

Supplement

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

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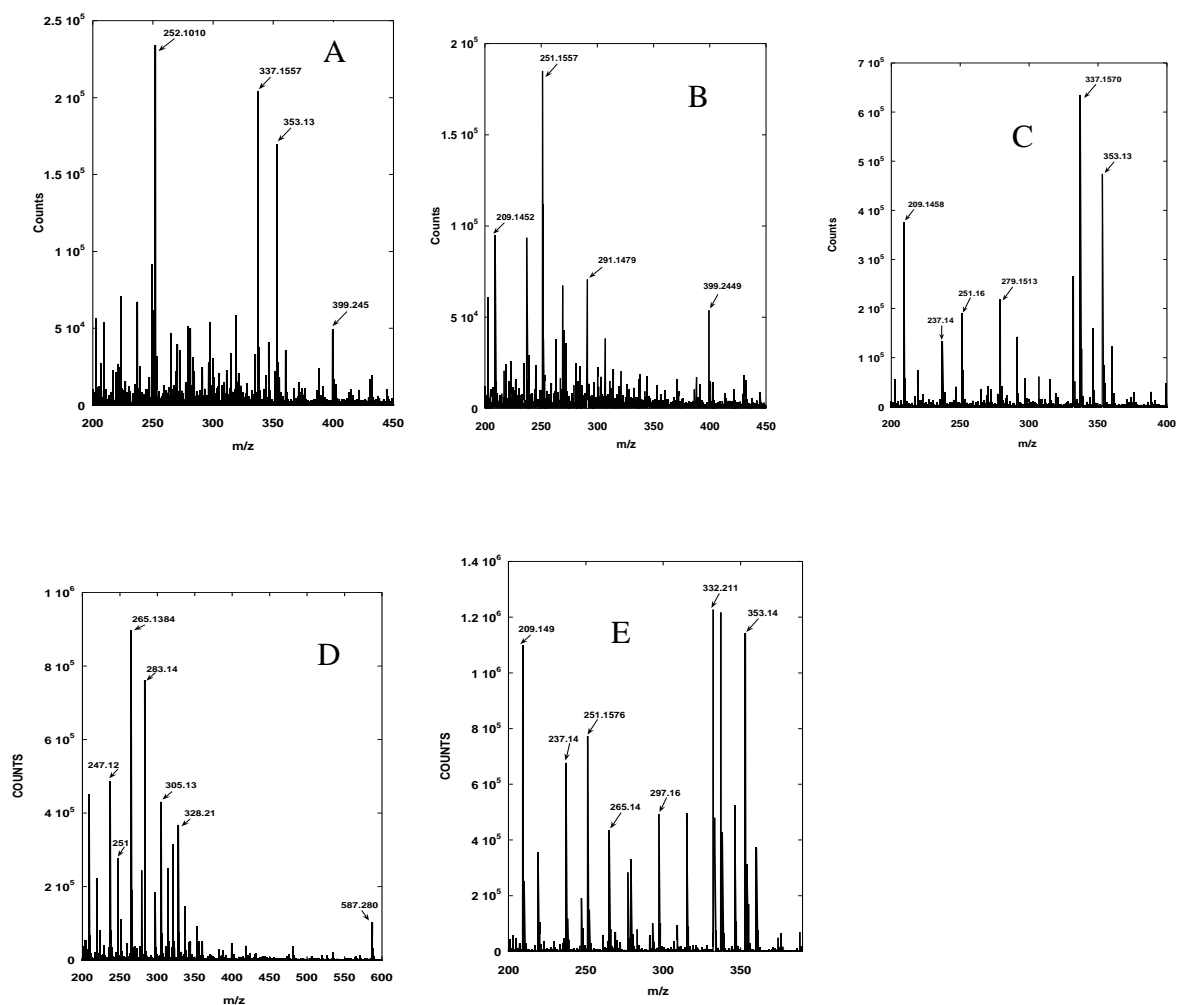
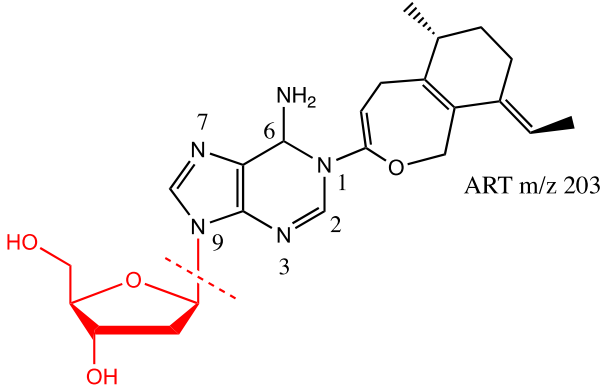
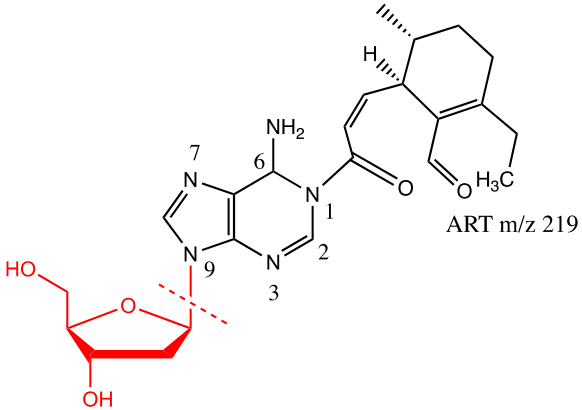
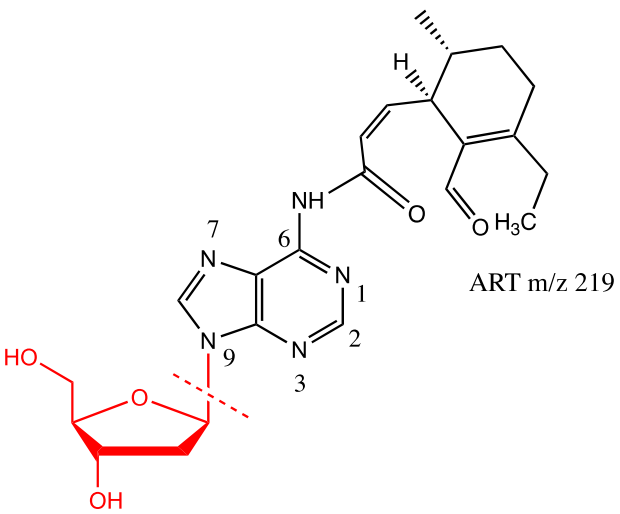


