



IUPHAR/BPS Guide to PHARMACOLOGY

Database Report

April 2024

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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 2023. Previous reports are online for [Nov 2023](#), [Apr 2023](#), [Nov 2022](#), [Apr 2022](#), [Nov 2021](#) and [April 2021](#). 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 by all means enquire).

Zenodo repository of reports:

- November 2023 doi: [10.5281/zenodo.1007801](https://doi.org/10.5281/zenodo.1007801)
- April 2023 doi: [10.5281/zenodo.7915909](https://doi.org/10.5281/zenodo.7915909)
- November 2022 doi: [10.5281/zenodo.7458274](https://doi.org/10.5281/zenodo.7458274)
- April 2022 doi: [10.5281/zenodo.7786340](https://doi.org/10.5281/zenodo.7786340)
- November 2021 doi: [10.5281/zenodo.7786355](https://doi.org/10.5281/zenodo.7786355)

Key Updates / Notifications

- 2 Database release (2023.3, 2024.1)
 - 28 new targets added, 24 with quantitative interactions.
 - 37 human targets with new quantitative interactions (total 1732)
 - 429 new ligands added (41 approved drugs), 231 with quantitative interactions
 - 245 ligands with new quantitative interactions (total 9204)
 - 683 new ligand-target interactions
- [~48,360 Engaged Sessions per month](#)
- [~36,100 Users per month](#)

The Guide to Pharmacology Database (GtoPdb)

GtoPdb Website Analytics

GtoPdb Website Access Statistics

<i>Monthly statistics</i>	Apr 2023 - March 2024 <i>(last report figures)</i>
<i>Engaged Sessions</i>	48,364 (52,014)
<i>Users</i>	36,113 (40,733)
<i>Page views</i>	291,706 (297,514)
<i>Pages / Session</i>	5.09 (4.64)
<i>Avg. Session Duration</i>	00:04:06 (00:03:48)
<i>Views per User</i>	8.08 (7.31)

The above table summarises the access statistics for the Guide to Pharmacology over the last year, comparing against our previous reporting period (Oct 2022 - Sep 2023). Data is generated using Google Analytics GA4.

In total there have been over 3.5 million page views during the last 12 months.

This second table shows the access stats by country (ordered by most engaged sessions). Around 54% of all engaged sessions come from the USA, China, UK and India. Engaged sessions are sessions lasting longer than 10 seconds, or containing 2 or more screen/page views.

Country	Total users	Sessions	↓ Engaged sessions	Engaged sessions per user	Views	Views per session
Totals	433,357	687,109	580,368	1.34	3,500,482	5.09
1 United States	127,952	178,453	152,944	1.2	683,627	3.83
2 United Kingdom	37,612	73,599	63,488	1.69	593,620	8.07
3 India	40,204	56,002	50,507	1.26	220,615	3.94
4 China	31,689	59,284	47,368	1.5	340,622	5.75
5 Germany	11,909	20,652	17,793	1.5	114,873	5.56
6 Japan	11,445	20,196	17,215	1.51	114,832	5.69
7 Australia	10,591	19,689	16,567	1.56	109,534	5.56
8 Canada	10,006	17,788	15,371	1.54	106,877	6.01
9 South Korea	10,376	16,424	14,151	1.36	71,937	4.38
10 France	7,051	11,380	9,746	1.39	71,462	6.28
11 Italy	6,365	10,098	8,712	1.37	57,376	5.68
12 Mexico	4,589	9,683	8,435	1.84	74,251	7.67
13 Spain	5,411	9,304	8,058	1.49	67,138	7.22
14 Brazil	4,926	9,051	7,954	1.62	54,724	6.05
15 Netherlands	5,145	8,354	7,331	1.43	47,791	5.72
16 Russia	4,276	7,138	6,155	1.44	38,708	5.42
17 Philippines	4,902	6,515	5,909	1.21	22,796	3.5
18 Hong Kong	3,161	6,590	5,439	1.74	39,678	6.02
19 Indonesia	4,663	5,855	5,334	1.14	19,793	3.38
20 Denmark	3,204	6,109	5,159	1.61	35,401	5.79

The third table, shown below, shows access stats from countries with a Human Development Index (HDI) of less than 0.8. The Human Development Index (HDI) is a summary measure of average achievement in key dimensions of human development: a long and healthy life, being knowledgeable and having a decent standard of living. The HDI is the geometric mean of normalised indices for each of the three dimensions. Countries with a HDI of 0.8 or above are considered ones with 'very high human development'.

Around 125,000 users for HDI<0.8 countries have accessed GtoPdb, which covers nearly 170,000 engaged sessions. This is about 29% of all sessions. If India and China are excluded it is around 70,000 sessions (~12% of all sessions).

	Total users	Sessions	Engaged sessions	Engaged sessions per user	Views
India	40,204	56,002	50,507	1.26	220,615
China	31,689	59,284	47,368	1.50	340,622
Mexico	4,589	9,683	8,435	1.84	74,251
Brazil	4,926	9,051	7,954	1.62	54,724
Philippines	4,902	6,515	5,909	1.21	22,796
Indonesia	4,663	5,855	5,334	1.14	19,793
Egypt	3,796	4,955	4,624	1.22	17,617
Pakistan	3,423	4,610	4,223	1.23	12,449
Nigeria	3,206	4,021	3,733	1.16	11,810
Iran	2,159	3,065	2,689	1.25	12,790
Colombia	1,495	2,803	2,457	1.64	22,585
Iraq	1,909	2,247	2,111	1.11	6,858
Vietnam	1,673	2,206	1,990	1.19	7,439
Bangladesh	1,487	1,900	1,735	1.17	5,525
South Africa	1,326	1,844	1,667	1.26	7,945
Ukraine	889	1,719	1,495	1.68	9,229
Peru	864	1,668	1,464	1.70	10,536
Jordan	951	1,519	1,410	1.48	7,536
Bulgaria	605	882	807	1.33	6,800
Algeria	611	862	804	1.32	6,165
Ghana	633	746	699	1.11	1,930
Kenya	587	747	684	1.17	2,295
Ethiopia	533	638	577	1.08	1,657
Morocco	319	597	533	1.68	3,630
Sri Lanka	461	540	506	1.10	1,657
Nepal	453	521	487	1.08	1,300
Yemen	416	518	484	1.16	2,243
Total for all HDI <0.8	125,308	193,339	168,228	133.66	924,103

Download Statistics

Previously, when using Google Universal Analytics we had recorded around 4,000 file downloads from GtoPdb between July 2022 and June 2023. We can't do an exact comparison with current data obtained via Google Analytics G4 due to issues with the transition from one method to the other.

However, as the table below shows, monthly file downloads are around the expected level but we don't have full data from before August 2023.

Data for April 2024 to March 2023 shows total file downloads of 4,247 during this period, which compares well against the previous method of tracking.

Year	Apr-Dec 2023	Jan-Mar 2024	Totals
Event name	Event count	Event count	↓ Event count
Totals	2,465 58.0% of total	1,782 42.0% of total	4,247 100.0% of total
1 file_download	2,465	1,782	4,247

GtoPdb Content

These database statistics were compiled on 26th March 2024 from the 2024.1 release. All database statistics can be found at <https://www.guidetopharmacology.org/databaseContent.jsp>.

