

Sample name: **D09**
Assay name: **UV-metric psKa**
Assay ID: **17J-06007**
Filename: **C:\Sirius_T3\17J-06007_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 8:04:20 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

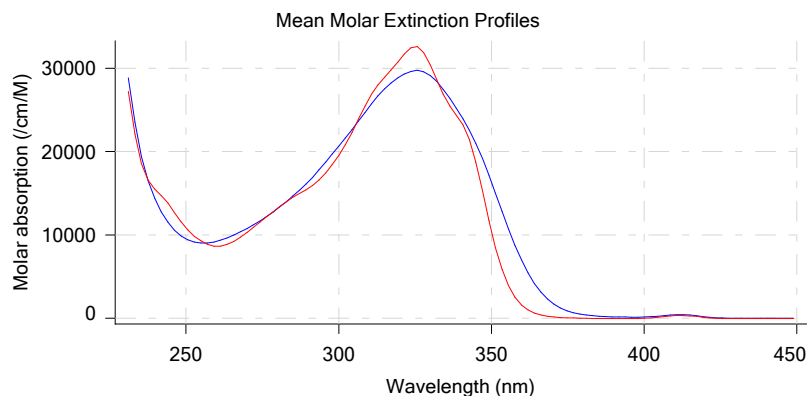
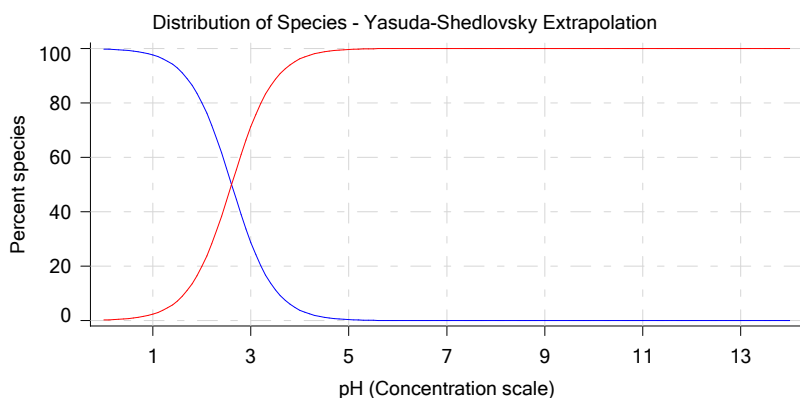
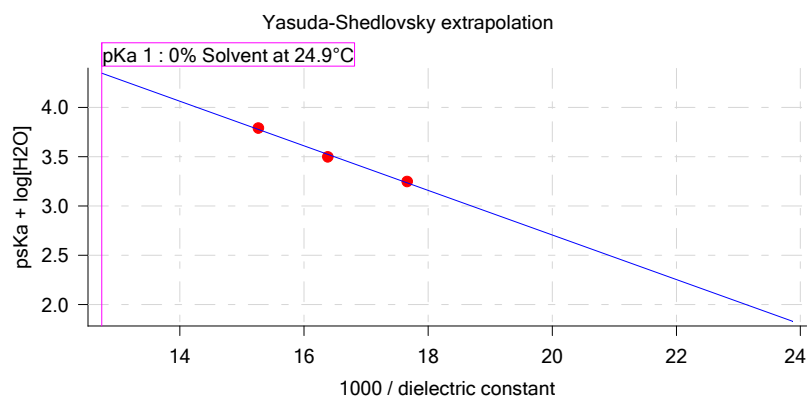
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	2.61	±0.07	7.23	-226.0326	0.9935	0.165 M	24.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1
17J-06007 Points 4 to 35	49.52 %	Up	UV-metric pKa	56.6	24.7 M	0.157 M	24.9°C	✓ 1.85
17J-06007 Points 37 to 75	39.95 %	Up	UV-metric pKa	61.0	30.0 M	0.166 M	24.9°C	✓ 2.02
17J-06007 Points 77 to 118	30.07 %	Up	UV-metric pKa	65.5	35.8 M	0.172 M	24.9°C	✓ 2.24

Graphs



UV-metric psKa Titration 1 of 3 17J-06007 Points 4 to 35

Results

pKa 1	1.85
RMSD	0.002 0.004
Chi squared	0.0074
PCA calculated number of pKas	4
Average ionic strength	0.157 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

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Results (continued)

