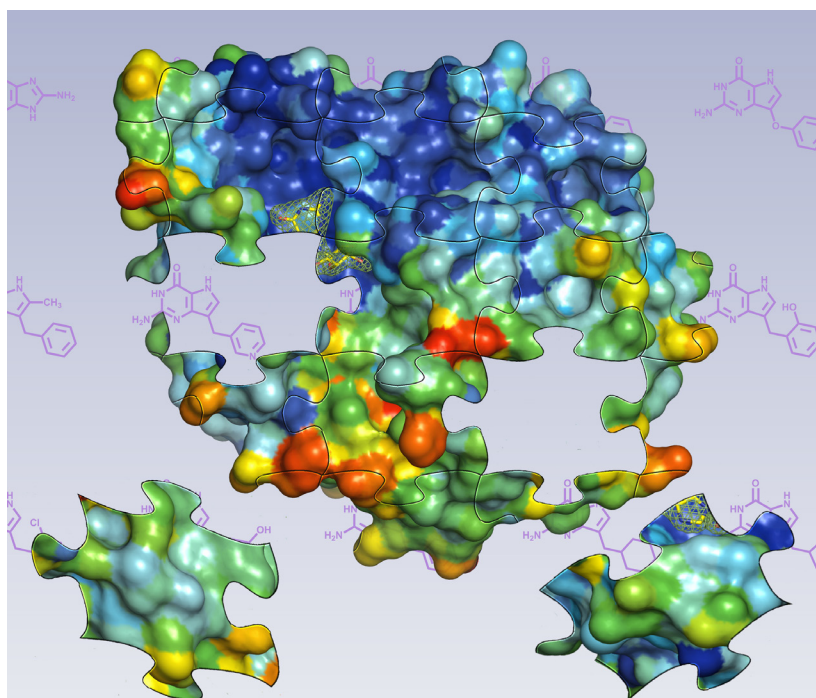


Cover Picture



Structure-based drug design (SBDD) methods play a crucial role in modern medicinal chemistry, and continue to expand and evolve in response to scientific and technological developments. These creative and knowledge driven approaches require a substantial understanding of the multiple intermolecular interactions that affect the binding affinities of protein-ligand complexes within well-defined binding pockets. The cover picture is a tridimensional flexible puzzle, which brings together a general idea of the components that describe the essential structural features of inhibitor drug design. Each piece of this puzzle is fitted into place and interacts with each other element, so that the real binding mode is revealed. These complex studies incorporate aspects of molecular biology, enzymology, biochemistry, structural biology, molecular modeling, medicinal chemistry and drug design. The cover picture also emphasizes how the integration of experimental and *in silico* strategies led to the identification of potent competitive inhibitors of the enzyme purine nucleoside phosphorylase from *Schistosoma mansoni* (SmpNP), as drug candidates for the treatment of schistosomiasis.

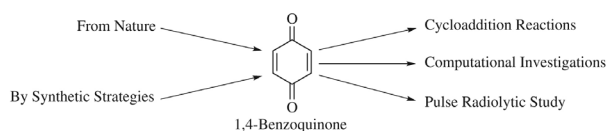
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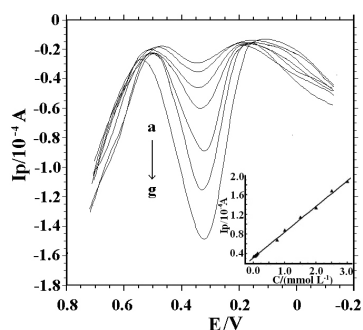
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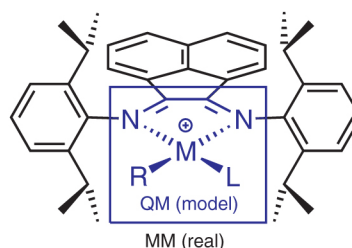


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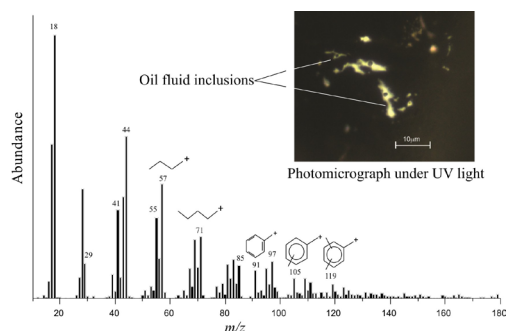


