

FIGURE S1. Determination of the site of sulfation on di- and tri- sulfated CCR5 1-18 peptides. Shown is (a) a MS/MS spectrum of acetylated, di-sulfated CCR5 1-18 from peak C' in Figure 1b. (b) MS/MS fragmentation scheme of di-sulfated CCR5 1-18. From the MS/MS spectrum it was determined that Tyr-10 and Tyr-15 were acetylated. (c) Structure of di-sulfated CCR5 1-18 from peak C' in Figure 1a. Since Tyr-3 and Tyr-14 were not acetylated, it was inferred that Tyr-3 and Tyr-14 were initially sulfated. (d) MS/MS spectrum of acetylated, di-sulfated CCR5 1-18 from peak D' in Figure 1b. (e) MS/MS fragmentation scheme of di-sulfated CCR5 1-18. From the MS/MS spectrum it was determined that Tyr-10 and Tyr-14 were acetylated. (f) Structure of di-sulfated CCR5 1-18 from peak D' in Figure 1a. Since Tyr-3 and Tyr-15 were not acetylated, it was inferred that Tyr-3 and Tyr-15 were initially sulfated. (g) MS/MS spectrum of acetylated, tri-sulfated CCR5 1-18 from peak E' in Figure 1b. (h) MS/MS fragmentation scheme of tri-sulfated CCR5 1-18. From the MS/MS spectrum it was determined that Tyr-10 was acetylated. (i) Structure of tri-sulfated CCR5 1-18. Since Tyr-3, Tyr-14 and Tyr-15 were not acetylated, it was inferred that Tyr-3, Tyr-14 and Tyr-15 were initially sulfated.

FIGURE S2. Determination of the site of sulfation on mono-sulfated CCR5 2-18 peptide. Shown are (a) a mass spectrum of mono-sulfated CCR5 2-18 from peak B in Figure 1a, (b) a mass spectrum of mono-sulfated CCR5 2-18 after reaction with S-NHSAc, and (c) a MS/MS spectrum of the acetylated, monosulfated CCR5 1-18 peptide. (d) MS/MS fragmentation scheme of CCR5 2-18. From the MS/MS spectrum it was determined that Tyr-3, Tyr-10, and Tyr-15 were acetylated. (e) Structure of mono-sulfated CCR5 2-18. Since Tyr-14 was not acetylated, it was inferred that Tyr-14 was initially sulfated.

FIGURE S3. Determination of the site of sulfation on mono-sulfated CCR5 2-18 peptide. Shown are (a) a mass spectrum of mono-sulfated CCR5 2-18 from peak C in Figure 1a, (b) a mass spectrum of mono-sulfated CCR5 2-18 after reaction with S-NHSAc, and (c) a MS/MS spectrum of the acetylated, mono-sulfated CCR5 2-18 peptide. (d) MS/MS fragmentation scheme of CCR5 2-18. From the MS/MS spectrum it was determined that Tyr-3, Tyr-10, and Tyr-14 were acetylated. (e) Structure of mono-sulfated CCR5 2-18. Since Tyr-15 was not acetylated, it was inferred that Tyr-15 was initially sulfated.

FIGURE S4. Time course of *in vitro* sulfation by TPST-2 for (a) CCR8 M1A 1-17, (b) CCR8 1-17 Nt-Ac, and (c) CCR8 2-17 Nt-Ac. At each time point, aliquots were taken and the reaction was quenched. The reaction was monitored by RP-HPLC. The relative amounts of each species were calculated by integrating the peak areas.

