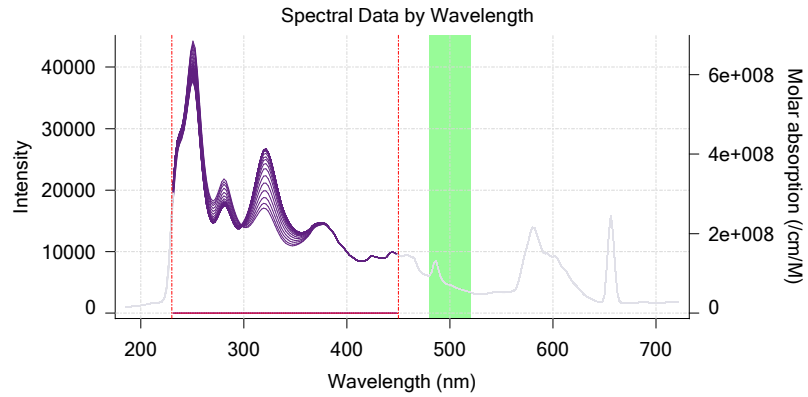
Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

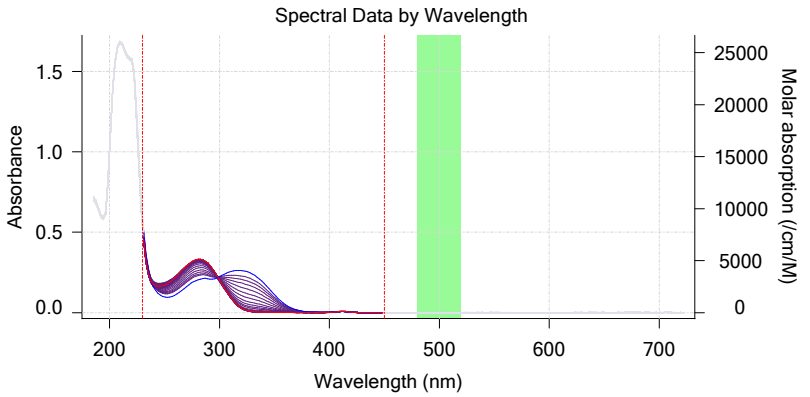
Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

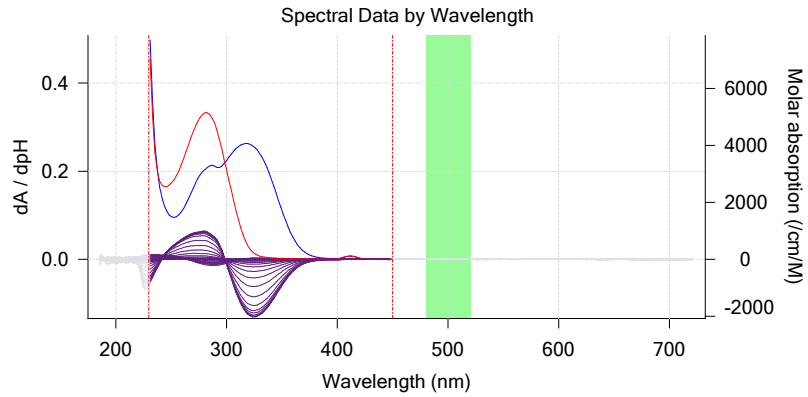
Assay Settings (continued)

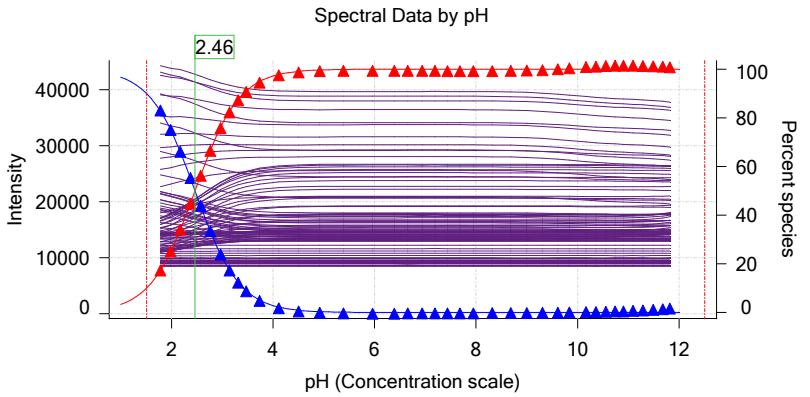
Setting	Value	Original Value	Date/Time changed	Imported from
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

