# Jean Loup M Faulon

## List of Publications by Citations



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|---|---|---|---|
| 99 papers | 3,569 citations | 37 h-index | 57 g-index |
| 114 ext. papers | 4,230 ext. citations | 6 avg, IF | 5.6 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 99 | Predicting protein-protein interactions using signature products. *Bioinformatics*, **2005**, 21, 218-26 | 7.2 | 299 |
| 98 | The signature molecular descriptor. 1. Using extended valence sequences in QSAR and QSPR studies. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 707-20 | | 185 |
| 97 | The signature molecular descriptor. 2. Enumerating molecules from their extended valence sequences. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 721-34 | | 120 |
| 96 | Genome scale enzyme-metabolite and drug-target interaction predictions using the signature molecular descriptor. *Bioinformatics*, **2008**, 24, 225-33 | 7.2 | 117 |
| 95 | Systems chemical biology. *Nature Chemical Biology*, **2007**, 3, 447-50 | 11.7 | 116 |
| 94 | Boolean dynamics of genetic regulatory networks inferred from microarray time series data. *Bioinformatics*, **2007**, 23, 866-74 | 7.2 | 113 |
| 93 | RetroPath2.0: A retrosynthesis workflow for metabolic engineers. *Metabolic Engineering*, **2018**, 45, 158-170 | 9.7 | 108 |
| 92 | An automated Design-Build-Test-Learn pipeline for enhanced microbial production of fine chemicals. *Communications Biology*, **2018**, 1, 66 | 6.7 | 97 |
| 91 | A retrosynthetic biology approach to metabolic pathway design for therapeutic production. *BMC Systems Biology*, **2011**, 5, 122 | 3.5 | 85 |
| 90 | XTMS: pathway design in an eXTended metabolic space. *Nucleic Acids Research*, **2014**, 42, W389-94 | 20.1 | 81 |
| 89 | Developing a methodology for an inverse quantitative structure-activity relationship using the signature molecular descriptor. *Journal of Molecular Graphics and Modelling*, **2002**, 20, 429-38 | 2.8 | 80 |
| 88 | The signature molecular descriptor. 3. Inverse-quantitative structure-activity relationship of ICAM-1 inhibitory peptides. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 263-73 | 2.8 | 72 |
| 87 | Is There Any Order in the Structure of Lignin?. *Energy & Fuels*, **1994**, 8, 402-407 | 4.1 | 66 |
| 86 | Stochastic Generator of Chemical Structure. 1. Application to the Structure Elucidation of Large Molecules. *Journal of Chemical Information and Computer Sciences*, **1994**, 34, 1204-1218 | | 66 |
| 85 | A three-dimensional model for lignocellulose from gymnospermous wood. *Organic Geochemistry*, **1994**, 21, 1169-1179 | 3.1 | 65 |
| 84 | Microbial Genes for a Circular and Sustainable Bio-PET Economy. *Genes*, **2019**, 10, | 4.2 | 64 |
| 83 | Retropath: automated pipeline for embedded metabolic circuits. *ACS Synthetic Biology*, **2014**, 3, 565-77 | 5.7 | 62 |

