Horse Chestnut saponins – Escins, Isoescins, Transescins, and Desacylescins

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Supporting information

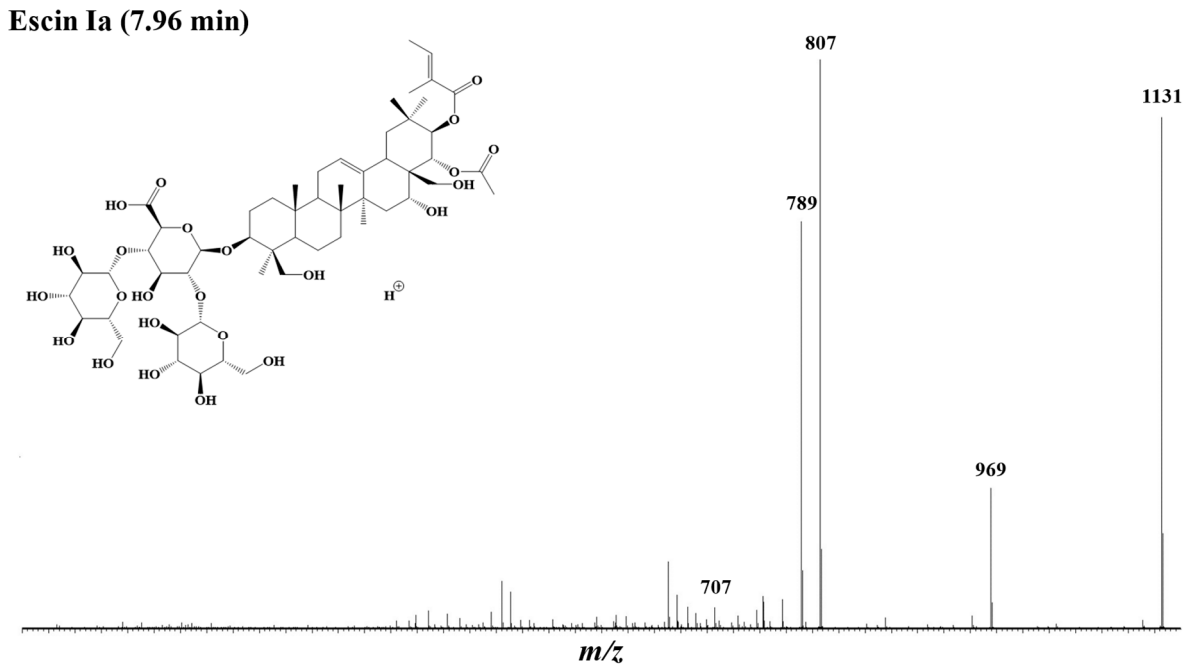

Figure S1: LC-MSMS(+) analysis of Escins I, II and III enriched-extract (EE): CID spectrum (15 eV) recorded for the *m/z* 1131 precursor ions $[M+H]^+$ at 7.96 min retention time (Escin Ia)

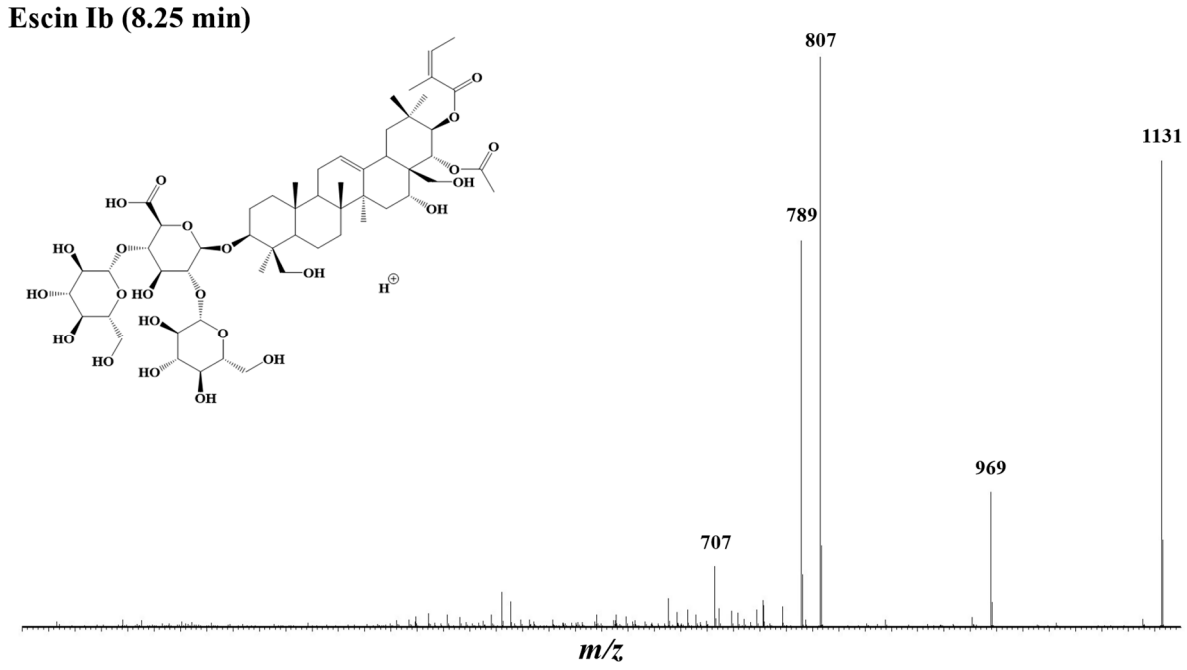

Figure S2: LC-MSMS(+) analysis of Escins I, II and III enriched-extract (EE): CID spectrum (15 eV) recorded for the *m/z* 1131 precursor ions $[M+H]^+$ at 8.25 min retention time (Escin Ib)

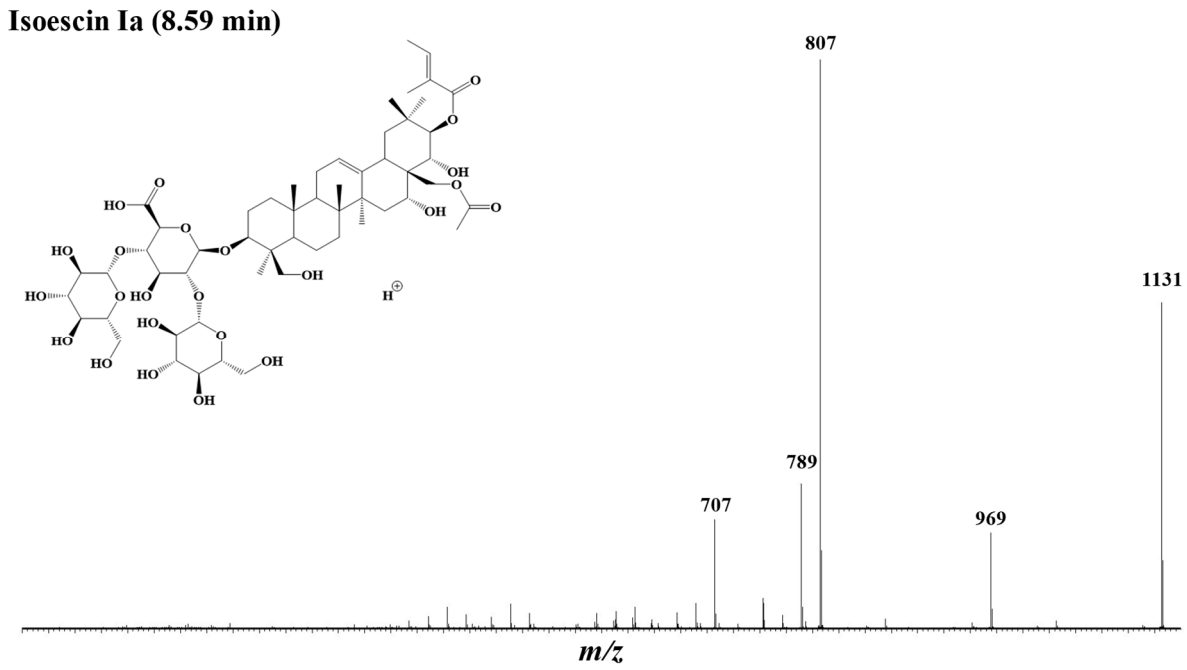

Figure S3: LC-MSMS(+) analysis of Escins I, II and III enriched-extract (EE): CID spectrum (15 eV) recorded for the *m/z* 1131 precursor ions $[M+H]^+$ at 8.59 min retention time (Isoescin Ia)

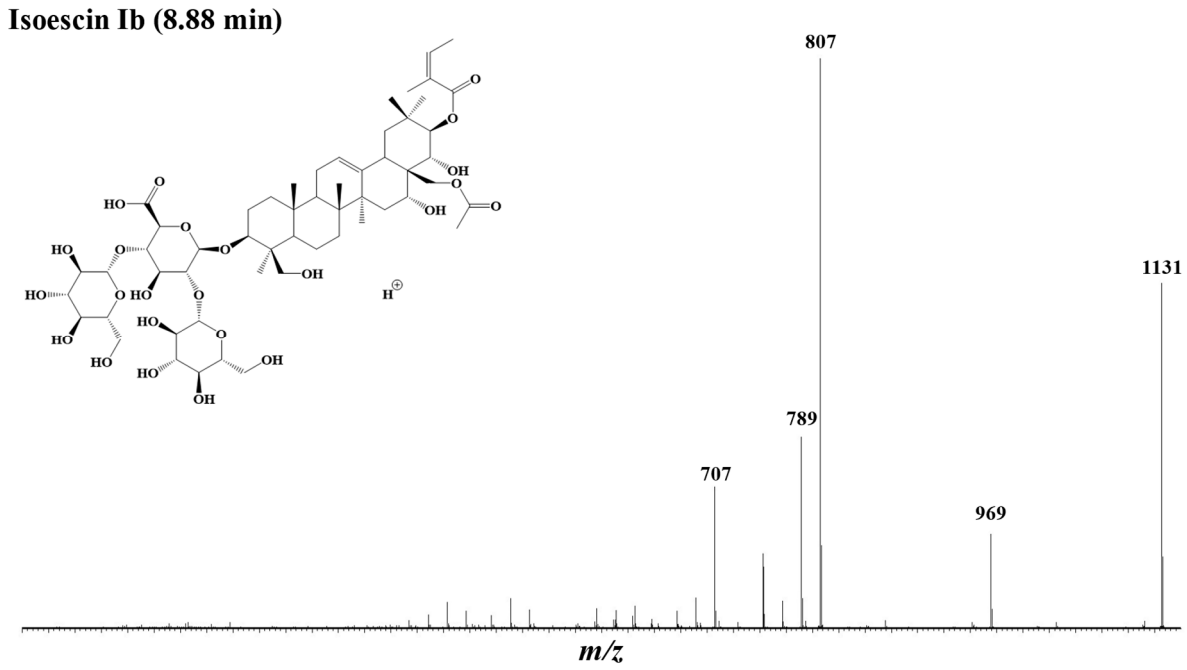

Figure S4: LC-MSMS(+) analysis of Escins I, II and III enriched-extract (EE): CID spectrum (15 eV) recorded for the *m/z* 1131 precursor ions $[M+H]^+$ at 8.88 min retention time (Isoescin Ib)

