A 1: Concept for study group Bioanalytics

Main purpose of this group is besides „listing“ of methods and „applications“ a help for deciding which to use for what and warn about pitfalls. It might be a help for those using analytics in fields like life science, environment and food analysis and not being a really well-trained Analyzer. Tools should be provided.

1. General

1.1 Find classification according to

1.1.1 Analytical Method

1.1.2 Targeted Molecule

1.1.3 Application

1.2 Key list for literature search (fundamental books, review articles….)

- Analytical Chemistry: A Modern Approach to Analytical Science, 2nd Edition, Robert Kellner (Editor), Jean-Michel Mermet (Editor), Matthias Otto (Editor), Miguel Valcárcel (Editor), H. Michael Widmer (Editor) ISBN: 978-3-527-30590-2, 1209 pages, Wiley-VCH, Weinheim, 2004
- Principles of instrumental analysis, Douglas A. Skoog, F. James Holler, Stanley R. Crouch. Belmont, CA : Thomson, Brooks/Cole, 1039 pages, ISBN 978-0-495-01201-6, Thomson, 2007.1998.
- Chemical Instrumentation: A Systematic Approach, 3rd Edition, Howard A. Strobel, William R. Heineman, Wiley, ISBN: 978-0-471-61223-0, 1248 pages, 1989
- Bioanalytics, (Analytical Methods and Concepts in Biochemistry and Molecular Biology), Lottspeich / Engels, 2018. 1000 S. Hardcover, Wiley-VCH ISBN 978-3-527-33919-8
- A. Manz, P. S. Dittrich, N. Pamme, D. Iossifidis. Bioanalytical Chemistry, 2nd ed., Imperial College Press, Londom, 2015
- G. Evans. A Handbook of Bioanalysis and Drug Metabolism, CRC Press, Boca Raton (2004).
- R. J. Reece. Analysis of Genes and Genomes, John Wiley & Sons Hoboken, NJ (2004).
- A. Lesk. Introduction to Genomics, Oxford University Press (2012).
- M. S. Poptsova, ed. Genome Analysis: Current Procedures and Applications, Caister Academic Press, Norfolk, UK (2014).
- J. Pevsner. Bioinformatics and Functional Genomics, 3rd ed., John Wiley and Sons Ltd, Chichester, UK (2015).
- W. W. Grody, R. M. Nakamura, F. L. Kiechle, C. Strom, eds. Molecular Diagnostics: Techniques and Applications for the Clinical Laboratory, 1st ed., Academic Press/Elsevier, London, UK (2009).
- G. P. Rédei. Encyclopedia of Genetics, Genomics, Proteomics, and Informatics, Springer Science & Business Media (2008).
- E. Buxbaum. Fundamentals of Protein Structure and Function, Springer International Publishing (2015).
- R. Westermeier, T. Naven, H.-R. Höpker. Proteomics in Practice: A Guide to Successful Experimental Design, John Wiley & Sons (2008).
- M. Soloviev. Peptidomics: Methods and Protocols, Humana Press (2010).
- T. Palzkill. Proteomics, Kluwer Academic Publishers, New York (2002).
- P. K. Ghosh. Introduction to Protein Mass Spectrometry, Academic Press, London, UK (2016).

- S. G. Villas-Boas, J. Nielsen, J. Smedsgaard, M. A. Hansen, U. Roessner-Tunali. Metabolome Analysis: An Introduction, John Wiley & Sons (2007).
- M. Lämmerhofer, W. Weckwerth, eds. Metabolomics in Practice: Successful Strategies to Generate and Analyze Metabolic Data, John Wiley & Sons (2013).
- W. L. Cabrera, J. S. Knapp, eds. Metabolomics: Metabolites, Metabonomics, and Analytical Technologies, Nova Science Publishers
- (2011).
- T. O. Metz. Metabolic Profiling, Springer (2011).
- A. Varki, R. D. Cummings, J. D. Esko, H. H. Freeze, G. W. Hart, M. E. Etzler, eds. Essentials of Glycobiology, Cold Spring Harbor Laboratory Press, USA (2008).
- H.-J. Gabius, ed. The Sugar Code: Fundamentals of Glycosciences, John Wiley & Sons (2011).
- Electrochemical Sensors in Bioanalysis, R.I. Stefan, J.F. van Staden and H.Y. Aboul-Enein, Marcel Dekker Inc., New York, USA, 2001.

