

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
 Data File : VV032443.D
 Acq On : 17 Oct 2023 14:16
 Operator : SY/MD
 Sample : 04903-10
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AF3

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_V\Method\SFAMVTR092923WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV032443.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.101	9	19	30	rVB2	54755	94560	9.70%	1.654%
2	1.278	66	74	86	rVB	70265	76041	7.80%	1.330%
3	1.362	92	100	103	rBV2	20831	27389	2.81%	0.479%
4	1.532	146	153	165	rVB	51886	64052	6.57%	1.120%
5	2.060	307	317	332	rBV	88196	133047	13.65%	2.327%
6	2.175	334	353	366	rVV5	11541	40707	4.18%	0.712%
7	2.240	367	373	384	rVB	9655	15716	1.61%	0.275%
8	2.889	565	575	586	rBV2	12793	27885	2.86%	0.488%
9	3.831	852	868	914	rBV2	61175	346379	35.54%	6.059%
10	4.256	985	1000	1023	rBV2	67836	195701	20.08%	3.423%
11	4.960	1203	1219	1240	rBV3	145762	383731	39.37%	6.712%
12	5.249	1296	1309	1326	rBV2	13837	35648	3.66%	0.624%
13	5.432	1354	1366	1382	rBV5	9567	25078	2.57%	0.439%
14	5.539	1387	1399	1415	rBV	137361	288685	29.62%	5.049%
15	5.844	1480	1494	1508	rBV9	7273	18622	1.91%	0.326%
16	5.992	1527	1540	1555	rBV2	85991	190170	19.51%	3.326%
17	6.439	1671	1679	1691	rBV3	7799	14418	1.48%	0.252%
18	6.921	1818	1829	1854	rBV2	38032	85029	8.72%	1.487%
19	7.191	1901	1913	1919	rBV6	5030	11174	1.15%	0.195%
20	7.246	1920	1930	1949	rVV	162701	315415	32.36%	5.517%
21	7.323	1949	1954	1966	rVV2	13533	26496	2.72%	0.463%
22	7.381	1968	1972	1989	rVB3	4640	9777	1.00%	0.171%
23	7.561	2018	2028	2043	rBV	22604	50218	5.15%	0.878%
24	7.908	2114	2136	2164	rBV	522504	974582	100.00%	17.047%
25	8.034	2164	2175	2209	rVV	248114	557193	57.17%	9.746%
