Proceedings of the British Pharmacological Society at http://www.pA2online.org/abstracts/Vol18Issue1abst129P.pdf

Navigating links between structures and papers: PubMed-to-PubChem connectivity from the Guide to PHARMACOLOGY and the British Journal of Pharmacology

C. Southan, E. Faccenda, J. L. Sharman, S. D. Harding, A. J. Pawson, J. A. Davies. IUPHAR/BPS Guide to PHARMACOLOGY, Edinburgh, United Kingdom.

Introduction: A crucial role of the pharmacological literature is providing connectivity between papers, SAR analogues, and clinical candidates. The IUPHAR/BPS Guide to PHARMACOLOGY (GtoPdb) enables this by expert curation of cross-references [1]. Our journal links are submitted to PubChem (PC), who incorporate links to PubMed (PM). These include selected British Journal of Pharmacology (BJP) articles where key structures get out-links to GtoPdb entries. Thus, both BJP readers and GtoPdb users are guided into the PM/PC system. This study presents statistics of connectivity and implications for user exploitation.

Methods: For GtoPdb entries in PC Substance we used the PC interface to count the PM links (query: pcsubstance_pubmed[filt] AND "IUPHAR/BPS Guide to PHARMACOLOGY"[SourceName]) . This gives the PC > PM mapping counts for this source from which we can analyse the PubMed links by journal. We then performed reciprocal analyses (i.e. PM > PC) by selecting PM sets; For BJP we counted structure links by year and source.

Results: From 8988 GtoPdb-submitted ligand substances in PC (release 2017.5) , 7309 are linked to 8980 PM entries. Of the 7309 there are 5632 links to chemical structures in PC compound entries, the rest being antibodies and larger peptides. From the 8980 PMIDs, the Journal of Medicinal Chemistry accounted for 1003 as our most frequently cited primary source of structure-to-activity mappings for drug discovery leads. For BJP most of the 345 cross-references were development compound reports. Dividing these by year for PC links showed an unexpected pattern. From 2014 to 2017 the BJP/PC links of ~ 30 structures per year are mostly from GtoPdb with some from the Comparative Toxicology Database. However, going back to 2010-12, this increased to 500-800 connections. These were mainly derived from the IBM source of automated chemical extraction from Medline abstracts. The specificity value of these different sources will be reviewed.

Conclusion: The ability to navigate between documents and bioactive chemistry databases is becoming an essential part of pharmacology education. GtoPdb is a major contributor of high-quality curated connections inside PC because of the precision of our cross-references to papers and patents. However, connections overall are complex and we have identified specificity issues with non-GtoPdb sources. Although navigating the NCBI Entrez system is challenging this presentation will help pharmacologists understand its potential. We are also expanding help documentation for exploiting the GtoPdb out-links from BJP.

References:

[1] Southan et al. (2016). Nucl. Acids Res. 44 (Database Issue): D1054-68.