1.3 Decision tree combining method, application, problem

1.3.1 Tutorial using analytics (adds and odds of methods)

During EuCheMS in Liverpool there will be a session "**ABCs of Analytics"** where recent developments are described, and advice on using instrumentation and evaluation procedures in the field of life sciences, environment and food analysis is given. First, young scientists receive information about publishing in analytical journals; at the end, there will be a panel discussion about challenges and solutions in analytics.

In TrAC Trends in Analytical Chemistry frequently tutorials are published on analytical methods.

1.3.2 Short courses organized at conferences such as EUROANALYSIS, EUCHEMs – for training of new researchers in the field

1.4 Classification of Bioanalytics

1.4.1 Definition

Analytical methods in biosciences like biochemistry, biology, biotechnology, molecular biology, molecular genetics, medicine, pharmacy as well as in environmental sciences.

Methods are used to get information on macromolecules related to their

- structure,
- dynamics,
- effects and impact

1.4.2 Bioinformatics

Especially in live sciences big data are produced using imaging techniques, high-throughput, arrays, dynamic measurements

2 Analytical methods

2.1 Separation sciences

2.1.1 GC, HPLC, CZE

2.2 Spectrometry

2.2.1 Mass Spectrometry

2.3 Spectroscopy

2.3.1 Colorimetric

2.3.2 Raman

- SERS

2.3.3 Fluorescence

Self-fluorescent biomolecules - bioluminescence,

Measurement of intensity, lifetime,

Lit.:

Joseph R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd edition (2006), Springer-Verlag, Heidelberg

Fluorescence Spectroscopy, New Methods and Applications, Otto S. Wolfbeis (Ed.) (1993), Springer-Verlag, Heidelberg

2.3.4 Direct optical

Measurement of product of refractive index times physical thickness of a layer

- Refractometric
  surface plasmon resonance, grating coupler, Mach-Zehnder, prism coupler, …..
- Reflectometric
  ellipsometry, reflectometric interference spectroscopy

Details in Handbook of Spectroscopy (Editors: G. Gauglitz, D.S. Moore), 2nd Completely Revised and Enlarged Edition, Vol. 3, “Direct Optical Detection in Bioanalytics” (G. Gauglitz, N.J. Goddard), Wiley-VCH 2014

2.4 Mass sensitive

2.4.1 QMB,

2.4.2 SAW

2.5 Electroanalytical methods

2.5.1 Amperometric Methods

2.5.2 Potentiometric Methods

2.5.3 Impedance

2.5.4 Stochastic Method

2.6 Hyphenated techniques

2.7 Tools for Bioanalysis

2.7.1 Biosensors (survey)

2.7.2 Stochastic sensors

3 Type of molecules to be determined

- Proteins
- Peptides
- Amino acids
- DNA/RNA
- Carbohydrates
- Lipids

4 Special Applications

- ✓ Screening of biological samples for early diagnosis
- ✓ Screening of food samples for quality control
- ✓ Quality control of pharmaceutical samples
- ✓ Enantioanalysis of biological samples
- ✓ Identification and characterization of new biomolecules in biological samples, environment

5 Web-Links

- http://b-analytics.net/

Links to additional networks

Further information on additional pages

A 2: 2.7.1 Biosensors (survey)

(1) ***Principle***

Biosensors are devices capable of providing specific quantitative or semi-quantitative analytical information using a biological recognition element which is in contact with a transduction element. Such a biosensor contains:

- a transduction element (electrochemical, optical, thermos, micro-balanced, surface-acoustic wave …). It transfers an effect offered by a biomolecular interaction process to an electronic signal;
- recognition elements (realizing biomolecular interaction processes between antigene/antibodies, analyte/biomimetics, proteins/proteins, peptide libraries), is responsible for selectivity; forming the sensitive layer, which inserts an effect to the transduction element;
- a shielding layer to suppress or avoid nonspecific interaction (especially in complex matrices such as blood or milk) and acting as an anchor layer for the recognition elements
- electronic read-out and data processing unit

