

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111323\
 Data File : VU056288.D
 Acq On : 14 Nov 2023 06:59
 Operator : MD/SY
 Sample : 05372-18
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GCDR2

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\SFAMUTR111323WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU056288.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	86	95	111	rVB	82768	101860	11.66%	1.167%
2	1.731	126	137	146	rBV	52392	66224	7.58%	0.758%
3	1.907	184	192	206	rVB	75618	104271	11.93%	1.194%
4	2.563	384	396	409	rBV	162670	261183	29.89%	2.991%
5	2.628	409	416	429	rVB	6677	12713	1.45%	0.146%
6	3.184	570	589	601	rBV	13525	36607	4.19%	0.419%
7	4.618	1019	1035	1071	rBV	108850	307088	35.14%	3.517%
8	4.804	1083	1093	1126	rVB2	37603	93376	10.68%	1.069%
9	5.058	1156	1172	1195	rBV2	149973	343630	39.32%	3.936%
10	5.721	1353	1378	1408	rBV3	286565	750569	85.88%	8.596%
11	6.245	1527	1541	1573	rBV	349674	691476	79.12%	7.919%
12	6.538	1618	1632	1651	rBV	411160	785794	89.91%	9.000%
13	6.685	1665	1678	1698	rBV	178310	354292	40.54%	4.058%
14	7.563	1939	1951	1969	rBV	85579	156226	17.88%	1.789%
15	7.894	2040	2054	2074	rBV	341149	617424	70.65%	7.071%
16	8.177	2127	2142	2161	rBV2	53489	95955	10.98%	1.099%
17	8.550	2246	2258	2271	rBV2	67495	117564	13.45%	1.346%
18	8.631	2271	2283	2296	rBV	378478	700586	80.16%	8.024%
19	8.743	2310	2318	2345	rVB3	45436	128619	14.72%	1.473%
20	8.926	2364	2375	2384	rBV6	20915	40059	4.58%	0.459%
21	8.978	2384	2391	2399	rVB4	9922	16819	1.92%	0.193%
22	9.058	2399	2416	2430	rBV8	17241	46737	5.35%	0.535%
23	9.129	2430	2438	2446	rVV3	12491	18259	2.09%	0.209%
24	9.181	2446	2454	2458	rVV4	7998	11157	1.28%	0.128%
25	9.219	2459	2466	2475	rVB3	12361	18296	2.09%	0.210%
26	9.344	2489	2505	2514	rBV5	36544	81162	9.29%	0.930%
27	9.412	2514	2526	2550	rVB	488796	873939	100.00%	10.009%