pH clipping 1.478 to 12.545

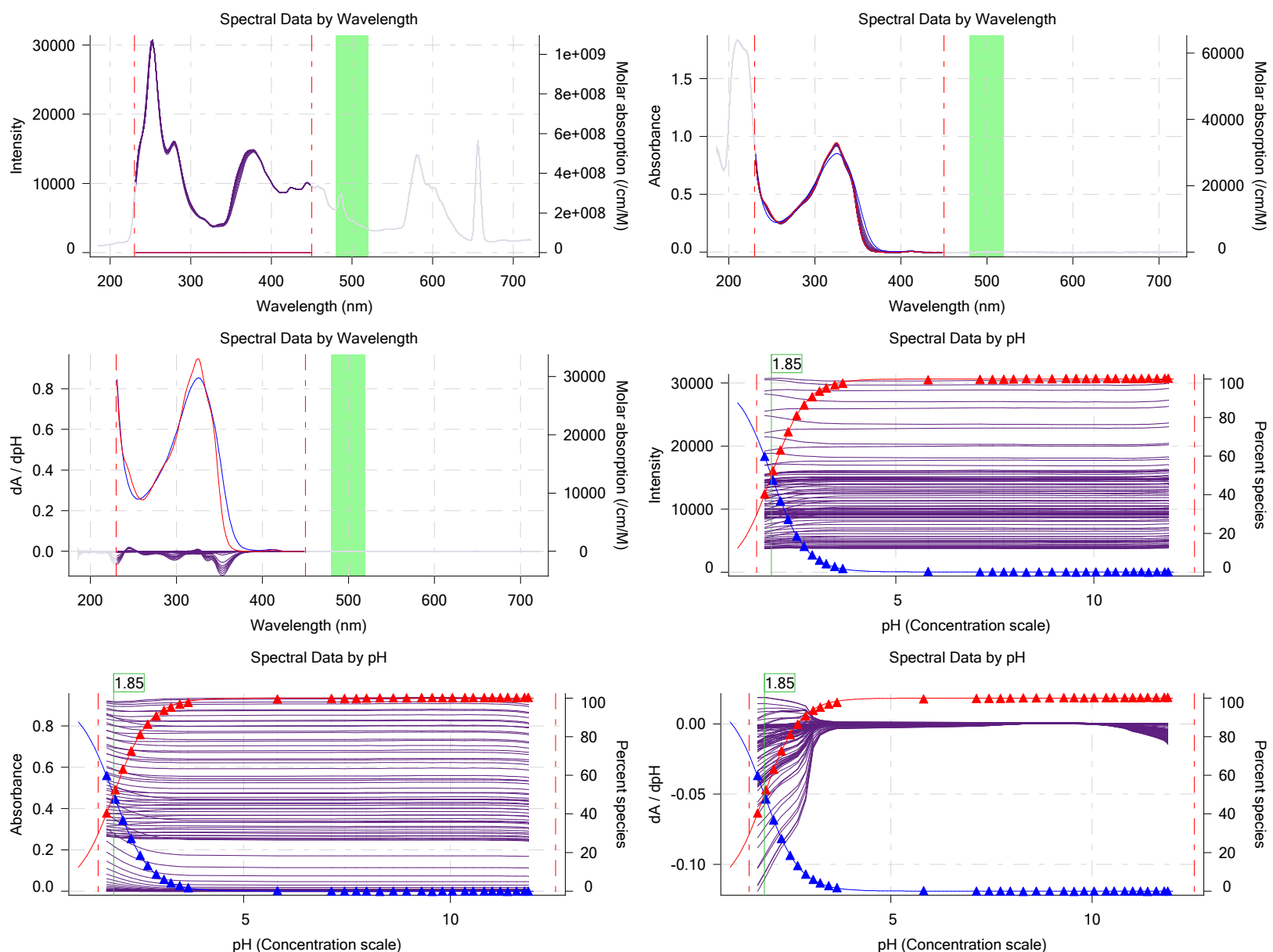
Warnings and errors

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			

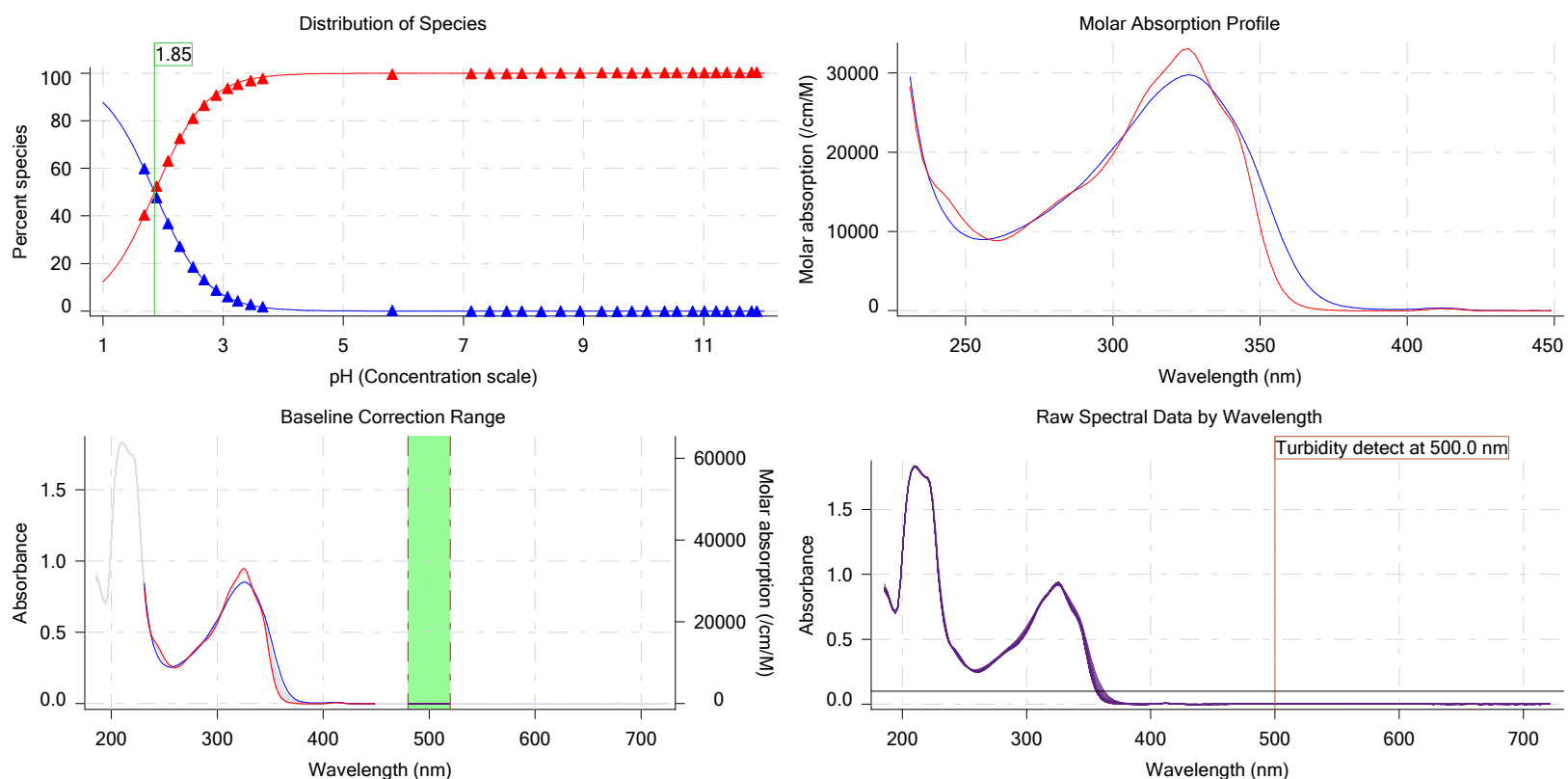
Graphs



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Graphs (continued)



UV-metric psKa Titration 2 of 3 17J-06007 Points 37 to 75

Results

pKa 1	2.02
RMSD	0.002 0.002
Chi squared	0.0030
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	1.506 to 12.542

