

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121423\
 Data File : VU056863.D
 Acq On : 15 Dec 2023 02:38
 Operator : MD/SY
 Sample : 05770-12
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EOY82

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\SFAMUTR121123WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU056863.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.358	14	21	37	rVB	169284	173572	21.79%	2.134%
2	1.486	54	61	67	rBV	100661	97910	12.29%	1.204%
3	1.515	67	70	76	rVB	9933	9551	1.20%	0.117%
4	1.599	86	96	107	rBV2	202693	237403	29.81%	2.919%
5	1.911	185	193	206	rVB	74384	99469	12.49%	1.223%
6	1.991	210	218	232	rVB	58535	81589	10.24%	1.003%
7	2.200	275	283	296	rVB	37395	53192	6.68%	0.654%
8	2.367	325	335	347	rVB5	8829	17214	2.16%	0.212%
9	2.563	381	396	415	rVB	139865	233096	29.26%	2.866%
10	2.682	421	433	443	rVB8	5568	11863	1.49%	0.146%
11	2.788	456	466	480	rVB	17053	29654	3.72%	0.365%
12	3.042	531	545	548	rBV7	4919	8937	1.12%	0.110%
13	3.078	548	556	565	rVV4	9533	19536	2.45%	0.240%
14	3.132	565	573	582	rVB4	5463	8850	1.11%	0.109%
15	3.357	628	643	654	rVB4	9357	19735	2.48%	0.243%
16	3.695	735	748	762	rBV4	11578	30242	3.80%	0.372%
17	4.528	993	1007	1025	rBV4	11989	29247	3.67%	0.360%
18	4.660	1031	1048	1079	rBV2	145972	490010	61.52%	6.026%
19	5.055	1156	1171	1199	rBV	156845	368687	46.29%	4.534%
20	5.380	1258	1272	1286	rVB5	11624	27896	3.50%	0.343%
21	5.721	1358	1378	1408	rBV4	279085	778094	97.69%	9.568%
22	6.245	1526	1541	1567	rBV	277126	552312	69.34%	6.792%
23	6.502	1606	1621	1629	rBV2	94716	204317	25.65%	2.513%
24	6.685	1664	1678	1693	rBV	182765	372379	46.75%	4.579%
25	6.753	1694	1699	1706	rVV2	16252	31853	4.00%	0.392%
26	6.801	1707	1714	1728	rVB4	32640	62324	7.82%	0.766%
27	6.975	1755	1768	1788	rBV8	6863	19737	2.48%	0.243%
28	7.560	1939	1950	1967	rBV2	84451	155993	19.58%	1.918%
