# Yasuda-Shedlovsky Result

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

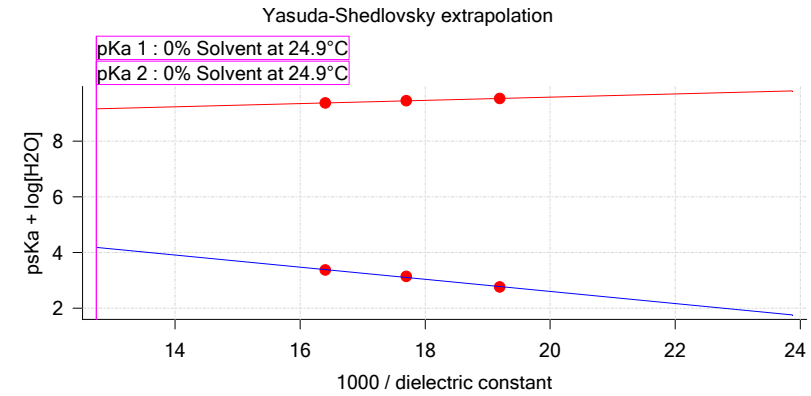
## Yasuda-Shedlovsky result

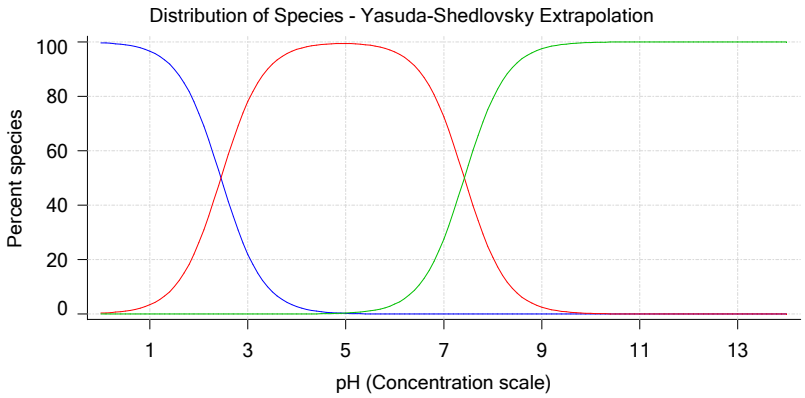
| Extrapolation type | pKa 0% | SD | Intercept | Slope | R² | Ionic strength | Temperature |
|---|---|---|---|---|---|---|---|
| Yasuda-Shedlovsky | 2.45 | ±0.10 | 6.98 | -218.9668 | 0.9925 | 0.166 M | 24.9°C |
| Yasuda-Shedlovsky | 7.42 | ±0.03 | 8.43 | 57.7140 | 0.9916 | 0.166 M | 24.9°C |

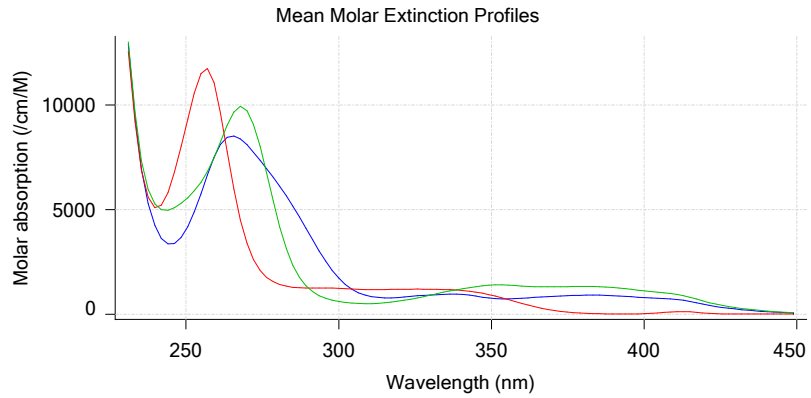
## Component assay results

| Titration | Methanol weight% | Direction | Result type | Dielectric constant | [H2O] | Ionic strength | Temperature | psKa 1 | psKa 2 |
|---|---|---|---|---|---|---|---|---|---|
| 17J-07003 Points 4 to 69 | 59.07 % | Up | UV-metric pKa | 52.1 | 19.6 M | 0.157 M | 24.9°C ☑ | 1.47 ☑ | 8.24 |
| 17J-07003 Points 71 to 140 | 49.72 % | Up | UV-metric pKa | 56.5 | 24.6 M | 0.167 M | 24.9°C ☑ | 1.75 ☑ | 8.07 |
| 17J-07003 Points 142 to 212 | 40.08 % | Up | UV-metric pKa | 61.0 | 30.0 M | 0.174 M | 24.9°C ☑ | 1.90 ☑ | 7.89 |

## Graphs




# UV-metric psKa Titration 1 of 3 17J-07003 Points 4 to 69

## Results

| | |
|---|---|
| pKa 1 | **1.47** |
| pKa 2 | **8.24** |
| RMSD | **0.004 0.002 0.005** |
| Chi squared | **0.0432** |
| PCA calculated number of pKas | **6** |
| Average ionic strength | **0.157 M** |
| Average temperature | **24.9°C** |
| Analyte concentration range | **81.2 µM to 76.3 µM** |
| Methanol weight % | **59.1 %** |
| Dielectric constant | **52.1** |
| Water concentration | **19.6 M** |

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

## Results (continued)

Number of pKas source **Predicted**
Wavelength clipping **230.0 nm to 450.0 nm**
pH clipping **1.462 to 12.542**

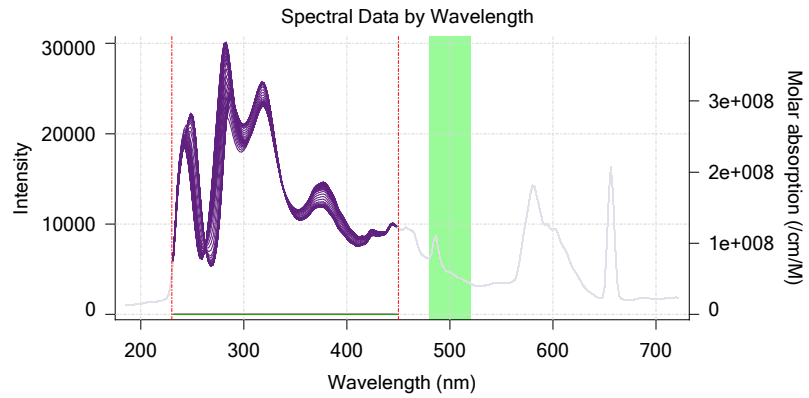
## Warnings and errors

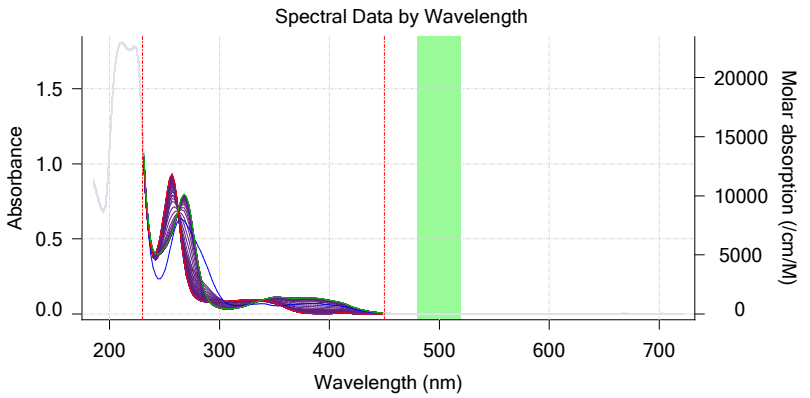
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

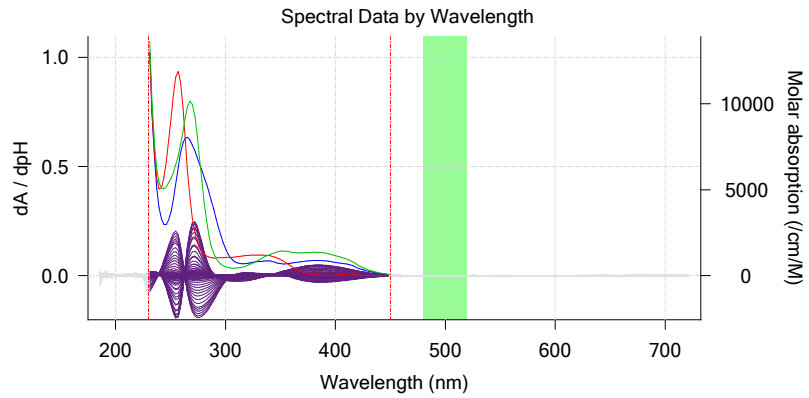
## Assay Settings

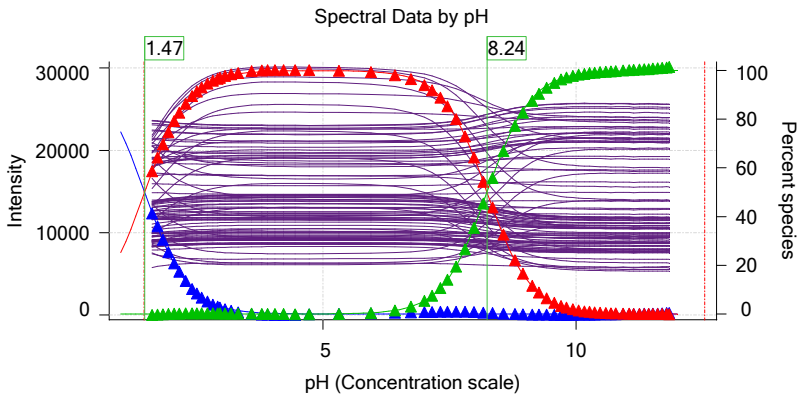
| Setting | Value | Original Value | Date/Time changed | Imported from |
|---|---|---|---|---|
| Buffer in use | Yes | | | |
| Buffer type | Phosphate Buffer | | | |
| ***Assay Medium*** | | | | |
| Volume of buffer introduced | 0.025000 mL | | | |
| Add buffer manually | Manual | | | |

