

Figure S1. EMANA EI-MS (SIM) proposed fragmentation mechanism.

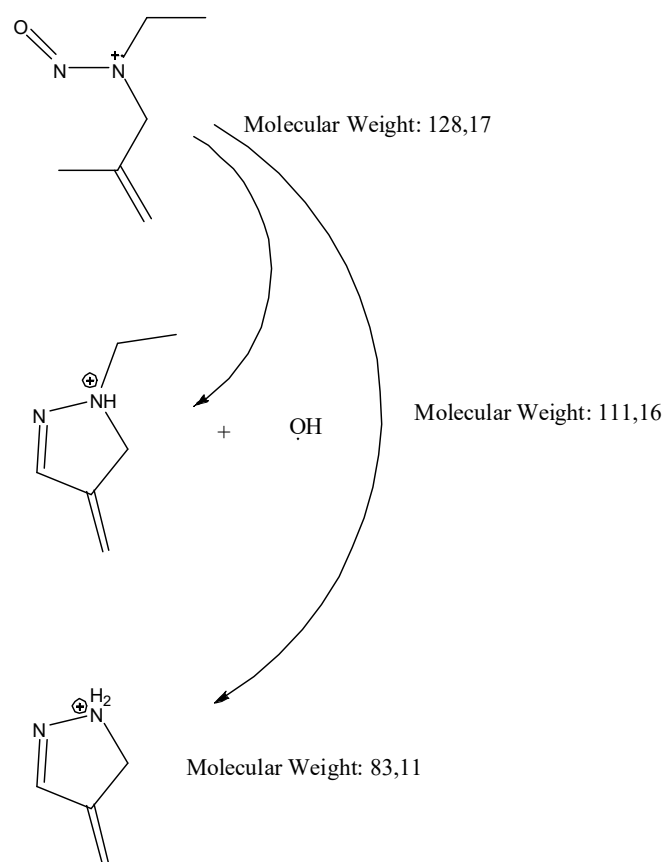


Figure S2. EMANA EI-MS/MS proposed fragmentation mechanism.

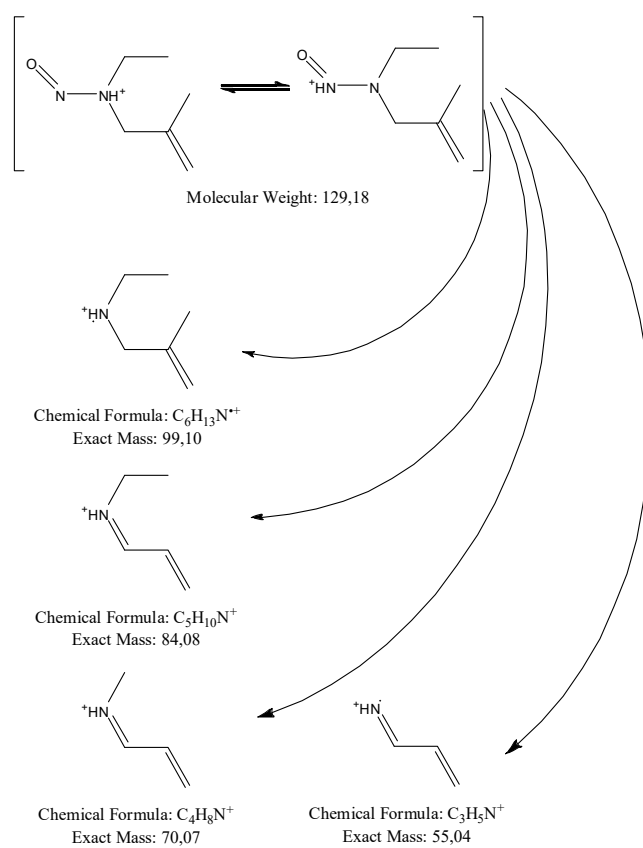


Figure S3. EMANA PCI-MS/MS proposed fragmentation mechanism.

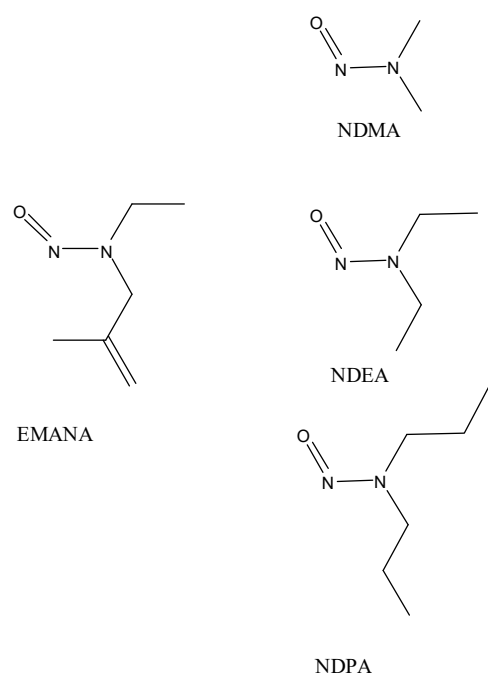


Figure S4. Structural resemblance of EMANA, NDMA and NDEA (IARC 2A classification-Probably carcinogenic to humans) and NDPA (IARC 2B classification-Possibly carcinogenic to humans).

