

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062524\
 Data File : VU059511.D
 Acq On : 26 Jun 2024 08:55
 Operator : MD/SY
 Sample : P2897-13
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 61 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COT60

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\SFAMUTR061724WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU059511.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	84	94	112	rBV2	59647	89402	18.19%	1.915%
2	1.682	113	122	143	rBV	107082	147455	30.00%	3.158%
3	1.911	183	193	210	rVB	52305	74513	15.16%	1.596%
4	2.329	314	323	337	rVB2	7994	13129	2.67%	0.281%
5	2.560	380	395	406	rBV	95222	156017	31.74%	3.341%
6	2.628	406	416	453	rVB	67397	149685	30.46%	3.206%
7	3.193	575	592	598	rBV4	5624	11563	2.35%	0.248%
8	4.438	961	979	1001	rBV6	15935	50877	10.35%	1.090%
9	4.621	1023	1036	1059	rBV2	67590	182389	37.11%	3.906%
10	5.055	1156	1171	1192	rBV	95495	211632	43.06%	4.532%
11	5.717	1358	1377	1405	rBV2	184719	484294	98.54%	10.372%
12	6.242	1526	1540	1561	rBV	162040	320787	65.27%	6.870%
13	6.682	1664	1677	1695	rBV	114929	227354	46.26%	4.869%
14	6.779	1700	1707	1718	rVV6	3093	6536	1.33%	0.140%
15	6.885	1731	1740	1752	rBV3	5300	9775	1.99%	0.209%
16	7.119	1801	1813	1820	rBV5	3993	7865	1.60%	0.168%
17	7.560	1939	1950	1973	rBV2	47584	87169	17.74%	1.867%
18	7.891	2040	2053	2071	rBV	216328	382003	77.72%	8.181%
19	7.965	2074	2076	2091	rVB4	3733	6120	1.25%	0.131%
20	8.177	2132	2142	2156	rBV2	28799	52993	10.78%	1.135%
21	8.627	2271	2282	2317	rBV	240248	491482	100.00%	10.525%
22	8.785	2322	2331	2351	rVB4	15842	30298	6.16%	0.649%
