

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061523\
 Data File : VU054543.D
 Acq On : 15 Jun 2023 23:07
 Operator : MD/SY
 Sample : 03253-18
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXYY5

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\SFAMUTR060723WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU054543.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.490	52	62	86	rBV	87547	298356	32.13%	3.671%
2	1.599	90	96	110	rVB	79425	111660	12.03%	1.374%
3	1.914	186	194	210	rVB	98582	136457	14.70%	1.679%
4	2.567	384	397	411	rBV	138694	232476	25.04%	2.861%
5	2.644	412	421	437	rVV2	16026	36102	3.89%	0.444%
6	3.049	535	547	561	rVB4	5804	11346	1.22%	0.140%
7	3.798	777	780	795	rVB	5137	10706	1.15%	0.132%
8	4.631	1027	1039	1079	rBV	130481	402723	43.37%	4.956%
9	5.059	1157	1172	1201	rVB	171229	403723	43.48%	4.968%
10	5.724	1357	1379	1397	rBV2	334005	873700	94.09%	10.751%
11	6.245	1528	1541	1565	rBV	327130	636343	68.53%	7.830%
12	6.686	1664	1678	1696	rBV	221148	443899	47.81%	5.462%
13	7.563	1936	1951	1969	rBV	84928	156237	16.83%	1.923%
14	7.894	2041	2054	2074	rBV	381792	674190	72.61%	8.296%
15	8.177	2130	2142	2161	rBV2	51776	94835	10.21%	1.167%
16	8.467	2221	2232	2243	rBV3	6944	13132	1.41%	0.162%
17	8.631	2270	2283	2319	rBV2	458570	928545	100.00%	11.426%
18	8.785	2323	2331	2342	rVV3	18994	34219	3.69%	0.421%
19	9.412	2514	2526	2554	rBV	442951	772479	83.19%	9.505%
20	10.753	2929	2943	2961	rBV	162050	269060	28.98%	3.311%
21	10.888	2973	2985	2999	rVB	15441	26421	2.85%	0.325%
22	11.685	3226	3233	3244	rBV7	7274	12497	1.35%	0.154%
23	11.808	3258	3271	3295	rBV	464841	756470	81.47%	9.308%
24	12.062	3340	3350	3377	rBV3	40498	104192	11.22%	1.282%
25	12.190	3377	3390	3409	rVV	384254	632709	68.14%	7.786%