Print Date: 23:45:31 Target Compound Report for #1 from 10-29-51 4387.xms

Sample ID:		Operator:	
Instrument ID:	Varian GC/MS #1	Last Calibration:	
Measurement Type:	Area	Calibration Type:	External Standard
Acquisition Date:	10:29	Data File:	...23 10-29-51 4387.xms
Calculation Date:	12:17	Method:	...ci ch4 v.0 final.mth
Sample Type:	Analysis		
Inj. Sample Notes:	None		

Compound Information

Peak Name:	EMANA	Compound Number:	1	CAS Number:	None	Identified
Result Index:	1					

Identification

Parameter	Specification	Actual	Status
Search Type	Spectrum		
Retention Time	5.996 +/- 0.200	5.978 min.	Pass
Match Result	N-R >= 700	955	Pass
Qual. Ion Ratio (1 ion)	m/z 55:1:86.0%	68.8%- 103.2% 85.3%	Pass

Integration and Quantitation

Parameter	Specification	Actual	Status
Quan Ions	84.0		
Calibration Equation	Linear, Ignore, None	y = +2.0459e+5x -1.5919e+4	
Area	>=500	15999	Pass
Height		11869	
Amount	>= 0.000 PPM	0.156 PPM	Pass

Match Types: N-R : Normal-Reverse

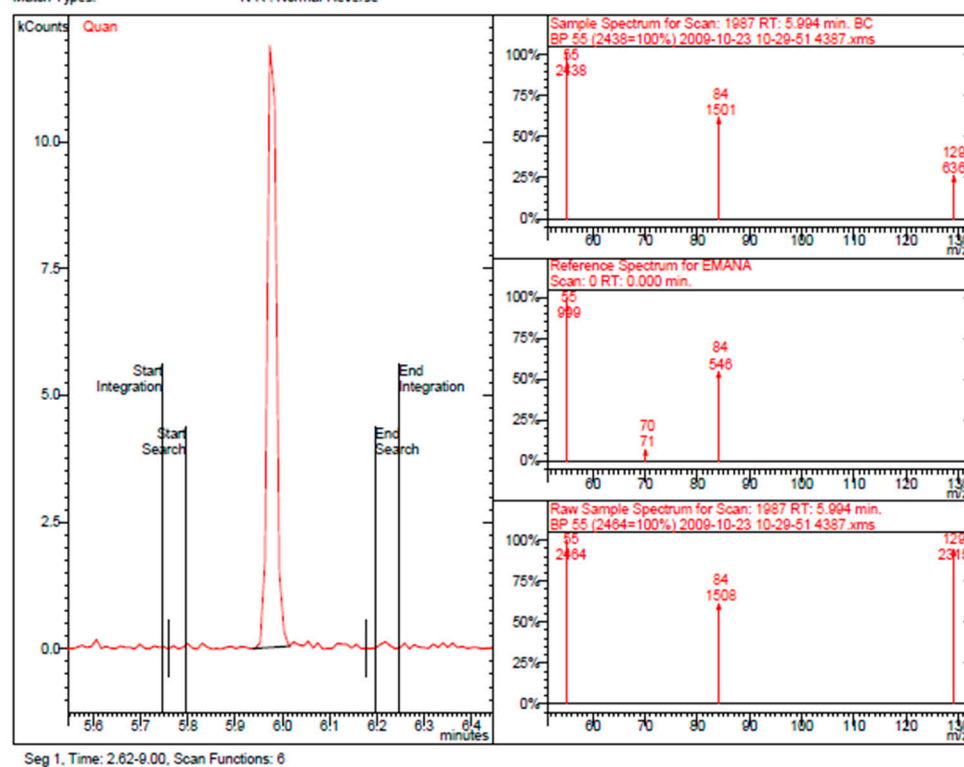


Figure S5. Target Compound Report from real sample with high interference.

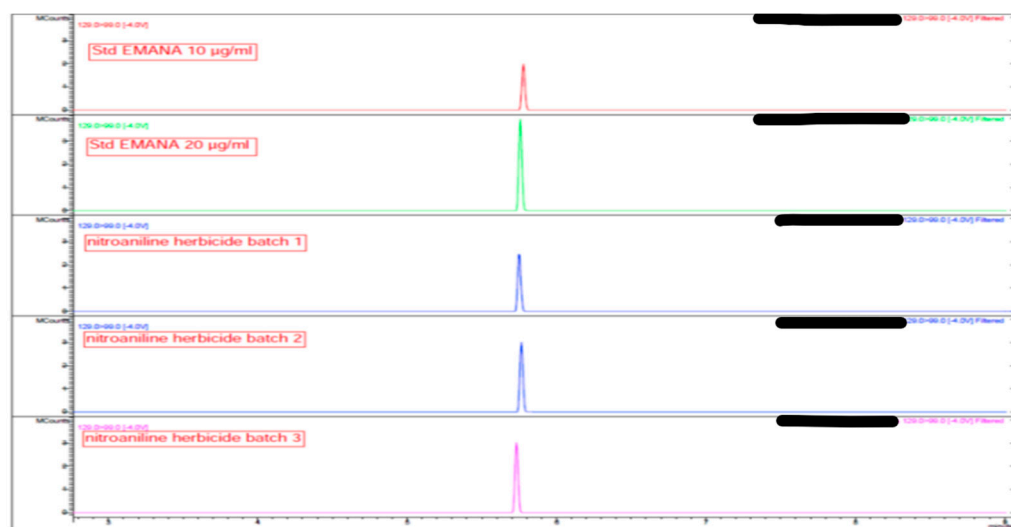


Figure S6. GC-PCI-MS/MS chromatograms of solutions of standard EMANA and non-compliant samples.