

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV022122\
 Data File : VV024771.D
 Acq On : 21 Feb 2022 13:09
 Operator : SY/MD
 Sample : N1625-01
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFY08

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\SFAMVTR021722WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV024771.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.111	15	22	37	rVB	250954	231440	35.54%	3.275%
2	1.179	38	43	46	rBV	10725	9781	1.50%	0.138%
3	1.204	46	51	61	rVB2	82821	85156	13.08%	1.205%
4	1.304	73	82	91	rBV2	168692	241172	37.03%	3.413%
5	1.420	112	118	130	rVB3	18243	23648	3.63%	0.335%
6	1.571	155	165	177	rVB	77131	92686	14.23%	1.312%
7	1.635	178	185	194	rVB	12225	14899	2.29%	0.211%
8	1.770	218	227	233	rBV	26579	34396	5.28%	0.487%
9	1.809	233	239	256	rVB4	19460	34910	5.36%	0.494%
10	1.986	284	294	301	rBV4	10000	15217	2.34%	0.215%
11	2.117	322	335	349	rBV4	297992	503824	77.36%	7.130%
12	2.452	427	439	449	rBV5	2970	7801	1.20%	0.110%
13	2.957	585	596	610	rVB5	5587	12144	1.86%	0.172%
14	3.191	652	669	693	rBV	308982	651252	100.00%	9.217%
15	3.896	877	888	945	rBV	47725	177152	27.20%	2.507%
16	4.352	1013	1030	1061	rBV	93234	248815	38.21%	3.521%
17	4.612	1094	1111	1129	rBV2	46380	119772	18.39%	1.695%
18	5.050	1231	1247	1294	rBV2	209681	545982	83.84%	7.727%
19	5.616	1410	1423	1454	rBV	194809	394594	60.59%	5.584%
20	5.915	1504	1516	1545	rBV2	108349	221109	33.95%	3.129%
21	6.069	1549	1564	1590	rBV	119071	245584	37.71%	3.476%
22	6.304	1628	1637	1656	rBV4	5650	13598	2.09%	0.192%
23	6.989	1838	1850	1875	rBV	57689	107275	16.47%	1.518%
24	7.317	1940	1952	1970	rBV	254038	443163	68.05%	6.272%
25	7.394	1970	1976	1992	rVB2	8644	17226	2.65%	0.244%
26	7.625	2038	2048	2070	rBV	31296	56654	8.70%	0.802%
27	7.979	2148	2158	2170	rVB3	20296	36507	5.61%	0.517%
28	8.088	2182	2192	2230	rBV	224603	445624	68.43%	6.306%
29	8.239	2230	2239	2265	rVV2	66709	119007	18.27%	1.684%
30	8.850	2418	2429	2454	rBV	281556	467572	71.80%	6.617%
31	9.808	2719	2727	2741	rBV2	24180	40455	6.21%	0.573%
32	10.214	2842	2853	2871	rVB	72477	113769	17.47%	1.610%
33	10.718	3001	3010	3020	rBV2	17129	25226	3.87%	0.357%
34	11.149	3134	3144	3156	rBV2	56514	87338	13.41%	1.236%
35	11.246	3164	3174	3194	rVB	286097	444927	68.32%	6.297%
36	11.622	3279	3291	3313	rVB	227553	359644	55.22%	5.090%

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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

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Peak separation: 5

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Title : TRACE VOA SFAM1.0

37	12.342	3500	3515	3531	rBV	224148	341244	52.40%	4.829%
38	14.175	4075	4085	4103	rBV4	21776	35577	5.46%	0.503%

