

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07007**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07007_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 10:32:05 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

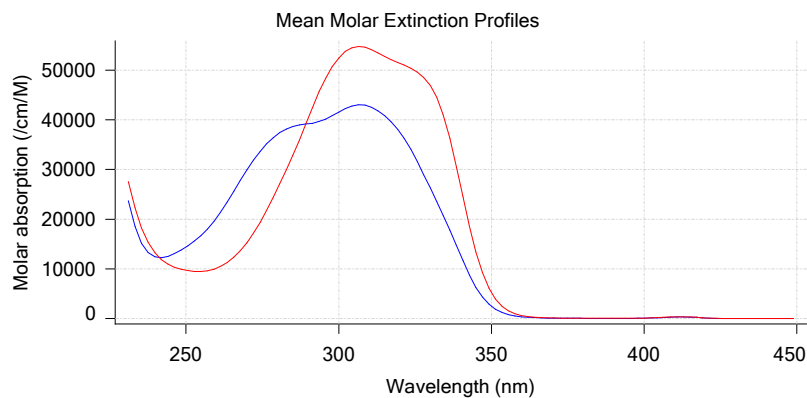
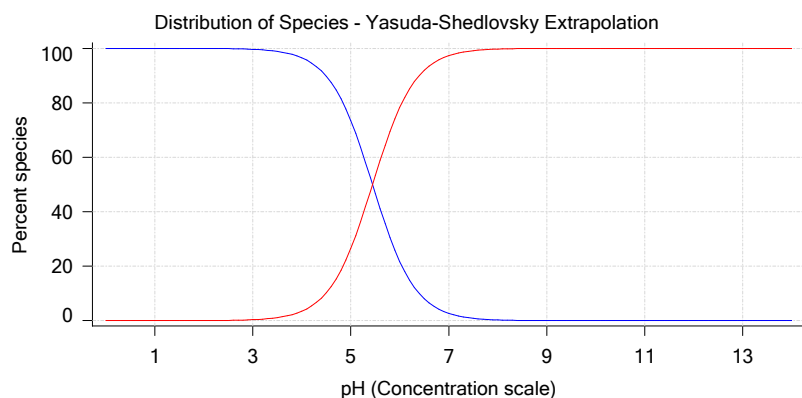
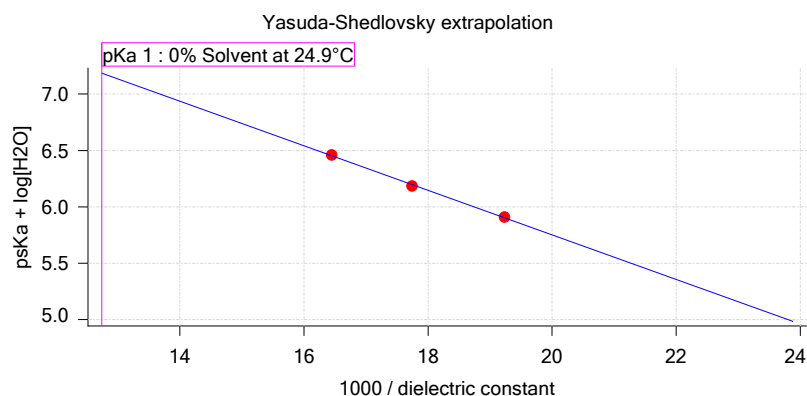
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.44	±0.05	9.70	-197.7237	0.9981	0.166 M	24.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1
17J-07007 Points 4 to 70	59.29 %	Up	UV-metric pKa	52.0	19.5 M	0.157 M	24.9°C	✓ 4.62
17J-07007 Points 72 to 139	50.03 %	Up	UV-metric pKa	56.4	24.4 M	0.167 M	24.9°C	✓ 4.80
17J-07007 Points 141 to 217	40.47 %	Up	UV-metric pKa	60.8	29.7 M	0.174 M	24.9°C	✓ 4.99

Graphs



UV-metric psKa Titration 1 of 3 17J-07007 Points 4 to 70

Results

pKa 1	4.62
RMSD	0.002 0.001
Chi squared	0.0075
PCA calculated number of pKas	3
Average ionic strength	0.157 M
Average temperature	24.9°C
Analyte concentration range	29.3 µM to 27.6 µM
Methanol weight %	59.3 %
Dielectric constant	52.0
Water concentration	19.5 M
Number of pKas source	Predicted
Wavelength clipping	230.0 nm to 450.0 nm

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Results (continued)

