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Delineation of Disease Phenotypes Associated with Esophageal Adenocarcinoma by MALDI-IMS-MS Analysis of Serum N-linked Glycans

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Supporting Information

In Figure 1, each one of the disease phenotypes, esophageal adenocarcinoma (EAC), high grade dysplasia (HGD), Barrett's esophagus (BE) and normal control (NC), are represented by a single individual chosen in the center of the corresponding group cluster represented in Figure 4. In order to assess the variability across all samples of the same disease group, mobility distributions for three additional individuals are represented in Figure S-1 (glycan ion $[S_1H_5N_4+Na]^+$), Figure S-2 (glycan ion $[F_1H_5N_4+Na]^+$) and Figure S-3 (glycan ion $[S_1F_1H_5N_4+Na]^+$). These individuals are chosen at the outside edge of each group cluster represented in Figure 4.

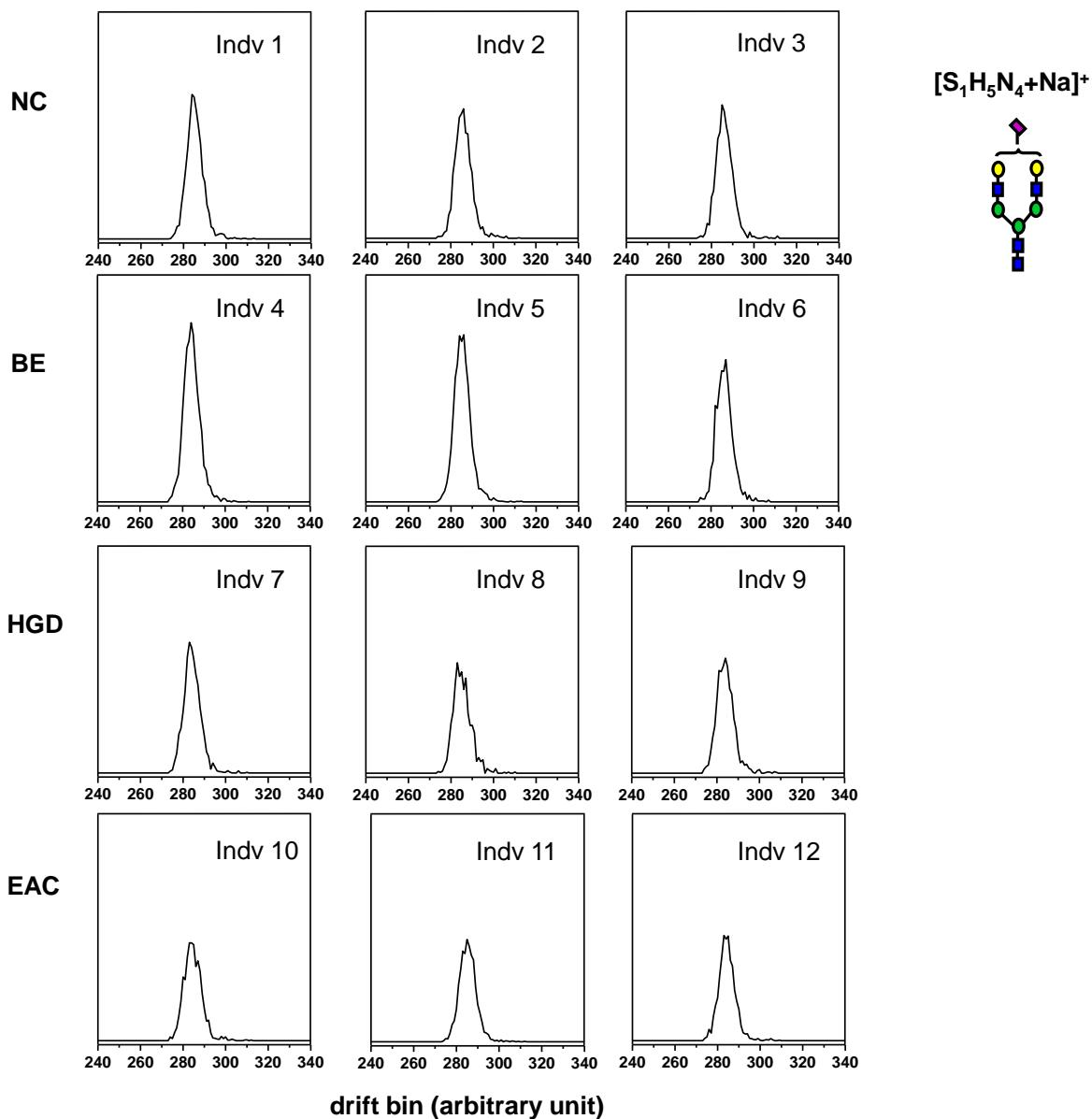


