

ARTICLE

Route Selection and Reaction Engineering for Sustainable Metabolite Synthesis

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Some specialized service companies, centers and research institutions are listed here, for example providing services for metabolite synthesis (see table 1 for a selection of service institutions), and for the analysis and identification of metabolites (see table 2 for a selection of service institutions).

Electronic Supplementary Information

Table 1 lists some service companies, centers and research institutions which are providing services for metabolite synthesis, isolation and purification.

Table 2: Organizations providing services for metabolite synthesis, isolation and purification

Organization	Services	Location	Website
Analyticon Discovery	Natural product isolation and purification Natural product synthesis	AnalytiCon Discovery GmbH Hermannswerder Haus 17 14473 Potsdam Germany	https://ac-discovery.com/
BOC Sciences	Custom metabolites synthesis	BOC Sciences 45-16 Ramsey Road, Shirley, NY 11967, USA	https://www.solutions.bocsci.com/metabolites-synthesis.htm
Chiroblock	Custom synthesis of commercially not available, complex and novel molecules	ChiroBlock Andresenstraße 1a 06766 Wolfen Germany	https://www.chiroblock.com/
HepatoChem	Oxidative drug metabolite synthesis Photochemical synthesis	HepatoChem Inc 100 Cummings Center, Suite 360 B Beverly, MA 01915 USA	https://www.hepatochem.com/

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Hypha Discovery	Synthesis of Metabolites of Drugs and Agrochemicals Synthesis of Stable isotope-labelled and radio-labelled metabolites Purification of metabolites, natural products and other small molecules	Hypha Discovery Limited 154B Brook Drive Milton Park Abingdon OX14 4SD, UK	https://www.hyphadiscovery.com/
LKT Labs	Natural product isolation and purification Custom synthesis	LKT Laboratories, Inc. 545 Phalen Blvd. St. Paul, MN 55130 USA	https://lktlabs.com/
NUVISAN	Oxidative drug metabolite synthesis Biocatalytic synthesis of glucuronides.	NUVISAN Pharma Holding GmbH Wegenerstraße 13 89231 Neu-Ulm Germany	https://www.nuvisan.com/value-chain/discovery/in-vivo-lead-generation/microbiology-metabolite-synthesis.html
Selcia Ltd.	Custom synthesis of metabolites Custom synthesis of compounds labelled with stable isotopes such as Carbon-13, Nitrogen-15, Deuterium	Selcia Ltd. Fyfield Business & Research Park, Fyfield Road, Ongar, Essex CM5 0GS United Kingdom	https://www.selcia.com/selcia-radiolabelling/glp-analytical-chemistry-services-and-metabolite-synthesis
SiChem GmbH	Custom synthesis of metabolites Custom synthesis of compounds labelled with stable isotopes such as Carbon-13, Nitrogen-15, Deuterium	Sirius Fine Chemicals Sichem GmbH Fahrenheitstresse 1 (BITZ) 28359 Bremen Germany	https://www.sichem.de/en/custom-synthesis/
Metabolite Standards Synthesis Center (MSSC)	Development of the synthesis of labeled and commercially unavailable compounds	Metabolite Standards Synthesis Center, Research Triangle Park 3040 East Cornwallis Road, P.O. Box 12194, Research Triangle Park, NC 27709-2194, USA	https://www.rti.org/impact/metabolite-standards-synthesis-center

Table 2 lists some service companies, centers and research institutions which are providing services for the analysis and identification of metabolites.

Table 2: Organizations providing services for the analysis and identification of metabolites

Organization	Services	Location	Website
Metabolon	Single Analyte Assays, Targeted Metabolomics, Untargeted Metabolomics	Metabolon, Inc., 617 Davis Drive, Suite 100, Morrisville, NC 27560, USA; Metabolon GmbH, Zeppelinstraße 3 85399 Hallbergmoos, Germany	https://www.metabolon.com/
Afekta	Metabolic profiling with LC-MS	Afekta Technologies Ltd. Microkatu 1 PL 1199 70210 Kuopio, Finland	https://afekta.com/
Biocrates	Metabolic phenotyping services Quantitative profiling assays Specialized quantitative assays Pathway analysis	biocrates life sciences AG Eduard-Bodem-Gasse 8 6020 Innsbruck Austria	https://biocrates.com/services/
Biogenity	Complete metabolomics workflow Metabolite analysis with mass spectrometry platforms	Biogenity ApS Niels Jernes Vej 10 9220 Aalborg Denmark	https://biogenity.com/metabolomics
CD Genomics	Lipidomics, Targeted Metabolomics, Untargeted Metabolomics	CD Genomics, SUITE 111, 17 Ramsey Road, Shirley, NY 11967, USA	https://multiomics.cd-genomics.com/
Creative Proteomics	Metabolite Profiling and Targeted Analysis, Metabolic Pathway Analysis, Metabolomics Data Analysis and Interpretation	Creative Proteomics, SUITE 115, 17 Ramsey Road, Shirley, NY 11967, USA	https://metabolomics.creative-proteomics.com/
Dalton Bioanalytics	MS-based biochemical identification, relative quantification, and statistical analysis of metabolites and lipids with data visualization	Dalton Bioanalytics California NanoSystems Institute 570 Westwood Plaza Bldg 114, Rm 6350H, Mail 722710 Los Angeles, California 90095-7227 USA	https://www.daltonbioanalytics.com/

