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	Design and Synthesis of Novel Epigenetic Inhibitors Targeting Histone Deacetylases, DNA Methyltransferase 1, and Lysine Methyltransferase G9a with In Vivo Efficacy in Multiple Myeloma. Journal of Medicinal Chemistry, 2021, 64, 3392-3426.	2.9	11
2	Fine tuning for success in structure-based virtual screening. Journal of Computer-Aided Molecular Design, 2021, 35, 1195-1206.	1.3	3
3	A novel FTY720 analogue targets SET-PP2A interaction and inhibits growth of acute myeloid leukemia cells without inducing cardiac toxicity. Cancer Letters, 2020, 468, 1-13.	3.2	26
4	Towards the understanding of the activity of G9a inhibitors: an activity landscape and molecular modeling approach. Journal of Computer-Aided Molecular Design, 2020, 34, 659-669.	1.3	19
5	MMP10 Promotes Efficient Thrombolysis After Ischemic Stroke in Mice with Induced Diabetes. Translational Stroke Research, 2019, 10, 389-401.	2.3	21
6	Dual Targeting of Histone Methyltransferase G9a and DNAâ€Methyltransferase 1 for the Treatment of Experimental Hepatocellular Carcinoma. Hepatology, 2019, 69, 587-603.	3.6	81
7	Taking Advantage of the Selectivity of Histone Deacetylases and Phosphodiesterase Inhibitors to Design Better Therapeutic Strategies to Treat Alzheimerâ€™s Disease. Frontiers in Aging Neuroscience, 2019, 11, 149.	1.7	32
8	Inhibition of a G9a/DNMT network triggers immune-mediated bladder cancer regression. Nature Medicine, 2019, 25, 1073-1081.	15.2	125
9	Multitarget Approach for the Treatment of Alzheimerâ€™s Disease: Inhibition of Phosphodiesterase 9 (PDE9) and Histone Deacetylases (HDACs) Covering Diverse Selectivity Profiles. ACS Chemical Neuroscience, 2019, 10, 4076-4101.	1.7	27
10	Discovery of in Vivo Chemical Probes for Treating Alzheimerâ€™s Disease: Dual Phosphodiesterase 5 (PDE5) and Class I Histone Deacetylase Selective Inhibitors. ACS Chemical Neuroscience, 2019, 10, 1765-1782.	1.7	28
11	Phenotypic Screening To Discover Novel Chemical Series as Efficient Antihemorrhagic Agents. ACS Medicinal Chemistry Letters, 2018, 9, 428-433.	1.3	2
12	Design, synthesis, biological evaluation and inÂvivo testing of dual phosphodiesterase 5 (PDE5) and histone deacetylase 6 (HDAC6)-selective inhibitors for the treatment of Alzheimer's disease. European Journal of Medicinal Chemistry, 2018, 150, 506-524.	2.6	48
13	Targeting the anion exchanger 2 with specific peptides as a new therapeutic approach in B lymphoid neoplasms. Haematologica, 2018, 103, 1065-1072.	1.7	10
14	Novel pharmacological maps of protein lysine methyltransferases: key for target deorphanization. Journal of Cheminformatics, 2018, 10, 32.	2.8	8
15	Discovery of Reversible DNA Methyltransferase and Lysine Methyltransferase G9a Inhibitors with Antitumoral in Vivo Efficacy. Journal of Medicinal Chemistry, 2018, 61, 6518-6545.	2.9	36
16	Development and Validation of Molecular Overlays Derived from Three-Dimensional Hydrophobic Similarity with PharmScreen. Journal of Chemical Information and Modeling, 2018, 58, 1596-1609.	2.5	14
17	Immunomodulatory Properties of Carvone Inhalation and Its Effects on Contextual Fear Memory in Mice. Frontiers in Immunology, 2018, 9, 68.	2.2	14
18	Detailed Exploration around 4-Aminoquinolines Chemical Space to Navigate the Lysine Methyltransferase G9a and DNA Methyltransferase Biological Spaces. Journal of Medicinal Chemistry, 2018, 61, 6546-6573.	2.9	19

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19	Information Retrieval and Text Mining Technologies for Chemistry. Chemical Reviews, 2017, 117, 7673-7761.	23.0	195
