pH-metric Result

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH +)   0.09   ±0.08 (n=50)
logP (neutral X)   2.99   ±0.03 (n=50)

18C-26010 Points 2 to 16

M13_octanol concentration factor   1.006
Carbonate   0.0000 mM
Acidity error   2.38959 mM

18C-26010 Points 17 to 40

M13_octanol concentration factor   0.639
Carbonate   0.1054 mM
Acidity error   2.15628 mM

18C-26010 Points 41 to 68

M13_octanol concentration factor   0.745
Carbonate   0.1125 mM
Acidity error   2.15554 mM
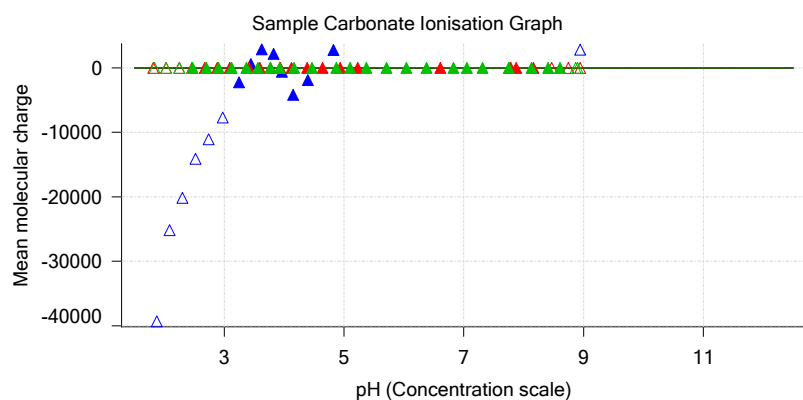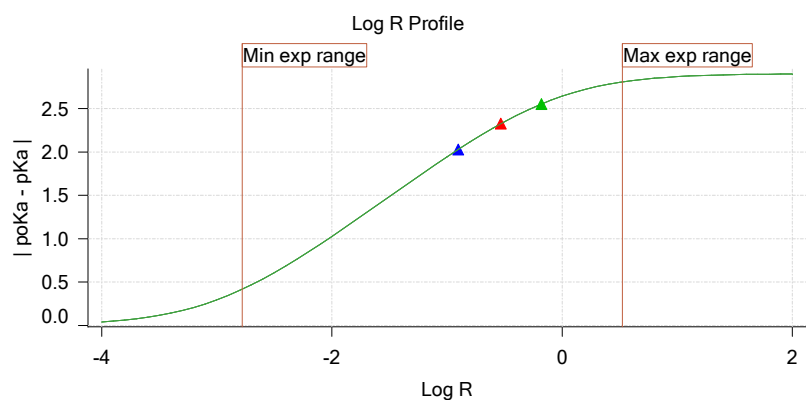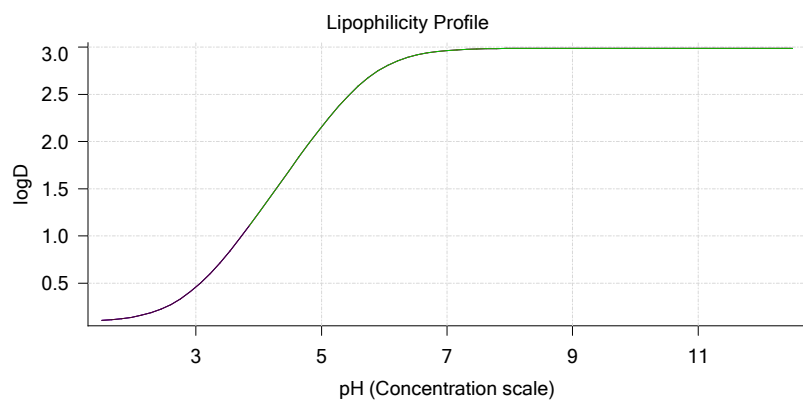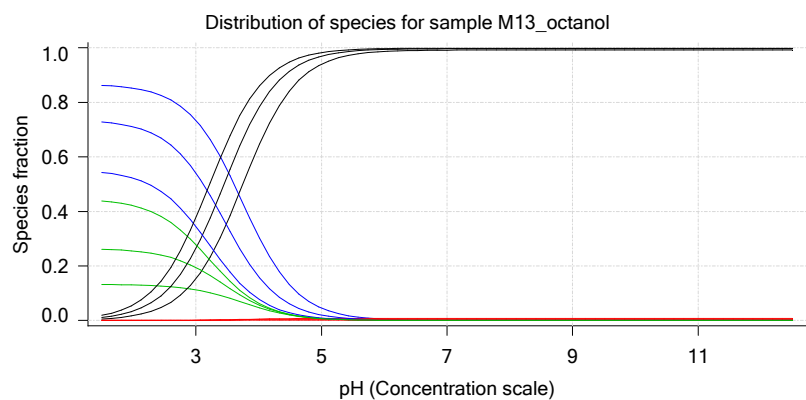
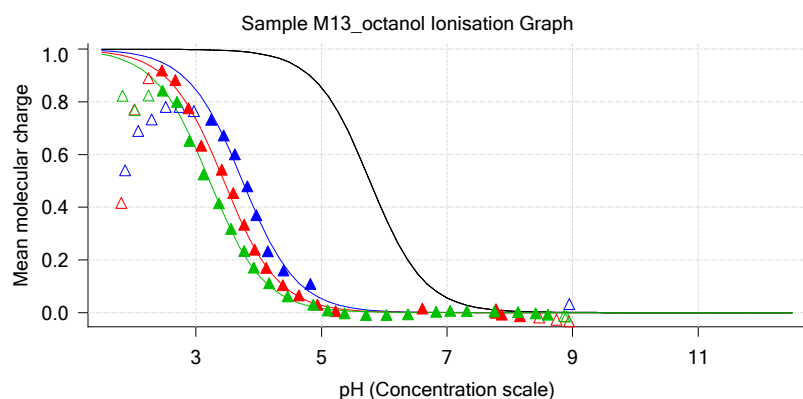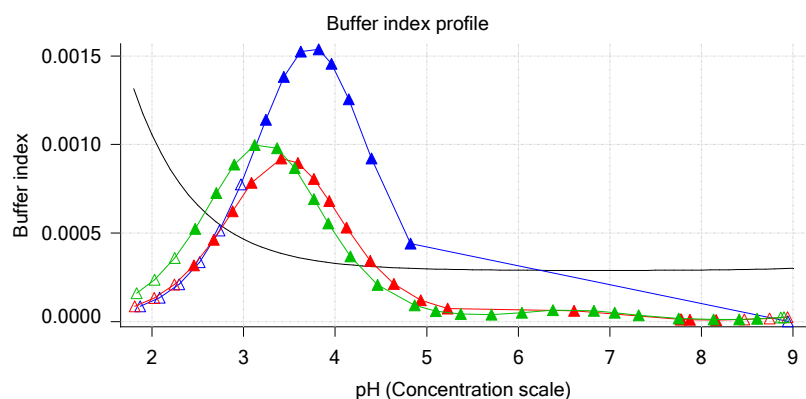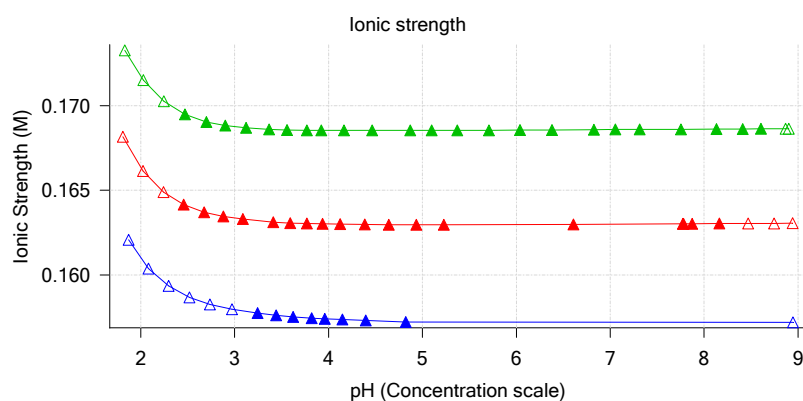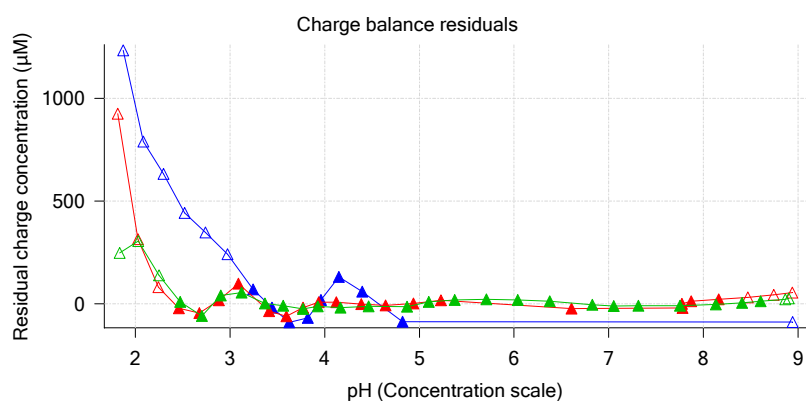## Warnings and errors

Errors   None
Warnings   None

Sample logD and percent species

pH	M13_octanol logD	M13_octanol M13_octanolH	M13_octanol M13_octanol	M13_octanol M13_octanolH*	M13_octanol M13_octanol*	Comment
1.000	0.09	44.67 %	0.00 %	54.60 %	0.74 %	
1.200	0.10	44.47 %	0.00 %	54.36 %	1.17 %	Stomach pH
2.000	0.14	41.88 %	0.01 %	51.19 %	6.93 %	
3.000	0.46	25.78 %	0.04 %	31.52 %	42.65 %	
4.000	1.24	5.32 %	0.09 %	6.51 %	88.08 %	
5.000	2.15	0.60 %	0.10 %	0.73 %	98.57 %	
6.000	2.79	0.06 %	0.10 %	0.07 %	99.76 %	
6.500	2.91	0.02 %	0.10 %	0.02 %	99.86 %	
7.000	2.96	0.01 %	0.10 %	0.01 %	99.88 %	
7.400	2.98	0.00 %	0.10 %	0.00 %	99.89 %	Blood pH
8.000	2.99	0.00 %	0.10 %	0.00 %	99.90 %	
9.000	2.99	0.00 %	0.10 %	0.00 %	99.90 %	
10.000	2.99	0.00 %	0.10 %	0.00 %	99.90 %	
11.000	2.99	0.00 %	0.10 %	0.00 %	99.90 %	
12.000	2.99	0.00 %	0.10 %	0.00 %	99.90 %	

Sample name: **M13_octanol** Experiment start time: **3/26/2018 4:16:35 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-26010** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M13_octanol Ionisation Graph

Distribution of species for sample M13_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Sample name: **M13_octanol**　　　　Experiment start time: **3/26/2018 4:16:35 PM**
Assay name: **pH-metric high logP**　　　　Analyst: **Pion**
Assay ID: **18C-26010**　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Graphs (continued)

Distribution of species for sample Carbonate

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

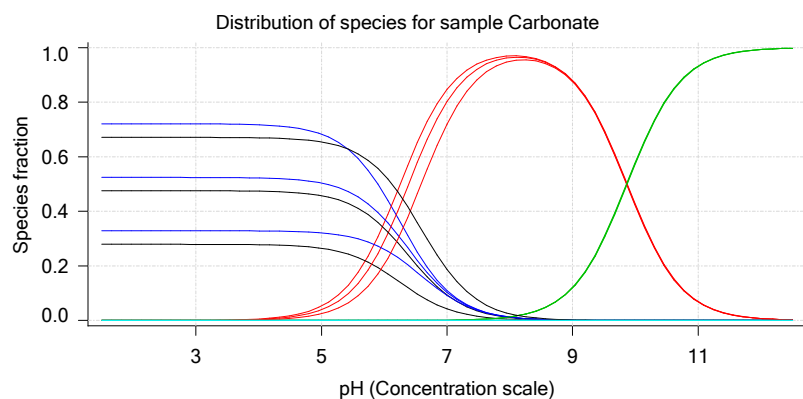# pH-metric high logP   Titration 1 of 3   18C-26010 Points 2 to 16