## Graphs



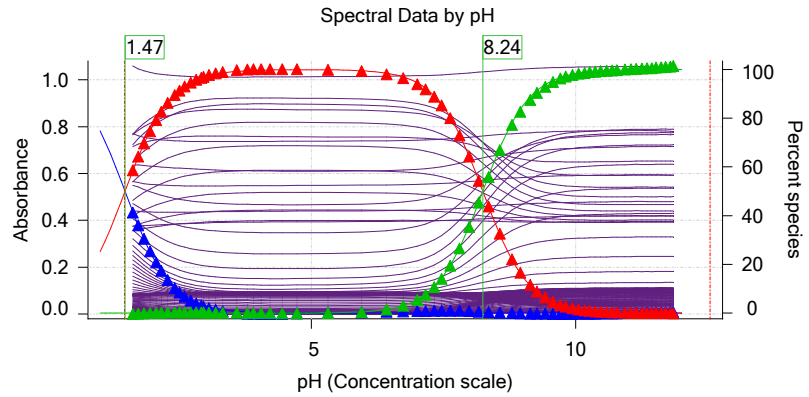



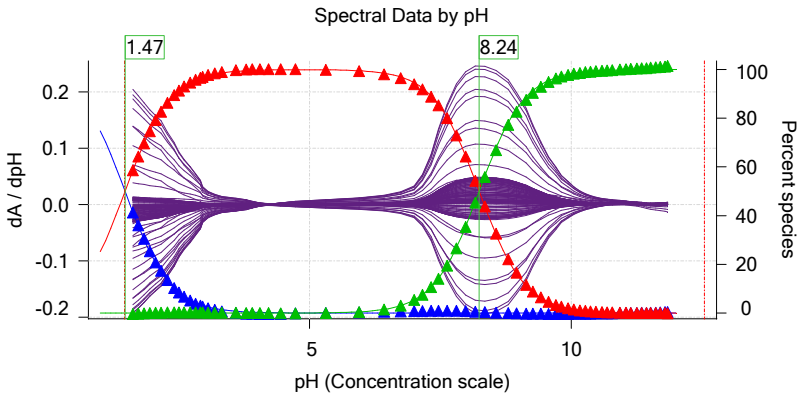



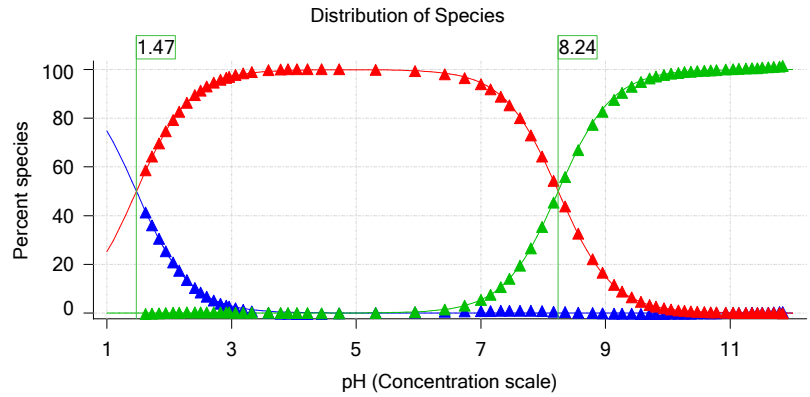
Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

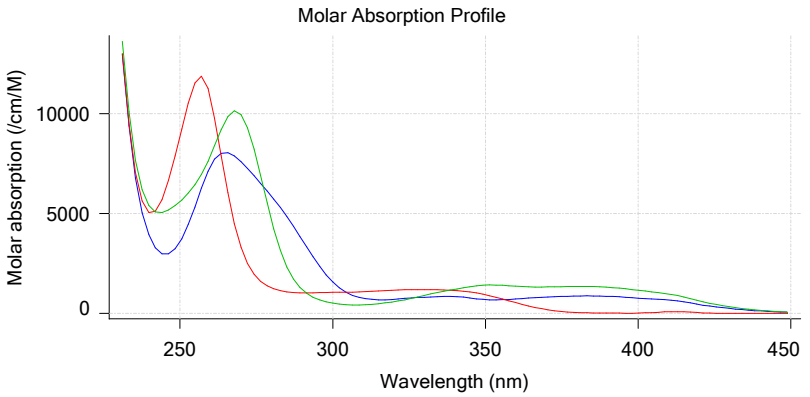
Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

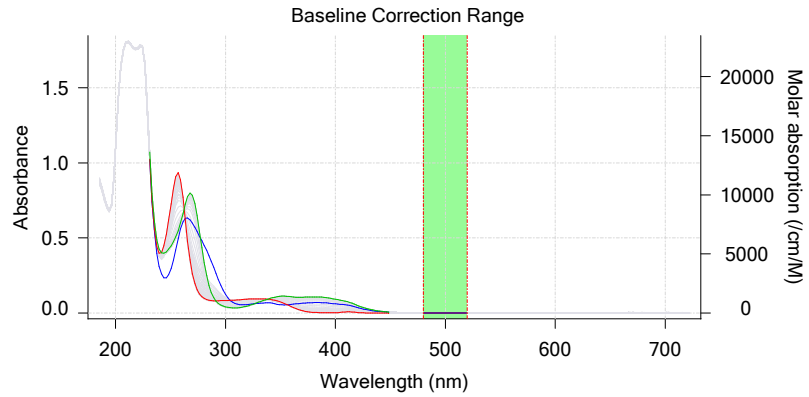
## Graphs (continued)

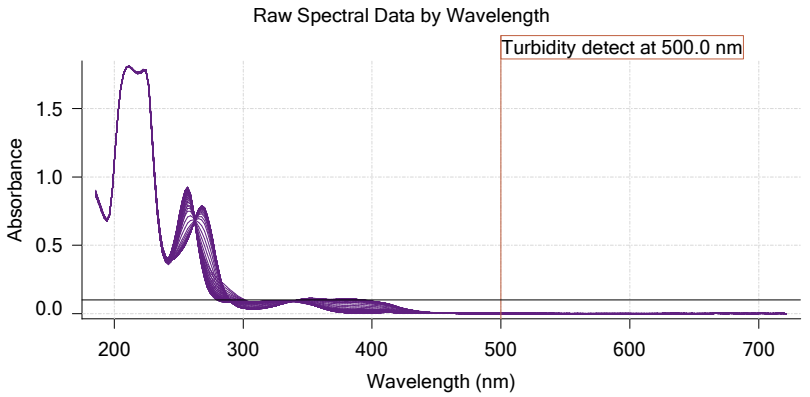



# UV-metric psKa Titration 2 of 3 17J-07003 Points 71 to 140

## Results

| | |
|---|---|
| pKa 1 | **1.75** |
| pKa 2 | **8.07** |
| RMSD | **0.005 0.007 0.005** |
| Chi squared | **0.0506** |
| PCA calculated number of pKas | **6** |
| Average ionic strength | **0.167 M** |
| Average temperature | **24.9°C** |
| Analyte concentration range | **69.4 µM to 65.5 µM** |
| Methanol weight % | **49.7 %** |
| Dielectric constant | **56.5** |
| Water concentration | **24.6 M** |

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

## Results (continued)

Number of pKas source **Predicted**
Wavelength clipping **230.0 nm to 450.0 nm**
pH clipping **1.495 to 12.539**

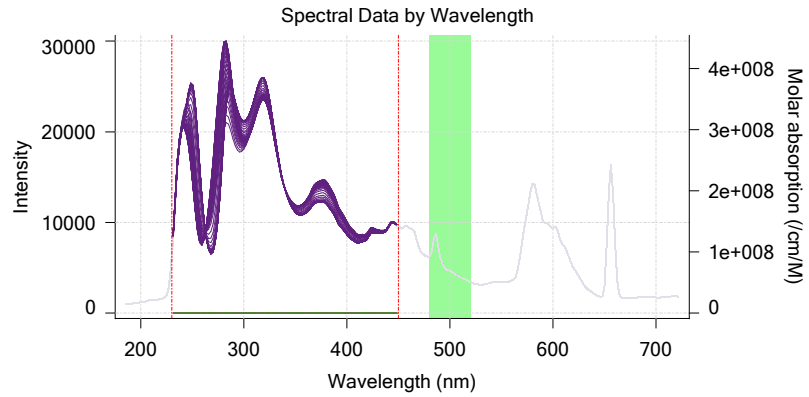
## Warnings and errors

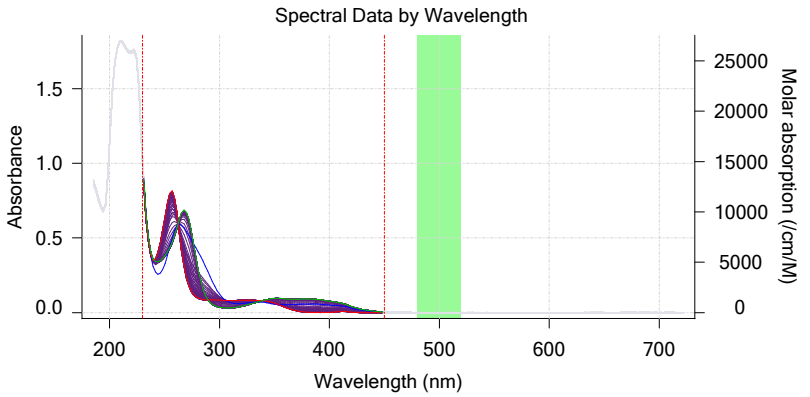
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

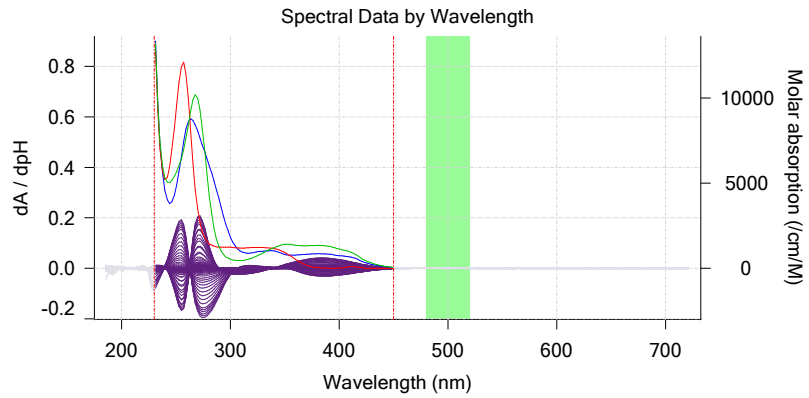
## Assay Settings

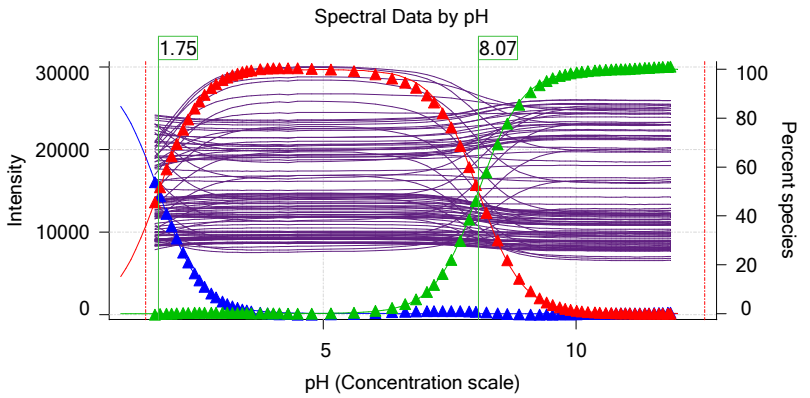
| Setting | Value | Original Value | Date/Time changed | Imported from |
|---|---|---|---|---|
| Buffer in use | Yes | | | |
| Buffer type | Phosphate Buffer | | | |
| ***Assay Medium*** | | | | |
| Volume of buffer introduced | 0.025000 mL | | | |
| Add buffer manually | Manual | | | |

