

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012524\
 Data File : VU057665.D
 Acq On : 25 Jan 2024 13:59
 Operator : MD/SY
 Sample : P1227-20
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0BF3

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\SFAMUTR012324WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU057665.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	85	95	109	rVB	22506	28195	14.82%	1.550%
2	1.689	116	124	131	rBV2	1735	2550	1.34%	0.140%
3	1.911	183	193	204	rBV	17269	23559	12.38%	1.295%
4	2.480	336	370	372	rBV4	5134	19315	10.15%	1.062%
5	2.563	386	396	413	rVB	39981	71843	37.76%	3.949%
6	2.647	415	422	439	rVB	5531	12712	6.68%	0.699%
7	3.177	575	587	596	rBV2	3396	7541	3.96%	0.415%
8	3.255	597	611	613	rBV4	2474	4697	2.47%	0.258%
9	4.431	963	977	988	rBV3	4013	10350	5.44%	0.569%
10	4.631	1027	1039	1062	rBV	20894	58364	30.67%	3.208%
11	5.055	1156	1171	1197	rVB2	35851	80938	42.54%	4.449%
12	5.721	1360	1378	1399	rBV2	68707	175764	92.38%	9.662%
13	6.242	1528	1540	1566	rBV	83558	159403	83.78%	8.762%
14	6.685	1665	1678	1699	rVB	41793	81808	43.00%	4.497%
15	7.123	1802	1814	1839	rBV	14249	31173	16.38%	1.714%
16	7.563	1937	1951	1967	rBV	21750	38546	20.26%	2.119%
17	7.894	2041	2054	2069	rBV	87381	153211	80.52%	8.422%
18	7.968	2071	2077	2093	rVB2	2441	4777	2.51%	0.263%
19	8.177	2133	2142	2158	rBV2	11440	20070	10.55%	1.103%
20	8.630	2272	2283	2314	rBV2	80003	163963	86.17%	9.013%
21	8.785	2322	2331	2349	rBV2	15000	27493	14.45%	1.511%
22	9.412	2511	2526	2551	rBV	111318	190272	100.00%	10.459%
23	9.569	2566	2575	2584	rBV	1657	2530	1.33%	0.139%
24	9.692	2604	2613	2627	rVB2	5637	8966	4.71%	0.493%
25	10.100	2729	2740	2748	rBV4	2521	4428	2.33%	0.243%
26	10.344	2803	2816	2833	rBV5	2964	6126	3.22%	0.337%
27	10.749	2932	2942	2956	rVB	27611	43708	22.97%	2.403%
