Sample name: **M11_octanol**	Experiment start time: **3/1/2018 12:11:22 AM**
Assay name: **pH-metric high logP**	Analyst: **Pion**
Assay ID: **18C-01001**	Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**	

pH-metric Result

logP (XH +)   0.55   ±0.07 (n=50)
logP (neutral X)   2.19   ±0.02 (n=50)

18C-01001 Points 1 to 23

M11_octanol concentration factor 1.023
Carbonate   0.0000 mM
Acidity error   0.03008 mM

18C-01001 Points 24 to 48

M11_octanol concentration factor 0.912
Carbonate   0.0957 mM
Acidity error   -0.30629 mM

18C-01001 Points 49 to 69

M11_octanol concentration factor 0.792
Carbonate   0.0733 mM
Acidity error   -0.81928 mM
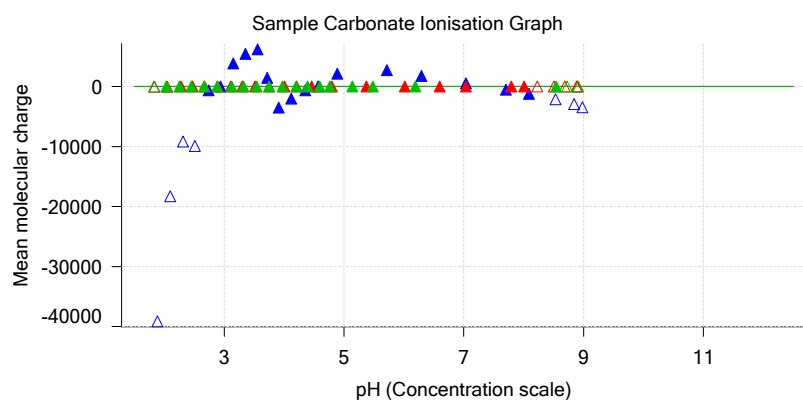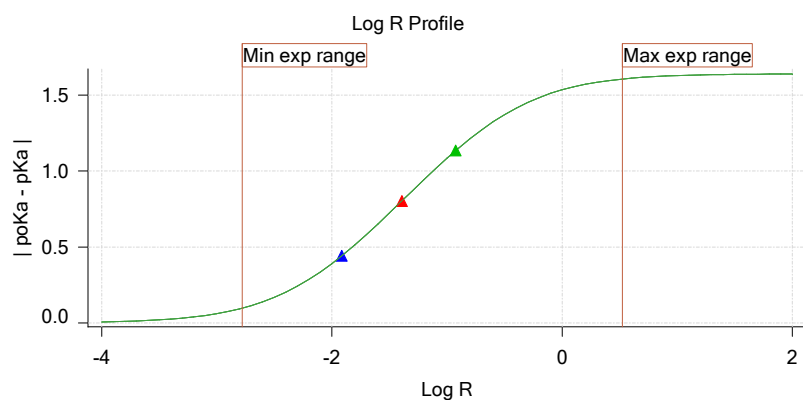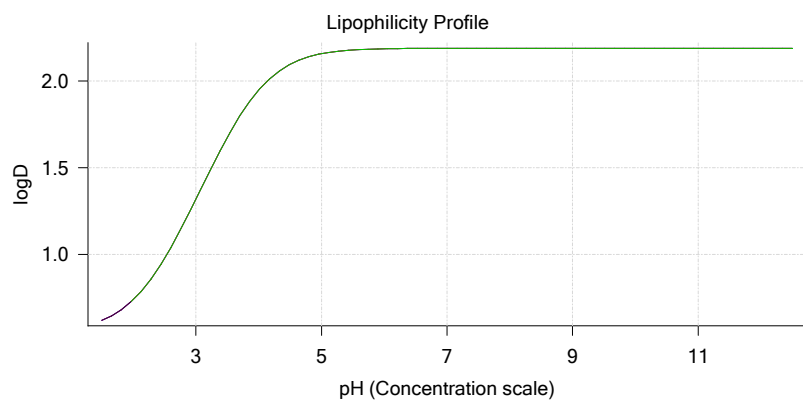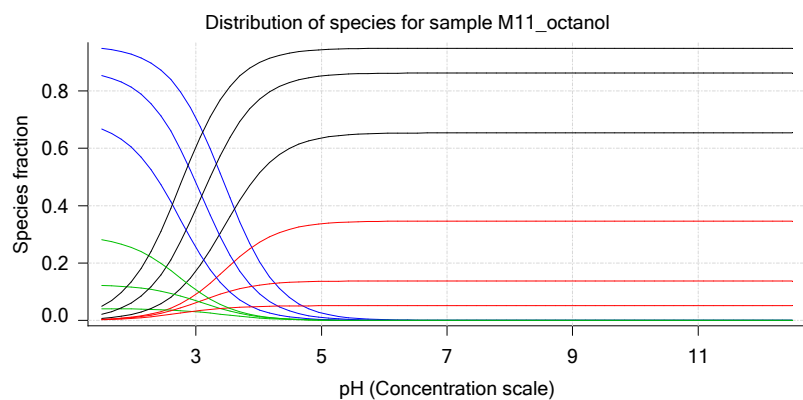
Warnings and errors

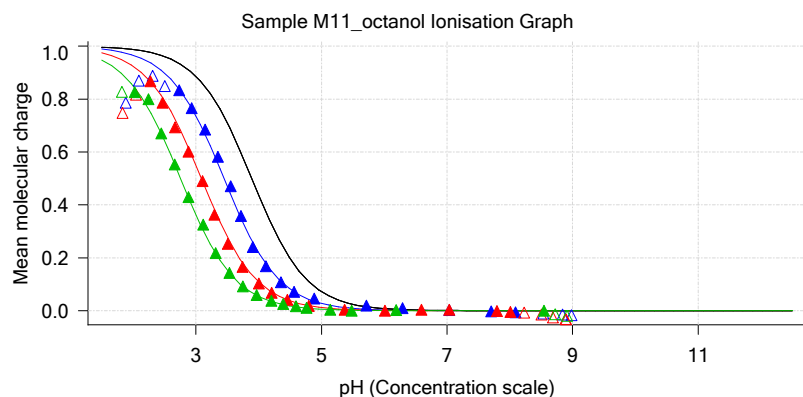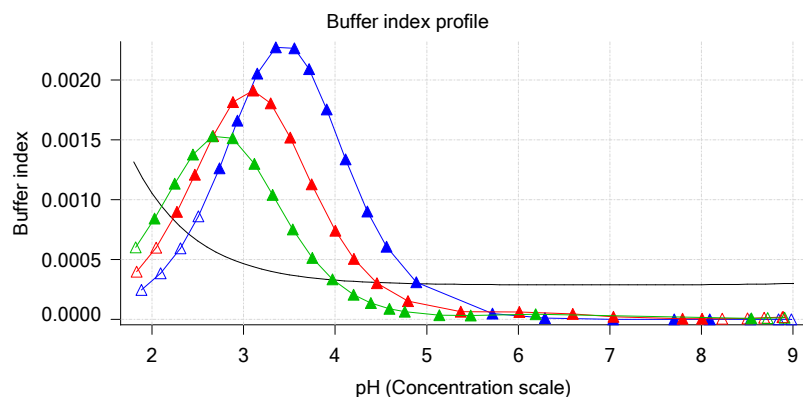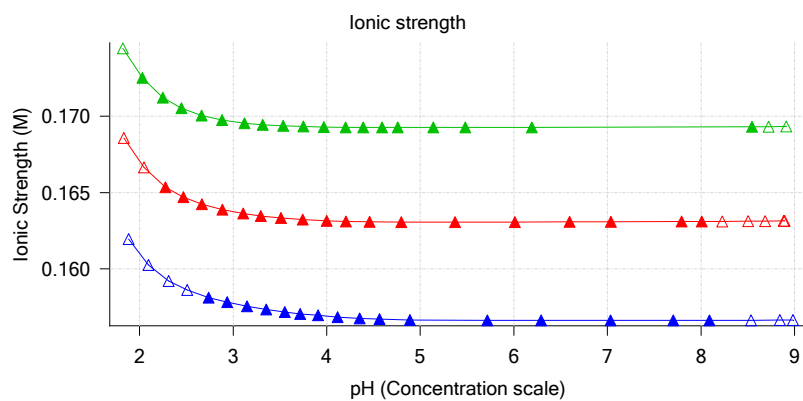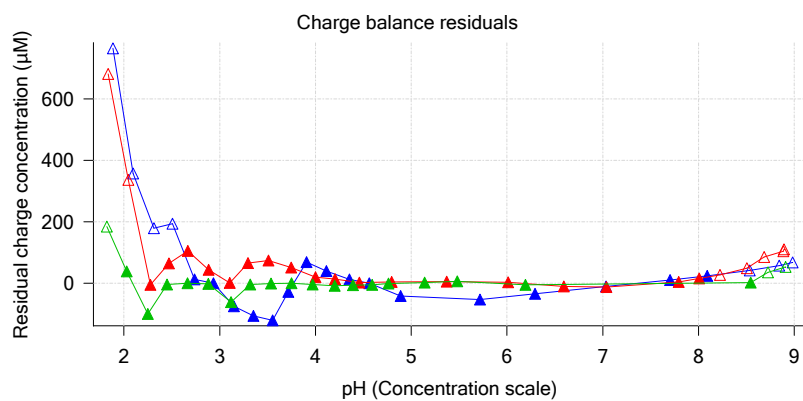Errors   None
Warnings   None

Sample logD and percent species

pH	M11_octanol logD	M11_octanol M11_octanolH	M11_octanol M11_octanol	M11_octanol M11_octanolH*	M11_octanol M11_octanol*	Comment
1.000	0.57	21.08 %	0.03 %	74.70 %	4.20 %	
1.200	0.59	20.57 %	0.04 %	72.90 %	6.49 %	Stomach pH
2.000	0.74	15.27 %	0.20 %	54.12 %	30.41 %	
3.000	1.32	4.07 %	0.52 %	14.42 %	80.99 %	
4.000	1.95	0.49 %	0.63 %	1.73 %	97.15 %	
5.000	2.16	0.05 %	0.64 %	0.18 %	99.13 %	
6.000	2.19	0.00 %	0.64 %	0.02 %	99.33 %	
6.500	2.19	0.00 %	0.64 %	0.01 %	99.35 %	
7.000	2.19	0.00 %	0.64 %	0.00 %	99.35 %	
7.400	2.19	0.00 %	0.64 %	0.00 %	99.36 %	Blood pH
8.000	2.19	0.00 %	0.64 %	0.00 %	99.36 %	
9.000	2.19	0.00 %	0.64 %	0.00 %	99.36 %	
10.000	2.19	0.00 %	0.64 %	0.00 %	99.36 %	
11.000	2.19	0.00 %	0.64 %	0.00 %	99.36 %	
12.000	2.19	0.00 %	0.64 %	0.00 %	99.36 %	

pH-metric Result

Sample name: **M11_octanol** Experiment start time: **3/1/2018 12:11:22 AM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-01001** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M11_octanol Ionisation Graph

Distribution of species for sample M11_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)

Distribution of species for sample Carbonate

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

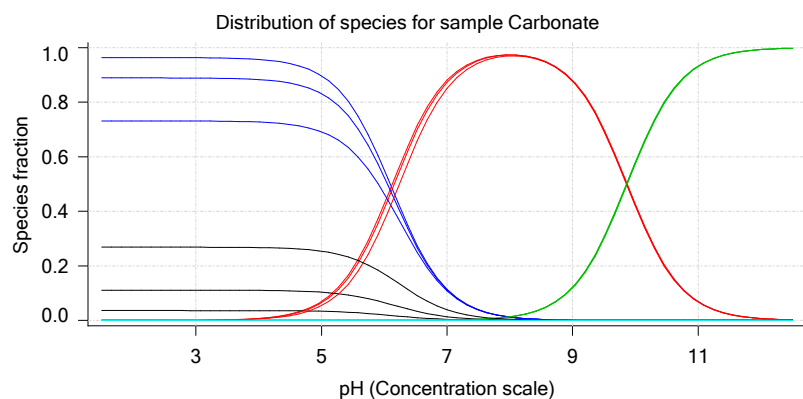Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 1 of 3   18C-01001 Points 1 to 23

