



IUPHAR/BPS Guide to PHARMACOLOGY

Database Report

April 2025

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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 April 2024. Previous reports are online for [Nov 2024](#), [Apr 2024](#), [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 2024 doi: [10.5281/zenodo.14046004](https://doi.org/10.5281/zenodo.14046004)
- April 2024 doi: [10.5281/zenodo.11046804](https://doi.org/10.5281/zenodo.11046804)
- 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 (2024.4, 2025.1)
 - 269 new ligands, including 45 approved drugs
 - 11 new targets added
 - Overall, 242 new ligand-target interactions added, 196 of which are quantitative
 - 144 new ligands with interactions, of which, 121 have quantitative interactions
- [~44,000 Engaged Sessions per month](#)
- [~33,200 Users per month](#)

GtoPdb Website Access Statistics

Monthly statistics	Apr 2024 - Mar 2025 <i>(last report figures)</i>
<i>Engaged Sessions</i>	43,835 (43,936)
<i>Users</i>	33,296 (32,549)
<i>Page views</i>	255,809 (266,390)
<i>Pages / Session</i>	4.87 (5.12)
<i>Avg. Session Duration</i>	00:03:59 (00:04:09)
<i>Views per User</i>	7.68 (8.19)

The above table summarises the access statistics for the Guide to Pharmacology over the last year, comparing against our previous reporting period (Oct 2023 - Sep 2024). Data are generated using Google Analytics GA4.

The website has had just over 3 million page views during the last 12 months. This is a slight decrease on the previous reporting period. Similarly the pages viewed per session, session duration and page views per user have all marginally decreased. Engaged sessions have remained just about the same with a slight increase in users.

This second table shows the access stats by country (ordered by most engaged sessions). Very similar to our last reporting period, 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 active user	Views	Views per session
Totals	399,551	629,976	526,026	1.32	3,069,713	4.87
1 United States	118,344	165,652	136,630	1.15	628,333	3.79
2 United Kingdom	32,073	66,404	55,717	1.74	458,229	6.9
3 India	44,844	60,872	53,142	1.19	205,017	3.37
4 China	23,140	48,783	38,103	1.65	280,312	5.75
5 Germany	10,363	19,278	16,156	1.56	112,542	5.84
6 Japan	10,215	18,549	15,310	1.5	95,937	5.17
7 Australia	8,883	16,948	13,892	1.57	90,754	5.35
8 Canada	9,457	15,596	13,311	1.41	90,050	5.77
9 South Korea	8,176	13,310	11,208	1.37	68,319	5.13
10 France	6,889	11,081	9,423	1.37	59,384	5.36
11 Italy	5,643	9,119	7,918	1.4	45,066	4.94
12 Spain	5,250	9,344	7,913	1.51	61,327	6.56
13 Brazil	4,948	8,837	7,611	1.54	49,451	5.6
14 Mexico	4,741	8,553	7,540	1.59	56,338	6.59
15 Netherlands	5,187	8,500	7,244	1.4	49,042	5.77
16 Russia	4,222	7,593	6,653	1.58	37,805	4.98
17 Hong Kong	5,317	9,472	6,231	1.18	44,024	4.65
18 Bangladesh	5,139	6,473	6,088	1.18	19,009	2.94
19 Indonesia	4,967	6,293	5,729	1.15	20,456	3.25
20 Türkiye	3,481	5,559	4,904	1.41	30,708	5.52

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 122,000 users for HDI<0.8 countries have accessed GtoPdb, which covers over 160,000 engaged sessions. This is about 30% of all sessions. If India and China are excluded it is around 77,000 sessions (~12% of all sessions). Previously we had reported around 114,000 users and 155,000 engaged sessions from HDI < 0.8 countries.

	Total users	Sessions	Engaged sessions	Engaged sessions per user	Views
India	44,844	60,872	53,142	1.19	205,017
China	23,140	48,783	38,103	1.65	280,312
Brazil	4,948	8,837	7,611	1.54	49,451
Mexico	4,741	8,553	7,540	1.59	56,338
Bangladesh	5,139	6,473	6,088	1.18	19,009
Indonesia	4,967	6,293	5,729	1.15	20,456
Egypt	3,462	4,593	4,254	1.23	15,726
Pakistan	3,599	4,580	3,967	1.10	13,420
Philippines	3,387	4,306	3,902	1.15	13,769
Thailand	2,629	3,358	2,988	1.14	10,010
Vietnam	2,318	2,848	2,632	1.14	9,068
Colombia	1,426	2,522	2,190	1.54	16,706
Nigeria	1,921	2,369	2,209	1.15	7,031
Iran	1,680	2,313	2,079	1.24	8,799
Peru	1,011	1,993	1,744	1.73	13,024
Ukraine	848	1,919	1,668	1.98	13,313
Iraq	1,460	1,755	1,616	1.11	5,670
South Africa	1,247	1,606	1,440	1.15	5,732
Jordan	586	913	825	1.41	3,481
Belarus	226	756	718	3.18	2,189
Algeria	459	626	562	1.22	2,359
Bulgaria	455	621	580	1.27	3,327
Sri Lanka	370	596	519	1.40	2,851
Ethiopia	453	577	514	1.14	1,675
Total for all HDI <0.8	122,318	187,018	160,765	132	810,113

Download Statistics

Data for April 2024 - March 2025 shows total file downloads of 7,927 during this period, which is a significant increase on our previous reporting period (6,890 (Oct 23-Sep 24)).

Year	Apr-Dec 2024	Jan-Mar 2025	Totals
Event name	Event count	Event count	↓ Event count
Totals	5,794 73.1% of total	2,133 26.9% of total	7,927 100.0% of total
1 file_download	5,794	2,133	7,927

GtoPdb Content

These database statistics were compiled on 2nd April 2025 from the 2025.1 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	1310
Transporters	555
Other protein targets	254
Human targets with ligand interactions	2015
Human targets with quantitative ligand interactions	1758
Human targets with approved drug interactions	755
Human Primary Targets with approved drug interactions	355
Total number of targets	3097

