Costas D Maranas

List of Publications by Year in Descending Order

245 papers	12,965 citations	62 h-index	106 g-index
265 ext. papers	15,284 ext. citations	6.5 avg, IF	6.86 L-index

#	Paper	IF	Citations
245	EnZymClass: Substrate specificity prediction tool of plant acyl-ACP thioesterases based on ensemble learning. *Current Research in Biotechnology*, **2022**, 4, 1-9	4.8	2
244	Multiple spillovers from humans and onward transmission of SARS-CoV-2 in white-tailed deer.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119,	11.5	26
243	Assessing the impact of substrate-level enzyme regulations limiting ethanol titer in Clostridium thermocellum using a core kinetic model.. *Metabolic Engineering*, **2022**, 69, 286-301	9.7	0
242	Metabolic engineering of Rhodotorula toruloides IFO0880 improves C16 and C18 fatty alcohol production from synthetic media.. *Microbial Cell Factories*, **2022**, 21, 26	6.4	1
241	Developmental changes in lignin composition are driven by both monolignol supply and laccase specificity.. *Science Advances*, **2022**, 8, eabm8145	14.3	1
240	Quantifying the propagation of parametric uncertainty on flux balance analysis. *Metabolic Engineering*, **2021**, 69, 26-39	9.7	0
239	Recombination and lineage-specific mutations linked to the emergence of SARS-CoV-2 **2021**,		15
238	A Genome-Scale Metabolic Model of 33047 to Guide Genetic Modifications to Overproduce Nylon Monomers. *Metabolites*, **2021**, 11,	5.6	1
237	Computationally Prospecting Potential Pathways from Lignin Monomers and Dimers toward Aromatic Compounds. *ACS Synthetic Biology*, **2021**, 10, 1064-1076	5.7	2
236	Elucidation of trophic interactions in an unusual single-cell nitrogen-fixing symbiosis using metabolic modeling. *PLoS Computational Biology*, **2021**, 17, e1008983	5	3
235	Engineering biology approaches for food and nutrient production by cyanobacteria. *Current Opinion in Biotechnology*, **2021**, 67, 1-6	11.4	11
234	Recent advances in constraint and machine learning-based metabolic modeling by leveraging stoichiometric balances, thermodynamic feasibility and kinetic law formalisms. *Metabolic Engineering*, **2021**, 63, 13-33	9.7	9
233	Modeling Growth Kinetics, Interspecies Cell Fusion, and Metabolism of a Clostridium acetobutylicum/Clostridium ljungdahlii Syntrophic Coculture. *MSystems*, **2021**, 6,	7.6	2
232	Building kinetic models for metabolic engineering. *Current Opinion in Biotechnology*, **2021**, 67, 35-41	11.4	9
231	Recombination and lineage-specific mutations linked to the emergence of SARS-CoV-2. *Genome Medicine*, **2021**, 13, 124	14.4	8
230	dGPredictor: Automated fragmentation method for metabolic reaction free energy prediction and de novo pathway design. *PLoS Computational Biology*, **2021**, 17, e1009448	5	0
229	Dissecting the Metabolic Reprogramming of Maize Root under Nitrogen-Deficient Stress Condition. *Journal of Experimental Botany*, **2021**,	7	3

228	Computational prediction of the effect of amino acid changes on the binding affinity between SARS-CoV-2 spike RBD and human ACE2. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	20
227	Functional analysis of H-pumping membrane-bound pyrophosphatase, ADP-glucose synthase, and pyruvate phosphate dikinase as pyrophosphate sources in .. *Applied and Environmental Microbiology* , **2021**, AEM0185721	4.8	0
226	Genome-scale metabolic reconstruction of the non-model yeast SD108 and its application to organic acids production. *Metabolic Engineering Communications*, **2020**, 11, e00148	6.5	5
225	Thermodynamic Analysis of Glycolysis in Clostridium thermocellum and Thermoanaerobacterium saccharolyticum Using C and H Tracers. *MSystems*, **2020**, 5,	7.6	20
224	K-FIT: An accelerated kinetic parameterization algorithm using steady-state fluxomic data. *Metabolic Engineering*, **2020**, 61, 197-205	9.7	17
223	SNPeffect: identifying functional roles of SNPs using metabolic networks. *Plant Journal*, **2020**, 103, 512-531	6.9	6
222	Metabolic flux analysis reaching genome wide coverage: lessons learned and future perspectives. *Current Opinion in Chemical Engineering*, **2020**, 30, 17-25	5.4	2
221	The importance and future of biochemical engineering. *Biotechnology and Bioengineering*, **2020**, 117, 2305-2318	4.9	7
220	Bacterial colonization reprograms the neonatal gut metabolome. *Nature Microbiology*, **2020**, 5, 838-847	26.6	37
219	Engineering sensitivity and specificity of AraC-based biosensors responsive to triacetic acid lactone and orsellinic acid. *Protein Engineering, Design and Selection*, **2020**, 33,	1.9	1
218	Artificial water channels enable fast and selective water permeation through water-wire networks. *Nature Nanotechnology*, **2020**, 15, 73-79	28.7	52
217	Computational biophysical characterization of the SARS-CoV-2 spike protein binding with the ACE2 receptor and implications for infectivity. *Computational and Structural Biotechnology Journal*, **2020**, 18, 2573-2582	6.8	26
216	IPRO+/-: Computational Protein Design Tool Allowing for Insertions and Deletions. *Structure*, **2020**, 28, 1344-1357.e4	5.2	3
215	Development of a Genome-Scale Metabolic Model of and Its Applications for Integration of Multi-Omics Datasets and Computational Strain Design. *Frontiers in Bioengineering and Biotechnology*, **2020**, 8, 772	5.8	9
214	Metabolic model guided strain design of cyanobacteria. *Current Opinion in Biotechnology*, **2020**, 64, 17-23	11.4	23
213	From directed evolution to computational enzyme engineering—A review. *AICHE Journal*, **2020**, 66, e16847	3.6	31
212	Challenges of cultivated meat production and applications of genome-scale metabolic modeling. *AICHE Journal*, **2020**, 66, e16235	3.6	4
211	A comprehensive genome-scale model for IFO0880 accounting for functional genomics and phenotypic data. *Metabolic Engineering Communications*, **2019**, 9, e00101	6.5	26