pH clipping 1.456 to 12.552

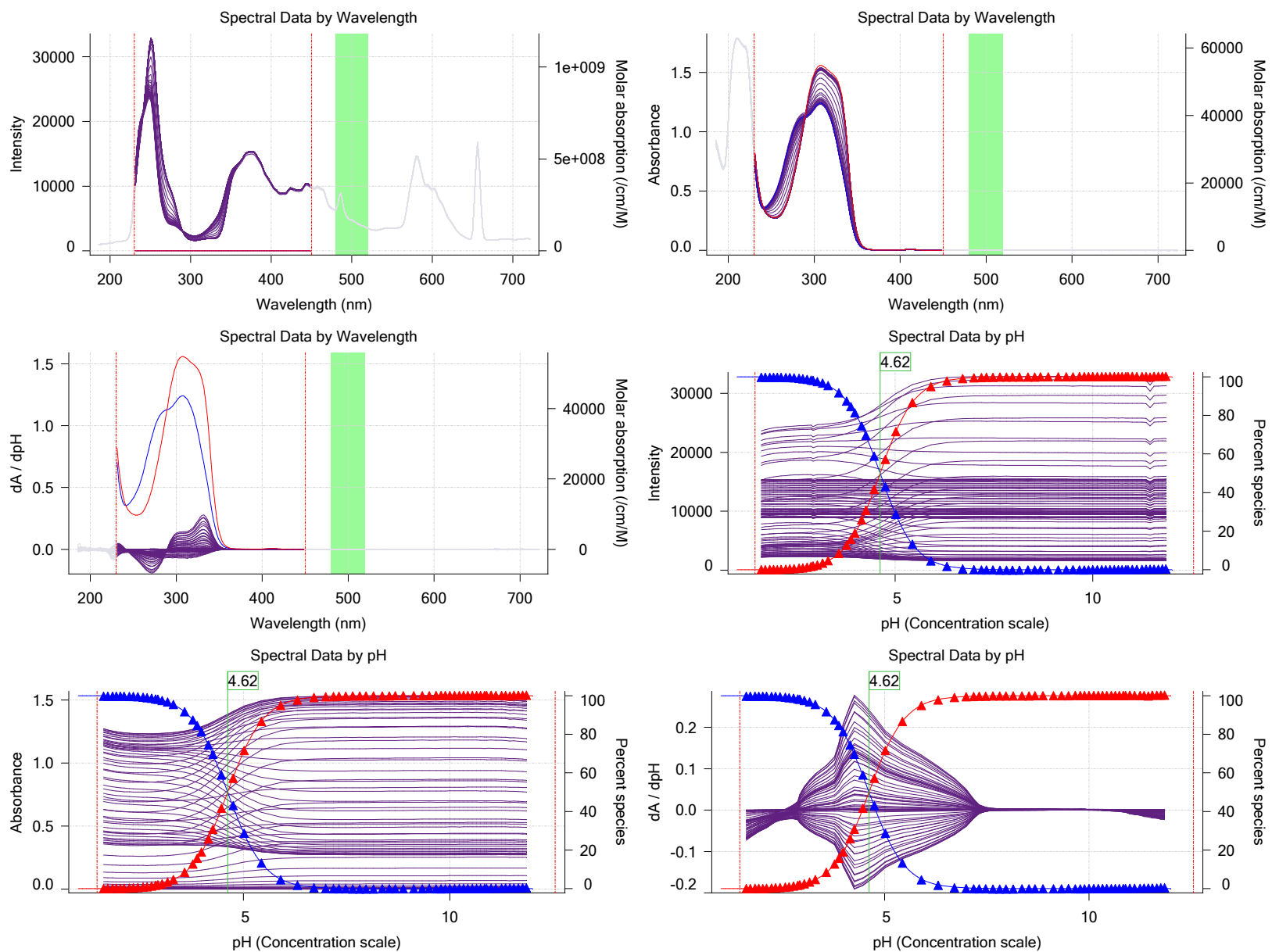
Warnings and errors

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			

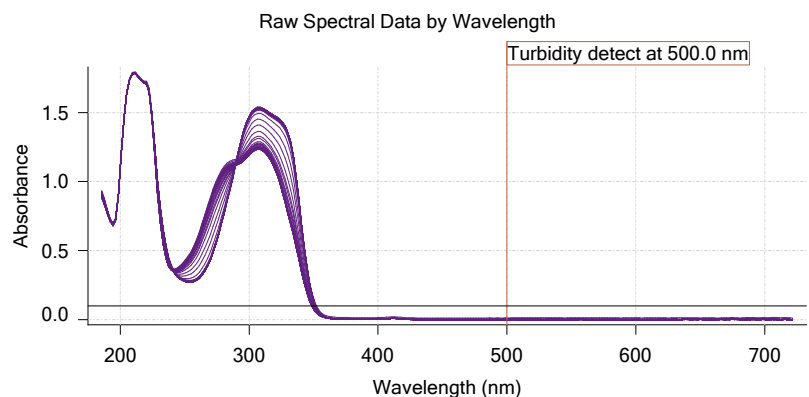
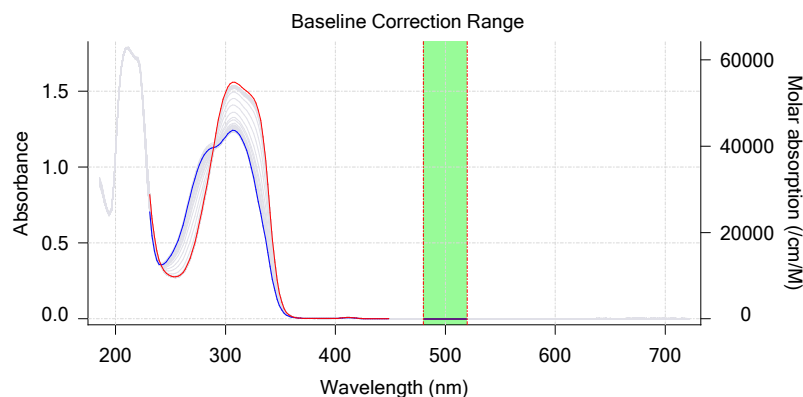
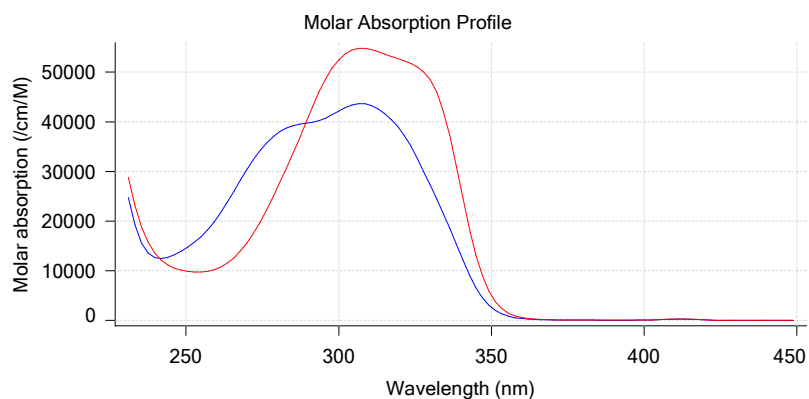
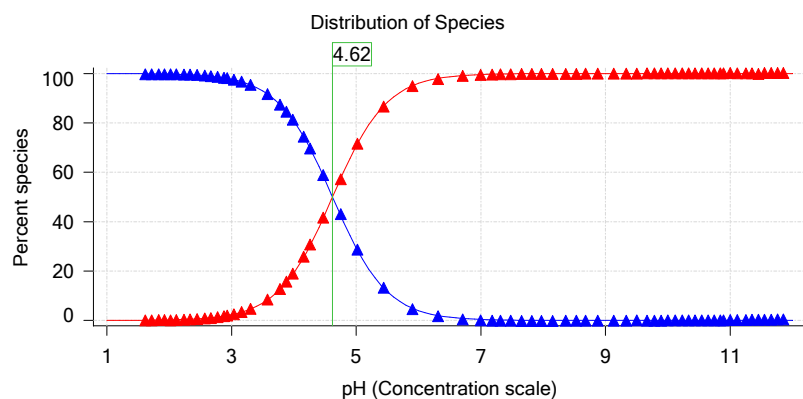
Graphs



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Experiment start time: **10/7/2017 10:32:05 AM**
Analyst: **Dorothy Leverse**
Instrument ID: **T311053**

Graphs (continued)



UV-metric psKa Titration 2 of 3 17J-07007 Points 72 to 139

Results

pKa 1	4.80
RMSD	0.002 0.002
Chi squared	0.0043
PCA calculated number of pKas	4
Average ionic strength	0.167 M
Average temperature	24.9°C
Analyte concentration range	25.1 µM to 23.7 µM
Methanol weight %	50.0 %
Dielectric constant	56.4
Water concentration	24.4 M
Number of pKas source	Predicted
Wavelength clipping	230.0 nm to 450.0 nm
pH clipping	1.472 to 12.541

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

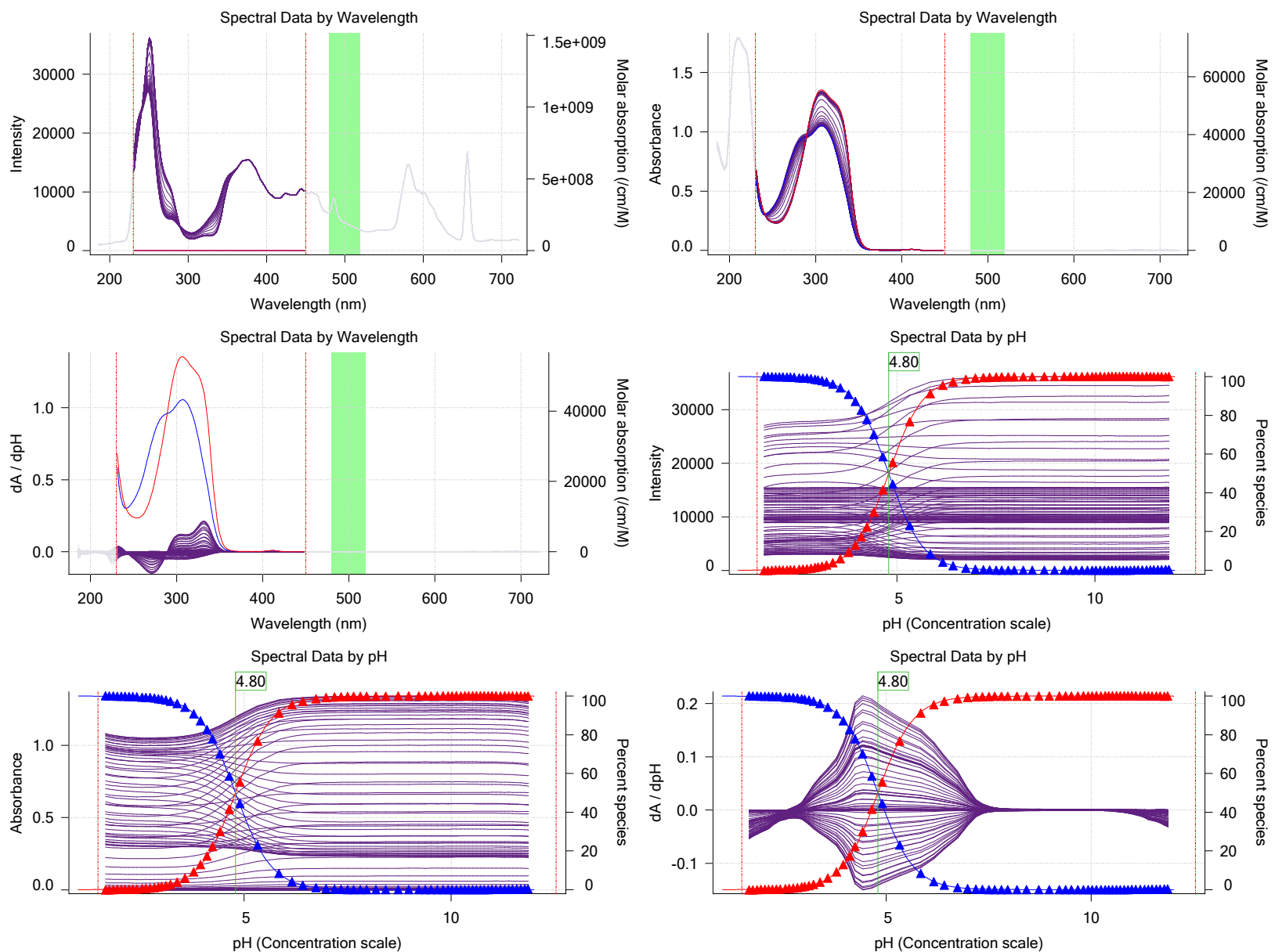
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Experiment start time: **10/7/2017 10:32:05 AM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Assay Settings (continued)

