Yasuda-Shedlovsky Result

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

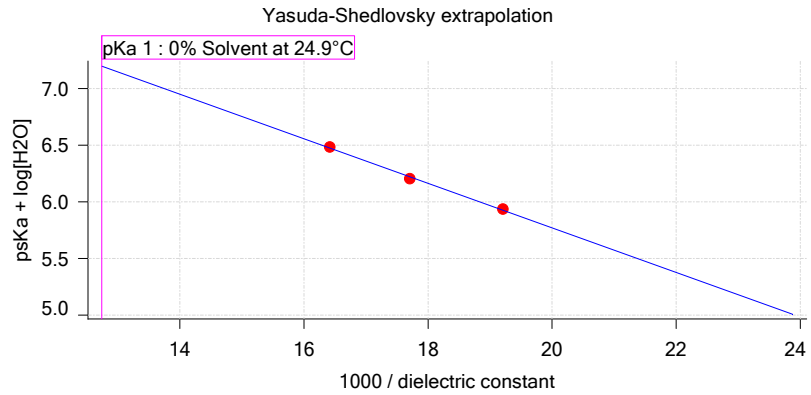
Yasuda-Shedlovsky result

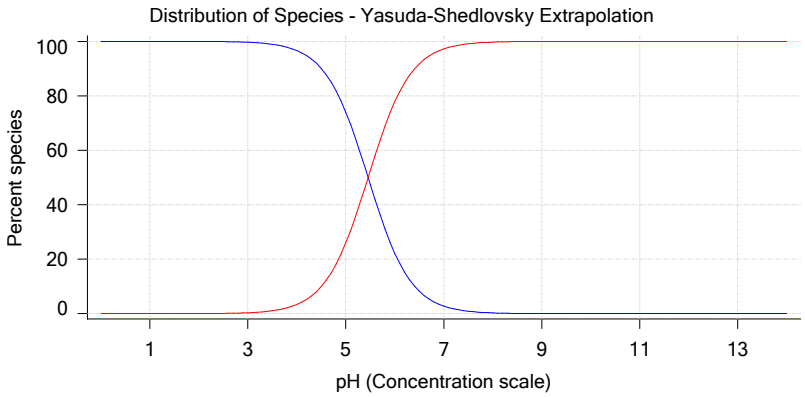
Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.45	±0.06	9.70	-196.5408	0.9968	0.166 M	24.9°C

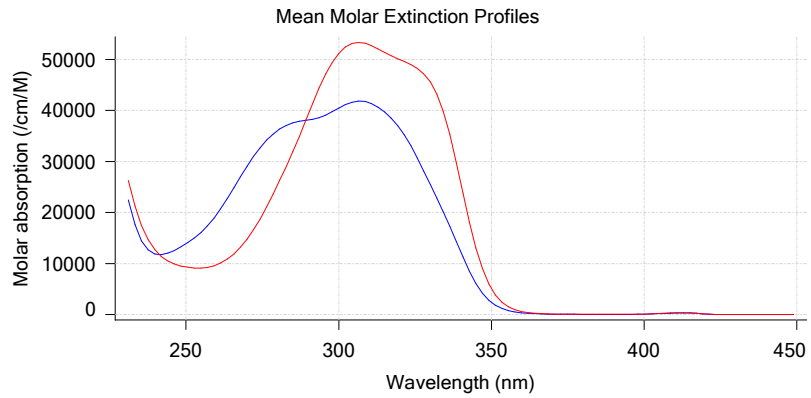
Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
17J-07008 Points 4 to 69	59.15 %	Up	UV-metric pKa	52.1	19.5 M	0.157 M	24.9°C	☑	4.64
17J-07008 Points 71 to 142	49.79 %	Up	UV-metric pKa	56.5	24.5 M	0.167 M	24.9°C	☑	4.81
17J-07008 Points 144 to 211	40.20 %	Up	UV-metric pKa	60.9	29.9 M	0.175 M	24.9°C	☑	5.01

Graphs







UV-metric psKa Titration 1 of 3 17J-07008 Points 4 to 69

Results

pKa 1	**4.64**
RMSD	**0.001 0.001**
Chi squared	**0.0057**
PCA calculated number of pKas	**3**
Average ionic strength	**0.157 M**
Average temperature	**24.9°C**
Analyte concentration range	**29.5 µM to 27.7 µM**
Methanol weight %	**59.1 %**
Dielectric constant	**52.1**
Water concentration	**19.5 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Results (continued)

pH clipping **1.468 to 12.523**

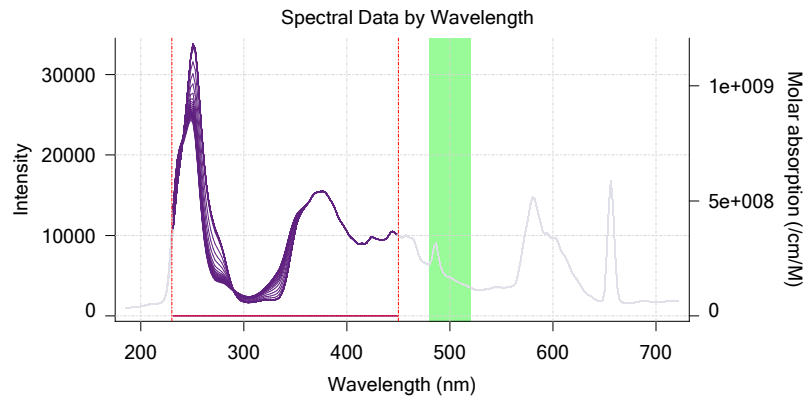
Warnings and errors

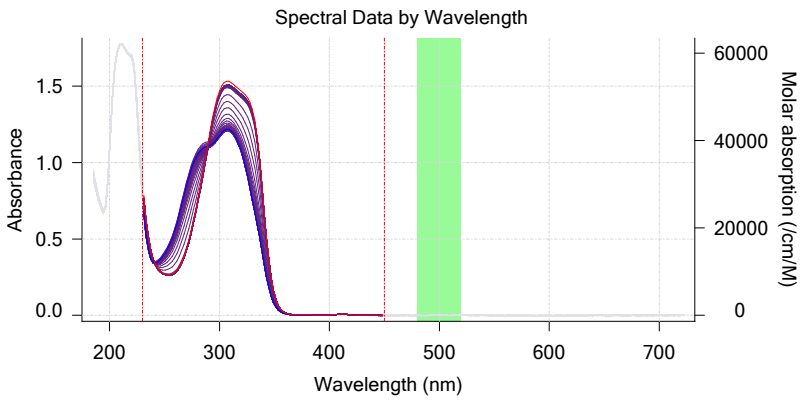
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

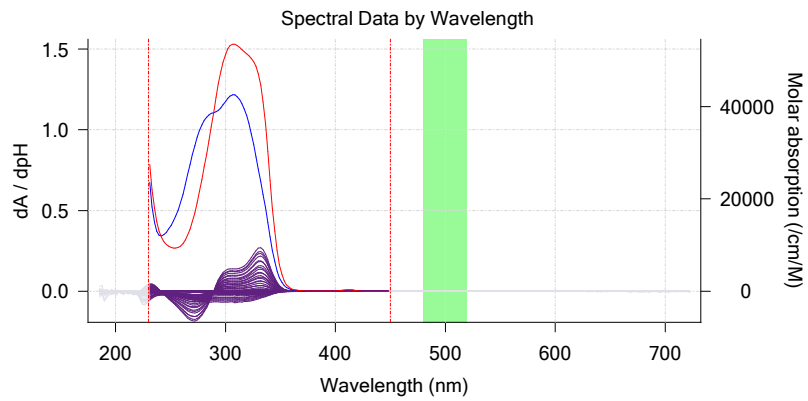
Assay Settings

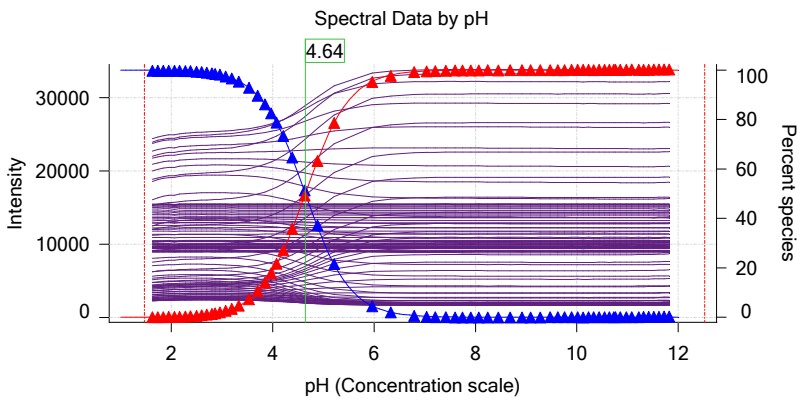
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

