Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

pH-metric Result

logP (XH +)   1.14   ±0.04 (n=50)
logP (neutral X)   4.16   ±0.01 (n=50)

18C-06015 Points 1 to 20

M02_octanol concentration factor 0.918
Carbonate   0.0000 mM
Acidity error   -0.42538 mM

18C-06015 Points 21 to 34

M02_octanol concentration factor 0.898
Carbonate   0.0001 mM
Acidity error   -0.16274 mM

18C-06015 Points 35 to 48

M02_octanol concentration factor 0.730
Carbonate   0.1987 mM
Acidity error   -0.19134 mM
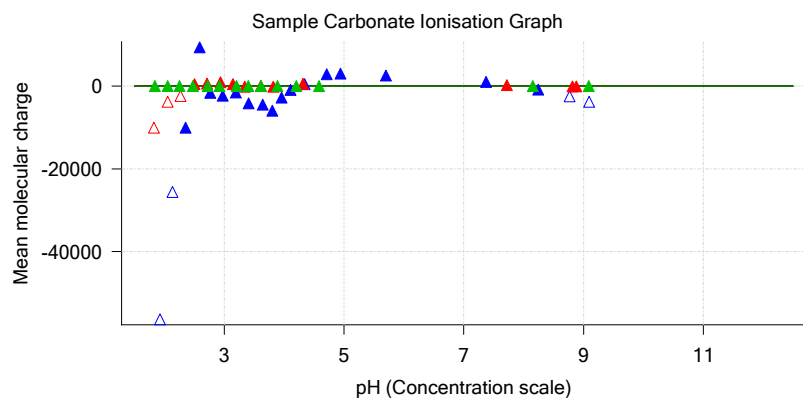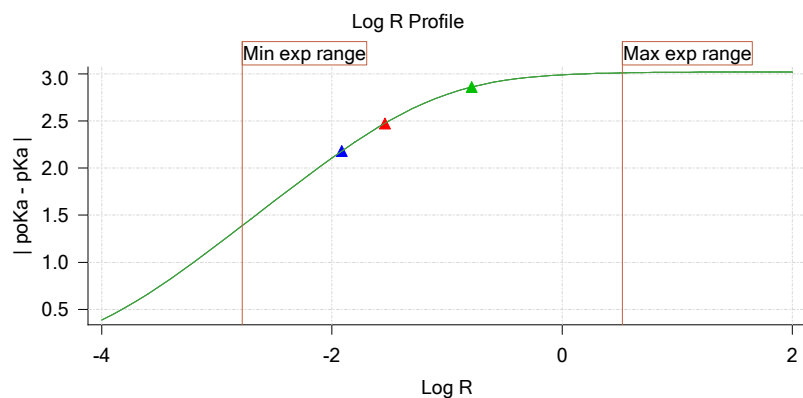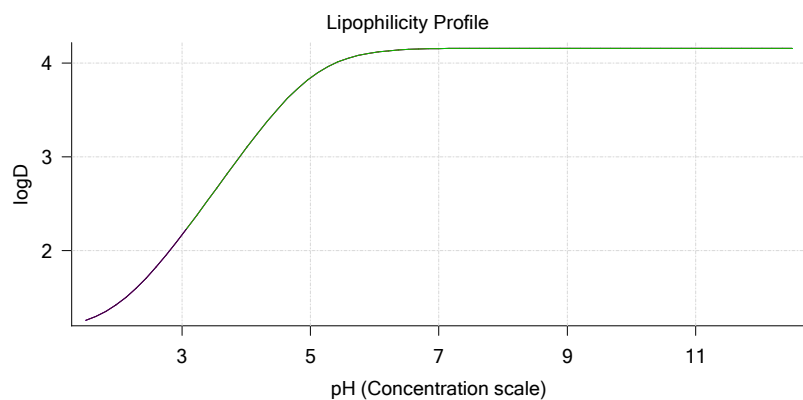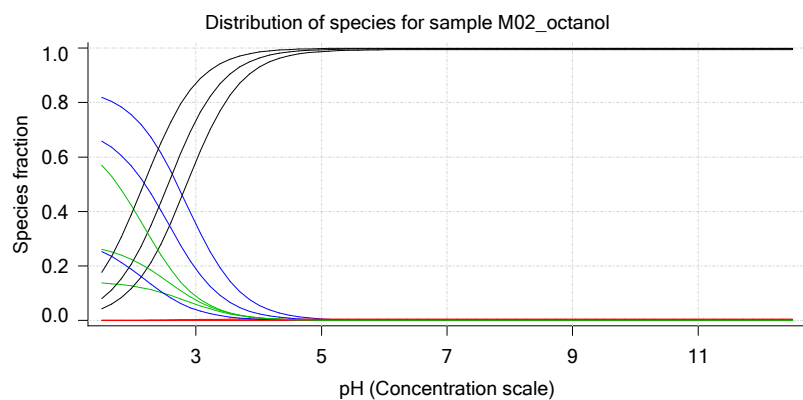
Warnings and errors
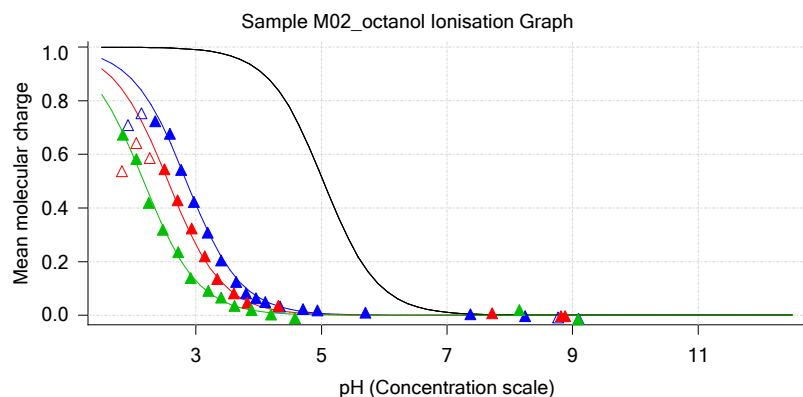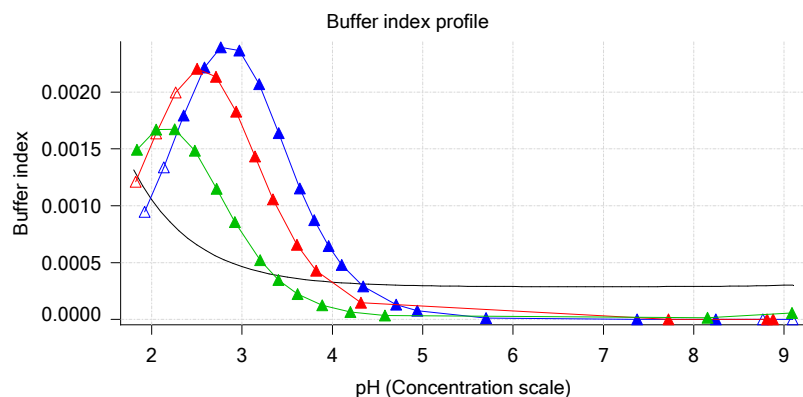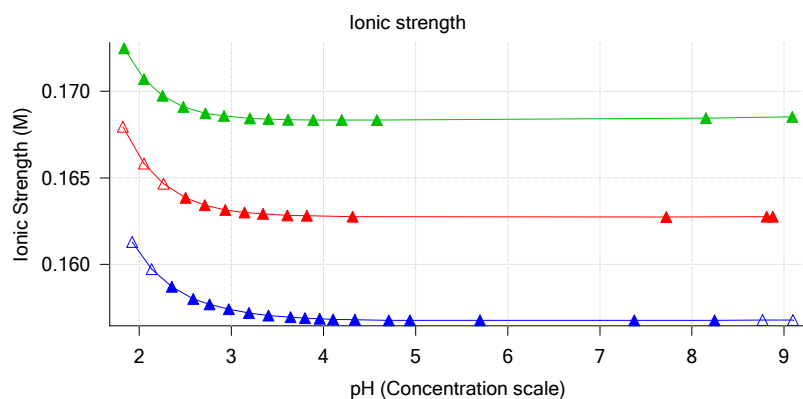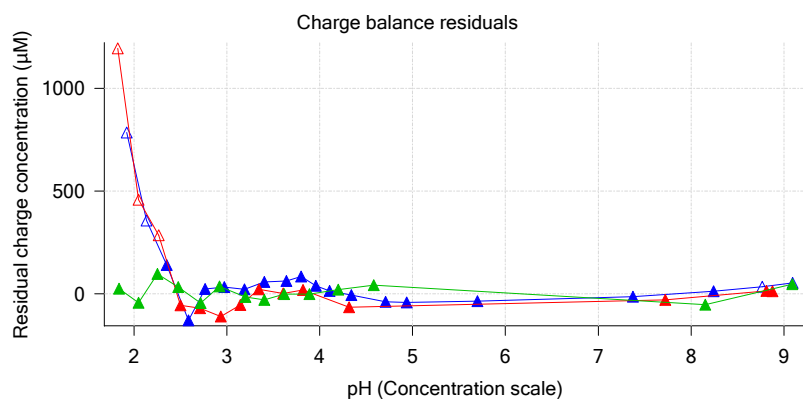
Errors   None
Warnings   None

Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanol	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.18	6.22 %	0.00 %	85.42 %	8.36 %	
1.200	1.20	5.93 %	0.00 %	81.44 %	12.64 %	Stomach pH
2.000	1.43	3.55 %	0.00 %	48.74 %	47.71 %	
3.000	2.17	0.67 %	0.01 %	9.21 %	90.12 %	
4.000	3.09	0.07 %	0.01 %	1.01 %	98.91 %	
5.000	3.84	0.01 %	0.01 %	0.10 %	99.88 %	
6.000	4.11	0.00 %	0.01 %	0.01 %	99.98 %	
6.500	4.14	0.00 %	0.01 %	0.00 %	99.99 %	
7.000	4.15	0.00 %	0.01 %	0.00 %	99.99 %	
7.400	4.16	0.00 %	0.01 %	0.00 %	99.99 %	Blood pH
8.000	4.16	0.00 %	0.01 %	0.00 %	99.99 %	
9.000	4.16	0.00 %	0.01 %	0.00 %	99.99 %	
10.000	4.16	0.00 %	0.01 %	0.00 %	99.99 %	
11.000	4.16	0.00 %	0.01 %	0.00 %	99.99 %	
12.000	4.16	0.00 %	0.01 %	0.00 %	99.99 %	

pH-metric Result

Sample name: **M02_octanol** Experiment start time: **3/6/2018 5:41:59 PM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **18C-06015** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M02_octanol Ionisation Graph

