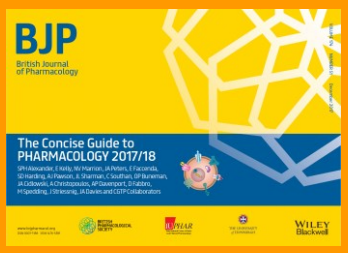
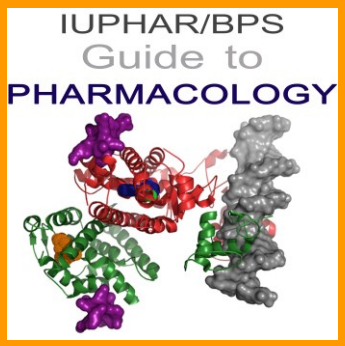
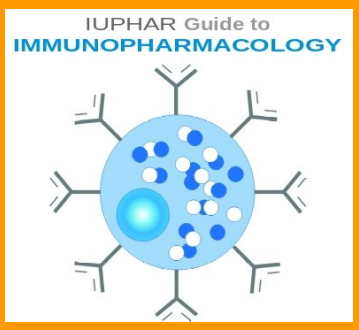
IUPHAR
International Union of Basic and Clinical Pharmacology

BRITISH PHARMACOLOGICAL SOCIETY







IUPHAR/MMV
Guide to MALARIA PHARMACOLOGY

DATABASE Report

April 2019

enquiries@guidetopharmacology.org

TABLE OF CONTENTS

INTRODUCTION

This database report provides an overview of recent progress and the current status of the IUPHAR/BPS Guide to PHARMACOLOGY (GtoPdb) since our last NC-IUPHAR meeting held in Edinburgh in October 2018. Previous reports are online for April 2017, Oct 2017, May 2018 and Oct 2018.

We have now reached the end of our 3-year Wellcome Trust funded project to develop the "The Guide to IMMUNOPHARMACOLOGY (GtoImmuPdb): Integration of targets, diseases and therapies into an expert-driven database". This grant began on the 1st of November 2015. More details can be found in our blog, which includes technical blog posts highlighting aspects of the development of the resource.

We again include details on the Guide to MALARIA PHARMACOLOGY (GtoMPdb), a project funded by Medicines for Malaria Venture (MMV) to add information about antimalarials to GtoPdb and to develop a purpose-built parasitologist-friendly portal for the website interface.

This report (along with the accompanying slide sets) will detail our progress on the GtoPdb, GtoImmuPdb and GtoMPdb projects. It is based on the May 2018 and October 2018 report versions as reference. A few general sections have been left in for context, but most have been updated. As usual, informal minutes will be taken at the April 2019 meeting in Paris, but please also talk to us regarding points, issues and suggestions from this report and the accompanying slide set.

GENERAL OVERVIEW OF DATABASE TEAM ACTIVITIES

PUBLIC ENGAGEMENT – PROMOTING OUR RESOURCES

CONFERENCES/MEETINGS (SINCE MAY 2018 AND UPCOMING)

- BioMalPar XV: Biology and Pathology of the Malaria Parasite, EMBL, Heidelberg, May 2019. Jane Armstrong will present a poster on the Guide to MALARIA PHARMACOLOGY
- BPS Pharmacology 2018, London, UK, Dec 2018. Simon Harding, Chris Southan, Jamie Davies
- Pharmacology Futures, Edinburgh, May 2018, Adam Pawson, Chris Southan, Jamie Davies
- ELIXIR All Hands 2018, Berlin, June 2018, Simon Harding
- 18th World Congress of Basic and Clinical Pharmacology (WCP 2018) July 2018, Kyoto, Adam Pawson and Chris Southan were in a Symposium on Computational Pharmacology, Databases and Drug Discovery, and had two talks and several posters
- 5th European Congress of Immunology, Amsterdam, September 2018, Simon Harding - presented poster on the Guide to IMMUNOPHARMACOLOGY

Our slideshare account includes slide sets and posters presented by team members. Some are also posted on Christopher Southan's own slideshare.

PUBLICATIONS

PUBLISHED (SINCE EARLY 2018)

- A new guide to immunopharmacology (2018). Simon D. Harding, Elena Faccenda, Chris Southan, Pasquale Maffia, Jamie A. Davies. Nat. Rev. Immunology (Web Watch). https://doi.org/10.1038/s41577-018-0079-2. Altmetric score of 24 since 16th Oct 2018.
- SynPharm: A Guide to PHARMACOLOGY Database Tool for Designing Drug Control into Engineered Proteins. Sam Ireland, Christopher Southan, Alazne Dominguez, Simon Harding, Joanna Sharman, Jamie Davies. ACS Omega. Jul 31;3(7):7993-8002. PMID: 30087931. The Rx version has garnered 2232, views, 87 downloads and an Altmetic score of 15 since March.
- Challenges of connecting chemistry to pharmacology: perspectives from curating the IUPHAR/BPS Guide to PHARMACOLOGY. Christopher Southan, Joanna L Sharman, Elena Faccenda, Adam J Pawson, Simon D Harding, Jamie A Davies. Jul 31;3(7):8408-8420. PMID:30087946. The Rx version has garnered 466 views and 109 downloads since May 2018.
- Accessing expert-curated pharmacological data in the IUPHAR/BPS Guide to PHARMACOLOGY. Joanna L Sharman, Elena Faccenda, Simon D Harding, Adam J Pawson, Christopher Southan, Jamie A Davies and NC-IUPHAR (2018). Current Protocols in Bioinformatics. 61: 1.34.1-1.34.46. PMID:30040201.

- Caveat usor: assessing differences between major chemistry databases. (2018) Chris Southan. ChemMedChem, 13(6):470-481. PMID 29451740 (Gold Open Access)

OUTREACH AND SOCIAL MEDIA

We use mainstream social media outlets for five primary purposes 1) outreach to potential new users and/or followers 2) informing on new features or releases 3) enhancing awareness of our publications and presentations 4) keeping collaborators and other followers (including many other databases) aware of our activities. 5) establishing reciprocity with key followers and collaborators.

FACEBOOK

The number of 'likes' increased to 4107 (March 2019), from 3749 in Sep 2018.

TWITTER

@GuidetoPHARM has just pipped 1,900 tweets, followers have increased to 2670 from 2186 in Sep 2018 and our re-tweet rate has also gone up. The value of this platform continues to increase as an alerting system for our blog posts, key papers, including from BJP, other pharmacology journals, immunology, biochemistry and medicinal chemistry, new PDB structures, etc. Most of our Hot Topics are now first picked up from Twitter. We also engage in a discrete re-tweeting for reciprocal outreach. These include @BritPharmSoc (who have been very active in promoting the Concise Guide) @BrJPharmacol, @PharmRevJournal, @PRandP_Journal @IUPHAR, @PharmacologyEd @immunopaedia @cdsouthan and @mqzspa (NC-IUPHAR chair). From our recent publications listed above we saw useful tweet boosts via @ChemRxiv as well as Wiley @currentprotocol and @ChemMedChem

LINKEDIN

The Curation Team have been encouraging Subcommittee Chairs and collaborators to increase their reciprocal connectivity as individual LinkedIN users. This expands our collective inter-network outreach for posting updates, new papers *etc*. (N.B. interested readers of this report are encouraged make connection requests from GtoPdb and IUPHAR scientists they know). Our own LinkedIN group page now has 191 followers.

BLOGGING

Our Edinburgh blog (http://blog.guidetopharmacology.org/) is receiving over 670 views on average per month over the last 6 months. This is our primary news feed and includes database release updates, new features, technical items or articles. Our regular posts with expert commentaries on hot topics relevant to pharmacology are particularly popular, always ranking in the top 5 posts for any given month. Team member Chris Southan maintains his own (http://cdsouthan.blogspot.com/) where relevant posts include cross-pointers to GtoPdb.

HOT TOPICS

As an established and popular feature our Hot Topics are seeded in the form of new significant pharmacology, drug discovery and key human genomics papers. These are communicated to us from Subcommittee members or picked up from Twitter. For a selection, as before, we commission concise commentaries from our expert contacts. We've had recent guest commentaries from Steve Alexander, Thomas Lundbäck, Jerold Chun, Nicola J. Smith, Anthony Davenport, David Gloriam, Jörg Striessnig, Emma Veale, Alastair Mathie and Chris Southan (all commentaries are posted under the Hot topic category on our blog).

SLIDESHARE

Our account (http://www.slideshare.net/GuidetoPHARM) allows the database team to share slide sets and posters with the community thereby extending the reach way beyond conference session direct attendees. Our slide sets received 3,444 (+486) views over the past year. We continue to provide a set of generic slides which can be used by anyone presenting or teaching on GtoPdb and a generic poster which can be printed out in various sizes and taken to meetings or handed out as flyers.

ENQUIRIES RECEIVED FROM USERS

We get a steady stream of user communications coming in to enquiries@guidetopharmacology.org. This is about one a week and they continue to cover a useful spectrum of (mostly minor) fixes that we promptly address. It is useful to catalogue these engagements as they provide valuable information (not readily captured by analytics) in how and why GtoPdb is used. They also provide useful ideas for future development.

DANIELA DIGLES (UNIVERSITY OF VIENNA)

Interested in accessing stoichiometry data for transporters. Helped us identify that this data could be added to API output.

CHARLES JOLY

Requested download of GPCR transduction mechanisms stored in GtoPdb. Helped us to update the transduction mechanism data to make it consistent between concise and target detailed views.

NOVO NORDISK (JO SHARMAN)

Jo has been helping to consolidate the data GtoPdb stores on endogenous and/or natural ligands. Hopefully this will lead to a permanent auto-generated download file for users.

REACTOME (LISA MATTHEWS, MANAGING EDITOR, NY)

Lisa requested disease to drug mapping data from GtoPdb as well as mappings between GtoPdb ligands and ChEBI. We were able to point her to our web-services but also provide a bespoke download of this data. This data was requested to provide a tool for analysis Reactome search results, ultimately looking for patterns or trends between Reactome queries (containing ligand names) and diseases.

BRAM WEYTJENS (LEAD BIOINFORMATICS ENGINEER, XAOP HTTPS://WWW.XAOP.COM/, BELGIUM)

Requested inclusion of selectivity data into interaction downloads. They had been accessing it *via* our API, but this particular data was absent from the static download.

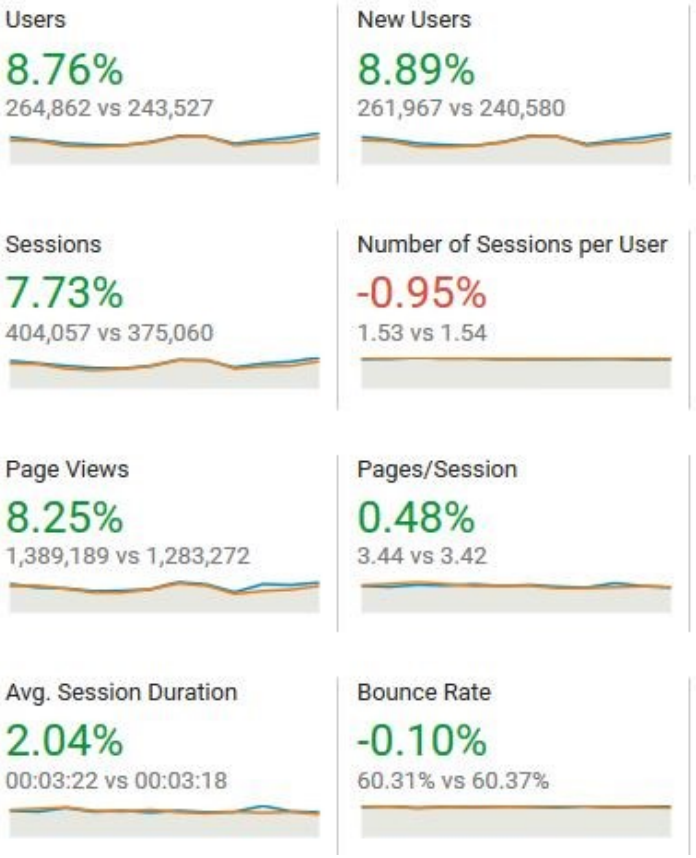
JAN BRAEKEN (GLPG.COM)

Contacted us off the back of communication with Bram. Asked if the Ensembl Gene Ids could be added to the interaction download and followed-up asking for a download of 2D structures. Also requested a list of our peptide structures and sequences (which we already provide as a download).

ENGAGING WITH US

As is implicit from the Social Media section above, it is crucial to extend our external presence and impact. Thus, the more readers of this document who “connect” with us, (*via* whichever of the channels above they use for their own professional profile) the more our outreach extends. This also has mutual advantages. In particular re-tweets and LinkedIN likes are useful for extending the alerting network for new releases, publications, meeting slide sets and blog posts. Note also that each time you either save one of our publications to your own Mendeley account or mention it in a tweet, blog or PubMed commons comment (but make sure you specify a DOI or PubMed link for the auto-indexing) the Altmetrics score.

