

Assay name: UV-metric psKa Analyst: Dorothy Levorse

Assay ID: 17J-11014 Instrument ID: T311053 Filename: C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

#### Yasuda-Shedlovsky result

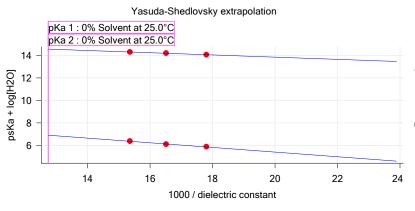
Extrapolation type pKa 0% SD Intercept Slope R<sup>2</sup> Ionic strength Temperature

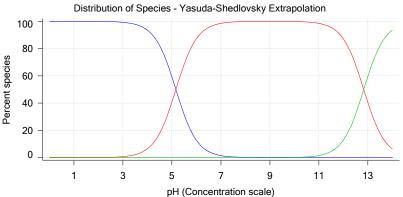
Yasuda-Shedlovsky 5.16 ±0.07 9.55 -207.1663 0.9931 0.166 M 25.0°C Yasuda-Shedlovsky 12.83 ±0.03 15.84 -99.3936 0.9946 0.166 M 25.0°C

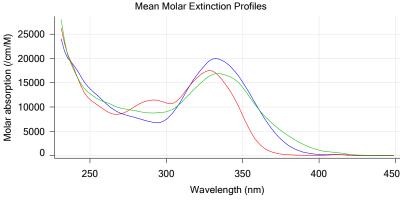
#### Component assay results

| Titration                   | Methanol | Direction | Result        | Dielectric | [H2O]  | lonic    | Temperature | )        | psKa   | psKa  |
|-----------------------------|----------|-----------|---------------|------------|--------|----------|-------------|----------|--------|-------|
|                             | weight%  |           | type          | constant   |        | strength |             |          | 1      | 2     |
| 17J-11014 Points 4 to 65    | 50.42 %  | Up        | UV-metric pKa | 56.2       | 24.2 M | 0.159 M  | 24.9°C      | <u></u>  | 4.49 🔽 | 12.69 |
| 17J-11014 Points 67 to 131  | 40.94 %  | Up        | UV-metric pKa | 60.6       | 29.5 M | 0.167 M  | 25.0°C      | <u></u>  | 4.63 🔽 | 12.74 |
| 17J-11014 Points 133 to 204 | 30.92 %  | Up        | UV-metric pKa | 65.1       | 35.3 M | 0.172 M  | 24.9°C      | <b>V</b> | 4.83 ▼ | 12.76 |

#### **Graphs**







# UV-metric psKa Titration 1 of 3 17J-11014 Points 4 to 65

#### Results

pKa 1 **4.49** pKa 2 **12.69** 

RMSD 0.002 0.004 0.005

Chi squared 0.2213

PCA calculated number of pKas 4

Average ionic strength
Average temperature

0.159 M
24.9°C

Analyte concentration range 71.3 µM to 67.1 µM

Methanol weight % 50.4 % Dielectric constant 56.2 Water concentration 24.2 M



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## Results (continued)

Number of pKas source Predicted

Wavelength clipping 237.3 nm to 450.0 nm

pH clipping 1.458 to 12.511

## Warnings and errors

Errors None

Warnings Calculated pKa outside clip range

PCA calculation disagrees with predicted number of pKas

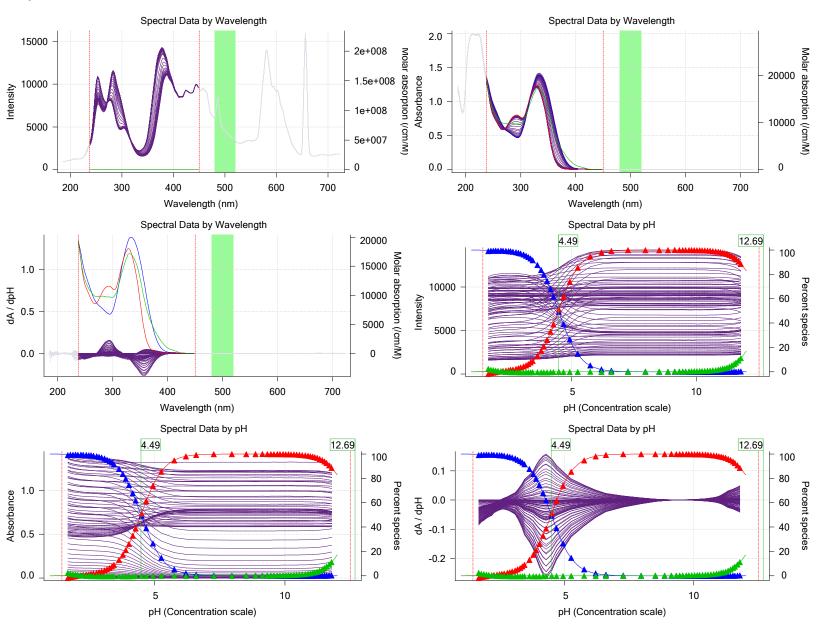
## Assay Settings

Setting Value Original Value Date/Time changed Imported from

Buffer in use

Assay Medium

#### **Graphs**

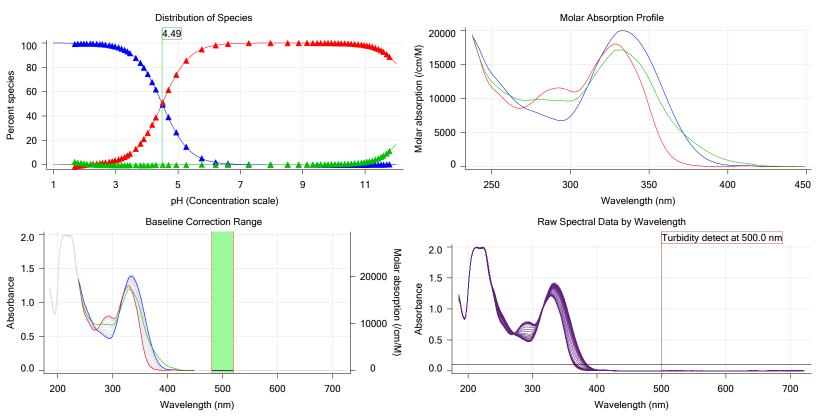




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## Graphs (continued)



# UV-metric psKa Titration 2 of 3 17J-11014 Points 67 to 131

#### Results

pKa 1 **4.63** pKa 2 **12.74** 

RMSD 0.001 0.003 0.003

Chi squared 0.1321

PCA calculated number of pKas 4

Average ionic strength 0.167 M Average temperature 25.0°C

Analyte concentration range 58.7 µM to 55.7 µM

Methanol weight % 40.9 %
Dielectric constant 60.6
Water concentration 29.5 M

Number of pKas source Predicted

Wavelength clipping 235.7 nm to 450.0 nm

pH clipping 1.484 to 12.503

## Warnings and errors

Errors Non-Warnings Calc

Calculated pKa outside clip range

PCA calculation disagrees with predicted number of pKas

#### **Assay Settings**

Setting Value Original Value Date/Time changed Imported from

Buffer in use No

Report by: Dorothy Levorse 10/12/2017 4:58:17 PM



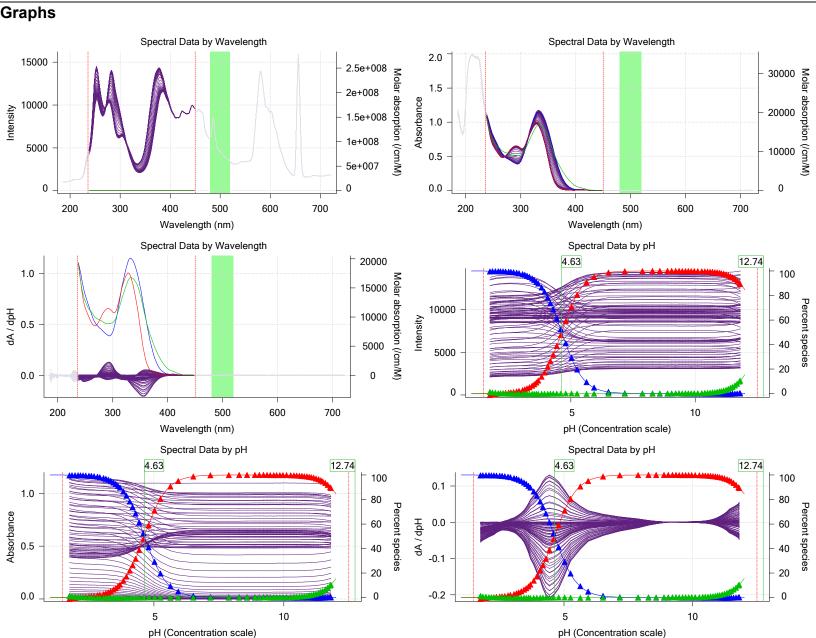
Assay name: UV-metric psKa Analyst: Dorothy Levorse

Assay ID: 17J-11014 Instrument ID: T311053 Filename: C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

# Assay Settings (continued)

Setting Value Original Value Date/Time changed Imported from

Assay Medium





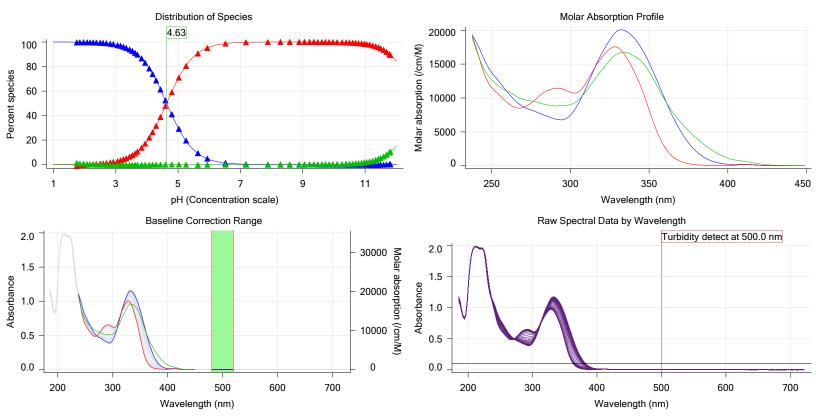
Filename:

Sample name: M12 Experiment start time: 10/11/2017 5:31:56 PM

Assay name: UV-metric psKa Analyst: Dorothy Levorse
Assay ID: 17J-11014 Instrument ID: T311053

C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

# Graphs (continued)



# UV-metric psKa Titration 3 of 3 17J-11014 Points 133 to 204

#### Results

pKa 1 **4.83** pKa 2 **12.76** 

RMSD 0.001 0.002 0.002

Chi squared 0.1134

PCA calculated number of pKas 4

Average ionic strength 0.172 M
Average temperature 24.9°C

Analyte concentration range 45.3 µM to 43.0 µM

Methanol weight % 30.9 % Dielectric constant 65.1 Water concentration 35.3 M

Number of pKas source Predicted

Wavelength clipping 230.0 nm to 450.0 nm

pH clipping 1.480 to 12.501

## Warnings and errors

Errors Non Warnings Cald

Calculated pKa outside clip range

PCA calculation disagrees with predicted number of pKas

#### **Assay Settings**

Setting Value Original Value Date/Time changed Imported from

Buffer in use No

Report by: Dorothy Levorse 10/12/2017 4:58:17 PM



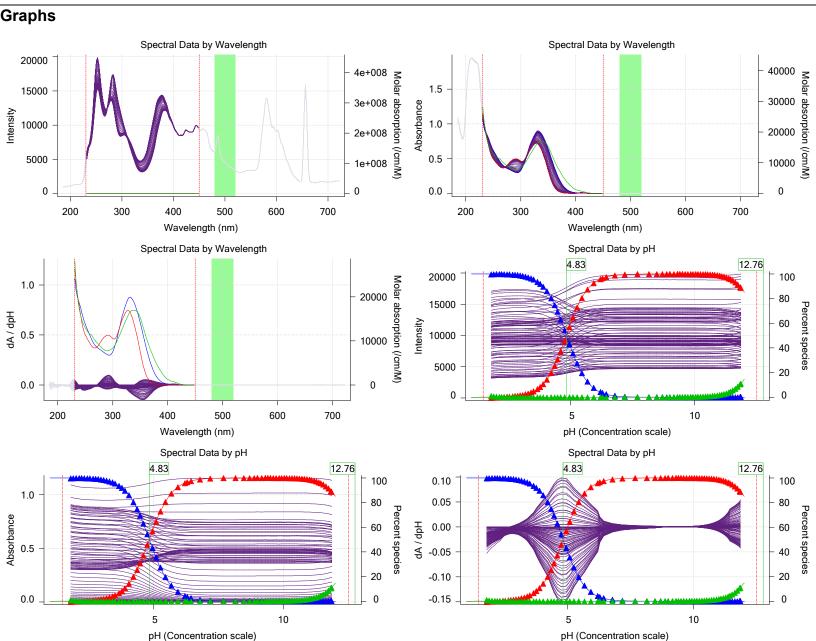
Assay name: UV-metric psKa Analyst: Dorothy Levorse

Assay ID: 17J-11014 Instrument ID: T311053 Filename: C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

## Assay Settings (continued)

Setting Value Original Value Date/Time changed Imported from

Assay Medium





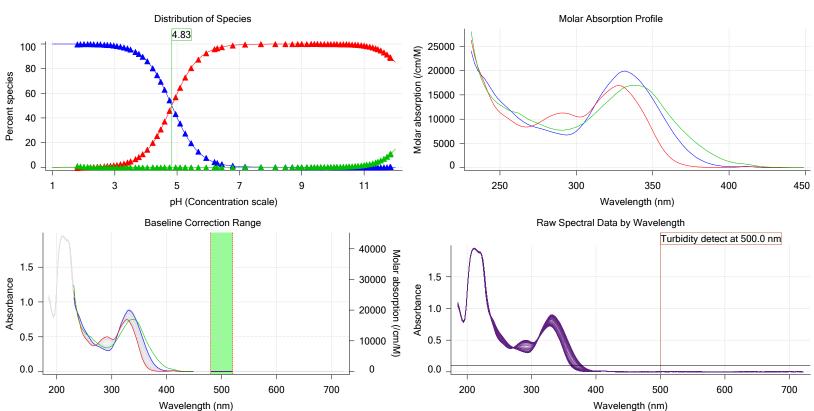
Filename:

Sample name: M12 Experiment start time: 10/11/2017 5:31:56 PM

Assay name: UV-metric psKa Analyst: Dorothy Levorse
Assay ID: 17J-11014 Instrument ID: T311053

17J-11014 Instrument ID: T31105
C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

# **Graphs** (continued)



## **Assay Model**

| rice and include                  |            |                      |                    |
|-----------------------------------|------------|----------------------|--------------------|
| Settings                          | Value      | Date/Time changed    | Imported from      |
| Sample name                       | M12        | 10/3/2017 3:44:45 PM | User entered value |
| Sample by                         | Volume     |                      | Default value      |
| Sample volume                     | 0.0030 mL  | 10/3/2017 3:44:45 PM | User entered value |
| Solvent                           | DMSO       |                      | Default value      |
| Sample concentration              | 0.037300 M | 10/3/2017 3:44:45 PM | User entered value |
| Solubility                        | Unknown    |                      | Default value      |
| Molecular weight                  | 292.16     | 10/3/2017 3:44:53 PM | User entered value |
| Individual pKa ionic environments | No         |                      | Default value      |
| Number of pKas                    | 2          | 10/3/2017 3:44:45 PM | User entered value |
| Sample is a                       | Base       | 10/3/2017 3:44:45 PM | User entered value |
| pKa 1                             | 3.40       | 10/3/2017 3:44:45 PM | User entered value |
| pKa 2                             | 5.60       | 10/3/2017 3:44:45 PM | User entered value |
| logP (XH2 2+)                     | -10.00     |                      | Default value      |
| logp (XH +)                       | -10.00     |                      | Default value      |
| logP (neutral X)                  | -10.00     | 10/3/2017 3:44:45 PM | User entered value |

## Events

| -         | -                  |
|-----------|--------------------|
|           | ,                  |
|           |                    |
|           |                    |
|           |                    |
| 0.85638 0 | 0.0011             |
| 0.43967 0 | 0.0005             |
| 0.79180 0 | 0.0006             |
| 0.87102 0 | 0.0007             |
| (         | 0.43967<br>0.79180 |



Sample name: M12 Experiment start time: 10/11/2017 5:31:56 PM

Assay name: UV-metric psKa Analyst: Dorothy Levorse

Assay ID: 17J-11014 Instrument ID: T311053
Filename: C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

