The results output for sodium laureth sulphate

a) Water Solubility

```
                Water Sol: 486.5 mg/L
```

(Estimated value)

```
SMILES : O([Na])S(=O)(=O)OCCOCCCCCCCCCCCC
CHEM   :
MOL FOR: C14 H29 O5 S1 Na1
MOL WT : 332.43
----------------------WSKOW v1.41 Results ----------
Log Kow  (estimated)  :  1.42
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  1.42

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
      (used when Melting Point NOT available)

      Correction(s):         Value
      --------------------   -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -2.835
   Water Solubility at 25 deg C (mg/L):  486.5

-----------------------------------------------------------------
```

Program and version used

Equation used for the estimate

b) Partition coefficient n-octanol/water

```
                Log Kow(version 1.67 estimate): 1.42
```

(Estimated value)

```
SMILES : O([Na])S(=O)(=O)OCCOCCCCCCCCCCCC
CHEM   :
MOL FOR: C14 H29 O5 S1 Na1
MOL WT : 332.43
```

Program and version used

```
---------- KOWwin v1.67 Results ----------

-------+----+-----------------------------------------+--------+-------
 TYPE  | NUM |        LOGKOW FRAGMENT DESCRIPTION       |  COEFF  |  VALUE
-------+----+-----------------------------------------+--------+-------
 Frag  |  1  |  -CH3    [aliphatic carbon]              | 0.5473  |  0.5473
 Frag  | 13  |  -CH2-   [aliphatic carbon]              | 0.4911  |  6.3843
 Frag  |  2  |  -O-     [oxygen, aliphatic attach]      |-1.2566  | -2.5132
 Frag  |  1  |  -O-SO2-O-     [sulfate, linear]         | 1.3500  |  1.3500
 Factor|  1  |  S-O-{Na,K,Li}   [coef*(1.3*(NUM-1))]   |-4.5800  | -4.5800
 Const |     |  Equation Constant                       |         |  0.2290
-------+----+-----------------------------------------+--------+-------
                                                        Log Kow   =   1.4174

-------------------------------------------------------------------------------
```

The method used to predict Kow. It is a fragment contribution method

C) Bioconcentration Factor (BCF)

```
                    Log BCF (v2.17 estimate): 1.85

SMILES : OS(=O)(=O)OCCOCCCCCCCCCCCC
CHEM   :
MOL FOR: C14 H30 O5 S1
MOL WT : 310.45
--------------------------Bcfwin v2.17 -----------------------
NOTE: Metals (Na, Li or K) are removed for BCF and log Kow evaluation!
Log Kow  (estimated)  :  2.15
Log Kow (experimental):  not available from database
Log Kow used by BCF estimates:  2.15

Equation Used to Make BCF estimate:
   Log BCF = 1.85 (Ionic; 11 or more -CH2- groups)


   Estimated Log BCF =  1.850  (BCF = 70.79)

-----------------------------------------------------------------
```

d) Soil Adsorption Coefficient (Koc/Kd)

```
                  Koc (estimated): 3.49e+003


SMILES : O([Na])S(=O)(=O)OCCOCCCCCCCCCCC
CHEM   :
MOL FOR: C14 H29 O5 S1 Na1
MOL WT : 332.43
--------------------------- PCKOCWIN v1.66 Results ------------------
NOTE: THE METAL (Na, Li or K) HAS BEEN REMOVED TO ALLOW ESTIMATION!
         First Order Molecular Connectivity Index  ..... :  9.561
         Non-Corrected Log Koc  ........................... :  5.7070
         Fragment Correction(s):
                  1   Ether, aliphatic  (-C-O-C-)  .....  : -1.2643
                  1   Miscellaneous  S(=O)  group  .....  : -0.9000
         Corrected Log Koc  ............................... :  3.5427

                        Estimated Koc:  3489

-----------------------------------------------------------------
```

