UV-metric pKa

Sample name:	**M07**	Experiment start time:	**9/15/2017 11:47:51 PM**
Assay name:	**UV-metric pKa**	Analyst:	**Dorothy Levorse**
Assay ID:	**17I-16002**	Instrument ID:	**T311053**
Filename:	**C:\Sirius_T3\17I-16002_M07_UV-metric pKa.t3r**		

Results

pKa 1	**6.07**
RMSD	**0.002 0.002**
Chi squared	**0.0116**
PCA calculated number of pKas	**3**
Average ionic strength	**0.158 M**
Average temperature	**24.9°C**
Analyte concentration range	**100.6 µM to 91.2 µM**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.276 to 12.701**

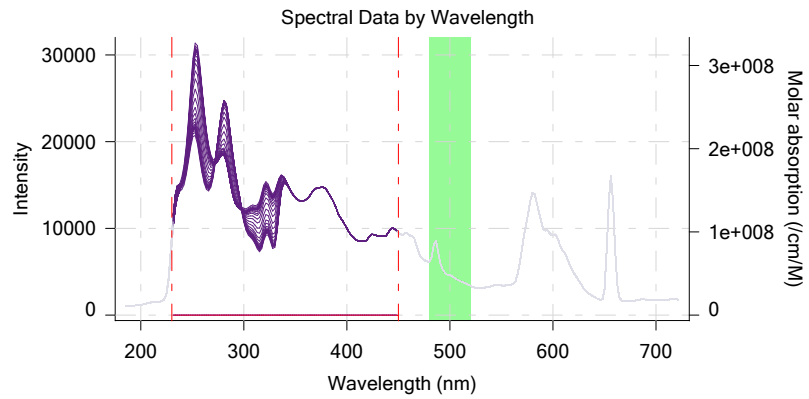
Warnings and errors

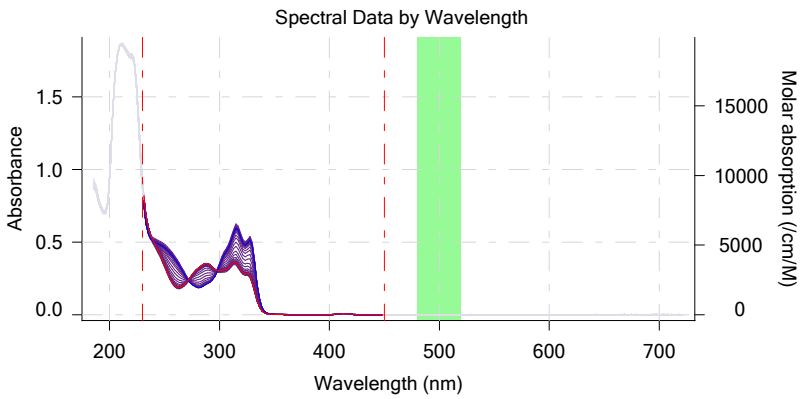
Errors	None
Warnings	PCA calculation disagrees with predicted number of pKas