28	10.901	2980	2989	3003	rVB5	1805	3635	1.91%	0.200%
29	11.527	3177	3184	3195	rVB3	5338	7937	4.17%	0.436%
30	11.688	3228	3234	3244	rBB4	1615	2156	1.13%	0.119%
31	11.807	3259	3271	3291	rBV	111638	179000	94.08%	9.840%
32	12.061	3342	3350	3364	rBV4	4730	9205	4.84%	0.506%
33	12.187	3379	3389	3405	rBV	75818	122903	64.59%	6.756%
34	12.521	3484	3493	3509	rBV	22890	36557	19.21%	2.010%
35	12.765	3556	3569	3583	rVB2	1727	2889	1.52%	0.159%
36	12.884	3594	3606	3617	rBV3	6771	10664	5.60%	0.586%

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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

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Title : TRACE VOA SFAM1.0

37	14.309	4043	4049	4058	rVB3	1770	2365	1.24%	0.130%
38	14.479	4095	4102	4110	rBV2	1742	2632	1.38%	0.145%
39	15.682	4469	4476	4484	rBV3	5251	6926	3.64%	0.381%

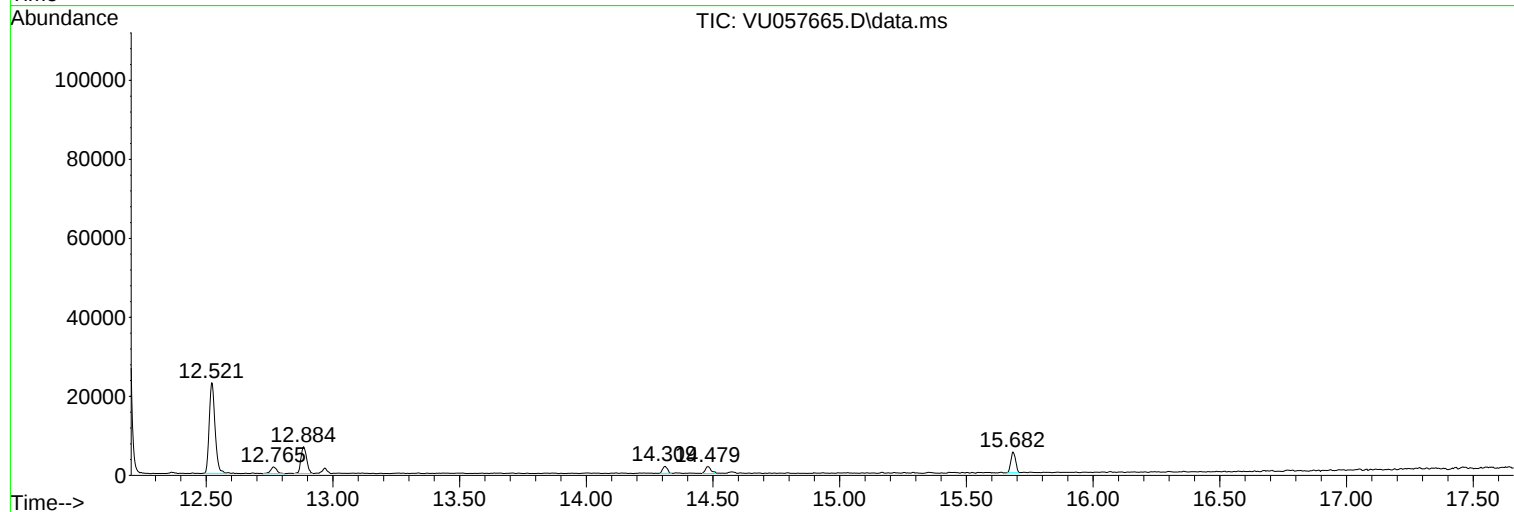
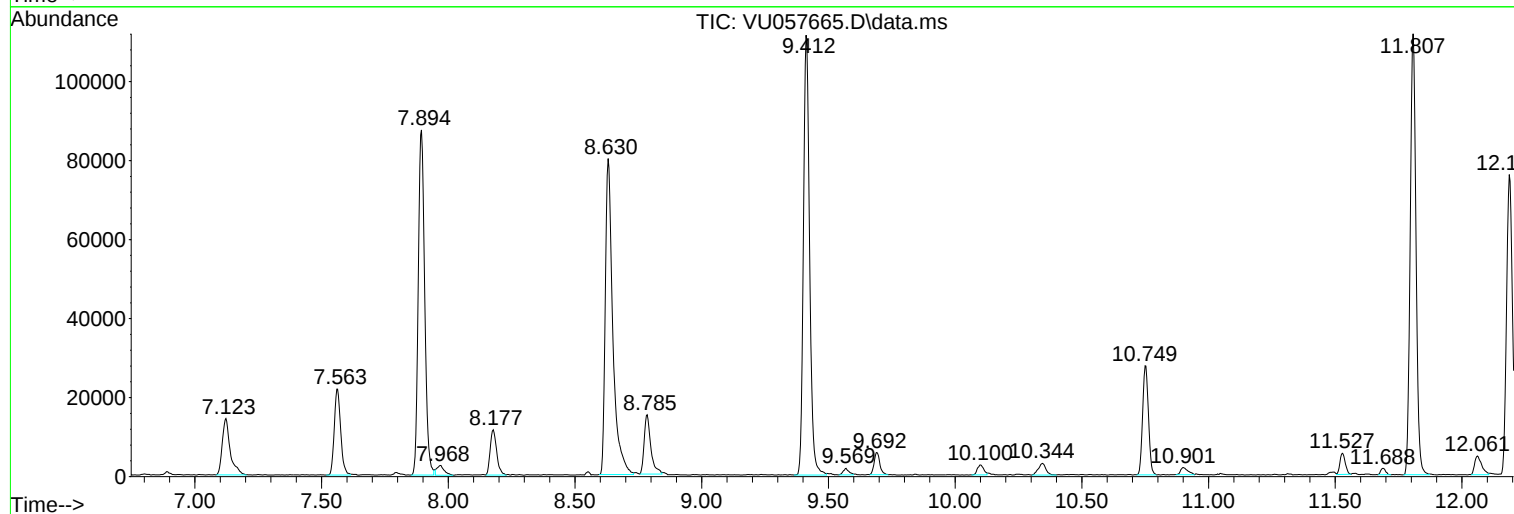
