IUPHAR/BPS Guide to PHARMACOLOGY

Database Report

April 2021

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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 November 2020. Previous reports are online for Apr 2019, Apr 2020 and Nov 2020. We have reduced redundancy between the reports by purging sections without significant changes. Thus, if you remember any aspect that is not here, it may well be in a previous report (and you can always enquire)

Updates over the last 5 months have focussed on preparations for the next edition of the Concise Guide to Pharmacology (2021/22). We have continued curation of data relevant to the pharmacological strategies aimed at mitigating SARS-CoV-2 infection (COVID-19) on our Coronavirus (COVID-19) information page and we provide updates on the Wellcome Trust funded Guide to IMMUNOPHARMACOLOGY (GtoImmuPdb) and the Medicines for Malaria Venture (MMV) funded Guide to MALARIA PHARMACOLOGY (GtoMPdb).

IUPHAR Fibrosis Symposium (Nov 2020)

NC-IUPHAR has organised high-level scientific meetings for receptor classifications for over three decades, and these meetings have underpinned the molecular basis for modern pharmacology. The meetings are traditionally held over a weekend in Paris, and have been made possible by educational grants from Servier. We therefore wished to develop these meetings, expanding the scientific part to have a one day symposium to progress certain fields thought to be crucial for pharmacology.

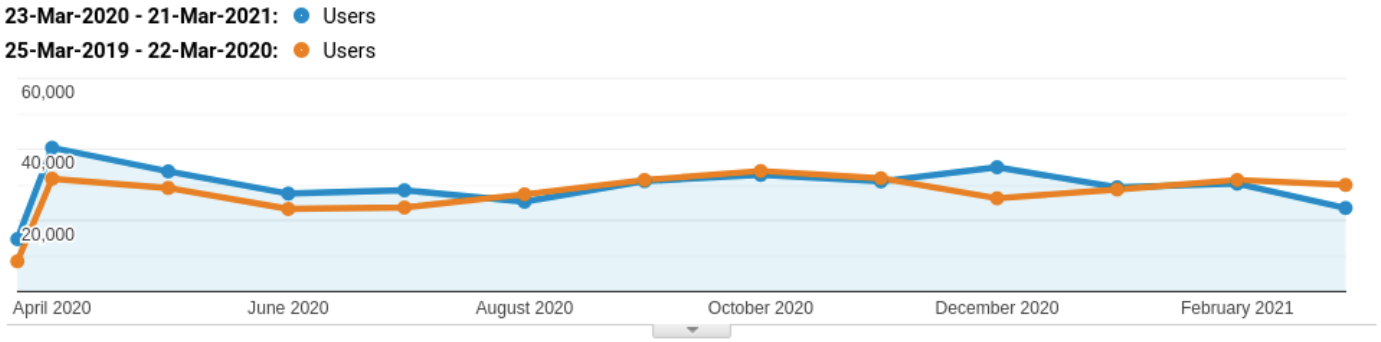
Last November the IUPHAR/Servier Fibrosis Symposium was held online and we like to thank Servier for their support and to all the speakers for contributing to an excellent meeting. The majority of the presentations (slides and videos) are available on the website www.guidetopharmacology.org/fibrosisSymposium20.jsp.

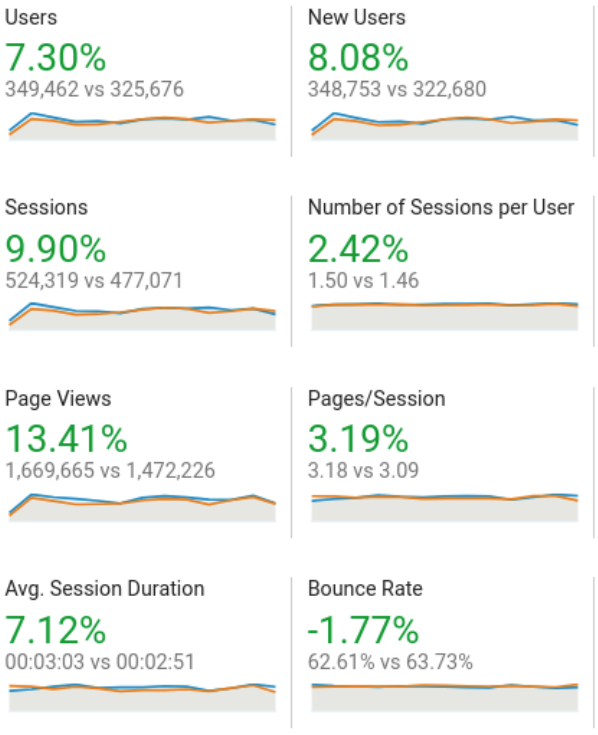
This includes the keynote lecture, dedicated to Paul Vanhoutte, delivered by Prof. Amrita Ahluwalia on "The non-canonical pathway for NO: NO_3^- -NO_2^- -NO".

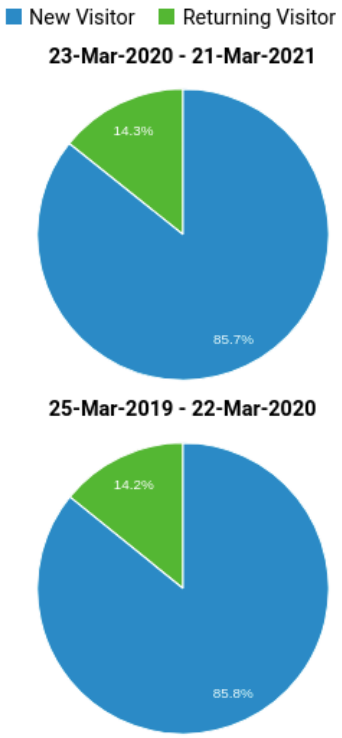
The IUPHAR Fibrosis Meeting Report can be read in the Dec 2020 issue of Pharmacology International.

GtoPdb Website Analytics

GtoPdb Website Access Statistics







Graphs comparing visitors to guidetopharmacology.org for the 12 months from March 2020 to March 2021, with the previous 12 months.

Monthly statistics	**Mar 2020 - Mar 2021 (previous 12 months)**
Sessions	43,693 (39,756)
Users	29,122 (27,140)
Page views	139138 (122,685)
Pages / Session	3.18 (3.09)
Avg. Session Duration	00:03:03 (00:02:51)

Acquisition & Google Search Console

To explore how the website performs in Google searches, we have made use of the Google Search Console (https://search.google.com/search-console/about). This allows us to see how many 'clicks' through to the GtoPdb website have been made from the results of different Google searches.

The figure below shows that there have been around 25,600 clicks through to GtoPdb from the results of Google searches in March 2021. The query that results in the most clicks through is 'iuphar' with 1,086. Impressions are the number of times a user will have seen a link to GtoPdb and the position shows the highest search result position for a link to GtoPdb. The CTR (click through rate) is the percentage of impressions that lead to clicks.

Reassuringly, we see that a query for GtoPdb specific terms (e.g. 'iuphar', 'guide to pharmacology'), gives an average position of 1 - so GtoPdb is the top hit for these searches. They also result in a high CTR - 64.8% for 'iuphar' and 88.1% for 'guide to pharmacology'. The tool enables us to observe the types of queries that create high 'impressions' and 'clicks'. In the table below, pharmacology specific search terms such as 'regdamvimab', 'phenylephrine mechanism of action' and 'muscarinic receptors' all give a GtoPdb page in the top 5 positions, each resulting in more than 100 clicks to GtoPdb. Their CTR is between 0.6% and 4.7%. The more specific search for 'pf-07304814 structure' (SARS-CoV-2 3CL protease (Mpro) inhibitor from Pfizer) gives a higher ranking for GtoPdb (to the ligand page), and produces a much higher CTR.

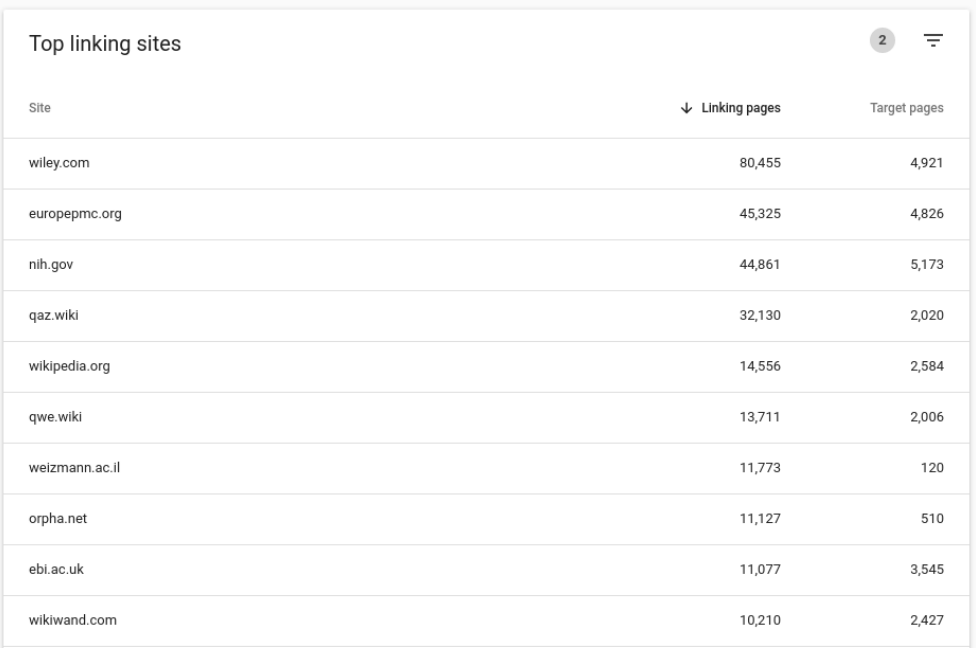
QUERIES | PAGES | COUNTRIES | DEVICES | SEARCH APPEARANCE | DATES

Query	Clicks	Impressions	CTR	Position
iuphar	1,088	1,679	64.8%	1.1
guide to pharmacology	467	530	88.1%	1
regdanvimab	237	5,023	4.7%	3.1
guidetopharmacology	139	150	92.7%	1
phenylephrine mechanism of action	131	3,907	3.4%	1.8
muscarinic receptors	113	20,394	0.6%	4.4
opioid receptors	79	4,819	1.6%	5.5
pf-07304814	79	674	11.7%	4.1
pf-07304814 structure	76	232	32.8%	1.2
sert	67	12,884	0.5%	8

Rows per page: 10 1-10 of 1000

Google Search Console - Performance data for guidetopharmacology.org (1 Mar 21 - 30 Mar 21)

The Google Search Console also allows us to pinpoint where external links into the Guide to Pharmacology are coming from. There are around 470,000 unique external links into GtoPdb. The following table shows the 10 sites with the highest number of links into GtoPdb. This covers Wiley, European PMC, NCBI (nih.gov), Wikipedia, EBI and GeneCard (there are a couple of wiki mirroring sites).



