pH-metric Result

Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09015**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 9:53:01 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH2 +)   -0.73   ±0.56 (n=50)
logP (neutral XH) 2.59   ±0.01 (n=50)
logP (X -)   0.46
RMSD   1.511

18C-09015 Points 2 to 20

M18_octanol concentration factor 1.192
Carbonate   0.0000 mM
Acidity error   0.28168 mM

18C-09015 Points 21 to 41

M18_octanol concentration factor 1.079
Carbonate   0.1008 mM
Acidity error   -0.00618 mM

18C-09015 Points 42 to 69

M18_octanol concentration factor 1.146
Carbonate   0.1707 mM
Acidity error   0.14218 mM
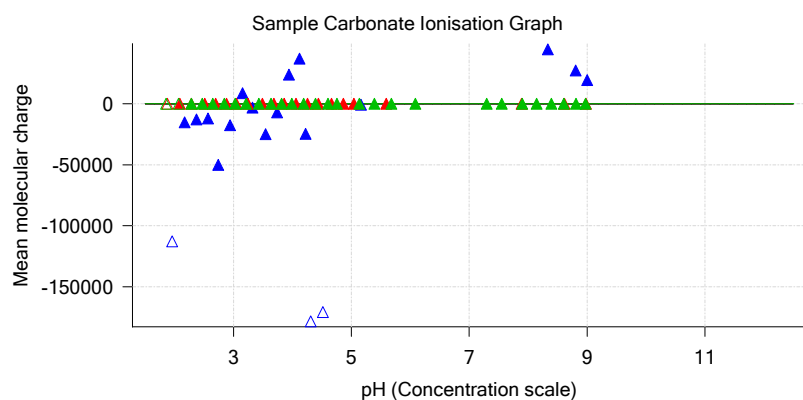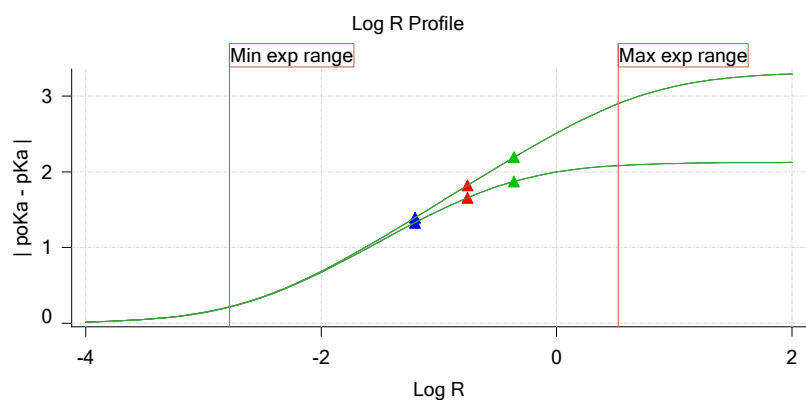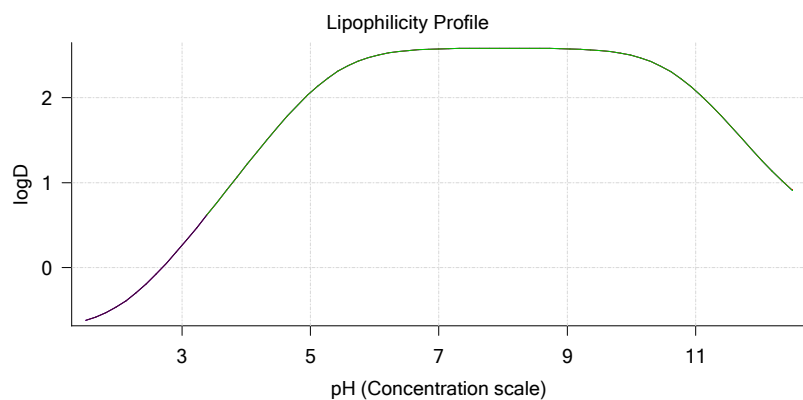
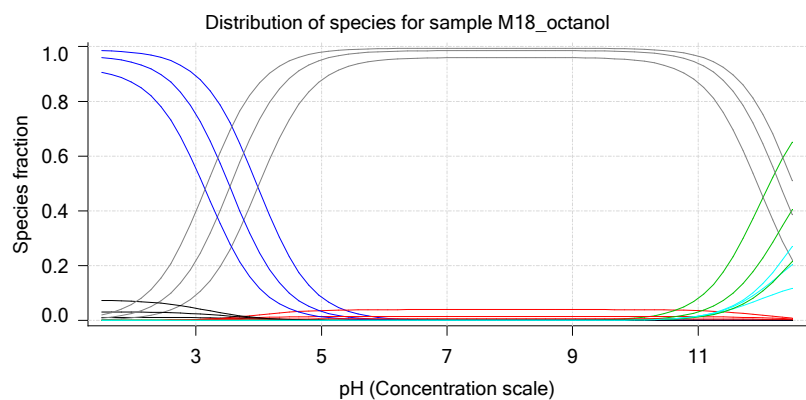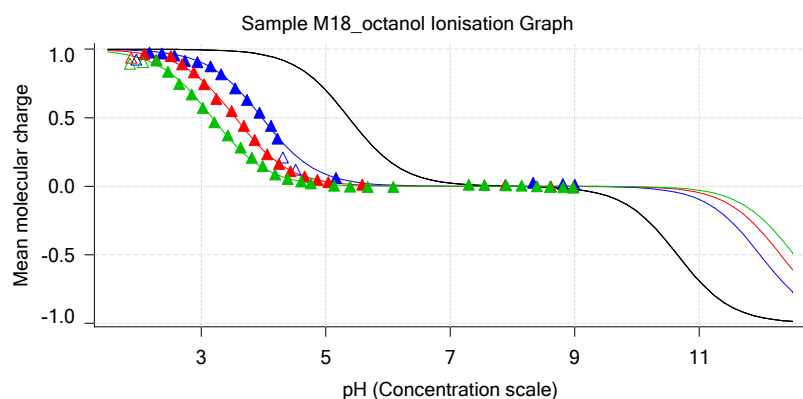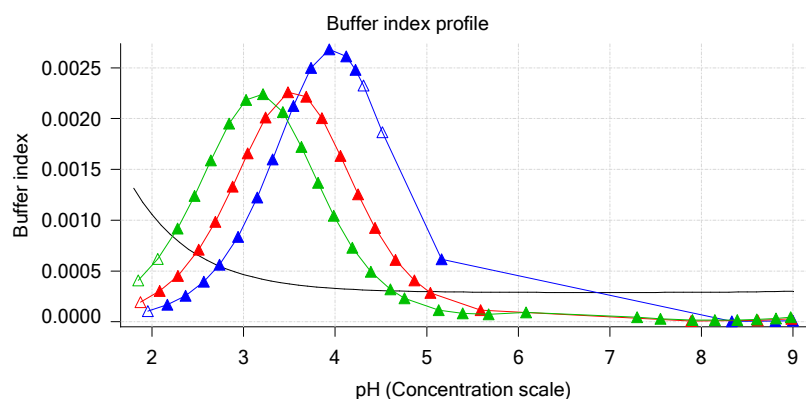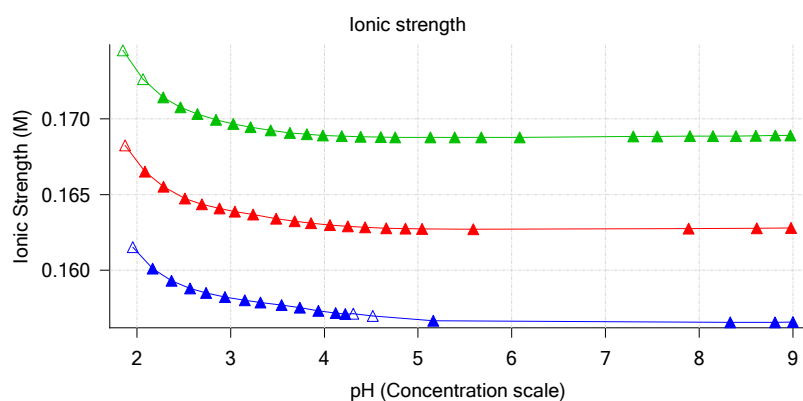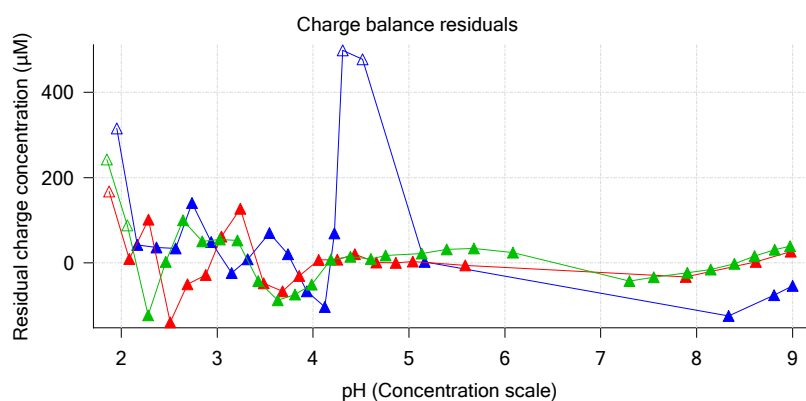## Warnings and errors

