

Sample name: **D05**
Assay name: **UV-metric psKa**
Assay ID: **17J-12002**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12002_D05_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:32:48 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

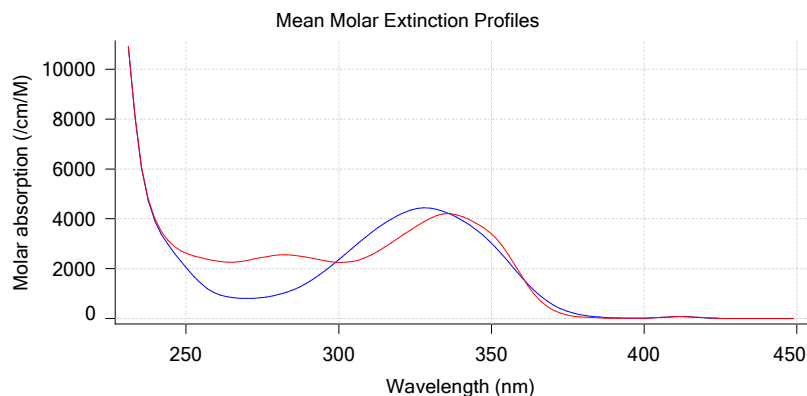
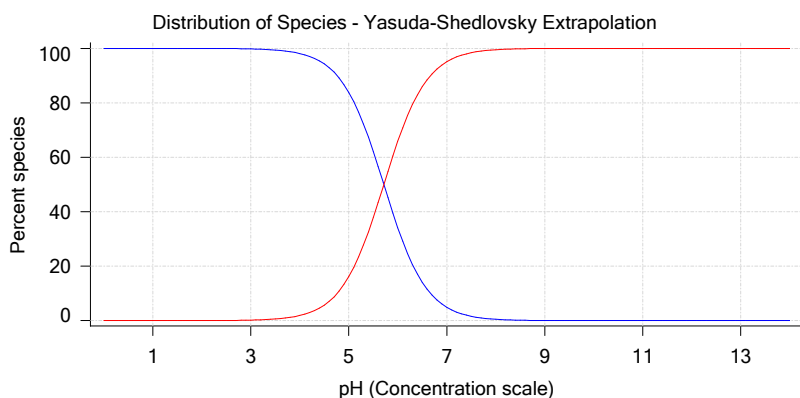
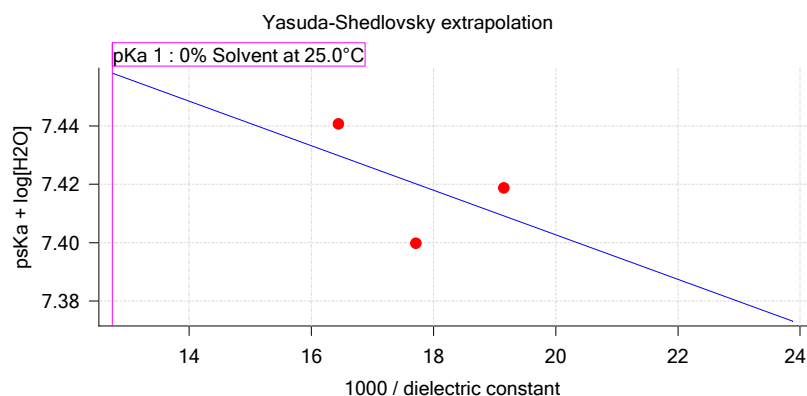
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.72	±0.07	7.56	-7.6396	0.2540	0.166 M	25.0°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1
17J-12002 Points 4 to 39	58.81 %	Up	UV-metric pKa	52.2	19.7 M	0.157 M	24.9°C	✓ 6.12
17J-12002 Points 41 to 80	49.80 %	Up	UV-metric pKa	56.5	24.5 M	0.166 M	25.0°C	✓ 6.01
17J-12002 Points 82 to 121	40.42 %	Up	UV-metric pKa	60.8	29.8 M	0.174 M	25.0°C	✓ 5.97

Graphs



UV-metric psKa Titration 1 of 3 17J-12002 Points 4 to 39

Results

pKa 1	6.12
RMSD	0.009 0.013
Chi squared	0.0373
PCA calculated number of pKas	2
Average ionic strength	0.157 M
Average temperature	24.9°C
Analyte concentration range	94.7 µM to 89.3 µM
Methanol weight %	58.8 %
Dielectric constant	52.2
Water concentration	19.7 M
Number of pKas source	Predicted
Wavelength clipping	230.0 nm to 450.0 nm

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Results (continued)

