

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112321\
 Data File : VU045966.D
 Acq On : 23 Nov 2021 19:18
 Operator : SY/MD
 Sample : M4722-06
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0G27

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\SFAMUTR111521WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU045966.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	15	rVB2	17629	16551	3.25%	0.475%
2	1.601	71	81	93	rBV5	45257	60611	11.91%	1.740%
3	1.919	171	180	195	rVB	35095	45565	8.95%	1.308%
4	2.572	370	383	397	rBV	60969	98498	19.36%	2.827%
5	2.800	441	454	472	rVB	19009	33187	6.52%	0.953%
6	3.051	523	532	543	rBV3	3946	6920	1.36%	0.199%
7	3.842	755	778	780	rBV	2372	6940	1.36%	0.199%
8	4.652	1011	1030	1087	rBV	47641	218665	42.97%	6.276%
9	5.067	1143	1159	1180	rBV	72369	172274	33.86%	4.945%
10	5.729	1344	1365	1399	rBV2	139572	378184	74.32%	10.855%
11	6.253	1512	1528	1545	rBV	110755	208177	40.91%	5.975%
12	6.694	1651	1665	1682	rBV	90284	172970	33.99%	4.965%
13	6.793	1686	1696	1706	rVB2	8942	15963	3.14%	0.458%
14	7.182	1809	1817	1834	rVB3	2821	5229	1.03%	0.150%
15	7.568	1925	1937	1954	rBV	32916	56301	11.06%	1.616%
16	7.796	1997	2008	2020	rBV3	7304	13795	2.71%	0.396%
17	7.899	2026	2040	2053	rBV	157474	279958	55.02%	8.036%
18	7.970	2053	2062	2088	rVB	55817	100307	19.71%	2.879%
19	8.182	2117	2128	2141	rBV	20921	33749	6.63%	0.969%
20	8.636	2256	2269	2312	rBV	245749	508851	100.00%	14.605%
21	9.420	2500	2513	2531	rBV	157904	266106	52.30%	7.638%
22	9.636	2569	2580	2589	rVV2	25013	40623	7.98%	1.166%
23	9.693	2589	2598	2609	rVB	13855	22824	4.49%	0.655%
24	10.102	2717	2725	2738	rBV2	6586	10289	2.02%	0.295%
