

Supplementary Information

Gas Chromatography-Mass Spectrometric Identification of Cyanide Using a Nucleophilic Substitution Based Derivatization with *s*-Phenyl benzenethiosulfonate

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Supplementary Information:

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1. General details

Reagents were obtained from commercial supplier, and used without further purification. Solvents used were purified by standard methods prior to use. The GC-MS analyses were performed on Agilent 6890 GC, with model 5973 mass selective detector. NMR spectra were recorded on a Bruker AVANCE II 400 MHz. TLC analysis was performed on silica gel 60 F₂₅₄ plates and column chromatography was conducted over silica gel (mesh 100-200).

2. Figures

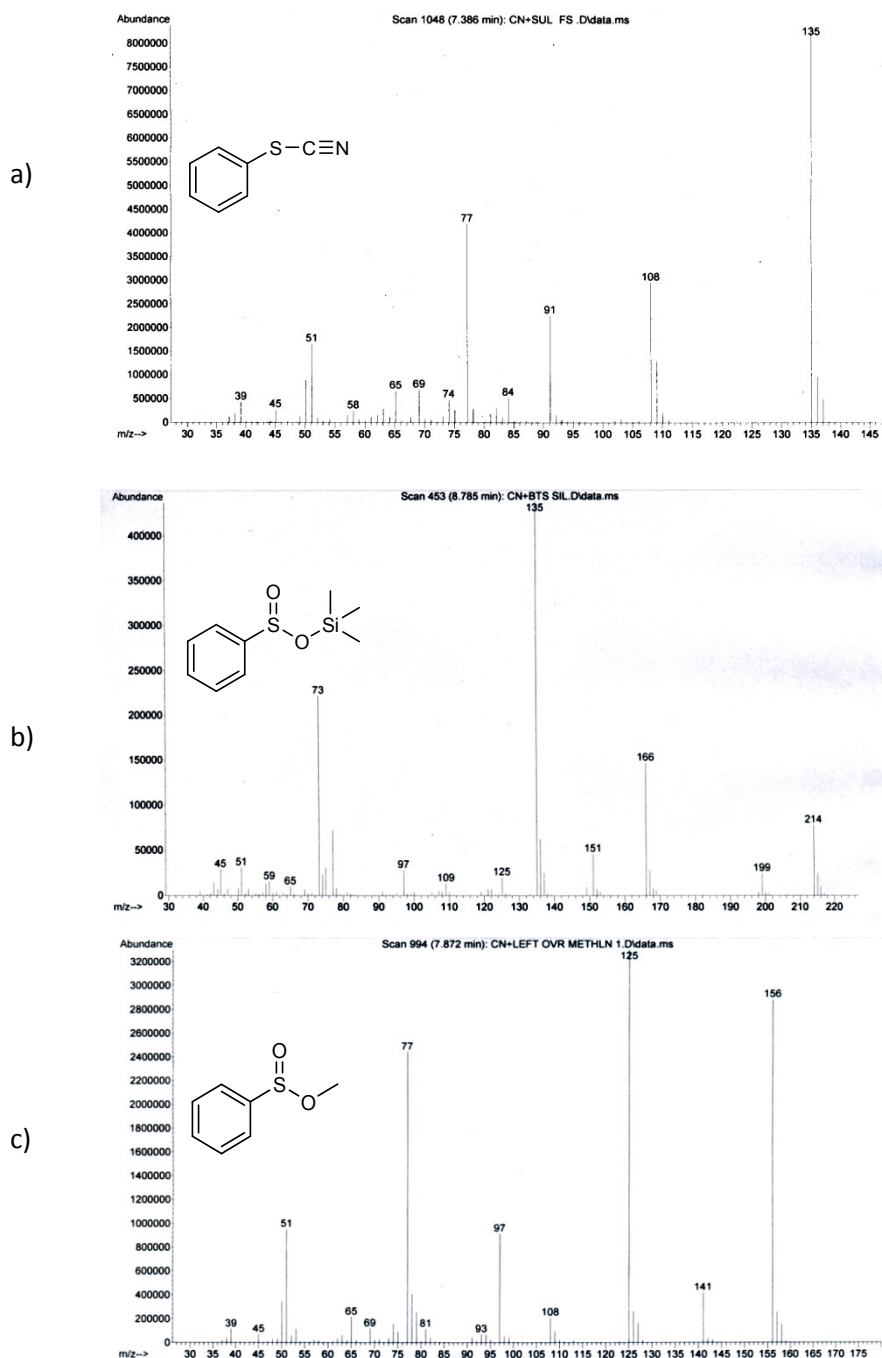


Figure-S1: a) Derivatized product phenyl thiocyanate in organic extraction b) Trimethyl silyl and c) methyl derivatives of reaction product Phenyl sulfinic acid in aqueous layer

