



IUPHAR/BPS Guide to PHARMACOLOGY Database Report

December 2025

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n	troduction	4
	Key Updates / Notifications	4
Γh	ne Guide to Pharmacology Database (GtoPdb)	5
	GtoPdb Website Analytics	5
	Download Statistics	7
	GtoPdb Content	8
	GtoPdb Entity Growth	g
	GtoPdb Updates	g
	Targets	g
	Ligands	11
	Concise Guide to Pharmacology	13
	Analysis of journals contributing to curated data	14
	AntibioticDB and Global Antibiotic Research and Development Partnership	16
	GtoPdb Web-Application Developments	17
	Drug Approvals	17
	Chemical structure search - highlighting substructures	18
	Connectivity	19
	Links to other resources	19
	Pubchem Connectivity	20
	PubChem Statistics for GtoPdb	21
	NCBI LinkOuts	21
	Europe PMC	22
	EBI UniProtKB/Swiss-Prot cross-references	23
	HGNC	25
	GPCRdb	25
	Bibliometrics	26
	Nucleic Acids Research Database Issue	26
	Concise Guide to Pharmacology	26
	CGTP and NAR Citations	26
	SARS-CoV-2 Review	27
	Other citation metrics	27
Ge	eneral overview of database team activities	29
	GtoPdb Team Interactions	29
	Global Core Biodata Resource	29
	ELIXIR	29
	Publications	30
	Outreach and Social Media	30
	BlueSky	30
	X (formerly Twitter)	30
	LinkedIn	30
	Guide to Pharmacology Blog	30

Hot Topics	31
Slides	31
Engaging with Us	31

Introduction

This database report provides an overview of recent progress and the current status of the <u>IUPHAR/BPS</u> <u>Guide to PHARMACOLOGY</u> (GtoPdb) since our last NC-IUPHAR meeting held in April 2025. Previous reports are online on our <u>downloads page</u>. Here are direct links to our most recent reports: <u>Apr 2025</u>, <u>Nov 2024</u>, <u>Apr 2024</u> and <u>Nov 2023</u>. 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:

April 2025 doi: <u>10.5281/zenodo.15342610</u>

• November 2024 doi: <u>10.5281/zenodo.14046004</u>

• April 2024 doi: <u>10.5281/zenodo.11046804</u>

• November 2023 doi: <u>10.5281/zenodo.1007801</u>

Key Updates / Notifications

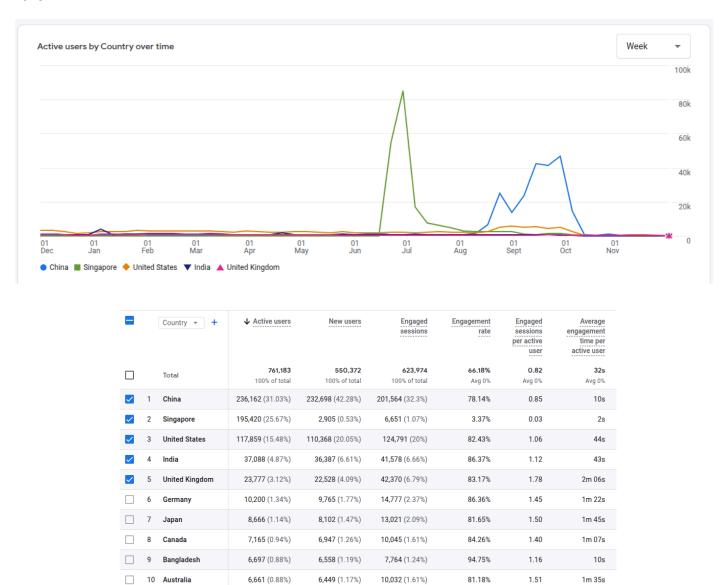
- 2 Database release (2025.2, 2025.3)
 - o 374 new ligands
 - 41 new and updated approved drugs
 - o 19 new targets added
 - o Overall, 570 new ligand-target interactions added, 467 of which are quantitative
- ~38,200 Engaged Sessions per month
- ~26,000 Active users per month

The Guide to Pharmacology Database (GtoPdb)

GtoPdb Website Analytics

We use Google Analytics GA4 to monitor access to the Guide to Pharmacology website and here we report users' access for the 12 months between 1 Dec 2024 and 30 Nov 2025.

The graph and table below show access stats, split by country. There are two quite obvious spikes in traffic to the GtoPdb site. The first, from Singapore, approximately between late-June 25 and mid-July 25, with tail-off into August and September. The second, from China, from mid-August 2025 and early-October 2025.



Given the very low engagement rate from Singapore (~3% compared to +80% from other countries), the spike from Singapore could well be unfiltered bot traffic. Google Analytics AI advisor identified this as a likely cause, supported by the fact the combination of a huge increase in "Direct" traffic and a "(not set)" landing page is often a sign of automated bots that are not being filtered out by Google Analytics.

