

SUPPLEMENTARY MATERIAL FOR:**Thermodynamic Analysis of Tyrosyl-tRNA Synthetases Revealed
Bacterial-Selective Tyrosine Derivatives**

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1. SDS-PAGE and mass spectral analyses of human TyrRS

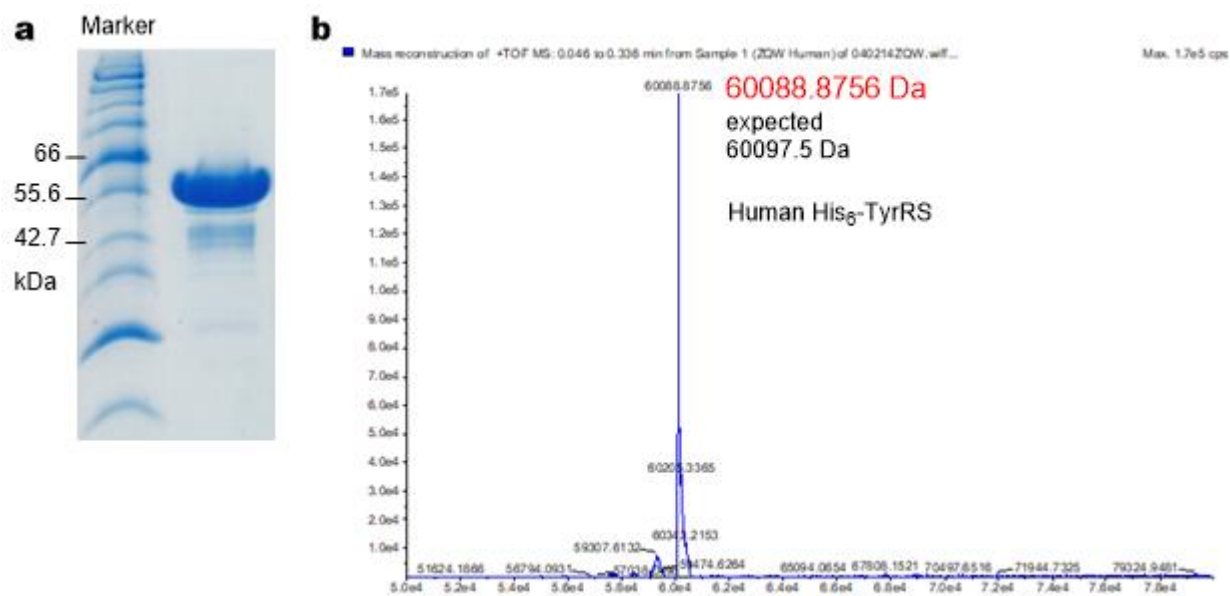


Figure S1. (a) Analysis of human His₆-TyrRS with SDS-PAGE containing 20% acrylamide; (b) mass spectral analyses of human His₆-TyrRS.

2. ITC data of *E. coli* His₆-TyrRS and human His₆-TyrRS with tyrosine analogues

2.1 ITC data of *E. coli* His₆-TyrRS and human His₆-TyrRS with tyrosine analogues

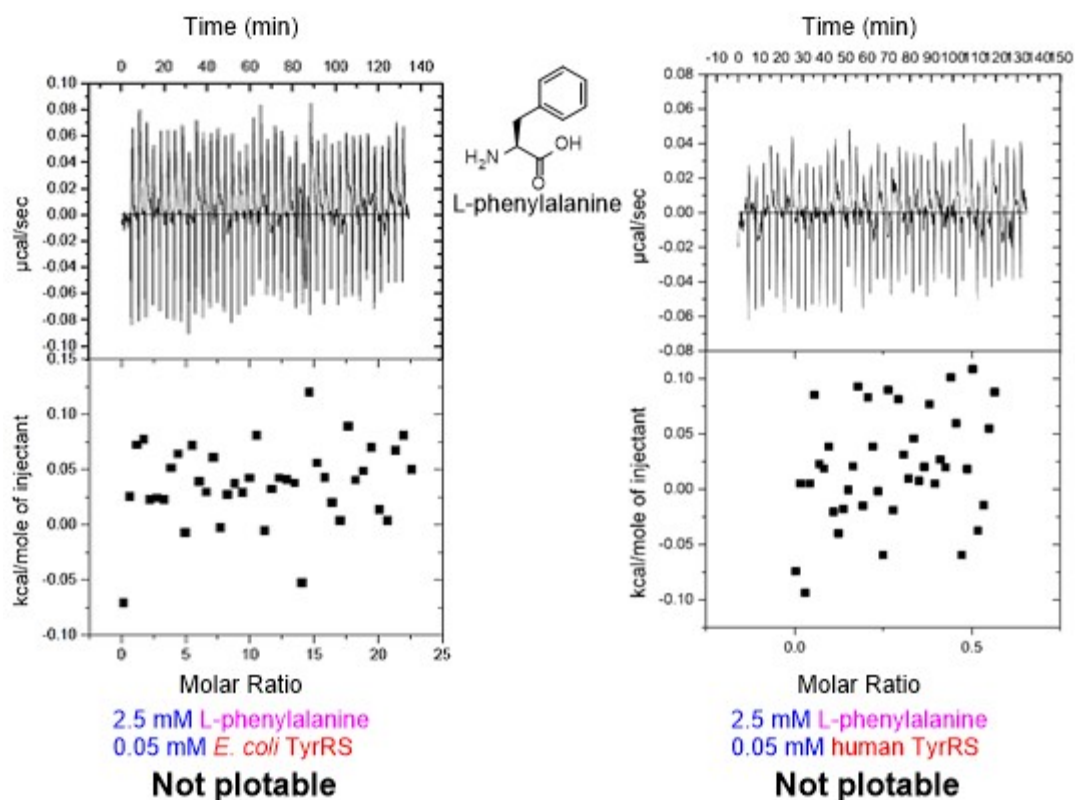


Figure S2. ITC of 0.05 mM *E. coli* TyrRS and human TyrRS with 2.5 mM L-phenylalanine.

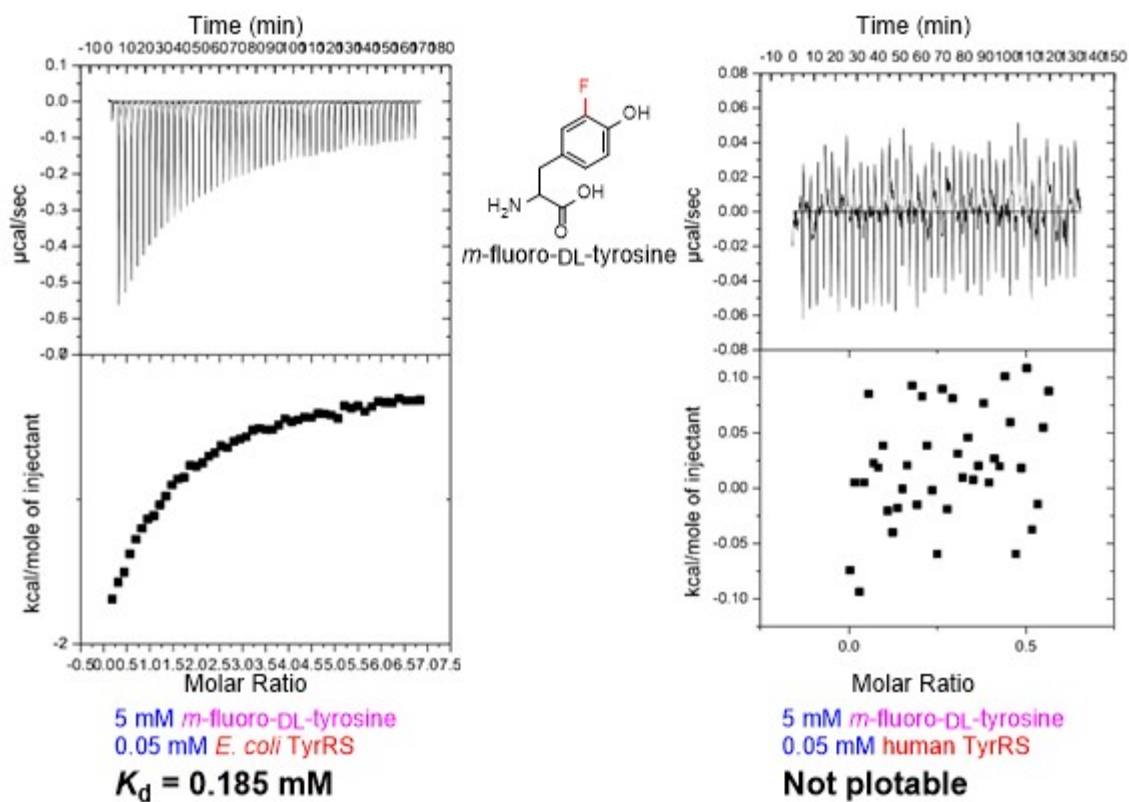


Figure S3. ITC of 0.05 mM *E. coli* TyrRS and human TyrRS with 5 mM *m*-fluoro-DL-tyrosine.

