pH-metric Result

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH +)   -9.50   ±0.85 (n=47)
logP (neutral X)   2.90   ±0.02 (n=47)

18C-02010 Points 1 to 22

M09_octanol concentration factor   1.064
Carbonate   0.0587 mM
Acidity error   -0.83134 mM

18C-02010 Points 23 to 44

M09_octanol concentration factor   0.800
Carbonate   0.0538 mM
Acidity error   -0.43636 mM

18C-02010 Points 45 to 64

M09_octanol concentration factor   1.103
Carbonate   0.1700 mM
Acidity error   -0.97715 mM

Warnings and errors

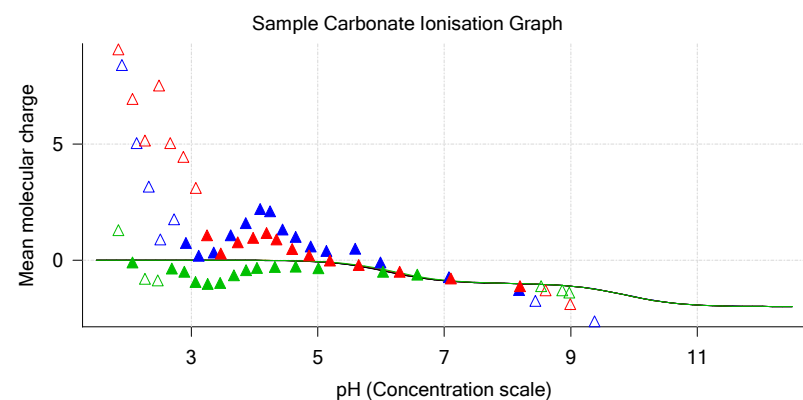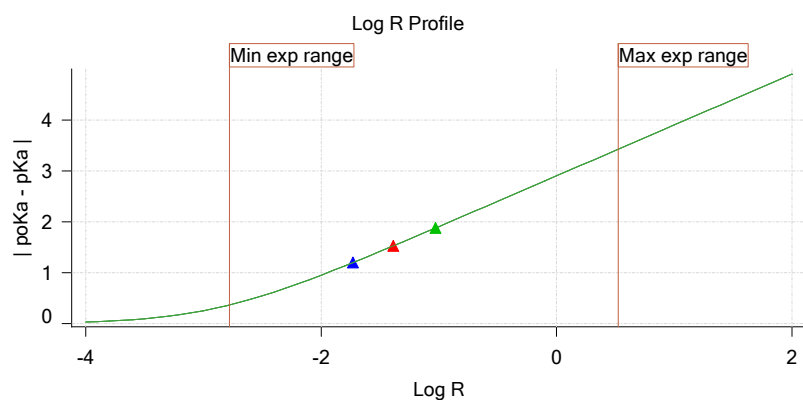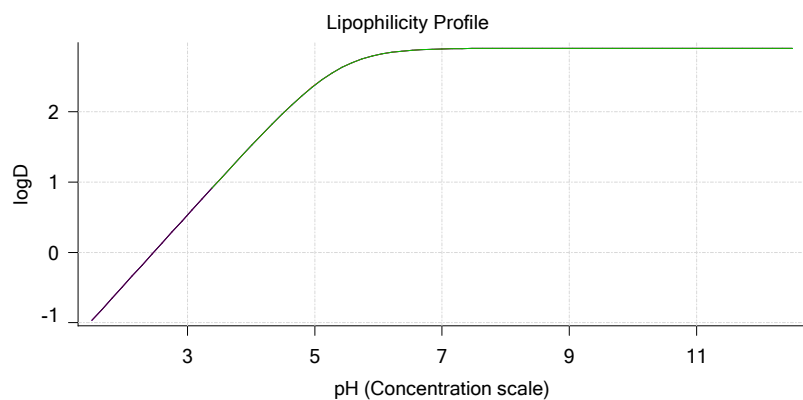Errors   None
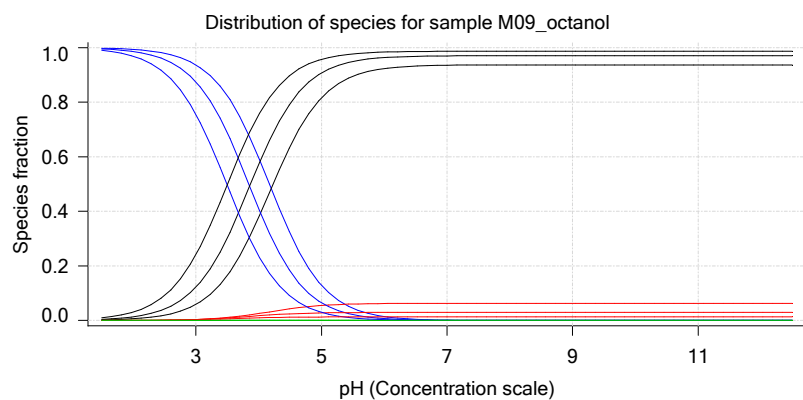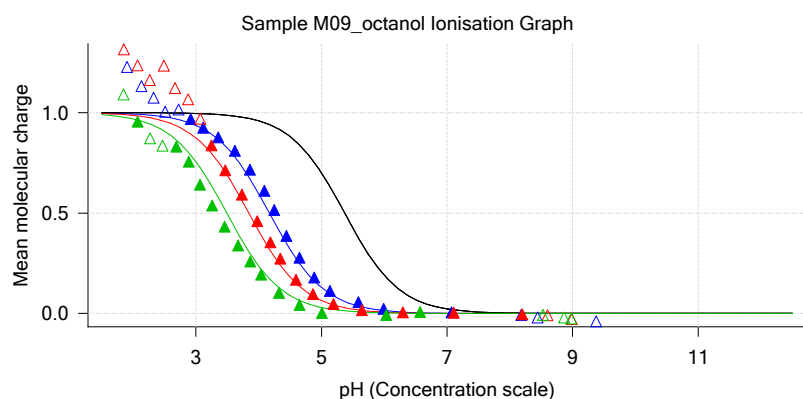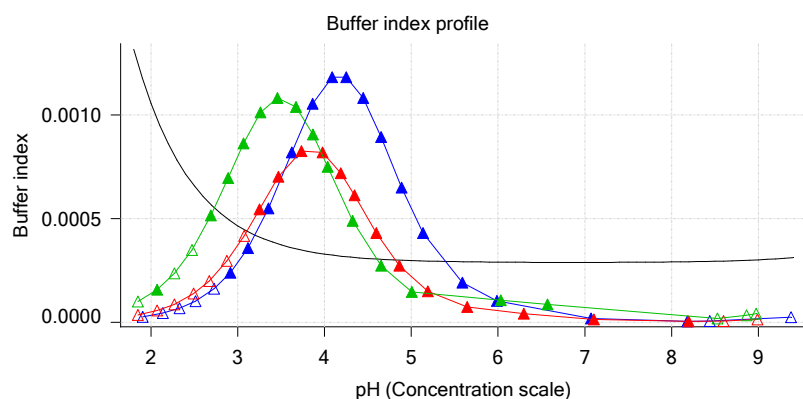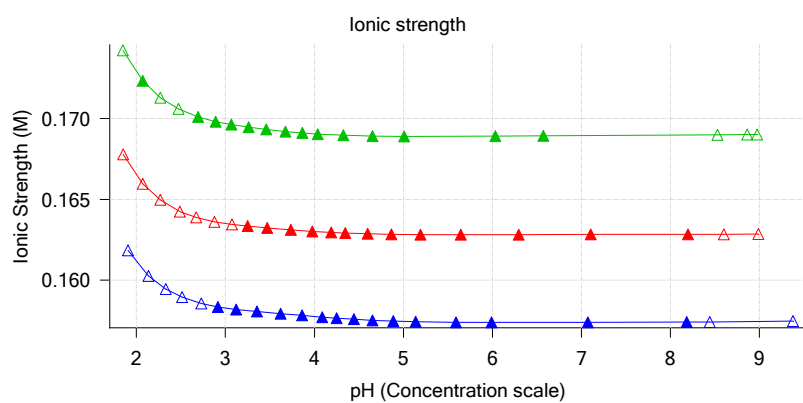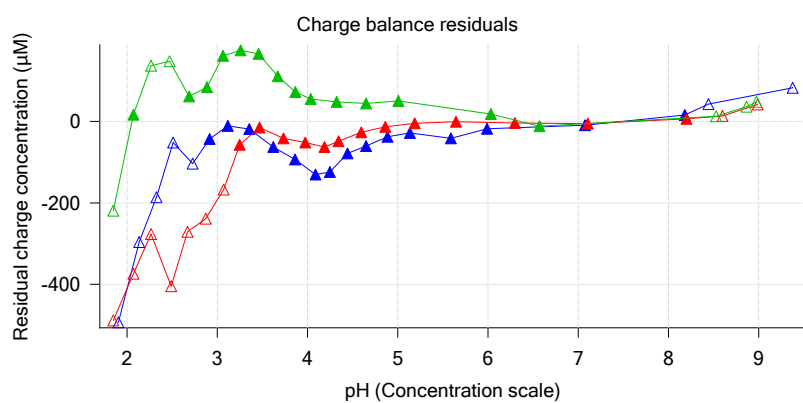Warnings   One or more logP values out of range

Sample logD and percent species

pH	M09_octanol logD	M09_octanol M09_octanolH	M09_octanol M09_octanol	M09_octanol M09_octanolH*	M09_octanol M09_octanol*	Comment
1.000	-1.47	96.71 %	0.00 %	0.00 %	3.29 %	
1.200	-1.27	94.88 %	0.01 %	0.00 %	5.11 %	Stomach pH
2.000	-0.47	74.60 %	0.03 %	0.00 %	25.37 %	
3.000	0.53	22.70 %	0.10 %	0.00 %	77.20 %	
4.000	1.51	2.85 %	0.12 %	0.00 %	97.03 %	
5.000	2.38	0.29 %	0.12 %	0.00 %	99.58 %	
6.000	2.81	0.03 %	0.13 %	0.00 %	99.85 %	
6.500	2.87	0.01 %	0.13 %	0.00 %	99.87 %	
7.000	2.89	0.00 %	0.13 %	0.00 %	99.87 %	
7.400	2.90	0.00 %	0.13 %	0.00 %	99.87 %	Blood pH
8.000	2.90	0.00 %	0.13 %	0.00 %	99.87 %	
9.000	2.90	0.00 %	0.13 %	0.00 %	99.87 %	
10.000	2.90	0.00 %	0.13 %	0.00 %	99.87 %	
11.000	2.90	0.00 %	0.13 %	0.00 %	99.87 %	
12.000	2.90	0.00 %	0.13 %	0.00 %	99.87 %	

pH-metric Result

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M09_octanol Ionisation Graph

Distribution of species for sample M09_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)

Distribution of species for sample Carbonate

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
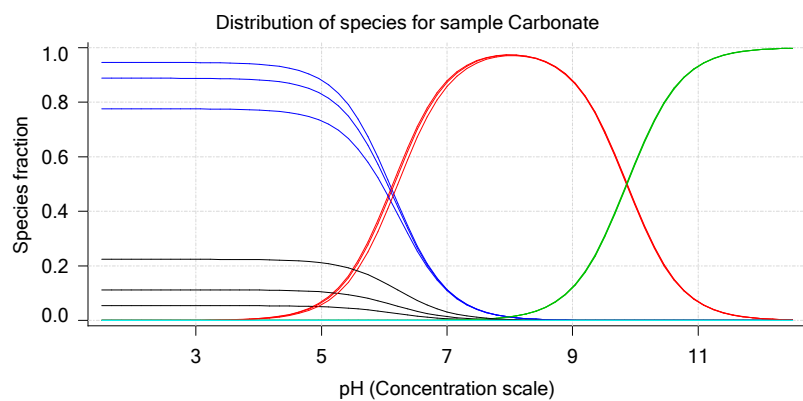Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 1 of 3   18C-02010 Points 1 to 22