Cou	intry	↑ Month	Active users	Sessions	Engaged sessions
	Totals		195,420	197,099	6,651
1	Singapore	Jan 25	201	310	265
2	Singapore	Feb 25	222	300	270
3	Singapore	Mar 25	288	393	295
4	Singapore	Apr 25	246	342	284
5	Singapore	May 25	243	313	281
6	Singapore	Jun 25	91,805	93,071	372
7	Singapore	Jul 25	82,645	82,184	355
8	Singapore	Aug 25	11,920	12,184	291
9	Singapore	Sep 25	6,225	6,397	2,270
10	Singapore	Oct 25	2,278	2,322	1,681
11	Singapore	Nov 25	946	962	172
12	Singapore	Dec 24	192	315	243

Singapore

The table on the left splits Singapore users by month.

The spike in users and sessions in June-August was not matched by an increase in engaged sessions, further supporting that this traffic was automated bots.

Whereas the less pronounced increase in September and October was reflected in increased engaged sessions - which may indicate an increase in genuine users.

China

The spike from China, while certainly unusual for GtoPdb, may not necessarily be a consequence of unfiltered automated bot.

The table to the right splits China users by month.

The increase in users and sessions is matched by an increase in engaged sessions show - which may indicate an increase in genuine users. This is further supported by the fact that the primary landing page from China was our homepage,

Cou	ntry	↑ Month	Active users	Sessions	Engaged sessions
	Totals		236,162	257,950	201,564
1	China	Jan 25	1,701	3,017	2,431
2	China	Feb 25	1,992	3,554	2,851
3	China	Mar 25	2,328	4,238	3,436
4	China	Apr 25	2,498	4,302	3,403
5	China	May 25	2,220	4,022	3,106
6	China	Jun 25	3,717	5,688	4,116
7	China	Jul 25	3,315	4,736	3,311
8	China	Aug 25	35,793	36,770	27,988
9	China	Sep 25	126,288	130,756	105,157
10	China	Oct 25	54,869	55,470	44,054
11	China	Nov 25	2,057	2,306	1,141
12	China	Dec 24	2,155	4,514	3,268

indicating traffic to be more likely from human users.

Monthly statistics	Dec 2024 - Nov 2025 adjusted	Dec 2024 - Nov 2025 non-adjusted
	(last report figures)	(last report figures)
Engaged Sessions	37,900 (43,835)	51,717 (43,835)
Active Users	29,550 (33,296)	46,963 (33,296)
Page views	208,885 (255,809)	238,423 (255,809)
Pages / Eng. Session	5.51 (4.87)**	4.61 (4.87)**
Avg. Session Duration	00:03:56* (00:03:59)	00:02:48 (00:03:59)
Views per Active User	7.07 (7.68)** (8.19)	5.07 (7.68)**

The above table summarises the access statistics for the Guide to Pharmacology over the last year, comparing against our previous reporting period (Apr 2024 - Mar 2025).

The adjusted figures use revised access stats that remove data from Singapore from mid-June to mid-August to account for the likely unfiltered automated bot traffic. It also uses typically average figures (taken for Jan 25 - Jul 25) for China instead of the recorded figures from August-October 2025 to account for the unusual spike.

** In this report we give pages per engaged session compared to pages per session and views per active user compared to views per users in the last report,

The website has had between 2.5-2.8 million page views during the last 12 months. The adjusted access figures show slight decline from previous reporting periods, with engaged sessions, active users and page views all lower than previously reported. However, including all data from China, shows a strong increase in traffic in terms of users and engaged sessions. The average session duration though in the non-adjusted figures

Cou	ntry	Total users	Active users	Sessions	↓Engaged sessions	Engaged sessions per active user	Views	Views per session
	Totals	564,205	563,564	749,662	620,612	1.1	2,861,080	3.82
1	China	236,236	236,162	257,950	201,564	0.85	615,715	2.39
2	United States	118,036	117,859	151,390	124,791	1.06	578,313	3.82
3	United Kingdom	23,836	23,777	50,944	42,370	1.78	338,639	6.65
4	India	37,102	37,088	48,142	41,578	1.12	158,181	3.29
5	Germany	10,215	10,200	17,111	14,777	1.45	88,833	5.19
6	Japan	8,678	8,666	15,947	13,021	1.5	80,701	5.06
7	Canada	7,175	7,165	11,921	10,045	1.4	53,170	4.46
8	Australia	6,670	6,661	12,358	10,032	1.51	66,112	5.35
9	South Korea	5,979	5,968	10,084	8,361	1.4	52,773	5.23
10	France	5,771	5,754	9,367	8,120	1.41	48,971	5.23
11	Bangladesh	6,697	6,697	8,194	7,764	1.16	23,350	2.85
12	Mexico	4,894	4,893	8,394	7,280	1.49	47,782	5.69
13	Brazil	4,945	4,941	8,316	7,000	1.42	45,389	5.46
14	Spain	4,347	4,334	7,620	6,439	1.49	47,905	6.29
15	Netherlands	3,950	3,943	7,302	6,099	1.55	44,683	6.12
16	Italy	4,286	4,278	6,908	6,002	1.4	37,271	5.4
17	Russia	3,188	3,182	6,034	5,356	1.68	30,985	5.14
18	Hong Kong	3,498	3,471	6,114	5,007	1.44	31,739	5.19
19	Türkiye	2,928	2,928	4,849	4,231	1.45	23,617	4.87

This above table shows the access stats by country (ordered by most engaged sessions). This highlights the high number of sessions from China, which when accounted for would put the engaged sessions closer to 454,800. Around 66% of all engaged sessions come from the USA, China, UK and India (up from 54% for the last reporting period). Engaged sessions are sessions lasting longer than 10 seconds, or containing 2 or more screen/page views.