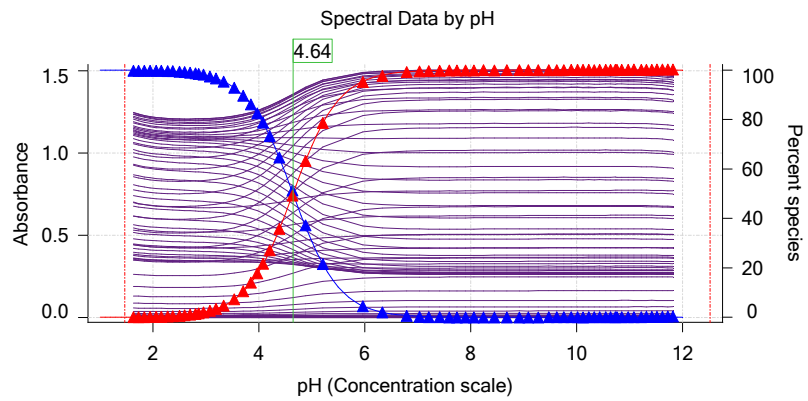
Graphs

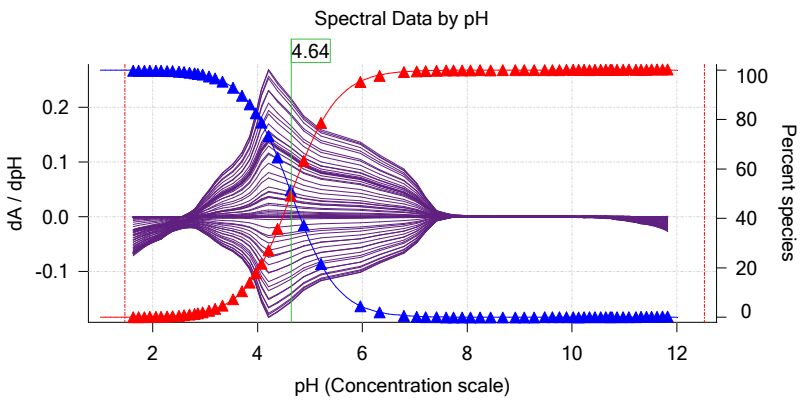








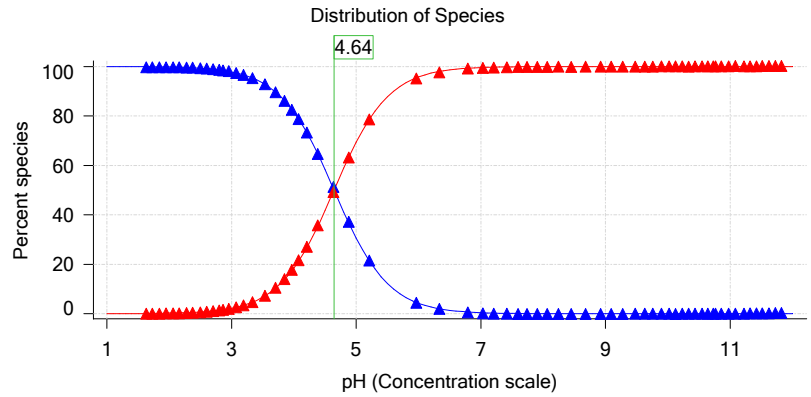


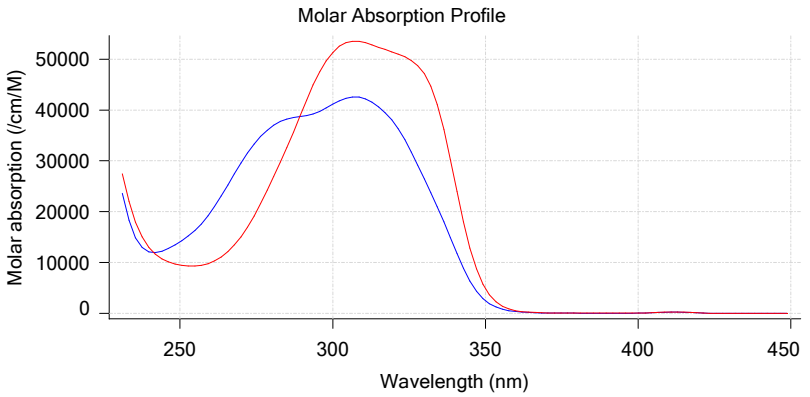


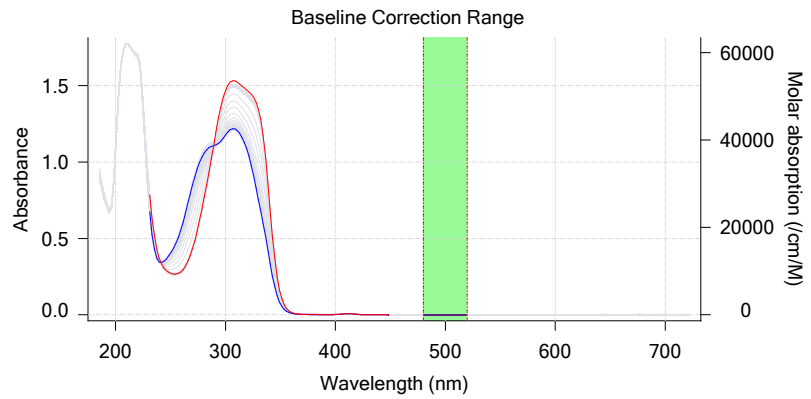
Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

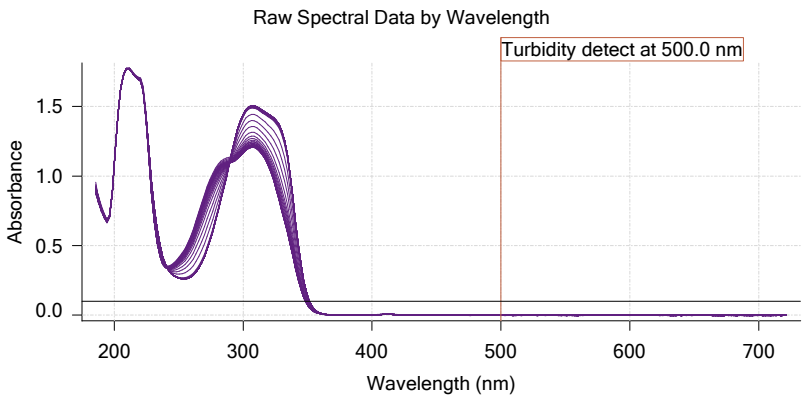
Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









UV-metric psKa Titration 2 of 3 17J-07008 Points 71 to 142

Results

pKa 1	**4.81**
RMSD	**0.002 0.002**
Chi squared	**0.0040**
PCA calculated number of pKas	**5**
Average ionic strength	**0.167 M**
Average temperature	**24.9°C**
Analyte concentration range	**25.2 µM to 23.8 µM**
Methanol weight %	**49.8 %**
Dielectric constant	**56.5**
Water concentration	**24.5 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.463 to 12.526**

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				

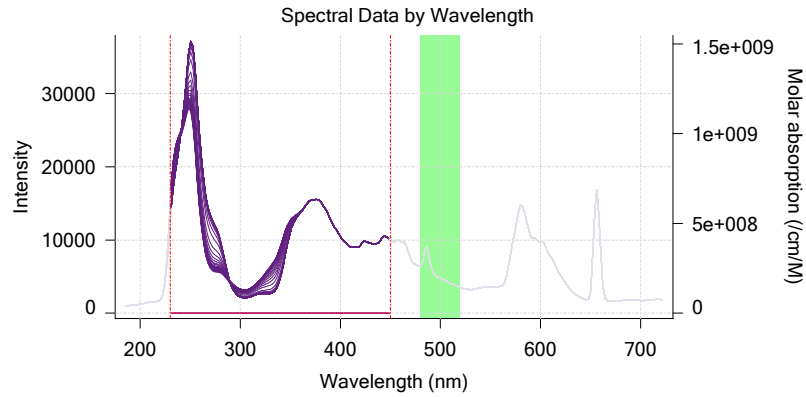
Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

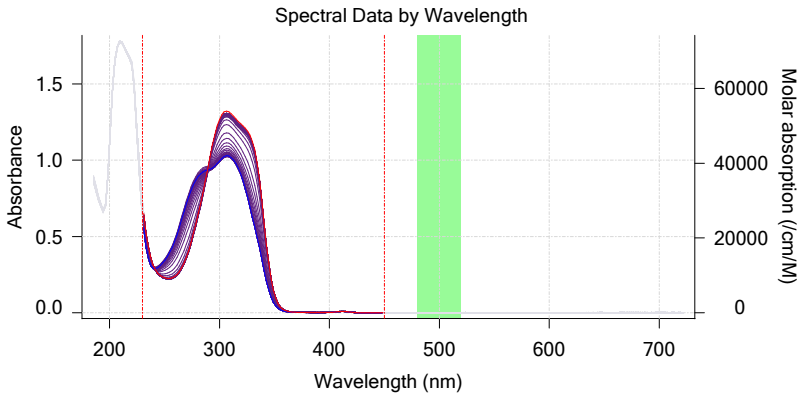
Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