28	9.795	2637	2645	2658	rVB2	14832	22523	2.58%	0.258%
29	10.750	2931	2942	2959	rVB2	128388	211775	24.23%	2.425%
30	10.936	2991	3000	3009	rVB6	6289	11088	1.27%	0.127%
31	11.389	3130	3141	3154	rVV2	35575	64136	7.34%	0.735%
32	11.479	3159	3169	3176	rVV4	12950	21614	2.47%	0.248%
33	11.518	3176	3181	3193	rVB4	9574	16138	1.85%	0.185%
34	11.631	3202	3216	3238	rBV4	73140	162094	18.55%	1.856%
35	11.807	3258	3271	3289	rBV	490219	836695	95.74%	9.583%
36	12.084	3346	3357	3371	rBV9	6455	14284	1.63%	0.164%

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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_U\Method\SFAMUTR111323WMA.M
Title : TRACE VOA SFAM1.0

37	12.187	3377	3389	3409	rBV	319797	539236	61.70%	6.176%
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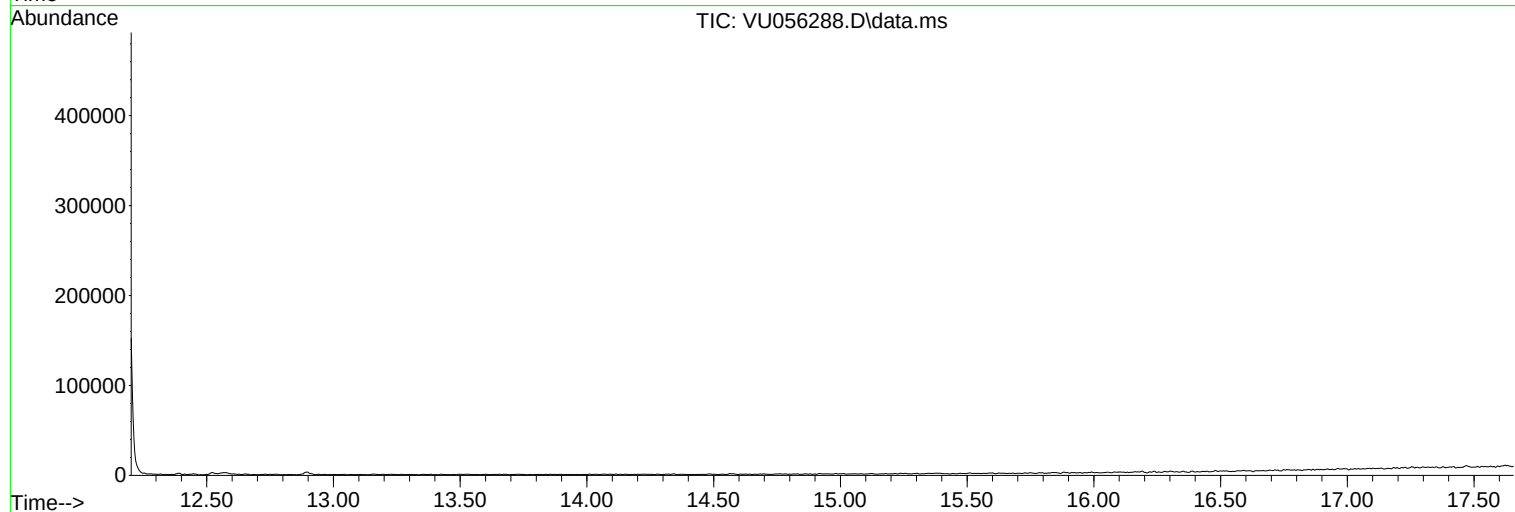
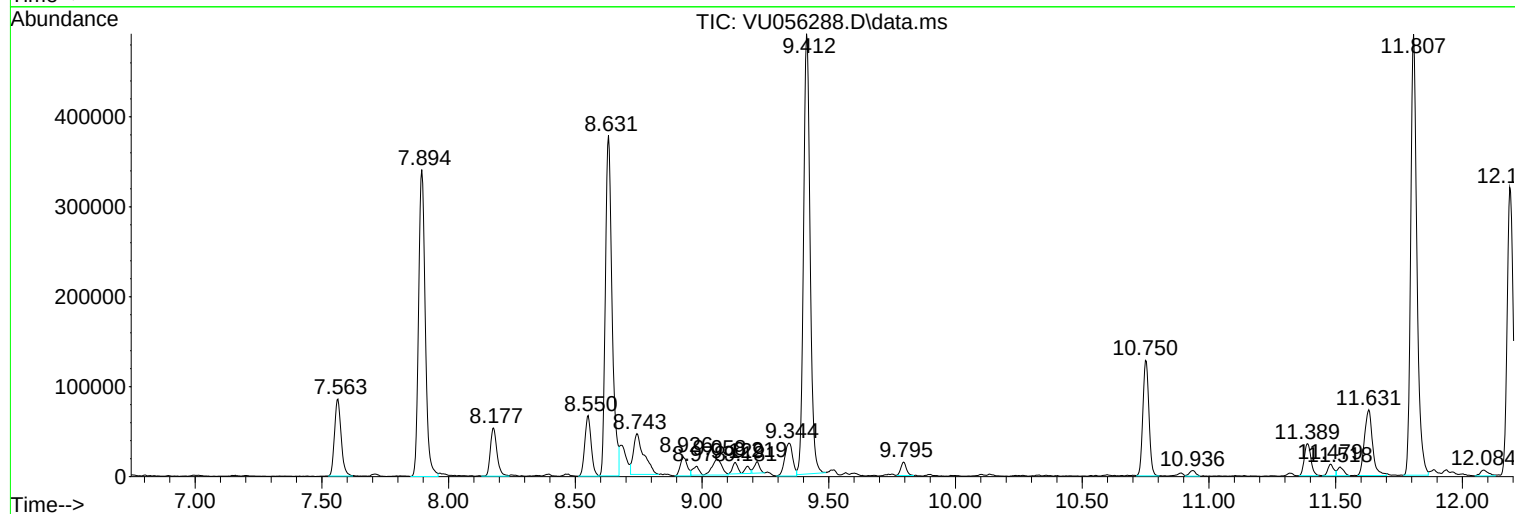
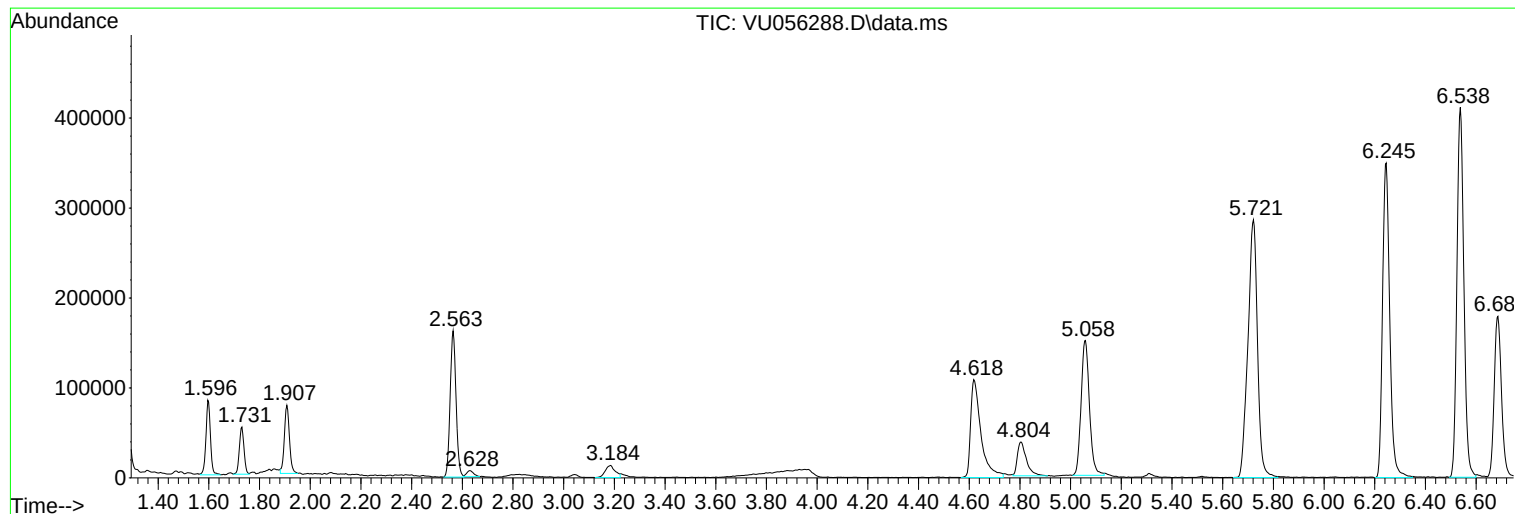