Overall results

RMSD   1.827
Average ionic strength   0.157 M
Average temperature   25.0°C
Partition ratio   0.0122 : 1
Analyte concentration range 3838.3 µM to 3962.6 µM
Total points considered   16 of 23

Warnings and errors

Errors   None
Warnings   One or more logP values out of range

Four-Plus parameters

Alpha   0.130   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
S   0.9970   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
jH   0.8   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
jOH   -0.4   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r

Titrants

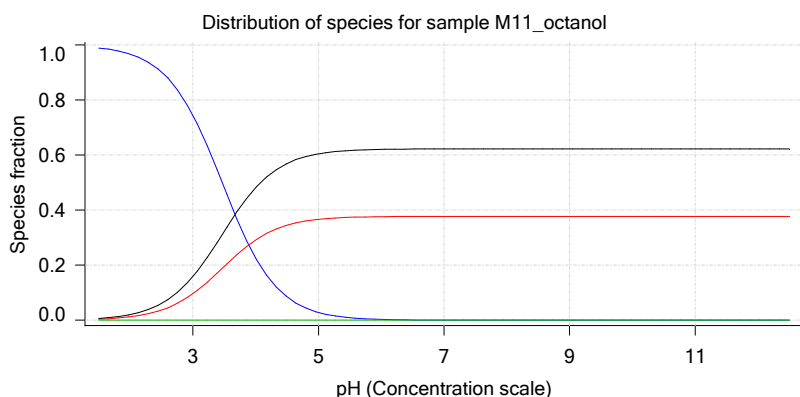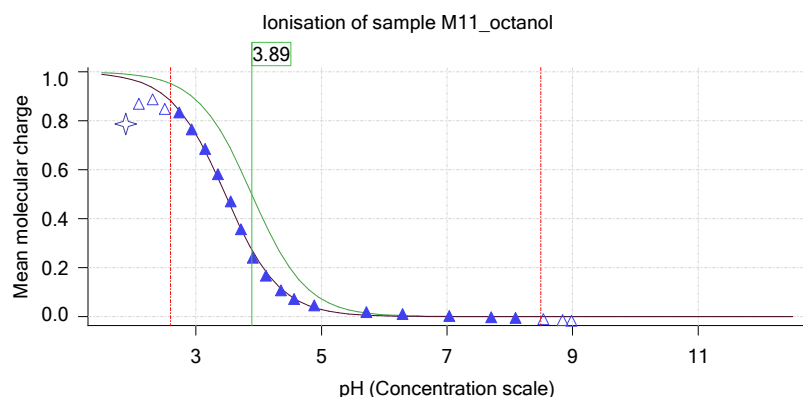0.50 M HCl   0.993513   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH   0.999845   3/1/2018 12:11:22 AM   C:\Sirius_T3\KOH18B27.t3r

Sample

M11_octanol concentration factor   1.023
Base pKa 1   3.89
logP (XH +)   -8.26
logP (neutral X)   2.13

Sample graphs

Ionisation of sample M11_octanol

Distribution of species for sample M11_octanol

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
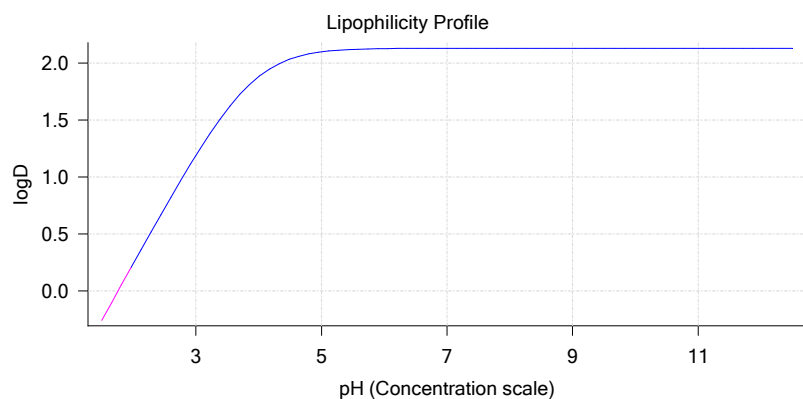
Sample logD and percent species

pH	M11_octanol logD	M11_octanol M11_octanolH	M11_octanol M11_octanol	M11_octanol M11_octanolH*	M11_octanol M11_octanol*	Comment
1.000	-0.76	99.66 %	0.13 %	0.00 %	0.21 %	
1.200	-0.56	99.46 %	0.20 %	0.00 %	0.34 %	Stomach pH
2.000	0.24	96.70 %	1.25 %	0.00 %	2.06 %	
3.000	1.19	74.55 %	9.60 %	0.00 %	15.84 %	
4.000	1.88	22.66 %	29.19 %	0.00 %	48.16 %	
5.000	2.10	2.85 %	36.66 %	0.00 %	60.49 %	
6.000	2.13	0.29 %	37.63 %	0.00 %	62.08 %	
6.500	2.13	0.09 %	37.70 %	0.00 %	62.20 %	
7.000	2.13	0.03 %	37.73 %	0.00 %	62.24 %	
7.400	2.13	0.01 %	37.73 %	0.00 %	62.25 %	Blood pH
8.000	2.13	0.00 %	37.74 %	0.00 %	62.26 %	
9.000	2.13	0.00 %	37.74 %	0.00 %	62.26 %	
10.000	2.13	0.00 %	37.74 %	0.00 %	62.26 %	
11.000	2.13	0.00 %	37.74 %	0.00 %	62.26 %	
12.000	2.13	0.00 %	37.74 %	0.00 %	62.26 %	

Carbonate and acidity

Carbonate   0.000 mM
Acidity error   0.030 mM

Other graphs

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
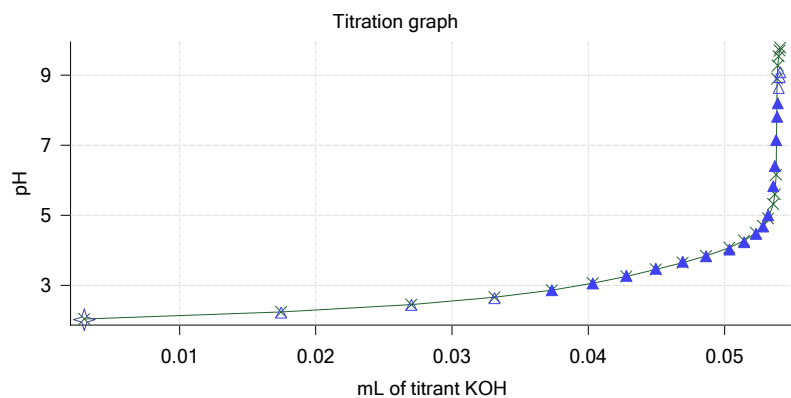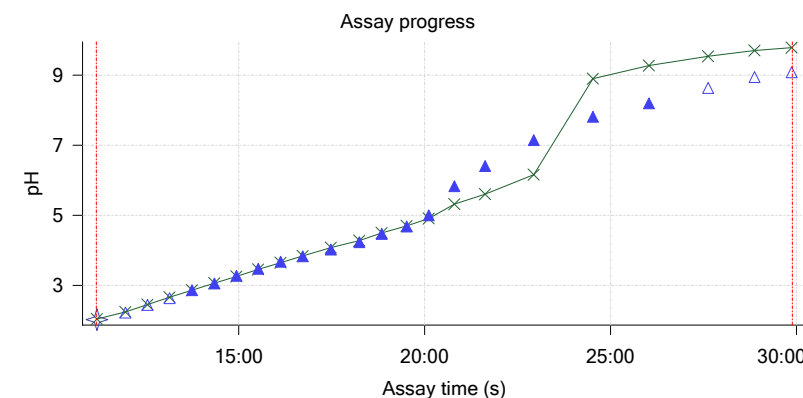Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
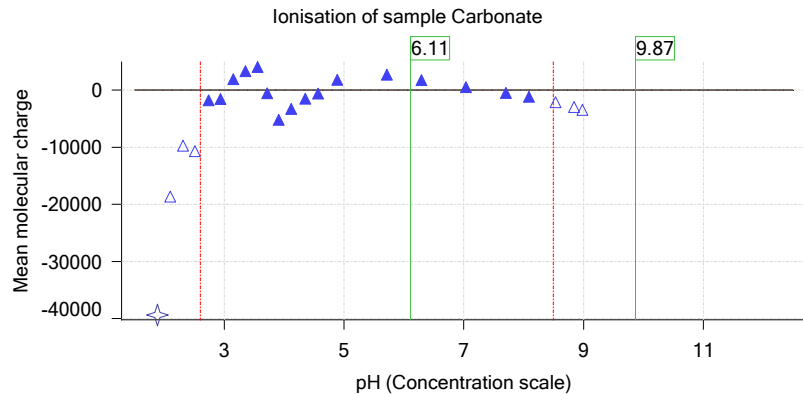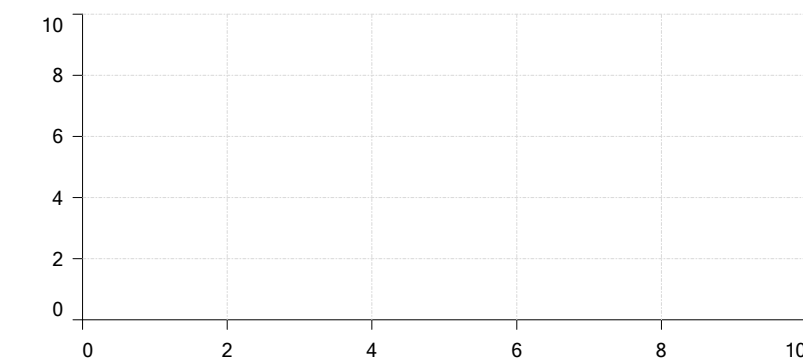
Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 2 of 3   18C-01001 Points 24 to 48

Overall results

RMSD   0.387
Average ionic strength   0.164 M
Average temperature   25.0°C
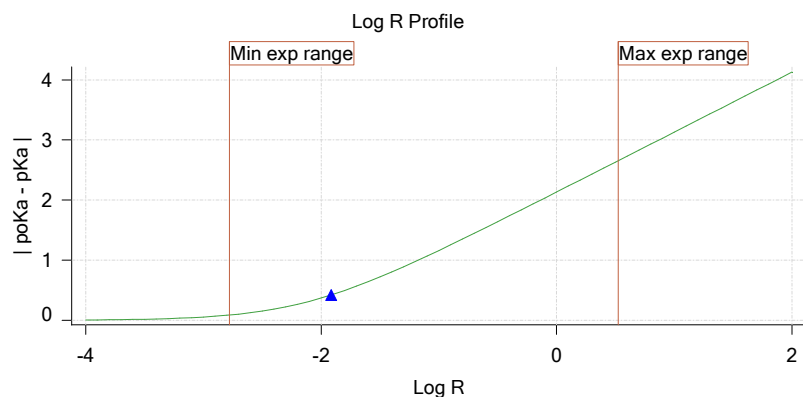Partition ratio   0.0404 : 1
Analyte concentration range   3480.1 µM to 3596.9 µM
Total points considered   18 of 25

Warnings and errors

Errors   None
Warnings   One or more logP values out of range

Four-Plus parameters

Alpha   0.130   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
S   0.9970   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
jH   0.8   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
jOH   -0.4   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r

Titrants

0.50 M HCl   0.993513   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH   0.999845   3/1/2018 12:11:22 AM   C:\Sirius_T3\KOH18B27.t3r

Sample

M11_octanol concentration factor   0.912
Base pKa 1   3.89
logP (XH +)   -4.46
logP (neutral X)   2.16

