

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV102023\
 Data File : VV032515.D
 Acq On : 20 Oct 2023 11:28
 Operator : SY/MD
 Sample : 04950-05
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A48Z5

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: VV032515.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.217	48	55	65	rBV	30233	36047	6.67%	0.833%
2	1.278	67	74	88	rVB	53228	57526	10.64%	1.329%
3	1.532	146	153	165	rVB	48314	56160	10.39%	1.298%
4	2.059	307	317	329	rBV	81048	120572	22.31%	2.786%
5	2.137	330	341	372	rVB	45317	137779	25.49%	3.183%
6	2.519	450	460	467	rBV5	4164	7639	1.41%	0.177%
7	3.632	797	806	811	rBV6	5671	10530	1.95%	0.243%
8	3.815	843	863	909	rBV3	120284	540433	100.00%	12.487%
9	4.252	984	999	1021	rBV	60132	157861	29.21%	3.647%
10	4.960	1203	1219	1238	rBV2	138971	359764	66.57%	8.312%
11	5.535	1387	1398	1415	rBV	113543	245999	45.52%	5.684%
12	5.992	1522	1540	1574	rBV2	84604	202270	37.43%	4.673%
13	6.220	1603	1611	1626	rBV2	12592	27870	5.16%	0.644%
14	6.918	1818	1828	1847	rBV	38114	79416	14.69%	1.835%
15	7.172	1896	1907	1919	rBV5	6972	16138	2.99%	0.373%
16	7.246	1919	1930	1947	rBV	147074	276755	51.21%	6.394%
17	7.558	2018	2027	2041	rBV	23526	44273	8.19%	1.023%
18	7.879	2114	2127	2139	rBV3	8365	17308	3.20%	0.400%
19	8.030	2162	2174	2207	rBV	221462	467078	86.43%	10.792%
20	8.181	2211	2221	2244	rBV	68002	129887	24.03%	3.001%
21	8.789	2399	2410	2434	rBV	180655	322286	59.63%	7.446%
22	9.078	2491	2500	2513	rBV2	9507	16531	3.06%	0.382%
23	9.487	2617	2627	2633	rBV3	6152	10014	1.85%	0.231%
24	9.654	2671	2679	2694	rBV	10066	20360	3.77%	0.470%
25	9.754	2702	2710	2723	rBV4	16285	26554	4.91%	0.614%
26	9.969	2770	2777	2789	rBV4	4608	8182	1.51%	0.189%
