

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062824\
 Data File : VU059571.D
 Acq On : 27 Jun 2024 18:49
 Operator : MD/SY
 Sample : P3006-04RE
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 JMRG9RE

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: VU059571.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.399	28	34	52	rVB	15305	20772	1.26%	0.287%
2	1.673	107	119	135	rBV	48013	73905	4.47%	1.022%
3	1.830	154	168	181	rBV	100949	149733	9.06%	2.070%
4	2.030	221	230	241	rBV	49686	74069	4.48%	1.024%
5	2.695	424	437	454	rBV	102065	185669	11.23%	2.567%
6	4.875	1078	1115	1146	rBV3	307412	1652828	100.00%	22.849%
7	5.181	1197	1210	1228	rVB	142415	318838	19.29%	4.408%
8	5.866	1404	1423	1444	rBV2	192393	451294	27.30%	6.239%
9	6.364	1566	1578	1597	rBV	135449	250722	15.17%	3.466%
10	6.640	1652	1664	1677	rBV5	17916	37539	2.27%	0.519%
11	6.788	1696	1710	1726	rBV	112237	216822	13.12%	2.997%
12	7.245	1833	1852	1877	rBV2	170232	350907	21.23%	4.851%
13	7.631	1956	1972	1990	rBV	46085	82179	4.97%	1.136%
14	7.779	2002	2018	2036	rBV	427964	810470	49.04%	11.204%
15	7.910	2051	2059	2062	rBV3	15845	22311	1.35%	0.308%
16	7.952	2062	2072	2088	rVV	218606	395830	23.95%	5.472%
17	8.020	2090	2093	2114	rVB2	19204	31876	1.93%	0.441%
18	8.226	2143	2157	2171	rBV3	28381	49128	2.97%	0.679%
19	8.592	2261	2271	2284	rBV4	26570	45330	2.74%	0.627%
20	8.673	2284	2296	2328	rBV	208911	445136	26.93%	6.154%
21	8.820	2332	2342	2353	rBV2	48286	86394	5.23%	1.194%
22	9.441	2524	2535	2560	rVB	193248	347709	21.04%	4.807%
23	9.595	2571	2583	2584	rBV2	21074	26630	1.61%	0.368%
24	9.615	2585	2589	2604	rVV	30128	49721	3.01%	0.687%
25	9.701	2604	2616	2631	rVB2	44511	80552	4.87%	1.114%
26	9.795	2637	2645	2655	rBV2	14942	25385	1.54%	0.351%
27	10.094	2728	2738	2746	rBV2	20132	33314	2.02%	0.461%
28	10.762	2934	2946	2961	rVB2	85296	139334	8.43%	1.926%
29	11.817	3261	3274	3295	rBV	184836	313221	18.95%	4.330%
30	12.068	3340	3352	3379	rBV2	32743	99807	6.04%	1.380%
31	12.193	3380	3391	3409	rVB	202446	348018	21.06%	4.811%
32	16.878	4836	4848	4860	rBV5	10875	18169	1.10%	0.251%

