

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121921\
 Data File : VV024097.D
 Acq On : 19 Dec 2021 18:38
 Operator : SY/MD
 Sample : M5134-11
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 GBBLO

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\SFAMVTR121021WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV024097.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.121	21	25	31	rVB	5090	5014	1.53%	0.165%
2	1.307	74	83	91	rBV	31832	33153	10.14%	1.089%
3	1.388	99	108	114	rBV2	13089	20804	6.36%	0.683%
4	1.471	128	134	141	rBV5	3714	5652	1.73%	0.186%
5	1.568	157	164	178	rVB	30899	34914	10.68%	1.147%
6	2.108	323	332	346	rVB	61301	88250	26.99%	2.898%
7	2.446	427	437	450	rBV2	8056	18264	5.59%	0.600%
8	2.510	451	457	467	rVB6	3485	5601	1.71%	0.184%
9	2.957	589	596	609	rBV7	2388	4870	1.49%	0.160%
10	3.121	634	647	669	rVB3	16413	34439	10.53%	1.131%
11	3.918	882	895	915	rBV2	12403	48037	14.69%	1.578%
12	4.365	1014	1034	1056	rBV3	66363	234290	71.66%	7.694%
13	4.828	1164	1178	1196	rVB3	11436	29385	8.99%	0.965%
14	5.050	1231	1247	1268	rBV3	93935	235768	72.11%	7.743%
15	5.179	1270	1287	1288	rBV7	5565	10884	3.33%	0.357%
16	5.616	1409	1423	1443	rBV	104146	209992	64.22%	6.896%
17	6.069	1546	1564	1593	rBV2	58832	127182	38.90%	4.177%
18	6.986	1839	1849	1867	rBV	25908	48647	14.88%	1.598%
19	7.317	1938	1952	1971	rBV	115676	203403	62.21%	6.680%
20	7.625	2037	2048	2061	rBV2	15784	29232	8.94%	0.960%
21	7.944	2134	2147	2172	rBV5	13601	47793	14.62%	1.570%
22	8.092	2183	2193	2218	rBV	96353	181159	55.41%	5.949%
23	8.243	2232	2240	2254	rVB6	13789	24610	7.53%	0.808%
24	8.850	2419	2429	2453	rBV	166979	282209	86.31%	9.268%
25	9.487	2617	2627	2651	rBV	124853	326968	100.00%	10.738%
26	9.809	2722	2727	2736	rVB6	2833	3592	1.10%	0.118%
27	9.934	2758	2766	2782	rVB2	9897	16435	5.03%	0.540%
28	10.217	2844	2854	2863	rBV2	39928	61905	18.93%	2.033%
29	10.381	2895	2905	2915	rBV3	13730	22267	6.81%	0.731%
30	10.821	3032	3042	3055	rBV4	18590	44862	13.72%	1.473%