GTOPDB WEB SITE ACCESS STATISTICS

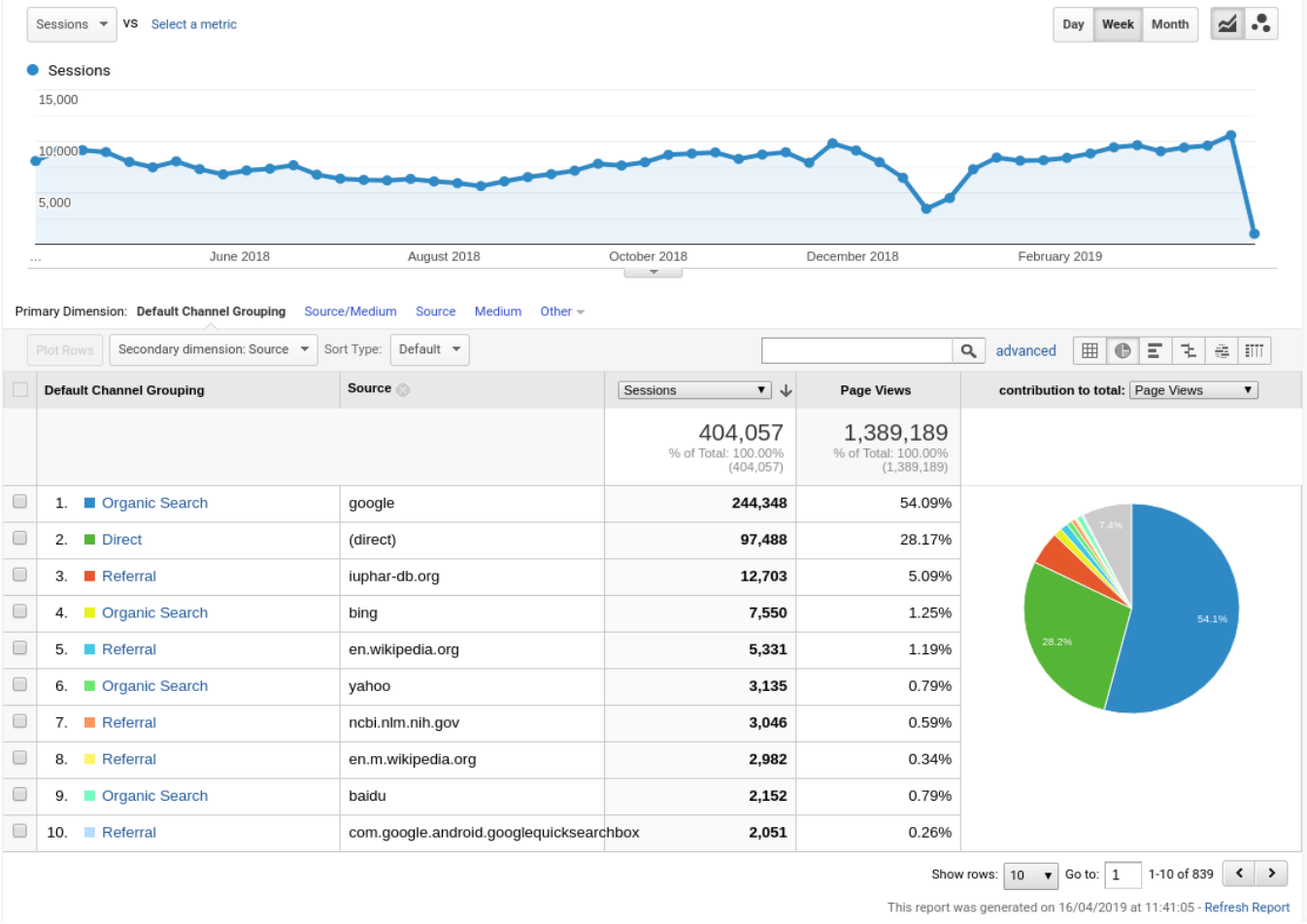


Graphs comparing visitors to guidetopharmacology.org for the 12 months from April 2018 to March 2019, with the previous 12 months.

Monthly statistics	**Apr 2018 - Mar 2019 (previous 12 months)**
Sessions	33,671 (31,255)
Users	22,071 (20,293)
Page views	115,765 (16,939)
Pages / Session	3.44 (3.42)
Avg. Session Duration	00:03:22 (00:03:18)

ACQUISITION, BROWSERS & DEVICES

It is useful to be aware of where users are accessing GtoPdb and what devices/browsers they are using. This can help us to better optimise the site and to ensure we test across the most popular platforms.



This shows acquisition data from Apr 2018 to Mar 2019.

	Browser	Device Category	Sessions	Sessions
			404,057 % of Total: 100.00% (404,057)	404,057 % of Total: 100.00% (404,057)
1.	Chrome	desktop	205,595	50.88%
2.	Firefox	desktop	42,100	10.42%
3.	Safari	desktop	35,331	8.74%
4.	Chrome	mobile	27,871	6.90%
5.	Internet Explorer	desktop	25,415	6.29%
6.	Safari	mobile	22,857	5.66%
7.	Edge	desktop	18,363	4.54%
8.	Safari	tablet	7,403	1.83%
9.	Samsung Internet	mobile	3,148	0.78%
10.	Opera	desktop	2,795	0.69%

Browser & Device Category of Session on GtoPdb (Apr 18 - Mar 19)

The majority of sessions on GtoPdb come *via* organic search (Google) and are performed predominantly from desktop devices. Chrome is also the browse of choice.

GTOPDB CONTENT

These database statistics were compiled from our March 28th release (v2019.2). All database statistics can be found at http://www.guidetopharmacology.org/about.jsp#content.

Targets	**Number of (Human) UniProt IDs**
7TM receptors	399
Nuclear hormone receptors	48
Catalytic receptors	245
Ligand-gated ion channels	81
Voltage-gated ion channels	144
Other ion channels	53
Enzymes	1209
Transporters	539
Other protein targets	202
Targets with ligand interactions	1764
Targets with quantitative ligand interactions	1505
Targets with approved drug interactions	630
Primary targets with approved drug interactions	324
Total number of targets	**2920**
Ligands	*Number of ligands*
Synthetic organics	6401
Metabolites	581
Endogenous peptides	789
Other peptides including synthetic peptides	1333
Natural products	264
Antibodies	255
Inorganics	39
Approved drugs	1421
Withdrawn drugs	70
Ligands with INNs	2307
Labelled ligands	609
Unique PubChem CIDs (total CID links)	7206 (7407)
Ligands with target interactions	8321
Ligands with quantitative interactions (approved drugs)	7316 (902)
Ligands with clinical use summaries (approved drugs)	2374 (1417)
Total number of ligands (PubChem SIDs)	**9670**
Number of binding constants	48071
Number of binding constants curated from the literature	16864

DOWNLOAD STATISTICS

Yearly period 1st April Year 1 to 31st March Year 2.

GOOGLE ANALYTICS COMPARISON OF DOWNLOADS

Event Category: Downloads
Event Label: Downloaded

	Count
2017-2018	2,810
2018-2019	2,704
Change	-3.77%

This corresponds to files downloaded from our main downloads page:
http://www.guidetopharmacology.org/download.jsp
and the slides page: http://www.guidetopharmacology.org/slides.jsp

A more specific breakdown is shown here:

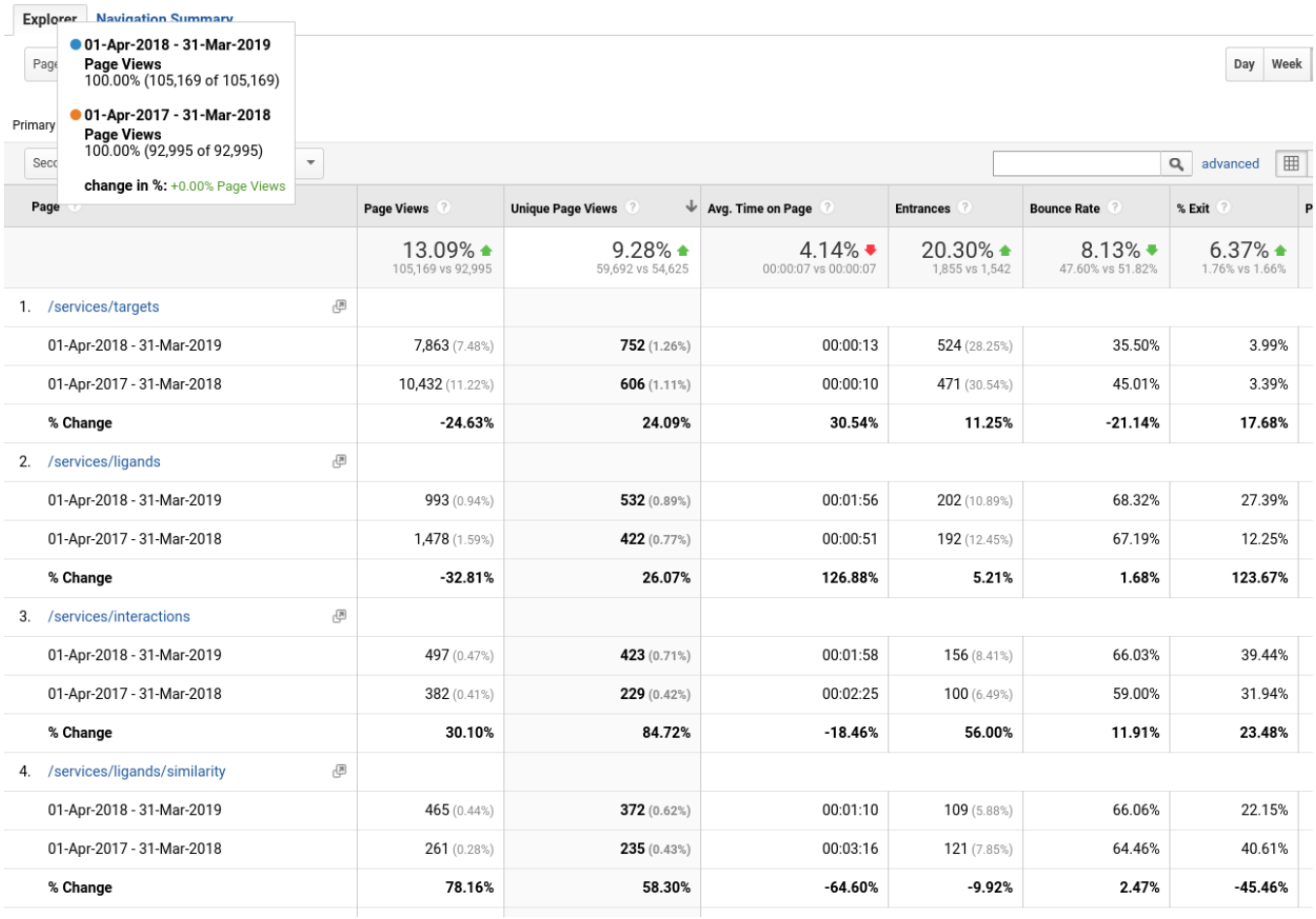
	2017-2018	2018-2019	Change
Targets CSV/TSV file	1084	1085	no change
Interactions CSV/TSV file	345	352	2%
Ligands CSV/TSV file	250	254	1.6%
UniProt Mapping file	165	170	3%
HGNC mapping file	98	118	20%
Peptides CSV file	99	121	22%
*PostgreSQL**	160	227	41%
Generic slides (PPT & PDF)	234	196	-16%
Generic poster	104	75	-27%
Other files			
Tutorial	492	472	-4%
Terms and Symbols	285	285	no change

* Total downloads of PostgreSQL database dump files (versions 2017.1 onwards).

WEB SERVICES

Tracking of our web-services has been in place since March 2017. Calls to the web-service are generally from client computers to our server and are not recorded in the same way as visits to our website. Therefore, we can't report details on specific users, such as location or number of visits. We can only record the number of hits for each distinct URL.

The image below shows that there were approximately **105,000** total hits over the year, an increase of around 13% on the previous period. Calls to target and ligands saw a reduction, but we note an increases in calls to interaction data and ligand similarity. There was also a large increase in web service calls for ligand substructures, diseases and database links.



Explorer | Navigation Summary

01-Apr-2018 - 31-Mar-2019
Page Views
100.00% (105,169 of 105,169)

01-Apr-2017 - 31-Mar-2018
Page Views
100.00% (92,995 of 92,995)

change in %: +0.00% Page Views

Day | Week

Primary

advanced

Page	Page Views	Unique Page Views	Avg. Time on Page	Entrances	Bounce Rate	% Exit	P
	13.09% ▲ 105,169 vs 92,995	9.28% ▲ 59,692 vs 54,625	4.14% ▼ 00:00:07 vs 00:00:07	20.30% ▲ 1,855 vs 1,542	8.13% ▼ 47.60% vs 51.82%	6.37% ▲ 1.76% vs 1.66%	
1. /services/targets							
01-Apr-2018 - 31-Mar-2019	7,863 (7.48%)	**752** (1.26%)	00:00:13	524 (28.25%)	35.50%	3.99%	
01-Apr-2017 - 31-Mar-2018	10,432 (11.22%)	**606** (1.11%)	00:00:10	471 (30.54%)	45.01%	3.39%	
% Change	**-24.63%**	**24.09%**	**30.54%**	**11.25%**	**-21.14%**	**17.68%**	
2. /services/ligands							
01-Apr-2018 - 31-Mar-2019	993 (0.94%)	**532** (0.89%)	00:01:56	202 (10.89%)	68.32%	27.39%	
01-Apr-2017 - 31-Mar-2018	1,478 (1.59%)	**422** (0.77%)	00:00:51	192 (12.45%)	67.19%	12.25%	
% Change	**-32.81%**	**26.07%**	**126.88%**	**5.21%**	**1.68%**	**123.67%**	
3. /services/interactions							
01-Apr-2018 - 31-Mar-2019	497 (0.47%)	**423** (0.71%)	00:01:58	156 (8.41%)	66.03%	39.44%	
01-Apr-2017 - 31-Mar-2018	382 (0.41%)	**229** (0.42%)	00:02:25	100 (6.49%)	59.00%	31.94%	
% Change	**30.10%**	**84.72%**	**-18.46%**	**56.00%**	**11.91%**	**23.48%**	
4. /services/ligands/similarity							
01-Apr-2018 - 31-Mar-2019	465 (0.44%)	**372** (0.62%)	00:01:10	109 (5.88%)	66.06%	22.15%	
01-Apr-2017 - 31-Mar-2018	261 (0.28%)	**235** (0.43%)	00:03:16	121 (7.85%)	64.46%	40.61%	
% Change	**78.16%**	**58.30%**	**-64.60%**	**-9.92%**	**2.47%**	**-45.46%**	

Traffic to GtoPdb web services URLs over the past year

SUPPLIER LINKS

In May 2018 we accepted sponsorship from Tocris (https://www.tocris.com) in return for providing product supplier links on our ligand summary pages. Tocris supplied a list of their compounds which we mapped to GtoPdb ligand *via* PubChem CIDs. This sponsorship was limited to one year. In total, we mapped 1258 GtoPdb ligand to Tocris compounds.

