

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012623\
 Data File : VV029961.D
 Acq On : 26 Jan 2023 14:10
 Operator : SY/MD
 Sample : VIBLK272
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VIBLK272

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\SFAMVTR011223WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV029961.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	77	82	101	rVB	186015	228585	25.92%	2.672%
2	1.384	102	107	122	rVB	34258	45165	5.12%	0.528%
3	1.564	157	163	178	rVB	144837	167100	18.95%	1.953%
4	2.050	306	314	322	rBV	38583	63929	7.25%	0.747%
5	2.105	322	331	345	rVB	250206	368008	41.73%	4.302%
6	2.500	446	454	465	rVB2	6907	11347	1.29%	0.133%
7	3.883	871	884	918	rBV	86945	276372	31.34%	3.231%
8	4.336	1006	1025	1053	rBV	160365	421471	47.79%	4.927%
9	5.037	1224	1243	1273	rBV2	353021	881973	100.00%	10.310%
10	5.606	1402	1420	1444	rBV	286321	582958	66.10%	6.814%
11	6.059	1544	1561	1583	rBV	203889	423840	48.06%	4.954%
12	6.976	1832	1846	1876	rBV	94271	177751	20.15%	2.078%
13	7.156	1881	1902	1906	rBV3	9667	28324	3.21%	0.331%
14	7.304	1936	1948	1981	rVB	427425	777239	88.13%	9.085%
15	7.609	2033	2043	2061	rVB	56664	98648	11.18%	1.153%
16	8.082	2178	2190	2223	rBV	390854	721306	81.78%	8.432%
17	8.233	2230	2237	2250	rVB8	5005	9958	1.13%	0.116%
18	8.841	2414	2426	2447	rBV	425819	688388	78.05%	8.047%
19	10.011	2776	2790	2807	rBV	5980	18356	2.08%	0.215%
20	10.204	2831	2850	2865	rBV	144560	230975	26.19%	2.700%
21	10.596	2958	2972	2974	rBV7	5762	10178	1.15%	0.119%
22	11.140	3132	3141	3149	rBV7	6012	9751	1.11%	0.114%
23	11.236	3159	3171	3189	rBV	464812	716327	81.22%	8.373%
24	11.609	3273	3287	3307	rBV	399303	630185	71.45%	7.367%
25	11.789	3333	3343	3356	rBV2	36809	64086	7.27%	0.749%
26	12.333	3504	3512	3524	rVB2	6905	11347	1.29%	0.133%
27	12.834	3657	3668	3678	rBV2	77037	123090	13.96%	1.439%
28	12.947	3695	3703	3714	rVB5	19935	31604	3.58%	0.369%
29	13.082	3729	3745	3762	rBV6	21561	44173	5.01%	0.516%
30	13.419	3843	3850	3860	rVB6	5817	10614	1.20%	0.124%
31	14.316	4121	4129	4137	rBV7	7226	12156	1.38%	0.142%
32	14.802	4272	4280	4289	rBV2	44088	61443	6.97%	0.718%
33	14.889	4302	4307	4315	rVB6	11789	15385	1.74%	0.180%
34	15.365	4446	4455	4474	rBV2	140400	228486	25.91%	2.671%
35	15.760	4570	4578	4594	rVB	81371	126111	14.30%	1.474%
36	16.281	4732	4740	4751	rBV	41323	61516	6.97%	0.719%

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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\SFAMVTR011223WMA.M
Title : TRACE VOA SFAM1.0

37	16.365	4759	4766	4778	rVB	38997	56646	6.42%	0.662%
38	16.545	4814	4822	4834	rBV	38690	65621	7.44%	0.767%
39	17.429	5090	5097	5111	rVB	32173	54322	6.16%	0.635%