27	10.156	2825	2835	2852	rVB	71369	115136	21.30%	2.660%
28	10.329	2873	2889	2898	rBV3	17731	30645	5.67%	0.708%
29	10.856	3040	3053	3059	rBV3	4905	10695	1.98%	0.247%
30	11.098	3119	3128	3136	rBV5	17572	29784	5.51%	0.688%
31	11.188	3145	3156	3174	rVB	208566	320754	59.35%	7.411%
32	11.490	3240	3250	3262	rBV3	18376	40522	7.50%	0.936%
33	11.564	3262	3273	3289	rVB	170734	269074	49.79%	6.217%
34	11.946	3384	3392	3402	rBV9	5634	11375	2.10%	0.263%
35	12.197	3459	3470	3476	rBV2	9102	15043	2.78%	0.348%
36	12.290	3490	3499	3516	rBV3	50001	81099	15.01%	1.874%

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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	13.991	4014	4028	4037	rBV2	4238	8682	1.61%	0.201%
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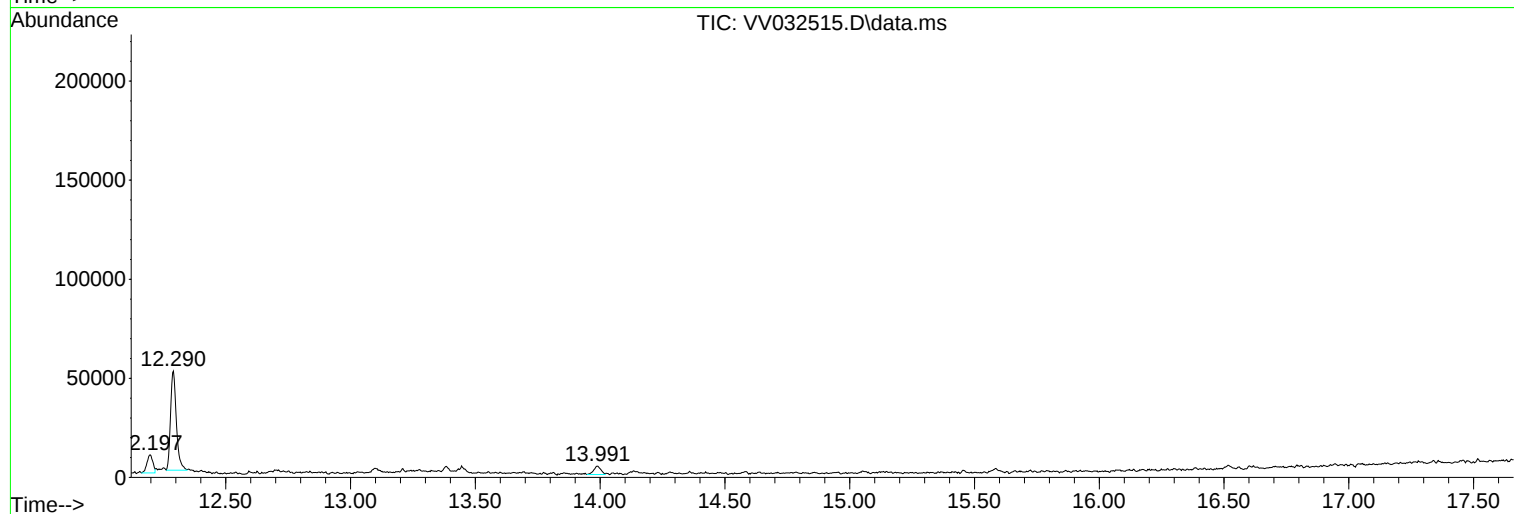
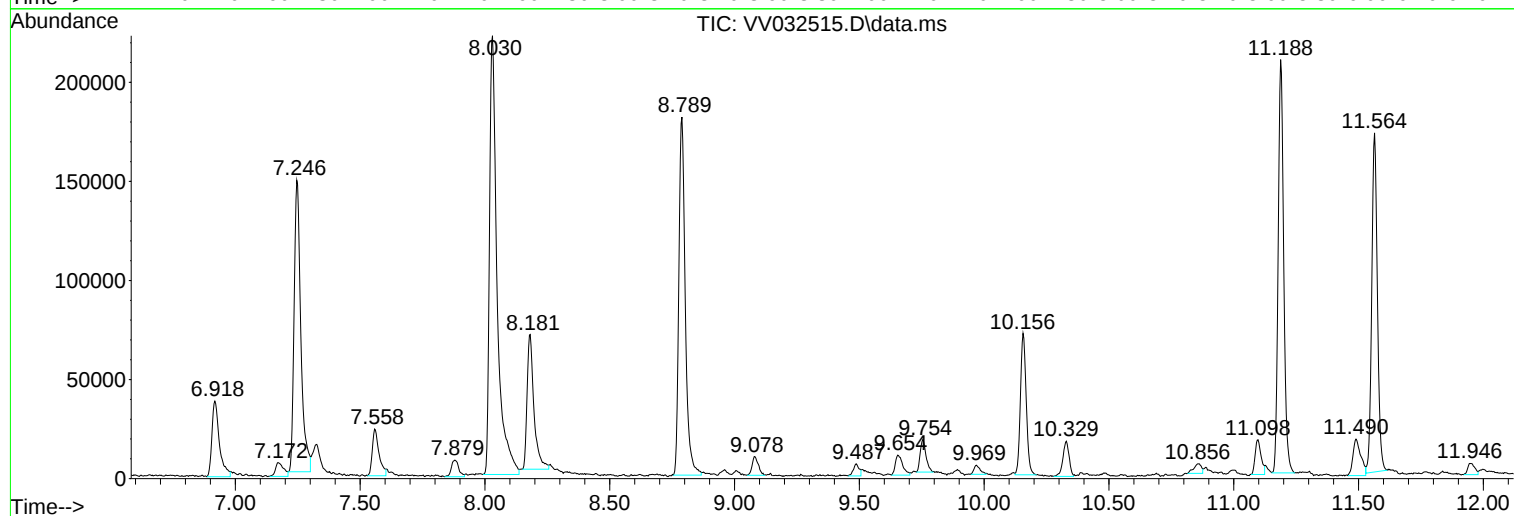
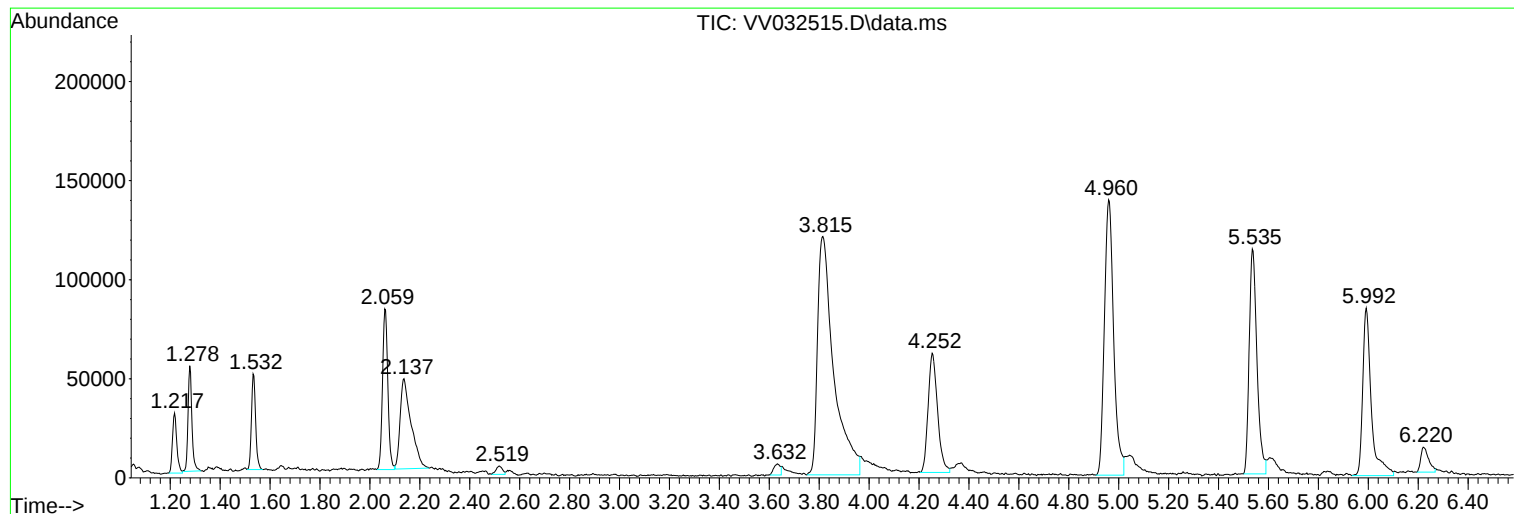
