Cover Picture

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The cover picture shows a model of the BACE-1 enzyme represented in ribbon mode with the catalytic site highlighted as a grey Connolly surface. The binding site is filled with six BACE-1 inhibitors in their docked conformations and coloured according to conserved interaction points. Theoretical studies of inhibitor binding allowed us to delineate an exhaustive nine-point pharmacophore model (upper right), which captures both the common geometric and the electronic features essential for enzyme inhibition. Interestingly, five of these points are present in all the inspected ligands (blue spheres), thus they can be referred to as essential features for inhibitor recognition and binding, whereas the other four points (light-blue spheres) contribute to BACE-1 selective inhibition. For more details, see the Full Paper by L. Marinelli et al. on p. 667 ff.