23	9.412	2514	2526	2554	rBV	244121	419301	85.31%	8.980%
24	9.647	2589	2599	2609	rBV4	7057	11512	2.34%	0.247%
25	10.132	2743	2750	2760	rVB3	3977	5865	1.19%	0.126%
26	10.235	2772	2782	2804	rBV2	32546	58765	11.96%	1.258%
27	10.749	2930	2942	2964	rVB	97340	160293	32.61%	3.433%
28	10.859	2964	2976	2994	rVB4	10190	19523	3.97%	0.418%
29	11.576	3189	3199	3213	rBV4	3472	6640	1.35%	0.142%
30	11.807	3257	3271	3293	rBV	237233	384575	78.25%	8.236%
31	12.061	3339	3350	3377	rBV3	15623	45578	9.27%	0.976%
32	12.187	3378	3389	3411	rVB	210089	355198	72.27%	7.607%
33	12.888	3597	3607	3618	rBV6	5914	8880	1.81%	0.190%

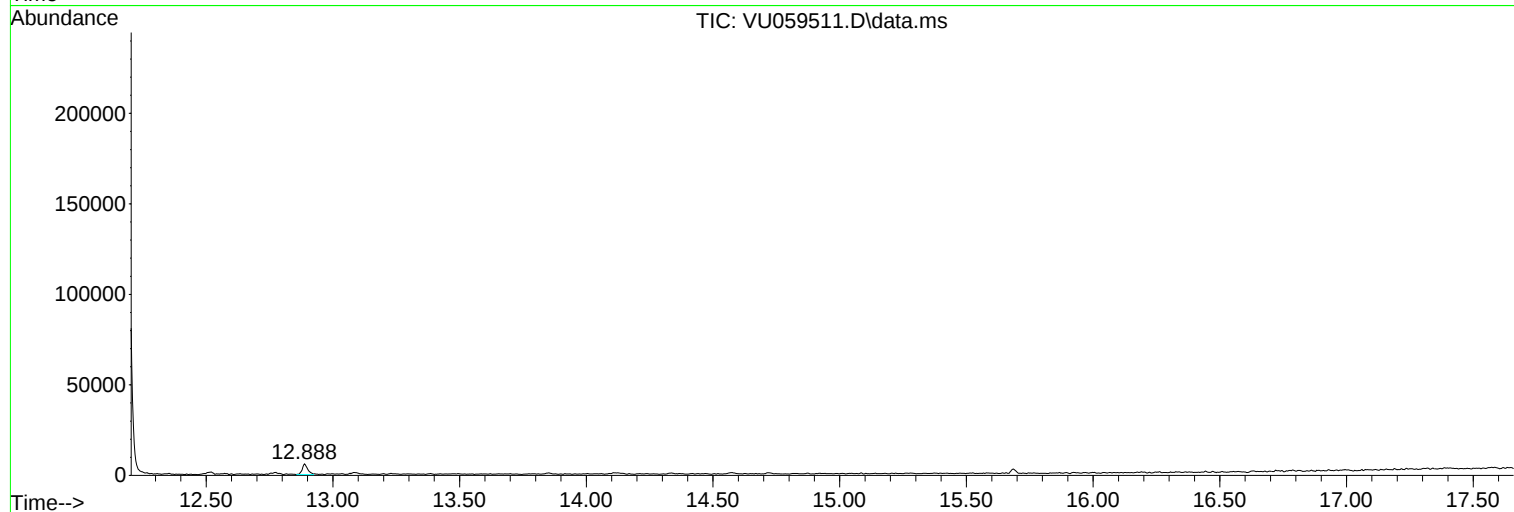
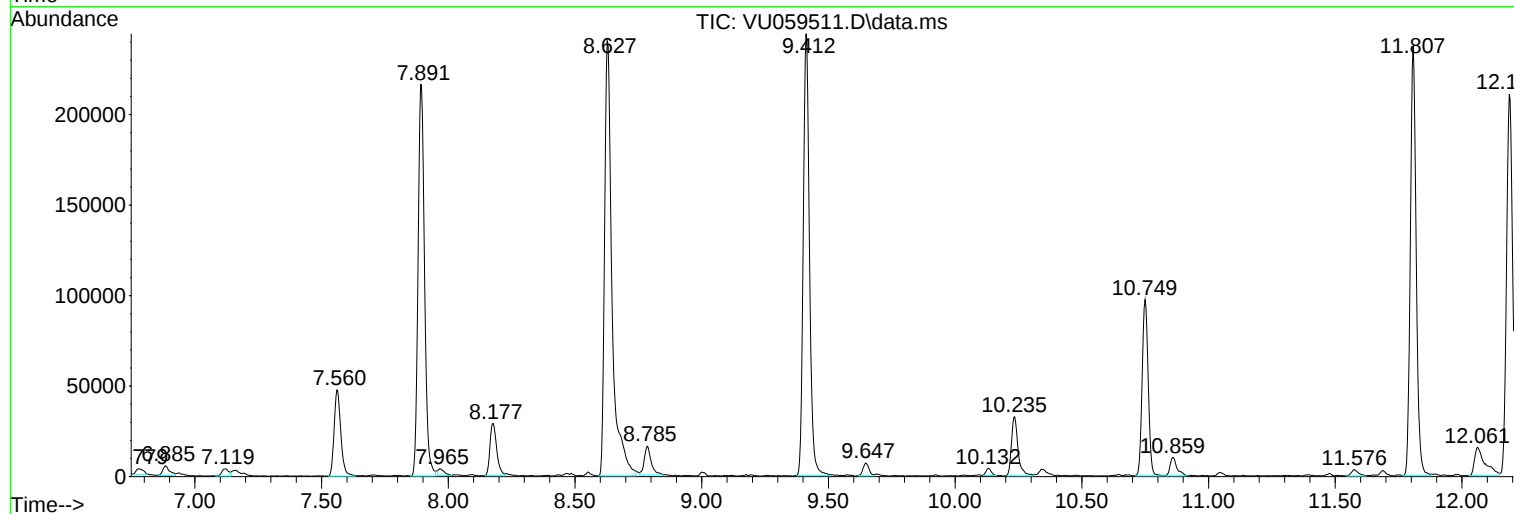
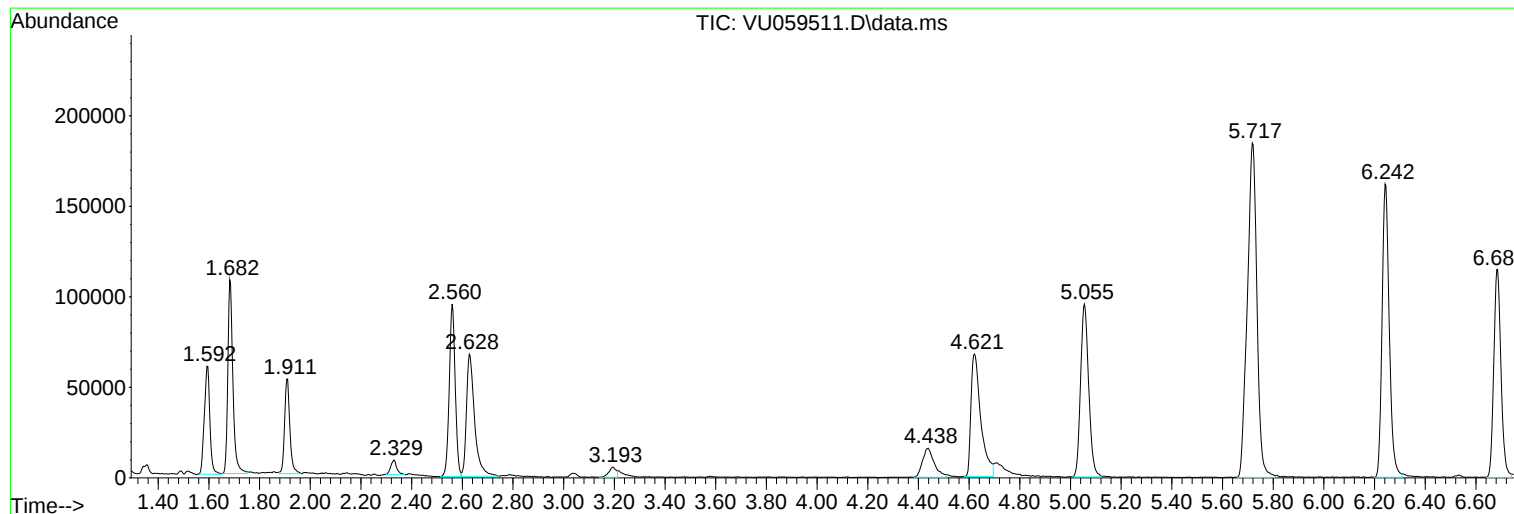
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COT60

