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Navigating between publications and databases for drug discovery: IUPHAR/BPS Guide to PHARMACOLOGY initiatives

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Making navigation between publications and databases more seamless offers major advantages in drug discovery informatics. A useful option is “live linking” where entities within the text of a manuscript (preferably open access) connect directly via a URL to an extrinsic database record for a bioactive chemical structure or a protein entry. This paper < > database navigation is complemented by paper < > paper connectivity via live-linked references. This has recently appeared in both PubMed Central and European PubMed Central (for abstracts and full-text) where names or IDs matching entities in the NCBI databases for the former and EBI in the later, are live-linked. Similarly, the web resource chemicalize.org can extract chemistry even from large patent documents (PMID 23618056). However the limited specificity of automated entity recognition produces many false positives and false negatives. Our own engagement arose from a pilot collaboration with the *British Journal of Pharmacology* (BJP) and its publisher Wiley that addresses this problem by expert manual link annotation (as a post-acceptance step) thereby ensuring relevance and accuracy. Examples can be seen in the Concise Guide to PHARMACOLOGY 2013/14 series of papers in BJP (http://www.guidetopharmacology.org/concise) and most recently for the IUPHAR reviews on epigenetic pathways (PMID 25060293) and endothelin (PMID 25131455). Tables display the target and ligand links from the publication to their corresponding entries in the IUPHAR/BPS Guide to PHARMACOLOGY database (GtoPdb). The next step will be to extend the document mark-up to all BJP authors with the introduction of new guidelines, whereby the addition of links will be led by authors during article submission. This has the advantage that it can drive the creation of new database content; authors will be encouraged to submit details of new protein and ligand entities with automatic alerts sent to the database curators. Given the success of this we have initiated other approaches to paper < > database coupling. We have explored retrospective and independent linking for relevant articles that include a high density of entities potentially linkable to GtoPdb but that had no mark-up at publication time. This was achieved by listing links on our blog and using PubMed Commons to cross-point between an article and our local mark-up (since we are already using this for our BJP marked-up articles). The result can be seen for a recent IUPHAR review on allosteric ligands in *Pharmacological Reviews* (PMID 25026896). Another initiative we have instigated is using document-binding synonyms in our ligand entries. This means we can link document-specific locators (e.g. “compound 11a” from a paper or “example 204” from a patent) directly to the document identifier as a PubMed ID or a patent number in the database entry. This enables users to immediately locate the specific structure we have mapped the activity data to, inside the document we extracted the data from. A bonus here is that these binding synonyms now surface in PubChem via

our submissions. Our engagements in this general theme of document < > database is expanding and we therefore welcome user opinions on the topic. Please note also that authors of pharmacology and/or drug discovery papers describing new ligands and/or targets that we have not yet captured in GtoPdb, are welcome to contact us.