



Sample name: **phenol** Experiment start time: **11/28/2017 12:07:50 PM**
Assay name: **pH-metric medium logP** Analyst: **Dorothy Levorse**
Assay ID: **17K-28007** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

pH-metric Result

logP (neutral XH) 1.49
logP (X -) -4.46
RMSD 0.550

17K-28007 Points 1 to 33

phenol concentration factor 1.106
Carbonate 0.4154 mM
Acidity error 0.03681 mM

17K-28007 Points 34 to 70

phenol concentration factor 1.032
Carbonate 0.2056 mM
Acidity error 0.20146 mM

17K-28007 Points 71 to 104

phenol concentration factor 1.023
Carbonate 0.3751 mM
Acidity error 0.08943 mM

Warnings and errors

Errors None
Warnings One or more logP values out of range

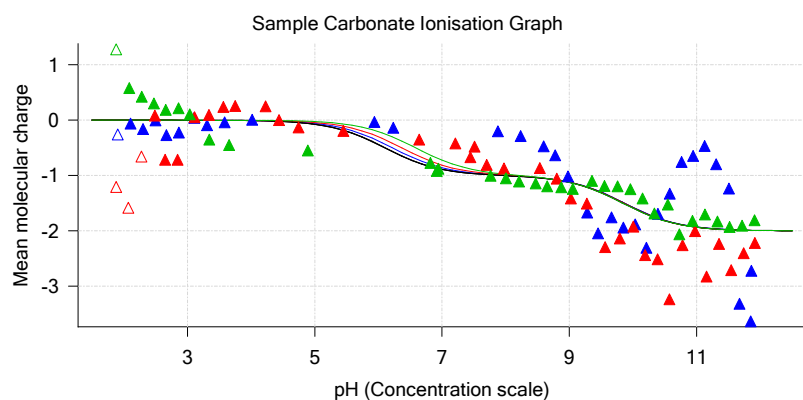
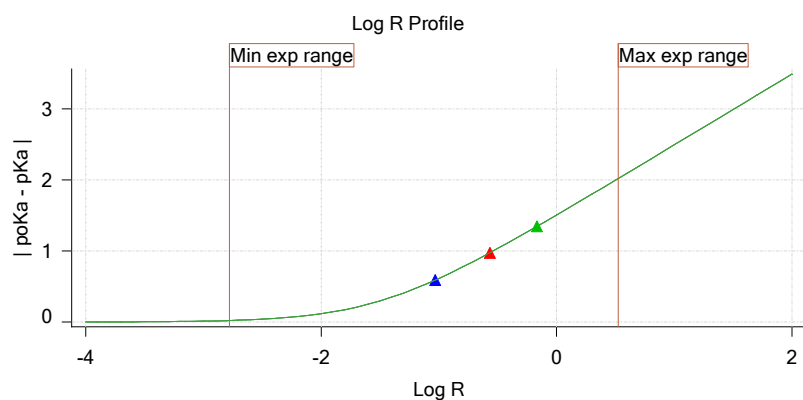
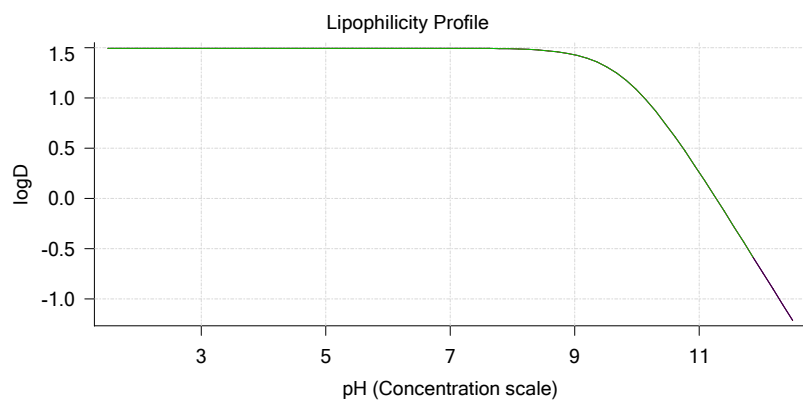
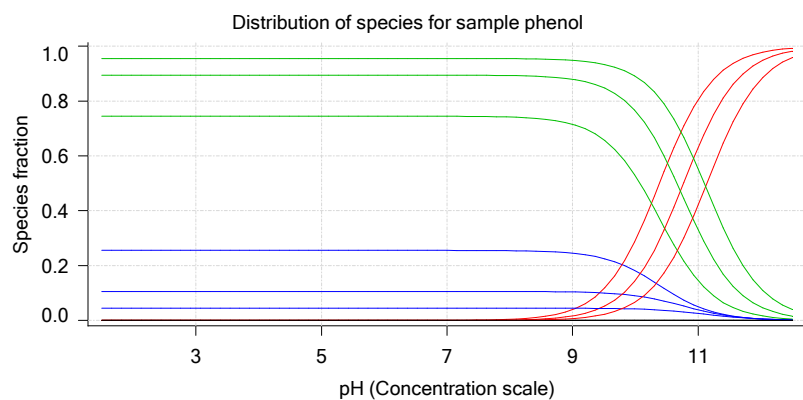
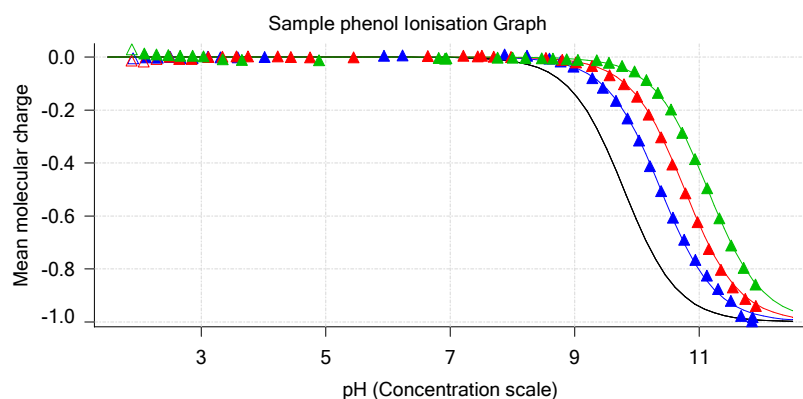
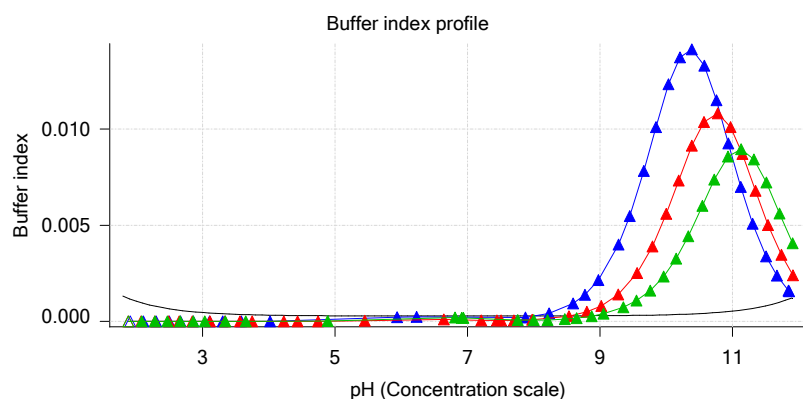
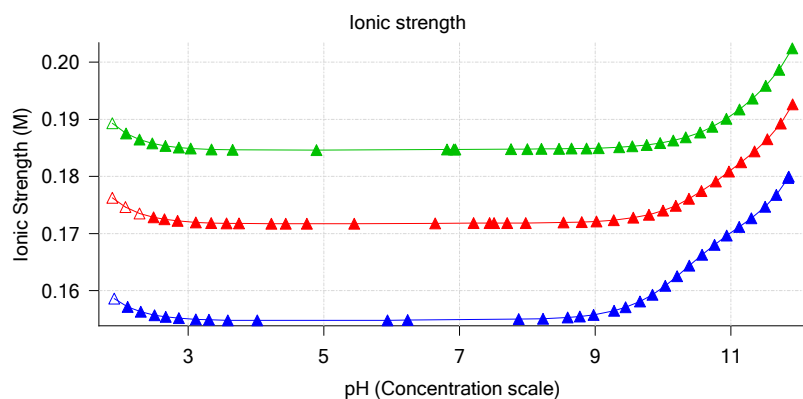
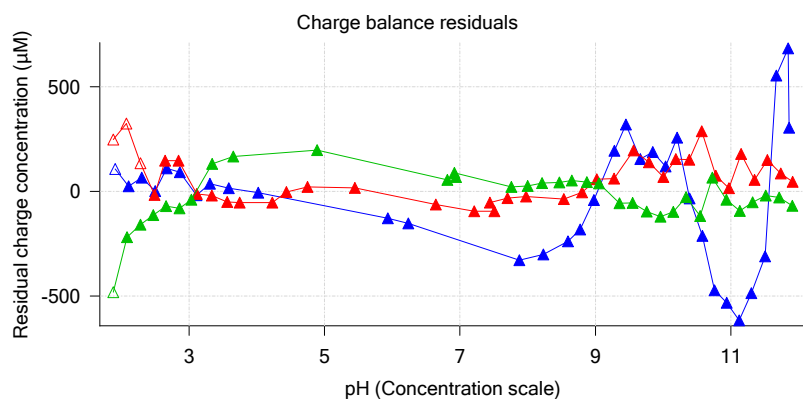
Sample logD and percent species

| pH | phenol logD | phenol phenolH | phenol phenol | phenol phenolH* | phenol phenol* | Comment |
|--------|----------------|-------------------|------------------|--------------------|-------------------|------------|
| 1.000 | 1.49 | 3.10 % | 0.00 % | 96.90 % | 0.00 % | Stomach pH |
| 1.200 | 1.49 | 3.10 % | 0.00 % | 96.90 % | 0.00 % | |
| 2.000 | 1.49 | 3.10 % | 0.00 % | 96.90 % | 0.00 % | |
| 3.000 | 1.49 | 3.10 % | 0.00 % | 96.90 % | 0.00 % | |
| 4.000 | 1.49 | 3.10 % | 0.00 % | 96.90 % | 0.00 % | |
| 5.000 | 1.49 | 3.10 % | 0.00 % | 96.90 % | 0.00 % | Blood pH |
| 6.000 | 1.49 | 3.10 % | 0.00 % | 96.90 % | 0.00 % | |
| 6.500 | 1.49 | 3.10 % | 0.00 % | 96.89 % | 0.00 % | |
| 7.000 | 1.49 | 3.10 % | 0.01 % | 96.89 % | 0.00 % | |
| 7.400 | 1.49 | 3.10 % | 0.01 % | 96.88 % | 0.00 % | |
| 8.000 | 1.49 | 3.10 % | 0.05 % | 96.85 % | 0.00 % | |
| 9.000 | 1.43 | 3.09 % | 0.50 % | 96.41 % | 0.00 % | |
| 10.000 | 1.08 | 2.95 % | 4.79 % | 92.25 % | 0.00 % | |
| 11.000 | 0.26 | 2.06 % | 33.48 % | 64.45 % | 0.00 % | |
| 12.000 | -0.72 | 0.51 % | 83.42 % | 16.06 % | 0.00 % | |