Top linking sites

Site	Linking pages	Target pages
wiley.com	80,455	4,921
europepmc.org	45,325	4,826
nih.gov	44,861	5,173
qaz.wiki	32,130	2,020
wikipedia.org	14,556	2,584
qwe.wiki	13,711	2,006
weizmann.ac.il	11,773	120
orpha.net	11,127	510
ebi.ac.uk	11,077	3,545
wikiwand.com	10,210	2,427

It is also possible to have a more detailed look at the pages in GtoPdb that external sites link to. The following tables are a snapshot of the top target and ligand pages linked to from external sites.

Table showing the top 20 targets linked to from external sites. 'Links' gives the total unique links to the page and 'Sites' shows the unique sites/domains

Target ID	Target Name	Family	Links	Sites
319	μ receptor	Opioid receptors	**880**	**128**
56	CB_1 receptor	Cannabinoid receptors	**776**	**103**
595	Peroxisome proliferator-activated receptor-γ	1C. Peroxisome proliferator-activated receptors	**751**	**59**
507	TRPV1	Transient Receptor Potential channels	**636**	**58**
1376	COX-2	Cyclooxygenase	**628**	**54**
57	CB_2 receptor	Cannabinoid receptors	**597**	**75**
34	AT_1 receptor	Angiotensin receptors	**596**	**76**
1337	CYP3A4	CYP3 family	**569**	**41**
1249	Endothelial NOS	Nitric oxide synthases	**562**	**39**
215	D_2 receptor	Dopamine receptors	**527**	**62**
1250	Inducible NOS	Nitric oxide synthases	**524**	**35**
29	β_2-adrenoceptor	Adrenoceptors	**495**	**55**
593	Peroxisome proliferator-activated receptor-α	1C. Peroxisome proliferator-activated receptors	**494**	**53**
317	δ receptor	Opioid receptors	**483**	**61**

485	TRPA1	Transient Receptor Potential channels	**477**	**70**
1	5-HT_{1A} receptor	5-Hydroxytryptamine receptors	**460**	**69**
1540	AMP kinase	AMPK subfamily	**427**	**26**
1619	Caspase 3	C14: Caspase	**422**	**26**
2109	mechanistic target of rapamycin kinase	FRAP subfamily	**404**	**35**
109	*GPR55*	GPR18, GPR55 and GPR119	**395**	**46**

Table showing the top 25 ligands linked to from external sites. 'Links' gives the total unique links to the page and 'Sites' shows the unique sites/domains

Ligand ID	Ligand Name	Type	Links	Sites
4998	IL-6	Peptide	**1342**	**64**
2509	NO	Inorganic	**1051**	**91**
4974	IL-1β	Peptide	**1020**	**53**
2352	cyclic AMP	Metabolite	**844**	**85**
294	acetylcholine	Metabolite	**766**	**106**
1713	ATP	Metabolite	**759**	**104**
1627	morphine	Natural product	**700**	**123**
5074	tumour necrosis factor shed form	Peptide	**700**	**33**
5	5-hydroxytryptamine	Metabolite	**684**	**109**
940	dopamine	Metabolite	**616**	**96**
5019	LPS	Natural product	**568**	**31**
4139	aspirin	Synthetic organic	**567**	**104**
2504	angiotensin II	Peptide	**555**	**38**
2424	δ^9-tetrahydrocannabinol	Natural product	**545**	**118**
1067	GABA	Metabolite	**544**	**117**
4968	IFN-γ	Peptide	**535**	**29**
5060	TGFβ1	Peptide	**522**	**31**
1883	PGE_2	Metabolite	**518**	**78**
5239	paracetamol	Synthetic organic	**517**	**99**
2347	cyclic GMP	Metabolite	**514**	**70**

2448	H_2O_2	Inorganic	**484**	**110**
2768	dexamethasone	Synthetic organic	**480**	**85**
4150	cannabidiol	Natural product	**475**	**105**
4779	metformin	Synthetic organic	**464**	**66**

Download Statistics

Yearly period 23 Mar 2020-21 Mar 2021 (comparing with 25 Mar 2019 - 22 Mar 2020)

Google Analytics: Comparison of Downloads

Event Category: Downloads

	Count
2019-2020	2,903
2020-2021	4,420
Change	52.26%

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

A more specific breakdown is shown here:

	2020-2021	**2019-2020**	**Change**
Targets CSV/TSV file	1396	1064	23%
Interactions CSV/TSV file	443	368	17%
*Ligands CSV/TSV file **	1105	462	58%
*Covid ligand/target files ***	167	60	178%
UniProt Mapping file	191	152	20%
HGNC mapping file	155	112	28%
*PostgreSQL****	195	145	26%

* The large increase in ligand downloads is attributable to the fact that we add a new way to download specific ligand sets from our ligand list pages (https://www.guidetopharmacology.org/GRAC/LigandListForward?database=all). Users can download any of the sets on this page in csv format.

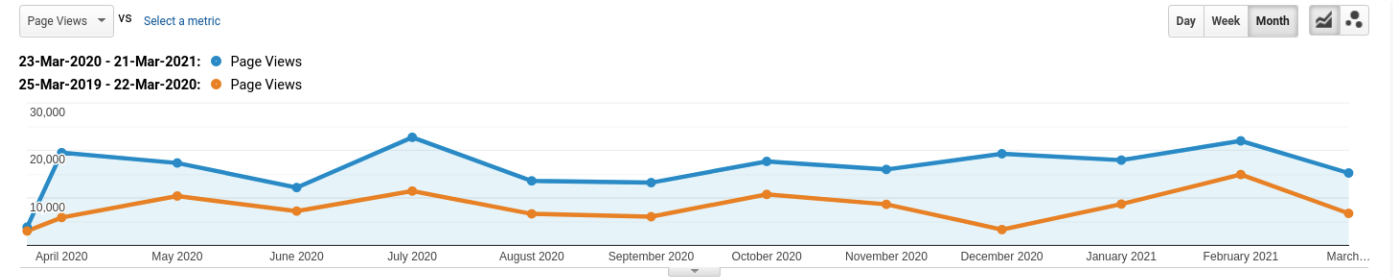
** This download was not available until April 2020.

*** Total downloads of PostgreSQL database dump files (versions 2018.4 onwards).

Web Services

We have tracked our web-services 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 not resolve these to specific users, locations or numberd of visits but we can record hits for each distinct URL.

The image below shows that there were approximately 210,571 total page views over the year, which is an increase on the following year (103,774).



Primary Dimension: **Page** Page Title Other

Plot Rows | Secondary dimension | Sort Type: Default | advanced

	Page	Page Views	Unique Page Views	Avg. Time on Page	Entrances	Bounce Rate	% Exit	Page Value
		102.91% 210,571 vs 103,774	79.55% 115,292 vs 64,213	28.90% 00:00:09 vs 00:00:13	53.61% 3,129 vs 2,037	15.37% 43.62% vs 51.55%	24.30% 1.49% vs 1.96%	0.00% US$0.00 vs US$0.00
1.	/services/targets							
	23-Mar-2020 - 21-Mar-2021	**27,490** (13.05%)	1,283 (1.11%)	00:00:12	850 (27.17%)	36.24%	2.14%	US$0.00 (0.00%)
	25-Mar-2019 - 22-Mar-2020	**13,342** (12.86%)	752 (1.17%)	00:00:13	556 (27.30%)	44.24%	2.86%	US$0.00 (0.00%)
	% Change	**106.04%**	**70.61%**	**-3.01%**	**52.88%**	**-18.10%**	**-24.97%**	**0.00%**
2.	/services/ligands							
	23-Mar-2020 - 21-Mar-2021	**9,413** (4.47%)	773 (0.67%)	00:00:23	433 (13.84%)	51.73%	4.06%	US$0.00 (0.00%)
	25-Mar-2019 - 22-Mar-2020	**3,933** (3.79%)	534 (0.83%)	00:00:28	326 (16.00%)	70.25%	8.77%	US$0.00 (0.00%)
	% Change	**139.33%**	**44.76%**	**-15.29%**	**32.82%**	**-26.36%**	**-53.74%**	**0.00%**

Traffic to GtoPdb web services over the past year

GtoPdb Content

These database statistics were compiled from our March 18th release (v2021.1). All database statistics can be found at http://www.guidetopharmacology.org/about.jsp#content.

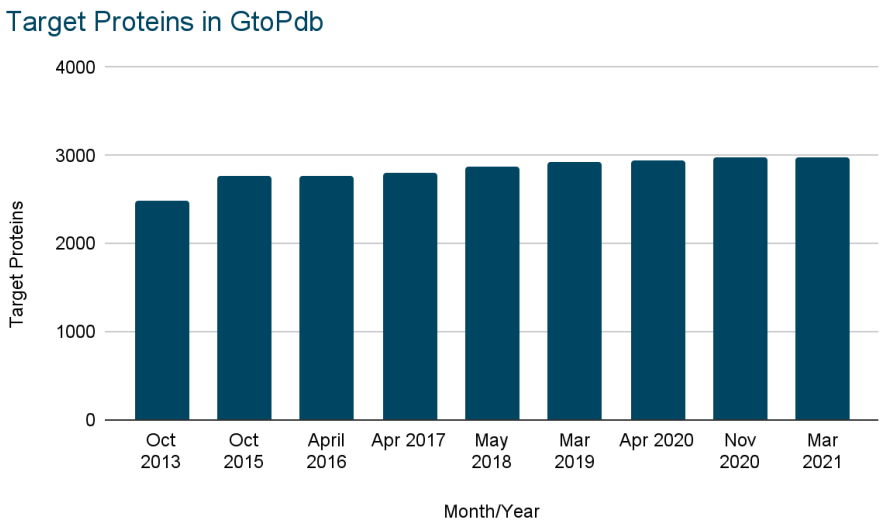
Targets	Number of (Human) UniProt IDs
7TM receptors	399
Nuclear hormone receptors	48
Catalytic receptors	249
Ligand-gated ion channels	81
Voltage-gated ion channels	144

