



# CAFFEINE EXTRACTION AND CHARACTERIZATION

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## ABSTRACT

Caffeine extracted and characterised from tea (black) leaves and coffee beans. Isolation was done by liquid-liquid extraction using di-chloromethane as an extracting agent. This extraction was done in four steps: steeping, evaporation, liquid-liquid extraction and recrystallization. The recrystallization was done using anhydrous sodium sulphate. The technique used for purity analysis and characterization were: High performance liquid chromatography, Differential scanning calorimeter, Fourier transform infrared spectroscopy and Melting point. First, the analysis was done using melting point analysis. The melting point of caffeine extracted from coffee beans and tea leaves was found to be 238°C. The absorption bands were compared with that available in literature and were found to be similar. Further, the purity check was done using High performance liquid chromatography method. Effective characterization of caffeine was achieved by determining Infrared spectrum, and employing a melting point apparatus and differential scanning calorimeter. The purity showed that the results that the extracted coffee was 90% pure. Further improvements in extraction efficiency will increase the yield and minimize wastage.

**Key Words:** Caffeine, Methyl xanthine, Theophylline, Differential scanning calorimeter, Fourier transform infrared spectroscopy, High performance liquid chromatography

## INTRODUCTION

Caffeine is a psychoactive CNS stimulant drug discovered by German chemist Friedrich Ferdinand Runge in 1819. He coined the term "Kaffein" which became Caffeine<sup>1</sup>. Caffeine is a methyl xanthine along with theophylline and theobromine. It is a natural pesticide. Caffeine does not counteract the effects of alcohol. Caffeine is a xanthine alkaloid compound that acts as a stimulant in humans. It is a central nervous stimulant, having the effect of temporarily warding off drowsiness and restoring alertness.<sup>2</sup> Every time we drink tea, coffee, cocoa, chocolate or cola we are giving our body a "hit" of caffeine. Along with nicotine and alcohol, caffeine is one of the three most widely used mood – affecting drugs in the world<sup>3</sup>.

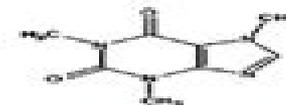
## OBJECTIVES

1. To extract caffeine from tea leaves and coffee beans by liquid-liquid extraction method.
2. To characterize the obtained caffeine by melting point, Infrared spectroscopy and Differential scanning calorimeter method.

3. To develop an easily adaptable method for the qualitative or purity analysis of caffeine

## PHYSICAL AND CHEMICAL PROPERTIES

Caffeine is sparingly soluble in most polar solvents but is highly soluble in less polar solvents. The melting point is 234°C-239°C and the chemical formula is C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>. It is an intensely bitter, white powder in its pure state. Caffeine is an alkaloid of the methylxanthine family, which also includes the similar compounds theophylline and theobromine<sup>3</sup>. The structure of caffeine is



## ADMET OF CAFFEINE

### Absorption & Distribution

Caffeine is absorbed orally with a max blood peak after 120 mins spreading quickly in all tissues. Caffeine is

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# Caffeine Extraction And Characterization

**Padhraic Smyth**



## **Caffeine Extraction And Characterization :**

**Direct Analysis in Real Time Mass Spectrometry** Yiyang Dong, 2018-04-09 Clear comprehensive and state of the art the groundbreaking book on the emerging technology of direct analysis in real time mass spectrometry Written by a noted expert in the field Direct Analysis in Real Time Mass Spectrometry offers a review of the background and the most recent developments in DART MS Invented in 2005 DART MS offers a wide range of applications for solving numerous analytical problems in various environments including food science forensics and clinical analysis The text presents an introduction to the history of the technology and includes information on the theoretical background for example on the ionization mechanism Chapters on sampling and coupling to different types of mass spectrometers are followed by a comprehensive discussion of a broad range of applications Unlike most other ionization methods DART does not require laborious sample preparation as ionization takes place directly on the sample surface This makes the technique especially attractive for applications in forensics and food science Comprehensive in scope this vital text Sets the standard on an important and emerging ionization technique Thoroughly discusses all the relevant aspects from instrumentation to applications Helps in solving numerous analytical problems in various applications for example food science forensics environmental and clinical analysis Covers mechanisms coupling to mass spectrometers and includes information on challenges and disadvantages of the technique Academics analytical chemists pharmaceutical chemists clinical chemists forensic scientists and others will find this illuminating text a must have resource for understanding the most recent developments in the field **Sustainable**