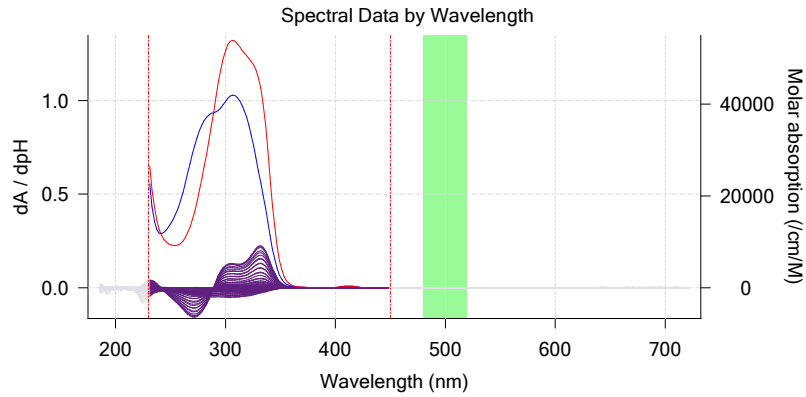
Assay Settings (continued)

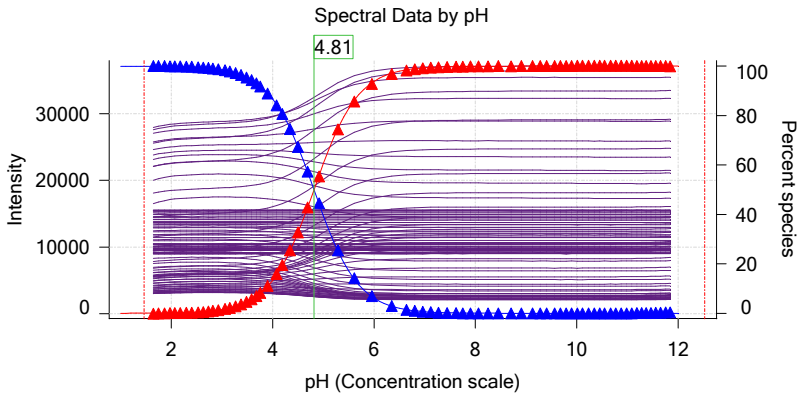
Setting	Value	Original Value	Date/Time changed	Imported from
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

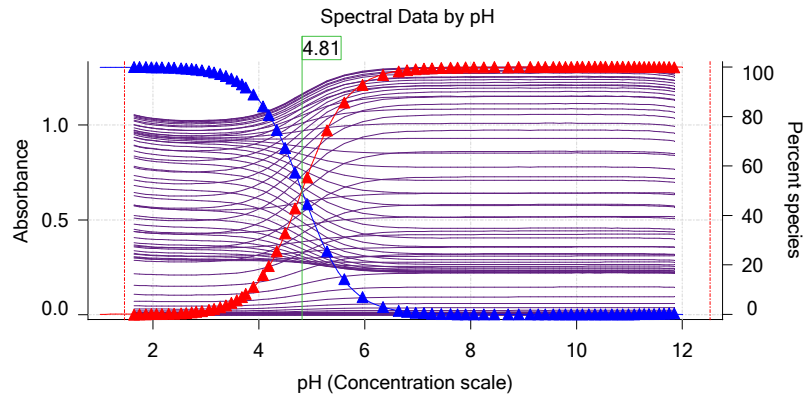
Graphs

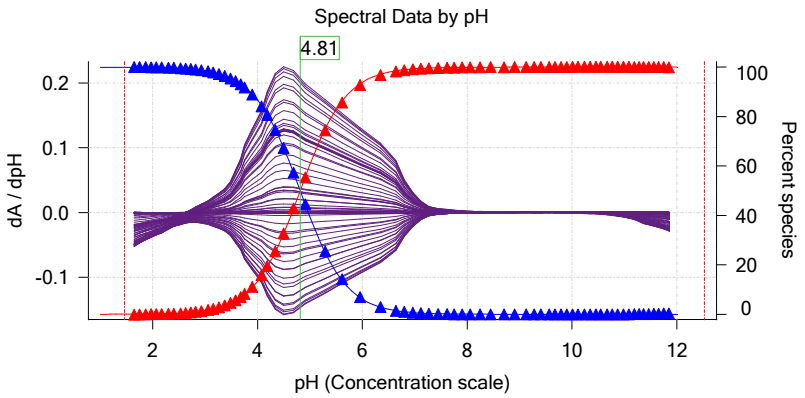








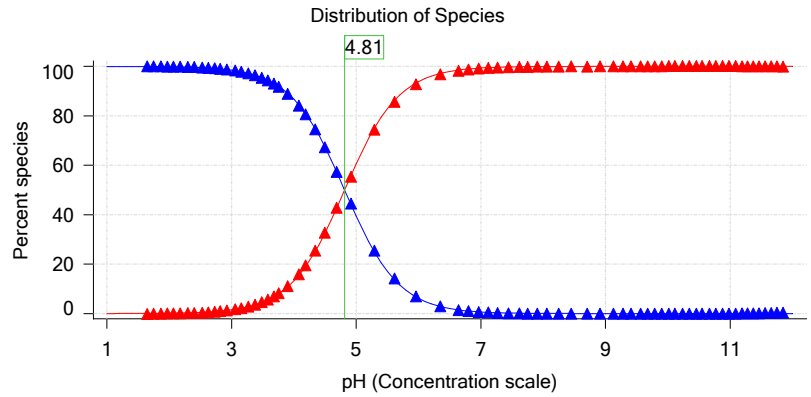


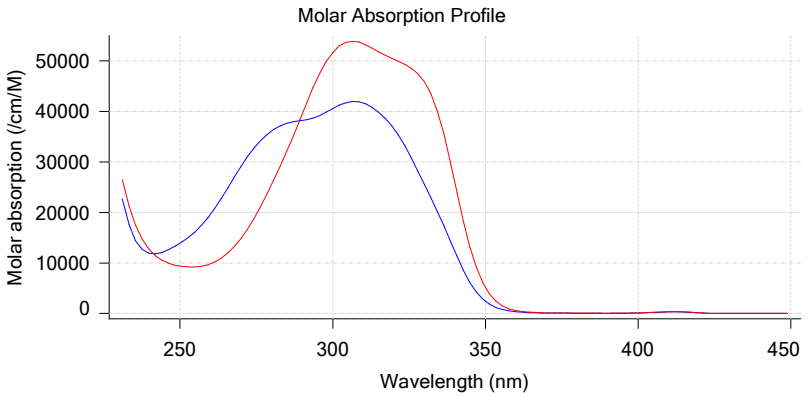


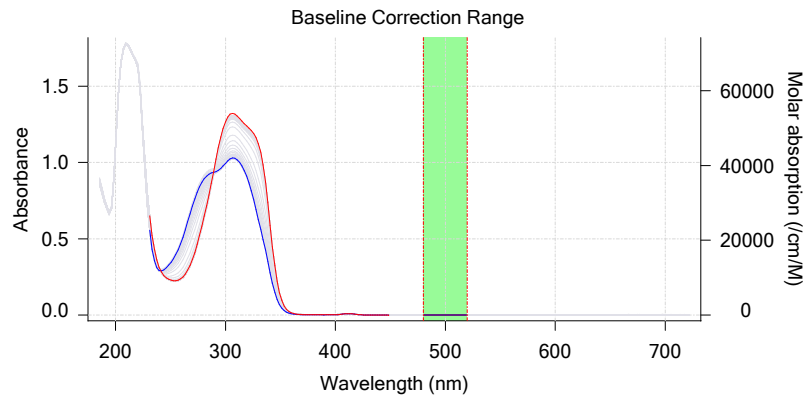
Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

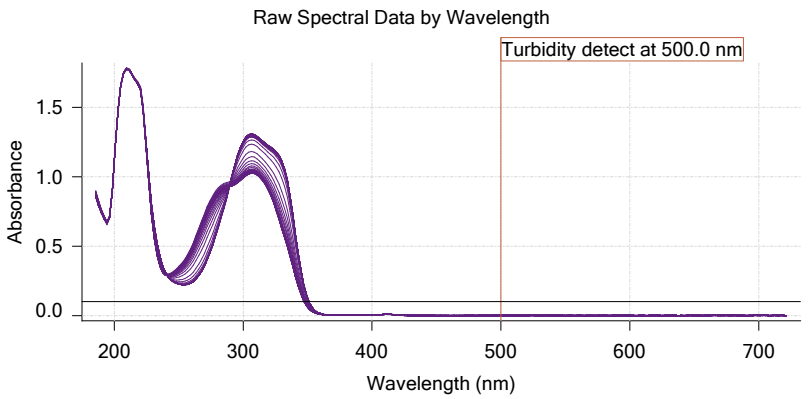
Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









UV-metric psKa Titration 3 of 3 17J-07008 Points 144 to 211

Results

pKa 1	**5.01**
RMSD	**0.003 0.003**
Chi squared	**0.0086**
PCA calculated number of pKas	**4**
Average ionic strength	**0.175 M**
Average temperature	**24.9°C**
Analyte concentration range	**20.7 µM to 19.6 µM**
Methanol weight %	**40.2 %**
Dielectric constant	**60.9**
Water concentration	**29.9 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.477 to 12.545**

