

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062824\
 Data File : VU059606.D
 Acq On : 28 Jun 2024 09:01
 Operator : MD/SY
 Sample : P3007-16
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 JMRG5

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\SFAMUTR061724WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU059606.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.354	13	20	32	rBV3	96060	106960	21.28%	2.019%
2	1.589	83	93	109	rBV2	69472	106951	21.28%	2.019%
3	1.724	130	135	142	rVB3	6987	7694	1.53%	0.145%
4	1.907	183	192	204	rBV	54352	71714	14.27%	1.354%
5	2.149	263	267	278	rVB5	3129	5516	1.10%	0.104%
6	2.557	381	394	413	rBV	99728	161422	32.12%	3.047%
7	2.673	413	430	446	rBV5	6842	21188	4.22%	0.400%
8	2.785	456	465	474	rVB	7237	11759	2.34%	0.222%
9	2.959	509	519	529	rBV2	3681	8380	1.67%	0.158%
10	3.036	534	543	553	rVB4	5461	10528	2.09%	0.199%
11	4.640	1028	1042	1083	rBV2	40150	172773	34.38%	3.261%
12	5.052	1156	1170	1193	rBV	98938	228476	45.46%	4.313%
13	5.718	1356	1377	1405	rBV2	194324	502540	100.00%	9.486%