Distribution of species for sample M02_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
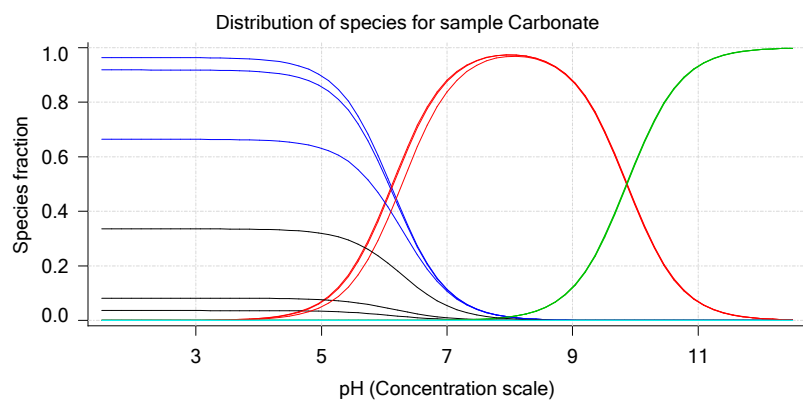Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Graphs (continued)

Distribution of species for sample Carbonate

Sample name: **M02_octanol** Experiment start time: **3/6/2018 5:41:59 PM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **18C-06015** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

pH-metric high logP   Titration 1 of 3   18C-06015 Points 1 to 20

Overall results

RMSD 2.836
Average ionic strength 0.157 M
Average temperature 24.9°C
Partition ratio 0.0122 : 1
Analyte concentration range 4481.9 µM to 4615.4 µM
Total points considered 16 of 20

Warnings and errors

Errors None
Warnings None

Four-Plus parameters

Alpha 0.124 3/6/2018 5:41:59 PM C:\Sirius_T3\18C-06006_Blank standardisation.t3r
S 0.9973 3/6/2018 5:41:59 PM C:\Sirius_T3\18C-06006_Blank standardisation.t3r
jH 0.9 3/6/2018 5:41:59 PM C:\Sirius_T3\18C-06006_Blank standardisation.t3r
jOH -0.7 3/6/2018 5:41:59 PM C:\Sirius_T3\18C-06006_Blank standardisation.t3r
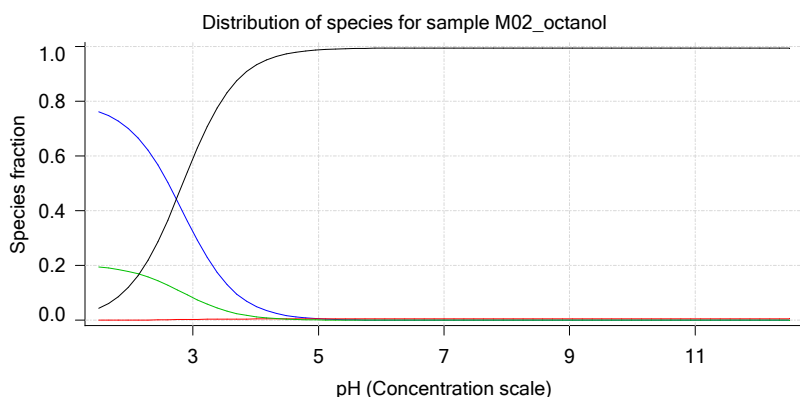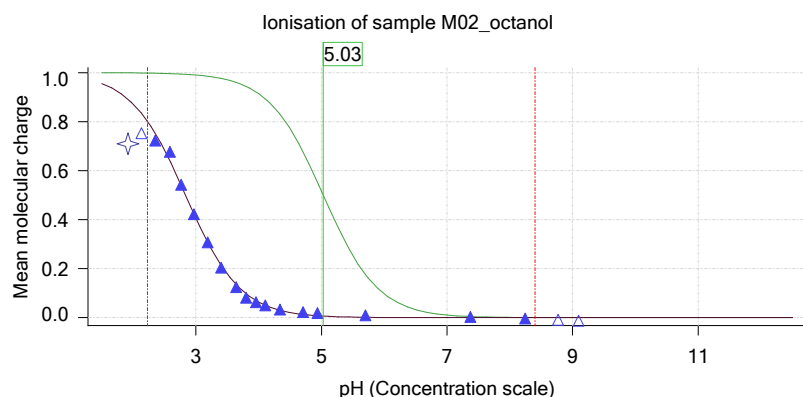
Titrants

0.50 M HCl 0.989131 3/6/2018 5:41:59 PM C:\Sirius_T3\18C-06006_Blank standardisation.t3r
0.50 M KOH 0.999845 3/6/2018 5:41:59 PM C:\Sirius_T3\KOH18B27.t3r

Sample

M02_octanol concentration factor 0.918
Base pKa 1 5.03
logP (XH +) 1.32
logP (neutral X) 4.20

Sample graphs

Ionisation of sample M02_octanol

Distribution of species for sample M02_octanol

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**
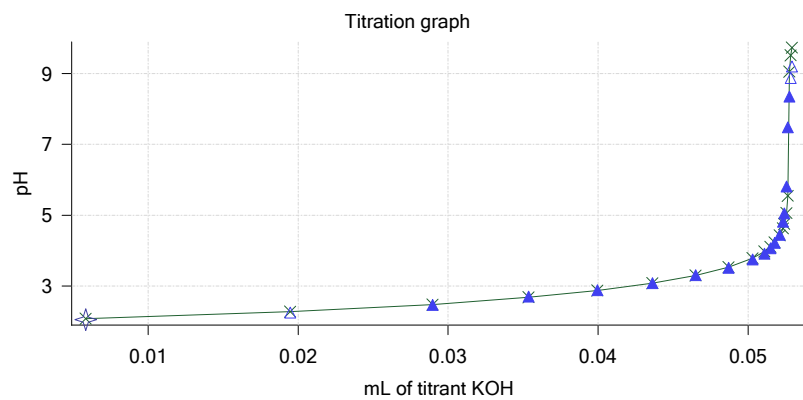
Sample graphs (continued)
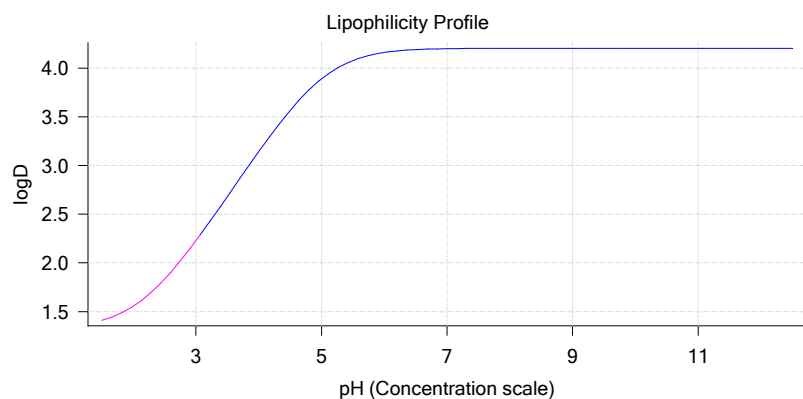
Lipophilicity Profile

Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanol	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.35	78.52 %	0.01 %	20.04 %	1.43 %	
1.200	1.37	77.87 %	0.01 %	19.87 %	2.25 %	Stomach pH
2.000	1.55	69.52 %	0.06 %	17.74 %	12.68 %	
3.000	2.23	32.38 %	0.30 %	8.26 %	59.05 %	
4.000	3.14	5.11 %	0.48 %	1.30 %	93.11 %	
5.000	3.89	0.54 %	0.51 %	0.14 %	98.81 %	
6.000	4.16	0.05 %	0.51 %	0.01 %	99.42 %	
6.500	4.19	0.02 %	0.51 %	0.00 %	99.47 %	
7.000	4.20	0.01 %	0.51 %	0.00 %	99.48 %	
7.400	4.20	0.00 %	0.51 %	0.00 %	99.49 %	Blood pH
8.000	4.20	0.00 %	0.51 %	0.00 %	99.49 %	
9.000	4.20	0.00 %	0.51 %	0.00 %	99.49 %	
10.000	4.20	0.00 %	0.51 %	0.00 %	99.49 %	
11.000	4.20	0.00 %	0.51 %	0.00 %	99.49 %	
12.000	4.20	0.00 %	0.51 %	0.00 %	99.49 %	

Carbonate and acidity

Carbonate   0.000 mM
Acidity error   -0.425 mM

Other graphs

Sample name: **M02_octanol**   Experiment start time: **3/6/2018 5:41:59 PM**
Assay name: **pH-metric high logP**   Analyst: **Dorothy Levorse**
Assay ID: **18C-06015**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_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
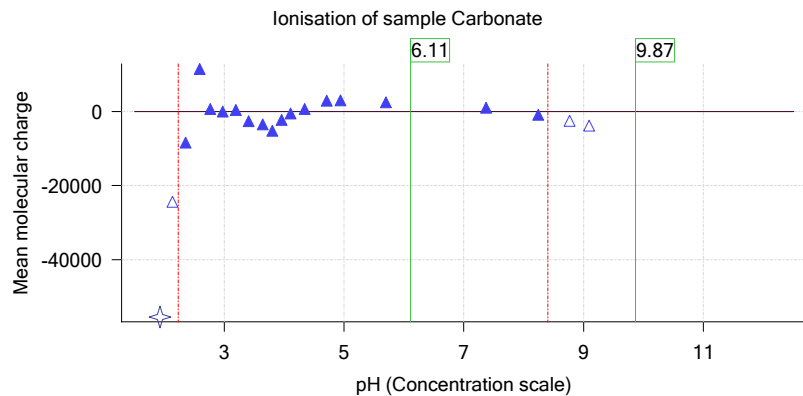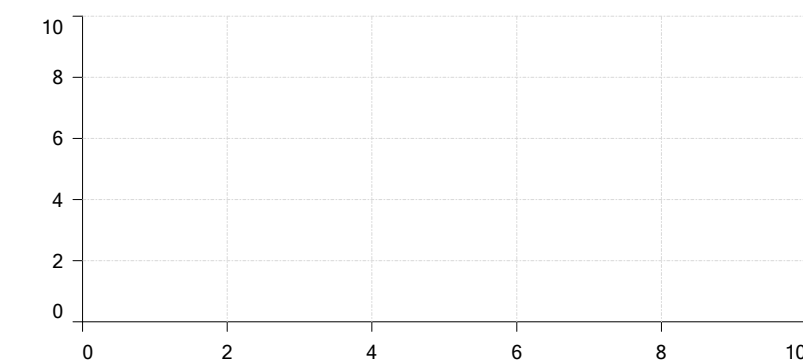
Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
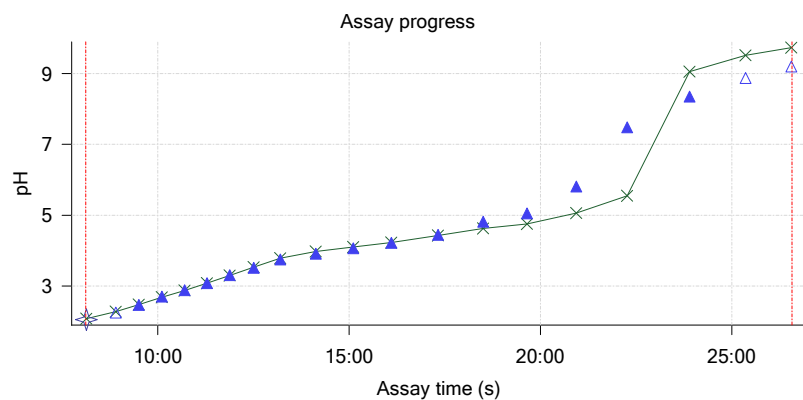Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

pH-metric high logP   Titration 2 of 3   18C-06015 Points 21 to 34

Overall results

RMSD	4.143
Average ionic strength	0.163 M
Average temperature	25.0°C
Partition ratio	0.0289 : 1
Analyte concentration range	4116.8 µM to 4254.1 µM
Total points considered	11 of 14

