

Sample name: **D05**
Assay name: **UV-metric psKa**
Assay ID: **17J-12003**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12003_D05_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 2:44:40 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

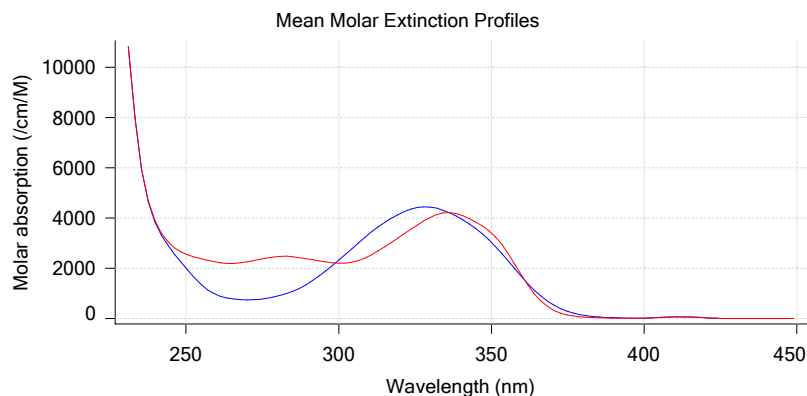
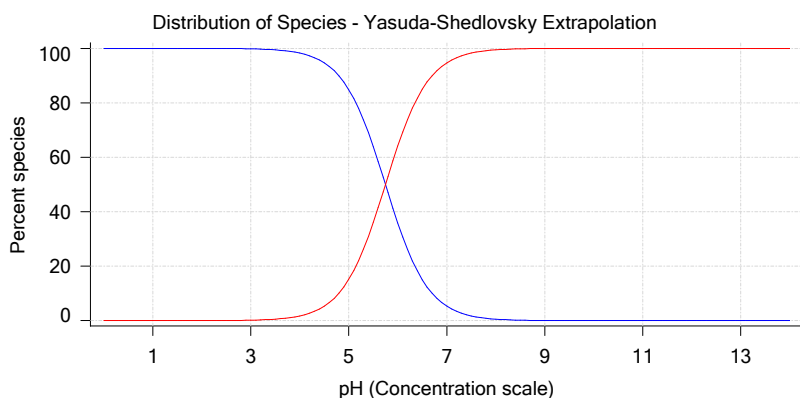
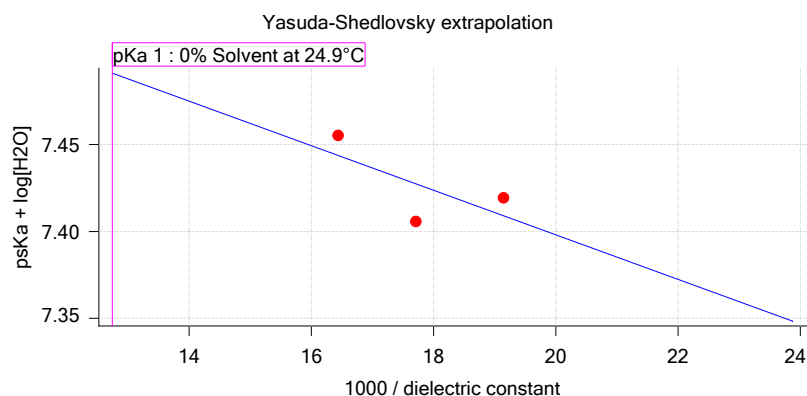
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.75	±0.07	7.65	-12.8140	0.4578	0.166 M	24.9°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1
17J-12003 Points 4 to 41	58.77 %	Up	UV-metric pKa	52.2	19.7 M	0.157 M	24.9°C	✓ 6.12
17J-12003 Points 43 to 82	49.77 %	Up	UV-metric pKa	56.5	24.5 M	0.166 M	25.0°C	✓ 6.02
17J-12003 Points 84 to 123	40.35 %	Up	UV-metric pKa	60.8	29.8 M	0.174 M	24.9°C	✓ 5.98

Graphs



UV-metric psKa Titration 1 of 3 17J-12003 Points 4 to 41

Results

pKa 1	6.12
RMSD	0.006 0.009
Chi squared	0.0274
PCA calculated number of pKas	2
Average ionic strength	0.157 M
Average temperature	24.9°C
Analyte concentration range	94.6 µM to 89.2 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 1.474 to 12.546