pH clipping 1.479 to 12.537

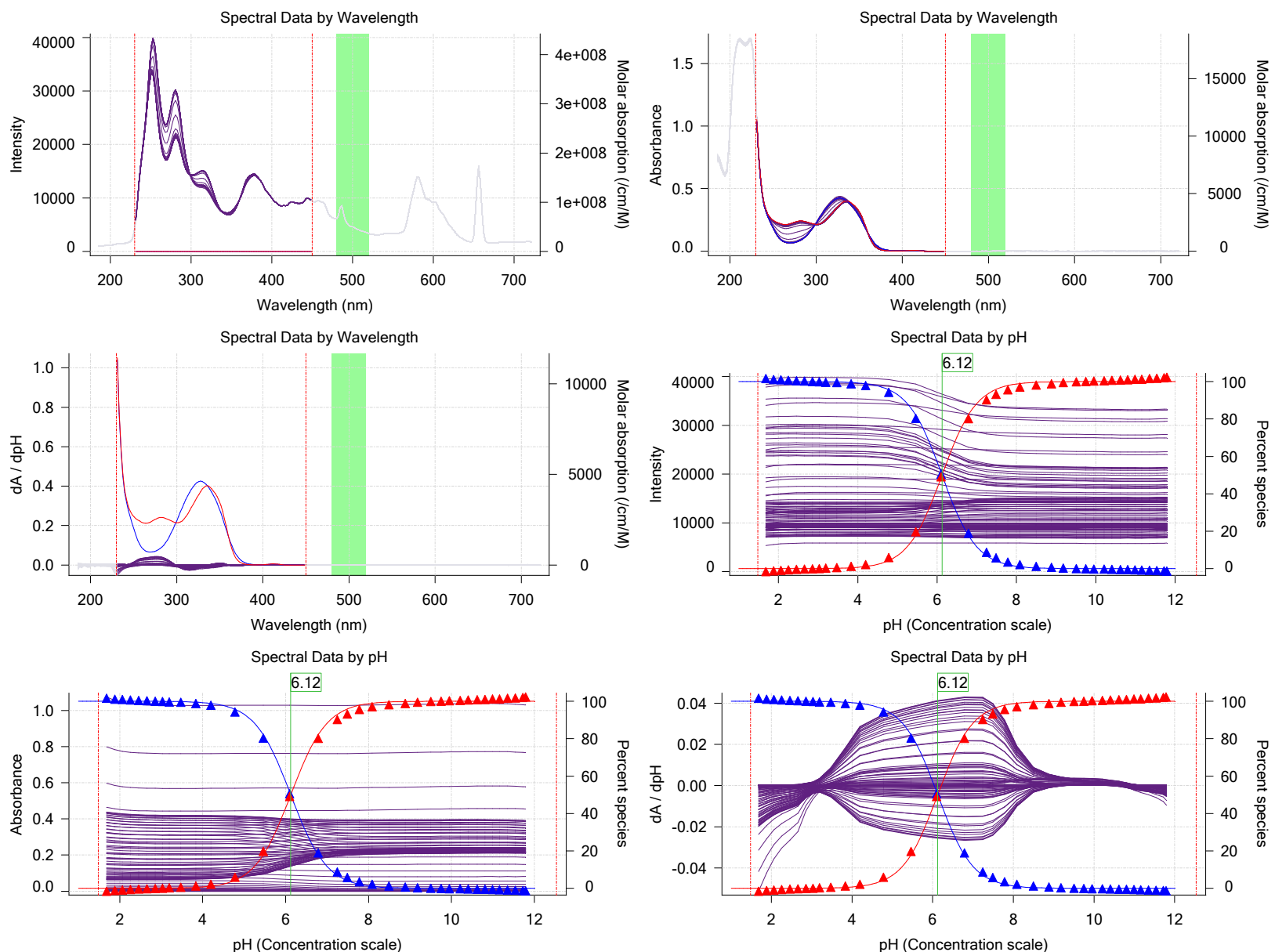
Warnings and errors

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				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

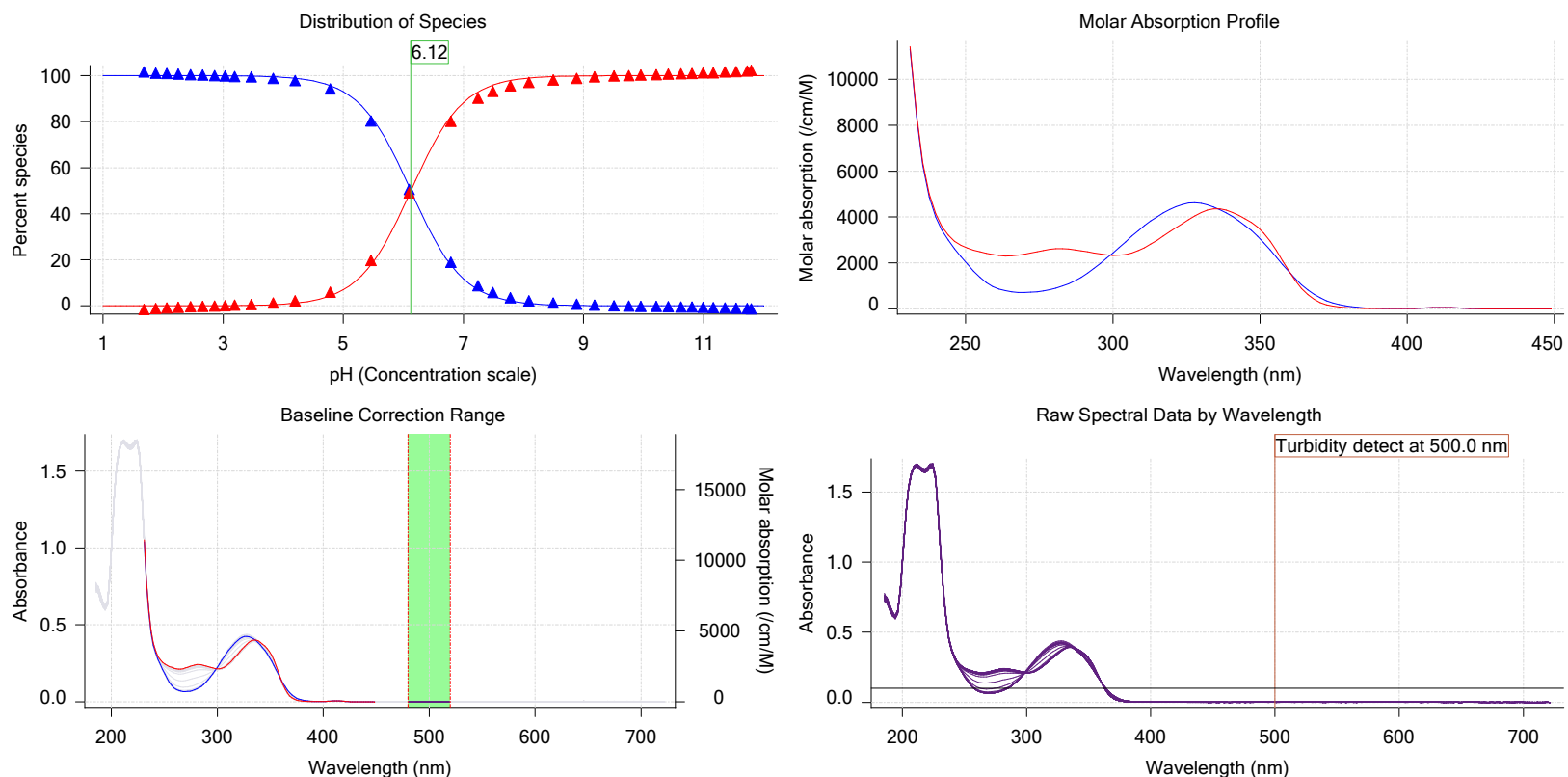
Graphs



Sample name: **D05**
Assay name: **UV-metric psKa**
Assay ID: **17J-12002**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12002_D05_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:32:48 AM**
Analyst: **Dorothy Leverse**
Instrument ID: **T311053**

Graphs (continued)



UV-metric psKa Titration 2 of 3 17J-12002 Points 41 to 80

Results

pKa 1	6.01
RMSD	0.004 0.004
Chi squared	0.0238
PCA calculated number of pKas	2
Average ionic strength	0.166 M
Average temperature	25.0°C
Analyte concentration range	81.6 µM to 77.2 µM
Methanol weight %	49.8 %
Dielectric constant	56.5
Water concentration	24.5 M
Number of pKas source	Predicted
Wavelength clipping	230.0 nm to 450.0 nm
pH clipping	1.490 to 12.509