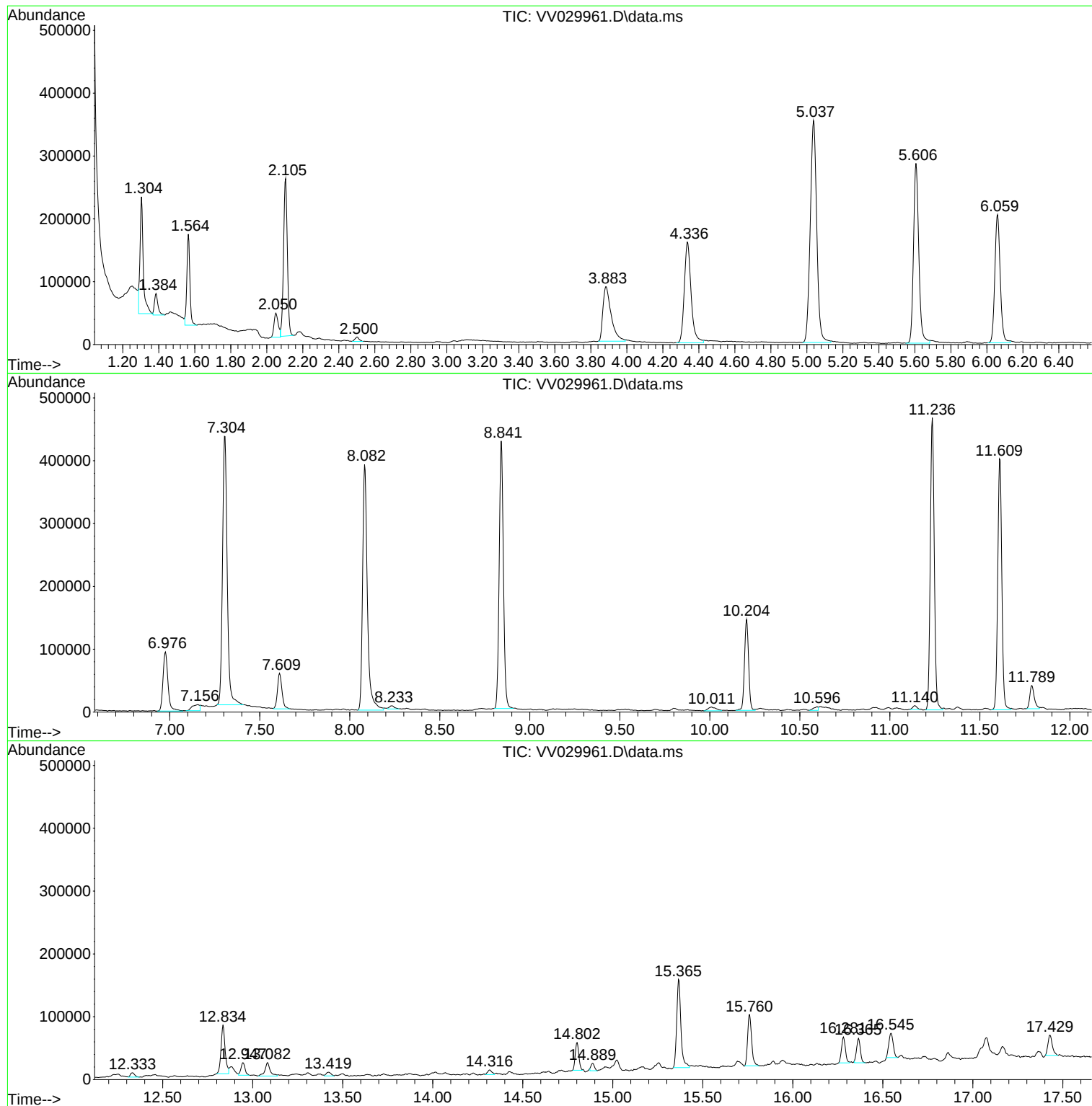
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Quant Title : TRACE VOA SFAM1.0

