Yasuda-Shedlovsky Result

Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

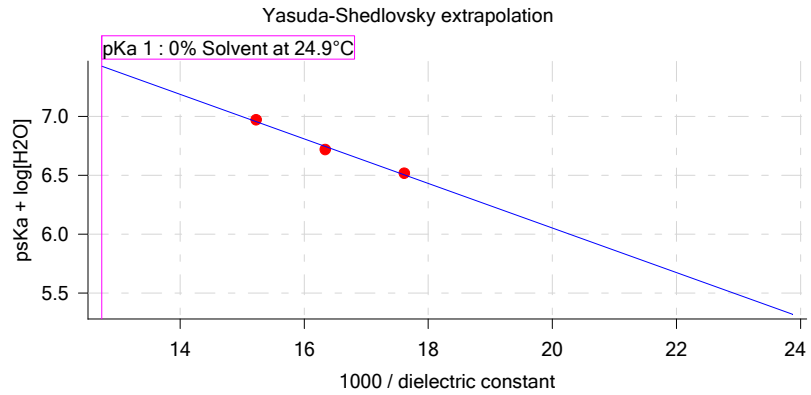
Yasuda-Shedlovsky result

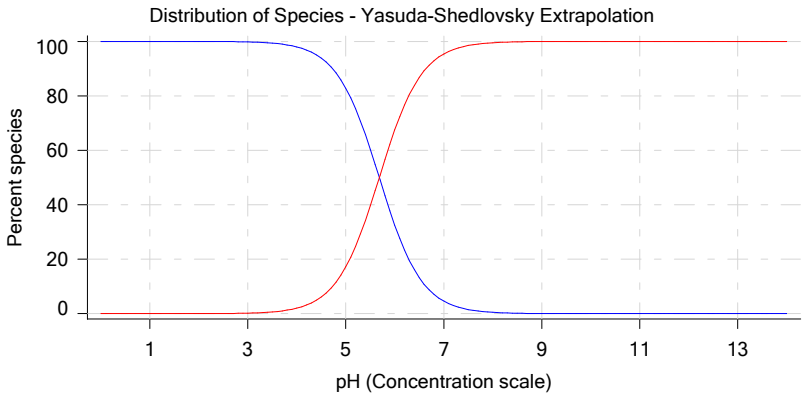
Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.68	±0.07	9.84	-189.2221	0.9904	0.166 M	24.9°C

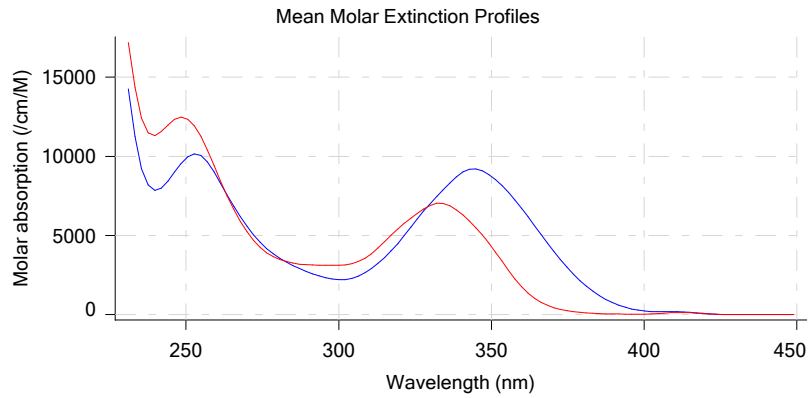
Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
17J-04005 Points 4 to 39	49.19 %	Up	UV-metric pKa	56.8	24.9 M	0.157 M	24.9°C	☑	5.12
17J-04005 Points 41 to 81	39.61 %	Up	UV-metric pKa	61.2	30.2 M	0.166 M	24.9°C	☑	5.24
17J-04005 Points 83 to 121	29.73 %	Up	UV-metric pKa	65.7	36.0 M	0.173 M	24.9°C	☑	5.41

Graphs







UV-metric psKa Titration 1 of 3 17J-04005 Points 4 to 39

Results

pKa 1	**5.12**
RMSD	**0.002 0.003**
Chi squared	**0.0053**
PCA calculated number of pKas	**2**
Average ionic strength	**0.157 M**
Average temperature	**24.9°C**
Analyte concentration range	**90.3 µM to 84.7 µM**
Methanol weight %	**49.2 %**
Dielectric constant	**56.8**
Water concentration	**24.9 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**

Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Results (continued)

pH clipping **1.459 to 12.504**

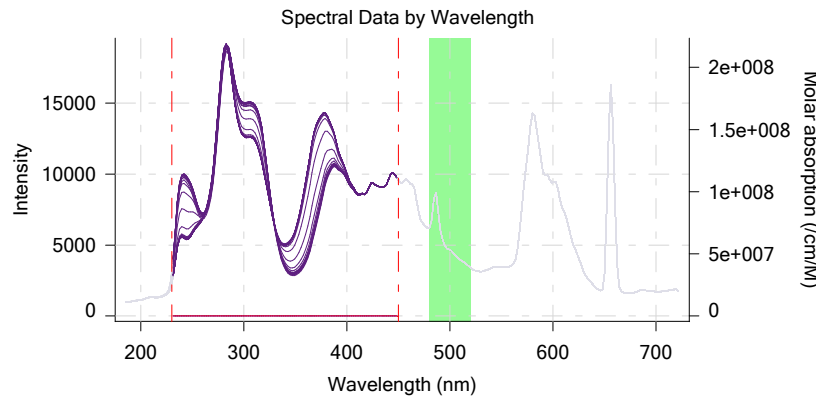
Warnings and errors

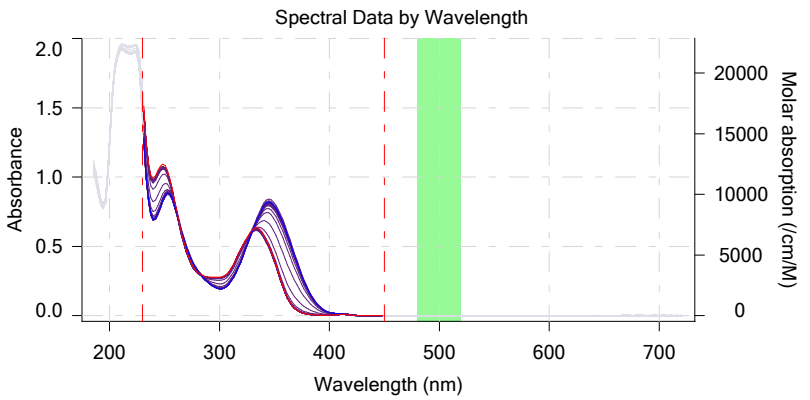
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