31	11.249	3161	3175	3194	rBV	197757	319524	97.72%	10.494%
32	11.548	3256	3268	3272	rBV7	4780	9498	2.90%	0.312%
33	11.622	3280	3291	3310	rVB	127879	202299	61.87%	6.644%
34	12.014	3404	3413	3431	rBV5	11573	28704	8.78%	0.943%
35	12.249	3477	3486	3493	rVB4	3269	5420	1.66%	0.178%
36	12.345	3506	3516	3520	rBV8	2339	3442	1.05%	0.113%

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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

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Title : TRACE VOA SFAM1.0

37	13.104	3743	3752	3762	rBV8	2579	5467	1.67%	0.180%
38	13.371	3828	3835	3851	rBV5	10931	22236	6.80%	0.730%
39	14.040	4034	4043	4053	rVB2	6028	8793	2.69%	0.289%

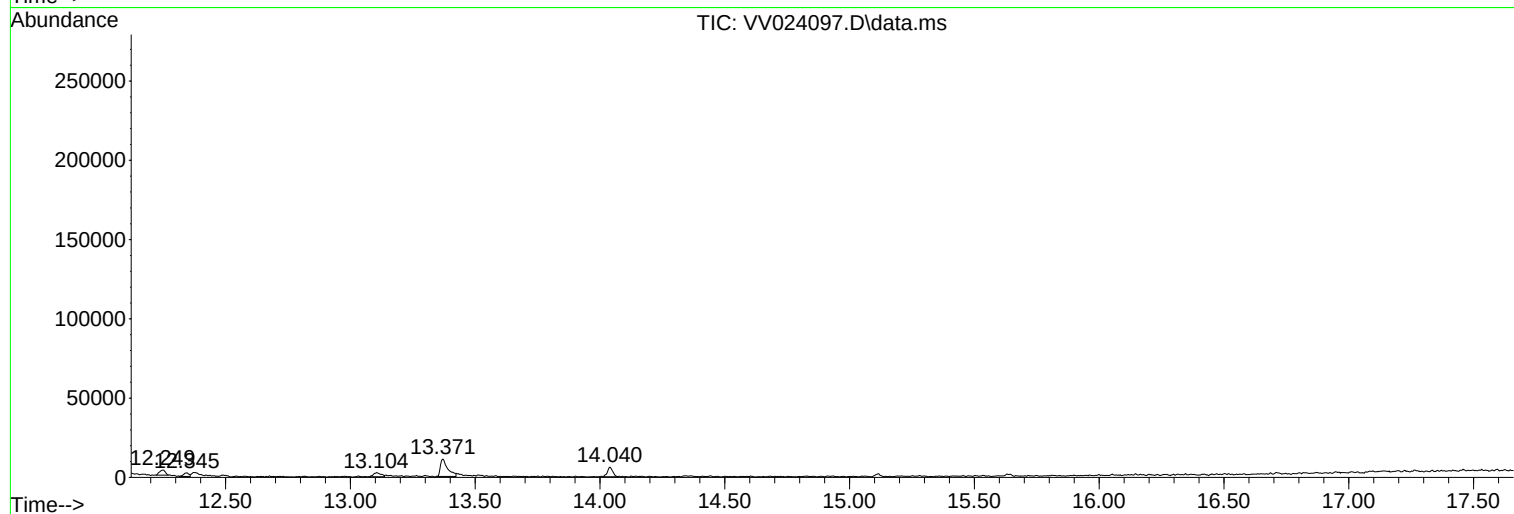
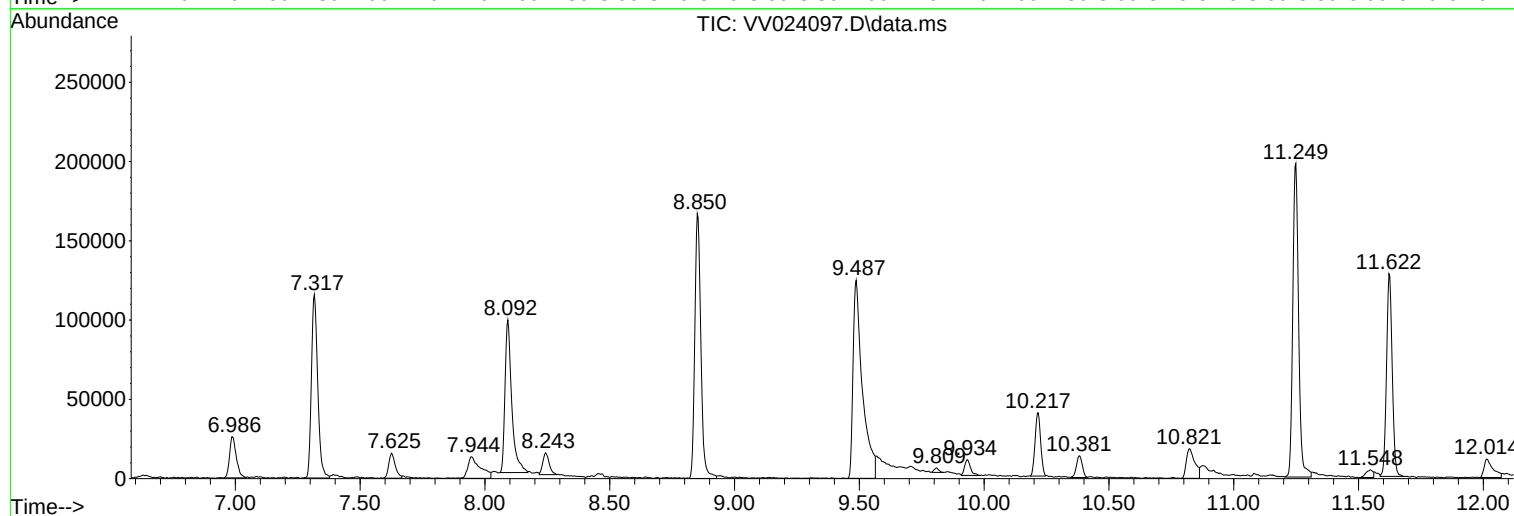
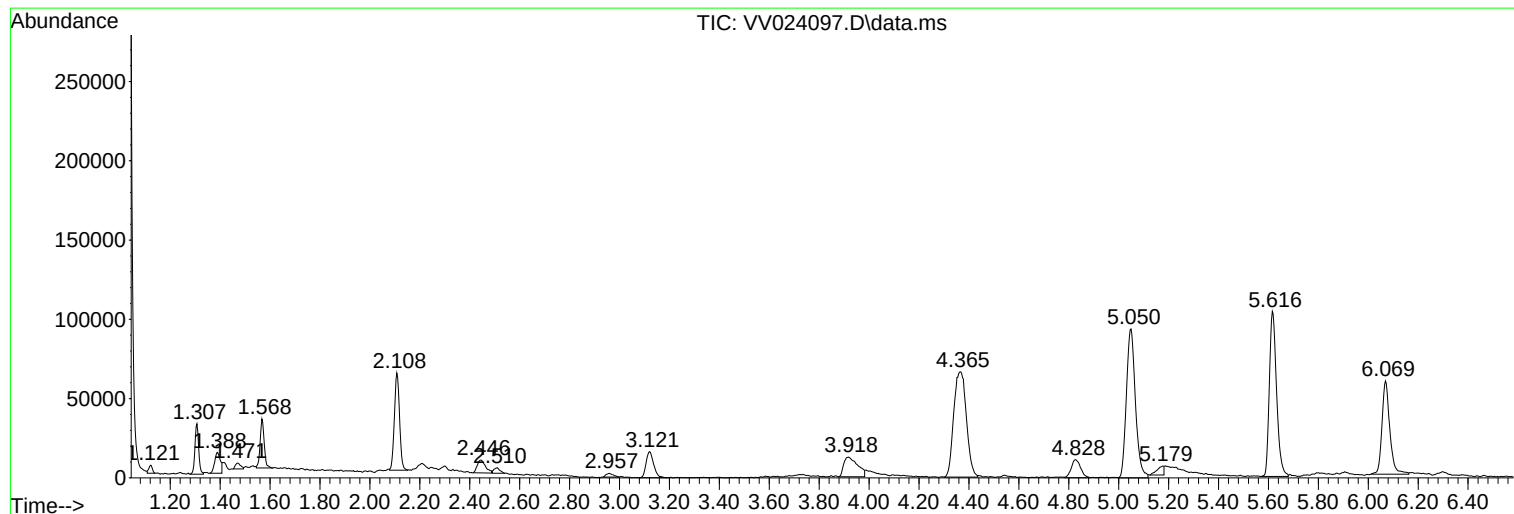
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR121021WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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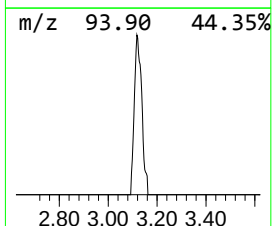
