UV-metric pKa

Sample name: **M06**
Assay name: **UV-metric pKa**
Assay ID: **17I-18023**
Filename: **C:\Sirius_T3\Mehtap\20170918_exp04_uv_M01-M14\17I-18023_M06_UV-metric pKa.t3r**

Experiment start time: **9/18/2017 11:44:44 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Results

pKa 1	**3.02**
pKa 2	**11.71**
RMSD	**0.031 0.024 0.015**
Chi squared	**0.1135**
PCA calculated number of pKas	**2**
Average ionic strength	**0.183 M**
Average temperature	**24.9°C**
Analyte concentration range	**86.8 µM to 70.2 µM**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.458 to 12.840**

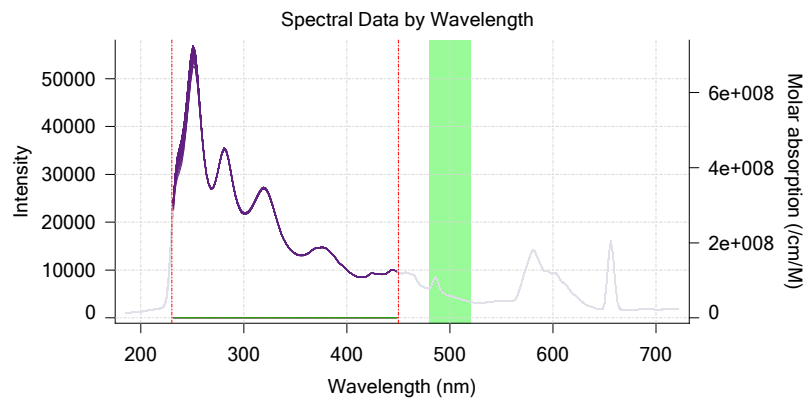
Warnings and errors

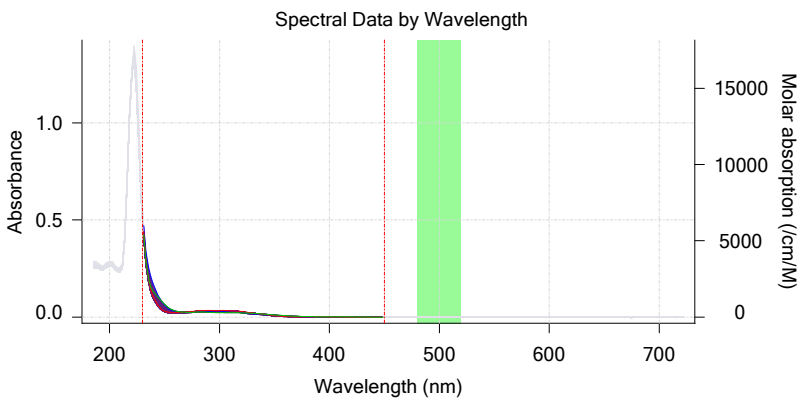
Errors None
Warnings None

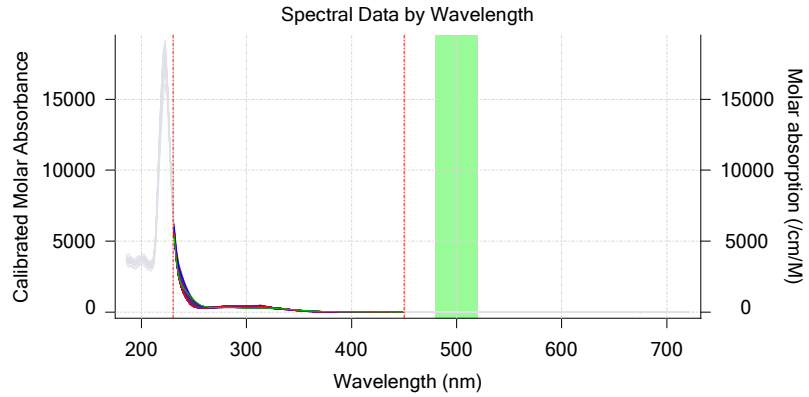
Assay Settings

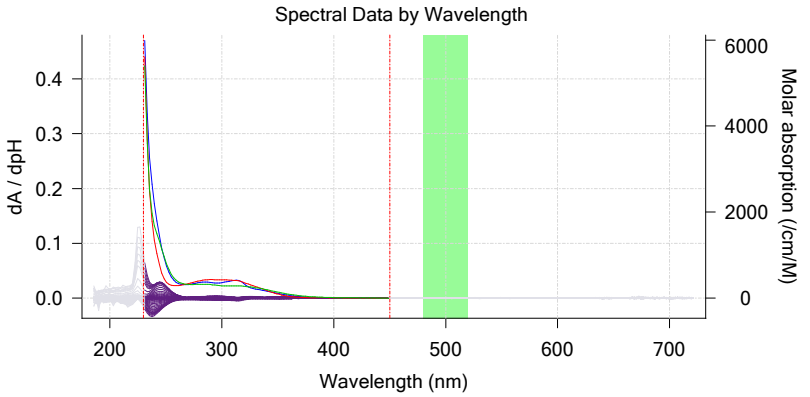
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

