

Supplementary data for “Conversion of Multiple Analyte Cation Types to a Single Analyte Anion Type via Ion/Ion Charge Inversion” by Kerry M. Hassell, Yves LeBlanc, and Scott A. McLuckey:

Supplementary figures:

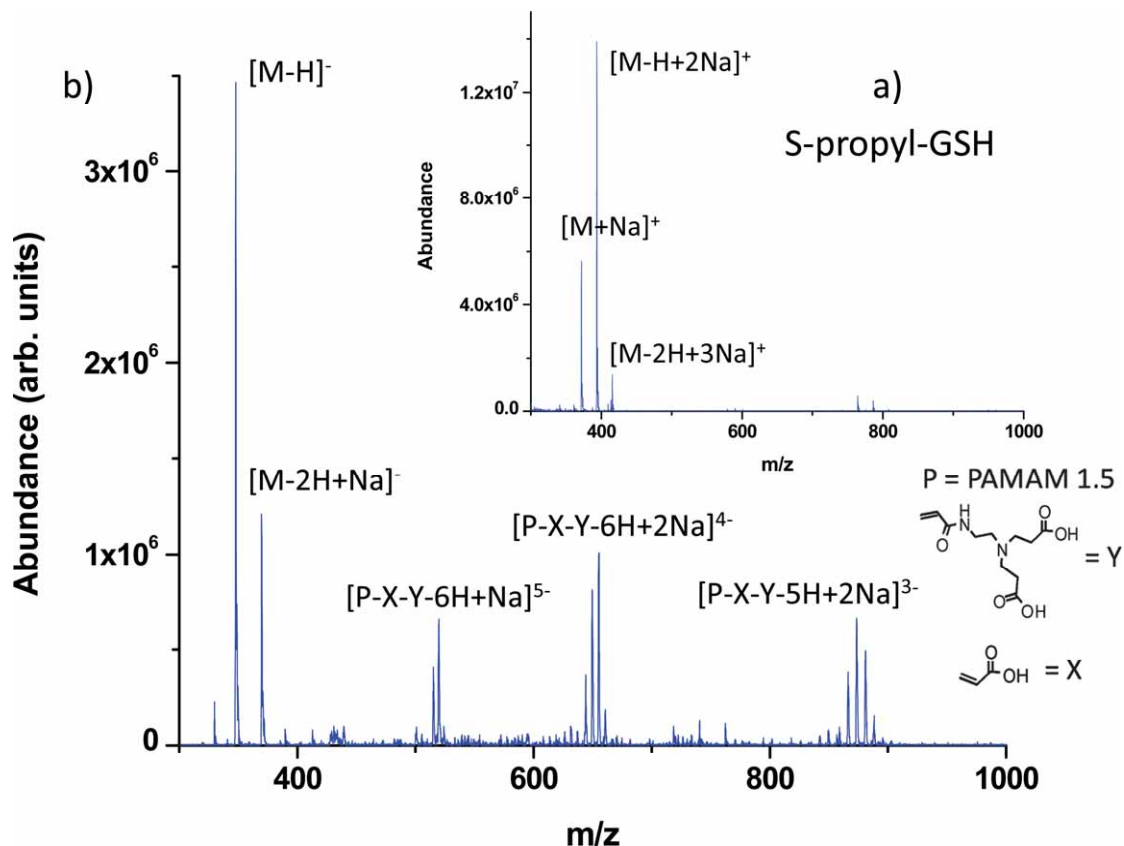


Figure S1 – a) Positive ion electrospray mass spectrum of S-propyl glutathione and b) negative ion spectrum after ion/ion charge inversion using [P-X-Y-6H]⁶⁻ reagent anions, where P = PAMAM generation 1.5.

