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COMPOSITE AROMATIC BOXES FOR ENZYMIC TRANSFORMATIONS OF QUATERNARY AMMONIUM SUBSTRATES

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Abstract:

Cation–p interactions to cognate ligands in enzymes have key roles in ligand binding and enzymatic catalysis. We have deciphered the key functional role of both charged and aromatic residues within the choline binding subsite of CTP:phosphocholine cytidyltransferase and choline kinase from *Plasmodium falciparum*. Comparison of quaternary ammonium binding site structures revealed a general composite aromatic box pattern of enzyme recognition sites, well distinguished from the aromatic box recognition site of receptors.

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