**Production of Bioactive Pigments** Wee Sim Choo, Laurent Dufossé, Lourdes Morales-Oyervides, 2021-05-24 Microbial

Bioprocessing of Agri-food Wastes Gustavo Molina, Minaxi Sharma, Rachid Benhida, Vijai Kumar Gupta, Ramesh Chander Kuhad, 2023-06-16 This book gives a comprehensive overview of recent advances in the valorization of agri food waste and discusses the main process conditions needed to overcome the difficulties of using waste as alternative raw materials It also discusses specific methodologies opportunistic microbes for biomass valorization the sustainable production of agri food waste as well as examines the assessment and management of bioactive molecules production from microbial valorization of agri food waste The authors provide technical concepts on the production of various bio products and their commercial interest including agri food waste utilization in the microbial synthesis of proteins the valorization of horticulture waste the sustainable production of pectin via microbial fermentation as well as other food and pharmacological applications This book is intended for bioengineers biologists biochemists biotechnologists microbiologists food technologists enzymologists and related professionals and researchers Explores recent advances in the valorization of agri food waste Provides technical concepts on the production of various bio products of commercial interest Discusses the main process conditions to overcome the difficulties of using waste as alternative raw materials Introduces technical economic details on the advantages and disadvantages of exploring the waste recovery chain Explores the main technological advances in the recovery of residues in

functional products     *Handbook of Coffee Processing By-Products* Charis M. Galanakis,2017-05-05 Handbook of Coffee Processing By Products Sustainable Applications presents alternative and sustainable solutions for coffee processing by products and specifies their industrial potential both as a source for the recovery of bioactive compounds and their reutilization in the pharmaceutical biotechnological food biotechnology and cosmetic industries also covering environmental and agronomic applications This book addresses key topics specific to sustainable management in the coffee industry placing an emphasis on integrated solutions for the valorization and upgrade of coffee processing by products biorefinery and different techniques for the separation extraction recovery and formulation of polyphenols Specifies potential for the use of by products as a source for the recovery of bioactive compounds and their reutilization in the pharmaceutical biotechnological food biotechnology and cosmetic industries Places emphasis on integrated solutions for the valorization and upgrade of coffee processing by products biorefinery and different techniques for the separation extraction recovery and formulation of polyphenols     **Achieving sustainable cultivation of coffee** Dr Philippe Lashermes,2018-01-09 Covers recent research on coffee genetics physiology and genetic diversity Reviews the latest developments in breeding new varieties Assesses advances in measuring and understanding the chemical composition and nutraceutical properties of coffee

**Coffee: From the Field to the Cup** Paulo Mazzafera,Sara Adrián López de Andrade,Sarada Krishnan,Herminia Prieto Martinez,Maria Beatriz A. Gloria,2022-08-08     *Coffee in Health and Disease Prevention* Victor R Preedy,2014-11-12 Coffee in Health and Disease Prevention presents a comprehensive look at the compounds in coffee their reported benefits or toxicity risks and also explores them on a health condition specific level providing researchers and academics with a single volume resource to help in identifying potential treatment uses No other book on the market considers all the varieties of coffee in one volume or takes the disease focused approach that will assist in directing further research and studies The book embraces a holistic approach and effectively investigates coffee and its specific compounds from the biochemical to the nutritional well being of geographical populations This book represents essential reading for researchers in nutrition dietetics food science biochemistry and public health Presents one comprehensive translational source for all aspects of how coffee plays a role in disease prevention and health Experts in nutrition diet and food chemistry from all areas of academic and medical research take readers from the bench research cellular and biochemical mechanisms of vitamins and nutrients to new preventive and therapeutic approaches Focuses on coffee composition nutritional aspects of coffee protective aspects of coffee related compounds specific coffee components and their effects on tissue and organ systems Features sections on both the general effects of coffee consumption on the body as well as the effects of specific coffee compounds on specific organ systems     **Food Science and Technology Abstracts** ,1986 Monthly References from world literature of books about 1000 journals and patents from 18 selected countries Classified arrangement according to 18 sections such as milk and dairy products eggs and egg products and food microbiology Author subject indexes     **Molecular and Computational**