Warnings and errors

Errors   None
Warnings None

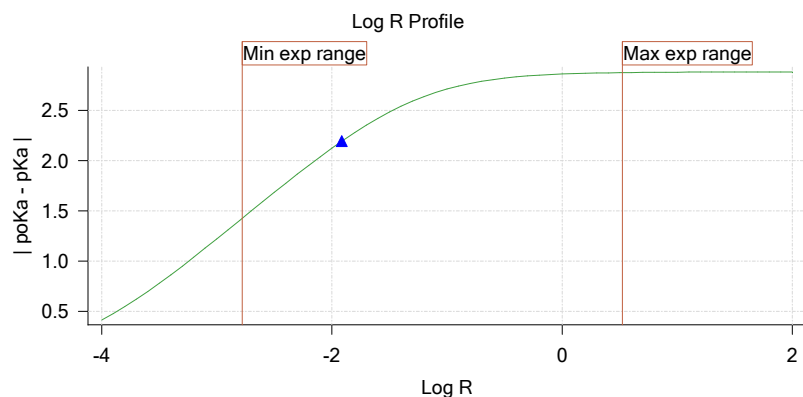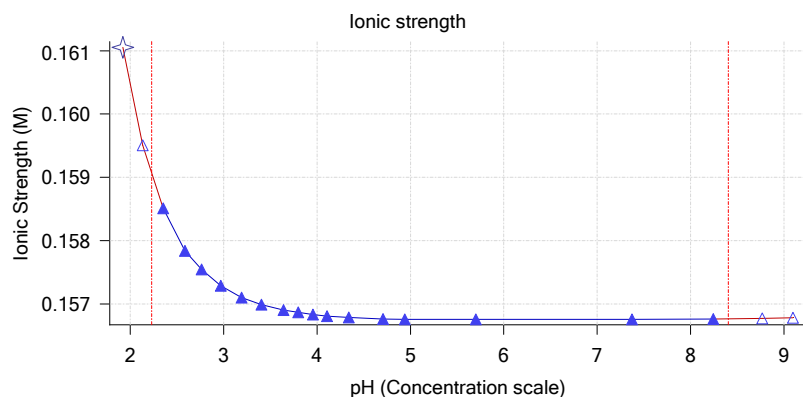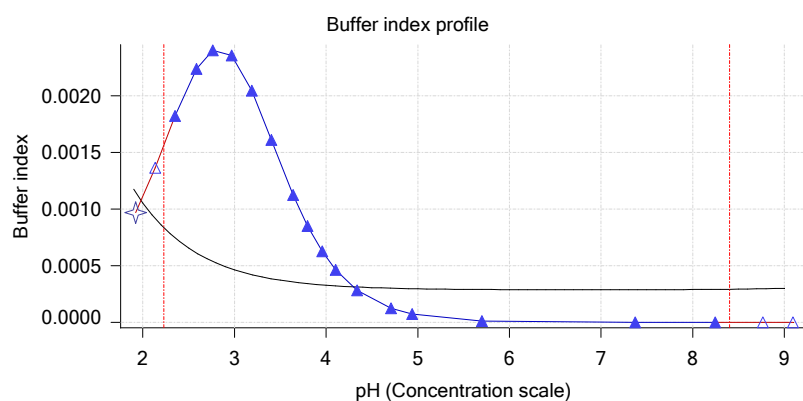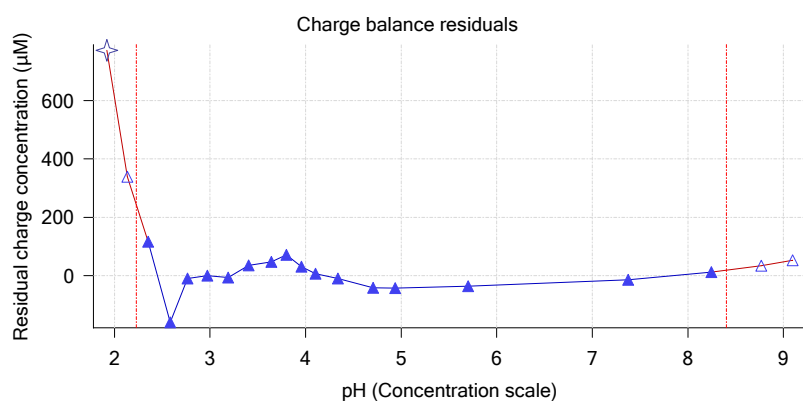## Four-Plus parameters

🔒 Alpha	0.124	3/6/2018 5:41:59 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
🔒 S	0.9973	3/6/2018 5:41:59 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
🔒 jH	0.9	3/6/2018 5:41:59 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
🔒 jOH	-0.7	3/6/2018 5:41:59 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r

Titrants

🔒 0.50 M HCl	0.989131	3/6/2018 5:41:59 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
🔒 0.50 M KOH	0.999845	3/6/2018 5:41:59 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

🔷 M02_octanol concentration factor	0.898
🔒 Base pKa 1	5.03
🔒 logP (XH +)	1.32
🔷 logP (neutral X)	4.19

Sample graphs

Ionisation of sample M02_octanol

Distribution of species for sample M02_octanol

Sample name: **M02_octanol** Experiment start time: **3/6/2018 5:41:59 PM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **18C-06015** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Sample graphs (continued)

Lipophilicity Profile
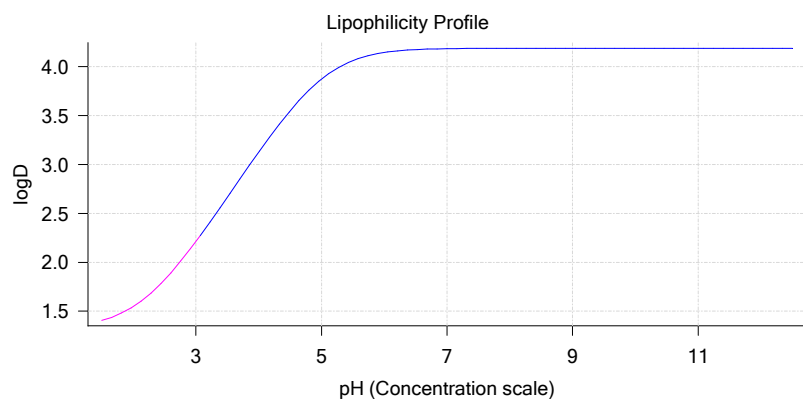
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanol	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.35	60.82 %	0.01 %	36.66 %	2.52 %	
1.200	1.36	59.93 %	0.01 %	36.13 %	3.93 %	Stomach pH
2.000	1.55	49.56 %	0.05 %	29.87 %	20.52 %	
3.000	2.21	17.38 %	0.16 %	10.48 %	71.97 %	
4.000	3.12	2.32 %	0.22 %	1.40 %	96.06 %	
5.000	3.87	0.24 %	0.22 %	0.14 %	99.39 %	
6.000	4.14	0.02 %	0.22 %	0.01 %	99.74 %	
6.500	4.17	0.01 %	0.22 %	0.00 %	99.76 %	
7.000	4.18	0.00 %	0.22 %	0.00 %	99.77 %	
7.400	4.19	0.00 %	0.22 %	0.00 %	99.77 %	Blood pH
8.000	4.19	0.00 %	0.22 %	0.00 %	99.77 %	
9.000	4.19	0.00 %	0.22 %	0.00 %	99.78 %	
10.000	4.19	0.00 %	0.22 %	0.00 %	99.78 %	
11.000	4.19	0.00 %	0.22 %	0.00 %	99.78 %	
12.000	4.19	0.00 %	0.22 %	0.00 %	99.78 %	

Carbonate and acidity

Carbonate 0.000 mM
Acidity error -0.163 mM

Other graphs

Assay progress

Titration graph

Sample name: **M02_octanol**   Experiment start time: **3/6/2018 5:41:59 PM**
Assay name: **pH-metric high logP**   Analyst: **Dorothy Levorse**
Assay ID: **18C-06015**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
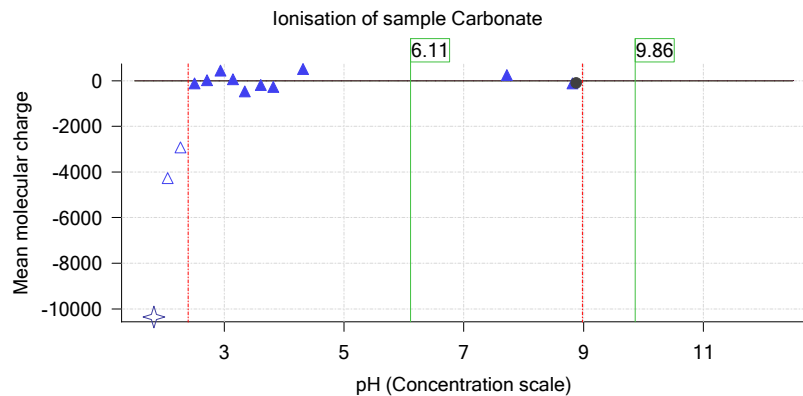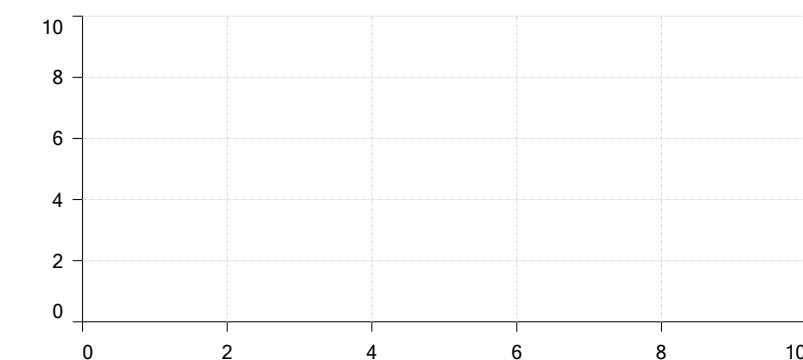
Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

