

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110122\
 Data File : VU051661.D
 Acq On : 01 Nov 2022 18:04
 Operator : JC/MD
 Sample : N5301-10
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBWU8

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\SFAMUTR102822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051661.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.466	30	39	51	rBV	328013	561971	66.29%	7.165%
2	1.546	53	64	66	rBV	63733	113074	13.34%	1.442%
3	1.598	75	80	102	rVB3	141413	243462	28.72%	3.104%
4	1.909	172	177	190	rVB	92431	124065	14.63%	1.582%
5	2.565	368	381	393	rBV	169720	277289	32.71%	3.535%
6	2.790	434	451	465	rBV	6660	13739	1.62%	0.175%
7	3.868	762	786	787	rBV	11587	27229	3.21%	0.347%
8	4.620	1009	1020	1048	rBV	124776	323942	38.21%	4.130%
9	5.060	1140	1157	1182	rBV	161432	369865	43.63%	4.716%
10	5.723	1339	1363	1395	rBV2	313875	847735	100.00%	10.808%
11	6.247	1513	1526	1543	rBV	236574	446082	52.62%	5.687%
12	6.543	1607	1618	1634	rBV2	41424	78423	9.25%	1.000%
13	6.691	1650	1664	1684	rBV	203486	397486	46.89%	5.068%
14	7.565	1924	1936	1955	rBV	86831	153889	18.15%	1.962%
15	7.896	2026	2039	2054	rBV	357539	620549	73.20%	7.912%
16	7.970	2054	2062	2078	rVB2	21637	39862	4.70%	0.508%
17	8.179	2114	2127	2147	rBV2	54020	93673	11.05%	1.194%
18	8.552	2232	2243	2256	rBV2	63586	104354	12.31%	1.330%
19	8.633	2256	2268	2302	rBV	419251	781036	92.13%	9.958%
20	9.417	2499	2512	2536	rBV2	352562	698706	82.42%	8.908%
21	9.691	2589	2597	2611	rVB6	6110	12957	1.53%	0.165%
22	10.755	2913	2928	2945	rBV	168371	273888	32.31%	3.492%
23	10.890	2960	2970	2982	rBV2	12441	19792	2.33%	0.252%
24	11.809	3242	3256	3277	rBV	315811	542370	63.98%	6.915%
25	12.060	3324	3334	3361	rBV2	32078	69621	8.21%	0.888%
26	12.192	3363	3375	3399	rVB	340215	580584	68.49%	7.402%