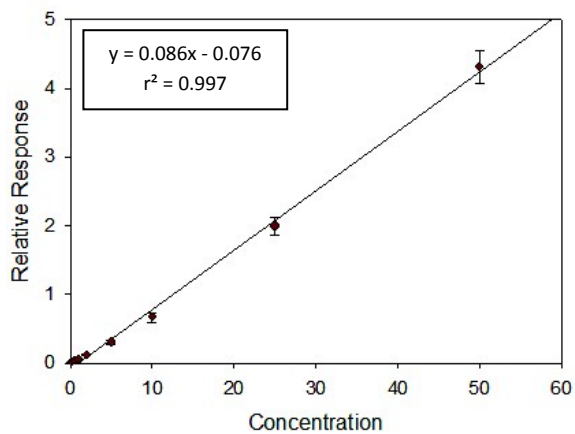


Figure-S2: Concentration Vs Relative response of derivatized product

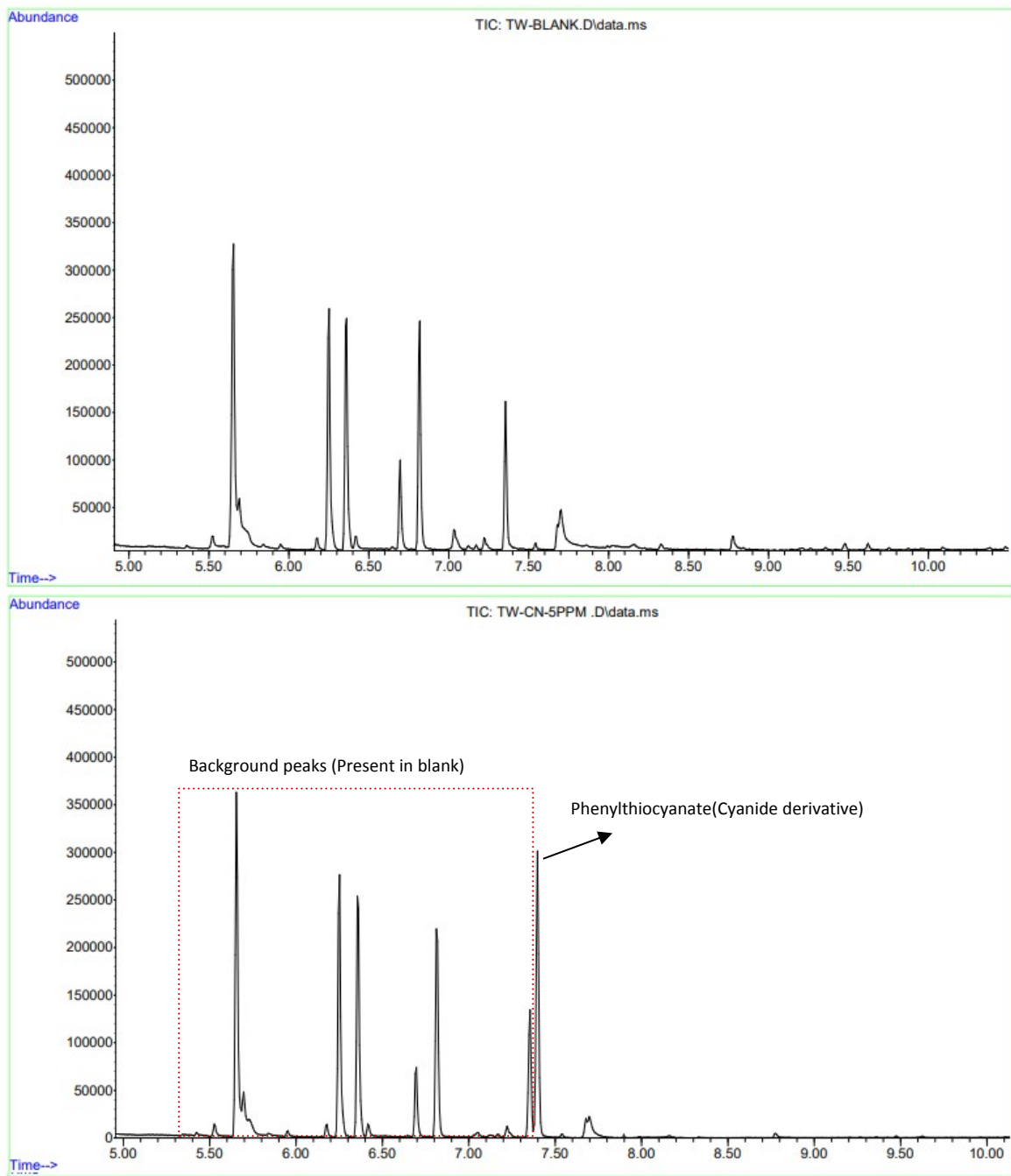


Figure-S3: Top: Total ion chromatogram of ethyl acetate extraction of blank sample of tap water after treating with derivatization reagent.

