

Sample name: **M18**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-12010**
 Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12010_M18_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 12:04:33 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

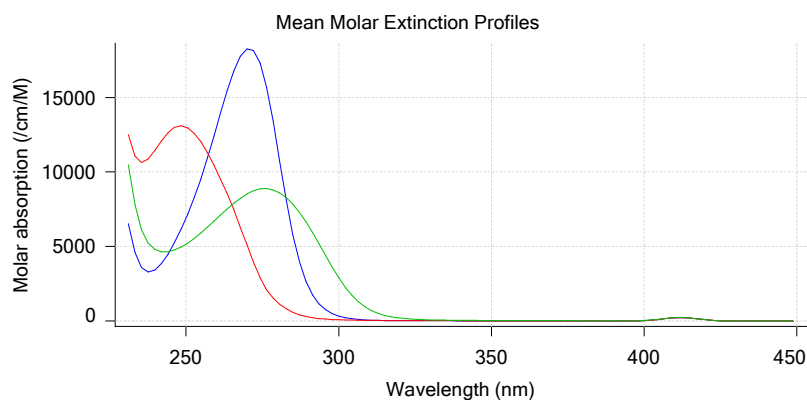
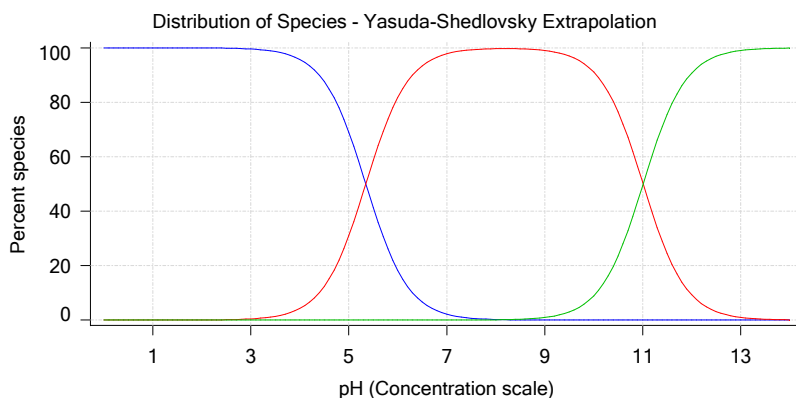
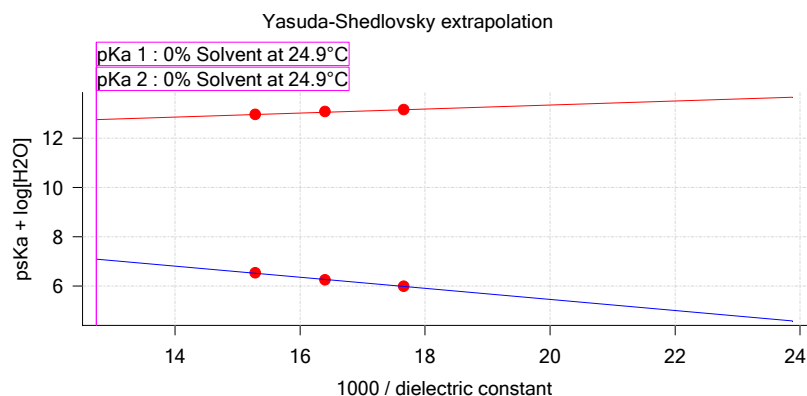
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.35	±0.06	9.97	-225.9587	0.9950	0.165 M	24.9°C
Yasuda-Shedlovsky	11.01	±0.05	11.71	81.7937	0.9745	0.165 M	24.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1	psKa 2
17J-12010 Points 4 to 39	49.47 %	Up	UV-metric pKa	56.6	24.7 M	0.157 M	24.9°C	✓	4.60 ✓
17J-12010 Points 41 to 78	40.05 %	Up	UV-metric pKa	61.0	30.0 M	0.166 M	25.0°C	✓	4.76 ✓
17J-12010 Points 80 to 116	30.24 %	Up	UV-metric pKa	65.4	35.7 M	0.172 M	24.9°C	✓	4.97 ✓

Graphs



UV-metric psKa Titration 1 of 3 17J-12010 Points 4 to 39

Results

pKa 1 **4.60**
 pKa 2 **11.75**
 RMSD **0.003 0.002 0.001**
 Chi squared **0.0250**
 PCA calculated number of pKas **2**
 Average ionic strength **0.157 M**
 Average temperature **24.9°C**
 Analyte concentration range **48.1 µM to 45.2 µM**
 Methanol weight % **49.5 %**
 Dielectric constant **56.6**
 Water concentration **24.7 M**

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Experiment start time: **10/12/2017 12:04:33 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.468 to 12.516**

