SUPPORTING INFORMATION

An H/D Exchange- and Protease Digestion-Based Screening Assay for the Detection of Protein-Ligand Binding

Erin D. Hopper,[†] Adrianne M. C. Pittman,[‡] Chandra L. Tucker,[‡]
Michael J. Campa,[§] Edward F. Patz,[§] and Michael C. Fitzgerald[†]

[†]Department of Chemistry, Duke University, Durham, North Carolina
[‡]Department of Biology, Duke University, Durham, North Carolina
[§]Department of Radiology, Duke University Medical Center, Durham, North Carolina

E-mail: michael.c.fitzgerald@duke.edu

CONTENTS:

The Supporting Information includes a table summarizing the SUPREX data used to evaluate the ΔG_f and *m*-values of the 11 AGTmi peptide fragments. It also includes six figures containing control screening data for CypA and AGTmi.

Table S-1: Transition midpoints of SUPREX curves obtained on apo-AGTmi using the SUPREX-protease digestion protocol.

Exchange Time (min)	3221 Da Fragment 1	3334 Da Fragment 2	3531 Da Fragment 3	3965 Da Fragment 4	4078 Da Fragment 5	4564 Da Fragment 6	5288 Da Fragment 7	5404 Da Fragment 8	5951 Da Fragment 9	6197 Da Fragment 10	6941 Da Fragment 11
0.5	2.0	2.0	1.9	2.0	2.1	1.7	2.0	1.9	1.7	1.7	1.8
2	1.9	1.9	1.8	1.8	1.8	1.5	1.8	1.7	1.7	1.5	1.7
5	1.7	1.7	1.6	1.7	1.6	1.3	1.7	1.5	1.5	1.4	1.5
25	1.4	1.5	1.4	1.4	1.4	1.0	1.5	1.3	1.4	1.3	1.4
40	1.4	1.4	1.3	1.2	1.2	1.1	1.5	1.2	1.4	1.2	1.3