## Graphs



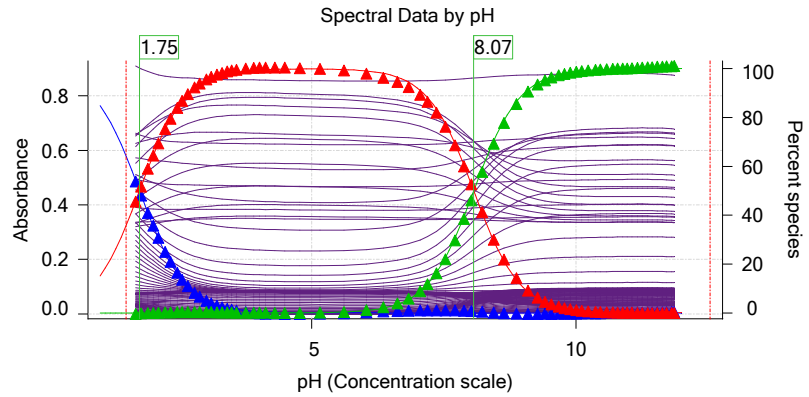



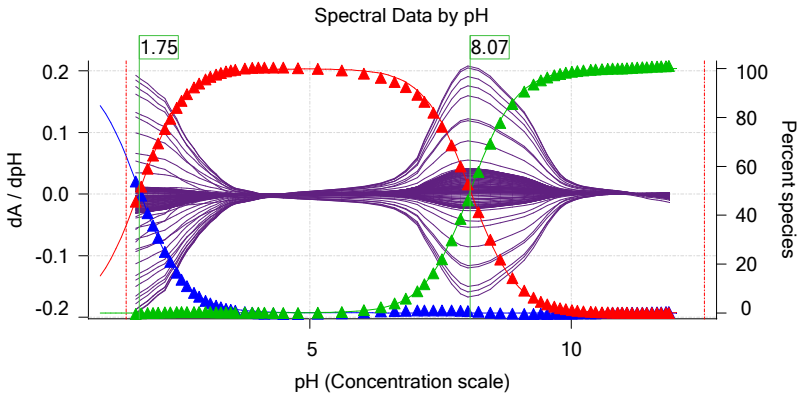



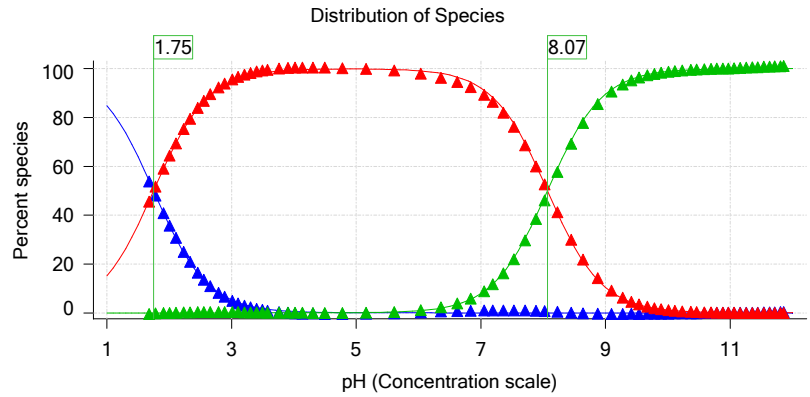
Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

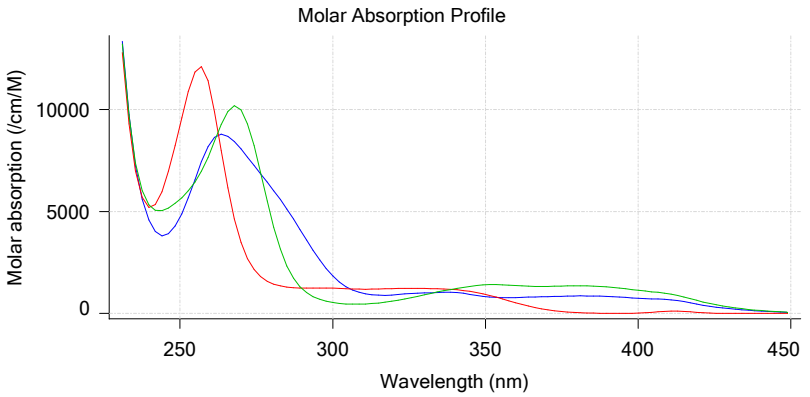
Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

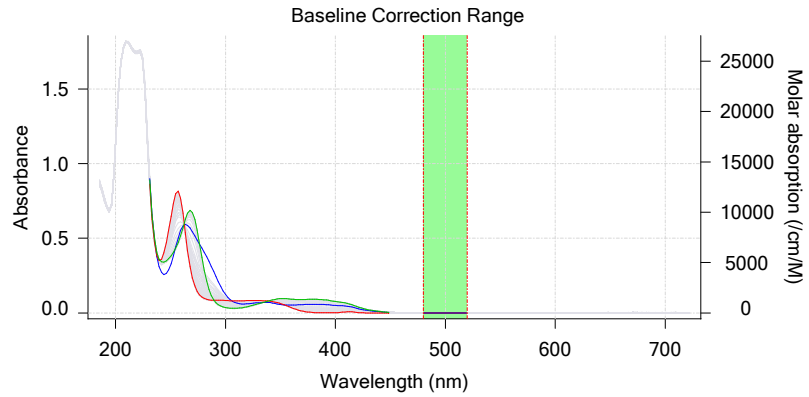
## Graphs (continued)

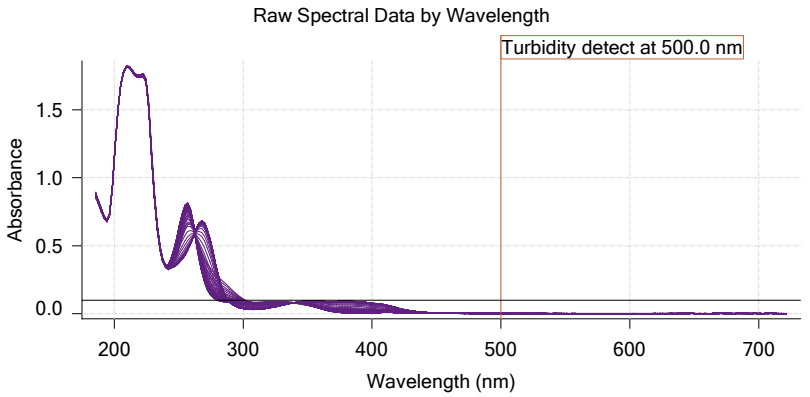



## UV-metric psKa Titration 3 of 3 17J-07003 Points 142 to 212

### Results

| | |
|---|---|
| pKa 1 | **1.90** |
| pKa 2 | **7.89** |
| RMSD | **0.020 0.012 0.023** |
| Chi squared | **0.1618** |
| PCA calculated number of pKas | **4** |
| Average ionic strength | **0.174 M** |
| Average temperature | **24.9°C** |
| Analyte concentration range | **57.0 µM to 54.0 µM** |
| Methanol weight % | **40.1 %** |
| Dielectric constant | **61.0** |
| Water concentration | **30.0 M** |

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

## Results (continued)

Number of pKas source **Predicted**
Wavelength clipping **230.0 nm to 450.0 nm**
pH clipping **1.497 to 12.522**

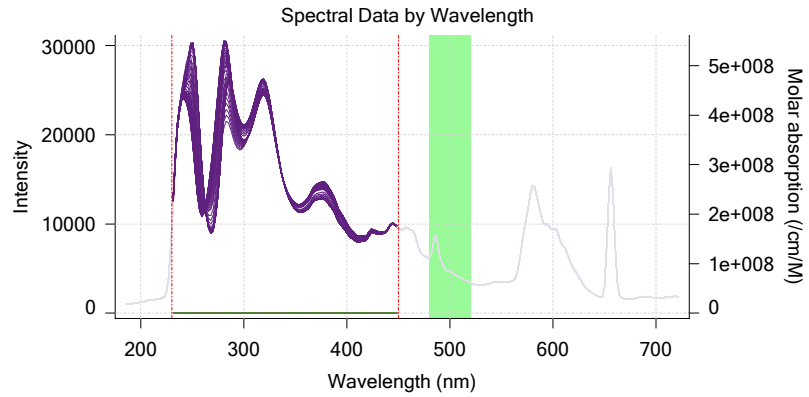
## Warnings and errors

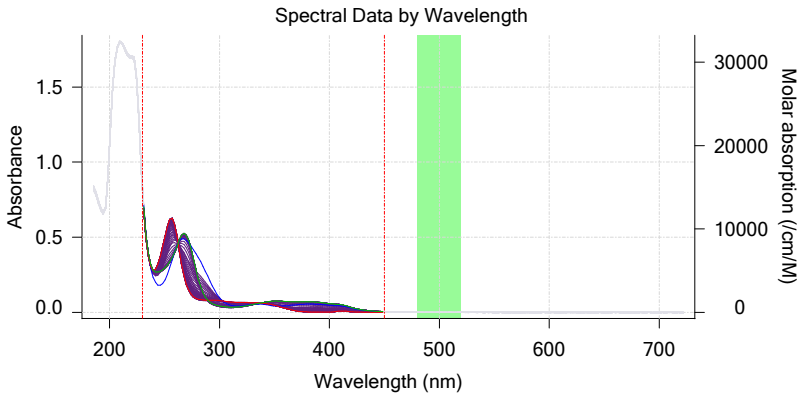
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

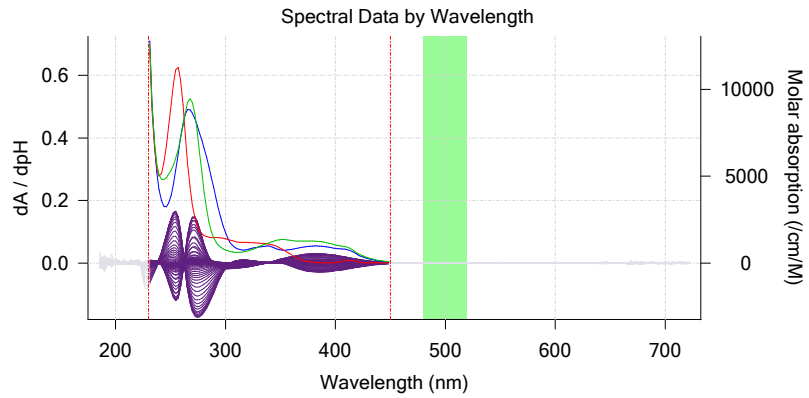
## Assay Settings

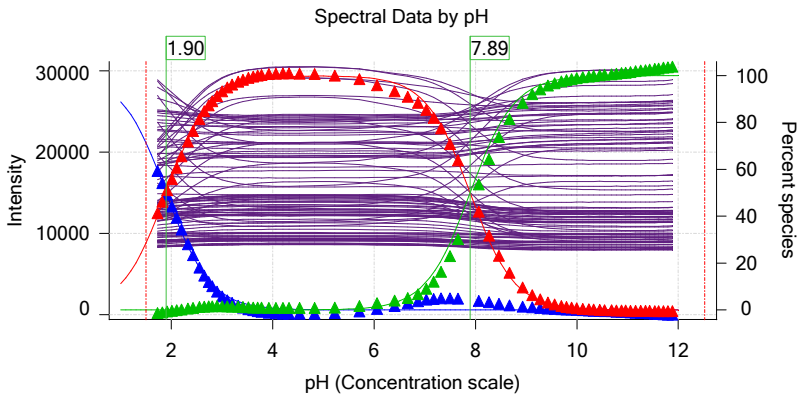
| Setting | Value | Original Value | Date/Time changed | Imported from |
|---|---|---|---|---|
| Buffer in use | Yes | | | |
| Buffer type | Phosphate Buffer | | | |
| ***Assay Medium*** | | | | |
| Volume of buffer introduced | 0.025000 mL | | | |
| Add buffer manually | Manual | | | |