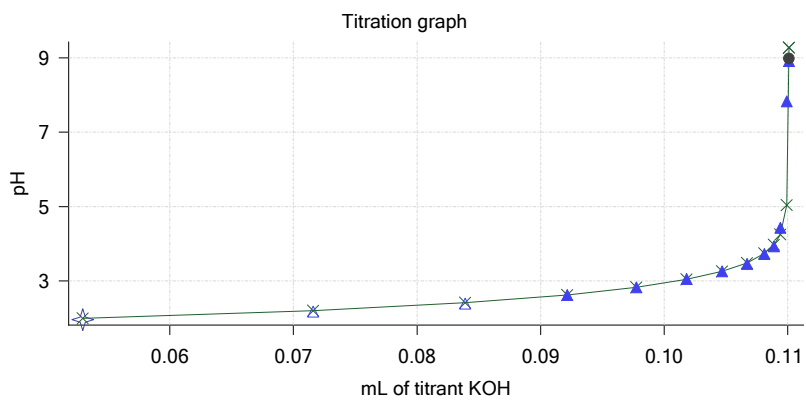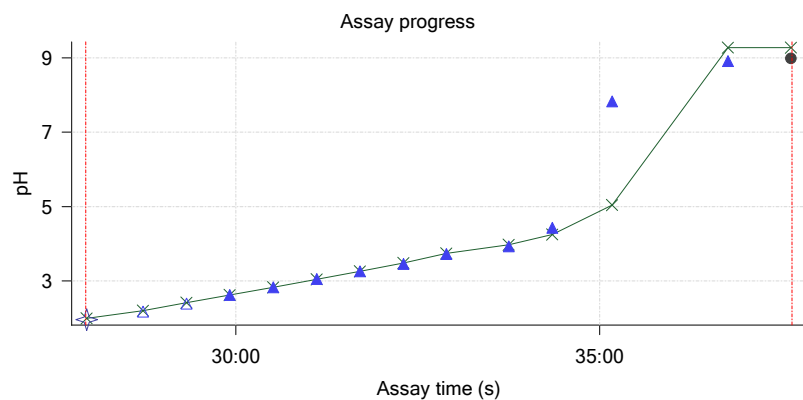# pH-metric high logP   Titration 3 of 3   18C-06015 Points 35 to 48

Overall results

RMSD   0.729
Average ionic strength   0.169 M
Average temperature   25.0°C
Partition ratio   0.1637 : 1
Analyte concentration range   3405.3 µM to 3503.8 µM
Total points considered   14 of 14

Warnings and errors

Errors   None
Warnings   None

Four-Plus parameters

Alpha   0.124   3/6/2018 5:41:59 PM   C:\Sirius_T3\18C-06006_Blank standardisation.t3r
S   0.9973   3/6/2018 5:41:59 PM   C:\Sirius_T3\18C-06006_Blank standardisation.t3r
jH   0.9   3/6/2018 5:41:59 PM   C:\Sirius_T3\18C-06006_Blank standardisation.t3r
jOH   -0.7   3/6/2018 5:41:59 PM   C:\Sirius_T3\18C-06006_Blank standardisation.t3r

Titrants

0.50 M HCl   0.989131   3/6/2018 5:41:59 PM   C:\Sirius_T3\18C-06006_Blank standardisation.t3r
0.50 M KOH   0.999845   3/6/2018 5:41:59 PM   C:\Sirius_T3\KOH18B27.t3r

Sample

M02_octanol concentration factor   0.730
Base pKa 1   5.03
logP (XH +)   1.32
logP (neutral X)   4.31

Sample graphs

Ionisation of sample M02_octanol

Distribution of species for sample M02_octanol

Sample name: **M02_octanol**   Experiment start time: **3/6/2018 5:41:59 PM**
Assay name: **pH-metric high logP**   Analyst: **Dorothy Levorse**
Assay ID: **18C-06015**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Sample graphs (continued)

Lipophilicity Profile
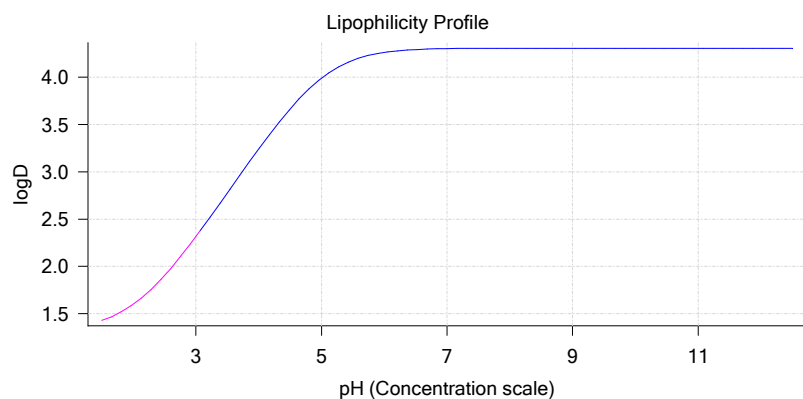
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanol	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.36	21.15 %	0.00 %	72.32 %	6.53 %	
1.200	1.38	20.37 %	0.00 %	69.66 %	9.97 %	Stomach pH
2.000	1.60	13.32 %	0.01 %	45.54 %	41.14 %	
3.000	2.32	2.83 %	0.03 %	9.68 %	87.46 %	
4.000	3.24	0.32 %	0.03 %	1.09 %	98.56 %	
5.000	3.99	0.03 %	0.03 %	0.11 %	99.83 %	
6.000	4.26	0.00 %	0.03 %	0.01 %	99.96 %	
6.500	4.29	0.00 %	0.03 %	0.00 %	99.97 %	
7.000	4.30	0.00 %	0.03 %	0.00 %	99.97 %	
7.400	4.30	0.00 %	0.03 %	0.00 %	99.97 %	Blood pH
8.000	4.31	0.00 %	0.03 %	0.00 %	99.97 %	
9.000	4.31	0.00 %	0.03 %	0.00 %	99.97 %	
10.000	4.31	0.00 %	0.03 %	0.00 %	99.97 %	
11.000	4.31	0.00 %	0.03 %	0.00 %	99.97 %	
12.000	4.31	0.00 %	0.03 %	0.00 %	99.97 %	

Carbonate and acidity

Carbonate   0.199 mM
Acidity error -0.191 mM
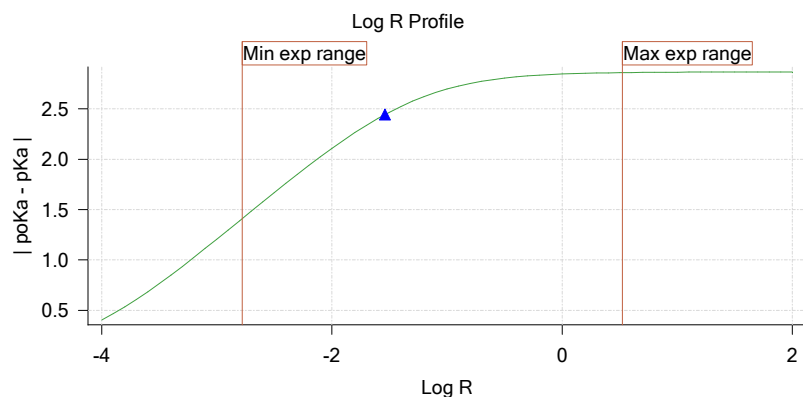
Other graphs
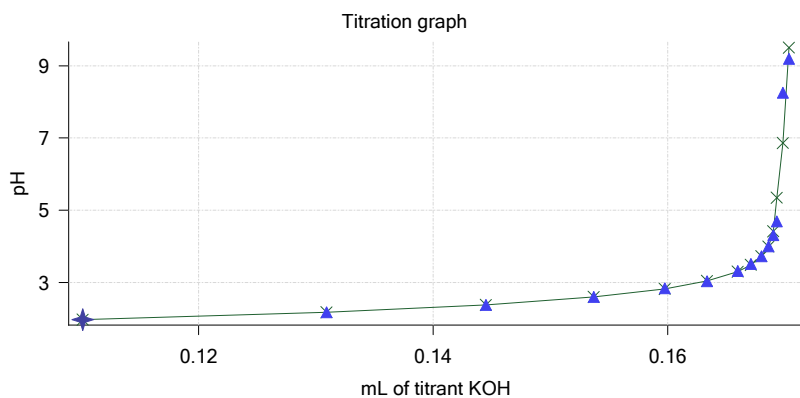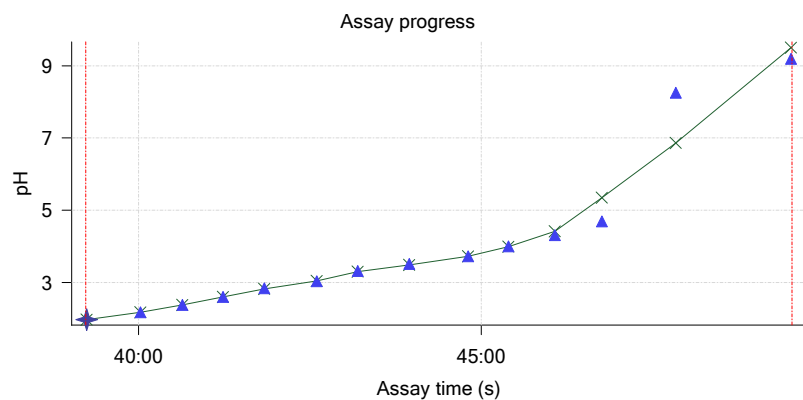
Assay progress