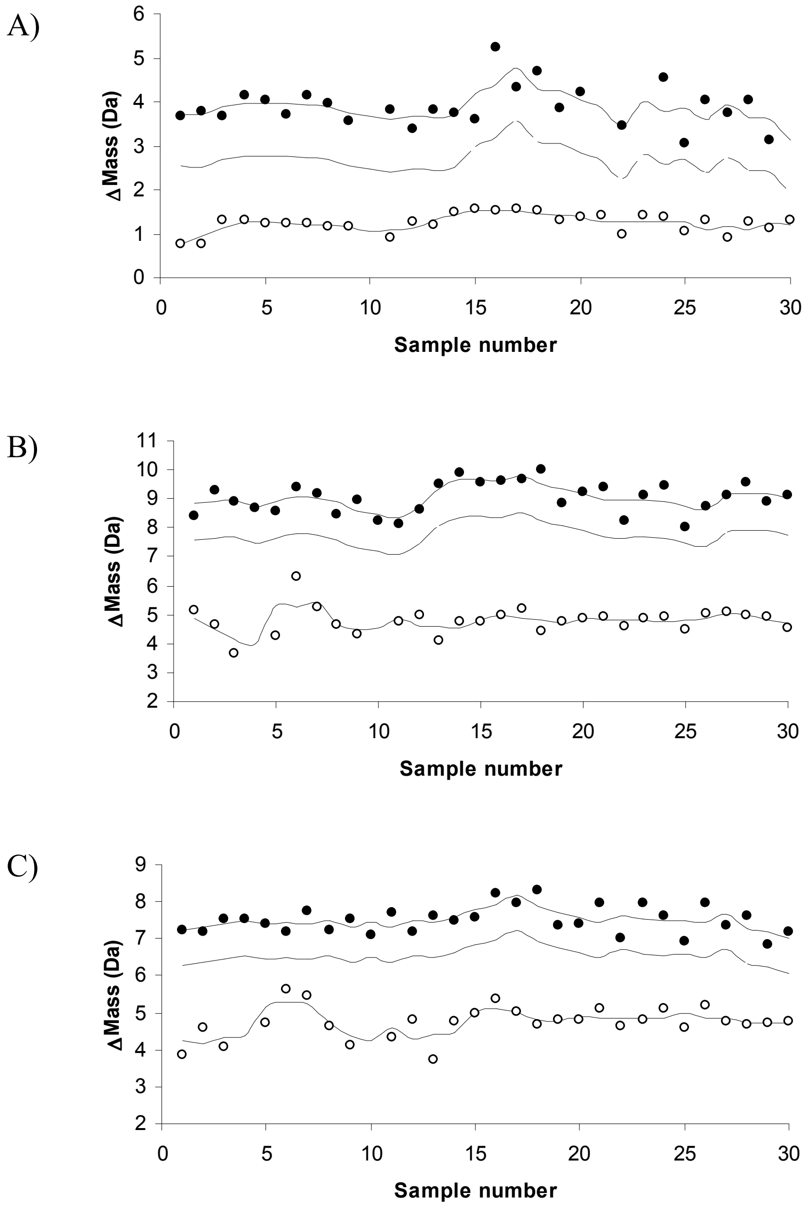


Figure S-1. Control screening data for CypA peptide fragments 1 (A), 3 (B) and 4 C) 4. ΔMass values are plotted for negative controls (filled circles) and positive controls (open circles), and the moving average for each control is represented by a solid line. The dashed line indicates the suggested cutoff values for each peptide.

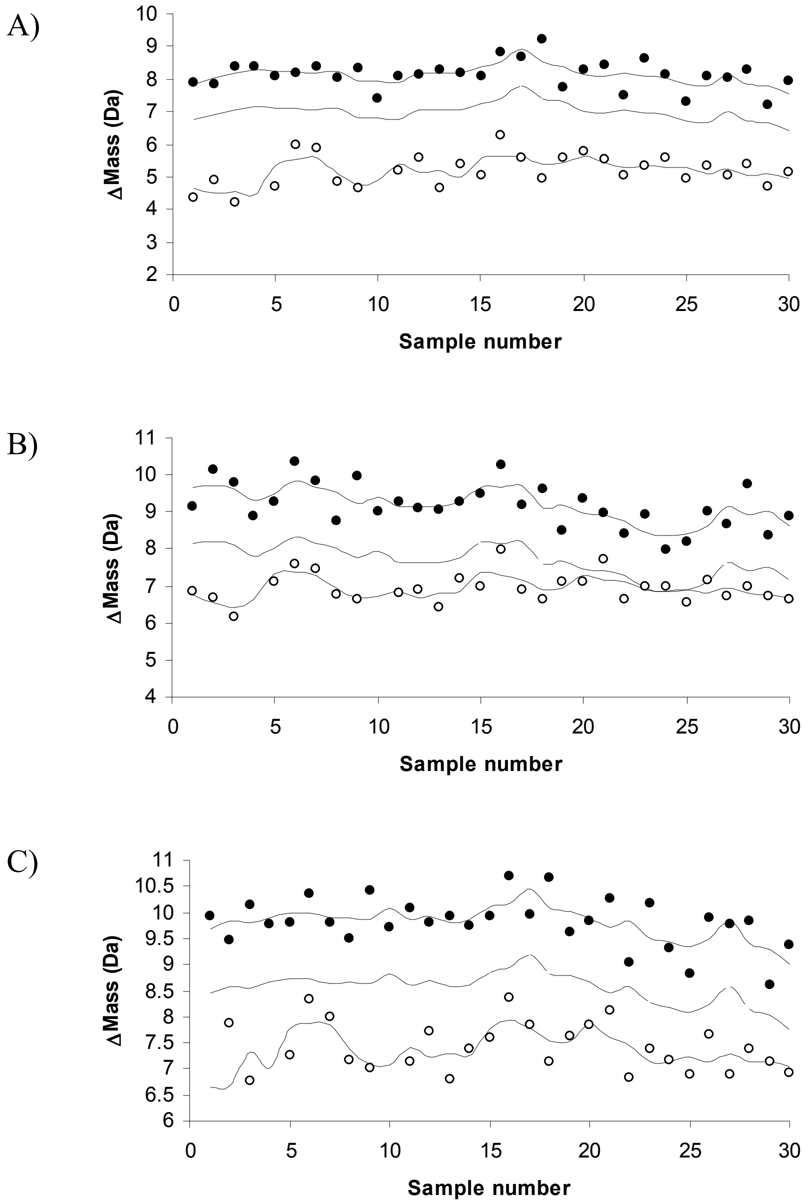
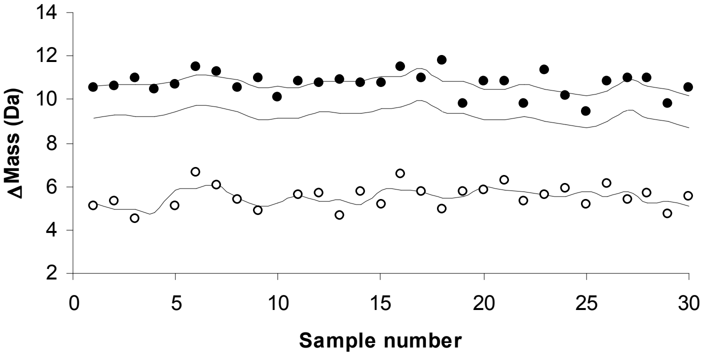