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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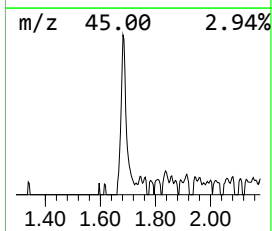
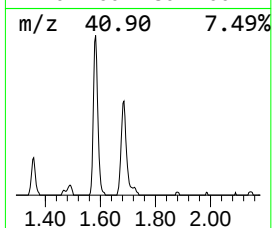
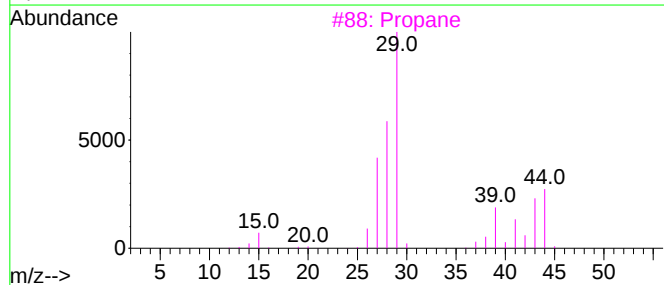
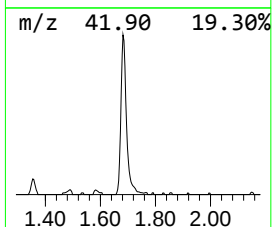
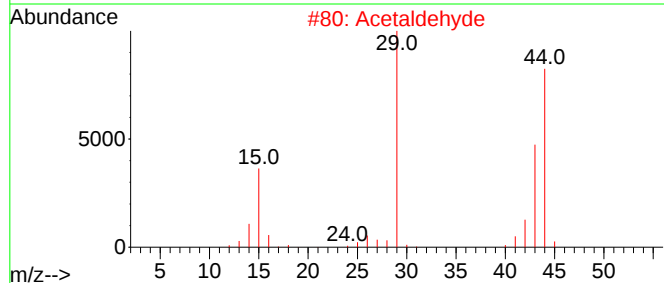
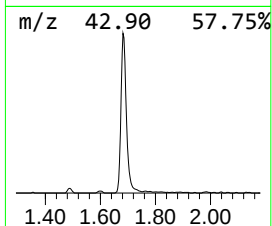
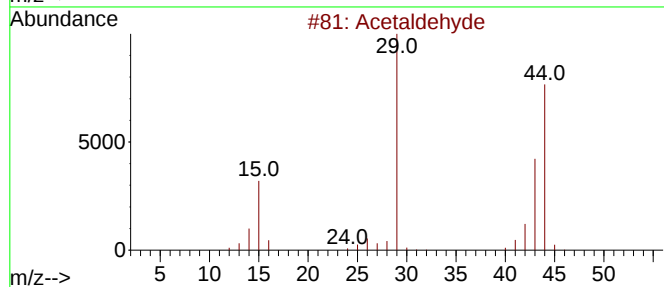
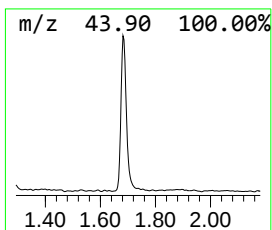
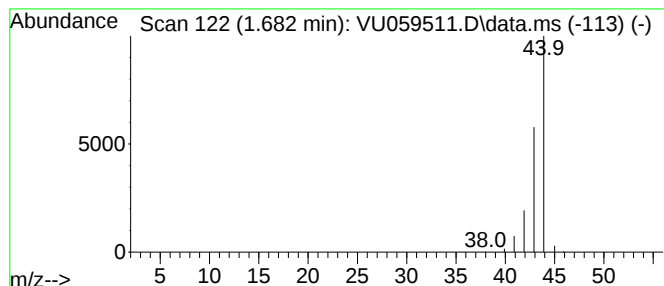
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.682	2.30 ug/L	147455	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Acetaldehyde	44	C2H4O	000075-07-0	74
3			Propane	44	C3H8	000074-98-6	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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Instrument :
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ClientSampleId :