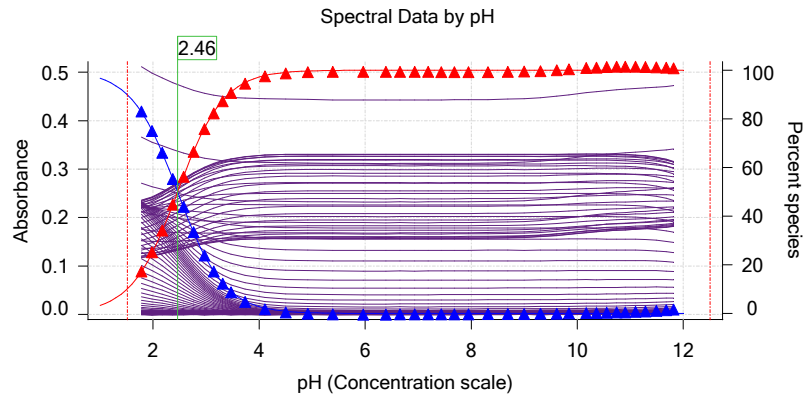
Graphs

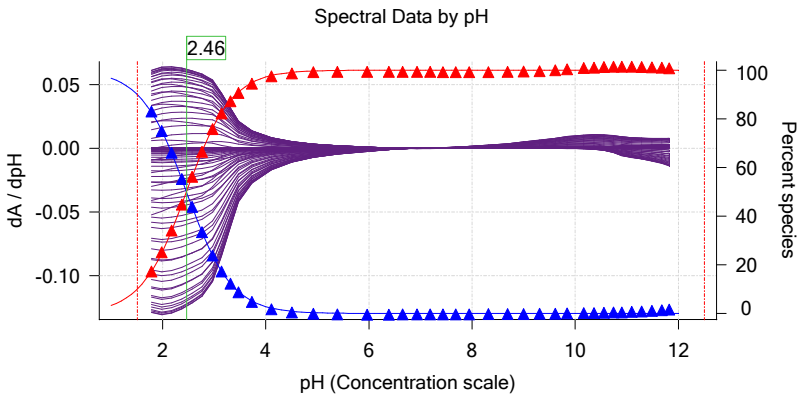








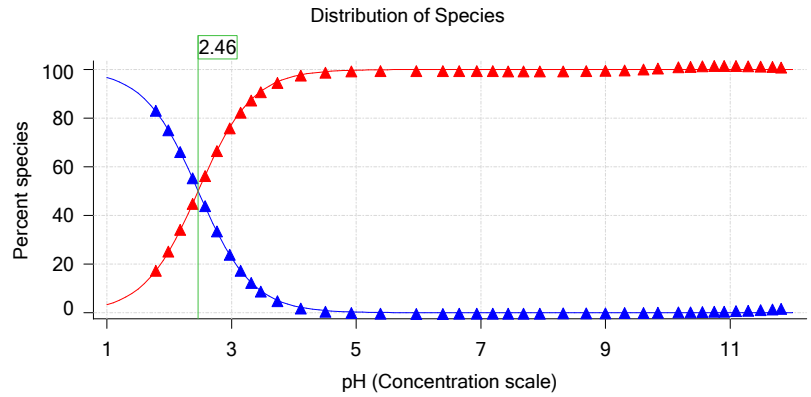


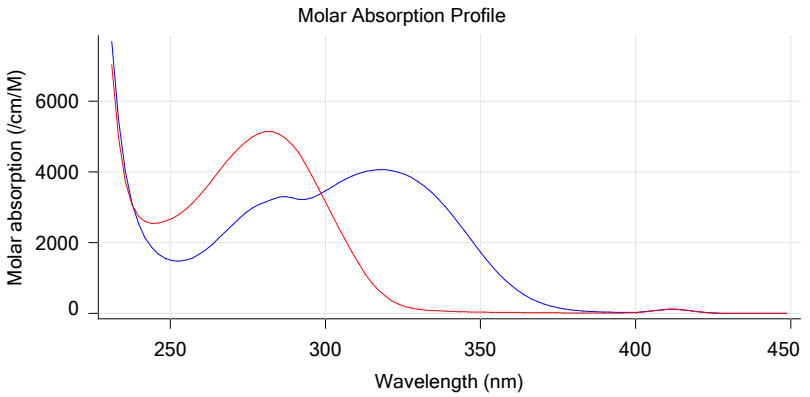


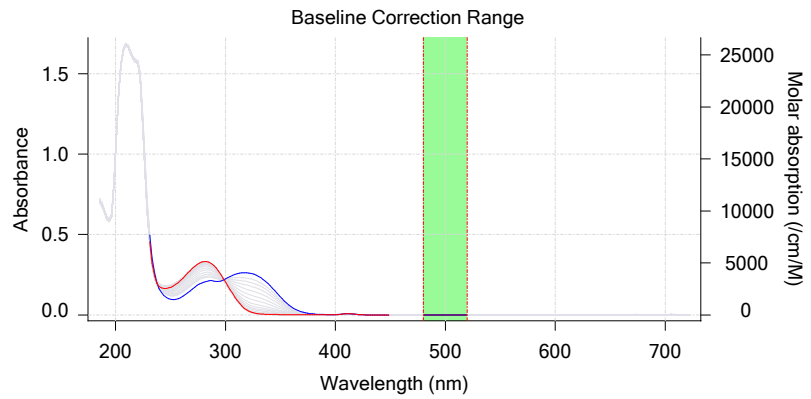
Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

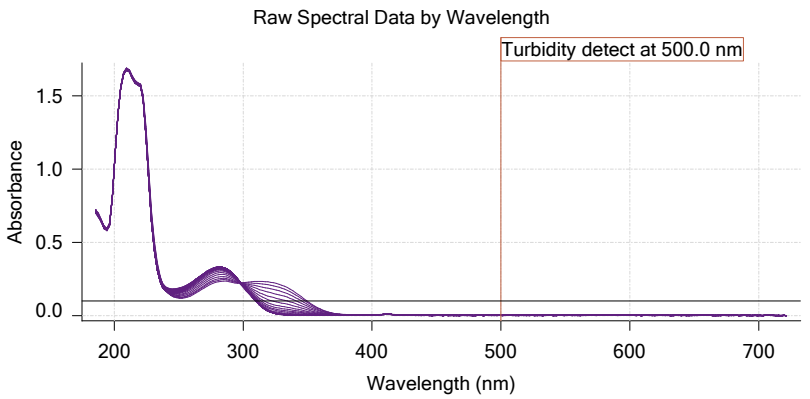
Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









