

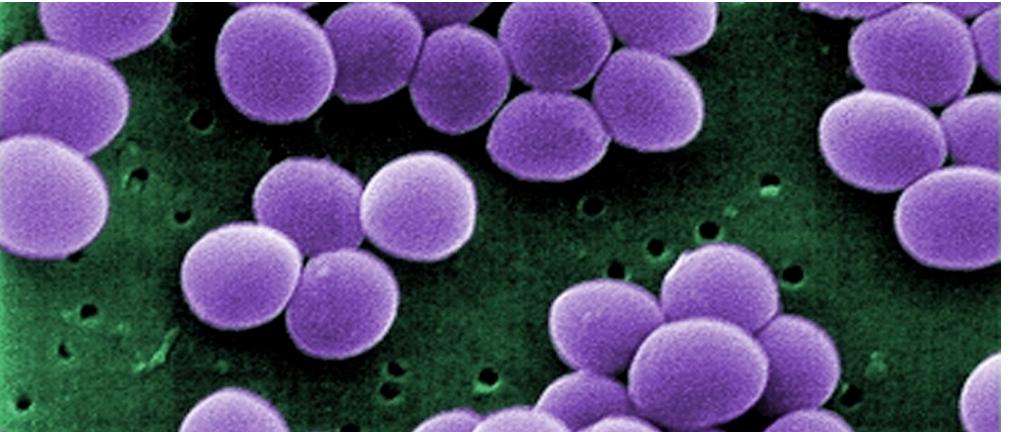
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Head of Literature Services
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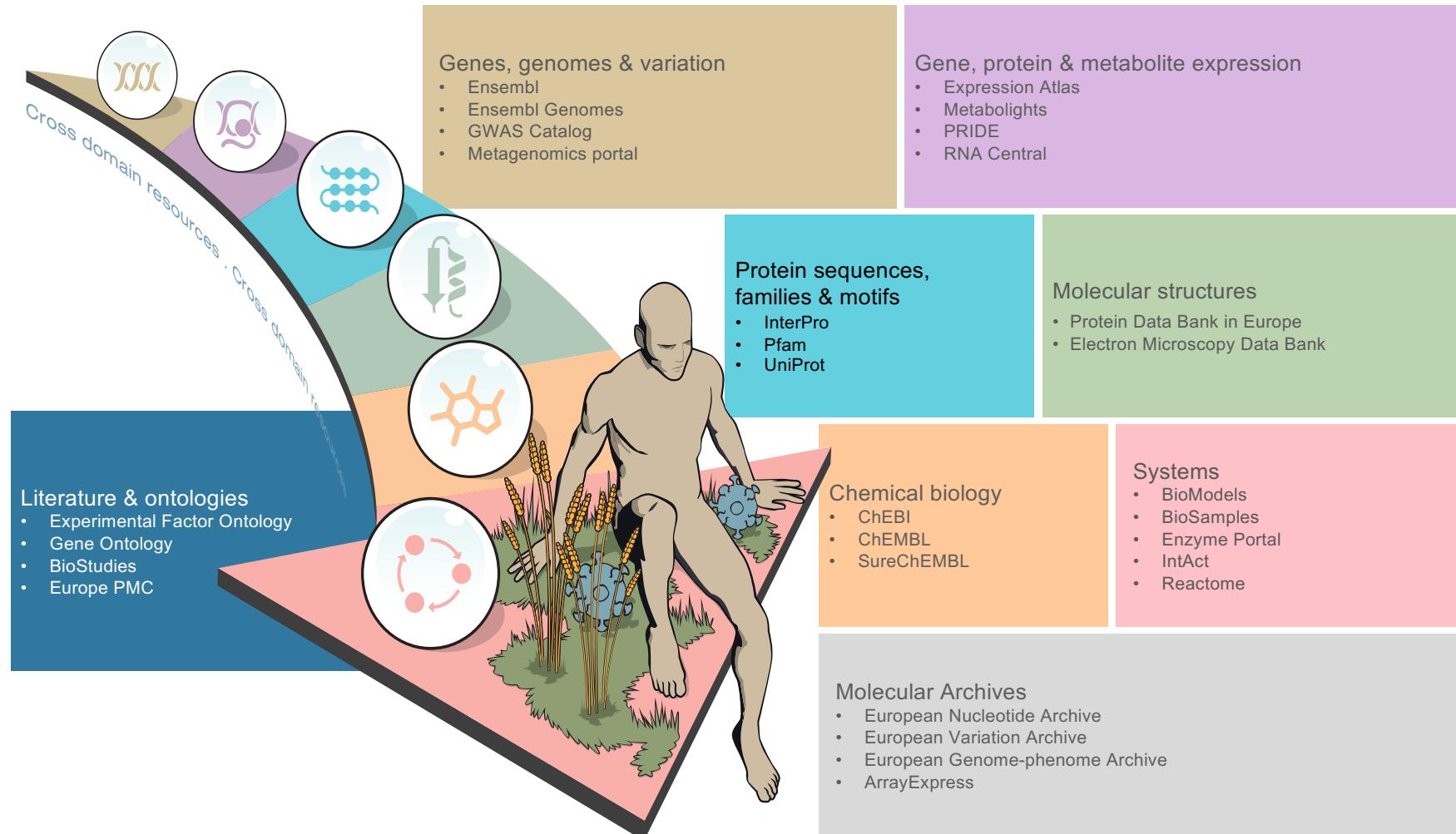
Life Sciences



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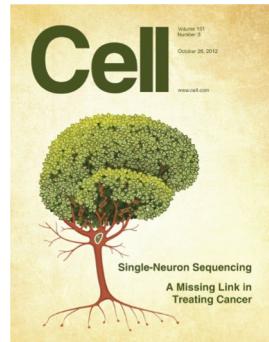


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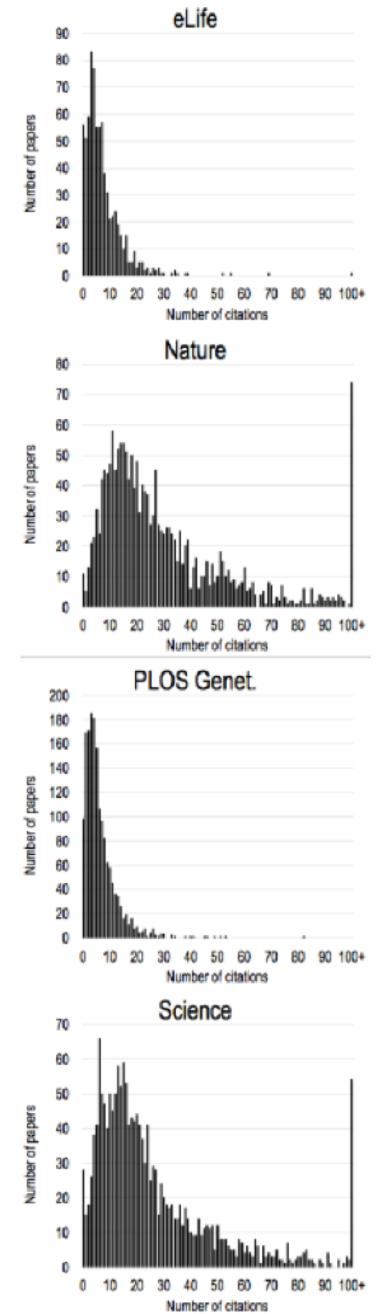


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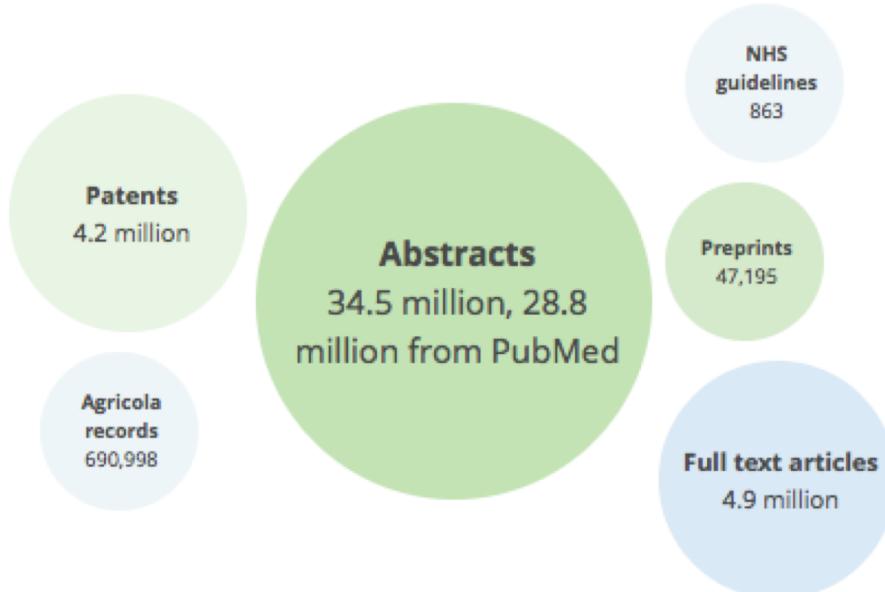




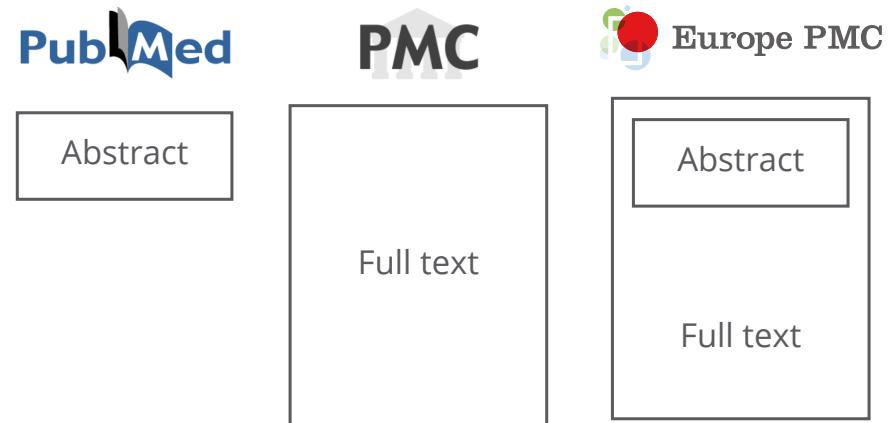
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[Metastatic HER2+ Breast Cancer: A Potentially Curable Disease?](#)

