

Sample name: **M04**
Assay name: **UV-metric psKa**
Assay ID: **17K-09020**
Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09020_M04_UV-metric psKa.t3r**

Experiment start time: **11/9/2017 5:32:22 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

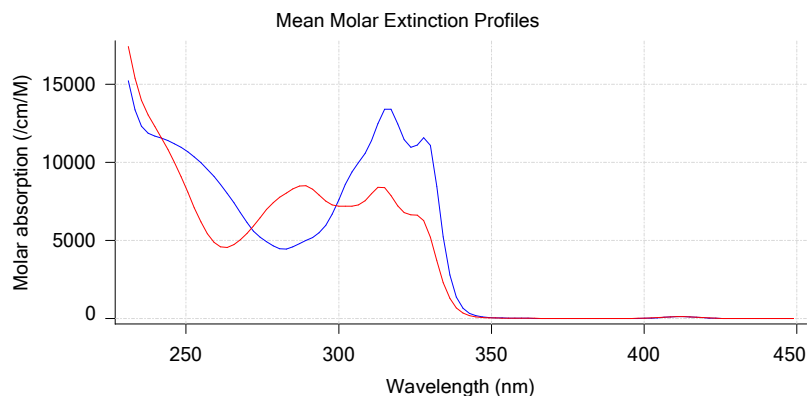
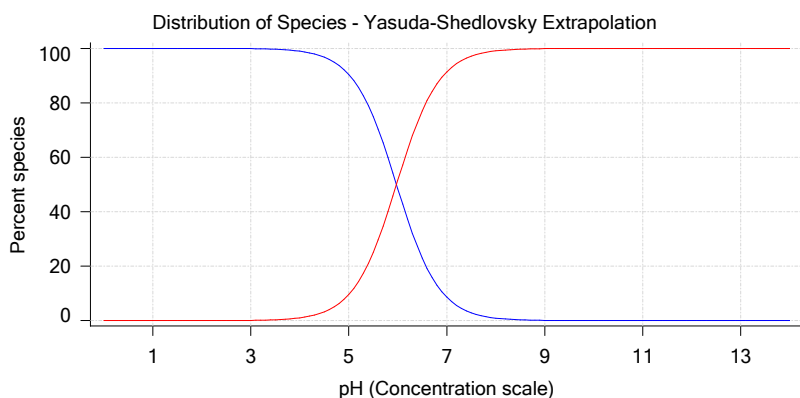
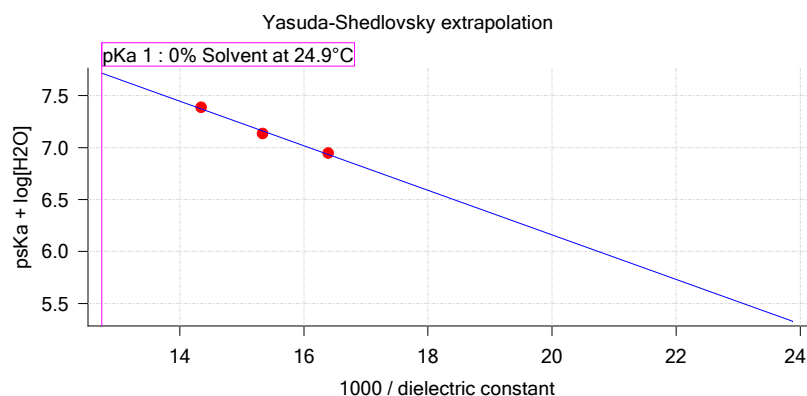
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.97	±0.06	10.45	-214.4690	0.9903	0.162 M	24.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1
17K-09020 Points 4 to 30	40.04 %	Up	UV-metric pKa	61.0	30.0 M	0.156 M	24.9°C	✓ 5.47
17K-09020 Points 32 to 74	30.67 %	Up	UV-metric pKa	65.2	35.5 M	0.163 M	25.0°C	✓ 5.59
17K-09020 Points 76 to 121	20.53 %	Up	UV-metric pKa	69.7	41.7 M	0.167 M	24.9°C	✓ 5.77

Graphs



UV-metric psKa Titration 1 of 3 17K-09020 Points 4 to 30

Results

pKa 1	5.47
RMSD	0.010 0.005
Chi squared	0.1418
PCA calculated number of pKas	1
Average ionic strength	0.156 M
Average temperature	24.9°C
Analyte concentration range	94.3 µM to 89.6 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

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Results (continued)

