

Supplement

Artemisinin DNA base interaction studies in presence of Fe (II): LC/TOF MS separation of reaction products.

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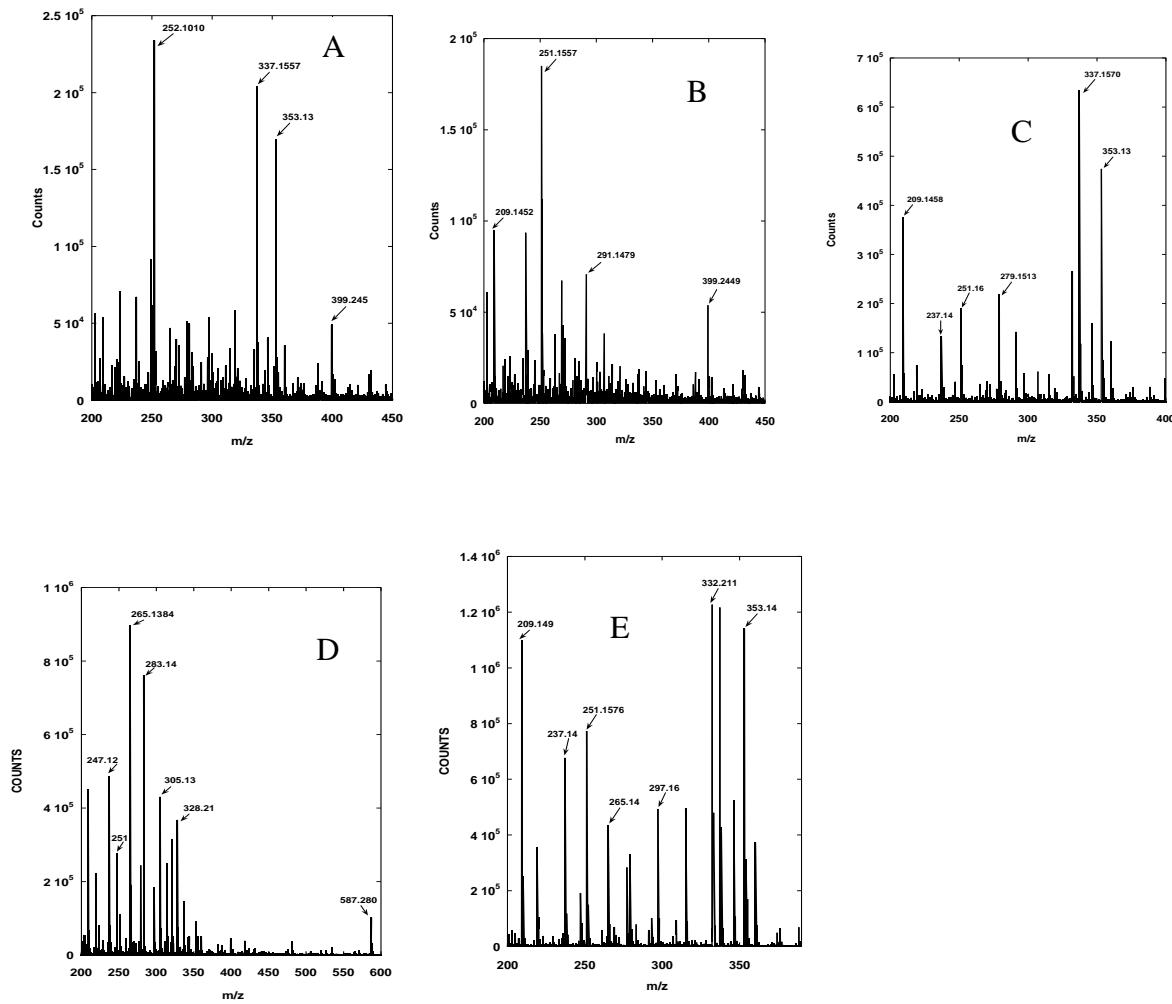
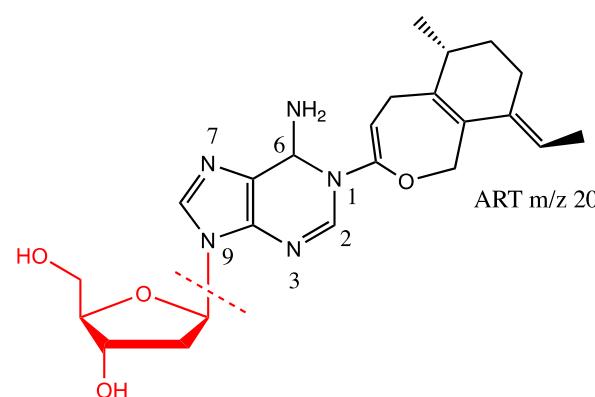
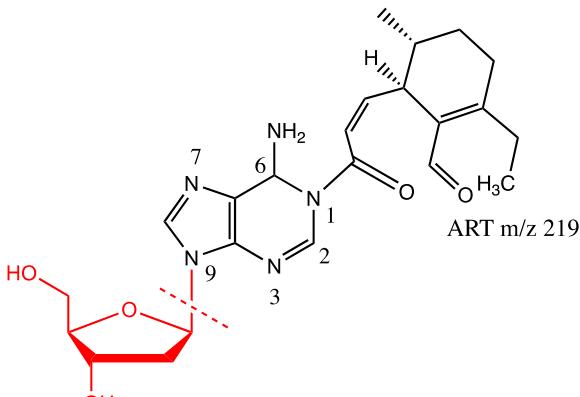
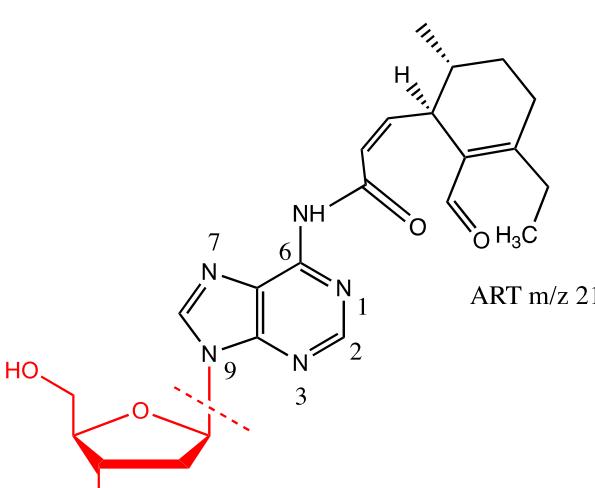