Human Metabolome Technologies (HMT)	Screening a wide range of metabolites in addition to energy metabolism Comprehensive analysis, including unknown metabolites Analysis of small amounts of sample, or when high sensitivity analysis is required Capturing energy metabolism Label analysis using stable isotopes Comprehensive analysis of lipophilic metabolites, in addition to hydrophilic and ionic metabolites Analysis of lipid mediators	Human Metabolome Technologies, Inc. 246-2 Mizukami Kakuganji, Tsuruoka, Yamagata 997-0052, Japan	https://humanmetabolome.com/ap/
Lipotype	Targeted lipidomics analysis Untargeted lipidomics analysis	Lipotype GmbH Tatzberg 47 01307 Dresden Germany	https://www.lipotype.com/
Metware Bio	Global Metabolite Profiling Targeted Metabolomics Lipidomics Multi-omics	Metware Biotechnology Inc. 8A Henshaw Street, Woburn, MA 01801 USA	https://www.metwarebio.com/
MS-Omics	Targeted Analysis of a limited List of predefined Compounds, Global Detection of Metabolites	MS-Omics, Bygstubben 9 DK-2950 Vedbæk, Denmark	https://www.msomics.com/
PANOMIX	Untargeted metabolome analysis Targeted metabolome analysis Quantitative metabolite analysis Metabolic flux analysis Lipidomics analysis	Suzhou PANOMIX Biotech Co., LTD 388 Xiping Street, Industrial Park, Suzhou city, Jiangsu Province China	https://en.panomix.com/

The Metabolomics Innovation Centre (TMIC)	Metabolic profiling including comprehensive metabolite identification, quantification and analysis, Quantitative Metabolomic Services for Biomarker Discovery and Validation, Semi-quantitative Metabolomics, Custom Solutions	National Canadian Core Facility consisting of University of Alberta, University of Victoria, McGill University, McMaster University, University of Calgary, Concordia University, The University of British Columbia	https://metabolomicscentre.ca/
EMBL Metabolomics Core Facility	Targeted Metabolomics Analysis, Untargeted Metabolomics and/or Lipidomics Analysis, Metabolite Identification, Lipid Identification, Drug and Drug Metabolite Analysis, Method Development	Metabolomics Core Facility EMBL Heidelberg, Meyerhofstraße 1, 69117 Heidelberg, Germany	https://www.embl.org/groups/metabolomics/
West Coast Metabolomics Center, UC Davis	Targeted Metabolite Analysis, Untargeted Metabolite Analysis, Metabolite Identification, Stable Isotope Tracer Analysis	UC Davis Genome Center, Metabolomics Central Service Core, Room 1212, 451 Health Sciences Drive Davis, CA 95616, USA	https://metabolomics.ucdavis.edu/
Michigan Regional Comprehensive Metabolomics Resource Core (MRC2)	Targeted Metabolomics, Untargeted Metabolomics, Targeted and untargeted Lipidomics, Fluxomics, Data analysis and visualization	Michigan Regional Comprehensive Metabolomics Resource Core (MRC2) University of Michigan at Ann Arbor WK Kellogg Eye Center @ Brehm Tower, 1000 Wall Street, Room 6309 Ann Arbor, MI 48105-5714, USA	https://brcf.medicine.umich.edu/cores/metabolomics/

