Peter Buchwald

List of Publications by Year in descending order

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133 papers 4,376 citations

34 h-index 56 g-index

157 all docs

157 docs citations

157 times ranked

5026 citing authors

#	Article	IF	CITATIONS
1	Soft drug design: General principles and recent applications. Medicinal Research Reviews, 2000, 20, 58-101.	10.5	220
2	Octanol-Water Partition: Searching for Predictive Models. Current Medicinal Chemistry, 1998, 5, 353-380.	2.4	159
3	Recent advances in the brain targeting of neuropharmaceuticals by chemical delivery systems. Advanced Drug Delivery Reviews, 1999, 36, 229-254.	13.7	157
4	Characterization of twenty-five ovarian tumour cell lines that phenocopy primary tumours. Nature Communications, 2015, 6, 7419.	12.8	149
5	Oscillatory Dynamics of Cdc42 GTPase in the Control of Polarized Growth. Science, 2012, 337, 239-243.	12.6	148
6	FEM-based oxygen consumption and cell viability models for avascular pancreatic islets. Theoretical Biology and Medical Modelling, 2009, 6, 5.	2.1	140
7	Smallâ€molecule protein–protein interaction inhibitors: Therapeutic potential in light of molecular size, chemical space, and ligand binding efficiency considerations. IUBMB Life, 2010, 62, 724-731.	3.4	115
8	A local glucose-and oxygen concentration-based insulin secretion model for pancreatic islets. Theoretical Biology and Medical Modelling, 2011, 8, 20.	2.1	104
9	Molecular Size Based Approach To Estimate Partition Properties for Organic Solutes. Journal of Physical Chemistry B, 1997, 101, 3404-3412.	2.6	96
10	Ophthalmic drug design based on the metabolic activity of the eye: Soft drugs and chemical delivery systems. AAPS Journal, 2005, 7, E820-E833.	4.4	86
11	Barriers to remember: brain-targeting chemical delivery systems and Alzheimer's disease. Drug Discovery Today, 2002, 7, 766-774.	6.4	79
12	Small-Molecule Inhibitors of the Coronavirus Spike: ACE2 Proteinâ€"Protein Interaction as Blockers of Viral Attachment and Entry for SARS-CoV-2. ACS Infectious Diseases, 2021, 7, 1519-1534.	3.8	77
13	Quantitative Structureâ°'Metabolism Relationships:Â Steric and Nonsteric Effects in the Enzymatic Hydrolysis of Noncongener Carboxylic Esters. Journal of Medicinal Chemistry, 1999, 42, 5160-5168.	6.4	74
14	Toward Small-Molecule Inhibition of Protein–Protein Interactions: General Aspects and Recent Progress in Targeting Costimulatory and Coinhibitory (Immune Checkpoint) Interactions. Current Topics in Medicinal Chemistry, 2018, 18, 674-699.	2.1	69
15	A simple, predictive, structure-based skin permeability model. Journal of Pharmacy and Pharmacology, 2010, 53, 1087-1098.	2.4	67
16	Methylene Blue Inhibits the SARS-CoV-2 Spikeâ€"ACE2 Protein-Protein Interactionâ€"a Mechanism that can Contribute to its Antiviral Activity Against COVID-19. Frontiers in Pharmacology, 2020, 11, 600372.	3.5	64
17	Glucoseâ€stimulated insulin release: Parallel perifusion studies of free and hydrogel encapsulated human pancreatic islets. Biotechnology and Bioengineering, 2018, 115, 232-245.	3.3	62
18	Quantitative Assessment of Islet Cell Products: Estimating the Accuracy of the Existing Protocol and Accounting for Islet Size Distribution. Cell Transplantation, 2009, 18, 1223-1235.	2.5	61