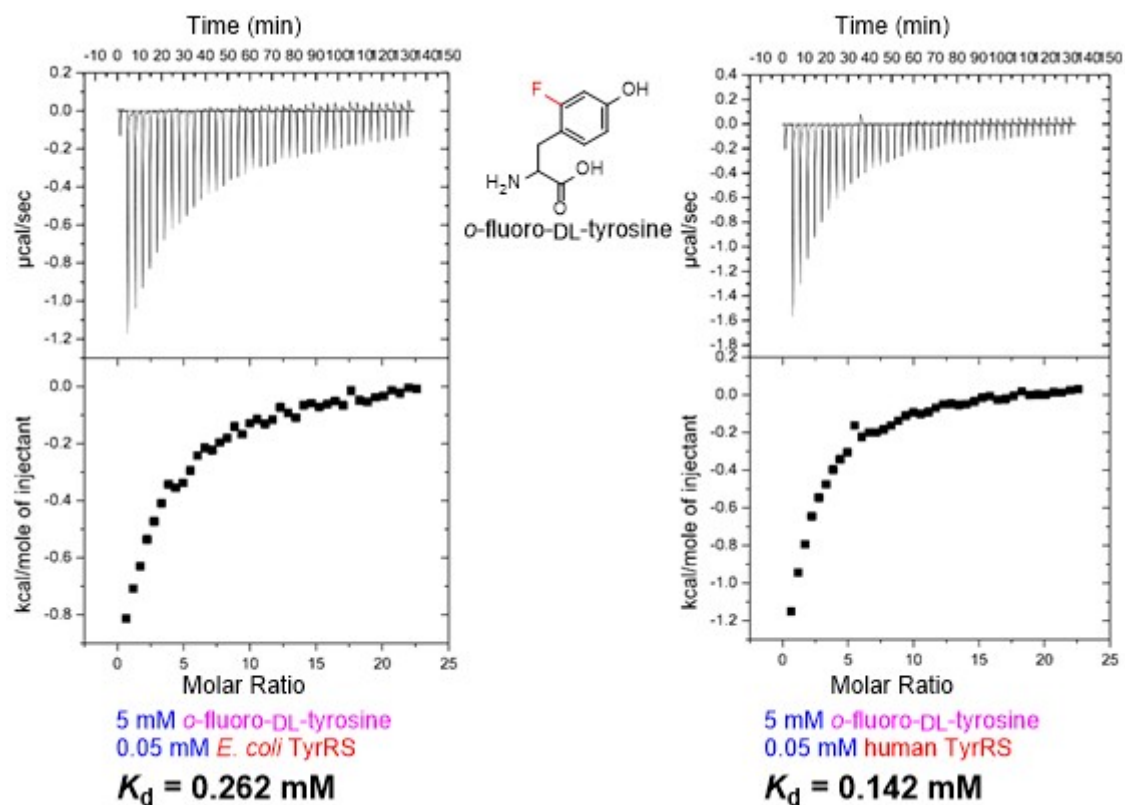


Figure S4. ITC of 0.05 mM *E. coli* TyrRS and human TyrRS with 5 mM *o*-fluoro-DL-tyrosine.

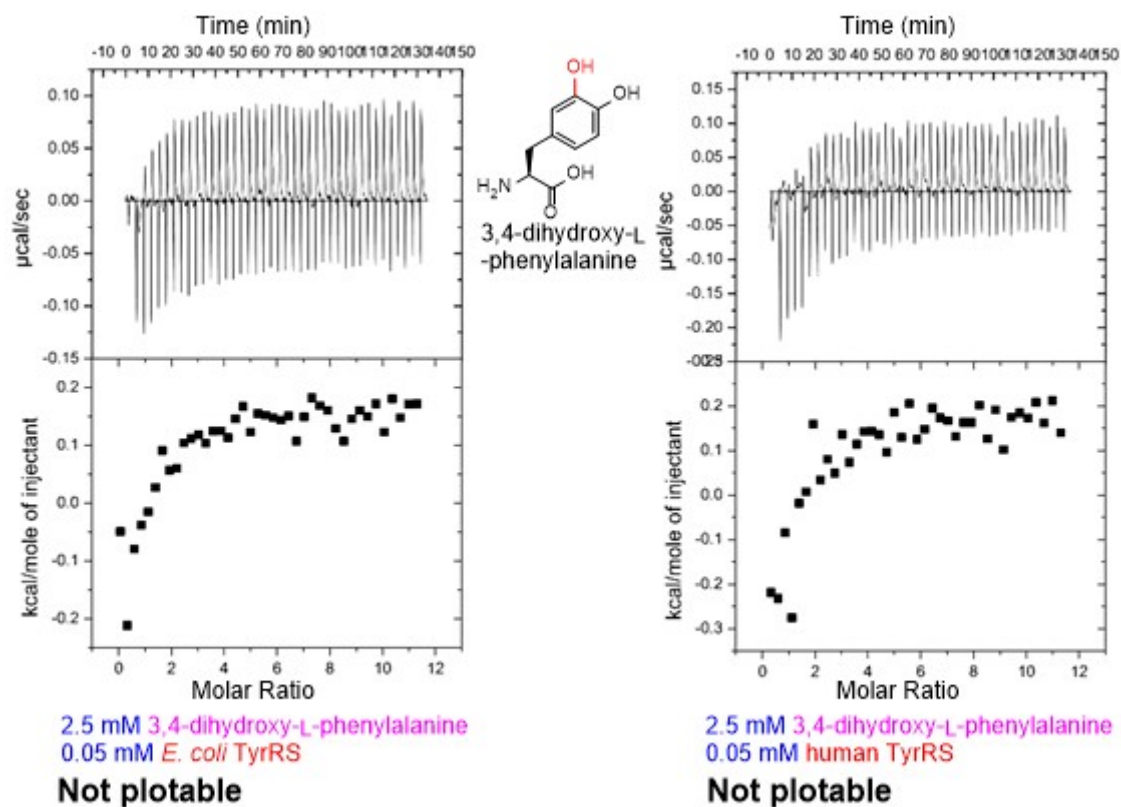


Figure S5. ITC of 0.05 mM *E. coli* TyrRS and human TyrRS with 2.5 mM 3,4-dihydroxy-L-phenylalanine.

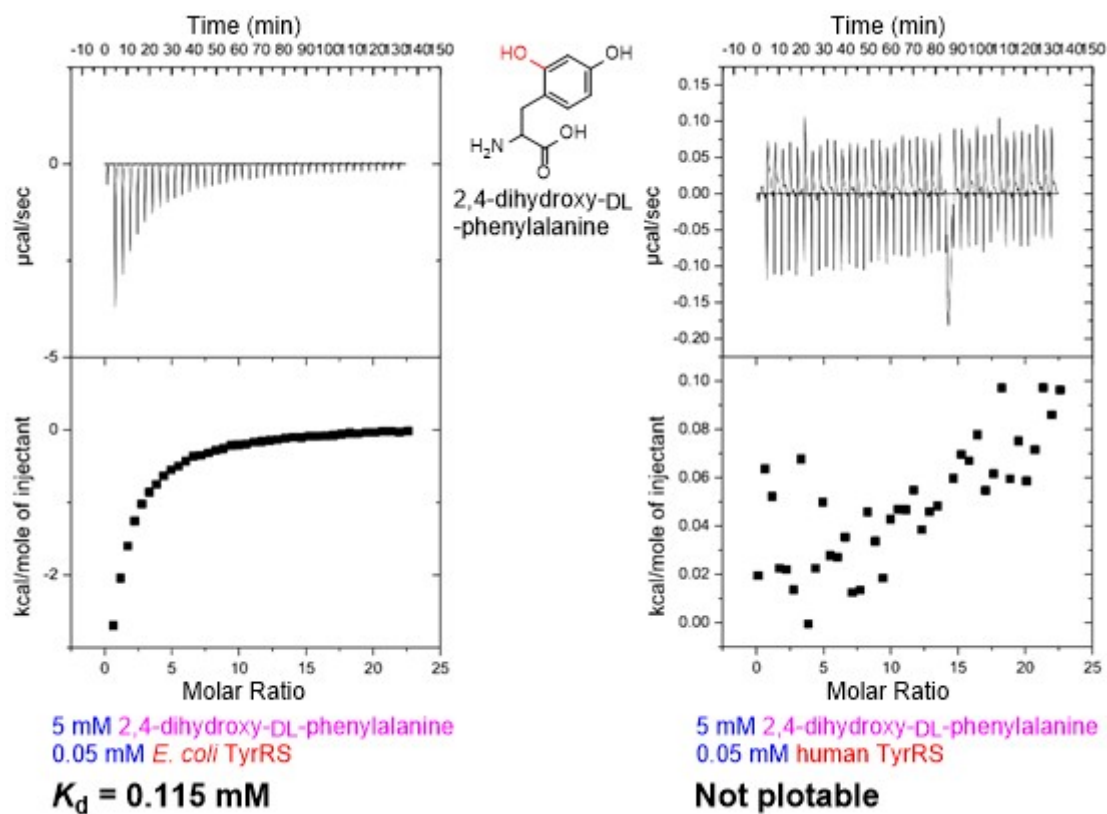


Figure S6. ITC of 0.05 mM *E. coli* TyrRS and human TyrRS with 5 mM 2,4-dihydroxy-DL-phenylalanine.

