

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100322\
 Data File : VV028298.D
 Acq On : 03 Oct 2022 23:15
 Operator : SY/MD
 Sample : N4820-18
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 CB8Q5

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_V\Method\SFAMVTR100322WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV028298.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.130	24	28	39	rVB	17485	20080	2.73%	0.292%
2	1.301	73	81	90	rBV	108757	113041	15.35%	1.644%
3	1.394	95	110	149	rBV2	65120	440878	59.88%	6.412%
4	1.561	156	162	174	rVB	99511	117374	15.94%	1.707%
5	2.101	320	330	348	rVB	202560	314160	42.67%	4.569%
6	2.767	523	537	554	rBV4	14675	32515	4.42%	0.473%
7	3.912	878	893	926	rBV2	44444	217860	29.59%	3.168%
8	4.342	1010	1027	1054	rBV	123822	323650	43.96%	4.707%
9	5.040	1225	1244	1270	rBV3	297468	736311	100.00%	10.708%
10	5.612	1411	1422	1444	rBV	206730	421891	57.30%	6.135%
11	6.066	1547	1563	1590	rBV	166846	351138	47.69%	5.107%
12	6.985	1839	1849	1872	rBV2	68748	131854	17.91%	1.918%
13	7.310	1938	1950	1972	rBV	329762	588023	79.86%	8.551%
14	7.622	2038	2047	2062	rBV	40904	74574	10.13%	1.085%
15	8.088	2182	2192	2231	rBV	307489	643447	87.39%	9.358%
16	8.850	2416	2429	2460	rBV2	323681	672495	91.33%	9.780%
17	9.107	2503	2509	2521	rVB2	4691	8981	1.22%	0.131%
18	9.493	2613	2629	2637	rBV10	4181	7628	1.04%	0.111%
19	10.120	2815	2824	2832	rBV10	5165	9251	1.26%	0.135%
20	10.214	2842	2853	2870	rVB	125071	204821	27.82%	2.979%
21	10.860	3044	3054	3063	rBV2	11571	17736	2.41%	0.258%
22	11.017	3094	3103	3108	rBV8	5302	8826	1.20%	0.128%
23	11.056	3109	3115	3126	rVB3	7320	11775	1.60%	0.171%
24	11.246	3162	3174	3200	rBV	333261	559317	75.96%	8.134%
25	11.529	3251	3262	3279	rBV	43699	88659	12.04%	1.289%
26	11.619	3279	3290	3311	rVB	334151	548237	74.46%	7.973%