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				

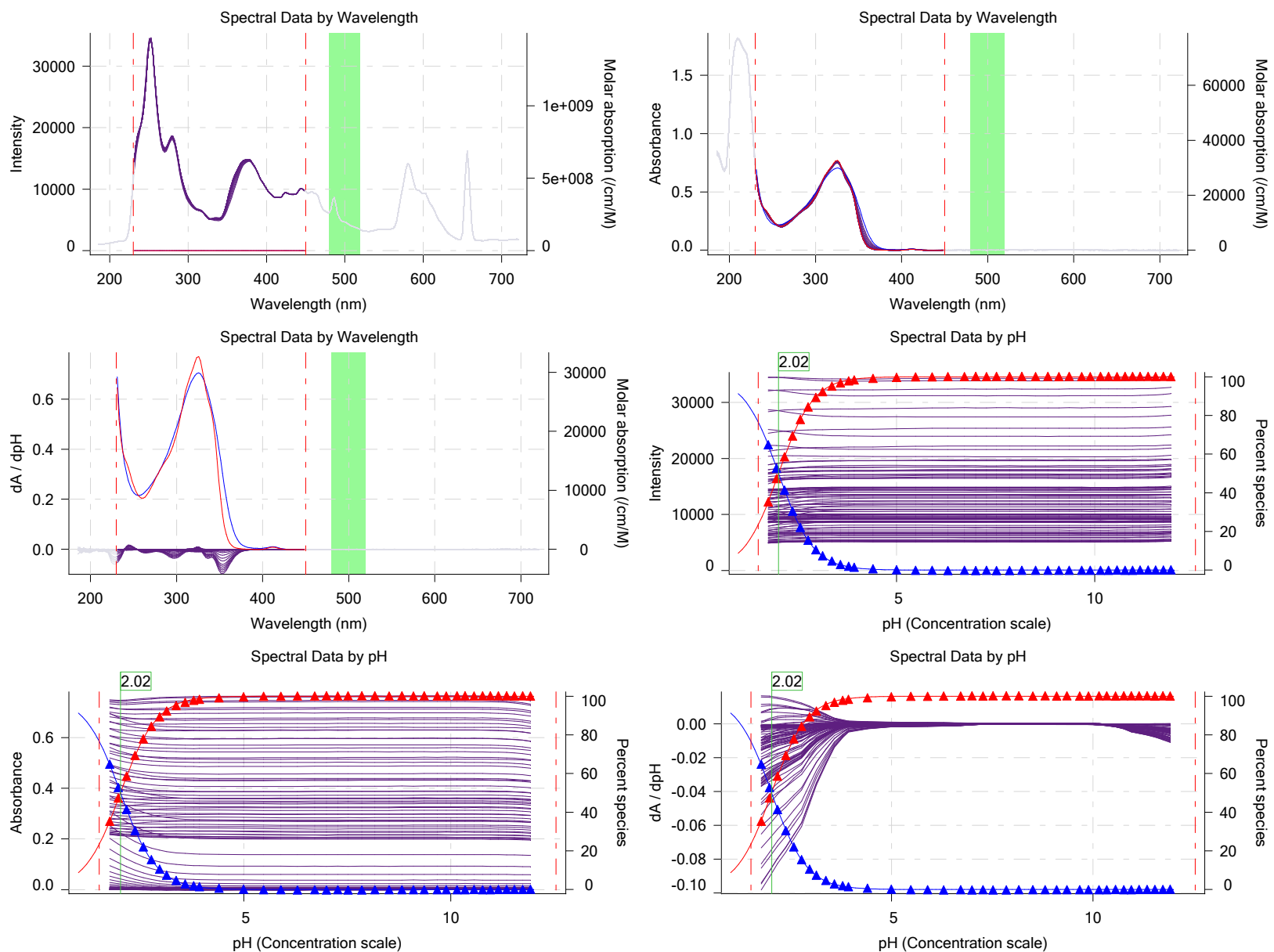
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 Assay name: **UV-metric psKa**
 Assay ID: **17J-06007**
 Filename: **C:\Sirius_T3\17J-06007_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 8:04:20 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			