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

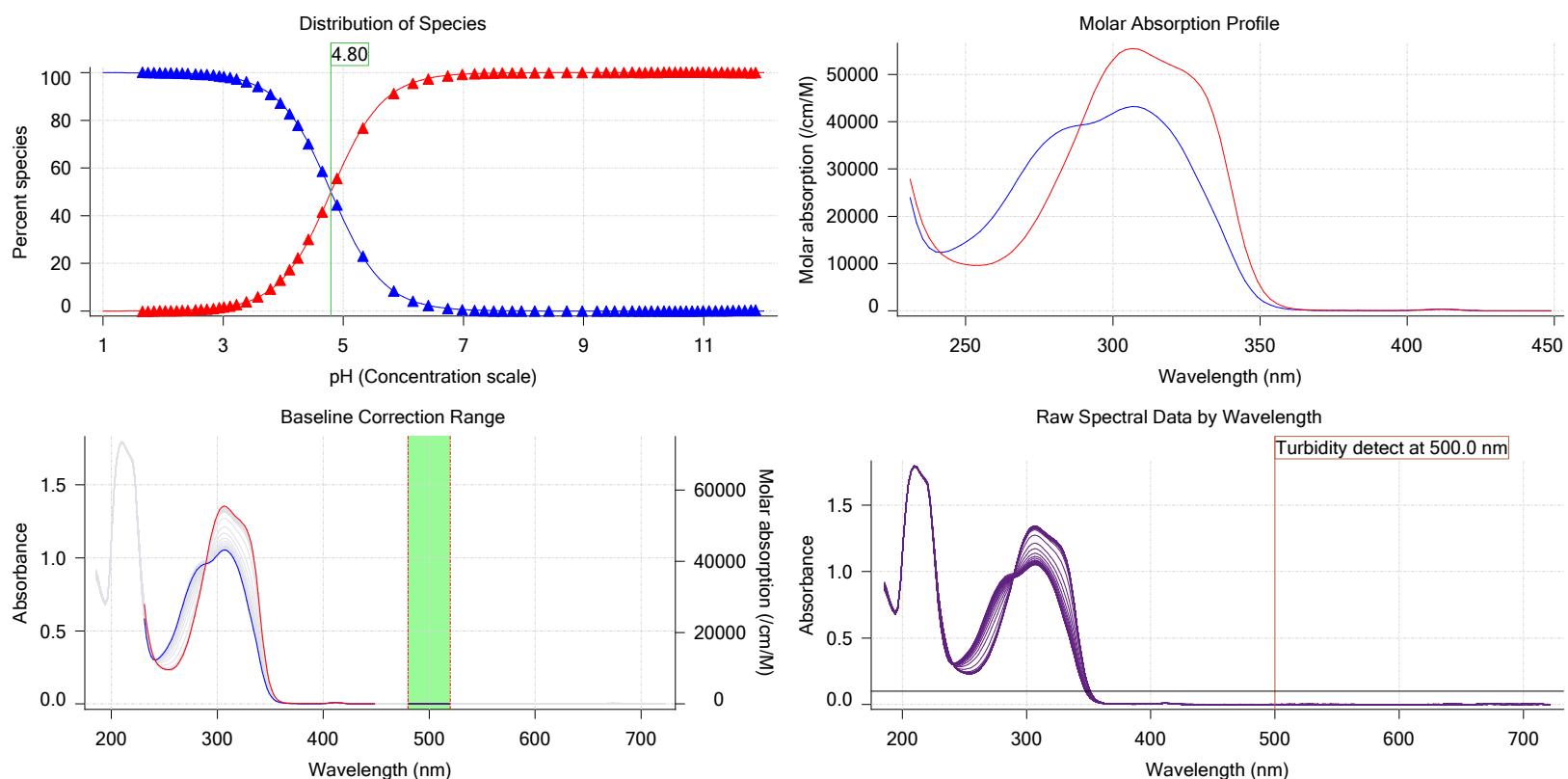
Graphs



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Experiment start time: **10/7/2017 10:32:05 AM**
Analyst: **Dorothy Levorse**
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Graphs (continued)



UV-metric psKa Titration 3 of 3 17J-07007 Points 141 to 217

Results

pKa 1	4.99
RMSD	0.003 0.004
Chi squared	0.0117
PCA calculated number of pKas	5
Average ionic strength	0.174 M
Average temperature	24.9°C
Analyte concentration range	20.7 µM to 19.6 µM
Methanol weight %	40.5 %
Dielectric constant	60.8
Water concentration	29.7 M
Number of pKas source	Predicted
Wavelength clipping	230.0 nm to 450.0 nm
pH clipping	1.480 to 12.547

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

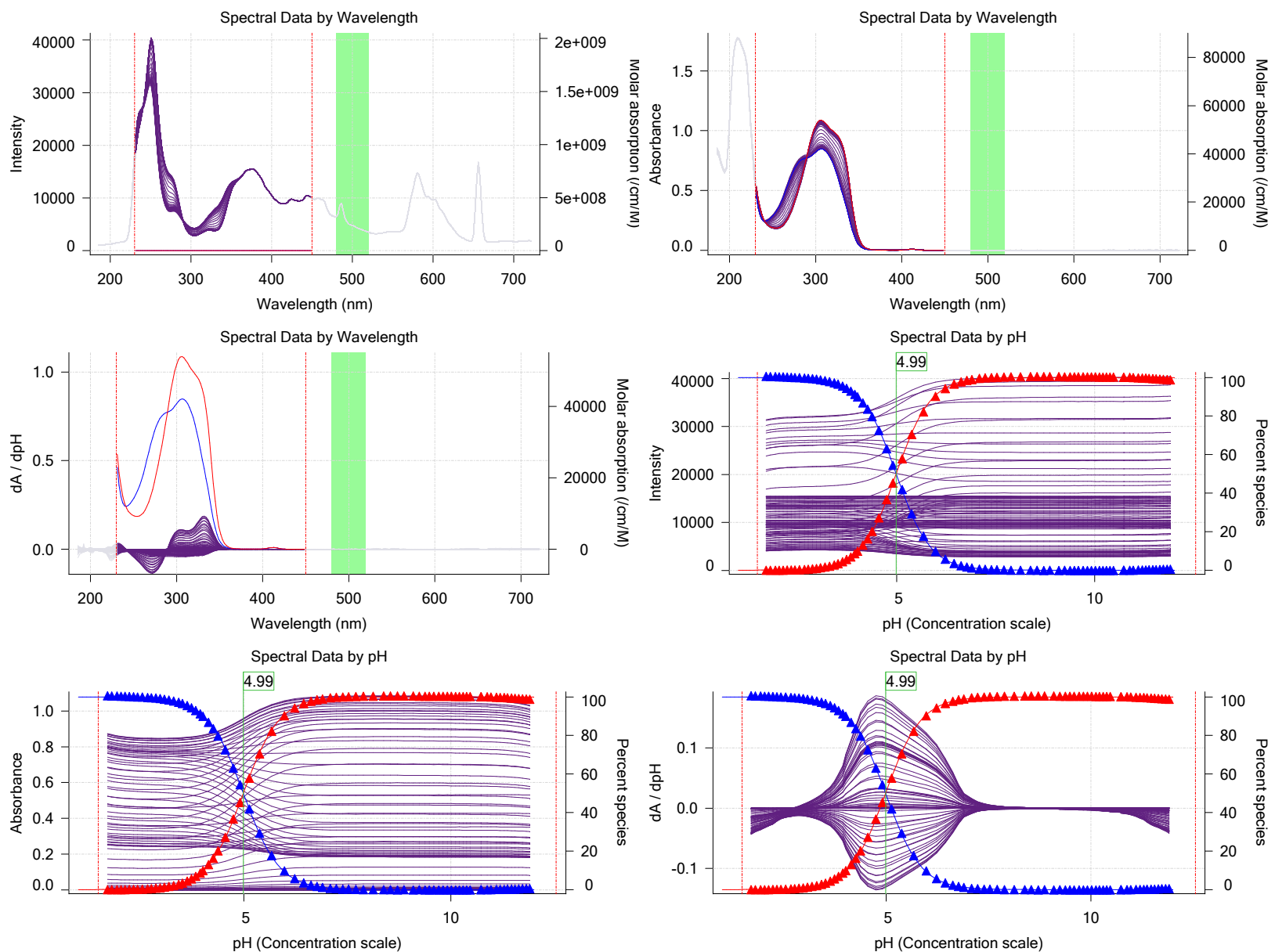
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 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Settings (continued)