25	10.758	2918	2929	2946	rVB	81382	128422	25.24%	3.686%
26	10.893	2961	2971	2980	rVB	4635	7209	1.42%	0.207%
27	11.812	3244	3257	3271	rBV	157923	247483	48.64%	7.103%
28	12.063	3325	3335	3352	rBV3	26227	53254	10.47%	1.529%
29	12.195	3364	3376	3390	rVB	170569	275096	54.06%	7.896%

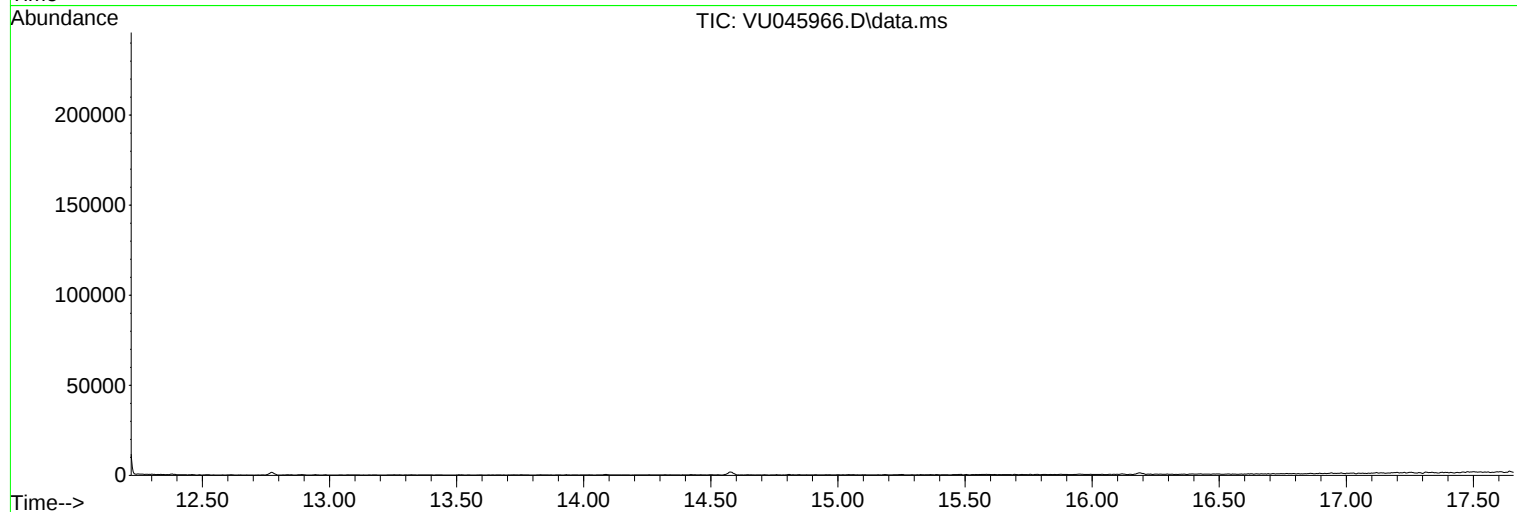
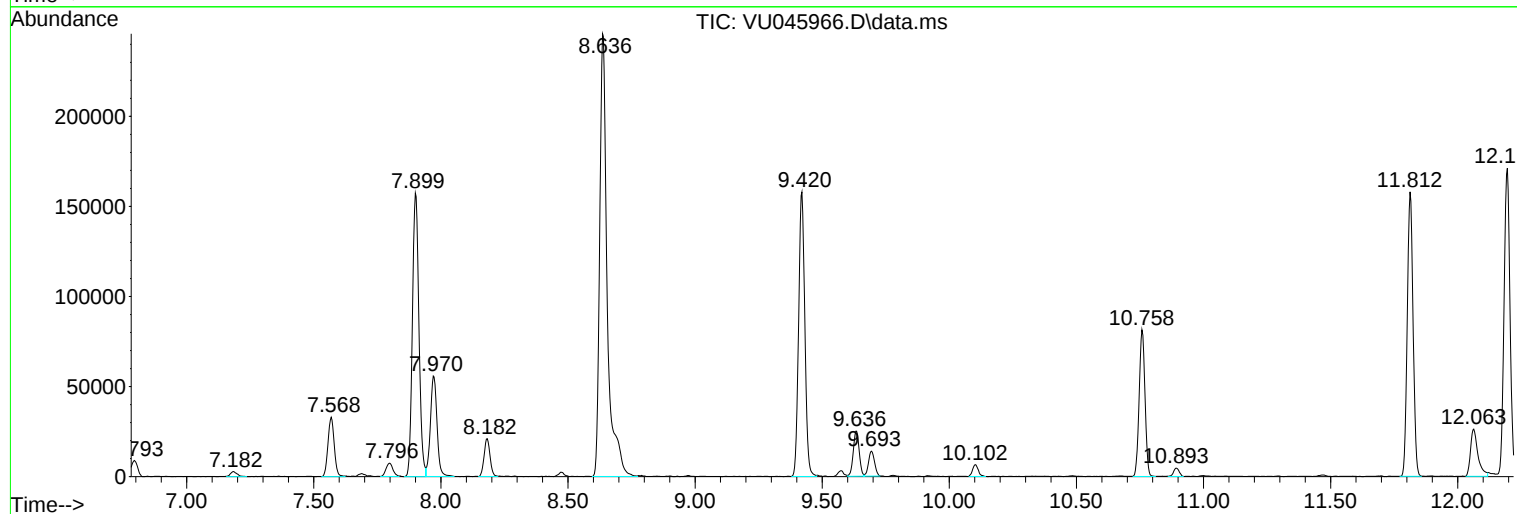
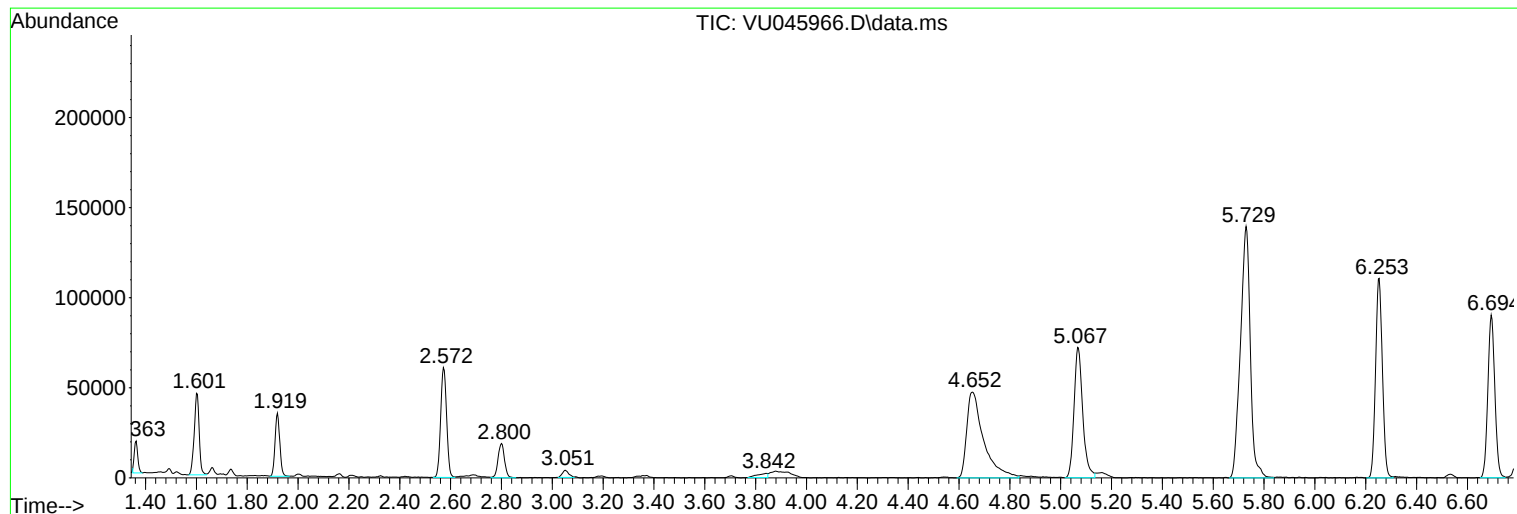
Sum of corrected areas: 3484001

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Instrument :
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ClientSampleId :
C0G27

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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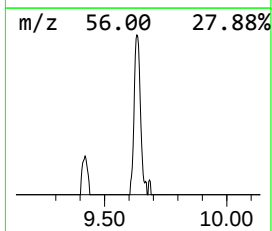
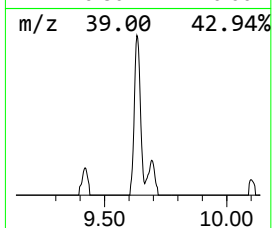
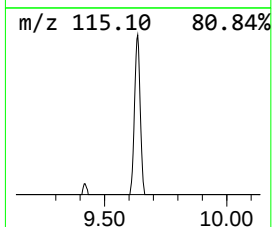
