

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07005**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07005_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 6:48:14 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

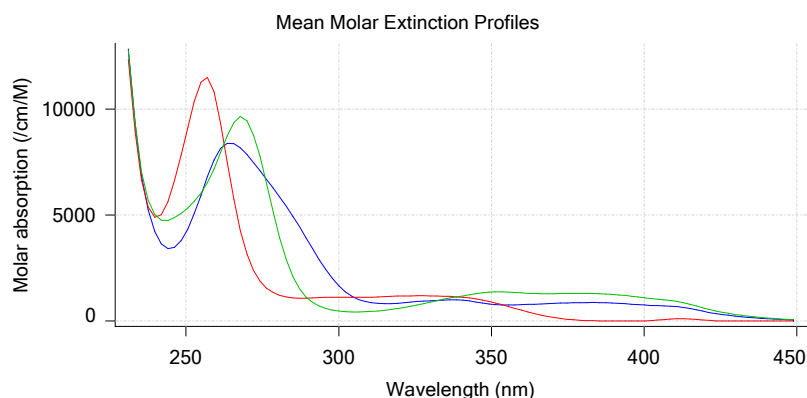
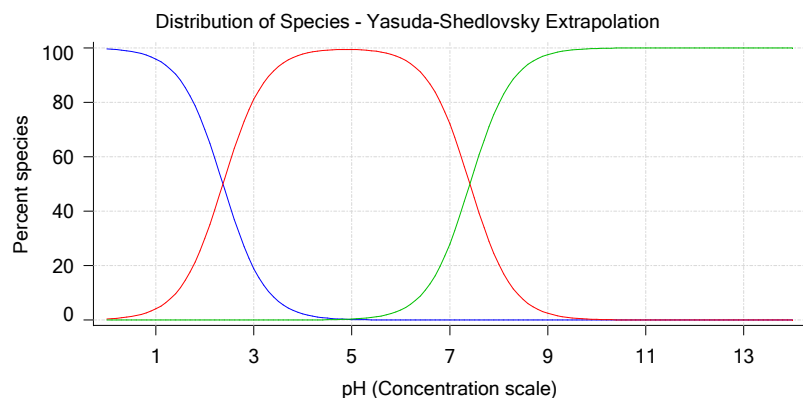
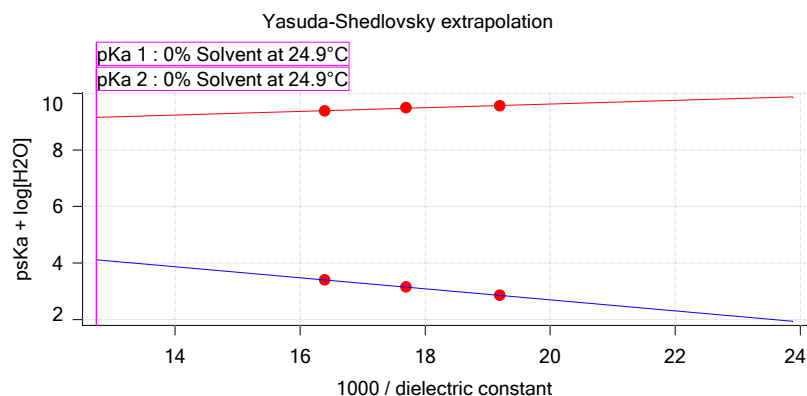
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	2.37	±0.02	6.59	-194.3321	0.9994	0.166 M	24.9°C
Yasuda-Shedlovsky	7.41	±0.04	8.34	64.2595	0.9851	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	psKa 2
17J-07005 Points 4 to 69	59.05 %	Up	UV-metric pKa	52.1	19.6 M	0.157 M	24.9°C	✓ 1.56	✓ 8.27
17J-07005 Points 71 to 142	49.70 %	Up	UV-metric pKa	56.5	24.6 M	0.167 M	24.9°C	✓ 1.76	✓ 8.09
17J-07005 Points 144 to 213	40.02 %	Up	UV-metric pKa	61.0	30.0 M	0.175 M	24.9°C	✓ 1.92	✓ 7.91

Graphs



UV-metric psKa Titration 1 of 3 17J-07005 Points 4 to 69

Results

pKa 1 **1.56**
 pKa 2 **8.27**
 RMSD **0.002 0.004 0.005**
 Chi squared **0.0225**
 PCA calculated number of pKas **4**
 Average ionic strength **0.157 M**
 Average temperature **24.9°C**
 Analyte concentration range **81.1 µM to 76.4 µM**
 Methanol weight % **59.1 %**
 Dielectric constant **52.1**
 Water concentration **19.6 M**

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 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.477 to 12.500**

