Yasuda-Shedlovsky Result

Sample name: **D09**	Experiment start time: **10/6/2017 9:09:14 AM**
Assay name: **UV-metric psKa**	Analyst: **Dorothy Levorse**
Assay ID: **17J-06008**	Instrument ID: **T311053**
Filename: **C:\Sirius_T3\17J-06008_D09_UV-metric psKa.t3r**	

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	2.58	±0.06	7.21	-226.8392	0.9949	0.165 M	24.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
17J-06008 Points 4 to 27	49.51 %	Up	UV-metric pKa	56.6	24.7 M	0.158 M	24.9°C	☑	1.83
17J-06008 Points 29 to 66	40.03 %	Up	UV-metric pKa	61.0	30.0 M	0.166 M	24.9°C	☑	1.99
17J-06008 Points 68 to 111	30.18 %	Up	UV-metric pKa	65.5	35.8 M	0.172 M	24.9°C	☑	2.21

Graphs

Yasuda-Shedlovsky extrapolation

pKa 1 : 0% Solvent at 24.9°C

Distribution of Species - Yasuda-Shedlovsky Extrapolation

Mean Molar Extinction Profiles

UV-metric psKa   Titration 1 of 3   17J-06008 Points 4 to 27

Results

pKa 1	**1.83**
RMSD	**0.001 0.002**
Chi squared	**0.0018**
PCA calculated number of pKas	**2**
Average ionic strength	**0.158 M**
Average temperature	**24.9°C**
Analyte concentration range	**29.5 µM to 27.8 µM**
Methanol weight %	**49.5 %**
Dielectric constant	**56.6**
Water concentration	**24.7 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**

Sample name: **D09**
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Experiment start time: **10/6/2017 9:09:14 AM**
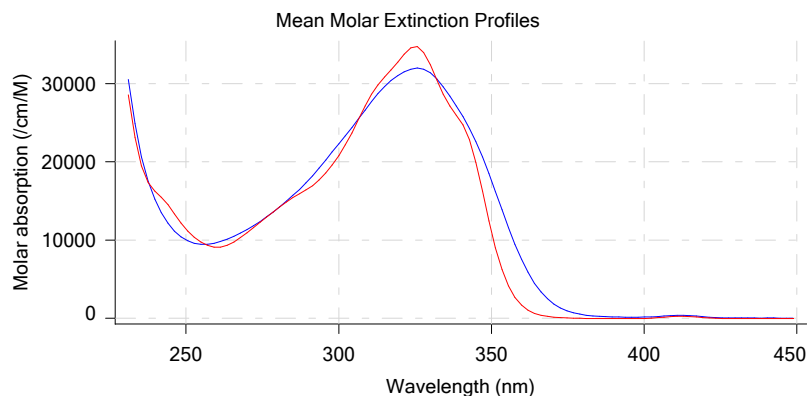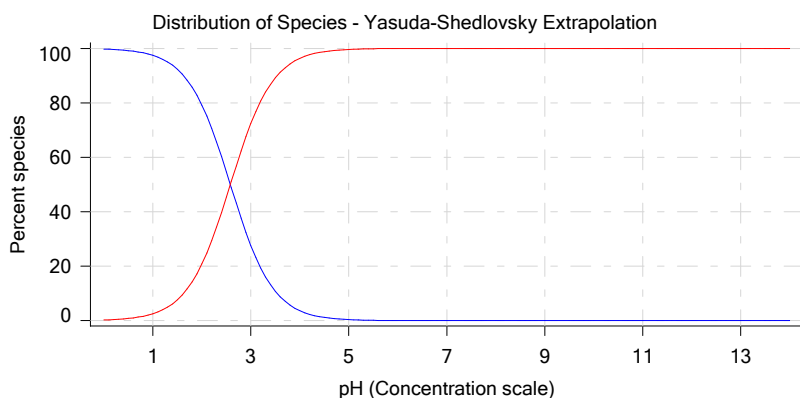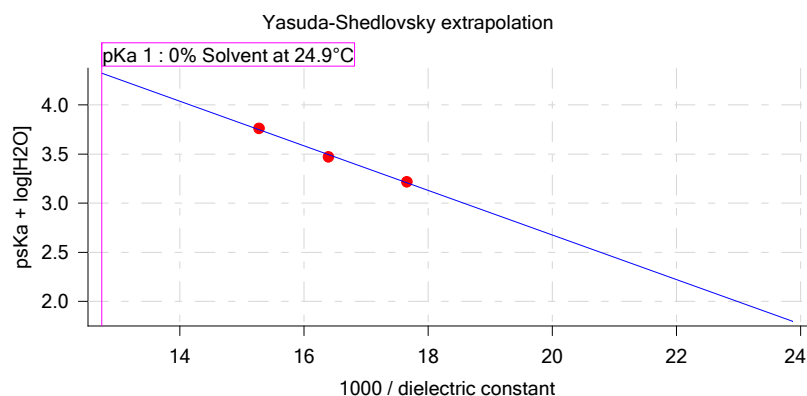Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Results (continued)
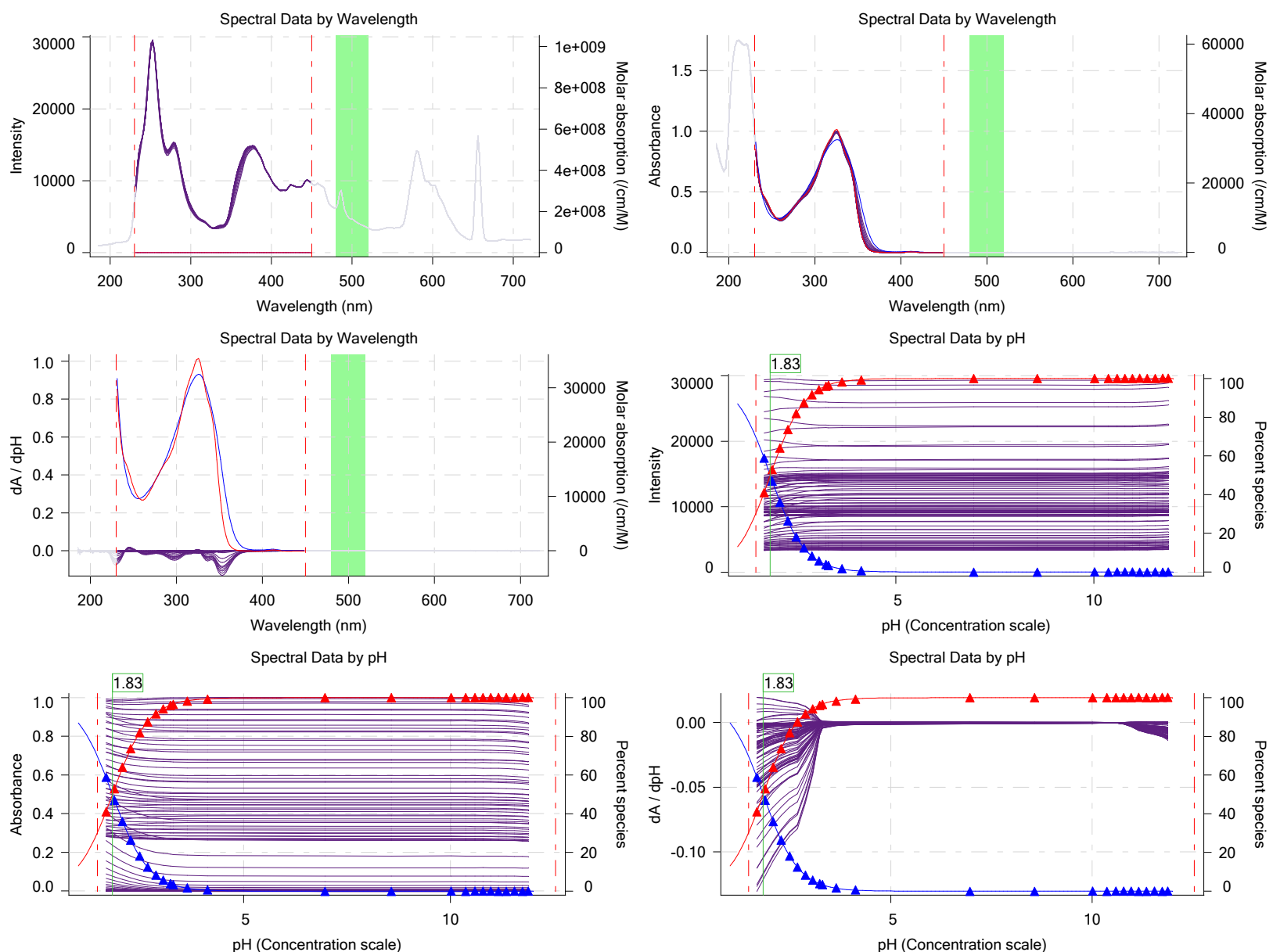
pH clipping **1.464 to 12.544**