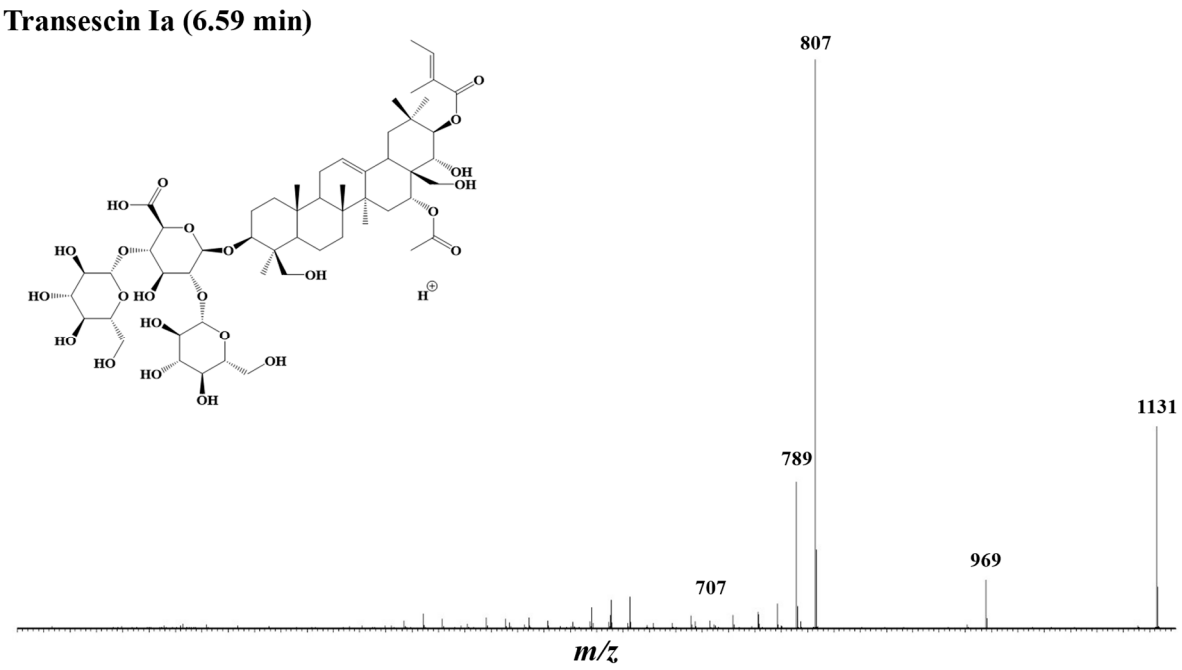

Figure S5: LC-MSMS(+) analysis of Transesterification extract (TE): CID spectrum (15 eV) recorded for the *m*/*z* 1131 precursor ions $[M+H]^+$ at 6.59 min retention time (Transescin Ia)

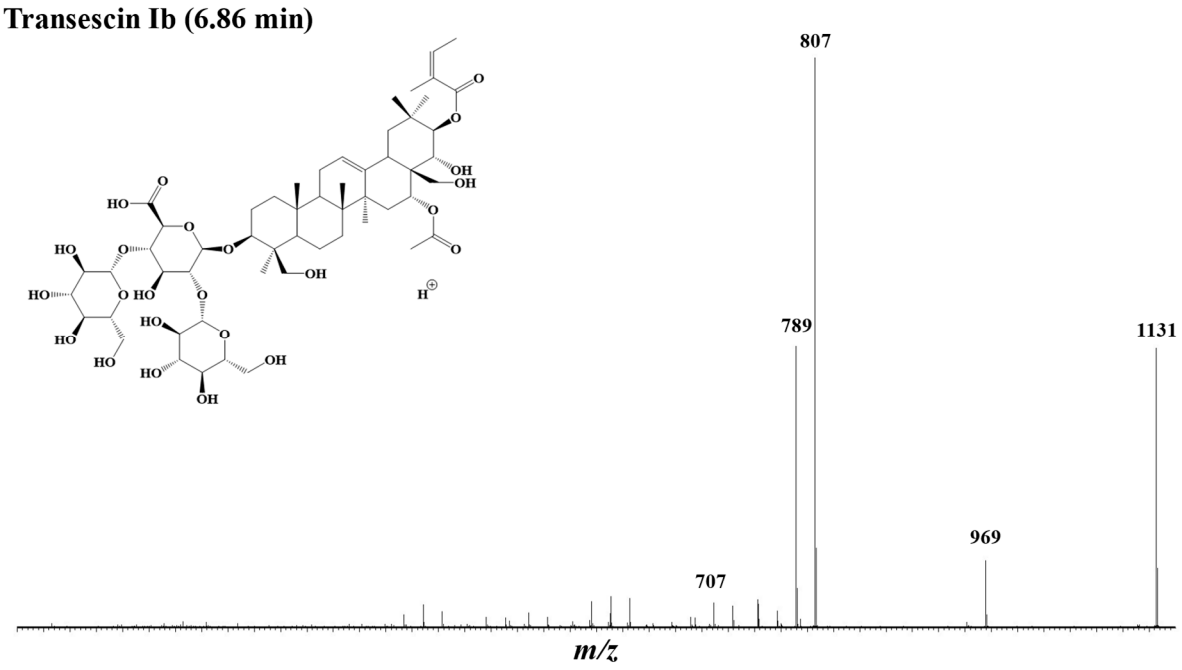

Figure S6: LC-MSMS(+) analysis of Transesterification extract (TE): CID spectrum (15 eV) recorded for the *m*/*z* 1131 precursor ions $[M+H]^+$ at 6.86 min retention time (Transescin Ib)

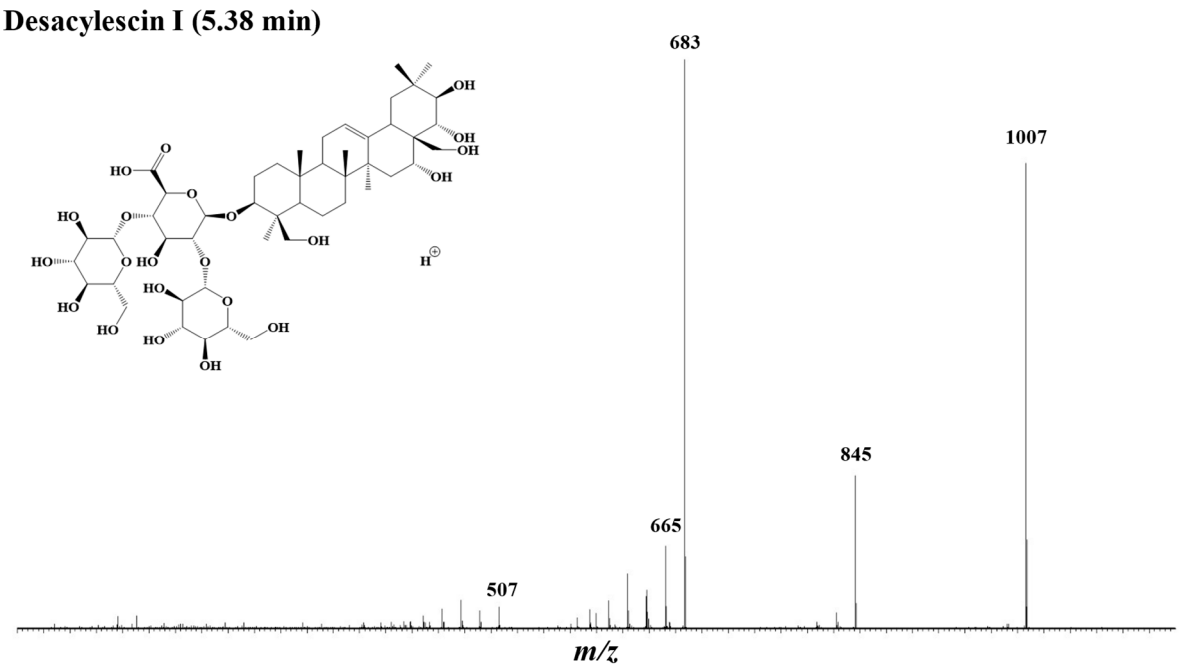

Figure S7: LC-MSMS(+) analysis of Hydrolysis extract (HE): CID spectrum (15 eV) recorded for the *m*/*z* 1007 precursor ions $[M+H]^+$ at 5.38 min retention time (Desacylescin I)

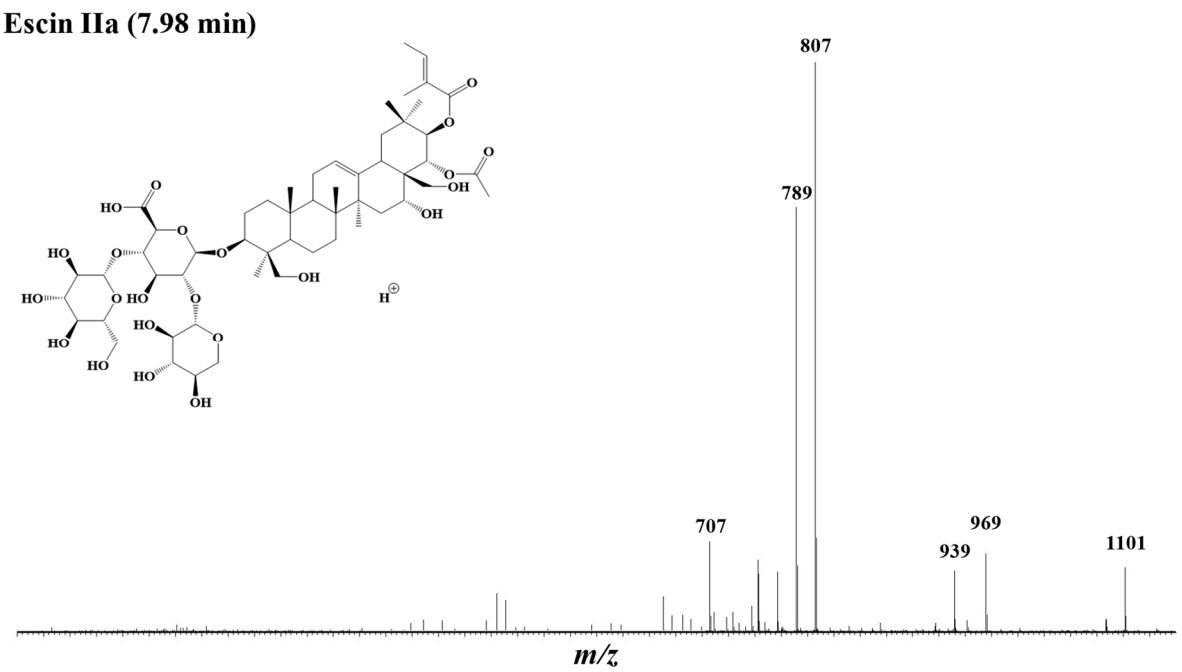

Figure S8: LC-MSMS(+) analysis of Escins I, II and III enriched-extract (EE): CID spectrum (15 eV) recorded for the *m*/*z* 1101 precursor ions $[M+H]^+$ at 7.98 min retention time (Escin IIa)