27	11.988	3393	3405	3413	rBV6	5603	9583	1.30%	0.139%
28	12.040	3413	3421	3436	rVB6	6741	14237	1.93%	0.207%
29	12.191	3459	3468	3477	rVB2	12786	17378	2.36%	0.253%
30	12.660	3605	3614	3629	rBV5	25355	48334	6.56%	0.703%
31	12.821	3656	3664	3676	rBV5	6289	8601	1.17%	0.125%
32	13.307	3807	3815	3828	rVB2	19376	35556	4.83%	0.517%
33	13.538	3878	3887	3897	rBV6	5861	8399	1.14%	0.122%
34	14.300	4113	4124	4133	rVB10	7833	14636	1.99%	0.213%
35	14.827	4275	4288	4298	rBV3	14195	27365	3.72%	0.398%
36	15.107	4367	4375	4382	rBV10	10013	14658	1.99%	0.213%

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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_V\Method\SFAMVTR100322WMA.M
Title : TRACE VOA SFAM1.0

37	15.303	4430	4436	4453	rVB9	5762	12990	1.76%	0.189%
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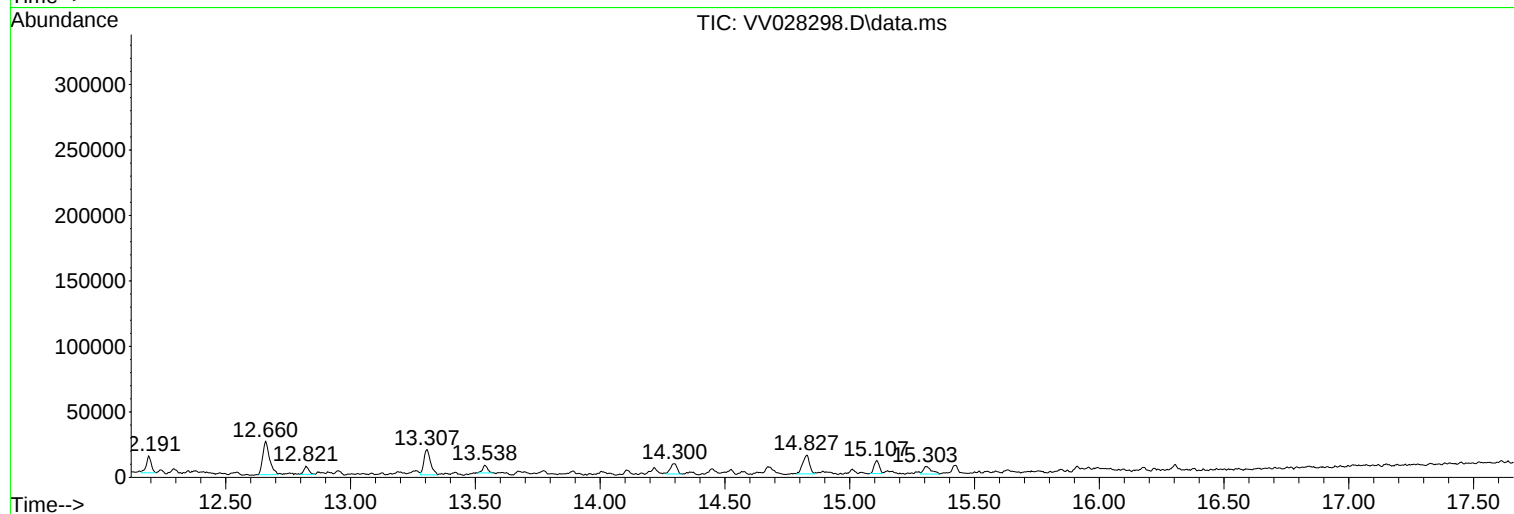
