

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061722\
 Data File : VU049272.D
 Acq On : 18 Jun 2022 02:30
 Operator : SY/MD
 Sample : N3256-08
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AH2

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

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_U\Method\SFAMUTR061422WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU049272.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.362	3	7	14	rVB2	12073	11099	1.12%	0.187%
2	1.510	41	53	64	rBV3	27719	92553	9.33%	1.562%
3	1.597	74	80	88	rBV	62162	65998	6.66%	1.114%
4	1.912	171	178	192	rVB	43782	56331	5.68%	0.951%
5	2.568	370	382	393	rBV	77593	126752	12.78%	2.140%
6	2.649	399	407	429	rVB	5057	12464	1.26%	0.210%
7	3.359	616	628	641	rBV8	5195	11180	1.13%	0.189%
8	4.665	1012	1034	1055	rBV2	156153	534360	53.88%	9.020%
9	5.066	1143	1159	1184	rVB2	81283	204583	20.63%	3.453%
10	5.726	1341	1364	1394	rBV2	153585	404280	40.77%	6.824%
11	6.250	1512	1527	1549	rBV	149706	284004	28.64%	4.794%
12	6.542	1600	1618	1647	rVB	162130	312387	31.50%	5.273%
13	6.690	1647	1664	1680	rBV	102911	199148	20.08%	3.362%
14	6.783	1682	1693	1704	rVB8	4685	10204	1.03%	0.172%
15	7.108	1780	1794	1801	rBV	21218	38859	3.92%	0.656%
16	7.163	1801	1811	1831	rVB3	49281	102460	10.33%	1.729%
17	7.565	1924	1936	1958	rBV	49309	88670	8.94%	1.497%
18	7.716	1970	1983	1997	rBV3	37486	69445	7.00%	1.172%
19	7.899	2027	2040	2053	rBV	177859	304828	30.74%	5.145%
20	7.970	2053	2062	2080	rVB	29735	52030	5.25%	0.878%
21	8.179	2117	2127	2140	rBV	30228	51031	5.15%	0.861%
22	8.552	2230	2243	2257	rBV	592607	991675	100.00%	16.739%