Overall results

RMSD   0.079
Average ionic strength   0.158 M
Average temperature   24.9°C
Partition ratio   0.1253 : 1
Analyte concentration range   2374.9 µM to 2437.5 µM
Total points considered   8 of 15

Warnings and errors

Errors   None
Warnings   One or more logP values out of range
           Excessive acidity error present

Four-Plus parameters

	Alpha	0.122	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r
	S	0.9974	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r
	jH	1.1	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r
	jOH	-0.5	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r

Titrants

	0.50 M HCl	0.994478	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r
	0.50 M KOH	1.003190	3/26/2018 4:16:35 PM	C:\Sirius_T3\KOH18C23.t3r

Sample

	M13_octanol concentration factor	1.006
	Base pKa 1	5.77
	logP (XH +)	-4.56
	logP (neutral X)	2.93

Sample graphs

Ionisation of sample M13_octanol

Distribution of species for sample M13_octanol

Sample name: **M13_octanol** Experiment start time: **3/26/2018 4:16:35 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-26010** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Sample graphs (continued)

Lipophilicity Profile
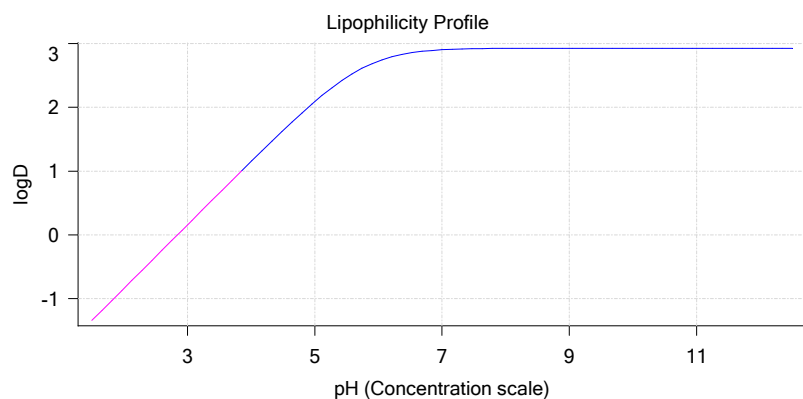
Sample logD and percent species

pH	M13_octanol logD	M13_octanol M13_octanolH	M13_octanol M13_octanol	M13_octanol M13_octanolH*	M13_octanol M13_octanol*	Comment
1.000	-1.84	99.82 %	0.00 %	0.00 %	0.18 %	
1.200	-1.64	99.71 %	0.00 %	0.00 %	0.28 %	Stomach pH
2.000	-0.84	98.21 %	0.02 %	0.00 %	1.77 %	
3.000	0.16	84.62 %	0.14 %	0.00 %	15.23 %	
4.000	1.15	35.50 %	0.60 %	0.00 %	63.90 %	
5.000	2.09	5.22 %	0.89 %	0.00 %	93.90 %	
6.000	2.73	0.55 %	0.93 %	0.00 %	98.52 %	
6.500	2.85	0.17 %	0.93 %	0.00 %	98.89 %	
7.000	2.90	0.05 %	0.93 %	0.00 %	99.01 %	
7.400	2.92	0.02 %	0.93 %	0.00 %	99.04 %	Blood pH
8.000	2.92	0.01 %	0.93 %	0.00 %	99.06 %	
9.000	2.93	0.00 %	0.93 %	0.00 %	99.06 %	
10.000	2.93	0.00 %	0.93 %	0.00 %	99.07 %	
11.000	2.93	0.00 %	0.93 %	0.00 %	99.07 %	
12.000	2.93	0.00 %	0.93 %	0.00 %	99.07 %	

Carbonate and acidity

Carbonate 0.000 mM
Acidity error 2.390 mM

Other graphs

Assay progress

Titration graph

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
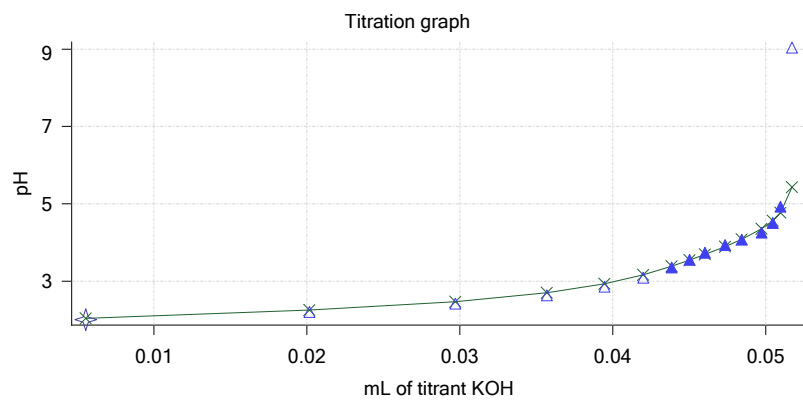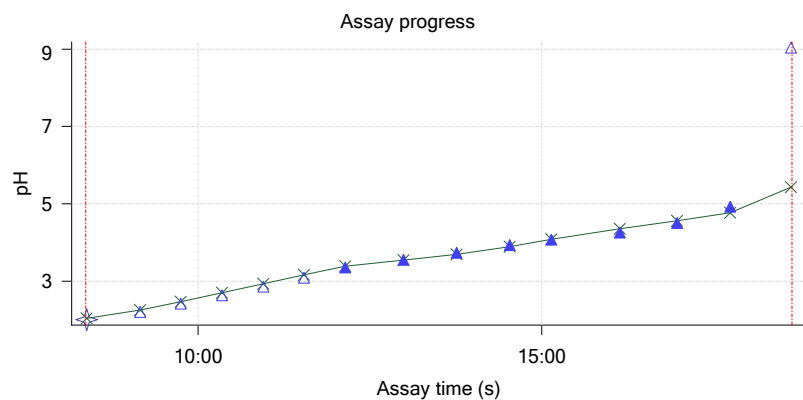Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
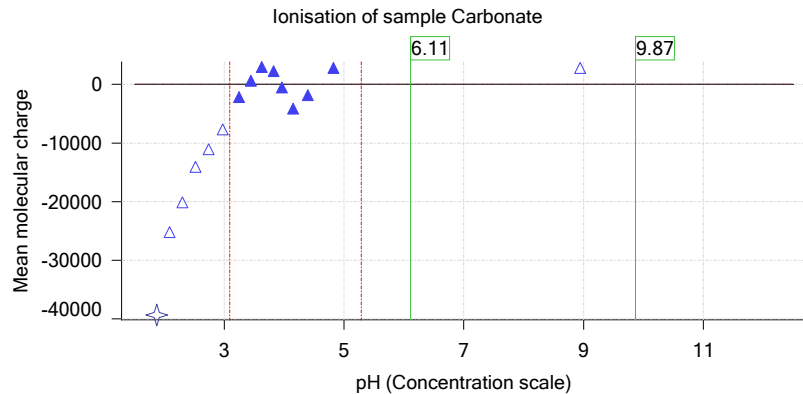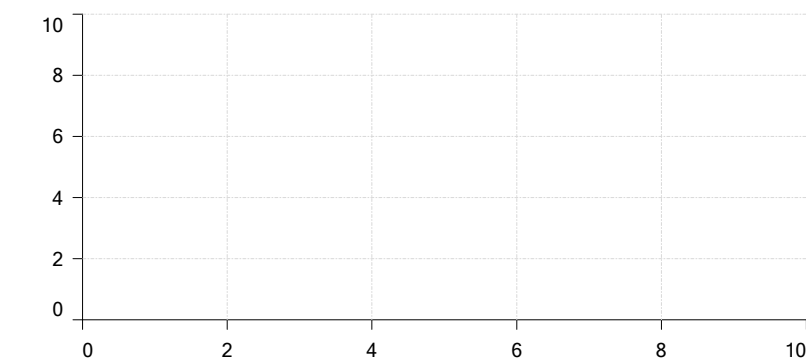
Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 2 of 3   18C-26010 Points 17 to 40

Overall results

RMSD   0.567
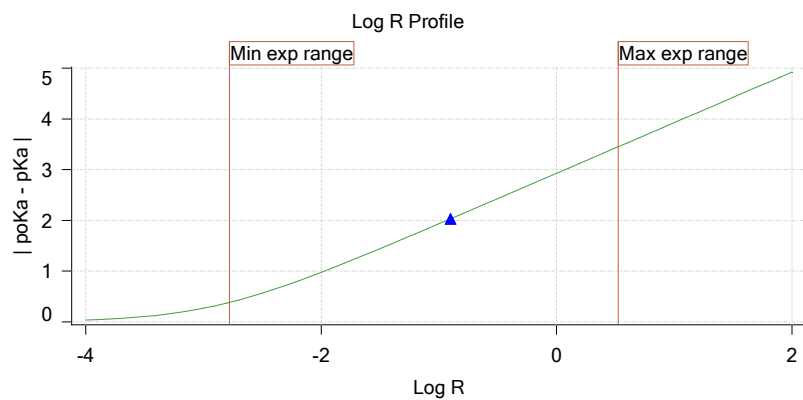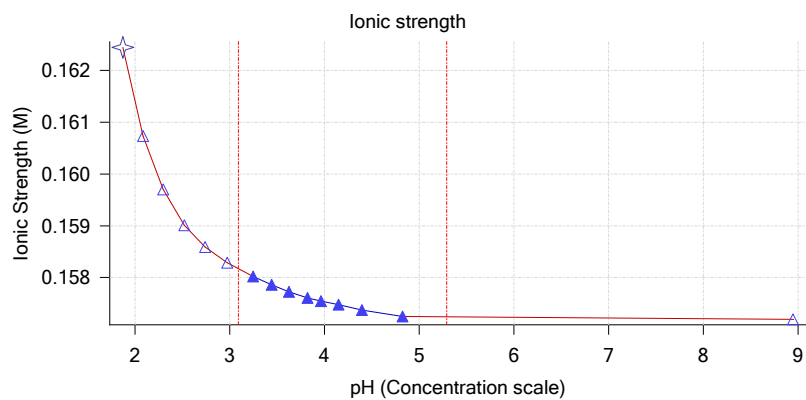Average ionic strength   0.163 M
Average temperature   25.0°C
Partition ratio   0.2937 : 1
Analyte concentration range   1935.6 µM to 1984.1 µM
Total points considered   18 of 24

Warnings and errors

Errors   None
Warnings Sample concentration factor out of range
          One or more logP values out of range
          Excessive acidity error present

Four-Plus parameters

Alpha   0.122   3/26/2018 4:16:34 PM   C:\Sirius_T3\18C-26006_Blank standardisation.t3r
S   0.9974   3/26/2018 4:16:34 PM   C:\Sirius_T3\18C-26006_Blank standardisation.t3r
jH   1.1   3/26/2018 4:16:34 PM   C:\Sirius_T3\18C-26006_Blank standardisation.t3r
jOH   -0.5   3/26/2018 4:16:34 PM   C:\Sirius_T3\18C-26006_Blank standardisation.t3r

Titrants

0.50 M HCl   0.994478   3/26/2018 4:16:34 PM   C:\Sirius_T3\18C-26006_Blank standardisation.t3r
0.50 M KOH   1.003190   3/26/2018 4:16:35 PM   C:\Sirius_T3\KOH18C23.t3r

Sample

M13_octanol concentration factor   0.639
Base pKa 1   5.77
logP (XH +)   -4.56
logP (neutral X)   2.85