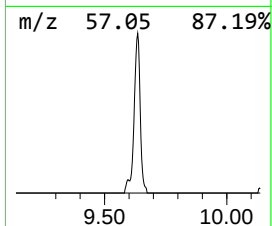
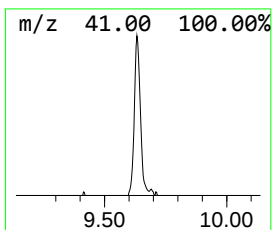
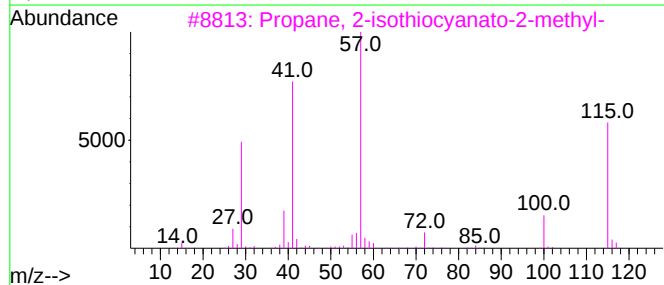
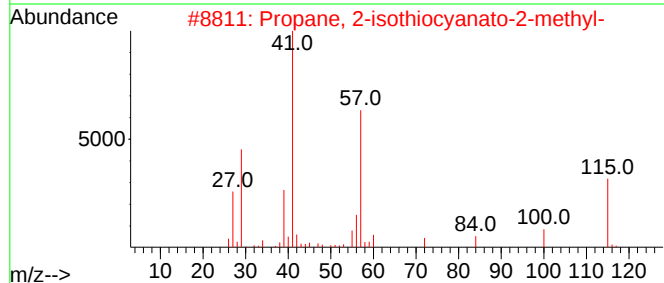
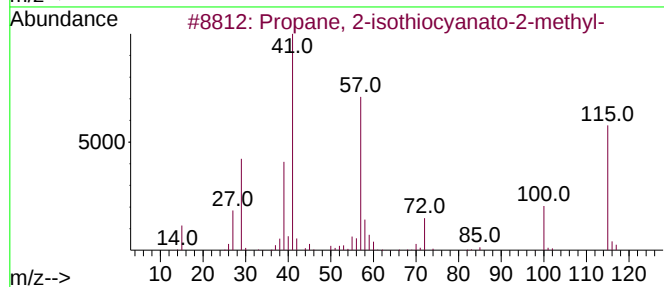
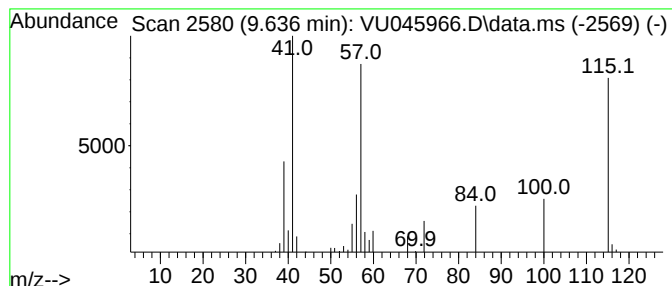
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 2-isothiocyanato-2... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.636	0.76 ug/L	40623	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-isothiocyanato-2-methyl-	115	C5H9NS	000590-42-1	74
2			Propane, 2-isothiocyanato-2-methyl-	115	C5H9NS	000590-42-1	64
3			Propane, 2-isothiocyanato-2-methyl-	115	C5H9NS	000590-42-1	46
4			Butane, 1-isothiocyanato-	115	C5H9NS	000592-82-5	43
5			1H-1,2,4-Triazole, 3-thiol-5-met...	115	C3H5N3S	007271-44-5	43



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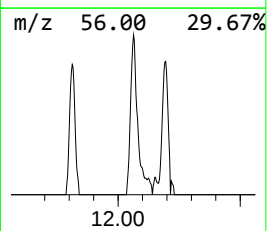