Errors   None
Warnings None

Sample logD and percent species

pH	M18_octanol logD	M18_octanol M18_octanolH2	M18_octanol M18_octanolH	M18_octanol M18_octanol	M18_octanol M18_octanolH2*	M18_octanol M18_octanolH*	M18_octanol M18_octanol*	Comment
1.000	-0.69	83.14 %	0.00 %	0.00 %	15.49 %	1.37 %	0.00 %	
1.200	-0.67	82.48 %	0.01 %	0.00 %	15.36 %	2.15 %	0.00 %	Stomach pH
2.000	-0.46	74.02 %	0.03 %	0.00 %	13.79 %	12.16 %	0.00 %	
3.000	0.26	35.30 %	0.15 %	0.00 %	6.57 %	57.98 %	0.00 %	
4.000	1.20	5.66 %	0.24 %	0.00 %	1.05 %	93.04 %	0.00 %	
5.000	2.06	0.60 %	0.26 %	0.00 %	0.11 %	99.03 %	0.00 %	
6.000	2.49	0.06 %	0.26 %	0.00 %	0.01 %	99.67 %	0.00 %	
6.500	2.55	0.02 %	0.26 %	0.00 %	0.00 %	99.72 %	0.00 %	
7.000	2.58	0.01 %	0.26 %	0.00 %	0.00 %	99.73 %	0.00 %	
7.400	2.58	0.00 %	0.26 %	0.00 %	0.00 %	99.74 %	0.00 %	Blood pH
8.000	2.58	0.00 %	0.26 %	0.00 %	0.00 %	99.74 %	0.00 %	
9.000	2.58	0.00 %	0.26 %	0.01 %	0.00 %	99.72 %	0.02 %	
10.000	2.50	0.00 %	0.26 %	0.06 %	0.00 %	99.52 %	0.17 %	
11.000	2.08	0.00 %	0.25 %	0.57 %	0.00 %	97.54 %	1.64 %	
12.000	1.28	0.00 %	0.21 %	4.73 %	0.00 %	81.41 %	13.65 %	

Sample name: **M18_octanol** Experiment start time: **3/9/2018 9:53:01 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-09015** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M18_octanol Ionisation Graph

Distribution of species for sample M18_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Sample name: **M18_octanol** Experiment start time: **3/9/2018 9:53:01 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-09015** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Graphs (continued)

Distribution of species for sample Carbonate

Sample name: **M18_octanol** Experiment start time: **3/9/2018 9:53:01 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-09015** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

pH-metric high logP   Titration 1 of 3   18C-09015 Points 2 to 20

Overall results

RMSD   2.905
Average ionic strength   0.158 M
Average temperature   24.9°C
Partition ratio   0.0626 : 1
Analyte concentration range   3669.6 µM to 3776.5 µM
Total points considered   16 of 19

Warnings and errors

Errors   None
Warnings   One or more logP values out of range

Four-Plus parameters

Alpha   0.102   3/9/2018 9:53:01 PM   C:\Sirius_T3\HCl18C09.t3r
S   0.9967   3/9/2018 9:53:01 PM   C:\Sirius_T3\HCl18C09.t3r
jH   1.2   3/9/2018 9:53:01 PM   C:\Sirius_T3\HCl18C09.t3r
jOH   0.0   3/9/2018 9:53:01 PM   C:\Sirius_T3\HCl18C09.t3r

Titrants

0.50 M HCl   0.999843   3/9/2018 9:53:01 PM   C:\Sirius_T3\HCl18C09.t3r
0.50 M KOH   0.999845   3/9/2018 9:53:01 PM   C:\Sirius_T3\KOH18B27.t3r

Sample

M18_octanol concentration factor   1.192
Base pKa 1   5.37
Acid pKa 2   10.65
logP (XH2 +)   -7.94
logP (neutral XH)   2.63
logP (X -)   0.46

Sample graphs

Ionisation of sample M18_octanol

Distribution of species for sample M18_octanol

Sample graphs (continued)

Lipophilicity Profile

Sample logD and percent species

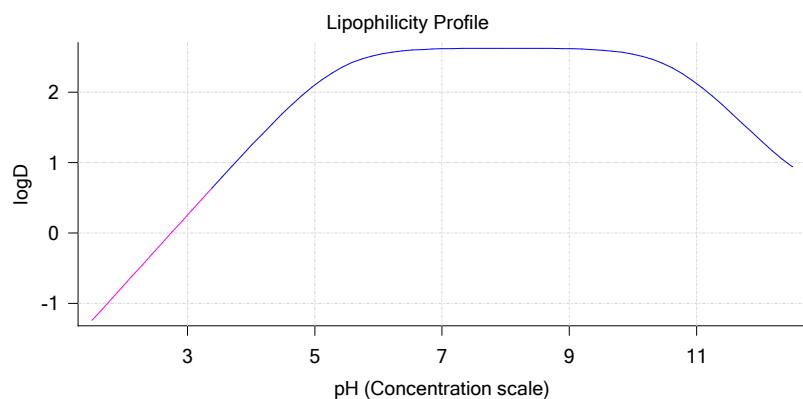| pH	M18_octanol logD	M18_octanol M18_octanolH2	M18_octanol M18_octanolH	M18_octanol M18_octanol	M18_octanol M18_octanolH2*	M18_octanol M18_octanolH*	M18_octanol M18_octanol*	Comment
1.000	-1.74	99.88 %	0.00 %	0.00 %	0.00 %	0.11 %	0.00 %	
1.200	-1.54	99.81 %	0.01 %	0.00 %	0.00 %	0.18 %	0.00 %	Stomach pH
2.000	-0.74	98.84 %	0.04 %	0.00 %	0.00 %	1.12 %	0.00 %	
3.000	0.26	89.50 %	0.38 %	0.00 %	0.00 %	10.12 %	0.00 %	
4.000	1.24	46.01 %	1.96 %	0.00 %	0.00 %	52.03 %	0.00 %	
5.000	2.10	7.85 %	3.35 %	0.00 %	0.00 %	88.80 %	0.00 %	
6.000	2.54	0.84 %	3.60 %	0.00 %	0.00 %	95.55 %	0.00 %	
6.500	2.60	0.27 %	3.63 %	0.00 %	0.00 %	96.11 %	0.00 %	
7.000	2.62	0.09 %	3.63 %	0.00 %	0.00 %	96.28 %	0.00 %	
7.400	2.62	0.03 %	3.63 %	0.00 %	0.00 %	96.33 %	0.00 %	Blood pH
8.000	2.63	0.01 %	3.63 %	0.01 %	0.00 %	96.35 %	0.00 %	
9.000	2.62	0.00 %	3.63 %	0.08 %	0.00 %	96.27 %	0.01 %	
10.000	2.54	0.00 %	3.60 %	0.81 %	0.00 %	95.45 %	0.15 %	
11.000	2.12	0.00 %	3.32 %	7.42 %	0.00 %	87.92 %	1.34 %	
12.000	1.32	0.00 %	1.85 %	41.51 %	0.00 %	49.15 %	7.49 %	

