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Biodegradation Model

Understanding biodegradation of chemicals in the environment is becoming increasingly important. There are several assays available to determine if a compound is biodegradable. Cheng (Cheng 2012) provided data and references for a set of 1,604 compounds that have undergone either the Japanese MITI (14 day) or the OECD 301C (28 day). After removing all metal containing compounds and retaining only a single stereoisomer or tautomer of structurally redundant entries, 1,581 compounds remained.

Under both protocols, the compound of interest is mixed with sludge from several different geographical locations then oxygen consumption is measured for the specified period of time. Biological oxygen demand (BOD) and percent biodegradation are calculated from the following equations:

$$\mathrm{BOD} = \frac{[\mathrm{O2\ uptake\ by\ test\ substance}] - [\mathrm{O2\ uptake\ by\ blank}]}{[\mathrm{amount\ of\ test\ substance}]}$$

The percentage biodegradation is obtained from:

$$\%\mathrm{biodegradation} = \frac{\mathrm{BOD}}{\mathrm{ThOD}} * 100\%$$

where ThOD represents the amount of oxygen consumed in converting all of the compound to carbon dioxide (CO_2), i.e., the theoretical oxygen demand. A compound was categorized as a positive (readily biodegradable) if %biodegradation is greater than or equal to 60% and as a negative otherwise. The model returns a "Yes" or "No" answer to the question: is this compound readily biodegradable?

Approximately 22% of the 1,581 compound data set was set aside as an external test set. The remaining 1,235 compounds were used as the training pool from which a 16 descriptor, 6 neuron artificial neural network ensemble was built. The model's sensitivity and specificity exceeded 82% on both the training pool and external data set.

Model	Set	Negatives	Positives	Total	Correct	Concordance	Sensitivity	Specificity
TOX_BIODEG	Training Pool	796	439	1235	1045	84.6%	82.5%	85.8%
	Test	202	144	346	289	83.5%	84.7%	82.7%

References

Cheng F, Ikenaga Y, Zhou Y, Yu Y, Li W, Shen J, Du Z, Chen L, Xu C, Liu G, Lee PW, Tang Y. "In silico assessment of chemical biodegradability." *J Chem Inf Model* **2012**; 52:655-669.