

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV042823\
 Data File : VV030933.D
 Acq On : 28 Apr 2023 20:11
 Operator : SY/MD
 Sample : 02488-19
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BHE74

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\SFAMVTR042823WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV030933.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.082	8	13	27	rBV2	58898	88096	7.15%	1.235%
2	1.269	62	71	85	rBV2	129052	205382	16.68%	2.878%
3	1.529	145	152	165	rVB	65167	85563	6.95%	1.199%
4	2.063	306	318	334	rBV3	340080	572520	46.49%	8.023%
5	2.236	364	372	382	rBV	98153	145688	11.83%	2.042%
6	3.905	880	891	894	rBV2	18119	34898	2.83%	0.489%
7	4.252	983	999	1017	rVB2	110278	278573	22.62%	3.904%
8	4.510	1065	1079	1095	rVB	31664	83000	6.74%	1.163%
9	4.953	1202	1217	1235	rBV2	217578	498792	40.50%	6.990%
10	5.535	1381	1398	1415	rBV	143813	301446	24.48%	4.224%
11	5.831	1472	1490	1518	rBV	617079	1231446	100.00%	17.257%
12	5.995	1528	1541	1561	rBV2	118750	246564	20.02%	3.455%
13	6.921	1816	1829	1844	rBV	44775	87195	7.08%	1.222%
14	7.246	1919	1930	1943	rBV	202375	366072	29.73%	5.130%
15	7.320	1943	1953	1977	rVB	200475	372524	30.25%	5.221%
16	7.564	2017	2029	2045	rBV2	27966	51948	4.22%	0.728%
17	7.908	2124	2136	2153	rBV	267671	463193	37.61%	6.491%
18	8.053	2170	2181	2214	rBV	142588	355962	28.91%	4.988%
19	8.198	2219	2226	2241	rVB	7520	15957	1.30%	0.224%
20	8.792	2399	2411	2442	rBV	205810	376771	30.60%	5.280%
21	9.474	2612	2623	2648	rBV3	17682	57328	4.66%	0.803%
22	9.757	2702	2711	2725	rBV4	35121	63240	5.14%	0.886%
23	10.162	2826	2837	2850	rBV2	76827	124807	10.13%	1.749%
24	10.988	3083	3094	3110	rBV	103436	169224	13.74%	2.371%
25	11.194	3147	3158	3177	rBV	225306	371197	30.14%	5.202%
