Engineering the OPAA Enzyme for Increased Catalytic Efficiency and Broadened Stereospecificity on Russian VX

Courtney M. Daczkowski [1], Scott D. Pegan*[1,2], and Steven P. Harvey*[3]

[1]Department of Pharmaceutical and Biomedical Sciences, University of Georgia, Athens, Georgia 30602, UGA. [2]U.S. Army Reserve 377th Sustainment Command Detachment 8, Aberdeen Proving Ground, MD 21010-5424, USA [3]U.S. Army Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD 21010-5424, USA

Supplementary Data

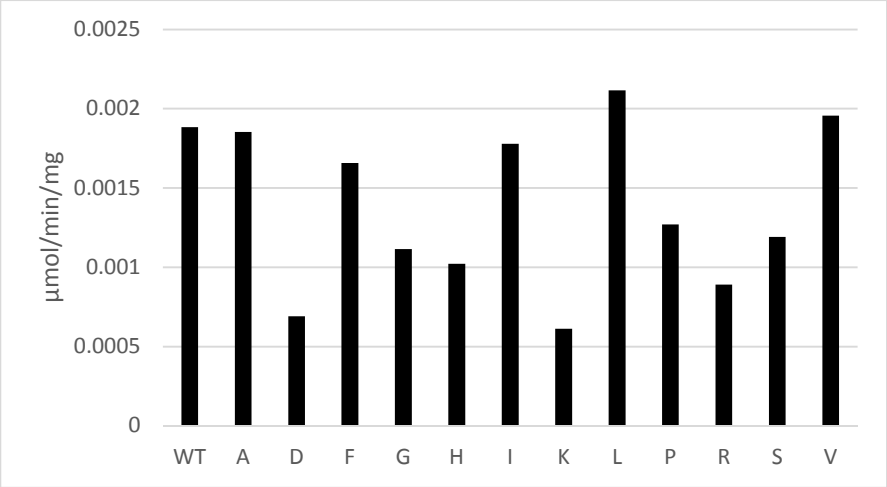

Figure S1. Screening data – specific activities of Y292 mutants on 3 mM VR.

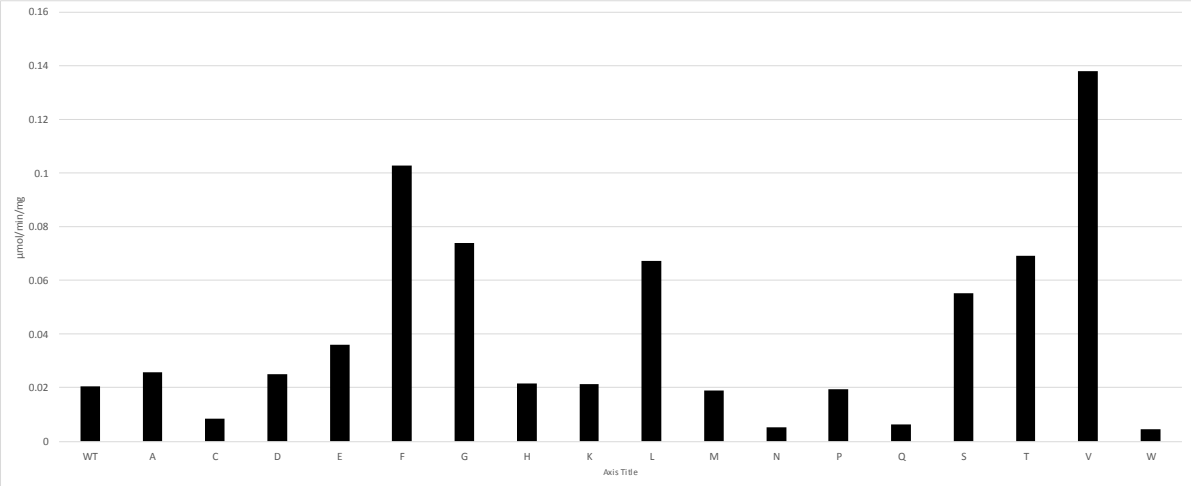

Figure S2. Screening data – specific activities of Y212 mutants on 3 mM VR.