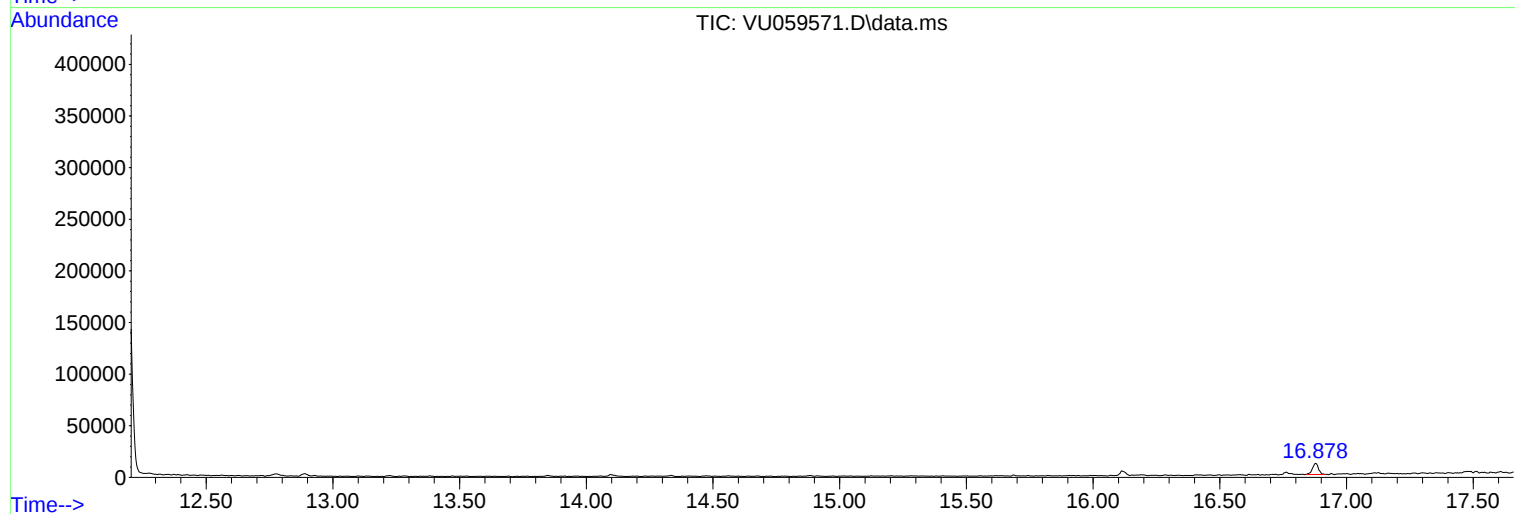
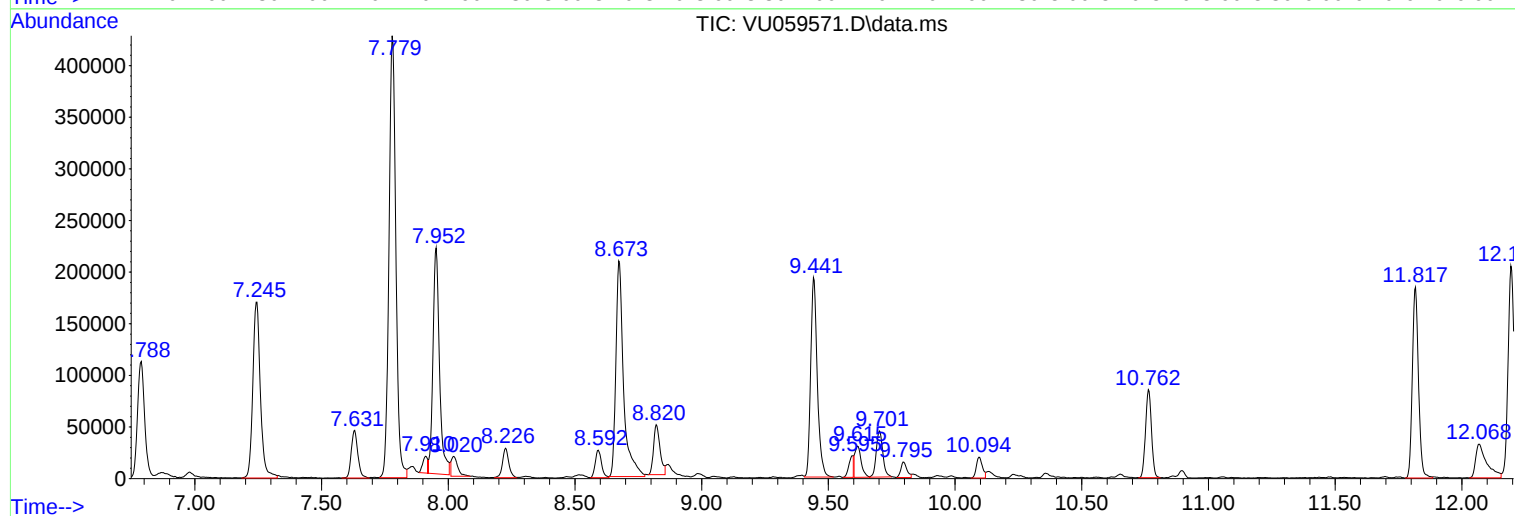
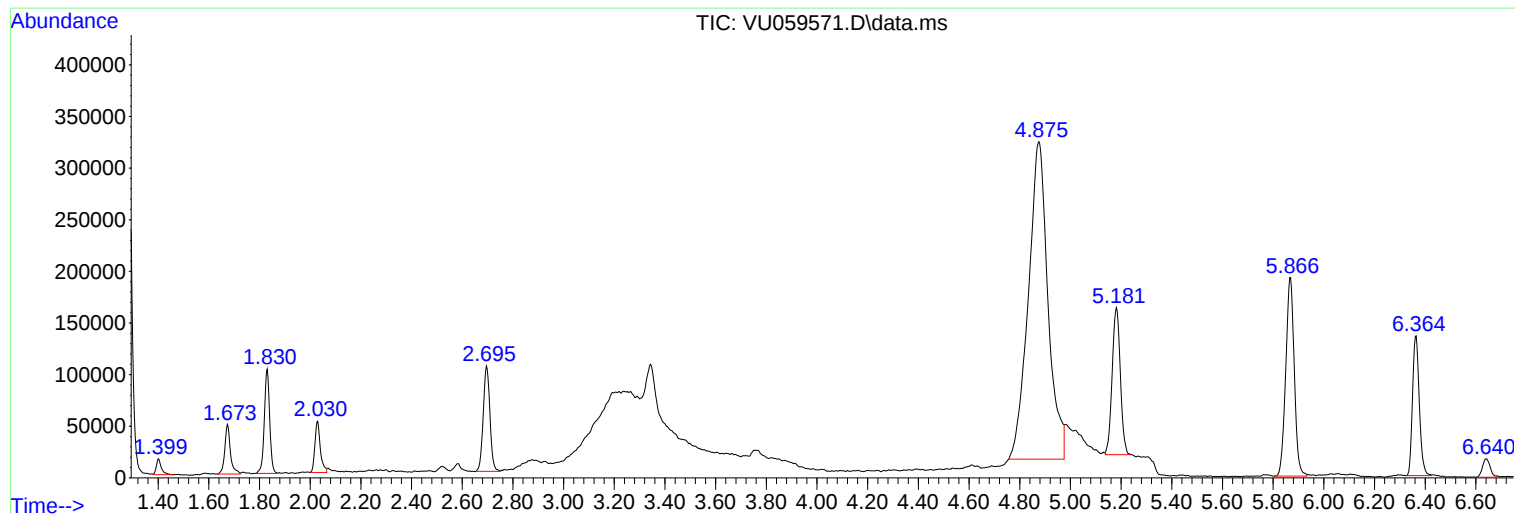
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ClientSampleId :
JMRG9RE