27	15.690	4455	4463	4479	rVB7	17129	27946	3.30%	0.356%

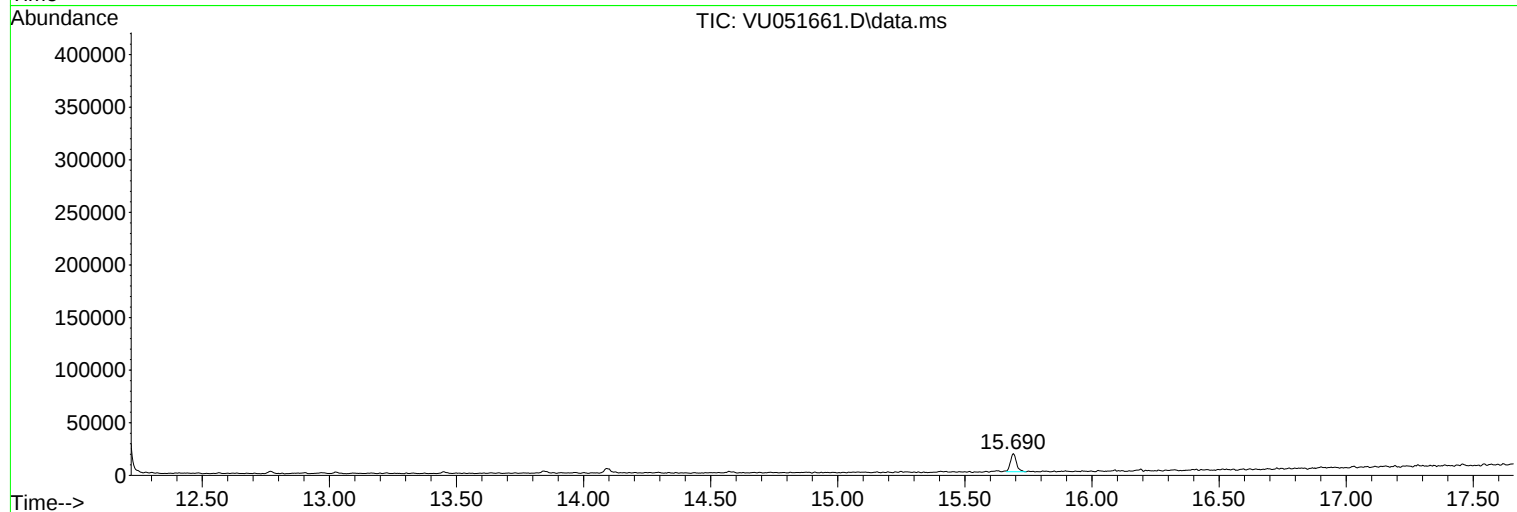
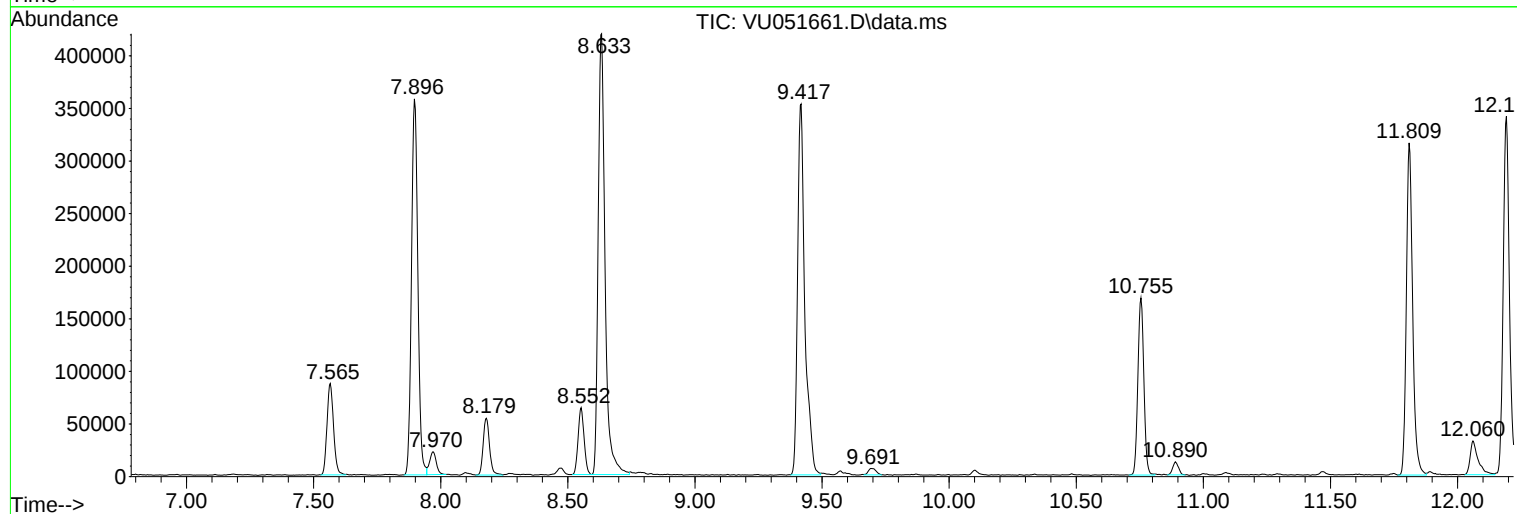
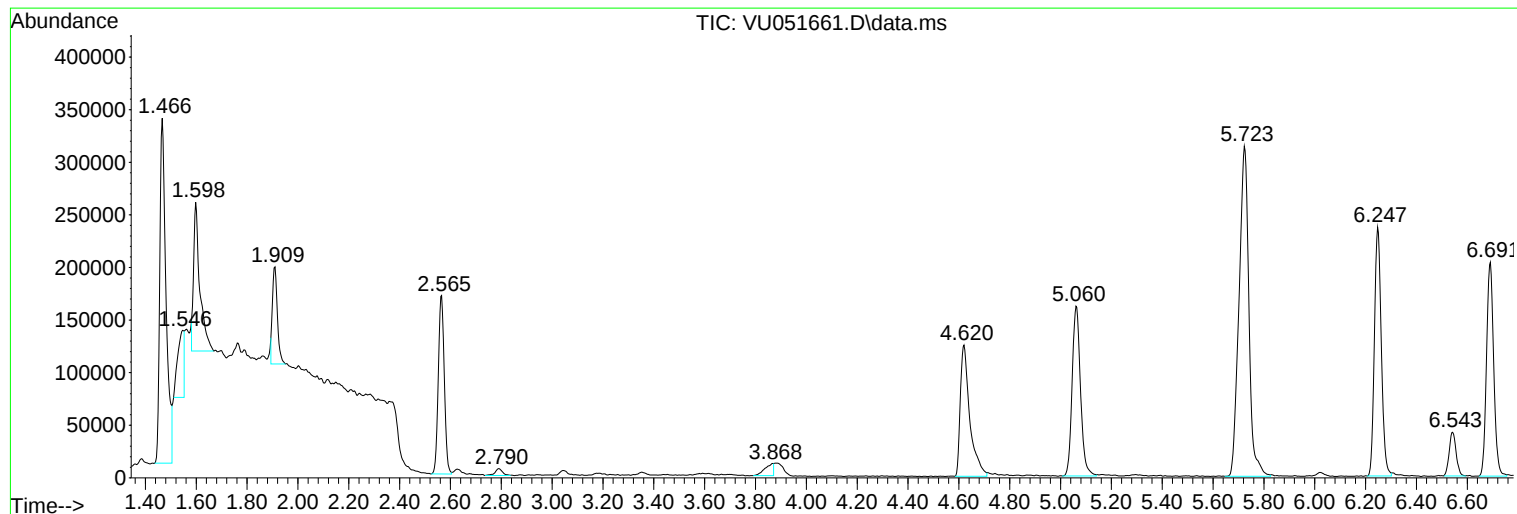
Sum of corrected areas: 7843589

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Instrument :
MSVOA_U
ClientSampleId :
DBWU8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.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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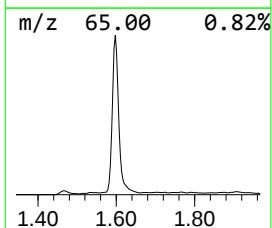
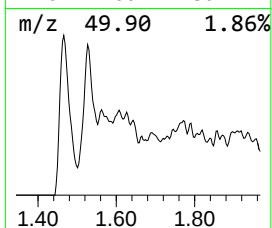
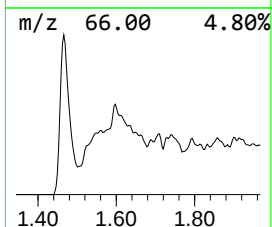
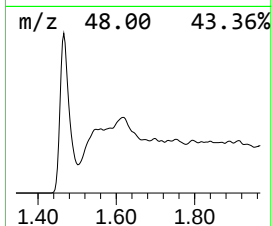
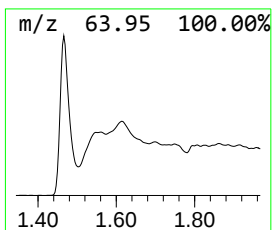
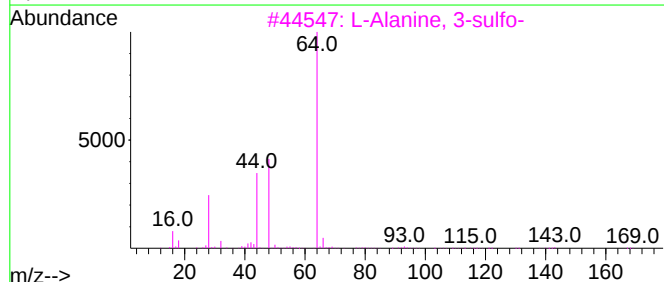
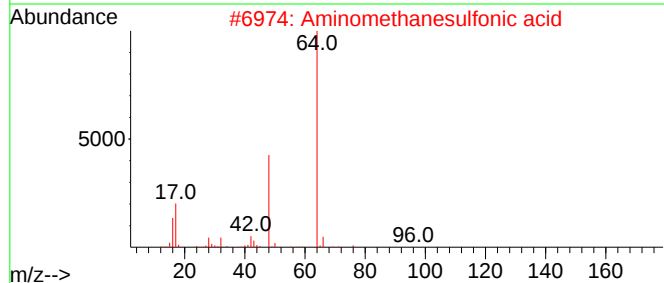
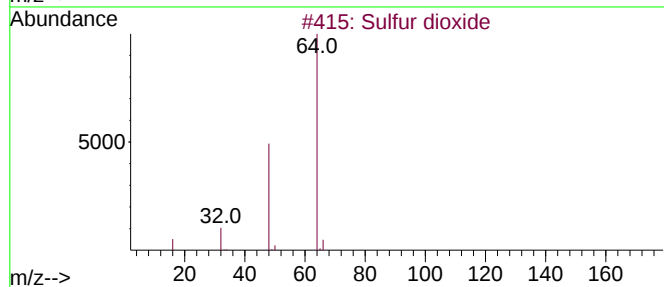
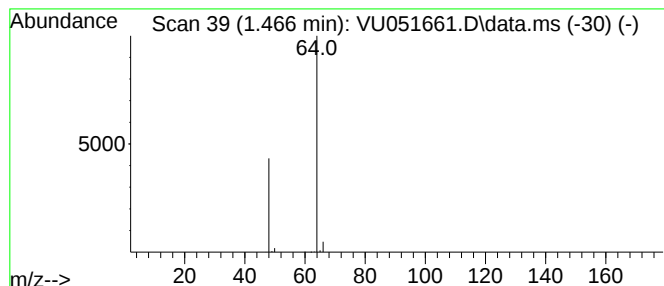