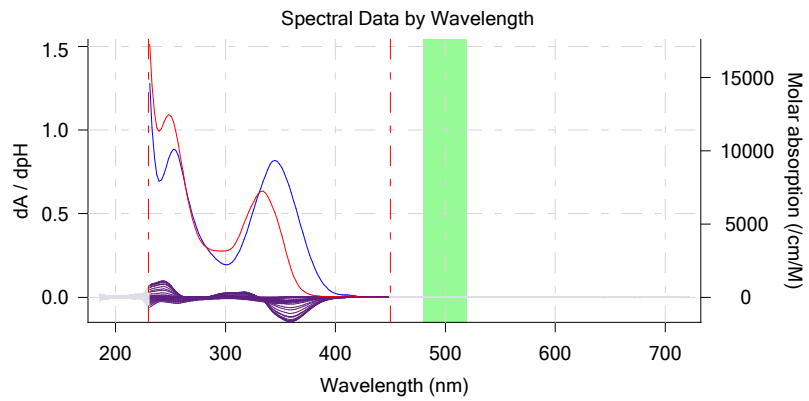
Assay Settings

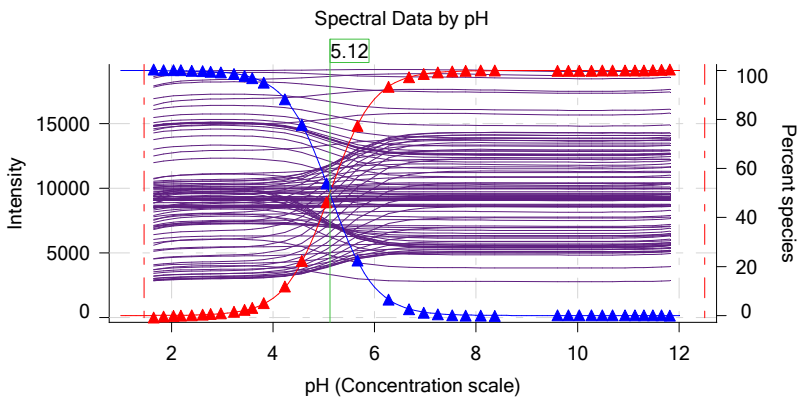
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

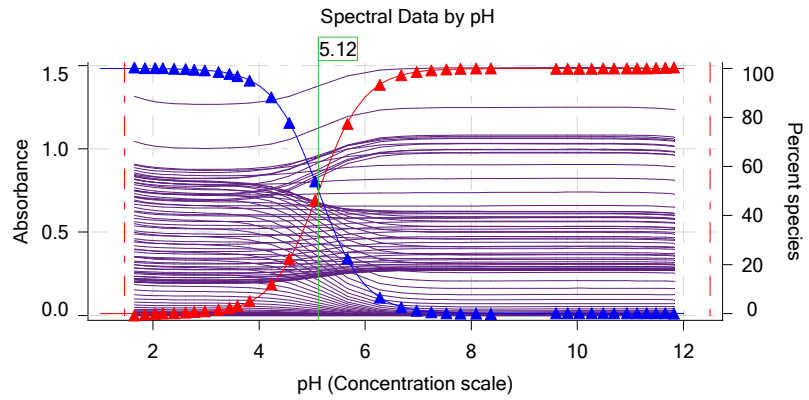
Graphs

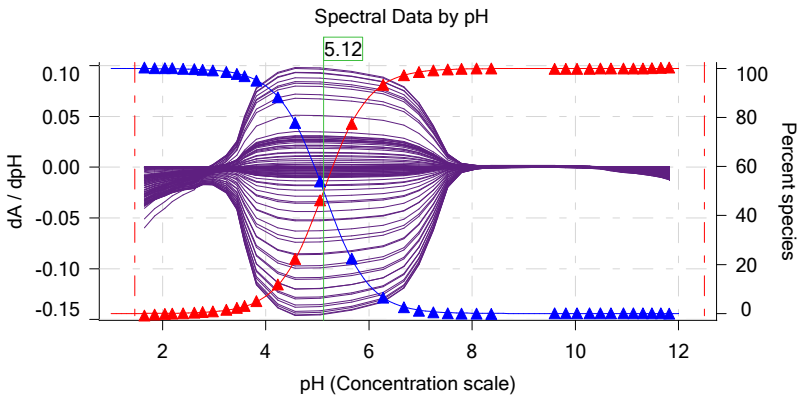








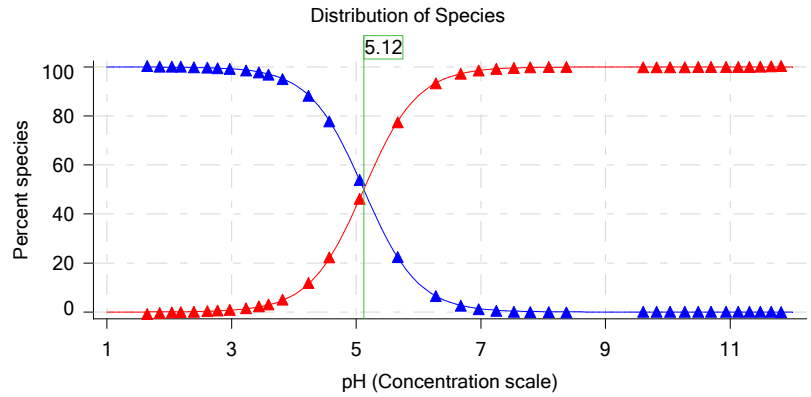


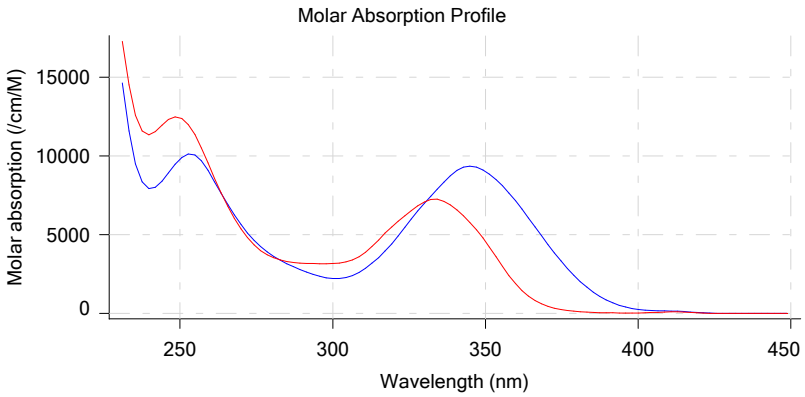


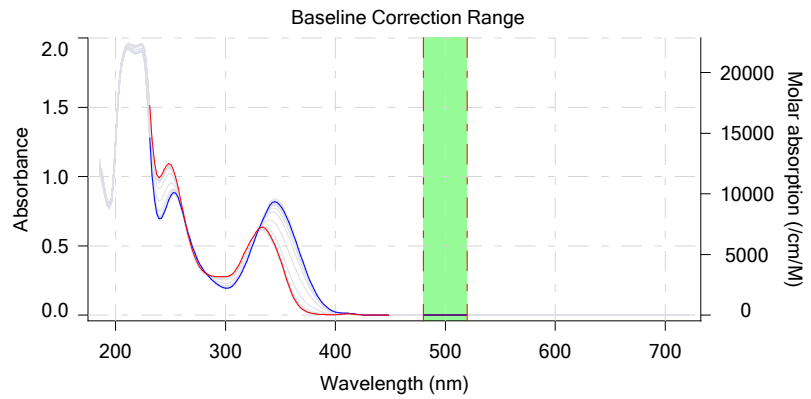
Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

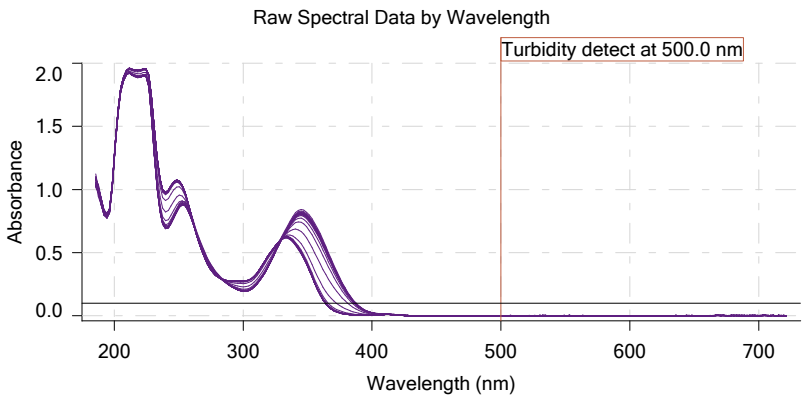
Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









