Sample name: **M08_octanol**   Experiment start time: **3/2/2018 6:51:30 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-02008**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

pH-metric Result

logP (neutral XH) 3.08 ±0.01 (n=50)
logP (X -)   -0.07 ±0.05 (n=50)

18C-02008 Points 2 to 33

M08_octanol concentration factor 1.008
Carbonate   0.0000 mM
Acidity error   -0.21439 mM

18C-02008 Points 34 to 67

M08_octanol concentration factor 1.106
Carbonate   0.0000 mM
Acidity error   -0.33976 mM

18C-02008 Points 68 to 106

M08_octanol concentration factor 0.984
Carbonate   0.2479 mM
Acidity error   -0.08487 mM
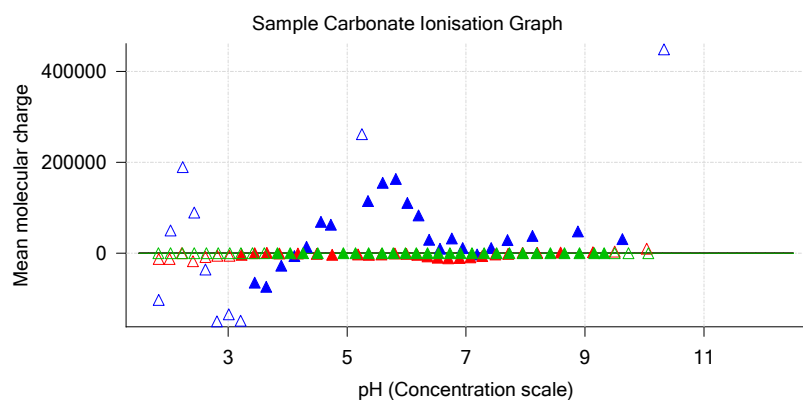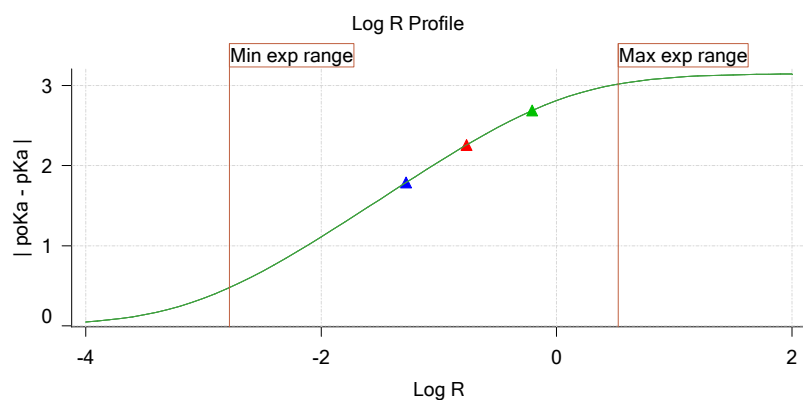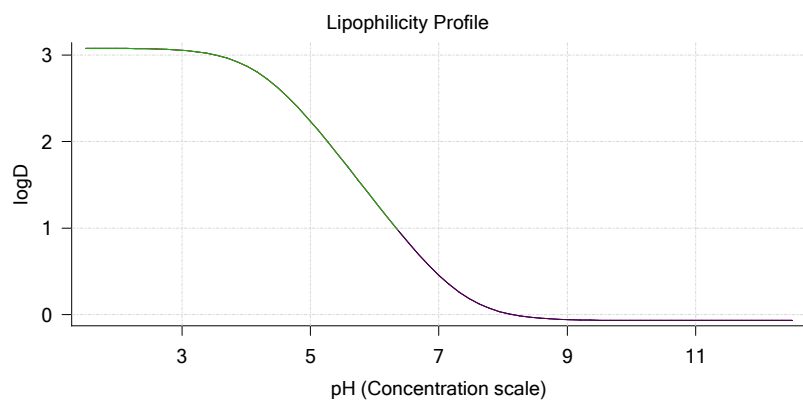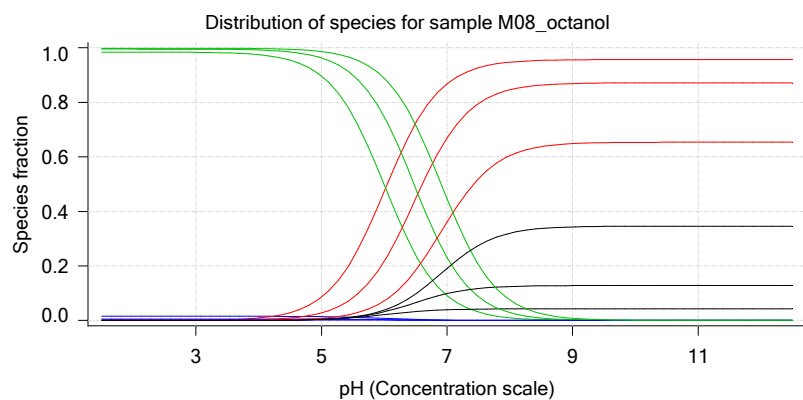
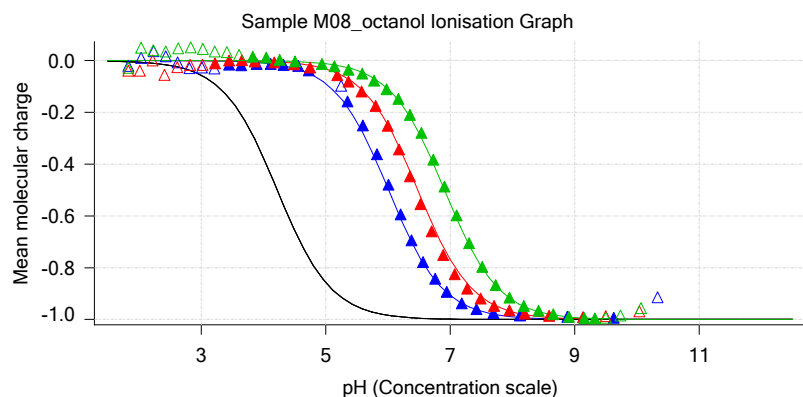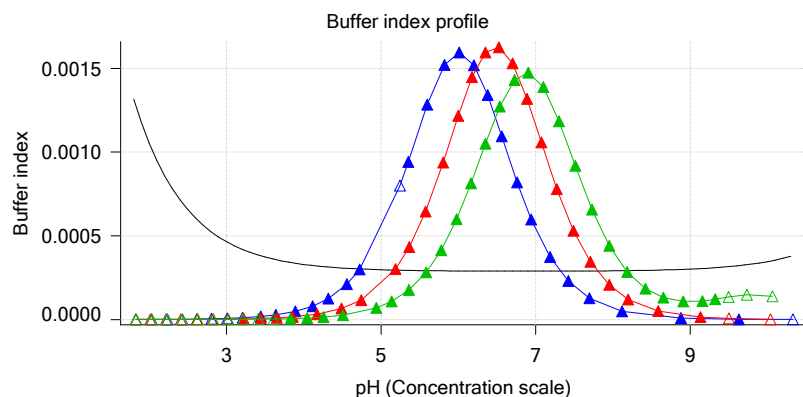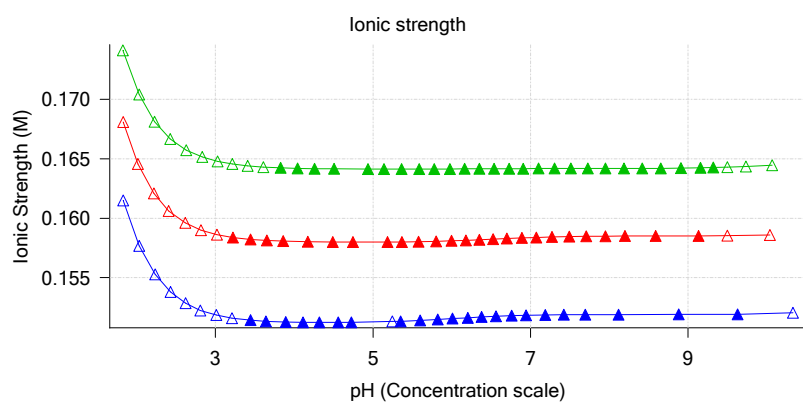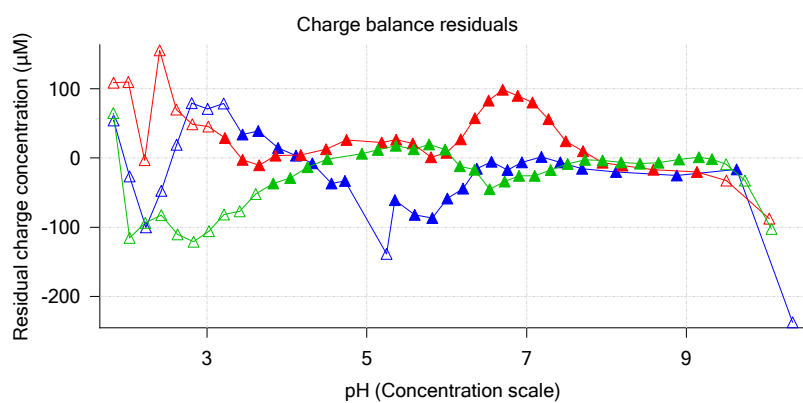## Warnings and errors

Errors   None
Warnings None

Sample logD and percent species

pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	3.08	0.08 %	0.00 %	99.92 %	0.00 %	
1.200	3.08	0.08 %	0.00 %	99.92 %	0.00 %	Stomach pH
2.000	3.08	0.08 %	0.00 %	99.92 %	0.00 %	
3.000	3.06	0.08 %	0.00 %	99.91 %	0.00 %	
4.000	2.88	0.08 %	0.05 %	99.82 %	0.04 %	
5.000	2.24	0.08 %	0.50 %	99.00 %	0.42 %	
6.000	1.31	0.08 %	4.58 %	91.44 %	3.91 %	
6.500	0.85	0.06 %	12.23 %	77.26 %	10.45 %	
7.000	0.45	0.04 %	25.94 %	51.84 %	22.18 %	
7.400	0.22	0.02 %	37.72 %	30.01 %	32.25 %	Blood pH
8.000	0.02	0.01 %	48.66 %	9.72 %	41.61 %	
9.000	-0.06	0.00 %	53.33 %	1.07 %	45.60 %	
10.000	-0.07	0.00 %	53.85 %	0.11 %	46.04 %	
11.000	-0.07	0.00 %	53.90 %	0.01 %	46.09 %	
12.000	-0.07	0.00 %	53.91 %	0.00 %	46.09 %	

pH-metric Result

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M08_octanol Ionisation Graph

Distribution of species for sample M08_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)

Distribution of species for sample Carbonate

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
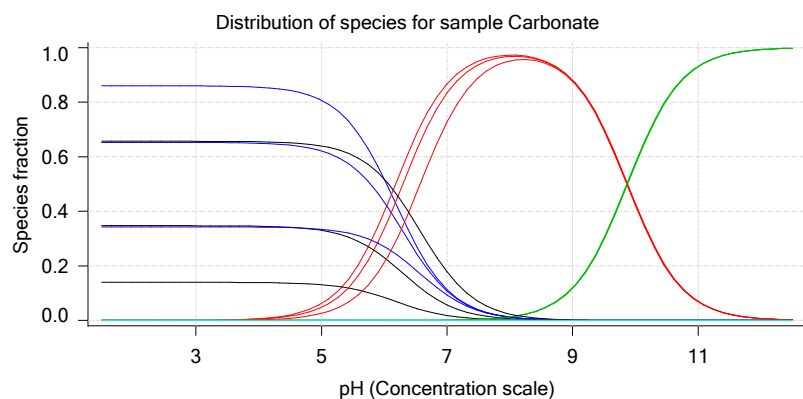Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 1 of 3   18C-02008 Points 2 to 33

Overall results

RMSD	0.161
Average ionic strength	0.152 M
Average temperature	24.9°C
Partition ratio	0.0526 : 1
Analyte concentration range	2531.4 µM to 2619.0 µM
Total points considered	22 of 32

Warnings and errors

Errors   None
Warnings   One or more logP values out of range

Four-Plus parameters

	Alpha	0.111	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
	S	0.9988	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
	jH	1.0	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
	jOH	-0.8	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r

Titrants

	0.50 M HCl	0.999058	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
	0.50 M KOH	0.999845	3/2/2018 6:51:30 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

	M08_octanol concentration factor	1.008
	Acid pKa 1	4.22
	logP (neutral XH)	3.10
	logP (X -)	-5.13

Sample graphs

Ionisation of sample M08_octanol

Distribution of species for sample M08_octanol

Sample name: **M08_octanol** Experiment start time: **3/2/2018 6:51:30 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02008** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Sample graphs (continued)

Lipophilicity Profile
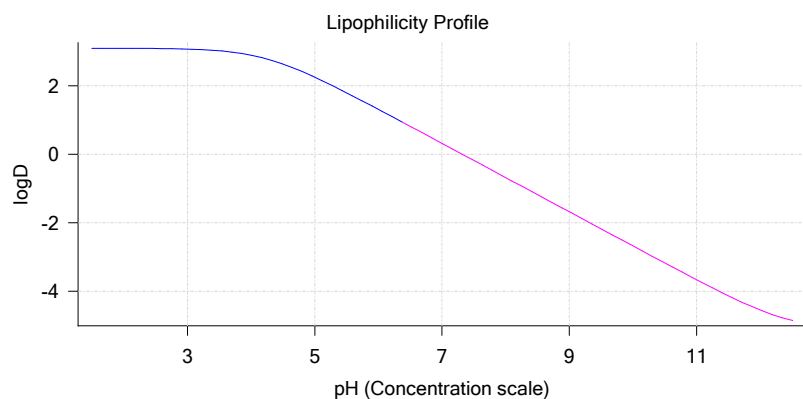
Sample logD and percent species

pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	3.10	1.49 %	0.00 %	98.50 %	0.00 %	
1.200	3.10	1.49 %	0.00 %	98.50 %	0.00 %	Stomach pH
2.000	3.10	1.49 %	0.01 %	98.50 %	0.00 %	
3.000	3.07	1.49 %	0.09 %	98.42 %	0.00 %	
4.000	2.89	1.48 %	0.89 %	97.63 %	0.00 %	
5.000	2.25	1.37 %	8.26 %	90.37 %	0.00 %	
6.000	1.31	0.79 %	47.38 %	51.83 %	0.00 %	
6.500	0.82	0.39 %	74.01 %	25.60 %	0.00 %	
7.000	0.32	0.15 %	90.01 %	9.84 %	0.00 %	
7.400	-0.08	0.06 %	95.77 %	4.17 %	0.00 %	Blood pH
8.000	-0.68	0.02 %	98.90 %	1.08 %	0.00 %	
9.000	-1.68	0.00 %	99.89 %	0.11 %	0.00 %	
10.000	-2.68	0.00 %	99.99 %	0.01 %	0.00 %	
11.000	-3.67	0.00 %	100.00 %	0.00 %	0.00 %	
12.000	-4.55	0.00 %	100.00 %	0.00 %	0.00 %	