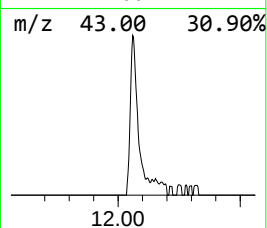
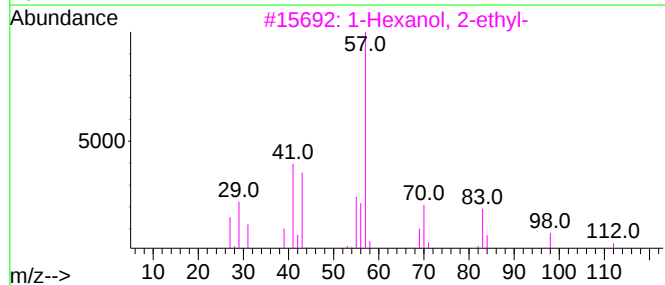
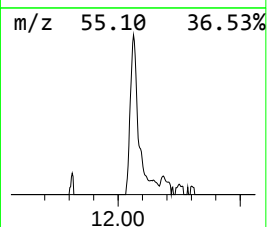
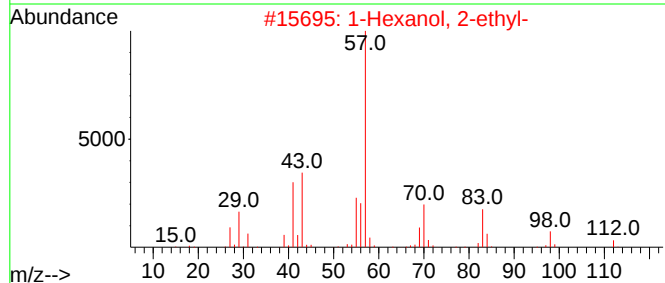
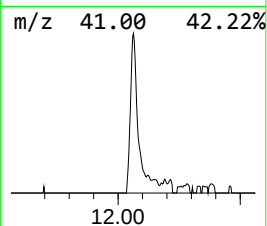
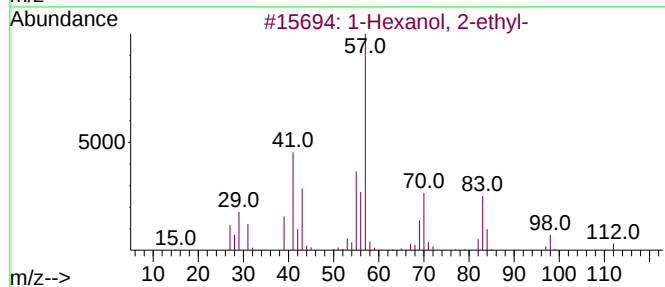
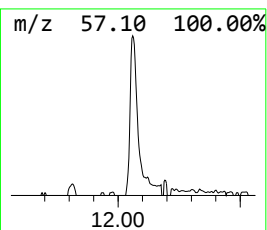
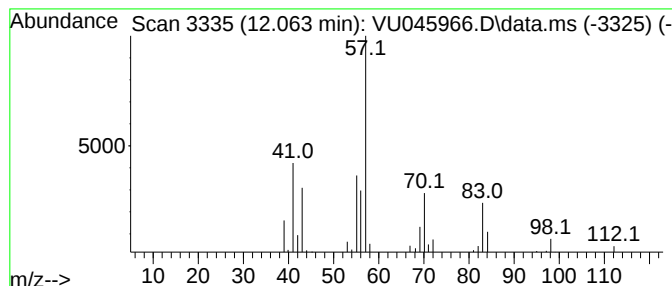
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Quant Title : TRACE VOA SFAM1.0

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	1.08 ug/L	53254	1,4-Dichlorobenzene-d4	11.812

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	83
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	80
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2-isot...	9.636	0.8	ug/L	40623	2	9.420	266106	5.0
1-Hexanol, 2-et...	12.063	1.1	ug/L	53254	3	11.812	247483	5.0