Graphs





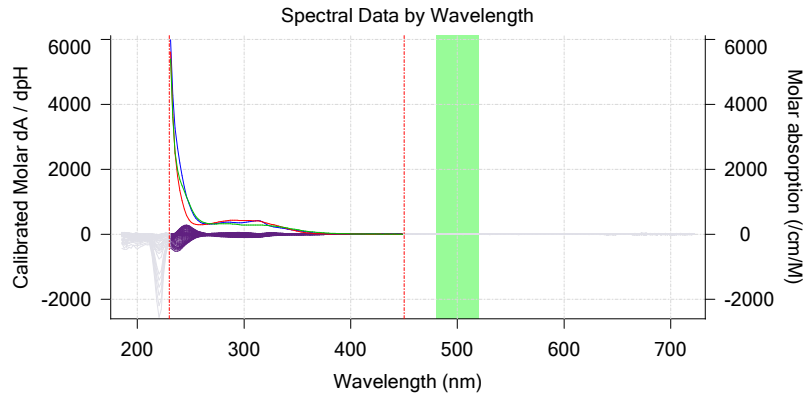


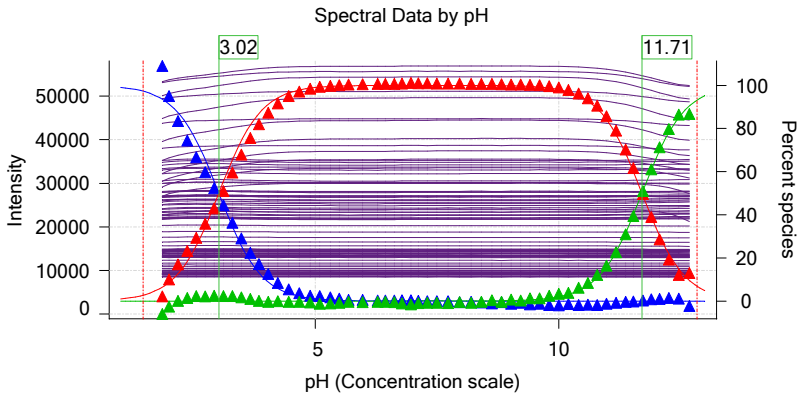


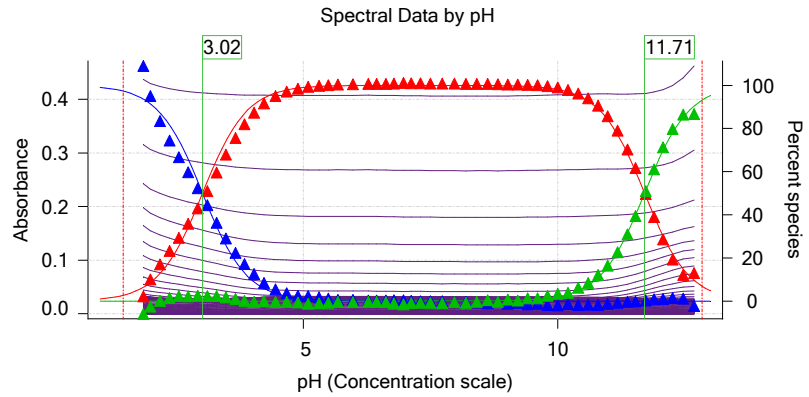
Sample name: **M06**
Assay name: **UV-metric pKa**
Assay ID: **17I-18023**
Filename: **C:\Sirius_T3\Mehtap\20170918_exp04_uv_M01-M14\17I-18023_M06_UV-metric pKa.t3r**

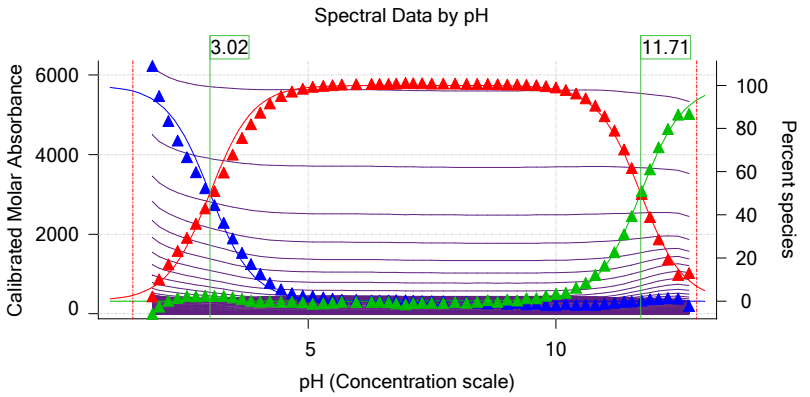
Experiment start time: **9/18/2017 11:44:44 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

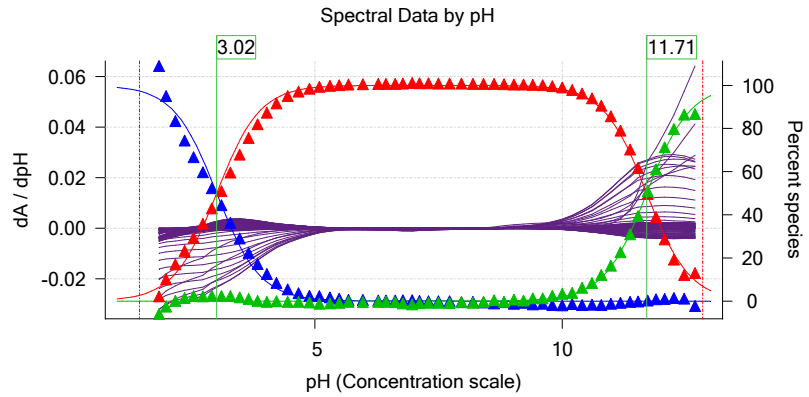
Graphs (continued)