Sample name: **phenol**
 Assay name: **pH-metric medium logP**
 Assay ID: **17K-28007**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

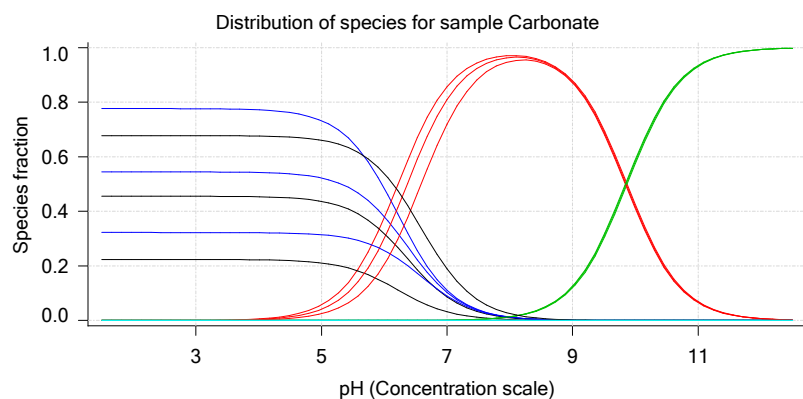
Experiment start time: **11/28/2017 12:07:50 PM**
 Analyst: **Dorothy Leverse**
 Instrument ID: **T311053**

Graphs



Sample name: **phenol** Experiment start time: **11/28/2017 12:07:50 PM**
 Assay name: **pH-metric medium logP** Analyst: **Dorothy Levorse**
 Assay ID: **17K-28007** Instrument ID: **T311053**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Graphs (continued)



Sample name: **phenol**
 Assay name: **pH-metric medium logP**
 Assay ID: **17K-28007**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

pH-metric medium logP Titration 1 of 3 17K-28007 Points 1 to 33

Overall results

RMSD 0.372
 Average ionic strength 0.161 M
 Average temperature 24.9°C
 Partition ratio 0.0933 : 1
 Analyte concentration range 19232.3 µM to 21058.4 µM
 Total points considered 32 of 33

Warnings and errors

Errors None
 Warnings One or more logP values out of range

Four-Plus parameters

Alpha 0.076 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28005_Blank standardisation.t3r
 S 1.0056 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28005_Blank standardisation.t3r
 jH 1.0 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28005_Blank standardisation.t3r
 jOH -0.9 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28005_Blank standardisation.t3r

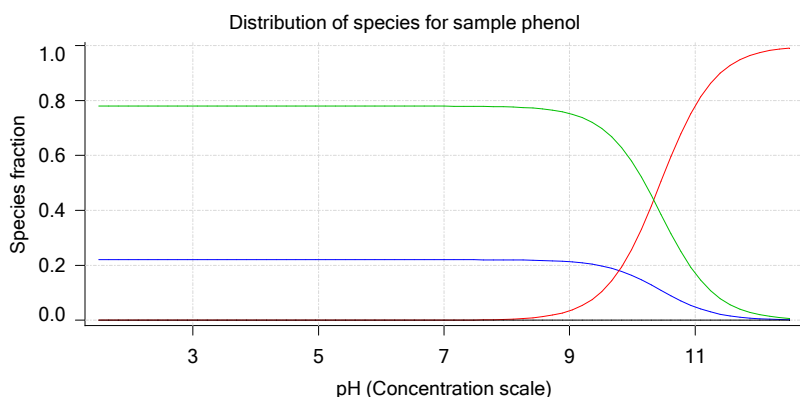
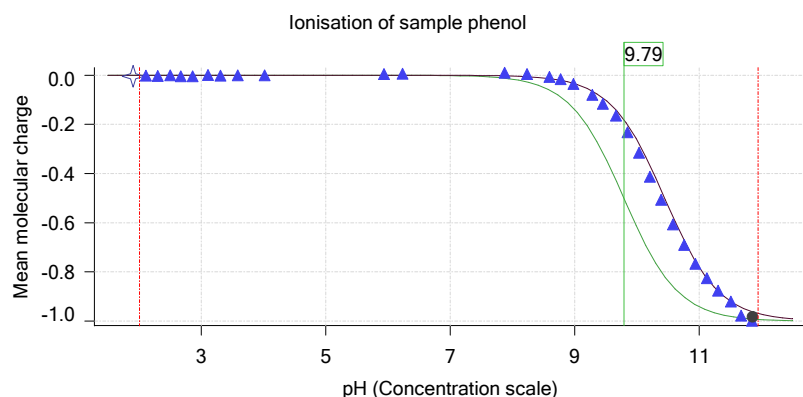
Titrants

0.50 M HCl 0.994563 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28006_Blank standardisation.t3r
 0.50 M KOH 1.000610 11/28/2017 12:07:50 PM C:\Sirius_T3\KOH17K27.t3r

Sample

phenol concentration factor 1.106
 Acid pKa 1 9.79
 logP (neutral XH) 1.58
 logP (X -) -9.00

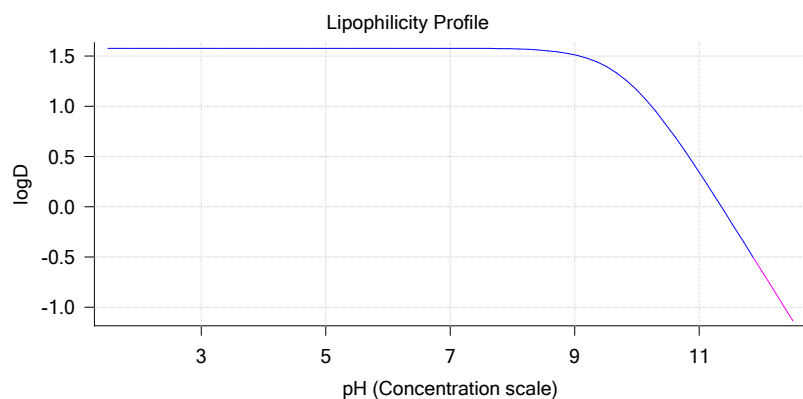
Sample graphs



Sample name: **phenol**
 Assay name: **pH-metric medium logP**
 Assay ID: **17K-28007**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**



Sample graphs (continued)



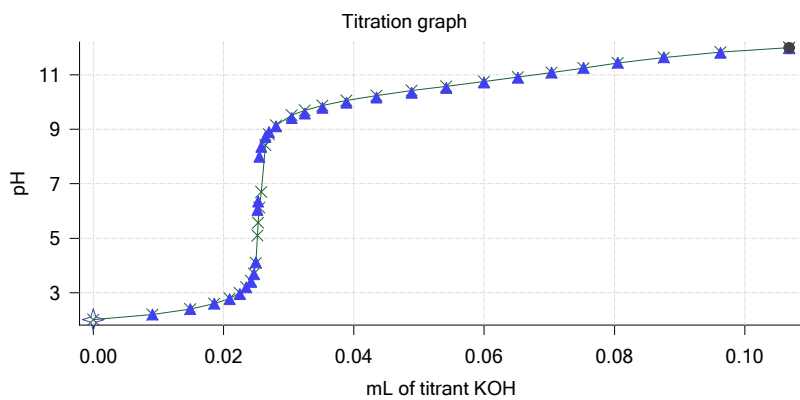
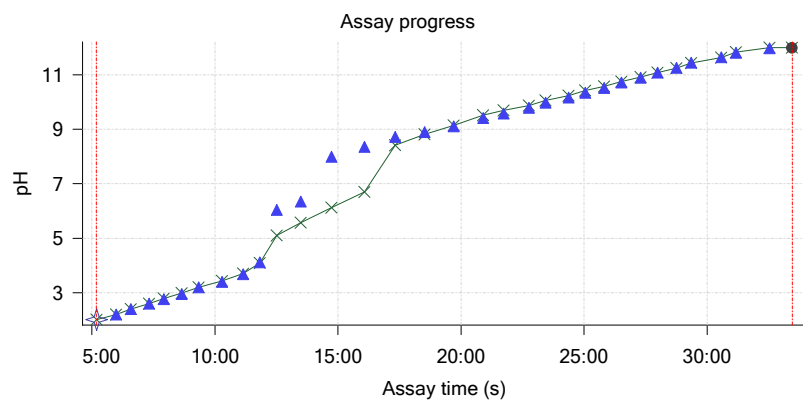
Sample logD and percent species

| pH | phenol logD | phenol phenolH | phenol phenol | phenol phenolH* | phenol phenol* | Comment |
|--------|----------------|-------------------|------------------|--------------------|-------------------|---------|
| 1.000 | 1.58 | 22.04 % | 0.00 % | 77.96 % | 0.00 % | |
| 1.200 | 1.58 | 22.04 % | 0.00 % | 77.96 % | 0.00 % | |
| 2.000 | 1.58 | 22.04 % | 0.00 % | 77.96 % | 0.00 % | |
| 3.000 | 1.58 | 22.04 % | 0.00 % | 77.96 % | 0.00 % | |
| 4.000 | 1.58 | 22.04 % | 0.00 % | 77.96 % | 0.00 % | |
| 5.000 | 1.58 | 22.04 % | 0.00 % | 77.96 % | 0.00 % | |
| 6.000 | 1.58 | 22.04 % | 0.00 % | 77.96 % | 0.00 % | |
| 6.500 | 1.58 | 22.04 % | 0.01 % | 77.95 % | 0.00 % | |
| 7.000 | 1.58 | 22.03 % | 0.04 % | 77.93 % | 0.00 % | |
| 7.400 | 1.58 | 22.02 % | 0.09 % | 77.89 % | 0.00 % | |
| 8.000 | 1.57 | 21.96 % | 0.36 % | 77.68 % | 0.00 % | |
| 9.000 | 1.51 | 21.28 % | 3.45 % | 75.27 % | 0.00 % | |
| 10.000 | 1.16 | 16.24 % | 26.33 % | 57.43 % | 0.00 % | |
| 11.000 | 0.34 | 4.82 % | 78.14 % | 17.04 % | 0.00 % | |
| 12.000 | -0.63 | 0.60 % | 97.28 % | 2.12 % | 0.00 % | |