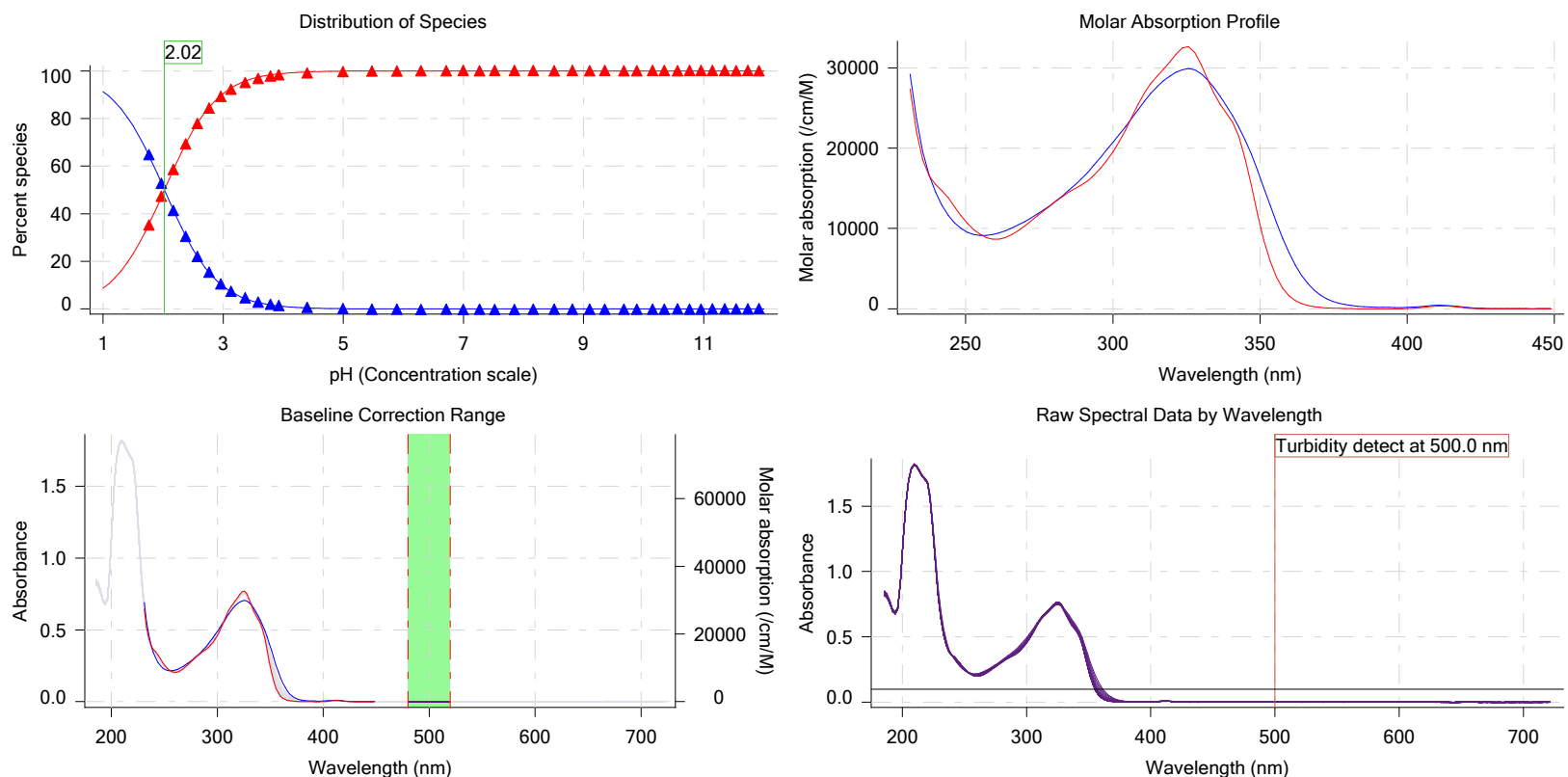
Graphs



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Graphs (continued)



UV-metric psKa Titration 3 of 3 17J-06007 Points 77 to 118

Results

pKa 1	2.24
RMSD	0.002 0.002
Chi squared	0.0027
PCA calculated number of pKas	4
Average ionic strength	0.172 M
Average temperature	24.9°C
Analyte concentration range	18.6 µM to 17.6 µM
Methanol weight %	30.1 %
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	1.506 to 12.537

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

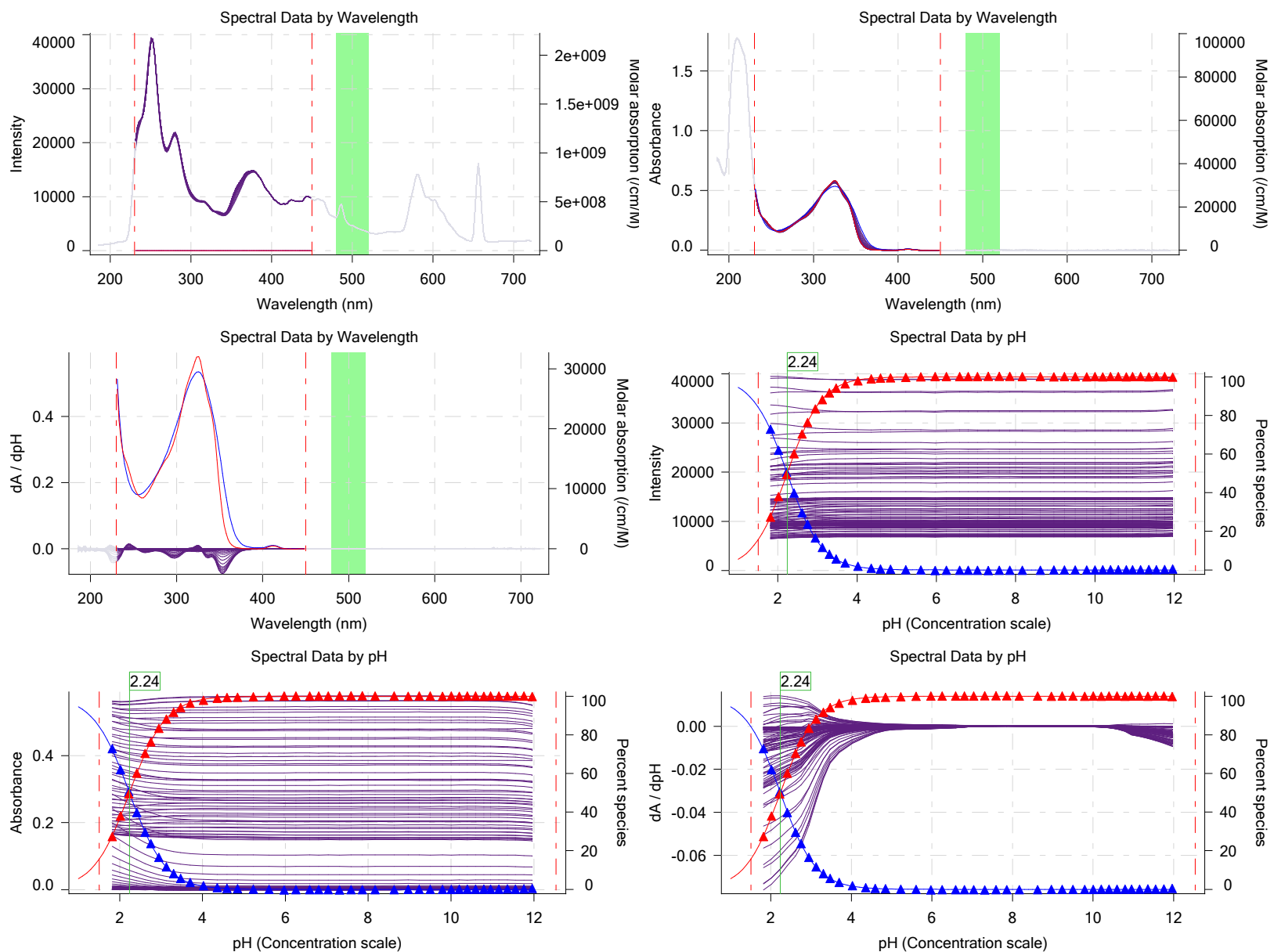
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Experiment start time: **10/6/2017 8:04:20 AM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Assay Settings (continued)