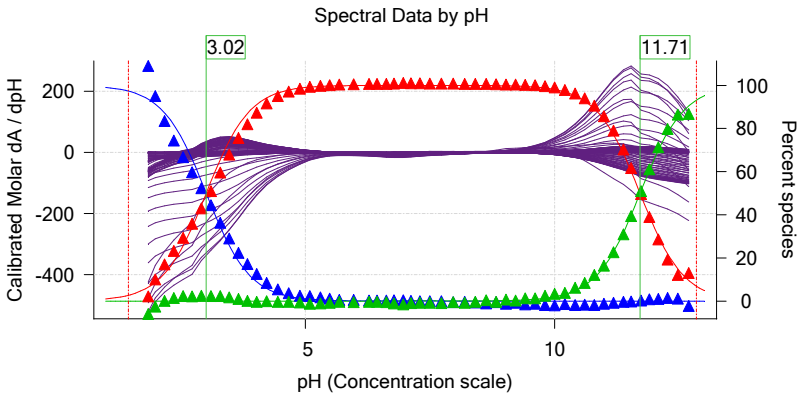


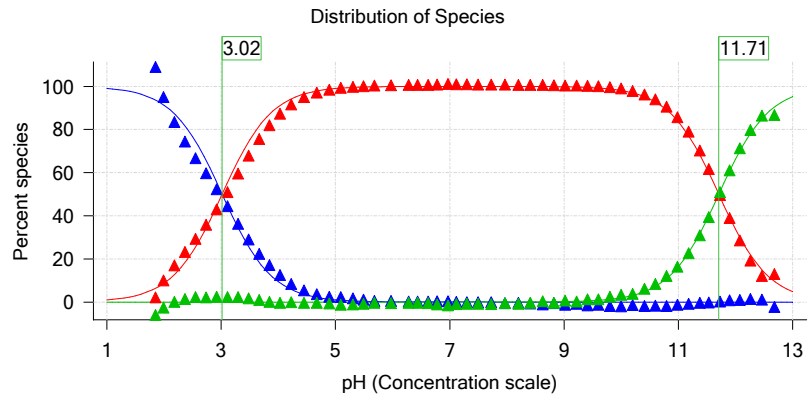


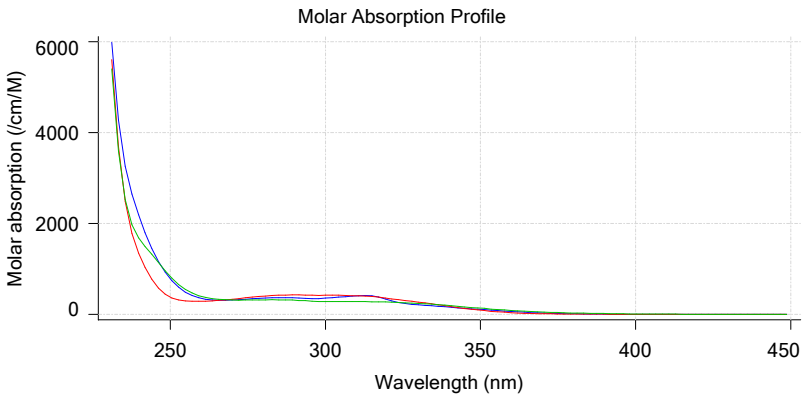








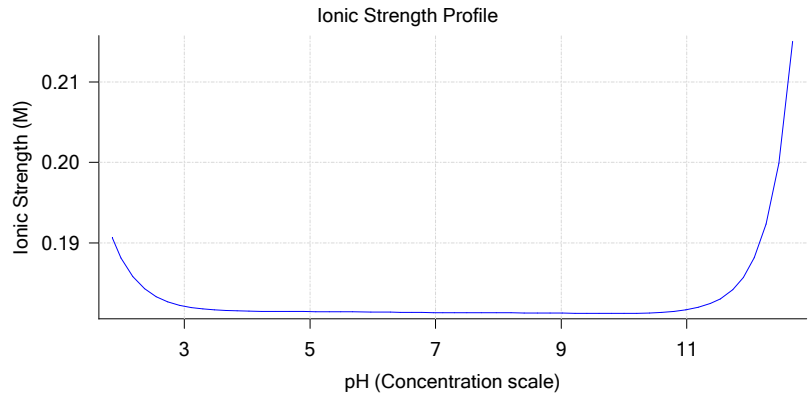


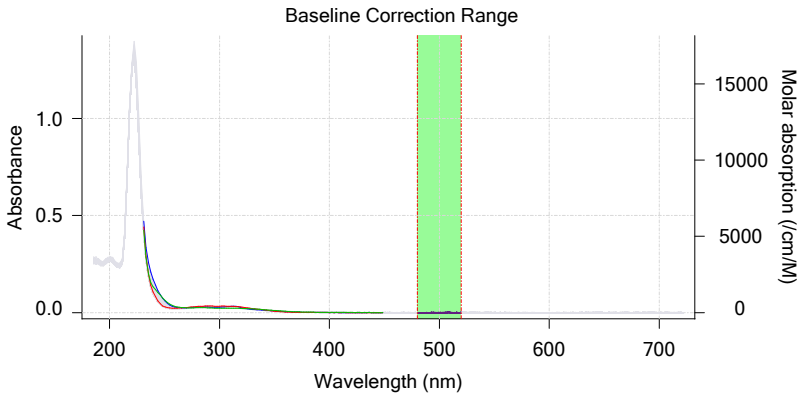


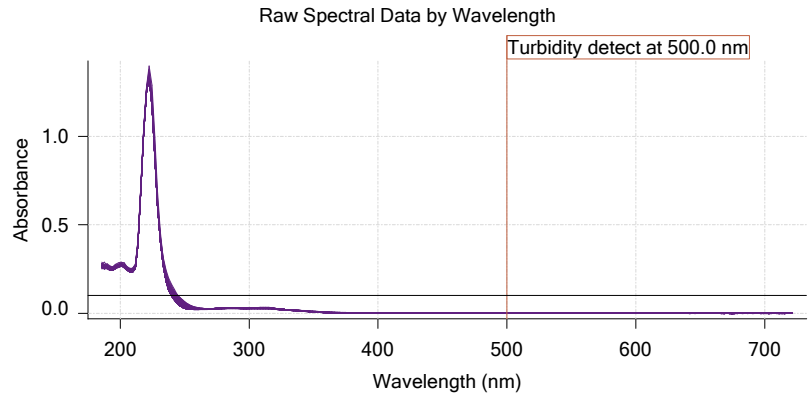
Sample name: **M06**
Assay name: **UV-metric pKa**
Assay ID: **17I-18023**
Filename: **C:\Sirius_T3\Mehtap\20170918_exp04_uv_M01-M14\17I-18023_M06_UV-metric pKa.t3r**

Experiment start time: **9/18/2017 11:44:44 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)