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19	Organoid microphysiological system preserves pancreatic islet function within 3D matrix. Science Advances, 2021, 7, .	10.3	59
20	The food colorant erythrosine is a promiscuous protein–protein interaction inhibitor. Biochemical Pharmacology, 2011, 81, 810-818.	4.4	57
21	Direct, differential-equation-based in-vitro–in-vivo correlation (IVIVC) method. Journal of Pharmacy and Pharmacology, 2010, 55, 495-504.	2.4	56
22	Drug targeting via retrometabolic approaches. , 1997, 76, 1-27.		54
23	Computer-aided drug design: the role of quantitative structure-property, structure-activity and structure-metabolism relationships (QSPR, QSAR, QSMR). Drugs of the Future, 2002, 27, 577.	0.1	54
24	Brain-Targeted Drug Delivery. American Journal of Drug Delivery, 2003, 1, 13-26.	0.6	53
25	Vitamin D and androgen receptor-targeted therapy for triple-negative breast cancer. Breast Cancer Research and Treatment, 2016, 157, 77-90.	2.5	52
26	Resealable, optically accessible, PDMS-free fluidic platform for ex vivo interrogation of pancreatic islets. Lab on A Chip, 2017, 17, 772-781.	6.0	52
27	Octanol–water partition of nonzwitterionic peptides: Predictive power of a molecular size-based model. , 1998, 30, 86-99.		50
28	High-Throughput Screening for Human Galactokinase Inhibitors. Journal of Biomolecular Screening, 2008, 13, 415-423.	2.6	45
29	Concentration-Dependency and Time Profile of Insulin Secretion: Dynamic Perifusion Studies With Human and Murine Islets. Frontiers in Endocrinology, 2019, 10, 680.	3.5	45
30	A general bilinear model to describe growth or decline time profiles. Mathematical Biosciences, 2007, 205, 108-136.	1.9	44
31	Corticosteroid Design for the Treatment of Asthma: Structural Insights and the Therapeutic Potential of Soft Corticosteroids. Current Pharmaceutical Design, 2006, 12, 3241-3260.	1.9	42
32	Phosphorylation-dependent inhibition of Cdc42 GEF Gef1 by 14-3-3 protein Rad24 spatially regulates Cdc42 GTPase activity and oscillatory dynamics during cell morphogenesis. Molecular Biology of the Cell, 2015, 26, 3520-3534.	2.1	40
33	A Collagen Based Cryogel Bioscaffold that Generates Oxygen for Islet Transplantation. Advanced Functional Materials, 2020, 30, 1902463.	14.9	40
34	Glucocorticoid receptor binding: A biphasic dependence on molecular size as revealed by the bilinear LinBiExp model. Steroids, 2008, 73, 193-208.	1.8	39
35	A Receptor Model With Binding Affinity, Activation Efficacy, and Signal Amplification Parameters for Complex Fractional Response Versus Occupancy Data. Frontiers in Pharmacology, 2019, 10, 605.	3.5	37
36	Receptor binding studies of soft anticholinergic agents. AAPS PharmSci, 2001, 3, 44-56.	1.3	36