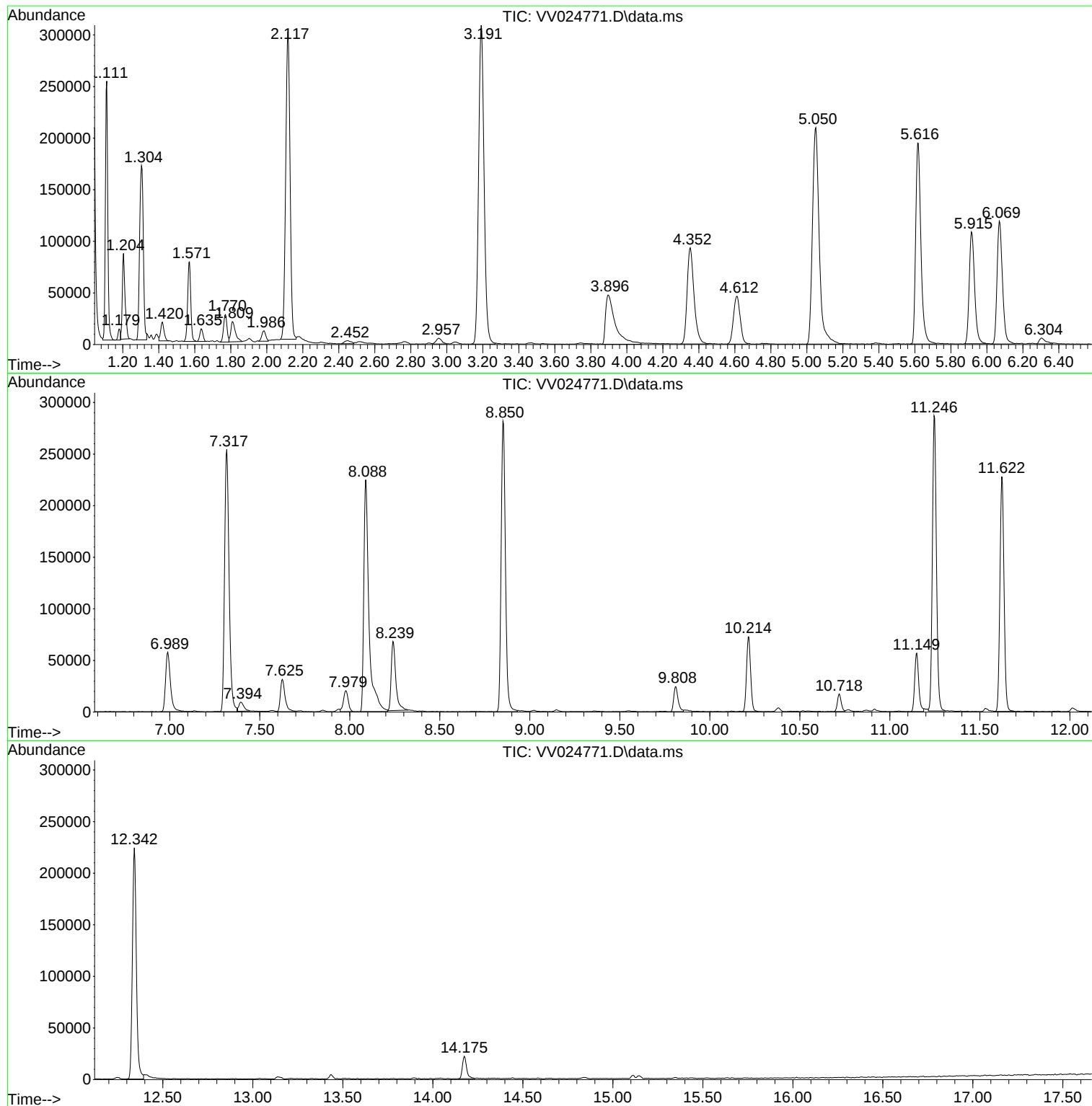
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TIC Library : C:\Database\NIST20.L
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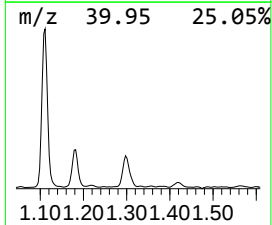
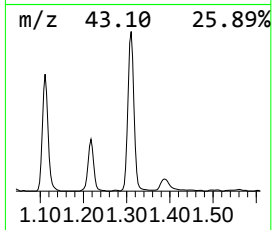
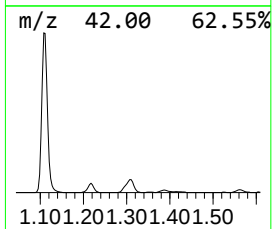
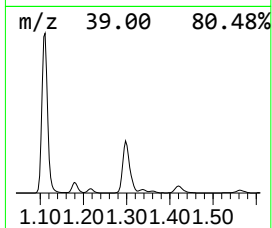
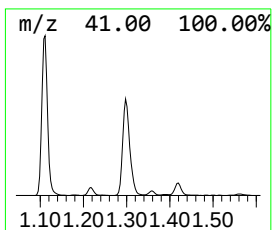
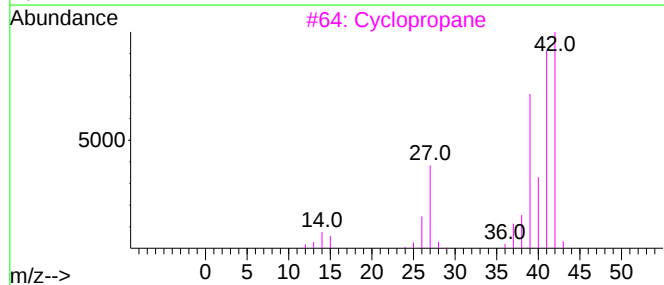