Carbonate and acidity

Carbonate 0.000 mM
Acidity error -0.214 mM

Other graphs

Assay progress

Titration graph

Sample name: **M08_octanol**

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

Assay ID: **18C-02008**

Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**

Analyst: **Pion**
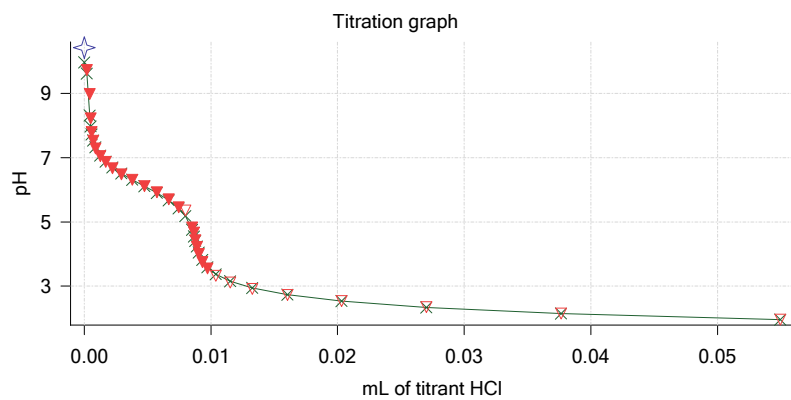
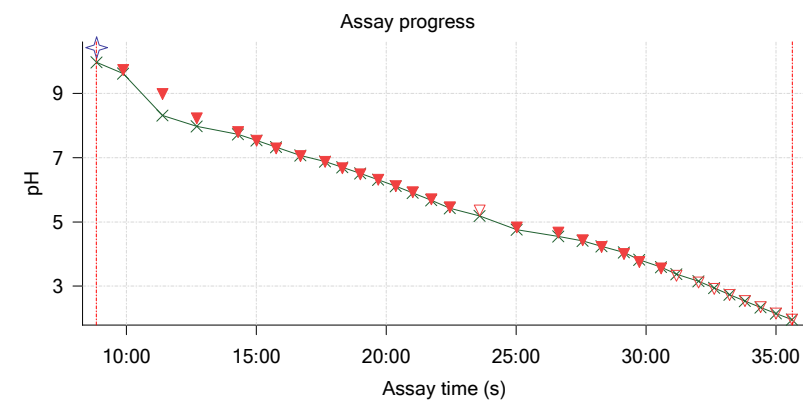Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
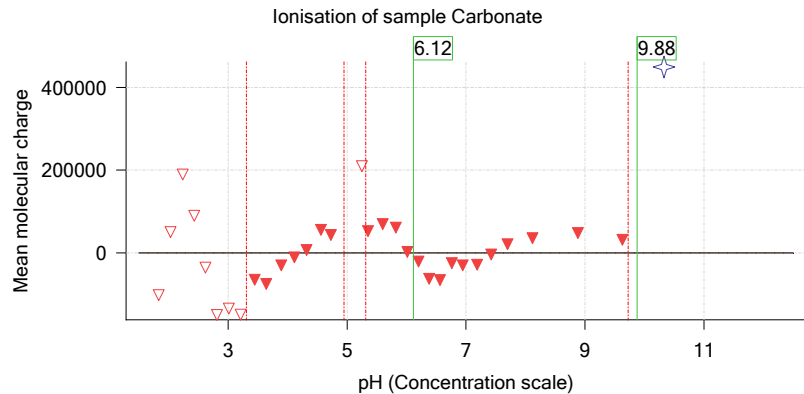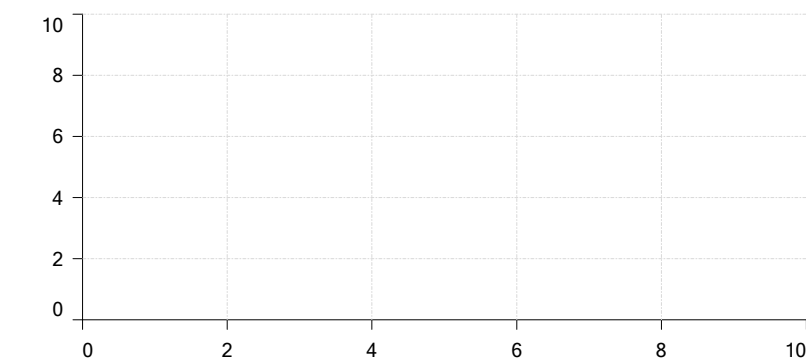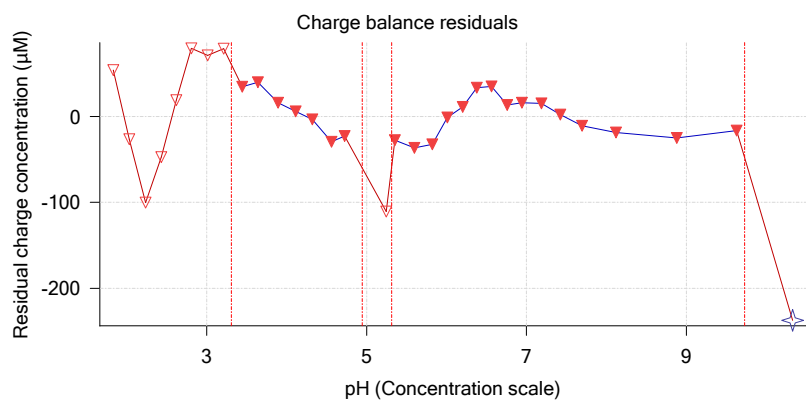
Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 2 of 3   18C-02008 Points 34 to 67

Overall results

RMSD   0.101
Average ionic strength   0.158 M
Average temperature   25.0°C
Partition ratio   0.1721 : 1
Analyte concentration range   2125.1 µM to 2191.1 µM
Total points considered   25 of 34

Warnings and errors

Errors   None
Warnings   One or more logP values out of range

Four-Plus parameters

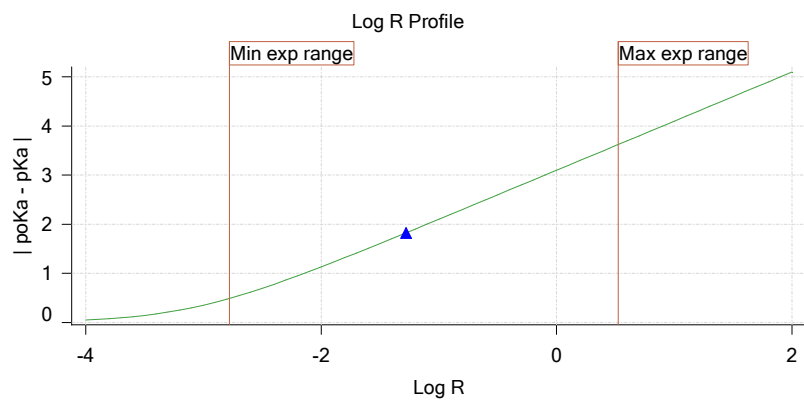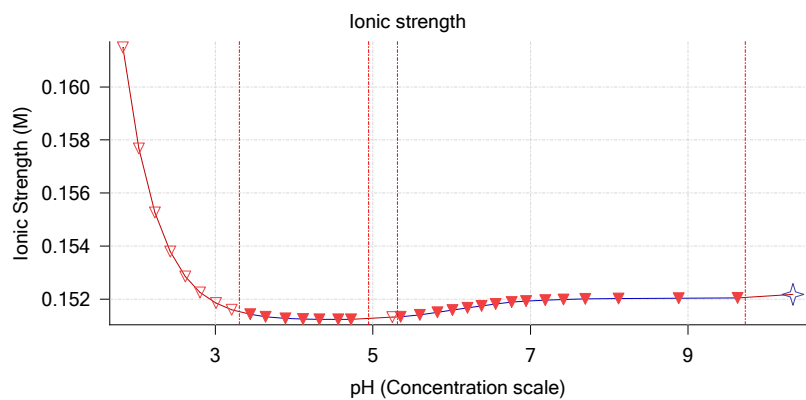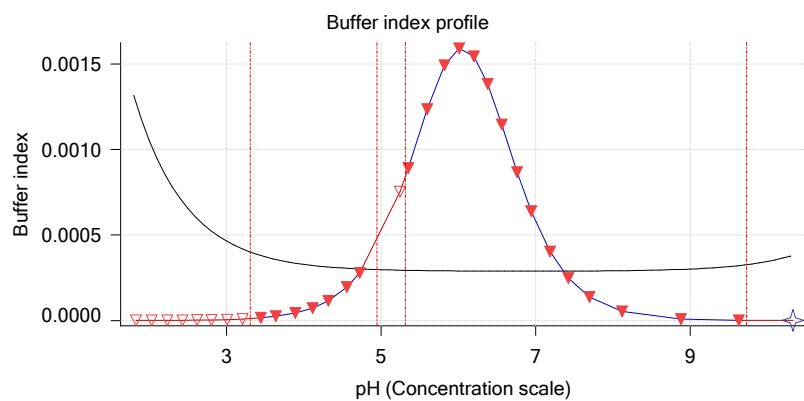|				
🔒	Alpha	0.111	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	S	0.9988	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	jH	1.0	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	jOH	-0.8	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r

Titrants

🔒	0.50 M HCl	0.999058	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	0.50 M KOH	0.999845	3/2/2018 6:51:30 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

🔷	M08_octanol concentration factor	1.106
🔒	Acid pKa 1	4.22
🔷	logP (neutral XH)	2.98
🔷	logP (X -)	-4.72

Sample graphs

Ionisation of sample M08_octanol

Distribution of species for sample M08_octanol

Sample name: **M08_octanol**　　　　　　　　　　　　　　Experiment start time: **3/2/2018 6:51:30 PM**
Assay name: **pH-metric high logP**　　　　　　　　　　　Analyst: **Pion**
Assay ID: **18C-02008**　　　　　　　　　　　　　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Sample graphs (continued)

Lipophilicity Profile
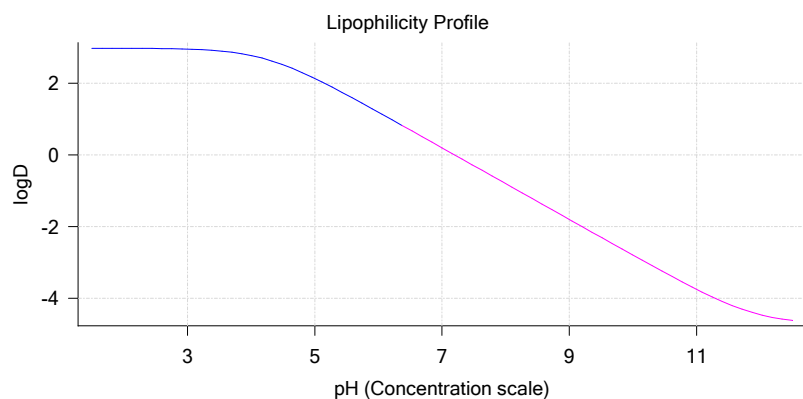
Sample logD and percent species

pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	2.98	0.61 %	0.00 %	99.39 %	0.00 %	
1.200	2.98	0.61 %	0.00 %	99.39 %	0.00 %	Stomach pH
2.000	2.98	0.61 %	0.00 %	99.39 %	0.00 %	
3.000	2.95	0.61 %	0.04 %	99.36 %	0.00 %	
4.000	2.77	0.61 %	0.36 %	99.03 %	0.00 %	
5.000	2.13	0.59 %	3.53 %	95.88 %	0.00 %	
6.000	1.19	0.44 %	26.80 %	72.76 %	0.00 %	
6.500	0.70	0.28 %	53.65 %	46.06 %	0.00 %	
7.000	0.20	0.13 %	78.54 %	21.32 %	0.00 %	
7.400	-0.20	0.06 %	90.19 %	9.75 %	0.00 %	Blood pH
8.000	-0.80	0.02 %	97.34 %	2.64 %	0.00 %	
9.000	-1.80	0.00 %	99.73 %	0.27 %	0.00 %	
10.000	-2.80	0.00 %	99.97 %	0.03 %	0.00 %	
11.000	-3.75	0.00 %	100.00 %	0.00 %	0.00 %	
12.000	-4.46	0.00 %	100.00 %	0.00 %	0.00 %	

