pH-metric Result

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH2 2+)   -5.50
logP (XH +)   -0.11   ±0.20 (n=50)
logP (neutral X) 1.92   ±0.01 (n=50)

18C-01004 Points 1 to 36

M15_octanol concentration factor   0.910
Carbonate   0.2391 mM
Acidity error   -0.31186 mM

18C-01004 Points 37 to 69

M15_octanol concentration factor   0.903
Carbonate   0.1847 mM
Acidity error   -0.25845 mM

18C-01004 Points 70 to 106

M15_octanol concentration factor   0.913
Carbonate   0.0779 mM
Acidity error   -0.09188 mM

Warnings and errors

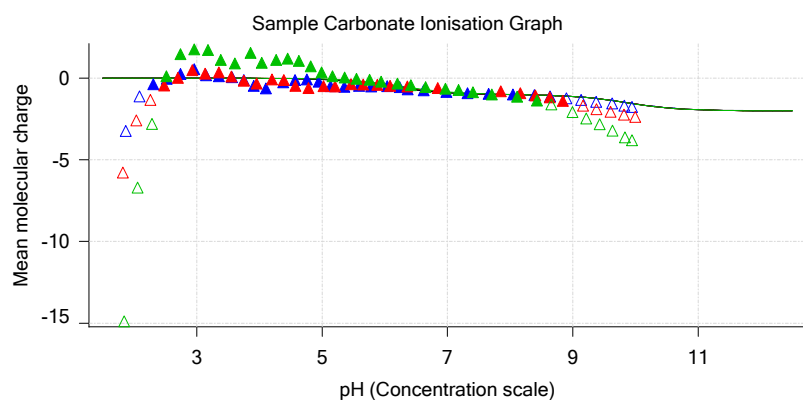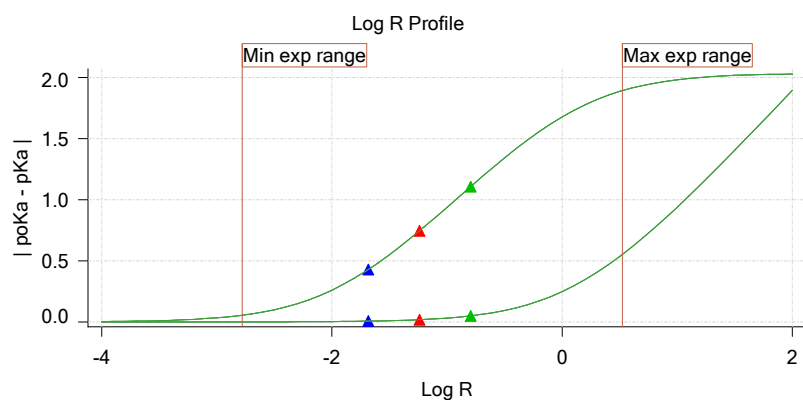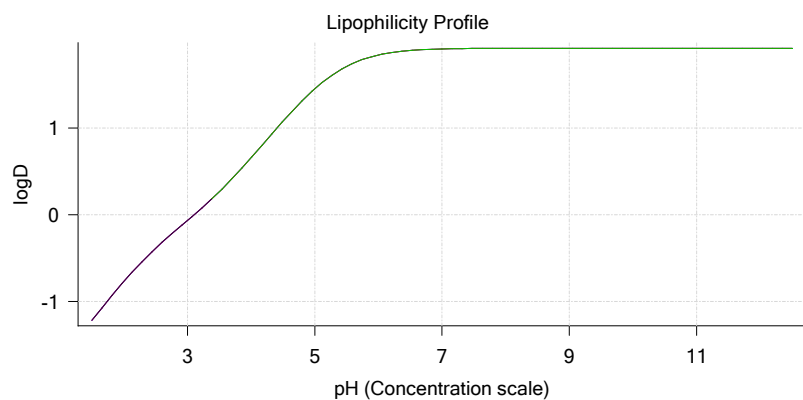Errors   None
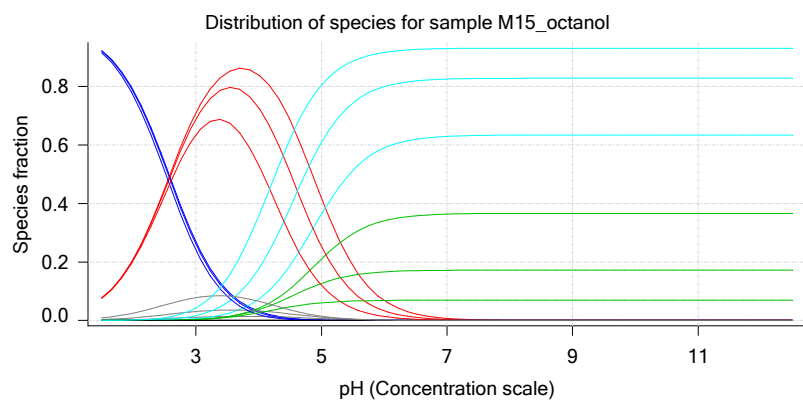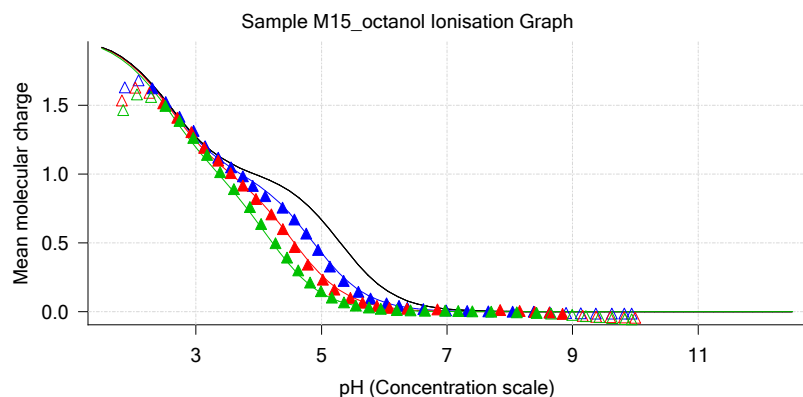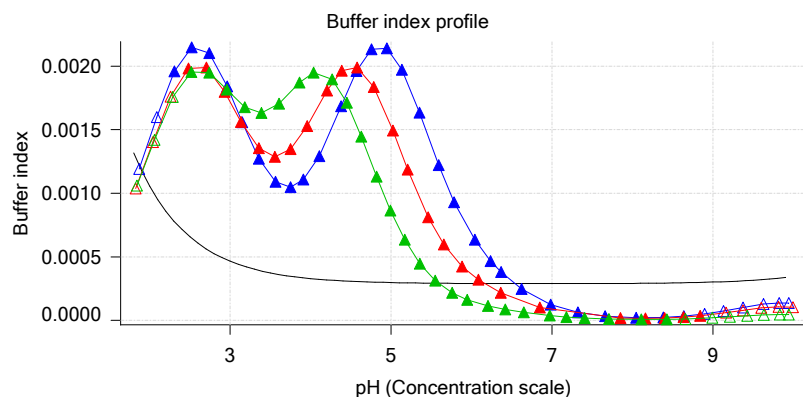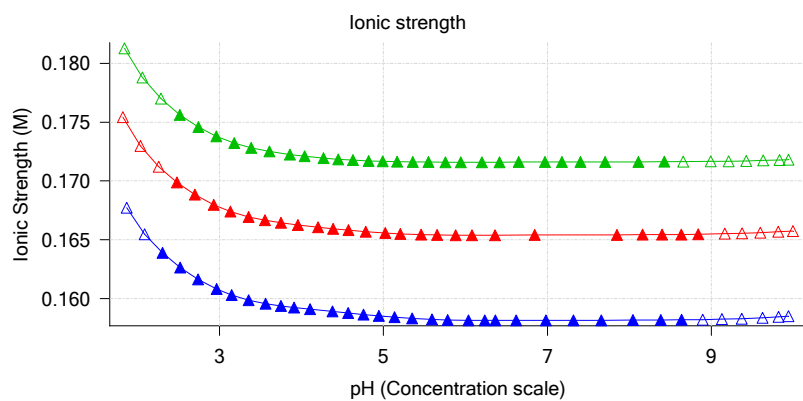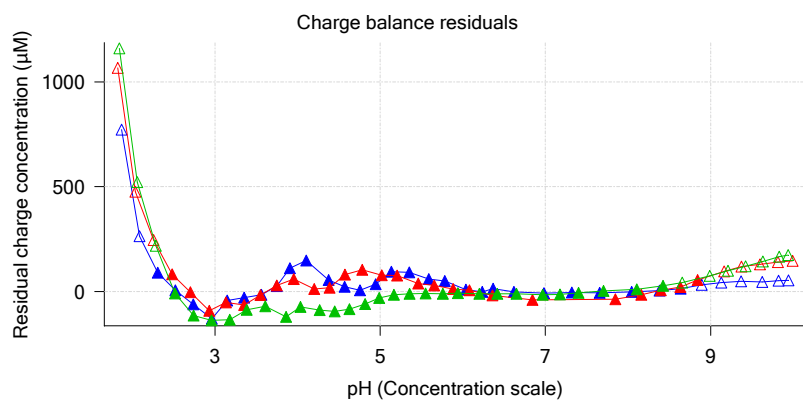Warnings   One or more logP values out of range

Sample logD and percent species

pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-1.70	95.54 %	2.51 %	0.00 %	0.00 %	1.94 %	0.01 %	
1.200	-1.51	93.10 %	3.88 %	0.00 %	0.00 %	3.00 %	0.03 %	Stomach pH
2.000	-0.77	67.69 %	17.81 %	0.01 %	0.00 %	13.75 %	0.74 %	
3.000	-0.07	14.76 %	38.83 %	0.19 %	0.00 %	29.98 %	16.23 %	
4.000	0.66	0.63 %	16.56 %	0.83 %	0.00 %	12.79 %	69.20 %	
5.000	1.45	0.01 %	2.27 %	1.14 %	0.00 %	1.75 %	94.83 %	
6.000	1.84	0.00 %	0.24 %	1.18 %	0.00 %	0.18 %	98.40 %	
6.500	1.89	0.00 %	0.07 %	1.18 %	0.00 %	0.06 %	98.68 %	
7.000	1.91	0.00 %	0.02 %	1.18 %	0.00 %	0.02 %	98.77 %	
7.400	1.92	0.00 %	0.01 %	1.18 %	0.00 %	0.01 %	98.80 %	Blood pH
8.000	1.92	0.00 %	0.00 %	1.19 %	0.00 %	0.00 %	98.81 %	
9.000	1.92	0.00 %	0.00 %	1.19 %	0.00 %	0.00 %	98.81 %	
10.000	1.92	0.00 %	0.00 %	1.19 %	0.00 %	0.00 %	98.81 %	
11.000	1.92	0.00 %	0.00 %	1.19 %	0.00 %	0.00 %	98.81 %	
12.000	1.92	0.00 %	0.00 %	1.19 %	0.00 %	0.00 %	98.81 %	

pH-metric Result

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M15_octanol Ionisation Graph

Distribution of species for sample M15_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)

Distribution of species for sample Carbonate

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

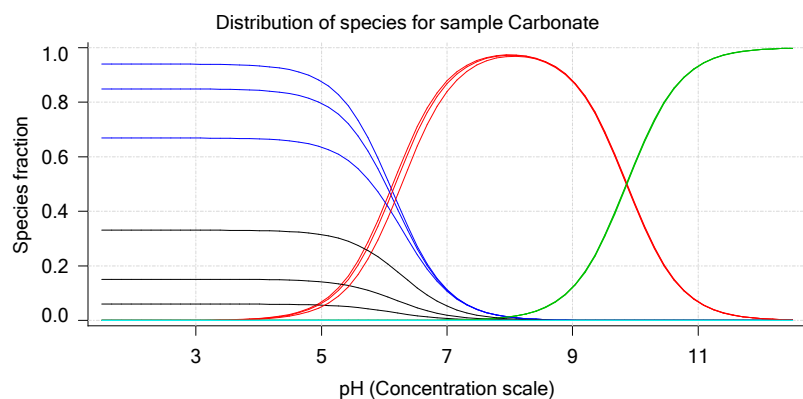# pH-metric high logP   Titration 1 of 3   18C-01004 Points 1 to 36

Overall results

RMSD   0.075
Average ionic strength   0.159 M
Average temperature   25.0°C
Partition ratio   0.0208 : 1
Analyte concentration range   3893.3 µM to 4047.6 µM
Total points considered   28 of 36

Warnings and errors

Errors   None
Warnings   One or more logP values out of range

Four-Plus parameters

Alpha	0.130	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r

Titrants

0.50 M HCl	0.993513	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	3/1/2018 4:33:50 AM	C:\Sirius_T3\KOH18B27.t3r

Sample

M15_octanol concentration factor	0.910
Base pKa 1	2.58
Base pKa 2	5.30
logP (XH2 2+)	-5.50
logP (XH +)	-4.16
logP (neutral X)	1.96

Sample graphs

Ionisation of sample M15_octanol

Distribution of species for sample M15_octanol

Sample graphs (continued)

Lipophilicity Profile

Sample logD and percent species

pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-3.91	97.44 %	2.56 %	0.00 %	0.00 %	0.00 %	0.00 %	
1.200	-3.52	96.00 %	4.00 %	0.00 %	0.00 %	0.00 %	0.00 %	Stomach pH
2.000	-2.02	79.15 %	20.82 %	0.01 %	0.00 %	0.00 %	0.02 %	
3.000	-0.48	27.26 %	71.69 %	0.36 %	0.00 %	0.00 %	0.69 %	
4.000	0.63	3.21 %	84.45 %	4.23 %	0.00 %	0.00 %	8.10 %	
5.000	1.49	0.15 %	40.58 %	20.34 %	0.00 %	0.00 %	38.93 %	
6.000	1.89	0.00 %	6.41 %	32.11 %	0.00 %	0.00 %	61.48 %	
6.500	1.94	0.00 %	2.12 %	33.58 %	0.00 %	0.00 %	64.30 %	
7.000	1.96	0.00 %	0.68 %	34.08 %	0.00 %	0.00 %	65.24 %	
7.400	1.96	0.00 %	0.27 %	34.22 %	0.00 %	0.00 %	65.51 %	Blood pH
8.000	1.96	0.00 %	0.07 %	34.29 %	0.00 %	0.00 %	65.64 %	
9.000	1.96	0.00 %	0.01 %	34.31 %	0.00 %	0.00 %	65.68 %	
10.000	1.96	0.00 %	0.00 %	34.31 %	0.00 %	0.00 %	65.69 %	
11.000	1.96	0.00 %	0.00 %	34.31 %	0.00 %	0.00 %	65.69 %	
12.000	1.96	0.00 %	0.00 %	34.31 %	0.00 %	0.00 %	65.69 %	