Figure S1. Mass spectrum of artemisinin-deoxyadenosine reaction products at 0.7 minutes (A), 0.8 mins (B), 0.9mins (C), 1.1mins (D) and 1.2 mins (E).

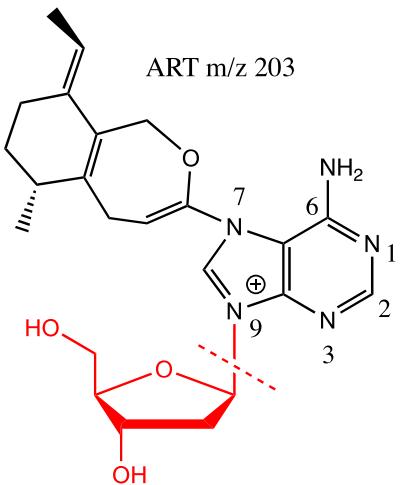
Table S1. Identification of mass fragments of artemisinin-deoxyadenosine reaction products.
(Repeated values indicated by asterisk*)

Retention time (min)	Main mass fragments (m/z)	Identification
0.7	251, 281, 337, 353, 399	 <p>ART m/z 203</p> <p>Artemisinin + Deoxyadenosine 337 at N1</p>  <p>ART m/z 219</p> <p>Artemisinin + Deoxyadenosine 353 at N1</p>
0.9	251*, 307*, 337* and 353*	 <p>ART m/z 219</p> <p>Artemisinin + Deoxyadenosine 353 at N6</p>