Carbonate and acidity

Carbonate   0.000 mM
Acidity error   0.282 mM

Other graphs

Assay progress

Titration graph

pH-metric

Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09015**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 9:53:01 PM**
Analyst: **Pion**
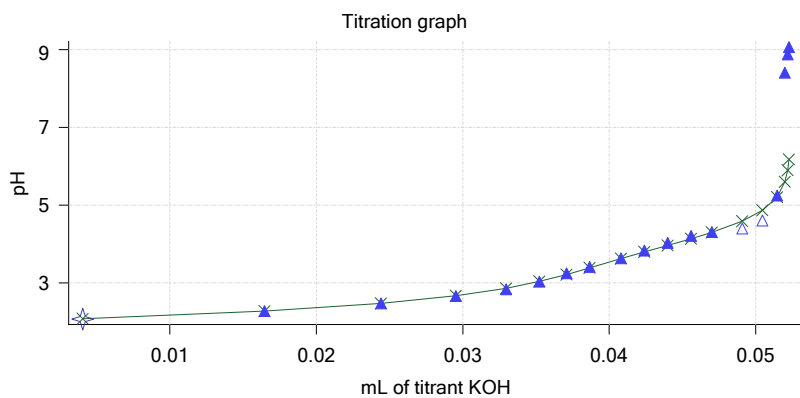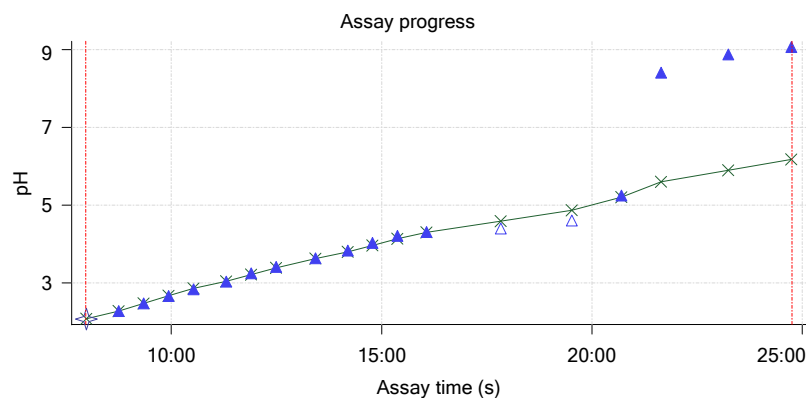Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
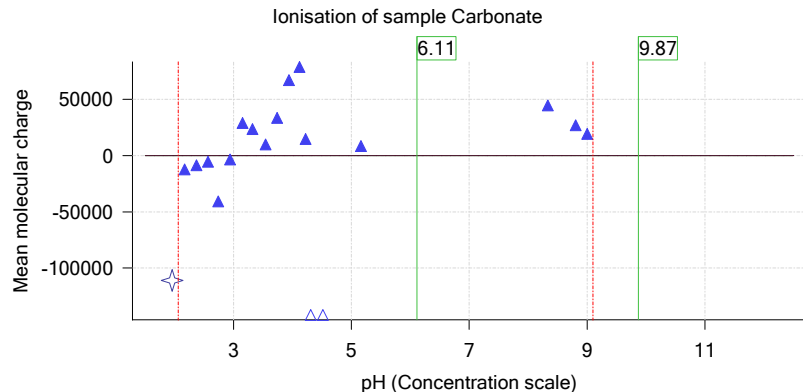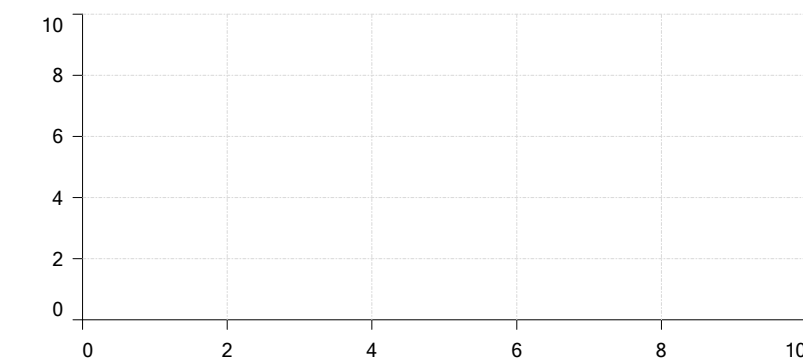
Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09015**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 9:53:01 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric high logP   Titration 2 of 3   18C-09015 Points 21 to 41

Overall results

RMSD   0.624
Average ionic strength   0.164 M
Average temperature   25.0°C
Partition ratio   0.1752 : 1
Analyte concentration range   3095.9 µM to 3187.0 µM
Total points considered   20 of 21

Warnings and errors

Errors   None
Warnings   One or more logP values out of range

Four-Plus parameters
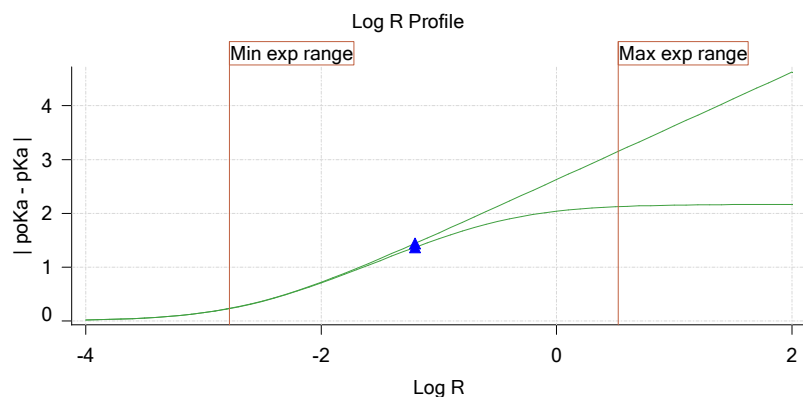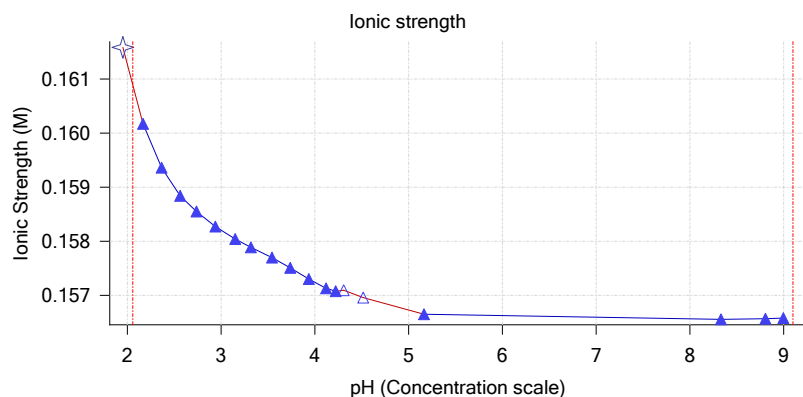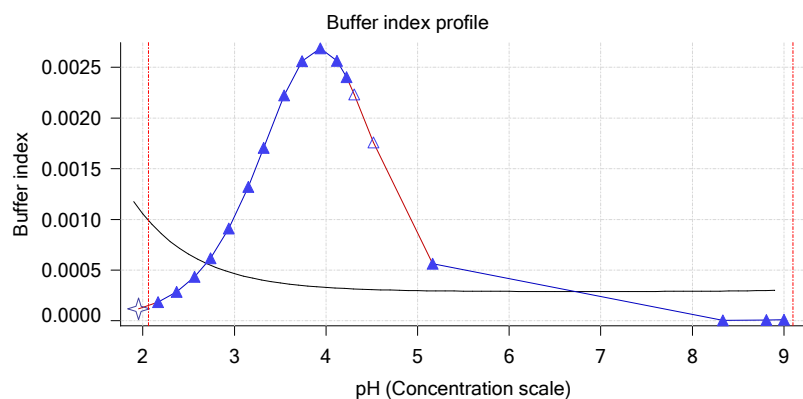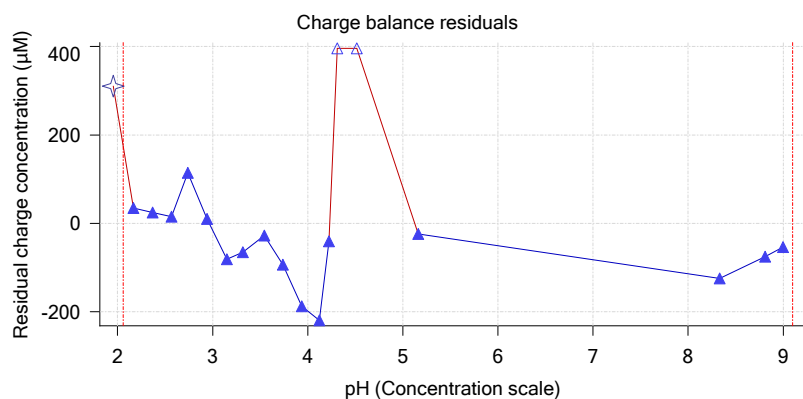
Alpha	0.102	3/9/2018 9:53:01 PM	C:\Sirius_T3\HCl18C09.t3r
S	0.9967	3/9/2018 9:53:01 PM	C:\Sirius_T3\HCl18C09.t3r
jH	1.2	3/9/2018 9:53:01 PM	C:\Sirius_T3\HCl18C09.t3r
jOH	0.0	3/9/2018 9:53:01 PM	C:\Sirius_T3\HCl18C09.t3r