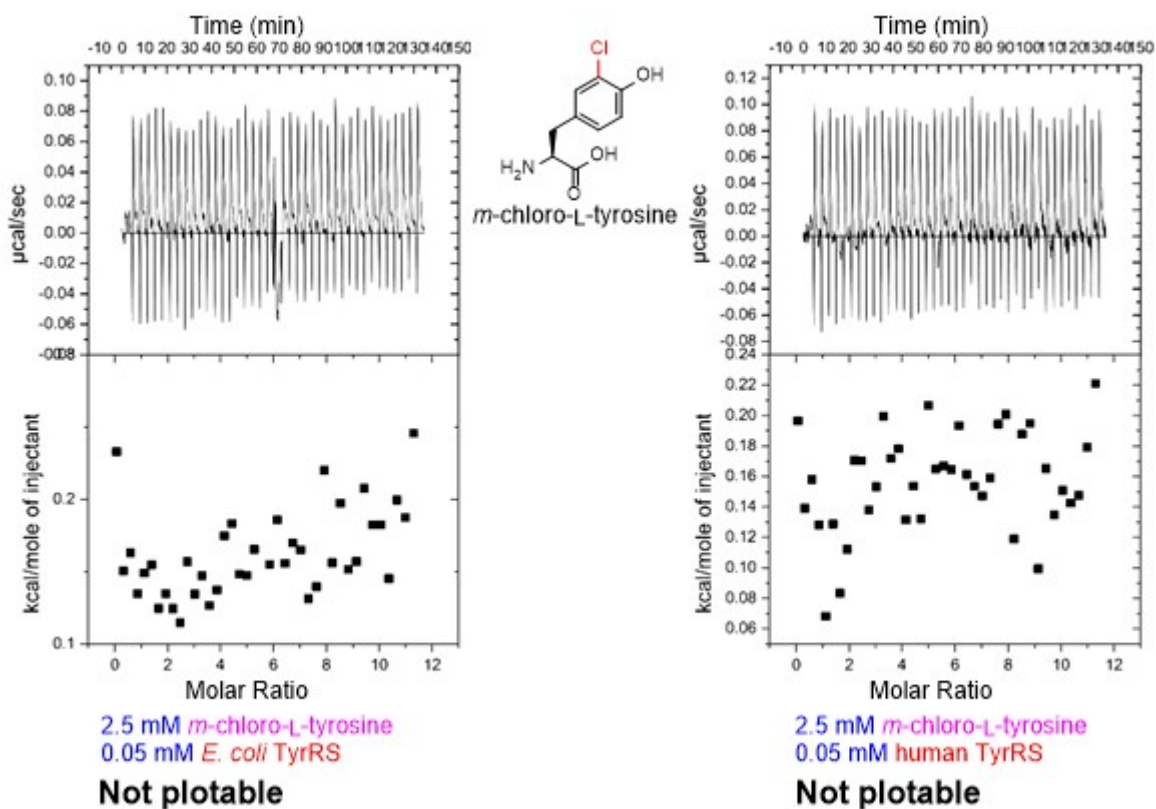


Figure S7. ITC of 0.05 mM *E. coli* TyrRS and human TyrRS with 2.5 mM *m*-chloro-L-tyrosine.

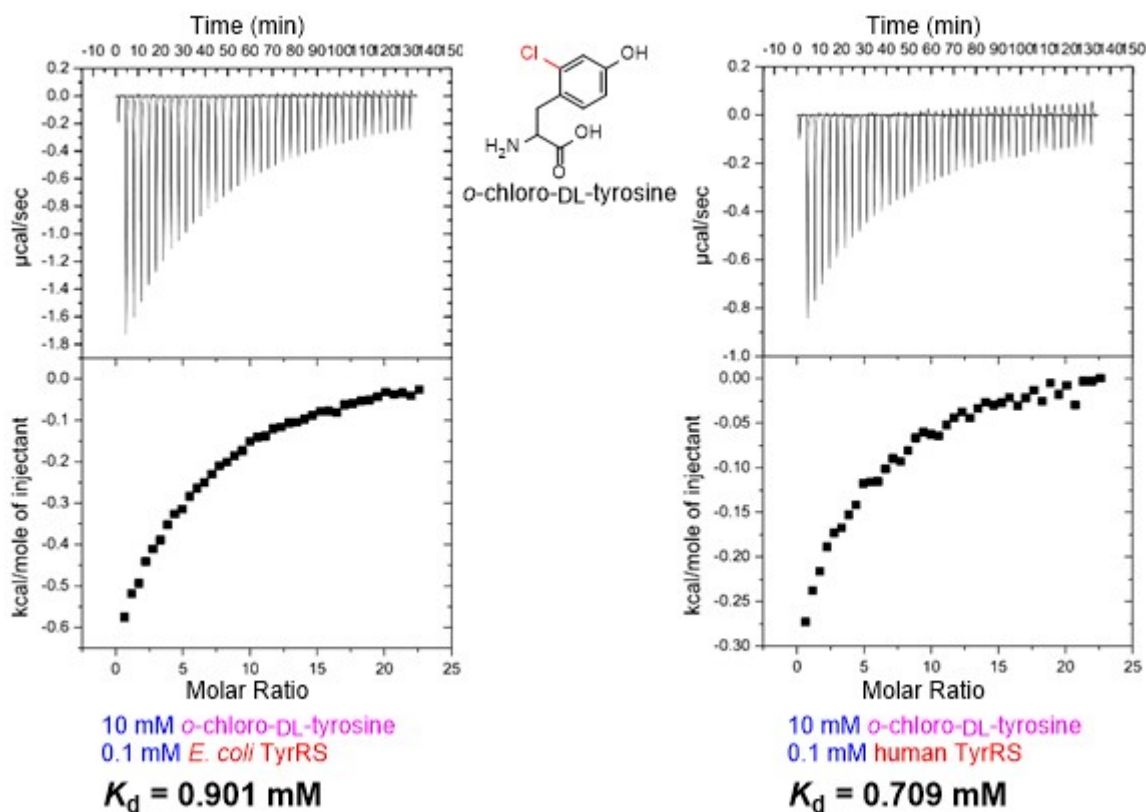


Figure S8. ITC of 0.1 mM *E. coli* TyrRS and human TyrRS with 10 mM *o*-chloro-DL-tyrosine.