Carbonate and acidity

 Carbonate 0.415 mM
 Acidity error 0.037 mM

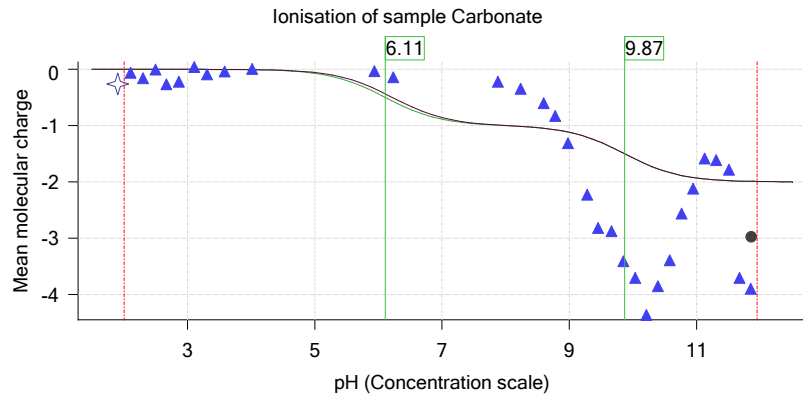
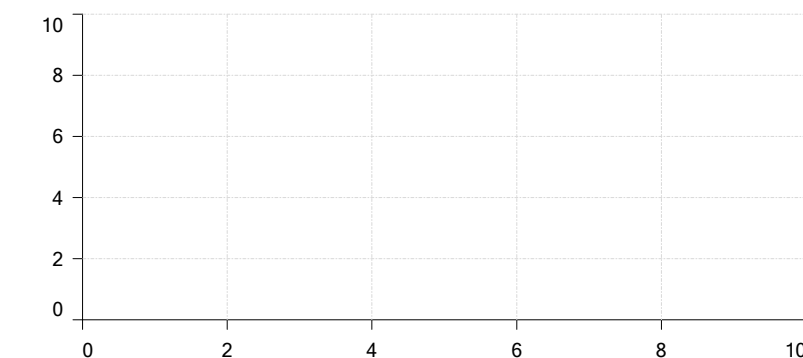
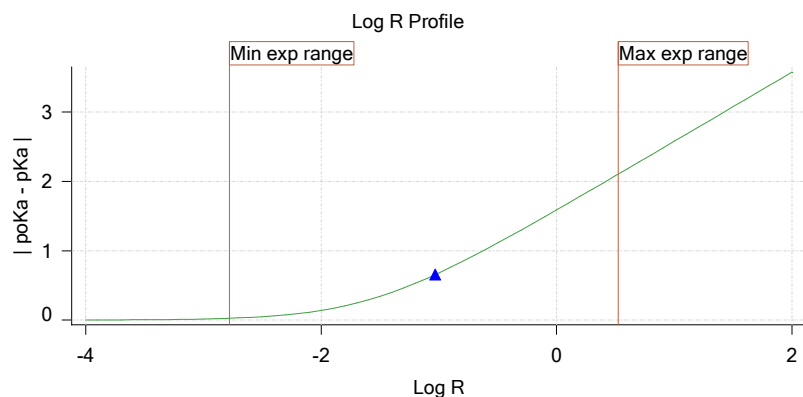
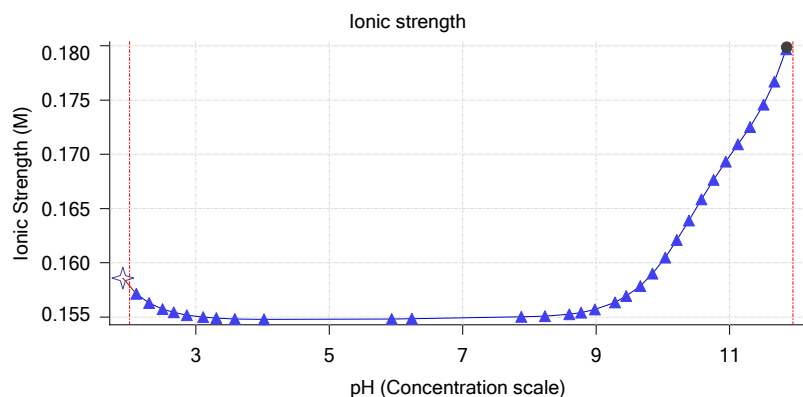
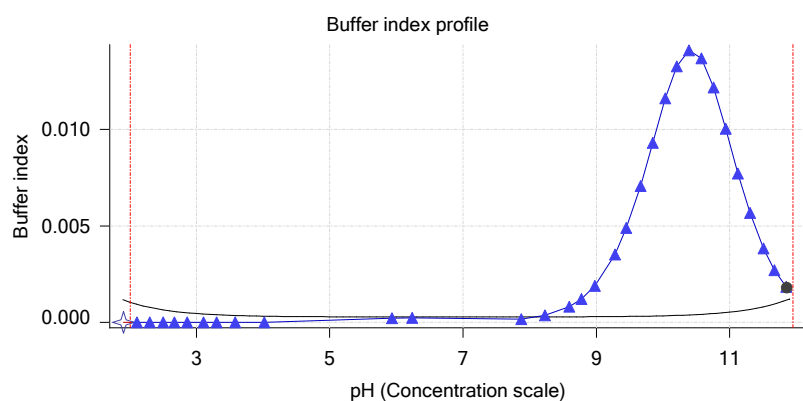
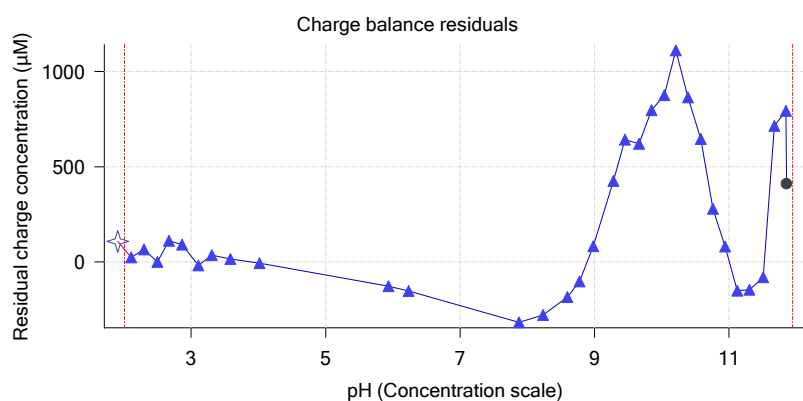
Other graphs



Sample name: **phenol**
 Assay name: **pH-metric medium logP**
 Assay ID: **17K-28007**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Other graphs (continued)



Sample name: **phenol**
 Assay name: **pH-metric medium logP**
 Assay ID: **17K-28007**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

pH-metric medium logP Titration 2 of 3 17K-28007 Points 34 to 70

Overall results

RMSD 0.453
 Average ionic strength 0.175 M
 Average temperature 25.0°C
 Partition ratio 0.2708 : 1
 Analyte concentration range 13821.0 µM to 14844.7 µM
 Total points considered 34 of 37

Warnings and errors

Errors None
 Warnings One or more logP values out of range

Four-Plus parameters

Alpha 0.076 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28005_Blank standardisation.t3r
 S 1.0056 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28005_Blank standardisation.t3r
 jH 1.0 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28005_Blank standardisation.t3r
 jOH -0.9 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28005_Blank standardisation.t3r

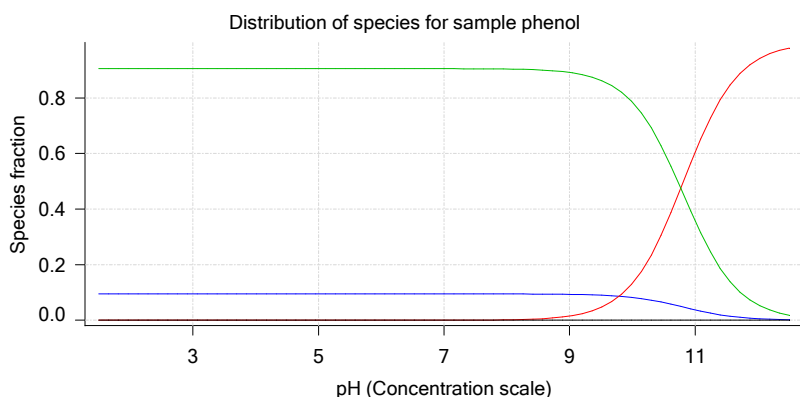
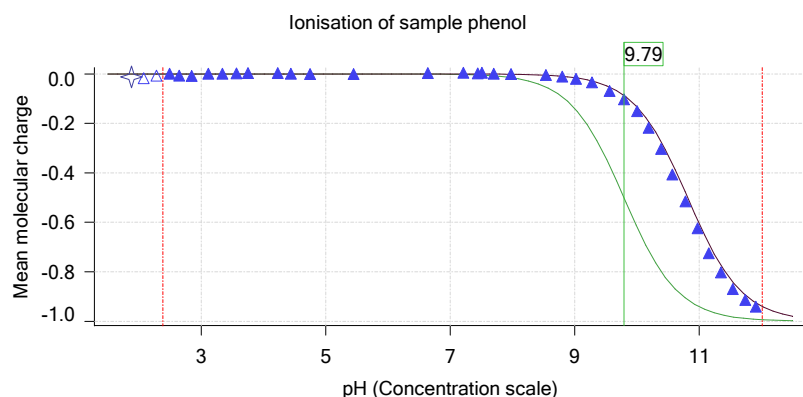
Titrants

0.50 M HCl 0.994563 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28006_Blank standardisation.t3r
 0.50 M KOH 1.000610 11/28/2017 12:07:50 PM C:\Sirius_T3\KOH17K27.t3r

Sample

phenol concentration factor 1.032
 Acid pKa 1 9.79
 logP (neutral XH) 1.55
 logP (X -) -9.00

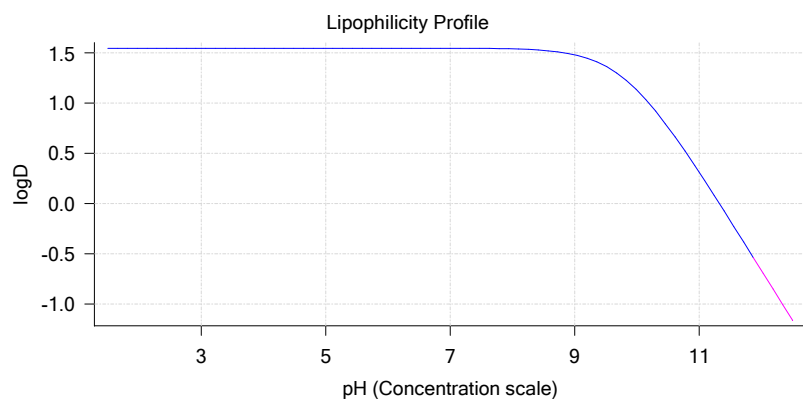
Sample graphs



Sample name: **phenol**
 Assay name: **pH-metric medium logP**
 Assay ID: **17K-28007**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**



Sample graphs (continued)



