

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
 Data File : VU051636.D
 Acq On : 01 Nov 2022 01:59
 Operator : JC/MD
 Sample : N5321-23
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBWW5

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\SFAMUTR102822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051636.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	34	43	52	rBV	208428	379475	34.19%	4.024%
2	1.787	133	139	155	rVB	192085	246449	22.20%	2.613%
3	2.469	346	351	363	rVB3	14817	22380	2.02%	0.237%
4	2.565	368	381	394	rVB	98102	160514	14.46%	1.702%
5	2.684	409	418	433	rVB	52114	92382	8.32%	0.980%
6	2.790	440	451	469	rVB	75205	126722	11.42%	1.344%
7	3.044	522	530	540	rVB5	6174	11472	1.03%	0.122%
8	4.626	1010	1022	1068	rBV	179355	553208	49.84%	5.866%
9	5.063	1142	1158	1186	rBV	156789	365961	32.97%	3.881%
10	5.723	1339	1363	1375	rBV2	265805	733080	66.05%	7.774%
11	6.022	1444	1456	1469	rVB2	21183	40749	3.67%	0.432%
12	6.247	1513	1526	1548	rBV	222077	431690	38.89%	4.578%
13	6.542	1604	1618	1639	rBV	229672	439730	39.62%	4.663%
14	6.690	1649	1664	1681	rBV	200307	388039	34.96%	4.115%
15	7.565	1924	1936	1955	rBV	68934	122511	11.04%	1.299%
16	7.896	2025	2039	2056	rBV	235840	417021	37.57%	4.422%
17	7.973	2056	2063	2075	rVB2	8325	15304	1.38%	0.162%
18	8.099	2090	2102	2117	rBV	111404	192758	17.37%	2.044%
19	8.179	2117	2127	2143	rVB2	43595	75142	6.77%	0.797%
20	8.552	2230	2243	2257	rBV	487874	821383	74.00%	8.710%
21	8.632	2257	2268	2301	rVB	613152	1109924	100.00%	11.770%
22	9.417	2496	2512	2541	rBV2	353139	712663	64.21%	7.557%
23	9.571	2550	2560	2569	rBV2	13083	20446	1.84%	0.217%
24	9.700	2580	2600	2614	rBV5	29612	68830	6.20%	0.730%
25	10.054	2701	2710	2716	rBV4	9630	15180	1.37%	0.161%
26	10.099	2716	2724	2743	rVB	23603	39598	3.57%	0.420%
27	10.755	2916	2928	2943	rBV	194967	308932	27.83%	3.276%
28	10.893	2963	2971	2982	rVB3	9031	15708	1.42%	0.167%