210	A diurnal flux balance model of Synechocystis sp. PCC 6803 metabolism. *PLoS Computational Biology*, **2019**, 15, e1006692	5	17
209	Thermodynamic analysis of the pathway for ethanol production from cellobiose in Clostridium thermocellum. *Metabolic Engineering*, **2019**, 55, 161-169	9.7	22
208	EcoFABs: advancing microbiome science through standardized fabricated ecosystems. *Nature Methods*, **2019**, 16, 567-571	21.6	39
207	Pareto Optimality Explanation of the Glycolytic Alternatives in Nature. *Scientific Reports*, **2019**, 9, 2633	4.9	13
206	Reply to Zhou and Li: Plasticity of the genomic haplotype of leads to rapid strain adaptation under laboratory conditions. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 3946-3947	11.5	2
205	Directed Evolution Reveals the Functional Sequence Space of an Adenylation Domain Specificity Code. *ACS Chemical Biology*, **2019**, 14, 2044-2054	4.9	9
204	Predicting the Longitudinally and Radially Varying Gut Microbiota Composition Using Multi-Scale Microbial Metabolic Modeling. *Processes*, **2019**, 7, 394	2.9	12
203	7 Log Virus Removal in a Simple Functionalized Sand Filter. *Environmental Science & Technology* , **2019**, 53, 12706-12714	10.3	10
202	Engineering microbial chemical factories using metabolic models. *BMC Chemical Engineering*, **2019**, 1,	3.5	3
201	Creation and analysis of biochemical constraint-based models using the COBRA Toolbox v.3.0. *Nature Protocols*, **2019**, 14, 639-702	18.8	385
200	From Escherichia coli mutant 13C labeling data to a core kinetic model: A kinetic model parameterization pipeline. *PLoS Computational Biology*, **2019**, 15, e1007319	5	21
199	Genome-Scale Fluxome of UTEX 2973 Using Transient C-Labeling Data. *Plant Physiology*, **2019**, 179, 761-769	7.4	36
198	Elucidation of photoautotrophic carbon flux topology in Synechocystis PCC 6803 using genome-scale carbon mapping models. *Metabolic Engineering*, **2018**, 47, 190-199	9.7	32
197	Exploring the combinatorial space of complete pathways to chemicals. *Biochemical Society Transactions*, **2018**, 46, 513-522	5.1	11
196	MinGenome: An In Silico Top-Down Approach for the Synthesis of Minimized Genomes. *ACS Synthetic Biology*, **2018**, 7, 462-473	5.7	22
195	Pathway design using de novo steps through uncharted biochemical spaces. *Nature Communications*, **2018**, 9, 184	17.4	49
194	Highly Active C-Acyl-ACP Thioesterase Variant Isolated by a Synthetic Selection Strategy. *ACS Synthetic Biology*, **2018**, 7, 2205-2215	5.7	32
193	Computationally Exploring and Alleviating the Kinetic Bottlenecks of Anaerobic Methane Oxidation. *Frontiers in Environmental Science*, **2018**, 6,	4.8	1