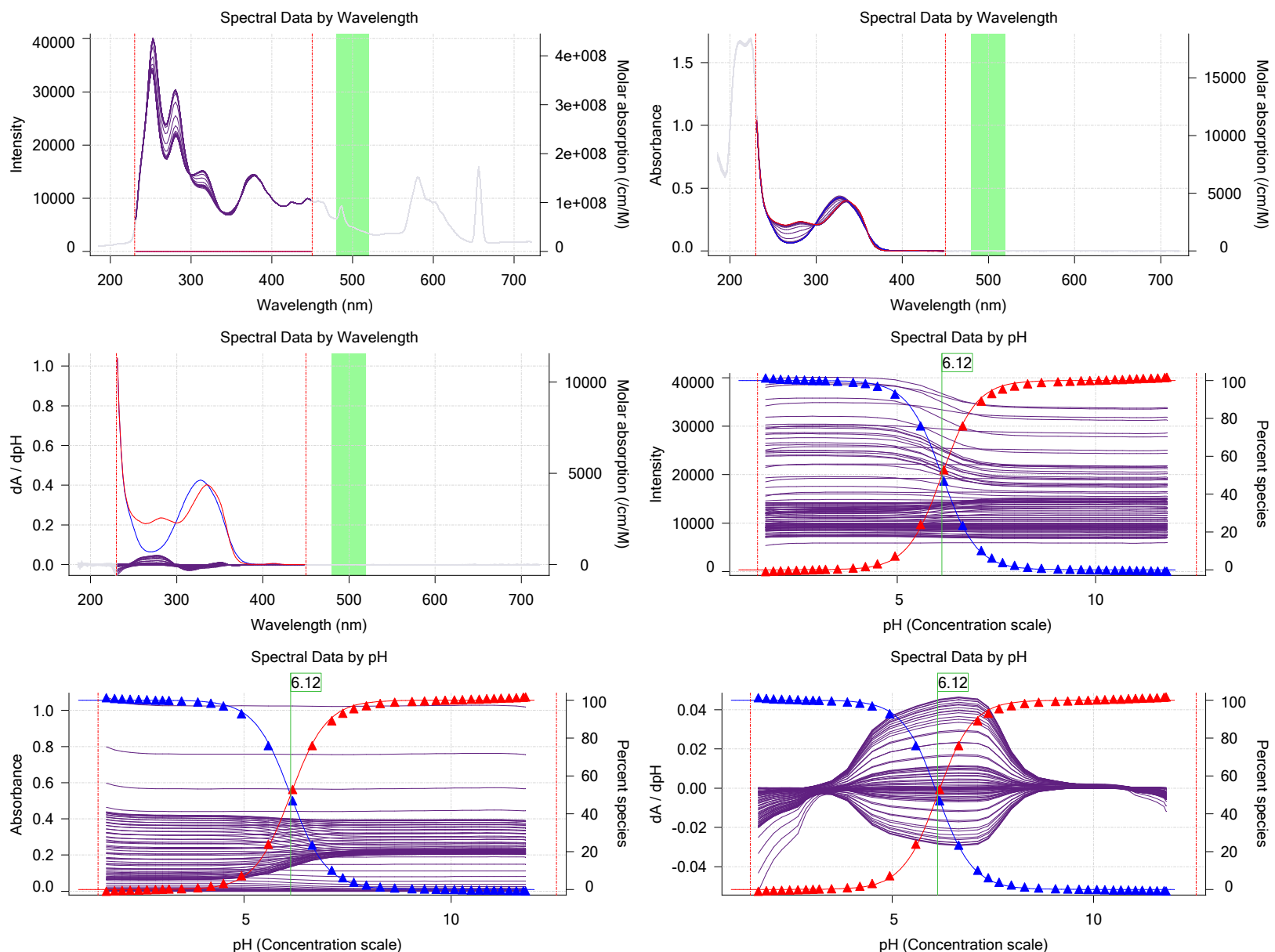
Warnings and errors

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

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

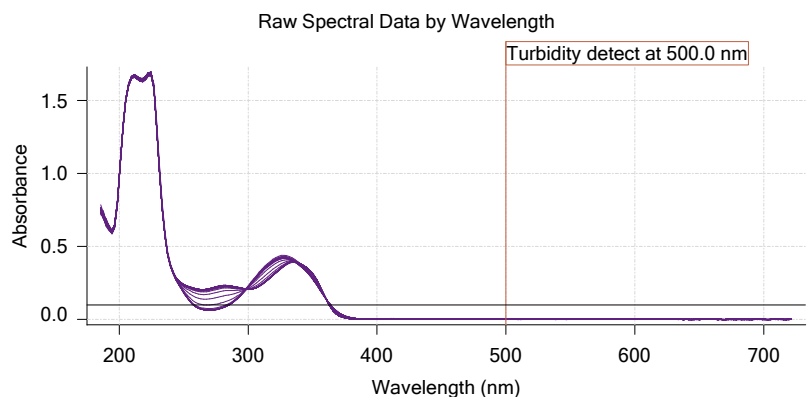
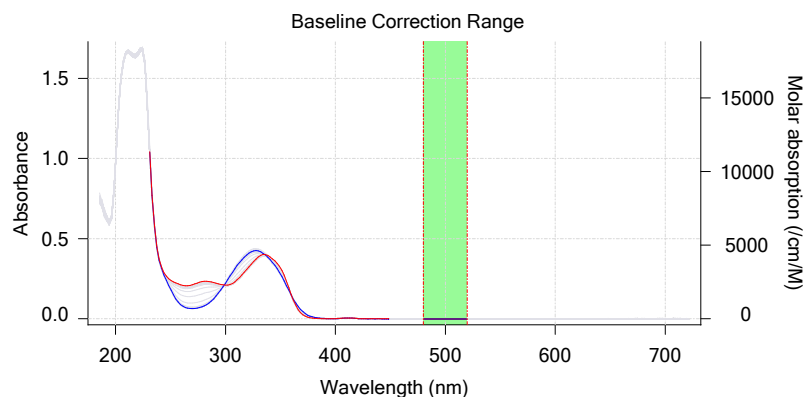
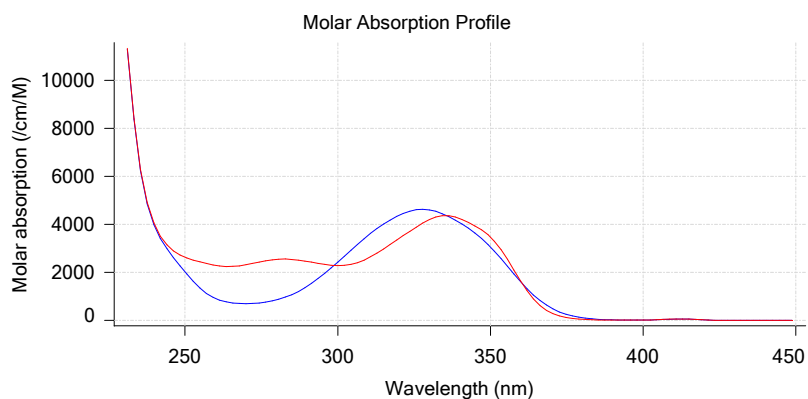
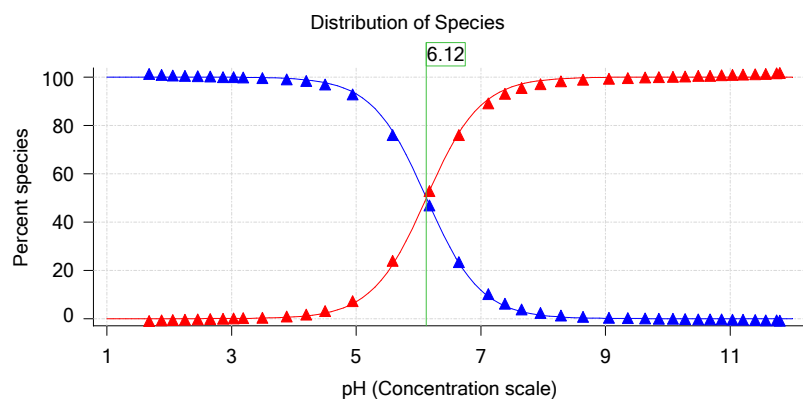
Graphs



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Experiment start time: **10/12/2017 2:44:40 AM**
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Graphs (continued)



UV-metric psKa Titration 2 of 3 17J-12003 Points 43 to 82

Results

pKa 1	6.02
RMSD	0.004 0.004
Chi squared	0.0217
PCA calculated number of pKas	2
Average ionic strength	0.166 M
Average temperature	25.0°C
Analyte concentration range	81.5 µM to 77.1 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	1.492 to 12.515

