Comparing biodegradability of molecules using Biowin

The goal of the waste presentation is to give participants an understanding of different approaches to deal with waste, and more importantly how to “design” waste if possible. One way to design waste is to build in biodegradation potential to the molecule so that when it undergoes degradation, the microbes can biodegrade it quickly and efficiently.

This exercise compares an output from publically available software, BIOWIN, for four distinct chemical groups. The program analyses the chemical structure of each molecule within the group, and assesses its biodegradation potential based on the molecule fragment and functional groups. The result is presented as a probability for degradation. If the number is greater or equal to 0.5, then the molecule will degrade faster. In contrast, values less than 0.5 indicate persistence and low biodegradation potential.

Each probability score consists of individual values for characteristic molecule fragments that make up the molecule. These individual values also indicate if the given fragment or a functional group contributes to or interferes with biodegradation. For example:

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	8	Aromatic alcohol [-OH]	0.4884	3.9074
Frag	6	Aromatic-H	0.1201	0.7208
MolWt	*	Molecular Weight Parameter		-11.7309
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0102

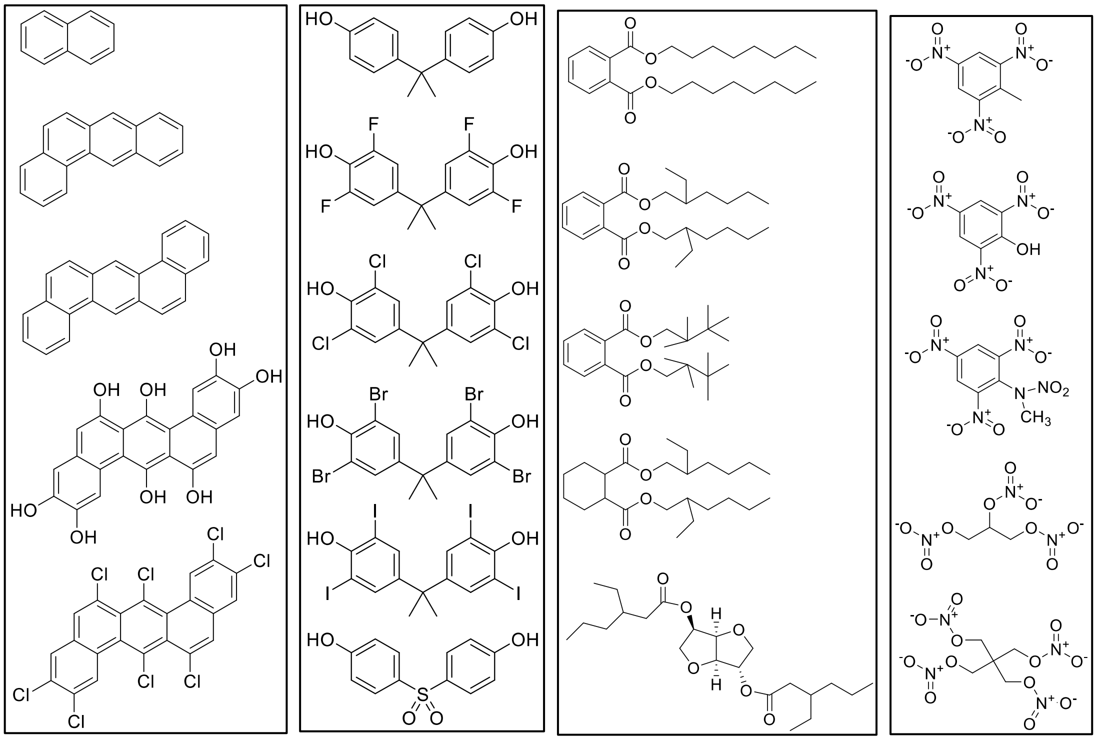
The biodegradation probability for that molecule is 0.0102. Given that the number is less than 0.5, it is safe to assume there is a low biodegradation potential for that molecule. However, parts of that molecule are biodegradable. Aromatic alcohol [–OH] had a value of 3.90, and improves the overall score.