26	11.400	3215	3222	3229	rBV2	12934	17863	1.45%	0.250%
27	11.496	3239	3252	3263	rBV5	10623	23646	1.92%	0.331%
28	11.567	3263	3274	3298	rVB	220324	370027	30.05%	5.186%
29	12.191	3460	3468	3476	rBV	8017	12930	1.05%	0.181%
30	13.275	3796	3805	3814	rBV8	10396	17133	1.39%	0.240%
31	16.258	4725	4733	4742	rVB4	31024	46756	3.80%	0.655%

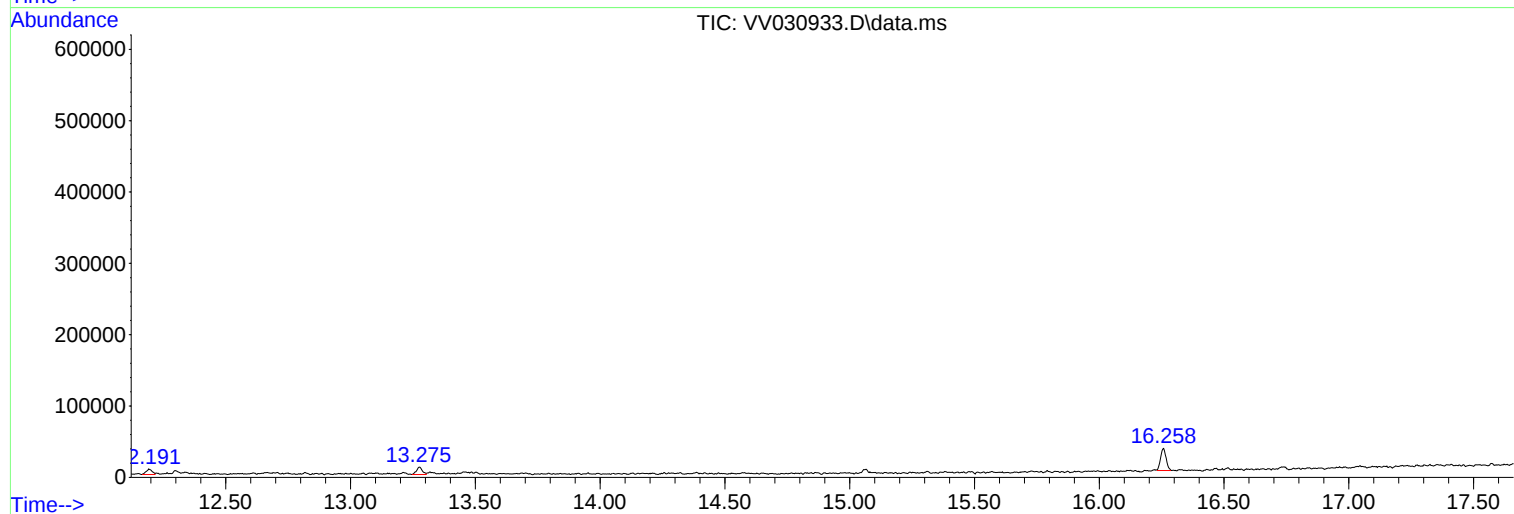
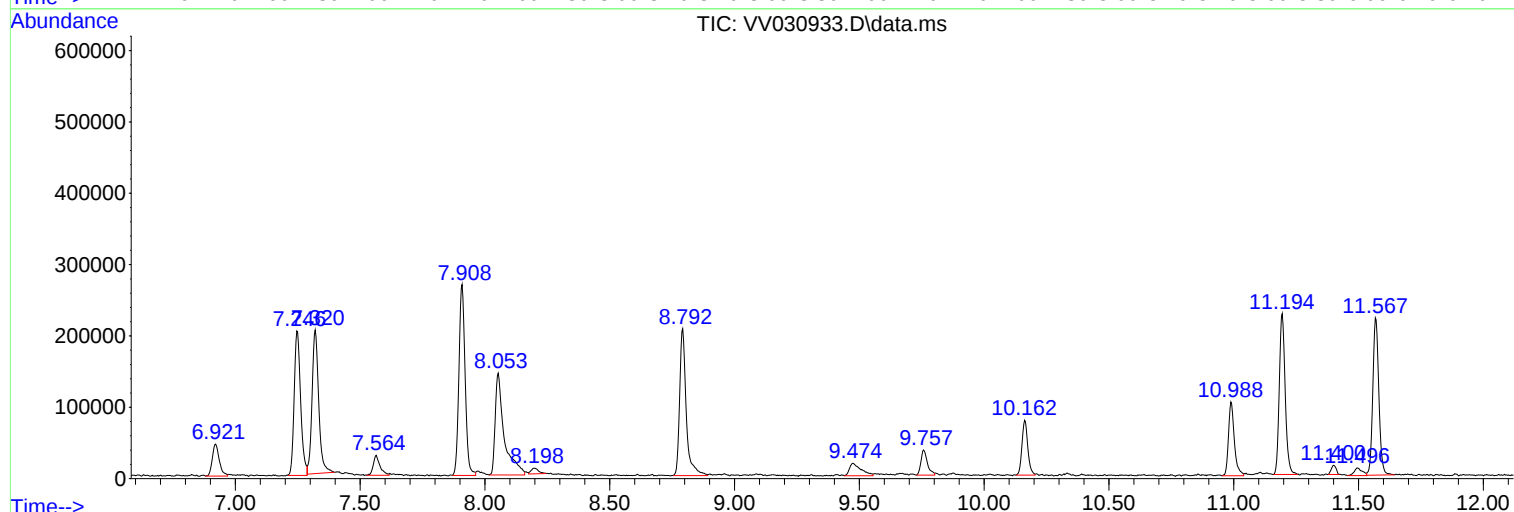
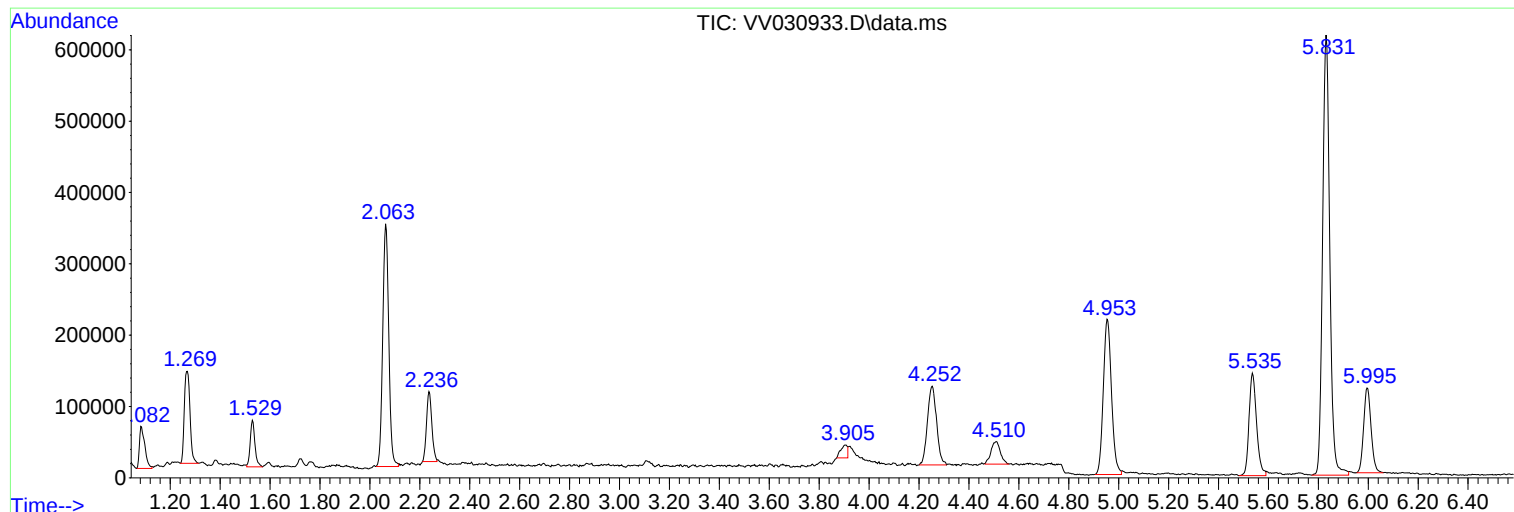
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Quant Title : TRACE VOA SFAM1.0

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



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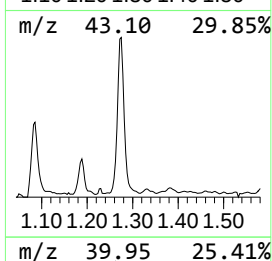
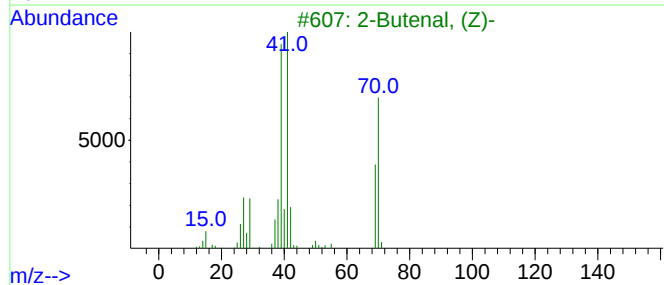
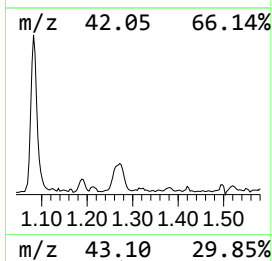
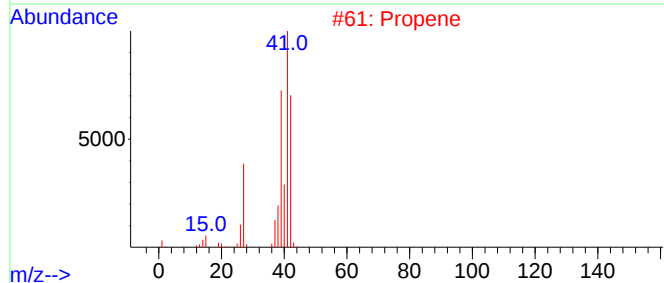
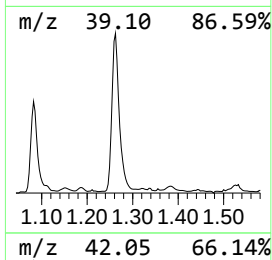
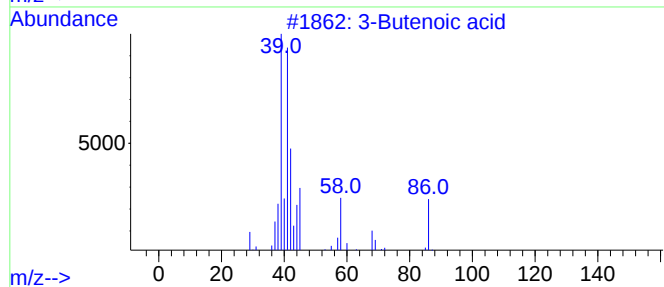