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

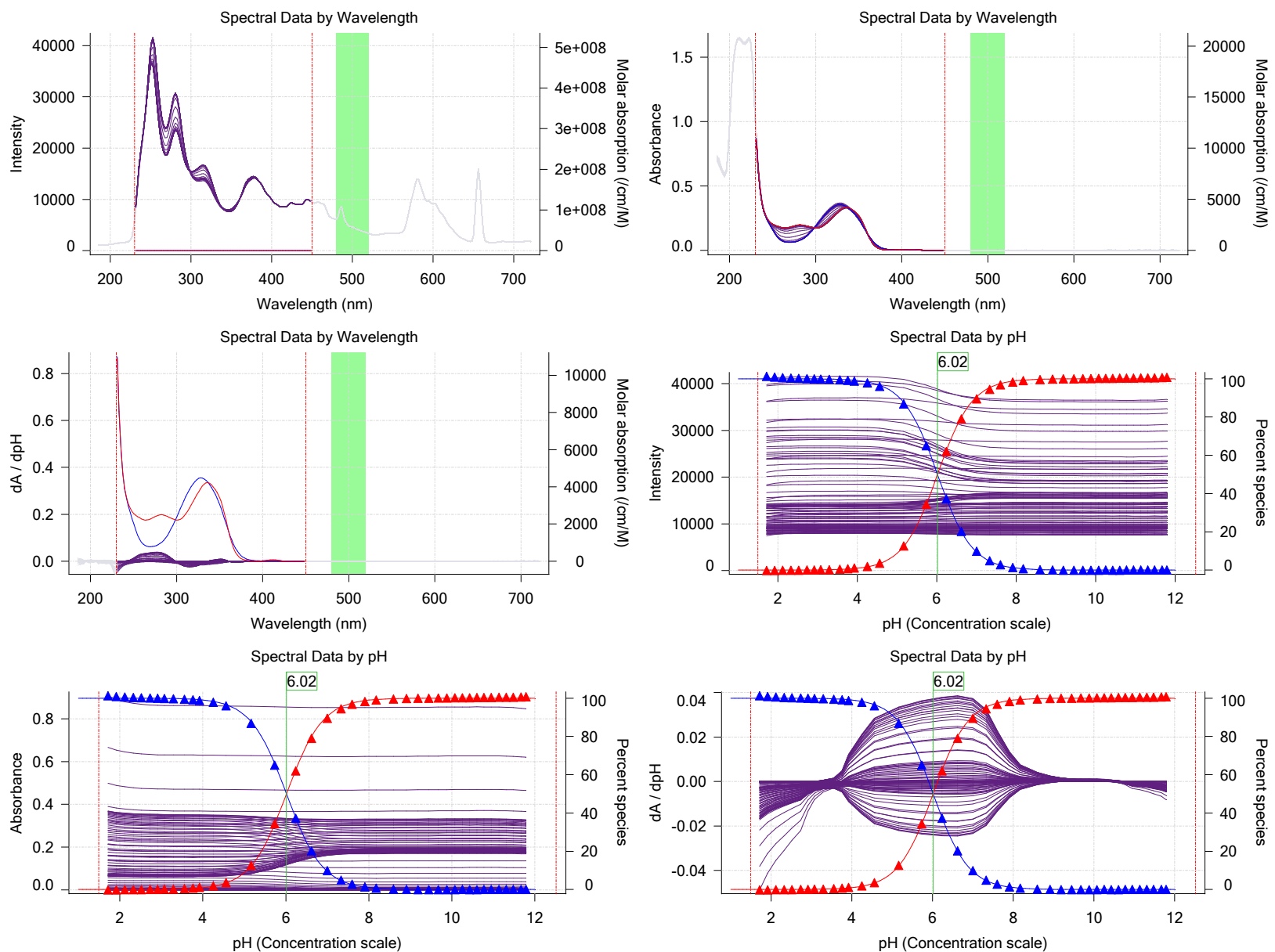
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Experiment start time: **10/12/2017 2:44:40 AM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Assay Settings (continued)

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

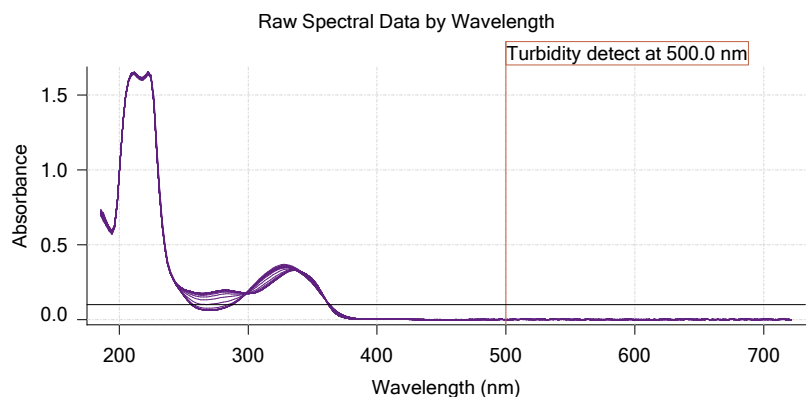
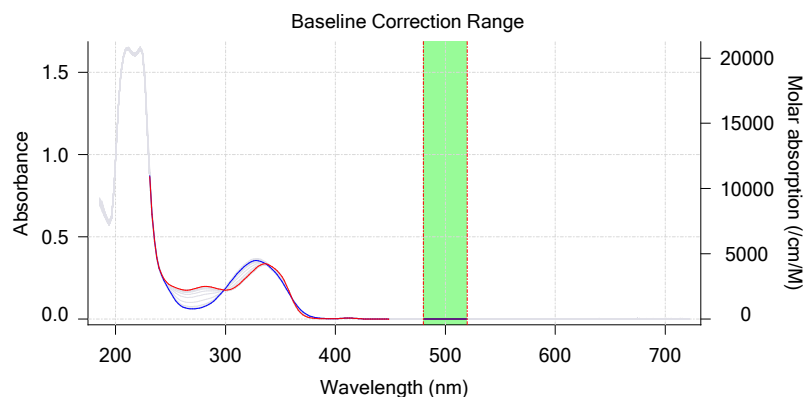
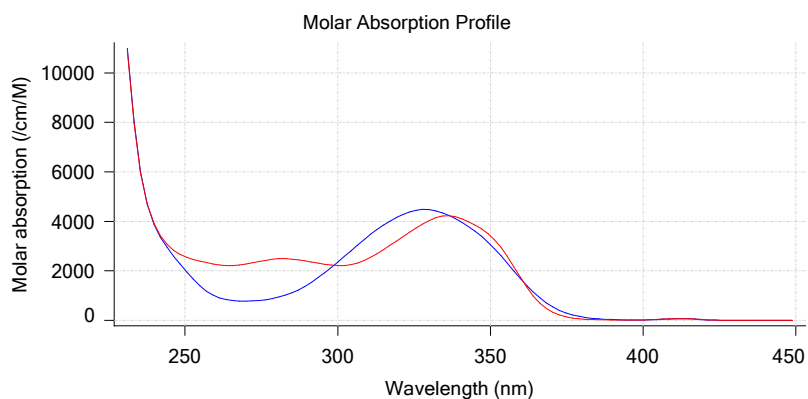
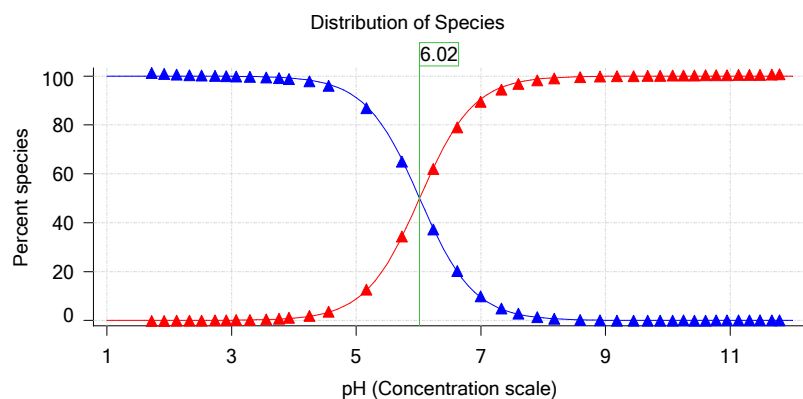
Graphs



