

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020222\
 Data File : VU046996.D
 Acq On : 02 Feb 2022 12:45
 Operator : SY/MD
 Sample : N1348-01 4X
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFX5

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\SFAMUTR011822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU046996.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	12	rVB2	7336	6554	1.42%	0.147%
2	1.604	72	82	97	rVB	61493	77251	16.78%	1.728%
3	1.919	171	180	201	rBV	45944	63383	13.76%	1.417%
4	2.575	368	384	400	rBV3	105833	199001	43.22%	4.450%
5	3.237	581	590	602	rVB5	4967	10166	2.21%	0.227%
6	3.877	772	789	802	rBV	15616	36681	7.97%	0.820%
7	3.970	802	818	844	rVB2	47963	131419	28.54%	2.939%
8	4.655	1013	1031	1066	rBV3	62249	250671	54.44%	5.606%
9	5.070	1143	1160	1181	rBV2	77531	178425	38.75%	3.990%
10	5.321	1225	1238	1249	rBV2	4919	9976	2.17%	0.223%
11	5.729	1345	1365	1394	rBV2	150427	403032	87.52%	9.013%
12	6.253	1515	1528	1545	rBV	121899	230911	50.15%	5.164%
13	6.546	1606	1619	1637	rBV	140989	261106	56.70%	5.839%
14	6.694	1650	1665	1684	rBV	93938	184957	40.17%	4.136%
15	6.887	1713	1725	1736	rBV3	5216	10093	2.19%	0.226%
16	7.568	1926	1937	1952	rBV	44201	76456	16.60%	1.710%
17	7.903	2028	2041	2056	rBV	155680	282682	61.39%	6.322%
18	7.973	2057	2063	2077	rVB	8570	15223	3.31%	0.340%
19	8.182	2114	2128	2144	rBV	27913	46506	10.10%	1.040%
20	8.475	2206	2219	2227	rBV2	3576	6065	1.32%	0.136%
21	8.555	2232	2244	2258	rVV	59932	102338	22.22%	2.289%
22	8.639	2258	2270	2304	rVV	237723	460481	100.00%	10.298%
23	8.790	2306	2317	2337	rVB2	66192	118996	25.84%	2.661%
24	9.420	2500	2513	2536	rBV	194317	343493	74.59%	7.682%
25	10.346	2793	2801	2815	rVB3	11749	18281	3.97%	0.409%
26	10.761	2917	2930	2947	rVB	79325	129060	28.03%	2.886%