Sample graphs
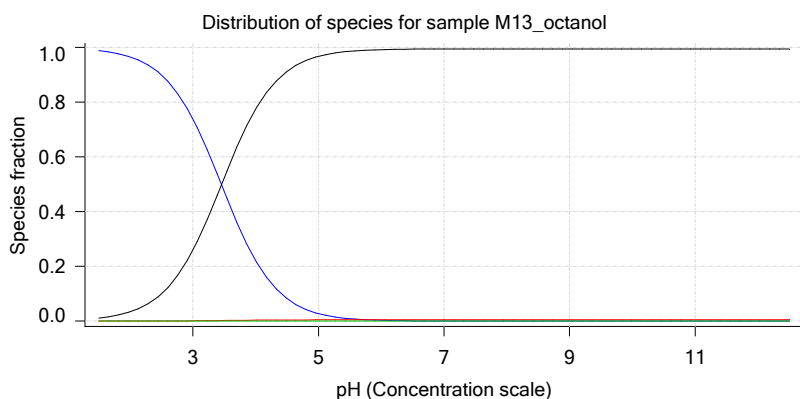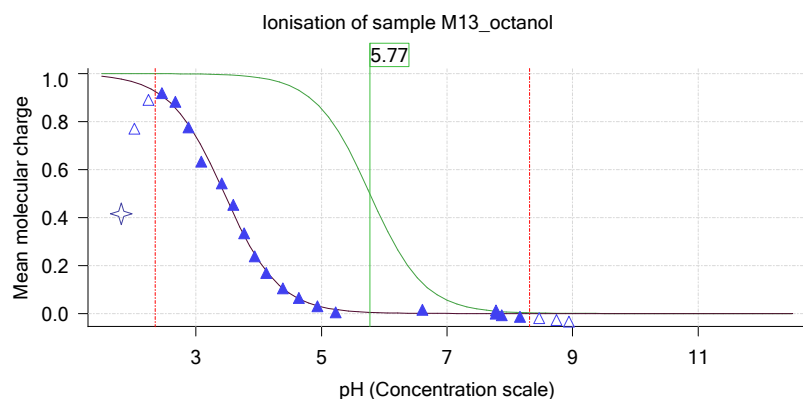
Ionisation of sample M13_octanol

Distribution of species for sample M13_octanol
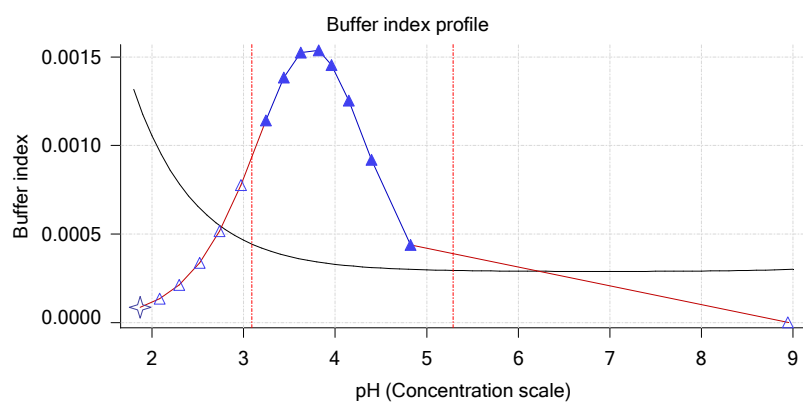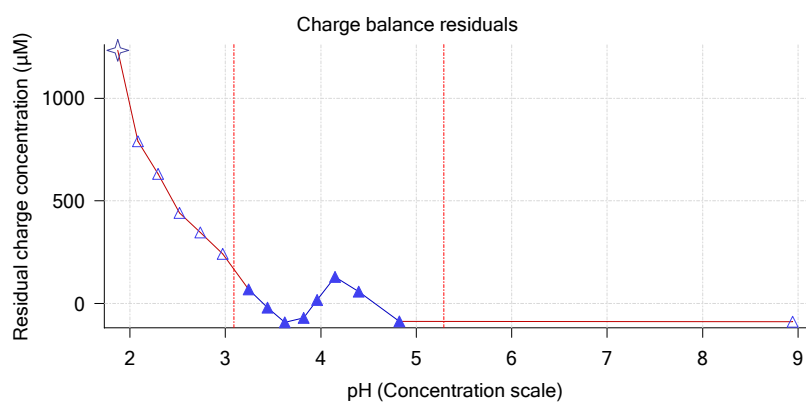
Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)
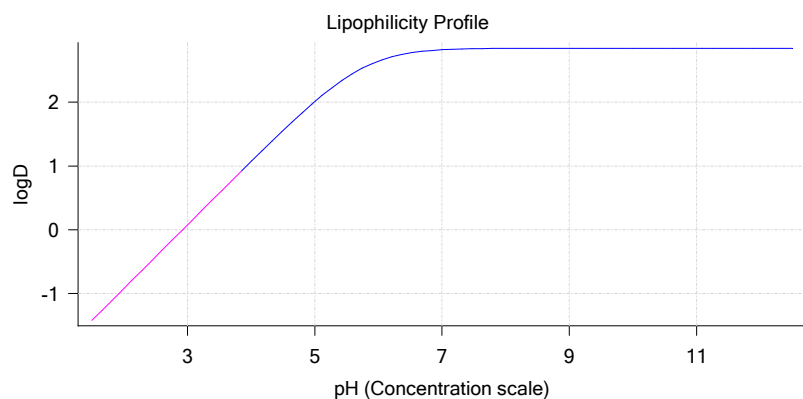
Lipophilicity Profile

Sample logD and percent species

pH	M13_octanol logD	M13_octanol M13_octanolH	M13_octanol M13_octanol	M13_octanol M13_octanolH*	M13_octanol M13_octanol*	Comment
1.000	-1.92	99.65 %	0.00 %	0.00 %	0.35 %	
1.200	-1.72	99.44 %	0.00 %	0.00 %	0.55 %	Stomach pH
2.000	-0.92	96.60 %	0.02 %	0.00 %	3.39 %	
3.000	0.08	73.95 %	0.13 %	0.00 %	25.93 %	
4.000	1.07	22.11 %	0.38 %	0.00 %	77.52 %	
5.000	2.01	2.76 %	0.47 %	0.00 %	96.77 %	
6.000	2.65	0.28 %	0.48 %	0.00 %	99.24 %	
6.500	2.77	0.09 %	0.48 %	0.00 %	99.43 %	
7.000	2.82	0.03 %	0.48 %	0.00 %	99.49 %	
7.400	2.84	0.01 %	0.48 %	0.00 %	99.51 %	Blood pH
8.000	2.84	0.00 %	0.48 %	0.00 %	99.52 %	
9.000	2.85	0.00 %	0.48 %	0.00 %	99.52 %	
10.000	2.85	0.00 %	0.48 %	0.00 %	99.52 %	
11.000	2.85	0.00 %	0.48 %	0.00 %	99.52 %	
12.000	2.85	0.00 %	0.48 %	0.00 %	99.52 %	

Carbonate and acidity

Carbonate   0.105 mM
Acidity error   2.156 mM

Other graphs

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
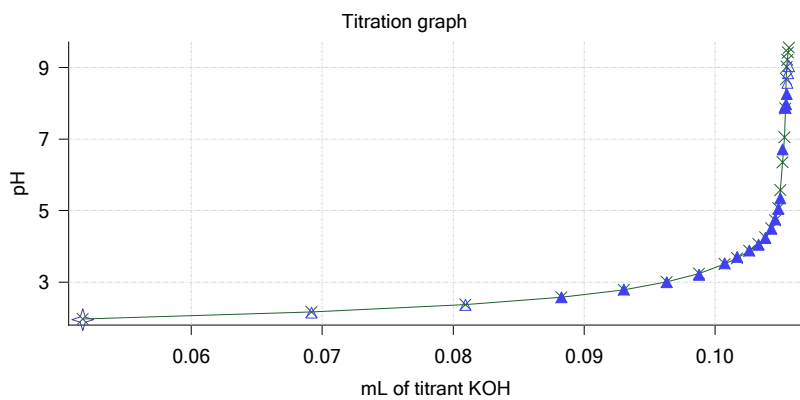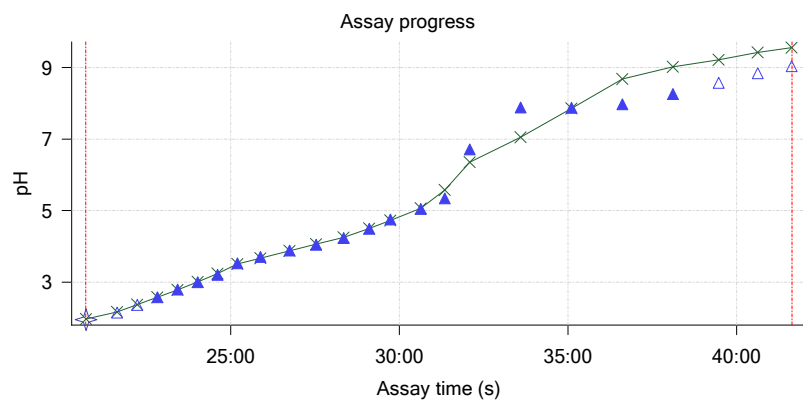Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
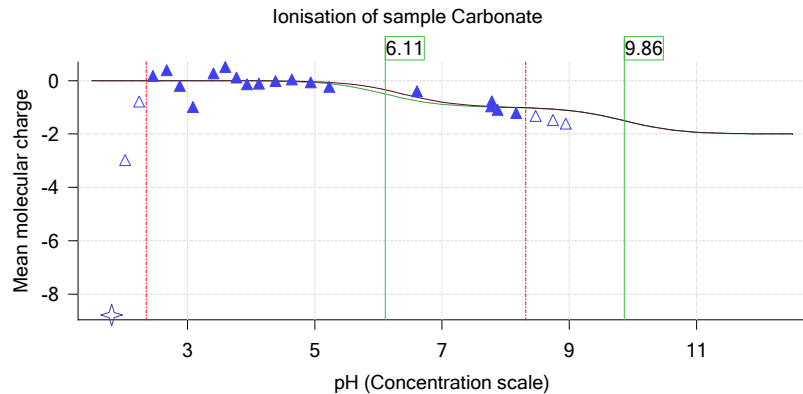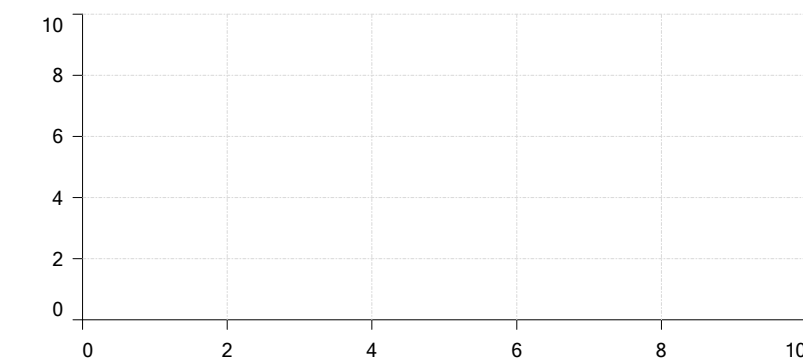
Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 3 of 3   18C-26010 Points 41 to 68

Overall results

RMSD	0.220
Average ionic strength	0.169 M
Average temperature	25.0°C
Partition ratio	0.6600 : 1
Analyte concentration range	1412.7 µM to 1440.3 µM
Total points considered	23 of 28

Warnings and errors

Errors   None
Warnings   One or more logP values out of range
            Excessive acidity error present

Four-Plus parameters

Alpha	0.122	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r
S	0.9974	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r
jH	1.1	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r
jOH	-0.5	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r

Titrants

0.50 M HCl	0.994478	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r
0.50 M KOH	1.003190	3/26/2018 4:16:35 PM	C:\Sirius_T3\KOH18C23.t3r

Sample

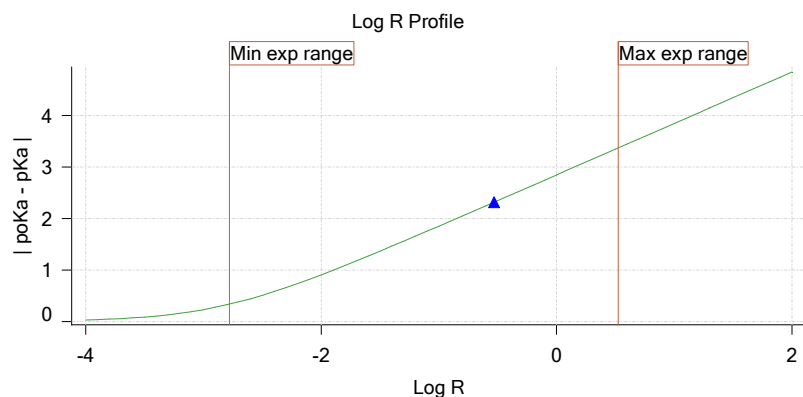|	
M13_octanol concentration factor	0.745
Base pKa 1	5.77
logP (XH +)	-4.56
logP (neutral X)	2.73