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

Graphs (continued)



UV-metric psKa Titration 3 of 3 17J-12003 Points 84 to 123

Results

pKa 1	5.98
RMSD	0.006 0.006
Chi squared	0.0458
PCA calculated number of pKas	2
Average ionic strength	0.174 M
Average temperature	24.9°C
Analyte concentration range	67.4 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	1.496 to 12.507

Warnings and errors

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

Assay Settings

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

Assay Medium

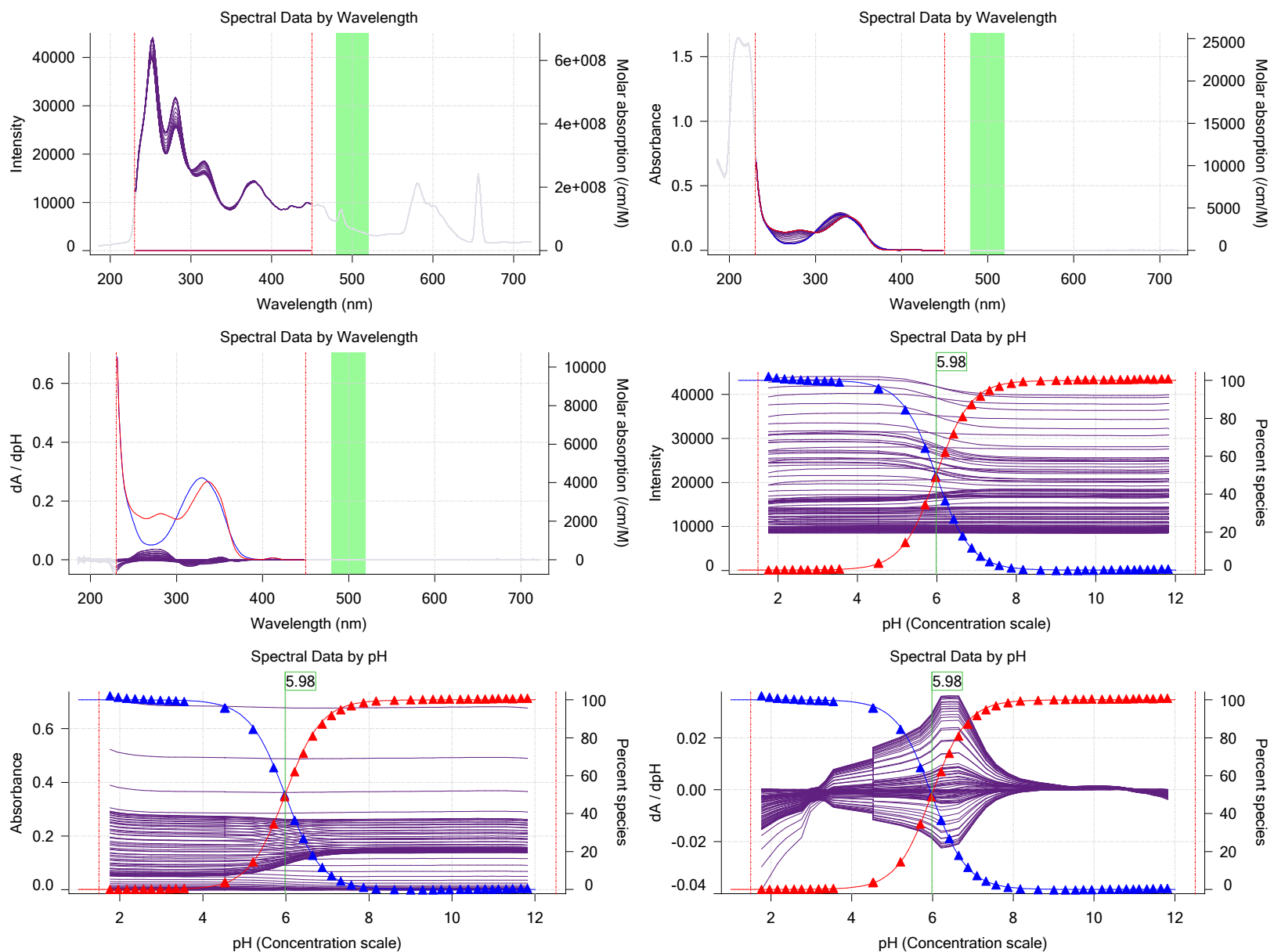
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Assay Settings (continued)