We have agreed to continue this arrangement and update these sponsored links from May 2019. We have begun preparations for the update and have been provided with an updated set of compounds from Tocris. These currently map to 1369 GtoPdb ligands. The new links will go live in May 2019.

This sponsorship is not exclusive, and we are in discussions with other suppliers about providing links to their compound catalogues.

GTOPDB TEAM INTERACTIONS

For more details of previous and continuing interactions please see the April 2017 and October 2018 reports. Only significant changes since October are reported below.

ELIXIR

Engagements continue with this important Europe-wide bioinformatics infrastructure initiative. As reported before, we have an entry in the ELIXIR bio-tools directory as one of the official UK ELIXIR Node Resources and part of the Excelerate initiative. We attend the ELIXIR-UK All-Hands Meeting held in November in Birmingham.

INTEROPERABILITY, RDF AND OPENPHACTS

One of ELIXIR's aims is to promote interoperability and FAIR (Findable, Accessible, Interoperable, Reusable) compliance (see **FAIR** Guiding **Principles** for scientific data management and stewardship. Wilkinson MD et al. Sci Data. (2016)). We have previously reported on our initiatives to increase interoperability of the GtoPdb data, including creating a new RDF version.

We continue to keep the RDF version of the Guide to Pharmacology up-to-date at each release. These are 4 data files in Notation3 (N3) format and 2 metadata files which include a general description of the dataset and specific information on the current version: 2019.2. The metadata have been generated in accordance with the W3C Health Care and Life Sciences Community (HCLS) Profile to ensure FAIR compliance.

We have implemented an 'early-stage' SPARQL endpoint that uses LodeStar as the web-application layer on top of the triple store. This provides a graphical frontend to the RDF data and allows control over SPARQL queries and provides the data in a human-readable format. This can be accessed at http://rdf.guidetopharmacology.org/

PUBCHEM

We continue our important interactions with PubChem, including by both mail and TC conversations with Evan Bolton, Paul Theissen and other members of the team. Some of our PubChem ligand content aspects are outlined in our latest NAR paper PMID 29149325. PubChem have recently piloted a new Classification Browser (https://pubchem.ncbi.nlm.nih.gov/classification/#hid=92) which displays the GtoPdb target hierarchy in a way that allows users to browse our PubChem Substances/Compounds. The GtoPdb target classification is also shown on PubChem Target pages (e.g. HTR1A). Note that PubChem specifically selected us for highlighting in this highly-visible global resource because of our acknowledged quality as a submitter.

Subsequent to our 2018.2 database release in May we have been submitting new BioAssays to PubChem, following on from a pilot exercise for the 5-HT receptor family in 2015. At this point all of our BioAssays have been submitted, following a re-generation step to improve the structure/content of the XML. We can report a good working relationship with Ben Shoemaker at PubChem who has been helpfully overseeing the upload of the assays. The Bioassays are also shown on Target and Compound pages in PubChem so this will increase exposure of the GtoPdb data.

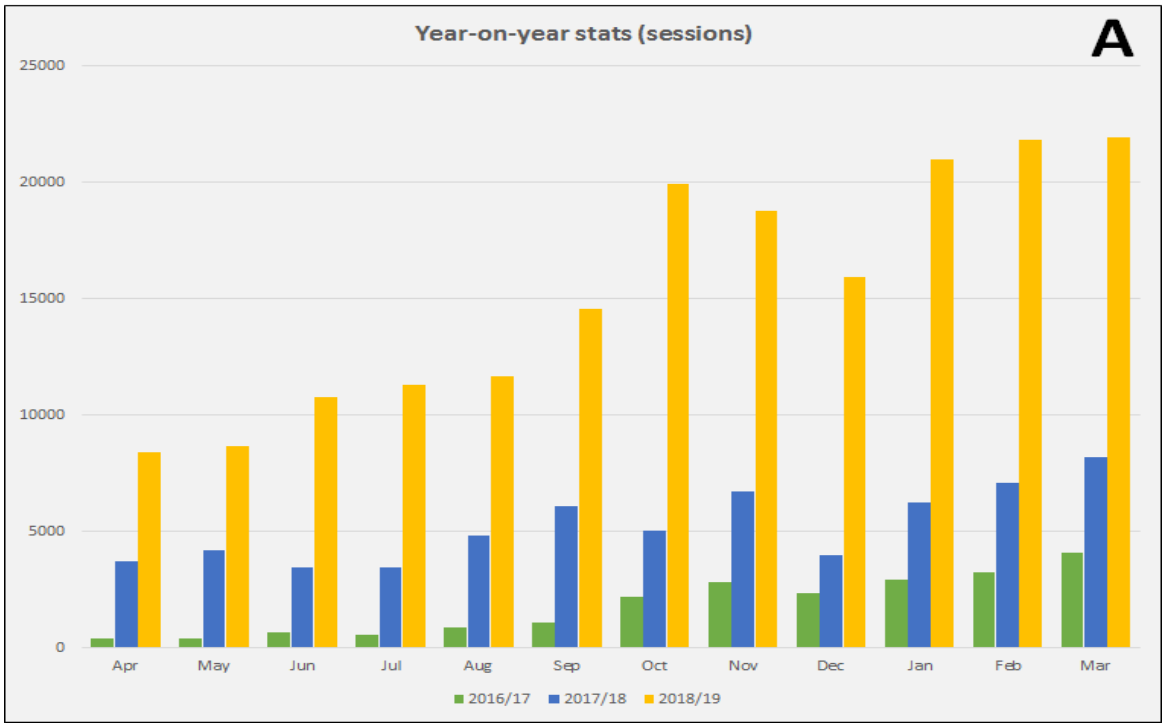
IUPHAR PHARMACOLOGY EDUCATION PROJECT (PEP)

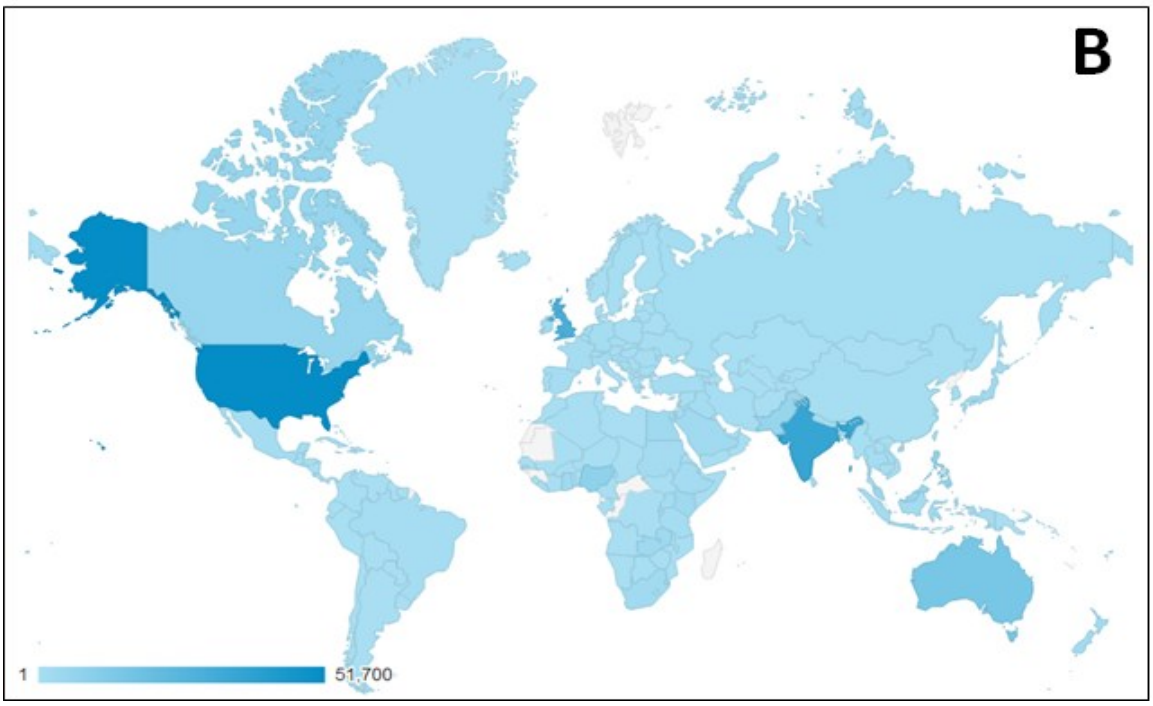
The IUPHAR Pharmacology Education project continues to be developed "*as a learning resource to support education and training in pharmacological sciences*". The PEP celebrated its 4th birthday on 1st April 2019.

Financial support is in place for one 0.5 FTE for the next 4-6 months. This comes from the Chinese, Japanese and Hungarian pharmacological societies.

Site Usage

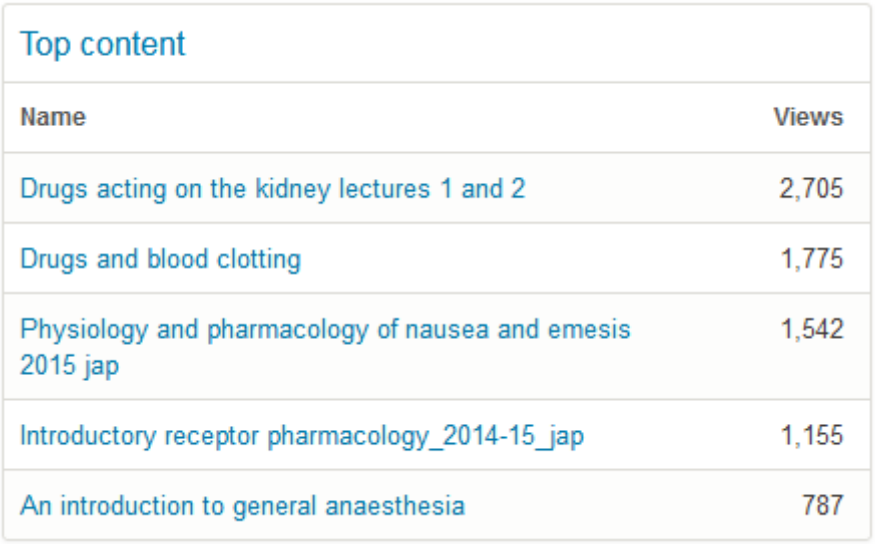
The figure below shows month to month data from Google Analytics of the recorded PEP user sessions (Panel A) and the global distribution of users (Panel B), from April 2016 when the PEP was launched up to the most current data. User sessions are continuing to grow, with >20K sessions recorded/month in 2019.





Google Analytics of access to IUPHAR PEP Website

We have noticed relatively high interest in our SlideShare offerings. We currently have 20 slide sets posted, and data analytics has recorded almost 11,500 views, and >400 downloads, in the last year. The top 5 (by number of views) are shown in the panel below.



Top content

Name	Views
Drugs acting on the kidney lectures 1 and 2	2,705
Drugs and blood clotting	1,775
Physiology and pharmacology of nausea and emesis 2015 jap	1,542
Introductory receptor pharmacology_2014-15_jap	1,155
An introduction to general anaesthesia	787

We also have embedded Vimeo videos by Simon Maxwell in some sections of PEP, and these have recorded ~2500 views coming from PEP.

PEP has 450 followers of our twitter handle, @PharmacologyEd.

A 'Practice article' entitled **The IUPHAR Pharmacology Education Project** was published in Clinical Pharmacology and Therapeutics in Jan 2019 PMID: 30588614. A short article that reported on PEP activities at WCP2018 was included in IUPHAR's latest Pharmacology International newsletter.