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.466	6.30 ug/L	561971	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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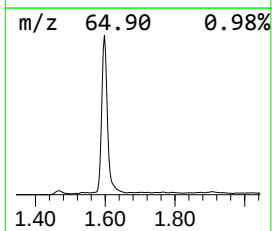
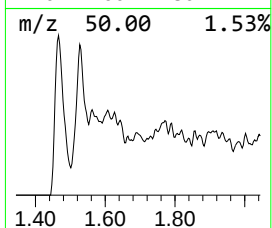
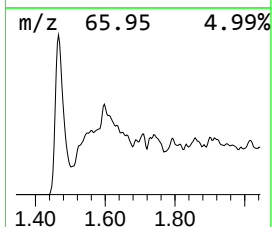
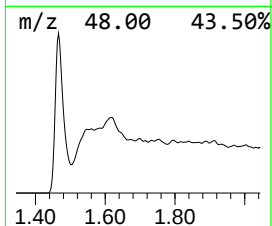
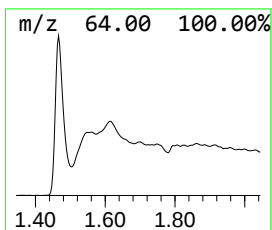
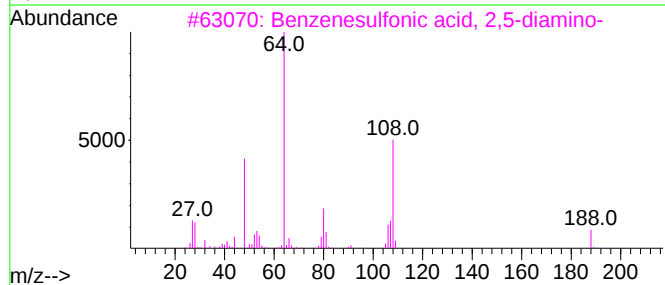
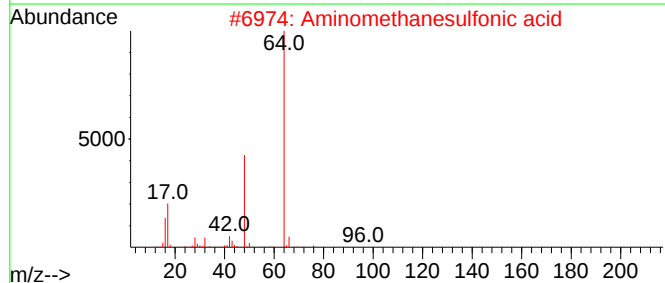
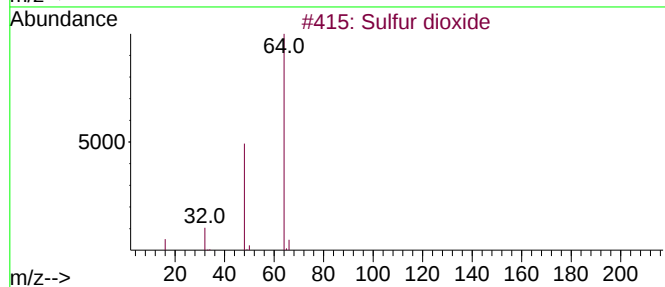
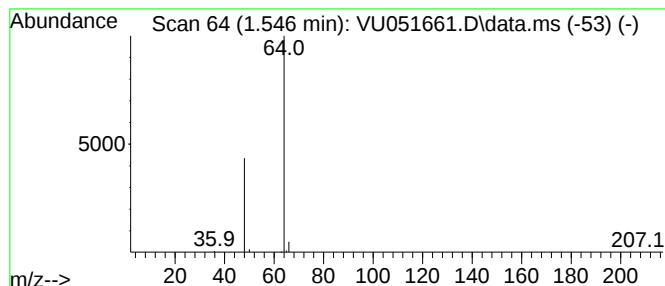
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Aminomethanesulfonic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.546	1.27 ug/L	113074	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Benzenesulfonic acid, 2,5-diamino-	188	C6H8N2O3S	000088-45-9	9
4			4,6-Diamino-5-pyrimidinyl hydrog...	206	C4H6N4O4S	071525-41-2	9
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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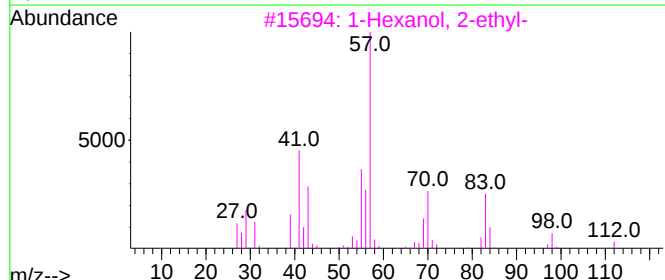