Sample graphs

Ionisation of sample M13_octanol

Distribution of species for sample M13_octanol

Sample name: **M13_octanol**   Experiment start time: **3/26/2018 4:16:35 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-26010**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Sample graphs (continued)

Lipophilicity Profile
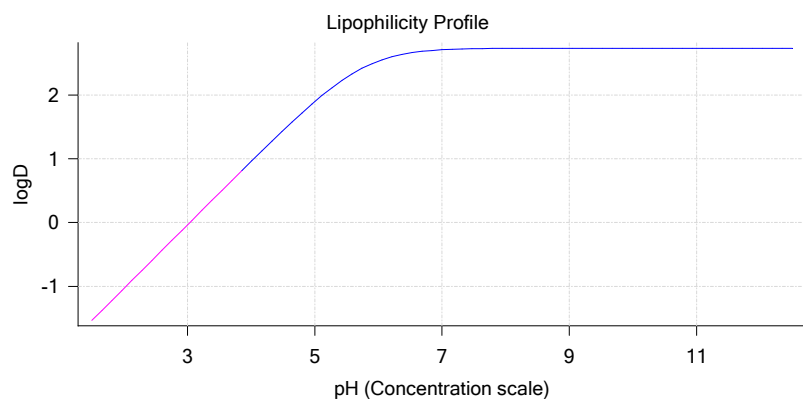
Sample logD and percent species

pH	M13_octanol logD	M13_octanol M13_octanolH	M13_octanol M13_octanol	M13_octanol M13_octanolH*	M13_octanol M13_octanol*	Comment
1.000	-2.04	99.39 %	0.00 %	0.00 %	0.60 %	
1.200	-1.84	99.04 %	0.00 %	0.00 %	0.95 %	Stomach pH
2.000	-1.04	94.26 %	0.02 %	0.00 %	5.72 %	
3.000	-0.04	62.18 %	0.11 %	0.00 %	37.72 %	
4.000	0.96	14.12 %	0.24 %	0.00 %	85.64 %	
5.000	1.90	1.62 %	0.27 %	0.00 %	98.11 %	
6.000	2.53	0.16 %	0.28 %	0.00 %	99.56 %	
6.500	2.66	0.05 %	0.28 %	0.00 %	99.67 %	
7.000	2.71	0.02 %	0.28 %	0.00 %	99.70 %	
7.400	2.72	0.01 %	0.28 %	0.00 %	99.71 %	Blood pH
8.000	2.73	0.00 %	0.28 %	0.00 %	99.72 %	
9.000	2.73	0.00 %	0.28 %	0.00 %	99.72 %	
10.000	2.73	0.00 %	0.28 %	0.00 %	99.72 %	
11.000	2.73	0.00 %	0.28 %	0.00 %	99.72 %	
12.000	2.73	0.00 %	0.28 %	0.00 %	99.72 %	

Carbonate and acidity

Carbonate   0.113 mM
Acidity error   2.156 mM

Other graphs

Other graphs (continued)

Charge balance residuals

Buffer index profile

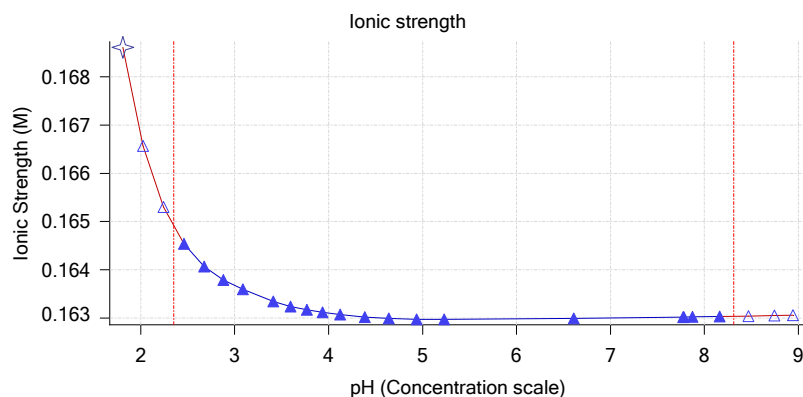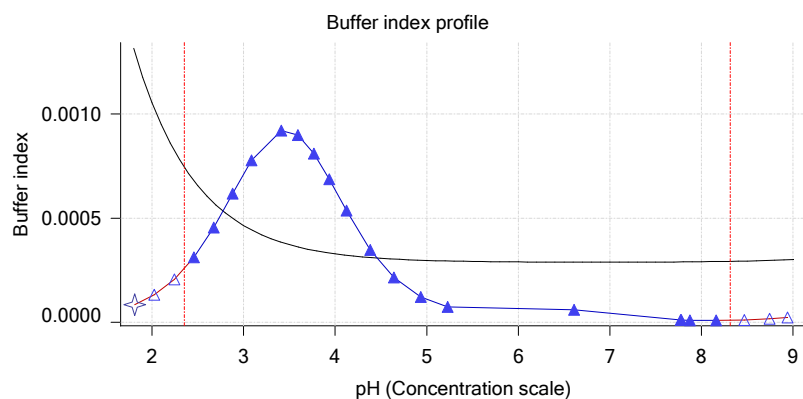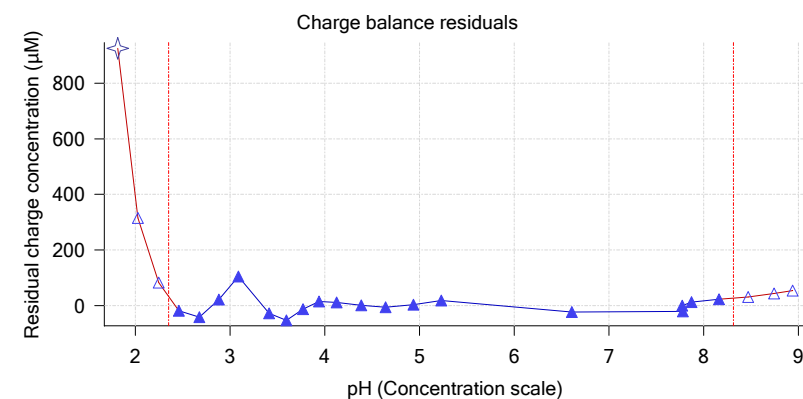Ionic strength

Log R Profile

Ionisation of sample Carbonate
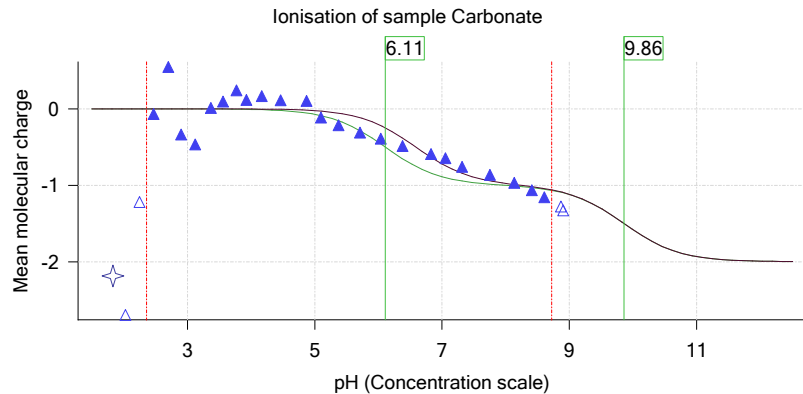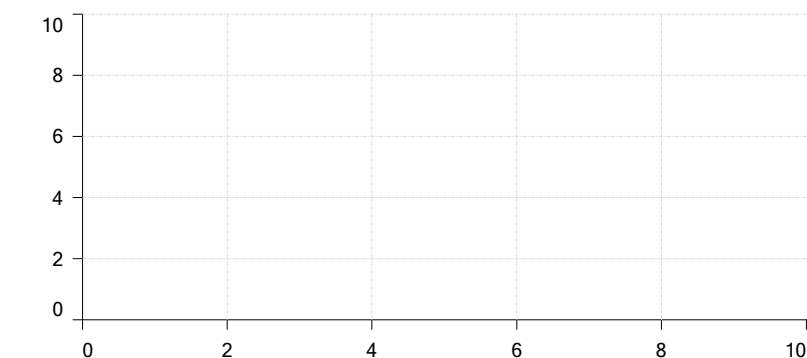
Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