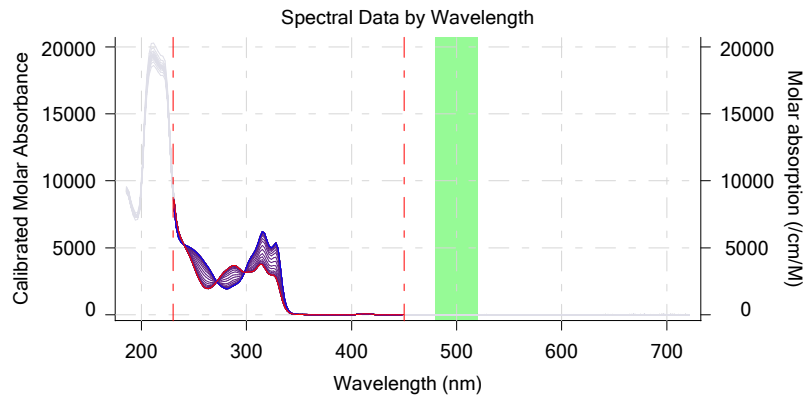
Assay Settings

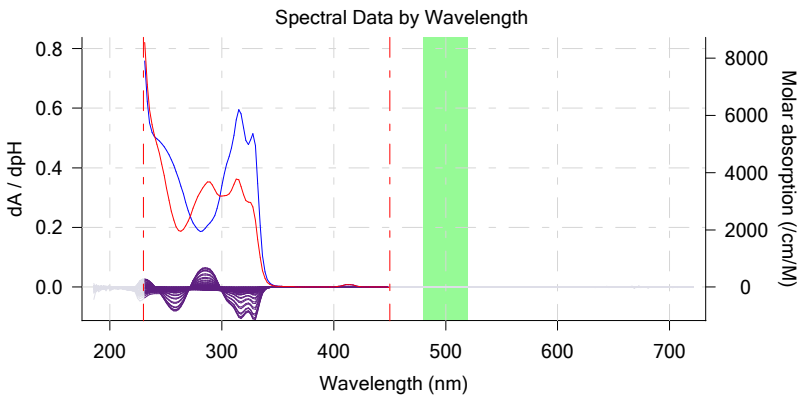
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

Graphs









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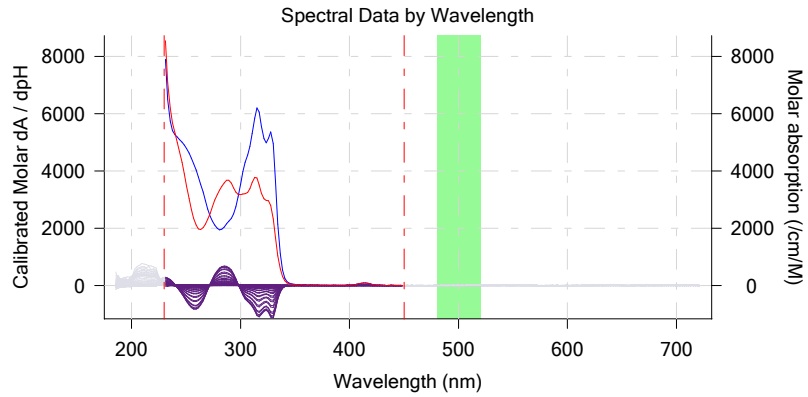
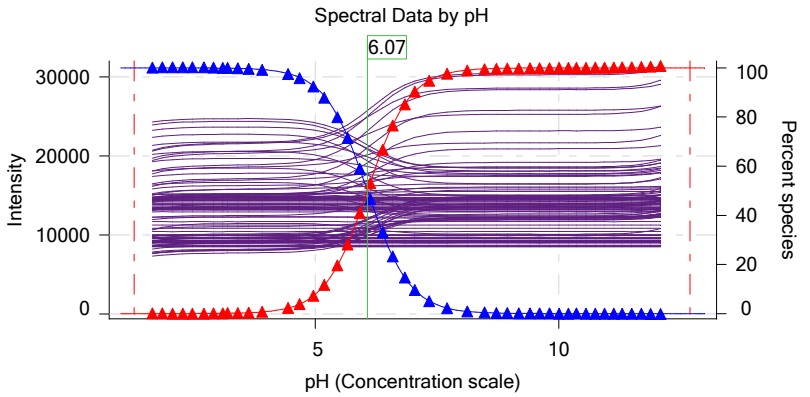
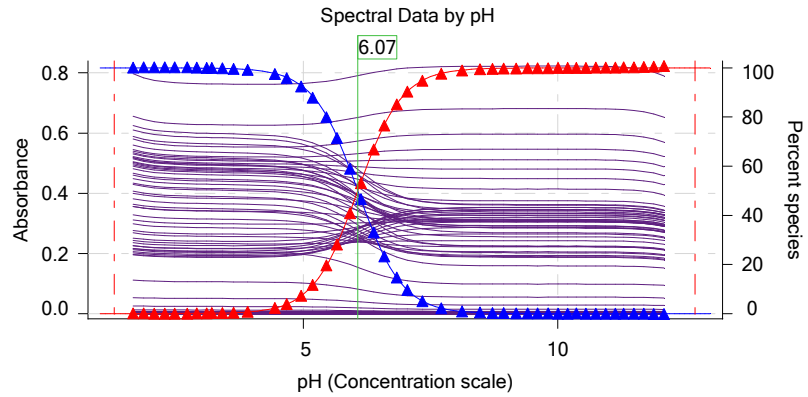
Filename: **C:\Sirius_T3\17I-16002_M07_UV-metric pKa.t3r**