Figure S-2. Control screening data for CypA peptide fragments 5 (A), 6 (B), and 7 (C). ΔMass values are plotted for negative controls (filled circles) and positive controls (open circles), and the moving average for each control is represented by a solid line. The dashed line indicates the suggested cutoff values for each peptide.

A)



B)

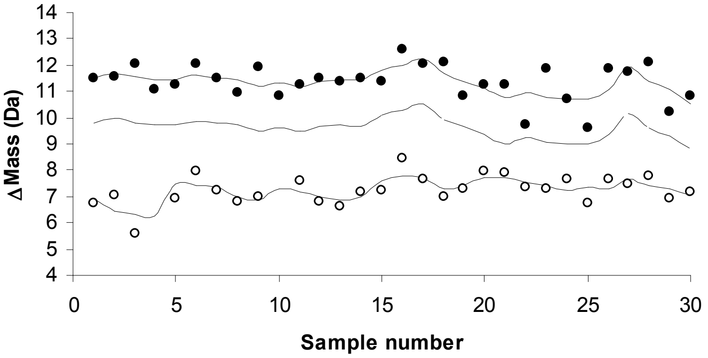


Figure S-3. Control screening data for CypA peptide fragments 8 (A) and 9 (B). ΔMass values are plotted for negative controls (filled circles) and positive controls (open circles), and the moving average for each control is represented by a solid line. The dashed line indicates the suggested cutoff values for each peptide.