Overall results

RMSD	0.413
Average ionic strength	0.158 M
Average temperature	24.9°C
Partition ratio	0.0186 : 1
Analyte concentration range	1902.7 µM to 1959.6 µM
Total points considered	15 of 22

Warnings and errors

Errors   None
Warnings None

Four-Plus parameters

Alpha	0.111	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r
S	0.9988	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r
jH	1.0	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r
jOH	-0.8	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r

Titrants

0.50 M HCl	0.999058	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH	0.999845	3/2/2018 10:00:20 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M09_octanol concentration factor	1.064
M09_octanol stoichiometry	1.000
Chloride stoichiometry	1.000
Base pKa 1	5.37
logP (XH +)	0.48
logP (neutral X)	2.84

Sample graphs

Ionisation of sample M09_octanol

Distribution of species for sample M09_octanol

Sample name: **M09_octanol**   Experiment start time: **3/2/2018 10:00:20 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-02010**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Sample graphs (continued)

Lipophilicity Profile
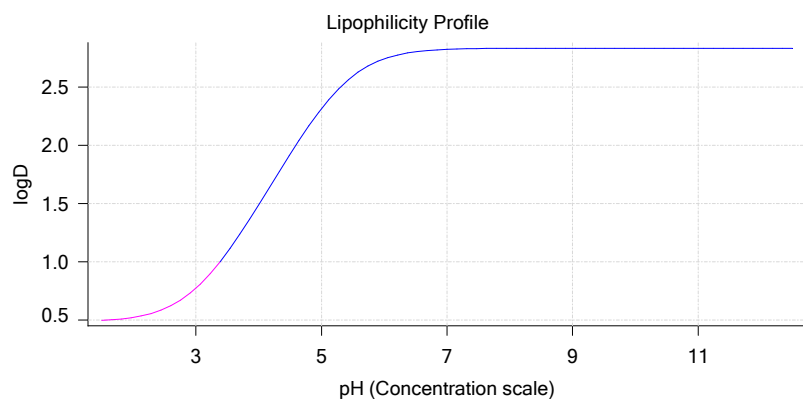
Sample logD and percent species

pH	M09_octanol logD	M09_octanol M09_octanolH	M09_octanol M09_octanol	M09_octanol M09_octanolH*	M09_octanol M09_octanol*	Comment
1.000	0.49	94.58 %	0.00 %	5.36 %	0.05 %	
1.200	0.49	94.55 %	0.01 %	5.36 %	0.08 %	Stomach pH
2.000	0.52	94.11 %	0.04 %	5.34 %	0.51 %	
3.000	0.77	89.67 %	0.38 %	5.08 %	4.86 %	
4.000	1.49	60.91 %	2.60 %	3.45 %	33.04 %	
5.000	2.32	14.48 %	6.17 %	0.82 %	78.53 %	
6.000	2.74	1.68 %	7.16 %	0.10 %	91.07 %	
6.500	2.80	0.54 %	7.25 %	0.03 %	92.18 %	
7.000	2.83	0.17 %	7.28 %	0.01 %	92.54 %	
7.400	2.83	0.07 %	7.28 %	0.00 %	92.64 %	Blood pH
8.000	2.83	0.02 %	7.29 %	0.00 %	92.69 %	
9.000	2.83	0.00 %	7.29 %	0.00 %	92.71 %	
10.000	2.84	0.00 %	7.29 %	0.00 %	92.71 %	
11.000	2.84	0.00 %	7.29 %	0.00 %	92.71 %	
12.000	2.84	0.00 %	7.29 %	0.00 %	92.71 %	

Carbonate and acidity

Carbonate   0.059 mM
Acidity error   -0.831 mM

Other graphs
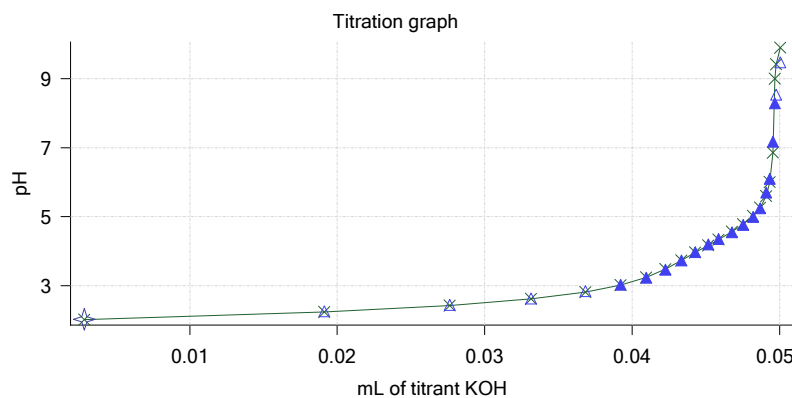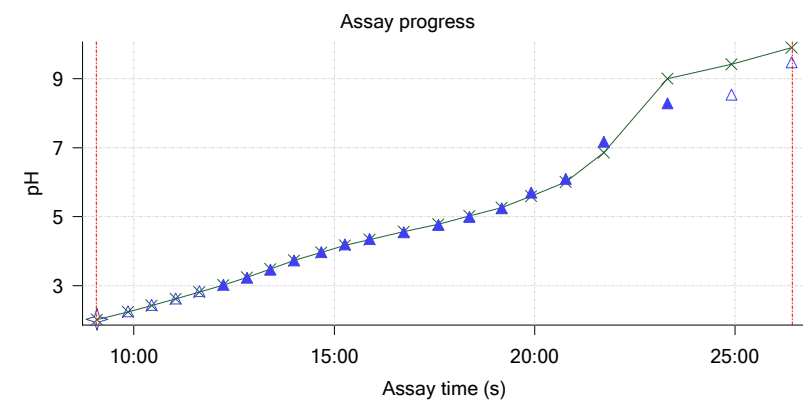
Assay progress

Titration graph

Sample name: **M09_octanol**　　　　　　　　　　　Experiment start time: **3/2/2018 10:00:20 PM**
Assay name: **pH-metric high logP**　　　　　　　　Analyst: **Pion**
Assay ID: **18C-02010**　　　　　　　　　　　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Min exp range　　　　　Max exp range

Ionisation of sample Carbonate

6.11　　　　9.87
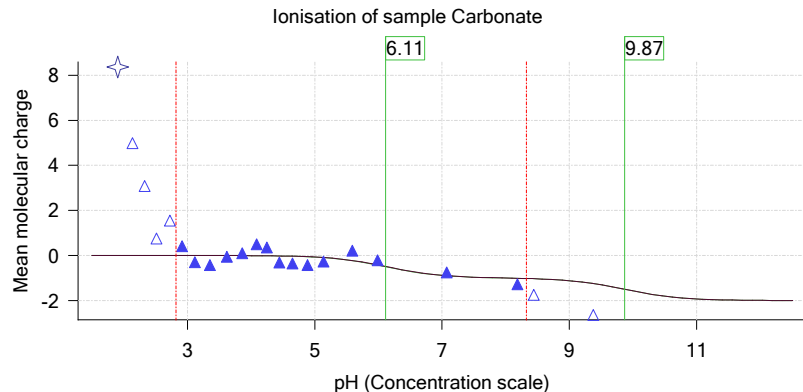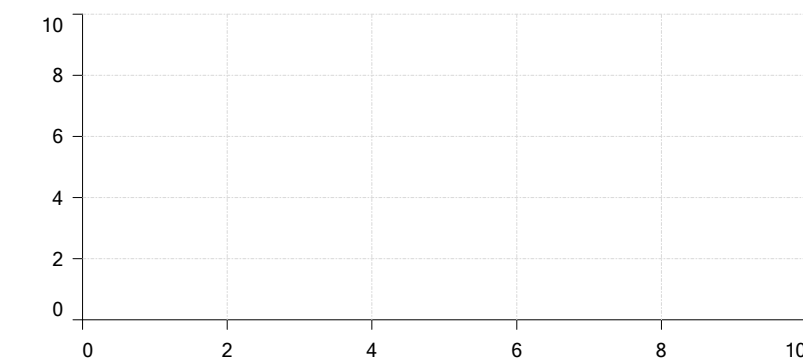
Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 2 of 3   18C-02010 Points 23 to 44

Overall results

RMSD	0.195
Average ionic strength	0.163 M
Average temperature	25.0°C
Partition ratio	0.0409 : 1
Analyte concentration range	1744.4 µM to 1798.6 µM
Total points considered	13 of 22

Warnings and errors

Errors   None
Warnings None

Four-Plus parameters

	Alpha	0.111	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r
	S	0.9988	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r
	jH	1.0	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r
	jOH	-0.8	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r

Titrants

	0.50 M HCl	0.999058	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r
	0.50 M KOH	0.999845	3/2/2018 10:00:20 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M09_octanol concentration factor	0.800
M09_octanol stoichiometry	1.000
Chloride stoichiometry	1.000
Base pKa 1	5.37
logP (XH +)	0.84
logP (neutral X)	2.95

Sample graphs

Ionisation of sample M09_octanol

Distribution of species for sample M09_octanol

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
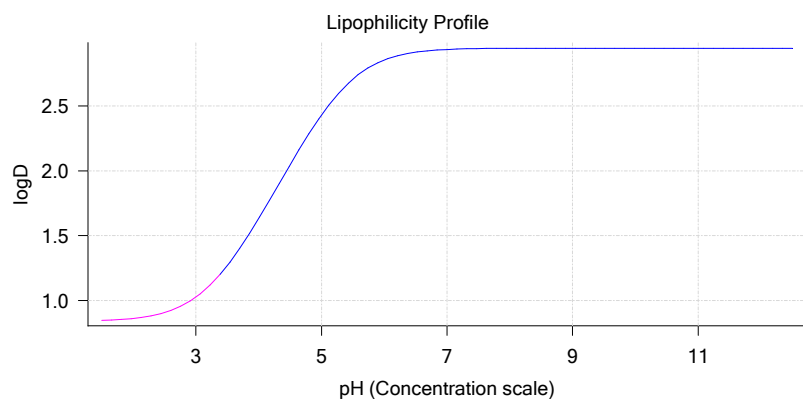
Sample logD and percent species

pH	M09_octanol logD	M09_octanol M09_octanolH	M09_octanol M09_octanol	M09_octanol M09_octanolH*	M09_octanol M09_octanol*	Comment
1.000	0.84	77.94 %	0.00 %	21.93 %	0.12 %	
1.200	0.84	77.89 %	0.01 %	21.92 %	0.19 %	Stomach pH
2.000	0.86	77.09 %	0.03 %	21.69 %	1.19 %	
3.000	1.03	69.45 %	0.30 %	19.54 %	10.72 %	
4.000	1.63	34.88 %	1.49 %	9.81 %	53.82 %	
5.000	2.43	5.83 %	2.49 %	1.64 %	90.04 %	
6.000	2.86	0.63 %	2.67 %	0.18 %	96.53 %	
6.500	2.92	0.20 %	2.68 %	0.06 %	97.06 %	
7.000	2.94	0.06 %	2.69 %	0.02 %	97.23 %	
7.400	2.94	0.03 %	2.69 %	0.01 %	97.28 %	Blood pH
8.000	2.95	0.01 %	2.69 %	0.00 %	97.30 %	
9.000	2.95	0.00 %	2.69 %	0.00 %	97.31 %	
10.000	2.95	0.00 %	2.69 %	0.00 %	97.31 %	
11.000	2.95	0.00 %	2.69 %	0.00 %	97.31 %	
12.000	2.95	0.00 %	2.69 %	0.00 %	97.31 %	