Bottom: Total ion chromatogram of ethyl acetate extraction of 5 ppm cyanide sample of tap water after treating with derivatization reagent. (derivatized product phenyl thiocyanate at 7.39 min)

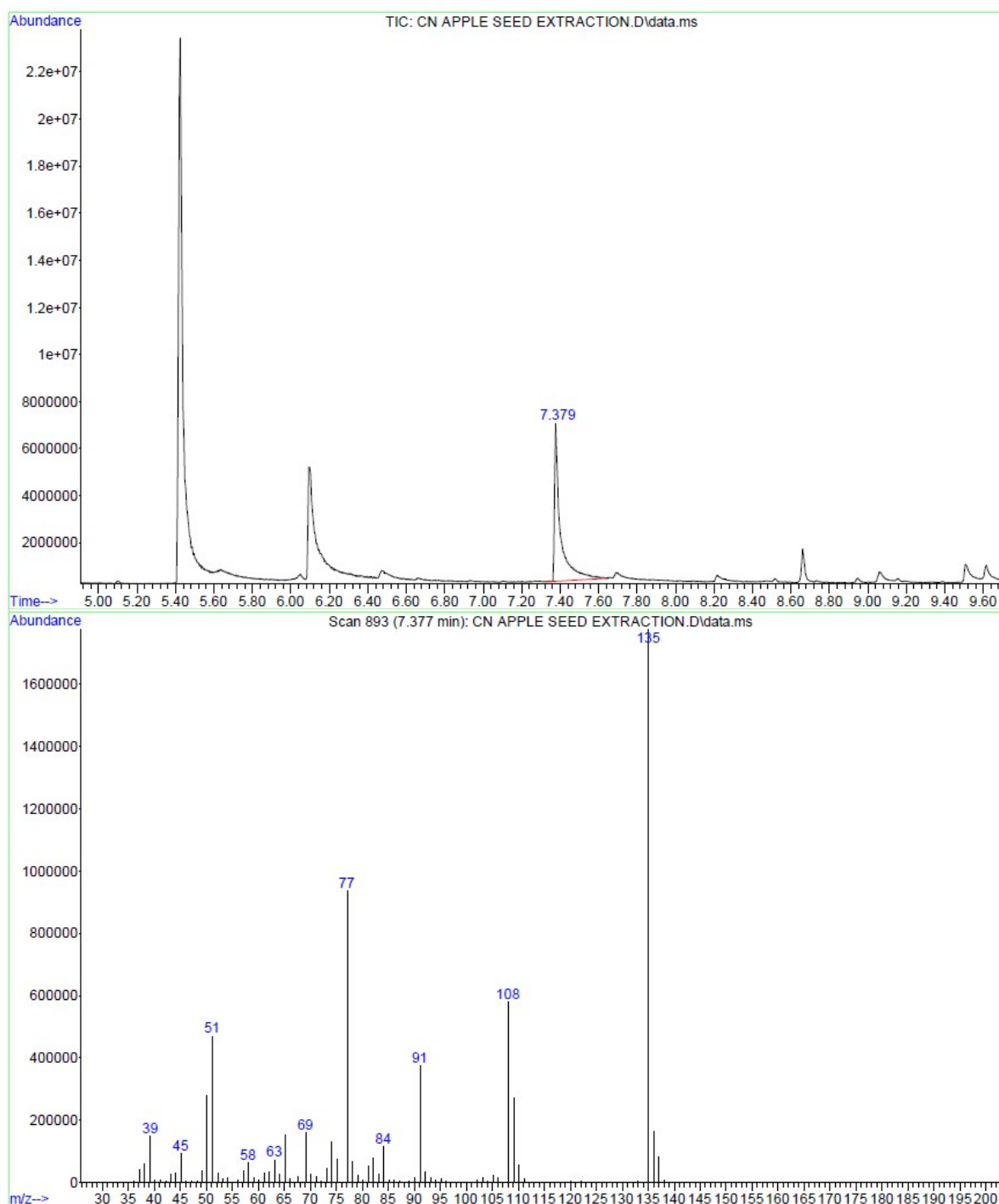


Figure-S4: Top: Total ion chromatogram of ethyl acetate extraction of sample of apple seed extraction after treating with derivatization reagent.

