

Rational Design of Cyclodextrin Glycosyltransferase with Improved Hesperidin Glycosylation Activity

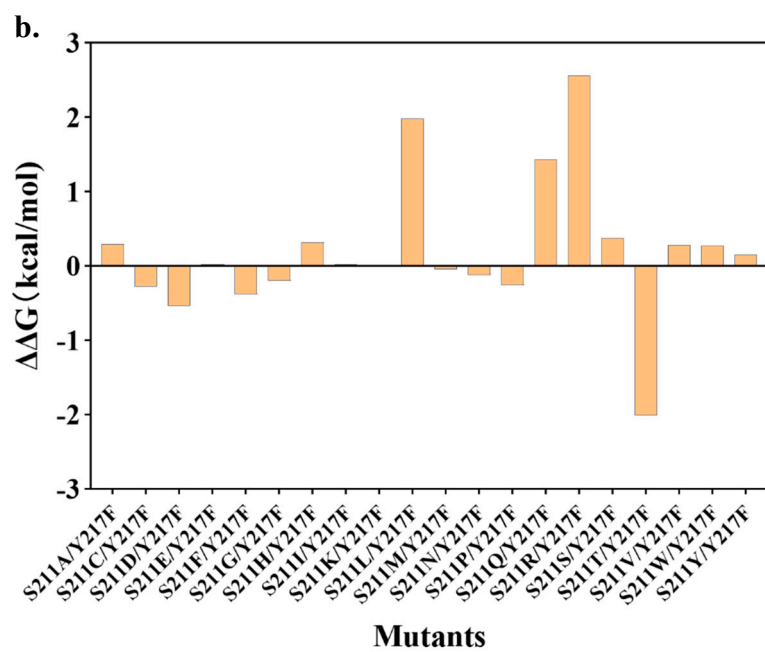
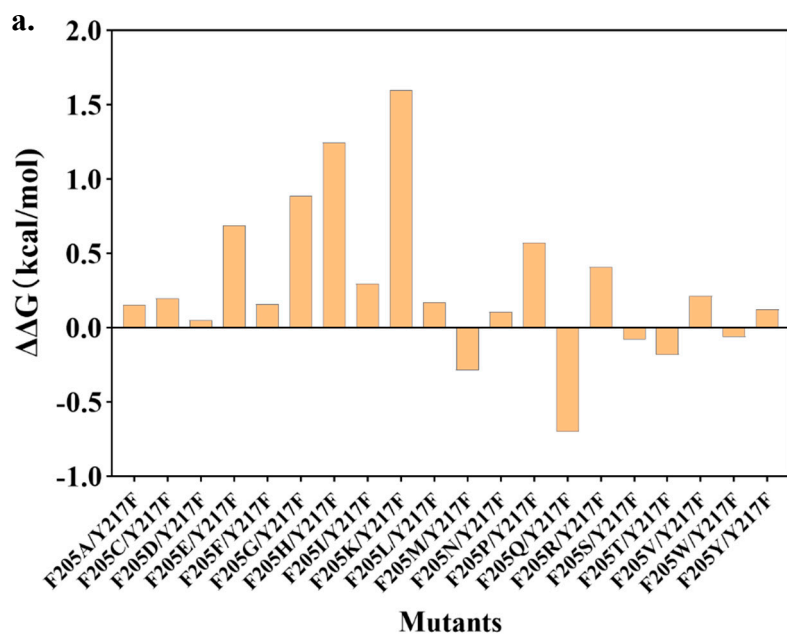
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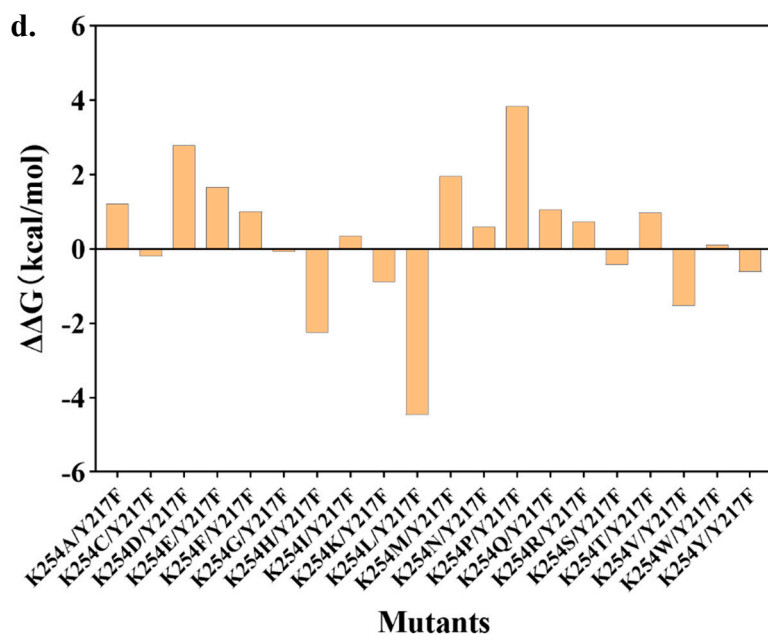
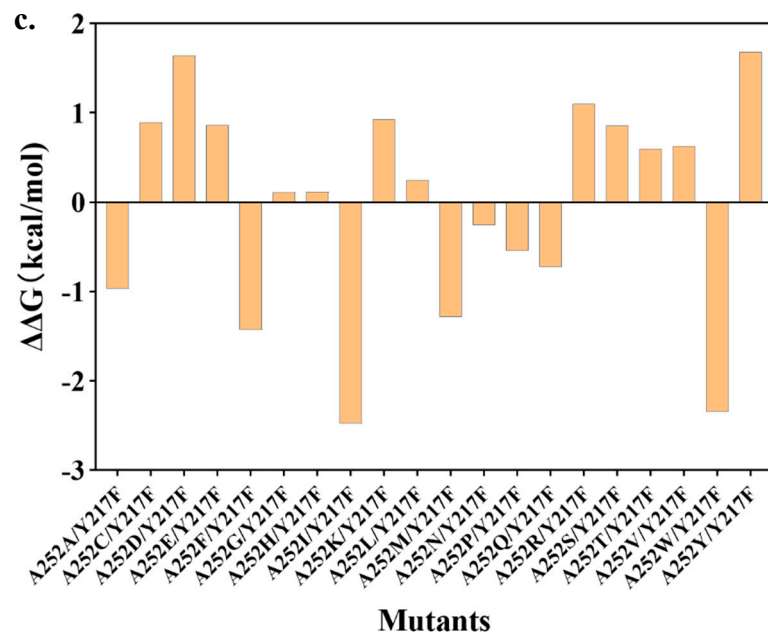