Carbonate and acidity

Carbonate 0.239 mM
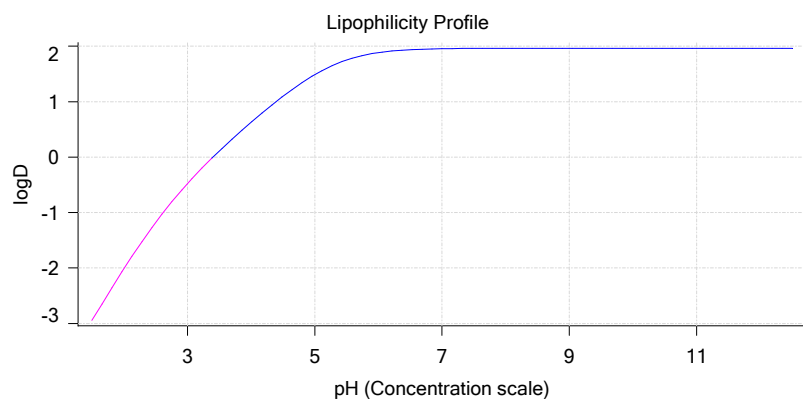Acidity error -0.312 mM

Other graphs

Assay progress

Titration graph

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
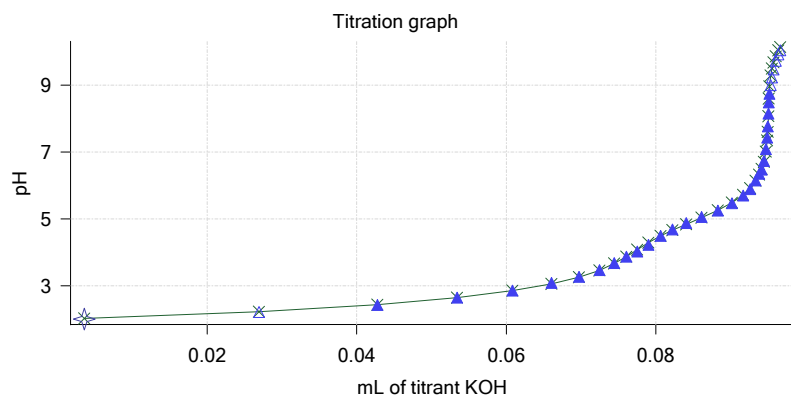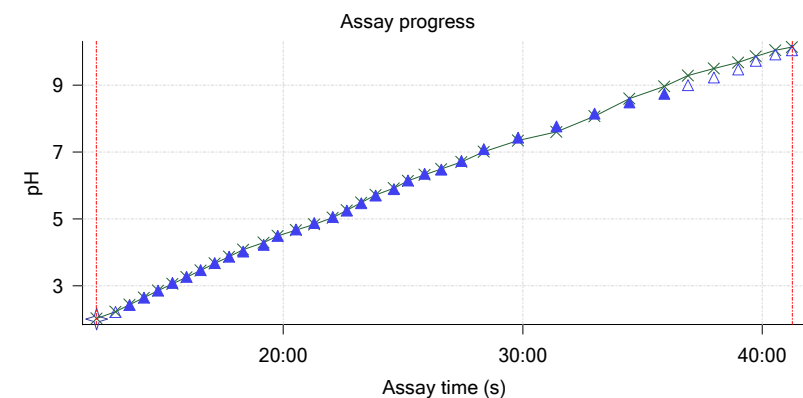Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
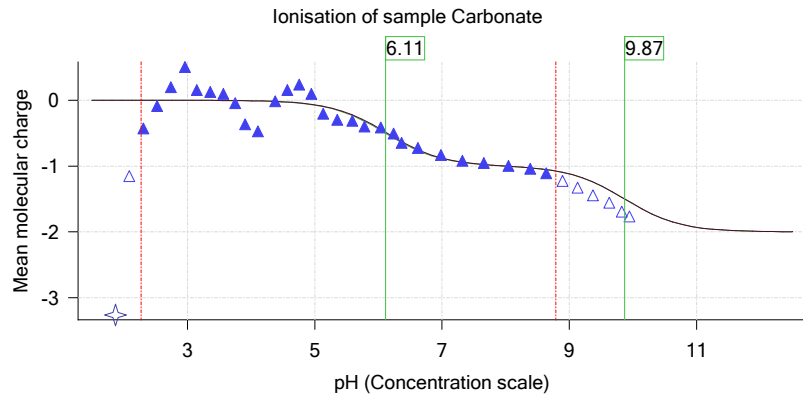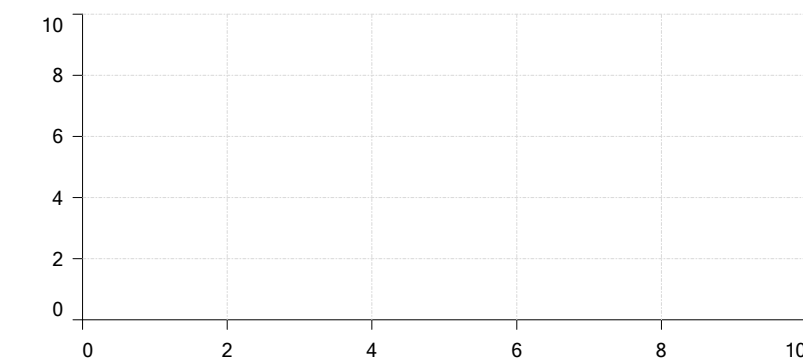
Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 2 of 3   18C-01004 Points 37 to 69

Overall results

RMSD   0.470
Average ionic strength   0.166 M
Average temperature   25.0°C
Partition ratio   0.0577 : 1
Analyte concentration range   3455.8 µM to 3592.3 µM
Total points considered   25 of 33

Warnings and errors

Errors   None
Warnings   One or more logP values out of range

Four-Plus parameters

	Alpha	0.130	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
	S	0.9970	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
	jH	0.8	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
	jOH	-0.4	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r

Titrants

	0.50 M HCl	0.993513	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
	0.50 M KOH	0.999845	3/1/2018 4:33:50 AM	C:\Sirius_T3\KOH18B27.t3r

Sample

	M15_octanol concentration factor	0.903
	Base pKa 1	2.58
	Base pKa 2	5.30
	logP (XH2 2+)	-5.50
	logP (XH +)	-3.58
	logP (neutral X)	1.94

Sample graphs

Ionisation of sample M15_octanol

Distribution of species for sample M15_octanol
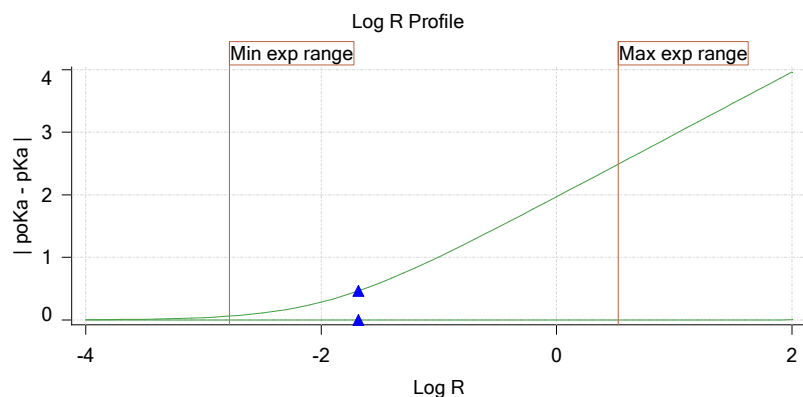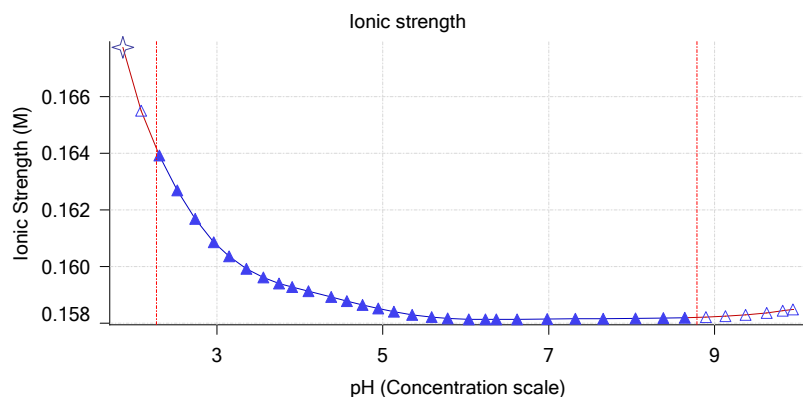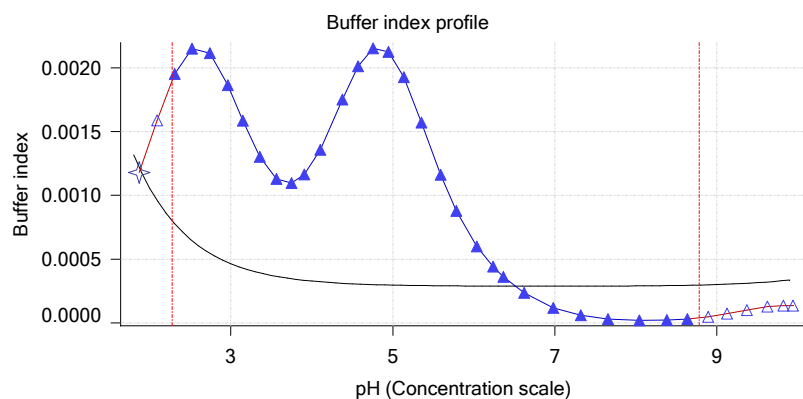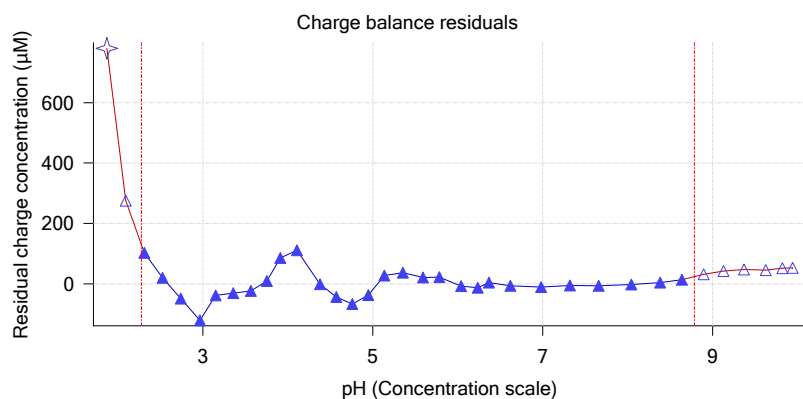
Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile

Sample logD and percent species

pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-3.91	97.44 %	2.56 %	0.00 %	0.00 %	0.00 %	0.00 %	
1.200	-3.54	96.00 %	4.00 %	0.00 %	0.00 %	0.00 %	0.00 %	Stomach pH
2.000	-2.04	79.12 %	20.81 %	0.01 %	0.00 %	0.00 %	0.05 %	
3.000	-0.50	26.96 %	70.90 %	0.36 %	0.00 %	0.00 %	1.79 %	
4.000	0.60	2.84 %	74.62 %	3.74 %	0.00 %	0.00 %	18.80 %	
5.000	1.46	0.09 %	24.85 %	12.46 %	0.00 %	0.00 %	62.60 %	
6.000	1.86	0.00 %	3.20 %	16.06 %	0.00 %	0.00 %	80.73 %	
6.500	1.91	0.00 %	1.04 %	16.42 %	0.00 %	0.00 %	82.54 %	
7.000	1.93	0.00 %	0.33 %	16.54 %	0.00 %	0.00 %	83.13 %	
7.400	1.94	0.00 %	0.13 %	16.57 %	0.00 %	0.00 %	83.30 %	Blood pH
8.000	1.94	0.00 %	0.03 %	16.59 %	0.00 %	0.00 %	83.38 %	
9.000	1.94	0.00 %	0.00 %	16.59 %	0.00 %	0.00 %	83.40 %	
10.000	1.94	0.00 %	0.00 %	16.60 %	0.00 %	0.00 %	83.40 %	
11.000	1.94	0.00 %	0.00 %	16.60 %	0.00 %	0.00 %	83.40 %	
12.000	1.94	0.00 %	0.00 %	16.60 %	0.00 %	0.00 %	83.40 %	

Carbonate and acidity

Carbonate   0.185 mM
Acidity error   -0.258 mM

Other graphs

Assay progress

Titration graph

Sample name: **M15_octanol**   Experiment start time: **3/1/2018 4:33:50 AM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-01004**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Other graphs (continued)

Charge balance residuals

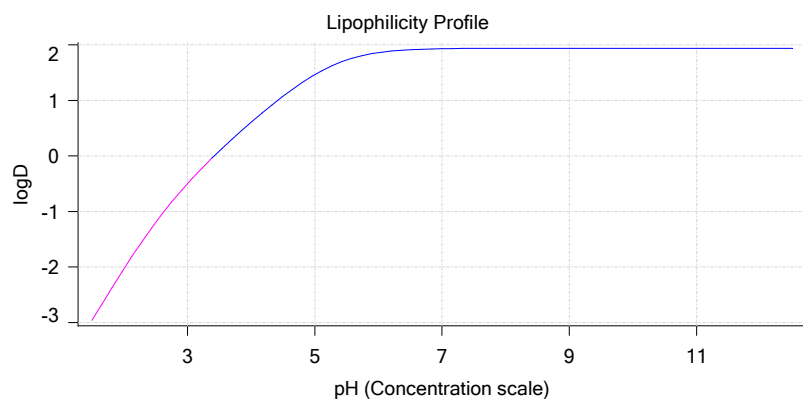Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
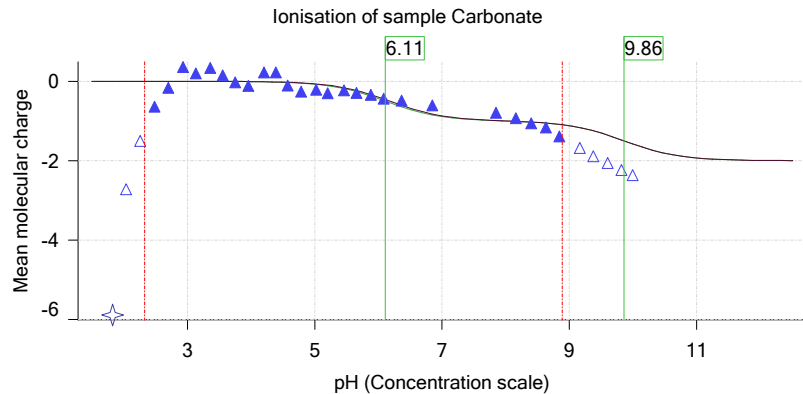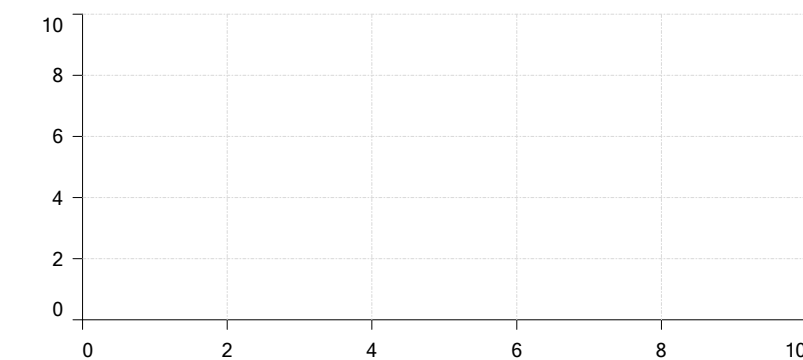
Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 3 of 3   18C-01004 Points 70 to 106