Sample graphs

Ionisation of sample M11_octanol

Distribution of species for sample M11_octanol
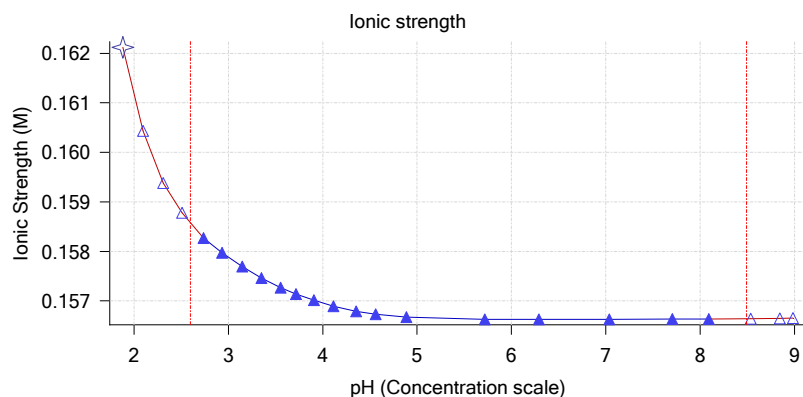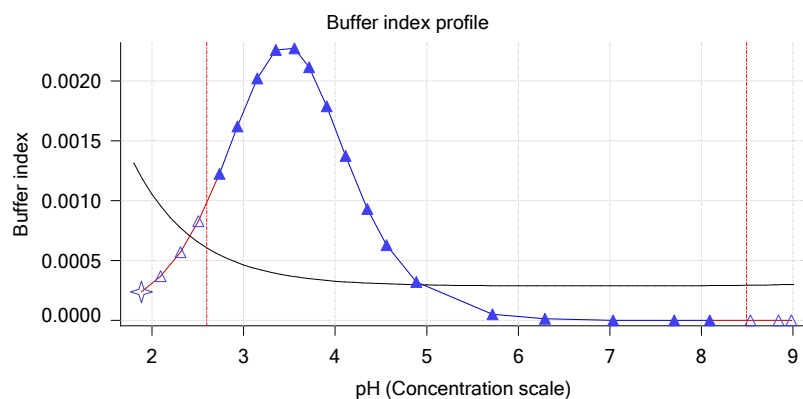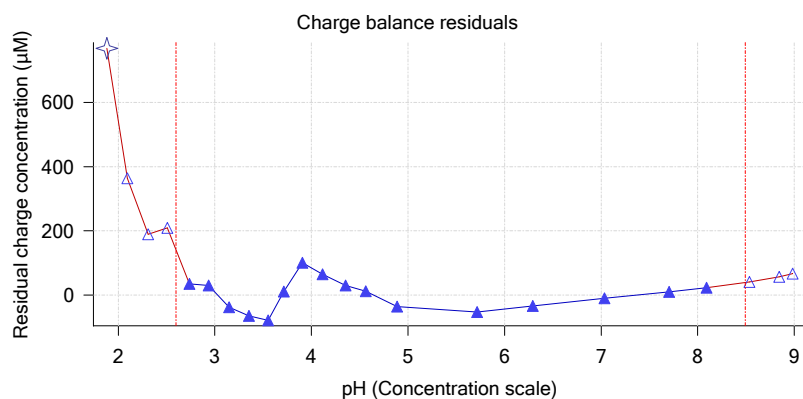
Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
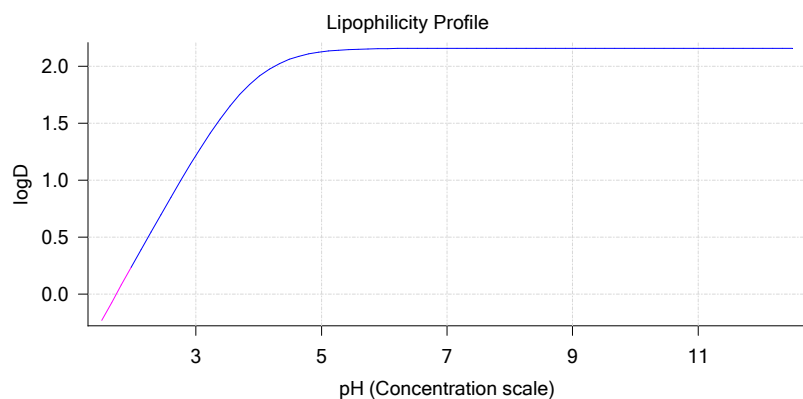
Sample logD and percent species

pH	M11_octanol logD	M11_octanol M11_octanolH	M11_octanol M11_octanol	M11_octanol M11_octanolH*	M11_octanol M11_octanol*	Comment
1.000	-0.73	99.13 %	0.13 %	0.00 %	0.74 %	
1.200	-0.53	98.62 %	0.20 %	0.00 %	1.17 %	Stomach pH
2.000	0.26	91.91 %	1.18 %	0.00 %	6.90 %	
3.000	1.22	53.20 %	6.85 %	0.00 %	39.94 %	
4.000	1.91	10.21 %	13.15 %	0.00 %	76.64 %	
5.000	2.13	1.12 %	14.48 %	0.00 %	84.40 %	
6.000	2.16	0.11 %	14.63 %	0.00 %	85.26 %	
6.500	2.16	0.04 %	14.64 %	0.00 %	85.32 %	
7.000	2.16	0.01 %	14.64 %	0.00 %	85.34 %	
7.400	2.16	0.00 %	14.64 %	0.00 %	85.35 %	Blood pH
8.000	2.16	0.00 %	14.65 %	0.00 %	85.35 %	
9.000	2.16	0.00 %	14.65 %	0.00 %	85.35 %	
10.000	2.16	0.00 %	14.65 %	0.00 %	85.35 %	
11.000	2.16	0.00 %	14.65 %	0.00 %	85.35 %	
12.000	2.16	0.00 %	14.65 %	0.00 %	85.35 %	

Carbonate and acidity

Carbonate 0.096 mM
Acidity error -0.306 mM

Other graphs

Assay progress

Titration graph

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
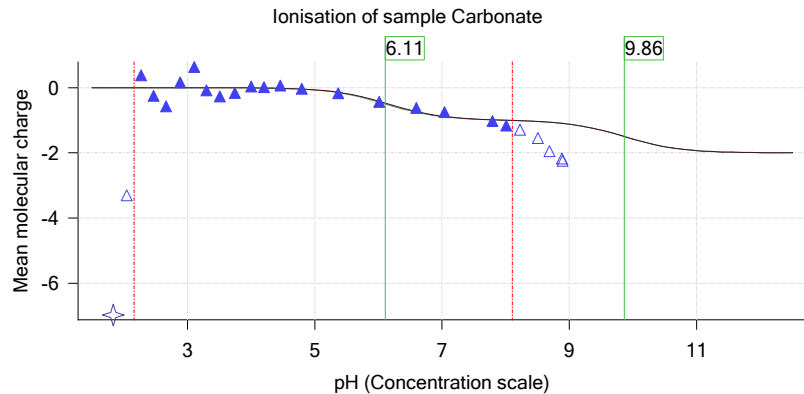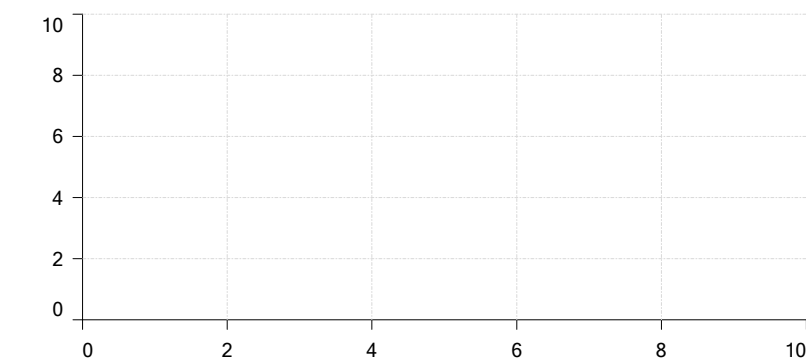
Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 3 of 3   18C-01001 Points 49 to 69

Overall results

RMSD   0.050
Average ionic strength   0.170 M
Average temperature   25.0°C
Partition ratio   0.1189 : 1
Analyte concentration range   3013.9 µM to 3107.7 µM
Total points considered   18 of 21

Warnings and errors

Errors   None
Warnings   One or more logP values out of range

Four-Plus parameters

Alpha   0.130   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
S   0.9970   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
jH   0.8   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
jOH   -0.4   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
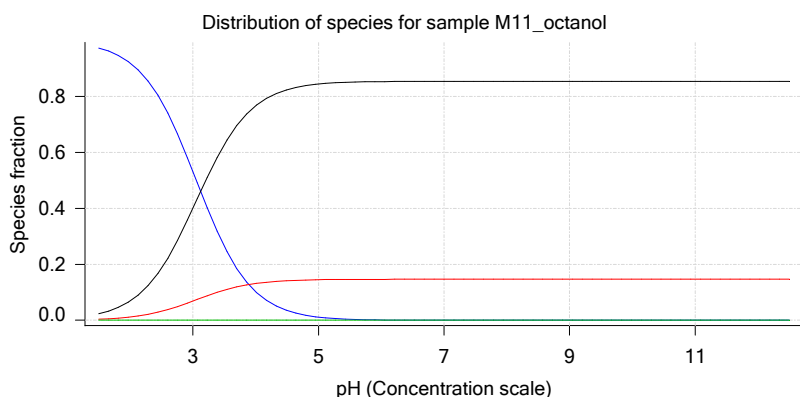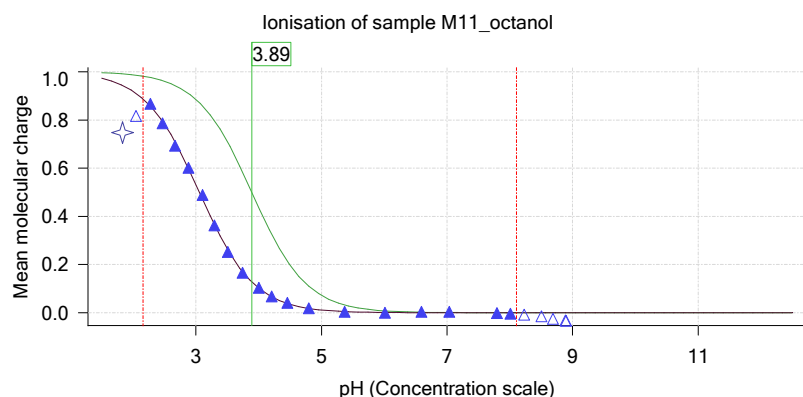
Titrants

0.50 M HCl   0.993513   3/1/2018 12:11:22 AM   C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH   0.999845   3/1/2018 12:11:22 AM   C:\Sirius_T3\KOH18B27.t3r

Sample

M11_octanol concentration factor   0.792
Base pKa 1   3.89
logP (XH +)   -5.10
logP (neutral X)   2.01

Sample graphs

Ionisation of sample M11_octanol

Distribution of species for sample M11_octanol

Sample name: **M11_octanol**   Experiment start time: **3/1/2018 12:11:22 AM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-01001**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Sample graphs (continued)