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| 82 | The signature molecular descriptor. 4. Canonizing molecules using extended valence sequences. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 427-36 | | 62 |
| 81 | Molecular signatures-based prediction of enzyme promiscuity. *Bioinformatics*, **2010**, 26, 2012-9 | 7.2 | 61 |
| 80 | OMG: Open Molecule Generator. *Journal of Cheminformatics*, **2012**, 4, 21 | 8.6 | 58 |
| 79 | Origins of specificity and promiscuity in metabolic networks. *Journal of Biological Chemistry*, **2011**, 286, 43994-44004 | 5.4 | 53 |
| 78 | Machine Learning of Designed Translational Control Allows Predictive Pathway Optimization in Escherichia coli. *ACS Synthetic Biology*, **2019**, 8, 127-136 | 5.7 | 53 |
| 77 | Isomorphism, Automorphism Partitioning, and Canonical Labeling Can Be Solved in Polynomial-Time for Molecular Graphs. *Journal of Chemical Information and Computer Sciences*, **1998**, 38, 432-444 | | 51 |
| 76 | Sensing new chemicals with bacterial transcription factors. *Current Opinion in Microbiology*, **2016**, 33, 105-112 | 7.9 | 49 |
| 75 | Enumerating metabolic pathways for the production of heterologous target chemicals in chassis organisms. *BMC Systems Biology*, **2012**, 6, 10 | 3.5 | 49 |
| 74 | Validation of RetroPath, a computer-aided design tool for metabolic pathway engineering. *Biotechnology Journal*, **2014**, 9, 1446-57 | 5.6 | 48 |
| 73 | Plug-and-play metabolic transducers expand the chemical detection space of cell-free biosensors. *Nature Communications*, **2019**, 10, 1697 | 17.4 | 47 |
| 72 | SensiPath: computer-aided design of sensing-enabling metabolic pathways. *Nucleic Acids Research*, **2016**, 44, W226-31 | 20.1 | 47 |
| 71 | Compound toxicity screening and structure-activity relationship modeling in Escherichia coli. *Biotechnology and Bioengineering*, **2012**, 109, 846-50 | 4.9 | 47 |
| 70 | Stereo signature molecular descriptor. *Journal of Chemical Information and Modeling*, **2013**, 53, 887-97 | 6.1 | 42 |
| 69 | Expanding Biosensing Abilities through Computer-Aided Design of Metabolic Pathways. *ACS Synthetic Biology*, **2016**, 5, 1076-1085 | 5.7 | 42 |
| 68 | Selenzyme: enzyme selection tool for pathway design. *Bioinformatics*, **2018**, 34, 2153-2154 | 7.2 | 41 |
| 67 | Correlation between Microporosity and Fractal Dimension of Bituminous Coal Based on Computer-Generated Models. *Energy & Fuels*, **1994**, 8, 408-414 | 4.1 | 40 |
| 66 | RetroRules: a database of reaction rules for engineering biology. *Nucleic Acids Research*, **2019**, 47, D1229-D1235 | 20.1 | 40 |
| 65 | Custom-made transcriptional biosensors for metabolic engineering. *Current Opinion in Biotechnology*, **2019**, 59, 78-84 | 11.4 | 38 |

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| 64 | Semisupervised Gaussian Process for Automated Enzyme Search. *ACS Synthetic Biology*, **2016**, 5, 518-28 | 5.7 | 37 |
| 63 | Data mining PubChem using a support vector machine with the Signature molecular descriptor: classification of factor XIa inhibitors. *Journal of Molecular Graphics and Modelling*, **2008**, 27, 466-75 | 2.8 | 37 |
| 62 | The Signature Molecular Descriptor. 5. The Design of Hydrofluoroether Foam Blowing Agents Using Inverse-QSAR. *Industrial & Engineering Chemistry Research*, **2005**, 44, 8883-8891 | 3.9 | 37 |
| 61 | Large scale active-learning-guided exploration for in vitro protein production optimization. *Nature Communications*, **2020**, 11, 1872 | 17.4 | 35 |
| 60 | Optimal bundling of transmembrane helices using sparse distance constraints. *Protein Science*, **2004**, 13, 2613-27 | 6.3 | 35 |
| 59 | Handbook of Chemoinformatics Algorithms | | 35 |
| 58 | Toward Quantitative Structure-Property Relationships for Charge Transfer Rates of Polycyclic Aromatic Hydrocarbons. *Journal of Chemical Theory and Computation*, **2011**, 7, 2549-55 | 6.4 | 34 |
| 57 | Pore Structure of Imogolite Computer Models. *Langmuir*, **1996**, 12, 4463-4468 | 4 | 32 |
| 56 | Metabolic perceptrons for neural computing in biological systems. *Nature Communications*, **2019**, 10, 3880 | 17.4 | 30 |
| 55 | Reinforcement Learning for Bioretrosynthesis. *ACS Synthetic Biology*, **2020**, 9, 157-168 | 5.7 | 30 |
| 54 | Designing novel polymers with targeted properties using the signature molecular descriptor. *Journal of Chemical Information and Modeling*, **2006**, 46, 826-35 | 6.1 | 28 |
| 53 | Molecular dynamics computer simulations of silica aerogels. *Journal of Non-Crystalline Solids*, **1995**, 186, 349-355 | 3.9 | 28 |
| 52 | Stochastic Generator of Chemical Structure. 2. Using Simulated Annealing To Search the Space of Constitutional Isomers. *Journal of Chemical Information and Computer Sciences*, **1996**, 36, 731-740 | | 28 |
| 51 | A computer-aided molecular model for high volatile bituminous coal. *Fuel Processing Technology*, **1993**, 34, 277-293 | 7.2 | 27 |
| 50 | Engineering antibiotic production and overcoming bacterial resistance. *Biotechnology Journal*, **2011** , 6, 812-25 | 5.6 | 24 |
| 49 | Stochastic generator of chemical structure. 3. Reaction network generation. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 894-908 | | 24 |
| 48 | Computer-aided design for metabolic engineering. *Journal of Biotechnology*, **2014**, 192 Pt B, 302-13 | 3.7 | 22 |
| 47 | A retrosynthetic biology approach to therapeutics: from conception to delivery. *Current Opinion in Biotechnology*, **2012**, 23, 948-56 | 11.4 | 20 |