## Graphs



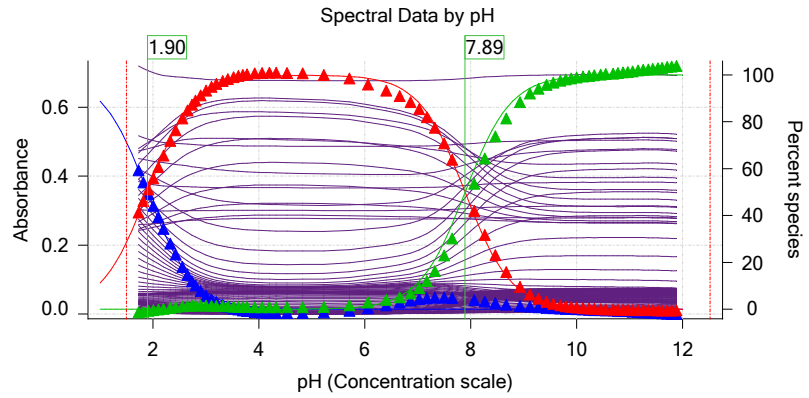



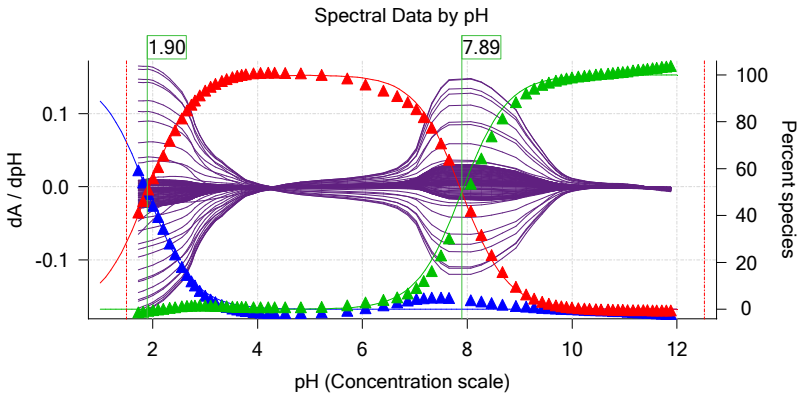



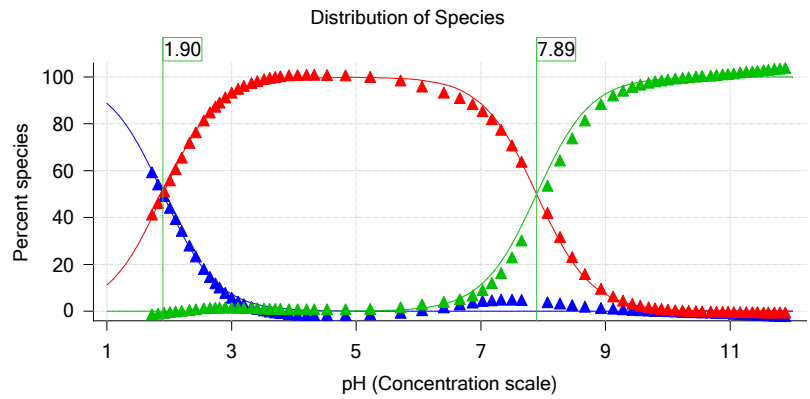
Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

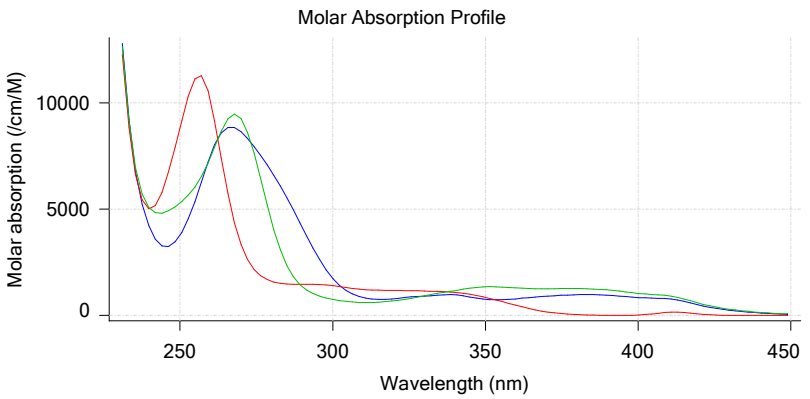
Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

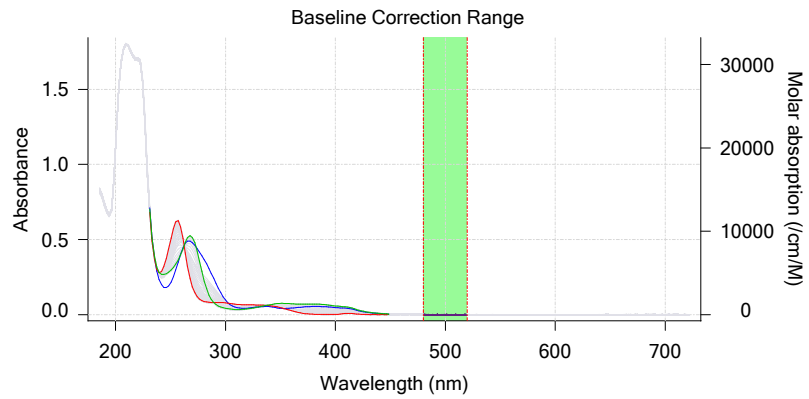
## Graphs (continued)

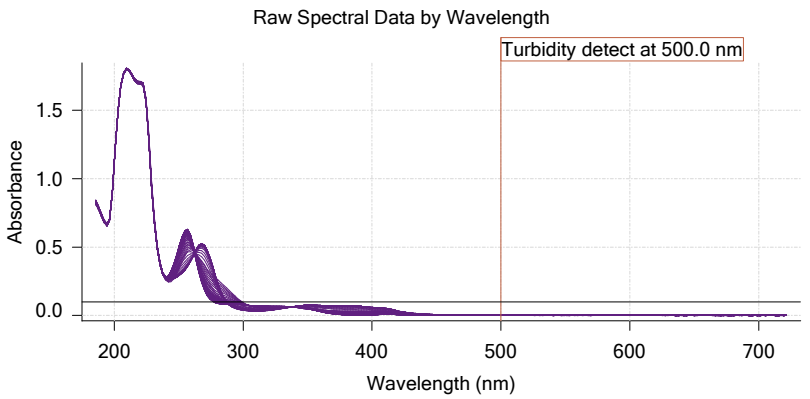



## Assay Model

| Settings | Value | Date/Time changed | Imported from |
|---|---|---|---|
| Sample name | D07 | 9/29/2017 6:39:44 PM | User entered value |
| Sample by | Volume | | Default value |
| Sample volume | 0.0040 mL | 10/6/2017 6:08:56 PM | User entered value |
| Solvent | DMSO | | Default value |
| Sample concentration | 0.032500 M | 10/2/2017 12:59:06 PM | User entered value |
| Solubility | Unknown | | Default value |
| Molecular weight | 396.95 | 9/29/2017 6:39:58 PM | User entered value |
| Individual pKa ionic environments | No | | Default value |
| Number of pKas | 2 | 9/29/2017 6:39:44 PM | User entered value |
| Sample is a | Ampholyte | 9/29/2017 6:39:44 PM | User entered value |
| pKa 1 | 2.43 | 9/29/2017 6:39:44 PM | User entered value |
| Type | Base | 9/29/2017 6:39:44 PM | User entered value |
| pKa 2 | 7.37 | 9/29/2017 6:39:44 PM | User entered value |
| Type | Acid | 9/29/2017 6:39:44 PM | User entered value |

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

## Assay Model (continued)

| Settings | Value | Date/Time changed | Imported from |
|---|---|---|---|
| logp (XH2 +) | -10.00 | | Default value |
| logP (neutral XH) | -10.00 | 9/29/2017 6:39:44 PM | User entered value |
| logP (X -) | -10.00 | | Default value |