Warnings and errors

Errors   None
Warnings   PCA calculation disagrees with predicted number of pKas

Assay Settings

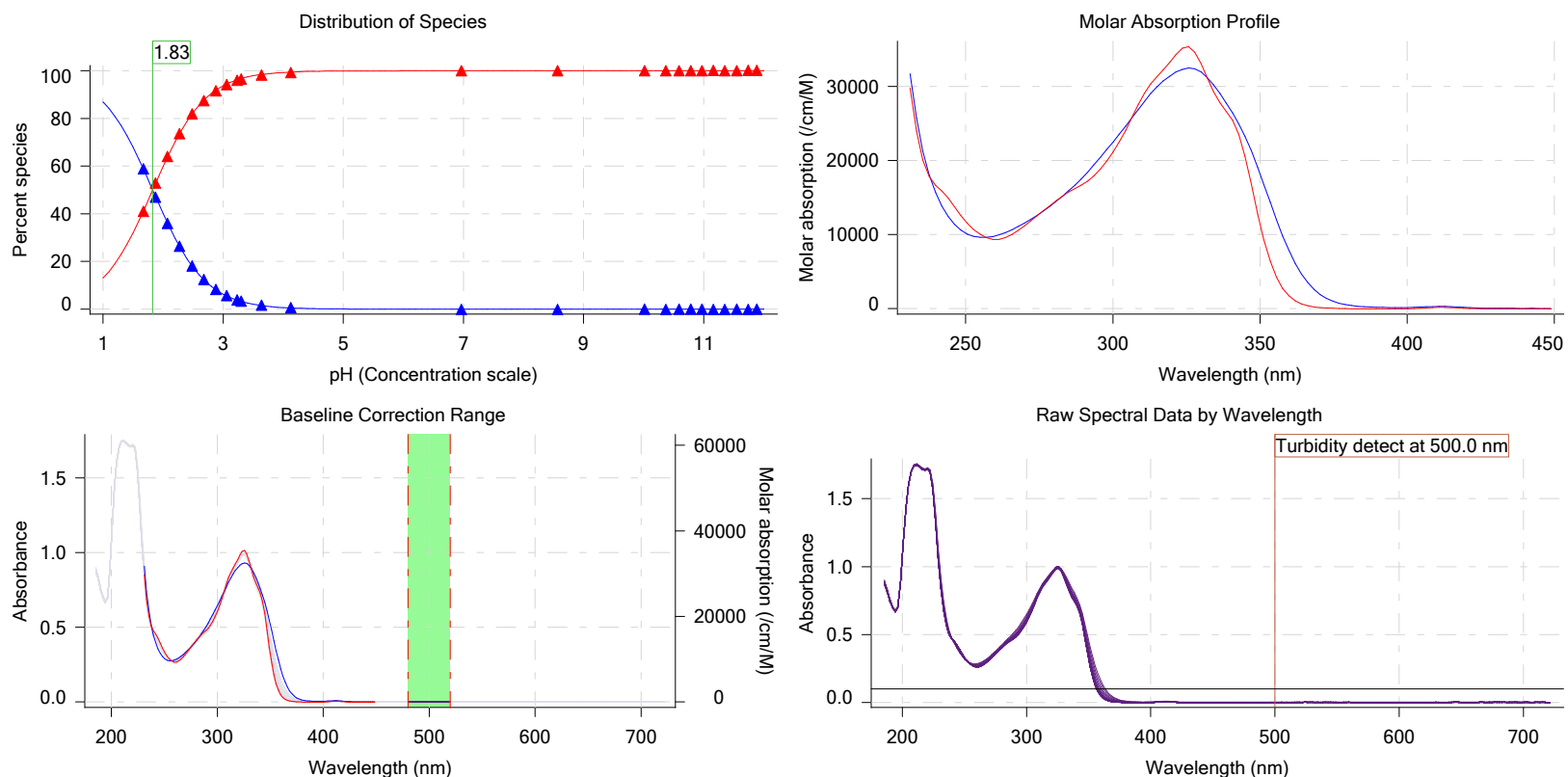| Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

Graphs

Sample name: **D09**
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Experiment start time: **10/6/2017 9:09:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)