Prior L, Lim M, Ward C, Featherstone H, Murray H, D'Arcy C, Crown J, Gullo G

[Cureus](#) [05 Sep 2017, 9(9):e1654]

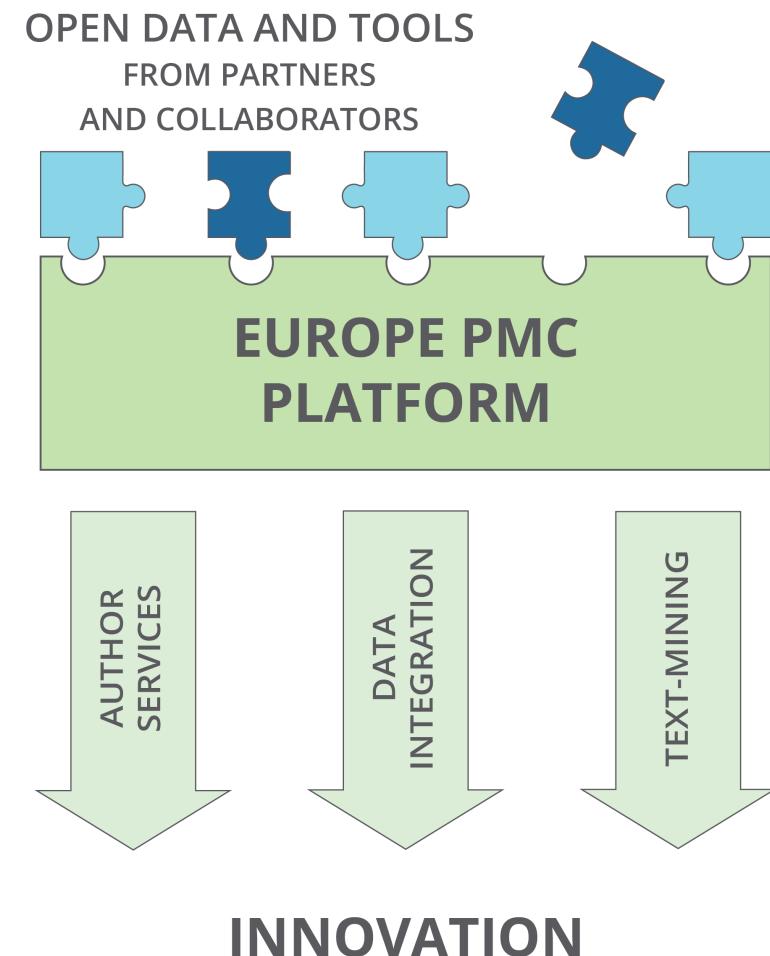
history of metastatic **HER2-positive breast cancer**, transforming it from an aggressive **cancer** subtype with a ... Predictor of Response to Dual **HER2 Blockade in HER2-positive Early Breast Cancer**) trial further evaluated

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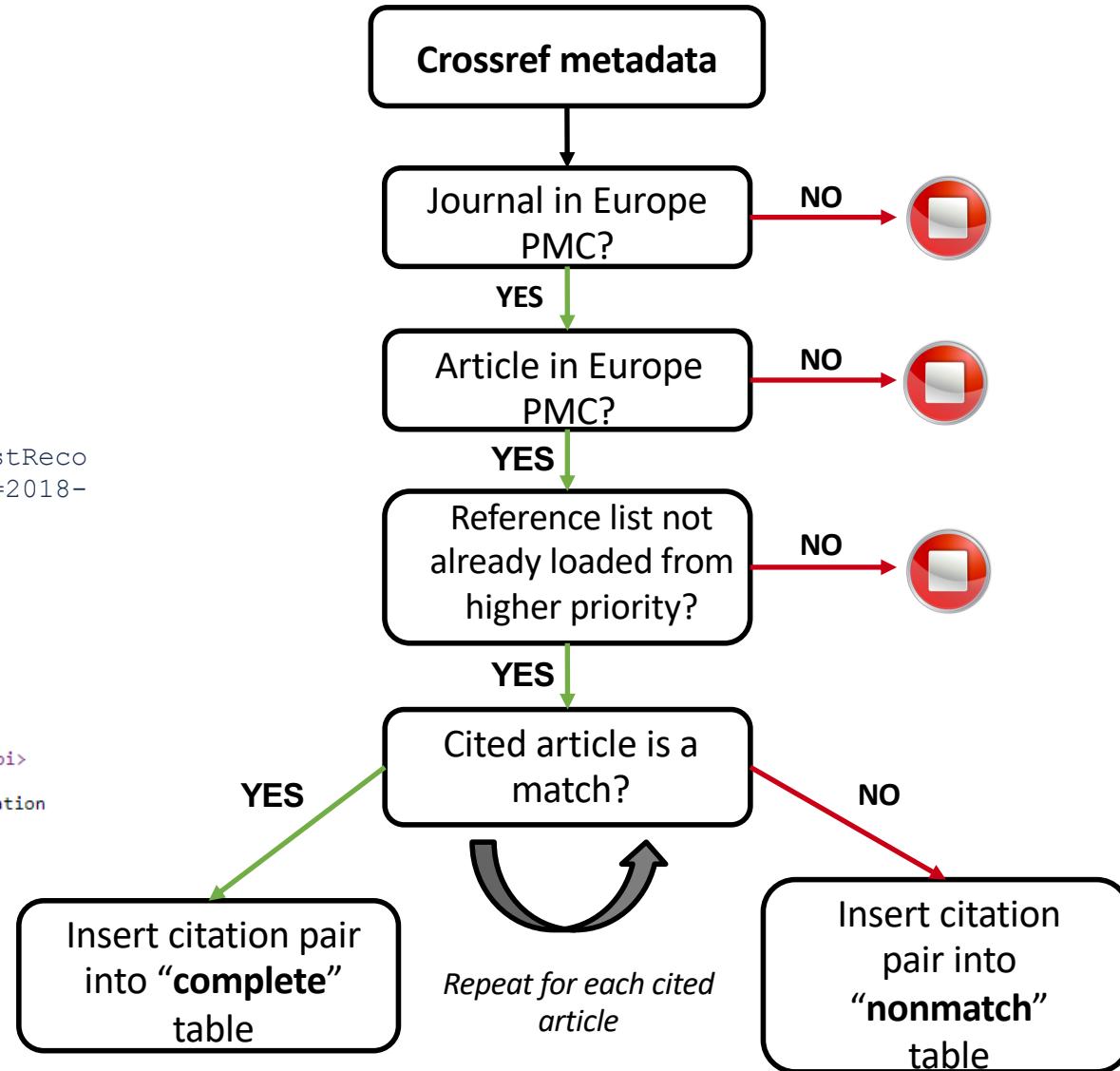
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</citation>
```



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[Tumour-associated macrophages as treatment targets in oncology.](#)
Mantovani A, Marchesi F, Malesci A, Laghi L, Allavena P