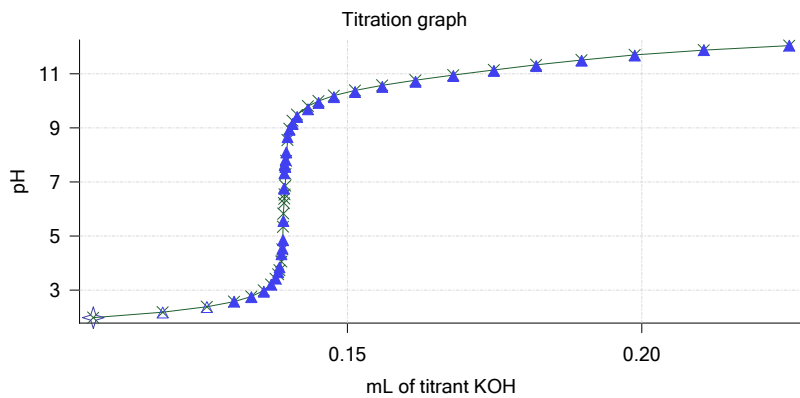
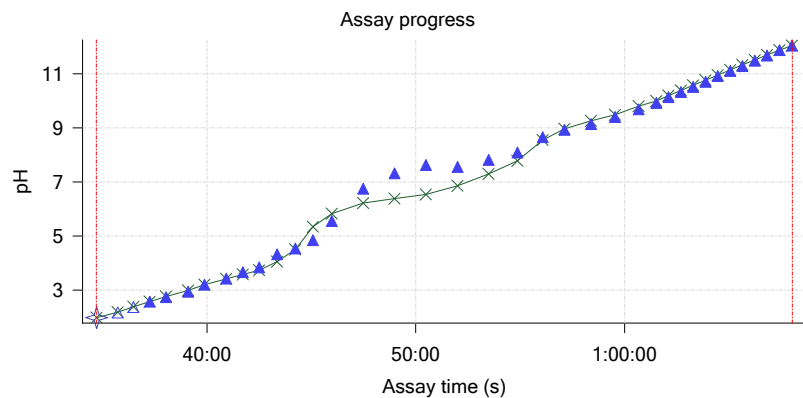
Sample logD and percent species

| pH | phenol logD | phenol phenolH | phenol phenol | phenol phenolH* | phenol phenol* | Comment |
|--------|-------------|----------------|---------------|-----------------|----------------|------------|
| 1.000 | 1.55 | 9.47 % | 0.00 % | 90.53 % | 0.00 % | |
| 1.200 | 1.55 | 9.47 % | 0.00 % | 90.53 % | 0.00 % | Stomach pH |
| 2.000 | 1.55 | 9.47 % | 0.00 % | 90.53 % | 0.00 % | |
| 3.000 | 1.55 | 9.47 % | 0.00 % | 90.53 % | 0.00 % | |
| 4.000 | 1.55 | 9.47 % | 0.00 % | 90.53 % | 0.00 % | |
| 5.000 | 1.55 | 9.47 % | 0.00 % | 90.53 % | 0.00 % | |
| 6.000 | 1.55 | 9.47 % | 0.00 % | 90.53 % | 0.00 % | |
| 6.500 | 1.55 | 9.47 % | 0.00 % | 90.52 % | 0.00 % | |
| 7.000 | 1.55 | 9.47 % | 0.02 % | 90.51 % | 0.00 % | |
| 7.400 | 1.55 | 9.47 % | 0.04 % | 90.49 % | 0.00 % | Blood pH |
| 8.000 | 1.54 | 9.46 % | 0.15 % | 90.39 % | 0.00 % | |
| 9.000 | 1.48 | 9.33 % | 1.51 % | 89.16 % | 0.00 % | |
| 10.000 | 1.13 | 8.21 % | 13.32 % | 78.47 % | 0.00 % | |
| 11.000 | 0.31 | 3.73 % | 60.57 % | 35.70 % | 0.00 % | |
| 12.000 | -0.67 | 0.58 % | 93.89 % | 5.53 % | 0.00 % | |

Carbonate and acidity

 Carbonate 0.206 mM
 Acidity error 0.201 mM

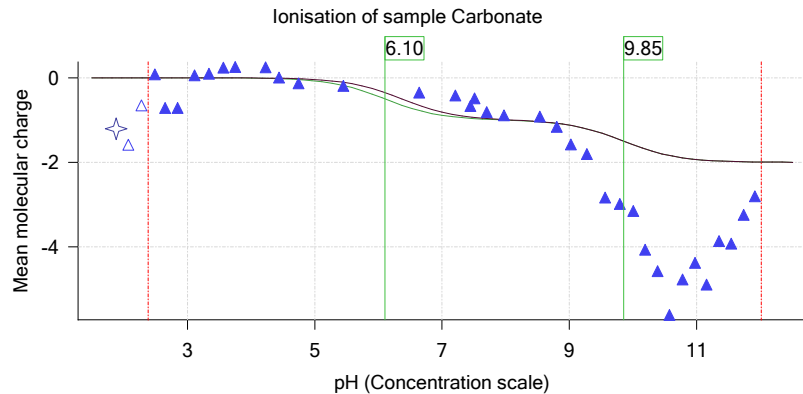
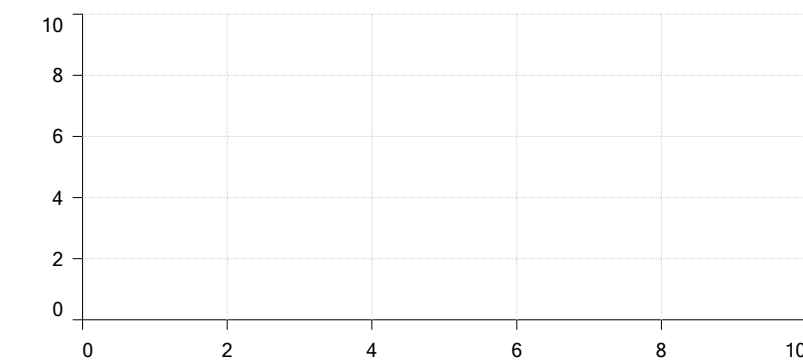
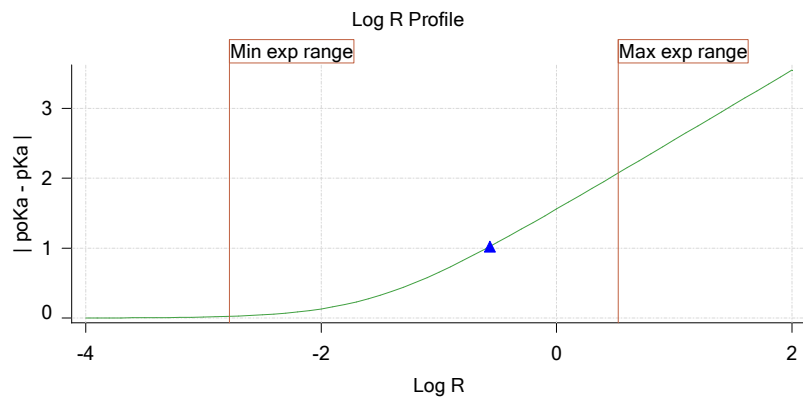
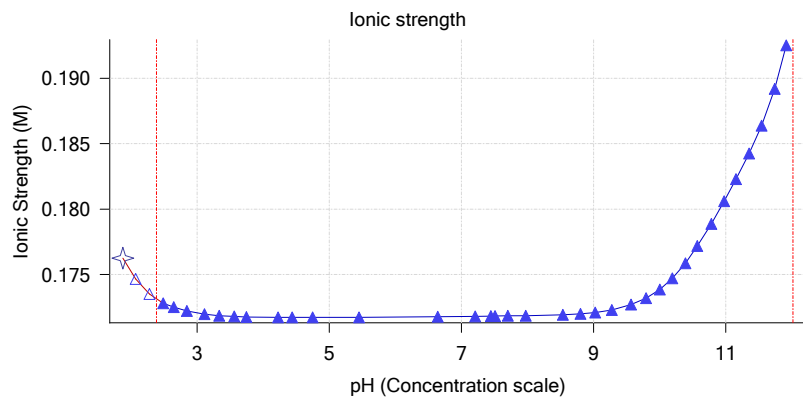
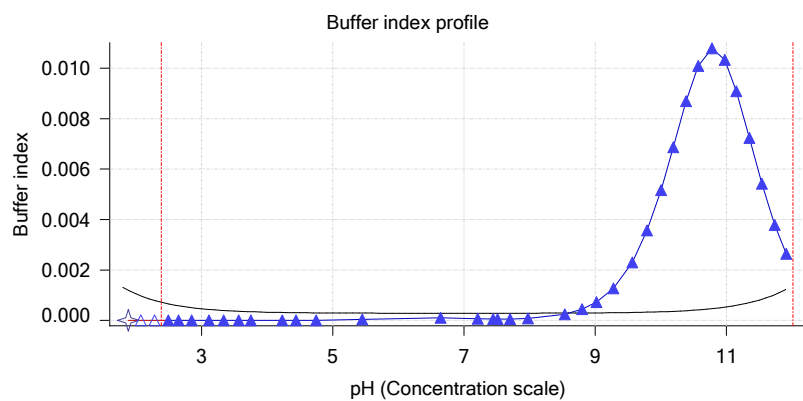
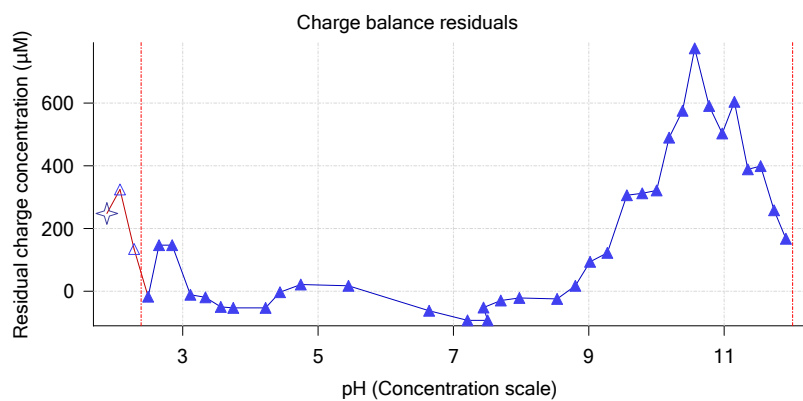
Other graphs



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 Assay name: **pH-metric medium logP**
 Assay ID: **17K-28007**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Other graphs (continued)



Sample name: **phenol**
 Assay name: **pH-metric medium logP**
 Assay ID: **17K-28007**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

pH-metric medium logP Titration 3 of 3 17K-28007 Points 71 to 104

Overall results

RMSD 0.773
 Average ionic strength 0.187 M
 Average temperature 25.0°C
 Partition ratio 0.6804 : 1
 Analyte concentration range 8865.9 µM to 9321.3 µM
 Total points considered 33 of 34

Warnings and errors

Errors None
 Warnings One or more logP values out of range

Four-Plus parameters

Alpha 0.076 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28005_Blank standardisation.t3r
 S 1.0056 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28005_Blank standardisation.t3r
 jH 1.0 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28005_Blank standardisation.t3r
 jOH -0.9 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28005_Blank standardisation.t3r

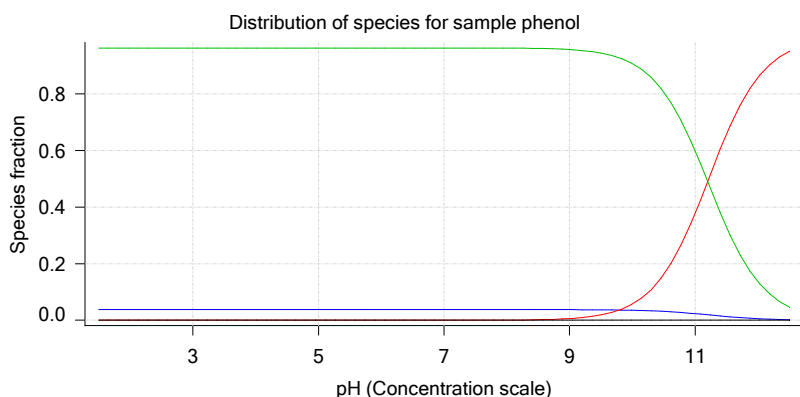
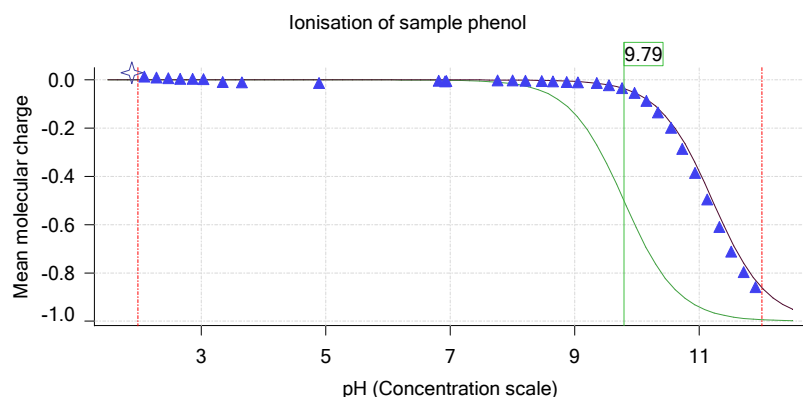
Titrants