Lipophilicity Profile
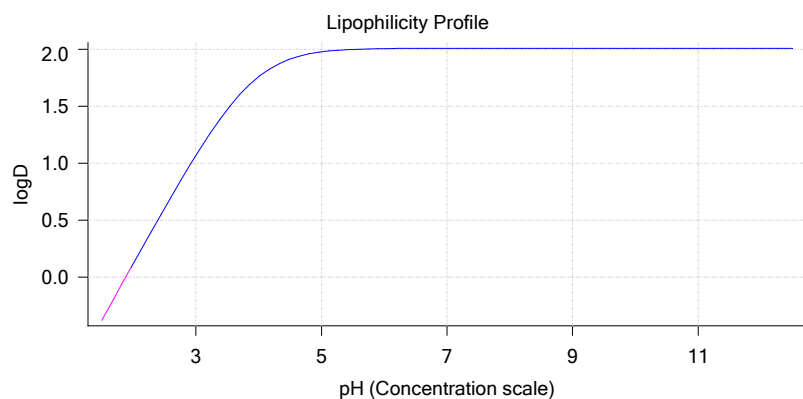
Sample logD and percent species

pH	M11_octanol logD	M11_octanol M11_octanolH	M11_octanol M11_octanol	M11_octanol M11_octanolH*	M11_octanol M11_octanol*	Comment
1.000	-0.88	98.33 %	0.13 %	0.00 %	1.54 %	
1.200	-0.68	97.38 %	0.20 %	0.00 %	2.42 %	Stomach pH
2.000	0.11	85.51 %	1.10 %	0.00 %	13.39 %	
3.000	1.07	37.11 %	4.78 %	0.00 %	58.11 %	
4.000	1.76	5.57 %	7.18 %	0.00 %	87.25 %	
5.000	1.98	0.59 %	7.56 %	0.00 %	91.86 %	
6.000	2.01	0.06 %	7.60 %	0.00 %	92.34 %	
6.500	2.01	0.02 %	7.60 %	0.00 %	92.38 %	
7.000	2.01	0.01 %	7.60 %	0.00 %	92.39 %	
7.400	2.01	0.00 %	7.60 %	0.00 %	92.40 %	Blood pH
8.000	2.01	0.00 %	7.60 %	0.00 %	92.40 %	
9.000	2.01	0.00 %	7.60 %	0.00 %	92.40 %	
10.000	2.01	0.00 %	7.60 %	0.00 %	92.40 %	
11.000	2.01	0.00 %	7.60 %	0.00 %	92.40 %	
12.000	2.01	0.00 %	7.60 %	0.00 %	92.40 %	

Carbonate and acidity

Carbonate   0.073 mM
Acidity error   -0.819 mM

Other graphs
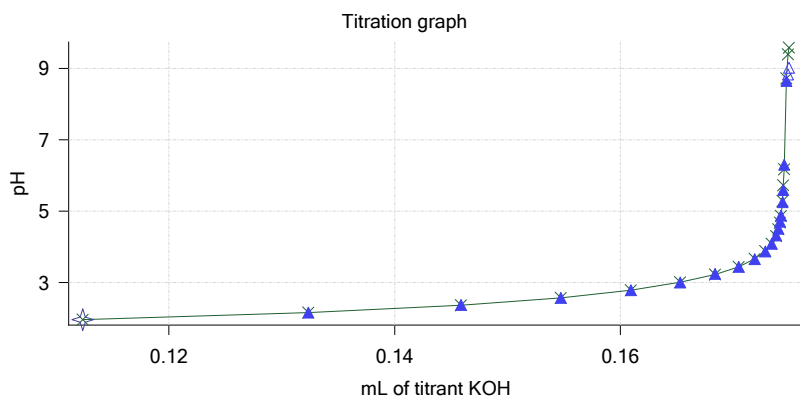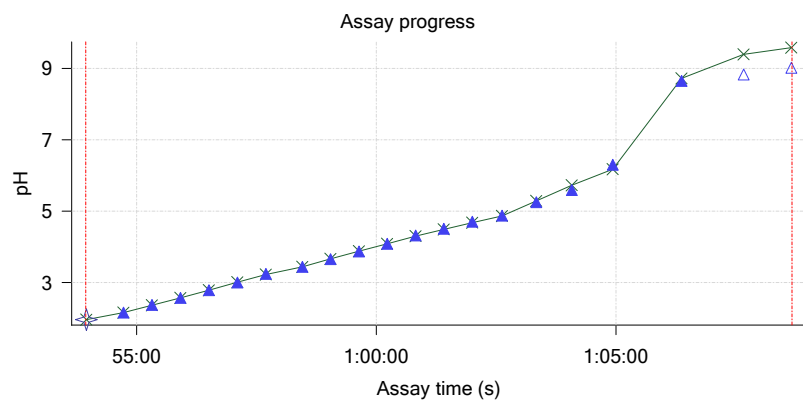
Assay progress

Titration graph

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
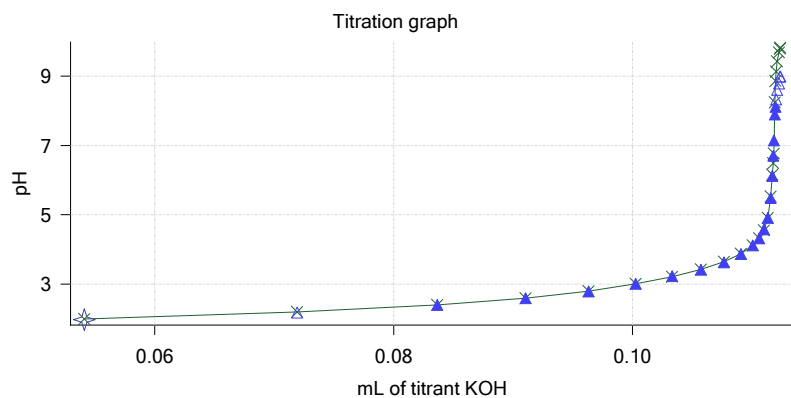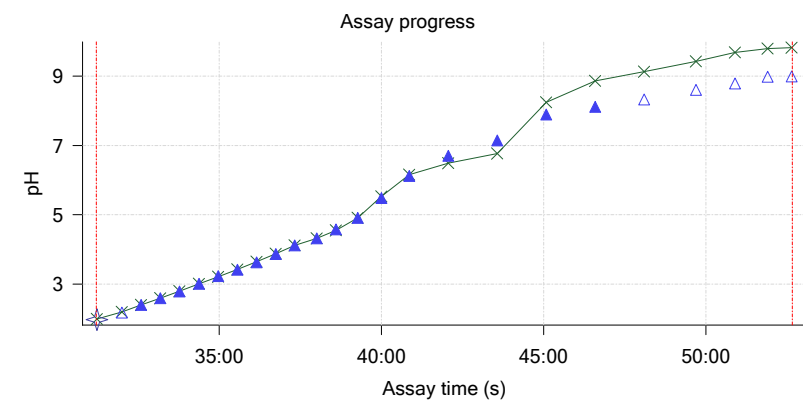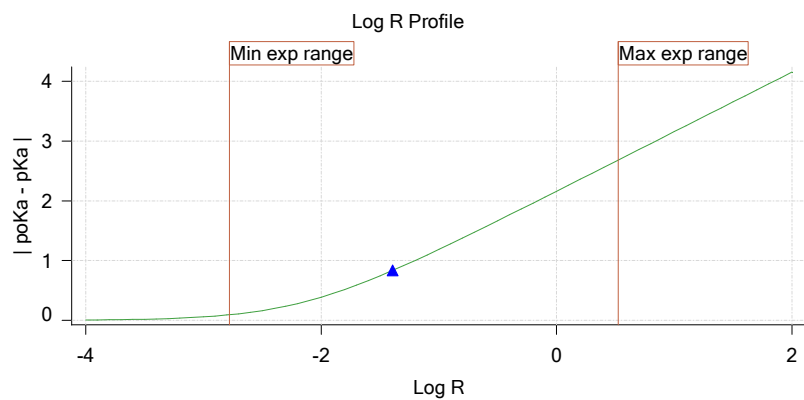Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
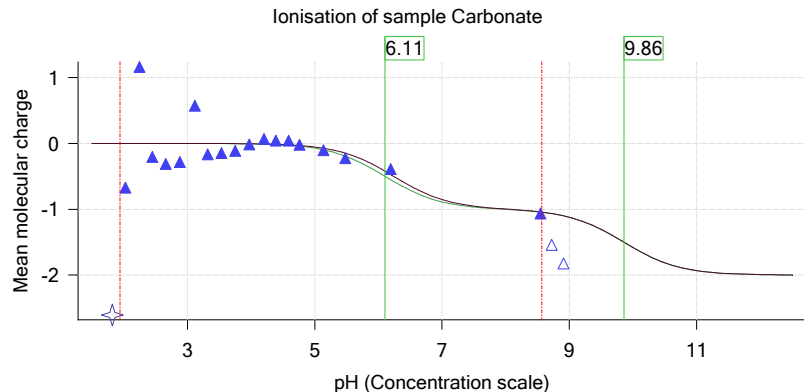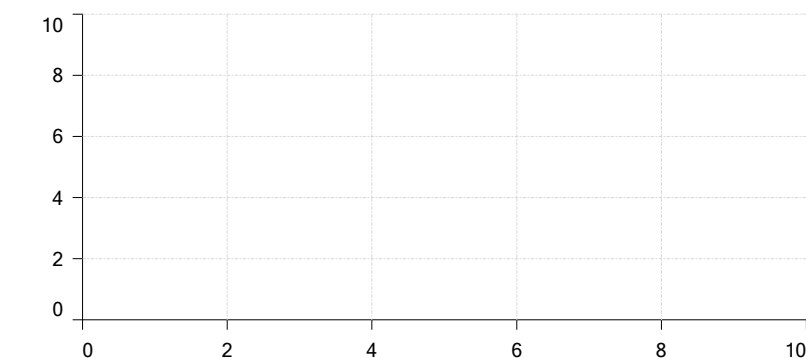
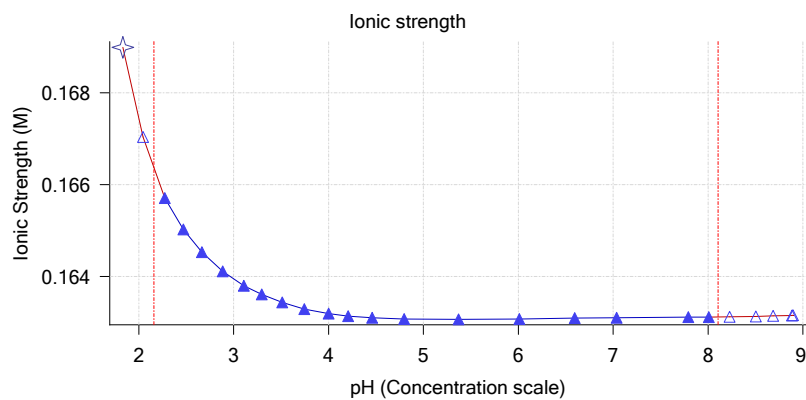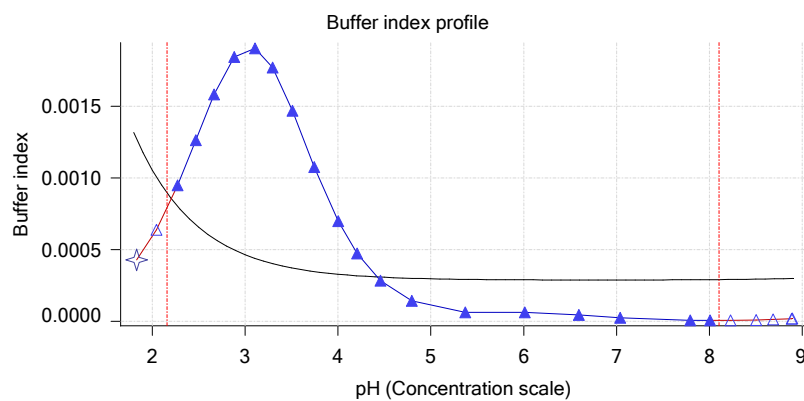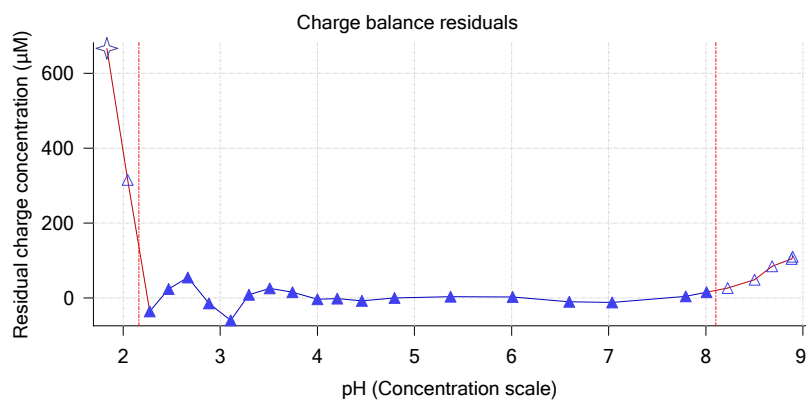Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M11_octanol	2/27/2018 4:54:30 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001320 g	2/28/2018 4:24:52 PM	User entered value
Formula weight	211.22 g/mol	2/27/2018 4:54:30 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	211.22	2/27/2018 4:54:30 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 4:54:30 PM	User entered value
Sample is a	Base	2/27/2018 4:54:30 PM	User entered value
pKa 1	3.89	2/27/2018 4:54:30 PM	User entered value
logp (XH +)	-5.60	2/28/2018 1:53:21 PM	User entered value
logP (neutral X)	2.09	2/28/2018 1:53:11 PM	User entered value