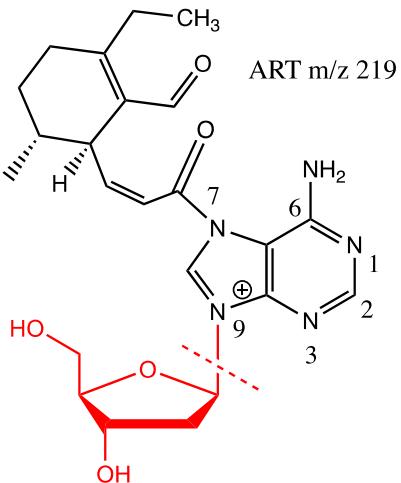
1.1

251*, 283, 337*, 353*, 587

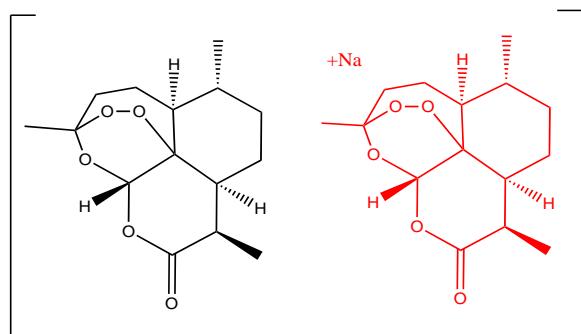
Dimer being formed
 Artemisinin formed dimer
 with itself.