27	10.893	2959	2971	2982	rBV2	7363	11848	2.57%	0.265%
28	11.259	3077	3085	3091	rBV	3609	4807	1.04%	0.108%
29	11.690	3210	3219	3233	rBV3	30524	46188	10.03%	1.033%
30	11.812	3245	3257	3279	rVB	205520	336029	72.97%	7.515%
31	12.195	3365	3376	3391	rBV	163345	264544	57.45%	5.916%
32	12.311	3404	3412	3422	rVB	3241	4892	1.06%	0.109%
33	12.549	3477	3486	3493	rBV7	3888	6075	1.32%	0.136%
34	12.889	3580	3592	3607	rBV2	55221	86489	18.78%	1.934%
35	13.063	3635	3646	3656	rBV4	7185	11595	2.52%	0.259%
36	14.449	4070	4077	4091	rBV4	4563	6261	1.36%	0.140%

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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_U\Method\SFAMUTR011822WMA.M
Title : TRACE VOA SFAM1.0

37	14.735	4154	4166	4178	rVB4	19726	30209	6.56%	0.676%
38	15.401	4365	4373	4383	rBV2	6498	9356	2.03%	0.209%

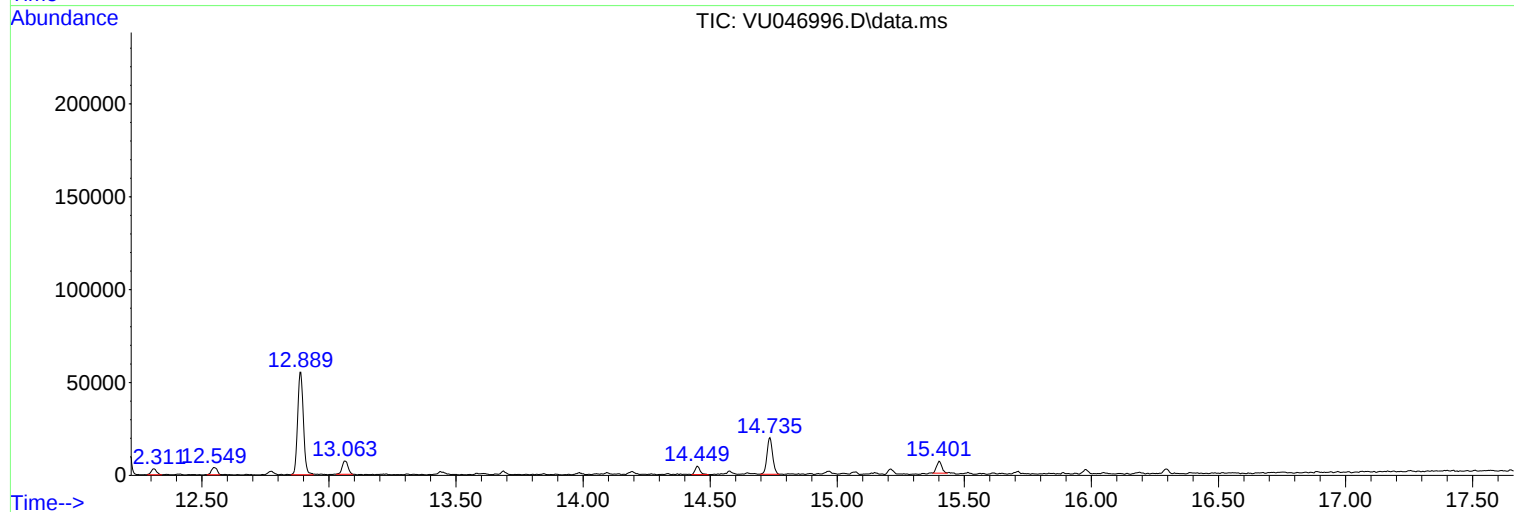
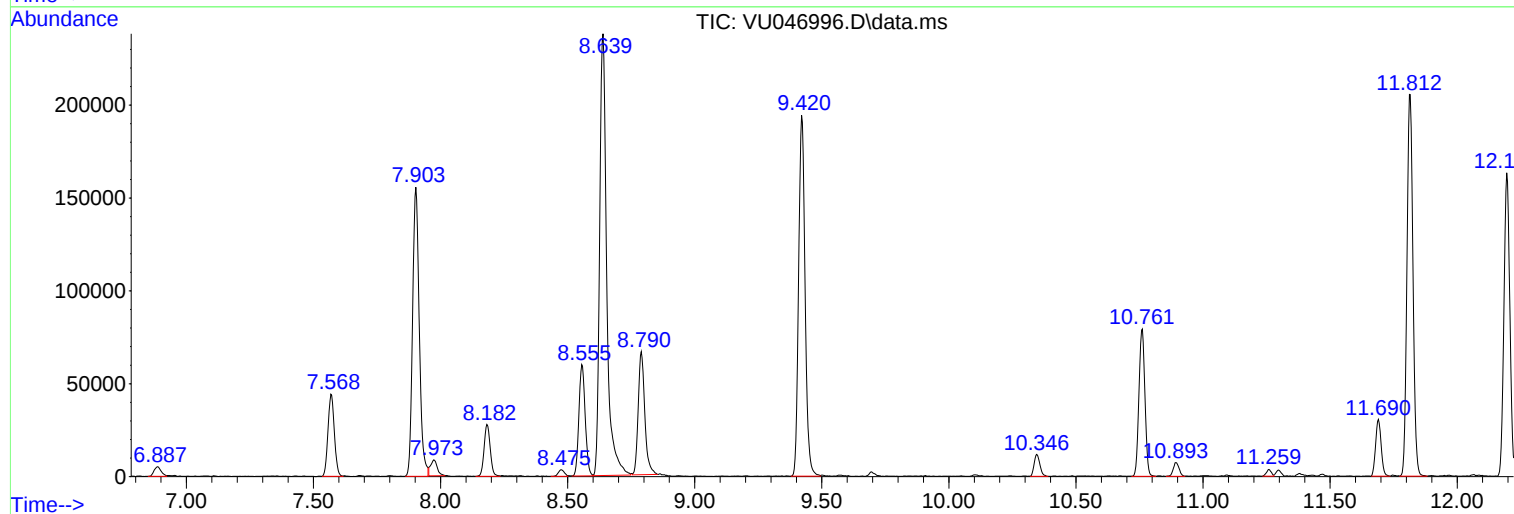
