

Sample name: **D05**  
Assay name: **UV-metric psKa**  
Assay ID: **17K-16013**  
Filename: **C:\Sirius\_T3\Mehtap\20171116\_exp18\_pKa\17K-16013\_D05\_UV-metric psKa.t3r**

Experiment start time: **11/16/2017 2:01:51 PM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

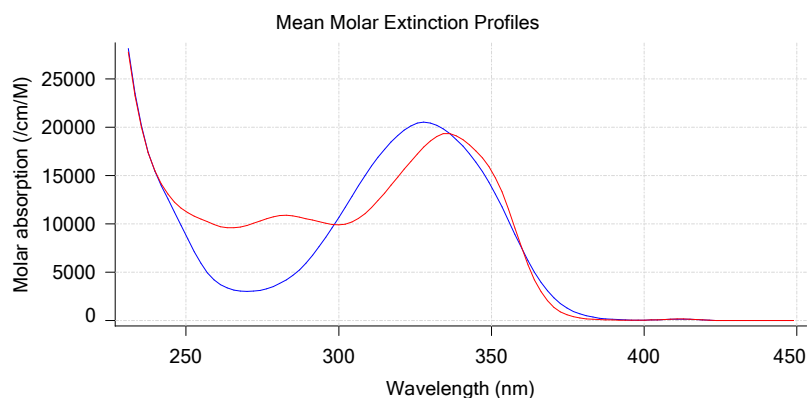
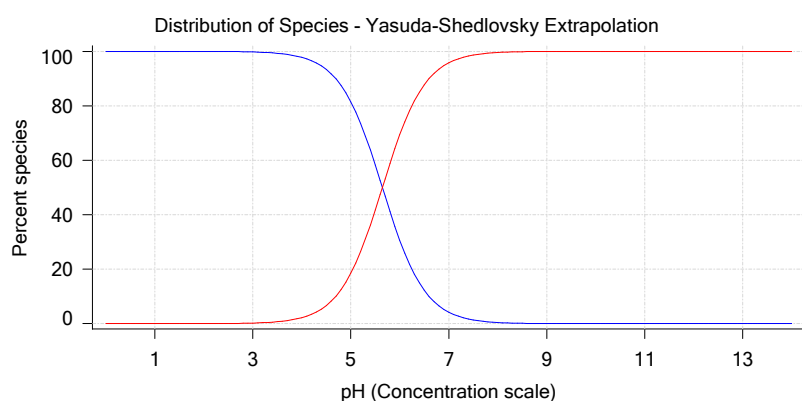
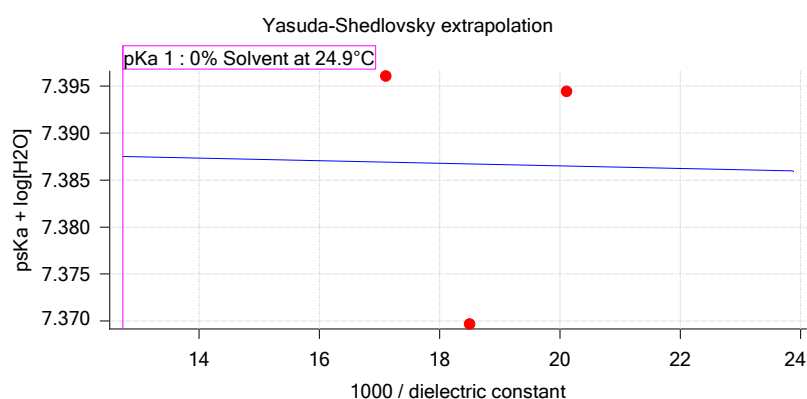
## Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R <sup>2</sup>	Ionic strength	Temperature
Yasuda-Shedlovsky	5.64	±0.06	7.39	-0.1369	0.0002	0.166 M	24.9°C

## Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1
17K-16013 Points 4 to 36	64.04 %	Up	UV-metric pKa	49.7	17.0 M	0.157 M	24.9°C	✓ 6.16
17K-16013 Points 38 to 75	54.96 %	Up	UV-metric pKa	54.0	21.7 M	0.166 M	24.9°C	✓ 6.03
17K-16013 Points 77 to 117	45.54 %	Up	UV-metric pKa	58.5	26.9 M	0.174 M	24.9°C	✓ 5.97

## Graphs



## UV-metric psKa Titration 1 of 3 17K-16013 Points 4 to 36

## Results

pKa 1	<b>6.16</b>
RMSD	<b>0.002 0.002</b>
Chi squared	<b>0.0017</b>
PCA calculated number of pKas	<b>3</b>
Average ionic strength	<b>0.157 M</b>
Average temperature	<b>24.9°C</b>
Analyte concentration range	<b>48.5 µM to 45.8 µM</b>
Methanol weight %	<b>64.0 %</b>
Dielectric constant	<b>49.7</b>
Water concentration	<b>17.0 M</b>
Number of pKas source	<b>Predicted</b>
Wavelength clipping	<b>235.2 nm to 450.0 nm</b>

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## Results (continued)