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

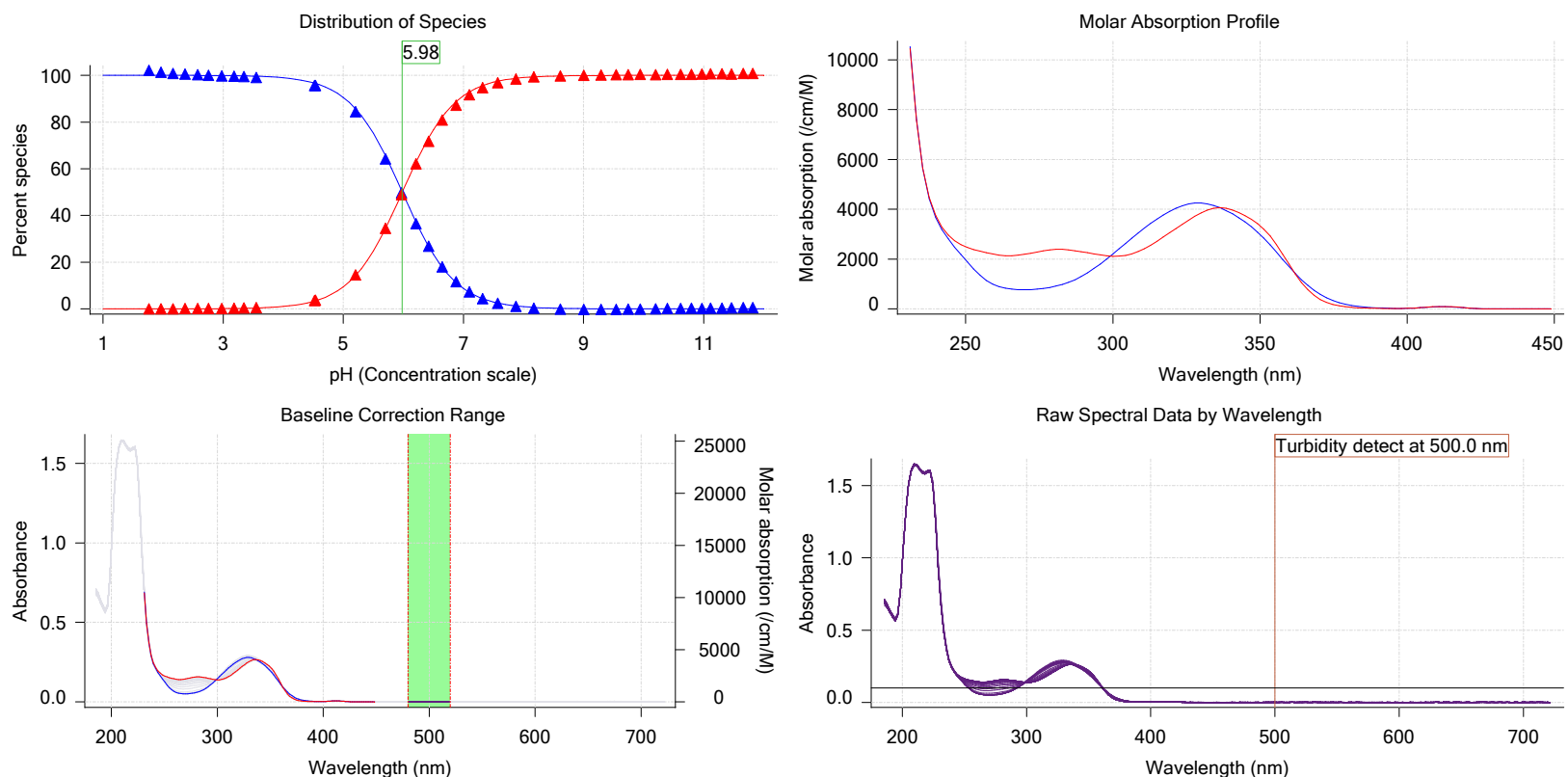
Graphs



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Graphs (continued)



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	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
3:05.7	Dark spectrum								
3:07.0	Reference spectrum								
3:34.6	Volume reset due to vial change								
5:05.4	Initial pH = 8.37								
6:00.9	Data point 4	0.16004 mL	0.07117 mL	0.00000 mL	1.34995 mL	0.02500 mL	1.974	-0.00256	0.21310
6:29.6	Data point 5	0.16004 mL	0.07117 mL	0.02502 mL	1.34995 mL	0.02500 mL	2.175	-0.00683	0.33375
6:46.6	Data point 6	0.16004 mL	0.07117 mL	0.04064 mL	1.34995 mL	0.02500 mL	2.360	0.02423	0.91641
7:03.3	Data point 7	0.16004 mL	0.07117 mL	0.05096 mL	1.34995 mL	0.02500 mL	2.556	0.02431	0.84355
7:19.9	Data point 8	0.16004 mL	0.07117 mL	0.05764 mL	1.34995 mL	0.02500 mL	2.758	0.02071	0.75996
7:36.6	Data point 9	0.16004 mL	0.07117 mL	0.06188 mL	1.34995 mL	0.02500 mL	2.960	0.01687	0.91173