Figure S-1: Ion mobility distribution of the N-linked glycan ion $[S_1H_5N_4+Na]^+$. Esophageal adenocarcinoma (EAC), high grade dysplasia (HGD), Barrett's esophagus (BE) and normal control (NC) phenotypes are represented by three individuals each. The glycan structure is shown on the right: F represents fucose (red triangle), H represents hexose (mannose green circle, galactose yellow circle), N represents N-acetylglucosamine (blue square) and S represents sialic acid (purple diamond).

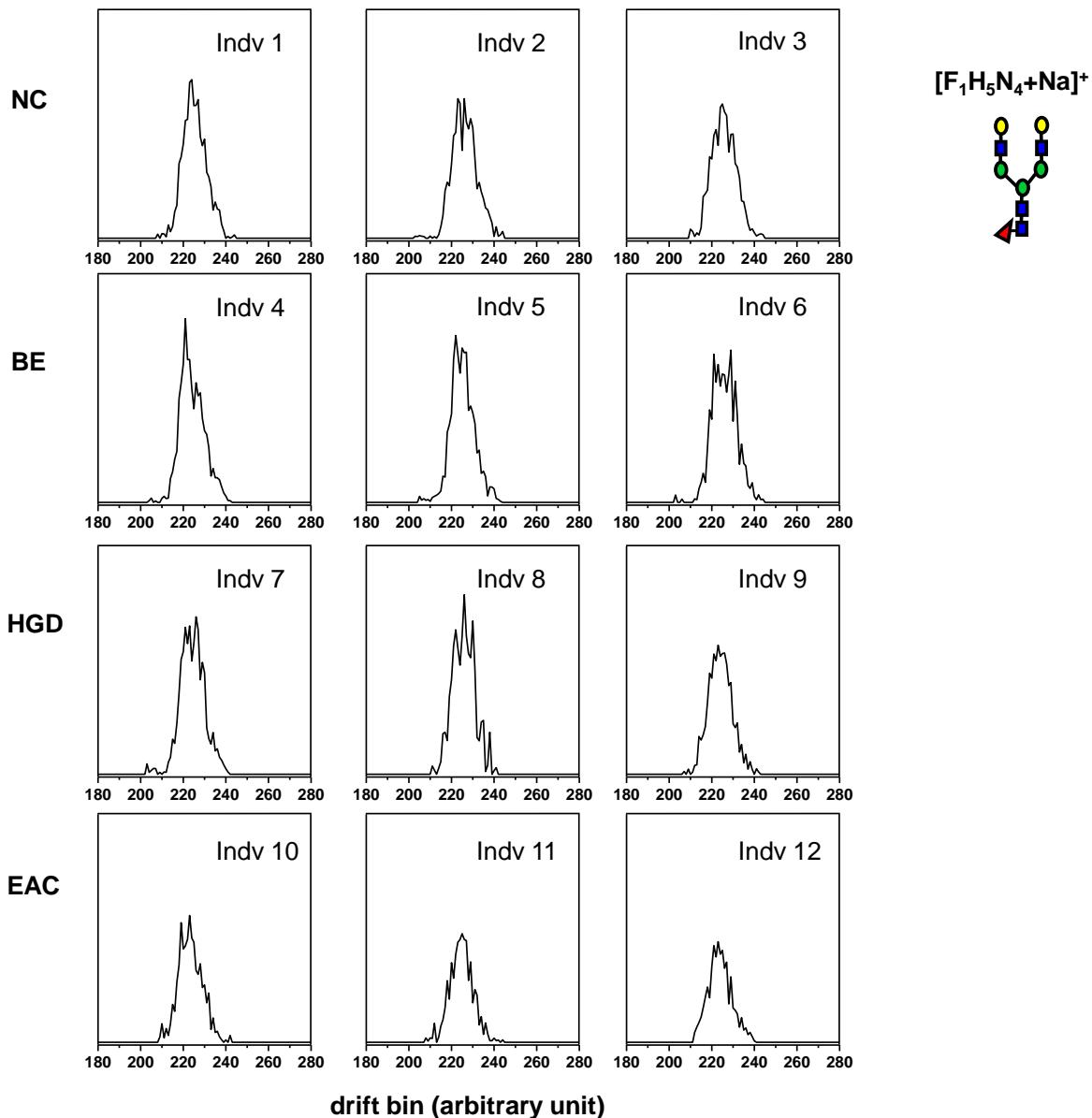


Figure S-2: Ion mobility distribution of the N-linked glycan ion $[F_1H_5N_4+Na]^+$. Esophageal adenocarcinoma (EAC), high grade dysplasia (HGD), Barrett's esophagus (BE) and normal control (NC) phenotypes are represented by three individuals each. The glycan structure is shown on the right: F represents fucose (red triangle), H represents hexose (mannose green circle, galactose yellow circle), N represents N-acetylglucosamine (blue square) and S represents sialic acid (purple diamond).