26	12.885	3594	3606	3619	rBV4	32903	54254	5.84%	0.668%

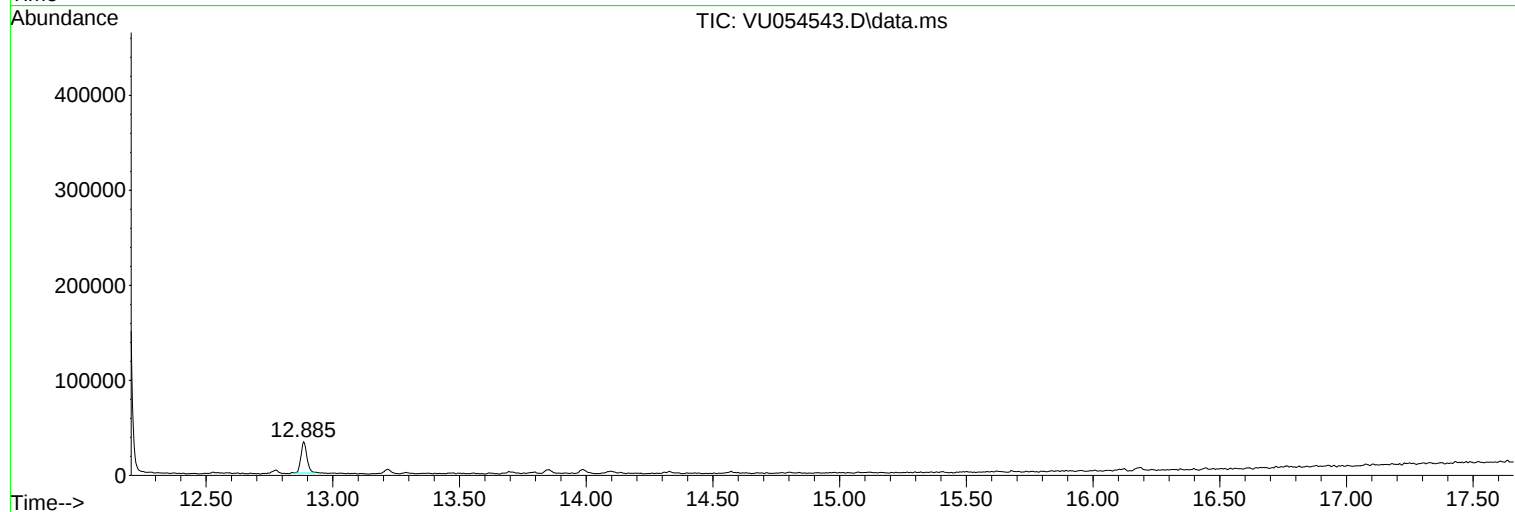
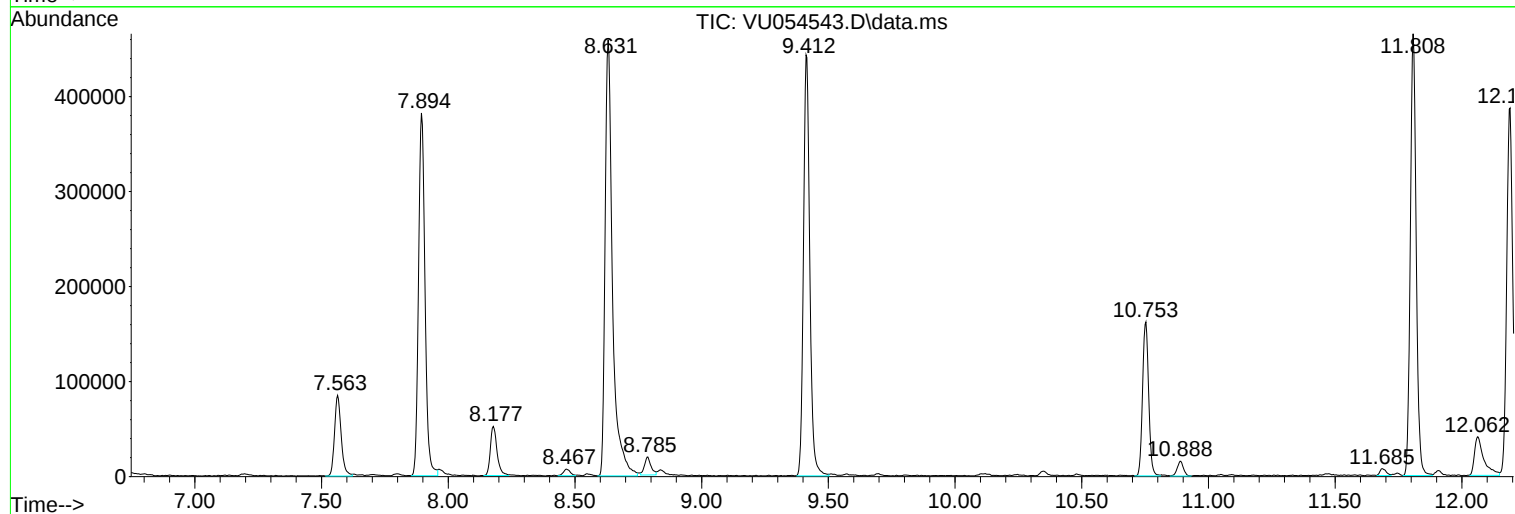
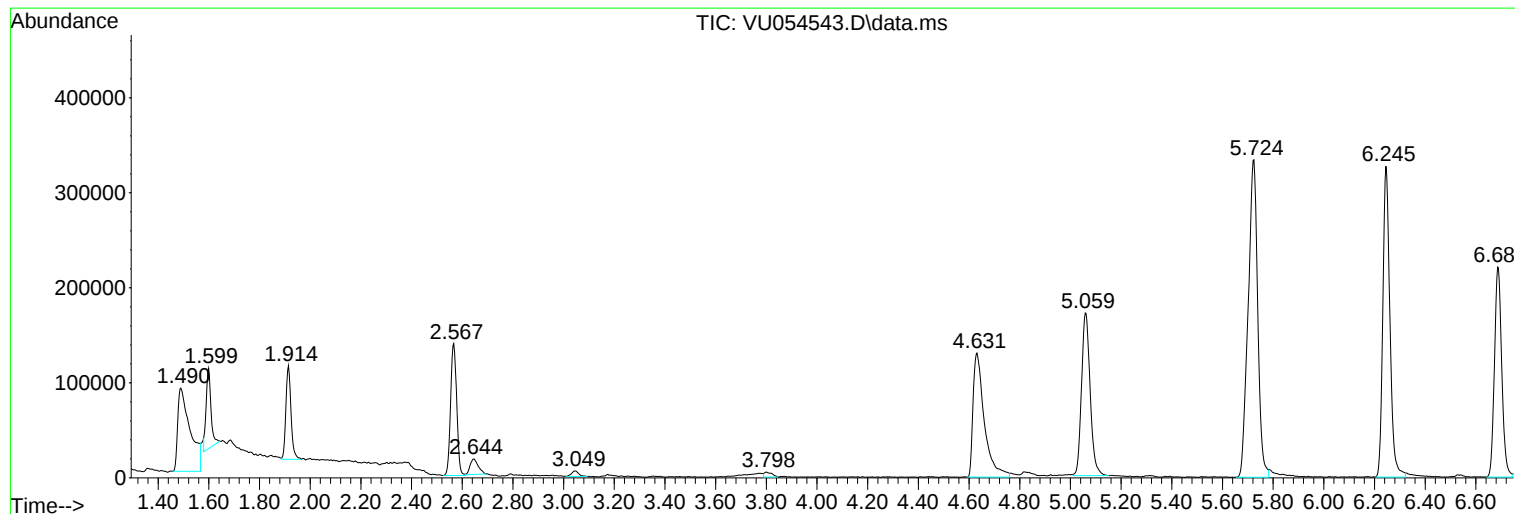
Sum of corrected areas: 8126731

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Instrument :
MSVOA_U
ClientSampleId :
EXYY5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.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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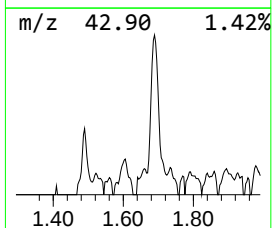
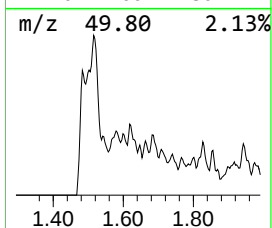
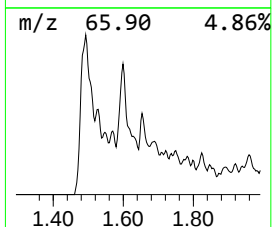
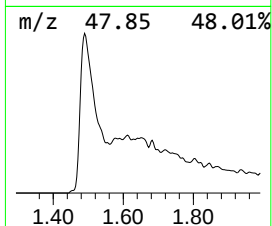
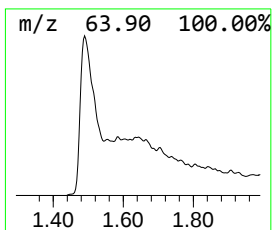
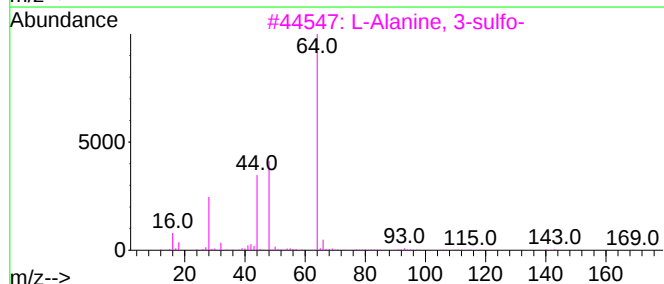
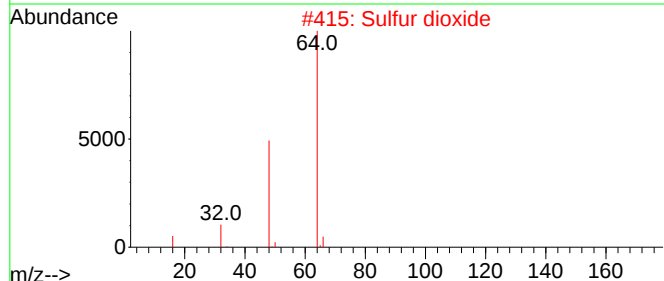
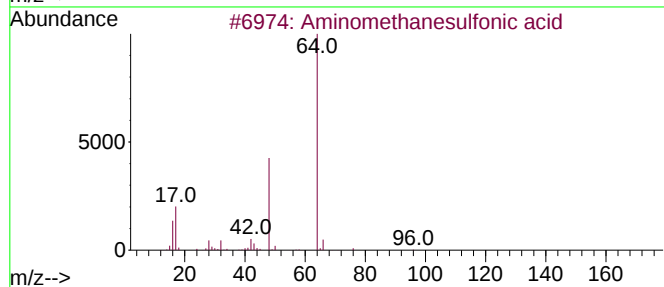
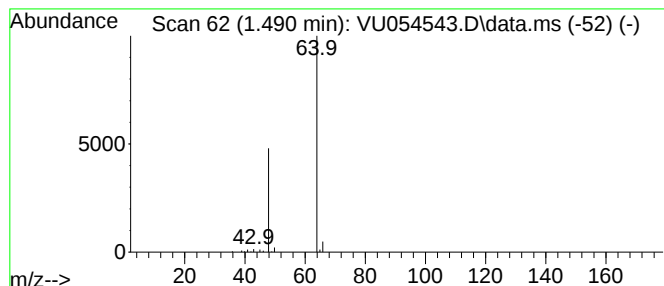
