

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111523\
 Data File : VU056369.D
 Acq On : 15 Nov 2023 20:53
 Operator : MD/SY
 Sample : 05372-18
 Misc : 25mL/MSVOA_U/WATER
 ALS Vial : 23 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: VU056369.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	86	95	107	rVB	154774	176204	15.81%	1.603%
2	1.727	128	136	146	rBV	69350	85637	7.69%	0.779%
3	1.907	183	192	207	rVB	121305	165853	14.88%	1.509%
4	2.563	384	396	410	rBV	263338	425699	38.20%	3.873%
5	2.811	453	473	476	rBV5	5762	15216	1.37%	0.138%
6	3.184	572	589	615	rBV2	22829	64200	5.76%	0.584%
7	4.618	1021	1035	1079	rBV	165372	458685	41.16%	4.174%
8	4.801	1082	1092	1120	rVB3	53164	126068	11.31%	1.147%
9	5.055	1157	1171	1196	rBV	221846	497193	44.62%	4.524%
10	5.721	1355	1378	1403	rBV2	427043	1114306	100.00%	10.139%
11	6.245	1528	1541	1568	rBV	326890	642001	57.61%	5.842%
12	6.537	1617	1632	1661	rBV	402460	771469	69.23%	7.020%
13	6.685	1664	1678	1707	rVB	268514	529235	47.49%	4.816%
14	7.563	1939	1951	1971	rBV	124859	231684	20.79%	2.108%
15	7.894	2039	2054	2077	rBV	519062	925110	83.02%	8.418%
16	8.174	2129	2141	2157	rBV	78987	140382	12.60%	1.277%
17	8.550	2245	2258	2271	rBV2	65591	113984	10.23%	1.037%
18	8.627	2271	2282	2310	rVV	557032	1095211	98.29%	9.965%
19	8.743	2310	2318	2347	rVB4	42753	125716	11.28%	1.144%
20	8.923	2364	2374	2384	rBV2	19909	37077	3.33%	0.337%
21	8.975	2385	2390	2400	rVV4	9984	15629	1.40%	0.142%
22	9.065	2400	2418	2431	rVV7	15802	43249	3.88%	0.394%
23	9.132	2431	2439	2446	rVV4	10442	16962	1.52%	0.154%
24	9.177	2447	2453	2459	rVV6	7077	11311	1.02%	0.103%
25	9.219	2459	2466	2474	rVV5	11381	18688	1.68%	0.170%
26	9.341	2491	2504	2514	rBV4	30924	67860	6.09%	0.617%
27	9.412	2514	2526	2548	rVB	463150	818172	73.42%	7.445%
