

Comparison of Beilstein CrossFire plus Reactions with ISIS Reaction Databases - Don Parkin

With easy access to reaction databases via desktop software programs, a large number of academics now have access to both selective and comprehensive reaction databases. The use of such databases is expected to increase, as more chemists become aware of the potential and ease of use of these databases. However, if most of the data is apparently available from a single monolithic database, it raises the question about the value of the smaller selective databases.

The Chemical Database Service (CDS) was in a position to address this question for two main reasons. The unique set up at Daresbury meant that we were able to host the National trial for UK academics of the comprehensive database, Beilstein. The CDS also hosts a wide range of smaller, selective reaction databases under ISIS.

A study was undertaken to assess the overlap in reference and reaction data, the role the small selective databases have to play in reaction searching and to answer the question "are small selective databases now redundant".

At present, the availability of Beilstein CrossFireplusReactions within the UK academic community has not caused the number of users or number of accesses to the smaller selective databases under ISIS to decrease - indeed this figure has risen.

1.1 Conclusions

A large overlap (over 90%) in bibliographic entries was shown for all the collective ISIS databases compared to Beilstein. The overlap in reaction data however is much smaller, partially due to a large percentage of reactions in Beilstein being not fully mapped, at the moment, and partially to the fact that the ISIS databases contain overall reaction schemes.

The use of one database over the other would appear to be dependent on the type of search query and the expected number of hits. When searching for a lead, the overall results for reaction searching indicate that it is better to search ISIS first, as the hit list is obtained quickly and can be manageable. Viewing and hit list manipulation facilities are currently better with ISIS as compared to Beilstein. If no hits or very few hits are obtained, then use Beilstein. For reference, fact or specific product searches, choose Beilstein; any other reaction search choose ISIS first then Beilstein.

Therefore the overall conclusion is that the two types of databases are complementary and that the smaller selective databases still maintain a key role in reaction searching.

Faiz A. Parkar and Don Parkin. *J. Chem. Inf. Comput. Sci.* **39**(2), 281-288.

