

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062322\
 Data File : VV026527.D
 Acq On : 23 Jun 2022 20:19
 Operator : SY/MD
 Sample : N3400-12
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AD9

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\SFAMVTR062322WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV026527.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.121	19	25	42	rVB	66526	67865	9.11%	0.981%
2	1.227	52	58	62	rBV	16079	14813	1.99%	0.214%
3	1.317	77	86	97	rBV2	188045	223678	30.03%	3.235%
4	1.426	115	120	129	rVB3	15320	18777	2.52%	0.272%
5	1.577	159	167	180	rBV	111267	140398	18.85%	2.030%
6	1.645	184	188	196	rVB2	10779	13016	1.75%	0.188%
7	1.777	223	229	236	rBV	20186	24048	3.23%	0.348%
8	1.815	237	241	250	rVB3	9209	11321	1.52%	0.164%
9	2.118	326	335	351	rVB	217344	319653	42.91%	4.623%
10	2.224	354	368	374	rBV2	7531	18508	2.48%	0.268%
11	2.519	452	460	473	rVB3	6315	11062	1.49%	0.160%
12	3.931	882	899	942	rBV3	39695	201517	27.05%	2.914%
13	4.359	1015	1032	1062	rBV	127109	313388	42.07%	4.532%
14	5.053	1233	1248	1284	rBV2	290466	744871	100.00%	10.773%
15	5.622	1413	1425	1460	rBV	238757	489612	65.73%	7.081%
16	6.076	1552	1566	1590	rBV	157417	323963	43.49%	4.685%
17	6.992	1841	1851	1867	rBV	57555	106894	14.35%	1.546%
18	7.317	1939	1952	1967	rBV	337459	591439	79.40%	8.554%
19	7.394	1967	1976	1997	rVB	62167	122107	16.39%	1.766%
20	7.629	2038	2049	2071	rBV2	30545	57831	7.76%	0.836%
21	8.095	2183	2194	2231	rBV	221837	473123	63.52%	6.843%
22	8.854	2419	2430	2454	rBV	352518	589315	79.12%	8.523%
23	9.021	2473	2482	2490	rBV2	5741	9541	1.28%	0.138%
24	9.143	2507	2520	2538	rBV2	18903	31987	4.29%	0.463%
25	9.548	2637	2646	2657	rBV	11469	18619	2.50%	0.269%
26	9.712	2689	2697	2708	rBV2	9261	16641	2.23%	0.241%
27	10.217	2842	2854	2871	rBV	106865	169106	22.70%	2.446%
