LC-MS/TOF Characterization and Stability Study of Artesunate in Different Solvent Systems

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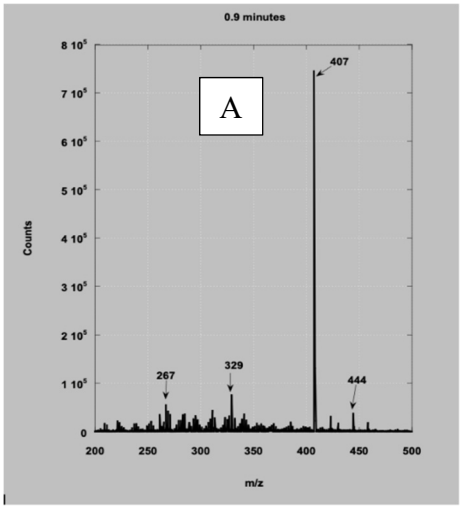
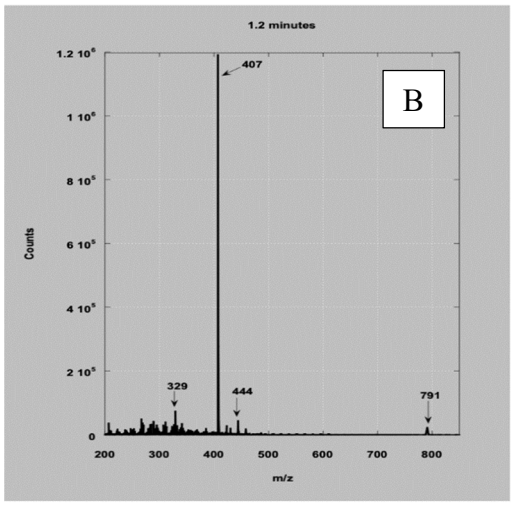
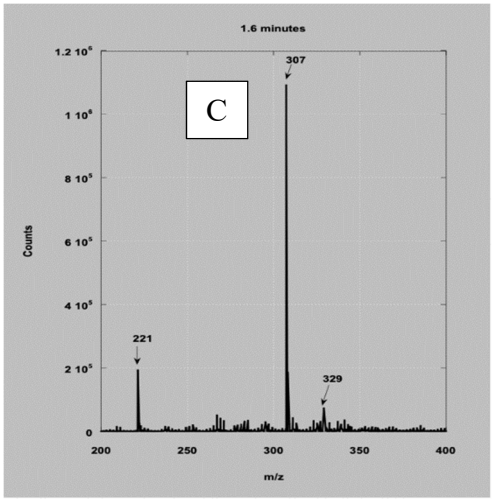
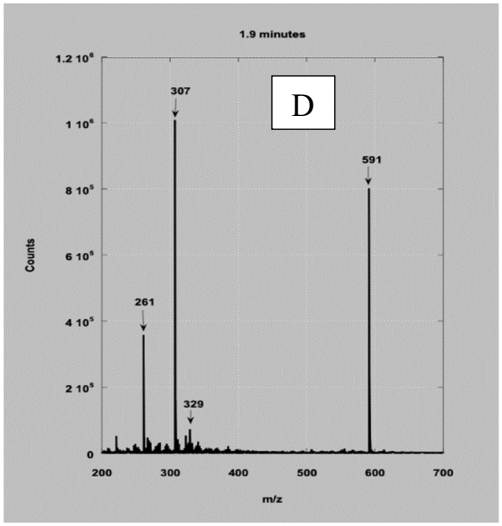
Supplementary