## Events

| Time | Event | Water | Acid | Base | Methanol | Buffer | pH | dpH/dt | pH R-squar |
|---|---|---|---|---|---|---|---|---|---|
| 3:34.6 | Dark spectrum | | | | | | | | |
| 3:36.0 | Reference spectrum | | | | | | | | |
| 4:03.7 | Volume reset due to vial change | | | | | | | | |
| 5:34.5 | Initial pH = 8.37 | | | | | | | | |
| 6:34.1 | Data point 4 | 0.15005 mL | 0.07237 mL | 0.00000 mL | 1.34995 mL | 0.02500 mL | 1.962 | -0.00317 | 0.25369 |
| 7:02.6 | Data point 5 | 0.15005 mL | 0.07237 mL | 0.01472 mL | 1.34995 mL | 0.02500 mL | 2.065 | 0.01126 | 0.32959 |
| 7:19.5 | Data point 6 | 0.15005 mL | 0.07237 mL | 0.02686 mL | 1.34995 mL | 0.02500 mL | 2.176 | -0.00084 | 0.02202 |
| 7:36.2 | Data point 7 | 0.15005 mL | 0.07237 mL | 0.03652 mL | 1.34995 mL | 0.02500 mL | 2.286 | 0.00238 | 0.15010 |
| 7:53.0 | Data point 8 | 0.15005 mL | 0.07237 mL | 0.04405 mL | 1.34995 mL | 0.02500 mL | 2.400 | 0.00446 | 0.59254 |
| 8:09.7 | Data point 9 | 0.15005 mL | 0.07237 mL | 0.04988 mL | 1.34995 mL | 0.02500 mL | 2.499 | 0.00544 | 0.32949 |
| 8:26.3 | Data point 10 | 0.15005 mL | 0.07237 mL | 0.05456 mL | 1.34995 mL | 0.02500 mL | 2.621 | 0.00918 | 0.76769 |
| 8:58.5 | Data point 11 | 0.15005 mL | 0.07237 mL | 0.05903 mL | 1.34995 mL | 0.02500 mL | 2.748 | 0.00811 | 0.83437 |
| 9:20.3 | Data point 12 | 0.15005 mL | 0.07237 mL | 0.06096 mL | 1.34995 mL | 0.02500 mL | 2.840 | 0.00400 | 0.55029 |
| 9:47.1 | Data point 13 | 0.15005 mL | 0.07237 mL | 0.06286 mL | 1.34995 mL | 0.02500 mL | 2.937 | 0.00510 | 0.63912 |
| 10:03.7 | Data point 14 | 0.15005 mL | 0.07237 mL | 0.06458 mL | 1.34995 mL | 0.02500 mL | 3.048 | 0.00318 | 0.31187 |
| 10:20.4 | Data point 15 | 0.15005 mL | 0.07237 mL | 0.06592 mL | 1.34995 mL | 0.02500 mL | 3.151 | 0.00762 | 0.65884 |
| 10:36.9 | Data point 16 | 0.15005 mL | 0.07237 mL | 0.06698 mL | 1.34995 mL | 0.02500 mL | 3.246 | 0.00954 | 0.86684 |
| 10:53.5 | Data point 17 | 0.15005 mL | 0.07237 mL | 0.06783 mL | 1.34995 mL | 0.02500 mL | 3.288 | 0.01355 | 0.91245 |
| 11:25.5 | Data point 18 | 0.15005 mL | 0.07237 mL | 0.06872 mL | 1.34995 mL | 0.02500 mL | 3.391 | 0.01638 | 0.94484 |
| 11:52.3 | Data point 19 | 0.15005 mL | 0.07237 mL | 0.06933 mL | 1.34995 mL | 0.02500 mL | 3.512 | 0.02210 | 0.97013 |
| 12:08.9 | Data point 20 | 0.15005 mL | 0.07237 mL | 0.06978 mL | 1.34995 mL | 0.02500 mL | 3.647 | 0.02941 | 0.98104 |
| 12:30.6 | Data point 21 | 0.15005 mL | 0.07237 mL | 0.07037 mL | 1.34995 mL | 0.02500 mL | 3.911 | 0.05472 | 0.98729 |
| 12:52.3 | Data point 22 | 0.15005 mL | 0.07237 mL | 0.07070 mL | 1.34995 mL | 0.02500 mL | 4.105 | 0.07329 | 0.98190 |
| 13:14.0 | Data point 23 | 0.15005 mL | 0.07237 mL | 0.07088 mL | 1.34995 mL | 0.02500 mL | 4.220 | 0.09781 | 0.99184 |
| 13:36.5 | Data point 24 | 0.15005 mL | 0.07237 mL | 0.07103 mL | 1.34995 mL | 0.02500 mL | 4.363 | 0.09852 | 0.98299 |
| 14:07.9 | Data point 25 | 0.15005 mL | 0.07237 mL | 0.07114 mL | 1.34995 mL | 0.02500 mL | 4.530 | 0.10026 | 0.98953 |
| 14:49.2 | Data point 26 | 0.15005 mL | 0.07237 mL | 0.07124 mL | 1.34995 mL | 0.02500 mL | 4.755 | 0.09606 | 0.95170 |
| 15:43.9 | Data point 27 | 0.15005 mL | 0.07237 mL | 0.07131 mL | 1.34995 mL | 0.02500 mL | 5.032 | 0.10080 | 0.99573 |
| 16:59.3 | Data point 28 | 0.15005 mL | 0.07237 mL | 0.07138 mL | 1.34995 mL | 0.02500 mL | 5.609 | 0.19851 | 0.99794 |
| 18:11.0 | Data point 29 | 0.15005 mL | 0.07237 mL | 0.07143 mL | 1.34995 mL | 0.02500 mL | 6.233 | 0.25243 | 0.99796 |
| 19:22.7 | Data point 30 | 0.15005 mL | 0.07237 mL | 0.07147 mL | 1.34995 mL | 0.02500 mL | 6.702 | 0.09218 | 0.90876 |
| 20:31.9 | Data point 31 | 0.15005 mL | 0.07237 mL | 0.07154 mL | 1.34995 mL | 0.02500 mL | 7.014 | 0.09806 | 0.98464 |
| 21:39.2 | Data point 32 | 0.15005 mL | 0.07237 mL | 0.07161 mL | 1.34995 mL | 0.02500 mL | 7.273 | 0.09965 | 0.99156 |
| 22:28.0 | Data point 33 | 0.15005 mL | 0.07237 mL | 0.07168 mL | 1.34995 mL | 0.02500 mL | 7.427 | 0.09774 | 0.98478 |
| 23:08.3 | Data point 34 | 0.15005 mL | 0.07237 mL | 0.07175 mL | 1.34995 mL | 0.02500 mL | 7.588 | 0.10115 | 0.99721 |
| 23:48.1 | Data point 35 | 0.15005 mL | 0.07237 mL | 0.07183 mL | 1.34995 mL | 0.02500 mL | 7.726 | 0.09814 | 0.98887 |
| 24:32.0 | Data point 36 | 0.15005 mL | 0.07237 mL | 0.07192 mL | 1.34995 mL | 0.02500 mL | 7.890 | 0.09673 | 0.98571 |
| 25:15.4 | Data point 37 | 0.15005 mL | 0.07237 mL | 0.07201 mL | 1.34995 mL | 0.02500 mL | 8.064 | 0.10002 | 0.99100 |
| 25:59.3 | Data point 38 | 0.15005 mL | 0.07237 mL | 0.07211 mL | 1.34995 mL | 0.02500 mL | 8.242 | 0.09908 | 0.99608 |
| 26:43.6 | Data point 39 | 0.15005 mL | 0.07237 mL | 0.07220 mL | 1.34995 mL | 0.02500 mL | 8.420 | 0.09965 | 0.98377 |
| 27:29.5 | Data point 40 | 0.15005 mL | 0.07237 mL | 0.07230 mL | 1.34995 mL | 0.02500 mL | 8.602 | 0.09934 | 0.99251 |
| 28:12.9 | Data point 41 | 0.15005 mL | 0.07237 mL | 0.07239 mL | 1.34995 mL | 0.02500 mL | 8.812 | 0.09587 | 0.94273 |
| 28:58.0 | Data point 42 | 0.15005 mL | 0.07237 mL | 0.07248 mL | 1.34995 mL | 0.02500 mL | 9.041 | 0.09908 | 0.97329 |
| 29:41.2 | Data point 43 | 0.15005 mL | 0.07237 mL | 0.07255 mL | 1.34995 mL | 0.02500 mL | 9.196 | 0.09414 | 0.96176 |
| 30:19.5 | Data point 44 | 0.15005 mL | 0.07237 mL | 0.07262 mL | 1.34995 mL | 0.02500 mL | 9.377 | 0.09721 | 0.98050 |
| 30:57.8 | Data point 45 | 0.15005 mL | 0.07237 mL | 0.07270 mL | 1.34995 mL | 0.02500 mL | 9.506 | 0.09828 | 0.96689 |
| 31:30.1 | Data point 46 | 0.15005 mL | 0.07237 mL | 0.07277 mL | 1.34995 mL | 0.02500 mL | 9.658 | 0.09564 | 0.95662 |
| 32:05.5 | Data point 47 | 0.15005 mL | 0.07237 mL | 0.07286 mL | 1.34995 mL | 0.02500 mL | 9.803 | 0.09391 | 0.96750 |
| 32:35.8 | Data point 48 | 0.15005 mL | 0.07237 mL | 0.07295 mL | 1.34995 mL | 0.02500 mL | 9.939 | 0.09720 | 0.98468 |
| 33:01.1 | Data point 49 | 0.15005 mL | 0.07237 mL | 0.07305 mL | 1.34995 mL | 0.02500 mL | 10.043 | 0.09565 | 0.94953 |