Targets	Number of (Human) UniProt IDs
7TM receptors	399
Nuclear hormone receptors	48
Catalytic receptors	253
Ligand-gated ion channels	81
Voltage-gated ion channels	144
Other ion channels	53
Enzymes	1301
Transporters	555
Other protein targets	233
Human targets with ligand interactions	1984
Human targets with quantitative ligand interactions	1732
Human targets with approved drug interactions	743
Human Primary Targets with approved drug interactions	350
Total number of targets	3067

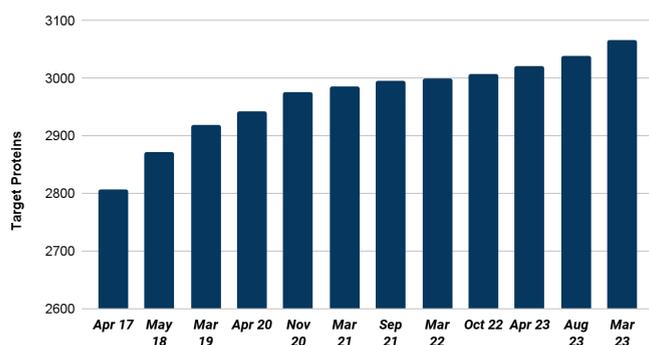
Ligands	Number of Ligands
Synthetic organics	8916
Metabolites	514
Endogenous peptides	817
Other peptides including synthetic peptides	1512
Natural products	416

Antibodies	376
Inorganics	39
Approved drugs	1981
Withdrawn drugs	109
Drugs with INNs	3446
Labelled ligands	649
Unique PubChem CIDs	10437
Ligands with target interactions	10405
Ligands with quantitative interactions (approved drugs)	9204 (1128)
Ligands with clinical use summaries (approved drugs)	3704 (1971)
Total number of ligands (PubChem SIDs)	12590
Number of binding constants curated from the literature	20,789

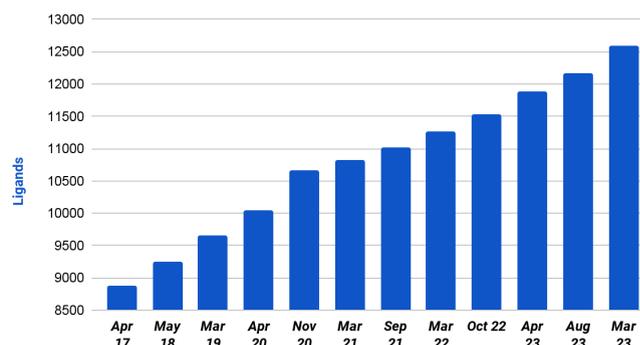
GtoPdb Entity Growth

Growth rates over the span of the previous Wellcome Trust grant are documented in earlier reports and our [2016](#), [2018](#), [2020](#), [2022](#) and [2024](#) 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.

Target Proteins in GtoPdb



Ligands in GtoPdb



	Mar 19	Apr 20	Nov 20	Mar 21	Sep 21	Mar 22	Oct 22	Apr 23	Aug 23	Mar 23
Target protein IDs	2920	2943	2976	2985	2995	3000	3007	3021	3039	3067
Ligands total	9662	10053	10659	10821	11025	11271	11532	11893	12164	12590
Approved drugs	1421	1471	1614	1643	1689	1734	1787	1865	1919	1981
PubChem CIDs	7407	7483	7994	8102	8262	8462	8633	9307	9852	10437

GtoPdb Updates

Targets

New protein targets:

We have curated 40 new protein targets since the last release of 2023. The top 24 in the table below were included in release 2024.1, with the remaining 14 added subsequently and pending release.

TID	Family	Gene	Name	Comment
3248	Lipid transfer/lipopolysaccharide binding proteins	CETP	cholesteryl ester transfer protein	atherosclerosis/dyslipidemia target- 6 sm inhibitors curated
3249	Carnitine palmitoyltransferases	CPT1A	carnitine palmitoyltransferase 1A	mitochondrial fatty acid β -oxidation; oncology target- 2 sm inhibitors curated
3250	Carnitine palmitoyltransferases	CPT1B	carnitine palmitoyltransferase 1B	mitochondrial fatty acid β -oxidation; oncology target- 1 sm inhibitors curated
3251	Carnitine palmitoyltransferases	CPT1C	carnitine palmitoyltransferase 1C	mitochondrial fatty acid β -oxidation; oncology target

3252	Carnitine palmitoyltransferases	CPT2	carnitine palmitoyltransferase 2	mitochondrial fatty acid β -oxidation; oncology target- 2 sm inhibitors curated
3253	Hydrolases & Lipases	PNPLA2	patatin like phospholipase domain containing 2	potential antiviral target- 1 sm inhibitor curated
3254	E3 ubiquitin ligase components	ZBTB25	zinc finger and BTB domain containing 25	E3 ligase activity is directly involved in ubiquitination of SARS-CoV-2 Mpro (main protease) leading to its degradation
3255	Protein tyrosine phosphatases non-receptor type (PTPN)	PTPN2	protein tyrosine phosphatase non-receptor type 2	oncology target- inhibition of PTPN1/2 promotes anti-tumour immunity- one sm inhibitor curated
3256	Diacylglycerol kinases	DGKA	diacylglycerol kinase alpha	2 sm inhibitors curated- potential to promote anti-tumour immunity
3257	Diacylglycerol kinases	GGKZ	diacylglycerol kinase zeta	one of the above inhibitors is a dual alpha/zeta inhibitor
3258	Hydrolases & Lipases	NEU2	neuraminidase 2	2 experimental sm inhibitors curated
3259	3.6.4.12 RecQ helicases family	WRN	WRN RecQ like helicase	WRN deficiency>Werner syndrome (a premature ageing disorder); oncology target, inhibition is synthetically lethal in cancers with microsatellite instability, 4 sm inhibitors curated in clinical candidate HRO761
3260	3.6.4.12 RecQ helicases family	BLM	BLM RecQ like helicase	BLM deficiency>Bloom syndrome- one sm NAM curated

3261	Coronavirus (CoV) proteins	ORF1ab	CoV Non-structural protein 13	helicase unwinding activity, crucial for viral replication- antiviral target 2 inhibitors & one NAM curated
3262	E3 ubiquitin ligase components	KLHDC2	kelch domain containing 2	tractable ubiquitin E3 ligase for PROTAC design and development- one PROTAC that binds KLHDC2 to engage the E3 ligase is curated
3263	Protein phosphatase catalytic subunits	PPP2CA	protein phosphatase 2 catalytic subunit alpha	Molecular target of natural marine toxins (okadaic acid, microcystin-LR, calyculin A)
3264	Protein phosphatase catalytic subunits	PPP1CA	protein phosphatase 1 catalytic subunit alpha	Molecular target of natural marine toxins (okadaic acid, microcystin-LR, calyculin A)
3265	SIGLECs (conserved)	SIGLEC15	sialic acid binding Ig like lectin 15	Anti-SIGLEC15 mAb demonstrated experimental anti-tumour potential
3266	Mono-ADP-ribosylating PARPs	TIPARP	TCDD inducible poly(ADP-ribose) polymerase	Inhibitors are proposed to promote immunomodulatory and antineoplastic actions (atamparib, (S)-XY-05)
3267	Mono-ADP-ribosylating PARPs	PARP10	poly(ADP-ribose) polymerase family member 10	Dual PARP10/PARP15 inhibition might be beneficial in cancer treatment (see compound 8a [PMID: 35500474])
3268	Mono-ADP-ribosylating PARPs	PARP11	poly(ADP-ribose) polymerase family member 11	The PARP11 inhibitor ITK7 is curated
3269	Mono-ADP-ribosylating PARPs	PARP14	poly(ADP-ribose) polymerase family member 14	Involved in the immune response and lymphocyte physiology; highly expressed in aggressive B cell lymphoma. RBN012759 used to

				explore anti-tumour potential of PARP14 inhibition.
3270	Mono-ADP-ribosylating PARPs	PARP15	poly(ADP-ribose) polymerase family member 15	Dual PARP10/PARP15 inhibition might be beneficial in cancer treatment (see compound 8a [PMID: 35500474])
3271	2.3.1.- Acyltransferases	ZDHHC3	zinc finger DHHC-type palmitoyltransferase 3	benzosceptrin C promotes T cell-mediated anti-tumour effect in vitro and in vivo; proposed as an alternative to anti-PD-L1 or anti-PD-1 immunotherapies
3272	S1: Chymotrypsin	CTRB1	chymotrypsinogen B1	Experimental inhibitor beta ph61 is curated
3273	AAA ATPases	CLPP	caseinolytic mitochondrial matrix peptidase proteolytic subunit	Validated target for the development of anti-tumour drugs; activator compound 16z [PMID: 35609303] and PAM ONC201 curated
3274	Methyllysine reader proteins	SPIN1	spindlin 1	anti-cancer drug development target-two inhibitor probes curated
3275	Coronavirus (CoV) proteins	ORF1ab	CoV Non-structural protein 10	nsp10/16 forms CoV 2'-O-methyltransferase (mRNA capping enzyme)- sinefungin inhibits enzyme function in vitro
3276	Coronavirus (CoV) proteins	ORF1ab	CoV Non-structural protein 16	nsp10/16 forms CoV 2'-O-methyltransferase (mRNA capping enzyme)- sinefungin inhibits enzyme function in vitro
3277	Coronavirus (CoV) proteins	ORF1ab	CoV 2'-O-methyltransferase (nsp10/16 complex)	sinefungin inhibits enzyme function in vitro

