Structural and histone binding ability characterization of the ARB2 domain of a histone deacetylase Hda1 from *Saccharomyces cerevisiae*

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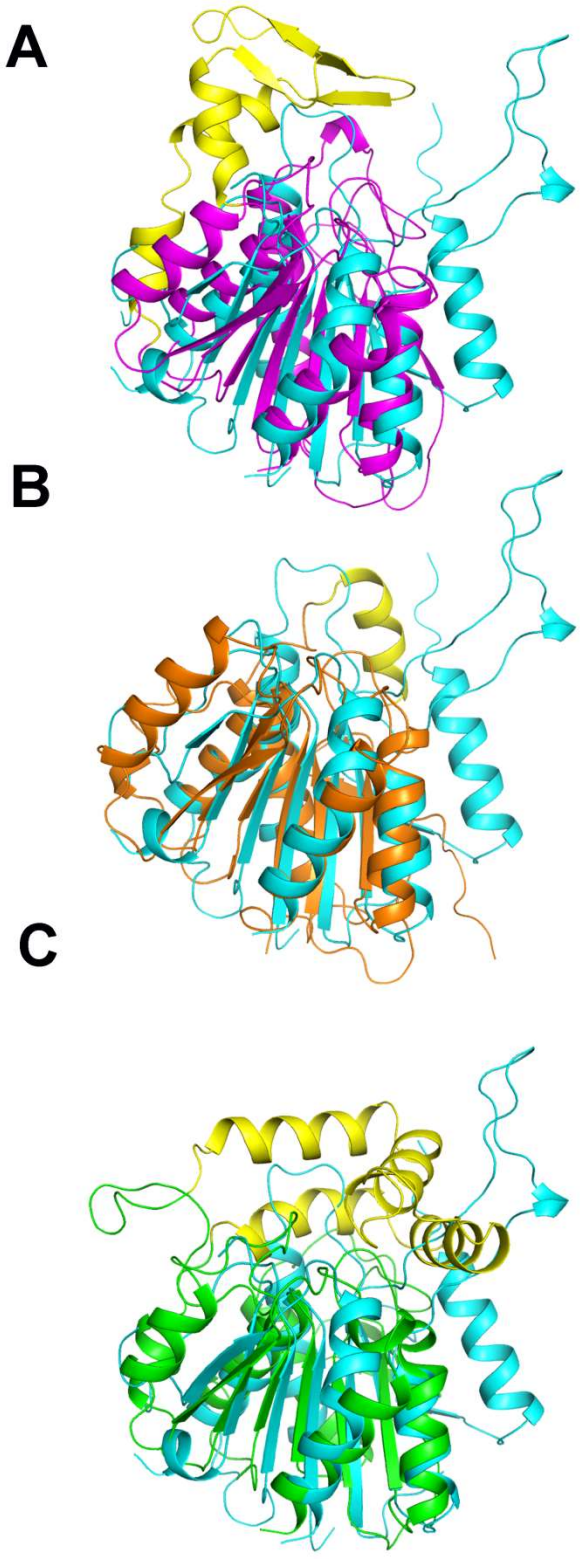
Supplementary Figure 1



Supplementary Figure 1. Structural superposition of the ARB2 domain of Hda1 with cinnamoyl esterase LJ0536 from *Lactobacillus johnsonii* (A), the dienelactone hydrolase (YP_324580.1) from *Anabaena variabilis* ATCC 29413 (B) and the methyl dl-beta-acetylthioisobutyrate esterase from *Pseudomonas putida* IFO 12996 (C). The ARB2 domain of Hda1 are colored in cyan. The cinnamoyl esterase LJ0536, dienelactone hydrolase (YP_324580.1) and methyl dl-beta-acetylthioisobutyrate esterase are colored in magenta, orange and green, respectively. The inserted subdomain of the cinnamoyl esterase LJ0536, dienelactone hydrolase (YP_324580.1) and methyl dl-beta-acetylthioisobutyrate esterase are colored in yellow. The inserted subdomain of the cinnamoyl esterase LJ0536 displays an open canal-like feature, consisting of three α-helices and two short β-hairpins. It constitutes the unique substrate binding pocket of the cinnamoyl esterase and is essential for the enzymatic activity. Instead, the dienelactone hydrolase (YP_324580.1) just contains an α-helix insertion between β4 and helix α1, and the substrate recognition mechanism is still unreported. The methyl dl-beta-acetylthioisobutyrate (dl-MATI) esterase assembles as a homotrimer in both crystals and solution. Each monomer possesses a four helices insertion that encloses a cavity used for substrate accommodation.