Titration graph

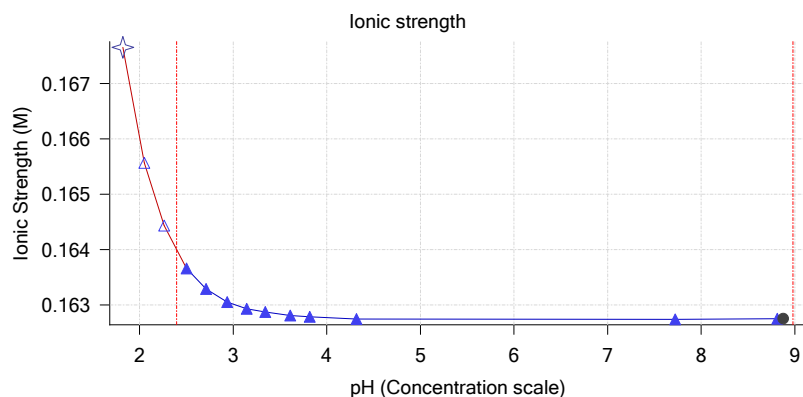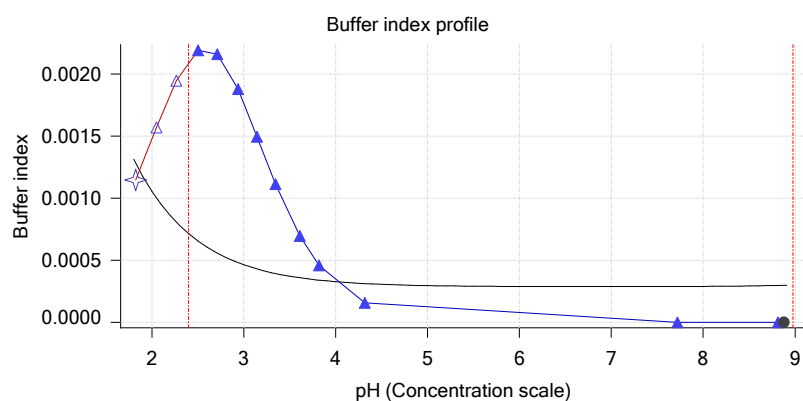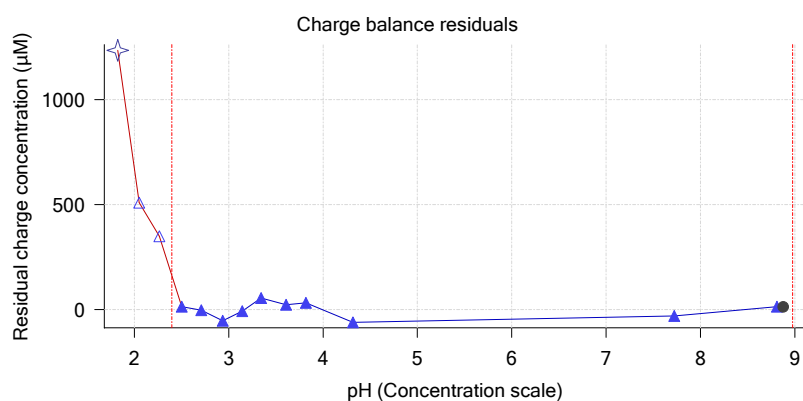Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Other graphs (continued)
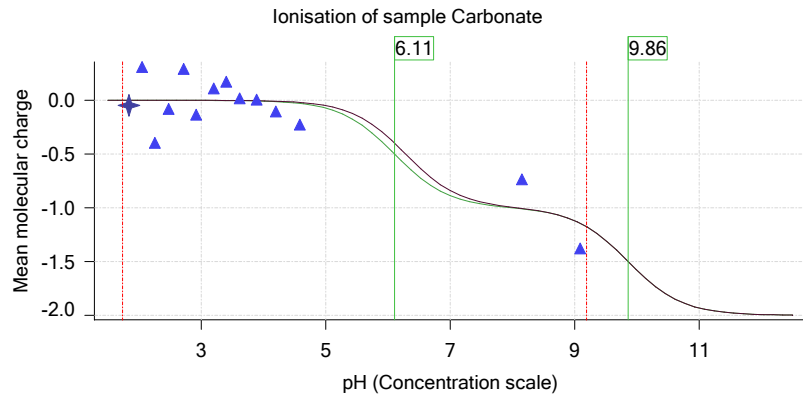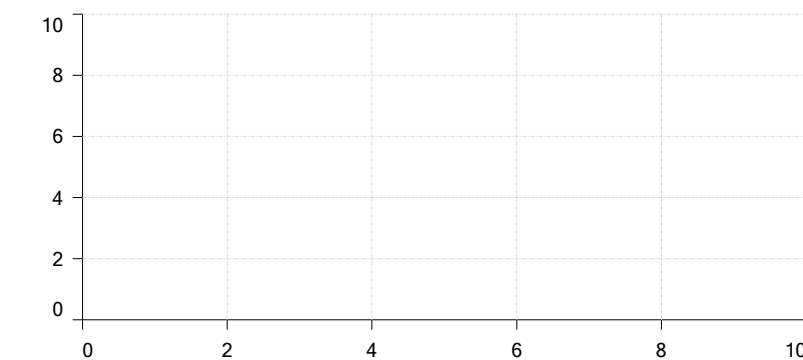
Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate

Sample name: **M02_octanol**   Experiment start time: **3/6/2018 5:41:59 PM**
Assay name: **pH-metric high logP**   Analyst: **Dorothy Levorse**
Assay ID: **18C-06015**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M02_octanol	12/6/2017 4:20:03 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.002110 g	3/6/2018 3:40:26 PM	User entered value
Formula weight	289.26 g/mol	12/6/2017 4:20:03 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	289.26	12/6/2017 4:20:03 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	12/6/2017 4:20:03 PM	User entered value
Sample is a	Base	12/6/2017 4:20:03 PM	User entered value
pKa 1	5.03	12/6/2017 4:20:03 PM	User entered value
logp (XH +)	1.32	3/2/2018 3:38:13 PM	User entered value
logP (neutral X)	4.10	3/2/2018 3:38:07 PM	User entered value

