

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121321\
 Data File : VN070056.D
 Acq On : 14 Dec 2021 2:41
 Operator : JC/MD
 Sample : M5007-13
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TB-2021.12.08

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M

Title : SW846 8260

Signal : TIC: VN070056.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.233	81	91	106	rBV5	263926	459799	5.75%	1.103%
2	8.024	2224	2250	2261	rBV	880352	2143878	26.80%	5.144%
3	8.086	2261	2273	2308	rVB	1439089	3295480	41.20%	7.907%
4	8.440	2381	2405	2433	rBV2	994203	2346838	29.34%	5.631%
5	8.968	2583	2602	2635	rBV	2483236	5153358	64.43%	12.365%
6	10.440	3131	3151	3191	rBV	4103647	7650618	95.65%	18.357%
7	11.744	3618	3637	3679	rBV	4450565	7998782	100.00%	19.192%
8	12.733	3986	4006	4037	rBV	3373278	6056100	75.71%	14.531%
9	13.675	4339	4357	4387	rBV	3729051	6572299	82.17%	15.770%

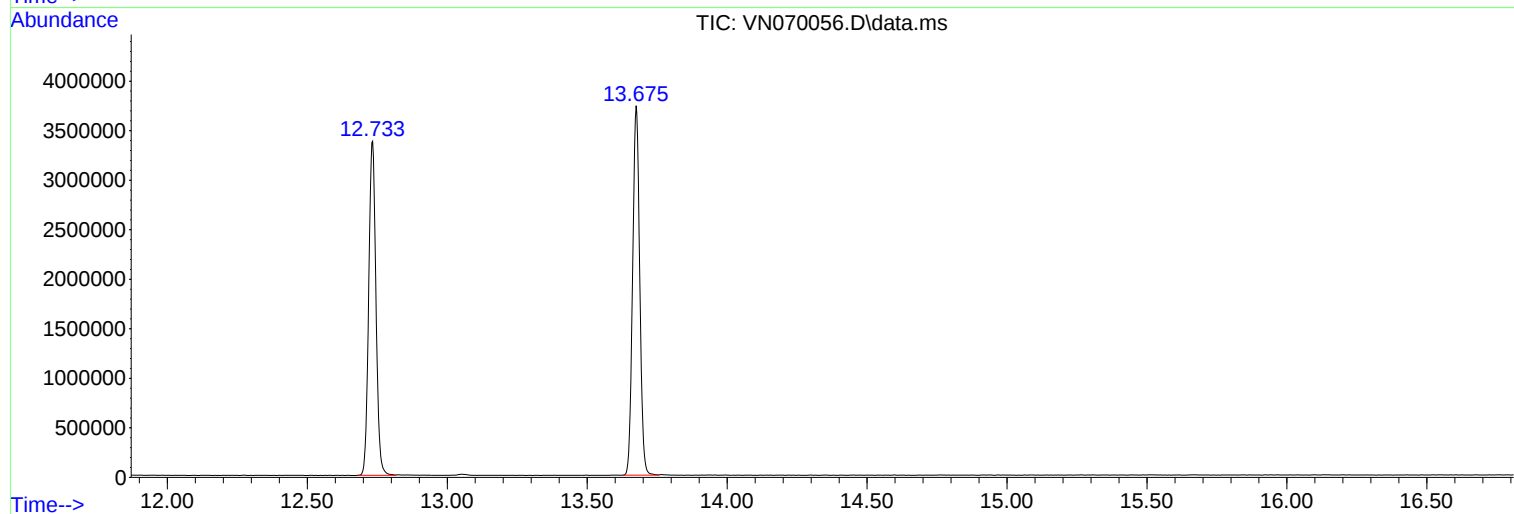
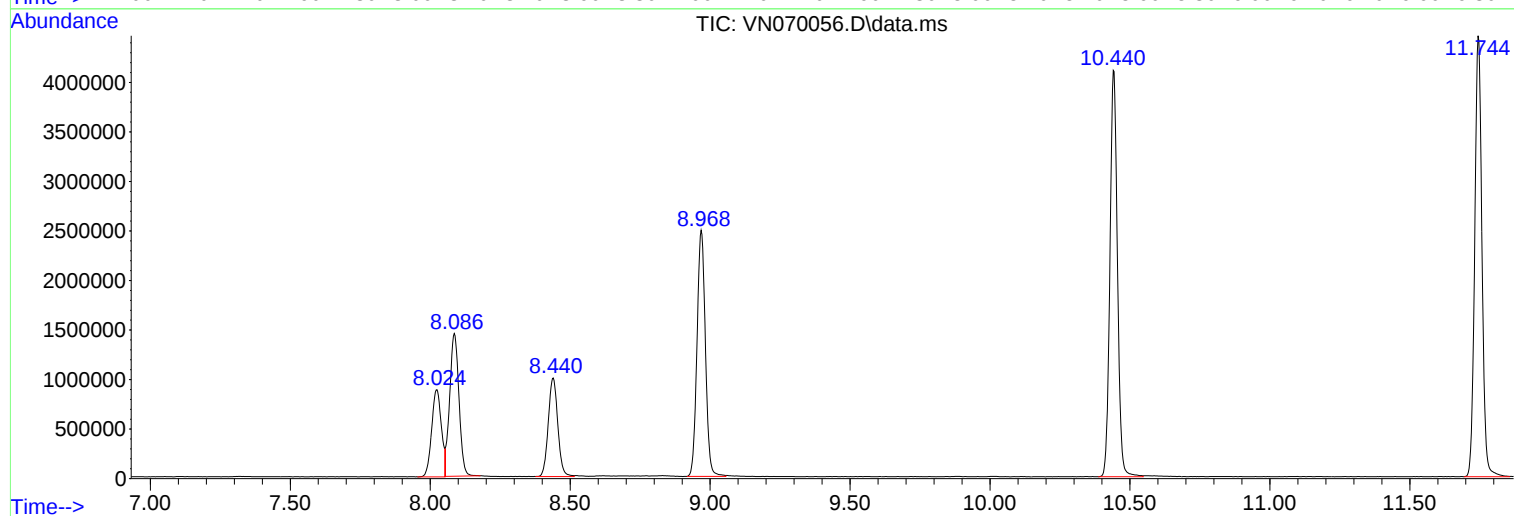
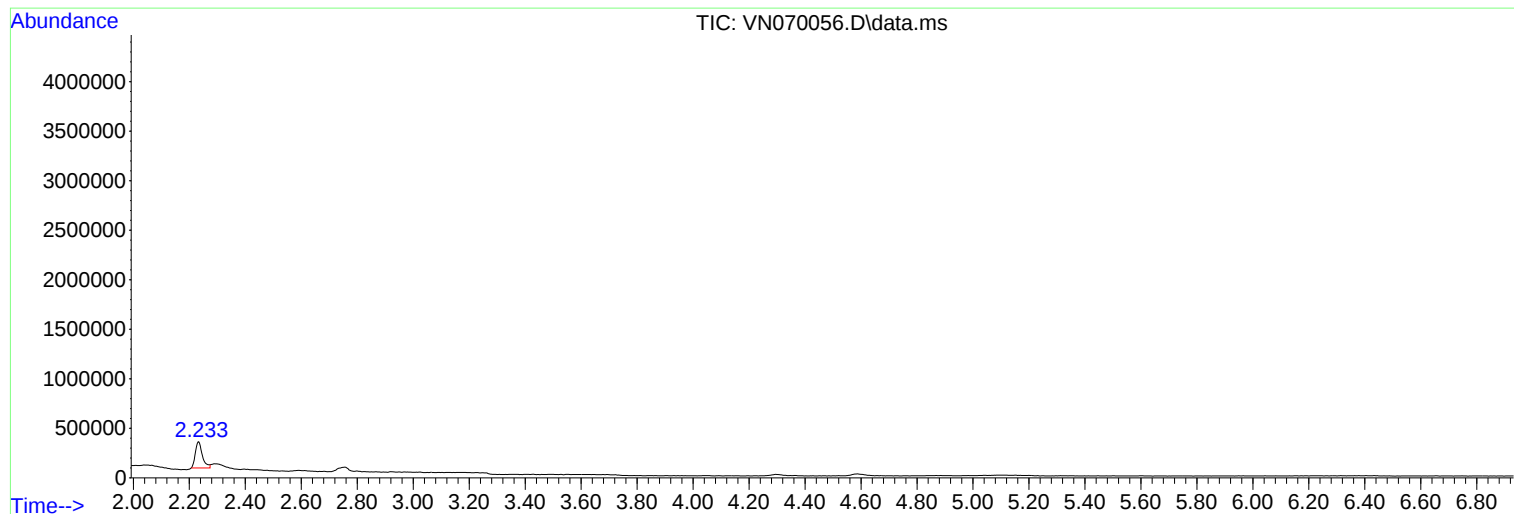
Sum of corrected areas: 41677152