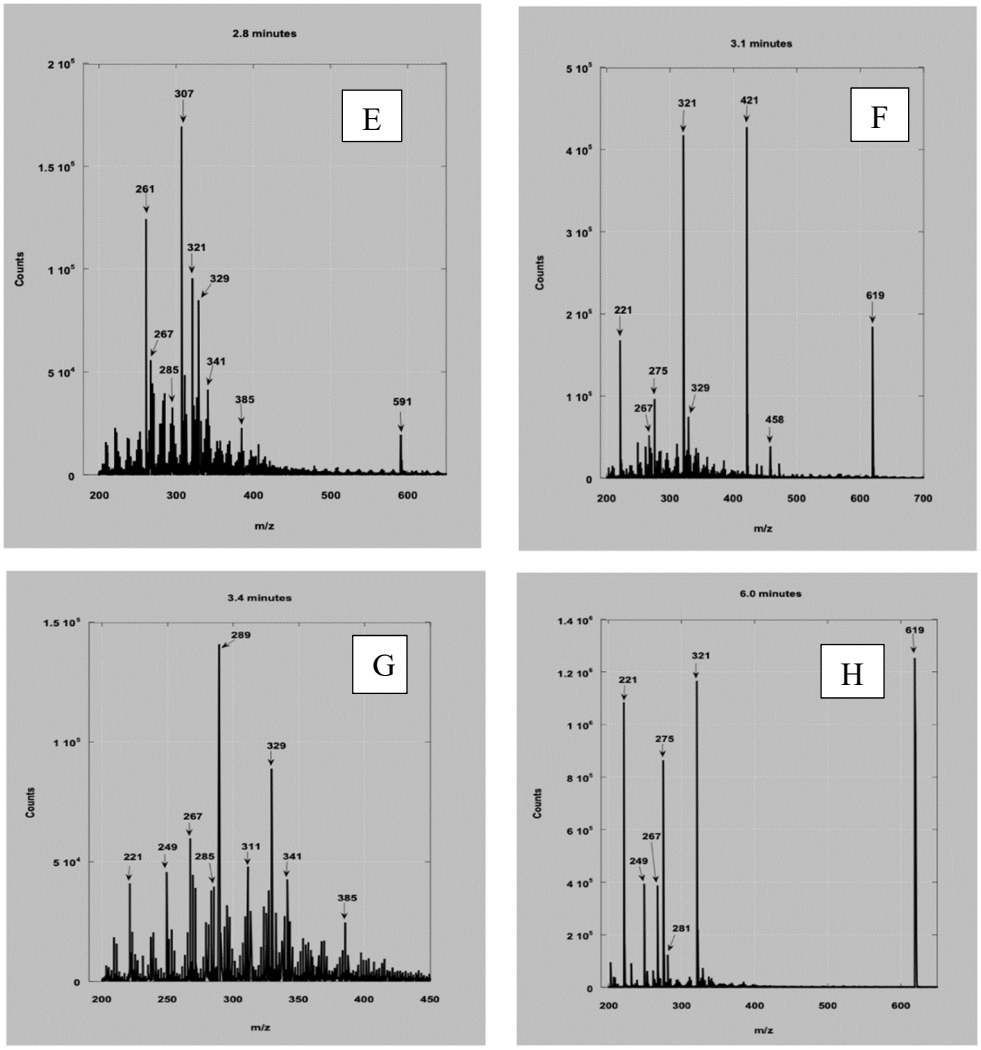
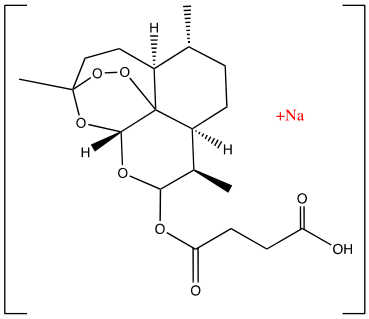
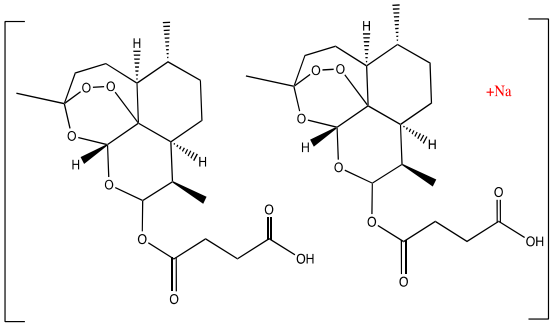
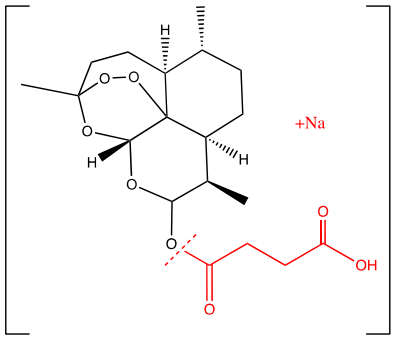
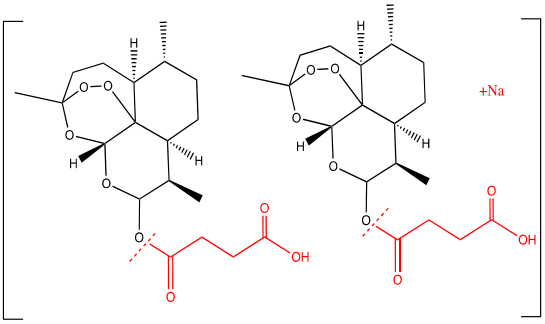