Artemisinin + Deoxyadenosine 337 at N7



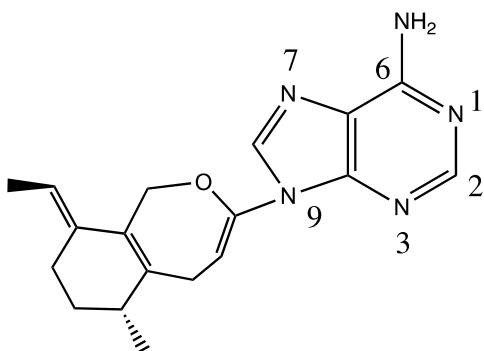
Artemisinin + Deoxyadenosine 353 at N7



Artemisinin 587 Dimer

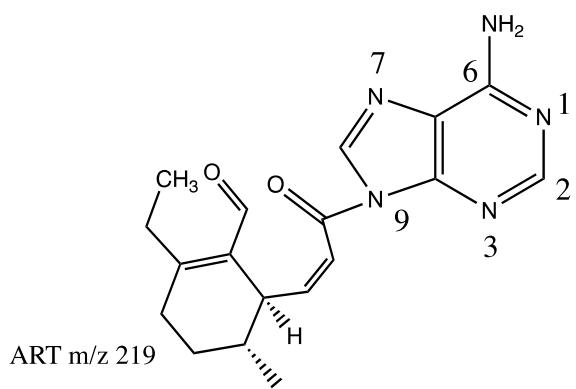
1.2

251*, 209, 237, 337* and,
353*



ART m/z 203

Artemisinin + Deoxyadenosine 337 at N9



ART m/z 219

Artemisinin + Deoxyadenosine 353 at N9

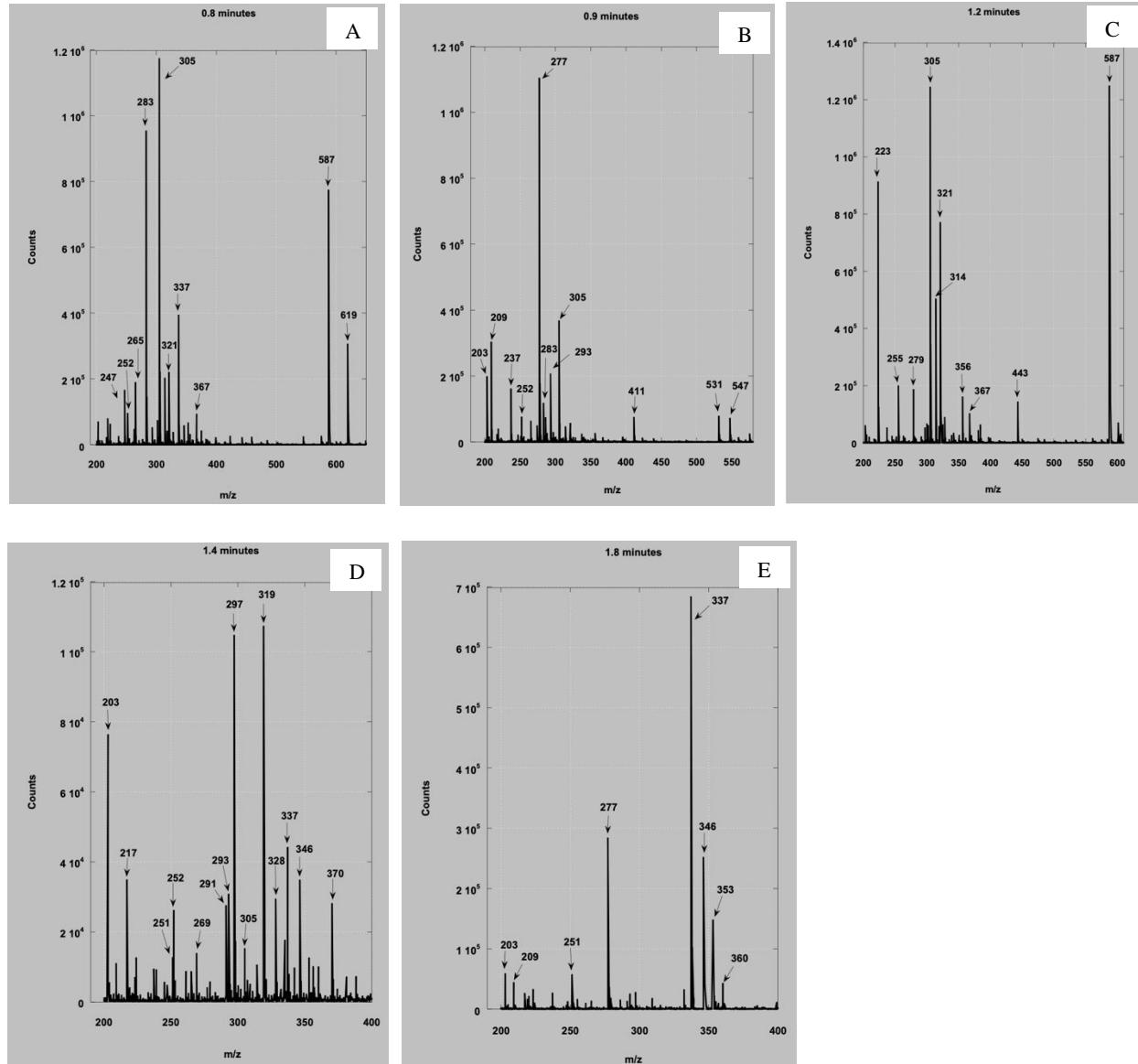
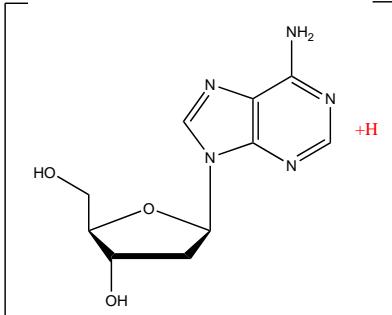
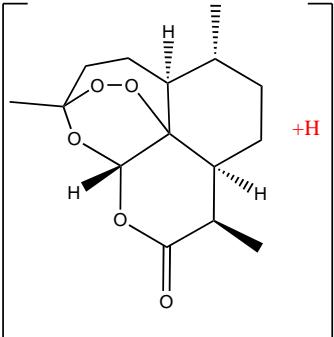
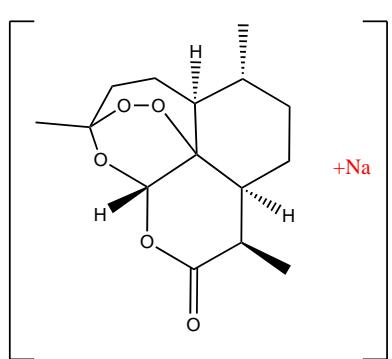
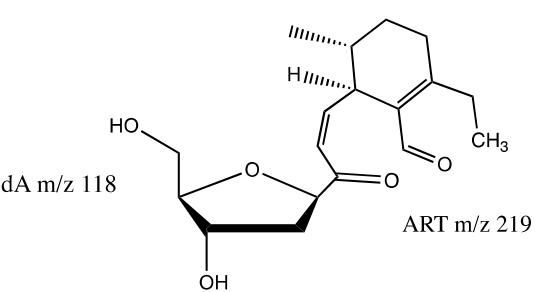