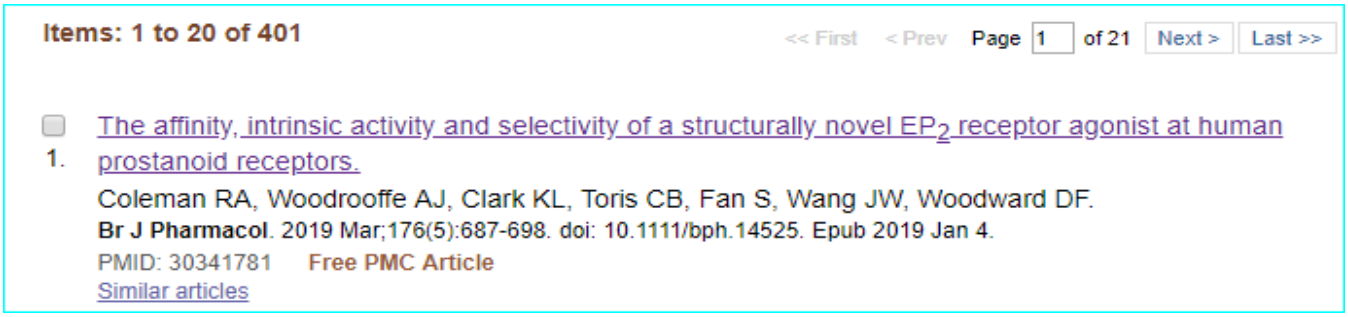
A brief survey designed to collect basic feedback from PEP users was initiated at the end of March 2019. We have had submissions from faculty and students, with most rating both the amount and quality of content as 'Excellent' and reporting that the site is 'Easy to navigate'. So far, IP address data shows completed surveys from users in Malaysia, Nigeria, Brazil, Romania, the Czech Republic and the UK.

JOURNAL < - > DATABASE CONNECTIVITY

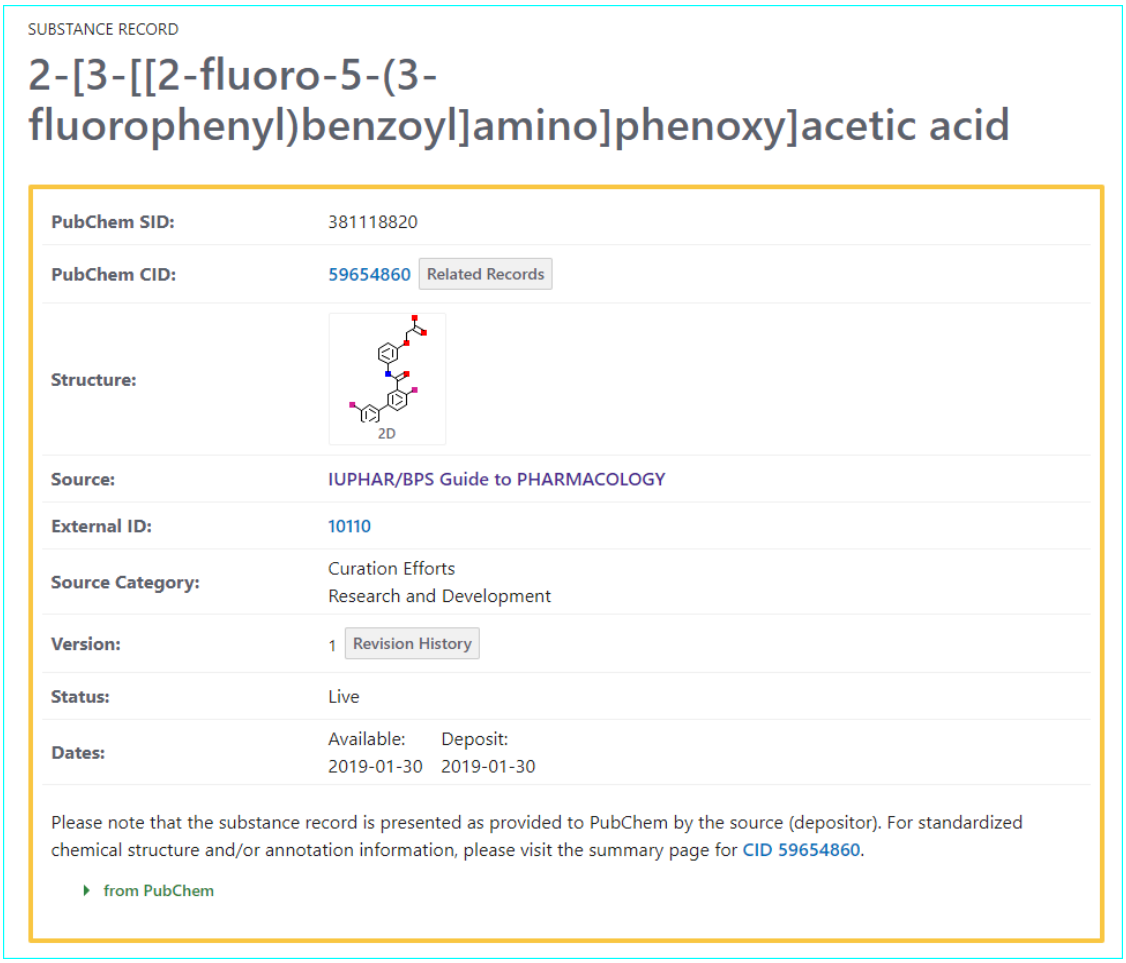
The journal-to-GtoPdb linking initiative PMID 25965085) for the BJP since Oct 2014 and BJCP since Nov 2016, can be counted via the reference citations to our Concise Guide and NAR papers. The results indicate out-links for ~ 80% of BJP papers and ~ 50% for BJCP, To ameliorate the retrospective "missing key link" problem we now have a prospective process whereby, on manuscript acceptance followed by their own marking-up of GtoPdb links, authors are advised to alert us directly to key entities that we do not yet have. In appropriate cases we then add these ligands and the new reference. This has the advantages, for both the author and the journal, of not only adding their reference into GtoPdb but also the paper gains PubChem-to-PubMed reciprocal linking derived from our PubChem ligand submissions (see below). Examples from the 2018.2 release include GS-458967 from BJP and esaxerenone from BJCP.

Another important type of connectivity mediated by us (for any journal) can be described as GtoPdb <> PubChem <> PubMed. Both journals and the authors benefit from the increasing traffic that goes around these links. We can select the headline statistics for our current 9670 SID > 10798 PubMed entries.

As our largest journal source of curation 1180 are J.Med.Chem papers but note also that 401 are from BJP. The most recent of these is shown below



In the “Related information” for all PubMed entries (in a facet down in the right hand of the web page) there is a PubChem Substance link to one of our SIDs for all 10798 entries. The one linked to the BJP reference above is shown below.

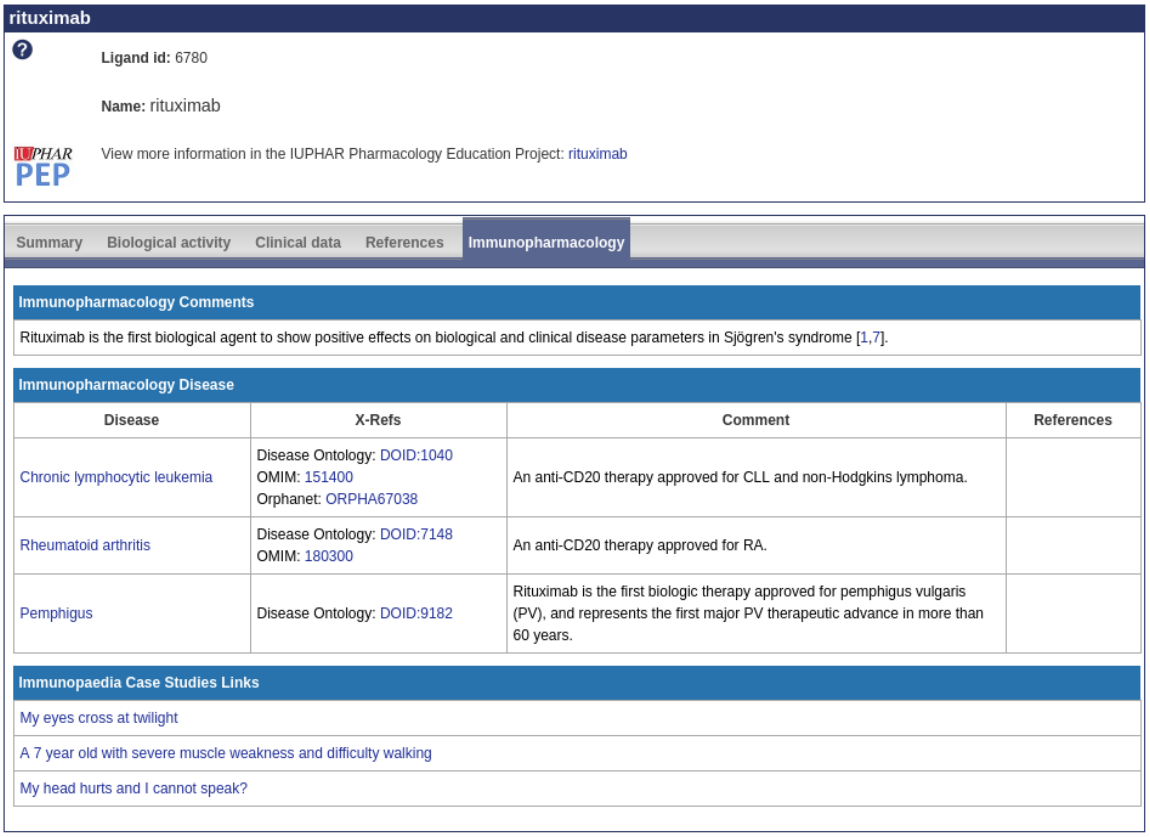


Note that for this recent BJP publication GtoPdb is the only source of the PubMed < > PubChem mapping (in this case the other four SID links came from automated patent extractions)

IMMUNOPAEDIA

Engagement continues with Immunopaedia, an open-access online platform freely available for learning and teaching immunology. The resource aims to improve engagement between core immunology and clinical practice, and it is the official International Union of Immunological Societies (IUIS) learning site. Immunopaedia provides clinical case studies to help highlight immunological concepts, online course to support teaching and learning in immunology, and it provides information on treatment and diagnostics on infectious diseases.

We have extended the immunopahrmacology links from ligand summary pages to provide links from relevant ligand to case studies at Immunopaedia.



rituximab

Ligand id: 6780

Name: rituximab

View more information in the IUPHAR Pharmacology Education Project: rituximab

Summary | Biological activity | Clinical data | References | Immunopharmacology

Immunopharmacology Comments

Rituximab is the first biological agent to show positive effects on biological and clinical disease parameters in Sjögren's syndrome [1,7].

Immunopharmacology Disease

Disease	X-Refs	Comment	References
Chronic lymphocytic leukemia	Disease Ontology: DOID:1040 OMIM: 151400 Orphanet: ORPHA67038	An anti-CD20 therapy approved for CLL and non-Hodgkins lymphoma.	
Rheumatoid arthritis	Disease Ontology: DOID:7148 OMIM: 180300	An anti-CD20 therapy approved for RA.	
Pemphigus	Disease Ontology: DOID:9182	Rituximab is the first biologic therapy approved for pemphigus vulgaris (PV), and represents the first major PV therapeutic advance in more than 60 years.	

Immunopaedia Case Studies Links

My eyes cross at twilight

A 7 year old with severe muscle weakness and difficulty walking

My head hurts and I cannot speak?

Screenshot showing links from rituximab and three Immunopaedia case studies

We are also looking at how we might best include links from targets and families to Immunopaedia. In total we have 48 links curated in GtoPdb and are currently curating a second set of links, which will be available in future database releases.

NEW DRUG APPROVALS

For our 2Q 2019 database releases there was a substantially increased our coverage of European Medicines Agency (EMA) drug approval data. There are 414 approved drugs with EMA marked as a source, up from 274 in 2018.1. In addition, at about this time of year considerable interest is generated from reviews of the previous year's FDA Drug Approvals (see https://cdsouthan.blogspot.com/2019/01/2018-approved-drugs-in-pubchem.html)

Reaching 59, 2018 was welcomed as a particularly prolific year. However, for our own capture, we have various exclusion criteria such as anti-infectives (with some exceptions including our antimalarials mentioned above), already-approved mixture components, topicals, non-antibody biologicals, undefined extracts (e.g. fish oil) and inorganics. Thus, our scorecard stands at 26 chemical entities that form PubChem Compound Identifiers. We also have database records and PubChem Substance submissions for 11 of the 12 newly-approved antibodies (excepting the anti-HIV one).

NEW GTOPDB WEBSITE FEATURES (SINCE OCTOBER 2018)

WEB-SERVICES

As part of the development of the GtoImmuPdb we have added target and ligands of immunological relevance, as well as the new immunopharmacology data types to our web services.
For example, targets tagged in the database as relevant to immunopharmacology can be retrieved from the following URL:
http://www.guidetopharmacology.org/services/targets?immuno=true
The API has also been extended to return immuno processes and cell types for specific targets. Here an example retrieving cell types associated with CD86 (target ID 2735):
http://www.guidetopharmacology.org/services/targets/2745/immunoCelltypes
We have also introduced disease data to the web services, so summarised data for any disease in GtoPdb can be retrieved, here using Psoriasis (disease ID 801) as an example:
http://www.guidetopharmacology.org/services/diseases/801

OTHER WORK

Updates on other ongoing new website features are:

- **Converting to HTTPS:** Using HTTPS (secure connection) on websites is becoming increasingly important (browsers and search engines are starting to warn users when they access an insecure site). JS/SH have been working with UofE Information Services to obtain security certificates from JISC which will allow us to install HTTPS on our web server. This is now at the final stage of implementation. All URLs currently redirect to https with the exception of the guidetopharmacology.org URL. We expect this final redirect to be in place in the next month.

- **ChEMBL target links:** We have updated all our outgoing target links to ChEMBL based on the most recent ChEMBL release (ChEMBL 25).