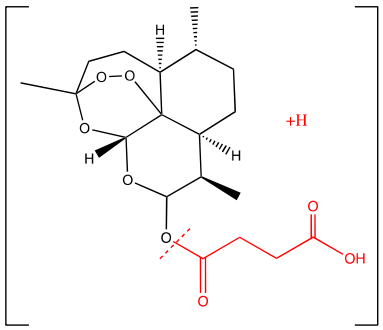
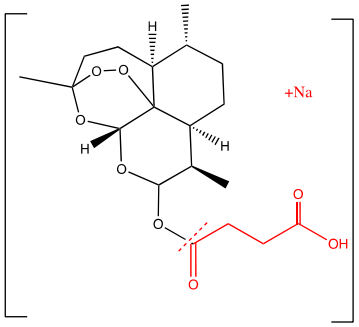
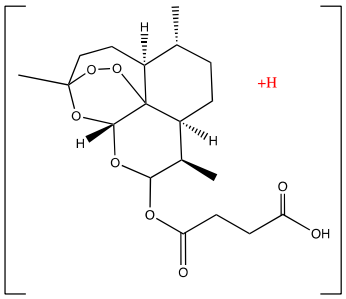
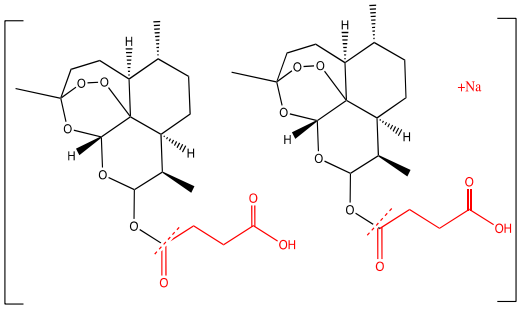
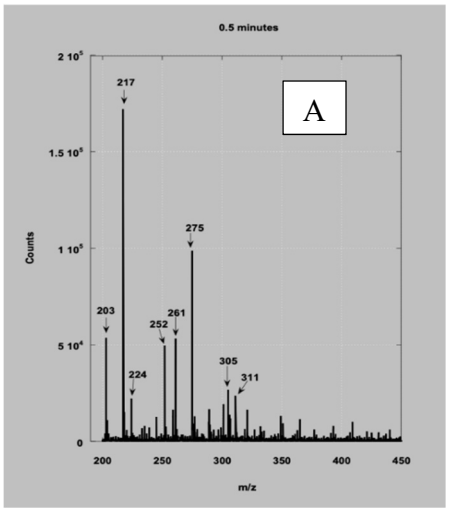