The table 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'. Figures for China use average figures (taken for Jan 25 - Jul 25) instead of the recorded figures from August-October 2025 to account for the unusually high traffic.

	Total users	Engaged sessions	Engaged Session per Active User
India	37102	48142	1.30
China	26248	92273	3.52
Bangladesh	6697	8194	1.22
Brazil	4945	8316	1.68
Mexico	4894	8394	1.72
Pakistan	3982	4923	1.24
Indonesia	3411	4254	1.25

Total for all HDI < 0.8	109,732	204,602	1.86
Ecuador	392	537	1.37
Jordan	403	620	1.54
Ukraine	657	1416	2.16
Peru	938	1575	1.68
Iraq	945	1160	1.23
South Africa	986	1321	1.34
Nigeria	1064	1294	1.22
Iran (Islamic Republic of)	1137	1587	1.40
Colombia	1444	2353	1.63
Philippines	2013	2495	1.24
Thailand	2143	2659	1.24
Egypt	2209	2875	1.30
Vietnam	2649	3187	1.20

Around 109,000 users for HDI<0.8 countries have accessed GtoPdb, which covers over 200,000 engaged sessions. This is about 32% of all sessions. If India and China are excluded it is around 64,000 sessions ($^{\sim}10\%$ of all sessions). Previously we had reported around 122,000 users and 160,000 engaged sessions from HDI < 0.8 countries.

Download Statistics

Data for Dec 2024 - November 2025 shows total file downloads of 7,523 during this period, which is a slight decrease on our previous reporting period (7,927 (Apr 24 - Mar 25)).

Year	Dec 2024	Jan-Nov 2025	Totals
Event name	Event count	Event count	√ Event count
Totals	6,859 91.17% of total	664 8.83% of total	7,523 100% of total
1 file_download	6,859	664	7,523

GtoPdb Content

These database statistics were compiled on 16th September 2025 from the 2025.3 release. All database statistics can be found at https://www.guidetopharmacology.org/databaseContent.jsp.

Targets	Number of (Human) UniProt IDs
7TM receptors	400
Nuclear hormone receptors	48
Catalytic receptors	253
Ligand-gated ion channels	81
Voltage-gated ion channels	144
Other ion channels	55
Enzymes	1320
Transporters	555
Other protein targets	256
Human targets with ligand interactions	2049
Human targets with quantitative ligand interactions	1790
Human targets with approved drug interactions	769
Human Primary Targets with approved drug interactions	356
Total number of targets	3112

Ligands	Number of Ligands
Synthetic organics	9509
Metabolites	513
Endogenous peptides	825
Other peptides including synthetic peptides	1580
Natural products	533
Antibodies	460
Inorganics	39
Approved drugs	2139
Withdrawn drugs	117
Drugs with INNs	3801
Labelled ligands	655
Unique PubChem CIDs	10938
Ligands with target interactions	10581
Ligands with quantitative interactions (approved drugs)	9758 (1201)
Ligands with clinical use summaries (approved drugs)	4133 (2138)

Total number of ligands (PubChem SIDs)	13503
Number of binding constants curated from the literature	21,968

GtoPdb Entity Growth

Growth rates are documented in earlier reports and our 2016, 2018, 2020, 2022, 2024 and 2026 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.

	Nov 20	Mar 21	Sep 21	Mar 22	Oct 22	Apr 23	Aug 23	Mar 24	Oct 24	Apr 25	Sep 25
Target protein											
IDs	2976	2985	2995	3000	3007	3021	3039	3067	3068	3097	3112
Ligands total	10659	10821	11025	11271	11532	11893	12164	12590	12862	13130	13503
Approved drugs	1614	1643	1689	1734	1787	1865	1919	1981	2019	2098	2139
PubChem CIDs	7994	8102	8262	8462	8633	9307	9852	10168	10469	10667	10938

GtoPdb Updates

Targets

New protein targets:

19 new proteins have been added since our last report, this covers additions made in both the 2025.2 and 2025.3 releases.

TID	Family	Gene	Name	Comment
3307	Hydrolases & Lipases	PNPLA3	patatin like domain 3, 1-acylglycerol-3-phosph ate O-acyltransferase	PNPLA3 ^{I148M} polymorphism is a driver of tissue damage in fatty liver disease. A small molecule degrader therapeutic candidate is curated.