26	8.185	2212	2222	2242	rVB2	37892	76628	7.86%	1.340%
27	8.789	2397	2410	2431	rBV	225871	400824	41.13%	7.011%
28	9.079	2490	2500	2514	rBV7	7107	13893	1.43%	0.243%
29	9.757	2701	2711	2725	rBV5	11720	22792	2.34%	0.399%
30	10.156	2819	2835	2855	rBV	78724	132181	13.56%	2.312%
31	10.329	2879	2889	2902	rVB2	18019	30636	3.14%	0.536%
32	10.452	2916	2927	2945	rBV	21213	37142	3.81%	0.650%
33	11.098	3119	3128	3143	rBV8	11736	21178	2.17%	0.370%
34	11.188	3145	3156	3178	rVV	236661	376559	38.64%	6.586%
35	11.487	3236	3249	3263	rBV	99911	213598	21.92%	3.736%
36	11.564	3264	3273	3301	rVB	207186	347880	35.70%	6.085%

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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 >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Title : TRACE VOA SFAM1.0

37	12.197	3463	3470	3482	rVB2	12609	20770	2.13%	0.363%
38	12.294	3492	3500	3513	rBV7	9698	15403	1.58%	0.269%

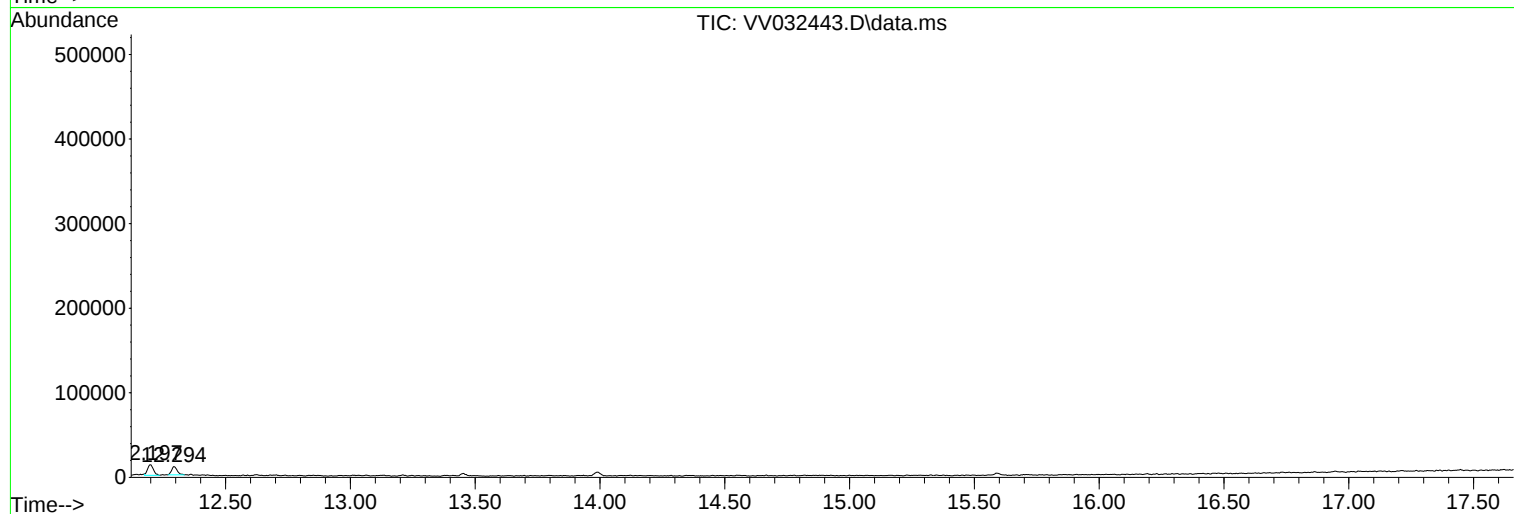
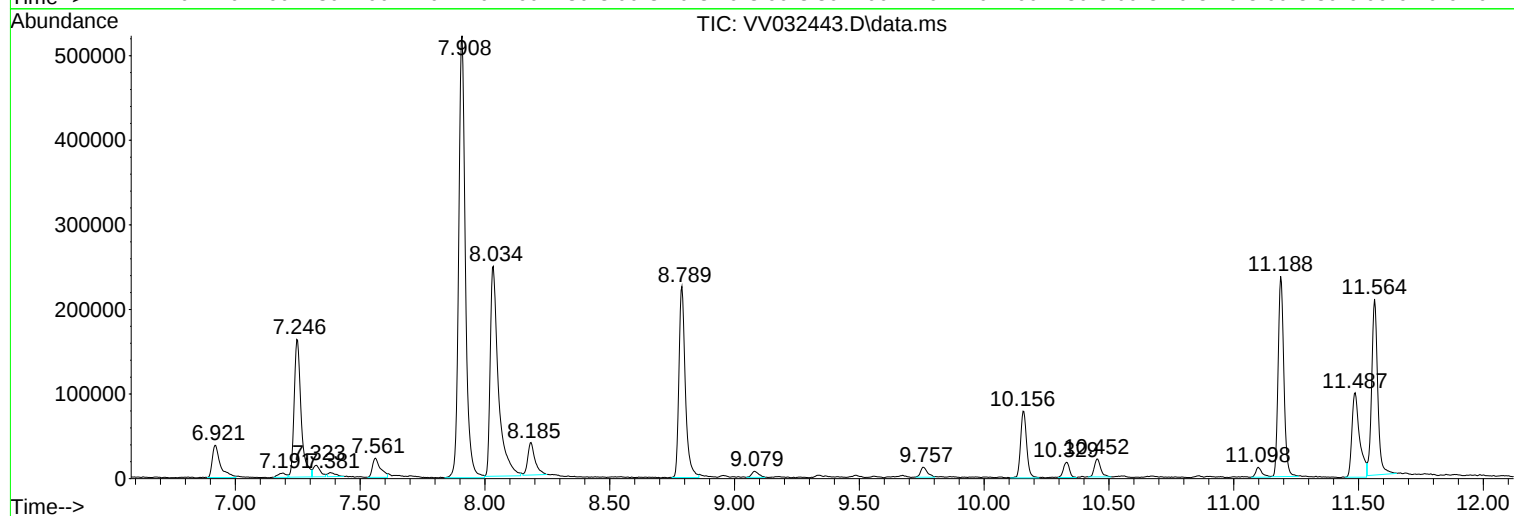
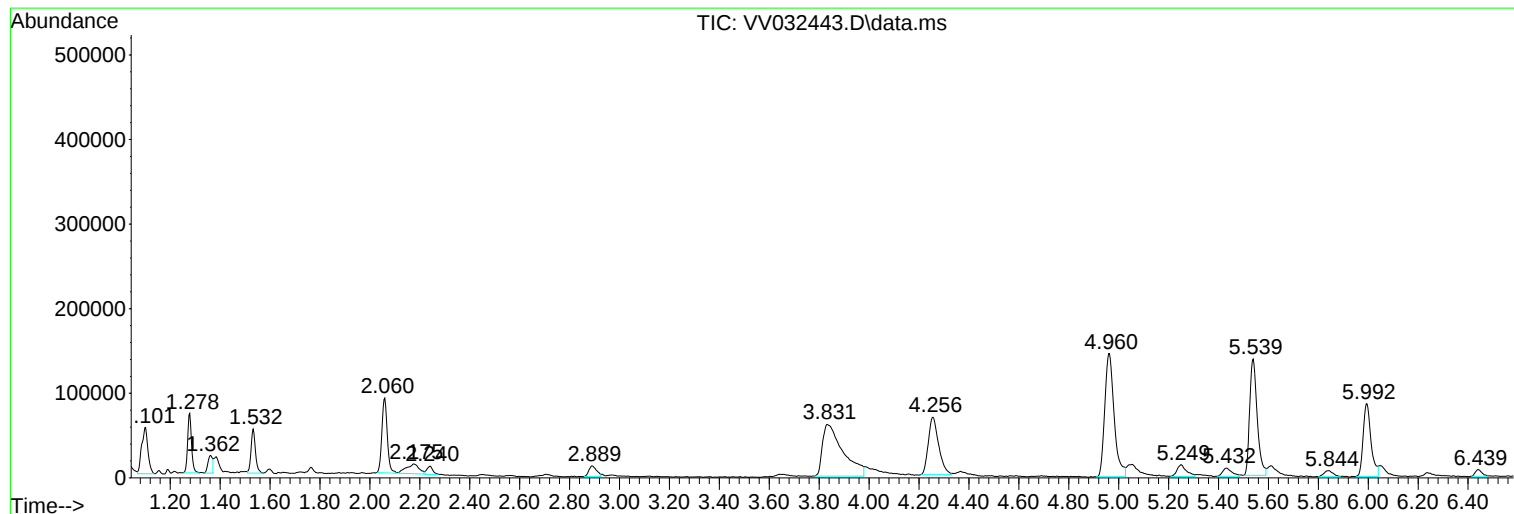
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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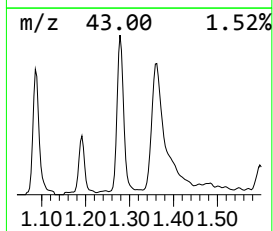
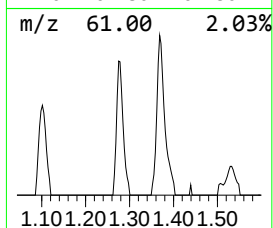
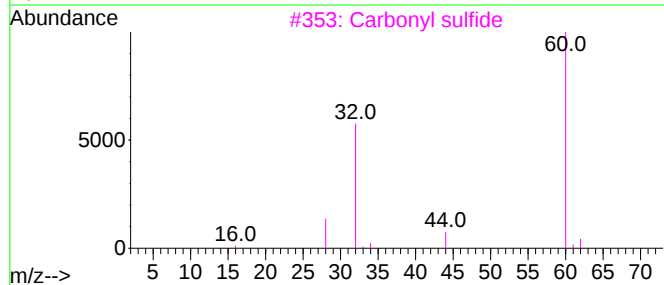
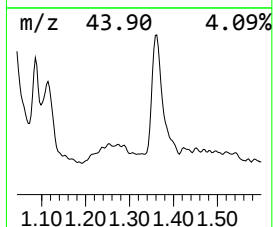
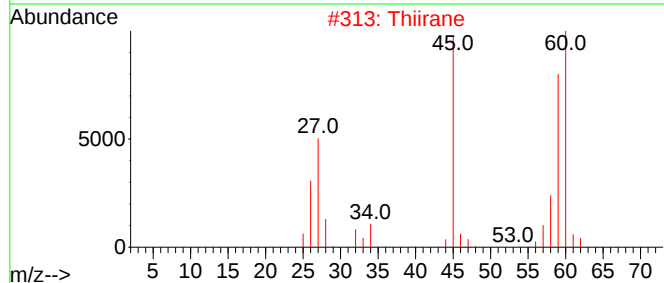
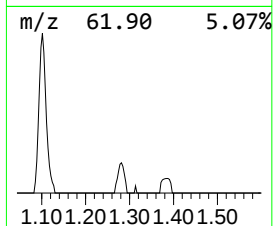
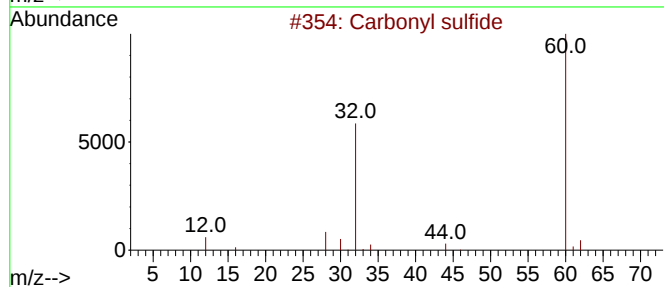
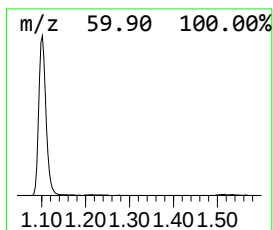
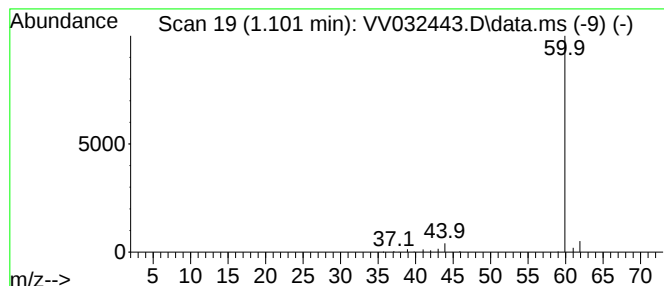
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.101	1.64 ug/L	94560	1,4-Difluorobenzene	5.539

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Carbonyl sulfide	60	COS	000463-58-1	9
2		Thiirane	60	C2H4S	000420-12-2	5
