Experimental Design in Clinical ‘Omics Biomarker Discovery

To avoid unpleasant surprises of statistical analysis, --avoids bias--to improve the chance of answering the clinical questions--statistical power, to avoid confounding factors

Jenny Forshed

Computer applications in chemistry
Chapter 11: Experimental designs

R Sambasiva Rao, G Nageswara Rao

The role of Simplex method in chemical research
Review: state-of-knowledge algorithms –applications kinetic method of analysis-chromatography-instrumental parameters

R. Sambasiva Rao

A Tasty Approach to Statistical Experimental Design in High School Chemistry: The Best Lemon Cake

Lucia Liguori

Extraction and Antibacterial Properties of Thyme Leaf Extracts: Authentic Practice of Green Chemistry

DOI: 10.1021/acs.jchemed.5b00891

Sean C. Purcell, Prithvi Pande, Yingxin Lin, Ernesto J. Rivera, Latisha Paw U, Luisa M. Smallwood, Geri A. Kerstiens, Laura B. Armstrong, maryann T. Robak, Anne M. Baranger, and Michelle C. Douskey

The Alcohol Dehydrogenase Kinetics Laboratory: Enhanced Data Analysis and Student-Designed Mini-Projects

DOI: 10.1021/acs.jchemed.5b00610

Todd P. Silverstein
The Coffee Project Revisited: Teaching Research Skills to Forensic Chemists

Hilary J. Hamnett and Ann-Sophie Korb

Nano Science

Understanding the Seed-Mediated Growth of Gold Nanorods through a Fractional Factorial Design of Experiments

Nathan D. Burrows, Samantha Harvey, Fred A. Idesis, and Catherine J. Murphy

DOI: 10.1021/acs.langmuir.6b03606

Laser Ablation of Silver in Liquid Organic Monomer: Influence of Experimental Parameters on the Synthesized Silver Nanoparticles/Graphite Colloids

Maxime Delmée, Grégory Mertz, Julien Bardon, Adeline Marguier, Lydie Ploux, Vincent Roucoules, and David Ruch

Nano Science

Submicrometric Magnetic Nanoporous Carbons Derived from Metal–Organic Frameworks Enabling Automated Electromagnet-Assisted Online Solid-Phase Extraction

Rejane M. Frizzarin, Carlos Palomino Cabello, Maria del Mar Bauzà, Lindomar A. Portugal, Fernando Maya, Víctor Cerdà, José M. Estela, and Gemma Turnes Palomino

Nano Science

Using Factorial Experimental Design To Prepare Size-Tuned Nanovesicles

Soft nanoparticles—suitable in food, cosmetic, pharmaceutical, or medical diagnosis/therapy

Pablo García-Manrique, María Matos, Gemma Gutiérrez, Oscar R. Estupiñán, María Carmen Blanco-López, and Carmen Pazos

Nano Science

Kriging-Based Design of Experiments for Multi-Source Exposure–Response Studies in Nanotoxicology

Ying Pei, Feng Yang, Xi Chen, Nianqiang Wu, and Kai Wang

Nano Science

Controlling the Interfacial Environment in the Electrosynthesis of Nanostructures for High-Performance Oxygen Reduction/Evolution Electro catalysis

Pooya Hosseini-Benhangi, Chun Haow Kung, Akram Alfantazi, and Előd L. Gyenge

Nano Science

Extraction of Cellulose Nanocrystals with a High Yield of 88% by Simultaneous Mechanochemical Activation and Phosphotungstic Acid Hydrolysis

Qilin Lu, Zhenghan Cai, Fengcai Lin, Lirong Tang, Siqun Wang, and Biao Huang

Nano Science

Evaluating the Combined Toxicity of Cu and ZnO Nanoparticles: Utility of the Concept of Additivity and a Nested Experimental Design

Yang Liu, Jan Baas, Willie J. G. M. Peijnenburg, and Martina G. Vijver

Nano Science

Advancement Application Announcement (AAA)
Hospital and Urban Residues

Fully Automated System for 99Tc Monitoring in Hospital and Urban Residues: A Simple Approach to Waste Management

Marina Villar, Antoni Borràs, Jessica Avivar, Fernando Vega, Víctor Cerdà, and Laura Ferrer

DOI: 10.1021/acs.analchem.7b00184

Proteomics

Identification of Analytical Factors Affecting Complex Proteomics Profiles Acquired in a Factorial Design Study with Analysis of Variance: Simultaneous Component Analysis

Two-level fractional factorial design; preprocessing: Threshold Avoiding Proteomics Pipeline

Vikram Mitra#, Natalia Govorukhina®, Gooitzen Zwanenburg, Huub Hoefsloot, Inge Westra, Age Smilde#, Theo Reijmers, Ate G. J. Van der Zee, Frank Suits, Rainer Bischoff#®, and Péter Horvatovich