Figure S1

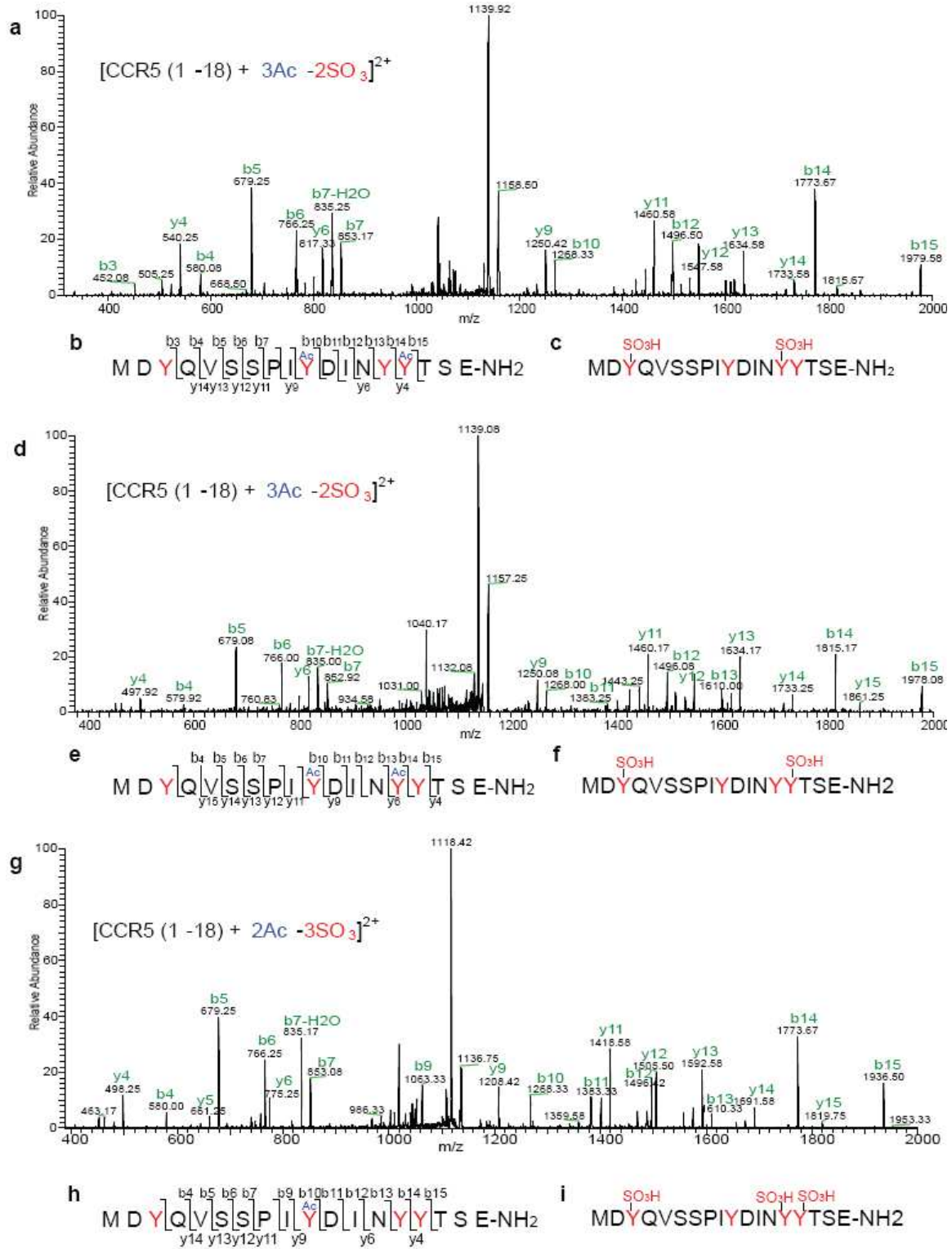


Figure S2

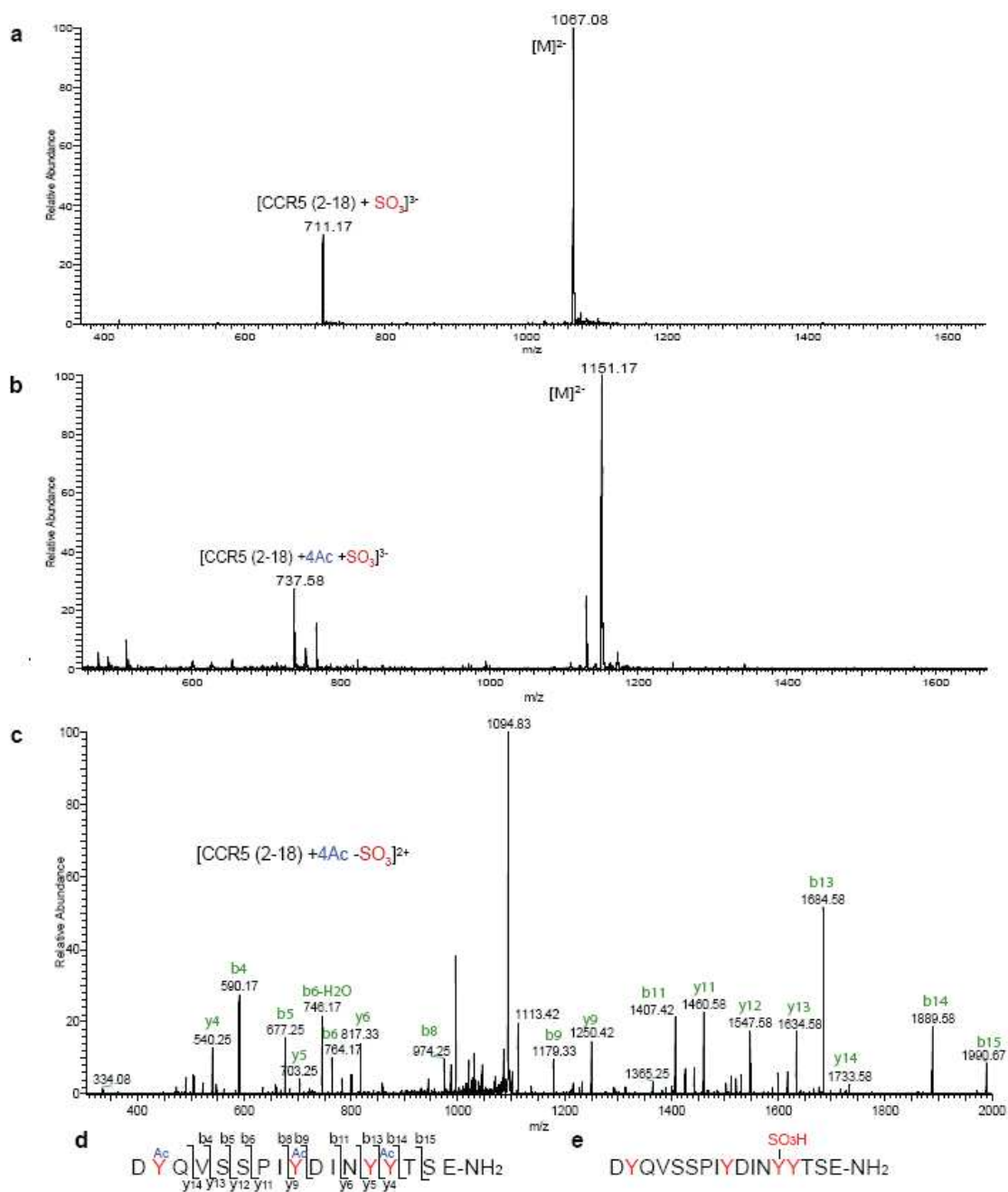


