

Nikolaos V Sahinidis

List of Publications by Year in descending order

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162
papers

11,058
citations

50170

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docs citations

170
times ranked

6561
citing authors

#	ARTICLE	IF	CITATIONS
1	SDP-quality bounds via convex quadratic relaxations for global optimization of mixed-integer quadratic programs. <i>Mathematical Programming</i> , 2022, 196, 203-233.	1.6	3
2	Deterministic symbolic regression with derivative information: General methodology and application to equations of state. <i>AIChE Journal</i> , 2022, 68, e17457.	1.8	6
3	Review and comparison of algorithms and software for mixed-integer derivative-free optimization. <i>Journal of Global Optimization</i> , 2022, 82, 433-462.	1.1	7
4	Computer-aided retrosynthetic design: fundamentals, tools, and outlook. <i>Current Opinion in Chemical Engineering</i> , 2022, 35, 100721.	3.8	11
5	Learning process patterns via multiple sequence alignment. <i>Computers and Chemical Engineering</i> , 2022, 159, 107676.	2.0	4
6	Stochastic analysis and modeling of pharmaceutical screw feeder mass flow rates. <i>International Journal of Pharmaceutics</i> , 2022, 621, 121776.	2.6	3
7	A triangulation and fill-reducing initialization procedure for the simplex algorithm. <i>Mathematical Programming Computation</i> , 2021, 13, 491-508.	3.2	1
8	Process Systems Engineering Perspective on the Design of Materials and Molecules. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 5194-5206.	1.8	22
9	ExtractionScore: A Quantitative Framework for Evaluating Synthetic Routes on Predicted Liquid-Liquid Extraction Performance. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2274-2282.	2.5	3
10	A New Functional Group Selection Method for Group Contribution Models and Its Application in the Design of Electronics Cooling Fluids. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 7291-7300.	1.8	5
11	Announcement: Howard Rosenbrock Prize 2020. <i>Optimization and Engineering</i> , 2021, 22, 1979-1980.	1.3	0
12	Backward Stepwise Elimination: Approximation Guarantee, a Batched GPU Algorithm, and Empirical Investigation. <i>SN Computer Science</i> , 2021, 2, 1.	2.3	0
13	Decomposition in derivative-free optimization. <i>Journal of Global Optimization</i> , 2021, 81, 269-292.	1.1	0
14	Efficient Bayesian inference using adversarial machine learning and low-complexity surrogate models. <i>Computers and Chemical Engineering</i> , 2021, 151, 107322.	2.0	6
15	Spectral Relaxations and Branching Strategies for Global Optimization of Mixed-Integer Quadratic Programs. <i>SIAM Journal on Optimization</i> , 2021, 31, 142-171.	1.2	8
16	HybridTuner: Tuning with Hybrid Derivative-Free Optimization Initialization Strategies. <i>Lecture Notes in Computer Science</i> , 2021, , 379-393.	1.0	1
17	GPU parameter tuning for tall and skinny dense linear least squares problems. <i>Optimization Methods and Software</i> , 2020, 35, 638-660.	1.6	9
18	On the impact of running intersection inequalities for globally solving polynomial optimization problems. <i>Mathematical Programming Computation</i> , 2020, 12, 165-191.	3.2	17

