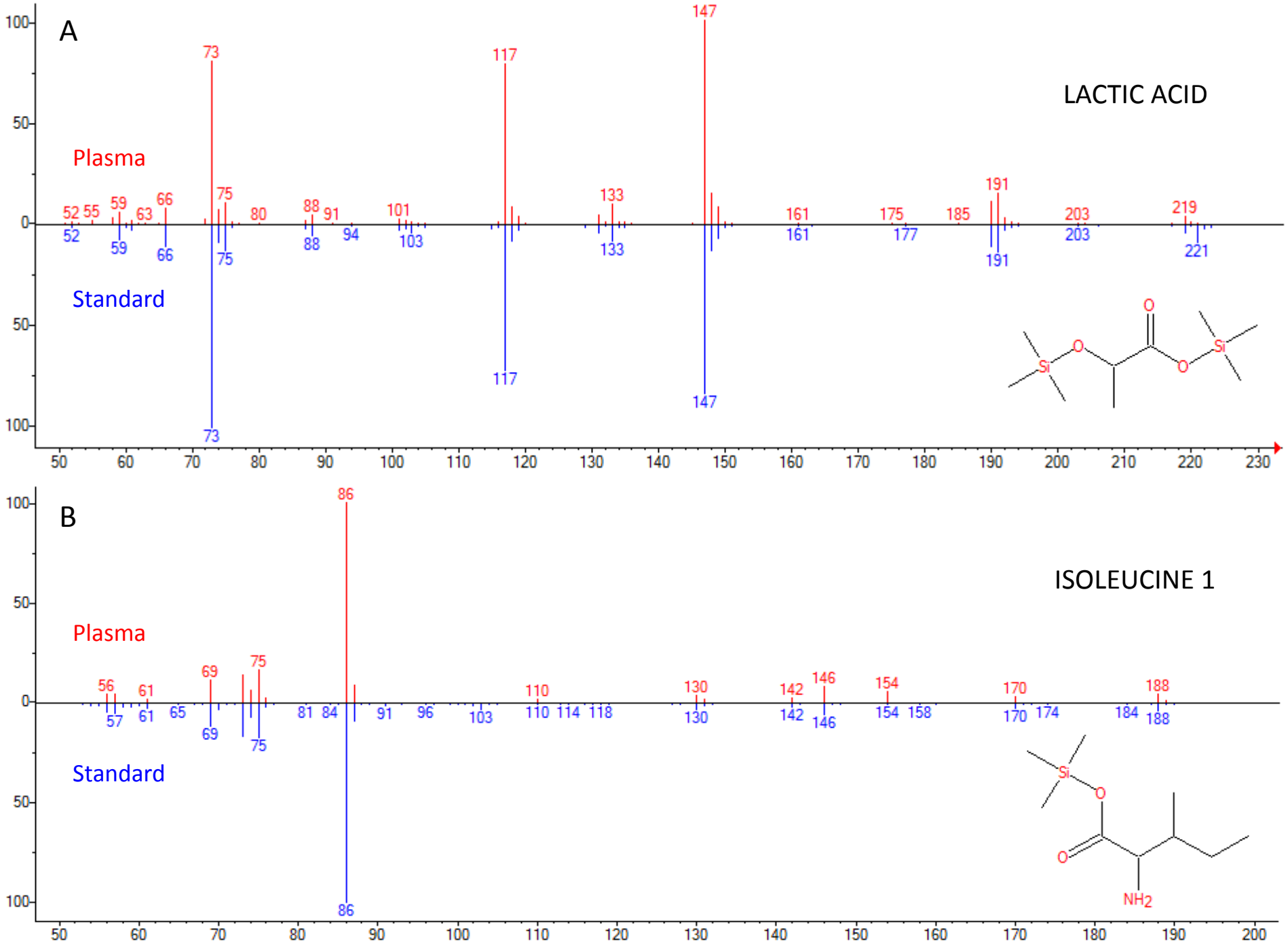
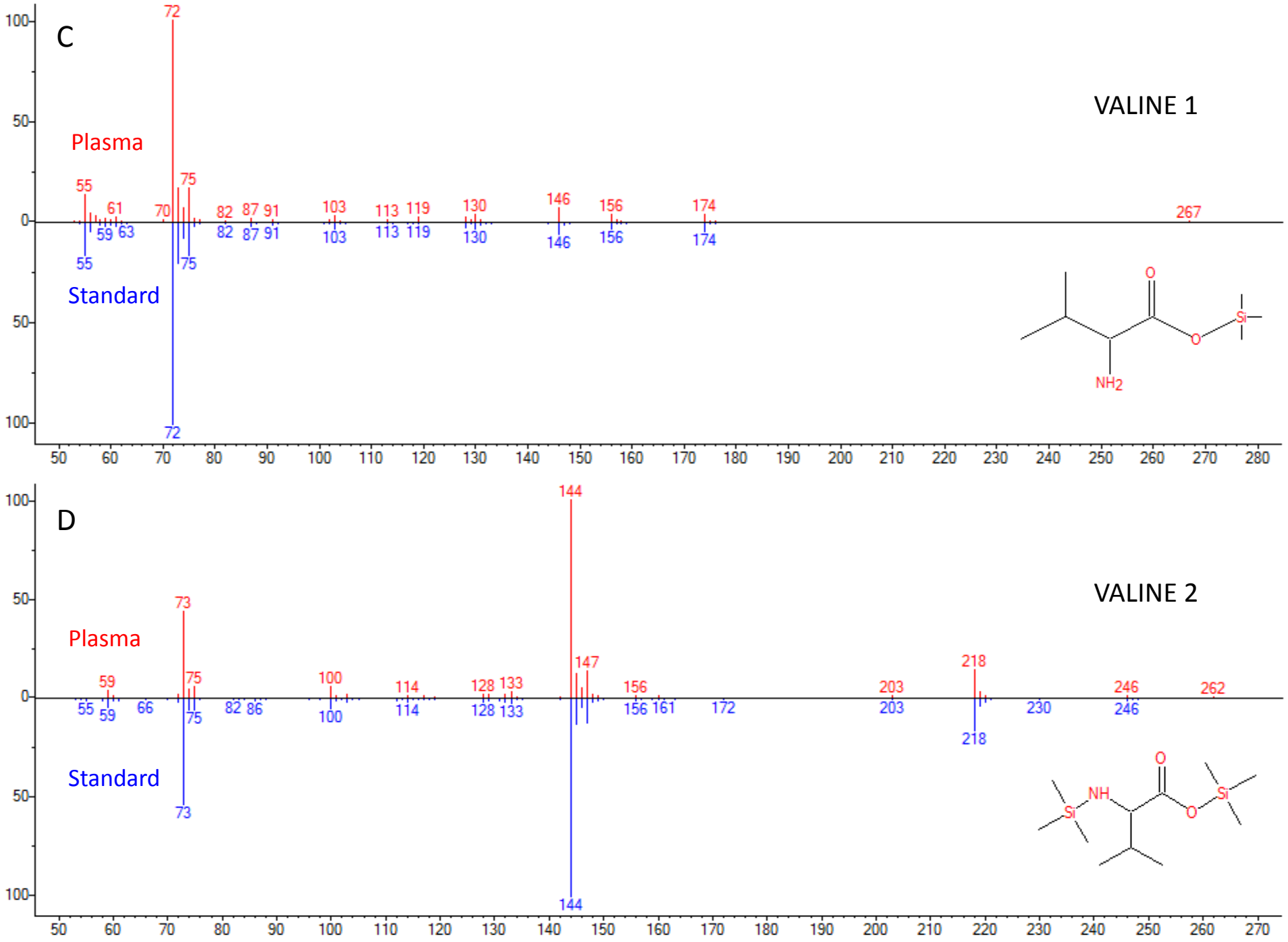
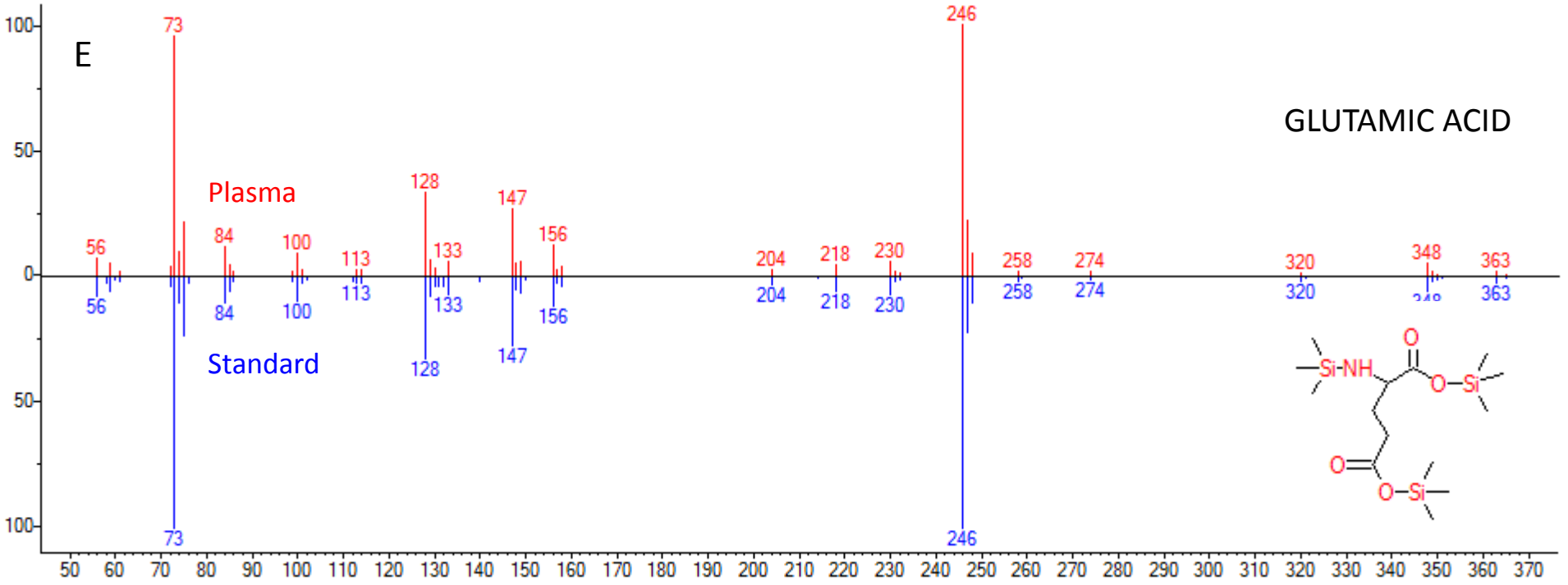
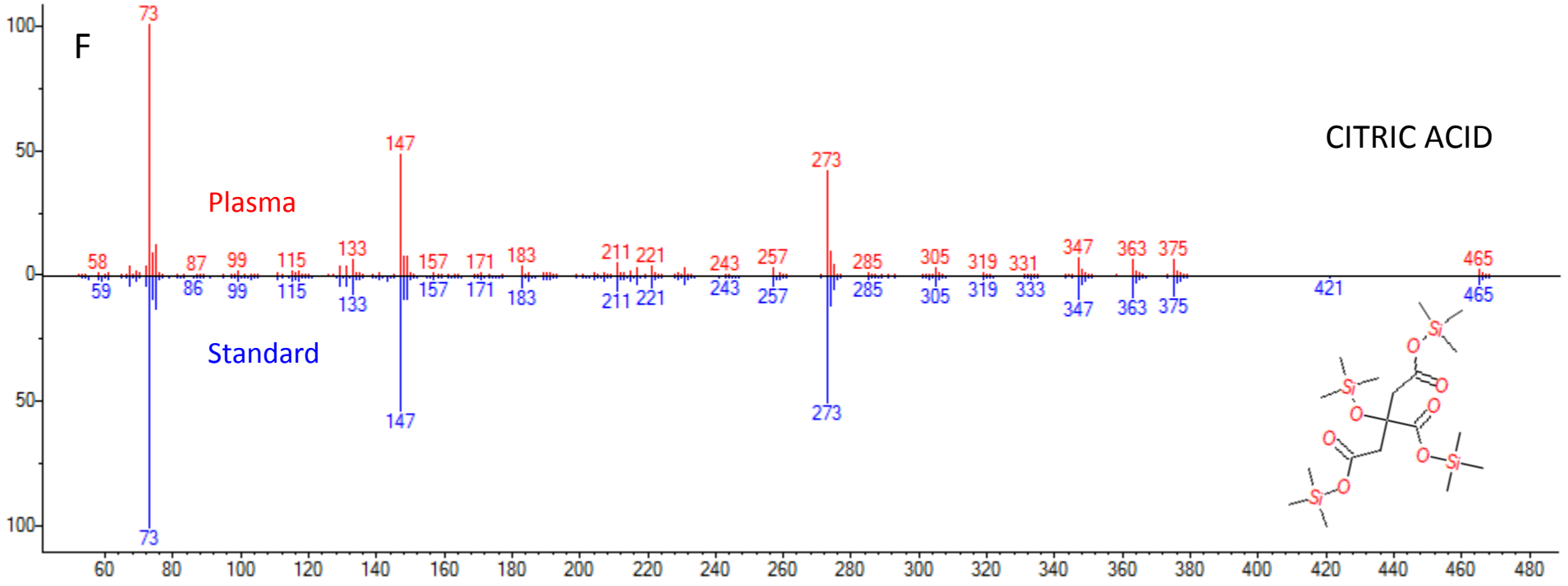
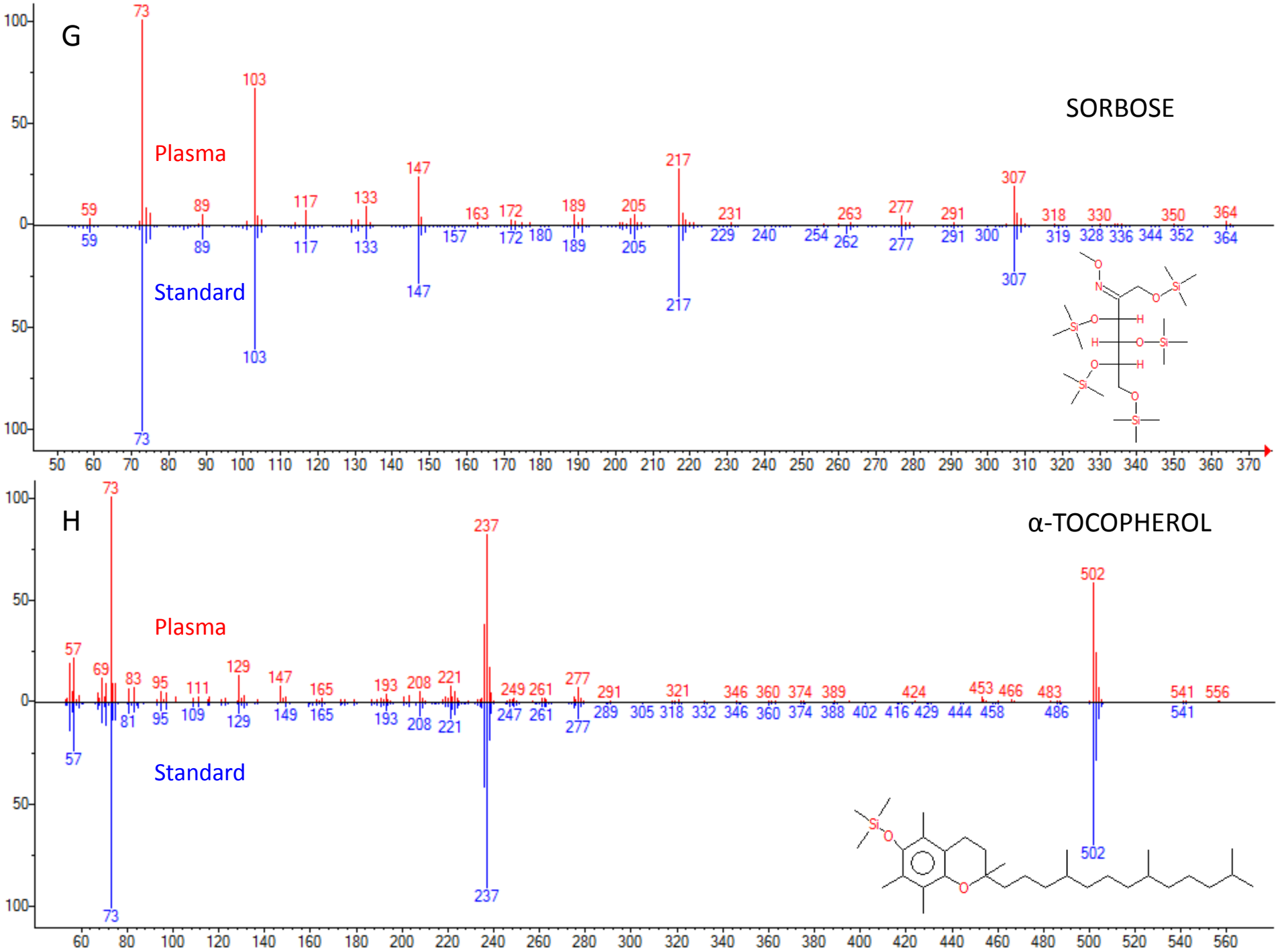

A
LACTIC ACID
Plasma
Standard
B
ISOLEUCINE 1
Plasma
Standard


C
VALINE 1
Plasma
Standard
D
VALINE 2
Plasma
Standard


E
GLUTAMIC ACID
Plasma
Standard