192	Modeling Plant Metabolism: Advancements and Future Capabilities **2018**, 57-76		2
191	Engineering of inherent fatty acid biosynthesis capacity to increase octanoic acid production. *Biotechnology for Biofuels*, **2018**, 11, 87	7.8	16
190	Comparative genomics reveals the molecular determinants of rapid growth of the cyanobacterium UTEX 2973. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E11761-E11770	11.5	64
189	OptMAVEn-2.0: De novo Design of Variable Antibody Regions against Targeted Antigen Epitopes. *Antibodies*, **2018**, 7,	7	22
188	A Prospective Study on the Fermentation Landscape of Gaseous Substrates to Biorenewables Using Metabolic Model. *Frontiers in Microbiology*, **2018**, 9, 1855	5.7	4
187	PoreDesigner for tuning solute selectivity in a robust and highly permeable outer membrane pore. *Nature Communications*, **2018**, 9, 3661	17.4	36
186	Accelerating flux balance calculations in genome-scale metabolic models by localizing the application of loopless constraints. *Bioinformatics*, **2018**, 34, 4248-4255	7.2	6
185	The Biochemistry and Physiology of Respiratory-Driven Reversed Methanogenesis **2018**, 183-197		2
184	Computational de novo design of antibodies binding to a peptide with high affinity. *Biotechnology and Bioengineering*, **2017**, 114, 1331-1342	4.9	19
183	Identifying the Metabolic Differences of a Fast-Growth Phenotype in Synechococcus UTEX 2973. *Scientific Reports*, **2017**, 7, 41569	4.9	40
182	Exploiting the Genetic Diversity of Maize Using a Combined Metabolomic, Enzyme Activity Profiling, and Metabolic Modeling Approach to Link Leaf Physiology to Kernel Yield. *Plant Cell*, **2017**, 29, 919-943	11.6	39
181	Computational Redesign of Acyl-ACP Thioesterase with Improved Selectivity toward Medium-Chain-Length Fatty Acids. *ACS Catalysis*, **2017**, 7, 3837-3849	13.1	49
180	Multilevel engineering of the upstream module of aromatic amino acid biosynthesis in Saccharomyces cerevisiae for high production of polymer and drug precursors. *Metabolic Engineering*, **2017**, 42, 134-144	9.7	51
179	Clostridium butyricum maximizes growth while minimizing enzyme usage and ATP production: metabolic flux distribution of a strain cultured in glycerol. *BMC Systems Biology*, **2017**, 11, 58	3.5	12
178	Computational Modeling of Microbial Communities **2017**, 163-189		4
177	Deciphering cyanobacterial phenotypes for fast photoautotrophic growth via isotopically nonstationary metabolic flux analysis. *Biotechnology for Biofuels*, **2017**, 10, 273	7.8	63
176	De novo design of antibody complementarity determining regions binding a FLAG tetra-peptide. *Scientific Reports*, **2017**, 7, 10295	4.9	20
175	Standardizing biomass reactions and ensuring complete mass balance in genome-scale metabolic models. *Bioinformatics*, **2017**, 33, 3603-3609	7.2	55

174	A review of computational tools for design and reconstruction of metabolic pathways. *Synthetic and Systems Biotechnology*, **2017**, 2, 243-252	4.2	73
173	Development of a core kinetic metabolic model consistent with multiple genetic perturbations. *Biotechnology for Biofuels*, **2017**, 10, 108	7.8	26
172	Facile Affinity Maturation of Antibody Variable Domains Using Natural Diversity Mutagenesis. *Frontiers in Immunology*, **2017**, 8, 986	8.4	36
171	SteadyCom: Predicting microbial abundances while ensuring community stability. *PLoS Computational Biology*, **2017**, 13, e1005539	5	91
170	NLP Applications in Metabolic Networks **2016**, 199-222		
169	Mathematical Optimization Fundamentals **2016**, 1-22		
168	LP and Duality Theory **2016**, 23-51		
167	Flux Balance Analysis and LP Problems **2016**, 53-80		2
166	Modeling with Binary Variables and MILP Fundamentals **2016**, 81-106		0
165	Thermodynamic Analysis of Metabolic Networks **2016**, 107-117		1
164	MINLP Fundamentals and Applications **2016**, 223-244		
163	Identification of Connected Paths to Target Metabolites **2016**, 137-153		
162	Computational Strain Design **2016**, 155-172		4
161	NLP Fundamentals **2016**, 173-198		
160	Resolving Network Gaps and Growth Prediction Inconsistencies in Metabolic Networks **2016**, 119-135		1
159	Farnesoid X Receptor Signaling Shapes the Gut Microbiota and Controls Hepatic Lipid Metabolism. *MSystems*, **2016**, 1,	7.6	67
158	Appendix A Coding Optimization Models in GAMS **2016**, 245-256		
157	Metabolic modeling of clostridia: current developments and applications. *FEMS Microbiology Letters*, **2016**, 363,	2.9	39