3308	N-myristoyltransferases	NMT1	N-myristoyltransferase 1	Oncology target; 3 inhibitors curated incl. Ph1 lead zelenirstat
3309	N-myristoyltransferases	NMT2	N-myristoyltransferase 2	
3310	DNA polymerases	POLG	DNA polymerase gamma, catalytic subunit	Ligand PZL-A disrupts POLG/POLG2 PPI, stabilises functional POLG
3311	COMMD proteins	COMMD1	copper metabolism domain containing 1	Oncology target and novel CFTR modulator; peptide ligand protein stabiliser curated
3312	Cyclic GMP-AMP turnover	ENPP1	ectonucleotide pyrophosphatase/phos phodiesterase 1	Oncology target (STING activation); 3 inhibitors curated
3313	2.1.1.43 Histone methyltransferases (HMTs)	SMYD3	SET and MYND domain containing 3	Oncology target; 3 inhibitors curated
3315	Taste 2 receptors	TAS2R2	TAS2R2	3 agonists curated as part of CG update process
3317	1 Oxidoreductases	CDO1	cysteine dioxygenase type 1	Discovered as a neo-substrate in a campaign to identify VHL-directed molecular glues
3318	Mitochondrial calcium uniporter (MCU) complex	MICU1	mitochondrial calcium uptake 1	2 inhibitors curated
3319	Mitochondrial calcium uniporter (MCU) complex	MICU2	mitochondrial calcium uptake 2	Added to complete family
3320	Mitochondrial calcium uniporter (MCU) complex	MICU3	mitochondrial calcium uptake 2	Added to complete family
3321	Mitochondrial calcium uniporter (MCU) complex	MCU	mitochondrial calcium uniporter	Added to complete family
3322	Mitochondrial calcium uniporter (MCU) complex	MCUB	mitochondrial calcium uniporter dominant negative subunit beta	Added to complete family
3323	Mitochondrial calcium uniporter (MCU) complex	SMDT1	single-pass membrane protein with aspartate rich tail 1 (aka EMRE)	Added to complete family

3324	RAS subfamily (small monomeric GTPases)	ARF6	ARF GTPase 6	Oncology target: allosteric inhibitor tool cmpd curated
3325	C19: Ubiquitin-specific protease	USP28	ubiquitin specific peptidase 28	Oncology target: 3 exp inhibitors curated
3326	Basic helix-loop-helix (BHLH) TFs (transcription factors subfamily)	TCF4	transcription factor 4	Oncology target: Ph1/2 zolucatetide inhibits β-catenin/TCF4 PPI
3327	Zinc finger TFs	ZBTB7A	zinc finger and BTB domain containing 7A	Ph1/2 molecular glue degrader curated (Sickle cell anemia)

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).

Approved drugs

We continue curating approved drugs, which now total 38 for 2025, across the approval agencies that we are able to easily follow- list available here

https://www.guidetopharmacology.org/GRAC/DrugApprovalsForward

First Disclosures 2025

Thirteen novel ligands were revealed during First Disclosures session at the ACS Fall 2025 meeting https://cen.acs.org/pharmaceuticals/drug-development/Structures-13-drug-candidates-unveiled/103/web/2025/08 -

We have been able to curate 12 of these novel compounds, adding extra content such as interaction data retrieved from patents, INNs and clinical trial information. The 13th (IID432) is a *Trypanosoma cruzi* topoisomerase II inhibitor for the treatment of Chagas disease, so is not appropriate for inclusion in the GtoPdb. The 13 are shown in the table below.

Name (clin phase; indication)	GtoPdb LID	Target & action	Company
BMS-986470 (Ph1/2; Sickle cell disease)	dual ZBTB7A/WIZ mol glue degrader		Bristol Myers Squibb
GS-1427/emvistegrast (Ph2; ulcerative colitis)	14189	α 4/β7 integrin inhibitor	Gilead
PF-07899895 (Ph1; ulcerative colitis, IBD)	14208	pan-SIK inhibitor	Pfizer
AZD0233 (Ph1: dilated cardiomyopathy SUSPENDED adverse tox)	14193	CX3CR1 antagonist	AZ
PF-07293893 (Ph1; congestive heart failure, dev ceased)	14198	AMPK gamma 3 activator	Pfizer
BMS-986463 (Ph1; adv solid tumours)	14190	WEE1 kinase mol glue degrader	Bristol Myers Squibb
TYRA-200 (Ph1; adv solid tumours with FGFR2 gene alterations)	14207	covalent FGFR2 inhibitor	Tyra Biosciences
MOMA-341 (Ph1; adv solid tumours)	14212	covalent WRN inhibitor	Moma Therapeutics
LRK-4189 (microsatellite stable CRC)	14199	lipid kinase PIP4K2C degrader	Larkspur Biosciences
FOG-001/zolucatetide (Ph1/2; adv solid tumours)	14191	beta-catenin/TCF4 interaction inhibitor	Parabilis Medicines
ETN029 (Ph1; DLL3-expressing solid tumors)	14192	DLL3-binding radioligand	Mariana Oncology
<u>MK-7337</u>	14213	lpha-synuclein binder; [11C]MK-7337 Parkinson's disease $lpha$ -synuclein imaging agent	Merck

IID432	n/a	topoisomerase II inhibitor	Novartis
		(Trypanosoma cruzi)	

Concise Guide to Pharmacology

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.

