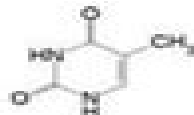




1. Cytosine
log P = -1.13



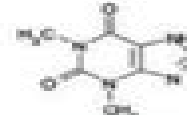
2. Hypoxanthine
log P = -1.99



3. Thymine
log P = -2.09



4. Theobromine
log P = -2.08



5. Theophylline
log P = -0.17



6. Caffeine
log P = -0.13

RPLC: 1 → 6 Elution Order



Column: ACE Excel C18, 150 x 4.6 mm, 5 μ m. Part number: EXL-121-15-00U. Mobile Phase: 0.1 % acetic acid in 95:5 v/v H₂O:MeCN. Flow Rate: 1.0 mL/min. Temperature: 22 °C. Detection: 254 nm. Injection: 5 μ L.

HILIC: 6 → 1 Elution Order



Column: ACE HILIC-N (neutral character phase), 150 x 4.6 mm, 5 μ m. Part number: HILN-5-15-00U. Mobile Phase: 0.1 % acetic acid in 5:95 v/v H₂O:MeCN. Flow Rate: 1.0 mL/min. Temperature: 22 °C. Detection: 254 nm. Injection: 5 μ L.

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HPLC and UHPLC for Practicing Scientists Michael W. Dong, 2019-07-10 A concise yet comprehensive reference guide on HPLC UHPLC that focuses on its fundamentals latest developments and best practices in the pharmaceutical and biotechnology industries Written for practitioners by an expert practitioner this new edition of HPLC and UHPLC for Practicing Scientists adds numerous updates to its coverage of high performance liquid chromatography including comprehensive information on UHPLC ultra high pressure liquid chromatography and the continuing migration of HPLC to UHPLC the modern standard platform In addition to introducing readers to HPLC s fundamentals applications and developments the book describes basic theory and terminology for the novice and reviews relevant concepts best practices and modern trends for the experienced practitioner HPLC and UHPLC for Practicing Scientists Second Edition offers three new chapters One is a standalone chapter on UHPLC covering concepts benefits practices and potential issues Another examines liquid chromatography mass spectrometry LC MS The third reviews at the analysis of recombinant biologics particularly monoclonal antibodies mAbs used as therapeutics While all chapters are revised in the new edition five chapters are essentially rewritten HPLC columns instrumentation pharmaceutical analysis method development and regulatory aspects The book also includes problem and answer sections at the end of each chapter Overviews fundamentals of HPLC to UHPLC including theories columns and instruments with an abundance of tables figures and key references Features brand new chapters on UHPLC LC MS and analysis of recombinant biologics Presents updated information on the best practices in method development validation operation troubleshooting and maintaining regulatory compliance for both HPLC and UHPLC Contains major revisions to all chapters of the first edition and substantial rewrites of chapters on HPLC columns instrumentation pharmaceutical analysis method development and regulatory aspects Includes end of chapter quizzes as assessment and learning aids Offers a reference guide to graduate students and practicing scientists in pharmaceutical biotechnology and other industries Filled with intuitive explanations case studies and clear figures HPLC and UHPLC for Practicing Scientists Second Edition is an essential resource for practitioners of all levels who need to understand and utilize this versatile analytical technology It will be a great benefit to every busy laboratory analyst and researcher

Hydrophilic Interaction Chromatography Bernard A. Olsen, Brian W. Pack, 2013-01-22 Discover how to use HILIC to analyze and better understand polar compounds An increasingly popular analytical method hydrophilic interaction chromatography HILIC has the ability to retain and separate polar compounds that are often difficult to analyze by reversed phase high performance liquid chromatography HPLC or other analytical methods Offering a comprehensive review this book enables readers to develop a fundamental understanding of how HILIC works and then apply that knowledge to develop and implement a variety of practical applications Hydrophilic Interaction Chromatography begins with discussions of HILIC retention mechanisms stationary phases and general method development This sets the foundation for the book s extensive coverage of applications

