

Figure 1: Chemical structures of dRTP and dPTP, nucleotide analogs used in the SeSaM method.



The screenshot shows the MAP2.0 3D Server interface. At the top, there are logos for Jacobs University, MAP2.0 3D, and RWTH Aachen University. Below the logos, a navigation bar includes links for Home, Submission, Instructions, References, and Contact Us. The main content area is divided into two sections: **Sequence based analysis** and **Structure based analysis**.

Sequence based analysis: This section contains a text input field labeled "Paste nucleotide sequence below", a file upload input labeled "Or upload sequence file [example file](#)", a checkbox for "Define mutagenesis method*", and buttons for "Submit" and "Reset". A note at the bottom of this section says: "Please mouse over the input labels for help!"

Structure based analysis: This section contains an input field for "Upload PDB file [example PDB](#)", a file search button "Durchsuchen...", a dropdown for "Chain" (set to "A"), a dropdown for "Select method" (set to "Non biased" with a note "(Default is Non biased)"), a dropdown for "Select the amino acid group" (set to "All" with a note "(Default is for all residues)"), and buttons for "Submit" and "Reset". A "Return to top" link is located at the bottom right of this section.

Figure 2: Overview of the query interface of the MAP2.0 3D server.

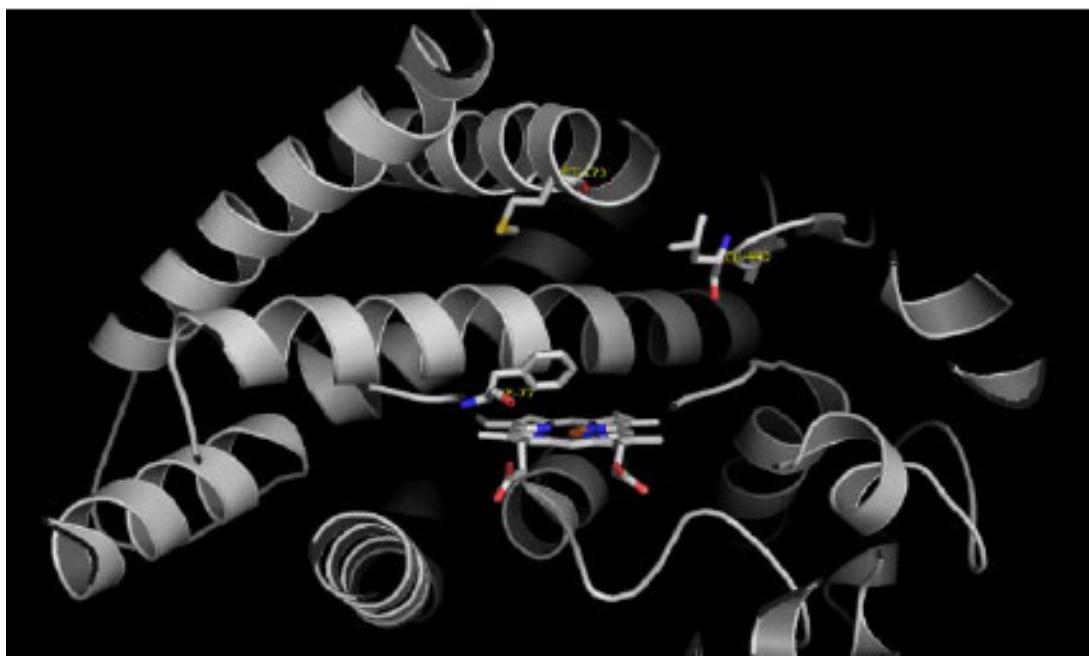


Figure 3: Close-up of the modeled E216M/F483L monooxygenases mutant.

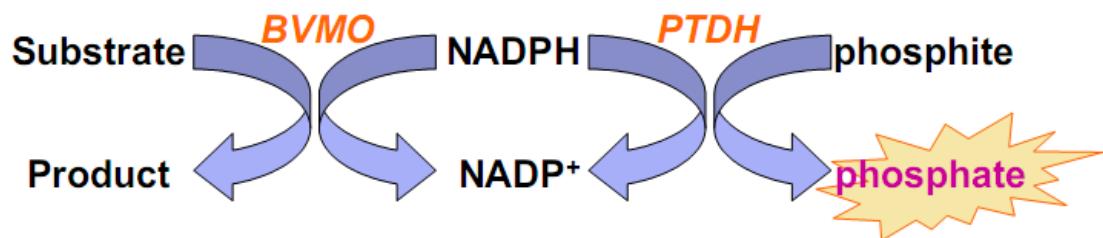


Figure 4. BVMO activity coupled to phosphate formation.