156	Reversing methanogenesis to capture methane for liquid biofuel precursors. *Microbial Cell Factories*, **2016**, 15, 11	6.4	91
155	Assessing methanotrophy and carbon fixation for biofuel production by Methanosarcina acetivorans. *Microbial Cell Factories*, **2016**, 15, 10	6.4	26
154	Identifying Regulatory Changes to Facilitate Nitrogen Fixation in the Nondiazotroph Synechocystis sp. PCC 6803. *ACS Synthetic Biology*, **2016**, 5, 250-8	5.7	14
153	A genome-scale Escherichia coli kinetic metabolic model k-ecoli457 satisfying flux data for multiple mutant strains. *Nature Communications*, **2016**, 7, 13806	17.4	135
152	A microbial factory for diverse chemicals. *Nature Biotechnology*, **2016**, 34, 513-5	44.5	2
151	Diurnal Regulation of Cellular Processes in the Cyanobacterium Synechocystis sp. Strain PCC 6803: Insights from Transcriptomic, Fluxomic, and Physiological Analyses. *MBio*, **2016**, 7,	7.8	59
150	Advances in de novo strain design using integrated systems and synthetic biology tools. *Current Opinion in Chemical Biology*, **2015**, 28, 105-14	9.7	23
149	Rational design of a synthetic Entner-Doudoroff pathway for improved and controllable NADPH regeneration. *Metabolic Engineering*, **2015**, 29, 86-96	9.7	115
148	13C metabolic flux analysis at a genome-scale. *Metabolic Engineering*, **2015**, 32, 12-22	9.7	58
147	Improving prediction fidelity of cellular metabolism with kinetic descriptions. *Current Opinion in Biotechnology*, **2015**, 36, 57-64	11.4	27
146	Personalized Kinetic Models for Predictive Healthcare. *Cell Systems*, **2015**, 1, 250-1	10.6	1
145	The Iterative Protein Redesign and Optimization (IPRO) suite of programs. *Journal of Computational Chemistry*, **2015**, 36, 251-63	3.5	27
144	Methane oxidation by anaerobic archaea for conversion to liquid fuels. *Journal of Industrial Microbiology and Biotechnology*, **2015**, 42, 391-401	4.2	23
143	Bilevel optimization techniques in computational strain design. *Computers and Chemical Engineering*, **2015**, 72, 363-372	4	30
142	Do genome-scale models need exact solvers or clearer standards?. *Molecular Systems Biology*, **2015**, 11, 831	12.2	41
141	Cyanobacterial Alkanes Modulate Photosynthetic Cyclic Electron Flow to Assist Growth under Cold Stress. *Scientific Reports*, **2015**, 5, 14894	4.9	32
140	Designing overall stoichiometric conversions and intervening metabolic reactions. *Scientific Reports* , **2015**, 5, 16009	4.9	36
139	Achieving Metabolic Flux Analysis for S. cerevisiae at a Genome-Scale: Challenges, Requirements, and Considerations. *Metabolites*, **2015**, 5, 521-35	5.6	12

138	Using Gene Essentiality and Synthetic Lethality Information to Correct Yeast and CHO Cell Genome-Scale Models. *Metabolites*, **2015**, 5, 536-70	5.6	26
137	Recent advances in the reconstruction of metabolic models and integration of omics data. *Current Opinion in Biotechnology*, **2014**, 29, 39-45	11.4	91
136	Coarse-grained optimization-driven design and piecewise linear modeling of synthetic genetic circuits. *European Journal of Operational Research*, **2014**, 237, 665-676	5.6	9
135	d-OptCom: Dynamic multi-level and multi-objective metabolic modeling of microbial communities. *ACS Synthetic Biology*, **2014**, 3, 247-57	5.7	133
134	Coupled enzyme reactions performed in heterogeneous reaction media: experiments and modeling for glucose oxidase and horseradish peroxidase in a PEG/citrate aqueous two-phase system. *Journal of Physical Chemistry B*, **2014**, 118, 2506-17	3.4	27
133	Nitrogen-use efficiency in maize (Zea mays L.): from 'omics' studies to metabolic modelling. *Journal of Experimental Botany*, **2014**, 65, 5657-71	7	61
132	A kinetic model of Escherichia coli core metabolism satisfying multiple sets of mutant flux data. *Metabolic Engineering*, **2014**, 25, 50-62	9.7	131
131	Succinate Overproduction: A Case Study of Computational Strain Design Using a Comprehensive Escherichia coli Kinetic Model. *Frontiers in Bioengineering and Biotechnology*, **2014**, 2, 76	5.8	39
130	OptMAVEn--a new framework for the de novo design of antibody variable region models targeting specific antigen epitopes. *PLoS ONE*, **2014**, 9, e105954	3.7	40
129	Capturing the response of Clostridium acetobutylicum to chemical stressors using a regulated genome-scale metabolic model. *Biotechnology for Biofuels*, **2014**, 7, 144	7.8	42
128	k-OptForce: integrating kinetics with flux balance analysis for strain design. *PLoS Computational Biology*, **2014**, 10, e1003487	5	98
127	Assessing the metabolic impact of nitrogen availability using a compartmentalized maize leaf genome-scale model. *Plant Physiology*, **2014**, 166, 1659-74	6.6	63
126	CLCA: maximum common molecular substructure queries within the MetRxn database. *Journal of Chemical Information and Modeling*, **2014**, 54, 3417-38	6.1	27
125	Systems metabolic engineering design: fatty acid production as an emerging case study. *Biotechnology and Bioengineering*, **2014**, 111, 849-57	4.9	61
124	MAPs: a database of modular antibody parts for predicting tertiary structures and designing affinity matured antibodies. *BMC Bioinformatics*, **2013**, 14, 168	3.6	21
123	Rapid construction of metabolic models for a family of Cyanobacteria using a multiple source annotation workflow. *BMC Systems Biology*, **2013**, 7, 142	3.5	26
122	Optimization-driven identification of genetic perturbations accelerates the convergence of model parameters in ensemble modeling of metabolic networks. *Biotechnology Journal*, **2013**, 8, 1090-104	5.6	22
121	OptZyme: computational enzyme redesign using transition state analogues. *PLoS ONE*, **2013**, 8, e75358	3.7	18