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

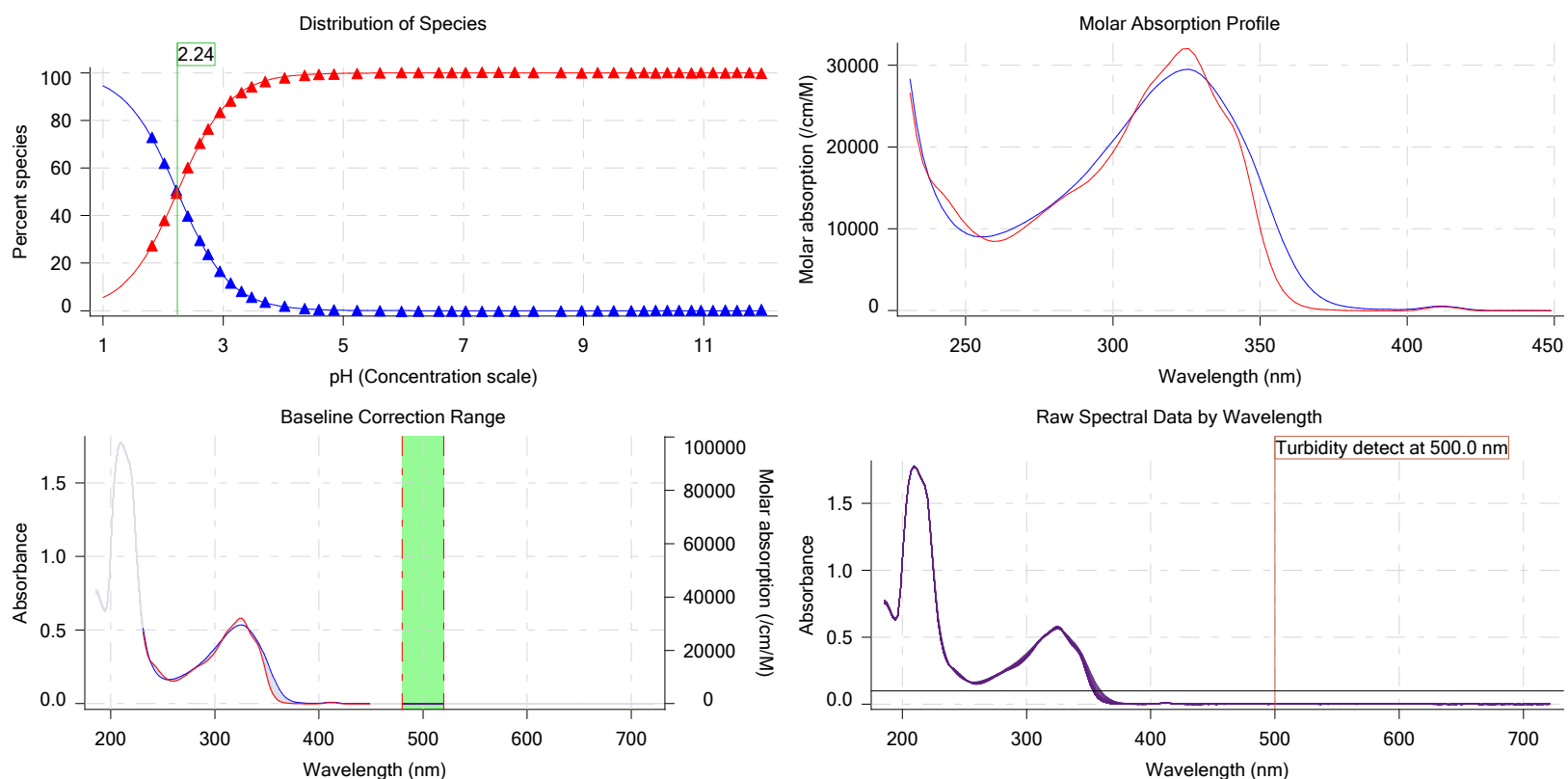
Graphs



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Graphs (continued)



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
3:09.7	Dark spectrum								
3:11.1	Reference spectrum								
3:38.8	Volume reset due to vial change								
4:22.9	Initial pH = 8.40								
5:31.6	Data point 4	0.34995 mL	0.06865 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.978	-0.01747	0.88859
6:00.3	Data point 5	0.34995 mL	0.06865 mL	0.02467 mL	1.15005 mL	0.02500 mL	2.179	0.00168	0.01966
6:17.3	Data point 6	0.34995 mL	0.06865 mL	0.03982 mL	1.15005 mL	0.02500 mL	2.367	0.02304	0.91296
6:34.1	Data point 7	0.34995 mL	0.06865 mL	0.04965 mL	1.15005 mL	0.02500 mL	2.560	0.00602	0.57190
6:50.9	Data point 8	0.34995 mL	0.06865 mL	0.05600 mL	1.15005 mL	0.02500 mL	2.774	0.00704	0.70747
7:07.6	Data point 9	0.34995 mL	0.06865 mL	0.05985 mL	1.15005 mL	0.02500 mL	2.957	0.01038	0.86741