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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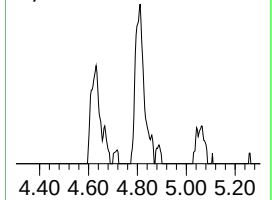
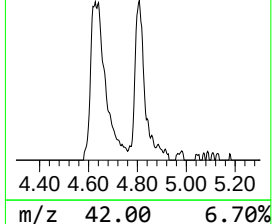
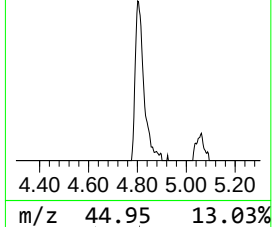
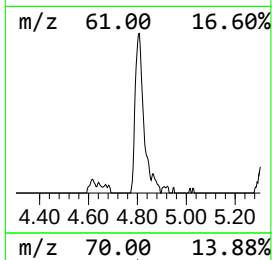
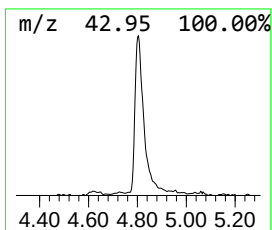
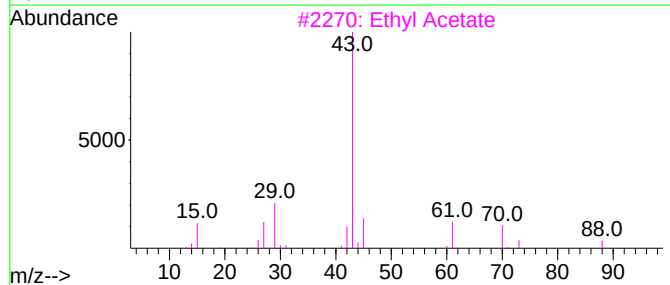
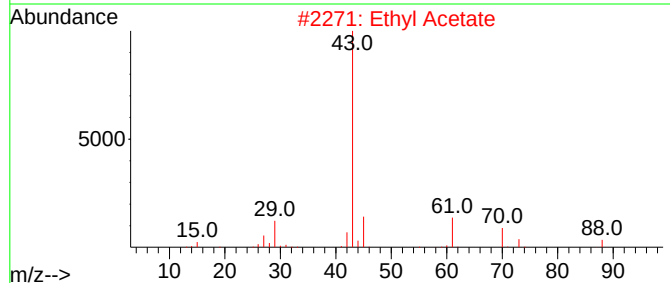
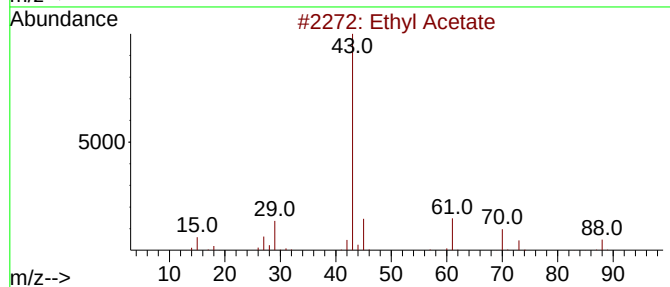
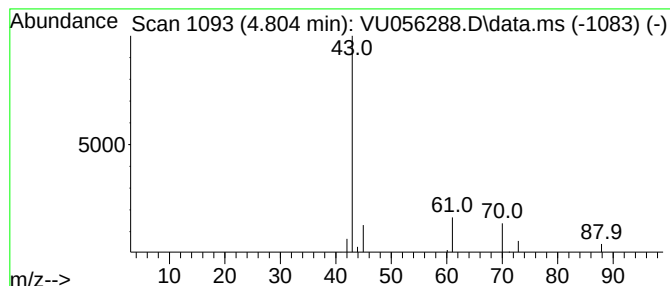
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Ethyl Acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.804	0.68 ug/L	93376	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	90
3			Ethyl Acetate	88	C4H8O2	000141-78-6	90
4			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	83
5			Ethyl Acetate	88	C4H8O2	000141-78-6	83



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Instrument :
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ClientSampleId :
GCDR2

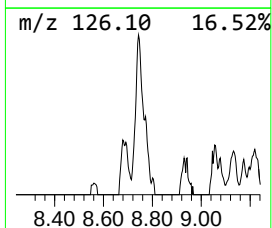