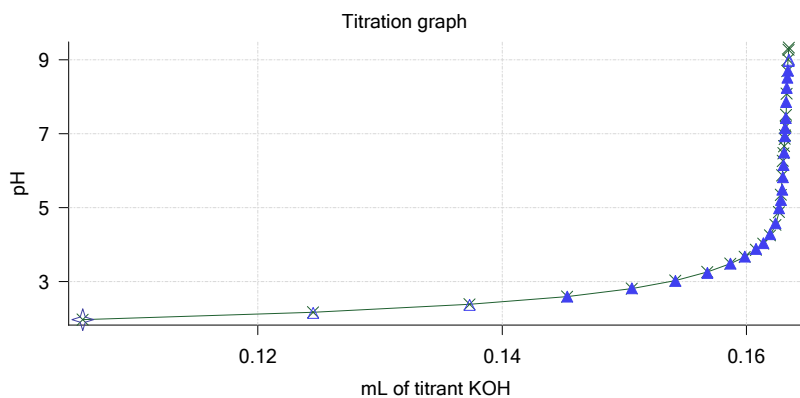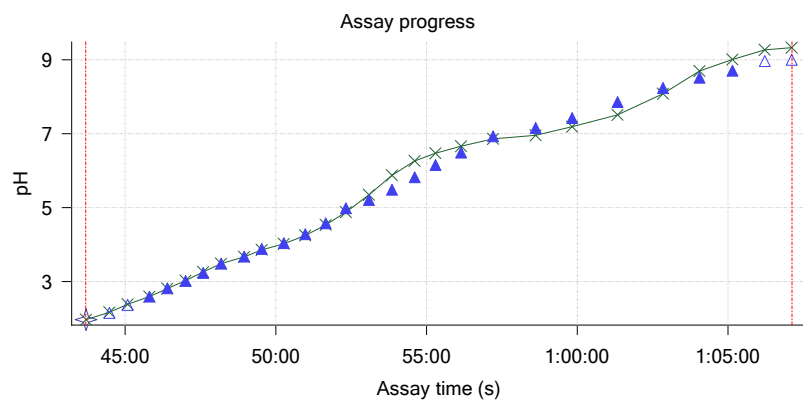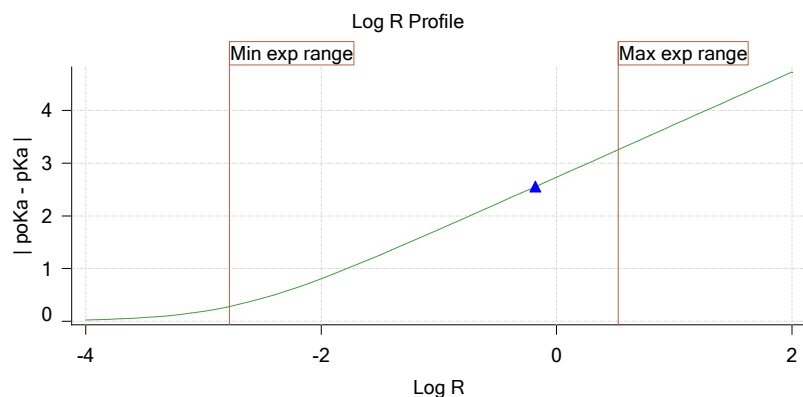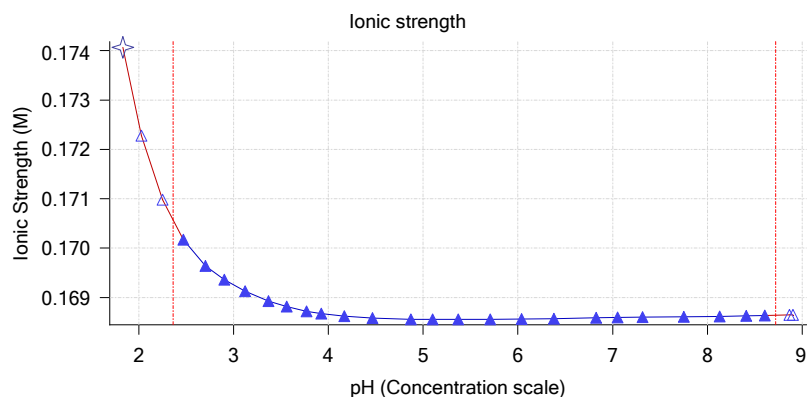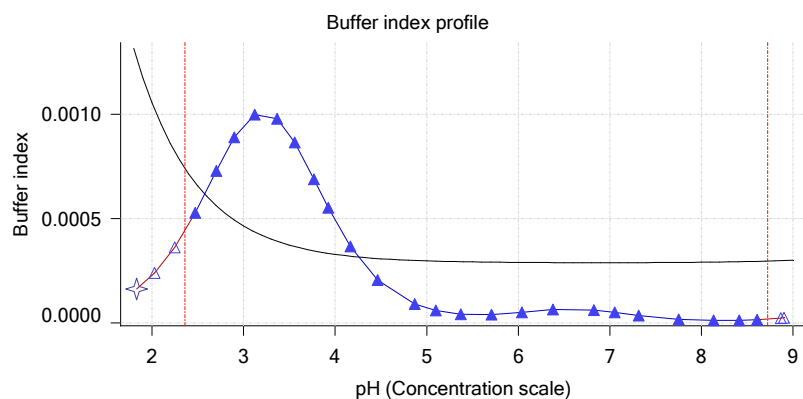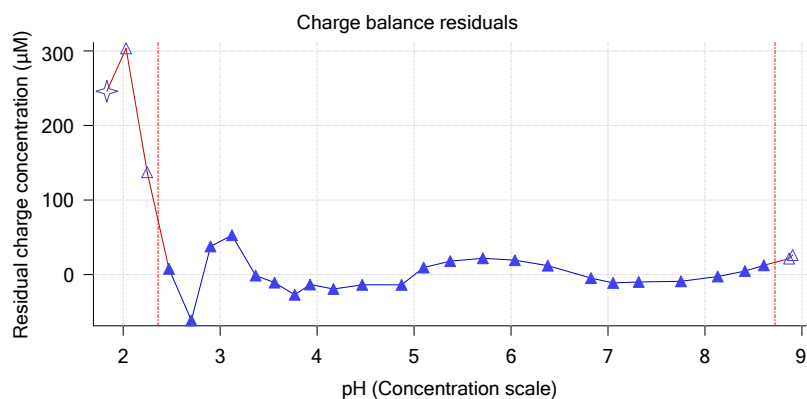| Settings	Value	Date/Time changed	Imported from
Sample name	M13_octanol	2/27/2018 5:57:49 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001260 g	3/26/2018 4:15:03 PM	User entered value
Formula weight	295.34 g/mol	2/27/2018 5:57:49 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	295.34	2/27/2018 5:57:49 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 5:57:49 PM	User entered value
Sample is a	Base	2/27/2018 5:57:49 PM	User entered value
pKa 1	5.77	2/27/2018 5:57:49 PM	User entered value
logp (XH +)	-4.56	3/2/2018 4:30:48 PM	User entered value
logP (neutral X)	2.99	3/2/2018 4:30:43 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/d time
5:17.0	Manual volume addition				0.20000 mL					
5:18.1	Initial pH = 3.49									
8:22.9	Data point 2	1.50000 mL	0.04473 mL	0.00553 mL	0.20000 mL	2.003	-0.00959	0.73625	0.00055	10.5 s
9:09.4	Data point 3	1.50000 mL	0.04473 mL	0.02016 mL	0.20000 mL	2.209	0.00564	0.12526	0.00079	10.0 s
9:45.0	Data point 4	1.50000 mL	0.04473 mL	0.02970 mL	0.20000 mL	2.418	0.01231	0.87847	0.00065	10.5 s
10:21.0	Data point 5	1.50000 mL	0.04473 mL	0.03568 mL	0.20000 mL	2.638	0.00365	0.22847	0.00038	10.5 s
10:57.1	Data point 6	1.50000 mL	0.04473 mL	0.03944 mL	0.20000 mL	2.855	-0.00035	0.00242	0.00035	10.0 s
11:32.6	Data point 7	1.50000 mL	0.04473 mL	0.04198 mL	0.20000 mL	3.087	0.00584	0.40770	0.00045	10.5 s
12:08.5	Data point 8	1.50000 mL	0.04473 mL	0.04384 mL	0.20000 mL	3.358	-0.00076	0.00844	0.00041	10.0 s
12:59.5	Data point 9	1.50000 mL	0.04473 mL	0.04501 mL	0.20000 mL	3.555	-0.00079	0.00582	0.00051	10.5 s
13:45.7	Data point 10	1.50000 mL	0.04473 mL	0.04603 mL	0.20000 mL	3.736	-0.01231	0.48567	0.00087	10.5 s
14:32.0	Data point 11	1.50000 mL	0.04473 mL	0.04734 mL	0.20000 mL	3.933	-0.00938	0.30311	0.00084	11.0 s
15:08.5	Data point 12	1.50000 mL	0.04473 mL	0.04842 mL	0.20000 mL	4.073	-0.01778	0.77327	0.00100	13.5 s
16:08.2	Data point 13	1.50000 mL	0.04473 mL	0.04972 mL	0.20000 mL	4.259	-0.01176	0.47760	0.00084	14.5 s
16:58.3	Data point 14	1.50000 mL	0.04473 mL	0.05045 mL	0.20000 mL	4.506	0.01843	0.89339	0.00096	21.0 s
17:44.7	Data point 15	1.50000 mL	0.04473 mL	0.05096 mL	0.20000 mL	4.931	0.01593	0.72074	0.00093	22.5 s
18:37.6	Data point 16	1.50000 mL	0.04473 mL	0.05172 mL	0.20000 mL	9.043	-0.08412	0.99442	0.00416	Timed out at
20:42.7	Data point 17	1.50000 mL	0.09854 mL	0.05172 mL	0.50000 mL	1.945	0.00587	0.10684	0.00089	19.0 s
21:38.0	Data point 18	1.50000 mL	0.09854 mL	0.06919 mL	0.50000 mL	2.151	-0.00296	0.10195	0.00046	10.0 s
22:13.6	Data point 19	1.50000 mL	0.09854 mL	0.08095 mL	0.50000 mL	2.366	0.00068	0.00245	0.00068	10.5 s
22:49.6	Data point 20	1.50000 mL	0.09854 mL	0.08826 mL	0.50000 mL	2.578	-0.01356	0.80667	0.00075	10.0 s

Sample name: **M13_octanol**　　　　　　　　　　Experiment start time: **3/26/2018 4:16:35 PM**
Assay name: **pH-metric high logP**　　　　　　　Analyst: **Pion**
Assay ID: **18C-26010**　　　　　　　　　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_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
23:25.1	Data point 21	1.50000 mL	0.09854 mL	0.09304 mL	0.50000 mL	2.792	0.00291	0.03033	0.00083	10.5 s
24:01.1	Data point 22	1.50000 mL	0.09854 mL	0.09631 mL	0.50000 mL	2.996	-0.00625	0.16494	0.00076	10.0 s
24:36.5	Data point 23	1.50000 mL	0.09854 mL	0.09878 mL	0.50000 mL	3.202	-0.00833	0.32865	0.00072	10.0 s
25:11.7	Data point 24	1.50000 mL	0.09854 mL	0.10073 mL	0.50000 mL	3.524	-0.01622	0.91829	0.00084	10.5 s
25:52.8	Data point 25	1.50000 mL	0.09854 mL	0.10167 mL	0.50000 mL	3.706	-0.01693	0.76864	0.00095	11.0 s
26:44.5	Data point 26	1.50000 mL	0.09854 mL	0.10261 mL	0.50000 mL	3.881	-0.01256	0.44869	0.00093	12.0 s
27:32.0	Data point 27	1.50000 mL	0.09854 mL	0.10332 mL	0.50000 mL	4.048	-0.01675	0.86339	0.00089	13.0 s
28:20.7	Data point 28	1.50000 mL	0.09854 mL	0.10383 mL	0.50000 mL	4.234	-0.01972	0.95699	0.00100	10.0 s
29:06.4	Data point 29	1.50000 mL	0.09854 mL	0.10430 mL	0.50000 mL	4.495	-0.01298	0.53508	0.00088	12.0 s
29:43.8	Data point 30	1.50000 mL	0.09854 mL	0.10459 mL	0.50000 mL	4.751	0.01337	0.62718	0.00083	23.5 s
30:37.9	Data point 31	1.50000 mL	0.09854 mL	0.10482 mL	0.50000 mL	5.045	-0.01188	0.50324	0.00083	12.5 s
31:21.0	Data point 32	1.50000 mL	0.09854 mL	0.10499 mL	0.50000 mL	5.337	-0.01679	0.75428	0.00095	13.5 s
32:05.0	Data point 33	1.50000 mL	0.09854 mL	0.10515 mL	0.50000 mL	6.712	-0.05259	0.99413	0.00261	Timed out at 59.5 s
33:35.6	Data point 34	1.50000 mL	0.09854 mL	0.10529 mL	0.50000 mL	7.882	-0.07582	0.99362	0.00376	Timed out at 59.5 s
35:06.1	Data point 35	1.50000 mL	0.09854 mL	0.10536 mL	0.50000 mL	7.874	-0.03303	0.99176	0.00164	Timed out at 59.5 s
36:36.6	Data point 36	1.50000 mL	0.09854 mL	0.10541 mL	0.50000 mL	7.975	-0.02481	0.97940	0.00124	Timed out at 59.5 s
38:07.1	Data point 37	1.50000 mL	0.09854 mL	0.10546 mL	0.50000 mL	8.262	-0.01947	0.94137	0.00099	50.5 s
39:28.1	Data point 38	1.50000 mL	0.09854 mL	0.10550 mL	0.50000 mL	8.569	-0.01705	0.77622	0.00096	34.0 s
40:37.7	Data point 39	1.50000 mL	0.09854 mL	0.10557 mL	0.50000 mL	8.843	-0.01363	0.52717	0.00093	24.5 s
41:37.8	Data point 40	1.50000 mL	0.09854 mL	0.10564 mL	0.50000 mL	9.039	-0.01553	0.70869	0.00091	19.0 s
43:42.7	Data point 41	1.50000 mL	0.15644 mL	0.10564 mL	1.20000 mL	1.964	-0.01340	0.57402	0.00087	10.0 s
44:28.9	Data point 42	1.50000 mL	0.15644 mL	0.12453 mL	1.20000 mL	2.154	0.00096	0.01426	0.00040	10.5 s
45:05.1	Data point 43	1.50000 mL	0.15644 mL	0.13735 mL	1.20000 mL	2.370	0.01091	0.34363	0.00092	18.0 s
45:48.7	Data point 44	1.50000 mL	0.15644 mL	0.14532 mL	1.20000 mL	2.589	-0.00436	0.09759	0.00069	10.0 s
46:24.3	Data point 45	1.50000 mL	0.15644 mL	0.15061 mL	1.20000 mL	2.818	-0.00140	0.02683	0.00042	10.5 s
47:00.3	Data point 46	1.50000 mL	0.15644 mL	0.15419 mL	1.20000 mL	3.015	-0.01292	0.43338	0.00097	10.0 s
47:35.8	Data point 47	1.50000 mL	0.15644 mL	0.15682 mL	1.20000 mL	3.235	-0.00551	0.33990	0.00047	10.0 s
48:11.2	Data point 48	1.50000 mL	0.15644 mL	0.15870 mL	1.20000 mL	3.480	-0.00486	0.44316	0.00036	10.0 s
48:57.0	Data point 49	1.50000 mL	0.15644 mL	0.15988 mL	1.20000 mL	3.672	-0.01560	0.96977	0.00078	10.0 s
49:32.4	Data point 50	1.50000 mL	0.15644 mL	0.16079 mL	1.20000 mL	3.881	0.00315	0.02822	0.00093	18.5 s
50:16.3	Data point 51	1.50000 mL	0.15644 mL	0.16138 mL	1.20000 mL	4.036	-0.01090	0.30494	0.00098	12.0 s
50:58.8	Data point 52	1.50000 mL	0.15644 mL	0.16195 mL	1.20000 mL	4.277	-0.01737	0.75358	0.00099	10.0 s
51:39.4	Data point 53	1.50000 mL	0.15644 mL	0.16239 mL	1.20000 mL	4.574	-0.01819	0.84303	0.00098	10.0 s
52:19.8	Data point 54	1.50000 mL	0.15644 mL	0.16268 mL	1.20000 mL	4.979	-0.01369	0.66561	0.00083	10.0 s
53:05.6	Data point 55	1.50000 mL	0.15644 mL	0.16284 mL	1.20000 mL	5.207	-0.00278	0.09353	0.00045	10.0 s
53:51.2	Data point 56	1.50000 mL	0.15644 mL	0.16294 mL	1.20000 mL	5.479	-0.00914	0.49731	0.00064	10.0 s
54:36.8	Data point 57	1.50000 mL	0.15644 mL	0.16301 mL	1.20000 mL	5.816	-0.01695	0.93689	0.00086	10.5 s
55:17.8	Data point 58	1.50000 mL	0.15644 mL	0.16305 mL	1.20000 mL	6.145	-0.00680	0.14161	0.00089	20.5 s
56:08.7	Data point 59	1.50000 mL	0.15644 mL	0.16310 mL	1.20000 mL	6.484	-0.01501	0.62688	0.00094	33.5 s
57:12.7	Data point 60	1.50000 mL	0.15644 mL	0.16315 mL	1.20000 mL	6.929	-0.01950	0.93593	0.00100	59.0 s
58:37.2	Data point 61	1.50000 mL	0.15644 mL	0.16317 mL	1.20000 mL	7.157	-0.01773	0.81355	0.00097	42.0 s
59:49.7	Data point 62	1.50000 mL	0.15644 mL	0.16322 mL	1.20000 mL	7.418	-0.02771	0.99293	0.00137	Timed out at 59.5 s
1:01:20.3	Data point 63	1.50000 mL	0.15644 mL	0.16326 mL	1.20000 mL	7.854	-0.03775	0.96659	0.00190	Timed out at 59.5 s
1:02:50.9	Data point 64	1.50000 mL	0.15644 mL	0.16331 mL	1.20000 mL	8.232	-0.01636	0.69169	0.00097	42.0 s
1:04:03.3	Data point 65	1.50000 mL	0.15644 mL	0.16336 mL	1.20000 mL	8.510	-0.01437	0.53636	0.00097	35.0 s
1:05:08.9	Data point 66	1.50000 mL	0.15644 mL	0.16340 mL	1.20000 mL	8.705	-0.01715	0.74002	0.00098	28.5 s
1:06:13.2	Data point 67	1.50000 mL	0.15644 mL	0.16348 mL	1.20000 mL	8.966	-0.00089	0.00198	0.00099	28.0 s
1:07:06.6	Data point 68	1.50000 mL	0.15644 mL	0.16350 mL	1.20000 mL	9.001	0.00342	0.03245	0.00094	26.5 s
1:07:42.2	Assay volumes	1.50000 mL	0.15644 mL	0.16350 mL	1.20000 mL					