Carbonate and acidity

Carbonate   0.054 mM
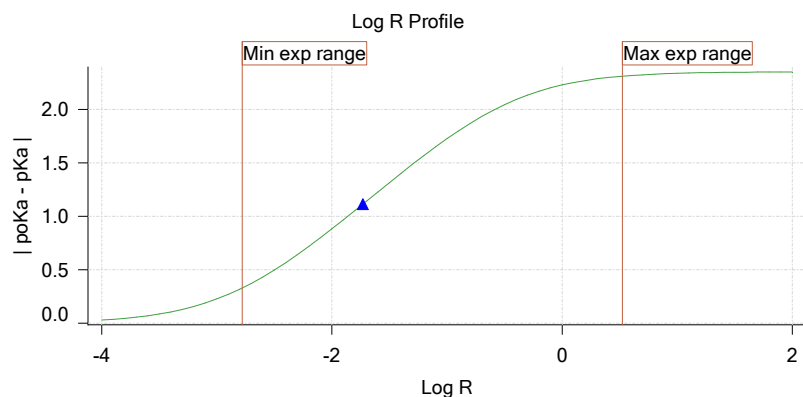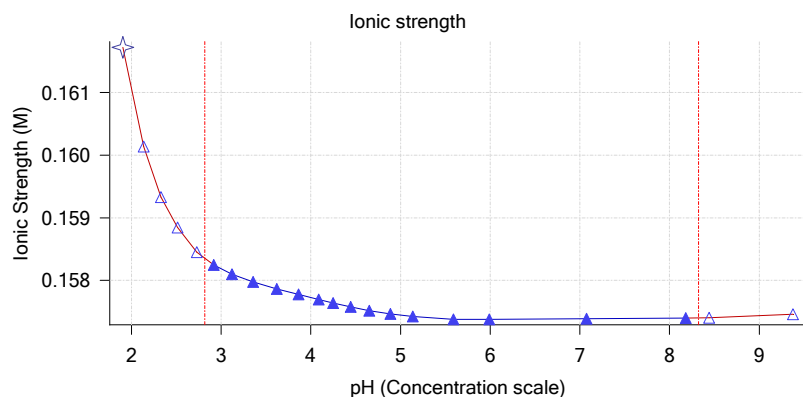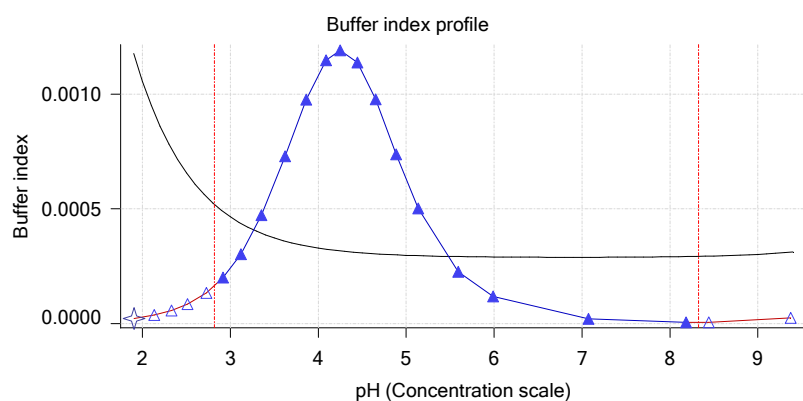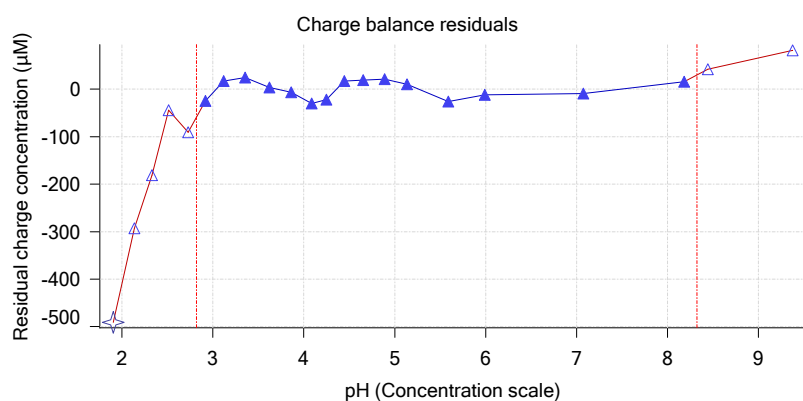Acidity error   -0.436 mM

Other graphs

Assay progress

Titration graph

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Min exp range   Max exp range

Ionisation of sample Carbonate

6.11   9.86
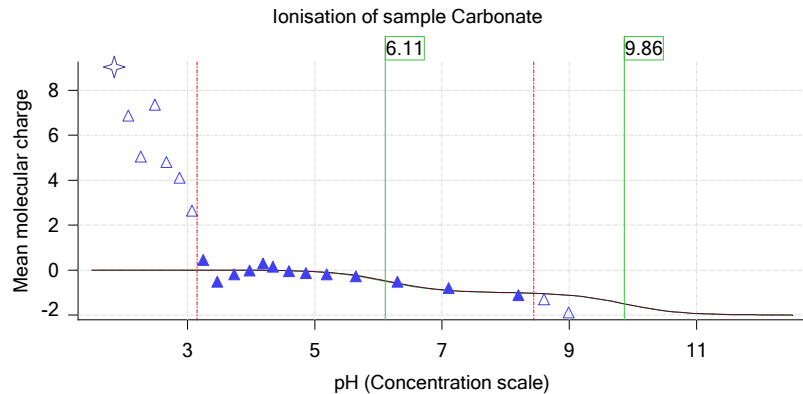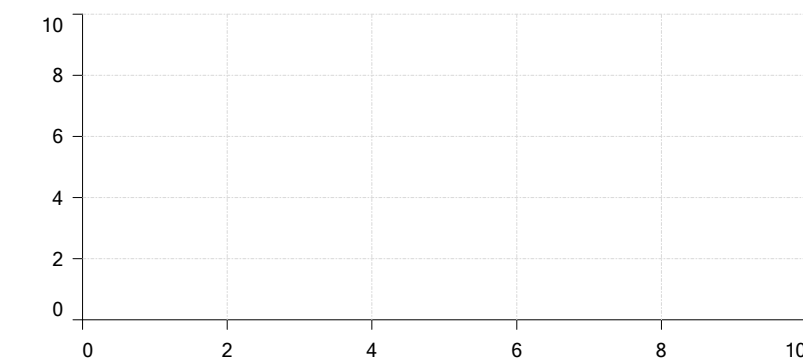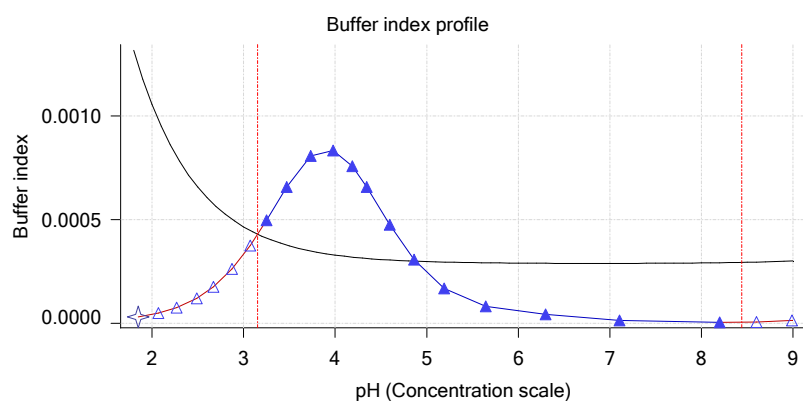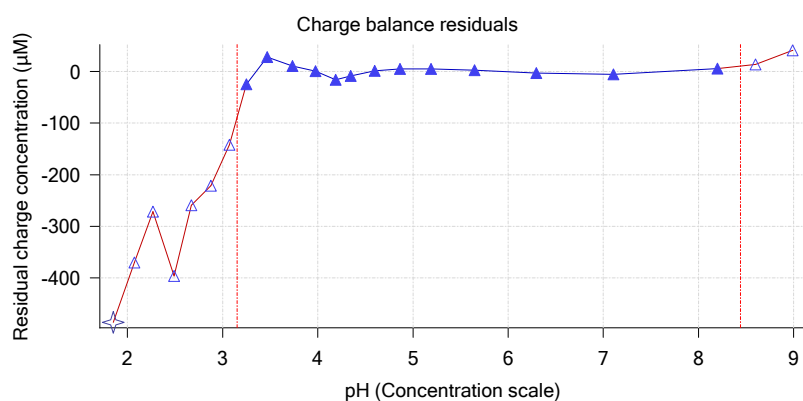
Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 3 of 3   18C-02010 Points 45 to 64

Overall results

RMSD   0.092
Average ionic strength   0.169 M
Average temperature   25.0°C
Partition ratio   0.0935 : 1
Analyte concentration range 1555.0 µM to 1601.8 µM
Total points considered   14 of 20

Warnings and errors

Errors   None
Warnings   None

Four-Plus parameters

Alpha   0.111   3/2/2018 10:00:20 PM   C:\Sirius_T3\HCl18C02.t3r
S   0.9988   3/2/2018 10:00:20 PM   C:\Sirius_T3\HCl18C02.t3r
jH   1.0   3/2/2018 10:00:20 PM   C:\Sirius_T3\HCl18C02.t3r
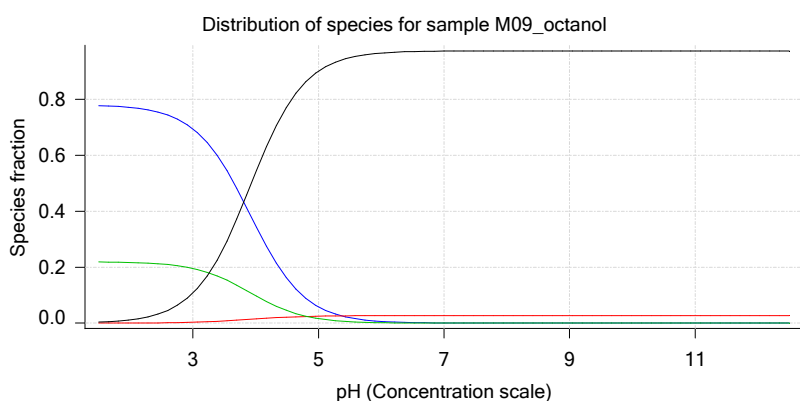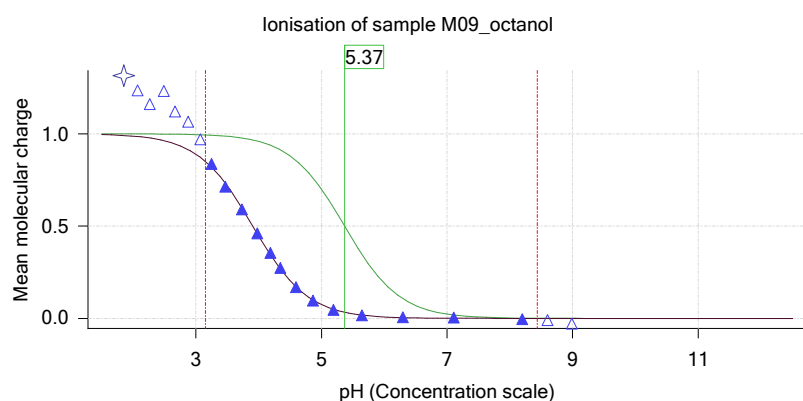jOH   -0.8   3/2/2018 10:00:20 PM   C:\Sirius_T3\HCl18C02.t3r

Titrants

0.50 M HCl   0.999058   3/2/2018 10:00:20 PM   C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH   0.999845   3/2/2018 10:00:20 PM   C:\Sirius_T3\KOH18B27.t3r

Sample

M09_octanol concentration factor   1.103
M09_octanol stoichiometry   1.000
Chloride stoichiometry   1.000
Base pKa 1   5.37
logP (XH +)   0.88
logP (neutral X)   3.27