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				

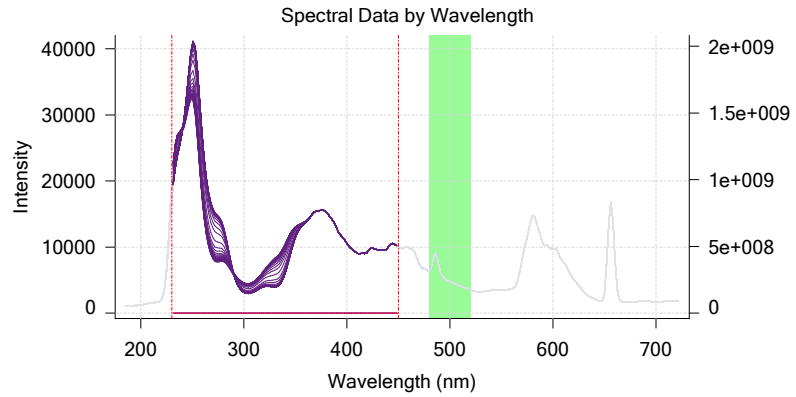
Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

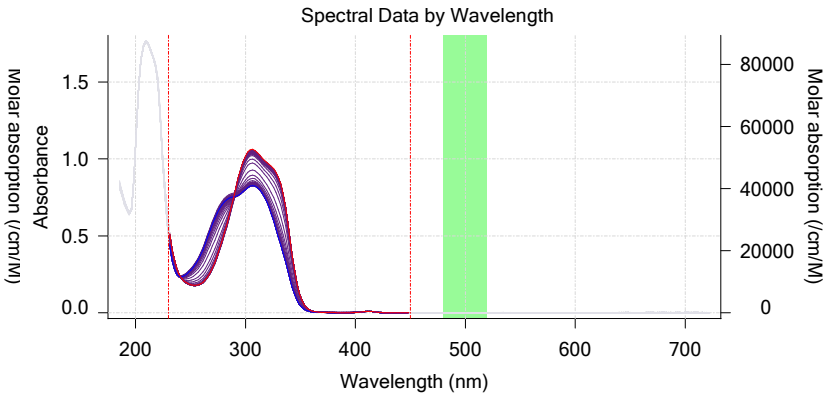
Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

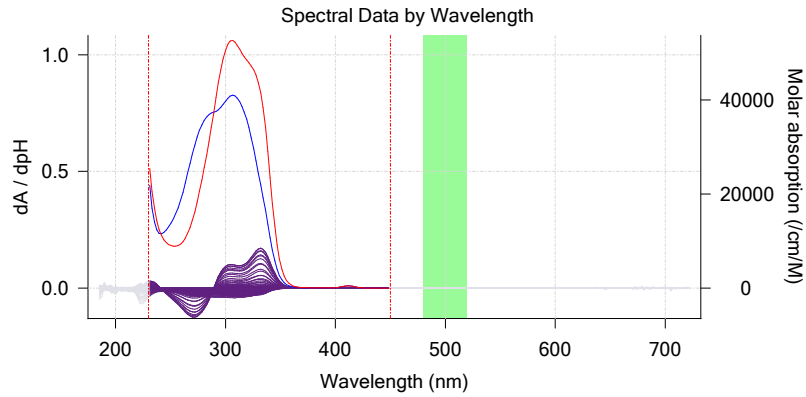
Assay Settings (continued)

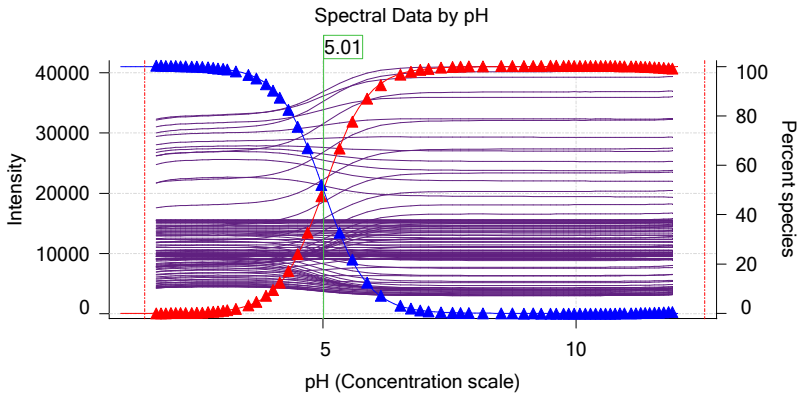
Setting	Value	Original Value	Date/Time changed	Imported from
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

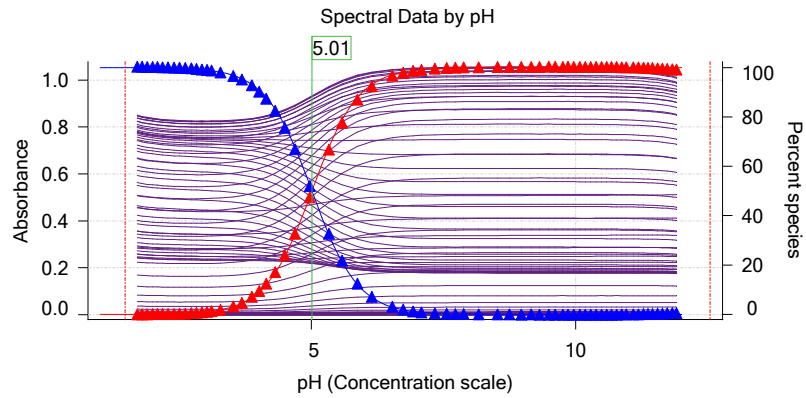
Graphs

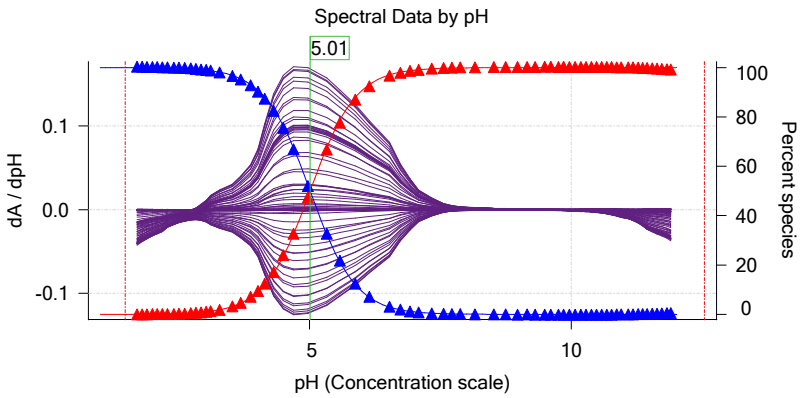








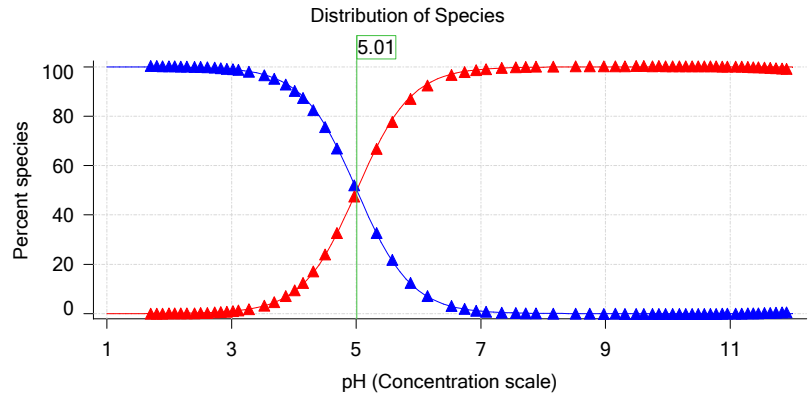


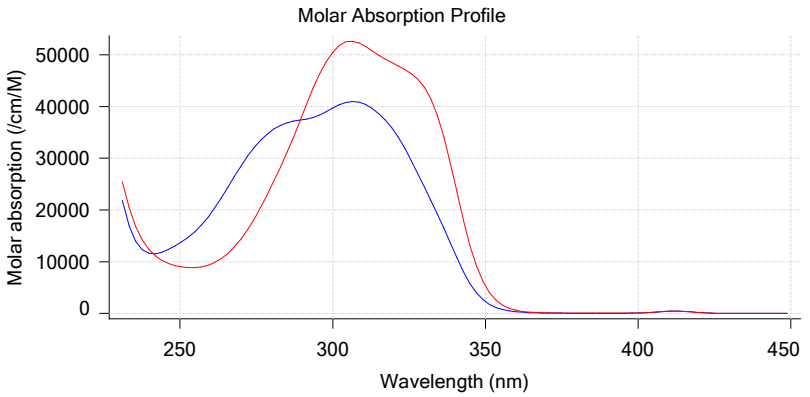


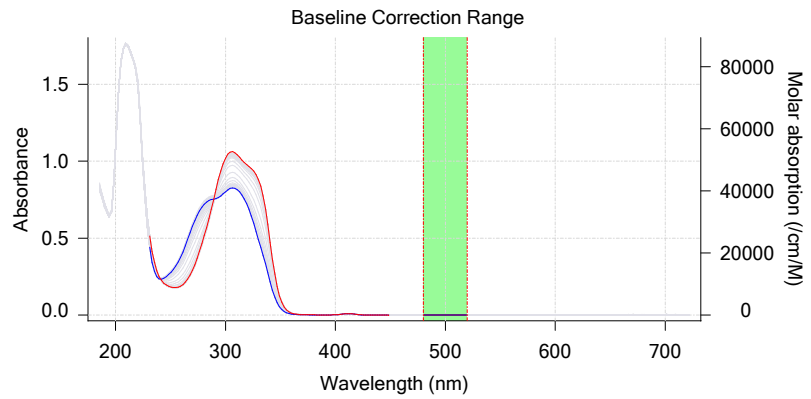
Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