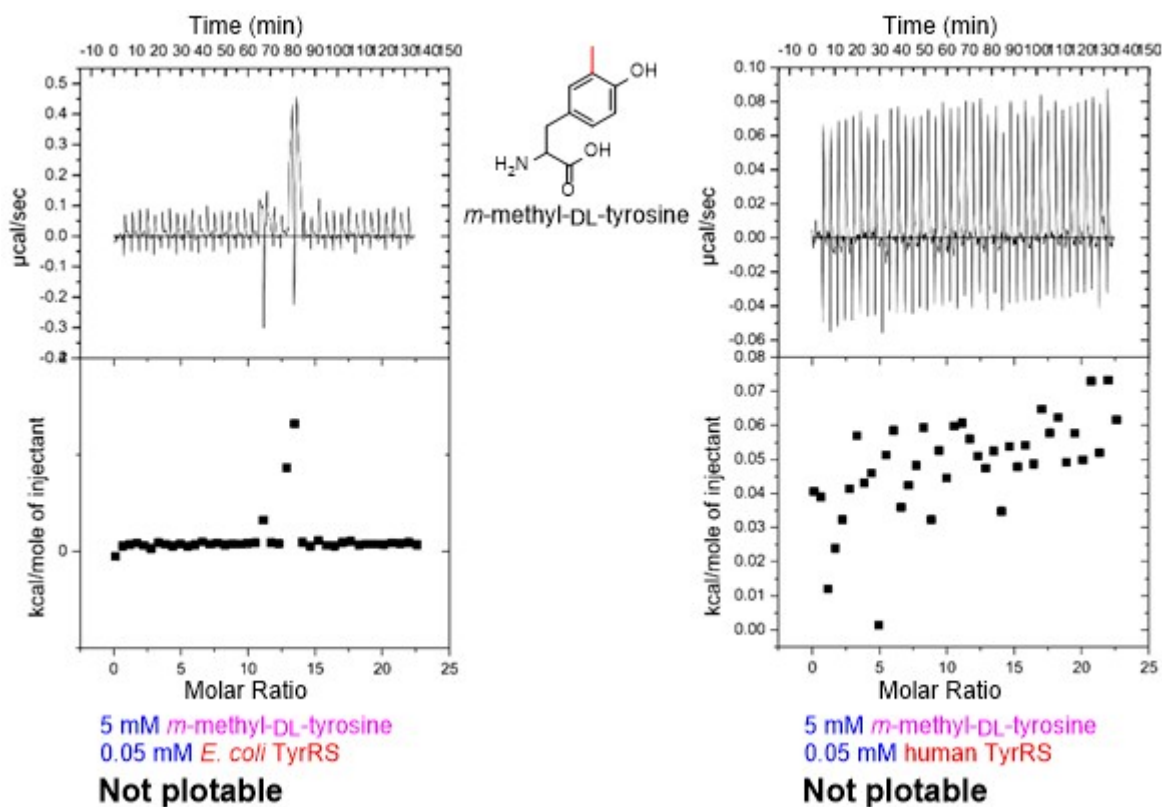


Figure S9. ITC of 0.05 mM *E. coli* TyrRS and human TyrRS with 5 mM *m*-methyl-DL-tyrosine.

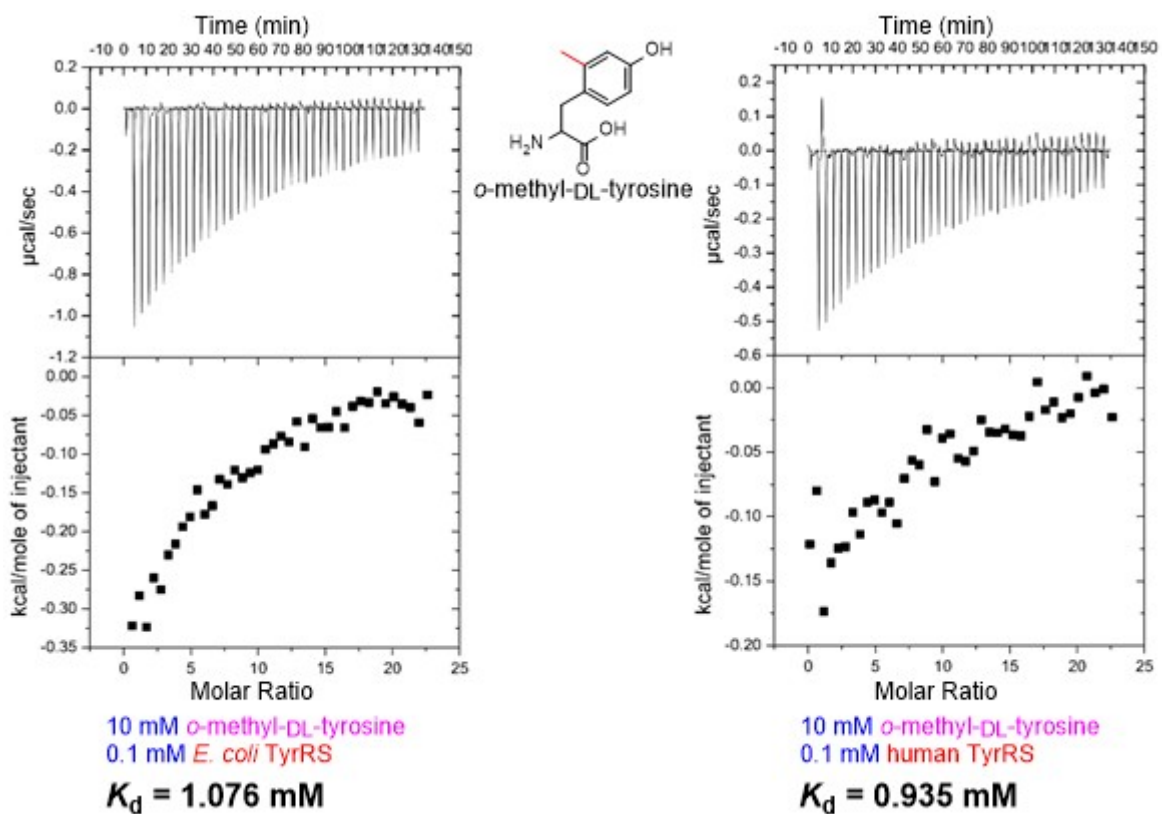


Figure S10. ITC of 0.1 mM *E. coli* TyrRS and human TyrRS with 10 mM *o*-methyl-DL-tyrosine.

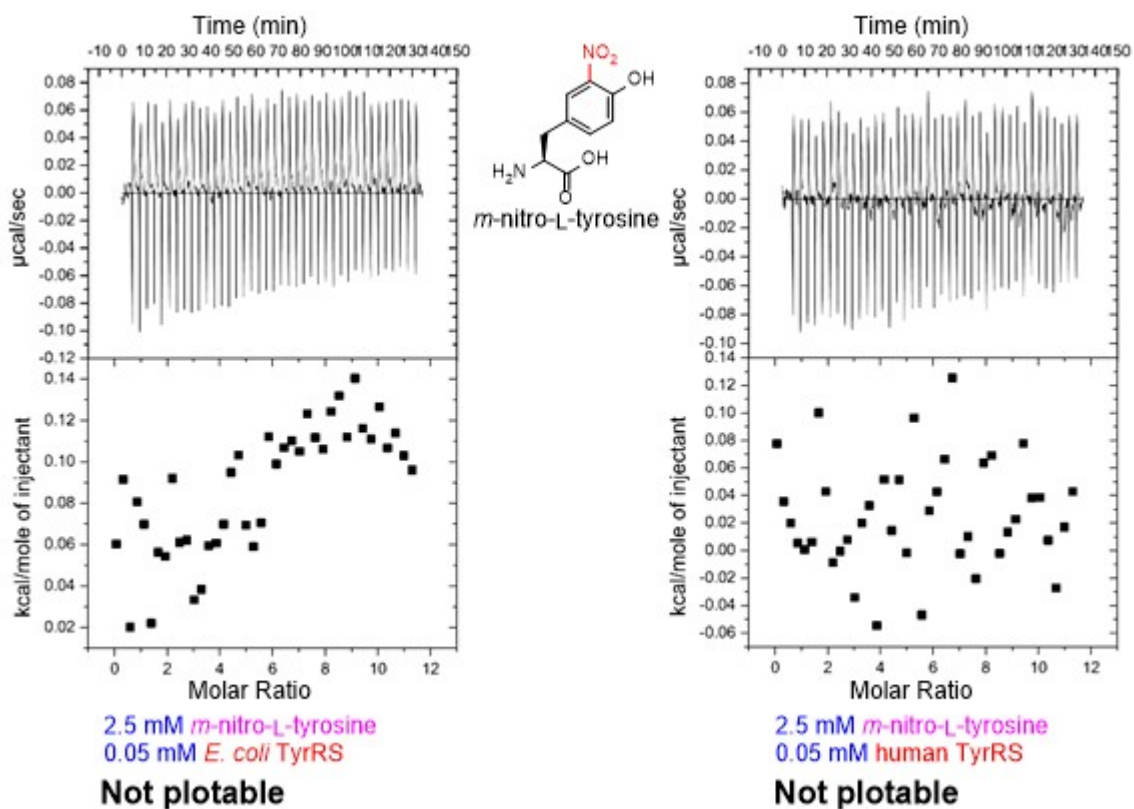


Figure S11. ITC of 0.05 mM *E. coli* TyrRS and human TyrRS with 2.5 mM *m*-nitro-L-tyrosine.