pH clipping 1.449 to 12.524

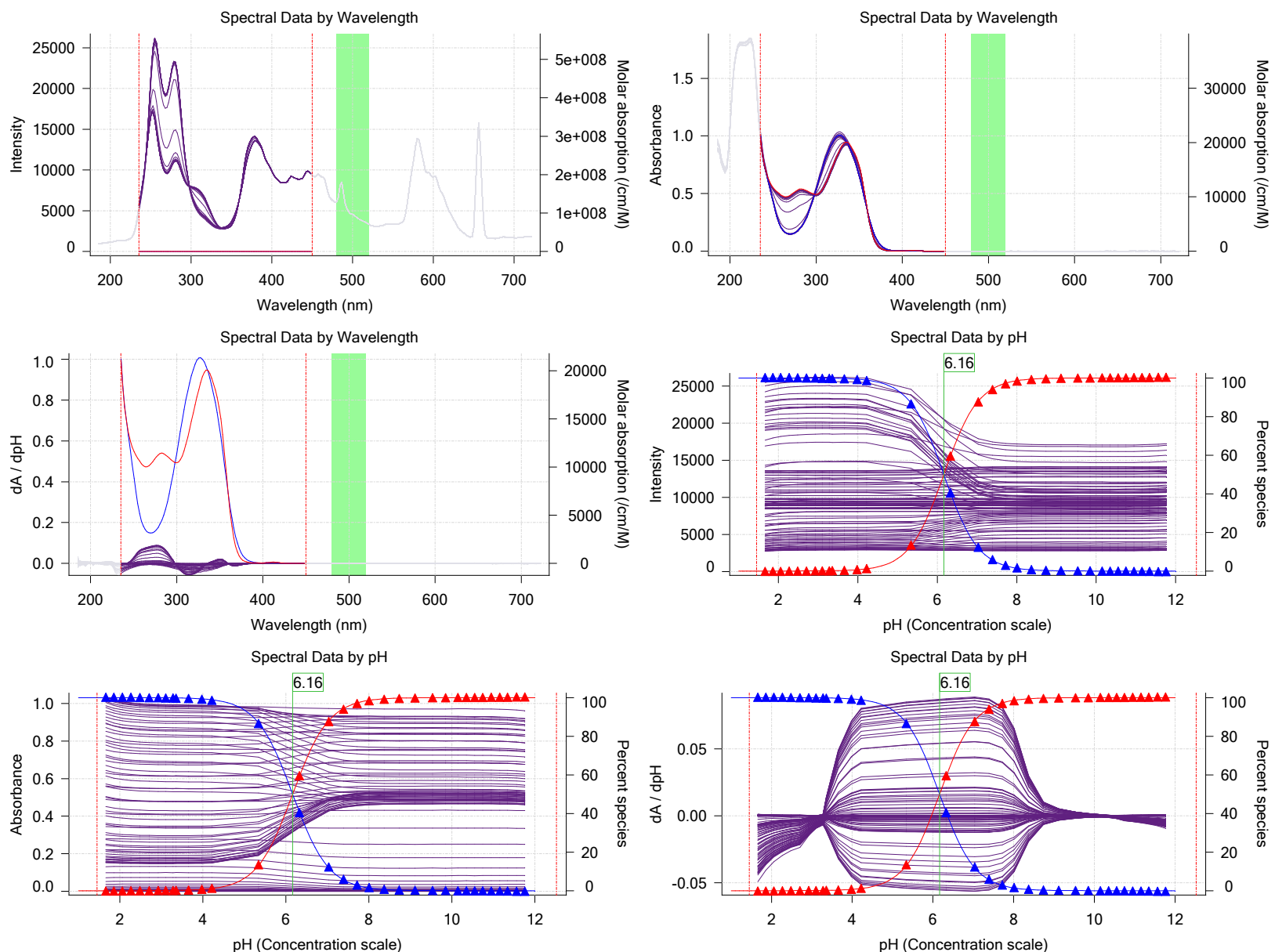
## Warnings and errors

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			
<b>Assay Medium</b>				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

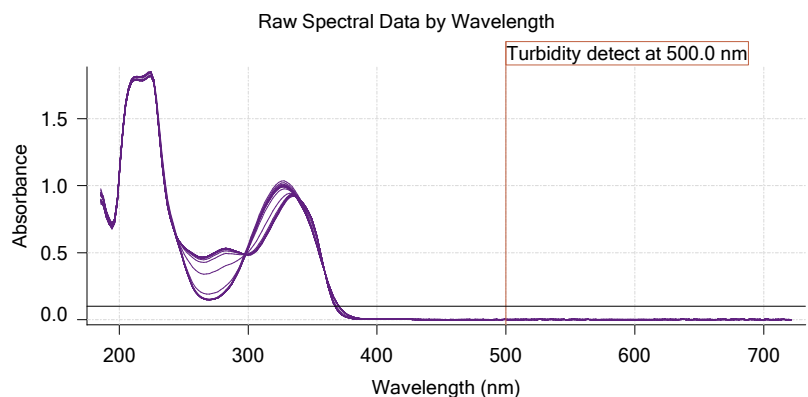
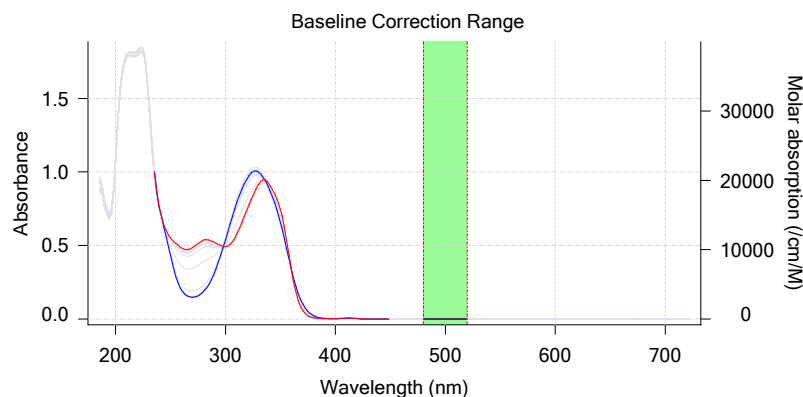
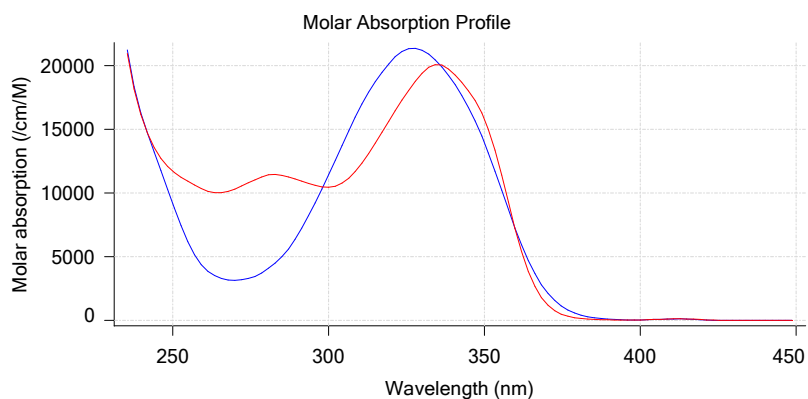
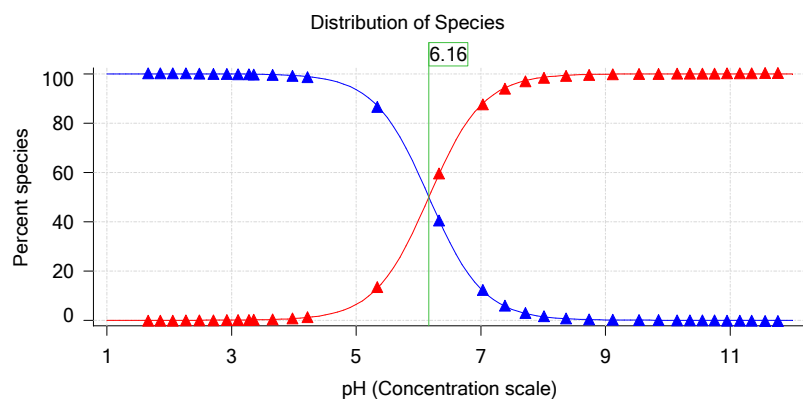
## Graphs



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Experiment start time: **11/16/2017 2:01:51 PM**  
Analyst: **Dorothy Levorse**  
Instrument ID: **T311053**

## Graphs (continued)



## UV-metric psKa Titration 2 of 3 17K-16013 Points 38 to 75

### Results

pKa 1 **6.03**  
RMSD **0.002 0.002**  
Chi squared **0.0069**  
PCA calculated number of pKas **3**  
Average ionic strength **0.166 M**  
Average temperature **24.9°C**  
Analyte concentration range **42.4 µM to 40.1 µM**  
Methanol weight % **55.0 %**  
Dielectric constant **54.0**  
Water concentration **21.7 M**