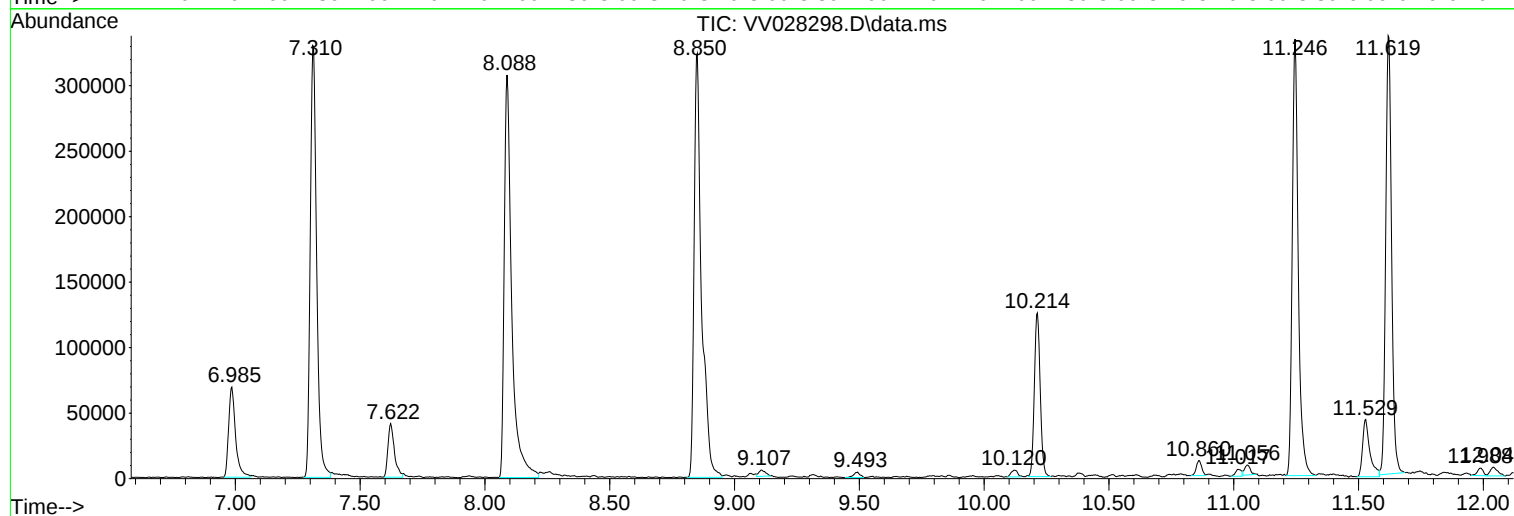
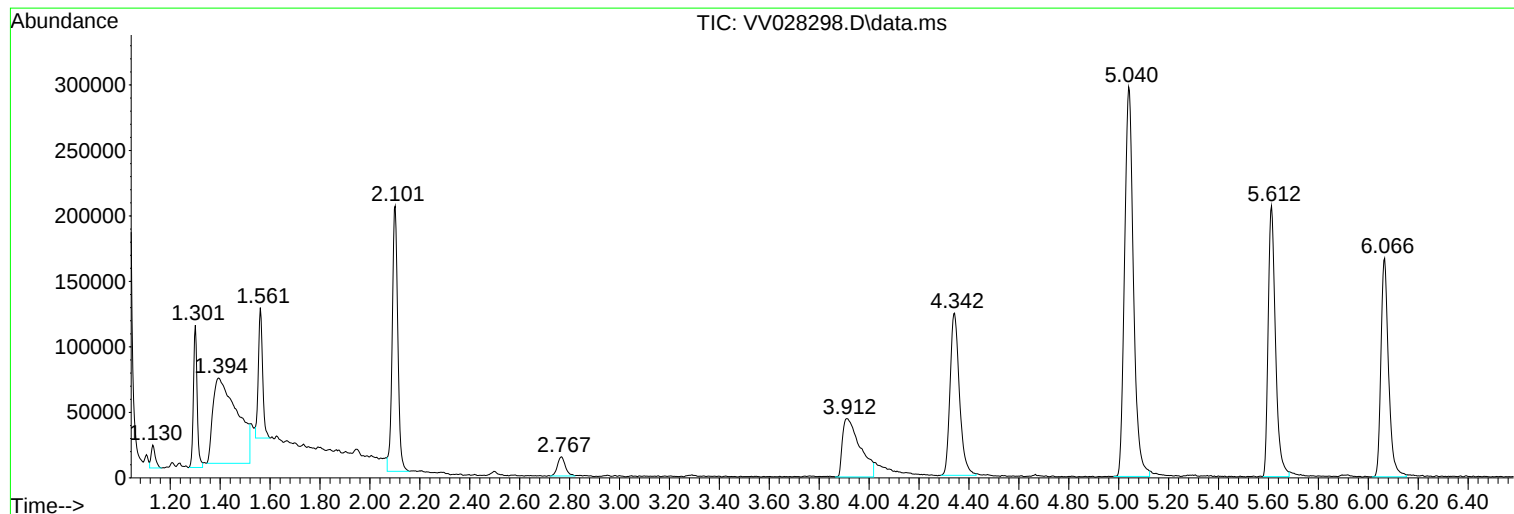
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR100322WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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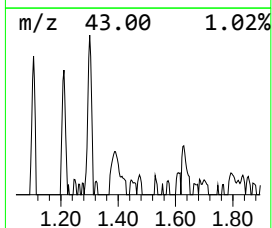
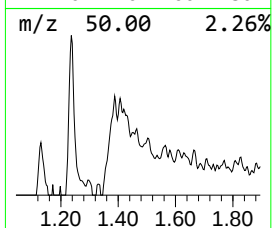
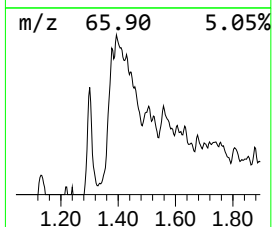
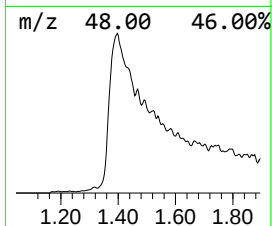
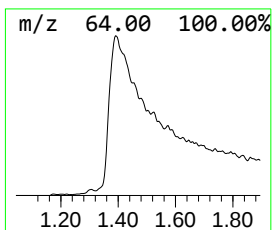
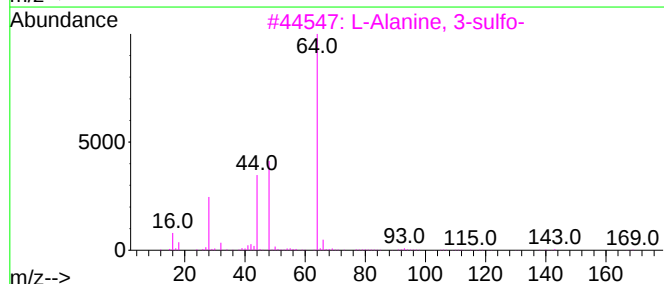
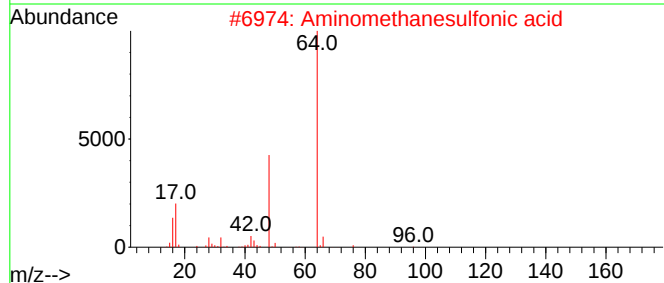
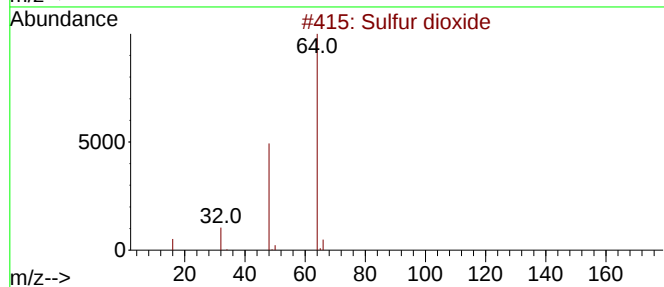
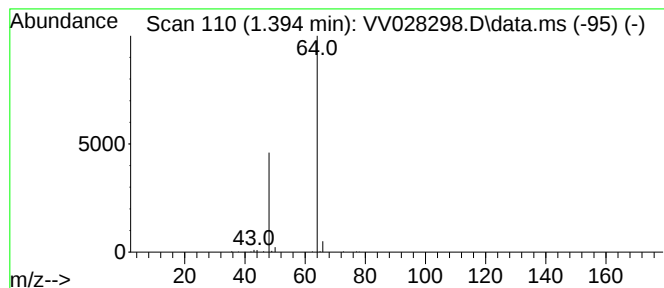
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR100322WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.394	5.23 ug/L	440878	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	7



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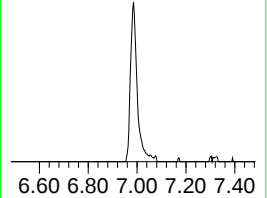
