DAVID S. WISHART

Distinguished University Professor (University of Alberta), FRSC

EDUCATION

1991 PhD	Molecular Biophysics & Biochemistry, Yale University, New Haven, U.S.A.
1986 MPhil	Molecular Biophysics & Biochemistry, Yale University, New Haven, U.S.A.
1983 BSc	(Honours, First Class) Physics, University of Alberta, Edmonton, Canada

ACADEMIC APPOINTMENTS

2016- Present	Distinguished University Professor, Depts. of Computing Science and Biological Sciences, University of Alberta, Edmonton, AB
2023-2030	Canada Research Chair (Tier 1) in Metabolomics and Precision Medicine
2016- Present	Chief Information Officer, Molecular You Corporation, Vancouver, BC
2012- Present	Adjunct Professor, Department of Laboratory Medicine and Pathology, University of Alberta
2012-2016	Program Coordinator for Metabolomic Sensors and Senior Research Office, NRC- National Institute of Nanotechnology (NINT)
2004-2012	Director of Nanobiology and Senior Research Officer, NRC-National Institute of Nanotechnology (NINT)
2003- Present	Professor, Department of Computing Science, University of Alberta, Edmonton, AB
2003- Present	Adjunct Professor, Faculty of Pharmacy, University of Alberta, Edmonton, AB
2002-2004	Cross-Appointed Member, NRC-National Institute of Nanotechnology (NINT)
2000-2003	Associate Professor (Bristol-Myers Squibb Chair), Faculty of Pharmacy, University of Alberta, Edmonton, AB
1995-2000	Assistant Professor (Bristol-Myers Squibb Chair), Faculty of Pharmacy, University of Alberta, Edmonton, AB

OVERALL CURRICULUM VITAE METRICS

Date	Category	Metrics
1986-Present	H-index	156
1986-Present	Total number of citations	173615
1980-Present	Provincial, National and International Awards, Honours & Prizes	45
1995-Present	Other Professional Activities (Businesses, Boards, Committees)	82
1995-Present	Membership of University Committees	18
1995-Present	Society/Organization Memberships and Society/Organization Board Memberships	14
1995-Present	National and International Conferences Chaired or Organized	30
1995-Present	Directorships of Research Service Centres and Service Cores	8
1995-Present	Grants and Awards Received (Applicant or Co-applicant)*	184
2020-Present	Awards to Graduate Students and Postdoctoral Fellows	15
1986-Present	Publications (Journals, Books, Book Chapters - Peer Reviewed)	646
1989-Present	Posters and Poster Abstracts Presented	485
1989-Present	Invited Conference, Workshop, Symposia or Public Lectures	636

1995-Present	Undergraduate Students Supervised**	183
1995-Present	Graduate Students Supervised**	58
1995-Present	Postdoctoral Fellows Supervised**	66
1995-Present	Research Associates Supervised**	27
1995-Present	Technician and Programmers Supervised**	124
1995-Present	Assistants and Research Coordinators Supervised**	23
1995-Present	Visiting Professors and Researchers hosted**	79
1995-Present	Courses Taught and/or developed	53
1995-Present	Graduate Student Examining Committee Member	51
1995-Present	Graduate Student Supervisory Committee Member	43
1995-Present	Patents Filed	14
1995-Present	Spin-off Companies Created	12
1995-present	Databases and Web-based Servers Created	65

Funds secured: over **$245 million through 184 Grants and Awards*

***Direct supervision and mentorship for about 600 students, technicians, researchers, and professors*

AWARDS, HONOURS, AND PRIZES (1997-2025)