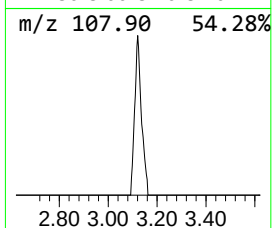
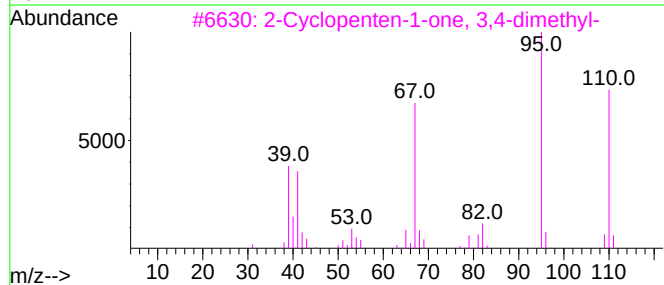
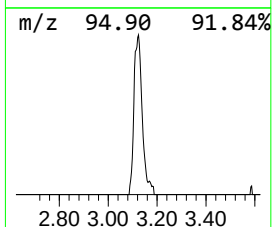
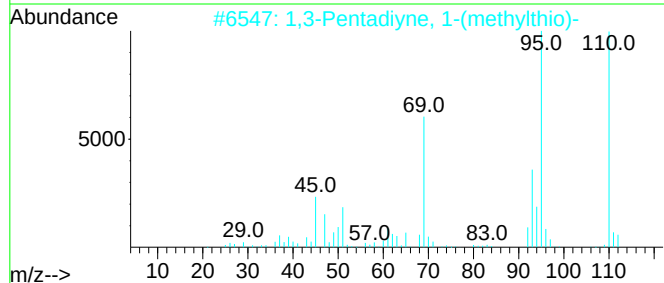
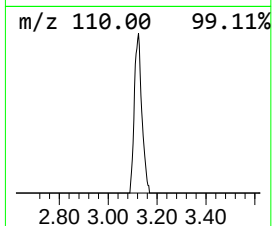
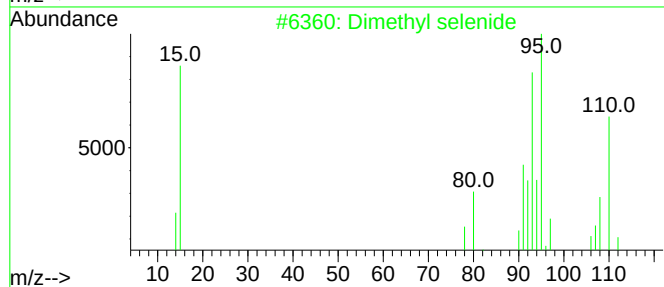
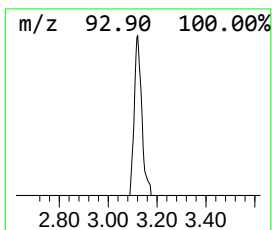
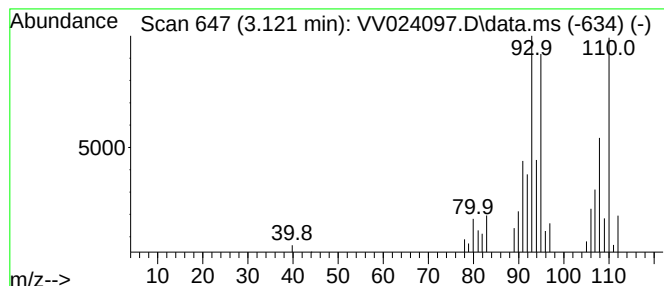
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR121021WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Dimethyl selenide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.121	0.82 ug/L	34439	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl selenide	110	C2H6Se	000593-79-3	64
2			1,3-Pentadiyne, 1-(methylthio)-	110	C6H6S	042875-80-9	25
3			2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	25
4			Cyclopentene, 3-ethylidene-1-met...	108	C8H12	062338-00-5	18
5			1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	16



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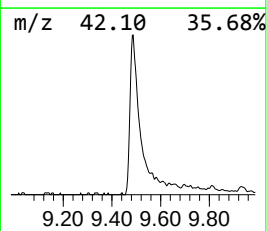