Events

Time	Event	Water	Acid	Base	Buffer	pH	dpH/dt	pH R-squared	pH SD
2:38.1	Dark spectrum								
2:39.6	Reference spectrum								
3:07.2	Volume reset due to vial change								
4:23.7	Initial pH = 12.84								
5:33.7	Data point 4	1.20002 mL	0.00000 mL	0.30000 mL	0.02500 mL	12.761	0.01226	0.83852	0.000
6:04.2	Data point 5	1.20002 mL	0.10308 mL	0.30000 mL	0.02500 mL	12.562	0.00252	0.19085	0.000
6:22.4	Data point 6	1.20002 mL	0.16997 mL	0.30000 mL	0.02500 mL	12.367	-0.00891	0.58210	0.000
6:39.9	Data point 7	1.20002 mL	0.21101 mL	0.30000 mL	0.02500 mL	12.187	-0.00754	0.20638	0.000
6:57.1	Data point 8	1.20002 mL	0.23742 mL	0.30000 mL	0.02500 mL	12.014	-0.01502	0.78492	0.000
7:14.0	Data point 9	1.20002 mL	0.25515 mL	0.30000 mL	0.02500 mL	11.847	-0.01627	0.95088	0.000
7:41.1	Data point 10	1.20002 mL	0.26867 mL	0.30000 mL	0.02500 mL	11.652	-0.01546	0.94608	0.000
7:57.9	Data point 11	1.20002 mL	0.27627 mL	0.30000 mL	0.02500 mL	11.495	-0.02120	0.97503	0.001
8:24.7	Data point 12	1.20002 mL	0.28255 mL	0.30000 mL	0.02500 mL	11.300	-0.02001	0.96462	0.001
8:51.7	Data point 13	1.20002 mL	0.28662 mL	0.30000 mL	0.02500 mL	11.103	-0.02166	0.93677	0.001
9:18.4	Data point 14	1.20002 mL	0.28935 mL	0.30000 mL	0.02500 mL	10.911	-0.01211	0.92136	0.000
9:45.2	Data point 15	1.20002 mL	0.29125 mL	0.30000 mL	0.02500 mL	10.720	-0.00182	0.11619	0.000
10:17.0	Data point 16	1.20002 mL	0.29269 mL	0.30000 mL	0.02500 mL	10.524	-0.01182	0.90519	0.000
10:53.9	Data point 17	1.20002 mL	0.29379 mL	0.30000 mL	0.02500 mL	10.320	-0.00914	0.68047	0.000
11:30.9	Data point 18	1.20002 mL	0.29471 mL	0.30000 mL	0.02500 mL	10.117	-0.01415	0.95268	0.000
12:07.7	Data point 19	1.20002 mL	0.29551 mL	0.30000 mL	0.02500 mL	9.920	-0.01073	0.85208	0.000
12:44.5	Data point 20	1.20002 mL	0.29626 mL	0.30000 mL	0.02500 mL	9.721	-0.00736	0.73002	0.000
13:21.2	Data point 21	1.20002 mL	0.29694 mL	0.30000 mL	0.02500 mL	9.525	-0.00759	0.87507	0.000
13:58.0	Data point 22	1.20002 mL	0.29753 mL	0.30000 mL	0.02500 mL	9.334	-0.01117	0.85348	0.000
14:34.6	Data point 23	1.20002 mL	0.29802 mL	0.30000 mL	0.02500 mL	9.137	-0.01868	0.89568	0.000
15:16.5	Data point 24	1.20002 mL	0.29842 mL	0.30000 mL	0.02500 mL	8.937	-0.02456	0.92960	0.001
15:53.5	Data point 25	1.20002 mL	0.29873 mL	0.30000 mL	0.02500 mL	8.739	-0.05543	0.96425	0.002

Sample name: **M06**
Assay name: **UV-metric pKa**
Assay ID: **17I-18023**
Filename: **C:\Sirius_T3\Mehtap\20170918_exp04_uv_M01-M14\17I-18023_M06_UV-metric pKa.t3r**

