**Homework 3 - Estimating Biodegradation of Organic Molecules**

**Introduction**

Biodegradation is nature’s waste management and recycling system. It breaks down everything from yard waste to crude oil. It is a natural process necessary to keep our planet clean and healthy. Unfortunately, the rate at which we are producing waste far outpaces the rate of natural biodegradation, making our current state unsustainable. Not to mention that most products are not designed to degrade due to optimized chemical and physical properties for high stability and resistance to external variables. As a result, landfills have been filling up at record rates, and air, water and soil pollution is increasing. This should be no surprise to many of you. Especially since this year’s Earth Day celebration shed light into the current state of plastic waste management and its’ subsequent pollution.

Instead of focusing on end of pipe solutions, this give scientists a great opportunity to tackle this challenge be creating safer and more sustainable chemistry through the innovative paradigm that is Green Chemistry. So what is the importance of Green Chemistry and why do scientists play a vital role? For most organic compounds, biodegradation is the most important parameter influencing the toxicity, persistence, and ultimate fate in aquatic and terrestrial ecosystems. Understanding how a molecule biodegrades give scientists a powerful tool to influence how materials and products are developed in a more benign manner.

The method that will you will be using in this exercise calculates an “index” factor that characterizes aerobic biodegradation rate in ambient environments. Hence, this offers the scope of the biodegradation of organic molecules to be identified as a constant variable. The method allows a scientist to calculate a **Biodegradation Index (BI)** that correlates the structural functionality of a molecules to its potential biodegradation. By looking at an organic molecule, a quantitative numerical factor is attributed to the functional groups that are present. The method is simple to use, calculating the probability timeframe for biodegradation, and has proven to be accurate for a wide range of chemical structures[1]. For this reason, it’s well recognized for the initial screening of organic compounds to aid in the determination of relative biodegradability. Curious??

Let’s begin!!

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**Calculating the Biodegradation Index (BI)**

***Biodegradation Equation:***

***BI = 3.199 + a1f1 + a2f2 +a3f3 + …. + anfn + amMW***

|  |  |
| --- | --- |
| **Variable** | **Meaning** |
| ***an*** | **Assigned contribution factor to functional group (see attached table)** |
| ***fn*** | **# of times/frequency a functional group in a molecule** |
| ***am*** | **Molecular weight contribution factor****(-0.00221)** |
| ***MW*** | **Molecule weight of molecule**  |

**\**BI*** is an indicator of aerobic biodegradation rate. A value to ***5*** indicates the compound is expected to degrade over **HOURS.** A value of ***4*** corresponds to a biodegradation of **DAYS.** Last, values of ***3,2, or 1*** correspond to biodegradation in **WEEKS**, **MONTHS, and YEARS** respectively. These values of ***BI*** should not be viewed as an accurate quantitative predictor of biodegradation. Rather, it should be viewed as a relative ranking of the probability that compound will degrade in the assigned timeframe.

**Examples:** *Estimate the Biodegradation Index of* ***1-propanol*** *&* ***Diphenyl ether***

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**BI = 3.19 + 0.160 – 0.00221(60) = 3.22 = WEEKS/DAYS**

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 **BI = 3.19 + 2(0.022) – 0.058 – 0.00221(170) = 2.81 = WEEKS**

**Calculate the Biodegradation Index (BI) for the following compounds using the indices table on the last page.**

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Atrazine (pesticide & contains a triazine ring)

PFOA

Toluene

Benzene

**BI** = - 2.74

**BI** = 2.33

**BI** = 2.44

**BI** = 2

****

BPA

BPS

Cinnamic Acid

PFOS

**BI** =-3.11

**BI** = 2.9

**BI** =2.6

**BI** = 2.98

**Comparison of Results**

**Do you notice any observations or trends associated to the molecular functionality to biodegradation? List these observations and be ready to express your findings.**

**The following trends should be identified:**

* **Halogens increase the time of aerobic degradation on molecules**
* **Aromatic OH decrease time for degradation. This applies to carboxylic acid functional groups.**
* **Heterocyclic compounds increase time for degradation.**
* **Aromaticity increases time for degradation.**

|  |  |
| --- | --- |
| **Structural Group** | **Group Contribution (an)** |
| **Molecular Weight** |   |   | -0.00221 |
|   |   |   |   |   |   |   |
| **Functional Groups** |   |   |   |   |   |
| Unsubstituted aromatic ring | -0.586 |
| Phosphate ester | 0.154 |
| Cyanide/nitrile | -0.082 |
| Aldehyde (CHO) | 0.022 |
| Amide (C(=O)N or C(=S)N) | -0.054 |
| Aromatic (C(=O)OH) |   |   | 0.088 |
| Ester |   |   |   | 0.14 |
| Aliphatic OH |   |   | 0.16 |
| Aliphatic NH2 or NH |   |   | 0.024 |
| Aromatic ether |   |   | -0.058 |
| Unsubstituted phenyl group (C6H5) |   | 0.022 |
| Aromatic OH |   |   | 0.056 |
| Linear C4 terminal |   |   | 0.298 |
| Aliphatic sulfonic acid or salt |   | 0.193 |
| Carbamate |   |   |   | -0.047 |
| Aliphatic (C(=O)OH) |   |   | 0.367 |
| Alkyl substituent on Aromatic ring |   | -0.075 |
| Triazine ring |   |   | -0.246 |
| Ketone |   |   |   | -0.023 |
|   |   |   |   |   |   |   |

**Biodegradation Indices Tables**

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|  |  |
| --- | --- |
| **Structural Group** | **Group Contribution (an)** |
| **Molecular Weight** |   |   | -0.00221 |
|   |   |   |   |   |   |   |
| **Functional Groups** |   |   |   |   |   |
| Polycyclic aromatic |   |   | -0.799 |
| N-nitroso (NN=O) |   |   | -0.385 |
| Trifluoromethyl (CF3) |   |   | -0.513 |
| Aliphatic ether |   |   | -0.0087 |
| Aromatic NO2 |   |   | -0.17 |
| Azo group (N=N) |   |   | -0.3 |
| Aromatic NH2 or NH |   |   | -0.135 |
| Aromatic sulfonic acid or salt |   | 0.142 |
| Tertiary amine |   |   | -0.255 |
| Carbon with four single bonds and no H | -0.212 |
| Aromatic Cl |   |   |   | -0.207 |
| Pyridine ring |   |   | -0.214 |
| Aliphatic Cl |   |   |   | -0.173 |
| Aromatic Br |   |   |   | -0.136 |
| Aliphatic Br |   |   |   | 0.029 |
| Aromatic F |   |   |   | -0.407 |
| Aromatic I |   |   |   | -0.045 |
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