Overall results

RMSD   0.356
Average ionic strength   0.172 M
Average temperature   25.0°C
Partition ratio   0.1602 : 1
Analyte concentration range   2913.6 µM to 3011.2 µM
Total points considered   27 of 37

Warnings and errors

Errors   None
Warnings   One or more logP values out of range

Four-Plus parameters

	Alpha	0.130	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
	S	0.9970	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
	jH	0.8	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
	jOH	-0.4	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r

Titrants

0.50 M HCl	0.993513	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	3/1/2018 4:33:50 AM	C:\Sirius_T3\KOH18B27.t3r

Sample

M15_octanol concentration factor	0.913
Base pKa 1	2.58
Base pKa 2	5.30
logP (XH2 2+)	-5.50
logP (XH +)	-1.60
logP (neutral X)	1.81

Sample graphs

Ionisation of sample M15_octanol

Distribution of species for sample M15_octanol

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
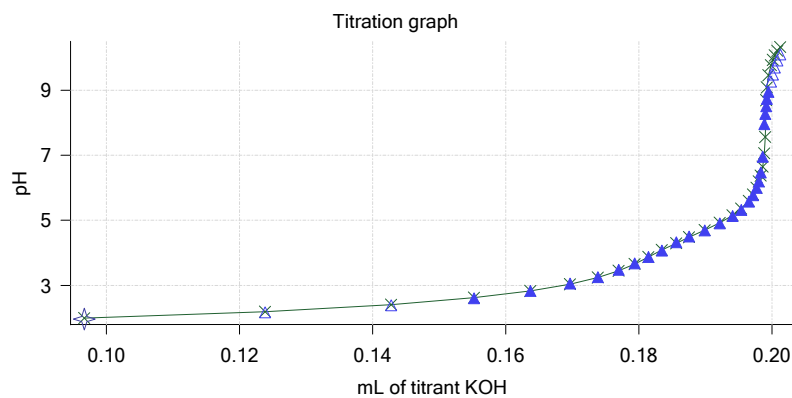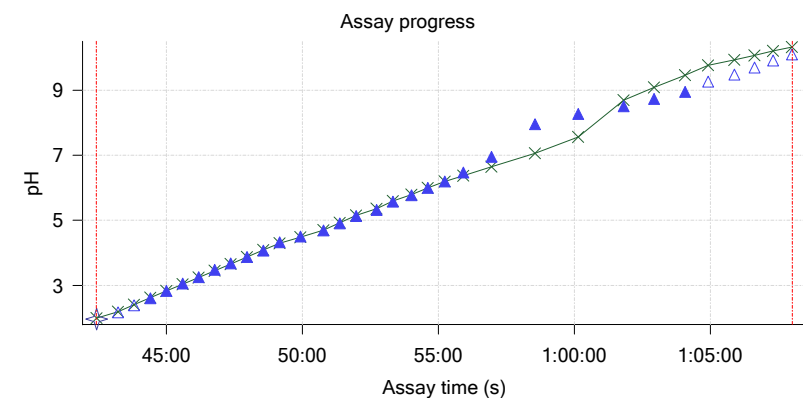Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
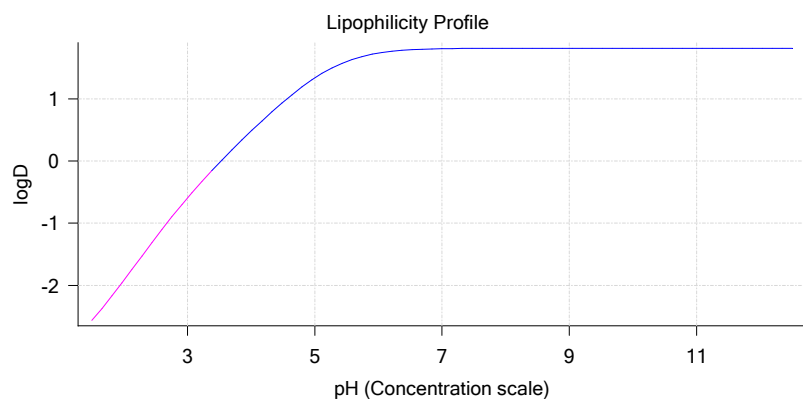
Sample logD and percent species

pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-3.13	97.43 %	2.56 %	0.00 %	0.00 %	0.01 %	0.00 %	
1.200	-2.91	95.98 %	4.00 %	0.00 %	0.00 %	0.02 %	0.00 %	Stomach pH
2.000	-1.92	79.01 %	20.78 %	0.01 %	0.00 %	0.08 %	0.11 %	
3.000	-0.60	26.38 %	69.38 %	0.35 %	0.00 %	0.28 %	3.62 %	
4.000	0.48	2.36 %	61.96 %	3.11 %	0.00 %	0.25 %	32.33 %	
5.000	1.34	0.06 %	14.87 %	7.45 %	0.00 %	0.06 %	77.56 %	
6.000	1.73	0.00 %	1.72 %	8.61 %	0.00 %	0.01 %	89.66 %	
6.500	1.79	0.00 %	0.55 %	8.72 %	0.00 %	0.00 %	90.73 %	
7.000	1.80	0.00 %	0.17 %	8.75 %	0.00 %	0.00 %	91.08 %	
7.400	1.81	0.00 %	0.07 %	8.76 %	0.00 %	0.00 %	91.17 %	Blood pH
8.000	1.81	0.00 %	0.02 %	8.76 %	0.00 %	0.00 %	91.22 %	
9.000	1.81	0.00 %	0.00 %	8.76 %	0.00 %	0.00 %	91.23 %	
10.000	1.81	0.00 %	0.00 %	8.76 %	0.00 %	0.00 %	91.24 %	
11.000	1.81	0.00 %	0.00 %	8.76 %	0.00 %	0.00 %	91.24 %	
12.000	1.81	0.00 %	0.00 %	8.76 %	0.00 %	0.00 %	91.24 %	

Carbonate and acidity

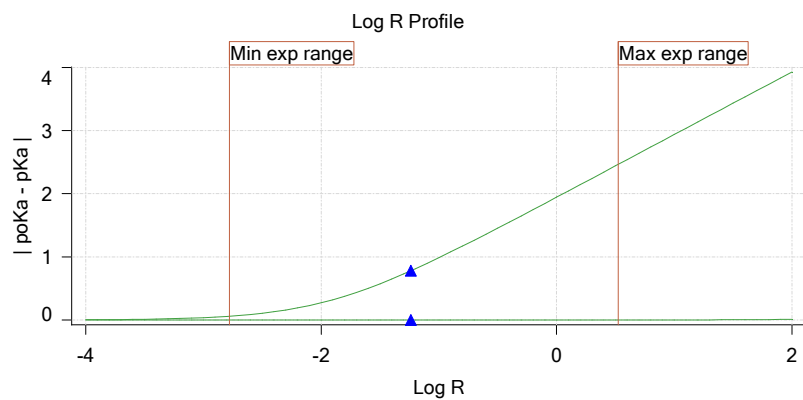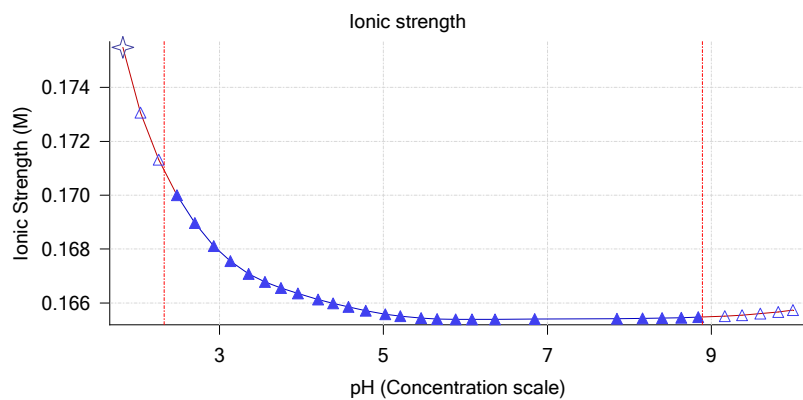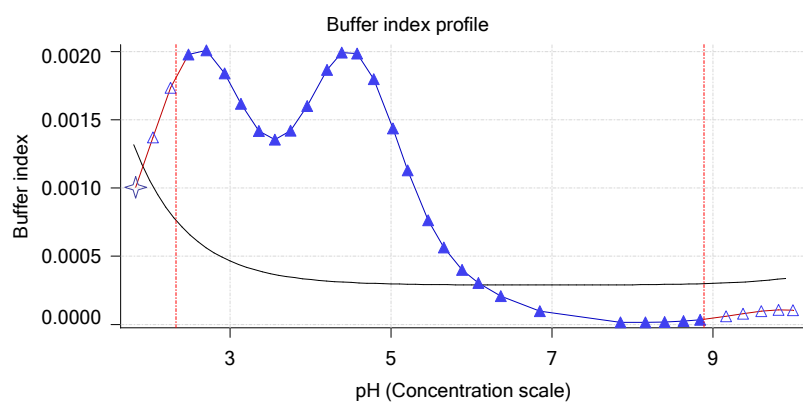Carbonate   0.078 mM
Acidity error   -0.092 mM
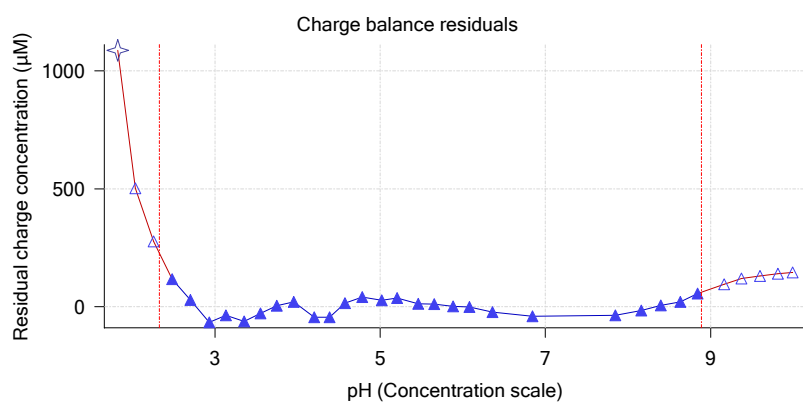
Other graphs

Assay progress

Titration graph

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Min exp range

Max exp range

Ionisation of sample Carbonate

6.10

9.85
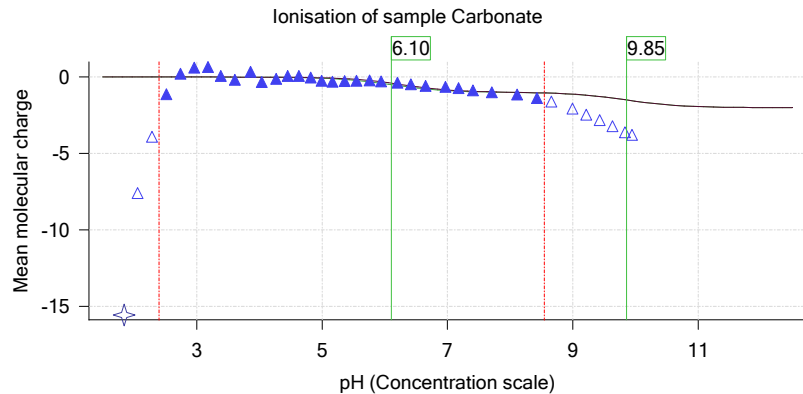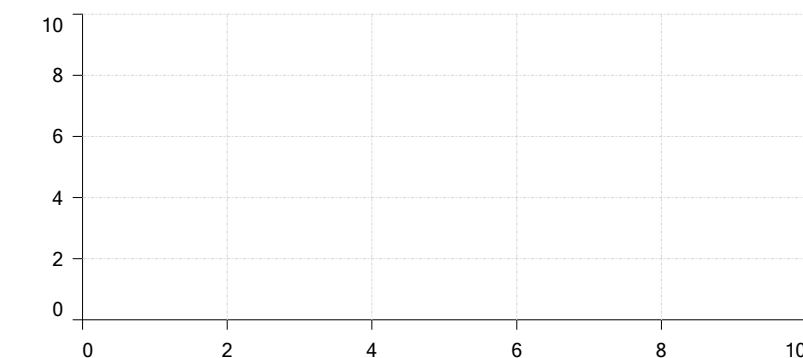
Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
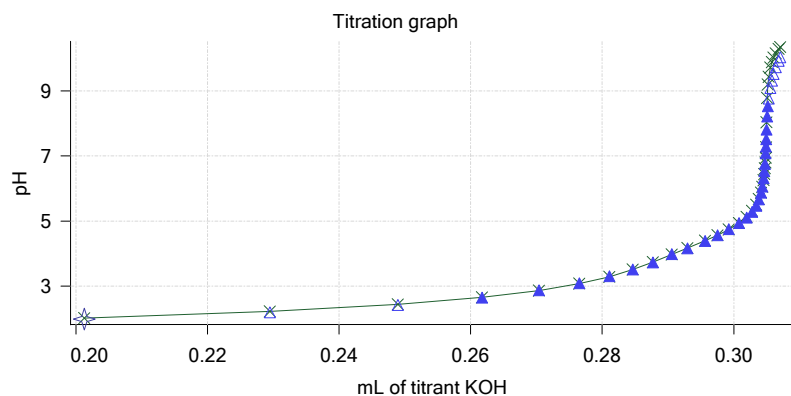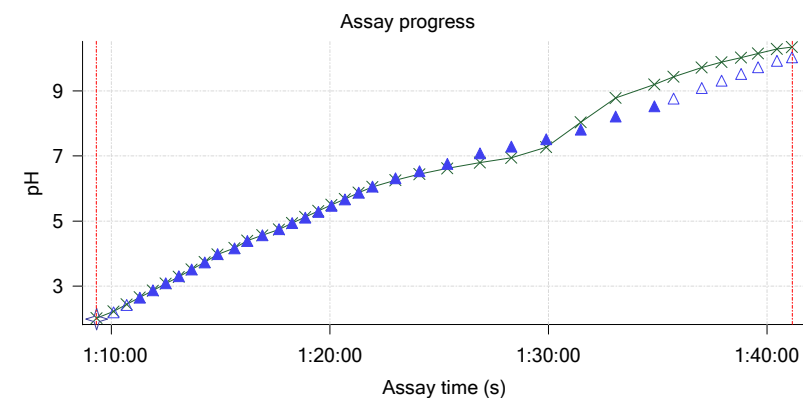Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M15_octanol	2/27/2018 5:03:03 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001990 g	2/28/2018 4:25:17 PM	User entered value
Formula weight	209.25 g/mol	2/27/2018 5:03:03 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	209.25	2/27/2018 5:03:03 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	2/27/2018 5:03:03 PM	User entered value
Sample is a	Base	2/27/2018 5:03:03 PM	User entered value
pKa 1	2.58	2/27/2018 5:03:03 PM	User entered value
pKa 2	5.30	2/27/2018 5:03:03 PM	User entered value
logP (XH2 2+)	-5.50	2/28/2018 2:10:35 PM	User entered value
logp (XH +)	-4.96	2/28/2018 2:10:28 PM	User entered value
logP (neutral X)	1.92	2/28/2018 2:10:15 PM	User entered value