Si-NH
O
O-Si
O=
O-Si


F
CITRIC ACID
Plasma
Standard
O
O
O
O
O
O
Si
Si
Si
Si


G
SORBOSE
Plasma
Standard
H
α-TOCOPHEROL
Plasma
Standard

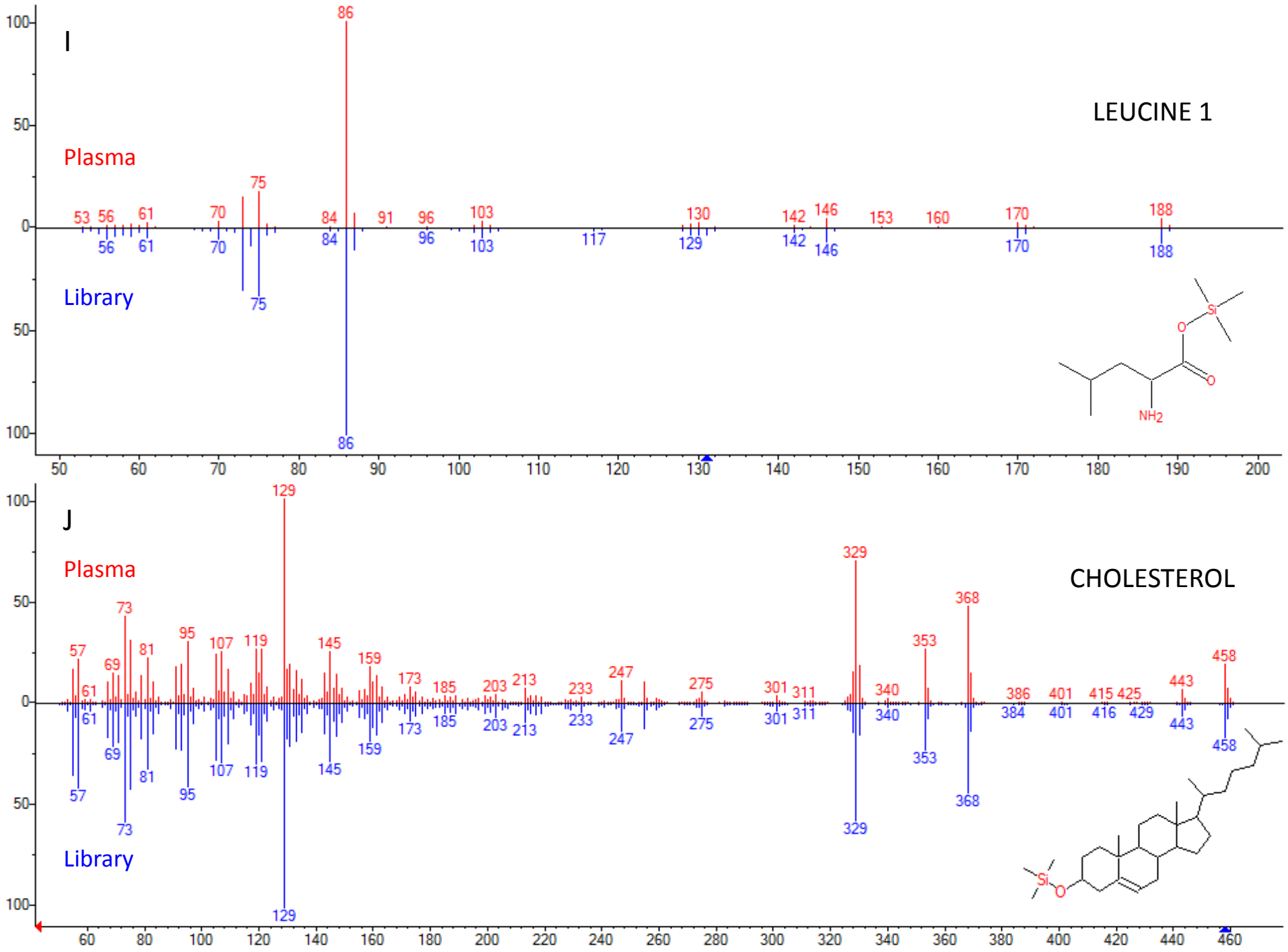

I
Plasma
Library
LEUCINE 1
J
Plasma
Library
CHOLESTEROL

Figure S1. Confirmation of metabolites' identities using standards. Identities of the following seven metabolites found to be significant in the targeted analyses were confirmed by the analysis of authentic compounds purchased from Sigma Aldrich: L-glutamic acid (95436), DL-alfa-tocopherol (47783), L-valine (PHR1172), L-(+)-lactic acid (46937), D-(+)-sorbose (S4887), DL-isoleucine (298689), and citric acid (94676). Individual 0.25 mg/mL stock standards solutions were prepared in appropriate solvent and stored at -20 °C until the analysis. Working standards solutions, at the concentration of 1.25 µg/mL, were prepared by appropriate dilution of the stock standard solutions in acetonitrile, isopropanol, and water (3:3:2). Standards were then concentrated to dryness and derivatized following the same procedure as for the serum samples described in the material and method paragraph. Each standard was analyzed in both GCq and GC-TOF platform, following the same GC and MS methods as previously described in the "Acquisition of GC-MS Data by Untargeted Method" section. Acquired spectra of the individual standards were cross matched with the corresponding spectra extracted from analysis of plasma samples. Representative spectra of the comparisons between the plasma metabolites and the standards are shown in Panels A-G. For two metabolites (leucine 1 and cholesterol), the comparisons were made between spectra from plasma samples and reference spectra extracted from the Fiehn library as illustrated in Panels H & I.