28	10.384	2889	2906	2915	rVB3	8815	15193	2.04%	0.220%
29	10.452	2919	2927	2940	rBV2	6547	12267	1.65%	0.177%
30	10.915	3061	3071	3087	rBV	17909	27996	3.76%	0.405%
31	11.024	3096	3105	3106	rBV3	7713	8324	1.12%	0.120%
32	11.249	3163	3175	3193	rBV	336491	523482	70.28%	7.571%
33	11.336	3196	3202	3211	rVB2	8885	12346	1.66%	0.179%
34	11.529	3251	3262	3281	rBV	219934	417461	56.04%	6.038%
35	11.622	3281	3291	3312	rVB	327432	528592	70.96%	7.645%
36	12.233	3472	3481	3495	rBV3	34921	56071	7.53%	0.811%

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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\SFAMVTR062322WMA.M
Title : TRACE VOA SFAM1.0

37	12.468	3545	3554	3565	rVB2	4690	8012	1.08%	0.116%
38	12.882	3671	3683	3692	rBV4	7195	10338	1.39%	0.150%
39	13.320	3808	3819	3837	rBV	83267	132506	17.79%	1.916%
40	13.506	3868	3877	3892	rBV	9396	16070	2.16%	0.232%
41	16.178	4700	4708	4716	rBV4	16152	22708	3.05%	0.328%

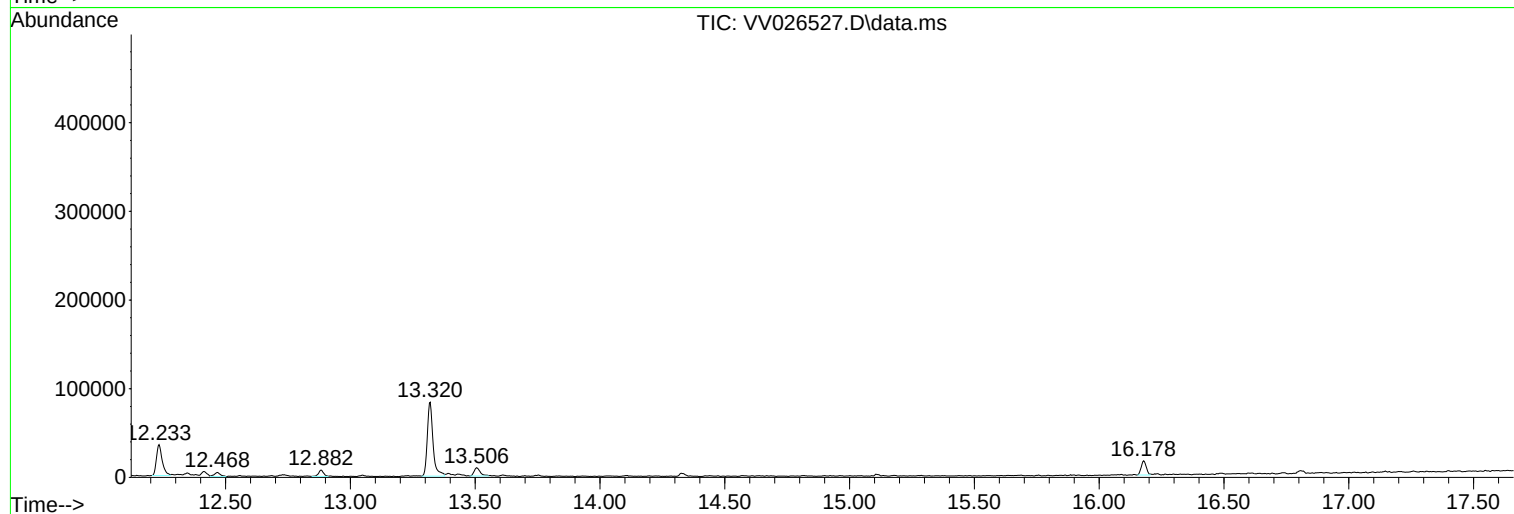
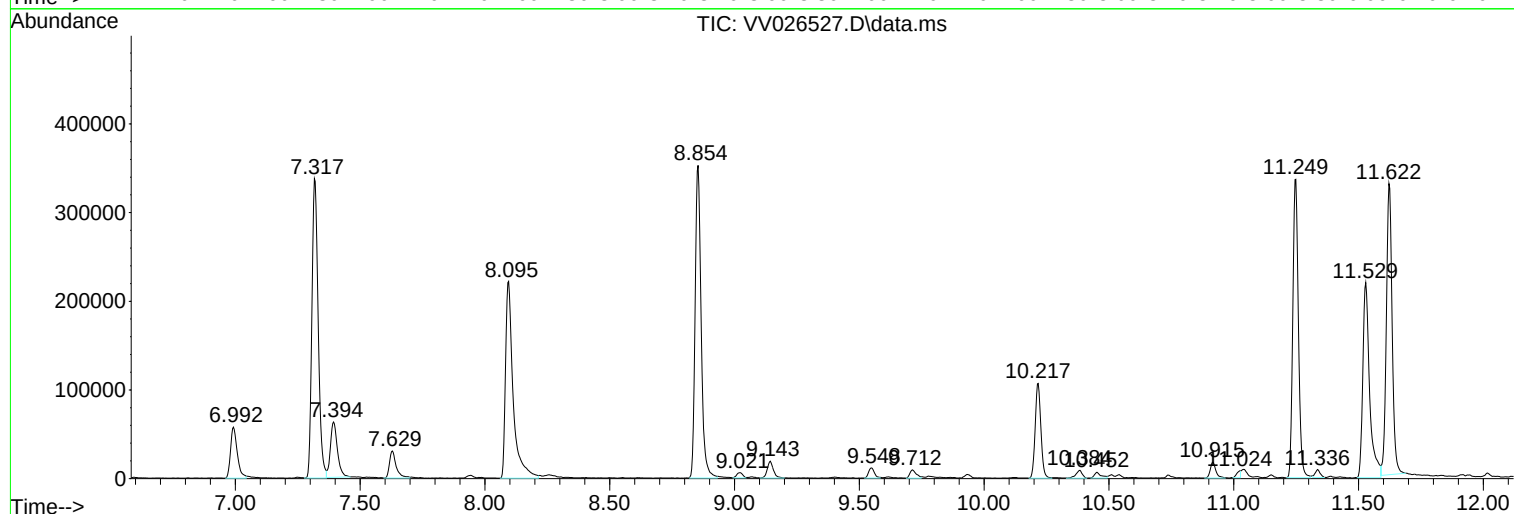
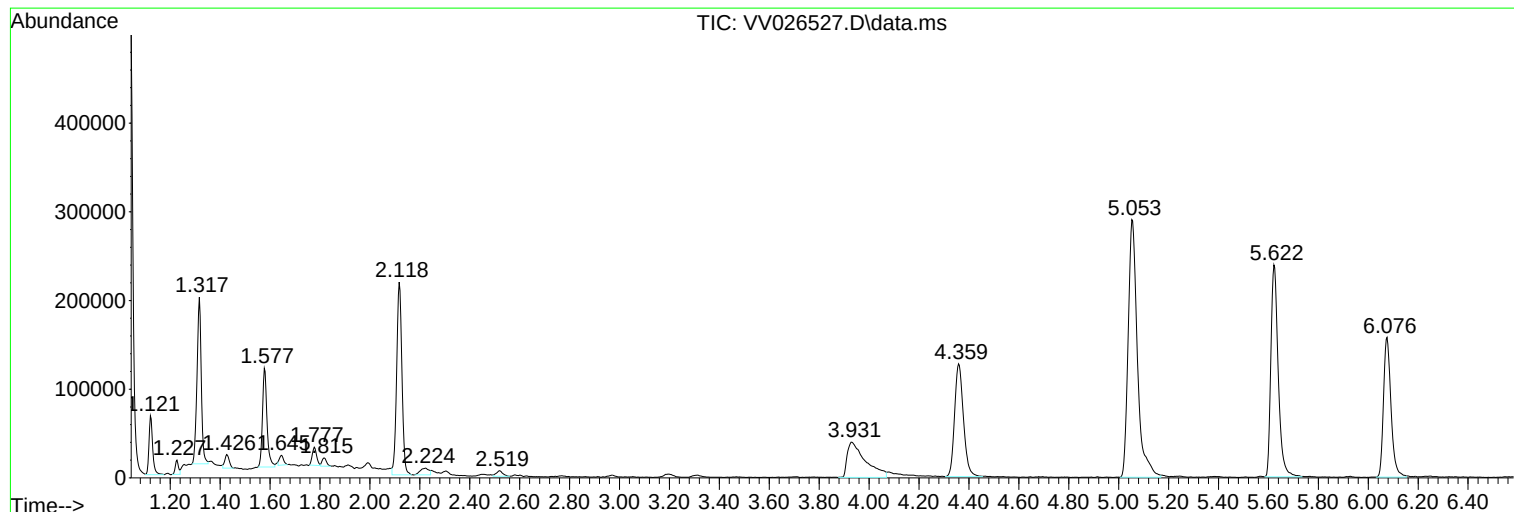
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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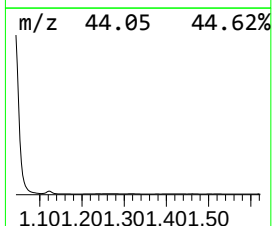
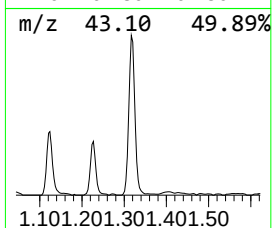
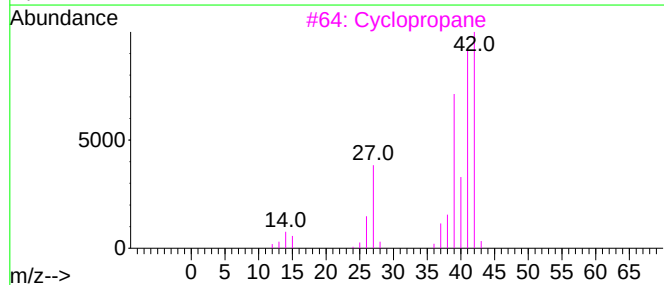
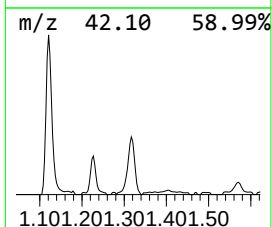
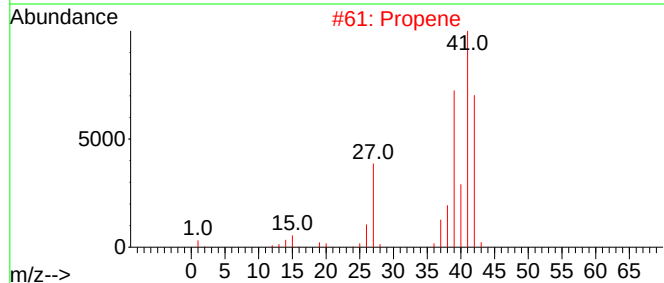
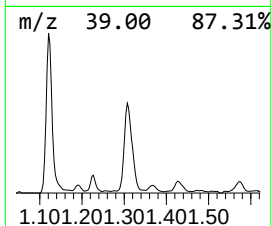
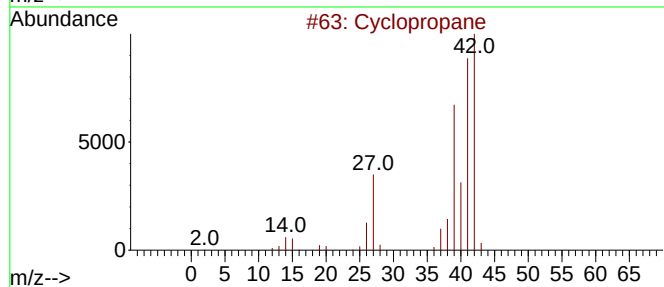
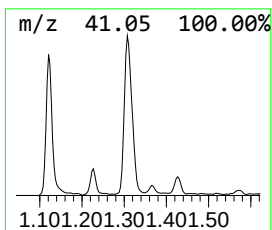
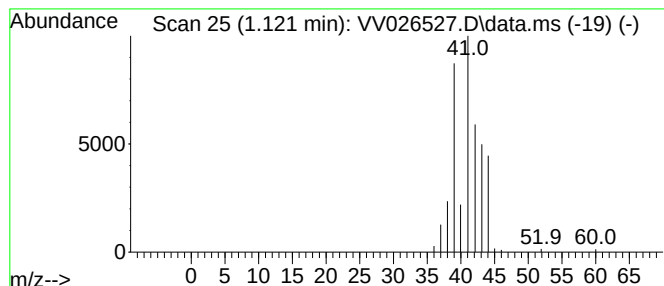
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Cyclic1.121 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.121	0.69 ug/L	67865	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane	42	C3H6	000075-19-4	40
2			Propene	42	C3H6	000115-07-1	10