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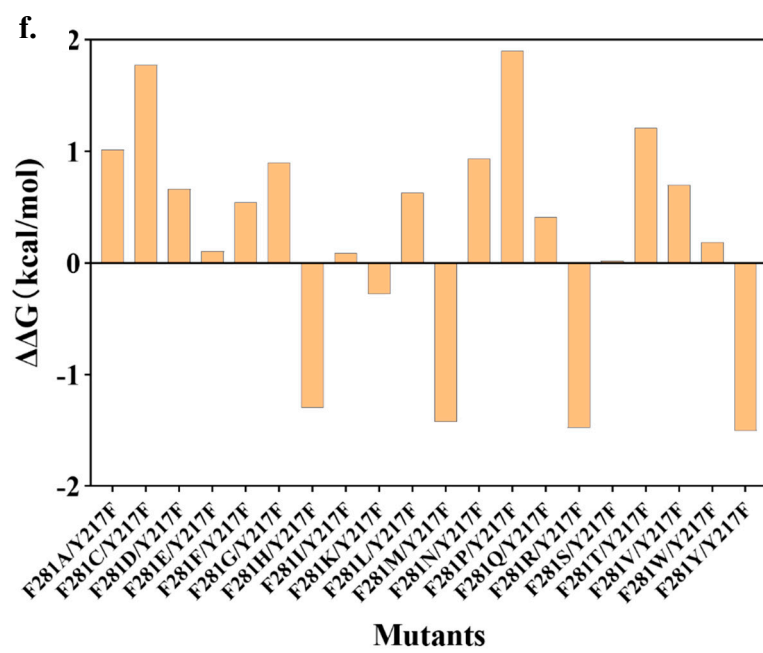
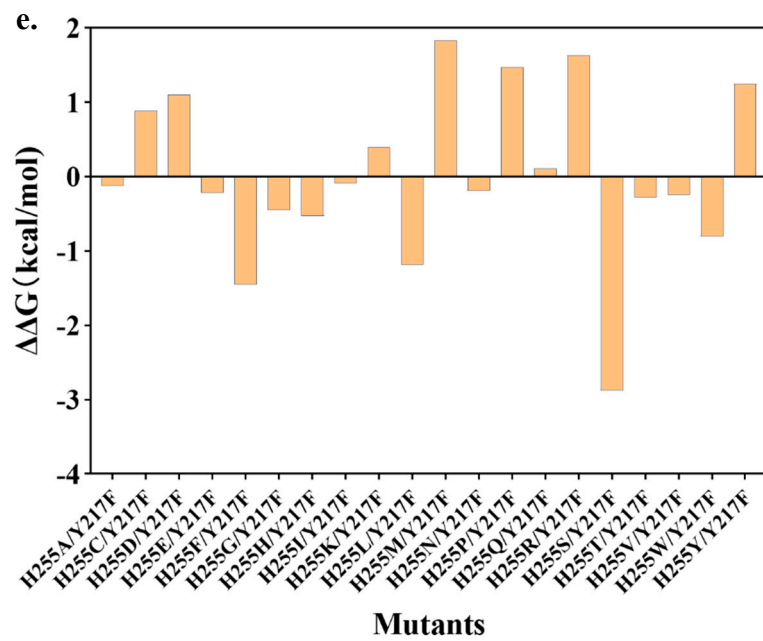
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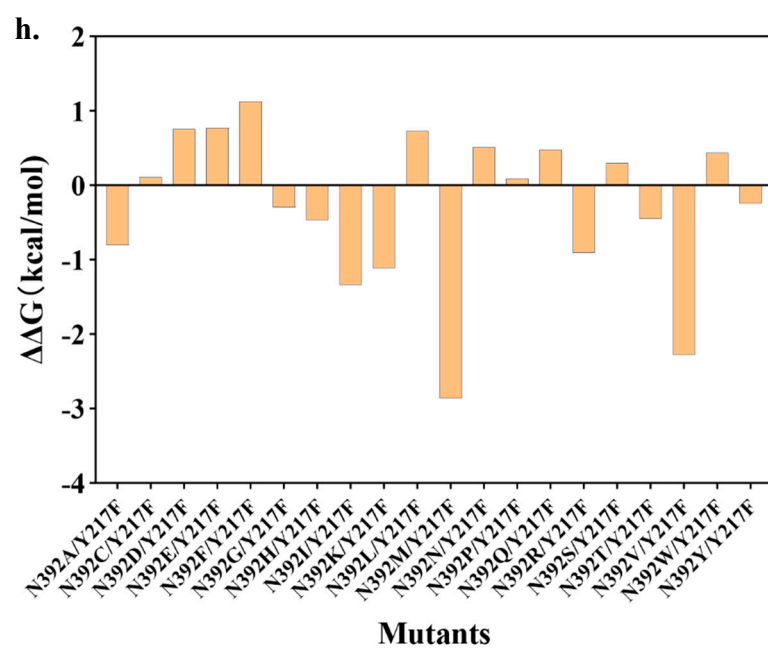
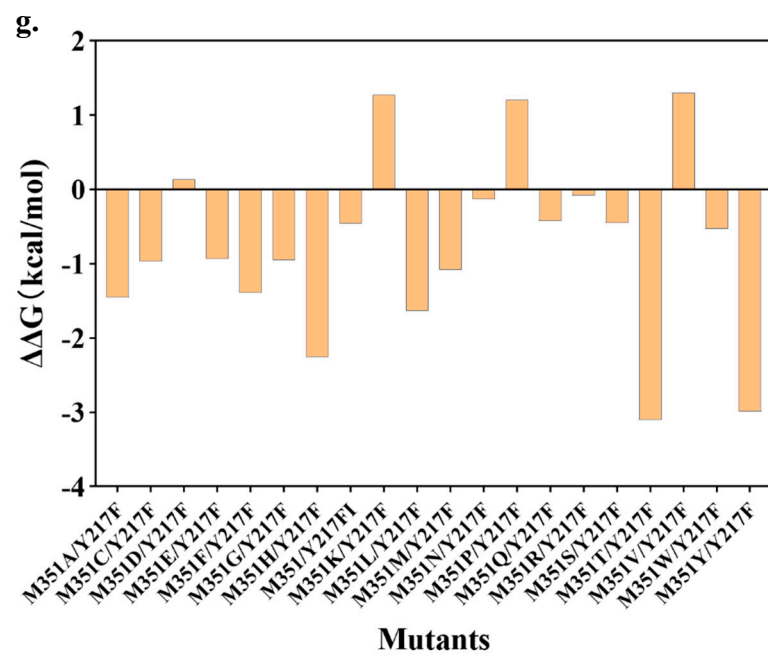
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Supplementary Materials









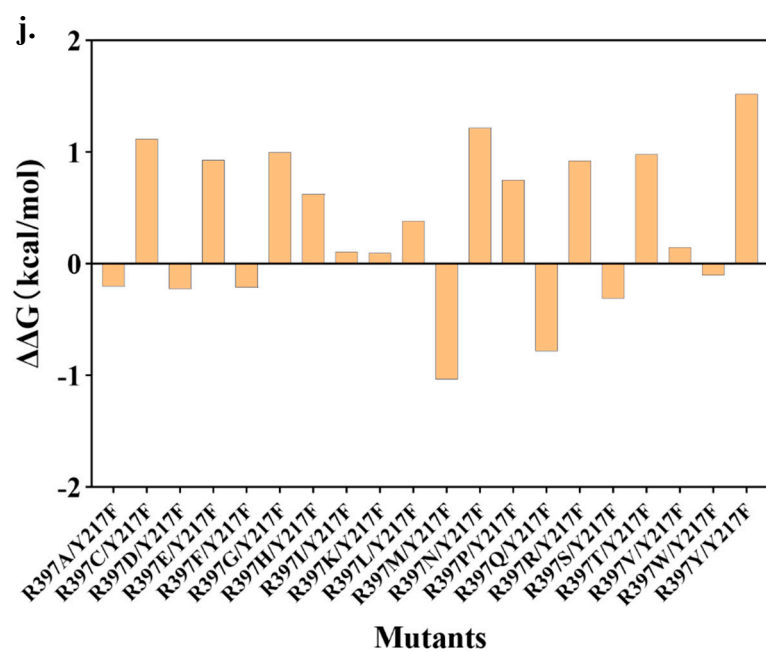