e) Henry's Law Constant

Two methods used to predict Henry's Constant

```
      Bond Est :  2.86E-009 atm-m3/mole
      Group Est:  Incomplete

SMILES : O([Na])S(=O)(=O)OCCOCCCCCCCCCCCC
CHEM   :
MOL FOR: C14 H29 O5 S1 Na1
MOL WT : 332.43
-------------------------- HENRYWIN v3.10 Results -------------------------
-
----------+-----------------------------------------------+--------+---------
   CLASS  |     BOND CONTRIBUTION DESCRIPTION             | COMMENT |  VALUE
----------+-----------------------------------------------+--------+---------
 HYDROGEN |  29  Hydrogen to Carbon (aliphatic) Bonds     |         | -3.4706
 FRAGMENT |  12  C-C                                      |         |  1.3956
 FRAGMENT |   3  C-O                                      |         |  3.2564
 FRAGMENT |   2  O-S                                      | ESTIMATE|  0.4200
 FRAGMENT |   2  O=S (sulfone-type)                       | ESTIMATE|  2.1000
 FRAGMENT |   1  O-Na                                     | ESTIMATE|  3.2300
----------+-----------------------------------------------+--------+---------
 RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE     |  TOTAL  |  6.931
----------+-----------------------------------------------+--------+---------
HENRYs LAW CONSTANT at 25 deg C = 2.86E-009 atm-m3/mole
                                = 1.17E-007 unitless

--------+-----------------------------------------------+-----------+-------
        |        GROUP CONTRIBUTION DESCRIPTION         |   COMMENT  |
VALUE
--------+-----------------------------------------------+-----------+-------
        |           1  CH3 (X)                          |            | -0.62
        |          10  CH2 (C)(C)                       |            | -1.50
        |           3  CH2 (C)(O)                       |            | -0.39
        |           1  O (C)(C)                         |            |  2.93
        |              MISSING Value for:  O (Na)(S)
        |              MISSING Value for:  UNTYPED(O)
        |              MISSING Value for:  S (=O)(=O)(O)(O)
        |              MISSING Value for:  O (C)(S)
--------+-----------------------------------------------+-----------+-------
 RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  | INCOMPLETE |  0.42
--------+-----------------------------------------------+-----------+-------
```

(1)

(2)

f) Half lives-t1/2 for Hydrolysis as a function of Ph

Can not be estimated

g) Half lives-t1/2 for Photolysis (Atmospheric OH Rate Constant)

```
SMILES : O([Na])S(=O)(=O)OCCOCCCCCCCCCCCC
CHEM   :
MOL FOR: C14 H29 O5 S1 Na1
MOL WT : 332.43
------------------- SUMMARY (AOP v1.92): HYDROXYL RADICALS ------
Hydrogen Abstraction       =  31.4611 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  31.4611 E-12 cm3/molecule-sec
   HALF-LIFE =     0.340 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     4.080 Hrs

------------------ SUMMARY (AOP v1.91): OZONE REACTION ---------
```

```
                ******  NO OZONE REACTION ESTIMATION ******
                (ONLY Olefins and Acetylenes are Estimated)

Experimental Database:  NO Structure Matches

-----------------------------------------------------------------
```

h) Biodegradability

```
SMILES : O([Na])S(=O)(=O)OCCOCCCCCCCCCCCC
CHEM   :
MOL FOR: C14 H29 O5 S1 Na1
MOL WT : 332.43
--------------------------- BIOWIN v4.10 Results ------------------------
-

   Biowin1 (Linear Model Prediction)    :  Does Not Biodegrade Fast
   Biowin2 (Non-Linear Model Prediction):  Does Not Biodegrade Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks
   Biowin4 (Primary  Biodegradation Timeframe):  Days-Weeks
   Biowin5 (MITI Linear Model Prediction)    :  Not Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Not Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Biodegrades Fast
   Ready Biodegradability Prediction:  NO
```

BIOWIN contains seven separate models to predict the biodegradation.