Warnings and errors

Errors: None
Warnings: PCA calculation disagrees with predicted number of pKas

Assay Settings

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

Assay Medium

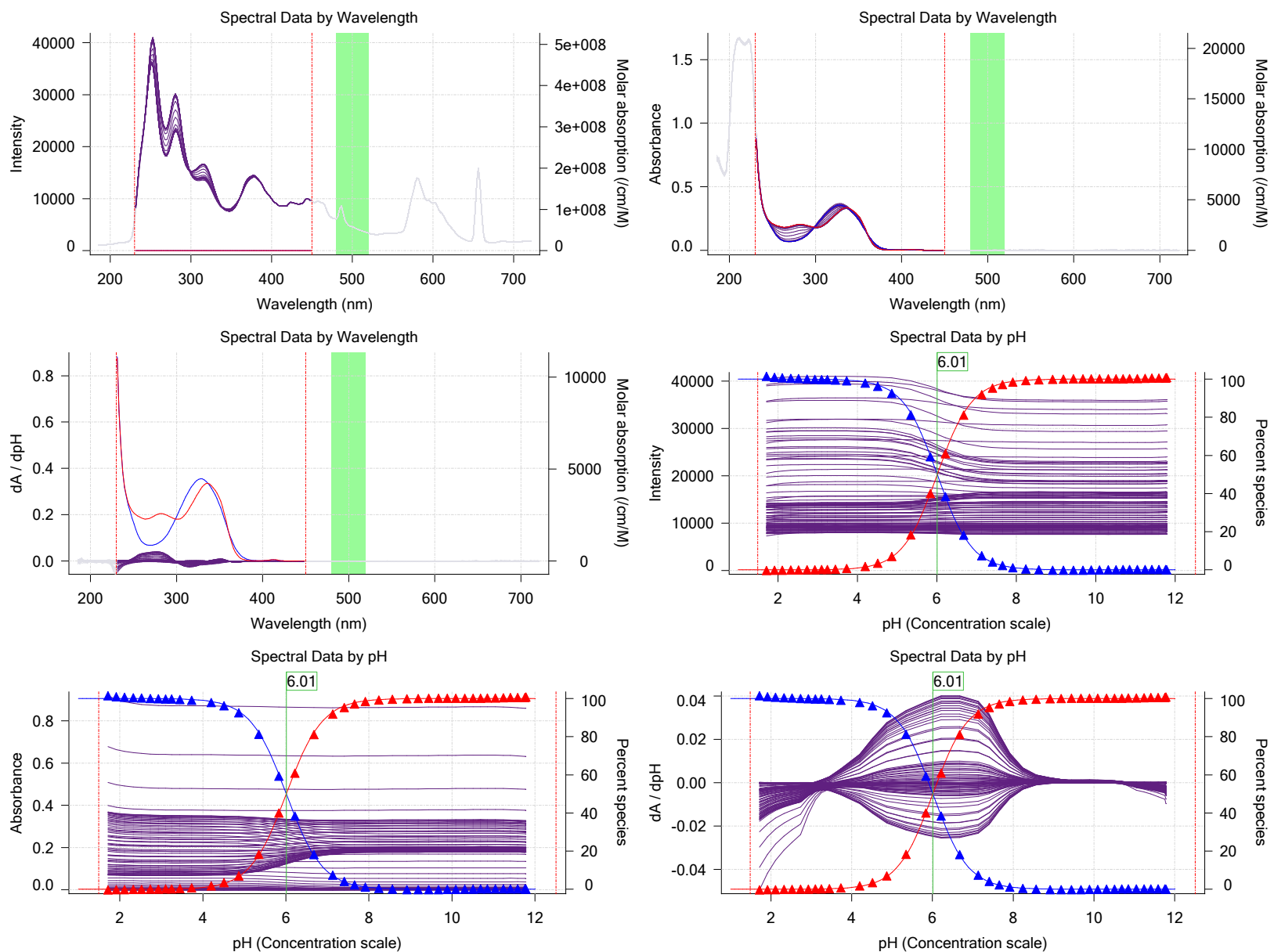
Sample name: **D05**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-12002**
 Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12002_D05_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:32:48 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			