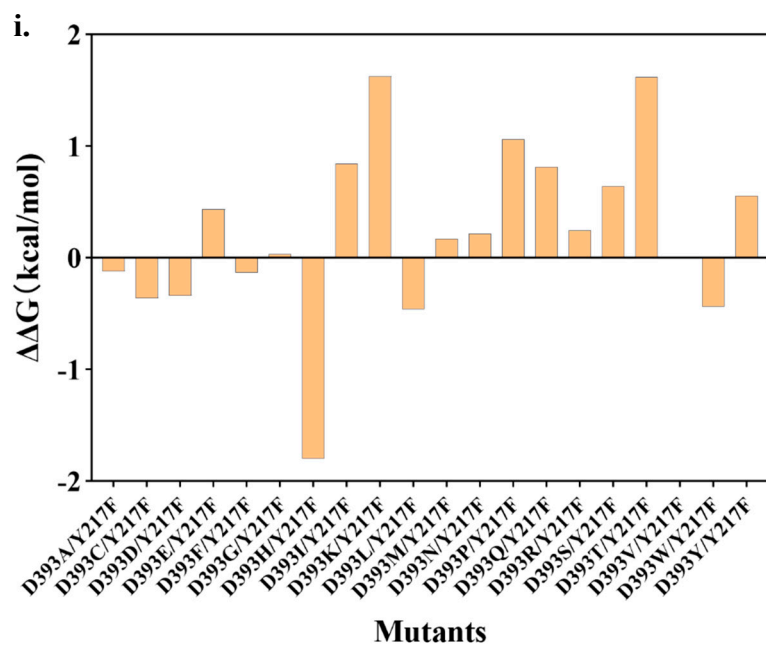


Figure S1. Using CGTase-Y217F as template, change of hesperidin binding energy calculated after saturated virtual mutation of selected residues. (a) F205; (b) S211; (c) A252; (d) K254; (e) H255; (f) F281; (g) M351; (h) N392; (i) D393; (j) R397

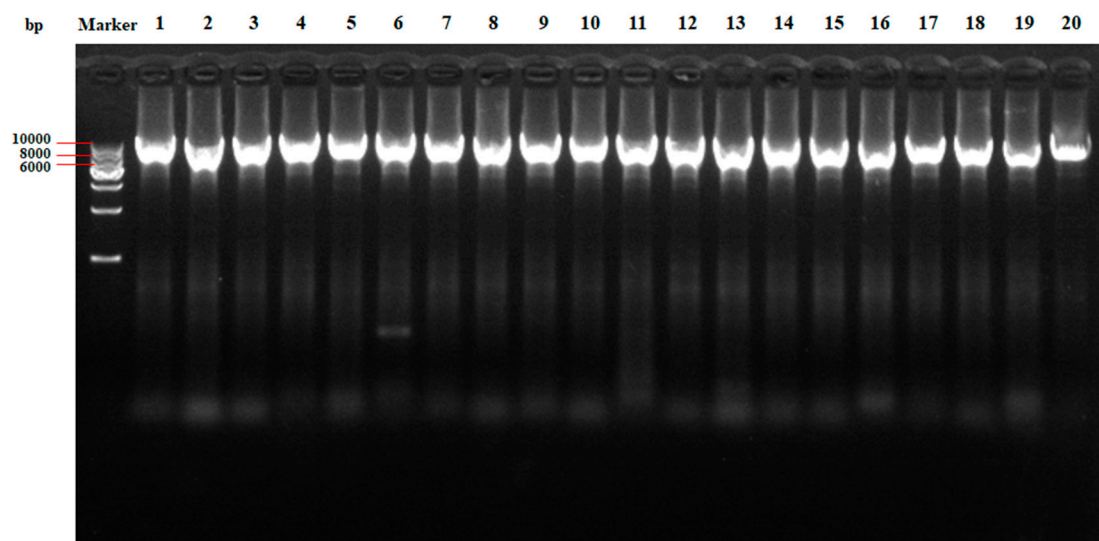