#### Events (continued)

| Event         | Water   | Acid         | Base   | Methanol   | рН   | dpH/dt  |   |  | dpH/dt time   |
|---------------|---|--------------|--|--|--|---|---|--|---|
| •             |   |              |  |  |  |   |   |  | 10.0 s  |
|               |   |              |  |  |  |   |   |  | 10.0 s  |
| •             |   |              |  |  |  |   |   |  | 10.0 s  |
| Data point 11 | 0.34995 mL  | 0.06679 mL   | 0.05348 mL   | 1.15005 mL   | 2.665  | 0.00114   | 0.06246   | 0.00022  | 10.0 s  |
| I             |   |              |  |  |  | 0.00945   | 0.76145   | 0.00053  | 10.0 s  |
|               |   |              |  |  |  | 0.00555   | 0.69061   | 0.00033  | 10.0 s  |
|               |   |              |  |  |  | 0.00787   | 0.74958   | 0.00045  | 10.0 s  |
| Data point 15 | 0.34995 mL  | 0.06679 mL   | 0.06136 mL   | 1.15005 mL   | 3.065  | 0.01215   | 0.82635   | 0.00066  | 10.0 s  |
| Data point 16 | 0.34995 mL  | 0.06679 mL   | 0.06225 mL   | 1.15005 mL   | 3.157  | 0.00779   | 0.81928   | 0.00043  | 10.0 s  |
| Data point 17 | 0.34995 mL  | 0.06679 mL   | 0.06305 mL   | 1.15005 mL   | 3.250  | 0.00959   | 0.83208   | 0.00052  | 10.0 s  |
| Data point 18 | 0.34995 mL  | 0.06679 mL   | 0.06376 mL   | 1.15005 mL   | 3.364  | 0.01534   | 0.89496   | 0.00080  | 10.0 s  |
| Data point 19 | 0.34995 mL  | 0.06679 mL   | 0.06430 mL   | 1.15005 mL   | 3.462  | 0.01836   | 0.95039   | 0.00093  | 10.0 s  |
| Data point 20 | 0.34995 mL  | 0.06679 mL   | 0.06475 mL   | 1.15005 mL   | 3.557  | 0.02502   | 0.96470   | 0.00126  | 10.0 s  |
| Data point 21 | 0.34995 mL  | 0.06679 mL   | 0.06510 mL   | 1.15005 mL   | 3.645  | 0.03039   | 0.98019   | 0.00152  | 10.0 s  |
| Data point 22 | 0.34995 mL  | 0.06679 mL   | 0.06538 mL   | 1.15005 mL   | 3.724  | 0.03659   | 0.98510   | 0.00182  | 10.0 s  |
| Data point 23 | 0.34995 mL  | 0.06679 mL   | 0.06583 mL   | 1.15005 mL   | 3.917  | 0.05070   | 0.97011   | 0.00254  | 10.0 s  |
| Data point 24 | 0.34995 mL  | 0.06679 mL   | 0.06613 mL   | 1.15005 mL   | 4.064  | 0.07456   | 0.97698   | 0.00372  | 10.0 s  |
| Data point 25 | 0.34995 mL  | 0.06679 mL   | 0.06635 mL   | 1.15005 mL   | 4.171  | 0.09155   | 0.99495   | 0.00453  | 10.0 s  |
| Data point 26 | 0.34995 mL  | 0.06679 mL   | 0.06656 mL   | 1.15005 mL   | 4.297  | 0.09988   | 0.99117   | 0.00495  | 13.5 s  |
| Data point 27 | 0.34995 mL  | 0.06679 mL   | 0.06679 mL   | 1.15005 mL   | 4.439  | 0.09985   | 0.99506   | 0.00494  | 19.0 s  |
| Data point 28 | 0.34995 mL  | 0.06679 mL   | 0.06710 mL   | 1.15005 mL   | 4.554  | 0.09604   | 0.95916   | 0.00484  | 14.5 s  |
| Data point 29 | 0.34995 mL  | 0.06679 mL   | 0.06731 mL   | 1.15005 mL   | 4.773  | 0.09812   | 0.98147   | 0.00489  | 26.0 s  |
| Data point 30 | 0.34995 mL  | 0.06679 mL   | 0.06738 mL   | 1.15005 mL   | 4.955  | 0.10035   | 0.99417   | 0.00497  | 31.5 s  |
| Data point 31 | 0.34995 mL  | 0.06679 mL   | 0.06747 mL   | 1.15005 mL   | 5.207  | 0.09776   | 0.98311   | 0.00486  | 43.5 s  |
| Data point 32 | 0.34995 mL  | 0.06679 mL   | 0.06754 mL   | 1.15005 mL   | 5.525  | 0.09943   | 0.99299   | 0.00492  | 53.0 s  |
|               |   |              |  |  |  | 0.13305   | 0.97740   | 0.00664  | Timed out at  |
| •             |   |              |  |  |  |   |   |  | 59.5 s  |
| Data point 34 | 0.34995 mL  | 0.06679 mL   | 0.06766 mL   | 1.15005 mL   | 6.463  | 0.16293   | 0.99741   | 0.00805  | Timed out at  |
|               | Data point 8 Data point 9 Data point 10 Data point 11 Data point 12 Data point 13 Data point 14 Data point 15 Data point 16 Data point 17 Data point 17 Data point 18 Data point 19 Data point 20 Data point 21 Data point 21 Data point 22 Data point 23 Data point 24 Data point 25 Data point 26 Data point 27 Data point 27 Data point 28 Data point 30 Data point 31 Data point 32 Data point 32 Data point 33 | Data point 8 | Data point 8         0.34995 mL         0.06679 mL           Data point 9         0.34995 mL         0.06679 mL           Data point 10         0.34995 mL         0.06679 mL           Data point 11         0.34995 mL         0.06679 mL           Data point 12         0.34995 mL         0.06679 mL           Data point 13         0.34995 mL         0.06679 mL           Data point 14         0.34995 mL         0.06679 mL           Data point 15         0.34995 mL         0.06679 mL           Data point 16         0.34995 mL         0.06679 mL           Data point 17         0.34995 mL         0.06679 mL           Data point 18         0.34995 mL         0.06679 mL           Data point 19         0.34995 mL         0.06679 mL           Data point 20         0.34995 mL         0.06679 mL           Data point 21         0.34995 mL         0.06679 mL           Data point 23         0.34995 mL         0.06679 mL           Data point 24         0.34995 mL         0.06679 mL           Data point 25         0.34995 mL         0.06679 mL           Data point 28         0.34995 mL         0.06679 mL           Data point 30         0.34995 mL         0.06679 mL           Data point | Data point 8         0.34995 mL         0.06679 mL         0.04008 mL           Data point 9         0.34995 mL         0.06679 mL         0.04563 mL           Data point 10         0.34995 mL         0.06679 mL         0.04993 mL           Data point 11         0.34995 mL         0.06679 mL         0.05348 mL           Data point 12         0.34995 mL         0.06679 mL         0.05616 mL           Data point 13         0.34995 mL         0.06679 mL         0.05833 mL           Data point 14         0.34995 mL         0.06679 mL         0.05992 mL           Data point 15         0.34995 mL         0.06679 mL         0.05992 mL           Data point 16         0.34995 mL         0.06679 mL         0.06305 mL           Data point 18         0.34995 mL         0.06679 mL         0.06305 mL           Data point 19         0.34995 mL         0.06679 mL         0.06376 mL           Data point 20         0.34995 mL         0.06679 mL         0.06475 mL           Data point 21         0.34995 mL         0.06679 mL         0.06538 mL           Data point 23         0.34995 mL         0.06679 mL         0.06633 mL           Data point 25         0.34995 mL         0.06679 mL         0.06635 mL           Data point 28 </td <td>Data point 8         0.34995 mL         0.06679 mL         0.04008 mL         1.15005 mL           Data point 10         0.34995 mL         0.06679 mL         0.04563 mL         1.15005 mL           Data point 11         0.34995 mL         0.06679 mL         0.04993 mL         1.15005 mL           Data point 12         0.34995 mL         0.06679 mL         0.05348 mL         1.15005 mL           Data point 13         0.34995 mL         0.06679 mL         0.05616 mL         1.15005 mL           Data point 14         0.34995 mL         0.06679 mL         0.05833 mL         1.15005 mL           Data point 15         0.34995 mL         0.06679 mL         0.05992 mL         1.15005 mL           Data point 16         0.34995 mL         0.06679 mL         0.06136 mL         1.15005 mL           Data point 17         0.34995 mL         0.06679 mL         0.06305 mL         1.15005 mL           Data point 18         0.34995 mL         0.06679 mL         0.06305 mL         1.15005 mL           Data point 19         0.34995 mL         0.06679 mL         0.06376 mL         1.15005 mL           Data point 20         0.34995 mL         0.06679 mL         0.06475 mL         1.15005 mL           Data point 21         0.34995 mL         0.06679 mL</td> <td>Data point 8         0.34995 mL         0.06679 mL         0.04008 mL         1.15005 mL         2.348           Data point 9         0.34995 mL         0.06679 mL         0.04563 mL         1.15005 mL         2.463           Data point 10         0.34995 mL         0.06679 mL         0.04993 mL         1.15005 mL         2.548           Data point 11         0.34995 mL         0.06679 mL         0.05348 mL         1.15005 mL         2.665           Data point 13         0.34995 mL         0.06679 mL         0.05616 mL         1.15005 mL         2.665           Data point 14         0.34995 mL         0.06679 mL         0.05833 mL         1.15005 mL         2.848           Data point 15         0.34995 mL         0.06679 mL         0.06679 mL         0.05992 mL         1.15005 mL         2.943           Data point 16         0.34995 mL         0.06679 mL         0.06625 mL         1.15005 mL         3.065           Data point 17         0.34995 mL         0.06679 mL         0.06625 mL         1.15005 mL         3.250           Data point 20         0.34995 mL         0.06679 mL         0.06430 mL         1.15005 mL         3.642           Data point 21         0.34995 mL         0.06679 mL         0.06679 mL         0.06538 mL         1.15</td> <td>Data point 8         0.34995 mL         0.06679 mL         0.04008 mL         1.15005 mL         2.348         -0.00140           Data point 9         0.34995 mL         0.06679 mL         0.04563 mL         1.15005 mL         2.463         0.00272           Data point 10         0.34995 mL         0.06679 mL         0.04993 mL         1.15005 mL         2.548         0.00026           Data point 11         0.34995 mL         0.06679 mL         0.05348 mL         1.15005 mL         2.665         0.00114           Data point 13         0.34995 mL         0.06679 mL         0.05616 mL         1.15005 mL         2.763         0.00945           Data point 14         0.34995 mL         0.06679 mL         0.05833 mL         1.15005 mL         2.848         0.00555           Data point 15         0.34995 mL         0.06679 mL         0.05992 mL         1.15005 mL         2.943         0.0077           Data point 16         0.34995 mL         0.06679 mL         0.06225 mL         1.15005 mL         3.065         0.01215           Data point 17         0.34995 mL         0.06679 mL         0.06305 mL         1.15005 mL         3.364         0.01534           Data point 20         0.34995 mL         0.06679 mL         0.06475 mL         1.15005 mL</td> <td>Data point 8         0.34995 mL         0.06679 mL         0.04008 mL         1.15005 mL         2.348         -0.00140         0.06513           Data point 9         0.34995 mL         0.06679 mL         0.04563 mL         1.15005 mL         2.463         0.00272         0.19537           Data point 10         0.34995 mL         0.06679 mL         0.04993 mL         1.15005 mL         2.665         0.00114         0.06246           Data point 12         0.34995 mL         0.06679 mL         0.05616 mL         1.15005 mL         2.665         0.00114         0.06246           Data point 13         0.34995 mL         0.06679 mL         0.05838 mL         1.15005 mL         2.665         0.00114         0.06246           Data point 14         0.34995 mL         0.06679 mL         0.05838 mL         1.15005 mL         2.848         0.00555         0.69061           Data point 16         0.34995 mL         0.06679 mL         0.06225 mL         1.15005 mL         3.065         0.01215         0.82635           Data point 17         0.34995 mL         0.06679 mL         0.06376 mL         1.15005 mL         3.250         0.00779         0.83208           Data point 29         0.34995 mL         0.06679 mL         0.06475 mL         1.15005 mL         3</td> <td>Data point 8         0.34995 mL         0.06679 mL         0.04008 mL         1.15005 mL         2.348         -0.00140         0.06513         0.00027           Data point 9         0.34995 mL         0.06679 mL         0.044563 mL         1.15005 mL         2.463         0.00272         0.19537         0.00030           Data point 10         0.34995 mL         0.06679 mL         0.04933 mL         1.15005 mL         2.548         0.00026         0.00238         0.00026           Data point 11         0.34995 mL         0.06679 mL         0.05348 mL         1.15005 mL         2.665         0.00114         0.06246         0.00022           Data point 13         0.34995 mL         0.06679 mL         0.05833 mL         1.15005 mL         2.763         0.00945         0.76145         0.00053           Data point 14         0.34995 mL         0.06679 mL         0.05833 mL         1.15005 mL         2.848         0.00575         0.69061         0.0033           Data point 15         0.34995 mL         0.06679 mL         0.06225 mL         1.15005 mL         3.065         0.01215         0.82635         0.00666           Data point 16         0.34995 mL         0.06679 mL         0.06225 mL         1.15005 mL         3.157         0.00779         0.8128</td> | Data point 8         0.34995 mL         0.06679 mL         0.04008 mL         1.15005 mL           Data point 10         0.34995 mL         0.06679 mL         0.04563 mL         1.15005 mL           Data point 11         0.34995 mL         0.06679 mL         0.04993 mL         1.15005 mL           Data point 12         0.34995 mL         0.06679 mL         0.05348 mL         1.15005 mL           Data point 13         0.34995 mL         0.06679 mL         0.05616 mL         1.15005 mL           Data point 14         0.34995 mL         0.06679 mL         0.05833 mL         1.15005 mL           Data point 15         0.34995 mL         0.06679 mL         0.05992 mL         1.15005 mL           Data point 16         0.34995 mL         0.06679 mL         0.06136 mL         1.15005 mL           Data point 17         0.34995 mL         0.06679 mL         0.06305 mL         1.15005 mL           Data point 18         0.34995 mL         0.06679 mL         0.06305 mL         1.15005 mL           Data point 19         0.34995 mL         0.06679 mL         0.06376 mL         1.15005 mL           Data point 20         0.34995 mL         0.06679 mL         0.06475 mL         1.15005 mL           Data point 21         0.34995 mL         0.06679 mL | Data point 8         0.34995 mL         0.06679 mL         0.04008 mL         1.15005 mL         2.348           Data point 9         0.34995 mL         0.06679 mL         0.04563 mL         1.15005 mL         2.463           Data point 10         0.34995 mL         0.06679 mL         0.04993 mL         1.15005 mL         2.548           Data point 11         0.34995 mL         0.06679 mL         0.05348 mL         1.15005 mL         2.665           Data point 13         0.34995 mL         0.06679 mL         0.05616 mL         1.15005 mL         2.665           Data point 14         0.34995 mL         0.06679 mL         0.05833 mL         1.15005 mL         2.848           Data point 15         0.34995 mL         0.06679 mL         0.06679 mL         0.05992 mL         1.15005 mL         2.943           Data point 16         0.34995 mL         0.06679 mL         0.06625 mL         1.15005 mL         3.065           Data point 17         0.34995 mL         0.06679 mL         0.06625 mL         1.15005 mL         3.250           Data point 20         0.34995 mL         0.06679 mL         0.06430 mL         1.15005 mL         3.642           Data point 21         0.34995 mL         0.06679 mL         0.06679 mL         0.06538 mL         1.15 | Data point 8         0.34995 mL         0.06679 mL         0.04008 mL         1.15005 mL         2.348         -0.00140           Data point 9         0.34995 mL         0.06679 mL         0.04563 mL         1.15005 mL         2.463         0.00272           Data point 10         0.34995 mL         0.06679 mL         0.04993 mL         1.15005 mL         2.548         0.00026           Data point 11         0.34995 mL         0.06679 mL         0.05348 mL         1.15005 mL         2.665         0.00114           Data point 13         0.34995 mL         0.06679 mL         0.05616 mL         1.15005 mL         2.763         0.00945           Data point 14         0.34995 mL         0.06679 mL         0.05833 mL         1.15005 mL         2.848         0.00555           Data point 15         0.34995 mL         0.06679 mL         0.05992 mL         1.15005 mL         2.943         0.0077           Data point 16         0.34995 mL         0.06679 mL         0.06225 mL         1.15005 mL         3.065         0.01215           Data point 17         0.34995 mL         0.06679 mL         0.06305 mL         1.15005 mL         3.364         0.01534           Data point 20         0.34995 mL         0.06679 mL         0.06475 mL         1.15005 mL | Data point 8         0.34995 mL         0.06679 mL         0.04008 mL         1.15005 mL         2.348         -0.00140         0.06513           Data point 9         0.34995 mL         0.06679 mL         0.04563 mL         1.15005 mL         2.463         0.00272         0.19537           Data point 10         0.34995 mL         0.06679 mL         0.04993 mL         1.15005 mL         2.665         0.00114         0.06246           Data point 12         0.34995 mL         0.06679 mL         0.05616 mL         1.15005 mL         2.665         0.00114         0.06246           Data point 13         0.34995 mL         0.06679 mL         0.05838 mL         1.15005 mL         2.665         0.00114         0.06246           Data point 14         0.34995 mL         0.06679 mL         0.05838 mL         1.15005 mL         2.848         0.00555         0.69061           Data point 16         0.34995 mL         0.06679 mL         0.06225 mL         1.15005 mL         3.065         0.01215         0.82635           Data point 17         0.34995 mL         0.06679 mL         0.06376 mL         1.15005 mL         3.250         0.00779         0.83208           Data point 29         0.34995 mL         0.06679 mL         0.06475 mL         1.15005 mL         3 | Data point 8         0.34995 mL         0.06679 mL         0.04008 mL         1.15005 mL         2.348         -0.00140         0.06513         0.00027           Data point 9         0.34995 mL         0.06679 mL         0.044563 mL         1.15005 mL         2.463         0.00272         0.19537         0.00030           Data point 10         0.34995 mL         0.06679 mL         0.04933 mL         1.15005 mL         2.548         0.00026         0.00238         0.00026           Data point 11         0.34995 mL         0.06679 mL         0.05348 mL         1.15005 mL         2.665         0.00114         0.06246         0.00022           Data point 13         0.34995 mL         0.06679 mL         0.05833 mL         1.15005 mL         2.763         0.00945         0.76145         0.00053           Data point 14         0.34995 mL         0.06679 mL         0.05833 mL         1.15005 mL         2.848         0.00575         0.69061         0.0033           Data point 15         0.34995 mL         0.06679 mL         0.06225 mL         1.15005 mL         3.065         0.01215         0.82635         0.00666           Data point 16         0.34995 mL         0.06679 mL         0.06225 mL         1.15005 mL         3.157         0.00779         0.8128 |

59.5 s



Sample name: M12 Experiment start time: 10/11/2017 5:31:56 PM

Assay name: UV-metric psKa Analyst: Dorothy Levorse

Assay ID: 17J-11014 Instrument ID: T311053 Filename: C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

37:29.9 Data point 61 0.34995 mL 0.06679 mL 0.08001 mL 1.15005 mL 11.658 -0.00469 0.53880