Distribution of Species

Molar Absorption Profile

Baseline Correction Range

Raw Spectral Data by Wavelength

UV-metric psKa   Titration 2 of 3   17J-06008 Points 29 to 66

Results

pKa 1	**1.99**
RMSD	**0.001 0.001**
Chi squared	**0.0027**
PCA calculated number of pKas	**4**
Average ionic strength	**0.166 M**
Average temperature	**24.9°C**
Analyte concentration range	**24.2 µM to 22.9 µM**
Methanol weight %	**40.0 %**
Dielectric constant	**61.0**
Water concentration	**30.0 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.515 to 12.540**

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: **D09**
Assay name: **UV-metric psKa**
Assay ID: **17J-06008**
Filename: **C:\Sirius_T3\17J-06008_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 9:09:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

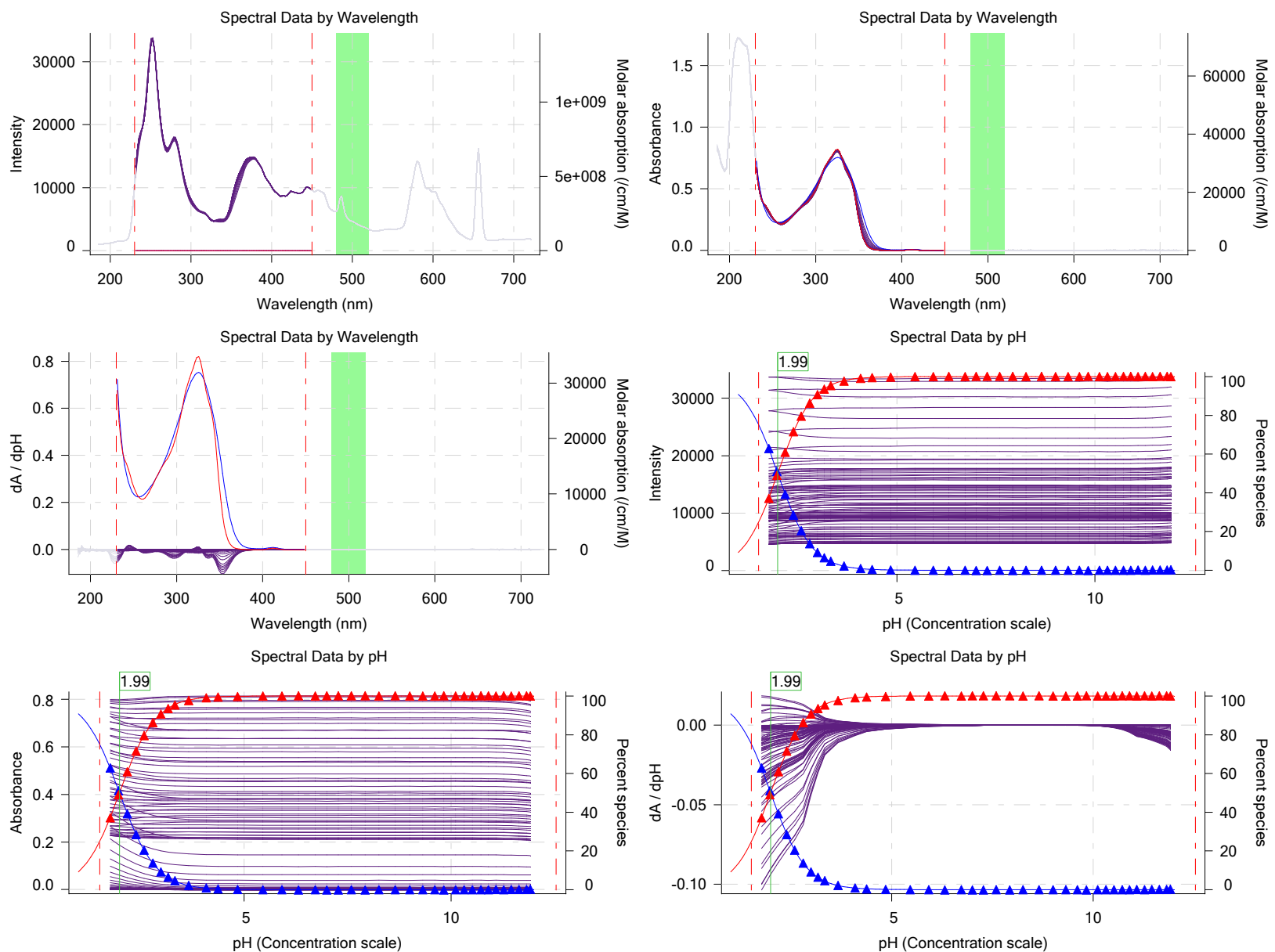| Setting	Value	Original Value	Date/Time changed	Imported from
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

Graphs

Sample name: **D09**
Assay name: **UV-metric psKa**
Assay ID: **17J-06008**
Filename: **C:\Sirius_T3\17J-06008_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 9:09:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)

Distribution of Species

Molar Absorption Profile

Baseline Correction Range

Raw Spectral Data by Wavelength

UV-metric psKa   Titration 3 of 3   17J-06008 Points 68 to 111

Results

pKa 1	**2.21**
RMSD	**0.002 0.001**
Chi squared	**0.0028**
PCA calculated number of pKas	**3**
Average ionic strength	**0.172 M**
Average temperature	**24.9°C**
Analyte concentration range	**18.7 µM to 17.7 µM**
Methanol weight %	**30.2 %**
Dielectric constant	**65.5**
Water concentration	**35.8 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.518 to 12.540**