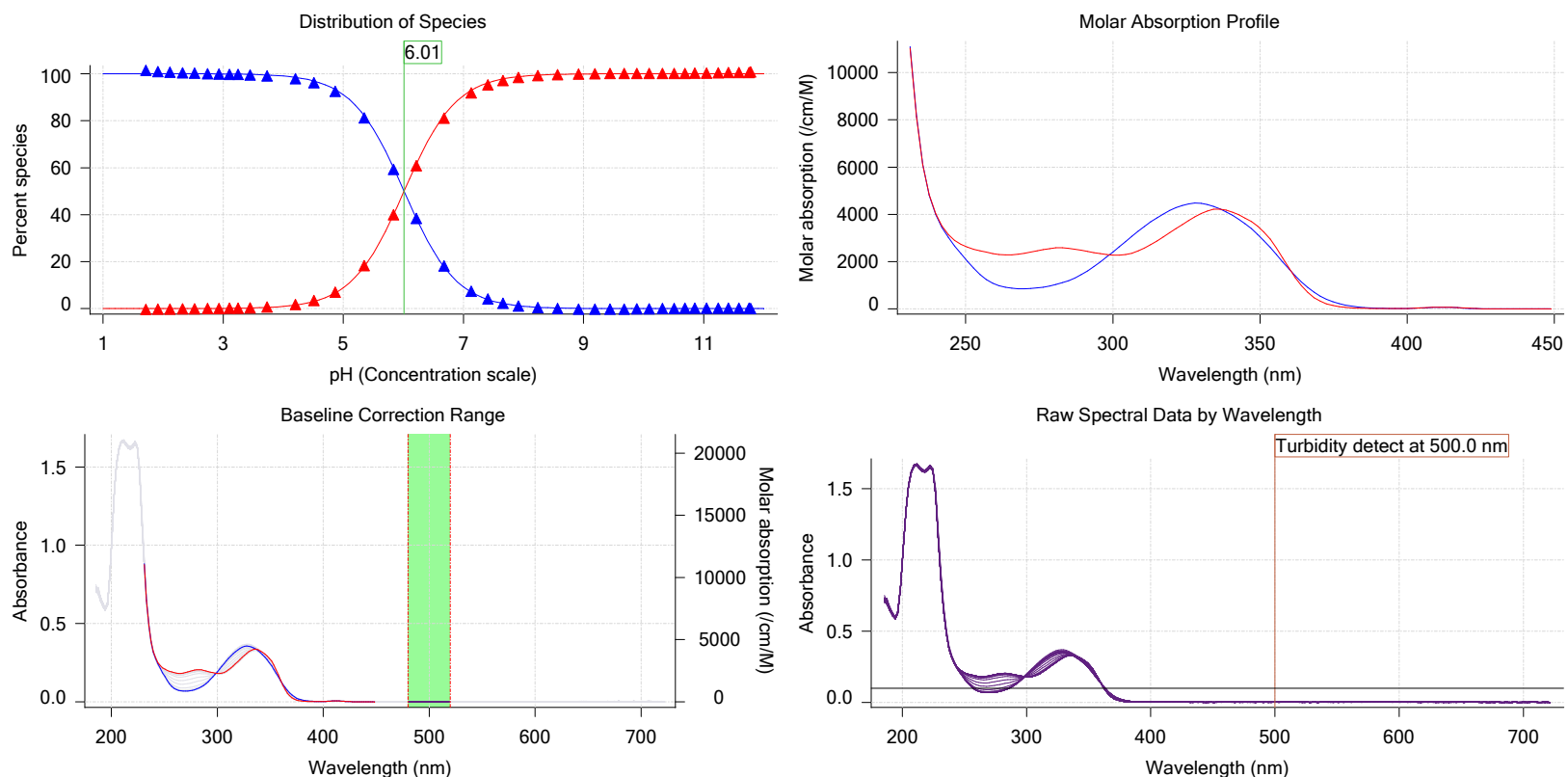
Graphs



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Experiment start time: **10/12/2017 1:32:48 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Graphs (continued)



UV-metric psKa Titration 3 of 3 17J-12002 Points 82 to 121

Results

pKa 1	5.97
RMSD	0.008 0.006
Chi squared	0.0517
PCA calculated number of pKas	3
Average ionic strength	0.174 M
Average temperature	25.0°C
Analyte concentration range	67.5 µM to 63.8 µM
Methanol weight %	40.4 %
Dielectric constant	60.8
Water concentration	29.8 M
Number of pKas source	Predicted
Wavelength clipping	230.0 nm to 450.0 nm
pH clipping	1.494 to 12.526

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

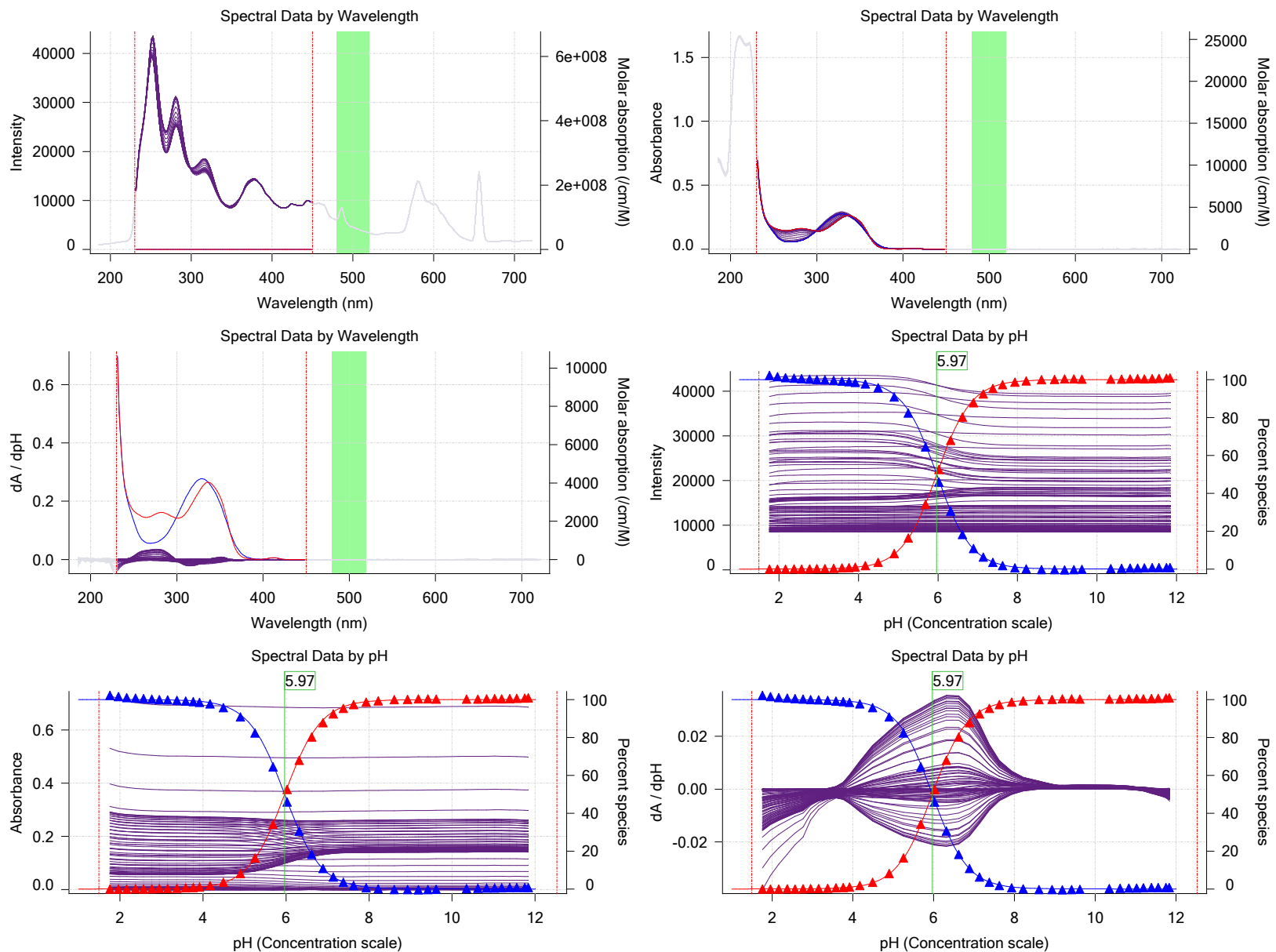
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Experiment start time: **10/12/2017 1:32:48 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Settings (continued)