120	Synthetic biology of cyanobacteria: unique challenges and opportunities. *Frontiers in Microbiology*, **2013**, 4, 246	5.7	205
119	Computational tools for metabolic engineering. *Metabolic Engineering*, **2012**, 14, 270-80	9.7	77
118	Mathematical optimization applications in metabolic networks. *Metabolic Engineering*, **2012**, 14, 672-86	9.7	100
117	Impact of stoichiometry representation on simulation of genotype-phenotype relationships in metabolic networks. *PLoS Computational Biology*, **2012**, 8, e1002758	5	27
116	An integrated computational and experimental study for overproducing fatty acids in Escherichia coli. *Metabolic Engineering*, **2012**, 14, 687-704	9.7	86
115	Orchestrating hi-fi annotations. *Nature Chemical Biology*, **2012**, 8, 810-1	11.7	
114	MetRxn: a knowledgebase of metabolites and reactions spanning metabolic models and databases. *BMC Bioinformatics*, **2012**, 13, 6	3.6	96
113	Down-regulation of HtrA1 activates the epithelial-mesenchymal transition and ATM DNA damage response pathways. *PLoS ONE*, **2012**, 7, e39446	3.7	25
112	Reconstruction and comparison of the metabolic potential of cyanobacteria Cyanothece sp. ATCC 51142 and Synechocystis sp. PCC 6803. *PLoS ONE*, **2012**, 7, e48285	3.7	73
111	OptCom: a multi-level optimization framework for the metabolic modeling and analysis of microbial communities. *PLoS Computational Biology*, **2012**, 8, e1002363	5	245
110	Zea mays iRS1563: a comprehensive genome-scale metabolic reconstruction of maize metabolism. *PLoS ONE*, **2011**, 6, e21784	3.7	146
109	Recent advances in computational protein design. *Current Opinion in Structural Biology*, **2011**, 21, 467-72	8.1	71
108	Genome-scale metabolic network modeling results in minimal interventions that cooperatively force carbon flux towards malonyl-CoA. *Metabolic Engineering*, **2011**, 13, 578-87	9.7	258
107	Model Simulations Reveal VCAM-1 Augment PAK Activation Rates to Amplify p38 MAPK and VE-Cadherin Phosphorylation. *Cellular and Molecular Bioengineering*, **2011**, 4, 656-669	3.9	4
106	Metabolic reconstruction of the archaeon methanogen Methanosarcina Acetivorans. *BMC Systems Biology*, **2011**, 5, 28	3.5	38
105	Construction of an E. Coli genome-scale atom mapping model for MFA calculations. *Biotechnology and Bioengineering*, **2011**, 108, 1372-82	4.9	36
104	An integrated computational and experimental study to increase the intra-cellular malonyl-CoA: Application to flavanone synthesis **2011**,		1
103	OptCDR: a general computational method for the design of antibody complementarity determining regions for targeted epitope binding. *Protein Engineering, Design and Selection*, **2010**, 23, 849-58	1.9	50