Experiment start time: **9/18/2017 11:44:44 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Buffer	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
16:35.4	Data point 26	1.20002 mL	0.29896 mL	0.30000 mL	0.02500 mL	8.524	-0.06657	0.97176	0.00334	10.0 s
17:12.2	Data point 27	1.20002 mL	0.29913 mL	0.30000 mL	0.02500 mL	8.312	-0.09201	0.97494	0.00460	10.0 s
17:53.8	Data point 28	1.20002 mL	0.29927 mL	0.30000 mL	0.02500 mL	8.079	-0.09533	0.96341	0.00479	10.5 s
18:31.0	Data point 29	1.20002 mL	0.29939 mL	0.30000 mL	0.02500 mL	7.839	-0.06445	0.91325	0.00336	10.0 s
19:07.9	Data point 30	1.20002 mL	0.29951 mL	0.30000 mL	0.02500 mL	7.608	0.02094	0.61563	0.00132	10.0 s
19:50.0	Data point 31	1.20002 mL	0.29965 mL	0.30000 mL	0.02500 mL	7.411	0.06661	0.98810	0.00331	10.0 s
20:31.7	Data point 32	1.20002 mL	0.29984 mL	0.30000 mL	0.02500 mL	7.228	0.09945	0.98942	0.00500	15.5 s
21:14.1	Data point 33	1.20002 mL	0.30005 mL	0.30000 mL	0.02500 mL	7.077	0.10028	0.98809	0.00497	19.0 s
22:10.0	Data point 34	1.20002 mL	0.30035 mL	0.30000 mL	0.02500 mL	6.889	0.09760	0.98579	0.00485	17.0 s
22:53.8	Data point 35	1.20002 mL	0.30063 mL	0.30000 mL	0.02500 mL	6.732	0.09704	0.97610	0.00489	19.0 s
23:39.7	Data point 36	1.20002 mL	0.30101 mL	0.30000 mL	0.02500 mL	6.548	0.09808	0.96377	0.00493	18.0 s
24:24.4	Data point 37	1.20002 mL	0.30136 mL	0.30000 mL	0.02500 mL	6.388	0.09482	0.96596	0.00482	14.0 s
25:10.8	Data point 38	1.20002 mL	0.30195 mL	0.30000 mL	0.02500 mL	6.080	0.08781	0.89213	0.00459	12.5 s
25:55.3	Data point 39	1.20002 mL	0.30242 mL	0.30000 mL	0.02500 mL	5.786	0.07060	0.85935	0.00376	10.5 s
26:32.7	Data point 40	1.20002 mL	0.30266 mL	0.30000 mL	0.02500 mL	5.599	0.03300	0.92085	0.00172	10.0 s
27:04.8	Data point 41	1.20002 mL	0.30282 mL	0.30000 mL	0.02500 mL	5.411	0.01731	0.72259	0.00100	10.0 s
27:41.5	Data point 42	1.20002 mL	0.30296 mL	0.30000 mL	0.02500 mL	5.197	-0.02053	0.87753	0.00108	10.0 s