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Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
7:53.2	Data point 10	0.16004 mL	0.07117 mL	0.06456 mL	1.34995 mL	0.02500 mL	3.162	0.01729	0.91992	0.00
8:09.8	Data point 11	0.16004 mL	0.07117 mL	0.06625 mL	1.34995 mL	0.02500 mL	3.335	0.01553	0.93331	0.00
8:26.4	Data point 12	0.16004 mL	0.07117 mL	0.06738 mL	1.34995 mL	0.02500 mL	3.488	0.01563	0.93935	0.00
8:48.2	Data point 13	0.16004 mL	0.07117 mL	0.06896 mL	1.34995 mL	0.02500 mL	3.790	0.02704	0.98199	0.00
9:09.9	Data point 14	0.16004 mL	0.07117 mL	0.06968 mL	1.34995 mL	0.02500 mL	4.179	0.06642	0.99021	0.00
9:31.5	Data point 15	0.16004 mL	0.07117 mL	0.06999 mL	1.34995 mL	0.02500 mL	4.491	0.09965	0.99464	0.00
10:01.4	Data point 16	0.16004 mL	0.07117 mL	0.07023 mL	1.34995 mL	0.02500 mL	4.793	0.09839	0.99022	0.00
10:53.1	Data point 17	0.16004 mL	0.07117 mL	0.07034 mL	1.34995 mL	0.02500 mL	5.229	0.07797	0.72726	0.00
11:46.0	Data point 18	0.16004 mL	0.07117 mL	0.07041 mL	1.34995 mL	0.02500 mL	5.871	0.13580	0.99228	0.00
13:02.8	Data point 19	0.16004 mL	0.07117 mL	0.07048 mL	1.34995 mL	0.02500 mL	6.458	0.08557	0.85614	0.00
14:12.4	Data point 20	0.16004 mL	0.07117 mL	0.07058 mL	1.34995 mL	0.02500 mL	6.926	0.06825	0.52714	0.00
14:57.0	Data point 21	0.16004 mL	0.07117 mL	0.07070 mL	1.34995 mL	0.02500 mL	7.395	0.07926	0.73304	0.00
15:22.1	Data point 22	0.16004 mL	0.07117 mL	0.07079 mL	1.34995 mL	0.02500 mL	7.660	0.09391	0.92659	0.00
15:53.5	Data point 23	0.16004 mL	0.07117 mL	0.07088 mL	1.34995 mL	0.02500 mL	7.925	0.09847	0.97907	0.00
16:33.9	Data point 24	0.16004 mL	0.07117 mL	0.07100 mL	1.34995 mL	0.02500 mL	8.227	0.09786	0.98932	0.00
17:19.0	Data point 25	0.16004 mL	0.07117 mL	0.07112 mL	1.34995 mL	0.02500 mL	8.553	0.10024	0.98946	0.00
18:08.0	Data point 26	0.16004 mL	0.07117 mL	0.07124 mL	1.34995 mL	0.02500 mL	8.902	0.09589	0.97982	0.00
18:59.8	Data point 27	0.16004 mL	0.07117 mL	0.07135 mL	1.34995 mL	0.02500 mL	9.317	0.09604	0.97049	0.00
19:46.7	Data point 28	0.16004 mL	0.07117 mL	0.07145 mL	1.34995 mL	0.02500 mL	9.617	0.09204	0.97468	0.00
20:25.5	Data point 29	0.16004 mL	0.07117 mL	0.07157 mL	1.34995 mL	0.02500 mL	9.896	0.10002	0.98700	0.00
20:55.0	Data point 30	0.16004 mL	0.07117 mL	0.07171 mL	1.34995 mL	0.02500 mL	10.116	0.09208	0.96660	0.00
21:17.1	Data point 31	0.16004 mL	0.07117 mL	0.07190 mL	1.34995 mL	0.02500 mL	10.336	0.05013	0.95823	0.00
21:43.9	Data point 32	0.16004 mL	0.07117 mL	0.07218 mL	1.34995 mL	0.02500 mL	10.531	0.02977	0.96557	0.00
22:00.5	Data point 33	0.16004 mL	0.07117 mL	0.07260 mL	1.34995 mL	0.02500 mL	10.741	0.01653	0.88289	0.00
22:17.2	Data point 34	0.16004 mL	0.07117 mL	0.07331 mL	1.34995 mL	0.02500 mL	10.932	0.00475	0.51628	0.00
22:33.8	Data point 35	0.16004 mL	0.07117 mL	0.07439 mL	1.34995 mL	0.02500 mL	11.112	-0.00957	0.73532	0.00
22:50.4	Data point 36	0.16004 mL	0.07117 mL	0.07603 mL	1.34995 mL	0.02500 mL	11.289	0.00165	0.13776	0.00
23:07.0	Data point 37	0.16004 mL	0.07117 mL	0.07848 mL	1.34995 mL	0.02500 mL	11.455	-0.00351	0.65913	0.00
23:33.9	Data point 38	0.16004 mL	0.07117 mL	0.08187 mL	1.34995 mL	0.02500 mL	11.649	-0.00502	0.63883	0.00
23:50.6	Data point 39	0.16004 mL	0.07117 mL	0.08746 mL	1.34995 mL	0.02500 mL	11.820	0.00171	0.07036	0.00
24:07.3	Data point 40	0.16004 mL	0.07117 mL	0.09574 mL	1.34995 mL	0.02500 mL	11.994	0.00916	0.82387	0.00
24:24.0	Data point 41	0.16004 mL	0.07117 mL	0.09864 mL	1.34995 mL	0.02500 mL	12.046	0.00229	0.18892	0.00
26:04.4	Reference spectrum									
27:07.0	Data point 43	0.22001 mL	0.17199 mL	0.09866 mL	1.34995 mL	0.02500 mL	1.992	-0.05362	0.93031	0.00
27:34.7	Data point 44	0.22001 mL	0.17199 mL	0.12533 mL	1.34995 mL	0.02500 mL	2.193	0.01156	0.85256	0.00
27:51.6	Data point 45	0.22001 mL	0.17199 mL	0.14189 mL	1.34995 mL	0.02500 mL	2.394	0.01487	0.83545	0.00
28:08.5	Data point 46	0.22001 mL	0.17199 mL	0.15245 mL	1.34995 mL	0.02500 mL	2.601	0.01220	0.80017	0.00
28:25.2	Data point 47	0.22001 mL	0.17199 mL	0.15906 mL	1.34995 mL	0.02500 mL	2.795	0.00625	0.25739	0.00
28:42.0	Data point 48	0.22001 mL	0.17199 mL	0.16329 mL	1.34995 mL	0.02500 mL	3.007	0.01666	0.88965	0.00
28:58.8	Data point 49	0.22001 mL	0.17199 mL	0.16590 mL	1.34995 mL	0.02500 mL	3.187	0.01879	0.96436	0.00
29:15.5	Data point 50	0.22001 mL	0.17199 mL	0.16761 mL	1.34995 mL	0.02500 mL	3.348	0.01899	0.96106	0.00
29:47.3	Data point 51	0.22001 mL	0.17199 mL	0.16898 mL	1.34995 mL	0.02500 mL	3.565	0.02363	0.94320	0.00
30:03.9	Data point 52	0.22001 mL	0.17199 mL	0.16971 mL	1.34995 mL	0.02500 mL	3.828	0.03718	0.97544	0.00
30:25.5	Data point 53	0.22001 mL	0.17199 mL	0.17016 mL	1.34995 mL	0.02500 mL	4.030	0.04910	0.98935	0.00
30:42.1	Data point 54	0.22001 mL	0.17199 mL	0.17039 mL	1.34995 mL	0.02500 mL	4.190	0.06742	0.96670	0.00
31:03.8	Data point 55	0.22001 mL	0.17199 mL	0.17067 mL	1.34995 mL	0.02500 mL	4.518	0.10009	0.98337	0.00
31:39.0	Data point 56	0.22001 mL	0.17199 mL	0.17084 mL	1.34995 mL	0.02500 mL	4.824	0.09906	0.98597	0.00
32:28.3	Data point 57	0.22001 mL	0.17199 mL	0.17098 mL	1.34995 mL	0.02500 mL	5.424	0.09724	0.99490	0.00
33:42.6	Data point 58	0.22001 mL	0.17199 mL	0.17107 mL	1.34995 mL	0.02500 mL	5.991	0.10009	0.99143	0.00
34:53.0	Data point 59	0.22001 mL	0.17199 mL	0.17117 mL	1.34995 mL	0.02500 mL	6.494	0.10091	0.99262	0.00
35:48.7	Data point 60	0.22001 mL	0.17199 mL	0.17126 mL	1.34995 mL	0.02500 mL	6.873	0.09961	0.99236	0.00
36:36.3	Data point 61	0.22001 mL	0.17199 mL	0.17138 mL	1.34995 mL	0.02500 mL	7.250	0.09789	0.98437	0.00
37:01.9	Data point 62	0.22001 mL	0.17199 mL	0.17150 mL	1.34995 mL	0.02500 mL	7.581	0.09970	0.99345	0.00
37:45.2	Data point 63	0.22001 mL	0.17199 mL	0.17164 mL	1.34995 mL	0.02500 mL	7.848	0.09861	0.97089	0.00
38:24.5	Data point 64	0.22001 mL	0.17199 mL	0.17178 mL	1.34995 mL	0.02500 mL	8.154	0.09668	0.98398	0.00
39:08.8	Data point 65	0.22001 mL	0.17199 mL	0.17190 mL	1.34995 mL	0.02500 mL	8.422	0.09933	0.97910	0.00
39:53.3	Data point 66	0.22001 mL	0.17199 mL	0.17201 mL	1.34995 mL	0.02500 mL	8.839	0.09591	0.96524	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 Slope