Events

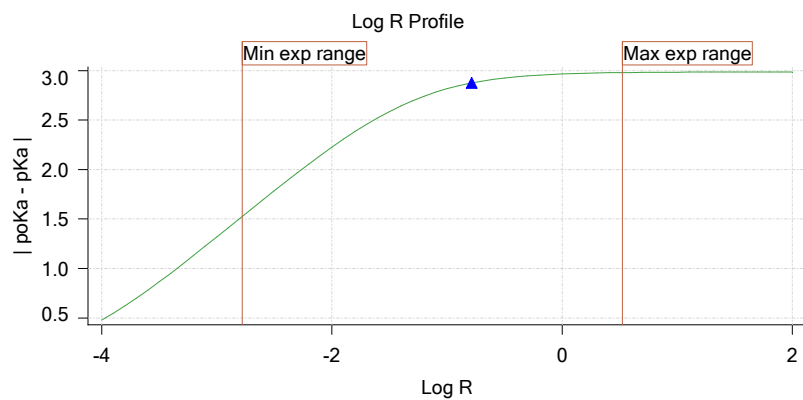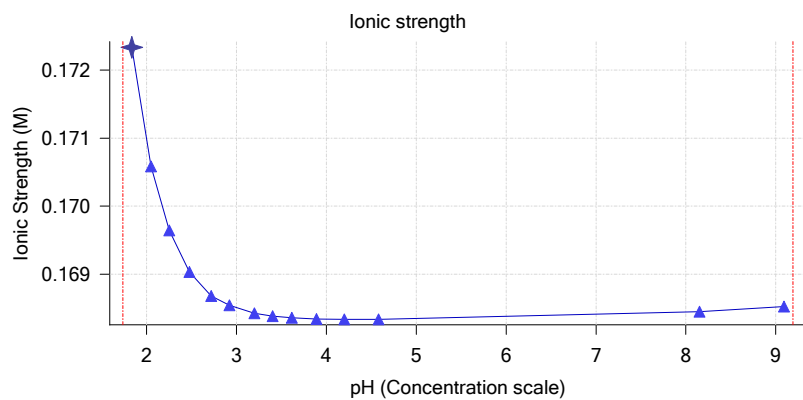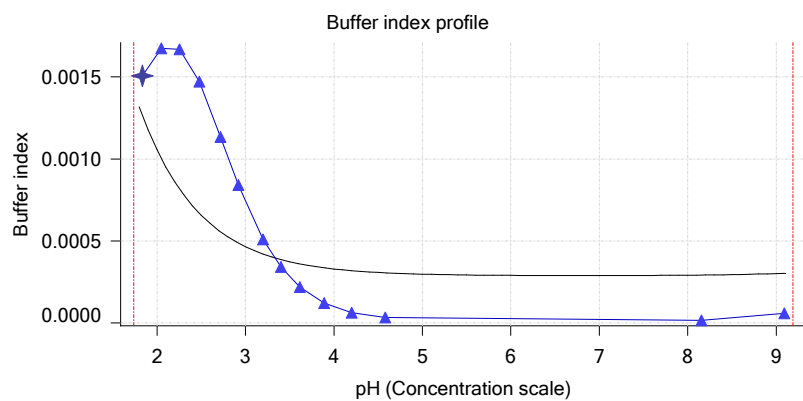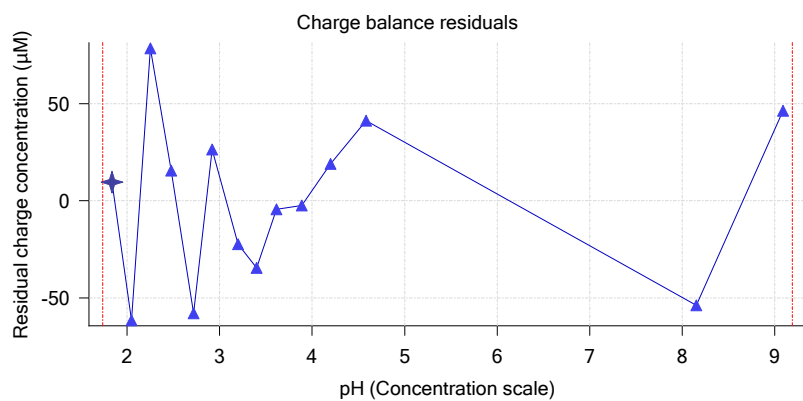| Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
5:08.1	Initial pH = 5.88									
8:07.7	Data point 1	1.50000 mL	0.05466 mL	0.00583 mL	0.01999 mL	2.051	0.00164	0.09342	0.00026	10.0 s
8:53.9	Data point 2	1.50000 mL	0.05466 mL	0.01947 mL	0.01999 mL	2.258	-0.00031	0.00286	0.00029	10.5 s
9:30.0	Data point 3	1.50000 mL	0.05466 mL	0.02897 mL	0.01999 mL	2.475	-0.00173	0.32401	0.00015	10.5 s
10:06.1	Data point 4	1.50000 mL	0.05466 mL	0.03537 mL	0.01999 mL	2.705	-0.01180	0.86985	0.00062	10.0 s
10:41.7	Data point 5	1.50000 mL	0.05466 mL	0.03996 mL	0.01999 mL	2.883	-0.00877	0.93188	0.00045	10.0 s
11:17.2	Data point 6	1.50000 mL	0.05466 mL	0.04363 mL	0.01999 mL	3.088	-0.01598	0.80563	0.00088	10.0 s
11:52.7	Data point 7	1.50000 mL	0.05466 mL	0.04652 mL	0.01999 mL	3.307	-0.01840	0.83749	0.00099	12.0 s
12:30.2	Data point 8	1.50000 mL	0.05466 mL	0.04871 mL	0.01999 mL	3.520	-0.01804	0.93551	0.00092	16.0 s
13:11.8	Data point 9	1.50000 mL	0.05466 mL	0.05031 mL	0.01999 mL	3.755	-0.01934	0.98232	0.00096	20.0 s
14:07.6	Data point 10	1.50000 mL	0.05466 mL	0.05111 mL	0.01999 mL	3.913	-0.01849	0.91937	0.00095	33.5 s
15:06.5	Data point 11	1.50000 mL	0.05466 mL	0.05151 mL	0.01999 mL	4.071	-0.01887	0.88004	0.00099	34.0 s
16:06.0	Data point 12	1.50000 mL	0.05466 mL	0.05179 mL	0.01999 mL	4.218	-0.01661	0.84054	0.00089	37.5 s
17:19.3	Data point 13	1.50000 mL	0.05466 mL	0.05212 mL	0.01999 mL	4.452	-0.01927	0.92356	0.00099	40.0 s
18:29.8	Data point 14	1.50000 mL	0.05466 mL	0.05233 mL	0.01999 mL	4.819	-0.01879	0.88303	0.00099	43.5 s
19:38.8	Data point 15	1.50000 mL	0.05466 mL	0.05242 mL	0.01999 mL	5.049	-0.01780	0.88852	0.00093	46.5 s
20:55.9	Data point 16	1.50000 mL	0.05466 mL	0.05256 mL	0.01999 mL	5.809	-0.01703	0.77107	0.00096	49.5 s
22:16.0	Data point 17	1.50000 mL	0.05466 mL	0.05266 mL	0.01999 mL	7.478	-0.01823	0.89028	0.00095	57.0 s
23:53.8	Data point 18	1.50000 mL	0.05466 mL	0.05275 mL	0.01999 mL	8.346	-0.01804	0.80184	0.00099	52.0 s
25:21.6	Data point 19	1.50000 mL	0.05466 mL	0.05285 mL	0.01999 mL	8.868	-0.01663	0.74418	0.00095	36.0 s
26:33.4	Data point 20	1.50000 mL	0.05466 mL	0.05294 mL	0.01999 mL	9.195	-0.01836	0.90519	0.00095	30.0 s
27:57.2	Data point 21	1.50000 mL	0.11178 mL	0.05294 mL	0.05000 mL	1.956	-0.00466	0.28331	0.00043	10.0 s
28:43.5	Data point 22	1.50000 mL	0.11178 mL	0.07159 mL	0.05000 mL	2.177	-0.01190	0.78202	0.00066	10.0 s
29:19.2	Data point 23	1.50000 mL	0.11178 mL	0.08389 mL	0.05000 mL	2.387	-0.00289	0.10680	0.00044	10.0 s
29:54.8	Data point 24	1.50000 mL	0.11178 mL	0.09214 mL	0.05000 mL	2.622	-0.00997	0.76942	0.00056	10.5 s
30:30.9	Data point 25	1.50000 mL	0.11178 mL	0.09774 mL	0.05000 mL	2.829	-0.01166	0.83145	0.00063	10.5 s
31:06.8	Data point 26	1.50000 mL	0.11178 mL	0.10181 mL	0.05000 mL	3.053	-0.01274	0.93127	0.00065	10.0 s
31:42.3	Data point 27	1.50000 mL	0.11178 mL	0.10468 mL	0.05000 mL	3.260	-0.01427	0.92797	0.00073	10.5 s
32:18.2	Data point 28	1.50000 mL	0.11178 mL	0.10670 mL	0.05000 mL	3.459	-0.00720	0.86970	0.00038	10.0 s
32:53.6	Data point 29	1.50000 mL	0.11178 mL	0.10811 mL	0.05000 mL	3.723	-0.01606	0.92694	0.00082	10.5 s
33:45.0	Data point 30	1.50000 mL	0.11178 mL	0.10889 mL	0.05000 mL	3.933	-0.01092	0.83346	0.00059	10.5 s
34:20.9	Data point 31	1.50000 mL	0.11178 mL	0.10941 mL	0.05000 mL	4.428	-0.01931	0.91819	0.00100	18.5 s
35:10.1	Data point 32	1.50000 mL	0.11178 mL	0.10992 mL	0.05000 mL	7.825	-0.06475	0.99712	0.00320	Timed out at 59.5 s
36:45.7	Data point 33	1.50000 mL	0.11178 mL	0.11011 mL	0.05000 mL	8.913	-0.01987	0.97328	0.00099	31.5 s
37:37.5	Data point 34	1.50000 mL	0.11178 mL	0.11011 mL	0.05000 mL	8.979	-0.01914	0.92668	0.00098	33.0 s
39:14.6	Data point 35	1.50000 mL	0.17180 mL	0.11011 mL	0.30000 mL	1.969	0.00151	0.00822	0.00082	10.5 s
40:01.6	Data point 36	1.50000 mL	0.17180 mL	0.13090 mL	0.30000 mL	2.177	-0.01405	0.55011	0.00094	11.0 s
40:38.3	Data point 37	1.50000 mL	0.17180 mL	0.14450 mL	0.30000 mL	2.376	-0.01463	0.74877	0.00083	10.0 s
41:13.9	Data point 38	1.50000 mL	0.17180 mL	0.15369 mL	0.30000 mL	2.598	-0.01418	0.73162	0.00082	10.5 s
41:50.1	Data point 39	1.50000 mL	0.17180 mL	0.15974 mL	0.30000 mL	2.837	0.01255	0.62249	0.00079	10.0 s
42:35.9	Data point 40	1.50000 mL	0.17180 mL	0.16336 mL	0.30000 mL	3.037	0.01290	0.63323	0.00080	10.5 s

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
43:11.9	Data point 41	1.50000 mL	0.17180 mL	0.16597 mL	0.30000 mL	3.316	-0.01737	0.82670	0.00094	14.5 s
43:57.2	Data point 42	1.50000 mL	0.17180 mL	0.16710 mL	0.30000 mL	3.518	-0.01034	0.83937	0.00056	10.5 s
44:48.5	Data point 43	1.50000 mL	0.17180 mL	0.16799 mL	0.30000 mL	3.731	0.01219	0.49410	0.00086	10.0 s
45:23.9	Data point 44	1.50000 mL	0.17180 mL	0.16858 mL	0.30000 mL	4.002	-0.01494	0.80259	0.00082	10.0 s
46:04.5	Data point 45	1.50000 mL	0.17180 mL	0.16900 mL	0.30000 mL	4.312	-0.01556	0.81871	0.00085	10.5 s
46:45.7	Data point 46	1.50000 mL	0.17180 mL	0.16928 mL	0.30000 mL	4.694	-0.01928	0.95047	0.00098	29.0 s
47:50.4	Data point 47	1.50000 mL	0.17180 mL	0.16980 mL	0.30000 mL	8.255	-0.04492	0.97778	0.00224	Timed out at 59.5 s
49:31.3	Data point 48	1.50000 mL	0.17180 mL	0.17034 mL	0.30000 mL	9.190	-0.01473	0.61216	0.00093	15.0 s
49:55.4	Assay volumes	1.50000 mL	0.17180 mL	0.17034 mL	0.30000 mL					

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.020 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	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	0.030 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: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
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	0.250 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	0.124	3/6/2018 5:41:59 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
Four-Plus S	0.9973	3/6/2018 5:41:59 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
Four-Plus jH	0.9	3/6/2018 5:41:59 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
Four-Plus jOH	-0.7	3/6/2018 5:41:59 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r
Base concentration factor	1.000	3/6/2018 5:41:59 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.989	3/6/2018 5:41:59 PM	C:\Sirius_T3\18C-06006_Blank standardisation.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 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)	02-08-2018	3/6/2018 9:28:59 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: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
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	+7.02 mV		3/6/2018 5:42:27 PM
Filling solution	3M KCl	KCL097	3/6/2018 9:23:20 AM
Liquids			
Wash 1	50% IPA:50% Water		3/6/2018 9:24:32 AM
Wash 2	0.5% Trition X-100 in H20		3/6/2018 9:24:35 AM
Buffer position 1	pH7 Wash		3/6/2018 9:24:38 AM
Buffer position 2	pH 7		3/6/2018 9:24:40 AM
Storage position			3/6/2018 9:24:07 AM
Wash water	5.8e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	9.8e+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	123:01:40		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: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
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

[49] Air gap released for Acid (0.5 M HCl)
[49] Air gap released for Base (0.5 M KOH)
[1:45] Air gap created for Water (0.15 M KCl)
[1:46] Air gap created for Acid (0.5 M HCl)
[1:46] Air gap created for Base (0.5 M KOH)
[1:46] Air gap released for Water (0.15 M KCl)
[1:50] Titrator arm moved over Titration position
[1:50] Titration 1 of 3
[1:50] Adding initial titrants
[1:50] Automatically add 1.50000 mL of water
[2:15] Dispensed 1.500000 mL of Water (0.15 M KCl)
[2:20] Titrator arm moved over Drain
[5:01] Titrator arm moved to Titration position
[5:01] Argon flow rate set to 100
[5:01] Stirrer speed set to 10
[5:06] Automatically add 0.02000 mL of Octanol
[5:07] Dispensed 0.019991 mL of Octanol
[5:08] Initial pH = 5.88
[5:08] Iterative adjust 5.88 -> 2.00
[5:08] pH 5.88 -> 2.00
[5:10] Air gap released for Acid (0.5 M HCl)
[5:10] Dispensed 0.054657 mL of Acid (0.5 M HCl)
[5:15] Holding pH 2.00
[7:15] Stirrer speed set to 0
[7:15] Stirrer speed set to 50
[7:15] Iterative adjust 1.95 -> 2.00
[7:15] pH 1.95 -> 2.00
[7:16] Air gap released for Base (0.5 M KOH)
[7:17] Dispensed 0.005833 mL of Base (0.5 M KOH)
[8:07] Stirrer speed set to 0
[8:17] Datapoint id 1 collected
[8:17] Stirrer speed set to 50
[8:22] pH 2.06 -> 2.26
[8:22] Using cautious pH adjust
[8:23] Dispensed 0.007197 mL of Base (0.5 M KOH)
[8:28] Stepping pH = 2.15
[8:28] Dispensed 0.005127 mL of Base (0.5 M KOH)
[8:33] Stepping pH = 2.23
[8:33] Dispensed 0.001317 mL of Base (0.5 M KOH)
[8:38] Stepping pH = 2.26
[8:54] Stirrer speed set to 0
[9:04] Datapoint id 2 collected