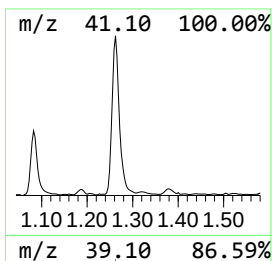
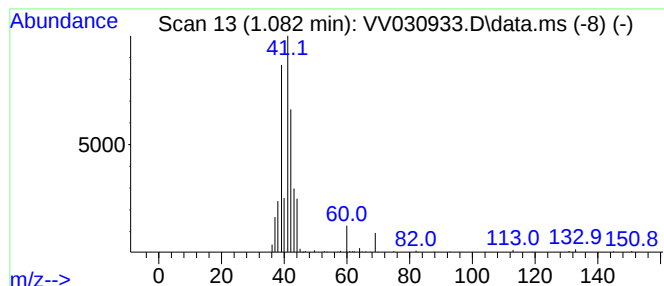
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 3-Butenoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.082	1.46 ug/L	88096	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Butenoic acid	86	C4H6O2	000625-38-7	83
2			Propene	42	C3H6	000115-07-1	78
3			2-Butenal, (Z)-	70	C4H6O	015798-64-8	64
4			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	64
5			2-Butenal, (E)-	70	C4H6O	000123-73-9	56



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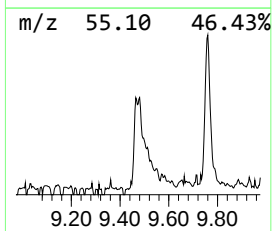
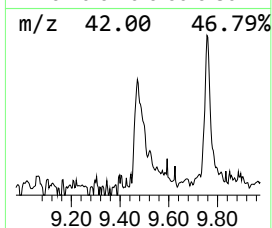
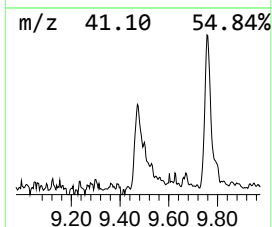
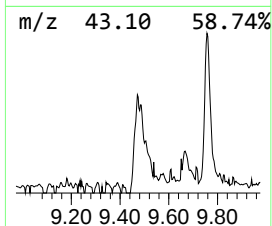
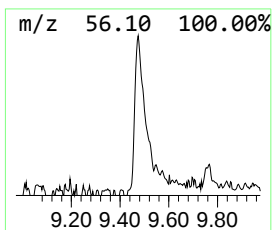
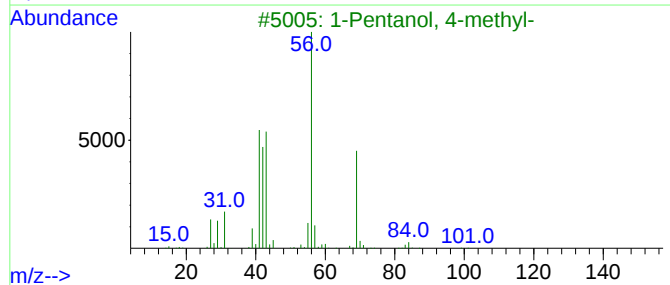
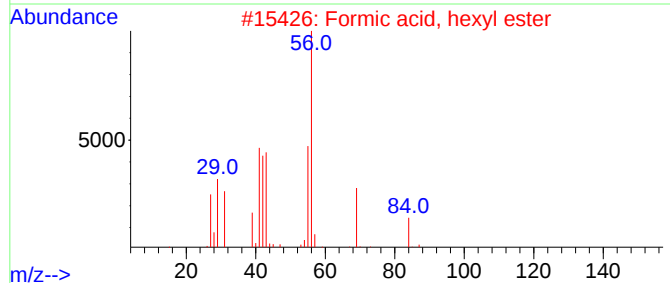
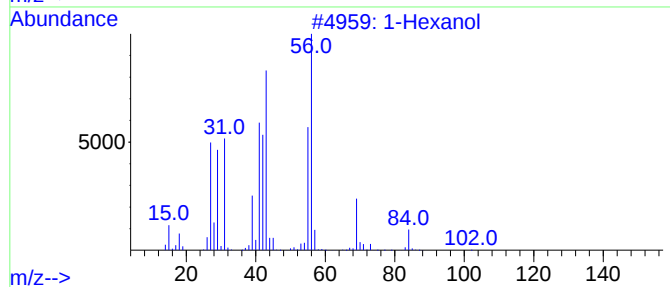