28:08.1	Data point 43	1.20002 mL	0.30306 mL	0.30000 mL	0.02500 mL	4.999	-0.03253	0.95352	0.00166	10.0 s
28:34.8	Data point 44	1.20002 mL	0.30315 mL	0.30000 mL	0.02500 mL	4.777	-0.04381	0.93273	0.00224	10.0 s
28:56.4	Data point 45	1.20002 mL	0.30325 mL	0.30000 mL	0.02500 mL	4.554	-0.04260	0.91692	0.00220	10.0 s
29:28.2	Data point 46	1.20002 mL	0.30339 mL	0.30000 mL	0.02500 mL	4.330	-0.02870	0.89663	0.00151	10.0 s
29:55.0	Data point 47	1.20002 mL	0.30355 mL	0.30000 mL	0.02500 mL	4.133	-0.01527	0.85433	0.00082	10.0 s
30:11.6	Data point 48	1.20002 mL	0.30376 mL	0.30000 mL	0.02500 mL	3.945	-0.00734	0.70992	0.00043	10.0 s
30:28.2	Data point 49	1.20002 mL	0.30407 mL	0.30000 mL	0.02500 mL	3.765	-0.00326	0.33320	0.00028	10.0 s
30:44.8	Data point 50	1.20002 mL	0.30454 mL	0.30000 mL	0.02500 mL	3.581	-0.00250	0.24906	0.00025	10.0 s
31:01.4	Data point 51	1.20002 mL	0.30524 mL	0.30000 mL	0.02500 mL	3.397	-0.00108	0.05183	0.00023	10.0 s
31:17.9	Data point 52	1.20002 mL	0.30633 mL	0.30000 mL	0.02500 mL	3.212	0.00018	0.00140	0.00024	10.0 s
31:34.5	Data point 53	1.20002 mL	0.30800 mL	0.30000 mL	0.02500 mL	3.022	-0.00290	0.23666	0.00029	10.0 s
31:51.1	Data point 54	1.20002 mL	0.31058 mL	0.30000 mL	0.02500 mL	2.836	-0.00373	0.40288	0.00029	10.0 s
32:07.8	Data point 55	1.20002 mL	0.31456 mL	0.30000 mL	0.02500 mL	2.652	-0.00325	0.46188	0.00024	10.0 s
32:24.4	Data point 56	1.20002 mL	0.32065 mL	0.30000 mL	0.02500 mL	2.468	-0.00366	0.54469	0.00024	10.0 s
32:41.1	Data point 57	1.20002 mL	0.33003 mL	0.30000 mL	0.02500 mL	2.282	-0.00607	0.65244	0.00037	10.0 s
32:58.0	Data point 58	1.20002 mL	0.34461 mL	0.30000 mL	0.02500 mL	2.099	-0.00274	0.20168	0.00030	10.0 s
33:14.9	Data point 59	1.20002 mL	0.36054 mL	0.30000 mL	0.02500 mL	1.962	-0.00716	0.76933	0.00040	10.0 s
36:10.9	Assay volumes	1.45002 mL	0.36054 mL	0.43008 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	1			
Minimum pH	2.000			
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				