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| 46 | Building a minimal and generalizable model of transcription factor-based biosensors: Showcasing flavonoids. *Biotechnology and Bioengineering*, **2018**, 115, 2292-2304 | 4.9 | 19 |
| 45 | Optimizing Cell-Free Biosensors to Monitor Enzymatic Production. *ACS Synthetic Biology*, **2019**, 8, 1952-1957 | 5.7 | 19 |
| 44 | Exploring the conformational space of membrane protein folds matching distance constraints. *Protein Science*, **2003**, 12, 1750-61 | 6.3 | 19 |
| 43 | Models for Cell-Free Synthetic Biology: Make Prototyping Easier, Better, and Faster. *Frontiers in Bioengineering and Biotechnology*, **2018**, 6, 182 | 5.8 | 19 |
| 42 | biochem4j: Integrated and extensible biochemical knowledge through graph databases. *PLoS ONE*, **2017**, 12, e0179130 | 3.7 | 18 |
| 41 | A dataset of small molecules triggering transcriptional and translational cellular responses. *Data in Brief*, **2018**, 17, 1374-1378 | 1.2 | 18 |
| 40 | Reverse engineering chemical structures from molecular descriptors: how many solutions?. *Journal of Computer-Aided Molecular Design*, **2005**, 19, 637-50 | 4.2 | 17 |
| 39 | Engineering towards production of gatekeeper (2)-flavanones: naringenin, pinocembrin, eriodictyol and homoeriodictyol. *Synthetic Biology*, **2020**, 5, ysaa012 | 3.3 | 17 |
| 38 | PartsGenie: an integrated tool for optimizing and sharing synthetic biology parts. *Bioinformatics*, **2018**, 34, 2327-2329 | 7.2 | 16 |
| 37 | Retrosynthetic design of heterologous pathways. *Methods in Molecular Biology*, **2013**, 985, 149-73 | 1.4 | 16 |
| 36 | Sensitivity analysis of a computational model of the IKK NF-kappaB IkappaBalpha A20 signal transduction network. *Annals of the New York Academy of Sciences*, **2007**, 1115, 221-39 | 6.5 | 16 |
| 35 | Thermodynamic Properties of Asphaltenes Through Computer Assisted Structure Elucidation and Atomistic Simulations. 1. Bulk Arabian Light Asphaltenes. *Petroleum Science and Technology*, **2004**, 22, 877-899 | 1.4 | 15 |
| 34 | Cheminformatics. *Communications of the ACM*, **2012**, 55, 65-75 | 2.5 | 13 |
| 33 | Molecular structures enumeration and virtual screening in the chemical space with RetroPath2.0. *Journal of Cheminformatics*, **2017**, 9, 64 | 8.6 | 10 |
| 32 | A Sense of Balance: Experimental Investigation and Modeling of a Malonyl-CoA Sensor in Escherichia coli. *Frontiers in Bioengineering and Biotechnology*, **2015**, 3, 46 | 5.8 | 10 |
| 31 | Stochastic generator of chemical structure. 4. Building polymeric systems with specified properties. *Journal of Computational Chemistry*, **2001**, 22, 580-590 | 3.5 | 10 |
| 30 | Mapping the patent landscape of synthetic biology for fine chemical production pathways. *Microbial Biotechnology*, **2016**, 9, 687-95 | 6.3 | 8 |
| 29 | Identification of expression patterns of IL-2-responsive genes in the murine T cell line CTLL-2. *Journal of Interferon and Cytokine Research*, **2007**, 27, 991-5 | 3.5 | 8 |