3			Cyclopropane	42	C3H6	000075-19-4	7
4			2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	4
5			Methylenecyclopropane	54	C4H6	006142-73-0	2



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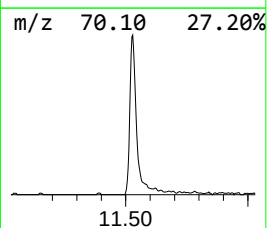
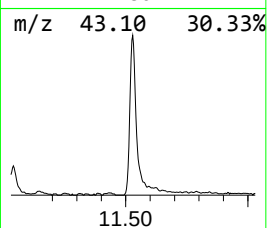
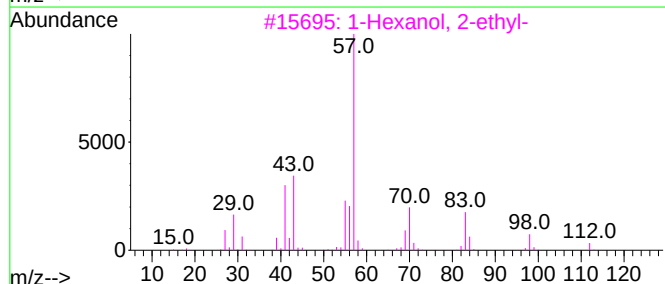
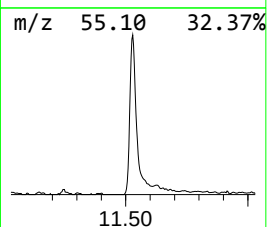
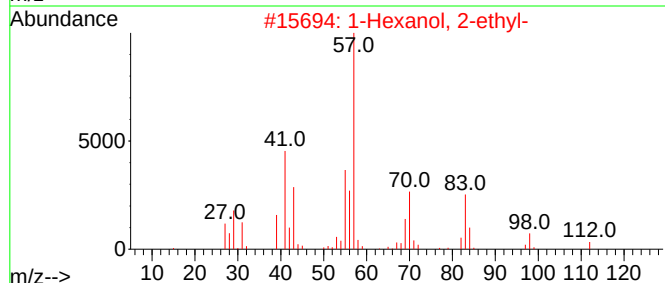
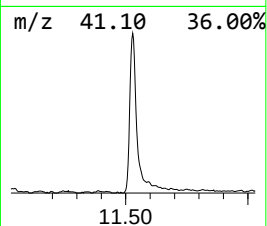
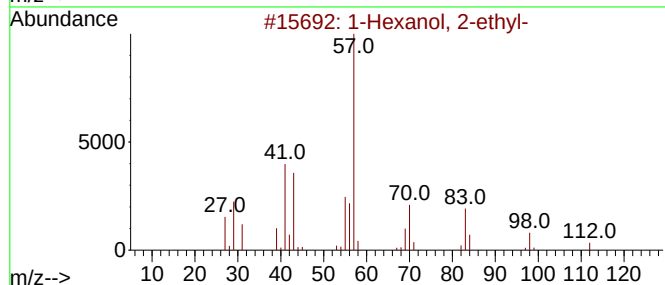
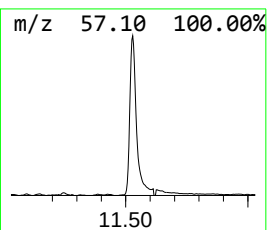
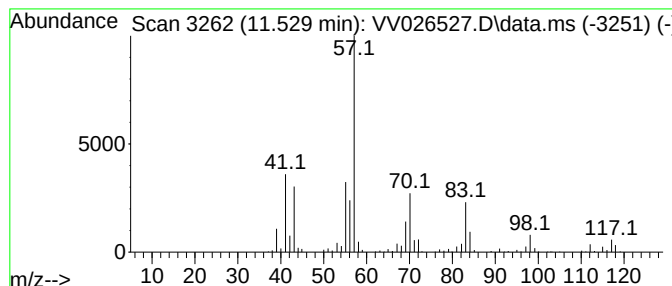
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.529	3.99 ug/L	417461	1,4-Dichlorobenzene-d4	11.249

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	72
5		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59



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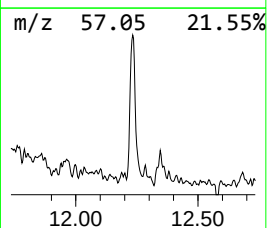
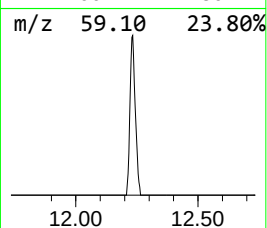