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

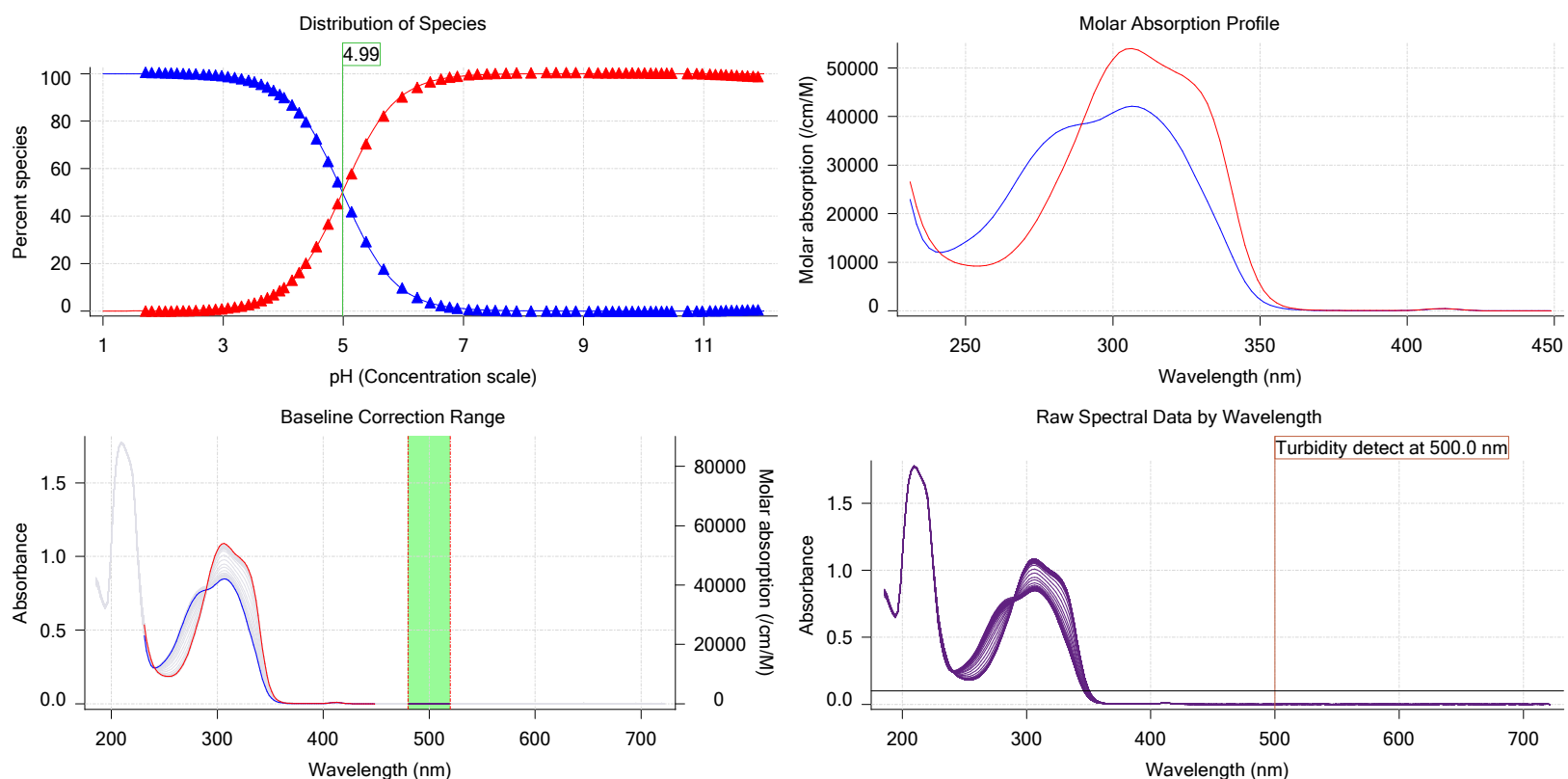
Graphs



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Experiment start time: **10/7/2017 10:32:05 AM**
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Graphs (continued)



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	D08	10/2/2017 12:57:31 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0010 mL	10/6/2017 6:10:30 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.047100 M	10/2/2017 12:59:19 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	420.46	9/29/2017 6:40:43 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	9/29/2017 6:40:34 PM	User entered value
Sample is a	Base	9/29/2017 6:40:34 PM	User entered value
pKa 1	6.16	9/29/2017 6:40:34 PM	User entered value
logp (XH +)	-10.00		Default value
logP (neutral X)	-10.00	9/29/2017 6:40:34 PM	User entered value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-square
3:10.1	Dark spectrum								
3:11.6	Reference spectrum								
3:39.2	Volume reset due to vial change								
8:43.3	Initial pH = 8.01								
9:03.3	Data point 4	0.15005 mL	0.07260 mL	0.00000 mL	1.35995 mL	0.02500 mL	1.956	-0.04734	0.98570
9:31.9	Data point 5	0.15005 mL	0.07260 mL	0.01496 mL	1.35995 mL	0.02500 mL	2.056	-0.00381	0.08449
9:48.8	Data point 6	0.15005 mL	0.07260 mL	0.02775 mL	1.35995 mL	0.02500 mL	2.171	0.01090	0.85724
10:10.8	Data point 7	0.15005 mL	0.07260 mL	0.03603 mL	1.35995 mL	0.02500 mL	2.266	0.00654	0.77235
10:32.7	Data point 8	0.15005 mL	0.07260 mL	0.04262 mL	1.35995 mL	0.02500 mL	2.362	0.00412	0.58281
10:59.8	Data point 9	0.15005 mL	0.07260 mL	0.04842 mL	1.35995 mL	0.02500 mL	2.454	0.00159	0.14512