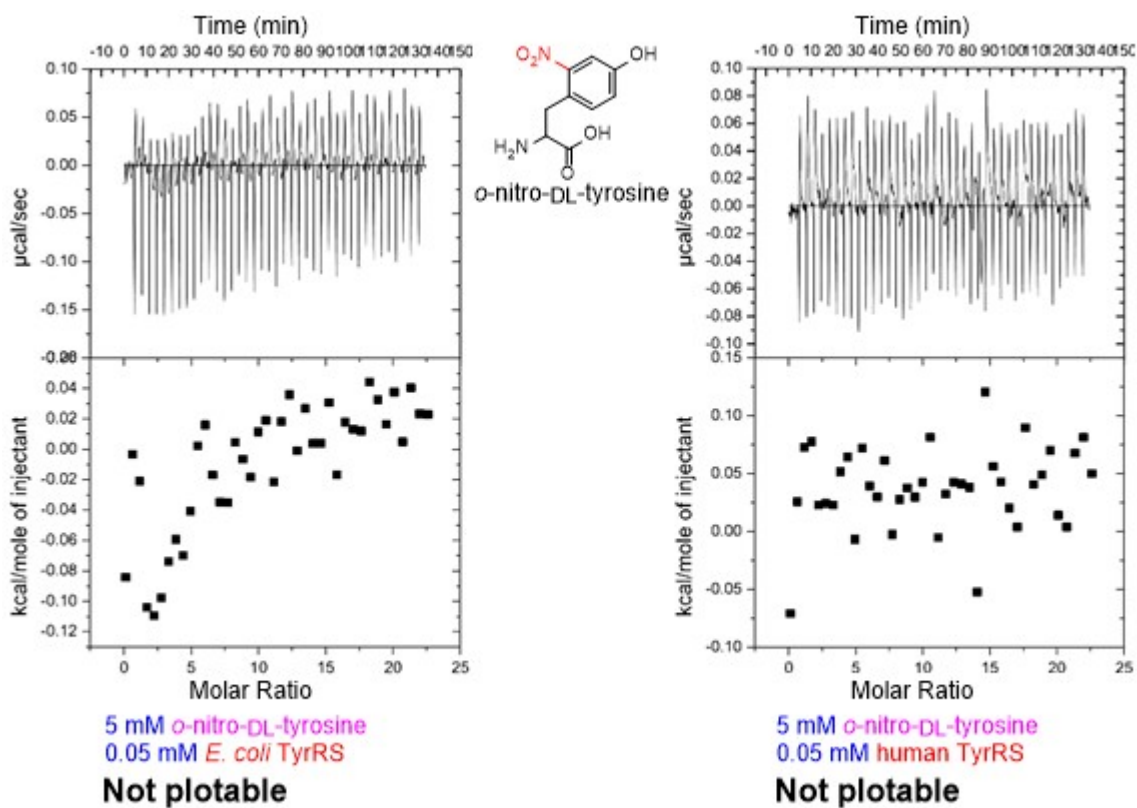


Figure S12. ITC of 0.05 mM *E. coli* TyrRS and human TyrRS with 5 mM *o*-nitro-DL-tyrosine.

2.2 Reproduce results of *E. coli* TyrRS with *m*-fluoro-DL-tyrosine and 2,4-dihydroxy-DL-phenylalanine under identical titration conditions

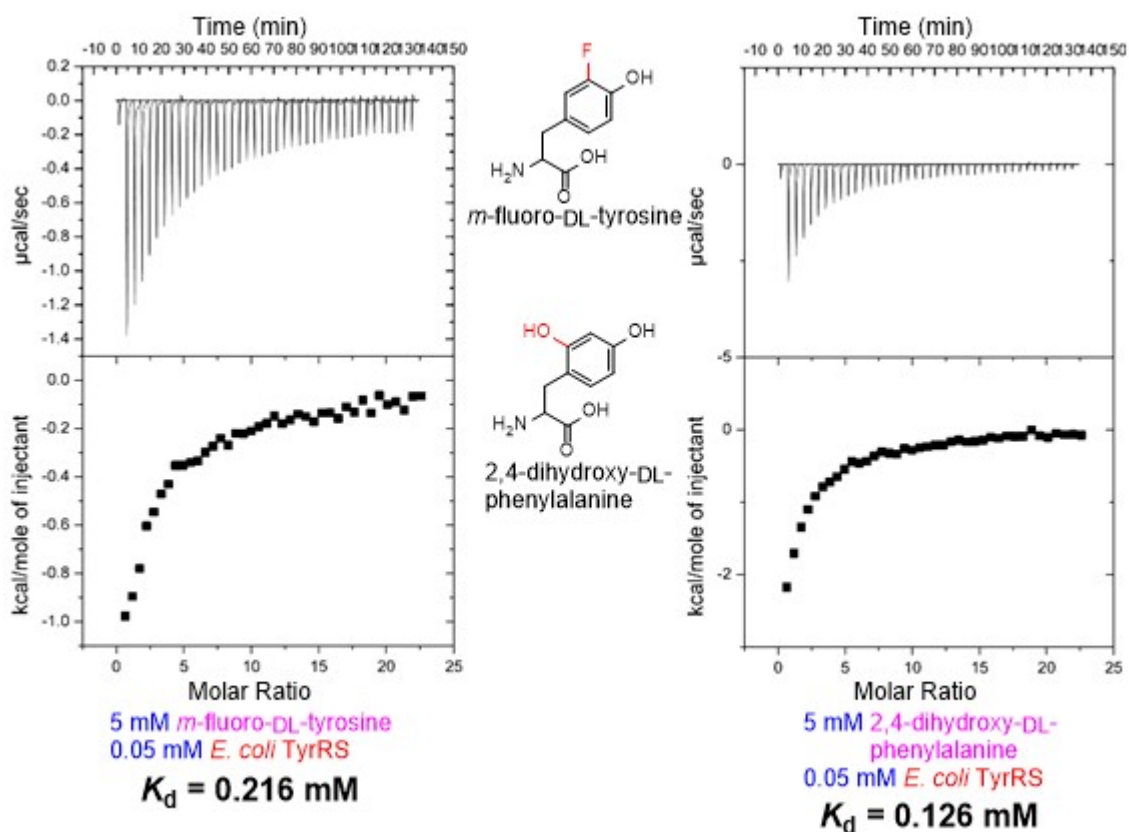


Figure S13. ITC of 0.05 mM *E. coli* TyrRS with 5 mM *m*-fluoro-DL-tyrosine and 5 mM 2,4-dihydroxy-DL-phenylalanine.

2.3 Reproduce results using different concentrations of human TyrRS and *m*-fluoro-DL-tyrosine

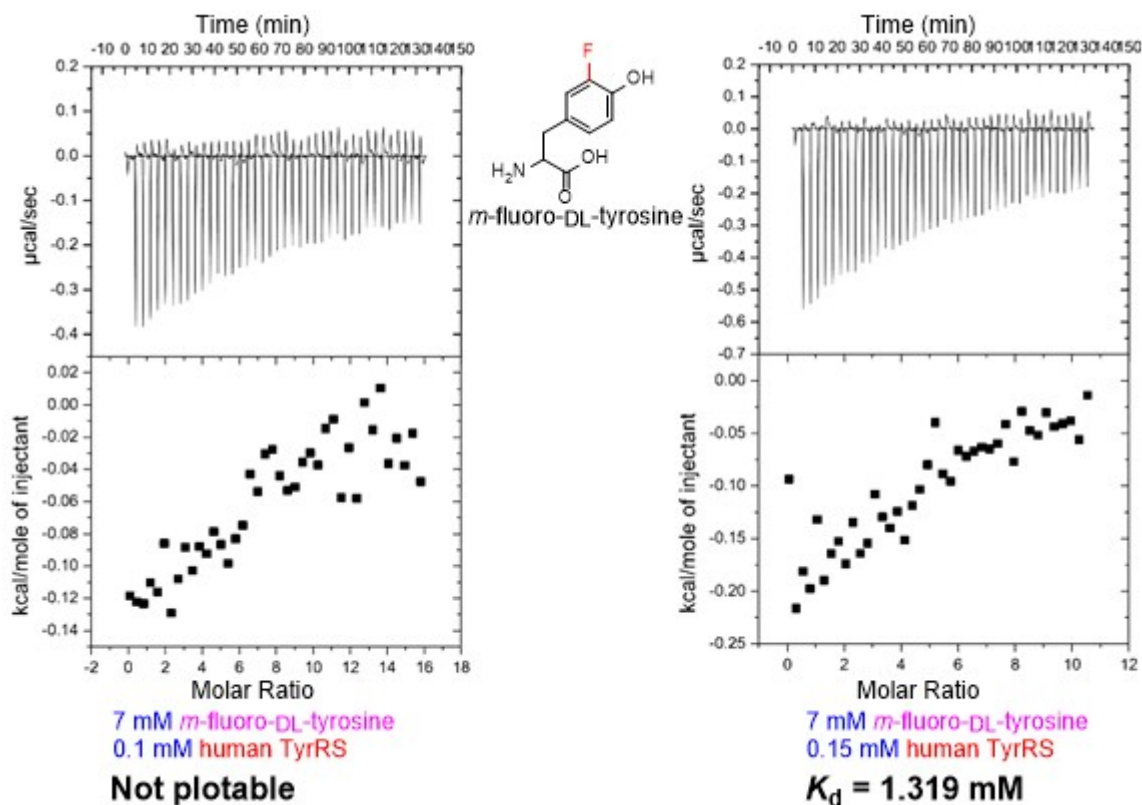


Figure S14. ITC of 0.1 and 0.15 mM human TyrRS with 7 mM *m*-fluoro-DL-tyrosine.