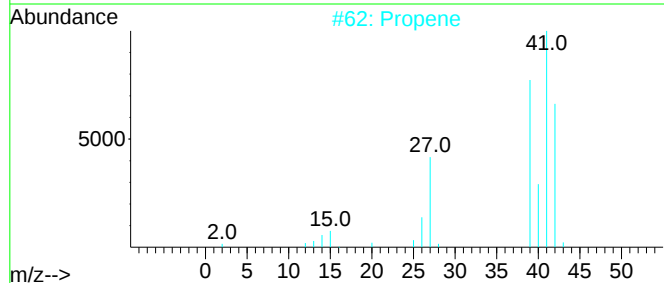
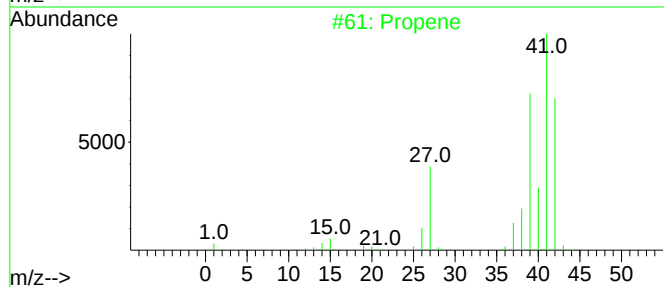
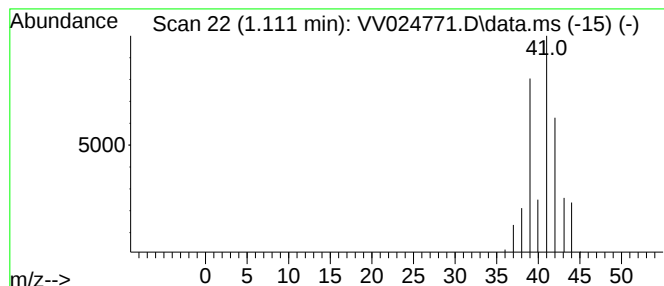
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR021722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.111	2.93 ug/L	231440	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Propene	42	C3H6	000115-07-1	42
3			Cyclopropane	42	C3H6	000075-19-4	9
4			Cyclopropene	40	C3H4	002781-85-3	9
5			Cyclopropane	42	C3H6	000075-19-4	7