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

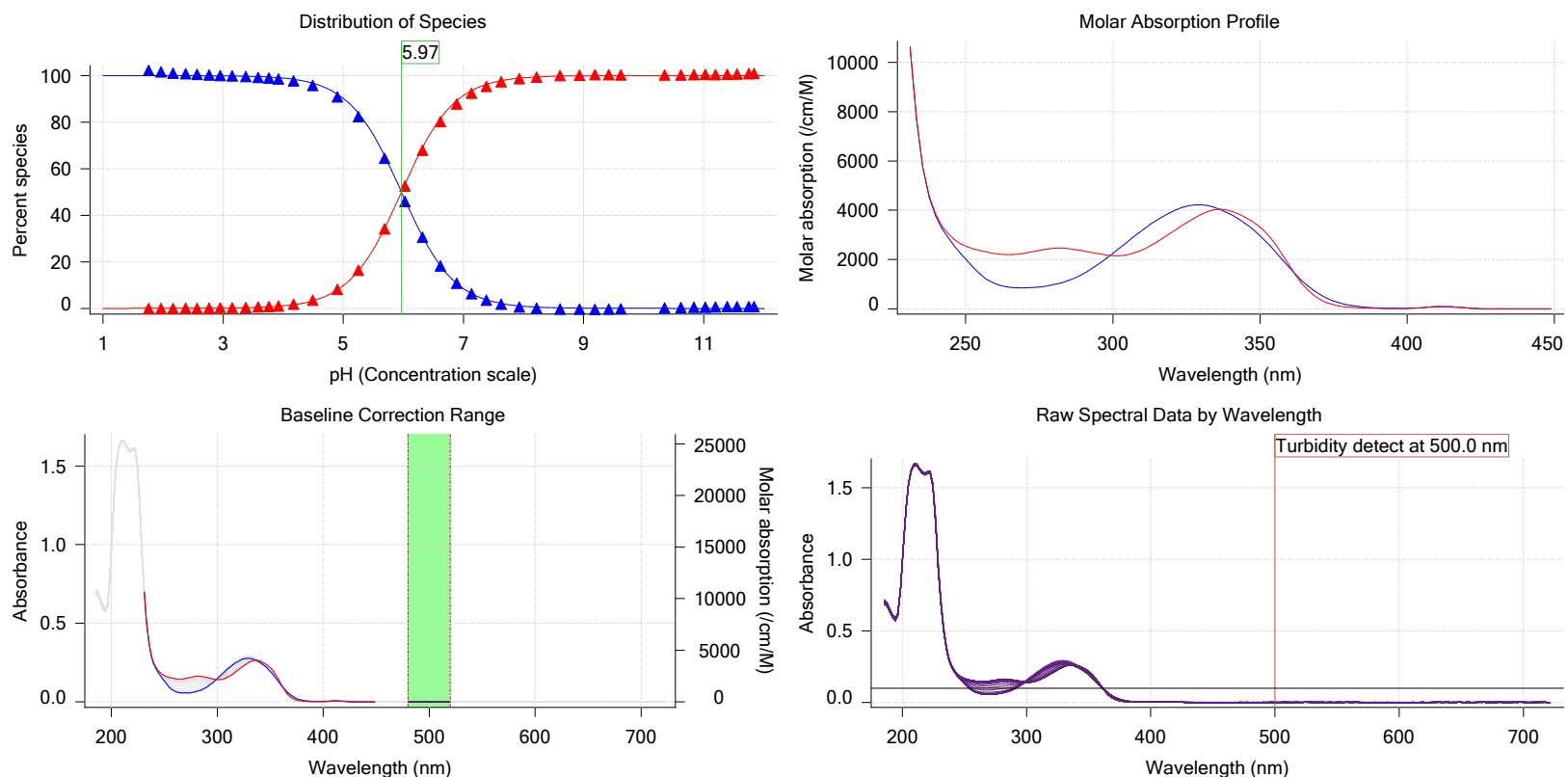
Graphs



Sample name: **D05**
 Assay name: **UV-metric pKa**
 Assay ID: **17J-12002**
 Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12002_D05_UV-metric pKa.t3r**

Experiment start time: **10/12/2017 1:32:48 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Graphs (continued)



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	D05	9/29/2017 6:38:13 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0040 mL	10/3/2017 3:25:30 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.038100 M	10/2/2017 12:58:32 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	380.25	9/29/2017 6:38:21 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	9/29/2017 6:38:13 PM	User entered value
Sample is a	Acid	9/29/2017 6:38:13 PM	User entered value
pKa 1	7.44	9/29/2017 6:38:13 PM	User entered value
logP (neutral XH)	-10.00	9/29/2017 6:38:13 PM	User entered value
logP (X -)	-10.00		Default value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:03.8	Dark spectrum								
3:05.2	Reference spectrum								
3:32.8	Volume reset due to vial change								
5:03.6	Initial pH = 8.38								
5:55.1	Data point 4	0.16004 mL	0.07084 mL	0.00000 mL	1.34995 mL	0.02500 mL	1.979	-0.00839	0.62270
6:23.8	Data point 5	0.16004 mL	0.07084 mL	0.02484 mL	1.34995 mL	0.02500 mL	2.178	0.00394	0.37693
6:40.8	Data point 6	0.16004 mL	0.07084 mL	0.04036 mL	1.34995 mL	0.02500 mL	2.363	0.02543	0.91071
6:57.7	Data point 7	0.16004 mL	0.07084 mL	0.05061 mL	1.34995 mL	0.02500 mL	2.557	0.02302	0.76767
7:14.4	Data point 8	0.16004 mL	0.07084 mL	0.05727 mL	1.34995 mL	0.02500 mL	2.759	0.02216	0.88733
7:31.1	Data point 9	0.16004 mL	0.07084 mL	0.06150 mL	1.34995 mL	0.02500 mL	2.958	0.01614	0.93237