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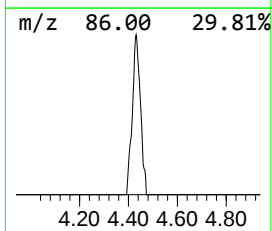
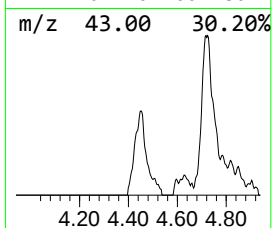
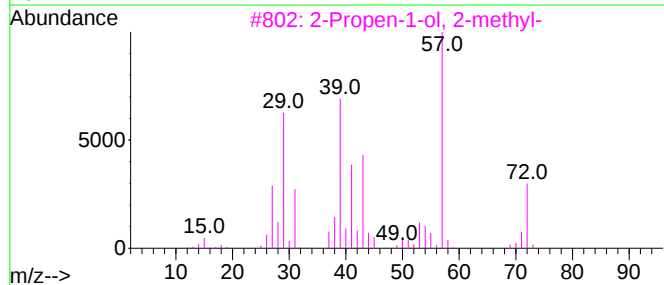
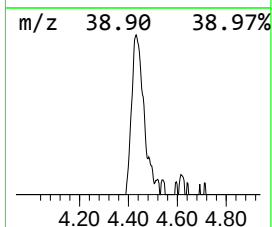
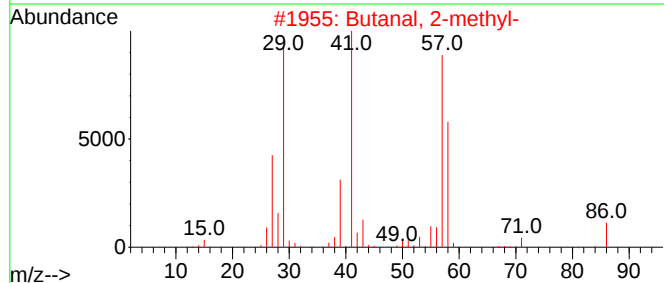
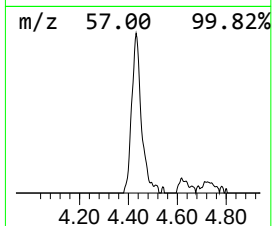
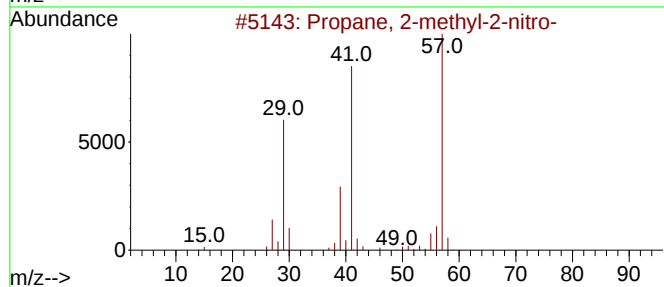
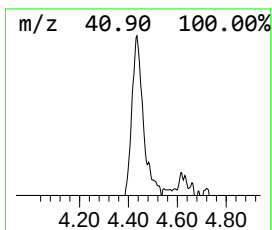
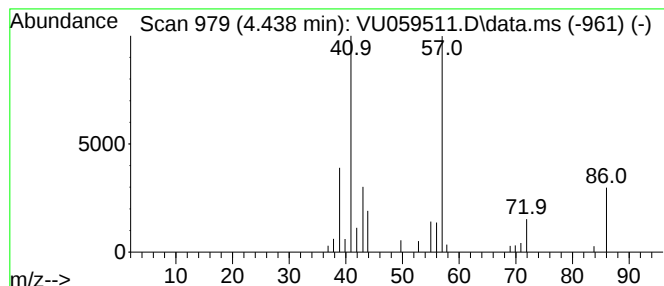
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.438	0.79 ug/L	50877	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	47
2			Butanal, 2-methyl-	86	C5H10O	000096-17-3	35
3			2-Propen-1-ol, 2-methyl-	72	C4H8O	000513-42-8	32
4			Oxirane, ethyl-	72	C4H8O	000106-88-7	23
5			Oxalic acid, allyl heptyl ester	228	C12H20O4	1000309-23-5	17