Number of pKas source **Predicted**  
Wavelength clipping **231.1 nm to 450.0 nm**  
pH clipping **1.703 to 11.761**

### 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**

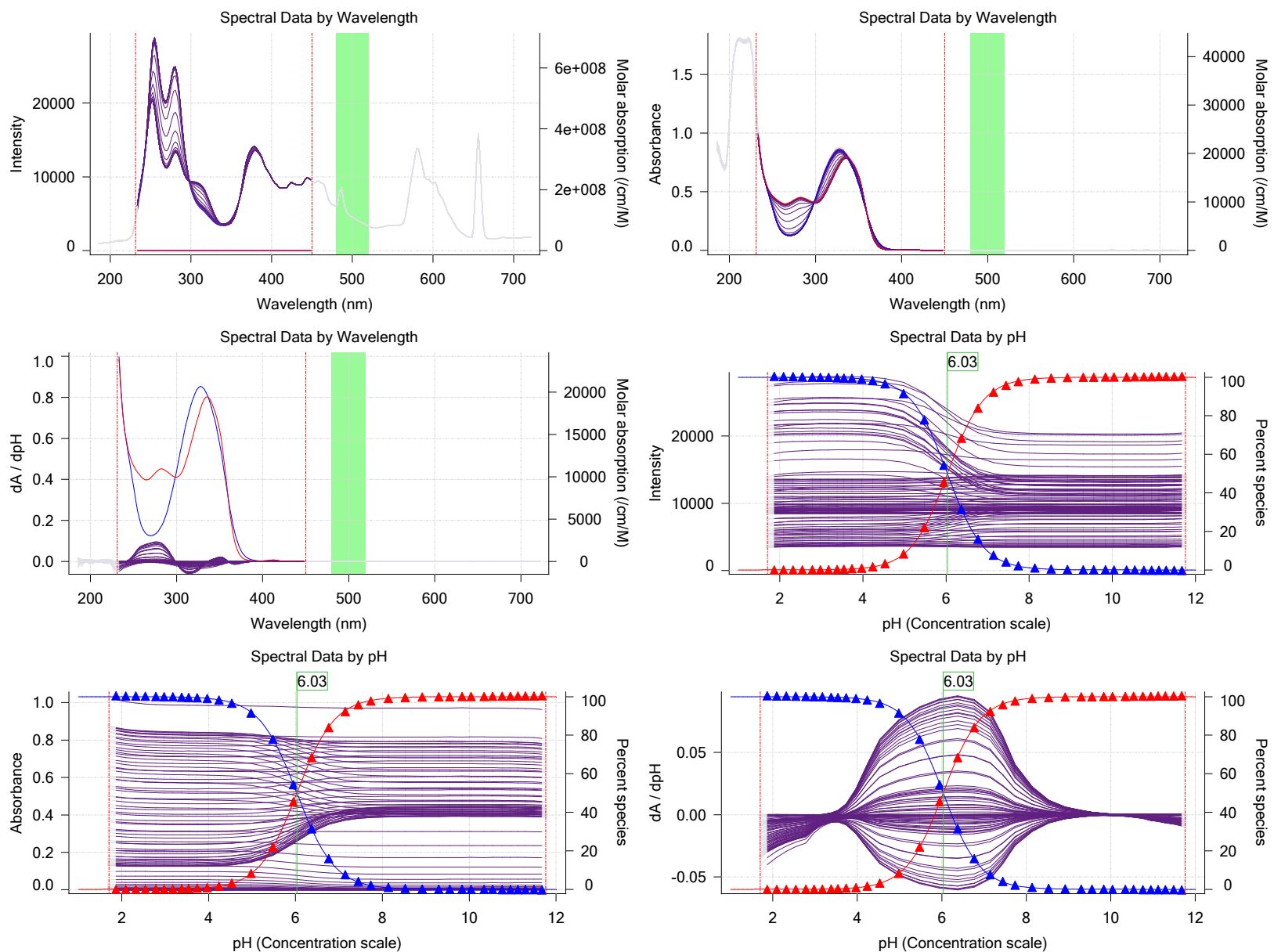
Sample name: **D05**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17K-16013**  
 Filename: **C:\Sirius\_T3\Mehtap\20171116\_exp18\_pKa\17K-16013\_D05\_UV-metric psKa.t3r**

Experiment start time: **11/16/2017 2:01:51 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			

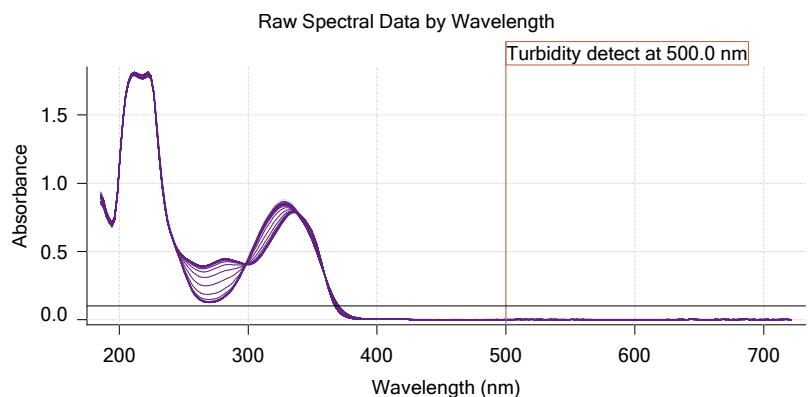
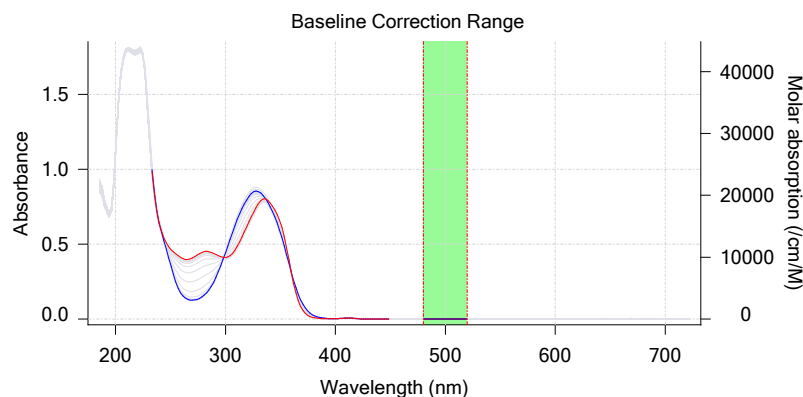
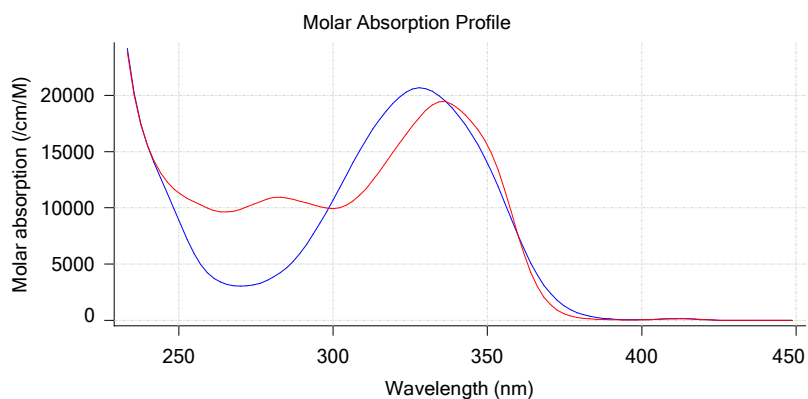
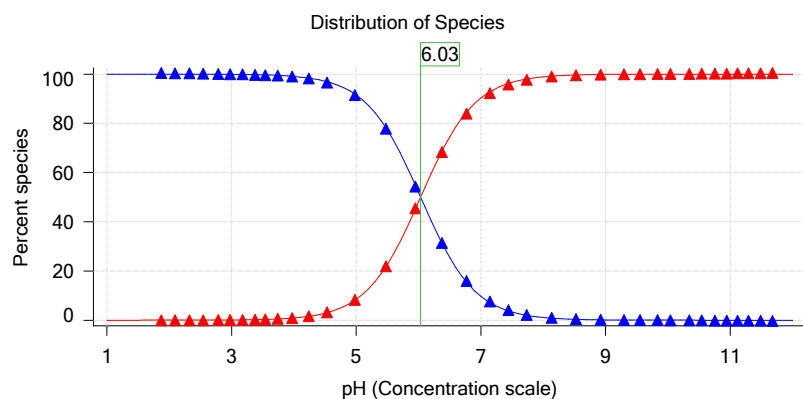
## Graphs