pH clipping 1.547 to 12.546

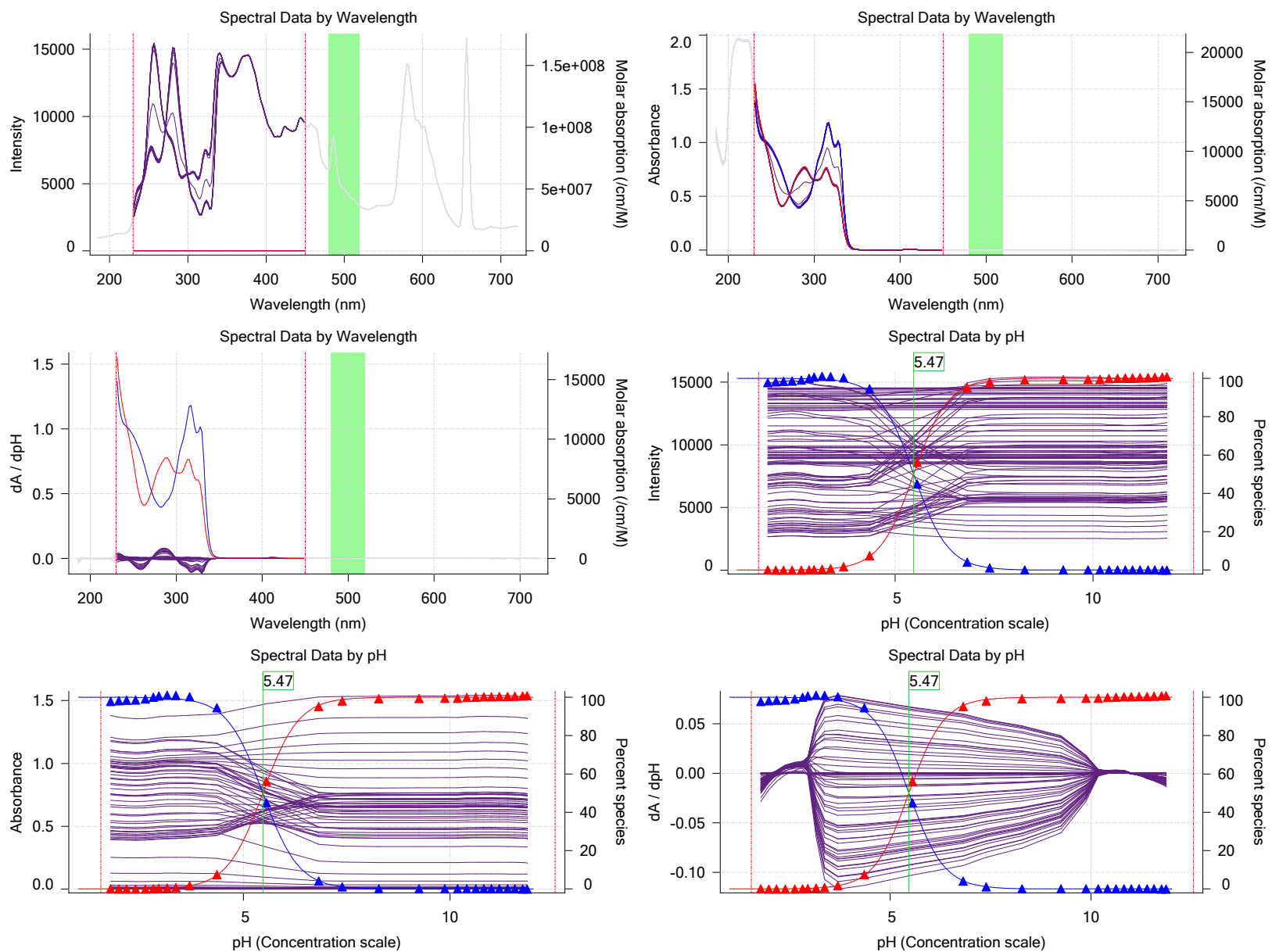
Warnings and errors

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			

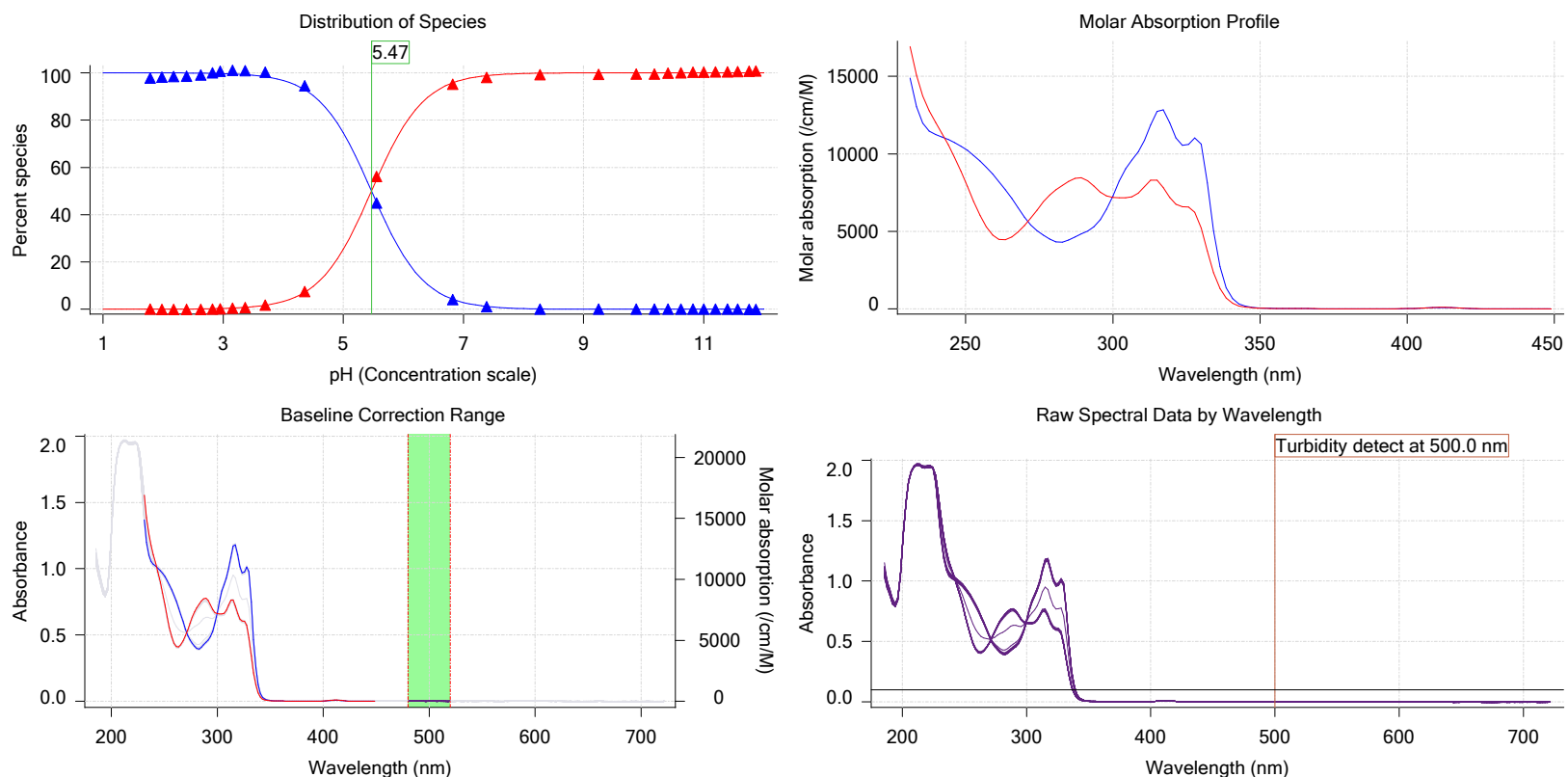
Graphs



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Experiment start time: **11/9/2017 5:32:22 PM**
Analyst: **Dorothy Leverse**
Instrument ID: **T311053**

Graphs (continued)



UV-metric psKa Titration 2 of 3 17K-09020 Points 32 to 74

Results

pKa 1	5.59
RMSD	0.004 0.002
Chi squared	0.0264
PCA calculated number of pKas	3
Average ionic strength	0.163 M
Average temperature	25.0°C
Analyte concentration range	73.5 µM to 70.1 µM
Methanol weight %	30.7 %
Dielectric constant	65.2
Water concentration	35.5 M
Number of pKas source	Predicted
Wavelength clipping	230.0 nm to 450.0 nm
pH clipping	1.553 to 12.541