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.490	2.34 ug/L	298356	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	5
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	4



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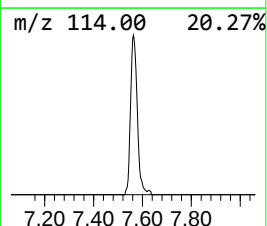
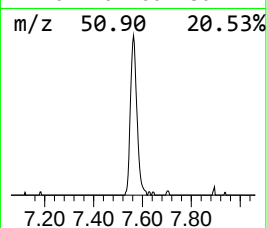
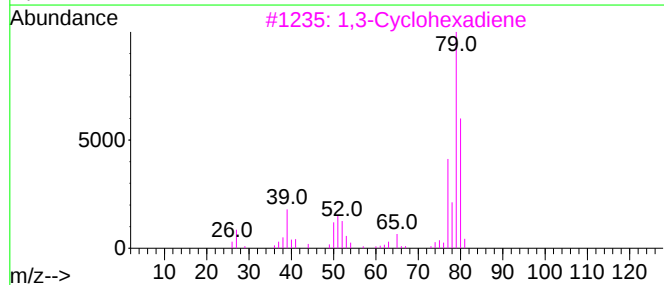
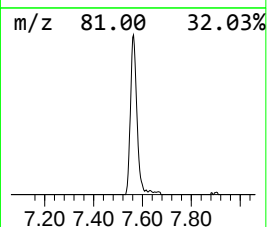
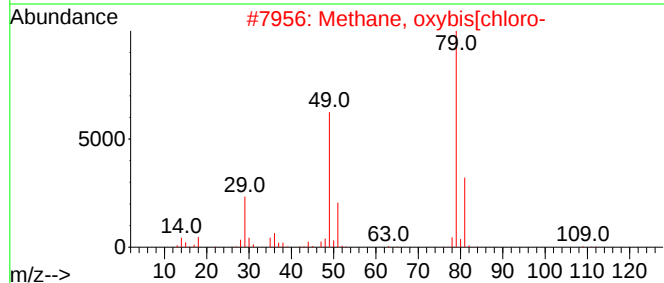
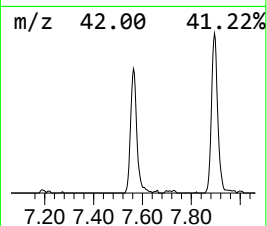
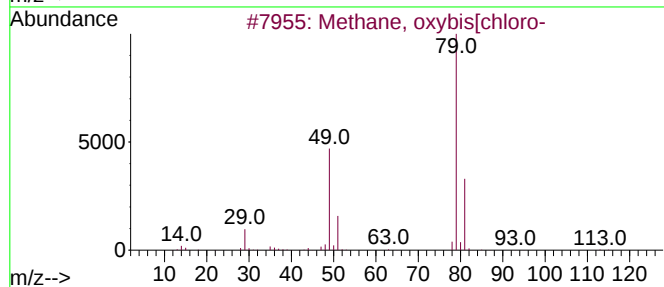
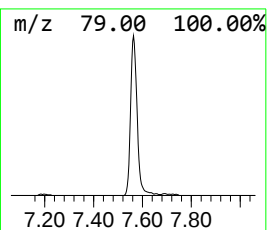
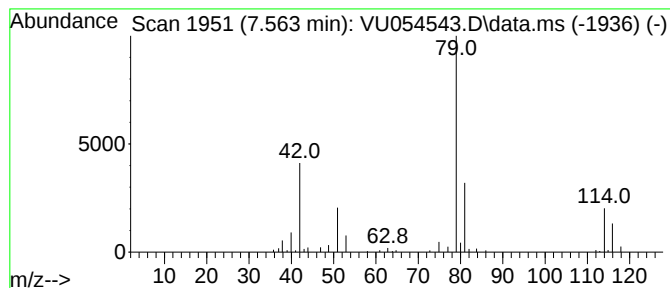
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	1.23 ug/L	156237	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	37
2			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	37
3			1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
4			Thiophosgene	114	CCl2S	000463-71-8	16