29	7.894	2032	2054	2067	rBV	304231	544739	68.39%	6.699%
30	7.965	2067	2076	2091	rVB	104607	188832	23.71%	2.322%
31	8.177	2132	2142	2155	rBV2	49885	88453	11.11%	1.088%
32	8.550	2248	2258	2267	rBV9	6331	11497	1.44%	0.141%
33	8.634	2270	2284	2318	rBV2	355911	796507	100.00%	9.795%
34	9.412	2514	2526	2552	rBV	398330	725187	91.05%	8.918%
35	9.569	2564	2575	2595	rVB2	14769	28248	3.55%	0.347%
36	9.692	2600	2613	2626	rBV2	20002	37166	4.67%	0.457%

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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	10.100	2731	2740	2752	rBV2	10027	17793	2.23%	0.219%
38	10.749	2931	2942	2958	rBV	145151	239871	30.12%	2.950%
39	11.466	3155	3165	3174	rBV2	9753	15011	1.88%	0.185%
40	11.807	3259	3271	3291	rBV	363683	617517	77.53%	7.594%
41	12.061	3341	3350	3366	rBV4	22257	50827	6.38%	0.625%
42	12.187	3376	3389	3406	rBV	311751	545565	68.49%	6.709%

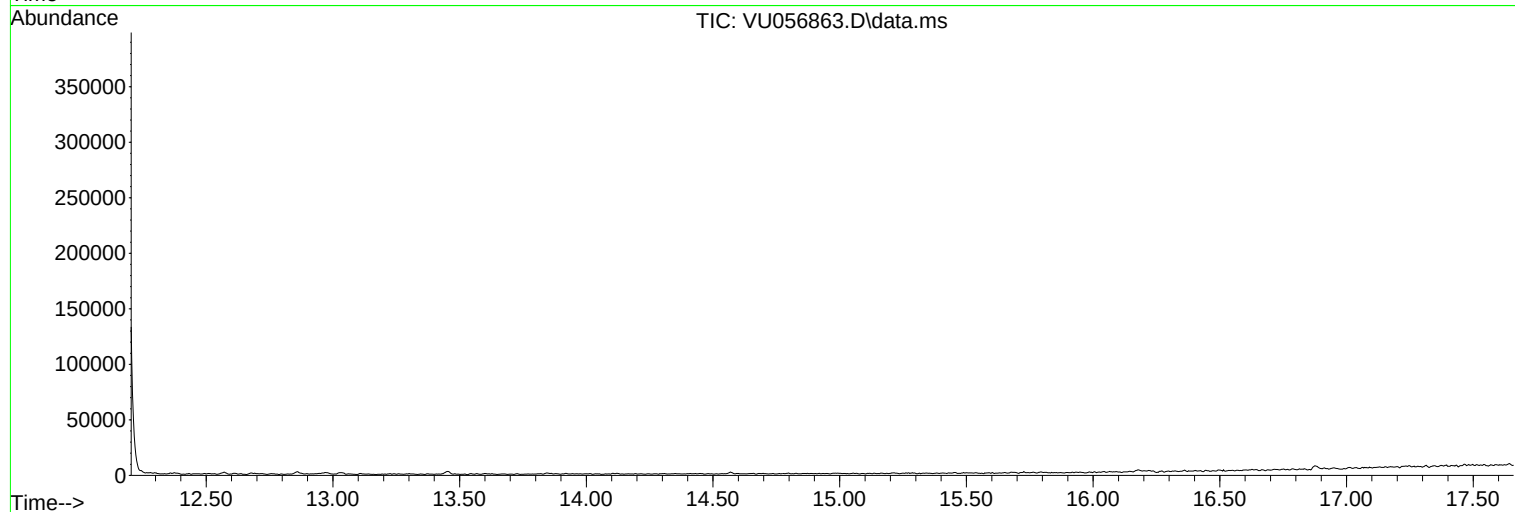
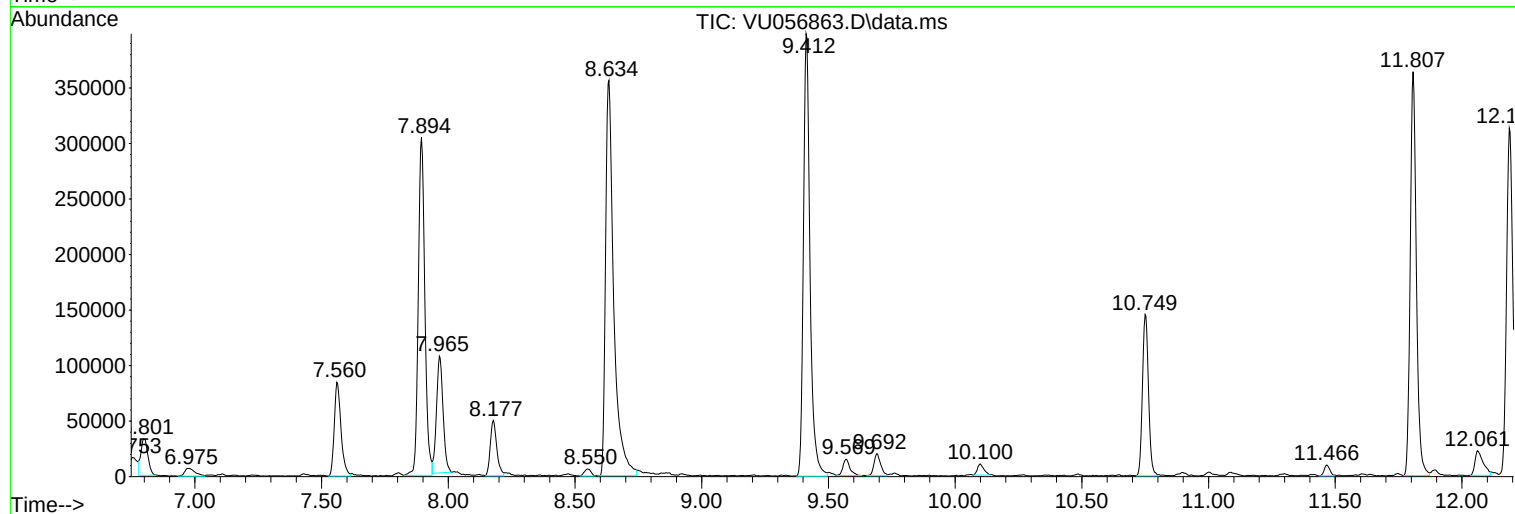