Figure S2. Mass spectrum of artemisinin-deoxyadenosine- Fe^{2+} at 0.8mins (A), 0.9mins (B), 1.2mins (C), 1.4 (D), and 1.8 (E).

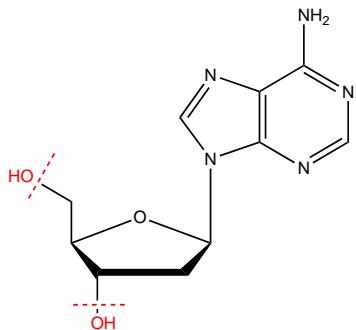
Table S2. Identification of mass fragments of artemisinin-deoxyadenosine- Fe^{2+} reaction products. (Repeated values indicated by asterisk*)

Retention time (min)	Main mass fragments (m/z)	Identification
0.8	252, 283, 305, 337, 423, 587 and 619	 Deoxyadenosine 252  Artemisinin 283  Artemisinin 305  Artemisinin + Deoxyadenosine 337

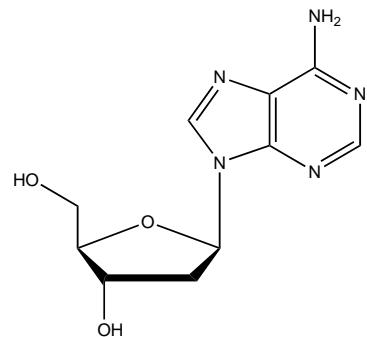
		<p>The first structure shows the chemical formula of Artemisinin, a sesquiterpenoid lactone. The second structure shows the same molecule with a sodium cation ($+Na$) added, indicating its salt form.</p> <p style="text-align: center;">Artemisinin 587</p>
0.9	209, 237, 277, 293, 305*, 321, 411, and 531	
1.2	277*, 321*, 337*, 346 and 353	<p>The left structure shows Artemisinin (ART) at m/z 219. The right structure shows Deoxyadenosine (dA) at m/z 135. Both structures are labeled with their respective mass-to-charge ratios.</p> <p style="text-align: center;">Artemisinin + Deoxyadenosine 353</p>