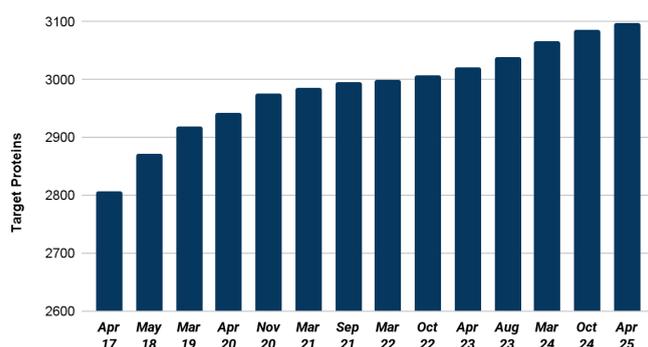
Ligands	Number of Ligands
Synthetic organics	9244
Metabolites	513
Endogenous peptides	822

Other peptides including synthetic peptides	1536
Natural products	502
Antibodies	433
Inorganics	39
Approved drugs	2098
Withdrawn drugs	113
Drugs with INNs	3701
Labelled ligands	649
Unique PubChem CIDs	10683
Ligands with target interactions	10581
Ligands with quantitative interactions (approved drugs)	9485 (1175)
Ligands with clinical use summaries (approved drugs)	3996 (2098)
Total number of ligands (PubChem SIDs)	13130
Number of binding constants curated from the literature	21,268

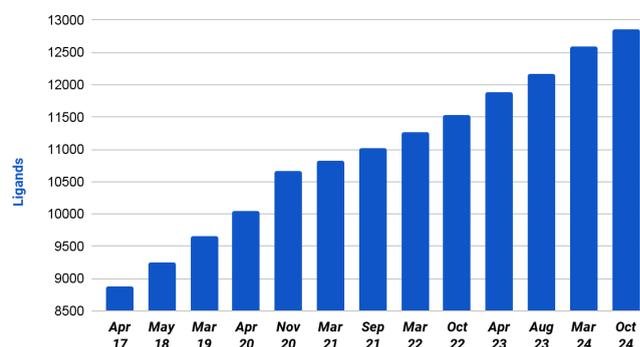
GtoPdb Entity Growth

Growth rates 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



	Apr 20	Nov 20	Mar 21	Sep 21	Mar 22	Oct 22	Apr 23	Aug 23	Mar 24	Oct 24	Apr 25
Target protein IDs	2943	2976	2985	2995	3000	3007	3021	3039	3067	3068	3097
Ligands total	10053	10659	10821	11025	11271	11532	11893	12164	12590	12862	13130
Approved drugs	1471	1614	1643	1689	1734	1787	1865	1919	1981	2019	2098
PubChem CIDs	7483	7994	8102	8262	8462	8633	9307	9852	10168	10469	10667

GtoPdb Updates

Targets

New protein targets:

We curated 11 new protein targets since our last report, this covers additions made in both the 2024.4 and 2025.1 releases.

TID	Family	Gene	Name	Comment
3296	Cholesterol biosynthesis pathway	<i>SC5D</i>	sterol-C5-desaturase	SC5D deficiency causes a rare autosomal recessive cholesterol biosynthesis disorder known as lathosterolosis
3297	Cholesterol biosynthesis pathway	<i>NSDHL</i>	NAD(P) dependent steroid dehydrogenase-like	Therapeutic potential for cholesterol-related diseases and carcinomas. Variants in <i>NSDHL</i> are associated with the lipid metabolism disorder CHILD syndrome. An inhibitor compound was curated
3298	Hydrolases & Lipases	<i>CES2</i>	carboxylesterase 2	detoxification of xenobiotics and activation of ester and amide prodrugs; natural product (+)-Yanhusanine B is an inhibitor

3299	Neuropilins and Plexins	<i>PLXND1</i>	plexin D1	Involved in axon guidance. Expression upregulated in prostate cancer, drives aggressiveness, invasiveness, and drug resistance. A preclinical synthetic PlexinD1:Fc decoy fusion protein (D1SP) is curated (oncology)
3300	Sortilin family proteins	<i>SORT1</i>	sortilin 1	Blocking sortilin 1 activity increases progranulin (PGRN) in a preclinical model of frontotemporal dementia and in patients- ? Translation to reduced disease progression. Two anti-SORT1 mAbs curated (neurodegeneration)
3301	CD33-related SIGLECs	<i>SIGLEC6</i>	sialic acid binding Ig like lectin 6	Considered as a therapeutic target for the treatment of eosinophil- and mast cell-mediated inflammation- development of anti-SIGLEC6 mAb discontinued at phase 1 (lack of efficacy)
3302	Thioredoxin (Trx) system proteins	<i>TXNRD1</i>	thioredoxin reductase 1	thioredoxin antioxidant system- overexpression is associated with drug resistance and poor prognosis in several types of cancer. Inhibitors hyperactivate ROS production -> ER stress and apoptosis. Synthetic and NP inhibitors curated (oncology)
3303	Tumour-associated antigens	<i>STEAP1</i>	STEAP family member 1	Antigen highly expressed on prostate cancer and metastases, functions in cell-cell junctions. Anti-STEAP1 mAb curated (oncology)
3304	T-box transcription factors	<i>TBXT</i>	T-box transcription factor T	Aka brachyury- oncogenic in chordoma (a bone cancer) – inhibitor compound curated (oncology)
3305	WD repeat-containing proteins	<i>SIGLEC6</i>	NACHT and WD repeat domain containing 1	Novel target for metabolic dysfunction-associated steatohepatitis (MASH) (metabolic disease)

3306	Lymphocyte antigens	LY75	lymphocyte antigen 75	Differentially expressed in malignancies from various histotypes- rapidly internalises so good target for delivery of cytotoxic agents to tumour cells- ADC OBT076 (maytansinoid microtubule disruptor payload) curated (oncology)
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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/PR&P 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).

A few ligand highlights for this report:

- We continue efforts to curate potential antiviral compounds that target SARS-CoV-2 proteins such as Mpro, PLpro, RdRp, nsp10/16 2'-O-methyltransferase complex, nsp13 helicase, and Mac1 domain of nsp3. We have 120 Mpro inhibitors with quantitative interaction data. We also curate ligands for human proteins that are targeted for anti-infection potential, such as TMPRSS2, a serine protease that plays a role in facilitating CoV entry into host cells. The most recent TMPRSS2 inhibitor to be added to GtoPdb was N-0920 which has demonstrated antiviral activity against prevalent SARS-CoV-2 variants.
- For 2024 we collected a total of 89 new drug approvals, from the FDA, EMA and other national regulatory agencies. Of the 89, 82 have full ligand entries in the GtoPdb. Those that are not included do not meet our inclusion criteria.
- All 7 of the newly FDA-approved drugs for 2025 are curated in the GtoPdb. We have also picked up non-FDA first approvals for two monoclonal antibodies (EMA, vilobelimab and China, serplulimab). The most recent FDA approval was a nucleic acid class drug fitusiran, a siRNA that targets antithrombin (*SERPINC1*) to prevent/reduce bleeding episode frequency in hemophilia A or B.
- The early 2025 release of WHO proposed INNs (PL132; with 249 INNs) offered the opportunity for curatorial sleuthing to try to match INNs either with lead compounds in declared company development pipelines, or to structures claimed in patents. We currently have 55 of this set of INNs in the GtoPdb, 31 of which are kinase inhibitors. We will continue to analyse PL132 to identify either new drug targets, or new pharmacological modalities for existing targets, to expand our coverage of emerging therapeutic targets.
- There are now 130 molecules in the GtoPdb 'PROTACs, molecular glues and other degraders' ligand family <https://www.guidetopharmacology.org/GRAC/FamilyDisplayForward?familyId=1030> (+10 since the last report). More than 10 of these degraders in early stage clinical trials. 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. Four of the chemical structures for clinical candidate PROTACs have been matched to INNs; zelebrudomide (NX2127) is a BTK PROTAC, zomiradomide (KT-413) degrades IRAK4, Ikaros and Aiolos, bavdegalutamide (ARV110) degrades the AR and vepdegrestrant (ARV471) targets the ER.

- In collaboration with Peter Ferdinandy and his team in Hungary, we have curated nucleic acid class drugs/ligands. The new ligand class tab <https://www.guidetopharmacology.org/GRAC/LigandListForward?type=Nucleic-acid> was published as part of our Database Release 2024.3 (October). We have continued to curate more compounds in this class, including any new clinical approvals. There are 10 nucleic acid class drugs in PL132 that have been added to the curation queue.

More information about new ligands and targets is included in our Database Updates blog posts <https://blog.guidetopharmacology.org/category/database-updates/>, which we generate for each Database release.

Summary of ligands added to GtoPdb in 2025.1 release (compared to 2024.3)

	New	Updated	Total (2025.1)	Total (2024.3)
Approved Drugs	45	34	2098	2019
Antibacterials	52	2	648	594
Interactions added (Ligands)				
Ligand Quantitative Interactions	121	8	9505	9376
All Ligands	269	-	13131	12862

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.

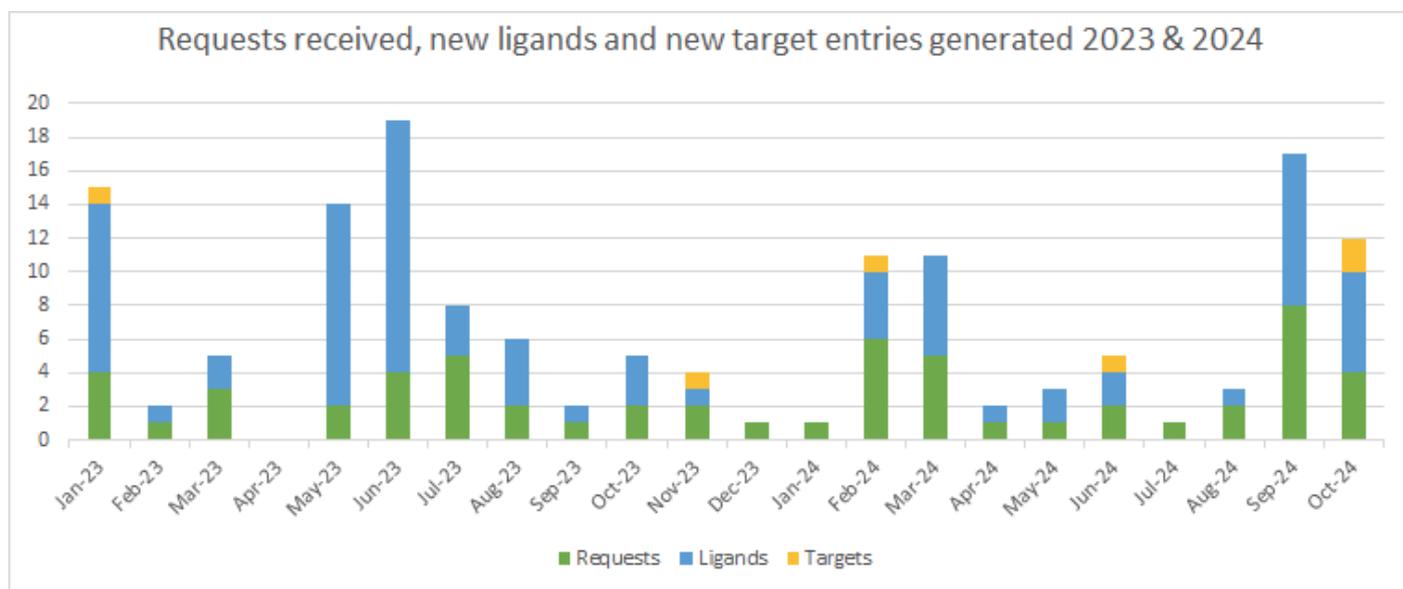
Comment Type	New Ligands	Updated Ligands
General	269	120
Clinical Use	150	101
Bioactivity	150	22
MOA	19	3

Tracking requests from BJP/BJCP authors for new ligand and target entries

Over the 2 years (to end Oct 24) we have received 58 requests from authors for additions to the GtoPdb; 27 from 2023, and 31 so far in 2024.

This process has resulted in the addition of 83 new ligands and 6 new targets, distributed as shown in the chart below.

The green bars show the count of individual requests made. Every inquiry that is received is carefully evaluated by the curators, before any decision is made to add new entries. Requests may result in multiple targets and/or ligands being added to the GtoP. However, it is also the case that for some requests, the targets and ligands don't meet our criteria for inclusion (exemplified by the green-only bars in the graph).



To date in 2025 we have had 6 requests re missing hyperlinks: 4 resulted in addition of new ligands (1 from each author), and 2 required no new additions (ligands and/or targets didn't meet our inclusion criteria).

Natural products project with Italian Society of Pharmacology (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, who earlier this year published a short editorial position piece to the BJP which outlines best-practice in NP research.

Visoli F. [Natural products: Call for hard evidence](#). Br J Pharmacol. 2024 181(16):3010-3011. doi:10.1111/bph.16437. PMID: [38783822](#)

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.