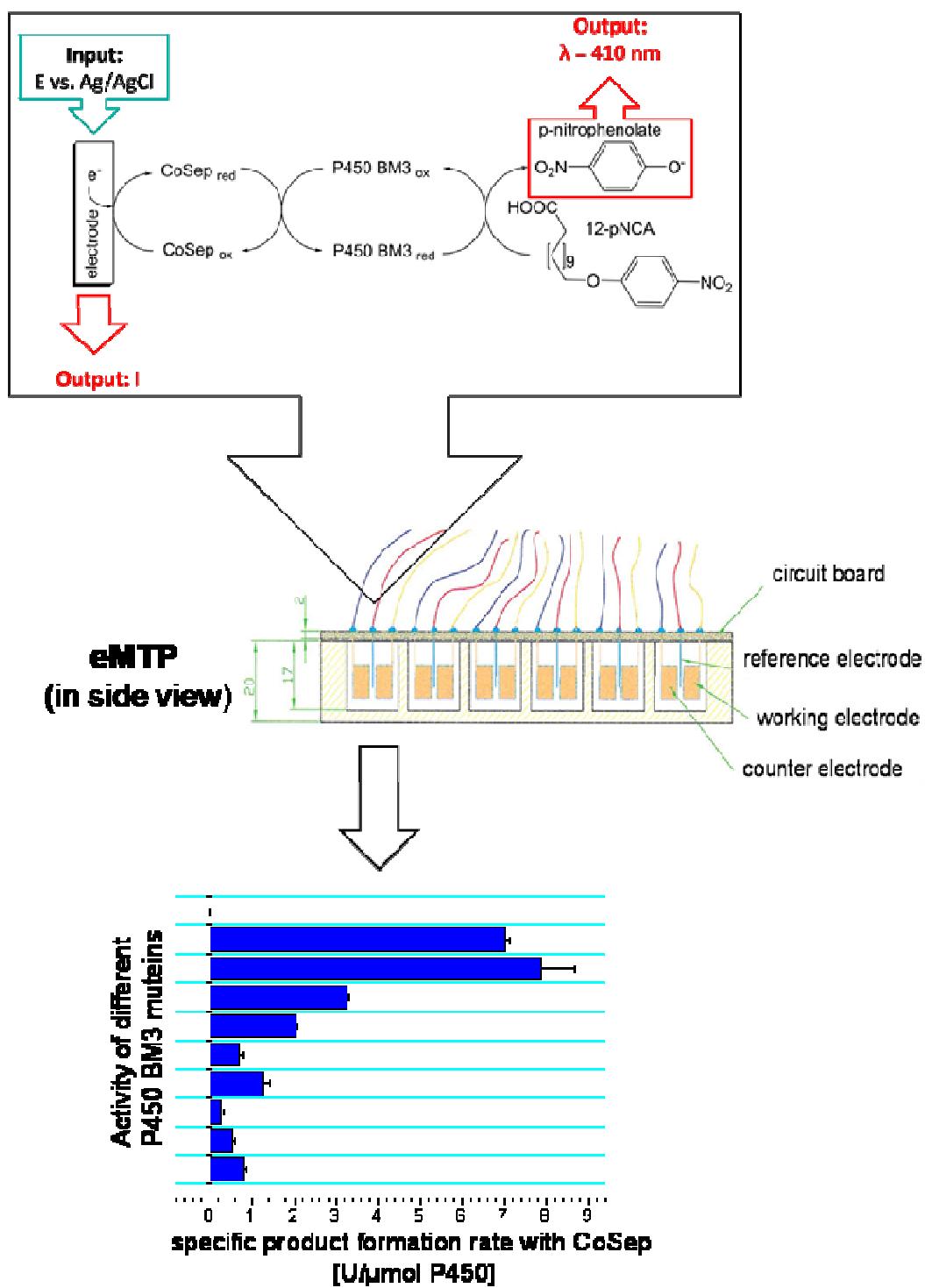


Figure 5

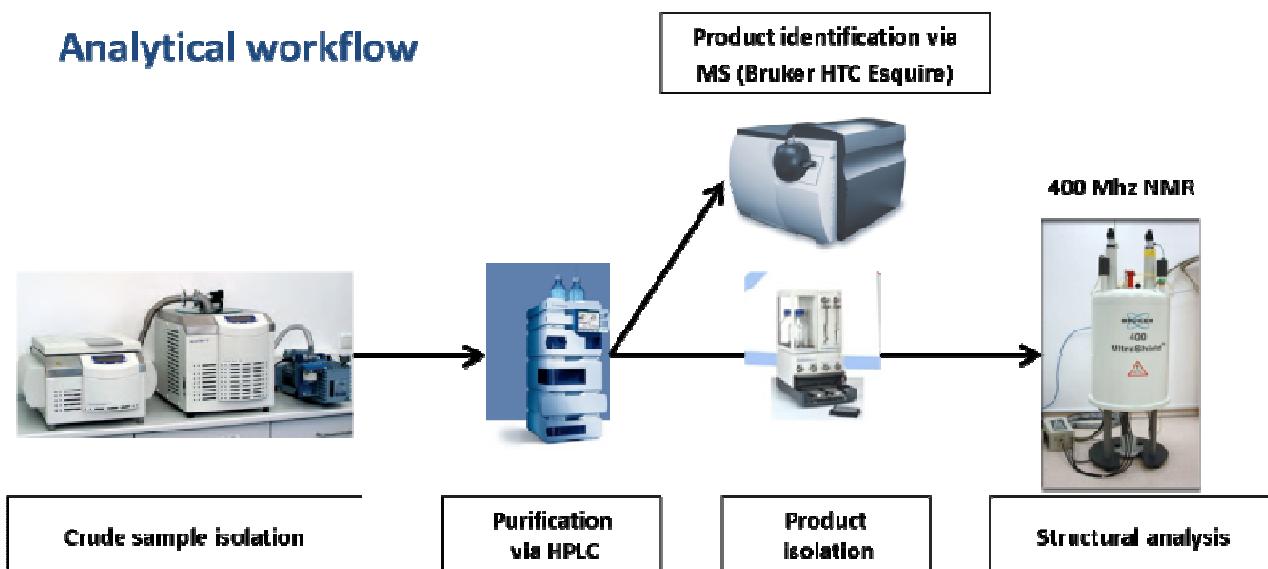


Figure 6

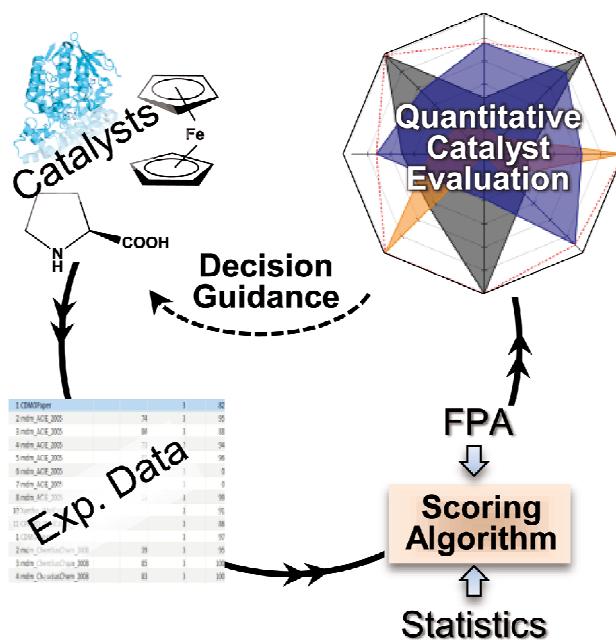


Figure 7. Logic process schematic for quantitative evaluation of the developed generic catalyst performance algorithm.