28	9.794	2636	2645	2656	rBV4	11900	18756	1.68%	0.171%
29	10.749	2930	2942	2966	rVB	176382	289323	25.96%	2.633%
30	11.389	3129	3141	3152	rVV	47028	78450	7.04%	0.714%
31	11.479	3160	3169	3175	rBV4	13648	22024	1.98%	0.200%
32	11.515	3175	3180	3193	rVB2	11032	17593	1.58%	0.160%
33	11.627	3201	3215	3234	rBV4	83560	180795	16.22%	1.645%
34	11.807	3259	3271	3290	rBV	471451	821112	73.69%	7.471%
35	12.074	3345	3354	3368	rBV	8996	21227	1.90%	0.193%
36	12.187	3377	3389	3415	rVB	482693	808086	72.52%	7.353%

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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

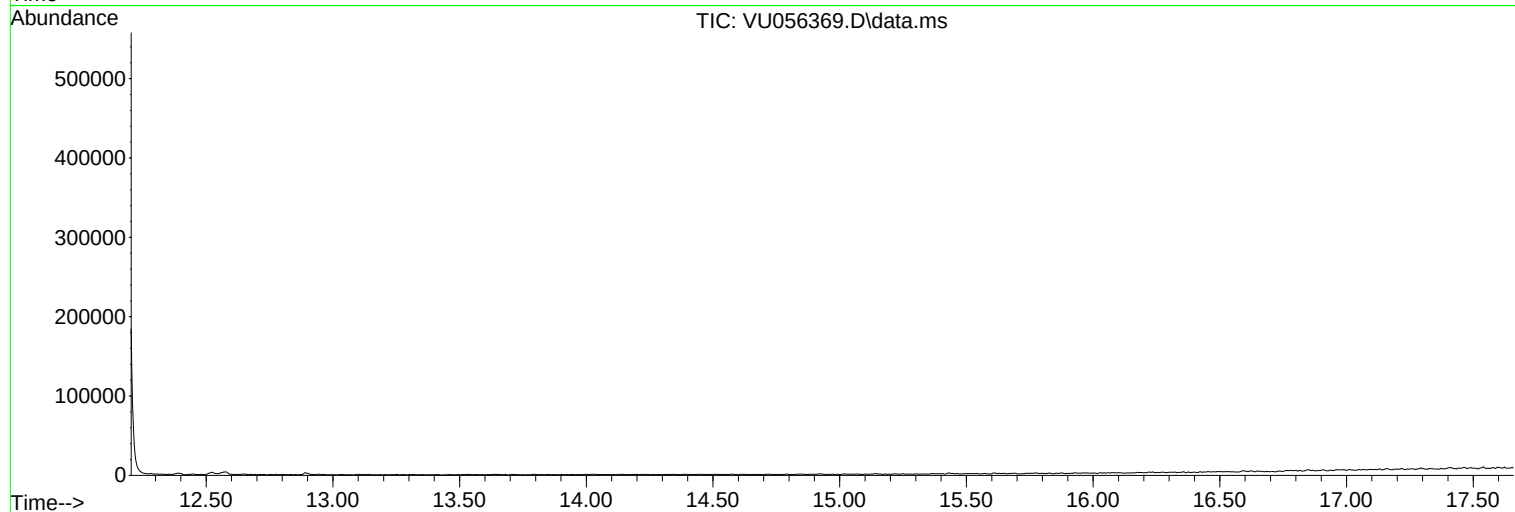
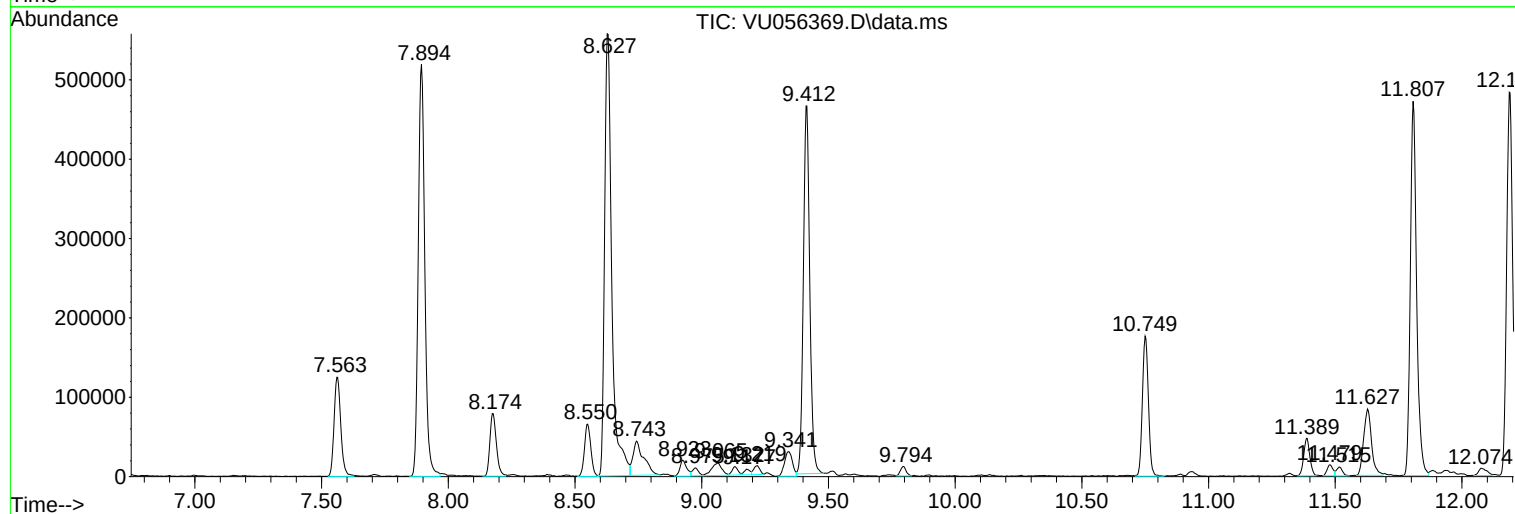
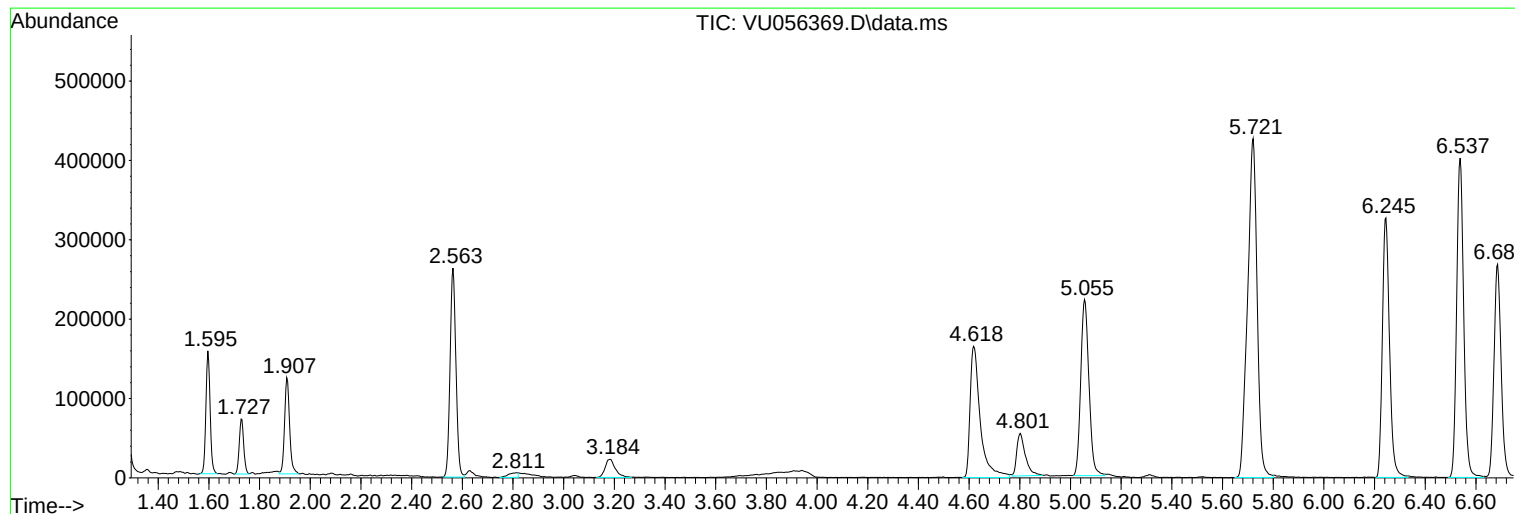
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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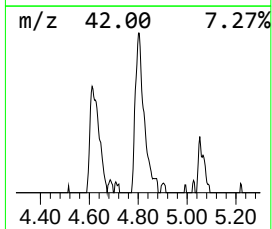