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

## Graphs (continued)



## UV-metric psKa Titration 3 of 3 17K-16013 Points 77 to 117

### Results

pKa 1	<b>5.97</b>
RMSD	<b>0.006 0.008</b>
Chi squared	<b>0.0890</b>
PCA calculated number of pKas	<b>3</b>
Average ionic strength	<b>0.174 M</b>
Average temperature	<b>24.9°C</b>
Analyte concentration range	<b>35.8 µM to 33.9 µM</b>
Methanol weight %	<b>45.5 %</b>
Dielectric constant	<b>58.5</b>
Water concentration	<b>26.9 M</b>
Number of pKas source	<b>Predicted</b>
Wavelength clipping	<b>230.0 nm to 450.0 nm</b>
pH clipping	<b>1.762 to 12.513</b>

### 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**

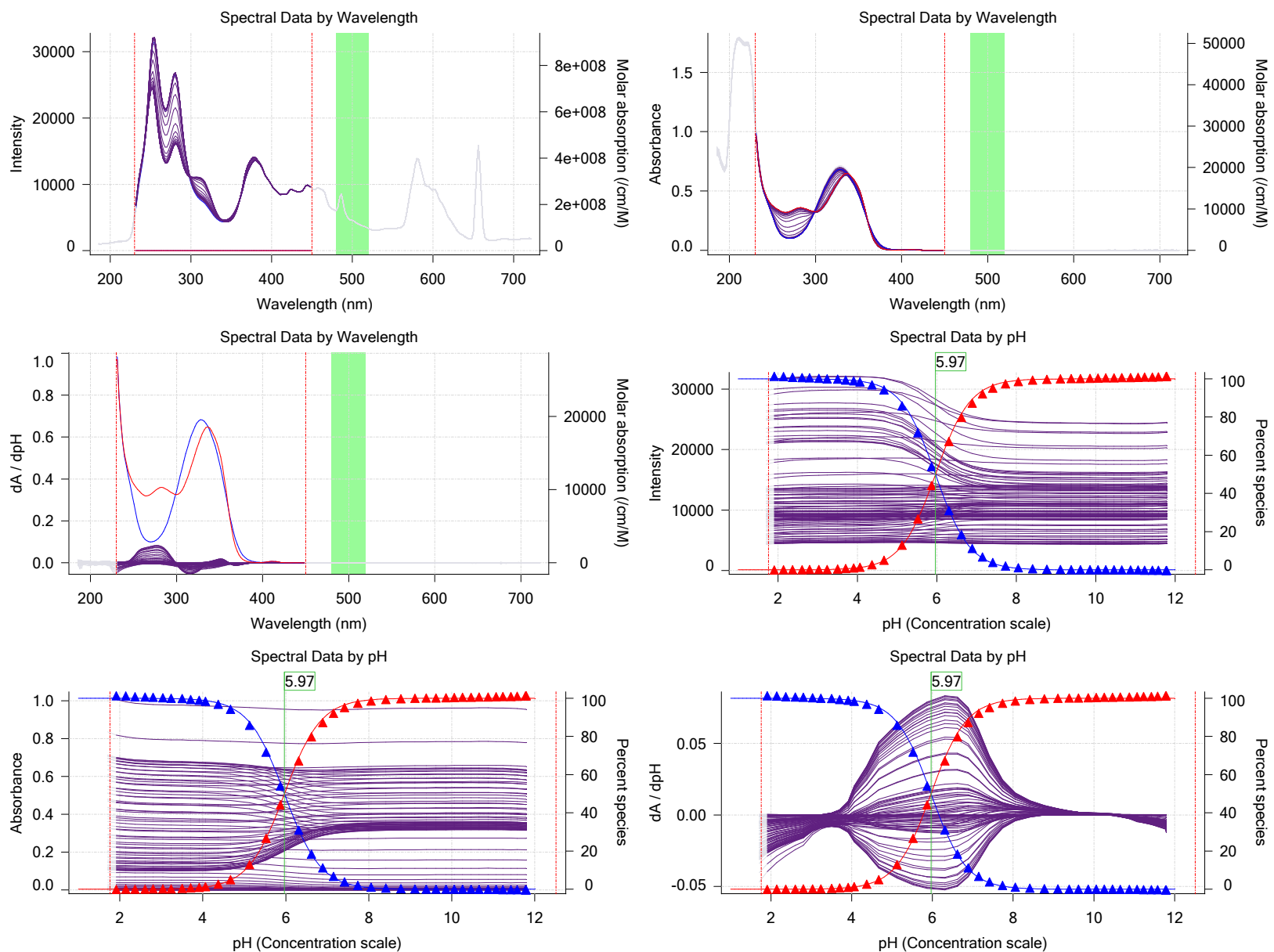
Sample name: **D05**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17K-16013**  
 Filename: **C:\Sirius\_T3\Mehtap\20171116\_exp18\_pKa\17K-16013\_D05\_UV-metric psKa.t3r**

Experiment start time: **11/16/2017 2:01:51 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