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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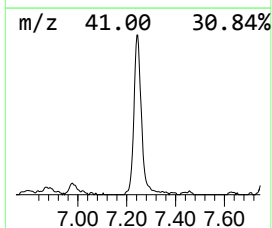
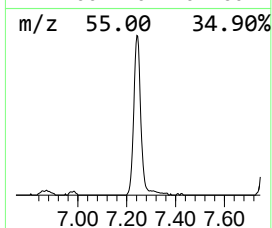
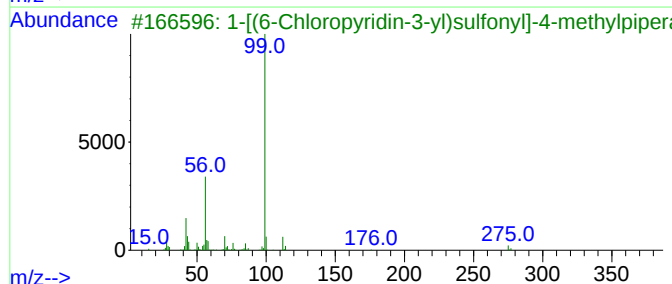
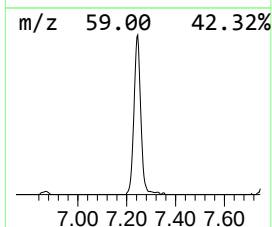
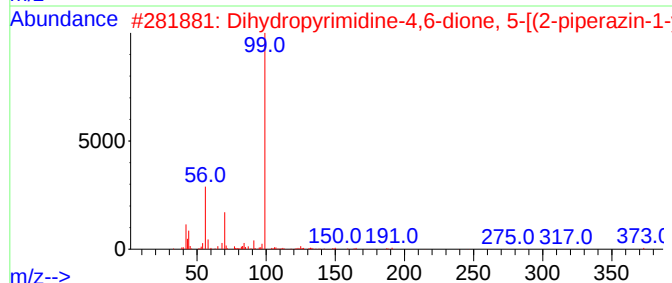
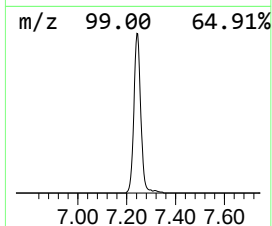
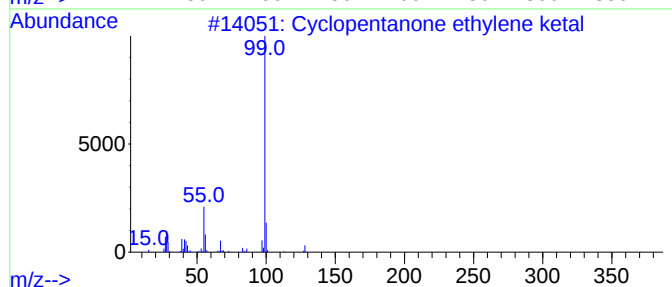
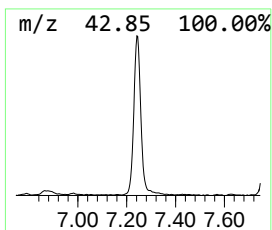
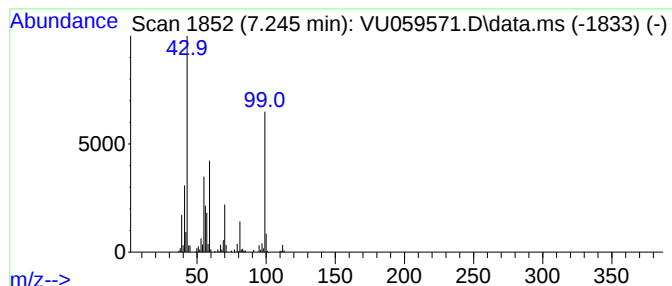
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.245	7.00 ug/L	350907	1,4-Difluorobenzene	6.364