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



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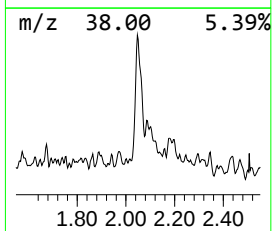
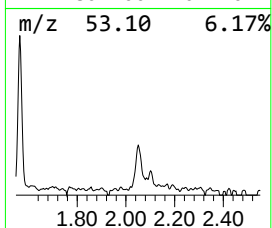
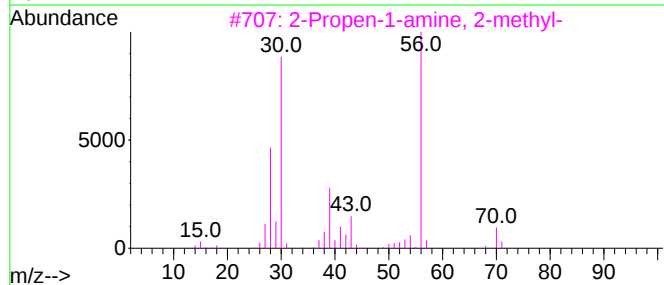
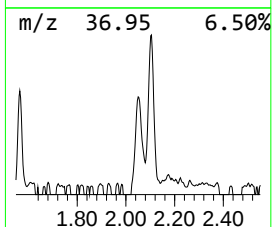
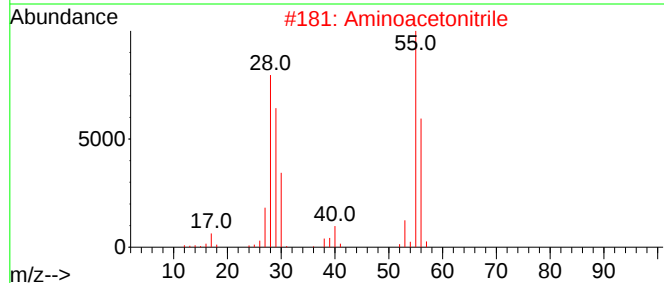
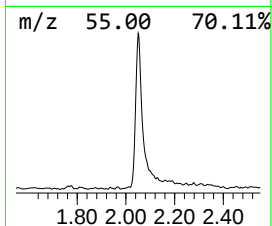
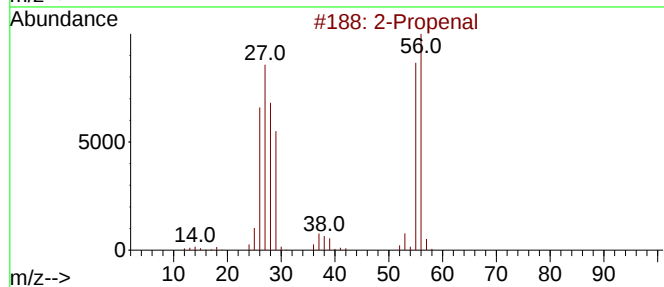
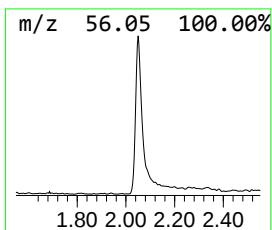
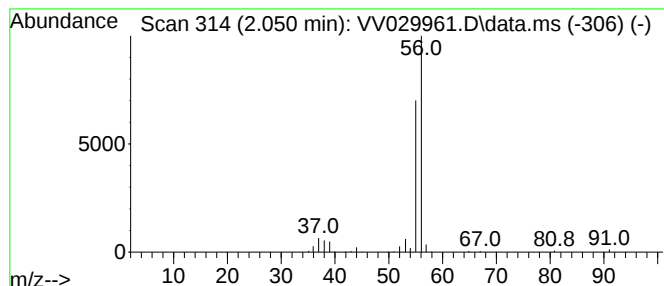
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 2-Propenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	0.55 ug/L	63929	1,4-Difluorobenzene	5.606

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propenal	56	C3H4O	000107-02-8	90
2		Aminoacetonitrile	56	C2H4N2	000540-61-4	9
3		2-Propen-1-amine, 2-methyl-	71	C4H9N	002878-14-0	9
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	9
5		2-Propenal	56	C3H4O	000107-02-8	7