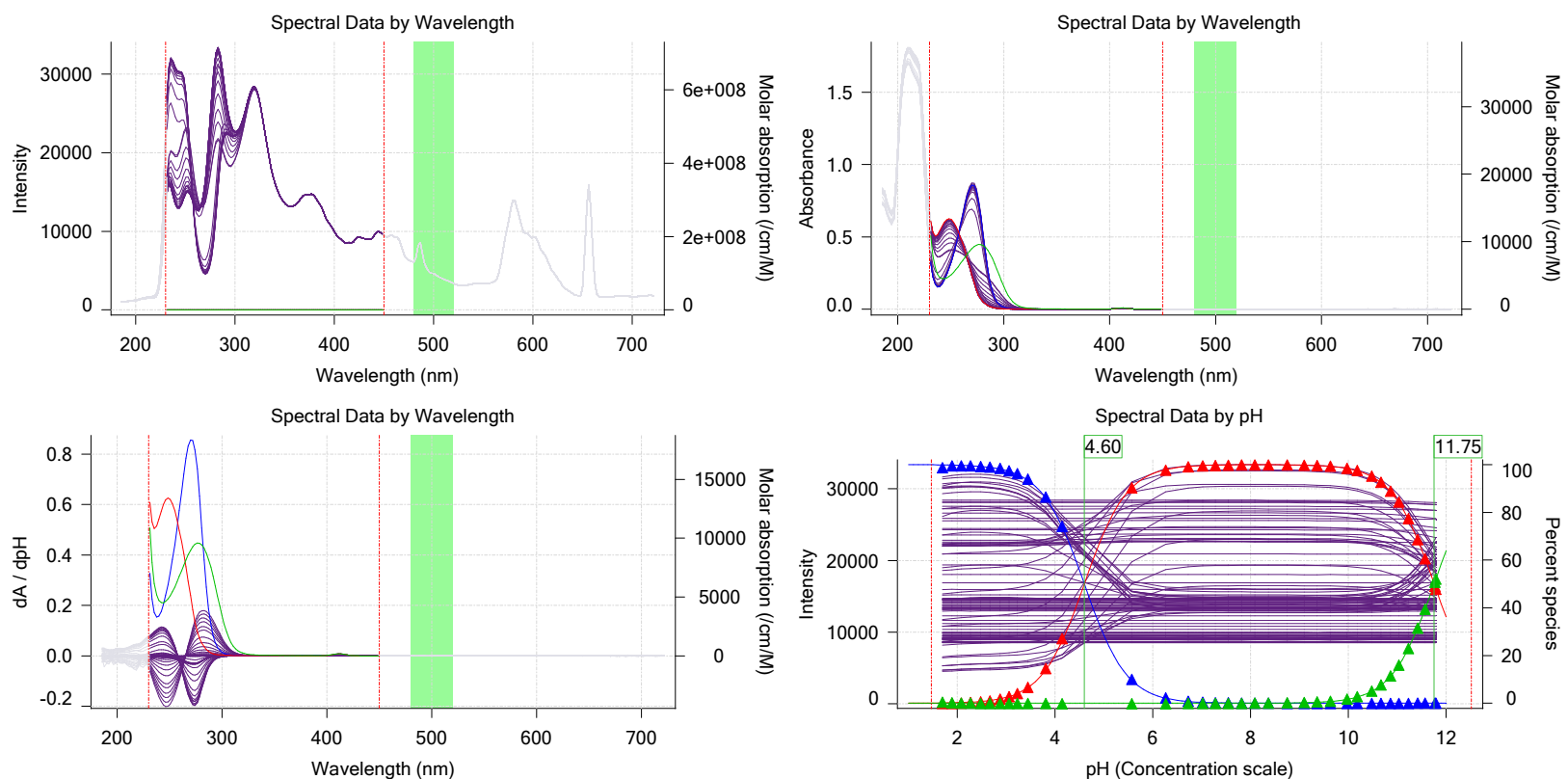
Warnings and errors

Errors None
 Warnings None

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			

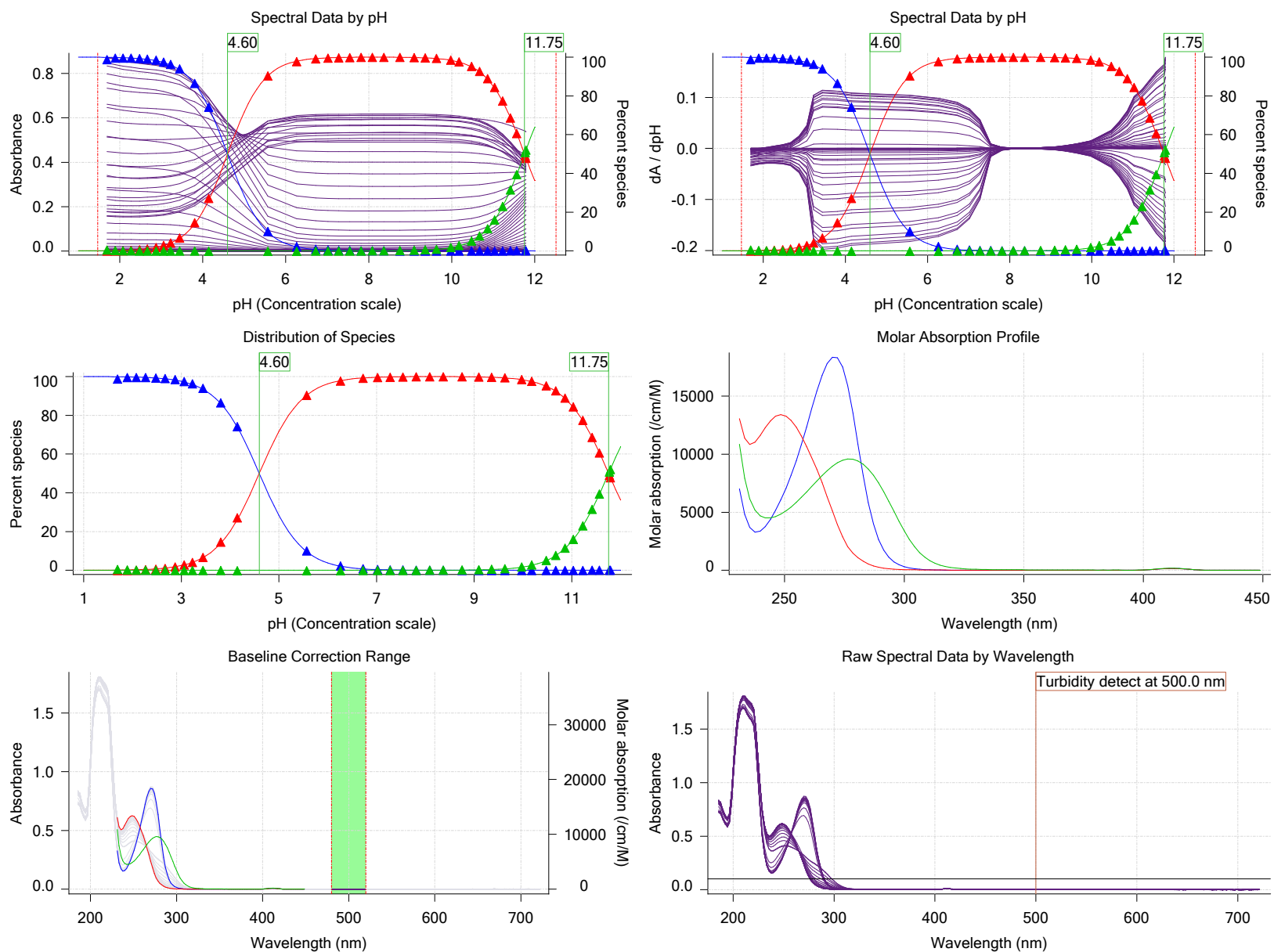
Graphs



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Experiment start time: **10/12/2017 12:04:33 PM**
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Graphs (continued)



UV-metric psKa Titration 2 of 3 17J-12010 Points 41 to 78

Results

pKa 1 **4.76**
 pKa 2 **11.59**
 RMSD **0.001 0.002 0.001**
 Chi squared **0.0136**
 PCA calculated number of pKas **2**
 Average ionic strength **0.166 M**
 Average temperature **25.0°C**
 Analyte concentration range **39.5 µM to 37.4 µM**
 Methanol weight % **40.0 %**
 Dielectric constant **61.0**
 Water concentration **30.0 M**

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Experiment start time: **10/12/2017 12:04:33 PM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.512 to 12.504**