Warnings and errors

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

Assay Settings

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

Assay Medium

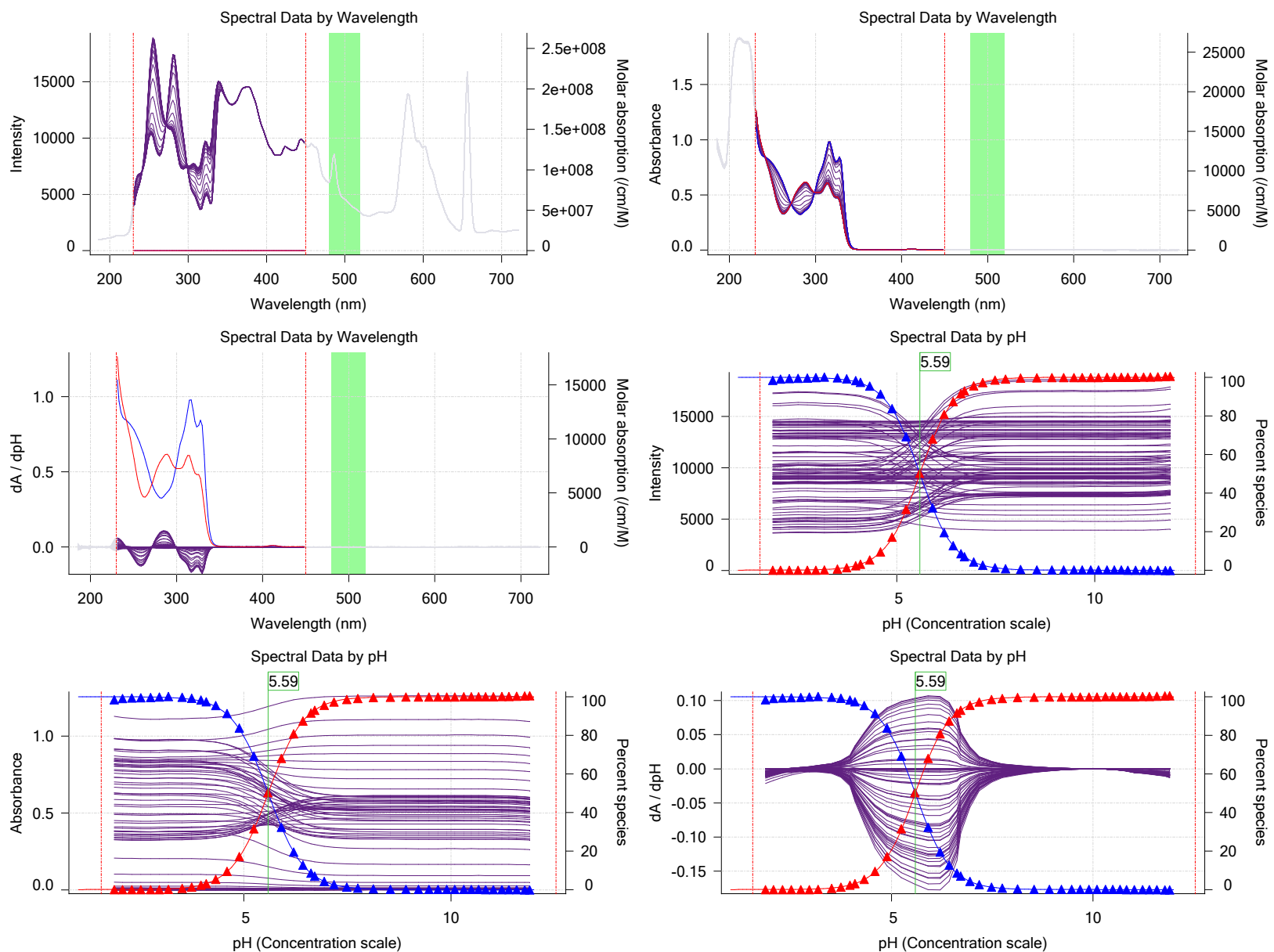
Sample name: **M04**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-09020**
 Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09020_M04_UV-metric psKa.t3r**

Experiment start time: **11/9/2017 5:32:22 PM**
 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			

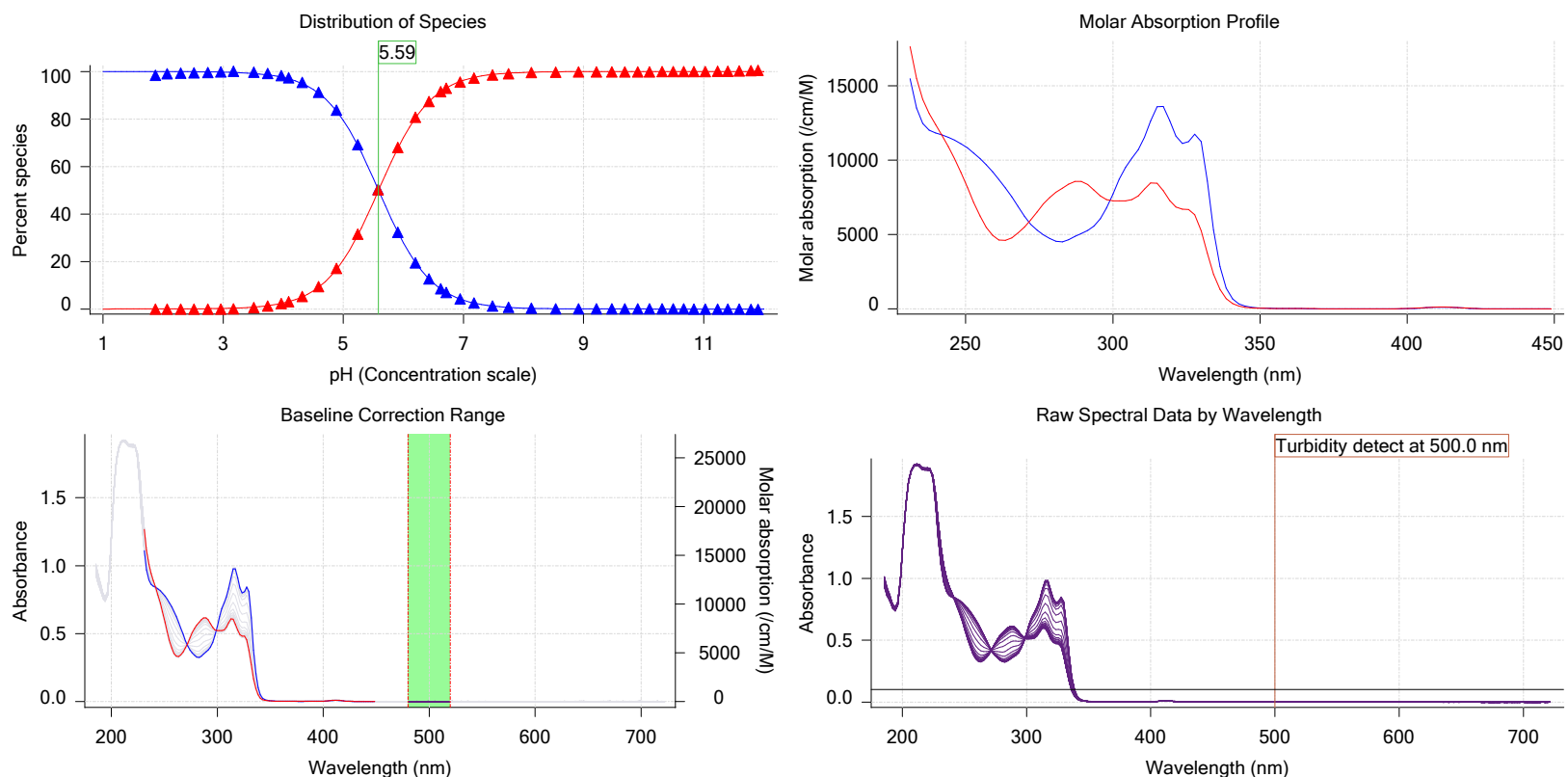
Graphs



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Experiment start time: **11/9/2017 5:32:22 PM**
Analyst: **Dorothy Leverse**
Instrument ID: **T311053**