Figure S1. Mass spectrum of artemisinin-deoxyadenosine reaction products at 0.7 minutes (A), 0.8 mins (B), 0.9mins (C), 1.1mins (D) and 1.2 mins (E).

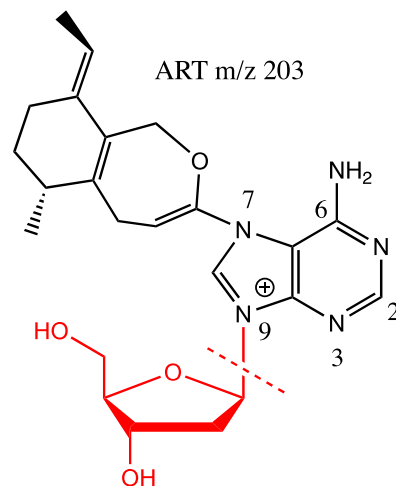
Table S1. Identification of mass fragments of artemisinin-deoxyadenosine reaction products. (Repeated values indicated by asterisk*)

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

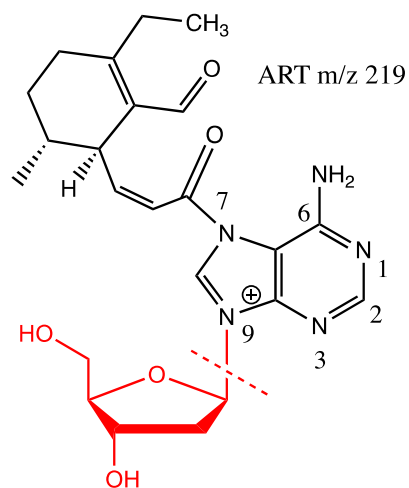
1.1

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

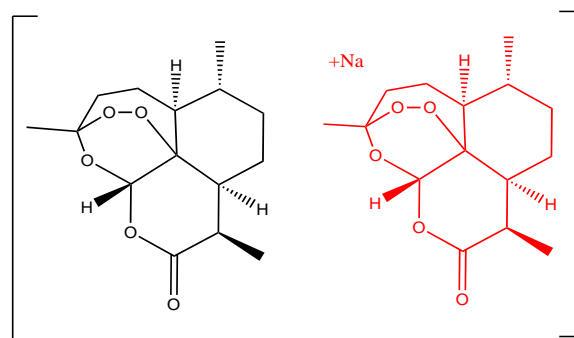
Dimer being formed
Artemisinin formed dimer
with itself.