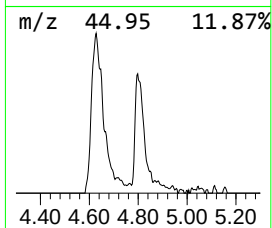
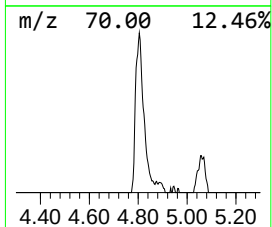
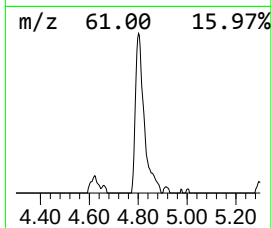
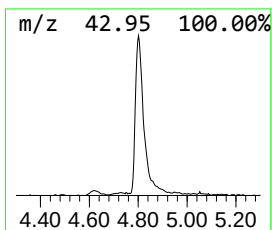
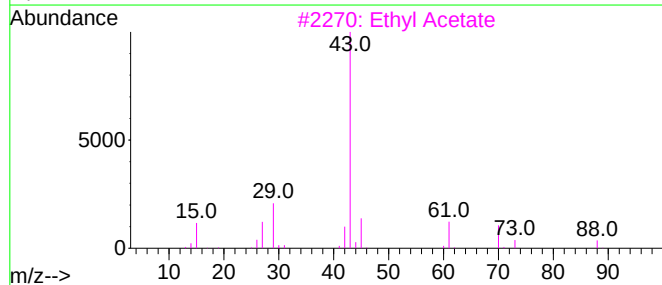
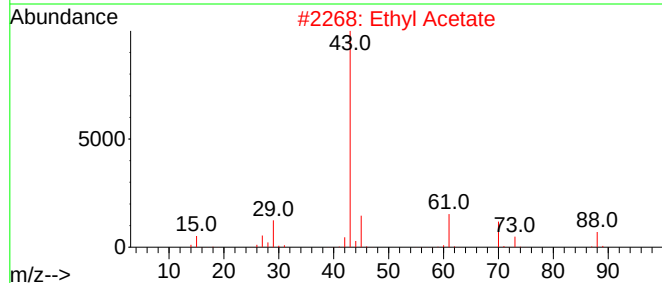
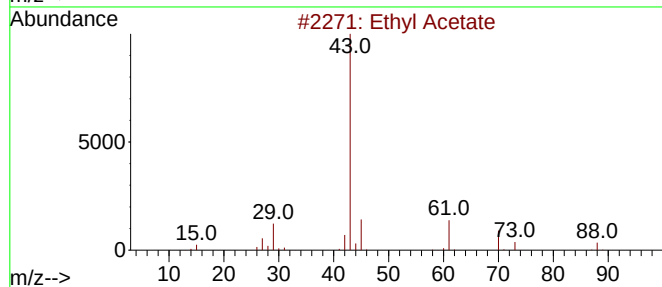
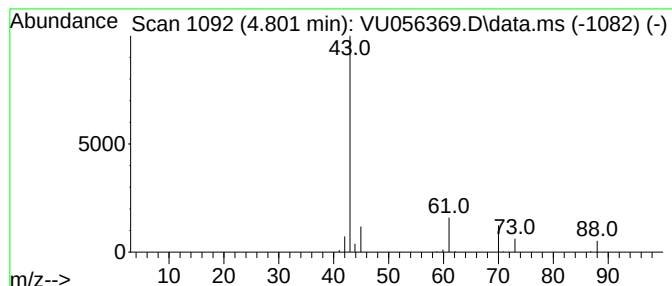
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Ethyl Acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.801	0.98 ug/L	126068	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			Ethyl Acetate	88	C4H8O2	000141-78-6	90
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40



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Instrument :
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ClientSampleId :
GCDR2

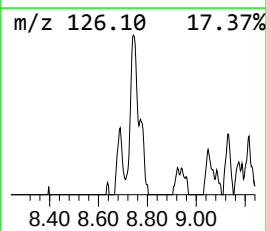
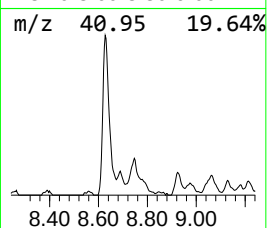
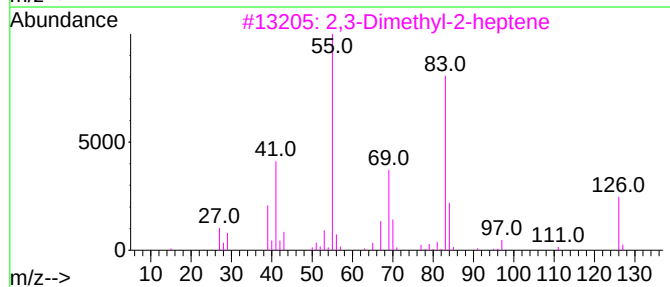