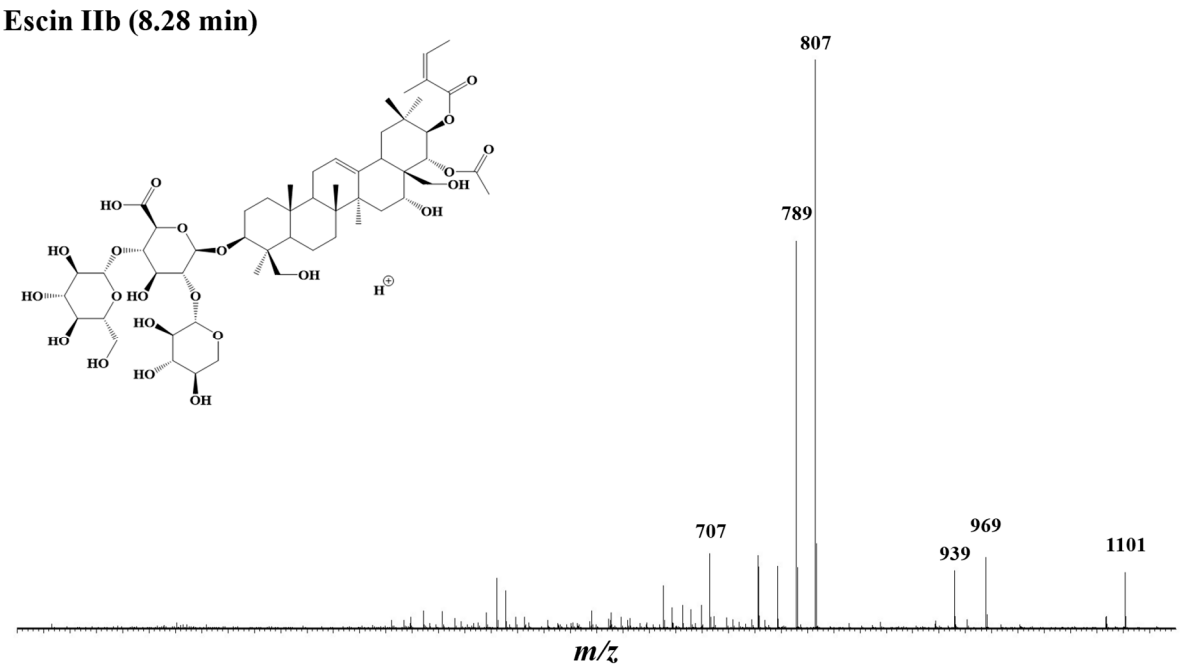

Figure S9: LC-MSMS(+) analysis of Escins I, II and III enriched-extract (EE): CID spectrum (15 eV) recorded for the *m*/*z* 1101 precursor ions $[M+H]^+$ at 8.28 min retention time (Escin IIb)

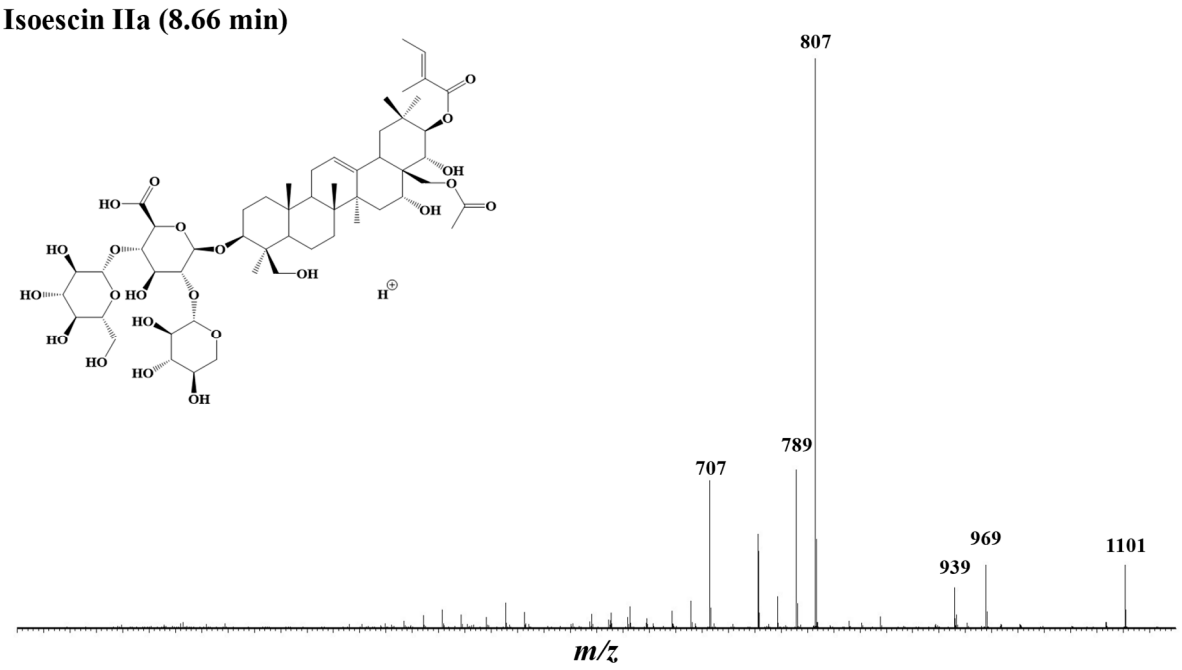

Figure S10: LC-MSMS(+) analysis of Escins I, II and III enriched-extract (EE): CID spectrum (15 eV) recorded for the *m*/*z* 1101 precursor ions $[M+H]^+$ at 8.66 min retention time (Isoescin IIa)

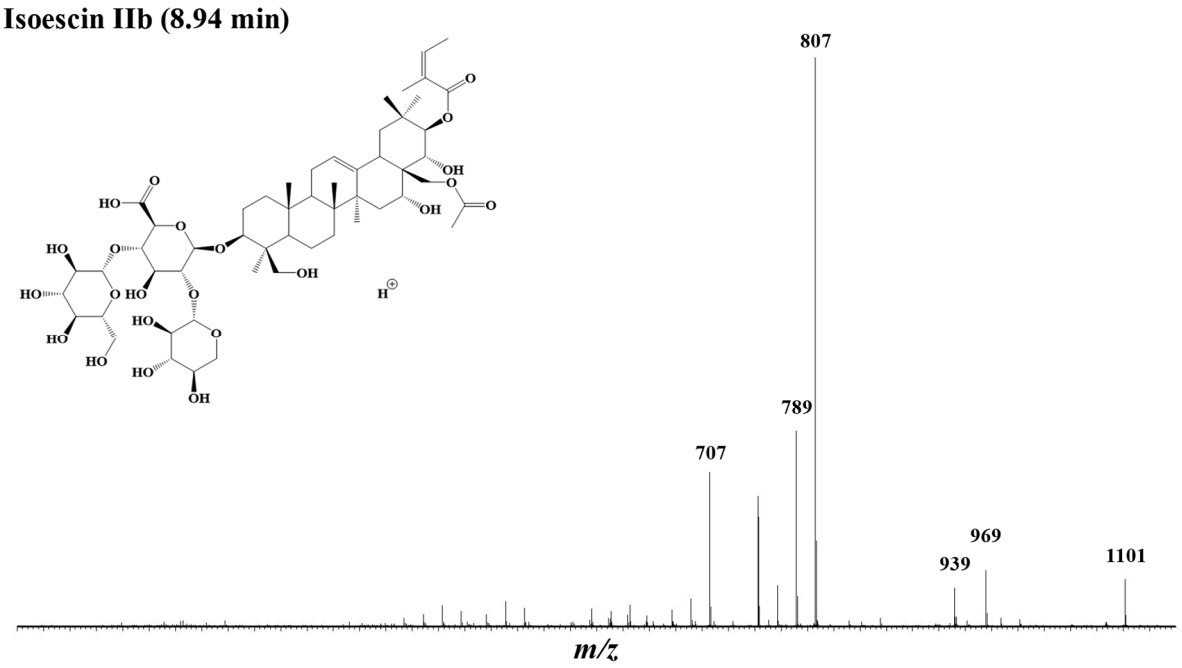

Figure S11: LC-MSMS(+) analysis of Escins I, II and III enriched-extract (EE): CID spectrum (15 eV) recorded for the *m*/*z* 1101 precursor ions $[M+H]^+$ at 8.94 min retention time (Isoescin IIb)

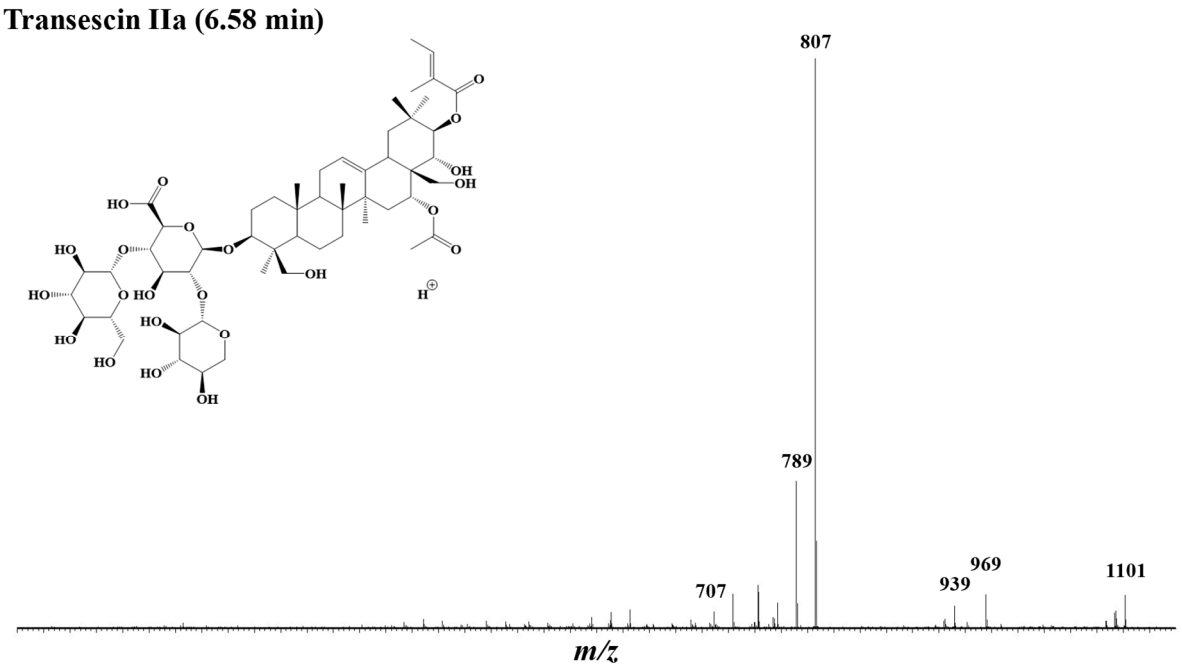

Figure S12: LC-MSMS(+) analysis of Transesterification extract (TE): CID spectrum (15 eV) recorded for the *m*/*z* 1101 precursor ions $[M+H]^+$ at 6.58 min retention time (Transescin IIa)