Artemisinin + Deoxyadenosine 337 at N7



Artemisinin + Deoxyadenosine 353 at N7



Artemisinin 587 Dimer

1.2	251*, 209, 237, 337* and, 353*	<div data-bbox="890 203 1369 551"> </div> <p data-bbox="932 573 1078 604">ART m/z 203</p> <p data-bbox="815 633 1353 669">Artemisinin + Deoxyadenosine 337 at N9</p> <div data-bbox="970 741 1401 1122"> </div> <p data-bbox="834 1070 981 1102">ART m/z 219</p> <p data-bbox="815 1167 1353 1202">Artemisinin + Deoxyadenosine 353 at N9</p>
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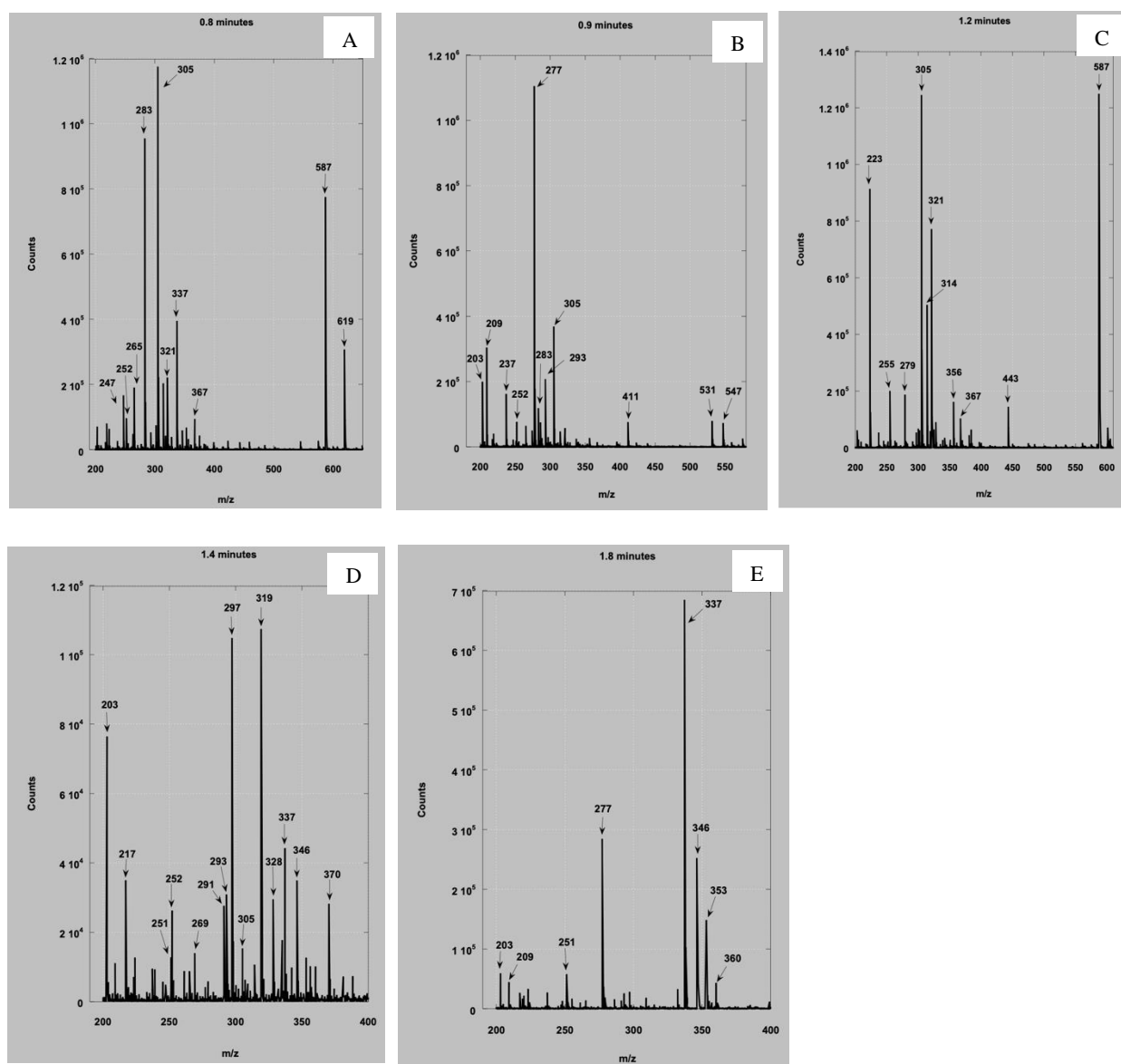
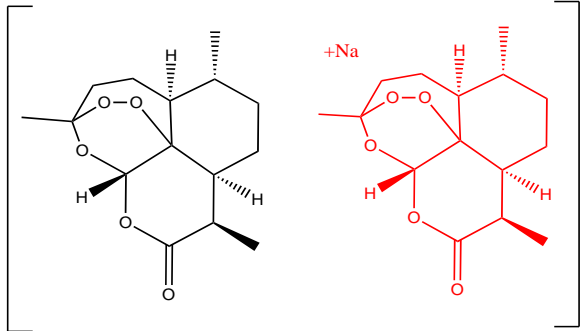
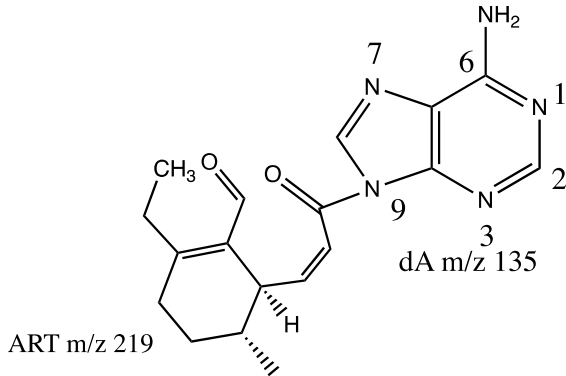