The authors address unique separation challenges for bioanalytical environmental pharmaceutical and biochemical applications Moreover there is a thorough discussion of HILIC in two dimensional chromatography With contributions from leading analytical scientists who have extensive experience in HILIC as well as HPLC Hydrophilic Interaction Chromatography serves as a practical guide for researchers featuring Detailed examples of HILIC methods and development approaches Thorough explanations of retention mechanisms and the impact of stationary phase and mobile phase properties on separations Step by step guidance for developing efficient sensitive and robust HILIC methods References to the primary literature at the end of each chapter Hydrophilic Interaction Chromatography is written for scientists who use or develop analytical methods for the separation of polar compounds In particular these researchers will discover how HILIC can be used to analyze and better understand the composition of pharmaceutical bioanalytical biochemical chemical food and environmental samples

Handbook of Advanced Chromatography /Mass Spectrometry Techniques Michal Holcapek,Wm. Craig Byrdwell,2017-09-07 Handbook of Advanced Chromatography Mass Spectrometry Techniques is a compendium of new and advanced analytical techniques that have been developed in recent years for analysis of all types of molecules in a variety of complex matrices from foods to fuel to pharmaceuticals and more Focusing on areas that are becoming widely used or growing rapidly this is a comprehensive volume that describes both theoretical and practical aspects of advanced methods for analysis Written by authors who have published the foundational works in the field the chapters have an emphasis on lipids but reach a broader audience by including advanced analytical techniques applied to a variety of fields Handbook of Advanced Chromatography Mass Spectrometry Techniques is the ideal reference for those just entering the analytical fields covered but also for those experienced analysts who want a combination of an overview of the techniques plus specific and pragmatic details not often covered in journal reports The authors provide in one source a synthesis of knowledge that is scattered across a multitude of literature articles The combination of pragmatic hints and tips with theoretical concepts and demonstrated applications provides both breadth and depth to produce a valuable and enduring reference manual It is well suited for advanced analytical instrumentation students as well as for analysts seeking additional knowledge or a deeper understanding of familiar techniques Includes UHPLC HILIC nano liquid chromatographic separations two dimensional LC MS LCxLC multiple parallel MS 2D GC GCxGC methodologies for lipids analysis and more Contains both practical and theoretical knowledge providing core understanding for implementing modern chromatographic and mass spectrometric techniques Presents chapters on the most popular and fastest growing new techniques being implemented in diverse areas of research

The Encyclopedia of Mass Spectrometry: Hyphenated methods Michael L. Gross,R. M. Caprioli,2003

The Encyclopedia of Mass Spectrometry Michael L. Gross,Wilfried Niessen,R. M. Caprioli,2006-10-30 Presents information on the biographies of recognized pioneers and innovators in the field of mass spectrometry Highlights over 120 innovators in mass spectrometry including several Nobel Prize winners Discusses instrumentation and their uses also

providing interesting information on the careers characters and life stories of the people who did the work Offers unique insight into the careers and personalities of luminaries in the field

Protein Digestion-Derived Peptides Cristina Martinez-Villaluenga, Blanca Hernandez-Ledesma, 2024-04-12 Protein Digestion Derived Peptides Chemistry Bioactivity and Health Effects presents the latest international advances in fundamental and applied research on the impact of gastrointestinal digestion on the release of bioactive peptides from food sources This book covers the fundamentals and applications of gastrointestinal digestion and absorption models as well as the impact of food matrices their components and protein characteristics and peptide bioaccessibility and bioavailability released during digestion Developed for nutrition researchers food scientists and pharmaceutical scientists this book is sure to be a welcomed for those who wish to understand the impact of peptides on chronic disease Includes applications literature reviews recent developments and methods Offers an overview of the main bioactivities of peptides released during the gastrointestinal digestion of food proteins Highlights mechanisms of action and health benefits of bioactive peptides released during gastrointestinal digestion