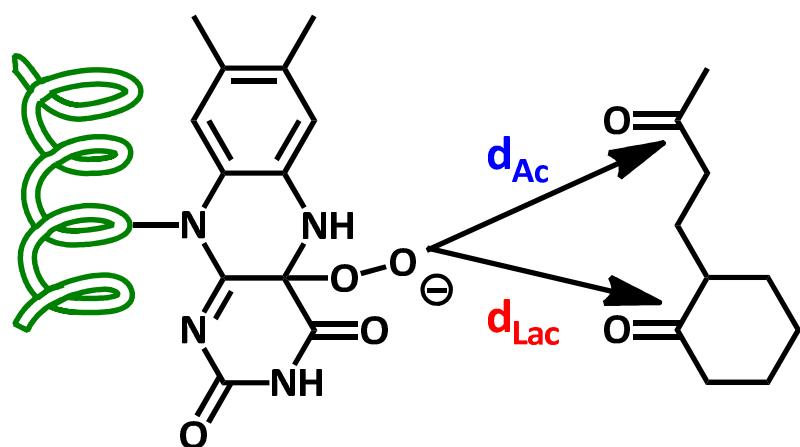


Figure 8. Illustration of the central hypothesis in regioselectivity prediction by distance measurement.

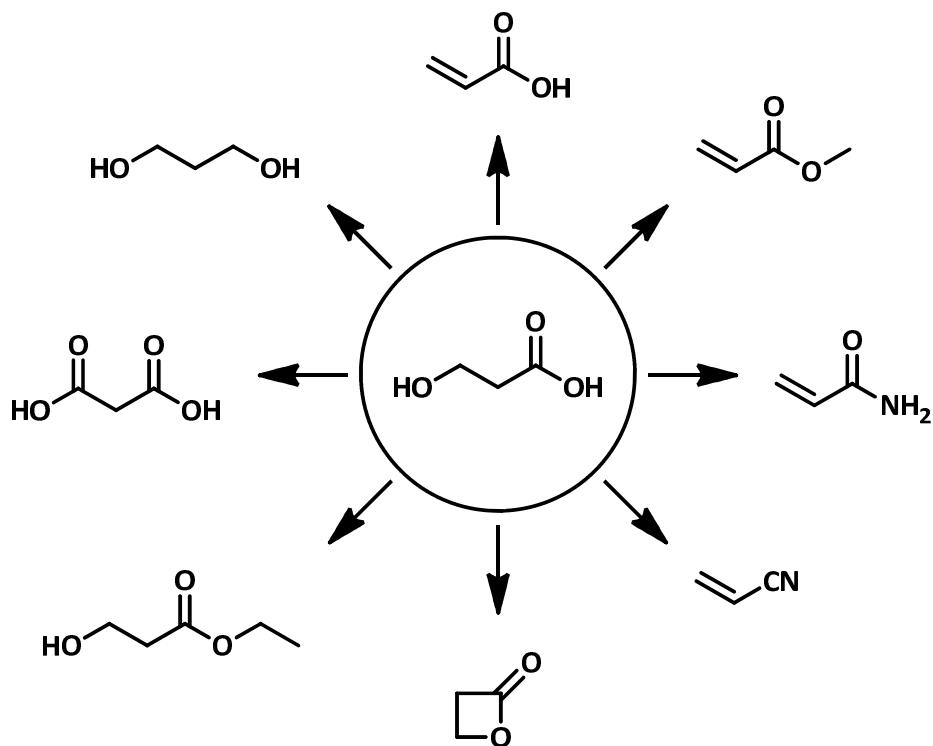


Figure 9. Derivatization pathways of 3-hydroxypropionic acid towards commodity chemicals.