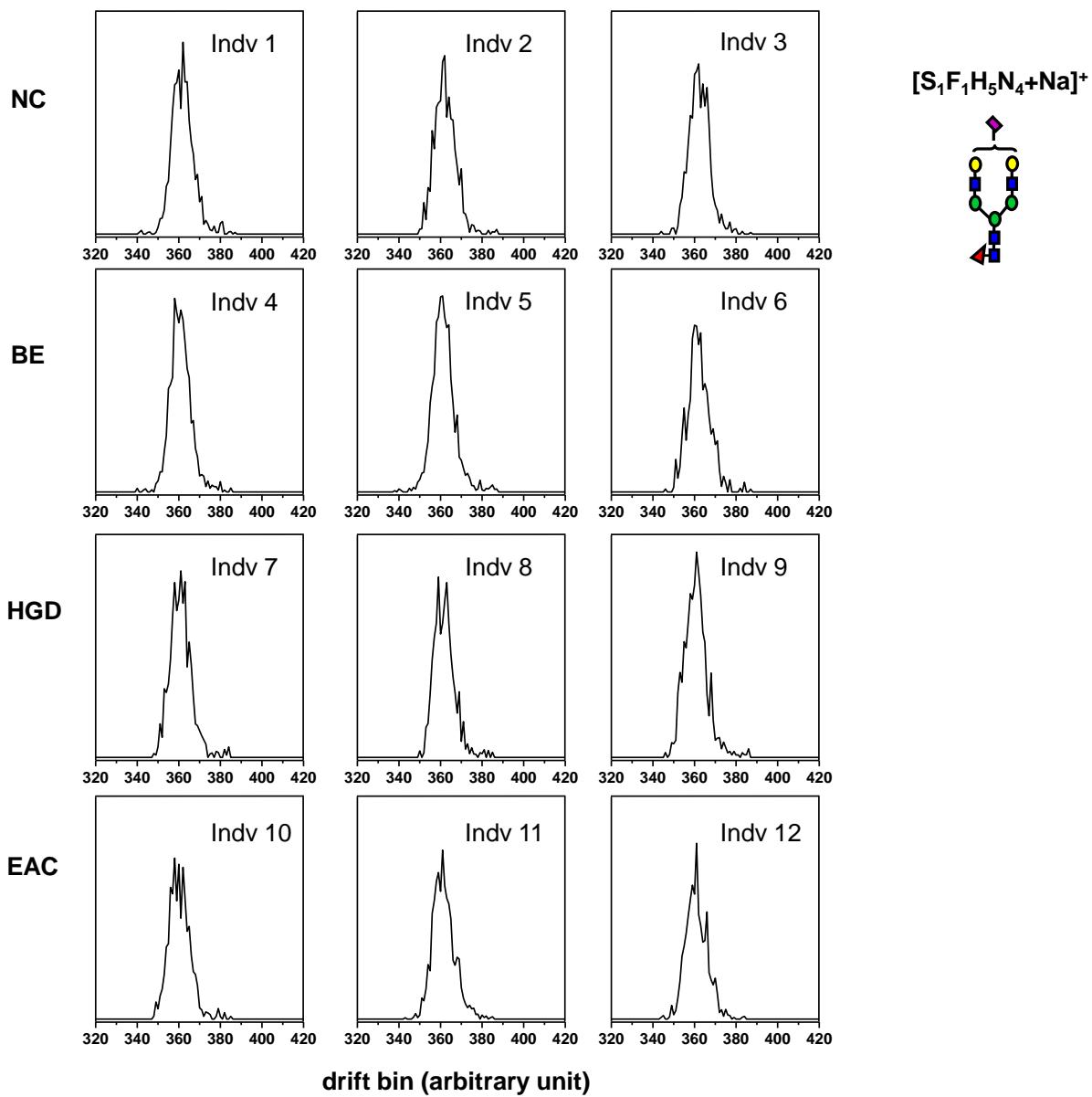


Figure S-3: Ion mobility distribution of the N-linked glycan ion $[S_1F_1H_5N_4+Na]^+$. Esophageal adenocarcinoma (EAC), high grade dysplasia (HGD), Barrett's esophagus (BE) and normal control (NC) phenotypes are represented by three individuals each. The glycan structure is shown on the right: F represents fucose (red triangle), H represents hexose (mannose green circle, galactose yellow circle), N represents N-acetylglucosamine (blue square) and S represents sialic acid (purple diamond).