1.9

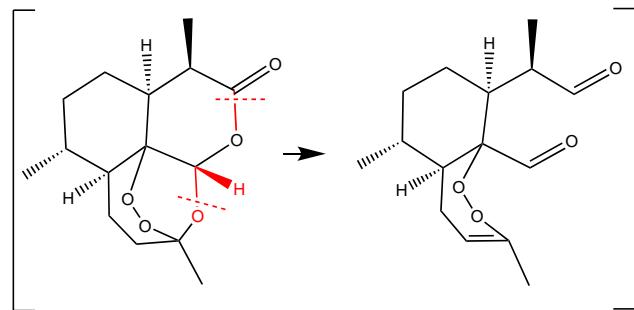
247, 251, 265, 283*, 305*,
328 and 587*



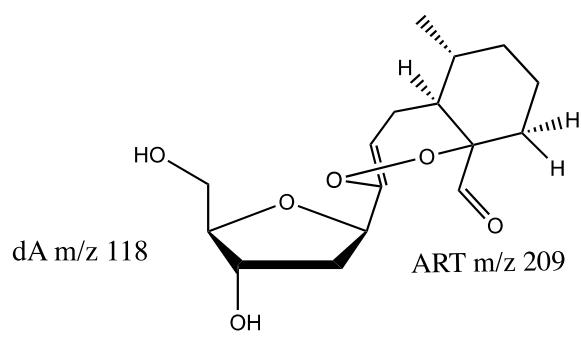
Deoxyadenosine 247



Deoxyadenosine 251



Artemisinin 265 [M+H-H₂O]⁺



Artemisinin + Deoxyadenosine 328

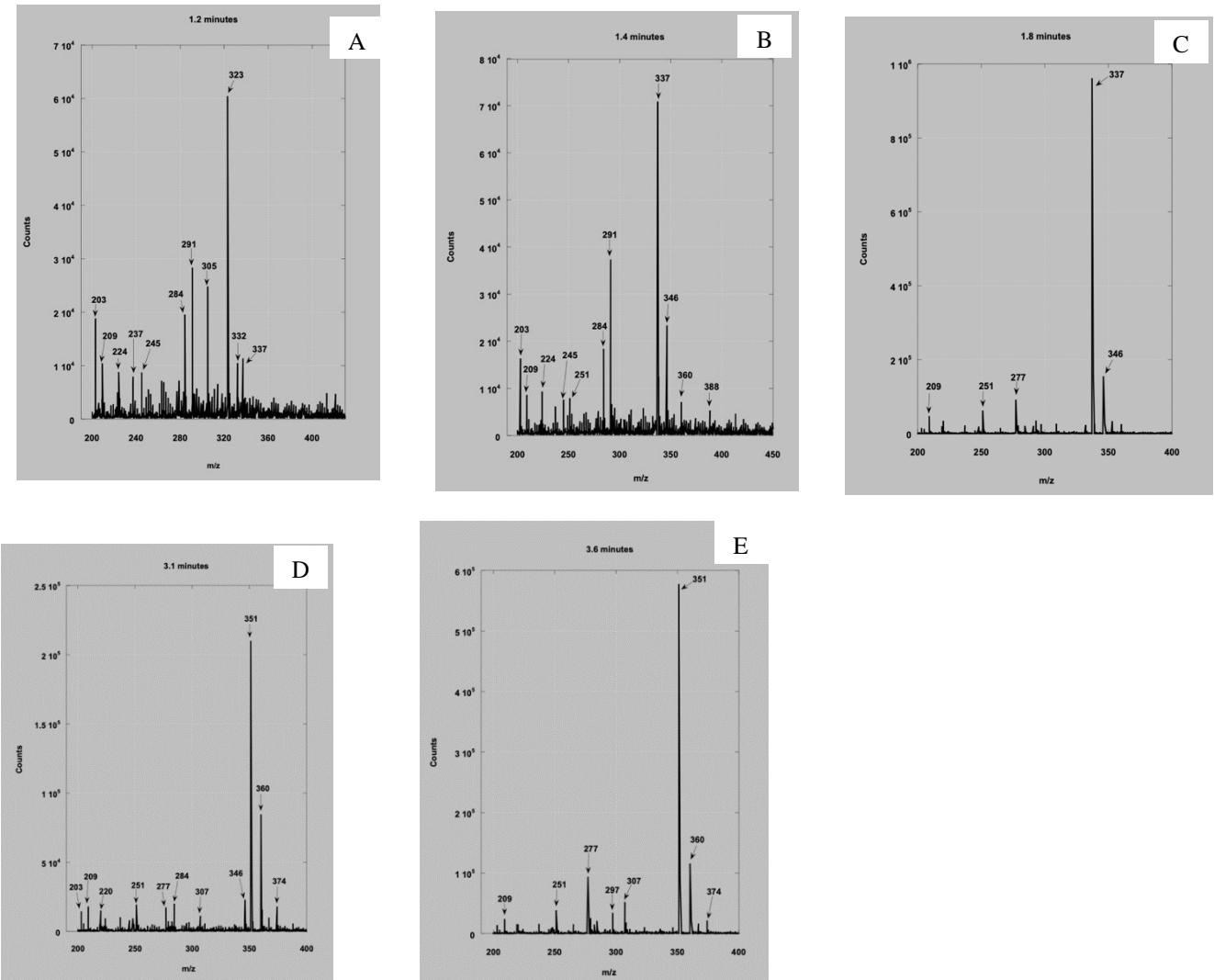


Figure S3. Mass spectrum of artemisinin-deoxycytidine reaction products at 1.2 minutes (A), 1.4 mins (B), 1.8 mins (C), 3.1 mins (D), and 3.6 mins (E).