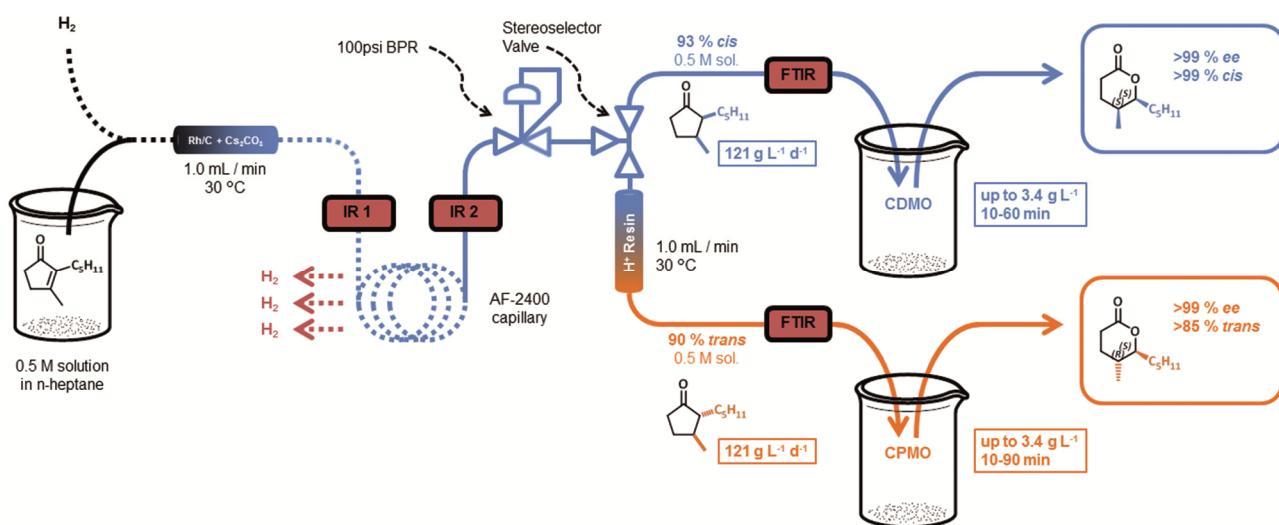


Figure 10. Process flow scheme for the combined continuous flow reactors for transition-metal-catalyzed heterogeneous hydrogenation and ion-exchange polymer catalyzed epimerization and the subsequent batch biotransformations.

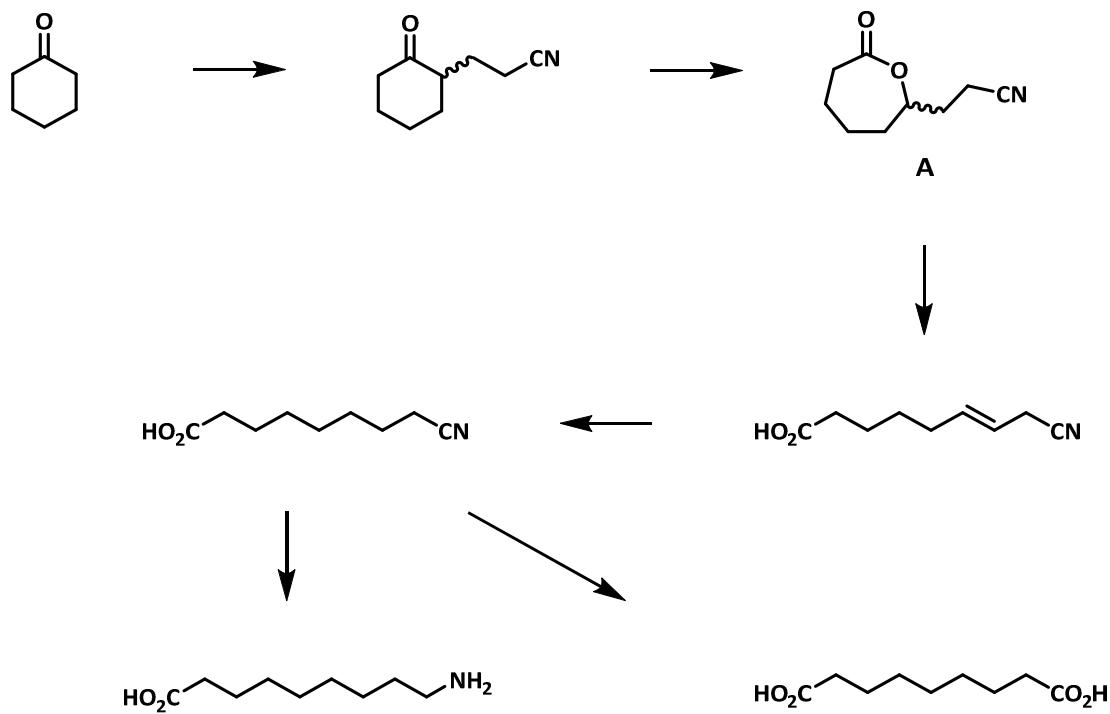


Figure 11. Cotarca's pathway towards polyamide-9 monomers, azelaic acid and 9-aminopalargonic acid via B-V oxidation and lactone pyrolysis.