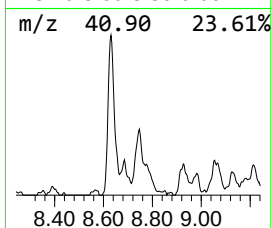
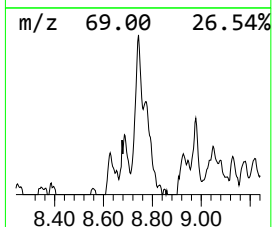
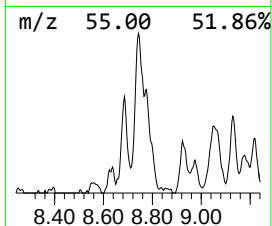
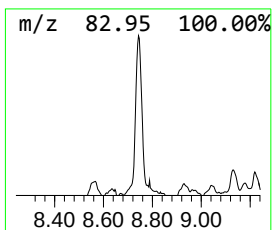
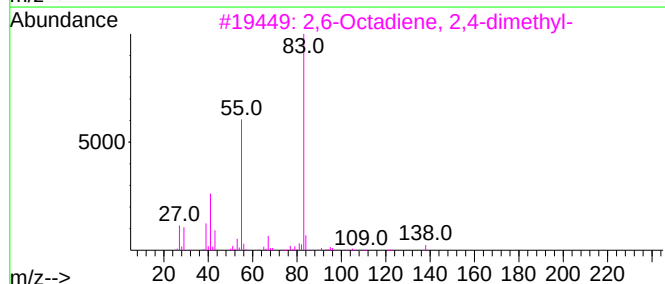
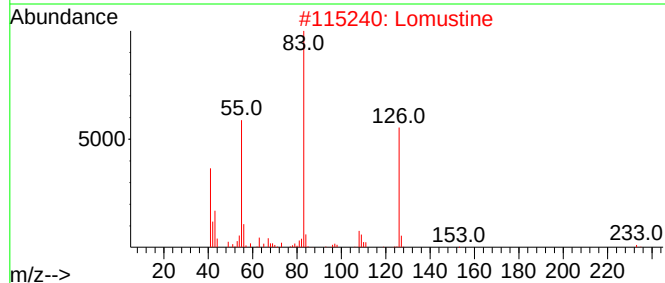
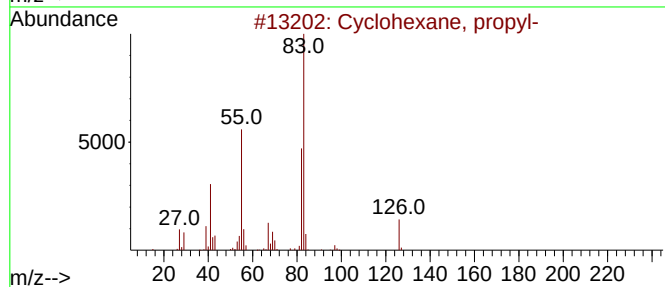
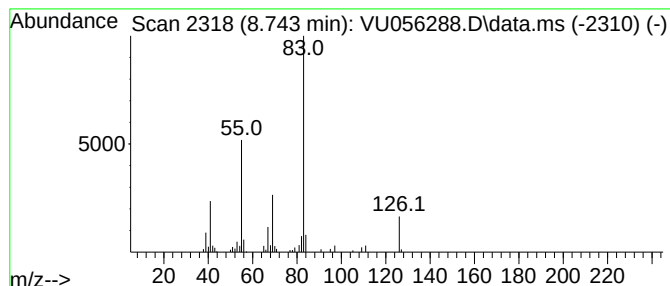
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Cyclic8.743 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.743	0.74 ug/L	128619	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, propyl-	126	C9H18	001678-92-8	83
2			Lomustine	233	C9H16ClN3O2	013010-47-4	78
3			2,6-Octadiene, 2,4-dimethyl-	138	C10H18	063843-03-8	72
4			Cyclohexane, propyl-	126	C9H18	001678-92-8	72
5			Hexanal 2E-hexenyl 3Z-hexenyl ac...	282	C18H34O2	1000431-43-4	64



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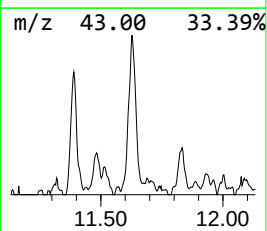
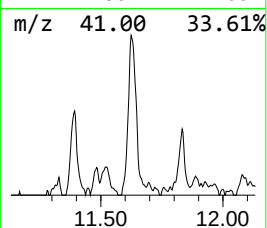