20	LimTox: a web tool for applied text mining of adverse event and toxicity associations of compounds, drugs and genes. Nucleic Acids Research, 2017, 45, W484-W489.	6.5	41
21	Discovery of first-in-class reversible dual small molecule inhibitors against G9a and DNMTs in hematological malignancies. Nature Communications, 2017, 8, 15424.	5.8	109
22	Impact of Scaffold Exploration on Novel Dual-Acting Histone Deacetylases and Phosphodiesterase 5 Inhibitors for the Treatment of Alzheimerâ€™s Disease. ACS Chemical Neuroscience, 2017, 8, 638-661.	1.7	30
23	Dual epigenetic modifiers for cancer therapy. Molecular and Cellular Oncology, 2017, 4, e1342748.	0.3	2
24	A First-in-Class Small-Molecule that Acts as a Dual Inhibitor of HDAC and PDE5 and that Rescues Hippocampal Synaptic Impairment in Alzheimerâ€™s Disease Mice. Neuropsychopharmacology, 2017, 42, 524-539.	2.8	86
25	Identification of LAG3 high affinity aptamers by HT-SELEX and Conserved Motif Accumulation (CMA). PLoS ONE, 2017, 12, e0185169.	1.1	29
26	Reversible dual inhibitor against G9a and DNMT1 improves human iPSC derivation enhancing MET and facilitating transcription factor engagement to the genome. PLoS ONE, 2017, 12, e0190275.	1.1	10
27	Blockage of FOXP3 transcription factor dimerization and FOXP3/AML1 interaction inhibits T regulatory cell activity: sequence optimization of a peptide inhibitor. Oncotarget, 2017, 8, 71709-71724.	0.8	27
28	Two Affinity Sites of the Cannabinoid Subtype 2 Receptor Identified by a Novel Homogeneous Binding Assay. Journal of Pharmacology and Experimental Therapeutics, 2016, 358, 580-587.	1.3	20
29	Design, Synthesis, and Biological Evaluation of First-in-Class Dual Acting Histone Deacetylases (HDACs) and Phosphodiesterase 5 (PDE5) Inhibitors for the Treatment of Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2016, 59, 8967-9004.	2.9	71
30	In Silico Aptamer Docking Studies: From a Retrospective Validation to a Prospective Case Study'TIM3 Aptamers Binding. Molecular Therapy - Nucleic Acids, 2016, 5, e376.	2.3	40
31	The Markyt visualisation, prediction and benchmark platform for chemical and gene entity recognition at BioCreative/CHEMDNER challenge. Database: the Journal of Biological Databases and Curation, 2016, 2016, baw120.	1.4	10
32	Hsp70 protects from stroke in atrial fibrillation patients by preventing thrombosis without increased bleeding risk. Cardiovascular Research, 2016, 110, 309-318.	1.8	30
33	CHEMDNER: The drugs and chemical names extraction challenge. Journal of Cheminformatics, 2015, 7, S1.	2.8	179
34	The CHEMDNER corpus of chemicals and drugs and its annotation principles. Journal of Cheminformatics, 2015, 7, S2.	2.8	166
35	Concomitant histone deacetylase and phosphodiesterase 5 inhibition synergistically prevents the disruption in synaptic plasticity and it reverses cognitive impairment in a mouse model of Alzheimerâ€™s disease. Clinical Epigenetics, 2015, 7, 108.	1.8	52
36	Discovery and Safety Profiling of a Potent Preclinical Candidate, (4-[4-[[(3R)-3-(Hydroxycarbamoyl)-8-azaspiro[4.5]decan-3-yl]sulfonyl]phenoxy]-N-methylbenzamide) (CM-352), for the Prevention and Treatment of Hemorrhage. Journal of Medicinal Chemistry, 2015, 58, 2941-2957.	2.9	11

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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. Journal of Medicinal Chemistry, 2015, 58, 2465-2488.	2.9	18
38	Novel Scaffold Fingerprint (SFP): Applications in Scaffold Hopping and Scaffold-Based Selection of Diverse Compounds. Journal of Chemical Information and Modeling, 2015, 55, 1-18.	2.5	26