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Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD	Comment
11:16.5	Data point 10	0.15005 mL	0.07260 mL	0.05360 mL	1.35995 mL	0.02500 mL	2.576	0.00885	0.79088	0.00049	1
11:43.6	Data point 11	0.15005 mL	0.07260 mL	0.05713 mL	1.35995 mL	0.02500 mL	2.673	-0.00369	0.41968	0.00028	1
12:00.2	Data point 12	0.15005 mL	0.07260 mL	0.06030 mL	1.35995 mL	0.02500 mL	2.782	0.00412	0.30674	0.00037	1
12:16.8	Data point 13	0.15005 mL	0.07260 mL	0.06275 mL	1.35995 mL	0.02500 mL	2.904	0.00254	0.17519	0.00030	1
12:43.8	Data point 14	0.15005 mL	0.07260 mL	0.06439 mL	1.35995 mL	0.02500 mL	3.001	0.00168	0.12367	0.00024	1
13:00.4	Data point 15	0.15005 mL	0.07260 mL	0.06587 mL	1.35995 mL	0.02500 mL	3.108	0.00755	0.77609	0.00042	1
13:17.0	Data point 16	0.15005 mL	0.07260 mL	0.06703 mL	1.35995 mL	0.02500 mL	3.207	0.00894	0.79214	0.00050	1
13:33.6	Data point 17	0.15005 mL	0.07260 mL	0.06794 mL	1.35995 mL	0.02500 mL	3.258	0.00930	0.79283	0.00052	1
14:05.4	Data point 18	0.15005 mL	0.07260 mL	0.06891 mL	1.35995 mL	0.02500 mL	3.364	0.01342	0.89463	0.00070	1
14:32.2	Data point 19	0.15005 mL	0.07260 mL	0.06954 mL	1.35995 mL	0.02500 mL	3.490	0.02031	0.96260	0.00102	1
14:48.6	Data point 20	0.15005 mL	0.07260 mL	0.07001 mL	1.35995 mL	0.02500 mL	3.630	0.02189	0.94286	0.00111	1
15:10.3	Data point 21	0.15005 mL	0.07260 mL	0.07063 mL	1.35995 mL	0.02500 mL	3.899	0.04326	0.99303	0.00214	1
15:32.1	Data point 22	0.15005 mL	0.07260 mL	0.07095 mL	1.35995 mL	0.02500 mL	4.094	0.08553	0.99488	0.00423	1
15:53.8	Data point 23	0.15005 mL	0.07260 mL	0.07114 mL	1.35995 mL	0.02500 mL	4.196	0.09115	0.99316	0.00452	1
16:15.5	Data point 24	0.15005 mL	0.07260 mL	0.07128 mL	1.35995 mL	0.02500 mL	4.299	0.08465	0.93556	0.00432	1
16:37.1	Data point 25	0.15005 mL	0.07260 mL	0.07140 mL	1.35995 mL	0.02500 mL	4.469	0.09753	0.98214	0.00486	2
17:14.8	Data point 26	0.15005 mL	0.07260 mL	0.07150 mL	1.35995 mL	0.02500 mL	4.573	0.04288	0.38469	0.00341	1
17:41.7	Data point 27	0.15005 mL	0.07260 mL	0.07157 mL	1.35995 mL	0.02500 mL	4.777	0.10053	0.98755	0.00499	3
18:32.6	Data point 28	0.15005 mL	0.07260 mL	0.07166 mL	1.35995 mL	0.02500 mL	5.056	0.09044	0.93158	0.00462	4
19:34.8	Data point 29	0.15005 mL	0.07260 mL	0.07173 mL	1.35995 mL	0.02500 mL	5.321	0.06685	0.50013	0.00466	3
20:22.4	Data point 30	0.15005 mL	0.07260 mL	0.07178 mL	1.35995 mL	0.02500 mL	5.734	0.18440	0.99709	0.00911	1
21:34.2	Data point 31	0.15005 mL	0.07260 mL	0.07183 mL	1.35995 mL	0.02500 mL	6.192	0.22980	0.99623	0.01136	1
22:45.8	Data point 32	0.15005 mL	0.07260 mL	0.07187 mL	1.35995 mL	0.02500 mL	6.593	0.09979	0.97140	0.00500	5
24:01.7	Data point 33	0.15005 mL	0.07260 mL	0.07194 mL	1.35995 mL	0.02500 mL	6.986	0.09786	0.98986	0.00486	5
25:13.0	Data point 34	0.15005 mL	0.07260 mL	0.07201 mL	1.35995 mL	0.02500 mL	7.267	0.09940	0.97611	0.00496	3
26:07.7	Data point 35	0.15005 mL	0.07260 mL	0.07208 mL	1.35995 mL	0.02500 mL	7.452	0.10039	0.99334	0.00497	3
26:56.4	Data point 36	0.15005 mL	0.07260 mL	0.07215 mL	1.35995 mL	0.02500 mL	7.581	0.09777	0.93909	0.00498	1
27:28.1	Data point 37	0.15005 mL	0.07260 mL	0.07222 mL	1.35995 mL	0.02500 mL	7.742	0.09960	0.99388	0.00493	2



