

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061522\
 Data File : VU049170.D
 Acq On : 15 Jun 2022 15:12
 Operator : SY/MD
 Sample : N3288-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGJ99

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\SFAMUTR061422WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU049170.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.610	77	84	93	rBV	69339	91478	3.09%	0.871%
2	1.803	138	144	154	rBV	31478	41147	1.39%	0.392%
3	1.925	176	182	194	rVB	52712	70894	2.39%	0.675%
4	2.594	376	390	405	rVB3	456001	817390	27.60%	7.787%
5	3.906	783	798	817	rVB	235182	549040	18.54%	5.230%
6	4.694	1027	1043	1065	rBV	863187	2018295	68.16%	19.227%
7	5.086	1153	1165	1181	rVB	81297	169688	5.73%	1.616%
8	5.748	1353	1371	1390	rBV2	210738	490765	16.57%	4.675%
9	5.999	1443	1449	1464	rBV	50960	73892	2.50%	0.704%
10	6.304	1532	1544	1563	rBV	166949	311339	10.51%	2.966%
11	6.591	1618	1633	1656	rBV	1622110	2961325	100.00%	28.210%
12	6.742	1668	1680	1696	rBV	122366	235858	7.96%	2.247%
13	7.600	1935	1947	1959	rBV	70202	121155	4.09%	1.154%
14	7.925	2036	2048	2061	rBV	246645	415605	14.03%	3.959%
15	8.205	2127	2135	2156	rVB2	52477	111790	3.77%	1.065%
16	8.661	2256	2277	2309	rBV	349190	667146	22.53%	6.355%
17	9.430	2500	2516	2538	rBV	218884	367941	12.42%	3.505%
18	10.764	2919	2931	2943	rBV	96081	153688	5.19%	1.464%
19	11.815	3245	3258	3280	rBV	238779	377027	12.73%	3.592%
20	12.060	3319	3334	3351	rBV	46271	84035	2.84%	0.801%
21	12.195	3364	3376	3391	rVB	229149	367800	12.42%	3.504%

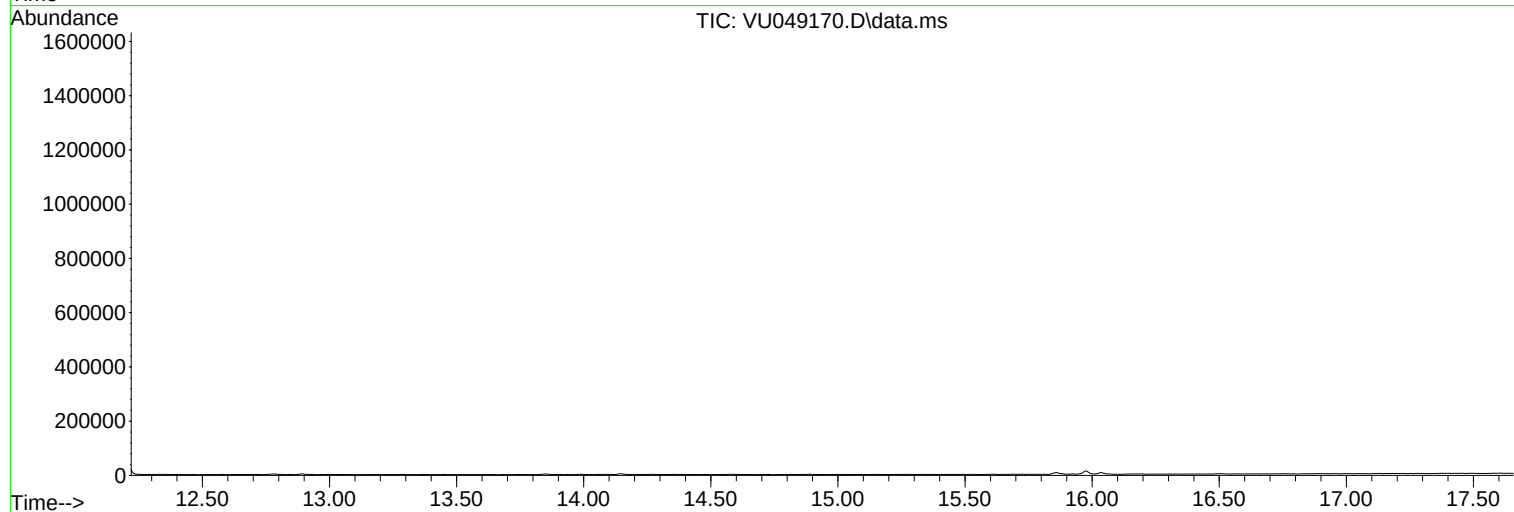
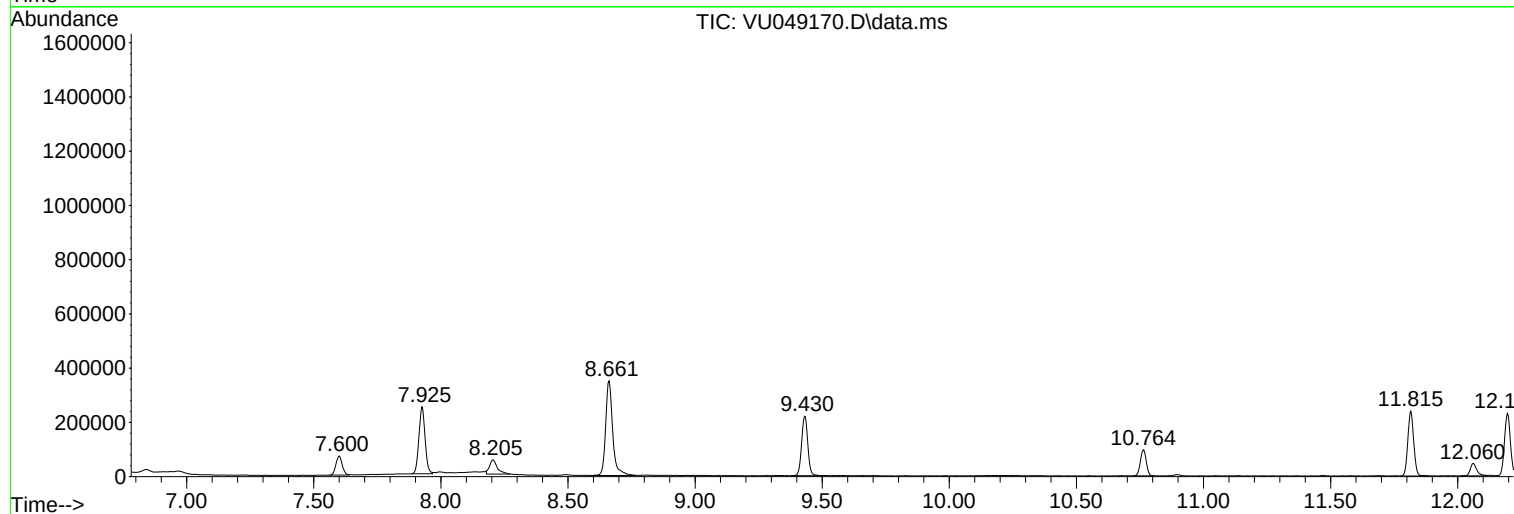
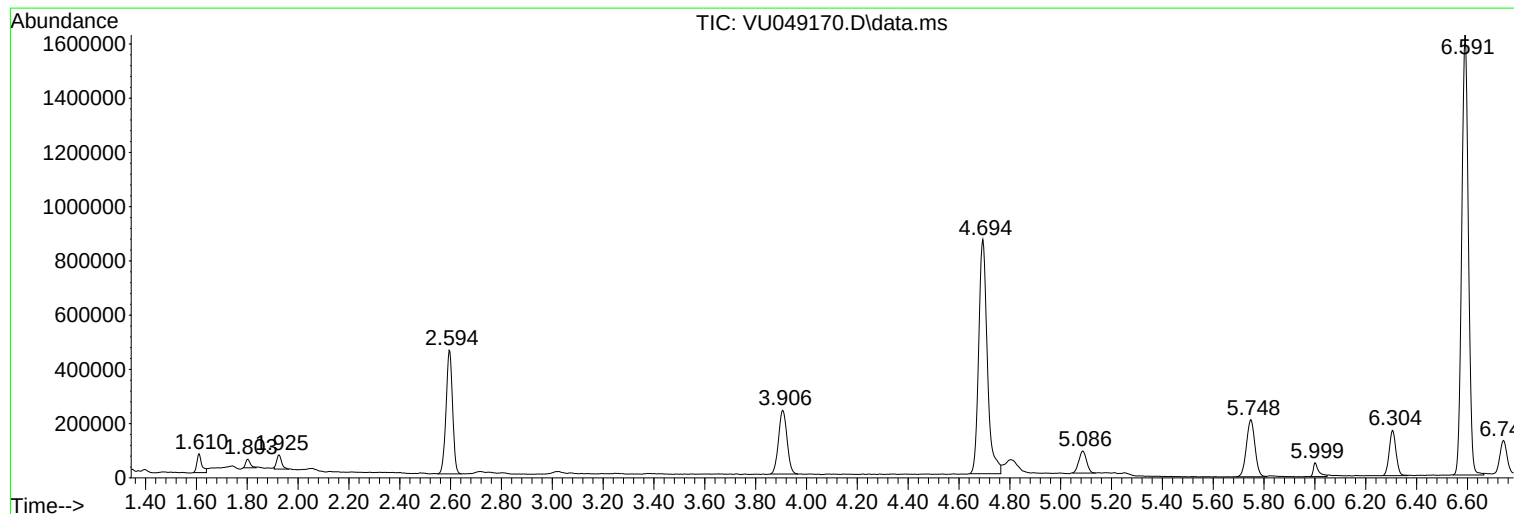