Sample graphs

Ionisation of sample M09_octanol

Distribution of species for sample M09_octanol

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
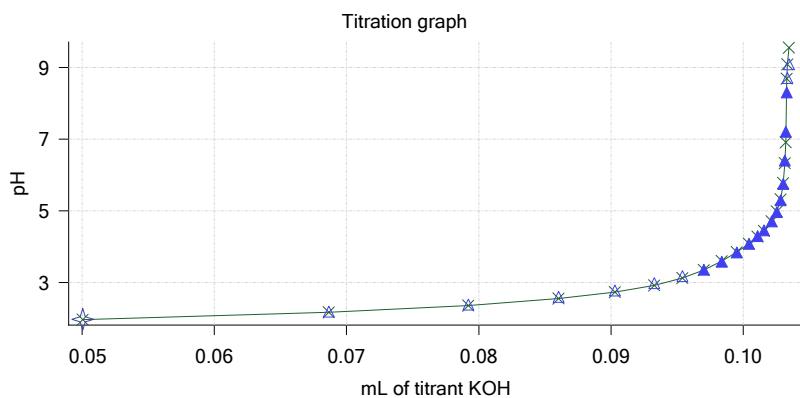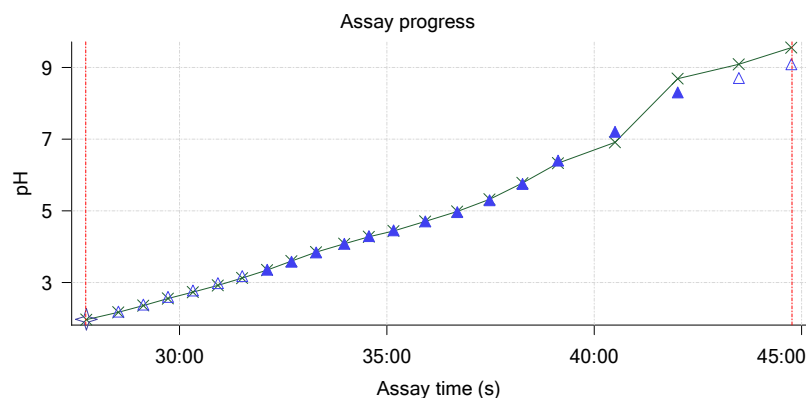Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
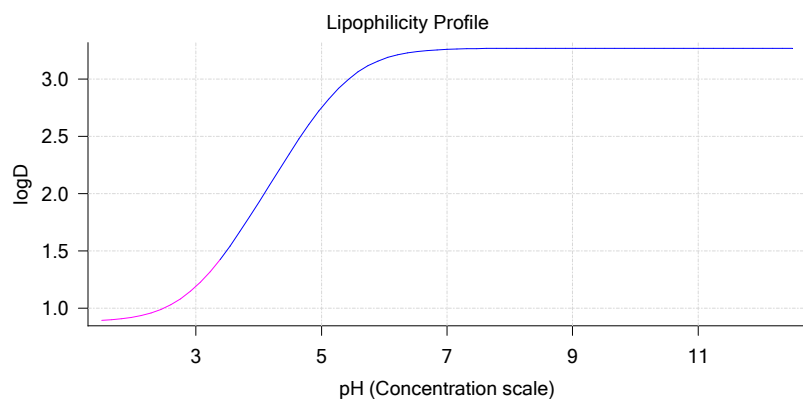
Sample logD and percent species

pH	M09_octanol logD	M09_octanol M09_octanolH	M09_octanol M09_octanol	M09_octanol M09_octanolH*	M09_octanol M09_octanol*	Comment
1.000	0.88	58.36 %	0.00 %	41.21 %	0.43 %	
1.200	0.89	58.21 %	0.00 %	41.10 %	0.69 %	Stomach pH
2.000	0.92	56.15 %	0.02 %	39.65 %	4.17 %	
3.000	1.19	40.76 %	0.17 %	28.78 %	30.28 %	
4.000	1.92	10.89 %	0.46 %	7.69 %	80.95 %	
5.000	2.75	1.31 %	0.56 %	0.92 %	97.21 %	
6.000	3.18	0.13 %	0.57 %	0.09 %	99.20 %	
6.500	3.24	0.04 %	0.57 %	0.03 %	99.36 %	
7.000	3.26	0.01 %	0.57 %	0.01 %	99.41 %	
7.400	3.27	0.01 %	0.57 %	0.00 %	99.42 %	Blood pH
8.000	3.27	0.00 %	0.57 %	0.00 %	99.43 %	
9.000	3.27	0.00 %	0.57 %	0.00 %	99.43 %	
10.000	3.27	0.00 %	0.57 %	0.00 %	99.43 %	
11.000	3.27	0.00 %	0.57 %	0.00 %	99.43 %	
12.000	3.27	0.00 %	0.57 %	0.00 %	99.43 %	

Carbonate and acidity

Carbonate 0.170 mM
Acidity error -0.977 mM

Other graphs
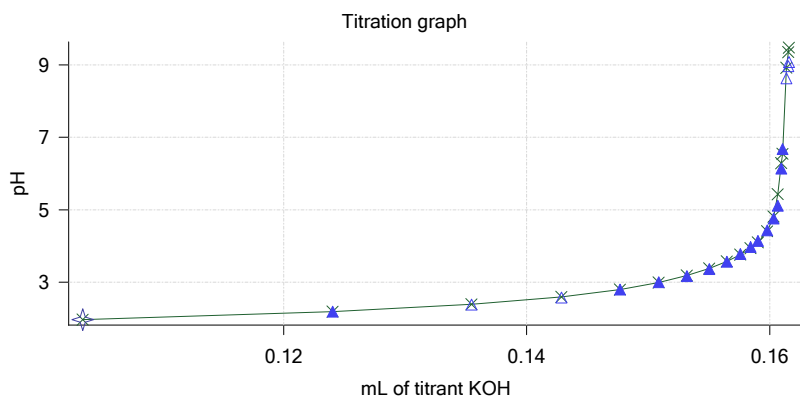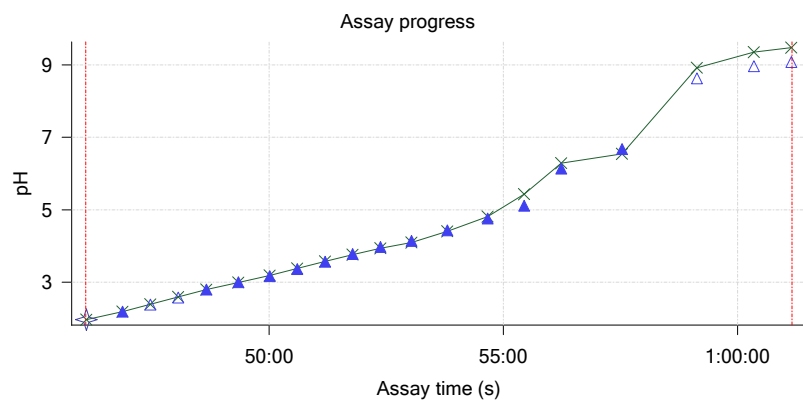
Assay progress

Titration graph
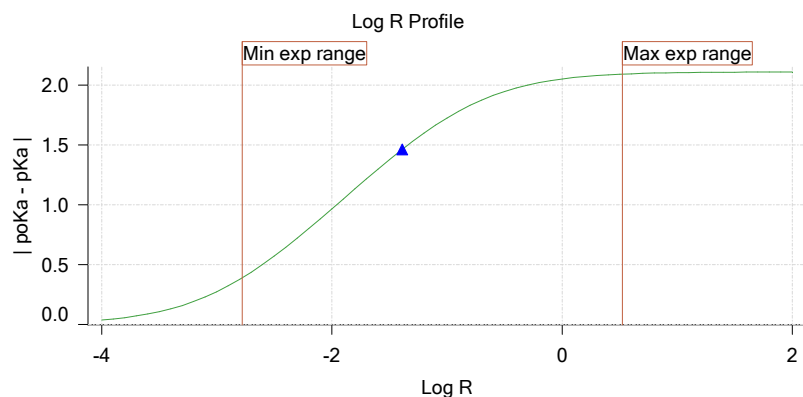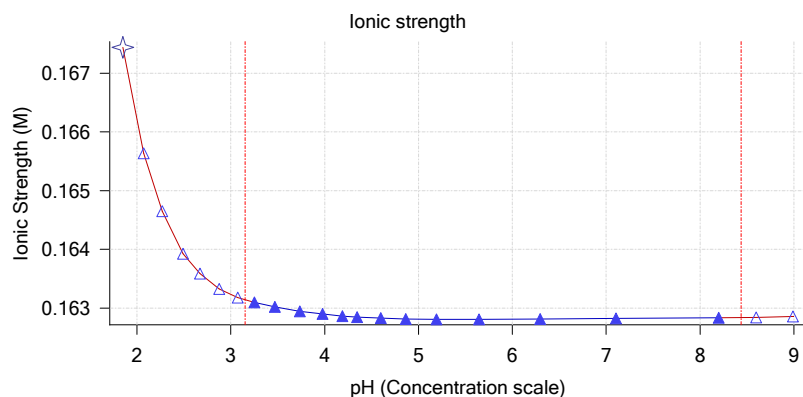
Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
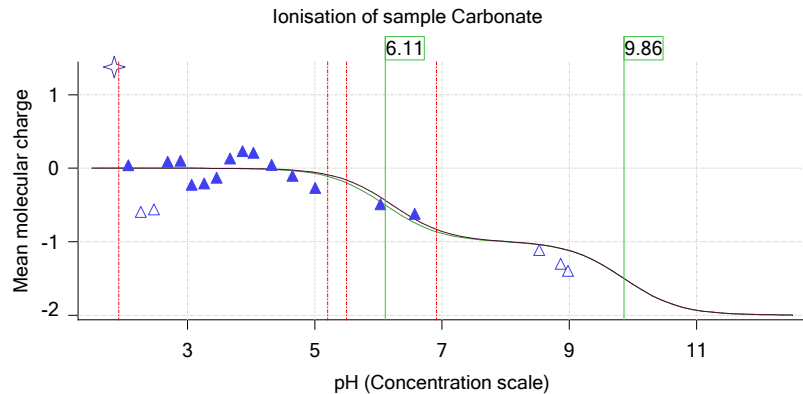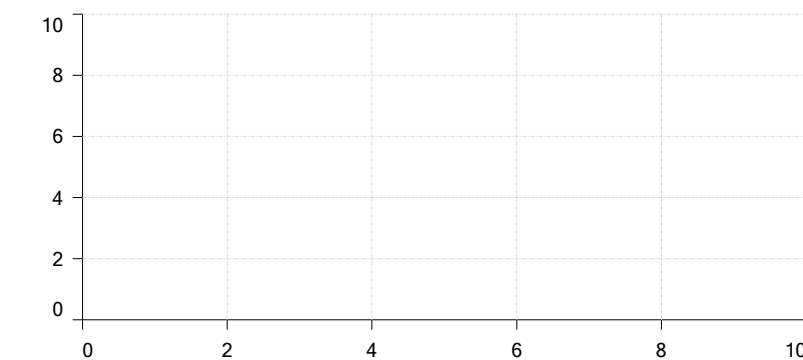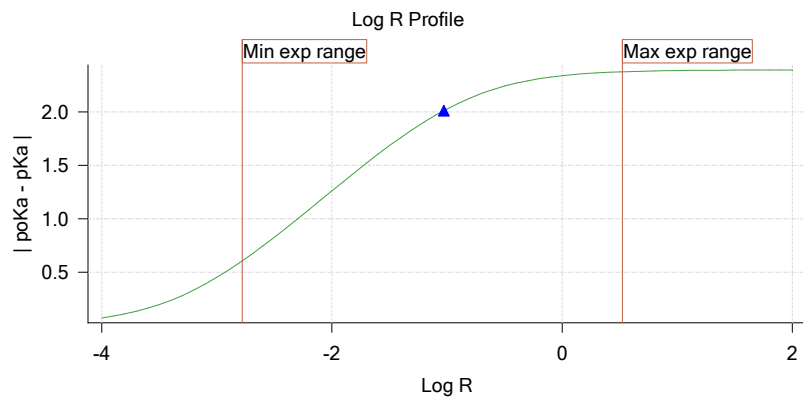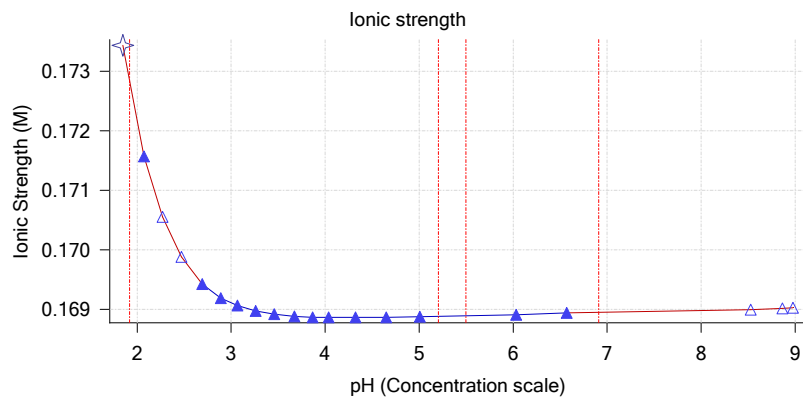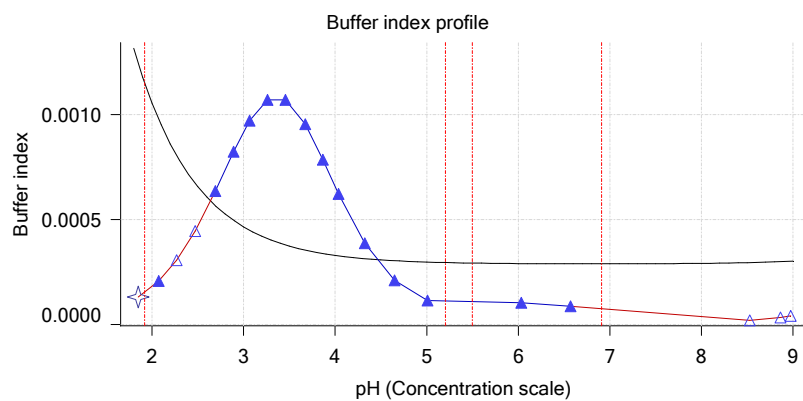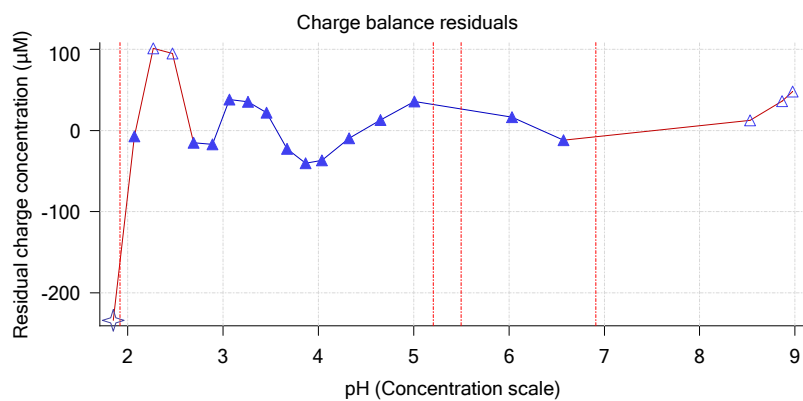
Sample name: **M09_octanol**   Experiment start time: **3/2/2018 10:00:20 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-02010**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M09_octanol	2/27/2018 4:56:17 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.000890 g	3/2/2018 5:08:29 PM	User entered value
Formula weight	287.74 g/mol	2/27/2018 4:45:45 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	251.28	2/27/2018 4:45:45 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 4:45:45 PM	User entered value
Sample is a	Base	2/27/2018 4:45:45 PM	User entered value
pKa 1	5.37	2/27/2018 4:45:45 PM	User entered value
logp (XH +)	0.76	3/2/2018 3:27:23 PM	User entered value
logP (neutral X)	3.27	3/2/2018 3:27:17 PM	User entered value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Events

| Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
6:00.1	Initial pH = 4.31									
9:04.7	Data point 1	1.50000 mL	0.04553 mL	0.00285 mL	0.03001 mL	2.026	-0.01138	0.33547	0.00097	10.0 s
9:51.0	Data point 2	1.50000 mL	0.04553 mL	0.01912 mL	0.03001 mL	2.251	-0.00371	0.21517	0.00040	10.0 s
10:26.6	Data point 3	1.50000 mL	0.04553 mL	0.02763 mL	0.03001 mL	2.442	-0.00300	0.28283	0.00028	10.5 s
11:02.7	Data point 4	1.50000 mL	0.04553 mL	0.03314 mL	0.03001 mL	2.623	-0.00261	0.52506	0.00018	10.0 s
11:38.3	Data point 5	1.50000 mL	0.04553 mL	0.03683 mL	0.03001 mL	2.836	-0.00461	0.55068	0.00031	10.0 s
12:13.7	Data point 6	1.50000 mL	0.04553 mL	0.03923 mL	0.03001 mL	3.025	-0.00570	0.58263	0.00037	10.0 s
12:49.2	Data point 7	1.50000 mL	0.04553 mL	0.04095 mL	0.03001 mL	3.227	-0.00639	0.77318	0.00036	10.0 s
13:24.6	Data point 8	1.50000 mL	0.04553 mL	0.04226 mL	0.03001 mL	3.462	-0.00426	0.73568	0.00025	10.0 s
14:00.0	Data point 9	1.50000 mL	0.04553 mL	0.04334 mL	0.03001 mL	3.728	-0.00671	0.78883	0.00037	10.0 s
14:40.6	Data point 10	1.50000 mL	0.04553 mL	0.04428 mL	0.03001 mL	3.968	-0.01073	0.80668	0.00059	10.0 s
15:16.1	Data point 11	1.50000 mL	0.04553 mL	0.04516 mL	0.03001 mL	4.194	-0.01846	0.90114	0.00096	11.5 s
15:53.0	Data point 12	1.50000 mL	0.04553 mL	0.04586 mL	0.03001 mL	4.354	-0.01589	0.68146	0.00095	10.5 s
16:44.4	Data point 13	1.50000 mL	0.04553 mL	0.04678 mL	0.03001 mL	4.549	-0.01839	0.87702	0.00097	10.5 s
17:35.9	Data point 14	1.50000 mL	0.04553 mL	0.04753 mL	0.03001 mL	4.756	-0.01781	0.86166	0.00095	11.0 s
18:22.6	Data point 15	1.50000 mL	0.04553 mL	0.04821 mL	0.03001 mL	4.992	-0.01766	0.92547	0.00091	12.5 s
19:10.8	Data point 16	1.50000 mL	0.04553 mL	0.04868 mL	0.03001 mL	5.240	-0.01809	0.83242	0.00098	13.5 s
19:54.9	Data point 17	1.50000 mL	0.04553 mL	0.04908 mL	0.03001 mL	5.694	-0.01649	0.87889	0.00087	16.0 s
20:46.7	Data point 18	1.50000 mL	0.04553 mL	0.04934 mL	0.03001 mL	6.092	-0.01930	0.92959	0.00099	21.0 s
21:43.4	Data point 19	1.50000 mL	0.04553 mL	0.04955 mL	0.03001 mL	7.176	-0.04769	0.99644	0.00236	Timed out at 59.5 s
23:19.0	Data point 20	1.50000 mL	0.04553 mL	0.04967 mL	0.03001 mL	8.283	-0.03268	0.96974	0.00164	Timed out at 59.5 s
24:54.6	Data point 21	1.50000 mL	0.04553 mL	0.04976 mL	0.03001 mL	8.541	-0.01854	0.89905	0.00097	54.5 s
26:24.8	Data point 22	1.50000 mL	0.04553 mL	0.05005 mL	0.03001 mL	9.474	-0.01874	0.97230	0.00094	21.5 s
27:45.4	Data point 23	1.50000 mL	0.09967 mL	0.05005 mL	0.07001 mL	1.973	-0.00556	0.20263	0.00061	10.0 s
28:31.7	Data point 24	1.50000 mL	0.09967 mL	0.06865 mL	0.07001 mL	2.188	-0.00175	0.27969	0.00016	10.5 s
29:07.8	Data point 25	1.50000 mL	0.09967 mL	0.07921 mL	0.07001 mL	2.381	-0.00137	0.05773	0.00028	10.0 s
29:43.5	Data point 26	1.50000 mL	0.09967 mL	0.08603 mL	0.07001 mL	2.600	-0.00181	0.18269	0.00021	10.5 s
30:19.5	Data point 27	1.50000 mL	0.09967 mL	0.09029 mL	0.07001 mL	2.780	-0.00959	0.84691	0.00052	10.5 s
30:55.5	Data point 28	1.50000 mL	0.09967 mL	0.09327 mL	0.07001 mL	2.984	-0.00603	0.12688	0.00083	10.0 s
31:31.0	Data point 29	1.50000 mL	0.09967 mL	0.09539 mL	0.07001 mL	3.180	-0.00463	0.68835	0.00028	10.5 s
32:07.0	Data point 30	1.50000 mL	0.09967 mL	0.09701 mL	0.07001 mL	3.357	-0.00337	0.46236	0.00024	10.0 s
32:42.4	Data point 31	1.50000 mL	0.09967 mL	0.09838 mL	0.07001 mL	3.576	-0.01194	0.46846	0.00086	10.0 s
33:17.9	Data point 32	1.50000 mL	0.09967 mL	0.09951 mL	0.07001 mL	3.840	-0.01046	0.33603	0.00089	10.0 s
33:58.5	Data point 33	1.50000 mL	0.09967 mL	0.10042 mL	0.07001 mL	4.082	-0.00936	0.85406	0.00050	10.5 s
34:34.4	Data point 34	1.50000 mL	0.09967 mL	0.10108 mL	0.07001 mL	4.294	-0.00407	0.09219	0.00066	10.0 s