Year(s)	Award/Recognition	Organization
International		
2018 - 2025	Top 200 Most Influential Researchers (Biological Sciences/Biochemistry)	Thomson Reuters/Clarivate Analytics
2014 - 2017	Top 100+ Most Influential Researchers (Biological Sciences)	Thomson Reuters/Clarivate Analytics
2016	Australian-New Zealand Magnetic Resonance Society	ANZMAG Lectureship
2014	Lifetime Honorary Fellow	International Metabolomics Society
2001	Young Investigator Prize	Astra-Zeneca-CFPS
1997	New Investigator Award	American Assoc. Colleges of Pharmacy
National/Provincial		
2026	Synergy Award for Innovation	Natural Sciences and Engineering Research Council
2026	Governor General's Innovation Award	The Rideau Hall Foundation (RHF)
2026	CAFA Distinguished Academic Award	Confederation of Alberta Faculty Associations
2025	Gerhard Herzberg Canada Gold Medal	Natural Sciences and Engineering Research Council
2025	ASTech Award for AI/ML and Quantum Computing	Alberta Science, Technology, and Leadership Awards
2024	Brockhouse Canada Prize for Interdisciplinary Research in Science and Engineering (Wishart & Greiner)	Natural Sciences and Engineering Research Council
2023	Canada Research Chair Tier 1	Government of Canada
2017	Fellow of the Royal Society of Canada	Royal Society of Canada
2005	Bristol-Myers Squibb Research Chair	CIHR-Rx&D and Bristol-Myers Squibb
Institutional		
2026	Killam Annual Professorship	University of Alberta, Edmonton, AB
2026	McCalla Professorship	University of Alberta, Edmonton, AB

2025	University Cup Award	University of Alberta, Edmonton, AB
2023	J. Gordin Kaplan Award for Excellence in Research	University of Alberta, Edmonton, AB
2022	Innovation Award for Q Boost Inc	University of Alberta, Edmonton, AB
2022	Innovation Award for MetabolomiX Inc	University of Alberta, Edmonton, AB
2021	Innovation Award for Molecular You Corporation	University of Alberta, Edmonton, AB
2021	Innovation Award for Tricca Technologies Inc.	University of Alberta, Edmonton, AB
2018	Distinguished University Professor	University of Alberta, Edmonton, AB
2018	University Alumni Award	University of Alberta, Edmonton, AB

DIRECTORSHIPS OF RESEARCH SERVICE CENTRES AND SERVICE CORES (2002-2025)

2002-2005	Director of the Alberta Cancer Board Polyomx Bioinformatics Core
2002-2011	Director of the Genome Canada Bioinformatics Help Desk
2002-2006	Director of the PENCE Bioinformatics Core Facility
2008-2012	Director of the Pan Alberta Metabolomics Platform – PANAMP
2010-2013	Director of the PrioNet Prion Protein and Plasmid Production (PrP5) Facility
2011-2019	Director of The Metabolomics Innovation Centre – TMIC
2014-2018	Director of the Metabolomics Technology Demonstration Centre
2019-Present	Co-director of The Metabolomics Innovation Centre – TMIC

MAJOR CONTRIBUTIONS TO SCIENCE

I have authored more than 640 peer-reviewed articles, including landmark papers in *Nature Communications*, *Nature Reviews Drug Discovery*, *Physiological Reviews*, *Nucleic Acids Research*, *Cell Reports Medicine*, *Analytical Chemistry*, and the *Proceedings of the National Academy of Sciences*. My research has advanced computational chemistry and chemical informatics through the development of methods and resources for identifying, classifying, representing, predicting, and interpreting small molecules. These contributions include foundational chemical databases such as HMDB and DrugBank; computational tools such as CFM-ID, ClassyFire, BioTransformer, MetaboAnalyst, and DeepMet foundational chemical databases such as HMDB and DrugBank; and standardized quantitative assays that have helped transform metabolomics into a rigorous, data-driven, and globally accessible discipline. My work has been cited more than 173,000 times and I have an H-index of over 156. A full and up-to-date list of my publications is available through my Google Scholar profile: https://scholar.google.com/citations?hl=es&user=-JSn-WgAAAAJ&view_op=list_works.

1) Computational Chemistry and Chemical Informatics for Small-Molecule Analysis

My early work in nuclear magnetic resonance (NMR) spectroscopy revealed fundamental relationships between chemical shifts and protein secondary structure. Building on this work, I demonstrated the power of computational approaches for interpreting complex spectral data, including some of the earliest applications of machine learning to biofluid NMR, enabling automated metabolite identification and quantification. These innovations led to the co-founding of Chenomx Inc., which pioneered widely adopted software for NMR-based metabolite analysis.