14	6.242	1526	1540	1564	rBV	170219	326891	65.05%	6.170%
15	6.534	1619	1631	1656	rBV2	101726	196654	39.13%	3.712%
16	6.682	1665	1677	1699	rBV	119772	236591	47.08%	4.466%
17	7.560	1937	1950	1964	rBV2	43489	78291	15.58%	1.478%
18	7.891	2041	2053	2066	rBV	228446	398077	79.21%	7.514%
19	7.965	2067	2076	2091	rVB	43220	76398	15.20%	1.442%
20	8.177	2130	2142	2166	rBV	27191	46086	9.17%	0.870%
21	8.631	2271	2283	2323	rBV	220028	477917	95.10%	9.021%
22	8.788	2323	2332	2343	rVB5	3971	7826	1.56%	0.148%
23	9.412	2514	2526	2546	rBV	254724	428367	85.24%	8.086%
24	10.749	2931	2942	2958	rBV2	99332	164322	32.70%	3.102%
25	11.807	3259	3271	3293	rBV	237425	388667	77.34%	7.337%
26	12.061	3339	3350	3375	rBV4	19560	53388	10.62%	1.008%
27	12.187	3377	3389	3410	rVB2	226497	380519	75.72%	7.183%
28	12.528	3487	3495	3507	rBV5	3376	6006	1.20%	0.113%
29	15.682	4468	4476	4487	rVB6	10146	14160	2.82%	0.267%
30	15.781	4498	4507	4520	rVB4	6456	9900	1.97%	0.187%
31	16.759	4802	4811	4825	rBV2	63901	101818	20.26%	1.922%