A brief summary of each model's prediction for sodium laureth sulphate

This prediction is based on BIOWIN3 and 5 results.

```
------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  0.1084 |  0.1084
 Frag |  1  |  Aliphatic ether  [C-O-C]               | -0.3474 | -0.3474
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.1583
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  0.3504
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  1.8437 |  1.8437
 Frag |  1  |  Aliphatic ether  [C-O-C]               | -3.4294 | -3.4294
 MolWt|  *  |  Molecular Weight Parameter             |         | -4.7206
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.0357
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  0.2983 |  0.2983
 Frag |  1  |  Aliphatic ether  [C-O-C]               | -0.0087 | -0.0087
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.7346
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|         |  2.7542
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  0.2691 |  0.2691
 Frag |  1  |  Aliphatic ether  [C-O-C]               | -0.0097 | -0.0097
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.4796
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|         |  3.6274
```

Fragments used in each model to derive the estimation

BIOWIN1 and 2 Results interpretation. For example, 0.0357<0.5 so Cetylpyridinium chloride does not biodegrade fast.

```
============+==========================================+=========+=========

 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer

------+-----+------------------------------------------+---------+---------
 TYPE | NUM |       Biowin5 FRAGMENT DESCRIPTION       |  COEFF  |  VALUE
------+-----+------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic ether  [C-O-C]                |  0.0015 |  0.0015
 Frag |  1  |  Methyl  [-CH3]                          |  0.0004 |  0.0004
 Frag | 13  |  -CH2-  [linear]                         |  0.0494 |  0.6424
 MolWt|  *  |  Molecular Weight Parameter              |         | -0.9890
 Const|  *  |  Equation Constant                       |         |  0.7121
============+==========================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)|         |  0.3674
============+==========================================+=========+=========

------+-----+------------------------------------------+---------+---------
 TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION       |  COEFF  |  VALUE
------+-----+------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic ether  [C-O-C]                | -0.1071 | -0.1071
 Frag |  1  |  Methyl  [-CH3]                          |  0.0194 |  0.0194
 Frag | 13  |  -CH2-  [linear]                         |  0.4295 |  5.5834
 MolWt|  *  |  Molecular Weight Parameter              |         | -9.5970
============+==========================================+=========+=========
   RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|         |  0.1714
============+==========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable


------+-----+------------------------------------------+---------+---------
 TYPE | NUM |       Biowin7 FRAGMENT DESCRIPTION       |  COEFF  |  VALUE
------+-----+------------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]     | -0.3177 | -0.3177
 Frag |  1  |  Aliphatic ether  [C-O-C]                | -0.2573 | -0.2573
 Frag |  1  |  Methyl  [-CH3]                          | -0.0796 | -0.0796
 Frag | 13  |  -CH2-  [linear]                         |  0.0260 |  0.3379
 Const|  *  |  Equation Constant                       |         |  0.8361
============+==========================================+=========+=========
   RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob) |         |  0.5194
============+==========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast



--------------------------------------------------------------------------------
```

BIOWIN3 and 4 Results interpretation.

i) Aquatic toxicity

```
SMILES : O([Na])S(=O)(=O)OCCOCCCCCCCCCCCC
CHEM   :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C14 H29 O5 S1 Na1
MOL WT : 332.43
Log Kow: 1.42  (KowWin estimate)
Melt Pt:
Wat Sol: 5772 mg/L  (calculated)

ECOSAR v0.99h Class(es) Found
-----------------------------
Surfactants-anionic



Predicted
ECOSAR Class                 Organism            Duration  End Pt   mg/L
(ppm)
===========================  ==================  ========  ======
==========
Neutral Organic SAR        : Fish                14-day    LC50     1428.518
(Baseline Toxicity)

 Note:  * = asterisk designates: Chemical may not be soluble
        enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: none
         Green algal EC50 toxicity log Kow cutoff: none
         Chronic toxicity log Kow cutoff: none
         MW cutoff: none


--------------------------------------------------------------------------------
--
```