3		Carbonyl sulfide	60	COS	000463-58-1	5
4		Formamidoxime	60	CH4N2O	000624-82-8	5
5		Methyl formate	60	C2H4O2	000107-31-3	5



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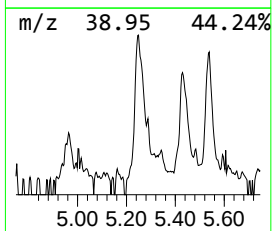
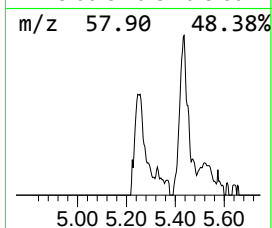
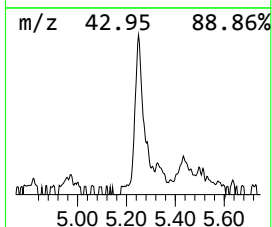
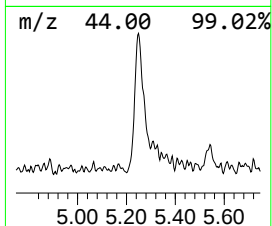
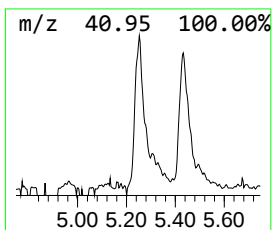
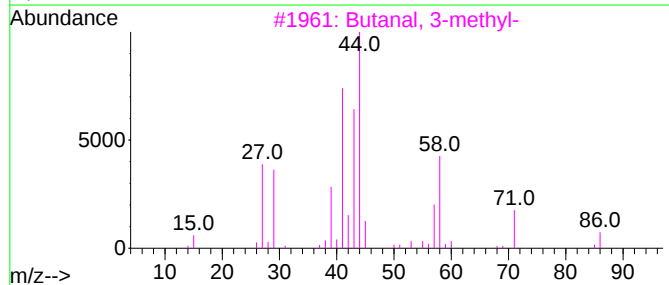
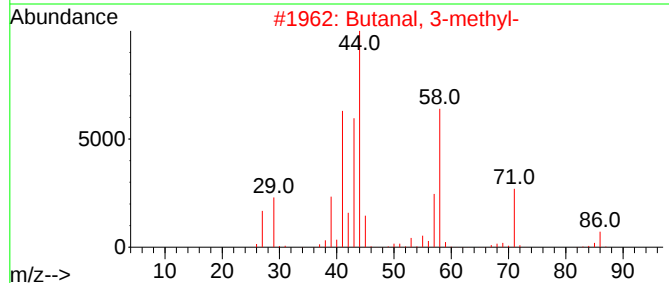
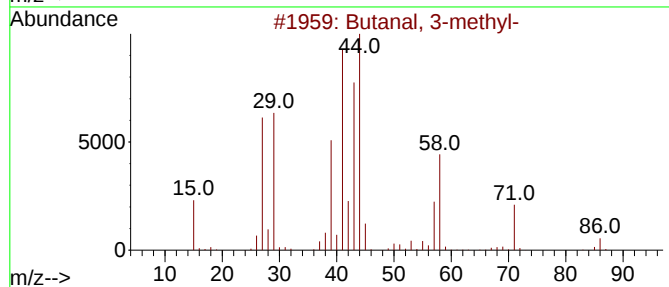
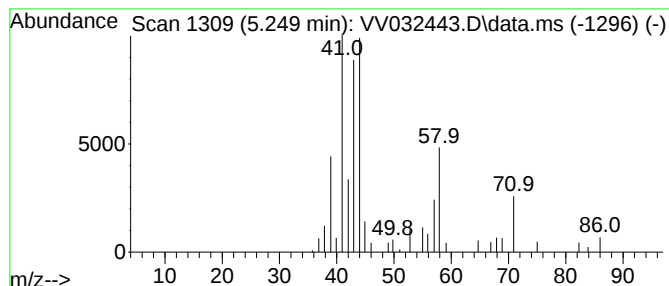
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butanal, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.249	0.62 ug/L	35648	1,4-Difluorobenzene	5.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 3-methyl-	86	C5H10O	000590-86-3	90
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	58
