

Obdulia Rabal

List of Publications by Year in descending order

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59
papers

2,216
citations

236612

25
h-index

233125

45
g-index

64
all docs

64
docs citations

64
times ranked

3302
citing authors

#	ARTICLE	IF	CITATIONS
1	Information Retrieval and Text Mining Technologies for Chemistry. <i>Chemical Reviews</i> , 2017, 117, 7673-7761.	23.0	195
2	CHEMDNER: The drugs and chemical names extraction challenge. <i>Journal of Cheminformatics</i> , 2015, 7, S1.	2.8	179
3	The CHEMDNER corpus of chemicals and drugs and its annotation principles. <i>Journal of Cheminformatics</i> , 2015, 7, S2.	2.8	166
4	Inhibition of a G9a/DNMT network triggers immune-mediated bladder cancer regression. <i>Nature Medicine</i> , 2019, 25, 1073-1081.	15.2	125
5	Discovery of first-in-class reversible dual small molecule inhibitors against G9a and DNMTs in hematological malignancies. <i>Nature Communications</i> , 2017, 8, 15424.	5.8	109
6	APIF: A New Interaction Fingerprint Based on Atom Pairs and Its Application to Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1245-1260.	2.5	102
7	A First-in-Class Small-Molecule that Acts as a Dual Inhibitor of HDAC and PDE5 and that Rescues Hippocampal Synaptic Impairment in Alzheimer's Disease Mice. <i>Neuropsychopharmacology</i> , 2017, 42, 524-539.	2.8	86
8	Dual Targeting of Histone Methyltransferase G9a and DNA Methyltransferase 1 for the Treatment of Experimental Hepatocellular Carcinoma. <i>Hepatology</i> , 2019, 69, 587-603.	3.6	81
9	Chemical Interrogation of FOXO3a Nuclear Translocation Identifies Potent and Selective Inhibitors of Phosphoinositide 3-Kinases. <i>Journal of Biological Chemistry</i> , 2009, 284, 28392-28400.	1.6	77
10	Design, Synthesis, and Biological Evaluation of First-in-Class Dual Acting Histone Deacetylases (HDACs) and Phosphodiesterase 5 (PDE5) Inhibitors for the Treatment of Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 8967-9004.	2.9	71
11	Comparison of Ligand-Based and Receptor-Based Virtual Screening of HIV Entry Inhibitors for the CXCR4 and CCR5 Receptors Using 3D Ligand Shape Matching and Ligand-Receptor Docking. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 509-533.	2.5	67
12	Concomitant histone deacetylase and phosphodiesterase 5 inhibition synergistically prevents the disruption in synaptic plasticity and it reverses cognitive impairment in a mouse model of Alzheimer's disease. <i>Clinical Epigenetics</i> , 2015, 7, 108.	1.8	52
13	Design, synthesis, biological evaluation and in vivo testing of dual phosphodiesterase 5 (PDE5) and histone deacetylase 6 (HDAC6)-selective inhibitors for the treatment of Alzheimer's disease. <i>European Journal of Medicinal Chemistry</i> , 2018, 150, 506-524.	2.6	48
14	LimTox: a web tool for applied text mining of adverse event and toxicity associations of compounds, drugs and genes. <i>Nucleic Acids Research</i> , 2017, 45, W484-W489.	6.5	41
15	In Silico Aptamer Docking Studies: From a Retrospective Validation to a Prospective Case Study TIM3 Aptamers Binding. <i>Molecular Therapy - Nucleic Acids</i> , 2016, 5, e376.	2.3	40
16	Design, synthesis and activity as acid ceramidase inhibitors of 2-oxooctanoyl and N-oleoylethanolamine analogues. <i>Chemistry and Physics of Lipids</i> , 2006, 144, 69-84.	1.5	39
17	Discovery of Mitogen-Activated Protein Kinase-Interacting Kinase 1 Inhibitors by a Comprehensive Fragment-Oriented Virtual Screening Approach. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 6618-6628.	2.9	38
18	Discovery of Reversible DNA Methyltransferase and Lysine Methyltransferase G9a Inhibitors with Antitumoral in Vivo Efficacy. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 6518-6545.	2.9	36