3278	Gasdermins (GSDM)	GSDMD	gasdermin D	All components of the NLRP3/caspase-1/GSDMD signalling pathway are targets for the development of drugs with anti-inflammatory potential- disulfiram and LDC7559 curated as experimental inhibitors
3279	High Mobility Group (HMG) proteins	HMGB1	high mobility group box 1	nuclear non-histone protein- anti-inflammatory potential- methotrexate and 3-AESA binding curated
3280	NF-kappa B TF proteins	RELA	RELA proto-oncogene, NF-kB subunit	inhibitors predicted to have anti-inflammatory or anti-cancer effects. Two inhibitors curated: one natural product that inhibits RelA nuclear translocation and a selective synthetic sm that inhibits RelA-DNA binding are curated
3281	NF-kappa B TF proteins	NFKB1	nuclear factor kappa B subunit 1	
3282	NF-kappa B TF proteins	NFKB2	nuclear factor kappa B subunit 2	
3283	NF-kappa B TF proteins	REL	REL proto-oncogene, NF-kB subunit	
3284	NF-kappa B TF proteins	RELB	RELB proto-oncogene, NF-kB subunit	
3285	Synuclein proteins	SNCA	synuclein alpha	target of mAbs as disease modifying PD therapeutics
3286	Synuclein proteins	SNCB	synuclein beta	

3287	Synuclein proteins	SNCG	synuclein gamma	
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Detailed page updates:

The Adrenoceptor family has been majorly updated by Roger Summers, Martin Michel and Jillian Baker. There is a brand new Detailed introduction, plus much more depth added to the ligand tables, physiological functions, tissue expression, functional assays sections etc.

Steve has recruited Nuria Casals and Rosalia Rodriguez to help with more detailed curation for the **Carnitine palmitoyltransferases family**.

Ligands

Curation of new ligands is generally guided by the target family subcommittees as part of routine update processes. Where targets don't have a formal GtoPdb subcommittee, curators are able to independently add ligands when pharmacological relevance is demonstrated. Caveat: new ligands will only be added to GtoPdb when the curators can confirm name-to-structure associations, find citable evidence that confirms MMOA and a source of quantitative interaction data.

Additional ligand sources include the medicinal chemistry literature, INN lists from the WHO, DrugHunter (<https://drughunter.com/>), first disclosures from scientific meetings (such as AACR and ACS) and patents. New ligands (and less frequently, targets) are also added on request by BJP/BJCP authors as part of the journal submission process, so that hyperlinks to the GtoPdb can be included in the published articles. The requests are vetted by the senior curator to ensure relevance before the decision is made to include in the GtoPdb (or not).

Release of the newest proposed INN list (PL130) in February provided the opportunity to curate new nominally clinically-relevant entities. There were 414 INNs in this list. So far we have curated 27 kinase inhibitors from PL130, and where possible we have endeavoured to match the INNs to research codes in disclosed clinical pipelines, primary literature sources and clinical trials. We hope that this depth of curation provides additional insight and information for users of the Guide. Sometimes the INNs match ligand structures that we have previously curated from other sources. Of note in PL130 was the inclusion of INNs for PROTAC type degrader molecules (zomiradomide, lirodegimod), and a kallikrein B1 gene editing agent (lonvoguran), both of which are relatively new classes of clinical interventions. We will continue to analyse this list to see if we can identify either new drug targets, or new pharmacological modalities for existing targets.

A few ligand highlights for this report:

- 6 new ligands targeting CoV proteins were added including novel tool cpds for the nsp10/16 2'-O-methyltransferase complex, nsp13 helicase, and Mac1 domain of nsp3 (which also encodes the papain-like protease)
- 9/11 of the drugs that have been approved by the FDA in 2024 are curated in the GtoPdb. The two absentees do not meet our inclusion criteria (one for a non-bacterial pathogen, and another botulinum toxin analogue for cosmetic use).
- Added two anti-alpha-synuclein mAbs (and see above for the synuclein proteins) to capture what's progressing positively in the Parkinson's disease field. Also updated a couple of the GLP-1 agonist pages with details about their potential efficacy in early clinical trials.

- There are now 111 molecules in the GtoPdb ‘PROTACs, molecular glues and other degraders’ ligand family <https://www.guidetopharmacology.org/GRAC/FamilyDisplayForward?familyId=1030>, with >10 PROTACS in early stage clinical trials. Several of the thalidomide analogue ‘glues’ are already approved immunomodulatory drugs. The majority of the PROTACs in CT are intended for use in cancer indications, and targets include the estrogen (ER) and androgen (AR) receptors, BRD9, BCL-XL, BTK and mutant BRAF. One clinical stage PROTAC with anti-inflammatory potential is designed to degrade IRAK4. Three of the chemical structures for clinical candidate PROTACs have been matched to INNs; zomiradomide (KT-413) degrades IRAK4, Ikaros and Aiolos, bavdegalutamide (ARV110) degrades the AR and vepdegrestrant (ARV471) targets the ER.

Summary of ligands added to GtoPdb in 2024.1 release (compared to 2023.2)

	New Ligands	Updated Ligands	Total Ligands (2024.1)	Total Ligands (2023.2)
Approved Drugs	41	22	1981	1918
WHO Essential Medicines	3	4	305	298
Ligands with Quantitative Interaction Data	231	14	9204	8959
Antibacterials	64	2	537	471
All Ligands	429	-	12590	12163

We also track the comment fields in GtoPdb to see which comments have been applied to new ligands, but also any updates to comments for existing ligands. Nearly all new ligands will have a general comment added.

Comment Type	New Ligands	Updated Ligands
General	429	126
Clinical Use	200	100
Bioactivity	235	22
MOA	14	1

Natural products project with SIF

This project began at the end of 2023, with SIF providing funding via IUPHAR that supports 0.4 FTE for a curator for 3 years. Our main liaison contact is Francesco Visoli, and he has just submitted a short editorial position piece to the BJP which outlines best-practice in NP research.

The first curation task was to review all of the ligands that were selected as ‘natural product’ in the GtoPdb dataset, and to rationalise which were truly NPs. A few were either semi-synthetic analogues or derivatives, so these were removed from the NP ligands set. The heading descriptor on the NPs page of the website

<https://www.guidetopharmacology.org/GRAC/LigandListForward?type=Natural-product> will be amended so that 'synthetic derivatives' is no longer included.

Many of the existing NP pages have been updated either with general comments, or information and references to targets, and interaction data where available.

Going forwards new ligands that meet the GtoPdb inclusion criteria will be added, with regular updates provided to SIF via Francesco.

Since January >40 new NPs have been added. These have been screened from primary med chem literature, natural product-specific journals and sources such as this 2024 review of GPCR-targeting NPs

> [Mol Pharmacol](#). 2024 Mar 8;MOLPHARM-MR-2023-000854. doi: 10.1124/molpharm.123.000854.
Online ahead of print.