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Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
7:24.2	Data point 10	0.34995 mL	0.06865 mL	0.06239 mL	1.15005 mL	0.02500 mL	3.156	0.00617	0.63755	0.00
7:40.9	Data point 11	0.34995 mL	0.06865 mL	0.06399 mL	1.15005 mL	0.02500 mL	3.341	0.01293	0.91518	0.00
7:57.6	Data point 12	0.34995 mL	0.06865 mL	0.06503 mL	1.15005 mL	0.02500 mL	3.511	0.01631	0.90014	0.00
8:29.6	Data point 13	0.34995 mL	0.06865 mL	0.06604 mL	1.15005 mL	0.02500 mL	3.723	0.02412	0.97892	0.00
9:01.4	Data point 14	0.34995 mL	0.06865 mL	0.06667 mL	1.15005 mL	0.02500 mL	3.924	0.03174	0.98189	0.00
9:28.3	Data point 15	0.34995 mL	0.06865 mL	0.06799 mL	1.15005 mL	0.02500 mL	6.054	0.09481	0.96314	0.00
10:40.6	Data point 16	0.34995 mL	0.06865 mL	0.06837 mL	1.15005 mL	0.02500 mL	7.352	0.05670	0.63722	0.00
11:14.7	Data point 17	0.34995 mL	0.06865 mL	0.06860 mL	1.15005 mL	0.02500 mL	7.659	0.09959	0.99062	0.00
11:58.2	Data point 18	0.34995 mL	0.06865 mL	0.06877 mL	1.15005 mL	0.02500 mL	7.941	0.09880	0.98927	0.00
12:44.3	Data point 19	0.34995 mL	0.06865 mL	0.06891 mL	1.15005 mL	0.02500 mL	8.185	0.09648	0.98745	0.00
13:30.2	Data point 20	0.34995 mL	0.06865 mL	0.06905 mL	1.15005 mL	0.02500 mL	8.505	0.09374	0.95342	0.00
14:22.0	Data point 21	0.34995 mL	0.06865 mL	0.06917 mL	1.15005 mL	0.02500 mL	8.827	0.09639	0.96543	0.00
15:07.4	Data point 22	0.34995 mL	0.06865 mL	0.06926 mL	1.15005 mL	0.02500 mL	9.148	0.09507	0.96438	0.00
15:52.1	Data point 23	0.34995 mL	0.06865 mL	0.06938 mL	1.15005 mL	0.02500 mL	9.503	0.09515	0.96837	0.00
16:30.4	Data point 24	0.34995 mL	0.06865 mL	0.06950 mL	1.15005 mL	0.02500 mL	9.754	0.09648	0.94763	0.00
17:00.6	Data point 25	0.34995 mL	0.06865 mL	0.06964 mL	1.15005 mL	0.02500 mL	10.000	0.09750	0.97405	0.00
17:23.7	Data point 26	0.34995 mL	0.06865 mL	0.06980 mL	1.15005 mL	0.02500 mL	10.243	0.07126	0.97779	0.00
17:40.1	Data point 27	0.34995 mL	0.06865 mL	0.07006 mL	1.15005 mL	0.02500 mL	10.539	0.02010	0.75324	0.00
18:07.0	Data point 28	0.34995 mL	0.06865 mL	0.07053 mL	1.15005 mL	0.02500 mL	10.741	0.00151	0.05467	0.00
18:23.5	Data point 29	0.34995 mL	0.06865 mL	0.07135 mL	1.15005 mL	0.02500 mL	10.999	-0.00291	0.35494	0.00
18:50.3	Data point 30	0.34995 mL	0.06865 mL	0.07279 mL	1.15005 mL	0.02500 mL	11.190	-0.00695	0.74136	0.00
19:07.0	Data point 31	0.34995 mL	0.06865 mL	0.07509 mL	1.15005 mL	0.02500 mL	11.381	-0.01053	0.83410	0.00
19:23.6	Data point 32	0.34995 mL	0.06865 mL	0.07872 mL	1.15005 mL	0.02500 mL	11.563	-0.01021	0.86215	0.00
19:40.3	Data point 33	0.34995 mL	0.06865 mL	0.08427 mL	1.15005 mL	0.02500 mL	11.767	-0.00499	0.58409	0.00
19:57.1	Data point 34	0.34995 mL	0.06865 mL	0.09330 mL	1.15005 mL	0.02500 mL	11.960	-0.00431	0.36013	0.00
20:13.8	Data point 35	0.34995 mL	0.06865 mL	0.09901 mL	1.15005 mL	0.02500 mL	12.045	-0.01444	0.88595	0.00
21:50.3	Reference spectrum									
22:54.3	Data point 37	0.50000 mL	0.16853 mL	0.09904 mL	1.15005 mL	0.02500 mL	2.006	-0.04801	0.95108	0.00
23:22.0	Data point 38	0.50000 mL	0.16853 mL	0.12444 mL	1.15005 mL	0.02500 mL	2.208	0.01300	0.93579	0.00
23:39.0	Data point 39	0.50000 mL	0.16853 mL	0.14005 mL	1.15005 mL	0.02500 mL	2.403	0.00720	0.33632	0.00
23:55.7	Data point 40	0.50000 mL	0.16853 mL	0.14998 mL	1.15005 mL	0.02500 mL	2.606	0.01099	0.72459	0.00
24:12.4	Data point 41	0.50000 mL	0.16853 mL	0.15616 mL	1.15005 mL	0.02500 mL	2.800	0.02694	0.87117	0.00
24:29.2	Data point 42	0.50000 mL	0.16853 mL	0.16011 mL	1.15005 mL	0.02500 mL	2.993	0.01965	0.91993	0.00
24:45.9	Data point 43	0.50000 mL	0.16853 mL	0.16263 mL	1.15005 mL	0.02500 mL	3.187	0.01447	0.96176	0.00
25:02.6	Data point 44	0.50000 mL	0.16853 mL	0.16423 mL	1.15005 mL	0.02500 mL	3.354	0.01212	0.85494	0.00
25:34.7	Data point 45	0.50000 mL	0.16853 mL	0.16597 mL	1.15005 mL	0.02500 mL	3.587	0.01856	0.94841	0.00
26:06.8	Data point 46	0.50000 mL	0.16853 mL	0.16686 mL	1.15005 mL	0.02500 mL	3.801	0.02738	0.98712	0.00
26:28.5	Data point 47	0.50000 mL	0.16853 mL	0.16726 mL	1.15005 mL	0.02500 mL	4.003	0.05089	0.98762	0.00
26:45.1	Data point 48	0.50000 mL	0.16853 mL	0.16750 mL	1.15005 mL	0.02500 mL	4.142	0.06270	0.98497	0.00
27:06.8	Data point 49	0.50000 mL	0.16853 mL	0.16783 mL	1.15005 mL	0.02500 mL	4.610	0.09965	0.98295	0.00
27:42.0	Data point 50	0.50000 mL	0.16853 mL	0.16809 mL	1.15005 mL	0.02500 mL	5.199	0.10034	0.98140	0.00
28:32.0	Data point 51	0.50000 mL	0.16853 mL	0.16818 mL	1.15005 mL	0.02500 mL	5.675	0.09148	0.99079	0.00
29:29.1	Data point 52	0.50000 mL	0.16853 mL	0.16825 mL	1.15005 mL	0.02500 mL	6.089	0.10022	0.98873	0.00
30:28.3	Data point 53	0.50000 mL	0.16853 mL	0.16832 mL	1.15005 mL	0.02500 mL	6.486	0.09966	0.99421	0.00
31:14.9	Data point 54	0.50000 mL	0.16853 mL	0.16842 mL	1.15005 mL	0.02500 mL	6.900	0.09871	0.96959	0.00
31:57.0	Data point 55	0.50000 mL	0.16853 mL	0.16851 mL	1.15005 mL	0.02500 mL	7.181	0.09627	0.97145	0.00
32:39.9	Data point 56	0.50000 mL	0.16853 mL	0.16863 mL	1.15005 mL	0.02500 mL	7.448	0.09998	0.98379	0.00
33:17.4	Data point 57	0.50000 mL	0.16853 mL	0.16872 mL	1.15005 mL	0.02500 mL	7.698	0.09725	0.98408	0.00
33:55.3	Data point 58	0.50000 mL	0.16853 mL	0.16881 mL	1.15005 mL	0.02500 mL	8.024	0.09999	0.97669	0.00
34:32.7	Data point 59	0.50000 mL	0.16853 mL	0.16889 mL	1.15005 mL	0.02500 mL	8.334	0.09867	0.98516	0.00
35:14.9	Data point 60	0.50000 mL	0.16853 mL	0.16896 mL	1.15005 mL	0.02500 mL	8.680	0.08676	0.88876	0.00
35:55.6	Data point 61	0.50000 mL	0.16853 mL	0.16903 mL	1.15005 mL	0.02500 mL	8.981	0.09673	0.97604	0.00
36:35.4	Data point 62	0.50000 mL	0.16853 mL	0.16910 mL	1.15005 mL	0.02500 mL	9.262	0.09926	0.96356	0.00
37:13.6	Data point 63	0.50000 mL	0.16853 mL	0.16919 mL	1.15005 mL	0.02500 mL	9.516	0.09952	0.97883	0.00
37:39.2	Data point 64	0.50000 mL	0.16853 mL	0.16931 mL	1.15005 mL	0.02500 mL	9.829	0.09568	0.99008	0.00
38:00.6	Data point 65	0.50000 mL	0.16853 mL	0.16945 mL	1.15005 mL	0.02500 mL	10.042	0.06233	0.96469	0.00
38:17.3	Data point 66	0.50000 mL	0.16853 mL	0.16969 mL	1.15005 mL	0.02500 mL	10.300	0.02378	0.94925	0.00