Nat Rev Clin Oncol [24 Jan 2017, 14(7):399-416]
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[Translation of CircRNAs.](#)
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Mol Cell [23 Mar 2017, 66(1):9-21.e7]
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[Treadmilling by FtsZ filaments drives peptidoglycan synthesis and bacterial cell division.](#)
Bisson-Filho AW, Hsu YP, Squyres GR, Kuru E, Wu F, Jukes C, Sun Y, Dekker C, Holden S, VanNieuwenhze MS, Brun YV, Garner EC
Science [01 Feb 2017, 355(6326):739-743]
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Select results 1 - 25

[Inflammation as target in cancer therapy.](#)
Marelli G, Sica A, Vannucci L, Allavena P
Curr Opin Pharmacol [12 Jun 2017, 35:57-65]
Cited: 13 times (PMID:28618326)

[Tumor-derived exosomes modulate PD-L1 expression in monocytes.](#)
Haderk F, Schulz R, Iskar M, Cid LL, Worst T, Willmund KV, Schulz A, Warnken U, Seiler J, Benner A, Nessling M, Zenz T, Göbel M, Dürig J [...] Seiffert M
Sci Immunol [01 Jul 2017, 2(13)]
Cited: 11 times (PMID:28754746)

[Cholangiocarcinoma - evolving concepts and therapeutic strategies.](#)
Rizvi S, Khan SA, Hallemeier CL, Kelley RK, Gores GJ
Nat Rev Clin Oncol [10 Oct 2017, 15(2):95-111]
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- Molecular docking screening using agonist-bound GPCR structures: probing the A2A adenosine receptor.