Carbonate and acidity

Carbonate　　0.000 mM
Acidity error　-0.340 mM

Other graphs
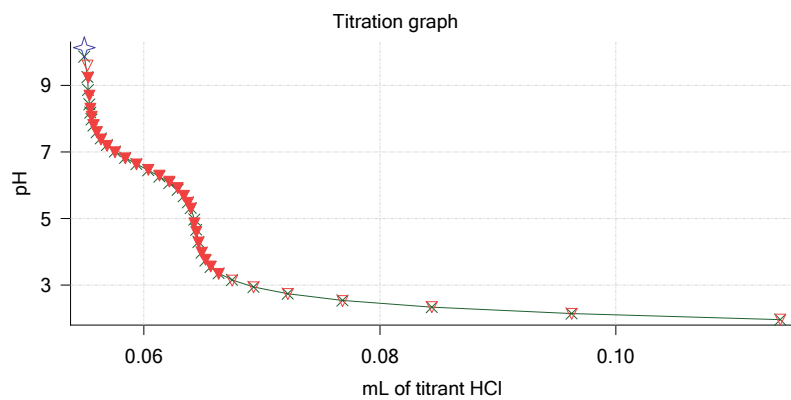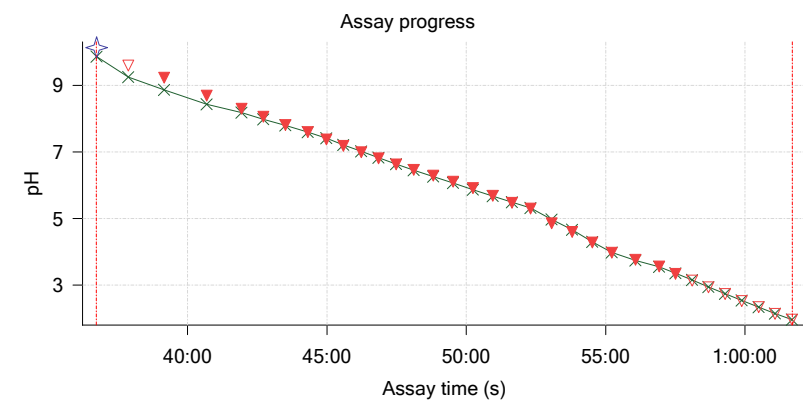
Assay progress

Titration graph

Sample name: **M08_octanol**   Experiment start time: **3/2/2018 6:51:30 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-02008**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
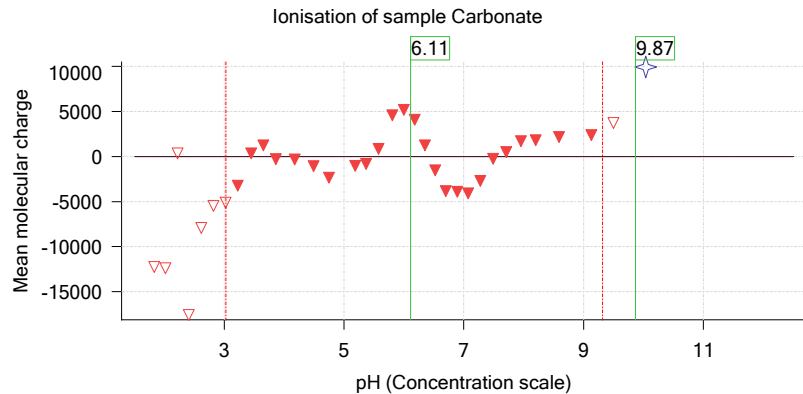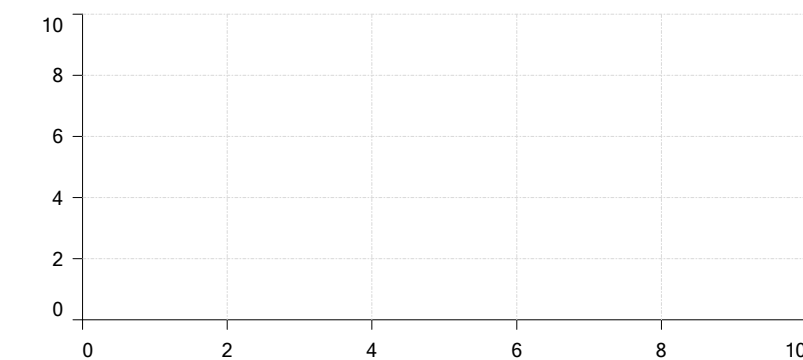
Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 3 of 3   18C-02008 Points 68 to 106

Overall results

RMSD   0.055
Average ionic strength   0.165 M
Average temperature   25.0°C
Partition ratio   0.6191 : 1
Analyte concentration range 1443.8 µM to 1476.3 µM
Total points considered   26 of 39

Warnings and errors

Errors   None
Warnings   One or more logP values out of range

Four-Plus parameters

🔒	Alpha	0.111	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	S	0.9988	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	jH	1.0	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	jOH	-0.8	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r

Titrants

🔒	0.50 M HCl	0.999058	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	0.50 M KOH	0.999845	3/2/2018 6:51:30 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

🔷	M08_octanol concentration factor	0.984
🔒	Acid pKa 1	4.22
🔷	logP (neutral XH)	2.91
🔒	logP (X -)	-5.22

Sample graphs
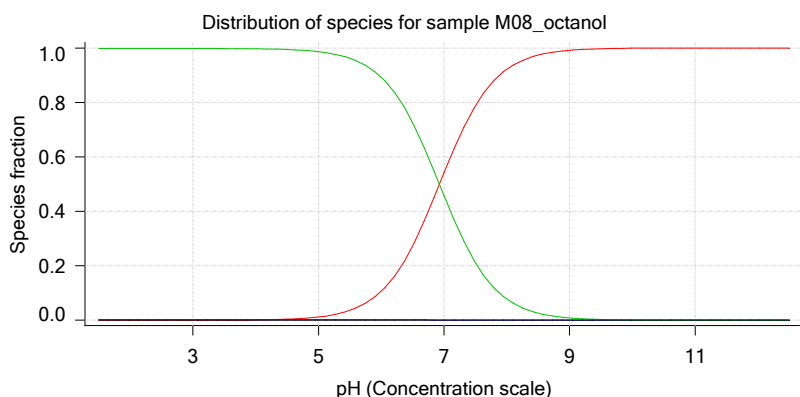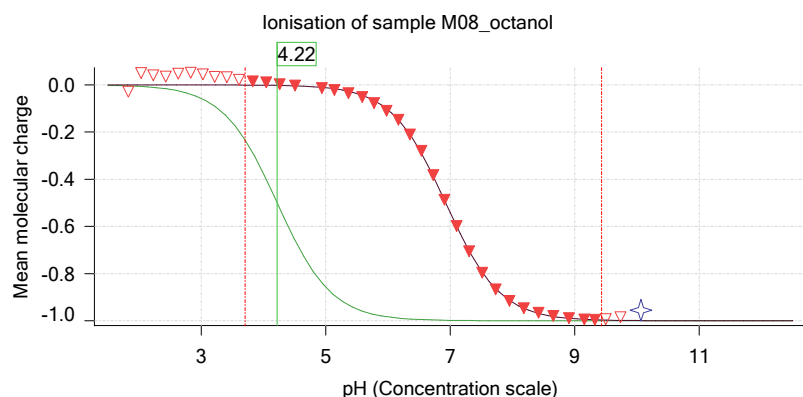
Ionisation of sample M08_octanol

Distribution of species for sample M08_octanol

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)
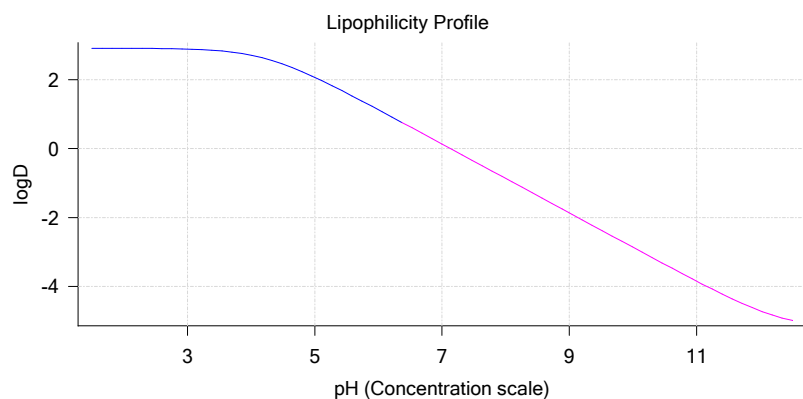
Lipophilicity Profile

Sample logD and percent species

pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	2.91	0.20 %	0.00 %	99.80 %	0.00 %	
1.200	2.91	0.20 %	0.00 %	99.80 %	0.00 %	Stomach pH
2.000	2.91	0.20 %	0.00 %	99.80 %	0.00 %	
3.000	2.89	0.20 %	0.01 %	99.79 %	0.00 %	
4.000	2.71	0.20 %	0.12 %	99.69 %	0.00 %	
5.000	2.07	0.19 %	1.17 %	98.64 %	0.00 %	
6.000	1.13	0.18 %	10.57 %	89.25 %	0.00 %	
6.500	0.63	0.14 %	27.22 %	72.64 %	0.00 %	
7.000	0.13	0.09 %	54.18 %	45.73 %	0.00 %	
7.400	-0.27	0.05 %	74.81 %	25.14 %	0.00 %	Blood pH
8.000	-0.87	0.02 %	92.20 %	7.78 %	0.00 %	
9.000	-1.87	0.00 %	99.16 %	0.84 %	0.00 %	
10.000	-2.86	0.00 %	99.92 %	0.08 %	0.00 %	
11.000	-3.85	0.00 %	99.99 %	0.01 %	0.00 %	
12.000	-4.71	0.00 %	100.00 %	0.00 %	0.00 %	

Carbonate and acidity
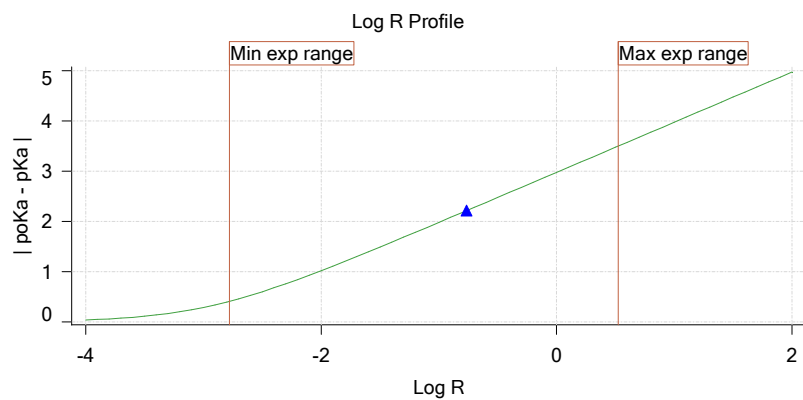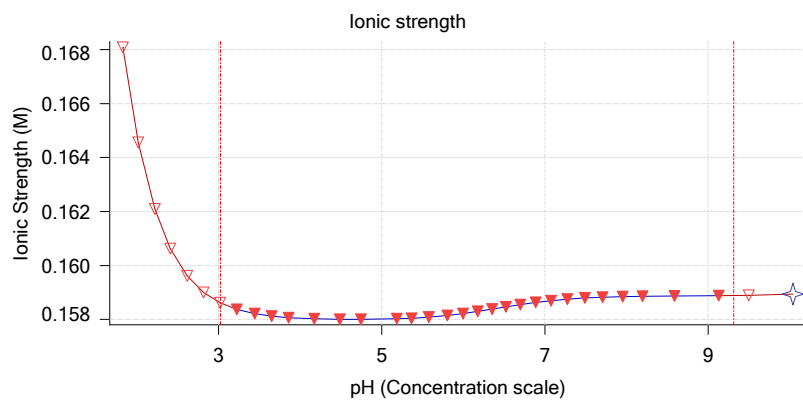
Carbonate   0.248 mM
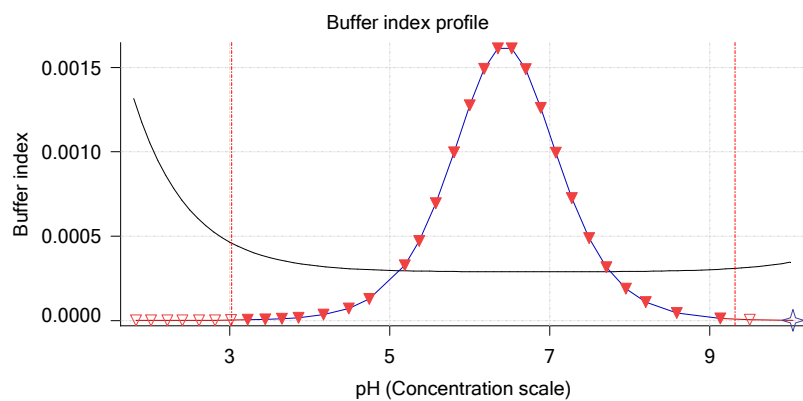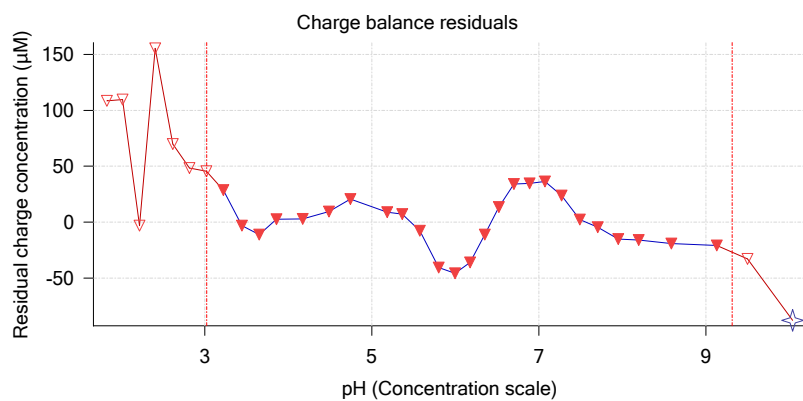Acidity error   -0.085 mM