Analytical Methods for Environmental Contaminants of Emerging Concern Nuria Fontanals, Rosa Maria Marce, 2022-05-02 Analytical Methods for Environmental Contaminants of Emerging Concern Provides the analytical methodology required to detect different families of organic compounds of emerging concern CECs from environmental samples Most contaminants of emerging concern CECs such as pharmaceuticals personal care products pesticides sunscreens perfluorinated compounds and microplastics have been present in the environment for years yet some have only recently been identified and many of these organic compounds remain unregulated Analytical methods have been developed to determine the toxicity and risk of different families of CECs Analytical Methods for Environmental Contaminants of Emerging Concern presents the methods currently available to determine families of organic CECs in environmental samples Each section of the book is devoted to a particular family of CECs covering different analytical methods supported by examples of both cutting edge research and commonly used methods An international panel of experts describes every step of the analytical procedures including sample preparation chromatographic separation coupled to mass spectrometry or other instrumental techniques Specific requirements are linked to the properties of the contaminants and the sample matrix for each procedure presented Throughout the book in depth case studies of analytical procedures for CEC extraction separation and determination are presented to help readers transfer the analytical methods to their laboratories Provides detailed descriptions of various approaches for determining each group of CECs in environmental samples Covers different types of aqueous solid and atmospheric samples Includes up to date information on CEC properties relevant legislation reported or potential metabolites transformation products and environmental occurrence Addresses CECs such as novel psychoactive substances artificial sweeteners musk fragrances disinfection byproducts and microplastics Offers practical tips and advice on special care procedures to assist readers in CEC determination Analytical Methods for Environmental

Contaminants of Emerging Concern is an essential reference and guide for advanced students and researchers in analytical chemistry and science environmental science forensic science and specialized subjects related to analytical chemistry

Handbook of Food Analysis - Two Volume Set Leo M.L. Nollet,Fidel Toldra,2015-06-10 Updated to reflect changes in the industry during the last ten years The Handbook of Food Analysis Third Edition covers the new analysis systems optimization of existing techniques and automation and miniaturization methods Under the editorial guidance of food science pioneer Leo M L Nollet and new editor Fidel Toldra the chapters take an in **Biological Chemistry Hoppe-Seyler** ,1992

Journal of Chromatography ,1997 **American Laboratory** ,2007 Federation Proceedings ,1985 **UHPLC in Life Sciences** Davy Guillardme,Jean-Luc Veuthey,2012 Since its commercial introduction in 2004 UHPLC Ultra High Performance Liquid Chromatography has begun to replace conventional HPLC in academia and industry and interest in this technique continues to grow Both the increases in speed and resolution make this an attractive method particularly to the life sciences and more than 1500 papers have been written on this strongly evolving topic to date This book provides a solid background on how to work with UHPLC and its application to the life sciences The first part of the book covers the basics of this approach and the specifics of a UHPLC system providing the reader with a solid background to working properly with such a system The second part examines the application of UHPLC to the life sciences with a focus on drug analysis strategies UHPLC MS a key technique in pharmaceutical and toxicological analyses is also examined in detail The editors Davy Guillardme and Jean Luc Veuthey were some of the earliest adopters of UHPLC and have published and lectured extensively on this topic Between them they have brought together an excellent team of contributors from Europe and the United States presenting a wealth of expertise and knowledge This book is an essential handbook for anyone wishing to adopt an UHPLC system in either an academic or industrial setting and will benefit postgraduate students and experienced workers alike *The HPLC Expert* Stavros Kromidas,2016-03-28 The rapid development of HPLC instrumentation and technology opens numerous possibilities and entails new questions Which column should I choose to obtain best results which gradient fits to my analytical problem what are recent and promising trends in detection techniques what is state of the art regarding LC MS coupling All these questions are answered by experts in ten self contained chapters Besides these more hardware related and technical chapters further related areas of interest are covered Comparison of recent chromatographic data systems and integration strategies smart documentation efficient information search in internet and tips for a successful FDA inspection This practical approach offers in a condensed manner recent trends and hints and will also display the advanced reader mistakes and errors he was not aware of so far Software-assisted Method Development In High Performance Liquid Chromatography Szabolcs Fekete,Imre Molnar,2018-08-01 The book is a useful contribution in the field of HPLC and may represent a valuable tool for chromatography practitioners in different fields as well as teachers and instructors The 12 chapters provide comprehensive insights of current day retention and resolution modelling in HPLC