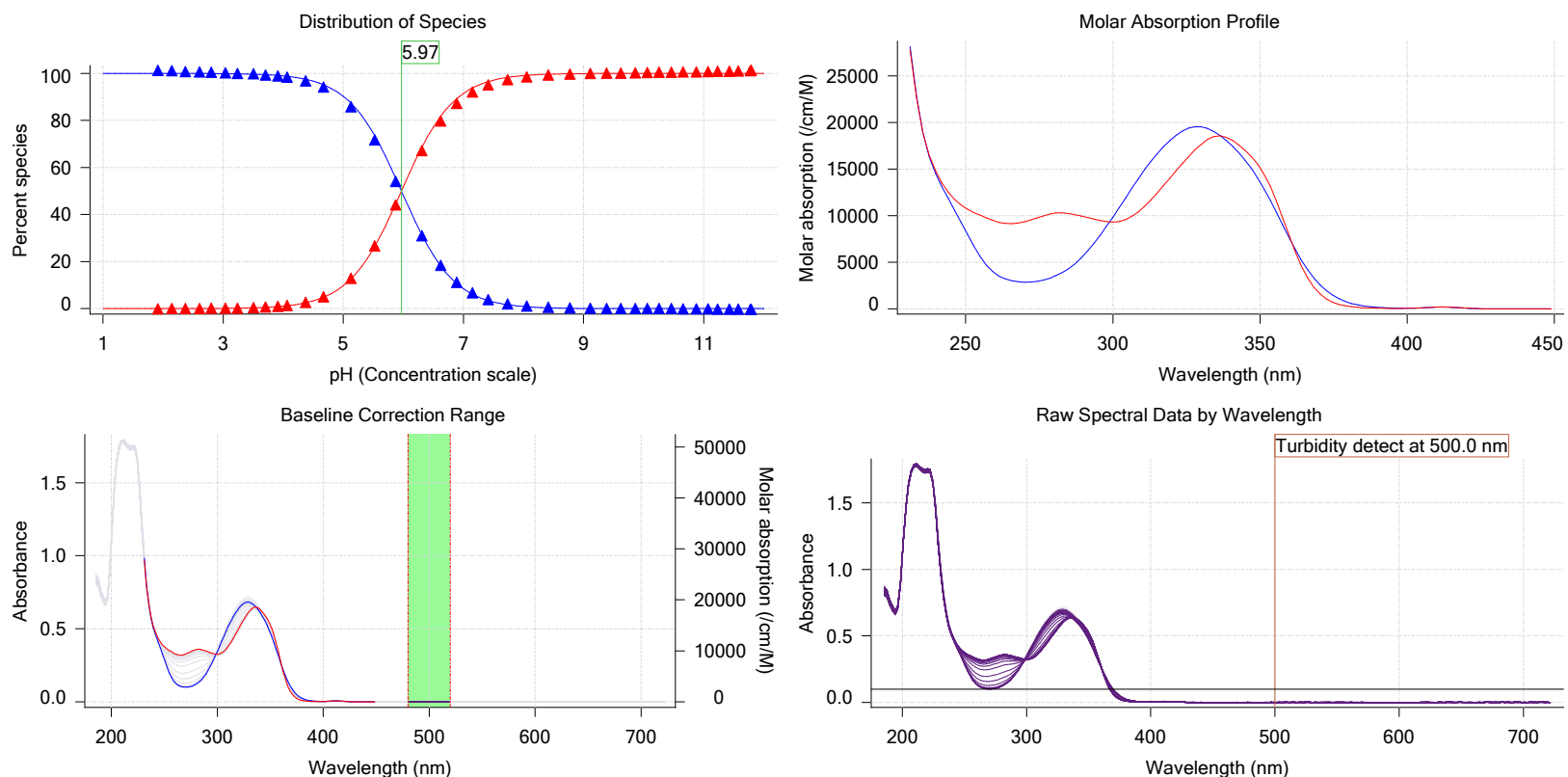




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 Assay ID: **17K-16013**  
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## Graphs (continued)



## Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	D05	11/10/2017 3:18:30 PM	User entered value
Sample by	Volume		Default value
Sample volume	0.0030 mL	11/16/2017 11:11:02 AM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.025800 M	11/10/2017 3:18:30 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	380.25	11/10/2017 3:18:39 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	11/10/2017 3:18:30 PM	User entered value
Sample is a	Acid	11/10/2017 3:18:30 PM	User entered value
pKa 1	7.44	11/10/2017 3:18:30 PM	User entered value
logP (neutral XH)	-10.00	11/10/2017 3:18:30 PM	User entered value
logP (X -)	-10.00		Default value

## Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-square
3:30.5	Dark spectrum								
3:31.8	Reference spectrum								
3:59.4	Volume reset due to vial change								
8:33.8	Initial pH = 7.90								
9:13.9	Data point 4	0.05997 mL	0.06933 mL	0.00000 mL	1.44003 mL	0.02500 mL	1.949	-0.02734	0.94557
9:42.5	Data point 5	0.05997 mL	0.06933 mL	0.02437 mL	1.44003 mL	0.02500 mL	2.149	-0.00254	0.08786
9:59.4	Data point 6	0.05997 mL	0.06933 mL	0.04076 mL	1.44003 mL	0.02500 mL	2.352	0.01910	0.75695
10:16.3	Data point 7	0.05997 mL	0.06933 mL	0.05122 mL	1.44003 mL	0.02500 mL	2.563	0.01590	0.85478
10:33.1	Data point 8	0.05997 mL	0.06933 mL	0.05771 mL	1.44003 mL	0.02500 mL	2.777	0.01417	0.88939
10:49.7	Data point 9	0.05997 mL	0.06933 mL	0.06169 mL	1.44003 mL	0.02500 mL	3.001	0.01325	0.91292