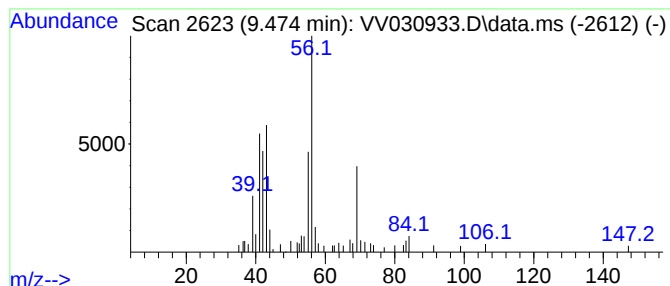
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR042823WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 1-Hexanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.474	0.76 ug/L	57328	Chlorobenzene-d5	8.792

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol		102	C6H14O	000111-27-3	72
2	Formic acid, hexyl ester		130	C7H14O2	000629-33-4	72
3	1-Pentanol, 4-methyl-		102	C6H14O	000626-89-1	64
4	Hexyl chloroformate		164	C7H13ClO2	006092-54-2	64
5	Oxirane, (1-methylbutyl)-		114	C7H14O	053229-39-3	64



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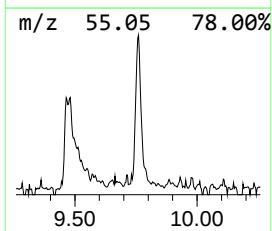
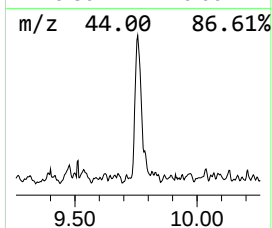
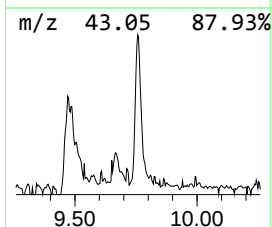
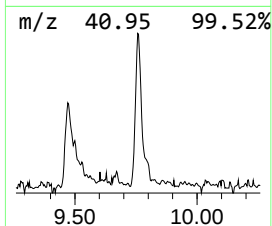
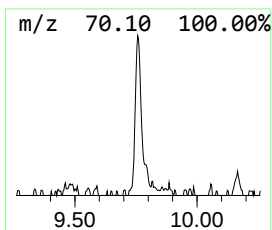
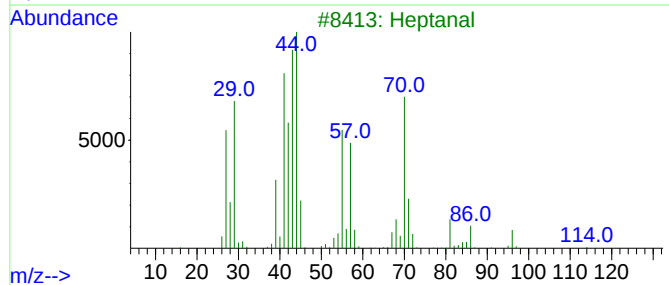