2023 Julius Axelrod Symposium: Plant-derived molecules acting on GPCRs

Nedjma Labani ¹, Florence Gbahou ², Shuangyu Lian ², Jianfeng Liu ³, Ralf Jockers ⁴

Affiliations + expand

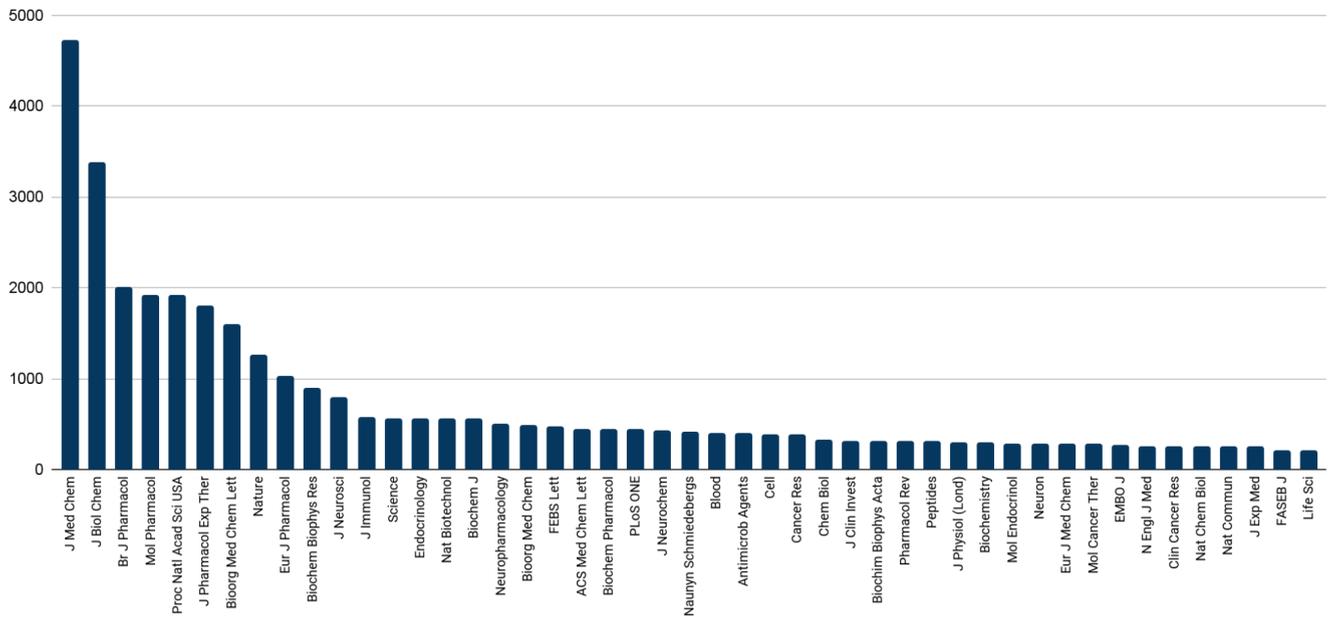
PMID: 38458772 DOI: [10.1124/molpharm.123.000854](https://doi.org/10.1124/molpharm.123.000854)

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	4733
J Biol Chem	3384
Br J Pharmacol	2008
Mol Pharmacol	1927
Proc Natl Acad Sci USA	1924
J Pharmacol Exp Ther	1799
Bioorg Med Chem Lett	1608
Nature	1265
Eur J Pharmacol	1032
Biochem Biophys Res Commun	899
J Neurosci	795
J Immunol	573

Science	563
Endocrinology	562
Nat Biotechnol	558
Biochem J	558



We have collaborated with Antibiotic DB (ADB; www.antibioticdb.com) since 2019, with the aim of extending the coverage of antibacterial compounds in GtoPdb and providing comprehensive chemistry and pharmacology for select antibacterials curated within ADB. This collaboration is supported by the Global Antibiotic Research and Development Partnership (GARDP; <https://gardp.org/>), with funding in place until March 2025. This includes continued financial support for a curator (with an increase from 0.2FTE to 0.3FTE) and additional funding for a software developer (0.5FTE), who is working on developing a 'Guide to ANTIMICROBIAL PHARMACOLOGY' portal to GtoPdb and the new ADB database and website (please see the section on [GtoPdb Web-Application Developments](#) for further details of this work).

Currently we have **537 ligands** tagged in GtoPdb as 'antibacterial' and **512** of these have links to compounds at ADB. The antibacterials in the GtoPdb include approved drugs, WHO essential Medicines-listed medicines, drugs in clinical development, and a number of investigational and experimental compounds. The focus of recent work has been the curation of antibacterial agents included in the WHO's report "2021 Antibacterial agents in clinical and preclinical development: an overview and analysis" (<https://www.who.int/publications/i/item/9789240047655>).

For further information about our work with ADB please refer to previous [Database Reports](#). This collaboration has also been described in more detail in our 2022 NAR update:

Harding SD, Armstrong JF, Faccenda E, Southan C, Alexander SPH, Davenport AP, Pawson AJ, Spedding M, Davies JA; NC-IUPHAR. The IUPHAR/BPS Guide to PHARMACOLOGY in 2022: curating pharmacology for COVID-19, malaria and antibacterials. *Nucleic Acids Research*, Volume 50, Issue D1, 7 January 2022, Pages D1282–D1294, <https://doi.org/10.1093/nar/gkab1010>. PMID: [34718737](https://pubmed.ncbi.nlm.nih.gov/34718737/).

Web-Application Updates

We have updated the [ligand substructure search](#) to fix an issue with searches returning no results when explicit hydrogen atoms are included in the query structure. The search also now opens a new tab for the results so that the original search tab with the query structure remains open and editable to support easier refinement by users of their query.

Our [web services](#) have been updated:

- Antibacterial tag is now include as filter for ligands
- Interaction JSON extended to include target names, ligand names and selectivity
- JSON file description updated to reflect these changes

We have added more download files to the [downloads page](#).

- A new approved drugs files that contain all approved drugs and their targets - including genes names, Entrez IDs and Ensembl identifiers.
- A new set of interaction downloads split by target class

We have also added a new [database content page](#) to house the summary tables of database content (moved from our about page).

AntibioticDB Collaboration

In our collaboration with AntibioticDB/GARDP we have been developing a new AntibioticDB website which is being hosted and maintained at the University of Edinburgh. The current status is as follows: The three main aspects we are currently working on are

- A PostgreSQL database is now set-up to store AntibioticDB data
- Script to load newly curated data from spreadsheet to PostgreSQL
- Java tool built to edit/curate data in the new database
- New website is now available internally (beta 2) to access the new database and present the data. This follows a similar style to the existing AntibioticDB website (<https://antibioticdb.com/>)

We have also begun to develop a new portal at the Guide to Pharmacology, similar to those created for the Guide to Malaria Pharmacology and Guide to Immunopharmacology. This will aim to provide optimised access to antibacterial and more broadly antimicrobial pharmacology data in the database.

Connectivity

Links to other resources

GtoPdb has built many collaborative connections with other resources, many of which are reciprocal. The table below shows the number of ligands and targets with out-links to each of the named resources. The table is not exhaustive, but shows those specialist resources we link with and resources that have reciprocal links back into GtoPdb.

Given we submit our ligand data to PubChem, all ligands with structural data linked to PubChem have out-links. Our recent and ongoing work with AntibioticDB has built links between antibacterials in GtoPdb (455) and AntibioticDB (<https://antibioticdb.com/>). Links from antibodies in GtoPdb are made to the IMGT/mAb-DB (<https://www.imgt.org/mAb-DB/>) database. We also link out to Wikipedia pages that describe ligands - often there are reciprocal links from these Wikipedia pages back to GtoPdb via the main 'chemical infoboxes'.