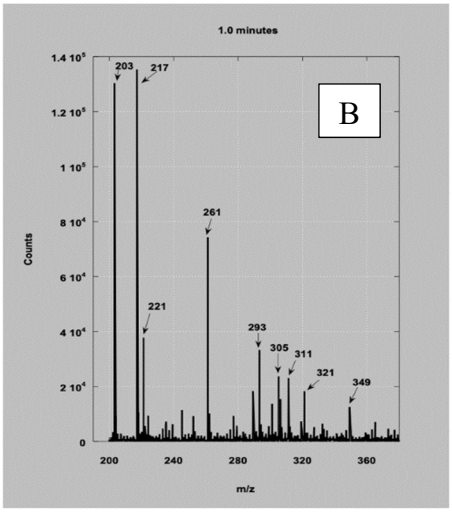
Figure S1. Mass spectrum of artesunate reaction products in methanol at 0.9mins (A), 1.2mins (B), 1.6mins (C), 1.9mins (D), 2.8mins (E), 3.1mins (F), 3.4mins (G) and 6.0mins (H).

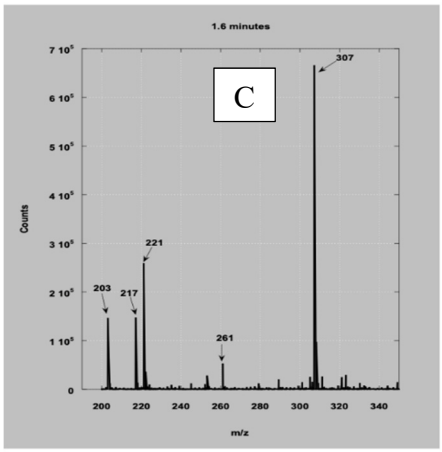
Table S1. Identification of mass fragments of artesunate reaction products in methanol.

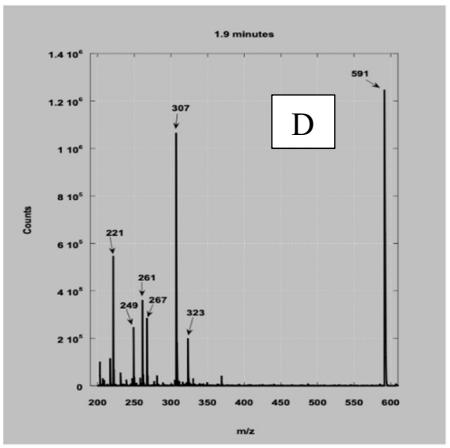
Retention time (min)	Main mass fragments (m/z)	Identification
0.9	407	 Artesunate 407
1.2	791	 Artesunate 791
1.6	307	 Artesunate 307
1.9	591	

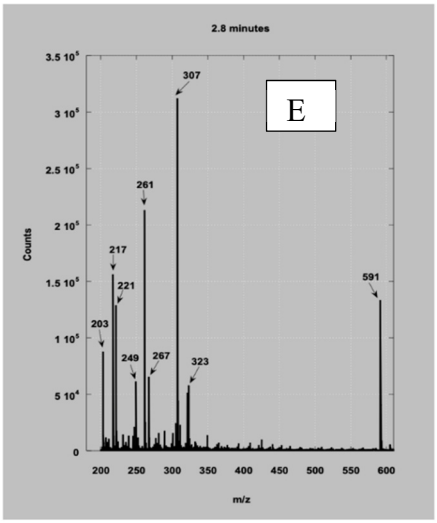
		Artesunate 591
2.8	285, 321, 385	 Artesunate 285  Artesunate 321  Artesunate 385
3.1	619	 Artesunate 619