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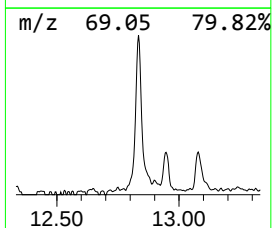
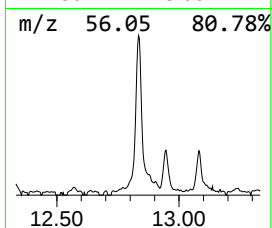
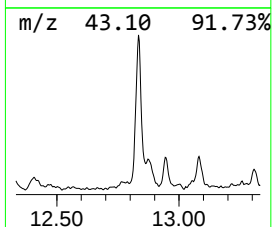
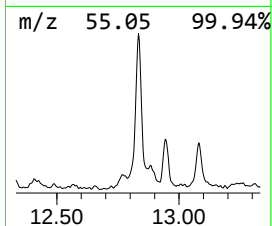
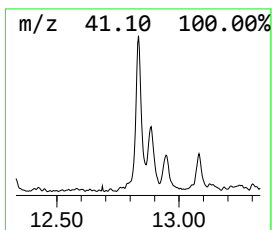
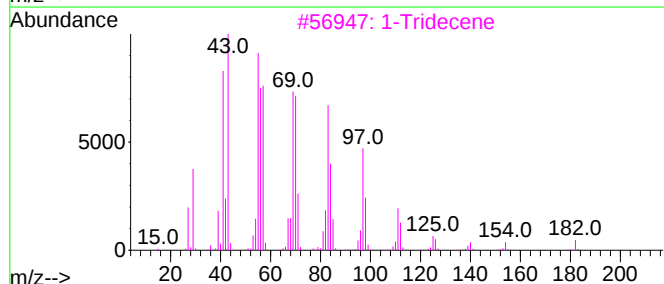
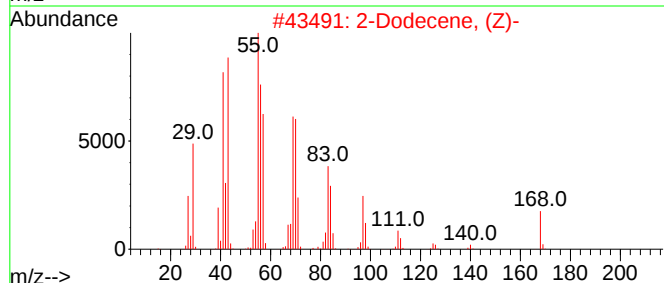
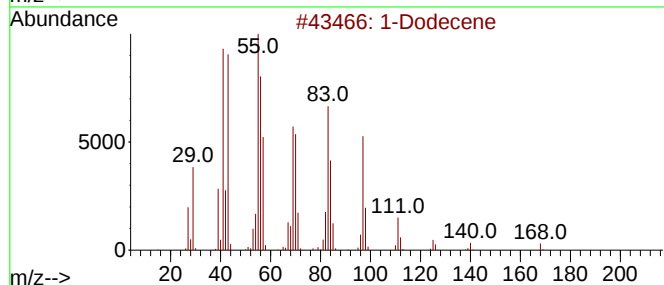
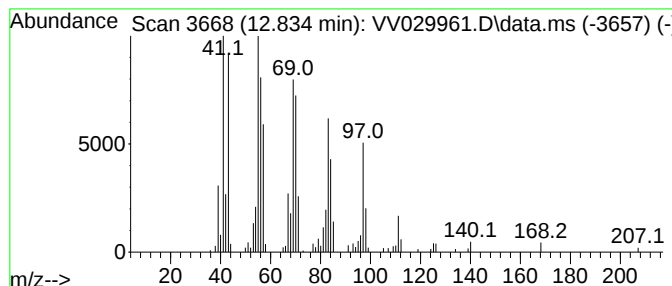
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011223WMA.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.834	0.86 ug/L	123090	1,4-Dichlorobenzene-d4	11.236

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Dodecene	168	C12H24	000112-41-4	96
2		2-Dodecene, (Z)-	168	C12H24	007206-26-0	93
3		1-Tridecene	182	C13H26	002437-56-1	91
4		1-Dodecene	168	C12H24	000112-41-4	91
5		Cyclododecane	168	C12H24	000294-62-2	87