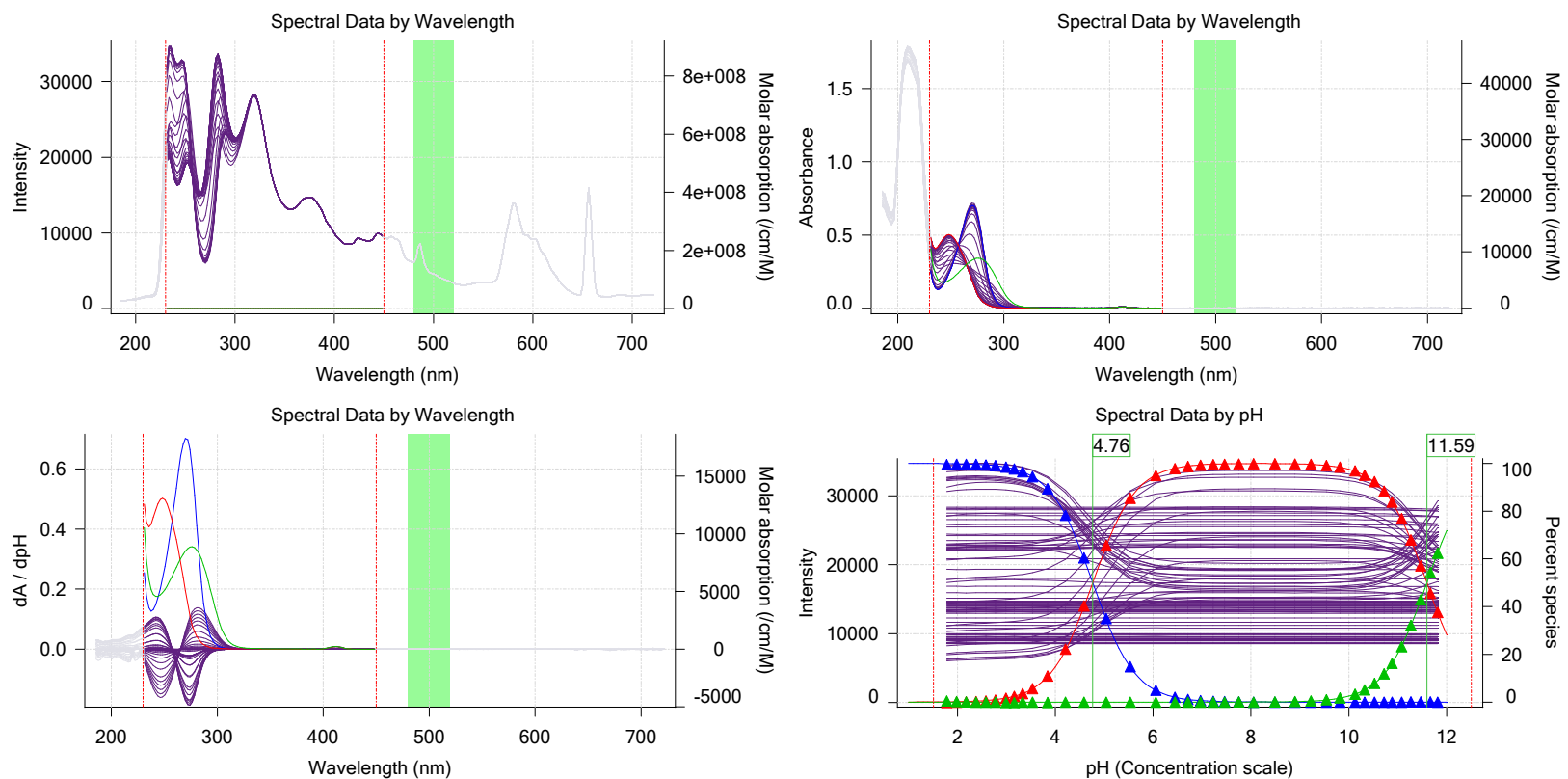
Warnings and errors

Errors None
 Warnings None

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			

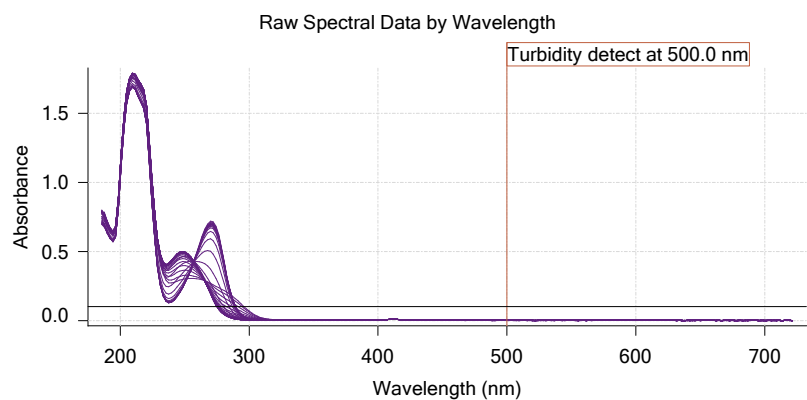
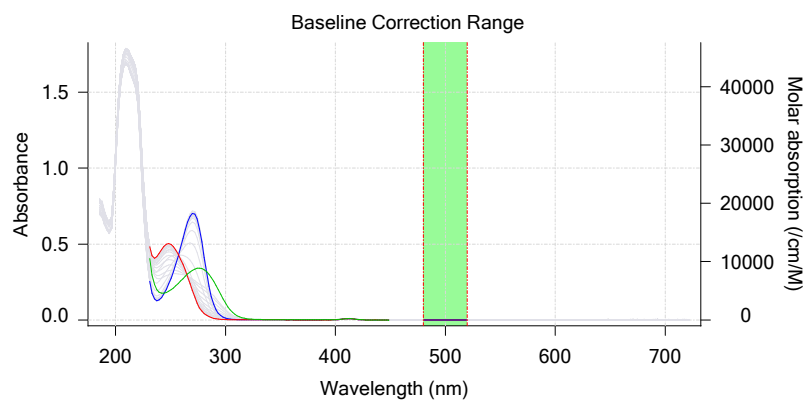
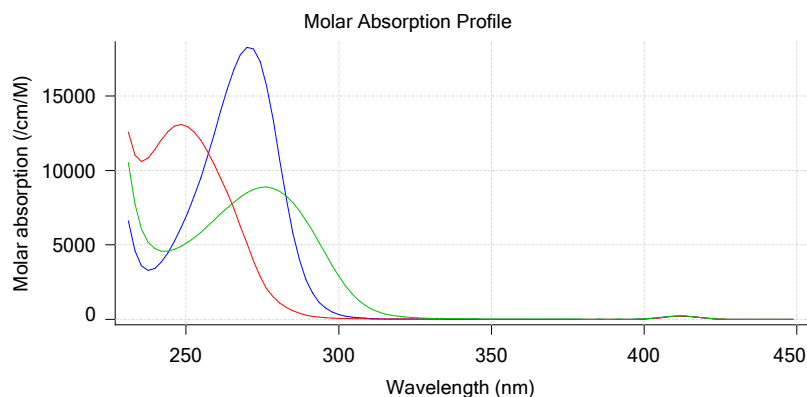
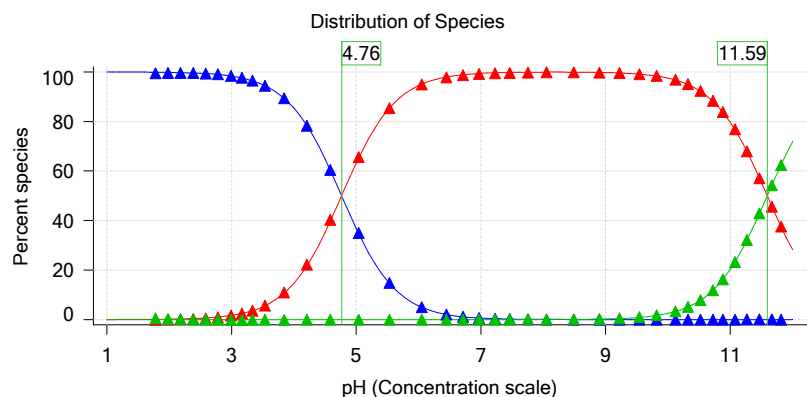
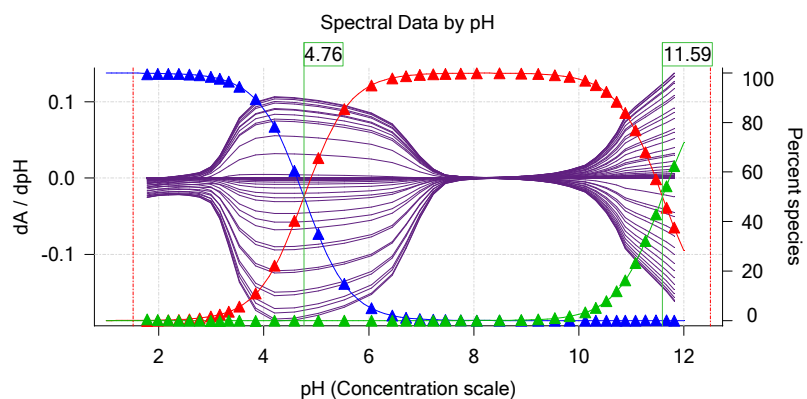
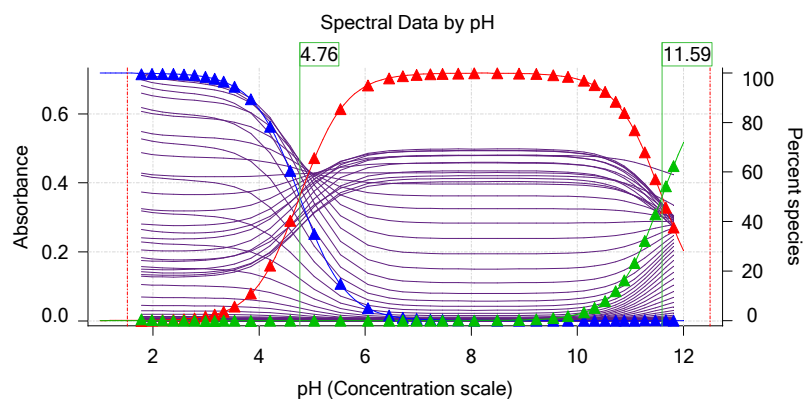
Graphs