UV-metric psKa Titration 2 of 3 17J-04005 Points 41 to 81

Results

pKa 1	**5.24**
RMSD	**0.002 0.002**
Chi squared	**0.0053**
PCA calculated number of pKas	**4**
Average ionic strength	**0.166 M**
Average temperature	**24.9°C**
Analyte concentration range	**73.8 µM to 69.6 µM**
Methanol weight %	**39.6 %**
Dielectric constant	**61.2**
Water concentration	**30.2 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.464 to 12.528**

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				

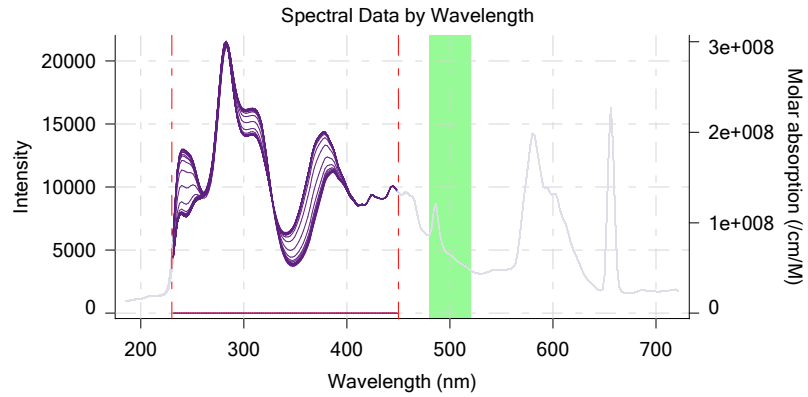
Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

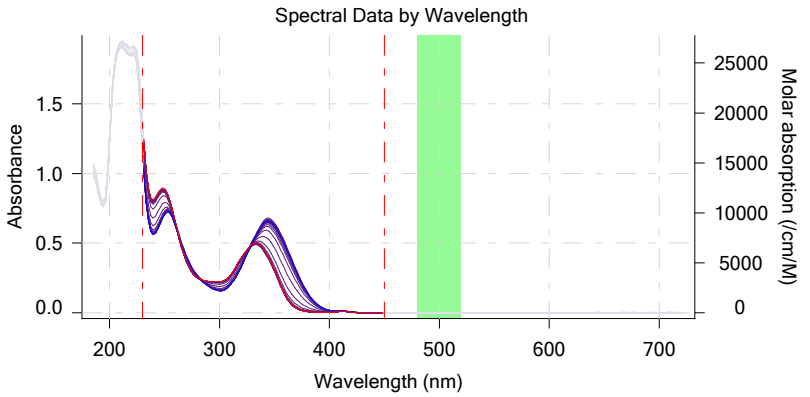
Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

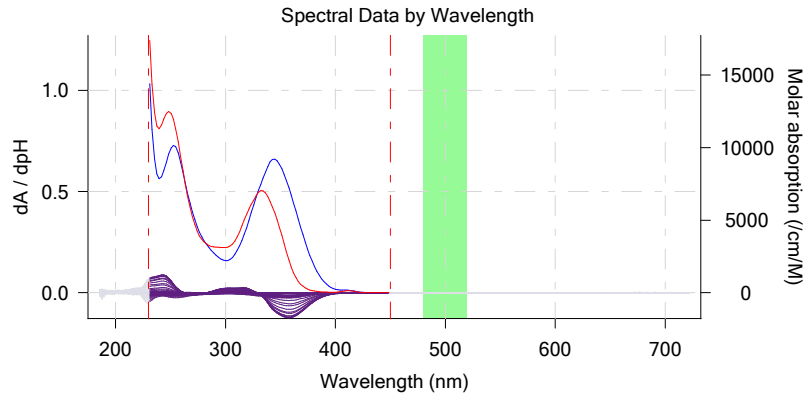
Assay Settings (continued)

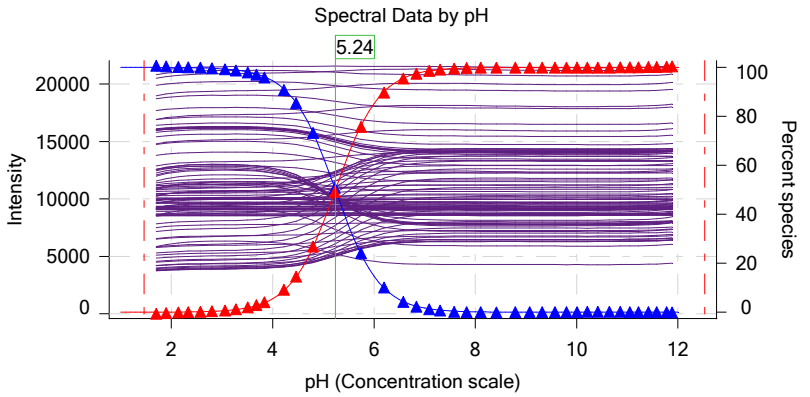
Setting	Value	Original Value	Date/Time changed	Imported from
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