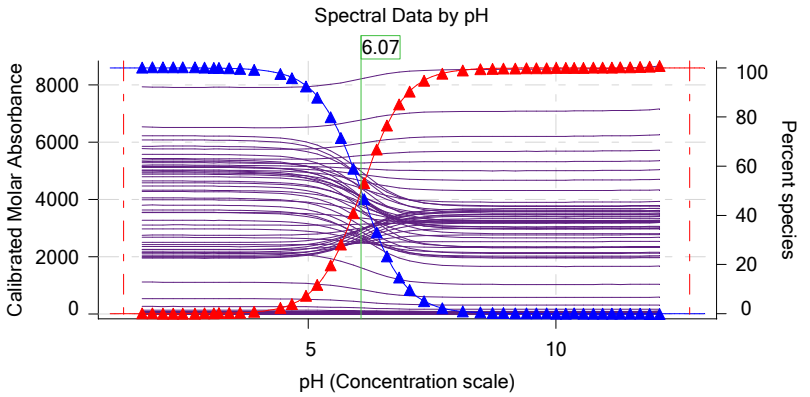
Experiment start time: **9/15/2017 11:47:51 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

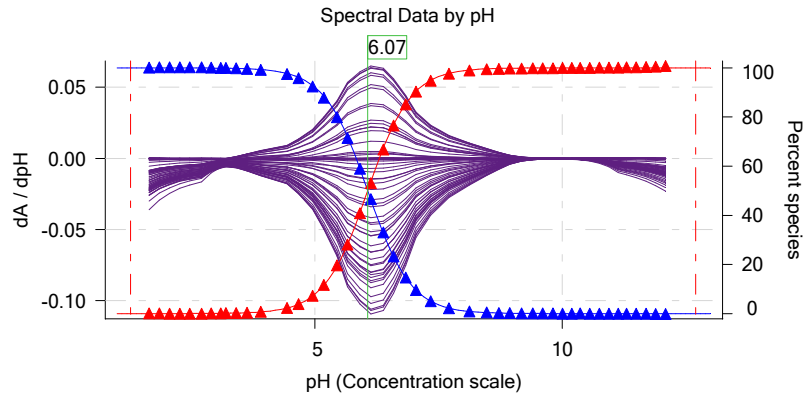
Graphs (continued)