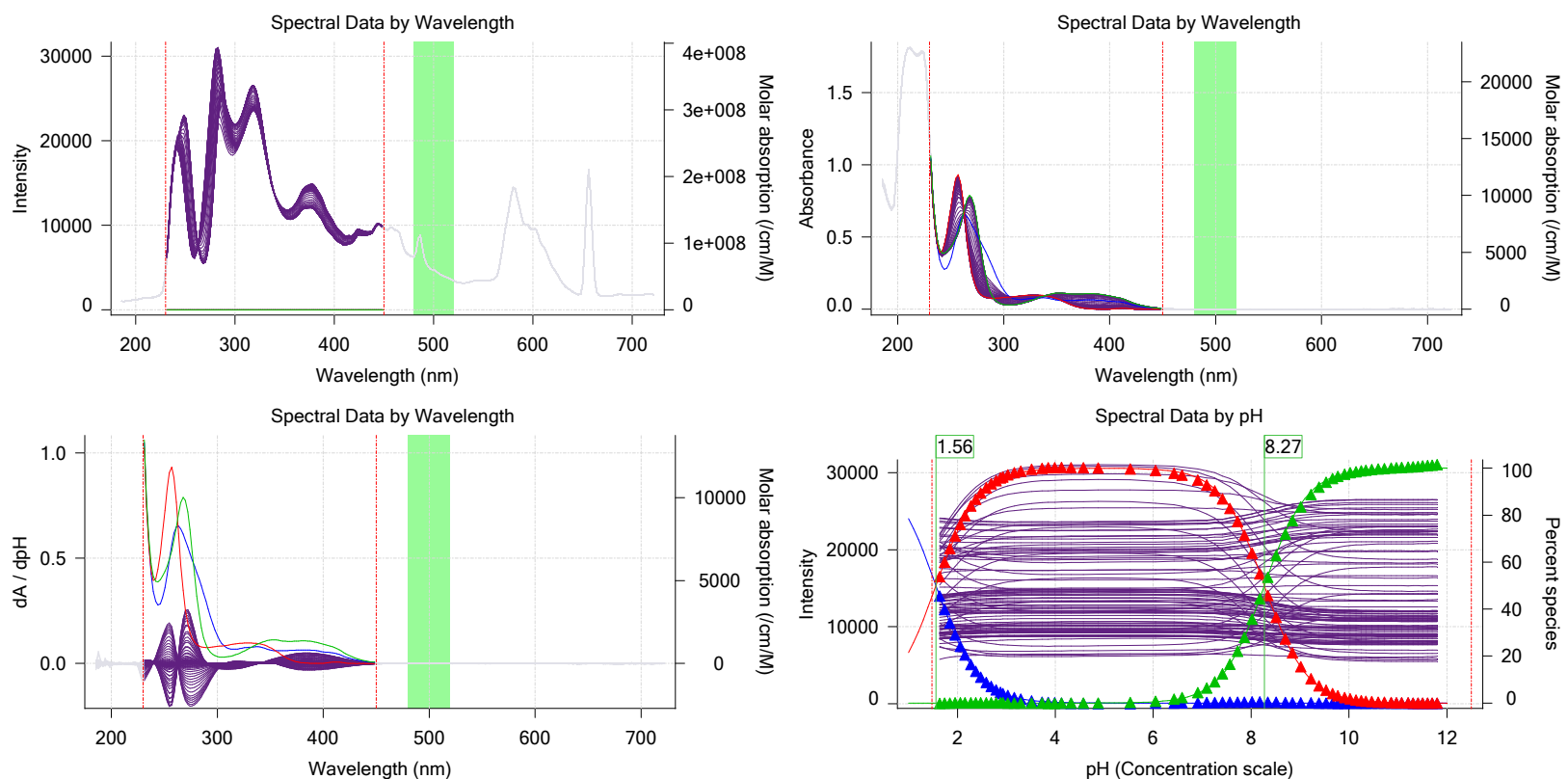
Warnings and errors

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			

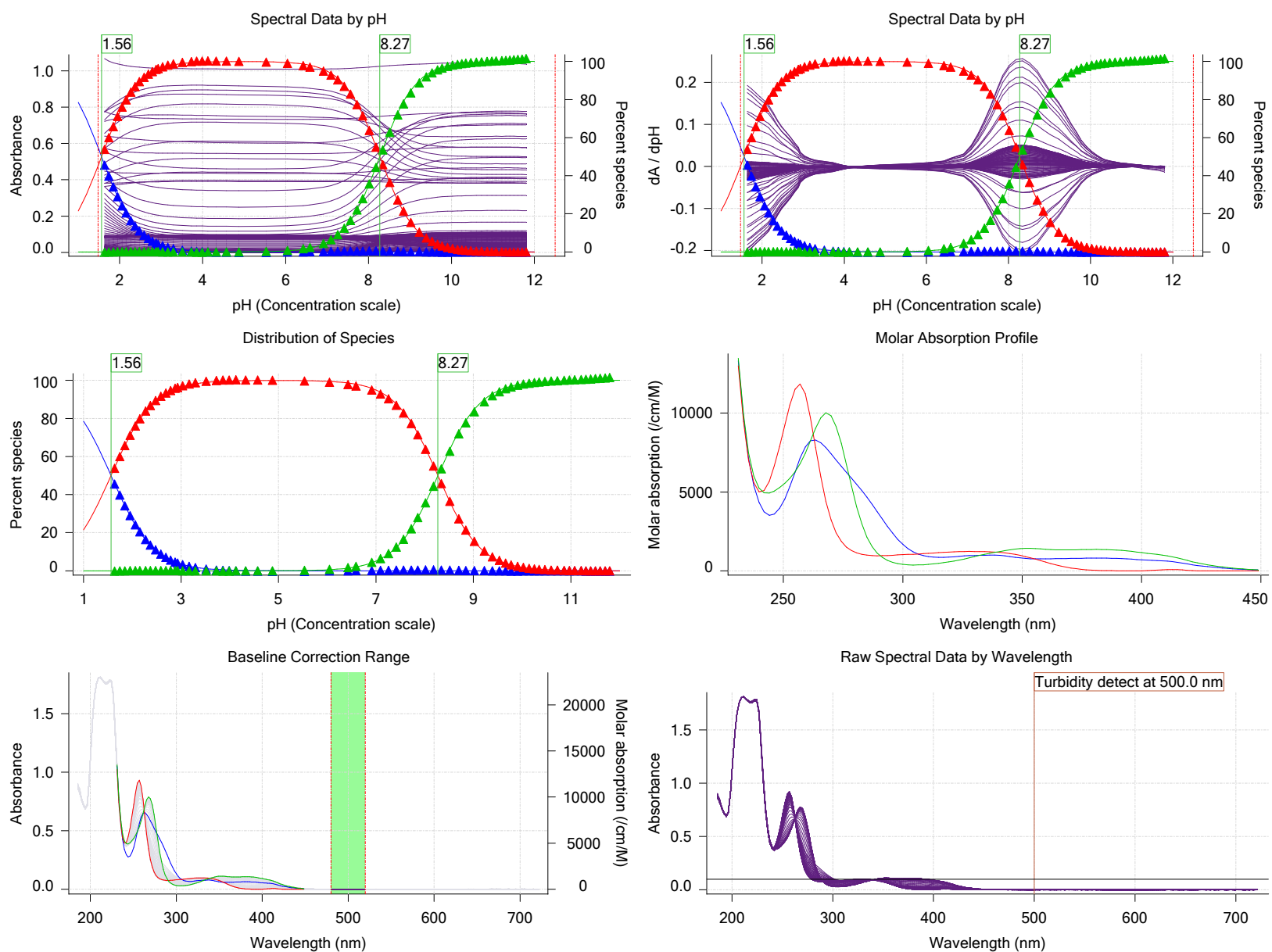
Graphs



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Graphs (continued)



UV-metric psKa Titration 2 of 3 17J-07005 Points 71 to 142

Results

pKa 1 **1.76**
 pKa 2 **8.09**
 RMSD **0.004 0.009 0.007**
 Chi squared **0.0514**
 PCA calculated number of pKas **6**
 Average ionic strength **0.167 M**
 Average temperature **24.9°C**
 Analyte concentration range **69.5 µM to 65.6 µM**
 Methanol weight % **49.7 %**
 Dielectric constant **56.5**
 Water concentration **24.6 M**

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Experiment start time: **10/7/2017 6:48:14 AM**
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Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.483 to 12.546**