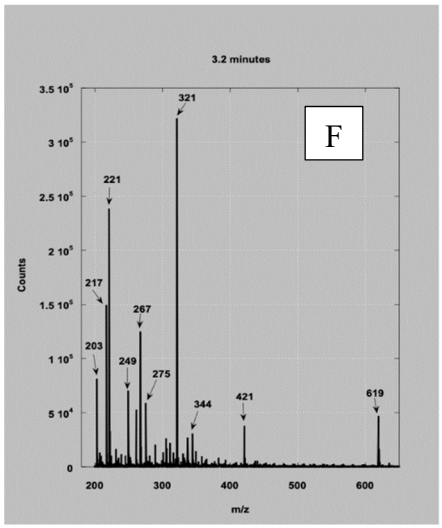

0.5 minutes
A
Counts
m/z
217
275
203
261
252
224
305
311


1.0 minutes
B
Counts
m/z
203
217
261
221
293
305
311
321
349


1.6 minutes
C
Counts
m/z
307
221
203
217
261


1.9 minutes
D
Counts
m/z
591
307
221
261
249
267
323


2.8 minutes
E
Counts
m/z
307
261
217
221
591
203
249
267
323


3.2 minutes
F
Counts
m/z
321
221
217
267
203
249
275
344
421
619

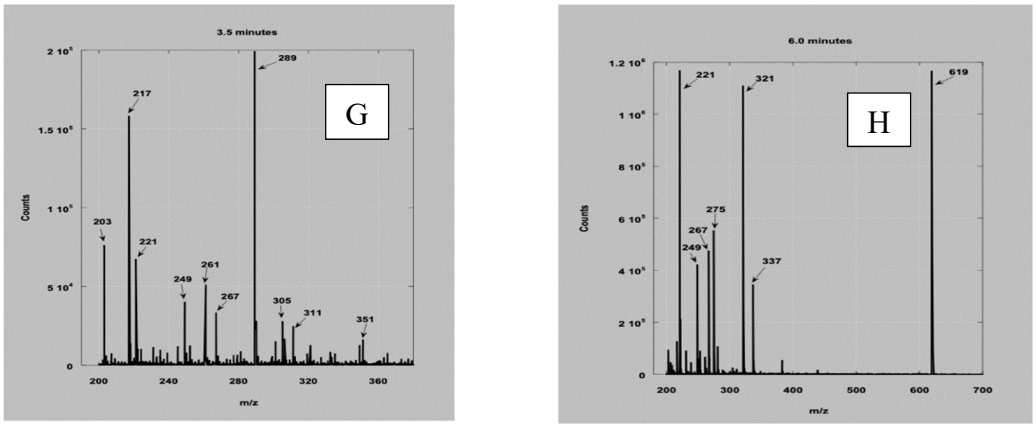
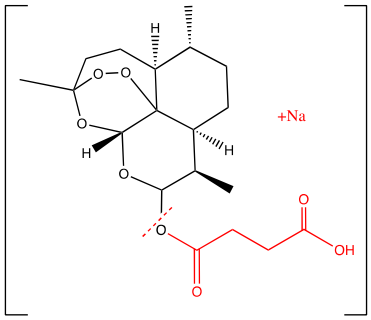
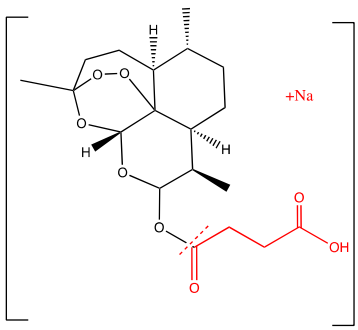
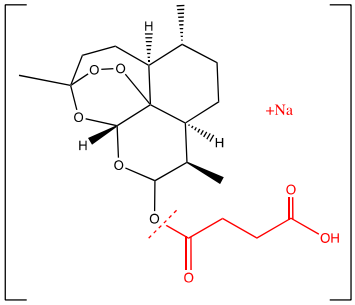
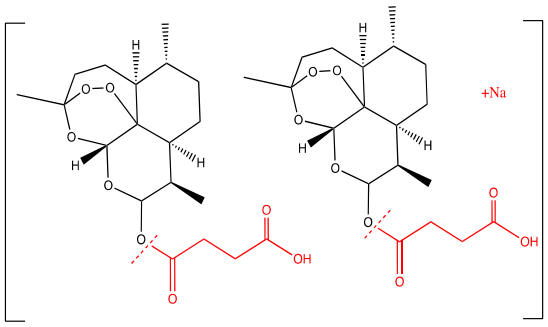
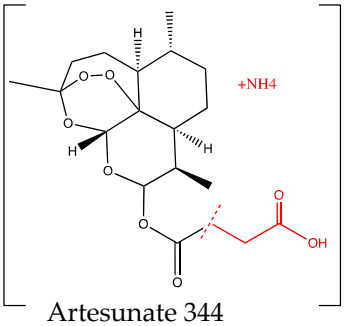
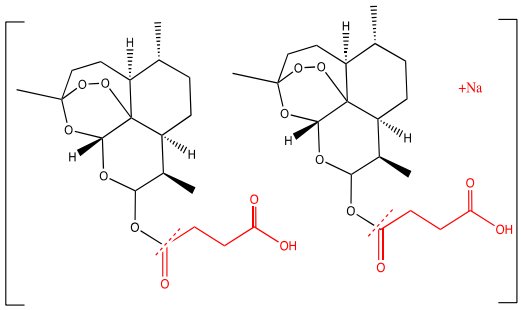
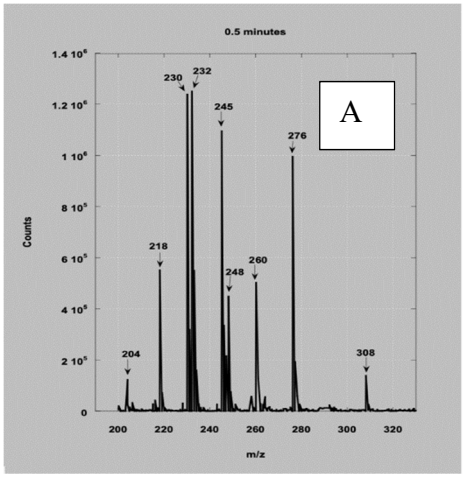