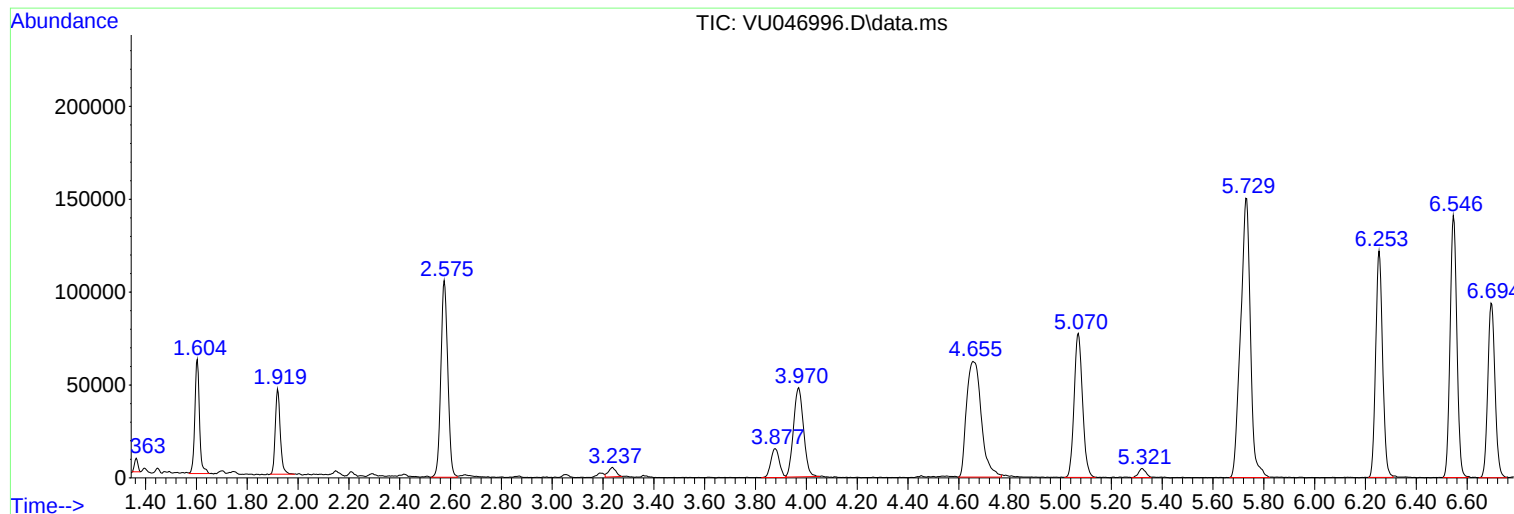
Sum of corrected areas: 4471500

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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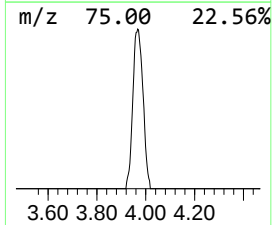
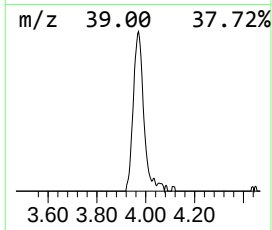
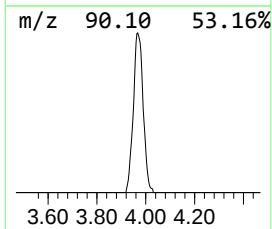
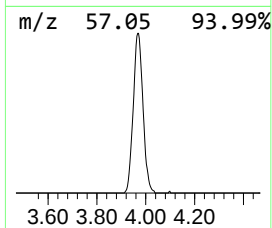
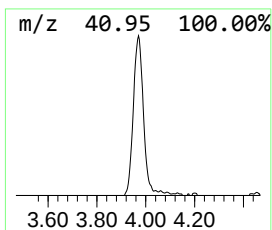
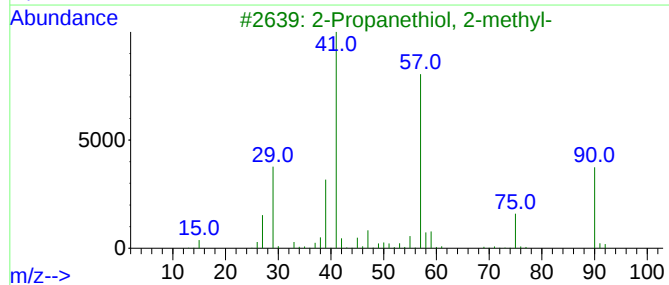
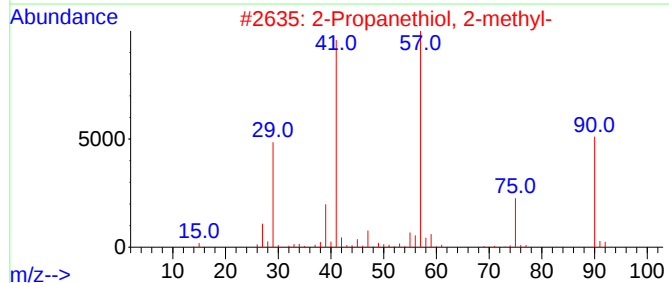
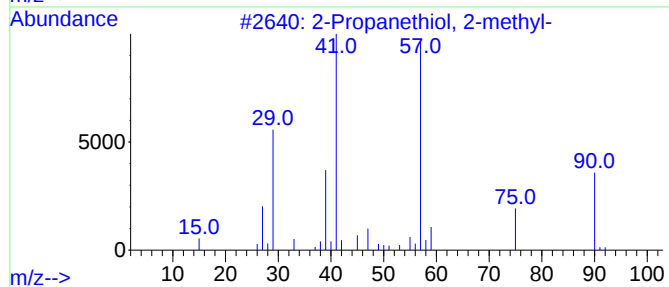
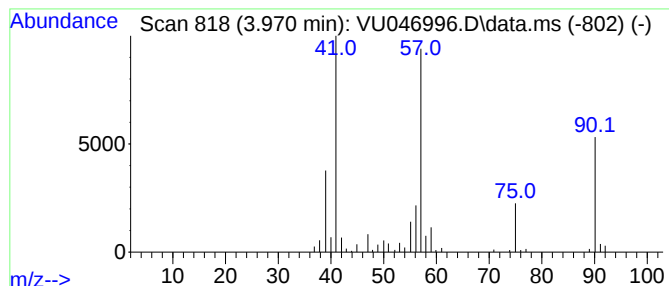
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 2-Propanethiol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.970	2.85 ug/L	131419	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-			90	C4H10S	000075-66-1	87
2	2-Propanethiol, 2-methyl-			90	C4H10S	000075-66-1	87
3	2-Propanethiol, 2-methyl-			90	C4H10S	000075-66-1	80