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19	Taking Advantage of the Selectivity of Histone Deacetylases and Phosphodiesterase Inhibitors to Design Better Therapeutic Strategies to Treat Alzheimer's Disease. <i>Frontiers in Aging Neuroscience</i> , 2019, 11, 149.	1.7	32
20	Hsp70 protects from stroke in atrial fibrillation patients by preventing thrombosis without increased bleeding risk. <i>Cardiovascular Research</i> , 2016, 110, 309-318.	1.8	30
21	Impact of Scaffold Exploration on Novel Dual-Acting Histone Deacetylases and Phosphodiesterase 5 Inhibitors for the Treatment of Alzheimer's Disease. <i>ACS Chemical Neuroscience</i> , 2017, 8, 638-661.	1.7	30
22	Imidazo[1,2-a]pyrazines as novel PI3K inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 1874-1878.	1.0	29
23	Identification of LAG3 high affinity aptamers by HT-SELEX and Conserved Motif Accumulation (CMA). <i>PLoS ONE</i> , 2017, 12, e0185169.	1.1	29
24	Discovery of <i>in Vivo</i> Chemical Probes for Treating Alzheimer's Disease: Dual Phosphodiesterase 5 (PDE5) and Class I Histone Deacetylase Selective Inhibitors. <i>ACS Chemical Neuroscience</i> , 2019, 10, 1765-1782.	1.7	28
25	Multitarget Approach for the Treatment of Alzheimer's Disease: Inhibition of Phosphodiesterase 9 (PDE9) and Histone Deacetylases (HDACs) Covering Diverse Selectivity Profiles. <i>ACS Chemical Neuroscience</i> , 2019, 10, 4076-4101.	1.7	27
26	Blockage of FOXP3 transcription factor dimerization and FOXP3/AML1 interaction inhibits T regulatory cell activity: sequence optimization of a peptide inhibitor. <i>Oncotarget</i> , 2017, 8, 71709-71724.	0.8	27
27	Novel Scaffold Fingerprint (SFP): Applications in Scaffold Hopping and Scaffold-Based Selection of Diverse Compounds. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1-18.	2.5	26
28	A novel FTY720 analogue targets SET-PP2A interaction and inhibits growth of acute myeloid leukemia cells without inducing cardiac toxicity. <i>Cancer Letters</i> , 2020, 468, 1-13.	3.2	26
29	Identification of ETP-46321, a potent and orally bioavailable PI3K $\hat{\pm}$, $\hat{\uparrow}$ inhibitor. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 3460-3466.	1.0	24
30	MMP10 Promotes Efficient Thrombolysis After Ischemic Stroke in Mice with Induced Diabetes. <i>Translational Stroke Research</i> , 2019, 10, 389-401.	2.3	21
31	Two Affinity Sites of the Cannabinoid Subtype 2 Receptor Identified by a Novel Homogeneous Binding Assay. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2016, 358, 580-587.	1.3	20
32	Fragment-Hopping-Based Discovery of a Novel Chemical Series of Proto-Oncogene PIM-1 Kinase Inhibitors. <i>PLoS ONE</i> , 2012, 7, e45964.	1.1	19
33	Rapid identification of ETP-46992, orally bioavailable PI3K inhibitor, selective versus mTOR. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 5208-5214.	1.0	19
34	Detailed Exploration around 4-Aminoquinolines Chemical Space to Navigate the Lysine Methyltransferase G9a and DNA Methyltransferase Biological Spaces. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 6546-6573.	2.9	19
35	Towards the understanding of the activity of G9a inhibitors: an activity landscape and molecular modeling approach. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 659-669.	1.3	19
36	Biologically Relevant Chemical Space Navigator: From Patent and Structure-Activity Relationship Analysis to Library Acquisition and Design. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 3123-3137.	2.5	18