Graphs (continued)



UV-metric psKa Titration 3 of 3 17K-09020 Points 76 to 121

Results

pKa 1	5.77
RMSD	0.002 0.004
Chi squared	0.0091
PCA calculated number of pKas	3
Average ionic strength	0.167 M
Average temperature	24.9°C
Analyte concentration range	50.4 µM to 48.0 µM
Methanol weight %	20.5 %
Dielectric constant	69.7
Water concentration	41.7 M
Number of pKas source	Predicted
Wavelength clipping	230.0 nm to 450.0 nm
pH clipping	1.543 to 12.552

Warnings and errors

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

Assay Settings

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

Assay Medium

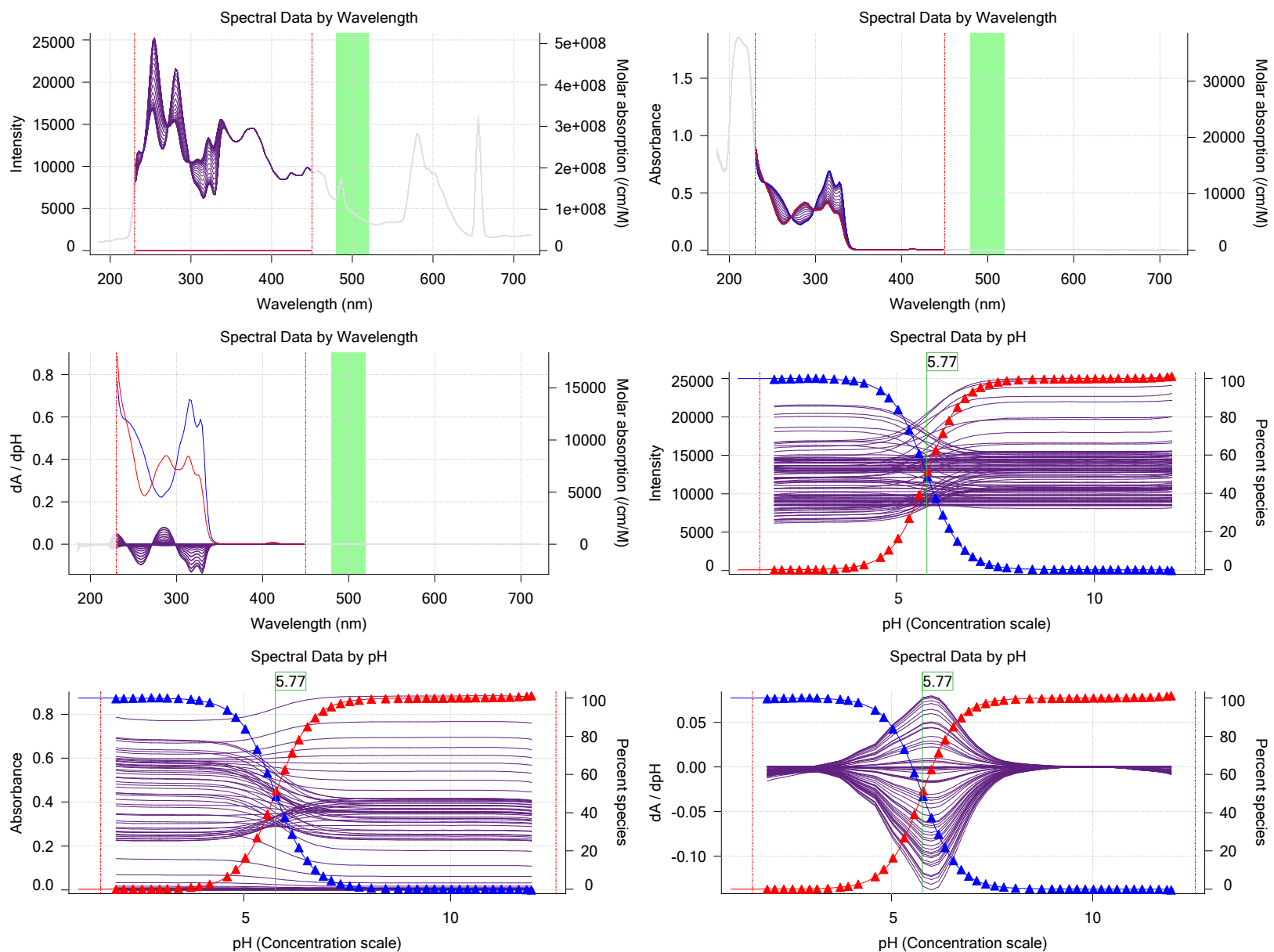
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Experiment start time: **11/9/2017 5:32:22 PM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Assay Settings (continued)

