# ecBLAST: A novel tool for searching similar enzymes based on chemical knowledge*

*Use of ECBlast is currently restricted, but is planned for release within the next few months. The tool will be available for testing by the Killer App judges.

**URL:** http://www.ebi.ac.uk/thornton-srv/software/rbl

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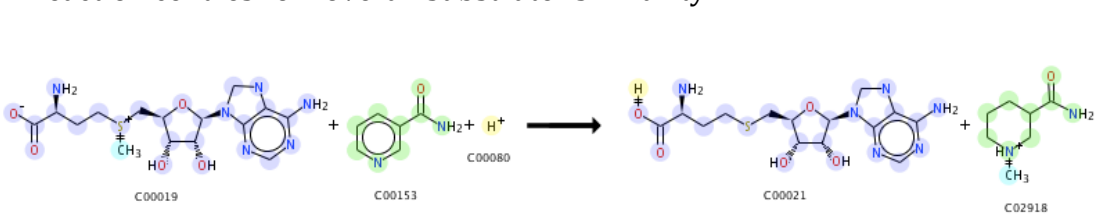
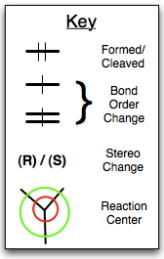
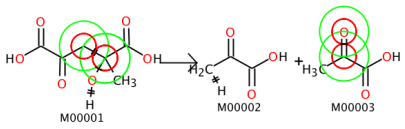
**How ecBLAST benefits biologists:**

- Using ecBLAST one can find similar reactions based on the "overall bond changes" and/or "reaction centres" or "overall substrate" similarity.

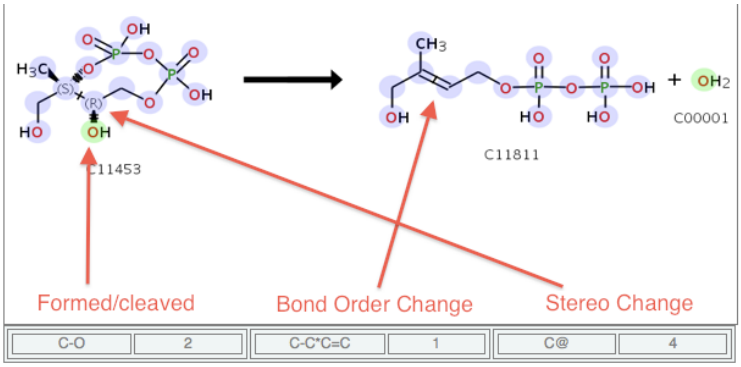



- This complements the sequence based homology search where top hits do not necessarily represent the chemistry depicted in the query enzyme.
- Many times one would like to find similar reactions where reaction centres are conserved e.g. in drug discovery to avoid toxicity effect.
- It may also have applications in protein design and metabolic pathway re-engineering (e.g. enzymes with similar reaction/or transformation).




- With ecBLAST one has the flexibility to search the chemistry encoded in the enzymes at various levels.
- This will bridge the gap between sequence and chemical based search results/annotation.
- Thus, ecBLAST can successfully annotate, search and highlight the chemistry of the enzyme performing a reaction.
- All this is done using in-house algorithms developed in our group and other available tools.



**Comparison to similar tools:**

There are currently no tools in the public domain that can do the equivalent task. However, we found two existing applications that are close to our tool.

1) App from SFLD (http://sfld.rbvi.ucsf.edu/django/reaction/search/)
    a. Searches reactions based on the substrate similarity.
    b. This app is specific for the SFLD i.e most EC numbers are not represented.
    c. This searches for the entries in the SFLD, which are in the mechanistic/active site DB. Therefore, has limited bond change information.
    d. Our tool also searches a background DB which has annotated reaction centres, bond changes.
    e. We contain all EC numbers and present detailed bond change information (currently we don't link back to mechanism but this on cards).
    f. We can search on bond change, reaction centres and substrate similarity.

2) Predict enzyme/reaction from KEGG (http://www.genome.jp/tools-bin/predict_reaction)
    a. This tool presents a search from compound to EC whereas our approach is from EC to reactions (compounds).
    b. KEGG's service is more transformation centric rather than overall similarity search.
    c. Our tool displays the result in an intuitive way and also display the bond changes, reactions centres and the highlighting of subgraphs is clearer.
    d. We also provide atom-atom mapping for the query reaction, which can be downloaded by users.