Bottom: Mass spectrum of cyanide derivatized product phenyl thiocyanate at 7.379 min)

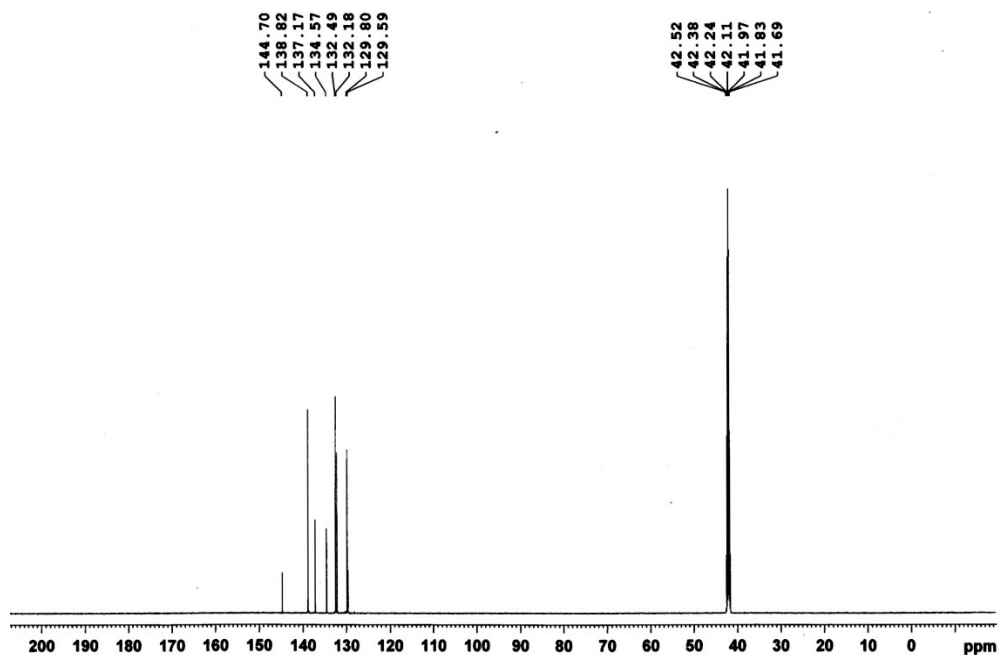


Figure-S6: ^{13}C NMR spectra of derivatization reagent *s*-phenyl benzenethiosulfonate

S.No.	Derivatization reagent	Analytical Technique	Limit of Detection (LOD)	Limit of Quantitation (LOQ)	Derivatization reaction conditions	Pre-concentration
1.	Pentafluoro benzylbromide (polymer bound phosphonium salt as catalyst) (Ref-24)	GC-MS	0.5 $\mu\text{g}/\text{mL}$ (Full Scan)	0.2 $\mu\text{g}/\text{mL}$ (SIM)	38/30min	---
2.	Two step derivatization 1. Benzaldehyde 2. heptafluorobutryl chloride Ref-26	GC-MS	0.01 $\mu\text{g}/\text{mL}$ (SIM)	0.02 $\mu\text{g}/\text{mL}$ (SIM)	Rt/20min	Evaporated to nearly drying
3.	1. cysteine, 2. Hypochloric acid (Ref-27)	LC-MS	0.07 $\mu\text{g}/\text{L}$	0.2 $\mu\text{g}/\text{L}$	Rt/ 10 min	---
4.	2-(dimethylamino)ethanethiol (Ref-30)	GC-MS/MS	0.02 $\mu\text{g}/\text{mL}$	0.07 $\mu\text{g}/\text{mL}$	60/ 20 min	10ml water to 100 EtOAc (100 times)
5.	<i>s</i> -Phenyl benzenethiosulfonate (present study)	GC-MS	0.075 $\mu\text{g}/\text{mL}$ (SIM)	0.25 $\mu\text{g}/\text{mL}$ (SIM)	Rt/ 5min	No pre-concentration

Table-S1: Comparison of reported methods for detection of cyanide and preset study