0.50 M HCl 0.994563 11/28/2017 12:07:50 PM C:\Sirius_T3\17K-28006_Blank standardisation.t3r
 0.50 M KOH 1.000610 11/28/2017 12:07:50 PM C:\Sirius_T3\KOH17K27.t3r

Sample

phenol concentration factor 1.023
 Acid pKa 1 9.79
 logP (neutral XH) 1.58
 logP (X -) -9.00

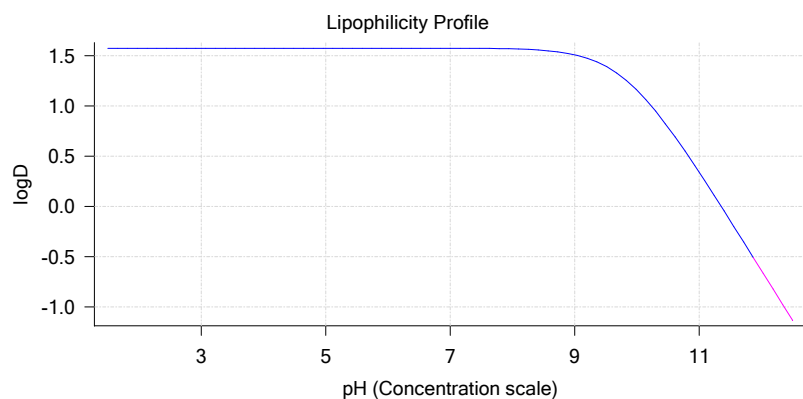
Sample graphs



Sample name: **phenol**
 Assay name: **pH-metric medium logP**
 Assay ID: **17K-28007**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**



Sample graphs (continued)



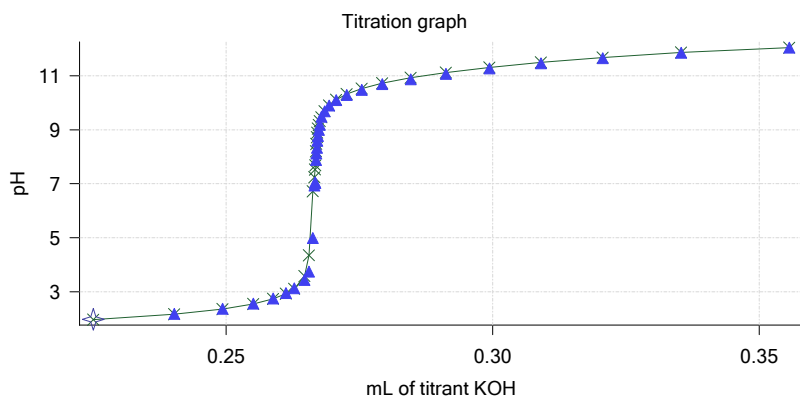
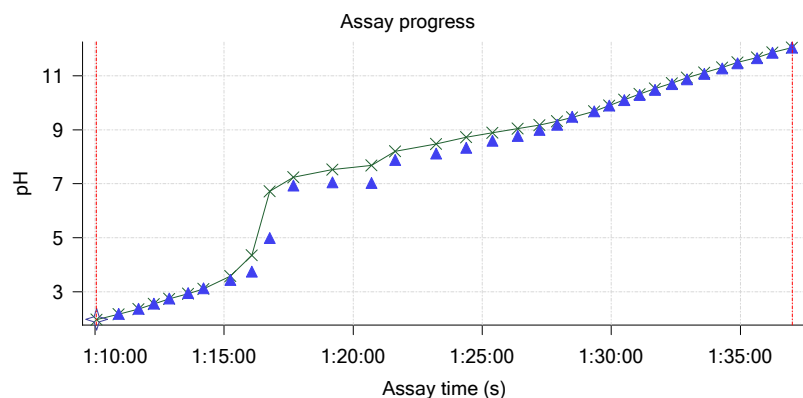
Sample logD and percent species

| pH | phenol logD | phenol phenolH | phenol phenol | phenol phenolH* | phenol phenol* | Comment |
|--------|-------------|----------------|---------------|-----------------|----------------|------------|
| 1.000 | 1.58 | 3.76 % | 0.00 % | 96.24 % | 0.00 % | Stomach pH |
| 1.200 | 1.58 | 3.76 % | 0.00 % | 96.24 % | 0.00 % | |
| 2.000 | 1.58 | 3.76 % | 0.00 % | 96.24 % | 0.00 % | |
| 3.000 | 1.58 | 3.76 % | 0.00 % | 96.24 % | 0.00 % | |
| 4.000 | 1.58 | 3.76 % | 0.00 % | 96.24 % | 0.00 % | |
| 5.000 | 1.58 | 3.76 % | 0.00 % | 96.24 % | 0.00 % | |
| 6.000 | 1.58 | 3.76 % | 0.00 % | 96.24 % | 0.00 % | Blood pH |
| 6.500 | 1.58 | 3.76 % | 0.00 % | 96.24 % | 0.00 % | |
| 7.000 | 1.57 | 3.76 % | 0.01 % | 96.23 % | 0.00 % | |
| 7.400 | 1.57 | 3.76 % | 0.02 % | 96.22 % | 0.00 % | |
| 8.000 | 1.57 | 3.76 % | 0.06 % | 96.18 % | 0.00 % | |
| 9.000 | 1.51 | 3.74 % | 0.61 % | 95.66 % | 0.00 % | |
| 10.000 | 1.16 | 3.54 % | 5.75 % | 90.71 % | 0.00 % | |
| 11.000 | 0.34 | 2.34 % | 37.88 % | 59.78 % | 0.00 % | |
| 12.000 | -0.64 | 0.53 % | 85.91 % | 13.56 % | 0.00 % | |

Carbonate and acidity

 Carbonate 0.375 mM
 Acidity error 0.089 mM

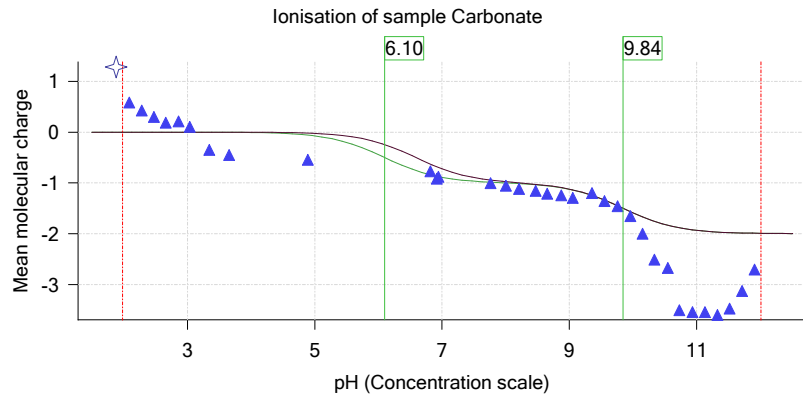
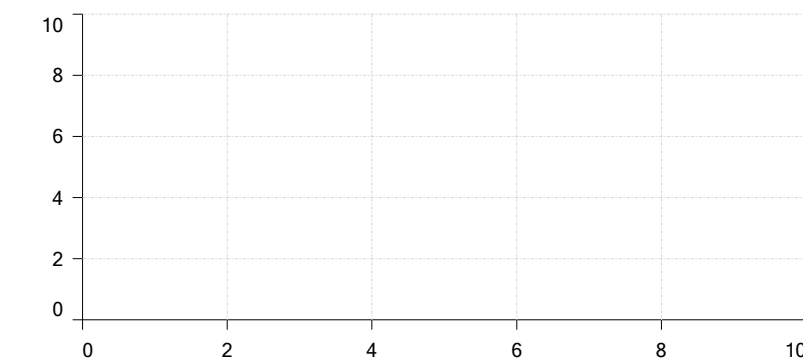
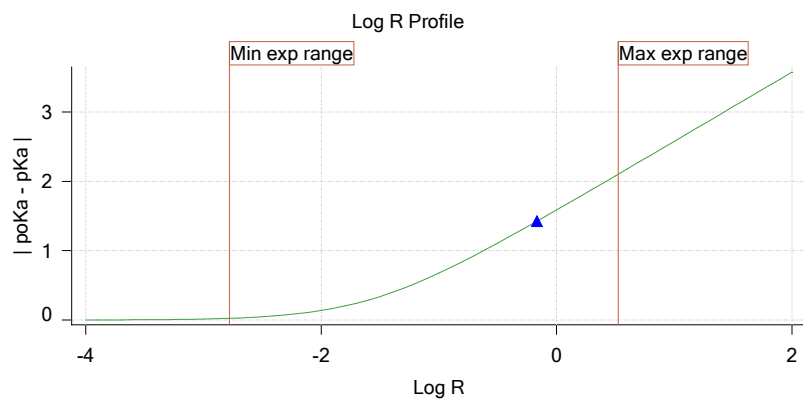
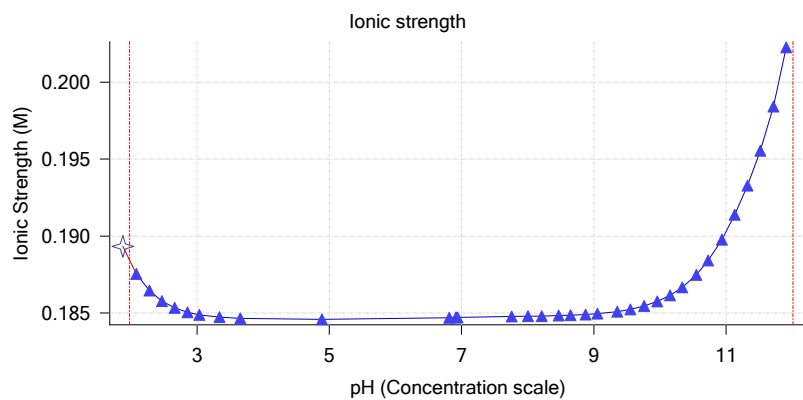
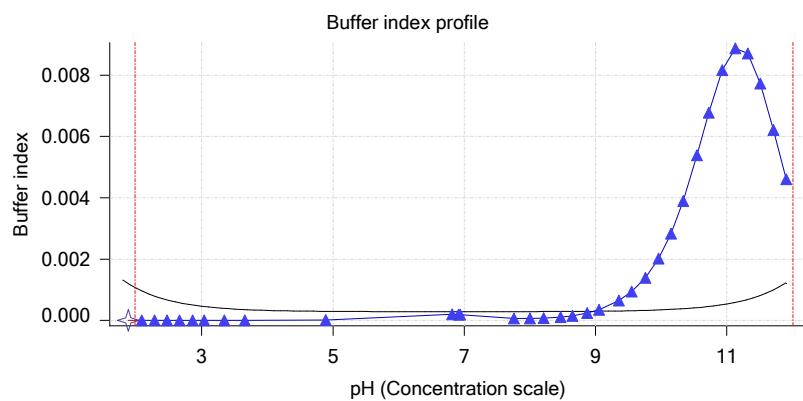
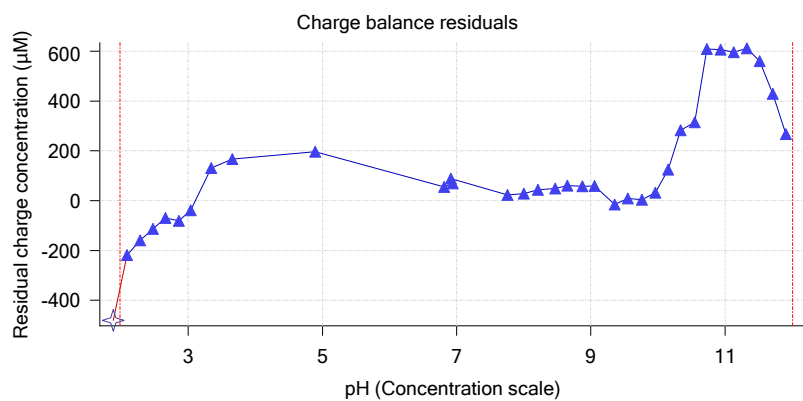
Other graphs