**Characterization of Translation in Zea Mays L.** Alan John Williams,2001      Tea in Health and Disease Prevention Victor R Preedy,Vinood Patel,2024-09-14 While there is a nearly universal agreement that drinking tea can benefit health information on the benefits or adverse effects of drinking tea is scattered leaving definitive answers difficult to ascertain *Tea in Health and Disease Prevention* Second Edition once again addresses this problem bringing together all the latest and most relevant information on tea and its health effects into one comprehensive resource This book covers compounds in black green and white teas and explores their health implications first more generally then in terms of specific organ systems and diseases With over 75% brand new content this fully reorganized updated edition covers a wider range of tea varieties and beneficial compounds found in tea such as epigallocatechin gallate and antioxidants *Tea in Health and Disease Prevention* Second Edition is an organized efficient resource that will help readers find quick answers to questions and will help inspire further studies for those interested in tea research This is a must have reference for researchers in food science and nutrition as well as nutritionists and dieticians Covers and compares features benefits and potential negative effects of the most important types of tea including green black and white Identifies therapeutic benefits of teas for new product development Offers a one stop shop for research in this area compiling both foundational and cutting edge topics into one resource Includes a dictionary of key terms other health effects of tea or extracts and a summary point section within each chapter for a quick reference

**Methods in Polyphenol Analysis** Celestino Santos-Buelga,Gary Williamson,2003 Polyphenols make a vital contribution to the colour tanning taste and astringency of so many of society s favourites from the unique taste of the British cup of tea to a glass of red wine Found widely in many foods of plant origin polyphenols are also becoming increasingly recognised as antioxidants in the body with action on long term health and reduction in the risk of chronic disease Due to the importance of polyphenols it is vital to conduct accurate and sensitive analysis Providing detailed state of the art research presented in a practical and effective way *Methods in Polyphenol Analysis* looks at the latest techniques in this developing field and includes among others New modern techniques such as LC MS LC NMR and LC coulometric detection Chemical and enzymatic synthesis of polyphenol conjugates and Characterization of oligomeric and polymeric tannins and complex polyphenols This timely publication is written by highly experienced practitioners in this field and will be invaluable to all academics and industrialists involved in phytochemistry biochemistry and food science

*Caffeinated Beverages* Thomas H. Parliment,Chi-Tang Ho,Peter Schieberle,2000 This book provides a comprehensive overview of the recent developments in the flavor and chemistry of caffeinated beverages It includes an update on the chemistry and flavor research on coffee tea and cocoa specifically addressing antioxidative phenolic compounds found in the beverages and an examination of the health benefits such as the anticancer anti aging and heat disease prevention properties of these beverages

**Quantitative Chemical Analysis** Daniel C. Harris,2010-04-30 The most widely used analytical chemistry textbook in the world Dan Harris s *Quantitative Chemical Analysis* provides a sound physical understanding of the principles

of analytical chemistry showing how these principles are applied in chemistry and related disciplines especially in life sciences and environmental science As always the new edition incorporates real data spreadsheets and a wealth of applications in a witty personable presentation that engages students without compromising the depth necessary for a thorough and practical understanding of analytical chemistry

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**Microscale Organic Laboratory** Dana W. Mayo, Ronald M. Pike, Samuel S. Butcher, 1989 A comprehensive coverage of organic chemistry experiments and techniques using milligram scale compared to the traditional multigrams scale The text is divided into seven chapters with the bulk of the techniques appearing in the first five chapters which represents one term of work Additional pre lab discussions and post lab questions and reports are included

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## Adopting the Beat of Expression: An Mental Symphony within **Caffeine Extraction And Characterization**

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