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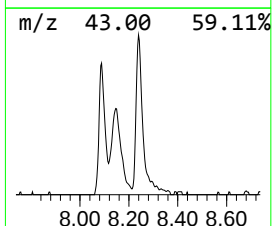
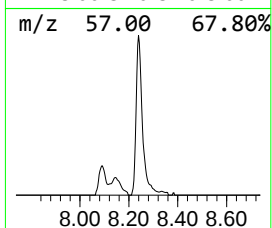
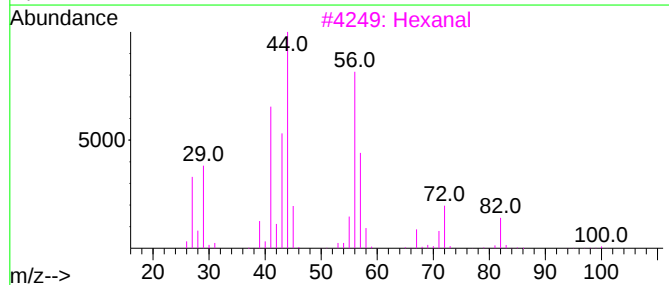
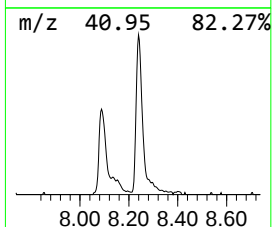
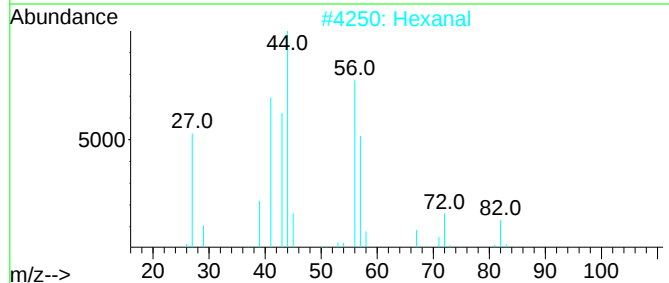
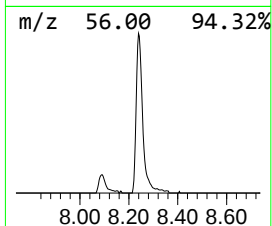
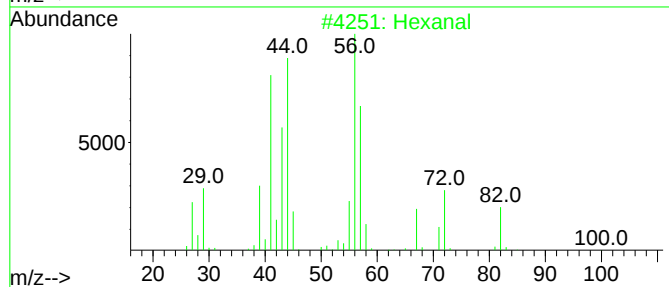
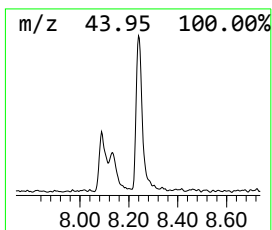
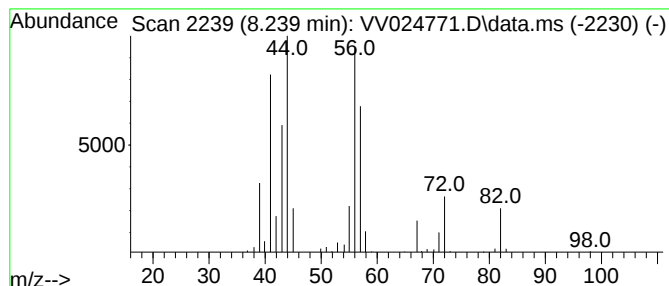
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR021722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.239	1.27 ug/L	119007	Chlorobenzene-d5	8.850