UV-metric psKa Titration 3 of 3 17J-12011 Points 71 to 113

Results

pKa 1	**2.72**
RMSD	**0.011 0.020**
Chi squared	**0.0314**
PCA calculated number of pKas	**3**
Average ionic strength	**0.171 M**
Average temperature	**25.0°C**
Analyte concentration range	**51.4 µM to 48.6 µM**
Methanol weight %	**30.3 %**
Dielectric constant	**65.4**
Water concentration	**35.7 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.516 to 12.505**

Warnings and errors

Errors None
Warnings PCA calculation disagrees with predicted number of pKas

Assay Settings

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

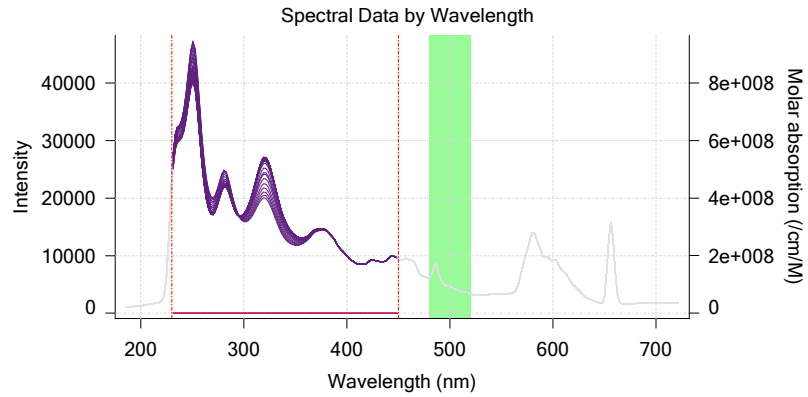
Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

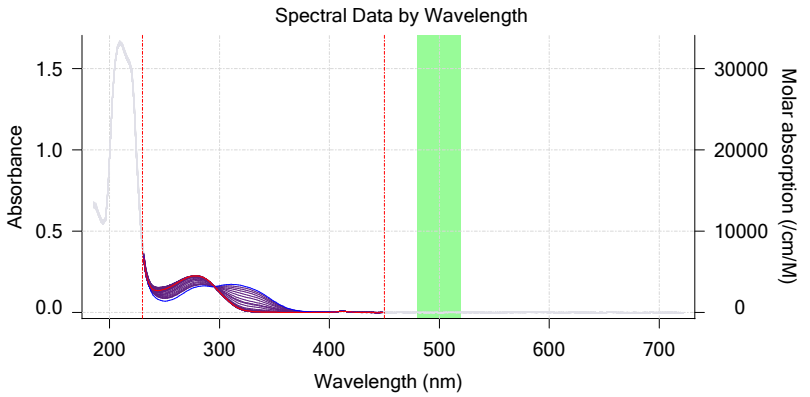
Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

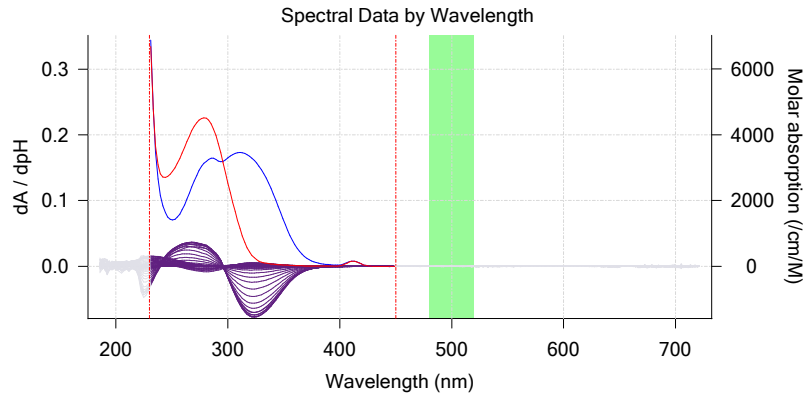
Assay Settings (continued)

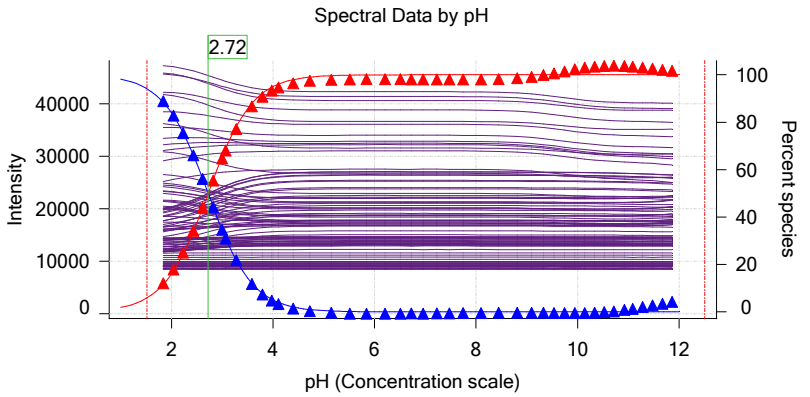
Setting	Value	Original Value	Date/Time changed	Imported from
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