In this exercise, participants will be given 4 groups of molecules

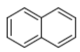
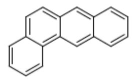
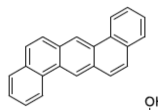
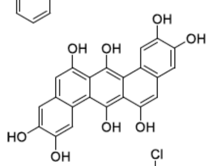
1. Ring structures
2. Bisphenol A derivatives
3. Plasticizers
4. Explosives

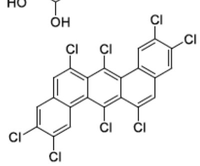
Based on BIOWIN 6 (aerobic biodegradation) and BIOWIN 7 (anaerobic biodegradation) output (these are provided), participants should:

- Predict which of the structures will or will not biodegrade.
- Rank the structures from most biodegradable to least biodegradable.
- Make a list of structures and functional groups, which favors and disfavors biodegradation.



TEAM 1

1. 
2. 
3. 
4. 

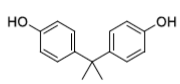
5. 

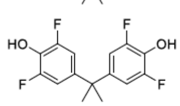
Increasing number of rings & molecular weight

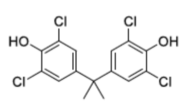
Favors biodegradation	**Disfavors biodegradation**
- OH - Low molecular weight	- High molecular weight - Cl

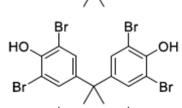
Most biodegradable (aerobic)	1>2>4>3>5	Least biodegradable
Most biodegradable (anaerobic)	4>1>2>3>5	Least biodegradable

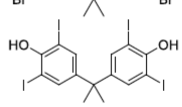
TEAM 2

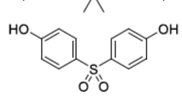
1. 

2. 

3. 

4. 

5. 

6. 

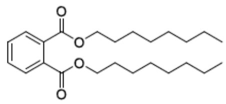
Poor biodegradation due to high MW (2–5)

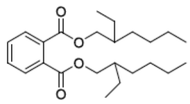
Bisphenol A derivatives: Halogenated and BPS

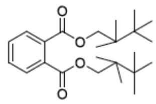
Favors biodegradation	**Disfavors biodegradation**
- Low molecular weight	- High molecular weight - Tertiary carbon BPA - Halogens, but F better than Cl

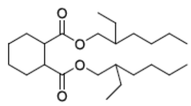
Most biodegradable (aerobic)	1>6>3>4>2>5	Least biodegradable
Most biodegradable (anaerobic)	6>2>4=5>3>1	Least biodegradable

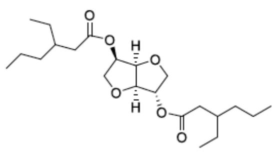
TEAM 3

1. 

2. 

3. 

4. 

5. 

Different plasticizers

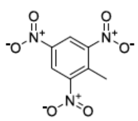
Linear and branched;
Two green plasticizers: Reduced ring to cyclo and isosorbide ring

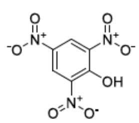
Favors biodegradation	**Disfavors biodegradation**
- Linear chains	- Side chains and branching
- Cyclo	- Ethers
- Esters	

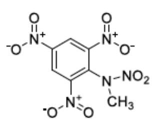
Most biodegradable (aerobic) 1>4>2>3>5 Least biodegradable

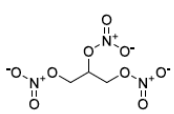
Most biodegradable (anaerobic) 1>5>2>4>3 Least biodegradable

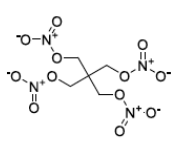
TEAM 4

1. 

2. 

3. 

4. 

5. 

Degrades faster due to small MW (4 and 5)

Explosives (TNT, nitroglycerine)

Favors biodegradation	**Disfavors biodegradation**
- Small molecular weight	- CH_3
- OH	- Large MW
	- NNO_2CH_3

Most biodegradable (aerobic) 4>5>1=2=3 Least biodegradable

Most biodegradable (anaerobic) 4>5>2>1>3 Least biodegradable