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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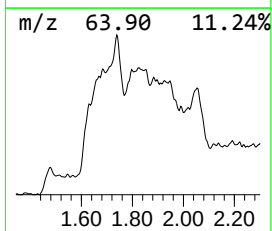
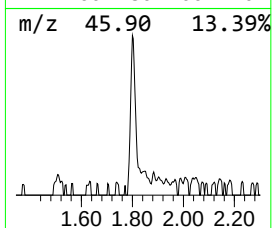
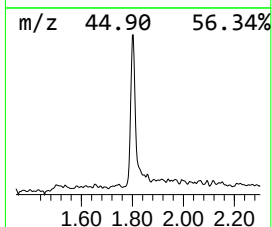
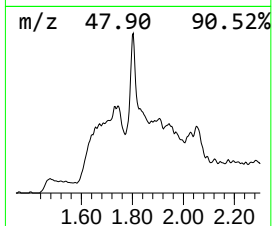
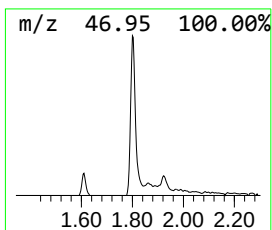
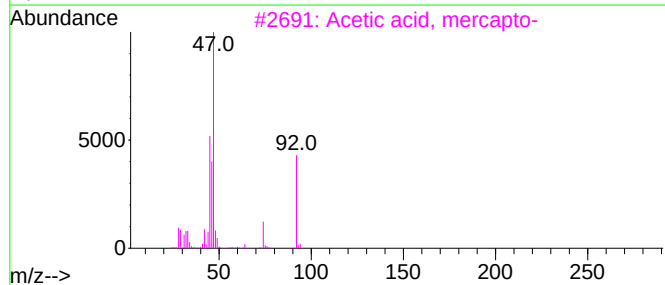
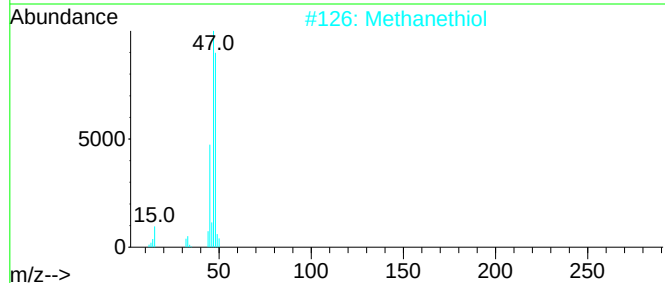
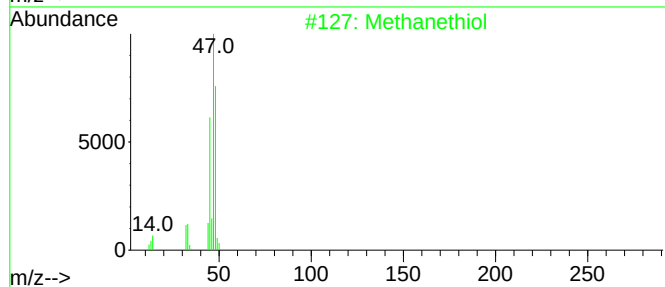
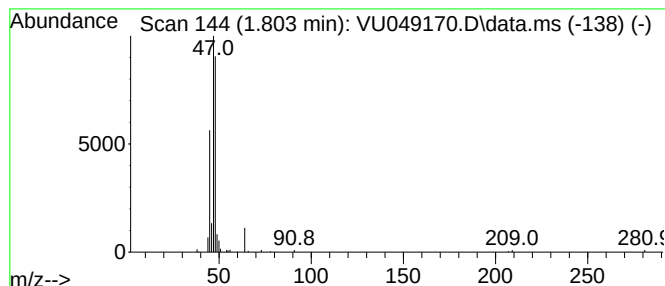
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Methanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.803	0.66 ug/L	41147	1,4-Difluorobenzene	6.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	86
2			Methanethiol	48	CH4S	000074-93-1	86
3			Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9
4			Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9
5			Methional	104	C4H8OS	003268-49-3	9