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone ethylene ketal	128	C7H12O2	000176-32-9	35
2			Dihydropyrimidine-4,6-dione, 5-[...]	373	C18H23N5O2S	1000304-28-2	35
3			1-[(6-Chloropyridin-3-yl)sulfonyl...]	275	C10H14ClN3O2S	064614-53-5	35
4			2-Ethylbutyl methylphosphonofluo...	182	C7H16FO2P	126204-48-6	35
5			3,7-Dimethyl-1-octyl methylphosp...	238	C11H24FO2P	345260-82-4	32



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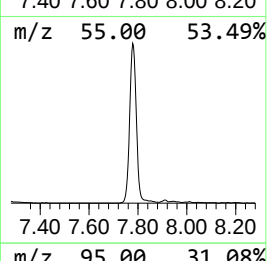
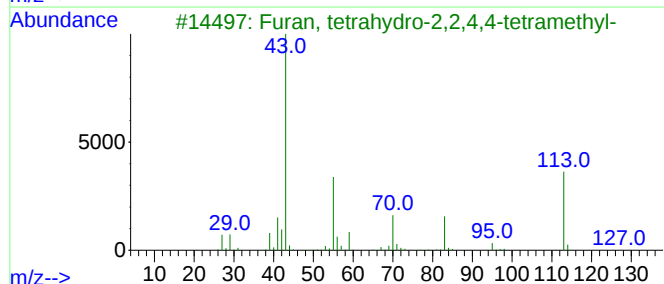
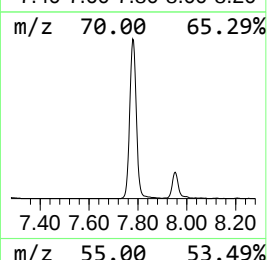
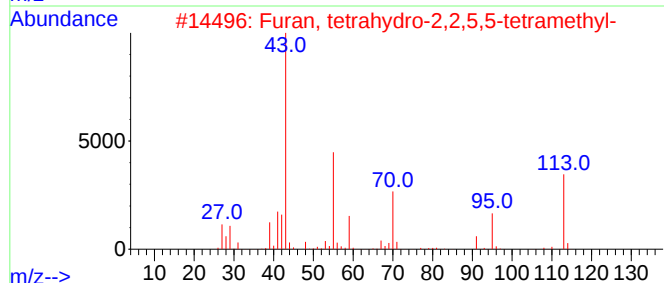
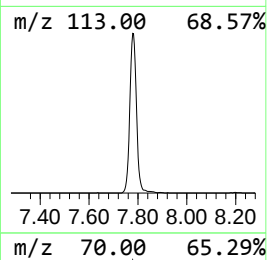
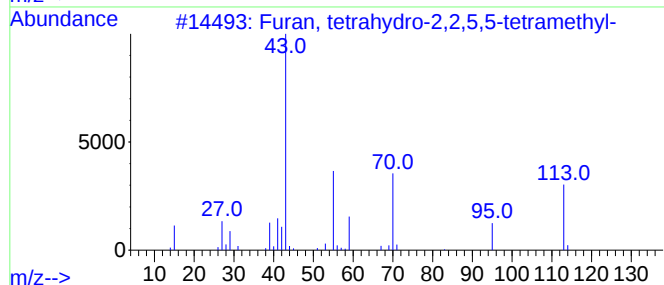
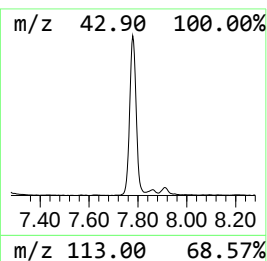
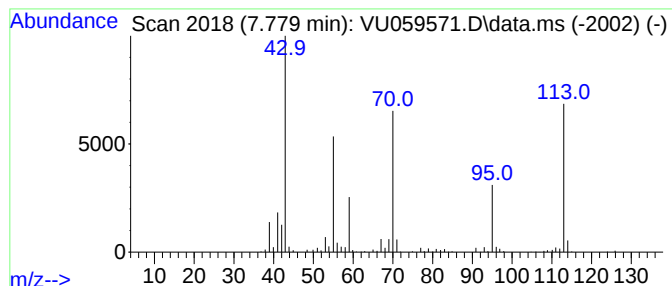
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.779	16.16 ug/L	810470	1,4-Difluorobenzene	6.364