Sample name: **phenol**
 Assay name: **pH-metric medium logP**
 Assay ID: **17K-28007**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Other graphs (continued)



Sample name: **phenol**
 Assay name: **pH-metric medium logP**
 Assay ID: **17K-28007**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

Assay Model

| Settings | Value | Date/Time changed | Imported from |
|-----------------------------------|-------------|------------------------|--------------------|
| Sample name | phenol | 11/17/2017 2:14:44 PM | User entered value |
| Sample by | Weight | | Default value |
| Sample weight | 0.002230 g | 11/28/2017 11:11:01 AM | User entered value |
| Formula weight | 94.11 g/mol | 11/17/2017 2:14:44 PM | User entered value |
| Solubility | Unknown | | Default value |
| Molecular weight | 94.11 | 11/17/2017 2:14:44 PM | User entered value |
| Individual pKa ionic environments | No | | Default value |
| Number of pKas | 1 | 11/17/2017 2:14:44 PM | User entered value |
| Sample is a | Acid | 11/17/2017 2:14:44 PM | User entered value |
| pKa 1 | 9.79 | 11/29/2017 1:00:18 PM | User entered value |
| logP (neutral XH) | 1.54 | 11/17/2017 2:56:09 PM | User entered value |
| logP (X -) | -9.00 | 11/27/2017 4:23:19 PM | User entered value |

Events

| Time | Event | Water | Acid | Base | Octanol | pH | dpH/dt | pH R-squared | pH SD | dpH/dt time |
|---------|-------------------|------------|------------|------------|------------|--------|----------|--------------|---------|-------------|
| 2:19.5 | Initial pH = 5.36 | | | | | | | | | |
| 5:11.8 | Data point 1 | 1.00000 mL | 0.02524 mL | 0.00000 mL | 0.10000 mL | 2.006 | 0.00335 | 0.06289 | 0.00066 | 10.0 s |
| 5:58.9 | Data point 2 | 1.00000 mL | 0.02524 mL | 0.00910 mL | 0.10000 mL | 2.204 | -0.01781 | 0.86156 | 0.00095 | 10.5 s |
| 6:34.8 | Data point 3 | 1.00000 mL | 0.02524 mL | 0.01489 mL | 0.10000 mL | 2.394 | 0.00782 | 0.15096 | 0.00099 | 19.5 s |
| 7:19.6 | Data point 4 | 1.00000 mL | 0.02524 mL | 0.01858 mL | 0.10000 mL | 2.594 | -0.01585 | 0.93109 | 0.00081 | 10.5 s |
| 7:55.4 | Data point 5 | 1.00000 mL | 0.02524 mL | 0.02091 mL | 0.10000 mL | 2.762 | -0.01950 | 0.92447 | 0.00100 | 13.5 s |
| 8:39.3 | Data point 6 | 1.00000 mL | 0.02524 mL | 0.02248 mL | 0.10000 mL | 2.956 | -0.01757 | 0.85425 | 0.00094 | 16.0 s |
| 9:20.6 | Data point 7 | 1.00000 mL | 0.02524 mL | 0.02349 mL | 0.10000 mL | 3.204 | -0.01417 | 0.60288 | 0.00090 | 16.5 s |
| 10:17.7 | Data point 8 | 1.00000 mL | 0.02524 mL | 0.02420 mL | 0.10000 mL | 3.401 | -0.01542 | 0.90376 | 0.00080 | 10.5 s |
| 11:09.0 | Data point 9 | 1.00000 mL | 0.02524 mL | 0.02465 mL | 0.10000 mL | 3.680 | -0.01761 | 0.93750 | 0.00090 | 10.5 s |
| 11:49.8 | Data point 10 | 1.00000 mL | 0.02524 mL | 0.02495 mL | 0.10000 mL | 4.118 | -0.01449 | 0.92180 | 0.00074 | 10.5 s |
| 12:30.7 | Data point 11 | 1.00000 mL | 0.02524 mL | 0.02519 mL | 0.10000 mL | 6.045 | -0.01897 | 0.89217 | 0.00099 | 28.5 s |
| 13:29.6 | Data point 12 | 1.00000 mL | 0.02524 mL | 0.02528 mL | 0.10000 mL | 6.346 | -0.01581 | 0.75316 | 0.00090 | 39.0 s |
| 14:44.2 | Data point 13 | 1.00000 mL | 0.02524 mL | 0.02549 mL | 0.10000 mL | 7.995 | 0.00039 | 0.00041 | 0.00097 | 50.0 s |
| 16:04.7 | Data point 14 | 1.00000 mL | 0.02524 mL | 0.02578 mL | 0.10000 mL | 8.354 | -0.01986 | 0.97475 | 0.00099 | 44.0 s |
| 17:19.3 | Data point 15 | 1.00000 mL | 0.02524 mL | 0.02641 mL | 0.10000 mL | 8.720 | -0.01802 | 0.87061 | 0.00095 | 42.0 s |
| 18:31.7 | Data point 16 | 1.00000 mL | 0.02524 mL | 0.02698 mL | 0.10000 mL | 8.901 | -0.00597 | 0.11324 | 0.00087 | 30.0 s |
| 19:42.4 | Data point 17 | 1.00000 mL | 0.02524 mL | 0.02803 mL | 0.10000 mL | 9.105 | -0.01848 | 0.88425 | 0.00097 | 36.0 s |
| 20:54.2 | Data point 18 | 1.00000 mL | 0.02524 mL | 0.03048 mL | 0.10000 mL | 9.409 | -0.01766 | 0.79490 | 0.00098 | 14.0 s |
| 21:43.9 | Data point 19 | 1.00000 mL | 0.02524 mL | 0.03248 mL | 0.10000 mL | 9.579 | -0.01709 | 0.81066 | 0.00094 | 36.0 s |
| 22:45.4 | Data point 20 | 1.00000 mL | 0.02524 mL | 0.03518 mL | 0.10000 mL | 9.792 | -0.01775 | 0.87272 | 0.00094 | 15.5 s |
| 23:26.3 | Data point 21 | 1.00000 mL | 0.02524 mL | 0.03888 mL | 0.10000 mL | 9.977 | -0.01923 | 0.95071 | 0.00097 | 20.0 s |
| 24:22.2 | Data point 22 | 1.00000 mL | 0.02524 mL | 0.04349 mL | 0.10000 mL | 10.168 | -0.01875 | 0.86644 | 0.00099 | 15.0 s |
| 25:02.7 | Data point 23 | 1.00000 mL | 0.02524 mL | 0.04887 mL | 0.10000 mL | 10.340 | -0.01471 | 0.86409 | 0.00078 | 10.5 s |
| 25:49.0 | Data point 24 | 1.00000 mL | 0.02524 mL | 0.05416 mL | 0.10000 mL | 10.524 | -0.01746 | 0.80957 | 0.00096 | 17.0 s |
| 26:31.4 | Data point 25 | 1.00000 mL | 0.02524 mL | 0.06000 mL | 0.10000 mL | 10.712 | -0.00762 | 0.44574 | 0.00056 | 10.5 s |
| 27:17.7 | Data point 26 | 1.00000 mL | 0.02524 mL | 0.06519 mL | 0.10000 mL | 10.896 | -0.01604 | 0.75614 | 0.00091 | 16.0 s |
| 27:59.3 | Data point 27 | 1.00000 mL | 0.02524 mL | 0.07034 mL | 0.10000 mL | 11.076 | -0.00603 | 0.46461 | 0.00044 | 10.5 s |
| 28:45.6 | Data point 28 | 1.00000 mL | 0.02524 mL | 0.07524 mL | 0.10000 mL | 11.261 | -0.01367 | 0.73900 | 0.00079 | 10.5 s |
| 29:21.6 | Data point 29 | 1.00000 mL | 0.02524 mL | 0.08050 mL | 0.10000 mL | 11.440 | -0.01796 | 0.84277 | 0.00097 | 32.0 s |
| 30:34.7 | Data point 30 | 1.00000 mL | 0.02524 mL | 0.08761 mL | 0.10000 mL | 11.643 | -0.01568 | 0.83548 | 0.00085 | 10.5 s |
| 31:10.7 | Data point 31 | 1.00000 mL | 0.02524 mL | 0.09628 mL | 0.10000 mL | 11.807 | -0.01827 | 0.83449 | 0.00099 | 51.0 s |
| 32:32.5 | Data point 32 | 1.00000 mL | 0.02524 mL | 0.10684 mL | 0.10000 mL | 11.979 | -0.01895 | 0.89783 | 0.00099 | 34.0 s |
| 33:26.8 | Data point 33 | 1.00000 mL | 0.02524 mL | 0.10684 mL | 0.10000 mL | 11.989 | -0.01286 | 0.84203 | 0.00069 | 10.5 s |
| 34:42.5 | Data point 34 | 1.00000 mL | 0.13939 mL | 0.10684 mL | 0.35000 mL | 1.979 | 0.01036 | 0.31629 | 0.00091 | 25.0 s |
| 35:43.4 | Data point 35 | 1.00000 mL | 0.13939 mL | 0.11863 mL | 0.35000 mL | 2.169 | -0.01840 | 0.92670 | 0.00094 | 19.0 s |
| 36:27.9 | Data point 36 | 1.00000 mL | 0.13939 mL | 0.12613 mL | 0.35000 mL | 2.374 | -0.01551 | 0.62902 | 0.00097 | 21.5 s |
| 37:14.8 | Data point 37 | 1.00000 mL | 0.13939 mL | 0.13079 mL | 0.35000 mL | 2.582 | -0.00548 | 0.09284 | 0.00089 | 22.0 s |
| 38:02.1 | Data point 38 | 1.00000 mL | 0.13939 mL | 0.13370 mL | 0.35000 mL | 2.740 | -0.01545 | 0.66175 | 0.00094 | 22.5 s |
| 39:05.5 | Data point 39 | 1.00000 mL | 0.13939 mL | 0.13580 mL | 0.35000 mL | 2.938 | -0.01148 | 0.37162 | 0.00093 | 21.5 s |
| 39:52.2 | Data point 40 | 1.00000 mL | 0.13939 mL | 0.13706 mL | 0.35000 mL | 3.206 | -0.01315 | 0.52952 | 0.00089 | 22.0 s |