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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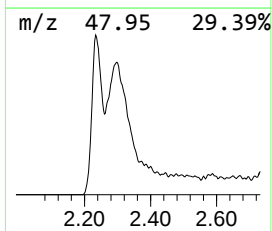
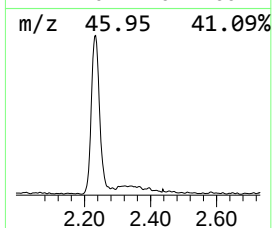
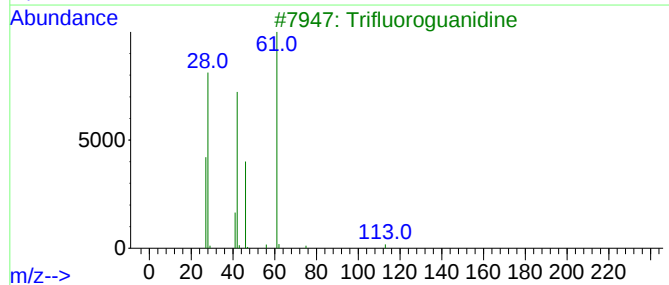
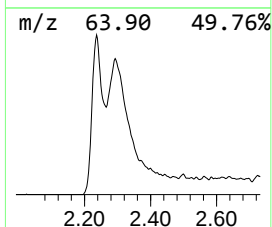
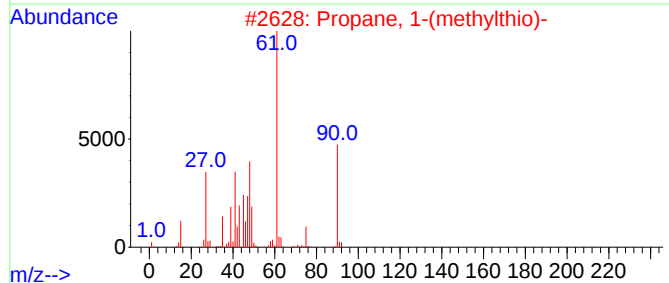
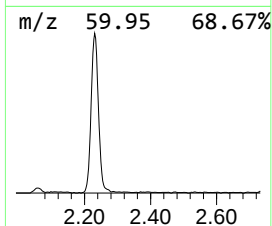
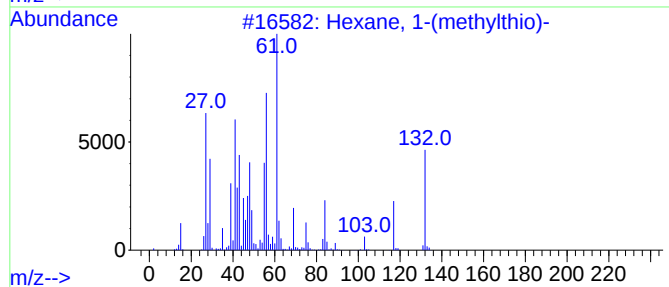
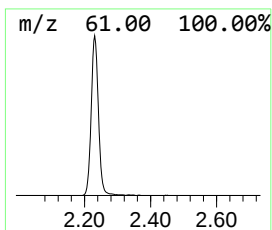
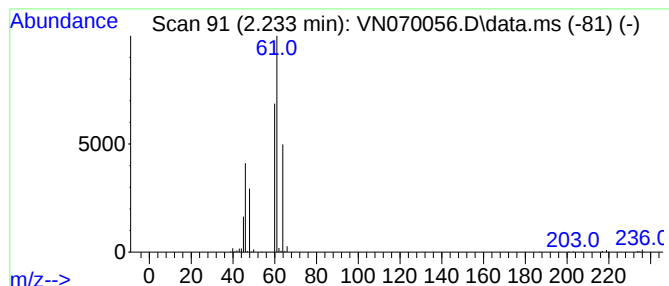
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.233 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.233	6.98 ug/l	459799	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 1-(methylthio)-	132	C7H16S	020291-60-5	9
2			Propane, 1-(methylthio)-	90	C4H10S	003877-15-4	9
3			Trifluoroguanidine	113	CH2F3N3	037950-72-4	9
4			Methanamine, N-methoxy-	61	C2H7NO	001117-97-1	7
5			S-Methyl-L-cysteine, N-(ethoxyca...	207	C7H13NO4S	1000453-28-8	5



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.233	2.233	7.0	ug/l	459799	1	8.086	3295480	50.0