Events

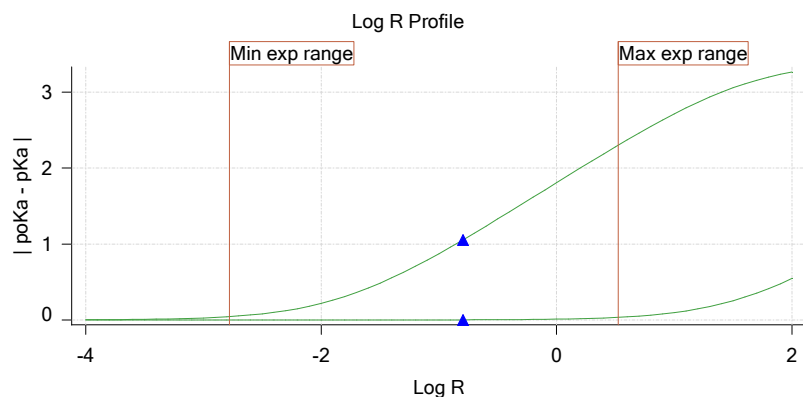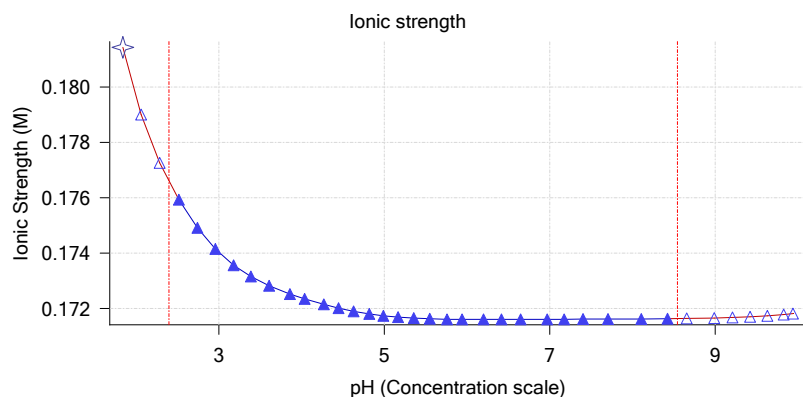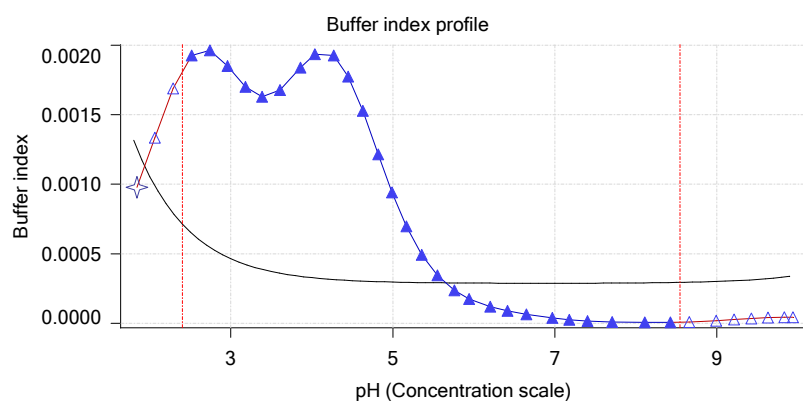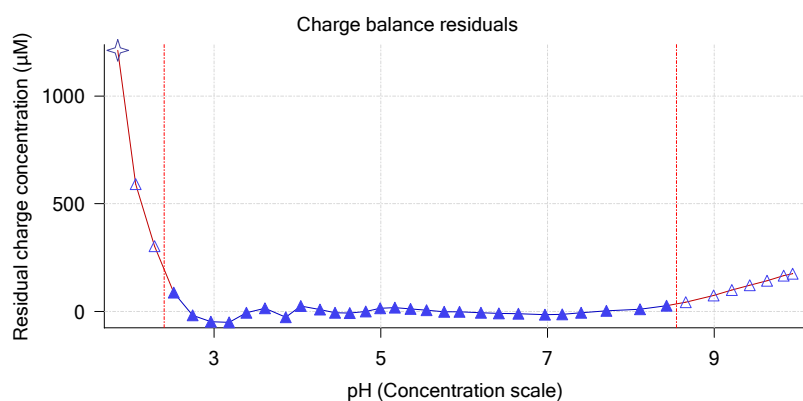| Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
9:11.8	Initial pH = 7.75									
12:12.6	Data point 1	2.20002 mL	0.09603 mL	0.00355 mL	0.05000 mL	2.004	-0.00004	0.00005	0.00026	10.5 s
12:59.6	Data point 2	2.20002 mL	0.09603 mL	0.02693 mL	0.05000 mL	2.218	-0.00410	0.09174	0.00067	10.0 s
13:35.4	Data point 3	2.20002 mL	0.09603 mL	0.04276 mL	0.05000 mL	2.434	-0.00622	0.41443	0.00048	10.0 s
14:11.0	Data point 4	2.20002 mL	0.09603 mL	0.05341 mL	0.05000 mL	2.647	-0.00112	0.17193	0.00013	10.0 s
14:46.6	Data point 5	2.20002 mL	0.09603 mL	0.06084 mL	0.05000 mL	2.863	-0.00762	0.16820	0.00092	10.0 s
15:22.1	Data point 6	2.20002 mL	0.09603 mL	0.06606 mL	0.05000 mL	3.086	-0.00070	0.05715	0.00014	10.0 s
15:57.6	Data point 7	2.20002 mL	0.09603 mL	0.06973 mL	0.05000 mL	3.269	-0.00182	0.13794	0.00024	10.0 s
16:33.1	Data point 8	2.20002 mL	0.09603 mL	0.07246 mL	0.05000 mL	3.476	-0.00683	0.20917	0.00074	10.0 s
17:08.6	Data point 9	2.20002 mL	0.09603 mL	0.07446 mL	0.05000 mL	3.682	-0.00883	0.24236	0.00089	10.0 s
17:44.1	Data point 10	2.20002 mL	0.09603 mL	0.07606 mL	0.05000 mL	3.870	-0.00207	0.48492	0.00015	10.5 s
18:20.0	Data point 11	2.20002 mL	0.09603 mL	0.07752 mL	0.05000 mL	4.027	-0.00297	0.52144	0.00020	10.0 s
19:11.0	Data point 12	2.20002 mL	0.09603 mL	0.07902 mL	0.05000 mL	4.224	0.00693	0.14332	0.00090	10.0 s
19:46.5	Data point 13	2.20002 mL	0.09603 mL	0.08067 mL	0.05000 mL	4.495	-0.00297	0.63948	0.00018	10.0 s
20:32.2	Data point 14	2.20002 mL	0.09603 mL	0.08224 mL	0.05000 mL	4.685	-0.00829	0.27907	0.00078	10.0 s
21:18.0	Data point 15	2.20002 mL	0.09603 mL	0.08405 mL	0.05000 mL	4.873	-0.00361	0.81281	0.00020	10.5 s
22:04.3	Data point 16	2.20002 mL	0.09603 mL	0.08615 mL	0.05000 mL	5.061	-0.00994	0.26388	0.00096	10.0 s
22:39.8	Data point 17	2.20002 mL	0.09603 mL	0.08831 mL	0.05000 mL	5.249	-0.01621	0.90472	0.00084	10.0 s
23:15.2	Data point 18	2.20002 mL	0.09603 mL	0.09019 mL	0.05000 mL	5.466	-0.00885	0.83876	0.00048	10.5 s
23:51.2	Data point 19	2.20002 mL	0.09603 mL	0.09167 mL	0.05000 mL	5.704	-0.01077	0.55398	0.00071	10.0 s
24:36.9	Data point 20	2.20002 mL	0.09603 mL	0.09262 mL	0.05000 mL	5.896	-0.01015	0.64626	0.00062	10.0 s
25:12.4	Data point 21	2.20002 mL	0.09603 mL	0.09337 mL	0.05000 mL	6.150	-0.01917	0.94736	0.00097	11.5 s
25:54.3	Data point 22	2.20002 mL	0.09603 mL	0.09384 mL	0.05000 mL	6.348	-0.01956	0.94838	0.00099	16.0 s
26:35.7	Data point 23	2.20002 mL	0.09603 mL	0.09417 mL	0.05000 mL	6.477	-0.01852	0.92877	0.00095	20.5 s
27:26.8	Data point 24	2.20002 mL	0.09603 mL	0.09447 mL	0.05000 mL	6.731	-0.01978	0.97668	0.00099	25.0 s
28:22.5	Data point 25	2.20002 mL	0.09603 mL	0.09476 mL	0.05000 mL	7.091	-0.01939	0.96778	0.00097	50.5 s
29:48.7	Data point 26	2.20002 mL	0.09603 mL	0.09492 mL	0.05000 mL	7.427	-0.02618	0.93832	0.00134	Timed out at 59.5 s
31:24.4	Data point 27	2.20002 mL	0.09603 mL	0.09499 mL	0.05000 mL	7.765	-0.02782	0.96820	0.00140	Timed out at 59.5 s
32:60.0	Data point 28	2.20002 mL	0.09603 mL	0.09506 mL	0.05000 mL	8.150	-0.01942	0.97507	0.00097	51.5 s
34:27.2	Data point 29	2.20002 mL	0.09603 mL	0.09513 mL	0.05000 mL	8.488	-0.01822	0.88544	0.00096	47.0 s
35:55.0	Data point 30	2.20002 mL	0.09603 mL	0.09523 mL	0.05000 mL	8.742	-0.01803	0.81814	0.00098	18.0 s
36:53.9	Data point 31	2.20002 mL	0.09603 mL	0.09539 mL	0.05000 mL	8.998	-0.01906	0.91802	0.00098	29.5 s
37:59.3	Data point 32	2.20002 mL	0.09603 mL	0.09556 mL	0.05000 mL	9.231	-0.01960	0.94492	0.00100	24.5 s
38:59.8	Data point 33	2.20002 mL	0.09603 mL	0.09577 mL	0.05000 mL	9.473	-0.01978	0.98072	0.00099	14.0 s
39:44.2	Data point 34	2.20002 mL	0.09603 mL	0.09605 mL	0.05000 mL	9.727	-0.01838	0.95975	0.00093	13.0 s
40:32.9	Data point 35	2.20002 mL	0.09603 mL	0.09640 mL	0.05000 mL	9.921	-0.01891	0.96239	0.00095	11.0 s
41:14.5	Data point 36	2.20002 mL	0.09603 mL	0.09666 mL	0.05000 mL	10.042	-0.01797	0.91702	0.00093	10.0 s