Assay Events

Sample name: **phenol** Experiment start time: **11/28/2017 12:07:50 PM**
Assay name: **pH-metric medium logP** Analyst: **Dorothy Levorse**
Assay ID: **17K-28007** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Events (continued)

| Time | Event | Water | Acid | Base | Octanol | pH | dpH/dt | pH R-squared | pH SD | dpH/dt time |
|-----------|---------------|------------|------------|------------|------------|--------|----------|--------------|---------|---------------------|
| 40:55.0 | Data point 41 | 1.00000 mL | 0.13939 mL | 0.13784 mL | 0.35000 mL | 3.432 | -0.01228 | 0.44436 | 0.00091 | 22.5 s |
| 41:42.8 | Data point 42 | 1.00000 mL | 0.13939 mL | 0.13824 mL | 0.35000 mL | 3.660 | 0.00935 | 0.23120 | 0.00096 | 21.5 s |
| 42:29.6 | Data point 43 | 1.00000 mL | 0.13939 mL | 0.13848 mL | 0.35000 mL | 3.846 | -0.01299 | 0.42567 | 0.00098 | 21.0 s |
| 43:21.0 | Data point 44 | 1.00000 mL | 0.13939 mL | 0.13878 mL | 0.35000 mL | 4.326 | -0.00991 | 0.35657 | 0.00082 | 22.5 s |
| 44:13.8 | Data point 45 | 1.00000 mL | 0.13939 mL | 0.13897 mL | 0.35000 mL | 4.539 | -0.01817 | 0.88379 | 0.00095 | 20.0 s |
| 45:04.2 | Data point 46 | 1.00000 mL | 0.13939 mL | 0.13909 mL | 0.35000 mL | 4.849 | -0.01538 | 0.80218 | 0.00085 | 23.5 s |
| 45:58.2 | Data point 47 | 1.00000 mL | 0.13939 mL | 0.13916 mL | 0.35000 mL | 5.555 | 0.15444 | 0.98187 | 0.00769 | Timed out at 59.5 s |
| 47:28.6 | Data point 48 | 1.00000 mL | 0.13939 mL | 0.13925 mL | 0.35000 mL | 6.755 | -0.03971 | 0.98862 | 0.00197 | Timed out at 59.5 s |
| 48:59.1 | Data point 49 | 1.00000 mL | 0.13939 mL | 0.13930 mL | 0.35000 mL | 7.325 | -0.03876 | 0.98498 | 0.00193 | Timed out at 59.5 s |
| 50:29.3 | Data point 50 | 1.00000 mL | 0.13939 mL | 0.13935 mL | 0.35000 mL | 7.627 | -0.02499 | 0.95193 | 0.00126 | Timed out at 59.5 s |
| 51:59.7 | Data point 51 | 1.00000 mL | 0.13939 mL | 0.13944 mL | 0.35000 mL | 7.561 | -0.01897 | 0.92280 | 0.00097 | 59.0 s |
| 53:29.3 | Data point 52 | 1.00000 mL | 0.13939 mL | 0.13953 mL | 0.35000 mL | 7.820 | -0.01928 | 0.91792 | 0.00099 | 52.5 s |
| 54:52.2 | Data point 53 | 1.00000 mL | 0.13939 mL | 0.13961 mL | 0.35000 mL | 8.095 | -0.01940 | 0.94220 | 0.00099 | 42.5 s |
| 56:05.1 | Data point 54 | 1.00000 mL | 0.13939 mL | 0.13982 mL | 0.35000 mL | 8.659 | -0.00168 | 0.00730 | 0.00097 | 31.5 s |
| 57:07.1 | Data point 55 | 1.00000 mL | 0.13939 mL | 0.14017 mL | 0.35000 mL | 8.926 | -0.01537 | 0.77096 | 0.00086 | 31.0 s |
| 58:24.1 | Data point 56 | 1.00000 mL | 0.13939 mL | 0.14071 mL | 0.35000 mL | 9.147 | -0.01563 | 0.75235 | 0.00089 | 33.0 s |
| 59:32.8 | Data point 57 | 1.00000 mL | 0.13939 mL | 0.14146 mL | 0.35000 mL | 9.404 | -0.01663 | 0.89354 | 0.00087 | 32.0 s |
| 1:00:40.4 | Data point 58 | 1.00000 mL | 0.13939 mL | 0.14330 mL | 0.35000 mL | 9.692 | -0.01393 | 0.84457 | 0.00075 | 10.0 s |
| 1:01:31.3 | Data point 59 | 1.00000 mL | 0.13939 mL | 0.14513 mL | 0.35000 mL | 9.922 | -0.00518 | 0.50297 | 0.00036 | 10.0 s |
| 1:02:06.6 | Data point 60 | 1.00000 mL | 0.13939 mL | 0.14769 mL | 0.35000 mL | 10.134 | 0.00161 | 0.09245 | 0.00026 | 10.0 s |
| 1:02:42.0 | Data point 61 | 1.00000 mL | 0.13939 mL | 0.15129 mL | 0.35000 mL | 10.322 | -0.00211 | 0.03053 | 0.00059 | 10.0 s |
| 1:03:17.3 | Data point 62 | 1.00000 mL | 0.13939 mL | 0.15593 mL | 0.35000 mL | 10.519 | -0.00918 | 0.73122 | 0.00053 | 10.0 s |
| 1:03:52.8 | Data point 63 | 1.00000 mL | 0.13939 mL | 0.16159 mL | 0.35000 mL | 10.703 | -0.00183 | 0.04565 | 0.00042 | 10.0 s |
| 1:04:28.2 | Data point 64 | 1.00000 mL | 0.13939 mL | 0.16799 mL | 0.35000 mL | 10.913 | 0.00207 | 0.07493 | 0.00037 | 10.0 s |
| 1:05:03.6 | Data point 65 | 1.00000 mL | 0.13939 mL | 0.17488 mL | 0.35000 mL | 11.109 | -0.00430 | 0.25596 | 0.00042 | 10.0 s |
| 1:05:39.1 | Data point 66 | 1.00000 mL | 0.13939 mL | 0.18208 mL | 0.35000 mL | 11.288 | 0.00192 | 0.03453 | 0.00051 | 10.0 s |
| 1:06:14.6 | Data point 67 | 1.00000 mL | 0.13939 mL | 0.18977 mL | 0.35000 mL | 11.487 | 0.00708 | 0.40896 | 0.00055 | 10.0 s |
| 1:06:50.1 | Data point 68 | 1.00000 mL | 0.13939 mL | 0.19882 mL | 0.35000 mL | 11.674 | 0.00339 | 0.04623 | 0.00078 | 10.0 s |
| 1:07:25.8 | Data point 69 | 1.00000 mL | 0.13939 mL | 0.21058 mL | 0.35000 mL | 11.871 | 0.00526 | 0.60434 | 0.00033 | 10.0 s |
| 1:08:01.4 | Data point 70 | 1.00000 mL | 0.13939 mL | 0.22507 mL | 0.35000 mL | 12.042 | -0.00641 | 0.34866 | 0.00054 | 10.0 s |
| 1:10:04.0 | Data point 71 | 1.00000 mL | 0.26703 mL | 0.22507 mL | 1.05000 mL | 1.981 | -0.01403 | 0.52120 | 0.00096 | 15.0 s |
| 1:10:55.2 | Data point 72 | 1.00000 mL | 0.26703 mL | 0.24026 mL | 1.05000 mL | 2.181 | -0.01307 | 0.43537 | 0.00098 | 20.5 s |
| 1:11:41.2 | Data point 73 | 1.00000 mL | 0.26703 mL | 0.24932 mL | 1.05000 mL | 2.374 | -0.01299 | 0.93367 | 0.00066 | 10.5 s |
| 1:12:17.1 | Data point 74 | 1.00000 mL | 0.26703 mL | 0.25508 mL | 1.05000 mL | 2.565 | -0.00045 | 0.00053 | 0.00097 | 10.5 s |
| 1:12:52.9 | Data point 75 | 1.00000 mL | 0.26703 mL | 0.25882 mL | 1.05000 mL | 2.754 | -0.01143 | 0.32177 | 0.00099 | 18.5 s |
| 1:13:36.8 | Data point 76 | 1.00000 mL | 0.26703 mL | 0.26122 mL | 1.05000 mL | 2.953 | 0.00008 | 0.00004 | 0.00064 | 10.0 s |
| 1:14:12.0 | Data point 77 | 1.00000 mL | 0.26703 mL | 0.26275 mL | 1.05000 mL | 3.129 | -0.00819 | 0.17990 | 0.00095 | 16.5 s |
| 1:15:14.6 | Data point 78 | 1.00000 mL | 0.26703 mL | 0.26470 mL | 1.05000 mL | 3.438 | -0.01482 | 0.61601 | 0.00093 | 19.5 s |
| 1:16:04.5 | Data point 79 | 1.00000 mL | 0.26703 mL | 0.26552 mL | 1.05000 mL | 3.750 | -0.00154 | 0.00771 | 0.00087 | 11.0 s |
| 1:16:46.0 | Data point 80 | 1.00000 mL | 0.26703 mL | 0.26627 mL | 1.05000 mL | 4.993 | 0.01309 | 0.44865 | 0.00096 | 20.0 s |
| 1:17:41.5 | Data point 81 | 1.00000 mL | 0.26703 mL | 0.26658 mL | 1.05000 mL | 6.929 | -0.15256 | 0.99781 | 0.00755 | Timed out at 59.5 s |
| 1:19:11.9 | Data point 82 | 1.00000 mL | 0.26703 mL | 0.26670 mL | 1.05000 mL | 7.055 | -0.02110 | 0.96462 | 0.00106 | Timed out at 59.5 s |
| 1:20:42.3 | Data point 83 | 1.00000 mL | 0.26703 mL | 0.26675 mL | 1.05000 mL | 7.030 | -0.01385 | 0.55321 | 0.00092 | 25.0 s |
| 1:21:37.6 | Data point 84 | 1.00000 mL | 0.26703 mL | 0.26686 mL | 1.05000 mL | 7.878 | -0.04906 | 0.98889 | 0.00243 | Timed out at 59.5 s |
| 1:23:13.2 | Data point 85 | 1.00000 mL | 0.26703 mL | 0.26693 mL | 1.05000 mL | 8.122 | -0.01878 | 0.89976 | 0.00098 | 39.0 s |
| 1:24:22.7 | Data point 86 | 1.00000 mL | 0.26703 mL | 0.26703 mL | 1.05000 mL | 8.332 | -0.01785 | 0.85890 | 0.00095 | 25.5 s |
| 1:25:23.8 | Data point 87 | 1.00000 mL | 0.26703 mL | 0.26712 mL | 1.05000 mL | 8.592 | -0.01295 | 0.45270 | 0.00095 | 23.0 s |
| 1:26:22.4 | Data point 88 | 1.00000 mL | 0.26703 mL | 0.26724 mL | 1.05000 mL | 8.774 | -0.01737 | 0.81890 | 0.00095 | 20.5 s |
| 1:27:13.5 | Data point 89 | 1.00000 mL | 0.26703 mL | 0.26738 mL | 1.05000 mL | 8.999 | 0.00113 | 0.00635 | 0.00070 | 10.0 s |
| 1:27:53.7 | Data point 90 | 1.00000 mL | 0.26703 mL | 0.26757 mL | 1.05000 mL | 9.180 | -0.01756 | 0.88832 | 0.00092 | 10.0 s |