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Experiment start time: **10/12/2017 1:32:48 AM**
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Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
7:47.8	Data point 10	0.16004 mL	0.07084 mL	0.06418 mL	1.34995 mL	0.02500 mL	3.158	0.01286	0.93466	0.00
8:04.2	Data point 11	0.16004 mL	0.07084 mL	0.06587 mL	1.34995 mL	0.02500 mL	3.331	0.01908	0.95814	0.00
8:20.8	Data point 12	0.16004 mL	0.07084 mL	0.06700 mL	1.34995 mL	0.02500 mL	3.492	0.01730	0.96040	0.00
8:42.5	Data point 13	0.16004 mL	0.07084 mL	0.06858 mL	1.34995 mL	0.02500 mL	3.768	0.02316	0.92748	0.00
9:04.1	Data point 14	0.16004 mL	0.07084 mL	0.06936 mL	1.34995 mL	0.02500 mL	4.131	0.05446	0.98788	0.00
9:25.8	Data point 15	0.16004 mL	0.07084 mL	0.06971 mL	1.34995 mL	0.02500 mL	4.490	0.09880	0.99059	0.00
10:03.7	Data point 16	0.16004 mL	0.07084 mL	0.07001 mL	1.34995 mL	0.02500 mL	5.071	0.09733	0.99035	0.00
11:10.2	Data point 17	0.16004 mL	0.07084 mL	0.07016 mL	1.34995 mL	0.02500 mL	5.748	0.12655	0.98678	0.00
12:26.8	Data point 18	0.16004 mL	0.07084 mL	0.07025 mL	1.34995 mL	0.02500 mL	6.382	0.09994	0.99135	0.00
13:30.9	Data point 19	0.16004 mL	0.07084 mL	0.07034 mL	1.34995 mL	0.02500 mL	7.066	0.09775	0.98625	0.00
14:25.5	Data point 20	0.16004 mL	0.07084 mL	0.07046 mL	1.34995 mL	0.02500 mL	7.519	0.09905	0.98975	0.00
15:04.6	Data point 21	0.16004 mL	0.07084 mL	0.07058 mL	1.34995 mL	0.02500 mL	7.762	0.09412	0.92581	0.00
15:42.0	Data point 22	0.16004 mL	0.07084 mL	0.07072 mL	1.34995 mL	0.02500 mL	8.052	0.10072	0.99298	0.00
16:21.1	Data point 23	0.16004 mL	0.07084 mL	0.07084 mL	1.34995 mL	0.02500 mL	8.359	0.10002	0.99011	0.00
17:11.3	Data point 24	0.16004 mL	0.07084 mL	0.07095 mL	1.34995 mL	0.02500 mL	8.762	0.09979	0.98281	0.00
18:02.6	Data point 25	0.16004 mL	0.07084 mL	0.07105 mL	1.34995 mL	0.02500 mL	9.150	0.09569	0.96974	0.00
18:50.8	Data point 26	0.16004 mL	0.07084 mL	0.07114 mL	1.34995 mL	0.02500 mL	9.443	0.09683	0.97796	0.00
19:36.0	Data point 27	0.16004 mL	0.07084 mL	0.07126 mL	1.34995 mL	0.02500 mL	9.767	0.09691	0.97468	0.00
20:14.3	Data point 28	0.16004 mL	0.07084 mL	0.07138 mL	1.34995 mL	0.02500 mL	10.010	0.09960	0.98396	0.00
20:41.5	Data point 29	0.16004 mL	0.07084 mL	0.07152 mL	1.34995 mL	0.02500 mL	10.211	0.08988	0.98856	0.00
20:58.0	Data point 30	0.16004 mL	0.07084 mL	0.07173 mL	1.34995 mL	0.02500 mL	10.466	0.04170	0.99046	0.00
21:29.9	Data point 31	0.16004 mL	0.07084 mL	0.07215 mL	1.34995 mL	0.02500 mL	10.663	0.02164	0.89734	0.00
21:46.5	Data point 32	0.16004 mL	0.07084 mL	0.07274 mL	1.34995 mL	0.02500 mL	10.874	0.00735	0.78760	0.00
22:03.1	Data point 33	0.16004 mL	0.07084 mL	0.07368 mL	1.34995 mL	0.02500 mL	11.060	0.00551	0.70376	0.00
22:19.7	Data point 34	0.16004 mL	0.07084 mL	0.07512 mL	1.34995 mL	0.02500 mL	11.241	0.00233	0.35922	0.00
22:36.2	Data point 35	0.16004 mL	0.07084 mL	0.07730 mL	1.34995 mL	0.02500 mL	11.410	0.00292	0.32719	0.00
23:03.0	Data point 36	0.16004 mL	0.07084 mL	0.08046 mL	1.34995 mL	0.02500 mL	11.605	0.00069	0.04038	0.00
23:19.8	Data point 37	0.16004 mL	0.07084 mL	0.08549 mL	1.34995 mL	0.02500 mL	11.790	0.00553	0.45504	0.00
23:36.5	Data point 38	0.16004 mL	0.07084 mL	0.09320 mL	1.34995 mL	0.02500 mL	11.970	0.00626	0.55601	0.00
23:53.1	Data point 39	0.16004 mL	0.07084 mL	0.09725 mL	1.34995 mL	0.02500 mL	12.037	-0.00287	0.27766	0.00
25:33.4	Reference spectrum									
26:36.0	Data point 41	0.22001 mL	0.17121 mL	0.09727 mL	1.34995 mL	0.02500 mL	1.990	-0.05763	0.94736	0.00
27:03.7	Data point 42	0.22001 mL	0.17121 mL	0.12462 mL	1.34995 mL	0.02500 mL	2.190	0.01129	0.86341	0.00
27:20.6	Data point 43	0.22001 mL	0.17121 mL	0.14128 mL	1.34995 mL	0.02500 mL	2.390	0.00839	0.73352	0.00
27:37.4	Data point 44	0.22001 mL	0.17121 mL	0.15193 mL	1.34995 mL	0.02500 mL	2.598	0.01259	0.87518	0.00
27:54.1	Data point 45	0.22001 mL	0.17121 mL	0.15858 mL	1.34995 mL	0.02500 mL	2.798	-0.00433	0.11172	0.00
28:10.8	Data point 46	0.22001 mL	0.17121 mL	0.16282 mL	1.34995 mL	0.02500 mL	3.012	0.01965	0.94146	0.00
28:27.5	Data point 47	0.22001 mL	0.17121 mL	0.16541 mL	1.34995 mL	0.02500 mL	3.201	0.01553	0.91759	0.00
28:44.1	Data point 48	0.22001 mL	0.17121 mL	0.16707 mL	1.34995 mL	0.02500 mL	3.375	0.01749	0.94154	0.00
29:00.7	Data point 49	0.22001 mL	0.17121 mL	0.16818 mL	1.34995 mL	0.02500 mL	3.520	0.02409	0.98566	0.00
29:32.7	Data point 50	0.22001 mL	0.17121 mL	0.16926 mL	1.34995 mL	0.02500 mL	3.719	0.03148	0.96915	0.00
29:59.5	Data point 51	0.22001 mL	0.17121 mL	0.16987 mL	1.34995 mL	0.02500 mL	4.002	0.02791	0.89372	0.00
30:21.3	Data point 52	0.22001 mL	0.17121 mL	0.17034 mL	1.34995 mL	0.02500 mL	4.467	0.10015	0.98327	0.00
30:51.1	Data point 53	0.22001 mL	0.17121 mL	0.17058 mL	1.34995 mL	0.02500 mL	4.778	0.09887	0.98710	0.00
31:31.3	Data point 54	0.22001 mL	0.17121 mL	0.17067 mL	1.34995 mL	0.02500 mL	5.130	0.08896	0.80586	0.00
32:19.9	Data point 55	0.22001 mL	0.17121 mL	0.17074 mL	1.34995 mL	0.02500 mL	5.609	0.09847	0.99249	0.00
33:28.7	Data point 56	0.22001 mL	0.17121 mL	0.17081 mL	1.34995 mL	0.02500 mL	6.093	0.09906	0.98838	0.00
34:35.8	Data point 57	0.22001 mL	0.17121 mL	0.17088 mL	1.34995 mL	0.02500 mL	6.471	0.09936	0.99655	0.00
35:33.5	Data point 58	0.22001 mL	0.17121 mL	0.17098 mL	1.34995 mL	0.02500 mL	6.930	0.10068	0.99138	0.00
36:20.2	Data point 59	0.22001 mL	0.17121 mL	0.17110 mL	1.34995 mL	0.02500 mL	7.382	0.09744	0.98145	0.00
36:50.9	Data point 60	0.22001 mL	0.17121 mL	0.17121 mL	1.34995 mL	0.02500 mL	7.655	0.09894	0.99130	0.00
37:25.2	Data point 61	0.22001 mL	0.17121 mL	0.17133 mL	1.34995 mL	0.02500 mL	7.905	0.10093	0.99321	0.00
38:00.4	Data point 62	0.22001 mL	0.17121 mL	0.17145 mL	1.34995 mL	0.02500 mL	8.163	0.09764	0.98141	0.00
38:44.7	Data point 63	0.22001 mL	0.17121 mL	0.17157 mL	1.34995 mL	0.02500 mL	8.486	0.10051	0.98559	0.00
39:27.3	Data point 64	0.22001 mL	0.17121 mL	0.17166 mL	1.34995 mL	0.02500 mL	8.812	0.09668	0.97549	0.00
40:18.7	Data point 65	0.22001 mL	0.17121 mL	0.17175 mL	1.34995 mL	0.02500 mL	9.157	0.09397	0.97462	0.00
41:03.9	Data point 66	0.22001 mL	0.17121 mL	0.17185 mL	1.34995 mL	0.02500 mL	9.428	0.09984	0.99450	0.00