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 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	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	0.200 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	60 seconds			
After sonication stir for	20 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	0.300 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
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Experiment start time: **3/26/2018 4:16:35 PM**
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	0.700 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	0.122	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r
Four-Plus S	0.9974	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r
Four-Plus jH	1.1	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r
Four-Plus jOH	-0.5	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.t3r
Base concentration factor	1.003	3/26/2018 4:16:35 PM	C:\Sirius_T3\KOH18C23.t3r
Acid concentration factor	0.994	3/26/2018 4:16:34 PM	C:\Sirius_T3\18C-26006_Blank standardisation.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 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	3/16/2018 11:09:18 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	03-16-2018	3/16/2018 10:56:23 AM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	3/22/2018	3/23/2018 9:34:17 AM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	02-08-2018	3/6/2018 10:28:59 AM
Port B	Cyclohexane	11-01-17	2/27/2018 11:37:57 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 11:18:04 AM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM

Sample name: **M13_octanol**
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Experiment start time: **3/26/2018 4:16:35 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 10:59:35 AM
Titrator		T3TM1200161	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 3:01:00 PM
E0 calibration	+5.08 mV		3/26/2018 4:17:19 PM
Filling solution	3M KCl	KCL097	3/26/2018 9:20:42 AM
Liquids			
Wash 1	50% IPA:50% Water		3/26/2018 9:21:48 AM
Wash 2	0.5% Trition X-100 in H20		3/26/2018 9:21:51 AM
Buffer position 1	pH7 Wash		3/26/2018 9:21:54 AM
Buffer position 2	pH 7		3/26/2018 9:21:57 AM
Storage position			3/26/2018 9:21:20 AM
Wash water	6.6e+003 mL	03-12-2018	3/12/2018 9:25:04 AM
Waste	3.7e+003 mL		3/12/2018 9:24:49 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		074811	11/23/2010 12:22:28 PM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	168:19:11		11/23/2010 12:22:28 PM
Calibrated on	2/27/2018 11:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M13_octanol** Experiment start time: **3/26/2018 4:16:35 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-26010** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

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

[2:41] Air gap created for Water (0.15 M KCl)
[2:41] Air gap created for Acid (0.5 M HCl)
[2:41] Air gap created for Base (0.5 M KOH)
[2:42] Air gap released for Water (0.15 M KCl)
[2:46] Titrator arm moved over Titration position
[2:46] Titration 1 of 3
[2:46] Adding initial titrants
[2:46] Automatically add 1.50000 mL of water
[3:11] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:15] Titrator arm moved over Drain
[4:56] Titrator arm moved to Titration position
[4:56] Argon flow rate set to 100
[4:56] Stirrer speed set to 10
[5:18] Initial pH = 3.49
[5:18] Iterative adjust 3.49 -> 2.00
[5:18] pH 3.49 -> 2.00
[5:19] Air gap released for Acid (0.5 M HCl)
[5:20] Dispensed 0.042404 mL of Acid (0.5 M HCl)
[5:25] pH 2.02 -> 2.00
[5:25] Dispensed 0.002328 mL of Acid (0.5 M HCl)
[5:30] Holding pH 2.00
[7:30] Stirrer speed set to 0
[7:30] Stirrer speed set to 50
[7:30] Iterative adjust 1.95 -> 2.00
[7:30] pH 1.95 -> 2.00
[7:31] Air gap released for Base (0.5 M KOH)
[7:32] Dispensed 0.005527 mL of Base (0.5 M KOH)
[8:22] Stirrer speed set to 0
[8:33] Datapoint id 2 collected
[8:33] Stirrer speed set to 50
[8:38] pH 2.01 -> 2.21
[8:38] Using cautious pH adjust
[8:38] Dispensed 0.007808 mL of Base (0.5 M KOH)
[8:43] Stepping pH = 2.09
[8:44] Dispensed 0.006068 mL of Base (0.5 M KOH)
[8:49] Stepping pH = 2.19
[8:49] Dispensed 0.000753 mL of Base (0.5 M KOH)
[8:54] Stepping pH = 2.21
[9:09] Stirrer speed set to 0
[9:19] Datapoint id 3 collected
[9:19] Charge balance equation is out by 6.4%
[9:19] Stirrer speed set to 50

Experiment Log (continued)

[9:24] pH 2.22 -> 2.42
[9:24] Using charge balance adjust
[9:24] Dispensed 0.009548 mL of Base (0.5 M KOH)
[9:45] Stirrer speed set to 0
[9:55] Datapoint id 4 collected
[9:55] Charge balance equation is out by -0.4%
[9:55] Stirrer speed set to 50
[10:00] pH 2.43 -> 2.63
[10:00] Using charge balance adjust
[10:00] Dispensed 0.005974 mL of Base (0.5 M KOH)
[10:21] Stirrer speed set to 0
[10:31] Datapoint id 5 collected
[10:31] Charge balance equation is out by 5.5%
[10:31] Stirrer speed set to 50
[10:36] pH 2.65 -> 2.85
[10:36] Using charge balance adjust
[10:36] Dispensed 0.003763 mL of Base (0.5 M KOH)
[10:57] Stirrer speed set to 0
[11:07] Datapoint id 6 collected
[11:07] Charge balance equation is out by 4.1%
[11:07] Stirrer speed set to 50
[11:12] pH 2.87 -> 3.07
[11:12] Using charge balance adjust
[11:12] Dispensed 0.002540 mL of Base (0.5 M KOH)
[11:32] Stirrer speed set to 0
[11:43] Datapoint id 7 collected
[11:43] Charge balance equation is out by 10.5%
[11:43] Stirrer speed set to 50
[11:48] pH 3.10 -> 3.30
[11:48] Using charge balance adjust
[11:48] Dispensed 0.001858 mL of Base (0.5 M KOH)
[12:08] Stirrer speed set to 0
[12:18] Datapoint id 8 collected
[12:18] Charge balance equation is out by 30.9%
[12:18] Stirrer speed set to 50
[12:23] pH 3.36 -> 3.56
[12:23] Using cautious pH adjust
[12:23] Dispensed 0.000753 mL of Base (0.5 M KOH)
[12:28] Stepping pH = 3.52
[12:29] Dispensed 0.000212 mL of Base (0.5 M KOH)
[12:34] Stepping pH = 3.55
[12:34] Dispensed 0.000094 mL of Base (0.5 M KOH)
[12:39] Stepping pH = 3.55
[12:39] Dispensed 0.000118 mL of Base (0.5 M KOH)
[12:44] Stepping pH = 3.57
[12:59] Stirrer speed set to 0
[13:10] Datapoint id 9 collected
[13:10] Charge balance equation is out by 23.3%
[13:10] Stirrer speed set to 50
[13:15] pH 3.56 -> 3.76
[13:15] Using cautious pH adjust
[13:15] Dispensed 0.000682 mL of Base (0.5 M KOH)
[13:20] Stepping pH = 3.73
[13:20] Dispensed 0.000141 mL of Base (0.5 M KOH)
[13:25] Stepping pH = 3.74
[13:25] Dispensed 0.000188 mL of Base (0.5 M KOH)
[13:30] Stepping pH = 3.77
[13:45] Stirrer speed set to 0
[13:56] Datapoint id 10 collected

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[13:56] Charge balance equation is out by 25.9%
[13:56] Stirrer speed set to 50
[14:01] pH 3.74 -> 3.94
[14:01] Using cautious pH adjust
[14:01] Dispensed 0.000635 mL of Base (0.5 M KOH)
[14:06] Stepping pH = 3.89
[14:06] Dispensed 0.000188 mL of Base (0.5 M KOH)
[14:11] Stepping pH = 3.90
[14:11] Dispensed 0.000494 mL of Base (0.5 M KOH)
[14:16] Stepping pH = 4.00
[14:32] Stirrer speed set to 0
[14:43] Datapoint id 11 collected
[14:43] Charge balance equation is out by -4.2%
[14:43] Stirrer speed set to 50
[14:48] pH 3.94 -> 4.14
[14:48] Using charge balance adjust
[14:48] Dispensed 0.001082 mL of Base (0.5 M KOH)
[15:08] Stirrer speed set to 0
[15:22] Datapoint id 12 collected
[15:22] Charge balance equation is out by -32.8%
[15:22] Stirrer speed set to 50
[15:27] pH 4.08 -> 4.28
[15:27] Using cautious pH adjust
[15:27] Dispensed 0.000470 mL of Base (0.5 M KOH)
[15:32] Stepping pH = 4.19
[15:32] Dispensed 0.000259 mL of Base (0.5 M KOH)
[15:37] Stepping pH = 4.23
[15:37] Dispensed 0.000212 mL of Base (0.5 M KOH)
[15:42] Stepping pH = 4.26
[15:42] Dispensed 0.000094 mL of Base (0.5 M KOH)
[15:47] Stepping pH = 4.26
[15:48] Dispensed 0.000259 mL of Base (0.5 M KOH)
[15:53] Stepping pH = 4.34
[16:08] Stirrer speed set to 0
[16:22] Datapoint id 13 collected
[16:22] Charge balance equation is out by -36.9%
[16:22] Stirrer speed set to 50
[16:27] pH 4.26 -> 4.46
[16:27] Using cautious pH adjust
[16:27] Dispensed 0.000376 mL of Base (0.5 M KOH)
[16:33] Stepping pH = 4.41
[16:33] Dispensed 0.000094 mL of Base (0.5 M KOH)
[16:38] Stepping pH = 4.41
[16:38] Dispensed 0.000259 mL of Base (0.5 M KOH)
[16:43] Stepping pH = 4.58
[16:58] Stirrer speed set to 0
[17:19] Datapoint id 14 collected
[17:19] Charge balance equation is out by -0.5%
[17:19] Stirrer speed set to 50
[17:24] pH 4.50 -> 4.70
[17:24] Using charge balance adjust
[17:24] Dispensed 0.000517 mL of Base (0.5 M KOH)
[17:44] Stirrer speed set to 0
[18:07] Datapoint id 15 collected
[18:07] Charge balance equation is out by 114.9%
[18:07] Stirrer speed set to 50
[18:12] pH 4.88 -> 5.08
[18:12] Using cautious pH adjust
[18:12] Dispensed 0.000118 mL of Base (0.5 M KOH)