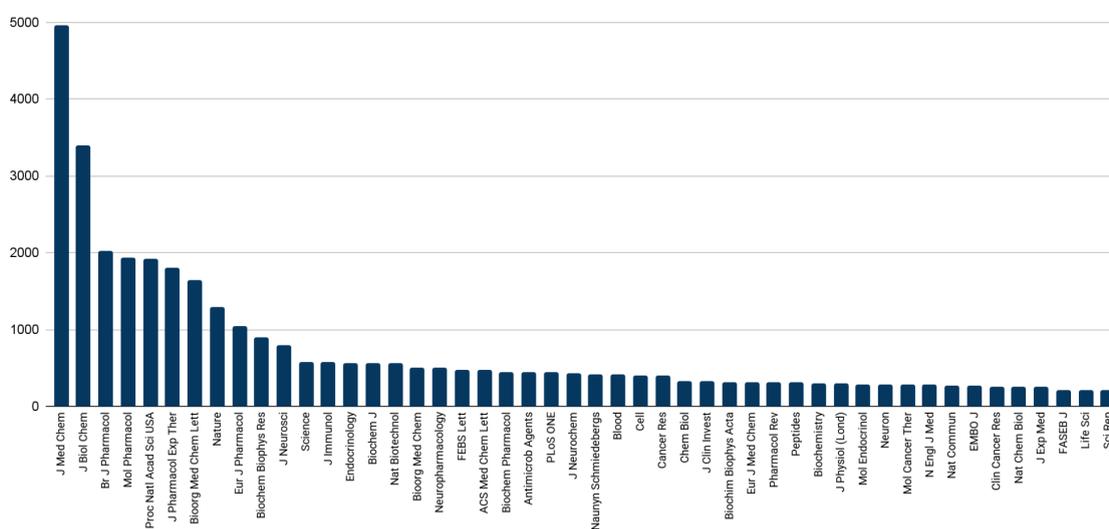
Since our last report ~30 new NPs have been added. These have been screened from primary med chem literature, natural product-specific journals and a few from BJP/BJCP author requests.

See the [Web-Application Update](#) section for information about a new natural products landing page

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	4955
J Biol Chem	3398
Br J Pharmacol	2023
Mol Pharmacol	1932
Proc Natl Acad Sci USA	1926
J Pharmacol Exp Ther	1811
Bioorg Med Chem Lett	1641
Nature	1294
Eur J Pharmacol	1048
Biochem Biophys Res Commun	907
J Neurosci	797
Science	576
J Immunol	574
Endocrinology	564
Biochem J	561
Nat Biotechnol	558
Bioorg Med Chem	502



AntibioticDB and Global Antibiotic Research and Development Partnership

We have collaborated with AntibioticDB (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

May 2026. This includes continued financial support for a curator and for a software developer, who are working on developing a landing page for antibacterial data on the Guide to Pharmacology website (please see the section on [GtoPdb Web-Application Developments](#) for further details of this work). The software developer will also continue to support the new ADB database and website that was launched in November 2024.

Currently we have **648 ligands** tagged in GtoPdb as ‘antibacterial’ and **628** 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 “2023 Antibacterial agents in clinical and preclinical development: an overview and analysis” (<https://www.who.int/publications/i/item/9789240094000>).

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

Drug Approvals

Each year, the Guide to Pharmacology Curation Team puts together a list of the latest approved drugs from FDA, EMA and MHRA as well as first-time approvals from other agencies.

We have now used this information to build a drug approvals page. This shows these approved drugs, in sortable tables, organised by year of approval. The majority of these drugs are curated in the database, and if so they are hyperlinked to their respective summary pages from the INN in the table. We still list drugs that we don't curate (because they don't meet our inclusion criteria), although these will not be hyperlinked.

A screenshot of the new page is shown below:

IUPHAR/BPS Guide to PHARMACOLOGY
An expert-curated resource of pharmacological targets and the substances that act on them

Home About Targets Ligands Diseases Resources Advanced search Immuno Portal Malaria Portal

Home Drug Approvals

Drug Approvals

Each year, the Guide to Pharmacology Curation Team puts together a list of the latest approved drugs from FDA, EMA and MHRA as well as first-time approvals from other agencies. The majority of these will be curated in the database, and they are hyperlinked to their respective summary pages from the INN in the tables below. There are some cases where we have listed an approved drug but it doesn't have a link because it will not have been curated.

2024 2023 2022 2021

Drug Approvals in 2024

INN	Trade Name	Type	Indication	Primary Target	Comments
acoramidis	Attruby	sm	To treat cardiomyopathy of wild-type or variant transthyretin-mediated amyloidosis		
ainuovirine		sm	To treat HIV type 1 infection		First approval in China Sep 2024
aprocitantan	Tryvio	sm	To treat hypertension		
arimoclomol	Miplyffa	sm	To treat Niemann-Pick disease type C		
axatilimab	Niktimvo	mAb	To treat chronic graft-versus-host disease		
benmelstobart	Andervi	mAb	To treat extensive-stage small cell lung cancer		First approval in China May 2024
benzgalantamine	Zurveyl	sm	To treat mild-to-moderate Alzheimer's disease	galantamine prodrug	galantamine prodrug
berdazimer	Zelsuvmi	sm	To treat molluscum contagiosum		
cefepime + enmetazobactam	Exblifep	sm	To treat complicated urinary tract infections		
ceftazidime	Zentox	sm	To treat certain bloodstream infections		

Natural Products

The [natural products landing page](https://www.guidetopharmacology.org/GRAC/NaturalProductsForward) (<https://www.guidetopharmacology.org/GRAC/NaturalProductsForward>) on the Guide to Pharmacology website gives details about our collaboration with the Italian Society of Pharmacology (SIF). It provides definition of natural products and explains our curation inclusion criteria. The page also shows content statistics for natural products and presents tables of the natural products curated in GtoPdb.

IUPHAR/SIF Guide to Natural Products

Quick links: [Citing](#) | [Ligands](#)

Introduction

Natural products (NPs) offer an invaluable source of biologically active compounds, and are well recognised for their potential in drug discovery and development. However, to realise their potential clinical benefits, extreme care must be taken to ensure consistency and safety throughout the processes from sample selection/collection, isolation methodologies, structure elucidation and biological evaluation. Of critical importance is the thorough validation of the pharmacological profile of any proposed new NP drug. To achieve these objectives IUPHAR (<https://iuphar.org/>) and the Italian Society of Pharmacology (SIF; <https://www.sifweb.org/>) are collaborating to provide an expert-driven project to curate NPs as a resource within the Guide to PHARMACOLOGY.

