

Article

Comparative Prediction of Gas Chromatographic Retention Indices for GC/MS Identification of Chemicals Related to Chemical Weapons Convention by Incremental and Machine Learning Methods

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Abstract: During on-site verification activities conducted by the Technical Secretariat of Organization for the Prohibition of Chemical Weapons, identification by gas chromatography retention indices (RI) data, in addition to mass spectrometry data, increase the reliability of factual findings. However, reference RIs do not cover all the possible chemical structures. That is why it is important to have models to predict RIs. Applicable only for narrow data sets of chemicals with a fixed scaffold (G- and V-series gases as example), the non-learning incremental method demonstrated predictive median absolute and percentage errors of 2–4 units and 0.1–0.2%; these are comparable with the experimental bias in RI measurements in the same laboratory with the same GC conditions. It outperforms the accuracy of two reported machine learning methods—median absolute and percentage errors of 11–52 units and 0.5–2.8%. However, for the whole Chemical Weapons Convention (CWC) data set of chemicals, when a fixed scaffold is absent, the incremental method is not applicable; essential machine learning methods achieved accuracy: median absolute and percentage errors of 29–33 units and 0.5–2.2%, depending on the machine learning method. In addition, we have developed a homology tree approach as a convenient method for the visualization of the CWC chemical space. We conclude that non-learning incremental methods may be more accurate than the state-of-the-art machine learning techniques in particular cases, such as predicting the RIs of homologues and isomers of chemicals related to CWC.

Keywords: gas chromatography; retention indexes; database; predictions; machine learning; deep learning



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1. Introduction

Gas chromatography (GC) is one of the core analytical methods recommended for the analysis of chemicals related to the Chemical Weapons Convention (CWC) [1]. GC hyphenated with electron ionization mass spectrometry (GC/MS) is a predominant experimental technique established by the Technical Secretariat of Organization for the Prohibition of Chemical Weapons (OPCW) for factual findings during on-site verification activities with sampling and analysis. The chemicals that have been identified for the application of verification measures are listed in the schedules contained in the Annex on Chemicals. In the sense of the Chemical Weapons Convention, Schedule 1 substances are chemicals that can either be used as chemical weapons themselves or used in the manufacture of chemical weapons; and which have no, or very limited, uses outside of chemical warfare.

Gas Chromatographic Retention Data

Christian Drosten



Gas Chromatographic Retention Data:

The book delves into Gas Chromatographic Retention Data. Gas Chromatographic Retention Data is a vital topic that needs to be grasped by everyone, ranging from students and scholars to the general public. This book will furnish comprehensive and in-depth insights into Gas Chromatographic Retention Data, encompassing both the fundamentals and more intricate discussions.

1. The book is structured into several chapters, namely:
 - Chapter 1: Introduction to Gas Chromatographic Retention Data
 - Chapter 2: Essential Elements of Gas Chromatographic Retention Data
 - Chapter 3: Gas Chromatographic Retention Data in Everyday Life
 - Chapter 4: Gas Chromatographic Retention Data in Specific Contexts
 - Chapter 5: Conclusion
2. In chapter 1, this book will provide an overview of Gas Chromatographic Retention Data. The first chapter will explore what Gas Chromatographic Retention Data is, why Gas Chromatographic Retention Data is vital, and how to effectively learn about Gas Chromatographic Retention Data.
3. In chapter 2, this book will delve into the foundational concepts of Gas Chromatographic Retention Data. The second chapter will elucidate the essential principles that must be understood to grasp Gas Chromatographic Retention Data in its entirety.
4. In chapter 3, this book will examine the practical applications of Gas Chromatographic Retention Data in daily life. The third chapter will showcase real-world examples of how Gas Chromatographic Retention Data can be effectively utilized in everyday scenarios.
5. In chapter 4, this book will scrutinize the relevance of Gas Chromatographic Retention Data in specific contexts. This chapter will explore how Gas Chromatographic Retention Data is applied in specialized fields, such as education, business, and technology.
6. In chapter 5, the author will draw a conclusion about Gas Chromatographic Retention Data. The final chapter will summarize the key points that have been discussed throughout the book.

The book is crafted in an easy-to-understand language and is complemented by engaging illustrations. It is highly recommended for anyone seeking to gain a comprehensive understanding of Gas Chromatographic Retention Data.

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