29	10.999	2994	3004	3022	rVB3	7100	14569	1.31%	0.154%
30	11.089	3022	3032	3043	rBV3	14055	22423	2.02%	0.238%
31	11.291	3083	3095	3103	rBV	8092	13135	1.18%	0.139%
32	11.468	3136	3150	3160	rBV	19493	31066	2.80%	0.329%
33	11.639	3184	3203	3210	rBV	4930	11492	1.04%	0.122%
34	11.809	3242	3256	3275	rBV	320044	590450	53.20%	6.261%
35	11.902	3275	3285	3298	rVB5	20743	48128	4.34%	0.510%
36	12.060	3324	3334	3342	rBV4	26024	50813	4.58%	0.539%

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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 >
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37	12.192	3362	3375	3396	rBV2	289276	525849	47.38%	5.576%
38	12.947	3599	3610	3625	rBV3	15838	34813	3.14%	0.369%
39	13.291	3709	3717	3736	rVB10	7048	12760	1.15%	0.135%
40	13.452	3757	3767	3776	rBV5	12391	20288	1.83%	0.215%
41	13.513	3778	3786	3796	rVB7	10080	18644	1.68%	0.198%
42	13.841	3877	3888	3901	rBV7	6749	12253	1.10%	0.130%
43	14.086	3955	3964	3983	rVB2	21905	42864	3.86%	0.455%