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 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH S
41:35.1	Data point 67	0.22001 mL	0.17121 mL	0.17194 mL	1.34995 mL	0.02500 mL	9.679	0.09816	0.96954	0.96954
42:10.9	Data point 68	0.22001 mL	0.17121 mL	0.17208 mL	1.34995 mL	0.02500 mL	9.914	0.09685	0.97696	0.97696
42:39.7	Data point 69	0.22001 mL	0.17121 mL	0.17225 mL	1.34995 mL	0.02500 mL	10.124	0.07138	0.88904	0.88904
43:06.4	Data point 70	0.22001 mL	0.17121 mL	0.17246 mL	1.34995 mL	0.02500 mL	10.328	0.03674	0.95340	0.95340
43:23.0	Data point 71	0.22001 mL	0.17121 mL	0.17279 mL	1.34995 mL	0.02500 mL	10.548	0.01521	0.85142	0.85142
43:39.5	Data point 72	0.22001 mL	0.17121 mL	0.17335 mL	1.34995 mL	0.02500 mL	10.742	0.00771	0.74721	0.74721
43:56.1	Data point 73	0.22001 mL	0.17121 mL	0.17422 mL	1.34995 mL	0.02500 mL	10.920	0.00160	0.09743	0.09743
44:12.6	Data point 74	0.22001 mL	0.17121 mL	0.17552 mL	1.34995 mL	0.02500 mL	11.085	-0.00294	0.43595	0.43595
44:44.7	Data point 75	0.22001 mL	0.17121 mL	0.17782 mL	1.34995 mL	0.02500 mL	11.277	-0.00712	0.69051	0.69051
45:11.5	Data point 76	0.22001 mL	0.17121 mL	0.18090 mL	1.34995 mL	0.02500 mL	11.470	-0.00545	0.67583	0.67583
45:28.2	Data point 77	0.22001 mL	0.17121 mL	0.18544 mL	1.34995 mL	0.02500 mL	11.640	-0.00052	0.01511	0.01511
45:44.9	Data point 78	0.22001 mL	0.17121 mL	0.19219 mL	1.34995 mL	0.02500 mL	11.814	0.00301	0.20833	0.20833
46:01.6	Data point 79	0.22001 mL	0.17121 mL	0.20233 mL	1.34995 mL	0.02500 mL	11.983	-0.00142	0.03221	0.03221
46:18.1	Data point 80	0.22001 mL	0.17121 mL	0.20447 mL	1.34995 mL	0.02500 mL	12.009	0.00057	0.02985	0.02985
47:59.9	Reference spectrum									
49:20.2	Data point 82	0.39005 mL	0.28511 mL	0.20449 mL	1.34995 mL	0.02500 mL	1.994	-0.07137	0.93327	0.93327
49:47.7	Data point 83	0.39005 mL	0.28511 mL	0.23401 mL	1.34995 mL	0.02500 mL	2.194	0.00477	0.40534	0.40534
50:04.7	Data point 84	0.39005 mL	0.28511 mL	0.25209 mL	1.34995 mL	0.02500 mL	2.396	0.00269	0.07457	0.07457
50:21.5	Data point 85	0.39005 mL	0.28511 mL	0.26357 mL	1.34995 mL	0.02500 mL	2.607	-0.00277	0.08324	0.08324
50:38.3	Data point 86	0.39005 mL	0.28511 mL	0.27067 mL	1.34995 mL	0.02500 mL	2.796	0.00635	0.34465	0.34465
50:54.9	Data point 87	0.39005 mL	0.28511 mL	0.27524 mL	1.34995 mL	0.02500 mL	2.996	-0.00383	0.27759	0.27759
51:11.6	Data point 88	0.39005 mL	0.28511 mL	0.27815 mL	1.34995 mL	0.02500 mL	3.179	0.00905	0.59388	0.59388
51:28.0	Data point 89	0.39005 mL	0.28511 mL	0.28003 mL	1.34995 mL	0.02500 mL	3.379	0.01228	0.80708	0.80708
51:44.6	Data point 90	0.39005 mL	0.28511 mL	0.28123 mL	1.34995 mL	0.02500 mL	3.600	0.01739	0.87535	0.87535
52:01.1	Data point 91	0.39005 mL	0.28511 mL	0.28194 mL	1.34995 mL	0.02500 mL	3.808	0.01735	0.88616	0.88616
52:17.6	Data point 92	0.39005 mL	0.28511 mL	0.28239 mL	1.34995 mL	0.02500 mL	3.988	0.02908	0.95915	0.95915
52:34.2	Data point 93	0.39005 mL	0.28511 mL	0.28267 mL	1.34995 mL	0.02500 mL	4.142	0.05437	0.98750	0.98750
52:56.0	Data point 94	0.39005 mL	0.28511 mL	0.28297 mL	1.34995 mL	0.02500 mL	4.395	0.09223	0.98961	0.98961
53:17.5	Data point 95	0.39005 mL	0.28511 mL	0.28318 mL	1.34995 mL	0.02500 mL	4.712	0.09954	0.99032	0.99032
53:56.6	Data point 96	0.39005 mL	0.28511 mL	0.28335 mL	1.34995 mL	0.02500 mL	5.120	0.09967	0.98087	0.98087
55:05.4	Data point 97	0.39005 mL	0.28511 mL	0.28344 mL	1.34995 mL	0.02500 mL	5.470	0.10034	0.98813	0.98813
56:06.1	Data point 98	0.39005 mL	0.28511 mL	0.28354 mL	1.34995 mL	0.02500 mL	5.902	0.09935	0.99153	0.99153
57:10.0	Data point 99	0.39005 mL	0.28511 mL	0.28363 mL	1.34995 mL	0.02500 mL	6.239	0.09615	0.98209	0.98209
57:55.7	Data point 100	0.39005 mL	0.28511 mL	0.28373 mL	1.34995 mL	0.02500 mL	6.532	0.10017	0.99128	0.99128
58:39.8	Data point 101	0.39005 mL	0.28511 mL	0.28384 mL	1.34995 mL	0.02500 mL	6.831	0.09042	0.92205	0.92205
59:02.3	Data point 102	0.39005 mL	0.28511 mL	0.28396 mL	1.34995 mL	0.02500 mL	7.102	0.09516	0.89477	0.89477
59:29.1	Data point 103	0.39005 mL	0.28511 mL	0.28410 mL	1.34995 mL	0.02500 mL	7.347	0.09978	0.98464	0.98464
59:57.9	Data point 104	0.39005 mL	0.28511 mL	0.28427 mL	1.34995 mL	0.02500 mL	7.588	0.09549	0.98997	0.98997
1:00:26.3	Data point 105	0.39005 mL	0.28511 mL	0.28441 mL	1.34995 mL	0.02500 mL	7.836	0.09943	0.97851	0.97851
1:01:04.6	Data point 106	0.39005 mL	0.28511 mL	0.28455 mL	1.34995 mL	0.02500 mL	8.140	0.09830	0.98992	0.98992
1:01:41.8	Data point 107	0.39005 mL	0.28511 mL	0.28467 mL	1.34995 mL	0.02500 mL	8.424	0.09986	0.97751	0.97751
1:02:28.5	Data point 108	0.39005 mL	0.28511 mL	0.28481 mL	1.34995 mL	0.02500 mL	8.812	0.09518	0.97012	0.97012
1:03:15.0	Data point 109	0.39005 mL	0.28511 mL	0.28495 mL	1.34995 mL	0.02500 mL	9.133	0.09701	0.98846	0.98846
1:03:54.9	Data point 110	0.39005 mL	0.28511 mL	0.28507 mL	1.34995 mL	0.02500 mL	9.389	0.09838	0.97772	0.97772
1:04:29.2	Data point 111	0.39005 mL	0.28511 mL	0.28521 mL	1.34995 mL	0.02500 mL	9.619	0.09853	0.97739	0.97739
1:04:57.4	Data point 112	0.39005 mL	0.28511 mL	0.28540 mL	1.34995 mL	0.02500 mL	9.820	0.07583	0.98273	0.98273
1:05:34.7	Data point 113	0.39005 mL	0.28511 mL	0.28563 mL	1.34995 mL	0.02500 mL	10.546	-0.02827	0.98764	0.98764
1:06:01.5	Data point 114	0.39005 mL	0.28511 mL	0.28895 mL	1.34995 mL	0.02500 mL	10.815	-0.01169	0.92381	0.92381
1:06:33.6	Data point 115	0.39005 mL	0.28511 mL	0.29057 mL	1.34995 mL	0.02500 mL	11.030	-0.01165	0.93499	0.93499
1:07:00.6	Data point 116	0.39005 mL	0.28511 mL	0.29273 mL	1.34995 mL	0.02500 mL	11.220	-0.01157	0.91241	0.91241
1:07:17.2	Data point 117	0.39005 mL	0.28511 mL	0.29624 mL	1.34995 mL	0.02500 mL	11.389	-0.01551	0.91321	0.91321
1:07:44.3	Data point 118	0.39005 mL	0.28511 mL	0.30207 mL	1.34995 mL	0.02500 mL	11.583	-0.00806	0.81300	0.81300
1:08:01.0	Data point 119	0.39005 mL	0.28511 mL	0.31014 mL	1.34995 mL	0.02500 mL	11.749	-0.00395	0.20371	0.20371
1:08:33.4	Data point 120	0.39005 mL	0.28511 mL	0.32477 mL	1.34995 mL	0.02500 mL	11.942	-0.00822	0.79638	0.79638
1:08:55.2	Data point 121	0.39005 mL	0.28511 mL	0.33314 mL	1.34995 mL	0.02500 mL	12.026	-0.00486	0.45836	0.45836
1:10:54.2	Assay volumes	0.64005 mL	0.41265 mL	0.33314 mL	1.34995 mL	0.02500 mL				