Other graphs

Assay progress

Titration graph

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
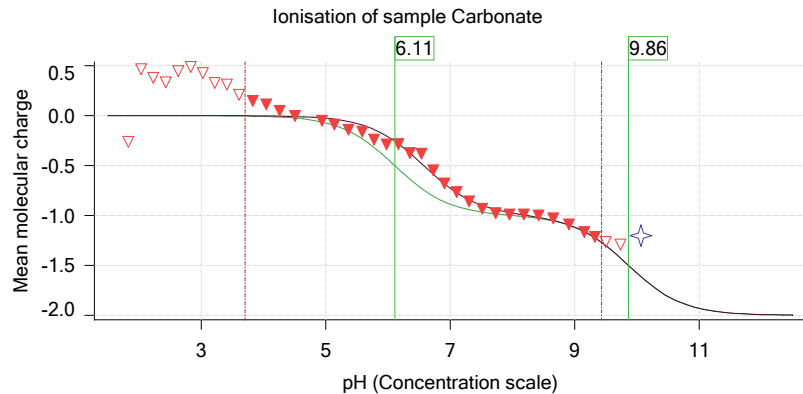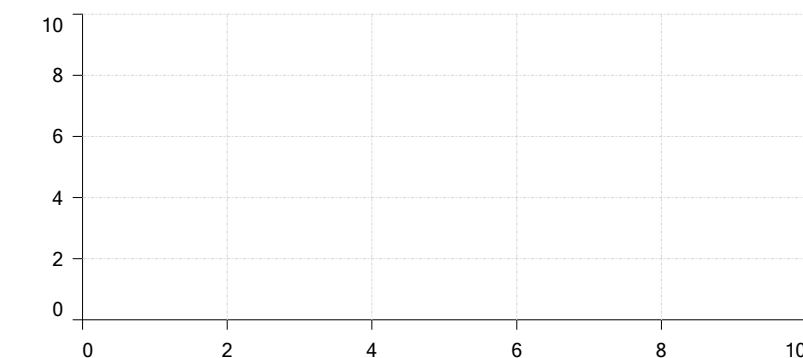
Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

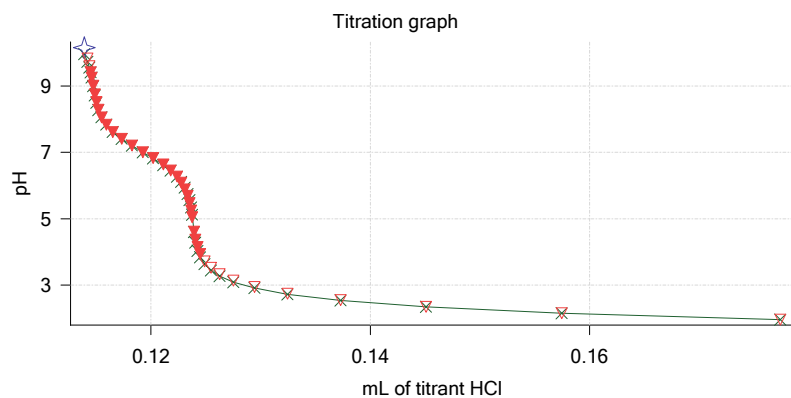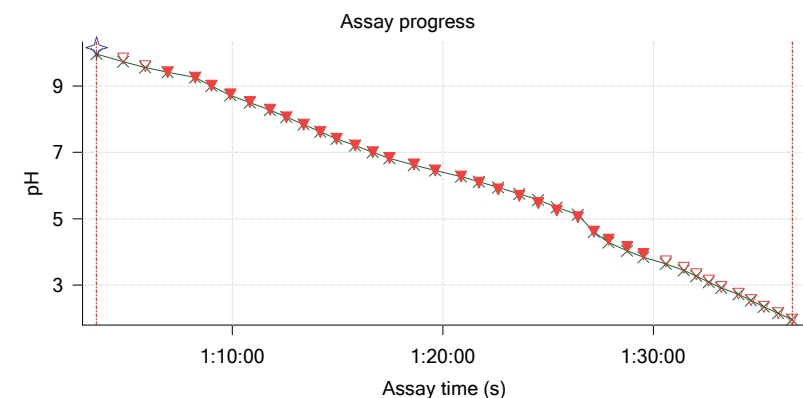| Settings	Value	Date/Time changed	Imported from
Sample name	M08_octanol	2/27/2018 4:33:51 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001220 g	3/2/2018 5:08:15 PM	User entered value
Formula weight	293.32 g/mol	2/27/2018 4:33:51 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	293.32	2/27/2018 4:33:51 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 4:33:51 PM	User entered value
Sample is a	Acid	2/27/2018 4:33:51 PM	User entered value
pKa 1	4.22	2/27/2018 4:33:51 PM	User entered value
logP (neutral XH)	2.98	3/2/2018 3:22:58 PM	User entered value
logP (X -)	-5.22	3/2/2018 3:23:03 PM	User entered value

Events

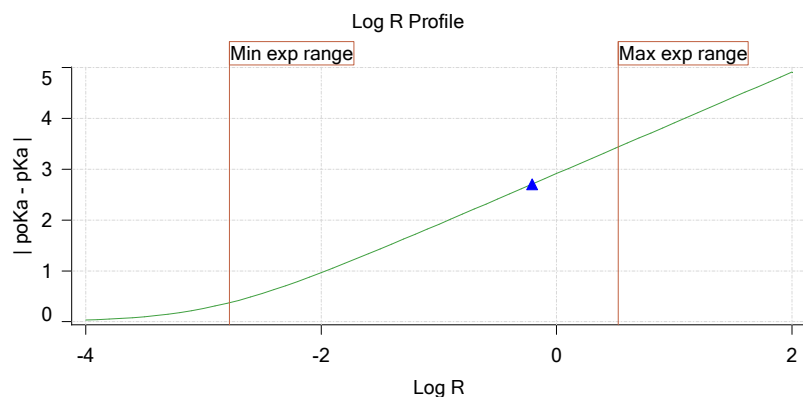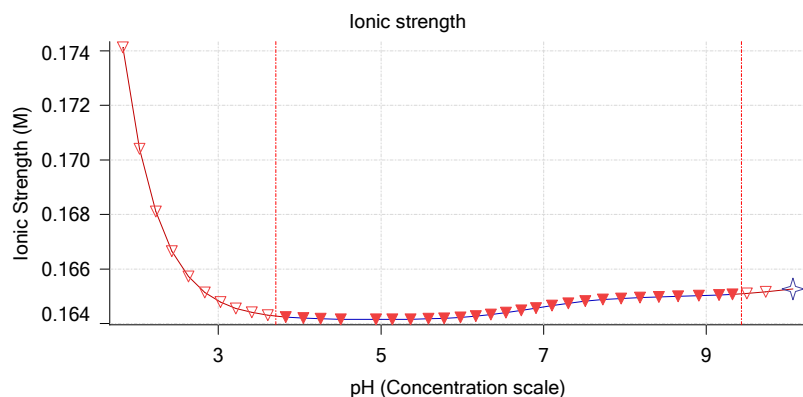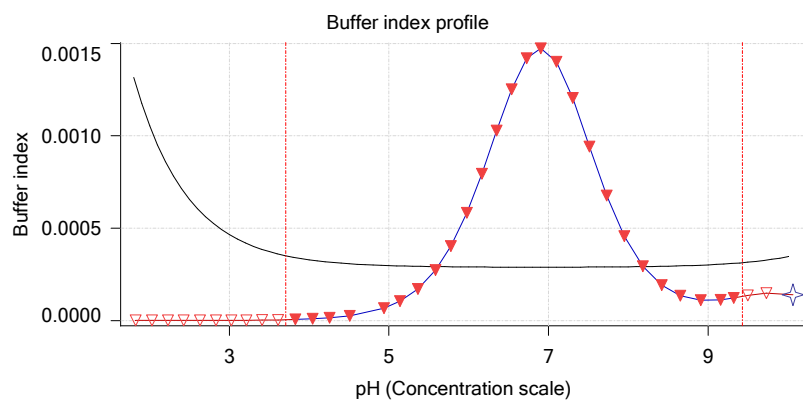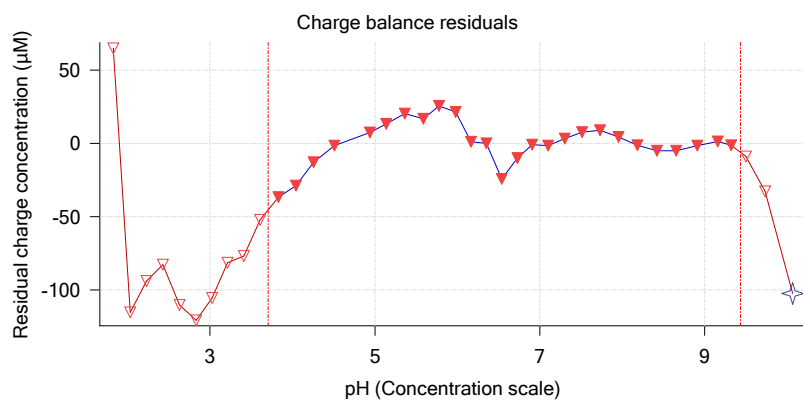| Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH time
5:58.6	Manual volume addition				0.08000 mL					
5:59.7	Initial pH = 5.21									
8:51.7	Data point 2	1.50000 mL	0.00000 mL	0.00811 mL	0.08000 mL	10.428	0.01958	0.93900	0.00100	34.0 s
9:52.4	Data point 3	1.50000 mL	0.00021 mL	0.00811 mL	0.08000 mL	9.727	0.01586	0.62733	0.00099	55.5 s
11:23.7	Data point 4	1.50000 mL	0.00042 mL	0.00811 mL	0.08000 mL	8.981	-0.01653	0.82499	0.00090	43.0 s
12:42.4	Data point 5	1.50000 mL	0.00049 mL	0.00811 mL	0.08000 mL	8.220	-0.04412	0.98170	0.00220	Time out at
14:17.9	Data point 6	1.50000 mL	0.00059 mL	0.00811 mL	0.08000 mL	7.798	0.01512	0.58186	0.00098	12.5 s
15:00.9	Data point 7	1.50000 mL	0.00071 mL	0.00811 mL	0.08000 mL	7.523	0.01618	0.67470	0.00097	14.5 s
15:46.0	Data point 8	1.50000 mL	0.00089 mL	0.00811 mL	0.08000 mL	7.289	0.01805	0.80919	0.00099	15.0 s
16:41.8	Data point 9	1.50000 mL	0.00127 mL	0.00811 mL	0.08000 mL	7.046	0.01754	0.75358	0.00100	16.0 s
17:38.7	Data point 10	1.50000 mL	0.00169 mL	0.00811 mL	0.08000 mL	6.863	0.01849	0.84615	0.00099	14.5 s
18:18.6	Data point 11	1.50000 mL	0.00223 mL	0.00811 mL	0.08000 mL	6.664	0.01638	0.78161	0.00092	16.0 s
18:59.9	Data point 12	1.50000 mL	0.00294 mL	0.00811 mL	0.08000 mL	6.481	0.01849	0.86308	0.00098	16.5 s
19:41.9	Data point 13	1.50000 mL	0.00379 mL	0.00811 mL	0.08000 mL	6.307	0.01848	0.90886	0.00096	15.0 s
20:22.3	Data point 14	1.50000 mL	0.00475 mL	0.00811 mL	0.08000 mL	6.113	0.01882	0.90673	0.00098	14.0 s
21:01.8	Data point 15	1.50000 mL	0.00574 mL	0.00811 mL	0.08000 mL	5.924	0.01677	0.83278	0.00091	17.0 s
21:44.2	Data point 16	1.50000 mL	0.00668 mL	0.00811 mL	0.08000 mL	5.702	0.01845	0.92173	0.00095	17.5 s
22:27.2	Data point 17	1.50000 mL	0.00746 mL	0.00811 mL	0.08000 mL	5.455	0.01862	0.94817	0.00094	28.0 s
23:36.2	Data point 18	1.50000 mL	0.00797 mL	0.00811 mL	0.08000 mL	5.350	0.09983	0.99423	0.00495	Time out at
25:01.6	Data point 19	1.50000 mL	0.00851 mL	0.00811 mL	0.08000 mL	4.830	0.04926	0.98780	0.00245	Time out at