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Quant Title : TRACE VOA SFAM1.0

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



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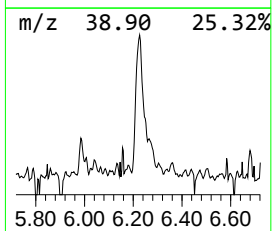
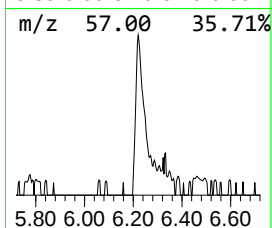
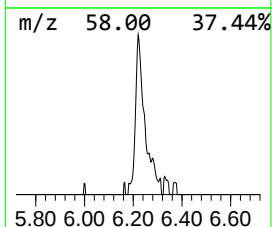
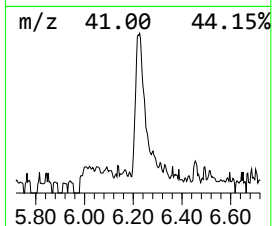
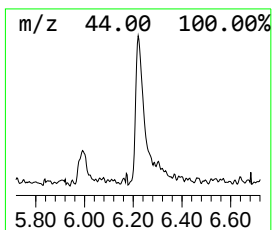
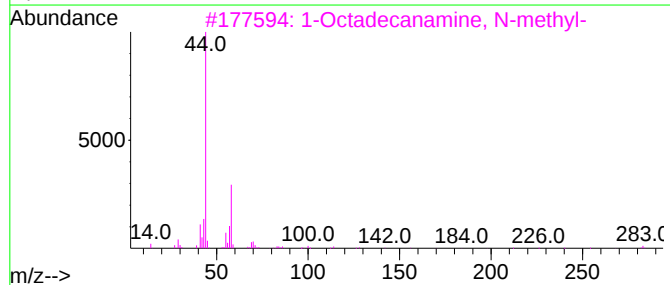
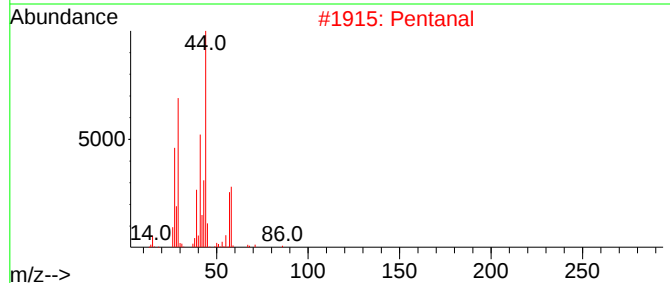
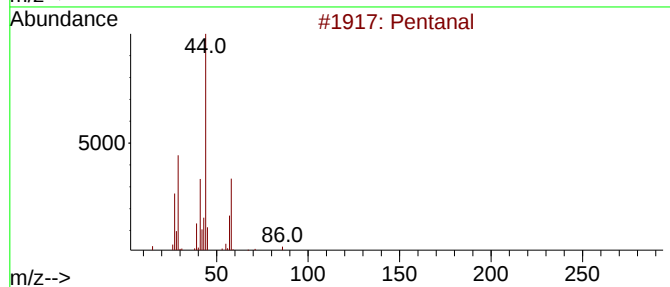
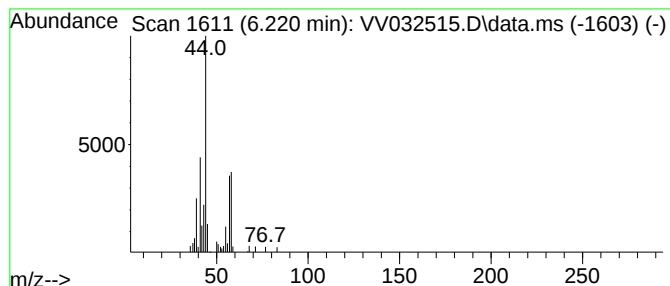
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Pentanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.220	0.57 ug/L	27870	1,4-Difluorobenzene	5.538

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentanal	86	C5H10O	000110-62-3	78
2		Pentanal	86	C5H10O	000110-62-3	72