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## Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
11:06.4	Data point 10	0.05997 mL	0.06933 mL	0.06406 mL	1.44003 mL	0.02500 mL	3.220	0.01673	0.94282	0.00
11:22.9	Data point 11	0.05997 mL	0.06933 mL	0.06550 mL	1.44003 mL	0.02500 mL	3.399	0.01738	0.90500	0.00
11:39.4	Data point 12	0.05997 mL	0.06933 mL	0.06644 mL	1.44003 mL	0.02500 mL	3.572	0.02110	0.95581	0.00
11:55.8	Data point 13	0.05997 mL	0.06933 mL	0.06707 mL	1.44003 mL	0.02500 mL	3.649	0.02161	0.94971	0.00
12:17.4	Data point 14	0.05997 mL	0.06933 mL	0.06811 mL	1.44003 mL	0.02500 mL	3.950	0.04439	0.91734	0.00
12:39.1	Data point 15	0.05997 mL	0.06933 mL	0.06863 mL	1.44003 mL	0.02500 mL	4.269	0.07467	0.88885	0.00
13:05.7	Data point 16	0.05997 mL	0.06933 mL	0.06891 mL	1.44003 mL	0.02500 mL	4.509	0.09974	0.99482	0.00
13:44.7	Data point 17	0.05997 mL	0.06933 mL	0.06921 mL	1.44003 mL	0.02500 mL	5.625	0.16420	0.99234	0.00
15:06.3	Data point 18	0.05997 mL	0.06933 mL	0.06945 mL	1.44003 mL	0.02500 mL	6.612	0.09978	0.97767	0.00
16:22.0	Data point 19	0.05997 mL	0.06933 mL	0.06964 mL	1.44003 mL	0.02500 mL	7.312	0.09411	0.94820	0.00
17:24.3	Data point 20	0.05997 mL	0.06933 mL	0.06978 mL	1.44003 mL	0.02500 mL	7.666	0.09457	0.98911	0.00
18:11.8	Data point 21	0.05997 mL	0.06933 mL	0.06992 mL	1.44003 mL	0.02500 mL	7.993	0.09905	0.99290	0.00
18:59.3	Data point 22	0.05997 mL	0.06933 mL	0.07006 mL	1.44003 mL	0.02500 mL	8.285	0.09417	0.97174	0.00
19:46.5	Data point 23	0.05997 mL	0.06933 mL	0.07020 mL	1.44003 mL	0.02500 mL	8.643	0.10106	0.99686	0.00
20:37.3	Data point 24	0.05997 mL	0.06933 mL	0.07030 mL	1.44003 mL	0.02500 mL	9.008	0.09521	0.96498	0.00
21:28.5	Data point 25	0.05997 mL	0.06933 mL	0.07039 mL	1.44003 mL	0.02500 mL	9.385	0.09702	0.92185	0.00
22:12.1	Data point 26	0.05997 mL	0.06933 mL	0.07051 mL	1.44003 mL	0.02500 mL	9.805	0.09246	0.94767	0.00
22:50.6	Data point 27	0.05997 mL	0.06933 mL	0.07065 mL	1.44003 mL	0.02500 mL	10.116	0.09311	0.94910	0.00
23:17.2	Data point 28	0.05997 mL	0.06933 mL	0.07084 mL	1.44003 mL	0.02500 mL	10.416	0.04379	0.80710	0.00
23:43.8	Data point 29	0.05997 mL	0.06933 mL	0.07110 mL	1.44003 mL	0.02500 mL	10.618	0.02703	0.78423	0.00
24:10.6	Data point 30	0.05997 mL	0.06933 mL	0.07152 mL	1.44003 mL	0.02500 mL	10.820	0.01658	0.62333	0.00
24:37.2	Data point 31	0.05997 mL	0.06933 mL	0.07220 mL	1.44003 mL	0.02500 mL	11.012	-0.00889	0.73783	0.00
25:08.8	Data point 32	0.05997 mL	0.06933 mL	0.07347 mL	1.44003 mL	0.02500 mL	11.216	-0.01001	0.52278	0.00
25:25.3	Data point 33	0.05997 mL	0.06933 mL	0.07547 mL	1.44003 mL	0.02500 mL	11.419	0.00203	0.13248	0.00
25:41.9	Data point 34	0.05997 mL	0.06933 mL	0.07865 mL	1.44003 mL	0.02500 mL	11.607	-0.00376	0.33291	0.00
25:58.6	Data point 35	0.05997 mL	0.06933 mL	0.08354 mL	1.44003 mL	0.02500 mL	11.824	0.00172	0.04788	0.00
26:15.3	Data point 36	0.05997 mL	0.06933 mL	0.09160 mL	1.44003 mL	0.02500 mL	12.024	0.00705	0.59233	0.00
27:54.6	Reference spectrum									
28:56.6	Data point 38	0.09995 mL	0.16555 mL	0.09163 mL	1.44003 mL	0.02500 mL	1.955	-0.06877	0.94489	0.00
29:23.9	Data point 39	0.09995 mL	0.16555 mL	0.11872 mL	1.44003 mL	0.02500 mL	2.153	-0.00322	0.08331	0.00
29:40.9	Data point 40	0.09995 mL	0.16555 mL	0.13699 mL	1.44003 mL	0.02500 mL	2.376	-0.00003	0.00001	0.00
29:57.9	Data point 41	0.09995 mL	0.16555 mL	0.14786 mL	1.44003 mL	0.02500 mL	2.603	0.01223	0.57117	0.00
30:14.6	Data point 42	0.09995 mL	0.16555 mL	0.15442 mL	1.44003 mL	0.02500 mL	2.825	0.01718	0.80422	0.00
30:31.3	Data point 43	0.09995 mL	0.16555 mL	0.15835 mL	1.44003 mL	0.02500 mL	3.064	0.01456	0.83713	0.00
30:58.1	Data point 44	0.09995 mL	0.16555 mL	0.16025 mL	1.44003 mL	0.02500 mL	3.257	0.03339	0.97755	0.00
31:29.7	Data point 45	0.09995 mL	0.16555 mL	0.16178 mL	1.44003 mL	0.02500 mL	3.455	0.02132	0.81856	0.00
31:46.4	Data point 46	0.09995 mL	0.16555 mL	0.16270 mL	1.44003 mL	0.02500 mL	3.657	0.02378	0.19126	0.00
32:02.9	Data point 47	0.09995 mL	0.16555 mL	0.16326 mL	1.44003 mL	0.02500 mL	3.820	0.04640	0.98700	0.00
32:29.7	Data point 48	0.09995 mL	0.16555 mL	0.16397 mL	1.44003 mL	0.02500 mL	4.018	0.06917	0.98776	0.00
32:51.4	Data point 49	0.09995 mL	0.16555 mL	0.16444 mL	1.44003 mL	0.02500 mL	4.247	0.10015	0.98993	0.00
33:13.6	Data point 50	0.09995 mL	0.16555 mL	0.16470 mL	1.44003 mL	0.02500 mL	4.514	0.09792	0.99302	0.00
33:52.6	Data point 51	0.09995 mL	0.16555 mL	0.16491 mL	1.44003 mL	0.02500 mL	4.808	0.09746	0.97875	0.00
34:39.2	Data point 52	0.09995 mL	0.16555 mL	0.16505 mL	1.44003 mL	0.02500 mL	5.254	0.09753	0.98723	0.00
35:44.8	Data point 53	0.09995 mL	0.16555 mL	0.16515 mL	1.44003 mL	0.02500 mL	5.750	0.09757	0.98194	0.00
36:59.9	Data point 54	0.09995 mL	0.16555 mL	0.16524 mL	1.44003 mL	0.02500 mL	6.221	0.09681	0.98559	0.00
38:04.0	Data point 55	0.09995 mL	0.16555 mL	0.16533 mL	1.44003 mL	0.02500 mL	6.644	0.09975	0.99691	0.00
39:01.6	Data point 56	0.09995 mL	0.16555 mL	0.16545 mL	1.44003 mL	0.02500 mL	7.038	0.09912	0.99181	0.00
39:59.9	Data point 57	0.09995 mL	0.16555 mL	0.16559 mL	1.44003 mL	0.02500 mL	7.414	0.09944	0.98223	0.00
40:48.4	Data point 58	0.09995 mL	0.16555 mL	0.16571 mL	1.44003 mL	0.02500 mL	7.712	0.09881	0.99056	0.00
41:28.6	Data point 59	0.09995 mL	0.16555 mL	0.16583 mL	1.44003 mL	0.02500 mL	8.003	0.09785	0.97211	0.00
42:20.7	Data point 60	0.09995 mL	0.16555 mL	0.16597 mL	1.44003 mL	0.02500 mL	8.402	0.10029	0.98746	0.00
43:17.4	Data point 61	0.09995 mL	0.16555 mL	0.16609 mL	1.44003 mL	0.02500 mL	8.792	0.10010	0.98630	0.00
44:10.9	Data point 62	0.09995 mL	0.16555 mL	0.16618 mL	1.44003 mL	0.02500 mL	9.184	0.09838	0.97175	0.00
44:59.5	Data point 63	0.09995 mL	0.16555 mL	0.16628 mL	1.44003 mL	0.02500 mL	9.561	0.10067	0.99423	0.00
45:39.6	Data point 64	0.09995 mL	0.16555 mL	0.16637 mL	1.44003 mL	0.02500 mL	9.814	0.09673	0.98761	0.00
46:12.6	Data point 65	0.09995 mL	0.16555 mL	0.16651 mL	1.44003 mL	0.02500 mL	10.095	0.09762	0.98196	0.00
46:39.2	Data point 66	0.09995 mL	0.16555 mL	0.16670 mL	1.44003 mL	0.02500 mL	10.302	0.06638	0.98559	0.00