102	OptForce: an optimization procedure for identifying all genetic manipulations leading to targeted overproductions. *PLoS Computational Biology*, **2010**, 6, e1000744	5	276
101	Microbial 1-butanol production: Identification of non-native production routes and in silico engineering interventions. *Biotechnology Journal*, **2010**, 5, 716-25	5.6	39
100	Improving the iMM904 S. cerevisiae metabolic model using essentiality and synthetic lethality data. *BMC Systems Biology*, **2010**, 4, 178	3.5	81
99	Improved computational performance of MFA using elementary metabolite units and flux coupling. *Metabolic Engineering*, **2010**, 12, 123-8	9.7	26
98	A genome-scale metabolic reconstruction of Mycoplasma genitalium, iPS189. *PLoS Computational Biology*, **2009**, 5, e1000285	5	105
97	GrowMatch: an automated method for reconciling in silico/in vivo growth predictions. *PLoS Computational Biology*, **2009**, 5, e1000308	5	169
96	Genome scale reconstruction of a Salmonella metabolic model: comparison of similarity and differences with a commensal Escherichia coli strain. *Journal of Biological Chemistry*, **2009**, 284, 29480-8	5.4	75
95	Analysis of NADPH supply during xylitol production by engineered Escherichia coli. *Biotechnology and Bioengineering*, **2009**, 102, 209-20	4.9	71
94	Computational design of Candida boidinii xylose reductase for altered cofactor specificity. *Protein Science*, **2009**, 18, 2125-38	6.3	76
93	Designing the substrate specificity of d-hydantoinase using a rational approach. *Enzyme and Microbial Technology*, **2009**, 44, 170-175	3.8	21
92	Genome-scale gene/reaction essentiality and synthetic lethality analysis. *Molecular Systems Biology*, **2009**, 5, 301	12.2	126
91	Using Systems Engineering to Reconstruct, Analyze and Redesign Metabolism. *Computer Aided Chemical Engineering*, **2009**, 113-115	0.6	
90	OptGraft: A computational procedure for transferring a binding site onto an existing protein scaffold. *Protein Science*, **2009**, 18, 180-95	6.3	30
89	Predicting biological system objectives de novo from internal state measurements. *BMC Bioinformatics*, **2008**, 9, 43	3.6	75
88	OptCircuit: an optimization based method for computational design of genetic circuits. *BMC Systems Biology*, **2008**, 2, 24	3.5	61
87	Identification of optimal measurement sets for complete flux elucidation in metabolic flux analysis experiments. *Biotechnology and Bioengineering*, **2008**, 100, 1039-49	4.9	32
86	Implication of dynamics in signal transduction and targeted disruption analyses of signaling networks. *Computers and Chemical Engineering*, **2008**, 32, 2065-2071	4	1
85	Extending Iterative Protein Redesign and Optimization (IPRO) in protein library design for ligand specificity. *Biophysical Journal*, **2007**, 92, 2120-30	2.9	24

84	Metabolic flux elucidation for large-scale models using 13C labeled isotopes. *Metabolic Engineering*, **2007**, 9, 387-405	9.7	94
83	Large-scale inference and graph-theoretical analysis of gene-regulatory networks in B. Subtilis. *Physica A: Statistical Mechanics and Its Applications*, **2007**, 373, 796-810	3.3	15
82	Optimization based automated curation of metabolic reconstructions. *BMC Bioinformatics*, **2007**, 8, 212	3.6	232
81	Optimal protein library design using recombination or point mutations based on sequence-based scoring functions. *Protein Engineering, Design and Selection*, **2007**, 20, 361-73	1.9	30
80	Elucidation of directionality for co-expressed genes: predicting intra-operon termination sites. *Bioinformatics*, **2006**, 22, 209-14	7.2	21
79	Bifurcation analysis of the metabolism of E. coli at optimal enzyme levels **2006**,		1
78	A computational framework for the topological analysis and targeted disruption of signal transduction networks. *Biophysical Journal*, **2006**, 91, 382-98	2.9	43
77	IPRO: an iterative computational protein library redesign and optimization procedure. *Biophysical Journal*, **2006**, 90, 4167-80	2.9	45
76	An optimization framework for identifying reaction activation/inhibition or elimination candidates for overproduction in microbial systems. *Metabolic Engineering*, **2006**, 8, 1-13	9.7	242
75	A Computational Procedure for Optimal Engineering Interventions Using Kinetic Models of Metabolism. *Biotechnology Progress*, **2006**, 22, 1507-1517	2.8	28
74	A computational procedure for optimal engineering interventions using kinetic models of metabolism. *Biotechnology Progress*, **2006**, 22, 1507-17	2.8	7
73	Design of combinatorial protein libraries of optimal size. *Proteins: Structure, Function and Bioinformatics*, **2005**, 60, 769-77	4.2	22
72	Elucidation and structural analysis of conserved pools for genome-scale metabolic reconstructions. *Biophysical Journal*, **2005**, 88, 37-49	2.9	42
71	Large-scale inference of the transcriptional regulation of Bacillus subtilis. *Computers and Chemical Engineering*, **2005**, 29, 565-576	4	15
70	In silico design and adaptive evolution of Escherichia coli for production of lactic acid. *Biotechnology and Bioengineering*, **2005**, 91, 643-8	4.9	300
69	Valuation and design of pharmaceutical R&D licensing deals. *AICHE Journal*, **2005**, 51, 198-209	3.6	18
68	DEMSIM: a discrete event based mechanistic simulation platform for gene expression and regulation dynamics. *Journal of Theoretical Biology*, **2005**, 232, 55-69	2.3	6
67	FamClash: a method for ranking the activity of engineered enzymes. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 4142-7	11.5	61