3		1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	40
4		Cyclopropyl carbinol	72	C4H8O	002516-33-8	9
5		Cyclopropyl carbinol	72	C4H8O	002516-33-8	9



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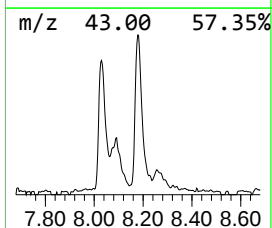
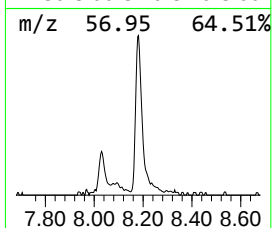
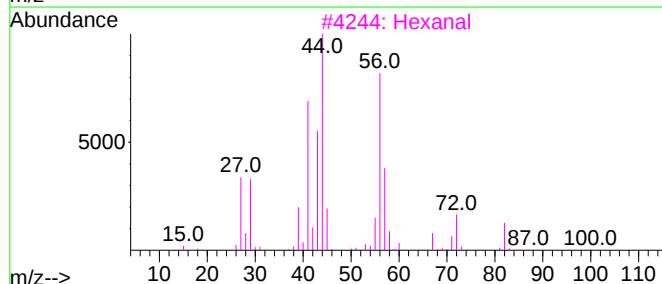
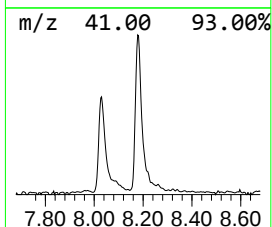
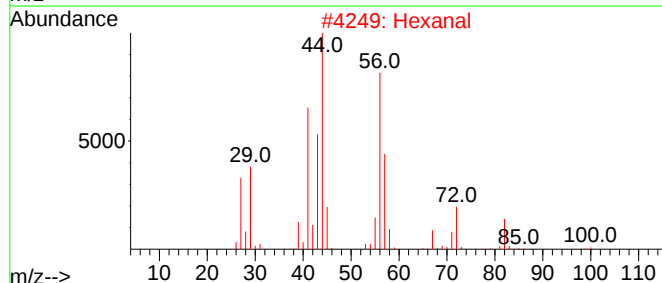
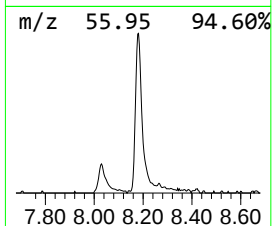
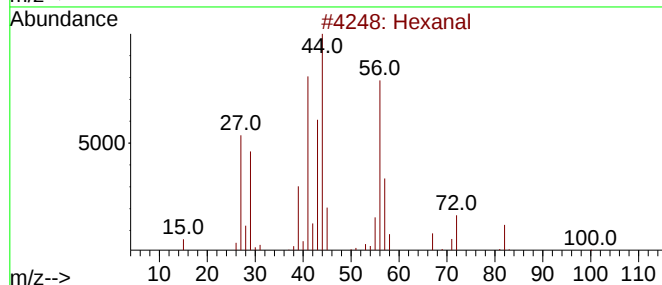
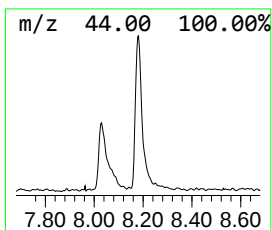
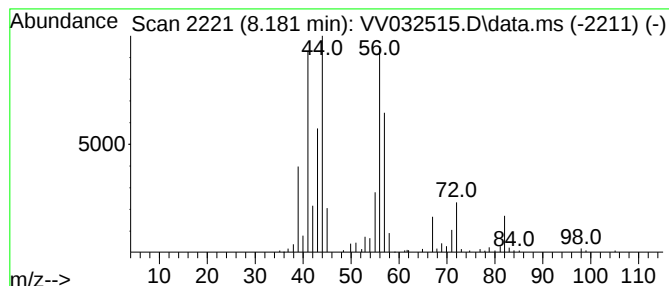
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.181	2.02 ug/L	129887	Chlorobenzene-d5	8.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	72
2	Hexanal			100	C6H12O	000066-25-1	64
3	Hexanal			100	C6H12O	000066-25-1	59
4	Hexanal			100	C6H12O	000066-25-1	58
5	Hexanal			100	C6H12O	000066-25-1	47