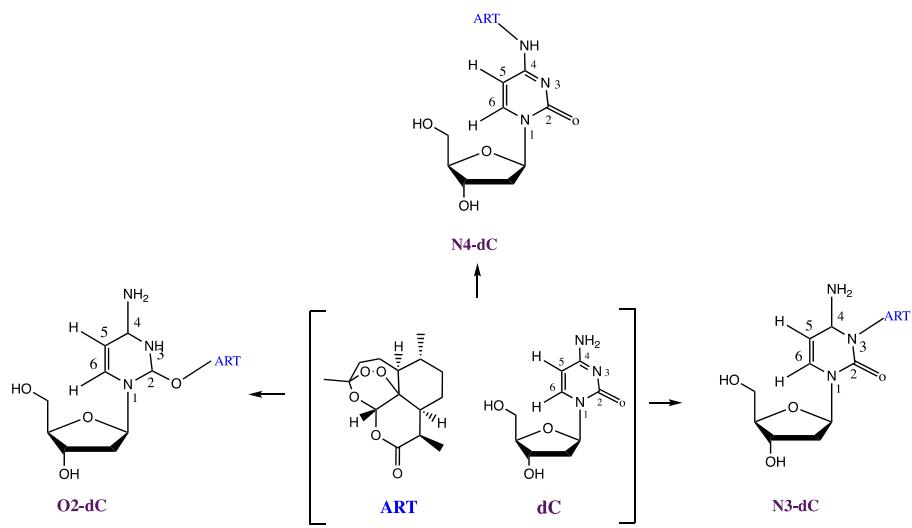
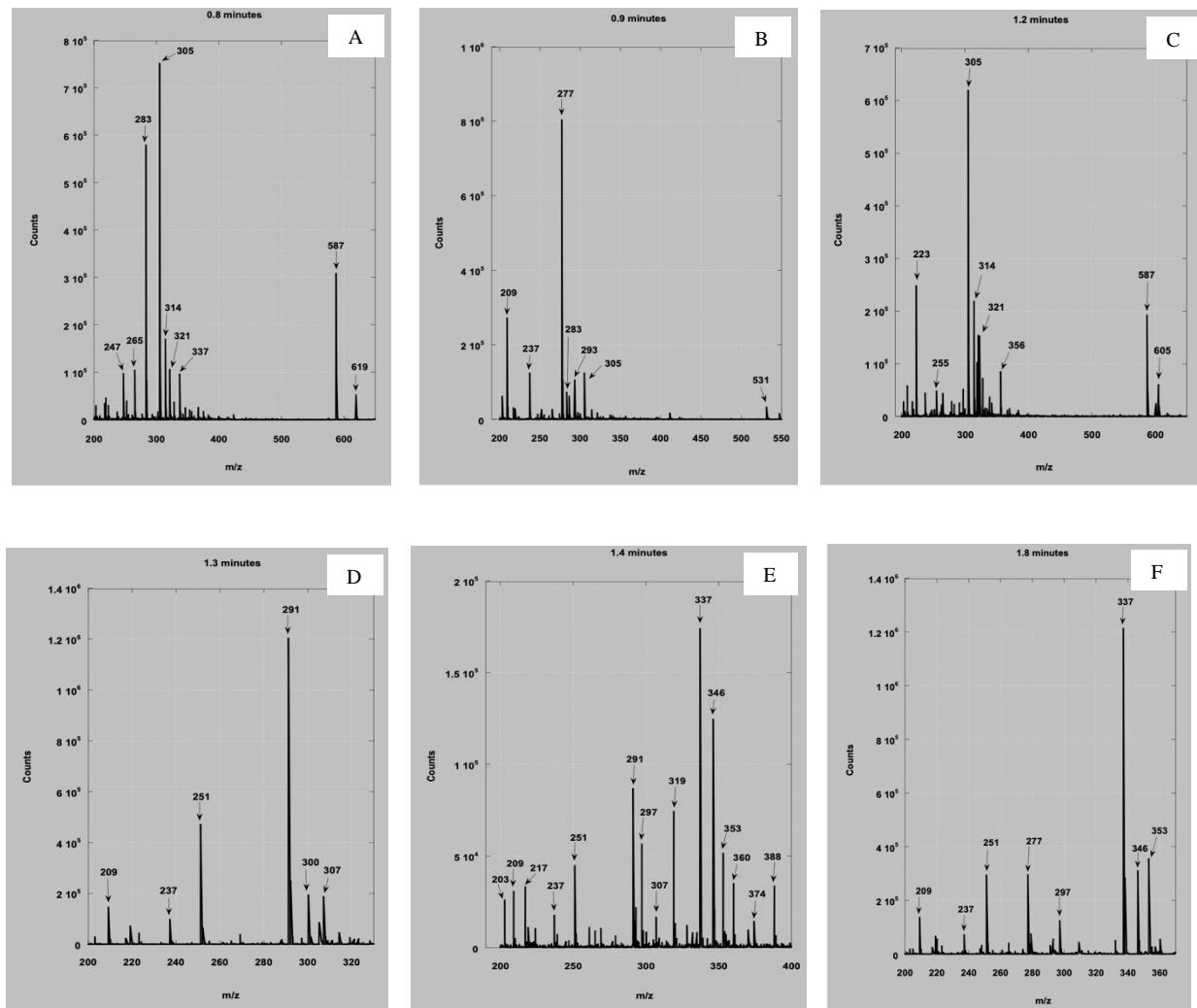