Further reading:

Visioli F. **Natural products: Call for hard evidence.** Br J Pharmacol. 2024 181(16):3010-3011. doi:10.1111/bph.16437. PMID: 38783822

Wang X, Izzo AA, Papapetropoulos A, et al. **Natural product pharmacology: the British Journal of Pharmacology perspective.** Br J Pharmacol. 2024 181(19):3547-3555. doi:10.1111/bph.17300. PMID: 39128855

Definition

Natural products may be simply defined as chemical substances produced by living organisms. Within the Guide to PHARMACOLOGY, we focus on single compounds (rather than mixtures) where there is validated evidence for biological impact, particularly in humans.

Inclusion Criteria

Natural products will be prioritised for considered in the Guide to PHARMACOLOGY if:

- They are single molecules (and, rarely, where there are naturally-occurring chiral mixtures)
- The chemical structure/s are fully defined
- There is validated (preferably quantitative) evidence for a molecular target or targets through which the biological effects of the purified natural product are mediated

Compounds of undisclosed formulation or undefined mixtures of compounds will not be included.

Data Content

Breakdown of natural product data in GtoPdb:
All Natural products: **502**
Natural products (with quantitative interactions): **302**
Natural products (Approved Drugs): **73**
Natural products (Approved Drugs with quantitative interactions): **38**

Antibacterials

We are in the process of developing a new landing page on the Guide to Pharmacology for antibacterial data. This has come about as part of our collaboration with ADB and GARDP. As the coverage of antibacterials in GtoPdb has increased, we decided to consolidate this information to a single page on the website. The page is modelled on the natural products landing page (see below) and will allow users to view and access all ligands in GtoPdb tagged as 'antibacterial' and also provide more information about how these are curated and further background reading and resources.

Antibacterial Data In GtoPdb

Quick links: [Resources](#) | [Inclusion Criteria](#) | [Data Content](#) | [Citing](#) | [Ligands](#) | [Targets](#)

Introduction

Modern medicine has been transformed by the discovery and use of antibacterial drugs, allowing previously fatal infectious diseases to be treated and enabling vital medical procedures to be carried out. However, the future utility of these therapies is threatened by a reduction in the development of new antibacterial compounds coupled with the growing challenge of antimicrobial resistance, which has been recognized by the World Health Organization (WHO) as a major global health threat [1]. The rapid spread of bacterial strains resistant to available antibacterial medicines is of particular concern, including the 'ESKAPE' pathogens (*Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, and *Enterobacter spp.*) that are responsible for many nosocomial infections [2-3].

IUPHAR/BPS Guide to Pharmacology (GtoPdb) has had a collaboration with **AntibioticDB**, (ADB; www.antibioticdb.com) that has been supported by the **Global Antibiotic Research and Development Partnership** (GARDP; <https://gardp.org>) since 2022. ADB is an open-access database of antibacterial agents, that was set up to serve as a reference and a source of starting points for future research and (re-)development of antibacterial therapeutics [4]. This collaboration has provided expert-driven oversight to increase the coverage of antibacterial compounds in GtoPdb.

Definition

An antibacterial can be defined as a drug, chemical or other substance that kills bacteria (bactericidal) or stops their growth (bacteriostatic). The term antibiotic refers to compounds with antimicrobial activity derived from bacteria or molds but is often used synonymously with antibacterial.

Inclusion Criteria

Antibacterials will be prioritised for inclusion in the Guide to PHARMACOLOGY if:

- They are single molecules
- The chemical structure/s are fully defined
- There are validated minimum inhibitory concentration (MIC) values against relevant bacterial species
- There is validated (preferably quantitative) evidence for a molecular target or targets through which the biological effects are mediated

Compounds of undisclosed formulation or undefined mixtures of compounds will not be included.

Data Content

Breakdown of antibacterial data in GtoPdb:

All Antibacterials: **648**

Antibacterials (Approved Drugs): **267**

Cite this page

The information on this page is curated by the [GtoPdb](#) curation team at the University of Edinburgh. If the information is useful to you, please cite it by referring to our [citation page](#).

Ligands		Targets	Resources	References / Further Reading
All	Approved			
Antibacterials that are approved drugs.				
Download all Antibacterials as CSV				
A B C D E F G H I J K L M N O P Q R S T V				
Ligand name		ID	Synonyms	
Back to top				
A				
amikacin	 	10894	Amikin®, AMK, Arikayce liposomal®, BB-K8	
amoxicillin	 	10895	Amoxil®, BRL-2333, co-amoxiclav (amoxicillin + clavulanic acid), Moxatag®, NSC-277174, Trimox®	
ampicillin	  	10896	aminobenzylpenicillin, KS-R1, Penbritin®, Polycillin, Principen®	
arbekacin	 	7345	arbekacin sulfate, habekacin, ME1100, NPC-14	
aspoxicillin		12293	Doyle®, TA-058	
auranofin	  	6306	MMV688978, Ridaura®, SK&F-39162, SK-39162	
avibactam	  	10761	AVI, Emblaveo® (aztreonam and avibactam), NXL 104, NXL-104, NXL104	
azidamfenicol		12397	azidamphenicol, azidoamfenicol, azidoamphenicol, Thilocof®	
azithromycin	    	6510		
azlocillin		12260	Azlin®, BAY-E-6905	
aztreonam	 	10763	Azactam®, Cayston®, Emblaveo® (aztreonam and avibactam), SQ 26776, SQ-26776	
Back to top				
B				
bacampicillin		12292	Penglobe®, Spectrobid®	
bacitracin A	 	12812		

Nucleic Acids

A few developments have been made as part of our collaboration with Prof Peter Ferdinandy's group at the Semmelweis University, Budapest, Hungary on curating nucleic acid ligands in GtoPdb.

Nucleic acid ligands can now be viewed and their data displayed. A new ligand category is now available on our ligand list page, <https://www.guidetopharmacology.org/GRAC/LigandListForward?type=Nucleic-acid>, note the new tab at the top of the page.