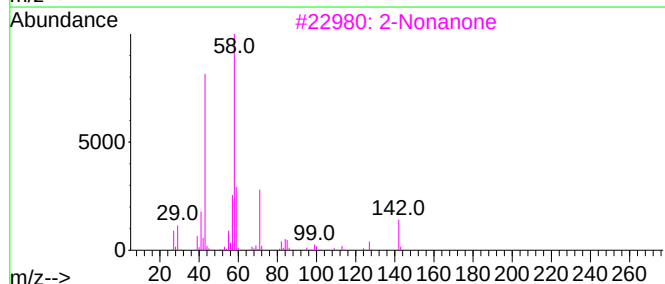
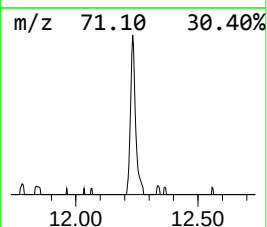
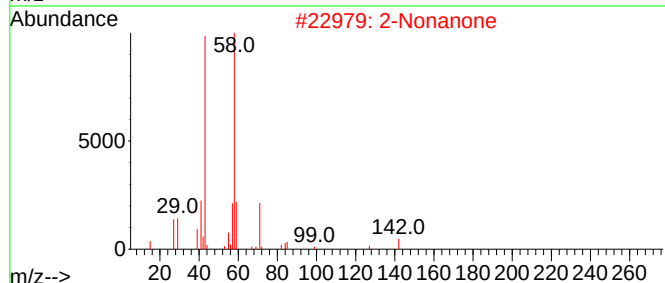
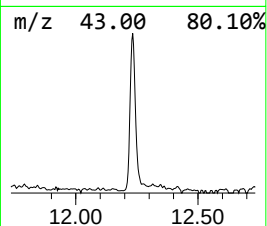
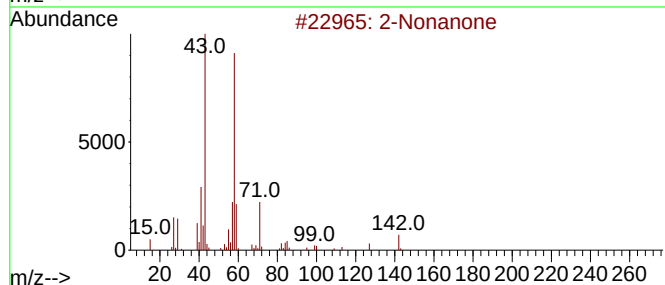
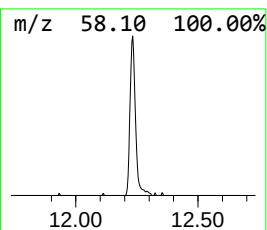
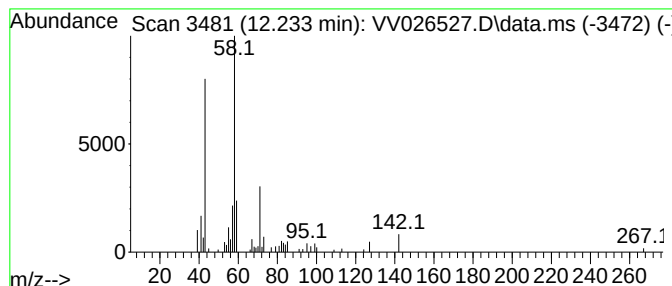
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 2-Nonanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.233	0.54 ug/L	56071	1,4-Dichlorobenzene-d4	11.249

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone		142	C9H18O	000821-55-6	91
2	2-Nonanone		142	C9H18O	000821-55-6	90
3	2-Nonanone		142	C9H18O	000821-55-6	78
4	2-Tridecanone		198	C13H26O	000593-08-8	64
5	2-Dodecanone		184	C12H24O	006175-49-1	64



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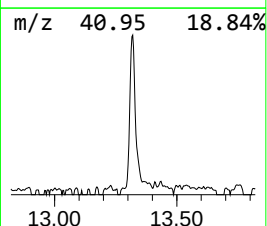
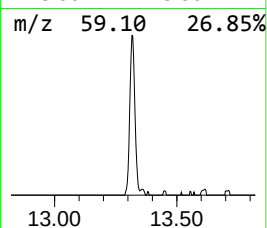
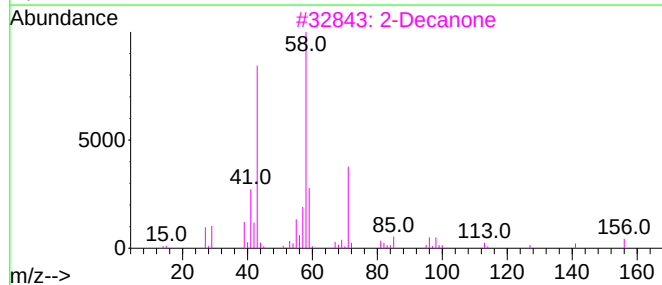