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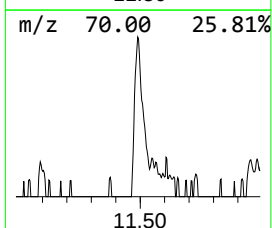
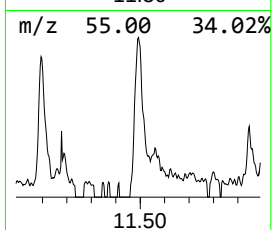
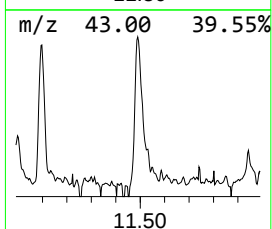
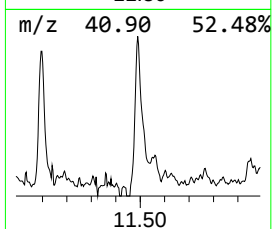
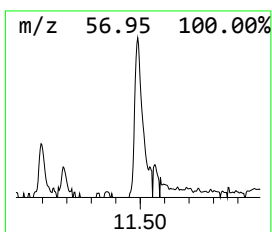
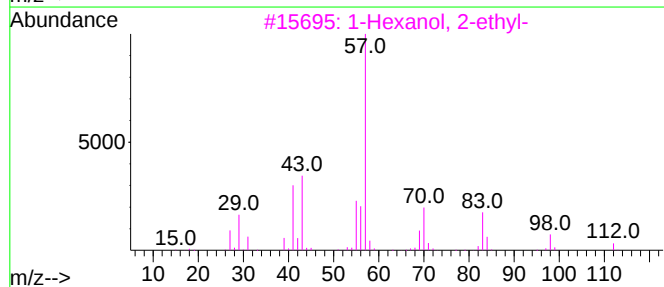
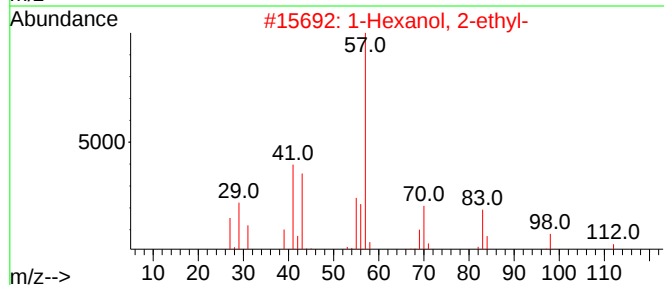
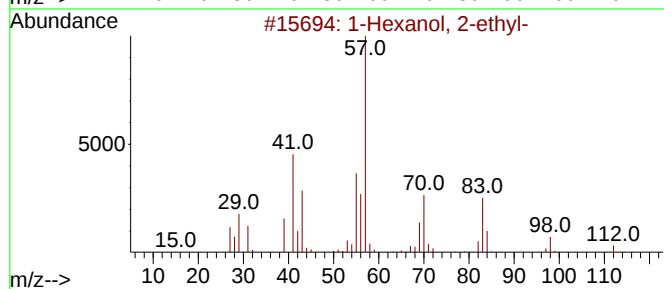
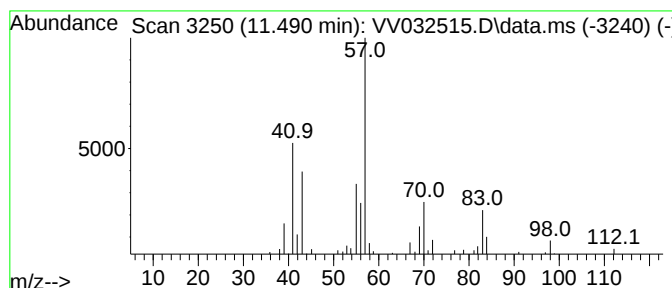
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.490	0.63 ug/L	40522	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	86
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59



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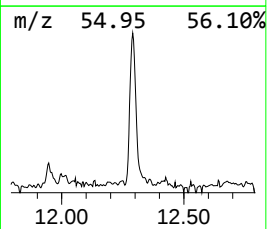
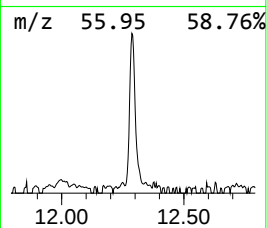
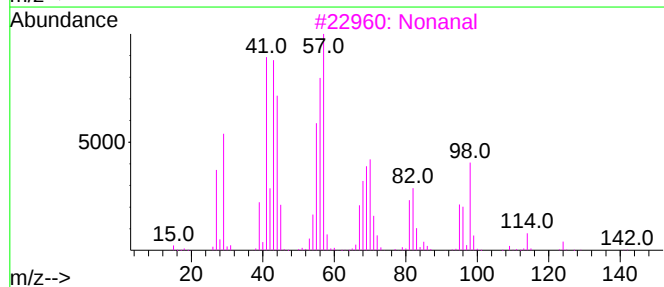
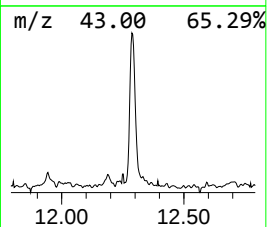
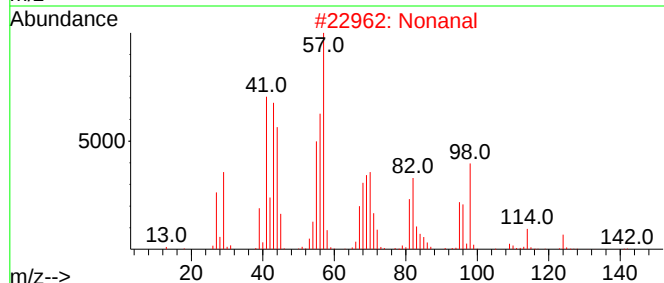
