Supporting Information

ARISTOLOCHIC ACID METABOLISM IN THE ISOLATED PERFUSED RAT KIDNEY

Horacio A. Priestap, M. Cecilia Torres, Robert A. Rieger, Kathleen G. Dickman, Tomoko Freshwater, David R. Taft, Mauel A. Barbieri, and Charles R. Iden

TOC

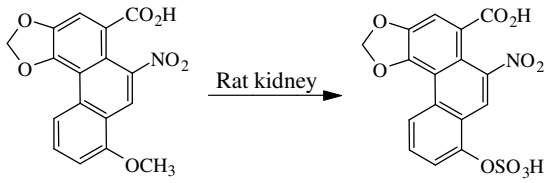


Figure 1. A. HPLC profile of urine of isolated rat kidney perfused with AA-I (detection at UV 254 nm); B and C, HPLC profiles of urine of rat injected with AA-I under fluorescence detection (excitation at 390 nm; emission at 480 nm) (B) and UV detection at 254 nm (C). Key to numbers and retentions times are shown in Scheme 1 and Table 1.

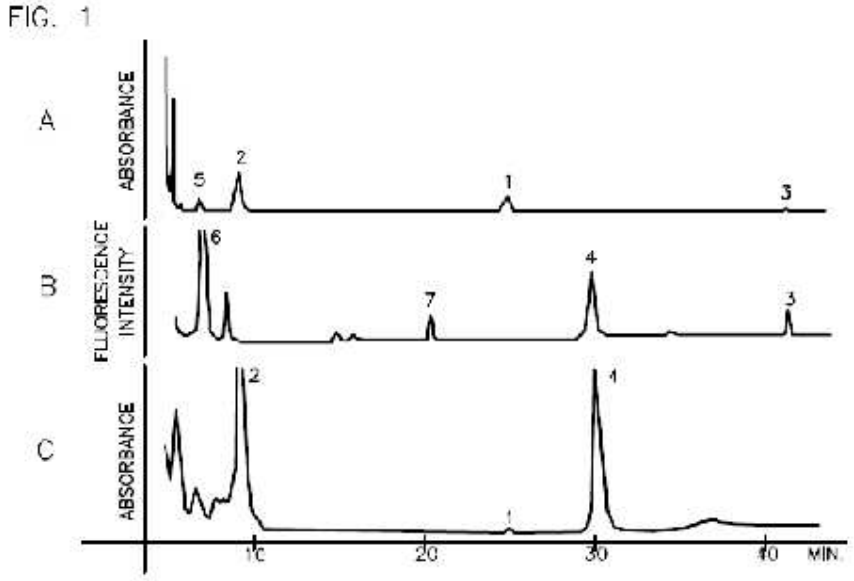
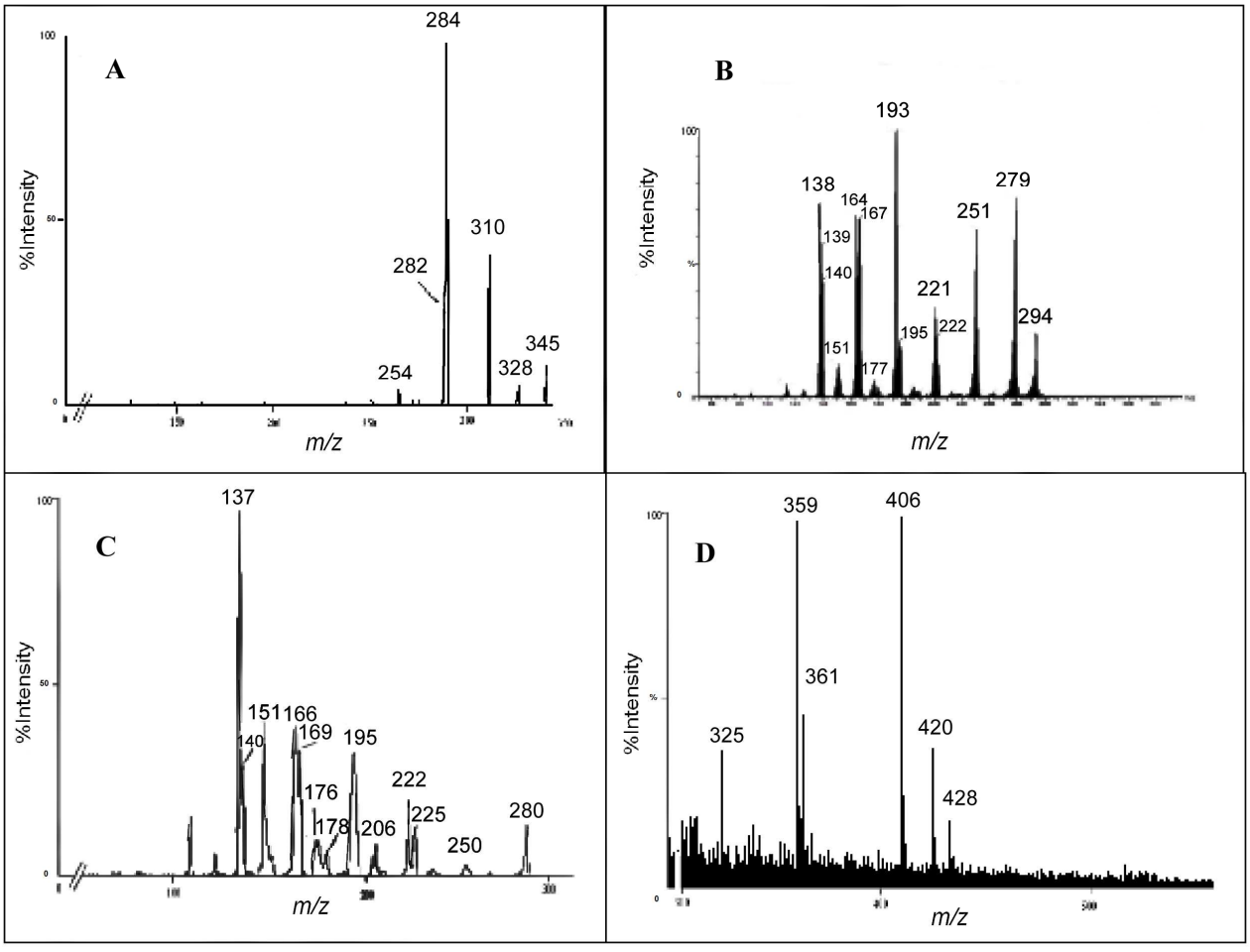
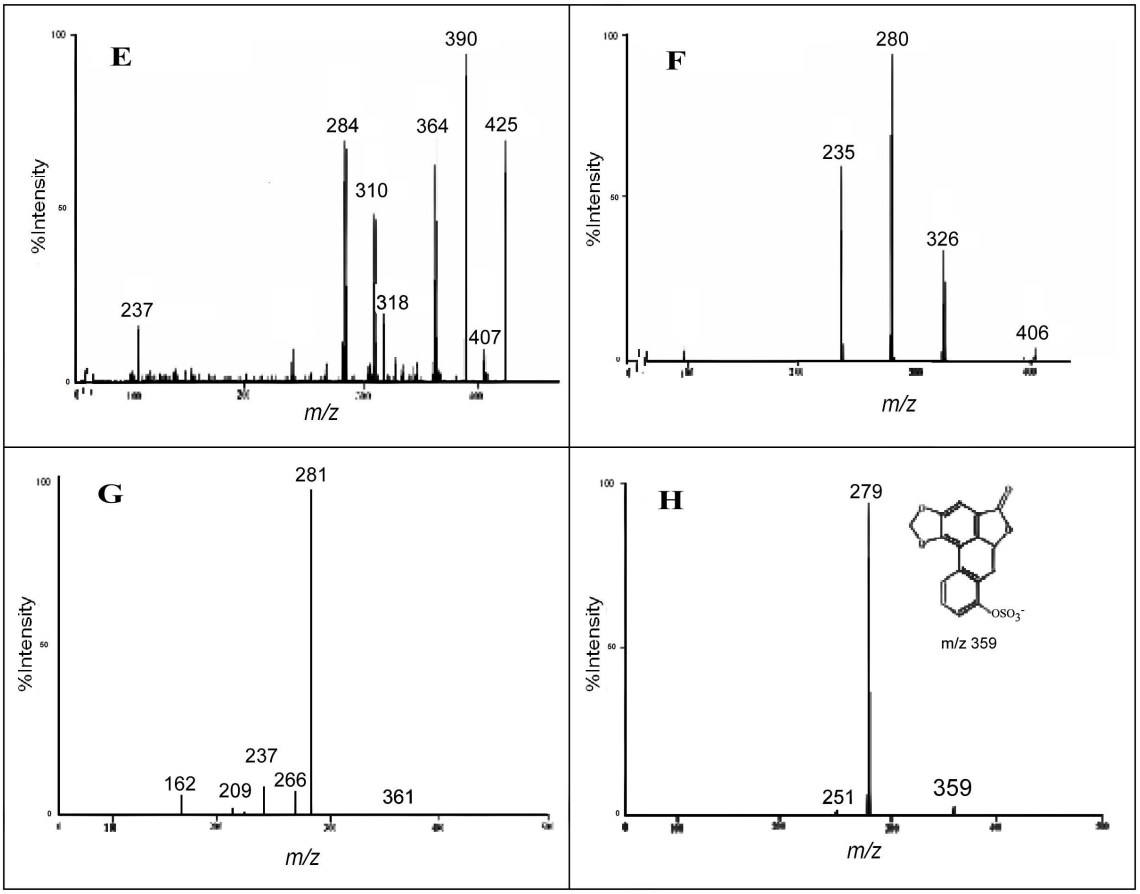
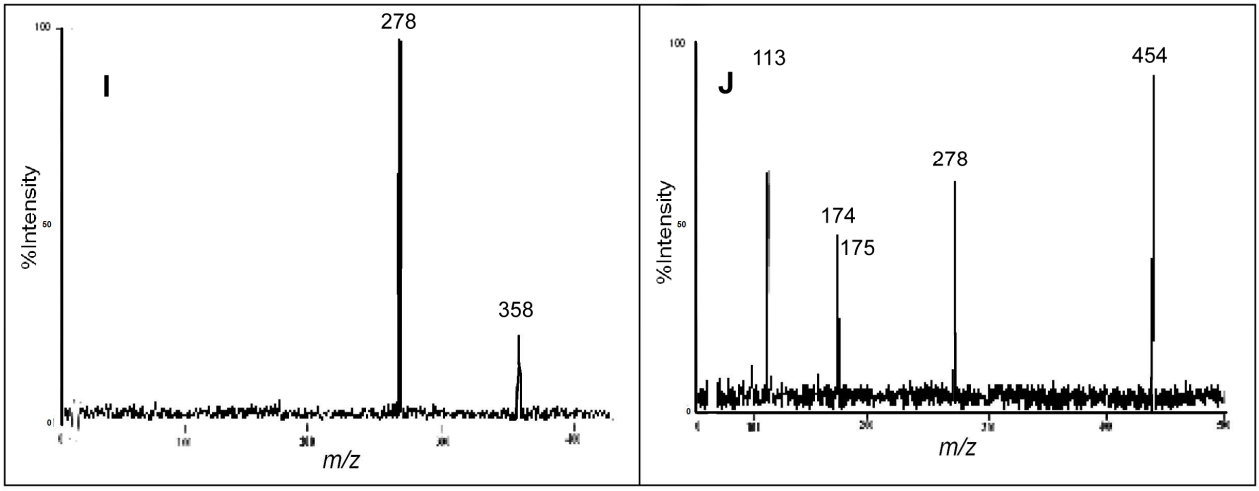