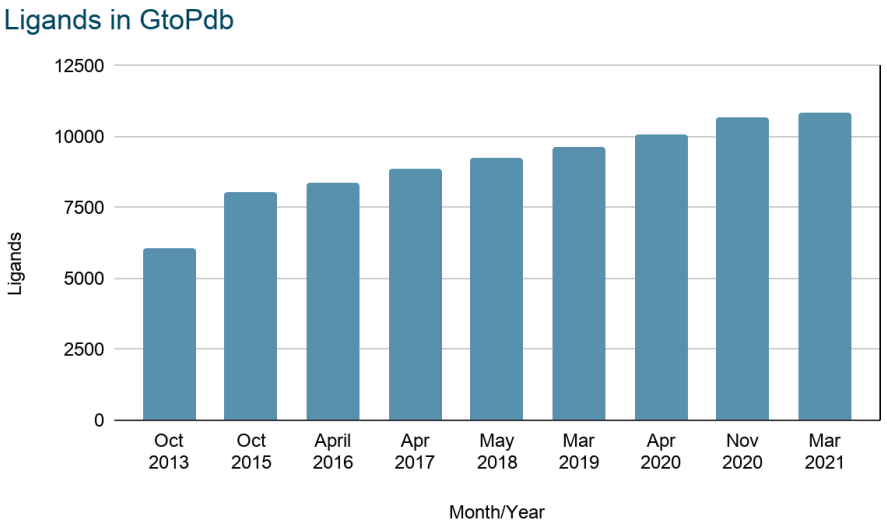
Other ion channels	53
Enzymes	1240
Transporters	555
Other protein targets	216
Targets with ligand interactions	1833
Targets with quantitative ligand interactions	1580
Targets with approved drug interactions	673
Primary Targets with approved drug interactions	333
Total number of targets	**2985**
Ligands	**Number of ligands**
Synthetic organics	7428
Metabolites	514
Endogenous peptides	803
Other peptides including synthetic peptides	1403
Natural products	331
Antibodies	303
Inorganics	39
Approved drugs	1643
Withdrawn drugs	86
Ligands with INNs	2789
Labelled ligands	630
Unique PubChem CIDs (total CID links)	8102 (8305)
Ligands with target interactions	9107
Ligands with quantitative interactions (approved drugs)	8016 (995)
Ligands with clinical use summaries (approved drugs)	2899 (1639)
Total number of ligands (PubChem SIDs)	**10659**
Number of binding constants	49558
Number of binding constants curated from the literature	18351

GtoPdb Entity Growth

Growth rates over the span of the previous Wellcome Trust grant are documented in earlier reports and our 2016, 2018 and 2020 NAR papers. Updates come via subcommittee contributions to the Concise Guide, and the continued tagging of pre-existing targets and ligands with comments and references to GtoImmuPdb and GtoMPdb. Note that, while we highlight newly-liganded targets in release notes, the growth of new targets is slow but ligand expansion continues.

	Oct 2013	Oct 2015	April 2016	Apr 2017	May 2018	Mar 2019	Apr 2020	Nov 2020	Mar 2021
Target protein IDs	**2485**	**2761**	**2775**	**2808**	**2872**	**2920**	**2943**	**2976**	**2985**
Ligands total	**6064**	**8024**	**8400**	**8872**	**9251**	**9662**	**10053**	**10659**	**10821**
Approved drugs	559	1233	1273	1322	1364	1421	1471	1614	1643
Antibodies	10	138	172	212	240	255	270	295	303
Peptides	1776	1981	2007	2063	2092	2122	2150	2180	2206
Synthetic small molecules	3504	5055	5363	5729	6048	6401	6816	7303	7428
PubChem SIDs	3107	8024	8328	8831	9251	9662	10053	10659	10821
PubChem CIDs	2694	6057	6163	6813	7109	7407	7483	7994	8102
Binding constants	41076	44691	45534	46287	47058	48071	48902	49363	49558
References	21774	27880	29247	31239	33245	35723	37261	39133	40022





GtoPdb Target Updates

These are lists of targets updated for the Concise Guide (21-22 ed), and new targets added since November 2020.

GPCRs:
Acetylcholine receptors
Adenosine receptors
Adhesion Class GPCRs
Adrenoceptors
Angiotensin receptors
Bradykinin receptor
Calcitonin receptors
Calcium-sensing receptor
Chemokine receptors
Cholecystokinin receptors
Class Frizzled GPCRs
Complement peptide receptors
Dopamine receptors
Formylpeptide receptors
G protein-coupled estrogen receptor
Galanin receptors
Ghrelin receptor
Gonadotropin-releasing hormone receptors
G protein-coupled estrogen receptor
Hydroxycarboxylic acid receptors
Leukotriene receptors
Lysophospholipid (LPA) receptors
Lysophospholipid (S1P) receptors
Melanocortin receptors
Metabotropic glutamate receptors
Motilin receptor
Neuromedin U receptors
Neuropeptide S receptor
Neurotensin receptors
Opioid receptors
Orexin receptors
P2Y receptors
Parathyroid hormone receptors
Prokineticin receptors
Prostanoid receptors (detailed updates rec'd)
QRFP receptor
Relaxin family peptide receptors
Succinate receptor
Tachykinin receptors
Thyrotropin-releasing hormone receptors
Urotensin receptor
Vasopressin and oxytocin receptors

Catalytic Receptors:
Integrins
Natriuretic peptide receptor family
Receptor Guanylyl Cyclase (RGC) family

NHRs:
3-Ketosteroid receptors
Tumour necrosis factor (TNF) receptor family

Ion Channels:
Acid-sensing (proton-gated) ion channels (ASICs)
Epithelial sodium channel (ENaC)
Cyclic nucleotide-regulated channels
Two P domain potassium channels
Voltage-gated calcium channels
Voltage-gated potassium channels
Aquaporins
Orai channels
Piezo channels

Enzymes and Other protein targets:
2-Acylglycerol ester turnover
N-Acyelthanolamine turnover
Cyclooxygenase
Cytochrome P450 (family overview)
CYP4 family
Haem oxygenase
Hydrogen sulphide synthesis
Lipoxygenases
Leukotriene and lipoxin metabolism
Peptidyl-prolyl cis/trans isomerases **NEW**
Prostaglandin synthases
Sphingosine 1-phosphate lyase
Sphingosine 1-phosphate phosphatase
Sphingosine 1-phosphate turnover
Sphingosine kinase
Blood coagulation components
RGS proteins

Transporters:

Glycine transporter subfamily
Organic anion transporters (OATs)
Organic cation transporters (OCT)
Organic zwitterions/cation transporters (OCTN)
Orphan or poorly characterized SLC22 family members
Neutral amino acid transporter subfamily
SLC1 family of amino acid transporters
SLC8 family of sodium/calcium exchangers
SLC14 family of facilitative urea transporters
SLC15 family of peptide transporters
SLC22 family of organic cation and anion transporters
SLC28 and SLC29 families of nucleoside transporters
SLC36 family of proton-coupled amino acid transporters
SLC47 family of multidrug and toxin extrusion transporters
SLC51 family of steroid-derived molecule transporters
SLC66 Lysosomal amino acid transporters

Urate transporter

New targets (not including Antimalarial targets):

AAA ATPases- LONP1

Peptidyl-prolyl cis/trans isomerases - FKBP38, FKBP51, FKBP52, FKBP prolyl isomerase like, peptidylprolyl cis/trans isomerase, NIMA-interacting 1, Cyclophilin D

CD24 molecule

sialic acid binding Ig like lectin 10 (SIGLEC10)

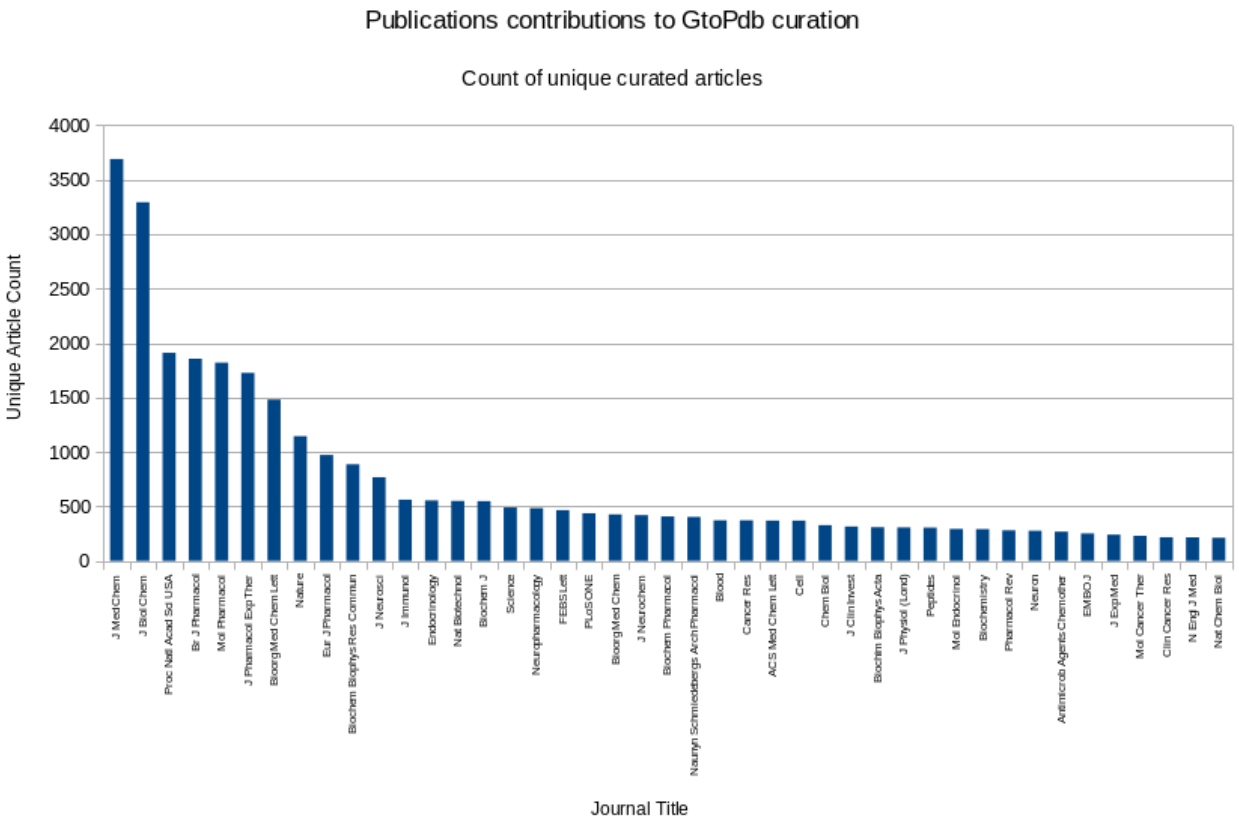
Cyclic GMP-AMP synthase

Analysis of journals contributing to curated data

The following table and graph show the count of unique articles from journals curated in the GtoPdb. The table is restricted to those journals with over 500 unique curated articles. The graph expands this to all journals with over 200 unique curated articles.

Title	Count
J Med Chem	3690
J Biol Chem	3293
Proc Natl Acad Sci USA	1910
Br J Pharmacol	1856
Mol Pharmacol	1820
J Pharmacol Exp Ther	1726
Bioorg Med Chem Lett	1481
Nature	1144
Eur J Pharmacol	971
Biochem Biophys Res Commun	886
J Neurosci	768
J Immunol	561

Endocrinology	555
Nat Biotechnol	550
Biochem J	548



Coronavirus (Covid-19) - GtoPdb information page

Since March 2020 we have been maintaining our coronavirus page that aims to collect many of the pharmacological strategies being considered to mitigate against COVID-19.

Many of these emerging strategies rely on repurposing existing drugs, and others are completely new, but all rely on existing scientific evidence of mechanistic approaches that are effective against either similar viral infections or the serious symptoms that are caused by COVID-19.

There are sections on the key targets and ligands of interest - linked into the more detailed GtoPdb pages, where we already have curated information in the database. As of April 2021 we have 91 unique entries in our table of COVID-19 relevant ligands. Of these, 73 have ligand summary pages in GtoPdb, 41 of which are approved drugs.