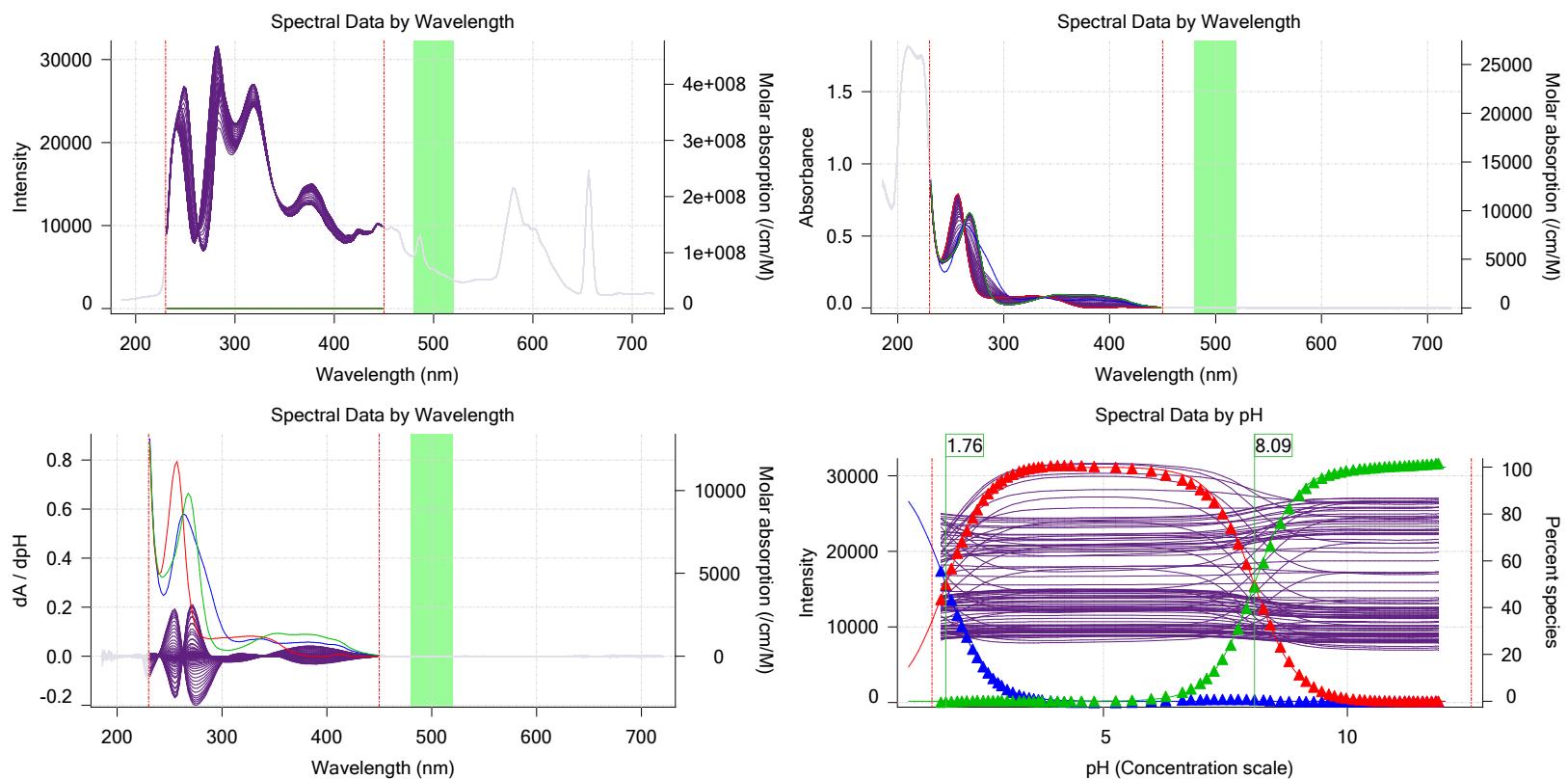
Warnings and errors

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			

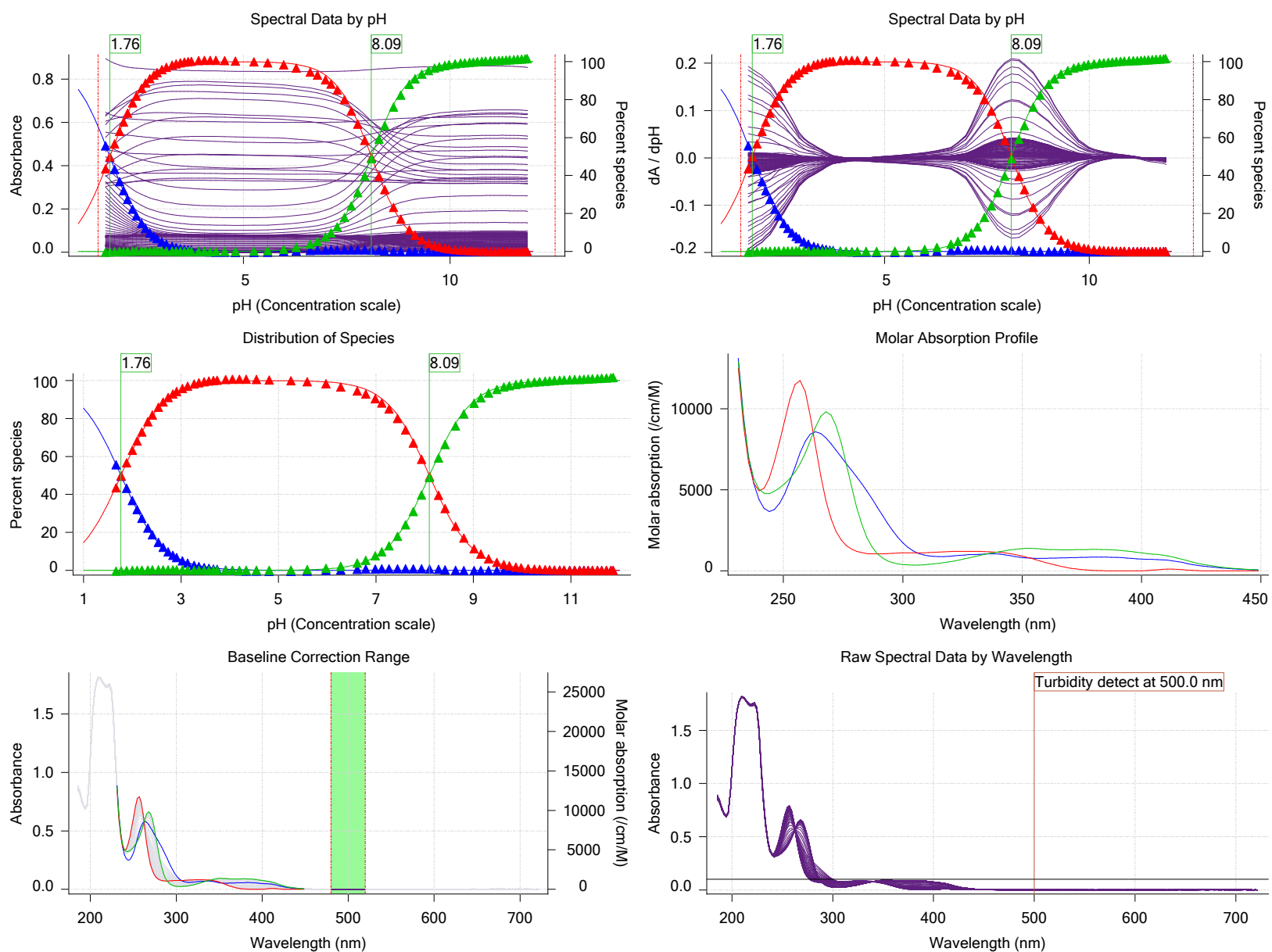
Graphs



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Graphs (continued)



UV-metric psKa Titration 3 of 3 17J-07005 Points 144 to 213

Results

pKa 1 **1.92**
 pKa 2 **7.91**
 RMSD **0.020 0.013 0.025**
 Chi squared **0.1635**
 PCA calculated number of pKas **4**
 Average ionic strength **0.175 M**
 Average temperature **24.9°C**
 Analyte concentration range **57.0 µM to 53.9 µM**
 Methanol weight % **40.0 %**
 Dielectric constant **61.0**
 Water concentration **30.0 M**

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Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.500 to 11.959**