Figure S2. Mass spectrum of artemisinin-deoxyadenosine- Fe^{2+} at 0.8mins (A), 0.9mins (B), 1.2mins (C), 1.4 (D), and 1.8 (E).

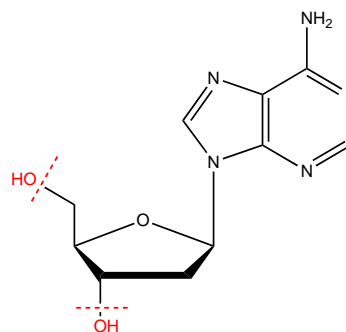
Table S2. Identification of mass fragments of artemisinin-deoxyadenosine- Fe^{2+} reaction products. (Repeated values indicated by asterisk*)

Retention time (min)	Main mass fragments (m/z)	Identification
0.8	252, 283, 305, 337, 423, 587 and 619	<div data-bbox="943 315 1342 636"> </div> <p>Deoxyadenosine 252</p> <div data-bbox="956 763 1294 1106"> </div> <p>Artemisinin 283</p> <div data-bbox="946 1207 1332 1550"> </div> <p>Artemisinin 305</p> <div data-bbox="860 1675 1398 1951"> </div> <p>Artemisinin + Deoxyadenosine 337</p>

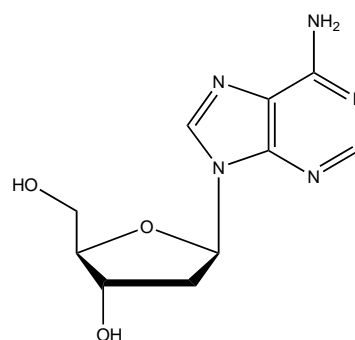
		 <p>Artemisinin 587</p>
0.9	209, 237, 277, 293, 305*, 321, 411, and 531	
1.2	277*, 321*, 337*, 346 and 353	 <p>Artemisinin + Deoxyadenosine 353</p>