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37	Design, Synthesis, and Biological Evaluation of Novel Matrix Metalloproteinase Inhibitors As Potent Antihemorrhagic Agents: From Hit Identification to an Optimized Lead. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 2465-2488.	2.9	18
38	Discovery of Novel Non- ϵ -Cyclam Polynitrogenated CXCR4 Coreceptor Inhibitors. <i>ChemMedChem</i> , 2008, 3, 1549-1557.	1.6	17
39	Computational medicinal chemistry in fragment-based drug discovery: what, how and when. <i>Future Medicinal Chemistry</i> , 2011, 3, 95-134.	1.1	17
40	Solid-phase synthesis of a combinatorial library of dihydroceramide analogues and its activity in human alveolar epithelial cells. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 50-62.	1.4	16
41	Conformational Selection versus Induced Fit in Kinases: The Case of PI3K β . <i>Angewandte Chemie - International Edition</i> , 2012, 51, 642-646.	7.2	16
42	Development and Validation of Molecular Overlays Derived from Three-Dimensional Hydrophobic Similarity with PharmScreen. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1596-1609.	2.5	14
43	Immunomodulatory Properties of Carvone Inhalation and Its Effects on Contextual Fear Memory in Mice. <i>Frontiers in Immunology</i> , 2018, 9, 68.	2.2	14
44	An integrated one-step system to extract, analyze and annotate all relevant information from image-based cell screening of chemical libraries. <i>Molecular BioSystems</i> , 2010, 6, 711.	2.9	11
45	Discovery and Safety Profiling of a Potent Preclinical Candidate, (4-[[3-(Hydroxycarbamoyl)-8-azaspiro[4.5]decan-3-yl]sulfonyl]phenoxy)-N-methylbenzamide), (CM-352), for the Prevention and Treatment of Hemorrhage. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 2941-2957.	2.9	11
46	Design and Synthesis of Novel Epigenetic Inhibitors Targeting Histone Deacetylases, DNA Methyltransferase 1, and Lysine Methyltransferase G9a with <i>In Vivo</i> Efficacy in Multiple Myeloma. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 3392-3426.	2.9	11
47	Structure-Based Virtual Screening of FGFR Inhibitors. <i>BioDrugs</i> , 2007, 21, 31-45.	2.2	10
48	The Markyt visualisation, prediction and benchmark platform for chemical and gene entity recognition at BioCreative/CHEMDNER challenge. <i>Database: the Journal of Biological Databases and Curation</i> , 2016, 2016, baw120.	1.4	10
49	Targeting the anion exchanger 2 with specific peptides as a new therapeutic approach in B lymphoid neoplasms. <i>Haematologica</i> , 2018, 103, 1065-1072.	1.7	10
50	Reversible dual inhibitor against G9a and DNMT1 improves human iPSC derivation enhancing MET and facilitating transcription factor engagement to the genome. <i>PLoS ONE</i> , 2017, 12, e0190275.	1.1	10
51	Using Novel Descriptor Accounting for Ligand-Receptor Interactions To Define and Visually Explore Biologically Relevant Chemical Space. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1086-1102.	2.5	9
52	Novel pharmacological maps of protein lysine methyltransferases: key for target deorphanization. <i>Journal of Cheminformatics</i> , 2018, 10, 32.	2.8	8
53	Centralizing Discovery Information: From Logistics to Knowledge at a Public Organization. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2011, 14, 429-449.	0.6	4
54	Cell-Integral-Diversity Criterion: A Proposal for Minimizing Cluster Artifact in Cell-Based Selections. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1886-1896.	2.5	3

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55	Fine tuning for success in structure-based virtual screening. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 1195-1206.	1.3	3
56	Dual epigenetic modifiers for cancer therapy. <i>Molecular and Cellular Oncology</i> , 2017, 4, e1342748.	0.3	2
57	Phenotypic Screening To Discover Novel Chemical Series as Efficient Antihemorrhagic Agents. <i>ACS Medicinal Chemistry Letters</i> , 2018, 9, 428-433.	1.3	2
58	Inhibition of the Methyltransferase G9a with Small Molecules As a New Therapeutic Strategy for Treatment of Hematological Malignancies. <i>Blood</i> , 2014, 124, 3532-3532.	0.6	2
59	P230Metalloproteinases inhibition: a new approach to reduce hemorrhage and blood transfusions. <i>Cardiovascular Research</i> , 2014, 103, S41.2-S41.	1.8	0