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	83
4	Hexanal			100	C6H12O	000066-25-1	83
5	Hexanal			100	C6H12O	000066-25-1	72



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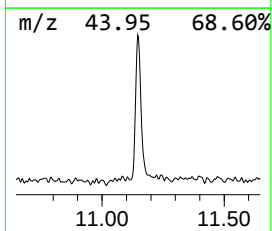
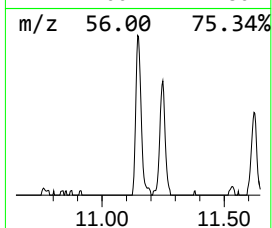
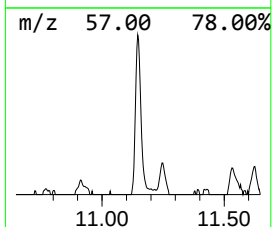
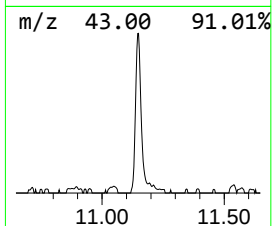
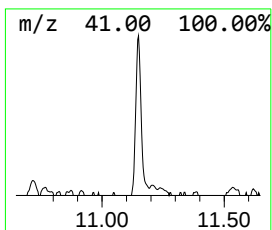
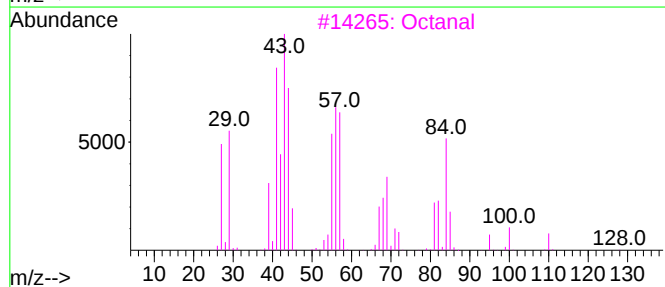
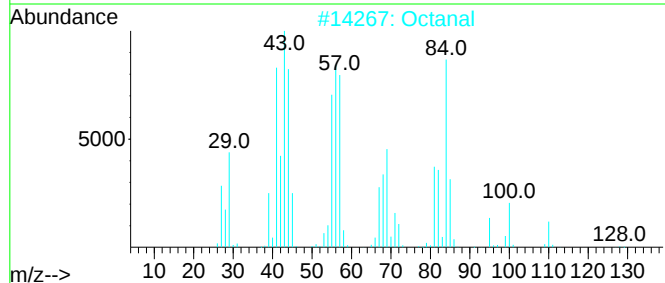
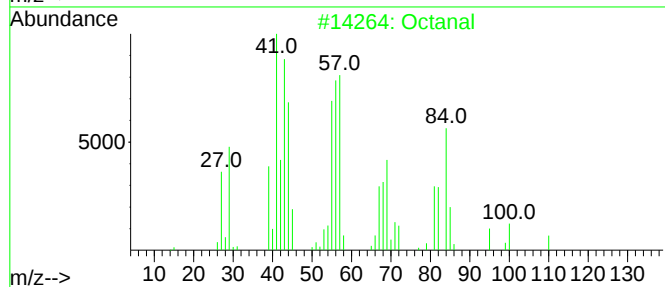
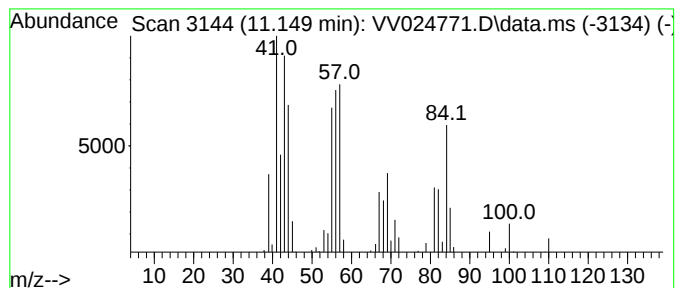
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Octanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.149	0.98 ug/L	87338	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal			128	C8H16O	000124-13-0	91
2	Octanal			128	C8H16O	000124-13-0	87
3	Octanal			128	C8H16O	000124-13-0	86
4	Octanal			128	C8H16O	000124-13-0	50
5	Piperazine, 2-methyl-			100	C5H12N2	000109-07-9	43



