Supporting Information (Figures)

Integration of semi-empirical MS/MS library with characteristic features for annotation of novel amino acid conjugated bile acids

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Figure S1. Comparison of MS intensities of amino acid conjugated lithocholic acid (LCA), deoxycholic acid (DCA) and cholic acid (CA) in negative and positive mode, normalized to the intensity of negative mode.
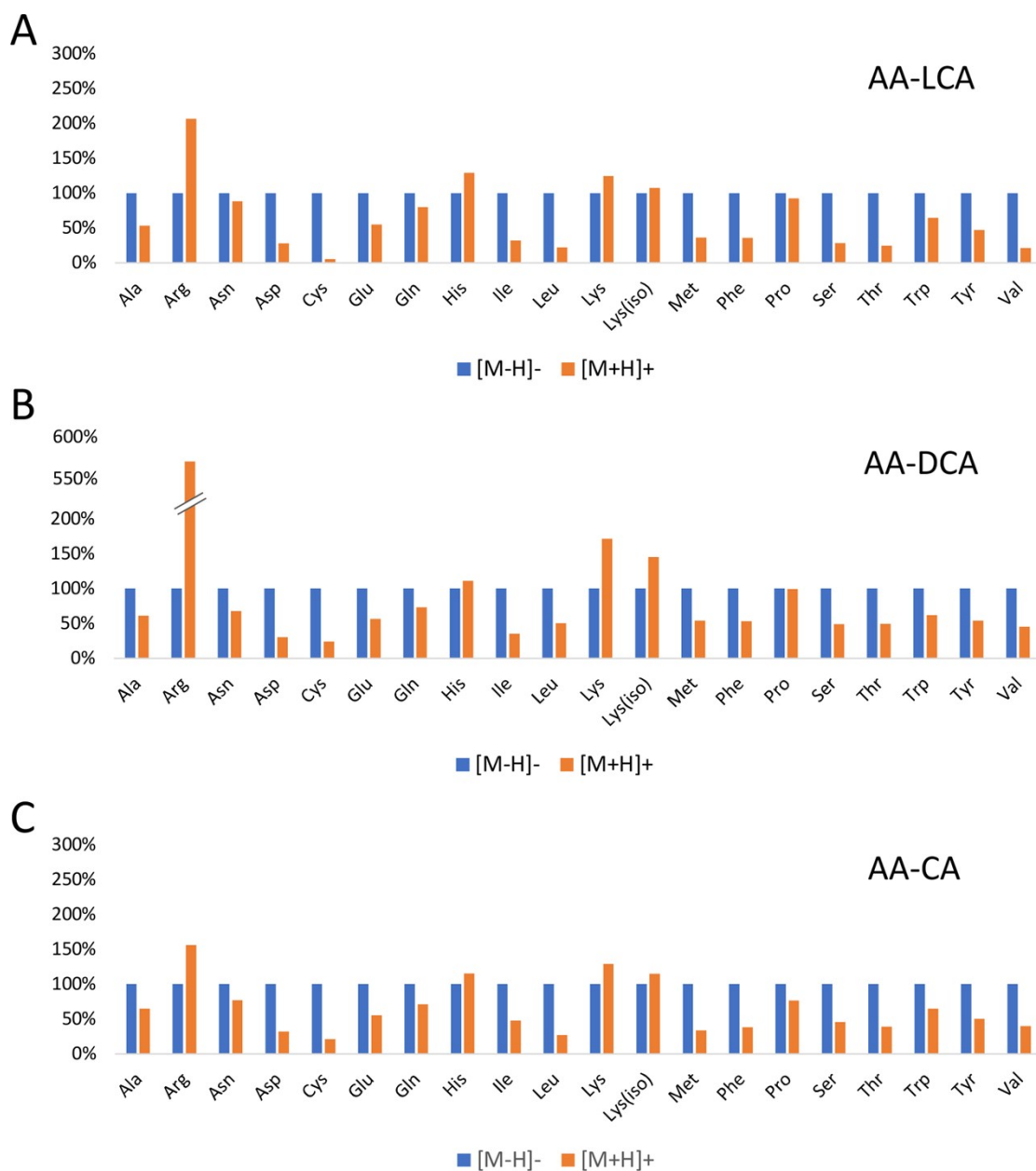
Figure S2. MS/MS spectra of cysteine conjugated lithocholic acid (LCA), deoxycholic acid (DCA) and cholic acid (CA) in negative mode.