There are 7 targets listed on the page all with detailed pages in GtoPdb. Six of these are protein targets: ACE2, CD147, furin, Neurophilin 1, SAR-CoV-2 main protease and TMPRSS2, and one, GM-CSF, is a ligand target.

In addition to the targets and ligands on the coronavirus page, many more entities in the GtoPdb have curator comments regarding evidence of a relationship to SARS-CoV-2 and/or COVID-19 (a search using SARS-CoV-2 retrieves 212 hits).

There are also sections providing useful links to other resources and key publications.

The GtoPdb Coronavirus page has been included in the following data hubs:

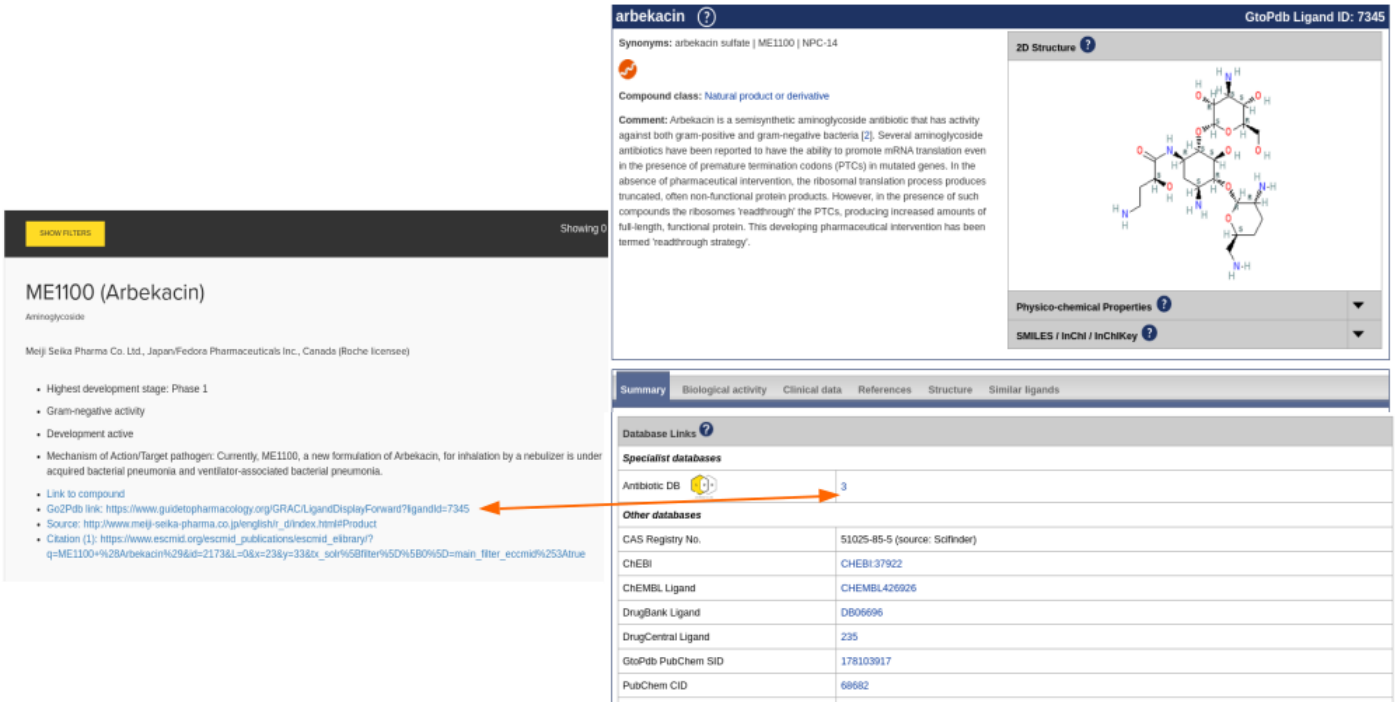
- European Data COVID-19 Data Portal, related resource (database) https://www.covid19dataportal.org/related-resources
- ELIXIR-UK https://elixiruknode.org/elixir-uk-our-support-to-covid-19-research/
- ELIXIR https://elixir-europe.org/services/covid-19#access
- BPS COVID-19 trusted resources https://www.bps.ac.uk/covid-19/resources-and-trusted-information/journals-and-publications

Antibiotic DB

We have continued our collaboration with Prof. Laura Piddock (University of Birmingham) and her team on incorporation of data contained in Antibiotic DB (https://www.antibioticdb.com/) into GtoPdb.

As part of a collaboration with AntibioticDB (https://www.antibioticdb.com/), we have identified and tagged a set of antibiotic ligands in GtoPdb. Where we have identified mappings between these and compounds in the AntibioticDB repository, we've put in place direct links.

Currently we have 303 ligands tagged in GtoPdb as 'antibiotic' and 247 of these have these links to compounds at AntibioticDB. The discrepancy is partly explained by AntibioticDBs focus on novel or development compounds for unmet clinical need, whereas GtoPdb have tried to include all approved antibiotics.



Showing the ligand summary page for arbekcin, with ADB links under the Summary tab, and subsequent landing page for compound 3 (ME1100 (Arbekacin)) at Antibiotic DB. The reciprocal link to GtoPdb is indicated

We are currently working on getting links from AntibioticDB into GtoPdb and expect this to be completed over the next month.

Ligand Download Files

Two new ligand download files are now available from the GtoPdb website: https://www.guidetopharmacology.org/download.jsp

The first, is an SDF (Structured-Data Format) file of all ligands in GtoPdb. SDF is a chemical-data file format developed by MDL. The format wraps individual ligands in molfile format, delineated by the line '$$$$'. The file is quite large, (~40MB) and only contains the structure connection table where we have a curated SMILES for the ligand.

https://www.guidetopharmacology.org/DATA/all_ligands.sdf

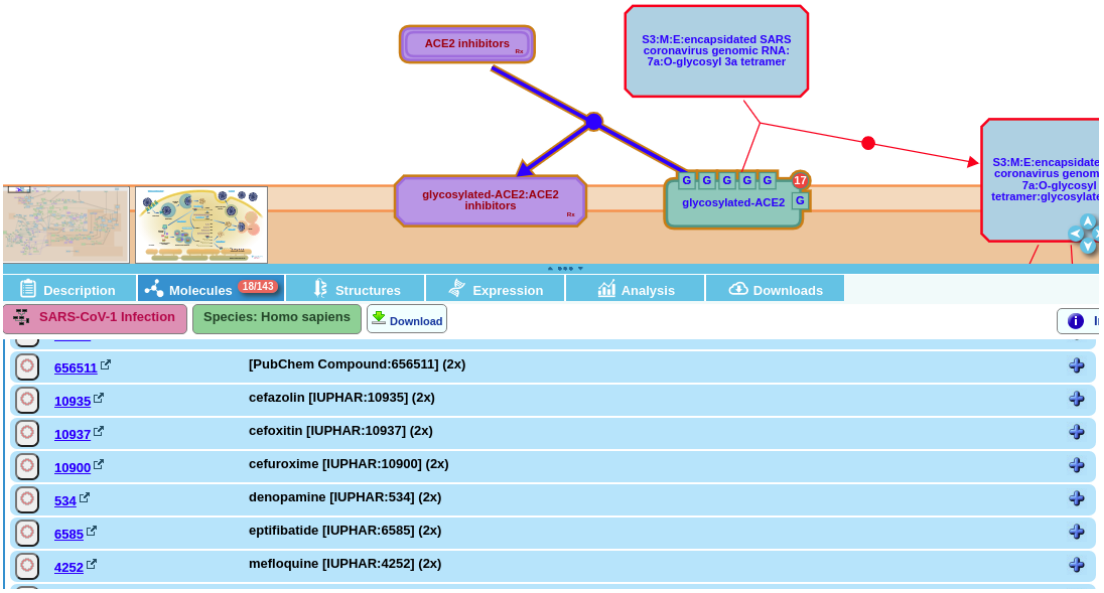
The second file is a Ligand ID Mapping file. This contains GtoPdb ligand IDs mapped to equivalent external resource IDs. The file includes PubChem CID, PubChem SID, ChEMBL, ChEBI, UniProt, IUPAC, INN, CAS, DrugBank and DrugCentral identifiers.

https://www.guidetopharmacology.org/DATA/ligand_id_mapping.csv

Links to Reactome

This collaboration was initiated when we were contacted by Bijay Jassal from Reactome, who inquired about mappings between GtoPdb ligand IDs (identifiers) and equivalent IDs in ChEMBL, ChEBI and DrugBank. Our ligand download file did contain some, but not all of these. We now provide a simple ligand identifier mapping csv file, so users can easily get hold of mapped identifiers from GtoPdb ligands and other resources. This is important in our aim to be FAIR compliant. This work is described in the above, new website features section.

This initial inquiry quickly led to an established strong engagement with Reactome over the last few months. Reactome already curated drugs/chemicals against Pathways and Reactions in their resource. They use GtoPdb identifiers for drugs, and are in the process of using GtoPdb interaction data to further curate drugs against reactions and pathways based on ligand interaction with proteins (UniProt IDs).

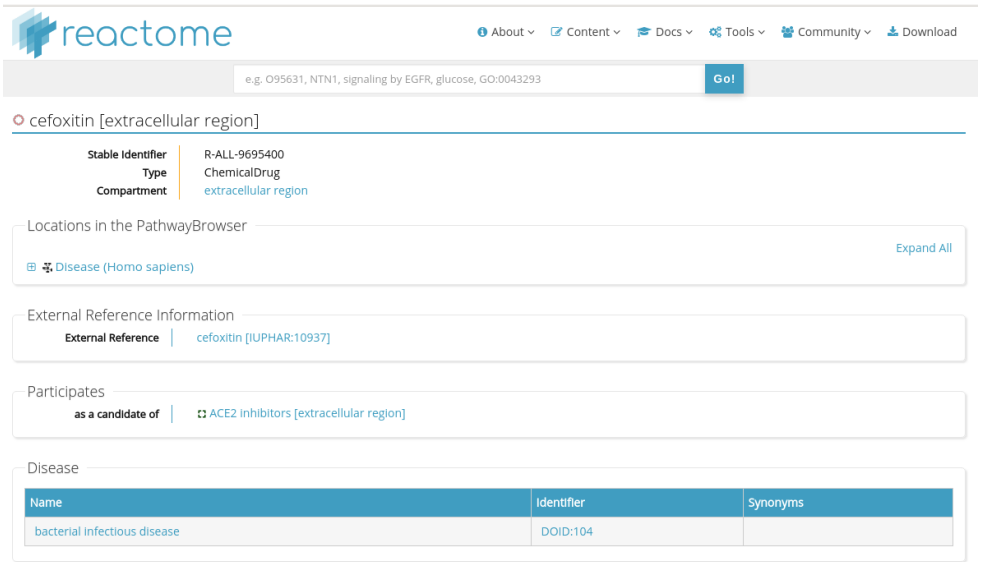


Zoomed in view of glycosylated-ACE2 binds ACE2 inhibitor reaction on Reactome Pathway Browser. The table underneath lists associated molecules (drugs), using IUPHAR (GtoPdb) IDs

Database Links	
Specialist databases	
Reactome Drug	R-ALL-9695400
Reactome Reaction	R-HSA-9695415

Reactome links on cefoxitin ligand summary page

In collaboration with Reactome we have now mapped GtoPdb ligands to appropriate Reactome Drug and Reaction pages. See the example below for the landing page for cefoxitin (GtoPdb: 10937).