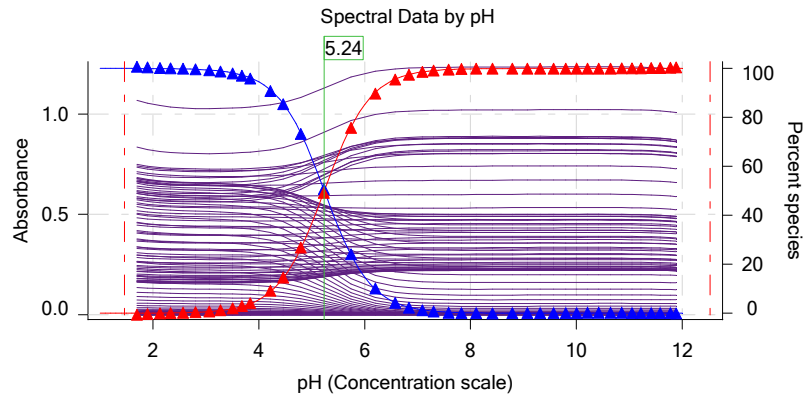
Graphs

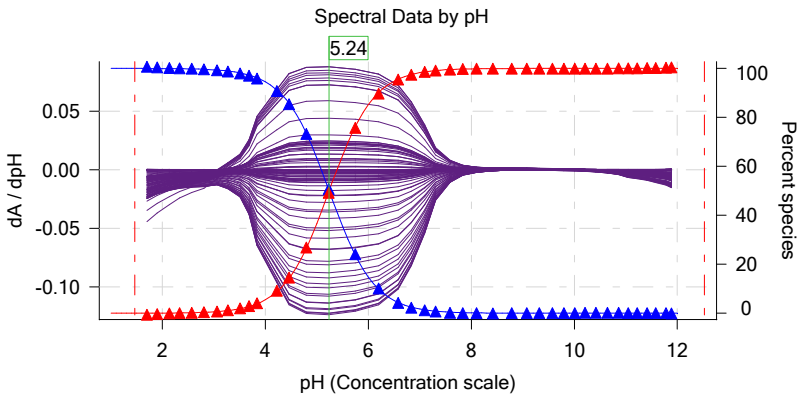








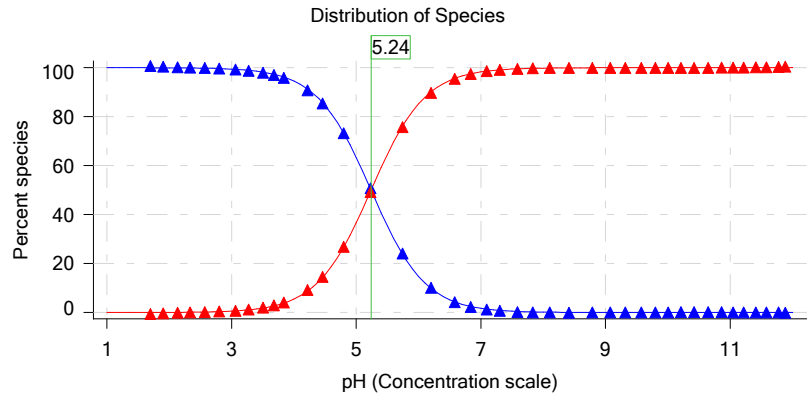


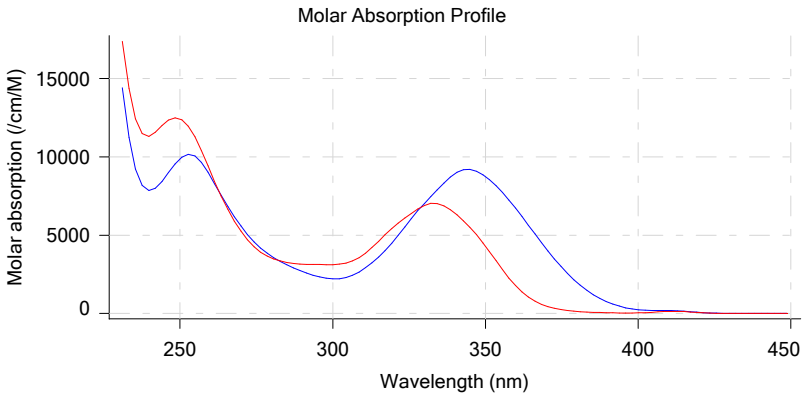


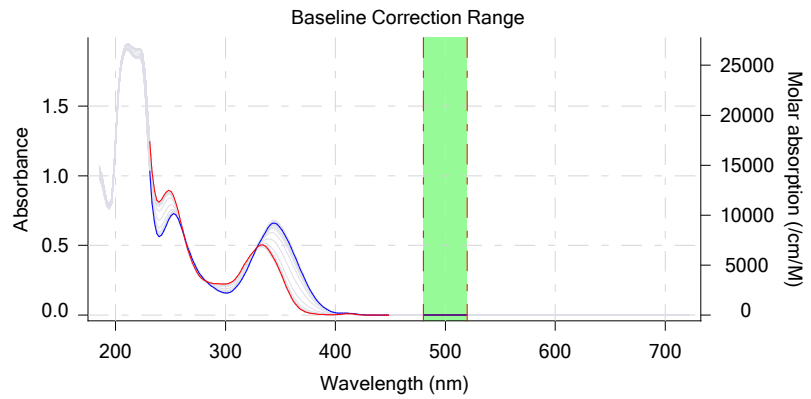
Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

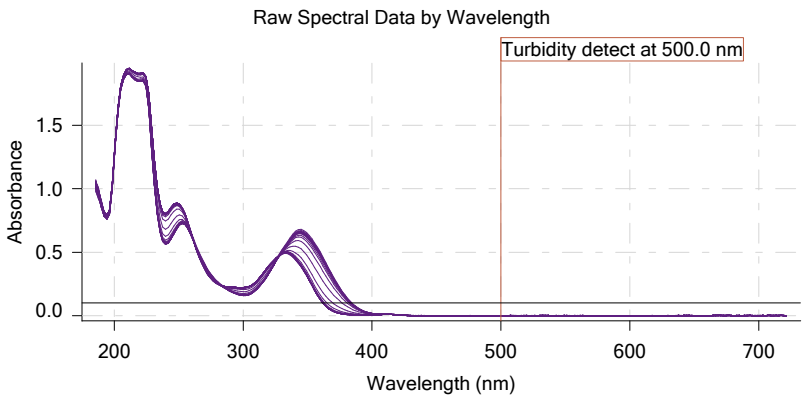
Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









UV-metric psKa Titration 3 of 3 17J-04005 Points 83 to 121

Results

pKa 1	**5.41**
RMSD	**0.002 0.002**
Chi squared	**0.0055**
PCA calculated number of pKas	**3**
Average ionic strength	**0.173 M**
Average temperature	**24.9°C**
Analyte concentration range	**56.6 µM to 53.4 µM**
Methanol weight %	**29.7 %**
Dielectric constant	**65.7**
Water concentration	**36.0 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.463 to 12.524**

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				

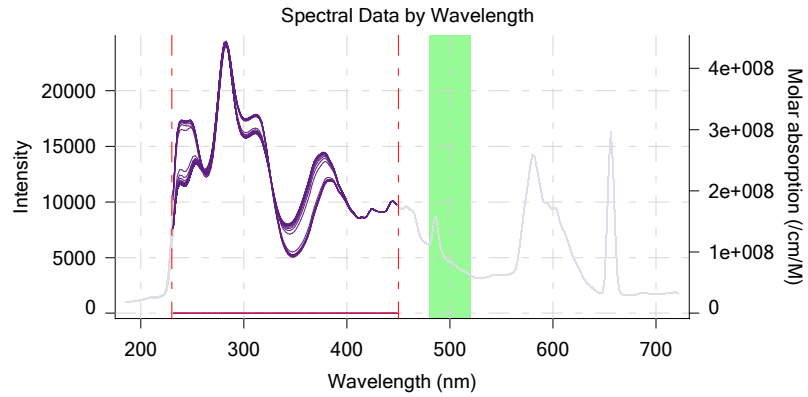
Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

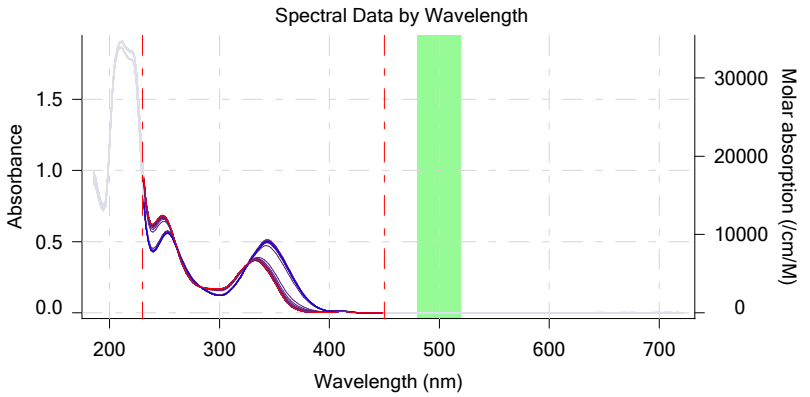
Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

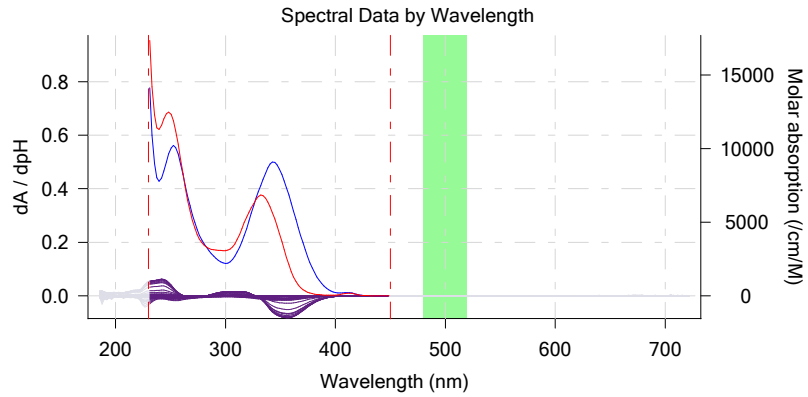
Assay Settings (continued)