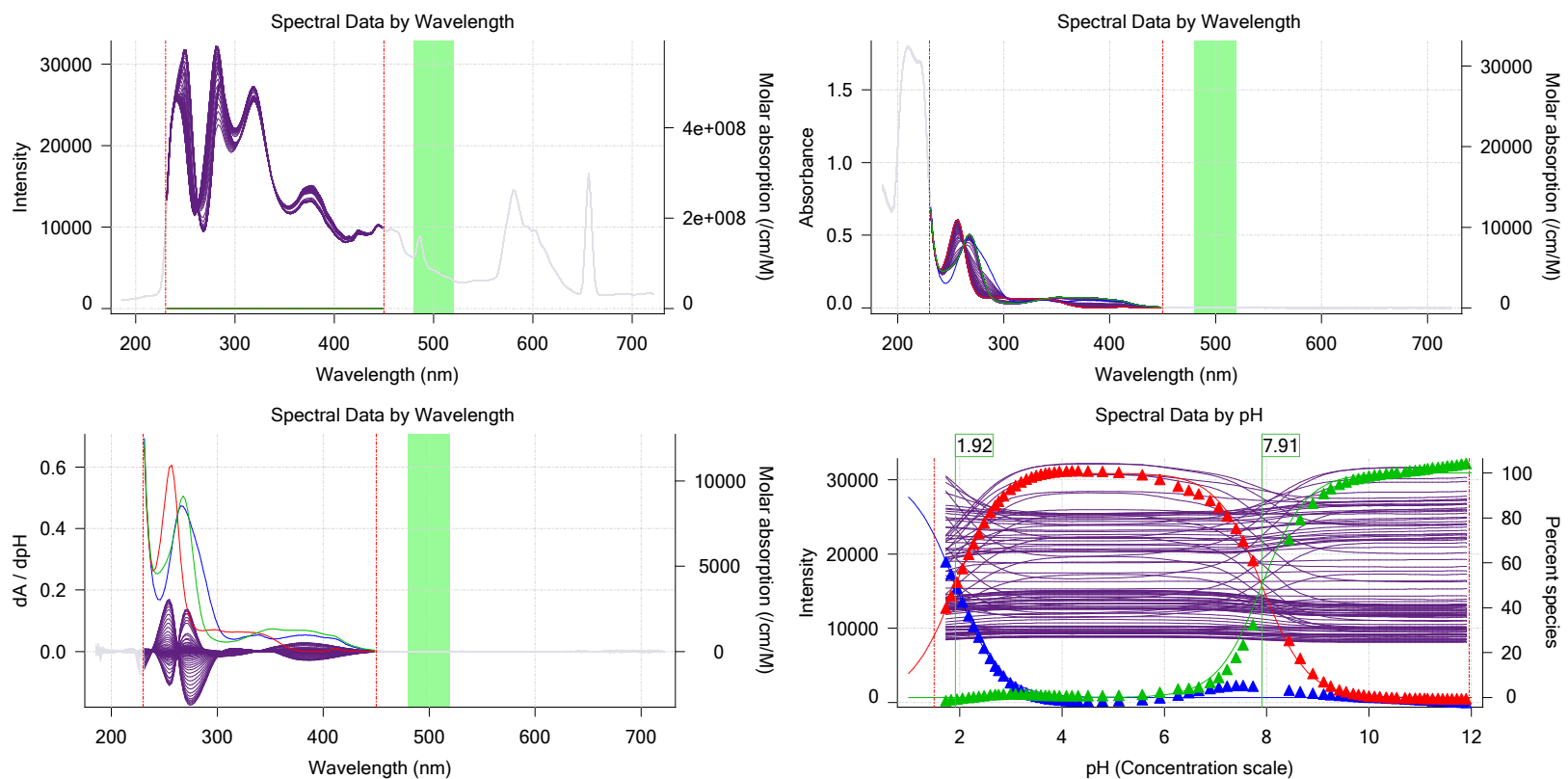
Warnings and errors

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			

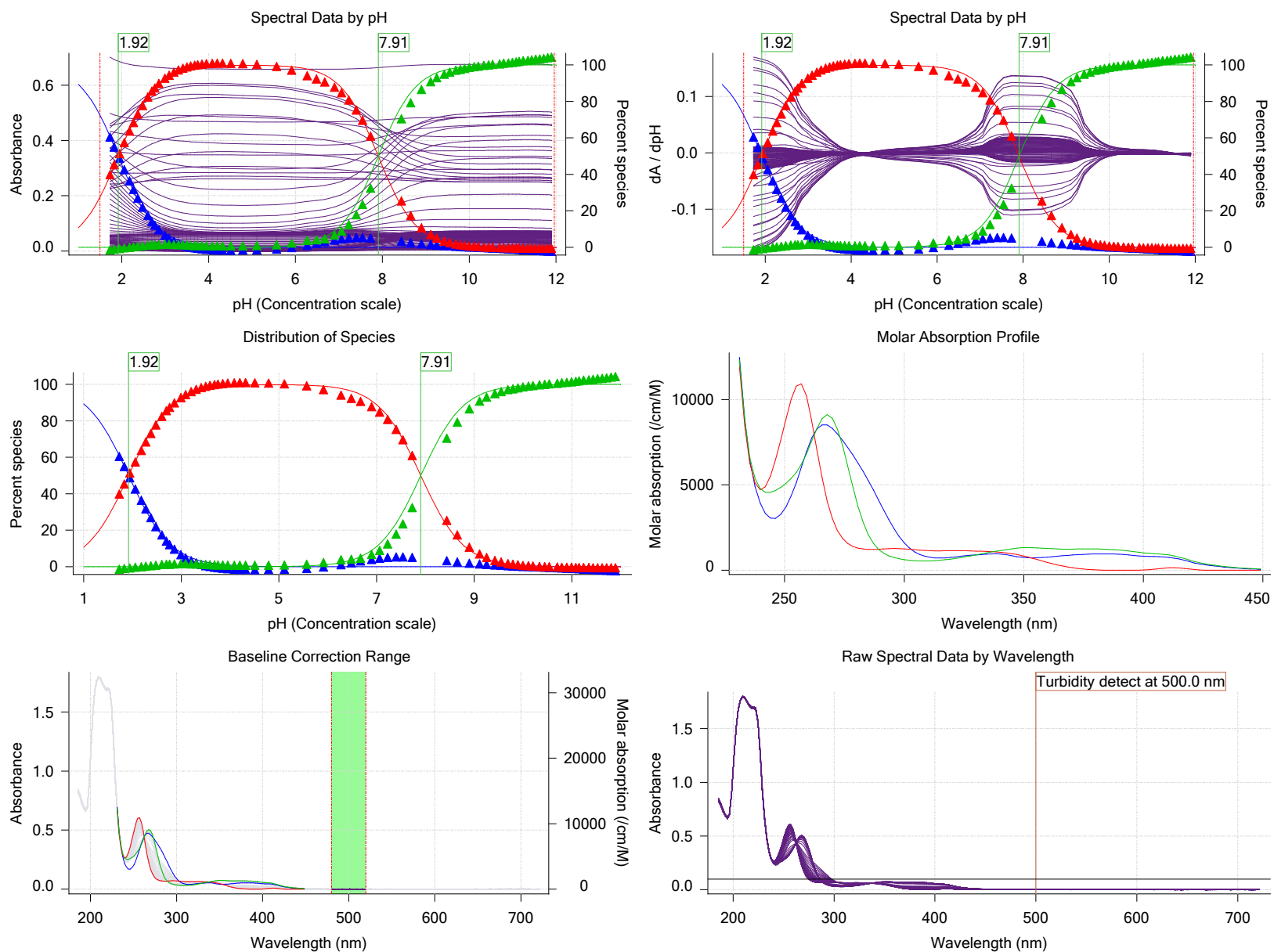
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 Analyst: **Dorothy Leverse**
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Graphs (continued)



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	D07	9/29/2017 6:39:44 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0040 mL	10/6/2017 6:08:56 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.032500 M	10/2/2017 12:59:06 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	396.95	9/29/2017 6:39:58 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	9/29/2017 6:39:44 PM	User entered value
Sample is a	Ampholyte	9/29/2017 6:39:44 PM	User entered value
pKa 1	2.43	9/29/2017 6:39:44 PM	User entered value
Type	Base	9/29/2017 6:39:44 PM	User entered value
pKa 2	7.37	9/29/2017 6:39:44 PM	User entered value
Type	Acid	9/29/2017 6:39:44 PM	User entered value

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Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logp (XH2 +)	-10.00		Default value
logP (neutral XH)	-10.00	9/29/2017 6:39:44 PM	User entered value
logP (X -)	-10.00		Default value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-square
3:12.6	Dark spectrum								
3:14.0	Reference spectrum								
3:41.6	Volume reset due to vial change								
5:12.4	Initial pH = 8.39								
6:07.0	Data point 4	0.15005 mL	0.07302 mL	0.00000 mL	1.34995 mL	0.02500 mL	1.977	-0.00844	0.60936
6:35.6	Data point 5	0.15005 mL	0.07302 mL	0.01489 mL	1.34995 mL	0.02500 mL	2.081	0.00741	0.24434
6:52.6	Data point 6	0.15005 mL	0.07302 mL	0.02672 mL	1.34995 mL	0.02500 mL	2.188	-0.00148	0.02996
7:09.5	Data point 7	0.15005 mL	0.07302 mL	0.03608 mL	1.34995 mL	0.02500 mL	2.293	-0.00052	0.00649
7:26.3	Data point 8	0.15005 mL	0.07302 mL	0.04351 mL	1.34995 mL	0.02500 mL	2.401	0.00848	0.77985
7:43.1	Data point 9	0.15005 mL	0.07302 mL	0.04932 mL	1.34995 mL	0.02500 mL	2.495	0.01395	0.88395
7:59.9	Data point 10	0.15005 mL	0.07302 mL	0.05402 mL	1.34995 mL	0.02500 mL	2.609	0.00871	0.88679
8:16.6	Data point 11	0.15005 mL	0.07302 mL	0.05764 mL	1.34995 mL	0.02500 mL	2.709	0.00843	0.88158
8:33.3	Data point 12	0.15005 mL	0.07302 mL	0.06051 mL	1.34995 mL	0.02500 mL	2.811	0.01517	0.89224
8:49.9	Data point 13	0.15005 mL	0.07302 mL	0.06277 mL	1.34995 mL	0.02500 mL	2.921	0.01823	0.84802
9:06.5	Data point 14	0.15005 mL	0.07302 mL	0.06453 mL	1.34995 mL	0.02500 mL	3.023	0.00585	0.59045
9:23.1	Data point 15	0.15005 mL	0.07302 mL	0.06595 mL	1.34995 mL	0.02500 mL	3.120	0.00694	0.69354
9:39.5	Data point 16	0.15005 mL	0.07302 mL	0.06707 mL	1.34995 mL	0.02500 mL	3.210	0.01370	0.92049
9:56.1	Data point 17	0.15005 mL	0.07302 mL	0.06799 mL	1.34995 mL	0.02500 mL	3.258	0.01130	0.89306
10:28.1	Data point 18	0.15005 mL	0.07302 mL	0.06898 mL	1.34995 mL	0.02500 mL	3.361	0.01821	0.93190
10:54.9	Data point 19	0.15005 mL	0.07302 mL	0.06966 mL	1.34995 mL	0.02500 mL	3.491	0.02144	0.98095