Sample name: **M15_octanol** Experiment start time: **3/1/2018 4:33:50 AM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-01004** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
42:26.2	Data point 37	2.20002 mL	0.20071 mL	0.09666 mL	0.15000 mL	1.959	-0.00249	0.02483	0.00078	10.0 s
43:12.8	Data point 38	2.20002 mL	0.20071 mL	0.12385 mL	0.15000 mL	2.169	0.00115	0.01005	0.00057	10.0 s
43:48.7	Data point 39	2.20002 mL	0.20071 mL	0.14278 mL	0.15000 mL	2.387	0.00292	0.23411	0.00030	10.0 s
44:24.4	Data point 40	2.20002 mL	0.20071 mL	0.15522 mL	0.15000 mL	2.607	0.00278	0.64171	0.00017	10.0 s
45:00.1	Data point 41	2.20002 mL	0.20071 mL	0.16369 mL	0.15000 mL	2.825	0.00765	0.45122	0.00056	10.0 s
45:35.6	Data point 42	2.20002 mL	0.20071 mL	0.16964 mL	0.15000 mL	3.053	0.00261	0.02150	0.00088	10.0 s
46:11.0	Data point 43	2.20002 mL	0.20071 mL	0.17382 mL	0.15000 mL	3.254	-0.00337	0.07118	0.00062	10.0 s
46:46.5	Data point 44	2.20002 mL	0.20071 mL	0.17695 mL	0.15000 mL	3.476	-0.00111	0.17901	0.00013	10.0 s
47:22.0	Data point 45	2.20002 mL	0.20071 mL	0.17935 mL	0.15000 mL	3.673	-0.00484	0.08087	0.00084	10.5 s
47:58.0	Data point 46	2.20002 mL	0.20071 mL	0.18144 mL	0.15000 mL	3.869	-0.00085	0.00291	0.00078	10.5 s
48:34.0	Data point 47	2.20002 mL	0.20071 mL	0.18347 mL	0.15000 mL	4.074	-0.00208	0.18891	0.00024	10.0 s
49:09.5	Data point 48	2.20002 mL	0.20071 mL	0.18561 mL	0.15000 mL	4.321	0.00313	0.03406	0.00084	10.5 s
49:55.8	Data point 49	2.20002 mL	0.20071 mL	0.18756 mL	0.15000 mL	4.505	-0.00239	0.41560	0.00018	10.0 s
50:46.8	Data point 50	2.20002 mL	0.20071 mL	0.18989 mL	0.15000 mL	4.692	0.00658	0.10707	0.00099	10.0 s
51:22.3	Data point 51	2.20002 mL	0.20071 mL	0.19215 mL	0.15000 mL	4.901	-0.00276	0.35548	0.00023	10.5 s
51:58.2	Data point 52	2.20002 mL	0.20071 mL	0.19410 mL	0.15000 mL	5.136	-0.00855	0.19756	0.00095	10.0 s
52:44.0	Data point 53	2.20002 mL	0.20071 mL	0.19539 mL	0.15000 mL	5.320	0.01104	0.48343	0.00078	10.5 s
53:19.9	Data point 54	2.20002 mL	0.20071 mL	0.19652 mL	0.15000 mL	5.575	-0.01538	0.61586	0.00097	10.0 s
54:00.5	Data point 55	2.20002 mL	0.20071 mL	0.19718 mL	0.15000 mL	5.767	-0.01599	0.72745	0.00093	10.5 s
54:36.4	Data point 56	2.20002 mL	0.20071 mL	0.19770 mL	0.15000 mL	5.995	-0.01720	0.89603	0.00090	12.5 s
55:14.3	Data point 57	2.20002 mL	0.20071 mL	0.19805 mL	0.15000 mL	6.194	-0.01773	0.93943	0.00090	15.0 s
55:54.8	Data point 58	2.20002 mL	0.20071 mL	0.19831 mL	0.15000 mL	6.473	-0.01702	0.93578	0.00087	32.0 s
56:57.3	Data point 59	2.20002 mL	0.20071 mL	0.19859 mL	0.15000 mL	6.955	-0.02431	0.97693	0.00121	Timed out at 59.5 s
58:33.1	Data point 60	2.20002 mL	0.20071 mL	0.19885 mL	0.15000 mL	7.955	-0.04787	0.97420	0.00240	Timed out at 59.5 s
1:00:08.8	Data point 61	2.20002 mL	0.20071 mL	0.19899 mL	0.15000 mL	8.265	-0.01855	0.84395	0.00100	59.0 s
1:01:48.7	Data point 62	2.20002 mL	0.20071 mL	0.19913 mL	0.15000 mL	8.503	-0.01414	0.67047	0.00085	31.5 s
1:02:55.9	Data point 63	2.20002 mL	0.20071 mL	0.19925 mL	0.15000 mL	8.736	-0.01917	0.92795	0.00098	28.0 s
1:04:04.8	Data point 64	2.20002 mL	0.20071 mL	0.19948 mL	0.15000 mL	8.945	-0.01399	0.56454	0.00092	14.5 s
1:04:54.9	Data point 65	2.20002 mL	0.20071 mL	0.19984 mL	0.15000 mL	9.265	-0.01776	0.81338	0.00097	22.5 s
1:05:53.3	Data point 66	2.20002 mL	0.20071 mL	0.20012 mL	0.15000 mL	9.476	-0.01942	0.96420	0.00098	13.5 s
1:06:37.4	Data point 67	2.20002 mL	0.20071 mL	0.20042 mL	0.15000 mL	9.700	-0.01799	0.94238	0.00092	11.0 s
1:07:18.9	Data point 68	2.20002 mL	0.20071 mL	0.20082 mL	0.15000 mL	9.916	-0.01678	0.93188	0.00086	10.5 s
1:08:00.0	Data point 69	2.20002 mL	0.20071 mL	0.20125 mL	0.15000 mL	10.094	-0.01862	0.92012	0.00096	13.5 s
1:09:19.8	Data point 70	2.20002 mL	0.30703 mL	0.20125 mL	0.45000 mL	1.978	-0.00661	0.17199	0.00079	10.0 s
1:10:06.4	Data point 71	2.20002 mL	0.30703 mL	0.22949 mL	0.45000 mL	2.191	0.00020	0.00450	0.00015	10.0 s
1:10:42.3	Data point 72	2.20002 mL	0.30703 mL	0.24894 mL	0.45000 mL	2.413	-0.00624	0.12108	0.00089	10.5 s
1:11:18.6	Data point 73	2.20002 mL	0.30703 mL	0.26174 mL	0.45000 mL	2.641	-0.00127	0.02629	0.00039	10.0 s
1:11:54.2	Data point 74	2.20002 mL	0.30703 mL	0.27039 mL	0.45000 mL	2.864	0.01123	0.56243	0.00074	10.0 s
1:12:29.8	Data point 75	2.20002 mL	0.30703 mL	0.27653 mL	0.45000 mL	3.082	0.00260	0.02083	0.00089	10.0 s
1:13:05.3	Data point 76	2.20002 mL	0.30703 mL	0.28109 mL	0.45000 mL	3.300	0.00115	0.17309	0.00014	10.0 s
1:13:40.9	Data point 77	2.20002 mL	0.30703 mL	0.28467 mL	0.45000 mL	3.507	-0.00125	0.06719	0.00024	10.0 s
1:14:16.4	Data point 78	2.20002 mL	0.30703 mL	0.28772 mL	0.45000 mL	3.728	-0.00003	0.00007	0.00016	10.0 s
1:14:51.9	Data point 79	2.20002 mL	0.30703 mL	0.29057 mL	0.45000 mL	3.979	0.00062	0.00143	0.00080	10.5 s
1:15:38.3	Data point 80	2.20002 mL	0.30703 mL	0.29299 mL	0.45000 mL	4.156	0.00694	0.12696	0.00096	10.0 s
1:16:13.8	Data point 81	2.20002 mL	0.30703 mL	0.29563 mL	0.45000 mL	4.386	-0.00283	0.55635	0.00019	10.0 s
1:16:54.4	Data point 82	2.20002 mL	0.30703 mL	0.29753 mL	0.45000 mL	4.567	0.00299	0.02388	0.00096	10.5 s
1:17:40.7	Data point 83	2.20002 mL	0.30703 mL	0.29925 mL	0.45000 mL	4.745	0.01034	0.46849	0.00075	10.5 s
1:18:16.7	Data point 84	2.20002 mL	0.30703 mL	0.30080 mL	0.45000 mL	4.934	-0.00687	0.30375	0.00062	10.5 s
1:18:52.6	Data point 85	2.20002 mL	0.30703 mL	0.30195 mL	0.45000 mL	5.106	-0.00848	0.37580	0.00068	10.5 s
1:19:28.6	Data point 86	2.20002 mL	0.30703 mL	0.30280 mL	0.45000 mL	5.282	-0.00416	0.04532	0.00097	10.5 s
1:20:04.5	Data point 87	2.20002 mL	0.30703 mL	0.30341 mL	0.45000 mL	5.472	0.00416	0.04632	0.00095	11.5 s
1:20:41.4	Data point 88	2.20002 mL	0.30703 mL	0.30383 mL	0.45000 mL	5.662	0.00750	0.22112	0.00079	12.5 s
1:21:19.3	Data point 89	2.20002 mL	0.30703 mL	0.30414 mL	0.45000 mL	5.871	-0.01602	0.74413	0.00092	12.5 s
1:21:57.2	Data point 90	2.20002 mL	0.30703 mL	0.30435 mL	0.45000 mL	6.055	-0.01729	0.85517	0.00092	32.5 s
1:23:00.4	Data point 91	2.20002 mL	0.30703 mL	0.30454 mL	0.45000 mL	6.313	-0.01803	0.92861	0.00092	40.0 s

Sample name: **M15_octanol**　　　　Experiment start time: **3/1/2018 4:33:50 AM**
Assay name: **pH-metric high logP**　　　　Analyst: **Pion**
Assay ID: **18C-01004**　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:24:05.7	Data point 92	2.20002 mL	0.30703 mL	0.30466 mL	0.45000 mL	6.527	-0.01857	0.95760	0.00094	51.0 s
1:25:22.1	Data point 93	2.20002 mL	0.30703 mL	0.30475 mL	0.45000 mL	6.759	-0.01815	0.93102	0.00093	59.5 s
1:26:52.2	Data point 94	2.20002 mL	0.30703 mL	0.30482 mL	0.45000 mL	7.078	-0.04861	0.94386	0.00247	Timed out at 59.5 s
1:28:17.6	Data point 95	2.20002 mL	0.30703 mL	0.30487 mL	0.45000 mL	7.285	-0.04933	0.98898	0.00245	Timed out at 59.5 s
1:29:53.3	Data point 96	2.20002 mL	0.30703 mL	0.30494 mL	0.45000 mL	7.511	-0.04973	0.95602	0.00251	Timed out at 59.5 s
1:31:28.9	Data point 97	2.20002 mL	0.30703 mL	0.30501 mL	0.45000 mL	7.812	-0.04080	0.98347	0.00203	Timed out at 59.5 s
1:33:04.5	Data point 98	2.20002 mL	0.30703 mL	0.30508 mL	0.45000 mL	8.214	-0.02455	0.95406	0.00124	Timed out at 59.5 s
1:34:50.4	Data point 99	2.20002 mL	0.30703 mL	0.30520 mL	0.45000 mL	8.531	-0.01310	0.49687	0.00092	17.0 s
1:35:43.0	Data point 100	2.20002 mL	0.30703 mL	0.30532 mL	0.45000 mL	8.762	-0.01738	0.82617	0.00094	31.5 s
1:37:00.5	Data point 101	2.20002 mL	0.30703 mL	0.30557 mL	0.45000 mL	9.094	-0.00556	0.09210	0.00091	13.5 s
1:37:54.9	Data point 102	2.20002 mL	0.30703 mL	0.30581 mL	0.45000 mL	9.313	-0.01317	0.45469	0.00096	18.0 s
1:38:48.6	Data point 103	2.20002 mL	0.30703 mL	0.30607 mL	0.45000 mL	9.526	-0.01066	0.32164	0.00093	11.0 s
1:39:35.3	Data point 104	2.20002 mL	0.30703 mL	0.30640 mL	0.45000 mL	9.732	-0.01018	0.39405	0.00080	11.0 s
1:40:27.1	Data point 105	2.20002 mL	0.30703 mL	0.30682 mL	0.45000 mL	9.932	-0.01216	0.85368	0.00065	10.5 s
1:41:08.2	Data point 106	2.20002 mL	0.30703 mL	0.30708 mL	0.45000 mL	10.040	-0.01217	0.84433	0.00065	10.0 s
1:41:27.3	Assay volumes	2.20002 mL	0.30703 mL	0.30708 mL	0.45000 mL					

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	10.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	2.20 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.050 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	300 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
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	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.100 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name:	**M15_octanol**	Experiment start time:	**3/1/2018 4:33:50 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-01004**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.300 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
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	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.130	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	3/1/2018 4:33:50 AM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	3/1/2018 4:33:50 AM	C:\Sirius_T3\HCl18B27.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M15_octanol**   Experiment start time: **3/1/2018 4:33:50 AM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-01004**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+3.15 mV		3/1/2018 4:34:18 AM
Filling solution	3M KCl	KCL097	2/27/2018 9:49:43 AM
Liquids			
Wash 1	50% IPA:50% Water		2/28/2018 10:23:32 AM
Wash 2	0.5% Trition X-100 in H20		2/28/2018 10:23:34 AM
Buffer position 1	pH7 Wash		2/28/2018 10:24:06 AM
Buffer position 2	pH 7		2/28/2018 10:24:08 AM
Storage position			2/28/2018 10:21:14 AM
Wash water	8.4e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	7e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	112:08:55		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
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	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:38] Air gap created for Water (0.15 M KCl)
[2:38] Air gap created for Acid (0.5 M HCl)
[2:38] Air gap created for Base (0.5 M KOH)
[2:39] Air gap released for Water (0.15 M KCl)
[2:42] Titrator arm moved over Titration position
[2:42] Titration 1 of 3
[2:42] Adding initial titrants
[2:42] Automatically add 2.20000 mL of water
[3:19] Dispensed 2.200024 mL of Water (0.15 M KCl)
[3:24] Titrator arm moved over Drain
[9:05] Titrator arm moved to Titration position
[9:05] Argon flow rate set to 100
[9:05] Stirrer speed set to 10
[9:10] Automatically add 0.05000 mL of Octanol
[9:11] Dispensed 0.050000 mL of Octanol
[9:12] Initial pH = 7.75
[9:12] Iterative adjust 7.75 -> 2.00
[9:12] pH 7.75 -> 2.00
[9:15] Air gap released for Acid (0.5 M HCl)
[9:16] Dispensed 0.096025 mL of Acid (0.5 M HCl)
[9:21] Holding pH 2.00
[11:21] Stirrer speed set to 0
[11:21] Stirrer speed set to 50
[11:21] Iterative adjust 1.98 -> 2.00
[11:21] pH 1.98 -> 2.00
[11:22] Air gap released for Base (0.5 M KOH)
[11:22] Dispensed 0.003551 mL of Base (0.5 M KOH)
[12:13] Stirrer speed set to 0
[12:23] Datapoint id 1 collected
[12:23] Stirrer speed set to 50
[12:29] pH 2.01 -> 2.21
[12:29] Using cautious pH adjust
[12:29] Dispensed 0.012159 mL of Base (0.5 M KOH)
[12:34] Stepping pH = 2.10
[12:34] Dispensed 0.009290 mL of Base (0.5 M KOH)
[12:40] Stepping pH = 2.19
[12:40] Dispensed 0.001929 mL of Base (0.5 M KOH)
[12:45] Stepping pH = 2.22
[13:00] Stirrer speed set to 0
[13:10] Datapoint id 2 collected
[13:10] Charge balance equation is out by 3.9%
[13:10] Stirrer speed set to 50