1.9

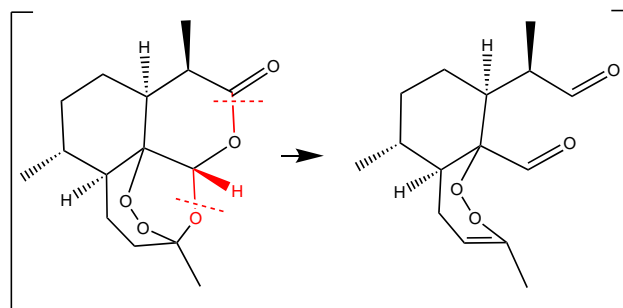
247, 251, 265, 283*, 305*,
328 and 587*



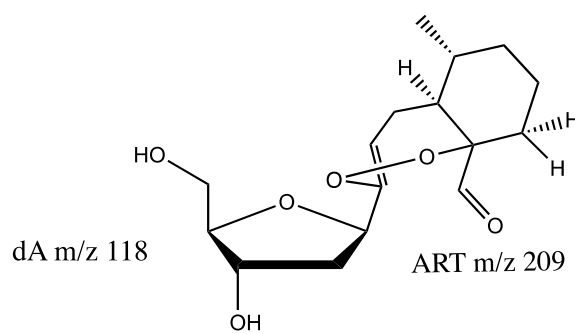
Deoxyadenosine 247



Deoxyadenosine 251



Artemisinin 265 [M+H-H₂O]⁺



Artemisinin + Deoxyadenosine 328

