Yasuda-Shedlovsky Result

Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

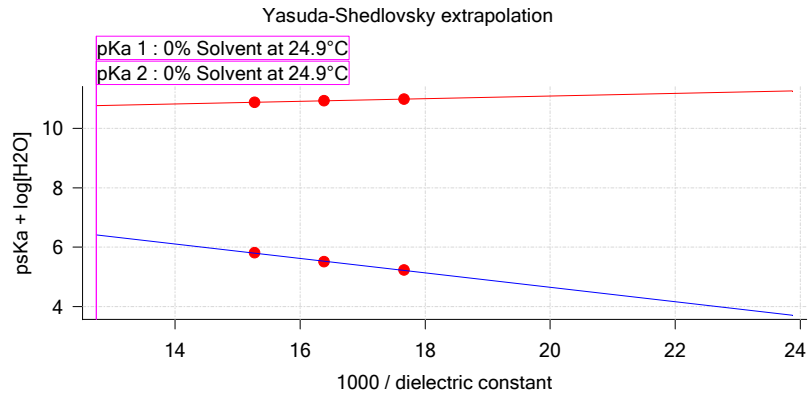
Yasuda-Shedlovsky result

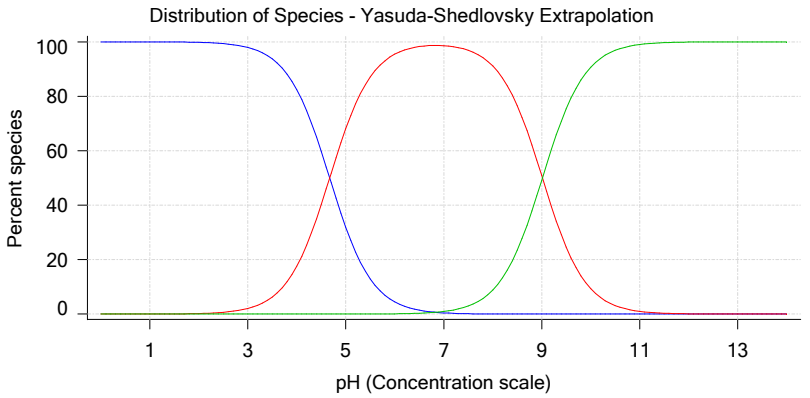
Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.67	±0.06	9.50	-242.2362	0.9963	0.165 M	24.9°C
Yasuda-Shedlovsky	9.01	±0.02	10.19	44.3207	0.9912	0.165 M	24.9°C

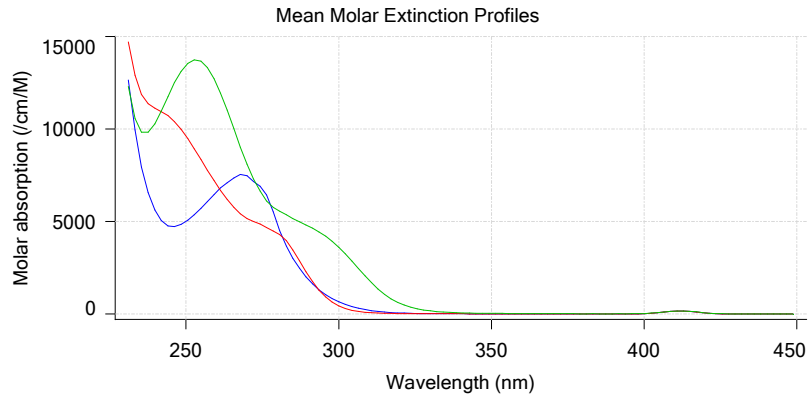
Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1	psKa 2
17J-12009 Points 4 to 42	49.50 %	Up	UV-metric pKa	56.6	24.7 M	0.157 M	24.9°C	3.84	9.58
17J-12009 Points 44 to 84	39.91 %	Up	UV-metric pKa	61.0	30.1 M	0.166 M	24.9°C	4.03	9.45
17J-12009 Points 86 to 128	30.13 %	Up	UV-metric pKa	65.5	35.8 M	0.172 M	24.9°C	4.26	9.31

Graphs







UV-metric psKa Titration 1 of 3 17J-12009 Points 4 to 42

Results

pKa 1	**3.84**
pKa 2	**9.58**
RMSD	**0.001 0.001 0.001**
Chi squared	**0.0049**
PCA calculated number of pKas	**2**
Average ionic strength	**0.157 M**
Average temperature	**24.9°C**
Analyte concentration range	**68.6 µM to 64.5 µM**
Methanol weight %	**49.5 %**
Dielectric constant	**56.6**
Water concentration	**24.7 M**

Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
Wavelength clipping **230.0 nm to 450.0 nm**
pH clipping **1.471 to 12.517**