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| 28 | Prediction of beta-strand packing interactions using the signature product. *Journal of Molecular Modeling*, **2006**, 12, 355-61 | 2 | 8 |
| 27 | Calculating the Number-Averaged Molecular Weight (M0) of Aromatic and Hydroaromatic Clusters in Coal using Rubber Elasticity Theory. *Energy & Fuels*, **1994**, 8, 1020-1023 | 4.1 | 8 |
| 26 | Statistical ensemble analysis for simulating extrinsic noise-driven response in NF-B signaling networks. *BMC Systems Biology*, **2013**, 7, 45 | 3.5 | 7 |
| 25 | PMG: Multi-core Metabolite Identification. *Electronic Notes in Theoretical Computer Science*, **2013**, 299, 53-60 | 0.7 | 7 |
| 24 | Development of a Biosensor for Detection of Benzoic Acid Derivatives in. *Frontiers in Bioengineering and Biotechnology*, **2019**, 7, 372 | 5.8 | 5 |
| 23 | SYNBIOCHEM Synthetic Biology Research Centre, Manchester - A UK foundry for fine and speciality chemicals production. *Synthetic and Systems Biotechnology*, **2016**, 1, 271-275 | 4.2 | 5 |
| 22 | PrecisePrimer: an easy-to-use web server for designing PCR primers for DNA library cloning and DNA shuffling. *Nucleic Acids Research*, **2014**, 42, W205-9 | 20.1 | 5 |
| 21 | SYNBIOCHEM-a SynBio foundry for the biosynthesis and sustainable production of fine and speciality chemicals. *Biochemical Society Transactions*, **2016**, 44, 675-7 | 5.1 | 5 |
| 20 | A deterministic algorithm for constrained enumeration of transmembrane protein folds. *Computational Biology and Chemistry*, **2005**, 29, 143-50 | 3.6 | 4 |
| 19 | Constrained walks and self-avoiding walks: implications for protein structure determination. *Journal of Physics A*, **2002**, 35, 1-19 | | 4 |
| 18 | Reaction Network Generation. *Chapman & Hall/CRC Mathematical and Computational Biology Series*, **2010**, 317-341 | | 4 |
| 17 | Disparate data fusion for protein phosphorylation prediction. *Annals of Operations Research*, **2010**, 174, 219-235 | 3.2 | 3 |
| 16 | The Signature Molecular Descriptor. Part 1. Using Extended Valence Sequences in QSAR and QSPR Studies.. *ChemInform*, **2003**, 34, no | | 3 |
| 15 | Plug-and-Play Metabolic Transducers Expand the Chemical Detection Space of Cell-Free Biosensors | | 3 |
| 14 | Efficient learning in metabolic pathway designs through optimal assembling. *IFAC-PapersOnLine*, **2019**, 52, 7-12 | 0.7 | 3 |
| 13 | Optimising protein synthesis in cell-free systems, a review. *Engineering Biology*, **2021**, 5, 10-19 | 1.1 | 3 |
| 12 | In silico, in vitro, and in vivo machine learning in synthetic biology and metabolic engineering. *Current Opinion in Chemical Biology*, **2021**, 65, 85-92 | 9.7 | 3 |
| 11 | Understanding virulence mechanisms in M. tuberculosis infection via a circuit-based simulation framework. *Annual International Conference of the IEEE Engineering in Medicine and Biology Society IEEE Engineering in Medicine and Biology Society Annual International Conference*, **2008**, 2008, 4953-5 | 0.9 | 2 |

# List of Publications

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|---|---|---|---|
| 10 | Using product kernels to predict protein interactions. *Advances in Biochemical Engineering/Biotechnology*, **2008**, 110, 215-45 | 1.7 | 1 |
| 9 | Synthetic Biology at the Hand of Cell-Free Systems **2020**, 275-288 | | 1 |
| 8 | Galaxy-SynBioCAD: Synthetic Biology Design Automation tools in Galaxy workflows | | 1 |
| 7 | Reinforcement Learning for Bio-Retrosynthesis | | 1 |
| 6 | RetroPath2.0: a retrosynthesis workflow for metabolic engineers | | 1 |
| 5 | Extended Metabolic Space Modeling. *Methods in Molecular Biology*, **2018**, 1671, 83-96 | 1.4 | 1 |
| 4 | Enzyme Discovery: Enzyme Selection and Pathway Design. *Methods in Enzymology*, **2018**, 608, 3-27 | 1.7 | 1 |
| 3 | Cell-Free Biosensors and AI Integration.. *Methods in Molecular Biology*, **2022**, 2433, 303-323 | 1.4 | 0 |
| 2 | Graphs: Flexible Representations of Molecular Structures and Biological Networks **2011**, 145-177 | | |
| 1 | XTMS in Action: Retrosynthetic Design in the Extended Metabolic Space of Heterologous Pathways for High-Value Compounds. *Lecture Notes in Computer Science*, **2014**, 256-259 | 0.9 | |