Connectivity

PubChem Statistics for GtoPdb, GtoImmuPdb and GtoMPdb

The stats for the 2021.1 release (with 2020.5 in brackets) are as follows (N.B. the links below can be slow but if they do time out try purging your browser cache).

1. Substances (SID) that we submit to PubChem (refreshing previous submissions) are up to 10826 (10585).
2. Those that have defined chemical structures are merged into 8704 (8371) Compound Identifiers, CIDs (i.e. small molecules and peptides below ~ 70 reisdues)
3. From our 8704 CIDs 6901 have vendor matches and 7287 have patent extraction matches
4. The select "IUPHAR/BPS Guide to PHARMACOLOGY"[SourceName] AND gtopdb_approved [Comment] now retrieves 1643 SIDs (1717) which link to 1454 approve drug CIDs
5. Of our SIDs, 1339 (1313) are tagged in GtoImmuPdb and 317 (310) of these are approved drugs
6. Of our CIDs 724 are tagged in GtoImmuPdb
7. Of our SIDs, 106 are tagged in GtoMPdb and 25 of these are approved drugs
8. Of our CIDs 51 are tagged in GtoMPdb
9. We have 2000 (2038) structures that ChEMBL does not have, 6135 not in DrugBank.
10. 312 (189) structures where GtoPdb is unique as the source. In most cases this is because we were first to extract the paper or patent and push the ligand structures into PubChem where they get linked to the PubMed entries (see Link out section below). There may be some cases where our stereo configuration is unique (InChIKey) but related to other entries (InChKey inner layer). Inspection of " Related Compounds" and "Same Connectivity" will indicate this.
11. We continue to curate clinical monoclonal antibodies with the PubChem Substance select "IUPHAR/BPS Guide to PHARMACOLOGY"[SourceName] gtopdb_antibody" returning 303 SIDs. Adding "gtopdb_approved" gives 105.

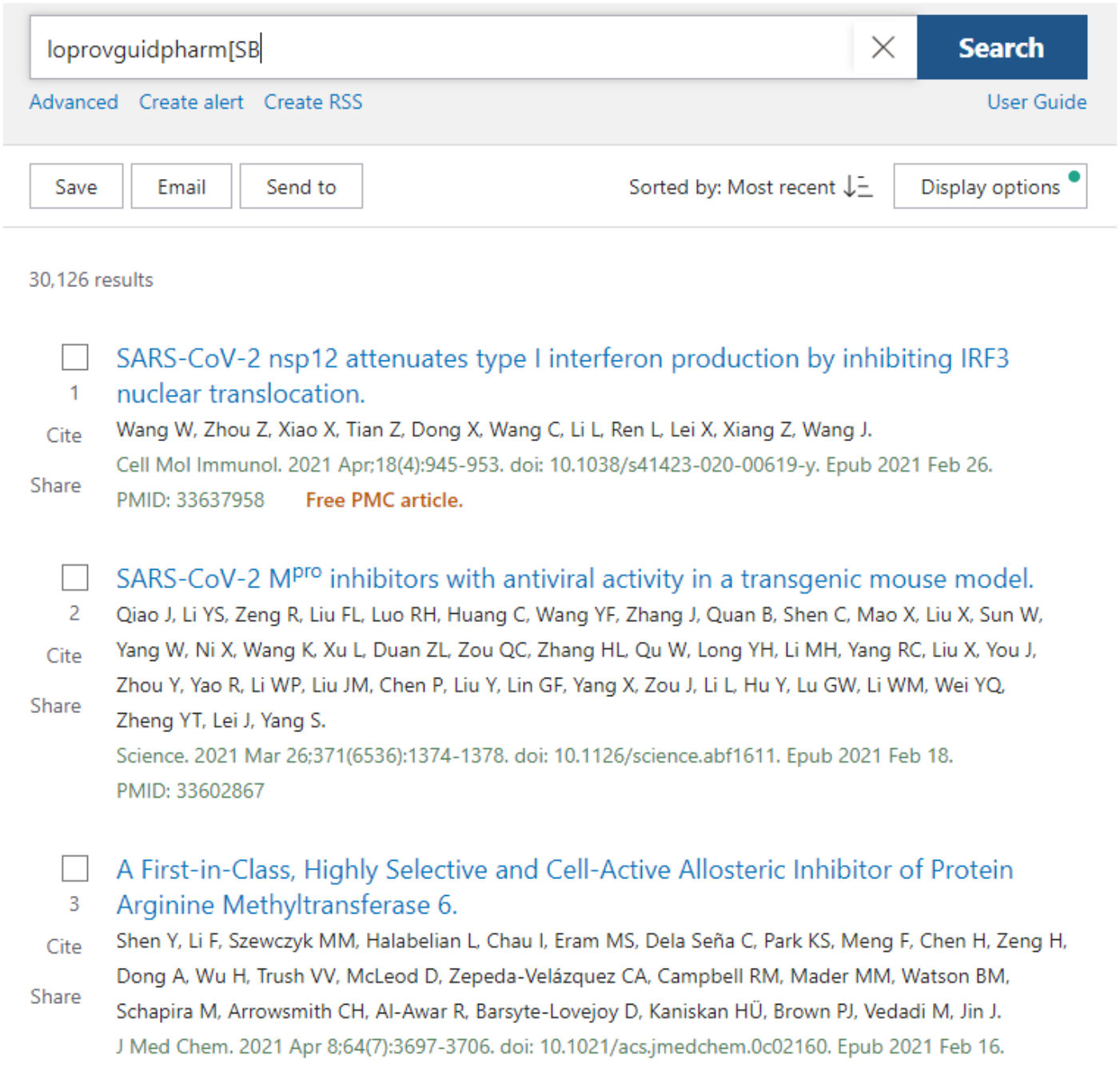
The ability to combine selects and filters of our own PubChem entries, find related linked sets (e.g. pivoting from Substances to Compounds) and compare these to other sources in PubChem becomes very informative and powerful. Users are also reminded that, via the InChIKeys or SMILES strings, any of our ligand downloads (including combinations or parts of) can be cast against PubChem using their Identifier Exchange Service to allow detailed exploration of the extensive PubChem links. Users needing guidance for PubChem interrogations are welcome to contact us.

NCBI LinkOuts

GtoPdb maintains sets of links in the NCBI LinkOut service, to the Protein, Nucleotide, Gene and PubMed databases. Our links are updated frequently.. Below is the count of all NCBI database records that contain 'LinkOuts' to GtoPdb. The PubMed count covers all references in the databases including reviews and additional reading for target families. Note these the LinkOut pointers link users back to the database

Protein	6003
Nucleotide	5950
Gene	8449
PubMed	30,095 (https://pubmed.ncbi.nlm.nih.gov/?term=loprovguidpharm[SB])

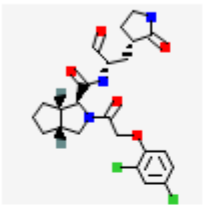
The screenshot shows the most recent of these references



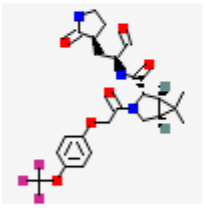
The first reverence is background reading for SARS.Cov-2 but the second has been curated for the most potent ligands against the M-Proteas. The “Related information” section towards the bottom of the PubMed entry (just above “Link Out), includes “PubChem substance” where we can click to see the three GtoPdb ligands below

Links from PubMed

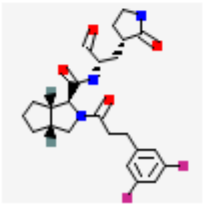
Items: 3

1. 

GTPL11441; MI-30; compound 18p [PMID:33602867] ...
Source: IUPHAR/BPS Guide to PHARMACOLOGY
Deposit Date: 2021-03-19 Available Date: 2021-03-19 Modify Date: 2021-03-19
SID: 440816810 [CID: 155817519]
Summary PubChem Same Compound

2. 

GTPL11440; MI-09; compound 11i [PMID: 33602867] ...
Source: IUPHAR/BPS Guide to PHARMACOLOGY
Deposit Date: 2021-03-19 Available Date: 2021-03-19 Modify Date: 2021-03-19
SID: 440816809 [CID: 155817518]
Summary PubChem Same Compound

3. 

GTPL11432; MI-23; compound 18i [PMID: 33602867]
Source: IUPHAR/BPS Guide to PHARMACOLOGY
Deposit Date: 2021-03-19 Available Date: 2021-03-19 Modify Date: 2021-03-19
SID: 440816801 [CID: 155804440]
Summary PubChem Same Compound

Europe PMC

We also maintain records in the Europe PMC External Links Service. Unlike the larger set of NCBI Outlinks, thes publication links are restricted to papers from which GtoPdb interaction data have been curated. These link targets and/or ligands mentioned in the article back to GtoPdb detailed pages.

As of April 2021 there are 7,359 articles in Europe PMC with links to GtoPdb targets and/or ligands. The EPMC interface query is (LABS_PUBS:"1969")

Full URL: https://europepmc.org/search?query=%28LABS_PUBS%3A%221969%22%29

Bibliometrics and Scholarly Portals

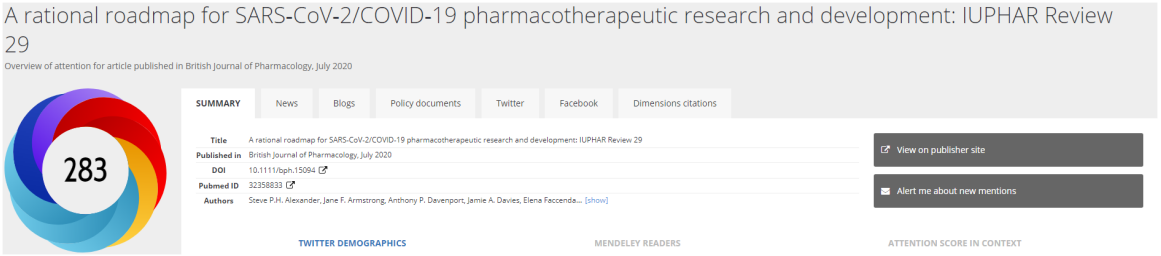
- As outlined in previous reports we track various metrics for the GtoPdb team and NC-IUPHAR affiliated papers in PubMed, PubMed Central , European Pub Med Central (EPMC) Kudos entries and Altmetrics.

- 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, SDH 0000-0002-9262-8318 and JFA 0000-0002-0524-0260.