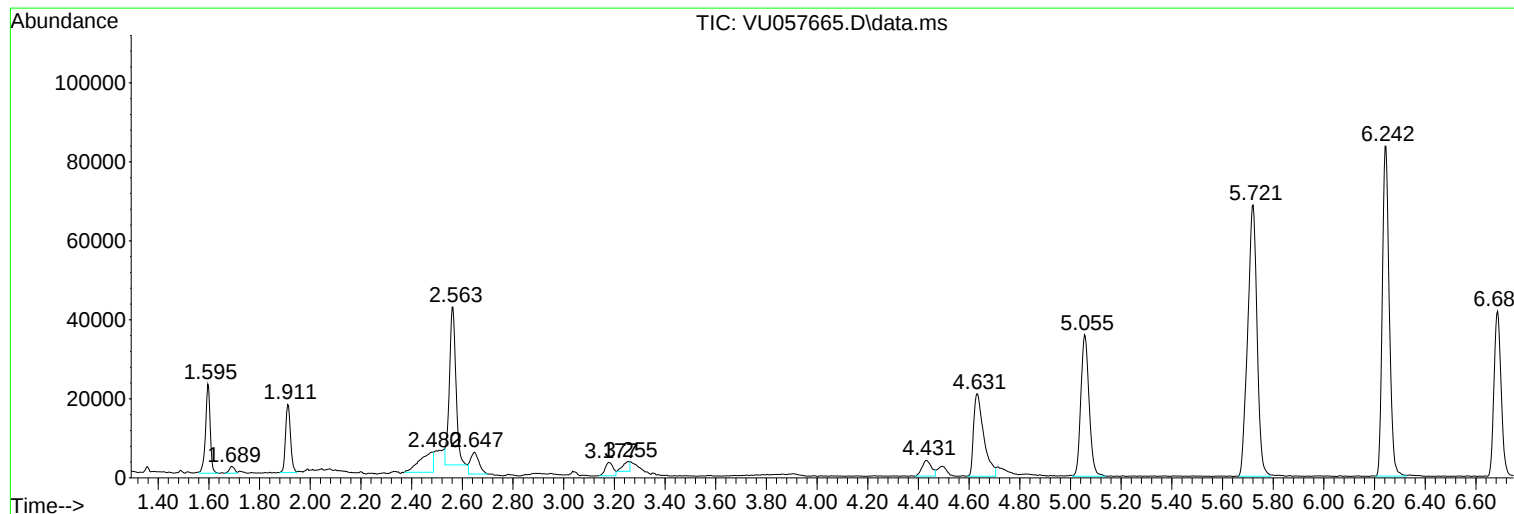
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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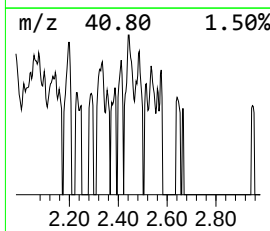
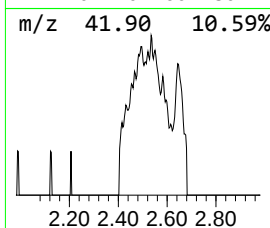
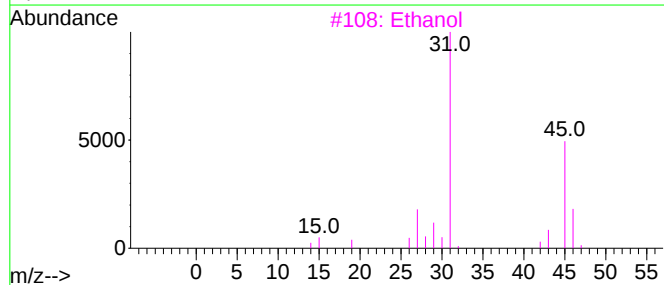
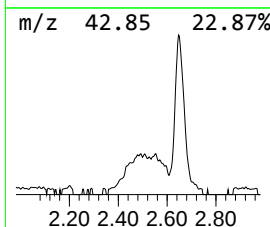
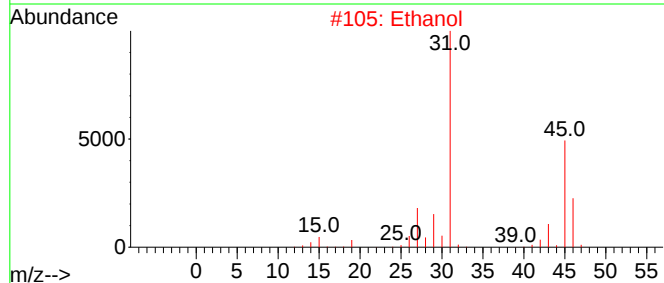
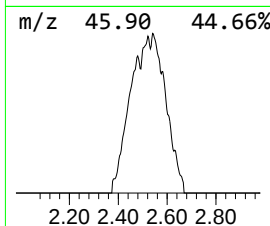
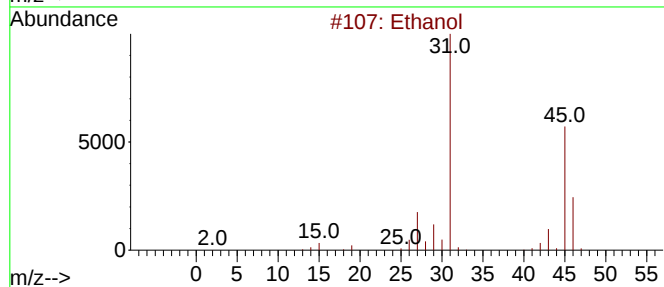
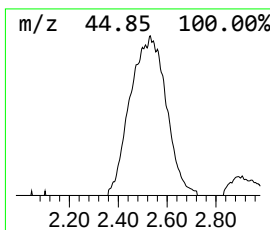
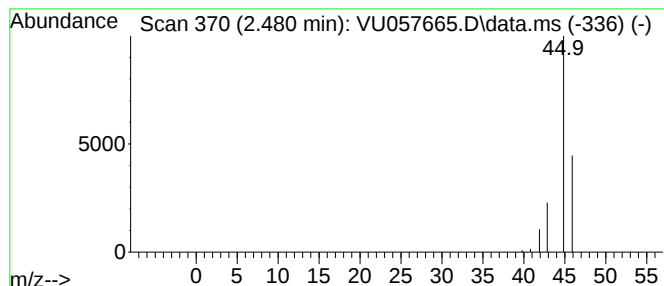
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.480	0.61 ug/L	19315	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	9
2	Ethanol			46	C2H6O	000064-17-5	9
3	Ethanol			46	C2H6O	000064-17-5	9
4	Ethanol			46	C2H6O	000064-17-5	9
5	Dimethyl ether			46	C2H6O	000115-10-6	5



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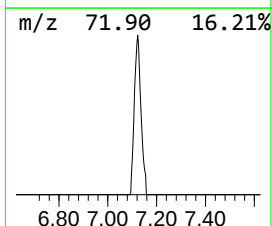