My team subsequently developed computational methods for processing, identifying, classifying, and predicting small molecules and their spectra, structures, properties, and metabolic products. These

include NMR spectral prediction and deconvolution tools such as MagMet, Bayesil, and PROSPRE [1]; mass spectral prediction and compound-identification tools such as CFM-ID [2] and GCMS-ID [3]; the structure-based chemical classification system ClassyFire [4] and its associated chemical ontology, ChemFOnt [5]; and BioTransformer [6], which predicts small-molecule metabolism and metabolic transformation products.

CFM-ID uses probabilistic graphical models to predict tandem mass spectra from chemical structures, annotate experimentally collected spectra, and identify compounds matching observed spectra. It has been integrated into resources including METLIN, HMDB, and DrugBank and has received more than 1,500 citations. ClassyFire is the first comprehensive, fully automated, structure-based chemical taxonomy system. It has been used to classify chemicals in more than a dozen databases, including PubChem, ChEBI, LIPID MAPS, and HMDB.

My group was also the first to apply machine-learning techniques to small-molecule metabolism prediction. This work produced BioTransformer, which uses machine-learning and knowledge-based approaches to predict metabolic reactions and their resulting chemical structures. BioTransformer has been expanded to predict small-molecule metabolism in human tissues and environmental systems.

More recently, I contributed to the development of DeepMet [7], a chemical language model trained on the structures of known metabolites. DeepMet anticipates previously unrecognized metabolite structures and integrates these predictions with mass-spectrometry data to support metabolite discovery. The approach has identified several dozen previously unrecognized mammalian metabolites and demonstrates the potential for chemical language models to expand existing maps of the metabolome. The paper was published in *Nature* in 2026.

My group also developed MetaboAnalyst [8], a web-based platform for metabolomic data processing, analysis, and interpretation. MetaboAnalyst is routinely used by metabolomics laboratories worldwide and received more than 15 million website accesses in the past year. Nearly half of published metabolomics papers cite MetaboAnalyst, and its principal publications have been cited more than 15,000 times. Together, these tools have established widely adopted computational methods for automated and reproducible small-molecule identification, classification, prediction, and analysis.

Selected Publications

[1] S. Ravanbakhsh, *et al*. Accurate, fully-automated NMR spectral profiling for metabolomics, *PLoS One*. **10** (2015) e0124219. doi:10.1371/journal.pone.0124219.

[2] F. Allen, *et al*. CFM-ID: A web server for annotation, spectrum prediction and metabolite identification from tandem mass spectra, *Nucleic Acids Res*. **42** (2014) W94–W99. doi:10.1093/NAR/GKU436.

[3] J. Wakoli, *et al*. GCMS-ID: A webserver for identifying compounds from gas chromatography mass spectrometry experiments, *Nucleic Acids Res*. **52** (2024) W381–W389. doi:10.1093/nar/gkae425.

[4] Y. Djoumbou Feunang, *et al*. ClassyFire: Automated chemical classification with a comprehensive, computable taxonomy, *J Cheminform*. **8** (2016) 61. doi:10.1186/S13321-016-0174-Y.

[5] D.S. Wishart et al., ChemFOnt: the chemical functional ontology resource, *Nucleic Acids Res*. **51** (2022) D1220–D1229. doi:10.1093/NAR/GKAC919.

[6] Y. Djoumbou-Feunang et al., BioTransformer: A comprehensive computational tool for small molecule metabolism prediction and metabolite identification, *J Cheminform*. **11** (2019) 2. doi:10.1186/s13321-018-0324-5.

[7] H. Qiang et al., Language model-guided anticipation and discovery of mammalian metabolites, Nature (2026). doi:10.1038/s41586-025-09969-x.

[8] J. Xia et al., MetaboAnalyst: a web server for metabolomic data analysis and interpretation., *Nucleic Acids Res*. **37** (2009) W652-60. doi:10.1093/nar/gkp356.