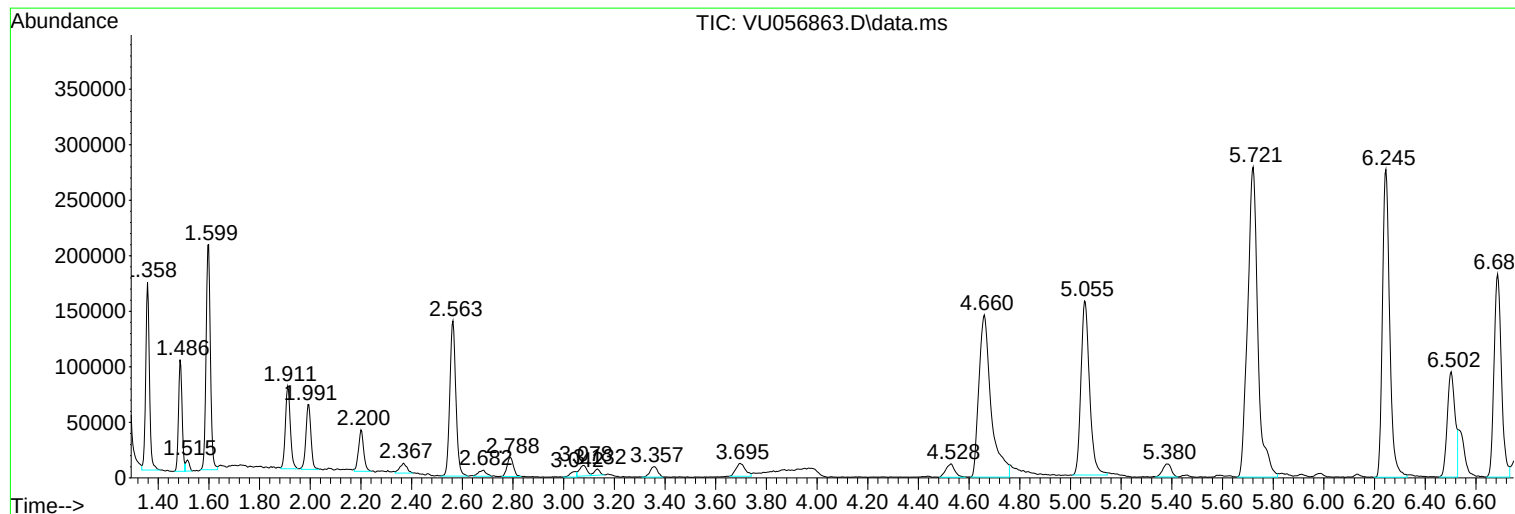
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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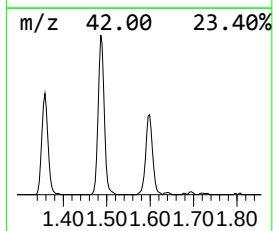
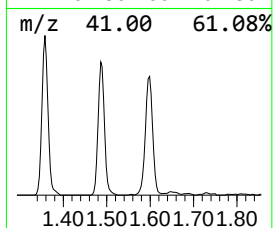
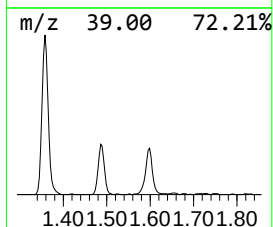
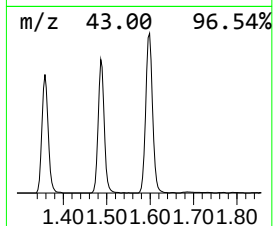
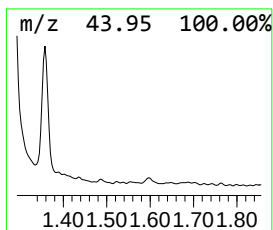
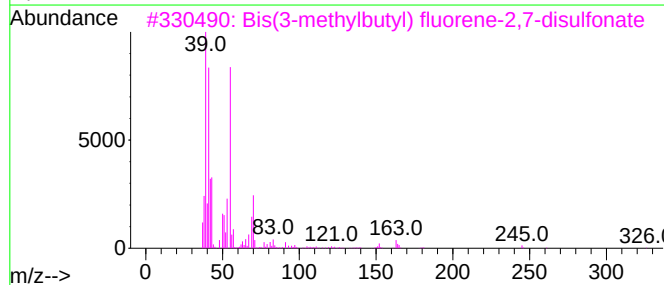
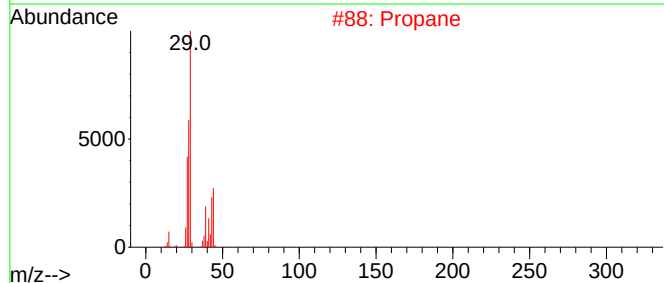
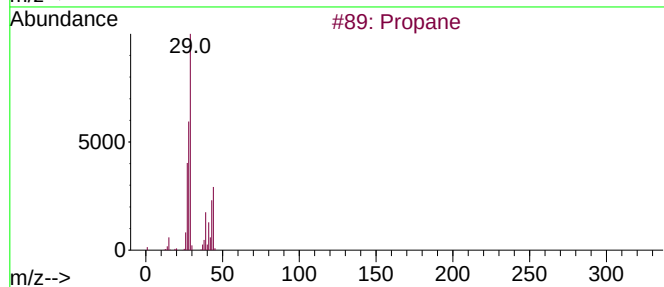
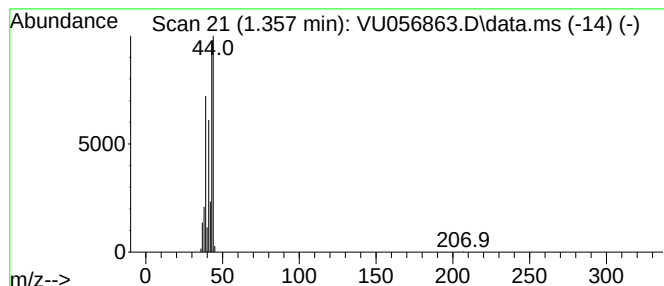
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.357	1.57 ug/L	173572	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	83
2			Propane	44	C3H8	000074-98-6	83
3			Bis(3-methylbutyl) fluorene-2,7-...	466	C23H30O6S2	253664-95-8	47
4			2-Hexynoic acid	112	C6H8O2	000764-33-0	39
5			Imidazol-5(2H)-one, 4-amino-2-(2...	196	C7H8N4O3	318259-17-5	38



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MSVOA_U
