Analysis and Isolation of Potential Artemisinin Precursors from Waste Streams of *Artemisia Annua* Extraction

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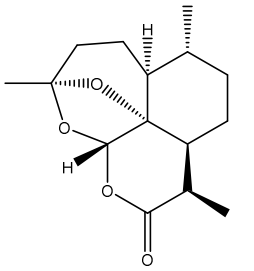
SUPPLEMENTAL INFORMATION

Includes ^{13}C NMR spectroscopic data for identified impurities
Includes HPLC chromatograms of partition samples
Includes HPLC assay results for partition samples

^{13}C NMR spectroscopic data
For component eluting at GC-MS RT=5.46 min

Scheme S1



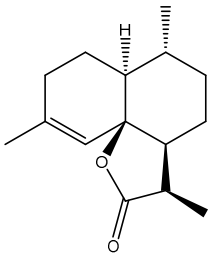
Deoxyartemisinin (**5**)

Table S1

assignment	Peak (ppm); this work	Peak (ppm); ref. 20 deoxyartemisinin
C-12	Nd	173.5
C-4	109.2	109.2
C-5	99.7	99.7
C-6	82.5	82.4
C-1	44.7	44.6
C-7	42.5	42.4
C-10	35.4	35.4
C-3	34.0	33.9
C-9	33.5	33.5
C-11	32.8	32.8
C-15	24.0	24.0
C-8	23.6	23.5
C-2	22.1	22.0
C-14	18.6	18.6
C-13	12.7	12.6

For component eluting at GC-MS RT=4.09 min

Scheme S2



Dihydro-*epi*-deoxy-arteannuiain B (**4**)

Table S2

assignment	Peak (ppm); this work	Peak (ppm); ref. 20 dihydro-*epi*-deoxy-arteannuin B	Peak (ppm); ref. 20 dihydro-deoxy-arteannuin B
C-12	179.3	179.4	180.6
C-4	142.1	142.2	142.3
C-5	121.8	121.8	120.5
C-6	83.1	83.2	86.7
C-1	46.6	46.6	46.6
C-7	42.8	42.8	49.8
C-11	39.6	39.7	39.0
C-9	32.5	32.5	35.3
C-3	30.9	30.8	26.0
C-10	29.7	29.7	30.7
C-15	23.8	23.5	24.1
C-8	23.4	23.4	22.0
C-2	21.0	21.0	20.1
C-14	19.6	19.6	19.9
C-13	9.4	9.5	13.1

HPLC Chromatograms

Overlay of chromatograms of the methanol extract (green) of the Guilin waste, the first heptane phase (red) and the final heptane phase (blue). Injection volumes were normalized to DHAA content to enable visual comparison of the enrichment obtained. Note that the response factor for AA is 2.5X that of DHAA so that its actual level is lower than it would appear. Similar chromatograms were observed for other waste materials