The Concise Guide provides concise overviews, mostly in tabular format, of the key properties of approximately 1900 drug targets, and about 7000 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 (2025/26) of the Concise Guide to Pharmacology was submitted to Wiley and proofs are being reviewed and re-submitted.

Editors:

Steve Alexander (Nottingham) Transporters, Enzymes, Other proteins

Eamonn Kelly (Bristol) GPCRs

Alistair Mathie (London), Emma Veale (Kent) Voltage-gated ion channels

Alasdair Gibb (London) Ligand-gated ion channels

Chloe Peach (Nottingham) Catalytic receptors

- In total >100 updates for protein families were received (summarised by target class in the table below).
- All updates were processed, and new content was included in GtoPdb release v2025.3 (10th Sept.)

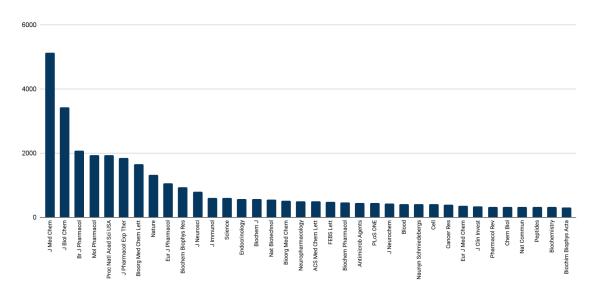
Target class	Number of families updated
GPCRs	45
Ion channels	17 (VGIC, LGIC & Other IC)
Transporters	7
Catalytic receptors	29

Enzymes	7 (plus Proteinases by Chris Southan, Kinases by Elena)
Nuclear hormone receptors	4

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	5125
J Biol Chem	3434
Br J Pharmacol	2087
Mol Pharmacol	1946
Proc Natl Acad Sci USA	1934
J Pharmacol Exp Ther	1844
Bioorg Med Chem Lett	1667
Nature	1321
Eur J Pharmacol	1071
Biochem Biophys Res Commun	931
J Neurosci	799
J Immunol	605
Science	605
Endocrinology	575
Biochem J	563
Nat Biotechnol	558
Bioorg Med Chem	516



AntibioticDB and Global Antibiotic Research and Development Partnership

Our collaboration with AntibioticDB (ADB; www.antibioticdb.com), which started in 2019, continues with the aim of extending the coverage of antibacterial compounds in GtoPdb and providing comprehensive chemistry and pharmacology for select antibacterials curated within ADB. The Global Antibiotic Research and Development Partnership (GARDP; https://gardp.org/) supports the collaboration with funding in place until May 2026.

Currently we have **688 ligands** tagged in GtoPdb as 'antibacterial' and **665** of these have links to compounds at ADB. **271** of the curated antibacterials are approved drugs. 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 <u>Database Reports</u>. 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.

As part of our work in curating antibacterial compounds in GtoPdb, we now have a dedicated landing page for antibacterials (https://www.guidetopharmacology.org/GRAC/AntibacterialsForward). This page consolidates information on antibacterials in GtoPdb, providing information on our collaboration with ADB and giving details about our inclusion criteria for curating antibacterials. The page includes a full table of all the antibacterial ligands curated in the database, with hyperlinks to the specific ligand summary pages for each compound. The table has separate tabs that provide information and links for the curated bacterial protein targets, additional resources and for references and further reading.

We continue to work with ADB to support the maintenance and development of their website. This includes recent work that provides 2D structure display with a short-term future aim to provide structure-based searching and improved filtering capabilities.

GtoPdb Web-Application Developments

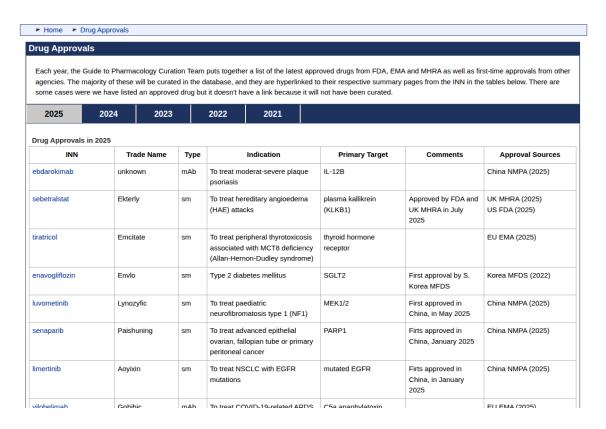
Drug Approvals

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.

Recently we have improved the drug approval tables to better display the primary targets and include a column showing the approval source (national authorities) and year. The table also includes a tab for 2025, showing the most recent approvals.

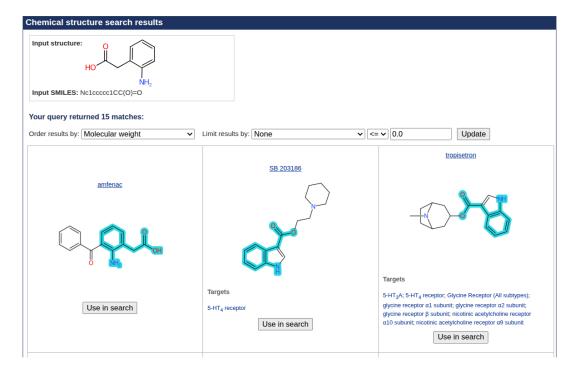
A screenshot of the drug approval page is shown below:



Chemical structure search - highlighting substructures

We have updated our <u>chemical structure search</u> to include highlighting the query structure in result sets from a substructure search. This uses Chemistry Development Kit's (CDK) depict feature and highlight functionality. When a user runs a chemical structure search and sets the type to substructure, the query structure will be highlighted in the results set.

