

Comparative oxidation state specific analysis of arsenic by high-performance liquid chromatography-inductively coupled plasma-mass spectrometry and hydride generation-cryotrapping-atomic absorption spectrometry

Jenna Currier,^a R. Jesse Saunders,^b Lan Ding,^b Wanda Bodnar,^c Peter Cable,^c Tomáš Matoušek,^d Jack Creed,^c and Miroslav Stýblo^{a,b,§}

SUPPLEMENTARY DATA

Table S1: The slopes of calibration curves generated by HG-CT-AAS (10^{-3} s/ng) and HPLC-ICP-MS (cps*s/pg) for As standards

HG-CT-AAS ^a						
Solvents	iAs ^{III+V}		MAs ^{III+V}		DMAs ^{III+V}	
DIW	814		808		788	
HPLC-ICP-MS ^b						
	iAs ^{III}	iAs ^V	MAs ^{III}	MAs ^V	DMAs ^{III}	DMAs ^V
DIW	1503	1461	1152	1543	632	1425
Reaction Mixture	1550	707	1145	1643	811	1486

^a Standards were prepared in DIW and were reduced with 2% cysteine prior to HG-CT-AAS analysis.

^b Standards were prepared in DIW or in the *in vitro* reaction mixture containing Tris-HCl buffer, SAM and TCEP, but not AS3MT.

Table S2: Limits of detection (LOD) for the analysis of As species by HPLC-ICP-MS and HG-CT-AAS

Method	LOD (pg mL ⁻¹)								
	iAs ^{III}	iAs ^V	iAs ^{III+V}	MAs ^{III}	MAs ^V	MAs ^{III+V}	DMAs ^{III}	DMAs ^V	DMAs ^{III+V}
HPLC-ICP-MS ^a	32	295		31	57		88	98	
HG-CT-AAS ^b	36	54	40	32	57	46	24	44	38

^a LODs were calculated as $(3*SD)/(slope*0.02)$ for 10 injections of DIW (20 μ l each).

^b LODs were calculated as $(3*SD)/(slope*0.5)$ for 10 injections of DIW or 2% cysteine in DIW (0.5 ml each).

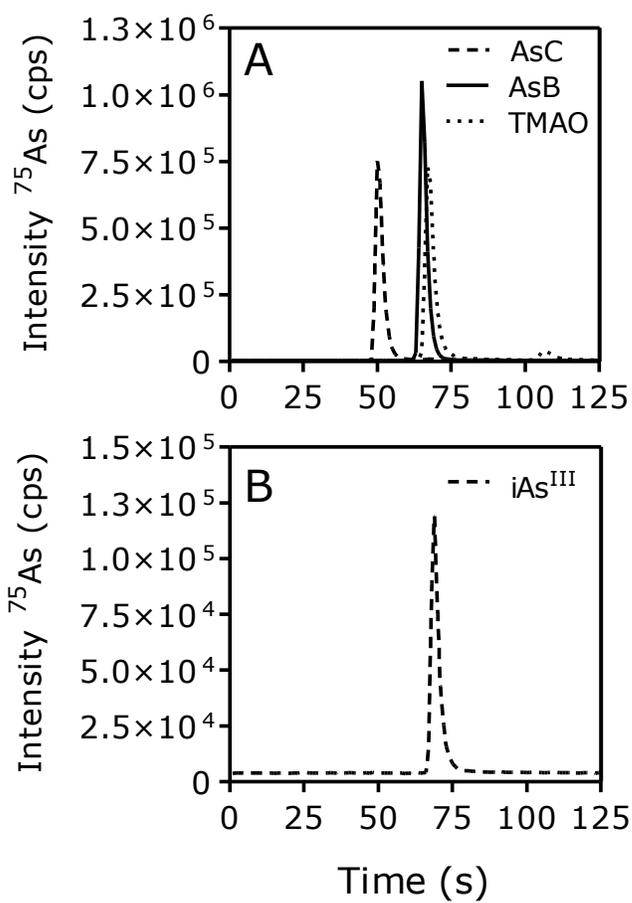


Figure S1: The HPLC-ICP-MS profiles of As standards in DIW, including AsC, AsB, TMAO (A, 2,000 pg each) and $i\text{As}^{\text{III}}$ (B, 280 pg). Detailed operating conditions are described in Table 1.