44	15.224	4307	4318	4327	rBV2	11784	19275	1.74%	0.204%
45	15.410	4367	4376	4388	rBV4	11968	21113	1.90%	0.224%
46	16.410	4677	4687	4694	rBV8	7182	13061	1.18%	0.139%

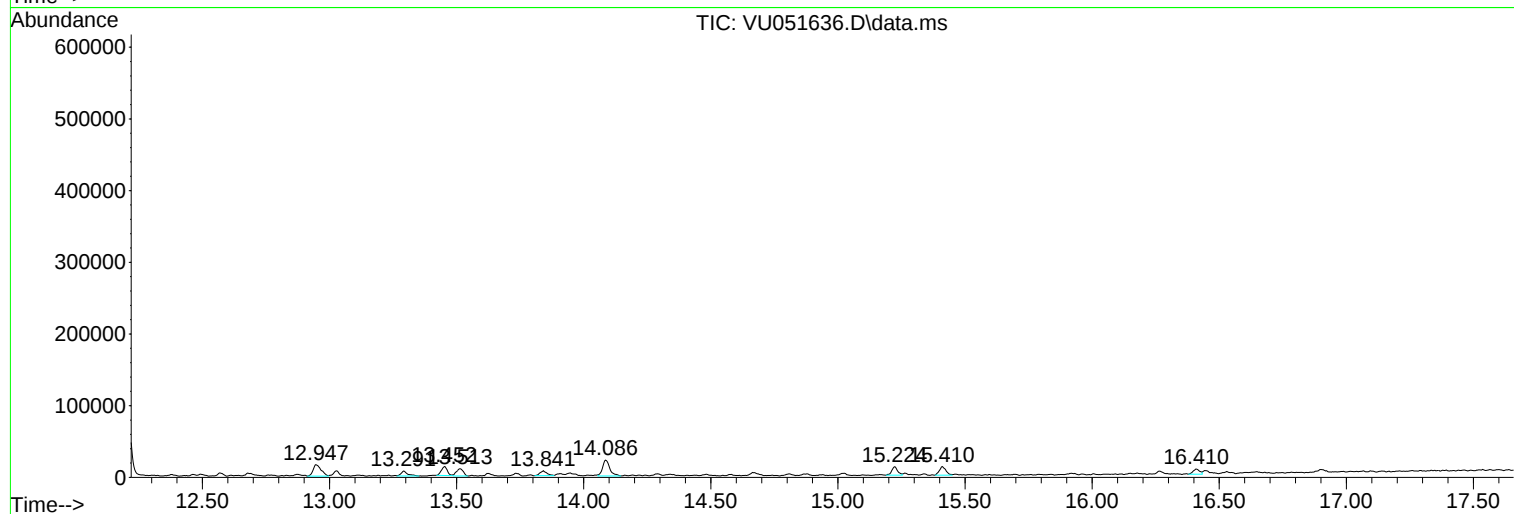
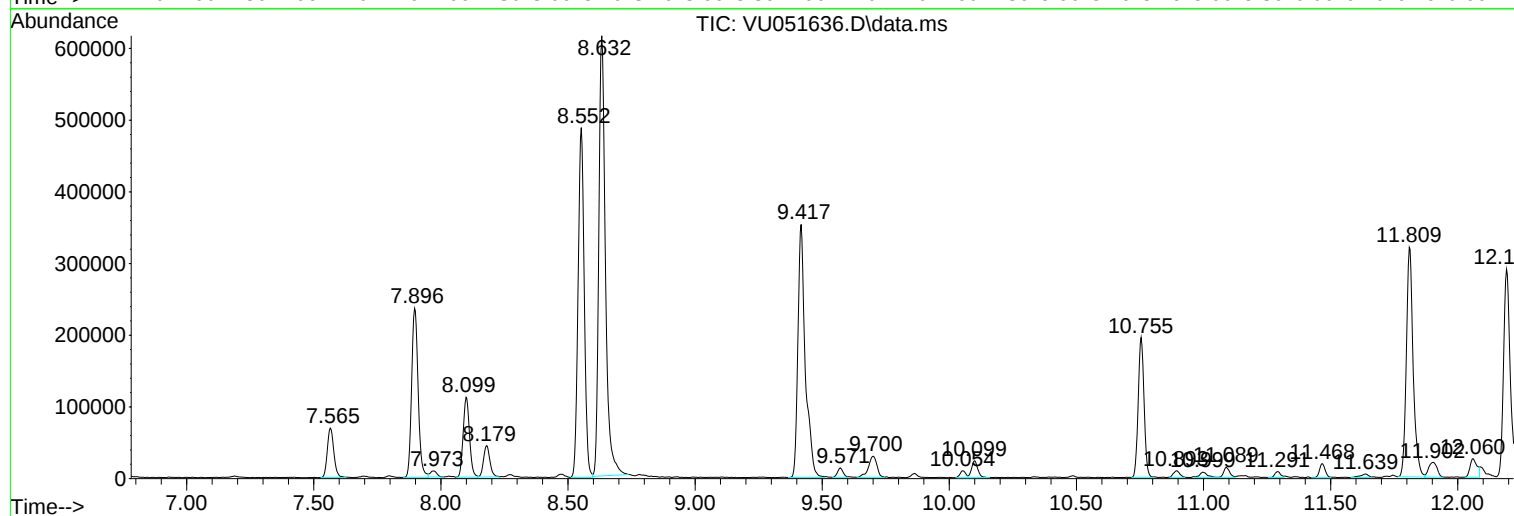
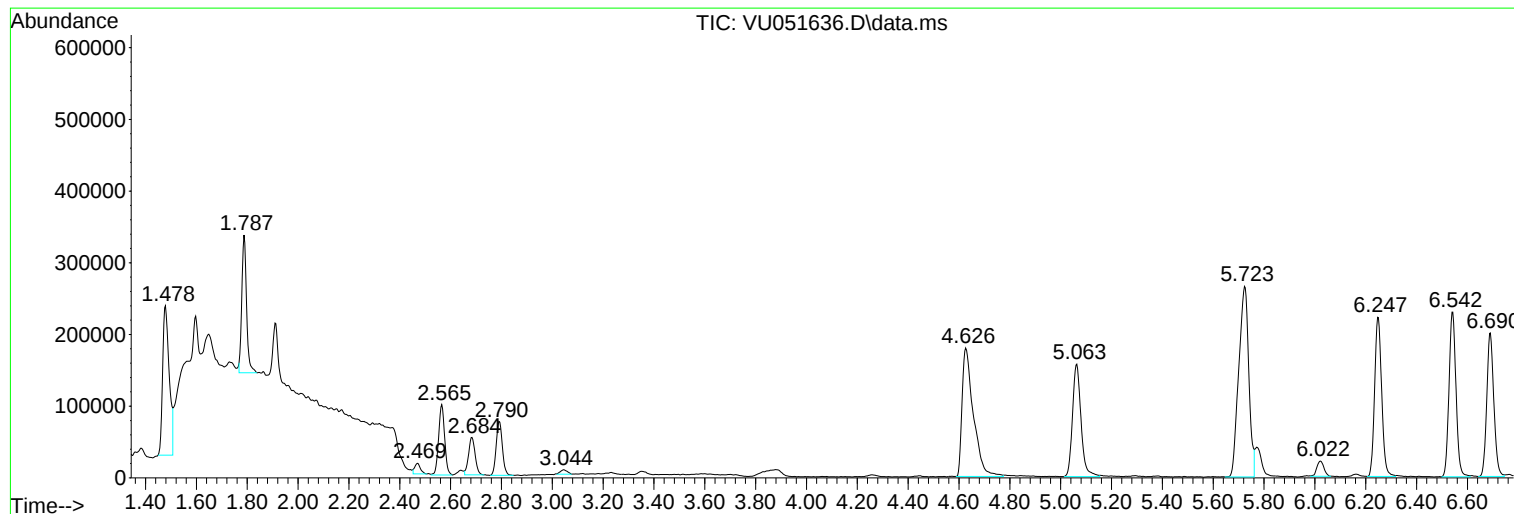
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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ClientSampleId :
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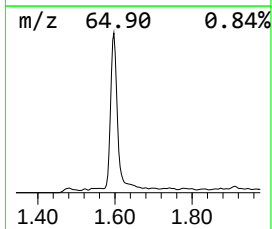
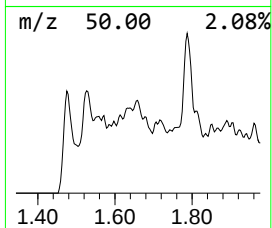
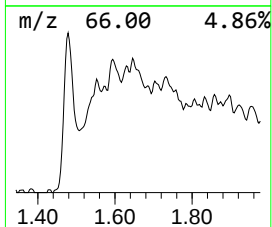
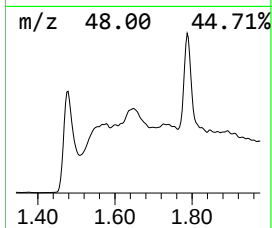
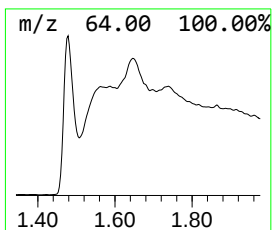
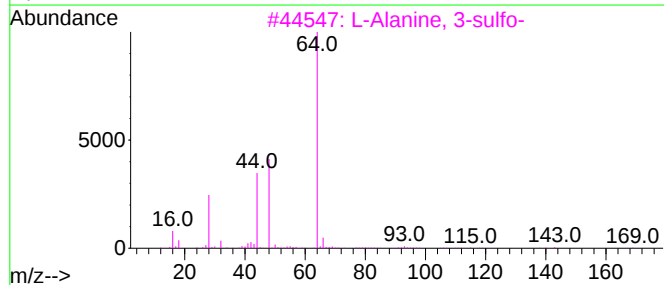
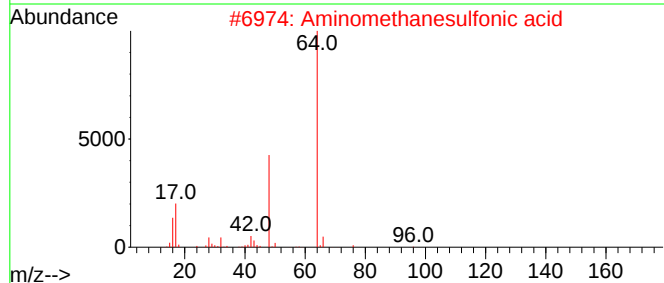
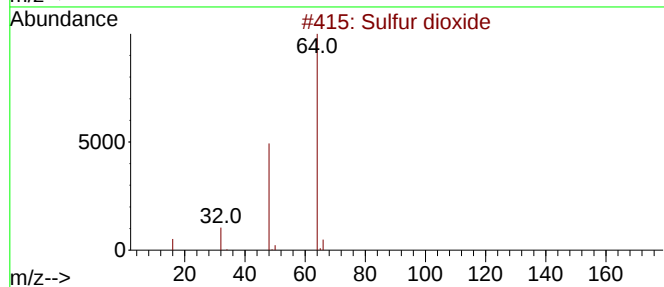
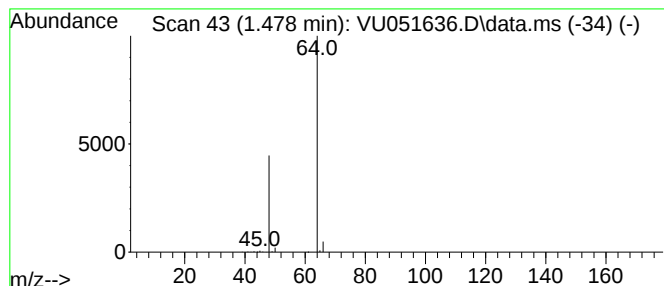