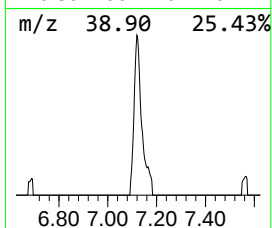
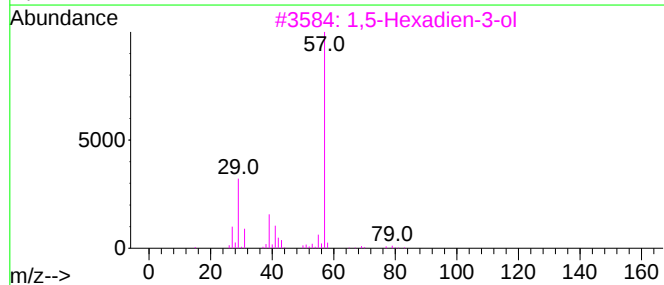
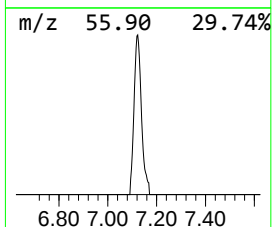
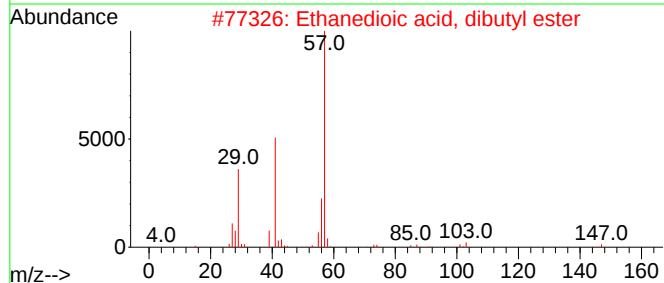
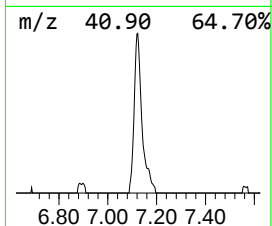
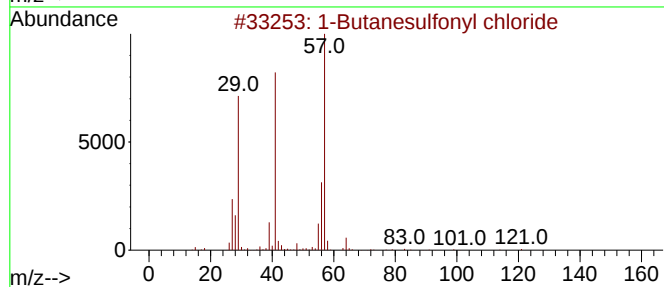
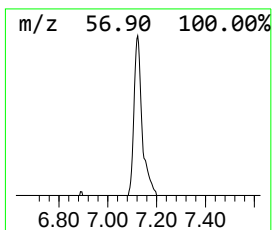
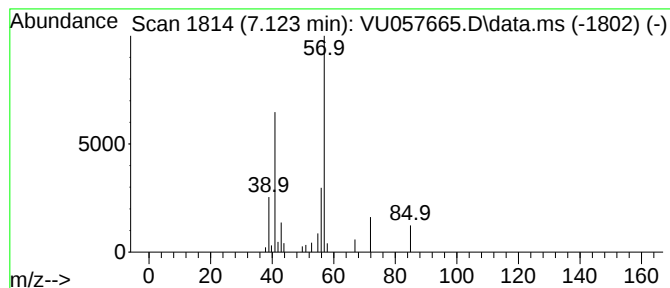
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.123	0.98 ug/L	31173	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	28
2			Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	28
3			1,5-Hexadien-3-ol	98	C6H10O	000924-41-4	25
4			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	23
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	12



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Misc : 25.0mL/MSVOA_U/WATER
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Instrument :
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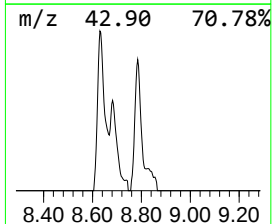