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[18:17] Stepping pH = 4.87
[18:17] Dispensed 0.000635 mL of Base (0.5 M KOH)
[18:22] Stepping pH = 9.43
[18:37] Stirrer speed set to 0
[19:37] Datapoint id 16 collected
[19:37] Charge balance equation is out by -207.2%
[19:37] Titration 2 of 3
[19:37] Adding initial titrants
[19:37] Automatically add 0.30000 mL of Octanol
[19:44] Dispensed 0.300000 mL of Octanol
[19:44] Stirrer speed set to 10
[19:45] Stirrer speed set to 55
[19:45] Iterative adjust 9.03 -> 2.00
[19:45] pH 9.03 -> 2.00
[19:47] Dispensed 0.052140 mL of Acid (0.5 M HCl)
[19:52] pH 2.02 -> 2.00
[19:52] Dispensed 0.001670 mL of Acid (0.5 M HCl)
[20:42] Stirrer speed set to 0
[21:01] Datapoint id 17 collected
[21:01] Stirrer speed set to 55
[21:06] pH 1.95 -> 2.15
[21:06] Using cautious pH adjust
[21:07] Dispensed 0.009525 mL of Base (0.5 M KOH)
[21:12] Stepping pH = 2.05
[21:12] Dispensed 0.006279 mL of Base (0.5 M KOH)
[21:17] Stepping pH = 2.13
[21:17] Dispensed 0.001670 mL of Base (0.5 M KOH)
[21:22] Stepping pH = 2.15
[21:38] Stirrer speed set to 0
[21:48] Datapoint id 18 collected
[21:48] Charge balance equation is out by 8.3%
[21:48] Stirrer speed set to 55
[21:53] pH 2.16 -> 2.36
[21:53] Using charge balance adjust
[21:53] Dispensed 0.011759 mL of Base (0.5 M KOH)
[22:13] Stirrer speed set to 0
[22:24] Datapoint id 19 collected
[22:24] Charge balance equation is out by 2.3%
[22:24] Stirrer speed set to 55
[22:29] pH 2.38 -> 2.58
[22:29] Using charge balance adjust
[22:29] Dispensed 0.007314 mL of Base (0.5 M KOH)
[22:49] Stirrer speed set to 0
[22:59] Datapoint id 20 collected
[22:59] Charge balance equation is out by 0.9%
[22:59] Stirrer speed set to 55
[23:04] pH 2.59 -> 2.79
[23:04] Using charge balance adjust
[23:05] Dispensed 0.004774 mL of Base (0.5 M KOH)
[23:25] Stirrer speed set to 0
[23:35] Datapoint id 21 collected
[23:35] Charge balance equation is out by 2.4%
[23:35] Stirrer speed set to 55
[23:40] pH 2.81 -> 3.01
[23:40] Using charge balance adjust
[23:40] Dispensed 0.003269 mL of Base (0.5 M KOH)
[24:01] Stirrer speed set to 0
[24:11] Datapoint id 22 collected
[24:11] Charge balance equation is out by -4.9%

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[24:11] Stirrer speed set to 55
[24:16] pH 3.01 -> 3.21
[24:16] Using charge balance adjust
[24:16] Dispensed 0.002469 mL of Base (0.5 M KOH)
[24:36] Stirrer speed set to 0
[24:46] Datapoint id 23 collected
[24:46] Charge balance equation is out by -3.0%
[24:46] Stirrer speed set to 55
[24:51] pH 3.21 -> 3.41
[24:51] Using charge balance adjust
[24:51] Dispensed 0.001952 mL of Base (0.5 M KOH)
[25:11] Stirrer speed set to 0
[25:22] Datapoint id 24 collected
[25:22] Charge balance equation is out by 54.8%
[25:22] Stirrer speed set to 55
[25:27] pH 3.53 -> 3.73
[25:27] Using cautious pH adjust
[25:27] Dispensed 0.000706 mL of Base (0.5 M KOH)
[25:32] Stepping pH = 3.68
[25:32] Dispensed 0.000235 mL of Base (0.5 M KOH)
[25:37] Stepping pH = 3.73
[25:52] Stirrer speed set to 0
[26:03] Datapoint id 25 collected
[26:03] Charge balance equation is out by 34.0%
[26:03] Stirrer speed set to 55
[26:08] pH 3.72 -> 3.92
[26:08] Using cautious pH adjust
[26:09] Dispensed 0.000564 mL of Base (0.5 M KOH)
[26:14] Stepping pH = 3.85
[26:14] Dispensed 0.000188 mL of Base (0.5 M KOH)
[26:19] Stepping pH = 3.89
[26:19] Dispensed 0.000094 mL of Base (0.5 M KOH)
[26:24] Stepping pH = 3.90
[26:24] Dispensed 0.000094 mL of Base (0.5 M KOH)
[26:29] Stepping pH = 3.92
[26:44] Stirrer speed set to 0
[26:56] Datapoint id 26 collected
[26:56] Charge balance equation is out by 15.5%
[26:56] Stirrer speed set to 55
[27:01] pH 3.89 -> 4.09
[27:01] Using cautious pH adjust
[27:01] Dispensed 0.000447 mL of Base (0.5 M KOH)
[27:06] Stepping pH = 4.03
[27:06] Dispensed 0.000141 mL of Base (0.5 M KOH)
[27:11] Stepping pH = 4.06
[27:11] Dispensed 0.000118 mL of Base (0.5 M KOH)
[27:16] Stepping pH = 4.09
[27:32] Stirrer speed set to 0
[27:45] Datapoint id 27 collected
[27:45] Charge balance equation is out by 19.9%
[27:45] Stirrer speed set to 55
[27:50] pH 4.06 -> 4.26
[27:50] Using cautious pH adjust
[27:50] Dispensed 0.000329 mL of Base (0.5 M KOH)
[27:55] Stepping pH = 4.19
[27:55] Dispensed 0.000118 mL of Base (0.5 M KOH)
[28:00] Stepping pH = 4.23
[28:00] Dispensed 0.000071 mL of Base (0.5 M KOH)
[28:05] Stepping pH = 4.25

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[28:20] Stirrer speed set to 0
[28:30] Datapoint id 28 collected
[28:30] Charge balance equation is out by 21.2%
[28:30] Stirrer speed set to 55
[28:35] pH 4.24 -> 4.44
[28:35] Using cautious pH adjust
[28:35] Dispensed 0.000235 mL of Base (0.5 M KOH)
[28:41] Stepping pH = 4.39
[28:41] Dispensed 0.000071 mL of Base (0.5 M KOH)
[28:46] Stepping pH = 4.39
[28:46] Dispensed 0.000165 mL of Base (0.5 M KOH)
[28:51] Stepping pH = 4.52
[29:06] Stirrer speed set to 0
[29:18] Datapoint id 29 collected
[29:18] Charge balance equation is out by -0.7%
[29:18] Stirrer speed set to 55
[29:23] pH 4.50 -> 4.70
[29:23] Using charge balance adjust
[29:23] Dispensed 0.000282 mL of Base (0.5 M KOH)
[29:43] Stirrer speed set to 0
[30:07] Datapoint id 30 collected
[30:07] Charge balance equation is out by 24.6%
[30:07] Stirrer speed set to 55
[30:12] pH 4.75 -> 4.95
[30:12] Using cautious pH adjust
[30:12] Dispensed 0.000094 mL of Base (0.5 M KOH)
[30:17] Stepping pH = 4.80
[30:17] Dispensed 0.000141 mL of Base (0.5 M KOH)
[30:22] Stepping pH = 5.09
[30:37] Stirrer speed set to 0
[30:50] Datapoint id 31 collected
[30:50] Charge balance equation is out by -26.9%
[30:50] Stirrer speed set to 55
[30:55] pH 5.05 -> 5.25
[30:55] Using cautious pH adjust
[30:55] Dispensed 0.000047 mL of Base (0.5 M KOH)
[31:00] Stepping pH = 5.07
[31:00] Dispensed 0.000118 mL of Base (0.5 M KOH)
[31:05] Stepping pH = 5.37
[31:21] Stirrer speed set to 0
[31:34] Datapoint id 32 collected
[31:34] Charge balance equation is out by -86.8%
[31:34] Stirrer speed set to 55
[31:39] pH 5.41 -> 5.61
[31:39] Using cautious pH adjust
[31:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[31:44] Stepping pH = 5.40
[31:44] Dispensed 0.000141 mL of Base (0.5 M KOH)
[31:49] Stepping pH = 6.97
[32:05] Stirrer speed set to 0
[33:05] Datapoint id 33 collected
[33:05] Charge balance equation is out by -201.9%
[33:05] Stirrer speed set to 55
[33:10] pH 6.45 -> 6.65
[33:10] Using cautious pH adjust
[33:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[33:15] Stepping pH = 6.42
[33:15] Dispensed 0.000118 mL of Base (0.5 M KOH)
[33:20] Stepping pH = 8.04

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[33:35] Stirrer speed set to 0
[34:35] Datapoint id 34 collected
[34:35] Charge balance equation is out by -241.6%
[34:35] Stirrer speed set to 55
[34:40] pH 7.57 -> 7.77
[34:40] Using cautious pH adjust
[34:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[34:45] Stepping pH = 7.53
[34:45] Dispensed 0.000047 mL of Base (0.5 M KOH)
[34:51] Stepping pH = 7.84
[35:06] Stirrer speed set to 0
[36:06] Datapoint id 35 collected
[36:06] Charge balance equation is out by -393.8%
[36:06] Stirrer speed set to 55
[36:11] pH 7.75 -> 7.95
[36:11] Using cautious pH adjust
[36:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:16] Stepping pH = 7.80
[36:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:21] Stepping pH = 8.02
[36:36] Stirrer speed set to 0
[37:36] Datapoint id 36 collected
[37:36] Charge balance equation is out by -332.8%
[37:36] Stirrer speed set to 55
[37:41] pH 8.03 -> 8.23
[37:41] Using cautious pH adjust
[37:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[37:46] Stepping pH = 8.20
[37:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[37:52] Stepping pH = 8.36
[38:07] Stirrer speed set to 0
[38:57] Datapoint id 37 collected
[38:57] Charge balance equation is out by -361.1%
[38:57] Stirrer speed set to 55
[39:02] pH 8.24 -> 8.44
[39:02] Using cautious pH adjust
[39:02] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:07] Stepping pH = 8.35
[39:07] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:13] Stepping pH = 8.60
[39:28] Stirrer speed set to 0
[40:02] Datapoint id 38 collected
[40:02] Charge balance equation is out by -280.6%
[40:02] Stirrer speed set to 55
[40:07] pH 8.66 -> 8.86
[40:07] Using cautious pH adjust
[40:07] Dispensed 0.000024 mL of Base (0.5 M KOH)
[40:12] Stepping pH = 8.70
[40:12] Dispensed 0.000024 mL of Base (0.5 M KOH)
[40:17] Stepping pH = 8.80
[40:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[40:22] Stepping pH = 8.89
[40:37] Stirrer speed set to 0
[41:02] Datapoint id 39 collected
[41:02] Charge balance equation is out by -172.2%
[41:02] Stirrer speed set to 55
[41:07] pH 8.88 -> 9.05
[41:07] Using cautious pH adjust
[41:07] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[41:12] Stepping pH = 8.90
[41:12] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:17] Stepping pH = 8.98
[41:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:22] Stepping pH = 9.07
[41:37] Stirrer speed set to 0
[41:56] Datapoint id 40 collected
[41:56] Charge balance equation is out by -170.5%
[41:56] Titration 3 of 3
[41:56] Adding initial titrants
[41:56] Automatically add 0.70000 mL of Octanol
[42:44] Dispensed 0.700000 mL of Octanol
[42:44] Stirrer speed set to 10
[42:45] Stirrer speed set to 60
[42:45] Iterative adjust 9.02 -> 2.00
[42:45] pH 9.02 -> 2.00
[42:47] Dispensed 0.054727 mL of Acid (0.5 M HCl)
[42:52] pH 2.03 -> 2.00
[42:52] Dispensed 0.003175 mL of Acid (0.5 M HCl)
[43:42] Stirrer speed set to 0
[43:52] Datapoint id 41 collected
[43:52] Stirrer speed set to 60
[43:57] pH 1.96 -> 2.16
[43:57] Using cautious pH adjust
[43:58] Dispensed 0.009972 mL of Base (0.5 M KOH)
[44:03] Stepping pH = 2.05
[44:03] Dispensed 0.007596 mL of Base (0.5 M KOH)
[44:08] Stepping pH = 2.14
[44:08] Dispensed 0.001317 mL of Base (0.5 M KOH)
[44:13] Stepping pH = 2.16
[44:28] Stirrer speed set to 0
[44:39] Datapoint id 42 collected
[44:39] Charge balance equation is out by 5.2%
[44:39] Stirrer speed set to 60
[44:44] pH 2.16 -> 2.36
[44:44] Using charge balance adjust
[44:44] Dispensed 0.012817 mL of Base (0.5 M KOH)
[45:05] Stirrer speed set to 0
[45:23] Datapoint id 43 collected
[45:23] Charge balance equation is out by 5.4%
[45:23] Stirrer speed set to 60
[45:28] pH 2.38 -> 2.58
[45:28] Using charge balance adjust
[45:28] Dispensed 0.007973 mL of Base (0.5 M KOH)
[45:48] Stirrer speed set to 0
[45:58] Datapoint id 44 collected
[45:58] Charge balance equation is out by 3.7%
[45:58] Stirrer speed set to 60
[46:03] pH 2.59 -> 2.79
[46:03] Using charge balance adjust
[46:04] Dispensed 0.005292 mL of Base (0.5 M KOH)
[46:24] Stirrer speed set to 0
[46:34] Datapoint id 45 collected
[46:34] Charge balance equation is out by 12.0%
[46:34] Stirrer speed set to 60
[46:39] pH 2.82 -> 3.02
[46:39] Using charge balance adjust
[46:40] Dispensed 0.003575 mL of Base (0.5 M KOH)
[47:00] Stirrer speed set to 0