Titrants

0.50 M HCl	0.999843	3/9/2018 9:53:01 PM	C:\Sirius_T3\HCl18C09.t3r
0.50 M KOH	0.999845	3/9/2018 9:53:01 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M18_octanol concentration factor   1.079
Base pKa 1   5.37
Acid pKa 2   10.65
logP (XH2 +)   -4.21
logP (neutral XH)   2.57
logP (X -)   0.46

Sample graphs

Ionisation of sample M18_octanol

Distribution of species for sample M18_octanol

Sample graphs (continued)

Lipophilicity Profile

Sample logD and percent species

pH	M18_octanol logD	M18_octanol M18_octanolH2	M18_octanol M18_octanolH	M18_octanol M18_octanol	M18_octanol M18_octanolH2*	M18_octanol M18_octanolH*	M18_octanol M18_octanol*	Comment
1.000	-1.80	99.72 %	0.00 %	0.00 %	0.00 %	0.28 %	0.00 %	
1.200	-1.60	99.55 %	0.01 %	0.00 %	0.00 %	0.44 %	0.00 %	Stomach pH
2.000	-0.80	97.25 %	0.04 %	0.00 %	0.00 %	2.71 %	0.00 %	
3.000	0.20	77.96 %	0.33 %	0.00 %	0.00 %	21.70 %	0.00 %	
4.000	1.18	26.13 %	1.11 %	0.00 %	0.00 %	72.75 %	0.00 %	
5.000	2.05	3.42 %	1.46 %	0.00 %	0.00 %	95.12 %	0.00 %	
6.000	2.48	0.35 %	1.50 %	0.00 %	0.00 %	98.14 %	0.00 %	
6.500	2.54	0.11 %	1.51 %	0.00 %	0.00 %	98.38 %	0.00 %	
7.000	2.56	0.04 %	1.51 %	0.00 %	0.00 %	98.46 %	0.00 %	
7.400	2.57	0.01 %	1.51 %	0.00 %	0.00 %	98.48 %	0.00 %	Blood pH
8.000	2.57	0.00 %	1.51 %	0.00 %	0.00 %	98.48 %	0.00 %	
9.000	2.56	0.00 %	1.51 %	0.03 %	0.00 %	98.44 %	0.02 %	
10.000	2.48	0.00 %	1.50 %	0.34 %	0.00 %	97.99 %	0.17 %	
11.000	2.07	0.00 %	1.44 %	3.22 %	0.00 %	93.72 %	1.62 %	
12.000	1.27	0.00 %	1.00 %	22.40 %	0.00 %	65.29 %	11.31 %	

Carbonate and acidity

Carbonate   0.101 mM
Acidity error   -0.006 mM

Other graphs

Assay progress

Titration graph
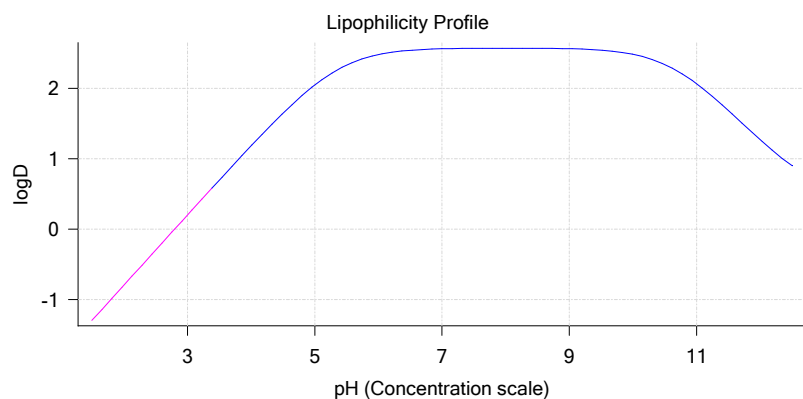
Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09015**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 9:53:01 PM**
Analyst: **Pion**
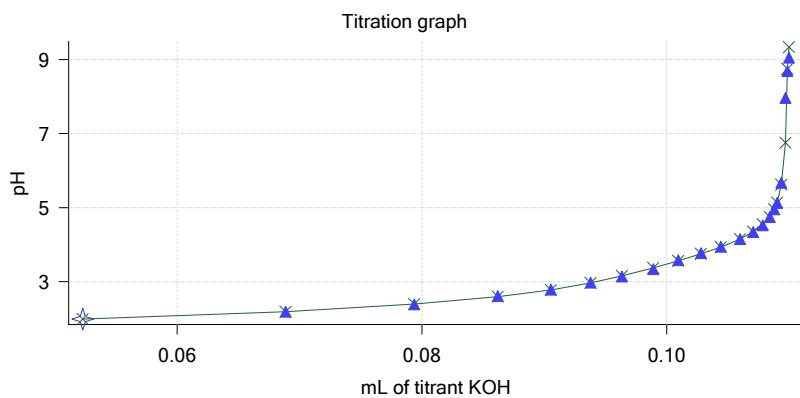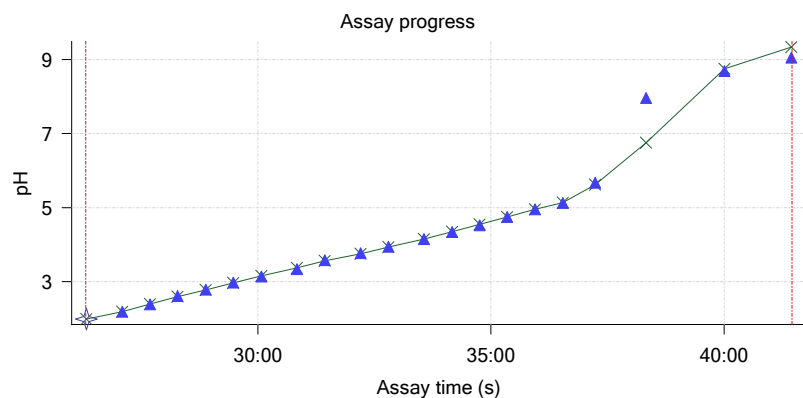Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
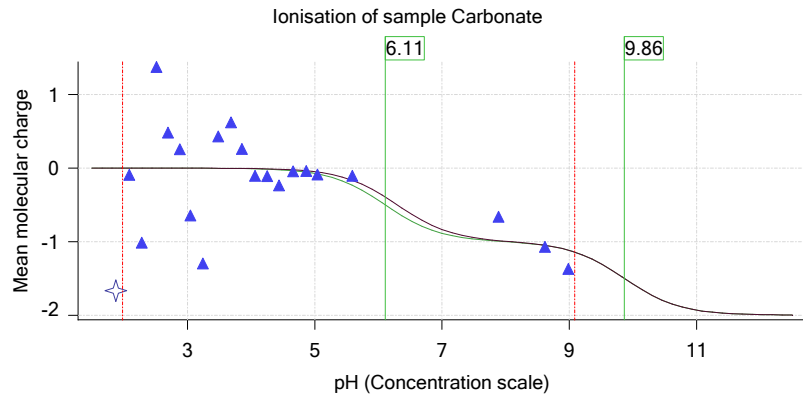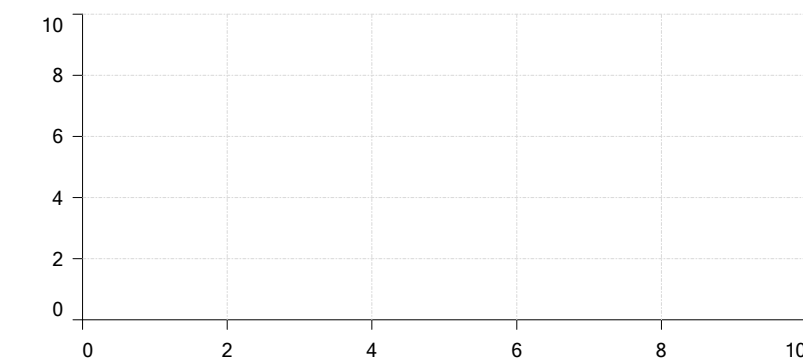
Sample name: **M18_octanol** Experiment start time: **3/9/2018 9:53:01 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-09015** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

pH-metric high logP   Titration 3 of 3   18C-09015 Points 42 to 69

Overall results

RMSD 0.425
Average ionic strength 0.169 M
Average temperature 25.0°C
Partition ratio 0.4343 : 1
Analyte concentration range 2362.4 µM to 2420.9 µM
Total points considered 26 of 28