For our targets, we use UniProtKB identifiers as our primary protein identifier. We use HGNC IDs to provide the primary human gene identifier for our targets. We also provide links to NCBI and Ensembl Gene resources. Specialist resources include GPCRdb (<https://gpcrdb.org/>), who we have a longstanding collaboration with, linking with GPCR targets. For transporter targets, we have links with Resolute and SLC tables at Bioparadigms.

We ensure that the cross-links are regularly refreshed through formal and informal contacts with database providers.

Site	Ligand Links	Site	Target Links
PubChem	10396	GPCRdb	372
ChEMBL	6688	ChEMBL	2256
Reactome	322	Resolute (SLC)	421
AntibioticDB	512	BioParadigms (SLC)	387
IMGT/mAb-DB	352	HGNC	3084
DrugCentral	1709	NCBI (Entrez) Gene	3063
Wikipedia	3031	Ensembl Gene	3087
GPCRdb	4246	UniProt	3149

Pubchem Connectivity

All GtoPdb ligands are submitted to PubChem after each database release, this gives them a PubChem Substance ID (SID).

PubChem Substances are community-provided compounds, and many entries may exist for the same molecule. Each may contain different information about the molecule, depending on the information

provided by the submitter. PubChem extracts the unique chemical structures from Substance records (standardisation) and stores them as PubChem Compounds. This means that substance records from different data sources about the same molecule are aggregated in a common Compound record in PubChem.

Following our last database release, 2024.1, all [12,590](#) ligands in GtoPdb have been submitted to PubChem and therefore have PubChem SIDs.

Our PubChem connectivity is enhanced by the addition of curatorial (depositor) comments that we provide when submitting compounds. These depositor comments can be viewed on a substance page at PubChem (see example for azithromycin below). We include ligand general comments, clinical use comments and flagged whether the compound is an approved drug and whether it is tagged as relevant to immunopharmacology, antimalarial pharmacology or antibacterial.

3 Depositor Comments



IUPHAR/BPS Guide to Pharmacology (GtoPdb) Comment: Azithromycin is a macrolide antibacterial with broad-spectrum activity against Gram-positive and atypical bacteria. The compound also has antimalarial activity. Azithromycin is one of the watch group antibacterials in the the World Health Organization's Model List of Essential Medicines (link provided in the Classification table below). The Malaria tab on this ligand page provides additional curator comments of relevance to the Guide to MALARIA PHARMACOLOGY.

gtopdb_approved - Substance is an approved drug in GtoPdb.

gtopdb_who - Substance is included in WHO Essential Medicines List.

gtopdb_antibacterial - Substance is tagged as an antibacterial in GtoPdb.

Clinical use: Azithromycin is approved for use in both the US and the UK. It is also available in other countries under various trade names, click here to link to Drugs.com's list of internationally marketed azithromycin drugs.

gtopdb_immuno - Substance is curated in IUPHAR Guide to Immunopharmacology (GtoImmuPdb).

GtoImmuPdb Comment: Azithromycin alleviates the severity of rheumatoid arthritis by antagonising the unfolded protein response component of heat shock protein family A (Hsp70) member 5 (HSPA5; a.k.a. glucose-regulated protein 78/GRP78) [PMID:34664264]. Direct binding of azithromycin to HSPA5 was suggested by a drug affinity responsive target stability (DARTS) screening assay, and was confirmed by cellular thermal shift assay. Azithromycin competes with ATP for binding to the ATPase active site of HSPA5.

gtopdb_malaria - Substance is curated in IUPHAR/MMV Guide to Malaria Pharmacology (GtoMPdb).

GtoMPdb Comments: Azithromycin alleviates the severity of rheumatoid arthritis by antagonising the unfolded protein response component of heat shock protein family A (Hsp70) member 5 (HSPA5; a.k.a. glucose-regulated protein 78/GRP78) [PMID:34664264]. Direct binding of azithromycin to HSPA5 was suggested by a drug affinity responsive target stability (DARTS) screening assay, and was confirmed by cellular thermal shift assay. Azithromycin competes with ATP for binding to the ATPase active site of HSPA5.

Depositor comments section of PubChem SID [178103124](#).

Our blog post from December 2022 illustrates [how users can exploit these tags](#) when using PubChem. This was reproduced with kind permission from Dr. Chris Southan's blog post: [Exploiting the Guide to Pharmacology substance \(SID\) tags in PubChem](#)

PubChem Statistics for GtoPdb, GtoImmuPdb and GtoMPdb

The stats for the 2024.1 release (with 2023.2 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 [12601](#) (12173).
2. Those that have defined chemical structures are merged into [10436](#) (10044) Compound Identifiers, CIDs (i.e. small molecules and peptides below ~ 70 residues)

3. From our 10211 CIDs [8532](#) have vendor matches
4. The select "IUPHAR/BPS Guide to PHARMACOLOGY"[SourceName] AND gtopdb_approved [Comment] now retrieves [1981](#) SIDs (1918) which link to 1746 approved drug CIDs
5. Of our SIDs, [1468](#) (1410) are tagged in GtoImmuPdb and [376](#) (361) of these are approved drugs
6. Of our CIDs 1022 are tagged in GtoImmuPdb
7. Of our SIDs, [136](#) are tagged in GtoMPdb and [25](#) of these are approved drugs
8. Of our CIDs 134 are tagged in GtoMPdb
9. Of our SIDs, [535](#) are tagged as antibacterial and [245](#) of these are approved drugs
10. Of our CIDs 534 are tagged as antibacterial
11. We have [2493](#) (2284) structures that ChEMBL does not have, [7586](#) (7237) not in DrugBank.
12. [116](#) (82) 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 (InChIKey inner layer). Inspection of "Related Compounds" and "Same Connectivity" will indicate this.
13. We continue to curate clinical monoclonal antibodies with the PubChem Substance select "IUPHAR/BPS Guide to PHARMACOLOGY"[SourceName] gtopdb_antibody" returning [376](#) SIDs. Adding "gtopdb_approved" gives [150](#).

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 that the LinkOut pointers link users back to the database. For various technical reasons associated with NCBI mapping stringencies the three sets of entity links have an element of over-counting with redundancy. However the PubMed links are clean because they are assigned via our own curation.

Protein [5893](#)

Nucleotide [5911](#)

Gene [8644](#)

Europe PMC

GtoPdb maintains records in the [Europe PMC External Links Service](#). Unlike the larger set of NCBI Outlinks, these 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.

The screenshot shows a Europe PMC article page. The main title is "Design of SARS-CoV-2 PLpro Inhibitors for COVID-19 Antiviral Therapy Leveraging Binding Cooperativity." The authors listed are Shen Z¹, Ratta K¹, Cooper L¹, Kong D¹, Lee H¹, Kwon Y¹, Li Y¹, Alqarni S¹, Huang F¹, Dubrovskiy O¹, Rong L¹, Thatcher GJF¹, and Xiong R¹. The article is from the Journal of Medicinal Chemistry, 19 Oct 2021, 65(4):2940-2955. The DOI is 10.1021/acs.jmedchem.1c01307, PMID: 34665619, and PMID: PMC547495. The article is available for free to read and use. The abstract states: "Antiviral agents that complement vaccination are urgently needed to end the COVID-19 pandemic. The SARS-CoV-2 papain-like protease (PLpro), one of only two essential cysteine proteases that regulate viral replication, also dysregulates host immune sensing by binding and deubiquitination of host protein substrates. PLpro is a promising therapeutic target, albeit challenging owing to featureless P1 and P2 sites recognizing glycine. To overcome this challenge, we leveraged the cooperativity of multiple shallow binding sites on the P1 non surface, yielding novel 2-". The article has 10 figures and is cited by 2 sources. The article is based on a previously available preprint. The article is shared on social media. The article is cited by 3 sources: IUPHAR/BPS Guide to Pharmacology (3). The article is funded by the National Institutes of Health (NIH).