23	8.635	2257	2269	2304	rVB	327792	596801	60.18%	10.074%
24	8.809	2309	2323	2341	rVB2	33413	61075	6.16%	1.031%
25	9.288	2462	2472	2484	rVB	7197	11852	1.20%	0.200%
26	9.417	2500	2512	2534	rBV	208062	341415	34.43%	5.763%
27	9.568	2551	2559	2570	rBV	6916	10662	1.08%	0.180%
28	9.687	2582	2596	2612	rVB4	17687	35324	3.56%	0.596%
29	10.291	2773	2784	2797	rVB2	21585	35051	3.53%	0.592%
30	10.758	2917	2929	2944	rBV	86953	140167	14.13%	2.366%
31	11.812	3244	3257	3274	rBV	214279	340114	34.30%	5.741%
32	12.063	3325	3335	3353	rBV3	13317	24748	2.50%	0.418%
33	12.192	3363	3375	3394	rVB	183403	302749	30.53%	5.110%

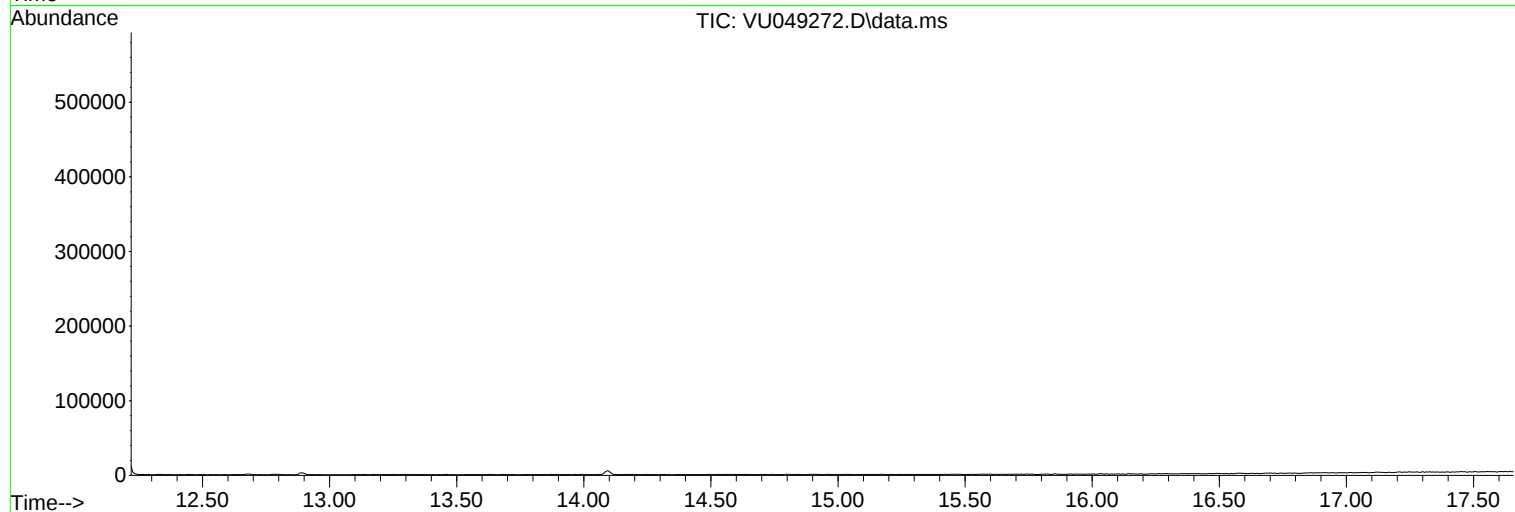
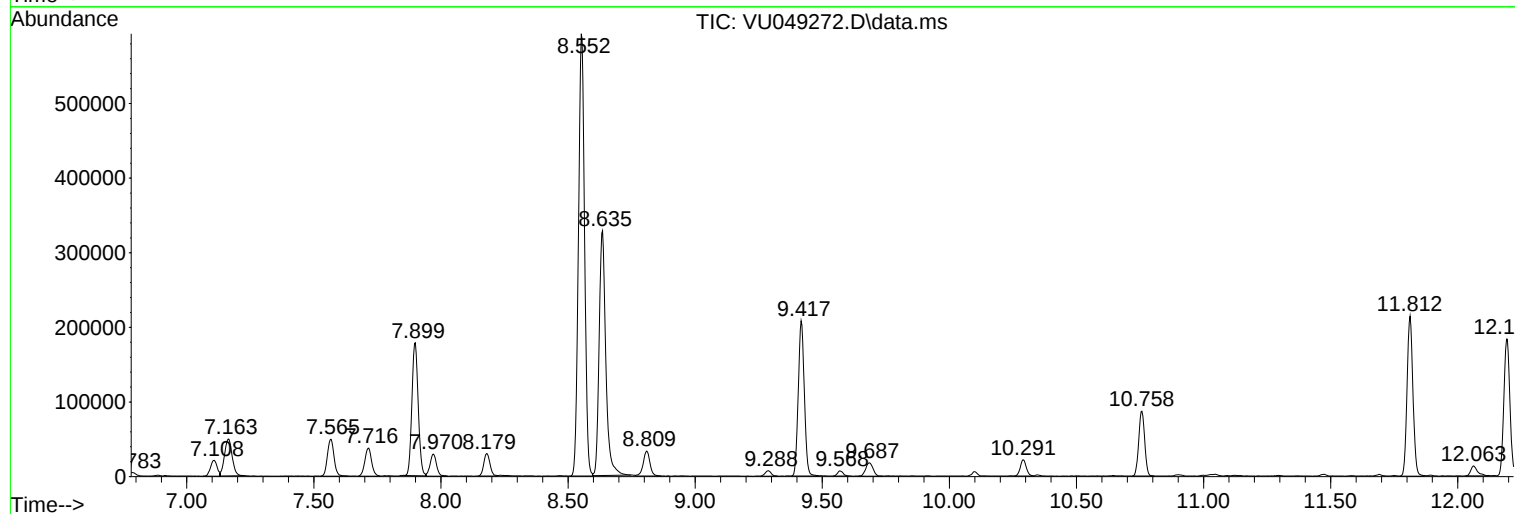
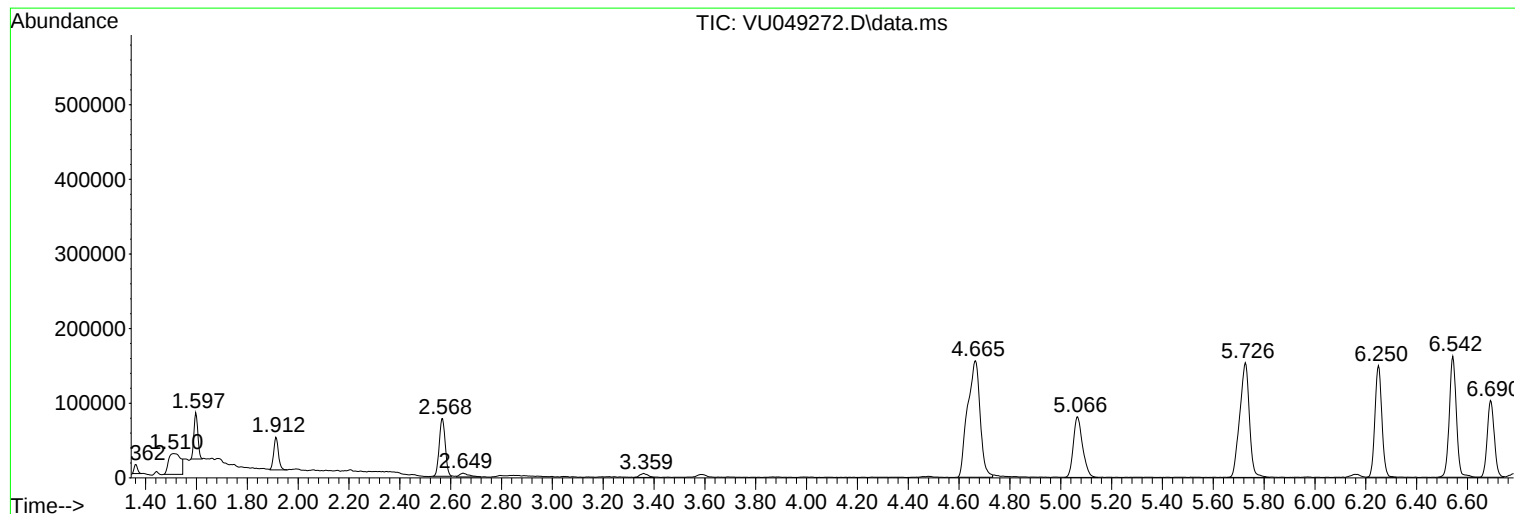
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Instrument :
MSVOA_U
ClientSampleId :