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Experiment start time: **10/12/2017 12:04:33 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Graphs (continued)



UV-metric psKa Titration 3 of 3 17J-12010 Points 80 to 116

Results

pKa 1 **4.97**
 pKa 2 **11.40**
 RMSD **0.001 0.002 0.001**
 Chi squared **0.0077**
 PCA calculated number of pKas **2**
 Average ionic strength **0.172 M**
 Average temperature **24.9°C**
 Analyte concentration range **30.4 µM to 28.8 µM**
 Methanol weight % **30.2 %**
 Dielectric constant **65.4**
 Water concentration **35.7 M**

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 Analyst: **Dorothy Leverage**
 Instrument ID: **T311053**

Results (continued)

Number of pKas source **Predicted**
 Wavelength clipping **230.0 nm to 450.0 nm**
 pH clipping **1.513 to 12.513**

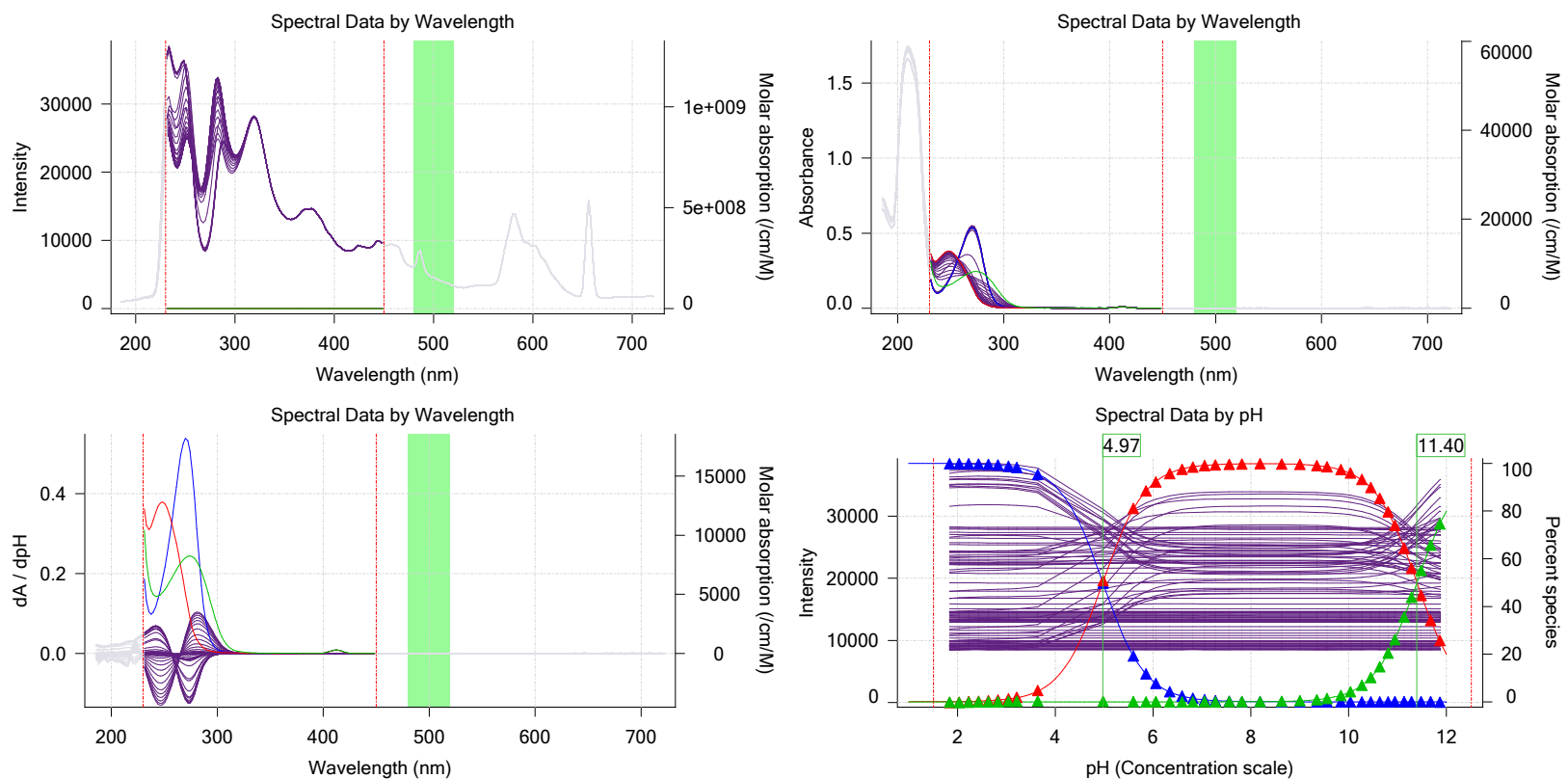
Warnings and errors

Errors None
 Warnings None

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			

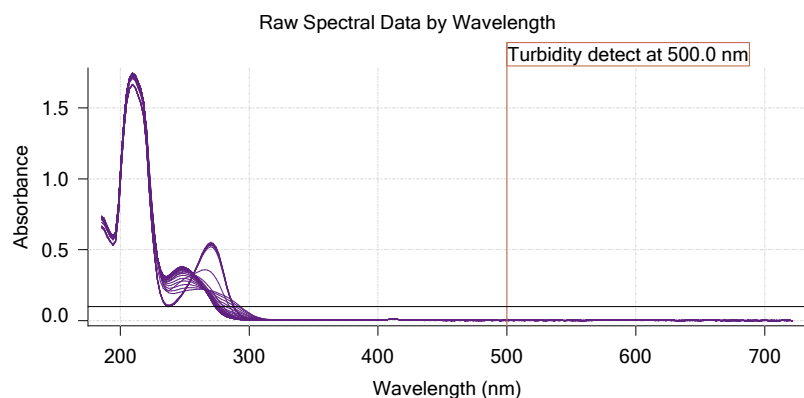
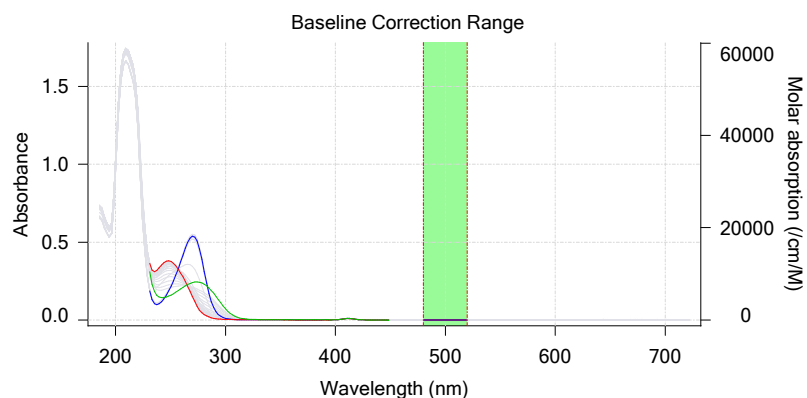