- **Switch to using Chemicalize Pro (ChemAxon):** A key feature of the IUPHAR Guide to Pharmacology website is the ability to perform searches by chemical structure (http://www.guidetopharmacology.org/GRAC/chemSearch.jsp). The chemical structure search tool utilises Marvin JS by ChemAxon. In the 2019.1 release we have updated the API control to use Chemicalize Pro (https://pro.chemicalize.com/). This update simplifies the integration of Marvin JS into our website

- **Update CDK libraries:** We have updated the Chemical Development Kit (CDK) library to version 2.2. This is used by the Guide to Pharmacology to calculate molecular properties of ligands curated in the database. As part of this update, we performed a re-calculation of all molecular properties in the database.

- **Endogenous ligands:** A new download file has been made available on our downloads page. This file contains a list of all ligands marked in the database as endogenous or natural ligands for a given target.

- **Transduction mechanisms:** We have undertaken curatorial work to consolidate our curated data on GPCR transduction mechanism. In some cases, the database contained inconsistent data between the transduction mechanism data on a targets detailed view and its concise view. Our analysis identified these cases and we've put in place curatorial protocols to fix.

- **Page Navigation:** We have updated our web-pages to feature a drop-down navigation bar, which is revealed when users scroll-down on longer pages. Many pages on GtoPdb are quite long, particularly detailed targets pages (e.g. CB_1 receptor) – the new drop-down menu keeps key menu items, and most importantly the site search, in focus at all time.

GTOPDB ENTITY GROWTH

Growth rates over the span of the previous Wellcome Trust grant are documented in earlier reports and our 2016 and 2018 NAR papers. While the subcommittees have submitted Concise Guide updates, most new entities have been added *via* the population of GtoImmuPdb and more recently the Guide to Malaria Pharmacology (GtoMPdb). However, significant curation effort goes towards tagging pre-existing targets and ligands with comments and references to GtoImmuPdb and GtoMPdb.

	Oct 2013	**Oct 2015**	**April 2016**	**Oct 2016**	**Apr 2017**	**Oct 2017**	**May 2018**	**Sep 2018**	**Mar 2019**
Target protein IDs	2485	2761	2775	2794	2808	2825	2872	2880	2920
Ligands total	6064	8024	8400	8674	8872	8978	9251	9405	9662
Approved drugs	559	1233	1273	1291	1322	1334	1364	1386	1421
Antibodies	10	138	172	205	212	223	240	248	255
Peptides	1776	1981	2007	2039	2063	2079	2092	2100	2122
Synthetic small molecules	3504	5055	5363	5563	5729	5807	6048	6180	6401
PubChem SIDs	3107	8024	8328	8674	8831	8978	9251	9405	9662
PubChem CIDs	2694	6057	6163	6337	6813	6822	7109	7224	7407
Binding constants	41076	44691	45534	45908	46287	46488	47058	47426	48071
References	21774	27880	29247	30251	31239	31733	33245	34382	35723

GTOPDB TARGET UPDATES (SINCE OCTOBER 2018)

In preparation for the next Concise Guide to PHARMACOLOGY (CGtP 2019/20 edition) our expert subcommittees and collaborators have been providing updates to the family summary pages across all target classes. Details of additional updates are listed below.

GPCRs:

Acetylcholine receptors (muscarinic)
Adenosine receptors
Bradykinin receptors
Cannabinoid receptors
Chemokine receptors
Class Frizzled GPCRs
Leukotriene receptors
Lysophospholipid (LPA) receptors
Lysophospholipid (S1P) receptors
Metabotropic glutamate receptors
Neuromedin U receptors
Neuropeptide S receptor
Parathyroid hormone receptors
Prostanoid receptors
Proteinase-activated receptors
Somatostatin receptors
Tachykinin receptors

Channels:

Aquaporins
Piezo channels
Transient Receptor Potential channels
Voltage-gated calcium channels
Voltage-gated sodium channels

NHRs:

Androgen receptor
Farnesoid X receptor
Retinoic acid-related orphans
Retinoid X receptors

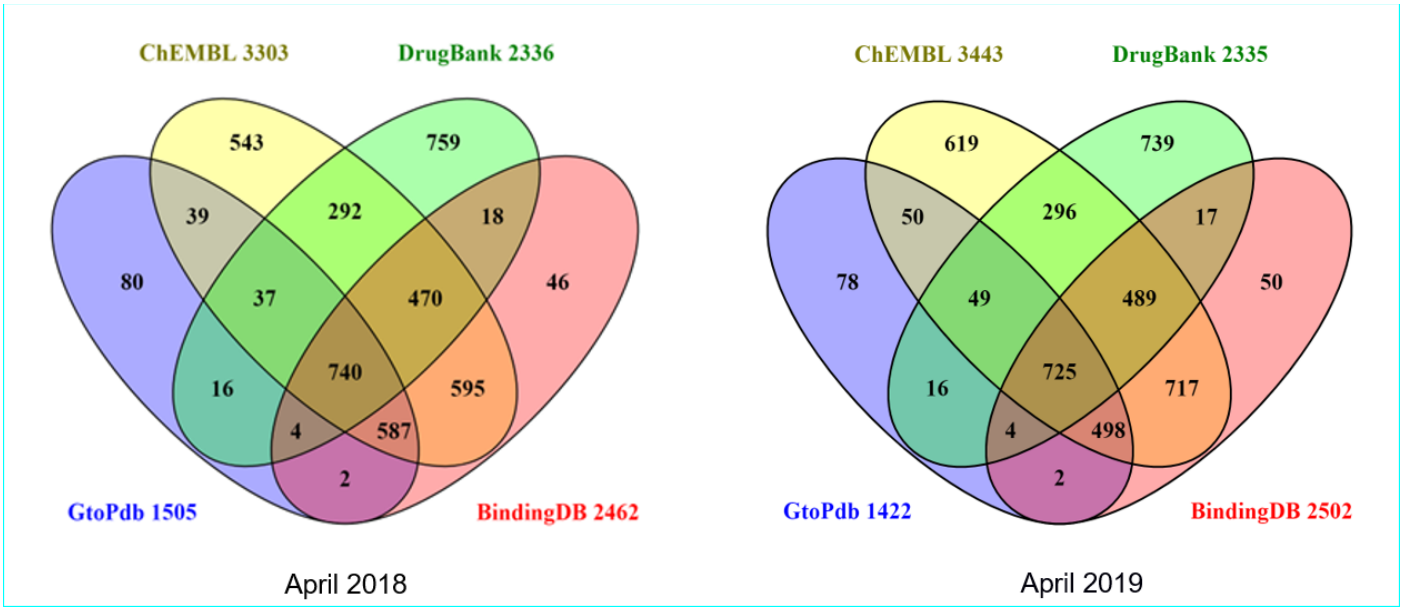
Enzymes:

Endocannabinoid turnover
Histone deacetylases (HDACs)
Histone demethylases
Fatty acid amide hydrolase (FAAH)
Sugar phosphatases
Dioxygenases
Oxidoreductases
Janus kinase (JakA) family
Carbonic anhydrases
Cytochrome P450s
Adenylyl cyclases (ACs)
Sphingosine kinases
Cyclooxygenases
2-Acylglycerol ester turnover
Eicosanoid turnover

Other protein targets:
Immune checkpoint proteins
CD molecules
Heat shock proteins
Non-catalytic pattern recognition receptors
STAT transcription factors

New targets (not including Antimalarial targets):
Poly ADP-ribose polymerases
Prolyl hydroxylases
Carbonic anhydrases
Paraoxonases
Vanin 1
AQP11
NRF2
CA IX
KIR3DL2 (CD158K)
AC10 (adenylyl cyclase 10)
αβ-Hydrolase 12
PVRIG
C-type lectin domain family 12 member A

Relative target growth and coverage: This can be assessed by comparing our own UniProt Human Swiss-Prot cross-references for targets with quantitative interactions against the other major chemogenomic resources that also have such cross-references, DrugBank, BindingDB and ChEMBL. The April 2018 and 2019 updates are shown below.



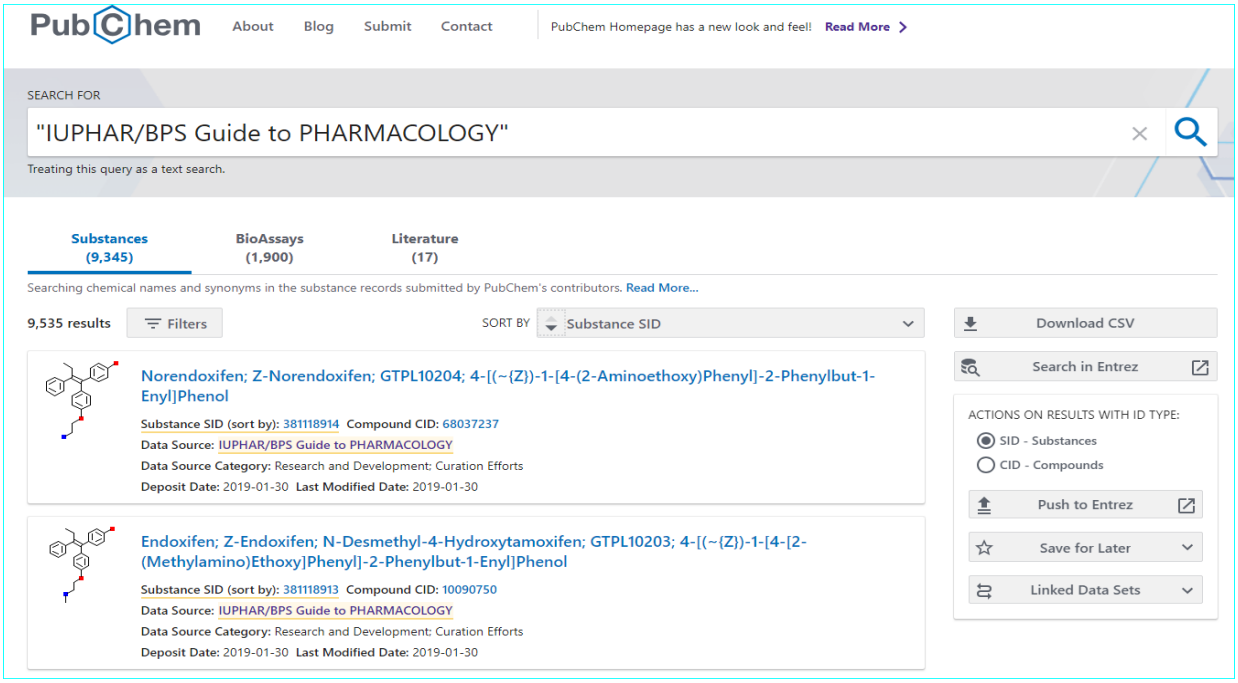
Our total has reduced since we increased the stringency of the mapping file that UniProt picks up for their releases. This was done by removing those kinases where the quantitative interaction data was only derived from old screening panels but confirmatory data from publications has never since appeared. The intersects and differences in the above figures are complex but note that the ChEMBL and BindingDB show some divergent target expansion (i.e. the 4-way consensus has dropped slightly). Not also that DrugBank includes interaction inferences based on literature co-occurrence rather than data-supported direct mechanisms of action (and their UniProt links have not updated). For more details see this slideshare set.

PUBCHEM STATISTICS FOR GTOPDB, GTOIMMUPDB AND GTOMPDB

The stats for the 2019.2 release (with 2018.4 in brackets) are as follows (n.b. because the NCBI Entrez system suffers from overload the links below may time out but should eventually return the result).

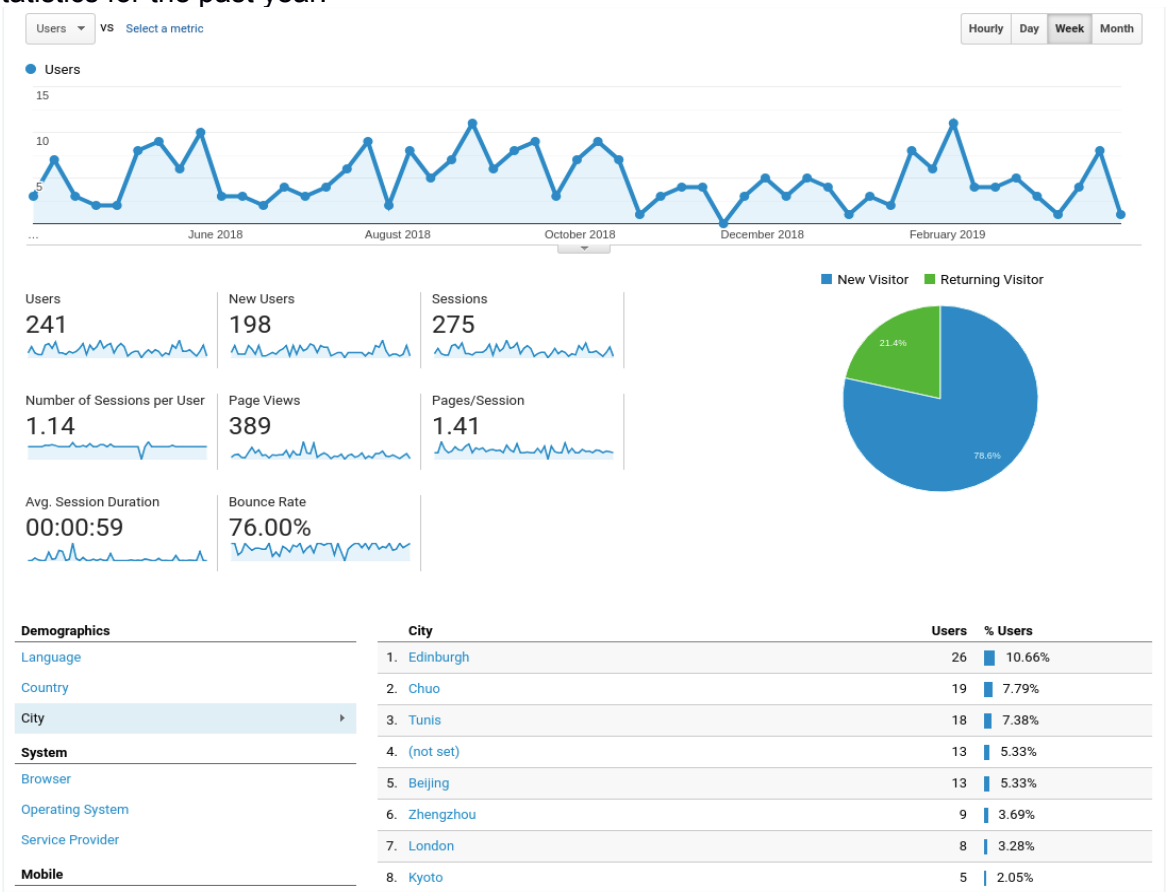
1. Substances (SID) that we submit to PubChem (refreshing previous submissions) are up to 9670 (9251).
2. Those that have defined chemical structures are merged into 7478 (6969) Compound Identifiers, CIDs (i.e. small molecules and moderate peptides)
3. The select "IUPHAR/BPS Guide to PHARMACOLOGY"[SourceName] AND approved [Comment] now retrieves 1518 SIDs (1457) .
4. Of these 1328 (1278) have CIDs (use the “Find Related Data” operator and select “same CIDs”.
5. Of our SIDs, 1151 (993) are tagged in GtoImmuPdb and 282 (258) of these are approved drugs
6. Of our CIDs 724 are tagged in GtoImmuPdb
7. Of our SIDs, 57 are tagged in GtoMPdb and 19 of these are approved drugs
8. Of our CIDs 51 are tagged in GtoMPdb
9. We have 1817 (1675) structures that ChEMBL23 does not have, 5456 not in DrugBank and 6151 not in DrugCentral.
10. 182 (95) structures unique to us as a source.