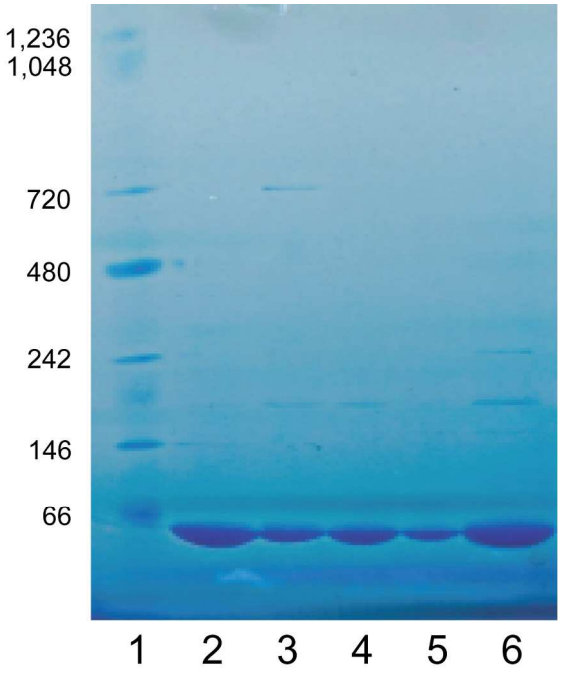

Figure S3. Native gel of wild-type OPAA as well as mutants Y212F, FL, FLY, and FLYD. Lane 1-6; Native MARK unstained protein ladder, wild-type OPAA, OPAA Y212F, OPAA Y212F/V342L (FL), OPAA Y212F/V342L/I215Y (FLY), OPAA Y212F/V342L/I215Y/H343D (FLYD).

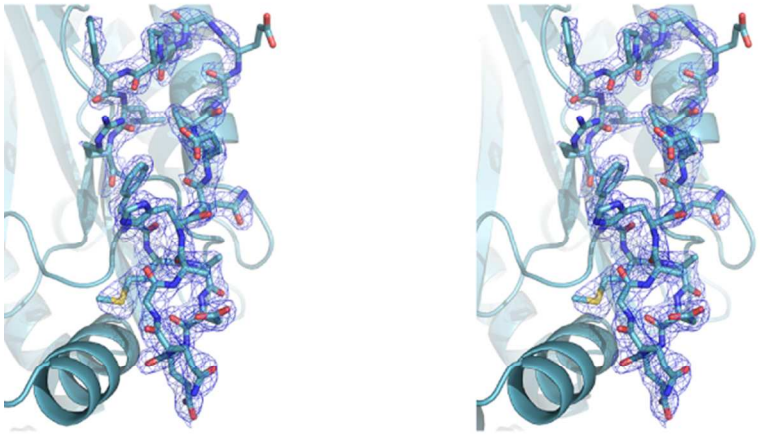

Figure S4. Close up of OPAA Y212 residues 348-365. Wall-eyed stereoview of the Y212F (krypton) with $2F_o$-F_c density scaled to 1 σ (blue mesh).

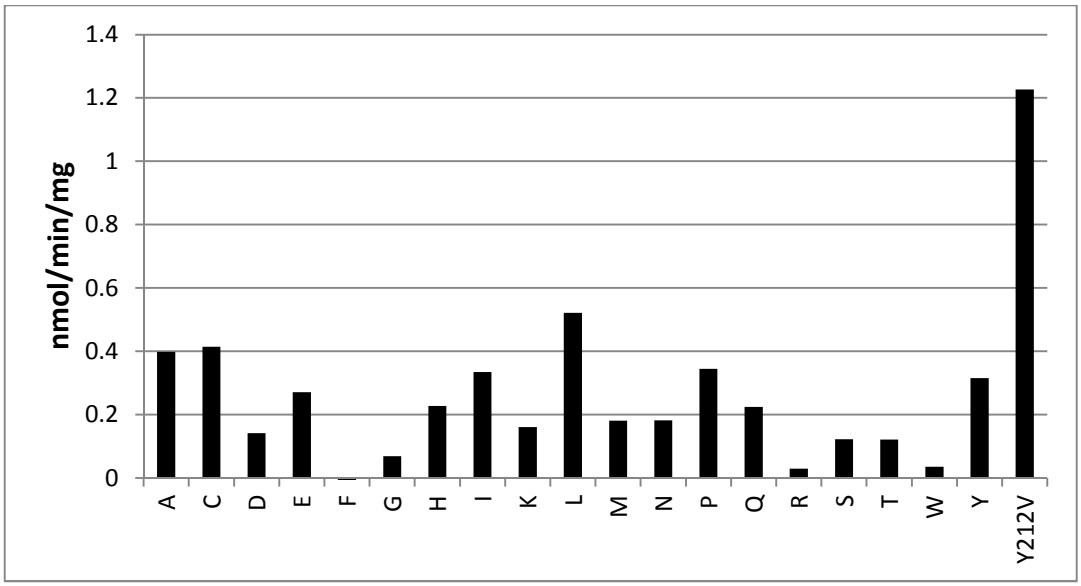

Figure S5. Screening data – specific activities of Y212V/V342 mutants on 3 mM VR.