The above screenshots show an example of the links from ([Shen et al. 2021](#)). Under the 'Data' tab on the left-hand side the data cited in the article can be found. This shows 3 links back to GtoPdb ligands and targets.

As of 8th April 2024 there were [8,198](#) 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 (screenshot below)

The screenshot shows the Europe PMC search interface. The search bar contains the query "(LABS_PUBS:"1969")". The search results show 1-25 of 8,418 results. The results are sorted by Relevance. The first result is "Developing inhibitory peptides against SARS-CoV-2 envelope protein." by Bekdash R, Yoshida K, Nair MS, Qiu L, Ahdout J, Tsai HY, Uryu K, Soni RK, Huang Y, Ho DD, Yazawa M. PLoS Biol, 22(3):e3002522, 14 Mar 2024. Cited by: 0 articles | PMID: 38483887. The second result is "Discovery of Clinical Candidate AZD5462, a Selective Oral Allosteric RFXFP1 Agonist for Treatment of Heart Failure." by Granberg KL, Sakamaki S, Larsson N, Bergström F, Fuchigami R, Niwa Y, Ryberg E, Backmark A, Kato H, Miyazaki S, Iguchi K, Sakamoto T, Persson M, Idei A, Prieto Garcia L, Villar IC, Gradén H, Bergonzini G, Arvidsson T, [...] Lai M. J Med Chem, 67(6):4419-4441, 19 Mar 2024. Cited by: 0 articles | PMID: 38502782. The third result is "Discovery of CBPD-268 as an Exceptionally Potent and Orally Efficacious CBP/p300 PROTAC Degradable Capable of Achieving Tumor Regression." by Chen Z, Wang M, Wu D, Bai L, Xu T, Metwally H, Wang Y, McEachern D, Zhao L, Li R, Takyi-Williams J, Wang M, Wang L, Li Q, Wen B, Sun D, Wang S. J Med Chem, 13 Mar 2024. Cited by: 0 articles | PMID: 38477974.

Bibliometrics and Scholarly Portals

Nucleic Acids Research Database Issue

Our latest submission to the Nucleic Acids Research Database Issue was accepted and published online in October 2023 and published in the Database Issue in January 2024.

Harding SD, Armstrong JF, Faccenda E, Southan C, Alexander SPH, Davenport AP, Spedding M, Davies JA. The IUPHAR/BPS Guide to PHARMACOLOGY in 2024. *Nucleic Acids Res.* 2024 Jan 5;52(D1):D1438-D1449. doi: [10.1093/nar/gkad944](https://doi.org/10.1093/nar/gkad944). PMID: [37897341](https://pubmed.ncbi.nlm.nih.gov/37897341/); PMCID: [PMC10767925](https://pubmed.ncbi.nlm.nih.gov/pmc/articles/PMC10767925/)

Already this publication has picked up [15](#) citations.

We note that the previous [NAR update in 2022](#) (PMID: [34718737](https://pubmed.ncbi.nlm.nih.gov/34718737/)), has received [107](#) citations ([59](#) in PubChem cited by), and that our [2020 NAR Database Issue](#) article has picked up [174](#) citations and ([106](#) in PubChem cited by).

Concise Guide to Pharmacology

The [6th Edition \(2023/24\) of the Concise Guide to Pharmacology](#) was accepted in October 2023 and first published online in December 2023.

The Concise Guide provides concise overviews, mostly in tabular format, of the key properties of approximately 1800 drug targets, and about 6000 interactions with about 3900 ligands. There is an emphasis on selective pharmacology (where available), plus links to the open access knowledgebase source of drug targets and their ligands (www.guidetopharmacology.org), which provides more detailed views of target and ligand properties. It is produced in close conjunction with the Nomenclature and Standards Committee of the International Union of Basic and Clinical Pharmacology (NC-IUPHAR), therefore, providing official IUPHAR classification and nomenclature for human drug targets, where appropriate

Bibliometrics

We continue to get high citation rates in our previous NAR Database Issues and Concise Guide articles because BJP and BJCP select these as [reference citations](#) for the GtoPdb outlinks. Top of the list is our NAR 2018 entry ([PMC5753190](https://pubmed.ncbi.nlm.nih.gov/pmc/articles/PMC5753190/)) with [1,302](#) citations (according to EPMC) or [1,336](#) (according to PubMed) and [1,623](#) by Google Scholar. This has over [1,500 citations](#) according to the publisher's metrics. This exceeds our 2016 paper ([PMC4702778](https://pubmed.ncbi.nlm.nih.gov/pmc/articles/PMC4702778/)), which has over [1,000 citations](#) via publisher metrics and [930](#) (via EPMC) / [934](#) (via PubMed) / [1,114](#) (via Google Scholar), and the 2014 paper ([PMC3965070](https://pubmed.ncbi.nlm.nih.gov/pmc/articles/PMC3965070/)) that has reached [714](#) (EPMC) / [740](#) (PubMed).

The "Concise Guide" citations are currently led by 2017/18 Enzymes ([PMC5650666](https://pubmed.ncbi.nlm.nih.gov/pmc/articles/PMC5650666/)) at [564](#) followed by 2015/16: Enzymes ([PMC4718211](https://pubmed.ncbi.nlm.nih.gov/pmc/articles/PMC4718211/)) at [513](#) and 2013/14: G protein-coupled receptors ([PMC3892287](https://pubmed.ncbi.nlm.nih.gov/pmc/articles/PMC3892287/)) at [476](#).

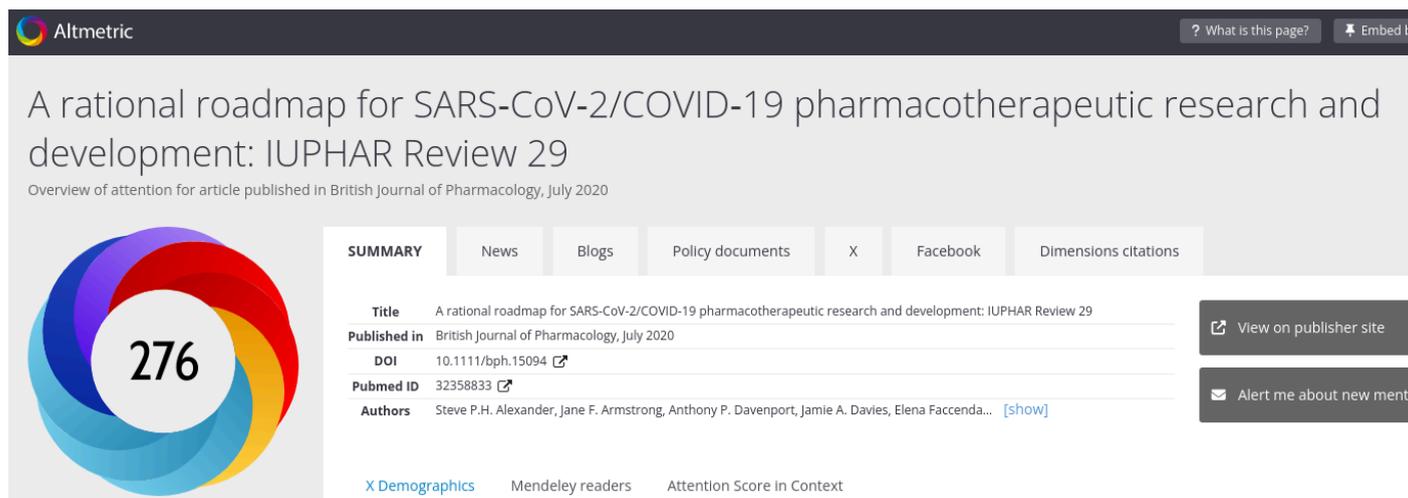
From the most recent edition of the Concise Guide, 2021/22 the [G protein-coupled receptors](#) has [119](#) citations and the [Ion Channels](#) has [166](#) citations (via CrossRef) and [73](#) citations (via PubMed).