PubChem has released a new interface that expands the indexing and search functionality for our own entries (see example query below) but there are still some minor discrepancies in the exact metrics returned compared to the Entrez interface.



SYNPHARM: A NEW DATABASE OF SMALL MOLECULES AND THEIR DRUG-RESPONSIVE PROTEIN SEQUENCES LINKED TO GTOPDB

For a detailed description of SynPHARM please see the October 2016 report or the website: http://synpharm.guidetopharmacology.org/. It is a database of drug-responsive protein sequences derived from GtoPdb interaction data. A paper describing SynPHARM has been published: Ireland et al. (2018) SynPharm: A Guide to PHARMACOLOGY Database Tool for Designing Drug Control into Engineered Proteins. ACS Omega. Jul 31;3(7):7993-8002. PMID: 30087931. The figure below shows the SynPHARM access statistics for the past year.



SynPharm access statistics for the past year

BIBLIOMETRICS AND SCHOLARLY PORTALS

- As outlined in previous reports we track various metrics for the GtoPdb team and NC-IUPHAR affiliated papers in PubMed, PubMed Central , European Pub Med Central (EPMC) Kudos entries and Altmetrics.
- Team members have individual Google Scholar pages as well as ResearchGate entries and Edinburgh Research Explorer profiles.
- However, the profile of choice (as EMPC linked with citation graphs) has now become ORCID IDs for which we have JLS 0000-0002-5275-6446 , EF 0000-0001-9855-7103 , AJP 0000-0003-2280-845X, CS 0000-0001-9580-0446 and SDH 0000-0002-9262-8318.

Below are the April 2019 live bibliometric updates compared to the November 2018 metrics. These are given with EPMC links which have the advantage over PubMed of directly generating a citation ranking for any set (but with significantly lower citation rates than PubMed, Google Scholar or WOS).

- Database team member cumulative co-authored publications have increased from 169 to 170 (this is a PubMed query that not so easy to do in EPMC).
- IUPHAR reviews in BJP increased by 1 to 26.
- IUPHAR Pharmacological Reviews remains at 103.
- The BJP “Concise Guide” sets from 2013 and 2015 added up to 17 with the 2017/18 set now taking us to 26 papers.
- Our publications in the NAR Database issues remains at six
- We continue to get high citation rates in our NAR and Concise Guide articles because the BJP and BJCP selected these as reference citations for the GtoPdb outlinks. These are topped by our NAR 2016 entry (PMID 24234439) with 689 citations, overtaking the 2014 paper (PMID 24234439) that reached 631.
- The “Concise Guide” citations are currently led by 2015/16: Enzymes (PMID 26650445) at 503 closely followed by 2013/14: G protein-coupled receptors (PMID 24517644) at 450.
- The overall citation performance of our papers resulted in team members JLS, EF and AJP, along IUPHAR co-authors, SPHA, MS, and APD being listed in the Clarivate 2018 ranking of Highly Cited Researchers.
- The Altmetric rankings for all our OA papers are now indexed in ScienceOpen.

THE GUIDE TO IMMUNOPHARMACOLOGY DATABASE (GTOIMMUPDB)

GTOIMMUPDB WEB INTERFACE AND DATABASE DEVELOPMENT STATUS

In October 2018 we officially launched the IUPHAR Guide to IMMUNOPHARMACOLOGY, have made the first public release back in June 2018. Full technical details on the development progress of GtoImmuPdb can be found on our blog.

As a reminder, GtoImmuPdb is an extension of GtoPdb and its development has involved modifications and extensions to the underlying GtoPdb schema to incorporate new immune system specific data types (such as processes, cell types and disease). It also involves further development of the existing GtoPdb website to surface this new data and incorporate it into the existing search and browse mechanisms. The GtoImmuPdb portal is available at (www.guidetoimmunopharmacology.org).

IMMUNOPHARMACOLOGY: CHALLENGES, OPPORTUNITIES AND RESEARCH TOOLS

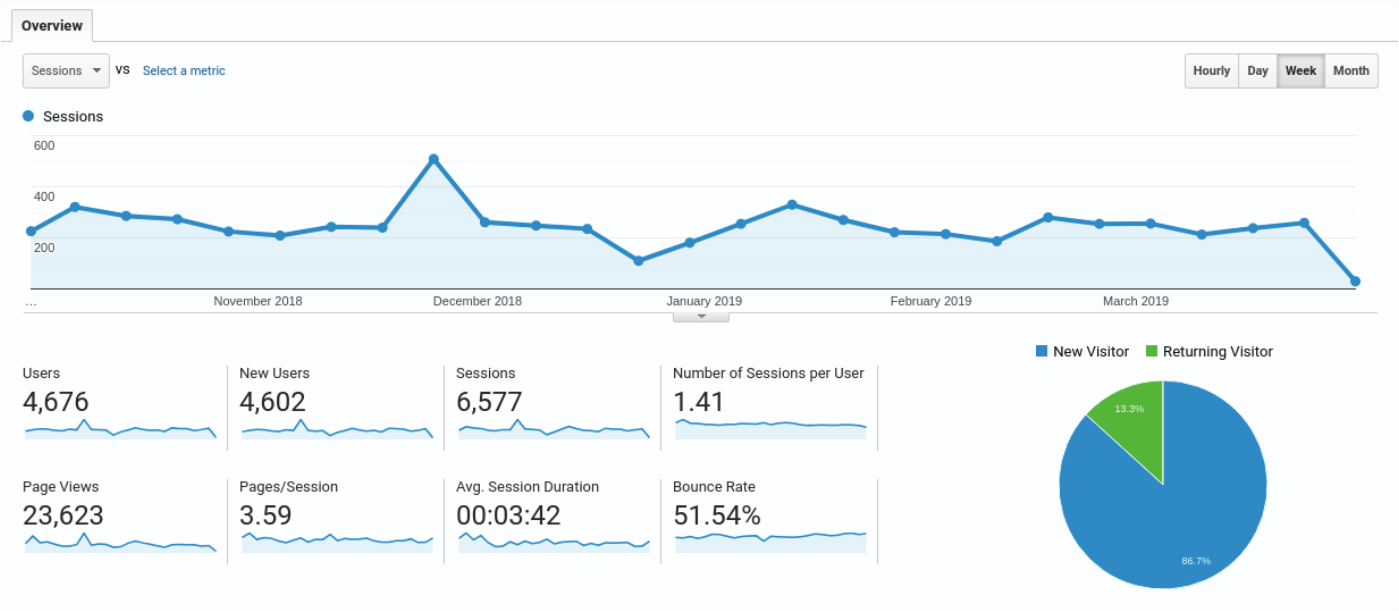
At the beginning of October 2018, we held a meeting in Edinburgh focussed on the launch of the IUPHAR Guide to IMMUNOPHARMACOLOGY. Invited speakers contributed to productive discussions on the varying challenges and opportunities in immunopharmacology research.

We have collated the presentations and written a detailed meeting report which are available on the website. Here is a direct download of the the Meeting Report (PDF).

The meeting included Prof. Tracy Hussell delivering the Anthony Harmar Memorial Lecture, details of which are given in a dedicated blog post.

GTOIMMUPDB ANALYTICS

Our analytics over the last 6 months (Oct 18 - Mar 19) shows an average of 1096 sessions per month.



Access statistics for GtoImmuPdb (October 2018-March 2019)

GTOIMMUPDB PORTAL AND SEARCHING

The CVR Onlife Interview with Prof. Alberto Mantovani and Prof. Michael Spedding was added to the GtoImmuPdb Portal. We have also added a link to the Immunopaedia resource.

The GtoImmuPdb portal, April 2019; Showing pop-up help with tutorial videos and inclusion of CVR Onlife Interview with Prof. Alberto Mantovani and Prof. Michael Spedding.

DISEASE DATA

Disease	GtoPdb Ligands	GtoPdb Targets
Rheumatoid arthritis	162	11
Asthma	77	6
Psoriasis	56	2
Chronic obstructive pulmonary disease	42	-
Crohn's disease	27	1
Osteoarthritis	25	4
Systemic lupus erythematosus	23	-
Ulcerative colitis	21	1
Psoriatic arthritis	16	-
Acute lymphocytic leukaemia (ALL)	2	2

This table gives a summary of the diseases with the most target and ligand associations in GtoImmuPdb.

IMMUNO PROCESS DATA

The table below summarises the unique target (UniProtKB) annotated to each category and the total target-GO annotations (data here is from 2018.4 release).

Process Category	GtoPdb Human UniProtKB	Target-GO annotations
Barrier integrity	47	63
Inflammation	630	1434
Antigen presentation	178	260
T cell (activation)	195	418
B cell (activation)	156	261
Immune regulation	481	1252
Tissue repair	21	21
Immune system development	240	428
Cytokine production & signalling	504	1347
Chemotaxis & migration	266	491
Cellular signalling	480	1177

IMMUNO CELL TYPE DATA

The table below shows the top-level cell type categories used in GtoImmuPdb along with the Cell Ontology (CO) terms mapped to each category. The Cell Ontology provides the formalised vocabulary against which we annotate targets to cell type associations.

Cell Type Category	Cell Ontology Terms	Targets annotated
B cells	CL:0000945 lymphocyte of B lineage	47
T cells	CL:0000789 alpha-beta T cell CL:0000815 regulatory T cell CL:0000911 effector T cell	72
Dendritic cells	CL:0000451 dendritic cell	41
Other T cells	CL:0000798 gamma-delta T cell CL:0000814 mature NK T cell CL:0000898 naive T cell CL:0000940 mucosal invariant T cell	3
Macrophages & monocytes	CL:0000235 macrophage CL:0000576 monocyte	55
Granulocytes	CL:0000094 granulocyte	45
Natural killer cells	CL:0000623 natural killer cell	23
Mast cells	CL:0000097 mast cell	37
Innate lymphoid cells	CL:0001065 innate lymphoid cell	3
Stromal cells	CL:0000499 stromal cell	1

GTOIMMUPDB TARGET AND LIGAND CURATION STATS

- 594 targets tagged as in GtoImmuPdb:
  - 148 catalytic receptors
  - 193 enzymes
  - 100 gpcrs
  - 25 voltage-gated ion channels
  - 99 other proteins
  - 8 nuclear hormone receptors
  - 9 transporters
  - 11 ligand-gated ion channels
- 1155 ligands tagged as in GtoImmuPdb:
  - 712 synthetic organic
  - 152 antibodies
  - 240 peptides
  - 37 metabolites
  - 13 natural products
  - 1 inorganic
  - 255 Approved drugs
- Detailed lists on:
  - www.guidetoimmunopharmacology.org/immuno/immunoHelpPage.jsp

SEARCHING, COLLATION, ALERTING

The different strategies we had used to retrieve papers was already described in the Oct 2018 report. However, in terms of using open reference managers to collate, tag, add curatorial notes and share papers of interest, we faced a major challenge in 1Q 2019 with the announcement of the closure of CiteUlike (the URL is already dead). We had been usefully using this over the last three years for intra-team and public sharing. Fortunately bulk migrations to Zotero worked fairly well and, crucially preserved the tagging and notes we had added to our CiteUlike entries. Example entries from our "Hot Topic" tagging are shown below from https://www.zotero.org/cdsouthan/items/collectionKey/4ZK4CW8S/tag/htopic

Title	Creator	Date Modified
Functional characterization of 3D protein structures informe...	Hicks et al.	4/17/2019 10:52 AM
A Brief Note About Alzheimer's	Lowe	4/17/2019 10:51 AM
Prioritization of cancer therapeutic targets using CRISPR-Ca...	Behan et al.	4/14/2019 7:59 PM
A reference map of the human protein interactome	Luck et al.	4/11/2019 10:08 PM
Microdeletion in a pseudogene identified in a patient with h...	Habib et al.	4/1/2019 1:14 PM
The past, present and future of anti-malarial medicines	Tse et al.	4/1/2019 10:27 AM
Biology must develop herd immunity against bad-actor molecul...	Plemper and Cox	4/1/2019 9:57 AM
A Diagnosis for All Rare Genetic Diseases: The Horizon and t...	Boycott et al.	3/30/2019 9:46 PM
Pharma R&DAnnual Review 2018	Llyod	2/26/2019 11:34 PM

Team members and collaborators are still adjusting to Zotero sharing features (and collaborators are welcome to connect to us) but we continue to use a variety of tags for our own triage in addition to adding pre-curation (e.g. PubChem IDs and patent numbers) and post curation notes (including to curated ligands). In terms of alerting we follow Twitter feeds from Immune Regulation News , Human Immune News British Society for Immunology, Edinburgh Centre for Inflammation Research as well as journals such as Nature Immunology and Journal of Immunology.