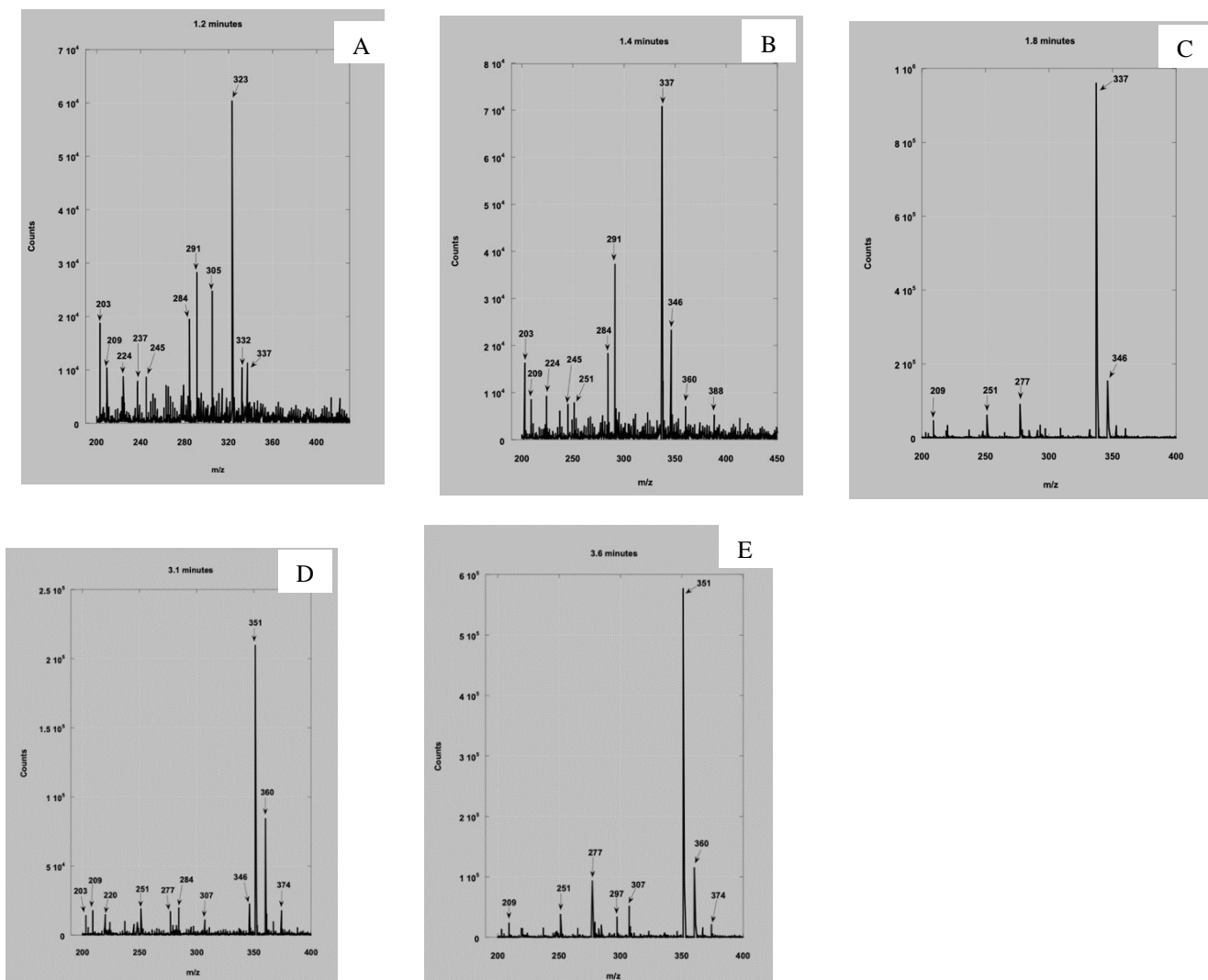


Figure S3. Mass spectrum of artemisinin-deoxycytidine reaction products at 1.2 minutes (A), 1.4 mins (B), 1.8 mins (C), 3.1 mins (D), and 3.6 mins (E).

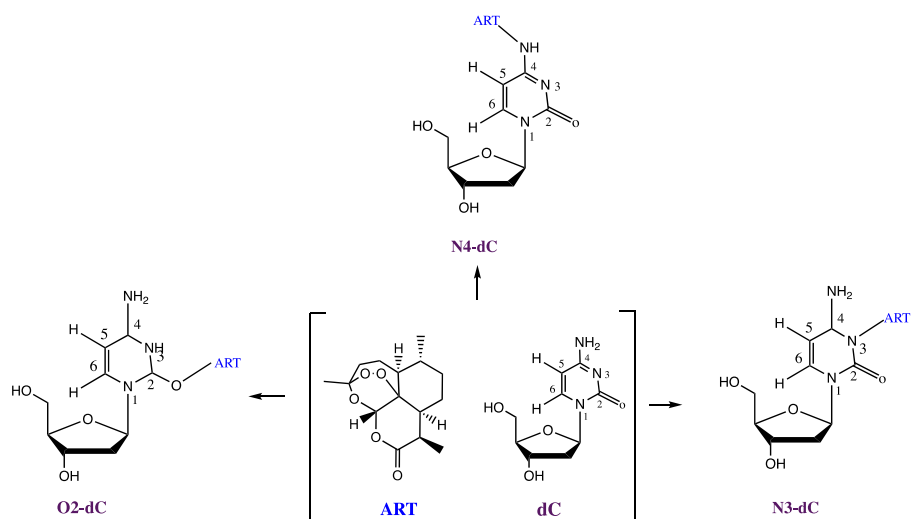
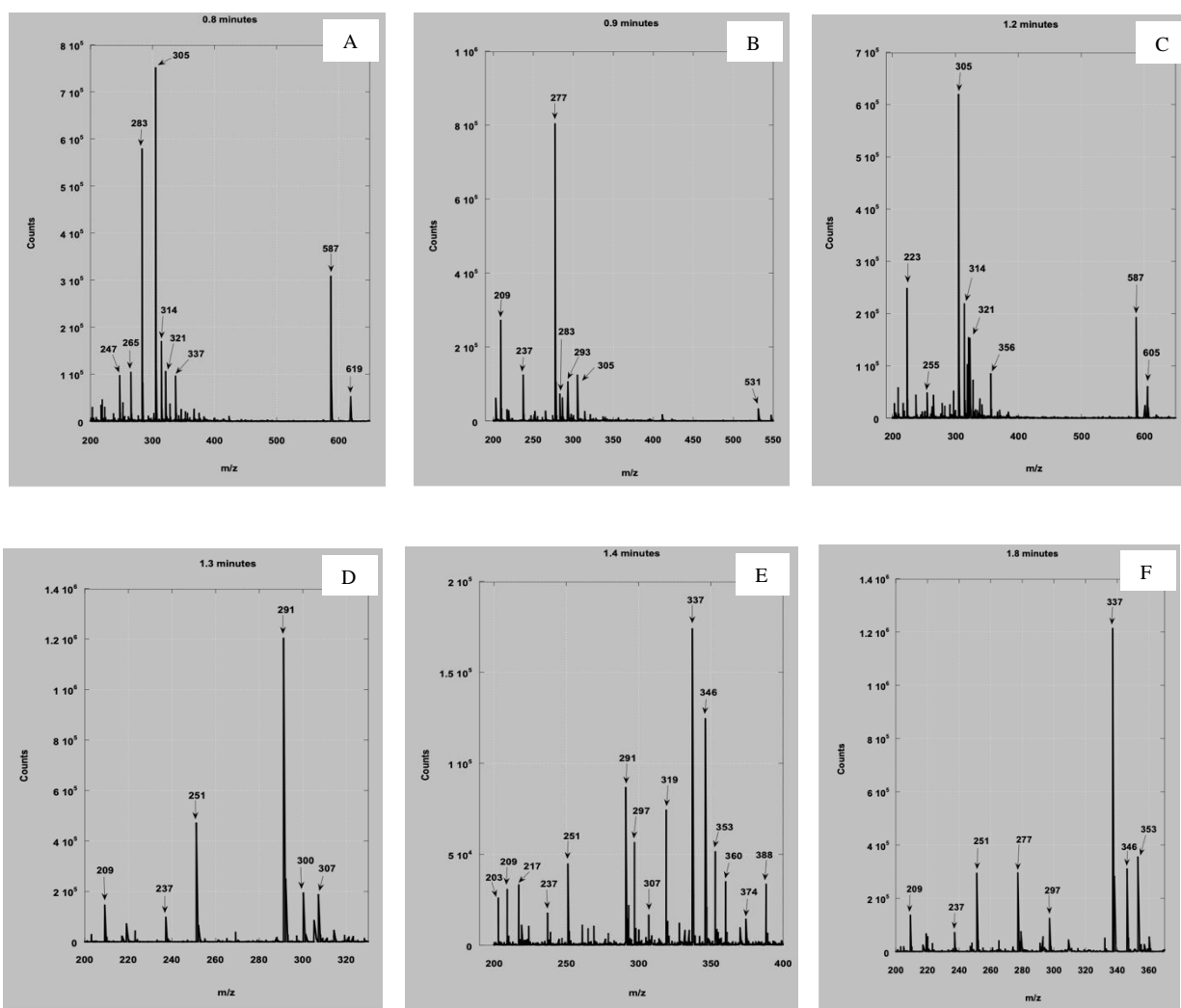


