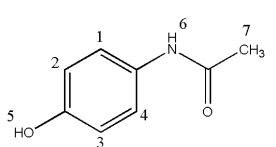
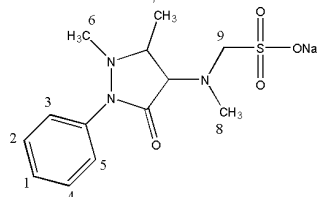
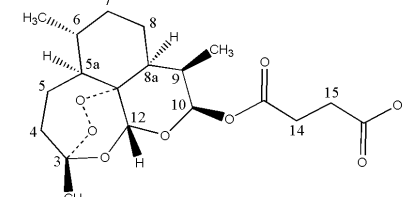
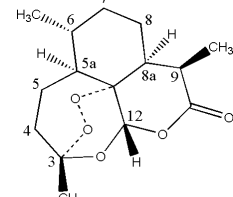


Electronic Supplementary Material for: “Combining Two-Dimensional Diffusion-Ordered Nuclear Magnetic Resonance Spectroscopy, Imaging Desorption Electrospray Ionization Mass Spectrometry and Direct Analysis in Real Time Mass Spectrometry for the Integral Investigation of Counterfeit Pharmaceuticals”, by Nyadong et al.

Table S-1. ¹H NMR data of active pharmaceutical ingredients detected in the artesunate antimalarial samples investigated in this study.

Acetaminophen			Dipyron			Artesunic acid			Artemisinin		
											
δ (ppm) ^a	Number of protons, multiplicity ^b (J, Hz)	N ^o	δ (ppm) ^a	Number of protons, multiplicity ^b (J, Hz)	N ^o	δ (ppm) ^a	Number of protons, multiplicity ^b (J, Hz)	N ^o	δ (ppm) ^a	Number of protons, multiplicity ^b (J, Hz)	N ^o
9.67	1H, s	6	7.48	2H, t (7.9)	2/4	5.69	1H, d (9.6)	10	6.15	1H, s	12
9.16	1H, s	5	7.38	2H, d (7.9)	3/5	5.57	1H, s	12	3.18	1H, m	9
7.35	2H, d (8.6)	1/4	7.28	1H, t (7.9)	1	2.62/2.52	4H, m	14/15	2.29	1H, m	4
6.69	2H, d (8.6)	2/3	3.68	2H, s	9	2.31	1H, m	9	2.08	1H, m	4
2.00	3H, s	7	2.91	3H, s	6	2.21	1H, m	4	1.95	1H, m	5
			2.90	3H, s	8	2.03	1H, m	4	1.81	1H, m	8a
			2.27	3H, s	7	1.84	1H, m	5	1.75	1H, m	8
						1.65	1H, m	8	1.66	1H, m	7
						1.65	1H, m	7	1.56	1H, m	6
						1.58	1H, m	8a	1.38	3H, s	3Me
						1.48	1H, m	8	1.36	1H, m	5a
						1.44	1H, m	6	1.34	1H, m	5
						1.35	1H, m	5	1.17	1H, m	8
						1.31	3H, s	3Me	1.09	3H, d (6.6)	9Me
						1.21	1H, m	5a	1.03	1H, m	7
						0.97	1H, m	7	0.94	3H, d (6.6)	6Me
						0.91	3H, d (6.6)	6Me			
						0.79	1H, d (6.6)	9Me			

^a Spectra were recorded at 298K in DMSO-d₆.

^b s: singlet; d: doublet; t: triplet; m: multiplet.

