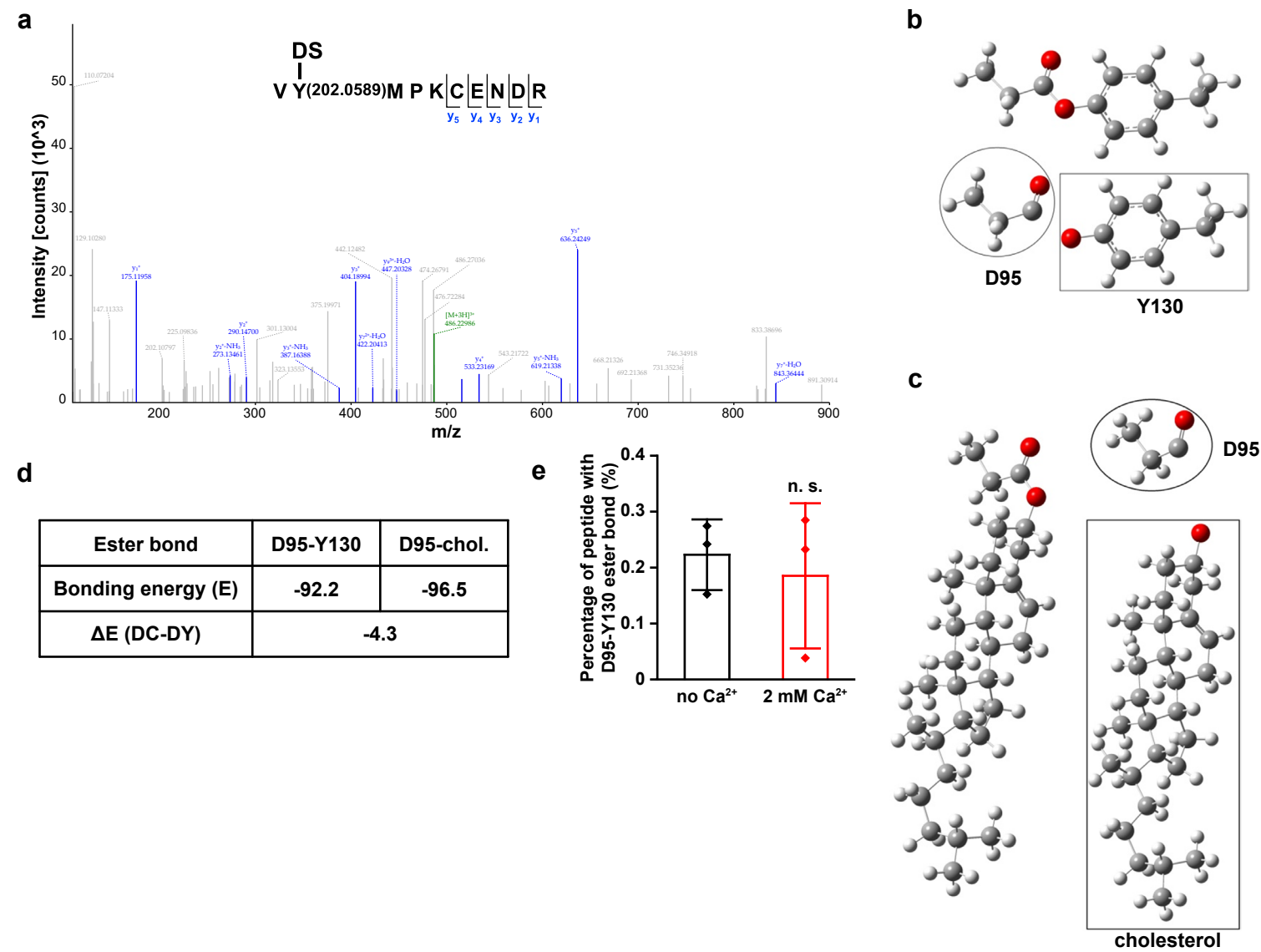


Fig. S2



**Fig. S2. Mass spectrum of intramolecular ester bond and calculation of the bonding energies.**

- a.** The mass spectrum of V129 to R138 peptide on protein backbone. The small fragment D95S96 was detected to be covalently linked to Y130 by the ester bond between D95 and Y130.
- b.** The molecular model of the intramolecular ester bond between side chains of D95 and Y130.
- c.** The ester bond between the side chain of D95 and cholesterol. Both models were constructed from the crystal structure of SMO (PDB: 5L7D).
- d.** The calculated bonding energies (in kcal/mol) of the ester bonds for D95-Y130, and D95-cholesterol after covalent modification were shown, using M06-2X/6-311+G\*. The ester bond energy is calculated by the energy of the bonding complex subtracting those of the two free radicals.
- e.** Quantification of D95-Y130 ester bond. The percentage of D95-Y130 ester bond-containing peptide was calculated by dividing the sum intensity of peptides containing crosslinked D95-Y130 by the sum intensity of D95 and Y130-containing peptides.  $p=0.6746$ . Two-sample T-test.