Warnings and errors

Errors   None
Warnings   PCA calculation disagrees with predicted number of pKas

Assay Settings

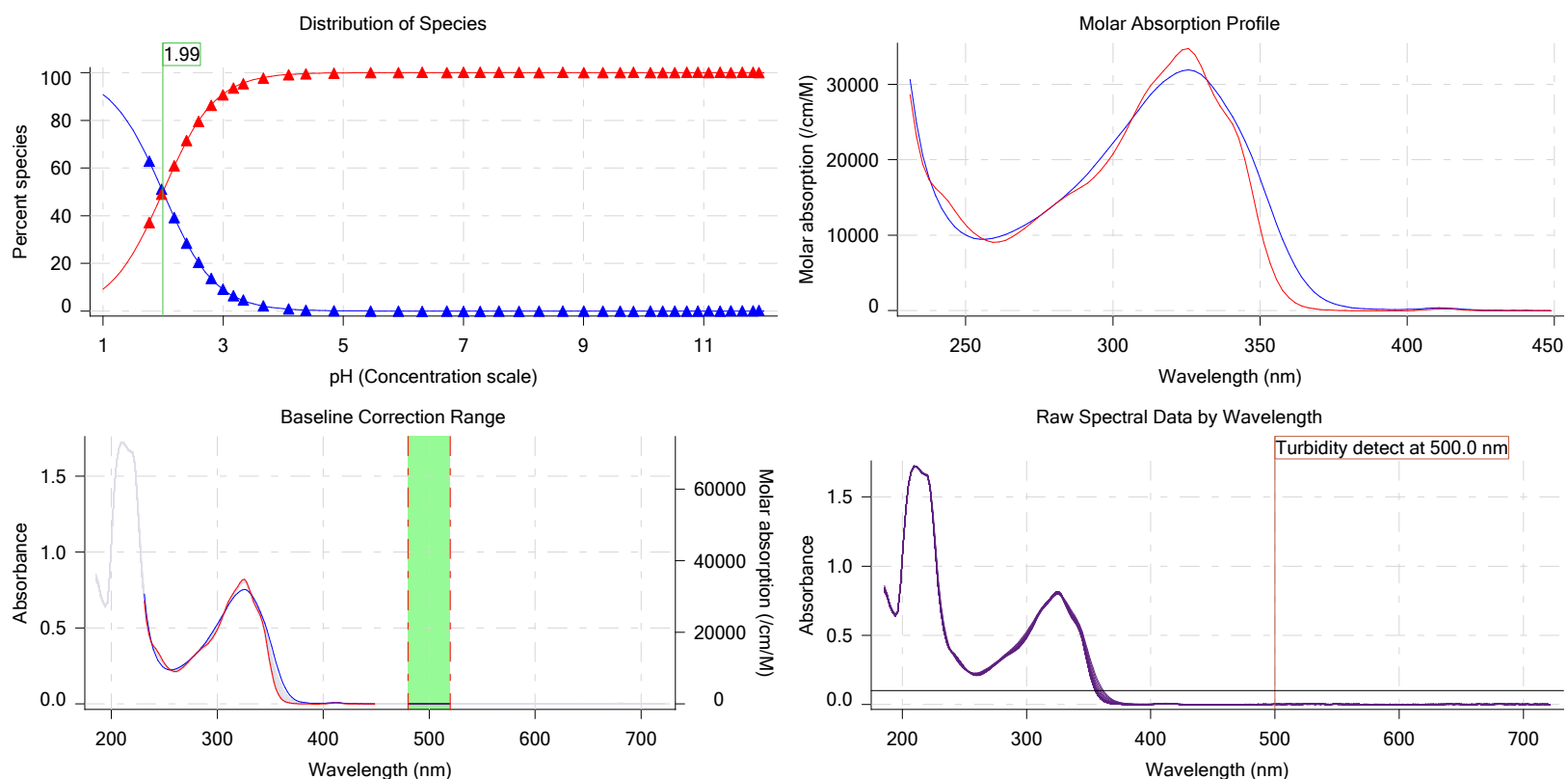| Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				

Sample name: **D09**
Assay name: **UV-metric psKa**
Assay ID: **17J-06008**
Filename: **C:\Sirius_T3\17J-06008_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 9:09:14 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