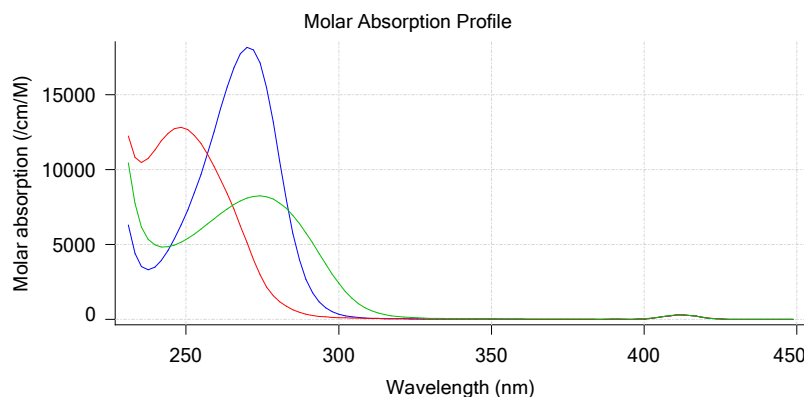
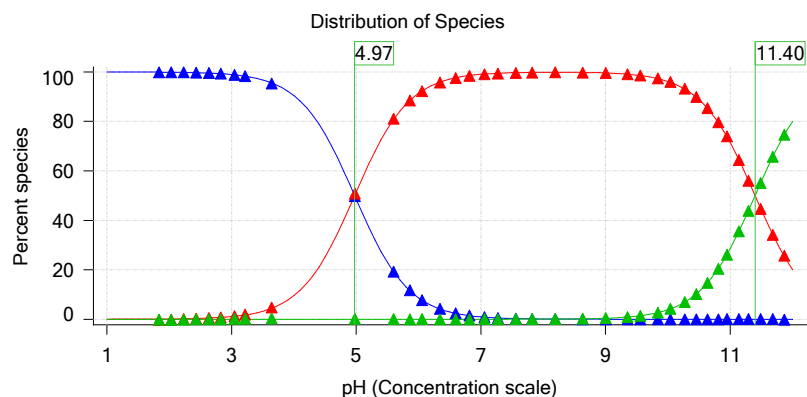
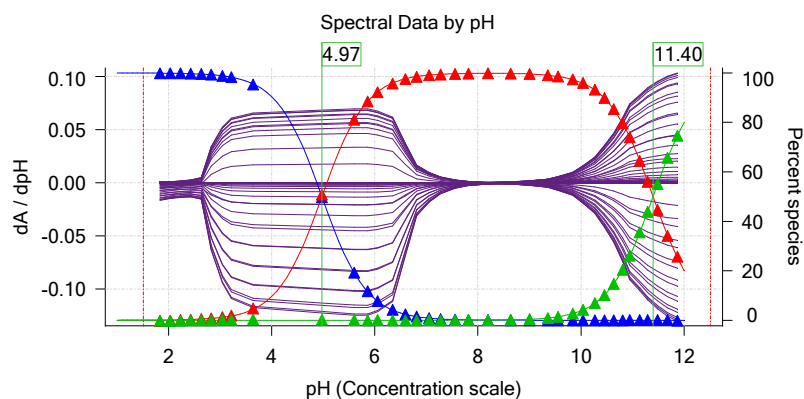
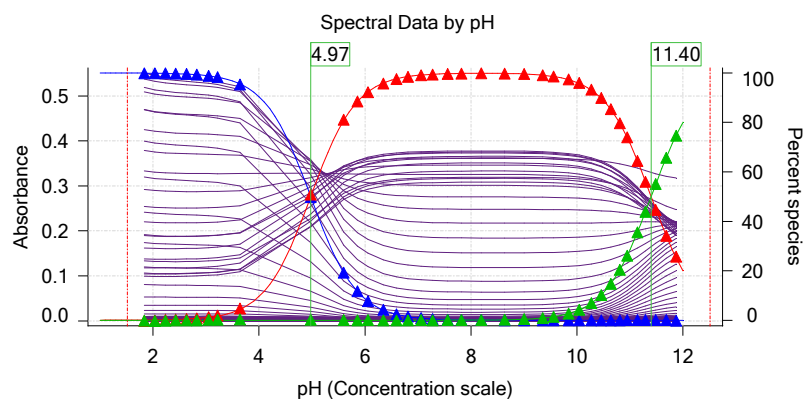
Graphs



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Experiment start time: **10/12/2017 12:04:33 PM**
 Analyst: **Dorothy Levorse**
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Graphs (continued)



Assay Model

Settings

Sample name	M18	10/11/2017 4:22:27 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0010 mL	10/11/2017 4:22:27 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.076700 M	10/11/2017 4:22:27 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	267.11	10/11/2017 4:22:36 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	10/11/2017 4:22:27 PM	User entered value
Sample is a	Ampholyte	10/11/2017 4:22:27 PM	User entered value
pKa 1	5.19	10/11/2017 4:22:27 PM	User entered value
Type	Base	10/11/2017 4:22:27 PM	User entered value
pKa 2	10.85	10/11/2017 4:22:27 PM	User entered value
Type	Acid	10/11/2017 4:22:27 PM	User entered value