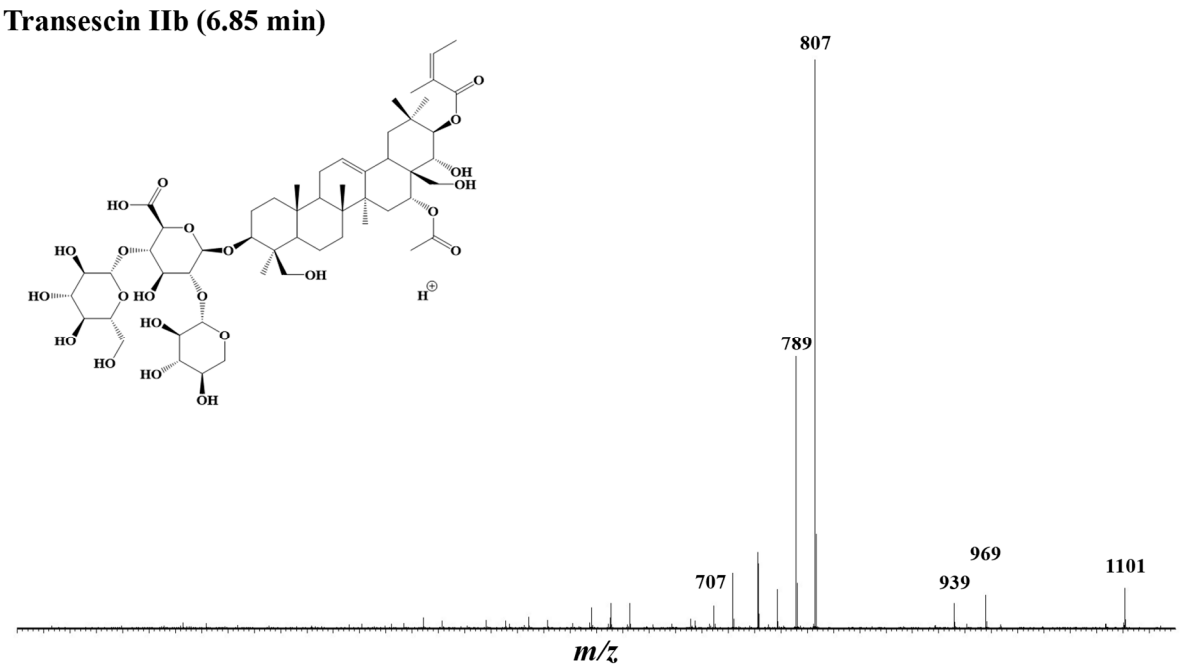

Figure S13: LC-MSMS(+) analysis of Transesterification extract (TE): CID spectrum (15 eV) recorded for the *m*/*z* 1101 precursor ions $[M+H]^+$ at 6.85 min retention time (Transecin IIb)

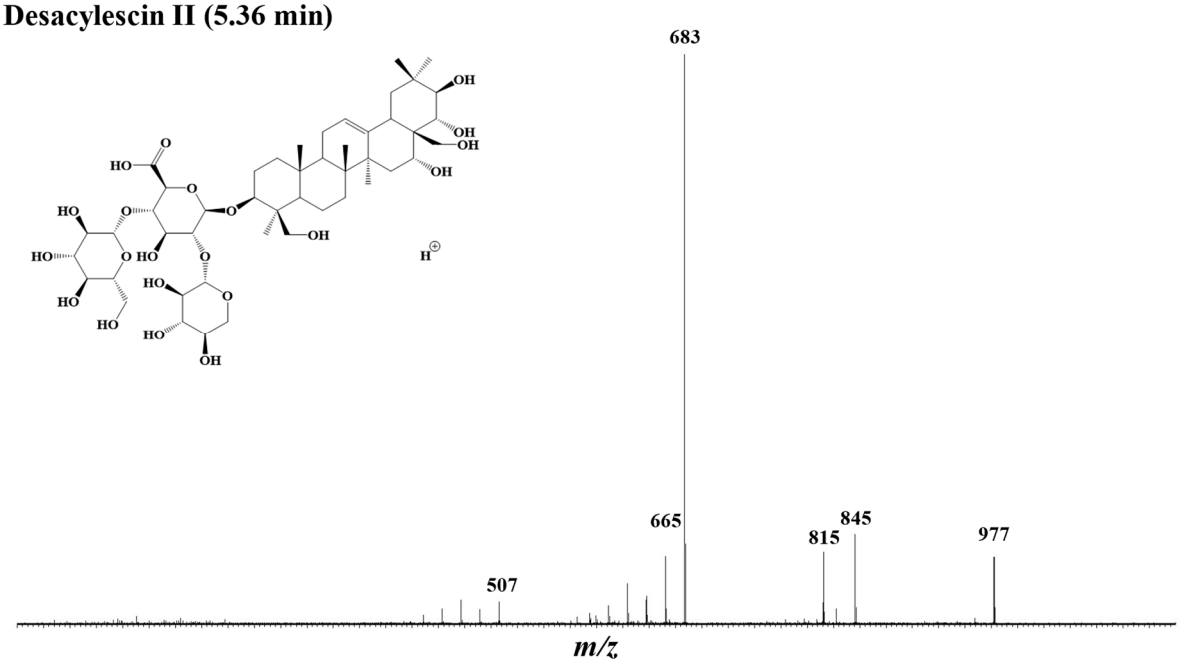

Figure S14: LC-MSMS(+) analysis of Hydrolysis extract (HE): CID spectrum (15 eV) recorded for the *m*/*z* 977 precursor ions $[M+H]^+$ at 5.36 min retention time (Desacylescin II)

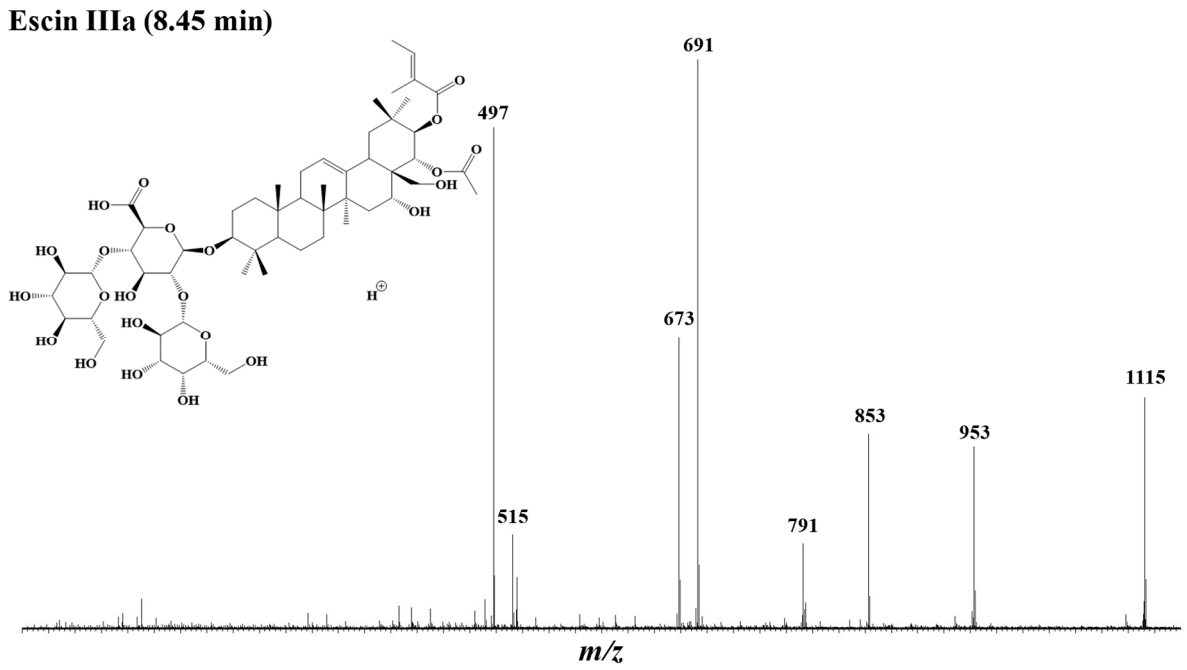

Figure S15: LC-MSMS(+) analysis of Escins I, II and III enriched-extract (EE): CID spectrum (15 eV) recorded for the *m*/*z* 1115 precursor ions $[M+H]^+$ at 8.45 min retention time (Escin IIIa)

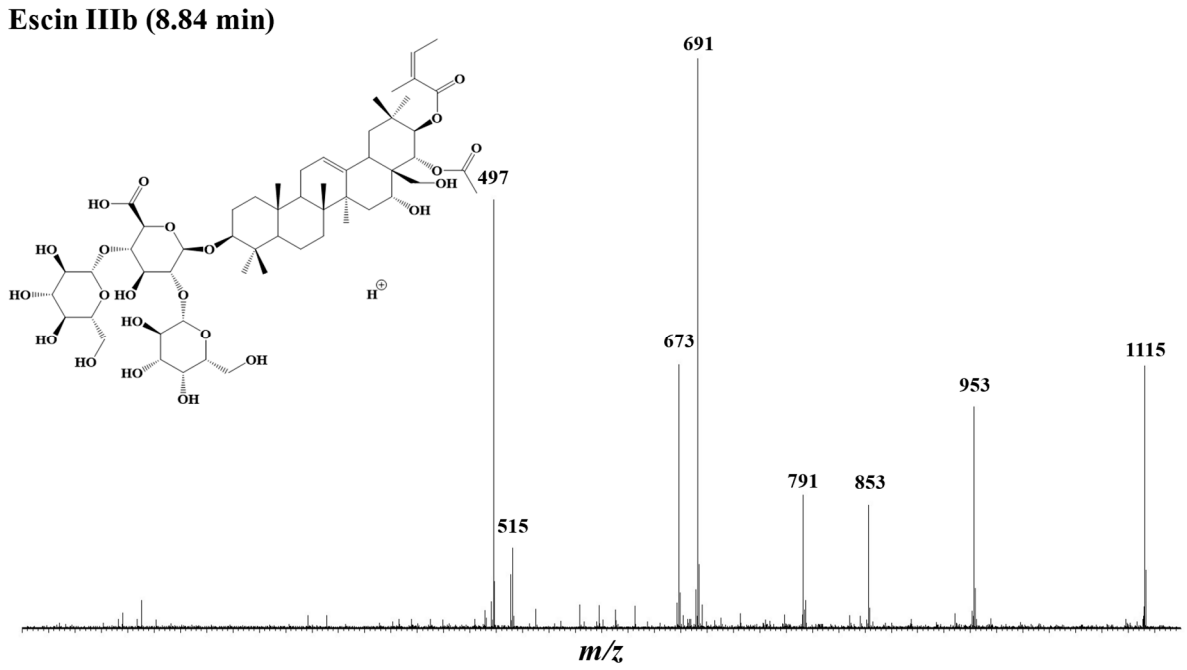

Figure S16: LC-MSMS(+) analysis of Escins I, II and III enriched-extract (EE): CID spectrum (15 eV) recorded for the *m*/*z* 1115 precursor ions $[M+H]^+$ at 8.84 min retention time (Escin IIIb)