66	OptStrain: a computational framework for redesign of microbial production systems. *Genome Research*, **2004**, 14, 2367-76	9.7	357
65	Flux coupling analysis of genome-scale metabolic network reconstructions. *Genome Research*, **2004**, 14, 301-12	9.7	285
64	Computational challenges in combinatorial library design for protein engineering. *AICHE Journal*, **2004**, 50, 262-272	3.6	27
63	Real-Options-Based Planning Strategies under Uncertainty. *Industrial & Engineering Chemistry Research*, **2004**, 43, 3870-3878	3.9	19
62	Molecular Design Using Quantum Chemical Calculations for Property Estimation. *Industrial & Engineering Chemistry Research*, **2004**, 43, 3419-3432	3.9	15
61	Identifying residue-residue clashes in protein hybrids by using a second-order mean-field approach. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 5091-6	11.5	42
60	Real options based approaches to decision making under uncertainty. *Computer Aided Chemical Engineering*, **2003**, 15, 310-315	0.6	
59	Using multiple sequence correlation analysis to characterize functionally important protein regions. *Protein Engineering, Design and Selection*, **2003**, 16, 397-406	1.9	25
58	Using a residue clash map to functionally characterize protein recombination hybrids. *Protein Engineering, Design and Selection*, **2003**, 16, 1025-34	1.9	20
57	Optimization-based framework for inferring and testing hypothesized metabolic objective functions. *Biotechnology and Bioengineering*, **2003**, 82, 670-7	4.9	159
56	Optknock: a bilevel programming framework for identifying gene knockout strategies for microbial strain optimization. *Biotechnology and Bioengineering*, **2003**, 84, 647-57	4.9	914
55	Exploring the overproduction of amino acids using the bilevel optimization framework OptKnock. *Biotechnology and Bioengineering*, **2003**, 84, 887-99	4.9	105
54	Managing demand uncertainty in supply chain planning. *Computers and Chemical Engineering*, **2003**, 27, 1219-1227	4	330
53	Review of the BRENDA Database. *Metabolic Engineering*, **2003**, 5, 71-3	9.7	40
52	Market-Based Pollution Abatement Strategies: Risk Management Using Emission Option Contracts. *Industrial & Engineering Chemistry Research*, **2003**, 42, 802-810	3.9	22
51	Predicting Out-of-Sequence Reassembly in DNA Shuffling. *Journal of Theoretical Biology*, **2002**, 219, 9-17	2.3	12
50	Review of the Biocatalysis/Biodegradation Database (UM-BBD). *Metabolic Engineering*, **2002**, 4, 111-113	9.7	2
49	Synthesis of Mixed Refrigerant Cascade Cycles. *Chemical Engineering Communications*, **2002**, 189, 1057-1078	2.8	59

48	eCodonOpt: a systematic computational framework for optimizing codon usage in directed evolution experiments. *Nucleic Acids Research*, **2002**, 30, 2407-16	20.1	15
47	Real Options Based Analysis of Optimal Pharmaceutical Research and Development Portfolios. *Industrial & Engineering Chemistry Research*, **2002**, 41, 6607-6620	3.9	74
46	Predicting Out-of-Sequence Reassembly in DNA Shuffling. *Journal of Theoretical Biology*, **2002**, 219, 9-17	2.3	11
45	Predicting out-of-sequence reassembly in DNA shuffling. *Journal of Theoretical Biology*, **2002**, 219, 9-17	2.3	4
44	Multiperiod planning of multisite supply chains under demand uncertainty. *Computer Aided Chemical Engineering*, **2001**, 9, 871-876	0.6	1
43	Review of EcoCyc and MetaCyc Databases. *Metabolic Engineering*, **2001**, 3, 98-99	9.7	6
42	Review of the Enzymes and Metabolic Pathways (EMP) Database. *Metabolic Engineering*, **2001**, 3, 193-194	9.7	11
41	Review of the TEIRESIAS-based tools of the IBM Bioinformatics and Pattern Discovery Group. *Metabolic Engineering*, **2001**, 3, 285-8	9.7	4
40	Probing the performance limits of the Escherichia coli metabolic network subject to gene additions or deletions. *Biotechnology and Bioengineering*, **2001**, 74, 364-75	4.9	99
39	Minimal reaction sets for Escherichia coli metabolism under different growth requirements and uptake environments. *Biotechnology Progress*, **2001**, 17, 791-7	2.8	116
38	Predicting crossover generation in DNA shuffling. *Proceedings of the National Academy of Sciences of the United States of America*, **2001**, 98, 3226-31	11.5	57
37	Creating multiple-crossover DNA libraries independent of sequence identity. *Proceedings of the National Academy of Sciences of the United States of America*, **2001**, 98, 11248-53	11.5	130
36	Optimization in molecular design and bioinformatics. *Computer Aided Chemical Engineering*, **2001**, 9, 1157-1164	0.6	
35	Modeling DNA mutation and recombination for directed evolution experiments. *Journal of Theoretical Biology*, **2000**, 205, 483-503	2.3	50
34	Modeling and optimization of DNA recombination. *Computers and Chemical Engineering*, **2000**, 24, 693-699	4	8
33	Mid-term supply chain planning under demand uncertainty: customer demand satisfaction and inventory management. *Computers and Chemical Engineering*, **2000**, 24, 2613-2621	4	112
32	A Two-Stage Modeling and Solution Framework for Multisite Midterm Planning under Demand Uncertainty. *Industrial & Engineering Chemistry Research*, **2000**, 39, 3799-3813	3.9	121
31	Design of surfactant solutions with optimal macroscopic properties. *Computers and Chemical Engineering*, **1999**, 23, S467-S470	4	6