3			Butanal, 3-methyl-	86	C5H10O	000590-86-3	52
4			Pentanal	86	C5H10O	000110-62-3	47
5			Butanal, 3-methyl-	86	C5H10O	000590-86-3	40



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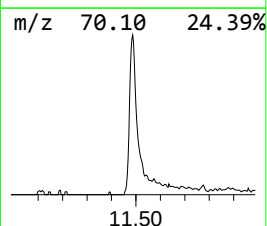
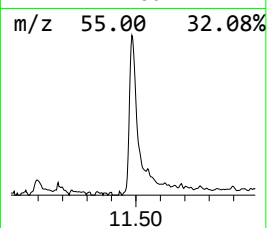
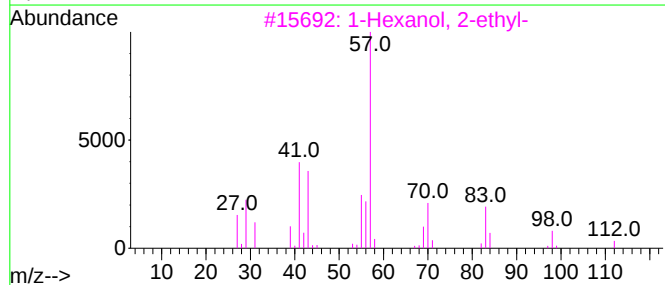
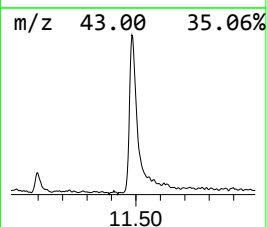
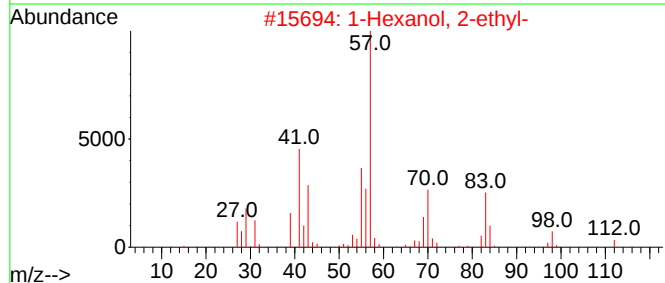
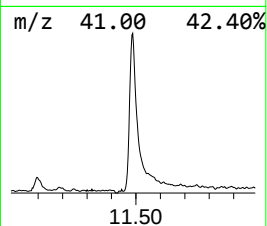
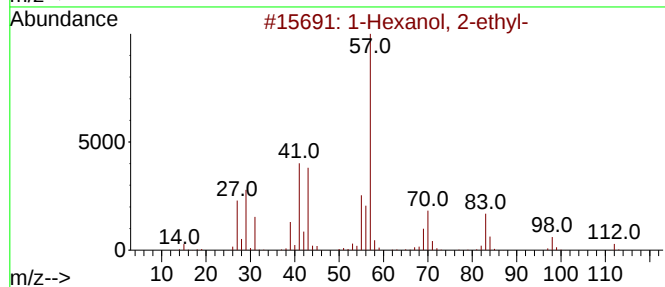
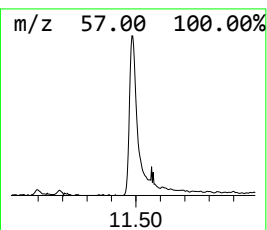
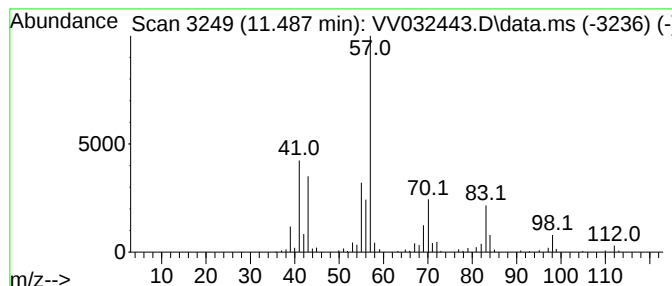
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.487	2.84 ug/L	213598	1,4-Dichlorobenzene-d4	11.188

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.101	1.6	ug/L	94560	1	5.539	288685	5.0
Butanal, 3-methyl-	5.249	0.6	ug/L	35648	1	5.539	288685	5.0
1-Hexanol, 2-et...	11.487	2.8	ug/L	213598	3	11.188	376559	5.0