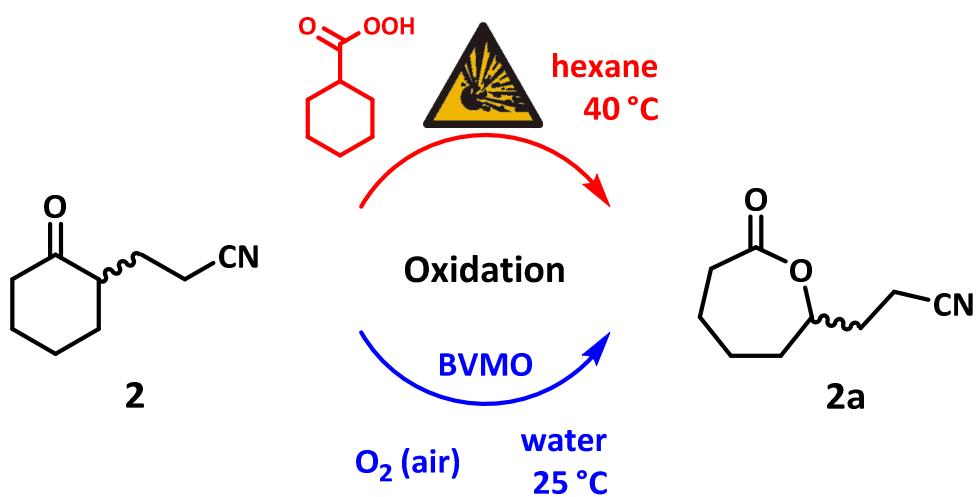
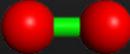


Figure 12. Green chemistry optimization potential in the biocatalytic synthesis of polyamid-9 monomers.

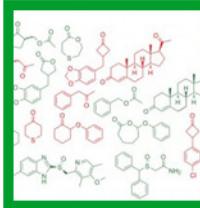

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Oxygreen Tools – Effective redesign of enzymes for green chemistry

Life is based on the ability of living systems to perform an enormous array of chemical reactions. This ability is made possible by the existence of enzymes, which can achieve rates that are simply beyond the limits of "classical" chemical methods. Such a terrific catalytic power is coupled to an exquisite degree of specificity: enzymes are extremely effective in dealing only with certain molecules and in avoiding the generation of unwanted byproducts. These features make enzymes obviously attractive for industrial applications. However often enzymes do need improvements before their use in industry is feasible. That is where we come in; Oxygreen services provides expertise for not only [Enzyme engineering](#), but also [Enzyme collection & Application testing](#), [Enzyme discovery & Production](#), [Enzyme Kinetics & Structures](#) and [Enzyme assays & Screening](#). This expertise was developed during our work for the [Oxygreen project](#). Although in the Oxygreen project work was done on oxygenating enzymes, in particular Baeyer-Villiger Monooxygenases, non-heme iron dioxygenases and P450 monooxygenases, most of the tools are useful for other types of enzymes as well. Please feel free to contact us in case of any questions.

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Enzyme Collections & Application Testing

During the Oxygreen-project a large number



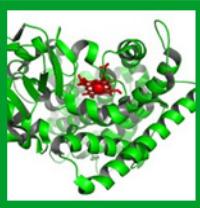
Enzyme Discovery & Production

We have ample experience in the discovery of novel



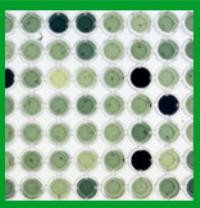
Enzyme Engineering Methods

We have ample experience in creating and screening mutants



Enzyme Kinetics & Structures

For engineering of enzymes it is important to know how the catalytic mechanism



Enzyme Assays & Screening Methods

We have ample expertise in developing and using numerous

Figure 13. Home page of the OxyGreen Services website www.enzymedesign.org.