(PMID:25625646 PMCID:PMC4474233)

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Rodríguez D¹, Gao ZG², Moss SM², Jacobson KA² , Carlsson J¹ 

Affiliations ▾

[Journal of Chemical Information and Modeling](#) [13 Feb 2015, 55(3):550-563]

Type: Research Support, Non-U.S. Gov't, research-article, Journal Article

DOI: [10.1021/ci500639g](https://doi.org/10.1021/ci500639g) 

Abstract

Crystal structures of G protein-coupled receptors (GPCRs) have recently revealed the molecular basis of ligand binding and activation, which has provided exciting opportunities for structure-based drug design. The A2A adenosine receptor (A2AAR) is a promising therapeutic target for cardiovascular diseases, but progress in this area is limited by the lack of novel agonist scaffolds. We carried out docking screens of 6.7 million commercially available molecules against active-like conformations of the A2AAR to investigate whether these structures could guide the discovery of agonists. Nine out of the 20 predicted agonists were confirmed to be A2AAR ligands, but none of these activated the ARs. The difficulties in discovering AR agonists using structure-based methods originated from limited atomic-level understanding of the activation mechanism and a chemical bias toward antagonists in the screened library. In particular, the composition of the screened library was found to strongly reduce the likelihood of identifying AR agonists, which reflected the high ligand complexity required for receptor activation. Extension of this analysis to other pharmaceutically relevant GPCRs suggested that library screening may not be suitable for targets requiring a complex receptor-ligand interaction network. Our results provide specific directions for the future development of novel A2AAR agonists and general strategies for structure-based drug discovery.

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Venkatesan A¹, Kim JH¹, Talo F¹, Ide-Smith M¹ , Gobeil J², Carter J³, Batista-Navarro R³, Ananiadou S³, Ruch P⁴, McEntyre J¹

Affiliations ▾

[Wellcome Open Research](#) [01 Jan 2016, 1:25]

Type: research-article, Journal Article

DOI: [10.12688/wellcomeopenres.10210.2](https://doi.org/10.12688/wellcomeopenres.10210.2)

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Jo McEntyre

European Bioinformatics Institute (EMBL-EBI)

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Abstract