2) Chemical Databases and Knowledge Resources

Recognizing the need for comprehensive chemical reference resources, I initiated a sustained research program focused on the systematic collection, curation, representation, and integration of small-molecule structures, spectra, properties, biological functions, and molecular interactions. Prior to this work, chemical and metabolomic knowledge was highly fragmented, with no unified resources linking chemical structures to reference spectra, biological concentrations, molecular targets, pathways, and disease associations.

Central to this effort was the Human Metabolome Project, which I initiated in 2006 to systematically identify, quantify, and catalogue metabolites present in human biofluids and tissues. Its principal outcome was the creation of the Human Metabolome Database (HMDB) [9,10], which now contains information on more than 250,000 metabolites, along with extensive spectral, concentration, and disease-association data. My team also completed comprehensive experimental characterizations of human serum, urine, cerebrospinal fluid, saliva, and feces, leading to the identification and annotation of more than 3,000 human metabolites.

Building on this foundation, I developed complementary resources linking metabolites, drugs, pathways, and biomarkers. These include DrugBank [11,12], which integrates detailed chemical, pharmacological, and molecular information on drugs and their targets; the Small Molecule Pathway Database [13] and PathBank [14], which provide maps of metabolic, signalling, and disease pathways; and MarkerDB [15], a curated collection of clinically validated genetic, metabolic, and protein biomarkers.

My group also developed specialized chemical resources supporting model-organism research, food science, natural-products chemistry, and environmental health. These include the Natural Products Magnetic Resonance Database [16], FooDB, YMDB, ECMDB, and Phenol-Explorer [17]. These resources contain chemical structures, molecular properties, biological annotations, and millions of reference NMR, GC-MS, and LC-MS spectra. They have established a globally adopted chemical knowledge infrastructure supporting metabolomics, drug discovery, natural-products research, nutrition science, and systems biology.

Selected Publications

[9] D.S. Wishart et al., HMDB: The human metabolome database, *Nucleic Acids Res*. **35** (2007) D521–D526. doi:10.1093/nar/gkl923.

[10] D.S. Wishart et al., HMDB 5.0: The Human Metabolome Database for 2022, *Nucleic Acids Res*. **50** (2022) D622–D631. doi:10.1093/nar/gkab1062.

[11] D.S. Wishart et al., DrugBank: a comprehensive resource for in silico drug discovery and exploration, *Nucleic Acids Res*. **34** (2006) D668–D672. doi:10.1093/NAR/GKJ067.

[12] C. Knox et al., DrugBank 6.0: the DrugBank knowledgebase for 2024, *Nucleic Acids Res*. **52** (2023) D1265–D1275. doi:10.1093/nar/gkad976.

[13] A. Frolkis et al., SMPDB: The Small Molecule Pathway Database, *Nucleic Acids Res*. **38** (2009) D408–D487. doi:10.1093/nar/gkp1002.

[14] D.S. Wishart et al., PathBank: A comprehensive pathway database for model organisms, *Nucleic Acids Res*. **48** (2020) D470–D478. doi:10.1093/nar/gkz861.

[15] D.S. Wishart et al., MarkerDB: an online database of molecular biomarkers, *Nucleic Acids Res*. **49** (2021) D1259–D1267. doi:10.1093/nar/gkaa1067.

[16] D.S. Wishart et al., NP-MRD: The Natural Products Magnetic Resonance Database, *Nucleic Acids Res*. **50** (2022) D665–D677. doi:10.1093/NAR/GKAB1052.

[17] V. Neveu et al., Phenol-Explorer: an online comprehensive database on polyphenol contents in foods, *Database (Oxford)* **2010** (2010). doi:10.1093/database/bap024.

3) Computational and Experimental Methods for Quantitative Metabolomics

I have had a long-standing interest in developing, assessing, and improving the performance of targeted quantitative metabolomic assays. My group developed computational and experimental approaches for the automated identification and quantification of metabolites using NMR and mass spectrometry. These include Bayesil [1] and MagMet [8] for automated NMR spectral profiling, as well as LC-MS assays designed to quantitatively measure large numbers of metabolites in serum, plasma, and urine [19,20].