#### Events (continued)

| <b>Time</b><br>24:08.1 | Event<br>Data point 35 | Water<br>0.34995 mL | <b>Acid</b> 0.06679 mL | <b>Base</b> 0.06771 mL | Methanol<br>1.15005 mL | <b>pH</b><br>6.857 | <b>dpH/dt</b><br>0.13768 | pH R-squared<br>0.99658 |         | dpH/dt time<br>Timed out at      |
|------------------------|------------------------|---------------------|------------------------|------------------------|------------------------|--------------------|--------------------------|-------------------------|---------|----------------------------------|
| 25:24.7                | Data point 36          | 0.34995 mL          | 0.06679 mL             | 0.06778 mL             | 1.15005 mL             | 7.523              | 0.14423                  | 0.99127                 | 0.00715 | 59.5 s<br>Timed out at<br>59.5 s |
| 26:41.5                | Data point 37          | 0.34995 mL          | 0.06679 mL             | 0.06785 mL             | 1.15005 mL             | 8.214              | 0.09750                  | 0.94493                 | 0.00495 | 49.0 s                           |
| 27:47.2                | Data point 38          | 0.34995 mL          | 0.06679 mL             | 0.06792 mL             | 1.15005 mL             | 8.763              | 0.08962                  | 0.92550                 | 0.00460 | 37.0 s                           |
| 28:40.8                | Data point 39          | 0.34995 mL          | 0.06679 mL             | 0.06799 mL             | 1.15005 mL             | 9.116              | 0.09810                  | 0.97641                 | 0.00490 | 29.0 s                           |
| 29:26.3                | Data point 40          | 0.34995 mL          | 0.06679 mL             | 0.06806 mL             | 1.15005 mL             | 9.379              | 0.09698                  | 0.97849                 | 0.00484 | 24.0 s                           |
| 30:07.1                | Data point 41          | 0.34995 mL          | 0.06679 mL             | 0.06813 mL             | 1.15005 mL             | 9.566              | 0.09846                  | 0.98624                 | 0.00489 | 20.0 s                           |
| 30:43.9                | Data point 42          | 0.34995 mL          | 0.06679 mL             | 0.06820 mL             | 1.15005 mL             | 9.700              | 0.09712                  | 0.96561                 | 0.00488 | 14.5 s                           |
| 31:15.0                | Data point 43          | 0.34995 mL          | 0.06679 mL             | 0.06827 mL             | 1.15005 mL             | 9.816              | 0.09664                  | 0.97191                 | 0.00484 | 13.5 s                           |
| 31:45.3                | Data point 44          | 0.34995 mL          | 0.06679 mL             | 0.06837 mL             | 1.15005 mL             | 9.949              | 0.09982                  | 0.97687                 | 0.00499 | 12.0 s                           |
| 32:08.9                | Data point 45          | 0.34995 mL          | 0.06679 mL             | 0.06846 mL             | 1.15005 mL             | 10.052             | 0.09983                  | 0.98026                 | 0.00498 | 10.0 s                           |
| 32:30.4                | Data point 46          | 0.34995 mL          | 0.06679 mL             | 0.06856 mL             | 1.15005 mL             | 10.162             | 0.08681                  | 0.96574                 | 0.00436 | 10.0 s                           |
| 32:57.2                | Data point 47          | 0.34995 mL          | 0.06679 mL             | 0.06867 mL             | 1.15005 mL             | 10.269             | 0.05613                  | 0.96822                 | 0.00282 | 10.0 s                           |
| 33:18.9                | Data point 48          | 0.34995 mL          | 0.06679 mL             | 0.06881 mL             | 1.15005 mL             | 10.374             | 0.04923                  | 0.97523                 | 0.00246 | 10.0 s                           |
| 33:40.5                | Data point 49          | 0.34995 mL          | 0.06679 mL             | 0.06898 mL             | 1.15005 mL             | 10.470             | 0.03422                  | 0.95947                 | 0.00172 | 10.0 s                           |
| 33:57.0                | Data point 50          | 0.34995 mL          | 0.06679 mL             | 0.06914 mL             | 1.15005 mL             | 10.578             | 0.02134                  | 0.90738                 | 0.00111 | 10.0 s                           |
| 34:13.6                | Data point 51          | 0.34995 mL          | 0.06679 mL             | 0.06936 mL             | 1.15005 mL             | 10.686             | 0.01080                  | 0.77963                 | 0.00060 | 10.0 s                           |
| 34:30.1                | Data point 52          | 0.34995 mL          | 0.06679 mL             | 0.06964 mL             | 1.15005 mL             | 10.790             | 0.01116                  | 0.91716                 | 0.00057 | 10.0 s                           |
| 34:46.6                | Data point 53          | 0.34995 mL          | 0.06679 mL             | 0.06999 mL             | 1.15005 mL             | 10.898             | 0.00536                  | 0.50282                 | 0.00037 | 10.0 s                           |
| 35:03.1                | Data point 54          | 0.34995 mL          | 0.06679 mL             | 0.07044 mL             | 1.15005 mL             | 11.012             | 0.00327                  | 0.44209                 | 0.00024 | 10.0 s                           |
| 35:19.6                | Data point 55          | 0.34995 mL          | 0.06679 mL             | 0.07103 mL             | 1.15005 mL             | 11.115             | 0.00076                  | 0.04103                 | 0.00019 | 10.0 s                           |
| 35:36.2                | Data point 56          | 0.34995 mL          | 0.06679 mL             | 0.07178 mL             | 1.15005 mL             | 11.205             | 0.00143                  | 0.12441                 | 0.00020 | 10.0 s                           |
| 35:52.8                |                        |                     |                        |                        |                        |                    | -0.00182                 | 0.17697                 | 0.00021 | 10.0 s                           |
| 36:09.4                | Data point 58          | 0.34995 mL          | 0.06679 mL             | 0.07382 mL             | 1.15005 mL             | 11.373             | -0.00305                 | 0.55352                 | 0.00020 | 10.0 s                           |
|                        | Data point 59          |                     |                        |                        |                        |                    | -0.00270                 | 0.41061                 | 0.00021 | 10.0 s                           |
| 37:03.2                | Data point 60          | 0.34995 mL          | 0.06679 mL             | 0.07787 mL             | 1.15005 mL             | 11.562             | -0.00360                 | 0.51552                 | 0.00025 | 10.0 s                           |
|                        |                        |                     |                        |                        |                        |                    |                          |                         |         |                                  |

0.00032 10.0 s



Sample name: M12 Experiment start time: 10/11/2017 5:31:56 PM

Assay name: UV-metric psKa Analyst: Dorothy Levorse

Assay ID: 17J-11014 Instrument ID: T311053
Filename: C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

#### Events (continued)

49:37.3 Data point 90

| Event              | Water  | Acid   | Base  | Methanol   | рН   | dpH/dt   | pH R-squared   | pH SD   | dpH/dt<br>time   |
|--------------------|--|--|---|--|--|--|--|---|--|
| Data point 62      | 0.34995 mL   | 0.06679 mL   | 0.08262 mL  | 1.15005 mL   | 11.746   | -0.00103   | 0.05891  | 0.00021   | 10.0 s   |
| Data point 63      |  |  |   |  |  | 0.00079  | 0.04545  | 0.00018   | 10.0 s   |
| Data point 64      | 0.34995 mL   | 0.06679 mL   | 0.09048 mL  | 1.15005 mL   | 11.920   | -0.00193   | 0.19582  | 0.00021   | 10.0 s   |
| Data point 65      | 0.34995 mL   | 0.06679 mL   | 0.09664 mL  | 1.15005 mL   | 12.011   | 0.00138  | 0.11564  | 0.00020   | 10.0 s   |
| Reference spectrum |  |  |   |  |  |  |  |   |  |
| Data point 67      | 0.50000 mL   | 0.15741 mL   | 0.09666 mL  | 1.15005 mL   | 1.984  | -0.05925   | 0.92666  | 0.00304   | 10.0 s   |
| Data point 68      | 0.50000 mL   | 0.15741 mL   | 0.10988 mL  | 1.15005 mL   | 2.082  | 0.00358  | 0.13224  | 0.00049   | 10.0 s   |
| Data point 69      | 0.50000 mL   | 0.15741 mL   | 0.12105 mL  | 1.15005 mL   | 2.197  | 0.01874  | 0.59829  | 0.00120   | 10.0 s   |
| Data point 70      | 0.50000 mL   | 0.15741 mL   | 0.12963 mL  | 1.15005 mL   | 2.313  | 0.00335  | 0.04368  | 0.00079   | 10.0 s   |
| Data point 71      | 0.50000 mL   | 0.15741 mL   | 0.13464 mL  | 1.15005 mL   | 2.407  | 0.01325  | 0.90450  | 0.00069   | 10.0 s   |
| Data point 72      | 0.50000 mL   | 0.15741 mL   | 0.13914 mL  | 1.15005 mL   | 2.507  | 0.01286  | 0.87351  | 0.00068   | 10.0 s   |
| Data point 73      |  |  |   |  |  | 0.00865  | 0.86302  | 0.00046   | 10.0 s   |
| Data point 74      |  |  |   |  |  |  |  | 0.00074   | 10.0 s   |
|                    |  |  |   |  |  | 0.00786  | 0.80929  | 0.00043   | 10.0 s   |
| Data point 76      |  |  |   |  |  | 0.01220  | 0.90713  | 0.00063   |  |
| •                  |  |  |   |  |  |  |  |   |  |
| •                  |  |  |   |  |  |  |  |   | 10.0 s   |
| <b> </b>           |  |  |   |  |  |  |  |   | 10.0 s   |
|                    |  |  |   |  |  |  |  |   |  |
| •                  |  |  |   |  |  |  |  |   |  |
|                    |  |  |   |  |  |  | * - *  |   | 10.0 s   |
| •                  |  |  |   |  |  |  |  |   | 10.0 s   |
| •                  |  |  |   |  |  |  |  |   |  |
| •                  |  |  |   |  |  |  |  |   |  |
| •                  |  |  |   |  |  |  |  |   |  |
| •                  |  |  |   |  |  |  |  |   | 10.0 s   |
|                    |  |  |   |  |  |  |  |   | 10.0 s   |
| Data point 89      |  |  |   |  |  |  |  |   | 10.0 s   |
|                    | Data point 62 Data point 63 Data point 64 Data point 65 Reference spectrum Data point 67 Data point 68 Data point 69 Data point 70 Data point 71 Data point 72 Data point 73 Data point 74 Data point 75 Data point 76 Data point 77 Data point 78 Data point 79 Data point 80 Data point 81 Data point 82 Data point 84 Data point 85 Data point 86 Data point 87 Data point 87 Data point 88 Data point 89 | Data point 62         0.34995 mL           Data point 63         0.34995 mL           Data point 64         0.34995 mL           Data point 65         0.34995 mL           Reference spectrum         0.50000 mL           Data point 68         0.50000 mL           Data point 70         0.50000 mL           Data point 71         0.50000 mL           Data point 72         0.50000 mL           Data point 73         0.50000 mL           Data point 74         0.50000 mL           Data point 75         0.50000 mL           Data point 76         0.50000 mL           Data point 77         0.50000 mL           Data point 78         0.50000 mL           Data point 80         0.50000 mL           Data point 81         0.50000 mL           Data point 82         0.50000 mL           Data point 83         0.50000 mL           Data point 84         0.50000 mL           Data point 85         0.50000 mL           Data point 86         0.50000 mL           Data point 87         0.50000 mL           Data point 88         0.50000 mL           Data point 88         0.50000 mL           Data point 88         0.50000 mL | Data point 62         0.34995 mL         0.06679 mL           Data point 63         0.34995 mL         0.06679 mL           Data point 64         0.34995 mL         0.06679 mL           Data point 65         0.34995 mL         0.06679 mL           Reference spectrum         0.50000 mL         0.15741 mL           Data point 68         0.50000 mL         0.15741 mL           Data point 70         0.50000 mL         0.15741 mL           Data point 71         0.50000 mL         0.15741 mL           Data point 72         0.50000 mL         0.15741 mL           Data point 73         0.50000 mL         0.15741 mL           Data point 74         0.50000 mL         0.15741 mL           Data point 75         0.50000 mL         0.15741 mL           Data point 76         0.50000 mL         0.15741 mL           Data point 79         0.50000 mL         0.15741 mL           Data point 80         0.50000 mL         0.15741 mL           Data point 81         0.50000 mL         0.15741 mL           Data point 82         0.50000 mL         0.15741 mL           Data point 84         0.50000 mL         0.15741 mL           Data point 85         0.50000 mL         0.15741 mL           Data | Data point 62         0.34995 mL         0.06679 mL         0.08262 mL           Data point 63         0.34995 mL         0.06679 mL         0.08582 mL           Data point 64         0.34995 mL         0.06679 mL         0.09048 mL           Data point 65         0.34995 mL         0.06679 mL         0.09664 mL           Reference spectrum         0.50000 mL         0.15741 mL         0.09666 mL           Data point 68         0.50000 mL         0.15741 mL         0.10988 mL           Data point 69         0.50000 mL         0.15741 mL         0.12963 mL           Data point 70         0.50000 mL         0.15741 mL         0.12963 mL           Data point 71         0.50000 mL         0.15741 mL         0.12963 mL           Data point 72         0.50000 mL         0.15741 mL         0.13464 mL           Data point 73         0.50000 mL         0.15741 mL         0.13914 mL           Data point 74         0.50000 mL         0.15741 mL         0.14638 mL           Data point 75         0.50000 mL         0.15741 mL         0.14638 mL           Data point 76         0.50000 mL         0.15741 mL         0.15075 mL           Data point 79         0.50000 mL         0.15741 mL         0.15235 mL           Data poi | Data point 62         0.34995 mL         0.06679 mL         0.08262 mL         1.15005 mL           Data point 63         0.34995 mL         0.06679 mL         0.08582 mL         1.15005 mL           Data point 64         0.34995 mL         0.06679 mL         0.09048 mL         1.15005 mL           Data point 65         0.34995 mL         0.06679 mL         0.09664 mL         1.15005 mL           Reference spectrum         0.50000 mL         0.15741 mL         0.09666 mL         1.15005 mL           Data point 68         0.50000 mL         0.15741 mL         0.10988 mL         1.15005 mL           Data point 69         0.50000 mL         0.15741 mL         0.12963 mL         1.15005 mL           Data point 70         0.50000 mL         0.15741 mL         0.12963 mL         1.15005 mL           Data point 71         0.50000 mL         0.15741 mL         0.13464 mL         1.15005 mL           Data point 72         0.50000 mL         0.15741 mL         0.13914 mL         1.15005 mL           Data point 73         0.50000 mL         0.15741 mL         0.14863 mL         1.15005 mL           Data point 74         0.50000 mL         0.15741 mL         0.14638 mL         1.15005 mL           Data point 75         0.50000 mL         0.15741 mL | Data point 62         0.34995 mL         0.06679 mL         0.08262 mL         1.15005 mL         11.746           Data point 63         0.34995 mL         0.06679 mL         0.08582 mL         1.15005 mL         11.823           Data point 64         0.34995 mL         0.06679 mL         0.09048 mL         1.15005 mL         11.920           Data point 65         0.34995 mL         0.06679 mL         0.09664 mL         1.15005 mL         12.011           Reference spectrum         Data point 67         0.50000 mL         0.15741 mL         0.09666 mL         1.15005 mL         1.984           Data point 68         0.50000 mL         0.15741 mL         0.10988 mL         1.15005 mL         2.082           Data point 70         0.50000 mL         0.15741 mL         0.12105 mL         1.15005 mL         2.197           Data point 71         0.50000 mL         0.15741 mL         0.13464 mL         1.15005 mL         2.407           Data point 72         0.50000 mL         0.15741 mL         0.13464 mL         1.15005 mL         2.507           Data point 73         0.50000 mL         0.15741 mL         0.13464 mL         1.15005 mL         2.507           Data point 73         0.50000 mL         0.15741 mL         0.14638 mL         1.15005 mL | Data point 62         0.34995 mL         0.06679 mL         0.08262 mL         1.15005 mL         11.746         -0.00103           Data point 63         0.34995 mL         0.06679 mL         0.08582 mL         1.15005 mL         11.823         0.00079           Data point 64         0.34995 mL         0.06679 mL         0.09048 mL         1.15005 mL         11.920         -0.00193           Reference spectrum Data point 67         0.50000 mL         0.15741 mL         0.09666 mL         1.15005 mL         12.011         0.00358           Data point 68         0.50000 mL         0.15741 mL         0.09866 mL         1.15005 mL         1.984         -0.05925           Data point 69         0.50000 mL         0.15741 mL         0.12963 mL         1.15005 mL         2.082         0.00358           Data point 70         0.50000 mL         0.15741 mL         0.12963 mL         1.15005 mL         2.197         0.01874           Data point 71         0.50000 mL         0.15741 mL         0.13464 mL         1.15005 mL         2.407         0.01325           Data point 72         0.50000 mL         0.15741 mL         0.13914 mL         1.15005 mL         2.407         0.01325           Data point 74         0.50000 mL         0.15741 mL         0.14638 mL | Data point 62         0.34995 mL         0.06679 mL         0.08262 mL         1.15005 mL         11.746         -0.00103         0.05891           Data point 63         0.34995 mL         0.06679 mL         0.08582 mL         1.15005 mL         11.823         0.00079         0.04545           Data point 64         0.34995 mL         0.06679 mL         0.09048 mL         1.15005 mL         11.920         -0.00193         0.19582           Data point 65         0.34995 mL         0.06679 mL         0.09048 mL         1.15005 mL         11.920         -0.00138         0.11564           Reference spectrum         Data point 67         0.50000 mL         0.15741 mL         0.09666 mL         1.15005 mL         1.984         -0.05925         0.92666           Data point 68         0.50000 mL         0.15741 mL         0.10988 mL         1.15005 mL         2.982         0.00358         0.13224           Data point 70         0.50000 mL         0.15741 mL         0.12963 mL         1.15005 mL         2.197         0.011874         0.59829           Data point 71         0.50000 mL         0.15741 mL         0.13464 mL         1.15005 mL         2.407         0.01325         0.90450           Data point 72         0.50000 mL         0.15741 mL         0.14306 mL< | Data point 62         0.34995 mL         0.06679 mL         0.08262 mL         1.15005 mL         11.746         -0.00103         0.05891         0.00021           Data point 63         0.34995 mL         0.06679 mL         0.08582 mL         1.15005 mL         11.823         0.00079         0.04545         0.00013           Data point 64         0.34995 mL         0.06679 mL         0.09048 mL         1.15005 mL         11.920         -0.00193         0.19582         0.00020           Reference spectrum         0.50000 mL         0.15741 mL         0.09666 mL         1.15005 mL         11.920         -0.00193         0.19582         0.00020           Data point 67         0.50000 mL         0.15741 mL         0.09666 mL         1.15005 mL         1.984         -0.05925         0.92666         0.00304           Data point 68         0.50000 mL         0.15741 mL         0.12963 mL         1.15005 mL         2.197         0.01874         0.59829         0.00120           Data point 70         0.50000 mL         0.15741 mL         0.12963 mL         1.15005 mL         2.407         0.01325         0.94368         0.00079           Data point 71         0.50000 mL         0.15741 mL         0.13964 mL         1.15005 mL         2.407         0.01325 <td< td=""></td<> |