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19	Announcement: Howard Rosenbrock Prize 2019. Optimization and Engineering, 2020, 21, 707-708.	1.3	0
20	Derivative-free optimization for chemical product design. Current Opinion in Chemical Engineering, 2020, 27, 98-106.	3.8	15
21	Optimality-based domain reduction for inequality-constrained NLP and MINLP problems. Journal of Global Optimization, 2020, 77, 425-454.	1.1	2
22	Industrial text analytics for reliability with derivative-free optimization. Computers and Chemical Engineering, 2020, 135, 106763.	2.0	6
23	A Discussion on Practical Considerations with Sparse Regression Methodologies. Statistical Science, 2020, 35, .	1.6	2
24	Announcement: Howard Rosenbrock Prize 2018. Optimization and Engineering, 2019, 20, 961-962.	1.3	0
25	Status report for optimization and engineering. Optimization and Engineering, 2019, 20, 963-964.	1.3	0
26	Heat Exchanger Circuitry Design by Decision Diagrams. Lecture Notes in Computer Science, 2019, , 461-471.	1.0	0
27	Mixed-integer nonlinear programming 2018. Optimization and Engineering, 2019, 20, 301-306.	1.3	50
28	Automated learning of chemical reaction networks. Computers and Chemical Engineering, 2019, 127, 88-98.	2.0	13
29	110th Anniversary: Design of Cooling Fluids for Electronic Equipment. Industrial & Engineering Chemistry Research, 2019, 58, 4925-4935.	1.8	5
30	Evaluating and ranking patents with multiple criteria: How many criteria are required to find the most promising patents?. Computers and Chemical Engineering, 2019, 123, 317-330.	2.0	6
31	Pattern recognition in chemical process flowsheets. AIChE Journal, 2019, 65, 592-603.	1.8	22
32	QPLIB: a library of quadratic programming instances. Mathematical Programming Computation, 2019, 11, 237-265.	3.2	38
33	Tuning BARON using derivative-free optimization algorithms. Journal of Global Optimization, 2019, 74, 611-637.	1.1	18
34	Long-Range Planning of Chemical Manufacturing Systems. , 2019, , 1-1-1-25.		0
35	An efficient strategy for the activation of MIP relaxations in a multicore global MINLP solver. Journal of Global Optimization, 2018, 70, 497-516.	1.1	18
36	Global optimization of nonconvex problems with convex-transformable intermediates. Journal of Global Optimization, 2018, 72, 255-276.	1.1	5

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37	Infeasibility resolution for multi-purpose batch process scheduling. Computers and Chemical Engineering, 2018, 116, 69-79.	2.0	1
38	Optimization of circuitry arrangements for heat exchangers using derivative-free optimization. Chemical Engineering Research and Design, 2018, 131, 16-28.	2.7	24
39	COSMO-based computer-aided molecular/mixture design: A focus on reaction solvents. AIChE Journal, 2018, 64, 104-122.	1.8	39
40	Exploiting integrality in the global optimization of mixed-integer nonlinear programming problems with BARON. Optimization Methods and Software, 2018, 33, 540-562.	1.6	107
41	A Machine Learning Approach to Correlation Development Applied to Fin-Tube Bundle Heat Exchangers. Energies, 2018, 11, 3450.	1.6	18
42	A hybrid LP/NLP paradigm for global optimization relaxations. Mathematical Programming Computation, 2018, 10, 383-421.	3.2	61
43	Announcement: Howard Rosenbrock Prize 2017. Optimization and Engineering, 2018, 19, 813-814.	1.3	0
44	Next Generation Multi-Scale Process Systems Engineering Framework. Computer Aided Chemical Engineering, 2018, , 2209-2214.	0.3	16
45	A global MINLP approach to symbolic regression. Mathematical Programming, 2018, 170, 97-119.	1.6	29
46	A COSMO-based approach to computer-aided mixture design. Chemical Engineering Science, 2017, 159, 93-105.	1.9	51
47	Domain reduction techniques for global NLP and MINLP optimization. Constraints, 2017, 22, 338-376.	0.4	47
48	Bounds tightening based on optimality conditions for nonconvex box-constrained optimization. Journal of Global Optimization, 2017, 67, 59-77.	1.1	11
49	The ALAMO approach to machine learning. Computers and Chemical Engineering, 2017, 106, 785-795.	2.0	128
50	Deletion Presolve for Accelerating Infeasibility Diagnosis in Optimization Models. INFORMS Journal on Computing, 2017, 29, 754-766.	1.0	7
51	Chapter 16: The Pooling Problem. , 2017, , 207-217.		3
52	Risk analysis of turnaround reschedule planning in integrated chemical sites. Computers and Chemical Engineering, 2017, 107, 381-394.	2.0	10
53	Chapter 21: State of the Art in Mixed-Integer Nonlinear Optimization. , 2017, , 273-292.		4
54	Innovative computational tools and models for the design, optimization and control of carbon capture processes. Computer Aided Chemical Engineering, 2016, 38, 2391-2396.	0.3	5