The tremendous growth in biological data has resulted in an increase in the number of research papers being published. This presents a great challenge for scientists in searching and assimilating facts described in those papers. Particularly, biological databases depend on curators to add highly precise and useful information that are usually extracted by reading research articles. Therefore, there is an urgent need to find ways to improve linking literature to the underlying data, thereby minimising the effort in browsing content and identifying key biological concepts. As part of the development of Europe PMC, we have developed a new platform, SciLite, which integrates text-mined annotations from different sources and overlays those outputs on research articles. The aim is to aid researchers and curators using Europe PMC in finding key concepts more easily and provide links to related resources or tools, bridging the gap between literature and biological data.

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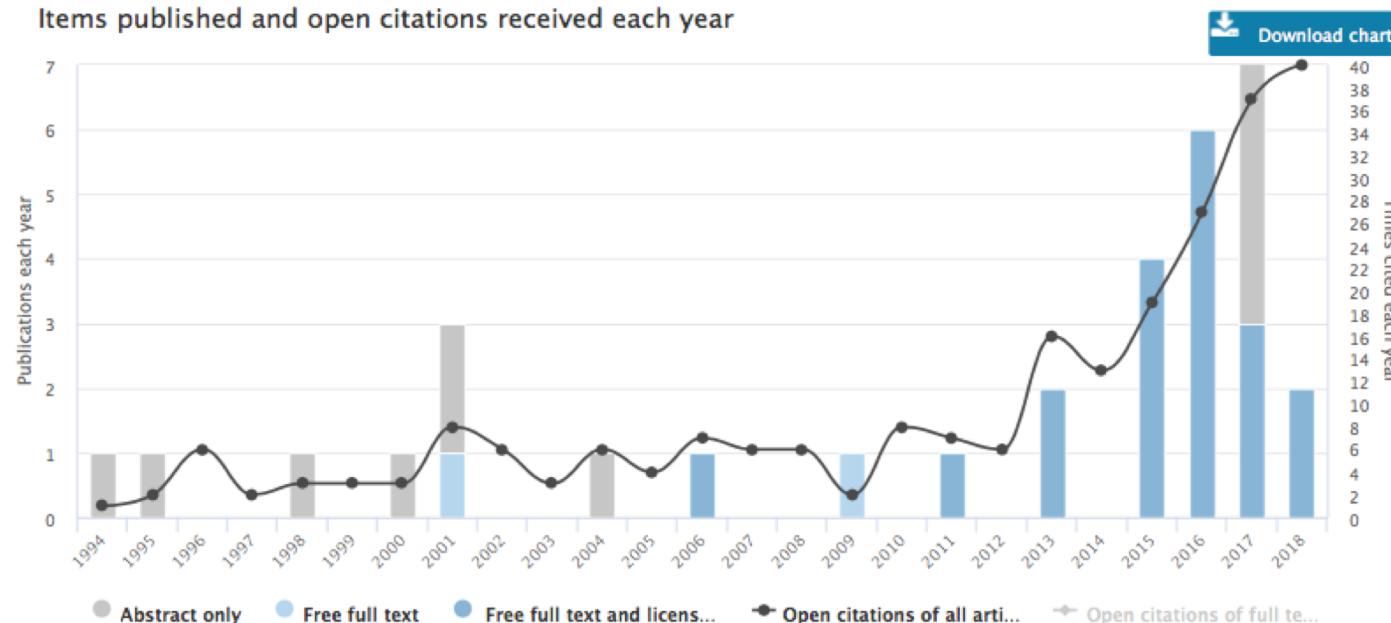
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B. Ian Hutchins, Xin Yuan, James M. Anderson, George M. Santangelo 

Published: September 6, 2016 • <https://doi.org/10.1371/journal.pbio.1002541> • >> See the preprint

Paper citations, data citations

PDB record: 3EML

The 2.6 angstrom crystal structure of a human A2A adenosine receptor bound to an antagonist.
(PMID:18832607 PMCID:PMC2586971)

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Jaakola VP¹ , Griffith MT, Hanson MA, Cherezov V, Chien EY, Lane JR , Ijzerman AP , Stevens RC

[Affiliations](#)

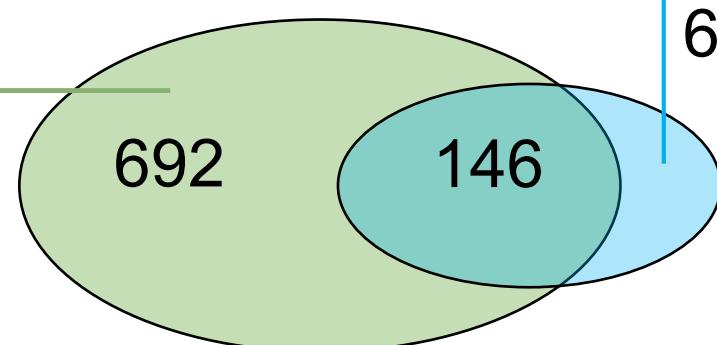
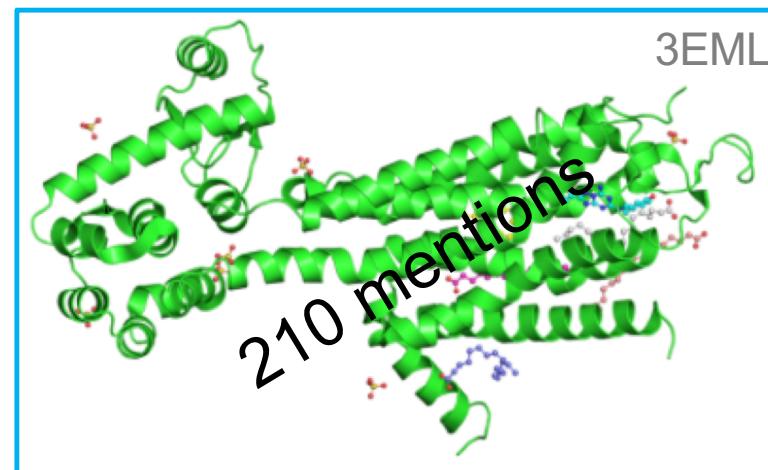
Science (New York, N.Y.) [02 Oct 2008, 322(5905):1211-1217]

Type: Research Support, Non-U.S. Gov't, research-article, Research Support, U.S. Gov't, Non-P.H.S., Journal Article, Research Support, N.I.H., Extramural
DOI: [10.1126/science.1164772](https://doi.org/10.1126/science.1164772)

Abstract

The adenosine class of heterotrimeric guanine nucleotide-binding protein (G protein)-coupled receptors (GPCRs) mediates the important role of extracellular adenosine in many physiological processes and is antagonized by caffeine. We have determined the crystal structure of the human A2A adenosine receptor, in complex with a high-affinity subtype-selective antagonist, ZM241385, to 2.6 angstrom resolution. Four disulfide bridges in the extracellular domain, combined with a subtle repacking of the transmembrane helices relative to the adrenergic and rhodopsin receptor structures, define a pocket distinct from that of other structurally determined GPCRs. The arrangement allows for the binding of the antagonist in an extended conformation, perpendicular to the membrane plane. The binding site highlights an integral role for the extracellular loops, together with the helical core, in ligand recognition by this class of GPCRs and suggests a role for ZM241385 in restricting the movement of a tryptophan residue important in the activation mechanism of the class A receptors.