Assay Events

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Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
42:42.0	Data point 67	0.15005 mL	0.07260 mL	0.08667 mL	1.35995 mL	0.02500 mL	11.756	-0.00185	0.19950	0.19950
42:58.6	Data point 68	0.15005 mL	0.07260 mL	0.09024 mL	1.35995 mL	0.02500 mL	11.864	-0.00486	0.39268	0.39268
43:15.3	Data point 69	0.15005 mL	0.07260 mL	0.09483 mL	1.35995 mL	0.02500 mL	11.962	-0.00252	0.16233	0.16233
43:32.1	Data point 70	0.15005 mL	0.07260 mL	0.09986 mL	1.35995 mL	0.02500 mL	12.052	-0.01020	0.76020	0.76020
45:07.8	Reference spectrum									
46:10.5	Data point 72	0.22001 mL	0.17260 mL	0.09988 mL	1.35995 mL	0.02500 mL	1.972	-0.04867	0.93802	0.93802
46:32.5	Data point 73	0.22001 mL	0.17260 mL	0.11315 mL	1.35995 mL	0.02500 mL	2.066	0.00820	0.64140	0.64140
46:54.6	Data point 74	0.22001 mL	0.17260 mL	0.12404 mL	1.35995 mL	0.02500 mL	2.163	0.02770	0.84315	0.84315
47:16.4	Data point 75	0.22001 mL	0.17260 mL	0.13236 mL	1.35995 mL	0.02500 mL	2.259	0.02476	0.82359	0.82359
47:38.4	Data point 76	0.22001 mL	0.17260 mL	0.13937 mL	1.35995 mL	0.02500 mL	2.352	0.02173	0.95165	0.95165
48:00.3	Data point 77	0.22001 mL	0.17260 mL	0.14443 mL	1.35995 mL	0.02500 mL	2.443	0.01312	0.92887	0.92887
48:22.1	Data point 78	0.22001 mL	0.17260 mL	0.14901 mL	1.35995 mL	0.02500 mL	2.537	0.01394	0.90993	0.90993
48:43.9	Data point 79	0.22001 mL	0.17260 mL	0.15245 mL	1.35995 mL	0.02500 mL	2.628	0.01046	0.88585	0.88585
49:10.9	Data point 80	0.22001 mL	0.17260 mL	0.15590 mL	1.35995 mL	0.02500 mL	2.720	0.01131	0.86202	0.86202
49:27.6	Data point 81	0.22001 mL	0.17260 mL	0.15894 mL	1.35995 mL	0.02500 mL	2.848	0.02014	0.92300	0.92300
49:49.5	Data point 82	0.22001 mL	0.17260 mL	0.16061 mL	1.35995 mL	0.02500 mL	2.939	0.00756	0.73547	0.73547
50:16.4	Data point 83	0.22001 mL	0.17260 mL	0.16230 mL	1.35995 mL	0.02500 mL	3.037	0.01326	0.89683	0.89683
50:33.1	Data point 84	0.22001 mL	0.17260 mL	0.16376 mL	1.35995 mL	0.02500 mL	3.139	0.01088	0.85467	0.85467
50:49.6	Data point 85	0.22001 mL	0.17260 mL	0.16491 mL	1.35995 mL	0.02500 mL	3.239	0.01338	0.91621	0.91621
51:06.2	Data point 86	0.22001 mL	0.17260 mL	0.16583 mL	1.35995 mL	0.02500 mL	3.313	0.01378	0.95817	0.95817
51:38.0	Data point 87	0.22001 mL	0.17260 mL	0.16672 mL	1.35995 mL	0.02500 mL	3.414	0.01714	0.96363	0.96363
52:04.8	Data point 88	0.22001 mL	0.17260 mL	0.16729 mL	1.35995 mL	0.02500 mL	3.522	0.02106	0.97407	0.97407
52:21.4	Data point 89	0.22001 mL	0.17260 mL	0.16776 mL	1.35995 mL	0.02500 mL	3.682	0.02456	0.96100	0.96100
52:43.0	Data point 90	0.22001 mL	0.17260 mL	0.16820 mL	1.35995 mL	0.02500 mL	3.870	0.03654	0.97689	0.97689
53:04.6	Data point 91	0.22001 mL	0.17260 mL	0.16858 mL	1.35995 mL	0.02500 mL	4.077	0.06142	0.99078	0.99078
53:26.4	Data point 92	0.22001 mL	0.17260 mL	0.16881 mL	1.35995 mL	0.02500 mL	4.241	0.08269	0.99169	0.99169
53:48.1	Data point 93	0.22001 mL	0.17260 mL	0.16898 mL	1.35995 mL	0.02500 mL	4.392	0.10027	0.98575	0.98575
54:17.9	Data point 94	0.22001 mL	0.17260 mL	0.16910 mL	1.35995 mL	0.02500 mL	4.528	0.10023	0.98300	0.98300
54:52.2	Data point 95	0.22001 mL	0.17260 mL	0.16919 mL	1.35995 mL	0.02500 mL	4.704	0.09984	0.99701	0.99701
55:42.2	Data point 96	0.22001 mL	0.17260 mL	0.16928 mL	1.35995 mL	0.02500 mL	4.929	0.09362	0.91224	0.91224
56:26.6	Data point 97	0.22001 mL	0.17260 mL	0.16936 mL	1.35995 mL	0.02500 mL	5.174	0.09632	0.97426	0.97426
57:22.0	Data point 98	0.22001 mL	0.17260 mL	0.16943 mL	1.35995 mL	0.02500 mL	5.600	0.10058	0.99374	0.99374
58:37.6	Data point 99	0.22001 mL	0.17260 mL	0.16950 mL	1.35995 mL	0.02500 mL	6.106	0.10986	0.98910	0.98910
59:49.2	Data point 100	0.22001 mL	0.17260 mL	0.16954 mL	1.35995 mL	0.02500 mL	6.420	0.10008	0.99268	0.99268
1:00:53.9	Data point 101	0.22001 mL	0.17260 mL	0.16959 mL	1.35995 mL	0.02500 mL	6.675	0.10046	0.99276	0.99276
1:01:59.7	Data point 102	0.22001 mL	0.17260 mL	0.16966 mL	1.35995 mL	0.02500 mL	6.994	0.09602	0.98741	0.98741
1:02:47.9	Data point 103	0.22001 mL	0.17260 mL	0.16973 mL	1.35995 mL	0.02500 mL	7.232	0.09890	0.99080	0.99080
1:03:35.3	Data point 104	0.22001 mL	0.17260 mL	0.16980 mL	1.35995 mL	0.02500 mL	7.432	0.09847	0.98637	0.98637
1:04:19.4	Data point 105	0.22001 mL	0.17260 mL	0.16987 mL	1.35995 mL	0.02500 mL	7.588	0.09830	0.99235	0.99235
1:05:00.6	Data point 106	0.22001 mL	0.17260 mL	0.16994 mL	1.35995 mL	0.02500 mL	7.747	0.09844	0.98737	0.98737
1:05:40.4	Data point 107	0.22001 mL	0.17260 mL	0.17001 mL	1.35995 mL	0.02500 mL	7.887	0.09936	0.99532	0.99532
1:06:19.6	Data point 108	0.22001 mL	0.17260 mL	0.17008 mL	1.35995 mL	0.02500 mL	8.048	0.09808	0.98886	0.98886
1:07:00.2	Data point 109	0.22001 mL	0.17260 mL	0.17016 mL	1.35995 mL	0.02500 mL	8.202	0.09972	0.99392	0.99392
1:07:39.8	Data point 110	0.22001 mL	0.17260 mL	0.17023 mL	1.35995 mL	0.02500 mL	8.422	0.09849	0.98935	0.98935
1:08:26.5	Data point 111	0.22001 mL	0.17260 mL	0.17030 mL	1.35995 mL	0.02500 mL	8.651	0.09564	0.97309	0.97309
1:09:12.7	Data point 112	0.22001 mL	0.17260 mL	0.17037 mL	1.35995 mL	0.02500 mL	8.949	0.09851	0.98423	0.98423
1:10:00.9	Data point 113	0.22001 mL	0.17260 mL	0.17044 mL	1.35995 mL	0.02500 mL	9.203	0.09711	0.98998	0.98998
1:10:45.5	Data point 114	0.22001 mL	0.17260 mL	0.17051 mL	1.35995 mL	0.02500 mL	9.442	0.09715	0.98298	0.98298
1:11:29.7	Data point 115	0.22001 mL	0.17260 mL	0.17058 mL	1.35995 mL	0.02500 mL	9.594	0.09722	0.98237	0.98237
1:12:07.5	Data point 116	0.22001 mL	0.17260 mL	0.17065 mL	1.35995 mL	0.02500 mL	9.734	0.09612	0.98244	0.98244
1:12:39.8	Data point 117	0.22001 mL	0.17260 mL	0.17074 mL	1.35995 mL	0.02500 mL	9.885	0.09521	0.97926	0.97926
1:13:03.9	Data point 118	0.22001 mL	0.17260 mL	0.17084 mL	1.35995 mL	0.02500 mL	10.019	0.09027	0.97727	0.97727
1:13:30.6	Data point 119	0.22001 mL	0.17260 mL	0.17096 mL	1.35995 mL	0.02500 mL	10.138	0.06985	0.97863	0.97863
1:13:52.2	Data point 120	0.22001 mL	0.17260 mL	0.17107 mL	1.35995 mL	0.02500 mL	10.235	0.05010	0.97944	0.97944
1:14:18.9	Data point 121	0.22001 mL	0.17260 mL	0.17124 mL	1.35995 mL	0.02500 mL	10.337	0.03962	0.97669	0.97669
1:14:35.5	Data point 122	0.22001 mL	0.17260 mL	0.17140 mL	1.35995 mL	0.02500 mL	10.443	0.03328	0.96453	0.96453
1:14:52.0	Data point 123	0.22001 mL	0.17260 mL	0.17161 mL	1.35995 mL	0.02500 mL	10.543	0.02062	0.96150	0.96150