Sample name: **M08_octanol** Experiment start time: **3/2/2018 6:51:30 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02008** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_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
26:37.2	Data point 20	1.50000 mL	0.00868 mL	0.00811 mL	0.08000 mL	4.665	0.01816	0.93657	0.00093	31.5 s
27:34.0	Data point 21	1.50000 mL	0.00877 mL	0.00811 mL	0.08000 mL	4.425	0.01775	0.90251	0.00092	12.5 s
28:17.1	Data point 22	1.50000 mL	0.00889 mL	0.00811 mL	0.08000 mL	4.219	0.01953	0.93075	0.00100	11.0 s
29:08.8	Data point 23	1.50000 mL	0.00905 mL	0.00811 mL	0.08000 mL	3.997	0.00018	0.00008	0.00098	10.0 s
29:44.2	Data point 24	1.50000 mL	0.00931 mL	0.00811 mL	0.08000 mL	3.747	0.00337	0.08202	0.00058	10.0 s
30:35.1	Data point 25	1.50000 mL	0.00974 mL	0.00811 mL	0.08000 mL	3.552	0.00143	0.03293	0.00039	10.0 s
31:10.5	Data point 26	1.50000 mL	0.01040 mL	0.00811 mL	0.08000 mL	3.317	0.00181	0.11529	0.00026	10.0 s
32:01.5	Data point 27	1.50000 mL	0.01152 mL	0.00811 mL	0.08000 mL	3.118	-0.00447	0.58442	0.00029	10.5 s
32:37.5	Data point 28	1.50000 mL	0.01326 mL	0.00811 mL	0.08000 mL	2.917	-0.00516	0.25417	0.00051	10.0 s
33:13.0	Data point 29	1.50000 mL	0.01604 mL	0.00811 mL	0.08000 mL	2.730	-0.01202	0.42201	0.00091	10.0 s
33:48.5	Data point 30	1.50000 mL	0.02032 mL	0.00811 mL	0.08000 mL	2.540	-0.00759	0.75110	0.00043	10.5 s
34:24.6	Data point 31	1.50000 mL	0.02702 mL	0.00811 mL	0.08000 mL	2.348	-0.00583	0.78723	0.00032	10.0 s
35:00.3	Data point 32	1.50000 mL	0.03765 mL	0.00811 mL	0.08000 mL	2.149	-0.01355	0.91748	0.00070	10.5 s
35:36.6	Data point 33	1.50000 mL	0.05496 mL	0.00811 mL	0.08000 mL	1.953	-0.01411	0.85512	0.00075	10.5 s
36:44.7	Data point 34	1.50000 mL	0.05496 mL	0.06333 mL	0.28000 mL	10.137	-0.00357	0.03271	0.00098	37.5 s
37:52.8	Data point 35	1.50000 mL	0.05522 mL	0.06333 mL	0.28000 mL	9.598	0.01355	0.57771	0.00088	51.5 s
39:09.8	Data point 36	1.50000 mL	0.05529 mL	0.06333 mL	0.28000 mL	9.232	0.01873	0.90967	0.00097	55.5 s
40:41.0	Data point 37	1.50000 mL	0.05539 mL	0.06333 mL	0.28000 mL	8.688	-0.00364	0.04343	0.00086	40.0 s
41:56.7	Data point 38	1.50000 mL	0.05548 mL	0.06333 mL	0.28000 mL	8.299	0.01075	0.31366	0.00095	10.5 s
42:43.0	Data point 39	1.50000 mL	0.05560 mL	0.06333 mL	0.28000 mL	8.053	0.01326	0.61367	0.00084	12.0 s
43:30.7	Data point 40	1.50000 mL	0.05576 mL	0.06333 mL	0.28000 mL	7.808	0.01660	0.85424	0.00089	12.5 s
44:18.9	Data point 41	1.50000 mL	0.05602 mL	0.06333 mL	0.28000 mL	7.592	0.01619	0.81503	0.00089	14.5 s
44:58.8	Data point 42	1.50000 mL	0.05637 mL	0.06333 mL	0.28000 mL	7.376	0.01819	0.83297	0.00098	11.5 s
45:35.7	Data point 43	1.50000 mL	0.05689 mL	0.06333 mL	0.28000 mL	7.176	0.01797	0.88644	0.00094	12.5 s
46:13.6	Data point 44	1.50000 mL	0.05757 mL	0.06333 mL	0.28000 mL	6.991	0.01928	0.96006	0.00097	12.0 s
46:51.1	Data point 45	1.50000 mL	0.05842 mL	0.06333 mL	0.28000 mL	6.803	0.01836	0.93846	0.00094	12.5 s
47:29.0	Data point 46	1.50000 mL	0.05938 mL	0.06333 mL	0.28000 mL	6.627	0.01804	0.92322	0.00093	12.5 s
48:06.9	Data point 47	1.50000 mL	0.06037 mL	0.06333 mL	0.28000 mL	6.455	0.01858	0.93024	0.00095	16.5 s
48:48.9	Data point 48	1.50000 mL	0.06134 mL	0.06333 mL	0.28000 mL	6.281	0.01664	0.78265	0.00093	17.5 s
49:31.9	Data point 49	1.50000 mL	0.06218 mL	0.06333 mL	0.28000 mL	6.101	0.01692	0.74989	0.00096	17.0 s
50:14.3	Data point 50	1.50000 mL	0.06289 mL	0.06333 mL	0.28000 mL	5.907	0.01653	0.76306	0.00093	17.5 s
50:57.3	Data point 51	1.50000 mL	0.06341 mL	0.06333 mL	0.28000 mL	5.681	0.01220	0.53640	0.00082	15.5 s
51:38.2	Data point 52	1.50000 mL	0.06376 mL	0.06333 mL	0.28000 mL	5.471	0.01147	0.51173	0.00079	15.0 s
52:18.6	Data point 53	1.50000 mL	0.06399 mL	0.06333 mL	0.28000 mL	5.290	0.01455	0.56277	0.00096	14.5 s
53:03.6	Data point 54	1.50000 mL	0.06430 mL	0.06333 mL	0.28000 mL	4.851	0.01470	0.53131	0.00100	14.0 s
53:48.2	Data point 55	1.50000 mL	0.06446 mL	0.06333 mL	0.28000 mL	4.594	0.01132	0.40356	0.00088	12.5 s
54:31.4	Data point 56	1.50000 mL	0.06465 mL	0.06333 mL	0.28000 mL	4.279	0.00590	0.14884	0.00076	11.5 s
55:13.4	Data point 57	1.50000 mL	0.06491 mL	0.06333 mL	0.28000 mL	3.965	0.00967	0.40120	0.00075	10.0 s
56:04.3	Data point 58	1.50000 mL	0.06524 mL	0.06333 mL	0.28000 mL	3.759	0.00813	0.49244	0.00057	10.0 s
56:55.2	Data point 59	1.50000 mL	0.06566 mL	0.06333 mL	0.28000 mL	3.552	-0.00215	0.16107	0.00027	10.0 s
57:30.6	Data point 60	1.50000 mL	0.06635 mL	0.06333 mL	0.28000 mL	3.331	-0.00414	0.34668	0.00035	10.0 s
58:06.0	Data point 61	1.50000 mL	0.06747 mL	0.06333 mL	0.28000 mL	3.126	-0.00603	0.61652	0.00038	10.0 s
58:41.5	Data point 62	1.50000 mL	0.06931 mL	0.06333 mL	0.28000 mL	2.927	-0.00487	0.09075	0.00080	10.0 s
59:17.0	Data point 63	1.50000 mL	0.07220 mL	0.06333 mL	0.28000 mL	2.726	0.00082	0.04244	0.00020	10.5 s
59:53.1	Data point 64	1.50000 mL	0.07683 mL	0.06333 mL	0.28000 mL	2.519	-0.00715	0.90269	0.00037	10.5 s
1:00:29.1	Data point 65	1.50000 mL	0.08441 mL	0.06333 mL	0.28000 mL	2.334	-0.01263	0.94471	0.00064	10.0 s
1:01:04.8	Data point 66	1.50000 mL	0.09624 mL	0.06333 mL	0.28000 mL	2.133	-0.01155	0.84750	0.00062	10.0 s
1:01:40.7	Data point 67	1.50000 mL	0.11392 mL	0.06333 mL	0.28000 mL	1.953	-0.00652	0.61375	0.00041	10.5 s
1:03:34.1	Data point 68	1.50000 mL	0.11392 mL	0.12345 mL	1.08000 mL	10.164	-0.01244	0.38157	0.00099	45.0 s
1:04:49.8	Data point 69	1.50000 mL	0.11423 mL	0.12345 mL	1.08000 mL	9.832	-0.00830	0.23375	0.00085	37.5 s
1:05:52.7	Data point 70	1.50000 mL	0.11439 mL	0.12345 mL	1.08000 mL	9.598	-0.01486	0.60594	0.00094	38.0 s
1:06:56.1	Data point 71	1.50000 mL	0.11451 mL	0.12345 mL	1.08000 mL	9.421	-0.00966	0.27141	0.00092	53.0 s
1:08:14.6	Data point 72	1.50000 mL	0.11461 mL	0.12345 mL	1.08000 mL	9.256	-0.00823	0.36404	0.00067	11.0 s
1:09:01.3	Data point 73	1.50000 mL	0.11475 mL	0.12345 mL	1.08000 mL	9.009	0.01389	0.51931	0.00095	18.0 s
1:09:55.0	Data point 74	1.50000 mL	0.11489 mL	0.12345 mL	1.08000 mL	8.754	0.00577	0.08155	0.00100	20.0 s
1:10:50.8	Data point 75	1.50000 mL	0.11503 mL	0.12345 mL	1.08000 mL	8.520	0.01828	0.95610	0.00092	21.5 s
1:11:48.1	Data point 76	1.50000 mL	0.11522 mL	0.12345 mL	1.08000 mL	8.286	0.01567	0.71329	0.00092	20.5 s

Sample name: **M08_octanol** Experiment start time: **3/2/2018 6:51:30 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02008** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_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
1:12:34.1	Data point 77	1.50000 mL	0.11550 mL	0.12345 mL	1.08000 mL	8.054	0.00873	0.25062	0.00086	24.0 s
1:13:23.5	Data point 78	1.50000 mL	0.11592 mL	0.12345 mL	1.08000 mL	7.830	0.01471	0.68425	0.00088	22.0 s
1:14:11.0	Data point 79	1.50000 mL	0.11653 mL	0.12345 mL	1.08000 mL	7.615	0.01082	0.31604	0.00095	21.0 s
1:14:57.5	Data point 80	1.50000 mL	0.11733 mL	0.12345 mL	1.08000 mL	7.406	0.01311	0.67015	0.00079	27.5 s
1:15:50.4	Data point 81	1.50000 mL	0.11827 mL	0.12345 mL	1.08000 mL	7.204	0.01583	0.70594	0.00093	24.5 s
1:16:40.4	Data point 82	1.50000 mL	0.11926 mL	0.12345 mL	1.08000 mL	7.008	0.01015	0.26007	0.00098	22.0 s
1:17:27.9	Data point 83	1.50000 mL	0.12020 mL	0.12345 mL	1.08000 mL	6.829	0.00824	0.26586	0.00079	29.0 s
1:18:37.8	Data point 84	1.50000 mL	0.12114 mL	0.12345 mL	1.08000 mL	6.639	0.01737	0.74638	0.00099	35.0 s
1:19:38.3	Data point 85	1.50000 mL	0.12180 mL	0.12345 mL	1.08000 mL	6.453	0.01561	0.66863	0.00094	33.0 s
1:20:52.2	Data point 86	1.50000 mL	0.12239 mL	0.12345 mL	1.08000 mL	6.268	0.01016	0.29466	0.00092	25.5 s
1:21:43.1	Data point 87	1.50000 mL	0.12277 mL	0.12345 mL	1.08000 mL	6.082	0.01424	0.61244	0.00090	24.0 s
1:22:37.7	Data point 88	1.50000 mL	0.12310 mL	0.12345 mL	1.08000 mL	5.882	0.00792	0.16581	0.00096	19.0 s
1:23:37.7	Data point 89	1.50000 mL	0.12335 mL	0.12345 mL	1.08000 mL	5.690	0.00115	0.00389	0.00091	23.5 s
1:24:31.7	Data point 90	1.50000 mL	0.12352 mL	0.12345 mL	1.08000 mL	5.467	0.01785	0.83193	0.00097	22.5 s
1:25:24.8	Data point 91	1.50000 mL	0.12366 mL	0.12345 mL	1.08000 mL	5.243	0.01854	0.86754	0.00098	29.5 s
1:26:24.8	Data point 92	1.50000 mL	0.12375 mL	0.12345 mL	1.08000 mL	5.042	0.00911	0.28586	0.00084	14.5 s
1:27:09.9	Data point 93	1.50000 mL	0.12392 mL	0.12345 mL	1.08000 mL	4.612	-0.01412	0.49010	0.00100	12.0 s
1:27:52.4	Data point 94	1.50000 mL	0.12406 mL	0.12345 mL	1.08000 mL	4.363	0.01967	0.96830	0.00099	17.0 s
1:28:45.1	Data point 95	1.50000 mL	0.12425 mL	0.12345 mL	1.08000 mL	4.149	0.00177	0.01471	0.00072	10.5 s
1:29:31.3	Data point 96	1.50000 mL	0.12448 mL	0.12345 mL	1.08000 mL	3.934	-0.00929	0.21345	0.00099	23.5 s
1:30:35.6	Data point 97	1.50000 mL	0.12488 mL	0.12345 mL	1.08000 mL	3.715	-0.00629	0.73094	0.00036	10.0 s
1:31:26.6	Data point 98	1.50000 mL	0.12547 mL	0.12345 mL	1.08000 mL	3.517	-0.01016	0.69269	0.00060	10.0 s
1:32:02.1	Data point 99	1.50000 mL	0.12627 mL	0.12345 mL	1.08000 mL	3.321	-0.01475	0.90060	0.00077	10.0 s
1:32:37.6	Data point 100	1.50000 mL	0.12752 mL	0.12345 mL	1.08000 mL	3.134	-0.00934	0.64893	0.00057	10.5 s
1:33:13.4	Data point 101	1.50000 mL	0.12945 mL	0.12345 mL	1.08000 mL	2.940	0.00025	0.00017	0.00095	23.5 s
1:34:02.5	Data point 102	1.50000 mL	0.13245 mL	0.12345 mL	1.08000 mL	2.741	-0.01740	0.87852	0.00092	10.0 s
1:34:38.0	Data point 103	1.50000 mL	0.13730 mL	0.12345 mL	1.08000 mL	2.539	-0.01964	0.96661	0.00099	10.5 s
1:35:14.2	Data point 104	1.50000 mL	0.14508 mL	0.12345 mL	1.08000 mL	2.343	0.00480	0.07839	0.00085	15.0 s
1:35:54.9	Data point 105	1.50000 mL	0.15746 mL	0.12345 mL	1.08000 mL	2.149	-0.01890	0.90387	0.00098	13.5 s
1:36:34.4	Data point 106	1.50000 mL	0.17738 mL	0.12345 mL	1.08000 mL	1.950	-0.01112	0.54218	0.00075	20.5 s
1:37:04.0	Assay volumes	1.50000 mL	0.17738 mL	0.12345 mL	1.08000 mL					

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
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	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.080 mL			
Partition solvent added	Manual in advance			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 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	High to low 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	High to low pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.200 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: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	High to low pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.800 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	0.111	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus S	0.9988	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jH	1.0	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jOH	-0.8	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.t3r
Base concentration factor	1.000	3/2/2018 6:51:30 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.999	3/2/2018 6:51:30 PM	C:\Sirius_T3\HCl18C02.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: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

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	+2.88 mV		3/2/2018 6:51:58 PM
Filling solution	3M KCl	KCL097	3/2/2018 9:43:24 AM
Liquids			
Wash 1	50% IPA:50% Water		3/2/2018 9:45:12 AM
Wash 2	0.5% Trition X-100 in H20		3/2/2018 9:45:15 AM
Buffer position 1	pH7 Wash		3/2/2018 9:45:18 AM
Buffer position 2	pH 7		3/2/2018 9:45:21 AM
Storage position			3/2/2018 9:44:44 AM
Wash water	7.3e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	8.1e+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	120:41:49		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: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
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)
[2:39] Air gap created for Base (0.5 M KOH)
[2:39] Air gap released for Water (0.15 M KCl)
[2:43] Titrator arm moved over Titration position
[2:43] Titration 1 of 3
[2:43] Adding initial titrants
[2:43] Automatically add 1.50000 mL of water
[3:08] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:12] Titrator arm moved over Drain
[5:54] Titrator arm moved to Titration position
[5:54] Argon flow rate set to 100
[5:54] Stirrer speed set to 10
[6:00] Initial pH = 5.21
[6:00] Iterative adjust 5.21 -> 10.00
[6:00] pH 5.21 -> 10.00
[6:01] Air gap released for Base (0.5 M KOH)
[6:02] Dispensed 0.008114 mL of Base (0.5 M KOH)
[6:07] Holding pH 10.00
[8:07] Stirrer speed set to 0
[8:07] Stirrer speed set to 50
[8:07] Iterative adjust 11.12 -> 10.00
[8:52] Stirrer speed set to 0
[9:26] Datapoint id 2 collected
[9:26] Stirrer speed set to 50
[9:31] pH 10.39 -> 10.19
[9:31] Using cautious pH adjust
[9:32] Air gap released for Acid (0.5 M HCl)
[9:33] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[9:38] Stepping pH = 10.07
[9:53] Stirrer speed set to 0
[10:48] Datapoint id 3 collected
[10:48] Charge balance equation is out by 50.1%
[10:48] Stirrer speed set to 50
[10:53] pH 9.64 -> 9.44
[10:53] Using cautious pH adjust
[10:54] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[10:59] Stepping pH = 9.60
[10:59] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[11:04] Stepping pH = 9.55
[11:04] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[11:09] Stepping pH = 9.35