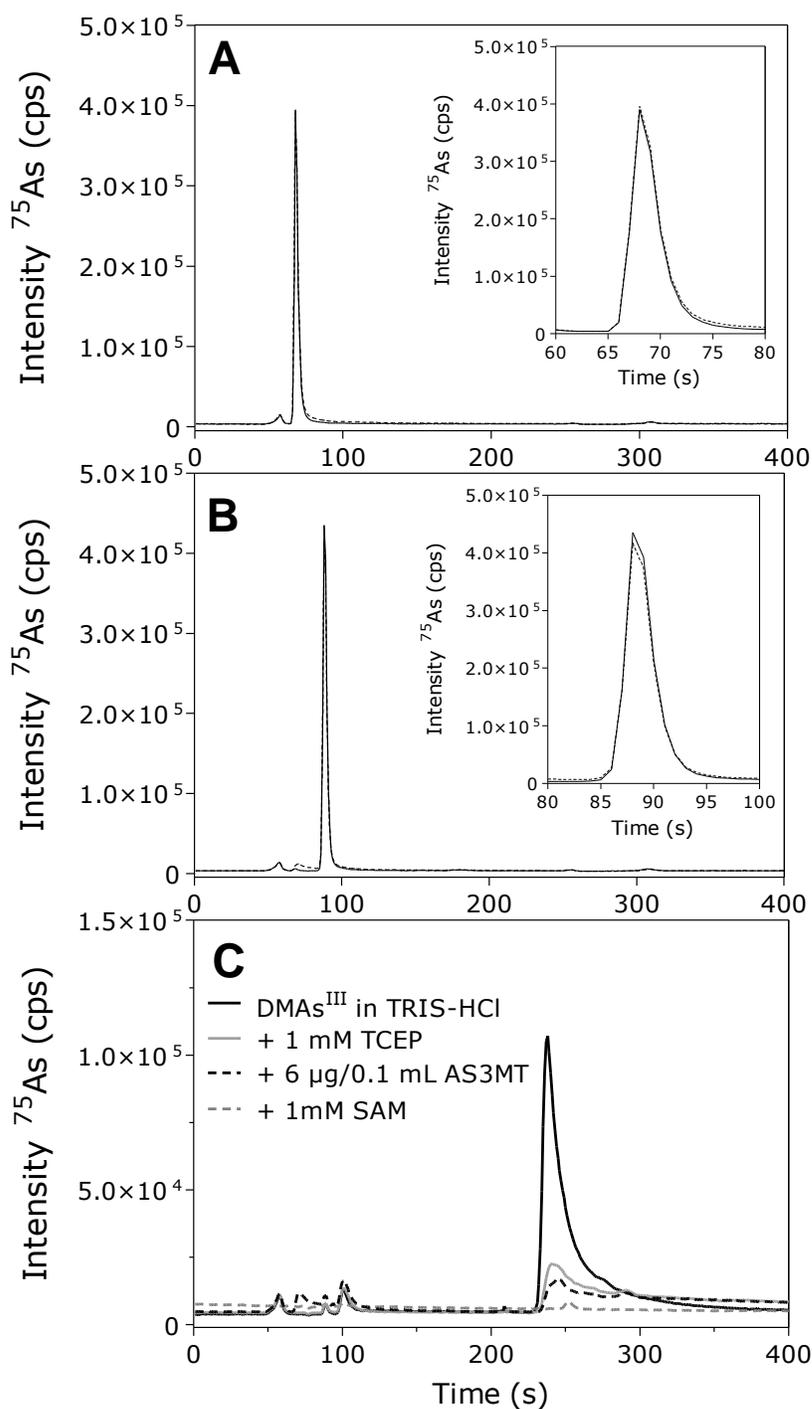


Figure S2: Comparison of the HPLC-ICP-MS profiles for As standards prepared in solutions containing the components of the *in vitro* methylation mixture: $0.5 \mu\text{M iAs}^{\text{III}}$ (A) and $0.5 \mu\text{M MAs}^{\text{III}}$ (B) in the 100 mM TRIS-HCl buffer (pH 7.4) in absence (—) and presence (---) of AS3MT (60 $\mu\text{g}/\text{mL}$). $0.5 \mu\text{M DMAs}^{\text{III}}$ (C) in a mixture with TRIS-HCl buffer (—), 1 mM TCEP (—), AS3MT (60 $\mu\text{g}/\text{mL}$; ---) or 1 mM SAM (---).