838 citations

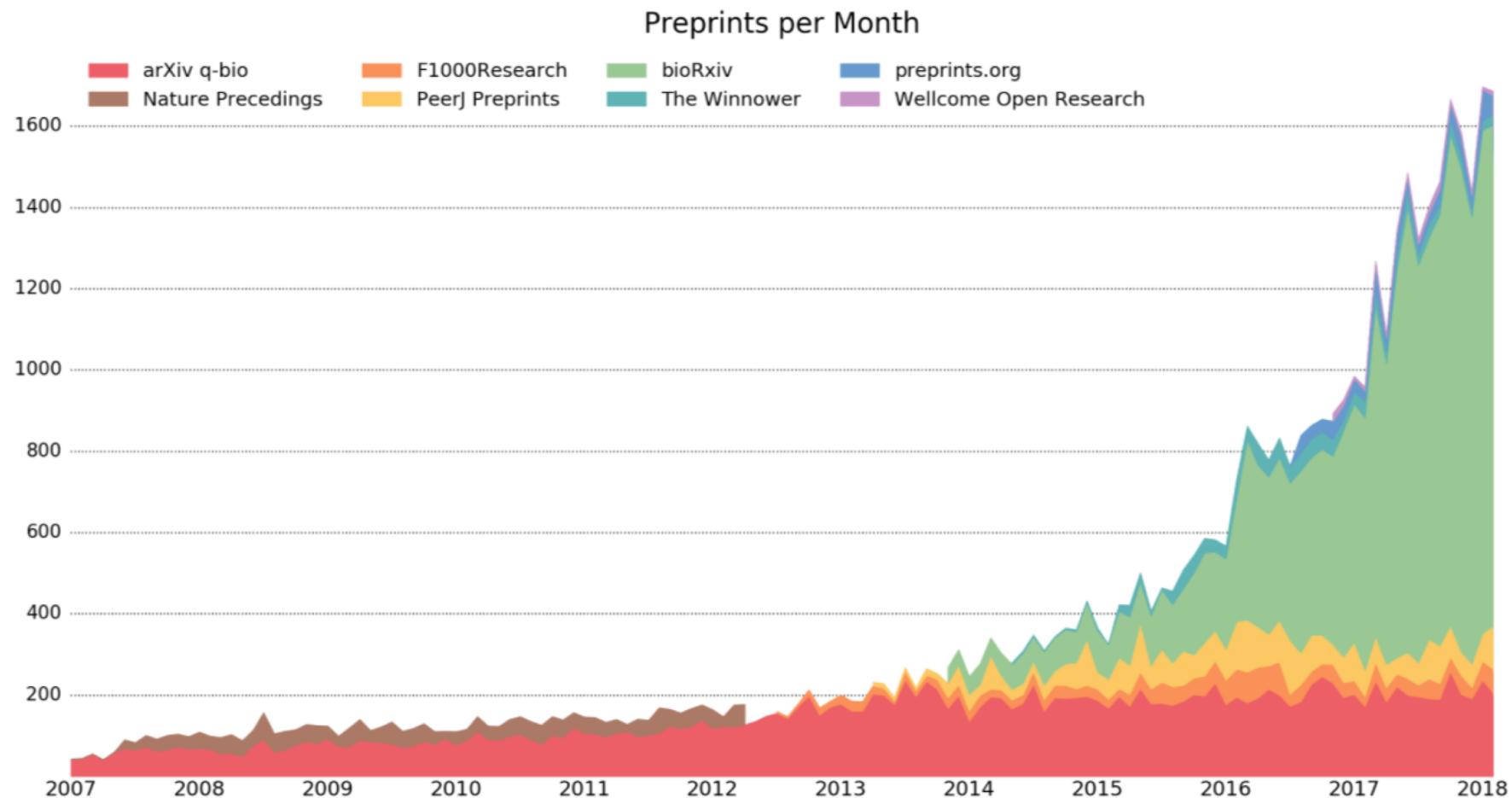


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□ Power Analysis of Single Cell RNA-Sequencing Experiments (PPR:PPR7010)

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Svensson V, Natarajan KN, Ly L, Miragaia RJ, Labalette C, Macaulay IC, Cvejic A, Teichmann SA

BioRxiv [08 Sep 2016]

Type: Preprint

DOI: [10.1101/073692](https://doi.org/10.1101/073692)

A later version of this preprint was published as "Power analysis of single-cell RNA-sequencing experiments." Nature methods. 2017 Apr;14(4):381-387.