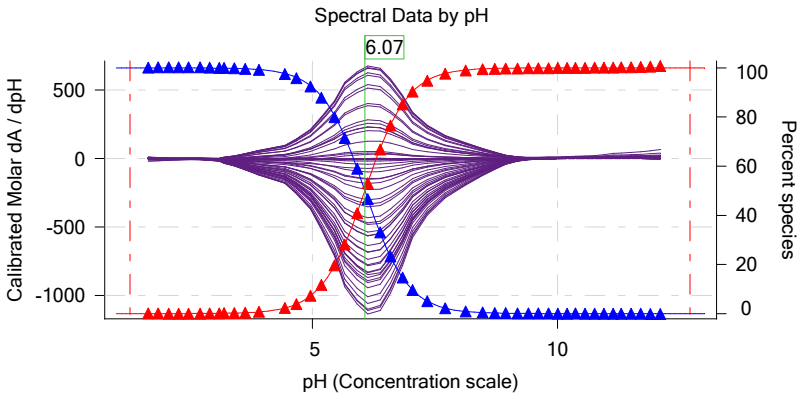


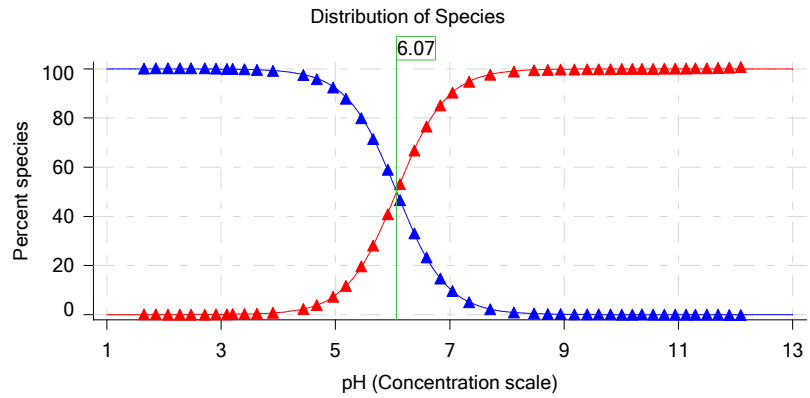


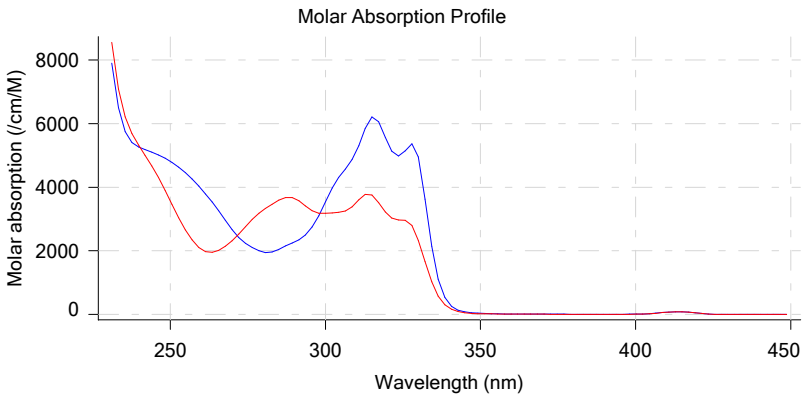












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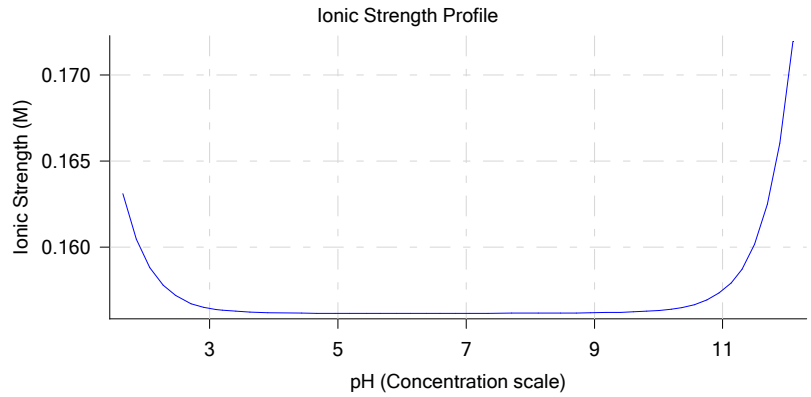
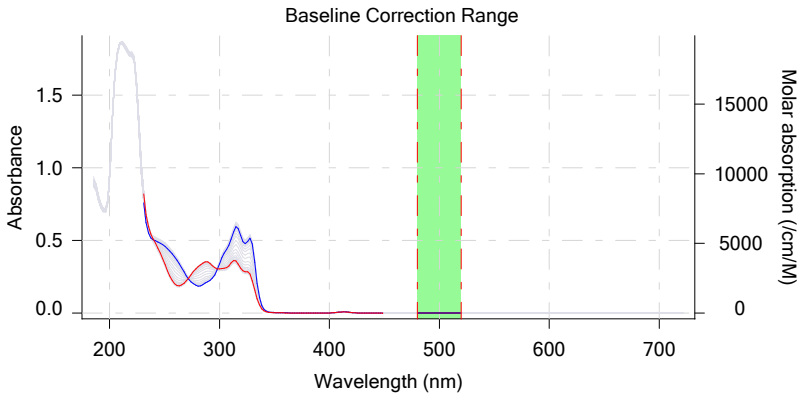
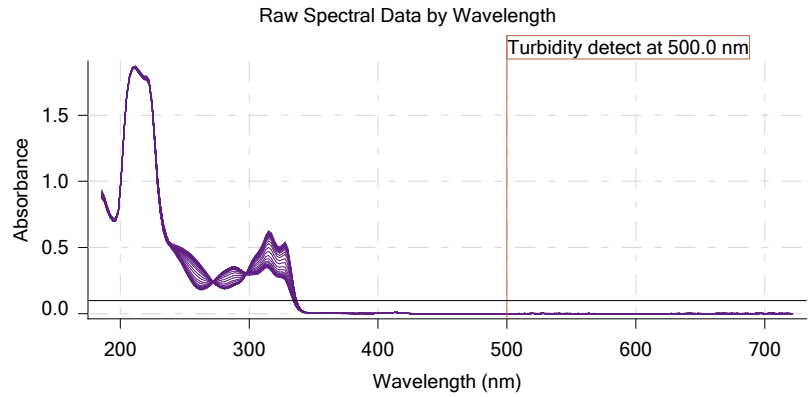
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)







Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M07	9/15/2017 3:35:09 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0030 mL	9/15/2017 3:35:09 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.053600 M	9/15/2017 3:35:09 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	235.28	9/15/2017 3:35:16 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	9/15/2017 3:35:09 PM	User entered value
Sample is a	Base	9/15/2017 3:35:09 PM	User entered value
pKa 1	5.70	9/15/2017 3:35:09 PM	User entered value
logp (XH +)	-10.00		Default value
logP (neutral X)	-10.00	9/15/2017 3:35:09 PM	User entered value

Events

Time	Event	Water	Acid	Base	Buffer	pH	dpH/dt	pH R-squared	pH SD
3:12.3	Dark spectrum								
3:13.8	Reference spectrum								
3:41.4	Volume reset due to vial change								
5:11.8	Initial pH = 7.61								
6:24.8	Data point 4	1.50000 mL	0.07084 mL	0.00000 mL	0.02500 mL	1.776	-0.00744	0.73426	0.00043
6:53.6	Data point 5	1.50000 mL	0.07084 mL	0.02547 mL	0.02500 mL	1.978	0.00458	0.17102	0.00055
7:10.8	Data point 6	1.50000 mL	0.07084 mL	0.04219 mL	0.02500 mL	2.184	0.00516	0.10363	0.00079
7:27.7	Data point 7	1.50000 mL	0.07084 mL	0.05252 mL	0.02500 mL	2.390	-0.01054	0.48727	0.00075
7:44.5	Data point 8	1.50000 mL	0.07084 mL	0.05894 mL	0.02500 mL	2.587	0.00719	0.47472	0.00051
8:01.3	Data point 9	1.50000 mL	0.07084 mL	0.06301 mL	0.02500 mL	2.826	0.00143	0.07186	0.00026

