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Supporting information for article:

A cautionary tale of structure-guided inhibitor development against an essential enzyme in the aspartate biosynthetic pathway

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Supplemental Figures

Figure S1

Model of 3-(3-carboxypropyl)phthalate docked in the active site in two alternative conformations (purple and orange) that each occupy the acetate binding pocket. The 2mFo-DFc electron density from the 1,2,3-benzenetricarboxylate complex with *sp*ASADH/NADP is shown as blue mesh.

Figure S2

Binding of 1,2,3-benzenetricarboxylate in subunit B of the *sp*ASADH complex with NADP. The lack of stabilizing interactions with the cofactor leads to much less well-ordered inhibitor binding.

Figure S3

Binding of 1,2,3-benzenetricarboxylate in subunit A of the *sp*ASADH complex with 2′,5′-ADP, superimposed with the electron density map for 2′,5′-ADP, inhibitor and acetate (2mFo-DFc, 1.9 Å resolution, contoured at 1.5 σ level).

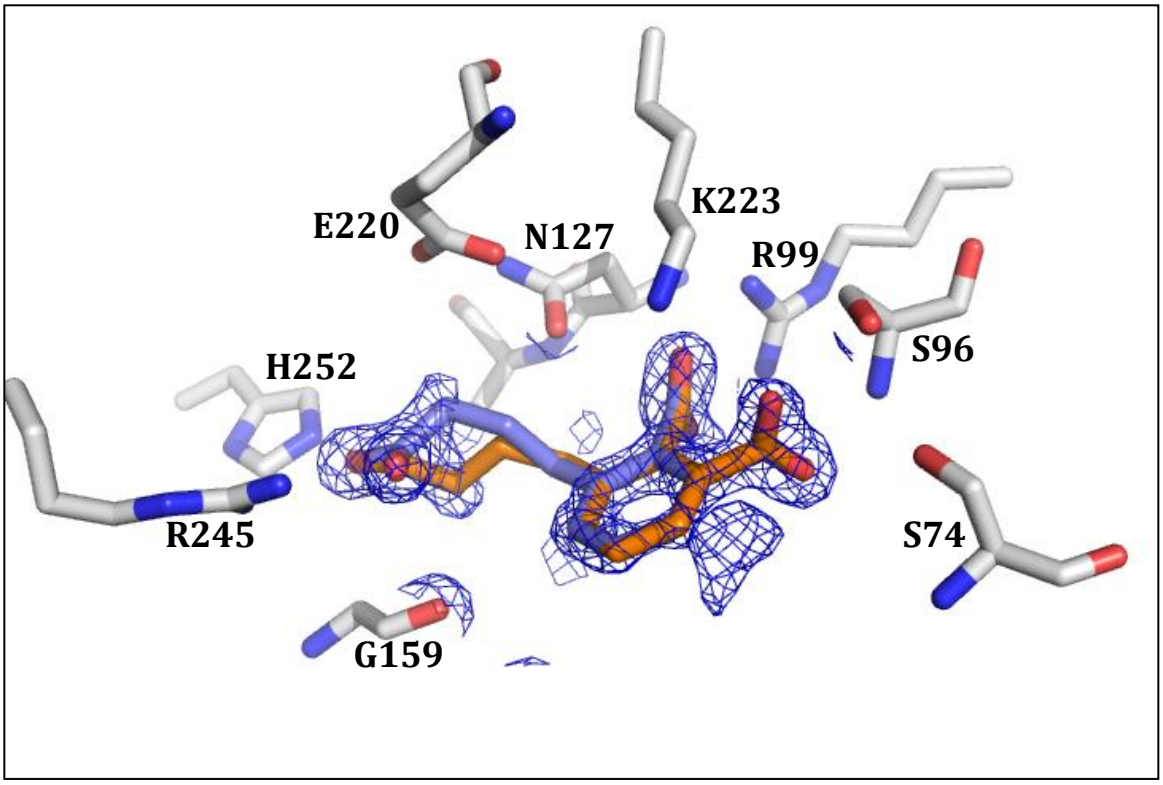

Figure S1

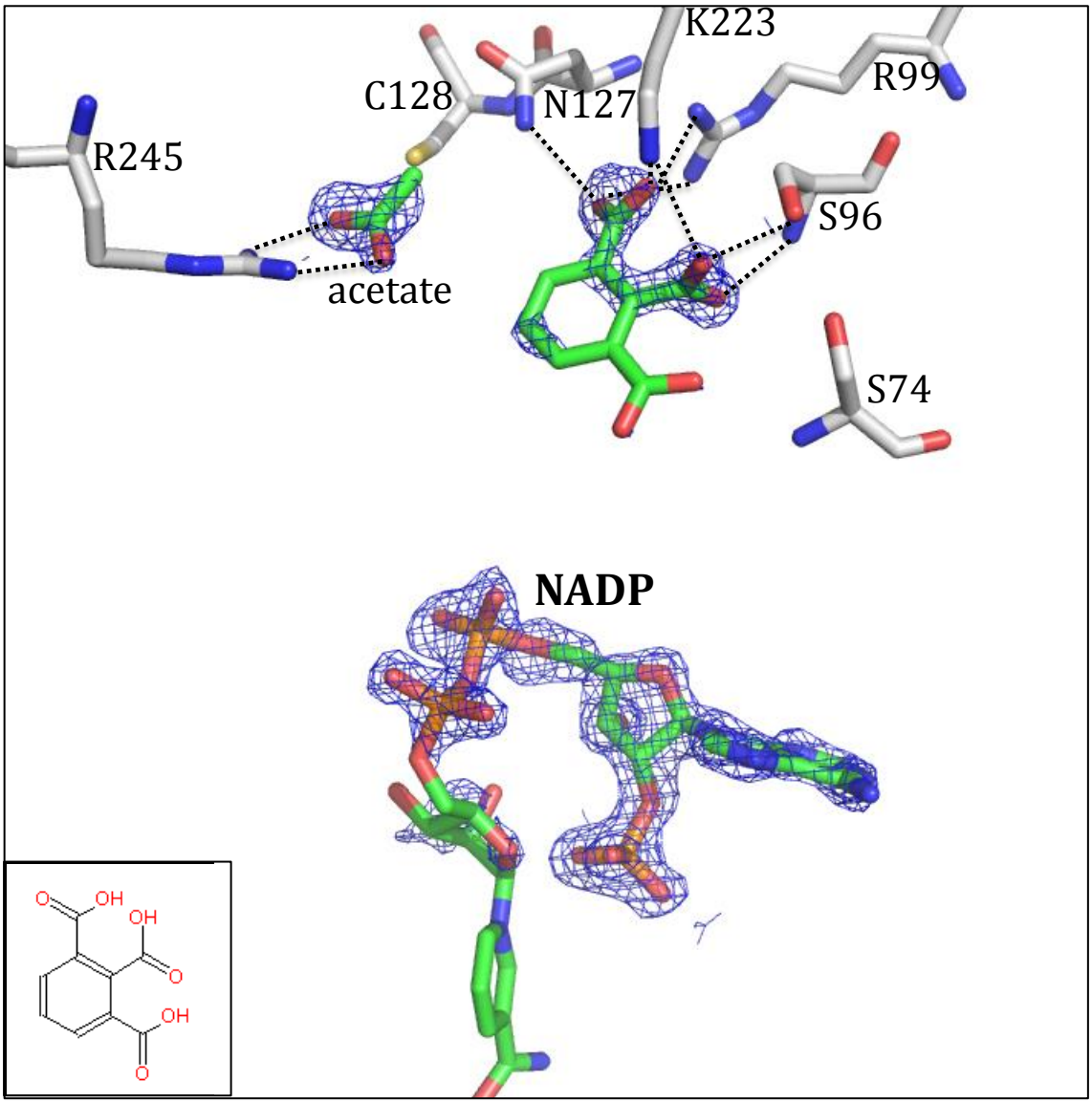

Figure S2

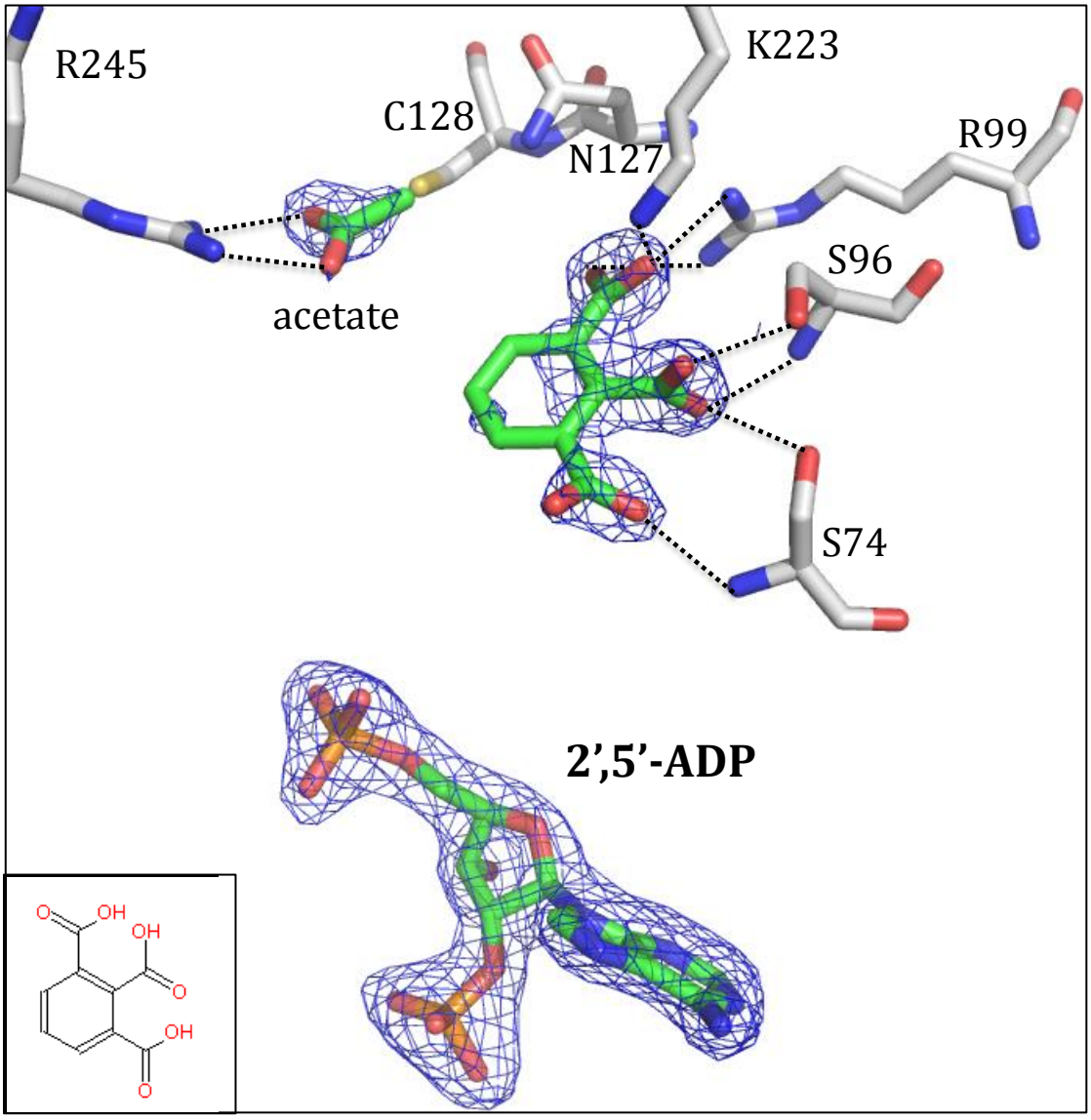

Figure S3