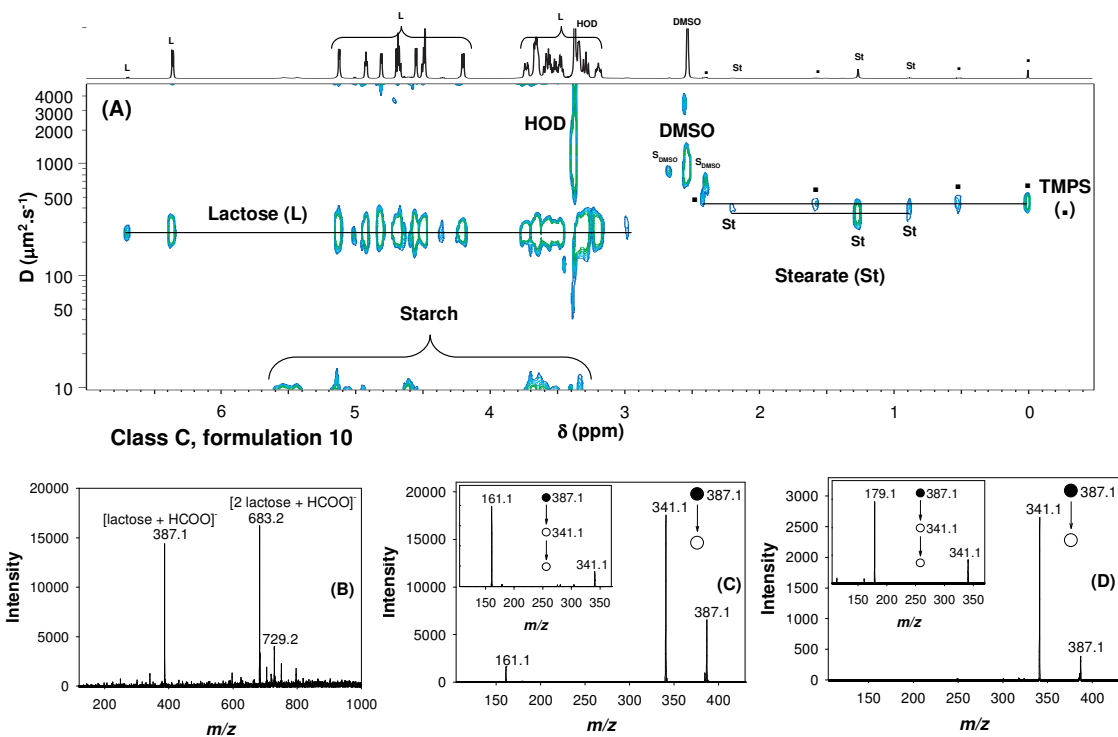


Figure S-1. Analysis of formulation **10** by: (A) 2D DOSY ^1H NMR in DMSO-d_6 with TMPS as internal reference standard (S_{DMSO} represents DMSO satellite signals), and (B) DESI MS in negative ion mode (using a spray solution of 99.9:0.1% v/v MeOH:HCOOH), (C) DESI MS 2 of the precursor ion at m/z 387.1 from sample **10** in negative ion mode, and (D) DESI MS 2 of the precursor ion at m/z 387.1 of sample **11** in negative ion mode. The inserts in (C) and (D) represent the corresponding DESI MS 3 spectra generated from the ions at m/z 341.1.