THE GUIDE TO MALARIA PHARMACOLOGY DATABASE (GTOMPDB)

INTRODUCTION

The Guide to MALARIA PHARMACOLOGY (GtoMPdb) has been developed as an extension to the main GtoPdb database, with the aim of providing optimized access for the malaria research community to the data in GtoPdb. In this section of the report we provide an update on both the curation effort and the status of web interface and database developments, including details of the public release of the GtoMPdb (now available at www.guidetomalariapharmacology.org).

GTOMPDB TARGET AND LIGAND CURATION

COLLECTING AND PRIORITISING CONTENT

The curation team use a similar strategy to the one employed by GtoImmuPdb and described in our previous reports. Following the announced closure of CiteUlike we have recently moved to Zotero, continuing to increase our collection of publications that we have tagged with antimalarial specific tags (antimalarial, antimalarial_targets). In addition, MMV have provided a list of targets and ligands that are of high priority and we will continue to build on this list with the advice of both MMV and our expert advisory committee.

CURATION SUMMARY

The number of ligands in the public database with antimalarial activity has continued to increase and we have also added to the number of *P. falciparum* targets. Our most recent database release (2019.2) contains:

- 57 ligands tagged as in GtoMPdb: http://www.guidetopharmacology.org/GRAC/FamilyDisplayForward?familyId=999
- 25 targets tagged as in GtoMPdb: http://www.guidetopharmacology.org/GRAC/FamilyDisplayForward?familyId=970

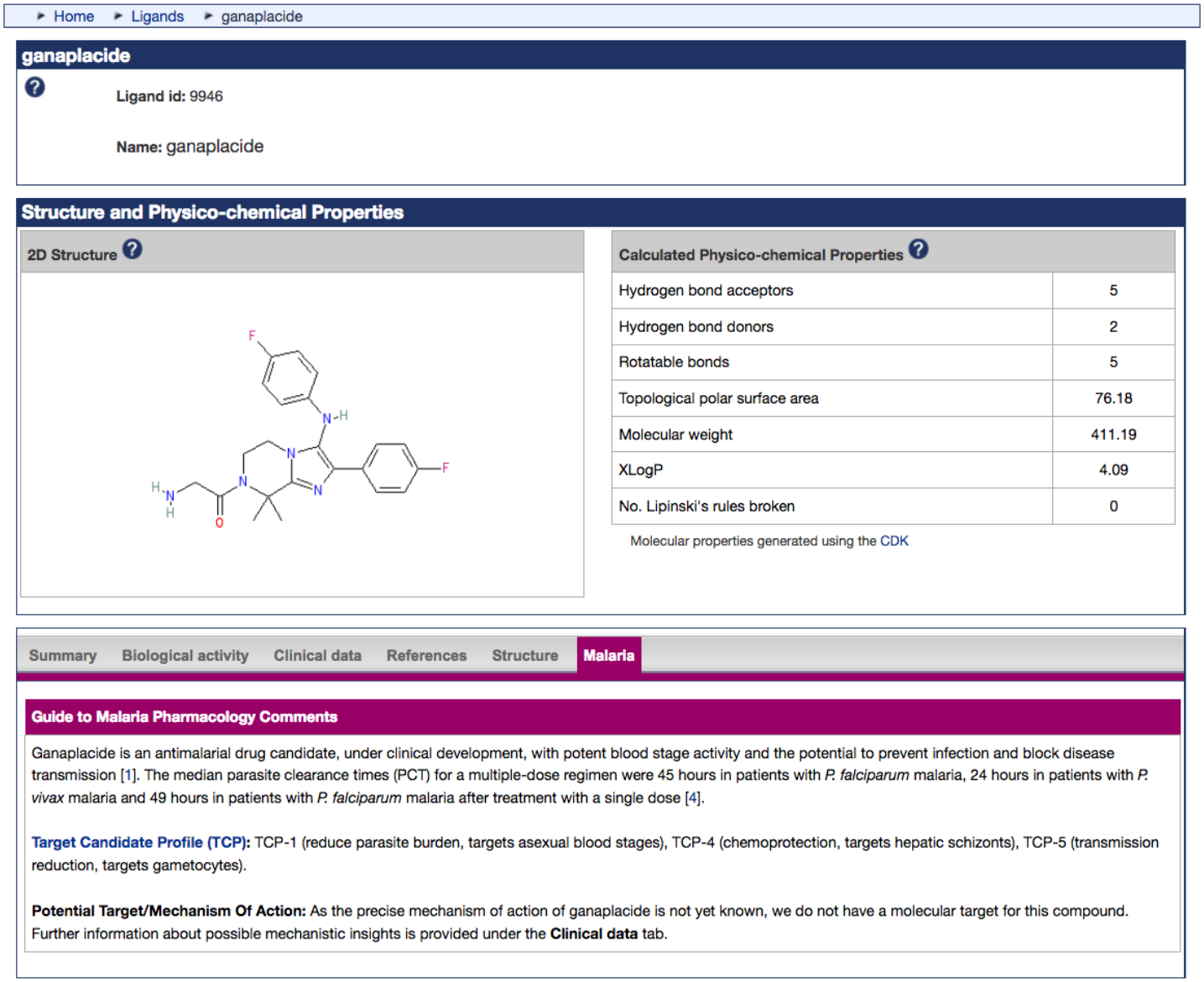
GTOMPDB WEB INTERFACE AND DATABASE DEVELOPMENT

The GtoMPdb uses the same underlying database as GtoPdb and in previous reports (May 2018 and October 2018) we have described a number of changes to the database structure and the web interface that were necessary for the capture and presentation of antimalarial data. To summarize this development work, we have:

- Introduced a project specific tag allowing us to identify all ligands and targets in the database that are to be included in the GtoMPdb.
- Many antimalarial compounds have a poorly understood mechanism of action and an unknown molecular target and we have extended the interactions table and updated the web interface to accommodate this.
- Introduced a new ‘whole organism’ assay type to capture data from the whole cell assays used routinely in antimalarial drug discovery.
- Information about the *Plasmodium* lifecycle activity of a ligand is now be stored in the database and is provided in the interactions table.
- Details about the *Plasmodium* species/strain can be stored in the database and displayed using a pop-up window that has been added to the interactions table.

This completed the major part of the required development work, but we have continued to implement improvements and in the last reporting period we have:

- Deployed a new malaria comments field for both ligands and targets.
- Extended the site search to incorporate the malaria comments field and to bring back targets from searches on parasite lifecycle stage or malaria species.
- For ligands we now include the Target Candidate Profile (TCP), where available, in the malaria comments field.



Ligand page for ganaplacide, illustrating the malaria comments field that now provides information on the Target Candidate Profile (TCP)

GTOMPDB PORTAL DEVELOPMENT

The GtoMPdb portal has been designed to provide optimized access to our antimalarial data and has been tailored for those involved in malaria research. Development of this portal has been a major focus of recent work, with a number of alpha-releases deployed to our (internal) development site for testing purposes and to gather feedback. In January 2019 we made the first public release of the GtoMPdb (beta-release v1.0), followed by a second release in March (beta-release v2.0), alongside the scheduled general database releases. These beta-releases contain most of the features that we expect to be included in the full official release but are considered to be under development at the present time. Release details and technical updates can be followed from our blog.

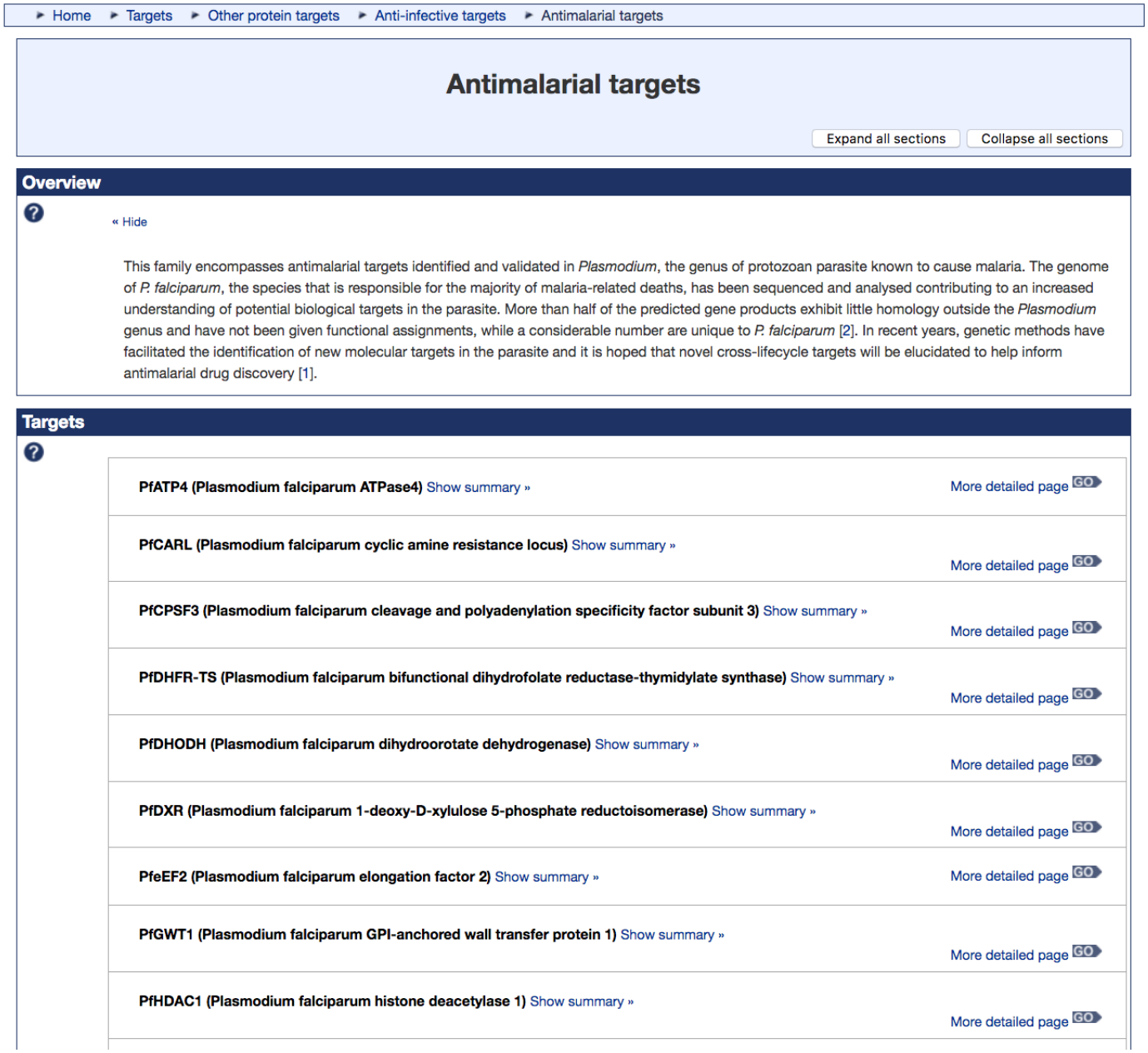
The development of the new portal draws on our experience from the GtoImmuPdb project with a dedicated domain for the GtoMPdb (www.guidetomalariapharmacology.org) and the design of a distinct identity (logo, header bar and colour scheme).

GtoMPdb portal (beta-release v2.0)

The portal provides tailored routes into browsing the antimalarial data. In addition to the existing ligand and target browse/search functionality available on the parent GtoPdb site we have developed customised views of the data that include parasite lifecycle and target species activity. Access to all is from the menu-bar or from the panels on the homepage.