(2) Literature

- Biosensing for the 21st century (Series Editor: T. Scheper; Volume Editors: R. Rennebert, F. Lisdat; Advances in Chemical Engineering/Biotechnologies 109; Springer Heidelberg, 2008
- Biosenors for Environmental Monitoring (Editors: U. Bilitewski, A.P.F. Turner); harwood academic publishers, 2000
- Biosensors and Biodetection Methods and Protocols (Editors: A. Rasooly, K.E. Herold), Methods in Molecular Biology 503; Springer Protocols; Methods and Protocols, Vol. 1, Optical-Based Detectors, Humana Press 2017
- Handbook of Biophotonics (Editors: J. Popp, V.V. Tuchin, A. Chiou, S.H. Heinemann), Vol. 3: Photnics in Pharmaceutics, Bioanalysis and Environmental Research; Wiley-VCH 2012
- Handbook of Spectroscopy (Editors: G. Gauglitz, D.S. Moore), 2nd Completely Revised and Enlarged Edition, Vol. 3, “Direct Optical Detection in Bioanalytics” (G. Gauglitz, N.J. Goddard), Wiley-VCH 2014
- Handbook of Spectroscopy (Editors: G. Gauglitz, D.S. Moore), 2nd Completely Revised and Enlarged Edition, Vol. 3, “Immunoassays” (G. Proll, M. Ehni), Wiley-VCH 2014
- D.R. Thevenot, K. Tóth, R.A. Durst, G.S. Wilson, “Electrochemical Biosensors: Recommended Definitions and Classifications”; Pure and Applied Chemistry, 71/12, 2333-2348, 1999

(3) Congresses

- Biosensors; international congress, every other year on a different continent in a different country;
- European Biosensor Symposium; every other year in a different European country;
- Workshop on Biosensors & Bioanalytical Microtechniques in Environment, Food & Clinical Analysis; every other year in different countries;

(4) Chances and pitfalls

- Avoiding nonspecific interaction;
- Suitable detection element
- selecting the best assay type (direct, competitive, binding inhibition, Sandwich);
- determination of limits of detection and limits of quantification because of sigmoid calibration curve;
- evaluation of binding curves (equilibrium, association and dissociation rate constants)

(5) Applications

Biosensors are used for trace analysis in case of environmental problems, to study

- imaging of DNA strands;
- protein/protein interactions;
- point-of-care diagnostics
- high through-put screening
- biomarker screening

5.7.2018 Gauglitz

A 3: 2.7.2 Stochastic sensors

(1) ***Principle***

Stochastic sensors are new tools developed for bioanalysis, based on a very simple principle: channel conductivity. When a molecule is entering the channel, it blocked it, and the current is getting to zero value until the molecule is entering the channel (this time is called t_{off} and is used for qualitative analysis), the time spent in the channel is called t_{on} and it is used the the quantitative measurements. Such a sensor comprise of:

- a membrane/active site of the sensor containing channels or pores.

(2) Literature

- Pattern recognition of 8-hydroxy-2′-deoxyguanosine in biological fluids, Anal Bioanal Chem, RI Stefan-van Staden et al., January 2018, Volume 410, Issue 1, pp 115–121
- Engineering of protein nanopores for sequencing, chemical or protein sensing and disease diagnosis, S Wang et al., Current Opinion in Biotechnology, Volume 51, June 2018, Pages 80-89
- Stochastic sensors inspired by biology, H. Bayley & P.S. Cremer, Nature, 413, pages 226–230 (13 September 2001).
- Stochastic sensors, J. Schmidt, Journal of Materials Chemistry, 2005,15, 831-840.
- Stochastic nanopore sensors for the detection of terrorist agents: Current status and challenges, A. Liu et al., Anal.Chim.Acta, 675, Issue 2, 24 August 2010, Pages 106-115

(3) Chances and pitfalls

- Reliable qualitative and quantitative analyses can be performed
- Suitable for multianalyte detection
- High selectivity
- Capable to perform analysis from very complex matrices because both quantitative and qualitative analysis are not influenced by the nature and complexity of the matrix from where the analytes are determined;

(4) Applications

Stochastic sensors are used for trace and ultra trace analysis in:

- Environmental analysis;
- Clinical analysis, including point-of-care diagnostics
- High through-put screening
- Pharmaceutical analysis
- Food analysis

RI van Staden