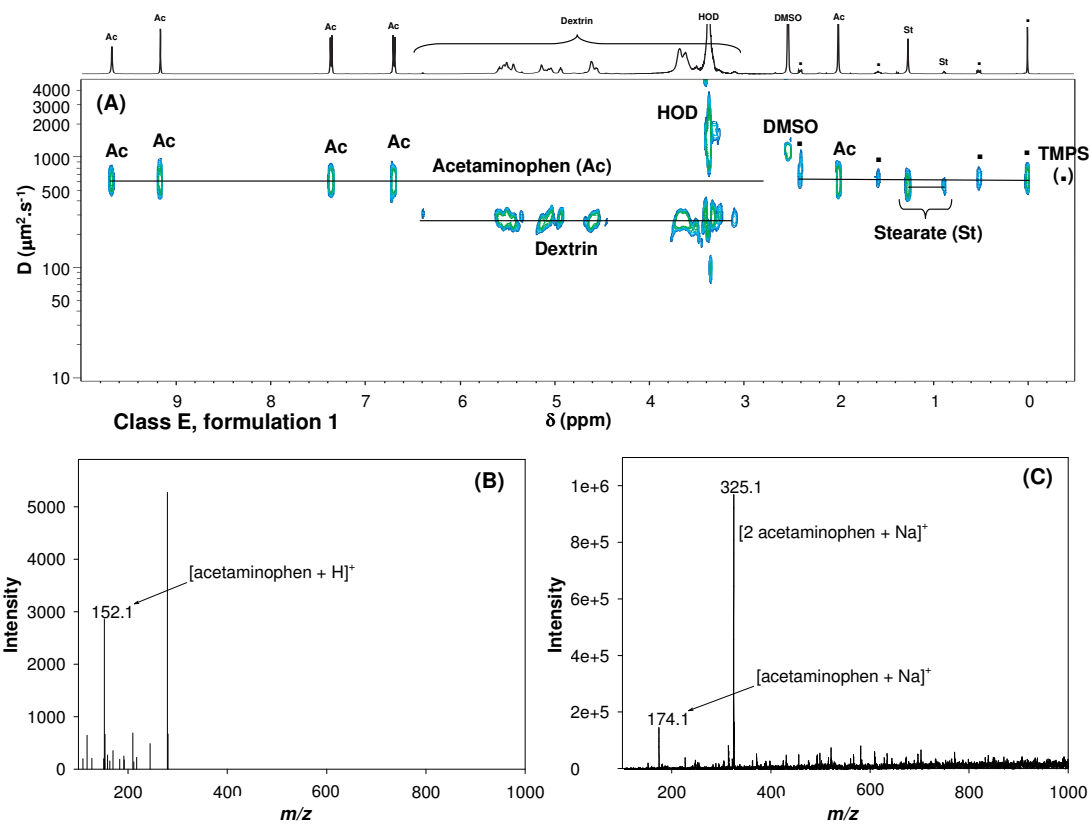


Figure S-2. Analysis of formulation **1** by: (A) 2D DOSY ^1H NMR in DMSO-d_6 with TMPS as internal reference standard, (B) DART MS in positive ion mode, and (C) DESI MS in positive ion mode.

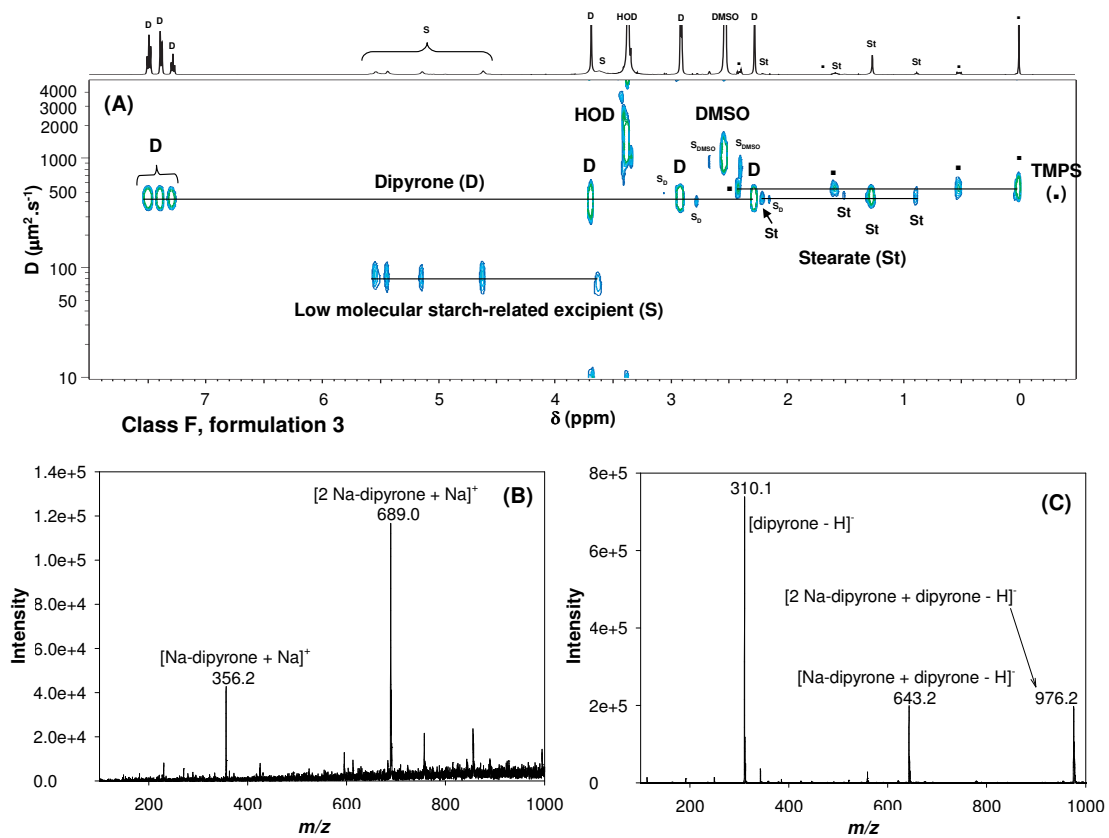


Figure S-3. Analysis of formulation 3 by: (A) 2D DOSY ^1H NMR in DMSO-d_6 with TMPS as internal reference standard (S_{DMSO} and S_D represent DMSO and dipyrone satellite peaks, respectively); and by DESI MS in (B) positive ion mode, and (C) negative ion mode.