The IUPHAR/BPS Guide to PHARMACOLOGY complete ligand list

Approved WHO Syn. Org. Metabolite Nat. Prod. Endo. Pep. Other Pep. Inorganic Antibody Labelled Immuno AntiMal AntiBac **Nuc. Acid** All

Nucleic acid ligands. Please note, this is a recently added ligand category and its curation is under development. Go to GtoPdb View OFF

A B C D E F G I L M N O P R T U V Z Download as CSV

Ligand name	ID	Synonyms
A Back to top		
Apta-1	13556	
avacincaptad pegol	12857	ARC-1905, ARC1905, Izervay®, Zimura
B Back to top		
bevasiranib	13629	
C Back to top		
casimersen	11444	Amondys 45®, SRP-4045, SRP4045
cenersen	8270	Aezea® (proposed proprietary name), EL625
D Back to top		
darvatirsén	13607	AZD-9150, AZD9150, ISIS STAT3Rx
donidalorsén	13610	IONIS-PKK-LRx, ISIS 721744, ISIS-721744, ISIS721744
drisapersén	13535	GSK2402968, Kyndrisa®, PRO051
E Back to top		
edifoligide	13633	CGT-003, CGT003, E2F Duplex Decoy
eplontersén	13606	AKCEA-TTR-LRx, Ionis-TTR-LRx, Wainua®, Wainzua®
F Back to top		
fltusiran	13630	ALN-57213, ALN-AT3, ALN-AT3SC
fomivirsén	13533	ISIS 2922, ISIS-2922, ISIS2922, Vitravene®

On a ligand summary page for a nucleic acid ligand there are now fields displaying nucleic acid subclass and target, along with the nucleic acid sequence and HELM notation (where curated) under the Structure tab

inotersen ? GtoPdb Ligand ID: 13543

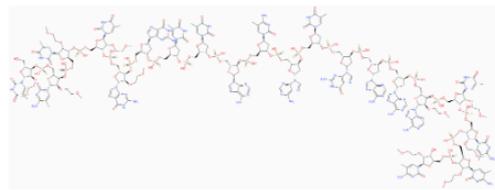
Synonyms: GSK-2998728 | GSK2998728 | ISIS-420915 | ISIS420915 | Tegsed[®]

 inotersen is an **approved drug** (EMA & FDA (2018), UK MHRA (2021))

Compound class: Nucleic acid

Comment: Inotersen is an antisense oligonucleotide that blocks expression of mutant transthyretin (TTR) protein that form pathogenic deposits in patients with hereditary transthyretin-mediated amyloidosis (hATTR).

2D Structure ?



Physico-chemical Properties ? ▼

SMILES / InChi / InChiKey ? ▼

Summary Biological activity Clinical data References **Structure** Similar ligands

Nucleic Acid Sequence ?

NNNNNGTTANATGAANNNNN

HELM Notation ?

RNA1[MOE](T).[sp][MOE]([5meC]).[sp][MOE](T).[sp][MOE](T).[sp][MOE](G).[sp][dR](G).[sp][dR](T).[sp][dR](T).[sp][dR](A).[sp][dR]([5meC]).[sp][dR](A).[sp][dR](T).[sp][dR](G).[sp][dR](A).[sp][dR](A).[sp][MOE](A).[sp][MOE](T).[sp][MOE]([5meC]).[sp][MOE]([5meC]).[sp][MOE]([5meC])\$\$\$\$

Honours Projects: Using LLMs for Text-to-SQL generation

In the last academic year (September 24 - April 25) we helped support two undergraduate, final-year projects (Honours Projects) that looked into uses of 'artificial intelligence' tools to improve access to or capabilities of the Guide to Pharmacology. Both projects focussed on the uses of Large Language Models (LLMs) (such as OpenAI's ChatGPT) to translating natural language queries to Structured Query Language (SQL) statements. This text-to-SQL conversion has the potential to enhance the ways users can ask questions of the data in the Guide to Pharmacology, removing the need to understand the database schema or SQL in order to retrieve data.

The two students, Ian Little and Nikita Rameshkumar, worked on individual projects with the same aims. Their work included analysing various LLMs to determine the ones most suitable to the task on text-to-SQL conversion in GtoPdb - these considered aspects such as cost, response time, performance and usability.

Each project developed its own model, which was trained using a set of 50 natural language queries (with associated gold standard SQL), and then tested using an previously unseen set of 30 natural language queries.

Their work investigated how the prompt for the LLM should be optimally constructed, this included looking at what degree of information about the database schema to provide, provision of example queries, query validation and error handling.

Ian and Nikita developed performance metrics in order to evaluate their models, which include a partial execution accuracy (PEX) score which indicates if the model was able to generate an SQL query for the natural language query that provides the same set of results as the gold-standard, without the SQL syntax having to be identical and allowing for addition column in the result set.

These projects were very interesting to be involved with and provided great insight into how one might go about developing a more robust and comprehensive LLM that can reliably and accurately convert natural

language queries into SQL. We are hoping to run further projects like these again in the next academic year that build on this work, perhaps by building in a user-interface to allow interaction with and refinement of the generated queries.

Their project dissertation are available here:

[Leveraging Large Language Models for Text-to-SQL on the IUPHAR/BPS Guide to Pharmacology Database](#)

Ian Little, 2025, 4th Year Project Report

Computer Science and Mathematics, School of Informatics, University of Edinburgh

[Tuning Large Language Models for Text-to-SQL on the IUPHAR/BPS Guide to Pharmacology](#)

Nikita Rameshkumar, 2025, MInf Project (Part 1) Report

Master of Informatics, School of Informatics, University of Edinburgh

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	10896	GPCRdb	372
ChEMBL	6932	ChEMBL	2256
Reactome	322	Resolute (SLC)	421

AntibioticDB	628	BioParadigms (SLC)	387
IMGT/mAb-DB	396	HGNC	3113
DrugCentral	1737	NCBI (Entrez) Gene	3077
Wikipedia	3039	Ensembl Gene	3117
CAS Registry	6517	RefSeq Protein	1968
GPCRdb	4325	UniProt	3181

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, 2025.1, all [13,131](#) 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](#)

A more recent blog post by Dr. Chris Southan speak to [Exploiting minable connectivity from GtoPdb](#)

PubChem Statistics for GtoPdb

The stats for the 2025.1 release (with 2024.3 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 [13,143](#) (12,874).
2. Those that have defined chemical structures are merged into [10,794](#) (10678) Compound Identifiers, CIDs (i.e. small molecules and peptides below ~ 70 residues)
3. From our 10211 CIDs [9,010](#) have vendor matches
4. The select "IUPHAR/BPS Guide to PHARMACOLOGY"[SourceName] AND gtopdb_approved [Comment] now retrieves [2,098](#) SIDs (2019) which link to 1,805 approved drug CIDs
5. Of our SIDs, [1,516](#) (1468) are tagged in GtoImmuPdb and [382](#) (382) of these are approved drugs
6. Of our CIDs 1031 are tagged in GtoImmuPdb
7. Of our SIDs, [143](#) are tagged in GtoMPdb and [25](#) of these are approved drugs
8. Of our CIDs 134 are tagged in GtoMPdb
9. Of our SIDs, [646](#) are tagged as antibacterial and [267](#) of these are approved drugs
10. Of our CIDs 551 are tagged as antibacterial

11. We have [2,460](#) (2472) structures that ChEMBL does not have, [7,810](#) (7810) not in DrugBank.
12. [37](#) (114) 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 [433](#) SIDs. Adding “gtopdb_approved” gives [181](#).