11:11.5	Data point 20	0.15005 mL	0.07302 mL	0.07013 mL	1.34995 mL	0.02500 mL	3.618	0.02815	0.96262
11:33.2	Data point 21	0.15005 mL	0.07302 mL	0.07070 mL	1.34995 mL	0.02500 mL	3.835	0.04153	0.98267
11:54.9	Data point 22	0.15005 mL	0.07302 mL	0.07110 mL	1.34995 mL	0.02500 mL	4.047	0.05932	0.99280
12:16.5	Data point 23	0.15005 mL	0.07302 mL	0.07133 mL	1.34995 mL	0.02500 mL	4.174	0.08941	0.98487
12:38.2	Data point 24	0.15005 mL	0.07302 mL	0.07150 mL	1.34995 mL	0.02500 mL	4.305	0.10041	0.99564
13:05.4	Data point 25	0.15005 mL	0.07302 mL	0.07161 mL	1.34995 mL	0.02500 mL	4.439	0.09853	0.99041
13:40.8	Data point 26	0.15005 mL	0.07302 mL	0.07173 mL	1.34995 mL	0.02500 mL	4.634	0.09888	0.97258
14:26.9	Data point 27	0.15005 mL	0.07302 mL	0.07183 mL	1.34995 mL	0.02500 mL	4.880	0.10093	0.99448
15:30.7	Data point 28	0.15005 mL	0.07302 mL	0.07190 mL	1.34995 mL	0.02500 mL	5.176	0.11714	0.99613
16:47.4	Data point 29	0.15005 mL	0.07302 mL	0.07197 mL	1.34995 mL	0.02500 mL	5.826	0.24342	0.99419
17:59.1	Data point 30	0.15005 mL	0.07302 mL	0.07201 mL	1.34995 mL	0.02500 mL	6.333	0.19128	0.99426
19:10.8	Data point 31	0.15005 mL	0.07302 mL	0.07206 mL	1.34995 mL	0.02500 mL	6.705	0.10630	0.99670
20:27.4	Data point 32	0.15005 mL	0.07302 mL	0.07213 mL	1.34995 mL	0.02500 mL	6.868	-0.05812	0.36422
20:49.1	Data point 33	0.15005 mL	0.07302 mL	0.07218 mL	1.34995 mL	0.02500 mL	7.185	0.09749	0.99339
21:40.8	Data point 34	0.15005 mL	0.07302 mL	0.07225 mL	1.34995 mL	0.02500 mL	7.363	0.09998	0.99177
22:26.2	Data point 35	0.15005 mL	0.07302 mL	0.07232 mL	1.34995 mL	0.02500 mL	7.528	0.10020	0.98258
23:08.6	Data point 36	0.15005 mL	0.07302 mL	0.07241 mL	1.34995 mL	0.02500 mL	7.683	0.09952	0.97569
23:42.4	Data point 37	0.15005 mL	0.07302 mL	0.07248 mL	1.34995 mL	0.02500 mL	7.828	0.09765	0.99147
24:23.2	Data point 38	0.15005 mL	0.07302 mL	0.07258 mL	1.34995 mL	0.02500 mL	7.984	0.09949	0.99227
25:05.2	Data point 39	0.15005 mL	0.07302 mL	0.07267 mL	1.34995 mL	0.02500 mL	8.120	0.09844	0.99386
25:45.0	Data point 40	0.15005 mL	0.07302 mL	0.07277 mL	1.34995 mL	0.02500 mL	8.276	0.09758	0.98996
26:26.1	Data point 41	0.15005 mL	0.07302 mL	0.07286 mL	1.34995 mL	0.02500 mL	8.435	0.09616	0.98564
27:10.3	Data point 42	0.15005 mL	0.07302 mL	0.07295 mL	1.34995 mL	0.02500 mL	8.595	0.09948	0.98929
27:53.7	Data point 43	0.15005 mL	0.07302 mL	0.07305 mL	1.34995 mL	0.02500 mL	8.764	0.09802	0.99189
28:39.0	Data point 44	0.15005 mL	0.07302 mL	0.07314 mL	1.34995 mL	0.02500 mL	8.950	0.09751	0.96520
29:16.0	Data point 45	0.15005 mL	0.07302 mL	0.07321 mL	1.34995 mL	0.02500 mL	9.091	0.09818	0.95920
29:50.2	Data point 46	0.15005 mL	0.07302 mL	0.07328 mL	1.34995 mL	0.02500 mL	9.261	0.09957	0.99220
30:33.7	Data point 47	0.15005 mL	0.07302 mL	0.07338 mL	1.34995 mL	0.02500 mL	9.463	0.09808	0.98699
31:16.6	Data point 48	0.15005 mL	0.07302 mL	0.07347 mL	1.34995 mL	0.02500 mL	9.627	0.09830	0.98101
31:51.3	Data point 49	0.15005 mL	0.07302 mL	0.07357 mL	1.34995 mL	0.02500 mL	9.766	0.09382	0.96644