Figure S3

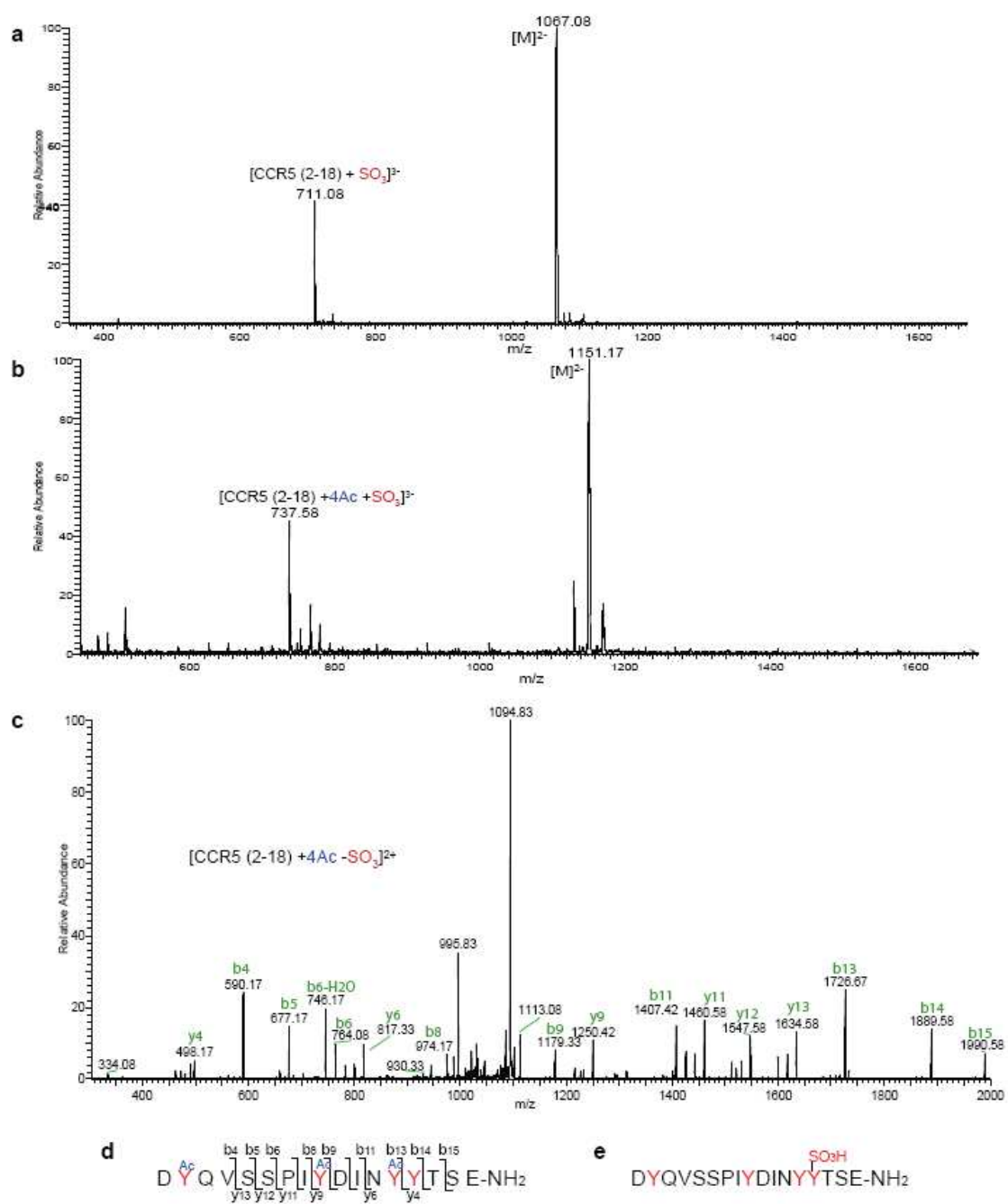


Figure S4