Sample name: **D08**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07007**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07007_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 10:32:05 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
1:15:08.7	Data point 124	0.22001 mL	0.17260 mL	0.17187 mL	1.35995 mL	0.02500 mL	10.631	0.01091	0.76280	0.76280
1:15:25.2	Data point 125	0.22001 mL	0.17260 mL	0.17220 mL	1.35995 mL	0.02500 mL	10.723	0.00916	0.88365	0.88365
1:15:41.9	Data point 126	0.22001 mL	0.17260 mL	0.17260 mL	1.35995 mL	0.02500 mL	10.817	0.00672	0.78919	0.78919
1:15:58.6	Data point 127	0.22001 mL	0.17260 mL	0.17310 mL	1.35995 mL	0.02500 mL	10.910	0.00120	0.11926	0.11926
1:16:15.1	Data point 128	0.22001 mL	0.17260 mL	0.17371 mL	1.35995 mL	0.02500 mL	11.002	-0.00133	0.11213	0.11213
1:16:31.6	Data point 129	0.22001 mL	0.17260 mL	0.17446 mL	1.35995 mL	0.02500 mL	11.093	-0.00095	0.05637	0.05637
1:16:48.1	Data point 130	0.22001 mL	0.17260 mL	0.17540 mL	1.35995 mL	0.02500 mL	11.187	-0.00353	0.55930	0.55930
1:17:04.7	Data point 131	0.22001 mL	0.17260 mL	0.17658 mL	1.35995 mL	0.02500 mL	11.280	-0.00204	0.25193	0.25193
1:17:21.3	Data point 132	0.22001 mL	0.17260 mL	0.17803 mL	1.35995 mL	0.02500 mL	11.387	-0.00222	0.27507	0.27507
1:17:37.8	Data point 133	0.22001 mL	0.17260 mL	0.17989 mL	1.35995 mL	0.02500 mL	11.491	-0.00370	0.52325	0.52325
1:17:54.4	Data point 134	0.22001 mL	0.17260 mL	0.18227 mL	1.35995 mL	0.02500 mL	11.583	-0.00730	0.66650	0.66650
1:18:11.1	Data point 135	0.22001 mL	0.17260 mL	0.18521 mL	1.35995 mL	0.02500 mL	11.674	-0.00269	0.28392	0.28392
1:18:27.8	Data point 136	0.22001 mL	0.17260 mL	0.18885 mL	1.35995 mL	0.02500 mL	11.774	-0.00385	0.45012	0.45012
1:18:44.7	Data point 137	0.22001 mL	0.17260 mL	0.19346 mL	1.35995 mL	0.02500 mL	11.866	-0.00502	0.63774	0.63774
1:19:01.4	Data point 138	0.22001 mL	0.17260 mL	0.19920 mL	1.35995 mL	0.02500 mL	11.965	-0.00561	0.65336	0.65336
1:19:18.2	Data point 139	0.22001 mL	0.17260 mL	0.20527 mL	1.35995 mL	0.02500 mL	12.041	-0.00298	0.40625	0.40625
1:21:00.3	Reference spectrum									
1:22:20.6	Data point 141	0.39005 mL	0.29487 mL	0.20529 mL	1.35995 mL	0.02500 mL	1.980	-0.07137	0.95498	0.95498
1:22:48.0	Data point 142	0.39005 mL	0.29487 mL	0.22187 mL	1.35995 mL	0.02500 mL	2.080	-0.00169	0.03564	0.03564
1:23:04.9	Data point 143	0.39005 mL	0.29487 mL	0.23638 mL	1.35995 mL	0.02500 mL	2.206	-0.01328	0.60032	0.60032
1:23:26.8	Data point 144	0.39005 mL	0.29487 mL	0.24457 mL	1.35995 mL	0.02500 mL	2.303	0.00608	0.24326	0.24326
1:23:48.9	Data point 145	0.39005 mL	0.29487 mL	0.25155 mL	1.35995 mL	0.02500 mL	2.399	0.01824	0.96245	0.96245
1:24:15.9	Data point 146	0.39005 mL	0.29487 mL	0.25736 mL	1.35995 mL	0.02500 mL	2.500	0.00966	0.85953	0.85953
1:24:37.7	Data point 147	0.39005 mL	0.29487 mL	0.26160 mL	1.35995 mL	0.02500 mL	2.598	0.01682	0.94637	0.94637
1:25:04.5	Data point 148	0.39005 mL	0.29487 mL	0.26543 mL	1.35995 mL	0.02500 mL	2.695	0.00832	0.86061	0.86061
1:25:21.1	Data point 149	0.39005 mL	0.29487 mL	0.26896 mL	1.35995 mL	0.02500 mL	2.808	0.01099	0.82268	0.82268
1:25:37.8	Data point 150	0.39005 mL	0.29487 mL	0.27166 mL	1.35995 mL	0.02500 mL	2.933	0.01698	0.86730	0.86730
1:26:04.6	Data point 151	0.39005 mL	0.29487 mL	0.27347 mL	1.35995 mL	0.02500 mL	3.027	0.00384	0.49968	0.49968
1:26:21.2	Data point 152	0.39005 mL	0.29487 mL	0.27512 mL	1.35995 mL	0.02500 mL	3.131	0.00128	0.08583	0.08583
1:26:37.8	Data point 153	0.39005 mL	0.29487 mL	0.27641 mL	1.35995 mL	0.02500 mL	3.234	0.00718	0.63231	0.63231
1:26:54.3	Data point 154	0.39005 mL	0.29487 mL	0.27742 mL	1.35995 mL	0.02500 mL	3.333	0.01000	0.86453	0.86453
1:27:10.9	Data point 155	0.39005 mL	0.29487 mL	0.27822 mL	1.35995 mL	0.02500 mL	3.444	0.01145	0.89193	0.89193
1:27:27.4	Data point 156	0.39005 mL	0.29487 mL	0.27883 mL	1.35995 mL	0.02500 mL	3.558	0.01369	0.86932	0.86932
1:27:44.0	Data point 157	0.39005 mL	0.29487 mL	0.27930 mL	1.35995 mL	0.02500 mL	3.675	0.02082	0.93278	0.93278
1:28:05.7	Data point 158	0.39005 mL	0.29487 mL	0.27963 mL	1.35995 mL	0.02500 mL	3.768	0.02169	0.94751	0.94751
1:28:22.3	Data point 159	0.39005 mL	0.29487 mL	0.27992 mL	1.35995 mL	0.02500 mL	3.881	0.02854	0.95475	0.95475
1:28:38.9	Data point 160	0.39005 mL	0.29487 mL	0.28013 mL	1.35995 mL	0.02500 mL	3.984	0.04244	0.98130	0.98130
1:28:55.5	Data point 161	0.39005 mL	0.29487 mL	0.28029 mL	1.35995 mL	0.02500 mL	4.085	0.04529	0.98378	0.98378
1:29:12.1	Data point 162	0.39005 mL	0.29487 mL	0.28043 mL	1.35995 mL	0.02500 mL	4.187	0.06041	0.98929	0.98929
1:29:28.6	Data point 163	0.39005 mL	0.29487 mL	0.28053 mL	1.35995 mL	0.02500 mL	4.256	0.06785	0.99216	0.99216
1:29:50.3	Data point 164	0.39005 mL	0.29487 mL	0.28064 mL	1.35995 mL	0.02500 mL	4.387	0.09669	0.97969	0.97969
1:30:06.7	Data point 165	0.39005 mL	0.29487 mL	0.28071 mL	1.35995 mL	0.02500 mL	4.503	0.09972	0.99362	0.99362
1:30:31.9	Data point 166	0.39005 mL	0.29487 mL	0.28079 mL	1.35995 mL	0.02500 mL	4.618	0.09956	0.98076	0.98076
1:31:02.2	Data point 167	0.39005 mL	0.29487 mL	0.28086 mL	1.35995 mL	0.02500 mL	4.788	0.09821	0.98948	0.98948
1:31:39.4	Data point 168	0.39005 mL	0.29487 mL	0.28093 mL	1.35995 mL	0.02500 mL	4.982	0.09922	0.98868	0.98868
1:32:16.5	Data point 169	0.39005 mL	0.29487 mL	0.28097 mL	1.35995 mL	0.02500 mL	5.140	0.09738	0.99136	0.99136
1:32:55.1	Data point 170	0.39005 mL	0.29487 mL	0.28102 mL	1.35995 mL	0.02500 mL	5.365	0.10040	0.99279	0.99279
1:33:42.8	Data point 171	0.39005 mL	0.29487 mL	0.28107 mL	1.35995 mL	0.02500 mL	5.607	0.10057	0.99188	0.99188
1:34:32.9	Data point 172	0.39005 mL	0.29487 mL	0.28112 mL	1.35995 mL	0.02500 mL	5.897	0.10044	0.99223	0.99223
1:35:23.4	Data point 173	0.39005 mL	0.29487 mL	0.28116 mL	1.35995 mL	0.02500 mL	6.198	0.09978	0.99240	0.99240
1:36:15.8	Data point 174	0.39005 mL	0.29487 mL	0.28121 mL	1.35995 mL	0.02500 mL	6.446	0.09927	0.99566	0.99566
1:36:58.5	Data point 175	0.39005 mL	0.29487 mL	0.28126 mL	1.35995 mL	0.02500 mL	6.660	0.09783	0.98595	0.98595
1:37:38.0	Data point 176	0.39005 mL	0.29487 mL	0.28130 mL	1.35995 mL	0.02500 mL	6.836	0.09727	0.98791	0.98791
1:38:14.2	Data point 177	0.39005 mL	0.29487 mL	0.28135 mL	1.35995 mL	0.02500 mL	6.981	0.09969	0.99007	0.99007
1:38:45.6	Data point 178	0.39005 mL	0.29487 mL	0.28140 mL	1.35995 mL	0.02500 mL	7.107	0.09940	0.99319	0.99319
1:39:19.7	Data point 179	0.39005 mL	0.29487 mL	0.28147 mL	1.35995 mL	0.02500 mL	7.295	0.09775	0.99021	0.99021
1:39:55.0	Data point 180	0.39005 mL	0.29487 mL	0.28154 mL	1.35995 mL	0.02500 mL	7.438	0.09674	0.97122	0.97122