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 Instrument ID: **T311053**

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logp (XH2 +)	-10.00		Default value
logP (neutral XH)	-10.00	10/11/2017 4:22:27 PM	User entered value
logP (X -)	-10.00		Default value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:31.4	Dark spectrum								
3:32.7	Reference spectrum								
4:00.4	Volume reset due to vial change								
4:44.7	Initial pH = 8.35								
5:39.1	Data point 4	0.34995 mL	0.06919 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.968	-0.02216	0.93220
6:07.9	Data point 5	0.34995 mL	0.06919 mL	0.02491 mL	1.15005 mL	0.02500 mL	2.168	-0.01140	0.51070
6:24.8	Data point 6	0.34995 mL	0.06919 mL	0.04008 mL	1.15005 mL	0.02500 mL	2.352	0.02310	0.86227
6:41.6	Data point 7	0.34995 mL	0.06919 mL	0.04988 mL	1.15005 mL	0.02500 mL	2.544	0.02591	0.86248
6:58.3	Data point 8	0.34995 mL	0.06919 mL	0.05628 mL	1.15005 mL	0.02500 mL	2.751	0.02119	0.81319
7:15.0	Data point 9	0.34995 mL	0.06919 mL	0.06028 mL	1.15005 mL	0.02500 mL	2.940	0.00531	0.69289
7:31.6	Data point 10	0.34995 mL	0.06919 mL	0.06289 mL	1.15005 mL	0.02500 mL	3.145	0.01086	0.71651
7:48.3	Data point 11	0.34995 mL	0.06919 mL	0.06451 mL	1.15005 mL	0.02500 mL	3.330	0.00949	0.76498
8:05.0	Data point 12	0.34995 mL	0.06919 mL	0.06557 mL	1.15005 mL	0.02500 mL	3.497	0.01228	0.83695
8:37.1	Data point 13	0.34995 mL	0.06919 mL	0.06670 mL	1.15005 mL	0.02500 mL	3.711	0.02264	0.95333
9:04.0	Data point 14	0.34995 mL	0.06919 mL	0.06783 mL	1.15005 mL	0.02500 mL	4.076	0.06944	0.98551
9:25.7	Data point 15	0.34995 mL	0.06919 mL	0.06820 mL	1.15005 mL	0.02500 mL	4.411	0.09971	0.99228
9:55.5	Data point 16	0.34995 mL	0.06919 mL	0.06863 mL	1.15005 mL	0.02500 mL	5.828	0.09719	0.97988
11:03.8	Data point 17	0.34995 mL	0.06919 mL	0.06884 mL	1.15005 mL	0.02500 mL	6.518	0.09753	0.98953
12:08.8	Data point 18	0.34995 mL	0.06919 mL	0.06898 mL	1.15005 mL	0.02500 mL	6.976	0.09815	0.98834
12:57.4	Data point 19	0.34995 mL	0.06919 mL	0.06910 mL	1.15005 mL	0.02500 mL	7.271	0.09986	0.98326
13:44.1	Data point 20	0.34995 mL	0.06919 mL	0.06921 mL	1.15005 mL	0.02500 mL	7.527	0.10032	0.99359
14:31.0	Data point 21	0.34995 mL	0.06919 mL	0.06936 mL	1.15005 mL	0.02500 mL	7.790	0.09965	0.99091
15:15.2	Data point 22	0.34995 mL	0.06919 mL	0.06950 mL	1.15005 mL	0.02500 mL	8.060	0.09971	0.98237
16:03.2	Data point 23	0.34995 mL	0.06919 mL	0.06961 mL	1.15005 mL	0.02500 mL	8.333	0.09994	0.97608
16:48.5	Data point 24	0.34995 mL	0.06919 mL	0.06971 mL	1.15005 mL	0.02500 mL	8.608	0.03826	0.16675
17:32.0	Data point 25	0.34995 mL	0.06919 mL	0.06980 mL	1.15005 mL	0.02500 mL	8.994	0.09896	0.98406
18:21.9	Data point 26	0.34995 mL	0.06919 mL	0.06990 mL	1.15005 mL	0.02500 mL	9.334	0.10061	0.98780
19:02.0	Data point 27	0.34995 mL	0.06919 mL	0.06999 mL	1.15005 mL	0.02500 mL	9.597	0.09781	0.98928
19:38.9	Data point 28	0.34995 mL	0.06919 mL	0.07011 mL	1.15005 mL	0.02500 mL	9.868	0.09614	0.98123
20:05.7	Data point 29	0.34995 mL	0.06919 mL	0.07027 mL	1.15005 mL	0.02500 mL	10.212	0.07694	0.96069
20:32.5	Data point 30	0.34995 mL	0.06919 mL	0.07051 mL	1.15005 mL	0.02500 mL	10.414	0.03263	0.92759
20:49.1	Data point 31	0.34995 mL	0.06919 mL	0.07088 mL	1.15005 mL	0.02500 mL	10.709	0.00864	0.78861
21:21.1	Data point 32	0.34995 mL	0.06919 mL	0.07171 mL	1.15005 mL	0.02500 mL	10.902	-0.00050	0.01117
21:53.0	Data point 33	0.34995 mL	0.06919 mL	0.07295 mL	1.15005 mL	0.02500 mL	11.094	-0.00659	0.71687
22:09.6	Data point 34	0.34995 mL	0.06919 mL	0.07462 mL	1.15005 mL	0.02500 mL	11.262	-0.00654	0.74297
22:36.6	Data point 35	0.34995 mL	0.06919 mL	0.07803 mL	1.15005 mL	0.02500 mL	11.455	-0.00627	0.67172
23:03.5	Data point 36	0.34995 mL	0.06919 mL	0.08208 mL	1.15005 mL	0.02500 mL	11.644	-0.00712	0.70022
23:20.2	Data point 37	0.34995 mL	0.06919 mL	0.08794 mL	1.15005 mL	0.02500 mL	11.794	-0.00717	0.74788
23:52.6	Data point 38	0.34995 mL	0.06919 mL	0.09899 mL	1.15005 mL	0.02500 mL	11.995	0.00175	0.11667
24:09.3	Data point 39	0.34995 mL	0.06919 mL	0.10052 mL	1.15005 mL	0.02500 mL	12.016	-0.00742	0.79563
25:50.8	Reference spectrum								
26:54.8	Data point 41	0.50000 mL	0.16660 mL	0.10054 mL	1.15005 mL	0.02500 mL	2.012	-0.04740	0.93961
27:22.3	Data point 42	0.50000 mL	0.16660 mL	0.12408 mL	1.15005 mL	0.02500 mL	2.211	0.00909	0.74636
27:39.3	Data point 43	0.50000 mL	0.16660 mL	0.13902 mL	1.15005 mL	0.02500 mL	2.409	0.01364	0.85662
27:56.1	Data point 44	0.50000 mL	0.16660 mL	0.14852 mL	1.15005 mL	0.02500 mL	2.611	0.00818	0.78053
28:12.8	Data point 45	0.50000 mL	0.16660 mL	0.15452 mL	1.15005 mL	0.02500 mL	2.812	0.02851	0.91765
28:29.3	Data point 46	0.50000 mL	0.16660 mL	0.15826 mL	1.15005 mL	0.02500 mL	3.007	0.00158	0.05553
28:45.9	Data point 47	0.50000 mL	0.16660 mL	0.16068 mL	1.15005 mL	0.02500 mL	3.216	0.01208	0.86564
29:02.5	Data point 48	0.50000 mL	0.16660 mL	0.16218 mL	1.15005 mL	0.02500 mL	3.390	0.01997	0.93839
29:19.1	Data point 49	0.50000 mL	0.16660 mL	0.16317 mL	1.15005 mL	0.02500 mL	3.559	0.01585	0.88400