Methods

Mouse embryonic stem (mES) cells culture

Wildtype E14 mouse ES cells (kindly provided by Pentao Liu, Wellcome Trust Sanger Institute) were cultured on gelatin coated dishes using Knockout DMEM (#10829; Gibco), 15% Fetal Calf Serum (FB 1001/500; batch tested from Labtech), 1x Penicillin-Streptomycin (#10378-016; Gibco), 1x MEM NEAA (11140-035; Gibco), 2-mercaptoethanol (31350-010; Gibco) and 1000U Leukemia Inhibitory Factor (LIF; #ESG1107). Mycoplasma-free tested mES cells were passaged every 2-3 days.

7. Bond MR, Hanover JA. A little sugar goes a long way: the cell biology of O-GlcNAc. J Cell Biol, 2015; 208: 869-880 <https://doi.org/10.1083/jcb.201501101> [Europe PMC Abstract] [Europe PMC Full Text]
8. Chepelianskii AD. Towards physical laws for software architecture. 2010
9. Choi I, Kim R, Lim H-W, Kaestner KH, Won K-J. 5-hydroxymethylcytosine represses the activity of enhancers in embryonic stem cells: a new epigenetic signature for gene regulation. BMC Genomics, 2014; 15: 670 <https://doi.org/10.1186/1471-2164-15-670> [Europe PMC Abstract] [Europe PMC Full Text]
10. Doege CA, Inoue K, Yamashita T, Rhee DB, Travis S, Fujita R, Guarnieri P, Bhagat G, Vanti WB, Shih A, Levine RL, et al. Early-stage epigenetic modification during somatic cell reprogramming by Parp1 and Tet2. Nature, 2012; 488: 652-655 <https://doi.org/10.1038/nature11333> [Europe PMC Abstract] [Europe PMC Full Text]

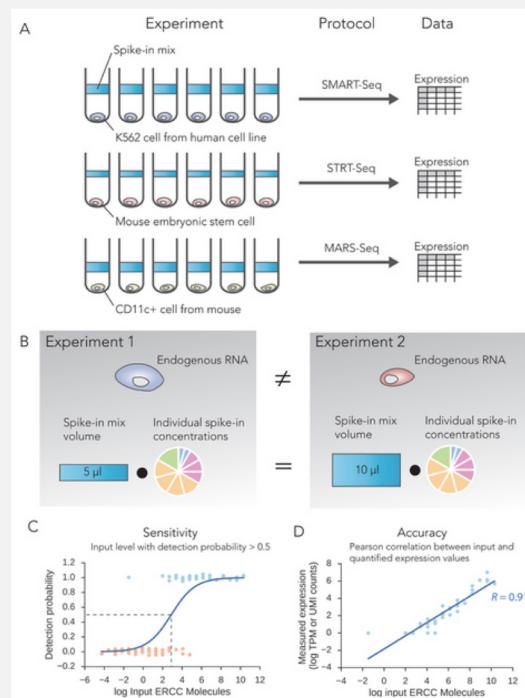
Figure 1: [Open in new tab](#)
Overview of protocol comparison strategy.

(A) The data we use are from different protocols and investigate diverse cell types.

(B) Comparing protocols by looking at properties relating to the cells would be distorted by the diverse cell types involved. Since the same standard spike-in mix has been used in all of them, albeit at different concentrations, we can base our assessment on these synthetic RNA molecules.

We define two global technical performance metrics based on these: (C) Spike-in sensitivity: the number of spike-in molecules which need to be present in a sample before there is at least 50% chance of detecting them. This is inferred by logistic regression.

(D) Spike-in quantification accuracy: How well preserved the log-linear relation between input spike-ins is when quantifying the measured expression. We formulate this as the Pearson correlation between input molecules and output expression.



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Turner SD
bioRxiv [14 May 2014]
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[Analysis of protein-coding genetic variation in 60,706 humans](#) Preprint
Exome Aggregation Consortium, Lek M, Karczewski K, Minikel E, Samocha K, Banks E, Fennell T, O'Donnell-Luria A, Ware J, Hill A, Cummings B [...] MacArthur D
bioRxiv [30 Oct 2015]
Cited: 29 times (PPR:PPR30268)

[Salmon provides accurate, fast, and bias-aware transcript expression estimates using dual-phase inference](#) Preprint
Patro R, Duggal G, Love MI, Irizarry RA, Kingsford C
bioRxiv [27 Jun 2015]
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[HTSeq - A Python framework to work with high-throughput sequencing data](#) Preprint
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bioRxiv [20 Feb 2014]
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