Experiment Log (continued)

[11:24] Stirrer speed set to 0
[12:07] Datapoint id 4 collected
[12:07] Charge balance equation is out by -137.2%
[12:07] Stirrer speed set to 50
[12:12] pH 8.90 -> 8.70
[12:12] Using cautious pH adjust
[12:12] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[12:17] Stepping pH = 8.82
[12:17] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[12:22] Stepping pH = 8.74
[12:22] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[12:28] Stepping pH = 8.61
[12:43] Stirrer speed set to 0
[13:43] Datapoint id 5 collected
[13:43] Charge balance equation is out by -121.9%
[13:43] Stirrer speed set to 50
[13:48] pH 8.13 -> 7.93
[13:48] Using cautious pH adjust
[13:48] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[13:53] Stepping pH = 8.08
[13:53] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[13:58] Stepping pH = 8.00
[13:58] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[14:03] Stepping pH = 7.90
[14:18] Stirrer speed set to 0
[14:31] Datapoint id 6 collected
[14:31] Charge balance equation is out by -91.6%
[14:31] Stirrer speed set to 50
[14:36] pH 7.77 -> 7.57
[14:36] Using cautious pH adjust
[14:36] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[14:41] Stepping pH = 7.72
[14:41] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[14:46] Stepping pH = 7.57
[15:01] Stirrer speed set to 0
[15:16] Datapoint id 7 collected
[15:16] Charge balance equation is out by -35.0%
[15:16] Stirrer speed set to 50
[15:21] pH 7.51 -> 7.31
[15:21] Using cautious pH adjust
[15:21] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[15:26] Stepping pH = 7.44
[15:26] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[15:31] Stepping pH = 7.28
[15:46] Stirrer speed set to 0
[16:01] Datapoint id 8 collected
[16:01] Charge balance equation is out by -17.3%
[16:01] Stirrer speed set to 50
[16:06] pH 7.29 -> 7.09
[16:06] Using cautious pH adjust
[16:06] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[16:12] Stepping pH = 7.20
[16:12] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[16:17] Stepping pH = 7.10
[16:17] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[16:22] Stepping pH = 7.10
[16:22] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[16:27] Stepping pH = 7.02
[16:42] Stirrer speed set to 0

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[16:58] Datapoint id 9 collected
[16:58] Charge balance equation is out by -48.6%
[16:58] Stirrer speed set to 50
[17:03] pH 7.04 -> 6.84
[17:03] Using cautious pH adjust
[17:03] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[17:08] Stepping pH = 6.92
[17:09] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[17:14] Stepping pH = 6.88
[17:14] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[17:19] Stepping pH = 6.86
[17:19] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[17:24] Stepping pH = 6.85
[17:39] Stirrer speed set to 0
[17:54] Datapoint id 10 collected
[17:54] Charge balance equation is out by -11.0%
[17:54] Stirrer speed set to 50
[17:59] pH 6.86 -> 6.66
[17:59] Using charge balance adjust
[17:59] Dispensed 0.000541 mL of Acid (0.5 M HCl)
[18:19] Stirrer speed set to 0
[18:35] Datapoint id 11 collected
[18:35] Charge balance equation is out by -2.2%
[18:35] Stirrer speed set to 50
[18:40] pH 6.66 -> 6.46
[18:40] Using charge balance adjust
[18:40] Dispensed 0.000706 mL of Acid (0.5 M HCl)
[19:00] Stirrer speed set to 0
[19:17] Datapoint id 12 collected
[19:17] Charge balance equation is out by -10.0%
[19:17] Stirrer speed set to 50
[19:22] pH 6.48 -> 6.28
[19:22] Using charge balance adjust
[19:22] Dispensed 0.000847 mL of Acid (0.5 M HCl)
[19:42] Stirrer speed set to 0
[19:57] Datapoint id 13 collected
[19:57] Charge balance equation is out by -11.9%
[19:57] Stirrer speed set to 50
[20:02] pH 6.31 -> 6.11
[20:02] Using charge balance adjust
[20:02] Dispensed 0.000964 mL of Acid (0.5 M HCl)
[20:23] Stirrer speed set to 0
[20:37] Datapoint id 14 collected
[20:37] Charge balance equation is out by -3.1%
[20:37] Stirrer speed set to 50
[20:42] pH 6.12 -> 5.92
[20:42] Using charge balance adjust
[20:42] Dispensed 0.000988 mL of Acid (0.5 M HCl)
[21:02] Stirrer speed set to 0
[21:19] Datapoint id 15 collected
[21:19] Charge balance equation is out by -3.5%
[21:19] Stirrer speed set to 50
[21:24] pH 5.93 -> 5.73
[21:24] Using charge balance adjust
[21:24] Dispensed 0.000941 mL of Acid (0.5 M HCl)
[21:45] Stirrer speed set to 0
[22:02] Datapoint id 16 collected
[22:02] Charge balance equation is out by 12.1%
[22:02] Stirrer speed set to 50

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[22:07] pH 5.71 -> 5.51
[22:07] Using charge balance adjust
[22:07] Dispensed 0.000776 mL of Acid (0.5 M HCl)
[22:28] Stirrer speed set to 0
[22:56] Datapoint id 17 collected
[22:56] Charge balance equation is out by 25.0%
[22:56] Stirrer speed set to 50
[23:01] pH 5.46 -> 5.26
[23:01] Using cautious pH adjust
[23:01] Dispensed 0.000282 mL of Acid (0.5 M HCl)
[23:06] Stepping pH = 5.35
[23:06] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[23:11] Stepping pH = 5.28
[23:11] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[23:16] Stepping pH = 5.28
[23:16] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[23:21] Stepping pH = 5.24
[23:36] Stirrer speed set to 0
[24:36] Datapoint id 18 collected
[24:36] Charge balance equation is out by 10.7%
[24:36] Stirrer speed set to 50
[24:42] pH 5.41 -> 5.21
[24:42] Using charge balance adjust
[24:42] Dispensed 0.000541 mL of Acid (0.5 M HCl)
[25:02] Stirrer speed set to 0
[26:02] Datapoint id 19 collected
[26:02] Charge balance equation is out by 187.7%
[26:02] Stirrer speed set to 50
[26:07] pH 4.89 -> 4.69
[26:07] Using cautious pH adjust
[26:07] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[26:12] Stepping pH = 4.73
[26:12] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[26:17] Stepping pH = 4.70
[26:17] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[26:22] Stepping pH = 4.65
[26:38] Stirrer speed set to 0
[27:09] Datapoint id 20 collected
[27:09] Charge balance equation is out by 31.0%
[27:09] Stirrer speed set to 50
[27:14] pH 4.68 -> 4.48
[27:14] Using cautious pH adjust
[27:14] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[27:19] Stepping pH = 4.44
[27:34] Stirrer speed set to 0
[27:47] Datapoint id 21 collected
[27:47] Charge balance equation is out by 50.0%
[27:47] Stirrer speed set to 50
[27:52] pH 4.43 -> 4.23
[27:52] Using cautious pH adjust
[27:52] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[27:57] Stepping pH = 4.32
[27:57] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[28:02] Stepping pH = 4.23
[28:17] Stirrer speed set to 0
[28:28] Datapoint id 22 collected
[28:28] Charge balance equation is out by 19.5%
[28:28] Stirrer speed set to 50
[28:34] pH 4.22 -> 4.02

Sample name: **M08_octanol** Experiment start time: **3/2/2018 6:51:30 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02008** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[28:34] Using cautious pH adjust
[28:34] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[28:39] Stepping pH = 4.08
[28:39] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[28:44] Stepping pH = 4.05
[28:44] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[28:49] Stepping pH = 4.04
[28:49] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[28:54] Stepping pH = 4.01
[29:09] Stirrer speed set to 0
[29:19] Datapoint id 23 collected
[29:19] Charge balance equation is out by 5.7%
[29:19] Stirrer speed set to 50
[29:24] pH 4.00 -> 3.80
[29:24] Using charge balance adjust
[29:24] Dispensed 0.000259 mL of Acid (0.5 M HCl)
[29:45] Stirrer speed set to 0
[29:55] Datapoint id 24 collected
[29:55] Charge balance equation is out by 26.5%
[29:55] Stirrer speed set to 50
[30:00] pH 3.75 -> 3.55
[30:00] Using cautious pH adjust
[30:00] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[30:05] Stepping pH = 3.64
[30:05] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[30:10] Stepping pH = 3.57
[30:10] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[30:15] Stepping pH = 3.56
[30:15] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[30:20] Stepping pH = 3.56
[30:35] Stirrer speed set to 0
[30:45] Datapoint id 25 collected
[30:45] Charge balance equation is out by 1.3%
[30:45] Stirrer speed set to 50
[30:51] pH 3.55 -> 3.35
[30:51] Using charge balance adjust
[30:51] Dispensed 0.000659 mL of Acid (0.5 M HCl)
[31:11] Stirrer speed set to 0
[31:21] Datapoint id 26 collected
[31:21] Charge balance equation is out by 18.1%
[31:21] Stirrer speed set to 50
[31:26] pH 3.32 -> 3.12
[31:26] Using cautious pH adjust
[31:26] Dispensed 0.000541 mL of Acid (0.5 M HCl)
[31:31] Stepping pH = 3.21
[31:31] Dispensed 0.000353 mL of Acid (0.5 M HCl)
[31:36] Stepping pH = 3.15
[31:36] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[31:42] Stepping pH = 3.13
[31:42] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[31:47] Stepping pH = 3.12
[32:02] Stirrer speed set to 0
[32:12] Datapoint id 27 collected
[32:12] Charge balance equation is out by -5.1%
[32:12] Stirrer speed set to 50
[32:17] pH 3.12 -> 2.92
[32:17] Using charge balance adjust
[32:18] Dispensed 0.001740 mL of Acid (0.5 M HCl)
[32:38] Stirrer speed set to 0

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[32:48] Datapoint id 28 collected
[32:48] Charge balance equation is out by 2.3%
[32:48] Stirrer speed set to 50
[32:53] pH 2.92 -> 2.72
[32:53] Using charge balance adjust
[32:53] Dispensed 0.002775 mL of Acid (0.5 M HCl)
[33:13] Stirrer speed set to 0
[33:23] Datapoint id 29 collected
[33:23] Charge balance equation is out by -4.1%
[33:23] Stirrer speed set to 50
[33:28] pH 2.73 -> 2.53
[33:28] Using charge balance adjust
[33:29] Dispensed 0.004280 mL of Acid (0.5 M HCl)
[33:49] Stirrer speed set to 0
[33:59] Datapoint id 30 collected
[33:59] Charge balance equation is out by -2.8%
[33:59] Stirrer speed set to 50
[34:04] pH 2.54 -> 2.34
[34:04] Using charge balance adjust
[34:05] Dispensed 0.006703 mL of Acid (0.5 M HCl)
[34:25] Stirrer speed set to 0
[34:35] Datapoint id 31 collected
[34:35] Charge balance equation is out by -1.5%
[34:35] Stirrer speed set to 50
[34:40] pH 2.35 -> 2.15
[34:40] Using charge balance adjust
[34:40] Dispensed 0.010630 mL of Acid (0.5 M HCl)
[35:01] Stirrer speed set to 0
[35:11] Datapoint id 32 collected
[35:11] Charge balance equation is out by 1.5%
[35:11] Stirrer speed set to 50
[35:16] pH 2.15 -> 1.95
[35:16] Using charge balance adjust
[35:17] Dispensed 0.017310 mL of Acid (0.5 M HCl)
[35:37] Stirrer speed set to 0
[35:47] Datapoint id 33 collected
[35:47] Charge balance equation is out by -0.1%
[35:47] Titration 2 of 3
[35:47] Adding initial titrants
[35:47] Automatically add 0.20000 mL of Octanol
[35:52] Dispensed 0.200000 mL of Octanol
[35:52] Stirrer speed set to 10
[35:53] Stirrer speed set to 55
[35:53] Iterative adjust 1.96 -> 10.00
[35:53] pH 1.96 -> 10.00
[35:55] Dispensed 0.055221 mL of Base (0.5 M KOH)
[36:45] Stirrer speed set to 0
[37:23] Datapoint id 34 collected
[37:23] Stirrer speed set to 55
[37:28] pH 10.05 -> 9.85
[37:28] Using cautious pH adjust
[37:28] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[37:33] Stepping pH = 9.99
[37:33] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[37:38] Stepping pH = 9.81
[37:53] Stirrer speed set to 0
[38:45] Datapoint id 35 collected
[38:45] Charge balance equation is out by -10.4%
[38:45] Stirrer speed set to 55