SARS-CoV-2 Review

Our BJP [SARS-Cov-2 review](#) has acquired [50](#) citations (according to CrossRef).

Alexander SPH et al. A rational roadmap for SARS-CoV-2/COVID-19 pharmacotherapeutic research and development: IUPHAR Review 29. *Br J Pharmacol.* 2020 Nov;177(21):4942-4966.

The [Altmetric](#) rankings for all our OA papers are indexed in [ScienceOpen](#). Top of the list by some margin at 276 is our [BJP SARS-Cov-2 review](#).



Other

- As outlined in previous reports we track various metrics for the GtoPdb team and NC-IUPHAR affiliated papers in [PubMed](#), [PubMed Central](#), [European PubMed Central](#) (EPMC) [Kudos entries](#) and [Altmetrics](#).
- Research output by members of the GtoPdb Curation team can be seen via [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](#).
- The overall citation performance has resulted in team members JFA, SDH, JLS, EF, AJP, CS and JAD, along with IUPHAR co-authors, SPHA, MS, and APD being listed in the Clarivate 2023 rankings of [Highly Cited Researchers](#).
- GtoPdb team members have [204](#) cumulative co-authored publications

Below are the (live) April 2024 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).

- The team is on their [9th NAR Database Issue](#) from 2009 to 2024
- IUPHAR reviews in BJP: [45](#).
- IUPHAR Pharmacological Reviews: [110](#)
- The cumulative BJP "Concise Guide" set now takes us to [47](#) papers

EBI UniProtKB/Swiss-Prot cross-references

Below are the metrics for UniProt 2024_02 chemistry sources. The context for these has been given in previous reports. They provide valuable protein < > chemistry mappings including our own targets where we have curated quantitative ligand interactions of generally < 1uM. Note that SwissLipids is the

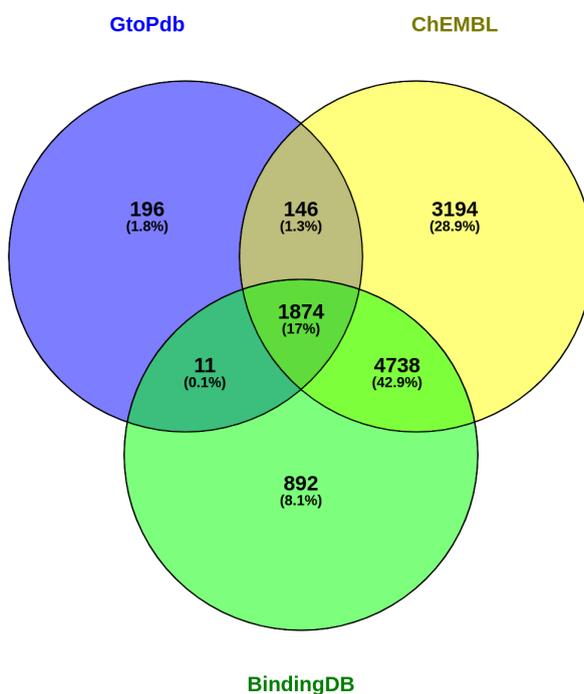
odd-man-out where the curated chemical interactions are for metabolites rather than activity modulators but nonetheless useful.

Cross-referenced databases 6 results

Download View: Cards Table Customize columns Share

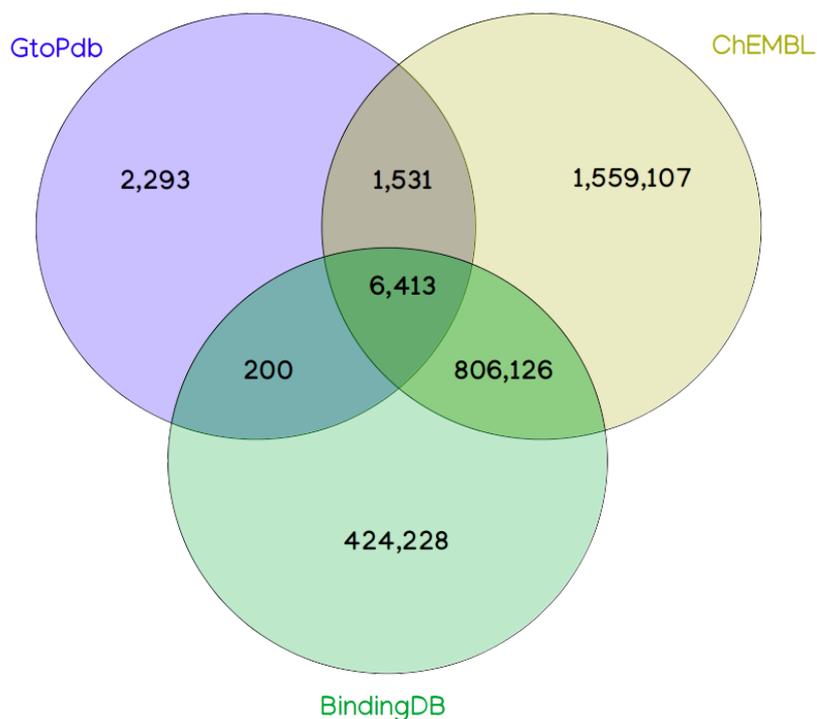
ID	Name	Abbreviation	Statistics	Category
<input type="checkbox"/> DB-0019	Drug and drug target database	DrugBank	5,220 UniProtKB entries 4,773 reviewed UniProtKB entries 447 unreviewed UniProtKB entries	Chemistry databases
<input type="checkbox"/> DB-0127	BindingDB database of measured binding affinities	BindingDB	7,515 UniProtKB entries 6,661 reviewed UniProtKB entries 854 unreviewed UniProtKB entries	Chemistry databases
<input type="checkbox"/> DB-0174	ChEMBL database of bioactive drug-like small molecules	ChEMBL	9,952 UniProtKB entries 8,835 reviewed UniProtKB entries 1,117 unreviewed UniProtKB entries	Chemistry databases
<input type="checkbox"/> DB-0182	IUPHAR/BPS Guide to PHARMACOLOGY	GuidetoPHARMACOLOGY	2,227 UniProtKB entries 2,206 reviewed UniProtKB entries 21 unreviewed UniProtKB entries	Chemistry databases
<input type="checkbox"/> DB-0197	SwissLipids knowledge resource for lipid biology	SwissLipids	1,398 UniProtKB entries 1,394 reviewed UniProtKB entries 4 unreviewed UniProtKB entries	Chemistry databases
<input type="checkbox"/> DB-0239	DrugCentral	DrugCentral	2,721 UniProtKB entries 2,565 reviewed UniProtKB entries 156 unreviewed UniProtKB entries	Chemistry databases

Even though these sources have different ways of curating, it is informative to compare and contrast. Below is a Venn diagram prepared for our recently accepted NAR issue showing the comparison of PubChem CIDs and UniProtKB between GtoPdb, ChEMBL and BindingDB.



This above Venn shows UniProtKB counts are taken from the UniProtKB Chemistry Databases (https://www.uniprot.org/database?query=*&facets=category_exact%3AChemistry+databases). Diagram drawn using Venny

2.1.0 (<https://csbg.cnb.csic.es/BioinfoGP/venny.html>). The update frequency of these cross-references may be variable depending on the sources.



CID counts are taken using the advanced PubChem Compound search (<https://www.ncbi.nlm.nih.gov/pccompound>), specifying source name in the query (i.e. 'IUPHAR/BPS Guide to PHARMACOLOGY'[SourceName]).

Around 24% of GtoPdb compounds do not overlap with ChEMBL. ChEMBL extracts all assay data, including ADMET determinations, from a paper whereas GtoPdb usually extracts just the lead compound but will also curate reported secondary target activity. In the comparison with BindingDB, 37% of GtoPdb compounds do not overlap. BindingDB's uniqueness is mainly their patent curation; it also has an arrangement with ChEMBL from which it subsumes just the individual protein target-mapped data. GtoPdb target overlap with both ChEMBL and BindingDB is extensive, GtoPdb has 207 not in ChEMBL and 342 not in BindingDB.