Spectral Data by Wavelength

Spectral Data by Wavelength

Spectral Data by Wavelength

Spectral Data by pH

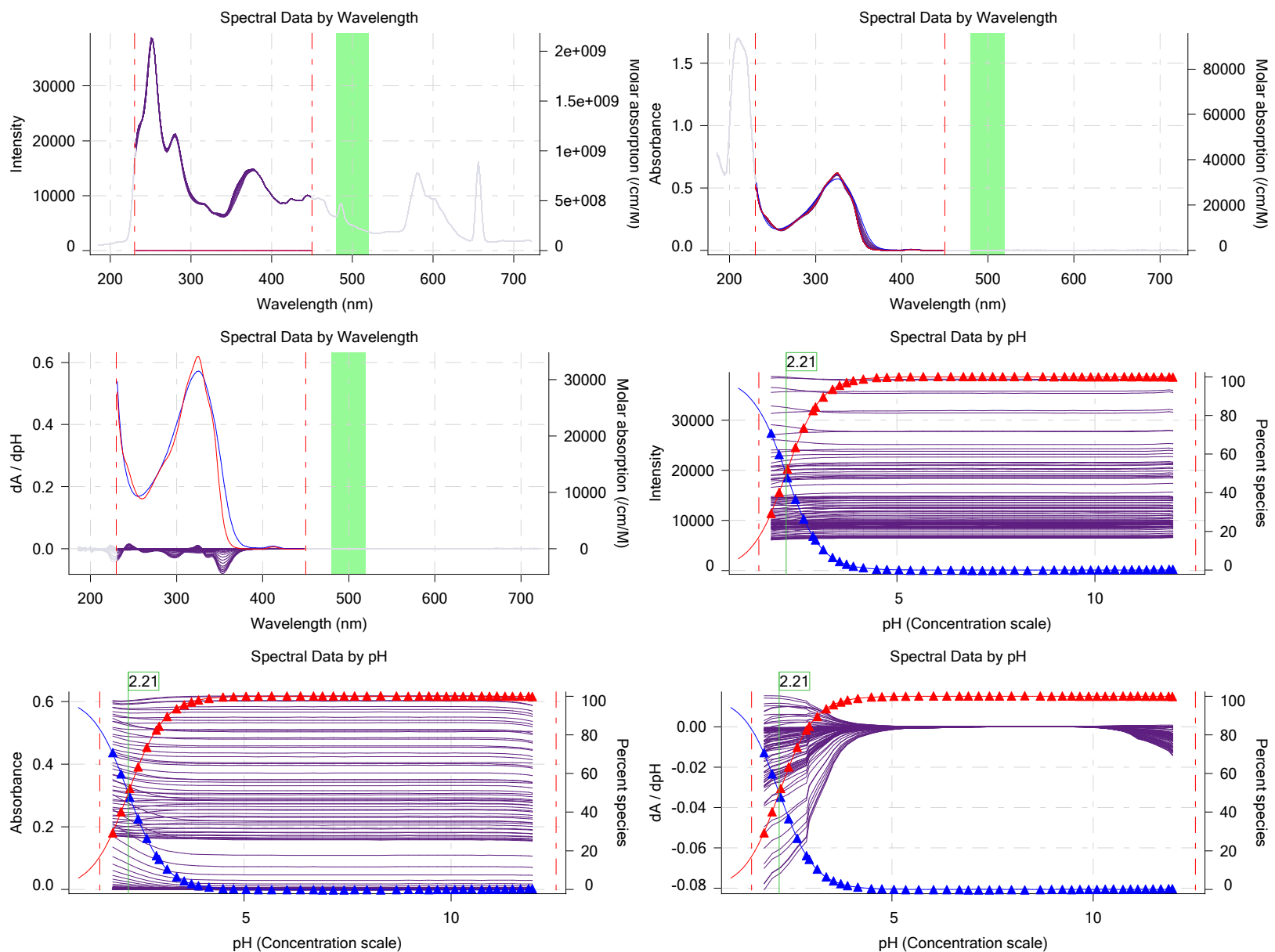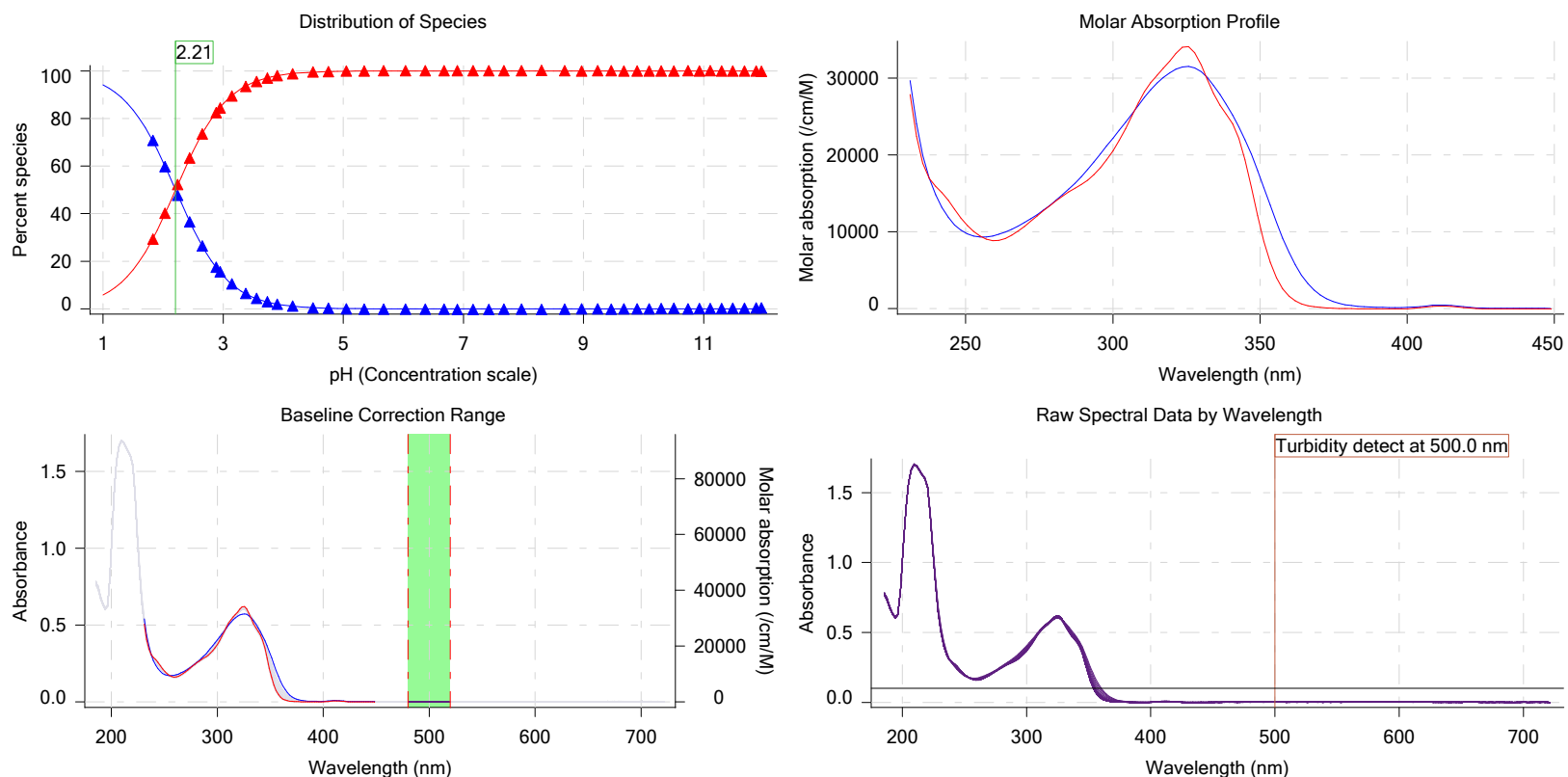Spectral Data by pH

Spectral Data by pH

Sample name: **D09**
Assay name: **UV-metric psKa**
Assay ID: **17J-06008**
Filename: **C:\Sirius_T3\17J-06008_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 9:09:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)

Distribution of Species

Molar Absorption Profile

Baseline Correction Range

Raw Spectral Data by Wavelength

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	D09	10/2/2017 11:57:35 AM	User entered value
Sample by	Volume		Default value
Sample volume	0.0015 mL	10/5/2017 3:30:01 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.031400 M	10/2/2017 11:59:31 AM	User entered value
Solubility	Unknown		Default value
Molecular weight	391.42	9/29/2017 5:41:30 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	9/29/2017 5:41:11 PM	User entered value
Sample is a	Base	9/29/2017 5:41:11 PM	User entered value
pKa 1	4.74	9/29/2017 5:41:11 PM	User entered value
logp (XH +)	-10.00		Default value
logP (neutral X)	-10.00	9/29/2017 5:41:11 PM	User entered value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:42.5	Dark spectrum								
3:43.9	Reference spectrum								
4:11.5	Volume reset due to vial change								
4:55.6	Initial pH = 8.37								
6:04.4	Data point 4	0.34995 mL	0.06912 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.964	-0.01609	0.86130
6:33.2	Data point 5	0.34995 mL	0.06912 mL	0.02493 mL	1.15005 mL	0.02500 mL	2.161	-0.00379	0.22209
6:50.2	Data point 6	0.34995 mL	0.06912 mL	0.04083 mL	1.15005 mL	0.02500 mL	2.355	0.03157	0.92164
7:07.0	Data point 7	0.34995 mL	0.06912 mL	0.05089 mL	1.15005 mL	0.02500 mL	2.551	0.02550	0.91609
7:23.7	Data point 8	0.34995 mL	0.06912 mL	0.05734 mL	1.15005 mL	0.02500 mL	2.761	0.01805	0.91638
7:40.4	Data point 9	0.34995 mL	0.06912 mL	0.06131 mL	1.15005 mL	0.02500 mL	2.954	0.01875	0.92905