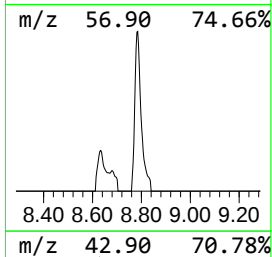
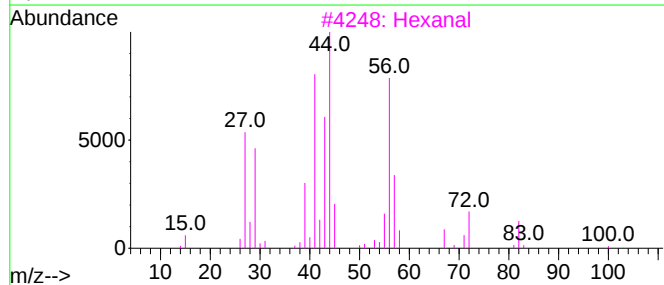
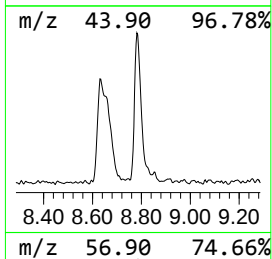
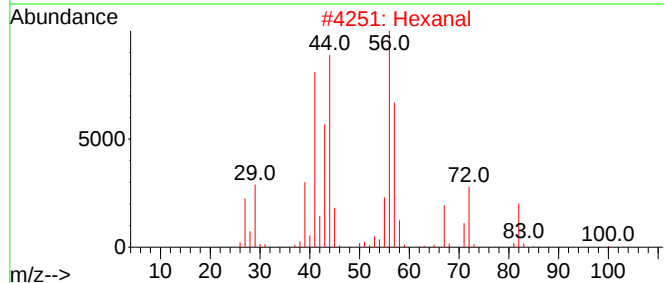
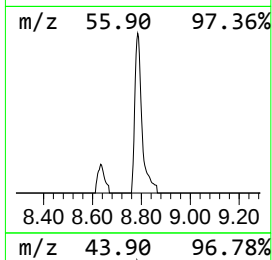
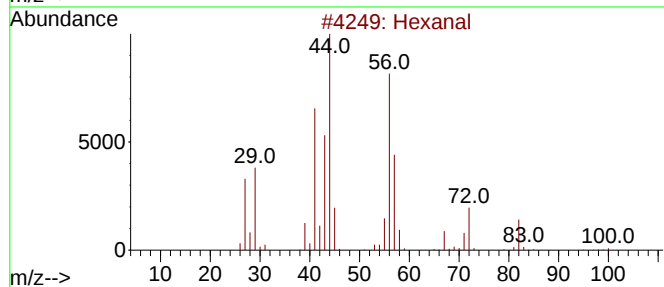
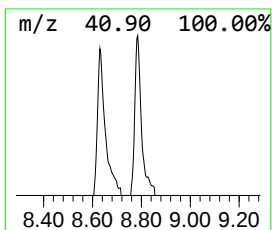
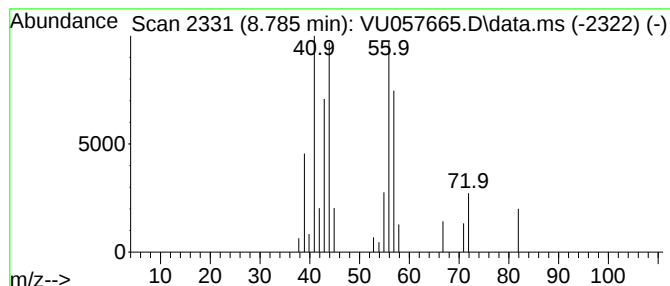
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
8.785	0.72 ug/L	27493	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	72
2	Hexanal			100	C6H12O	000066-25-1	72
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	59
5	Hexanal			100	C6H12O	000066-25-1	53



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ClientSampleId :
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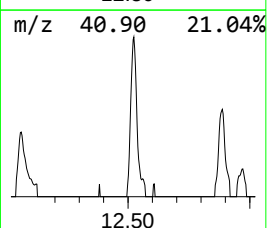
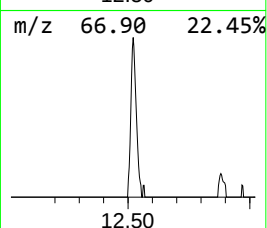
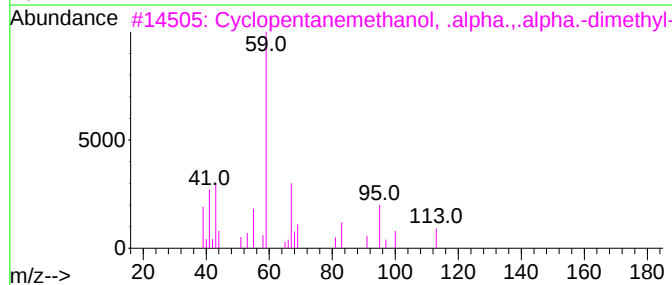
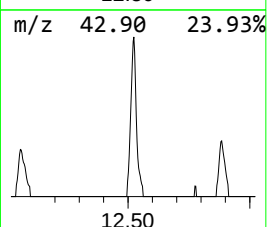