Events

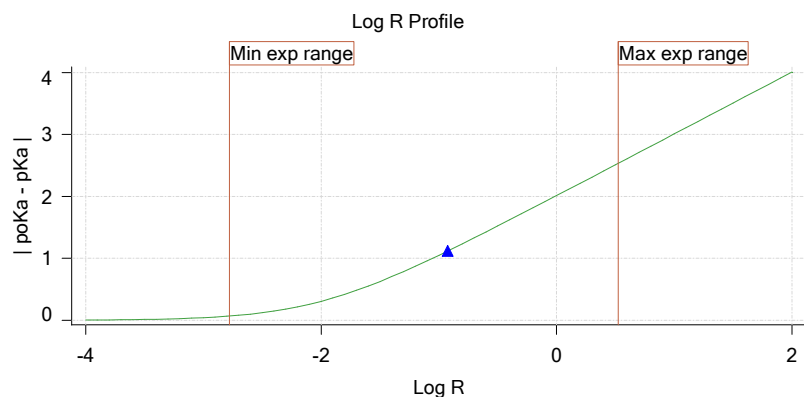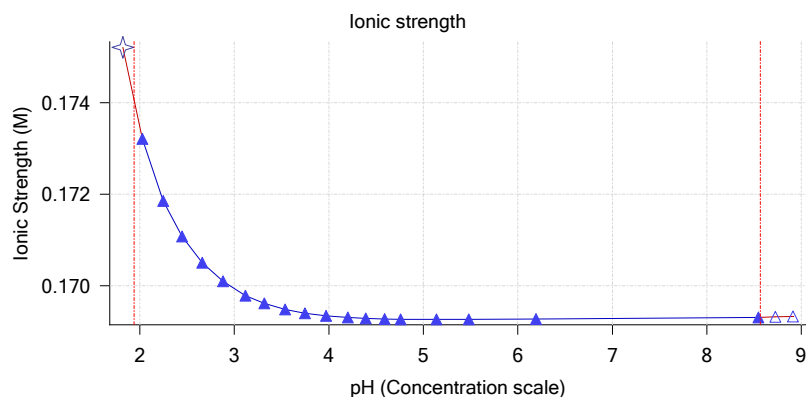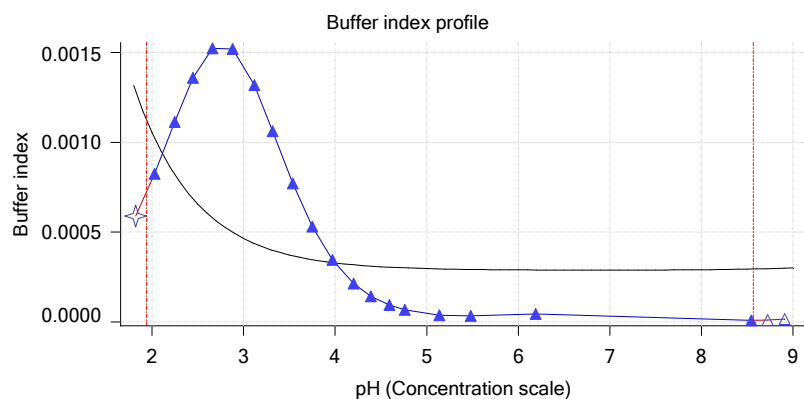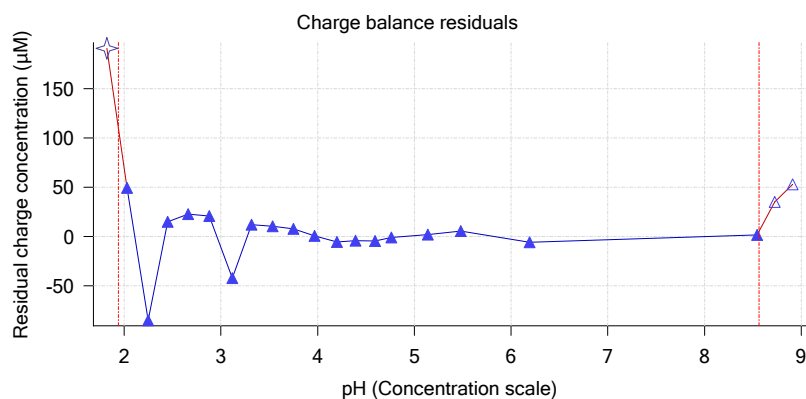| Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
8:11.4	Initial pH = 9.64									
11:11.0	Data point 1	1.50000 mL	0.05407 mL	0.00301 mL	0.01999 mL	2.018	-0.00907	0.79017	0.00050	10.0 s
11:57.2	Data point 2	1.50000 mL	0.05407 mL	0.01745 mL	0.01999 mL	2.225	-0.00501	0.21160	0.00054	10.0 s
12:32.9	Data point 3	1.50000 mL	0.05407 mL	0.02702 mL	0.01999 mL	2.438	-0.00560	0.18844	0.00064	10.0 s
13:08.5	Data point 4	1.50000 mL	0.05407 mL	0.03311 mL	0.01999 mL	2.633	-0.00265	0.48730	0.00019	10.5 s
13:44.5	Data point 5	1.50000 mL	0.05407 mL	0.03732 mL	0.01999 mL	2.860	-0.01106	0.66289	0.00067	10.5 s
14:20.5	Data point 6	1.50000 mL	0.05407 mL	0.04033 mL	0.01999 mL	3.057	-0.01232	0.47963	0.00088	10.0 s
14:56.0	Data point 7	1.50000 mL	0.05407 mL	0.04280 mL	0.01999 mL	3.270	-0.00677	0.19054	0.00077	10.5 s
15:31.5	Data point 8	1.50000 mL	0.05407 mL	0.04497 mL	0.01999 mL	3.472	-0.00166	0.35149	0.00014	10.5 s
16:07.5	Data point 9	1.50000 mL	0.05407 mL	0.04692 mL	0.01999 mL	3.673	-0.00781	0.35544	0.00065	10.0 s
16:42.9	Data point 10	1.50000 mL	0.05407 mL	0.04864 mL	0.01999 mL	3.835	-0.01388	0.51424	0.00096	10.0 s
17:28.7	Data point 11	1.50000 mL	0.05407 mL	0.05035 mL	0.01999 mL	4.027	-0.01025	0.38200	0.00082	10.0 s
18:14.5	Data point 12	1.50000 mL	0.05407 mL	0.05143 mL	0.01999 mL	4.232	-0.00787	0.92490	0.00040	10.5 s
18:50.5	Data point 13	1.50000 mL	0.05407 mL	0.05230 mL	0.01999 mL	4.470	-0.00601	0.45130	0.00044	10.0 s
19:31.0	Data point 14	1.50000 mL	0.05407 mL	0.05282 mL	0.01999 mL	4.679	-0.00976	0.57077	0.00064	10.0 s
20:06.4	Data point 15	1.50000 mL	0.05407 mL	0.05320 mL	0.01999 mL	5.003	-0.01866	0.86396	0.00099	11.0 s
20:48.0	Data point 16	1.50000 mL	0.05407 mL	0.05357 mL	0.01999 mL	5.829	-0.01903	0.91633	0.00098	19.0 s
21:37.5	Data point 17	1.50000 mL	0.05407 mL	0.05369 mL	0.01999 mL	6.403	-0.02005	0.98528	0.00100	42.5 s
22:55.8	Data point 18	1.50000 mL	0.05407 mL	0.05379 mL	0.01999 mL	7.144	-0.04872	0.99706	0.00241	Timed out at 59.5 s
24:31.4	Data point 19	1.50000 mL	0.05407 mL	0.05386 mL	0.01999 mL	7.810	-0.04860	0.99788	0.00240	Timed out at 59.5 s
26:01.9	Data point 20	1.50000 mL	0.05407 mL	0.05390 mL	0.01999 mL	8.196	-0.02409	0.99122	0.00119	Timed out at 59.5 s
27:37.5	Data point 21	1.50000 mL	0.05407 mL	0.05397 mL	0.01999 mL	8.638	-0.02003	0.99205	0.00099	39.0 s
28:52.2	Data point 22	1.50000 mL	0.05407 mL	0.05405 mL	0.01999 mL	8.945	-0.02002	0.98473	0.00100	29.5 s
29:52.2	Data point 23	1.50000 mL	0.05407 mL	0.05409 mL	0.01999 mL	9.084	-0.01992	0.97892	0.00099	22.5 s
31:14.1	Data point 24	1.50000 mL	0.11336 mL	0.05409 mL	0.06999 mL	1.969	-0.01287	0.76123	0.00073	10.0 s
32:00.4	Data point 25	1.50000 mL	0.11336 mL	0.07192 mL	0.06999 mL	2.176	-0.00432	0.09399	0.00070	10.0 s
32:36.1	Data point 26	1.50000 mL	0.11336 mL	0.08365 mL	0.06999 mL	2.402	0.00539	0.49157	0.00038	10.0 s
33:11.7	Data point 27	1.50000 mL	0.11336 mL	0.09104 mL	0.06999 mL	2.594	-0.00764	0.16492	0.00093	10.0 s
33:47.2	Data point 28	1.50000 mL	0.11336 mL	0.09631 mL	0.06999 mL	2.790	-0.00104	0.07057	0.00019	10.0 s
34:22.7	Data point 29	1.50000 mL	0.11336 mL	0.10026 mL	0.06999 mL	3.007	-0.00433	0.31139	0.00038	10.0 s
34:58.2	Data point 30	1.50000 mL	0.11336 mL	0.10332 mL	0.06999 mL	3.227	-0.00212	0.02826	0.00062	10.0 s
35:33.8	Data point 31	1.50000 mL	0.11336 mL	0.10572 mL	0.06999 mL	3.417	0.00173	0.09499	0.00028	10.0 s
36:09.3	Data point 32	1.50000 mL	0.11336 mL	0.10764 mL	0.06999 mL	3.630	-0.00346	0.60333	0.00022	10.0 s
36:44.7	Data point 33	1.50000 mL	0.11336 mL	0.10908 mL	0.06999 mL	3.864	-0.00645	0.48290	0.00046	10.0 s
37:20.1	Data point 34	1.50000 mL	0.11336 mL	0.11007 mL	0.06999 mL	4.119	-0.00379	0.54985	0.00025	10.0 s
38:00.7	Data point 35	1.50000 mL	0.11336 mL	0.11061 mL	0.06999 mL	4.322	-0.00366	0.30464	0.00033	10.0 s
38:36.1	Data point 36	1.50000 mL	0.11336 mL	0.11101 mL	0.06999 mL	4.575	-0.01448	0.78873	0.00080	10.0 s
39:16.6	Data point 37	1.50000 mL	0.11336 mL	0.11134 mL	0.06999 mL	4.912	-0.01854	0.87629	0.00098	13.0 s