The below shows an example of a result set from a substructure search. Showing the query structure highlighted (in cyan).



In addition to adding highlighting on substructure searches, we are also implementing the display of the Tanimoto Coefficient value used when a similarity search is run.

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.

We submit GtoPdb ligands (as substances) to PubChem at each database release. One of the strengths of GtoPdb is our regular release cycle, with new database releases approximately every quarter. As a consequence, GtoPdb can often be the first submitter of a substance to PubChem. For example, a query of PubChem for compounds where IUPHAR/BPS GtoPdb is the source and where there is only one depositor, shows 68 compounds as of 28th November 2025.

We have a long-standing collaboration with HGNC on shared nomenclature interests and our adherence to mapping HGNC-approved human gene symbols and names to NC-IUPHAR nomenclature. In addition, we have built links between more specialist resources such as GPCRdb. GtoPdb submits data to NCBI via their link-out utility, which indexes our PMIDs (https://pubmed.ncbi.nlm.nih.gov/?term=loprovguidpharm[SB], 33 449 PMIDs) with additional links for genes, nucleotides, and proteins. We also submit to Europe PMC (https://europepmc.org/) through their external links service (https://europepmc.org/LabsLink). Using this service, links are added from Europe PMC articles to related GtoPdb target and ligand data where the article is a reference to a curated pharmacological interaction in GtoPdb. A full list of the 8677 Europe PMC articles with GtoPdb data links (at the time of writing) can be retrieved from

https://europepmc.org/search?query=%28LABS_PUBS%3A%221969%22%29. Wherever we have cross-links to other resources, we maintain contacts with the teams concerned and do our best to ensure these are regularly refreshed.

Site	Ligand Links	Site	Target Links
PubChem	10938	GPCRdb	372
ChEMBL	7060	ChEMBL	2257
Reactome	322	Resolute (SLC)	421
AntibioticDB	665	BioParadigms (SLC)	387
IMGT/mAb-DB	411	HGNC	3133
DrugCentral	1742	NCBI (Entrez) Gene	3132
Wikipedia	3038	Ensembl Gene	3088
CAS Registry	6695	RefSeq Protein	1968
GPCRdb	4326	UniProt	3196
BindingDB	2116		

Pubchem Connectivity

As mentioned, 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 September 2025 database release, 2025.3, all <u>13,503</u> 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 <u>how users can exploit these tags</u> when using PubChem. This was reproduced with kind permission from Dr. Chris Southan's blog post: <u>Exploiting the Guide to Pharmacology substance (SID) tags in PubChem</u>

A more recent blog post by Dr. Chris Southan speak to Exploiting minable connectivity from GtoPdb

PubChem Statistics for GtoPdb

The stats for the 2025.3 release (with 2025.1 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 <u>13,520</u> (13,143).
- 2. Those that have defined chemical structures are merged into 11,211 (10,794) Compound Identifiers, CIDs (i.e. small molecules and peptides below ~ 70 residues)
- 3. From our 10,938 CIDs 9,308 have vendor matches
- 4. The select "IUPHAR/BPS Guide to PHARMACOLOGY" [SourceName] AND gtopdb_approved [Comment] now retrieves 2,139 SIDs (2,098) which link to 1,850 approved drug CIDs
- 5. Of our SIDs, 1,543 (1,516) are tagged in GtoImmuPdb and 394 (382) of these are approved drugs
- 6. Of our CIDs 1,065 are tagged in GtoImmuPdb
- 7. Of our SIDs, 143 are tagged in GtoMPdb and 25 of these are approved drugs
- 8. Of our CIDs 140 are tagged in GtoMPdb
- 9. Of our SIDs, <u>688</u> are tagged as antibacterial and <u>271</u> of these are approved drugs

- 10. Of our CIDs 671 are tagged as antibacterial
- 11. We have 2,372 (2,460) structures that ChEMBL does not have, 8,226 (7,810) not in DrugBank.
- 12. <u>68</u> (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 (InChKey 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 460 SIDs. Adding "gtopdb_approved" gives 190.