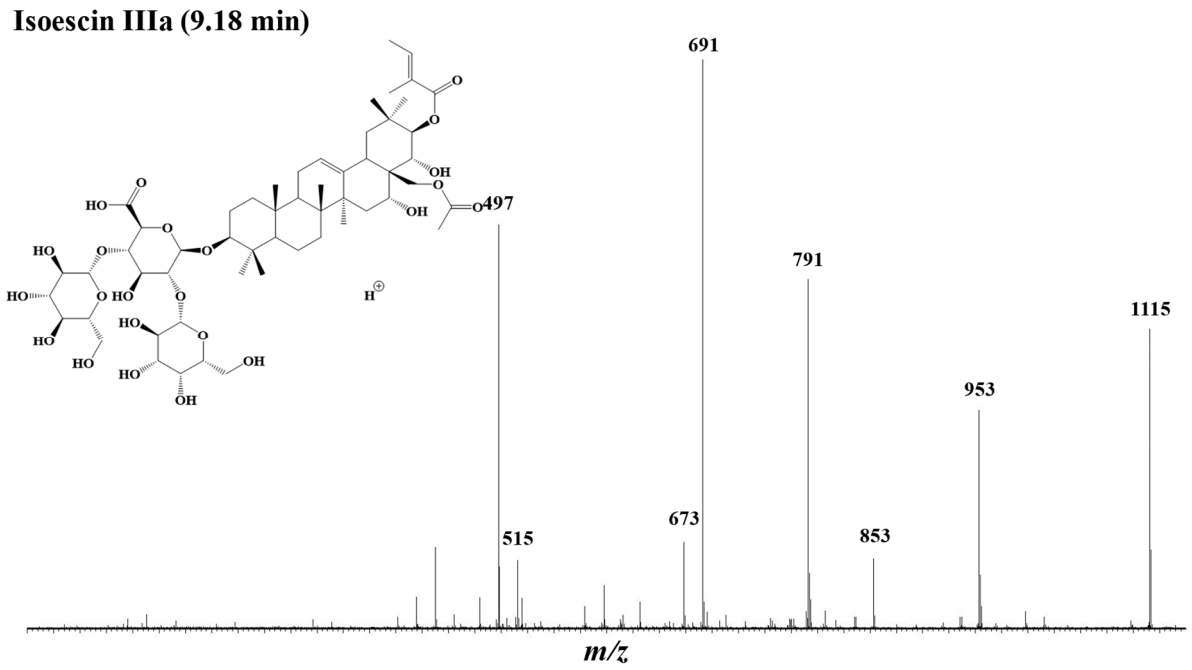

Figure S17: LC-MSMS(+) analysis of Escins I, II and III enriched-extract (EE): CID spectrum (15 eV) recorded for the *m*/*z* 1115 precursor ions $[M+H]^+$ at 9.18 min retention time (Isoescin IIIa)

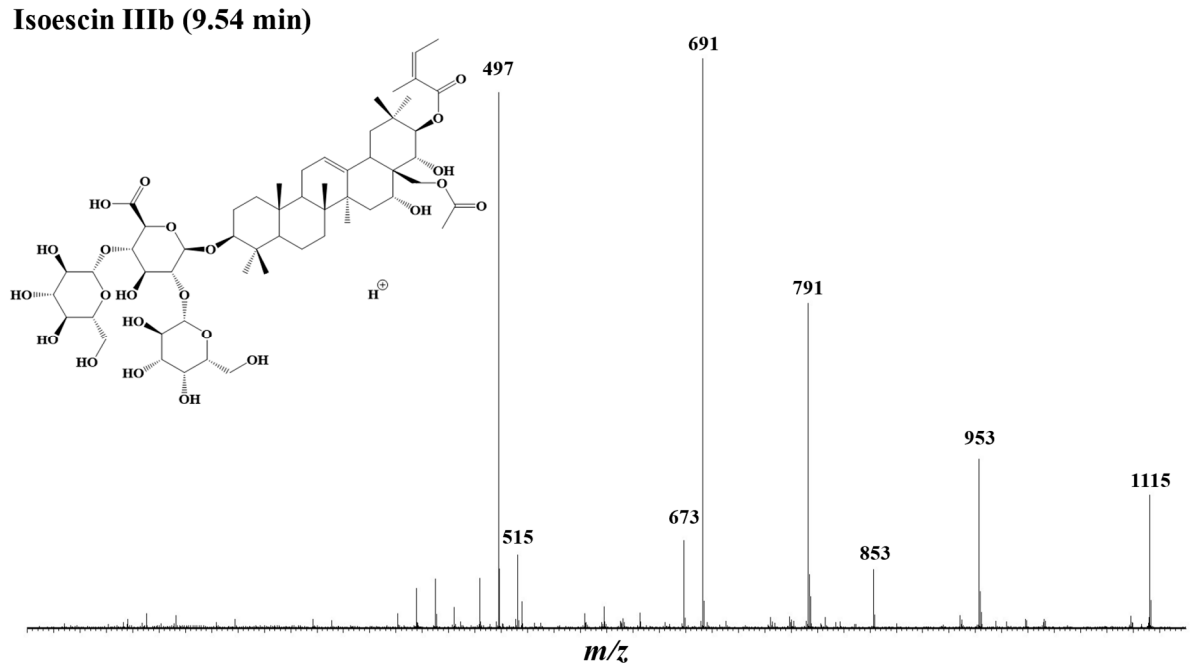

Figure S18: LC-MSMS(+) analysis of Escins I, II and III enriched-extract (EE): CID spectrum (15 eV) recorded for the *m*/*z* 1115 precursor ions $[M+H]^+$ at 9.54 min retention time (Isoescin IIIb)

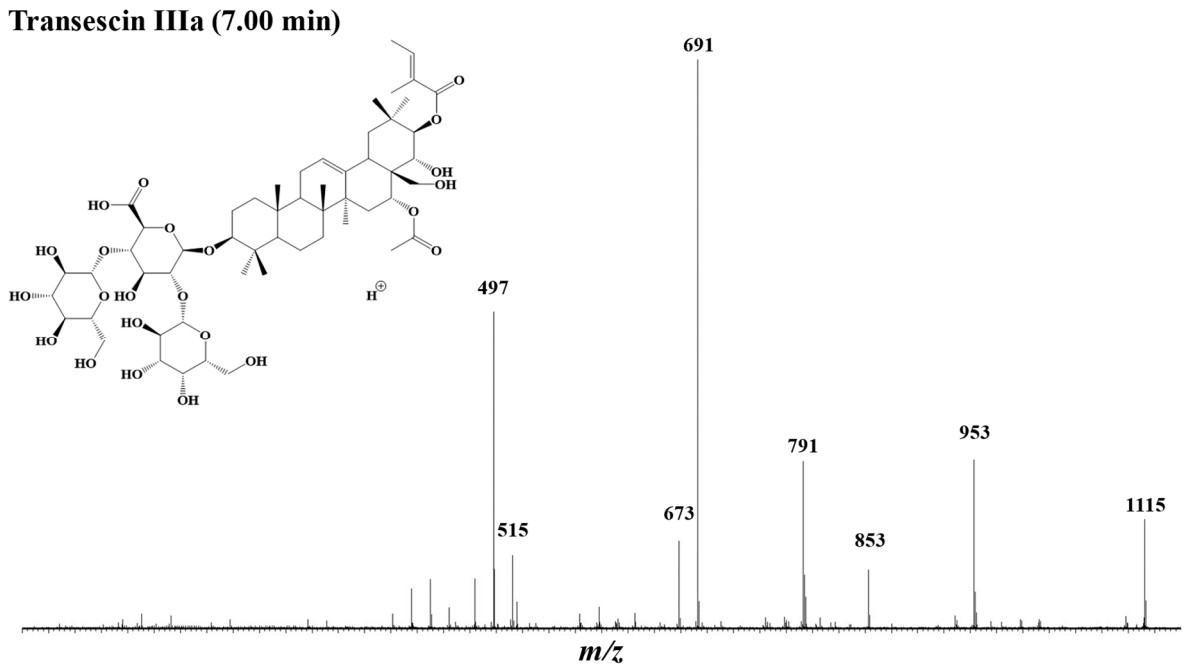

Figure S19: LC-MSMS(+) analysis of Transesterification extract (TE): CID spectrum (15 eV) recorded for the *m*/*z* 1115 precursor ions $[M+H]^+$ at 7.00 min retention time (Transescin IIIa)

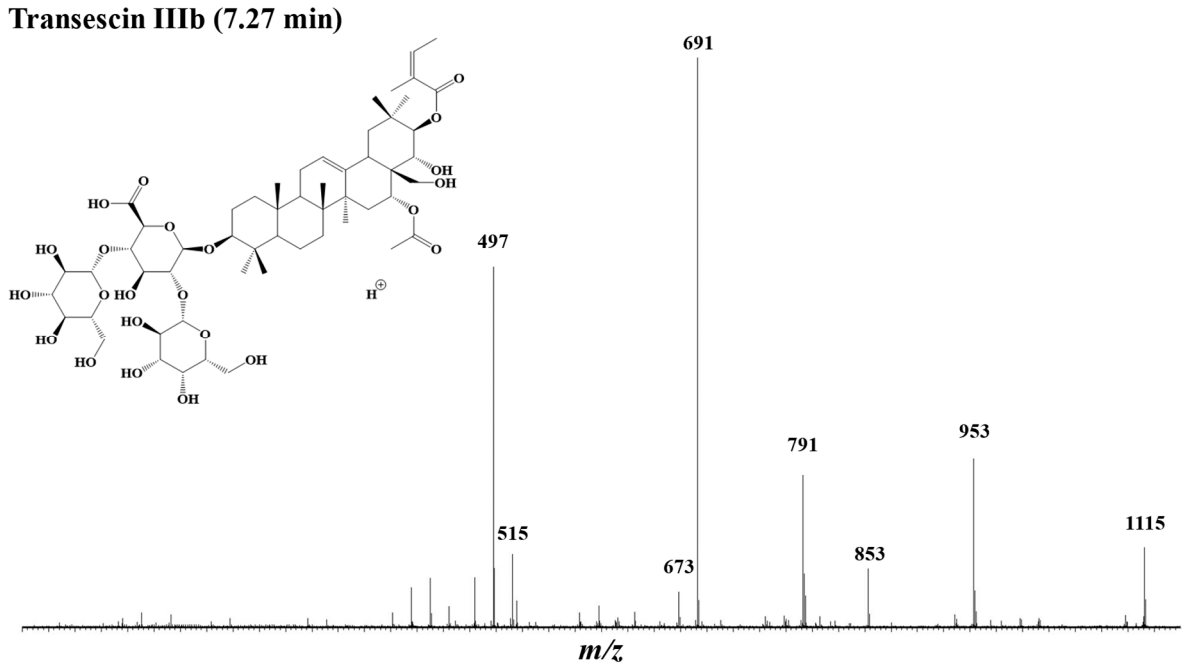

Figure S20: LC-MSMS(+) analysis of Transesterification extract (TE): CID spectrum (15 eV) recorded for the *m*/*z* 1115 precursor ions $[M+H]^+$ at 7.27 min retention time (Transescin IIIb)

Desacylescin III (5.39 min)

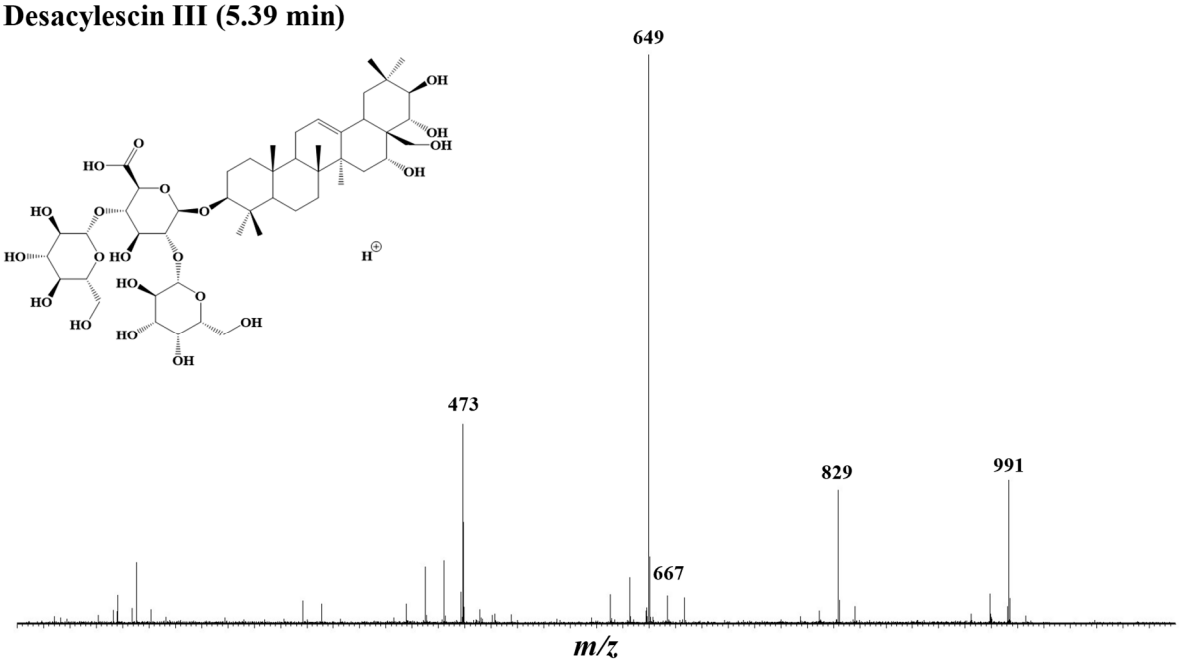

Figure S21: LC-MSMS(+) analysis of Hydrolysis extract (HE): CID spectrum (15 eV) recorded for the *m*/*z* 991 precursor ions $[M+H]^+$ at 5.39 min retention time (Desacylescin III)