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.478	4.40 ug/L	379475	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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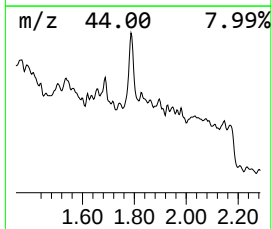
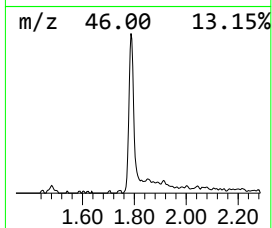
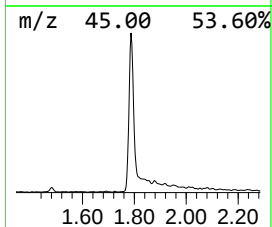
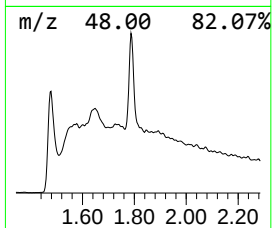
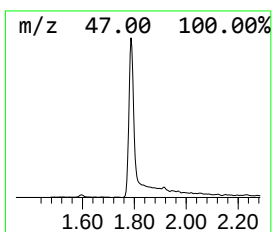
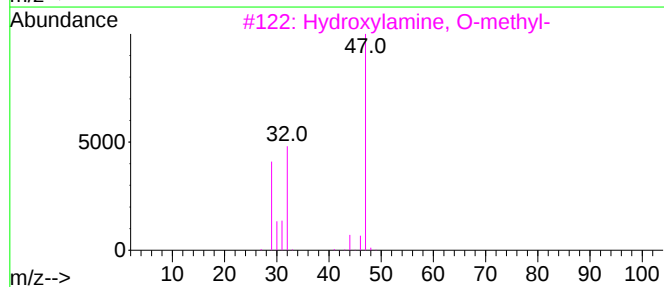
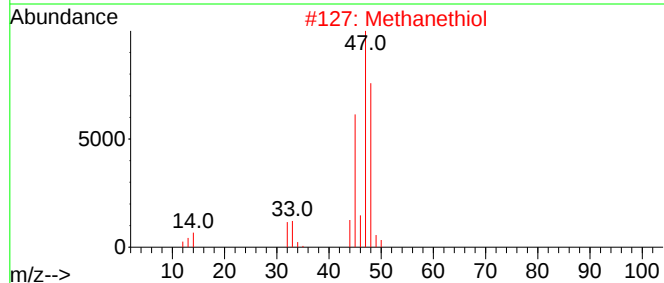
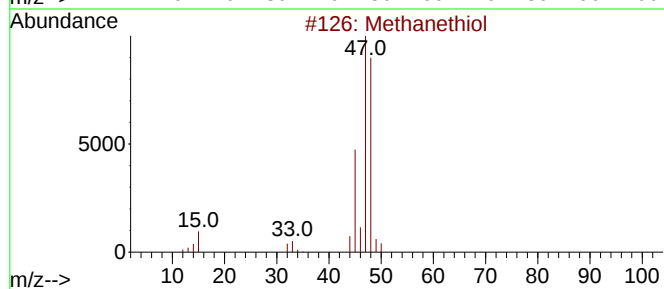
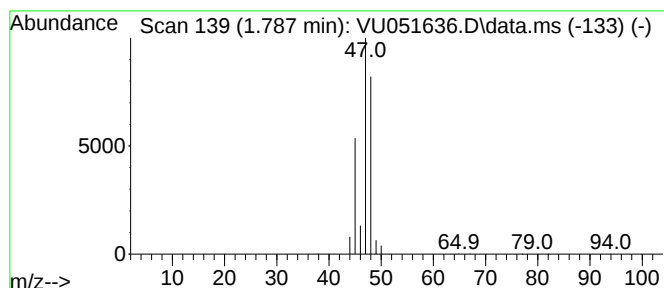
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Methanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.787	2.85 ug/L	246449	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	90
2			Methanethiol	48	CH4S	000074-93-1	83
3			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5			Methane, nitroso-	45	CH3NO	000865-40-7	5



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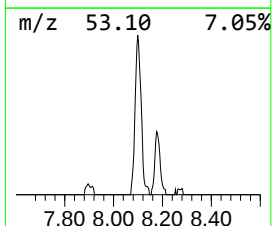
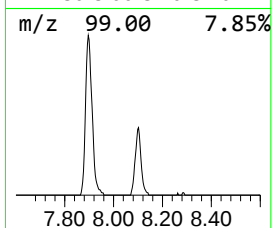
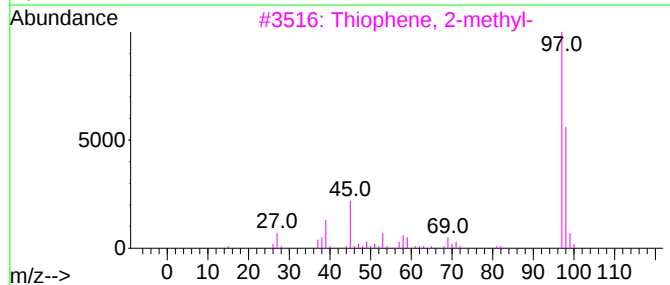