39	P230Metalloproteinases inhibition: a new approach to reduce hemorrhage and blood transfusions. Cardiovascular Research, 2014, 103, S41.2-S41.	1.8	0
40	Inhibition of the Methyltransferase G9a with Small Molecules As a New Therapeutic Strategy for Treatment of Hematological Malignancies. Blood, 2014, 124, 3532-3532.	0.6	2
41	Fragment-Hopping-Based Discovery of a Novel Chemical Series of Proto-Oncogene PIM-1 Kinase Inhibitors. PLoS ONE, 2012, 7, e45964.	1.1	19
42	Using Novel Descriptor Accounting for Ligandâ€“Receptor Interactions To Define and Visually Explore Biologically Relevant Chemical Space. Journal of Chemical Information and Modeling, 2012, 52, 1086-1102.	2.5	9
43	Biologically Relevant Chemical Space Navigator: From Patent and Structureâ€“Activity Relationship Analysis to Library Acquisition and Design. Journal of Chemical Information and Modeling, 2012, 52, 3123-3137.	2.5	18
44	Rapid identification of ETP-46992, orally bioavailable PI3K inhibitor, selective versus mTOR. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 5208-5214.	1.0	19
45	Imidazo[1,2-a]pyrazines as novel PI3K inhibitors. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 1874-1878.	1.0	29
46	Identification of ETP-46321, a potent and orally bioavailable PI3K Î±, Î´ inhibitor. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 3460-3466.	1.0	24
47	Conformational Selection versus Induced Fit in Kinases: The Case of PI3Kâ€Î³. Angewandte Chemie - International Edition, 2012, 51, 642-646.	7.2	16
48	Computational medicinal chemistry in fragment-based drug discovery: what, how and when. Future Medicinal Chemistry, 2011, 3, 95-134.	1.1	17
49	Centralizing Discovery Information: From Logistics to Knowledge at a Public Organization. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 429-449.	0.6	4
50	Discovery of Mitogen-Activated Protein Kinase-Interacting Kinase 1 Inhibitors by a Comprehensive Fragment-Oriented Virtual Screening Approach. Journal of Medicinal Chemistry, 2010, 53, 6618-6628.	2.9	38
51	An integrated one-step system to extract, analyze and annotate all relevant information from image-based cell screening of chemical libraries. Molecular BioSystems, 2010, 6, 711.	2.9	11
52	Chemical Interrogation of FOXO3a Nuclear Translocation Identifies Potent and Selective Inhibitors of Phosphoinositide 3-Kinases. Journal of Biological Chemistry, 2009, 284, 28392-28400.	1.6	77
53	APIF: A New Interaction Fingerprint Based on Atom Pairs and Its Application to Virtual Screening. Journal of Chemical Information and Modeling, 2009, 49, 1245-1260.	2.5	102
54	Discovery of Novel Nonâ€Cyclam Polynitrogenated CXCR4 Coreceptor Inhibitors. ChemMedChem, 2008, 3, 1549-1557.	1.6	17

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55	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 Ligandâ"Receptor Docking. Journal of Chemical Information and Modeling, 2008, 48, 509-533.	2.5	67
56	Structure-Based Virtual Screening of FGFR Inhibitors. BioDrugs, 2007, 21, 31-45.	2.2	10
57	Cell-Integral-Diversity Criterion:â€‰ A Proposal for Minimizing Cluster Artifact in Cell-Based Selections. Journal of Chemical Information and Modeling, 2007, 47, 1886-1896.	2.5	3
58	Solid-phase synthesis of a combinatorial library of dihydroceramide analogues and its activity in human alveolar epithelial cells. Bioorganic and Medicinal Chemistry, 2007, 15, 50-62.	1.4	16
59	Design, synthesis and activity as acid ceramidase inhibitors of 2-oxooctanoyl and N-oleoylethanolamine analogues. Chemistry and Physics of Lipids, 2006, 144, 69-84.	1.5	39