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55	Global optimization of an industrial gas network operation. <i>AICHE Journal</i> , 2016, 62, 3215-3224.	1.8	16
56	Mixture design using derivative-free optimization in the space of individual component properties. <i>AICHE Journal</i> , 2016, 62, 1514-1530.	1.8	20
57	Computer-aided molecular design: An introduction and review of tools, applications, and solution techniques. <i>Chemical Engineering Research and Design</i> , 2016, 116, 2-26.	2.7	149
58	Simulation optimization: a review of algorithms and applications. <i>Annals of Operations Research</i> , 2016, 240, 351-380.	2.6	315
59	Medium-term maintenance turnaround planning under uncertainty for integrated chemical sites. <i>Computers and Chemical Engineering</i> , 2016, 84, 422-433.	2.0	26
60	Global optimization of mathematical programs with complementarity constraints and application to clean energy deployment. <i>Optimization Letters</i> , 2016, 10, 325-340.	0.9	4
61	The ALAMO approach to machine learning. <i>Computer Aided Chemical Engineering</i> , 2016, 38, 2410.	0.3	3
62	A combined first-principles and data-driven approach to model building. <i>Computers and Chemical Engineering</i> , 2015, 73, 116-127.	2.0	77
63	Long-term turnaround planning for integrated chemical sites. <i>Computers and Chemical Engineering</i> , 2015, 72, 145-158.	2.0	21
64	Global optimization of nonconvex problems with multilinear intermediates. <i>Mathematical Programming Computation</i> , 2015, 7, 1-37.	3.2	33
65	Global optimization of general nonconvex problems with intermediate polynomial substructures. <i>Journal of Global Optimization</i> , 2014, 59, 673-693.	1.1	5
66	Simulation optimization: a review of algorithms and applications. <i>4or</i> , 2014, 12, 301-333.	1.0	95
67	Relaxations of factorable functions with convex-transformable intermediates. <i>Mathematical Programming</i> , 2014, 144, 107-140.	1.6	12
68	Preface: Honoring the 60th birthday of Panos M. Pardalos. <i>Journal of Global Optimization</i> , 2014, 59, 207-207.	1.1	0
69	Optimal Source-Sink Matching in Carbon Capture and Storage Systems under Uncertainty. <i>Industrial & Engineering Chemistry Research</i> , 2014, 53, 778-785.	1.8	39
70	Carbon Capture Simulation Initiative: A Case Study in Multiscale Modeling and New Challenges. <i>Annual Review of Chemical and Biomolecular Engineering</i> , 2014, 5, 301-323.	3.3	66
71	Global optimization of general non-convex problems with intermediate bilinear substructures. <i>Optimization Methods and Software</i> , 2014, 29, 442-462.	1.6	21
72	Learning surrogate models for simulation-based optimization. <i>AICHE Journal</i> , 2014, 60, 2211-2227.	1.8	305

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73	Evaluation of rapid performance reservoir models for quantitative risk assessment. Energy Procedia, 2014, 63, 3425-3431.	1.8	12
74	A Framework for Optimization and Quantification of Uncertainty and Sensitivity for Developing Carbon Capture Systems. Energy Procedia, 2014, 63, 1055-1063.	1.8	13
75	Optimization-based framework for computer-aided molecular design. AIChE Journal, 2013, 59, 3686-3701.	1.8	92
76	Design of Heat-Transfer Media Components for Retail Food Refrigeration. Industrial & Engineering Chemistry Research, 2013, 52, 8518-8526.	1.8	27
77	Computational Experience with Applications of Bilinear Cutting Planes. Industrial & Engineering Chemistry Research, 2013, 52, 7514-7525.	1.8	7
78	Derivative-free optimization: a review of algorithms and comparison of software implementations. Journal of Global Optimization, 2013, 56, 1247-1293.	1.1	886
79	Uncertainty Quantification in CO ₂ Sequestration Using Surrogate Models from Polynomial Chaos Expansion. Industrial & Engineering Chemistry Research, 2013, 52, 3121-3132.	1.8	54
80	Convex envelopes generated from finitely many compact convex sets. Mathematical Programming, 2013, 137, 371-408.	1.6	34
81	A review of LU factorisation in the simplex algorithm. International Journal of Mathematics in Operational Research, 2012, 4, 319.	0.1	2
82	A review of the LU update in the simplex algorithm. International Journal of Mathematics in Operational Research, 2012, 4, 366.	0.1	7
83	SAS-Pro: Simultaneous Residue Assignment and Structure Superposition for Protein Structure Alignment. PLoS ONE, 2012, 7, e37493.	1.1	4
84	Scaling linear optimization problems prior to application of the simplex method. Computational Optimization and Applications, 2012, 52, 345-371.	0.9	21
85	Global optimization of nonlinear least-squares problems by branch-and-bound and optimality constraints. Top, 2012, 20, 154-172.	1.1	7
86	Convex envelopes of products of convex and component-wise concave functions. Journal of Global Optimization, 2012, 52, 391-409.	1.1	32
87	Semidefinite relaxations for quadratically constrained quadratic programming: A review and comparisons. Mathematical Programming, 2011, 129, 129-157.	1.6	90
88	Steady-state process optimization with guaranteed robust stability under parametric uncertainty. AIChE Journal, 2011, 57, 3395-3407.	1.8	9
89	An integer programming approach to DNA sequence assembly. Computational Biology and Chemistry, 2011, 35, 251-258.	1.1	7
90	GPU simulations for risk assessment in CO ₂ geologic sequestration. Computers and Chemical Engineering, 2011, 35, 1631-1644.	2.0	20