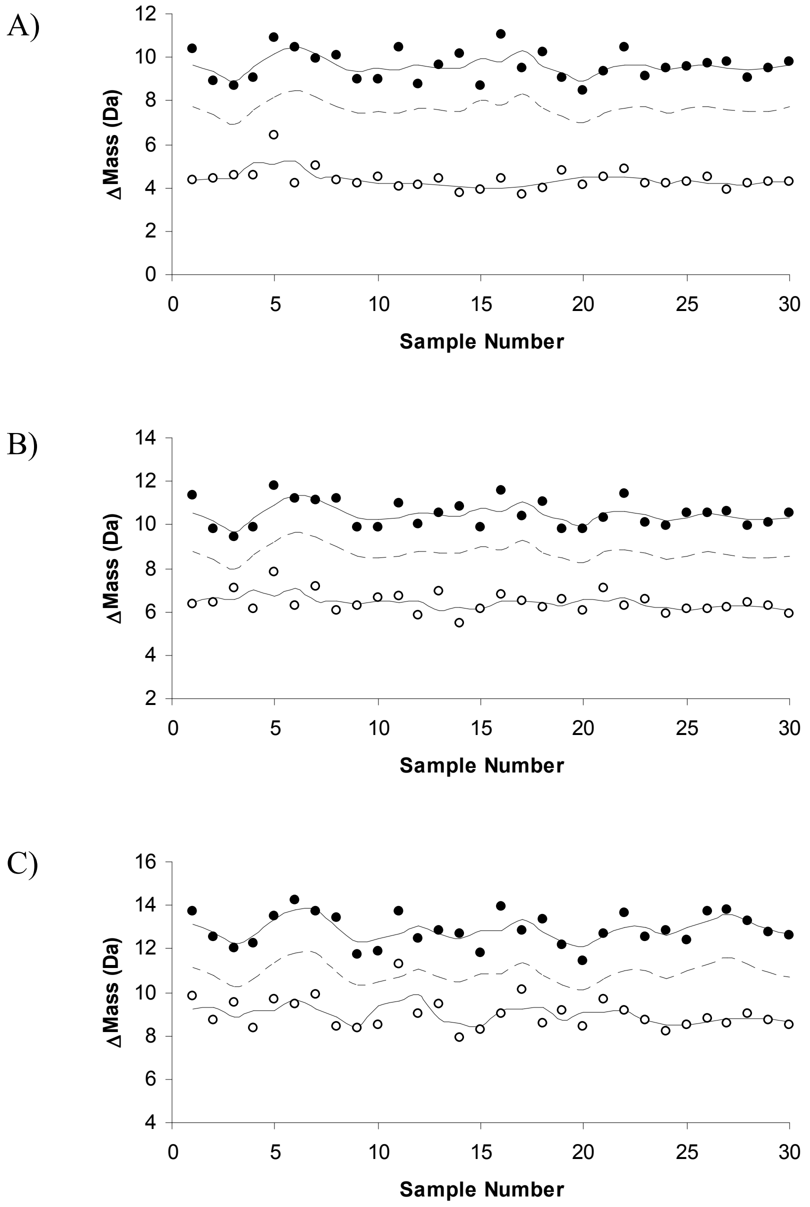


Figure S-4. Control screening data for AGTmi peptide fragments 1 (A), 3 (B), and 4 (C). ΔMass values are plotted for negative controls (filled circles) and positive controls (open circles), and the moving average for each control is represented by a solid line. The dashed line indicates the suggested cutoff values for each peptide.