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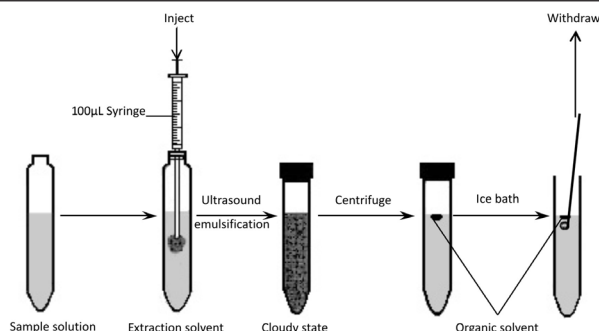


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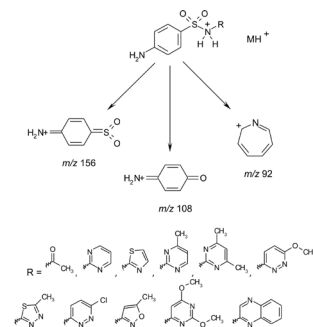


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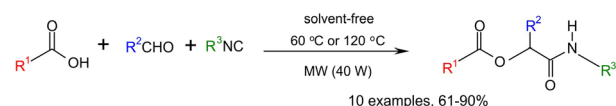
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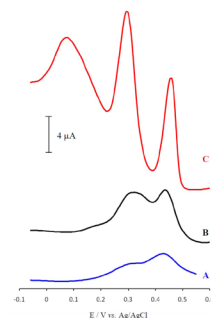
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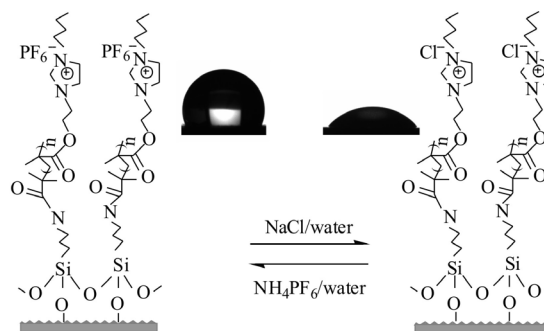
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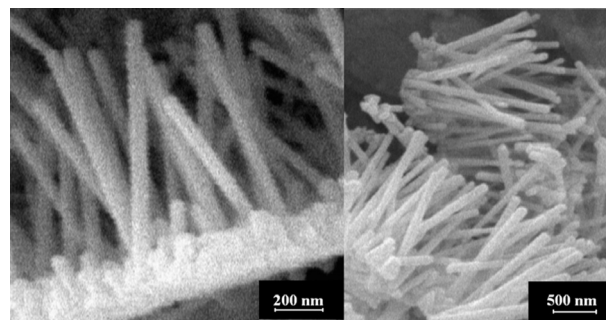
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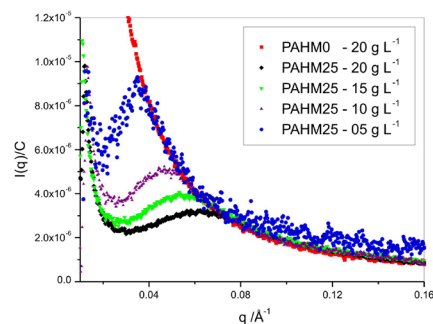
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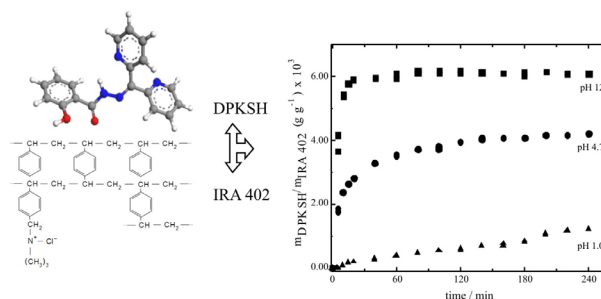
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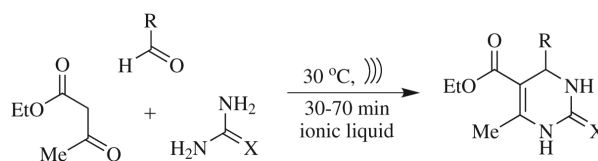
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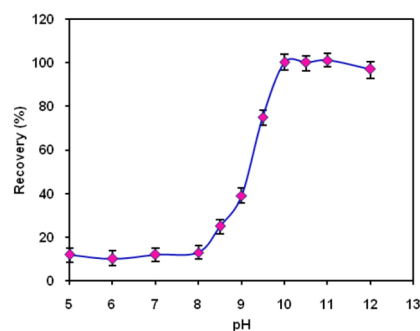
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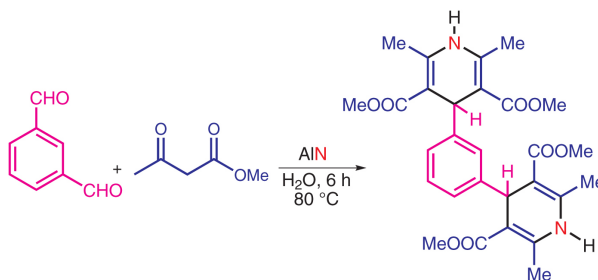
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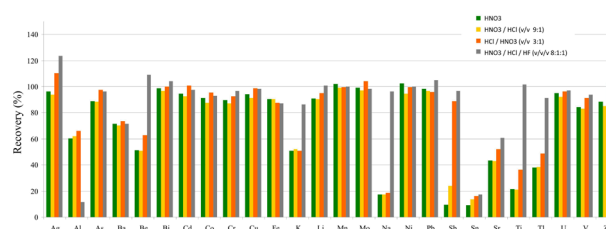
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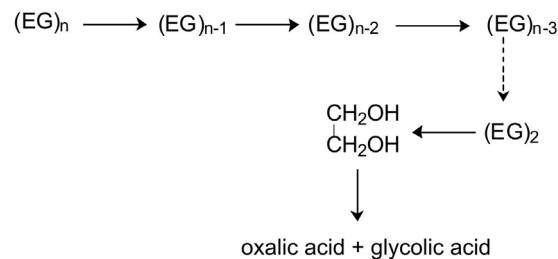