Sample name: **M06**
Assay name: **UV-metric pKa**
Assay ID: **17I-18023**
Filename: **C:\Sirius_T3\Mehtap\20170918_exp04_uv_M01-M14\17I-18023_M06_UV-metric pKa.t3r**

Experiment start time: **9/18/2017 11:44:44 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titrant pre-dose	Base Titrant			
Base titrant volume	0.30000 mL			
Allow to stand for	15 seconds			
Assay Medium				
Cosolvent in use	No			
ISA water volume	1.20 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	High to low pH			
Adjust to start pH	No			
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	0.094	9/18/2017 11:44:43 PM	C:\Sirius_T3\17I-18009_Blank standardisation.t3r
Four-Plus S	1.0023	9/18/2017 11:44:43 PM	C:\Sirius_T3\17I-18009_Blank standardisation.t3r
Four-Plus jH	0.8	9/18/2017 11:44:43 PM	C:\Sirius_T3\17I-18009_Blank standardisation.t3r
Four-Plus jOH	-0.5	9/18/2017 11:44:43 PM	C:\Sirius_T3\17I-18009_Blank standardisation.t3r
Base concentration factor	1.015	9/18/2017 11:44:44 PM	C:\Sirius_T3\KOH17I11.t3r
Acid concentration factor	1.006	9/18/2017 11:44:43 PM	C:\Sirius_T3\17I-18009_Blank standardisation.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		

Sample name: **M06**
Assay name: **UV-metric pKa**
Assay ID: **17I-18023**
Filename: **C:\Sirius_T3\Mehtap\20170918_exp04_uv_M01-M14\17I-18023_M06_UV-metric pKa.t3r**

Experiment start time: **9/18/2017 11:44:44 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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	9/18/2017 9:13:04 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)	01/06/17	9/8/2017 9:20:03 AM
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)	8-15-17	9/13/2017 12:23:11 PM
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	-7.55 mV		9/18/2017 11:45:07 PM
Filling solution	3M KCl	KCL095	9/18/2017 9:17:15 AM
Liquids			
Wash 1	50% IPA:50% Water		9/18/2017 9:09:36 AM
Wash 2	0.5% Trition X-100 in H20		9/18/2017 9:09:39 AM
Buffer position 1	pH7 Wash		9/18/2017 9:09:41 AM
Buffer position 2	pH 7		9/18/2017 9:09:44 AM
Storage position			9/18/2017 9:10:43 AM
Wash water	8.3e+003 mL	9-18-17	9/18/2017 8:54:32 AM
Waste	1.7e+003 mL		9/18/2017 8:54:39 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	143:53:30		11/23/2010 12:22:28 PM
Calibrated on	9/18/2017 9:35:14 AM		
Integration time	11		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 10:34:13 AM

Sample name: **M06**
Assay name: **UV-metric pKa**
Assay ID: **17I-18023**
Filename: **C:\Sirius_T3\Mehtap\20170918_exp04_uv_M01-M14\17I-18023_M06_UV-metric pKa.t3r**

Experiment start time: **9/18/2017 11:44:44 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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