Below are the (live) April 2021 live bibliometric updates compared to the November 2020 metrics. These are given with EPMC links which have the advantage over PubMed of directly generating a citation ranking for any set (but with lower citation rates than PubMed, Google Scholar or WOS).

- Database team members have 184 cumulative co-authored publications
- The team is on their 7the NAR Database Issue from 2009 to 2020
- IUPHAR reviews in BJP increased by 1 to 31.
- IUPHAR Pharmacological Reviews increased by 2 to 108
- The cumulative BJP "Concise Guide" set now takes us to 33 papers
- 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 2018 entry (PMC5753190) with 1,055 citations (according to EPMC) or 1,134 (according to PubMed). This thus overtakes our 2016 paper (PMC4702778) with 901 (EMPC) or 905 (PubMed) citations, and the 2014 paper (PMC3965070) that reached 688 / 719 .
- The "Concise Guide" citations are currently led by 2017/18 Enzymes (PMC5650666) at 555 followed by 2015/16: Enzymes (PMC4718211) at 510 and 2013/14: G protein-coupled receptors (PMC3892287) at 464.
- While these two papers are not BJP reference citations, we are pleased to note that our 2020 NAR article has already picked up 28 citations. Impressively, no less than seven of these are from the 2021 annual NAR Database edition, confirming increased recognition of GtoPdb in the wider informatics domain. Our BJP SARS-Cov-2 review acquired 16 citations in a similarly short time frame which rises to 46 in Google Scholar.
- The overall citation performance has resulted in team members JLS, EF, AJP, CS and JAD, along with IUPHAR co-authors, SPHA, MS, and APD being listed in both the Clarivate 2019 and 2020 rankings of Highly Cited Researchers.
- The Altmetric rankings for all our OA papers are indexed in ScienceOpen. Top of the list by some margin at 283 is our BJP SARS-Cov-2 review



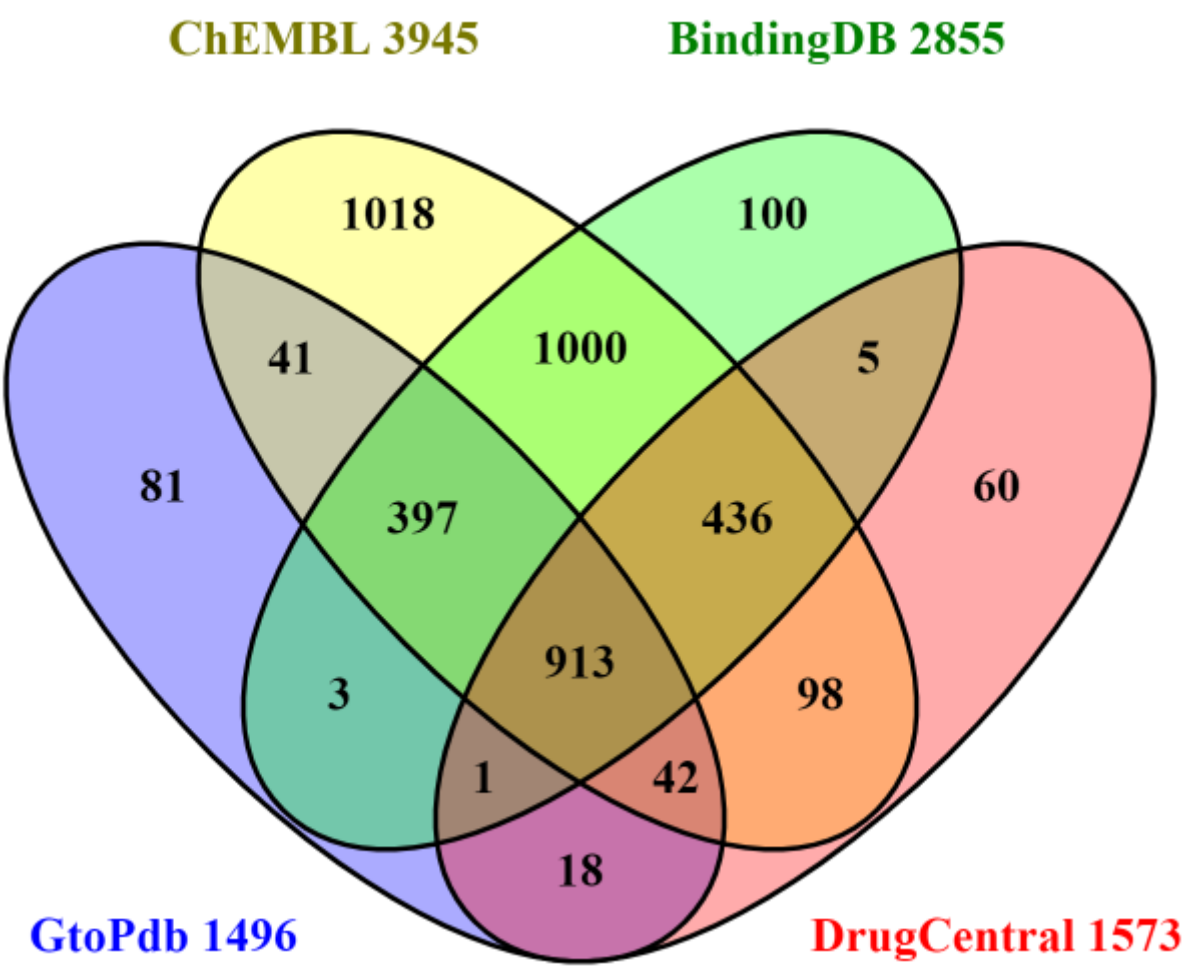
In second place we have The Concise Guide to PHARMACOLOGY 2015/16: Enzymes. The more modest score of 55 still puts this in the top 5% of all research outputs scored by Altmetric (n.b. Altmentric sores are also displayed under the "Citations & impact" tab in EPMC for both open or paywalled articles).

EBI UniProtKB/Swiss-Prot cross-references

Below are the metrics for UniProt 2021_02 chemistry sources. Context for these has been given in previous reports as complementary sources to intersect protein < > chemistry mappings including our own targets where we have curated quantitative ligand interactions of generally < 1uM. Note that SwissLipids is the odd-man-out where the curated chemical interactions are for metabolites rather that activity modulators but nonetheless useful.

Cross-reference
BindingDB BindingDB database of measured binding affinities · UniProtKB (8,247) Category: Chemistry databases
ChEMBL ChEMBL database of bioactive drug-like small molecules · UniProtKB (8,738) Category: Chemistry databases
DrugBank Drug and drug target database · UniProtKB (5,159) Category: Chemistry databases
DrugCentral DrugCentral · UniProtKB (2,783) Category: Chemistry databases
GuidetoPHARMACOLOGY IUPHAR/BPS Guide to PHARMACOLOGY · UniProtKB (2,056) Category: Chemistry databases
SwissLipids SwissLipids knowledge resource for lipid biology · UniProtKB (1,396) Category: Chemistry databases

Even though these sources have slightly different ways of going about their curatorial business it is informative to compare and contrast the four below (omitting DrugBank which has a tendency to over-map) to give both a druggable proteome snapshot and our unique contribution to the aggregate coverage. The Venn diagram for the human Swiss-Prot entries are shown below.



There are interesting aspects of relative coverage that cannot be expanded on here (n.b. individual entries can be followed through to their sources via UniProt). However salient observations include that ~20% of the human proteome (4113 as the OR union of these four divided by the current Swiss-Prot human total of 20,395) has some kind of modulatory ligand (n.b. as discussed in PMID 28529709 the more stringent HGNC protein coding gene total is lower at 19207 that would < coverage but only by ~1%). A second observation is that each source has complementary unique content, including the 81 GtoPdb-only targets. Biases in coverage and extraction strategies that may contribute to the divergences above are of interest but need deeper analysis plus the inspection of unique entries.

ChEMBL

We have updated our pharmacology search and ligand activity charts to use the latest ChEMBL database release - version 28 (released in Jan 2021, updated in GtoPdb in Feb 2021).

HGNC

We continued to use HGNC gene identifiers and names for targets in GtoPdb. In total this covers 3,000 human targets. We also use HGNC nomenclature for updating protein names in some cases.

GPCRdb

372 targets in GtoPdb have links to GPCRdb. https://gpcrdb.org/

DrugCentral and Pharos

We continue to engage with these two resources that are part of the Illuminating the Druggable Genome (IDG) program. We now include links from ligand pages to DrugCentral where we are one of their acknowledged sources and cited in their latest NAR PMID 33151287 . The process for mapping our ligands to their compounds is downloading the structures in SMILES/InChI format from DrugCentral (https://unmtid-shinyapps.net/download/structures.smiles.tsv) and map, via InChI Key to GtoPdb ligands. In our latest release (2021.1) this mapped **1554 GtoPdb ligands to 1498 DrugCentral compounds**. The links to DrugCentral are shown on our ligand summary pages and DrugCentral IDs are included in the new ligand ID mapping file (https://www.guidetopharmacology.org/DATA/ligand_id_mapping.csv). On the protein side the role of Pharos in the IDG is enriching knowledge around human targets and monitoring their therapeutic development levels. We are also a declared source and cited in their recent NAR PMID 33156327. Because Pharos offers a particularly rich set of functional genomic and genetic links for targets we have now added this as one of our protein links.

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” and celebrated its 5th birthday on 1st April 2021.

Financial support is in place for one 0.5 FTE for the next 6 months from IUPHAR.

Site Usage

Google Analytics shows that user sessions continue to average >30K/month.

PEP has >1200 followers of our twitter handle, @PharmacologyEd.

Succession Planning

Dr Clare Guilding (Newcastle University, Vice-Chair of IUPHAR’s Education Section & works with BPS Education and Training Committee) has accepted the role of Deputy Director of PEP, to help take on some of the activities that John Szarek is currently responsible for. Clare will be responsible for regular meetings of the Management Team and quarterly Board meetings. John and Simon Maxwell will continue in their current roles as co-directors, and will work closely with Clare in stewardship of PEP.