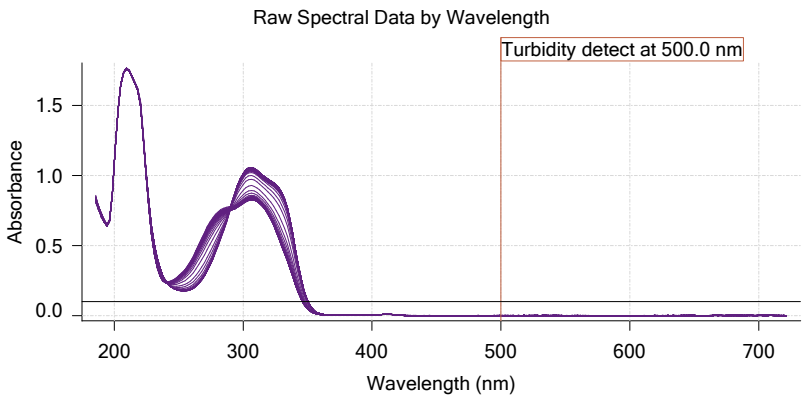
Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









Assay Model

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

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-square
3:11.6	Dark spectrum								
3:13.0	Reference spectrum								
3:40.6	Volume reset due to vial change								
8:45.0	Initial pH = 8.03								
9:05.0	Data point 4	0.15005 mL	0.07331 mL	0.00000 mL	1.34995 mL	0.02500 mL	1.968	-0.04384	0.97174
9:33.7	Data point 5	0.15005 mL	0.07331 mL	0.01545 mL	1.34995 mL	0.02500 mL	2.071	-0.00569	0.17964
9:50.5	Data point 6	0.15005 mL	0.07331 mL	0.02773 mL	1.34995 mL	0.02500 mL	2.180	0.00971	0.79084
10:07.2	Data point 7	0.15005 mL	0.07331 mL	0.03723 mL	1.34995 mL	0.02500 mL	2.288	0.01064	0.86455
10:24.1	Data point 8	0.15005 mL	0.07331 mL	0.04466 mL	1.34995 mL	0.02500 mL	2.401	0.00798	0.72819
10:41.0	Data point 9	0.15005 mL	0.07331 mL	0.05045 mL	1.34995 mL	0.02500 mL	2.499	0.00925	0.90538

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD	d t
10:57.8	Data point 10	0.15005 mL	0.07331 mL	0.05508 mL	1.34995 mL	0.02500 mL	2.616	0.01286	0.90473	0.00067	1 s
11:24.8	Data point 11	0.15005 mL	0.07331 mL	0.05875 mL	1.34995 mL	0.02500 mL	2.714	0.00948	0.76175	0.00054	1 s
11:41.5	Data point 12	0.15005 mL	0.07331 mL	0.06157 mL	1.34995 mL	0.02500 mL	2.836	0.00838	0.83587	0.00045	1 s
12:08.5	Data point 13	0.15005 mL	0.07331 mL	0.06350 mL	1.34995 mL	0.02500 mL	2.933	0.00085	0.03139	0.00024	1 s
12:25.1	Data point 14	0.15005 mL	0.07331 mL	0.06522 mL	1.34995 mL	0.02500 mL	3.035	0.00299	0.19328	0.00034	1 s
12:41.7	Data point 15	0.15005 mL	0.07331 mL	0.06658 mL	1.34995 mL	0.02500 mL	3.134	0.00556	0.56405	0.00037	1 s
12:58.3	Data point 16	0.15005 mL	0.07331 mL	0.06766 mL	1.34995 mL	0.02500 mL	3.193	0.01007	0.85873	0.00054	1 s
13:25.3	Data point 17	0.15005 mL	0.07331 mL	0.06867 mL	1.34995 mL	0.02500 mL	3.285	0.00942	0.86087	0.00050	1 s
13:41.9	Data point 18	0.15005 mL	0.07331 mL	0.06943 mL	1.34995 mL	0.02500 mL	3.402	0.01064	0.80976	0.00058	1 s
14:03.6	Data point 19	0.15005 mL	0.07331 mL	0.07001 mL	1.34995 mL	0.02500 mL	3.516	0.02132	0.96984	0.00107	1 s
14:20.1	Data point 20	0.15005 mL	0.07331 mL	0.07046 mL	1.34995 mL	0.02500 mL	3.658	0.02802	0.98020	0.00140	1 s
14:41.9	Data point 21	0.15005 mL	0.07331 mL	0.07098 mL	1.34995 mL	0.02500 mL	3.856	0.04042	0.98885	0.00201	1 s
15:03.5	Data point 22	0.15005 mL	0.07331 mL	0.07133 mL	1.34995 mL	0.02500 mL	4.026	0.06251	0.99491	0.00309	1 s
15:25.3	Data point 23	0.15005 mL	0.07331 mL	0.07157 mL	1.34995 mL	0.02500 mL	4.166	0.07947	0.99285	0.00394	1 s
15:46.8	Data point 24	0.15005 mL	0.07331 mL	0.07173 mL	1.34995 mL	0.02500 mL	4.284	0.09990	0.99028	0.00496	1 s
16:11.6	Data point 25	0.15005 mL	0.07331 mL	0.07185 mL	1.34995 mL	0.02500 mL	4.391	0.09735	0.98849	0.00483	1 s
16:39.3	Data point 26	0.15005 mL	0.07331 mL	0.07194 mL	1.34995 mL	0.02500 mL	4.520	0.10069	0.99307	0.00499	2 s
17:17.2	Data point 27	0.15005 mL	0.07331 mL	0.07204 mL	1.34995 mL	0.02500 mL	4.694	0.09903	0.99552	0.00490	2 s
18:03.5	Data point 28	0.15005 mL	0.07331 mL	0.07213 mL	1.34995 mL	0.02500 mL	4.940	0.09004	0.88669	0.00472	3 s
18:59.2	Data point 29	0.15005 mL	0.07331 mL	0.07220 mL	1.34995 mL	0.02500 mL	5.183	0.09773	0.98421	0.00486	4 s
20:02.4	Data point 30	0.15005 mL	0.07331 mL	0.07227 mL	1.34995 mL	0.02500 mL	5.509	0.14412	0.99800	0.00712	T o a
21:19.1	Data point 31	0.15005 mL	0.07331 mL	0.07234 mL	1.34995 mL	0.02500 mL	6.252	0.18732	0.99659	0.00926	T o a
22:30.7	Data point 32	0.15005 mL	0.07331 mL	0.07239 mL	1.34995 mL	0.02500 mL	6.613	0.07325	0.58421	0.00473	5 s
23:41.4	Data point 33	0.15005 mL	0.07331 mL	0.07248 mL	1.34995 mL	0.02500 mL	7.067	0.10012	0.99249	0.00496	4 s
24:45.2	Data point 34	0.15005 mL	0.07331 mL	0.07255 mL	1.34995 mL	0.02500 mL	7.305	0.10049	0.99172	0.00498	3 s
25:40.1	Data point 35	0.15005 mL	0.07331 mL	0.07262 mL	1.34995 mL	0.02500 mL	7.476	0.09956	0.99376	0.00493	3 s
26:31.9	Data point 36	0.15005 mL	0.07331 mL	0.07272 mL	1.34995 mL	0.02500 mL	7.681	0.09843	0.99531	0.00487	2 s
27:20.8	Data point 37	0.15005 mL	0.07331 mL	0.07281 mL	1.34995 mL	0.02500 mL	7.861	0.10092	0.99292	0.00500	2 s