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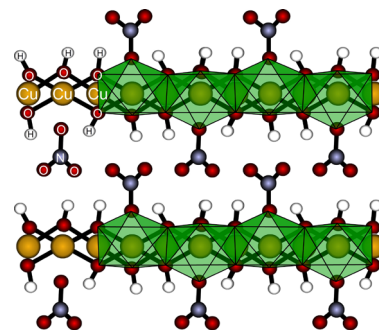


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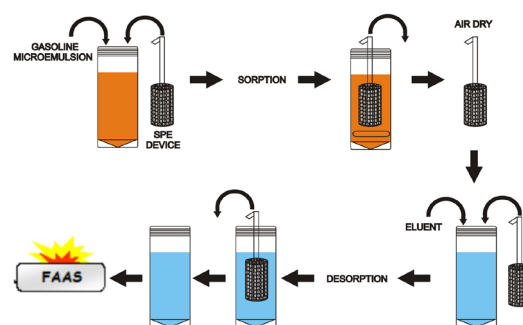


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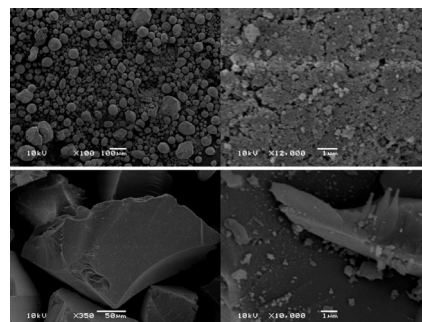
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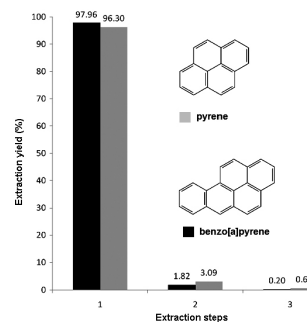


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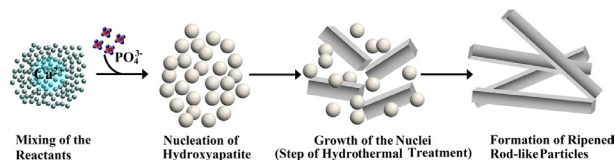


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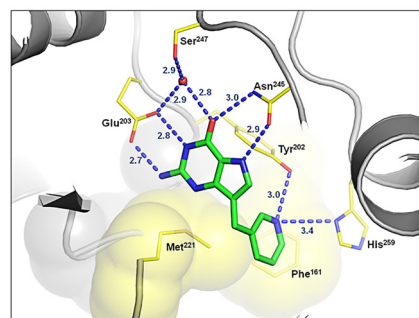


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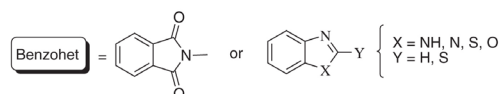
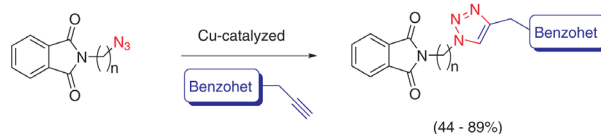
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