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 <u>Identifier Exchange Service</u> 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 <u>5,940</u>

Nucleotide <u>5,887</u>

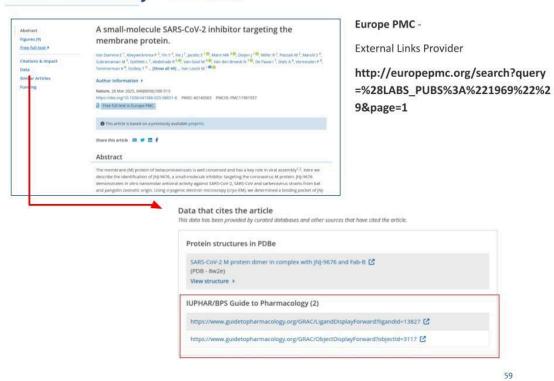
Gene <u>8,678</u>

PubMed 33,449 (https://pubmed.ncbi.nlm.nih.gov/?term=loprovguidpharm[SB])

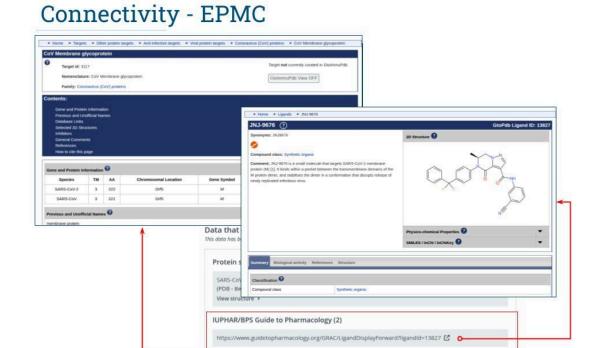
Europe PMC

GtoPdb maintains records in the <u>Europe PMC External Links Service</u>. 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.

Connectivity - EPMC



The above figure shows an example of the links from <u>PMID:40140563</u>. 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. Below shows how these data links navigate users to GtoPdb Target and Ligand pages.



v.guidetopharmacology.org/GRAC/ObjectDisplayForward?objectid=3117 🛂

60

As of 28th November 2025 there were <u>8,677</u> 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)

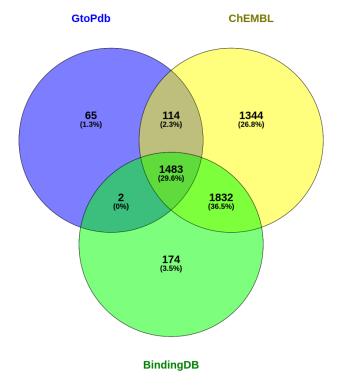
EBI UniProtKB/Swiss-Prot cross-references

Below are the metrics for <u>UniProt 2025_04 chemistry sources</u>. 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.

C	Cross-referenced databases 6 results					
≜ T	ools▼ ±	Download (6) View: Cards O Tab	le Customize columns	% Share ▼		
	ID .	Name	Abbreviation .	Statistics	Category .	
	DB-0127	BindingDB database of measured binding affinities	BindingDB	7,850 UniProtKB entries 6,928 reviewed UniProtKB entries 922 unreviewed UniProtKB entries	Chemistry databases	
	DB-0174	ChEMBL database of bioactive drug-like small molecules	ChEMBL	10,290 UniProtKB entries 9,109 reviewed UniProtKB entries 1,181 unreviewed UniProtKB entries	Chemistry databases	
	DB-0019	Drug and drug target database	DrugBank	5,345 UniProtKB entries 4,937 reviewed UniProtKB entries 408 unreviewed UniProtKB entries	Chemistry databases	
	DB-0239	DrugCentral	DrugCentral	3,270 UniProtKB entries 2,982 reviewed UniProtKB entries 288 unreviewed UniProtKB entries	Chemistry databases	
	DB-0182	IUPHAR/BPS Guide to PHARMACOLOGY	GuidetoPHARMACOLOGY	2,296 UniProtKB entries 2,278 reviewed UniProtKB entries 18 unreviewed UniProtKB entries	Chemistry databases	
	DB-0197	SwissLipids knowledge resource for lipid biology	SwissLipids	1,398 UniProtKB entries 1,394 reviewed UniProtKB entries 4 unreviewed UniProtKB entries	Chemistry databases	

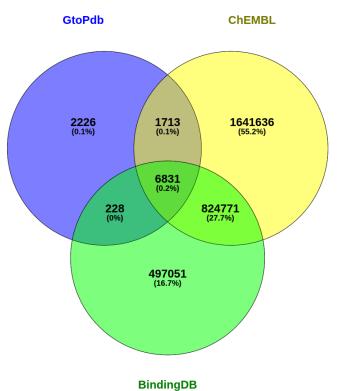
Even though these sources have different ways of curating, it is informative to compare and contrast. Below is a Venn diagram (taken from our NAR update) showing the comparison of UniProtKB identifiers between GtoPdb, ChEMBL and BindingDB. GtoPdb target overlap with both ChEMBL and BindingDB is extensive, GtoPdb has 67 not in ChEMBL and 179 not in BindingDB.

B. Human UniProtKB



This second 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]).

A. PubChem CID



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.

Bibliometrics

Nucleic Acids Research Database Issue

Our latest submission to the Nucleic Acids Research Database Issue was accepted and published online in November 2025 and due to be published in the Database Issue in January 2026.

Harding SD, Armstrong JF, Faccenda E, Southan C, Alexander SPH, Davenport AP, Spedding M, Davies JA. The IUPHAR/BPS Guide to Pharmacology in 2026. Nucleic Acids Res. 2025 Epub ahead of print. doi: 10.1093/nar/gkaf1067. PMID: 41160876.