These assays have since been expanded to measure more than 1,000 compounds in serum and plasma and applied to the comprehensive analysis of the National Institute of Standards and Technology Standard Reference Material 1950 [21]. This work has contributed to more accurate, efficient, and reproducible metabolite measurement across plasma, serum, urine, cerebrospinal fluid, and stool.

The resulting methods have been used to study lung, colorectal, and pancreatic cancers, as well as metabolic, cardiovascular, cognitive, diabetic, and maternal health conditions. My group's biomarker discoveries have contributed to colorectal-cancer screening in Nigeria [22], early-detection strategies for pancreatic cancer in Canada [23], and lung-cancer diagnostics in Canada and China [24,25].

Selected Publications

[18] M. Rout et al., MagMet: A fully automated web server for targeted nuclear magnetic resonance metabolomics of plasma and serum, *Magn Reson Chem*. **61** (2023) 681–704. doi:10.1002/mrc.5371.

[19] L. Zhang et al., A comprehensive LC–MS metabolomics assay for quantitative analysis of serum and plasma, *Metabolites* **14** (2024) 622. doi:10.3390/metabo14110622.

[20] J. Zheng et al., Comprehensive targeted metabolomic assay for urine analysis, *Anal Chem*. **92** (2020) 10627–10634. doi:10.1021/ACS.ANALCHEM.0C01682.

[21] R. Mandal et al., Comprehensive, quantitative analysis of SRM 1950: the NIST human plasma reference material, *Anal Chem*. **97** (2025) 667–675. doi:10.1021/acs.analchem.4c05018.

[22] L. Zhang et al., Identification of urinary biomarkers of colorectal cancer: Towards the development of a colorectal screening test in limited resource settings, *Cancer Biomark*. **36** (2023) 17–30. doi:10.3233/CBM-220034.

[23] M.A. Anwar et al., Blood-based multiomics-guided detection of a precancerous pancreatic tumor, *OMICS* **28** (2024) 182–192. doi:10.1089/omi.2023.0278.

[24] L. Zhang et al., A high-performing plasma metabolite panel for early-stage lung cancer detection, *Cancers* **12** (2020) 622. doi:10.3390/cancers12030622.

[25] Z. Chen et al., Identification of high-performing blood metabolite biomarkers of lung cancer in a Chinese population, *Phenomics* (2026). doi:10.1007/s43657-024-00206-5.

4) Chemical Exposomics and Microbiome–Metabolite Interactions

I have played a leading role in expanding metabolomics into the field of the chemical exposome, changing how environmental exposures are catalogued, measured, and interpreted in human health research. My group developed Exposome-Explorer [26], the first database dedicated to biomarkers of environmental and dietary exposures, and the Toxin and Toxin Target Database, a comprehensive resource cataloguing toxic substances and their molecular targets. These databases provide the chemical and computational infrastructure needed to connect environmental, dietary, and toxic exposures with validated biomarkers.

My work has also highlighted the "blood exposome" [27], the diverse set of endogenous, dietary, pharmaceutical, and pollutant-derived chemicals circulating in human blood. By demonstrating that these chemicals exceed genome-encoded metabolites in number, diversity, and dynamic range, this work helped motivate data-driven approaches to identifying environmental contributors to chronic disease.

I also led the development of the Human Microbial Metabolome Database (MiMeDB) [28], the first resource to integrate microbial genomics, metabolomics, protein function, metabolic pathways, and exposure sources into a unified searchable platform. MiMeDB contains data on 1,904 microbes, 24,254 metabolites, and 626 health effects. It connects microbial metabolites with their biosynthetic enzymes, human protein targets, physiological roles, concentration ranges, exposure sources, and documented health effects. Together, this work frames the metabolome as an integrative chemical readout of the combined influences of environmental exposures, diet, the microbiome, and the genome.

Selected Publications

[26] V. Neveu et al., Exposome-Explorer: A manually-curated database on biomarkers of exposure to dietary and environmental factors, *Nucleic Acids Res*. **45** (2017) D979–D984. doi:10.1093/nar/gkw980.