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Experiment start time: **9/15/2017 11:47:51 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
8:33.4	Data point 10	1.50000 mL	0.07084 mL	0.06540 mL	0.02500 mL	3.020	0.00892	0.78278	0.00050	10.0 s
8:50.0	Data point 11	1.50000 mL	0.07084 mL	0.06691 mL	0.02500 mL	3.211	0.01230	0.89789	0.00064	10.0 s
9:06.6	Data point 12	1.50000 mL	0.07084 mL	0.06787 mL	0.02500 mL	3.313	0.00426	0.47301	0.00031	10.0 s
9:38.6	Data point 13	1.50000 mL	0.07084 mL	0.06881 mL	0.02500 mL	3.522	0.01169	0.87789	0.00062	10.0 s
10:05.2	Data point 14	1.50000 mL	0.07084 mL	0.06931 mL	0.02500 mL	3.741	0.02154	0.93404	0.00110	10.0 s
10:21.9	Data point 15	1.50000 mL	0.07084 mL	0.06959 mL	0.02500 mL	4.021	0.03685	0.89652	0.00192	10.0 s
10:43.4	Data point 16	1.50000 mL	0.07084 mL	0.06987 mL	0.02500 mL	4.551	0.06049	0.91743	0.00312	10.0 s
11:10.2	Data point 17	1.50000 mL	0.07084 mL	0.07001 mL	0.02500 mL	4.788	0.09184	0.95650	0.00469	10.5 s
11:32.4	Data point 18	1.50000 mL	0.07084 mL	0.07011 mL	0.02500 mL	5.072	0.09633	0.97713	0.00481	13.5 s
11:57.6	Data point 19	1.50000 mL	0.07084 mL	0.07016 mL	0.02500 mL	5.295	0.09549	0.97449	0.00478	12.5 s
12:21.8	Data point 20	1.50000 mL	0.07084 mL	0.07023 mL	0.02500 mL	5.565	0.04991	0.96241	0.00251	10.0 s
12:43.5	Data point 21	1.50000 mL	0.07084 mL	0.07027 mL	0.02500 mL	5.775	0.02473	0.56978	0.00164	10.0 s
13:00.1	Data point 22	1.50000 mL	0.07084 mL	0.07034 mL	0.02500 mL	6.030	-0.00122	0.00203	0.00134	10.0 s
13:21.6	Data point 23	1.50000 mL	0.07084 mL	0.07041 mL	0.02500 mL	6.247	0.02532	0.48669	0.00180	10.0 s
13:43.3	Data point 24	1.50000 mL	0.07084 mL	0.07051 mL	0.02500 mL	6.499	0.01222	0.17135	0.00146	10.0 s
14:10.2	Data point 25	1.50000 mL	0.07084 mL	0.07060 mL	0.02500 mL	6.707	0.01306	0.27836	0.00124	10.0 s
14:42.3	Data point 26	1.50000 mL	0.07084 mL	0.07072 mL	0.02500 mL	6.953	0.05092	0.71439	0.00300	10.0 s
15:09.1	Data point 27	1.50000 mL	0.07084 mL	0.07081 mL	0.02500 mL	7.161	0.08383	0.84268	0.00451	10.0 s
15:35.7	Data point 28	1.50000 mL	0.07084 mL	0.07088 mL	0.02500 mL	7.456	0.07496	0.77394	0.00420	11.5 s
16:04.0	Data point 29	1.50000 mL	0.07084 mL	0.07095 mL	0.02500 mL	7.826	0.08509	0.82167	0.00469	13.5 s
16:34.5	Data point 30	1.50000 mL	0.07084 mL	0.07103 mL	0.02500 mL	8.239	0.07265	0.70504	0.00432	13.5 s
17:04.8	Data point 31	1.50000 mL	0.07084 mL	0.07110 mL	0.02500 mL	8.591	0.06777	0.70972	0.00397	11.5 s
17:33.1	Data point 32	1.50000 mL	0.07084 mL	0.07117 mL	0.02500 mL	8.835	0.07881	0.81206	0.00432	11.0 s
18:06.1	Data point 33	1.50000 mL	0.07084 mL	0.07126 mL	0.02500 mL	9.058	0.06474	0.87630	0.00342	10.0 s
18:33.0	Data point 34	1.50000 mL	0.07084 mL	0.07138 mL	0.02500 mL	9.300	0.02884	0.79122	0.00160	10.0 s
19:05.0	Data point 35	1.50000 mL	0.07084 mL	0.07152 mL	0.02500 mL	9.525	0.01333	0.62782	0.00083	10.0 s
19:26.7	Data point 36	1.50000 mL	0.07084 mL	0.07168 mL	0.02500 mL	9.725	0.00622	0.17959	0.00073	10.0 s
19:58.5	Data point 37	1.50000 mL	0.07084 mL	0.07194 mL	0.02500 mL	9.931	-0.00266	0.11481	0.00039	10.0 s
20:25.4	Data point 38	1.50000 mL	0.07084 mL	0.07222 mL	0.02500 mL	10.126	-0.00793	0.58188	0.00051	10.0 s
20:42.0	Data point 39	1.50000 mL	0.07084 mL	0.07260 mL	0.02500 mL	10.316	-0.01107	0.92163	0.00057	10.0 s
20:58.7	Data point 40	1.50000 mL	0.07084 mL	0.07314 mL	0.02500 mL	10.484	-0.01598	0.94608	0.00081	10.0 s
21:30.8	Data point 41	1.50000 mL	0.07084 mL	0.07422 mL	0.02500 mL	10.676	-0.01260	0.88860	0.00066	10.0 s
22:07.8	Data point 42	1.50000 mL	0.07084 mL	0.07594 mL	0.02500 mL	10.871	-0.01405	0.89635	0.00074	10.0 s
22:34.9	Data point 43	1.50000 mL	0.07084 mL	0.07829 mL	0.02500 mL	11.061	-0.01459	0.92807	0.00075	10.0 s
23:01.7	Data point 44	1.50000 mL	0.07084 mL	0.08116 mL	0.02500 mL	11.251	-0.01209	0.89220	0.00063	10.0 s
23:18.5	Data point 45	1.50000 mL	0.07084 mL	0.08570 mL	0.02500 mL	11.417	-0.00955	0.91159	0.00049	10.0 s
23:50.9	Data point 46	1.50000 mL	0.07084 mL	0.09393 mL	0.02500 mL	11.614	-0.00899	0.93119	0.00046	10.0 s
24:23.4	Data point 47	1.50000 mL	0.07084 mL	0.10745 mL	0.02500 mL	11.811	-0.00933	0.84361	0.00050	10.0 s
24:50.9	Data point 48	1.50000 mL	0.07084 mL	0.12801 mL	0.02500 mL	12.002	-0.00561	0.69123	0.00033	10.0 s
25:24.0	Data point 49	1.50000 mL	0.07084 mL	0.16409 mL	0.02500 mL	12.201	-0.00522	0.79337	0.00029	10.0 s
27:24.3	Assay volumes	1.75000 mL	0.24443 mL	0.16409 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	1.800			
Maximum pH	12.200			
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				