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 and gene names as part of our regular database update process.

GPCRdb

There are 943 links from 372 GPCR protein targets in GtoPdb to GPCRdb (<https://gpcrdb.org/>). This gives users specific pointers to GPCRdb's detailed features, curation of mutations, sequence display toolbox and residue numbering system. There are also now links from GPCRdb and GtoPdb ligand pages following work done by GPCRdb to pick up endogenous ligand data from GtoPdb.

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 7th birthday on 1st April 2023.

Financial support ended on 31.10.2023. The University of Edinburgh will continue to host the website, so that it’s still available for users.

Succession Planning

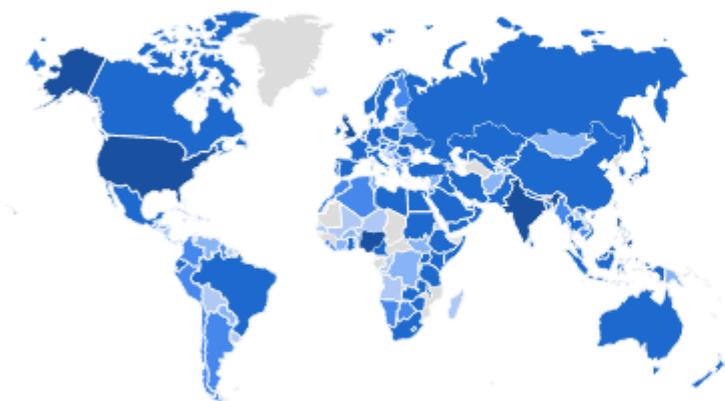
Under the stewardship of Clare Guilding (PEP Deputy Director; Newcastle University, Vice-Chair of IUPHAR’s Education Section & contributor to BPS Education and Training Committee), John Szarek and Simon Maxwell (PEP co-Directors) PEP has been integrated into the IUPHAR-ed section’s jurisdiction. We hold quarterly combined PEP/IUPHAR-ed meetings. These meetings rotate around reports from PEP, IUPHAR-ed and the Core Concepts working group.

Google Analytics data charts for PEP site usage since 1st April 2016

Google Analytics shows that user sessions continue to average >20K/month. Accumulated page views total >1.8 million.

Global Access

Users ▾ by Country



COUNTRY	USERS
India	40K
United States	30K
United Kingdom	27K
Nigeria	15K
Philippines	9.3K
Australia	7.7K
Pakistan	5.2K

[View countries](#) →

The website has been revised to handle the new Google Analytics 4 (GA4). This required technical input from the University of Edinburgh Drupal team who developed and now maintain the site. To date, data collection is comparable between the current Universal Analytics (UA) and the new GA4 system.

Social Media

PEP has >2000 followers (+300 since last report) of our twitter handle, @PharmacologyEd. IUPHAR-Ed & PEP have established a combined social media team, to try to increase exposure of both resources on social media.

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 April 23 are reported below.

Global Core Biodata Resource

The IUPHAR/BPS Guide to Pharmacology was announced as one of 15 new Global Core Biodata Resources (GCBRs) in December 2023. The announce news article can be viewed here:

<https://globalbiodata.org/global-biodata-coalition-announces-outcome-of-2023-global-core-biodata-resource-selection-process/>



GLOBAL
CORE
BIODATA
RESOURCE

This means that GtoPdb is now one of 52 GCBR designated by the Global Biodata Coalition (GBC). Through the GCBR designation, the Global Biodata Coalition (GBC) seeks to draw attention to the most critical set of global biodata resources and to better understand the challenges and needs for biodata long-term stability. GCBRs are resources of fundamental importance to global life sciences and biomedical research communities, providing open access and long-term preservation of key biological data.

[The GCBR selection process](#) was open to biodata resources globally that were able to meet several stringent eligibility criteria and more than 90 resources submitted expressions of interest across the two rounds of GCBR selection. The assessment process for GCBRs was undertaken by a panel of more than 50 independent expert reviewers against a series of criteria that included scientific focus, the size and reach of the user communities, quality of service, governance, and impact on global research.

ELIXIR

Engagement continues 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.

We are part of ELIXIR-UK though as one facet of the University of Edinburgh's membership. As reported before, we have an entry in the [ELIXIR bio-tools directory](#) as one of the official [UK ELIXIR Node Services](#).

We have been engaging locally with other groups in Edinburgh to help strengthen our involvement, this includes engaging with the [BioFAIR](#) project and their roadshow in Edinburgh on May 22nd 2024.

Publications

Listed here are our most recent/upcoming publications.

The next edition (6th) of the Concise Guide to Pharmacology (2023/24) was published in December 2023.

In October 2023 our latest database update paper was accepted and published online in the annual Nucleic Acids Research Database Issue.

Harding SD, Armstrong JF, Faccenda E, Southan C, Alexander SPH, Davenport AP, Spedding M, Davies JA. **The IUPHAR/BPS Guide to PHARMACOLOGY in 2024**. Nucleic Acids Res. 2024 Jan 5;52(D1):D1438-D1449. doi: [10.1093/nar/gkad944](https://doi.org/10.1093/nar/gkad944). PMID: [37897341](https://pubmed.ncbi.nlm.nih.gov/37897341/); PMCID: [PMC10767925](https://pubmed.ncbi.nlm.nih.gov/PMC10767925/)

An IUPHAR review 'Advances in Malaria Pharmacology and the online Guide to MALARIA PHARMACOLOGY: IUPHAR Review 38' was published:

Armstrong, J. F., Campo, B., Alexander, S. P. H., Arendse, L. B., Cheng, X., Davenport, A. P., Faccenda, E., Fidock, D. A., Godinez-Macias, K. P., Harding, S. D., Kato, N., Lee, M. C. S., Luth, M. R., Mazitschek, R., Mittal, N., Niles, J. C., Okombo, J., Otilie, S., Pasaje, C. F. A., ... Davies, J. A. (2023). Advances in malaria pharmacology and the online guide to MALARIA PHARMACOLOGY: IUPHAR review 38. *British Journal of Pharmacology*, 180(15), 1899–1929. PMID: [37197802](https://pubmed.ncbi.nlm.nih.gov/37197802/). <https://doi.org/10.1111/bph.16144>

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](https://twitter.com/GuidetoPHARM) has, as of 15th April 2024, 5,465 followers (increased from 5,336). This platform remains useful 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](https://twitter.com/BritPharmSoc) (who are active in promoting the Concise Guide) [@BrJPharmacol](https://twitter.com/BrJPharmacol), [@PharmRevJournal](https://twitter.com/PharmRevJournal), [@PRandP_Journal](https://twitter.com/PRandP_Journal) [@IUPHAR](https://twitter.com/IUPHAR), [@PharmacologyEd](https://twitter.com/PharmacologyEd) [@immunopaedia](https://twitter.com/immunopaedia) [@cdsouthan](https://twitter.com/cdsouthan) and [@mqzspa](https://twitter.com/mqzspa) (NC-IUPHAR chair).

(NB readers of this document are most welcome to follow [@GuidetoPHARM](https://twitter.com/GuidetoPHARM) and [@Steve Alexander \(@mqzspa\)](https://twitter.com/SteveAlexander) and re-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 **496 followers**, up from 457 in November 2023.

Guide to Pharmacology Blog

Our Edinburgh blog (<http://blog.guidetopharmacology.org/>) has received over 1,100 visitors between Nov 2022 and Mar 2023 - an average of 222 visitors per month. Over the same period there have been 1,540 views of our blog, which gives an average views per visitor of 1.38.

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 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 2023 we have added 15 new hot topic articles.

Slides

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.