Figure S2. Agarose gel electrophoresis of the designed 20 mutants. Lane 1: S211T/Y217F; Lane 2: Y217F/K254V; Lane 3: Y217F/K254L; Lane 4: Y217F/K254H; Lane 5: Y217F/H255S; Lane 6: Y217F/H255L; Lane 7: Y217F/H255F; Lane 8: Y217F/F281M; Lane 9 : Y217F/F281Y; Lane 10: Y217F/F281R; Lane 11: Y217F/F281H; Lane 12: Y217F/M351T; Lane 13: Y217F/M351F; Lane 14: Y217F/M351L; Lane 15: Y217F/M351A; Lane 16: Y217F/M351Y; Lane 17: Y217F/M351H; Lane 18: Y217F/N392V; Lane 19: Y217F/N392M; Lane 20: Y217F/D393H.

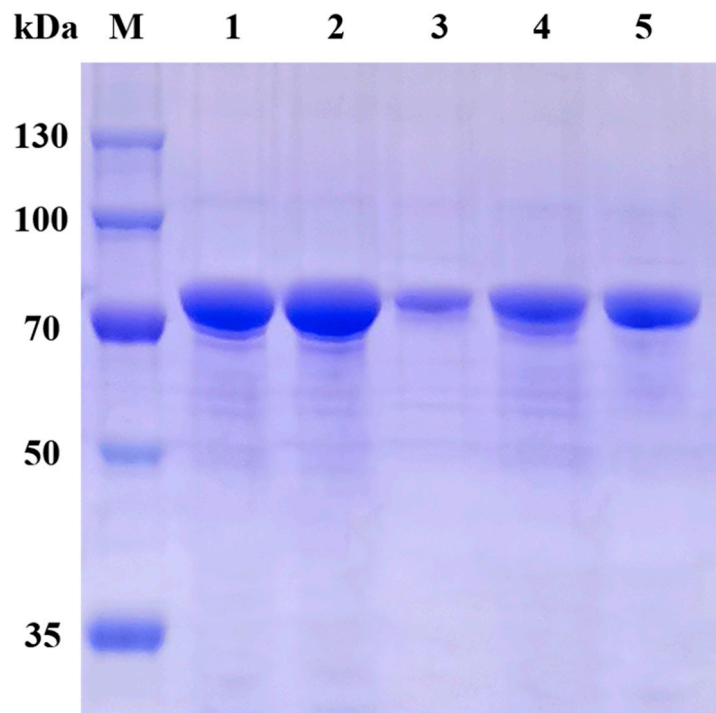


Figure S3: SDS-PAGE of purified CGTase variants. Lanes M: protein marker; Lane 1: Y217F/D393H; Lane 2: Y217F/ M351L; Lane 3: Y217F/ M351F; Lane 4: Y217F/ F281Y; Lane 5: Y217F/ K254L.