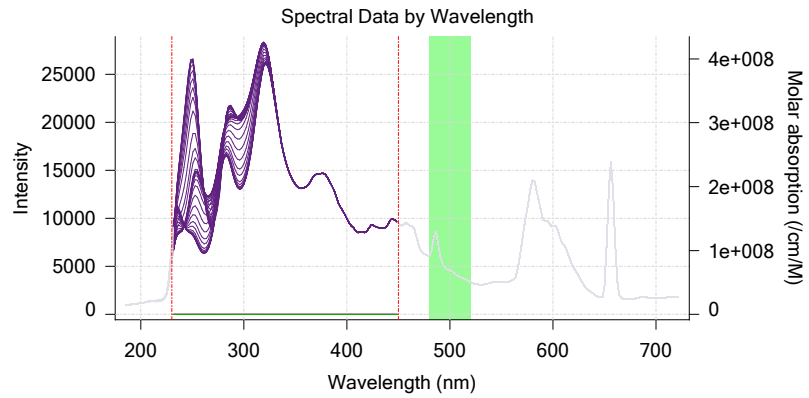
Warnings and errors

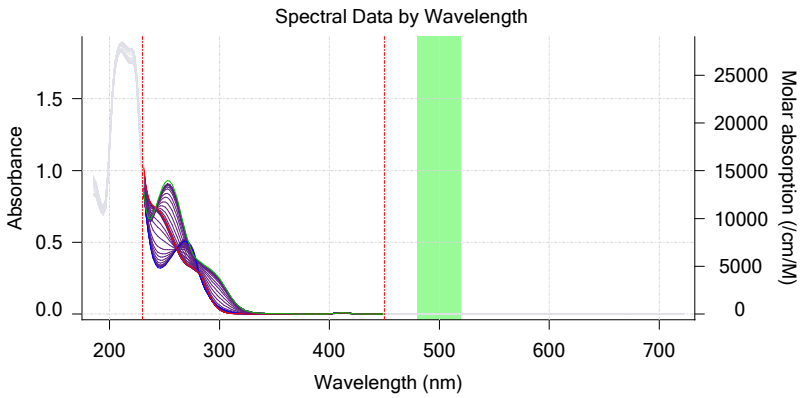
Errors None
Warnings None

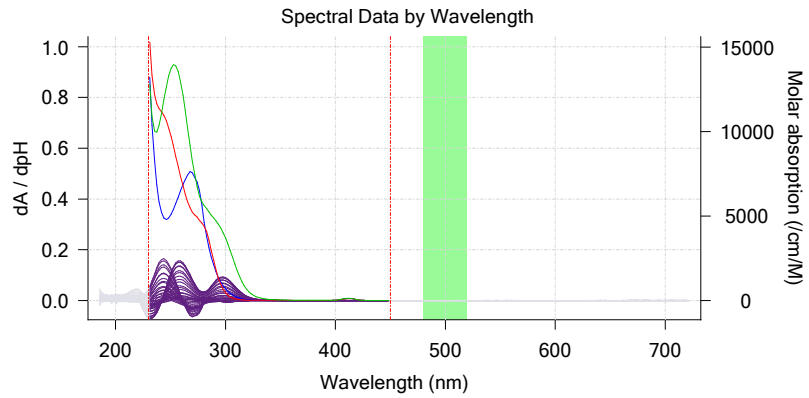
Assay Settings

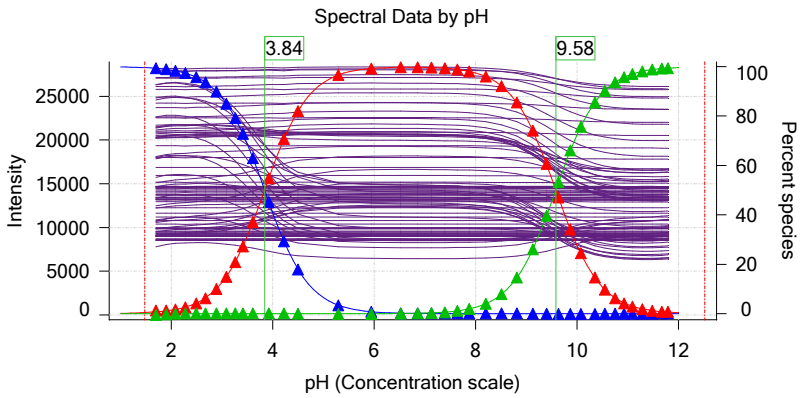
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

Graphs





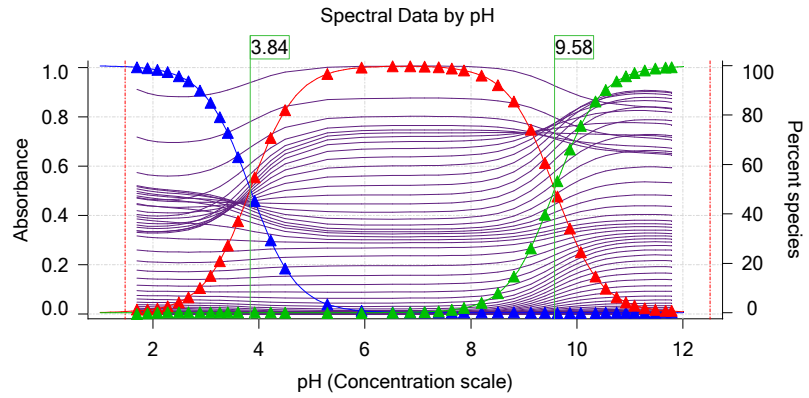


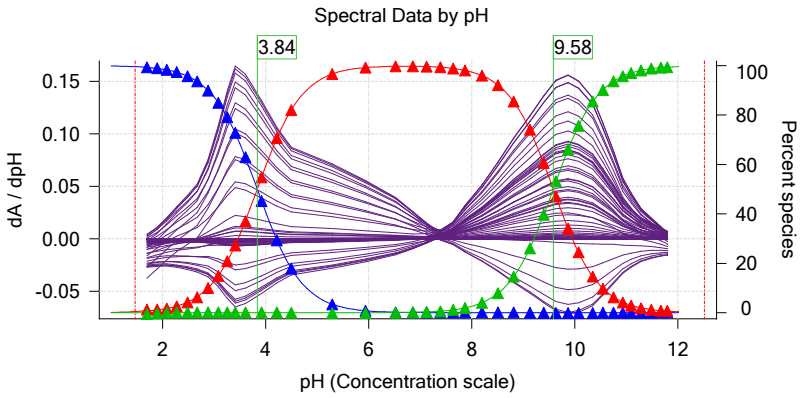


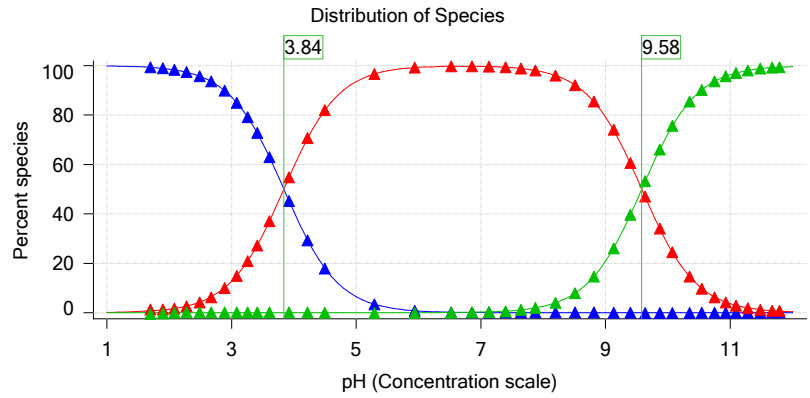
Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**

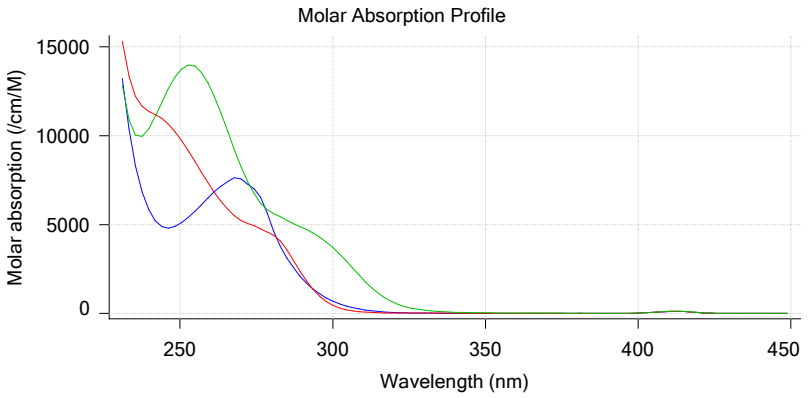
Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

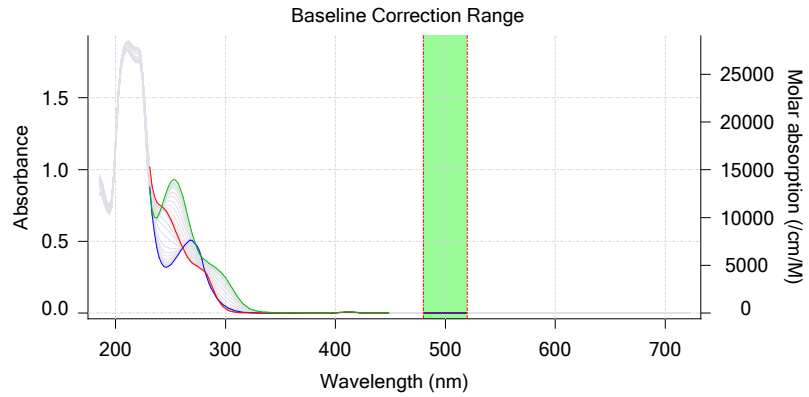
Graphs (continued)

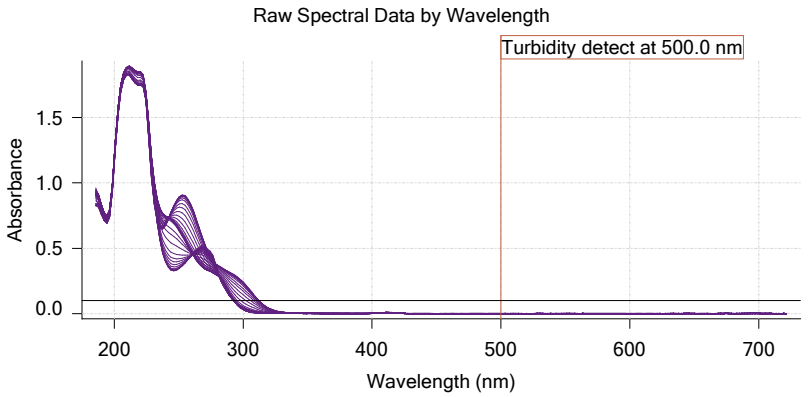












UV-metric psKa Titration 2 of 3 17J-12009 Points 44 to 84

Results

pKa 1	**4.03**
pKa 2	**9.45**
RMSD	**0.001 0.002 0.002**
Chi squared	**0.0062**
PCA calculated number of pKas	**2**
Average ionic strength	**0.166 M**
Average temperature	**24.9°C**
Analyte concentration range	**56.2 µM to 53.1 µM**
Methanol weight %	**39.9 %**
Dielectric constant	**61.0**
Water concentration	**30.1 M**

Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
Wavelength clipping **230.0 nm to 450.0 nm**
pH clipping **1.487 to 12.519**

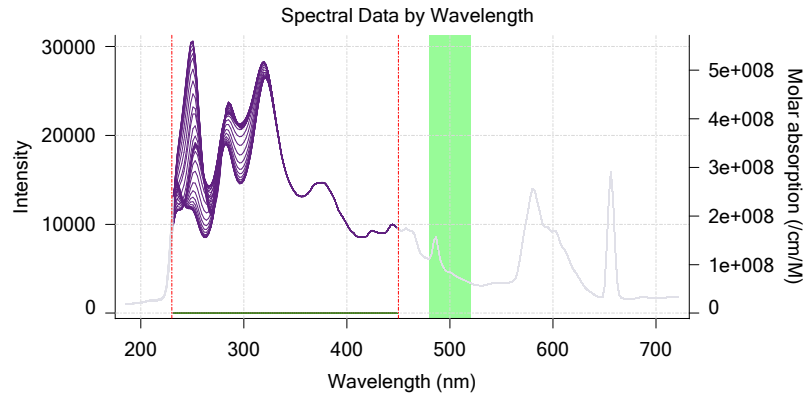
Warnings and errors

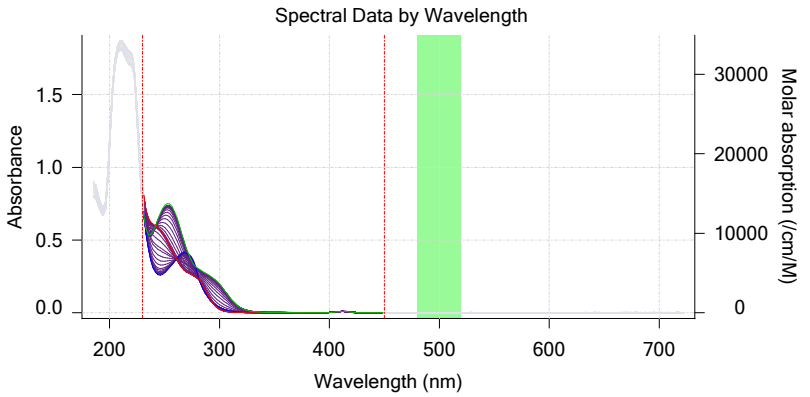
Errors None
Warnings None

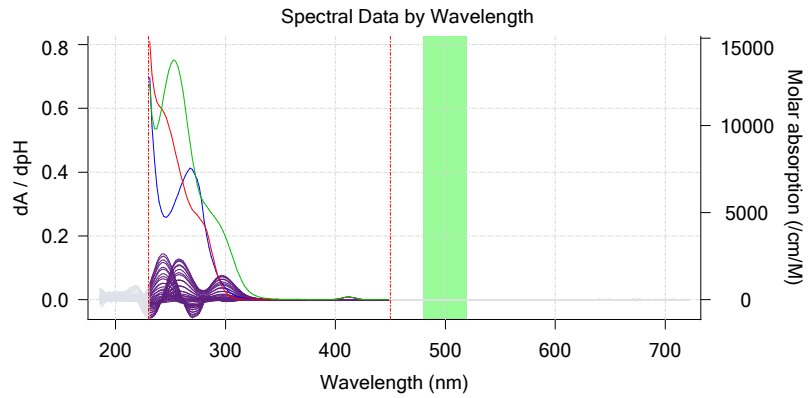
Assay Settings

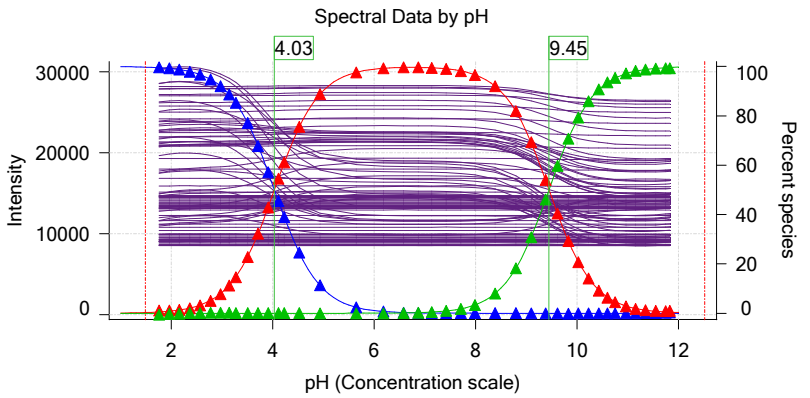
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

Graphs





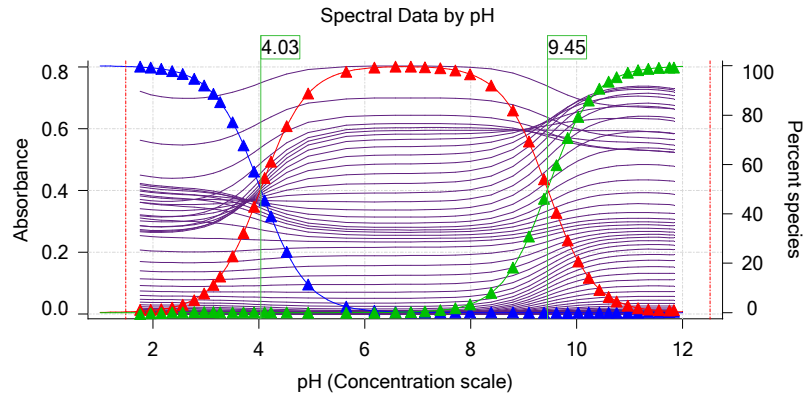


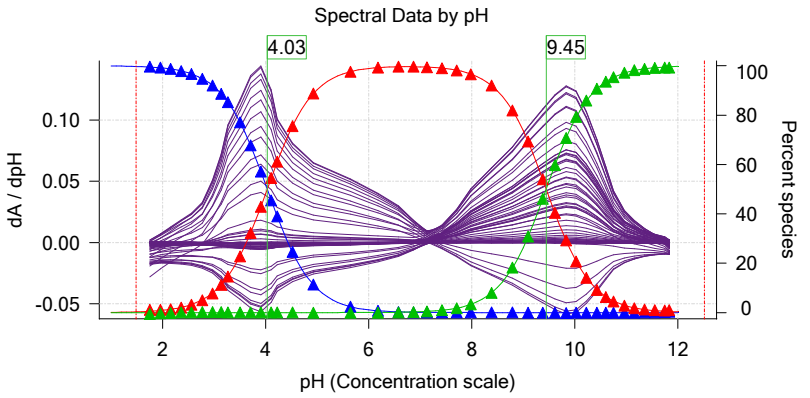


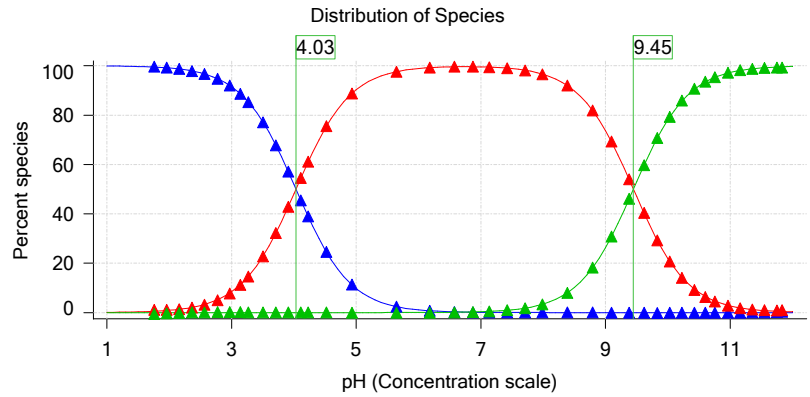
Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**