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
2			Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
3			Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
4			4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50
5			1,3,5-Triazine-2,4(1H,3H)-dione	113	C3H3N3O2	000071-33-0	38



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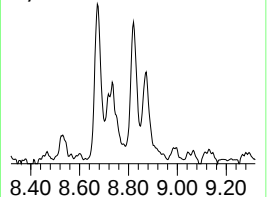
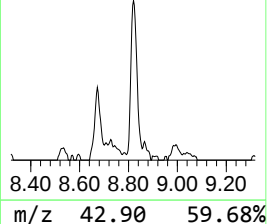
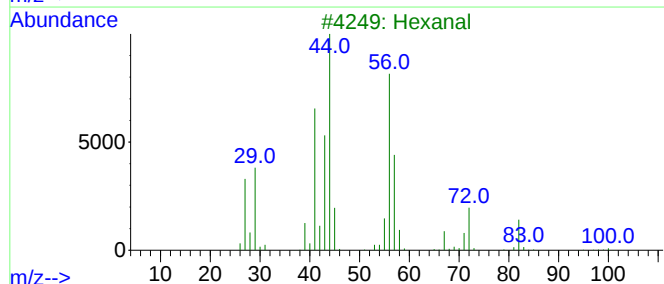
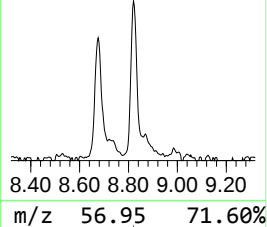
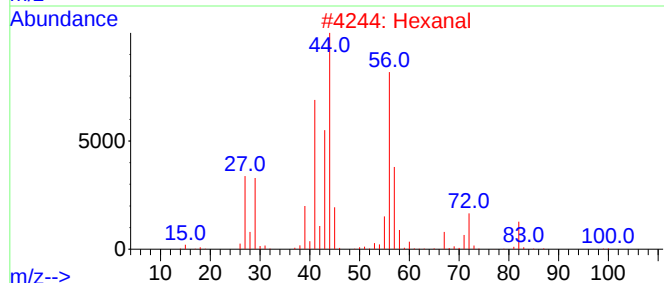
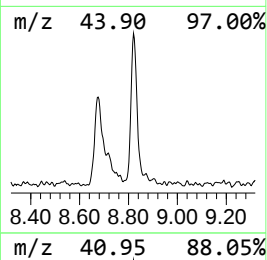
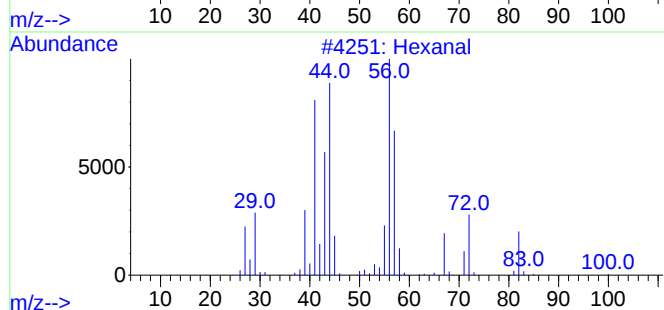
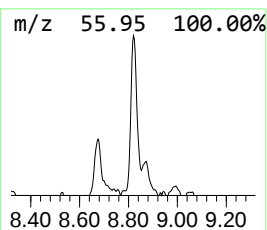
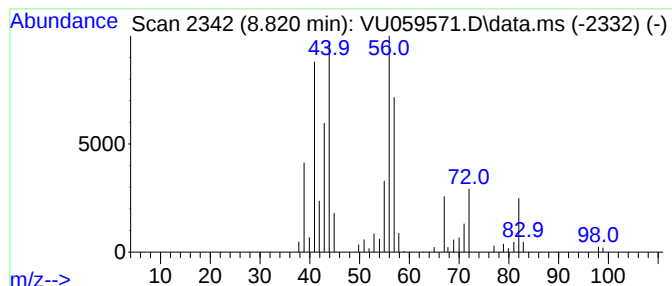
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Hexanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.820	1.24 ug/L	86394	Chlorobenzene-d5	9.441