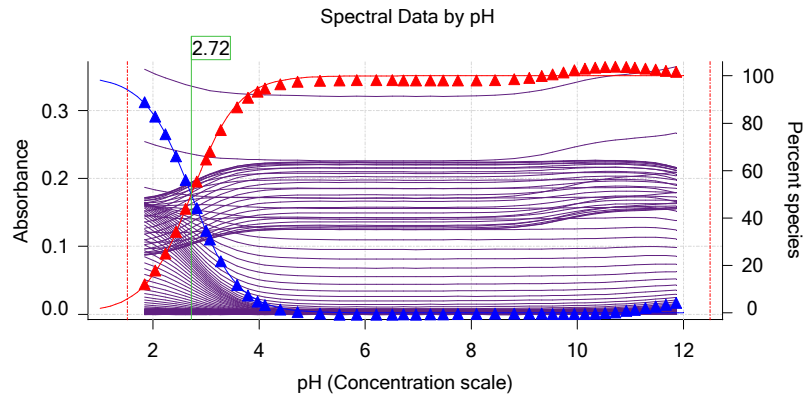
Graphs

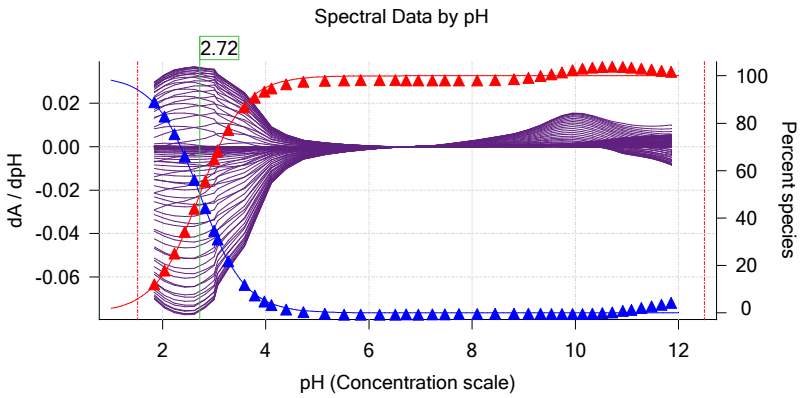








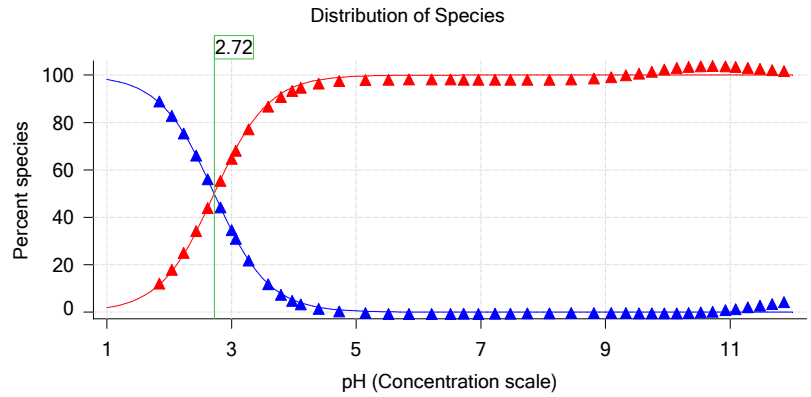


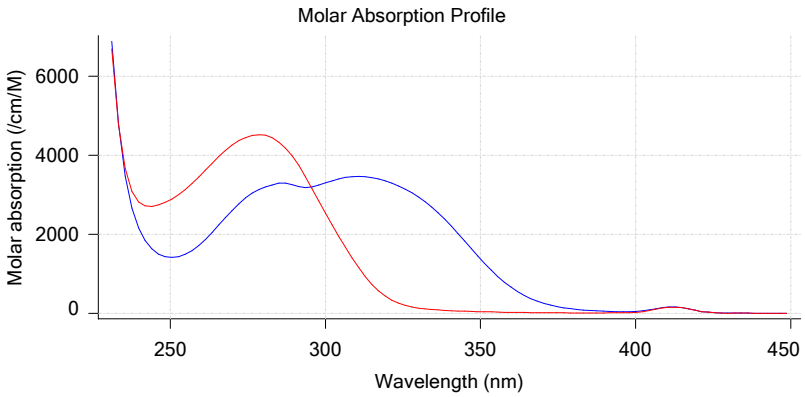


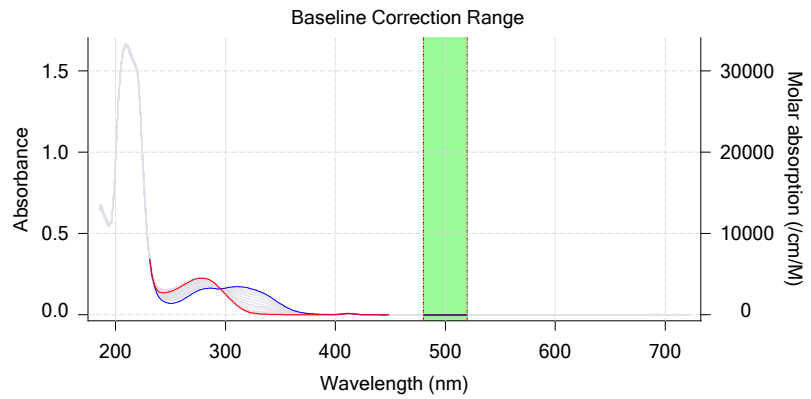
Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