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[38:50] pH 9.48 -> 9.28
[38:50] Using charge balance adjust
[38:50] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[39:10] Stirrer speed set to 0
[40:06] Datapoint id 36 collected
[40:06] Charge balance equation is out by 26.4%
[40:06] Stirrer speed set to 55
[40:11] pH 9.11 -> 8.91
[40:11] Using cautious pH adjust
[40:11] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[40:16] Stepping pH = 9.08
[40:16] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[40:21] Stepping pH = 8.95
[40:21] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[40:26] Stepping pH = 8.86
[40:41] Stirrer speed set to 0
[41:21] Datapoint id 37 collected
[41:21] Charge balance equation is out by -100.8%
[41:21] Stirrer speed set to 55
[41:27] pH 8.60 -> 8.40
[41:27] Using cautious pH adjust
[41:27] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[41:32] Stepping pH = 8.56
[41:32] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[41:37] Stepping pH = 8.42
[41:37] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[41:42] Stepping pH = 8.36
[41:57] Stirrer speed set to 0
[42:08] Datapoint id 38 collected
[42:08] Charge balance equation is out by -78.4%
[42:08] Stirrer speed set to 55
[42:13] pH 8.28 -> 8.08
[42:13] Using cautious pH adjust
[42:13] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[42:18] Stepping pH = 8.21
[42:18] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[42:23] Stepping pH = 8.11
[42:23] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[42:28] Stepping pH = 8.08
[42:43] Stirrer speed set to 0
[42:55] Datapoint id 39 collected
[42:55] Charge balance equation is out by -33.8%
[42:55] Stirrer speed set to 55
[43:00] pH 8.04 -> 7.84
[43:00] Using cautious pH adjust
[43:00] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[43:06] Stepping pH = 7.94
[43:06] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[43:11] Stepping pH = 7.89
[43:11] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[43:16] Stepping pH = 7.83
[43:31] Stirrer speed set to 0
[43:44] Datapoint id 40 collected
[43:44] Charge balance equation is out by -18.6%
[43:44] Stirrer speed set to 55
[43:49] pH 7.80 -> 7.60
[43:49] Using cautious pH adjust
[43:49] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[43:54] Stepping pH = 7.70

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[43:54] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[43:59] Stepping pH = 7.63
[43:59] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[44:04] Stepping pH = 7.60
[44:19] Stirrer speed set to 0
[44:34] Datapoint id 41 collected
[44:34] Charge balance equation is out by -7.6%
[44:34] Stirrer speed set to 55
[44:39] pH 7.59 -> 7.39
[44:39] Using charge balance adjust
[44:39] Dispensed 0.000353 mL of Acid (0.5 M HCl)
[44:59] Stirrer speed set to 0
[45:11] Datapoint id 42 collected
[45:11] Charge balance equation is out by 4.7%
[45:11] Stirrer speed set to 55
[45:16] pH 7.37 -> 7.17
[45:16] Using charge balance adjust
[45:16] Dispensed 0.000517 mL of Acid (0.5 M HCl)
[45:36] Stirrer speed set to 0
[45:49] Datapoint id 43 collected
[45:49] Charge balance equation is out by -1.7%
[45:49] Stirrer speed set to 55
[45:54] pH 7.17 -> 6.97
[45:54] Using charge balance adjust
[45:54] Dispensed 0.000682 mL of Acid (0.5 M HCl)
[46:14] Stirrer speed set to 0
[46:26] Datapoint id 44 collected
[46:26] Charge balance equation is out by -8.7%
[46:26] Stirrer speed set to 55
[46:31] pH 6.99 -> 6.79
[46:31] Using charge balance adjust
[46:31] Dispensed 0.000847 mL of Acid (0.5 M HCl)
[46:51] Stirrer speed set to 0
[47:04] Datapoint id 45 collected
[47:04] Charge balance equation is out by -5.3%
[47:04] Stirrer speed set to 55
[47:09] pH 6.80 -> 6.60
[47:09] Using charge balance adjust
[47:09] Dispensed 0.000964 mL of Acid (0.5 M HCl)
[47:29] Stirrer speed set to 0
[47:42] Datapoint id 46 collected
[47:42] Charge balance equation is out by -11.4%
[47:42] Stirrer speed set to 55
[47:47] pH 6.63 -> 6.43
[47:47] Using charge balance adjust
[47:47] Dispensed 0.000988 mL of Acid (0.5 M HCl)
[48:07] Stirrer speed set to 0
[48:24] Datapoint id 47 collected
[48:24] Charge balance equation is out by -13.9%
[48:24] Stirrer speed set to 55
[48:29] pH 6.45 -> 6.25
[48:29] Using charge balance adjust
[48:29] Dispensed 0.000964 mL of Acid (0.5 M HCl)
[48:49] Stirrer speed set to 0
[49:07] Datapoint id 48 collected
[49:07] Charge balance equation is out by -14.7%
[49:07] Stirrer speed set to 55
[49:12] pH 6.28 -> 6.08
[49:12] Using charge balance adjust

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[49:12] Dispensed 0.000847 mL of Acid (0.5 M HCl)
[49:32] Stirrer speed set to 0
[49:49] Datapoint id 49 collected
[49:49] Charge balance equation is out by -13.2%
[49:49] Stirrer speed set to 55
[49:54] pH 6.09 -> 5.89
[49:54] Using charge balance adjust
[49:54] Dispensed 0.000706 mL of Acid (0.5 M HCl)
[50:15] Stirrer speed set to 0
[50:32] Datapoint id 50 collected
[50:32] Charge balance equation is out by -7.5%
[50:32] Stirrer speed set to 55
[50:37] pH 5.90 -> 5.70
[50:37] Using charge balance adjust
[50:37] Dispensed 0.000517 mL of Acid (0.5 M HCl)
[50:58] Stirrer speed set to 0
[51:13] Datapoint id 51 collected
[51:13] Charge balance equation is out by 7.5%
[51:13] Stirrer speed set to 55
[51:18] pH 5.67 -> 5.47
[51:18] Using charge balance adjust
[51:18] Dispensed 0.000353 mL of Acid (0.5 M HCl)
[51:38] Stirrer speed set to 0
[51:54] Datapoint id 52 collected
[51:54] Charge balance equation is out by -2.1%
[51:54] Stirrer speed set to 55
[51:59] pH 5.46 -> 5.26
[51:59] Using charge balance adjust
[51:59] Dispensed 0.000235 mL of Acid (0.5 M HCl)
[52:19] Stirrer speed set to 0
[52:33] Datapoint id 53 collected
[52:33] Charge balance equation is out by -17.6%
[52:33] Stirrer speed set to 55
[52:39] pH 5.27 -> 5.07
[52:39] Using cautious pH adjust
[52:39] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[52:44] Stepping pH = 5.25
[52:44] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[52:49] Stepping pH = 4.83
[53:04] Stirrer speed set to 0
[53:18] Datapoint id 54 collected
[53:18] Charge balance equation is out by -65.9%
[53:18] Stirrer speed set to 55
[53:23] pH 4.84 -> 4.64
[53:23] Using cautious pH adjust
[53:23] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[53:28] Stepping pH = 4.81
[53:28] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[53:33] Stepping pH = 4.59
[53:48] Stirrer speed set to 0
[54:01] Datapoint id 55 collected
[54:01] Charge balance equation is out by -62.4%
[54:01] Stirrer speed set to 55
[54:06] pH 4.59 -> 4.39
[54:06] Using cautious pH adjust
[54:06] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[54:11] Stepping pH = 4.59
[54:12] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[54:17] Stepping pH = 4.27

Sample name: **M08_octanol** Experiment start time: **3/2/2018 6:51:30 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02008** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[54:32] Stirrer speed set to 0
[54:43] Datapoint id 56 collected
[54:43] Charge balance equation is out by -100.0%
[54:43] Stirrer speed set to 55
[54:48] pH 4.28 -> 4.08
[54:48] Using cautious pH adjust
[54:48] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[54:54] Stepping pH = 4.25
[54:54] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[54:59] Stepping pH = 3.97
[55:14] Stirrer speed set to 0
[55:24] Datapoint id 57 collected
[55:24] Charge balance equation is out by -70.8%
[55:24] Stirrer speed set to 55
[55:29] pH 3.96 -> 3.76
[55:29] Using cautious pH adjust
[55:29] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[55:34] Stepping pH = 3.87
[55:34] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[55:39] Stepping pH = 3.79
[55:39] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[55:44] Stepping pH = 3.77
[55:44] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[55:49] Stepping pH = 3.76
[56:05] Stirrer speed set to 0
[56:15] Datapoint id 58 collected
[56:15] Charge balance equation is out by -19.0%
[56:15] Stirrer speed set to 55
[56:20] pH 3.76 -> 3.56
[56:20] Using cautious pH adjust
[56:20] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[56:25] Stepping pH = 3.63
[56:25] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[56:30] Stepping pH = 3.59
[56:30] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[56:35] Stepping pH = 3.57
[56:35] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[56:40] Stepping pH = 3.56
[56:55] Stirrer speed set to 0
[57:06] Datapoint id 59 collected
[57:06] Charge balance equation is out by 3.2%
[57:06] Stirrer speed set to 55
[57:11] pH 3.55 -> 3.35
[57:11] Using charge balance adjust
[57:11] Dispensed 0.000682 mL of Acid (0.5 M HCl)
[57:31] Stirrer speed set to 0
[57:41] Datapoint id 60 collected
[57:41] Charge balance equation is out by 10.1%
[57:41] Stirrer speed set to 55
[57:46] pH 3.33 -> 3.13
[57:46] Using charge balance adjust
[57:46] Dispensed 0.001129 mL of Acid (0.5 M HCl)
[58:06] Stirrer speed set to 0
[58:16] Datapoint id 61 collected
[58:16] Charge balance equation is out by 3.9%
[58:16] Stirrer speed set to 55
[58:21] pH 3.13 -> 2.93
[58:21] Using charge balance adjust
[58:22] Dispensed 0.001834 mL of Acid (0.5 M HCl)

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[58:42] Stirrer speed set to 0
[58:52] Datapoint id 62 collected
[58:52] Charge balance equation is out by 1.2%
[58:52] Stirrer speed set to 55
[58:57] pH 2.93 -> 2.73
[58:57] Using charge balance adjust
[58:57] Dispensed 0.002893 mL of Acid (0.5 M HCl)
[59:17] Stirrer speed set to 0
[59:28] Datapoint id 63 collected
[59:28] Charge balance equation is out by 3.2%
[59:28] Stirrer speed set to 55
[59:33] pH 2.73 -> 2.53
[59:33] Using charge balance adjust
[59:33] Dispensed 0.004633 mL of Acid (0.5 M HCl)
[59:53] Stirrer speed set to 0
[1:00:04] Datapoint id 64 collected
[1:00:04] Charge balance equation is out by 5.3%
[1:00:04] Stirrer speed set to 55
[1:00:09] pH 2.52 -> 2.32
[1:00:09] Using charge balance adjust
[1:00:09] Dispensed 0.007573 mL of Acid (0.5 M HCl)
[1:00:29] Stirrer speed set to 0
[1:00:39] Datapoint id 65 collected
[1:00:39] Charge balance equation is out by -5.8%
[1:00:39] Stirrer speed set to 55
[1:00:45] pH 2.34 -> 2.14
[1:00:45] Using charge balance adjust
[1:00:45] Dispensed 0.011830 mL of Acid (0.5 M HCl)
[1:01:05] Stirrer speed set to 0
[1:01:15] Datapoint id 66 collected
[1:01:15] Charge balance equation is out by 1.7%
[1:01:15] Stirrer speed set to 55
[1:01:20] pH 2.14 -> 1.95
[1:01:20] Using charge balance adjust
[1:01:21] Dispensed 0.017686 mL of Acid (0.5 M HCl)
[1:01:41] Stirrer speed set to 0
[1:01:52] Datapoint id 67 collected
[1:01:52] Charge balance equation is out by -8.3%
[1:01:52] Titration 3 of 3
[1:01:52] Adding initial titrants
[1:01:52] Automatically add 0.80000 mL of Octanol
[1:02:42] Dispensed 0.800000 mL of Octanol
[1:02:42] Stirrer speed set to 10
[1:02:43] Stirrer speed set to 60
[1:02:43] Iterative adjust 1.94 -> 10.00
[1:02:43] pH 1.94 -> 10.00
[1:02:44] Dispensed 0.060113 mL of Base (0.5 M KOH)
[1:03:34] Stirrer speed set to 0
[1:04:20] Datapoint id 68 collected
[1:04:20] Stirrer speed set to 60
[1:04:25] pH 10.13 -> 9.93
[1:04:25] Using cautious pH adjust
[1:04:25] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[1:04:30] Stepping pH = 10.07
[1:04:30] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:04:35] Stepping pH = 9.92
[1:04:50] Stirrer speed set to 0
[1:05:28] Datapoint id 69 collected
[1:05:28] Charge balance equation is out by -4.4%

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:05:28] Stirrer speed set to 60
[1:05:33] pH 9.82 -> 9.62
[1:05:33] Using charge balance adjust
[1:05:33] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:05:53] Stirrer speed set to 0
[1:06:31] Datapoint id 70 collected
[1:06:31] Charge balance equation is out by 12.1%
[1:06:31] Stirrer speed set to 60
[1:06:36] pH 9.60 -> 9.40
[1:06:36] Using charge balance adjust
[1:06:36] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[1:06:56] Stirrer speed set to 0
[1:07:50] Datapoint id 71 collected
[1:07:50] Charge balance equation is out by -11.8%
[1:07:50] Stirrer speed set to 60
[1:07:55] pH 9.39 -> 9.19
[1:07:55] Using charge balance adjust
[1:07:55] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:08:15] Stirrer speed set to 0
[1:08:26] Datapoint id 72 collected
[1:08:26] Charge balance equation is out by -31.9%
[1:08:26] Stirrer speed set to 60
[1:08:31] pH 9.25 -> 9.05
[1:08:31] Using cautious pH adjust
[1:08:31] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:08:36] Stepping pH = 9.20
[1:08:36] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:08:41] Stepping pH = 9.08
[1:08:41] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:08:47] Stepping pH = 9.04
[1:09:02] Stirrer speed set to 0
[1:09:20] Datapoint id 73 collected
[1:09:20] Charge balance equation is out by -49.6%
[1:09:20] Stirrer speed set to 60
[1:09:25] pH 9.00 -> 8.80
[1:09:25] Using cautious pH adjust
[1:09:25] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:09:30] Stepping pH = 8.94
[1:09:30] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:09:35] Stepping pH = 8.86
[1:09:35] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:09:40] Stepping pH = 8.78
[1:09:55] Stirrer speed set to 0
[1:10:15] Datapoint id 74 collected
[1:10:15] Charge balance equation is out by -58.1%
[1:10:15] Stirrer speed set to 60
[1:10:20] pH 8.72 -> 8.52
[1:10:20] Using cautious pH adjust
[1:10:21] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:10:26] Stepping pH = 8.63
[1:10:26] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:10:31] Stepping pH = 8.56
[1:10:31] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:10:36] Stepping pH = 8.52
[1:10:51] Stirrer speed set to 0
[1:11:13] Datapoint id 75 collected
[1:11:13] Charge balance equation is out by -17.8%
[1:11:13] Stirrer speed set to 60
[1:11:18] pH 8.50 -> 8.30