40:39.0	Data point 67	0.22001 mL	0.17199 mL	0.17211 mL	1.34995 mL	0.02500 mL	9.153	0.09578	0.95530	0.00000
41:21.7	Data point 68	0.22001 mL	0.17199 mL	0.17220 mL	1.34995 mL	0.02500 mL	9.426	0.09992	0.98405	0.00000
42:00.9	Data point 69	0.22001 mL	0.17199 mL	0.17232 mL	1.34995 mL	0.02500 mL	9.687	0.09469	0.96789	0.00000
42:38.7	Data point 70	0.22001 mL	0.17199 mL	0.17248 mL	1.34995 mL	0.02500 mL	9.915	0.09148	0.96960	0.00000
43:05.5	Data point 71	0.22001 mL	0.17199 mL	0.17267 mL	1.34995 mL	0.02500 mL	10.115	0.06079	0.98716	0.00000
43:27.2	Data point 72	0.22001 mL	0.17199 mL	0.17291 mL	1.34995 mL	0.02500 mL	10.312	0.03664	0.97913	0.00000
43:43.8	Data point 73	0.22001 mL	0.17199 mL	0.17324 mL	1.34995 mL	0.02500 mL	10.488	0.01540	0.91648	0.00000
44:00.5	Data point 74	0.22001 mL	0.17199 mL	0.17373 mL	1.34995 mL	0.02500 mL	10.662	0.00517	0.55692	0.00000
44:17.1	Data point 75	0.22001 mL	0.17199 mL	0.17446 mL	1.34995 mL	0.02500 mL	10.838	0.00446	0.50501	0.00000
44:33.7	Data point 76	0.22001 mL	0.17199 mL	0.17554 mL	1.34995 mL	0.02500 mL	11.009	-0.00368	0.52829	0.00000
44:50.4	Data point 77	0.22001 mL	0.17199 mL	0.17714 mL	1.34995 mL	0.02500 mL	11.182	-0.00956	0.80557	0.00000
45:07.0	Data point 78	0.22001 mL	0.17199 mL	0.17952 mL	1.34995 mL	0.02500 mL	11.367	-0.00536	0.56823	0.00000
45:23.7	Data point 79	0.22001 mL	0.17199 mL	0.18311 mL	1.34995 mL	0.02500 mL	11.539	-0.00320	0.56390	0.00000
45:40.3	Data point 80	0.22001 mL	0.17199 mL	0.18845 mL	1.34995 mL	0.02500 mL	11.707	0.00338	0.25474	0.00000
46:07.5	Data point 81	0.22001 mL	0.17199 mL	0.19763 mL	1.34995 mL	0.02500 mL	11.898	-0.00281	0.23613	0.00000
46:29.5	Data point 82	0.22001 mL	0.17199 mL	0.20602 mL	1.34995 mL	0.02500 mL	12.015	0.00102	0.03106	0.00000
48:11.3	Reference spectrum									
49:31.7	Data point 84	0.39005 mL	0.28662 mL	0.20604 mL	1.34995 mL	0.02500 mL	1.996	-0.06802	0.93696	0.00000
49:59.2	Data point 85	0.39005 mL	0.28662 mL	0.23533 mL	1.34995 mL	0.02500 mL	2.194	0.00228	0.11348	0.00000
50:16.1	Data point 86	0.39005 mL	0.28662 mL	0.25336 mL	1.34995 mL	0.02500 mL	2.397	0.00331	0.25966	0.00000
50:33.1	Data point 87	0.39005 mL	0.28662 mL	0.26482 mL	1.34995 mL	0.02500 mL	2.597	-0.01203	0.48344	0.00000
50:49.8	Data point 88	0.39005 mL	0.28662 mL	0.27220 mL	1.34995 mL	0.02500 mL	2.803	0.02105	0.81589	0.00000
51:06.4	Data point 89	0.39005 mL	0.28662 mL	0.27667 mL	1.34995 mL	0.02500 mL	2.985	-0.00985	0.52910	0.00000
51:23.1	Data point 90	0.39005 mL	0.28662 mL	0.27968 mL	1.34995 mL	0.02500 mL	3.202	0.00774	0.65158	0.00000
51:39.7	Data point 91	0.39005 mL	0.28662 mL	0.28149 mL	1.34995 mL	0.02500 mL	3.405	0.00991	0.82690	0.00000
51:56.3	Data point 92	0.39005 mL	0.28662 mL	0.28262 mL	1.34995 mL	0.02500 mL	3.574	0.01768	0.89629	0.00000
52:28.2	Data point 93	0.39005 mL	0.28662 mL	0.28370 mL	1.34995 mL	0.02500 mL	3.775	0.02353	0.89783	0.00000
53:05.5	Data point 94	0.39005 mL	0.28662 mL	0.28422 mL	1.34995 mL	0.02500 mL	4.758	-0.06373	0.99352	0.00000
53:22.0	Data point 95	0.39005 mL	0.28662 mL	0.28427 mL	1.34995 mL	0.02500 mL	4.743	-0.05410	0.98073	0.00000
53:59.1	Data point 96	0.39005 mL	0.28662 mL	0.28594 mL	1.34995 mL	0.02500 mL	5.425	-0.06043	0.94220	0.00000
54:25.8	Data point 97	0.39005 mL	0.28662 mL	0.28622 mL	1.34995 mL	0.02500 mL	5.918	0.09779	0.96295	0.00000
54:52.7	Data point 98	0.39005 mL	0.28662 mL	0.28638 mL	1.34995 mL	0.02500 mL	6.185	0.04794	0.97865	0.00000
55:24.7	Data point 99	0.39005 mL	0.28662 mL	0.28652 mL	1.34995 mL	0.02500 mL	6.425	0.10015	0.99230	0.00000
55:49.4	Data point 100	0.39005 mL	0.28662 mL	0.28664 mL	1.34995 mL	0.02500 mL	6.634	-0.00652	0.05249	0.00000
56:21.2	Data point 101	0.39005 mL	0.28662 mL	0.28678 mL	1.34995 mL	0.02500 mL	6.859	0.09121	0.96469	0.00000
56:47.9	Data point 102	0.39005 mL	0.28662 mL	0.28692 mL	1.34995 mL	0.02500 mL	7.089	0.06823	0.96255	0.00000
57:14.6	Data point 103	0.39005 mL	0.28662 mL	0.28707 mL	1.34995 mL	0.02500 mL	7.309	0.09002	0.89954	0.00000
57:41.4	Data point 104	0.39005 mL	0.28662 mL	0.28721 mL	1.34995 mL	0.02500 mL	7.531	0.09248	0.96862	0.00000
58:09.1	Data point 105	0.39005 mL	0.28662 mL	0.28735 mL	1.34995 mL	0.02500 mL	7.782	0.09878	0.98698	0.00000
58:45.8	Data point 106	0.39005 mL	0.28662 mL	0.28749 mL	1.34995 mL	0.02500 mL	8.080	0.09955	0.97934	0.00000
59:20.6	Data point 107	0.39005 mL	0.28662 mL	0.28761 mL	1.34995 mL	0.02500 mL	8.378	0.09790	0.97476	0.00000
1:00:07.0	Data point 108	0.39005 mL	0.28662 mL	0.28772 mL	1.34995 mL	0.02500 mL	8.818	0.09430	0.96839	0.00000
1:00:58.7	Data point 109	0.39005 mL	0.28662 mL	0.28784 mL	1.34995 mL	0.02500 mL	9.207	0.09800	0.97920	0.00000
1:01:37.0	Data point 110	0.39005 mL	0.28662 mL	0.28796 mL	1.34995 mL	0.02500 mL	9.494	0.09948	0.96547	0.00000
1:02:12.8	Data point 111	0.39005 mL	0.28662 mL	0.28810 mL	1.34995 mL	0.02500 mL	9.741	0.09553	0.94777	0.00000
1:02:36.0	Data point 112	0.39005 mL	0.28662 mL	0.28826 mL	1.34995 mL	0.02500 mL	9.940	0.06177	0.95583	0.00000
1:03:02.6	Data point 113	0.39005 mL	0.28662 mL	0.28848 mL	1.34995 mL	0.02500 mL	10.140	0.03939	0.90864	0.00000
1:03:19.2	Data point 114	0.39005 mL	0.28662 mL	0.28878 mL	1.34995 mL	0.02500 mL	10.396	0.00702	0.76538	0.00000
1:03:45.9	Data point 115	0.39005 mL	0.28662 mL	0.28928 mL	1.34995 mL	0.02500 mL	10.592	0.00240	0.22134	0.00000
1:04:02.5	Data point 116	0.39005 mL	0.28662 mL	0.29012 mL	1.34995 mL	0.02500 mL	10.809	-0.01224	0.89642	0.00000
1:04:19.1	Data point 117	0.39005 mL	0.28662 mL	0.29151 mL	1.34995 mL	0.02500 mL	10.993	-0.01300	0.90612	0.00000
1:04:35.6	Data point 118	0.39005 mL	0.28662 mL	0.29360 mL	1.34995 mL	0.02500 mL	11.163	-0.01146	0.92351	0.00000
1:04:52.2	Data point 119	0.39005 mL	0.28662 mL	0.29668 mL	1.34995 mL	0.02500 mL	11.309	-0.01322	0.86140	0.00000
1:05:19.3	Data point 120	0.39005 mL	0.28662 mL	0.30089 mL	1.34995 mL	0.02500 mL	11.498	-0.01023	0.85640	0.00000
1:05:35.9	Data point 121	0.39005 mL	0.28662 mL	0.30753 mL	1.34995 mL	0.02500 mL	11.655	-0.00996	0.81412	0.00000
1:06:03.2	Data point 122	0.39005 mL	0.28662 mL	0.31842 mL	1.34995 mL	0.02500 mL	11.848	-0.00853	0.68656	0.00000
1:06:20.1	Data point 123	0.39005 mL	0.28662 mL	0.33342 mL	1.34995 mL	0.02500 mL	12.007	-0.00508	0.51348	0.00000