Eastern Regional Comprehensive Metabolomics Resource Core (ERCMRC) at UNC Chapel Hill	Mass spectrometry and NMR Spectroscopy for broad spectrum and targeted metabolomics	Eastern Regional Comprehensive Metabolomics Resource Core (ERCMRC), Department of Nutrition, University of North Carolina at Chapel Hill, UNC Nutrition Research Institute 500 Laureate Way, Kannapolis, NC, 28081. USA	https://www.rti.org/impact/eastern-regional-comprehensive-metabolomics-research-core-rti-rcmrc
Southeast Center for Integrated Metabolomics (SECIM)	Global Metabolite Analysis, Targeted Metabolite Analysis.	Southeast Center for Integrated Metabolomics (SECIM), University of Florida, Analytical Chemistry, Chemistry Laboratory Building, Room 210, PO Box 117200, Gainesville, FL 32611-7200, USA	http://secim.ufl.edu/
Resource Center for Stable Isotope-Resolved Metabolomics (RC-SIRM)	Sample Preparation; Analytical Measurements by NMR, FTMS, GC & LC, ICPMS; Data reduction/interpretation of complex labeling.	Resource Center for Stable Isotope-Resolved Metabolomics (RC-SIRM) University of Kentucky, Markey Cancer Center, 800 Rose St., Lexington, KY 40536-0093, USA	http://bioinformatics.cesb.uky.edu/bin/view/RCSIRM/
Metabolomics Core at Mayo Clinic	Untargeted Metabolomics Targeted Metabolomics Isotope Ratio Measurements NMR Specialty Tools	Metabolomics Core at Mayo Clinic, Mayo Clinic, Division of Endocrinology 200 First Street SW, Rochester, MN 55905, USA	https://www.mayo.edu/research/core-resources/metabolomics-core/overview

NIEHS Metabolomics Core Facility	Untargeted Metabolomics, Metabolite Identification, Measurement of Molecular Weight Measurement of MS/MS or MSn Measurement of Collisional Cross-section, Untargeted Metabolomics Data Analysis	National Institute of Environmental Health Sciences (NIEHS), Metabolomics Core Facility 111w Alexander Dr David P Rall Building Research Triangle Park, NC 27709, USA	https://www.niehs.nih.gov/research/atniehs/facilities/metabolomics/index.cfm
Scripps Center for Metabolomics and Mass Spectrometry	ESI High Accuracy m/z measurements with mass errors <5 ppm for small molecules typically < 2000 Da; 3000 Da limit ESI Unit Mass results in positive or negative mode, typically 100 - 3,000 Da MALDI Unit mass results Metabolic Pathway Analysis LC/MS and GC/MS Quantitative Analysis Open Access Single Quad, TOF, Rapid-MS	Scripps Center for Metabolomics and Mass Spectrometry The Scripps Research Institute 10650 North Torrey Pines Rd La Jolla, CA 92037 USA	https://masspec.scripps.edu/
PHRT Center for Metabolomics and Lipidomics	Untargeted Metabolomics (LC-MS) HT Metabolomics (FIA-MS, untargeted): CHF 30 per sample and mode. Normally, only negative mode analysis is needed. Recommended for cellular extracts and supernatants. Lipidomics (LC-MS, untargeted): CH	PHRT Center for Metabolomics and Lipidomics Institute of Molecular Systems Biology ETH Zurich Otto-Stern-Weg 3 8093 Zürich Switzerland	https://imsb.ethz.ch/research/zamboni/ext/srv.html

Functional Genomics Center Zurich	Absolute metabolite quantification (targeted) Global metabolite profiling Global small molecules profiling Method development Statistical analysis and cross-omics support	Functional Genomics Center Zurich Joint Facility of ETH Zürich and the University of Zurich Irchel Campus Winterthurerstrasse 190 8057 Zürich Switzerland	https://fgcz.ch/the-center.html
Metabolomics Unit	Single pathway targeted analyses (absolute quantification), Multiple pathway targeted analyses - polar metabolites (relative quantification) Multiple pathway targeted analyses - complex lipids (absolute quantification), Stable isotope-assisted analyses (Untargeted analyses)	Metabolomics Unit, Faculty of Biology and Medicine, Université de Lausanne Metabolomics Platform (MEP) Quartier UNIL-CHUV, Rue du Bugnon 19, CH-1005 Lausanne Switzerland	https://www.unil.ch/metabolomics/en/home.html
National Phenome Centre	Complete solutions for the Metabolome	National Phenome Centre Imperial College London South Kensington Campus London SW7 2AZ United Kingdom	https://phenomecentre.org/
MetaboHUB	Metabolomic profiling Metabolite identification and quantitation Isotopic enrichment measurement and fluxomics	MetaboHUB National infrastructure in metabolomics & fluxomics 135 Avenue de Rangueil, 31400, Toulouse, France	https://www.metabohub.fr/home.html

Table 2.