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Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH Slope
32:22.4	Data point 50	0.15005 mL	0.07302 mL	0.07366 mL	1.34995 mL	0.02500 mL	9.896	0.09514	0.98329	0.98329
32:47.0	Data point 51	0.15005 mL	0.07302 mL	0.07375 mL	1.34995 mL	0.02500 mL	10.004	0.09535	0.96735	0.96735
33:15.3	Data point 52	0.15005 mL	0.07302 mL	0.07387 mL	1.34995 mL	0.02500 mL	10.138	0.09499	0.97067	0.97067
33:42.6	Data point 53	0.15005 mL	0.07302 mL	0.07401 mL	1.34995 mL	0.02500 mL	10.255	0.07895	0.96512	0.96512
34:04.3	Data point 54	0.15005 mL	0.07302 mL	0.07418 mL	1.34995 mL	0.02500 mL	10.372	0.04171	0.98169	0.98169
34:25.9	Data point 55	0.15005 mL	0.07302 mL	0.07437 mL	1.34995 mL	0.02500 mL	10.474	0.03086	0.91333	0.91333
34:47.6	Data point 56	0.15005 mL	0.07302 mL	0.07458 mL	1.34995 mL	0.02500 mL	10.571	0.02794	0.96847	0.96847
35:04.2	Data point 57	0.15005 mL	0.07302 mL	0.07481 mL	1.34995 mL	0.02500 mL	10.687	0.01768	0.86505	0.86505
35:25.9	Data point 58	0.15005 mL	0.07302 mL	0.07524 mL	1.34995 mL	0.02500 mL	10.817	0.00521	0.46073	0.46073
35:47.7	Data point 59	0.15005 mL	0.07302 mL	0.07585 mL	1.34995 mL	0.02500 mL	10.944	0.00746	0.71056	0.71056
36:09.4	Data point 60	0.15005 mL	0.07302 mL	0.07691 mL	1.34995 mL	0.02500 mL	11.077	0.00470	0.46090	0.46090
36:41.3	Data point 61	0.15005 mL	0.07302 mL	0.07789 mL	1.34995 mL	0.02500 mL	11.186	-0.00207	0.23717	0.23717
37:13.4	Data point 62	0.15005 mL	0.07302 mL	0.07890 mL	1.34995 mL	0.02500 mL	11.291	-0.00206	0.21221	0.21221
37:30.1	Data point 63	0.15005 mL	0.07302 mL	0.08010 mL	1.34995 mL	0.02500 mL	11.423	-0.00172	0.08215	0.08215
37:57.1	Data point 64	0.15005 mL	0.07302 mL	0.08168 mL	1.34995 mL	0.02500 mL	11.519	-0.00318	0.48627	0.48627
38:13.6	Data point 65	0.15005 mL	0.07302 mL	0.08373 mL	1.34995 mL	0.02500 mL	11.616	-0.00247	0.44097	0.44097
38:30.2	Data point 66	0.15005 mL	0.07302 mL	0.08629 mL	1.34995 mL	0.02500 mL	11.710	-0.00108	0.06764	0.06764
38:46.9	Data point 67	0.15005 mL	0.07302 mL	0.08946 mL	1.34995 mL	0.02500 mL	11.808	-0.00268	0.19359	0.19359
39:03.7	Data point 68	0.15005 mL	0.07302 mL	0.09349 mL	1.34995 mL	0.02500 mL	11.906	-0.00482	0.47391	0.47391
39:20.5	Data point 69	0.15005 mL	0.07302 mL	0.09857 mL	1.34995 mL	0.02500 mL	12.000	-0.00719	0.80490	0.80490
40:55.2	Reference spectrum									
41:57.9	Data point 71	0.22001 mL	0.17302 mL	0.09859 mL	1.34995 mL	0.02500 mL	1.983	-0.05063	0.92399	0.92399
42:25.3	Data point 72	0.22001 mL	0.17302 mL	0.11395 mL	1.34995 mL	0.02500 mL	2.085	0.01345	0.87942	0.87942
42:42.3	Data point 73	0.22001 mL	0.17302 mL	0.12683 mL	1.34995 mL	0.02500 mL	2.198	0.02163	0.93717	0.93717
42:59.1	Data point 74	0.22001 mL	0.17302 mL	0.13697 mL	1.34995 mL	0.02500 mL	2.314	0.01343	0.85378	0.85378
43:21.1	Data point 75	0.22001 mL	0.17302 mL	0.14344 mL	1.34995 mL	0.02500 mL	2.409	0.00728	0.25975	0.25975
43:48.2	Data point 76	0.22001 mL	0.17302 mL	0.14918 mL	1.34995 mL	0.02500 mL	2.508	0.01458	0.90346	0.90346
44:04.9	Data point 77	0.22001 mL	0.17302 mL	0.15414 mL	1.34995 mL	0.02500 mL	2.626	0.01400	0.88701	0.88701
44:31.9	Data point 78	0.22001 mL	0.17302 mL	0.15781 mL	1.34995 mL	0.02500 mL	2.718	0.01821	0.92354	0.92354
44:48.6	Data point 79	0.22001 mL	0.17302 mL	0.16087 mL	1.34995 mL	0.02500 mL	2.842	0.00862	0.88959	0.88959
45:15.7	Data point 80	0.22001 mL	0.17302 mL	0.16296 mL	1.34995 mL	0.02500 mL	2.939	0.00662	0.83628	0.83628
45:32.4	Data point 81	0.22001 mL	0.17302 mL	0.16482 mL	1.34995 mL	0.02500 mL	3.040	0.01214	0.80762	0.80762
45:49.1	Data point 82	0.22001 mL	0.17302 mL	0.16628 mL	1.34995 mL	0.02500 mL	3.135	0.01585	0.94010	0.94010
46:05.8	Data point 83	0.22001 mL	0.17302 mL	0.16743 mL	1.34995 mL	0.02500 mL	3.210	0.00827	0.82895	0.82895
46:37.9	Data point 84	0.22001 mL	0.17302 mL	0.16860 mL	1.34995 mL	0.02500 mL	3.327	0.01344	0.89929	0.89929
47:04.8	Data point 85	0.22001 mL	0.17302 mL	0.16928 mL	1.34995 mL	0.02500 mL	3.435	0.01072	0.80236	0.80236
47:21.4	Data point 86	0.22001 mL	0.17302 mL	0.16987 mL	1.34995 mL	0.02500 mL	3.568	0.02319	0.97954	0.97954
47:48.3	Data point 87	0.22001 mL	0.17302 mL	0.17034 mL	1.34995 mL	0.02500 mL	3.664	0.02265	0.95978	0.95978
48:04.7	Data point 88	0.22001 mL	0.17302 mL	0.17067 mL	1.34995 mL	0.02500 mL	3.768	0.02828	0.97186	0.97186
48:21.3	Data point 89	0.22001 mL	0.17302 mL	0.17093 mL	1.34995 mL	0.02500 mL	3.862	0.03672	0.98754	0.98754
48:37.8	Data point 90	0.22001 mL	0.17302 mL	0.17114 mL	1.34995 mL	0.02500 mL	3.954	0.03215	0.97041	0.97041
48:54.5	Data point 91	0.22001 mL	0.17302 mL	0.17131 mL	1.34995 mL	0.02500 mL	4.033	0.05531	0.98418	0.98418
49:16.1	Data point 92	0.22001 mL	0.17302 mL	0.17154 mL	1.34995 mL	0.02500 mL	4.203	0.06936	0.99118	0.99118
49:37.7	Data point 93	0.22001 mL	0.17302 mL	0.17171 mL	1.34995 mL	0.02500 mL	4.342	0.09502	0.99211	0.99211
49:59.2	Data point 94	0.22001 mL	0.17302 mL	0.17183 mL	1.34995 mL	0.02500 mL	4.481	0.09857	0.98803	0.98803
50:26.8	Data point 95	0.22001 mL	0.17302 mL	0.17192 mL	1.34995 mL	0.02500 mL	4.617	0.09946	0.99064	0.99064
51:04.1	Data point 96	0.22001 mL	0.17302 mL	0.17201 mL	1.34995 mL	0.02500 mL	4.827	0.10024	0.99062	0.99062
51:53.8	Data point 97	0.22001 mL	0.17302 mL	0.17208 mL	1.34995 mL	0.02500 mL	5.083	0.09873	0.99152	0.99152
52:55.9	Data point 98	0.22001 mL	0.17302 mL	0.17215 mL	1.34995 mL	0.02500 mL	5.524	0.11129	0.99586	0.99586
54:07.5	Data point 99	0.22001 mL	0.17302 mL	0.17220 mL	1.34995 mL	0.02500 mL	5.854	0.09011	0.87481	0.87481
55:06.2	Data point 100	0.22001 mL	0.17302 mL	0.17225 mL	1.34995 mL	0.02500 mL	6.238	0.08159	0.75439	0.75439
56:09.9	Data point 101	0.22001 mL	0.17302 mL	0.17230 mL	1.34995 mL	0.02500 mL	6.537	0.09892	0.98567	0.98567
57:22.7	Data point 102	0.22001 mL	0.17302 mL	0.17237 mL	1.34995 mL	0.02500 mL	6.870	0.09945	0.97989	0.97989
58:14.8	Data point 103	0.22001 mL	0.17302 mL	0.17244 mL	1.34995 mL	0.02500 mL	7.043	0.09911	0.99070	0.99070
58:57.7	Data point 104	0.22001 mL	0.17302 mL	0.17251 mL	1.34995 mL	0.02500 mL	7.232	0.09990	0.99074	0.99074
59:40.9	Data point 105	0.22001 mL	0.17302 mL	0.17258 mL	1.34995 mL	0.02500 mL	7.366	0.10064	0.99226	0.99226
1:00:16.1	Data point 106	0.22001 mL	0.17302 mL	0.17265 mL	1.34995 mL	0.02500 mL	7.511	0.09962	0.98854	0.98854



