Isidro Cortes-Ciriano

List of Publications by Year in Descending Order

58 papers	3,213 citations	25 h-index	56 g-index
68 ext. papers	4,737 ext. citations	12.8 avg, IF	5.56 L-index

#	Paper	IF	Citations
58	Patient-derived models of brain metastases recapitulate human disseminated disease.. *Cell Reports Medicine*, **2022**, 3, 100623	18	0
57	Rearrangement-mediated cis-regulatory alterations in advanced patient tumors reveal interactions with therapy. *Cell Reports*, **2021**, 37, 110023	10.6	0
56	Reconstructing the Lineage Histories and Differentiation Trajectories of Individual Cancer Cells in Myeloproliferative Neoplasms. *Cell Stem Cell*, **2021**, 28, 514-523.e9	18	42
55	Artificial intelligence in drug discovery: what is realistic, what are illusions? Part 2: a discussion of chemical and biological data. *Drug Discovery Today*, **2021**, 26, 1040-1052	8.8	22
54	A semi-supervised learning framework for quantitative structure-activity regression modelling. *Bioinformatics*, **2021**, 37, 342-350	7.2	2
53	Artificial intelligence in drug discovery: what is realistic, what are illusions? Part 1: Ways to make an impact, and why we are not there yet. *Drug Discovery Today*, **2021**, 26, 511-524	8.8	39
52	Computational analysis of cancer genome sequencing data. *Nature Reviews Genetics*, **2021**,	30.1	2
51	QSAR-derived affinity fingerprints (part 1): fingerprint construction and modeling performance for similarity searching, bioactivity classification and scaffold hopping. *Journal of Cheminformatics*, **2020**, 12, 39	8.6	13
50	A user guide for the online exploration and visualization of PCAWG data. *Nature Communications*, **2020**, 11, 3400	17.4	7
49	QSAR-derived affinity fingerprints (part 2): modeling performance for potency prediction. *Journal of Cheminformatics*, **2020**, 12, 41	8.6	7
48	Genomic footprints of activated telomere maintenance mechanisms in cancer. *Nature Communications*, **2020**, 11, 733	17.4	40
47	Comprehensive analysis of chromothripsis in 2,658 human cancers using whole-genome sequencing. *Nature Genetics*, **2020**, 52, 331-341	36.3	168
46	Reconstructing the Lineage Histories and Differentiation Trajectories of Individual Hematopoietic Stem Cells in JAK2-Mutant Myeloproliferative Neoplasms. *Blood*, **2020**, 136, 7-8	2.2	4
45	Accurate detection of mosaic variants in sequencing data without matched controls. *Nature Biotechnology*, **2020**, 38, 314-319	44.5	20
44	Mechanisms and therapeutic implications of hypermutation in gliomas. *Nature*, **2020**, 580, 517-523	50.4	172
43	Genomics of MPNST (GeM) Consortium: Rationale and Study Design for Multi-Omic Characterization of NF1-Associated and Sporadic MPNSTs. *Genes*, **2020**, 11,	4.2	6
42	KekuleScope: prediction of cancer cell line sensitivity and compound potency using convolutional neural networks trained on compound images. *Journal of Cheminformatics*, **2019**, 11, 41	8.6	29

41	Reliable Prediction Errors for Deep Neural Networks Using Test-Time Dropout. *Journal of Chemical Information and Modeling*, **2019**, 59, 3330-3339	6.1	18
40	A decision-theoretic approach to the evaluation of machine learning algorithms in computational drug discovery. *Bioinformatics*, **2019**, 35, 4656-4663	7.2	7
39	Linked-read analysis identifies mutations in single-cell DNA-sequencing data. *Nature Genetics*, **2019**, 51, 749-754	36.3	42
38	Detecting the mutational signature of homologous recombination deficiency in clinical samples. *Nature Genetics*, **2019**, 51, 912-919	36.3	96
37	Elucidating Compound Mechanism of Action and Predicting Cytotoxicity Using Machine Learning Approaches, Taking Prediction Confidence into Account. *Current Protocols in Chemical Biology*, **2019** , 11, e73	1.8	1
36	Deep Confidence: A Computationally Efficient Framework for Calculating Reliable Prediction Errors for Deep Neural Networks. *Journal of Chemical Information and Modeling*, **2019**, 59, 1269-1281	6.1	40
35	Comprehensive Characterization of Cancer Driver Genes and Mutations. *Cell*, **2018**, 173, 371-385.e18	56.2	854
34	Perspective on Oncogenic Processes at the End of the Beginning of Cancer Genomics. *Cell*, **2018**, 173, 305-320.e10	56.2	166
33	Conformal Regression for Quantitative Structure-Activity Relationship Modeling-Quantifying Prediction Uncertainty. *Journal of Chemical Information and Modeling*, **2018**, 58, 1132-1140	6.1	27
32	Discovering Highly Potent Molecules from an Initial Set of Inactives Using Iterative Screening. *Journal of Chemical Information and Modeling*, **2018**, 58, 2000-2014	6.1	21
31	Abstract LB-378: Comprehensive analysis of chromothripsis in 2,658 human cancers using whole-genome sequencing **2018**,		2
30	Intersection of diverse neuronal genomes and neuropsychiatric disease: The Brain Somatic Mosaicism Network. *Science*, **2017**, 356,	33.3	152
29	A molecular portrait of microsatellite instability across multiple cancers. *Nature Communications*, **2017**, 8, 15180	17.4	288
28	Improved large-scale prediction of growth inhibition patterns using the NCI60 cancer cell line panel. *Bioinformatics*, **2016**, 32, 85-95	7.2	60
27	Bioalerts: a python library for the derivation of structural alerts from bioactivity and toxicity data sets. *Journal of Cheminformatics*, **2016**, 8, 13	8.6	19
26	The Impact of Environmental and Endogenous Damage on Somatic Mutation Load in Human Skin Fibroblasts. *PLoS Genetics*, **2016**, 12, e1006385	6	55
25	Current Trends in Drug Sensitivity Prediction. *Current Pharmaceutical Design*, **2016**, 22, 6918-6927	3.3	9
24	Improving the prediction of organism-level toxicity through integration of chemical, protein target and cytotoxicity qHTS data. *Toxicology Research*, **2016**, 5, 883-894	2.6	7