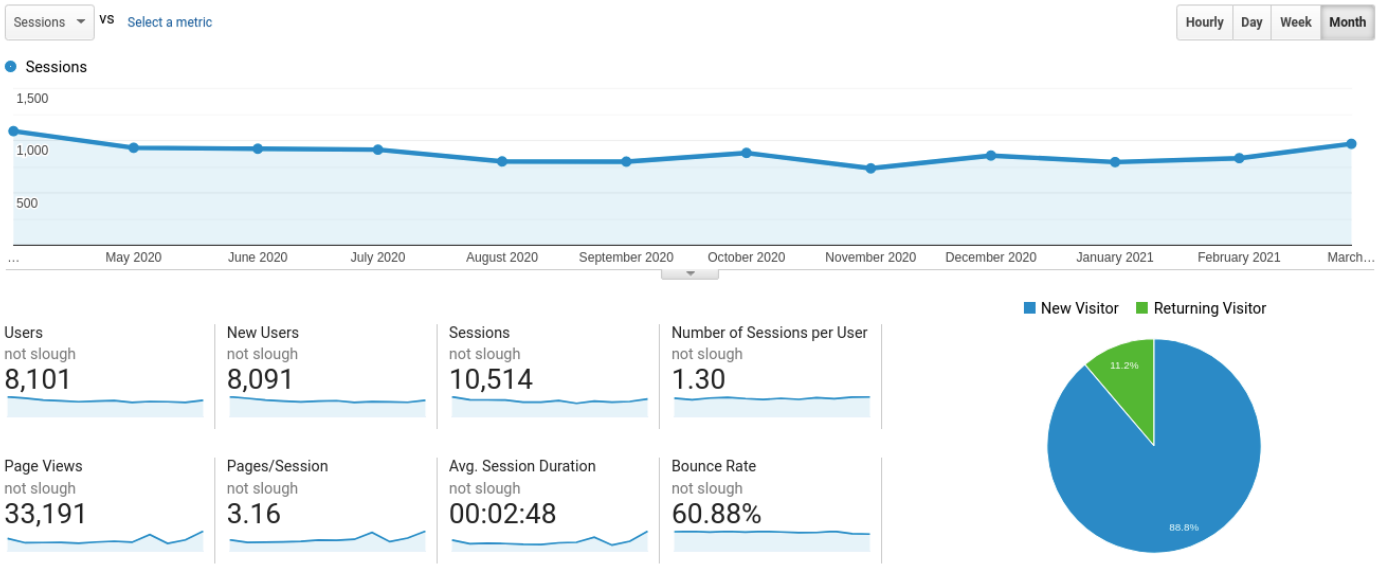
The Guide to Immunopharmacology Database (GtoImmuPdb)

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).

In October 2018, we officially launched the IUPHAR Guide to IMMUNOPHARMACOLOGY, having made the first public release back in June 2018. Technical details on its development and blog posts related to the resource can be found here.

GtoImmuPdb analytics

Our analytics over the last year (April 20 - March 21) shows an average of ~870 sessions per month. Note, this removes a particular set of sessions that were run as part of a site accessibility check.



Access statistics for GtoImmuPdb (April 2020 - March 2021)

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 the 2021.1 release).

Process Category	**GtoPdb Human UniProtKB**	**Target-GO annotations**
Barrier integrity	51	66
Inflammation	677	1544
Antigen presentation	161	247
T cell (activation)	230	535
B cell (activation)	183	320
Immune regulation	554	1429
Tissue repair	27	28
Immune system development	290	554

Cytokine production & signalling	559	1630
Chemotaxis & migration	281	613
Cellular signalling	517	1195

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	58
T cells	CL:0000789 alpha-beta T cell CL:0000815 regulatory T cell CL:0000911 effector T cell	84
Dendritic cells	CL:0000451 dendritic cell	44
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	4
Macrophages & monocytes	CL:0000235 macrophage CL:0000576 monocyte	60
Granulocytes	CL:0000094 granulocyte	48
Natural killer cells	CL:0000623 natural killer cell	30
Mast cells	CL:0000097 mast cell	39
Innate lymphoid cells	CL:0001065 innate lymphoid cell	6
Stromal cells	CL:0000499 stromal cell	1

GtoImmuPdb target and ligand curation stats

- 641 (+10) targets tagged as in GtoImmuPdb:
  - 150 catalytic receptors
  - 214 enzymes
  - 104 gpcrs
  - 40 ion channels
  - 116 other proteins
  - 9 nuclear hormone receptors
  - 10 transporters
- 1337 (+17) ligands tagged as in GtoImmuPdb:
  - 863 synthetic organic
  - 169 antibodies
  - 260 peptides
  - 28 metabolites
  - 16 natural products
  - 1 inorganic
  - 283 Approved drugs

Detailed lists on:

- www.guidetoimmunopharmacology.org/immuno/immunoHelpPage.jsp

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. Although the initial phase of the project has been completed, MMV have provided further funding (0.2 FTE until December 2021) to allow malaria pharmacology content to be maintained and expanded.

IUPHAR/MMV
Guide to MALARIA PHARMACOLOGY

The IUPHAR/MMV Guide to MALARIA PHARMACOLOGY was officially released in September 2019 and the resource is available at www.guidetomalariapharmacology.org. Blog posts related to the resource and technical reports on its development can be found here.

GtoMPdb Target and Ligand Curation

Curation Summary

The number of ligands in the public database with antimalarial activity has continued to increase. The most recent database release (2021.1) contains:

- 105 ligands tagged as in GtoMPdb (selectable in PubChem, see section)

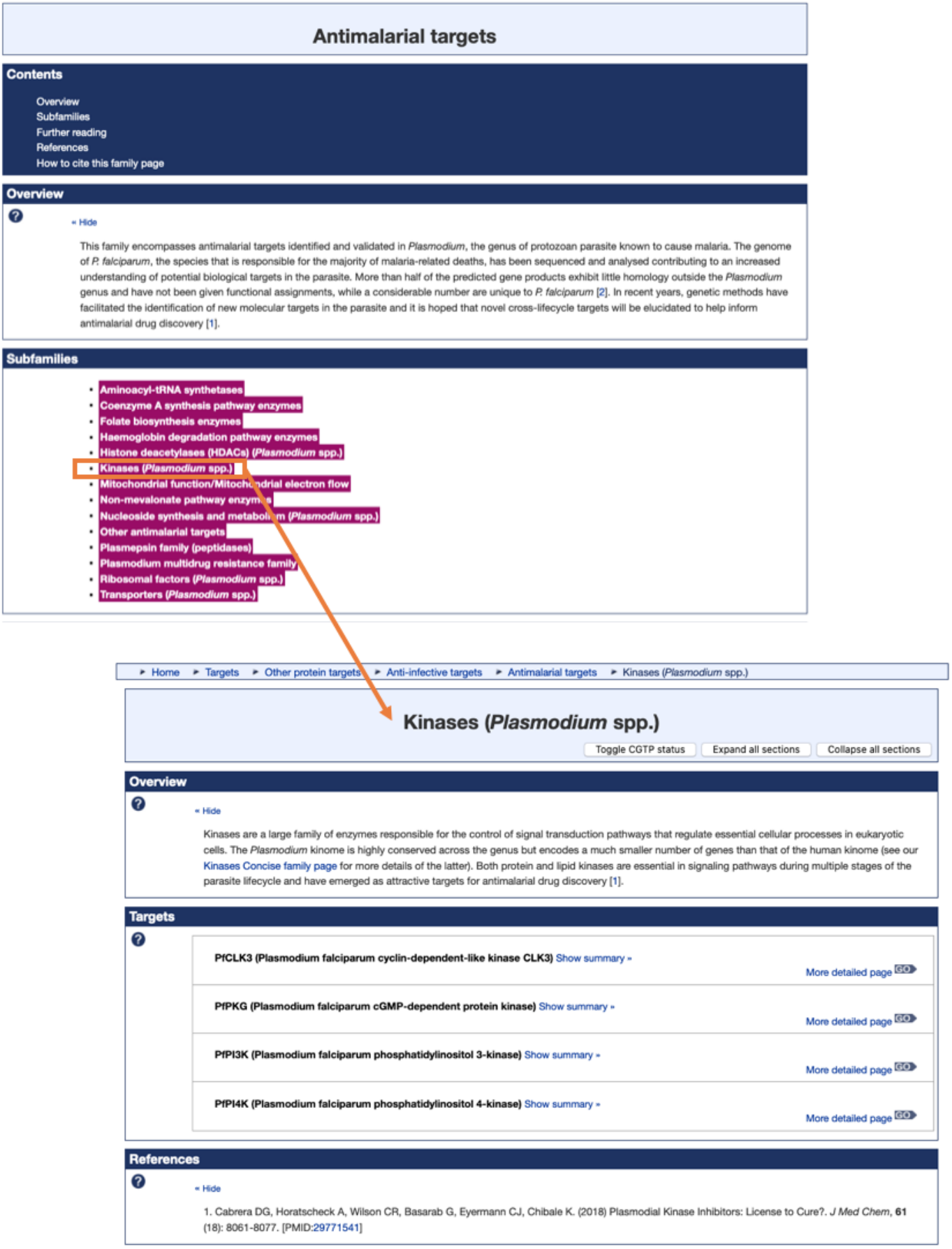
http://www.guidetopharmacology.org/GRAC/FamilyDisplayForward?familyId=999

- 37 targets tagged as in GtoMPdb:

http://www.guidetopharmacology.org/GRAC/FamilyDisplayForward?familyId=970

Target Subfamilies

A major focus of work over the period covered by this report has been the addition of subfamilies to the 'Antimalarial targets' family (see figure below). This new classification is still under review but has allowed additional information to be added as overviews on the subfamily pages. It is hoped that these pages will continue to be developed following feedback from expert contributors.



The ‘Antimalarial targets’ family page now displays a list of subfamilies. These are linked to new pages with the page for ‘Kinases (Plasmodium spp.)’ shown as an example.

GtoMPdb Web Interface and Database Development

The GtoMPdb uses the same underlying database as GtoPdb and in previous reports we have described changes to the database structure and the web interface that were necessary for the capture and presentation of antimalarial data (please see our November 2020 report for a summary). The major part of the required development work was completed prior to the public release of the GtoMPdb but we have continued to implement updates and improvements following user recommendations.

GtoMPdb Page View Analytics

In November 2020 we ran a more detailed analysis of page views for malaria content in GtoMPdb. The figures in the table below are taken from our Google Analytics for the period Nov 19-Nov 20. Much of the malaria content is available when using the guidetopharmacology domain (as well as from guidetomalariapharmacology.org). So the figures are split in the table by domain.

Total shows over 6,000 unique views (~500 per month).

		page views	per month	unique page views	per month
malaria domain	**index**	1628	136	1325	110
	Parasite Lifecycle	715	60	581	48
	Species	64	5	44	4
	about	53	4	44	4
	help	65	5	44	4
gtpdb domain	**Family 970 (antimalarial targets)**	711	59	453	38
	Family 999 (antimalarial ligands)	191	16	100	8
	Targets	911	76	745	62
	Ligands	1943	162	1623	135
	Species	246	21	202	17
	Parasite Lifecycle	991	83	856	71
	Total	**7518**	**627**	**6017**	**501**

General overview of database team activities

GtoPdb Team Interactions

For more details of previous and continuing interactions please see previous reports. Only significant changes since November 2020 are reported below.

ELIXIR

Engagements continue with this important Europe-wide bioinformatics infrastructure initiative. Our involvement with ELIXIR-UK brings closer ties with other key UK bioinformatics resources and facilitates collaboration on the use of standard ontologies and identifiers. This is valuable as we continue seeking to ensure GtoPdb is a FAIR-compliant (Findable, Accessible, Interoperable, Reusable) resource.