Escin IV (6.10 min)

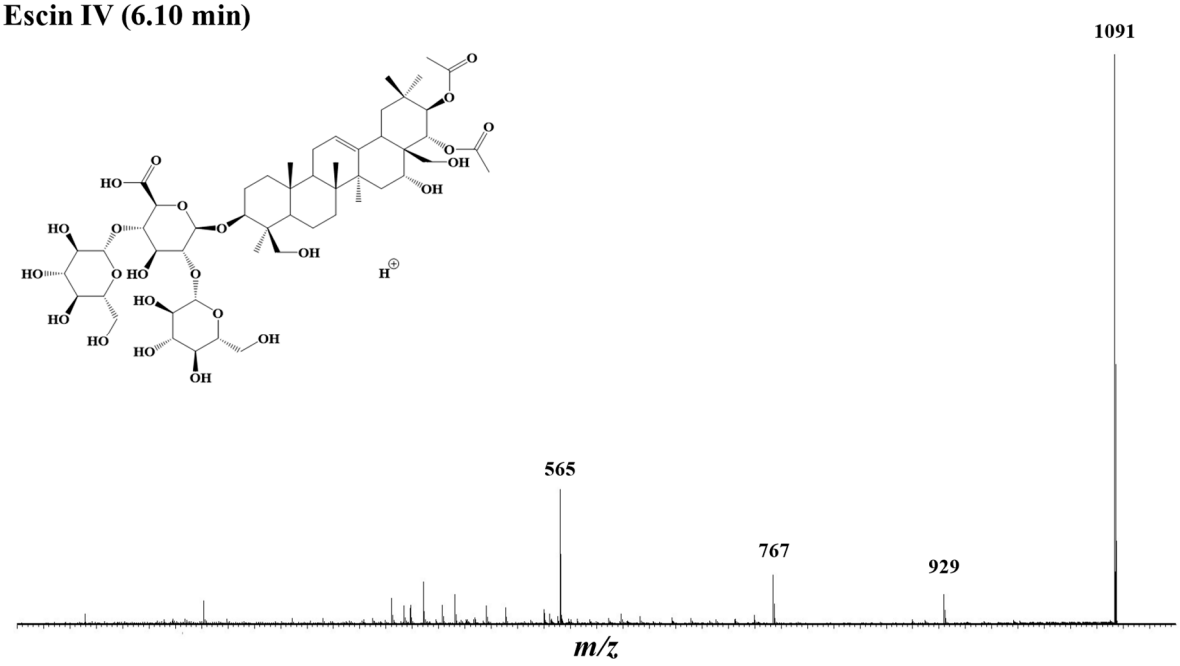

Figure S22: LC-MSMS(+) analysis of Natural extract (NE): CID spectrum (15 eV) recorded for the *m*/*z* 1091 precursor ions $[M+H]^+$ at 6.10 min retention time (Escin IV)

Isoescin IV (6.56 min)

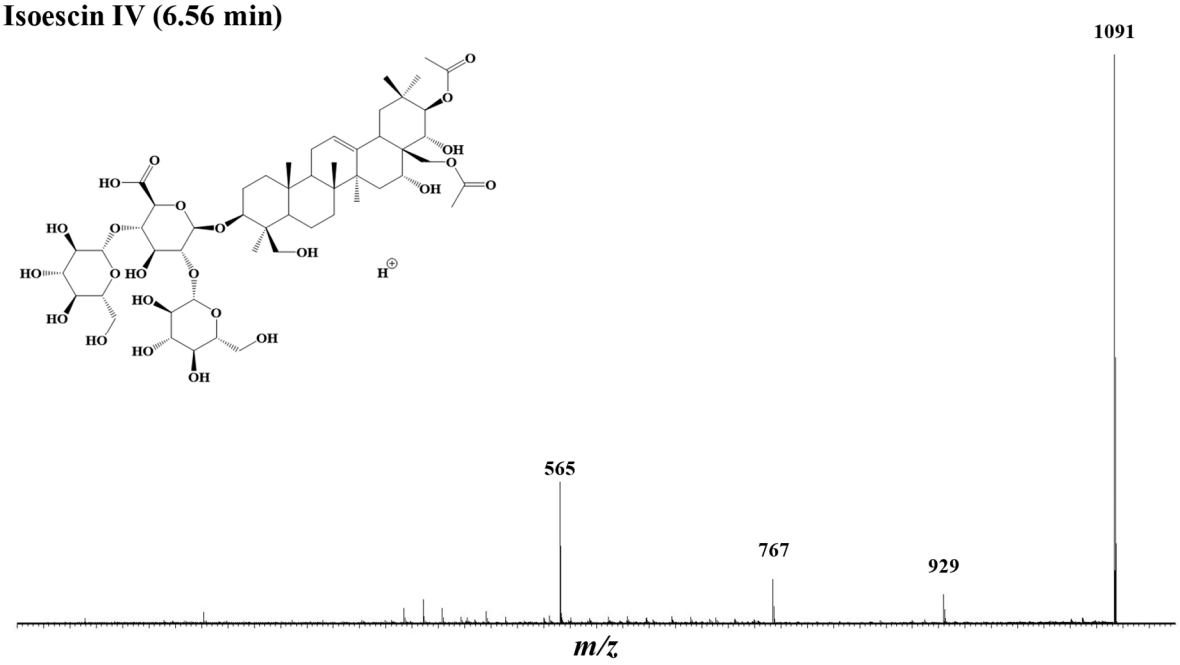

Figure S23: LC-MSMS(+) analysis of Natural extract (NE): CID spectrum (15 eV) recorded for the *m*/*z* 1091 precursor ions $[M+H]^+$ at 6.56 min retention time (Isoescin IV)

Escin V (7.71 min)

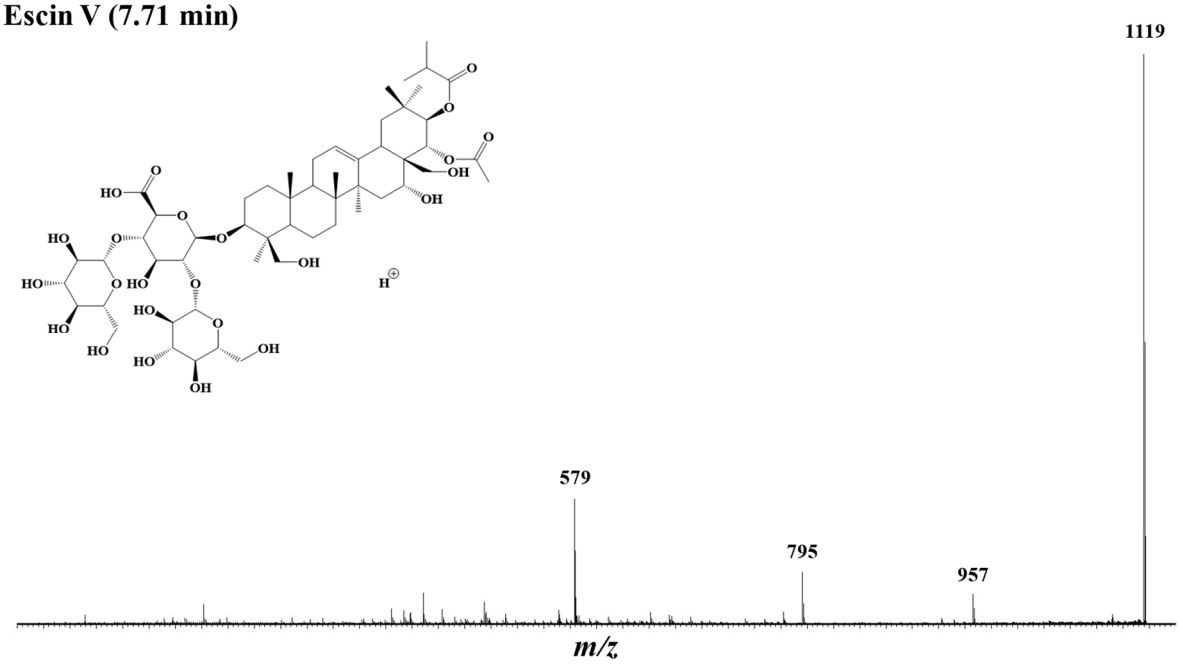

Figure S24: LC-MSMS(+) analysis of Natural extract (NE): CID spectrum (15 eV) recorded for the *m*/*z* 1119 precursor ions $[M+H]^+$ at 7.71 min retention time (Escin V)

Isoescin V (8.20 min)

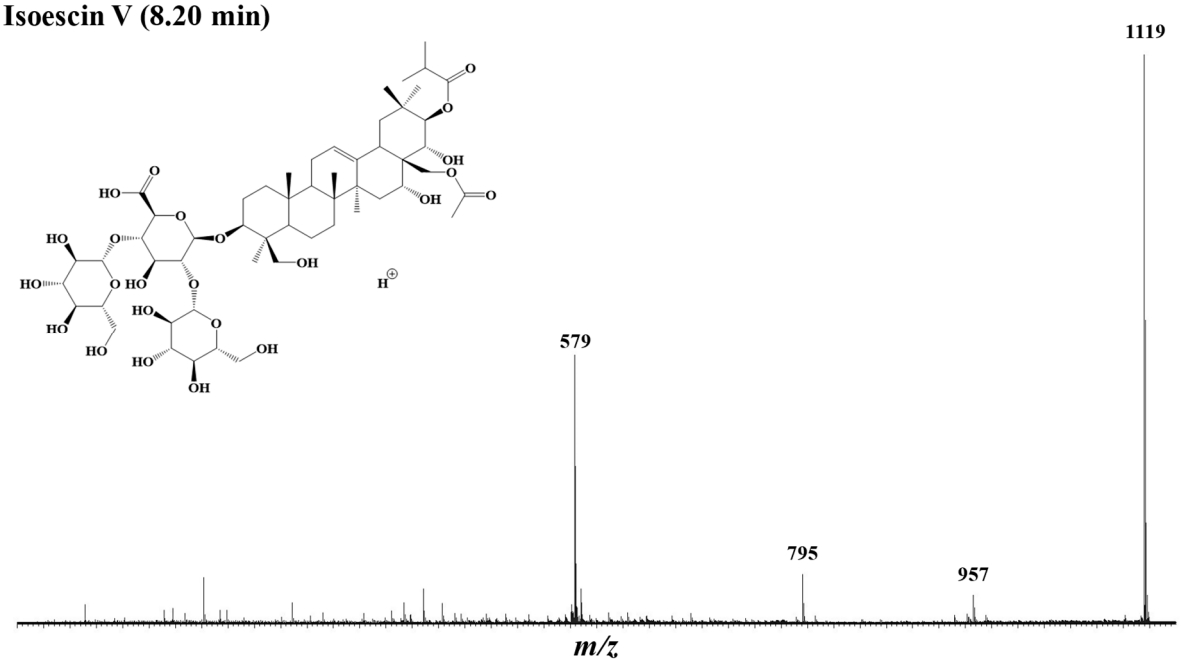

Figure S25: LC-MSMS(+) analysis of Natural extract (NE): CID spectrum (15 eV) recorded for the *m*/*z* 1119 precursor ions $[M+H]^+$ at 8.20 min retention time (Isoescin V)