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[13:15] pH 2.22 -> 2.42
[13:15] Using charge balance adjust
[13:15] Dispensed 0.015828 mL of Base (0.5 M KOH)
[13:36] Stirrer speed set to 0
[13:46] Datapoint id 3 collected
[13:46] Charge balance equation is out by 5.0%
[13:46] Stirrer speed set to 50
[13:51] pH 2.44 -> 2.64
[13:51] Using charge balance adjust
[13:51] Dispensed 0.010654 mL of Base (0.5 M KOH)
[14:11] Stirrer speed set to 0
[14:21] Datapoint id 4 collected
[14:21] Charge balance equation is out by 4.3%
[14:21] Stirrer speed set to 50
[14:26] pH 2.65 -> 2.85
[14:26] Using charge balance adjust
[14:27] Dispensed 0.007432 mL of Base (0.5 M KOH)
[14:47] Stirrer speed set to 0
[14:57] Datapoint id 5 collected
[14:57] Charge balance equation is out by 5.6%
[14:57] Stirrer speed set to 50
[15:02] pH 2.87 -> 3.07
[15:02] Using charge balance adjust
[15:02] Dispensed 0.005221 mL of Base (0.5 M KOH)
[15:22] Stirrer speed set to 0
[15:32] Datapoint id 6 collected
[15:32] Charge balance equation is out by 7.8%
[15:32] Stirrer speed set to 50
[15:38] pH 3.09 -> 3.29
[15:38] Using charge balance adjust
[15:38] Dispensed 0.003669 mL of Base (0.5 M KOH)
[15:58] Stirrer speed set to 0
[16:08] Datapoint id 7 collected
[16:08] Charge balance equation is out by -10.7%
[16:08] Stirrer speed set to 50
[16:13] pH 3.27 -> 3.47
[16:13] Using charge balance adjust
[16:13] Dispensed 0.002728 mL of Base (0.5 M KOH)
[16:33] Stirrer speed set to 0
[16:43] Datapoint id 8 collected
[16:43] Charge balance equation is out by 1.1%
[16:43] Stirrer speed set to 50
[16:49] pH 3.48 -> 3.68
[16:49] Using charge balance adjust
[16:49] Dispensed 0.001999 mL of Base (0.5 M KOH)
[17:09] Stirrer speed set to 0
[17:19] Datapoint id 9 collected
[17:19] Charge balance equation is out by 0.9%
[17:19] Stirrer speed set to 50
[17:24] pH 3.69 -> 3.89
[17:24] Using charge balance adjust
[17:24] Dispensed 0.001599 mL of Base (0.5 M KOH)
[17:44] Stirrer speed set to 0
[17:55] Datapoint id 10 collected
[17:55] Charge balance equation is out by -8.5%
[17:55] Stirrer speed set to 50
[18:00] pH 3.87 -> 4.07
[18:00] Using charge balance adjust
[18:00] Dispensed 0.001458 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[18:20] Stirrer speed set to 0
[18:30] Datapoint id 11 collected
[18:30] Charge balance equation is out by -23.7%
[18:30] Stirrer speed set to 50
[18:35] pH 4.03 -> 4.23
[18:35] Using cautious pH adjust
[18:35] Dispensed 0.000729 mL of Base (0.5 M KOH)
[18:41] Stepping pH = 4.13
[18:41] Dispensed 0.000564 mL of Base (0.5 M KOH)
[18:46] Stepping pH = 4.21
[18:46] Dispensed 0.000118 mL of Base (0.5 M KOH)
[18:51] Stepping pH = 4.22
[18:51] Dispensed 0.000094 mL of Base (0.5 M KOH)
[18:56] Stepping pH = 4.23
[19:11] Stirrer speed set to 0
[19:21] Datapoint id 12 collected
[19:21] Charge balance equation is out by -3.6%
[19:21] Stirrer speed set to 50
[19:26] pH 4.23 -> 4.43
[19:26] Using charge balance adjust
[19:27] Dispensed 0.001646 mL of Base (0.5 M KOH)
[19:47] Stirrer speed set to 0
[19:57] Datapoint id 13 collected
[19:57] Charge balance equation is out by 33.3%
[19:57] Stirrer speed set to 50
[20:02] pH 4.50 -> 4.70
[20:02] Using cautious pH adjust
[20:02] Dispensed 0.001011 mL of Base (0.5 M KOH)
[20:07] Stepping pH = 4.63
[20:07] Dispensed 0.000447 mL of Base (0.5 M KOH)
[20:12] Stepping pH = 4.68
[20:12] Dispensed 0.000118 mL of Base (0.5 M KOH)
[20:17] Stepping pH = 4.69
[20:32] Stirrer speed set to 0
[20:42] Datapoint id 14 collected
[20:42] Charge balance equation is out by 22.0%
[20:42] Stirrer speed set to 50
[20:48] pH 4.69 -> 4.89
[20:48] Using cautious pH adjust
[20:48] Dispensed 0.001105 mL of Base (0.5 M KOH)
[20:53] Stepping pH = 4.82
[20:53] Dispensed 0.000517 mL of Base (0.5 M KOH)
[20:58] Stepping pH = 4.87
[20:58] Dispensed 0.000188 mL of Base (0.5 M KOH)
[21:03] Stepping pH = 4.88
[21:18] Stirrer speed set to 0
[21:29] Datapoint id 15 collected
[21:29] Charge balance equation is out by 17.8%
[21:29] Stirrer speed set to 50
[21:34] pH 4.88 -> 5.08
[21:34] Using cautious pH adjust
[21:34] Dispensed 0.001129 mL of Base (0.5 M KOH)
[21:39] Stepping pH = 4.99
[21:39] Dispensed 0.000706 mL of Base (0.5 M KOH)
[21:44] Stepping pH = 5.05
[21:44] Dispensed 0.000259 mL of Base (0.5 M KOH)
[21:49] Stepping pH = 5.07
[22:05] Stirrer speed set to 0
[22:15] Datapoint id 16 collected

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[22:15] Charge balance equation is out by 7.7%
[22:15] Stirrer speed set to 50
[22:20] pH 5.07 -> 5.27
[22:20] Using charge balance adjust
[22:20] Dispensed 0.002164 mL of Base (0.5 M KOH)
[22:40] Stirrer speed set to 0
[22:50] Datapoint id 17 collected
[22:50] Charge balance equation is out by -8.1%
[22:50] Stirrer speed set to 50
[22:55] pH 5.25 -> 5.45
[22:55] Using charge balance adjust
[22:55] Dispensed 0.001881 mL of Base (0.5 M KOH)
[23:15] Stirrer speed set to 0
[23:26] Datapoint id 18 collected
[23:26] Charge balance equation is out by 7.2%
[23:26] Stirrer speed set to 50
[23:31] pH 5.47 -> 5.67
[23:31] Using charge balance adjust
[23:31] Dispensed 0.001482 mL of Base (0.5 M KOH)
[23:51] Stirrer speed set to 0
[24:02] Datapoint id 19 collected
[24:02] Charge balance equation is out by 17.3%
[24:02] Stirrer speed set to 50
[24:07] pH 5.71 -> 5.91
[24:07] Using cautious pH adjust
[24:07] Dispensed 0.000517 mL of Base (0.5 M KOH)
[24:12] Stepping pH = 5.80
[24:12] Dispensed 0.000376 mL of Base (0.5 M KOH)
[24:17] Stepping pH = 5.90
[24:17] Dispensed 0.000047 mL of Base (0.5 M KOH)
[24:22] Stepping pH = 5.90
[24:37] Stirrer speed set to 0
[24:47] Datapoint id 20 collected
[24:47] Charge balance equation is out by 10.0%
[24:47] Stirrer speed set to 50
[24:52] pH 5.90 -> 6.10
[24:52] Using charge balance adjust
[24:52] Dispensed 0.000753 mL of Base (0.5 M KOH)
[25:13] Stirrer speed set to 0
[25:24] Datapoint id 21 collected
[25:24] Charge balance equation is out by 24.3%
[25:24] Stirrer speed set to 50
[25:29] pH 6.15 -> 6.35
[25:29] Using cautious pH adjust
[25:29] Dispensed 0.000235 mL of Base (0.5 M KOH)
[25:34] Stepping pH = 6.23
[25:34] Dispensed 0.000235 mL of Base (0.5 M KOH)
[25:39] Stepping pH = 6.35
[25:55] Stirrer speed set to 0
[26:11] Datapoint id 22 collected
[26:11] Charge balance equation is out by 3.5%
[26:11] Stirrer speed set to 50
[26:16] pH 6.36 -> 6.56
[26:16] Using charge balance adjust
[26:16] Dispensed 0.000329 mL of Base (0.5 M KOH)
[26:36] Stirrer speed set to 0
[26:57] Datapoint id 23 collected
[26:57] Charge balance equation is out by -39.1%
[26:57] Stirrer speed set to 50

Sample name: **M15_octanol**

Assay name: **pH-metric high logP**

Assay ID: **18C-01004**

Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**

Analyst: **Pion**

Instrument ID: **T312060**

Experiment Log (continued)

[27:02] pH 6.48 -> 6.68
[27:02] Using cautious pH adjust
[27:02] Dispensed 0.000118 mL of Base (0.5 M KOH)
[27:07] Stepping pH = 6.53
[27:07] Dispensed 0.000188 mL of Base (0.5 M KOH)
[27:12] Stepping pH = 6.72
[27:27] Stirrer speed set to 0
[27:52] Datapoint id 24 collected
[27:52] Charge balance equation is out by -27.4%
[27:52] Stirrer speed set to 50
[27:57] pH 6.75 -> 6.95
[27:57] Using cautious pH adjust
[27:57] Dispensed 0.000071 mL of Base (0.5 M KOH)
[28:02] Stepping pH = 6.77
[28:03] Dispensed 0.000212 mL of Base (0.5 M KOH)
[28:08] Stepping pH = 7.07
[28:23] Stirrer speed set to 0
[29:13] Datapoint id 25 collected
[29:13] Charge balance equation is out by -83.1%
[29:13] Stirrer speed set to 50
[29:18] pH 7.12 -> 7.32
[29:18] Using cautious pH adjust
[29:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:24] Stepping pH = 7.13
[29:24] Dispensed 0.000094 mL of Base (0.5 M KOH)
[29:29] Stepping pH = 7.23
[29:29] Dispensed 0.000047 mL of Base (0.5 M KOH)
[29:34] Stepping pH = 7.42
[29:49] Stirrer speed set to 0
[30:49] Datapoint id 26 collected
[30:49] Charge balance equation is out by -166.1%
[30:49] Stirrer speed set to 50
[30:54] pH 7.49 -> 7.69
[30:54] Using cautious pH adjust
[30:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[30:59] Stepping pH = 7.55
[30:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[31:04] Stepping pH = 7.61
[31:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[31:10] Stepping pH = 7.74
[31:25] Stirrer speed set to 0
[32:25] Datapoint id 27 collected
[32:25] Charge balance equation is out by -89.7%
[32:25] Stirrer speed set to 50
[32:30] pH 7.81 -> 8.01
[32:30] Using cautious pH adjust
[32:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[32:35] Stepping pH = 7.86
[32:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[32:40] Stepping pH = 7.97
[32:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[32:45] Stepping pH = 8.12
[33:00] Stirrer speed set to 0
[33:52] Datapoint id 28 collected
[33:52] Charge balance equation is out by -214.6%
[33:52] Stirrer speed set to 50
[33:57] pH 8.22 -> 8.42
[33:57] Using cautious pH adjust
[33:57] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**   Experiment start time: **3/1/2018 4:33:50 AM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-01004**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[34:02] Stepping pH = 8.27
[34:02] Dispensed 0.000024 mL of Base (0.5 M KOH)
[34:07] Stepping pH = 8.37
[34:07] Dispensed 0.000024 mL of Base (0.5 M KOH)
[34:12] Stepping pH = 8.48
[34:27] Stirrer speed set to 0
[35:15] Datapoint id 29 collected
[35:15] Charge balance equation is out by -257.9%
[35:15] Stirrer speed set to 50
[35:20] pH 8.53 -> 8.73
[35:20] Using cautious pH adjust
[35:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[35:25] Stepping pH = 8.56
[35:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[35:30] Stepping pH = 8.62
[35:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[35:35] Stepping pH = 8.68
[35:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[35:40] Stepping pH = 8.74
[35:55] Stirrer speed set to 0
[36:13] Datapoint id 30 collected
[36:13] Charge balance equation is out by -326.8%
[36:13] Stirrer speed set to 50
[36:18] pH 8.76 -> 8.96
[36:18] Using cautious pH adjust
[36:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:24] Stepping pH = 8.78
[36:24] Dispensed 0.000047 mL of Base (0.5 M KOH)
[36:29] Stepping pH = 8.83
[36:29] Dispensed 0.000071 mL of Base (0.5 M KOH)
[36:34] Stepping pH = 8.95
[36:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:39] Stepping pH = 9.00
[36:54] Stirrer speed set to 0
[37:24] Datapoint id 31 collected
[37:24] Charge balance equation is out by -326.2%
[37:24] Stirrer speed set to 50
[37:29] pH 9.02 -> 9.22
[37:29] Using cautious pH adjust
[37:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[37:34] Stepping pH = 9.03
[37:34] Dispensed 0.000094 mL of Base (0.5 M KOH)
[37:39] Stepping pH = 9.14
[37:39] Dispensed 0.000047 mL of Base (0.5 M KOH)
[37:44] Stepping pH = 9.23
[38:00] Stirrer speed set to 0
[38:24] Datapoint id 32 collected
[38:24] Charge balance equation is out by -182.2%
[38:24] Stirrer speed set to 50
[38:29] pH 9.24 -> 9.44
[38:29] Using cautious pH adjust
[38:29] Dispensed 0.000047 mL of Base (0.5 M KOH)
[38:34] Stepping pH = 9.26
[38:34] Dispensed 0.000141 mL of Base (0.5 M KOH)
[38:40] Stepping pH = 9.43
[38:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[38:45] Stepping pH = 9.47
[39:00] Stirrer speed set to 0
[39:14] Datapoint id 33 collected

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[39:14] Charge balance equation is out by -108.6%
[39:14] Stirrer speed set to 50
[39:19] pH 9.49 -> 9.69
[39:19] Using cautious pH adjust
[39:19] Dispensed 0.000071 mL of Base (0.5 M KOH)
[39:24] Stepping pH = 9.51
[39:24] Dispensed 0.000212 mL of Base (0.5 M KOH)
[39:29] Stepping pH = 9.72
[39:45] Stirrer speed set to 0
[39:58] Datapoint id 34 collected
[39:58] Charge balance equation is out by -84.8%
[39:58] Stirrer speed set to 50
[40:03] pH 9.73 -> 9.93
[40:03] Using cautious pH adjust
[40:03] Dispensed 0.000141 mL of Base (0.5 M KOH)
[40:08] Stepping pH = 9.80
[40:08] Dispensed 0.000165 mL of Base (0.5 M KOH)
[40:13] Stepping pH = 9.90
[40:13] Dispensed 0.000047 mL of Base (0.5 M KOH)
[40:18] Stepping pH = 9.93
[40:33] Stirrer speed set to 0
[40:44] Datapoint id 35 collected
[40:44] Charge balance equation is out by -29.7%
[40:44] Stirrer speed set to 50
[40:49] pH 9.93 -> 10.05
[40:49] Using cautious pH adjust
[40:49] Dispensed 0.000118 mL of Base (0.5 M KOH)
[40:55] Stepping pH = 9.97
[40:55] Dispensed 0.000141 mL of Base (0.5 M KOH)
[41:00] Stepping pH = 10.04
[41:15] Stirrer speed set to 0
[41:25] Datapoint id 36 collected
[41:25] Charge balance equation is out by -12.1%
[41:25] Titration 2 of 3
[41:25] Adding initial titrants
[41:25] Automatically add 0.10000 mL of Octanol
[41:27] Dispensed 0.100000 mL of Octanol
[41:27] Stirrer speed set to 10
[41:28] Stirrer speed set to 55
[41:28] Iterative adjust 10.05 -> 2.00
[41:28] pH 10.05 -> 2.00
[41:31] Dispensed 0.100000 mL of Acid (0.5 M HCl)
[41:36] pH 2.03 -> 2.00
[41:36] Dispensed 0.004680 mL of Acid (0.5 M HCl)
[42:26] Stirrer speed set to 0
[42:36] Datapoint id 37 collected
[42:36] Stirrer speed set to 55
[42:42] pH 1.96 -> 2.16
[42:42] Using cautious pH adjust
[42:42] Dispensed 0.014675 mL of Base (0.5 M KOH)
[42:47] Stepping pH = 2.05
[42:48] Dispensed 0.010466 mL of Base (0.5 M KOH)
[42:53] Stepping pH = 2.14
[42:53] Dispensed 0.002046 mL of Base (0.5 M KOH)
[42:58] Stepping pH = 2.17
[43:13] Stirrer speed set to 0
[43:23] Datapoint id 38 collected
[43:23] Charge balance equation is out by 7.4%
[43:23] Stirrer speed set to 55