Warnings and errors

Errors None
Warnings One or more logP values out of range

Four-Plus parameters

Alpha 0.102 3/9/2018 9:53:01 PM C:\Sirius_T3\HCl18C09.t3r
S 0.9967 3/9/2018 9:53:01 PM C:\Sirius_T3\HCl18C09.t3r
jH 1.2 3/9/2018 9:53:01 PM C:\Sirius_T3\HCl18C09.t3r
jOH 0.0 3/9/2018 9:53:01 PM C:\Sirius_T3\HCl18C09.t3r

Titrants

0.50 M HCl 0.999843 3/9/2018 9:53:01 PM C:\Sirius_T3\HCl18C09.t3r
0.50 M KOH 0.999845 3/9/2018 9:53:01 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M18_octanol concentration factor 1.146
Base pKa 1 5.37
Acid pKa 2 10.65
logP (XH2 +) -3.41
logP (neutral XH) 2.55
logP (X -) 0.46

Sample graphs
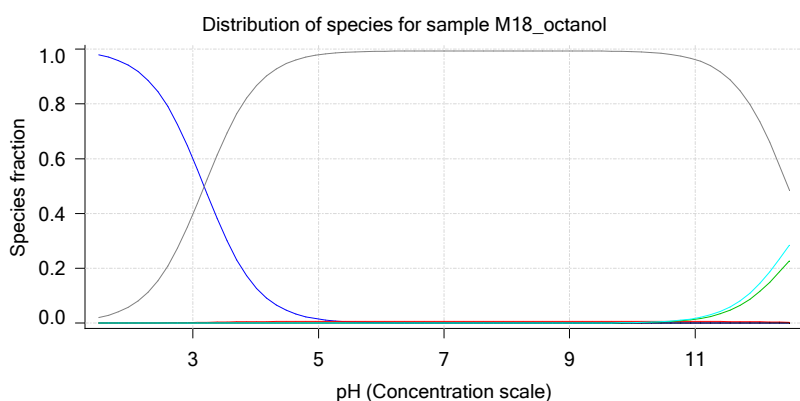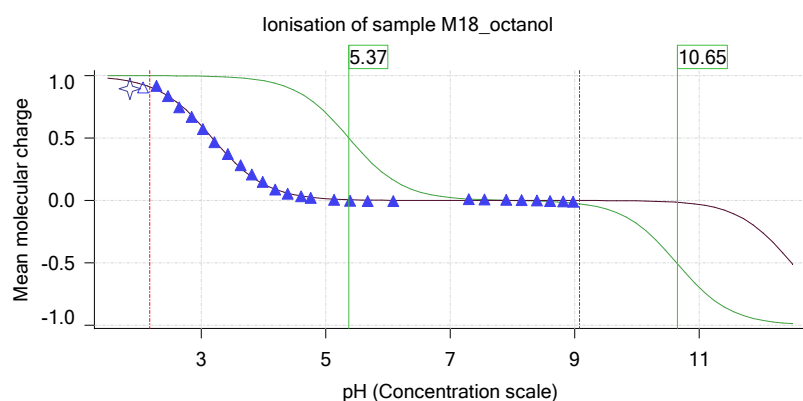
Ionisation of sample M18_octanol

Distribution of species for sample M18_octanol

Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09015**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 9:53:01 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)
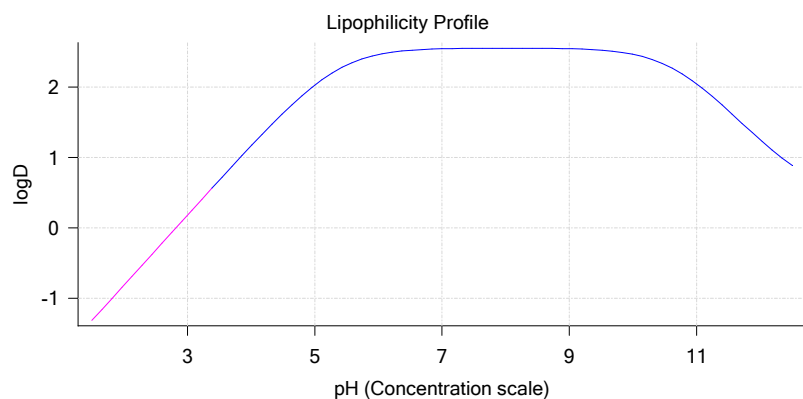
Lipophilicity Profile

Sample logD and percent species

pH	M18_octanol logD	M18_octanol M18_octanolH2	M18_octanol M18_octanolH	M18_octanol M18_octanol	M18_octanol M18_octanolH2*	M18_octanol M18_octanolH*	M18_octanol M18_octanol*	Comment
1.000	-1.80	99.32 %	0.00 %	0.00 %	0.02 %	0.66 %	0.00 %	
1.200	-1.61	98.94 %	0.01 %	0.00 %	0.02 %	1.04 %	0.00 %	Stomach pH
2.000	-0.81	93.72 %	0.04 %	0.00 %	0.02 %	6.22 %	0.00 %	
3.000	0.18	59.93 %	0.26 %	0.00 %	0.01 %	39.80 %	0.00 %	
4.000	1.17	13.02 %	0.56 %	0.00 %	0.00 %	86.43 %	0.00 %	
5.000	2.03	1.47 %	0.63 %	0.00 %	0.00 %	97.90 %	0.00 %	
6.000	2.46	0.15 %	0.64 %	0.00 %	0.00 %	99.21 %	0.00 %	
6.500	2.52	0.05 %	0.64 %	0.00 %	0.00 %	99.31 %	0.00 %	
7.000	2.54	0.01 %	0.64 %	0.00 %	0.00 %	99.35 %	0.00 %	
7.400	2.55	0.01 %	0.64 %	0.00 %	0.00 %	99.35 %	0.00 %	Blood pH
8.000	2.55	0.00 %	0.64 %	0.00 %	0.00 %	99.36 %	0.00 %	
9.000	2.54	0.00 %	0.64 %	0.01 %	0.00 %	99.33 %	0.02 %	
10.000	2.47	0.00 %	0.64 %	0.14 %	0.00 %	99.04 %	0.18 %	
11.000	2.05	0.00 %	0.62 %	1.38 %	0.00 %	96.26 %	1.73 %	
12.000	1.26	0.00 %	0.48 %	10.81 %	0.00 %	75.17 %	13.54 %	