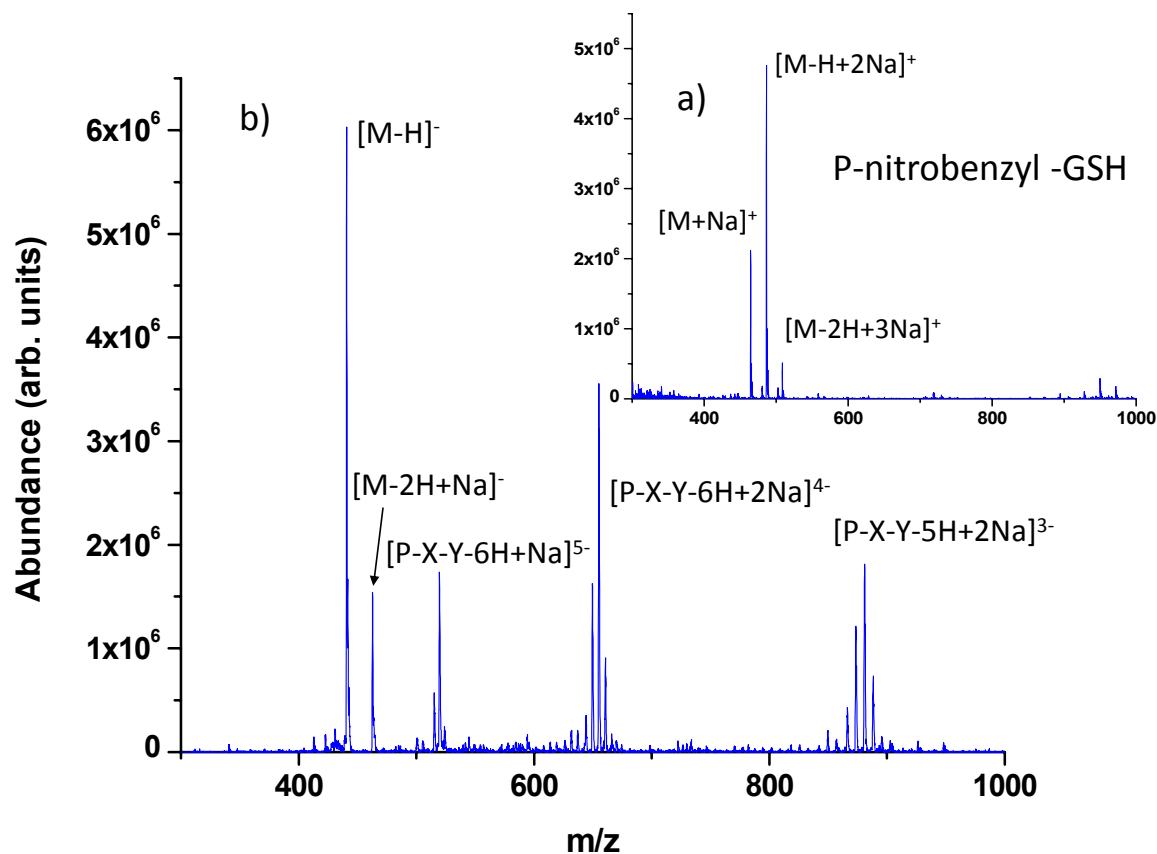


Figure S2 – a) Positive ion electrospray mass spectrum of P-nitrobenzyl glutathione and b) negative ion spectrum after ion/ion charge inversion using $[P-X-Y-6H]^{0-}$ reagent anions, where P = PAMAM generation 1.5 (see Figure S1 for structures of X and Y).