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
40:00.2	Data point 38	1.50000 mL	0.11336 mL	0.11157 mL	0.06999 mL	5.485	-0.01247	0.47642	0.00089	16.0 s
40:51.8	Data point 39	1.50000 mL	0.11336 mL	0.11171 mL	0.06999 mL	6.124	-0.01978	0.97231	0.00099	36.5 s
42:04.0	Data point 40	1.50000 mL	0.11336 mL	0.11178 mL	0.06999 mL	6.704	-0.02890	0.99478	0.00143	Timed out at 59.5 s
43:34.5	Data point 41	1.50000 mL	0.11336 mL	0.11183 mL	0.06999 mL	7.146	-0.04871	0.99489	0.00241	Timed out at 59.5 s
45:05.1	Data point 42	1.50000 mL	0.11336 mL	0.11192 mL	0.06999 mL	7.900	-0.05502	0.99571	0.00272	Timed out at 59.5 s
46:35.6	Data point 43	1.50000 mL	0.11336 mL	0.11197 mL	0.06999 mL	8.113	-0.02606	0.99186	0.00129	Timed out at 59.5 s
48:06.1	Data point 44	1.50000 mL	0.11336 mL	0.11202 mL	0.06999 mL	8.331	-0.01989	0.98982	0.00099	55.0 s
49:41.9	Data point 45	1.50000 mL	0.11336 mL	0.11211 mL	0.06999 mL	8.608	-0.01909	0.97284	0.00096	31.0 s
50:53.8	Data point 46	1.50000 mL	0.11336 mL	0.11225 mL	0.06999 mL	8.789	-0.01955	0.99182	0.00097	25.0 s
51:54.4	Data point 47	1.50000 mL	0.11336 mL	0.11235 mL	0.06999 mL	8.987	-0.01750	0.90247	0.00091	19.0 s
52:38.8	Data point 48	1.50000 mL	0.11336 mL	0.11237 mL	0.06999 mL	8.997	-0.01930	0.96484	0.00097	16.5 s
53:57.2	Data point 49	1.50000 mL	0.17855 mL	0.11237 mL	0.21999 mL	1.958	-0.00753	0.72606	0.00044	10.0 s
54:43.6	Data point 50	1.50000 mL	0.17855 mL	0.13236 mL	0.21999 mL	2.160	-0.00028	0.00344	0.00023	10.0 s
55:19.4	Data point 51	1.50000 mL	0.17855 mL	0.14588 mL	0.21999 mL	2.375	0.00030	0.00453	0.00022	10.0 s
55:55.0	Data point 52	1.50000 mL	0.17855 mL	0.15473 mL	0.21999 mL	2.574	-0.00751	0.16614	0.00091	10.0 s
56:30.6	Data point 53	1.50000 mL	0.17855 mL	0.16091 mL	0.21999 mL	2.786	-0.00360	0.47623	0.00026	10.0 s
57:06.1	Data point 54	1.50000 mL	0.17855 mL	0.16529 mL	0.21999 mL	3.003	0.00336	0.12158	0.00048	10.0 s
57:41.6	Data point 55	1.50000 mL	0.17855 mL	0.16837 mL	0.21999 mL	3.241	-0.01332	0.90714	0.00069	10.0 s
58:27.4	Data point 56	1.50000 mL	0.17855 mL	0.17046 mL	0.21999 mL	3.438	-0.00073	0.01099	0.00034	10.0 s
59:02.8	Data point 57	1.50000 mL	0.17855 mL	0.17190 mL	0.21999 mL	3.656	-0.00412	0.83143	0.00022	10.0 s
59:38.3	Data point 58	1.50000 mL	0.17855 mL	0.17281 mL	0.21999 mL	3.868	-0.00343	0.75983	0.00019	10.0 s
1:00:13.7	Data point 59	1.50000 mL	0.17855 mL	0.17340 mL	0.21999 mL	4.088	-0.00449	0.80203	0.00025	10.0 s
1:00:49.1	Data point 60	1.50000 mL	0.17855 mL	0.17378 mL	0.21999 mL	4.318	-0.00344	0.13702	0.00046	10.0 s
1:01:24.5	Data point 61	1.50000 mL	0.17855 mL	0.17399 mL	0.21999 mL	4.508	-0.01637	0.76668	0.00092	10.0 s
1:01:59.9	Data point 62	1.50000 mL	0.17855 mL	0.17413 mL	0.21999 mL	4.709	-0.01145	0.54777	0.00076	12.0 s
1:02:37.3	Data point 63	1.50000 mL	0.17855 mL	0.17422 mL	0.21999 mL	4.876	-0.00617	0.20813	0.00067	12.5 s
1:03:20.3	Data point 64	1.50000 mL	0.17855 mL	0.17434 mL	0.21999 mL	5.253	-0.01491	0.67066	0.00090	14.0 s
1:04:04.7	Data point 65	1.50000 mL	0.17855 mL	0.17441 mL	0.21999 mL	5.593	-0.01977	0.97774	0.00099	20.5 s
1:04:55.7	Data point 66	1.50000 mL	0.17855 mL	0.17448 mL	0.21999 mL	6.302	-0.01947	0.98219	0.00097	55.5 s
1:06:21.7	Data point 67	1.50000 mL	0.17855 mL	0.17469 mL	0.21999 mL	8.648	-0.01798	0.88440	0.00094	37.0 s
1:07:39.6	Data point 68	1.50000 mL	0.17855 mL	0.17483 mL	0.21999 mL	8.828	-0.01767	0.82826	0.00096	24.0 s
1:08:39.2	Data point 69	1.50000 mL	0.17855 mL	0.17493 mL	0.21999 mL	9.013	-0.01774	0.89128	0.00093	16.0 s
1:09:04.2	Assay volumes	1.50000 mL	0.17855 mL	0.17493 mL	0.21999 mL					

Sample name: **M11_octanol**   Experiment start time: **3/1/2018 12:11:22 AM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-01001**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

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	9.000			
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	0.020 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	0.050 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: **M11_octanol**
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Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

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	0.150 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 12:11:22 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	3/1/2018 12:11:22 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	3/1/2018 12:11:22 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	3/1/2018 12:11:22 AM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	3/1/2018 12:11:22 AM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	3/1/2018 12:11:22 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: **M11_octanol**   Experiment start time: **3/1/2018 12:11:22 AM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-01001**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_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	+3.86 mV		3/1/2018 12:11:50 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	8.5e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	6.9e+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: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 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

[1:49] Air gap created for Water (0.15 M KCl)
[1:49] Air gap created for Acid (0.5 M HCl)
[1:50] Air gap created for Base (0.5 M KOH)
[1:50] Air gap released for Water (0.15 M KCl)
[1:54] Titrator arm moved over Titration position
[1:54] Titration 1 of 3
[1:54] Adding initial titrants
[1:54] Automatically add 1.50000 mL of water
[2:19] Dispensed 1.500000 mL of Water (0.15 M KCl)
[2:23] Titrator arm moved over Drain
[8:05] Titrator arm moved to Titration position
[8:05] Argon flow rate set to 100
[8:05] Stirrer speed set to 10
[8:10] Automatically add 0.02000 mL of Octanol
[8:10] Dispensed 0.019991 mL of Octanol
[8:11] Initial pH = 9.64
[8:11] Iterative adjust 9.64 -> 2.00
[8:11] pH 9.64 -> 2.00
[8:13] Air gap released for Acid (0.5 M HCl)
[8:14] Dispensed 0.054069 mL of Acid (0.5 M HCl)
[8:19] Holding pH 2.00
[10:19] Stirrer speed set to 0
[10:19] Stirrer speed set to 50
[10:19] Iterative adjust 1.97 -> 2.00
[10:19] pH 1.97 -> 2.00
[10:20] Air gap released for Base (0.5 M KOH)
[10:21] Dispensed 0.003010 mL of Base (0.5 M KOH)
[11:11] Stirrer speed set to 0
[11:21] Datapoint id 1 collected
[11:21] Stirrer speed set to 50
[11:26] pH 2.02 -> 2.22
[11:26] Using cautious pH adjust
[11:26] Dispensed 0.007643 mL of Base (0.5 M KOH)
[11:32] Stepping pH = 2.11
[11:32] Dispensed 0.005833 mL of Base (0.5 M KOH)
[11:37] Stepping pH = 2.20
[11:37] Dispensed 0.000964 mL of Base (0.5 M KOH)
[11:42] Stepping pH = 2.22
[11:57] Stirrer speed set to 0
[12:07] Datapoint id 2 collected
[12:07] Charge balance equation is out by 5.6%
[12:07] Stirrer speed set to 50

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[12:12] pH 2.23 -> 2.43
[12:12] Using charge balance adjust
[12:13] Dispensed 0.009572 mL of Base (0.5 M KOH)
[12:33] Stirrer speed set to 0
[12:43] Datapoint id 3 collected
[12:43] Charge balance equation is out by 3.5%
[12:43] Stirrer speed set to 50
[12:48] pH 2.44 -> 2.64
[12:48] Using charge balance adjust
[12:48] Dispensed 0.006091 mL of Base (0.5 M KOH)
[13:09] Stirrer speed set to 0
[13:19] Datapoint id 4 collected
[13:19] Charge balance equation is out by -5.3%
[13:19] Stirrer speed set to 50
[13:24] pH 2.64 -> 2.84
[13:24] Using charge balance adjust
[13:24] Dispensed 0.004210 mL of Base (0.5 M KOH)
[13:45] Stirrer speed set to 0
[13:55] Datapoint id 5 collected
[13:55] Charge balance equation is out by 10.7%
[13:55] Stirrer speed set to 50
[14:00] pH 2.87 -> 3.07
[14:00] Using charge balance adjust
[14:00] Dispensed 0.003010 mL of Base (0.5 M KOH)
[14:21] Stirrer speed set to 0
[14:31] Datapoint id 6 collected
[14:31] Charge balance equation is out by -4.5%
[14:31] Stirrer speed set to 50
[14:36] pH 3.06 -> 3.26
[14:36] Using charge balance adjust
[14:36] Dispensed 0.002469 mL of Base (0.5 M KOH)
[14:56] Stirrer speed set to 0
[15:06] Datapoint id 7 collected
[15:06] Charge balance equation is out by 4.2%
[15:06] Stirrer speed set to 50
[15:11] pH 3.27 -> 3.47
[15:11] Using charge balance adjust
[15:11] Dispensed 0.002164 mL of Base (0.5 M KOH)
[15:32] Stirrer speed set to 0
[15:42] Datapoint id 8 collected
[15:42] Charge balance equation is out by 0.1%
[15:42] Stirrer speed set to 50
[15:47] pH 3.48 -> 3.68
[15:47] Using charge balance adjust
[15:47] Dispensed 0.001952 mL of Base (0.5 M KOH)
[16:07] Stirrer speed set to 0
[16:18] Datapoint id 9 collected
[16:18] Charge balance equation is out by -1.5%
[16:18] Stirrer speed set to 50
[16:23] pH 3.67 -> 3.87
[16:23] Using charge balance adjust
[16:23] Dispensed 0.001717 mL of Base (0.5 M KOH)
[16:43] Stirrer speed set to 0
[16:53] Datapoint id 10 collected
[16:53] Charge balance equation is out by -16.9%
[16:53] Stirrer speed set to 50
[16:58] pH 3.84 -> 4.04
[16:58] Using cautious pH adjust
[16:58] Dispensed 0.000729 mL of Base (0.5 M KOH)