[27] S.M. Rappaport et al., The blood exposome and its role in discovering causes of disease, *Environ Health Perspect*. **122** (2014) 769–774. doi:10.1289/ehp.1308015.

[28] D.S. Wishart et al., MiMeDB: The Human Microbial Metabolome Database, *Nucleic Acids Res*. **51** (2023) D611–D620. doi:10.1093/NAR/GKAC868.

5) Translation of Small-Molecule Technologies into Clinical Applications

From 2012 to 2018, I oversaw the Metabolomic Tricorder Project, in which University of Alberta and National Research Council laboratories developed metabolomic test kits and portable devices for small-molecule detection. More recently, my group developed point-of-care colorimetric assays to detect ascorbate, hippuric acid, diacetylspermine, carnitine, succinate, and creatinine [29].

These biosensor platforms have been translated into point-of-care clinical tests, including a urine metabolomics assay for colorectal-cancer screening in southwestern Nigeria [30]. The assay demonstrated high sensitivity, specificity, and patient acceptance, supporting its feasibility for broader clinical implementation. The University of Alberta spin-off Tricca Technologies Inc. is adapting these biosensor platforms for commercialization. This work demonstrates how small-molecule measurement technologies can move from analytical development to practical diagnostic applications.

Selected Publications

[29] S. Bai et al., Development of a point-of-care colorimetric metabolomic sensor platform, *Biosens Bioelectron*. **253** (2024) 116186. doi:10.1016/j.bios.2024.116186.

[30] A.A. Adeomi et al., Point-of-care urine metabolomics test to diagnose colorectal cancers in low- and middle-income countries: a pilot controlled trial in southwestern Nigeria, *JCO Glob Oncol*. **11** (2025) e2500062. doi:10.1200/GO-25-00062.

MENTIONED WEB-BASED RESOURCES (Open Access; *partially Open Access)

Databases	***Web-based Metabolomics Tools***
1) DrugBank* https://www.drugbank.com/	1) Bayesil http://bayesil.ca/
2) ECMDB https://ecmdb.ca/	2) Biotransformer https://biotransformer.ca/new
3) FooDB https://foodb.ca/	3) CFM-ID https://cfmid.wishartlab.com/
4) HMDB https://hmdb.ca/	4) ClassyFire http://classyfire.wishartlab.com/
5) MarkerDB https://markerdb.ca/	5) NMRlib http://nmrlib.wishartlab.com/
6) MiMeDB https://mimedb.org/	6) GC-Autofit http://gc-autofit.wishartlab.com/
7) NP-MRD https://np-mrd.org/	7) MagMet* http://magmet.ca/users/login
8) PathBank https://pathbank.org/	8) MetaboAnalyst https://www.metaboanalyst.ca/
9) SMPDB https://smpdb.ca/	9) PROSPRE https://prospre.ca/
10) T3DB http://www.t3db.ca/	10) GCMS-ID https://www.gcms-id.ca/
11) YMDB http://www.ymdb.ca/	11) RT-Pred https://rtpred.ca/
12) Serum Metabolome https://serummetabolome.ca/	
13) SRM1950 https://srm1950-data.wishartlab.com/	
14) CSF Metabolome https://csfmetabolome.ca/	
15) Phenol Explorer http://phenol-explorer.eu/	

SELECTED NOTABLE PRESENTATIONS

1. "The Human Metabolome Project and its Impact on Human Disease," presented at the 1st Annual Meeting of the Metabolomics Society, Tsuruoka City, Japan (2005).
2. "Automated Metabolite Identification and Quantification by NMR," presented at the 5th Gordon Research Conference on Computational Aspects of Biomolecular NMR, Il Ciocco, Italy (2008).
3. "New Software Tools and Resources for MS-based Metabolomics," presented at the University of Copenhagen, Copenhagen, Denmark (2016).
4. "New Technologies for Large Scale Analysis of Small Molecules," presented at the 2017 HUPO Meeting, San Diego, CA (2017).
5. "Bioinformatic Tools for Clinical Metabolomics", presented at the Clinical Metabolomics Copenhagen Conference, Copenhagen, DK (2018).