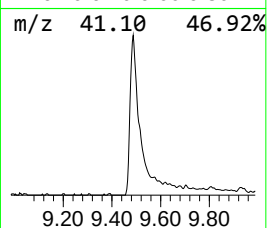
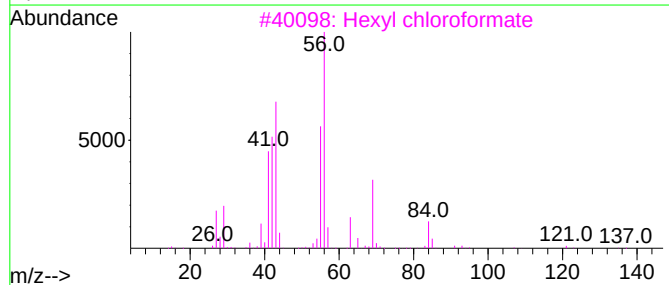
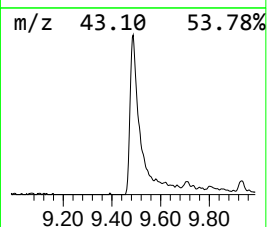
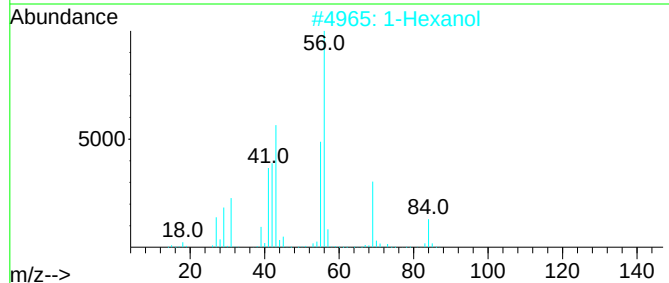
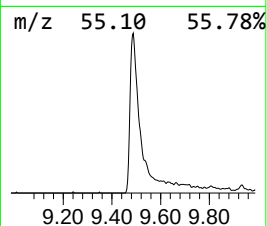
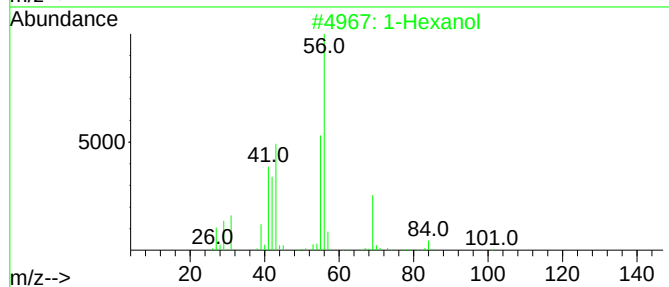
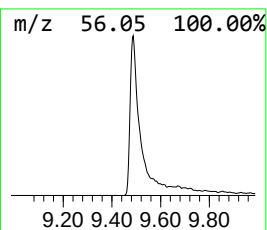
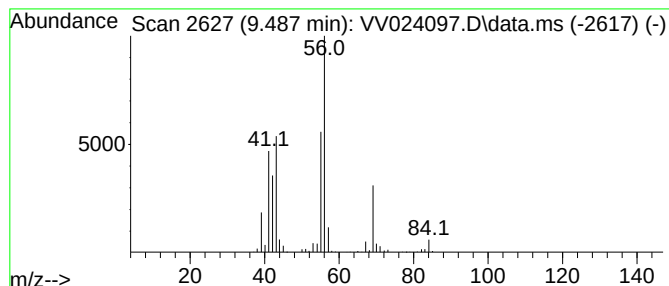
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR121021WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 1-Hexanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.487	5.79 ug/L	326968	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol			102	C6H14O	000111-27-3	83
2	1-Hexanol			102	C6H14O	000111-27-3	83
3	Hexyl chloroformate			164	C7H13ClO2	006092-54-2	78
4	Cyclopentane, methyl-			84	C6H12	000096-37-7	78
5	1-Hexanol			102	C6H14O	000111-27-3	78



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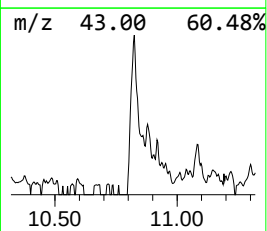
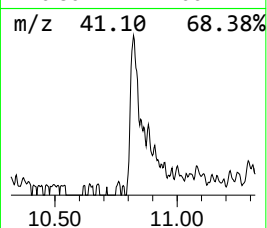
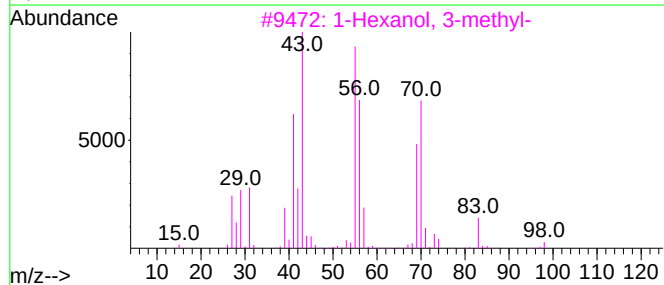