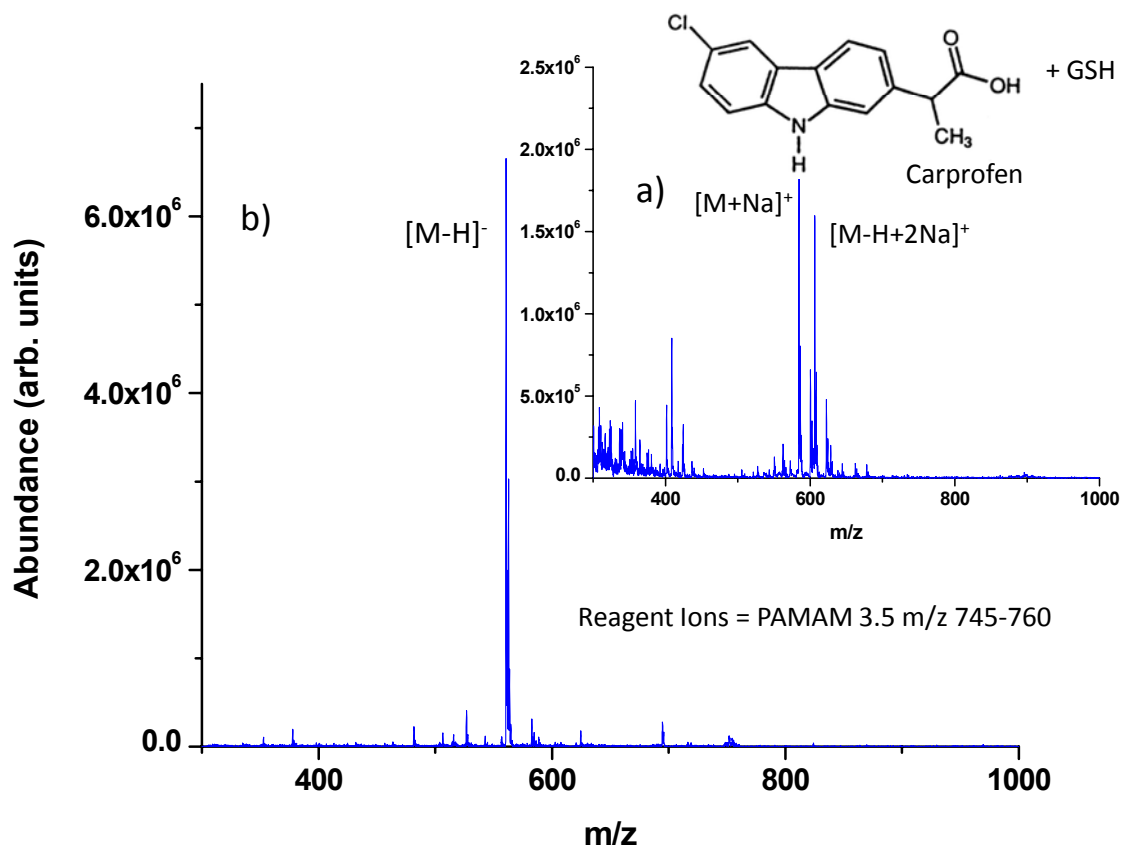


Figure S3 – a) Positive ion electrospray mass spectrum of the GSH conjugate of carprofen (see structure in the figure) and b) negative ion spectrum after ion/ion charge inversion using anions in the m/z region of 745-760 derived from nanoelectrospray of PAMAM generation 3.5.

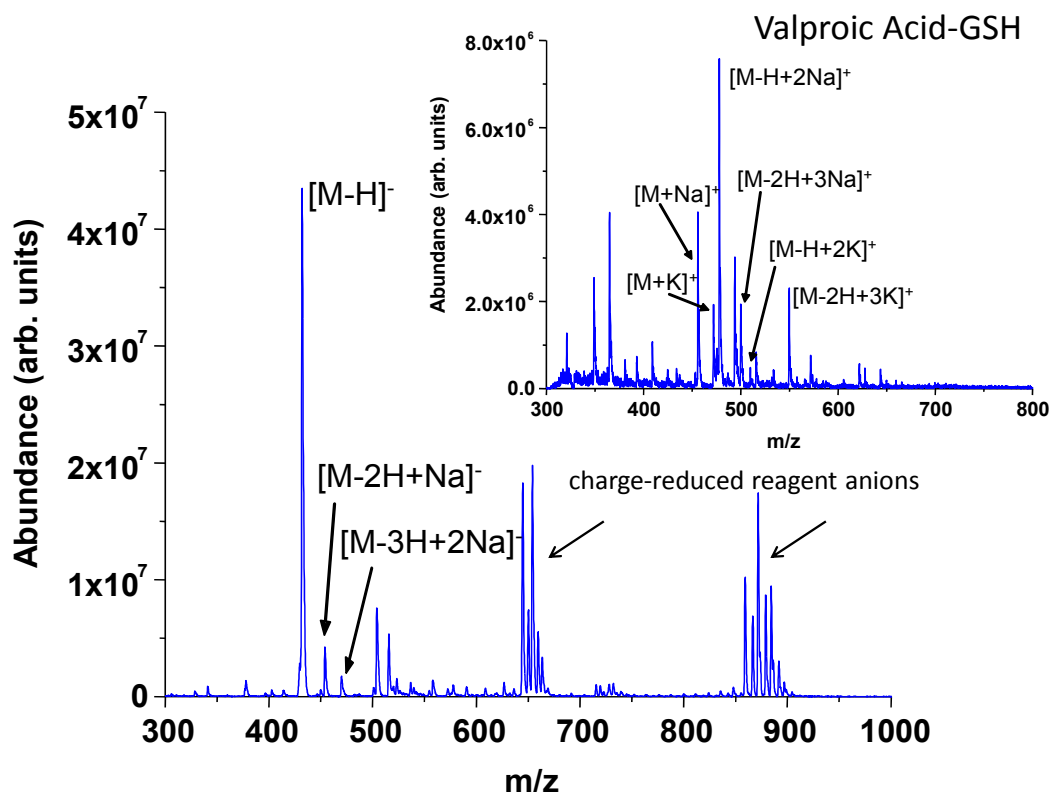


Figure S4 –a) Positive electrospray mass spectrum of valproic acid-GSH with significant $[M+K]^+$ signal and b) negative ion spectrum after ion/ion charge inversion using $[P-X-Y-6H]^{6-}$ reagent anions, where P = PAMAM generation 1.5 (see Figure S1 for structures of X and Y).