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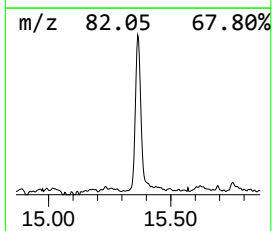
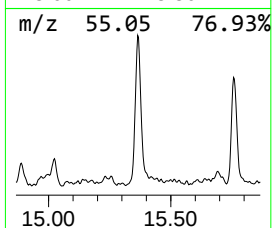
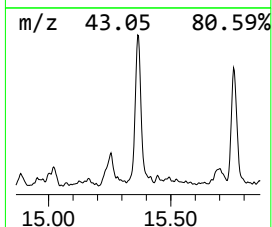
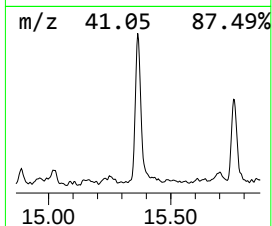
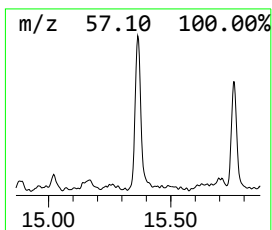
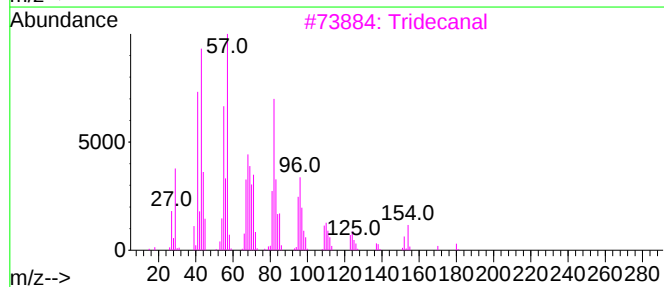
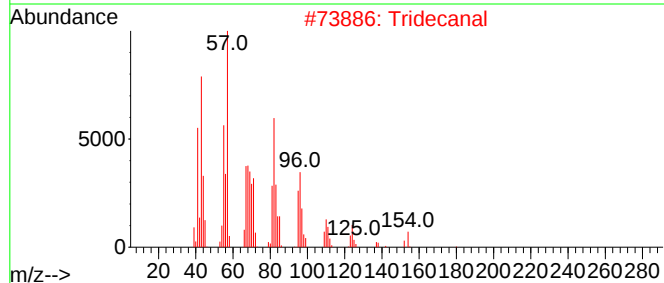
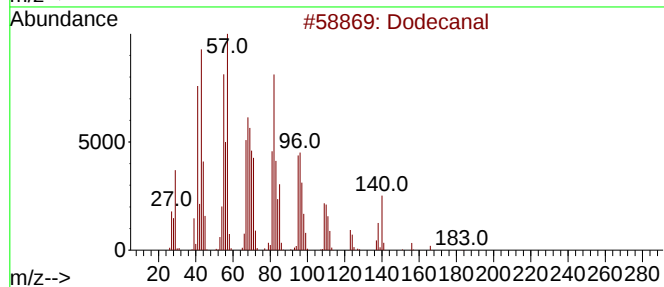
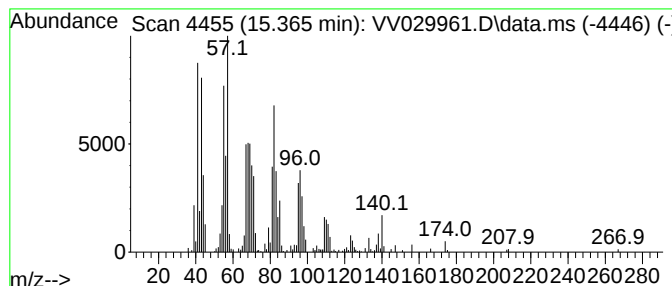
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011223WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Dodecanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.365	1.59 ug/L	228486	1,4-Dichlorobenzene-d4	11.236

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecanal	184	C12H24O	000112-54-9	95
2		Tridecanal	198	C13H26O	010486-19-8	91
3		Tridecanal	198	C13H26O	010486-19-8	90
4		Dodecanal	184	C12H24O	000112-54-9	87
5		Dodecanal	184	C12H24O	000112-54-9	87