Carbonate and acidity

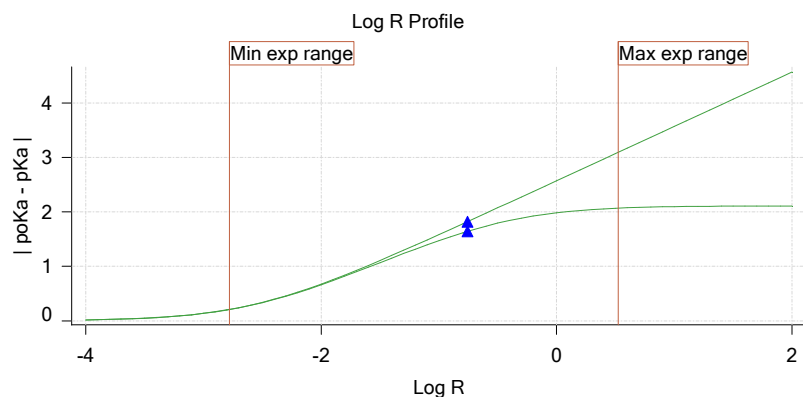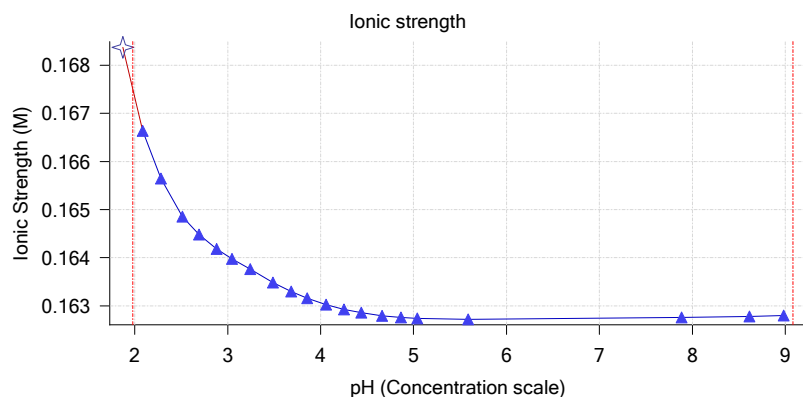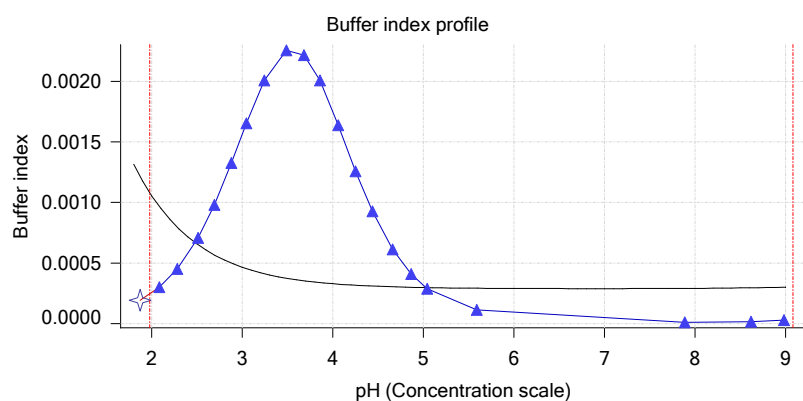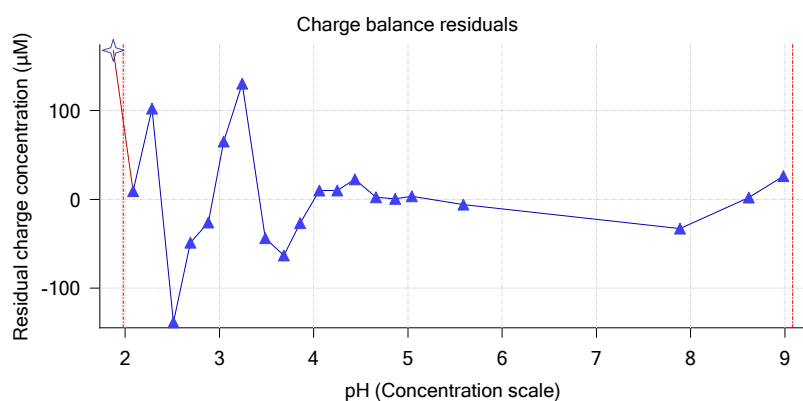Carbonate   0.171 mM
Acidity error   0.142 mM

Other graphs

Sample name: **M18_octanol** Experiment start time: **3/9/2018 9:53:01 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-09015** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate

Sirius
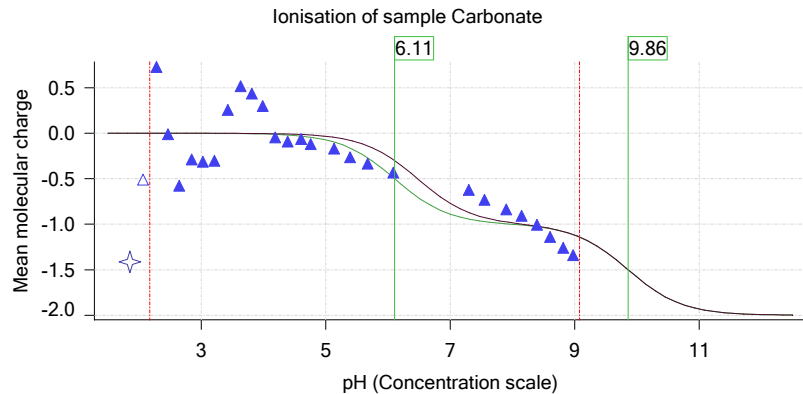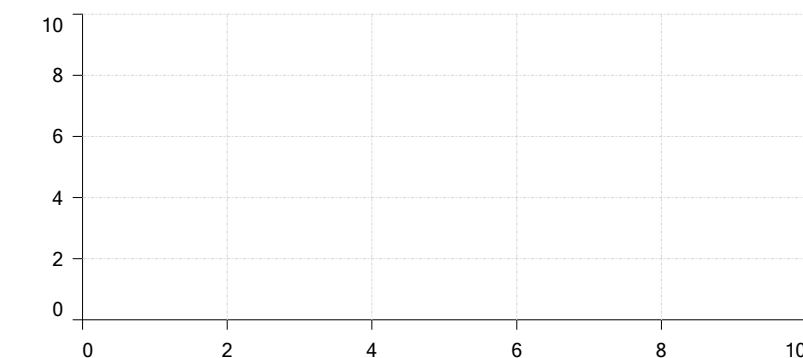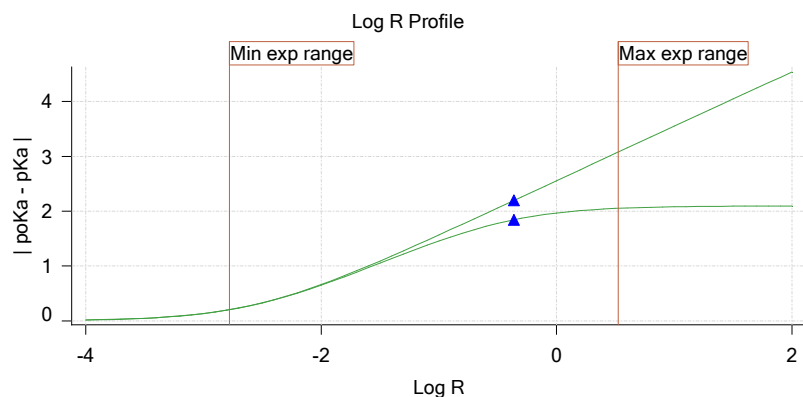
Sample name:	**M18_octanol**
Assay name:	**pH-metric high logP**
Assay ID:	**18C-09015**
Filename:	**C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Experiment start time:	**3/9/2018 9:53:01 PM**
Analyst:	**Pion**
Instrument ID:	**T312060**

Assay Model

| Settings	Value	Date/Time changed	Imported from
Sample name	M18_octanol	2/27/2018 7:08:39 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001670 g	3/9/2018 2:22:44 PM	User entered value
Formula weight	267.11 g/mol	2/27/2018 7:08:39 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	267.11	2/27/2018 7:08:39 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	2/27/2018 7:08:39 PM	User entered value
Sample is a	Ampholyte	2/27/2018 7:08:39 PM	User entered value
pKa 1	5.37	2/27/2018 7:08:39 PM	User entered value
Type	Base	2/27/2018 7:08:39 PM	User entered value
pKa 2	10.65	2/27/2018 7:08:39 PM	User entered value
Type	Acid	2/27/2018 7:08:39 PM	User entered value
logp (XH2 +)	-0.35	2/28/2018 3:20:28 PM	User entered value
logP (neutral XH)	2.57	3/2/2018 4:34:50 PM	User entered value
logP (X -)	0.46	2/27/2018 7:09:34 PM	User entered value