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 [5,946](#)

Nucleotide [5,893](#)

Gene [8650](#)

PubMed [33,319](#) ([https://pubmed.ncbi.nlm.nih.gov/?term=loprovguidpharm\[SB\]](https://pubmed.ncbi.nlm.nih.gov/?term=loprovguidpharm[SB]))

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 the Europe PMC search interface. The search query is "(LABS_PUBS:'1969') AND (FIRST_PDATE:[2023 TO 2023])". The search results display the abstract for the paper "Structural basis of efficacy-driven ligand selectivity at GPCRs." by Powers AS et al. The abstract text is partially visible. On the right side, there are sections for "Data that cites the article" and "IUPHAR/BPS Guide to Pharmacology (Showing 5 of 6)", both containing links to the GtoPdb database.

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 2025 there were [8,564](#) 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 displays the Europe PMC search results page for the query (LABS_PUBS:"1969"). The page shows 8,564 results. The search bar contains the query and a 'Search' button. Below the search bar, there are filters for 'Free full text access', 'Type', and 'Date published'. The 'Free full text access' filter shows options for 'Full text in Europe PMC (2,621)' and 'Link to free full text (1,871)'. The 'Type' filter shows options for 'Research articles (8,292)', 'Review articles (272)', 'Preprints (0)', and 'Books & documents (0)'. The 'Date published' filter shows a histogram and options for 'The last year (91)', 'The last 3 years (424)', and 'The last 5 years (871)'. The search results are sorted by 'Relevance'. The first three results are:

- Discovery of selective Orai channel blockers bearing an indazole or a pyrazole scaffold.**
Liardo E, Pham AT, Ghilardi AF, Zhelay T, Sztayn K, Gandi NL, Ekkati A, Koerner S, Kozak JA, Sun L
Eur J Med Chem, 278:116805, 28 Aug 2024
Cited by: 0 articles | PMID: 39232360
+ Add to export list
- Identification of an m6A Natural Inhibitor, Lobeline, That Reverses Lenvatinib Resistance in Hepatocellular Tumors.**
Zhao L, Ma H, Jiang Y, Li Y, Qiao L, Chen Y, Jiang X, Wang L, Wang S, Fan X
J Nat Prod, 87(8):1983-1993, 13 Aug 2024
Cited by: 1 article | PMID: 39136667
+ Add to export list
- Chalcone-Monoterpene Derivatives from the Buds of *Cleistocalyx operculatus* and Their Potential as Protein Tyrosine Phosphatase 1B Inhibitors.**
Mai VH, Ponce-Zea JE, Doan TP, Vu QH, Ryu B, Lee CH, Oh WK
J Nat Prod, 87(8):1903-1913, 24 Jul 2024
Cited by: 1 article | PMID: 39046805
+ Add to export list

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/PMC10767925/)

This publication has so far picked up [45](#) citations (European PMC) or [30](#) (in PubChem).

We note that the previous [NAR update in 2022](#) (PMID: [34718737](https://pubmed.ncbi.nlm.nih.gov/34718737/)), has received [86](#) citations ([73](#) PubChem), and that our [2020 NAR Database Issue](#) article has picked up [118](#) citations and ([111](#) PubChem).

Concise Guide to Pharmacology

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 Guide to Pharmacology database, 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.

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

The 7th Edition of the Concise Guide to Pharmacology is currently undergoing editing and we anticipate that it will be submitted this summer before publication towards the end of 2025.

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](#)) with [1,442](#) citations (according to EPMC) or [1,379](#) (according to PubMed) and [1,812](#) by Google Scholar. See the table below for links and details of other highly cited NAR and CGTP papers.

	EPMC	PubMed	Google Scholar
NAR 2018	1,442	1,379	1,812
NAR 2016	962	936	1,209
NAR 2014	768	740	916
NAR 2020	118	111	229
NAR 2022	86	73	152
CGTP 17/18 Enzymes	567	564	645
CGTP 15/16 Enzymes	518	514	576
CGTP 13/14 GPCRs	486	465	921
CGTP 17/18 GPCRs	483	465	720

From the most recent edition of the Concise Guide, 2023/24, the [G protein-coupled receptors](#) has [105](#) citations and the [Ion Channel chapter](#) and [Enzyme chapter](#) both have 71 and 195 citations respectively (all via EPMC).

CGTP Chapter	Citations (obtained from EPMC)
Enzymes	127
G protein-coupled receptors	105
Introduction and Other Proteins	68
Catalytic Receptors	58

Ion Channels	55
Transporters	38
Nuclear Hormone Receptors	22

SARS-CoV-2 Review

Our BJP [SARS-Cov-2 review](#) has acquired [43](#) citations (EPMC).

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 275 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 2024 rankings of [Highly Cited Researchers](#).
- GtoPdb team members have [206](#) 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: [57](#).
- IUPHAR Pharmacological Reviews: [116](#)
- The cumulative BJP “Concise Guide” set now takes us to [47](#) papers