Figure S4. Possible mechanism of deoxycytidine (dC) alkylation on the N3, N4, and 2O positions by Artemisinin (ART) under temperature control.



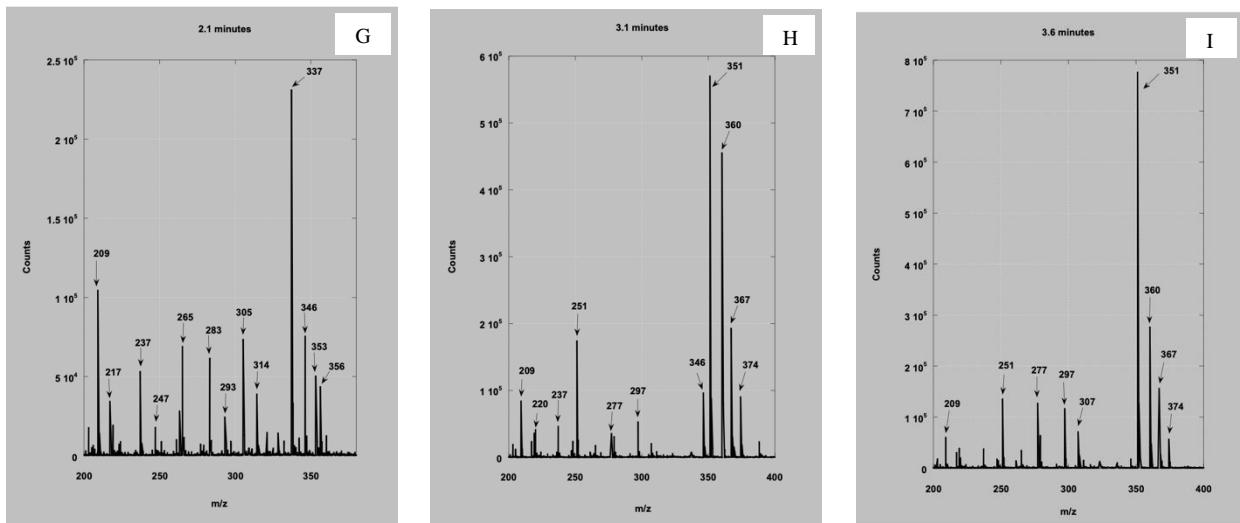


Figure S5. Mass spectrum of artemisinin-deoxycytidine- Fe^{2+} at 0.8mins (A), 0.9mins (B), 1.2mins (C), 1.3 mins (D), 1.4 (E), 1.8 (F), 2.1 (G), 3.1 (H) and 3.6 (I).