Sample name: **M13_octanol**   Experiment start time: **3/26/2018 4:16:35 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-26010**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[47:10] Datapoint id 46 collected
[47:10] Charge balance equation is out by -4.8%
[47:10] Stirrer speed set to 60
[47:15] pH 3.02 -> 3.22
[47:15] Using charge balance adjust
[47:15] Dispensed 0.002634 mL of Base (0.5 M KOH)
[47:35] Stirrer speed set to 0
[47:45] Datapoint id 47 collected
[47:45] Charge balance equation is out by 7.7%
[47:45] Stirrer speed set to 60
[47:50] pH 3.25 -> 3.45
[47:50] Using charge balance adjust
[47:51] Dispensed 0.001881 mL of Base (0.5 M KOH)
[48:11] Stirrer speed set to 0
[48:21] Datapoint id 48 collected
[48:21] Charge balance equation is out by 17.5%
[48:21] Stirrer speed set to 60
[48:26] pH 3.49 -> 3.69
[48:26] Using cautious pH adjust
[48:26] Dispensed 0.000635 mL of Base (0.5 M KOH)
[48:31] Stepping pH = 3.59
[48:31] Dispensed 0.000400 mL of Base (0.5 M KOH)
[48:36] Stepping pH = 3.66
[48:36] Dispensed 0.000141 mL of Base (0.5 M KOH)
[48:41] Stepping pH = 3.68
[48:57] Stirrer speed set to 0
[49:07] Datapoint id 49 collected
[49:07] Charge balance equation is out by 7.9%
[49:07] Stirrer speed set to 60
[49:12] pH 3.68 -> 3.88
[49:12] Using charge balance adjust
[49:12] Dispensed 0.000917 mL of Base (0.5 M KOH)
[49:32] Stirrer speed set to 0
[49:51] Datapoint id 50 collected
[49:51] Charge balance equation is out by 2.2%
[49:51] Stirrer speed set to 60
[49:56] pH 3.90 -> 4.10
[49:56] Using charge balance adjust
[49:56] Dispensed 0.000588 mL of Base (0.5 M KOH)
[50:16] Stirrer speed set to 0
[50:28] Datapoint id 51 collected
[50:28] Charge balance equation is out by -30.8%
[50:28] Stirrer speed set to 60
[50:33] pH 4.05 -> 4.25
[50:33] Using cautious pH adjust
[50:33] Dispensed 0.000212 mL of Base (0.5 M KOH)
[50:38] Stepping pH = 4.09
[50:38] Dispensed 0.000353 mL of Base (0.5 M KOH)
[50:43] Stepping pH = 4.29
[50:58] Stirrer speed set to 0
[51:08] Datapoint id 52 collected
[51:08] Charge balance equation is out by -28.1%
[51:08] Stirrer speed set to 60
[51:14] pH 4.27 -> 4.47
[51:14] Using cautious pH adjust
[51:14] Dispensed 0.000141 mL of Base (0.5 M KOH)
[51:19] Stepping pH = 4.30
[51:19] Dispensed 0.000306 mL of Base (0.5 M KOH)
[51:24] Stepping pH = 4.59

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[51:39] Stirrer speed set to 0
[51:49] Datapoint id 53 collected
[51:49] Charge balance equation is out by -65.4%
[51:49] Stirrer speed set to 60
[51:54] pH 4.58 -> 4.78
[51:54] Using cautious pH adjust
[51:54] Dispensed 0.000071 mL of Base (0.5 M KOH)
[51:59] Stepping pH = 4.59
[51:59] Dispensed 0.000212 mL of Base (0.5 M KOH)
[52:04] Stepping pH = 4.99
[52:19] Stirrer speed set to 0
[52:29] Datapoint id 54 collected
[52:29] Charge balance equation is out by -96.2%
[52:29] Stirrer speed set to 60
[52:35] pH 4.97 -> 5.17
[52:35] Using cautious pH adjust
[52:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[52:40] Stepping pH = 4.97
[52:40] Dispensed 0.000094 mL of Base (0.5 M KOH)
[52:45] Stepping pH = 5.07
[52:45] Dispensed 0.000047 mL of Base (0.5 M KOH)
[52:50] Stepping pH = 5.19
[53:05] Stirrer speed set to 0
[53:15] Datapoint id 55 collected
[53:15] Charge balance equation is out by -183.3%
[53:15] Stirrer speed set to 60
[53:20] pH 5.19 -> 5.39
[53:20] Using cautious pH adjust
[53:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:25] Stepping pH = 5.20
[53:25] Dispensed 0.000047 mL of Base (0.5 M KOH)
[53:31] Stepping pH = 5.35
[53:31] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:36] Stepping pH = 5.46
[53:51] Stirrer speed set to 0
[54:01] Datapoint id 56 collected
[54:01] Charge balance equation is out by -136.9%
[54:01] Stirrer speed set to 60
[54:06] pH 5.47 -> 5.67
[54:06] Using cautious pH adjust
[54:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:11] Stepping pH = 5.50
[54:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:16] Stepping pH = 5.63
[54:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:21] Stepping pH = 5.79
[54:36] Stirrer speed set to 0
[54:47] Datapoint id 57 collected
[54:47] Charge balance equation is out by -142.7%
[54:47] Stirrer speed set to 60
[54:52] pH 5.85 -> 6.05
[54:52] Using cautious pH adjust
[54:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:57] Stepping pH = 5.91
[54:57] Dispensed 0.000024 mL of Base (0.5 M KOH)
[55:02] Stepping pH = 6.14
[55:17] Stirrer speed set to 0
[55:38] Datapoint id 58 collected
[55:38] Charge balance equation is out by -37.8%

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[55:38] Stirrer speed set to 60
[55:43] pH 6.09 -> 6.29
[55:43] Using cautious pH adjust
[55:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[55:48] Stepping pH = 6.20
[55:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[55:53] Stepping pH = 6.54
[56:08] Stirrer speed set to 0
[56:42] Datapoint id 59 collected
[56:42] Charge balance equation is out by -15.1%
[56:42] Stirrer speed set to 60
[56:47] pH 6.56 -> 6.76
[56:47] Using cautious pH adjust
[56:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:52] Stepping pH = 6.65
[56:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:57] Stepping pH = 6.97
[57:12] Stirrer speed set to 0
[58:11] Datapoint id 60 collected
[58:11] Charge balance equation is out by 3.8%
[58:11] Stirrer speed set to 60
[58:16] pH 6.99 -> 7.19
[58:16] Using charge balance adjust
[58:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:37] Stirrer speed set to 0
[59:19] Datapoint id 61 collected
[59:19] Charge balance equation is out by -18.2%
[59:19] Stirrer speed set to 60
[59:24] pH 6.94 -> 7.14
[59:24] Using cautious pH adjust
[59:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:29] Stepping pH = 6.99
[59:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:34] Stepping pH = 7.34
[59:49] Stirrer speed set to 0
[1:00:49] Datapoint id 62 collected
[1:00:49] Charge balance equation is out by -30.8%
[1:00:49] Stirrer speed set to 60
[1:00:54] pH 7.34 -> 7.54
[1:00:54] Using cautious pH adjust
[1:00:55] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:00] Stepping pH = 7.38
[1:01:00] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:05] Stepping pH = 7.84
[1:01:20] Stirrer speed set to 0
[1:02:20] Datapoint id 63 collected
[1:02:20] Charge balance equation is out by -73.9%
[1:02:20] Stirrer speed set to 60
[1:02:25] pH 7.88 -> 8.08
[1:02:25] Using cautious pH adjust
[1:02:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:30] Stepping pH = 7.97
[1:02:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:02:35] Stepping pH = 8.26
[1:02:50] Stirrer speed set to 0
[1:03:33] Datapoint id 64 collected
[1:03:33] Charge balance equation is out by -237.4%
[1:03:33] Stirrer speed set to 60
[1:03:38] pH 8.20 -> 8.40

Sample name: **M13_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-26010**
Filename: **C:\Sirius_T3\Mehtap\20180327_exp34_logP_T3-2\18C-26010_M13_octanol_pH-metric high logP.t3r**

Experiment start time: **3/26/2018 4:16:35 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:03:38] Using cautious pH adjust
[1:03:38] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:43] Stepping pH = 8.28
[1:03:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:48] Stepping pH = 8.53
[1:04:03] Stirrer speed set to 0
[1:04:38] Datapoint id 65 collected
[1:04:38] Charge balance equation is out by -230.0%
[1:04:38] Stirrer speed set to 60
[1:04:43] pH 8.49 -> 8.69
[1:04:43] Using cautious pH adjust
[1:04:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:48] Stepping pH = 8.55
[1:04:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:53] Stepping pH = 8.71
[1:05:08] Stirrer speed set to 0
[1:05:37] Datapoint id 66 collected
[1:05:37] Charge balance equation is out by -127.2%
[1:05:37] Stirrer speed set to 60
[1:05:42] pH 8.71 -> 8.91
[1:05:42] Using cautious pH adjust
[1:05:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:05:47] Stepping pH = 8.74
[1:05:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:05:53] Stepping pH = 8.87
[1:05:53] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:05:58] Stepping pH = 8.98
[1:06:13] Stirrer speed set to 0
[1:06:41] Datapoint id 67 collected
[1:06:41] Charge balance equation is out by -152.4%
[1:06:41] Stirrer speed set to 60
[1:06:46] pH 8.97 -> 9.05
[1:06:46] Using cautious pH adjust
[1:06:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:06:51] Stepping pH = 9.00
[1:07:06] Stirrer speed set to 0
[1:07:33] Datapoint id 68 collected
[1:07:33] Charge balance equation is out by -27.6%
[1:07:33] Argon flow rate set to 0
[1:07:37] Titrator arm moved over Titration position
[1:07:58] The autoloader failed to pick at location "Sample position"