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[43:28] pH 2.17 -> 2.37
[43:28] Using charge balance adjust
[43:29] Dispensed 0.018932 mL of Base (0.5 M KOH)
[43:49] Stirrer speed set to 0
[43:59] Datapoint id 39 collected
[43:59] Charge balance equation is out by 7.7%
[43:59] Stirrer speed set to 55
[44:04] pH 2.39 -> 2.59
[44:04] Using charge balance adjust
[44:05] Dispensed 0.012441 mL of Base (0.5 M KOH)
[44:25] Stirrer speed set to 0
[44:35] Datapoint id 40 collected
[44:35] Charge balance equation is out by 8.0%
[44:35] Stirrer speed set to 55
[44:40] pH 2.61 -> 2.81
[44:40] Using charge balance adjust
[44:40] Dispensed 0.008467 mL of Base (0.5 M KOH)
[45:00] Stirrer speed set to 0
[45:10] Datapoint id 41 collected
[45:10] Charge balance equation is out by 6.4%
[45:10] Stirrer speed set to 55
[45:15] pH 2.83 -> 3.03
[45:15] Using charge balance adjust
[45:16] Dispensed 0.005950 mL of Base (0.5 M KOH)
[45:36] Stirrer speed set to 0
[45:46] Datapoint id 42 collected
[45:46] Charge balance equation is out by 10.4%
[45:46] Stirrer speed set to 55
[45:51] pH 3.06 -> 3.26
[45:51] Using charge balance adjust
[45:51] Dispensed 0.004186 mL of Base (0.5 M KOH)
[46:11] Stirrer speed set to 0
[46:21] Datapoint id 43 collected
[46:21] Charge balance equation is out by -2.9%
[46:21] Stirrer speed set to 55
[46:26] pH 3.26 -> 3.46
[46:26] Using charge balance adjust
[46:27] Dispensed 0.003128 mL of Base (0.5 M KOH)
[46:47] Stirrer speed set to 0
[46:57] Datapoint id 44 collected
[46:57] Charge balance equation is out by 9.8%
[46:57] Stirrer speed set to 55
[47:02] pH 3.48 -> 3.68
[47:02] Using charge balance adjust
[47:02] Dispensed 0.002399 mL of Base (0.5 M KOH)
[47:22] Stirrer speed set to 0
[47:33] Datapoint id 45 collected
[47:33] Charge balance equation is out by -4.0%
[47:33] Stirrer speed set to 55
[47:38] pH 3.68 -> 3.88
[47:38] Using charge balance adjust
[47:38] Dispensed 0.002093 mL of Base (0.5 M KOH)
[47:58] Stirrer speed set to 0
[48:09] Datapoint id 46 collected
[48:09] Charge balance equation is out by -4.6%
[48:09] Stirrer speed set to 55
[48:14] pH 3.87 -> 4.07
[48:14] Using charge balance adjust
[48:14] Dispensed 0.002023 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[48:34] Stirrer speed set to 0
[48:44] Datapoint id 47 collected
[48:44] Charge balance equation is out by 0.6%
[48:44] Stirrer speed set to 55
[48:49] pH 4.07 -> 4.27
[48:49] Using charge balance adjust
[48:50] Dispensed 0.002140 mL of Base (0.5 M KOH)
[49:10] Stirrer speed set to 0
[49:20] Datapoint id 48 collected
[49:20] Charge balance equation is out by 22.9%
[49:20] Stirrer speed set to 55
[49:25] pH 4.32 -> 4.52
[49:25] Using cautious pH adjust
[49:25] Dispensed 0.001176 mL of Base (0.5 M KOH)
[49:31] Stepping pH = 4.44
[49:31] Dispensed 0.000635 mL of Base (0.5 M KOH)
[49:36] Stepping pH = 4.51
[49:36] Dispensed 0.000141 mL of Base (0.5 M KOH)
[49:41] Stepping pH = 4.52
[49:56] Stirrer speed set to 0
[50:06] Datapoint id 49 collected
[50:06] Charge balance equation is out by 16.8%
[50:06] Stirrer speed set to 55
[50:11] pH 4.51 -> 4.71
[50:11] Using cautious pH adjust
[50:11] Dispensed 0.001176 mL of Base (0.5 M KOH)
[50:16] Stepping pH = 4.61
[50:16] Dispensed 0.000800 mL of Base (0.5 M KOH)
[50:22] Stepping pH = 4.68
[50:22] Dispensed 0.000212 mL of Base (0.5 M KOH)
[50:27] Stepping pH = 4.70
[50:27] Dispensed 0.000141 mL of Base (0.5 M KOH)
[50:32] Stepping pH = 4.70
[50:47] Stirrer speed set to 0
[50:57] Datapoint id 50 collected
[50:57] Charge balance equation is out by 1.4%
[50:57] Stirrer speed set to 55
[51:02] pH 4.69 -> 4.89
[51:02] Using charge balance adjust
[51:02] Dispensed 0.002258 mL of Base (0.5 M KOH)
[51:23] Stirrer speed set to 0
[51:33] Datapoint id 51 collected
[51:33] Charge balance equation is out by 4.7%
[51:33] Stirrer speed set to 55
[51:38] pH 4.90 -> 5.10
[51:38] Using charge balance adjust
[51:38] Dispensed 0.001952 mL of Base (0.5 M KOH)
[51:58] Stirrer speed set to 0
[52:09] Datapoint id 52 collected
[52:09] Charge balance equation is out by 16.1%
[52:09] Stirrer speed set to 55
[52:14] pH 5.14 -> 5.34
[52:14] Using cautious pH adjust
[52:14] Dispensed 0.000753 mL of Base (0.5 M KOH)
[52:19] Stepping pH = 5.25
[52:19] Dispensed 0.000447 mL of Base (0.5 M KOH)
[52:24] Stepping pH = 5.32
[52:24] Dispensed 0.000094 mL of Base (0.5 M KOH)
[52:29] Stepping pH = 5.33

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[52:44] Stirrer speed set to 0
[52:55] Datapoint id 53 collected
[52:55] Charge balance equation is out by 13.9%
[52:55] Stirrer speed set to 55
[53:00] pH 5.33 -> 5.53
[53:00] Using charge balance adjust
[53:00] Dispensed 0.001129 mL of Base (0.5 M KOH)
[53:20] Stirrer speed set to 0
[53:30] Datapoint id 54 collected
[53:30] Charge balance equation is out by 23.2%
[53:30] Stirrer speed set to 55
[53:35] pH 5.58 -> 5.78
[53:35] Using cautious pH adjust
[53:35] Dispensed 0.000376 mL of Base (0.5 M KOH)
[53:41] Stepping pH = 5.67
[53:41] Dispensed 0.000282 mL of Base (0.5 M KOH)
[53:46] Stepping pH = 5.77
[54:01] Stirrer speed set to 0
[54:11] Datapoint id 55 collected
[54:11] Charge balance equation is out by 11.5%
[54:11] Stirrer speed set to 55
[54:16] pH 5.77 -> 5.97
[54:16] Using charge balance adjust
[54:16] Dispensed 0.000517 mL of Base (0.5 M KOH)
[54:37] Stirrer speed set to 0
[54:49] Datapoint id 56 collected
[54:49] Charge balance equation is out by 10.2%
[54:49] Stirrer speed set to 55
[54:54] pH 6.00 -> 6.20
[54:54] Using charge balance adjust
[54:54] Dispensed 0.000353 mL of Base (0.5 M KOH)
[55:15] Stirrer speed set to 0
[55:30] Datapoint id 57 collected
[55:30] Charge balance equation is out by -5.4%
[55:30] Stirrer speed set to 55
[55:35] pH 6.21 -> 6.41
[55:35] Using charge balance adjust
[55:35] Dispensed 0.000259 mL of Base (0.5 M KOH)
[55:55] Stirrer speed set to 0
[56:27] Datapoint id 58 collected
[56:27] Charge balance equation is out by 31.8%
[56:27] Stirrer speed set to 55
[56:32] pH 6.50 -> 6.70
[56:32] Using cautious pH adjust
[56:32] Dispensed 0.000071 mL of Base (0.5 M KOH)
[56:37] Stepping pH = 6.51
[56:37] Dispensed 0.000212 mL of Base (0.5 M KOH)
[56:42] Stepping pH = 6.96
[56:58] Stirrer speed set to 0
[57:58] Datapoint id 59 collected
[57:58] Charge balance equation is out by -84.9%
[57:58] Stirrer speed set to 55
[58:03] pH 6.98 -> 7.18
[58:03] Using cautious pH adjust
[58:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:08] Stepping pH = 7.01
[58:08] Dispensed 0.000071 mL of Base (0.5 M KOH)
[58:13] Stepping pH = 7.02
[58:13] Dispensed 0.000165 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[58:18] Stepping pH = 7.94
[58:33] Stirrer speed set to 0
[59:33] Datapoint id 60 collected
[59:33] Charge balance equation is out by -331.1%
[59:33] Stirrer speed set to 55
[59:39] pH 8.01 -> 8.21
[59:39] Using cautious pH adjust
[59:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:44] Stepping pH = 8.02
[59:44] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:49] Stepping pH = 8.02
[59:49] Dispensed 0.000094 mL of Base (0.5 M KOH)
[59:54] Stepping pH = 8.25
[1:00:09] Stirrer speed set to 0
[1:01:08] Datapoint id 61 collected
[1:01:08] Charge balance equation is out by -895.9%
[1:01:08] Stirrer speed set to 55
[1:01:13] pH 8.29 -> 8.49
[1:01:13] Using cautious pH adjust
[1:01:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:18] Stepping pH = 8.30
[1:01:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:24] Stepping pH = 8.31
[1:01:24] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:01:29] Stepping pH = 8.46
[1:01:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:34] Stepping pH = 8.51
[1:01:49] Stirrer speed set to 0
[1:02:21] Datapoint id 62 collected
[1:02:21] Charge balance equation is out by -675.6%
[1:02:21] Stirrer speed set to 55
[1:02:26] pH 8.53 -> 8.73
[1:02:26] Using cautious pH adjust
[1:02:26] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:31] Stepping pH = 8.55
[1:02:31] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:36] Stepping pH = 8.59
[1:02:36] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:02:41] Stepping pH = 8.73
[1:02:56] Stirrer speed set to 0
[1:03:24] Datapoint id 63 collected
[1:03:24] Charge balance equation is out by -363.9%
[1:03:24] Stirrer speed set to 55
[1:03:29] pH 8.75 -> 8.95
[1:03:29] Using cautious pH adjust
[1:03:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:34] Stepping pH = 8.77
[1:03:35] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:03:40] Stepping pH = 8.81
[1:03:40] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:03:45] Stepping pH = 8.88
[1:03:45] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:03:50] Stepping pH = 8.94
[1:04:05] Stirrer speed set to 0
[1:04:20] Datapoint id 64 collected
[1:04:20] Charge balance equation is out by -534.8%
[1:04:20] Stirrer speed set to 55
[1:04:25] pH 8.96 -> 9.16
[1:04:25] Using cautious pH adjust

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:04:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:30] Stepping pH = 8.97
[1:04:30] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:04:35] Stepping pH = 8.99
[1:04:35] Dispensed 0.000235 mL of Base (0.5 M KOH)
[1:04:40] Stepping pH = 9.25
[1:04:55] Stirrer speed set to 0
[1:05:18] Datapoint id 65 collected
[1:05:18] Charge balance equation is out by -466.4%
[1:05:18] Stirrer speed set to 55
[1:05:23] pH 9.28 -> 9.48
[1:05:23] Using cautious pH adjust
[1:05:23] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:05:28] Stepping pH = 9.28
[1:05:28] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:05:33] Stepping pH = 9.42
[1:05:33] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:05:38] Stepping pH = 9.47
[1:05:54] Stirrer speed set to 0
[1:06:07] Datapoint id 66 collected
[1:06:07] Charge balance equation is out by -157.2%
[1:06:07] Stirrer speed set to 55
[1:06:12] pH 9.48 -> 9.68
[1:06:12] Using cautious pH adjust
[1:06:12] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:06:17] Stepping pH = 9.51
[1:06:17] Dispensed 0.000212 mL of Base (0.5 M KOH)
[1:06:23] Stepping pH = 9.69
[1:06:38] Stirrer speed set to 0
[1:06:49] Datapoint id 67 collected
[1:06:49] Charge balance equation is out by -70.6%
[1:06:49] Stirrer speed set to 55
[1:06:54] pH 9.71 -> 9.91
[1:06:54] Using cautious pH adjust
[1:06:54] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:06:59] Stepping pH = 9.75
[1:06:59] Dispensed 0.000259 mL of Base (0.5 M KOH)
[1:07:04] Stepping pH = 9.91
[1:07:19] Stirrer speed set to 0
[1:07:30] Datapoint id 68 collected
[1:07:30] Charge balance equation is out by -45.5%
[1:07:30] Stirrer speed set to 55
[1:07:35] pH 9.92 -> 10.05
[1:07:35] Using cautious pH adjust
[1:07:35] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:07:40] Stepping pH = 9.94
[1:07:40] Dispensed 0.000306 mL of Base (0.5 M KOH)
[1:07:45] Stepping pH = 10.09
[1:08:00] Stirrer speed set to 0
[1:08:14] Datapoint id 69 collected
[1:08:14] Charge balance equation is out by -72.3%
[1:08:14] Titration 3 of 3
[1:08:14] Adding initial titrants
[1:08:14] Automatically add 0.30000 mL of Octanol
[1:08:21] Dispensed 0.300000 mL of Octanol
[1:08:21] Stirrer speed set to 10
[1:08:22] Stirrer speed set to 60
[1:08:22] Iterative adjust 10.10 -> 2.00
[1:08:22] pH 10.10 -> 2.00