5			3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	9



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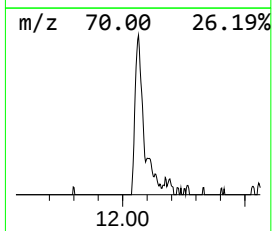
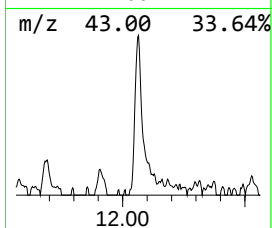
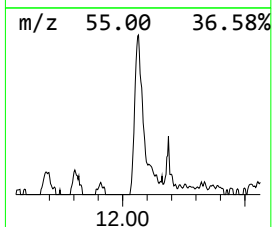
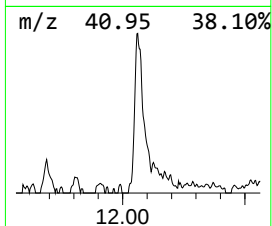
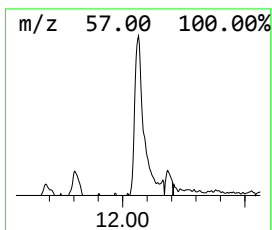
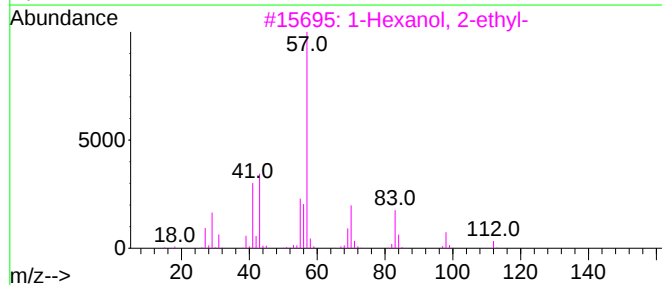
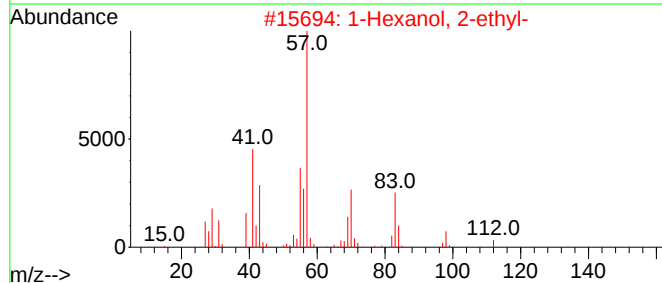
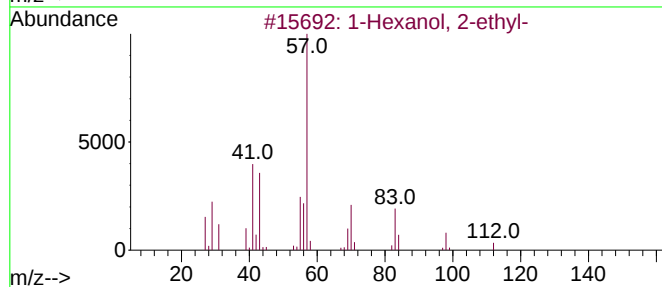
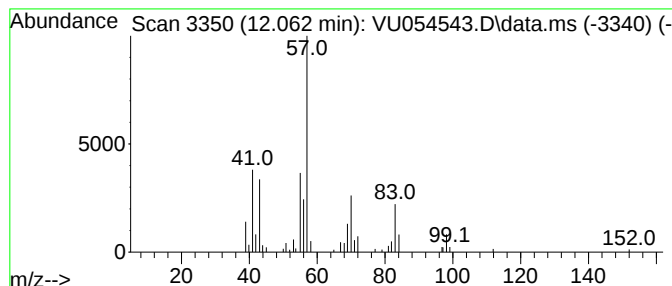
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.062	0.69 ug/L	104192	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
5	1-Pentanol, 2-ethyl-4-methyl-			130	C8H18O	000106-67-2	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
Aminomethanesul...	1.490	2.3	ug/L	298356	1	6.245	636343	5.0
unknown-01	7.563	1.2	ug/L	156237	1	6.245	636343	5.0
1-Hexanol, 2-et...	12.062	0.7	ug/L	104192	3	11.807	756470	5.0