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

## Events (continued)

| Time | Event | Water | Acid | Base | Methanol | Buffer | pH | dpH/dt | pH R-squared | pH S |
|---|---|---|---|---|---|---|---|---|---|---|
| 33:27.9 | Data point 50 | 0.15005 mL | 0.07237 mL | 0.07317 mL | 1.34995 mL | 0.02500 mL | 10.166 | 0.07720 | 0.98213 | 0. |
| 33:54.6 | Data point 51 | 0.15005 mL | 0.07237 mL | 0.07331 mL | 1.34995 mL | 0.02500 mL | 10.280 | 0.05739 | 0.97585 | 0. |
| 34:16.4 | Data point 52 | 0.15005 mL | 0.07237 mL | 0.07347 mL | 1.34995 mL | 0.02500 mL | 10.394 | 0.04054 | 0.97814 | 0. |
| 34:38.1 | Data point 53 | 0.15005 mL | 0.07237 mL | 0.07366 mL | 1.34995 mL | 0.02500 mL | 10.492 | 0.03080 | 0.96824 | 0. |
| 35:04.7 | Data point 54 | 0.15005 mL | 0.07237 mL | 0.07389 mL | 1.34995 mL | 0.02500 mL | 10.591 | 0.02015 | 0.92835 | 0. |
| 35:26.3 | Data point 55 | 0.15005 mL | 0.07237 mL | 0.07418 mL | 1.34995 mL | 0.02500 mL | 10.695 | 0.01433 | 0.92400 | 0. |
| 35:48.0 | Data point 56 | 0.15005 mL | 0.07237 mL | 0.07455 mL | 1.34995 mL | 0.02500 mL | 10.807 | 0.00595 | 0.60447 | 0. |
| 36:09.7 | Data point 57 | 0.15005 mL | 0.07237 mL | 0.07502 mL | 1.34995 mL | 0.02500 mL | 10.907 | 0.00411 | 0.41576 | 0. |
| 36:31.4 | Data point 58 | 0.15005 mL | 0.07237 mL | 0.07559 mL | 1.34995 mL | 0.02500 mL | 10.999 | 0.00111 | 0.04235 | 0. |
| 36:58.3 | Data point 59 | 0.15005 mL | 0.07237 mL | 0.07700 mL | 1.34995 mL | 0.02500 mL | 11.146 | 0.00306 | 0.32740 | 0. |
| 37:30.1 | Data point 60 | 0.15005 mL | 0.07237 mL | 0.07820 mL | 1.34995 mL | 0.02500 mL | 11.261 | -0.00453 | 0.67584 | 0. |
| 37:57.0 | Data point 61 | 0.15005 mL | 0.07237 mL | 0.07923 mL | 1.34995 mL | 0.02500 mL | 11.353 | -0.00467 | 0.63841 | 0. |
| 38:13.5 | Data point 62 | 0.15005 mL | 0.07237 mL | 0.08062 mL | 1.34995 mL | 0.02500 mL | 11.464 | -0.00235 | 0.33895 | 0. |
| 38:30.2 | Data point 63 | 0.15005 mL | 0.07237 mL | 0.08241 mL | 1.34995 mL | 0.02500 mL | 11.557 | -0.00365 | 0.56650 | 0. |
| 38:46.8 | Data point 64 | 0.15005 mL | 0.07237 mL | 0.08462 mL | 1.34995 mL | 0.02500 mL | 11.645 | -0.00534 | 0.57589 | 0. |
| 39:03.4 | Data point 65 | 0.15005 mL | 0.07237 mL | 0.08735 mL | 1.34995 mL | 0.02500 mL | 11.722 | -0.00389 | 0.24919 | 0. |
| 39:30.4 | Data point 66 | 0.15005 mL | 0.07237 mL | 0.09052 mL | 1.34995 mL | 0.02500 mL | 11.818 | -0.00314 | 0.48821 | 0. |
| 39:47.0 | Data point 67 | 0.15005 mL | 0.07237 mL | 0.09461 mL | 1.34995 mL | 0.02500 mL | 11.904 | -0.00339 | 0.33145 | 0. |
| 40:03.7 | Data point 68 | 0.15005 mL | 0.07237 mL | 0.09965 mL | 1.34995 mL | 0.02500 mL | 11.993 | -0.00341 | 0.11203 | 0. |
| 40:20.4 | Data point 69 | 0.15005 mL | 0.07237 mL | 0.10303 mL | 1.34995 mL | 0.02500 mL | 12.042 | -0.00654 | 0.68141 | 0. |
| 41:55.3 | Reference spectrum | | | | | | | | | |
| 42:57.9 | Data point 71 | 0.22001 mL | 0.17237 mL | 0.10306 mL | 1.34995 mL | 0.02500 mL | 1.995 | -0.03620 | 0.90558 | 0. |
| 43:25.3 | Data point 72 | 0.22001 mL | 0.17237 mL | 0.11729 mL | 1.34995 mL | 0.02500 mL | 2.097 | 0.01250 | 0.84397 | 0. |
| 43:42.1 | Data point 73 | 0.22001 mL | 0.17237 mL | 0.12989 mL | 1.34995 mL | 0.02500 mL | 2.221 | 0.01481 | 0.89996 | 0. |
| 44:04.1 | Data point 74 | 0.22001 mL | 0.17237 mL | 0.13791 mL | 1.34995 mL | 0.02500 mL | 2.319 | 0.00201 | 0.04028 | 0. |
| 44:31.3 | Data point 75 | 0.22001 mL | 0.17237 mL | 0.14473 mL | 1.34995 mL | 0.02500 mL | 2.419 | 0.00710 | 0.45161 | 0. |
| 44:48.1 | Data point 76 | 0.22001 mL | 0.17237 mL | 0.15080 mL | 1.34995 mL | 0.02500 mL | 2.543 | 0.01931 | 0.94787 | 0. |
| 45:15.3 | Data point 77 | 0.22001 mL | 0.17237 mL | 0.15503 mL | 1.34995 mL | 0.02500 mL | 2.645 | 0.01186 | 0.93909 | 0. |
| 45:31.9 | Data point 78 | 0.22001 mL | 0.17237 mL | 0.15865 mL | 1.34995 mL | 0.02500 mL | 2.768 | 0.00845 | 0.75201 | 0. |
| 45:58.9 | Data point 79 | 0.22001 mL | 0.17237 mL | 0.16124 mL | 1.34995 mL | 0.02500 mL | 2.860 | 0.01125 | 0.91798 | 0. |
| 46:15.4 | Data point 80 | 0.22001 mL | 0.17237 mL | 0.16345 mL | 1.34995 mL | 0.02500 mL | 2.964 | 0.00515 | 0.52568 | 0. |
| 46:32.0 | Data point 81 | 0.22001 mL | 0.17237 mL | 0.16522 mL | 1.34995 mL | 0.02500 mL | 3.092 | 0.01000 | 0.85148 | 0. |
| 46:58.8 | Data point 82 | 0.22001 mL | 0.17237 mL | 0.16637 mL | 1.34995 mL | 0.02500 mL | 3.189 | 0.01480 | 0.89927 | 0. |
| 47:15.4 | Data point 83 | 0.22001 mL | 0.17237 mL | 0.16740 mL | 1.34995 mL | 0.02500 mL | 3.311 | 0.01299 | 0.91139 | 0. |
| 47:42.0 | Data point 84 | 0.22001 mL | 0.17237 mL | 0.16820 mL | 1.34995 mL | 0.02500 mL | 3.404 | 0.01010 | 0.84899 | 0. |
| 47:58.8 | Data point 85 | 0.22001 mL | 0.17237 mL | 0.16884 mL | 1.34995 mL | 0.02500 mL | 3.507 | 0.01955 | 0.95806 | 0. |
| 48:15.3 | Data point 86 | 0.22001 mL | 0.17237 mL | 0.16933 mL | 1.34995 mL | 0.02500 mL | 3.603 | 0.01623 | 0.95327 | 0. |
| 48:31.8 | Data point 87 | 0.22001 mL | 0.17237 mL | 0.16973 mL | 1.34995 mL | 0.02500 mL | 3.698 | 0.02643 | 0.98573 | 0. |
| 48:48.4 | Data point 88 | 0.22001 mL | 0.17237 mL | 0.17004 mL | 1.34995 mL | 0.02500 mL | 3.787 | 0.03247 | 0.98103 | 0. |
| 49:04.9 | Data point 89 | 0.22001 mL | 0.17237 mL | 0.17030 mL | 1.34995 mL | 0.02500 mL | 3.872 | 0.04010 | 0.97518 | 0. |
| 49:26.6 | Data point 90 | 0.22001 mL | 0.17237 mL | 0.17067 mL | 1.34995 mL | 0.02500 mL | 4.050 | 0.05652 | 0.99131 | 0. |
| 49:48.3 | Data point 91 | 0.22001 mL | 0.17237 mL | 0.17093 mL | 1.34995 mL | 0.02500 mL | 4.194 | 0.08109 | 0.99149 | 0. |
| 50:14.9 | Data point 92 | 0.22001 mL | 0.17237 mL | 0.17114 mL | 1.34995 mL | 0.02500 mL | 4.303 | 0.08356 | 0.98509 | 0. |
| 50:36.8 | Data point 93 | 0.22001 mL | 0.17237 mL | 0.17128 mL | 1.34995 mL | 0.02500 mL | 4.420 | 0.10028 | 0.99587 | 0. |
| 51:08.6 | Data point 94 | 0.22001 mL | 0.17237 mL | 0.17140 mL | 1.34995 mL | 0.02500 mL | 4.590 | 0.09894 | 0.99362 | 0. |
| 51:48.3 | Data point 95 | 0.22001 mL | 0.17237 mL | 0.17150 mL | 1.34995 mL | 0.02500 mL | 4.776 | 0.10106 | 0.99749 | 0. |
| 52:36.7 | Data point 96 | 0.22001 mL | 0.17237 mL | 0.17159 mL | 1.34995 mL | 0.02500 mL | 5.055 | 0.09968 | 0.98619 | 0. |
| 53:42.5 | Data point 97 | 0.22001 mL | 0.17237 mL | 0.17166 mL | 1.34995 mL | 0.02500 mL | 5.430 | 0.13278 | 0.99578 | 0. |
| 54:59.2 | Data point 98 | 0.22001 mL | 0.17237 mL | 0.17173 mL | 1.34995 mL | 0.02500 mL | 5.878 | 0.13190 | 0.99307 | 0. |
| 56:15.9 | Data point 99 | 0.22001 mL | 0.17237 mL | 0.17180 mL | 1.34995 mL | 0.02500 mL | 6.297 | 0.11466 | 0.99478 | 0. |
| 57:32.6 | Data point 100 | 0.22001 mL | 0.17237 mL | 0.17187 mL | 1.34995 mL | 0.02500 mL | 6.618 | 0.09887 | 0.99142 | 0. |
| 58:33.4 | Data point 101 | 0.22001 mL | 0.17237 mL | 0.17194 mL | 1.34995 mL | 0.02500 mL | 6.876 | 0.10094 | 0.99357 | 0. |
| 59:31.6 | Data point 102 | 0.22001 mL | 0.17237 mL | 0.17201 mL | 1.34995 mL | 0.02500 mL | 7.088 | 0.09921 | 0.99227 | 0. |
| 1:00:17.9 | Data point 103 | 0.22001 mL | 0.17237 mL | 0.17211 mL | 1.34995 mL | 0.02500 mL | 7.301 | 0.09330 | 0.95086 | 0. |
| 1:00:57.2 | Data point 104 | 0.22001 mL | 0.17237 mL | 0.17218 mL | 1.34995 mL | 0.02500 mL | 7.439 | 0.10014 | 0.99140 | 0. |
| 1:01:38.9 | Data point 105 | 0.22001 mL | 0.17237 mL | 0.17227 mL | 1.34995 mL | 0.02500 mL | 7.606 | 0.09813 | 0.98979 | 0. |
| 1:02:21.9 | Data point 106 | 0.22001 mL | 0.17237 mL | 0.17244 mL | 1.34995 mL | 0.02500 mL | 7.770 | 0.09790 | 0.99627 | 0. |