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91	Optimization of IMC-PID Tuning Parameters for Adaptive Control: Part 1. Computer Aided Chemical Engineering, 2011, 29, 758-762.	0.3	5
92	GPU-BLAST: using graphics processors to accelerate protein sequence alignment. Bioinformatics, 2011, 27, 182-188.	1.8	179
93	Portfolio optimization for wealth-dependent risk preferences. Annals of Operations Research, 2010, 177, 63-90.	2.6	8
94	GPU computing with Kaczmarz's and other iterative algorithms for linear systems. Parallel Computing, 2010, 36, 215-231.	1.3	52
95	Global optimization. Optimization Methods and Software, 2009, 24, 479-482.	1.6	2
96	Paclitaxel delivery from PLGA foams for controlled release in post-surgical chemotherapy against glioblastoma multiforme. Biomaterials, 2009, 30, 3189-3196.	5.7	123
97	Optimization techniques in molecular structure and function elucidation. Computers and Chemical Engineering, 2009, 33, 2055-2062.	2.0	4
98	Multiterm polyhedral relaxations for nonconvex, quadratically constrained quadratic programs. Optimization Methods and Software, 2009, 24, 485-504.	1.6	72
99	Design of Secondary Refrigerants. , 2009, , 879-886.		2
100	Selection, acquisition, and allocation of manufacturing technology in a multi-period environment. European Journal of Operational Research, 2008, 189, 807-821.	3.5	12
101	SnBversion 2.3: triplet sieve phasing for centrosymmetric structures. Journal of Applied Crystallography, 2008, 41, 644-646.	1.9	5
102	A branch-and-bound algorithm for the continuous facility layout problem. Computers and Chemical Engineering, 2008, 32, 1016-1028.	2.0	66
103	A Reduction-Based Exact Algorithm for the Contact Map Overlap Problem. Journal of Computational Biology, 2007, 14, 637-654.	0.8	33
104	In vivo performance of implantable biodegradable preparations delivering Paclitaxel and Etanidazole for the treatment of glioma. Biomaterials, 2007, 28, 886-894.	5.7	47
105	An integer minimal principle and triplet sieve method for phasing centrosymmetric structures. Acta Crystallographica Section A: Foundations and Advances, 2007, 63, 164-171.	0.3	6
106	Global optimization in stabilizing controller design. Journal of Global Optimization, 2007, 38, 509-526.	1.1	17
107	Residue-rotamer-reduction algorithm for the protein side-chain conformation problem. Bioinformatics, 2006, 22, 188-194.	1.8	37
108	A Branch-and-Reduce Algorithm for the Contact Map Overlap Problem. Lecture Notes in Computer Science, 2006, , 516-529.	1.0	10