C0AH2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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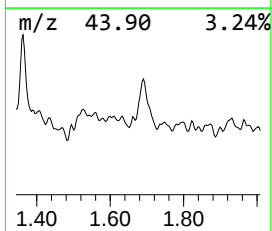
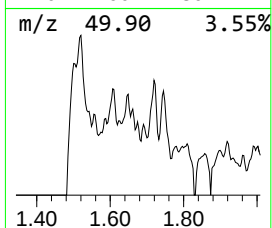
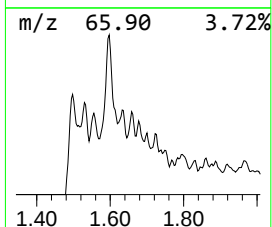
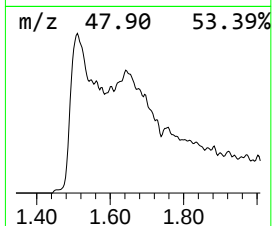
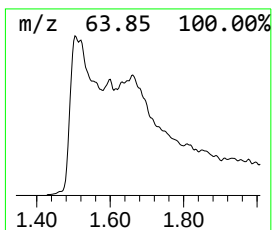
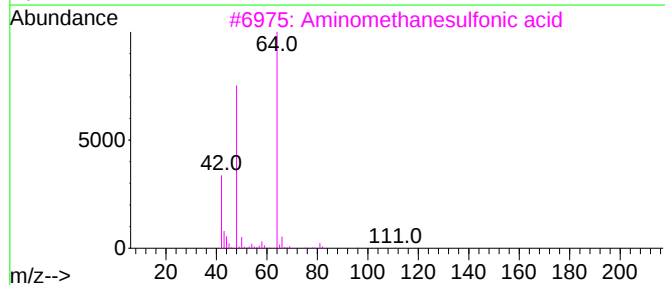
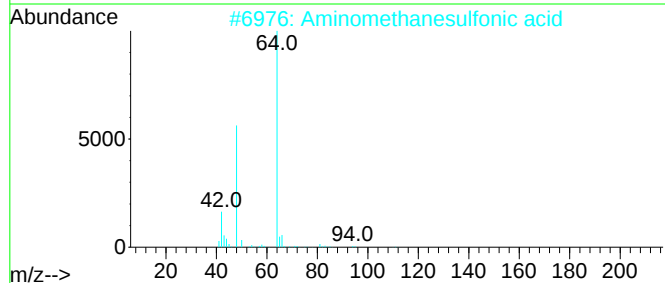
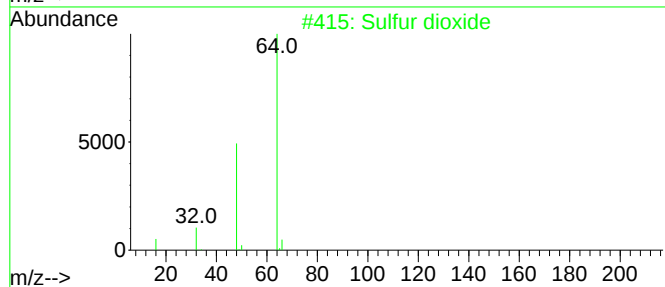
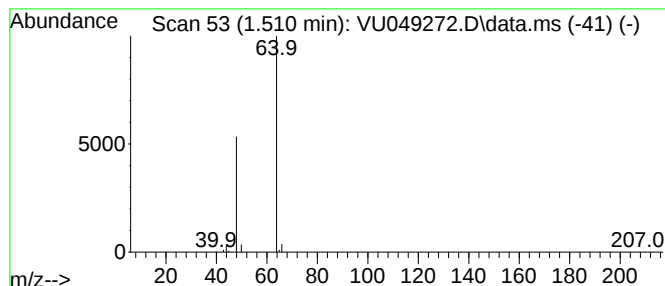
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.510	1.63 ug/L	92553	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AH2

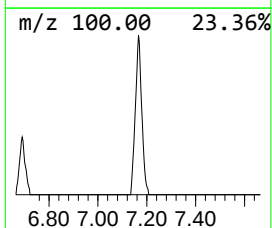
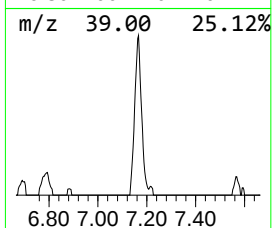
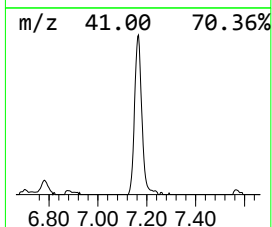
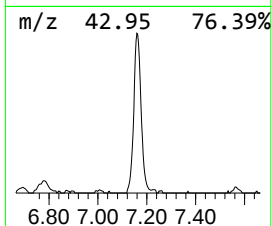
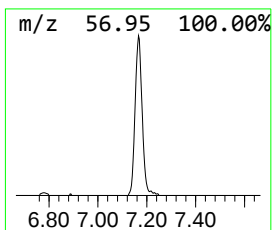