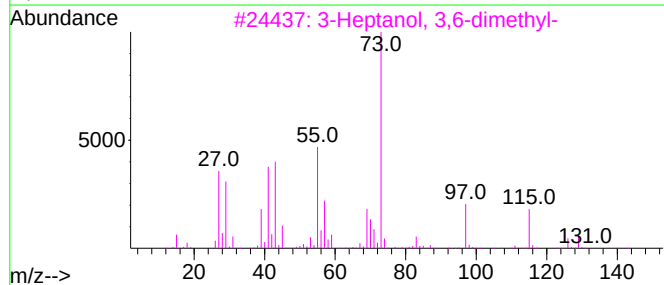
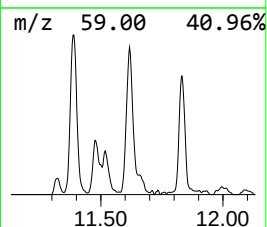
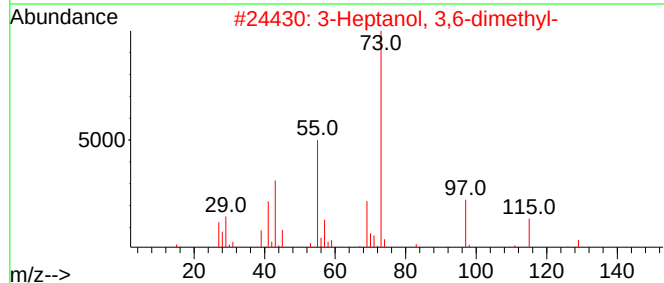
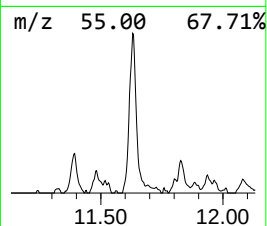
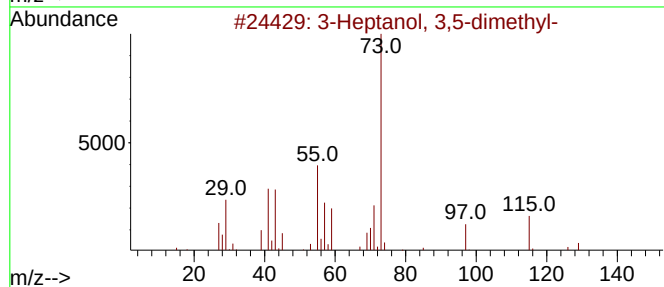
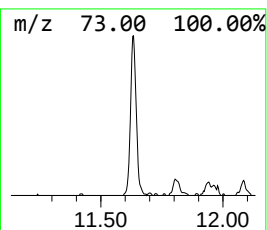
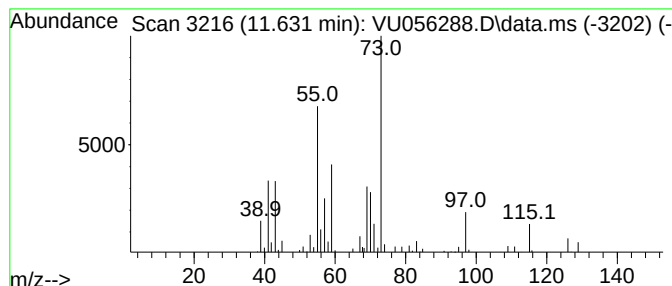
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.631	0.97 ug/L	162094	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	32
2			3-Heptanol, 3,6-dimethyl-	144	C9H20O	001573-28-0	25
3			3-Heptanol, 3,6-dimethyl-	144	C9H20O	001573-28-0	17
4			3-Hepten-2-one, 5-methyl-	126	C8H14O	005090-16-4	11
5			Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	10



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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
Ethyl Acetate	4.804	0.7	ug/L	93376	1	6.245	691476	5.0
(DEL) Alkane: C...	8.743	0.7	ug/L	128619	2	9.412	873939	5.0
unknown-01	11.631	1.0	ug/L	162094	3	11.807	836695	5.0