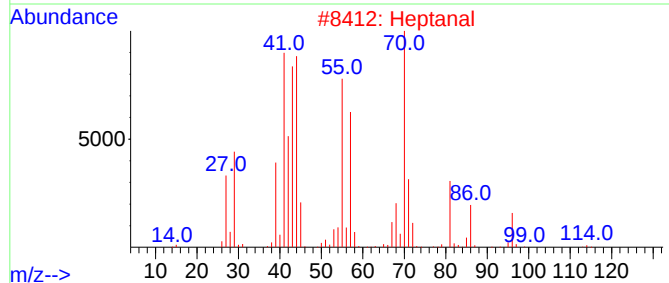
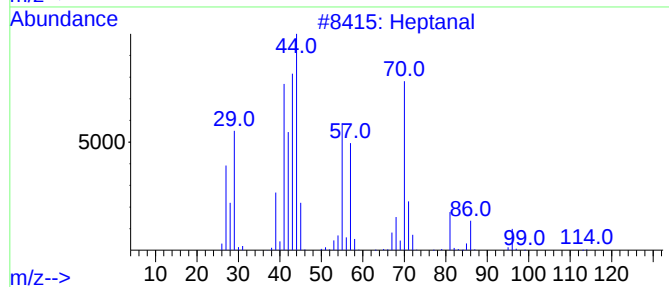
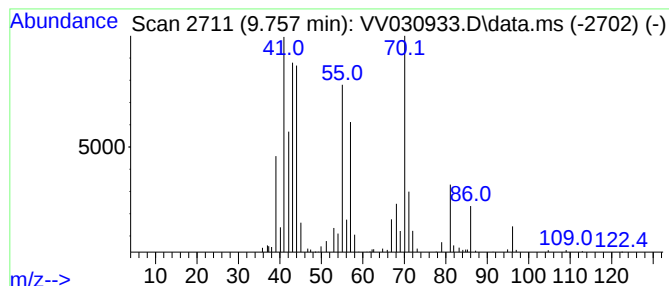
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR042823WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Heptanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.757	0.84 ug/L	63240	Chlorobenzene-d5	8.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	59
2			Heptanal	114	C7H14O	000111-71-7	53
3			Heptanal	114	C7H14O	000111-71-7	50
4			1-Butene, 3-methyl-	70	C5H10	000563-45-1	35
5			cis-1,2-Cyclohexanediol	116	C6H12O2	001792-81-0	35



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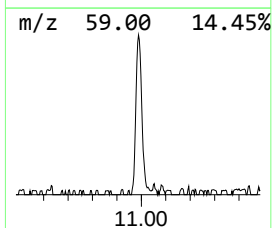
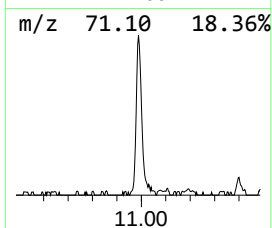
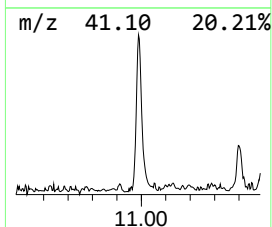
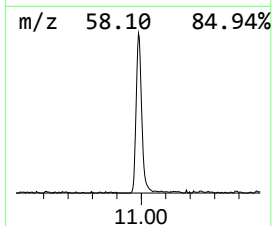
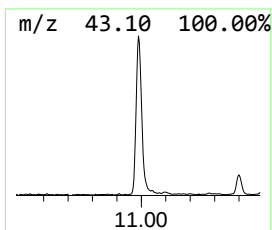
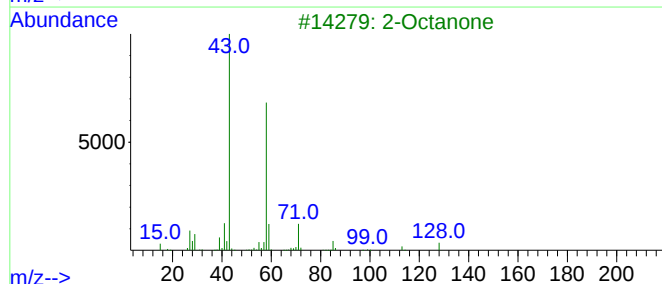