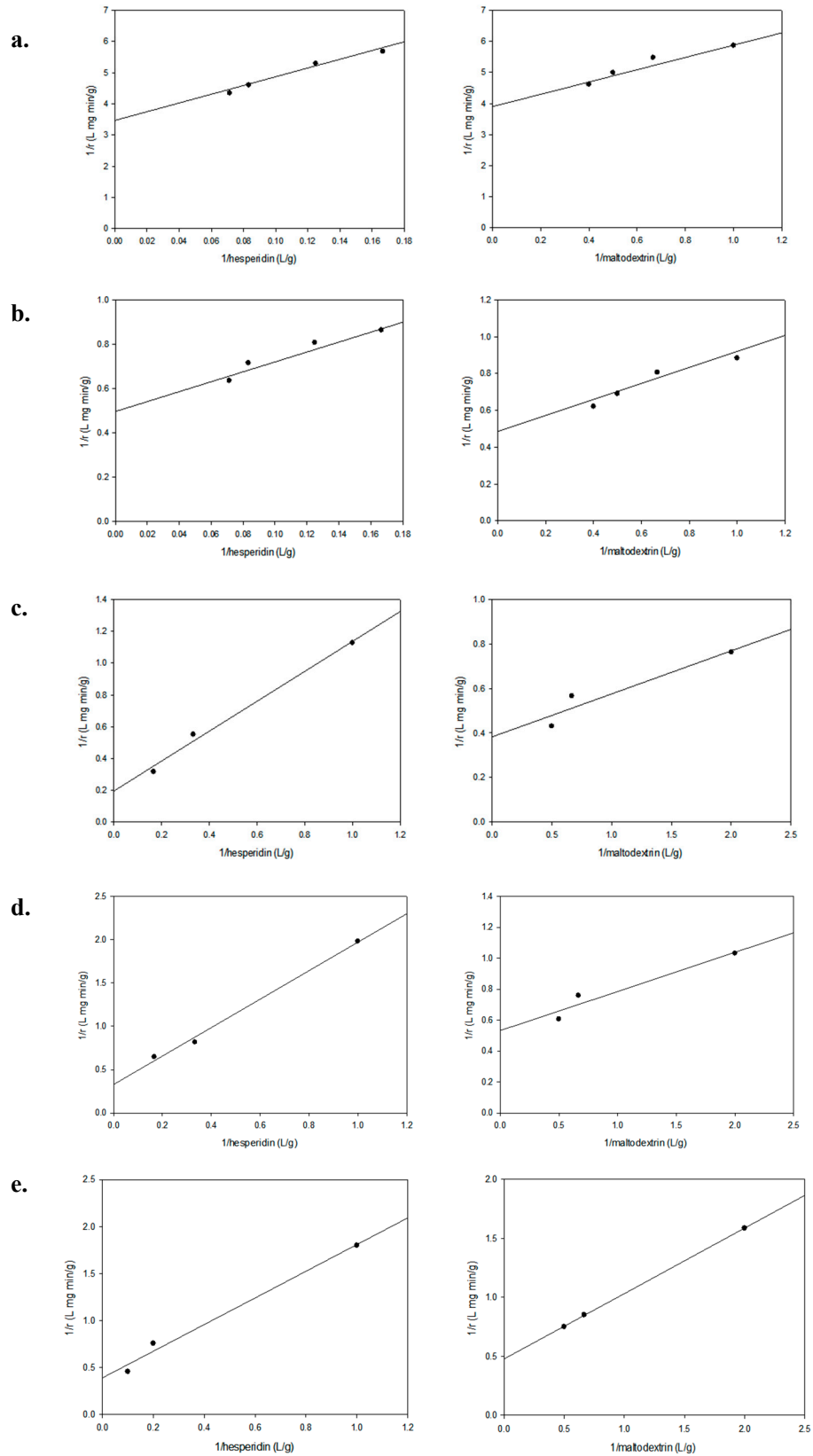


Figure S4. Linearly regressed Lineweaver-Burk plot based on ping-pong mechanism. (a) wild-type; (b) Y217F; (c) Y217F/D393H; (d) Y217F/M351L; (e) Y217F/M351F.