Sample name: **M02_octanol**　　　　　　　　　　　Experiment start time: **3/6/2018 5:41:59 PM**
Assay name: **pH-metric high logP**　　　　　　　　Analyst: **Dorothy Levorse**
Assay ID: **18C-06015**　　　　　　　　　　　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[9:04] Charge balance equation is out by 5.2%
[9:04] Stirrer speed set to 50
[9:09] pH 2.26 -> 2.46
[9:09] Using charge balance adjust
[9:09] Dispensed 0.009501 mL of Base (0.5 M KOH)
[9:30] Stirrer speed set to 0
[9:40] Datapoint id 3 collected
[9:40] Charge balance equation is out by 5.9%
[9:40] Stirrer speed set to 50
[9:45] pH 2.48 -> 2.68
[9:45] Using charge balance adjust
[9:46] Dispensed 0.006397 mL of Base (0.5 M KOH)
[10:06] Stirrer speed set to 0
[10:16] Datapoint id 4 collected
[10:16] Charge balance equation is out by 10.6%
[10:16] Stirrer speed set to 50
[10:21] pH 2.71 -> 2.91
[10:21] Using charge balance adjust
[10:21] Dispensed 0.004586 mL of Base (0.5 M KOH)
[10:41] Stirrer speed set to 0
[10:51] Datapoint id 5 collected
[10:51] Charge balance equation is out by -13.3%
[10:51] Stirrer speed set to 50
[10:56] pH 2.89 -> 3.09
[10:56] Using charge balance adjust
[10:57] Dispensed 0.003669 mL of Base (0.5 M KOH)
[11:17] Stirrer speed set to 0
[11:27] Datapoint id 6 collected
[11:27] Charge balance equation is out by -1.0%
[11:27] Stirrer speed set to 50
[11:32] pH 3.09 -> 3.29
[11:32] Using charge balance adjust
[11:32] Dispensed 0.002893 mL of Base (0.5 M KOH)
[11:52] Stirrer speed set to 0
[12:04] Datapoint id 7 collected
[12:04] Charge balance equation is out by 7.5%
[12:04] Stirrer speed set to 50
[12:09] pH 3.31 -> 3.51
[12:09] Using charge balance adjust
[12:10] Dispensed 0.002187 mL of Base (0.5 M KOH)
[12:30] Stirrer speed set to 0
[12:46] Datapoint id 8 collected
[12:46] Charge balance equation is out by 5.8%
[12:46] Stirrer speed set to 50
[12:51] pH 3.52 -> 3.72
[12:51] Using charge balance adjust
[12:51] Dispensed 0.001599 mL of Base (0.5 M KOH)
[13:11] Stirrer speed set to 0
[13:32] Datapoint id 9 collected
[13:32] Charge balance equation is out by 17.6%
[13:32] Stirrer speed set to 50
[13:37] pH 3.76 -> 3.96
[13:37] Using cautious pH adjust
[13:37] Dispensed 0.000541 mL of Base (0.5 M KOH)
[13:42] Stepping pH = 3.90
[13:42] Dispensed 0.000165 mL of Base (0.5 M KOH)
[13:47] Stepping pH = 3.93
[13:47] Dispensed 0.000094 mL of Base (0.5 M KOH)
[13:52] Stepping pH = 3.95

Sample name: **M02_octanol**　　　　　　　　　Experiment start time: **3/6/2018 5:41:59 PM**
Assay name: **pH-metric high logP**　　　　　　Analyst: **Dorothy Levorse**
Assay ID: **18C-06015**　　　　　　　　　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[14:07] Stirrer speed set to 0
[14:41] Datapoint id 10 collected
[14:41] Charge balance equation is out by 24.5%
[14:41] Stirrer speed set to 50
[14:46] pH 3.92 -> 4.12
[14:46] Using cautious pH adjust
[14:46] Dispensed 0.000400 mL of Base (0.5 M KOH)
[14:51] Stepping pH = 4.14
[15:06] Stirrer speed set to 0
[15:40] Datapoint id 11 collected
[15:40] Charge balance equation is out by 50.0%
[15:40] Stirrer speed set to 50
[15:45] pH 4.08 -> 4.28
[15:45] Using cautious pH adjust
[15:45] Dispensed 0.000282 mL of Base (0.5 M KOH)
[15:51] Stepping pH = 4.29
[16:06] Stirrer speed set to 0
[16:43] Datapoint id 12 collected
[16:43] Charge balance equation is out by 50.0%
[16:43] Stirrer speed set to 50
[16:48] pH 4.23 -> 4.43
[16:48] Using cautious pH adjust
[16:48] Dispensed 0.000212 mL of Base (0.5 M KOH)
[16:53] Stepping pH = 4.38
[16:54] Dispensed 0.000047 mL of Base (0.5 M KOH)
[16:59] Stepping pH = 4.39
[16:59] Dispensed 0.000071 mL of Base (0.5 M KOH)
[17:04] Stepping pH = 4.48
[17:19] Stirrer speed set to 0
[17:59] Datapoint id 13 collected
[17:59] Charge balance equation is out by 17.5%
[17:59] Stirrer speed set to 50
[18:04] pH 4.49 -> 4.69
[18:04] Using cautious pH adjust
[18:04] Dispensed 0.000118 mL of Base (0.5 M KOH)
[18:09] Stepping pH = 4.58
[18:09] Dispensed 0.000094 mL of Base (0.5 M KOH)
[18:14] Stepping pH = 4.81
[18:29] Stirrer speed set to 0
[19:13] Datapoint id 14 collected
[19:13] Charge balance equation is out by 11.3%
[19:13] Stirrer speed set to 50
[19:18] pH 4.89 -> 5.09
[19:18] Using charge balance adjust
[19:18] Dispensed 0.000094 mL of Base (0.5 M KOH)
[19:38] Stirrer speed set to 0
[20:25] Datapoint id 15 collected
[20:25] Charge balance equation is out by -19.7%
[20:25] Stirrer speed set to 50
[20:30] pH 5.10 -> 5.30
[20:30] Using cautious pH adjust
[20:30] Dispensed 0.000047 mL of Base (0.5 M KOH)
[20:35] Stepping pH = 5.11
[20:35] Dispensed 0.000094 mL of Base (0.5 M KOH)
[20:40] Stepping pH = 5.54
[20:56] Stirrer speed set to 0
[21:45] Datapoint id 16 collected
[21:45] Charge balance equation is out by -87.8%
[21:45] Stirrer speed set to 50

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[21:50] pH 6.10 -> 6.30
[21:50] Using cautious pH adjust
[21:50] Dispensed 0.000024 mL of Base (0.5 M KOH)
[21:55] Stepping pH = 6.11
[21:55] Dispensed 0.000071 mL of Base (0.5 M KOH)
[22:01] Stepping pH = 6.60
[22:16] Stirrer speed set to 0
[23:13] Datapoint id 17 collected
[23:13] Charge balance equation is out by -96.1%
[23:13] Stirrer speed set to 50
[23:18] pH 7.61 -> 7.81
[23:18] Using cautious pH adjust
[23:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[23:23] Stepping pH = 7.64
[23:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[23:28] Stepping pH = 7.64
[23:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[23:33] Stepping pH = 7.71
[23:33] Dispensed 0.000024 mL of Base (0.5 M KOH)
[23:38] Stepping pH = 7.95
[23:53] Stirrer speed set to 0
[24:46] Datapoint id 18 collected
[24:46] Charge balance equation is out by -1,094.0%
[24:46] Stirrer speed set to 50
[24:51] pH 8.41 -> 8.61
[24:51] Using cautious pH adjust
[24:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:56] Stepping pH = 8.43
[24:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[25:01] Stepping pH = 8.43
[25:01] Dispensed 0.000047 mL of Base (0.5 M KOH)
[25:06] Stepping pH = 8.72
[25:21] Stirrer speed set to 0
[25:57] Datapoint id 19 collected
[25:57] Charge balance equation is out by -649.6%
[25:57] Stirrer speed set to 50
[26:02] pH 8.94 -> 9.05
[26:02] Using cautious pH adjust
[26:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:08] Stepping pH = 8.95
[26:08] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:13] Stepping pH = 8.97
[26:13] Dispensed 0.000047 mL of Base (0.5 M KOH)
[26:18] Stepping pH = 9.10
[26:33] Stirrer speed set to 0
[27:03] Datapoint id 20 collected
[27:03] Charge balance equation is out by -476.6%
[27:03] Titration 2 of 3
[27:03] Adding initial titrants
[27:03] Automatically add 0.03000 mL of Octanol
[27:04] Dispensed 0.030009 mL of Octanol
[27:04] Stirrer speed set to 10
[27:05] Stirrer speed set to 55
[27:05] Iterative adjust 9.21 -> 2.00
[27:05] pH 9.21 -> 2.00
[27:06] Dispensed 0.057126 mL of Acid (0.5 M HCl)
[27:57] Stirrer speed set to 0
[28:07] Datapoint id 21 collected
[28:07] Stirrer speed set to 55

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[28:12] pH 1.97 -> 2.17
[28:12] Using cautious pH adjust
[28:12] Dispensed 0.009666 mL of Base (0.5 M KOH)
[28:17] Stepping pH = 2.05
[28:18] Dispensed 0.007361 mL of Base (0.5 M KOH)
[28:23] Stepping pH = 2.14
[28:23] Dispensed 0.001623 mL of Base (0.5 M KOH)
[28:28] Stepping pH = 2.17
[28:43] Stirrer speed set to 0
[28:53] Datapoint id 22 collected
[28:53] Charge balance equation is out by 3.5%
[28:53] Stirrer speed set to 55
[28:58] pH 2.18 -> 2.38
[28:58] Using charge balance adjust
[28:59] Dispensed 0.012300 mL of Base (0.5 M KOH)
[29:19] Stirrer speed set to 0
[29:29] Datapoint id 23 collected
[29:29] Charge balance equation is out by 2.4%
[29:29] Stirrer speed set to 55
[29:34] pH 2.40 -> 2.60
[29:34] Using charge balance adjust
[29:34] Dispensed 0.008255 mL of Base (0.5 M KOH)
[29:54] Stirrer speed set to 0
[30:05] Datapoint id 24 collected
[30:05] Charge balance equation is out by 12.9%
[30:05] Stirrer speed set to 55
[30:10] pH 2.63 -> 2.83
[30:10] Using charge balance adjust
[30:10] Dispensed 0.005597 mL of Base (0.5 M KOH)
[30:31] Stirrer speed set to 0
[30:41] Datapoint id 25 collected
[30:41] Charge balance equation is out by 0.3%
[30:41] Stirrer speed set to 55
[30:46] pH 2.83 -> 3.03
[30:46] Using charge balance adjust
[30:46] Dispensed 0.004069 mL of Base (0.5 M KOH)
[31:06] Stirrer speed set to 0
[31:16] Datapoint id 26 collected
[31:16] Charge balance equation is out by 8.9%
[31:16] Stirrer speed set to 55
[31:22] pH 3.06 -> 3.26
[31:22] Using charge balance adjust
[31:22] Dispensed 0.002869 mL of Base (0.5 M KOH)
[31:42] Stirrer speed set to 0
[31:52] Datapoint id 27 collected
[31:52] Charge balance equation is out by 0.5%
[31:52] Stirrer speed set to 55
[31:57] pH 3.26 -> 3.46
[31:57] Using charge balance adjust
[31:58] Dispensed 0.002023 mL of Base (0.5 M KOH)
[32:18] Stirrer speed set to 0
[32:28] Datapoint id 28 collected
[32:28] Charge balance equation is out by -2.6%
[32:28] Stirrer speed set to 55
[32:33] pH 3.47 -> 3.67
[32:33] Using charge balance adjust
[32:33] Dispensed 0.001411 mL of Base (0.5 M KOH)
[32:53] Stirrer speed set to 0
[33:04] Datapoint id 29 collected