4	2-Propanethiol, 2-methyl-			90	C4H10S	000075-66-1	64
5	2-Butanethiol			90	C4H10S	000513-53-1	36



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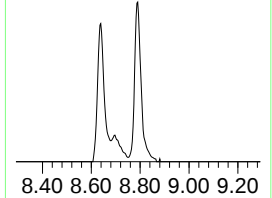
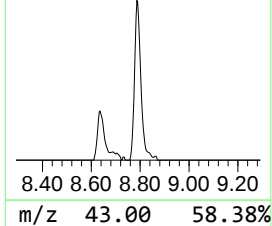
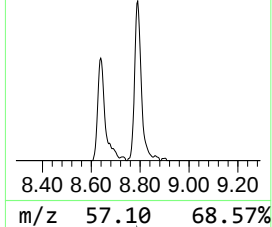
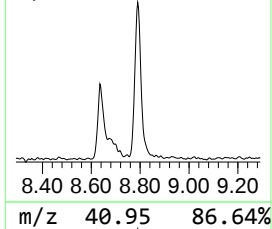
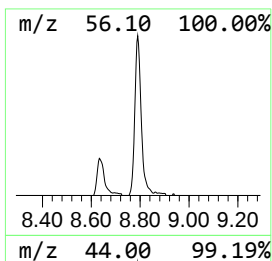
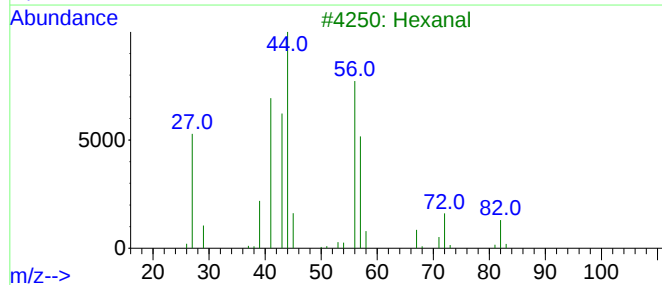
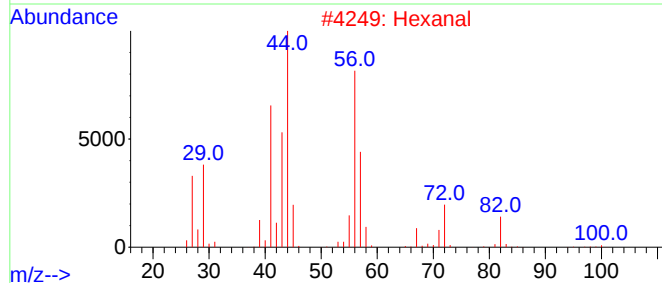
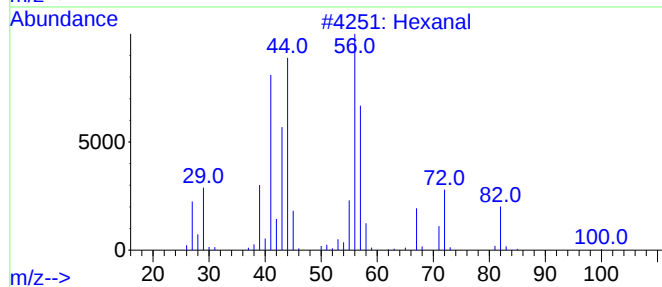
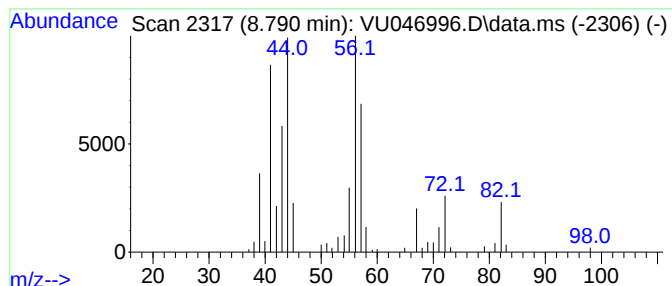
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.790	1.73 ug/L	118996	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	90
2	Hexanal			100	C6H12O	000066-25-1	86
3	Hexanal			100	C6H12O	000066-25-1	86
4	Hexanal			100	C6H12O	000066-25-1	78
5	Hexanal			100	C6H12O	000066-25-1	78



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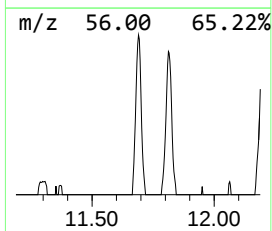