A

$[M-H-CO_2-H_2S]^-$
400.3218

Cys-LCA

$[M-H-Cys]^-$
357.2783

300.1697

B

$[M-H-Cys-H_2O]^-$
355.2645

Cys-DCA

$[M-H-CO_2-H_2S]^-$
416.3183

297.2229

C

$[M-H-Cys-2H_2O]^-$
353.2484

Cys-CA

95.0490

$[M-H-Cys-H_2O]^-$
371.2595

$[M-H-CO_2-H_2S]^-$
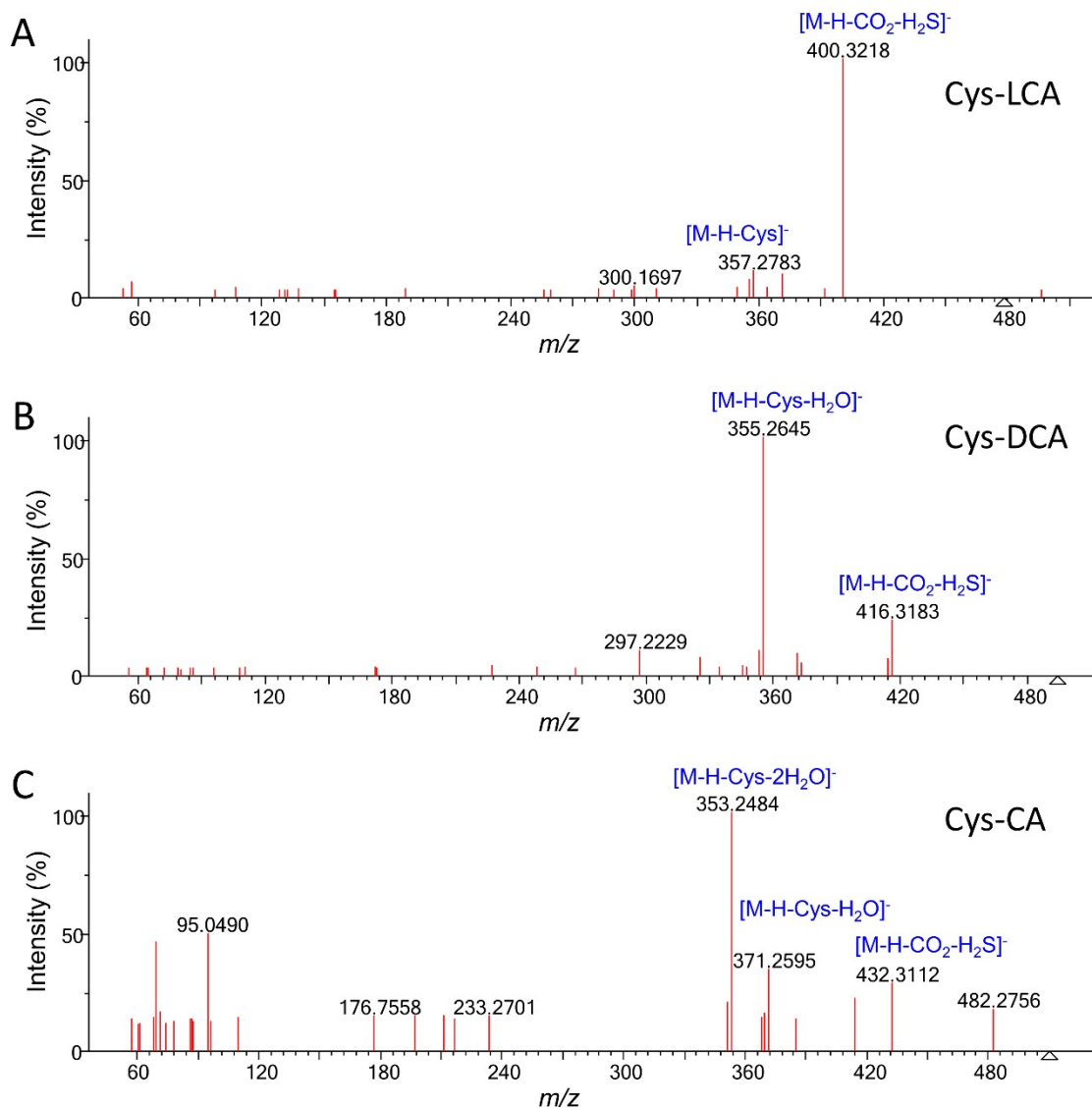432.3112

482.2756

176.7558   233.2701

Figure S3. Workflow of semi-empirical library development in negative mode.
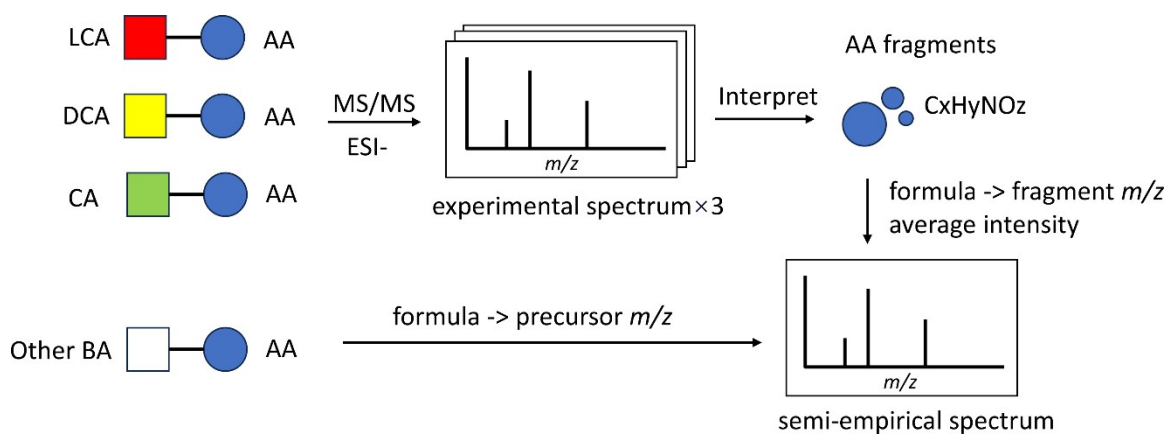
Figure S3: MS/MS spectra of amino acid conjugated cholic acid (CA) in positive mode, compared with MS/MS spectra of unconjugated CA.

m/z of amino acid-related fragments are labeled. Triangles on the *m/z* axis show the positions of precursors.

H

110.071 156.077

His-CA

CA

m/z 110,156 removed

I

86.097

132.102

Leu-CA

CA

J

86.097

132.102

Ile-CA

CA

S7

K

84.082
130.086
147.113

Lys-CA

CA

L

84.081
130.086
147.113

Lys(iso)-CA

CA

M

104.053 133.032 150.058

Met-CA

CA

N

120.081
166.086

Phe-CA

CA

O

116.071

70.066

Pro-CA

CA

⇨

m/z 70,116 removed

P

106.050

60.045

Ser-CA

CA

Q

120.066

102.056

74.061

Thr-CA

CA