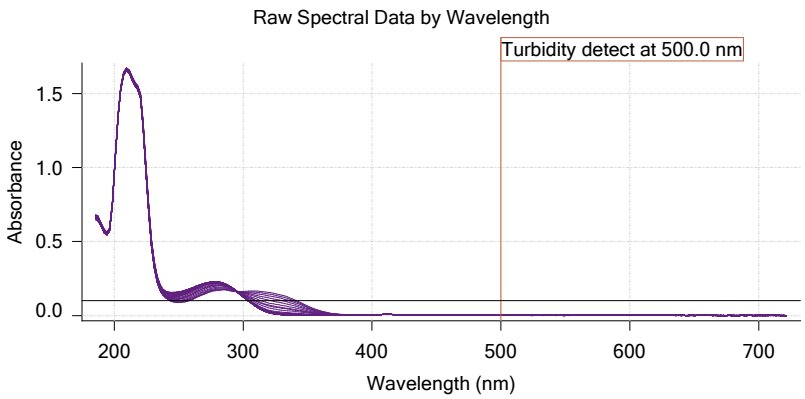
Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M19	10/11/2017 4:23:37 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0020 mL	10/11/2017 4:23:37 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.064600 M	10/11/2017 4:23:37 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	269.32	10/11/2017 4:23:44 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	10/11/2017 4:23:37 PM	User entered value
Sample is a	Base	10/11/2017 4:23:37 PM	User entered value
pKa 1	0.99	10/11/2017 4:23:37 PM	User entered value
logp (XH +)	-10.00		Default value
logP (neutral X)	-10.00	10/11/2017 4:23:37 PM	User entered value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:36.6	Dark spectrum								
3:37.9	Reference spectrum								
4:05.5	Volume reset due to vial change								
4:49.7	Initial pH = 8.37								
6:02.6	Data point 4	0.34995 mL	0.06818 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.967	-0.01439	0.85460
6:31.3	Data point 5	0.34995 mL	0.06818 mL	0.02467 mL	1.15005 mL	0.02500 mL	2.169	-0.00944	0.54316
6:48.2	Data point 6	0.34995 mL	0.06818 mL	0.03965 mL	1.15005 mL	0.02500 mL	2.354	-0.00389	0.07916
7:05.0	Data point 7	0.34995 mL	0.06818 mL	0.04965 mL	1.15005 mL	0.02500 mL	2.553	0.02038	0.78717
7:21.7	Data point 8	0.34995 mL	0.06818 mL	0.05593 mL	1.15005 mL	0.02500 mL	2.768	0.01572	0.82898
7:38.3	Data point 9	0.34995 mL	0.06818 mL	0.05978 mL	1.15005 mL	0.02500 mL	2.957	0.00649	0.53915

Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
7:54.9	Data point 10	0.34995 mL	0.06818 mL	0.06228 mL	1.15005 mL	0.02500 mL	3.165	0.01286	0.91150	0.00
8:11.5	Data point 11	0.34995 mL	0.06818 mL	0.06383 mL	1.15005 mL	0.02500 mL	3.363	0.00929	0.82971	0.00
8:28.0	Data point 12	0.34995 mL	0.06818 mL	0.06482 mL	1.15005 mL	0.02500 mL	3.533	0.00369	0.22518	0.00
8:44.6	Data point 13	0.34995 mL	0.06818 mL	0.06548 mL	1.15005 mL	0.02500 mL	3.689	0.01572	0.91478	0.00
9:16.8	Data point 14	0.34995 mL	0.06818 mL	0.06616 mL	1.15005 mL	0.02500 mL	3.887	0.03266	0.94775	0.00
9:38.5	Data point 15	0.34995 mL	0.06818 mL	0.06663 mL	1.15005 mL	0.02500 mL	4.195	0.07746	0.96380	0.00
10:10.4	Data point 16	0.34995 mL	0.06818 mL	0.06762 mL	1.15005 mL	0.02500 mL	6.687	0.09623	0.98783	0.00
11:10.2	Data point 17	0.34995 mL	0.06818 mL	0.06820 mL	1.15005 mL	0.02500 mL	8.216	0.09814	0.96358	0.00
11:57.8	Data point 18	0.34995 mL	0.06818 mL	0.06858 mL	1.15005 mL	0.02500 mL	9.484	0.09907	0.96793	0.00
12:40.1	Data point 19	0.34995 mL	0.06818 mL	0.06886 mL	1.15005 mL	0.02500 mL	9.997	0.09994	0.98521	0.00
13:03.4	Data point 20	0.34995 mL	0.06818 mL	0.06912 mL	1.15005 mL	0.02500 mL	10.272	0.04390	0.95642	0.00
13:25.1	Data point 21	0.34995 mL	0.06818 mL	0.06954 mL	1.15005 mL	0.02500 mL	10.582	0.01186	0.79887	0.00
13:57.1	Data point 22	0.34995 mL	0.06818 mL	0.07020 mL	1.15005 mL	0.02500 mL	10.782	-0.00023	0.00342	0.00
14:23.9	Data point 23	0.34995 mL	0.06818 mL	0.07098 mL	1.15005 mL	0.02500 mL	11.012	-0.01328	0.92169	0.00
14:40.5	Data point 24	0.34995 mL	0.06818 mL	0.07234 mL	1.15005 mL	0.02500 mL	11.194	-0.01004	0.84771	0.00
14:57.2	Data point 25	0.34995 mL	0.06818 mL	0.07441 mL	1.15005 mL	0.02500 mL	11.359	-0.00773	0.73134	0.00
15:24.4	Data point 26	0.34995 mL	0.06818 mL	0.07848 mL	1.15005 mL	0.02500 mL	11.551	-0.00980	0.88034	0.00
15:56.4	Data point 27	0.34995 mL	0.06818 mL	0.08398 mL	1.15005 mL	0.02500 mL	11.747	-0.01132	0.86562	0.00
16:28.8	Data point 28	0.34995 mL	0.06818 mL	0.09377 mL	1.15005 mL	0.02500 mL	11.944	-0.00719	0.61157	0.00
16:50.6	Data point 29	0.34995 mL	0.06818 mL	0.09991 mL	1.15005 mL	0.02500 mL	12.030	0.00067	0.01403	0.00
18:32.1	Reference spectrum									
19:36.1	Data point 31	0.50000 mL	0.16714 mL	0.09993 mL	1.15005 mL	0.02500 mL	2.012	-0.04590	0.94420	0.00
20:03.5	Data point 32	0.50000 mL	0.16714 mL	0.12399 mL	1.15005 mL	0.02500 mL	2.213	0.00706	0.74726	0.00
20:20.5	Data point 33	0.50000 mL	0.16714 mL	0.13883 mL	1.15005 mL	0.02500 mL	2.402	0.00480	0.50543	0.00
20:37.3	Data point 34	0.50000 mL	0.16714 mL	0.14849 mL	1.15005 mL	0.02500 mL	2.601	0.00095	0.02147	0.00
20:54.0	Data point 35	0.50000 mL	0.16714 mL	0.15468 mL	1.15005 mL	0.02500 mL	2.803	-0.01137	0.49269	0.00
21:10.7	Data point 36	0.50000 mL	0.16714 mL	0.15858 mL	1.15005 mL	0.02500 mL	2.991	0.00169	0.01882	0.00
21:27.4	Data point 37	0.50000 mL	0.16714 mL	0.16108 mL	1.15005 mL	0.02500 mL	3.196	0.00121	0.03244	0.00
21:44.2	Data point 38	0.50000 mL	0.16714 mL	0.16265 mL	1.15005 mL	0.02500 mL	3.368	0.01084	0.87315	0.00