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

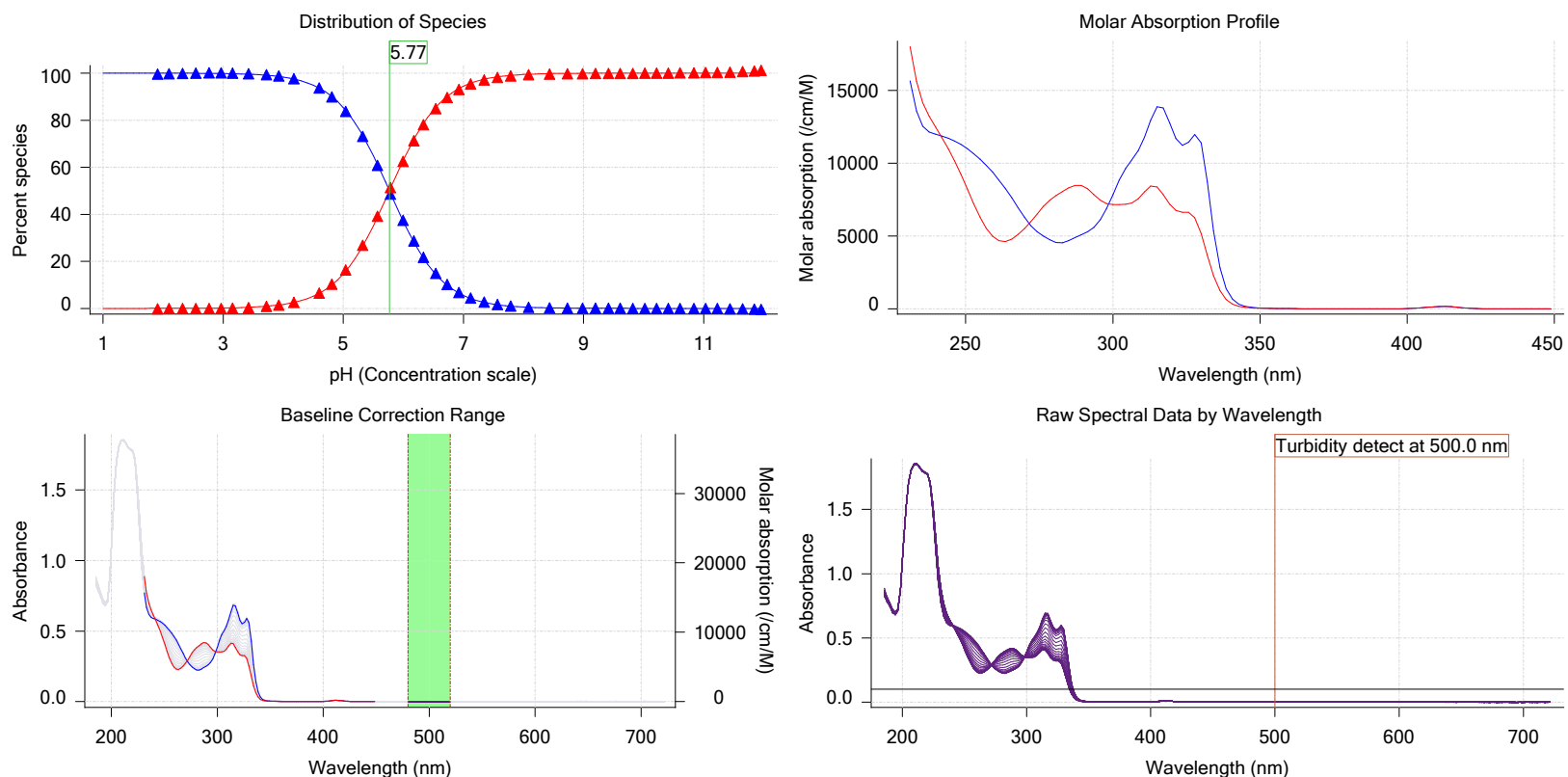
Graphs



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Experiment start time: **11/9/2017 5:32:22 PM**
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 Instrument ID: **T311053**

Graphs (continued)



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M04	11/9/2017 5:25:47 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0030 mL	11/9/2017 5:25:47 PM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.051900 M	11/10/2017 2:16:17 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	269.73	11/9/2017 5:25:56 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	11/9/2017 5:25:47 PM	User entered value
Sample is a	Base	11/9/2017 5:25:47 PM	User entered value
pKa 1	6.01	11/9/2017 5:25:47 PM	User entered value
logp (XH +)	-10.00		Default value
logP (neutral X)	-10.00	11/9/2017 5:25:47 PM	User entered value

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-square
16:50.5	Dark spectrum								
16:52.0	Reference spectrum								
17:19.6	Volume reset due to vial change								
18:03.8	Initial pH = 8.20								
19:11.5	Data point 4	0.55997 mL	0.06192 mL	0.00000 mL	0.94003 mL	0.02500 mL	2.018	-0.02107	0.91847
19:40.0	Data point 5	0.55997 mL	0.06192 mL	0.01900 mL	0.94003 mL	0.02500 mL	2.214	0.00003	0.00002
19:56.8	Data point 6	0.55997 mL	0.06192 mL	0.03126 mL	0.94003 mL	0.02500 mL	2.405	0.00692	0.47443
20:13.6	Data point 7	0.55997 mL	0.06192 mL	0.03921 mL	0.94003 mL	0.02500 mL	2.619	0.01556	0.89489
20:30.2	Data point 8	0.55997 mL	0.06192 mL	0.04403 mL	0.94003 mL	0.02500 mL	2.854	0.01613	0.96154
20:57.2	Data point 9	0.55997 mL	0.06192 mL	0.04682 mL	0.94003 mL	0.02500 mL	3.047	0.01687	0.89461