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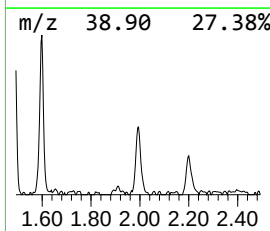
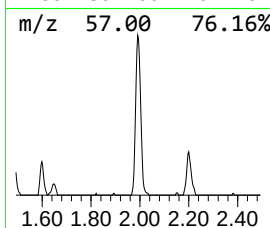
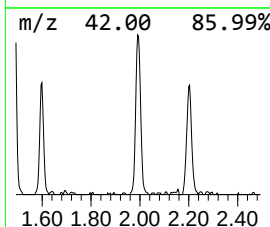
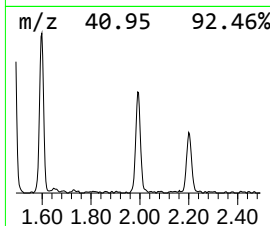
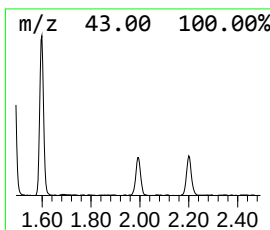
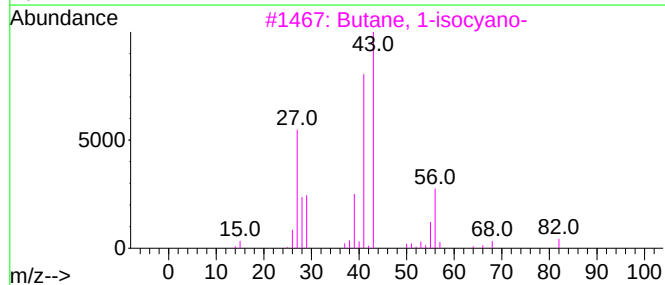
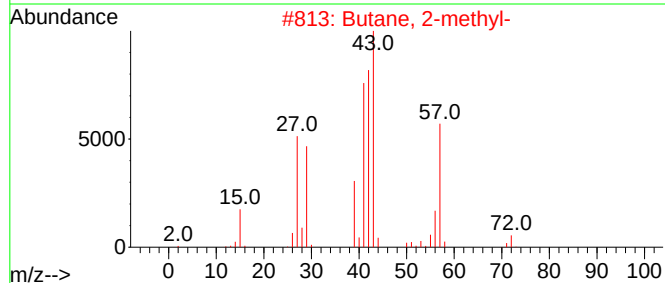
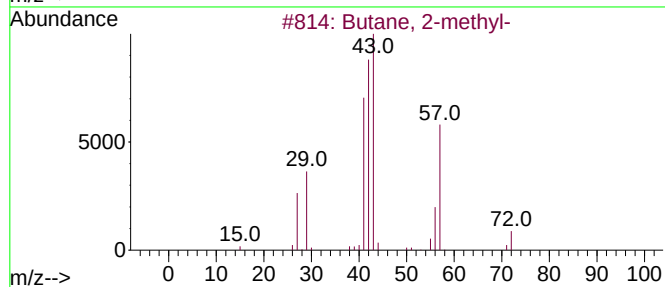
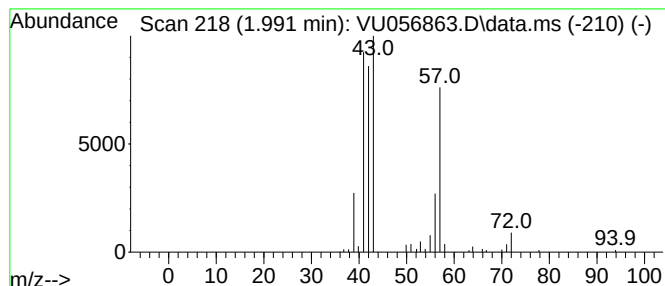
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.991	0.74 ug/L	81589	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Butane, 2-methyl-	72	C5H12	000078-78-4	86
3			Butane, 1-isocyano-	83	C5H9N	002769-64-4	10
4			Methane, isocyanato-	57	C2H3NO	000624-83-9	9
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	9



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

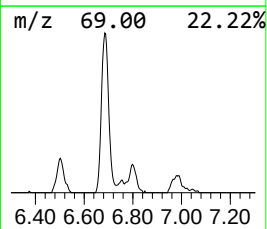
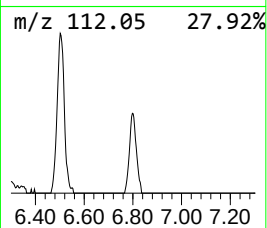
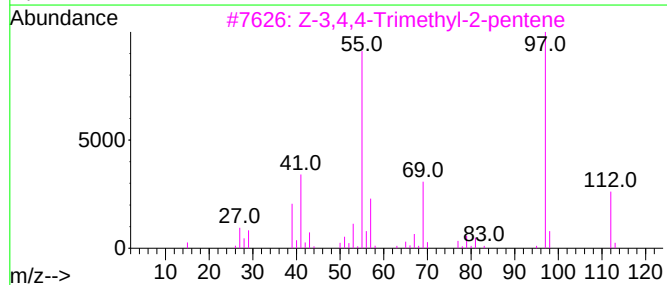
