

Supplemental Data I: Usage Example - ST8Sia IV

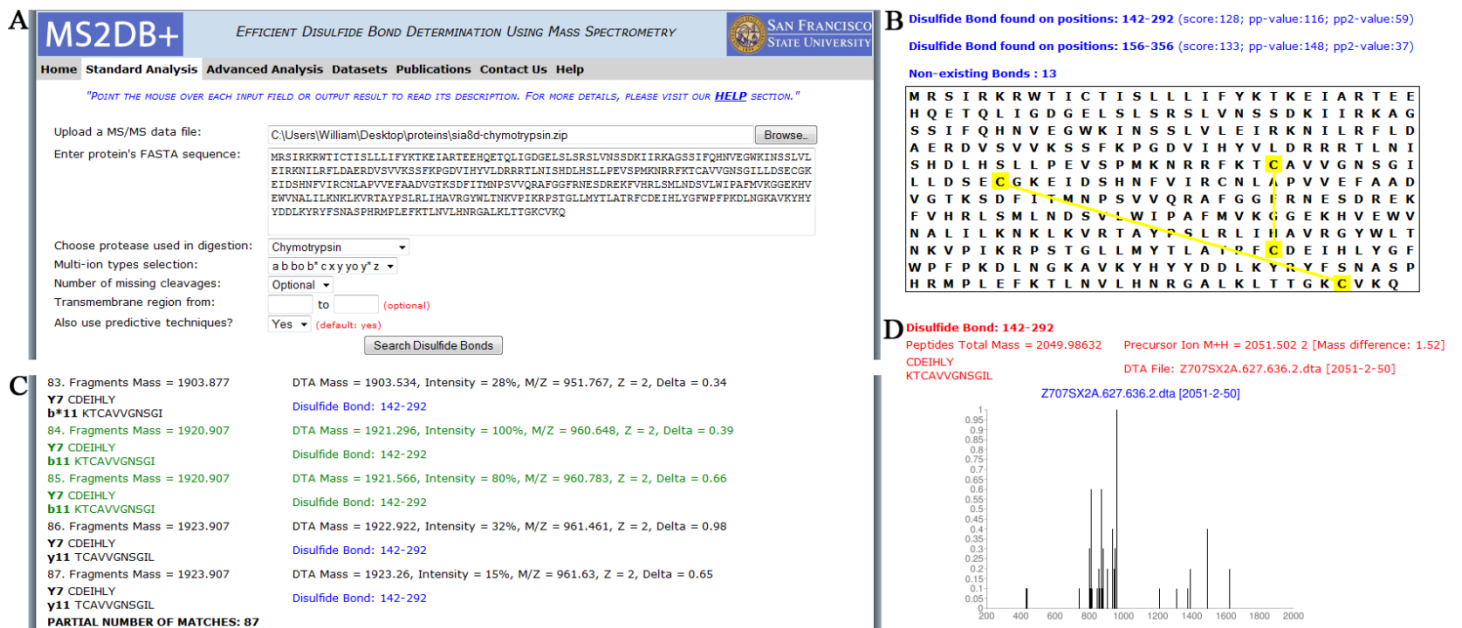


Figure 2. (A) The standard analysis interface of MS2DB+ showing the key inputs for the molecule ST8SiaIV. (B) Disulfide bonds (in yellow) found for ST8SiaIV. (C) Some of the confirmatory matches found for the S-S bond between cysteines C¹⁴²-C²⁹². Matches whose MS/MS fragment's normalized intensity equal or exceed 50% are marked in green). (D) The confirmatory spectrum for an initial match (in red) containing the most abundant confirmatory peaks found while determining the S-S bond between cysteines C¹⁴²-C²⁹².

Here, we describe a walkthrough demonstrating the use of MS2DB+ using the protein Syalyltransferase ST8Sia IV (UniProt ID Q92187). This example is one of nine Glycosyltransferases with varying S-S bonding topologies, the MS/MS data for which have been made available in the *Datasets* page of the MS2DB+ site. As a first step, in the standard analysis page (Fig.2.A), the user needs to upload the MS/MS data file(s), enter the protein's FASTA sequence and select the protease used during digestion. Next, MS2DB+ analyzes the data and lists the disulfide bonds found with their empirical and statistical scores calculated. Each bond is shown graphically, as in Fig.2.B where two bonds (C¹⁴²-C²⁹² and C¹⁵⁶-C³⁵⁶) are shown. MS2DB+ also provides other relevant information for each disulfide bond in the other sections of the figure presented above (Fig.2.C and Fig.2.D).