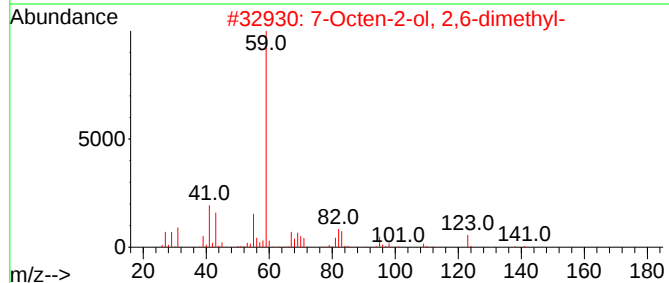
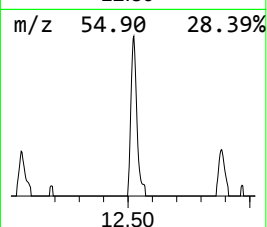
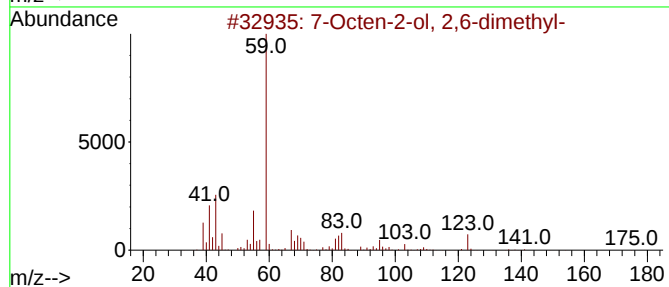
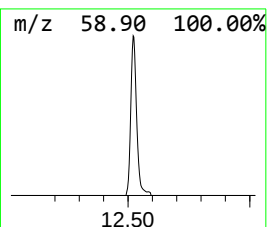
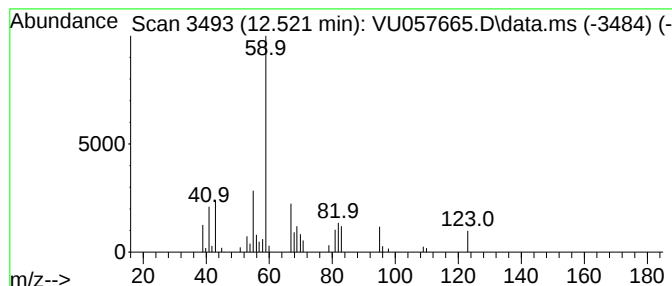
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.521	1.02 ug/L	36557	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	59
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	56
3			Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	53
4			1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	50
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	47



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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
unknown-01	2.480	0.6	ug/L	19315	1	6.245	159403	5.0
unknown-02	7.123	1.0	ug/L	31173	1	6.245	159403	5.0
Hexanal	8.785	0.7	ug/L	27493	2	9.412	190272	5.0
7-Octen-2-ol, 2...	12.521	1.0	ug/L	36557	3	11.807	179000	5.0