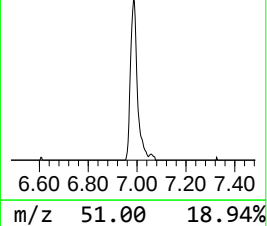
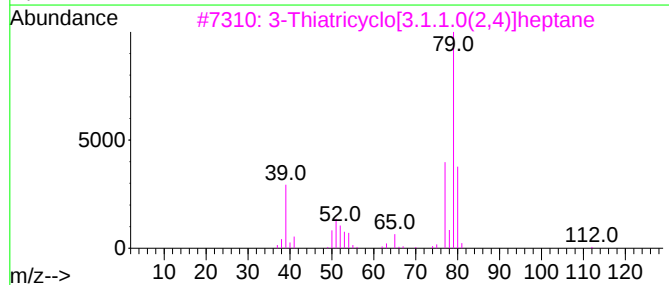
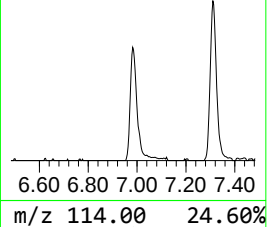
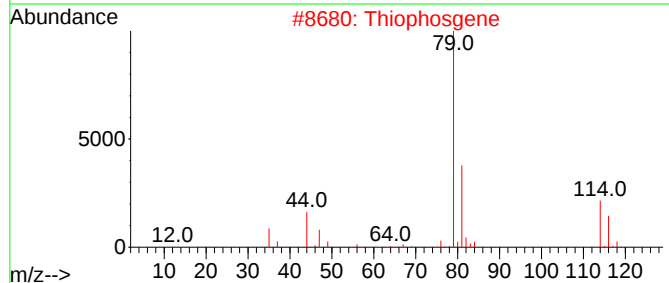
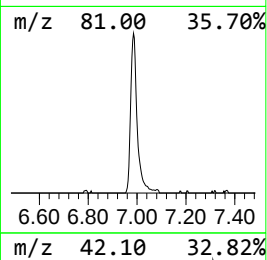
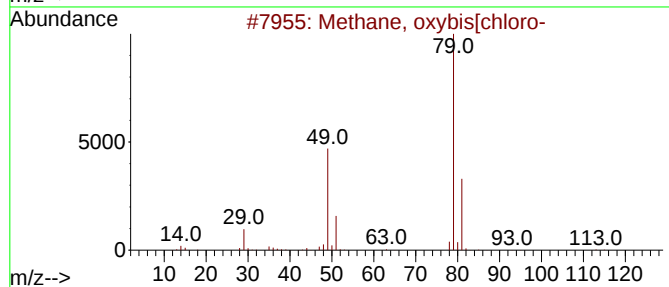
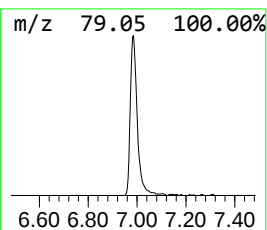
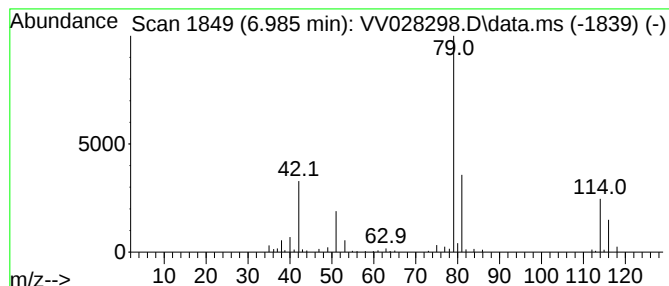
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Methane, oxybis[chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.985	1.56 ug/L	131854	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	50
2			Thiophosgene	114	CCl2S	000463-71-8	45
3			3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	38
4			1,3-Cyclohexadiene	80	C6H8	000592-57-4	28
5			2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	9



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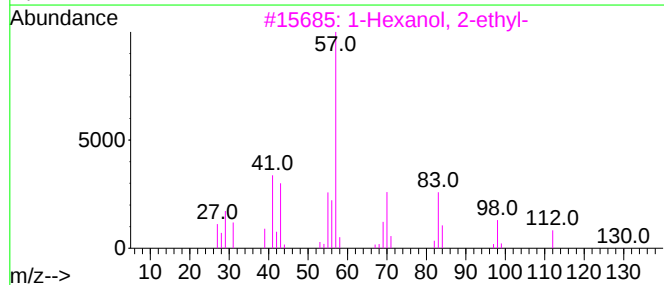
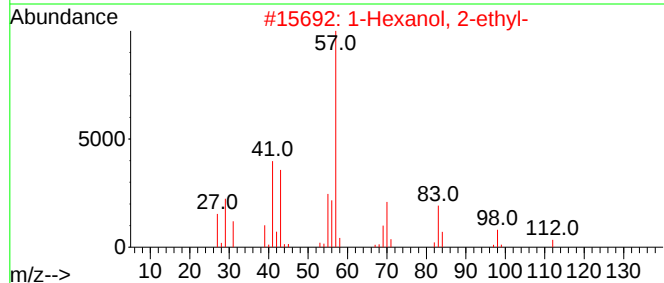