Assay Events

Sample name: **D07** Experiment start time: **10/7/2017 6:48:14 AM**
Assay name: **UV-metric psKa** Analyst: **Dorothy Leverse**
Assay ID: **17J-07005** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07005_D07_UV-metric psKa.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
1:00:58.7	Data point 107	0.22001 mL	0.17302 mL	0.17274 mL	1.34995 mL	0.02500 mL	7.684	0.10096	0.99397	0.99397
1:01:39.3	Data point 108	0.22001 mL	0.17302 mL	0.17284 mL	1.34995 mL	0.02500 mL	7.849	0.10002	0.99327	0.99327
1:02:20.2	Data point 109	0.22001 mL	0.17302 mL	0.17293 mL	1.34995 mL	0.02500 mL	8.002	0.10003	0.99713	0.99713
1:02:59.0	Data point 110	0.22001 mL	0.17302 mL	0.17302 mL	1.34995 mL	0.02500 mL	8.172	0.09890	0.98826	0.98826
1:03:39.6	Data point 111	0.22001 mL	0.17302 mL	0.17312 mL	1.34995 mL	0.02500 mL	8.334	0.10076	0.98883	0.98883
1:04:22.9	Data point 112	0.22001 mL	0.17302 mL	0.17321 mL	1.34995 mL	0.02500 mL	8.514	0.09665	0.99231	0.99231
1:05:00.5	Data point 113	0.22001 mL	0.17302 mL	0.17328 mL	1.34995 mL	0.02500 mL	8.648	0.09960	0.98753	0.98753
1:05:34.8	Data point 114	0.22001 mL	0.17302 mL	0.17335 mL	1.34995 mL	0.02500 mL	8.858	0.09603	0.98432	0.98432
1:06:16.0	Data point 115	0.22001 mL	0.17302 mL	0.17342 mL	1.34995 mL	0.02500 mL	9.029	0.09671	0.95840	0.95840
1:06:51.2	Data point 116	0.22001 mL	0.17302 mL	0.17350 mL	1.34995 mL	0.02500 mL	9.235	0.09804	0.98515	0.98515
1:07:30.0	Data point 117	0.22001 mL	0.17302 mL	0.17357 mL	1.34995 mL	0.02500 mL	9.371	0.09679	0.98598	0.98598
1:08:00.9	Data point 118	0.22001 mL	0.17302 mL	0.17364 mL	1.34995 mL	0.02500 mL	9.531	0.09358	0.97557	0.97557
1:08:39.3	Data point 119	0.22001 mL	0.17302 mL	0.17373 mL	1.34995 mL	0.02500 mL	9.693	0.09988	0.98946	0.98946
1:09:10.5	Data point 120	0.22001 mL	0.17302 mL	0.17382 mL	1.34995 mL	0.02500 mL	9.836	0.09673	0.96626	0.96626
1:09:35.6	Data point 121	0.22001 mL	0.17302 mL	0.17392 mL	1.34995 mL	0.02500 mL	9.950	0.08926	0.97905	0.97905
1:09:57.3	Data point 122	0.22001 mL	0.17302 mL	0.17404 mL	1.34995 mL	0.02500 mL	10.082	0.06782	0.97556	0.97556
1:10:24.0	Data point 123	0.22001 mL	0.17302 mL	0.17418 mL	1.34995 mL	0.02500 mL	10.187	0.04198	0.95103	0.95103
1:10:45.6	Data point 124	0.22001 mL	0.17302 mL	0.17436 mL	1.34995 mL	0.02500 mL	10.327	0.03213	0.96574	0.96574
1:11:07.2	Data point 125	0.22001 mL	0.17302 mL	0.17460 mL	1.34995 mL	0.02500 mL	10.458	0.02160	0.93956	0.93956
1:11:28.8	Data point 126	0.22001 mL	0.17302 mL	0.17488 mL	1.34995 mL	0.02500 mL	10.563	0.01488	0.95717	0.95717
1:11:50.6	Data point 127	0.22001 mL	0.17302 mL	0.17524 mL	1.34995 mL	0.02500 mL	10.671	0.01106	0.82578	0.82578
1:12:17.3	Data point 128	0.22001 mL	0.17302 mL	0.17568 mL	1.34995 mL	0.02500 mL	10.764	0.00535	0.67749	0.67749
1:12:49.2	Data point 129	0.22001 mL	0.17302 mL	0.17627 mL	1.34995 mL	0.02500 mL	10.862	0.00173	0.14978	0.14978
1:13:21.1	Data point 130	0.22001 mL	0.17302 mL	0.17705 mL	1.34995 mL	0.02500 mL	10.965	-0.00057	0.02373	0.02373
1:13:47.9	Data point 131	0.22001 mL	0.17302 mL	0.17771 mL	1.34995 mL	0.02500 mL	11.058	-0.00042	0.01281	0.01281
1:14:04.6	Data point 132	0.22001 mL	0.17302 mL	0.17858 mL	1.34995 mL	0.02500 mL	11.168	-0.00440	0.57017	0.57017
1:14:21.3	Data point 133	0.22001 mL	0.17302 mL	0.17970 mL	1.34995 mL	0.02500 mL	11.271	-0.00310	0.47272	0.47272
1:14:38.0	Data point 134	0.22001 mL	0.17302 mL	0.18112 mL	1.34995 mL	0.02500 mL	11.370	-0.00258	0.28840	0.28840
1:14:54.7	Data point 135	0.22001 mL	0.17302 mL	0.18290 mL	1.34995 mL	0.02500 mL	11.458	-0.00442	0.55498	0.55498
1:15:11.4	Data point 136	0.22001 mL	0.17302 mL	0.18509 mL	1.34995 mL	0.02500 mL	11.543	-0.00453	0.65818	0.65818
1:15:28.0	Data point 137	0.22001 mL	0.17302 mL	0.18775 mL	1.34995 mL	0.02500 mL	11.631	-0.00587	0.70934	0.70934
1:15:44.7	Data point 138	0.22001 mL	0.17302 mL	0.19104 mL	1.34995 mL	0.02500 mL	11.729	-0.00311	0.38730	0.38730
1:16:01.3	Data point 139	0.22001 mL	0.17302 mL	0.19520 mL	1.34995 mL	0.02500 mL	11.817	-0.00369	0.37333	0.37333
1:16:17.9	Data point 140	0.22001 mL	0.17302 mL	0.20033 mL	1.34995 mL	0.02500 mL	11.912	-0.00266	0.31087	0.31087
1:16:34.6	Data point 141	0.22001 mL	0.17302 mL	0.20675 mL	1.34995 mL	0.02500 mL	11.999	-0.00479	0.61370	0.61370
1:16:51.3	Data point 142	0.22001 mL	0.17302 mL	0.21056 mL	1.34995 mL	0.02500 mL	12.046	-0.00294	0.37781	0.37781
1:18:33.3	Reference spectrum									
1:19:53.7	Data point 144	0.39005 mL	0.30014 mL	0.21058 mL	1.34995 mL	0.02500 mL	2.000	-0.06697	0.94722	0.94722
1:20:20.9	Data point 145	0.39005 mL	0.30014 mL	0.22737 mL	1.34995 mL	0.02500 mL	2.101	0.00989	0.90045	0.90045
1:20:37.7	Data point 146	0.39005 mL	0.30014 mL	0.24106 mL	1.34995 mL	0.02500 mL	2.214	0.01213	0.63503	0.63503
1:20:54.6	Data point 147	0.39005 mL	0.30014 mL	0.25160 mL	1.34995 mL	0.02500 mL	2.324	-0.00585	0.30179	0.30179
1:21:11.3	Data point 148	0.39005 mL	0.30014 mL	0.25995 mL	1.34995 mL	0.02500 mL	2.442	0.00223	0.06292	0.06292
1:21:33.1	Data point 149	0.39005 mL	0.30014 mL	0.26512 mL	1.34995 mL	0.02500 mL	2.536	0.01213	0.94494	0.94494
1:22:00.1	Data point 150	0.39005 mL	0.30014 mL	0.26973 mL	1.34995 mL	0.02500 mL	2.635	0.01288	0.91124	0.91124
1:22:16.8	Data point 151	0.39005 mL	0.30014 mL	0.27375 mL	1.34995 mL	0.02500 mL	2.740	0.00602	0.72228	0.72228
1:22:33.5	Data point 152	0.39005 mL	0.30014 mL	0.27695 mL	1.34995 mL	0.02500 mL	2.857	0.01695	0.86723	0.86723
1:23:00.3	Data point 153	0.39005 mL	0.30014 mL	0.27942 mL	1.34995 mL	0.02500 mL	2.953	0.00427	0.45003	0.45003
1:23:32.6	Data point 154	0.39005 mL	0.30014 mL	0.28137 mL	1.34995 mL	0.02500 mL	3.018	0.01061	0.85581	0.85581
1:23:54.4	Data point 155	0.39005 mL	0.30014 mL	0.28314 mL	1.34995 mL	0.02500 mL	3.111	0.00838	0.75933	0.75933
1:24:11.1	Data point 156	0.39005 mL	0.30014 mL	0.28448 mL	1.34995 mL	0.02500 mL	3.244	0.00188	0.11929	0.11929
1:24:37.8	Data point 157	0.39005 mL	0.30014 mL	0.28535 mL	1.34995 mL	0.02500 mL	3.342	0.01176	0.94564	0.94564
1:24:54.3	Data point 158	0.39005 mL	0.30014 mL	0.28612 mL	1.34995 mL	0.02500 mL	3.451	0.00876	0.81858	0.81858
1:25:10.9	Data point 159	0.39005 mL	0.30014 mL	0.28674 mL	1.34995 mL	0.02500 mL	3.554	0.01069	0.84161	0.84161
1:25:27.4	Data point 160	0.39005 mL	0.30014 mL	0.28723 mL	1.34995 mL	0.02500 mL	3.654	0.01455	0.91454	0.91454
1:25:44.0	Data point 161	0.39005 mL	0.30014 mL	0.28761 mL	1.34995 mL	0.02500 mL	3.746	0.01642	0.93127	0.93127
1:26:00.6	Data point 162	0.39005 mL	0.30014 mL	0.28791 mL	1.34995 mL	0.02500 mL	3.834	0.02678	0.92693	0.92693
1:26:17.2	Data point 163	0.39005 mL	0.30014 mL	0.28817 mL	1.34995 mL	0.02500 mL	3.925	0.02740	0.98730	0.98730