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[33:04] Charge balance equation is out by 27.7%
[33:04] Stirrer speed set to 55
[33:09] pH 3.73 -> 3.93
[33:09] Using cautious pH adjust
[33:09] Dispensed 0.000423 mL of Base (0.5 M KOH)
[33:14] Stepping pH = 3.84
[33:14] Dispensed 0.000235 mL of Base (0.5 M KOH)
[33:19] Stepping pH = 3.92
[33:19] Dispensed 0.000047 mL of Base (0.5 M KOH)
[33:24] Stepping pH = 3.92
[33:24] Dispensed 0.000071 mL of Base (0.5 M KOH)
[33:30] Stepping pH = 3.94
[33:45] Stirrer speed set to 0
[33:55] Datapoint id 30 collected
[33:55] Charge balance equation is out by 7.6%
[33:55] Stirrer speed set to 55
[34:00] pH 3.95 -> 4.15
[34:00] Using charge balance adjust
[34:00] Dispensed 0.000517 mL of Base (0.5 M KOH)
[34:21] Stirrer speed set to 0
[34:39] Datapoint id 31 collected
[34:39] Charge balance equation is out by 139.7%
[34:39] Stirrer speed set to 55
[34:44] pH 4.47 -> 4.67
[34:44] Using cautious pH adjust
[34:44] Dispensed 0.000094 mL of Base (0.5 M KOH)
[34:49] Stepping pH = 4.47
[34:50] Dispensed 0.000423 mL of Base (0.5 M KOH)
[34:55] Stepping pH = 7.49
[35:10] Stirrer speed set to 0
[36:10] Datapoint id 32 collected
[36:10] Charge balance equation is out by -201.6%
[36:10] Stirrer speed set to 55
[36:15] pH 8.18 -> 8.38
[36:15] Using cautious pH adjust
[36:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:20] Stepping pH = 8.14
[36:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[36:25] Stepping pH = 8.10
[36:25] Dispensed 0.000141 mL of Base (0.5 M KOH)
[36:30] Stepping pH = 8.92
[36:45] Stirrer speed set to 0
[37:17] Datapoint id 33 collected
[37:17] Charge balance equation is out by -2,089.2%
[37:17] Stirrer speed set to 55
[37:22] pH 9.03 -> 9.05
[37:22] Using cautious pH adjust
[37:37] Stirrer speed set to 0
[38:10] Datapoint id 34 collected
[38:10] Charge balance equation is out by 100.0%
[38:10] Titration 3 of 3
[38:10] Adding initial titrants
[38:10] Automatically add 0.25000 mL of Octanol
[38:16] Dispensed 0.250000 mL of Octanol
[38:16] Stirrer speed set to 10
[38:17] Stirrer speed set to 60
[38:17] Iterative adjust 9.00 -> 2.00
[38:17] pH 9.00 -> 2.00
[38:19] Dispensed 0.058725 mL of Acid (0.5 M HCl)

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[38:24] pH 2.01 -> 2.00
[38:24] Dispensed 0.001294 mL of Acid (0.5 M HCl)
[39:14] Stirrer speed set to 0
[39:25] Datapoint id 35 collected
[39:25] Stirrer speed set to 60
[39:30] pH 1.98 -> 2.18
[39:30] Using cautious pH adjust
[39:30] Dispensed 0.010254 mL of Base (0.5 M KOH)
[39:35] Stepping pH = 2.06
[39:36] Dispensed 0.008043 mL of Base (0.5 M KOH)
[39:41] Stepping pH = 2.15
[39:41] Dispensed 0.002493 mL of Base (0.5 M KOH)
[39:46] Stepping pH = 2.18
[40:01] Stirrer speed set to 0
[40:12] Datapoint id 36 collected
[40:12] Charge balance equation is out by -1.3%
[40:12] Stirrer speed set to 60
[40:17] pH 2.18 -> 2.38
[40:17] Using charge balance adjust
[40:18] Dispensed 0.013594 mL of Base (0.5 M KOH)
[40:38] Stirrer speed set to 0
[40:48] Datapoint id 37 collected
[40:48] Charge balance equation is out by -1.2%
[40:48] Stirrer speed set to 60
[40:53] pH 2.38 -> 2.58
[40:53] Using charge balance adjust
[40:53] Dispensed 0.009196 mL of Base (0.5 M KOH)
[41:14] Stirrer speed set to 0
[41:24] Datapoint id 38 collected
[41:24] Charge balance equation is out by 9.4%
[41:24] Stirrer speed set to 60
[41:29] pH 2.60 -> 2.80
[41:29] Using charge balance adjust
[41:30] Dispensed 0.006044 mL of Base (0.5 M KOH)
[41:50] Stirrer speed set to 0
[42:00] Datapoint id 39 collected
[42:00] Charge balance equation is out by 16.8%
[42:00] Stirrer speed set to 60
[42:05] pH 2.85 -> 3.05
[42:05] Using cautious pH adjust
[42:05] Dispensed 0.001929 mL of Base (0.5 M KOH)
[42:10] Stepping pH = 2.94
[42:10] Dispensed 0.001435 mL of Base (0.5 M KOH)
[42:15] Stepping pH = 3.03
[42:15] Dispensed 0.000259 mL of Base (0.5 M KOH)
[42:20] Stepping pH = 3.04
[42:36] Stirrer speed set to 0
[42:46] Datapoint id 40 collected
[42:46] Charge balance equation is out by 5.9%
[42:46] Stirrer speed set to 60
[42:51] pH 3.05 -> 3.25
[42:51] Using charge balance adjust
[42:51] Dispensed 0.002611 mL of Base (0.5 M KOH)
[43:12] Stirrer speed set to 0
[43:26] Datapoint id 41 collected
[43:26] Charge balance equation is out by 35.1%
[43:26] Stirrer speed set to 60
[43:31] pH 3.32 -> 3.52
[43:31] Using cautious pH adjust

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[43:31] Dispensed 0.000729 mL of Base (0.5 M KOH)
[43:36] Stepping pH = 3.43
[43:37] Dispensed 0.000400 mL of Base (0.5 M KOH)
[43:42] Stepping pH = 3.52
[43:57] Stirrer speed set to 0
[44:07] Datapoint id 42 collected
[44:07] Charge balance equation is out by 22.8%
[44:07] Stirrer speed set to 60
[44:12] pH 3.53 -> 3.73
[44:12] Using cautious pH adjust
[44:12] Dispensed 0.000470 mL of Base (0.5 M KOH)
[44:18] Stepping pH = 3.63
[44:18] Dispensed 0.000306 mL of Base (0.5 M KOH)
[44:23] Stepping pH = 3.71
[44:23] Dispensed 0.000047 mL of Base (0.5 M KOH)
[44:28] Stepping pH = 3.72
[44:28] Dispensed 0.000071 mL of Base (0.5 M KOH)
[44:33] Stepping pH = 3.73
[44:48] Stirrer speed set to 0
[44:58] Datapoint id 43 collected
[44:58] Charge balance equation is out by 5.5%
[44:58] Stirrer speed set to 60
[45:03] pH 3.75 -> 3.95
[45:03] Using charge balance adjust
[45:03] Dispensed 0.000588 mL of Base (0.5 M KOH)
[45:24] Stirrer speed set to 0
[45:34] Datapoint id 44 collected
[45:34] Charge balance equation is out by 26.0%
[45:34] Stirrer speed set to 60
[45:39] pH 4.03 -> 4.23
[45:39] Using cautious pH adjust
[45:39] Dispensed 0.000165 mL of Base (0.5 M KOH)
[45:44] Stepping pH = 4.07
[45:44] Dispensed 0.000259 mL of Base (0.5 M KOH)
[45:49] Stepping pH = 4.31
[46:04] Stirrer speed set to 0
[46:15] Datapoint id 45 collected
[46:15] Charge balance equation is out by -34.4%
[46:15] Stirrer speed set to 60
[46:20] pH 4.37 -> 4.57
[46:20] Using cautious pH adjust
[46:20] Dispensed 0.000071 mL of Base (0.5 M KOH)
[46:25] Stepping pH = 4.37
[46:25] Dispensed 0.000212 mL of Base (0.5 M KOH)
[46:30] Stepping pH = 4.68
[46:45] Stirrer speed set to 0
[47:14] Datapoint id 46 collected
[47:14] Charge balance equation is out by -97.4%
[47:14] Stirrer speed set to 60
[47:19] pH 4.84 -> 5.04
[47:19] Using cautious pH adjust
[47:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[47:25] Stepping pH = 4.84
[47:25] Dispensed 0.000141 mL of Base (0.5 M KOH)
[47:30] Stepping pH = 4.86
[47:30] Dispensed 0.000353 mL of Base (0.5 M KOH)
[47:35] Stepping pH = 8.18
[47:50] Stirrer speed set to 0
[48:50] Datapoint id 47 collected

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-06015**
Filename: **C:\Sirius_T3\Mehtap\20180306_exp30_logP_T3-2\18C-06015_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/6/2018 5:41:59 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[48:50] Charge balance equation is out by -866.5%
[48:50] Stirrer speed set to 60
[48:55] pH 8.41 -> 8.61
[48:55] Using cautious pH adjust
[48:55] Dispensed 0.000024 mL of Base (0.5 M KOH)
[49:00] Stepping pH = 8.38
[49:00] Dispensed 0.000047 mL of Base (0.5 M KOH)
[49:05] Stepping pH = 8.35
[49:06] Dispensed 0.000235 mL of Base (0.5 M KOH)
[49:11] Stepping pH = 8.46
[49:11] Dispensed 0.000235 mL of Base (0.5 M KOH)
[49:16] Stepping pH = 9.22
[49:31] Stirrer speed set to 0
[49:46] Datapoint id 48 collected
[49:46] Charge balance equation is out by -3,486.6%
[49:46] Argon flow rate set to 0
[49:50] Titrator arm moved over Titration position
[50:12] The autoloader failed to pick at location "Sample position"