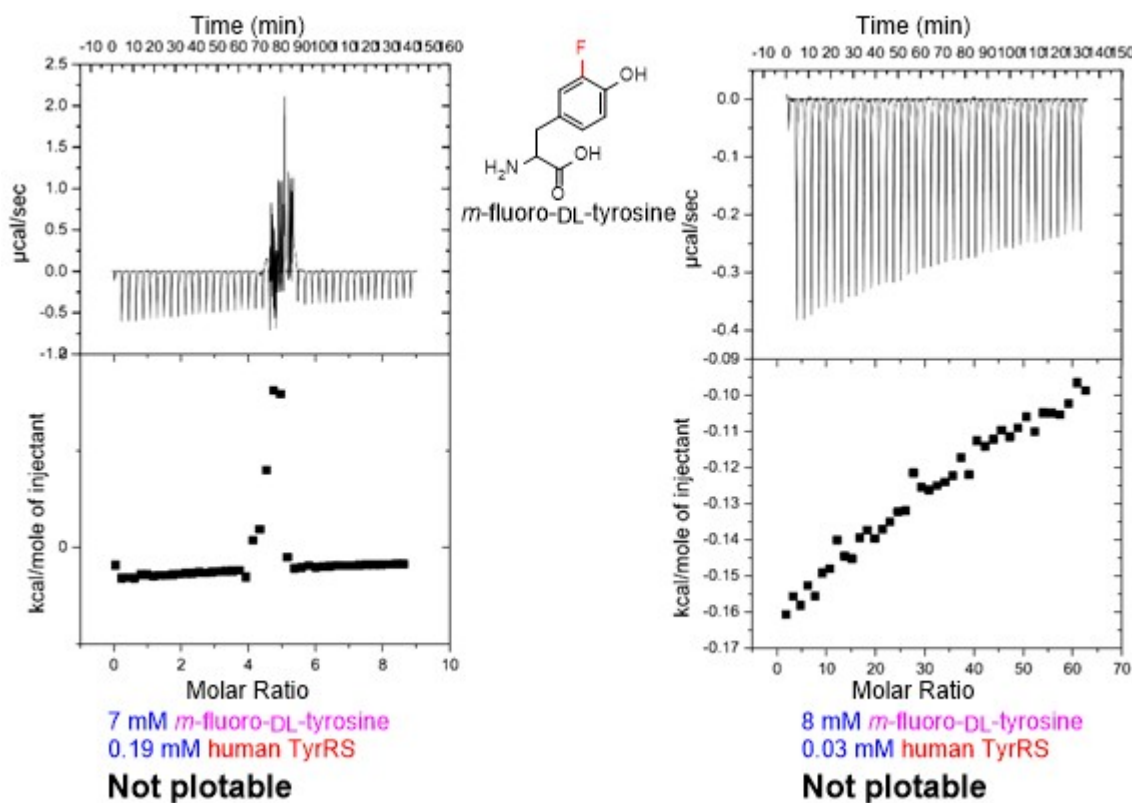


Figure S15. ITC of 0.19 and 0.03 mM human TyrRS with 7 and 8 mM *m*-fluoro-DL-tyrosine.

2.4 Reproduce results using different concentrations of human TyrRS with 2,4-dihydroxy-DL-phenylalanine

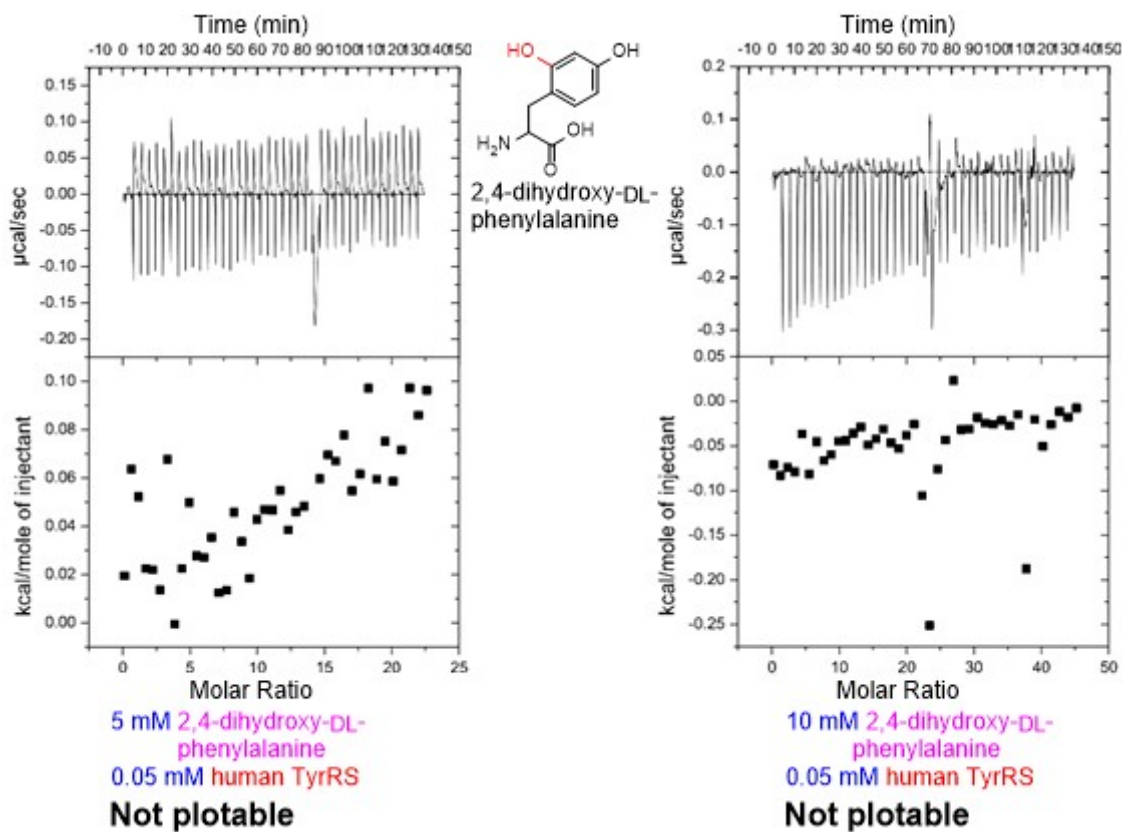


Figure S16. ITC of 0.05 human TyrRS with 5 and 10 mM *m*-fluoro-DL-tyrosine.

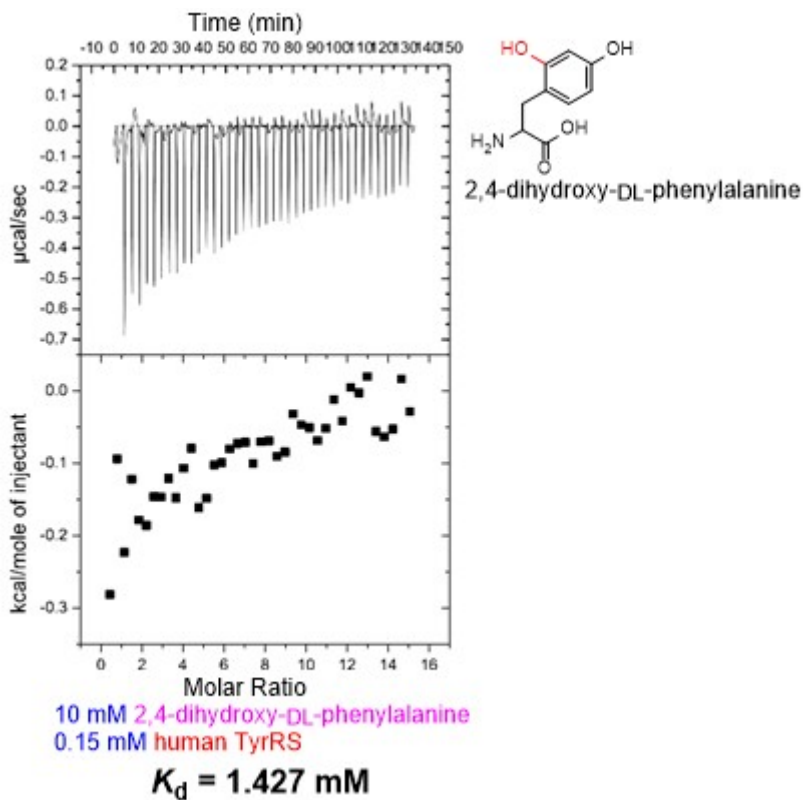


Figure S17. ITC of 0.15 human TyrRS with 10 mM *m*-fluoro-DL-tyrosine.