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

## Events (continued)

| Time | Event | Water | Acid | Base | Methanol | Buffer | pH | dpH/dt | pH R-squared | pH SD |
|---|---|---|---|---|---|---|---|---|---|---|
| 1:03:03.7 | Data point 107 | 0.22001 mL | 0.17237 mL | 0.17253 mL | 1.34995 mL | 0.02500 mL | 7.949 | 0.09742 | 0.98928 | 0. |
| 1:03:46.6 | Data point 108 | 0.22001 mL | 0.17237 mL | 0.17263 mL | 1.34995 mL | 0.02500 mL | 8.119 | 0.09898 | 0.98251 | 0. |
| 1:04:21.9 | Data point 109 | 0.22001 mL | 0.17237 mL | 0.17269 mL | 1.34995 mL | 0.02500 mL | 8.255 | 0.09851 | 0.99305 | 0. |
| 1:05:04.4 | Data point 110 | 0.22001 mL | 0.17237 mL | 0.17279 mL | 1.34995 mL | 0.02500 mL | 8.458 | 0.09964 | 0.99038 | 0. |
| 1:05:52.4 | Data point 111 | 0.22001 mL | 0.17237 mL | 0.17288 mL | 1.34995 mL | 0.02500 mL | 8.677 | 0.09820 | 0.97334 | 0. |
| 1:06:36.2 | Data point 112 | 0.22001 mL | 0.17237 mL | 0.17295 mL | 1.34995 mL | 0.02500 mL | 8.865 | 0.09898 | 0.98259 | 0. |
| 1:07:16.9 | Data point 113 | 0.22001 mL | 0.17237 mL | 0.17302 mL | 1.34995 mL | 0.02500 mL | 9.096 | 0.09553 | 0.96258 | 0. |
| 1:08:00.8 | Data point 114 | 0.22001 mL | 0.17237 mL | 0.17310 mL | 1.34995 mL | 0.02500 mL | 9.317 | 0.10068 | 0.98735 | 0. |
| 1:08:42.0 | Data point 115 | 0.22001 mL | 0.17237 mL | 0.17317 mL | 1.34995 mL | 0.02500 mL | 9.492 | 0.09603 | 0.96675 | 0. |
| 1:09:17.1 | Data point 116 | 0.22001 mL | 0.17237 mL | 0.17324 mL | 1.34995 mL | 0.02500 mL | 9.632 | 0.10064 | 0.98729 | 0. |
| 1:09:49.8 | Data point 117 | 0.22001 mL | 0.17237 mL | 0.17331 mL | 1.34995 mL | 0.02500 mL | 9.751 | 0.09893 | 0.98396 | 0. |
| 1:10:19.7 | Data point 118 | 0.22001 mL | 0.17237 mL | 0.17340 mL | 1.34995 mL | 0.02500 mL | 9.884 | 0.09891 | 0.98270 | 0. |
| 1:10:43.9 | Data point 119 | 0.22001 mL | 0.17237 mL | 0.17350 mL | 1.34995 mL | 0.02500 mL | 9.994 | 0.09691 | 0.96615 | 0. |
| 1:11:06.1 | Data point 120 | 0.22001 mL | 0.17237 mL | 0.17359 mL | 1.34995 mL | 0.02500 mL | 10.102 | 0.07482 | 0.98156 | 0. |
| 1:11:22.7 | Data point 121 | 0.22001 mL | 0.17237 mL | 0.17368 mL | 1.34995 mL | 0.02500 mL | 10.216 | 0.05591 | 0.97990 | 0. |
| 1:11:39.1 | Data point 122 | 0.22001 mL | 0.17237 mL | 0.17380 mL | 1.34995 mL | 0.02500 mL | 10.319 | 0.04210 | 0.96595 | 0. |
| 1:11:55.7 | Data point 123 | 0.22001 mL | 0.17237 mL | 0.17397 mL | 1.34995 mL | 0.02500 mL | 10.437 | 0.01994 | 0.96637 | 0. |
| 1:12:17.4 | Data point 124 | 0.22001 mL | 0.17237 mL | 0.17422 mL | 1.34995 mL | 0.02500 mL | 10.573 | 0.00987 | 0.87943 | 0. |
| 1:12:44.2 | Data point 125 | 0.22001 mL | 0.17237 mL | 0.17453 mL | 1.34995 mL | 0.02500 mL | 10.665 | 0.00483 | 0.45081 | 0. |
| 1:13:00.8 | Data point 126 | 0.22001 mL | 0.17237 mL | 0.17488 mL | 1.34995 mL | 0.02500 mL | 10.783 | 0.00177 | 0.11866 | 0. |
| 1:13:32.6 | Data point 127 | 0.22001 mL | 0.17237 mL | 0.17549 mL | 1.34995 mL | 0.02500 mL | 10.893 | -0.00141 | 0.09861 | 0. |
| 1:13:59.5 | Data point 128 | 0.22001 mL | 0.17237 mL | 0.17608 mL | 1.34995 mL | 0.02500 mL | 10.983 | -0.00165 | 0.17162 | 0. |
| 1:14:16.0 | Data point 129 | 0.22001 mL | 0.17237 mL | 0.17681 mL | 1.34995 mL | 0.02500 mL | 11.080 | -0.00431 | 0.51872 | 0. |
| 1:14:32.6 | Data point 130 | 0.22001 mL | 0.17237 mL | 0.17773 mL | 1.34995 mL | 0.02500 mL | 11.164 | -0.00259 | 0.37464 | 0. |
| 1:14:59.4 | Data point 131 | 0.22001 mL | 0.17237 mL | 0.17907 mL | 1.34995 mL | 0.02500 mL | 11.256 | -0.00503 | 0.69652 | 0. |
| 1:15:26.4 | Data point 132 | 0.22001 mL | 0.17237 mL | 0.18097 mL | 1.34995 mL | 0.02500 mL | 11.352 | -0.00558 | 0.60743 | 0. |
| 1:15:53.4 | Data point 133 | 0.22001 mL | 0.17237 mL | 0.18288 mL | 1.34995 mL | 0.02500 mL | 11.446 | -0.00454 | 0.68900 | 0. |
| 1:16:10.0 | Data point 134 | 0.22001 mL | 0.17237 mL | 0.18502 mL | 1.34995 mL | 0.02500 mL | 11.544 | -0.00521 | 0.54566 | 0. |
| 1:16:26.7 | Data point 135 | 0.22001 mL | 0.17237 mL | 0.18770 mL | 1.34995 mL | 0.02500 mL | 11.629 | -0.00375 | 0.36915 | 0. |
| 1:16:53.9 | Data point 136 | 0.22001 mL | 0.17237 mL | 0.19156 mL | 1.34995 mL | 0.02500 mL | 11.723 | -0.00627 | 0.69405 | 0. |
| 1:17:20.7 | Data point 137 | 0.22001 mL | 0.17237 mL | 0.19591 mL | 1.34995 mL | 0.02500 mL | 11.818 | -0.00407 | 0.56951 | 0. |
| 1:17:37.4 | Data point 138 | 0.22001 mL | 0.17237 mL | 0.20103 mL | 1.34995 mL | 0.02500 mL | 11.895 | -0.00193 | 0.24057 | 0. |
| 1:18:04.6 | Data point 139 | 0.22001 mL | 0.17237 mL | 0.20783 mL | 1.34995 mL | 0.02500 mL | 11.989 | -0.00263 | 0.47878 | 0. |
| 1:18:21.3 | Data point 140 | 0.22001 mL | 0.17237 mL | 0.21235 mL | 1.34995 mL | 0.02500 mL | 12.039 | -0.00584 | 0.60456 | 0. |
| 1:20:03.4 | Reference spectrum | | | | | | | | | |
| 1:21:23.7 | Data point 142 | 0.39005 mL | 0.29857 mL | 0.21237 mL | 1.34995 mL | 0.02500 mL | 1.997 | -0.05261 | 0.96918 | 0. |
| 1:21:45.8 | Data point 143 | 0.39005 mL | 0.29857 mL | 0.22683 mL | 1.34995 mL | 0.02500 mL | 2.091 | 0.01063 | 0.84683 | 0. |
| 1:22:07.9 | Data point 144 | 0.39005 mL | 0.29857 mL | 0.23798 mL | 1.34995 mL | 0.02500 mL | 2.185 | 0.00938 | 0.42022 | 0. |
| 1:22:29.9 | Data point 145 | 0.39005 mL | 0.29857 mL | 0.24699 mL | 1.34995 mL | 0.02500 mL | 2.276 | 0.00648 | 0.27027 | 0. |
| 1:22:51.9 | Data point 146 | 0.39005 mL | 0.29857 mL | 0.25421 mL | 1.34995 mL | 0.02500 mL | 2.369 | 0.01077 | 0.81160 | 0. |
| 1:23:18.8 | Data point 147 | 0.39005 mL | 0.29857 mL | 0.26065 mL | 1.34995 mL | 0.02500 mL | 2.466 | 0.00949 | 0.87743 | 0. |
| 1:23:35.4 | Data point 148 | 0.39005 mL | 0.29857 mL | 0.26663 mL | 1.34995 mL | 0.02500 mL | 2.588 | 0.01036 | 0.88790 | 0. |
| 1:24:02.4 | Data point 149 | 0.39005 mL | 0.29857 mL | 0.27081 mL | 1.34995 mL | 0.02500 mL | 2.688 | 0.00637 | 0.72041 | 0. |
| 1:24:19.1 | Data point 150 | 0.39005 mL | 0.29857 mL | 0.27441 mL | 1.34995 mL | 0.02500 mL | 2.813 | 0.00903 | 0.75955 | 0. |
| 1:24:46.1 | Data point 151 | 0.39005 mL | 0.29857 mL | 0.27693 mL | 1.34995 mL | 0.02500 mL | 2.909 | 0.00426 | 0.47875 | 0. |
| 1:25:18.5 | Data point 152 | 0.39005 mL | 0.29857 mL | 0.27909 mL | 1.34995 mL | 0.02500 mL | 2.996 | 0.00319 | 0.38398 | 0. |
| 1:25:35.1 | Data point 153 | 0.39005 mL | 0.29857 mL | 0.28086 mL | 1.34995 mL | 0.02500 mL | 3.060 | 0.00886 | 0.78262 | 0. |
| 1:25:56.8 | Data point 154 | 0.39005 mL | 0.29857 mL | 0.28215 mL | 1.34995 mL | 0.02500 mL | 3.155 | 0.01045 | 0.87755 | 0. |
| 1:26:23.7 | Data point 155 | 0.39005 mL | 0.29857 mL | 0.28309 mL | 1.34995 mL | 0.02500 mL | 3.257 | 0.00522 | 0.63048 | 0. |
| 1:26:50.6 | Data point 156 | 0.39005 mL | 0.29857 mL | 0.28387 mL | 1.34995 mL | 0.02500 mL | 3.356 | 0.01107 | 0.93400 | 0. |
| 1:27:17.6 | Data point 157 | 0.39005 mL | 0.29857 mL | 0.28455 mL | 1.34995 mL | 0.02500 mL | 3.450 | 0.01542 | 0.86338 | 0. |
| 1:27:34.1 | Data point 158 | 0.39005 mL | 0.29857 mL | 0.28516 mL | 1.34995 mL | 0.02500 mL | 3.567 | 0.01197 | 0.90756 | 0. |
| 1:28:01.0 | Data point 159 | 0.39005 mL | 0.29857 mL | 0.28565 mL | 1.34995 mL | 0.02500 mL | 3.661 | 0.01862 | 0.95448 | 0. |
| 1:28:17.5 | Data point 160 | 0.39005 mL | 0.29857 mL | 0.28603 mL | 1.34995 mL | 0.02500 mL | 3.768 | 0.02292 | 0.97802 | 0. |
| 1:28:34.1 | Data point 161 | 0.39005 mL | 0.29857 mL | 0.28631 mL | 1.34995 mL | 0.02500 mL | 3.859 | 0.02973 | 0.97889 | 0. |
| 1:28:50.6 | Data point 162 | 0.39005 mL | 0.29857 mL | 0.28655 mL | 1.34995 mL | 0.02500 mL | 3.945 | 0.03108 | 0.96810 | 0. |
| 1:29:07.1 | Data point 163 | 0.39005 mL | 0.29857 mL | 0.28674 mL | 1.34995 mL | 0.02500 mL | 4.024 | 0.03775 | 0.97611 | 0. |