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:11:18] Using cautious pH adjust
[1:11:18] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:11:23] Stepping pH = 8.39
[1:11:23] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:11:28] Stepping pH = 8.31
[1:11:28] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:11:33] Stepping pH = 8.29
[1:11:48] Stirrer speed set to 0
[1:12:09] Datapoint id 76 collected
[1:12:09] Charge balance equation is out by 5.6%
[1:12:09] Stirrer speed set to 60
[1:12:14] pH 8.27 -> 8.07
[1:12:14] Using charge balance adjust
[1:12:14] Dispensed 0.000282 mL of Acid (0.5 M HCl)
[1:12:34] Stirrer speed set to 0
[1:12:58] Datapoint id 77 collected
[1:12:58] Charge balance equation is out by 6.1%
[1:12:58] Stirrer speed set to 60
[1:13:04] pH 8.03 -> 7.83
[1:13:04] Using charge balance adjust
[1:13:04] Dispensed 0.000423 mL of Acid (0.5 M HCl)
[1:13:24] Stirrer speed set to 0
[1:13:46] Datapoint id 78 collected
[1:13:46] Charge balance equation is out by -1.0%
[1:13:46] Stirrer speed set to 60
[1:13:51] pH 7.81 -> 7.61
[1:13:51] Using charge balance adjust
[1:13:51] Dispensed 0.000611 mL of Acid (0.5 M HCl)
[1:14:11] Stirrer speed set to 0
[1:14:32] Datapoint id 79 collected
[1:14:32] Charge balance equation is out by -0.6%
[1:14:32] Stirrer speed set to 60
[1:14:37] pH 7.59 -> 7.39
[1:14:37] Using charge balance adjust
[1:14:38] Dispensed 0.000800 mL of Acid (0.5 M HCl)
[1:14:58] Stirrer speed set to 0
[1:15:25] Datapoint id 80 collected
[1:15:25] Charge balance equation is out by -5.5%
[1:15:25] Stirrer speed set to 60
[1:15:30] pH 7.38 -> 7.18
[1:15:30] Using charge balance adjust
[1:15:31] Dispensed 0.000941 mL of Acid (0.5 M HCl)
[1:15:51] Stirrer speed set to 0
[1:16:15] Datapoint id 81 collected
[1:16:15] Charge balance equation is out by -10.4%
[1:16:15] Stirrer speed set to 60
[1:16:20] pH 7.18 -> 6.98
[1:16:20] Using charge balance adjust
[1:16:21] Dispensed 0.000988 mL of Acid (0.5 M HCl)
[1:16:41] Stirrer speed set to 0
[1:17:03] Datapoint id 82 collected
[1:17:03] Charge balance equation is out by -12.8%
[1:17:03] Stirrer speed set to 60
[1:17:08] pH 6.99 -> 6.79
[1:17:08] Using charge balance adjust
[1:17:08] Dispensed 0.000941 mL of Acid (0.5 M HCl)
[1:17:28] Stirrer speed set to 0
[1:17:57] Datapoint id 83 collected
[1:17:57] Charge balance equation is out by -21.6%

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:17:57] Stirrer speed set to 60
[1:18:02] pH 6.79 -> 6.59
[1:18:02] Using cautious pH adjust
[1:18:02] Dispensed 0.000423 mL of Acid (0.5 M HCl)
[1:18:08] Stepping pH = 6.70
[1:18:08] Dispensed 0.000329 mL of Acid (0.5 M HCl)
[1:18:13] Stepping pH = 6.62
[1:18:13] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:18:18] Stepping pH = 6.61
[1:18:18] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:18:23] Stepping pH = 6.59
[1:18:38] Stirrer speed set to 0
[1:19:13] Datapoint id 84 collected
[1:19:13] Charge balance equation is out by -11.6%
[1:19:13] Stirrer speed set to 60
[1:19:18] pH 6.59 -> 6.39
[1:19:18] Using charge balance adjust
[1:19:18] Dispensed 0.000659 mL of Acid (0.5 M HCl)
[1:19:39] Stirrer speed set to 0
[1:20:12] Datapoint id 85 collected
[1:20:12] Charge balance equation is out by -31.3%
[1:20:12] Stirrer speed set to 60
[1:20:17] pH 6.40 -> 6.20
[1:20:17] Using cautious pH adjust
[1:20:17] Dispensed 0.000259 mL of Acid (0.5 M HCl)
[1:20:22] Stepping pH = 6.31
[1:20:22] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[1:20:27] Stepping pH = 6.23
[1:20:27] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:20:32] Stepping pH = 6.21
[1:20:32] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:20:37] Stepping pH = 6.20
[1:20:53] Stirrer speed set to 0
[1:21:18] Datapoint id 86 collected
[1:21:18] Charge balance equation is out by -13.3%
[1:21:18] Stirrer speed set to 60
[1:21:23] pH 6.22 -> 6.02
[1:21:23] Using charge balance adjust
[1:21:23] Dispensed 0.000376 mL of Acid (0.5 M HCl)
[1:21:43] Stirrer speed set to 0
[1:22:08] Datapoint id 87 collected
[1:22:08] Charge balance equation is out by -33.3%
[1:22:08] Stirrer speed set to 60
[1:22:13] pH 6.01 -> 5.81
[1:22:13] Using cautious pH adjust
[1:22:13] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[1:22:18] Stepping pH = 5.97
[1:22:18] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[1:22:23] Stepping pH = 5.81
[1:22:38] Stirrer speed set to 0
[1:22:57] Datapoint id 88 collected
[1:22:57] Charge balance equation is out by -32.4%
[1:22:57] Stirrer speed set to 60
[1:23:02] pH 5.82 -> 5.62
[1:23:02] Using cautious pH adjust
[1:23:02] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:23:07] Stepping pH = 5.76
[1:23:08] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[1:23:13] Stepping pH = 5.65

Sample name: **M08_octanol** Experiment start time: **3/2/2018 6:51:30 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02008** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[1:23:13] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:23:18] Stepping pH = 5.63
[1:23:18] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:23:23] Stepping pH = 5.62
[1:23:38] Stirrer speed set to 0
[1:24:02] Datapoint id 89 collected
[1:24:02] Charge balance equation is out by -35.8%
[1:24:02] Stirrer speed set to 60
[1:24:07] pH 5.62 -> 5.42
[1:24:07] Using cautious pH adjust
[1:24:07] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:24:12] Stepping pH = 5.59
[1:24:12] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[1:24:17] Stepping pH = 5.42
[1:24:32] Stirrer speed set to 0
[1:24:55] Datapoint id 90 collected
[1:24:55] Charge balance equation is out by -48.7%
[1:24:55] Stirrer speed set to 60
[1:25:00] pH 5.41 -> 5.21
[1:25:00] Using cautious pH adjust
[1:25:00] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:25:05] Stepping pH = 5.39
[1:25:05] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:25:10] Stepping pH = 5.20
[1:25:25] Stirrer speed set to 0
[1:25:55] Datapoint id 91 collected
[1:25:55] Charge balance equation is out by -72.9%
[1:25:55] Stirrer speed set to 60
[1:26:00] pH 5.20 -> 5.00
[1:26:00] Using cautious pH adjust
[1:26:00] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:26:05] Stepping pH = 5.17
[1:26:05] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:26:10] Stepping pH = 5.00
[1:26:25] Stirrer speed set to 0
[1:26:40] Datapoint id 92 collected
[1:26:40] Charge balance equation is out by -79.7%
[1:26:40] Stirrer speed set to 60
[1:26:45] pH 4.97 -> 4.77
[1:26:45] Using cautious pH adjust
[1:26:45] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:26:50] Stepping pH = 4.97
[1:26:50] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[1:26:55] Stepping pH = 4.59
[1:27:10] Stirrer speed set to 0
[1:27:22] Datapoint id 93 collected
[1:27:22] Charge balance equation is out by -206.8%
[1:27:22] Stirrer speed set to 60
[1:27:27] pH 4.58 -> 4.38
[1:27:27] Using cautious pH adjust
[1:27:27] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:27:32] Stepping pH = 4.55
[1:27:33] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:27:38] Stepping pH = 4.36
[1:27:53] Stirrer speed set to 0
[1:28:10] Datapoint id 94 collected
[1:28:10] Charge balance equation is out by -82.7%
[1:28:10] Stirrer speed set to 60
[1:28:15] pH 4.35 -> 4.15

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:28:15] Using cautious pH adjust
[1:28:15] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:28:20] Stepping pH = 4.29
[1:28:20] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:28:25] Stepping pH = 4.17
[1:28:25] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:28:30] Stepping pH = 4.15
[1:28:45] Stirrer speed set to 0
[1:28:56] Datapoint id 95 collected
[1:28:56] Charge balance equation is out by -35.8%
[1:28:56] Stirrer speed set to 60
[1:29:01] pH 4.13 -> 3.93
[1:29:01] Using cautious pH adjust
[1:29:01] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:29:06] Stepping pH = 4.05
[1:29:06] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:29:11] Stepping pH = 3.97
[1:29:11] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:29:17] Stepping pH = 3.94
[1:29:32] Stirrer speed set to 0
[1:29:55] Datapoint id 96 collected
[1:29:55] Charge balance equation is out by -17.3%
[1:29:55] Stirrer speed set to 60
[1:30:00] pH 3.92 -> 3.72
[1:30:00] Using cautious pH adjust
[1:30:00] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:30:05] Stepping pH = 3.83
[1:30:05] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[1:30:11] Stepping pH = 3.75
[1:30:11] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:30:16] Stepping pH = 3.74
[1:30:16] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:30:21] Stepping pH = 3.72
[1:30:36] Stirrer speed set to 0
[1:30:46] Datapoint id 97 collected
[1:30:46] Charge balance equation is out by -21.4%
[1:30:46] Stirrer speed set to 60
[1:30:51] pH 3.72 -> 3.52
[1:30:51] Using cautious pH adjust
[1:30:51] Dispensed 0.000259 mL of Acid (0.5 M HCl)
[1:30:56] Stepping pH = 3.61
[1:30:56] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[1:31:01] Stepping pH = 3.55
[1:31:02] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:31:07] Stepping pH = 3.53
[1:31:07] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:31:12] Stepping pH = 3.52
[1:31:27] Stirrer speed set to 0
[1:31:37] Datapoint id 98 collected
[1:31:37] Charge balance equation is out by -13.3%
[1:31:37] Stirrer speed set to 60
[1:31:42] pH 3.52 -> 3.32
[1:31:42] Using charge balance adjust
[1:31:42] Dispensed 0.000800 mL of Acid (0.5 M HCl)
[1:32:02] Stirrer speed set to 0
[1:32:12] Datapoint id 99 collected
[1:32:12] Charge balance equation is out by -0.9%
[1:32:12] Stirrer speed set to 60
[1:32:18] pH 3.32 -> 3.12

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02008**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02008_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 6:51:30 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:32:18] Using charge balance adjust
[1:32:18] Dispensed 0.001246 mL of Acid (0.5 M HCl)
[1:32:38] Stirrer speed set to 0
[1:32:48] Datapoint id 100 collected
[1:32:48] Charge balance equation is out by -4.4%
[1:32:48] Stirrer speed set to 60
[1:32:53] pH 3.14 -> 2.94
[1:32:53] Using charge balance adjust
[1:32:54] Dispensed 0.001929 mL of Acid (0.5 M HCl)
[1:33:14] Stirrer speed set to 0
[1:33:37] Datapoint id 101 collected
[1:33:37] Charge balance equation is out by -0.5%
[1:33:37] Stirrer speed set to 60
[1:33:42] pH 2.94 -> 2.74
[1:33:42] Using charge balance adjust
[1:33:43] Dispensed 0.003010 mL of Acid (0.5 M HCl)
[1:34:03] Stirrer speed set to 0
[1:34:13] Datapoint id 102 collected
[1:34:13] Charge balance equation is out by 1.9%
[1:34:13] Stirrer speed set to 60
[1:34:18] pH 2.74 -> 2.54
[1:34:18] Using charge balance adjust
[1:34:18] Dispensed 0.004845 mL of Acid (0.5 M HCl)
[1:34:38] Stirrer speed set to 0
[1:34:49] Datapoint id 103 collected
[1:34:49] Charge balance equation is out by 1.5%
[1:34:49] Stirrer speed set to 60
[1:34:54] pH 2.54 -> 2.34
[1:34:54] Using charge balance adjust
[1:34:54] Dispensed 0.007785 mL of Acid (0.5 M HCl)
[1:35:15] Stirrer speed set to 0
[1:35:30] Datapoint id 104 collected
[1:35:30] Charge balance equation is out by -0.7%
[1:35:30] Stirrer speed set to 60
[1:35:35] pH 2.35 -> 2.15
[1:35:35] Using charge balance adjust
[1:35:35] Dispensed 0.012371 mL of Acid (0.5 M HCl)
[1:35:55] Stirrer speed set to 0
[1:36:09] Datapoint id 105 collected
[1:36:09] Charge balance equation is out by -0.3%
[1:36:09] Stirrer speed set to 60
[1:36:14] pH 2.15 -> 1.95
[1:36:14] Using charge balance adjust
[1:36:14] Dispensed 0.019920 mL of Acid (0.5 M HCl)
[1:36:35] Stirrer speed set to 0
[1:36:55] Datapoint id 106 collected
[1:36:55] Charge balance equation is out by 1.4%
[1:36:55] Argon flow rate set to 0
[1:36:59] Titrator arm moved over Titration position