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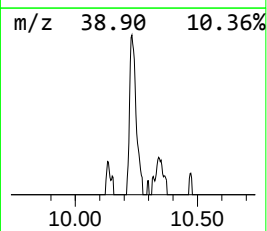
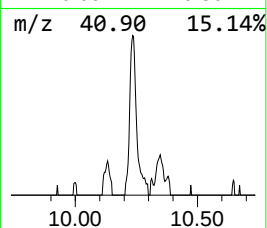
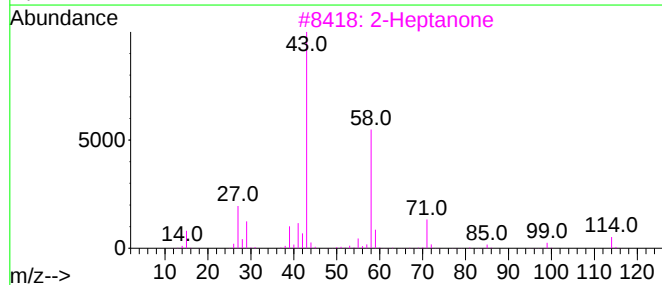
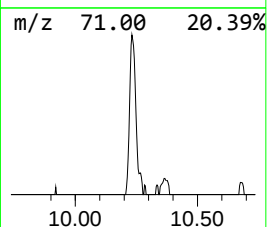
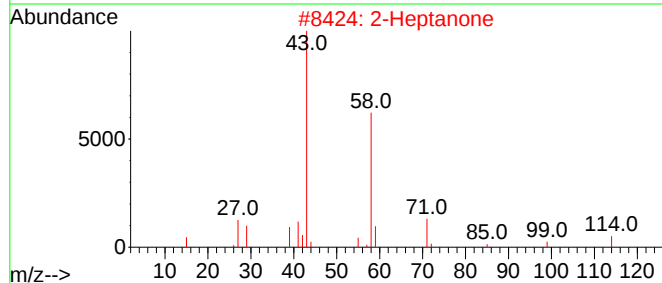
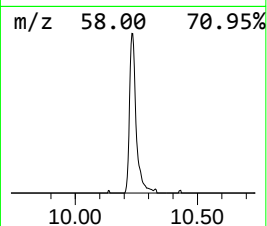
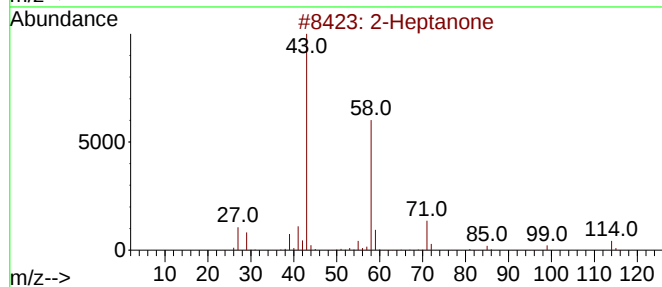
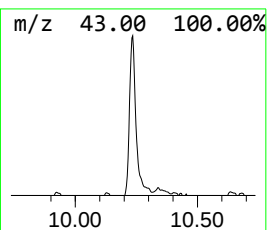
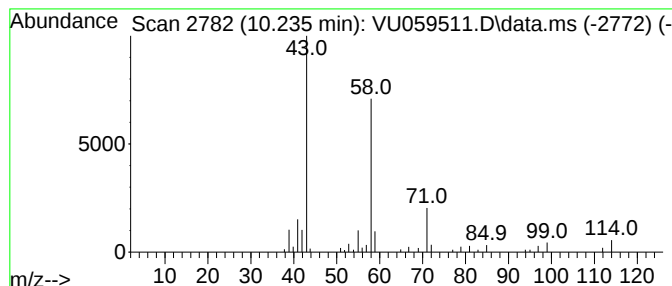
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.235	0.70 ug/L	58765	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone			114	C7H14O	000110-43-0	87
2	2-Heptanone			114	C7H14O	000110-43-0	80
3	2-Heptanone			114	C7H14O	000110-43-0	80
4	2-Heptanone			114	C7H14O	000110-43-0	80
5	2-Heptanone			114	C7H14O	000110-43-0	53



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Instrument :