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	64
2	Hexanal			100	C6H12O	000066-25-1	64
3	Hexanal			100	C6H12O	000066-25-1	59
4	Hexanal			100	C6H12O	000066-25-1	59
5	Hexanal			100	C6H12O	000066-25-1	53



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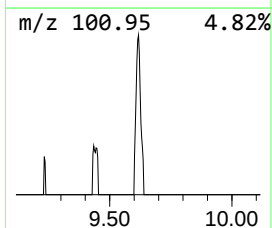
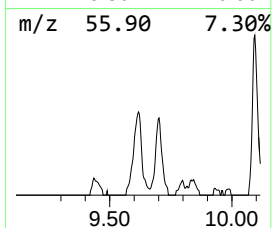
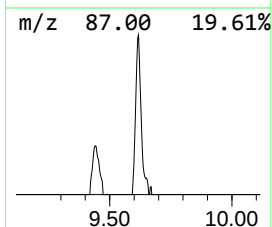
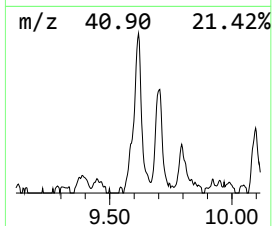
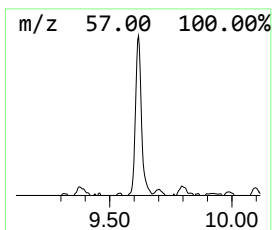
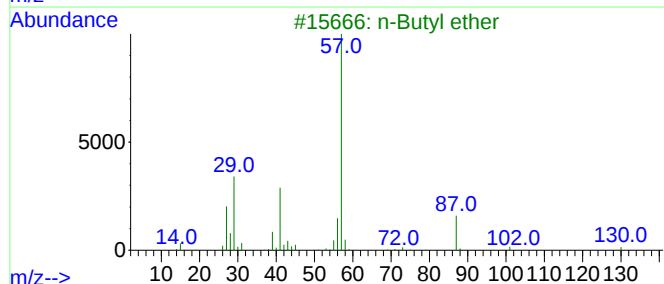
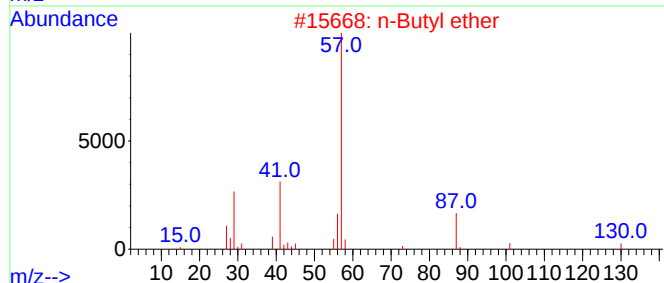
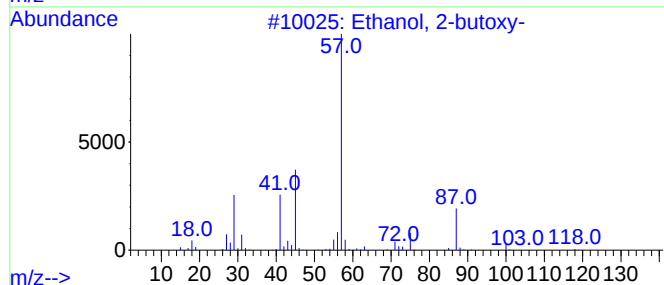
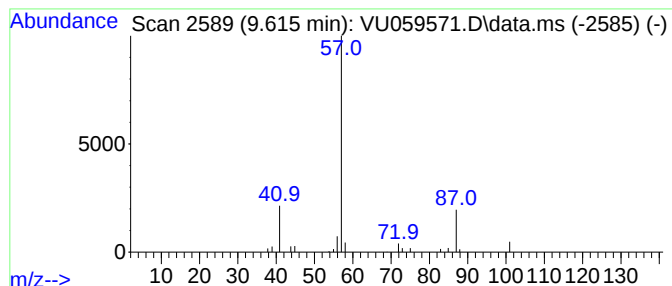
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Ethanol, 2-butoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.615	0.71 ug/L	49721	Chlorobenzene-d5	9.441