30	Optimal synthesis of refrigeration cycles and selection of refrigerants. *AICHE Journal*, **1999**, 45, 997-1017	3.6	58
29	A Hierarchical Lagrangean Relaxation Procedure for Solving Midterm Planning Problems. *Industrial & Engineering Chemistry Research*, **1999**, 38, 1937-1947	3.9	62
28	Optimization in Polymer Design Using Connectivity Indices. *Industrial & Engineering Chemistry Research*, **1999**, 38, 1884-1892	3.9	81
27	Design of single-product campaign batch plants under demand uncertainty. *AICHE Journal*, **1998**, 44, 896-911	3.6	49
26	Optimization in product design with properties correlated with topological indices. *Computers and Chemical Engineering*, **1998**, 22, 747-763	4	53
25	Design of multiproduct batch plants under demand uncertainty with staged capacity expansions. *Computers and Chemical Engineering*, **1998**, 22, S789-S792	4	7
24	Multiperiod Planning and Scheduling of Multiproduct Batch Plants under Demand Uncertainty. *Industrial & Engineering Chemistry Research*, **1997**, 36, 4864-4881	3.9	129
23	Locating All Homogeneous Azeotropes in Multicomponent Mixtures. *Industrial & Engineering Chemistry Research*, **1997**, 36, 160-178	3.9	53
22	Prediction of Oligopeptide Conformations via Deterministic Global Optimization. *Journal of Global Optimization*, **1997**, 11, 1-34	1.5	52
21	Solving long-term financial planning problems via global optimization. *Journal of Economic Dynamics and Control*, **1997**, 21, 1405-1425	1.3	73
20	Global optimization in generalized geometric programming. *Computers and Chemical Engineering*, **1997**, 21, 351-369	4	159
19	Optimization accounting for property prediction uncertainty in polymer design. *Computers and Chemical Engineering*, **1997**, 21, S1019-S1024	4	7
18	Optimal molecular design under property prediction uncertainty. *AICHE Journal*, **1997**, 43, 1250-1264	3.6	78
17	Quantitative assessment of uncertainty in the optimization of metabolic pathways. *Biotechnology and Bioengineering*, **1997**, 56, 145-61	4.9	21
16	Optimal Computer-Aided Molecular Design: A Polymer Design Case Study. *Industrial & Engineering Chemistry Research*, **1996**, 35, 3403-3414	3.9	98
15	Locating all azeotropes in homogeneous azeotropic systems. *Computers and Chemical Engineering*, **1996**, 20, S413-S418	4	14
14	A global optimization method, ɃB, for process design. *Computers and Chemical Engineering*, **1996**, 20, S419-S424	4	86
13	Finding all solutions of nonlinearly constrained systems of equations. *Journal of Global Optimization* , **1995**, 7, 143-182	1.5	166

12	BB: A global optimization method for general constrained nonconvex problems. *Journal of Global Optimization*, **1995**, 7, 337-363	1.5	308
11	New results in the packing of equal circles in a square. *Discrete Mathematics*, **1995**, 142, 287-293	0.7	56
10	A deterministic global optimization approach for molecular structure determination. *Journal of Chemical Physics*, **1994**, 100, 1247-1261	3.9	85
9	Global minimum potential energy conformations of small molecules. *Journal of Global Optimization*, **1994**, 4, 135-170	1.5	137
8	A Global Optimization Method For Weber Problem With Attraction And Repulsion **1994**, 259-285		8
7	Global optimization for molecular conformation problems. *Annals of Operations Research*, **1993**, 42, 85-11	3.2	30
6	A global optimization approach for Lennard-Jones microclusters. *Journal of Chemical Physics*, **1992**, 97, 7667-7678	3.9	117
5	Toward low-cost biological and hybrid biological/catalytic conversion of cellulosic biomass to fuels. *Energy and Environmental Science*,	35.4	7
4	Biophysical characterization of the SARS-CoV-2 spike protein binding with the ACE2 receptor and implications for infectivity		15
3	De novo design of high-affinity antibody variable regions (Fv) against the SARS-CoV-2 spike protein		2
2	K-FIT: An accelerated kinetic parameterization algorithm using steady-state fluxomic data		2
1	Computational prediction of the effect of amino acid changes on the binding affinity between SARS-CoV-2 spike protein and the human ACE2 receptor		4