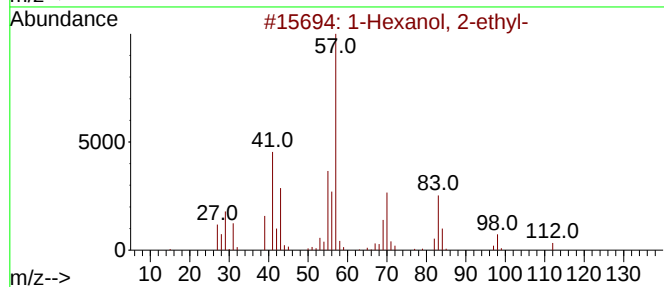
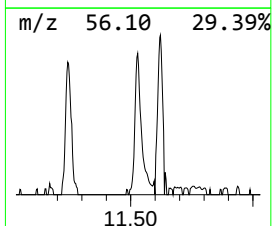
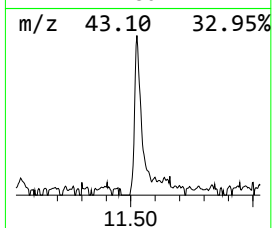
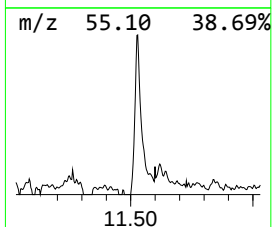
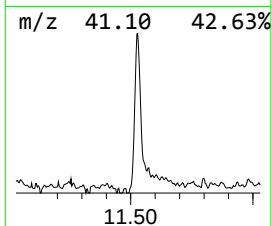
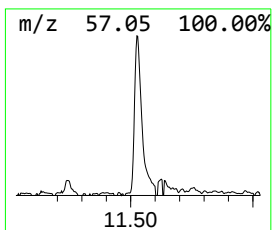
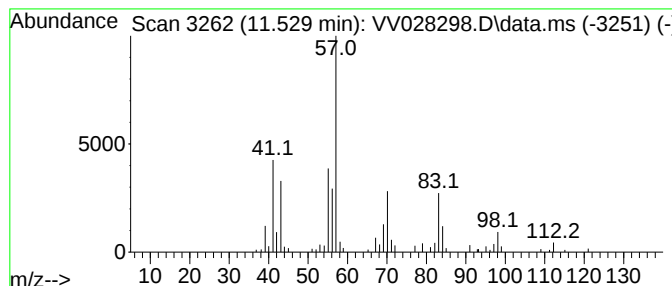
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR100322WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
11.529	0.79 ug/L	88659	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	86
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	83
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72



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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
Sulfur dioxide	1.394	5.2	ug/L	440878	1	5.612	421891	5.0
Methane, oxybis...	6.985	1.6	ug/L	131854	1	5.612	421891	5.0
1-Hexanol, 2-et...	11.529	0.8	ug/L	88659	3	11.246	559317	5.0