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[17:03] Stepping pH = 3.91
[17:03] Dispensed 0.000823 mL of Base (0.5 M KOH)
[17:08] Stepping pH = 4.01
[17:09] Dispensed 0.000165 mL of Base (0.5 M KOH)
[17:14] Stepping pH = 4.04
[17:29] Stirrer speed set to 0
[17:39] Datapoint id 11 collected
[17:39] Charge balance equation is out by -17.2%
[17:39] Stirrer speed set to 50
[17:44] pH 4.03 -> 4.23
[17:44] Using cautious pH adjust
[17:44] Dispensed 0.000588 mL of Base (0.5 M KOH)
[17:49] Stepping pH = 4.12
[17:49] Dispensed 0.000447 mL of Base (0.5 M KOH)
[17:54] Stepping pH = 4.22
[17:54] Dispensed 0.000047 mL of Base (0.5 M KOH)
[17:59] Stepping pH = 4.24
[18:14] Stirrer speed set to 0
[18:25] Datapoint id 12 collected
[18:25] Charge balance equation is out by 7.9%
[18:25] Stirrer speed set to 50
[18:30] pH 4.24 -> 4.44
[18:30] Using charge balance adjust
[18:30] Dispensed 0.000870 mL of Base (0.5 M KOH)
[18:50] Stirrer speed set to 0
[19:01] Datapoint id 13 collected
[19:01] Charge balance equation is out by 17.3%
[19:01] Stirrer speed set to 50
[19:06] pH 4.47 -> 4.67
[19:06] Using cautious pH adjust
[19:06] Dispensed 0.000282 mL of Base (0.5 M KOH)
[19:11] Stepping pH = 4.56
[19:11] Dispensed 0.000235 mL of Base (0.5 M KOH)
[19:16] Stepping pH = 4.67
[19:31] Stirrer speed set to 0
[19:41] Datapoint id 14 collected
[19:41] Charge balance equation is out by 9.3%
[19:41] Stirrer speed set to 50
[19:46] pH 4.69 -> 4.89
[19:46] Using charge balance adjust
[19:46] Dispensed 0.000376 mL of Base (0.5 M KOH)
[20:06] Stirrer speed set to 0
[20:17] Datapoint id 15 collected
[20:17] Charge balance equation is out by 58.7%
[20:17] Stirrer speed set to 50
[20:23] pH 5.01 -> 5.21
[20:23] Using cautious pH adjust
[20:23] Dispensed 0.000094 mL of Base (0.5 M KOH)
[20:28] Stepping pH = 5.02
[20:28] Dispensed 0.000282 mL of Base (0.5 M KOH)
[20:33] Stepping pH = 5.74
[20:48] Stirrer speed set to 0
[21:07] Datapoint id 16 collected
[21:07] Charge balance equation is out by -91.3%
[21:07] Stirrer speed set to 50
[21:12] pH 5.85 -> 6.05
[21:12] Using cautious pH adjust
[21:12] Dispensed 0.000024 mL of Base (0.5 M KOH)
[21:17] Stepping pH = 5.87

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[21:17] Dispensed 0.000094 mL of Base (0.5 M KOH)
[21:22] Stepping pH = 6.25
[21:38] Stirrer speed set to 0
[22:20] Datapoint id 17 collected
[22:20] Charge balance equation is out by -85.8%
[22:20] Stirrer speed set to 50
[22:25] pH 6.40 -> 6.60
[22:25] Using cautious pH adjust
[22:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[22:30] Stepping pH = 6.43
[22:30] Dispensed 0.000047 mL of Base (0.5 M KOH)
[22:36] Stepping pH = 6.55
[22:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[22:41] Stepping pH = 6.90
[22:56] Stirrer speed set to 0
[23:56] Datapoint id 18 collected
[23:56] Charge balance equation is out by -113.3%
[23:56] Stirrer speed set to 50
[24:01] pH 7.16 -> 7.36
[24:01] Using cautious pH adjust
[24:01] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:06] Stepping pH = 7.21
[24:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:11] Stepping pH = 7.34
[24:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:16] Stepping pH = 7.64
[24:31] Stirrer speed set to 0
[25:31] Datapoint id 19 collected
[25:31] Charge balance equation is out by -330.3%
[25:31] Stirrer speed set to 50
[25:37] pH 7.74 -> 7.94
[25:37] Using cautious pH adjust
[25:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[25:42] Stepping pH = 7.80
[25:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[25:47] Stepping pH = 8.00
[26:02] Stirrer speed set to 0
[27:02] Datapoint id 20 collected
[27:02] Charge balance equation is out by -530.4%
[27:02] Stirrer speed set to 50
[27:07] pH 8.20 -> 8.40
[27:07] Using cautious pH adjust
[27:07] Dispensed 0.000024 mL of Base (0.5 M KOH)
[27:12] Stepping pH = 8.24
[27:12] Dispensed 0.000024 mL of Base (0.5 M KOH)
[27:17] Stepping pH = 8.38
[27:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[27:22] Stepping pH = 8.62
[27:38] Stirrer speed set to 0
[28:17] Datapoint id 21 collected
[28:17] Charge balance equation is out by -617.9%
[28:17] Stirrer speed set to 50
[28:22] pH 8.66 -> 8.86
[28:22] Using cautious pH adjust
[28:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[28:27] Stepping pH = 8.68
[28:27] Dispensed 0.000024 mL of Base (0.5 M KOH)
[28:32] Stepping pH = 8.76
[28:32] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M11_octanol** Experiment start time: **3/1/2018 12:11:22 AM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-01001** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[28:37] Stepping pH = 8.92
[28:52] Stirrer speed set to 0
[29:22] Datapoint id 22 collected
[29:22] Charge balance equation is out by -250.7%
[29:22] Stirrer speed set to 50
[29:27] pH 8.95 -> 9.05
[29:27] Using cautious pH adjust
[29:27] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:32] Stepping pH = 8.95
[29:32] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:37] Stepping pH = 9.06
[29:52] Stirrer speed set to 0
[30:15] Datapoint id 23 collected
[30:15] Charge balance equation is out by -155.3%
[30:15] Titration 2 of 3
[30:15] Adding initial titrants
[30:15] Automatically add 0.05000 mL of Octanol
[30:16] Dispensed 0.050000 mL of Octanol
[30:16] Stirrer speed set to 10
[30:17] Stirrer speed set to 55
[30:17] Iterative adjust 9.09 -> 2.00
[30:17] pH 9.09 -> 2.00
[30:19] Dispensed 0.056421 mL of Acid (0.5 M HCl)
[30:24] pH 2.03 -> 2.00
[30:24] Dispensed 0.002869 mL of Acid (0.5 M HCl)
[31:14] Stirrer speed set to 0
[31:24] Datapoint id 24 collected
[31:24] Stirrer speed set to 55
[31:29] pH 1.97 -> 2.17
[31:29] Using cautious pH adjust
[31:30] Dispensed 0.009313 mL of Base (0.5 M KOH)
[31:35] Stepping pH = 2.07
[31:35] Dispensed 0.006303 mL of Base (0.5 M KOH)
[31:40] Stepping pH = 2.14
[31:40] Dispensed 0.002211 mL of Base (0.5 M KOH)
[31:45] Stepping pH = 2.17
[32:00] Stirrer speed set to 0
[32:10] Datapoint id 25 collected
[32:10] Charge balance equation is out by 4.3%
[32:10] Stirrer speed set to 55
[32:16] pH 2.18 -> 2.38
[32:16] Using charge balance adjust
[32:16] Dispensed 0.011736 mL of Base (0.5 M KOH)
[32:36] Stirrer speed set to 0
[32:46] Datapoint id 26 collected
[32:46] Charge balance equation is out by 10.1%
[32:46] Stirrer speed set to 55
[32:51] pH 2.41 -> 2.61
[32:51] Using charge balance adjust
[32:52] Dispensed 0.007385 mL of Base (0.5 M KOH)
[33:12] Stirrer speed set to 0
[33:22] Datapoint id 27 collected
[33:22] Charge balance equation is out by -6.9%
[33:22] Stirrer speed set to 55
[33:27] pH 2.60 -> 2.80
[33:27] Using charge balance adjust
[33:27] Dispensed 0.005268 mL of Base (0.5 M KOH)
[33:47] Stirrer speed set to 0
[33:57] Datapoint id 28 collected

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[33:57] Charge balance equation is out by -4.7%
[33:57] Stirrer speed set to 55
[34:02] pH 2.80 -> 3.00
[34:02] Using charge balance adjust
[34:03] Dispensed 0.003951 mL of Base (0.5 M KOH)
[34:23] Stirrer speed set to 0
[34:33] Datapoint id 29 collected
[34:33] Charge balance equation is out by 5.7%
[34:33] Stirrer speed set to 55
[34:38] pH 3.01 -> 3.21
[34:38] Using charge balance adjust
[34:38] Dispensed 0.003057 mL of Base (0.5 M KOH)
[34:58] Stirrer speed set to 0
[35:08] Datapoint id 30 collected
[35:08] Charge balance equation is out by 7.6%
[35:08] Stirrer speed set to 55
[35:13] pH 3.23 -> 3.43
[35:13] Using charge balance adjust
[35:14] Dispensed 0.002399 mL of Base (0.5 M KOH)
[35:34] Stirrer speed set to 0
[35:44] Datapoint id 31 collected
[35:44] Charge balance equation is out by -7.7%
[35:44] Stirrer speed set to 55
[35:49] pH 3.42 -> 3.62
[35:49] Using charge balance adjust
[35:49] Dispensed 0.001929 mL of Base (0.5 M KOH)
[36:09] Stirrer speed set to 0
[36:19] Datapoint id 32 collected
[36:19] Charge balance equation is out by 4.5%
[36:19] Stirrer speed set to 55
[36:24] pH 3.63 -> 3.83
[36:24] Using charge balance adjust
[36:25] Dispensed 0.001435 mL of Base (0.5 M KOH)
[36:45] Stirrer speed set to 0
[36:55] Datapoint id 33 collected
[36:55] Charge balance equation is out by 14.8%
[36:55] Stirrer speed set to 55
[37:00] pH 3.87 -> 4.07
[37:00] Using charge balance adjust
[37:00] Dispensed 0.000988 mL of Base (0.5 M KOH)
[37:20] Stirrer speed set to 0
[37:30] Datapoint id 34 collected
[37:30] Charge balance equation is out by 25.2%
[37:30] Stirrer speed set to 55
[37:35] pH 4.13 -> 4.33
[37:35] Using cautious pH adjust
[37:35] Dispensed 0.000306 mL of Base (0.5 M KOH)
[37:40] Stepping pH = 4.21
[37:41] Dispensed 0.000235 mL of Base (0.5 M KOH)
[37:46] Stepping pH = 4.32
[38:01] Stirrer speed set to 0
[38:11] Datapoint id 35 collected
[38:11] Charge balance equation is out by 9.9%
[38:11] Stirrer speed set to 55
[38:16] pH 4.33 -> 4.53
[38:16] Using charge balance adjust
[38:16] Dispensed 0.000400 mL of Base (0.5 M KOH)
[38:36] Stirrer speed set to 0
[38:46] Datapoint id 36 collected