TARGETS

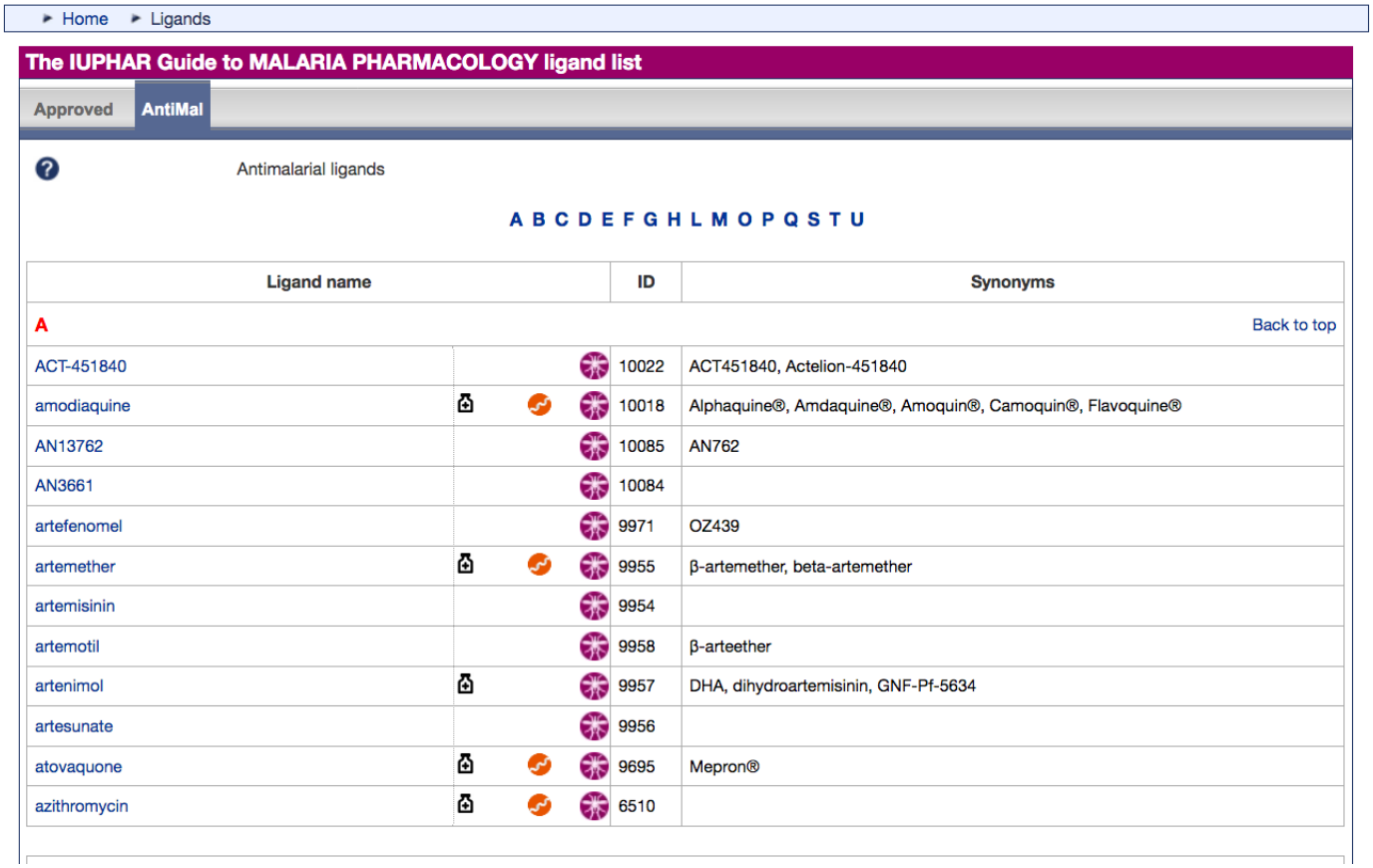
The entry point to our *P. falciparum* targets is the 'Antimalarial targets' subfamily, a new subdivision of the existing 'Anti-infective targets' family. All *P. falciparum* targets have a more detailed page that is modelled on the GtoPdb target pages, with the addition of a comments section for information of relevance to malaria.



Antimalarial targets subfamily

LIGANDS

A ligand list page has been developed for the GtoMPdb. At present two categories are provided, one showing all antimalarials (AntiMal) and a second showing just those that are approved drugs.



Home ▸ Ligands

The IUPHAR Guide to MALARIA PHARMACOLOGY ligand list

Approved | AntiMal

Antimalarial ligands

A B C D E F G H L M O P Q S T U

Ligand name	ID	Synonyms
A		Back to top
ACT-451840	10022	ACT451840, Actelion-451840
amodiaquine	10018	Alphaquine®, Amdaquine®, Amoquin®, Camoquin®, Flavoquine®
AN13762	10085	AN762
AN3661	10084	
artefenomel	9971	OZ439
artemether	9955	β-artemether, beta-artemether
artemisinin	9954	
artemotil	9958	β-arteether
artenimol	9957	DHA, dihydroartemisinin, GNF-Pf-5634
artesunate	9956	
atovaquone	9695	Mepron®
azithromycin	6510	

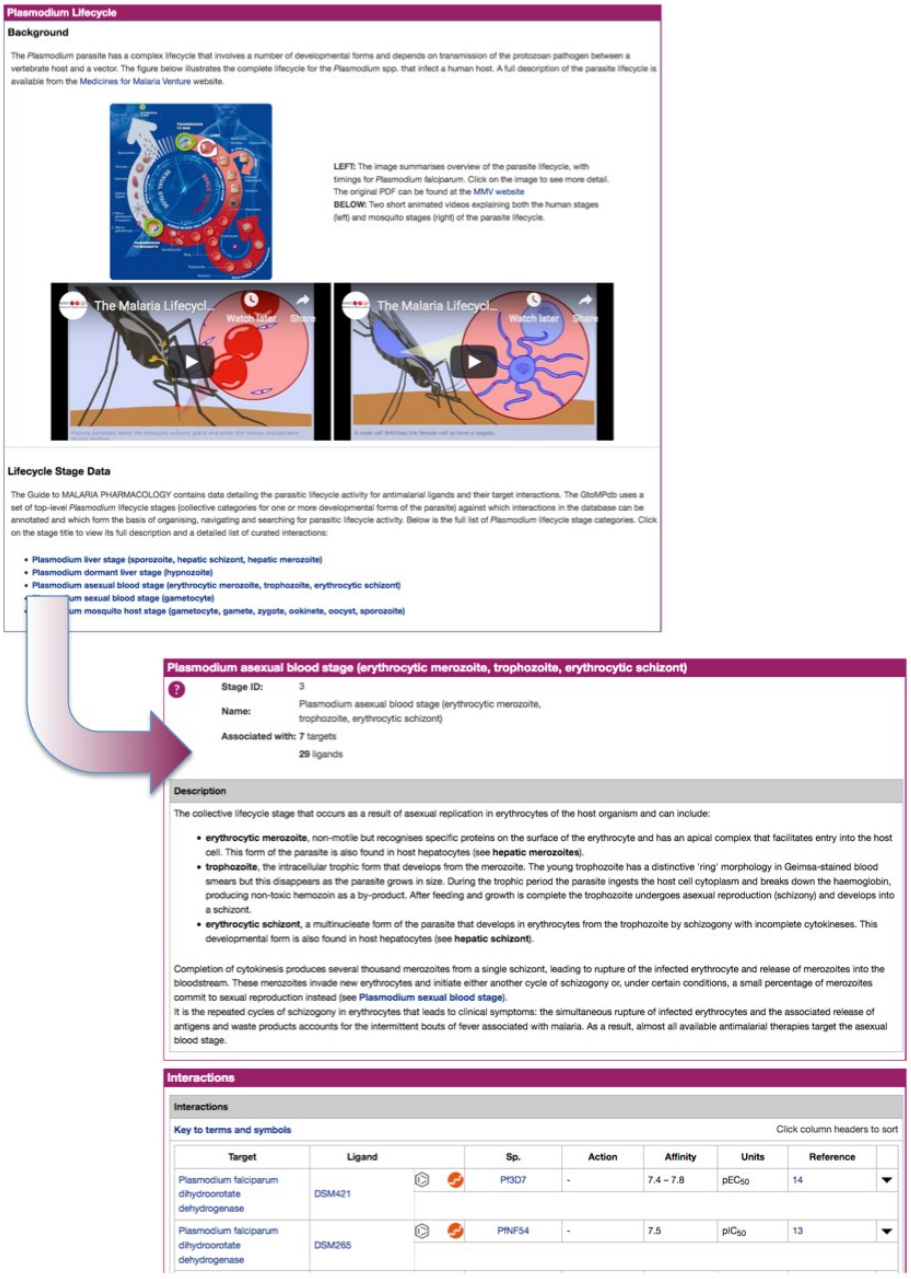
GtoMPdb ligand list, showing AntiMal tab selected.

The AntiMal tab provides a discrete list of all ligands that have the GtoMPdb tag. These ligands are also highlighted in all other lists by the appearance of a new ‘antimalarial ligand' icon next to the ligand name.

Icon/Table heading	Definition
	Indicates that the ligand has been tagged in the database as being relevant to GtoMPdb

PARASITE LIFECYCLE ACTIVITY DATA

The GtoMPdb uses a set of top-level Plasmodium lifecycle stages (collective categories for one or more developmental forms of the parasite) against which interactions in the database can be annotated and which form the basis of organising, navigating and searching for parasitic lifecycle activity. We have developed a new Parasite Lifecycle homepage that provides a short introduction and links to additional pages for each of the top-level lifecycle stages. These in turn contain a more detailed description and a table of interactions for that lifecycle stage.

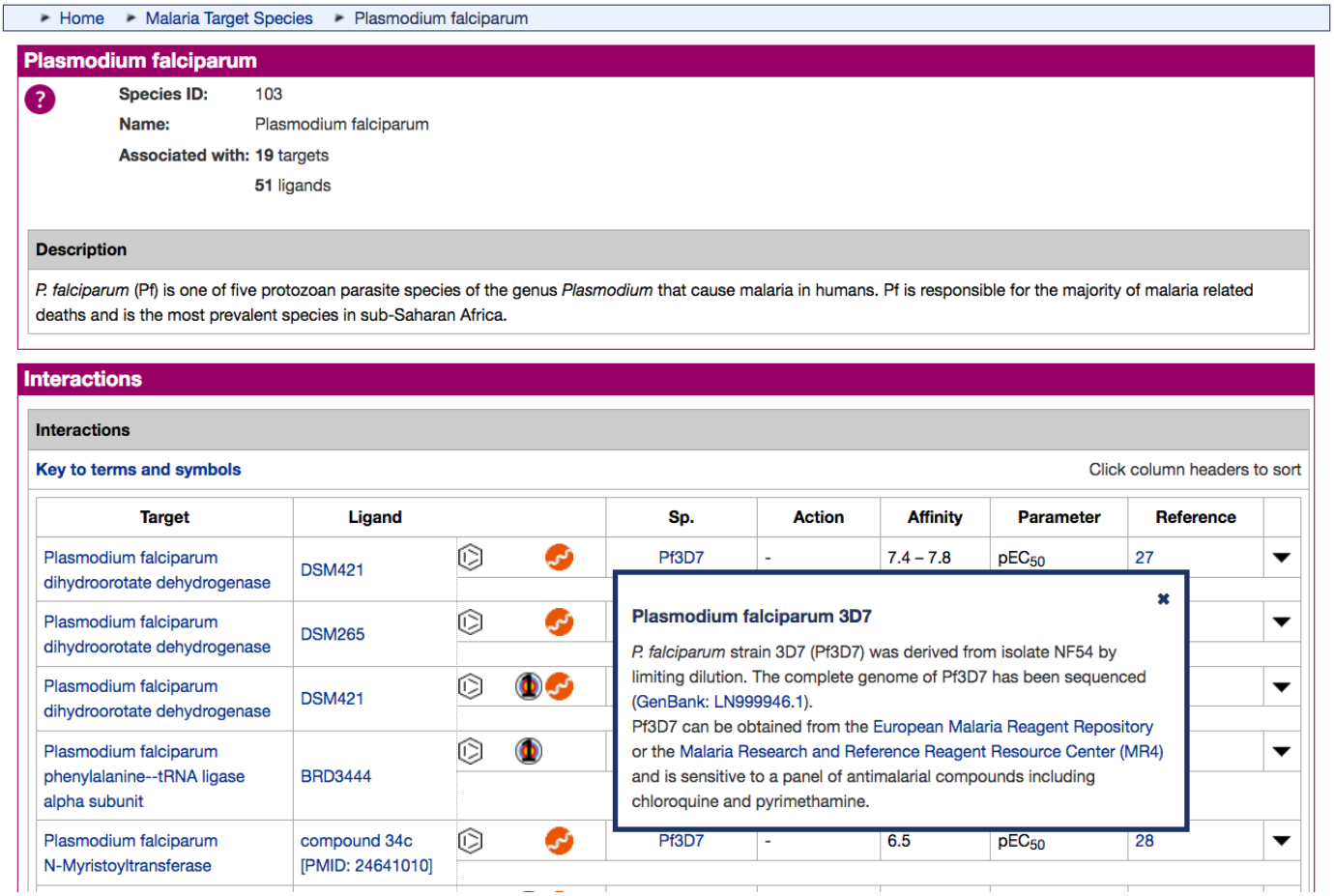


Parasite Lifecycle homepage with links to individual lifecycle pages

TARGET SPECIES

The Target Species homepage provides a short description for *Plasmodium* species that are of clinical or research importance. It also includes a resource section and links to individual pages for species that have annotated interactions in the database. The figure below illustrates an example of an individual species page. The interactions table displays affinity data for the species but also provides additional details, when available, for the strain used.

We continue to develop these pages and expand the number of species, with the recent introduction of a description section on each page and the addition of a page for *P. yoelii*.



Individual Target Species page for *P. falciparum* showing interaction data and an example of the pop-up strain window

HELP AND ABOUT PAGES

The menu-bar provides access to the new ‘Help’ and ‘About’ pages for GtoMPdb. We have included ‘Help’ pop-ups on both the main panels of the homepage and on the parasite lifecycle and target species pages.

A section for Contributor details has been added (under About) with both our Expert Advisory Committee and Scientific Advisors listed.