Figure 2. Collision induced dissociation spectra of (A) ammoniated aristolochic acid Ia (**2**) (*m/z* 345); (B) protonated aristolactam I (**3**) (*m/z* 294) and (C) protonated aristolactam Ia (**4**) (*m/z* 280); (D) Negative ion nano-ESI mass spectrum of the collected fractions containing aristolochic acid Ia O-sulfate (**5**) ; (E) MS/MS spectrum of the ammonium adduct of aristolochic acid Ia O-sulfate (**5**) ($[M+NH_4]^+$, *m/z* 425); (F) MS/MS spectrum of the negative ion of aristolochic acid Ia O-sulfate (**5**) ($[M-H]^-$; *m/z* 406); (G and H) MS/MS spectra of the negative *m/z* 361 and 359 fragment ions, respectively, from AA-Ia-O-S (**5**); (I) negative ion of aristolactam Ia O-sulfate (**7**); (J) negative ion of aristolactam Ia O-glucuronide (**6**) (*m/z* 454);




E
390
284
364
425
310
318
237
407
%Intensity
m/z
F
280
235
326
406
%Intensity
m/z
G
281
237
162
209
266
361
%Intensity
m/z
H
279
359
251
%Intensity
m/z
m/z 359


I
278
358
%Intensity
m/z
J
113
454
278
174
175
%Intensity
m/z

Scheme 2. Collision induced fragmentation pathways of the positive ammonium adduct of aristolochic acid Ia O-sulfate.

Scheme 2