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Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
21:13.8	Data point 10	0.55997 mL	0.06192 mL	0.04864 mL	0.94003 mL	0.02500 mL	3.178	0.01542	0.88065	0.00
21:45.8	Data point 11	0.55997 mL	0.06192 mL	0.05026 mL	0.94003 mL	0.02500 mL	3.379	0.04592	0.96024	0.00
22:12.6	Data point 12	0.55997 mL	0.06192 mL	0.05108 mL	0.94003 mL	0.02500 mL	3.590	0.06958	0.98751	0.00
22:29.1	Data point 13	0.55997 mL	0.06192 mL	0.05158 mL	0.94003 mL	0.02500 mL	3.921	0.10012	0.98158	0.00
22:55.7	Data point 14	0.55997 mL	0.06192 mL	0.05202 mL	0.94003 mL	0.02500 mL	4.576	0.09924	0.98746	0.00
23:43.0	Data point 15	0.55997 mL	0.06192 mL	0.05235 mL	0.94003 mL	0.02500 mL	5.770	0.10050	0.99516	0.00
24:58.5	Data point 16	0.55997 mL	0.06192 mL	0.05266 mL	0.94003 mL	0.02500 mL	7.031	0.09846	0.99397	0.00
25:45.8	Data point 17	0.55997 mL	0.06192 mL	0.05292 mL	0.94003 mL	0.02500 mL	7.597	0.10010	0.99272	0.00
26:40.2	Data point 18	0.55997 mL	0.06192 mL	0.05322 mL	0.94003 mL	0.02500 mL	8.481	0.09711	0.95398	0.00
27:49.3	Data point 19	0.55997 mL	0.06192 mL	0.05348 mL	0.94003 mL	0.02500 mL	9.452	0.09821	0.98838	0.00
28:48.7	Data point 20	0.55997 mL	0.06192 mL	0.05376 mL	0.94003 mL	0.02500 mL	10.074	0.09615	0.97429	0.00
29:20.2	Data point 21	0.55997 mL	0.06192 mL	0.05412 mL	0.94003 mL	0.02500 mL	10.377	0.09653	0.98006	0.00
29:47.4	Data point 22	0.55997 mL	0.06192 mL	0.05459 mL	0.94003 mL	0.02500 mL	10.603	0.10073	0.99360	0.00
30:19.3	Data point 23	0.55997 mL	0.06192 mL	0.05539 mL	0.94003 mL	0.02500 mL	10.817	0.03239	0.95743	0.00
30:51.1	Data point 24	0.55997 mL	0.06192 mL	0.05651 mL	0.94003 mL	0.02500 mL	11.014	0.02827	0.96747	0.00
31:07.7	Data point 25	0.55997 mL	0.06192 mL	0.05802 mL	0.94003 mL	0.02500 mL	11.193	0.01550	0.91190	0.00
31:24.3	Data point 26	0.55997 mL	0.06192 mL	0.06032 mL	0.94003 mL	0.02500 mL	11.385	0.00968	0.81127	0.00
31:40.9	Data point 27	0.55997 mL	0.06192 mL	0.06390 mL	0.94003 mL	0.02500 mL	11.582	0.00642	0.60087	0.00
31:57.5	Data point 28	0.55997 mL	0.06192 mL	0.06959 mL	0.94003 mL	0.02500 mL	11.754	0.00951	0.73803	0.00
32:14.3	Data point 29	0.55997 mL	0.06192 mL	0.07815 mL	0.94003 mL	0.02500 mL	11.937	0.01332	0.78854	0.00
32:31.1	Data point 30	0.55997 mL	0.06192 mL	0.08490 mL	0.94003 mL	0.02500 mL	12.046	0.00718	0.81421	0.00
34:14.1	Reference spectrum									
35:18.5	Data point 32	0.83996 mL	0.14727 mL	0.08490 mL	0.94003 mL	0.02500 mL	2.053	-0.08490	0.97066	0.00
35:46.9	Data point 33	0.83996 mL	0.14727 mL	0.10499 mL	0.94003 mL	0.02500 mL	2.247	-0.00097	0.03078	0.00
36:03.8	Data point 34	0.83996 mL	0.14727 mL	0.11797 mL	0.94003 mL	0.02500 mL	2.469	-0.00085	0.02547	0.00
36:20.5	Data point 35	0.83996 mL	0.14727 mL	0.12582 mL	0.94003 mL	0.02500 mL	2.689	-0.00928	0.65064	0.00
36:37.2	Data point 36	0.83996 mL	0.14727 mL	0.13053 mL	0.94003 mL	0.02500 mL	2.923	-0.00784	0.54716	0.00
37:04.0	Data point 37	0.83996 mL	0.14727 mL	0.13384 mL	0.94003 mL	0.02500 mL	3.135	0.02551	0.87325	0.00
37:35.8	Data point 38	0.83996 mL	0.14727 mL	0.13556 mL	0.94003 mL	0.02500 mL	3.347	0.01898	0.93662	0.00
37:52.4	Data point 39	0.83996 mL	0.14727 mL	0.13657 mL	0.94003 mL	0.02500 mL	3.681	0.02123	0.94711	0.00
38:14.0	Data point 40	0.83996 mL	0.14727 mL	0.13706 mL	0.94003 mL	0.02500 mL	3.912	0.04480	0.98589	0.00
38:30.7	Data point 41	0.83996 mL	0.14727 mL	0.13735 mL	0.94003 mL	0.02500 mL	4.136	0.06611	0.97366	0.00
38:47.2	Data point 42	0.83996 mL	0.14727 mL	0.13751 mL	0.94003 mL	0.02500 mL	4.261	0.09679	0.98546	0.00
39:09.8	Data point 43	0.83996 mL	0.14727 mL	0.13768 mL	0.94003 mL	0.02500 mL	4.489	0.09750	0.98486	0.00
39:38.9	Data point 44	0.83996 mL	0.14727 mL	0.13779 mL	0.94003 mL	0.02500 mL	4.760	0.09716	0.98021	0.00
40:15.5	Data point 45	0.83996 mL	0.14727 mL	0.13789 mL	0.94003 mL	0.02500 mL	5.055	0.10049	0.99231	0.00
41:00.7	Data point 46	0.83996 mL	0.14727 mL	0.13798 mL	0.94003 mL	0.02500 mL	5.407	0.09743	0.97920	0.00
41:45.4	Data point 47	0.83996 mL	0.14727 mL	0.13808 mL	0.94003 mL	0.02500 mL	5.746	0.09688	0.97780	0.00
42:27.2	Data point 48	0.83996 mL	0.14727 mL	0.13817 mL	0.94003 mL	0.02500 mL	6.072	0.09849	0.98349	0.00
43:04.8	Data point 49	0.83996 mL	0.14727 mL	0.13826 mL	0.94003 mL	0.02500 mL	6.367	0.10025	0.98914	0.00
43:35.8	Data point 50	0.83996 mL	0.14727 mL	0.13834 mL	0.94003 mL	0.02500 mL	6.591	0.09999	0.98856	0.00
44:07.3	Data point 51	0.83996 mL	0.14727 mL	0.13841 mL	0.94003 mL	0.02500 mL	6.786	0.10034	0.98530	0.00
44:32.7	Data point 52	0.83996 mL	0.14727 mL	0.13845 mL	0.94003 mL	0.02500 mL	6.877	0.09729	0.99076	0.00
45:05.8	Data point 53	0.83996 mL	0.14727 mL	0.13855 mL	0.94003 mL	0.02500 mL	7.106	0.09797	0.97290	0.00
45:39.0	Data point 54	0.83996 mL	0.14727 mL	0.13866 mL	0.94003 mL	0.02500 mL	7.337	0.09925	0.97859	0.00
46:16.4	Data point 55	0.83996 mL	0.14727 mL	0.13881 mL	0.94003 mL	0.02500 mL	7.644	0.09849	0.97976	0.00
46:57.3	Data point 56	0.83996 mL	0.14727 mL	0.13892 mL	0.94003 mL	0.02500 mL	7.910	0.09786	0.98027	0.00
47:43.6	Data point 57	0.83996 mL	0.14727 mL	0.13904 mL	0.94003 mL	0.02500 mL	8.288	0.09395	0.98391	0.00
48:30.7	Data point 58	0.83996 mL	0.14727 mL	0.13914 mL	0.94003 mL	0.02500 mL	8.696	0.09313	0.97131	0.00
49:20.4	Data point 59	0.83996 mL	0.14727 mL	0.13923 mL	0.94003 mL	0.02500 mL	9.073	0.09571	0.96497	0.00
50:01.6	Data point 60	0.83996 mL	0.14727 mL	0.13932 mL	0.94003 mL	0.02500 mL	9.373	0.09962	0.98877	0.00
50:39.6	Data point 61	0.83996 mL	0.14727 mL	0.13944 mL	0.94003 mL	0.02500 mL	9.629	0.09628	0.96633	0.00
51:05.9	Data point 62	0.83996 mL	0.14727 mL	0.13958 mL	0.94003 mL	0.02500 mL	9.841	0.09370	0.96956	0.00
51:32.7	Data point 63	0.83996 mL	0.14727 mL	0.13979 mL	0.94003 mL	0.02500 mL	10.055	0.05056	0.94750	0.00
51:59.3	Data point 64	0.83996 mL	0.14727 mL	0.14010 mL	0.94003 mL	0.02500 mL	10.251	0.03259	0.89794	0.00
52:15.9	Data point 65	0.83996 mL	0.14727 mL	0.14052 mL	0.94003 mL	0.02500 mL	10.463	0.00605	0.55881	0.00
52:32.6	Data point 66	0.83996 mL	0.14727 mL	0.14118 mL	0.94003 mL	0.02500 mL	10.644	0.00488	0.59095	0.00