Figure S1. Overlay of Chromatograms from Guilin Extraction

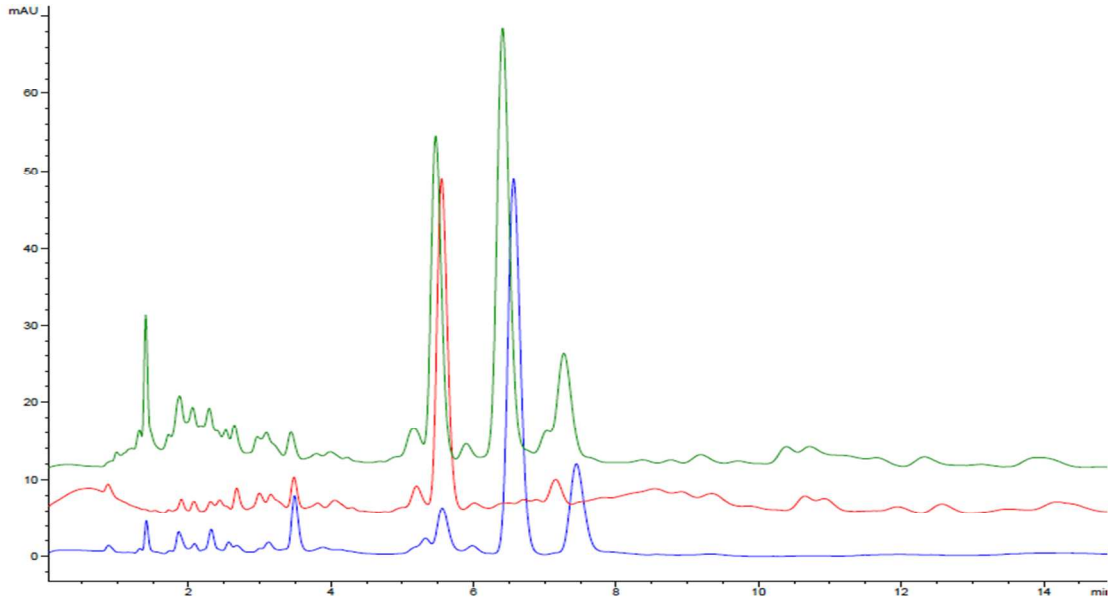
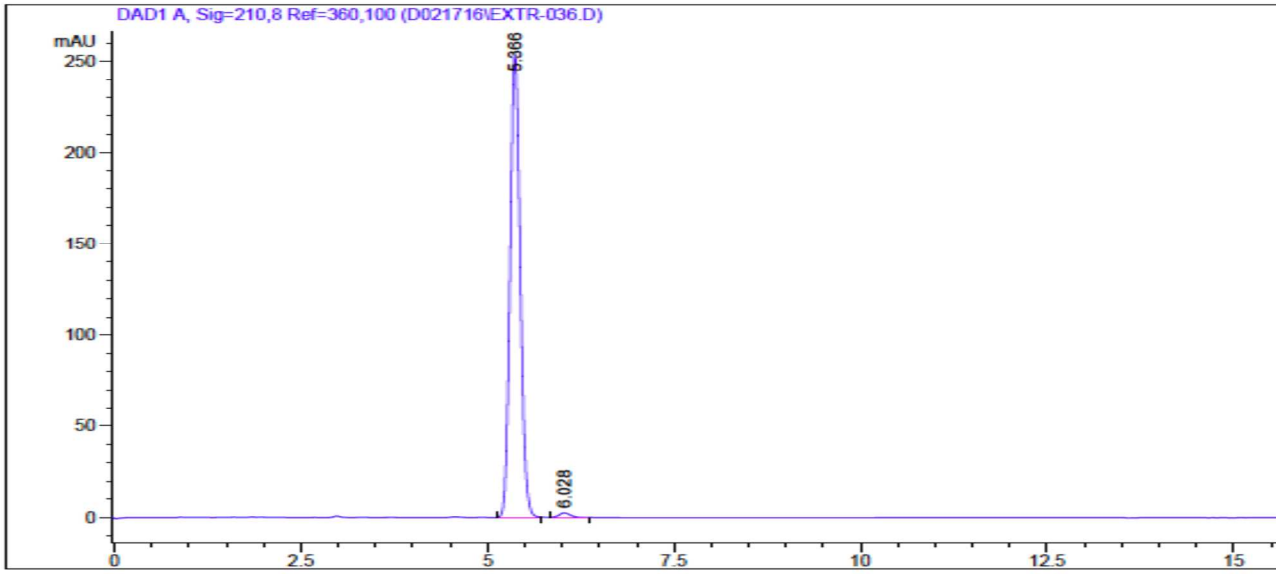


Figure S2. DHAA crystallized from cold acetonitrile



Results of HPLC Assay of Extraction Samples

Guilin Waste – Table S3

5.36 g waste containing 8.0% DHAA and 0.88% AA
Theoretical DHAA = 429 mg
Theoretical AA = 47 mg

Sample	DHAA	% theory	AA	% theory
Extract -1	430 mg	100%	49 mg	104%
Heptane-2	354 mg	83%	42 mg	89%
Aqueous-2	44 mg	10%	6 mg	13%
Heptane-3	49 mg	11%	9 mg	19%
Aqueous-3	7 mg	2%	3 mg	8%
Final oil	448 mg	104%	49 mg	104%

Botanical Extracts – Table S4

5.12 g waste containing 5.0% DHAA and 0.9% AA
Theoretical DHAA = 256 mg
Theoretical AA = 46 mg

Sample	DHAA	% theory	AA	% theory
Extract -1	248 mg	98%	46 mg	100%
Heptane-2	208 mg	83%	42 mg	91%
Aqueous-2	17 mg	7%	4 mg	9%
Heptane-3	23 mg	9%	5 mg	11%
Aqueous-3	0 mg	0%	0 mg	0%
Final oil	243 mg	96%	50 mg	109%

Bionexx Extracts – Table S5

7.57g waste containing 6.4% DHAA and 1.4% AA (not quantified)
Theoretical DHAA = 484 mg

Sample	DHAA	% theory
Extract -1	381 mg	79%
Aqueous-1	345 mg	72%
Final oil	376 mg	78%

Sample explanation
Extract -1 = methanol extract after cooling and filtration
Aqueous-1= aqueous layer after first heptane partition and pH adjustment
Heptane-2 = heptane layer after pH adjustment showing partition of acids from aqueous
Aqueous-2 = aqueous layer after pH adjustment and partition of acids into heptane
Heptane-3 = second heptane extraction of Aqueous-2

Aqueous-3 = aqueous layer after second heptane extraction of Aqueous-2
Final Oil= combined heptane fractions of partitioned acids