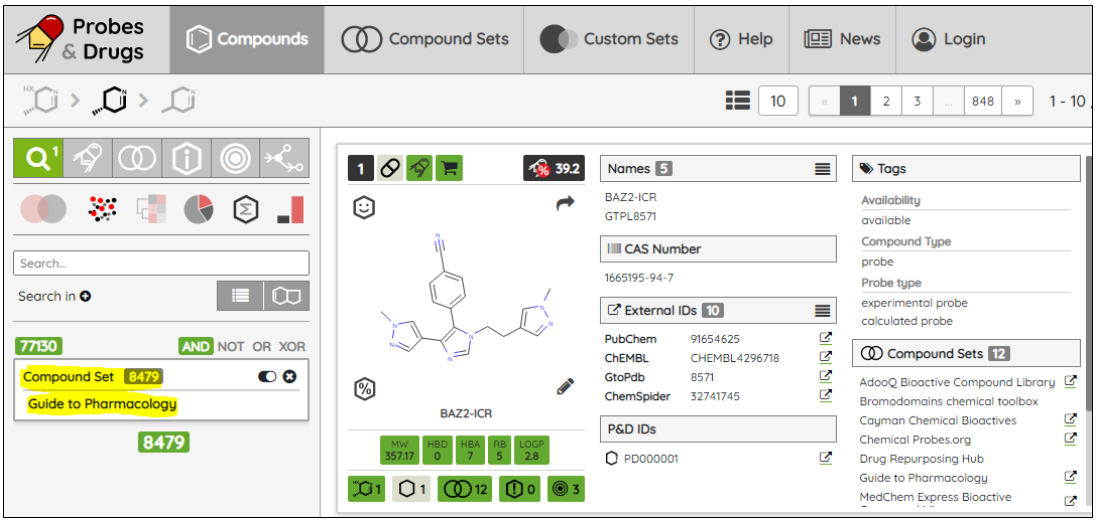
As reported before, we have an entry in the ELIXIR bio-tools directory as one of the official UK ELIXIR Node Services and part of the Excelerate initiative.

Dr. Simon Harding attended the virtual ELIXIR-UK All-Hands Meeting held in December 2020, where he presented an update on the IUPHAR/BPS Guide to Pharmacology (slideshare link).

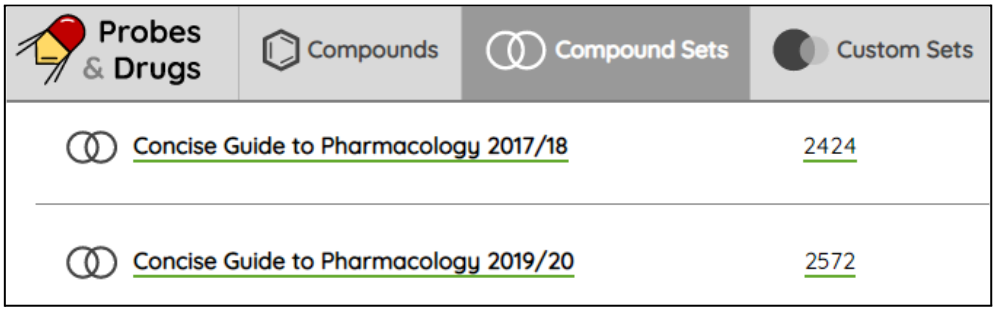
Part of the meeting was given over to contributing to an ELIXIR-UK feasibility study for a new initiative for life science data management and bioinformatics, BioFAIR.

Probes and Drugs

We continue useful interactions with The Probes & Drugs portal (P&D) They have just released a major update with probe scores, redesigned compound details and new compound sets. They are the quickest metasource to pick up the chemistry from each of our releases and provide an independant, very detailed and filterable breakdown of cheminformatic properties and links. The analytics for GtoPdb can be drilled down into from this link (representative screenshot below).



Note also, via scraping the urls, they have indexed two editions of our Concise Guides.



This facilitates metrics that would be difficult to establish from our side. This includes recording an increase of 148 ligands for the newest CG set and that the latter covered ~ 30% of our small-molecule ligand content. P&D have also uniquely downloaded many boutique compound sets (some of which we have recommended) that can be directly compared with GtoPdb and the individual intersections inspected. As examples, we can simply read off the following numbers of compounds-in-common we have with other sources in P&D

1348 from 2503 ChEMBL approved drugs

127 from 481 in BiasDB

204 from 362 in Chemical Probes.org

2531 from 2536 extracted from Concise Guide to Pharmacology 2019/20

76 from 4485 in CovalentDB

23 from 1662 in PROTAC-DB

141 From 299 in the NURSA ligand set

196 from 242 Clinical kinase drugs (PMID: 29191878)

BindingDB

We continue interactions on complementary coverage aspects, including general strategic iteration since Chris Southan is on their SAB. One of these is their extensive and unique curation of SAR data sets from patents. We also do limited curation of patents as bioactivity sources where papers have not yet appeared or will in many cases point to a patent where a lead compound has explicit SAR from exemplified analogue assay data (usually more than the paper). The complementarity is that BindingDB will curate entire patent SAR sets, up to several 100s of compounds. GtoPdb users can exploit this by connecting between us and BindingDB either via the PubChem records (CIDs in-common) and/or via the patent number in PubChem (but note our WO numbers need to be mapped forwards to the later-publishing USPTO numbers). Another important connection is that they recently embarked on the extraction of SAR sets from COVID-19 literature and patents as well as pointing across to us as a source. The advantage for users is that we typically curate one or two leads from a paper on an SARS CoV-2 target (e,g, the M-protease) whereas BindingDB will extract all compound data from the same papers.

PubChem

We continue our important interactions with Evan Bolton, Paul Theissen and other members of the team. The intersection statistics are shown in the section above. Aspects of our PubChem ligand content were outlined in our 2020 NAR paper PMID 31691834 and detailed in previous recent database reports. We were pleased this was cited by the PubChem team in their 2021 NAR contribution PMID 33151290.

Public Engagement and Promotion

BPS Fellowships

We are pleased to highlight and congratulate Prof. Anthony Davenport, Prof. Jamie Davies and Dr. Christopher Southan for their award of British Pharmacological Society Fellowships and Honorary Fellowships in 2020.

Professor Anthony Davenport was awarded an Honorary Fellowship in recognition of sustained excellence and leadership in science, healthcare, and public service.

Professor Jamie Davies and Dr. Christopher Southan were both awarded Fellowships, which are given to members who have demonstrated distinction and peer recognition in pharmacology.

https://www.bps.ac.uk/publishing/blog/november-2020/announcing-our-new-fellows-for-2020

Conferences/meetings (since November 2020 and upcoming)

- ELIXIR-UK All Hands 2020 (e-poster - Simon Harding - Dec 10 2020) https://www.slideshare.net/GuidetoPHARM/guide-to-pharmacology-poster-elixir-all-hands-2020
- BPS Pharmacology 2020 (iPoster 14 Dec- Simon Harding). IUPHAR/BPS Guide to PHARMACOLOGY: Expansion for antimalarials, antibiotics and COVID-19
- BPS Pharmacology 2020 (Oral Communication 15 Dec - Chris Southan). Curating SARS-CoV-2 viral targets for the IUPHAR/BPS Guide to Pharmacology' (Zendo link)
- BPS Pharmacology 2020 (submitted Late Breaking abstract - Chris Southan). SARS-CoV-2/COVID-19 pharmacological roadmap: a strategy for curating and updating drug targets in the Guide to Pharmacology Coronavirus

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

Publications

Published or pre-printed (since early April 2020)

No publications have been made since November 2020. Listed here are our most recent publications, as recorded in our November 2020 report. We are preparing for the next edition (2021/22) of the Concise Guide to Pharmacology and will also be submitting our database update to the NAR database issue later in the year.

- Steve P.H. Alexander Jane F. Armstrong Anthony P. Davenport Jamie A. Davies Elena Faccenda Simon D. Harding Francesca Levi-Schaffer Janet J. Maguire Adam J. Pawson Christopher Southan Michael Spedding. A rational roadmap for SARS-CoV-2/COVID-19 pharmacotherapeutic research and development. Br J Pharmacol. 2020 Nov;177(21):4942-4966. April 13, 2020. DOI: https://doi.org/10.1111/bph.15094. PMID: 32358833.
    - front cover of special joint BJP, BJCP & PR&P virtual issue COVID-19 Research
- Simon Fowler, Simon D. Harding, Joanna Sharman, James Cheney. Cross-tier web programming for curated databases: A case study. International Journal of Digital Curation, 2020 Vol 15 No 1. DOI: https://doi.org/10.2218/ijdc.v15i1.717. https://arxiv.org/abs/2003.03845
- Christopher Southan. Opening up connectivity between documents, structures and bioactivity. Beilstein J Org Chem. 2020 Apr 2;16:596-606. doi: 10.3762/bjoc.16.54. eCollection 2020. Review. PMID: 32280387
- Simon Milling, Michael Spedding & Pasquale Maffia. Guide to Immunopharmacology: a database to boost immunology education, research and therapy. Milling S, Spedding M, Maffia P. Immunology. 2020 May;160(1):1-2. doi: 10.1111/imm.13201. PMID: 32297319
- Ctibor Škuta, Christopher Southan & Petr Bartůněk "Will the chemical probes please stand up?", submitted April 2021 and should appear as a ChemRxiv preprint in May.

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) fostering contacts with our direct collaborators and other followers (including many other databases) 5) establishing reciprocity with key followers and collaborators.

Twitter

@GuidetoPHARM has, as of 31st March 2021, output 2,237 tweets, followers have increased to 4,248, from 3,977 in October 2020. 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.

At each database release, our Twitter announcement usually gathers ~3,000 impressions with an engagement rate ~3%. The most recent release announcement, tweeted on 23 March has gathered ~500 impressions and an engagement rate of 3.7% in one week.

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 are active in promoting the Concise Guide) @BrJPharmacol, @PharmRevJournal, @PRandP_Journal @IUPHAR, @PharmacologyEd @immunopaedia @cdsouthan and @mqzspa (NC-IUPHAR chair).

(NB readers of this document are most welcome to follow @GuidetoPHARM and tre-tweet posts of interest).

LinkedIn

The Curation Team continues to encourage Subcommittee Chairs and collaborators to increase their reciprocal connectivity as individual LinkedIN users. This expands our collective inter-network reach for posting updates, new papers etc. (N.B. interested readers of this report are encouraged to make connection requests from GtoPdb and IUPHAR scientists they know). Our own LinkedIN group page now has 297 followers, up from 2800 in October 2020.

Guide to Pharmacology Blog

Our Edinburgh blog (http://blog.guidetopharmacology.org/) has received ~420 views on average per month since November 2020. This is a reduction from an average in the previous 6 months of ~470 views.

The blog 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

An established and popular feature, our Hot Topics in Pharmacology track and highlight new significant papers in pharmacology and drug discovery. These are communicated to us from Subcommittee members or picked up from Social Media. For a selection we commission concise commentaries from our expert contacts.

Since November 2020 we've added 36 new hot topic articles, which include a commentary by Dr. Chris Southan on "Gene Symbol usage and the need to do better", examining the importance of eliminating equivocality in gene and gene product naming as raised in an opinion paper by in PNAS (Fujiyoshi et al. 2021).

Slides

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 3,993 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.

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.