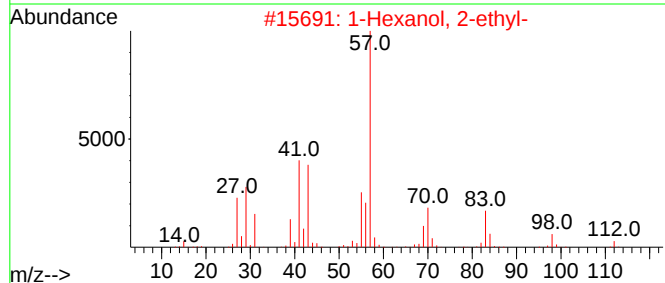
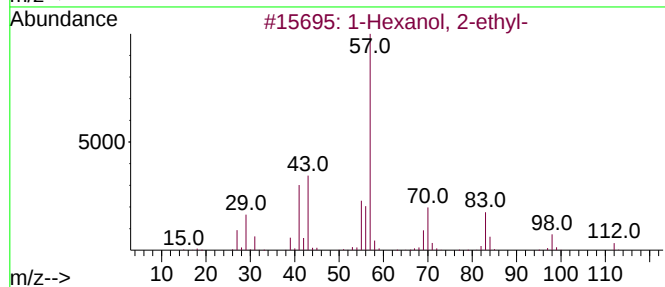
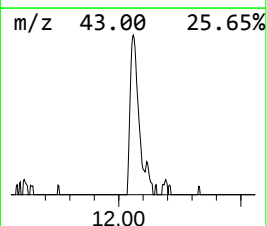
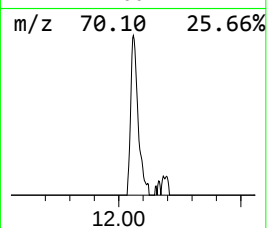
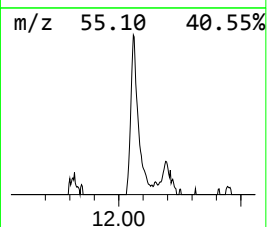
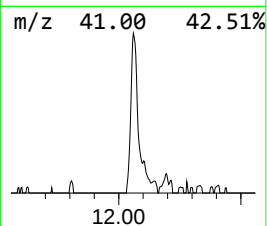
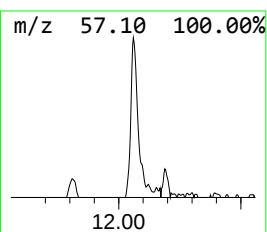
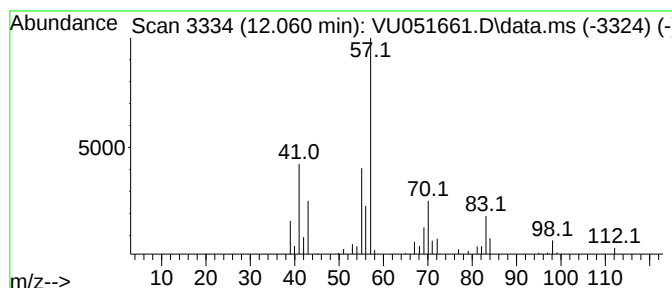
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	0.64 ug/L	69621	1,4-Dichlorobenzene-d4	11.809

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			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53



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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
Sulfur dioxide	1.466	6.3	ug/L	561971	1	6.247	446082	5.0
Aminomethanesul...	1.546	1.3	ug/L	113074	1	6.247	446082	5.0
1-Hexanol, 2-et...	12.060	0.6	ug/L	69621	3	11.809	542370	5.0