Our previous update published in 2024 has so far picked up $\underline{102}$ citations (European PMC) or $\underline{81}$ (in PubChem).

We note that the previous <u>NAR update in 2022</u> (PMID: <u>34718737</u>), has received <u>121</u> citations (<u>87</u> PubChem), and that our <u>2020 NAR Database Issue</u> article has picked up <u>148</u> citations and (<u>113</u> PubChem).

Concise Guide to Pharmacology

Details of our work in curating and preparing the Concise Guide are in the <u>curation section of the report</u>.

CGTP and NAR Citations

We continue to get high citation rates in our previous NAR Database Issues and Concise Guide articles because BJP and BJCP select these as <u>reference citations</u> for the GtoPdb outlinks. Top of the list is our NAR 2018 entry (<u>PMC5753190</u>) with <u>1,530</u> citations (according to EPMC) or <u>1,423</u> (according to PubMed) and

1,850 by Google Scholar. See the table below for links and details of other highly cited NAR and CGTP papers.

	ЕРМС	PubMed	Google Scholar
NAR 2018	<u>1,533</u>	<u>1,423</u>	<u>1,850</u>
NAR 2016	989	939	1,224
NAR 2014	<u>786</u>	<u>743</u>	918
NAR 2020	<u>148</u>	<u>113</u>	238
NAR 2022	121	<u>87</u>	<u>162</u>
CGTP 17/18 Enzymes	<u>573</u>	<u>564</u>	<u>646</u>
CGTP 15/16 Enzymes	518	<u>515</u>	<u>577</u>
CGTP 13/14 GPCRs	499	466	<u>685</u>
CGTP 17/18 GPCRs	515	471	730

From the most recent edition of the Concise Guide, 2023/24, the <u>G protein-coupled receptors</u> has <u>219</u> citations and the <u>Ion Channel chapter</u> and <u>Enzyme chapter</u> both have 126 and 271 citations respectively (all via EPMC).

CGTP Chapter	Citations (obtained from EPMC)
<u>Enzymes</u>	<u>271</u>
G protein-coupled receptors	219
Introduction and Other Proteins	127
Catalytic Receptors	106
<u>Ion Channels</u>	126
<u>Transporters</u>	92
Nuclear Hormone Receptors	<u>52</u>

SARS-CoV-2 Review

Our BJP <u>SARS-Cov-2 review</u> has acquired <u>51</u> 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 <u>Altmetric</u> rankings for all our OA papers are indexed in <u>ScienceOpen</u>. Top of the list by some margin at 274 is our <u>BJP SARS-Cov-2 review</u>.

Other citation metrics

- As outlined in previous reports we track various metrics for the GtoPdb team and NC-IUPHAR affiliated papers in <u>PubMed</u>, <u>PubMed Central</u>, <u>European PubMed Central</u> (EPMC) <u>Kudos entries</u> and <u>Altmetrics</u>.
- Research output by members of the GtoPdb Curation team can be seen via $\underline{\mathsf{ORCID\ IDs}}$ for which we have JLS $\underline{\mathsf{0000-0002-5275-6446}}$, EF $\underline{\mathsf{0000-0001-9855-7103}}$, AJP $\underline{\mathsf{0000-0003-2280-845X}}$, CS $\underline{\mathsf{0000-0001-9580-0446}}$, SDH $\underline{\mathsf{0000-0002-9262-8318}}$ and JFA $\underline{\mathsf{0000-0002-0524-0260}}$.
- 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 2025 rankings of <u>Highly Cited Researchers</u>.
- GtoPdb team members have <u>210</u> 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 <u>10th NAR Database Issue</u> from 2009 to 2026
- IUPHAR reviews in BJP: 41.
- IUPHAR Pharmacological Reviews: <u>118</u>
- The cumulative BJP "Concise Guide" set is 47 papers (before the 2025/26 edition)

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 were represented by Dr. Chris Southan at the ELIXIR UK All-Hands Meeting, Exeter, in October 2025.

Publications

Listed here are our most recent publications.

The 7th edition of the Concise Guide to Pharmacology (2025/26) is in preparation (Nov 2025).

As mentioned, in September 2025 our latest database update paper was accepted and published online shortly thereafter 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 2026**. Nucleic Acids Res. 2025 Epub ahead of print. doi: 10.1093/nar/gkaf1067. PMID: 41160876.

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 <u>gtopdb.bsky.social</u>. As of 1st December 2025 we have 85 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)

<u>@GuidetoPHARM</u> has, as of 1st December 2025, 5,455 followers (decreased from 5,470). 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 <u>LinkedIN</u> group page now has **652 followers**, up from 585 in April 2025.

Guide to Pharmacology Blog

Our Edinburgh blog (http://blog.guidetopharmacology.org/) has received 2,213 visitors between Dec 24 and Nov 25 - an average of 184 visitors per month. Over the same period there have been 3,737 views of our blog (311 per month). This is a slight increase on the 1,993 visitors and 3,581 views in our last report.

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 <u>Hot Topics in Pharmacology</u> 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 March 2025, we have added 150 new hot topic articles.

Slides

We continue to provide a set of <u>generic slides</u> 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.