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[38:46] Charge balance equation is out by 23.7%
[38:46] Stirrer speed set to 55
[38:51] pH 4.58 -> 4.78
[38:51] Using cautious pH adjust
[38:51] Dispensed 0.000118 mL of Base (0.5 M KOH)
[38:56] Stepping pH = 4.62
[38:56] Dispensed 0.000212 mL of Base (0.5 M KOH)
[39:02] Stepping pH = 4.90
[39:17] Stirrer speed set to 0
[39:30] Datapoint id 37 collected
[39:30] Charge balance equation is out by -32.8%
[39:30] Stirrer speed set to 55
[39:35] pH 4.93 -> 5.13
[39:35] Using cautious pH adjust
[39:35] Dispensed 0.000071 mL of Base (0.5 M KOH)
[39:40] Stepping pH = 4.94
[39:40] Dispensed 0.000165 mL of Base (0.5 M KOH)
[39:45] Stepping pH = 5.45
[40:00] Stirrer speed set to 0
[40:16] Datapoint id 38 collected
[40:16] Charge balance equation is out by -85.1%
[40:16] Stirrer speed set to 55
[40:21] pH 5.53 -> 5.73
[40:21] Using cautious pH adjust
[40:21] Dispensed 0.000024 mL of Base (0.5 M KOH)
[40:26] Stepping pH = 5.56
[40:27] Dispensed 0.000047 mL of Base (0.5 M KOH)
[40:32] Stepping pH = 5.61
[40:32] Dispensed 0.000071 mL of Base (0.5 M KOH)
[40:37] Stepping pH = 6.14
[40:52] Stirrer speed set to 0
[41:28] Datapoint id 39 collected
[41:28] Charge balance equation is out by -212.4%
[41:28] Stirrer speed set to 55
[41:34] pH 6.23 -> 6.43
[41:34] Using cautious pH adjust
[41:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:39] Stepping pH = 6.29
[41:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:44] Stepping pH = 6.37
[41:44] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:49] Stepping pH = 6.60
[42:04] Stirrer speed set to 0
[43:04] Datapoint id 40 collected
[43:04] Charge balance equation is out by -59.8%
[43:04] Stirrer speed set to 55
[43:09] pH 6.71 -> 6.91
[43:09] Using cautious pH adjust
[43:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[43:14] Stepping pH = 6.85
[43:14] Dispensed 0.000024 mL of Base (0.5 M KOH)
[43:19] Stepping pH = 7.05
[43:35] Stirrer speed set to 0
[44:35] Datapoint id 41 collected
[44:35] Charge balance equation is out by -35.1%
[44:35] Stirrer speed set to 55
[44:40] pH 6.87 -> 7.07
[44:40] Using cautious pH adjust
[44:40] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[44:45] Stepping pH = 6.82
[44:45] Dispensed 0.000071 mL of Base (0.5 M KOH)
[44:50] Stepping pH = 7.44
[45:05] Stirrer speed set to 0
[46:05] Datapoint id 42 collected
[46:05] Charge balance equation is out by -316.2%
[46:05] Stirrer speed set to 55
[46:10] pH 7.84 -> 8.04
[46:10] Using cautious pH adjust
[46:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[46:15] Stepping pH = 7.89
[46:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[46:20] Stepping pH = 8.09
[46:36] Stirrer speed set to 0
[47:36] Datapoint id 43 collected
[47:36] Charge balance equation is out by -492.9%
[47:36] Stirrer speed set to 55
[47:41] pH 8.08 -> 8.28
[47:41] Using cautious pH adjust
[47:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[47:46] Stepping pH = 8.16
[47:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[47:51] Stepping pH = 8.30
[48:06] Stirrer speed set to 0
[49:01] Datapoint id 44 collected
[49:01] Charge balance equation is out by -412.6%
[49:01] Stirrer speed set to 55
[49:06] pH 8.32 -> 8.52
[49:06] Using cautious pH adjust
[49:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:11] Stepping pH = 8.36
[49:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:17] Stepping pH = 8.42
[49:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:22] Stepping pH = 8.50
[49:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:27] Stepping pH = 8.61
[49:42] Stirrer speed set to 0
[50:13] Datapoint id 45 collected
[50:13] Charge balance equation is out by -623.6%
[50:13] Stirrer speed set to 55
[50:18] pH 8.59 -> 8.79
[50:18] Using cautious pH adjust
[50:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[50:23] Stepping pH = 8.61
[50:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[50:28] Stepping pH = 8.66
[50:28] Dispensed 0.000047 mL of Base (0.5 M KOH)
[50:34] Stepping pH = 8.69
[50:34] Dispensed 0.000047 mL of Base (0.5 M KOH)
[50:39] Stepping pH = 8.79
[50:54] Stirrer speed set to 0
[51:19] Datapoint id 46 collected
[51:19] Charge balance equation is out by -667.4%
[51:19] Stirrer speed set to 55
[51:24] pH 8.78 -> 8.98
[51:24] Using cautious pH adjust
[51:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
[51:29] Stepping pH = 8.79

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[51:29] Dispensed 0.000047 mL of Base (0.5 M KOH)
[51:34] Stepping pH = 8.93
[51:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[51:39] Stepping pH = 9.00
[51:54] Stirrer speed set to 0
[52:14] Datapoint id 47 collected
[52:14] Charge balance equation is out by -185.9%
[52:14] Stirrer speed set to 55
[52:19] pH 8.99 -> 9.05
[52:19] Using cautious pH adjust
[52:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[52:24] Stepping pH = 9.00
[52:39] Stirrer speed set to 0
[52:55] Datapoint id 48 collected
[52:55] Charge balance equation is out by -80.3%
[52:55] Titration 3 of 3
[52:55] Adding initial titrants
[52:55] Automatically add 0.15000 mL of Octanol
[52:59] Dispensed 0.150000 mL of Octanol
[52:59] Stirrer speed set to 10
[53:00] Stirrer speed set to 60
[53:00] Iterative adjust 9.00 -> 2.00
[53:00] pH 9.00 -> 2.00
[53:02] Dispensed 0.058678 mL of Acid (0.5 M HCl)
[53:07] pH 2.06 -> 2.00
[53:07] Dispensed 0.006515 mL of Acid (0.5 M HCl)
[53:57] Stirrer speed set to 0
[54:07] Datapoint id 49 collected
[54:07] Stirrer speed set to 60
[54:12] pH 1.96 -> 2.16
[54:12] Using cautious pH adjust
[54:13] Dispensed 0.010466 mL of Base (0.5 M KOH)
[54:18] Stepping pH = 2.05
[54:18] Dispensed 0.007667 mL of Base (0.5 M KOH)
[54:23] Stepping pH = 2.13
[54:23] Dispensed 0.001858 mL of Base (0.5 M KOH)
[54:28] Stepping pH = 2.16
[54:44] Stirrer speed set to 0
[54:54] Datapoint id 50 collected
[54:54] Charge balance equation is out by 4.5%
[54:54] Stirrer speed set to 60
[54:59] pH 2.16 -> 2.36
[54:59] Using charge balance adjust
[54:59] Dispensed 0.013523 mL of Base (0.5 M KOH)
[55:19] Stirrer speed set to 0
[55:29] Datapoint id 51 collected
[55:29] Charge balance equation is out by 5.4%
[55:29] Stirrer speed set to 60
[55:35] pH 2.38 -> 2.58
[55:35] Using charge balance adjust
[55:35] Dispensed 0.008843 mL of Base (0.5 M KOH)
[55:55] Stirrer speed set to 0
[56:05] Datapoint id 52 collected
[56:05] Charge balance equation is out by -2.8%
[56:05] Stirrer speed set to 60
[56:10] pH 2.58 -> 2.78
[56:10] Using charge balance adjust
[56:10] Dispensed 0.006185 mL of Base (0.5 M KOH)
[56:31] Stirrer speed set to 0

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[56:41] Datapoint id 53 collected
[56:41] Charge balance equation is out by 2.9%
[56:41] Stirrer speed set to 60
[56:46] pH 2.79 -> 2.99
[56:46] Using charge balance adjust
[56:46] Dispensed 0.004374 mL of Base (0.5 M KOH)
[57:06] Stirrer speed set to 0
[57:16] Datapoint id 54 collected
[57:16] Charge balance equation is out by 5.5%
[57:16] Stirrer speed set to 60
[57:21] pH 3.01 -> 3.21
[57:21] Using charge balance adjust
[57:21] Dispensed 0.003081 mL of Base (0.5 M KOH)
[57:42] Stirrer speed set to 0
[57:52] Datapoint id 55 collected
[57:52] Charge balance equation is out by 17.6%
[57:52] Stirrer speed set to 60
[57:57] pH 3.25 -> 3.45
[57:57] Using cautious pH adjust
[57:57] Dispensed 0.001035 mL of Base (0.5 M KOH)
[58:02] Stepping pH = 3.33
[58:02] Dispensed 0.000823 mL of Base (0.5 M KOH)
[58:07] Stepping pH = 3.42
[58:07] Dispensed 0.000235 mL of Base (0.5 M KOH)
[58:12] Stepping pH = 3.44
[58:27] Stirrer speed set to 0
[58:37] Datapoint id 56 collected
[58:37] Charge balance equation is out by -2.1%
[58:37] Stirrer speed set to 60
[58:42] pH 3.44 -> 3.64
[58:42] Using charge balance adjust
[58:43] Dispensed 0.001435 mL of Base (0.5 M KOH)
[59:03] Stirrer speed set to 0
[59:13] Datapoint id 57 collected
[59:13] Charge balance equation is out by 5.6%
[59:13] Stirrer speed set to 60
[59:18] pH 3.66 -> 3.86
[59:18] Using charge balance adjust
[59:18] Dispensed 0.000917 mL of Base (0.5 M KOH)
[59:38] Stirrer speed set to 0
[59:48] Datapoint id 58 collected
[59:48] Charge balance equation is out by 2.8%
[59:48] Stirrer speed set to 60
[59:53] pH 3.88 -> 4.08
[59:53] Using charge balance adjust
[59:53] Dispensed 0.000588 mL of Base (0.5 M KOH)
[1:00:14] Stirrer speed set to 0
[1:00:24] Datapoint id 59 collected
[1:00:24] Charge balance equation is out by 5.7%
[1:00:24] Stirrer speed set to 60
[1:00:29] pH 4.09 -> 4.29
[1:00:29] Using charge balance adjust
[1:00:29] Dispensed 0.000376 mL of Base (0.5 M KOH)
[1:00:49] Stirrer speed set to 0
[1:00:59] Datapoint id 60 collected
[1:00:59] Charge balance equation is out by 11.7%
[1:00:59] Stirrer speed set to 60
[1:01:04] pH 4.33 -> 4.53
[1:01:04] Using charge balance adjust

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:01:04] Dispensed 0.000212 mL of Base (0.5 M KOH)
[1:01:24] Stirrer speed set to 0
[1:01:35] Datapoint id 61 collected
[1:01:35] Charge balance equation is out by -11.9%
[1:01:35] Stirrer speed set to 60
[1:01:40] pH 4.52 -> 4.72
[1:01:40] Using charge balance adjust
[1:01:40] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:02:00] Stirrer speed set to 0
[1:02:12] Datapoint id 62 collected
[1:02:12] Charge balance equation is out by -7.5%
[1:02:12] Stirrer speed set to 60
[1:02:17] pH 4.73 -> 4.93
[1:02:17] Using charge balance adjust
[1:02:17] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:02:37] Stirrer speed set to 0
[1:02:50] Datapoint id 63 collected
[1:02:50] Charge balance equation is out by -28.9%
[1:02:50] Stirrer speed set to 60
[1:02:55] pH 4.92 -> 5.12
[1:02:55] Using cautious pH adjust
[1:02:55] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:00] Stepping pH = 4.94
[1:03:00] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:03:05] Stepping pH = 5.24
[1:03:20] Stirrer speed set to 0
[1:03:34] Datapoint id 64 collected
[1:03:34] Charge balance equation is out by -82.8%
[1:03:34] Stirrer speed set to 60
[1:03:39] pH 5.35 -> 5.55
[1:03:39] Using cautious pH adjust
[1:03:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:44] Stepping pH = 5.38
[1:03:45] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:03:50] Stepping pH = 5.57
[1:04:05] Stirrer speed set to 0
[1:04:25] Datapoint id 65 collected
[1:04:25] Charge balance equation is out by -49.2%
[1:04:25] Stirrer speed set to 60
[1:04:30] pH 5.71 -> 5.91
[1:04:30] Using cautious pH adjust
[1:04:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:35] Stepping pH = 5.75
[1:04:36] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:04:41] Stepping pH = 6.27
[1:04:56] Stirrer speed set to 0
[1:05:51] Datapoint id 66 collected
[1:05:51] Charge balance equation is out by -57.7%
[1:05:51] Stirrer speed set to 60
[1:05:56] pH 6.32 -> 6.52
[1:05:56] Using cautious pH adjust
[1:05:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:06:01] Stepping pH = 6.20
[1:06:02] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:06:07] Stepping pH = 8.64
[1:06:22] Stirrer speed set to 0
[1:06:59] Datapoint id 67 collected
[1:06:59] Charge balance equation is out by -355.4%
[1:06:59] Stirrer speed set to 60

Sample name: **M11_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-01001**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01001_M11_octanol_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 12:11:22 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:07:04] pH 8.65 -> 8.85
[1:07:04] Using cautious pH adjust
[1:07:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:09] Stepping pH = 8.61
[1:07:09] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:07:14] Stepping pH = 8.77
[1:07:14] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:19] Stepping pH = 8.81
[1:07:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:24] Stepping pH = 8.85
[1:07:40] Stirrer speed set to 0
[1:08:04] Datapoint id 68 collected
[1:08:04] Charge balance equation is out by -499.1%
[1:08:04] Stirrer speed set to 60
[1:08:09] pH 8.85 -> 9.05
[1:08:09] Using cautious pH adjust
[1:08:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:08:14] Stepping pH = 8.87
[1:08:14] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:08:19] Stepping pH = 8.98
[1:08:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:08:24] Stepping pH = 9.02
[1:08:39] Stirrer speed set to 0
[1:08:55] Datapoint id 69 collected
[1:08:55] Charge balance equation is out by -147.2%
[1:08:55] Argon flow rate set to 0
[1:08:59] Titrator arm moved over Titration position