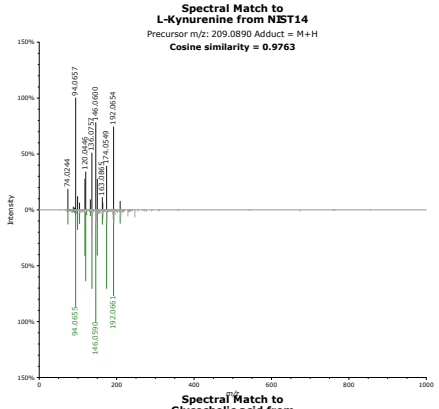
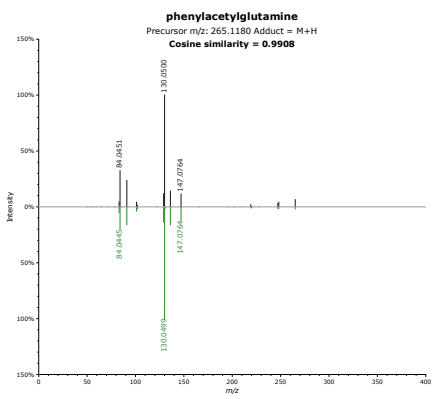
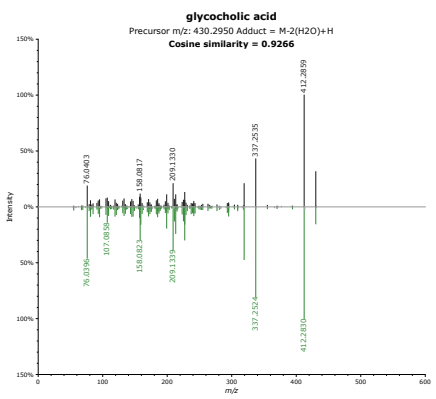
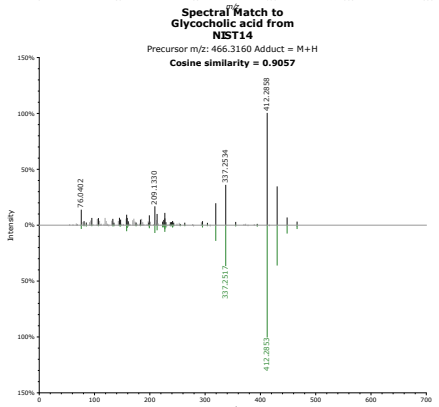
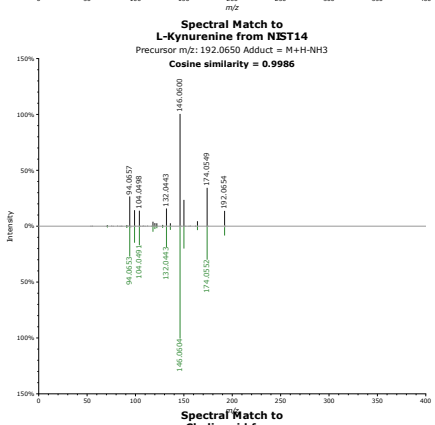
Figurere 2S

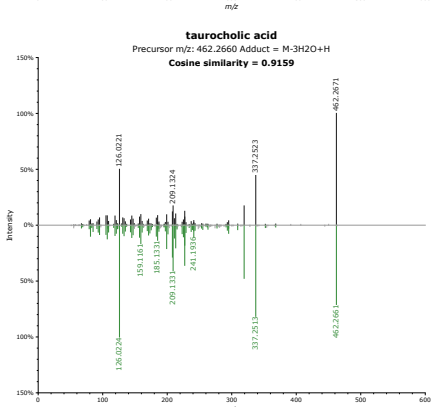

Spectral Match to
L-Kynurenine from NIST14
Precursor m/z: 209.0890 Adduct = M+H
Cosine similarity = 0.9763
Intensity
m/z

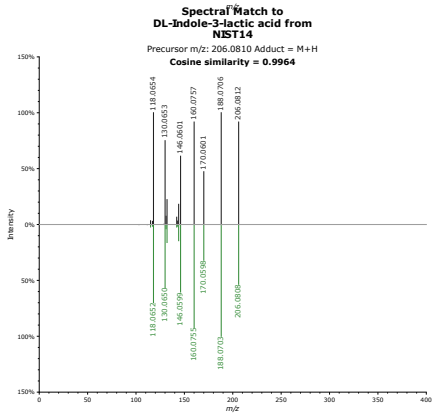

phenylacetylglutamine
Precursor m/z: 265.1180 Adduct = M+H
Cosine similarity = 0.9908
Intensity
m/z

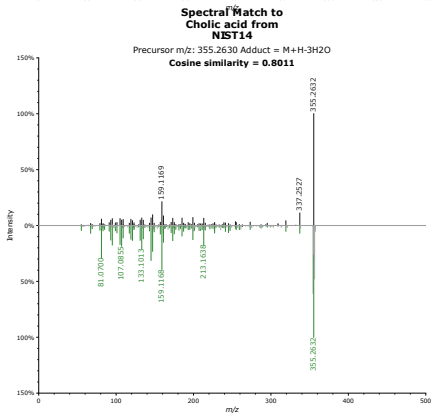

glycocholic acid
Precursor m/z: 430.2950 Adduct = M-2(H2O)+H
Cosine similarity = 0.9266
Intensity
m/z