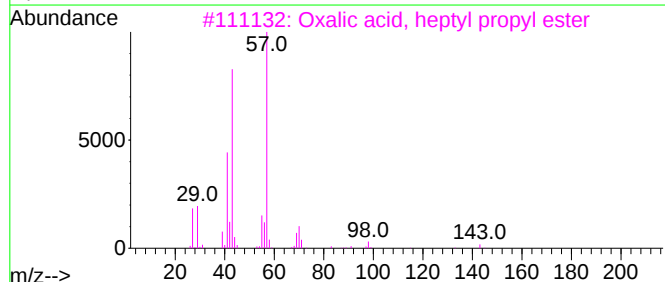
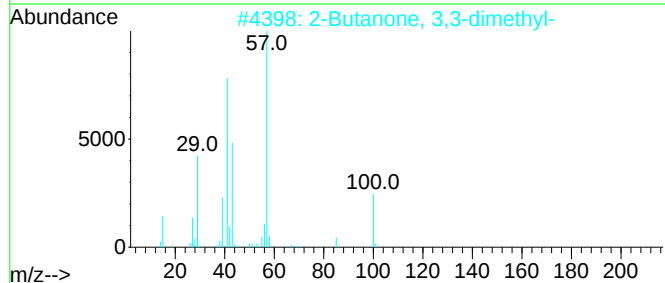
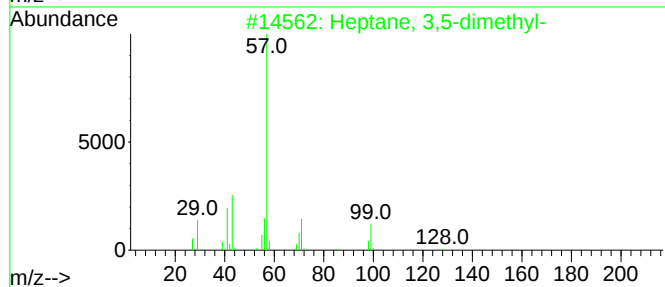
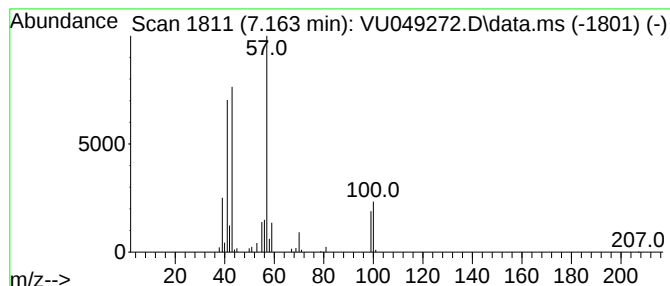
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.163	1.80 ug/L	102460	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	50
2			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	47
3			Oxalic acid, heptyl propyl ester	230	C12H22O4	1000309-26-0	47
4			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	42
5			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	40



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ClientSampleId :
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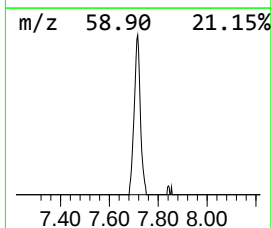
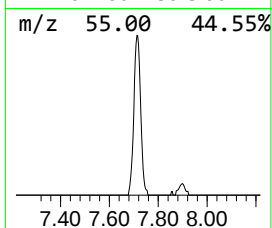
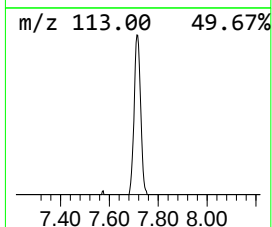
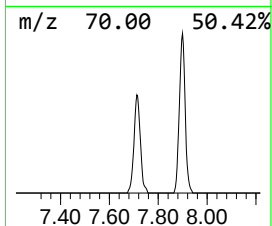