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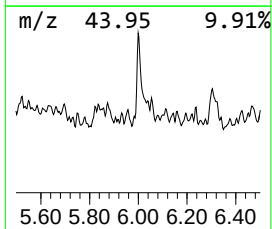
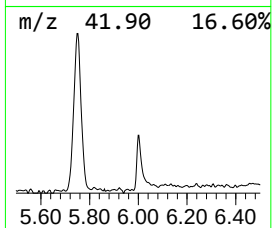
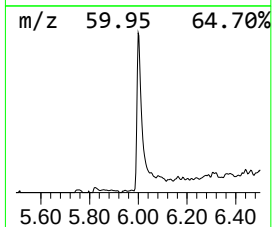
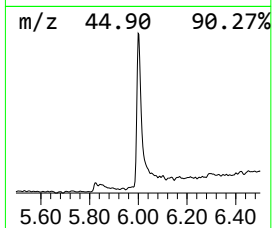
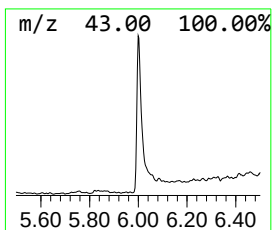
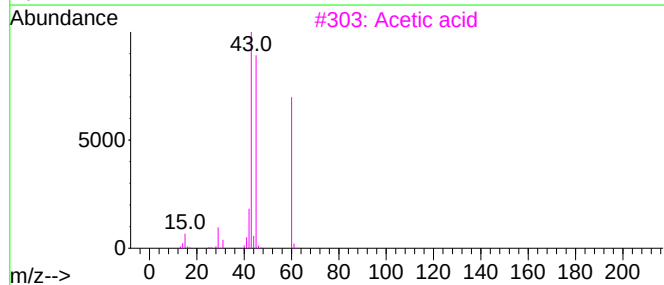
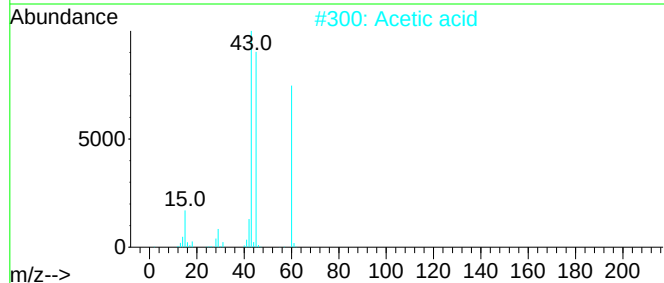
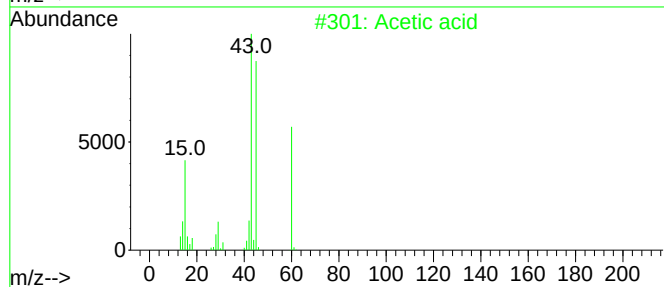
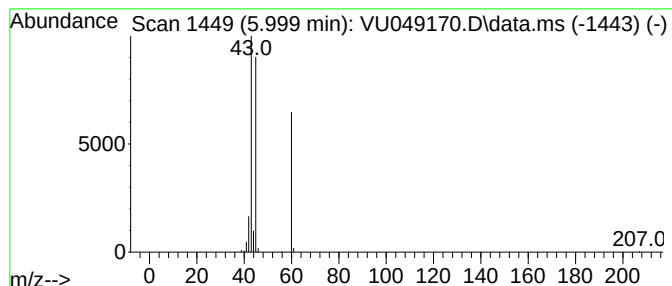
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Acetic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.999	1.19 ug/L	73892	1,4-Difluorobenzene	6.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid			60	C2H4O2	000064-19-7	90
2	Acetic acid			60	C2H4O2	000064-19-7	90
3	Acetic acid			60	C2H4O2	000064-19-7	90
4	Acetic acid			60	C2H4O2	000064-19-7	90
5	Acetic acid			60	C2H4O2	000064-19-7	78



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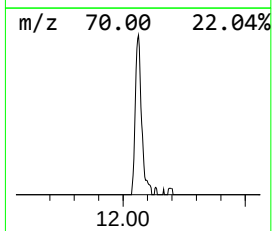