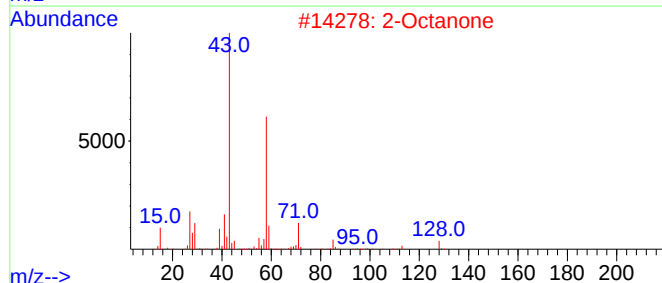
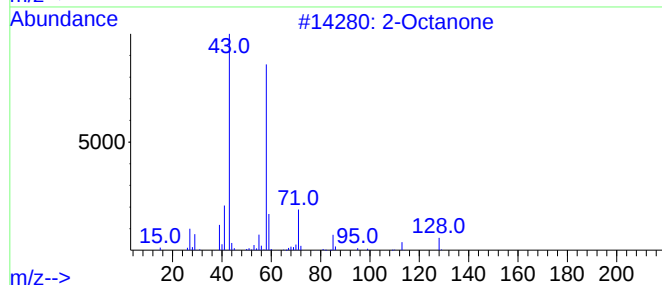
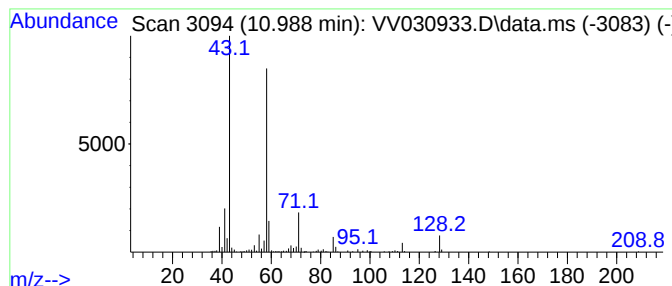
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 2-Octanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.988	2.28 ug/L	169224	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone			128	C8H16O	000111-13-7	94
2	2-Octanone			128	C8H16O	000111-13-7	91
3	2-Octanone			128	C8H16O	000111-13-7	91
4	2-Octanone			128	C8H16O	000111-13-7	91
5	2-Octanone			128	C8H16O	000111-13-7	87



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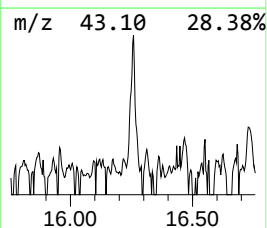
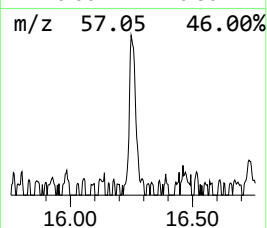
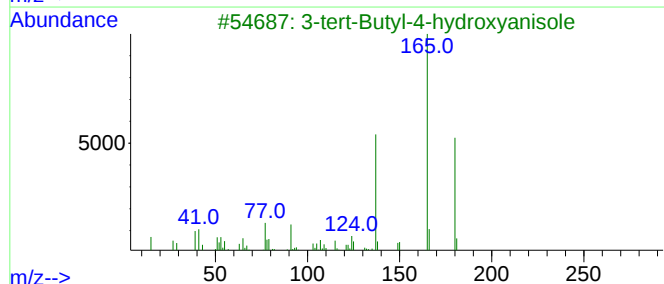
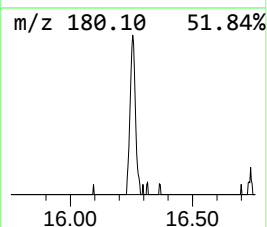
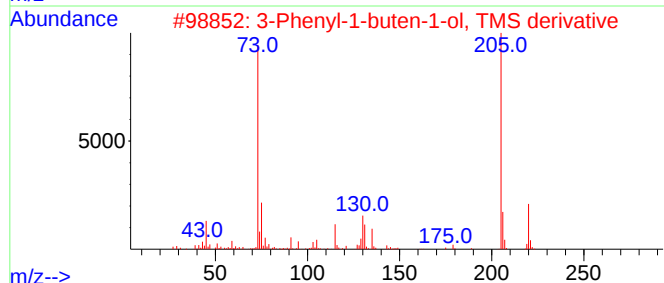
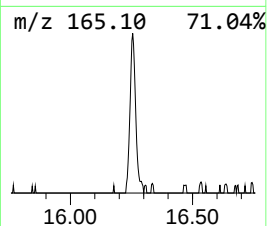
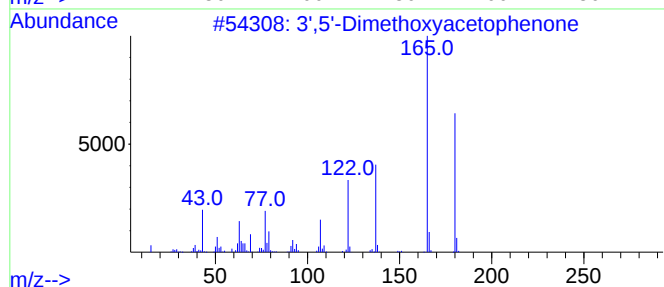
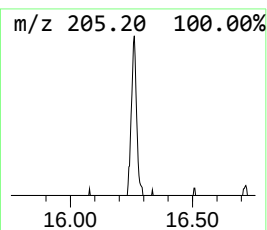