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

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH Slope
29:46.0	Data point 50	0.50000 mL	0.16660 mL	0.16432 mL	1.15005 mL	0.02500 mL	3.760	0.02862	0.97119	0.97119
30:07.8	Data point 51	0.50000 mL	0.16660 mL	0.16498 mL	1.15005 mL	0.02500 mL	4.068	0.04928	0.98585	0.98585
30:29.6	Data point 52	0.50000 mL	0.16660 mL	0.16538 mL	1.15005 mL	0.02500 mL	4.427	0.09688	0.99530	0.99530
30:56.4	Data point 53	0.50000 mL	0.16660 mL	0.16571 mL	1.15005 mL	0.02500 mL	4.805	0.09983	0.99043	0.99043
31:36.3	Data point 54	0.50000 mL	0.16660 mL	0.16590 mL	1.15005 mL	0.02500 mL	5.259	0.09611	0.95932	0.95932
32:34.2	Data point 55	0.50000 mL	0.16660 mL	0.16602 mL	1.15005 mL	0.02500 mL	5.750	0.09659	0.98588	0.98588
33:30.9	Data point 56	0.50000 mL	0.16660 mL	0.16611 mL	1.15005 mL	0.02500 mL	6.267	0.09792	0.98701	0.98701
34:25.6	Data point 57	0.50000 mL	0.16660 mL	0.16620 mL	1.15005 mL	0.02500 mL	6.660	0.09938	0.97707	0.97707
35:03.3	Data point 58	0.50000 mL	0.16660 mL	0.16630 mL	1.15005 mL	0.02500 mL	6.923	0.10057	0.99505	0.99505
35:42.0	Data point 59	0.50000 mL	0.16660 mL	0.16639 mL	1.15005 mL	0.02500 mL	7.179	0.09757	0.99359	0.99359
36:22.5	Data point 60	0.50000 mL	0.16660 mL	0.16651 mL	1.15005 mL	0.02500 mL	7.435	0.09462	0.97663	0.97663
37:01.3	Data point 61	0.50000 mL	0.16660 mL	0.16663 mL	1.15005 mL	0.02500 mL	7.668	0.09781	0.99247	0.99247
37:45.8	Data point 62	0.50000 mL	0.16660 mL	0.16675 mL	1.15005 mL	0.02500 mL	7.960	0.09633	0.98309	0.98309
38:28.7	Data point 63	0.50000 mL	0.16660 mL	0.16684 mL	1.15005 mL	0.02500 mL	8.260	0.09940	0.98649	0.98649
39:14.2	Data point 64	0.50000 mL	0.16660 mL	0.16693 mL	1.15005 mL	0.02500 mL	8.692	0.09572	0.97048	0.97048
40:04.2	Data point 65	0.50000 mL	0.16660 mL	0.16703 mL	1.15005 mL	0.02500 mL	9.104	0.09854	0.98929	0.98929
40:47.4	Data point 66	0.50000 mL	0.16660 mL	0.16712 mL	1.15005 mL	0.02500 mL	9.427	0.09929	0.96392	0.96392
41:20.1	Data point 67	0.50000 mL	0.16660 mL	0.16722 mL	1.15005 mL	0.02500 mL	9.744	0.09517	0.97511	0.97511
41:44.8	Data point 68	0.50000 mL	0.16660 mL	0.16733 mL	1.15005 mL	0.02500 mL	10.020	0.06934	0.95893	0.95893
42:01.3	Data point 69	0.50000 mL	0.16660 mL	0.16755 mL	1.15005 mL	0.02500 mL	10.322	0.01941	0.88056	0.88056
42:33.2	Data point 70	0.50000 mL	0.16660 mL	0.16804 mL	1.15005 mL	0.02500 mL	10.519	0.00425	0.52856	0.52856
43:05.3	Data point 71	0.50000 mL	0.16660 mL	0.16874 mL	1.15005 mL	0.02500 mL	10.718	-0.00079	0.04953	0.04953
43:22.0	Data point 72	0.50000 mL	0.16660 mL	0.16973 mL	1.15005 mL	0.02500 mL	10.915	-0.00777	0.77415	0.77415
43:38.6	Data point 73	0.50000 mL	0.16660 mL	0.17126 mL	1.15005 mL	0.02500 mL	11.078	-0.00404	0.40114	0.40114
44:10.7	Data point 74	0.50000 mL	0.16660 mL	0.17415 mL	1.15005 mL	0.02500 mL	11.270	-0.01018	0.91389	0.91389
44:37.7	Data point 75	0.50000 mL	0.16660 mL	0.17806 mL	1.15005 mL	0.02500 mL	11.461	-0.01191	0.91645	0.91645
45:10.1	Data point 76	0.50000 mL	0.16660 mL	0.18535 mL	1.15005 mL	0.02500 mL	11.659	-0.00968	0.85015	0.85015
45:42.6	Data point 77	0.50000 mL	0.16660 mL	0.19617 mL	1.15005 mL	0.02500 mL	11.857	-0.00576	0.66939	0.66939
46:04.7	Data point 78	0.50000 mL	0.16660 mL	0.20889 mL	1.15005 mL	0.02500 mL	12.004	-0.00665	0.65235	0.65235
47:49.5	Reference spectrum									
49:12.9	Data point 80	0.83996 mL	0.29548 mL	0.20891 mL	1.15005 mL	0.02500 mL	2.013	-0.03025	0.95923	0.95923
49:40.6	Data point 81	0.83996 mL	0.29548 mL	0.23584 mL	1.15005 mL	0.02500 mL	2.209	0.01165	0.71144	0.71144
49:57.5	Data point 82	0.83996 mL	0.29548 mL	0.25299 mL	1.15005 mL	0.02500 mL	2.408	0.00774	0.43737	0.43737
50:14.3	Data point 83	0.83996 mL	0.29548 mL	0.26392 mL	1.15005 mL	0.02500 mL	2.604	-0.03359	0.83216	0.83216
50:31.1	Data point 84	0.83996 mL	0.29548 mL	0.27107 mL	1.15005 mL	0.02500 mL	2.808	0.00980	0.53331	0.53331
50:47.8	Data point 85	0.83996 mL	0.29548 mL	0.27545 mL	1.15005 mL	0.02500 mL	3.002	-0.01498	0.82438	0.82438
51:04.3	Data point 86	0.83996 mL	0.29548 mL	0.27827 mL	1.15005 mL	0.02500 mL	3.220	-0.00773	0.40725	0.40725
51:20.9	Data point 87	0.83996 mL	0.29548 mL	0.27996 mL	1.15005 mL	0.02500 mL	3.388	0.00254	0.11739	0.11739
52:02.4	Data point 88	0.83996 mL	0.29548 mL	0.28140 mL	1.15005 mL	0.02500 mL	3.812	-0.01429	0.83687	0.83687
52:29.4	Data point 89	0.83996 mL	0.29548 mL	0.28443 mL	1.15005 mL	0.02500 mL	5.145	-0.06232	0.60070	0.60070
52:58.1	Data point 90	0.83996 mL	0.29548 mL	0.28469 mL	1.15005 mL	0.02500 mL	5.765	0.09540	0.95384	0.95384
53:30.6	Data point 91	0.83996 mL	0.29548 mL	0.28481 mL	1.15005 mL	0.02500 mL	6.024	0.09838	0.96697	0.96697
54:00.4	Data point 92	0.83996 mL	0.29548 mL	0.28490 mL	1.15005 mL	0.02500 mL	6.221	-0.03478	0.34071	0.34071
54:22.1	Data point 93	0.83996 mL	0.29548 mL	0.28502 mL	1.15005 mL	0.02500 mL	6.509	-0.07557	0.70744	0.70744
54:48.1	Data point 94	0.83996 mL	0.29548 mL	0.28514 mL	1.15005 mL	0.02500 mL	6.757	-0.09151	0.92688	0.92688
55:19.4	Data point 95	0.83996 mL	0.29548 mL	0.28525 mL	1.15005 mL	0.02500 mL	6.975	0.03002	0.62417	0.62417
55:51.4	Data point 96	0.83996 mL	0.29548 mL	0.28540 mL	1.15005 mL	0.02500 mL	7.218	0.08354	0.85166	0.85166
56:18.3	Data point 97	0.83996 mL	0.29548 mL	0.28551 mL	1.15005 mL	0.02500 mL	7.435	0.09524	0.94381	0.94381
56:51.3	Data point 98	0.83996 mL	0.29548 mL	0.28563 mL	1.15005 mL	0.02500 mL	7.717	0.09909	0.98255	0.98255
57:26.7	Data point 99	0.83996 mL	0.29548 mL	0.28572 mL	1.15005 mL	0.02500 mL	7.979	0.09940	0.97982	0.97982
58:07.1	Data point 100	0.83996 mL	0.29548 mL	0.28582 mL	1.15005 mL	0.02500 mL	8.351	0.09745	0.98546	0.98546
58:55.6	Data point 101	0.83996 mL	0.29548 mL	0.28591 mL	1.15005 mL	0.02500 mL	8.791	0.08853	0.90914	0.90914
59:39.5	Data point 102	0.83996 mL	0.29548 mL	0.28601 mL	1.15005 mL	0.02500 mL	9.159	0.09262	0.96900	0.96900
1:00:10.2	Data point 103	0.83996 mL	0.29548 mL	0.28610 mL	1.15005 mL	0.02500 mL	9.509	0.09447	0.94462	0.94462
1:00:35.9	Data point 104	0.83996 mL	0.29548 mL	0.28619 mL	1.15005 mL	0.02500 mL	9.712	0.08737	0.95857	0.95857
1:00:52.4	Data point 105	0.83996 mL	0.29548 mL	0.28636 mL	1.15005 mL	0.02500 mL	9.994	0.01804	0.91104	0.91104
1:01:14.0	Data point 106	0.83996 mL	0.29548 mL	0.28664 mL	1.15005 mL	0.02500 mL	10.194	0.00435	0.41151	0.41151