23	Benchmarking the Predictive Power of Ligand Efficiency Indices in QSAR. *Journal of Chemical Information and Modeling*, **2016**, 56, 1576-87	6.1	28
22	How Consistent are Publicly Reported Cytotoxicity Data? Large-Scale Statistical Analysis of the Concordance of Public Independent Cytotoxicity Measurements. *ChemMedChem*, **2016**, 11, 57-71	3.7	19
21	Prediction of the potency of mammalian cyclooxygenase inhibitors with ensemble proteochemometric modeling. *Journal of Cheminformatics*, **2015**, 7, 1	8.6	70
20	Temperature Accelerated Molecular Dynamics with Soft-Ratcheting Criterion Orients Enhanced Sampling by Low-Resolution Information. *Journal of Chemical Theory and Computation*, **2015**, 11, 3446-54	6.4	11
19	Identification of binding sites and favorable ligand binding moieties by virtual screening and self-organizing map analysis. *BMC Bioinformatics*, **2015**, 16, 93	3.6	11
18	Proteochemometric modelling coupled to in silico target prediction: an integrated approach for the simultaneous prediction of polypharmacology and binding affinity/potency of small molecules. *Journal of Cheminformatics*, **2015**, 7, 15	8.6	26
17	Prediction of PARP Inhibition with Proteochemometric Modelling and Conformal Prediction. *Molecular Informatics*, **2015**, 34, 357-66	3.8	20
16	Chemically Aware Model Builder (camb): an R package for property and bioactivity modelling of small molecules. *Journal of Cheminformatics*, **2015**, 7, 45	8.6	31
15	Polypharmacology modelling using proteochemometrics (PCM): recent methodological developments, applications to target families, and future prospects. *MedChemComm*, **2015**, 6, 24-50	5	74
14	Improved Chemical Structure-Activity Modeling Through Data Augmentation. *Journal of Chemical Information and Modeling*, **2015**, 55, 2682-92	6.1	23
13	Applications of proteochemometrics - from species extrapolation to cell line sensitivity modelling. *BMC Bioinformatics*, **2015**, 16,	3.6	3
12	Comparing the Influence of Simulated Experimental Errors on 12 Machine Learning Algorithms in Bioactivity Modeling Using 12 Diverse Data Sets. *Journal of Chemical Information and Modeling*, **2015**, 55, 1413-25	6.1	21
11	Extending in silico mechanism-of-action analysis by annotating targets with pathways: application to cellular cytotoxicity readouts. *Future Medicinal Chemistry*, **2014**, 6, 2029-56	4.1	16
10	Modelling ligand selectivity of serine proteases using integrative proteochemometric approaches improves model performance and allows the multi-target dependent interpretation of features. *Integrative Biology (United Kingdom)*, **2014**, 6, 1023-33	3.7	23
9	Proteochemometric modeling in a Bayesian framework. *Journal of Cheminformatics*, **2014**, 6, 35	8.6	32
8	Experimental validation of in silico target predictions on synergistic protein targets. *Journal of Cheminformatics*, **2013**, 5,	8.6	78
7	Benchmarking of protein descriptor sets in proteochemometric modeling (part 2): modeling performance of 13 amino acid descriptor sets. *Journal of Cheminformatics*, **2013**, 5, 42	8.6	48
6	Experimental validation of in silico target predictions on synergistic protein targets. *MedChemComm*, **2013**, 4, 278-288	5	7

List of Publications

5	Clonal diversification and histogenesis of malignant germ cell tumours	1
4	A user guide to the online resources for data exploration, visualization, and discovery for the Pan-Cancer Analysis of Whole Genomes project (PCAWG)	3
3	Reconstructing the lineage histories and differentiation trajectories of individual cancer cells in JAK2-mutant myeloproliferative neoplasms	1
2	Comprehensive analysis of chromothripsis in 2,658 human cancers using whole-genome sequencing	12
1	Cancer Cell Line Profiler (CCLP): a webserver for the prediction of compound activity across the NCI60 panel	1