David F Grant

List of Publications by Year
in descending order

33 papers	2,019 citations	361413 20 h-index	395702 33 g-index
35 all docs	35 docs citations	35 times ranked	2354 citing authors

#	Article	IF	Citations
1	High-Throughput Non-targeted Chemical Structure Identification Using Gas-Phase Infrared Spectra. Analytical Chemistry, 2021, 93, 10688-10696.	6.5	4
2	Comprehensive Assessment of GFN Tight-Binding and Composite Density Functional Theory Methods for Calculating Gas-Phase Infrared Spectra. Journal of Chemical Theory and Computation, 2020, 16, 7044-7060.	5.3	32
3	MolFind2: A Protocol for Acquiring and Integrating MS3 Data to Improve In Silico Chemical Structure Elucidation for Metabolomics. Methods in Molecular Biology, 2020, 2084, 283-295.	0.9	1
4	Development of a Reverse Phase HPLC Retention Index Model for Nontargeted Metabolomics Using Synthetic Compounds. Journal of Chemical Information and Modeling, 2018, 58, 591-604.	5.4	21
5	Evaluation of an Artificial Neural Network Retention Index Model for Chemical Structure Identification in Nontargeted Metabolomics. Analytical Chemistry, 2018, 90, 12752-12760.	6.5	40
6	Development of Database Assisted Structure Identification (DASI) Methods for Nontargeted Metabolomics. Metabolites, 2016, 6, 17.	2.9	5
7	Correction of precursor and product ion relative abundances in order to standardize CID spectra and improve Ecom50 accuracy for non-targeted metabolomics. Metabolomics, 2015, 11, 753-763.	3.0	9
8	Ion Mobility-Derived Collision Cross Section As an Additional Measure for Lipid Fingerprinting and Identification. Analytical Chemistry, 2015, 87, 1137-1144.	6.5	245
9	Optimizing artificial neural network models for metabolomics and systems biology: an example using HPLC retention index data. Bioanalysis, 2015, 7, 939-955.	1.5	20
10	Ion Mobility Derived Collision Cross Sections to Support Metabolomics Applications. Analytical Chemistry, 2014, 86, 3985-3993.	6.5	279
11	BioSM: Metabolomics Tool for Identifying Endogenous Mammalian Biochemical Structures in Chemical Structure Space. Journal of Chemical Information and Modeling, 2013, 53, 601-612.	5.4	30
12	CHEMICAL STRUCTURE IDENTIFICATION IN METABOLOMICS: COMPUTATIONAL MODELING OF EXPERIMENTAL FEATURES. Computational and Structural Biotechnology Journal, 2013, 5, e201302005.	4.1	12
13	In Silico Enzymatic Synthesis of a 400â€‰000 Compound Biochemical Database for Nontargeted Metabolomics. Journal of Chemical Information and Modeling, 2013, 53, 2483-2492.	5.4	37
14	Development of Ecom₅₀ and Retention Index Models for Nontargeted Metabolomics: Identification of 1,3-Dicyclohexylurea in Human Serum by HPLC/Mass Spectrometry. Journal of Chemical Information and Modeling, 2012, 52, 1222-1237.	5.4	46
15	Correlation of Ecom₅₀ values between mass spectrometers: effect of collision cell radiofrequency voltage on calculated survival yield. Rapid Communications in Mass Spectrometry, 2012, 26, 2303-2310.	1.5	20
16	MolFind: A Software Package Enabling HPLC/MS-Based Identification of Unknown Chemical Structures. Analytical Chemistry, 2012, 84, 9388-9394.	6.5	65
17	CE₅₀: Quantifying collision induced dissociation energy for small molecule characterization and identification. Journal of the American Society for Mass Spectrometry, 2009, 20, 1759-1767.	2.8	93
18	Prediction of HPLC Retention Index Using Artificial Neural Networks and IGroup E-State Indices. Journal of Chemical Information and Modeling, 2009, 49, 788-799.	5.4	25

#	Article	IF	Citations
19	Database searching for structural identification of metabolites in complex biofluids for mass spectrometry-based metabonomics. Bioanalysis, 2009, 1, 1627-1643.	1.5	15
20	Mass Spectral Metabonomics beyond Elemental Formula: Chemical Database Querying by Matching Experimental with Computational Fragmentation Spectra. Analytical Chemistry, 2008, 80, 5574-5582.	6.5	117
21	A semiparametric modeling framework for potential biomarker discovery and the development of metabonomic profiles. BMC Bioinformatics, 2008, 9, 38.	2.6	9
22	Effects of human soluble epoxide hydrolase polymorphisms on isoprenoid phosphate hydrolysis. Biochemical and Biophysical Research Communications, 2006, 341, 254-260.	2.1	57
23	NMR and HPLC-MS/MS analysis of synthetically prepared linoleic acid diol glucuronides. Chemistry and Physics of Lipids, 2006, 140, 75-87.	3.2	8
24	Distribution of soluble epoxide hydrolase, cytochrome P450 2C8, 2C9 and 2J2 in human malignant neoplasms. Journal of Molecular Histology, 2006, 37, 133-141.	2.2	75
25	Alignment of high resolution mass spectra: development of a heuristic approach for metabolomics. Metabolomics, 2006, 2, 75-83.	3.0	19
26	Distribution of Soluble Epoxide Hydrolase and of Cytochrome P450 2C8, 2C9, and 2J2 in Human Tissues. Journal of Histochemistry and Cytochemistry, 2004, 52, 447-454.	2.5	221
27	Polymorphisms in Human Soluble Epoxide Hydrolase. Molecular Pharmacology, 2003, 64, 482-490.	2.3	142
28	Linoleic Acid Metabolites Act to Increase Contractility in Isolated Rat Heart. Cardiovascular Toxicology, 2002, 2, 219-230.	2.7	1
29	Defining Mechanisms of Toxicity for Linoleic Acid Monoepoxides and Diols in Sf-21 Cells. Chemical Research in Toxicology, 2001, 14, 431-437.	3.3	23
30	Identification of the Î³-Aminobutyric Acid Receptor Î²2 and Î²3 Subunits in Rat, Rabbit, and Human Kidneys. Journal of the American Society of Nephrology: JASN, 2001, 12, 1107-1113.	6.1	12
31	Linoleic Acid Diols Are Novel Substrates for Human UDP-Glucuronosyltransferases. Archives of Biochemistry and Biophysics, 2000, 380, 294-302.	3.0	28
32	Differential subcellular localization of endogenous and transfected soluble epoxide hydrolase in mammalian cells: evidence for isozyme variants. FEBS Letters, 1999, 445, 301-305.	2.8	16
33	Bioactivation of leukotoxins to their toxic diols by epoxide hydrolase. Nature Medicine, 1997, 3, 562-566.	30.7	268