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Experiment start time: **10/6/2017 9:09:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
7:57.0	Data point 10	0.34995 mL	0.06912 mL	0.06385 mL	1.15005 mL	0.02500 mL	3.151	0.02292	0.96725	0.00
8:13.6	Data point 11	0.34995 mL	0.06912 mL	0.06545 mL	1.15005 mL	0.02500 mL	3.328	0.03872	0.92382	0.00
8:30.1	Data point 12	0.34995 mL	0.06912 mL	0.06651 mL	1.15005 mL	0.02500 mL	3.499	0.04154	0.97486	0.00
8:46.6	Data point 13	0.34995 mL	0.06912 mL	0.06722 mL	1.15005 mL	0.02500 mL	3.566	0.05839	0.95736	0.00
9:08.3	Data point 14	0.34995 mL	0.06912 mL	0.06839 mL	1.15005 mL	0.02500 mL	3.903	0.09831	0.99104	0.00
9:34.4	Data point 15	0.34995 mL	0.06912 mL	0.06891 mL	1.15005 mL	0.02500 mL	4.382	0.09888	0.99120	0.00
10:30.8	Data point 16	0.34995 mL	0.06912 mL	0.06950 mL	1.15005 mL	0.02500 mL	7.191	0.08887	0.90891	0.00
11:50.8	Data point 17	0.34995 mL	0.06912 mL	0.07001 mL	1.15005 mL	0.02500 mL	8.778	0.19196	0.99612	0.00
13:17.8	Data point 18	0.34995 mL	0.06912 mL	0.07048 mL	1.15005 mL	0.02500 mL	10.210	0.09659	0.97959	0.00
13:53.6	Data point 19	0.34995 mL	0.06912 mL	0.07095 mL	1.15005 mL	0.02500 mL	10.557	0.09596	0.96115	0.00
14:19.3	Data point 20	0.34995 mL	0.06912 mL	0.07152 mL	1.15005 mL	0.02500 mL	10.777	0.04804	0.90264	0.00
14:36.0	Data point 21	0.34995 mL	0.06912 mL	0.07241 mL	1.15005 mL	0.02500 mL	10.969	0.02265	0.91127	0.00
14:52.6	Data point 22	0.34995 mL	0.06912 mL	0.07380 mL	1.15005 mL	0.02500 mL	11.153	0.00300	0.24716	0.00
15:09.3	Data point 23	0.34995 mL	0.06912 mL	0.07592 mL	1.15005 mL	0.02500 mL	11.340	-0.00241	0.27355	0.00
15:25.8	Data point 24	0.34995 mL	0.06912 mL	0.07919 mL	1.15005 mL	0.02500 mL	11.526	0.00024	0.00435	0.00
15:42.5	Data point 25	0.34995 mL	0.06912 mL	0.08424 mL	1.15005 mL	0.02500 mL	11.721	-0.00751	0.70887	0.00
15:59.2	Data point 26	0.34995 mL	0.06912 mL	0.09233 mL	1.15005 mL	0.02500 mL	11.908	0.00256	0.05338	0.00
16:16.0	Data point 27	0.34995 mL	0.06912 mL	0.10071 mL	1.15005 mL	0.02500 mL	12.044	-0.00474	0.51580	0.00
17:52.2	Reference spectrum									
18:56.1	Data point 29	0.50000 mL	0.16595 mL	0.10073 mL	1.15005 mL	0.02500 mL	2.015	-0.04738	0.92455	0.00
19:23.6	Data point 30	0.50000 mL	0.16595 mL	0.12444 mL	1.15005 mL	0.02500 mL	2.213	0.00668	0.61846	0.00
19:40.6	Data point 31	0.50000 mL	0.16595 mL	0.13982 mL	1.15005 mL	0.02500 mL	2.419	0.01045	0.60319	0.00
19:57.4	Data point 32	0.50000 mL	0.16595 mL	0.14944 mL	1.15005 mL	0.02500 mL	2.625	0.00090	0.01332	0.00
20:14.2	Data point 33	0.50000 mL	0.16595 mL	0.15539 mL	1.15005 mL	0.02500 mL	2.820	0.02466	0.82507	0.00
20:31.0	Data point 34	0.50000 mL	0.16595 mL	0.15917 mL	1.15005 mL	0.02500 mL	3.030	0.00649	0.42170	0.00
20:47.6	Data point 35	0.50000 mL	0.16595 mL	0.16148 mL	1.15005 mL	0.02500 mL	3.222	0.01370	0.88874	0.00
21:04.2	Data point 36	0.50000 mL	0.16595 mL	0.16296 mL	1.15005 mL	0.02500 mL	3.393	0.01307	0.87294	0.00
21:20.9	Data point 37	0.50000 mL	0.16595 mL	0.16395 mL	1.15005 mL	0.02500 mL	3.556	0.02447	0.93527	0.00
21:42.7	Data point 38	0.50000 mL	0.16595 mL	0.16526 mL	1.15005 mL	0.02500 mL	3.885	0.03007	0.96171	0.00
22:04.3	Data point 39	0.50000 mL	0.16595 mL	0.16587 mL	1.15005 mL	0.02500 mL	4.303	0.07572	0.98283	0.00
22:26.0	Data point 40	0.50000 mL	0.16595 mL	0.16613 mL	1.15005 mL	0.02500 mL	4.587	0.09824	0.98871	0.00
23:05.8	Data point 41	0.50000 mL	0.16595 mL	0.16634 mL	1.15005 mL	0.02500 mL	5.053	0.09796	0.98183	0.00
24:05.7	Data point 42	0.50000 mL	0.16595 mL	0.16644 mL	1.15005 mL	0.02500 mL	5.656	0.09996	0.98667	0.00
25:15.9	Data point 43	0.50000 mL	0.16595 mL	0.16651 mL	1.15005 mL	0.02500 mL	6.113	0.10039	0.99187	0.00
26:22.2	Data point 44	0.50000 mL	0.16595 mL	0.16658 mL	1.15005 mL	0.02500 mL	6.507	0.09893	0.98901	0.00
27:11.4	Data point 45	0.50000 mL	0.16595 mL	0.16667 mL	1.15005 mL	0.02500 mL	6.913	0.10063	0.98956	0.00
27:48.3	Data point 46	0.50000 mL	0.16595 mL	0.16677 mL	1.15005 mL	0.02500 mL	7.187	0.09753	0.97522	0.00
28:28.8	Data point 47	0.50000 mL	0.16595 mL	0.16689 mL	1.15005 mL	0.02500 mL	7.459	0.10045	0.98899	0.00
29:06.7	Data point 48	0.50000 mL	0.16595 mL	0.16700 mL	1.15005 mL	0.02500 mL	7.772	0.09878	0.98556	0.00
29:48.0	Data point 49	0.50000 mL	0.16595 mL	0.16710 mL	1.15005 mL	0.02500 mL	8.101	0.09733	0.96752	0.00
30:24.8	Data point 50	0.50000 mL	0.16595 mL	0.16717 mL	1.15005 mL	0.02500 mL	8.429	0.09964	0.97005	0.00
31:09.1	Data point 51	0.50000 mL	0.16595 mL	0.16724 mL	1.15005 mL	0.02500 mL	8.822	0.09813	0.96851	0.00
31:49.5	Data point 52	0.50000 mL	0.16595 mL	0.16731 mL	1.15005 mL	0.02500 mL	9.168	0.09759	0.98936	0.00
32:32.1	Data point 53	0.50000 mL	0.16595 mL	0.16740 mL	1.15005 mL	0.02500 mL	9.482	0.09858	0.97035	0.00
32:59.7	Data point 54	0.50000 mL	0.16595 mL	0.16752 mL	1.15005 mL	0.02500 mL	9.767	0.09392	0.93006	0.00
33:27.4	Data point 55	0.50000 mL	0.16595 mL	0.16766 mL	1.15005 mL	0.02500 mL	9.986	0.07180	0.95217	0.00
33:44.0	Data point 56	0.50000 mL	0.16595 mL	0.16787 mL	1.15005 mL	0.02500 mL	10.266	0.01792	0.93639	0.00
34:16.2	Data point 57	0.50000 mL	0.16595 mL	0.16834 mL	1.15005 mL	0.02500 mL	10.468	0.00468	0.35720	0.00
34:48.1	Data point 58	0.50000 mL	0.16595 mL	0.16900 mL	1.15005 mL	0.02500 mL	10.666	0.00181	0.12449	0.00
35:04.7	Data point 59	0.50000 mL	0.16595 mL	0.16997 mL	1.15005 mL	0.02500 mL	10.867	-0.00413	0.54026	0.00
35:21.4	Data point 60	0.50000 mL	0.16595 mL	0.17147 mL	1.15005 mL	0.02500 mL	11.048	-0.00808	0.75855	0.00
35:38.1	Data point 61	0.50000 mL	0.16595 mL	0.17378 mL	1.15005 mL	0.02500 mL	11.227	-0.01003	0.85193	0.00
35:54.7	Data point 62	0.50000 mL	0.16595 mL	0.17723 mL	1.15005 mL	0.02500 mL	11.411	-0.01094	0.90092	0.00
36:11.4	Data point 63	0.50000 mL	0.16595 mL	0.18257 mL	1.15005 mL	0.02500 mL	11.589	-0.01443	0.86365	0.00
36:28.2	Data point 64	0.50000 mL	0.16595 mL	0.19073 mL	1.15005 mL	0.02500 mL	11.773	-0.00975	0.82764	0.00
36:45.1	Data point 65	0.50000 mL	0.16595 mL	0.20341 mL	1.15005 mL	0.02500 mL	11.949	-0.00912	0.79476	0.00
37:01.7	Data point 66	0.50000 mL	0.16595 mL	0.21223 mL	1.15005 mL	0.02500 mL	12.040	-0.01524	0.88425	0.00