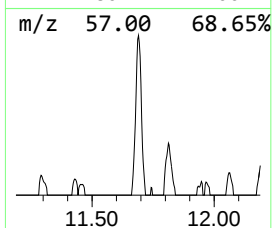
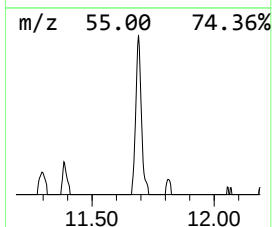
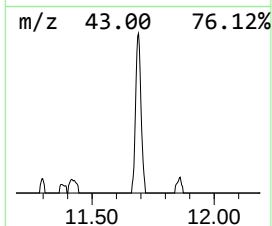
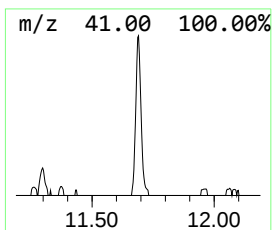
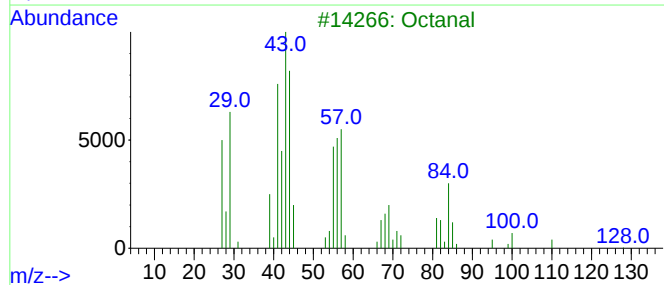
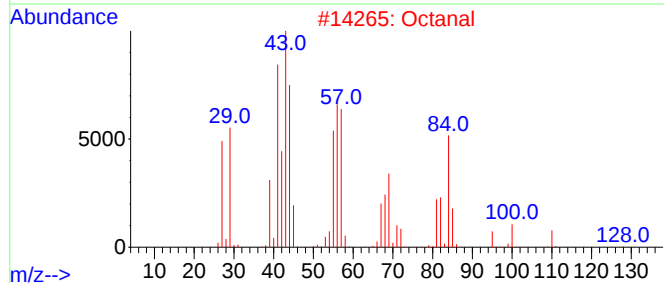
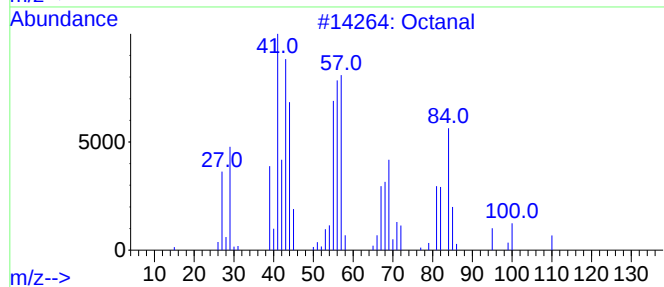
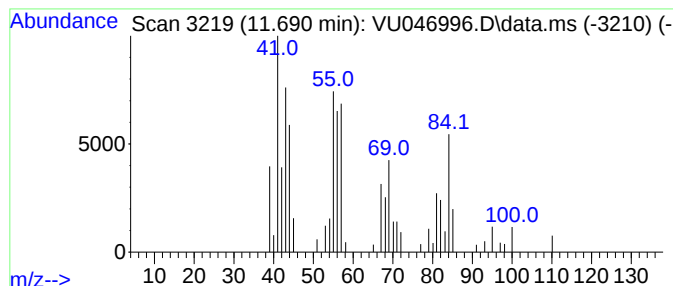
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Octanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.690	0.69 ug/L	46188	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal			128	C8H16O	000124-13-0	91
2	Octanal			128	C8H16O	000124-13-0	91
3	Octanal			128	C8H16O	000124-13-0	86
4	Octanal			128	C8H16O	000124-13-0	86
5	Octanal			128	C8H16O	000124-13-0	86



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ClientSampleId :
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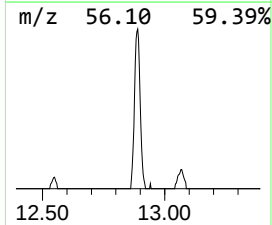