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SI
42:33.9	Data point 67	0.15005 mL	0.07331 mL	0.08958 mL	1.34995 mL	0.02500 mL	11.825	-0.00428	0.49302	0.
42:50.6	Data point 68	0.15005 mL	0.07331 mL	0.09374 mL	1.34995 mL	0.02500 mL	11.926	-0.00582	0.66314	0.
43:07.3	Data point 69	0.15005 mL	0.07331 mL	0.09904 mL	1.34995 mL	0.02500 mL	12.023	-0.00195	0.17577	0.
44:42.4	Reference spectrum									
45:45.1	Data point 71	0.22001 mL	0.17331 mL	0.09906 mL	1.34995 mL	0.02500 mL	1.963	-0.04858	0.92277	0.
46:12.4	Data point 72	0.22001 mL	0.17331 mL	0.11437 mL	1.34995 mL	0.02500 mL	2.066	0.00539	0.35675	0.
46:29.4	Data point 73	0.22001 mL	0.17331 mL	0.12801 mL	1.34995 mL	0.02500 mL	2.184	0.00805	0.46264	0.
46:56.6	Data point 74	0.22001 mL	0.17331 mL	0.13657 mL	1.34995 mL	0.02500 mL	2.285	0.02048	0.56559	0.
47:18.6	Data point 75	0.22001 mL	0.17331 mL	0.14313 mL	1.34995 mL	0.02500 mL	2.382	0.02354	0.95170	0.
47:45.7	Data point 76	0.22001 mL	0.17331 mL	0.14915 mL	1.34995 mL	0.02500 mL	2.484	0.01338	0.88956	0.
48:02.5	Data point 77	0.22001 mL	0.17331 mL	0.15440 mL	1.34995 mL	0.02500 mL	2.609	0.01721	0.93345	0.
48:29.5	Data point 78	0.22001 mL	0.17331 mL	0.15818 mL	1.34995 mL	0.02500 mL	2.710	0.00917	0.85110	0.
48:46.2	Data point 79	0.22001 mL	0.17331 mL	0.16131 mL	1.34995 mL	0.02500 mL	2.837	0.01568	0.91796	0.
49:13.1	Data point 80	0.22001 mL	0.17331 mL	0.16340 mL	1.34995 mL	0.02500 mL	2.935	0.01372	0.90142	0.
49:29.7	Data point 81	0.22001 mL	0.17331 mL	0.16524 mL	1.34995 mL	0.02500 mL	3.034	0.00221	0.18916	0.
49:46.3	Data point 82	0.22001 mL	0.17331 mL	0.16672 mL	1.34995 mL	0.02500 mL	3.120	0.00983	0.79296	0.
50:02.9	Data point 83	0.22001 mL	0.17331 mL	0.16792 mL	1.34995 mL	0.02500 mL	3.229	0.01122	0.87851	0.
50:19.5	Data point 84	0.22001 mL	0.17331 mL	0.16886 mL	1.34995 mL	0.02500 mL	3.358	0.01253	0.93394	0.
50:46.5	Data point 85	0.22001 mL	0.17331 mL	0.16950 mL	1.34995 mL	0.02500 mL	3.453	0.01761	0.95688	0.
51:03.0	Data point 86	0.22001 mL	0.17331 mL	0.17004 mL	1.34995 mL	0.02500 mL	3.565	0.01962	0.95692	0.
51:19.6	Data point 87	0.22001 mL	0.17331 mL	0.17046 mL	1.34995 mL	0.02500 mL	3.672	0.02712	0.97628	0.
51:36.0	Data point 88	0.22001 mL	0.17331 mL	0.17079 mL	1.34995 mL	0.02500 mL	3.777	0.03251	0.96671	0.
51:52.6	Data point 89	0.22001 mL	0.17331 mL	0.17105 mL	1.34995 mL	0.02500 mL	3.875	0.03668	0.98245	0.
52:09.2	Data point 90	0.22001 mL	0.17331 mL	0.17126 mL	1.34995 mL	0.02500 mL	3.970	0.04093	0.97316	0.
52:25.8	Data point 91	0.22001 mL	0.17331 mL	0.17142 mL	1.34995 mL	0.02500 mL	4.045	0.04723	0.98797	0.
52:47.6	Data point 92	0.22001 mL	0.17331 mL	0.17164 mL	1.34995 mL	0.02500 mL	4.186	0.07494	0.99220	0.
53:09.3	Data point 93	0.22001 mL	0.17331 mL	0.17183 mL	1.34995 mL	0.02500 mL	4.364	0.10097	0.99430	0.
53:31.9	Data point 94	0.22001 mL	0.17331 mL	0.17194 mL	1.34995 mL	0.02500 mL	4.473	0.09850	0.99243	0.
54:02.0	Data point 95	0.22001 mL	0.17331 mL	0.17206 mL	1.34995 mL	0.02500 mL	4.624	0.10108	0.99650	0.
54:39.7	Data point 96	0.22001 mL	0.17331 mL	0.17215 mL	1.34995 mL	0.02500 mL	4.779	0.09962	0.98985	0.
55:22.1	Data point 97	0.22001 mL	0.17331 mL	0.17222 mL	1.34995 mL	0.02500 mL	4.965	0.10012	0.97767	0.
56:13.4	Data point 98	0.22001 mL	0.17331 mL	0.17230 mL	1.34995 mL	0.02500 mL	5.190	0.09577	0.98450	0.
57:11.2	Data point 99	0.22001 mL	0.17331 mL	0.17237 mL	1.34995 mL	0.02500 mL	5.562	0.09982	0.99195	0.
58:18.3	Data point 100	0.22001 mL	0.17331 mL	0.17241 mL	1.34995 mL	0.02500 mL	5.879	0.09752	0.99132	0.
59:29.1	Data point 101	0.22001 mL	0.17331 mL	0.17246 mL	1.34995 mL	0.02500 mL	6.219	0.09862	0.99637	0.
1:00:41.3	Data point 102	0.22001 mL	0.17331 mL	0.17253 mL	1.34995 mL	0.02500 mL	6.604	0.10103	0.99470	0.
1:01:43.6	Data point 103	0.22001 mL	0.17331 mL	0.17260 mL	1.34995 mL	0.02500 mL	6.892	0.10018	0.99236	0.
1:02:38.8	Data point 104	0.22001 mL	0.17331 mL	0.17267 mL	1.34995 mL	0.02500 mL	7.053	0.09709	0.98546	0.
1:03:20.9	Data point 105	0.22001 mL	0.17331 mL	0.17274 mL	1.34995 mL	0.02500 mL	7.214	0.09976	0.99383	0.
1:04:01.2	Data point 106	0.22001 mL	0.17331 mL	0.17281 mL	1.34995 mL	0.02500 mL	7.364	0.09888	0.99221	0.
1:04:42.9	Data point 107	0.22001 mL	0.17331 mL	0.17288 mL	1.34995 mL	0.02500 mL	7.514	0.09989	0.99145	0.
1:05:28.1	Data point 108	0.22001 mL	0.17331 mL	0.17298 mL	1.34995 mL	0.02500 mL	7.687	0.09737	0.99313	0.
1:06:07.9	Data point 109	0.22001 mL	0.17331 mL	0.17307 mL	1.34995 mL	0.02500 mL	7.859	0.09751	0.98830	0.
1:06:45.7	Data point 110	0.22001 mL	0.17331 mL	0.17314 mL	1.34995 mL	0.02500 mL	7.991	0.09914	0.99100	0.
1:07:22.0	Data point 111	0.22001 mL	0.17331 mL	0.17321 mL	1.34995 mL	0.02500 mL	8.140	0.09745	0.96937	0.
1:07:59.8	Data point 112	0.22001 mL	0.17331 mL	0.17328 mL	1.34995 mL	0.02500 mL	8.294	0.09867	0.98752	0.
1:08:40.6	Data point 113	0.22001 mL	0.17331 mL	0.17335 mL	1.34995 mL	0.02500 mL	8.481	0.09862	0.98927	0.
1:09:25.8	Data point 114	0.22001 mL	0.17331 mL	0.17342 mL	1.34995 mL	0.02500 mL	8.680	0.10063	0.99049	0.
1:10:11.6	Data point 115	0.22001 mL	0.17331 mL	0.17350 mL	1.34995 mL	0.02500 mL	8.933	0.09978	0.98381	0.
1:10:58.4	Data point 116	0.22001 mL	0.17331 mL	0.17357 mL	1.34995 mL	0.02500 mL	9.131	0.10000	0.98307	0.
1:11:40.8	Data point 117	0.22001 mL	0.17331 mL	0.17364 mL	1.34995 mL	0.02500 mL	9.349	0.09478	0.97546	0.
1:12:21.1	Data point 118	0.22001 mL	0.17331 mL	0.17371 mL	1.34995 mL	0.02500 mL	9.496	0.09924	0.98988	0.
1:12:55.7	Data point 119	0.22001 mL	0.17331 mL	0.17378 mL	1.34995 mL	0.02500 mL	9.625	0.10027	0.98245	0.
1:13:28.4	Data point 120	0.22001 mL	0.17331 mL	0.17387 mL	1.34995 mL	0.02500 mL	9.779	0.09867	0.98336	0.
1:13:54.5	Data point 121	0.22001 mL	0.17331 mL	0.17397 mL	1.34995 mL	0.02500 mL	9.891	0.10059	0.98974	0.
1:14:22.0	Data point 122	0.22001 mL	0.17331 mL	0.17406 mL	1.34995 mL	0.02500 mL	10.002	0.09832	0.96383	0.
1:14:48.6	Data point 123	0.22001 mL	0.17331 mL	0.17418 mL	1.34995 mL	0.02500 mL	10.111	0.07626	0.98232	0.