Escin VI (8.62 min)

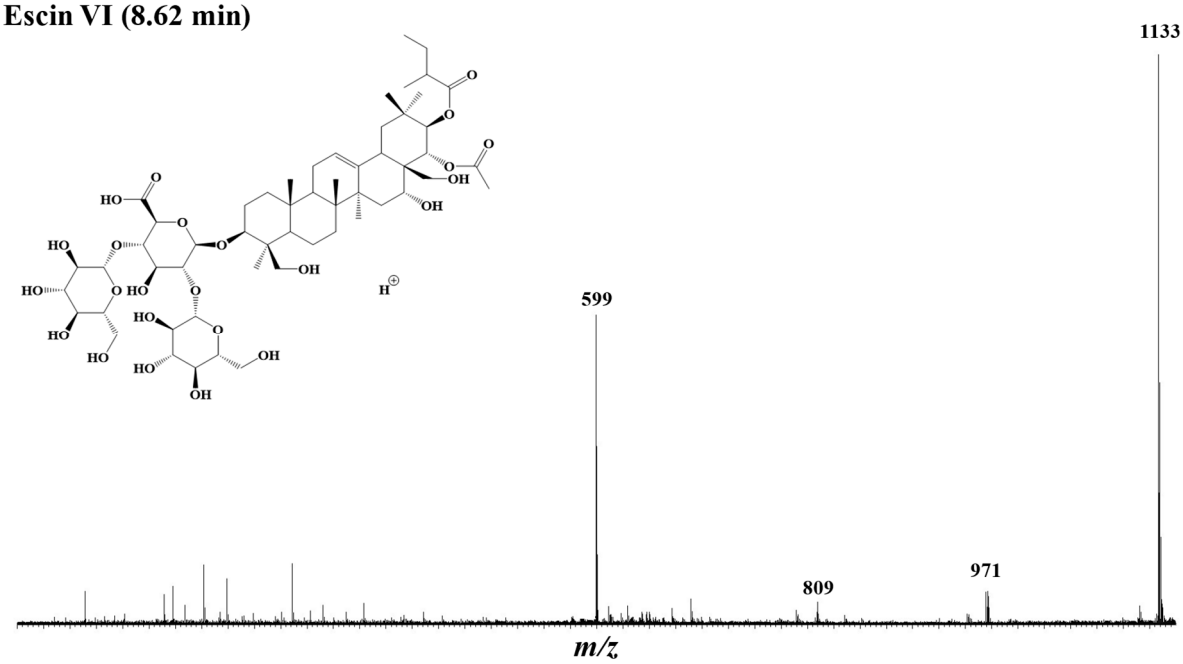

Figure S26: LC-MSMS(+) analysis of Natural extract (NE): CID spectrum (15 eV) recorded for the *m*/*z* 1133 precursor ions $[M+H]^+$ at 8.62 min retention time (Escin VI)

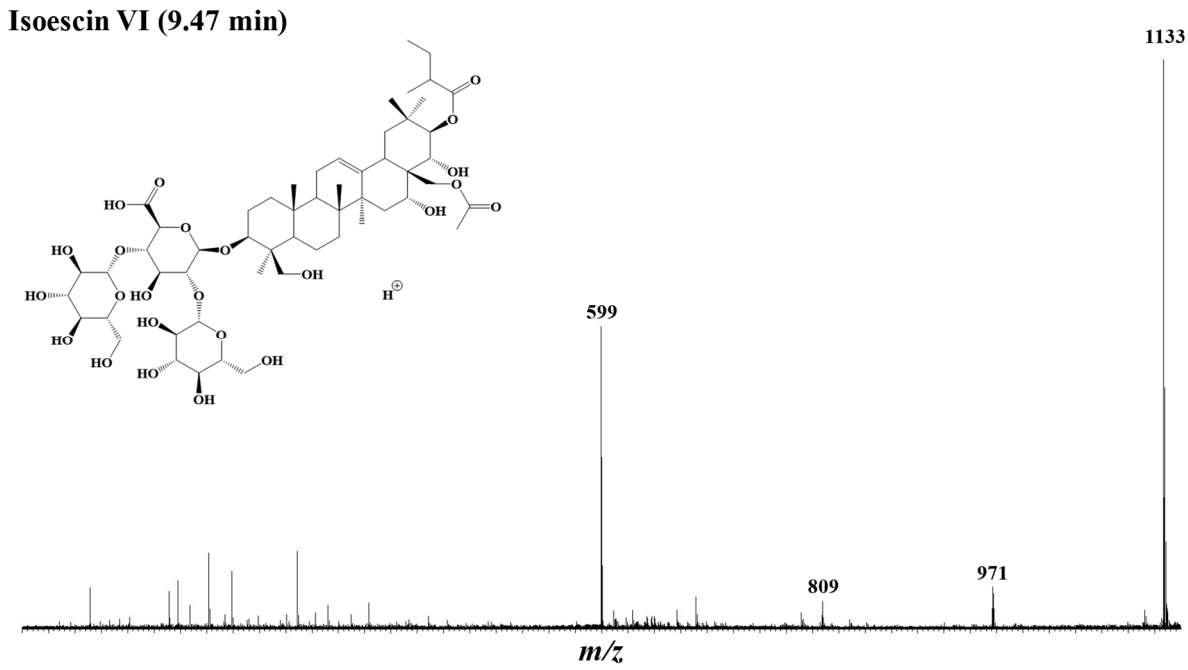

Figure S27: LC-MSMS(+) analysis of Natural extract (NE): CID spectrum (15 eV) recorded for the *m*/*z* 1133 precursor ions $[M+H]^+$ at 9.47 min retention time (Isoescin VI)

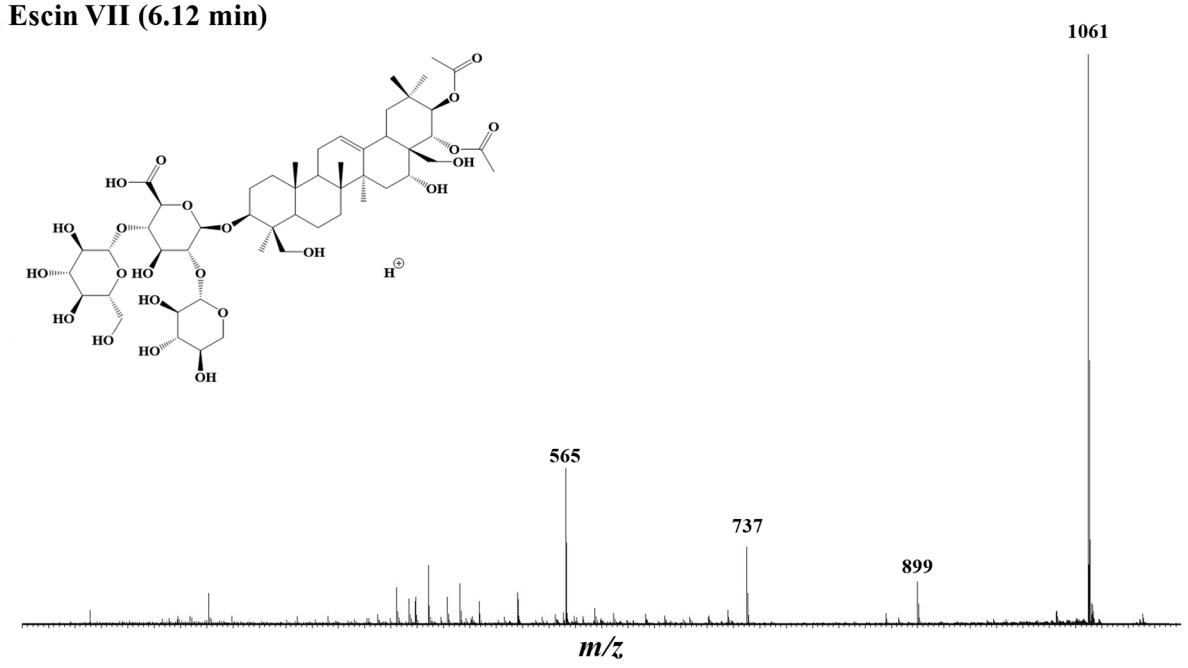

Figure S28: LC-MSMS(+) analysis of Natural extract (NE): CID spectrum (15 eV) recorded for the *m*/*z* 1061 precursor ions $[M+H]^+$ at 6.12 min retention time (Escin VII)

Isoescin VII (6.59 min)

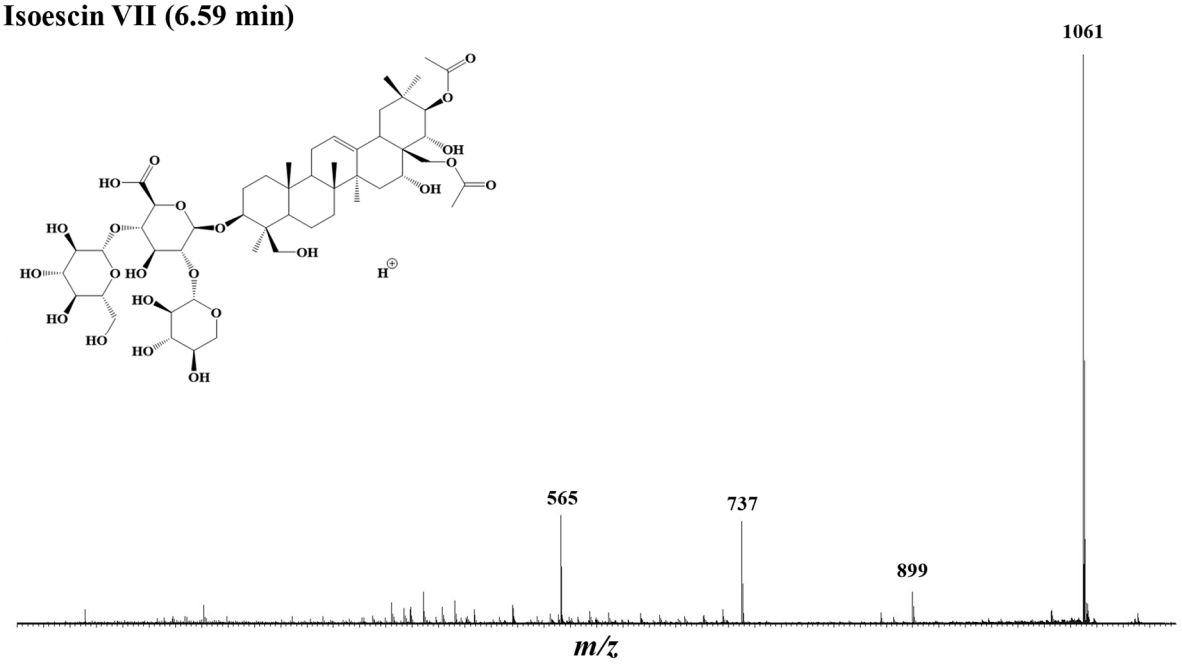

Figure S29: LC-MSMS(+) analysis of Natural extract (NE): CID spectrum (15 eV) recorded for the *m*/*z* 1061 precursor ions $[M+H]^+$ at 6.59 min retention time (Isoescin VII)