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Experiment start time: **11/9/2017 5:32:22 PM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH Slope
52:49.2	Data point 67	0.83996 mL	0.14727 mL	0.14217 mL	0.94003 mL	0.02500 mL	10.821	0.00122	0.06281	0.00000
53:05.8	Data point 68	0.83996 mL	0.14727 mL	0.14365 mL	0.94003 mL	0.02500 mL	10.987	-0.00296	0.33725	0.00000
53:32.8	Data point 69	0.83996 mL	0.14727 mL	0.14553 mL	0.94003 mL	0.02500 mL	11.179	-0.00384	0.41183	0.00000
53:49.5	Data point 70	0.83996 mL	0.14727 mL	0.14885 mL	0.94003 mL	0.02500 mL	11.378	-0.00494	0.50693	0.00000
54:06.2	Data point 71	0.83996 mL	0.14727 mL	0.15412 mL	0.94003 mL	0.02500 mL	11.550	0.00202	0.09538	0.00000
54:23.1	Data point 72	0.83996 mL	0.14727 mL	0.16202 mL	0.94003 mL	0.02500 mL	11.734	-0.00211	0.17341	0.00000
54:39.9	Data point 73	0.83996 mL	0.14727 mL	0.17429 mL	0.94003 mL	0.02500 mL	11.925	0.00359	0.33042	0.00000
54:56.7	Data point 74	0.83996 mL	0.14727 mL	0.18532 mL	0.94003 mL	0.02500 mL	12.041	0.00111	0.02805	0.00000
56:47.2	Reference spectrum									
59:03.1	Data point 76	1.54998 mL	0.27509 mL	0.18535 mL	0.94003 mL	0.02500 mL	2.043	0.06917	0.90848	0.00000
59:30.5	Data point 77	1.54998 mL	0.27509 mL	0.20908 mL	0.94003 mL	0.02500 mL	2.231	-0.03092	0.92001	0.00000
59:47.6	Data point 78	1.54998 mL	0.27509 mL	0.22679 mL	0.94003 mL	0.02500 mL	2.453	-0.09132	0.88155	0.00000
1:00:05.5	Data point 79	1.54998 mL	0.27509 mL	0.23770 mL	0.94003 mL	0.02500 mL	2.672	-0.09315	0.91500	0.00000
1:00:23.3	Data point 80	1.54998 mL	0.27509 mL	0.24431 mL	0.94003 mL	0.02500 mL	2.894	-0.07997	0.85624	0.00000
1:00:42.0	Data point 81	1.54998 mL	0.27509 mL	0.24824 mL	0.94003 mL	0.02500 mL	3.092	-0.08802	0.90741	0.00000
1:00:59.5	Data point 82	1.54998 mL	0.27509 mL	0.25073 mL	0.94003 mL	0.02500 mL	3.280	-0.08458	0.86944	0.00000
1:01:17.1	Data point 83	1.54998 mL	0.27509 mL	0.25235 mL	0.94003 mL	0.02500 mL	3.549	-0.08753	0.87041	0.00000
1:01:51.2	Data point 84	1.54998 mL	0.27509 mL	0.25336 mL	0.94003 mL	0.02500 mL	3.848	-0.04767	0.75820	0.00000
1:02:23.0	Data point 85	1.54998 mL	0.27509 mL	0.25381 mL	0.94003 mL	0.02500 mL	4.049	0.02522	0.90913	0.00000
1:02:39.5	Data point 86	1.54998 mL	0.27509 mL	0.25407 mL	0.94003 mL	0.02500 mL	4.300	-0.08312	0.75633	0.00000
1:03:01.6	Data point 87	1.54998 mL	0.27509 mL	0.25435 mL	0.94003 mL	0.02500 mL	4.723	-0.06595	0.68190	0.00000
1:03:29.6	Data point 88	1.54998 mL	0.27509 mL	0.25449 mL	0.94003 mL	0.02500 mL	4.931	0.09400	0.91805	0.00000
1:03:54.7	Data point 89	1.54998 mL	0.27509 mL	0.25459 mL	0.94003 mL	0.02500 mL	5.163	0.09873	0.98876	0.00000
1:04:26.3	Data point 90	1.54998 mL	0.27509 mL	0.25468 mL	0.94003 mL	0.02500 mL	5.443	0.09870	0.98949	0.00000
1:04:54.9	Data point 91	1.54998 mL	0.27509 mL	0.25477 mL	0.94003 mL	0.02500 mL	5.692	0.01325	0.06621	0.00000
1:05:21.7	Data point 92	1.54998 mL	0.27509 mL	0.25487 mL	0.94003 mL	0.02500 mL	5.907	0.06181	0.87322	0.00000
1:05:38.2	Data point 93	1.54998 mL	0.27509 mL	0.25496 mL	0.94003 mL	0.02500 mL	6.115	-0.07344	0.65835	0.00000
1:05:56.8	Data point 94	1.54998 mL	0.27509 mL	0.25506 mL	0.94003 mL	0.02500 mL	6.294	-0.08268	0.73202	0.00000
1:06:15.8	Data point 95	1.54998 mL	0.27509 mL	0.25515 mL	0.94003 mL	0.02500 mL	6.454	-0.07814	0.81176	0.00000
1:06:40.3	Data point 96	1.54998 mL	0.27509 mL	0.25527 mL	0.94003 mL	0.02500 mL	6.658	-0.09654	0.90825	0.00000
1:07:05.5	Data point 97	1.54998 mL	0.27509 mL	0.25539 mL	0.94003 mL	0.02500 mL	6.850	-0.09683	0.96364	0.00000
1:07:30.1	Data point 98	1.54998 mL	0.27509 mL	0.25550 mL	0.94003 mL	0.02500 mL	7.043	-0.09332	0.96755	0.00000
1:07:59.8	Data point 99	1.54998 mL	0.27509 mL	0.25564 mL	0.94003 mL	0.02500 mL	7.238	-0.03640	0.92189	0.00000
1:08:26.6	Data point 100	1.54998 mL	0.27509 mL	0.25579 mL	0.94003 mL	0.02500 mL	7.462	-0.05094	0.91797	0.00000
1:08:53.2	Data point 101	1.54998 mL	0.27509 mL	0.25590 mL	0.94003 mL	0.02500 mL	7.685	0.01861	0.28988	0.00000
1:09:24.9	Data point 102	1.54998 mL	0.27509 mL	0.25600 mL	0.94003 mL	0.02500 mL	7.907	0.09187	0.94881	0.00000
1:09:59.6	Data point 103	1.54998 mL	0.27509 mL	0.25609 mL	0.94003 mL	0.02500 mL	8.201	0.09616	0.97201	0.00000
1:10:37.4	Data point 104	1.54998 mL	0.27509 mL	0.25619 mL	0.94003 mL	0.02500 mL	8.549	0.09436	0.97163	0.00000
1:11:13.9	Data point 105	1.54998 mL	0.27509 mL	0.25628 mL	0.94003 mL	0.02500 mL	8.849	0.09191	0.96244	0.00000
1:11:44.6	Data point 106	1.54998 mL	0.27509 mL	0.25637 mL	0.94003 mL	0.02500 mL	9.102	0.09229	0.91849	0.00000
1:12:06.2	Data point 107	1.54998 mL	0.27509 mL	0.25647 mL	0.94003 mL	0.02500 mL	9.312	0.01044	0.38198	0.00000
1:12:38.0	Data point 108	1.54998 mL	0.27509 mL	0.25661 mL	0.94003 mL	0.02500 mL	9.532	0.03931	0.82740	0.00000
1:12:59.6	Data point 109	1.54998 mL	0.27509 mL	0.25677 mL	0.94003 mL	0.02500 mL	9.727	-0.03138	0.83158	0.00000
1:13:16.2	Data point 110	1.54998 mL	0.27509 mL	0.25701 mL	0.94003 mL	0.02500 mL	9.933	-0.07363	0.90245	0.00000
1:13:32.8	Data point 111	1.54998 mL	0.27509 mL	0.25738 mL	0.94003 mL	0.02500 mL	10.136	-0.07387	0.87320	0.00000
1:13:49.4	Data point 112	1.54998 mL	0.27509 mL	0.25795 mL	0.94003 mL	0.02500 mL	10.330	-0.09289	0.88014	0.00000
1:14:05.9	Data point 113	1.54998 mL	0.27509 mL	0.25882 mL	0.94003 mL	0.02500 mL	10.523	-0.07971	0.90032	0.00000
1:14:22.5	Data point 114	1.54998 mL	0.27509 mL	0.26014 mL	0.94003 mL	0.02500 mL	10.720	-0.09100	0.93166	0.00000
1:14:39.0	Data point 115	1.54998 mL	0.27509 mL	0.26218 mL	0.94003 mL	0.02500 mL	10.950	-0.08999	0.90341	0.00000
1:15:10.9	Data point 116	1.54998 mL	0.27509 mL	0.26548 mL	0.94003 mL	0.02500 mL	11.143	-0.01967	0.88519	0.00000
1:15:27.6	Data point 117	1.54998 mL	0.27509 mL	0.27074 mL	0.94003 mL	0.02500 mL	11.339	-0.06521	0.91501	0.00000
1:15:44.3	Data point 118	1.54998 mL	0.27509 mL	0.27916 mL	0.94003 mL	0.02500 mL	11.544	-0.08685	0.90700	0.00000
1:16:01.2	Data point 119	1.54998 mL	0.27509 mL	0.29292 mL	0.94003 mL	0.02500 mL	11.752	-0.09127	0.91726	0.00000
1:16:34.4	Data point 120	1.54998 mL	0.27509 mL	0.31562 mL	0.94003 mL	0.02500 mL	11.946	-0.03952	0.94871	0.00000
1:16:51.5	Data point 121	1.54998 mL	0.27509 mL	0.33248 mL	0.94003 mL	0.02500 mL	12.052	-0.05360	0.90316	0.00000
1:18:16.9	Assay volumes	1.54998 mL	0.43561 mL	0.33248 mL	0.94003 mL	0.02500 mL				