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37	Quantification of the Islet Product: Presentation of a Standardized Current Good Manufacturing Practices Compliant System With Minimal Variability. Transplantation, 2011, 91, 677-683.	1.0	36
38	Differences in the glucocorticoid to progesterone receptor selectivity of inhaled glucocorticoids. European Respiratory Journal, 2006, 27, 511-516.	6.7	35
39	Metabolomics Study of the Effects of Inflammation, Hypoxia, and High Glucose on Isolated Human Pancreatic Islets. Journal of Proteome Research, 2017, 16, 2294-2306.	3.7	35
40	Small-molecule costimulatory blockade: organic dye inhibitors of the CD40–CD154 interaction. Journal of Molecular Medicine, 2009, 87, 1133-1143.	3.9	34
41	Octanoic acid in alcohol-responsive essential tremor. Neurology, 2013, 80, 933-940.	1.1	34
42	Structure-Metabolism Relationships Steric Effects and the Enzymatic Hydrolysis of Carboxylic Esters. Mini-Reviews in Medicinal Chemistry, 2001, 1, 101-111.	2.4	33
43	General Linearized Biexponential Model for QSAR Data Showing Bilinear-Type Distribution. Journal of Pharmaceutical Sciences, 2005, 94, 2355-2379.	3.3	33
44	A Double Fail-Safe Approach to Prevent Tumorigenesis and Select Pancreatic \hat{l}^2 Cells from Human Embryonic Stem Cells. Stem Cell Reports, 2019, 12, 611-623.	4.8	32
45	Complexation Thermodynamics of Cyclodextrins in the Framework of a Molecular Size-Based Model for Nonassociative Organic Liquids That Includes a Modified Hydration-Shell Hydrogen-Bond Model for Water. Journal of Physical Chemistry B, 2002, 106, 6864-6870.	2.6	31
46	An Open-Label, Single-Dose, Crossover Study of the Pharmacokinetics and Metabolism of Two Oral Formulations of 1-Octanol in Patients with Essential Tremor. Neurotherapeutics, 2011, 8, 753-762.	4.4	31
47	Controlled Release of Dexamethasone from Organosilicone Constructs for Local Modulation of Inflammation in Islet Transplantation. Tissue Engineering - Part A, 2015, 21, 2250-2261.	3.1	31
48	Molecular Size-Based Model To Describe Simple Organic Liquids. Journal of Physical Chemistry B, 1998, 102, 5715-5726.	2.6	30
49	Designing Safer (Soft) Drugs by Avoiding the Formation of Toxic and Oxidative Metabolites. Molecular Biotechnology, 2004, 26, 123-132.	2.4	30
50	Targeted drug delivery to the brain via phosphonate derivatives II. Anionic chemical delivery system for zidovudine (AZT). International Journal of Pharmaceutics, 1998, 166, 27-35.	5.2	29
51	Targeted drug delivery to the brain via phosphonate derivatives. International Journal of Pharmaceutics, 1998, 166, 15-26.	5.2	29
52	Local delivery of fingolimod from threeâ€dimensional scaffolds impacts islet graft efficacy and microenvironment in a murine diabetic model. Journal of Tissue Engineering and Regenerative Medicine, 2018, 12, 393-404.	2.7	29
53	Suramin inhibits the CD40–CD154 costimulatory interaction: A possible mechanism for immunosuppressive effects. Biochemical Pharmacology, 2009, 77, 1236-1245.	4.4	28
54	TNF Superfamily Protein-Protein Interactions: Feasibility of Small- Molecule Modulation. Current Drug Targets, 2015, 16, 393-408.	2.1	28

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55	Smallâ€molecule modulators of the <scp>OX</scp> 40– <scp>OX40</scp> ligand coâ€stimulatory protein–protein interaction. British Journal of Pharmacology, 2014, 171, 4955-4969.	5.4	27
56	Computer-Assisted Design of New Drugs Based on Retrometabolic Concepts. SAR and QSAR in Environmental Research, 1998, 8, 41-92.	2.2	26
57	The time-profile of cell growth in fission yeast: model selection criteria favoring bilinear models over exponential ones. Theoretical Biology and Medical Modelling, 2006, 3, 16.	2.1	26
58	Experimental evaluation and computational modeling of the effects of encapsulation on the time-profile of glucose-stimulated insulin release of pancreatic islets. BioMedical Engineering OnLine, 2015, 14, 28.	2.7	25
59	Octanol-water partition: searching for predictive models. Current Medicinal Chemistry, 1998, 5, 353-80.	2.4	25
60	Cell length growth in fission yeast: an analysis of its bilinear character and the nature of its rate change transition. FEMS Yeast Research, 2013, 13, 635-649.	2.3	24
61	Small-Molecule Inhibitors of the CD40–CD40L Costimulatory Protein–Protein Interaction. Journal of Medicinal Chemistry, 2017, 60, 8906-8922.	6.4	22
62	Soft glucocorticoid design: structural elements and physicochemical parameters determining receptor-binding affinity. Die Pharmazie, 2004, 59, 396-404.	0.5	22
63	Simple Model for Nonassociative Organic Liquids and Water. Journal of the American Chemical Society, 2000, 122, 10671-10679.	13.7	21
64	In Vitro and In Vivo Evaluations of Dihydroquinoline- and Dihydroisoquinoline-based Targetor Moieties for Brain-specific Chemical Delivery Systems. Journal of Drug Targeting, 2002, 10, 63-71.	4.4	21
65	Retrometabolic drug design: Principles and recent developments. Pure and Applied Chemistry, 2008, 80, 1669-1682.	1.9	21
66	A threeâ€parameter twoâ€state model of receptor function that incorporates affinity, efficacy, and signal amplification. Pharmacology Research and Perspectives, 2017, 5, e00311.	2.4	21
67	In vivo imaging of type 1 diabetes immunopathology using eye-transplanted islets in NOD mice. Diabetologia, 2019, 62, 1237-1250.	6.3	20
68	Physicochemical aspects of the enzymatic hydrolysis of carboxylic esters. Die Pharmazie, 2002, 57, 87-93.	0.5	20
69	Theoretical Insights into the Formation, Structure, and Energetics of Some Cyclodextrin Complexes. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2002, 44, 9-14.	1.6	19
70	Fully Automated Islet Cell Counter (ICC) for the Assessment of Islet Mass, Purity, and Size Distribution by Digital Image Analysis. Cell Transplantation, 2016, 25, 1747-1761.	2.5	19
71	A single unified model for fitting simple to complex receptor response data. Scientific Reports, 2020, 10, 13386.	3.3	19
72	Feasibility of localized immunosuppression: 1. Exploratory studies with glucocorticoids in a biohybrid device designed for cell transplantation. Die Pharmazie, 2010, 65, 421-8.	0.5	19