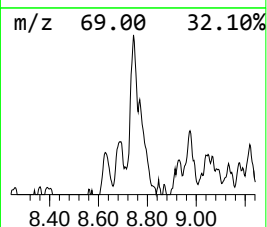
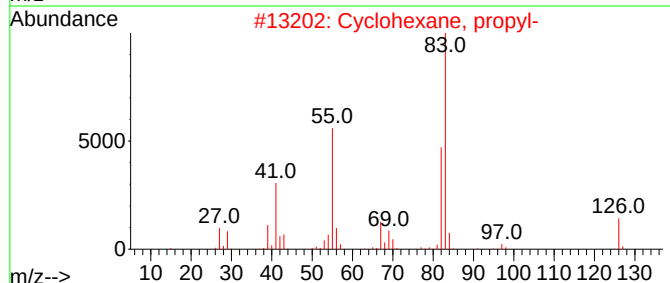
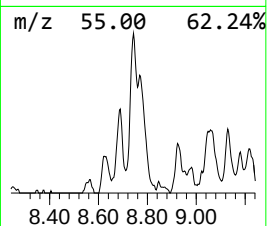
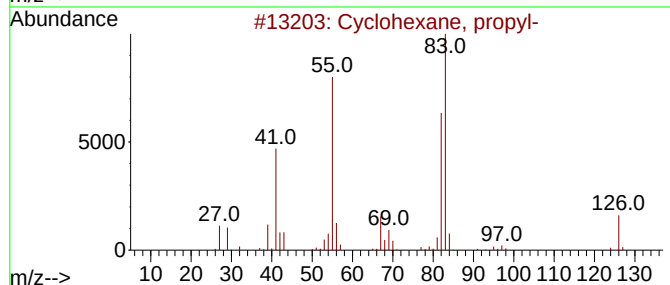
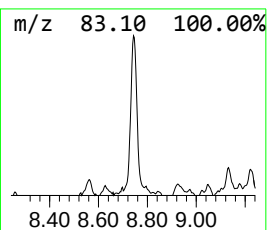
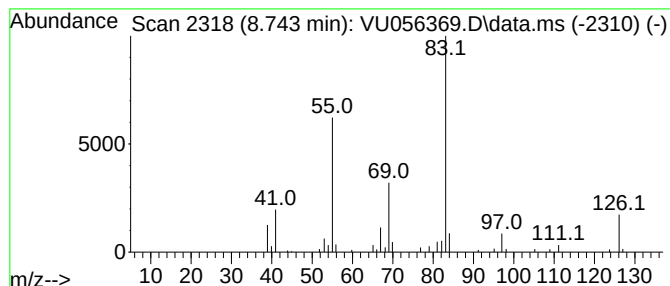
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Cyclic8.743 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.743	0.77 ug/L	125716	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, propyl-	126	C9H18	001678-92-8	91
2			Cyclohexane, propyl-	126	C9H18	001678-92-8	86
3			2,3-Dimethyl-2-heptene	126	C9H18	003074-64-4	86
4			Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	72
5			Cyclohexanecarboxylic acid, 4-ni...	249	C13H15NO4	1000307-70-8	72



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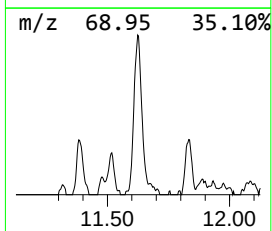
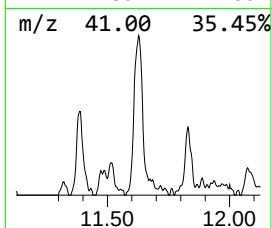
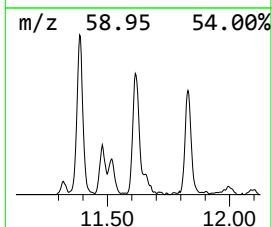