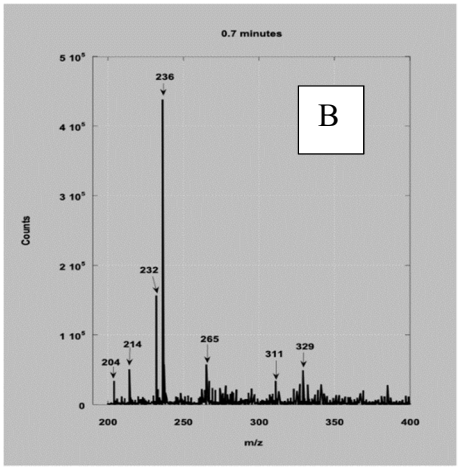
Figure S2. Mass spectrum of reaction products in methanol:water at 0.5mins (A), 1.0mins (B), 1.6mins (C), 1.9mins (D), 2.8mins (E), 3.2mins (F), 3.5mins (G) and 6.0mins (H).

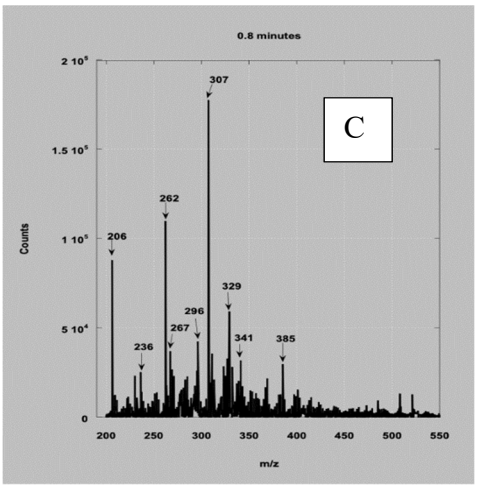
Table S2. Identification of mass fragments of artesunate reaction products in methanol:water.

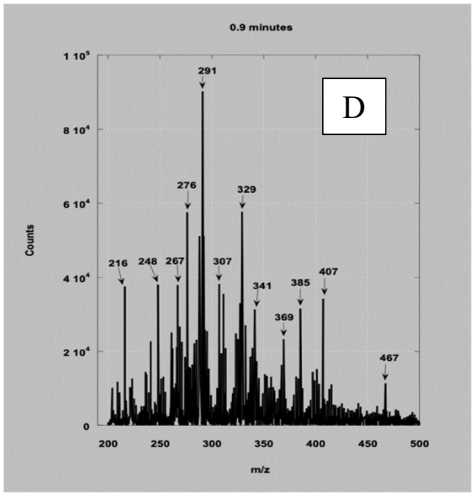
Retention time (min)	**Main mass fragments (m/z)**	**Identification**
0.5	305	 Artesunate 305
1.0	305*, and 321	 Artesunate 321
1.6	307	 Artesunate 307

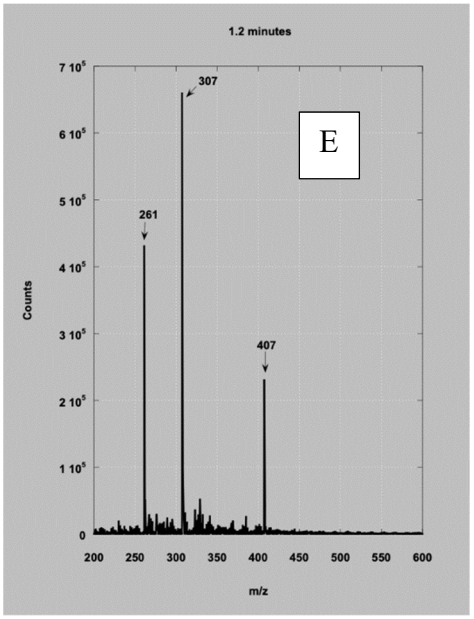
1.9	307*, 591	 Artesunate 591
3.2	321*, 344, 619	 Artesunate 344  Artesunate 691