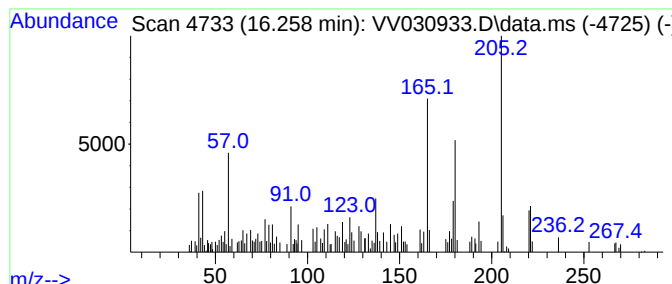
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 3',5'-Dimethoxyacetophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.258	0.63 ug/L	46756	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	51
2			3-Phenyl-1-buten-1-ol, TMS deriv...	220	C13H20OSi	055543-95-8	38
3			3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	38
4			2-Phenazincarbonitrile	205	C13H7N3	006479-93-2	38
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	38



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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
3-Butenoic acid	1.082	1.5	ug/L	88096	1	5.535	301446	5.0
1-Hexanol	9.474	0.8	ug/L	57328	2	8.792	376771	5.0
Heptanal	9.757	0.8	ug/L	63240	2	8.792	376771	5.0
2-Octanone	10.988	2.3	ug/L	169224	3	11.194	371197	5.0
3',5'-Dimethoxy...	16.258	0.6	ug/L	46756	3	11.194	371197	5.0