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109	Optimization of metabolic pathways under stability considerations. Computers and Chemical Engineering, 2005, 29, 467-479.	2.0	30
110	A polyhedral branch-and-cut approach to global optimization. Mathematical Programming, 2005, 103, 225-249.	1.6	983
111	Accelerating Branch-and-Bound through a Modeling Language Construct for Relaxation-Specific Constraints. Journal of Global Optimization, 2005, 32, 259-280.	1.1	28
112	Polynomial-time algorithms for the integer minimal principle for centrosymmetric structures. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, 445-452.	0.3	3
113	Establishing a master's degree programme in Bioinformatics: challenges and opportunities. IET Systems Biology, 2005, 152, 269.	2.0	5
114	Approximation Algorithms for the Minimum Number of Matches Problem in Heat Exchanger Network Synthesis. Industrial & Engineering Chemistry Research, 2004, 43, 3554-3565.	1.8	22
115	Global optimization of mixed-integer nonlinear programs: A theoretical and computational study. Mathematical Programming, 2004, 99, 563-591.	1.6	439
116	A finite branch-and-bound algorithm for two-stage stochastic integer programs. Mathematical Programming, 2004, 100, 355-377.	1.6	169
117	Optimization under uncertainty: state-of-the-art and opportunities. Computers and Chemical Engineering, 2004, 28, 971-983.	2.0	893
118	Global Optimization of Multiplicative Programs. Journal of Global Optimization, 2003, 26, 387-418.	1.1	83
119	Design of alternative refrigerants via global optimization. AIChE Journal, 2003, 49, 1761-1775.	1.8	93
120	Simultaneous parameter estimation and model structure determination in FTIR spectroscopy by global MINLP optimization. Computers and Chemical Engineering, 2003, 27, 763-779.	2.0	12
121	An integer programming approach to the phase problem for centrosymmetric structures. Acta Crystallographica Section A: Foundations and Advances, 2003, 59, 452-458.	0.3	7
122	An Approximation Scheme for Stochastic Integer Programs Arising in Capacity Expansion. Operations Research, 2003, 51, 461-471.	1.2	97
123	Global Optimization and Constraint Satisfaction: The Branch-and-Reduce Approach. Lecture Notes in Computer Science, 2003, , 1-16.	1.0	22
124	Convexification and Global Optimization in Continuous and Mixed-Integer Nonlinear Programming. Nonconvex Optimization and Its Applications, 2002, , .	0.1	392
125	A Critical Review and Annotated Bibliography for Heat Exchanger Network Synthesis in the 20th Century. Industrial & Engineering Chemistry Research, 2002, 41, 2335-2370.	1.8	391
126	Exact Algorithms for Global Optimization of Mixed-Integer Nonlinear Programs. Nonconvex Optimization and Its Applications, 2002, , 65-85.	0.1	28

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127	Convex extensions and envelopes of lower semi-continuous functions. <i>Mathematical Programming</i> , 2002, 93, 247-263.	1.6	101
128	Product Disaggregation in Global Optimization and Relaxations of Rational Programs. <i>Optimization and Engineering</i> , 2002, 3, 281-303.	1.3	15
129	Global Optimization of 0-1 Hyperbolic Programs. <i>Journal of Global Optimization</i> , 2002, 24, 385-416.	1.1	52
130	Computational complexity of heat exchanger network synthesis. <i>Computers and Chemical Engineering</i> , 2001, 25, 1371-1390.	2.0	126
131	Semidefinite Relaxations of Fractional Programs via Novel Convexification Techniques. <i>Journal of Global Optimization</i> , 2001, 20, 133-154.	1.1	97
132	Analysis of Bounds for Multilinear Functions. <i>Journal of Global Optimization</i> , 2001, 19, 403-424.	1.1	78
133	Solving Global Optimization Problems with Baron. <i>Nonconvex Optimization and Its Applications</i> , 2001, 205-230.	0.1	12
134	Applications of global optimization to process and molecular design. <i>Computers and Chemical Engineering</i> , 2000, 24, 2157-2169.	2.0	42
135	Analytical investigations of the process planning problem. <i>Computers and Chemical Engineering</i> , 2000, 23, 1605-1621.	2.0	20
136	An improved decomposition algorithm for optimization under uncertainty. <i>Computers and Chemical Engineering</i> , 2000, 23, 1589-1604.	2.0	26
137	Globally optimal robust process control. <i>Journal of Process Control</i> , 1999, 9, 375-383.	1.7	27
138	A Lagrangian Approach to the Pooling Problem. <i>Industrial & Engineering Chemistry Research</i> , 1999, 38, 1956-1972.	1.8	115
139	A Finite Algorithm for Global Minimization of Separable Concave Programs. <i>Journal of Global Optimization</i> , 1998, 12, 1-36.	1.1	72
140	Robust Process Planning under Uncertainty. <i>Industrial & Engineering Chemistry Research</i> , 1998, 37, 1883-1892.	1.8	181
141	Process planning in a fuzzy environment. <i>European Journal of Operational Research</i> , 1997, 100, 142-169.	3.5	88
142	Globally optimal robust control for systems with time-varying nonlinear perturbations. <i>Computers and Chemical Engineering</i> , 1997, 21, S125-S130.	2.0	25
143	Bridging the gap between heuristics and optimization: Capacity expansion case. <i>AIChE Journal</i> , 1997, 43, 2289-2299.	1.8	16
144	The assignment problem with external interactions. <i>Networks</i> , 1997, 30, 171-185.	1.6	3