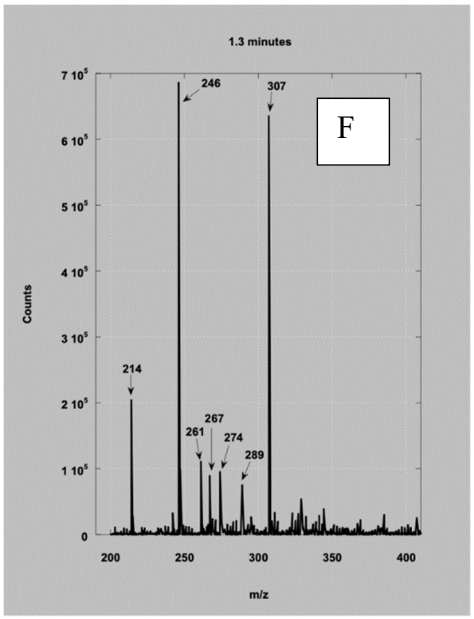

0.5 minutes
A
Counts
m/z
204
218
230
232
245
248
260
276
308

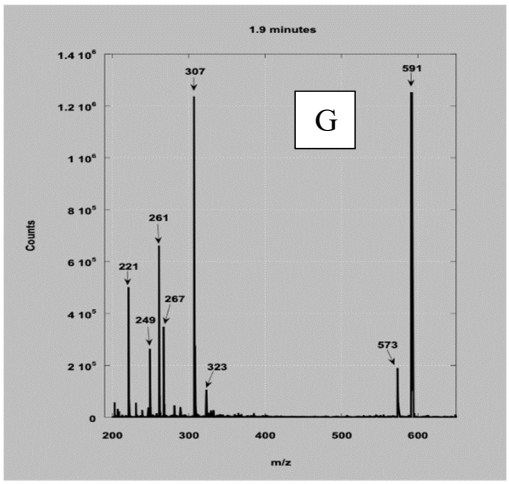

0.7 minutes
B
Counts
m/z
204
214
232
236
265
311
329

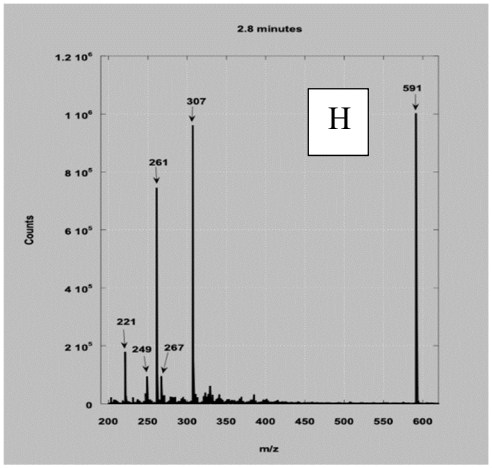

0.8 minutes
C
Counts
m/z
206
236
262
267
296
307
329
341
385


0.9 minutes
D
Counts
m/z
216
248
267
276
291
307
329
341
369
385
407
467


1.2 minutes
E
Counts
m/z
261
307
407


1.3 minutes
F
Counts
m/z
214
246
261
267
274
289
307





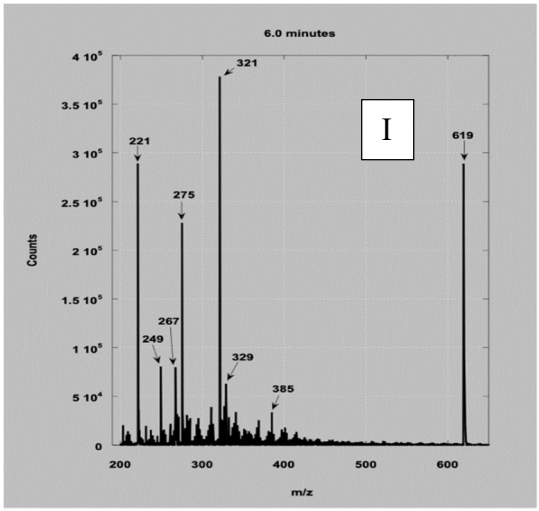
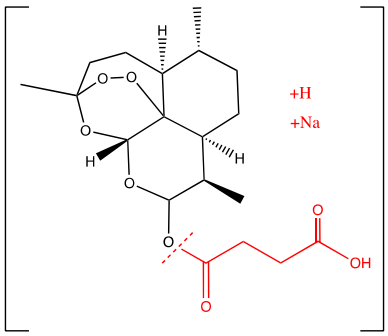
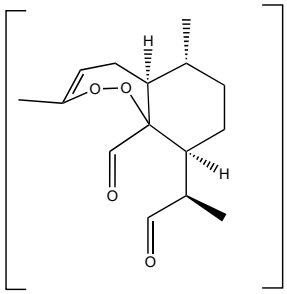
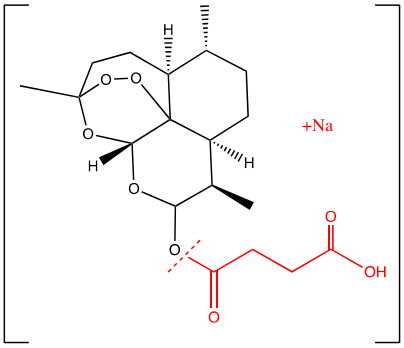
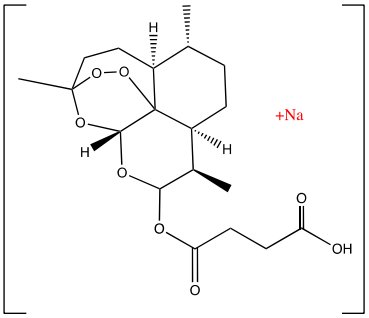
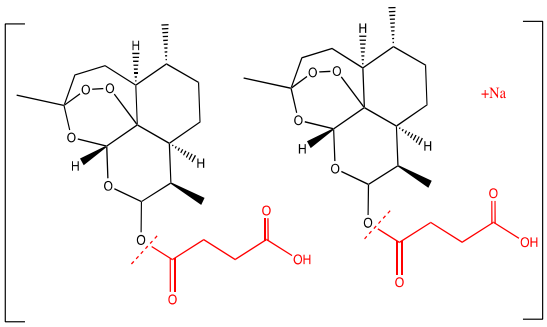
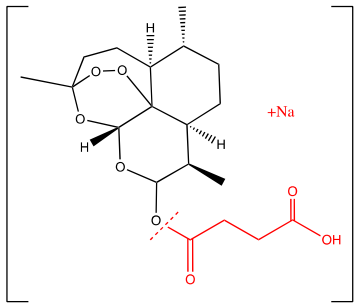
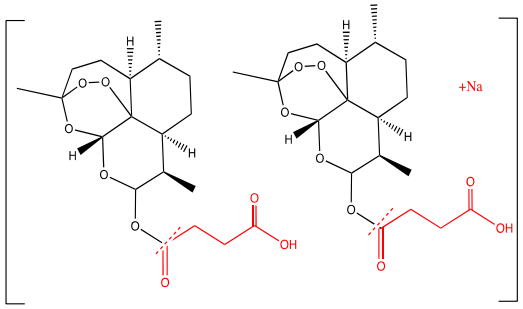


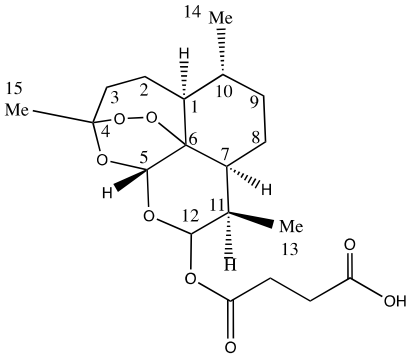