Assay Events

Sample name: **phenol** Experiment start time: **11/28/2017 12:07:50 PM**
Assay name: **pH-metric medium logP** Analyst: **Dorothy Levorse**
Assay ID: **17K-28007** Instrument ID: **T311053**
Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Events (continued)

| Time | Event | Water | Acid | Base | Octanol | pH | dpH/dt | pH R-squared | pH SD | dpH/dt time |
|-----------|----------------|------------|------------|------------|------------|--------|----------|--------------|---------|-------------|
| 1:28:29.1 | Data point 91 | 1.00000 mL | 0.26703 mL | 0.26785 mL | 1.05000 mL | 9.484 | 0.01232 | 0.38407 | 0.00098 | 10.0 s |
| 1:29:20.0 | Data point 92 | 1.00000 mL | 0.26703 mL | 0.26846 mL | 1.05000 mL | 9.679 | -0.00089 | 0.00221 | 0.00093 | 10.0 s |
| 1:29:55.2 | Data point 93 | 1.00000 mL | 0.26703 mL | 0.26931 mL | 1.05000 mL | 9.890 | -0.00234 | 0.06095 | 0.00047 | 10.0 s |
| 1:30:30.5 | Data point 94 | 1.00000 mL | 0.26703 mL | 0.27063 mL | 1.05000 mL | 10.092 | 0.00700 | 0.76968 | 0.00039 | 10.0 s |
| 1:31:05.9 | Data point 95 | 1.00000 mL | 0.26703 mL | 0.27260 mL | 1.05000 mL | 10.284 | 0.00810 | 0.73675 | 0.00047 | 10.0 s |
| 1:31:41.3 | Data point 96 | 1.00000 mL | 0.26703 mL | 0.27542 mL | 1.05000 mL | 10.470 | 0.00776 | 0.19387 | 0.00087 | 14.0 s |
| 1:32:20.7 | Data point 97 | 1.00000 mL | 0.26703 mL | 0.27930 mL | 1.05000 mL | 10.682 | 0.00999 | 0.79618 | 0.00055 | 10.0 s |
| 1:32:56.1 | Data point 98 | 1.00000 mL | 0.26703 mL | 0.28462 mL | 1.05000 mL | 10.862 | 0.01097 | 0.37770 | 0.00088 | 14.5 s |
| 1:33:36.0 | Data point 99 | 1.00000 mL | 0.26703 mL | 0.29125 mL | 1.05000 mL | 11.069 | 0.01105 | 0.55241 | 0.00073 | 16.5 s |
| 1:34:18.1 | Data point 100 | 1.00000 mL | 0.26703 mL | 0.29939 mL | 1.05000 mL | 11.267 | 0.01005 | 0.56097 | 0.00066 | 10.0 s |
| 1:34:53.5 | Data point 101 | 1.00000 mL | 0.26703 mL | 0.30906 mL | 1.05000 mL | 11.460 | 0.01330 | 0.66088 | 0.00081 | 19.5 s |
| 1:35:38.6 | Data point 102 | 1.00000 mL | 0.26703 mL | 0.32065 mL | 1.05000 mL | 11.649 | 0.00451 | 0.19942 | 0.00050 | 10.0 s |
| 1:36:14.4 | Data point 103 | 1.00000 mL | 0.26703 mL | 0.33535 mL | 1.05000 mL | 11.845 | 0.01594 | 0.67856 | 0.00095 | 19.5 s |
| 1:36:59.7 | Data point 104 | 1.00000 mL | 0.26703 mL | 0.35564 mL | 1.05000 mL | 12.037 | 0.01099 | 0.50532 | 0.00076 | 10.0 s |
| 1:37:18.6 | Assay volumes | 1.00000 mL | 0.26703 mL | 0.35564 mL | 1.05000 mL | | | | | |

Sample name: **phenol**
 Assay name: **pH-metric medium logP**
 Assay ID: **17K-28007**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T311053**

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 | 12.000 | | | |
| 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% | | | |
| Titration Pre-Dose | | | | |
| Titration pre-dose | None | | | |
| Assay Medium | | | | |
| ISA water volume | 1.00 mL | | | |
| Water added | Automatic | | | |
| After water addition, stir for | 5 seconds | | | |
| At a speed of | 10% | | | |
| Partition solvent type | Octanol | | | |
| Partition volume | 0.100 mL | | | |
| Partition solvent added | Automatic | | | |
| After partition addition, stir for | 1 seconds | | | |
| Sample Sonication | | | | |
| Sonicate | No | | | |
| 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 | 0.250 mL | | | |
| Additional partition solvent added | Automatic | | | |
| After pH adjust stir for | 30 seconds | | | |
| Stir to allow partitioning for | 15 seconds | | | |
| Stirrer speed for partitioning | 55% | | | |
| Titration 3 | | | | |

Sample name: **phenol** Experiment start time: **11/28/2017 12:07:50 PM**
 Assay name: **pH-metric medium logP** Analyst: **Dorothy Levorse**
 Assay ID: **17K-28007** Instrument ID: **T311053**
 Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Assay Settings (continued)

| Setting | Value | Original Value | Date/Time changed | Imported from |
|-------------------------------------|----------------|----------------|-------------------|---------------|
| Titrate from | Low to high pH | | | |
| Add additional water | 0.00 mL | | | |
| Additional partition solvent volume | 0.700 mL | | | |
| Additional partition solvent added | Automatic | | | |
| After pH adjust stir for | 30 seconds | | | |
| Stir to allow partitioning for | 15 seconds | | | |
| Stirrer speed for partitioning | 60% | | | |
| Data Point Stability | | | | |
| Stir during data point collection | No | | | |
| Delay before data point collection | 0 seconds | | | |
| Number of points to average | 20 points | | | |
| Time interval between points | 0.50 seconds | | | |
| Required maximum standard deviation | 0.00100 dpH/dt | | | |
| Stability timeout after | 60 seconds | | | |

Calibration Settings

| Setting | Value | Date/Time changed | Imported from |
|---------------------------|--------|------------------------|--|
| Four-Plus alpha | 0.076 | 11/28/2017 12:07:50 PM | C:\Sirius_T3\17K-28005_Blank standardisation.t3r |
| Four-Plus S | 1.0056 | 11/28/2017 12:07:50 PM | C:\Sirius_T3\17K-28005_Blank standardisation.t3r |
| Four-Plus jH | 1.0 | 11/28/2017 12:07:50 PM | C:\Sirius_T3\17K-28005_Blank standardisation.t3r |
| Four-Plus jOH | -0.9 | 11/28/2017 12:07:50 PM | C:\Sirius_T3\17K-28005_Blank standardisation.t3r |
| Base concentration factor | 1.001 | 11/28/2017 12:07:50 PM | C:\Sirius_T3\KOH17K27.t3r |
| Acid concentration factor | 0.995 | 11/28/2017 12:07:50 PM | C:\Sirius_T3\17K-28006_Blank standardisation.t3r |

Instrument Settings

| Setting | Value | Batch Id | Install date |
|----------------------|----------------------------|-------------|-----------------------|
| Instrument owner | Merck | | |
| Instrument ID | T311053 | | |
| Instrument type | T3 Simulator | | |
| Software version | 1.1.3.0 | | |
| Dispenser module | | T3DM1100253 | 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) | 10-10-2017 | 11/8/2017 11:33:30 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) | 11-8-17 | 11/8/2017 11:32:21 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) | 09-22-17 | 11/27/2017 9:30:45 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) | 9-26-17 | 11/16/2017 9:31:07 AM |
| Port B | Cyclohexane | | 10/19/2017 2:11:05 PM |
| Port C | MeCN (50%, 0.15 M KCl) | 10-30-17 | 11/27/2017 9:21:50 AM |
| Port D | Dodecane | 11-17-2017 | 11/17/2017 4:39:13 PM |
| Dispenser 3 | Buffer | | 8/3/2010 5:05:16 AM |
| Syringe volume | 0.5 mL | | |
| Firmware version | 1.2.1(r2) | | |
| Titrant | Phosphate Buffer | | 11/8/2017 11:32:27 AM |

Sample name: **phenol**
Assay name: **pH-metric medium logP**
Assay ID: **17K-28007**
Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

| Setting | Value | Batch Id | Install date |
|---|----------------------------|-------------|------------------------|
| Dispenser 6 | Octanol | | 10/22/2010 10:52:43 AM |
| Syringe volume | 0.5 mL | | |
| Firmware version | 1.2.1(r2) | | |
| Titration | Octanol | 9-14-17 | 10/13/2017 7:46:59 AM |
| Titration | | T3TM1100153 | 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 | T3E0769 | 8/15/2017 9:21:54 AM |
| E0 calibration | -4.51 mV | | 11/28/2017 12:08:18 PM |
| Filling solution | 3M KCl | KCL095 | 11/27/2017 9:15:10 AM |
| Liquids | | | |
| Wash 1 | 50% IPA:50% Water | | 11/28/2017 10:29:51 AM |
| Wash 2 | 0.5% Triton X-100 in H2O | | 11/28/2017 10:29:54 AM |
| Buffer position 1 | pH7 Wash | | 11/28/2017 10:29:57 AM |
| Buffer position 2 | pH 7 | | 11/28/2017 10:30:05 AM |
| Storage position | | | 11/28/2017 10:31:10 AM |
| Wash water | 9.7e+003 mL | 11-28-17 | 11/28/2017 10:30:22 AM |
| Waste | 3e+002 mL | | 11/28/2017 10:30:33 AM |
| Temperature controller | | | 8/5/2010 6:35:13 AM |
| Turbidity detector | | | 3/31/2009 5:24:45 AM |
| Spectrometer | | 072390 | 11/23/2010 11:22:28 AM |
| Dip probe | | 11086 | |
| Wavelength coefficient A0 | 185.563 | | |
| Wavelength coefficient A1 | 2.17439 | | |
| Wavelength coefficient A2 | -0.000285622 | | |
| Total lamp lit time | 565:42:53 | | 11/23/2010 11:22:28 AM |
| Calibrated on | 11/8/2017 1:14:37 PM | | |
| Integration time | 10 | | |
| Scans averaged | 10 | | |
| Autoloader | | T3AL1100237 | 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) | | |
| Titration 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% | | |



Assay Settings

Sample name: **phenol**
Assay name: **pH-metric medium logP**
Assay ID: **17K-28007**
Filename: **C:\Sirius_T3\Mehtap\20171128_exp20_logP_training\17K-28007_phenol_pH-metric medium logP_pHpKa.t3r**

Experiment start time: **11/28/2017 12:07:50 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T311053**

Instrument Settings (continued)

| Setting | Value | Batch Id | Install date |
|---|---------|----------|--------------|
| E0 calibration reading stir speed | 0% | | |
| 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 |