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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 S
46:55.8	Data point 67	0.09995 mL	0.16555 mL	0.16698 mL	1.44003 mL	0.02500 mL	10.602	0.02666	0.93997	0.93997
47:27.4	Data point 68	0.09995 mL	0.16555 mL	0.16759 mL	1.44003 mL	0.02500 mL	10.800	0.01312	0.84960	0.84960
47:43.9	Data point 69	0.09995 mL	0.16555 mL	0.16849 mL	1.44003 mL	0.02500 mL	11.015	0.00299	0.21893	0.21893
48:00.5	Data point 70	0.09995 mL	0.16555 mL	0.16997 mL	1.44003 mL	0.02500 mL	11.203	-0.00447	0.51130	0.51130
48:17.1	Data point 71	0.09995 mL	0.16555 mL	0.17222 mL	1.44003 mL	0.02500 mL	11.376	-0.00252	0.09763	0.09763
48:33.6	Data point 72	0.09995 mL	0.16555 mL	0.17556 mL	1.44003 mL	0.02500 mL	11.549	-0.00056	0.01331	0.01331
48:50.2	Data point 73	0.09995 mL	0.16555 mL	0.18055 mL	1.44003 mL	0.02500 mL	11.743	-0.00341	0.36509	0.36509
49:06.8	Data point 74	0.09995 mL	0.16555 mL	0.18840 mL	1.44003 mL	0.02500 mL	11.929	0.00221	0.14855	0.14855
49:23.4	Data point 75	0.09995 mL	0.16555 mL	0.19506 mL	1.44003 mL	0.02500 mL	12.032	-0.00387	0.28829	0.28829
51:04.3	Reference spectrum									
52:23.6	Data point 77	0.21990 mL	0.27606 mL	0.19509 mL	1.44003 mL	0.02500 mL	1.958	-0.09499	0.96118	0.96118
52:51.2	Data point 78	0.21990 mL	0.27606 mL	0.22528 mL	1.44003 mL	0.02500 mL	2.160	0.00591	0.54637	0.54637
53:08.2	Data point 79	0.21990 mL	0.27606 mL	0.24497 mL	1.44003 mL	0.02500 mL	2.389	0.01743	0.72389	0.72389
53:25.1	Data point 80	0.21990 mL	0.27606 mL	0.25661 mL	1.44003 mL	0.02500 mL	2.613	0.00778	0.27779	0.27779
53:41.7	Data point 81	0.21990 mL	0.27606 mL	0.26355 mL	1.44003 mL	0.02500 mL	2.851	0.00035	0.00199	0.00199
54:08.4	Data point 82	0.21990 mL	0.27606 mL	0.26754 mL	1.44003 mL	0.02500 mL	3.044	0.01908	0.96793	0.96793
54:25.1	Data point 83	0.21990 mL	0.27606 mL	0.27011 mL	1.44003 mL	0.02500 mL	3.277	0.02798	0.93967	0.93967
54:57.0	Data point 84	0.21990 mL	0.27606 mL	0.27143 mL	1.44003 mL	0.02500 mL	3.480	0.01614	0.69953	0.69953
55:13.5	Data point 85	0.21990 mL	0.27606 mL	0.27237 mL	1.44003 mL	0.02500 mL	3.744	0.02510	0.97464	0.97464
55:45.2	Data point 86	0.21990 mL	0.27606 mL	0.27293 mL	1.44003 mL	0.02500 mL	3.947	0.06531	0.98793	0.98793
56:01.7	Data point 87	0.21990 mL	0.27606 mL	0.27324 mL	1.44003 mL	0.02500 mL	4.153	0.08496	0.99481	0.99481
56:18.2	Data point 88	0.21990 mL	0.27606 mL	0.27342 mL	1.44003 mL	0.02500 mL	4.305	0.09856	0.97872	0.97872
56:40.3	Data point 89	0.21990 mL	0.27606 mL	0.27366 mL	1.44003 mL	0.02500 mL	4.612	0.09795	0.98408	0.98408
57:23.5	Data point 90	0.21990 mL	0.27606 mL	0.27382 mL	1.44003 mL	0.02500 mL	4.909	0.09839	0.99096	0.99096
58:14.2	Data point 91	0.21990 mL	0.27606 mL	0.27394 mL	1.44003 mL	0.02500 mL	5.366	0.09790	0.98011	0.98011
59:11.9	Data point 92	0.21990 mL	0.27606 mL	0.27404 mL	1.44003 mL	0.02500 mL	5.762	0.09893	0.99259	0.99259
1:00:07.5	Data point 93	0.21990 mL	0.27606 mL	0.27413 mL	1.44003 mL	0.02500 mL	6.110	0.10073	0.99253	0.99253
1:01:00.7	Data point 94	0.21990 mL	0.27606 mL	0.27427 mL	1.44003 mL	0.02500 mL	6.545	0.09921	0.98338	0.98338
1:01:49.9	Data point 95	0.21990 mL	0.27606 mL	0.27439 mL	1.44003 mL	0.02500 mL	6.857	0.09713	0.98102	0.98102
1:02:33.6	Data point 96	0.21990 mL	0.27606 mL	0.27451 mL	1.44003 mL	0.02500 mL	7.125	0.09798	0.99618	0.99618
1:03:08.0	Data point 97	0.21990 mL	0.27606 mL	0.27465 mL	1.44003 mL	0.02500 mL	7.384	0.09955	0.99393	0.99393
1:03:48.3	Data point 98	0.21990 mL	0.27606 mL	0.27484 mL	1.44003 mL	0.02500 mL	7.648	0.09876	0.98256	0.98256
1:04:23.2	Data point 99	0.21990 mL	0.27606 mL	0.27500 mL	1.44003 mL	0.02500 mL	7.969	0.09831	0.98185	0.98185
1:05:07.1	Data point 100	0.21990 mL	0.27606 mL	0.27514 mL	1.44003 mL	0.02500 mL	8.288	0.09359	0.96918	0.96918
1:05:54.0	Data point 101	0.21990 mL	0.27606 mL	0.27528 mL	1.44003 mL	0.02500 mL	8.647	0.09769	0.97253	0.97253
1:06:42.4	Data point 102	0.21990 mL	0.27606 mL	0.27542 mL	1.44003 mL	0.02500 mL	9.005	0.09762	0.97344	0.97344
1:07:31.2	Data point 103	0.21990 mL	0.27606 mL	0.27556 mL	1.44003 mL	0.02500 mL	9.344	0.09180	0.94792	0.94792
1:08:09.2	Data point 104	0.21990 mL	0.27606 mL	0.27571 mL	1.44003 mL	0.02500 mL	9.617	0.09522	0.96768	0.96768
1:08:42.9	Data point 105	0.21990 mL	0.27606 mL	0.27589 mL	1.44003 mL	0.02500 mL	9.848	0.09539	0.96938	0.96938
1:09:12.6	Data point 106	0.21990 mL	0.27606 mL	0.27636 mL	1.44003 mL	0.02500 mL	10.090	0.05741	0.97395	0.97395
1:09:34.2	Data point 107	0.21990 mL	0.27606 mL	0.27667 mL	1.44003 mL	0.02500 mL	10.290	0.03026	0.85412	0.85412
1:10:06.1	Data point 108	0.21990 mL	0.27606 mL	0.27714 mL	1.44003 mL	0.02500 mL	10.487	0.01691	0.83469	0.83469
1:10:38.0	Data point 109	0.21990 mL	0.27606 mL	0.27789 mL	1.44003 mL	0.02500 mL	10.693	0.00924	0.79263	0.79263
1:11:10.1	Data point 110	0.21990 mL	0.27606 mL	0.27886 mL	1.44003 mL	0.02500 mL	10.885	-0.00308	0.13715	0.13715
1:11:26.6	Data point 111	0.21990 mL	0.27606 mL	0.28029 mL	1.44003 mL	0.02500 mL	11.105	-0.01014	0.83705	0.83705
1:11:43.2	Data point 112	0.21990 mL	0.27606 mL	0.28264 mL	1.44003 mL	0.02500 mL	11.299	-0.00549	0.72084	0.72084
1:11:59.9	Data point 113	0.21990 mL	0.27606 mL	0.28626 mL	1.44003 mL	0.02500 mL	11.459	-0.01166	0.84409	0.84409
1:12:26.9	Data point 114	0.21990 mL	0.27606 mL	0.29179 mL	1.44003 mL	0.02500 mL	11.651	-0.00894	0.81693	0.81693
1:12:59.3	Data point 115	0.21990 mL	0.27606 mL	0.30000 mL	1.44003 mL	0.02500 mL	11.802	-0.00699	0.66627	0.66627
1:13:31.4	Data point 116	0.21990 mL	0.27606 mL	0.31395 mL	1.44003 mL	0.02500 mL	11.999	-0.00743	0.57020	0.57020
1:13:48.1	Data point 117	0.21990 mL	0.27606 mL	0.31597 mL	1.44003 mL	0.02500 mL	12.013	-0.01061	0.76050	0.76050
1:15:46.8	Assay volumes	0.46990 mL	0.39238 mL	0.31597 mL	1.44003 mL	0.02500 mL				

## Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
<b>General Settings</b>				

Sample name: **D05**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17K-16013**  
 Filename: **C:\Sirius\_T3\Mehtap\20171116\_exp18\_pKa\17K-16013\_D05\_UV-metric psKa.t3r**

Experiment start time: **11/16/2017 2:01:51 PM**  
 Analyst: **Dorothy Levorse**  
 Instrument ID: **T311053**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
<b>Standard Experiment Settings</b>				
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			
<b>Advanced General Settings</b>				
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%			
<b>Titration Pre-Dose</b>				
Titration pre-dose	None			
<b>Assay Medium</b>				
Cosolvent in use	Yes			
Cosolvent type	Methanol			
Cosolvent volume	1.44 mL			
Cosolvent added	Automatic			
ISA water volume	0.06 mL			
Water added	Automatic			
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			
<b>Sample Sonication</b>				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	30 seconds			
<b>Sample Dissolution</b>				
Perform a dissolution stage	No			
<b>Carbonate purge</b>				
Perform a carbonate purge	No			
<b>Temperature Control</b>				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
<b>Titration 1</b>				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	10 seconds			
<b>Titration 2</b>				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.04 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
<b>Titration 3</b>				

Sample name: **D05**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17K-16013**  
 Filename: **C:\Sirius\_T3\Mehtap\20171116\_exp18\_pKa\17K-16013\_D05\_UV-metric psKa.t3r**

Experiment start time: **11/16/2017 2:01:51 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	0.12 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
<b>Data Point Stability</b>				
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			
<b>Experiment cleanup</b>				
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	0.088	11/16/2017 2:01:51 PM	C:\Sirius_T3\HCl17K16.t3r
Four-Plus S	1.0037	11/16/2017 2:01:51 PM	C:\Sirius_T3\HCl17K16.t3r
Four-Plus jH	0.7	11/16/2017 2:01:51 PM	C:\Sirius_T3\HCl17K16.t3r
Four-Plus jOH	-0.7	11/16/2017 2:01:51 PM	C:\Sirius_T3\HCl17K16.t3r
Base concentration factor	1.008	11/16/2017 2:01:51 PM	C:\Sirius_T3\KOH17K09.t3r
Acid concentration factor	1.004	11/16/2017 2:01:51 PM	C:\Sirius_T3\HCl17K16.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	11/16/2017 9:31:07 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: **D05**  
 Assay name: **UV-metric psKa**  
 Assay ID: **17K-16013**  
 Filename: **C:\Sirius\_T3\Mehtap\20171116\_exp18\_pKa\17K-16013\_D05\_UV-metric psKa.t3r**

Experiment start time: **11/16/2017 2:01:51 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	-8.28 mV		11/16/2017 2:02:15 PM
Filling solution	3M KCl	KCL095	11/16/2017 9:28:10 AM
Liquids			
Wash 1	50% IPA:50% Water		11/16/2017 9:31:35 AM
Wash 2	0.5% Triton X-100 in H2O		11/16/2017 9:31:38 AM
Buffer position 1	pH7 Wash		11/16/2017 9:31:40 AM
Buffer position 2	pH 7		11/16/2017 9:31:42 AM
Storage position			11/16/2017 9:32:48 AM
Wash water	7.1e+003 mL	11-10-17	11/10/2017 10:14:37 AM
Waste	1e+004 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	535:10:13		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: **D05**  
Assay name: **UV-metric psKa**  
Assay ID: **17K-16013**  
Filename: **C:\Sirius\_T3\Mehtap\20171116\_exp18\_pKa\17K-16013\_D05\_UV-metric psKa.t3r**

Experiment start time: **11/16/2017 2:01:51 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 C1