EBI UniProtKB/Swiss-Prot cross-references

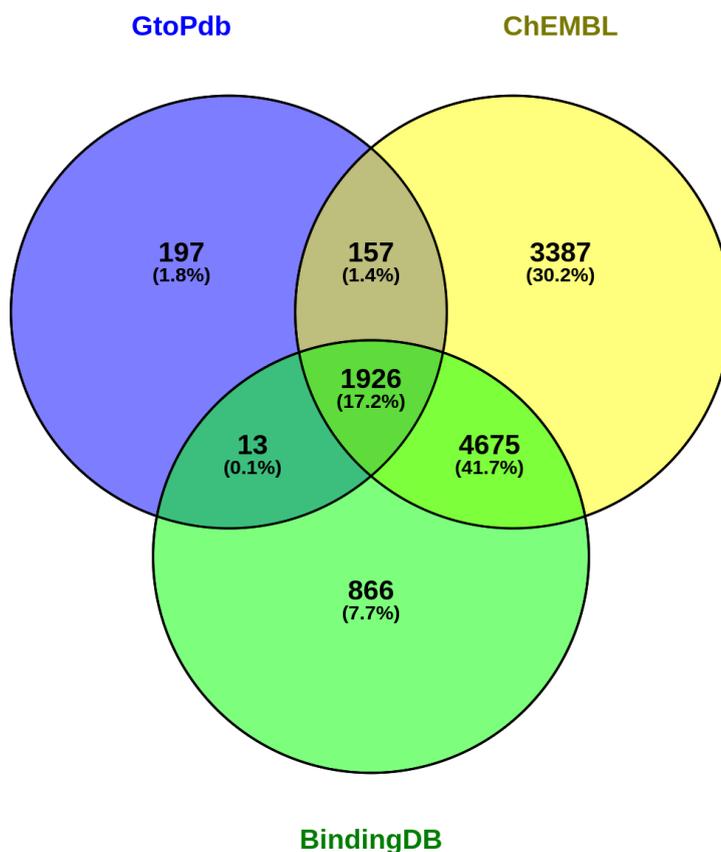
Below are the metrics for [UniProt 2024 04 chemistry sources](#). The context for these has been given in previous reports. They provide valuable protein < > chemistry mappings including our own targets where we have curated quantitative ligand interactions of generally < 1uM. Note that SwissLipids curated chemical interactions are for metabolites rather than activity modulators.

Cross-referenced databases 6 results

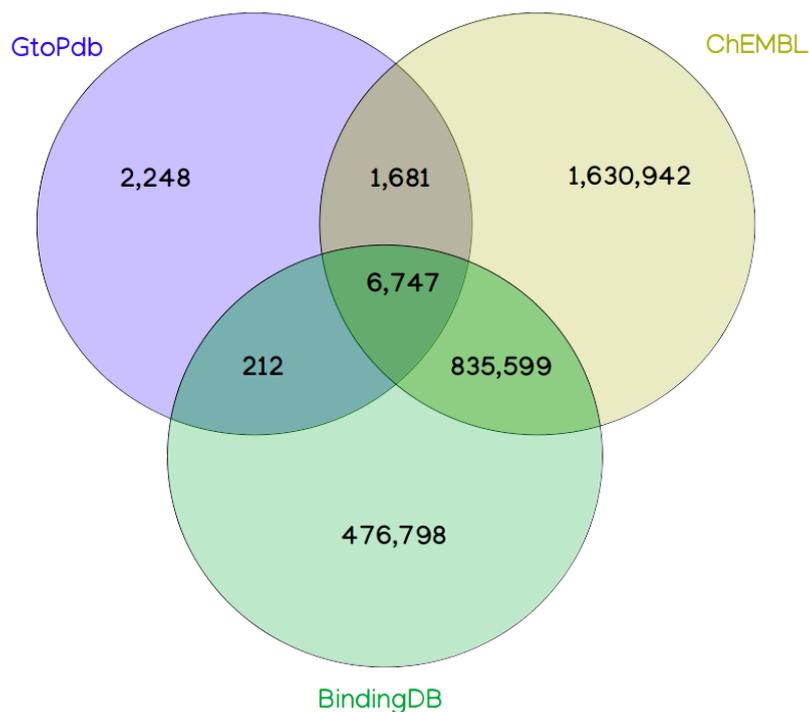
Tools ▼ Download (6) View: Cards ○ Table ● Customize columns ↗ Share ▼

ID	Name	Abbreviation	Statistics	Category
<input type="checkbox"/> DB-0019	Drug and drug target database	DrugBank	5,210 UniProtKB entries 4,788 reviewed UniProtKB entries 422 unreviewed UniProtKB entries	Chemistry databases
<input type="checkbox"/> DB-0127	BindingDB database of measured binding affinities	BindingDB	7,480 UniProtKB entries 6,662 reviewed UniProtKB entries 818 unreviewed UniProtKB entries	Chemistry databases
<input type="checkbox"/> DB-0174	ChEMBL database of bioactive drug-like small molecules	ChEMBL	10,145 UniProtKB entries 8,955 reviewed UniProtKB entries 1,190 unreviewed UniProtKB entries	Chemistry databases
<input type="checkbox"/> DB-0182	IUPHAR/BPS Guide to PHARMACOLOGY	GuidetoPHARMACOLOGY	2,293 UniProtKB entries 2,273 reviewed UniProtKB entries 20 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	3,285 UniProtKB entries 2,982 reviewed UniProtKB entries 303 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 showing the comparison of UniProtKB identifiers between GtoPdb, ChEMBL and BindingDB. GtoPdb target overlap with both ChEMBL and BindingDB is extensive, GtoPdb has 202 not in ChEMBL and 349 not in 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 25% 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, 40% 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..

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 938 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 4,263 links from GtoPdb ligand pages to GPCRdb, following work done by GPCRdb to pick up endogenous ligand data from GtoPdb.

General overview of database team activities

GtoPdb Team Interactions

For more details of previous and continuing interactions please see previous reports.

Global Core Biodata Resource

Since December 2023, the IUPHAR/BPS Guide to Pharmacology has been a Global Core Biodata Resources (GCBRs). The original announcement article can be viewed here:

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



This makes GtoPdb 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 included engaging with the [BioFAIR](#) project and their roadshow in Edinburgh on May 22nd 2024.

Publications

Listed here are our most recent publications.

The 6th edition 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/)

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.

BlueSky

We have established a BlueSky Profile [gtopdb.bsky.social](https://bsky.app/profile/gtopdb.bsky.social). As of 8th April 2025 we have 56 followers. Please connect with us if you use this platform and would like to be kept up-to-date with GtoPdb database release and other news.

X (formerly Twitter)

[@GuidetoPHARM](https://twitter.com/GuidetoPHARM) has, as of 8th April 2025, 5,470 followers (increased from 5,509). Although 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., we no longer use it as a primary way to disseminate information about the resource.

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 **585 followers**, up from 532 in November 2024.

Guide to Pharmacology Blog

Our Edinburgh blog (<http://blog.guidetopharmacology.org/>) has received 1,993 visitors between Apr 24 and Mar 25 - an average of 166 visitors per month. Over the same period there have been 3,581 views of our blog (298 per month), which gives an average views per visitor of 1.79.

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 the end of October 2024, we have added 54 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.