Sample name: **D09**
Assay name: **UV-metric psKa**
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Filename: **C:\Sirius_T3\17J-06008_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 9:09:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
38:46.7	Reference spectrum									
40:09.9	Data point 68	0.83996 mL	0.29621 mL	0.21225 mL	1.15005 mL	0.02500 mL	2.018	-0.02376	0.92739	0.
40:37.4	Data point 69	0.83996 mL	0.29621 mL	0.23876 mL	1.15005 mL	0.02500 mL	2.214	0.01282	0.74048	0.
40:54.4	Data point 70	0.83996 mL	0.29621 mL	0.25628 mL	1.15005 mL	0.02500 mL	2.423	0.00828	0.44148	0.
41:11.3	Data point 71	0.83996 mL	0.29621 mL	0.26710 mL	1.15005 mL	0.02500 mL	2.620	-0.01671	0.37820	0.
41:28.0	Data point 72	0.83996 mL	0.29621 mL	0.27397 mL	1.15005 mL	0.02500 mL	2.828	-0.00608	0.64601	0.
42:00.3	Data point 73	0.83996 mL	0.29621 mL	0.27820 mL	1.15005 mL	0.02500 mL	3.057	0.00353	0.34434	0.
42:16.9	Data point 74	0.83996 mL	0.29621 mL	0.28067 mL	1.15005 mL	0.02500 mL	3.122	0.00275	0.30774	0.
42:38.6	Data point 75	0.83996 mL	0.29621 mL	0.28271 mL	1.15005 mL	0.02500 mL	3.317	-0.00176	0.08259	0.
42:55.2	Data point 76	0.83996 mL	0.29621 mL	0.28408 mL	1.15005 mL	0.02500 mL	3.543	0.00202	0.02570	0.
43:11.7	Data point 77	0.83996 mL	0.29621 mL	0.28488 mL	1.15005 mL	0.02500 mL	3.721	0.00263	0.14055	0.
43:28.3	Data point 78	0.83996 mL	0.29621 mL	0.28542 mL	1.15005 mL	0.02500 mL	3.898	0.00353	0.23098	0.
43:44.9	Data point 79	0.83996 mL	0.29621 mL	0.28577 mL	1.15005 mL	0.02500 mL	4.065	0.01689	0.87069	0.
44:06.5	Data point 80	0.83996 mL	0.29621 mL	0.28612 mL	1.15005 mL	0.02500 mL	4.315	0.04798	0.93421	0.
44:28.2	Data point 81	0.83996 mL	0.29621 mL	0.28638 mL	1.15005 mL	0.02500 mL	4.651	0.07034	0.96728	0.
44:49.9	Data point 82	0.83996 mL	0.29621 mL	0.28652 mL	1.15005 mL	0.02500 mL	4.907	0.09406	0.94367	0.
45:18.5	Data point 83	0.83996 mL	0.29621 mL	0.28662 mL	1.15005 mL	0.02500 mL	5.204	0.09917	0.99382	0.
45:53.5	Data point 84	0.83996 mL	0.29621 mL	0.28669 mL	1.15005 mL	0.02500 mL	5.497	0.09644	0.93676	0.
46:31.2	Data point 85	0.83996 mL	0.29621 mL	0.28676 mL	1.15005 mL	0.02500 mL	5.817	0.09548	0.93897	0.
47:12.8	Data point 86	0.83996 mL	0.29621 mL	0.28685 mL	1.15005 mL	0.02500 mL	6.182	0.00850	0.04370	0.
47:34.4	Data point 87	0.83996 mL	0.29621 mL	0.28695 mL	1.15005 mL	0.02500 mL	6.505	-0.04813	0.60332	0.
47:56.0	Data point 88	0.83996 mL	0.29621 mL	0.28707 mL	1.15005 mL	0.02500 mL	6.818	-0.05306	0.54919	0.
48:22.8	Data point 89	0.83996 mL	0.29621 mL	0.28718 mL	1.15005 mL	0.02500 mL	7.036	0.07330	0.92151	0.
48:54.7	Data point 90	0.83996 mL	0.29621 mL	0.28732 mL	1.15005 mL	0.02500 mL	7.293	0.09292	0.93029	0.
49:33.1	Data point 91	0.83996 mL	0.29621 mL	0.28747 mL	1.15005 mL	0.02500 mL	7.553	0.09885	0.96936	0.
50:08.5	Data point 92	0.83996 mL	0.29621 mL	0.28758 mL	1.15005 mL	0.02500 mL	7.803	0.09709	0.96489	0.
50:46.8	Data point 93	0.83996 mL	0.29621 mL	0.28770 mL	1.15005 mL	0.02500 mL	8.096	0.09742	0.97677	0.
51:32.0	Data point 94	0.83996 mL	0.29621 mL	0.28779 mL	1.15005 mL	0.02500 mL	8.423	0.09473	0.94304	0.
52:18.2	Data point 95	0.83996 mL	0.29621 mL	0.28791 mL	1.15005 mL	0.02500 mL	8.805	0.09169	0.94413	0.
53:00.5	Data point 96	0.83996 mL	0.29621 mL	0.28803 mL	1.15005 mL	0.02500 mL	9.087	0.09683	0.97010	0.
53:35.7	Data point 97	0.83996 mL	0.29621 mL	0.28815 mL	1.15005 mL	0.02500 mL	9.351	0.09850	0.96983	0.
54:07.9	Data point 98	0.83996 mL	0.29621 mL	0.28831 mL	1.15005 mL	0.02500 mL	9.576	0.09618	0.96754	0.
54:35.2	Data point 99	0.83996 mL	0.29621 mL	0.28862 mL	1.15005 mL	0.02500 mL	9.784	0.06374	0.95433	0.
55:07.0	Data point 100	0.83996 mL	0.29621 mL	0.28920 mL	1.15005 mL	0.02500 mL	10.000	0.03155	0.95343	0.
55:39.0	Data point 101	0.83996 mL	0.29621 mL	0.28961 mL	1.15005 mL	0.02500 mL	10.198	0.01997	0.85406	0.
56:05.7	Data point 102	0.83996 mL	0.29621 mL	0.29017 mL	1.15005 mL	0.02500 mL	10.401	-0.00113	0.05107	0.
56:22.3	Data point 103	0.83996 mL	0.29621 mL	0.29097 mL	1.15005 mL	0.02500 mL	10.605	-0.01868	0.82537	0.
56:38.8	Data point 104	0.83996 mL	0.29621 mL	0.29224 mL	1.15005 mL	0.02500 mL	10.841	-0.02077	0.91357	0.
57:05.8	Data point 105	0.83996 mL	0.29621 mL	0.29419 mL	1.15005 mL	0.02500 mL	11.029	-0.01197	0.86448	0.
57:22.6	Data point 106	0.83996 mL	0.29621 mL	0.29753 mL	1.15005 mL	0.02500 mL	11.207	-0.02108	0.91807	0.
57:39.2	Data point 107	0.83996 mL	0.29621 mL	0.30256 mL	1.15005 mL	0.02500 mL	11.395	-0.02076	0.93747	0.
57:56.0	Data point 108	0.83996 mL	0.29621 mL	0.31042 mL	1.15005 mL	0.02500 mL	11.577	-0.02447	0.89468	0.
58:12.9	Data point 109	0.83996 mL	0.29621 mL	0.32255 mL	1.15005 mL	0.02500 mL	11.766	-0.02604	0.94446	0.
58:30.0	Data point 110	0.83996 mL	0.29621 mL	0.34179 mL	1.15005 mL	0.02500 mL	11.953	-0.02504	0.94492	0.
58:46.8	Data point 111	0.83996 mL	0.29621 mL	0.35503 mL	1.15005 mL	0.02500 mL	12.040	-0.01997	0.91781	0.
1:00:46.4	Assay volumes	1.08996 mL	0.44266 mL	0.35503 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			