Escin VIII (7.42 min)

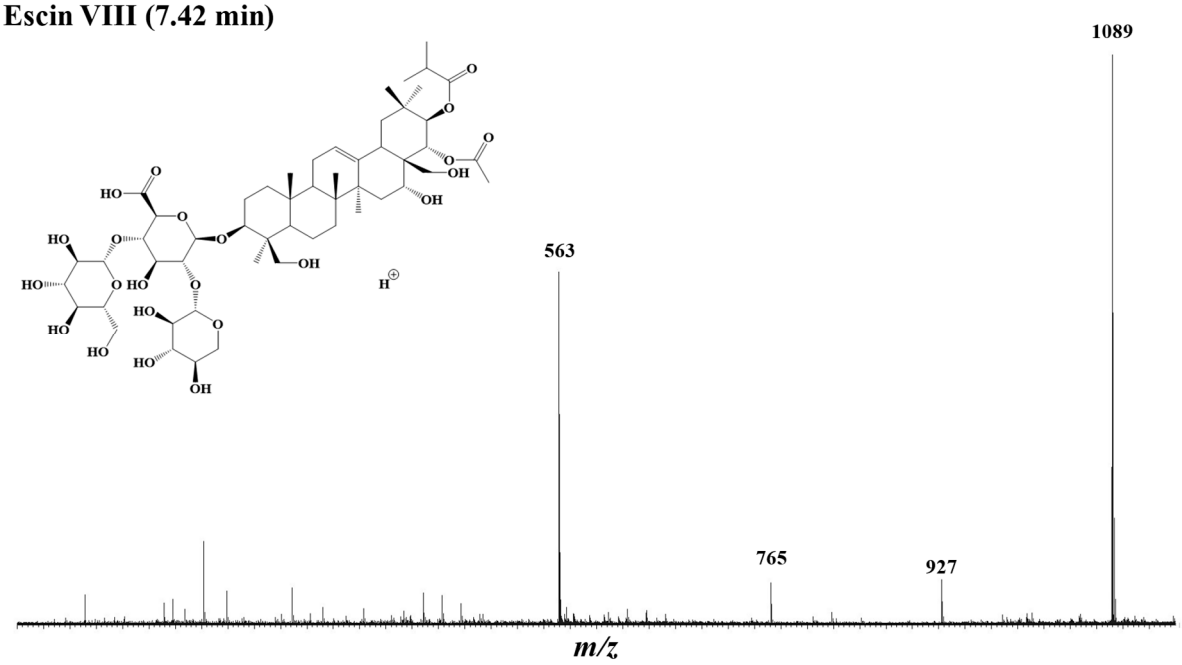

Figure S30: LC-MSMS(+) analysis of Natural extract (NE): CID spectrum (15 eV) recorded for the *m*/*z* 1089 precursor ions $[M+H]^+$ at 7.42 min retention time (Escin VIII)

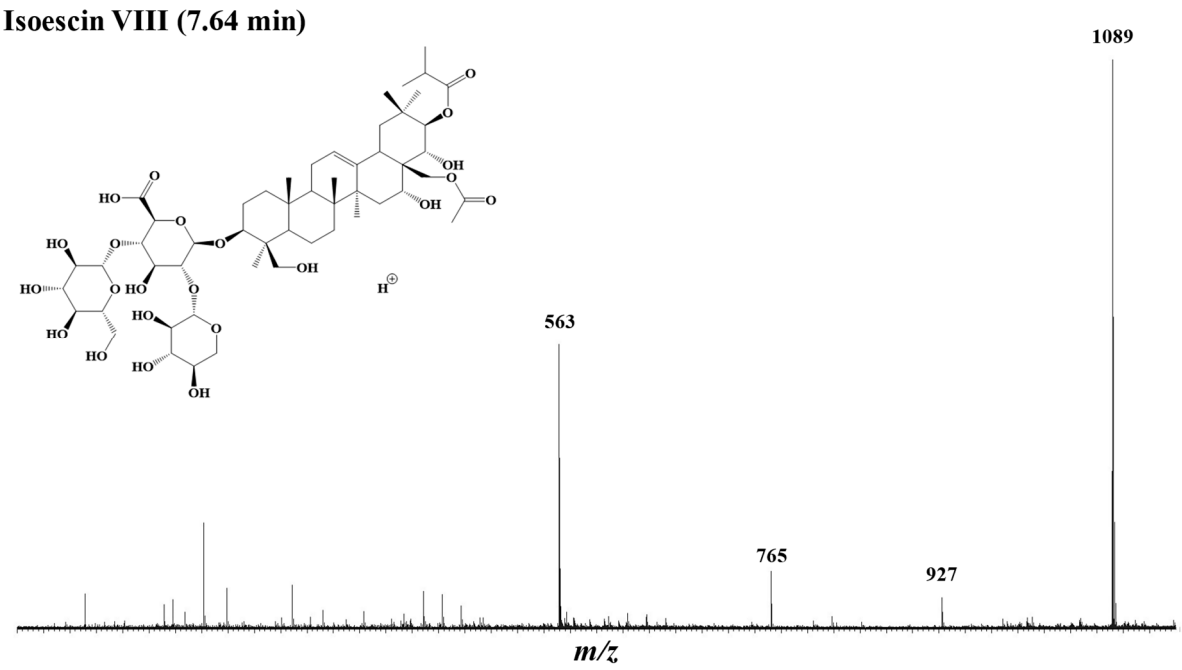

Figure S31: LC-MSMS(+) analysis of Natural extract (NE): CID spectrum (15 eV) recorded for the *m*/*z* 1089 precursor ions $[M+H]^+$ at 7.64 min retention time (Isoescin VIII)

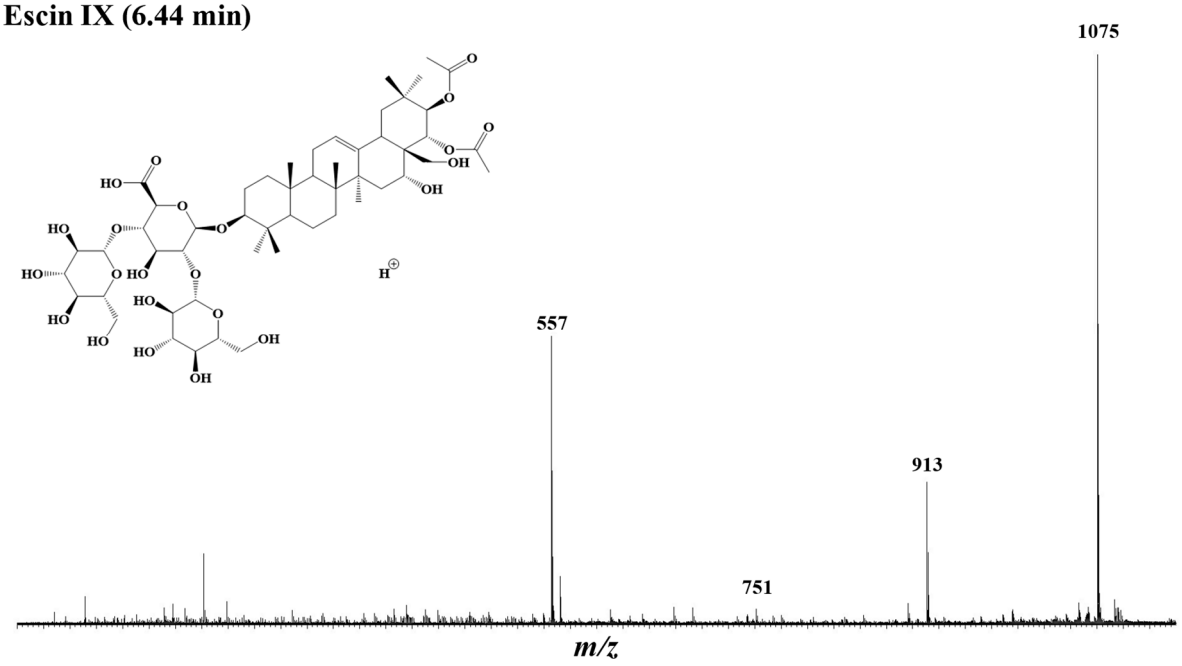

Figure S32: LC-MSMS(+) analysis of Natural extract (NE): CID spectrum (15 eV) recorded for the *m*/*z* 1075 precursor ions $[M+H]^+$ at 6.44 min retention time (Escin IX)

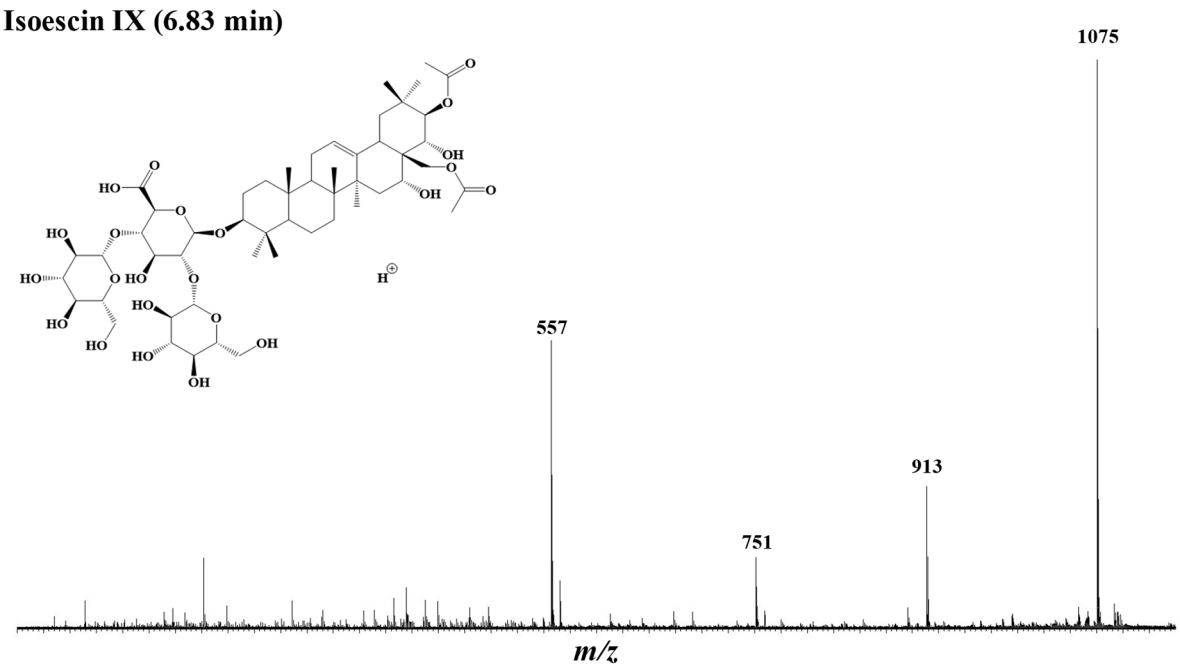

Figure S33: LC-MSMS(+) analysis of Natural extract (NE): CID spectrum (15 eV) recorded for the *m*/*z* 1075 precursor ions $[M+H]^+$ at 6.83 min retention time (Isoescin IX)