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:08:24] Dispensed 0.100000 mL of Acid (0.5 M HCl)
[1:08:30] pH 2.04 -> 2.00
[1:08:30] Dispensed 0.006326 mL of Acid (0.5 M HCl)
[1:09:20] Stirrer speed set to 0
[1:09:30] Datapoint id 70 collected
[1:09:30] Stirrer speed set to 60
[1:09:35] pH 1.99 -> 2.19
[1:09:35] Using cautious pH adjust
[1:09:36] Dispensed 0.015052 mL of Base (0.5 M KOH)
[1:09:41] Stepping pH = 2.08
[1:09:41] Dispensed 0.010818 mL of Base (0.5 M KOH)
[1:09:46] Stepping pH = 2.16
[1:09:46] Dispensed 0.002375 mL of Base (0.5 M KOH)
[1:09:52] Stepping pH = 2.19
[1:10:07] Stirrer speed set to 0
[1:10:17] Datapoint id 71 collected
[1:10:17] Charge balance equation is out by 6.2%
[1:10:17] Stirrer speed set to 60
[1:10:22] pH 2.19 -> 2.39
[1:10:22] Using charge balance adjust
[1:10:22] Dispensed 0.019450 mL of Base (0.5 M KOH)
[1:10:43] Stirrer speed set to 0
[1:10:53] Datapoint id 72 collected
[1:10:53] Charge balance equation is out by 9.2%
[1:10:53] Stirrer speed set to 60
[1:10:58] pH 2.41 -> 2.61
[1:10:58] Using charge balance adjust
[1:10:59] Dispensed 0.012794 mL of Base (0.5 M KOH)
[1:11:19] Stirrer speed set to 0
[1:11:29] Datapoint id 73 collected
[1:11:29] Charge balance equation is out by 13.1%
[1:11:29] Stirrer speed set to 60
[1:11:34] pH 2.64 -> 2.84
[1:11:34] Using charge balance adjust
[1:11:34] Dispensed 0.008655 mL of Base (0.5 M KOH)
[1:11:54] Stirrer speed set to 0
[1:12:05] Datapoint id 74 collected
[1:12:05] Charge balance equation is out by 9.7%
[1:12:05] Stirrer speed set to 60
[1:12:10] pH 2.87 -> 3.07
[1:12:10] Using charge balance adjust
[1:12:10] Dispensed 0.006138 mL of Base (0.5 M KOH)
[1:12:30] Stirrer speed set to 0
[1:12:40] Datapoint id 75 collected
[1:12:40] Charge balance equation is out by 5.4%
[1:12:40] Stirrer speed set to 60
[1:12:45] pH 3.09 -> 3.29
[1:12:45] Using charge balance adjust
[1:12:45] Dispensed 0.004563 mL of Base (0.5 M KOH)
[1:13:06] Stirrer speed set to 0
[1:13:16] Datapoint id 76 collected
[1:13:16] Charge balance equation is out by 6.3%
[1:13:16] Stirrer speed set to 60
[1:13:21] pH 3.30 -> 3.50
[1:13:21] Using charge balance adjust
[1:13:21] Dispensed 0.003575 mL of Base (0.5 M KOH)
[1:13:41] Stirrer speed set to 0
[1:13:51] Datapoint id 77 collected
[1:13:51] Charge balance equation is out by 2.0%

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:13:51] Stirrer speed set to 60
[1:13:56] pH 3.51 -> 3.71
[1:13:56] Using charge balance adjust
[1:13:57] Dispensed 0.003057 mL of Base (0.5 M KOH)
[1:14:17] Stirrer speed set to 0
[1:14:27] Datapoint id 78 collected
[1:14:27] Charge balance equation is out by 10.2%
[1:14:27] Stirrer speed set to 60
[1:14:32] pH 3.73 -> 3.93
[1:14:32] Using charge balance adjust
[1:14:32] Dispensed 0.002846 mL of Base (0.5 M KOH)
[1:14:52] Stirrer speed set to 0
[1:15:03] Datapoint id 79 collected
[1:15:03] Charge balance equation is out by 26.2%
[1:15:03] Stirrer speed set to 60
[1:15:08] pH 3.98 -> 4.18
[1:15:08] Using cautious pH adjust
[1:15:08] Dispensed 0.001364 mL of Base (0.5 M KOH)
[1:15:13] Stepping pH = 4.08
[1:15:13] Dispensed 0.000894 mL of Base (0.5 M KOH)
[1:15:18] Stepping pH = 4.16
[1:15:18] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:15:23] Stepping pH = 4.17
[1:15:39] Stirrer speed set to 0
[1:15:49] Datapoint id 80 collected
[1:15:49] Charge balance equation is out by 10.9%
[1:15:49] Stirrer speed set to 60
[1:15:54] pH 4.16 -> 4.36
[1:15:54] Using charge balance adjust
[1:15:54] Dispensed 0.002634 mL of Base (0.5 M KOH)
[1:16:14] Stirrer speed set to 0
[1:16:24] Datapoint id 81 collected
[1:16:24] Charge balance equation is out by 15.1%
[1:16:24] Stirrer speed set to 60
[1:16:29] pH 4.38 -> 4.58
[1:16:29] Using cautious pH adjust
[1:16:29] Dispensed 0.001152 mL of Base (0.5 M KOH)
[1:16:34] Stepping pH = 4.48
[1:16:34] Dispensed 0.000753 mL of Base (0.5 M KOH)
[1:16:40] Stepping pH = 4.57
[1:16:55] Stirrer speed set to 0
[1:17:05] Datapoint id 82 collected
[1:17:05] Charge balance equation is out by 17.4%
[1:17:05] Stirrer speed set to 60
[1:17:10] pH 4.56 -> 4.76
[1:17:10] Using cautious pH adjust
[1:17:10] Dispensed 0.000964 mL of Base (0.5 M KOH)
[1:17:16] Stepping pH = 4.67
[1:17:16] Dispensed 0.000611 mL of Base (0.5 M KOH)
[1:17:21] Stepping pH = 4.74
[1:17:21] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:17:26] Stepping pH = 4.76
[1:17:41] Stirrer speed set to 0
[1:17:52] Datapoint id 83 collected
[1:17:52] Charge balance equation is out by 12.3%
[1:17:52] Stirrer speed set to 60
[1:17:57] pH 4.75 -> 4.95
[1:17:57] Using charge balance adjust
[1:17:57] Dispensed 0.001552 mL of Base (0.5 M KOH)

Sample name: **M15_octanol** Experiment start time: **3/1/2018 4:33:50 AM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-01004** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[1:18:17] Stirrer speed set to 0
[1:18:27] Datapoint id 84 collected
[1:18:27] Charge balance equation is out by -6.1%
[1:18:27] Stirrer speed set to 60
[1:18:33] pH 4.93 -> 5.13
[1:18:33] Using charge balance adjust
[1:18:33] Dispensed 0.001152 mL of Base (0.5 M KOH)
[1:18:53] Stirrer speed set to 0
[1:19:03] Datapoint id 85 collected
[1:19:03] Charge balance equation is out by -13.9%
[1:19:03] Stirrer speed set to 60
[1:19:09] pH 5.11 -> 5.31
[1:19:09] Using charge balance adjust
[1:19:09] Dispensed 0.000847 mL of Base (0.5 M KOH)
[1:19:29] Stirrer speed set to 0
[1:19:39] Datapoint id 86 collected
[1:19:39] Charge balance equation is out by -13.8%
[1:19:39] Stirrer speed set to 60
[1:19:44] pH 5.29 -> 5.49
[1:19:44] Using charge balance adjust
[1:19:45] Dispensed 0.000611 mL of Base (0.5 M KOH)
[1:20:05] Stirrer speed set to 0
[1:20:16] Datapoint id 87 collected
[1:20:16] Charge balance equation is out by -8.9%
[1:20:16] Stirrer speed set to 60
[1:20:21] pH 5.48 -> 5.68
[1:20:21] Using charge balance adjust
[1:20:21] Dispensed 0.000423 mL of Base (0.5 M KOH)
[1:20:42] Stirrer speed set to 0
[1:20:54] Datapoint id 88 collected
[1:20:54] Charge balance equation is out by -11.2%
[1:20:54] Stirrer speed set to 60
[1:20:59] pH 5.68 -> 5.88
[1:20:59] Using charge balance adjust
[1:20:59] Dispensed 0.000306 mL of Base (0.5 M KOH)
[1:21:20] Stirrer speed set to 0
[1:21:32] Datapoint id 89 collected
[1:21:32] Charge balance equation is out by -4.3%
[1:21:32] Stirrer speed set to 60
[1:21:37] pH 5.89 -> 6.09
[1:21:37] Using charge balance adjust
[1:21:37] Dispensed 0.000212 mL of Base (0.5 M KOH)
[1:21:58] Stirrer speed set to 0
[1:22:30] Datapoint id 90 collected
[1:22:30] Charge balance equation is out by -17.7%
[1:22:30] Stirrer speed set to 60
[1:22:35] pH 6.08 -> 6.28
[1:22:35] Using cautious pH adjust
[1:22:35] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:22:40] Stepping pH = 6.15
[1:22:40] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:22:46] Stepping pH = 6.33
[1:23:01] Stirrer speed set to 0
[1:23:41] Datapoint id 91 collected
[1:23:41] Charge balance equation is out by -5.1%
[1:23:41] Stirrer speed set to 60
[1:23:46] pH 6.35 -> 6.55
[1:23:46] Using charge balance adjust
[1:23:46] Dispensed 0.000118 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:24:06] Stirrer speed set to 0
[1:24:57] Datapoint id 92 collected
[1:24:57] Charge balance equation is out by -13.5%
[1:24:57] Stirrer speed set to 60
[1:25:02] pH 6.61 -> 6.81
[1:25:02] Using charge balance adjust
[1:25:02] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:25:22] Stirrer speed set to 0
[1:26:22] Datapoint id 93 collected
[1:26:22] Charge balance equation is out by -26.4%
[1:26:22] Stirrer speed set to 60
[1:26:27] pH 6.83 -> 7.03
[1:26:27] Using cautious pH adjust
[1:26:27] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:26:32] Stepping pH = 6.90
[1:26:32] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:26:37] Stepping pH = 7.10
[1:26:53] Stirrer speed set to 0
[1:27:53] Datapoint id 94 collected
[1:27:53] Charge balance equation is out by -5.1%
[1:27:53] Stirrer speed set to 60
[1:27:58] pH 7.15 -> 7.35
[1:27:58] Using charge balance adjust
[1:27:58] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:28:18] Stirrer speed set to 0
[1:29:18] Datapoint id 95 collected
[1:29:18] Charge balance equation is out by -32.1%
[1:29:18] Stirrer speed set to 60
[1:29:23] pH 7.27 -> 7.47
[1:29:23] Using cautious pH adjust
[1:29:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:29:28] Stepping pH = 7.34
[1:29:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:29:33] Stepping pH = 7.40
[1:29:33] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:29:38] Stepping pH = 7.52
[1:29:54] Stirrer speed set to 0
[1:30:54] Datapoint id 96 collected
[1:30:54] Charge balance equation is out by -94.3%
[1:30:54] Stirrer speed set to 60
[1:30:59] pH 7.53 -> 7.73
[1:30:59] Using cautious pH adjust
[1:30:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:31:04] Stepping pH = 7.55
[1:31:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:31:09] Stepping pH = 7.63
[1:31:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:31:14] Stepping pH = 7.75
[1:31:29] Stirrer speed set to 0
[1:32:29] Datapoint id 97 collected
[1:32:29] Charge balance equation is out by -237.6%
[1:32:29] Stirrer speed set to 60
[1:32:34] pH 7.96 -> 8.16
[1:32:34] Using cautious pH adjust
[1:32:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:32:39] Stepping pH = 8.09
[1:32:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:32:45] Stepping pH = 8.13
[1:32:45] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:32:50] Stepping pH = 8.22
[1:33:05] Stirrer speed set to 0
[1:34:05] Datapoint id 98 collected
[1:34:05] Charge balance equation is out by -329.5%
[1:34:05] Stirrer speed set to 60
[1:34:10] pH 8.28 -> 8.48
[1:34:10] Using cautious pH adjust
[1:34:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:34:15] Stepping pH = 8.35
[1:34:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:34:20] Stepping pH = 8.41
[1:34:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:34:25] Stepping pH = 8.43
[1:34:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:34:30] Stepping pH = 8.44
[1:34:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:34:36] Stepping pH = 8.50
[1:34:51] Stirrer speed set to 0
[1:35:08] Datapoint id 99 collected
[1:35:08] Charge balance equation is out by -520.9%
[1:35:08] Stirrer speed set to 60
[1:35:13] pH 8.57 -> 8.77
[1:35:13] Using cautious pH adjust
[1:35:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:35:18] Stepping pH = 8.59
[1:35:18] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:35:23] Stepping pH = 8.67
[1:35:23] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:35:28] Stepping pH = 8.76
[1:35:43] Stirrer speed set to 0
[1:36:15] Datapoint id 100 collected
[1:36:15] Charge balance equation is out by -224.9%
[1:36:15] Stirrer speed set to 60
[1:36:20] pH 8.79 -> 8.99
[1:36:20] Using cautious pH adjust
[1:36:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:36:25] Stepping pH = 8.82
[1:36:25] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:36:30] Stepping pH = 8.90
[1:36:30] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:36:35] Stepping pH = 8.97
[1:36:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:36:41] Stepping pH = 8.96
[1:36:41] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:36:46] Stepping pH = 9.08
[1:37:01] Stirrer speed set to 0
[1:37:14] Datapoint id 101 collected
[1:37:14] Charge balance equation is out by -394.5%
[1:37:14] Stirrer speed set to 60
[1:37:19] pH 9.11 -> 9.31
[1:37:19] Using cautious pH adjust
[1:37:20] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:37:25] Stepping pH = 9.14
[1:37:25] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:37:30] Stepping pH = 9.26
[1:37:30] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:37:35] Stepping pH = 9.30
[1:37:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:37:40] Stepping pH = 9.31

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01004**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01004_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 4:33:50 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:37:55] Stirrer speed set to 0
[1:38:13] Datapoint id 102 collected
[1:38:13] Charge balance equation is out by -152.8%
[1:38:13] Stirrer speed set to 60
[1:38:18] pH 9.33 -> 9.53
[1:38:18] Using cautious pH adjust
[1:38:18] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:38:23] Stepping pH = 9.37
[1:38:24] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:38:29] Stepping pH = 9.50
[1:38:29] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:38:34] Stepping pH = 9.52
[1:38:49] Stirrer speed set to 0
[1:39:00] Datapoint id 103 collected
[1:39:00] Charge balance equation is out by -71.5%
[1:39:00] Stirrer speed set to 60
[1:39:05] pH 9.54 -> 9.74
[1:39:05] Using cautious pH adjust
[1:39:05] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:39:10] Stepping pH = 9.58
[1:39:10] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:39:15] Stepping pH = 9.71
[1:39:15] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:39:20] Stepping pH = 9.73
[1:39:36] Stirrer speed set to 0
[1:39:47] Datapoint id 104 collected
[1:39:47] Charge balance equation is out by -52.8%
[1:39:47] Stirrer speed set to 60
[1:39:52] pH 9.74 -> 9.94
[1:39:52] Using cautious pH adjust
[1:39:52] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:39:57] Stepping pH = 9.82
[1:39:57] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:40:02] Stepping pH = 9.91
[1:40:02] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:40:07] Stepping pH = 9.93
[1:40:07] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:40:12] Stepping pH = 9.94
[1:40:27] Stirrer speed set to 0
[1:40:38] Datapoint id 105 collected
[1:40:38] Charge balance equation is out by -33.7%
[1:40:38] Stirrer speed set to 60
[1:40:43] pH 9.94 -> 10.05
[1:40:43] Using cautious pH adjust
[1:40:43] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:40:48] Stepping pH = 9.97
[1:40:48] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:40:53] Stepping pH = 10.04
[1:41:08] Stirrer speed set to 0
[1:41:18] Datapoint id 106 collected
[1:41:18] Charge balance equation is out by -10.7%
[1:41:18] Argon flow rate set to 0
[1:41:22] Titrator arm moved over Titration position