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Experiment start time: **9/15/2017 11:47:51 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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	No			
ISA water volume	1.50 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			
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	0.112	9/15/2017 11:47:51 PM	C:\Sirius_T3\HCl17I15.t3r
Four-Plus S	1.0006	9/15/2017 11:47:51 PM	C:\Sirius_T3\HCl17I15.t3r
Four-Plus jH	0.7	9/15/2017 11:47:51 PM	C:\Sirius_T3\HCl17I15.t3r
Four-Plus jOH	-0.6	9/15/2017 11:47:51 PM	C:\Sirius_T3\HCl17I15.t3r
Base concentration factor	1.015	9/15/2017 11:47:51 PM	C:\Sirius_T3\KOH17I11.t3r

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Instrument ID: **T311053**

Calibration Settings (continued)

Setting	Value	Date/Time changed	Imported from
Acid concentration factor	1.003	9/15/2017 11:47:51 PM	C:\Sirius_T3\HCl17I15.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 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	8-18-17	9/8/2017 8:22:43 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	166940	9/8/2017 8:21:27 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	01/06/17	9/8/2017 8:20:03 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	8-15-17	9/13/2017 11:23:11 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Phosphate Buffer		9/12/2017 11:32:29 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	9-14-17	9/14/2017 9:30:38 AM
Titrator		T3TM1100153	3/31/2009 5:24:17 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 9:21:54 AM
E0 calibration	-8.33 mV		9/15/2017 11:48:15 PM
Filling solution	3M KCl	KCL095	9/13/2017 8:16:19 AM
Liquids			
Wash 1	50% IPA:50% Water		9/15/2017 8:38:18 AM
Wash 2	0.5% Trition X-100 in H20		9/15/2017 8:38:22 AM
Buffer position 1	pH7 Wash		9/15/2017 8:38:24 AM
Buffer position 2	pH 7		9/15/2017 8:38:27 AM
Storage position			9/15/2017 8:38:55 AM
Wash water	3.6e+003 mL	9-11-17	9/11/2017 3:28:43 PM
Waste	6.5e+003 mL		9/11/2017 3:28:49 PM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		072390	11/23/2010 11:22:28 AM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		

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Assay name: **UV-metric pKa**
Assay ID: **17I-16002**
Filename: **C:\Sirius_T3\17I-16002_M07_UV-metric pKa.t3r**

Experiment start time: **9/15/2017 11:47:51 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	114:03:31		11/23/2010 11:22:28 AM
Calibrated on	9/6/2017 8:33:02 AM		
Integration time	11		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 9:34:13 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