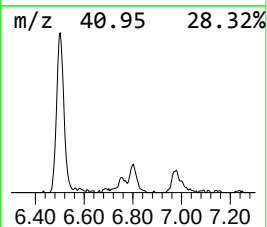
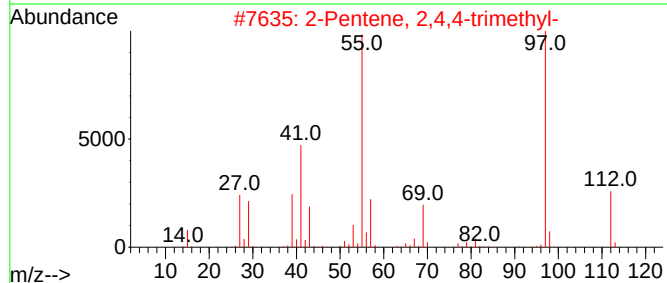
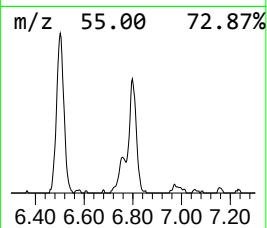
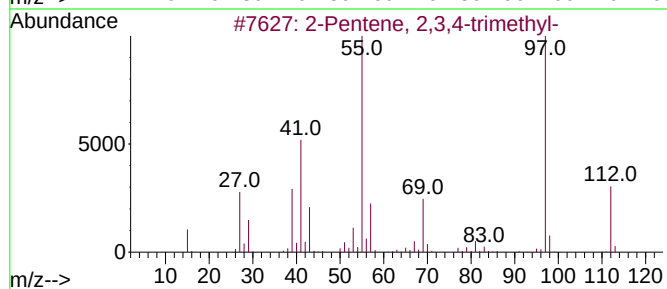
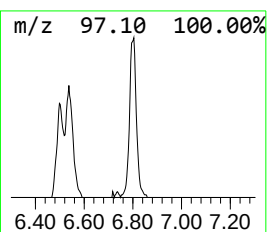
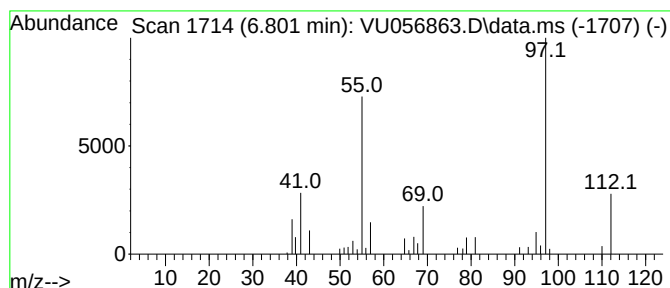
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.801	0.56 ug/L	62324	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentene, 2,3,4-trimethyl-	112	C8H16	000565-77-5	72
2		2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	64
3		Z-3,4,4-Trimethyl-2-pentene	112	C8H16	039761-64-3	64
4		3-Hepten-2-one, (Z)-	112	C7H12O	069668-88-8	59
5		2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	59



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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
(DEL) Alkane: S...	1.357	1.6	ug/L	173572	1	6.245	552312	5.0
(DEL) Alkane: S...	1.991	0.7	ug/L	81589	1	6.245	552312	5.0
(DEL) Alkane: S...	6.801	0.6	ug/L	62324	1	6.245	552312	5.0