Sample name: **M09_octanol**   Experiment start time: **3/2/2018 10:00:20 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-02010**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_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
35:09.9	Data point 35	1.50000 mL	0.09967 mL	0.10155 mL	0.07001 mL	4.450	-0.01452	0.77733	0.00081	10.0 s
35:55.6	Data point 36	1.50000 mL	0.09967 mL	0.10214 mL	0.07001 mL	4.702	-0.01411	0.84297	0.00076	10.5 s
36:41.9	Data point 37	1.50000 mL	0.09967 mL	0.10254 mL	0.07001 mL	4.968	-0.01431	0.68972	0.00085	11.0 s
37:28.6	Data point 38	1.50000 mL	0.09967 mL	0.10282 mL	0.07001 mL	5.294	-0.01678	0.70413	0.00099	12.0 s
38:16.4	Data point 39	1.50000 mL	0.09967 mL	0.10301 mL	0.07001 mL	5.750	-0.01457	0.79249	0.00081	15.5 s
39:07.6	Data point 40	1.50000 mL	0.09967 mL	0.10313 mL	0.07001 mL	6.399	-0.01829	0.88102	0.00096	47.0 s
40:30.3	Data point 41	1.50000 mL	0.09967 mL	0.10320 mL	0.07001 mL	7.207	-0.05114	0.99091	0.00254	Timed out at 59.5 s
42:00.8	Data point 42	1.50000 mL	0.09967 mL	0.10327 mL	0.07001 mL	8.299	-0.01875	0.88424	0.00099	58.0 s
43:29.5	Data point 43	1.50000 mL	0.09967 mL	0.10332 mL	0.07001 mL	8.699	-0.01983	0.98147	0.00099	35.0 s
44:45.3	Data point 44	1.50000 mL	0.09967 mL	0.10346 mL	0.07001 mL	9.089	-0.01827	0.94147	0.00093	20.5 s
46:06.3	Data point 45	1.50000 mL	0.15753 mL	0.10346 mL	0.17001 mL	1.972	-0.01076	0.86425	0.00057	10.0 s
46:52.6	Data point 46	1.50000 mL	0.15753 mL	0.12404 mL	0.17001 mL	2.189	-0.00758	0.73014	0.00044	10.0 s
47:28.3	Data point 47	1.50000 mL	0.15753 mL	0.13547 mL	0.17001 mL	2.382	-0.00182	0.17529	0.00021	10.0 s
48:03.9	Data point 48	1.50000 mL	0.15753 mL	0.14285 mL	0.17001 mL	2.583	0.00231	0.53001	0.00016	10.5 s
48:39.9	Data point 49	1.50000 mL	0.15753 mL	0.14767 mL	0.17001 mL	2.800	0.01463	0.61912	0.00092	15.5 s
49:20.9	Data point 50	1.50000 mL	0.15753 mL	0.15087 mL	0.17001 mL	2.998	0.01486	0.59518	0.00095	14.5 s
50:00.9	Data point 51	1.50000 mL	0.15753 mL	0.15320 mL	0.17001 mL	3.174	-0.00236	0.06490	0.00046	10.0 s
50:36.4	Data point 52	1.50000 mL	0.15753 mL	0.15503 mL	0.17001 mL	3.369	-0.00368	0.52645	0.00025	10.0 s
51:11.8	Data point 53	1.50000 mL	0.15753 mL	0.15647 mL	0.17001 mL	3.564	-0.00334	0.04831	0.00075	10.0 s
51:47.3	Data point 54	1.50000 mL	0.15753 mL	0.15760 mL	0.17001 mL	3.779	-0.00287	0.06293	0.00056	10.0 s
52:22.7	Data point 55	1.50000 mL	0.15753 mL	0.15842 mL	0.17001 mL	3.972	0.01222	0.41308	0.00094	14.5 s
53:02.6	Data point 56	1.50000 mL	0.15753 mL	0.15903 mL	0.17001 mL	4.143	-0.00657	0.60274	0.00042	10.0 s
53:48.4	Data point 57	1.50000 mL	0.15753 mL	0.15981 mL	0.17001 mL	4.429	0.01474	0.60321	0.00094	16.0 s
54:40.1	Data point 58	1.50000 mL	0.15753 mL	0.16033 mL	0.17001 mL	4.755	0.01365	0.52664	0.00093	11.0 s
55:26.8	Data point 59	1.50000 mL	0.15753 mL	0.16065 mL	0.17001 mL	5.112	-0.00952	0.31084	0.00084	11.5 s
56:14.0	Data point 60	1.50000 mL	0.15753 mL	0.16096 mL	0.17001 mL	6.134	-0.01828	0.87737	0.00096	42.5 s
57:32.1	Data point 61	1.50000 mL	0.15753 mL	0.16105 mL	0.17001 mL	6.674	-0.03582	0.95893	0.00181	Timed out at 59.5 s
59:07.8	Data point 62	1.50000 mL	0.15753 mL	0.16138 mL	0.17001 mL	8.628	-0.01937	0.92742	0.00099	32.0 s
1:00:20.6	Data point 63	1.50000 mL	0.15753 mL	0.16152 mL	0.17001 mL	8.963	-0.00684	0.12695	0.00095	17.5 s
1:01:08.6	Data point 64	1.50000 mL	0.15753 mL	0.16159 mL	0.17001 mL	9.075	-0.01927	0.95912	0.00097	15.0 s
1:01:32.7	Assay volumes	1.50000 mL	0.15753 mL	0.16159 mL	0.17001 mL					

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 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	0.030 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	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	0.040 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: **M09_octanol**   Experiment start time: **3/2/2018 10:00:20 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-02010**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.100 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.111	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus S	0.9988	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jH	1.0	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jOH	-0.8	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r
Base concentration factor	1.000	3/2/2018 10:00:20 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.999	3/2/2018 10:00:20 PM	C:\Sirius_T3\HCl18C02.t3r

Instrument Settings

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

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+3.23 mV		3/2/2018 10:00:48 PM
Filling solution	3M KCl	KCL097	3/2/2018 9:43:24 AM
Liquids			
Wash 1	50% IPA:50% Water		3/2/2018 9:45:12 AM
Wash 2	0.5% Trition X-100 in H20		3/2/2018 9:45:15 AM
Buffer position 1	pH7 Wash		3/2/2018 9:45:18 AM
Buffer position 2	pH 7		3/2/2018 9:45:21 AM
Storage position			3/2/2018 9:44:44 AM
Wash water	7.2e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	8.2e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	120:41:49		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:37] Air gap created for Water (0.15 M KCl)
[2:38] Air gap created for Acid (0.5 M HCl)
[2:38] Air gap created for Base (0.5 M KOH)
[2:39] Air gap released for Water (0.15 M KCl)
[2:42] Titrator arm moved over Titration position
[2:42] Titration 1 of 3
[2:42] Adding initial titrants
[2:42] Automatically add 1.50000 mL of water
[3:08] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:12] Titrator arm moved over Drain
[5:53] Titrator arm moved to Titration position
[5:53] Argon flow rate set to 100
[5:53] Stirrer speed set to 10
[5:58] Automatically add 0.03000 mL of Octanol
[5:59] Dispensed 0.030009 mL of Octanol
[6:00] Initial pH = 4.31
[6:00] Iterative adjust 4.31 -> 2.00
[6:00] pH 4.31 -> 2.00
[6:02] Air gap released for Acid (0.5 M HCl)
[6:03] Dispensed 0.043815 mL of Acid (0.5 M HCl)
[6:08] pH 2.02 -> 2.00
[6:08] Dispensed 0.001717 mL of Acid (0.5 M HCl)
[6:13] Holding pH 2.00
[8:13] Stirrer speed set to 0
[8:13] Stirrer speed set to 50
[8:13] Iterative adjust 1.97 -> 2.00
[8:13] pH 1.97 -> 2.00
[8:14] Air gap released for Base (0.5 M KOH)
[8:15] Dispensed 0.002846 mL of Base (0.5 M KOH)
[9:05] Stirrer speed set to 0
[9:15] Datapoint id 1 collected
[9:15] Stirrer speed set to 50
[9:20] pH 2.03 -> 2.23
[9:20] Using cautious pH adjust
[9:20] Dispensed 0.007173 mL of Base (0.5 M KOH)
[9:25] Stepping pH = 2.10
[9:26] Dispensed 0.007832 mL of Base (0.5 M KOH)
[9:31] Stepping pH = 2.21
[9:31] Dispensed 0.001270 mL of Base (0.5 M KOH)
[9:36] Stepping pH = 2.24
[9:51] Stirrer speed set to 0
[10:01] Datapoint id 2 collected

Sample name: **M09_octanol** Experiment start time: **3/2/2018 10:00:20 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02010** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[10:01] Charge balance equation is out by -13.4%
[10:01] Stirrer speed set to 50
[10:06] pH 2.26 -> 2.46
[10:06] Using charge balance adjust
[10:07] Dispensed 0.008514 mL of Base (0.5 M KOH)
[10:27] Stirrer speed set to 0
[10:37] Datapoint id 3 collected
[10:37] Charge balance equation is out by -7.5%
[10:37] Stirrer speed set to 50
[10:42] pH 2.45 -> 2.65
[10:42] Using charge balance adjust
[10:43] Dispensed 0.005503 mL of Base (0.5 M KOH)
[11:03] Stirrer speed set to 0
[11:13] Datapoint id 4 collected
[11:13] Charge balance equation is out by -12.9%
[11:13] Stirrer speed set to 50
[11:18] pH 2.63 -> 2.83
[11:18] Using charge balance adjust
[11:18] Dispensed 0.003692 mL of Base (0.5 M KOH)
[11:38] Stirrer speed set to 0
[11:48] Datapoint id 5 collected
[11:48] Charge balance equation is out by 3.3%
[11:48] Stirrer speed set to 50
[11:54] pH 2.84 -> 3.04
[11:54] Using charge balance adjust
[11:54] Dispensed 0.002399 mL of Base (0.5 M KOH)
[12:14] Stirrer speed set to 0
[12:24] Datapoint id 6 collected
[12:24] Charge balance equation is out by -8.2%
[12:24] Stirrer speed set to 50
[12:29] pH 3.03 -> 3.23
[12:29] Using charge balance adjust
[12:29] Dispensed 0.001717 mL of Base (0.5 M KOH)
[12:49] Stirrer speed set to 0
[12:59] Datapoint id 7 collected
[12:59] Charge balance equation is out by -2.1%
[12:59] Stirrer speed set to 50
[13:04] pH 3.23 -> 3.43
[13:04] Using charge balance adjust
[13:05] Dispensed 0.001317 mL of Base (0.5 M KOH)
[13:25] Stirrer speed set to 0
[13:35] Datapoint id 8 collected
[13:35] Charge balance equation is out by 15.0%
[13:35] Stirrer speed set to 50
[13:40] pH 3.47 -> 3.67
[13:40] Using charge balance adjust
[13:40] Dispensed 0.001082 mL of Base (0.5 M KOH)
[14:00] Stirrer speed set to 0
[14:10] Datapoint id 9 collected
[14:10] Charge balance equation is out by 31.3%
[14:10] Stirrer speed set to 50
[14:15] pH 3.73 -> 3.93
[14:15] Using cautious pH adjust
[14:15] Dispensed 0.000494 mL of Base (0.5 M KOH)
[14:21] Stepping pH = 3.81
[14:21] Dispensed 0.000447 mL of Base (0.5 M KOH)
[14:26] Stepping pH = 3.94
[14:41] Stirrer speed set to 0
[14:51] Datapoint id 10 collected

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[14:51] Charge balance equation is out by 3.1%
[14:51] Stirrer speed set to 50
[14:56] pH 3.97 -> 4.17
[14:56] Using charge balance adjust
[14:56] Dispensed 0.000870 mL of Base (0.5 M KOH)
[15:16] Stirrer speed set to 0
[15:28] Datapoint id 11 collected
[15:28] Charge balance equation is out by 10.9%
[15:28] Stirrer speed set to 50
[15:33] pH 4.20 -> 4.40
[15:33] Using charge balance adjust
[15:33] Dispensed 0.000706 mL of Base (0.5 M KOH)
[15:53] Stirrer speed set to 0
[16:04] Datapoint id 12 collected
[16:04] Charge balance equation is out by -22.6%
[16:04] Stirrer speed set to 50
[16:09] pH 4.36 -> 4.56
[16:09] Using cautious pH adjust
[16:09] Dispensed 0.000306 mL of Base (0.5 M KOH)
[16:14] Stepping pH = 4.41
[16:14] Dispensed 0.000447 mL of Base (0.5 M KOH)
[16:19] Stepping pH = 4.52
[16:19] Dispensed 0.000118 mL of Base (0.5 M KOH)
[16:24] Stepping pH = 4.55
[16:24] Dispensed 0.000047 mL of Base (0.5 M KOH)
[16:29] Stepping pH = 4.56
[16:45] Stirrer speed set to 0
[16:55] Datapoint id 13 collected
[16:55] Charge balance equation is out by -53.1%
[16:55] Stirrer speed set to 50
[17:00] pH 4.56 -> 4.76
[17:00] Using cautious pH adjust
[17:00] Dispensed 0.000235 mL of Base (0.5 M KOH)
[17:06] Stepping pH = 4.60
[17:06] Dispensed 0.000329 mL of Base (0.5 M KOH)
[17:11] Stepping pH = 4.70
[17:11] Dispensed 0.000165 mL of Base (0.5 M KOH)
[17:16] Stepping pH = 4.75
[17:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[17:21] Stepping pH = 4.76
[17:36] Stirrer speed set to 0
[17:47] Datapoint id 14 collected
[17:47] Charge balance equation is out by -67.5%
[17:47] Stirrer speed set to 50
[17:52] pH 4.77 -> 4.97
[17:52] Using cautious pH adjust
[17:52] Dispensed 0.000165 mL of Base (0.5 M KOH)
[17:57] Stepping pH = 4.79
[17:57] Dispensed 0.000400 mL of Base (0.5 M KOH)
[18:03] Stepping pH = 4.92
[18:03] Dispensed 0.000118 mL of Base (0.5 M KOH)
[18:08] Stepping pH = 4.98
[18:23] Stirrer speed set to 0
[18:35] Datapoint id 15 collected
[18:35] Charge balance equation is out by -106.8%
[18:35] Stirrer speed set to 50
[18:40] pH 5.01 -> 5.21
[18:40] Using cautious pH adjust
[18:41] Dispensed 0.000094 mL of Base (0.5 M KOH)