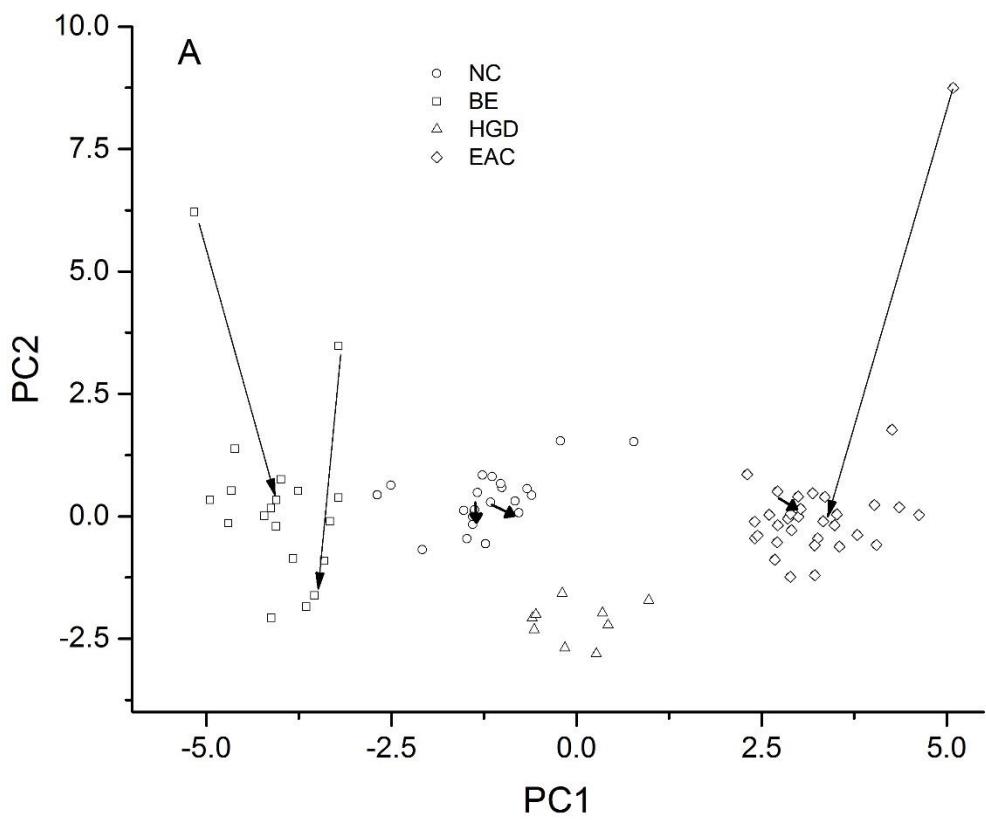


Figure S-4: Arrows indicating matched-pairs of replicate measurements overlaid on the PC plot of the 38 features selected after 200 generations of the genetic algorithm for pattern recognition shown in Figure 3 A of the manuscript.