Sample name: **D09**
Assay name: **UV-metric psKa**
Assay ID: **17J-06008**
Filename: **C:\Sirius_T3\17J-06008_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 9:09:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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				
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			

Sample name: **D09**
Assay name: **UV-metric psKa**
Assay ID: **17J-06008**
Filename: **C:\Sirius_T3\17J-06008_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 9:09:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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	0.125	10/6/2017 9:09:14 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus S	0.9949	10/6/2017 9:09:14 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jH	0.8	10/6/2017 9:09:14 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jOH	-1.3	10/6/2017 9:09:14 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Base concentration factor	1.011	10/6/2017 9:09:14 AM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	1.003	10/6/2017 9:09:14 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.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	9/26/2017 8:05:04 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)	9-22-17	9/22/2017 3:02:42 PM
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)	9-26-17	10/5/2017 4:02:03 PM
Port B	Cyclohexane		9/19/2017 1:15:02 PM
Port C	MeCN (50%, 0.15 M KCl)	10-2-17	10/2/2017 10:28:55 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)		

Sample name: **D09**
Assay name: **UV-metric psKa**
Assay ID: **17J-06008**
Filename: **C:\Sirius_T3\17J-06008_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 9:09:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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	-9.26 mV		10/6/2017 9:09:38 AM
Filling solution	3M KCI	KCL095	10/4/2017 2:50:10 PM
Liquids			
Wash 1	50% IPA:50% Water		10/5/2017 8:59:12 AM
Wash 2	0.5% Trition X-100 in H20		10/5/2017 8:59:14 AM
Buffer position 1	pH7 Wash		10/5/2017 8:59:17 AM
Buffer position 2	pH 7		10/5/2017 8:59:19 AM
Storage position			10/5/2017 8:58:45 AM
Wash water	4.2e+003 mL	10-3-17	10/3/2017 8:04:49 AM
Waste	5.9e+003 mL		10/3/2017 8:04:54 AM
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		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	366:44:47		11/23/2010 11:22:28 AM
Calibrated on	10/5/2017 9:23:25 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%		

Sample name: **D09**
Assay name: **UV-metric psKa**
Assay ID: **17J-06008**
Filename: **C:\Sirius_T3\17J-06008_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 9:09:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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   F3