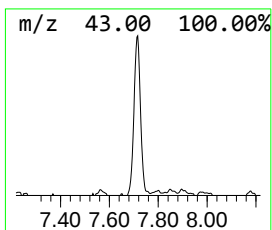
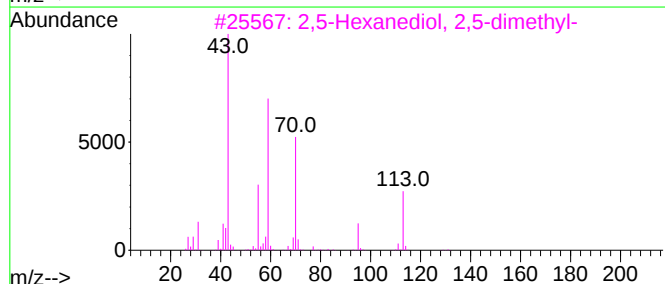
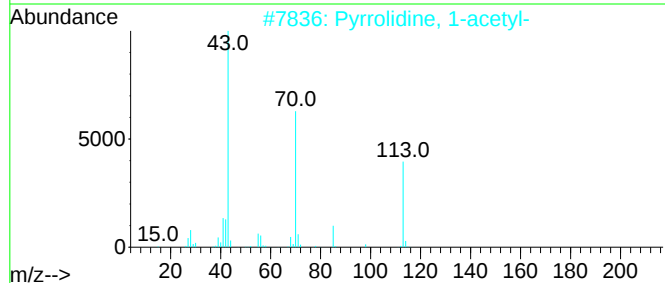
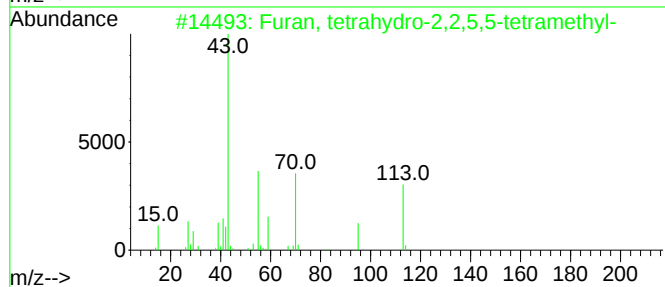
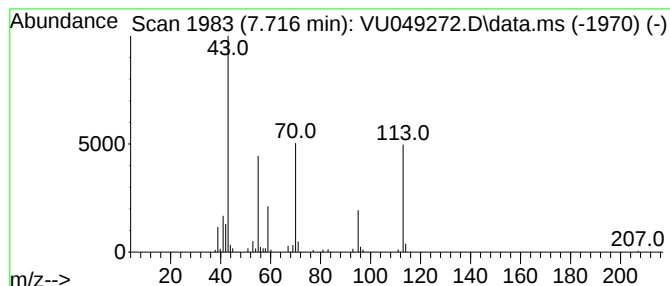
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.716	1.22 ug/L	69445	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	64
2			Pyrrolidine, 1-acetyl-	113	C6H11NO	004030-18-6	53
3			2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	50
4			Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	50
5			Piperazine, 1-[(2,4-dichlorobenz...	286	C13H16Cl2N2O	1000137-95-1	43



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.510	1.6	ug/L	92553	1	6.250	284004	5.0
(DEL) Alkane: S...	7.163	1.8	ug/L	102460	1	6.250	284004	5.0
Furan, tetrahyd...	7.716	1.2	ug/L	69445	1	6.250	284004	5.0