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145	Planning of Chemical Process Networks via Global Concave Minimization. <i>Nonconvex Optimization and Its Applications</i> , 1996, , 195-230.	0.1	10
146	Optimization in Process Planning under Uncertainty. <i>Industrial & Engineering Chemistry Research</i> , 1996, 35, 4154-4165.	1.8	182
147	Long range planning in the process industries: A projection approach. <i>Computers and Operations Research</i> , 1996, 23, 237-253.	2.4	24
148	An exact solution approach for the time-dependent traveling-salesman problem. <i>Naval Research Logistics</i> , 1996, 43, 797-820.	1.4	33
149	A branch-and-reduce approach to global optimization. <i>Journal of Global Optimization</i> , 1996, 8, 107-138.	1.1	257
150	BARON: A general purpose global optimization software package. <i>Journal of Global Optimization</i> , 1996, 8, 201-205.	1.1	595
151	A Finite Algorithm for Global Minimization of Separable Concave Programs. <i>Nonconvex Optimization and Its Applications</i> , 1996, , 303-339.	0.1	2
152	Global optimization of nonconvex NLPs and MINLPs with applications in process design. <i>Computers and Chemical Engineering</i> , 1995, 19, 551-566.	2.0	344
153	GLOBAL OPTIMIZATION ALGORITHMS FOR CHIP LAYOUT AND COMPACTION. <i>Engineering Optimization</i> , 1995, 25, 131-154.	1.5	56
154	Heuristic Bounds and Test Problem Generation for the Time-Dependent Traveling Salesman Problem. <i>Transportation Science</i> , 1995, 29, 167-183.	2.6	27
155	Computational Trends and Effects of Approximations in an MILP Model for Process Planning. <i>Industrial & Engineering Chemistry Research</i> , 1995, 34, 1662-1673.	1.8	28
156	Reformulation of the Multiperiod MILP Model for Capacity Expansion of Chemical Processes. <i>Operations Research</i> , 1992, 40, S127-S144.	1.2	45
157	Multiperiod investment model for processing networks with dedicated and flexible plants. <i>Industrial & Engineering Chemistry Research</i> , 1991, 30, 1165-1171.	1.8	44
158	Reformulation of multiperiod MILP models for planning and scheduling of chemical processes. <i>Computers and Chemical Engineering</i> , 1991, 15, 255-272.	2.0	106
159	Convergence properties of generalized benders decomposition. <i>Computers and Chemical Engineering</i> , 1991, 15, 481-491.	2.0	121
160	MINLP model for cyclic multiproduct scheduling on continuous parallel lines. <i>Computers and Chemical Engineering</i> , 1991, 15, 85-103.	2.0	140
161	Optimization model for long range planning in the chemical industry. <i>Computers and Chemical Engineering</i> , 1989, 13, 1049-1063.	2.0	163
162	Hyperparameter autotuning of programs with HybridTuner. <i>Annals of Mathematics and Artificial Intelligence</i> , 0, , .	0.9	0