Figure S3. Mass spectrum of artesunate reaction products in 20 mM Ammonium Acetate: methanol at 0.5mins (A), 0.7mins (B), 0.8mins (C), 0.9mins (D), 1.2mins (E), 1.3mins (F), 1.9mins (G), 2.8mins (H), and 6.0mins (I).

Table S3. Identification of mass fragments of artesunate reaction products in 20 mM Ammonium Acetate: methanol.

Retention time (min)	Main mass fragments (m/z)	Identification
0.5	308	 Artesunate 308

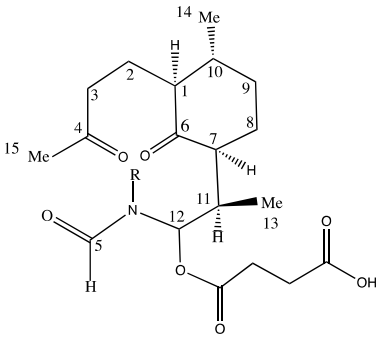
0.7	265	Addition of H to 282 gives m/z 283. Removal of water from m/z 283 resulted in fragment ion m/z 265.  Artesunate 265
0.8	307	 Artesunate 307
0.9	307*, 407	 Artesunate 407
1.9	267*, 307*, 591	 Artesunate 591

6.0	321, and 619	 Artesunate 321  Artesunate 619



1

artesunate



2 R=H

conjugated artesunate

Figure S4. Mechanism of conjugation between artesunate and nitrogen in 20 mM Ammonium Acetate : Methanol at 37°C.