and its applications for small and large molecule analysis It may be a useful reference for specialists in pharmaceuticals but not limited to It may be a valuable resource to assist scientists involved in method development aiming to achieve the best results with reduced costs time and efforts Analytical and Bioanalytical Chemistry This handbook gives a general overview of the possibilities in recent developments in chromatographic retention modeling As a result of the latest developments in modeling software several new features are now accessible opening a new level in HPLC method development Many of these current possibilities in software assisted liquid chromatographic method modeling for analytical purposes are presented Several modes of chromatography including Reversed Phase Liquid Chromatography RPLC Ion Exchange Chromatography IEX Hydrophobic Interaction Chromatography HIC and Hydrophilic Interaction Liquid Chromatography HILIC are explained in detail For all these chromatographic modes the most important variables for tuning retention and selectivity are exposed Beside the industrial and practical benefits of retention modeling the possibilities in teaching and education are also illustrated Finally numerous representative industrial examples are shown to highlight the benefits time and cost savings offered by state of the art software assisted HPLC method development

Ultra-High Performance Liquid Chromatography and Its Applications Q. Alan Xu, 2013-04-01 Explores both the benefits and limitations of new UHPLC technology High performance liquid chromatography HPLC has been widely used in analytical chemistry and biochemistry to separate identify and quantify compounds for decades The science of liquid chromatography however was revolutionized a few years ago with the advent of ultra high performance liquid chromatography UHPLC which made it possible for researchers to analyze sample compounds with greater speed resolution and sensitivity Ultra High Performance Liquid Chromatography and Its Applications enables readers to maximize the performance of UHPLC as well as develop UHPLC methods tailored to their particular research needs Readers familiar with HPLC methods will learn how to transfer these methods to a UHPLC platform and vice versa In addition the book explores a variety of UHPLC applications designed to support research in such fields as pharmaceuticals food safety clinical medicine and environmental science The book begins with discussions of UHPLC method development and method transfer between HPLC and UHPLC platforms It then examines practical aspects of UHPLC Next the book covers Coupling UHPLC with mass spectrometry Potential of shell particles in fast liquid chromatography Determination of abused drugs in human biological matrices Analyses of isoflavones and flavonoids Therapeutic protein characterization Analysis of illicit drugs The final chapter of the book explores the use of UHPLC in drug metabolism and pharmacokinetics studies for traditional Chinese medicine With its frank discussions of UHPLC s benefits and limitations Ultra High Performance Liquid Chromatography and Its Applications equips analytical scientists with the skills and knowledge needed to take full advantage of this new separation technology

Optimization in HPLC Stavros Kromidas, 2021-11-08 Learn to maximize the performance of your HPLC or UHPLC system with this resource from leading experts in the field Optimization in HPLC Concepts and Strategies delivers tried and tested strategies for optimizing the