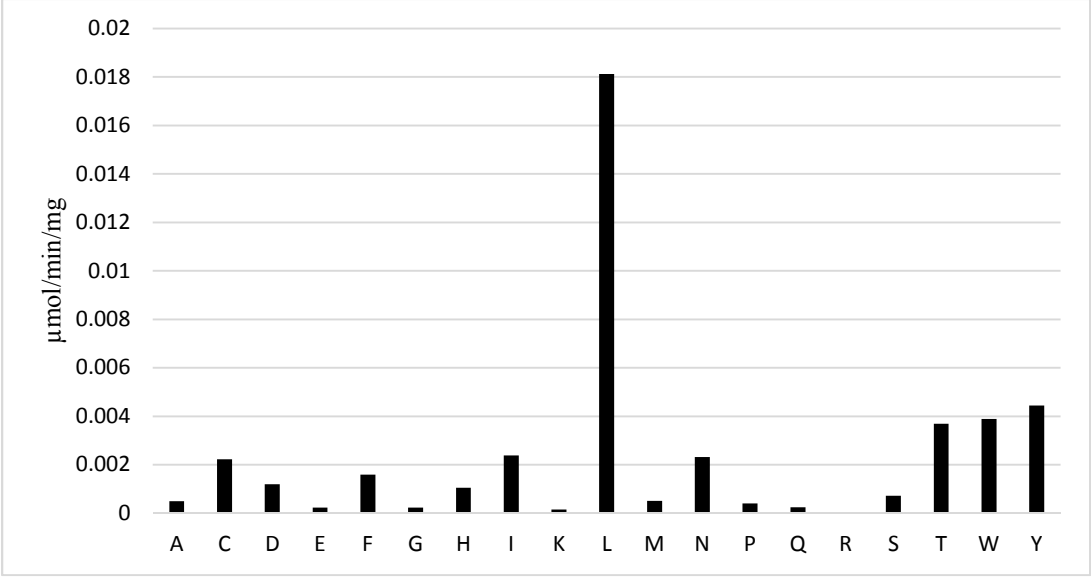

Figure S6. Screening data – specific activities of Y212F/V342 mutants on 3 mM VR.

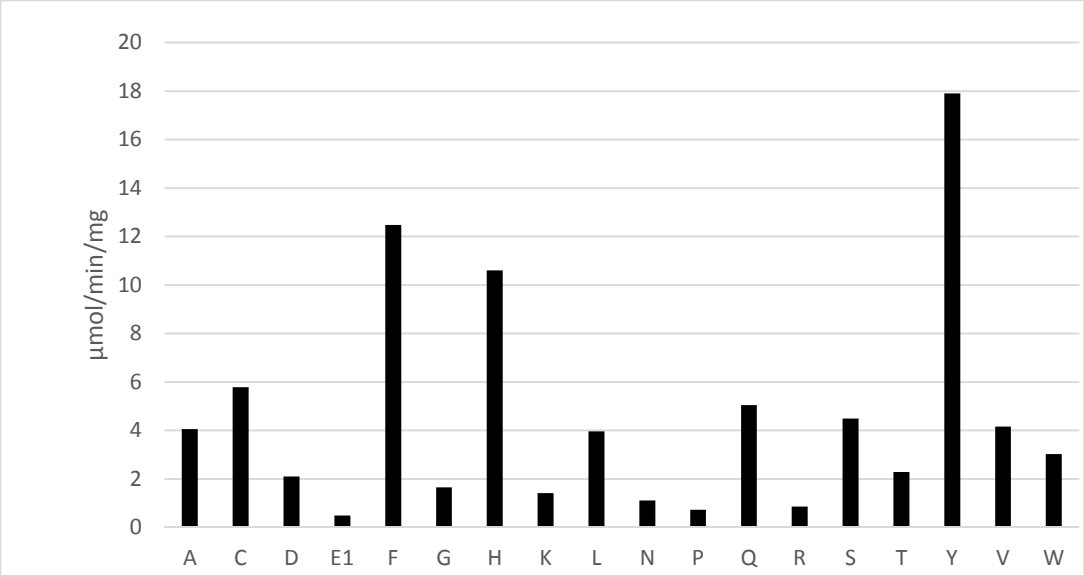

Figure S7. Screening data – specific activities of Y212F/V342L/I215 mutants on 3 mM VR.