Sample name: **M09_octanol** Experiment start time: **3/2/2018 10:00:20 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02010** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[18:46] Stepping pH = 5.01
[18:46] Dispensed 0.000306 mL of Base (0.5 M KOH)
[18:51] Stepping pH = 5.16
[18:51] Dispensed 0.000071 mL of Base (0.5 M KOH)
[18:56] Stepping pH = 5.22
[19:11] Stirrer speed set to 0
[19:25] Datapoint id 16 collected
[19:25] Charge balance equation is out by -128.8%
[19:25] Stirrer speed set to 50
[19:30] pH 5.26 -> 5.46
[19:30] Using cautious pH adjust
[19:30] Dispensed 0.000071 mL of Base (0.5 M KOH)
[19:35] Stepping pH = 5.26
[19:35] Dispensed 0.000329 mL of Base (0.5 M KOH)
[19:40] Stepping pH = 5.52
[19:55] Stirrer speed set to 0
[20:11] Datapoint id 17 collected
[20:11] Charge balance equation is out by -200.5%
[20:11] Stirrer speed set to 50
[20:16] pH 5.72 -> 5.92
[20:16] Using cautious pH adjust
[20:16] Dispensed 0.000047 mL of Base (0.5 M KOH)
[20:21] Stepping pH = 5.73
[20:22] Dispensed 0.000094 mL of Base (0.5 M KOH)
[20:27] Stepping pH = 5.79
[20:27] Dispensed 0.000118 mL of Base (0.5 M KOH)
[20:32] Stepping pH = 5.94
[20:47] Stirrer speed set to 0
[21:08] Datapoint id 18 collected
[21:08] Charge balance equation is out by -265.1%
[21:08] Stirrer speed set to 50
[21:13] pH 6.11 -> 6.31
[21:13] Using cautious pH adjust
[21:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[21:18] Stepping pH = 6.11
[21:18] Dispensed 0.000141 mL of Base (0.5 M KOH)
[21:23] Stepping pH = 6.26
[21:23] Dispensed 0.000047 mL of Base (0.5 M KOH)
[21:29] Stepping pH = 6.65
[21:44] Stirrer speed set to 0
[22:44] Datapoint id 19 collected
[22:44] Charge balance equation is out by -268.6%
[22:44] Stirrer speed set to 50
[22:49] pH 7.06 -> 7.26
[22:49] Using cautious pH adjust
[22:49] Dispensed 0.000024 mL of Base (0.5 M KOH)
[22:54] Stepping pH = 7.04
[22:54] Dispensed 0.000047 mL of Base (0.5 M KOH)
[22:59] Stepping pH = 7.13
[22:59] Dispensed 0.000047 mL of Base (0.5 M KOH)
[23:04] Stepping pH = 7.50
[23:19] Stirrer speed set to 0
[24:19] Datapoint id 20 collected
[24:19] Charge balance equation is out by -526.7%
[24:19] Stirrer speed set to 50
[24:24] pH 8.19 -> 8.39
[24:24] Using cautious pH adjust
[24:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:29] Stepping pH = 8.16

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[24:29] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:35] Stepping pH = 8.20
[24:35] Dispensed 0.000047 mL of Base (0.5 M KOH)
[24:40] Stepping pH = 8.49
[24:55] Stirrer speed set to 0
[25:49] Datapoint id 21 collected
[25:49] Charge balance equation is out by -997.9%
[25:49] Stirrer speed set to 50
[25:55] pH 8.47 -> 8.67
[25:55] Using cautious pH adjust
[25:55] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:00] Stepping pH = 8.43
[26:00] Dispensed 0.000047 mL of Base (0.5 M KOH)
[26:05] Stepping pH = 8.40
[26:05] Dispensed 0.000212 mL of Base (0.5 M KOH)
[26:10] Stepping pH = 9.23
[26:25] Stirrer speed set to 0
[26:47] Datapoint id 22 collected
[26:47] Charge balance equation is out by -1,935.7%
[26:47] Titration 2 of 3
[26:47] Adding initial titrants
[26:47] Automatically add 0.04000 mL of Octanol
[26:48] Dispensed 0.040005 mL of Octanol
[26:48] Stirrer speed set to 10
[26:49] Stirrer speed set to 55
[26:49] Iterative adjust 9.48 -> 2.00
[26:49] pH 9.48 -> 2.00
[26:50] Dispensed 0.048871 mL of Acid (0.5 M HCl)
[26:55] pH 2.05 -> 2.00
[26:55] Dispensed 0.005268 mL of Acid (0.5 M HCl)
[27:46] Stirrer speed set to 0
[27:56] Datapoint id 23 collected
[27:56] Stirrer speed set to 55
[28:01] pH 1.98 -> 2.18
[28:01] Using cautious pH adjust
[28:01] Dispensed 0.008702 mL of Base (0.5 M KOH)
[28:06] Stepping pH = 2.05
[28:06] Dispensed 0.008302 mL of Base (0.5 M KOH)
[28:12] Stepping pH = 2.15
[28:12] Dispensed 0.001599 mL of Base (0.5 M KOH)
[28:17] Stepping pH = 2.18
[28:32] Stirrer speed set to 0
[28:42] Datapoint id 24 collected
[28:42] Charge balance equation is out by -6.9%
[28:42] Stirrer speed set to 55
[28:47] pH 2.19 -> 2.39
[28:47] Using charge balance adjust
[28:48] Dispensed 0.010560 mL of Base (0.5 M KOH)
[29:08] Stirrer speed set to 0
[29:18] Datapoint id 25 collected
[29:18] Charge balance equation is out by -5.9%
[29:18] Stirrer speed set to 55
[29:23] pH 2.39 -> 2.59
[29:23] Using charge balance adjust
[29:23] Dispensed 0.006820 mL of Base (0.5 M KOH)
[29:44] Stirrer speed set to 0
[29:54] Datapoint id 26 collected
[29:54] Charge balance equation is out by 6.5%
[29:54] Stirrer speed set to 55

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[29:59] pH 2.61 -> 2.81
[29:59] Using charge balance adjust
[30:00] Dispensed 0.004257 mL of Base (0.5 M KOH)
[30:20] Stirrer speed set to 0
[30:30] Datapoint id 27 collected
[30:30] Charge balance equation is out by -12.7%
[30:30] Stirrer speed set to 55
[30:35] pH 2.78 -> 2.98
[30:35] Using charge balance adjust
[30:36] Dispensed 0.002987 mL of Base (0.5 M KOH)
[30:56] Stirrer speed set to 0
[31:06] Datapoint id 28 collected
[31:06] Charge balance equation is out by 0.0%
[31:06] Stirrer speed set to 55
[31:11] pH 2.99 -> 3.19
[31:11] Using charge balance adjust
[31:11] Dispensed 0.002117 mL of Base (0.5 M KOH)
[31:31] Stirrer speed set to 0
[31:42] Datapoint id 29 collected
[31:42] Charge balance equation is out by -3.1%
[31:42] Stirrer speed set to 55
[31:47] pH 3.18 -> 3.38
[31:47] Using charge balance adjust
[31:47] Dispensed 0.001623 mL of Base (0.5 M KOH)
[32:07] Stirrer speed set to 0
[32:17] Datapoint id 30 collected
[32:17] Charge balance equation is out by -13.1%
[32:17] Stirrer speed set to 55
[32:22] pH 3.36 -> 3.56
[32:22] Using charge balance adjust
[32:22] Dispensed 0.001364 mL of Base (0.5 M KOH)
[32:43] Stirrer speed set to 0
[32:53] Datapoint id 31 collected
[32:53] Charge balance equation is out by 7.5%
[32:53] Stirrer speed set to 55
[32:58] pH 3.58 -> 3.78
[32:58] Using charge balance adjust
[32:58] Dispensed 0.001129 mL of Base (0.5 M KOH)
[33:18] Stirrer speed set to 0
[33:28] Datapoint id 32 collected
[33:28] Charge balance equation is out by 30.1%
[33:28] Stirrer speed set to 55
[33:33] pH 3.84 -> 4.04
[33:33] Using cautious pH adjust
[33:33] Dispensed 0.000447 mL of Base (0.5 M KOH)
[33:38] Stepping pH = 3.91
[33:38] Dispensed 0.000470 mL of Base (0.5 M KOH)
[33:44] Stepping pH = 4.03
[33:59] Stirrer speed set to 0
[34:09] Datapoint id 33 collected
[34:09] Charge balance equation is out by -3.9%
[34:09] Stirrer speed set to 55
[34:14] pH 4.08 -> 4.28
[34:14] Using charge balance adjust
[34:14] Dispensed 0.000659 mL of Base (0.5 M KOH)
[34:35] Stirrer speed set to 0
[34:45] Datapoint id 34 collected
[34:45] Charge balance equation is out by 5.3%
[34:45] Stirrer speed set to 55

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[34:50] pH 4.30 -> 4.50
[34:50] Using charge balance adjust
[34:50] Dispensed 0.000470 mL of Base (0.5 M KOH)
[35:10] Stirrer speed set to 0
[35:20] Datapoint id 35 collected
[35:20] Charge balance equation is out by -24.5%
[35:20] Stirrer speed set to 55
[35:25] pH 4.46 -> 4.66
[35:25] Using cautious pH adjust
[35:25] Dispensed 0.000188 mL of Base (0.5 M KOH)
[35:30] Stepping pH = 4.50
[35:30] Dispensed 0.000306 mL of Base (0.5 M KOH)
[35:36] Stepping pH = 4.61
[35:36] Dispensed 0.000094 mL of Base (0.5 M KOH)
[35:41] Stepping pH = 4.67
[35:56] Stirrer speed set to 0
[36:06] Datapoint id 36 collected
[36:06] Charge balance equation is out by -61.6%
[36:06] Stirrer speed set to 55
[36:11] pH 4.71 -> 4.91
[36:11] Using cautious pH adjust
[36:12] Dispensed 0.000118 mL of Base (0.5 M KOH)
[36:17] Stepping pH = 4.74
[36:17] Dispensed 0.000235 mL of Base (0.5 M KOH)
[36:22] Stepping pH = 4.88
[36:22] Dispensed 0.000047 mL of Base (0.5 M KOH)
[36:27] Stepping pH = 4.93
[36:42] Stirrer speed set to 0
[36:53] Datapoint id 37 collected
[36:53] Charge balance equation is out by -76.9%
[36:53] Stirrer speed set to 55
[36:58] pH 4.98 -> 5.18
[36:58] Using cautious pH adjust
[36:58] Dispensed 0.000071 mL of Base (0.5 M KOH)
[37:03] Stepping pH = 5.00
[37:03] Dispensed 0.000188 mL of Base (0.5 M KOH)
[37:09] Stepping pH = 5.17
[37:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[37:14] Stepping pH = 5.23
[37:29] Stirrer speed set to 0
[37:41] Datapoint id 38 collected
[37:41] Charge balance equation is out by -100.4%
[37:41] Stirrer speed set to 55
[37:46] pH 5.31 -> 5.51
[37:46] Using cautious pH adjust
[37:46] Dispensed 0.000047 mL of Base (0.5 M KOH)
[37:51] Stepping pH = 5.32
[37:51] Dispensed 0.000118 mL of Base (0.5 M KOH)
[37:56] Stepping pH = 5.49
[37:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[38:01] Stepping pH = 5.62
[38:17] Stirrer speed set to 0
[38:32] Datapoint id 39 collected
[38:32] Charge balance equation is out by -114.7%
[38:32] Stirrer speed set to 55
[38:37] pH 5.77 -> 5.97
[38:37] Using cautious pH adjust
[38:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[38:42] Stepping pH = 5.78