2.5 Titration of amino acids into buffer that contained no *E. coli* TyrRS or human TyrRS

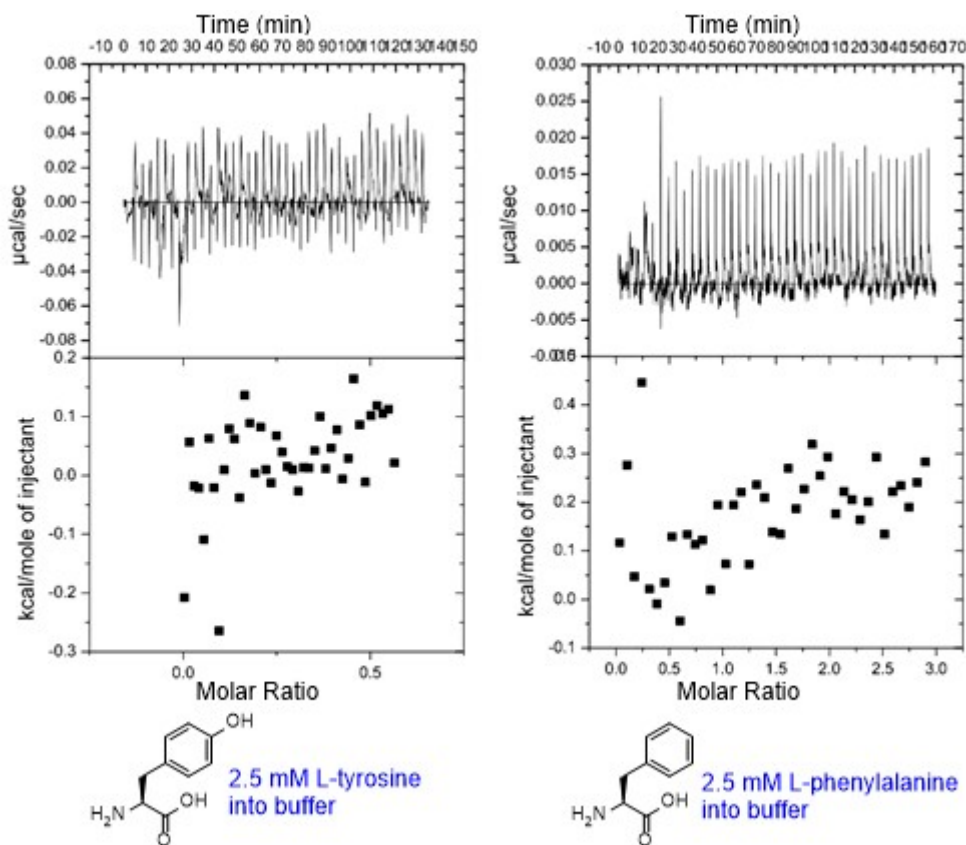


Figure S18. Titration of 2.5 mM L-tyrosine and L-phenylalanine into buffer that contained no enzyme.

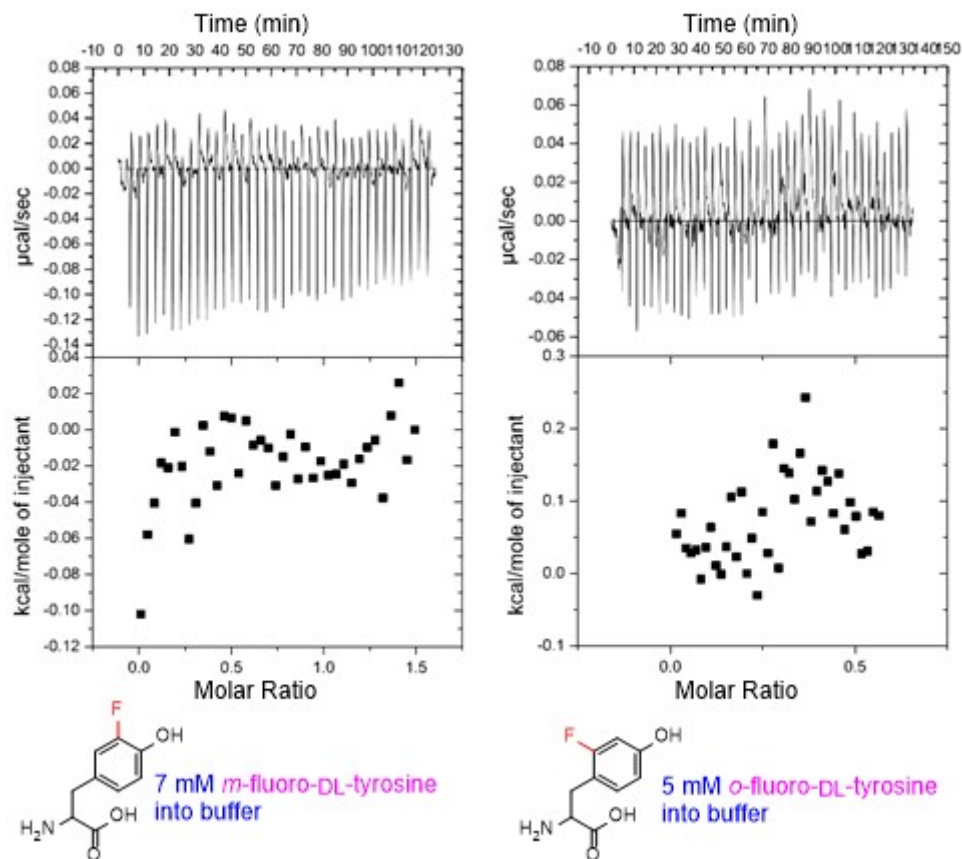


Figure S19. Titration of 7 mM *m*-fluoro-L-tyrosine and 5 mM *o*-fluoro-L-tyrosine into buffer that contained

no enzyme.

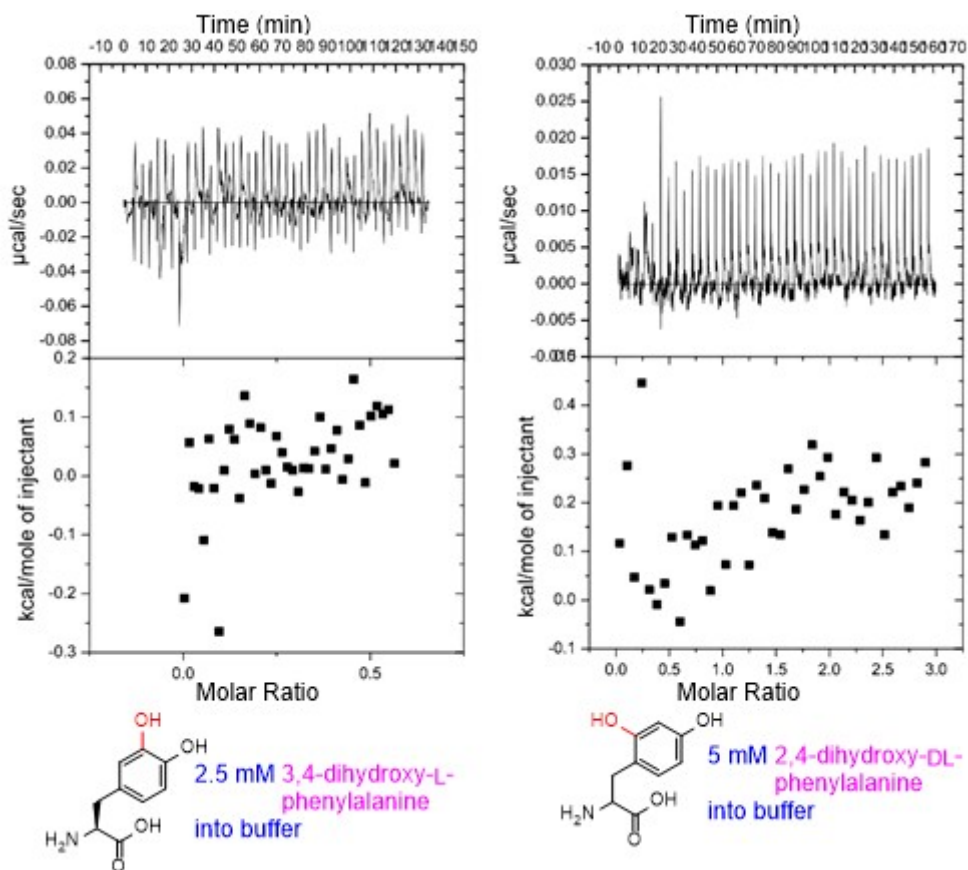


Figure S20. Titration of 2.5 mM 3,4-dihydroxy-L-phenylalanine and 5 mM 2,4-dihydroxy-DL-phenylalanine into buffer that contained no enzyme.