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	56
2			n-Butyl ether	130	C8H18O	000142-96-1	45
3			n-Butyl ether	130	C8H18O	000142-96-1	38
4			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	9
5			Trimethylaluminum	72	C3H9Al	000075-24-1	9



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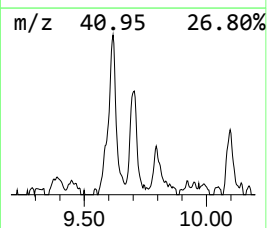
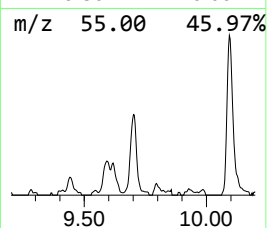
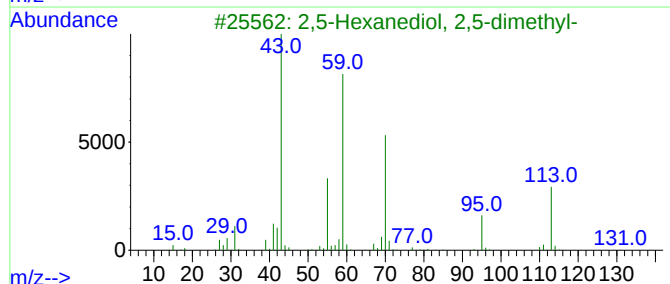
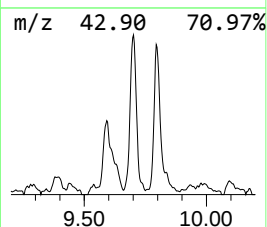
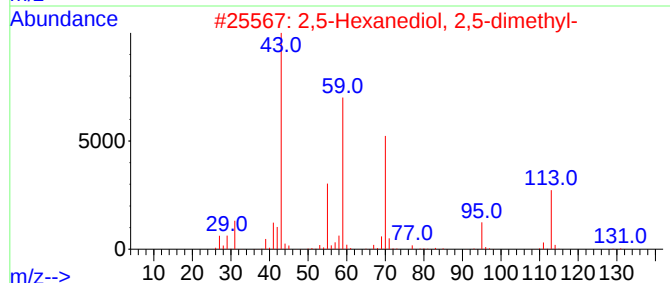
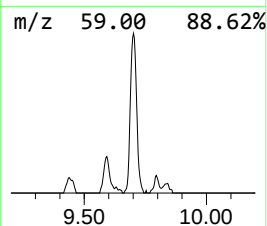
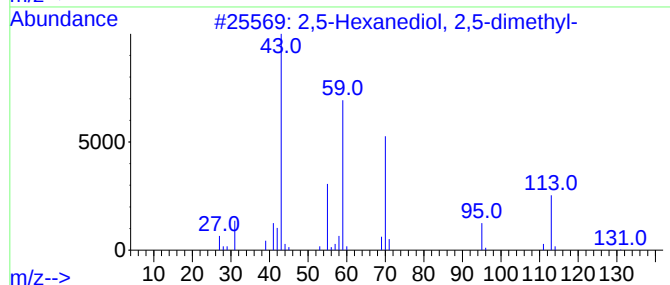
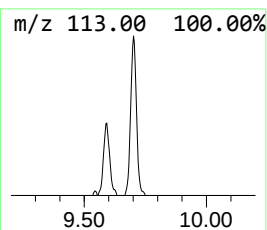
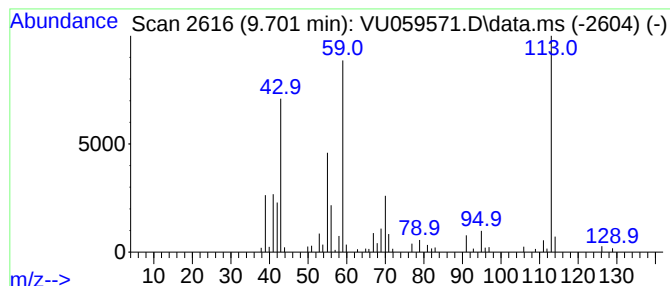
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 2,5-Hexanediol, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.701	1.16 ug/L	80552	Chlorobenzene-d5	9.441

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	59		
2	2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	53		
3	2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	53		
4	Ethyl 3-[(4-ethylpiperazin-1-yl)...	330	C13H22N4O4S	1000514-46-7	43		
5	Ethyl 3-[(4-ethylpiperazin-1-yl)...	358	C14H22N4O5S	1000514-46-6	43		