Sample name: **D08**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07007**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07007_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 10:32:05 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
1:40:28.4	Data point 181	0.39005 mL	0.29487 mL	0.28161 mL	1.35995 mL	0.02500 mL	7.593	0.09763	0.99343	0.0048
1:41:03.1	Data point 182	0.39005 mL	0.29487 mL	0.28168 mL	1.35995 mL	0.02500 mL	7.731	0.10004	0.99163	0.0049
1:41:36.8	Data point 183	0.39005 mL	0.29487 mL	0.28175 mL	1.35995 mL	0.02500 mL	7.906	0.09725	0.98022	0.0048
1:42:13.1	Data point 184	0.39005 mL	0.29487 mL	0.28182 mL	1.35995 mL	0.02500 mL	8.083	0.09714	0.98580	0.0048
1:42:49.8	Data point 185	0.39005 mL	0.29487 mL	0.28189 mL	1.35995 mL	0.02500 mL	8.318	0.09678	0.98984	0.0048
1:43:31.5	Data point 186	0.39005 mL	0.29487 mL	0.28196 mL	1.35995 mL	0.02500 mL	8.571	0.09889	0.98218	0.0049
1:44:08.6	Data point 187	0.39005 mL	0.29487 mL	0.28201 mL	1.35995 mL	0.02500 mL	8.731	0.09923	0.97318	0.0049
1:44:41.6	Data point 188	0.39005 mL	0.29487 mL	0.28206 mL	1.35995 mL	0.02500 mL	8.899	0.09574	0.98392	0.0047
1:45:14.8	Data point 189	0.39005 mL	0.29487 mL	0.28210 mL	1.35995 mL	0.02500 mL	9.053	0.09833	0.98354	0.0048
1:45:52.1	Data point 190	0.39005 mL	0.29487 mL	0.28217 mL	1.35995 mL	0.02500 mL	9.275	0.09963	0.98195	0.0049
1:46:28.5	Data point 191	0.39005 mL	0.29487 mL	0.28224 mL	1.35995 mL	0.02500 mL	9.420	0.09758	0.97973	0.0048
1:46:59.1	Data point 192	0.39005 mL	0.29487 mL	0.28231 mL	1.35995 mL	0.02500 mL	9.554	0.10035	0.98769	0.0049
1:47:28.3	Data point 193	0.39005 mL	0.29487 mL	0.28239 mL	1.35995 mL	0.02500 mL	9.660	0.09177	0.97030	0.0046
1:47:50.0	Data point 194	0.39005 mL	0.29487 mL	0.28246 mL	1.35995 mL	0.02500 mL	9.763	0.08241	0.95920	0.0041
1:48:11.6	Data point 195	0.39005 mL	0.29487 mL	0.28255 mL	1.35995 mL	0.02500 mL	9.884	0.07236	0.96151	0.0036
1:48:38.5	Data point 196	0.39005 mL	0.29487 mL	0.28267 mL	1.35995 mL	0.02500 mL	9.985	0.04900	0.95527	0.0024
1:49:00.1	Data point 197	0.39005 mL	0.29487 mL	0.28281 mL	1.35995 mL	0.02500 mL	10.086	0.03562	0.97890	0.0017
1:49:21.6	Data point 198	0.39005 mL	0.29487 mL	0.28297 mL	1.35995 mL	0.02500 mL	10.187	0.02935	0.95122	0.0014
1:49:38.2	Data point 199	0.39005 mL	0.29487 mL	0.28314 mL	1.35995 mL	0.02500 mL	10.287	0.01696	0.93225	0.0008
1:49:54.6	Data point 200	0.39005 mL	0.29487 mL	0.28335 mL	1.35995 mL	0.02500 mL	10.374	0.01188	0.93142	0.0006
1:50:11.3	Data point 201	0.39005 mL	0.29487 mL	0.28361 mL	1.35995 mL	0.02500 mL	10.464	0.00826	0.78693	0.0004
1:50:27.9	Data point 202	0.39005 mL	0.29487 mL	0.28391 mL	1.35995 mL	0.02500 mL	10.549	0.00560	0.52204	0.0003
1:50:44.3	Data point 203	0.39005 mL	0.29487 mL	0.28429 mL	1.35995 mL	0.02500 mL	10.634	0.00415	0.43999	0.0003
1:51:21.6	Data point 204	0.39005 mL	0.29487 mL	0.28476 mL	1.35995 mL	0.02500 mL	10.891	-0.01451	0.94552	0.0007
1:51:38.1	Data point 205	0.39005 mL	0.29487 mL	0.28558 mL	1.35995 mL	0.02500 mL	10.894	-0.01373	0.93433	0.0007
1:51:59.9	Data point 206	0.39005 mL	0.29487 mL	0.28805 mL	1.35995 mL	0.02500 mL	11.040	-0.01075	0.83367	0.0005
1:52:26.9	Data point 207	0.39005 mL	0.29487 mL	0.28925 mL	1.35995 mL	0.02500 mL	11.131	-0.00569	0.72089	0.0003
1:52:43.5	Data point 208	0.39005 mL	0.29487 mL	0.29066 mL	1.35995 mL	0.02500 mL	11.258	-0.00925	0.77963	0.0005
1:53:10.5	Data point 209	0.39005 mL	0.29487 mL	0.29257 mL	1.35995 mL	0.02500 mL	11.352	-0.00804	0.86528	0.0004
1:53:27.0	Data point 210	0.39005 mL	0.29487 mL	0.29490 mL	1.35995 mL	0.02500 mL	11.444	-0.00959	0.83028	0.0005
1:53:43.6	Data point 211	0.39005 mL	0.29487 mL	0.29781 mL	1.35995 mL	0.02500 mL	11.520	-0.01099	0.86837	0.0005
1:54:10.4	Data point 212	0.39005 mL	0.29487 mL	0.30078 mL	1.35995 mL	0.02500 mL	11.616	-0.00636	0.74874	0.0003
1:54:27.0	Data point 213	0.39005 mL	0.29487 mL	0.30513 mL	1.35995 mL	0.02500 mL	11.698	-0.00875	0.74135	0.0005
1:54:48.7	Data point 214	0.39005 mL	0.29487 mL	0.30997 mL	1.35995 mL	0.02500 mL	11.789	-0.00763	0.75897	0.0004
1:55:05.6	Data point 215	0.39005 mL	0.29487 mL	0.31653 mL	1.35995 mL	0.02500 mL	11.876	-0.00898	0.81222	0.0004
1:55:22.4	Data point 216	0.39005 mL	0.29487 mL	0.32462 mL	1.35995 mL	0.02500 mL	11.966	-0.00516	0.52777	0.0003
1:55:39.1	Data point 217	0.39005 mL	0.29487 mL	0.33293 mL	1.35995 mL	0.02500 mL	12.047	-0.00676	0.68026	0.0004
1:57:38.0	Assay volumes	0.64005 mL	0.42161 mL	0.33293 mL	1.35995 mL	0.02500 mL				

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.100			
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			

Sample name: **D08**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07007**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07007_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 10:32:05 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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	1.35 mL			
Cosolvent added	Automatic			
ISA water volume	0.15 mL			
Water added	Automatic			
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	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	60 seconds			
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	0.07 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	0.17 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			

Sample name:	D08	Experiment start time:	10/7/2017 10:32:05 AM
Assay name:	UV-metric psKa	Analyst:	Dorothy Levorse
Assay ID:	17J-07007	Instrument ID:	T311053
Filename:	C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07007_D08_UV-metric psKa.t3r		

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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	0.161	10/7/2017 10:32:05 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus S	0.9927	10/7/2017 10:32:05 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus jH	0.5	10/7/2017 10:32:05 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus jOH	-0.7	10/7/2017 10:32:05 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Base concentration factor	1.011	10/7/2017 10:32:05 AM	C:\Sirius_T3\KOH17122.t3r
Acid concentration factor	1.003	10/7/2017 10:32:05 AM	C:\Sirius_T3\17J-06018_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 and 172875	10/6/2017 2:55:40 PM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9-22-17	9/22/2017 4:02:42 PM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	9-26-17	10/5/2017 5:02:03 PM
Port B	Cyclohexane		9/19/2017 2:15:02 PM
Port C	MeCN (50%, 0.15 M KCl)	10-2-17	10/2/2017 11:28:55 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Phosphate Buffer		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
Titration		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	-7.91 mV		10/7/2017 10:32:29 AM



Assay Settings

Sample name: **D08** Experiment start time: **10/7/2017 10:32:05 AM**
Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse**
Assay ID: **17J-07007** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07007_D08_UV-metric psKa.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Filling solution	3M KCl	KCL095	10/4/2017 3:50:10 PM
Liquids			
Wash 1	50% IPA:50% Water		10/6/2017 2:50:08 PM
Wash 2	0.5% Triton X-100 in H2O		10/6/2017 2:50:11 PM
Buffer position 1	pH7 Wash		10/6/2017 2:50:17 PM
Buffer position 2	pH 7		10/6/2017 2:50:19 PM
Storage position			10/6/2017 2:50:25 PM
Wash water	8.4e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	1.6e+003 mL		10/6/2017 3:04:33 PM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	391:10:29		11/23/2010 12:22:28 PM
Calibrated on	10/5/2017 10:23:25 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		
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		



Assay Settings

Sample name: **D08**
Assay name: **UV-metric psKa**
Assay ID: **17J-07007**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07007_D08_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 10:32:05 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

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 G3