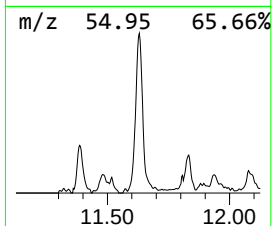
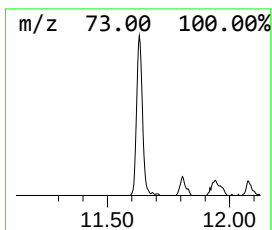
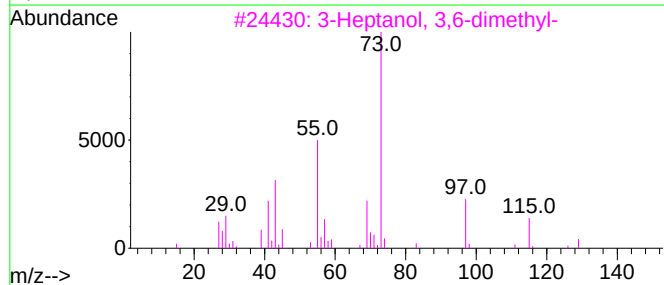
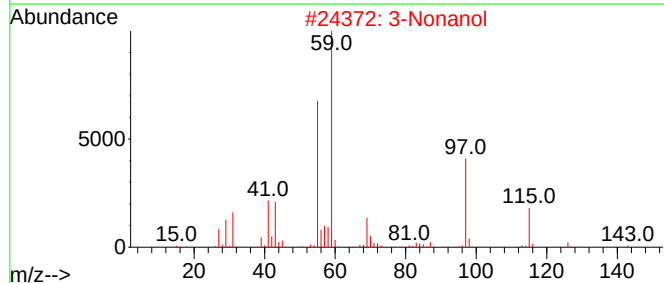
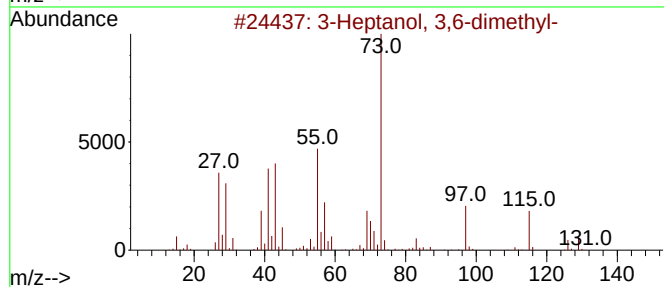
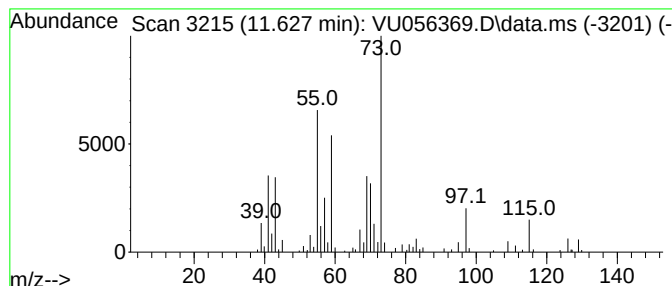
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.627	1.10 ug/L	180795	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanol, 3,6-dimethyl-	144	C9H20O	001573-28-0	37
2			3-Nonanol	144	C9H20O	000624-51-1	32
3			3-Heptanol, 3,6-dimethyl-	144	C9H20O	001573-28-0	32
4			Silane, butyltrimethyl-	130	C7H18Si	001000-49-3	23
5			N,N-Dimethylformamide-di-t-butyl...	203	C11H25NO2	036805-97-7	16



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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	4.801	1.0	ug/L	126068	1	6.245	642001	5.0
(DEL) Alkane: C...	8.743	0.8	ug/L	125716	2	9.415	818172	5.0
unknown-01	11.627	1.1	ug/L	180795	3	11.807	821112	5.0