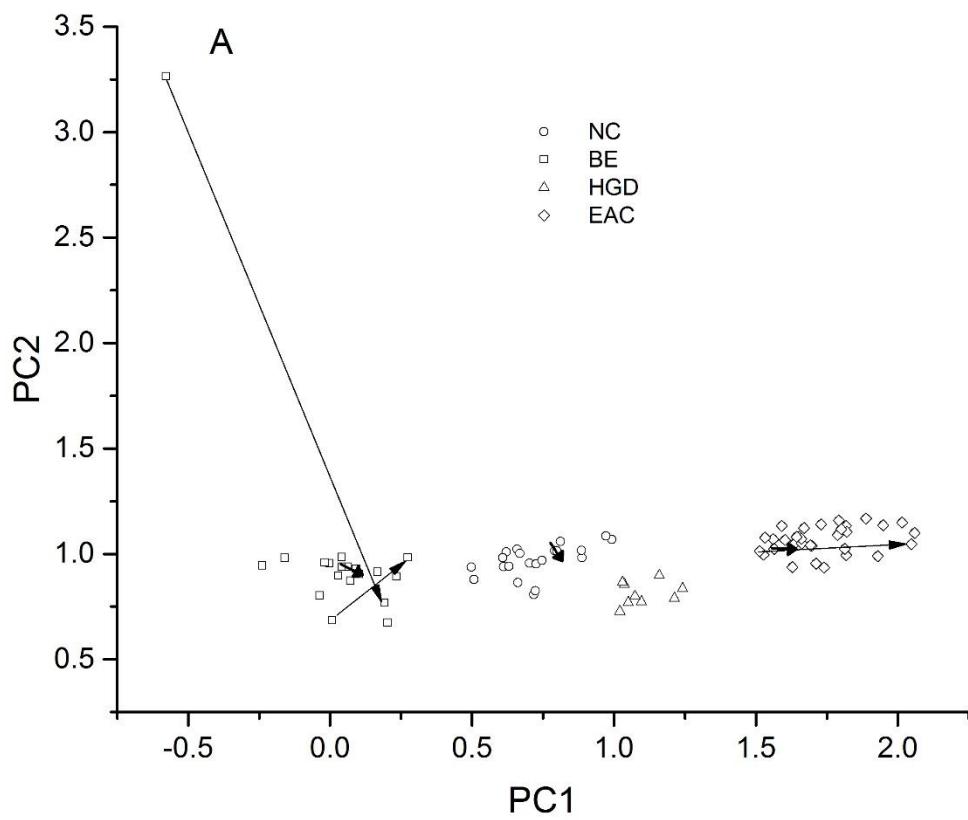


Figure S-5: Arrows indicating matched-pairs of replicate measurements overlaid on the Plot of the two largest PC of the 24 features obtained after 200 generations of the genetic algorithm for pattern recognition shown in Figure 4 A of the manuscript.

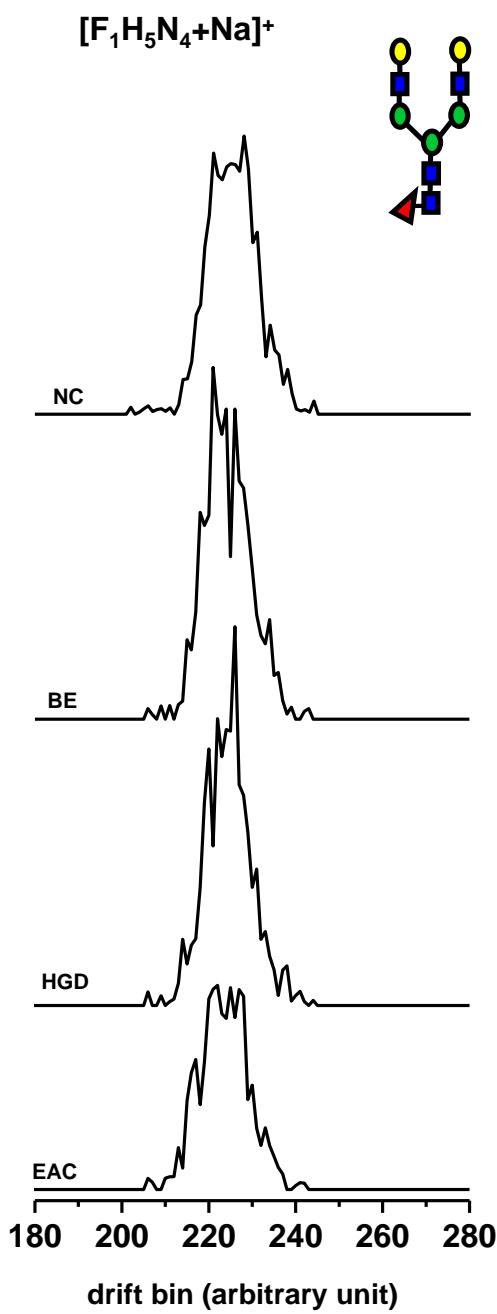


Figure S-7: Enlarged view of the ion mobility distribution of the N-linked glycan ion $[F_1H_5N_4+Na]^+$ presented in Figure 1, middle trace. Esophageal adenocarcinoma (EAC), high grade dysplasia (HGD), Barrett's esophagus (BE) and normal control (NC) phenotypes are represented by three individuals each. The glycan structure is shown on the right: F represents fucose (red triangle), H represents hexose (mannose green circle, galactose yellow circle), N represents N-acetylglucosamine (blue square) and S represents sialic acid (purple diamond).