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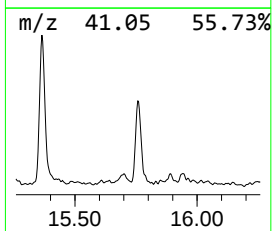
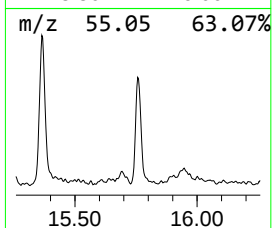
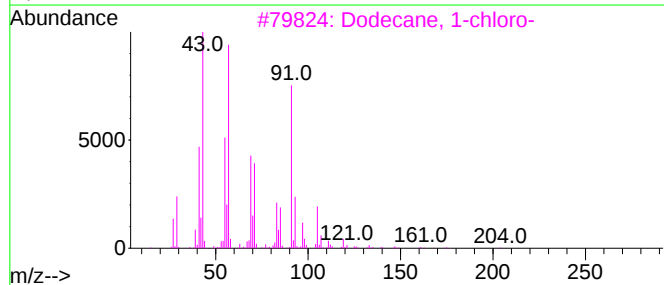
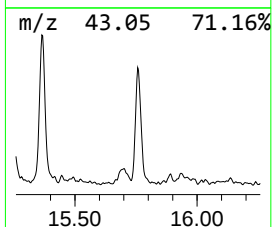
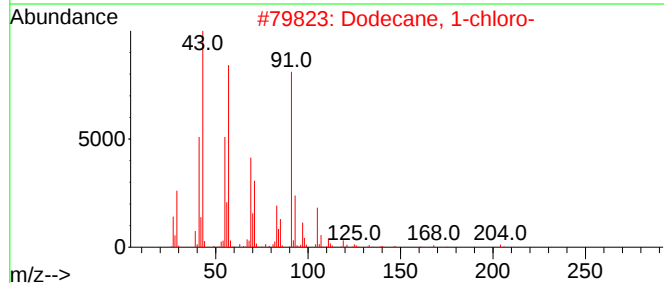
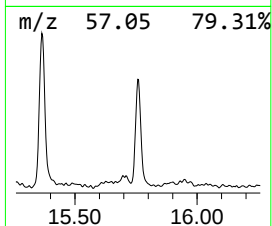
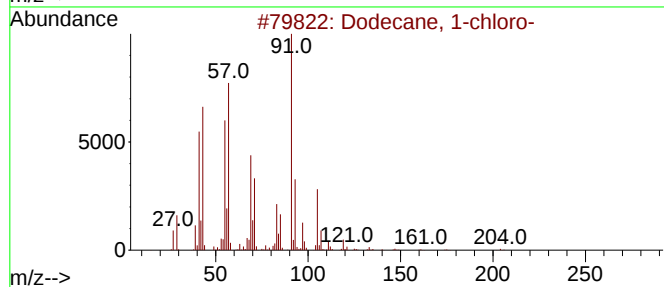
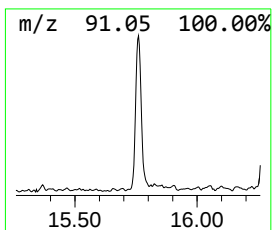
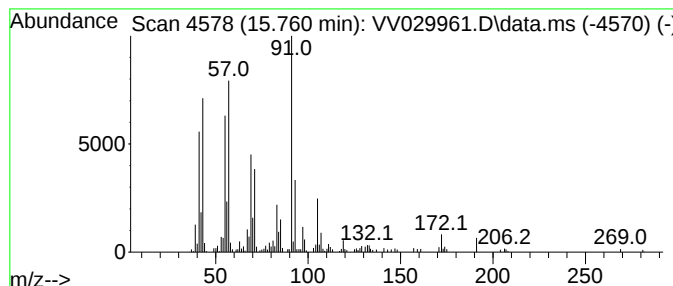
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Peak Number 5 Dodecane, 1-chloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.760	0.88 ug/L	126111	1,4-Dichlorobenzene-d4	11.236

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	98
2			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	95
3			Dodecane, 1-chloro-	204	C12H25Cl	000112-52-7	93
4			Decane, 1-chloro-	176	C10H21Cl	001002-69-3	83
5			1-Chloroundecane	190	C11H23Cl	002473-03-2	80



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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
2-Propenal	2.050	0.6	ug/L	63929	1	5.606	582958	5.0
(DEL) Alkane: S...	12.834	0.9	ug/L	123090	3	11.236	716327	5.0
Dodecanal	15.365	1.6	ug/L	228486	3	11.236	716327	5.0
Dodecane, 1-chl...	15.760	0.9	ug/L	126111	3	11.236	716327	5.0