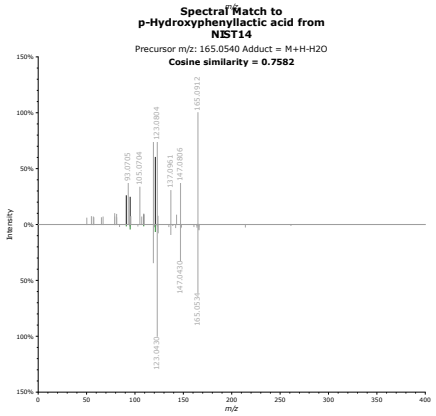

Spectral Match to
Glycocholic acid from
NIST14
Precursor m/z: 466.3160 Adduct = M+H
Cosine similarity = 0.9057
Intensity
m/z

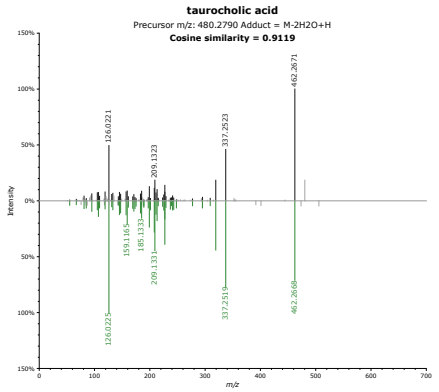

Spectral Match to
L-Kynurenine from NIST14
Precursor m/z: 192.0650 Adduct = M+H-NH3
Cosine similarity = 0.9986
Intensity
m/z

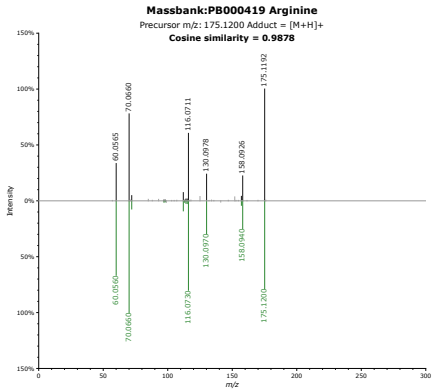

taurocholic acid
Precursor m/z: 462.2660 Adduct = M-3H2O+H
Cosine similarity = 0.9159
Intensity
m/z

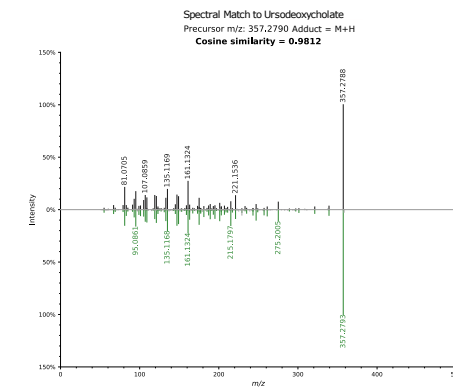

Spectral Match to
DL-Indole-3-lactic acid from
NIST14
Precursor m/z: 206.0810 Adduct = M+H
Cosine similarity = 0.9964
Intensity
m/z

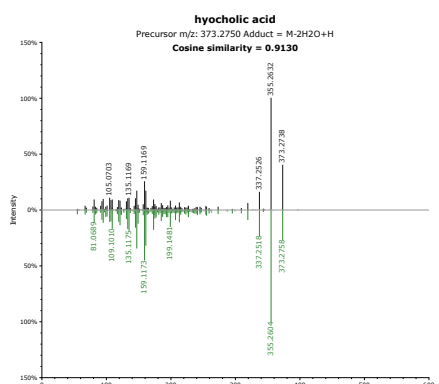

Spectral Match to
Cholic acid from
NIST14
Precursor m/z: 355.2630 Adduct = M+H-3H2O
Cosine similarity = 0.8011
Intensity
m/z

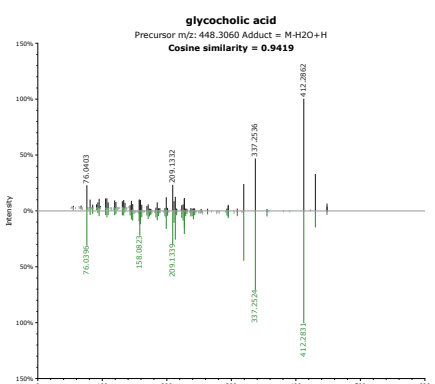

Spectral Match to
p-Hydroxyphenyllactic acid from
NIST14
Precursor m/z: 165.0540 Adduct = M+H-H2O
Cosine similarity = 0.7582
Intensity
m/z

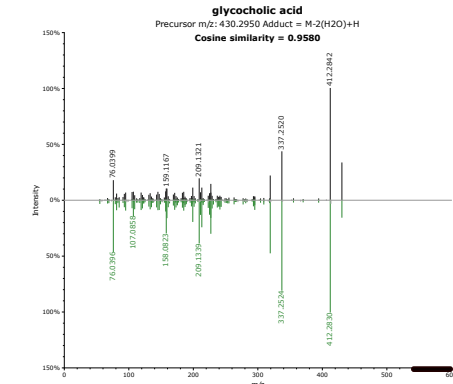

taurocholic acid
Precursor m/z: 480.2790 Adduct = M-2H2O+H
Cosine similarity = 0.9119
Intensity
m/z


Massbank:PB000419 Arginine
Precursor m/z: 175.1200 Adduct = [M+H]+
Cosine similarity = 0.9878
Intensity
m/z


Spectral Match to Ursodeoxycholate
Precursor m/z: 357.2790 Adduct = M+H
Cosine similarity = 0.9812
Intensity
m/z


hyocholic acid
Precursor m/z: 373.2750 Adduct = M-2H2O+H
Cosine similarity = 0.9130
Intensity


glycocholic acid
Precursor m/z: 448.3060 Adduct = M-H2O+H
Cosine similarity = 0.9419
Intensity


glycocholic acid
Precursor m/z: 430.2950 Adduct = M-2(H2O)+H
Cosine similarity = 0.9580
Intensity