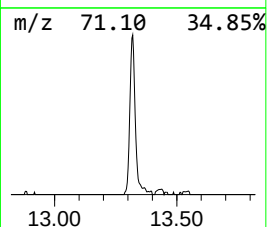
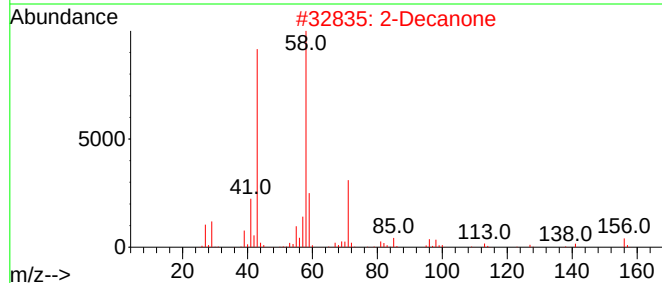
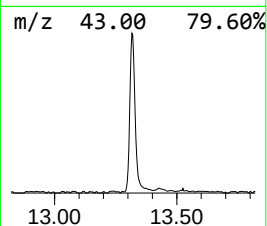
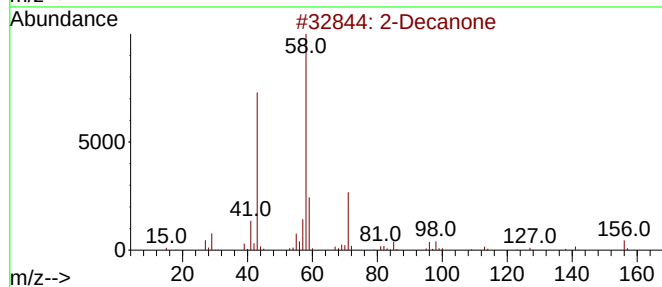
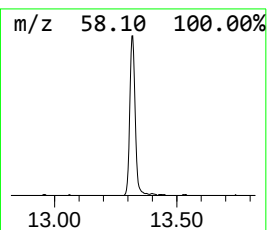
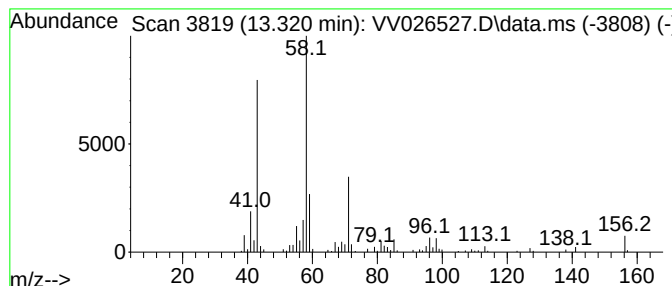
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Decanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.320	1.27 ug/L	132506	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Decanone			156	C10H20O	000693-54-9	97
2	2-Decanone			156	C10H20O	000693-54-9	97
3	2-Decanone			156	C10H20O	000693-54-9	93
4	2-Decanone			156	C10H20O	000693-54-9	91
5	2-Undecanone			170	C11H22O	000112-12-9	78



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	1.121	0.7	ug/L	67865	1	5.622	489612	5.0
1-Hexanol, 2-et...	11.529	4.0	ug/L	417461	3	11.249	523482	5.0
2-Nonanone	12.233	0.5	ug/L	56071	3	11.249	523482	5.0
2-Decanone	13.320	1.3	ug/L	132506	3	11.249	523482	5.0