performance of HPLC and UHPLC systems for a wide variety of analytical tasks The book explains how to optimize the different HPLC operation modes for a range of analyses including small molecules chiral substances and biomolecules It also shows readers when and how computational tools may be used to optimize performance The practice oriented text describes common challenges faced by users and developers of HPLC and UHPLC systems as well as how those challenges can be overcome Written for first time and experienced users of HPLC technology and keeping pace with recent developments in HPLC instrumentation and operation modes this comprehensive guide leaves few questions unanswered Readers will also benefit from the inclusion of A thorough introduction to optimization strategies for different modes and uses of HPLC including working under regulatory constraints An exploration of computer aided HPLC optimization including ChromSwordAuto and Fusion QbD A treatment of current challenges for HPLC users in industry as well as large and small analytical service providers Discussions of current challenges for HPLC equipment suppliers Tailor made for analytical chemists chromatographers pharmacologists toxicologists and lab technicians Optimization in HPLC Concepts and Strategies will also earn a place on the shelves of analytical laboratories in academia and industry who seek a one stop reference for optimizing the performance of HPLC systems *Essentials in Modern HPLC Separations* Serban C. Moldoveanu,Victor David,2012-11-08 *Essentials in Modern HPLC Separations* discusses the role of separation in high performance liquid chromatography HPLC This up to date reference systematically covers new developments in types and characteristics of stationary phases mobile phases and other factors of this technique that influence separation of compounds being analyzed The volume also considers the selection process for stationary and mobile phases in relation to the molecules being separated and examined as well as their matrices The book includes a section on the contemporary applications of HPLC particularly the analysis of pharmaceutical and biological samples food and beverages environmental samples and more Discusses key parameters in HPLC separation Describes interrelation between various HPLC features solvent pressure separation detection Includes a large number of references *Method Development in Analytical HPLC* Serban C. Moldoveanu,Victor David,2024-10-22 *Method Development in Analytical HPLC* presents the essential information for understanding the process of developing an HPLC method of analysis It includes foundational information related to HPLC as well as discussion of sample types the properties of analytes and matrices in the samples and sample preparation The core of the book describes the best ways for approaching method development in various types of HPLC and the criteria for method optimization and validation This book provides clear guidance for adopting analytical methods from the literature and describes the development of original methods with selection of the suitable type of HPLC of specific columns mobile phase and detection techniques with an emphasis on the use of mass spectrometry for detection as well as optimization and validation of the chosen analytical method The book includes useful details on method development for specific types of chromatography such as RP HPLC HILIC ion exchange size exclusion and chiral Method Development in Analytical HPLC

also includes information about green chemistry in analytical methods computer assisted method development and other key contemporary aspects of the subject Offers a systematic and logical presentation of the foundational of analytical HPLC Goes in depth on method development for specific types of chromatography such as RP HPLC HILIC ion exchange and size exclusion Includes methods with an emphasis on the use of mass spectrometry for detection

HPLC and UHPLC for Practicing Scientists Michael W. Dong, 2019-07-10 A concise yet comprehensive reference guide on HPLC UHPLC that focuses on its fundamentals latest developments and best practices in the pharmaceutical and biotechnology industries Written for practitioners by an expert practitioner this new edition of HPLC and UHPLC for Practicing Scientists adds numerous updates to its coverage of high performance liquid chromatography including comprehensive information on UHPLC ultra high pressure liquid chromatography and the continuing migration of HPLC to UHPLC the modern standard platform In addition to introducing readers to HPLC s fundamentals applications and developments the book describes basic theory and terminology for the novice and reviews relevant concepts best practices and modern trends for the experienced practitioner HPLC and UHPLC for Practicing Scientists Second Edition offers three new chapters One is a standalone chapter on UHPLC covering concepts benefits practices and potential issues Another examines liquid chromatography mass spectrometry LC MS The third reviews the analysis of recombinant biologics particularly monoclonal antibodies mAbs used as therapeutics While all chapters are revised in the new edition five chapters are essentially rewritten HPLC columns instrumentation pharmaceutical analysis method development and regulatory aspects The book also includes problem and answer sections at the end of each chapter Overviews fundamentals of HPLC to UHPLC including theories columns and instruments with an abundance of tables figures and key references Features brand new chapters on UHPLC LC MS and analysis of recombinant biologics Presents updated information on the best practices in method development validation operation troubleshooting and maintaining regulatory compliance for both HPLC and UHPLC Contains major revisions to all chapters of the first edition and substantial rewrites of chapters on HPLC columns instrumentation pharmaceutical analysis method development and regulatory aspects Includes end of chapter quizzes as assessment and learning aids Offers a reference guide to graduate students and practicing scientists in pharmaceutical biotechnology and other industries Filled with intuitive explanations case studies and clear figures HPLC and UHPLC for Practicing Scientists Second Edition is an essential resource for practitioners of all levels who need to understand and utilize this versatile analytical technology It will be a great benefit to every busy laboratory analyst and researcher

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