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SE
1:15:10.1	Data point 124	0.22001 mL	0.17331 mL	0.17432 mL	1.34995 mL	0.02500 mL	10.221	0.05511	0.97660	0.
1:15:36.9	Data point 125	0.22001 mL	0.17331 mL	0.17448 mL	1.34995 mL	0.02500 mL	10.320	0.04439	0.96712	0.
1:15:58.6	Data point 126	0.22001 mL	0.17331 mL	0.17469 mL	1.34995 mL	0.02500 mL	10.440	0.02578	0.94578	0.
1:16:20.2	Data point 127	0.22001 mL	0.17331 mL	0.17495 mL	1.34995 mL	0.02500 mL	10.549	0.02330	0.93104	0.
1:16:42.1	Data point 128	0.22001 mL	0.17331 mL	0.17528 mL	1.34995 mL	0.02500 mL	10.657	0.01355	0.92117	0.
1:17:08.9	Data point 129	0.22001 mL	0.17331 mL	0.17568 mL	1.34995 mL	0.02500 mL	10.749	0.00874	0.87357	0.
1:17:30.6	Data point 130	0.22001 mL	0.17331 mL	0.17625 mL	1.34995 mL	0.02500 mL	10.868	0.00182	0.16369	0.
1:17:52.4	Data point 131	0.22001 mL	0.17331 mL	0.17686 mL	1.34995 mL	0.02500 mL	10.967	0.00138	0.13374	0.
1:18:09.0	Data point 132	0.22001 mL	0.17331 mL	0.17756 mL	1.34995 mL	0.02500 mL	11.072	-0.00357	0.48066	0.
1:18:25.7	Data point 133	0.22001 mL	0.17331 mL	0.17846 mL	1.34995 mL	0.02500 mL	11.177	-0.00354	0.56868	0.
1:18:42.4	Data point 134	0.22001 mL	0.17331 mL	0.17961 mL	1.34995 mL	0.02500 mL	11.282	-0.00181	0.20866	0.
1:18:59.0	Data point 135	0.22001 mL	0.17331 mL	0.18107 mL	1.34995 mL	0.02500 mL	11.380	-0.00299	0.55467	0.
1:19:15.6	Data point 136	0.22001 mL	0.17331 mL	0.18290 mL	1.34995 mL	0.02500 mL	11.470	-0.00400	0.60052	0.
1:19:32.2	Data point 137	0.22001 mL	0.17331 mL	0.18516 mL	1.34995 mL	0.02500 mL	11.558	-0.00242	0.23718	0.
1:19:48.8	Data point 138	0.22001 mL	0.17331 mL	0.18791 mL	1.34995 mL	0.02500 mL	11.652	-0.00300	0.23074	0.
1:20:05.5	Data point 139	0.22001 mL	0.17331 mL	0.19137 mL	1.34995 mL	0.02500 mL	11.748	-0.00235	0.25129	0.
1:20:22.2	Data point 140	0.22001 mL	0.17331 mL	0.19570 mL	1.34995 mL	0.02500 mL	11.839	-0.00581	0.71745	0.
1:20:38.9	Data point 141	0.22001 mL	0.17331 mL	0.20106 mL	1.34995 mL	0.02500 mL	11.934	-0.00791	0.80166	0.
1:20:55.6	Data point 142	0.22001 mL	0.17331 mL	0.20781 mL	1.34995 mL	0.02500 mL	12.026	-0.00189	0.10747	0.
1:22:37.7	Reference spectrum									
1:23:57.9	Data point 144	0.39005 mL	0.29744 mL	0.20783 mL	1.34995 mL	0.02500 mL	1.977	-0.06981	0.94029	0.
1:24:20.1	Data point 145	0.39005 mL	0.29744 mL	0.22338 mL	1.34995 mL	0.02500 mL	2.070	0.00795	0.81074	0.
1:24:42.2	Data point 146	0.39005 mL	0.29744 mL	0.23492 mL	1.34995 mL	0.02500 mL	2.161	-0.00095	0.01039	0.
1:25:09.4	Data point 147	0.39005 mL	0.29744 mL	0.24494 mL	1.34995 mL	0.02500 mL	2.262	0.00917	0.64449	0.
1:25:31.4	Data point 148	0.39005 mL	0.29744 mL	0.25205 mL	1.34995 mL	0.02500 mL	2.355	0.01358	0.91979	0.
1:25:53.4	Data point 149	0.39005 mL	0.29744 mL	0.25826 mL	1.34995 mL	0.02500 mL	2.449	0.01106	0.87642	0.
1:26:20.4	Data point 150	0.39005 mL	0.29744 mL	0.26359 mL	1.34995 mL	0.02500 mL	2.548	0.01580	0.91264	0.
1:26:37.1	Data point 151	0.39005 mL	0.29744 mL	0.26851 mL	1.34995 mL	0.02500 mL	2.667	0.00615	0.61367	0.
1:27:04.1	Data point 152	0.39005 mL	0.29744 mL	0.27194 mL	1.34995 mL	0.02500 mL	2.765	0.01093	0.77080	0.
1:27:20.7	Data point 153	0.39005 mL	0.29744 mL	0.27493 mL	1.34995 mL	0.02500 mL	2.870	0.00845	0.74527	0.
1:27:37.4	Data point 154	0.39005 mL	0.29744 mL	0.27728 mL	1.34995 mL	0.02500 mL	2.987	0.00366	0.40073	0.
1:28:04.3	Data point 155	0.39005 mL	0.29744 mL	0.27876 mL	1.34995 mL	0.02500 mL	3.084	0.00494	0.50342	0.
1:28:31.1	Data point 156	0.39005 mL	0.29744 mL	0.28008 mL	1.34995 mL	0.02500 mL	3.181	0.00940	0.79795	0.
1:28:47.8	Data point 157	0.39005 mL	0.29744 mL	0.28121 mL	1.34995 mL	0.02500 mL	3.277	0.00604	0.63168	0.
1:29:04.4	Data point 158	0.39005 mL	0.29744 mL	0.28210 mL	1.34995 mL	0.02500 mL	3.361	0.01007	0.77002	0.
1:29:36.6	Data point 159	0.39005 mL	0.29744 mL	0.28248 mL	1.34995 mL	0.02500 mL	3.532	-0.00152	0.10276	0.
1:30:03.4	Data point 160	0.39005 mL	0.29744 mL	0.28518 mL	1.34995 mL	0.02500 mL	3.771	0.00997	0.74172	0.
1:30:25.3	Data point 161	0.39005 mL	0.29744 mL	0.28570 mL	1.34995 mL	0.02500 mL	3.931	0.01461	0.81103	0.
1:30:46.9	Data point 162	0.39005 mL	0.29744 mL	0.28608 mL	1.34995 mL	0.02500 mL	4.115	0.04120	0.96745	0.
1:31:08.6	Data point 163	0.39005 mL	0.29744 mL	0.28631 mL	1.34995 mL	0.02500 mL	4.254	0.06548	0.97763	0.
1:31:30.3	Data point 164	0.39005 mL	0.29744 mL	0.28648 mL	1.34995 mL	0.02500 mL	4.385	0.08087	0.98063	0.
1:31:51.9	Data point 165	0.39005 mL	0.29744 mL	0.28659 mL	1.34995 mL	0.02500 mL	4.551	0.09725	0.97763	0.
1:32:17.5	Data point 166	0.39005 mL	0.29744 mL	0.28669 mL	1.34995 mL	0.02500 mL	4.735	0.09745	0.98744	0.
1:32:49.1	Data point 167	0.39005 mL	0.29744 mL	0.28676 mL	1.34995 mL	0.02500 mL	4.926	0.09973	0.98884	0.
1:33:30.8	Data point 168	0.39005 mL	0.29744 mL	0.28683 mL	1.34995 mL	0.02500 mL	5.199	0.09817	0.98669	0.
1:34:22.6	Data point 169	0.39005 mL	0.29744 mL	0.28690 mL	1.34995 mL	0.02500 mL	5.556	0.09906	0.96844	0.
1:35:10.1	Data point 170	0.39005 mL	0.29744 mL	0.28695 mL	1.34995 mL	0.02500 mL	5.802	0.09844	0.98937	0.
1:36:00.7	Data point 171	0.39005 mL	0.29744 mL	0.28699 mL	1.34995 mL	0.02500 mL	6.091	0.09916	0.99165	0.
1:36:53.4	Data point 172	0.39005 mL	0.29744 mL	0.28704 mL	1.34995 mL	0.02500 mL	6.361	0.09941	0.98339	0.
1:37:37.6	Data point 173	0.39005 mL	0.29744 mL	0.28711 mL	1.34995 mL	0.02500 mL	6.740	0.09890	0.97644	0.
1:38:14.9	Data point 174	0.39005 mL	0.29744 mL	0.28716 mL	1.34995 mL	0.02500 mL	6.946	0.09673	0.96899	0.
1:38:47.6	Data point 175	0.39005 mL	0.29744 mL	0.28721 mL	1.34995 mL	0.02500 mL	7.129	0.09352	0.95173	0.
1:39:20.2	Data point 176	0.39005 mL	0.29744 mL	0.28725 mL	1.34995 mL	0.02500 mL	7.289	0.09862	0.97685	0.
1:39:57.5	Data point 177	0.39005 mL	0.29744 mL	0.28732 mL	1.34995 mL	0.02500 mL	7.536	0.09491	0.96581	0.
1:40:36.4	Data point 178	0.39005 mL	0.29744 mL	0.28739 mL	1.34995 mL	0.02500 mL	7.759	0.09960	0.98267	0.
1:41:08.0	Data point 179	0.39005 mL	0.29744 mL	0.28744 mL	1.34995 mL	0.02500 mL	7.919	0.09611	0.94766	0.
1:41:40.0	Data point 180	0.39005 mL	0.29744 mL	0.28749 mL	1.34995 mL	0.02500 mL	8.078	0.09317	0.96561	0.