Sample name: **D05**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-12002**
 Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12002_D05_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:32:48 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	1.34 mL			
Cosolvent added	Automatic			
ISA water volume	0.16 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	0.06 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Titration 3				

Sample name: **D05**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-12002**
 Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12002_D05_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:32:48 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	0.17 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Data Point Stability				
Stir during data point collection	Yes			
For point collection, stir at	15%			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00500 dpH/dt			
Stability timeout after	60 seconds			
Experiment cleanup				
Adjust pH to cleanup	To start pH			
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 1:32:48 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus S	1.0007	10/12/2017 1:32:48 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jH	0.3	10/12/2017 1:32:48 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jOH	-0.2	10/12/2017 1:32:48 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Base concentration factor	1.011	10/12/2017 1:32:48 AM	C:\Sirius_T3\KOH17122.t3r
Acid concentration factor	0.995	10/12/2017 1:32:48 AM	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
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

Sample name: **D05**
Assay name: **UV-metric psKa**
Assay ID: **17J-12002**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12002_D05_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:32:48 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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
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	-8.48 mV		10/12/2017 1:33:12 AM
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	5.1e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	5e+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		
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		



Assay Settings

Sample name: **D05**
Assay name: **UV-metric psKa**
Assay ID: **17J-12002**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12002_D05_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 1:32:48 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 F3