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ClientSampleId :
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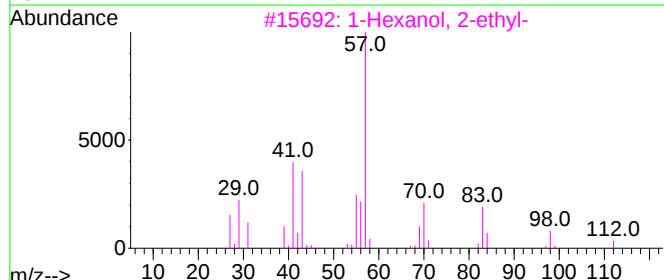
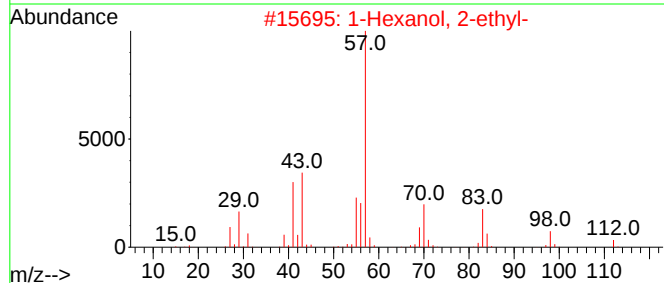
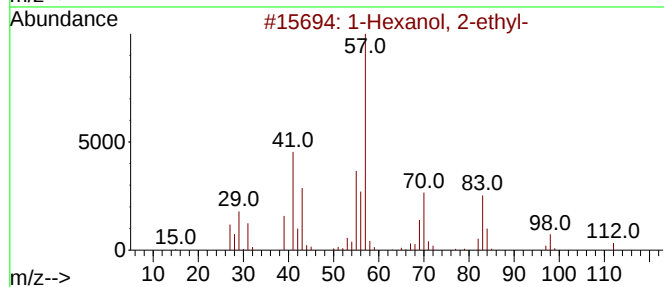
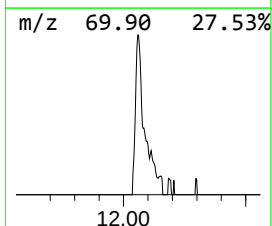
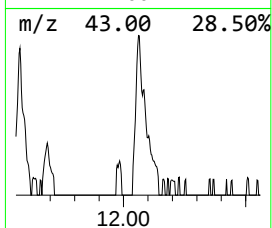
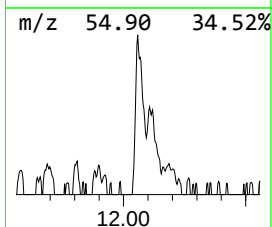
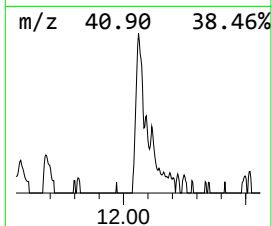
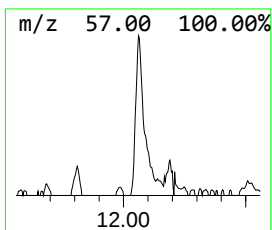
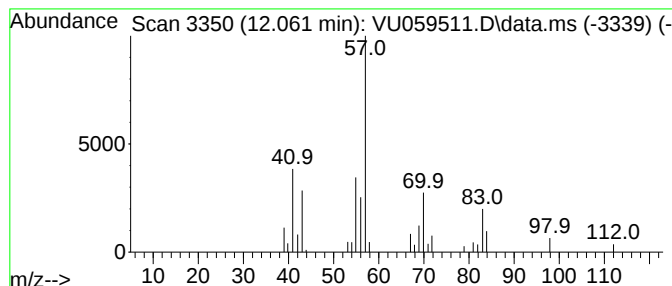
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.061	0.59 ug/L	45578	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.682	2.3	ug/L	147455	1	6.245	320787	5.0
unknown-01	4.438	0.8	ug/L	50877	1	6.245	320787	5.0
2-Heptanone	10.235	0.7	ug/L	58765	2	9.412	419301	5.0
1-Hexanol, 2-et...	12.061	0.6	ug/L	45578	3	11.807	384575	5.0