0.50000 mL 0.15741 mL 0.15767 mL 1.15005 mL 4.407 0.10061 0.99318

0.00499 11.5 s



Sample name: M12 Experiment start time: 10/11/2017 5:31:56 PM

Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse** 

Assay ID: 17J-11014 Instrument ID: T311053 Filename: C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

## Events (continued)

| Time                   | Event                            | Water      | Acid       | Base       | Methanol   | рН     | dpH/dt              | pH R-squared       | pH SD              | dpH/dt<br>time   |
|------------------------|----------------------------------|------------|------------|------------|------------|--------|---------------------|--------------------|--------------------|------------------|
| 50:00.5                | Data point 91                    | 0.50000 mL | 0.15741 mL | 0.15776 mL | 1.15005 mL | 4.520  | 0.09756             | 0.98213            | 0.00486            | 12.5 s           |
| 50:29.6                | Data point 92                    | 0.50000 mL | 0.15741 mL | 0.15786 mL | 1.15005 mL | 4.659  | 0.09953             | 0.96637            | 0.00500            | 15.5 s           |
| 51:01.8                | Data point 93                    | 0.50000 mL | 0.15741 mL | 0.15795 mL | 1.15005 mL | 4.818  | 0.10081             | 0.99136            | 0.00500            | 19.5 s           |
| 51:37.9                | Data point 94                    | 0.50000 mL | 0.15741 mL | 0.15804 mL | 1.15005 mL | 5.019  | 0.09825             | 0.98646            | 0.00488            | 26.5 s           |
| 52:26.1                | Data point 95                    | 0.50000 mL | 0.15741 mL | 0.15814 mL | 1.15005 mL | 5.249  | 0.10046             | 0.98612            | 0.00499            | 31.5 s           |
| 53:14.5                | Data point 96                    | 0.50000 mL | 0.15741 mL | 0.15821 mL | 1.15005 mL | 5.475  | 0.09871             | 0.96815            | 0.00495            | 32.0 s           |
| 54:03.2                | Data point 97                    | 0.50000 mL | 0.15741 mL | 0.15828 mL | 1.15005 mL | 5.855  | 0.09887             | 0.98512            | 0.00491            | 47.0 s           |
| 55:01.8                | Data point 98                    | 0.50000 mL | 0.15741 mL | 0.15832 mL | 1.15005 mL | 6.157  | 0.10057             | 0.99257            | 0.00498            | 52.0 s           |
| 56:05.4                | Data point 99                    |            |            |            | 1.15005 mL |        | 0.09961             | 0.99016            | 0.00494            | 52.0 s           |
| 57:14.2                | Data point 100                   | 0.50000 mL | 0.15741 mL | 0.15847 mL | 1.15005 mL | 7.386  | 0.09533             | 0.97305            | 0.00477            | 59.0 s           |
| 58:29.8                | Data point 101                   | 0.50000 mL | 0.15741 mL | 0.15854 mL | 1.15005 mL | 8.091  | 0.09725             | 0.96315            | 0.00489            | 48.5 s           |
| 59:34.9                | Data point 102                   |            |            |            |            |        | 0.09711             | 0.93091            | 0.00497            | 36.5 s           |
| 1:00:28.2              | Data point 103                   |            |            |            |            |        | 0.07960             | 0.70096            | 0.00469            | 34.0 s           |
| 1:01:23.9              | Data point 104                   |            |            |            |            |        | 0.09401             | 0.93387            | 0.00480            | 26.5 s           |
| 1:02:07.0              | Data point 105                   |            |            |            |            |        | 0.09051             | 0.83639            | 0.00488            |                  |
| 1:02:45.2              | Data point 106                   |            |            |            |            |        | 0.09569             | 0.97559            | 0.00478            | 19.5 s           |
| 1:03:21.4              | Data point 107                   |            |            |            |            |        | 0.09939             | 0.97818            | 0.00496            | 16.5 s           |
| 1:03:59.7              | Data point 108                   |            |            |            |            |        | 0.10033             | 0.98212            | 0.00500            | 12.5 s           |
| 1:04:33.9              | Data point 109                   |            |            |            |            |        | 0.09460             | 0.98316            | 0.00471            | 11.5 s           |
| 1:05:02.0              | Data point 110                   |            |            |            |            |        | 0.09291             | 0.96791            | 0.00466            | 10.0 s           |
| 1:05:23.7              | Data point 111                   |            |            |            |            | 10.047 | 0.07931             | 0.96996            | 0.00397            | 10.0 s           |
| 1:05:50.4              | Data point 112                   |            |            |            |            | 10.164 |                     | 0.98159            | 0.00242            |                  |
| 1:06:11.9              | Data point 113                   |            |            |            |            | 10.304 | 0.03228             | 0.96029            | 0.00162            |                  |
| 1:06:33.5              | Data point 114                   |            |            |            |            | 10.464 |                     | 0.90610            | 0.00080            |                  |
| 1:06:55.1              | Data point 115                   |            |            |            |            |        |                     | 0.79797            | 0.00043            | 10.0 s           |
| 1:07:16.8              | Data point 116                   |            |            |            |            |        |                     | 0.75121            | 0.00036            | 10.0 s           |
| 1:07:33.2<br>1:07:49.9 | Data point 117<br>Data point 118 |            |            |            |            |        | 0.00060<br>-0.00053 | 0.01368<br>0.01894 | 0.00025<br>0.00019 | 10.0 s<br>10.0 s |
| 1.5                    | p 110                            |            | <u>-</u>   | <b>-</b>   |            |        | 2.0000              |                    |                    |                  |



Sample name: M12 Experiment start time: 10/11/2017 5:31:56 PM Analyst: Assay name: **UV-metric psKa Dorothy Levorse** 

| Assay ID:<br>Filename: |                | \Mehtap\201710 | )11_exp15_pl |            | rument ID:<br><b>_M12_UV-m</b> e |        | 311053<br>a.t3r |              |         |
|------------------------|----------------|----------------|--------------|------------|----------------------------------|--------|-----------------|--------------|---------|
| Events                 | (continued)    |                |              |            |                                  |        |                 |              |         |
| Time                   | Event          | Water          | Acid         | Base       | Methanol                         | рН     | dpH/dt          | pH R-squared | pH SD   |
| 1:08:06.6              | Data point 119 | 0.50000 mL     | 0.15741 mL   | 0.16228 mL | 1.15005 mL                       | 10.990 | -0.00336        | 0.47444      | 0.00024 |
| 1:08:23.3              | Data point 120 | 0.50000 mL     | 0.15741 mL   | 0.16305 mL | 1.15005 mL                       | 11.083 | -0.00375        | 0.47086      | 0.00027 |
| 1:08:39.9              | Data point 121 | 0.50000 mL     | 0.15741 mL   | 0.16399 mL | 1.15005 mL                       | 11.170 | -0.00533        | 0.75131      | 0.00030 |
| 1:08:56.4              | Data point 122 | 0.50000 mL     | 0.15741 mL   | 0.16515 mL | 1.15005 mL                       | 11.250 | -0.00548        | 0.68104      | 0.00033 |
| 1:09:23.3              | Data point 123 | 0.50000 mL     | 0.15741 mL   | 0.16693 mL | 1.15005 mL                       | 11.343 | -0.00508        | 0.52133      | 0.00035 |

1:09:50.3 Data point 124

1:10:17.2 Data point 125

1:10:33.7 Data point 126

1:10:50.4 Data point 127

1:11:17.3 Data point 128

1:11:44.5 Data point 129

1:12:11.7 Data point 130

1:12:28.4 Data point 131

1:16:03.6 Data point 134

1:16:20.5 Data point 135

1:16:37.2 Data point 136

1:16:59.1 Data point 137

1:17:26.1 Data point 138

1:17:42.8 Data point 139

1:18:09.9 Data point 140

1:18:26.5 Data point 141

1:18:53.5 Data point 142

1:19:20.2 Data point 143

1:19:36.8 Data point 144

1:19:53.4 Data point 145

1:20:09.9 Data point 146

1:20:26.5 Data point 147

Report by: Dorothy Levorse 10/12/2017 4:58:17 PM

1:14:13.0 Reference spectrum 1:15:36.2 Data point 133

0.83996 mL 0.27954 mL 0.19828 mL 1.15005 mL 1.980

0.83996 mL 0.27954 mL 0.21355 mL 1.15005 mL 2.079

0.83996 mL 0.27954 mL 0.22615 mL 1.15005 mL 2.190

0.83996 mL 0.27954 mL 0.23638 mL 1.15005 mL 2.306

0.83996 mL 0.27954 mL 0.24203 mL 1.15005 mL 2.398

0.83996 mL 0.27954 mL 0.24770 mL 1.15005 mL 2.500

0.83996 mL 0.27954 mL 0.25252 mL 1.15005 mL 2.618

0.83996 mL 0.27954 mL 0.25621 mL 1.15005 mL 2.715

0.83996 mL 0.27954 mL 0.25920 mL 1.15005 mL 2.841

0.83996 mL 0.27954 mL 0.26110 mL 1.15005 mL 2.939

0.83996 mL 0.27954 mL 0.26293 mL 1.15005 mL 3.038

0.83996 mL 0.27954 mL 0.26435 mL 1.15005 mL 3.141

0.83996 mL 0.27954 mL 0.26548 mL 1.15005 mL 3.246

0.83996 mL 0.27954 mL 0.26637 mL 1.15005 mL 3.355

0.83996 mL 0.27954 mL 0.26705 mL 1.15005 mL 3.467

0.50000 mL 0.15741 mL 0.17161 mL 1.15005 mL 11.532 -0.00432 0.50207

0.50000 mL 0.15741 mL 0.17425 mL 1.15005 mL 11.619 -0.00193 0.17949

0.50000 mL 0.15741 mL 0.17749 mL 1.15005 mL 11.694 -0.00478 0.58682

0.50000 mL 0.15741 mL 0.18213 mL 1.15005 mL 11.790 -0.00530 0.64616

0.50000 mL 0.15741 mL 0.18831 mL 1.15005 mL 11.882 -0.00366 0.51598

0.50000 mL 0.15741 mL 0.19551 mL 1.15005 mL 11.974 -0.00286 0.28361

0.50000 mL 0.15741 mL 0.19826 mL 1.15005 mL 12.003 -0.00532 0.60244

0.50000 mL 0.15741 mL 0.16928 mL 1.15005 mL 11.438 -0.00707 0.81328

-0.05713 0.98577

-0.00199 0.06407

0.06127

0.87682

0.47603

0.95489

0.49761

0.69643

0.39174

0.71541

0.81058

0.76956

0.79190

0.85204

0.58455

0.00240

0.02878

0.00607

0.01670

0.00541

0.00844

0.00417

0.01077

0.01309

0.00876

0.00885

0.01111

0.00792

10.0 033 0.00035 10.0 0.00039 0.00030

0.00031

0.00027

0.00034

0.00284

0.00048

0.00039

0.00152

0.00043

0.00084

0.00038

0.00033

0.00063

0.00072

0.00049

0.00049

0.00059

0.00051

10.0 10.0 0.00022 10.0 10.0 0.00033 10.0 0.00025 10.0 10.0

dpH/e time

10.0

10.0

10.0

10.0 s 10.0

10.0

10.0 10.0 10.0

10.0 10.0 0.00050 10.0

10.0

10.0

10.0

10.0

10.0

10.0

10.0

S

Page 12 of 17

| Events (continued) |                |            |            |            |            |        |  |  |  |  |  |
|--------------------|----------------|------------|------------|------------|------------|--------|--|--|--|--|--|
| Time               | Event          | Water      | Acid       | Base       | Methanol   | рН     |  |  |  |  |  |
| 1:08:06.6          | Data point 119 | 0.50000 mL | 0.15741 mL | 0.16228 mL | 1.15005 mL | 10.990 |  |  |  |  |  |
|                    |                |            |            |            |            |        |  |  |  |  |  |



Experiment start time: 10/11/2017 5:31:56 PM Sample name: M12

Assay name: UV-metric psKa Analyst: **Dorothy Levorse** 

Assay ID: 17J-11014 Instrument ID: T311053 Filename:

 $C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric\ psKa.t3r$ 

# Events (continued)

| 120-43.1   Data point 148   0.83996 mL   0.27954 mL   0.26759 mL   1.15005 mL   3.583   0.01443   0.84501   0.00077   10.0 s   1.21:09.8   Data point 140   0.83996 mL   0.27954 mL   0.26759 mL   1.15005 mL   3.681   0.02073   0.96001   0.00077   10.0 s   1.21:48.0   Data point 150   0.3996 mL   0.27954 mL   0.26856 mL   1.15005 mL   3.861   0.02073   0.96001   0.000174   10.0 s   1.21:48.0   Data point 151   0.83996 mL   0.27954 mL   0.26856 mL   1.15005 mL   3.084   0.03448   0.96106   0.00026   10.0 s   1.22:26.2   Data point 152   0.83996 mL   0.27954 mL   0.26856 mL   1.15005 mL   4.066   0.04100   0.97169   0.00026   10.0 s   1.22:26.2   Data point 154   0.83996 mL   0.27954 mL   0.26803 mL   1.15005 mL   4.066   0.04911   0.97762   0.00245   10.0 s   1.23:09.4   Data point 154   0.83996 mL   0.27954 mL   0.26921 mL   1.15005 mL   4.391   0.09778   0.99200   0.00336   10.0 s   1.23:09.4   Data point 156   0.83996 mL   0.27954 mL   0.26921 mL   1.15005 mL   4.545   0.09811   0.98940   0.00457   10.0 s   1.24:03.3   Data point 156   0.83996 mL   0.27954 mL   0.26921 mL   1.15005 mL   4.645   0.09865   0.98461   0.00490   10.5 s   1.24:03.3   Data point 156   0.83996 mL   0.27954 mL   0.26925 mL   1.15005 mL   4.547   0.09949   0.99151   0.00493   14.0 s   1.25:04.7   Data point 150   0.3996 mL   0.27954 mL   0.26925 mL   1.15005 mL   4.927   0.09949   0.99151   0.00493   18.0 s   1.25:04.7   Data point 150   0.3996 mL   0.27954 mL   0.26965 mL   1.15005 mL   4.267   0.09620   0.9983   0.00479   2.25 s   1.26:15.3   Data point 161   0.83996 mL   0.27954 mL   0.26965 mL   1.15005 mL   5.261   0.009620   0.9983   0.00479   2.25 s   1.26:15.3   Data point 161   0.83996 mL   0.27954 mL   0.26966 mL   1.15005 mL   5.247   0.009620   0.9983   0.00479   2.25 s   1.26:15.3   Data point 161   0.83996 mL   0.27954 mL   0.26966 mL   1.15005 mL   5.647   0.10071   0.96322   0.00493   3.00 s   1.27:254 mL   0.26966 mL   1.15005 mL   5.647   0.10071   0.96322   0.00493   3.00 s   1.27554 mL   0.26966 mL   1.15005 mL   5.   | Events (  | Events (continued) |            |            |            |            |        |          |              |         |        |  |  |
|--|-----------|--------------------|------------|------------|------------|------------|--------|----------|--------------|---------|--------|--|--|
| 121:19.8 Data point 149 0.83996 mL 0.27954 mL 0.26799 mL 1.15005 mL 3.841 0.02073 0.96001 0.00104 10.0 s 121:14.80 Data point 150 0.83996 mL 0.27954 mL 0.26856 mL 1.15005 mL 3.944 0.03448 0.96106 0.00114 10.0 s 121:14.80 Data point 151 0.83996 mL 0.27954 mL 0.26856 mL 1.15005 mL 3.944 0.03448 0.96106 0.00114 10.0 s 121:22.62 Data point 152 0.83996 mL 0.27954 mL 0.26893 mL 1.15005 mL 4.215 0.04911 0.97782 0.0025 10.0 s 122:26.2 Data point 154 0.83996 mL 0.27954 mL 0.26893 mL 1.15005 mL 4.215 0.04911 0.97782 0.0025 10.0 s 123:09.4 Data point 154 0.83996 mL 0.27954 mL 0.26893 mL 1.15005 mL 4.215 0.04911 0.97782 0.00336 10.0 s 123:09.4 Data point 154 0.83996 mL 0.27954 mL 0.26931 mL 1.15005 mL 4.215 0.04911 0.9895 0.00336 10.0 s 123:09.4 Data point 154 0.83996 mL 0.27954 mL 0.26932 mL 1.15005 mL 4.215 0.04911 0.0027 0.98450 0.00336 10.0 s 124:03.3 Data point 156 0.83996 mL 0.27954 mL 0.26938 mL 1.5005 mL 4.777 0.10027 0.98450 0.00498 14.0 s 124:04.0 Data point 156 0.83996 mL 0.27954 mL 0.26935 mL 1.5005 mL 4.777 0.10027 0.98451 0.00498 14.0 s 125:411 0.0445 point 156 0.83996 mL 0.27954 mL 0.26935 mL 1.5005 mL 4.777 0.10027 0.98451 0.00498 14.0 s 125:411 0.0445 point 156 0.83996 mL 0.27954 mL 0.26935 mL 1.5005 mL 5.224 0.08620 0.97833 0.00492 0.255 mL 1.25641 0.0445 point 156 0.83996 mL 0.27954 mL 0.26956 mL 1.15005 mL 5.224 0.08620 0.97833 0.00492 0.255 mL 1.25641 0.0445 point 156 0.83996 mL 0.27954 mL 0.26956 mL 1.15005 mL 5.427 0.10038 0.98171 0.00492 0.25 s 12.2565 0.0448 point 156 0.83996 mL 0.27954 mL 0.26956 mL 1.15005 mL 5.427 0.10038 0.98171 0.00492 0.25 s 12.2565 0.0448 point 156 0.83996 mL 0.27954 mL 0.26956 mL 1.15005 mL 5.427 0.10038 0.98171 0.00492 0.25 s 12.2565 0.0448 point 156 0.83996 mL 0.27954 mL 0.26956 mL 1.15005 mL 5.427 0.10038 0.98171 0.00498 0.25 s 12.2565 0.0448 point 156 0.83996 mL 0.27954 mL 0.26956 mL 1.15005 mL 5.427 0.10038 0.9810 0.99126 0.00498 0.25 s 12.2565 0.0448 point 156 0.83996 mL 0.27954 mL 0.26996 mL 1.15005 mL 5.457 0.00471 0.99126 0.00498 0.25 s 12.2565 0.0449 0.0449 0.0448 | Time      | Event              | Water      | Acid       | Base       | Methanol   | рН     | dpH/dt   | pH R-squared | pH SD   |        |  |  |
| 1212:63. Data point 150 0.83996 mL 0.27954 mL 0.26832 mL 1.15005 mL 3.846 0.02474 0.91122 0.00112 10.0 s 12:20-44 Data point 151 0.83996 mL 0.27954 mL 0.26874 mL 1.15005 mL 4.066 0.04100 0.97169 0.00025 10.0 s 12:20-42 Data point 152 0.83996 mL 0.27954 mL 0.268974 mL 1.15005 mL 4.066 0.04100 0.97169 0.00025 10.0 s 12:24-79 Data point 153 0.83996 mL 0.27954 mL 0.26991 mL 1.15005 mL 4.215 0.04911 0.0776 0.00025 10.0 s 12:23-30 Data point 156 0.83996 mL 0.27954 mL 0.26991 mL 1.15005 mL 4.391 0.06778 0.99200 0.0036 10.0 s 12:33-30 Data point 157 0.83996 mL 0.27954 mL 0.26991 mL 1.15005 mL 4.391 0.06778 0.99461 0.00049 14.0 s 12:33-30 Data point 157 0.83996 mL 0.27954 mL 0.26991 mL 1.15005 mL 4.0004 0.09816 0.99461 0.00049 14.0 s 12:43-430 Data point 157 0.83996 mL 0.27954 mL 0.26993 mL 1.15005 mL 4.0004 0.09816 0.99461 0.00049 14.0 s 12:43-430 Data point 157 0.83996 mL 0.27954 mL 0.26993 mL 1.15005 mL 4.0004 0.09820 0.99580 0.00049 14.0 s 12:43-430 Data point 159 0.83996 mL 0.27954 mL 0.26995 mL 1.15005 mL 5.123 0.99860 0.98592 0.00049 12.0 s 12:54-11 Data point 160 0.83996 mL 0.27954 mL 0.26995 mL 1.15005 mL 5.123 0.99860 0.98592 0.00049 12.0 s 12:55-14 Data point 150 0.83996 mL 0.27954 mL 0.26995 mL 1.15005 mL 5.23 0.99860 0.98592 0.00049 12.0 s 12:55-14 Data point 150 0.83996 mL 0.27954 mL 0.26995 mL 1.15005 mL 5.23 0.99860 0.98592 0.00049 12.0 s 12:55-14 Data point 150 0.83996 mL 0.27954 mL 0.26995 mL 1.15005 mL 5.43 0.99860 0.98592 0.00049 12.0 s 12:55-14 Data point 150 0.83996 mL 0.27954 mL 0.26995 mL 1.15005 mL 5.43 0.99860 0.98960 0.00049 12:55 0.00049 0.00049 12:55 0.00049 0 | 1:20:43.1 |                    |            |            |            |            |        | 0.01443  | 0.84501      |         |        |  |  |
| 121:48.0 Data point 150 0.83996 mL 0.27954 mL 0.26866 mL 1.15005 mL 3,944 0.03448 0.96106 0.00026 10.0 s 1:22:22-0 Data point 150 0.83996 mL 0.27954 mL 0.26893 mL 1.15005 mL 4.066 0.04100 0.97780 0.00265 10.0 s 1:22:24-19 Data point 154 0.83996 mL 0.27954 mL 0.26993 mL 1.15005 mL 4.391 0.09778 0.99200 0.00336 10.0 s 1:23:09.4 Data point 156 0.83996 mL 0.27954 mL 0.26993 mL 1.15005 mL 4.832 0.09214 0.98940 0.00036 10.0 s 1:23:09.4 Data point 156 0.83996 mL 0.27954 mL 0.26921 mL 1.15005 mL 4.645 0.09865 0.98461 0.00490 10.5 s 1:24:03.3 Data point 156 0.83996 mL 0.27954 mL 0.26993 mL 1.15005 mL 4.645 0.09865 0.98461 0.00490 10.5 s 1:24:03.3 Data point 156 0.83996 mL 0.27954 mL 0.26995 mL 1.15005 mL 4.645 0.09949 0.99151 0.00493 18.0 s 1:25:08.7 Data point 150 0.83996 mL 0.27954 mL 0.26958 mL 1.15005 mL 4.927 0.09949 0.99151 0.00493 18.0 s 1:25:08.7 Data point 150 0.83996 mL 0.27954 mL 0.26958 mL 1.15005 mL 4.927 0.09620 0.99893 0.00479 22.5 s 1:26:15.3 Data point 160 0.83996 mL 0.27954 mL 0.26965 mL 1.15005 mL 5.264 0.00620 0.99893 0.00479 22.5 s 1:26:15.3 Data point 160 0.83996 mL 0.27954 mL 0.26966 mL 1.15005 mL 5.264 0.00620 0.9983 0.00479 22.5 s 1:27:29.6 Data point 162 0.83996 mL 0.27954 mL 0.26966 mL 1.15005 mL 5.264 0.00860 0.98592 0.00499 23.0 s 1:27:29.6 Data point 162 0.83996 mL 0.27954 mL 0.26966 mL 1.15005 mL 5.264 0.00893 0.99317 0.00500 26.0 s 1:27:29.6 Data point 162 0.83996 mL 0.27954 mL 0.26967 mL 1.15005 mL 5.645 0.00881 0.99317 0.00500 26.0 s 1:28:254 Data point 160 0.83996 mL 0.27954 mL 0.26968 mL 1.15005 mL 6.150 0.09821 0.99820 0.00498 23.0 s 1:29:59.0 Data point 167 0.83996 mL 0.27954 mL 0.26968 mL 1.15005 mL 6.150 0.09821 0.99820 0.00498 23.0 s 1:29:59.0 Data point 167 0.83996 mL 0.27954 mL 0.26968 mL 1.15005 mL 6.150 0.09820 0.99826 0.00498 23.5 s 1:29:59.0 Data point 167 0.83996 mL 0.27954 mL 0.26968 mL 1.15005 mL 6.150 0.09820 0.99820 0.00498 23.0 s 1:29:59.0 Data point 167 0.83996 mL 0.27954 mL 0.26968 mL 1.15005 mL 6.150 0.09820 0.99820 0.00498 23.0 s 1:29:250 0.00489 0.0048 0.00482 0. | 1:21:09.8 |                    |            |            |            |            |        |          |              |         |        |  |  |
| 12224.2 Data point 152 0.83996 mL 0.27954 mL 0.28974 mL 1.15005 mL 4.215 0.04911 0.9782 0.00245 10.0 s   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 122242 Data point 150 0.83996 mL 0.27954 mL 0.28983 mL 1.15005 mL 4.391 0.97782 0.00245 10.0 s 123094 Data point 150 0.83996 mL 0.27954 mL 0.28921 mL 1.15005 mL 4.391 0.09778 0.98200 0.00336 10.0 s 123094 Data point 150 0.83996 mL 0.27954 mL 0.28921 mL 1.15005 mL 4.645 0.09845 0.98461 0.00490 10.5 s 124033 Data point 150 0.83996 mL 0.27954 mL 0.28931 mL 1.15005 mL 4.645 0.09845 0.98461 0.00490 10.5 s 124033 Data point 150 0.83996 mL 0.27954 mL 0.28938 mL 1.15005 mL 4.645 0.09940 0.98151 0.00491 11.0 s 12503. Data point 150 0.83996 mL 0.27954 mL 0.28958 mL 1.15005 mL 4.297 0.09845 0.99151 0.00491 11.0 s 125041 Data point 150 0.83996 mL 0.27954 mL 0.28957 mL 1.15005 mL 5.264 0.09860 0.98592 0.00490 21.0 s 126541. Data point 160 0.83996 mL 0.27954 mL 0.28957 mL 1.15005 mL 5.264 0.09860 0.98592 0.00490 21.0 s 12665. Data point 161 0.83996 mL 0.27954 mL 0.28966 mL 1.15005 mL 5.264 0.09860 0.98592 0.00490 22.0 s 127:29.6 Data point 162 0.83996 mL 0.27954 mL 0.28966 mL 1.15005 mL 5.264 0.00880 0.98592 0.00490 25.0 s 127:29.6 Data point 162 0.83996 mL 0.27954 mL 0.28967 mL 1.15005 mL 5.264 0.00880 0.989171 0.00500 26.0 s 127:29.6 Data point 160 0.83996 mL 0.27954 mL 0.28967 mL 1.15005 mL 5.264 0.00881 0.99171 0.00500 26.0 s 128:254 Data point 160 0.83996 mL 0.27954 mL 0.28967 mL 1.15005 mL 6.151 0.00987 0.99126 0.00493 30.0 s 128:554 Data point 160 0.83996 mL 0.27954 mL 0.28968 mL 1.15005 mL 6.151 0.00987 0.99126 0.00493 30.5 s 129:559 Data point 160 0.83996 mL 0.27954 mL 0.28968 mL 1.15005 mL 6.150 0.09820 0.98826 0.00498 83.5 s 129:559 Data point 160 0.83996 mL 0.27954 mL 0.28968 mL 1.15005 mL 6.455 0.09820 0.99821 0.00493 30.5 s 131:28.1 Data point 160 0.83996 mL 0.27954 mL 0.28968 mL 1.15005 mL 6.455 0.09820 0.99821 0.00493 30.5 s 131:28.1 Data point 170 0.83996 mL 0.27954 mL 0.28968 mL 1.15005 mL 6.455 0.09820 0.99821 0.00498 30.5 s 131:28.1 Data point 170 0.83996 mL 0.27954 mL 0.28968 mL 1.15005 mL 6.455 0.09820 0.99821 0.00498 30.5 s 131:28.1 Data point 170 0.83996 mL 0.27954 mL 0.27906 mL 1.15005 mL 0.1500 mL 0 |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:22:47.9 Data point 156 0.83996 mL 0.27954 mL 0.26910 mL 1.15005 mL 4.530 0.06214 0.99200 0.00336 10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:23:36.0 D Ala point 155 0.83996 ml 0.27954 ml 0.26931 ml 1.15005 ml 4.530 0.09246 0.09460 0.00457 10.0 s 1:23:36.0 D Ala point 156 0.83996 ml 0.27954 ml 0.26931 ml 1.15005 ml 4.645 0.09865 0.98866 0.00490 10.5 s 1:24:03.3 Data point 158 0.83996 ml 0.27954 ml 0.26934 ml 1.15005 ml 4.771 0.10027 0.98458 0.00409 11.5 s 1:25:06.7 D Ala point 158 0.83996 ml 0.27954 ml 0.26945 ml 1.15005 ml 4.771 0.10027 0.99459 0.00409 11.0 s 1:25:06.7 D Ala point 159 0.83996 ml 0.27954 ml 0.26952 ml 1.15005 ml 5.123 0.09860 0.98592 0.00409 21.0 s 1:25:06.7 D Ala point 160 0.83996 ml 0.27954 ml 0.26957 ml 1.15005 ml 5.123 0.09860 0.98592 0.00409 21.0 s 1:26:15.3 D Ala point 161 0.83996 ml 0.27954 ml 0.26961 ml 1.15005 ml 5.431 0.10011 0.99398 0.00409 22.5 s 1:26:15.3 D Ala point 162 0.83996 ml 0.27954 ml 0.26961 ml 1.15005 ml 5.431 0.10011 0.99398 0.00409 22.5 s 1:27:29.6 D Ala point 162 0.83996 ml 0.27954 ml 0.26976 ml 1.15005 ml 5.847 0.10017 0.99632 0.00498 32.5 s 1:28:55.4 D Ala point 165 0.83996 ml 0.27954 ml 0.26987 ml 1.15005 ml 6.369 0.09902 0.98826 0.00498 32.5 s 1:28:55.4 D Ala point 165 0.83996 ml 0.27954 ml 0.26980 ml 1.15005 ml 6.369 0.09902 0.98826 0.00498 32.5 s 1:29:59.0 D Ala point 167 0.83996 ml 0.27954 ml 0.26985 ml 1.15005 ml 6.633 0.09902 0.98869 0.00498 32.5 s 1:29:59.0 D Ala point 167 0.83996 ml 0.27954 ml 0.26985 ml 1.15005 ml 6.603 0.09902 0.98826 0.00498 32.5 s 1:31:28.1 D Ala point 169 0.83996 ml 0.27954 ml 0.26985 ml 1.15005 ml 6.803 0.09902 0.98826 0.00498 32.5 s 1:31:28.1 D Ala point 169 0.83996 ml 0.27954 ml 0.26994 ml 1.15005 ml 6.903 0.09924 0.98921 0.00498 30.5 s 1:31:24.1 D Ala point 169 0.83996 ml 0.27954 ml 0.27954 ml 0.20004 ml 1.15005 ml 6.903 0.09920 0.98921 0.00498 30.5 s 1:31:32.1 D Ala point 178 0.83996 ml 0.27954 ml 0.27954 ml 0.27004 ml 1.15005 ml 8.331 0.08320 0.09923 0.09033 0.0048 30.5 s 1:33:24.5 D Ala point 179 0.83996 ml 0.27954 ml 0.27954 ml 0.27004 ml 1.15005 ml 9.0052 0.09824 0.00489 30.5 s 1:33:24.5 D Ala point 171 0.83996 ml 0.27954 ml 0.27954 ml 0.27005 ml 9.15005 ml 0.09963 |           | •                  |            |            |            |            |        |          |              |         |        |  |  |
| 123360 Data point 156 0.83996 ml 0.27954 ml 0.26931 ml 1.15005 ml 4.645 0.09865 0.98461 0.00490 14.0 s 124240.3 Data point 157 0.83996 ml 0.27954 ml 0.26945 ml 1.15005 ml 4.721 0.10027 0.98458 0.00490 14.0 s 12554.1 Data point 158 0.83996 ml 0.27954 ml 0.26952 ml 1.15005 ml 4.927 0.09849 0.99151 0.00493 18.0 s 12554.1 Data point 150 0.83996 ml 0.27954 ml 0.26957 ml 1.15005 ml 5.264 0.09860 0.98652 0.00490 21.0 s 12554.1 Data point 160 0.83996 ml 0.27954 ml 0.26957 ml 1.15005 ml 5.264 0.09860 0.99893 0.00479 22.5 s 123615.3 Data point 161 0.83996 ml 0.27954 ml 0.26996 ml 1.15005 ml 5.621 0.10038 0.98171 0.00900 26.0 s 123613.3 Data point 162 0.83996 ml 0.27954 ml 0.26996 ml 1.15005 ml 5.621 0.10038 0.98171 0.00900 26.0 s 123613.3 Data point 165 0.83996 ml 0.27954 ml 0.26996 ml 1.15005 ml 5.621 0.10038 0.98171 0.00900 26.0 s 123613.3 Data point 165 0.83996 ml 0.27954 ml 0.26996 ml 1.15005 ml 6.405 0.00820 0.98060 0.00498 30.0 s 1239340 Data point 165 0.83996 ml 0.27954 ml 0.26983 ml 1.15005 ml 6.405 0.00820 0.98266 0.00498 30.5 s 123939.0 Data point 166 0.83996 ml 0.27954 ml 0.26993 ml 1.15005 ml 6.405 0.00820 0.98859 0.00488 18.5 s 123939.0 Data point 166 0.83996 ml 0.27954 ml 0.26993 ml 1.15005 ml 6.405 0.00820 0.98266 0.00492 32.0 s 131281.1 Data point 169 0.83996 ml 0.27954 ml 0.26990 ml 1.15005 ml 6.405 0.00820 0.98291 0.00489 36.5 s 131281.1 Data point 160 0.83996 ml 0.27954 ml 0.26990 ml 1.15005 ml 6.405 0.00820 0.98291 0.00489 36.5 s 131281.1 Data point 160 0.83996 ml 0.27954 ml 0.26990 ml 1.15005 ml 6.405 0.00820 0.98291 0.00489 36.5 s 133246.1 Data point 170 0.83996 ml 0.27954 ml 0.26990 ml 1.15005 ml 6.405 0.09820 0.99331 0.00482 36.0 s 133246.1 Data point 170 0.83996 ml 0.27954 ml 0.27018 ml 1.15005 ml 6.405 0.09820 0.99331 0.00482 36.0 s 133246.1 Data point 170 0.83996 ml 0.27954 ml 0.27018 ml 1.15005 ml 6.405 0.09820 0.99331 0.00482 36.0 s 133246.1 Data point 170 0.83996 ml 0.27954 ml 0.27018 ml 1.15005 ml 9.406 0.09931 0.09331 0.00482 0.00483 1.00483 0.00483 0.00483 0.00483 0.00483 0.00483 0.00483  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:24:93.0 Data point 157 0.83996 ml 0.27954 ml 0.26938 ml 1.15005 ml 4.771 0.10027 0.99458 0.00499 14.0 s 12:508.7 Data point 158 0.83996 ml 0.27954 ml 0.26945 ml 1.15005 ml 5.123 0.09960 0.99592 0.00490 21.0 s 12:508.7 Data point 169 0.83996 ml 0.27954 ml 0.26957 ml 1.15005 ml 5.123 0.09960 0.99592 0.00490 21.0 s 12:508.7 Data point 160 0.83996 ml 0.27954 ml 0.26957 ml 1.15005 ml 5.123 0.09960 0.99593 0.00490 21.0 s 12:65:51.0 Data point 160 0.83996 ml 0.27954 ml 0.26961 ml 1.15005 ml 5.431 0.10011 0.99398 0.00490 22.5 s 12:65:52.0 Data point 162 0.83996 ml 0.27954 ml 0.26961 ml 1.15005 ml 5.431 0.10013 0.9931 0.00490 22.0 s 12:72:96 Data point 163 0.83996 ml 0.27954 ml 0.26976 ml 1.15005 ml 5.847 0.10071 0.99632 0.00498 30.0 s 12:8:55.4 Data point 164 0.83996 ml 0.27954 ml 0.26996 ml 1.15005 ml 6.369 0.09902 0.98826 0.00498 32.5 s 12:8:55.4 Data point 165 0.83996 ml 0.27954 ml 0.26980 ml 1.15005 ml 6.369 0.09902 0.98826 0.00498 32.5 s 12:9:59.0 Data point 167 0.83996 ml 0.27954 ml 0.26985 ml 1.15005 ml 6.603 0.09902 0.98826 0.00498 32.5 s 12:9:59.0 Data point 167 0.83996 ml 0.27954 ml 0.26985 ml 1.15005 ml 6.603 0.09902 0.98826 0.00498 32.5 s 13:12:21.5 Data point 168 0.83996 ml 0.27954 ml 0.26994 ml 1.15005 ml 6.603 0.09903 0.98951 0.00490 29.5 s 13:13:23.1 Data point 169 0.83996 ml 0.27954 ml 0.26994 ml 1.15005 ml 6.803 0.09903 0.98951 0.00490 29.5 s 13:13:24.1 Data point 169 0.83996 ml 0.27954 ml 0.22954 ml 0.25005 ml 6.803 0.09903 0.9903 0.9035 0.00498 36.5 s 13:13:24.1 Data point 170 0.83996 ml 0.27954 ml 0.27954 ml 0.27954 ml 0.2005 ml 6.803 0.09950 0.09924 0.98921 0.00498 32.5 s 13:13:24.1 Data point 171 0.83996 ml 0.27954 ml 0.27954 ml 0.27050 ml 8.15005 ml 8.304 0.09930 0.99031 0.00480 29.5 s 13:13:24.1 Data point 172 0.83996 ml 0.27954 ml 0.27954 ml 0.27050 ml 8.15005 ml 9.00492 0.09924 0.09924 0.00498 32.5 s 13:13:24.1 Data point 173 0.83996 ml 0.27954 ml 0.27954 ml 0.27050 ml 9.1500 ml 9.00492 0.09924 0.00498 30.00498 30.00498 30.00498 30.00498 30.00498 30.00498 30.00498 30.00498 30.00498 30.00498 |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 12:43:40. Data point 158 0.83996 mL 0.27954 mL 0.26945 mL 1.15005 mL 5.125 0.0986 0.98592 0.00499 21.0 s 1:25504.7 Data point 159 0.83996 mL 0.27954 mL 0.26957 mL 1.15005 mL 5.125 0.09860 0.98592 0.00499 22.5 s 1:2552.1 Data point 161 0.83996 mL 0.27954 mL 0.26961 mL 1.15005 mL 5.264 0.09620 0.97893 0.00479 22.5 s 1:2652.0 Data point 162 0.83996 mL 0.27954 mL 0.26961 mL 1.15005 mL 5.431 0.10011 0.99396 0.00496 25.0 s 1:2652.0 Data point 162 0.83996 mL 0.27954 mL 0.26961 mL 1.15005 mL 5.434 0.10011 0.99396 0.00498 30.0 s 1:2851.3 Data point 164 0.83996 mL 0.27954 mL 0.26976 mL 1.15005 mL 5.434 0.10011 0.99396 0.00498 32.5 s 1:2854.0 Data point 168 0.83996 mL 0.27954 mL 0.26980 mL 1.15005 mL 6.4010 0.09871 0.99622 0.00488 32.5 s 1:29540 Data point 166 0.83996 mL 0.27954 mL 0.26980 mL 1.15005 mL 6.9399 0.09020 0.98826 0.00493 32.5 s 1:30340.2 Data point 167 0.83996 mL 0.27954 mL 0.26986 mL 1.15005 mL 6.950 0.09820 0.98859 0.00488 18.5 s 1:30340.2 Data point 167 0.83996 mL 0.27954 mL 0.26990 mL 1.15005 mL 6.950 0.09820 0.98851 0.00488 36.5 s 1:30340.2 Data point 167 0.83996 mL 0.27954 mL 0.26990 mL 1.15005 mL 6.950 0.09824 0.98291 0.00488 36.5 s 1:30345.5 Data point 170 0.83996 mL 0.27954 mL 0.26990 mL 1.15005 mL 6.950 0.09824 0.98291 0.00489 36.5 s 1:33346.1 Data point 170 0.83996 mL 0.27954 mL 0.26990 mL 1.15005 mL 6.950 0.09824 0.98391 0.00489 37.5 s 1:33346.1 Data point 170 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 6.950 0.09872 0.98306 0.00467 30.0 s 1:33346.1 Data point 170 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 6.950 0.09872 0.98336 0.00487 33.5 s 1:33346.1 Data point 170 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 9.950 0.005872 0.09336 0.00487 33.5 s 1:35221.4 Data point 177 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 9.950 0.00582 0.97306 0.00487 1.5355.2 Data point 177 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 9.950 0.00582 0.97306 0.00487 1.5355.2 Data point 178 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 9.950 0.00682 0.99338 0.000487 1.0088 1.33707.8 Data point 178 0.83996 mL 0.27954 mL 0.270 |           |                    |            |            |            |            |        |          |              |         |        |  |  |