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[38:42] Dispensed 0.000071 mL of Base (0.5 M KOH)
[38:48] Stepping pH = 5.95
[38:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[38:53] Stepping pH = 6.16
[39:08] Stirrer speed set to 0
[39:55] Datapoint id 40 collected
[39:55] Charge balance equation is out by -131.1%
[39:55] Stirrer speed set to 55
[40:00] pH 6.40 -> 6.60
[40:00] Using cautious pH adjust
[40:00] Dispensed 0.000024 mL of Base (0.5 M KOH)
[40:05] Stepping pH = 6.45
[40:05] Dispensed 0.000024 mL of Base (0.5 M KOH)
[40:10] Stepping pH = 6.54
[40:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[40:15] Stepping pH = 6.77
[40:31] Stirrer speed set to 0
[41:31] Datapoint id 41 collected
[41:31] Charge balance equation is out by -75.8%
[41:31] Stirrer speed set to 55
[41:36] pH 7.09 -> 7.29
[41:36] Using cautious pH adjust
[41:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[41:41] Stepping pH = 7.03
[41:41] Dispensed 0.000047 mL of Base (0.5 M KOH)
[41:46] Stepping pH = 7.49
[42:01] Stirrer speed set to 0
[42:59] Datapoint id 42 collected
[42:59] Charge balance equation is out by -364.7%
[42:59] Stirrer speed set to 55
[43:04] pH 8.28 -> 8.48
[43:04] Using cautious pH adjust
[43:04] Dispensed 0.000024 mL of Base (0.5 M KOH)
[43:09] Stepping pH = 8.37
[43:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[43:15] Stepping pH = 8.52
[43:30] Stirrer speed set to 0
[44:05] Datapoint id 43 collected
[44:05] Charge balance equation is out by -286.1%
[44:05] Stirrer speed set to 55
[44:10] pH 8.68 -> 8.88
[44:10] Using cautious pH adjust
[44:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[44:15] Stepping pH = 8.68
[44:15] Dispensed 0.000047 mL of Base (0.5 M KOH)
[44:20] Stepping pH = 8.76
[44:20] Dispensed 0.000047 mL of Base (0.5 M KOH)
[44:25] Stepping pH = 8.85
[44:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[44:30] Stepping pH = 8.98
[44:46] Stirrer speed set to 0
[45:06] Datapoint id 44 collected
[45:06] Charge balance equation is out by -572.8%
[45:06] Titration 3 of 3
[45:06] Adding initial titrants
[45:06] Automatically add 0.10000 mL of Octanol
[45:08] Dispensed 0.100000 mL of Octanol
[45:08] Stirrer speed set to 10
[45:10] Stirrer speed set to 60

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[45:10] Iterative adjust 9.09 -> 2.00
[45:10] pH 9.09 -> 2.00
[45:11] Dispensed 0.051529 mL of Acid (0.5 M HCl)
[45:16] pH 2.06 -> 2.00
[45:16] Dispensed 0.006326 mL of Acid (0.5 M HCl)
[46:07] Stirrer speed set to 0
[46:17] Datapoint id 45 collected
[46:17] Stirrer speed set to 60
[46:22] pH 1.97 -> 2.17
[46:22] Using cautious pH adjust
[46:22] Dispensed 0.009431 mL of Base (0.5 M KOH)
[46:27] Stepping pH = 2.04
[46:27] Dispensed 0.009525 mL of Base (0.5 M KOH)
[46:32] Stepping pH = 2.15
[46:33] Dispensed 0.001623 mL of Base (0.5 M KOH)
[46:38] Stepping pH = 2.18
[46:53] Stirrer speed set to 0
[47:03] Datapoint id 46 collected
[47:03] Charge balance equation is out by -9.2%
[47:03] Stirrer speed set to 60
[47:08] pH 2.19 -> 2.39
[47:08] Using charge balance adjust
[47:08] Dispensed 0.011430 mL of Base (0.5 M KOH)
[47:28] Stirrer speed set to 0
[47:38] Datapoint id 47 collected
[47:38] Charge balance equation is out by -4.3%
[47:38] Stirrer speed set to 60
[47:44] pH 2.39 -> 2.59
[47:44] Using charge balance adjust
[47:44] Dispensed 0.007385 mL of Base (0.5 M KOH)
[48:04] Stirrer speed set to 0
[48:15] Datapoint id 48 collected
[48:15] Charge balance equation is out by -1.9%
[48:15] Stirrer speed set to 60
[48:20] pH 2.59 -> 2.79
[48:20] Using charge balance adjust
[48:20] Dispensed 0.004821 mL of Base (0.5 M KOH)
[48:40] Stirrer speed set to 0
[48:56] Datapoint id 49 collected
[48:56] Charge balance equation is out by 5.6%
[48:56] Stirrer speed set to 60
[49:01] pH 2.81 -> 3.01
[49:01] Using charge balance adjust
[49:01] Dispensed 0.003198 mL of Base (0.5 M KOH)
[49:21] Stirrer speed set to 0
[49:36] Datapoint id 50 collected
[49:36] Charge balance equation is out by -4.8%
[49:36] Stirrer speed set to 60
[49:41] pH 3.00 -> 3.20
[49:41] Using charge balance adjust
[49:41] Dispensed 0.002328 mL of Base (0.5 M KOH)
[50:01] Stirrer speed set to 0
[50:11] Datapoint id 51 collected
[50:11] Charge balance equation is out by -14.6%
[50:11] Stirrer speed set to 60
[50:16] pH 3.18 -> 3.38
[50:16] Using charge balance adjust
[50:16] Dispensed 0.001834 mL of Base (0.5 M KOH)
[50:37] Stirrer speed set to 0

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[50:47] Datapoint id 52 collected
[50:47] Charge balance equation is out by -5.0%
[50:47] Stirrer speed set to 60
[50:52] pH 3.37 -> 3.57
[50:52] Using charge balance adjust
[50:52] Dispensed 0.001435 mL of Base (0.5 M KOH)
[51:12] Stirrer speed set to 0
[51:22] Datapoint id 53 collected
[51:22] Charge balance equation is out by -4.5%
[51:22] Stirrer speed set to 60
[51:27] pH 3.57 -> 3.77
[51:27] Using charge balance adjust
[51:27] Dispensed 0.001129 mL of Base (0.5 M KOH)
[51:47] Stirrer speed set to 0
[51:57] Datapoint id 54 collected
[51:57] Charge balance equation is out by 5.2%
[51:57] Stirrer speed set to 60
[52:03] pH 3.78 -> 3.98
[52:03] Using charge balance adjust
[52:03] Dispensed 0.000823 mL of Base (0.5 M KOH)
[52:23] Stirrer speed set to 0
[52:37] Datapoint id 55 collected
[52:37] Charge balance equation is out by -5.8%
[52:37] Stirrer speed set to 60
[52:43] pH 3.98 -> 4.18
[52:43] Using charge balance adjust
[52:43] Dispensed 0.000611 mL of Base (0.5 M KOH)
[53:03] Stirrer speed set to 0
[53:13] Datapoint id 56 collected
[53:13] Charge balance equation is out by -17.3%
[53:13] Stirrer speed set to 60
[53:18] pH 4.15 -> 4.35
[53:18] Using cautious pH adjust
[53:18] Dispensed 0.000235 mL of Base (0.5 M KOH)
[53:23] Stepping pH = 4.19
[53:23] Dispensed 0.000400 mL of Base (0.5 M KOH)
[53:28] Stepping pH = 4.30
[53:28] Dispensed 0.000141 mL of Base (0.5 M KOH)
[53:33] Stepping pH = 4.38
[53:49] Stirrer speed set to 0
[54:05] Datapoint id 57 collected
[54:05] Charge balance equation is out by -71.6%
[54:05] Stirrer speed set to 60
[54:10] pH 4.43 -> 4.63
[54:10] Using cautious pH adjust
[54:10] Dispensed 0.000118 mL of Base (0.5 M KOH)
[54:15] Stepping pH = 4.44
[54:15] Dispensed 0.000353 mL of Base (0.5 M KOH)
[54:20] Stepping pH = 4.61
[54:20] Dispensed 0.000047 mL of Base (0.5 M KOH)
[54:25] Stepping pH = 4.70
[54:40] Stirrer speed set to 0
[54:51] Datapoint id 58 collected
[54:51] Charge balance equation is out by -107.6%
[54:51] Stirrer speed set to 60
[54:56] pH 4.76 -> 4.96
[54:56] Using cautious pH adjust
[54:56] Dispensed 0.000071 mL of Base (0.5 M KOH)
[55:02] Stepping pH = 4.77

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02010**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02010_M09_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[55:02] Dispensed 0.000188 mL of Base (0.5 M KOH)
[55:07] Stepping pH = 4.90
[55:07] Dispensed 0.000071 mL of Base (0.5 M KOH)
[55:12] Stepping pH = 5.01
[55:27] Stirrer speed set to 0
[55:39] Datapoint id 59 collected
[55:39] Charge balance equation is out by -151.8%
[55:39] Stirrer speed set to 60
[55:44] pH 5.13 -> 5.33
[55:44] Using cautious pH adjust
[55:44] Dispensed 0.000024 mL of Base (0.5 M KOH)
[55:49] Stepping pH = 5.14
[55:49] Dispensed 0.000094 mL of Base (0.5 M KOH)
[55:54] Stepping pH = 5.17
[55:54] Dispensed 0.000188 mL of Base (0.5 M KOH)
[55:59] Stepping pH = 5.59
[56:14] Stirrer speed set to 0
[56:57] Datapoint id 60 collected
[56:57] Charge balance equation is out by -376.9%
[56:57] Stirrer speed set to 60
[57:02] pH 6.13 -> 6.33
[57:02] Using cautious pH adjust
[57:02] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:07] Stepping pH = 6.17
[57:07] Dispensed 0.000047 mL of Base (0.5 M KOH)
[57:12] Stepping pH = 6.29
[57:12] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:17] Stepping pH = 6.46
[57:32] Stirrer speed set to 0
[58:32] Datapoint id 61 collected
[58:32] Charge balance equation is out by -74.4%
[58:32] Stirrer speed set to 60
[58:37] pH 6.61 -> 6.81
[58:37] Using cautious pH adjust
[58:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:43] Stepping pH = 6.59
[58:43] Dispensed 0.000094 mL of Base (0.5 M KOH)
[58:48] Stepping pH = 6.63
[58:48] Dispensed 0.000212 mL of Base (0.5 M KOH)
[58:53] Stepping pH = 7.68
[59:08] Stirrer speed set to 0
[59:40] Datapoint id 62 collected
[59:40] Charge balance equation is out by -805.8%
[59:40] Stirrer speed set to 60
[59:45] pH 8.62 -> 8.82
[59:45] Using cautious pH adjust
[59:45] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:50] Stepping pH = 8.65
[59:50] Dispensed 0.000024 mL of Base (0.5 M KOH)
[59:55] Stepping pH = 8.68
[59:55] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:00:01] Stepping pH = 8.75
[1:00:01] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:00:06] Stepping pH = 8.87
[1:00:21] Stirrer speed set to 0
[1:00:38] Datapoint id 63 collected
[1:00:38] Charge balance equation is out by -507.2%
[1:00:38] Stirrer speed set to 60
[1:00:43] pH 8.96 -> 9.05

Sample name: **M09_octanol**
Assay name: **pH-metric high logP**
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Experiment start time: **3/2/2018 10:00:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:00:43] Using cautious pH adjust
[1:00:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:49] Stepping pH = 8.96
[1:00:49] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:00:54] Stepping pH = 9.00
[1:01:09] Stirrer speed set to 0
[1:01:24] Datapoint id 64 collected
[1:01:24] Charge balance equation is out by -267.3%
[1:01:24] Argon flow rate set to 0
[1:01:28] Titrator arm moved over Titration position