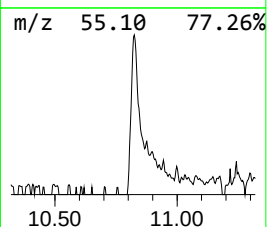
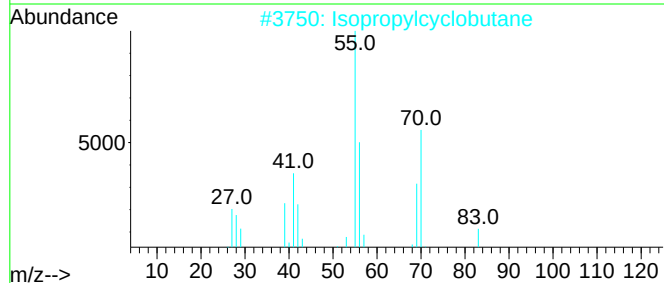
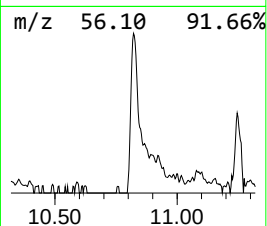
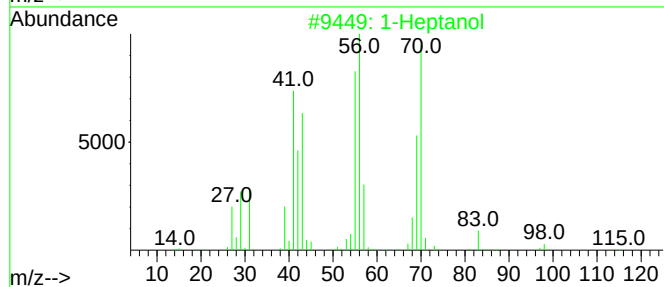
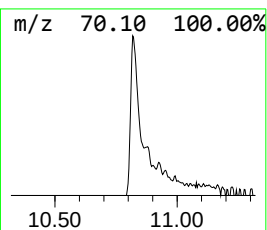
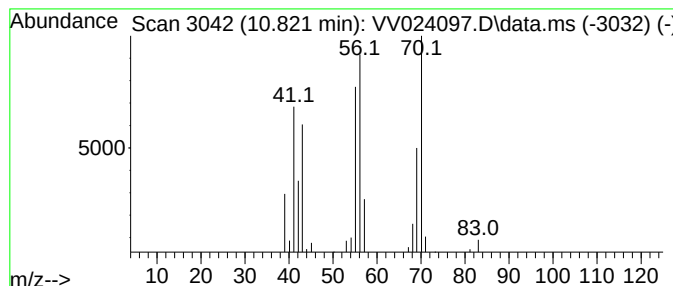
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR121021WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 1-Heptanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.821	0.70 ug/L	44862	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptanol	116	C7H16O	000111-70-6	83
2			Isopropylcyclobutane	98	C7H14	000872-56-0	50
3			1-Hexanol, 3-methyl-	116	C7H16O	013231-81-7	50
4			1-Pentene, 3,4-dimethyl-	98	C7H14	007385-78-6	50
5			Butane, 2-cyclopropyl-	98	C7H14	005750-02-7	47



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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
Dimethyl selenide	3.121	0.8	ug/L	34439	1	5.616	209992	5.0
1-Hexanol	9.487	5.8	ug/L	326968	2	8.850	282209	5.0
1-Heptanol	10.821	0.7	ug/L	44862	3	11.249	319524	5.0