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| 1:27:29.6 Data point 163 0.83996 mL 0.27954 mL 0.26976 mL 1.5005 mL 5.847 0.10071 0.99632 0.0048 30.0 s 1:28:55.4 Data point 164 0.83996 mL 0.27954 mL 0.26976 mL 1.5005 mL 6.101 0.09870 0.99826 0.0048 32.5 s 1:28:55.4 Data point 165 0.83996 mL 0.27954 mL 0.26980 mL 1.15005 mL 6.603 0.0980 0.98859 0.00488 18.5 s 1:29:54.0 Data point 167 0.83996 mL 0.27954 mL 0.26994 mL 1.5005 mL 6.603 0.0980 0.98951 0.00480 29.5 s 1:30:40.2 Data point 168 0.83996 mL 0.27954 mL 0.26994 mL 1.15005 mL 6.603 0.0980 0.98951 0.00480 29.5 s 1:30:40.2 Data point 168 0.83996 mL 0.27954 mL 0.26994 mL 1.15005 mL 6.950 0.09824 0.98921 0.00489 36.5 s 1:32:16.8 Data point 170 0.83996 mL 0.27954 mL 0.26994 mL 1.15005 mL 6.950 0.09824 0.98921 0.00489 36.5 s 1:32:16.8 Data point 170 0.83996 mL 0.27954 mL 0.26994 mL 1.15005 mL 7.843 0.09930 0.97035 0.00496 37.0 s 1:32:16.8 Data point 170 0.83996 mL 0.27954 mL 0.27094 mL 1.15005 mL 7.851 0.09450 0.93391 0.00482 36.0 s 1:33:46.1 Data point 172 0.83996 mL 0.27954 mL 0.27004 mL 1.15005 mL 8.634 0.09732 0.98046 0.00457 30.0 s 1:33:46.1 Data point 174 0.83996 mL 0.27954 mL 0.27013 mL 1.15005 mL 8.634 0.09732 0.96336 0.00482 23.5 s 1:34:52.4 Data point 174 0.83996 mL 0.27954 mL 0.27013 mL 1.15005 mL 9.00450 0.99321 0.00480 17.5 s 1:35:52.1 Data point 176 0.83996 mL 0.27954 mL 0.27013 mL 1.15005 mL 9.301 0.09301 0.90532 0.00481 17.5 s 1:35:52.1 Data point 177 0.83996 mL 0.27954 mL 0.27013 mL 1.15005 mL 9.301 0.09301 0.90532 0.00481 10.0 s 1:36:64.1 Data point 178 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 9.509 0.00621 0.96283 0.00481 10.0 s 1:33:74.6 Data point 179 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 9.650 0.09943 0.90528 0.00481 10.0 s 1:33:74.8 Data point 180 0.83996 mL 0.27954 mL 0.27054 mL 1.15005 mL 9.650 0.09943 0.90528 0.00481 10.0 s 1:33:74.8 Data point 180 0.83996 mL 0.27954 mL 0.27054 mL 1.15005 mL 9.650 0.09943 0.90528 0.00481 10.0 s 1:33:74.8 Data point 180 0.83996 mL 0.27954 mL 0.27056 mL 1.15005 mL 1.0080 0.00747 0.90628 0.00043 10.0 s 1:33:74.1 Data point 180 0.83996 mL 0.27954 m |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:28:11.3 Data point 164 0.83996 mL 0.27954 mL 0.26980 mL 1.15005 mL 6.101 0.09871 0.99126 0.00429 32.0 s 1:29:34.0 Data point 165 0.83996 mL 0.27954 mL 0.26980 mL 1.15005 mL 6.359 0.09802 0.98265 0.00492 32.0 s 1:29:58.0 Data point 167 0.83996 mL 0.27954 mL 0.26980 mL 1.15005 mL 6.550 0.09820 0.98265 0.00490 32.0 s 1:39:321.0 Data point 169 0.83996 mL 0.27954 mL 0.26990 mL 1.15005 mL 6.550 0.09820 0.98261 0.00489 36.5 s 1:31:28.1 Data point 169 0.83996 mL 0.27954 mL 0.26990 mL 1.15005 mL 6.550 0.09820 0.98261 0.00489 36.5 s 1:33:261.6 Data point 171 0.83996 mL 0.27954 mL 0.26999 mL 1.15005 mL 7.343 0.09903 0.93031 0.00480 36.5 s 1:33:261.6 Data point 171 0.83996 mL 0.27954 mL 0.27094 mL 1.15005 mL 8.313 0.08732 0.89046 0.00457 30.0 s 1:33:04.5 Data point 173 0.83996 mL 0.27954 mL 0.27004 mL 1.15005 mL 8.343 0.09903 0.93391 0.00480 23.5 s 1:34:524 Data point 174 0.83996 mL 0.27954 mL 0.27013 mL 1.15005 mL 8.634 0.09550 0.97504 0.00478 19.5 s 1:34:524 Data point 174 0.83996 mL 0.27954 mL 0.27013 mL 1.15005 mL 9.150 0.09502 0.97504 0.00478 19.5 s 1:35:522 Data point 176 0.83996 mL 0.27954 mL 0.27023 mL 1.15005 mL 9.150 0.09605 0.97504 0.00478 17.5 s 1:35:54.0 Data point 176 0.83996 mL 0.27954 mL 0.27023 mL 1.15005 mL 9.150 0.90605 0.97504 0.00461 14.0 s 1:35:522 Data point 176 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.150 0.90605 0.97504 0.00461 14.0 s 1:35:54.0 Data point 177 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.460 0.99943 0.96283 0.00033 10.0 s 1:35:54.0 Data point 178 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.460 0.99943 0.96283 0.00033 10.0 s 1:35:54.0 Data point 178 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.460 0.99943 0.96283 0.00033 10.0 s 1:35:361.8 Data point 178 0.83996 mL 0.27954 mL 0.27056 mL 0.2705 |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:28:554 Data point 166 0.83996 mL 0.27954 mL 0.26983 mL 1.15005 mL 6.369 0.09920 0.98650 0.00482 32.0 s 1:29:590 Data point 166 0.83996 mL 0.27954 mL 0.26983 mL 1.15005 mL 6.635 0.09820 0.98650 0.00480 29.5 s 1:29:590 Data point 167 0.83996 mL 0.27954 mL 0.26989 mL 1.15005 mL 6.635 0.09820 0.98650 0.00480 36.5 s 1:31:28.1 Data point 168 0.83996 mL 0.27954 mL 0.26994 mL 1.15005 mL 7.531 0.09930 0.97035 0.00480 37.0 s 1:32:168 Data point 170 0.83996 mL 0.27954 mL 0.26994 mL 1.15005 mL 7.851 0.09450 0.93391 0.00482 36.0 s 1:33:46.1 Data point 172 0.83996 mL 0.27954 mL 0.27004 mL 1.15005 mL 8.343 0.09930 0.97035 0.00480 37.0 s 1:33:46.1 Data point 172 0.83996 mL 0.27954 mL 0.27004 mL 1.15005 mL 8.854 0.09732 0.89046 0.00457 30.0 s 1:33:46.1 Data point 174 0.83996 mL 0.27954 mL 0.27018 mL 1.15005 mL 8.654 0.09556 0.97504 0.00478 19.5 s 1:34:52.2 Data point 174 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 9.131 0.99556 0.97504 0.00478 19.5 s 1:35:52.2 Data point 176 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 9.131 0.09301 0.9632 0.00483 17.5 s 1:35:52.2 Data point 177 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 9.131 0.08760 0.80852 0.00483 10.0 s 1:35:52.2 Data point 177 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 9.351 0.08760 0.80852 0.00483 10.0 s 1:35:52.2 Data point 179 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 9.559 0.08621 0.96283 0.00333 10.0 s 1:37:07.8 Data point 180 0.83996 mL 0.27954 mL 0.27034 mL 1.15005 mL 9.559 0.06621 0.96283 0.00333 10.0 s 1:37:07.8 Data point 180 0.83996 mL 0.27954 mL 0.27054 mL 0.27056 mL 1.15005 mL 9.768 0.96240 0.96240 0.00487 10.0 s 1:38:22.8 Data point 181 0.83996 mL 0.27954 mL 0.27056 mL 1.15005 mL 9.768 0.96240 0.96240 0.00481 10.0 s 1:38:39:37.9 Data point 183 0.83996 mL 0.27954 mL 0.27056 mL 1.15005 mL 1.15005 mL 0.08621 0.96283 0.00333 10.0 s 1:38:22.8 Data point 185 0.83996 mL 0.27954 mL 0.27056 mL 1.15005 mL 1.15005 mL 1.15005 mL 0.08621 0.96240 0.00047 10.0 s 1:38:39:37.9 Data point 180 0.83996 mL 0.27954 mL 0.27056 mL 1.15005 mL 1.15005 mL 1.15005 mL 1.0282 0.00033 |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:29:34.0 Data point 166   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:29:59.0 Data point 167 0.83996 mL 0.27954 mL 0.26985 mL 1.15005 mL 6.950 0.09824 0.98951 0.00489 36.5 s 1:31:28.1 Data point 168 0.83996 mL 0.27954 mL 0.26999 mL 1.15005 mL 6.950 0.09824 0.98291 0.00489 36.5 s 1:31:28.1 Data point 170 0.83996 mL 0.27954 mL 0.26999 mL 1.15005 mL 7.381 0.09450 0.93391 0.00482 36.0 s 1:33:46.1 Data point 171 0.83996 mL 0.27954 mL 0.27009 mL 1.15005 mL 8.313 0.08732 0.89046 0.00457 30.0 s 1:33:46.1 Data point 172 0.83996 mL 0.27954 mL 0.27009 mL 1.15005 mL 8.634 0.09732 0.96336 0.00489 32.5 s 1:33:46.1 Data point 174 0.83996 mL 0.27954 mL 0.27009 mL 1.15005 mL 8.634 0.09732 0.96336 0.00489 23.5 s 1:34:21.3 Data point 174 0.83996 mL 0.27954 mL 0.27018 mL 1.15005 mL 8.634 0.09732 0.96336 0.00489 23.5 s 1:34:52.4 Data point 174 0.83996 mL 0.27954 mL 0.27018 mL 1.15005 mL 8.634 0.09732 0.96336 0.00489 23.5 s 1:35:21.4 Data point 175 0.83996 mL 0.27954 mL 0.27023 mL 1.15005 mL 9.156 0.09205 0.97180 0.00478 19.5 s 1:35:52.2 Data point 176 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.156 0.09205 0.97180 0.00481 14.0 s 1:36:46.1 Data point 177 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.56 0.09205 0.97180 0.00481 14.0 s 1:36:46.1 Data point 177 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.460 0.09843 0.96283 0.00500 10.5 s 1:37:07.8 Data point 176 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.667 0.06621 0.96283 0.00333 10.0 s 1:37:07.8 Data point 176 0.83996 mL 0.27954 mL 0.27056 mL 1.15005 mL 9.667 0.06624 0.96283 0.00333 10.0 s 1:37:07.8 Data point 180 0.83996 mL 0.27954 mL 0.27056 mL 1.15005 mL 9.678 0.06621 0.96283 0.00333 10.0 s 1:37:07.8 Data point 180 0.83996 mL 0.27954 mL 0.27056 mL 1.15005 mL 9.678 0.06624 0.92144 0.0010 10.0 s 1:33:11.2 Data point 181 0.83996 mL 0.27954 mL 0.27056 mL 1.15005 mL 9.678 0.00625 0.93067 0.00238 10.0 s 1:33:13.9 0.00060 0.00 |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:30:40.2 Data point 168   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:31:28.1 Data point 169   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:32:16.8 Data point 170   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:33:04.5 Data point 171   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:33:46.1 Data point 172   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:34:21.3 Data point 173 0.83996 mL 0.27954 mL 0.27013 mL 1.15005 mL 8.854 0.09556 0.97504 0.00478 19.5 s 1:35:52.4 Data point 175 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.031 0.09050 0.97180 0.00461 14.0 s 1:35:52.2 Data point 176 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.460 0.09205 0.97180 0.00461 14.0 s 1:35:52.2 Data point 177 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.460 0.09205 0.97180 0.00463 10.0 s 1:35:63.2 Data point 178 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.460 0.0943 0.96283 0.00500 10.5 s 1:35:07.8 Data point 179 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.659 0.06621 0.96283 0.0033 10.0 s 1:37:07.8 Data point 180 0.83996 mL 0.27954 mL 0.27051 mL 1.15005 mL 9.659 0.06621 0.96283 0.0033 10.0 s 1:37:34.6 Data point 180 0.83996 mL 0.27954 mL 0.27060 mL 1.15005 mL 9.678 0.0946 0.9948 0.9946 0.9948  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:34:52.4 Data point 174 0.83996 mL 0.27954 mL 0.27030 mL 1.15005 mL 9.156 0.09205 0.97180 0.00461 14.0 s 1:35:51.2 Data point 175 0.83996 mL 0.27954 mL 0.27030 mL 1.15005 mL 9.251 0.08796 0.80852 0.00483 10.0 s 1:35:53.2 Data point 177 0.83996 mL 0.27954 mL 0.27030 mL 1.15005 mL 9.251 0.08796 0.80852 0.00483 10.0 s 1:36:46.1 Data point 178 0.83996 mL 0.27954 mL 0.27037 mL 1.15005 mL 9.657 0.06621 0.96283 0.00500 10.5 s 1:37:37:07.8 Data point 179 0.83996 mL 0.27954 mL 0.27051 mL 1.15005 mL 9.657 0.06621 0.96283 0.00333 10.0 s 1:37:34.6 Data point 180 0.83996 mL 0.27954 mL 0.27051 mL 1.15005 mL 9.657 0.06624 0.97101 0.00348 10.0 s 1:37:34.6 Data point 181 0.83996 mL 0.27954 mL 0.27060 mL 1.15005 mL 9.657 0.06624 0.97101 0.00348 10.0 s 1:38:49.6 Data point 182 0.83996 mL 0.27954 mL 0.27060 mL 1.15005 mL 9.878 0.03288 0.94322 0.00167 10.0 s 1:38:49.6 Data point 183 0.83996 mL 0.27954 mL 0.27105 mL 1.15005 mL 9.993 0.02142 0.92144 0.00110 10.0 s 1:38:49.6 Data point 185 0.83996 mL 0.27954 mL 0.27105 mL 1.15005 mL 9.993 0.02142 0.92144 0.00110 10.0 s 1:39:39.7 Data point 185 0.83996 mL 0.27954 mL 0.27156 mL 1.15005 mL 10.282 0.00655 0.59948 0.00042 10.0 s 1:39:39.6 Data point 186 0.83996 mL 0.27954 mL 0.27165 mL 1.15005 mL 10.282 0.00655 0.59948 0.00042 10.0 s 1:43:00.2 Data point 188 0.83996 mL 0.27954 mL 0.27286 mL 1.15005 mL 10.283 0.00033 0.05079 0.00028 10.0 s 1:44:00.2 Data point 188 0.83996 mL 0.27954 mL 0.27286 mL 1.15005 mL 10.583 0.00034 0.00982 0.00017 10.0 s 1:44:00.2 Data point 189 0.83996 mL 0.27954 mL 0.27286 mL 1.15005 mL 10.583 0.00034 0.00982 0.00017 10.0 s 1:44:00.2 Data point 190 0.83996 mL 0.27954 mL 0.27286 mL 1.15005 mL 10.684 0.00034 0.00982 0.00017 10.0 s 1:44:00.2 Data point 191 0.83996 mL 0.27954 mL 0.27286 mL 1.15005 mL 10.686 0.00034 0.00982 0.00017 10.0 s 1:44:00.2 Data point 190 0.83996 mL 0.27954 mL 0.27512 mL 1.15005 mL 10.686 0.00034 0.00982 0.00017 10.0 s 1:44:00.3 Data point 191 0.83996 mL 0.27954 mL 0.27512 mL 1.15005 mL 10.686 0.00034 0.00034 0.00034 10.0 s 1:44:30.3 Data point |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:36:52.2 Data point 176   |           |                    |            |            |            |            |        | 0.09301  |              |         |        |  |  |
| 1:36:46.1 Data point 177   |           |                    |            |            |            |            |        | 0.09205  |              |         |        |  |  |
| 1:36:46.1 Data point 178   | 1:35:52.2 | Data point 176     | 0.83996 mL | 0.27954 mL | 0.27030 mL | 1.15005 mL | 9.321  | 0.08796  | 0.80852      | 0.00483 | 10.0 s |  |  |
| 1:37:07.8 Data point 179   | 1:36:18.9 |                    |            |            |            |            |        | 0.09943  |              |         |        |  |  |
| 1:37:34.6 Data point 180 0.83996 mL 0.27954 mL 0.27060 mL 1.15005 mL 9.768 0.04967 0.93667 0.00253 10.0 s 1:38:01.2 Data point 181 0.83996 mL 0.27954 mL 0.27072 mL 1.15005 mL 9.878 0.03288 0.94322 0.00167 10.0 s 1:38:22.8 Data point 182 0.83996 mL 0.27954 mL 0.27086 mL 1.15005 mL 9.993 0.02142 0.92144 0.00110 10.0 s 1:38:39:11.2 Data point 183 0.83996 mL 0.27954 mL 0.27105 mL 1.15005 mL 10.086 0.01737 0.85820 0.00093 10.0 s 1:39:37.9 Data point 185 0.83996 mL 0.27954 mL 0.27124 mL 1.15005 mL 10.191 0.00828 0.65791 0.00050 10.0 s 1:39:37.9 Data point 186 0.83996 mL 0.27954 mL 0.27124 mL 1.15005 mL 10.191 0.00828 0.65791 0.00050 10.0 s 1:39:37.9 Data point 187 0.83996 mL 0.27954 mL 0.27124 mL 1.15005 mL 10.388 -0.00075 0.01811 0.00028 10.0 s 1:40:31.5 Data point 187 0.83996 mL 0.27954 mL 0.27232 mL 1.15005 mL 10.388 -0.00075 0.01811 0.00028 10.0 s 1:41:30.2 Data point 188 0.83996 mL 0.27954 mL 0.27232 mL 1.15005 mL 10.883 -0.00075 0.01811 0.00028 10.0 s 1:41:30.2 Data point 189 0.83996 mL 0.27954 mL 0.27342 mL 1.15005 mL 10.674 -0.00102 0.05048 0.00022 10.0 s 1:42:03.9 Data point 190 0.83996 mL 0.27954 mL 0.27342 mL 1.15005 mL 10.674 -0.00102 0.05048 0.00022 10.0 s 1:42:03.9 Data point 191 0.83996 mL 0.27954 mL 0.27512 mL 1.15005 mL 10.674 -0.00102 0.05048 0.00022 10.0 s 1:43:30.6 Data point 192 0.83996 mL 0.27954 mL 0.27512 mL 1.15005 mL 10.679 -0.00678 0.60168 0.00043 10.0 s 1:43:37.1 Data point 193 0.83996 mL 0.27954 mL 0.27512 mL 1.15005 mL 10.599 -0.00679 0.41179 0.00039 10.0 s 1:43:50.3 Data point 194 0.83996 mL 0.27954 mL 0.2893 mL 1.15005 mL 11.590 -0.00670 0.75163 0.00050 10.0 s 1:44:44.4 Data point 196 0.83996 mL 0.27954 mL 0.2894 mL 0.28950 mL 1.15005 mL 11.500 mL 11.500 -0.00670 0.51564 0.00043 10.0 s 1:44:44.4 Data point 199 0.83996 mL 0.27954 mL 0.2894 mL 0.28950 mL 1.15005 mL 11.500 mL 11.500 -0.00614 0.55576 0.00041 10.0 s 1:46:50.5 Data point 199 0.83996 mL 0.27954 mL 0.28980 mL 1.15005 mL 11.500 mL 11.500 -0.00014 0.0084 0.00043 10.0 s 1:46:50.5 Data point 200 0.83996 mL 0.27954 mL 0.28980 mL 1. | 1:36:46.1 |                    |            |            |            |            |        | 0.06621  |              |         |        |  |  |
| 1:38:01.2 Data point 181   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:38:22.8       Data point 182       0.83996 mL       0.27954 mL       0.27086 mL       1.15005 mL       9.993       0.02142       0.92144       0.00110       10.0 s         1:38:49.6       Data point 184       0.83996 mL       0.27954 mL       0.27105 mL       1.15005 mL       10.086       0.01737       0.85820       0.00093       10.0 s         1:39:11.2       Data point 186       0.83996 mL       0.27954 mL       0.27124 mL       1.15005 mL       10.086       0.0655       0.59948       0.000042       10.0 s         1:39:37.9       Data point 186       0.83996 mL       0.27954 mL       0.27124 mL       1.15005 mL       10.388       -0.00075       0.01811       0.00022       10.0 s         1:40:31.5       Data point 187       0.83996 mL       0.27954 mL       0.27282 mL       1.15005 mL       10.488       0.00075       0.01811       0.00022       10.0 s         1:41:30.4       Data point 188       0.83996 mL       0.27954 mL       0.27342 mL       1.15005 mL       10.488       0.00133       0.05079       0.00029       10.0 s         1:42:02.1       Data point 190       0.83996 mL       0.27954 mL       0.27342 mL       1.15005 mL       10.674       -0.00102       0.05048       0.00022       10.0 s </td <td></td>   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:38:49.6       Data point 183       0.83996 mL       0.27954 mL       0.27105 mL       1.15005 mL       10.086       0.01737       0.85820       0.00093       10.0 s         1:39:17.2       Data point 185       0.83996 mL       0.27954 mL       0.27150 mL       1.15005 mL       10.191       0.00828       0.65791       0.00050       10.0 s         1:39:37.9       Data point 186       0.83996 mL       0.27954 mL       0.27150 mL       1.15005 mL       10.282       0.00655       0.59948       0.00022       10.0 s         1:40:31.5       Data point 187       0.83996 mL       0.27954 mL       0.27232 mL       1.15005 mL       10.488       0.00133       0.05079       0.00022       10.0 s         1:41:03.4       Data point 188       0.83996 mL       0.27954 mL       0.27286 mL       1.15005 mL       10.583       -0.00034       0.0982       0.00017       10.0 s         1:42:30.2       Data point 189       0.83996 mL       0.27954 mL       0.27954 mL       1.15005 mL       10.583       -0.00044       0.00982       0.00017       10.0 s         1:42:30.2       Data point 190       0.83996 mL       0.27954 mL       0.27512 mL       1.15005 mL       10.664       -0.00102       0.05048       0.00022       10.0 s     <   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:39:11.2       Data point 184       0.83996 mL       0.27954 mL       0.27124 mL       1.15005 mL       10.191       0.00828       0.65791       0.00050       10.0 s         1:39:59.6       Data point 186       0.83996 mL       0.27954 mL       0.27150 mL       1.15005 mL       10.282       0.00655       0.59948       0.00042       10.0 s         1:40:31.5       Data point 187       0.83996 mL       0.27954 mL       0.27232 mL       1.15005 mL       10.388       -0.00073       0.01811       0.00028       10.0 s         1:41:03.4       Data point 188       0.83996 mL       0.27954 mL       0.27286 mL       1.15005 mL       10.684       0.00133       0.05079       0.00029       10.0 s         1:41:30.2       Data point 189       0.83996 mL       0.27954 mL       0.27286 mL       1.15005 mL       10.674       -0.00102       0.05048       0.00022       10.0 s         1:42:02.1       Data point 190       0.83996 mL       0.27954 mL       0.27427 mL       1.15005 mL       10.674       -0.0012       0.5048       0.00022       10.0 s         1:43:30.9       Data point 191       0.83996 mL       0.27954 mL       0.275599 mL       1.15005 mL       10.674       -0.00328       0.60168       0.00043       10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:39:37.9       Data point 185       0.83996 mL       0.27954 mL       0.27150 mL       1.15005 mL       10.282       0.00655       0.59948       0.00042       10.0 s         1:39:59.6       Data point 186       0.83996 mL       0.27954 mL       0.27182 mL       1.15005 mL       10.488       -0.00075       0.01811       0.00028       10.0 s         1:40:30.4       Data point 187       0.83996 mL       0.27954 mL       0.27286 mL       1.15005 mL       10.488       -0.00033       0.05079       0.00029       10.0 s         1:41:30.4       Data point 189       0.83996 mL       0.27954 mL       0.27286 mL       1.15005 mL       10.674       -0.00102       0.05048       0.00022       10.0 s         1:42:02.1       Data point 190       0.83996 mL       0.27954 mL       0.27427 mL       1.15005 mL       10.674       -0.00102       0.05048       0.00022       10.0 s         1:42:33.9       Data point 191       0.83996 mL       0.27954 mL       0.27559 mL       1.15005 mL       10.868       -0.00507       0.41179       0.00039       10.0 s         1:43:30.6       Data point 192       0.83996 mL       0.27954 mL       0.27759 mL       1.15005 mL       11.059       -0.00678       0.60168       0.00043       10.0 s   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:39:59.6       Data point 186       0.83996 mL       0.27954 mL       0.27182 mL       1.15005 mL       10.388       -0.00075       0.01811       0.00028       10.0 s         1:40:31.5       Data point 187       0.83996 mL       0.27954 mL       0.27228 mL       1.15005 mL       10.488       0.00133       0.05079       0.00029       10.0 s         1:41:30.2       Data point 188       0.83996 mL       0.27954 mL       0.27228 mL       1.15005 mL       10.674       -0.00102       0.05048       0.00022       10.0 s         1:42:30.2       Data point 199       0.83996 mL       0.27954 mL       0.27427 mL       1.15005 mL       10.674       -0.00102       0.05048       0.00022       10.0 s         1:42:30.9       Data point 191       0.83996 mL       0.27954 mL       0.27512 mL       1.15005 mL       10.770       -0.00328       0.29122       0.00030       10.0 s         1:43:17.1       Data point 192       0.83996 mL       0.27954 mL       0.27512 mL       1.15005 mL       10.959       -0.00678       0.60168       0.00043       10.0 s         1:43:17.1       Data point 193       0.83996 mL       0.27954 mL       0.27843 mL       1.15005 mL       11.154       -0.00832       0.77640       0.00047       10.0 s   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:40:31.5       Data point 187       0.83996 mL       0.27954 mL       0.27232 mL       1.15005 mL       10.488       0.00133       0.05079       0.00029       10.0 s         1:41:03.4       Data point 188       0.83996 mL       0.27954 mL       0.27286 mL       1.15005 mL       10.583       -0.00034       0.00982       0.00017       10.0 s         1:41:30.2       Data point 189       0.83996 mL       0.27954 mL       0.27427 mL       1.15005 mL       10.674       -0.00102       0.05048       0.00022       10.0 s         1:42:33.9       Data point 191       0.83996 mL       0.27954 mL       0.27427 mL       1.15005 mL       10.770       -0.00328       0.29122       0.00030       10.0 s         1:43:00.6       Data point 191       0.83996 mL       0.27954 mL       0.27599 mL       1.15005 mL       10.959       -0.00678       0.60168       0.00043       10.0 s         1:43:31.7       Data point 192       0.83996 mL       0.27954 mL       0.27707 mL       1.15005 mL       11.059       -0.00632       0.77640       0.00047       10.0 s         1:44:17.2       Data point 195       0.83996 mL       0.27954 mL       0.28013 mL       1.15005 mL       11.237       -0.00901       0.79163       0.00054       10.0 s   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:41:03.4       Data point 188       0.83996 mL       0.27954 mL       0.27286 mL       1.15005 mL       10.583       -0.00034       0.00982       0.00017       10.0 s         1:41:30.2       Data point 189       0.83996 mL       0.27954 mL       0.27342 mL       1.15005 mL       10.674       -0.00102       0.05048       0.00022       10.0 s         1:42:02.1       Data point 190       0.83996 mL       0.27954 mL       0.27427 mL       1.15005 mL       10.770       -0.00328       0.29122       0.00030       10.0 s         1:42:33.9       Data point 191       0.83996 mL       0.27954 mL       0.275512 mL       1.15005 mL       10.868       -0.00507       0.41179       0.00039       10.0 s         1:43:00.6       Data point 192       0.83996 mL       0.27954 mL       0.27707 mL       1.15005 mL       11.059       -0.00678       0.60168       0.00043       10.0 s         1:43:50.3       Data point 194       0.83996 mL       0.27954 mL       0.27954 mL       0.28013 mL       1.15005 mL       11.154       -0.00988       0.80264       0.00054       10.0 s         1:44:41.7.2       Data point 195       0.83996 mL       0.27954 mL       0.28279 mL       1.15005 mL       11.5005 mL       11.237       -0.00901       0.7  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:41:30.2       Data point 189       0.83996 mL       0.27954 mL       0.27342 mL       1.15005 mL       10.674       -0.00102       0.05048       0.00022       10.0 s         1:42:02.1       Data point 190       0.83996 mL       0.27954 mL       0.27427 mL       1.15005 mL       10.770       -0.00328       0.29122       0.00030       10.0 s         1:42:33.9       Data point 191       0.83996 mL       0.27954 mL       0.27512 mL       1.15005 mL       10.868       -0.00507       0.41179       0.00039       10.0 s         1:43:17.1       Data point 193       0.83996 mL       0.27954 mL       0.27707 mL       1.15005 mL       11.059       -0.00678       0.60168       0.00043       10.0 s         1:43:33.7       Data point 194       0.83996 mL       0.27954 mL       0.27843 mL       1.15005 mL       11.154       -0.00988       0.80264       0.00047       10.0 s         1:44:41.7.2       Data point 196       0.83996 mL       0.27954 mL       0.28279 mL       1.15005 mL       11.331       -0.00630       0.51564       0.00043       10.0 s         1:44:44.1       Data point 197       0.83996 mL       0.27954 mL       0.288584 mL       1.15005 mL       11.427       -0.00714       0.67877       0.00043       10.0 s <td></td>   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:42:02.1       Data point 190       0.83996 mL       0.27954 mL       0.27427 mL       1.15005 mL       10.770       -0.00328       0.29122       0.00030       10.0 s         1:42:33.9       Data point 191       0.83996 mL       0.27954 mL       0.27512 mL       1.15005 mL       10.868       -0.00507       0.41179       0.00039       10.0 s         1:43:00.6       Data point 192       0.83996 mL       0.27954 mL       0.27599 mL       1.15005 mL       10.959       -0.00678       0.60168       0.00043       10.0 s         1:43:33.7       Data point 194       0.83996 mL       0.27954 mL       0.27707 mL       1.15005 mL       11.059       -0.00832       0.77640       0.00047       10.0 s         1:43:50.3       Data point 195       0.83996 mL       0.27954 mL       0.28013 mL       1.15005 mL       11.154       -0.00988       0.80264       0.00054       10.0 s         1:44:17.2       Data point 196       0.83996 mL       0.27954 mL       0.28279 mL       1.15005 mL       11.331       -0.00630       0.51564       0.00043       10.0 s         1:45:11.1       Data point 197       0.83996 mL       0.27954 mL       0.28923 mL       1.15005 mL       11.520       -0.00614       0.55576       0.00041       10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:42:33.9       Data point 191       0.83996 mL       0.27954 mL       0.27512 mL       1.15005 mL       10.868       -0.00507       0.41179       0.00039       10.0 s         1:43:00.6       Data point 192       0.83996 mL       0.27954 mL       0.27599 mL       1.15005 mL       10.959       -0.00678       0.60168       0.00043       10.0 s         1:43:17.1       Data point 193       0.83996 mL       0.27954 mL       0.27707 mL       1.15005 mL       11.059       -0.00832       0.77640       0.00047       10.0 s         1:43:33.7       Data point 194       0.83996 mL       0.27954 mL       0.27943 mL       1.15005 mL       11.154       -0.00988       0.80264       0.00054       10.0 s         1:43:50.3       Data point 195       0.83996 mL       0.27954 mL       0.28013 mL       1.15005 mL       11.237       -0.00901       0.79163       0.00050       10.0 s         1:44:47.2       Data point 196       0.83996 mL       0.27954 mL       0.28584 mL       1.15005 mL       11.427       -0.00714       0.67877       0.00043       10.0 s         1:45:11.1       Data point 198       0.83996 mL       0.27954 mL       0.28923 mL       1.15005 mL       11.593       -0.00614       0.55576       0.00041       10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:43:00.6       Data point 192       0.83996 mL       0.27954 mL       0.27559 mL       1.15005 mL       10.959       -0.00678       0.60168       0.00043       10.0 s         1:43:17.1       Data point 193       0.83996 mL       0.27954 mL       0.27707 mL       1.15005 mL       11.059       -0.00832       0.77640       0.00047       10.0 s         1:43:33.7       Data point 194       0.83996 mL       0.27954 mL       0.27843 mL       1.15005 mL       11.154       -0.00988       0.80264       0.00054       10.0 s         1:43:50.3       Data point 195       0.83996 mL       0.27954 mL       0.28013 mL       1.15005 mL       11.237       -0.00901       0.79163       0.00050       10.0 s         1:44:17.2       Data point 196       0.83996 mL       0.27954 mL       0.28279 mL       1.15005 mL       11.331       -0.00630       0.51564       0.00043       10.0 s         1:45:11.1       Data point 197       0.83996 mL       0.27954 mL       0.28923 mL       1.15005 mL       11.520       -0.00614       0.55576       0.00041       10.0 s         1:46:05.3       Data point 200       0.83996 mL       0.27954 mL       0.29880 mL       1.15005 mL       11.684       -0.00807       0.69880       0.00048       10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:43:17.1       Data point 193       0.83996 mL       0.27954 mL       0.27707 mL       1.15005 mL       11.059       -0.00832       0.77640       0.00047       10.0 s         1:43:33.7       Data point 194       0.83996 mL       0.27954 mL       0.27843 mL       1.15005 mL       11.154       -0.00988       0.80264       0.00054       10.0 s         1:43:50.3       Data point 195       0.83996 mL       0.27954 mL       0.28013 mL       1.15005 mL       11.237       -0.00901       0.79163       0.00050       10.0 s         1:44:17.2       Data point 196       0.83996 mL       0.27954 mL       0.28279 mL       1.15005 mL       11.331       -0.00630       0.51564       0.00043       10.0 s         1:44:17.1       Data point 197       0.83996 mL       0.27954 mL       0.28584 mL       1.15005 mL       11.427       -0.00714       0.67877       0.00043       10.0 s         1:45:11.1       Data point 198       0.83996 mL       0.27954 mL       0.28923 mL       1.15005 mL       11.520       -0.00614       0.55576       0.00041       10.0 s         1:46:05.3       Data point 200       0.83996 mL       0.27954 mL       0.29880 mL       1.15005 mL       11.684       -0.00807       0.69880       0.00048       10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:43:33.7       Data point 194       0.83996 mL       0.27954 mL       0.27843 mL       1.15005 mL       11.154       -0.00988       0.80264       0.00054       10.0 s         1:43:50.3       Data point 195       0.83996 mL       0.27954 mL       0.28013 mL       1.15005 mL       11.237       -0.00901       0.79163       0.00050       10.0 s         1:44:17.2       Data point 196       0.83996 mL       0.27954 mL       0.28279 mL       1.15005 mL       11.331       -0.00630       0.51564       0.00043       10.0 s         1:44:44.1       Data point 197       0.83996 mL       0.27954 mL       0.28584 mL       1.15005 mL       11.427       -0.00714       0.67877       0.00043       10.0 s         1:45:11.1       Data point 198       0.83996 mL       0.27954 mL       0.28923 mL       1.15005 mL       11.520       -0.00614       0.55576       0.00041       10.0 s         1:46:05.3       Data point 200       0.83996 mL       0.27954 mL       0.29880 mL       1.15005 mL       11.583       -0.00911       0.75680       0.00048       10.0 s         1:46:32.4       Data point 201       0.83996 mL       0.27954 mL       0.30649 mL       1.15005 mL       11.785       -0.00734       0.62077       0.00048       10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:43:50.3       Data point 195       0.83996 mL       0.27954 mL       0.28013 mL       1.15005 mL       11.237       -0.00901       0.79163       0.00050       10.0 s         1:44:17.2       Data point 196       0.83996 mL       0.27954 mL       0.28279 mL       1.15005 mL       11.331       -0.00630       0.51564       0.00043       10.0 s         1:44:44.1       Data point 197       0.83996 mL       0.27954 mL       0.28584 mL       1.15005 mL       11.427       -0.00714       0.67877       0.00043       10.0 s         1:45:11.1       Data point 198       0.83996 mL       0.27954 mL       0.28923 mL       1.15005 mL       11.520       -0.00614       0.55576       0.00041       10.0 s         1:45:43.5       Data point 199       0.83996 mL       0.27954 mL       0.29316 mL       1.15005 mL       11.593       -0.00911       0.75680       0.00042       10.0 s         1:46:05.3       Data point 200       0.83996 mL       0.27954 mL       0.29880 mL       1.15005 mL       11.684       -0.00807       0.69880       0.00048       10.0 s         1:46:32.4       Data point 202       0.83996 mL       0.27954 mL       0.31599 mL       1.15005 mL       11.883       -0.00847       0.74340       0.00049       10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:44:17.2       Data point 196       0.83996 mL       0.27954 mL       0.28279 mL       1.15005 mL       11.331       -0.00630       0.51564       0.00043       10.0 s         1:44:44.1       Data point 197       0.83996 mL       0.27954 mL       0.28584 mL       1.15005 mL       11.427       -0.00714       0.67877       0.00043       10.0 s         1:45:11.1       Data point 198       0.83996 mL       0.27954 mL       0.28923 mL       1.15005 mL       11.520       -0.00614       0.55576       0.00041       10.0 s         1:45:43.5       Data point 199       0.83996 mL       0.27954 mL       0.29316 mL       1.15005 mL       11.593       -0.00911       0.75680       0.00052       10.0 s         1:46:05.3       Data point 200       0.83996 mL       0.27954 mL       0.29880 mL       1.15005 mL       11.684       -0.00807       0.69880       0.00048       10.0 s         1:46:32.4       Data point 201       0.83996 mL       0.27954 mL       0.30649 mL       1.15005 mL       11.785       -0.00734       0.62077       0.00046       10.0 s         1:46:59.5       Data point 202       0.83996 mL       0.27954 mL       0.31599 mL       1.15005 mL       11.883       -0.00847       0.74340       0.00049       10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:44:44.1       Data point 197       0.83996 mL       0.27954 mL       0.28584 mL       1.15005 mL       11.427       -0.00714       0.67877       0.00043       10.0 s         1:45:11.1       Data point 198       0.83996 mL       0.27954 mL       0.28923 mL       1.15005 mL       11.520       -0.00614       0.55576       0.00041       10.0 s         1:45:43.5       Data point 199       0.83996 mL       0.27954 mL       0.29316 mL       1.15005 mL       11.593       -0.00911       0.75680       0.00052       10.0 s         1:46:05.3       Data point 200       0.83996 mL       0.27954 mL       0.29880 mL       1.15005 mL       11.684       -0.00807       0.69880       0.00048       10.0 s         1:46:32.4       Data point 201       0.83996 mL       0.27954 mL       0.30649 mL       1.15005 mL       11.785       -0.00734       0.62077       0.00046       10.0 s         1:46:59.5       Data point 202       0.83996 mL       0.27954 mL       0.31599 mL       1.15005 mL       11.883       -0.00847       0.74340       0.00049       10.0 s         1:47:26.6       Data point 203       0.83996 mL       0.27954 mL       0.32723 mL       1.15005 mL       11.979       -0.00379       0.37547       0.00031       10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:45:43.5       Data point 199       0.83996 mL       0.27954 mL       0.29316 mL       1.15005 mL       11.593       -0.00911       0.75680       0.00052       10.0 s         1:46:05.3       Data point 200       0.83996 mL       0.27954 mL       0.29880 mL       1.15005 mL       11.684       -0.00807       0.69880       0.00048       10.0 s         1:46:32.4       Data point 201       0.83996 mL       0.27954 mL       0.30649 mL       1.15005 mL       11.785       -0.00734       0.62077       0.00046       10.0 s         1:46:59.5       Data point 202       0.83996 mL       0.27954 mL       0.31599 mL       1.15005 mL       11.883       -0.00847       0.74340       0.00049       10.0 s         1:47:26.6       Data point 203       0.83996 mL       0.27954 mL       0.32723 mL       1.15005 mL       11.979       -0.00379       0.37547       0.00031       10.0 s  |           |                    |            |            |            |            |        |          |              | 0.00043 | 10.0 s |  |  |
| 1:46:05.3 Data point 200 0.83996 mL 0.27954 mL 0.29880 mL 1.15005 mL 11.684 -0.00807 0.69880 0.00048 10.0 s<br>1:46:32.4 Data point 201 0.83996 mL 0.27954 mL 0.30649 mL 1.15005 mL 11.785 -0.00734 0.62077 0.00046 10.0 s<br>1:46:59.5 Data point 202 0.83996 mL 0.27954 mL 0.31599 mL 1.15005 mL 11.883 -0.00847 0.74340 0.00049 10.0 s<br>1:47:26.6 Data point 203 0.83996 mL 0.27954 mL 0.32723 mL 1.15005 mL 11.979 -0.00379 0.37547 0.00031 10.0 s   | 1:45:11.1 | Data point 198     | 0.83996 mL | 0.27954 mL | 0.28923 mL | 1.15005 mL | 11.520 | -0.00614 | 0.55576      | 0.00041 | 10.0 s |  |  |
| 1:46:32.4 Data point 201 0.83996 mL 0.27954 mL 0.30649 mL 1.15005 mL 11.785 -0.00734 0.62077 0.00046 10.0 s<br>1:46:59.5 Data point 202 0.83996 mL 0.27954 mL 0.31599 mL 1.15005 mL 11.883 -0.00847 0.74340 0.00049 10.0 s<br>1:47:26.6 Data point 203 0.83996 mL 0.27954 mL 0.32723 mL 1.15005 mL 11.979 -0.00379 0.37547 0.00031 10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:46:59.5 Data point 202 0.83996 mL 0.27954 mL 0.31599 mL 1.15005 mL 11.883 -0.00847 0.74340 0.00049 10.0 s<br>1:47:26.6 Data point 203 0.83996 mL 0.27954 mL 0.32723 mL 1.15005 mL 11.979 -0.00379 0.37547 0.00031 10.0 s   |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:47:26.6 Data point 203 0.83996 mL 0.27954 mL 0.32723 mL 1.15005 mL 11.979 -0.00379 0.37547 0.00031 10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
|  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
| 1:47:43.3 Data point 204 0.83996 mL 0.27954 mL 0.33121 mL 1.15005 mL 12.001 -0.00521 0.53217 0.00035 10.0 s  |           |                    |            |            |            |            |        |          |              |         |        |  |  |
|  | 1:47:43.3 | Data point 204     | 0.83996 mL | 0.27954 mL | 0.33121 mL | 1.15005 mL | 12.001 | -0.00521 | 0.5321/      | 0.00035 | 10.0 s |  |  |



Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse** 

Assay ID: 17J-11014 Instrument ID: T311053

Filename: C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

#### Events (continued)

Time **Event** Water Acid **Base** Methanol pH dpH/dt pH R-squared pH SD dpH/dt time Ten

1:49:42.4 Assay volumes 1.08996 mL 0.41228 mL 0.33121 mL 1.15005 mL

#### Assay Settings

| Setting | \ /- I | Out at the all Males a | Date/Time changed      | lance and a self-record |
|---------|--------|------------------------|------------------------|-------------------------|
| Sattina | Value  | Original Vallid        | Hate/ Lime change      | IMPORTED TROM           |
| Octuing | value  | Original Value         | Date, i iiie ciialigea |                         |

General Settings

Analyst name **Dorothy Levorse** 

Separate reference vial

Standard Experiment Settings

Number of titrations

2.000 Minimum pH Maximum pH 12.000

pH step between points of 0.100 0.00002 mL

Minimum titrant addition 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 1.15 mL

Cosolvent added Automatic ISA water volume 0.35 mL Water added Automatic Buffer in use

After medium addition, stir for 5 seconds

Sample Sonication

Sonicate Yes

Adjust pH for sonication No

Sonicate for 120 seconds After sonication stir for 30 seconds

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 0.15 mL

Report by: Dorothy Levorse 10/12/2017 4:58:17 PM



Assay name: **UV-metric psKa** Analyst: **Dorothy Levorse** 

Instrument ID: Assay ID: 17J-11014 T311053 Filename: C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

#### Assay Settings (continued)

| Setting | Value | Original Value | Date/Time changed | Imported from |
|---------|-------|----------------|-------------------|---------------|
|         |       |                |                   |               |

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 0.34 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

Value

#### Calibration Settings

| Setting                   | Value  | Date/Time changed     | Imported from                                    |
|---------------------------|--------|-----------------------|--|
| Four-Plus alpha           | 0.109  | 10/11/2017 5:31:56 PM | C:\Sirius_T3\17J-11006_Blank standardisation.t3r |
| Four-Plus S               | 1.0007 | 10/11/2017 5:31:56 PM | C:\Sirius_T3\17J-11006_Blank standardisation.t3r |
| Four-Plus jH              | 0.3    | 10/11/2017 5:31:56 PM | C:\Sirius_T3\17J-11006_Blank standardisation.t3r |
| Four-Plus jOH             | -0.2   | 10/11/2017 5:31:56 PM | C:\Sirius_T3\17J-11006_Blank standardisation.t3r |
| Base concentration factor | 1.011  | 10/11/2017 5:31:56 PM | C:\Sirius_T3\KOH17I22.t3r                        |
| Acid concentration factor | 0.995  | 10/11/2017 5:31:56 PM | C:\Sirius_T3\17J-11005_Blank standardisation.t3r |

Install date

#### Instrument Settings

Setting

| Instrument owner Instrument ID Instrument type Software version | Merck<br>T311053<br>T3 Simulator<br>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 KCI)                          | 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 HCI)                            | 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  |   |                   | 3/31/2009 6:28:19 AM   |
| Firmware version  | 1.1.3                                       |                   |                        |

Batch Id



Assay name: UV-metric psKa Analyst: Dorothy Levorse

Assay ID: 17J-11014 Instrument ID: T311053
Filename: C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

## Instrument Settings (continued)

| <b>Setting</b><br>Port A   | Value<br>Methanol (80%, 0.15 M KCI)                  | <b>Batch Id</b> 9-26-17 | Install date<br>10/5/2017 5:02:03 PM |
|--|--|-------------------------|--------------------------------------|
| Port B   | Cyclohexane  |                         | 9/19/2017 2:15:02 PM                 |
| Port C   | MeCN (50%, 0.15 M KCI)                               | 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)  | 0.44.47                 | 0/44/0047 40:00:00 ANA               |
| Titrant  | Octanol  | 9-14-17<br>T2TM1100152  | 9/14/2017 10:30:38 AM                |
| Titrator  Horizontal axis firmware version                         | 1 17 AI1DI2DO2 Stopper 2                             | 1311111100133           | 3/31/2009 6:24:17 AM                 |
| Vertical axis firmware version                                     | 1.17 Al1Dl2DO2 Stepper 2<br>1.17 Al1Dl2DO2 Stepper 2 |                         |                                      |
| Chassis I/O firmware version                                       | 1.11 AI1DI0DO2 Stepper 2                             |                         |                                      |
| Probe I/O firmware version   | 1.11 A 1 D 10 D 0 4 No 1 g 1 e 1 1 / 0 1             |                         |                                      |
| Electrode  | T3 Electrode   | T3E0769                 | 8/15/2017 10:21:54 AM                |
| E0 calibration   | -8.44 mV   | 1000700                 | 10/11/2017 5:32:40 PM                |
| Filling solution   | 3M KCI   | KCL095                  | 10/10/2017 9:58:43 AM                |
| Liquids  |  | 1102000                 | 16/16/2017 0:00:107 111              |
| Wash 1   | 50% IPA:50% Water                                    |                         | 10/11/2017 8:31:15 AM                |
| Wash 2   | 0.5% Trition X-100 in H20                            |                         | 10/11/2017 8:31:17 AM                |
| Buffer position 1  | pH7 Wash   |                         | 10/11/2017 8:31:21 AM                |
| Buffer position 2  | pH 7   |                         | 10/11/2017 8:31:23 AM                |
| Storage position   | •  |                         | 10/11/2017 8:31:26 AM                |
| Wash water   | 5.6e+003 mL  | 10-6-17                 | 10/6/2017 3:04:25 PM                 |
| Waste  | 4.5e+003 mL  |                         | 10/6/2017 3:04:33 PM                 |
| Temperature controller   |  |                         | 8/5/2010 7:35:13 AM                  |
| Turbidity detector   |  |                         | 3/31/2009 6:24:45 AM                 |
| Spectrometer   |  | 072390                  | 11/23/2010 12:22:28 PM               |
| Dip probe  |  | 11086                   |                                      |
| Wavelength coefficient A0  | 185.563  |                         |                                      |
| Wavelength coefficient A1  | 2.17439  |                         |                                      |
| Wavelength coefficient A2  | -0.000285622   |                         | 44/00/0040 40 00 00 014              |
| 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   | T2AL4400227             | 44/40/2045 40:24:42 AM               |
| Autoloader   | 1 17 AI1DI2DO2 Stannar 2                             | 13AL1100237             | 11/10/2015 10:34:13 AM               |
| Left-right axis firmware version                                   | 1.17 Al1Dl2DO2 Stepper 2<br>1.17 Al1Dl2DO2 Stepper 2 |                         |                                      |
| Front-back axis firmware version<br>Vertical axis firmware version | 1.17 AI1DI2DO2 Stepper 2                             |                         |                                      |
| Chassis I/O firmware version                                       | 1.11 AI1DI0DO4 Norgren I/O                           |                         |                                      |
| Configuration  | 1.11 ATIDIODO4 Norgien I/O                           |                         |                                      |
| 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 week atir anded   | 200/   |                         |                                      |

Surfactant wash stir speed

30%



Assay name: UV-metric psKa Analyst: Dorothy Levorse

Assay ID: 17J-11014 Instrument ID: T311053
Filename: C:\Sirius\_T3\Mehtap\20171011\_exp15\_pKa\17J-11014\_M12\_UV-metric psKa.t3r

# Instrument Settings (continued)

| Setting                                     | Value   | Batch Id | l Install date |
|---|---------|----------|----------------|
| 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 A1