6. “BioTransformer: An Accurate, Freely Available Tool for Predicting Small Molecule Metabolism-Applications in Drug Discovery,” presented at the 255th American Chemical Society National Meeting, New Orleans, LA, USA (2018).
7. “Using Artificial Intelligence to Predict the Next Designer Drugs,” presented at the Ohio Narcotics Intelligence Center Drug Summit, Columbus, Ohio, USA (2022).
8. “A Quantitative Assay for Measuring 1000 Metabolites in Serum and Plasma” presented at 6th Annual MANA Conference 2024, Tampa, FL (2024).
9. “Automating Targeted and Untargeted MS-Based Microbial Metabolomics,” presented at the PacifiChem 2025 Symposium on MS in Microbiome Research, Honolulu, Hawaii, USA (2025).

SPIN-OFF COMPANIES (Founded and/or Scientific Officer)

1. BioTools Inc. (1997-2011), Canada’s first bioinformatics company, developed sequence-analysis software that reached more than $1 million in annual sales.

2. Chenomx Inc. (2000 – pres.), the world’s first and oldest metabolomics company. For more than 25 years, it has sold software that uses advanced algorithms to identify and quantify metabolites from NMR spectra.
3. OMx Personal Health Analytics Inc., also known as OMx or DrugBank.com (2012 – pres.) is Canada’s first drug-informatics company. DrugBank is used by major pharmaceutical companies, and ideas generated from it are estimated to have contributed to more than $1 billion in new or repurposed drug sales.
4. Molecular You Corporation or MYCo (2014 – pres.), Canada’s and the world’s first precision-medicine company, uses proteomic and metabolomic profiles for personalized health management and has secured over $20 million in financing.
5. MetaSci Inc. (2017 – pres.) supplies more than 20 chemical reference libraries derived from approximately 1,250 human, plant, bacterial, and food metabolites.
6. Tricca Technologies Inc. (2017 – pres.) develops automated systems for metabolomics kits and commercialized IceKube for transporting biological samples at sub-zero temperatures.
7. MetabolomiX Inc., or MTX Inc. (2019 – pres.) develops metabolomics kits for NMR, GC-MS, and LC-MS platforms. Its kits are compatible with multiple instrument models and can be adapted for different biofluids.
8. Metabolomics Innovations Inc. or MII (2020 – pres.) licenses and enhances HMDB, FooDB, T3DB, MarkerDB, and SMPDB and develops machine-learning software for agriculture.
9. Q Boost Inc. (2021 – pres.) provides quality-management and regulatory-compliance services to academic, commercial, and clinical laboratories.
10. Metabosensor (2022–pres.) develops portable biosensors for real-time metabolite detection, disease diagnosis, and patient monitoring.
11. Linearis (2022–pres.) develops non-invasive, portable technologies for real-time metabolite detection and monitoring, with applications in early disease detection, diagnostics, and personalized medicine.
12. iollo (2022-pres.) based in San Francisco, CA uses metabolomics and AI for at-home testing, personalized health recommendations, and pharmaceutical applications, generating approximately US$440,000 in 2025.
13. Nutrowell (2025-pres.) integrates metabolomics, proteomics, and microbiome analysis for personalized nutrition, disease prevention, and healthy aging.

SELECTED PATENTS

1. D.S. Wishart et al. **Compound Identification and Quantitation in Liquid Mixtures—Method and Process Using an Automated Nuclear Magnetic Resonance Measurement System.** UK Patent GB2410559, awarded June 2005.

2. D.S. Wishart, K. Azyat and D. Golec. **Heterobifunctional Linker.** U.S. Patent 10,562,863 B2, issued February 18, 2020.

3. S. MacKay, J. Chen, P. Hermansen and D.S. Wishart. **Devices and Methods for Nanoparticle Enhanced Impedance-Based Molecular Sensing.** U.S. Patent 10,585,094 B2, issued March 10, 2020.

4. R. Kaddurah-Daouk, D.S. Wishart and D.Y. Rayat. **Systems and Devices for Coupling Metabolomics Data with Digital Monitors for Precision Health.** U.S. Patent Application 18/837,460, filed January 25, 2023.