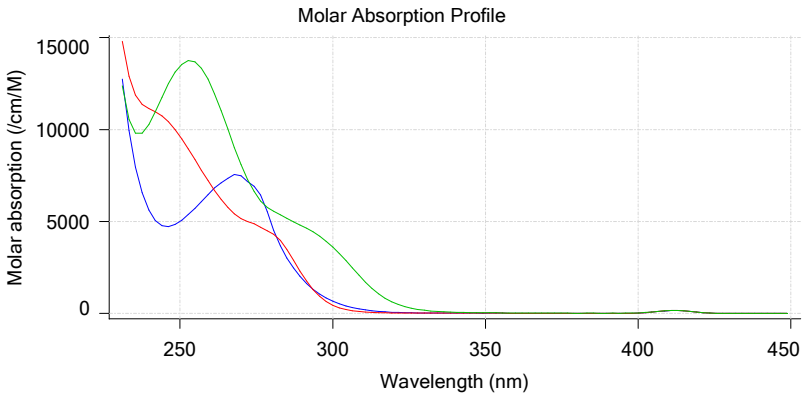
Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

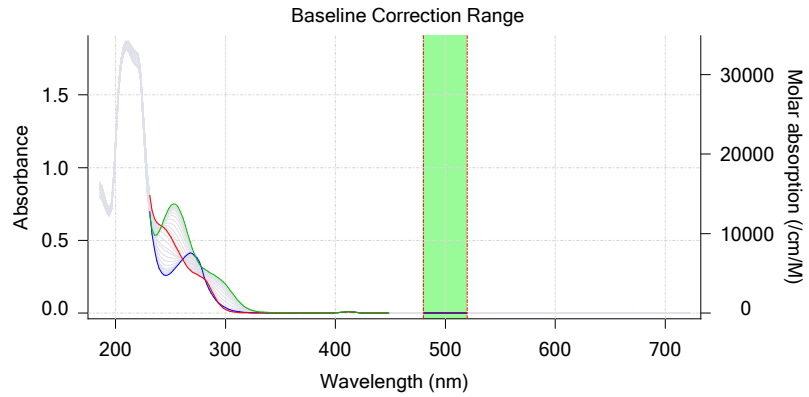
Graphs (continued)

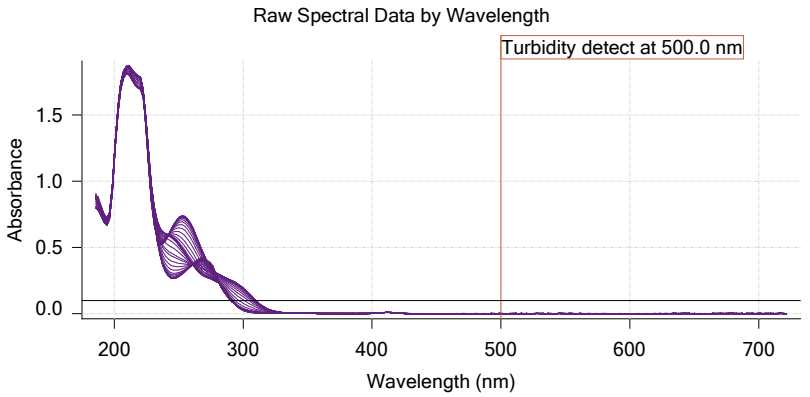












UV-metric psKa Titration 3 of 3 17J-12009 Points 86 to 128

Results

pKa 1	**4.26**
pKa 2	**9.31**
RMSD	**0.002 0.003 0.003**
Chi squared	**0.0098**
PCA calculated number of pKas	**3**
Average ionic strength	**0.172 M**
Average temperature	**24.9°C**
Analyte concentration range	**43.3 µM to 40.9 µM**
Methanol weight %	**30.1 %**
Dielectric constant	**65.5**
Water concentration	**35.8 M**

Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
Wavelength clipping **230.0 nm to 450.0 nm**
pH clipping **1.494 to 12.527**

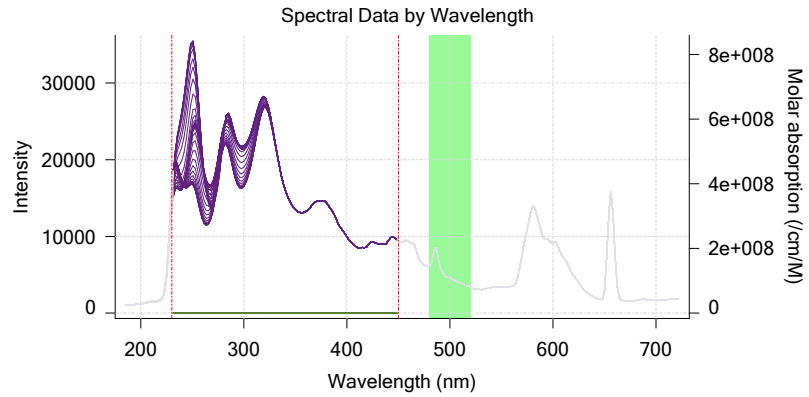
Warnings and errors

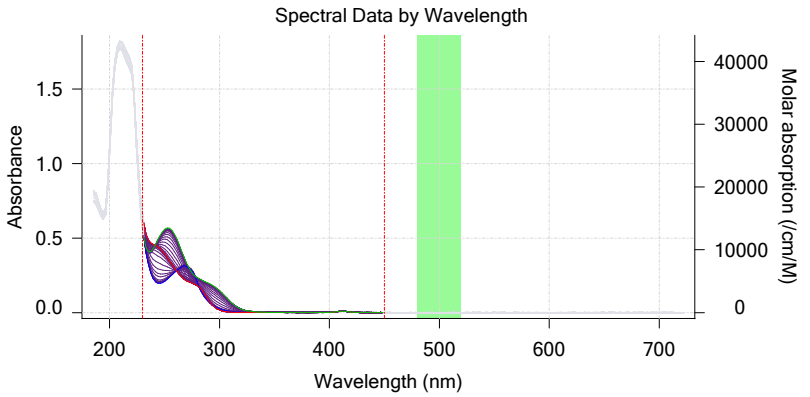
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