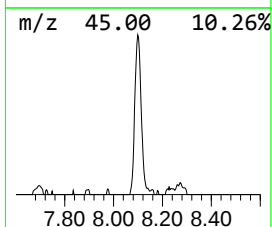
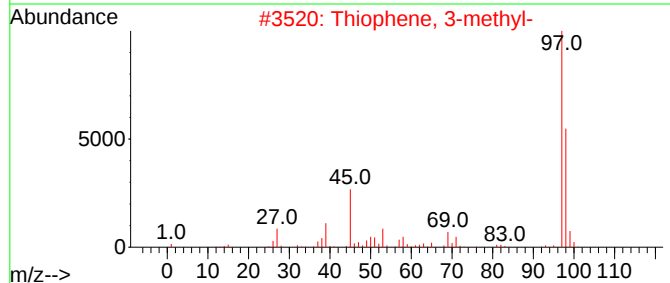
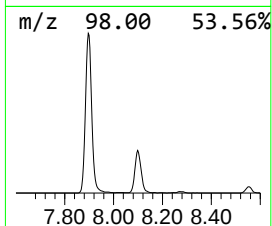
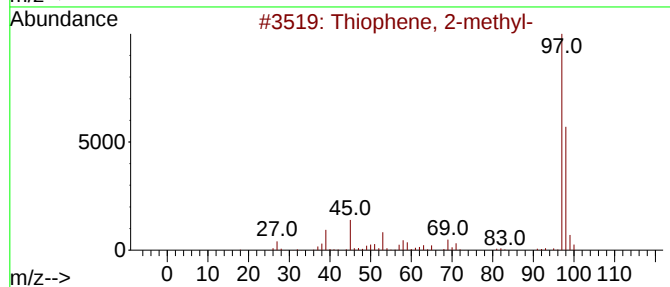
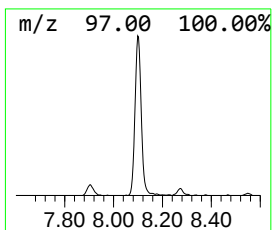
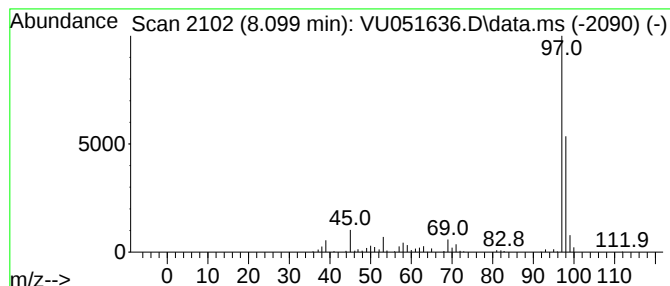
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Thiophene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.099	1.35 ug/L	192758	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 2-methyl-	98	C5H6S	000554-14-3	93
2			Thiophene, 3-methyl-	98	C5H6S	000616-44-4	91
3			Thiophene, 2-methyl-	98	C5H6S	000554-14-3	91
4			Thiophene, 2-methyl-	98	C5H6S	000554-14-3	91
5			Thiophene, 3-methyl-	98	C5H6S	000616-44-4	91



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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	1.478	4.4	ug/L	379475	1	6.250	431690	5.0
Methanethiol	1.787	2.9	ug/L	246449	1	6.250	431690	5.0
Thiophene, 2-me...	8.099	1.4	ug/L	192758	2	9.417	712663	5.0