Events

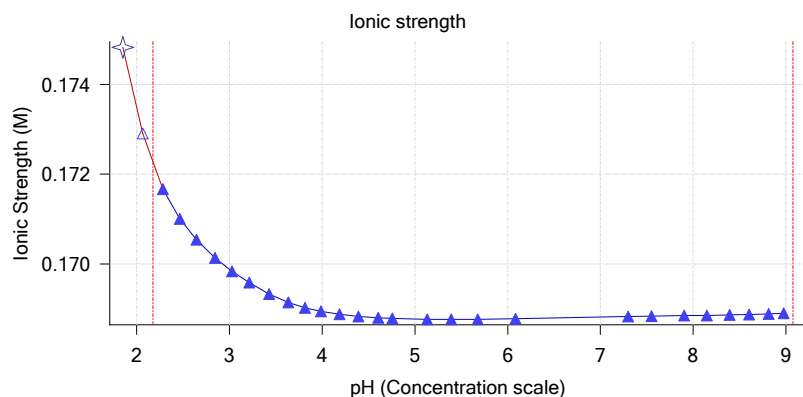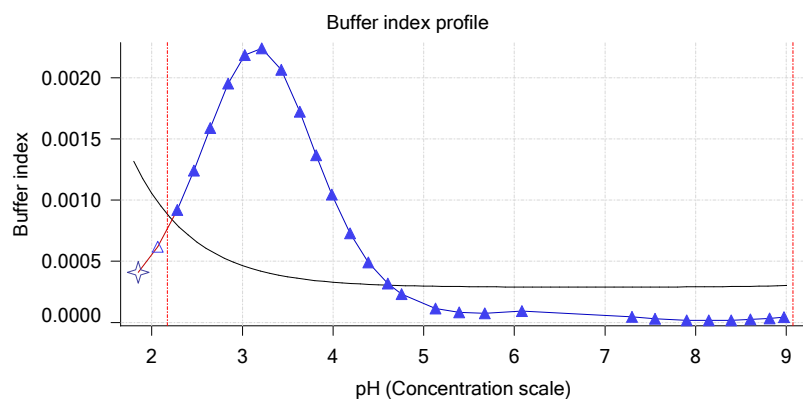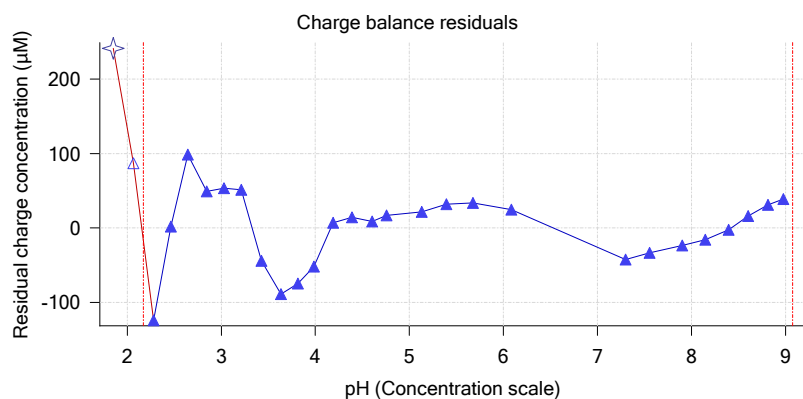| Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/time
4:58.2	Manual volume addition				0.10000 mL					
4:59.3	Initial pH = 8.13									
7:58.9	Data point 2	1.50000 mL	0.05148 mL	0.00405 mL	0.10000 mL	2.064	-0.00398	0.61752	0.00025	10.0 s
8:45.1	Data point 3	1.50000 mL	0.05148 mL	0.01646 mL	0.10000 mL	2.270	0.00032	0.01048	0.00015	10.0 s
9:20.7	Data point 4	1.50000 mL	0.05148 mL	0.02441 mL	0.10000 mL	2.467	0.00127	0.33156	0.00011	10.0 s
9:56.2	Data point 5	1.50000 mL	0.05148 mL	0.02954 mL	0.10000 mL	2.663	-0.00044	0.05449	0.00009	10.0 s
10:31.9	Data point 6	1.50000 mL	0.05148 mL	0.03295 mL	0.10000 mL	2.835	-0.00106	0.08335	0.00018	10.5 s
11:18.2	Data point 7	1.50000 mL	0.05148 mL	0.03523 mL	0.10000 mL	3.034	-0.00637	0.44601	0.00047	10.0 s
11:53.8	Data point 8	1.50000 mL	0.05148 mL	0.03709 mL	0.10000 mL	3.244	-0.00918	0.56183	0.00060	10.5 s
12:29.7	Data point 9	1.50000 mL	0.05148 mL	0.03866 mL	0.10000 mL	3.411	-0.01473	0.74716	0.00084	10.0 s
13:25.9	Data point 10	1.50000 mL	0.05148 mL	0.04080 mL	0.10000 mL	3.635	-0.01009	0.71263	0.00059	10.0 s
14:11.7	Data point 11	1.50000 mL	0.05148 mL	0.04240 mL	0.10000 mL	3.828	-0.01257	0.80770	0.00069	10.0 s
14:47.2	Data point 12	1.50000 mL	0.05148 mL	0.04400 mL	0.10000 mL	4.027	-0.00532	0.89260	0.00028	10.0 s
15:22.6	Data point 13	1.50000 mL	0.05148 mL	0.04558 mL	0.10000 mL	4.210	-0.01823	0.90318	0.00095	16.0 s
16:04.1	Data point 14	1.50000 mL	0.05148 mL	0.04701 mL	0.10000 mL	4.312	-0.10209	0.99736	0.00505	Timed out at
17:50.2	Data point 15	1.50000 mL	0.05148 mL	0.04908 mL	0.10000 mL	4.398	-0.03232	0.99319	0.00160	Timed out at
19:31.1	Data point 16	1.50000 mL	0.05148 mL	0.05047 mL	0.10000 mL	4.604	-0.02003	0.98669	0.00100	45.5 s
20:42.0	Data point 17	1.50000 mL	0.05148 mL	0.05146 mL	0.10000 mL	5.249	-0.01859	0.86523	0.00099	26.0 s