Figure S4. Possible mechanism of deoxycytidine (dC) alkylation on the N3, N4, and 2O positions by Artemisinin (ART) under temperature control.



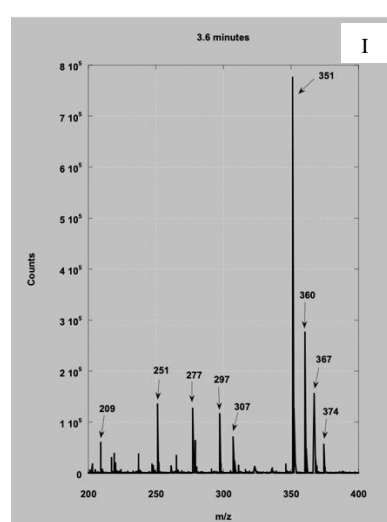
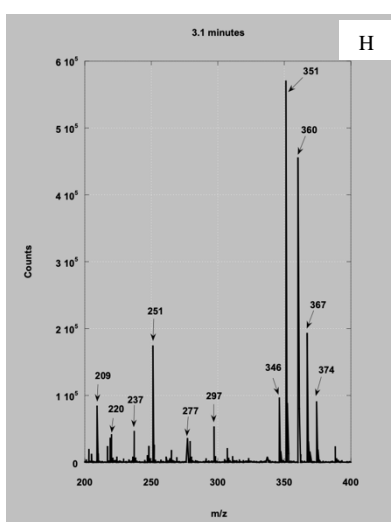
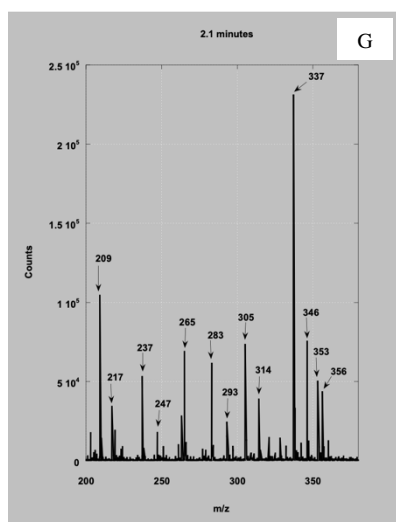


Figure S5. Mass spectrum of artemisinin-deoxycytidine- Fe^{2+} at 0.8mins (A), 0.9mins (B), 1.2mins (C), 1.3 mins (D), 1.4 (E), 1.8 (F), 2.1 (G), 3.1 (H) and 3.6 (I).