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
1:42:17.7	Data point 181	0.39005 mL	0.29744 mL	0.28756 mL	1.34995 mL	0.02500 mL	8.355	0.09741	0.97011	0.0048
1:42:58.0	Data point 182	0.39005 mL	0.29744 mL	0.28763 mL	1.34995 mL	0.02500 mL	8.707	0.09914	0.97165	0.0049
1:43:36.3	Data point 183	0.39005 mL	0.29744 mL	0.28768 mL	1.34995 mL	0.02500 mL	8.930	0.09927	0.97636	0.0049
1:44:11.6	Data point 184	0.39005 mL	0.29744 mL	0.28772 mL	1.34995 mL	0.02500 mL	9.155	0.09973	0.96892	0.0050
1:44:47.0	Data point 185	0.39005 mL	0.29744 mL	0.28777 mL	1.34995 mL	0.02500 mL	9.335	0.09604	0.95852	0.0048
1:45:18.1	Data point 186	0.39005 mL	0.29744 mL	0.28782 mL	1.34995 mL	0.02500 mL	9.492	0.09738	0.97167	0.0048
1:45:52.3	Data point 187	0.39005 mL	0.29744 mL	0.28789 mL	1.34995 mL	0.02500 mL	9.669	0.09897	0.95758	0.0049
1:46:19.4	Data point 188	0.39005 mL	0.29744 mL	0.28796 mL	1.34995 mL	0.02500 mL	9.787	0.09290	0.93810	0.0047
1:46:42.1	Data point 189	0.39005 mL	0.29744 mL	0.28805 mL	1.34995 mL	0.02500 mL	9.928	0.08998	0.98097	0.0044
1:47:03.9	Data point 190	0.39005 mL	0.29744 mL	0.28815 mL	1.34995 mL	0.02500 mL	10.029	0.06065	0.95194	0.0030
1:47:20.4	Data point 191	0.39005 mL	0.29744 mL	0.28826 mL	1.34995 mL	0.02500 mL	10.136	0.03958	0.93883	0.0020
1:47:36.9	Data point 192	0.39005 mL	0.29744 mL	0.28841 mL	1.34995 mL	0.02500 mL	10.245	0.02909	0.93027	0.0014
1:47:53.4	Data point 193	0.39005 mL	0.29744 mL	0.28859 mL	1.34995 mL	0.02500 mL	10.351	0.01660	0.91925	0.0008
1:48:10.0	Data point 194	0.39005 mL	0.29744 mL	0.28883 mL	1.34995 mL	0.02500 mL	10.451	0.01348	0.92579	0.0006
1:48:26.6	Data point 195	0.39005 mL	0.29744 mL	0.28913 mL	1.34995 mL	0.02500 mL	10.553	0.00437	0.64112	0.0002
1:48:43.3	Data point 196	0.39005 mL	0.29744 mL	0.28951 mL	1.34995 mL	0.02500 mL	10.651	0.00110	0.04060	0.0002
1:48:59.8	Data point 197	0.39005 mL	0.29744 mL	0.28998 mL	1.34995 mL	0.02500 mL	10.748	-0.00185	0.10871	0.0002
1:49:16.4	Data point 198	0.39005 mL	0.29744 mL	0.29057 mL	1.34995 mL	0.02500 mL	10.842	-0.00406	0.39231	0.0003
1:49:33.1	Data point 199	0.39005 mL	0.29744 mL	0.29130 mL	1.34995 mL	0.02500 mL	10.935	-0.00701	0.76110	0.0004
1:49:49.7	Data point 200	0.39005 mL	0.29744 mL	0.29219 mL	1.34995 mL	0.02500 mL	11.029	-0.00651	0.57533	0.0004
1:50:06.3	Data point 201	0.39005 mL	0.29744 mL	0.29330 mL	1.34995 mL	0.02500 mL	11.113	-0.00996	0.83015	0.0005
1:50:28.1	Data point 202	0.39005 mL	0.29744 mL	0.29567 mL	1.34995 mL	0.02500 mL	11.246	-0.00908	0.86719	0.0004
1:50:49.9	Data point 203	0.39005 mL	0.29744 mL	0.29704 mL	1.34995 mL	0.02500 mL	11.338	-0.00730	0.73018	0.0004
1:51:16.8	Data point 204	0.39005 mL	0.29744 mL	0.29922 mL	1.34995 mL	0.02500 mL	11.433	-0.00814	0.69283	0.0004
1:51:33.4	Data point 205	0.39005 mL	0.29744 mL	0.30207 mL	1.34995 mL	0.02500 mL	11.520	-0.01019	0.87198	0.0005
1:51:50.1	Data point 206	0.39005 mL	0.29744 mL	0.30555 mL	1.34995 mL	0.02500 mL	11.604	-0.00959	0.89477	0.0005
1:52:17.2	Data point 207	0.39005 mL	0.29744 mL	0.30945 mL	1.34995 mL	0.02500 mL	11.699	-0.00717	0.74050	0.0004
1:52:33.9	Data point 208	0.39005 mL	0.29744 mL	0.31475 mL	1.34995 mL	0.02500 mL	11.786	-0.01036	0.87388	0.0005
1:52:50.7	Data point 209	0.39005 mL	0.29744 mL	0.32128 mL	1.34995 mL	0.02500 mL	11.877	-0.00754	0.69783	0.0004
1:53:07.6	Data point 210	0.39005 mL	0.29744 mL	0.32942 mL	1.34995 mL	0.02500 mL	11.973	-0.00797	0.74702	0.0004
1:53:24.4	Data point 211	0.39005 mL	0.29744 mL	0.33714 mL	1.34995 mL	0.02500 mL	12.045	-0.00727	0.71021	0.0004
1:55:23.5	Assay volumes	0.64005 mL	0.42665 mL	0.33714 mL	1.34995 mL	0.02500 mL				

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.100			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	Spectrometer			
Monitor at a wavelength of	500.0 nm			
Absorbance threshold of	0.100			
Collect turbidity sensor data	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	15%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Cosolvent in use	Yes			
Cosolvent type	Methanol			
Cosolvent volume	1.35 mL			
Cosolvent added	Automatic			
ISA water volume	0.15 mL			
Water added	Automatic			
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			
After medium addition, stir for	5 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	60 seconds			
Sample Dissolution				
Perform a dissolution stage	No			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	10 seconds			
Titration 2				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.07 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Titration 3				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.17 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Data Point Stability				
Stir during data point collection	Yes			
For point collection, stir at	15%			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00500 dpH/dt			
Stability timeout after	60 seconds			
Experiment cleanup				
Adjust pH to cleanup	To start pH			
And then stir for	60 seconds			
For cleaning, stir at	20%			
Then add water volume	0.25 mL			
And then stir for	30 seconds			

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.161	10/7/2017 12:30:45 PM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus S	0.9927	10/7/2017 12:30:45 PM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus jH	0.5	10/7/2017 12:30:45 PM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus jOH	-0.7	10/7/2017 12:30:45 PM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Base concentration factor	1.011	10/7/2017 12:30:45 PM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	1.003	10/7/2017 12:30:45 PM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T311053		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1100253	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	8-18-17	9/26/2017 9:05:04 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	166940 and 172875	10/6/2017 2:55:40 PM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9-22-17	9/22/2017 4:02:42 PM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	9-26-17	10/5/2017 5:02:03 PM
Port B	Cyclohexane		9/19/2017 2:15:02 PM
Port C	MeCN (50%, 0.15 M KCl)	10-2-17	10/2/2017 11:28:55 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Phosphate Buffer		9/12/2017 12:32:29 PM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	9-14-17	9/14/2017 10:30:38 AM
Titrator		T3TM1100153	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 10:21:54 AM
E0 calibration	-7.50 mV		10/7/2017 12:31:09 PM
Filling solution	3M KCl	KCL095	10/4/2017 3:50:10 PM
Liquids			
Wash 1	50% IPA:50% Water		10/6/2017 2:50:08 PM
Wash 2	0.5% Trition X-100 in H20		10/6/2017 2:50:11 PM
Buffer position 1	pH7 Wash		10/6/2017 2:50:17 PM
Buffer position 2	pH 7		10/6/2017 2:50:19 PM
Storage position			10/6/2017 2:50:25 PM
Wash water	8.2e+003 mL	10-6-17	10/6/2017 3:04:25 PM

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Waste	1.8e+003 mL		10/6/2017 3:04:33 PM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	391:10:29		11/23/2010 12:22:28 PM
Calibrated on	10/5/2017 10:23:25 AM		
Integration time	11		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
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

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07008**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07008_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 12:30:45 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Refinement Settings (continued)

Setting	Value	Default value
Maximum RMSD severe warning	0.250	0.250
Maximum RMSD warning	0.050	0.050

Tray Information

Title
Location G5