CLASSIFICATION OF CHEMICAL BIODEGRADATION

TEAM - 3

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Problem Statement

Background:

Non-biodegradable substances can remain in ecosystems without degrading, and if the chemical's effects are not fully understood, detrimental repercussions may occur at some point. These negative consequences can endure indefinitely and have an influence on wildlife and human health

Problem:

- Increased regulation is making non biodegradable chemicals harder to get to market
- Is there a cost effective way to determine biodegradability without extensive chemical testing?

Solution:

Develop a systematic predictive model to determine biodegradability based solely on existing data of molecular attributes

(Boethling et al., 2007)

Problem Approach

What are Ready Biodegradable (RB) and Non-Ready biodegradable (NRB) variables?

- Ready Biodegradable consistent of chemicals that are capable of decomposing.
- Non Ready Biodegradable do not decompose and can linger for an indefinite amount of time.

How the analysis was done?

- Used existing data with generally available modeling techniques.
- Working towards a simplified model relative to published techniques which in general had a better balance of prediction for both those chemicals that are ready biodegradability and those that are not.
- Looking to achieve better results with less resources to maintain.

Results

- Determined relationships between chemical attributes that enable prediction of non biodegradable.
- Improved upon published results (~40% improvement in correctly identifying a chemical biodegradability status).
- Specialized methods were not required.

Conclusion

- Investigated the chemical attributes to understand the degradation mechanism
- Found a method that would require less time and funding to get to production
  - Chemicals can be identified early into research/development phase, which would make effective use of a limited funding budget
  - Researchers can utilize our model to find more insights about their specified chemicals
- 1 out of a 100 chemicals may be misidentified, but when used with current chemical analysis that ratio may be further reduced

References

Boethling, R. S., Sommer, E., & DiFiore, D. (2007). Designing small molecules for biodegradability. *Chemical Reviews*, *107*(6), 2207–2227. https://doi.org/10.1021/cr050952t