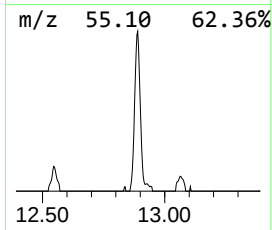
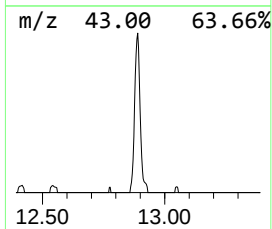
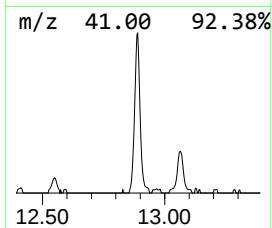
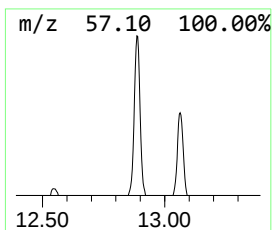
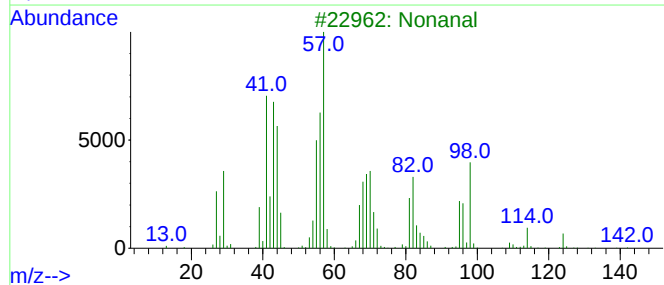
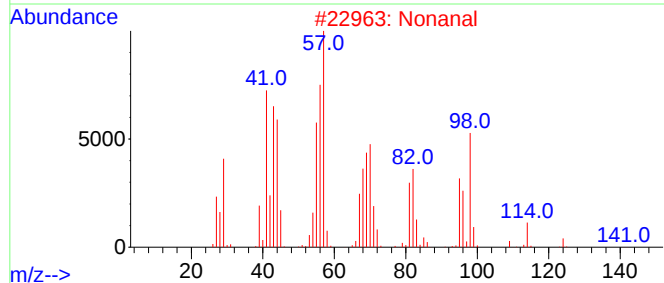
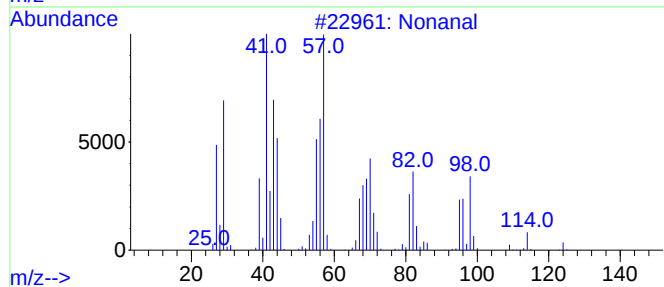
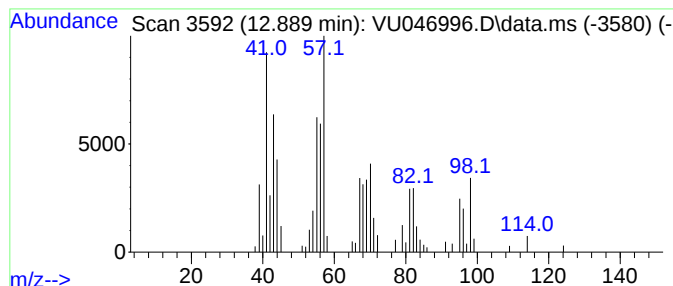
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.890	1.29 ug/L	86489	1,4-Dichlorobenzene-d4	11.816

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	80
4			2-Nonen-1-ol, (E)-	142	C9H18O	031502-14-4	38
5			2-Nonen-1-ol	142	C9H18O	022104-79-6	35



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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
2-Propanethiol,...	3.970	2.9	ug/L	131419	1	6.253	230911	5.0
Hexanal	8.790	1.7	ug/L	118996	2	9.420	343493	5.0
Octanal	11.690	0.7	ug/L	46188	3	11.816	336029	5.0
Nonanal	12.890	1.3	ug/L	86489	3	11.816	336029	5.0