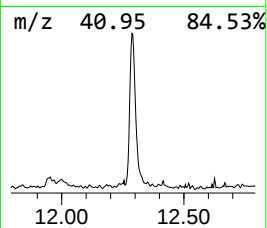
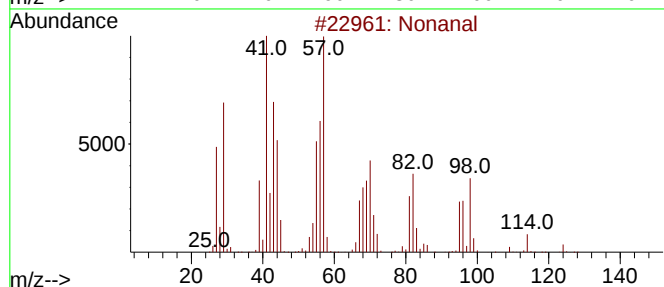
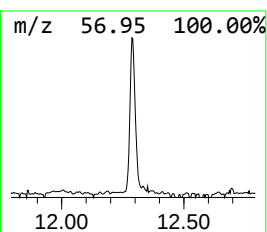
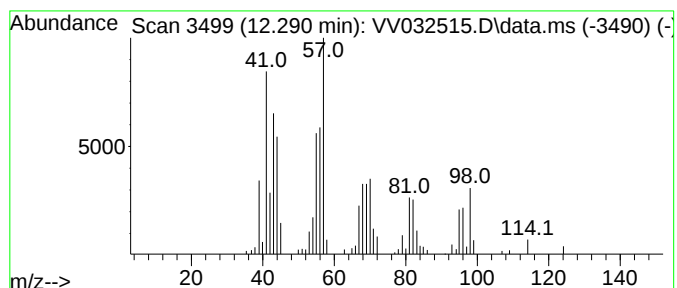
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Nonanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.291	1.26 ug/L	81099	1,4-Dichlorobenzene-d4	11.188

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	91
2			Nonanal	142	C9H18O	000124-19-6	90
3			Nonanal	142	C9H18O	000124-19-6	86
4			Nonanal	142	C9H18O	000124-19-6	80
5			2-Nonen-1-ol	142	C9H18O	022104-79-6	35



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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
Pentanal	6.220	0.6	ug/L	27870	1	5.538	245999	5.0
Hexanal	8.181	2.0	ug/L	129887	2	8.789	322286	5.0
1-Hexanol, 2-et...	11.490	0.6	ug/L	40522	3	11.188	320754	5.0
Nonanal	12.291	1.3	ug/L	81099	3	11.188	320754	5.0