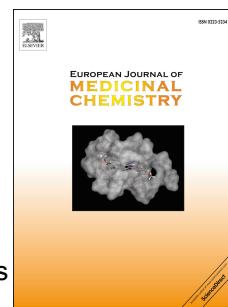


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Rational design of novel TLR4 ligands by *in silico* screening and their functional and structural characterization *in vitro*

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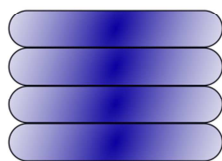
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Ligand database



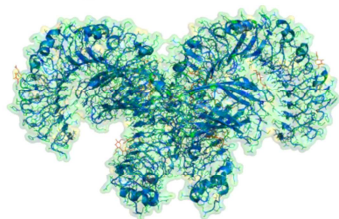
Supercomputer



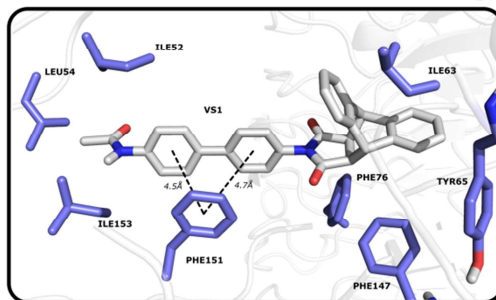
Organic synthesis



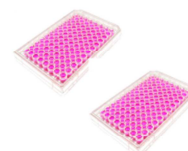
Target TLR4-MD2



Structure-based virtual screening



Biochemistry



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