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07005**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07005_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 6:48:14 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
1:26:33.8	Data point 164	0.39005 mL	0.30014 mL	0.28836 mL	1.34995 mL	0.02500 mL	3.994	0.03465	0.97320	0.0017
1:26:55.6	Data point 165	0.39005 mL	0.30014 mL	0.28857 mL	1.34995 mL	0.02500 mL	4.093	0.04878	0.98344	0.0024
1:27:17.2	Data point 166	0.39005 mL	0.30014 mL	0.28874 mL	1.34995 mL	0.02500 mL	4.192	0.06520	0.99095	0.0032
1:27:38.9	Data point 167	0.39005 mL	0.30014 mL	0.28890 mL	1.34995 mL	0.02500 mL	4.326	0.08586	0.98674	0.0042
1:28:00.6	Data point 168	0.39005 mL	0.30014 mL	0.28902 mL	1.34995 mL	0.02500 mL	4.437	0.09701	0.96350	0.0048
1:28:24.9	Data point 169	0.39005 mL	0.30014 mL	0.28911 mL	1.34995 mL	0.02500 mL	4.556	0.09990	0.98951	0.0049
1:28:56.1	Data point 170	0.39005 mL	0.30014 mL	0.28920 mL	1.34995 mL	0.02500 mL	4.743	0.09989	0.97405	0.0049
1:29:35.8	Data point 171	0.39005 mL	0.30014 mL	0.28930 mL	1.34995 mL	0.02500 mL	5.021	0.09871	0.99244	0.0048
1:30:25.6	Data point 172	0.39005 mL	0.30014 mL	0.28937 mL	1.34995 mL	0.02500 mL	5.338	0.10052	0.99039	0.0049
1:31:24.4	Data point 173	0.39005 mL	0.30014 mL	0.28944 mL	1.34995 mL	0.02500 mL	5.789	0.09680	0.98229	0.0048
1:32:28.5	Data point 174	0.39005 mL	0.30014 mL	0.28951 mL	1.34995 mL	0.02500 mL	6.129	0.10015	0.98565	0.0049
1:33:26.8	Data point 175	0.39005 mL	0.30014 mL	0.28961 mL	1.34995 mL	0.02500 mL	6.484	0.09837	0.99411	0.0048
1:34:13.9	Data point 176	0.39005 mL	0.30014 mL	0.28968 mL	1.34995 mL	0.02500 mL	6.692	0.10045	0.99615	0.0049
1:34:56.0	Data point 177	0.39005 mL	0.30014 mL	0.28975 mL	1.34995 mL	0.02500 mL	6.880	0.09783	0.99169	0.0048
1:35:38.3	Data point 178	0.39005 mL	0.30014 mL	0.28984 mL	1.34995 mL	0.02500 mL	7.104	0.09953	0.97819	0.0049
1:36:16.6	Data point 179	0.39005 mL	0.30014 mL	0.28993 mL	1.34995 mL	0.02500 mL	7.266	0.09959	0.99677	0.0049
1:36:54.3	Data point 180	0.39005 mL	0.30014 mL	0.29008 mL	1.34995 mL	0.02500 mL	7.432	0.09444	0.96454	0.0047
1:37:36.2	Data point 181	0.39005 mL	0.30014 mL	0.29022 mL	1.34995 mL	0.02500 mL	7.601	0.09990	0.97808	0.0049
1:38:10.8	Data point 182	0.39005 mL	0.30014 mL	0.29036 mL	1.34995 mL	0.02500 mL	7.741	0.09950	0.99219	0.0049
1:38:50.7	Data point 183	0.39005 mL	0.30014 mL	0.29052 mL	1.34995 mL	0.02500 mL	7.927	0.09994	0.97305	0.0050
1:39:41.1	Data point 184	0.39005 mL	0.30014 mL	0.29099 mL	1.34995 mL	0.02500 mL	8.624	0.09588	0.97408	0.0048
1:40:27.8	Data point 185	0.39005 mL	0.30014 mL	0.29109 mL	1.34995 mL	0.02500 mL	8.840	0.09513	0.96720	0.0047
1:41:15.7	Data point 186	0.39005 mL	0.30014 mL	0.29118 mL	1.34995 mL	0.02500 mL	9.082	0.09857	0.98444	0.0049
1:42:02.6	Data point 187	0.39005 mL	0.30014 mL	0.29128 mL	1.34995 mL	0.02500 mL	9.291	0.09502	0.97033	0.0047
1:42:41.4	Data point 188	0.39005 mL	0.30014 mL	0.29137 mL	1.34995 mL	0.02500 mL	9.430	0.10068	0.98902	0.0050
1:43:16.5	Data point 189	0.39005 mL	0.30014 mL	0.29146 mL	1.34995 mL	0.02500 mL	9.598	0.09937	0.98121	0.0049
1:43:49.3	Data point 190	0.39005 mL	0.30014 mL	0.29156 mL	1.34995 mL	0.02500 mL	9.727	0.09444	0.97354	0.0047
1:44:18.5	Data point 191	0.39005 mL	0.30014 mL	0.29168 mL	1.34995 mL	0.02500 mL	9.862	0.09188	0.95840	0.0046
1:44:40.7	Data point 192	0.39005 mL	0.30014 mL	0.29179 mL	1.34995 mL	0.02500 mL	9.963	0.07308	0.96379	0.0036
1:45:07.5	Data point 193	0.39005 mL	0.30014 mL	0.29191 mL	1.34995 mL	0.02500 mL	10.065	0.05923	0.95556	0.0029
1:45:34.1	Data point 194	0.39005 mL	0.30014 mL	0.29207 mL	1.34995 mL	0.02500 mL	10.171	0.04543	0.97196	0.0022
1:45:55.9	Data point 195	0.39005 mL	0.30014 mL	0.29226 mL	1.34995 mL	0.02500 mL	10.278	0.02809	0.94991	0.0014
1:46:17.5	Data point 196	0.39005 mL	0.30014 mL	0.29247 mL	1.34995 mL	0.02500 mL	10.374	0.01814	0.95638	0.0009
1:46:34.1	Data point 197	0.39005 mL	0.30014 mL	0.29273 mL	1.34995 mL	0.02500 mL	10.502	0.00407	0.41907	0.0003
1:46:55.9	Data point 198	0.39005 mL	0.30014 mL	0.29311 mL	1.34995 mL	0.02500 mL	10.609	0.00228	0.16611	0.0002
1:47:22.7	Data point 199	0.39005 mL	0.30014 mL	0.29353 mL	1.34995 mL	0.02500 mL	10.702	0.00513	0.45222	0.0003
1:47:39.3	Data point 200	0.39005 mL	0.30014 mL	0.29407 mL	1.34995 mL	0.02500 mL	10.862	-0.00309	0.38025	0.0002
1:48:06.1	Data point 201	0.39005 mL	0.30014 mL	0.29478 mL	1.34995 mL	0.02500 mL	10.953	-0.00209	0.20834	0.0002
1:48:22.6	Data point 202	0.39005 mL	0.30014 mL	0.29572 mL	1.34995 mL	0.02500 mL	11.058	-0.00598	0.72367	0.0003
1:48:39.2	Data point 203	0.39005 mL	0.30014 mL	0.29692 mL	1.34995 mL	0.02500 mL	11.151	-0.00723	0.82657	0.0003
1:48:55.8	Data point 204	0.39005 mL	0.30014 mL	0.29840 mL	1.34995 mL	0.02500 mL	11.238	-0.00735	0.74722	0.0004
1:49:12.4	Data point 205	0.39005 mL	0.30014 mL	0.30021 mL	1.34995 mL	0.02500 mL	11.301	-0.00605	0.65585	0.0003
1:49:39.5	Data point 206	0.39005 mL	0.30014 mL	0.30252 mL	1.34995 mL	0.02500 mL	11.396	-0.00581	0.61242	0.0003
1:49:56.1	Data point 207	0.39005 mL	0.30014 mL	0.30513 mL	1.34995 mL	0.02500 mL	11.500	-0.01051	0.88275	0.0005
1:50:12.6	Data point 208	0.39005 mL	0.30014 mL	0.30849 mL	1.34995 mL	0.02500 mL	11.588	-0.00866	0.75820	0.0004
1:50:29.3	Data point 209	0.39005 mL	0.30014 mL	0.31261 mL	1.34995 mL	0.02500 mL	11.676	-0.00604	0.65971	0.0003
1:50:46.0	Data point 210	0.39005 mL	0.30014 mL	0.31769 mL	1.34995 mL	0.02500 mL	11.767	-0.00536	0.68040	0.0003
1:51:02.7	Data point 211	0.39005 mL	0.30014 mL	0.32399 mL	1.34995 mL	0.02500 mL	11.859	-0.00920	0.71813	0.0005
1:51:19.4	Data point 212	0.39005 mL	0.30014 mL	0.33184 mL	1.34995 mL	0.02500 mL	11.948	-0.00711	0.79766	0.0003
1:51:36.3	Data point 213	0.39005 mL	0.30014 mL	0.34156 mL	1.34995 mL	0.02500 mL	12.035	-0.00761	0.82800	0.0004
1:53:35.3	Assay volumes	0.64005 mL	0.43217 mL	0.34156 mL	1.34995 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			

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07005**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07005_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 6:48:14 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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			
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			
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	0.07 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			

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07005**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07005_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 6:48:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Data Point Stability				
Stir during data point collection	Yes			
For point collection, stir at	15%			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00500 dpH/dt			
Stability timeout after	60 seconds			
Experiment cleanup				
Adjust pH to cleanup	To start pH			
And then stir for	60 seconds			
For cleaning, stir at	20%			
Then add water volume	0.25 mL			
And then stir for	30 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.161	10/7/2017 6:48:14 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus S	0.9927	10/7/2017 6:48:14 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus jH	0.5	10/7/2017 6:48:14 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Four-Plus jOH	-0.7	10/7/2017 6:48:14 AM	C:\Sirius_T3\17J-06018_Blank standardisation.t3r
Base concentration factor	1.011	10/7/2017 6:48:14 AM	C:\Sirius_T3\KOH17122.t3r
Acid concentration factor	1.003	10/7/2017 6:48:14 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)		

Sample name: **D07**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-07005**
 Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07005_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 6:48:14 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Titration	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)		
Titration	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	-7.72 mV		10/7/2017 6:48:38 AM
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	8.7e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	1.3e+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)		
Titration 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		



Assay Settings

Sample name: **D07**
Assay name: **UV-metric pKa**
Assay ID: **17J-07005**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07005_D07_UV-metric pKa.t3r**

Experiment start time: **10/7/2017 6:48:14 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	Spectrometer	Spectrometer
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00
Exclude turbid points	Yes	Yes
Low intensity warning threshold	100	100
Minimum absorbance change threshold	0.100	0.100
Eigenvector autocorrelation threshold	0.80	0.80
Maximum RMSD severe warning	0.250	0.250
Maximum RMSD warning	0.050	0.050

Tray Information

Title
Location F5