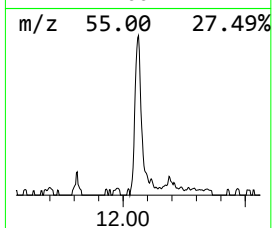
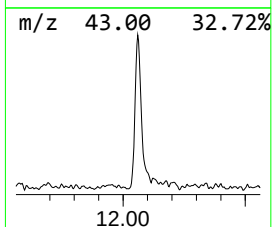
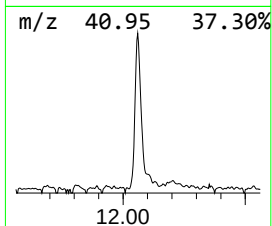
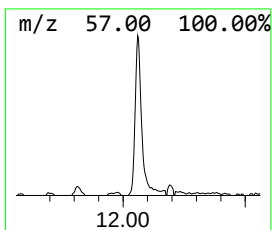
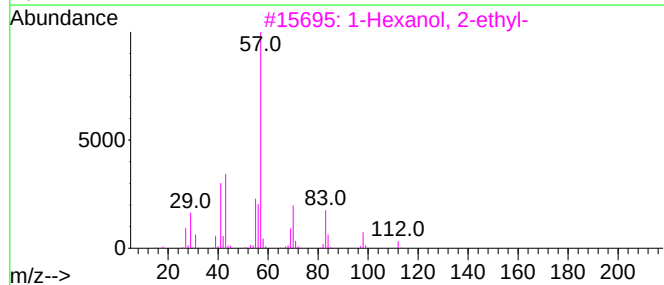
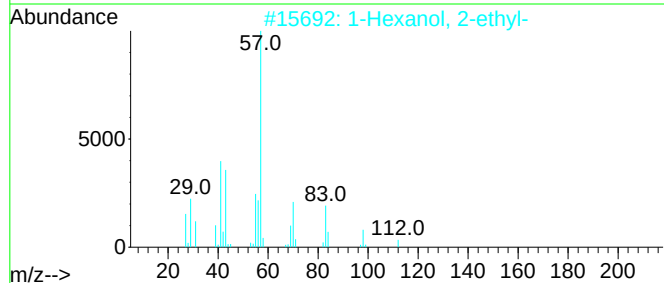
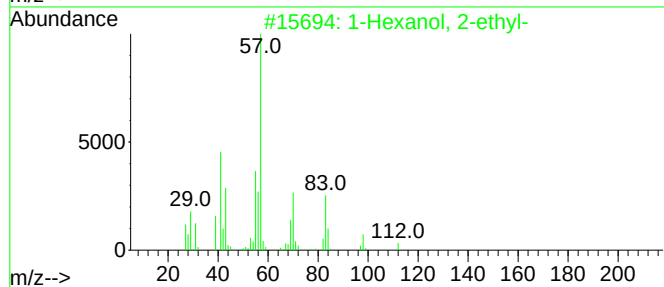
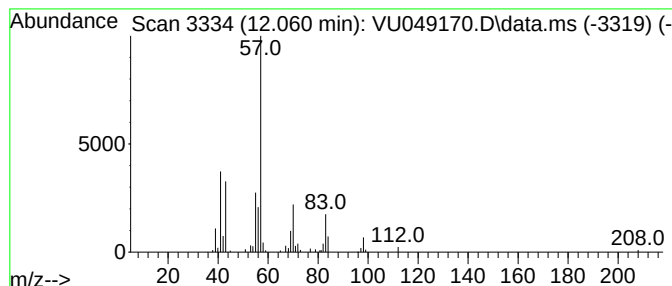
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Quant Title : TRACE VOA SFAM1.0

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TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	1.11 ug/L	84035	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	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
Methanethiol	1.803	0.7	ug/L	41147	1	6.304	311339	5.0
Acetic acid	5.999	1.2	ug/L	73892	1	6.304	311339	5.0
1-Hexanol, 2-et...	12.060	1.1	ug/L	84035	3	11.816	377027	5.0