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73	Soft Quaternary Anticholinergics:Â Comprehensive Quantitative Structureâ 'Activity Relationship (QSAR) with a Linearized Biexponential (LinBiExp) Model. Journal of Medicinal Chemistry, 2006, 49, 883-891.	6.4	18
74	Recent advances in the design and development of soft drugs. Die Pharmazie, 2014, 69, 403-13.	0.5	18
75	Modeling liquid properties, solvation, and hydrophobicity: A molecular size-based perspective. Journal of Computer - Aided Molecular Design, 2000, 19, 19-45.	1.0	17
76	Synthesis and pharmacological effects of new, N-substituted soft anticholinergics based on glycopyrrolate. Journal of Pharmacy and Pharmacology, 2010, 57, 1427-1435.	2.4	17
77	Research Article: Effective and Specific Inhibition of the CD40–CD154 Costimulatory Interaction by a Naphthalenesulphonic Acid Derivative. Chemical Biology and Drug Design, 2010, 76, 305-313.	3.2	17
78	Molecular Organization of the Complex between the Muscarinic M3 Receptor and the Regulator of G Protein Signaling, $G^2 < sub > 5 < /sub > 3^RGS7$. Biochemistry, 2010, 49, 4998-5006.	2.5	17
79	Effects of representative glucocorticoids on TNFα- and CD40L-induced NF-κB activation in sensor cells. Steroids, 2014, 85, 36-43.	1.8	17
80	Dose-escalation study of octanoic acid in patients with essential tremor. Journal of Clinical Investigation, 2016, 126, 1451-1457.	8.2	17
81	Parallel Multi-Omics in High-Risk Subjects for the Identification of Integrated Biomarker Signatures of Type 1 Diabetes. Biomolecules, 2021 , 11 , 383 .	4.0	17
82	Brain-Targeting Chemical Delivery Systems and Their Cyclodextrin-Based Formulations in Light of the Contributions of Marcus E. Brewster. Journal of Pharmaceutical Sciences, 2016, 105, 2589-2600.	3.3	16
83	Controlled Nutrient Delivery to Pancreatic Islets Using Polydopamine-Coated Mesoporous Silica Nanoparticles. Nano Letters, 2020, 20, 7220-7229.	9.1	16
84	Soft drugs: design principles, success stories, and future perspectives. Expert Opinion on Drug Metabolism and Toxicology, 2020, 16, 645-650.	3 . 3	16
85	The Role of Computational Techniques in Retrometabolic Drug Design Strategies. Theoretical and Computational Chemistry, 1999, , 569-618.	0.4	14
86	The promiscuous protein binding ability of erythrosine B studied by metachromasy (metachromasia). Journal of Molecular Recognition, 2013, 26, 181-189.	2.1	14
87	Soft corticosteroids for local immunosuppression: exploring the possibility for the use of loteprednol etabonate for islet transplantation. Die Pharmazie, 2008, 63, 226-32.	0.5	14
88	Structural studies on the chiral selector capacity of cyclodextrin derivatives. Journal of Proteomics, 2008, 70, 1276-1282.	2.4	13
89	Novel, cell-penetrating molecular transporters with flexible backbones and permanently charged side-chains. Journal of Pharmacy and Pharmacology, 2010, 59, 1065-1076.	2.4	13
90	Comprehensive Metabolomics Study To Assess Longitudinal Biochemical Changes and Potential Early Biomarkers in Nonobese Diabetic Mice That Progress to Diabetes. Journal of Proteome Research, 2017, 16, 3873-3890.	3.7	13