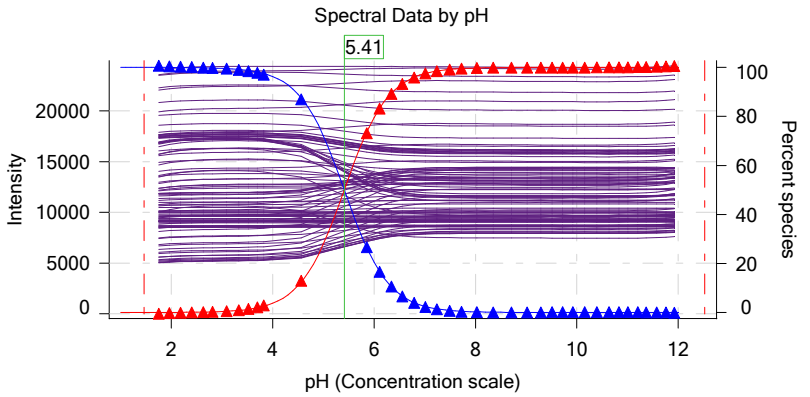
Setting	Value	Original Value	Date/Time changed	Imported from
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

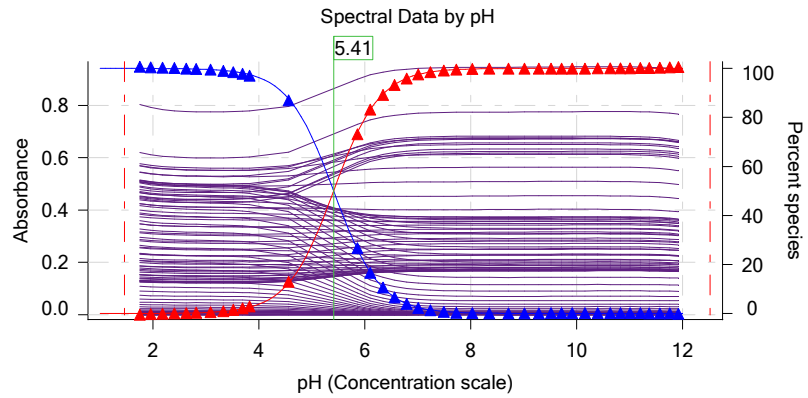
Graphs

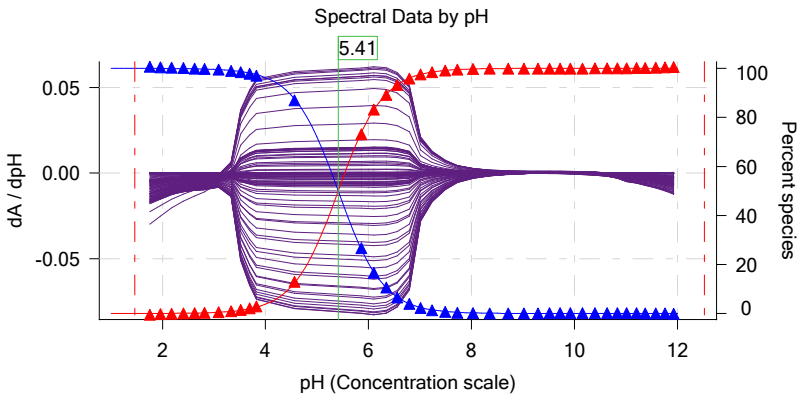








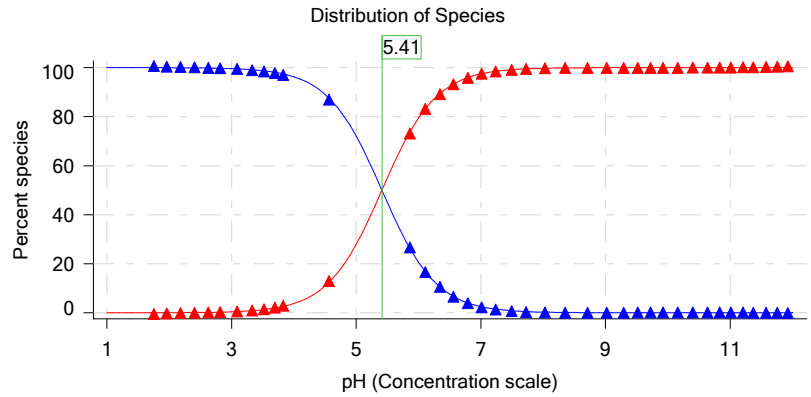


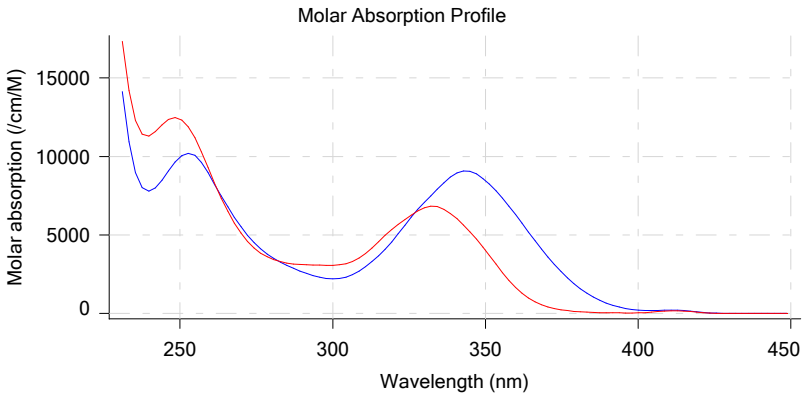


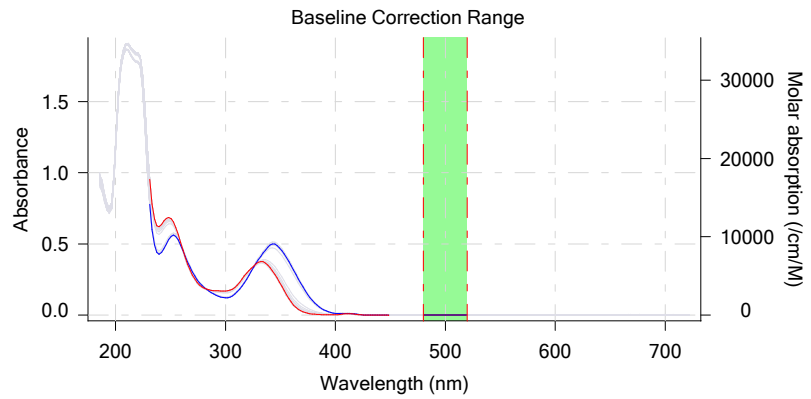
Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

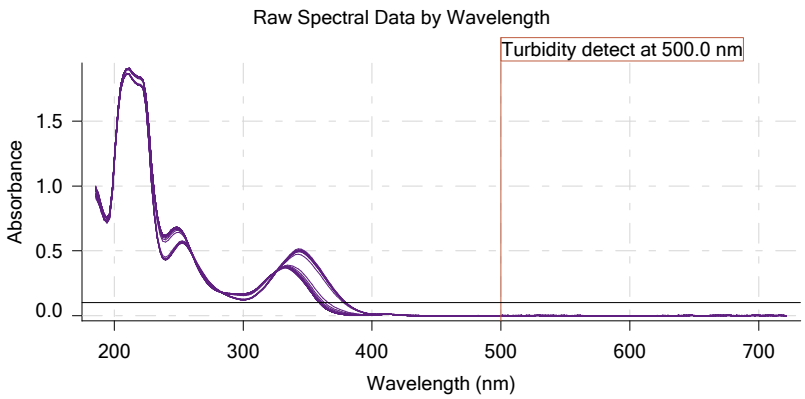
Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)









Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M13	10/3/2017 3:53:41 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0040 mL	10/3/2017 3:53:41 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.036100 M	10/3/2017 3:53:41 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	295.34	10/3/2017 3:53:56 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	4/11/2018 1:43:49 PM	User entered value
Sample is a	Base	4/11/2018 1:43:53 PM	User entered value
pKa 1	3.20	10/3/2017 3:53:41 PM	User entered value
logp (XH +)	-10.00	10/3/2017 3:53:41 PM	User entered value
logP (neutral X)	-10.00		Default value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:36.1	Dark spectrum								
3:37.5	Reference spectrum								
4:05.2	Volume reset due to vial change								
4:49.5	Initial pH = 8.11								
6:02.4	Data point 4	0.34995 mL	0.06987 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.959	-0.01494	0.88981
6:31.1	Data point 5	0.34995 mL	0.06987 mL	0.02556 mL	1.15005 mL	0.02500 mL	2.154	-0.01491	0.59662
6:48.0	Data point 6	0.34995 mL	0.06987 mL	0.04271 mL	1.15005 mL	0.02500 mL	2.348	0.00926	0.33184
7:04.9	Data point 7	0.34995 mL	0.06987 mL	0.05357 mL	1.15005 mL	0.02500 mL	2.490	-0.00524	0.36332
7:32.0	Data point 8	0.34995 mL	0.06987 mL	0.06112 mL	1.15005 mL	0.02500 mL	2.697	0.00746	0.78083
7:48.8	Data point 9	0.34995 mL	0.06987 mL	0.06604 mL	1.15005 mL	0.02500 mL	2.911	0.00830	0.79193

Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
8:05.5	Data point 10	0.34995 mL	0.06987 mL	0.06905 mL	1.15005 mL	0.02500 mL	3.070	0.00550	0.51679	0.00
8:27.2	Data point 11	0.34995 mL	0.06987 mL	0.07058 mL	1.15005 mL	0.02500 mL	3.266	0.00853	0.85502	0.00
8:59.3	Data point 12	0.34995 mL	0.06987 mL	0.07201 mL	1.15005 mL	0.02500 mL	3.525	0.02252	0.96832	0.00
9:15.9	Data point 13	0.34995 mL	0.06987 mL	0.07274 mL	1.15005 mL	0.02500 mL	3.725	0.03586	0.95370	0.00
9:32.4	Data point 14	0.34995 mL	0.06987 mL	0.07321 mL	1.15005 mL	0.02500 mL	3.876	0.04672	0.97603	0.00
9:53.9	Data point 15	0.34995 mL	0.06987 mL	0.07371 mL	1.15005 mL	0.02500 mL	4.101	0.06799	0.99465	0.00
10:15.5	Data point 16	0.34995 mL	0.06987 mL	0.07408 mL	1.15005 mL	0.02500 mL	4.511	0.10053	0.99194	0.00
10:53.6	Data point 17	0.34995 mL	0.06987 mL	0.07434 mL	1.15005 mL	0.02500 mL	4.843	0.09828	0.97568	0.00
11:44.2	Data point 18	0.34995 mL	0.06987 mL	0.07448 mL	1.15005 mL	0.02500 mL	5.324	0.09862	0.98372	0.00
12:50.8	Data point 19	0.34995 mL	0.06987 mL	0.07460 mL	1.15005 mL	0.02500 mL	5.930	0.10050	0.99631	0.00
14:01.0	Data point 20	0.34995 mL	0.06987 mL	0.07472 mL	1.15005 mL	0.02500 mL	6.533	0.09796	0.98347	0.00
15:07.1	Data point 21	0.34995 mL	0.06987 mL	0.07484 mL	1.15005 mL	0.02500 mL	6.927	0.10007	0.99445	0.00
16:00.5	Data point 22	0.34995 mL	0.06987 mL	0.07498 mL	1.15005 mL	0.02500 mL	7.214	0.10070	0.98815	0.00
16:38.3	Data point 23	0.34995 mL	0.06987 mL	0.07509 mL	1.15005 mL	0.02500 mL	7.491	0.10029	0.99212	0.00
17:27.6	Data point 24	0.34995 mL	0.06987 mL	0.07531 mL	1.15005 mL	0.02500 mL	7.771	0.09876	0.97800	0.00
18:14.1	Data point 25	0.34995 mL	0.06987 mL	0.07554 mL	1.15005 mL	0.02500 mL	8.031	0.09566	0.98180	0.00
19:03.5	Data point 26	0.34995 mL	0.06987 mL	0.07571 mL	1.15005 mL	0.02500 mL	8.323	0.09563	0.98275	0.00
19:56.8	Data point 27	0.34995 mL	0.06987 mL	0.07589 mL	1.15005 mL	0.02500 mL	8.600	0.10045	0.98741	0.00
20:45.6	Data point 28	0.34995 mL	0.06987 mL	0.07636 mL	1.15005 mL	0.02500 mL	9.818	0.09419	0.96340	0.00
21:18.9	Data point 29	0.34995 mL	0.06987 mL	0.07662 mL	1.15005 mL	0.02500 mL	10.033	0.09016	0.95040	0.00
21:40.7	Data point 30	0.34995 mL	0.06987 mL	0.07683 mL	1.15005 mL	0.02500 mL	10.246	0.04531	0.96508	0.00
22:02.3	Data point 31	0.34995 mL	0.06987 mL	0.07714 mL	1.15005 mL	0.02500 mL	10.480	0.02178	0.95559	0.00
22:34.0	Data point 32	0.34995 mL	0.06987 mL	0.07780 mL	1.15005 mL	0.02500 mL	10.691	0.00650	0.63605	0.00
23:00.7	Data point 33	0.34995 mL	0.06987 mL	0.07853 mL	1.15005 mL	0.02500 mL	10.894	-0.00274	0.31828	0.00
23:17.2	Data point 34	0.34995 mL	0.06987 mL	0.07966 mL	1.15005 mL	0.02500 mL	11.133	-0.00616	0.80076	0.00
23:43.9	Data point 35	0.34995 mL	0.06987 mL	0.08159 mL	1.15005 mL	0.02500 mL	11.325	-0.00851	0.80661	0.00
24:00.6	Data point 36	0.34995 mL	0.06987 mL	0.08464 mL	1.15005 mL	0.02500 mL	11.504	-0.00683	0.80154	0.00
24:17.2	Data point 37	0.34995 mL	0.06987 mL	0.08928 mL	1.15005 mL	0.02500 mL	11.676	-0.00731	0.72297	0.00
24:33.9	Data point 38	0.34995 mL	0.06987 mL	0.09624 mL	1.15005 mL	0.02500 mL	11.845	-0.01143	0.86800	0.00
24:55.6	Data point 39	0.34995 mL	0.06987 mL	0.10517 mL	1.15005 mL	0.02500 mL	12.004	-0.00877	0.73189	0.00
26:37.3	Reference spectrum									
27:41.4	Data point 41	0.50000 mL	0.17187 mL	0.10520 mL	1.15005 mL	0.02500 mL	1.964	-0.04942	0.90955	0.00
28:08.9	Data point 42	0.50000 mL	0.17187 mL	0.13133 mL	1.15005 mL	0.02500 mL	2.161	0.01175	0.86793	0.00
28:25.9	Data point 43	0.50000 mL	0.17187 mL	0.14958 mL	1.15005 mL	0.02500 mL	2.392	0.01031	0.62895	0.00
28:53.0	Data point 44	0.50000 mL	0.17187 mL	0.15922 mL	1.15005 mL	0.02500 mL	2.587	-0.01032	0.50004	0.00
29:09.7	Data point 45	0.50000 mL	0.17187 mL	0.16613 mL	1.15005 mL	0.02500 mL	2.822	0.00594	0.77267	0.00
29:41.6	Data point 46	0.50000 mL	0.17187 mL	0.17065 mL	1.15005 mL	0.02500 mL	3.051	0.00439	0.61230	0.00
29:58.2	Data point 47	0.50000 mL	0.17187 mL	0.17302 mL	1.15005 mL	0.02500 mL	3.308	0.00724	0.80181	0.00
30:29.9	Data point 48	0.50000 mL	0.17187 mL	0.17427 mL	1.15005 mL	0.02500 mL	3.516	0.00885	0.73530	0.00
30:46.4	Data point 49	0.50000 mL	0.17187 mL	0.17509 mL	1.15005 mL	0.02500 mL	3.746	0.02917	0.96458	0.00
31:02.9	Data point 50	0.50000 mL	0.17187 mL	0.17556 mL	1.15005 mL	0.02500 mL	3.918	0.02853	0.97912	0.00
31:19.5	Data point 51	0.50000 mL	0.17187 mL	0.17589 mL	1.15005 mL	0.02500 mL	4.075	0.03886	0.96737	0.00
31:41.1	Data point 52	0.50000 mL	0.17187 mL	0.17632 mL	1.15005 mL	0.02500 mL	4.452	0.08509	0.87669	0.00
32:08.0	Data point 53	0.50000 mL	0.17187 mL	0.17658 mL	1.15005 mL	0.02500 mL	4.690	0.09884	0.98828	0.00
32:37.6	Data point 54	0.50000 mL	0.17187 mL	0.17672 mL	1.15005 mL	0.02500 mL	5.023	0.09815	0.98524	0.00
33:23.0	Data point 55	0.50000 mL	0.17187 mL	0.17683 mL	1.15005 mL	0.02500 mL	5.450	0.09974	0.98582	0.00
34:14.7	Data point 56	0.50000 mL	0.17187 mL	0.17698 mL	1.15005 mL	0.02500 mL	5.962	0.10023	0.99543	0.00
35:08.2	Data point 57	0.50000 mL	0.17187 mL	0.17714 mL	1.15005 mL	0.02500 mL	6.413	0.09852	0.97264	0.00
35:59.8	Data point 58	0.50000 mL	0.17187 mL	0.17730 mL	1.15005 mL	0.02500 mL	6.786	0.10044	0.99093	0.00
36:36.4	Data point 59	0.50000 mL	0.17187 mL	0.17742 mL	1.15005 mL	0.02500 mL	7.041	0.09723	0.98345	0.00
37:16.6	Data point 60	0.50000 mL	0.17187 mL	0.17756 mL	1.15005 mL	0.02500 mL	7.294	0.09676	0.98747	0.00
38:04.6	Data point 61	0.50000 mL	0.17187 mL	0.17782 mL	1.15005 mL	0.02500 mL	7.505	0.09673	0.97655	0.00
38:41.9	Data point 62	0.50000 mL	0.17187 mL	0.17818 mL	1.15005 mL	0.02500 mL	7.782	0.09808	0.99281	0.00
39:20.6	Data point 63	0.50000 mL	0.17187 mL	0.17832 mL	1.15005 mL	0.02500 mL	8.027	0.10018	0.98289	0.00
40:07.2	Data point 64	0.50000 mL	0.17187 mL	0.17843 mL	1.15005 mL	0.02500 mL	8.296	0.10061	0.99264	0.00
40:49.8	Data point 65	0.50000 mL	0.17187 mL	0.17853 mL	1.15005 mL	0.02500 mL	8.604	0.09865	0.98819	0.00
41:36.4	Data point 66	0.50000 mL	0.17187 mL	0.17862 mL	1.15005 mL	0.02500 mL	8.972	0.09264	0.96514	0.00

Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
42:18.5	Data point 67	0.50000 mL	0.17187 mL	0.17872 mL	1.15005 mL	0.02500 mL	9.258	0.10013	0.99142	0.
42:57.4	Data point 68	0.50000 mL	0.17187 mL	0.17881 mL	1.15005 mL	0.02500 mL	9.497	0.09800	0.98730	0.
43:30.6	Data point 69	0.50000 mL	0.17187 mL	0.17898 mL	1.15005 mL	0.02500 mL	9.749	0.09641	0.96984	0.
43:55.8	Data point 70	0.50000 mL	0.17187 mL	0.17914 mL	1.15005 mL	0.02500 mL	9.975	0.05745	0.97083	0.
44:22.4	Data point 71	0.50000 mL	0.17187 mL	0.17937 mL	1.15005 mL	0.02500 mL	10.180	0.03285	0.93515	0.
44:54.2	Data point 72	0.50000 mL	0.17187 mL	0.17975 mL	1.15005 mL	0.02500 mL	10.380	0.01412	0.87362	0.
45:20.9	Data point 73	0.50000 mL	0.17187 mL	0.18027 mL	1.15005 mL	0.02500 mL	10.589	0.00176	0.22115	0.
45:37.6	Data point 74	0.50000 mL	0.17187 mL	0.18104 mL	1.15005 mL	0.02500 mL	10.811	-0.00633	0.72956	0.
45:54.3	Data point 75	0.50000 mL	0.17187 mL	0.18234 mL	1.15005 mL	0.02500 mL	11.023	-0.00950	0.89894	0.
46:11.0	Data point 76	0.50000 mL	0.17187 mL	0.18443 mL	1.15005 mL	0.02500 mL	11.210	-0.01127	0.92533	0.
46:27.7	Data point 77	0.50000 mL	0.17187 mL	0.18765 mL	1.15005 mL	0.02500 mL	11.376	-0.00906	0.88383	0.
46:54.7	Data point 78	0.50000 mL	0.17187 mL	0.19278 mL	1.15005 mL	0.02500 mL	11.569	-0.01129	0.90364	0.
47:11.5	Data point 79	0.50000 mL	0.17187 mL	0.20026 mL	1.15005 mL	0.02500 mL	11.733	-0.01085	0.88951	0.
47:38.8	Data point 80	0.50000 mL	0.17187 mL	0.21261 mL	1.15005 mL	0.02500 mL	11.926	-0.00959	0.80487	0.
47:55.6	Data point 81	0.50000 mL	0.17187 mL	0.22260 mL	1.15005 mL	0.02500 mL	12.028	-0.00784	0.78373	0.
49:40.8	Reference spectrum									
51:04.4	Data point 83	0.83996 mL	0.31122 mL	0.22262 mL	1.15005 mL	0.02500 mL	1.963	-0.02208	0.92470	0.
51:32.1	Data point 84	0.83996 mL	0.31122 mL	0.25301 mL	1.15005 mL	0.02500 mL	2.163	0.00890	0.66642	0.
52:04.7	Data point 85	0.83996 mL	0.31122 mL	0.27387 mL	1.15005 mL	0.02500 mL	2.381	-0.01331	0.55053	0.
52:21.6	Data point 86	0.83996 mL	0.31122 mL	0.28667 mL	1.15005 mL	0.02500 mL	2.603	0.00167	0.07564	0.
52:38.3	Data point 87	0.83996 mL	0.31122 mL	0.29426 mL	1.15005 mL	0.02500 mL	2.823	-0.00962	0.34492	0.
52:55.2	Data point 88	0.83996 mL	0.31122 mL	0.29885 mL	1.15005 mL	0.02500 mL	3.010	-0.01611	0.70036	0.
53:11.9	Data point 89	0.83996 mL	0.31122 mL	0.30186 mL	1.15005 mL	0.02500 mL	3.282	-0.01901	0.61878	0.
53:43.8	Data point 90	0.83996 mL	0.31122 mL	0.30365 mL	1.15005 mL	0.02500 mL	3.519	0.00807	0.81936	0.
54:00.3	Data point 91	0.83996 mL	0.31122 mL	0.30459 mL	1.15005 mL	0.02500 mL	3.707	-0.00486	0.22709	0.
54:16.9	Data point 92	0.83996 mL	0.31122 mL	0.30520 mL	1.15005 mL	0.02500 mL	3.880	0.00581	0.23143	0.
54:33.3	Data point 93	0.83996 mL	0.31122 mL	0.30560 mL	1.15005 mL	0.02500 mL	4.010	0.02162	0.87736	0.
55:00.2	Data point 94	0.83996 mL	0.31122 mL	0.30680 mL	1.15005 mL	0.02500 mL	4.741	-0.01995	0.17650	0.
55:27.0	Data point 95	0.83996 mL	0.31122 mL	0.30729 mL	1.15005 mL	0.02500 mL	6.025	-0.05252	0.31919	0.
56:02.4	Data point 96	0.83996 mL	0.31122 mL	0.30750 mL	1.15005 mL	0.02500 mL	6.269	0.10021	0.97854	0.
56:25.7	Data point 97	0.83996 mL	0.31122 mL	0.30762 mL	1.15005 mL	0.02500 mL	6.505	-0.09636	0.92033	0.
56:52.9	Data point 98	0.83996 mL	0.31122 mL	0.30774 mL	1.15005 mL	0.02500 mL	6.719	0.01824	0.63932	0.
57:14.4	Data point 99	0.83996 mL	0.31122 mL	0.30785 mL	1.15005 mL	0.02500 mL	6.948	-0.08519	0.98106	0.
57:46.3	Data point 100	0.83996 mL	0.31122 mL	0.30800 mL	1.15005 mL	0.02500 mL	7.168	0.05657	0.88823	0.
58:18.2	Data point 101	0.83996 mL	0.31122 mL	0.30814 mL	1.15005 mL	0.02500 mL	7.390	0.07489	0.83646	0.
58:49.8	Data point 102	0.83996 mL	0.31122 mL	0.30828 mL	1.15005 mL	0.02500 mL	7.642	0.09148	0.91360	0.
59:24.1	Data point 103	0.83996 mL	0.31122 mL	0.30840 mL	1.15005 mL	0.02500 mL	7.875	0.09992	0.97999	0.
1:00:05.8	Data point 104	0.83996 mL	0.31122 mL	0.30851 mL	1.15005 mL	0.02500 mL	8.176	0.09857	0.96991	0.
1:00:47.0	Data point 105	0.83996 mL	0.31122 mL	0.30861 mL	1.15005 mL	0.02500 mL	8.496	0.09271	0.95727	0.
1:01:31.7	Data point 106	0.83996 mL	0.31122 mL	0.30870 mL	1.15005 mL	0.02500 mL	8.851	0.09687	0.97511	0.
1:02:10.3	Data point 107	0.83996 mL	0.31122 mL	0.30880 mL	1.15005 mL	0.02500 mL	9.154	0.09684	0.96233	0.
1:02:45.5	Data point 108	0.83996 mL	0.31122 mL	0.30891 mL	1.15005 mL	0.02500 mL	9.422	0.09855	0.96632	0.
1:03:10.7	Data point 109	0.83996 mL	0.31122 mL	0.30906 mL	1.15005 mL	0.02500 mL	9.647	0.06219	0.98437	0.
1:03:37.5	Data point 110	0.83996 mL	0.31122 mL	0.30924 mL	1.15005 mL	0.02500 mL	9.850	0.04151	0.97249	0.
1:04:04.2	Data point 111	0.83996 mL	0.31122 mL	0.30950 mL	1.15005 mL	0.02500 mL	10.048	0.03235	0.89904	0.
1:04:20.8	Data point 112	0.83996 mL	0.31122 mL	0.30985 mL	1.15005 mL	0.02500 mL	10.282	-0.01175	0.83447	0.
1:04:47.6	Data point 113	0.83996 mL	0.31122 mL	0.31051 mL	1.15005 mL	0.02500 mL	10.522	-0.01448	0.89249	0.
1:05:04.2	Data point 114	0.83996 mL	0.31122 mL	0.31155 mL	1.15005 mL	0.02500 mL	10.757	-0.02586	0.94230	0.
1:05:36.2	Data point 115	0.83996 mL	0.31122 mL	0.31350 mL	1.15005 mL	0.02500 mL	10.951	-0.01301	0.85335	0.
1:05:52.8	Data point 116	0.83996 mL	0.31122 mL	0.31623 mL	1.15005 mL	0.02500 mL	11.128	-0.02671	0.94173	0.
1:06:09.6	Data point 117	0.83996 mL	0.31122 mL	0.32032 mL	1.15005 mL	0.02500 mL	11.320	-0.02476	0.94965	0.
1:06:26.4	Data point 118	0.83996 mL	0.31122 mL	0.32669 mL	1.15005 mL	0.02500 mL	11.484	-0.02253	0.94614	0.
1:06:58.8	Data point 119	0.83996 mL	0.31122 mL	0.33737 mL	1.15005 mL	0.02500 mL	11.683	-0.01396	0.91516	0.
1:07:15.8	Data point 120	0.83996 mL	0.31122 mL	0.35247 mL	1.15005 mL	0.02500 mL	11.863	-0.02079	0.91507	0.
1:07:32.8	Data point 121	0.83996 mL	0.31122 mL	0.37396 mL	1.15005 mL	0.02500 mL	12.024	-0.02214	0.95039	0.
1:09:32.4	Assay volumes	1.08996 mL	0.45830 mL	0.37396 mL	1.15005 mL	0.02500 mL				

Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
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				

Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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	0.150	10/4/2017 4:54:41 AM	C:\Sirius_T3\17J-03018_Blank standardisation.t3r
Four-Plus S	0.9943	10/4/2017 4:54:41 AM	C:\Sirius_T3\17J-03018_Blank standardisation.t3r
Four-Plus jH	0.6	10/4/2017 4:54:41 AM	C:\Sirius_T3\17J-03018_Blank standardisation.t3r
Four-Plus jOH	-0.8	10/4/2017 4:54:41 AM	C:\Sirius_T3\17J-03018_Blank standardisation.t3r
Base concentration factor	1.011	10/4/2017 4:54:41 AM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	1.007	10/4/2017 4:54:41 AM	C:\Sirius_T3\17J-03018_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	9/8/2017 9:21:27 AM
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	9/29/2017 9:58:40 AM
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

Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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	-9.45 mV		10/4/2017 4:55:05 AM
Filling solution	3M KCl	KCL095	10/2/2017 9:26:59 AM
Liquids			
Wash 1	50% IPA:50% Water		10/3/2017 9:05:00 AM
Wash 2	0.5% Trition X-100 in H20		10/3/2017 9:05:01 AM
Buffer position 1	pH7 Wash		10/3/2017 9:05:03 AM
Buffer position 2	pH 7		10/3/2017 9:05:05 AM
Storage position			10/3/2017 9:05:10 AM
Wash water	7.4e+003 mL	10-3-17	10/3/2017 9:04:49 AM
Waste	2.6e+003 mL		10/3/2017 9:04:54 AM
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	313:32:06		11/23/2010 12:22:28 PM
Calibrated on	9/26/2017 9:22:07 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		

Sample name: **M13**
Assay name: **UV-metric psKa**
Assay ID: **17J-04005**
Filename: **C:\Sirius_T3\17J-04005_M13_UV-metric psKa_1_pKa.t3r**

Experiment start time: **10/4/2017 4:54:41 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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 G1