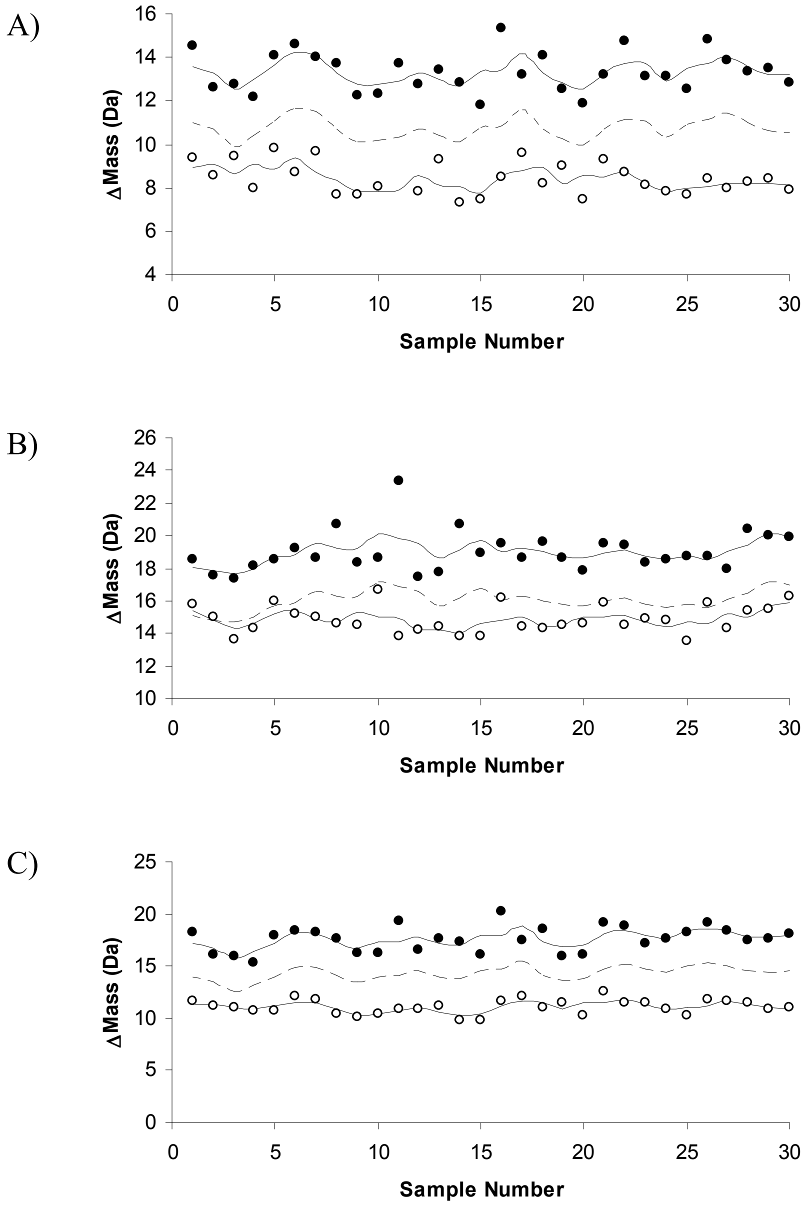


Figure S-5. Control screening data for AGTmi peptide fragments 5 (A), 6 (B), and 7 (C). ΔMass values are plotted for negative controls (filled circles) and positive controls (open circles), and the moving average for each control is represented by a solid line. The dashed line indicates the suggested cutoff values for each peptide.

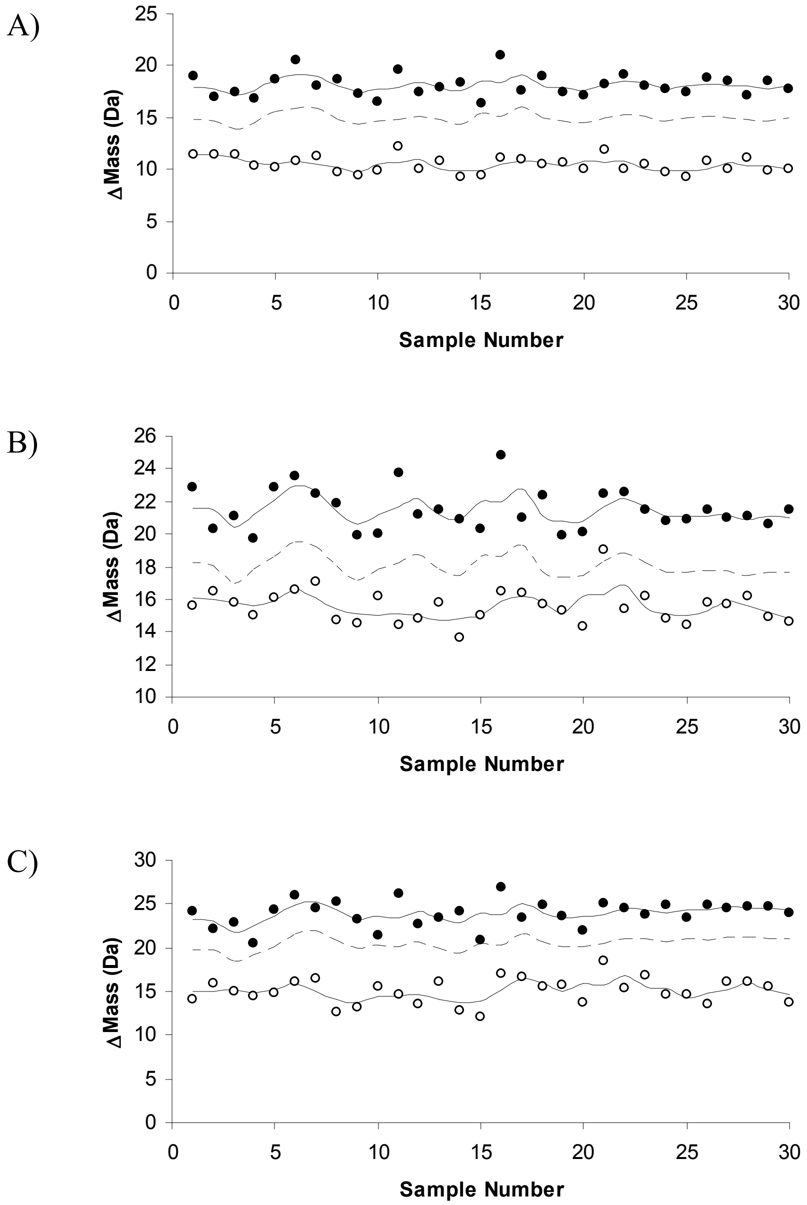


Figure S-6. Control screening data for AGTmi peptide fragments 8 (A), 9 (B), and 10 (C). ΔMass values are plotted for negative controls (filled circles) and positive controls (open circles), and the moving average for each control is represented by a solid line. The dashed line indicates the suggested cutoff values for each peptide.