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91	Design, Synthesis, and Evaluation of Novel Immunomodulatory Small Molecules Targeting the CD40–CD154 Costimulatory Protein-Protein Interaction. Molecules, 2018, 23, 1153.	3.8	13
92	Structure-based estimation of enzymatic hydrolysis rates and its application in computer-aided retrometabolic drug design. Die Pharmazie, 2000, 55, 210-7.	0.5	13
93	Design and evaluation of new soft anticholinergic agents. Drug Development Research, 1998, 43, 117-127.	2.9	12
94	Choice of Immunosuppression Influences Cytomegalovirus DNAemia in Cynomolgus Monkey (<i>Macaca fascicularis</i>) Islet Allograft Recipients. Cell Transplantation, 2010, 19, 1547-1561.	2.5	12
95	Cell length growth patterns in fission yeast reveal a novel size control mechanism operating in late G2 phase. Biology of the Cell, 2016, 108, 259-277.	2.0	12
96	Growth hormone-releasing hormone agonists ameliorate chronic kidney disease-induced heart failure with preserved ejection fraction. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	12
97	Brain-Targeted Delivery of Estradiol. American Journal of Drug Delivery, 2006, 4, 161-175.	0.6	11
98	Pharmacokinetic and Pharmacodynamic Evaluations of the Zwitterionic Metabolite of a New Series of N-Substituted Soft Anticholinergics. Pharmaceutical Research, 2005, 22, 2035-2044.	3.5	10
99	Organic dyes as small molecule protein–protein interaction inhibitors for the CD40–CD154 costimulatory interaction. Journal of Molecular Recognition, 2010, 23, 65-73.	2.1	9
100	Feasibility of Localized Metabolomics in the Study of Pancreatic Islets and Diabetes. Metabolites, 2019, 9, 207.	2.9	9
101	Longitudinal proteomics analysis in the immediate microenvironment of islet allografts during progression of rejection. Journal of Proteomics, 2020, 223, 103826.	2.4	9
102	Pharmacokinetics of the sequential metabolites of loteprednol etabonate in rats. Journal of Pharmacy and Pharmacology, 2010, 60, 291-297.	2.4	8
103	Biphasic decline of βâ€cell function with age in euglycemic nonobese diabetic mice parallels diabetes onset. IUBMB Life, 2015, 67, 634-644.	3.4	8
104	Drug-Integrating Amphiphilic Nanomaterial Assemblies: 1. Spatiotemporal control of cyclosporine delivery and activity using nanomicelles and nanofibrils. Journal of Controlled Release, 2021, 329, 955-970.	9.9	8
105	Feasibility of localized immunosuppression: 3. Preliminary evaluation of organosilicone constructs designed for sustained drug release in a cell transplant environment using dexamethasone. Die Pharmazie, 2012, 67, 394-9.	0.5	8
106	Methylene Blue Is a Nonspecific Protein–Protein Interaction Inhibitor with Potential for Repurposing as an Antiviral for COVID-19. Pharmaceuticals, 2022, 15, 621.	3.8	8
107	NMR investigation and secondary structure of domains I and II of rat brain calbindin D28k (1-93). FEBS Journal, 1999, 262, 933-938.	0.2	7
108	QSAR Study of 2,3-Benzodiazepin-4(thi)one- and 1,2-Phthalazine-Related Negative Allosteric Modulators of the AMPA Receptor: A Structural Descriptors-Based Reassessment. QSAR and Combinatorial Science, 2005, 24, 325-331.	1.4	7