DOI: 10.1021/acs.analchem.5b03483

Pharmaceutical Analysis

Rapid Method Development in Hydrophilic Interaction Liquid Chromatography for Pharmaceutical Analysis Using a Combination of Quantitative Structure–Retention Relationships and Design of Experiments

Maryam Taraji, Paul R. Haddad, Ruth I. J. Amos, Mohammad Talebi, Roman Szucs, John W. Dolan, and Chris A. Pohl

DOI: 10.1021/acs.analchem.6b04282

Technology

Probability-Based Design of Experiments for Batch Process Optimization with End-Point Specifications; Find optimal policies for runs involving stochastic binary outcomes; acetoacetylation of pyrrole with diketene

Estefanía Colombo, Martin Luna, and Ernesto Martínez

Optimization of Catalytic Glycerol Etherification with Ethanol in a Continuous Reactor

Caroline O. T. Lemos, Leticia L. Rade, Marcos A. De S. Barrozo, Linovald D. Fernandes, Lucio Cardozo-Filho, and Carla E. Hori

DOI: 10.1021/acs.energyfuels.7b00194

Experimental and Statistical Optimization of the Tensile Strength of Carbon Fibers from Pitches with Different Composition

Factorial design;

Noel Diez, Patricia Álvarez, Clara Blanco, Ricardo Santamaría, Marcos Granda, and Rosa Menéndez

Ultrademo-Photoassisted Advanced Oxidation of Parabens Catalyzed by Hydrogen Peroxide and Titanium Dioxide. Improving the System

Factorial central composite orthogonal and rotatable design

Eduardo M. Cuerda-Correa, Joaquin R. Domínguez-Vargas, María J. Muñoz-Peña, and Teresa González

DOI: 10.1021/acs.iecr.5b04560
**Biodiesel**

Biodiesel Production via Transesterification of Soybean Oil Catalyzed by Superhydrophobic Porous Poly(ionic liquid) Solid Base

Three-level and three-factorial central composite

Bin Jiang, Yumei Wang, Luhong Zhang, Yongli Sun, Huawei Yang, Baoyu Wang, and Na Yang

Steam Deacidification of High Free Fatty Acid in Jatropha Oil for Biodiesel Production

Central composite design; temperature; amount of steam

Godlisten G. Kombe and Abraham K. Temu

Combination of Dispersive Liquid–Liquid Micro-extraction and Emulsion Breaking for the Determination of Cu(II) and Pb(II) in Biodiesel and Oil Samples

Central composite design and a univariate analysis; exptvar: [complexant concentration, pH value, and extractant solvent volume]


**Chemical Kinetics**

Reaction Kinetic Study of Solketal Production from Glycerol Ketalization with Acetone

Ketalization reaction [catalyst: zeolite H-BEA]: glycerol + acetone

Solketal is a green solvent

Vinicius Rossa, Yolanda da S. P. Pessanha, Gisel Ch. Díaz, Léoncio Diógenes Tavares Câmara, Síbele B. C. Pergher, and Donato A. G. Aranda

Experimental Design for Discrimination of Chemical Kinetic Models for Oxy-Methane Combustion

Liming Cai, Stephan Kruse, Daniel Felsmann, Christoph Thies, Kiran K. Yalamanchi, and Heinz Pitsch

Enzymatic Hydrolysis of Steam-Treated Sugarcane Bagasse: Effect of Enzyme Loading and Substrate Total Solids on Its Fractal Kinetic Modeling and Rheological Properties

Douglas H. Fockink, Mateus B. Urio, Jorge H. Sánchez, and Luiz P. Ramos

**Multi-variate Analysis**

Multivariate Analysis in Selective Nitroacetophenone Conversion by Hydrogen Sulfide under Phase Transfer Catalysis

Ujjal Mondal and Sujit Sen

**Miscellaneous**

Development of an Adaptive Experimental Design Method Based on Probability of Achieving a Target Range through Parallel Experiments

Adaptive experimental design- parallel experiments–Gaussian process regression


Energy Fuels, 2017, 31 (6), pp 6206–6210 DOI: 10.1021/acs.energyfuels.7b00700

Energy Fuels, 2017, 31 (9), pp 9491–9497 DOI: 10.1021/acs.energyfuels.7b01430

Energy Fuels, 2017, 31 (5), pp 5533–5542 DOI: 10.1021/acs.energyfuels.6b03025

Energy Fuels, 2017, 31 (6), pp 6211–6220 DOI: 10.1021/acs.energyfuels.7b00818

Experimental and Theoretical Investigation of Inhibition Efficiency of 2-(2-Hydroxyphenyl)-benzothiazole Using Impedance Spectroscopy, Experimental Design, and Quantum Chemical Calculations