22:00.8	Data point 39	0.50000 mL	0.16714 mL	0.16371 mL	1.15005 mL	0.02500 mL	3.539	0.01760	0.94016	0.00
22:17.4	Data point 40	0.50000 mL	0.16714 mL	0.16442 mL	1.15005 mL	0.02500 mL	3.694	0.02398	0.96615	0.00
22:39.0	Data point 41	0.50000 mL	0.16714 mL	0.16536 mL	1.15005 mL	0.02500 mL	3.957	0.02315	0.88697	0.00
23:00.7	Data point 42	0.50000 mL	0.16714 mL	0.16587 mL	1.15005 mL	0.02500 mL	4.333	0.09390	0.97697	0.00
23:27.6	Data point 43	0.50000 mL	0.16714 mL	0.16623 mL	1.15005 mL	0.02500 mL	4.725	0.09935	0.98569	0.00
24:09.8	Data point 44	0.50000 mL	0.16714 mL	0.16639 mL	1.15005 mL	0.02500 mL	5.140	0.08200	0.72341	0.00
24:53.6	Data point 45	0.50000 mL	0.16714 mL	0.16646 mL	1.15005 mL	0.02500 mL	5.605	0.09836	0.97863	0.00
25:55.8	Data point 46	0.50000 mL	0.16714 mL	0.16656 mL	1.15005 mL	0.02500 mL	6.176	0.09387	0.94260	0.00
26:54.1	Data point 47	0.50000 mL	0.16714 mL	0.16665 mL	1.15005 mL	0.02500 mL	6.602	0.09965	0.99284	0.00
27:38.3	Data point 48	0.50000 mL	0.16714 mL	0.16675 mL	1.15005 mL	0.02500 mL	6.865	0.09633	0.90835	0.00
28:13.5	Data point 49	0.50000 mL	0.16714 mL	0.16684 mL	1.15005 mL	0.02500 mL	7.146	0.09784	0.96140	0.00
28:55.8	Data point 50	0.50000 mL	0.16714 mL	0.16696 mL	1.15005 mL	0.02500 mL	7.399	0.09993	0.99492	0.00
29:35.8	Data point 51	0.50000 mL	0.16714 mL	0.16707 mL	1.15005 mL	0.02500 mL	7.644	0.09746	0.98450	0.00
30:16.3	Data point 52	0.50000 mL	0.16714 mL	0.16719 mL	1.15005 mL	0.02500 mL	7.889	0.09031	0.93972	0.00
30:56.2	Data point 53	0.50000 mL	0.16714 mL	0.16729 mL	1.15005 mL	0.02500 mL	8.153	0.09727	0.97020	0.00
31:40.1	Data point 54	0.50000 mL	0.16714 mL	0.16738 mL	1.15005 mL	0.02500 mL	8.522	0.09488	0.94984	0.00
32:24.4	Data point 55	0.50000 mL	0.16714 mL	0.16745 mL	1.15005 mL	0.02500 mL	8.891	0.09682	0.91682	0.00
33:08.6	Data point 56	0.50000 mL	0.16714 mL	0.16752 mL	1.15005 mL	0.02500 mL	9.200	0.09321	0.95778	0.00
33:49.6	Data point 57	0.50000 mL	0.16714 mL	0.16761 mL	1.15005 mL	0.02500 mL	9.508	0.09637	0.93988	0.00
34:19.6	Data point 58	0.50000 mL	0.16714 mL	0.16773 mL	1.15005 mL	0.02500 mL	9.810	0.09435	0.95565	0.00
34:49.4	Data point 59	0.50000 mL	0.16714 mL	0.16787 mL	1.15005 mL	0.02500 mL	10.039	0.06063	0.38639	0.00
35:07.0	Data point 60	0.50000 mL	0.16714 mL	0.16809 mL	1.15005 mL	0.02500 mL	10.364	0.01889	0.88765	0.00
35:39.0	Data point 61	0.50000 mL	0.16714 mL	0.16863 mL	1.15005 mL	0.02500 mL	10.559	0.00511	0.53193	0.00
36:11.0	Data point 62	0.50000 mL	0.16714 mL	0.16938 mL	1.15005 mL	0.02500 mL	10.750	-0.00454	0.44530	0.00
36:27.6	Data point 63	0.50000 mL	0.16714 mL	0.17041 mL	1.15005 mL	0.02500 mL	10.938	-0.01034	0.92463	0.00
36:44.3	Data point 64	0.50000 mL	0.16714 mL	0.17201 mL	1.15005 mL	0.02500 mL	11.095	-0.00894	0.82242	0.00
37:16.6	Data point 65	0.50000 mL	0.16714 mL	0.17509 mL	1.15005 mL	0.02500 mL	11.287	-0.00892	0.85565	0.00
37:43.7	Data point 66	0.50000 mL	0.16714 mL	0.17919 mL	1.15005 mL	0.02500 mL	11.479	-0.00924	0.83468	0.00

Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pI S
38:16.0	Data point 67	0.50000 mL	0.16714 mL	0.18690 mL	1.15005 mL	0.02500 mL	11.678	-0.00959	0.82388	0.
38:43.2	Data point 68	0.50000 mL	0.16714 mL	0.19795 mL	1.15005 mL	0.02500 mL	11.868	-0.00516	0.45775	0.
39:05.2	Data point 69	0.50000 mL	0.16714 mL	0.21065 mL	1.15005 mL	0.02500 mL	12.006	-0.00116	0.02185	0.
40:50.4	Reference spectrum									
42:13.7	Data point 71	0.83996 mL	0.28713 mL	0.21068 mL	1.15005 mL	0.02500 mL	2.016	-0.01170	0.72167	0.
42:41.2	Data point 72	0.83996 mL	0.28713 mL	0.23798 mL	1.15005 mL	0.02500 mL	2.215	0.00193	0.09658	0.
42:58.2	Data point 73	0.83996 mL	0.28713 mL	0.25492 mL	1.15005 mL	0.02500 mL	2.408	-0.00034	0.00184	0.
43:15.1	Data point 74	0.83996 mL	0.28713 mL	0.26587 mL	1.15005 mL	0.02500 mL	2.606	-0.00810	0.54430	0.
43:31.8	Data point 75	0.83996 mL	0.28713 mL	0.27286 mL	1.15005 mL	0.02500 mL	2.788	-0.03251	0.85240	0.
43:48.5	Data point 76	0.83996 mL	0.28713 mL	0.27752 mL	1.15005 mL	0.02500 mL	2.997	0.00337	0.05939	0.
44:20.8	Data point 77	0.83996 mL	0.28713 mL	0.28034 mL	1.15005 mL	0.02500 mL	3.174	0.00189	0.10386	0.
44:37.5	Data point 78	0.83996 mL	0.28713 mL	0.28222 mL	1.15005 mL	0.02500 mL	3.243	-0.00057	0.01132	0.
45:09.4	Data point 79	0.83996 mL	0.28713 mL	0.28401 mL	1.15005 mL	0.02500 mL	3.447	0.01910	0.91167	0.
45:26.0	Data point 80	0.83996 mL	0.28713 mL	0.28500 mL	1.15005 mL	0.02500 mL	3.758	-0.02077	0.60664	0.
45:47.7	Data point 81	0.83996 mL	0.28713 mL	0.28551 mL	1.15005 mL	0.02500 mL	3.961	0.01204	0.78145	0.
46:04.3	Data point 82	0.83996 mL	0.28713 mL	0.28582 mL	1.15005 mL	0.02500 mL	4.143	0.02546	0.90904	0.
46:20.9	Data point 83	0.83996 mL	0.28713 mL	0.28601 mL	1.15005 mL	0.02500 mL	4.281	0.04191	0.34039	0.
46:42.5	Data point 84	0.83996 mL	0.28713 mL	0.28624 mL	1.15005 mL	0.02500 mL	4.566	0.09776	0.97686	0.
47:04.1	Data point 85	0.83996 mL	0.28713 mL	0.28638 mL	1.15005 mL	0.02500 mL	4.896	0.09980	0.98859	0.
47:43.9	Data point 86	0.83996 mL	0.28713 mL	0.28650 mL	1.15005 mL	0.02500 mL	5.314	0.09759	0.96536	0.
48:24.1	Data point 87	0.83996 mL	0.28713 mL	0.28657 mL	1.15005 mL	0.02500 mL	5.682	0.09617	0.93333	0.
49:09.1	Data point 88	0.83996 mL	0.28713 mL	0.28664 mL	1.15005 mL	0.02500 mL	6.008	0.10044	0.98335	0.
49:50.4	Data point 89	0.83996 mL	0.28713 mL	0.28674 mL	1.15005 mL	0.02500 mL	6.372	0.00814	0.07566	0.
50:11.9	Data point 90	0.83996 mL	0.28713 mL	0.28683 mL	1.15005 mL	0.02500 mL	6.673	-0.00536	0.00954	0.
50:33.6	Data point 91	0.83996 mL	0.28713 mL	0.28692 mL	1.15005 mL	0.02500 mL	6.884	0.07720	0.86182	0.
51:00.9	Data point 92	0.83996 mL	0.28713 mL	0.28704 mL	1.15005 mL	0.02500 mL	7.120	0.09612	0.90453	0.
51:32.8	Data point 93	0.83996 mL	0.28713 mL	0.28718 mL	1.15005 mL	0.02500 mL	7.389	0.09749	0.96621	0.
52:04.1	Data point 94	0.83996 mL	0.28713 mL	0.28730 mL	1.15005 mL	0.02500 mL	7.633	0.09759	0.94139	0.
52:42.5	Data point 95	0.83996 mL	0.28713 mL	0.28742 mL	1.15005 mL	0.02500 mL	7.905	0.09648	0.97918	0.
53:28.4	Data point 96	0.83996 mL	0.28713 mL	0.28753 mL	1.15005 mL	0.02500 mL	8.256	0.09453	0.97996	0.
54:13.7	Data point 97	0.83996 mL	0.28713 mL	0.28763 mL	1.15005 mL	0.02500 mL	8.606	0.09912	0.96732	0.
54:59.5	Data point 98	0.83996 mL	0.28713 mL	0.28772 mL	1.15005 mL	0.02500 mL	8.969	0.09712	0.97105	0.
55:39.8	Data point 99	0.83996 mL	0.28713 mL	0.28782 mL	1.15005 mL	0.02500 mL	9.248	0.09591	0.95450	0.
56:17.1	Data point 100	0.83996 mL	0.28713 mL	0.28794 mL	1.15005 mL	0.02500 mL	9.484	0.09700	0.95486	0.
56:43.3	Data point 101	0.83996 mL	0.28713 mL	0.28808 mL	1.15005 mL	0.02500 mL	9.690	0.09092	0.96085	0.
57:10.1	Data point 102	0.83996 mL	0.28713 mL	0.28829 mL	1.15005 mL	0.02500 mL	9.895	0.04856	0.96544	0.
57:42.1	Data point 103	0.83996 mL	0.28713 mL	0.28862 mL	1.15005 mL	0.02500 mL	10.097	0.03276	0.92705	0.
58:14.0	Data point 104	0.83996 mL	0.28713 mL	0.28911 mL	1.15005 mL	0.02500 mL	10.294	0.01018	0.75773	0.
58:46.1	Data point 105	0.83996 mL	0.28713 mL	0.28989 mL	1.15005 mL	0.02500 mL	10.486	0.00595	0.56537	0.
59:13.1	Data point 106	0.83996 mL	0.28713 mL	0.29135 mL	1.15005 mL	0.02500 mL	10.678	-0.00915	0.67111	0.
59:40.0	Data point 107	0.83996 mL	0.28713 mL	0.29287 mL	1.15005 mL	0.02500 mL	10.866	-0.01371	0.90545	0.
59:56.6	Data point 108	0.83996 mL	0.28713 mL	0.29492 mL	1.15005 mL	0.02500 mL	11.073	-0.01954	0.86666	0.
1:00:13.2	Data point 109	0.83996 mL	0.28713 mL	0.29819 mL	1.15005 mL	0.02500 mL	11.236	-0.02047	0.88414	0.
1:00:40.2	Data point 110	0.83996 mL	0.28713 mL	0.30419 mL	1.15005 mL	0.02500 mL	11.430	-0.01511	0.86175	0.
1:01:07.3	Data point 111	0.83996 mL	0.28713 mL	0.31352 mL	1.15005 mL	0.02500 mL	11.625	-0.01524	0.91479	0.
1:01:39.7	Data point 112	0.83996 mL	0.28713 mL	0.32912 mL	1.15005 mL	0.02500 mL	11.818	-0.01330	0.89789	0.
1:02:07.3	Data point 113	0.83996 mL	0.28713 mL	0.35212 mL	1.15005 mL	0.02500 mL	12.005	-0.00465	0.28612	0.
1:04:06.7	Assay volumes	1.08996 mL	0.42808 mL	0.35212 mL	1.15005 mL	0.02500 mL				

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				
Number of titrations	3			

Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	Spectrometer			
Monitor at a wavelength of	500.0 nm			
Absorbance threshold of	0.100			
Collect turbidity sensor data	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	15%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
Cosolvent in use	Yes			
Cosolvent type	Methanol			
Cosolvent volume	1.15 mL			
Cosolvent added	Automatic			
ISA water volume	0.35 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	15%			
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			
After medium addition, stir for	5 seconds			
Sample Sonication				
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	No			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	10 seconds			
Titration 2				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.15 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			
Add additional water	0.34 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			

Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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 1:12:22 PM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus S	1.0007	10/12/2017 1:12:22 PM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jH	0.3	10/12/2017 1:12:22 PM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jOH	-0.2	10/12/2017 1:12:22 PM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Base concentration factor	1.011	10/12/2017 1:12:22 PM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	0.995	10/12/2017 1:12:22 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		
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

Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	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	-9.63 mV		10/12/2017 1:12:46 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	3.7e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	6.3e+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%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M19**
Assay name: **UV-metric psKa**
Assay ID: **17J-12011**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12011_M19_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:12:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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 H1