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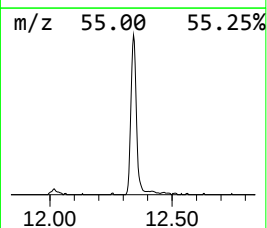
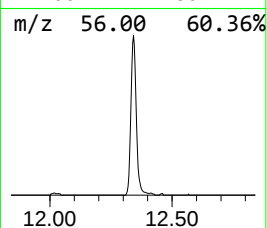
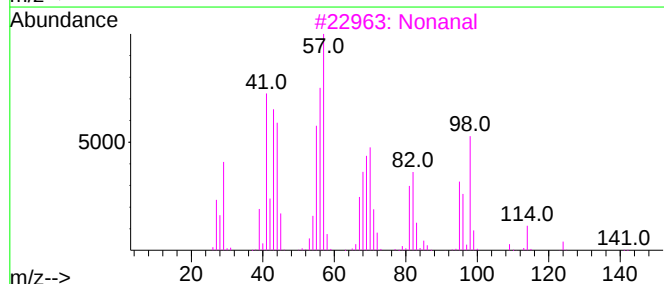
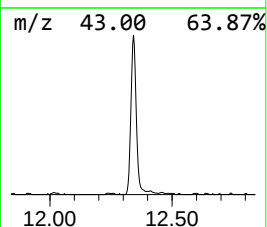
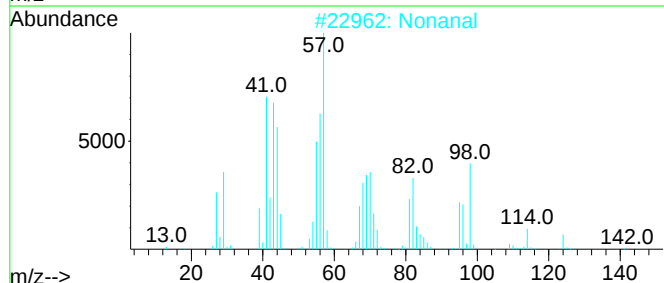
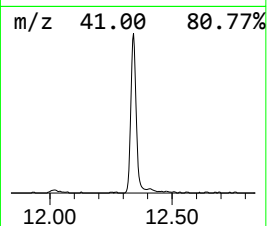
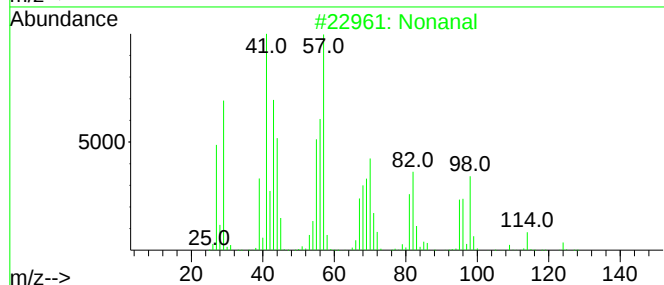
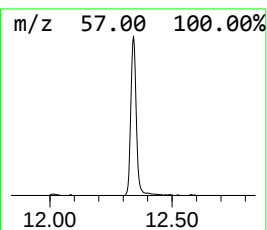
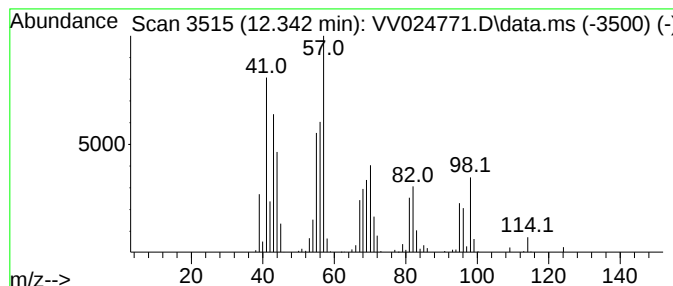
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
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Peak Number 6 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.342	3.83 ug/L	341244	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	91
2			Nonanal	142	C9H18O	000124-19-6	91
3			Nonanal	142	C9H18O	000124-19-6	90
4			Nonanal	142	C9H18O	000124-19-6	90
5			Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27



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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
(DEL) Alkane: S...	1.111	2.9	ug/L	231440	1	5.619	394594	5.0
Hexanal	8.239	1.3	ug/L	119007	2	8.850	467572	5.0
Octanal	11.149	1.0	ug/L	87338	3	11.249	444927	5.0
Nonanal	12.342	3.8	ug/L	341244	3	11.249	444927	5.0