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

## Events (continued)

| Time | Event | Water | Acid | Base | Methanol | Buffer | pH | dpH/dt | pH R-squared | pH SD |
|---|---|---|---|---|---|---|---|---|---|---|
| 1:29:28.8 | Data point 164 | 0.39005 mL | 0.29857 mL | 0.28697 mL | 1.34995 mL | 0.02500 mL | 4.164 | 0.05879 | 0.98975 | 0.0029 |
| 1:29:50.4 | Data point 165 | 0.39005 mL | 0.29857 mL | 0.28716 mL | 1.34995 mL | 0.02500 mL | 4.301 | 0.08405 | 0.97612 | 0.0042 |
| 1:30:17.1 | Data point 166 | 0.39005 mL | 0.29857 mL | 0.28730 mL | 1.34995 mL | 0.02500 mL | 4.440 | 0.09859 | 0.98587 | 0.0049 |
| 1:30:42.3 | Data point 167 | 0.39005 mL | 0.29857 mL | 0.28739 mL | 1.34995 mL | 0.02500 mL | 4.562 | 0.09992 | 0.98719 | 0.0049 |
| 1:31:16.6 | Data point 168 | 0.39005 mL | 0.29857 mL | 0.28749 mL | 1.34995 mL | 0.02500 mL | 4.765 | 0.09955 | 0.98099 | 0.0049 |
| 1:31:59.5 | Data point 169 | 0.39005 mL | 0.29857 mL | 0.28758 mL | 1.34995 mL | 0.02500 mL | 5.059 | 0.09922 | 0.98040 | 0.0049 |
| 1:32:54.7 | Data point 170 | 0.39005 mL | 0.29857 mL | 0.28765 mL | 1.34995 mL | 0.02500 mL | 5.452 | 0.10011 | 0.98504 | 0.0049 |
| 1:33:59.6 | Data point 171 | 0.39005 mL | 0.29857 mL | 0.28775 mL | 1.34995 mL | 0.02500 mL | 5.932 | 0.09917 | 0.99271 | 0.0049 |
| 1:35:11.5 | Data point 172 | 0.39005 mL | 0.29857 mL | 0.28782 mL | 1.34995 mL | 0.02500 mL | 6.275 | 0.09977 | 0.97803 | 0.0049 |
| 1:36:10.9 | Data point 173 | 0.39005 mL | 0.29857 mL | 0.28791 mL | 1.34995 mL | 0.02500 mL | 6.617 | 0.09856 | 0.99153 | 0.0048 |
| 1:37:00.2 | Data point 174 | 0.39005 mL | 0.29857 mL | 0.28801 mL | 1.34995 mL | 0.02500 mL | 6.870 | 0.09994 | 0.99323 | 0.0049 |
| 1:37:43.0 | Data point 175 | 0.39005 mL | 0.29857 mL | 0.28810 mL | 1.34995 mL | 0.02500 mL | 7.073 | 0.09566 | 0.98828 | 0.0047 |
| 1:38:20.5 | Data point 176 | 0.39005 mL | 0.29857 mL | 0.28822 mL | 1.34995 mL | 0.02500 mL | 7.233 | 0.09883 | 0.98534 | 0.0049 |
| 1:38:57.3 | Data point 177 | 0.39005 mL | 0.29857 mL | 0.28834 mL | 1.34995 mL | 0.02500 mL | 7.377 | 0.09790 | 0.97920 | 0.0048 |
| 1:39:34.4 | Data point 178 | 0.39005 mL | 0.29857 mL | 0.28848 mL | 1.34995 mL | 0.02500 mL | 7.524 | 0.09827 | 0.98393 | 0.0048 |
| 1:40:15.8 | Data point 179 | 0.39005 mL | 0.29857 mL | 0.28862 mL | 1.34995 mL | 0.02500 mL | 7.697 | 0.09793 | 0.98043 | 0.0048 |
| 1:40:57.3 | Data point 180 | 0.39005 mL | 0.29857 mL | 0.28876 mL | 1.34995 mL | 0.02500 mL | 7.850 | 0.09979 | 0.98171 | 0.0049 |
| 1:41:45.0 | Data point 181 | 0.39005 mL | 0.29857 mL | 0.28918 mL | 1.34995 mL | 0.02500 mL | 8.260 | 0.10001 | 0.99182 | 0.0049 |
| 1:42:26.1 | Data point 182 | 0.39005 mL | 0.29857 mL | 0.28925 mL | 1.34995 mL | 0.02500 mL | 8.458 | 0.09931 | 0.96677 | 0.0049 |
| 1:43:08.4 | Data point 183 | 0.39005 mL | 0.29857 mL | 0.28932 mL | 1.34995 mL | 0.02500 mL | 8.652 | 0.09790 | 0.97894 | 0.0048 |
| 1:43:52.1 | Data point 184 | 0.39005 mL | 0.29857 mL | 0.28939 mL | 1.34995 mL | 0.02500 mL | 8.856 | 0.09466 | 0.96836 | 0.0047 |
| 1:44:40.4 | Data point 185 | 0.39005 mL | 0.29857 mL | 0.28949 mL | 1.34995 mL | 0.02500 mL | 9.110 | 0.09498 | 0.95807 | 0.0048 |
| 1:45:28.3 | Data point 186 | 0.39005 mL | 0.29857 mL | 0.28958 mL | 1.34995 mL | 0.02500 mL | 9.300 | 0.09832 | 0.97764 | 0.0049 |
| 1:46:07.0 | Data point 187 | 0.39005 mL | 0.29857 mL | 0.28968 mL | 1.34995 mL | 0.02500 mL | 9.457 | 0.09695 | 0.96428 | 0.0048 |
| 1:46:41.9 | Data point 188 | 0.39005 mL | 0.29857 mL | 0.28977 mL | 1.34995 mL | 0.02500 mL | 9.607 | 0.10029 | 0.98383 | 0.0050 |
| 1:47:12.1 | Data point 189 | 0.39005 mL | 0.29857 mL | 0.28986 mL | 1.34995 mL | 0.02500 mL | 9.734 | 0.09666 | 0.95866 | 0.0048 |
| 1:47:40.9 | Data point 190 | 0.39005 mL | 0.29857 mL | 0.28998 mL | 1.34995 mL | 0.02500 mL | 9.864 | 0.09726 | 0.97509 | 0.0048 |
| 1:48:08.0 | Data point 191 | 0.39005 mL | 0.29857 mL | 0.29010 mL | 1.34995 mL | 0.02500 mL | 9.967 | 0.07318 | 0.97891 | 0.0036 |
| 1:48:29.6 | Data point 192 | 0.39005 mL | 0.29857 mL | 0.29024 mL | 1.34995 mL | 0.02500 mL | 10.066 | 0.04385 | 0.92217 | 0.0022 |
| 1:48:56.4 | Data point 193 | 0.39005 mL | 0.29857 mL | 0.29041 mL | 1.34995 mL | 0.02500 mL | 10.167 | 0.02883 | 0.79342 | 0.0016 |
| 1:49:17.9 | Data point 194 | 0.39005 mL | 0.29857 mL | 0.29062 mL | 1.34995 mL | 0.02500 mL | 10.286 | 0.01558 | 0.89519 | 0.0008 |
| 1:49:39.5 | Data point 195 | 0.39005 mL | 0.29857 mL | 0.29087 mL | 1.34995 mL | 0.02500 mL | 10.402 | 0.01094 | 0.82769 | 0.0005 |
| 1:50:01.2 | Data point 196 | 0.39005 mL | 0.29857 mL | 0.29116 mL | 1.34995 mL | 0.02500 mL | 10.496 | 0.00872 | 0.85603 | 0.0004 |
| 1:50:17.8 | Data point 197 | 0.39005 mL | 0.29857 mL | 0.29149 mL | 1.34995 mL | 0.02500 mL | 10.616 | 0.00055 | 0.02138 | 0.0001 |
| 1:50:39.4 | Data point 198 | 0.39005 mL | 0.29857 mL | 0.29191 mL | 1.34995 mL | 0.02500 mL | 10.711 | -0.00003 | 0.00005 | 0.0002 |
| 1:50:56.0 | Data point 199 | 0.39005 mL | 0.29857 mL | 0.29245 mL | 1.34995 mL | 0.02500 mL | 10.847 | -0.00342 | 0.31328 | 0.0003 |
| 1:51:22.7 | Data point 200 | 0.39005 mL | 0.29857 mL | 0.29318 mL | 1.34995 mL | 0.02500 mL | 10.939 | -0.00425 | 0.58470 | 0.0002 |
| 1:51:39.3 | Data point 201 | 0.39005 mL | 0.29857 mL | 0.29410 mL | 1.34995 mL | 0.02500 mL | 11.036 | -0.00829 | 0.88051 | 0.0004 |
| 1:51:55.9 | Data point 202 | 0.39005 mL | 0.29857 mL | 0.29523 mL | 1.34995 mL | 0.02500 mL | 11.121 | -0.00666 | 0.76426 | 0.0003 |
| 1:52:22.8 | Data point 203 | 0.39005 mL | 0.29857 mL | 0.29685 mL | 1.34995 mL | 0.02500 mL | 11.212 | -0.00656 | 0.75724 | 0.0003 |
| 1:52:49.8 | Data point 204 | 0.39005 mL | 0.29857 mL | 0.29946 mL | 1.34995 mL | 0.02500 mL | 11.314 | -0.00713 | 0.74880 | 0.0004 |
| 1:53:16.7 | Data point 205 | 0.39005 mL | 0.29857 mL | 0.30176 mL | 1.34995 mL | 0.02500 mL | 11.411 | -0.00690 | 0.83867 | 0.0003 |
| 1:53:33.4 | Data point 206 | 0.39005 mL | 0.29857 mL | 0.30447 mL | 1.34995 mL | 0.02500 mL | 11.506 | -0.00927 | 0.76917 | 0.0005 |
| 1:53:50.2 | Data point 207 | 0.39005 mL | 0.29857 mL | 0.30785 mL | 1.34995 mL | 0.02500 mL | 11.587 | -0.00782 | 0.83981 | 0.0004 |
| 1:54:17.1 | Data point 208 | 0.39005 mL | 0.29857 mL | 0.31235 mL | 1.34995 mL | 0.02500 mL | 11.684 | -0.00788 | 0.74468 | 0.0004 |
| 1:54:33.8 | Data point 209 | 0.39005 mL | 0.29857 mL | 0.31750 mL | 1.34995 mL | 0.02500 mL | 11.759 | -0.00891 | 0.80597 | 0.0004 |
| 1:55:00.8 | Data point 210 | 0.39005 mL | 0.29857 mL | 0.32406 mL | 1.34995 mL | 0.02500 mL | 11.853 | -0.00651 | 0.66133 | 0.0004 |
| 1:55:17.6 | Data point 211 | 0.39005 mL | 0.29857 mL | 0.33180 mL | 1.34995 mL | 0.02500 mL | 11.939 | -0.00758 | 0.91302 | 0.0003 |
| 1:55:34.4 | Data point 212 | 0.39005 mL | 0.29857 mL | 0.34137 mL | 1.34995 mL | 0.02500 mL | 12.022 | -0.00881 | 0.75425 | 0.0005 |
| 1:57:33.6 | Assay volumes | 0.64005 mL | 0.42959 mL | 0.34137 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*** | | | | |

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

## Assay Settings (continued)

| Setting | Value | Original Value | Date/Time changed | Imported from |
|---|---|---|---|---|
| Number of titrations | 3 | | | |
| Minimum pH | 2.000 | | | |
| Maximum pH | 12.000 | | | |
| pH step between points of | 0.100 | | | |
| 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 | 1.35 mL | | | |
| Cosolvent added | Automatic | | | |
| ISA water volume | 0.15 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 | 0.07 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 | | | |

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

## Assay Settings (continued)

| Setting | Value | Original Value | Date/Time changed | Imported from |
|---|---|---|---|---|
| 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 | 0.161 | 10/7/2017 2:51:21 AM | C:\Sirius_T3\17J-06018_Blank standardisation.t3r |
| Four-Plus S | 0.9927 | 10/7/2017 2:51:21 AM | C:\Sirius_T3\17J-06018_Blank standardisation.t3r |
| Four-Plus jH | 0.5 | 10/7/2017 2:51:21 AM | C:\Sirius_T3\17J-06018_Blank standardisation.t3r |
| Four-Plus jOH | -0.7 | 10/7/2017 2:51:21 AM | C:\Sirius_T3\17J-06018_Blank standardisation.t3r |
| Base concentration factor | 1.011 | 10/7/2017 2:51:21 AM | C:\Sirius_T3\KOH17I22.t3r |
| Acid concentration factor | 1.003 | 10/7/2017 2:51:21 AM | C:\Sirius_T3\17J-06018_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) | 8-18-17 | 9/26/2017 9:05:04 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 |
| Dispenser 3 | Buffer | | 8/3/2010 6:05:16 AM |
| Syringe volume | 0.5 mL | | |
| Firmware version | 1.2.1(r2) | | |
| Titrant | Phosphate Buffer | | 9/12/2017 12:32:29 PM |

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

## Instrument Settings (continued)

| Setting | Value | Batch Id | Install date |
|---|---|---|---|
| Dispenser 6 | Octanol | | 10/22/2010 11:52:43 AM |
| Syringe volume | 0.5 mL | | |
| Firmware version | 1.2.1(r2) | | |
| Titrant | Octanol | 9-14-17 | 9/14/2017 10:30:38 AM |
| Titrator | | T3TM1100153 | 3/31/2009 6:24:17 AM |
| Horizontal axis firmware version | 1.17 AI1DI2DO2 Stepper 2 | | |
| Vertical axis firmware version | 1.17 AI1DI2DO2 Stepper 2 | | |
| Chassis I/O firmware version | 1.11 AI1DI0DO4 Norgren I/O | | |
| Probe I/O firmware version | 1.1.1 | | |
| Electrode | T3 Electrode | T3E0769 | 8/15/2017 10:21:54 AM |
| E0 calibration | -9.13 mV | | 10/7/2017 2:51:45 AM |
| Filling solution | 3M KCl | KCL095 | 10/4/2017 3:50:10 PM |
| Liquids | | | |
| Wash 1 | 50% IPA:50% Water | | 10/6/2017 2:50:08 PM |
| Wash 2 | 0.5% Trition X-100 in H20 | | 10/6/2017 2:50:11 PM |
| Buffer position 1 | pH7 Wash | | 10/6/2017 2:50:17 PM |
| Buffer position 2 | pH 7 | | 10/6/2017 2:50:19 PM |
| Storage position | | | 10/6/2017 2:50:25 PM |
| Wash water | 9e+003 mL | 10-6-17 | 10/6/2017 3:04:25 PM |
| Waste | 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 | 391:10:29 | | 11/23/2010 12:22:28 PM |
| Calibrated on | 10/5/2017 10:23:25 AM | | |
| Integration time | 11 | | |
| 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) | | |
| Titrant tube volume | 1.3 mL | | |
| Syringe flush count | 3.50 | | |
| Flowing wash pump volume | 20.0 mL | | |
| Flowing wash stir duration | 5 s | | |
| Flowing wash stir speed | 30% | | |
| Solvent wash stir duration | 5 s | | |
| Solvent wash stir speed | 30% | | |
| Surfactant wash stir duration | 5 s | | |
| Surfactant wash stir speed | 30% | | |
| E0 calibration minimum number of points | 10 | | |
| E0 calibration maximum standard deviation | 0.01500 | | |
| E0 calibration timeout period | 60 s | | |
| E0 calibration stir duration | 5 s | | |
| E0 calibration preparation stir speed | 30% | | |
| E0 calibration buffer wash stir duration | 5 s | | |
| E0 calibration buffer wash stir speed | 30% | | |

Sample name: **D07**
Assay name: **UV-metric psKa**
Assay ID: **17J-07003**
Filename: **C:\Sirius_T3\Mehtap\20171006_exp14_pKa\17J-07003_D07_UV-metric psKa.t3r**

Experiment start time: **10/7/2017 2:51:21 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

## Instrument Settings (continued)

| Setting | Value | Batch Id | Install date |
|---|---|---|---|
| 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 F1