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Technical Report

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Classification Models for Ready Biodegradability

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Contents

1	Introduction	3
2	Materials and Methods	4
2.1	Data Set Construction	4
2.2	Calculation of Molecular Descriptors	4
2.3	Calculation of Molecular Fingerprints	4
2.4	Modeling Methods	4
2.5	Definition of Model Applicability Domain	4
2.6	Privileged Substructures Analysis	4
2.7	Performance Evaluation of Models	4
3	Results	5
3.1	Chemical Space Analysis	5
3.2	Performance of Descriptor-Based Models	5
3.3	Performance of Fingerprint-Based Models	5
3.4	Role of the Applicability Domain (AD)	5
3.5	Privileged Substructure for Chemical Biodegradation	5
4	Discussion	6
4.1	Comparison of Different Modeling Methods	6
4.2	Diversity of the Data Set	6
4.3	Relevance of Selected Chemical Descriptors to the Biodegradability Mechanism	6
4.4	Visual Analysis of Substructure Alerts for Chemical Biodegradation	6
5	Conclusion	7
6	Associated Content	8
7	References	9

Chapter 1

Introduction

Chapter 2

Materials and Methods

2.1 Data Set Construction

2.2 Calculation of Molecular Descriptors

2.3 Calculation of Molecular Fingerprints

2.4 Modeling Methods

2.5 Definition of Model Applicability Domain

2.6 Privileged Substructures Analysis

2.7 Performance Evaluation of Models

Chapter 3

Results

3.1 Chemical Space Analysis

3.2 Performance of Descriptor-Based Models

3.3 Performance of Fingerprint-Based Models

3.4 Role of the Applicability Domain (AD)

3.5 Privileged Substructure for Chemical Biodegradation

Chapter 4

Discussion

- 4.1 Comparison of Different Modeling Methods
- 4.2 Diversity of the Data Set
- 4.3 Relevance of Selected Chemical Descriptors to the Biodegradability Mechanism
- 4.4 Visual Analysis of Substructure Alerts for Chemical Biodegradation

Chapter 5

Conclusion

Chapter 6

Associated Content

Chapter 7

References