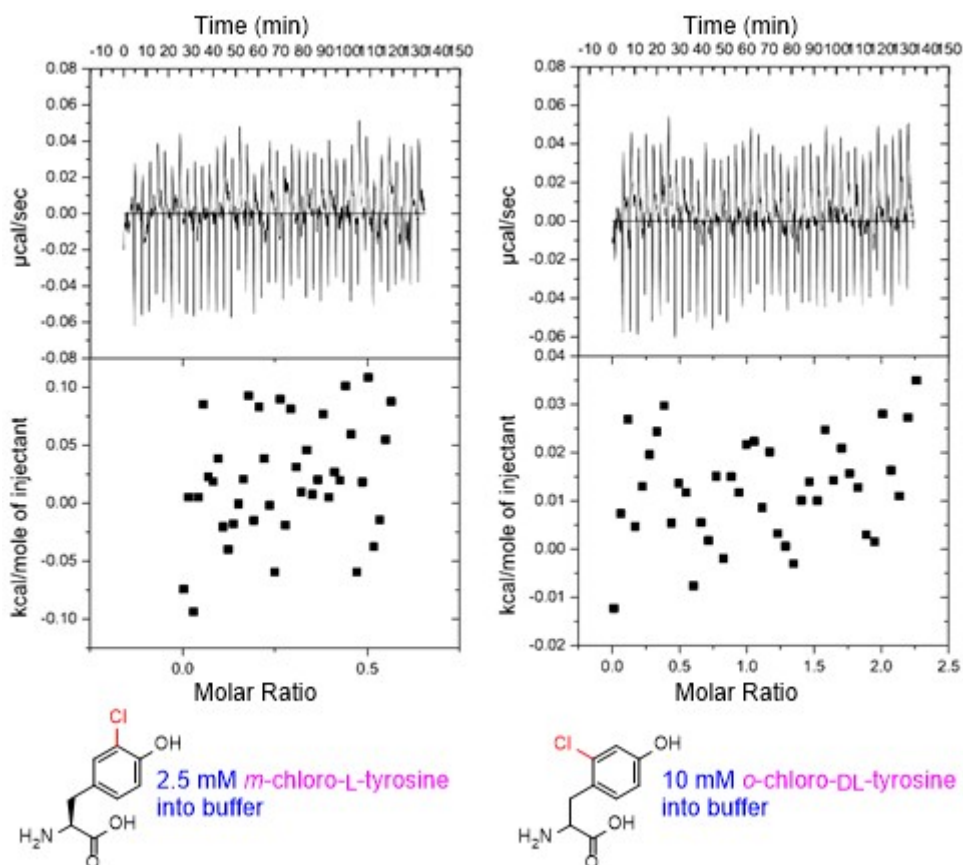


Figure S21. Titration of 2.5 mM *m*-chloro-L-tyrosine and 10 mM *o*-chloro-L-tyrosine into buffer that contained no enzyme.

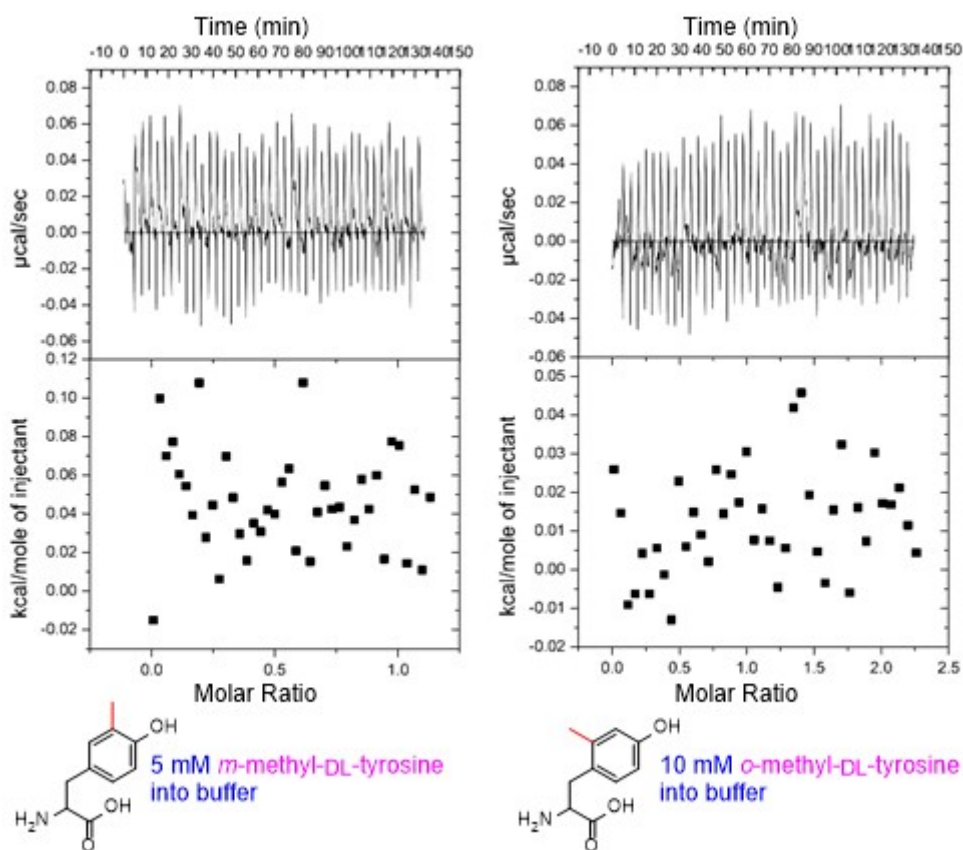


Figure S22. Titration of 5 mM *m*-methyl-L-tyrosine and 10 mM *o*-methyl-L-tyrosine into buffer that

contained no enzyme.

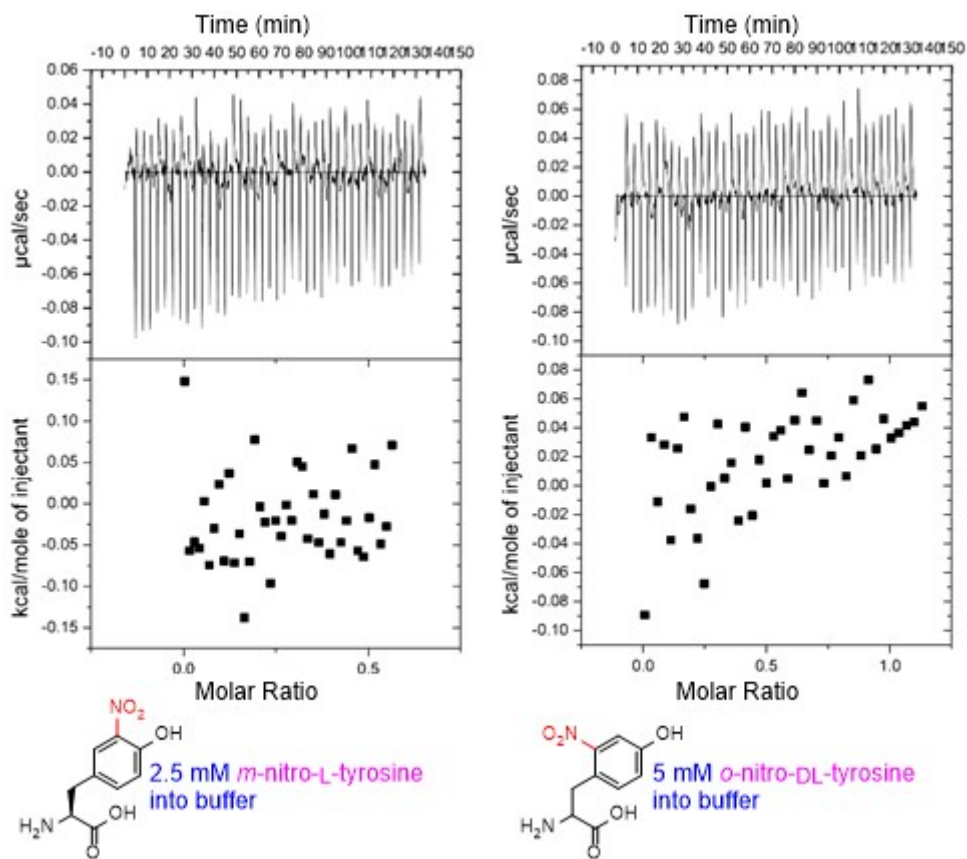


Figure S23. Titration of 2.5 mM *m*-nitro-L-tyrosine and 5 mM *o*-nitro-DL-tyrosine into buffer that contained no enzyme.