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ClientSampleId :
JMRG9RE

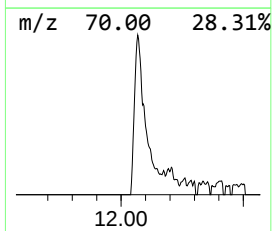
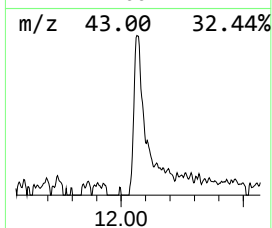
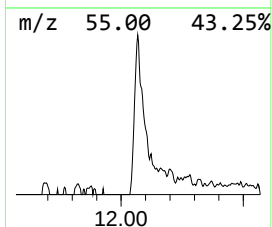
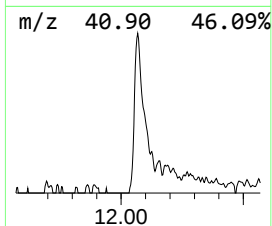
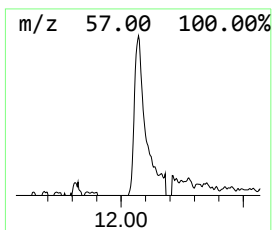
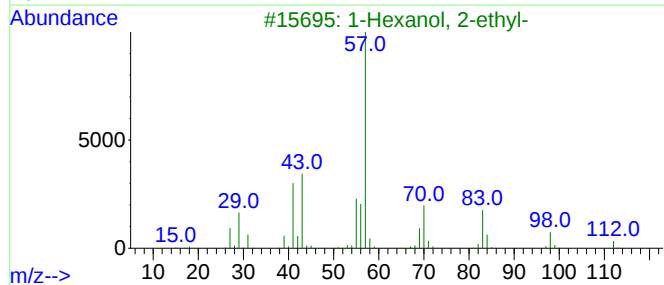
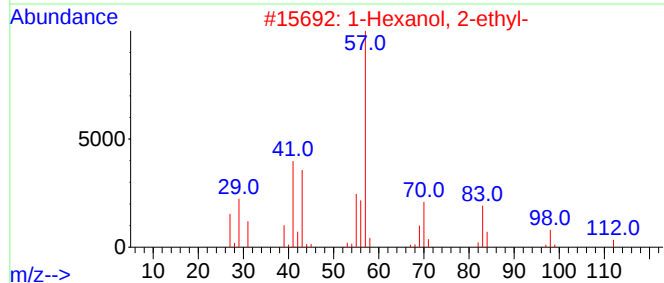
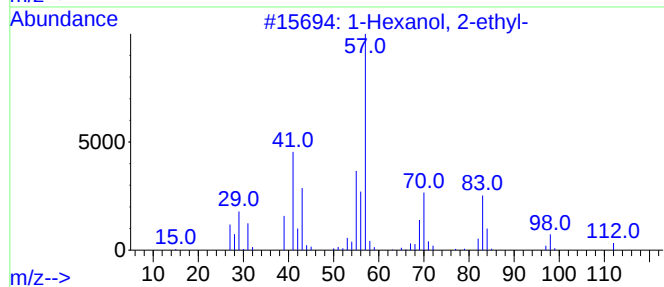
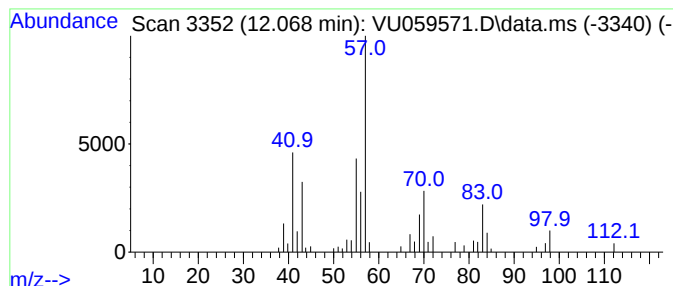
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.068	1.59 ug/L	99807	1,4-Dichlorobenzene-d4	11.817

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	72
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062824\
Data File : VU059571.D
Acq On : 27 Jun 2024 18:49
Operator : MD/SY
Sample : P3006-04RE
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JMRG9RE

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	7.245	7.0	ug/L	350907	1	6.364	250722	5.0
Furan, tetrahyd...	7.779	16.2	ug/L	810470	1	6.364	250722	5.0
Hexanal	8.820	1.2	ug/L	86394	2	9.441	347709	5.0
Ethanol, 2-butoxy-	9.615	0.7	ug/L	49721	2	9.441	347709	5.0
2,5-Hexanediol,...	9.701	1.2	ug/L	80552	2	9.441	347709	5.0
1-Hexanol, 2-et...	12.068	1.6	ug/L	99807	3	11.817	313221	5.0