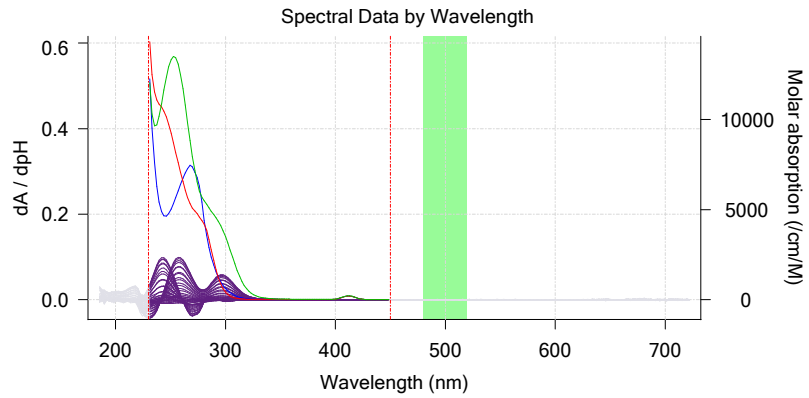
Assay Settings

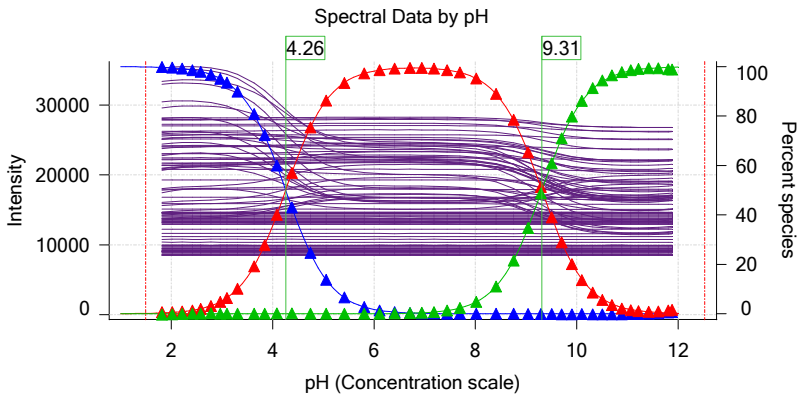
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

Graphs





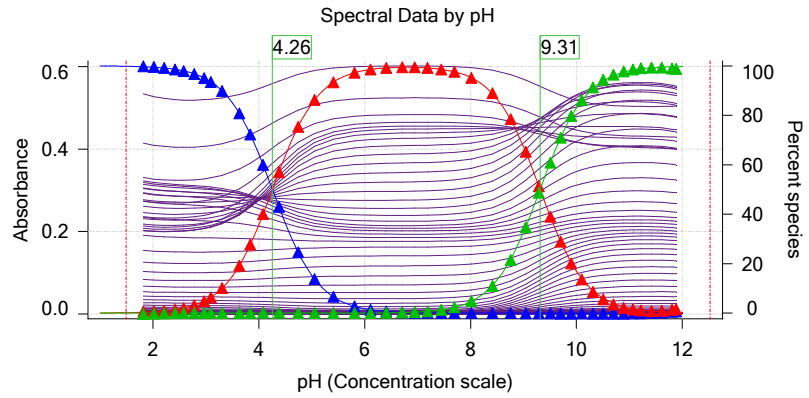


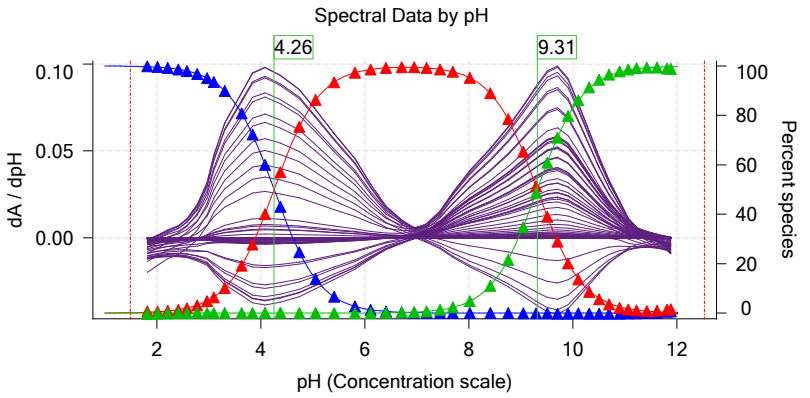


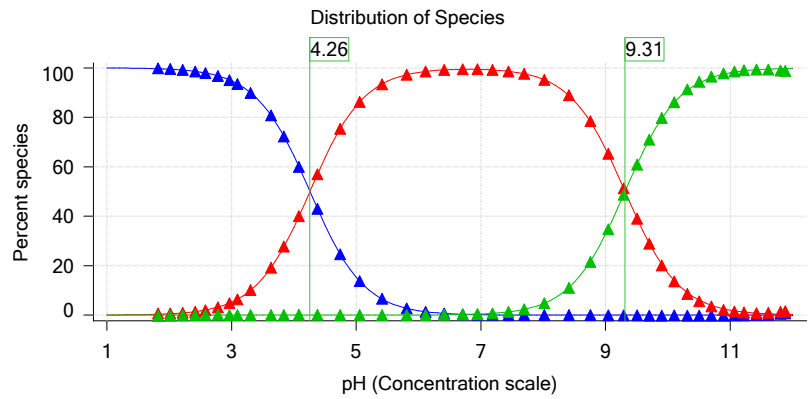
Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**

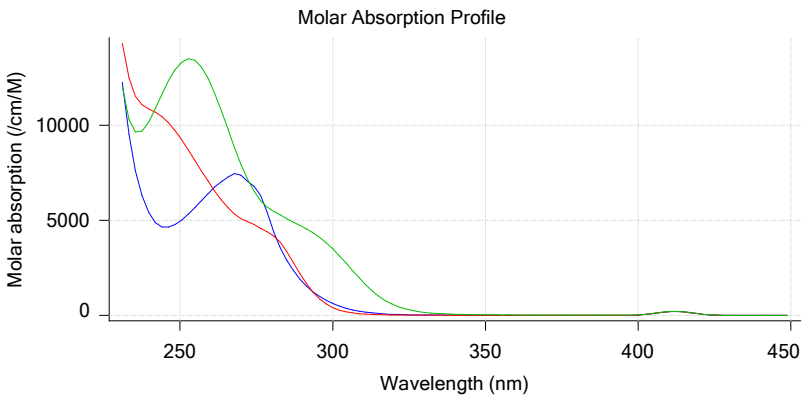
Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

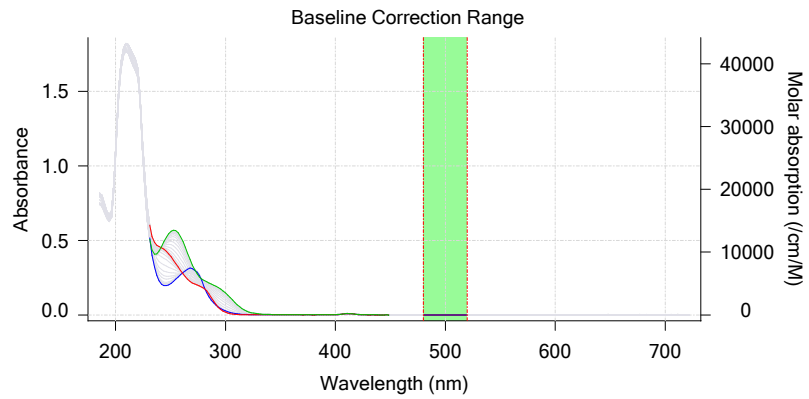
Graphs (continued)

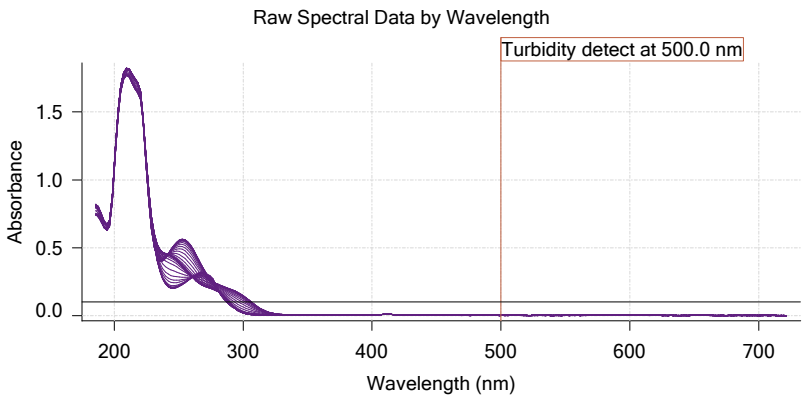












Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M16	10/11/2017 4:21:12 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0020 mL	10/11/2017 4:21:12 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.054700 M	10/11/2017 4:21:12 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	210.23	10/11/2017 4:21:22 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	10/11/2017 4:21:12 PM	User entered value
Sample is a	Ampholyte	10/11/2017 4:21:12 PM	User entered value
pKa 1	4.86	10/11/2017 4:21:12 PM	User entered value
Type	Base	10/11/2017 4:21:12 PM	User entered value
pKa 2	9.07	10/11/2017 4:21:12 PM	User entered value
Type	Acid	10/11/2017 4:21:12 PM	User entered value

Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logp (XH2 +)	-10.00		Default value
logP (neutral XH)	-10.00	10/11/2017 4:21:12 PM	User entered value
logP (X -)	-10.00		Default value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squar
3:40.5	Dark spectrum								
3:42.0	Reference spectrum								
4:09.7	Volume reset due to vial change								
4:53.9	Initial pH = 8.07								
5:59.4	Data point 4	0.34995 mL	0.06860 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.971	-0.00967	0.69536
6:28.2	Data point 5	0.34995 mL	0.06860 mL	0.02465 mL	1.15005 mL	0.02500 mL	2.172	-0.01785	0.72737
6:45.1	Data point 6	0.34995 mL	0.06860 mL	0.03963 mL	1.15005 mL	0.02500 mL	2.357	0.01480	0.92168
7:01.9	Data point 7	0.34995 mL	0.06860 mL	0.04936 mL	1.15005 mL	0.02500 mL	2.552	0.02578	0.84828
7:18.6	Data point 8	0.34995 mL	0.06860 mL	0.05567 mL	1.15005 mL	0.02500 mL	2.764	0.01968	0.80361
7:35.2	Data point 9	0.34995 mL	0.06860 mL	0.05955 mL	1.15005 mL	0.02500 mL	2.944	0.01316	0.85269
7:51.8	Data point 10	0.34995 mL	0.06860 mL	0.06211 mL	1.15005 mL	0.02500 mL	3.159	0.00948	0.75581
8:08.3	Data point 11	0.34995 mL	0.06860 mL	0.06369 mL	1.15005 mL	0.02500 mL	3.357	0.01152	0.78578
8:24.9	Data point 12	0.34995 mL	0.06860 mL	0.06468 mL	1.15005 mL	0.02500 mL	3.530	0.01310	0.90115
8:41.4	Data point 13	0.34995 mL	0.06860 mL	0.06533 mL	1.15005 mL	0.02500 mL	3.681	0.03201	0.96874
9:08.3	Data point 14	0.34995 mL	0.06860 mL	0.06595 mL	1.15005 mL	0.02500 mL	3.877	0.03400	0.97813
9:29.9	Data point 15	0.34995 mL	0.06860 mL	0.06651 mL	1.15005 mL	0.02500 mL	4.187	0.08154	0.99377
10:01.9	Data point 16	0.34995 mL	0.06860 mL	0.06736 mL	1.15005 mL	0.02500 mL	4.485	0.09919	0.99482
10:39.6	Data point 17	0.34995 mL	0.06860 mL	0.06754 mL	1.15005 mL	0.02500 mL	4.761	0.09769	0.98949
11:15.2	Data point 18	0.34995 mL	0.06860 mL	0.06773 mL	1.15005 mL	0.02500 mL	5.551	0.11230	0.99525
12:32.1	Data point 19	0.34995 mL	0.06860 mL	0.06783 mL	1.15005 mL	0.02500 mL	6.196	0.11157	0.99182
13:49.0	Data point 20	0.34995 mL	0.06860 mL	0.06794 mL	1.15005 mL	0.02500 mL	6.777	0.10014	0.99485
14:49.2	Data point 21	0.34995 mL	0.06860 mL	0.06804 mL	1.15005 mL	0.02500 mL	7.108	0.09753	0.98842
15:38.5	Data point 22	0.34995 mL	0.06860 mL	0.06816 mL	1.15005 mL	0.02500 mL	7.378	0.10099	0.99390
16:26.8	Data point 23	0.34995 mL	0.06860 mL	0.06830 mL	1.15005 mL	0.02500 mL	7.644	0.09933	0.99346
17:09.7	Data point 24	0.34995 mL	0.06860 mL	0.06844 mL	1.15005 mL	0.02500 mL	7.889	0.09867	0.98767
17:50.5	Data point 25	0.34995 mL	0.06860 mL	0.06858 mL	1.15005 mL	0.02500 mL	8.119	0.08217	0.72434
18:28.2	Data point 26	0.34995 mL	0.06860 mL	0.06872 mL	1.15005 mL	0.02500 mL	8.445	0.09452	0.96667
19:06.5	Data point 27	0.34995 mL	0.06860 mL	0.06884 mL	1.15005 mL	0.02500 mL	8.752	0.09935	0.99241
19:44.8	Data point 28	0.34995 mL	0.06860 mL	0.06893 mL	1.15005 mL	0.02500 mL	9.053	0.09736	0.98825
20:27.1	Data point 29	0.34995 mL	0.06860 mL	0.06905 mL	1.15005 mL	0.02500 mL	9.370	0.09941	0.98377
21:08.0	Data point 30	0.34995 mL	0.06860 mL	0.06917 mL	1.15005 mL	0.02500 mL	9.636	0.09723	0.97756
21:41.7	Data point 31	0.34995 mL	0.06860 mL	0.06931 mL	1.15005 mL	0.02500 mL	9.873	0.10040	0.98895
22:06.8	Data point 32	0.34995 mL	0.06860 mL	0.06947 mL	1.15005 mL	0.02500 mL	10.105	0.07554	0.97877
22:33.5	Data point 33	0.34995 mL	0.06860 mL	0.06968 mL	1.15005 mL	0.02500 mL	10.307	0.04184	0.93948
22:50.0	Data point 34	0.34995 mL	0.06860 mL	0.06997 mL	1.15005 mL	0.02500 mL	10.584	0.01590	0.90148
23:11.7	Data point 35	0.34995 mL	0.06860 mL	0.07044 mL	1.15005 mL	0.02500 mL	10.778	0.00406	0.39940
23:28.3	Data point 36	0.34995 mL	0.06860 mL	0.07124 mL	1.15005 mL	0.02500 mL	10.983	-0.00419	0.36656
23:44.8	Data point 37	0.34995 mL	0.06860 mL	0.07253 mL	1.15005 mL	0.02500 mL	11.159	-0.00606	0.49103
24:01.5	Data point 38	0.34995 mL	0.06860 mL	0.07444 mL	1.15005 mL	0.02500 mL	11.320	-0.00736	0.63490
24:28.6	Data point 39	0.34995 mL	0.06860 mL	0.07827 mL	1.15005 mL	0.02500 mL	11.513	-0.00938	0.89098
25:00.7	Data point 40	0.34995 mL	0.06860 mL	0.08323 mL	1.15005 mL	0.02500 mL	11.709	-0.00915	0.76515
25:27.8	Data point 41	0.34995 mL	0.06860 mL	0.09170 mL	1.15005 mL	0.02500 mL	11.899	-0.00817	0.77154
25:49.8	Data point 42	0.34995 mL	0.06860 mL	0.09955 mL	1.15005 mL	0.02500 mL	12.017	-0.00561	0.60495
27:31.3	Reference spectrum								
28:35.4	Data point 44	0.50000 mL	0.16928 mL	0.09958 mL	1.15005 mL	0.02500 mL	1.987	-0.04742	0.92670
29:02.9	Data point 45	0.50000 mL	0.16928 mL	0.12439 mL	1.15005 mL	0.02500 mL	2.188	0.00964	0.81669
29:19.9	Data point 46	0.50000 mL	0.16928 mL	0.14012 mL	1.15005 mL	0.02500 mL	2.386	0.01430	0.79035
29:36.7	Data point 47	0.50000 mL	0.16928 mL	0.15014 mL	1.15005 mL	0.02500 mL	2.592	0.00124	0.02477
29:53.3	Data point 48	0.50000 mL	0.16928 mL	0.15644 mL	1.15005 mL	0.02500 mL	2.790	0.02782	0.86790
30:10.0	Data point 49	0.50000 mL	0.16928 mL	0.16042 mL	1.15005 mL	0.02500 mL	3.002	0.01190	0.82364

Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SI
30:26.6	Data point 50	0.50000 mL	0.16928 mL	0.16287 mL	1.15005 mL	0.02500 mL	3.194	0.01465	0.92113	0.
30:43.3	Data point 51	0.50000 mL	0.16928 mL	0.16444 mL	1.15005 mL	0.02500 mL	3.366	0.00927	0.80485	0.
30:59.8	Data point 52	0.50000 mL	0.16928 mL	0.16550 mL	1.15005 mL	0.02500 mL	3.495	0.02401	0.92832	0.
31:31.7	Data point 53	0.50000 mL	0.16928 mL	0.16660 mL	1.15005 mL	0.02500 mL	3.726	0.01485	0.78700	0.
32:03.8	Data point 54	0.50000 mL	0.16928 mL	0.16722 mL	1.15005 mL	0.02500 mL	3.931	0.04364	0.98886	0.
32:25.5	Data point 55	0.50000 mL	0.16928 mL	0.16750 mL	1.15005 mL	0.02500 mL	4.129	0.06512	0.98133	0.
32:42.1	Data point 56	0.50000 mL	0.16928 mL	0.16769 mL	1.15005 mL	0.02500 mL	4.331	0.09337	0.99119	0.
32:58.6	Data point 57	0.50000 mL	0.16928 mL	0.16780 mL	1.15005 mL	0.02500 mL	4.448	0.09931	0.98052	0.
33:23.2	Data point 58	0.50000 mL	0.16928 mL	0.16794 mL	1.15005 mL	0.02500 mL	4.742	0.09999	0.99406	0.
34:00.5	Data point 59	0.50000 mL	0.16928 mL	0.16806 mL	1.15005 mL	0.02500 mL	5.148	0.09881	0.97125	0.
34:46.2	Data point 60	0.50000 mL	0.16928 mL	0.16816 mL	1.15005 mL	0.02500 mL	5.862	0.09761	0.98120	0.
35:42.3	Data point 61	0.50000 mL	0.16928 mL	0.16823 mL	1.15005 mL	0.02500 mL	6.393	0.10013	0.99317	0.
36:35.5	Data point 62	0.50000 mL	0.16928 mL	0.16830 mL	1.15005 mL	0.02500 mL	6.788	0.10099	0.99485	0.
37:12.1	Data point 63	0.50000 mL	0.16928 mL	0.16837 mL	1.15005 mL	0.02500 mL	7.080	0.09927	0.98962	0.
37:49.7	Data point 64	0.50000 mL	0.16928 mL	0.16846 mL	1.15005 mL	0.02500 mL	7.341	0.10010	0.98426	0.
38:29.6	Data point 65	0.50000 mL	0.16928 mL	0.16858 mL	1.15005 mL	0.02500 mL	7.630	0.09718	0.98219	0.
39:08.4	Data point 66	0.50000 mL	0.16928 mL	0.16870 mL	1.15005 mL	0.02500 mL	7.916	0.09773	0.97502	0.
39:50.3	Data point 67	0.50000 mL	0.16928 mL	0.16879 mL	1.15005 mL	0.02500 mL	8.191	0.09950	0.98346	0.
40:32.7	Data point 68	0.50000 mL	0.16928 mL	0.16889 mL	1.15005 mL	0.02500 mL	8.588	0.09613	0.96963	0.
41:16.5	Data point 69	0.50000 mL	0.16928 mL	0.16898 mL	1.15005 mL	0.02500 mL	8.995	0.09558	0.97693	0.
41:52.6	Data point 70	0.50000 mL	0.16928 mL	0.16907 mL	1.15005 mL	0.02500 mL	9.298	0.09442	0.96942	0.
42:24.7	Data point 71	0.50000 mL	0.16928 mL	0.16919 mL	1.15005 mL	0.02500 mL	9.580	0.09533	0.93985	0.
42:51.8	Data point 72	0.50000 mL	0.16928 mL	0.16933 mL	1.15005 mL	0.02500 mL	9.816	0.08831	0.97822	0.
43:23.7	Data point 73	0.50000 mL	0.16928 mL	0.16952 mL	1.15005 mL	0.02500 mL	10.029	0.04734	0.94350	0.
43:55.4	Data point 74	0.50000 mL	0.16928 mL	0.16978 mL	1.15005 mL	0.02500 mL	10.224	0.03020	0.94846	0.
44:22.0	Data point 75	0.50000 mL	0.16928 mL	0.17013 mL	1.15005 mL	0.02500 mL	10.421	0.00656	0.39990	0.
44:38.6	Data point 76	0.50000 mL	0.16928 mL	0.17063 mL	1.15005 mL	0.02500 mL	10.623	0.00409	0.37662	0.
44:55.0	Data point 77	0.50000 mL	0.16928 mL	0.17140 mL	1.15005 mL	0.02500 mL	10.796	-0.00702	0.60318	0.
45:11.6	Data point 78	0.50000 mL	0.16928 mL	0.17255 mL	1.15005 mL	0.02500 mL	10.948	-0.00557	0.68474	0.
45:48.7	Data point 79	0.50000 mL	0.16928 mL	0.17495 mL	1.15005 mL	0.02500 mL	11.159	-0.00838	0.90101	0.
46:15.8	Data point 80	0.50000 mL	0.16928 mL	0.17808 mL	1.15005 mL	0.02500 mL	11.349	-0.00924	0.85101	0.
46:48.0	Data point 81	0.50000 mL	0.16928 mL	0.18342 mL	1.15005 mL	0.02500 mL	11.544	-0.01208	0.87745	0.
47:20.2	Data point 82	0.50000 mL	0.16928 mL	0.19182 mL	1.15005 mL	0.02500 mL	11.741	-0.00938	0.82417	0.
47:52.7	Data point 83	0.50000 mL	0.16928 mL	0.20562 mL	1.15005 mL	0.02500 mL	11.936	-0.01072	0.80276	0.
48:14.7	Data point 84	0.50000 mL	0.16928 mL	0.21383 mL	1.15005 mL	0.02500 mL	12.019	-0.00860	0.76892	0.
49:59.7	Reference spectrum									
51:23.3	Data point 86	0.83996 mL	0.29421 mL	0.21385 mL	1.15005 mL	0.02500 mL	1.994	-0.02349	0.94569	0.
51:50.9	Data point 87	0.83996 mL	0.29421 mL	0.24224 mL	1.15005 mL	0.02500 mL	2.191	0.01188	0.78011	0.
52:07.8	Data point 88	0.83996 mL	0.29421 mL	0.26011 mL	1.15005 mL	0.02500 mL	2.388	0.00437	0.31795	0.
52:24.7	Data point 89	0.83996 mL	0.29421 mL	0.27161 mL	1.15005 mL	0.02500 mL	2.589	-0.02030	0.82416	0.
52:57.1	Data point 90	0.83996 mL	0.29421 mL	0.27895 mL	1.15005 mL	0.02500 mL	2.756	0.00976	0.65367	0.
53:24.2	Data point 91	0.83996 mL	0.29421 mL	0.28335 mL	1.15005 mL	0.02500 mL	2.951	0.00170	0.14583	0.
53:40.9	Data point 92	0.83996 mL	0.29421 mL	0.28652 mL	1.15005 mL	0.02500 mL	3.140	-0.00336	0.21309	0.
53:57.5	Data point 93	0.83996 mL	0.29421 mL	0.28857 mL	1.15005 mL	0.02500 mL	3.268	0.00344	0.27724	0.
54:29.4	Data point 94	0.83996 mL	0.29421 mL	0.29022 mL	1.15005 mL	0.02500 mL	3.477	0.01189	0.87382	0.
54:45.9	Data point 95	0.83996 mL	0.29421 mL	0.29116 mL	1.15005 mL	0.02500 mL	3.802	-0.00531	0.16094	0.
55:17.7	Data point 96	0.83996 mL	0.29421 mL	0.29168 mL	1.15005 mL	0.02500 mL	4.009	0.03675	0.96951	0.
55:34.1	Data point 97	0.83996 mL	0.29421 mL	0.29196 mL	1.15005 mL	0.02500 mL	4.250	0.04055	0.97110	0.
55:55.7	Data point 98	0.83996 mL	0.29421 mL	0.29224 mL	1.15005 mL	0.02500 mL	4.547	0.07033	0.94381	0.
56:17.3	Data point 99	0.83996 mL	0.29421 mL	0.29243 mL	1.15005 mL	0.02500 mL	4.910	0.09976	0.97446	0.
56:50.0	Data point 100	0.83996 mL	0.29421 mL	0.29255 mL	1.15005 mL	0.02500 mL	5.222	0.09875	0.97662	0.
57:25.7	Data point 101	0.83996 mL	0.29421 mL	0.29264 mL	1.15005 mL	0.02500 mL	5.577	0.09753	0.98708	0.
58:07.8	Data point 102	0.83996 mL	0.29421 mL	0.29273 mL	1.15005 mL	0.02500 mL	5.971	0.10016	0.99125	0.
58:46.4	Data point 103	0.83996 mL	0.29421 mL	0.29283 mL	1.15005 mL	0.02500 mL	6.275	-0.03907	0.55717	0.
59:08.1	Data point 104	0.83996 mL	0.29421 mL	0.29292 mL	1.15005 mL	0.02500 mL	6.571	-0.08584	0.94201	0.
59:29.6	Data point 105	0.83996 mL	0.29421 mL	0.29304 mL	1.15005 mL	0.02500 mL	6.871	-0.09713	0.94088	0.
1:00:05.2	Data point 106	0.83996 mL	0.29421 mL	0.29318 mL	1.15005 mL	0.02500 mL	7.107	0.09337	0.95943	0.

Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
1:00:37.2	Data point 107	0.83996 mL	0.29421 mL	0.29332 mL	1.15005 mL	0.02500 mL	7.346	0.08825	0.95666	0.0044
1:01:14.5	Data point 108	0.83996 mL	0.29421 mL	0.29346 mL	1.15005 mL	0.02500 mL	7.603	0.09465	0.96757	0.0047
1:01:49.7	Data point 109	0.83996 mL	0.29421 mL	0.29358 mL	1.15005 mL	0.02500 mL	7.851	0.09726	0.98075	0.0048
1:02:28.5	Data point 110	0.83996 mL	0.29421 mL	0.29370 mL	1.15005 mL	0.02500 mL	8.175	0.09974	0.98165	0.0049
1:03:12.6	Data point 111	0.83996 mL	0.29421 mL	0.29381 mL	1.15005 mL	0.02500 mL	8.568	0.09761	0.94615	0.0049
1:03:53.5	Data point 112	0.83996 mL	0.29421 mL	0.29393 mL	1.15005 mL	0.02500 mL	8.911	0.09881	0.98625	0.0049
1:04:30.8	Data point 113	0.83996 mL	0.29421 mL	0.29405 mL	1.15005 mL	0.02500 mL	9.197	0.09677	0.98197	0.0048
1:05:04.0	Data point 114	0.83996 mL	0.29421 mL	0.29419 mL	1.15005 mL	0.02500 mL	9.447	0.09347	0.95203	0.0047
1:05:26.6	Data point 115	0.83996 mL	0.29421 mL	0.29436 mL	1.15005 mL	0.02500 mL	9.661	0.05370	0.97656	0.0026
1:05:48.1	Data point 116	0.83996 mL	0.29421 mL	0.29457 mL	1.15005 mL	0.02500 mL	9.854	0.03229	0.87936	0.0017
1:06:20.0	Data point 117	0.83996 mL	0.29421 mL	0.29490 mL	1.15005 mL	0.02500 mL	10.055	0.02379	0.93949	0.0012
1:06:41.8	Data point 118	0.83996 mL	0.29421 mL	0.29532 mL	1.15005 mL	0.02500 mL	10.252	-0.00051	0.01469	0.0002
1:07:18.8	Data point 119	0.83996 mL	0.29421 mL	0.29654 mL	1.15005 mL	0.02500 mL	10.464	-0.00045	0.01218	0.0002
1:07:50.8	Data point 120	0.83996 mL	0.29421 mL	0.29758 mL	1.15005 mL	0.02500 mL	10.654	-0.01243	0.71782	0.0007
1:08:23.0	Data point 121	0.83996 mL	0.29421 mL	0.29908 mL	1.15005 mL	0.02500 mL	10.846	-0.00991	0.73895	0.0005
1:08:55.1	Data point 122	0.83996 mL	0.29421 mL	0.30101 mL	1.15005 mL	0.02500 mL	11.043	-0.01277	0.71584	0.0007
1:09:11.8	Data point 123	0.83996 mL	0.29421 mL	0.30407 mL	1.15005 mL	0.02500 mL	11.214	-0.01678	0.90057	0.0008
1:09:28.6	Data point 124	0.83996 mL	0.29421 mL	0.30858 mL	1.15005 mL	0.02500 mL	11.369	-0.02172	0.91506	0.0011
1:10:00.9	Data point 125	0.83996 mL	0.29421 mL	0.31733 mL	1.15005 mL	0.02500 mL	11.568	-0.01344	0.85187	0.0007
1:10:28.1	Data point 126	0.83996 mL	0.29421 mL	0.32952 mL	1.15005 mL	0.02500 mL	11.759	-0.01385	0.84697	0.0007
1:10:55.7	Data point 127	0.83996 mL	0.29421 mL	0.34993 mL	1.15005 mL	0.02500 mL	11.949	-0.01210	0.82759	0.0006
1:11:17.8	Data point 128	0.83996 mL	0.29421 mL	0.36197 mL	1.15005 mL	0.02500 mL	12.027	-0.01064	0.72154	0.0006
1:13:17.2	Assay volumes	1.08996 mL	0.43921 mL	0.36197 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			
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			

Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**
Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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			
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 10:50:14 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus S	1.0007	10/12/2017 10:50:14 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jH	0.3	10/12/2017 10:50:14 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jOH	-0.2	10/12/2017 10:50:14 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Base concentration factor	1.011	10/12/2017 10:50:14 AM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	0.995	10/12/2017 10:50:14 AM	C:\Sirius_T3\17J-11005_Blank standardisation.t3r

Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

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
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	-9.65 mV		10/12/2017 10:50:38 AM
Filling solution	3M KCl	KCL095	10/10/2017 9:58:43 AM
Liquids			
Wash 1	50% IPA:50% Water		10/11/2017 8:31:15 AM
Wash 2	0.5% Trition X-100 in H20		10/11/2017 8:31:17 AM
Buffer position 1	pH7 Wash		10/11/2017 8:31:21 AM
Buffer position 2	pH 7		10/11/2017 8:31:23 AM
Storage position			10/11/2017 8:31:26 AM
Wash water	4e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	6e+003 mL		10/6/2017 3:04:33 PM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	419:28:33		11/23/2010 12:22:28 PM
Calibrated on	10/11/2017 8:30:19 AM		

Sample name: **M16**
Assay name: **UV-metric psKa**
Assay ID: **17J-12009**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12009_M16_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 10:50:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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%		
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 F1