Assay Events

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Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
38:49.1	Data point 67	0.50000 mL	0.16853 mL	0.17013 mL	1.15005 mL	0.02500 mL	10.496	0.00649	0.56509	0.00000
39:05.6	Data point 68	0.50000 mL	0.16853 mL	0.17079 mL	1.15005 mL	0.02500 mL	10.712	0.00056	0.03026	0.00000
39:22.2	Data point 69	0.50000 mL	0.16853 mL	0.17185 mL	1.15005 mL	0.02500 mL	10.911	-0.00505	0.72757	0.00000
39:38.8	Data point 70	0.50000 mL	0.16853 mL	0.17352 mL	1.15005 mL	0.02500 mL	11.100	-0.00607	0.66239	0.00000
39:55.4	Data point 71	0.50000 mL	0.16853 mL	0.17611 mL	1.15005 mL	0.02500 mL	11.287	-0.00816	0.78710	0.00000
40:11.9	Data point 72	0.50000 mL	0.16853 mL	0.18010 mL	1.15005 mL	0.02500 mL	11.486	-0.00762	0.80640	0.00000
40:28.6	Data point 73	0.50000 mL	0.16853 mL	0.18650 mL	1.15005 mL	0.02500 mL	11.672	-0.01543	0.88607	0.00000
40:45.4	Data point 74	0.50000 mL	0.16853 mL	0.19647 mL	1.15005 mL	0.02500 mL	11.864	-0.01222	0.78574	0.00000
41:02.3	Data point 75	0.50000 mL	0.16853 mL	0.21105 mL	1.15005 mL	0.02500 mL	12.042	-0.00331	0.59498	0.00000
42:47.4	Reference spectrum									
44:10.9	Data point 77	0.83996 mL	0.30200 mL	0.21108 mL	1.15005 mL	0.02500 mL	2.006	-0.04882	0.94930	0.00000
44:38.6	Data point 78	0.83996 mL	0.30200 mL	0.24010 mL	1.15005 mL	0.02500 mL	2.203	0.01561	0.80400	0.00000
44:55.6	Data point 79	0.83996 mL	0.30200 mL	0.25814 mL	1.15005 mL	0.02500 mL	2.402	0.01037	0.58227	0.00000
45:12.5	Data point 80	0.83996 mL	0.30200 mL	0.26952 mL	1.15005 mL	0.02500 mL	2.589	-0.01647	0.68573	0.00000
45:29.3	Data point 81	0.83996 mL	0.30200 mL	0.27698 mL	1.15005 mL	0.02500 mL	2.788	-0.00998	0.67261	0.00000
46:01.8	Data point 82	0.83996 mL	0.30200 mL	0.28168 mL	1.15005 mL	0.02500 mL	2.924	0.00853	0.80202	0.00000
46:23.6	Data point 83	0.83996 mL	0.30200 mL	0.28476 mL	1.15005 mL	0.02500 mL	3.116	0.00008	0.00017	0.00000
46:40.2	Data point 84	0.83996 mL	0.30200 mL	0.28692 mL	1.15005 mL	0.02500 mL	3.295	0.00119	0.02422	0.00000
46:56.7	Data point 85	0.83996 mL	0.30200 mL	0.28836 mL	1.15005 mL	0.02500 mL	3.470	-0.00043	0.00427	0.00000
47:13.3	Data point 86	0.83996 mL	0.30200 mL	0.28932 mL	1.15005 mL	0.02500 mL	3.639	-0.00368	0.22755	0.00000
47:40.0	Data point 87	0.83996 mL	0.30200 mL	0.29073 mL	1.15005 mL	0.02500 mL	3.863	0.01484	0.87853	0.00000
48:01.8	Data point 88	0.83996 mL	0.30200 mL	0.29142 mL	1.15005 mL	0.02500 mL	4.185	0.01855	0.72851	0.00000
48:23.5	Data point 89	0.83996 mL	0.30200 mL	0.29177 mL	1.15005 mL	0.02500 mL	4.514	0.06399	0.97428	0.00000
48:50.3	Data point 90	0.83996 mL	0.30200 mL	0.29198 mL	1.15005 mL	0.02500 mL	4.750	0.09874	0.98468	0.00000
49:18.2	Data point 91	0.83996 mL	0.30200 mL	0.29210 mL	1.15005 mL	0.02500 mL	5.000	0.10010	0.98033	0.00000
49:50.4	Data point 92	0.83996 mL	0.30200 mL	0.29219 mL	1.15005 mL	0.02500 mL	5.378	0.09674	0.97574	0.00000
50:26.5	Data point 93	0.83996 mL	0.30200 mL	0.29226 mL	1.15005 mL	0.02500 mL	5.755	0.09673	0.97641	0.00000
51:08.2	Data point 94	0.83996 mL	0.30200 mL	0.29236 mL	1.15005 mL	0.02500 mL	6.115	0.07515	0.71635	0.00000
51:34.9	Data point 95	0.83996 mL	0.30200 mL	0.29243 mL	1.15005 mL	0.02500 mL	6.394	0.09826	0.98462	0.00000
52:01.5	Data point 96	0.83996 mL	0.30200 mL	0.29255 mL	1.15005 mL	0.02500 mL	6.727	-0.05152	0.64149	0.00000
52:23.3	Data point 97	0.83996 mL	0.30200 mL	0.29264 mL	1.15005 mL	0.02500 mL	6.942	0.06476	0.82035	0.00000
52:50.0	Data point 98	0.83996 mL	0.30200 mL	0.29273 mL	1.15005 mL	0.02500 mL	7.170	0.09172	0.96440	0.00000
53:22.7	Data point 99	0.83996 mL	0.30200 mL	0.29285 mL	1.15005 mL	0.02500 mL	7.441	0.09816	0.97937	0.00000
53:57.1	Data point 100	0.83996 mL	0.30200 mL	0.29297 mL	1.15005 mL	0.02500 mL	7.718	0.09901	0.98602	0.00000
54:35.0	Data point 101	0.83996 mL	0.30200 mL	0.29306 mL	1.15005 mL	0.02500 mL	7.983	0.09865	0.96697	0.00000
55:14.2	Data point 102	0.83996 mL	0.30200 mL	0.29316 mL	1.15005 mL	0.02500 mL	8.293	0.09855	0.97869	0.00000
55:59.9	Data point 103	0.83996 mL	0.30200 mL	0.29325 mL	1.15005 mL	0.02500 mL	8.746	0.09755	0.96339	0.00000
56:38.1	Data point 104	0.83996 mL	0.30200 mL	0.29332 mL	1.15005 mL	0.02500 mL	9.083	0.09823	0.98103	0.00000
57:11.2	Data point 105	0.83996 mL	0.30200 mL	0.29339 mL	1.15005 mL	0.02500 mL	9.350	0.09065	0.91820	0.00000
57:39.4	Data point 106	0.83996 mL	0.30200 mL	0.29349 mL	1.15005 mL	0.02500 mL	9.613	0.09717	0.94635	0.00000
57:58.0	Data point 107	0.83996 mL	0.30200 mL	0.29363 mL	1.15005 mL	0.02500 mL	9.905	0.03601	0.93295	0.00000
58:24.9	Data point 108	0.83996 mL	0.30200 mL	0.29386 mL	1.15005 mL	0.02500 mL	10.114	0.02698	0.94292	0.00000
58:46.4	Data point 109	0.83996 mL	0.30200 mL	0.29410 mL	1.15005 mL	0.02500 mL	10.308	0.00571	0.48619	0.00000
59:13.2	Data point 110	0.83996 mL	0.30200 mL	0.29466 mL	1.15005 mL	0.02500 mL	10.501	-0.00352	0.40238	0.00000
59:45.2	Data point 111	0.83996 mL	0.30200 mL	0.29565 mL	1.15005 mL	0.02500 mL	10.695	-0.00930	0.77587	0.00000
1:00:02.0	Data point 112	0.83996 mL	0.30200 mL	0.29723 mL	1.15005 mL	0.02500 mL	10.895	-0.01887	0.91154	0.00000
1:00:18.7	Data point 113	0.83996 mL	0.30200 mL	0.29969 mL	1.15005 mL	0.02500 mL	11.053	-0.02360	0.96644	0.00000
1:00:45.7	Data point 114	0.83996 mL	0.30200 mL	0.30310 mL	1.15005 mL	0.02500 mL	11.253	-0.01510	0.92679	0.00000
1:01:02.5	Data point 115	0.83996 mL	0.30200 mL	0.30875 mL	1.15005 mL	0.02500 mL	11.452	-0.02445	0.95395	0.00000
1:01:19.3	Data point 116	0.83996 mL	0.30200 mL	0.31780 mL	1.15005 mL	0.02500 mL	11.644	-0.02318	0.93610	0.00000
1:01:36.3	Data point 117	0.83996 mL	0.30200 mL	0.33215 mL	1.15005 mL	0.02500 mL	11.842	-0.02202	0.96176	0.00000
1:01:53.5	Data point 118	0.83996 mL	0.30200 mL	0.35555 mL	1.15005 mL	0.02500 mL	12.037	-0.02473	0.89513	0.00000
1:03:53.0	Assay volumes	1.08996 mL	0.44636 mL	0.35555 mL	1.15005 mL	0.02500 mL				