Sample name: **M18_octanol**   Experiment start time: **3/9/2018 9:53:01 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-09015**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_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
21:38.6	Data point 18	1.50000 mL	0.05148 mL	0.05200 mL	0.10000 mL	8.408	-0.02877	0.97980	0.00144	Timed out at 59.5 s
23:14.2	Data point 19	1.50000 mL	0.05148 mL	0.05219 mL	0.10000 mL	8.882	-0.01997	0.97577	0.00100	54.5 s
24:44.4	Data point 20	1.50000 mL	0.05148 mL	0.05228 mL	0.10000 mL	9.072	-0.01991	0.96826	0.00100	32.0 s
26:19.4	Data point 21	1.50000 mL	0.10948 mL	0.05228 mL	0.30000 mL	1.985	-0.00807	0.73649	0.00046	10.0 s
27:05.6	Data point 22	1.50000 mL	0.10948 mL	0.06886 mL	0.30000 mL	2.191	-0.00302	0.06536	0.00058	10.0 s
27:41.3	Data point 23	1.50000 mL	0.10948 mL	0.07937 mL	0.30000 mL	2.384	0.00289	0.58885	0.00019	10.0 s
28:16.9	Data point 24	1.50000 mL	0.10948 mL	0.08619 mL	0.30000 mL	2.610	-0.00234	0.02222	0.00078	10.5 s
28:52.9	Data point 25	1.50000 mL	0.10948 mL	0.09055 mL	0.30000 mL	2.789	-0.00887	0.28002	0.00083	10.0 s
29:28.4	Data point 26	1.50000 mL	0.10948 mL	0.09377 mL	0.30000 mL	2.975	-0.00368	0.74326	0.00021	10.5 s
30:04.5	Data point 27	1.50000 mL	0.10948 mL	0.09633 mL	0.30000 mL	3.139	-0.00884	0.23194	0.00091	10.0 s
30:50.3	Data point 28	1.50000 mL	0.10948 mL	0.09889 mL	0.30000 mL	3.334	-0.01064	0.80030	0.00059	10.5 s
31:26.3	Data point 29	1.50000 mL	0.10948 mL	0.10094 mL	0.30000 mL	3.577	-0.01028	0.41136	0.00079	10.0 s
32:12.0	Data point 30	1.50000 mL	0.10948 mL	0.10280 mL	0.30000 mL	3.773	-0.00666	0.87855	0.00035	10.5 s
32:48.0	Data point 31	1.50000 mL	0.10948 mL	0.10442 mL	0.30000 mL	3.947	-0.01424	0.74500	0.00081	10.0 s
33:33.8	Data point 32	1.50000 mL	0.10948 mL	0.10600 mL	0.30000 mL	4.149	-0.00724	0.88195	0.00038	10.5 s
34:09.8	Data point 33	1.50000 mL	0.10948 mL	0.10706 mL	0.30000 mL	4.340	-0.00713	0.59165	0.00046	10.0 s
34:45.3	Data point 34	1.50000 mL	0.10948 mL	0.10786 mL	0.30000 mL	4.525	-0.01579	0.72847	0.00091	10.0 s
35:20.7	Data point 35	1.50000 mL	0.10948 mL	0.10842 mL	0.30000 mL	4.747	-0.01335	0.78441	0.00074	10.5 s
35:56.6	Data point 36	1.50000 mL	0.10948 mL	0.10880 mL	0.30000 mL	4.951	-0.00800	0.24231	0.00080	10.5 s
36:32.5	Data point 37	1.50000 mL	0.10948 mL	0.10903 mL	0.30000 mL	5.127	-0.01493	0.70300	0.00088	11.0 s
37:14.0	Data point 38	1.50000 mL	0.10948 mL	0.10936 mL	0.30000 mL	5.672	-0.01880	0.88256	0.00099	29.5 s
38:19.4	Data point 39	1.50000 mL	0.10948 mL	0.10969 mL	0.30000 mL	7.963	-0.08034	0.99469	0.00398	Timed out at 59.5 s
40:00.2	Data point 40	1.50000 mL	0.10948 mL	0.10985 mL	0.30000 mL	8.691	-0.01737	0.90449	0.00090	50.5 s
41:26.4	Data point 41	1.50000 mL	0.10948 mL	0.11000 mL	0.30000 mL	9.055	-0.02009	0.98442	0.00100	30.0 s
43:22.0	Data point 42	1.50000 mL	0.17251 mL	0.11000 mL	0.80000 mL	1.964	-0.00989	0.81980	0.00054	10.0 s
44:08.3	Data point 43	1.50000 mL	0.17251 mL	0.12900 mL	0.80000 mL	2.170	0.00443	0.37114	0.00036	10.0 s
44:44.0	Data point 44	1.50000 mL	0.17251 mL	0.14088 mL	0.80000 mL	2.382	0.00263	0.03724	0.00067	10.5 s
45:20.1	Data point 45	1.50000 mL	0.17251 mL	0.14857 mL	0.80000 mL	2.564	-0.00827	0.25892	0.00080	10.0 s
45:55.7	Data point 46	1.50000 mL	0.17251 mL	0.15404 mL	0.80000 mL	2.741	-0.00871	0.52375	0.00059	10.0 s
46:31.2	Data point 47	1.50000 mL	0.17251 mL	0.15818 mL	0.80000 mL	2.939	0.00202	0.06322	0.00040	10.5 s
47:07.2	Data point 48	1.50000 mL	0.17251 mL	0.16141 mL	0.80000 mL	3.121	-0.00814	0.90284	0.00042	10.0 s
47:42.7	Data point 49	1.50000 mL	0.17251 mL	0.16409 mL	0.80000 mL	3.304	0.00201	0.05752	0.00041	10.5 s
48:18.7	Data point 50	1.50000 mL	0.17251 mL	0.16634 mL	0.80000 mL	3.520	-0.01362	0.46718	0.00098	10.0 s
48:54.2	Data point 51	1.50000 mL	0.17251 mL	0.16813 mL	0.80000 mL	3.724	-0.00424	0.07060	0.00079	10.0 s
49:29.6	Data point 52	1.50000 mL	0.17251 mL	0.16950 mL	0.80000 mL	3.903	-0.00679	0.94080	0.00035	10.5 s
50:05.6	Data point 53	1.50000 mL	0.17251 mL	0.17053 mL	0.80000 mL	4.076	0.00436	0.17804	0.00051	10.0 s
50:56.5	Data point 54	1.50000 mL	0.17251 mL	0.17154 mL	0.80000 mL	4.276	-0.00388	0.13097	0.00053	10.0 s
51:47.4	Data point 55	1.50000 mL	0.17251 mL	0.17211 mL	0.80000 mL	4.477	-0.01051	0.37200	0.00085	10.0 s
52:22.7	Data point 56	1.50000 mL	0.17251 mL	0.17246 mL	0.80000 mL	4.690	-0.01333	0.59091	0.00086	11.0 s
52:59.1	Data point 57	1.50000 mL	0.17251 mL	0.17267 mL	0.80000 mL	4.843	-0.01303	0.56430	0.00086	11.0 s
53:40.6	Data point 58	1.50000 mL	0.17251 mL	0.17295 mL	0.80000 mL	5.218	-0.01867	0.86298	0.00099	28.0 s
54:39.2	Data point 59	1.50000 mL	0.17251 mL	0.17310 mL	0.80000 mL	5.477	-0.01831	0.92742	0.00094	31.0 s
55:40.7	Data point 60	1.50000 mL	0.17251 mL	0.17319 mL	0.80000 mL	5.760	-0.01927	0.92709	0.00099	35.5 s
56:46.8	Data point 61	1.50000 mL	0.17251 mL	0.17328 mL	0.80000 mL	6.166	-0.01962	0.94684	0.00100	59.0 s
58:16.4	Data point 62	1.50000 mL	0.17251 mL	0.17342 mL	0.80000 mL	7.377	-0.12941	0.99771	0.00639	Timed out at 59.5 s
59:46.9	Data point 63	1.50000 mL	0.17251 mL	0.17350 mL	0.80000 mL	7.630	-0.07477	0.98222	0.00373	Timed out at 59.5 s
1:01:22.5	Data point 64	1.50000 mL	0.17251 mL	0.17357 mL	0.80000 mL	7.978	-0.05777	0.98086	0.00288	Timed out at 59.5 s
1:02:53.1	Data point 65	1.50000 mL	0.17251 mL	0.17361 mL	0.80000 mL	8.222	-0.03185	0.98956	0.00158	Timed out at 59.5 s
1:04:28.8	Data point 66	1.50000 mL	0.17251 mL	0.17368 mL	0.80000 mL	8.468	-0.02381	0.91426	0.00123	Timed out at 59.5 s
1:06:09.5	Data point 67	1.50000 mL	0.17251 mL	0.17378 mL	0.80000 mL	8.677	-0.01737	0.85617	0.00093	43.5 s

Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09015**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 9:53:01 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:07:28.7	Data point 68	1.50000 mL	0.17251 mL	0.17387 mL	0.80000 mL	8.888	-0.01877	0.89665	0.00098	35.5 s
1:08:34.8	Data point 69	1.50000 mL	0.17251 mL	0.17394 mL	0.80000 mL	9.048	-0.01938	0.95152	0.00098	14.0 s
1:08:57.9	Assay volumes	1.50000 mL	0.17251 mL	0.17394 mL	0.80000 mL					

Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09015**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 9:53:01 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	0.100 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	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	0.200 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09015**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 9:53:01 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	0.500 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	0.102	3/9/2018 9:53:01 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus S	0.9967	3/9/2018 9:53:01 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus jH	1.2	3/9/2018 9:53:01 PM	C:\Sirius_T3\HCl18C09.t3r
Four-Plus jOH	0.0	3/9/2018 9:53:01 PM	C:\Sirius_T3\HCl18C09.t3r
Base concentration factor	1.000	3/9/2018 9:53:01 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	1.000	3/9/2018 9:53:01 PM	C:\Sirius_T3\HCl18C09.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	2/27/2018 11:05:59 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)	02-27-2018	2/27/2018 11:27:22 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)	9/22/2017	2/27/2018 11:21:22 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: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09015**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 9:53:01 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	+4.36 mV		3/9/2018 9:53:29 PM
Filling solution	3M KCl	KCL097	3/9/2018 11:05:42 AM
Liquids			
Wash 1	50% IPA:50% Water		3/9/2018 11:04:22 AM
Wash 2	0.5% Trition X-100 in H20		3/9/2018 11:04:25 AM
Buffer position 1	pH7 Wash		3/9/2018 11:04:27 AM
Buffer position 2	pH 7		3/9/2018 11:04:30 AM
Storage position			3/9/2018 11:05:04 AM
Wash water	5e+003 mL	02-27-2018	2/27/2018 10:54:39 AM
Waste	1.1e+004 mL		11/28/2017 11:36:29 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	123:16:41		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: **M18_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-09015**
Filename: **C:\Sirius_T3\Mehtap\20180309_exp31_logP_T3-2\18C-09015_M18_octanol_pH-metric high logP.t3r**

Experiment start time: **3/9/2018 9:53:01 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