Sample name: **D05**
 Assay name: **UV-metric pKa**
 Assay ID: **17J-12003**
 Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12003_D05_UV-metric pKa.t3r**

Experiment start time: **10/12/2017 2:44:40 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD	dpH time
1:08:19.2	Assay volumes	0.64005 mL	0.41244 mL	0.33342 mL	1.34995 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	1.34 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				

Sample name: **D05**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-12003**
 Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12003_D05_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 2:44:40 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	0.06 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	0.17 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 2:44:40 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus S	1.0007	10/12/2017 2:44:40 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jH	0.3	10/12/2017 2:44:40 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Four-Plus jOH	-0.2	10/12/2017 2:44:40 AM	C:\Sirius_T3\17J-11006_Blank standardisation.t3r
Base concentration factor	1.011	10/12/2017 2:44:40 AM	C:\Sirius_T3\KOH17122.t3r
Acid concentration factor	0.995	10/12/2017 2:44:40 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		

Sample name: **D05**
 Assay name: **UV-metric psKa**
 Assay ID: **17J-12003**
 Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12003_D05_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 2:44:40 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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
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	-8.63 mV		10/12/2017 2:45:04 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	5e+003 mL	10-6-17	10/6/2017 3:04:25 PM
Waste	5.1e+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		



Assay Settings

Sample name: **D05**
Assay name: **UV-metric psKa**
Assay ID: **17J-12003**
Filename: **C:\Sirius_T3\Mehtap\20171011_exp15_pKa\17J-12003_D05_UV-metric psKa.t3r**

Experiment start time: **10/12/2017 2:44:40 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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 F5