Assay Settings

Sample name: **D09**
Assay name: **UV-metric psKa**
Assay ID: **17J-06007**
Filename: **C:\Sirius_T3\17J-06007_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 8:04:20 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

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	0.200			
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%			
Titration Pre-Dose				
Titration 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				



Assay Settings

Sample name: **D09**
Assay name: **UV-metric psKa**
Assay ID: **17J-06007**
Filename: **C:\Sirius_T3\17J-06007_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 8:04:20 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
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			
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 8:04:20 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus S	0.9949	10/6/2017 8:04:20 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jH	0.8	10/6/2017 8:04:20 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Four-Plus jOH	-1.3	10/6/2017 8:04:20 AM	C:\Sirius_T3\Mehtap\20171003_exp12_pKa\HCl17J03.t3r
Base concentration factor	1.011	10/6/2017 8:04:20 AM	C:\Sirius_T3\KOH17I22.t3r
Acid concentration factor	1.003	10/6/2017 8:04:20 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

Sample name: **D09**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-06007**
 Filename: **C:\Sirius_T3\17J-06007_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 8:04:20 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Phosphate Buffer		9/12/2017 11:32:29 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	9-14-17	9/14/2017 9:30:38 AM
Titrator		T3TM1100153	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 9:21:54 AM
E0 calibration	-8.20 mV		10/6/2017 8:04:44 AM
Filling solution	3M KCl	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% Triton X-100 in H2O		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	4.3e+003 mL	10-3-17	10/3/2017 8:04:49 AM
Waste	5.7e+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		



Assay Settings

Sample name: **D09**
Assay name: **UV-metric psKa**
Assay ID: **17J-06007**
Filename: **C:\Sirius_T3\17J-06007_D09_UV-metric psKa.t3r**

Experiment start time: **10/6/2017 8:04:20 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

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

Refinement Settings

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

Tray Information

Title
Location F1