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109	Computer-aided retrometabolic drug design: soft drugs. Expert Opinion on Drug Discovery, 2007, 2, 923-933.	5.0	7
110	Glucose-stimulated insulin secretion in isolated pancreatic islets: Multiphysics FEM model calculations compared to results of perifusion experiments with human islets. Journal of Biomedical Science and Engineering, 2013, 06, 26-35.	0.4	7
111	Drug targeting via retrometabolic approaches. , 1997, 76, 1-27.		7
112	Stereoisomers of N-substituted soft anticholinergics and their zwitterionic metabolite based on glycopyrrolate-syntheses and pharmacological evaluations. Die Pharmazie, 2008, 63, 200-9.	0.5	7
113	Extended covalent solid forms of carbon dioxide with carbon–oxygen single bonds. Chemical Physics Letters, 2000, 319, 645-649.	2.6	6
114	Activity-Limiting Role of Molecular Size: Size-Dependency of Maximum Activity for P450 Inhibition as Revealed by qHTS Data. Drug Metabolism and Disposition, 2014, 42, 1785-1790.	3.3	6
115	RNA aptamers specific for transmembrane p24 trafficking protein 6 and Clusterin for the targeted delivery of imaging reagents and RNA therapeutics to human \hat{l}^2 cells. Nature Communications, 2022, 13, 1815.	12.8	6
116	DRUG TARGETING BY RETROMETABOLIC DESIGN: SOFT DRUGS AND CHEMICAL DELIVERY SYSTEMS. Journal of Receptor and Signal Transduction Research, 2001, 21, 287-310.	2.5	5
117	Is there a universal rule for cellular growth? - Problems in studying and interpreting this phenomenon. FEMS Yeast Research, 2014, 14, 679-682.	2.3	5
118	CD40-targeting KGYY15 peptides do not efficiently block the CD40–CD40L interaction. Diabetologia, 2019, 62, 2158-2160.	6.3	5
119	Developing Small-Molecule Inhibitors of Protein-Protein Interactions Involved in Viral Entry as Potential Antivirals for COVID-19. Frontiers in Drug Discovery, 2022, 2, .	2.8	5
120	Designing Safer (Soft) Drugs by Avoiding the Formation of Toxic and Oxidative Metabolites., 2002, 186, 301-312.		4
121	Unified Pharmacogenetics-Based Parent–Metabolite Pharmacokinetic Model Incorporating Acetylation Polymorphism for Talampanel in Humans. Journal of Pharmacokinetics and Pharmacodynamics, 2005, 32, 377-400.	1.8	4
122	Cdc42 GTPase-activating proteins (GAPs) regulate generational inheritance of cell polarity and cell shape in fission yeast. Molecular Biology of the Cell, 2021, 32, ar14.	2.1	4
123	Effect of Arginase-1 Inhibition on the Incidence of Autoimmune Diabetes in NOD Mice. Current Research in Diabetes & Obesity Journal, 2018, 5, .	0.0	4
124	Exploratory computational assessment of possible binding modes for small molecule inhibitors of the CD40-CD154 co-stimulatory interaction. Die Pharmazie, 2012, 67, 374-9.	0.5	4
125	Parallel Evaluation of Polyethylene Glycol Conformal Coating and Alginate Microencapsulation as Immunoisolation Strategies for Pancreatic Islet Transplantation. Frontiers in Bioengineering and Biotechnology, 2022, 10 , .	4.1	4
126	Attempts of Ranking in a Series of Synthetic Nonpsychotropic Cannabinoids. SAR and QSAR in Environmental Research, 2001, 12, 113-127.	2.2	2

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127	Bilinear Model for the Sizeâ€Dependency of the CYP3A4 Inhibitory Activity of Structurally Diverse Compounds. Molecular Informatics, 2014, 33, 8-14.	2.5	2
128	The quantitative characterization of free radical sources and traps by electromigration applications. Journal of Proteomics, 2008, 70, 1317-1323.	2.4	1
129	Modeling Fission-Yeast Growth Partitioning and Oscillating Cortical Cdc42 Populations. Biophysical Journal, 2011, 100, 445a.	0.5	1
130	Islet Transplantation: A Collagen Based Cryogel Bioscaffold that Generates Oxygen for Islet Transplantation (Adv. Funct. Mater. 15/2020). Advanced Functional Materials, 2020, 30, 2070099.	14.9	1
131	Predicting Insulin Secretion Profiles for Immunoisolating Devices with Transplanted Islets. Diabetes, 2018, 67, 27-OR.	0.6	1
132	Drug Targeting by Retrometabolic Design. Drugs and the Pharmaceutical Sciences, 2001, , .	0.1	0
133	The Effect of Recovery Warm-up Time Following Cold Storage on the Dynamic Glucose-stimulated Insulin Secretion of Isolated Human Islets. Cell Transplantation, 2020, 29, 096368972090827.	2.5	0