Atsuyuki Nakao, Hiromasa Kaneko, and Kimito Funatsu

DOI: 10.1021/acs.iecr.7b02030

Optimization of Solketalacetin Synthesis as a Green Fuel Additive from Ketalization of Monoacetin with Acetone

Central composite design-RSM

Yadollah M. Gorji and Hassan S. Ghaziaskar

DOI: 10.1021/acs.iecr.6b00929

Direct Determination of Contaminants and Major and Minor Nutrients in Solid Fertilizers Using Laser-Induced Breakdown Spectroscopy (LIBS)

Factorial design- using laser-induced breakdown spectroscopy (LIBS) parameters

Daniel F. Andrade and Edenir Rodrigues Pereira-Filho

DOI: 10.1021/acssuschemeng.6b02008

A Bioinspired Alginate-Gum Arabic Hydrogel with Micro-/Nanoscale Structures for Controlled Drug Release in Chronic Wound Healing

Orthogonal experimental design

Mi Li, Haichang LiV, Xiangguang Li#, Hua Zhu, Zihui Xu, Lianqing Liu, Jianjie Ma, and Mingjun Zhang

Statistical Optimization of Heavy Metal (Cu2+ and Co2+) Extraction from Printed Circuit Boards and Mobile Batteries Using Chelation Technology

Box–Behnken design + central compositedesign

Nitin Sharma, Garia Chauhan, Arinjay Kumar, and S. K. Sharma

DOI: 10.1021/acs.oprd.6b00153

Optimization of Salts Supplementation on Xylitol Production by Debaryomyces hansenii Using a Synthetic Medium or Corncob Hemicellulosic Hydrolyzates and Further Scaled Up

☼ Central composite design:

Guadalupe Bustos Vázquez, Noelia Pérez-Rodríguez, José Manuel Salgado, Ricardo Pinheiro de Souza Oliveira, and José Manuel Domínguez

J. Agric. Food Chem., 2016, 64 (41), pp 7890–7898
DOI: 10.1021/acs.jafc.6b04028

Adsorbent Screening for Postcombustion CO2 Capture: A Method Relating Equilibrium Isotherm Characteristics to an Optimum Vacuum Swing Adsorption Process Performance

Centralcomposite; neural-network-based model; meta-models

Maninder Khurana and Shamsuzzaman Farooq

DOI: 10.1021/acsami.7b04428

ADSorption for Puriﬁcation of Curcumin by Cooling Crystallization

Nitin Sharma, Garima Chauhan, Arinjay Kumar, and S. K. Sharma

DOI: 10.1021/acs.oprd.6b00153
An In-Depth Study of the Use of Eosin Y for the Solar Photocatalytic Oxidative Coupling of Benzylic Amines

Joshua D. Tibbetts, David R. Carbery, and Emma A. C. Emanuelsson

An In-Depth Study of the Use of Eosin Y for the Solar Photocatalytic Oxidative Coupling of Benzylic Amines

Marko Ukrainczyk, B. Kieran Hodnett, and Åke C. Rasmuson

ACS Sustainable Chem. Eng., Article ASAP
DOI: 10.1021/acssuschemeng.7b01754

Single-Step Assembly of Multifunctional Poly(tannic acid)–Graphene Oxide Coating To Reduce Biofouling of Forward Osmosis Membranes

Joshua D. Tibbetts, David R. Carbery, and Emma A. C. Emanuelsson

ACS Appl. Mater. Interfaces, 2016, 8 (27), pp 17519–17528
DOI: 10.1021/acsami.6b03719

Taguchi’s design

Hanaa M. Hegab, Ahmed elmekawy, Thomas G. Barclay, Andrew Michelmore, Linda Zou#, Christopher P. Saint, and Milena Ginic-Markovic

Hitchhiker’s Guide to Voltammetry: Acute and Chronic Electrodes for in Vivo Fast-Scan Cyclic Voltammetry

Nathan T. Rodeberg, Stefan G. Sandberg, Justin A. Johnson, Paul E. M. Phillips, and R. Mark Wightman

DOI: 10.1021/acschemneuro.6b00393

Strecker Aldehyde Formation in Wine: New Insights into the Role of Gallic Acid, Glucose, and Metals in Phenylacetaldehyde Formation

Ana Rita Monforte, Sara I. F. S. Martins#, and Antonio C. Silva Ferreira

Elementary Transformation of Glycerol to Trivalerin: Design of an Experimental Approach

Kamalpreet Kaur, Ravinder Kumar Wanchoo, and Amrit Pal Toor

DOI: 10.1021/acssuschemeng.6b02133

Credit: Acs.org