Sample name: **M04**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-09020**
 Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09020_M04_UV-metric psKa.t3r**

Experiment start time: **11/9/2017 5:32:22 PM**
 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	0.94 mL			
Cosolvent added	Automatic			
ISA water volume	0.56 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	0.28 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Titration 3				

Sample name: **M04**
 Assay name: **UV-metric psKa**
 Assay ID: **17K-09020**
 Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09020_M04_UV-metric psKa.t3r**

Experiment start time: **11/9/2017 5:32:22 PM**
 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	0.71 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	11/9/2017 5:32:22 PM	C:\Sirius_T3\HCl17K09.t3r
Four-Plus S	1.0008	11/9/2017 5:32:22 PM	C:\Sirius_T3\HCl17K09.t3r
Four-Plus jH	0.6	11/9/2017 5:32:22 PM	C:\Sirius_T3\HCl17K09.t3r
Four-Plus jOH	-1.2	11/9/2017 5:32:22 PM	C:\Sirius_T3\HCl17K09.t3r
Base concentration factor	1.008	11/9/2017 5:32:22 PM	C:\Sirius_T3\KOH17K09.t3r
Acid concentration factor	0.998	11/9/2017 5:32:22 PM	C:\Sirius_T3\HCl17K09.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)	10-10-2017	11/8/2017 11:33:30 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)	11-8-17	11/8/2017 11:32:21 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)	10-30-17	10/30/2017 8:01:46 AM
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	11/1/2017 10:56:16 AM
Port B	Cyclohexane		10/19/2017 2:11:05 PM
Port C	MeCN (50%, 0.15 M KCl)	10-30-17	10/30/2017 8:02:00 AM

Sample name: **M04**
 Assay name: **UV-metric psKa**
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 Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09020_M04_UV-metric psKa.t3r**

Experiment start time: **11/9/2017 5:32:22 PM**
 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		11/8/2017 11:32:27 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	10/13/2017 7:46:59 AM
Titration		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	-7.05 mV		11/9/2017 5:33:06 PM
Filling solution	3M KCl	KCL095	11/8/2017 11:31:02 AM
Liquids			
Wash 1	50% IPA:50% Water		11/9/2017 8:31:16 AM
Wash 2	0.5% Triton X-100 in H2O		11/9/2017 8:31:19 AM
Buffer position 1	pH7 Wash		11/9/2017 8:31:22 AM
Buffer position 2	pH 7		11/9/2017 8:31:24 AM
Storage position			11/9/2017 8:31:29 AM
Wash water	3.4e+003 mL	10-13-17	10/13/2017 8:58:01 AM
Waste	7e+003 mL		10/13/2017 8:58:05 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	512:14:04		11/23/2010 11:22:28 AM
Calibrated on	11/8/2017 1:14:37 PM		
Integration time	10		
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)		
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: **M04**
Assay name: **UV-metric psKa**
Assay ID: **17K-09020**
Filename: **C:\Sirius_T3\Mehtap\20171109_exp16_pKa\17K-09020_M04_UV-metric psKa.t3r**

Experiment start time: **11/9/2017 5:32:22 PM**
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 A1