Sample name: **M18**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-12010**
 Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12010_M18_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 12:04:33 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
1:01:30.6	Data point 107	0.83996 mL	0.29548 mL	0.28711 mL	1.15005 mL	0.02500 mL	10.424	-0.01587	0.92501	0.0008
1:01:47.3	Data point 108	0.83996 mL	0.29548 mL	0.28789 mL	1.15005 mL	0.02500 mL	10.607	-0.01835	0.89412	0.0009
1:02:03.9	Data point 109	0.83996 mL	0.29548 mL	0.28906 mL	1.15005 mL	0.02500 mL	10.788	-0.02060	0.94692	0.0010
1:02:20.6	Data point 110	0.83996 mL	0.29548 mL	0.29080 mL	1.15005 mL	0.02500 mL	10.960	-0.02285	0.92858	0.0011
1:02:37.2	Data point 111	0.83996 mL	0.29548 mL	0.29334 mL	1.15005 mL	0.02500 mL	11.097	-0.02119	0.92066	0.0010
1:03:04.2	Data point 112	0.83996 mL	0.29548 mL	0.29673 mL	1.15005 mL	0.02500 mL	11.287	-0.01817	0.95686	0.0009
1:03:20.9	Data point 113	0.83996 mL	0.29548 mL	0.30207 mL	1.15005 mL	0.02500 mL	11.439	-0.01973	0.92653	0.0010
1:03:53.3	Data point 114	0.83996 mL	0.29548 mL	0.31101 mL	1.15005 mL	0.02500 mL	11.634	-0.01396	0.92329	0.0007
1:04:20.6	Data point 115	0.83996 mL	0.29548 mL	0.32587 mL	1.15005 mL	0.02500 mL	11.828	-0.01381	0.93854	0.0007
1:04:48.3	Data point 116	0.83996 mL	0.29548 mL	0.34875 mL	1.15005 mL	0.02500 mL	12.013	-0.00961	0.71039	0.0005
1:06:47.6	Assay volumes	1.08996 mL	0.43631 mL	0.34875 mL	1.15005 mL	0.02500 mL				

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	Spectrometer			
Monitor at a wavelength of	500.0 nm			
Absorbance threshold of	0.100			
Collect turbidity sensor data	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	15%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
Cosolvent in use	Yes			
Cosolvent type	Methanol			
Cosolvent volume	1.15 mL			
Cosolvent added	Automatic			
ISA water volume	0.35 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	15%			
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			
After medium addition, stir for	5 seconds			
Sample Sonication				
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	No			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			

Sample name:	M18	Experiment start time:	10/12/2017 12:04:33 PM
Assay name:	UV-metric psKa	Analyst:	Dorothy Levorse
Assay ID:	17J-12010	Instrument ID:	T311053
Filename:	C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12010_M18_UV-metric psKa.t3r		

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	10 seconds			
Titration 2				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.15 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Titration 3				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.34 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Data Point Stability				
Stir during data point collection	Yes			
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	0.109	10/12/2017 12:04:33 PM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus S	1.0007	10/12/2017 12:04:33 PM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jH	0.3	10/12/2017 12:04:33 PM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jOH	-0.2	10/12/2017 12:04:33 PM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Base concentration factor	1.011	10/12/2017 12:04:33 PM	C:\Sirius_T3\KOH17122.t3r
Acid concentration factor	0.995	10/12/2017 12:04:33 PM	C:\Sirius_T3\17J-11005_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)	10-10-2017	10/10/2017 10:48:53 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM

Sample name: **M18**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-12010**
 Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12010_M18_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 12:04:33 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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		10/10/2017 9:57:33 AM
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
Titrator		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	-9.42 mV		10/12/2017 12:04:57 PM
Filling solution	3M KCl	KCL095	10/10/2017 9:58:43 AM
Liquids			
Wash 1	50% IPA:50% Water		10/11/2017 8:31:15 AM
Wash 2	0.5% Triton X-100 in H2O		10/11/2017 8:31:17 AM
Buffer position 1	pH7 Wash		10/11/2017 8:31:21 AM
Buffer position 2	pH 7		10/11/2017 8:31:23 AM
Storage position			10/11/2017 8:31:26 AM
Wash water	3.9e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	6.2e+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	419:28:33		11/23/2010 12:22:28 PM
Calibrated on	10/11/2017 8:30:19 AM		
Integration time	10		
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		



Assay Settings

Sample name: **M18** Experiment start time: **10/12/2017 12:04:33 PM**
Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse**
Assay ID: **17J-12010** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12010_M18_UV-metric psKa.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

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

Tray Information

Title
Location G1