32	16.878	4837	4848	4863	rBV	317617	489935	97.49%	9.248%

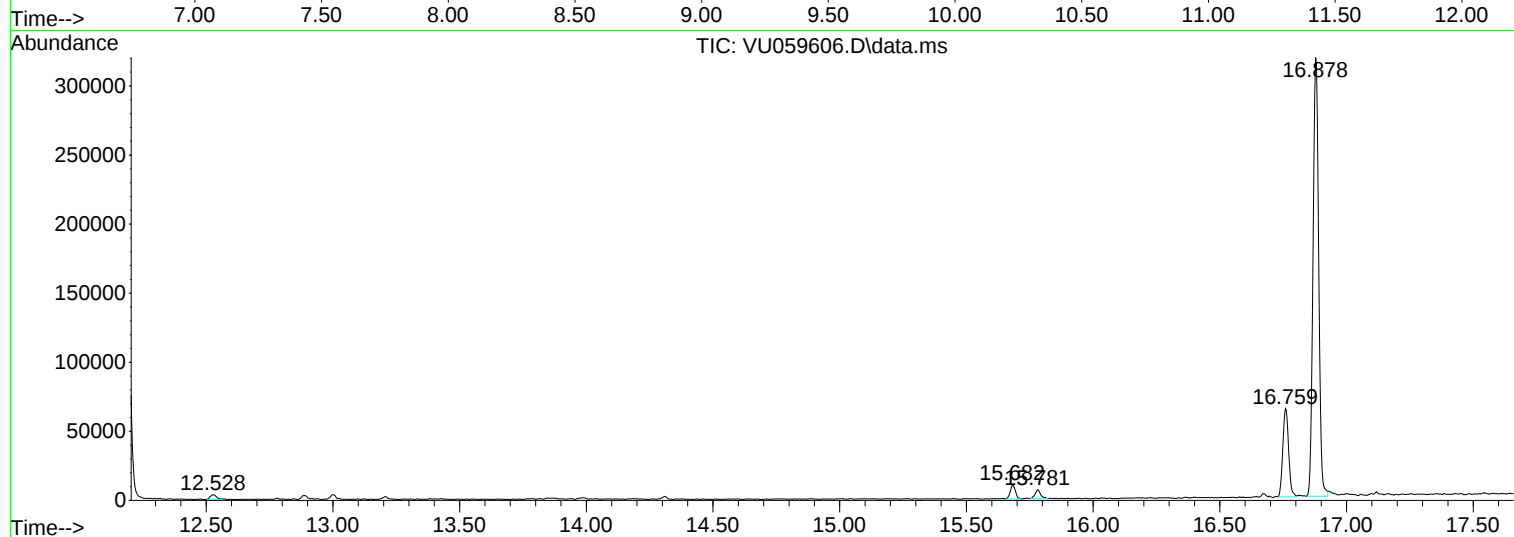
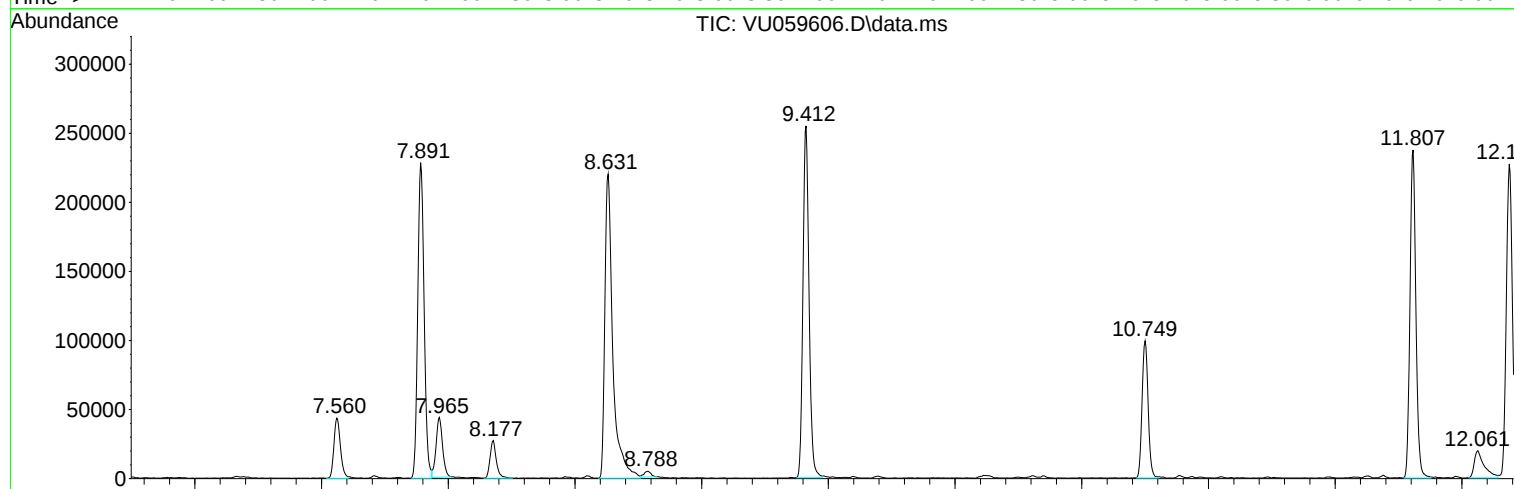
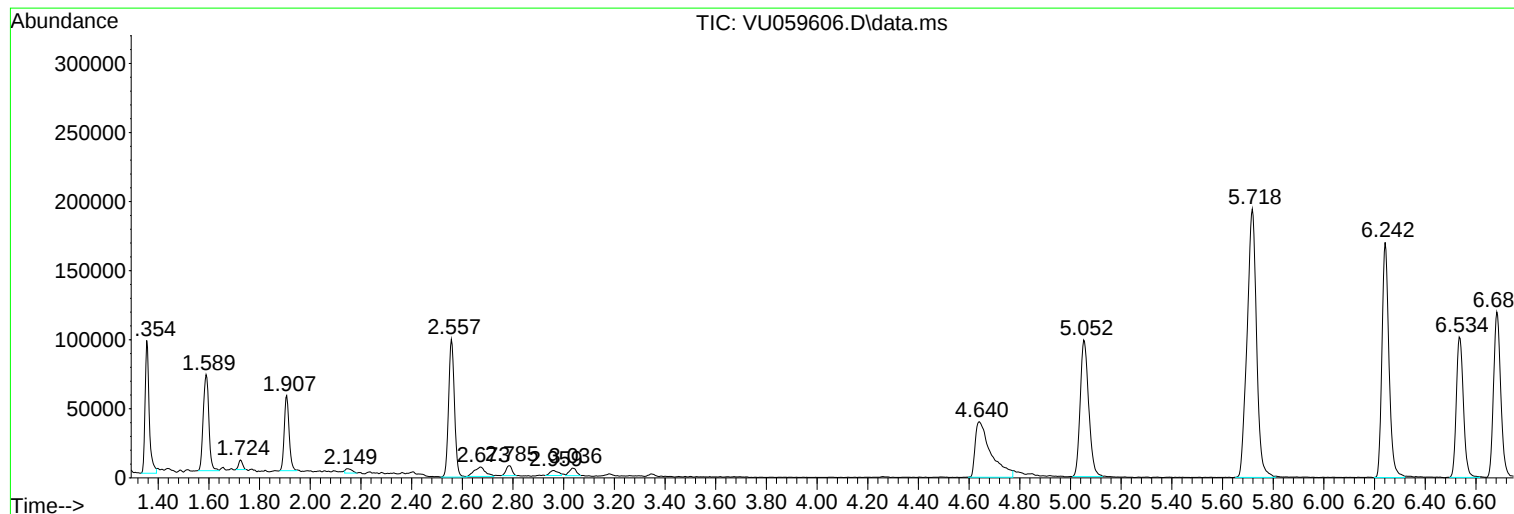
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JMRG5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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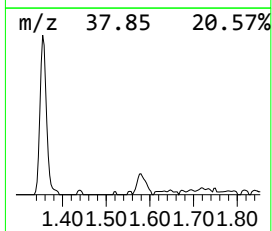
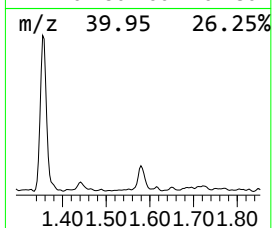
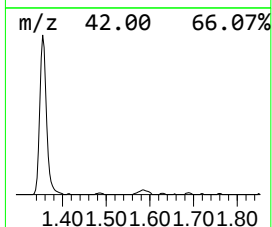
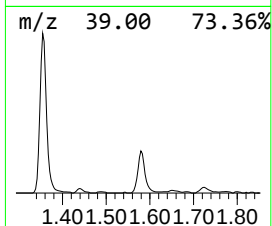
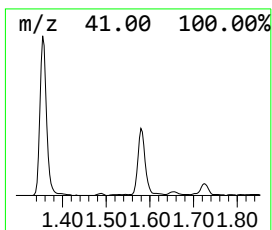
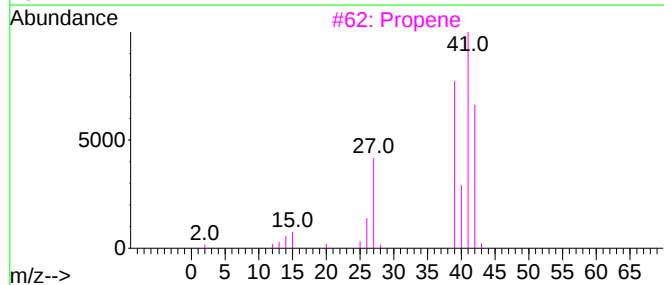
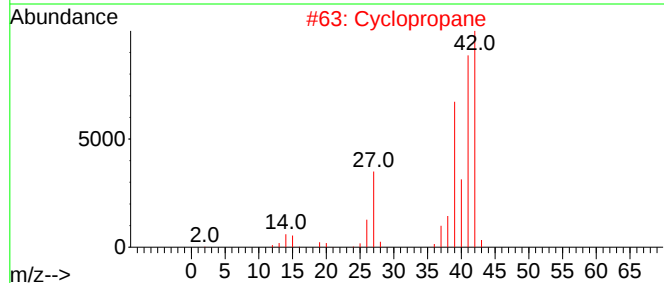
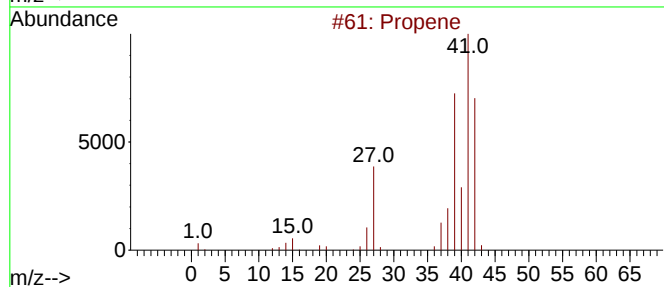
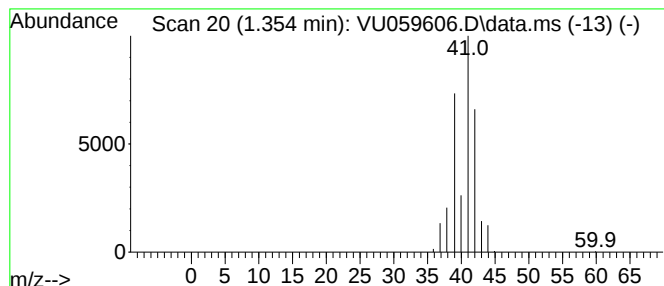
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.354	1.64 ug/L	106960	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Cyclopropane	42	C3H6	000075-19-4	64
3			Propene	42	C3H6	000115-07-1	45
4			Cyclopropane	42	C3H6	000075-19-4	9
5			Cyclopropene	40	C3H4	002781-85-3	9



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
JMRG5

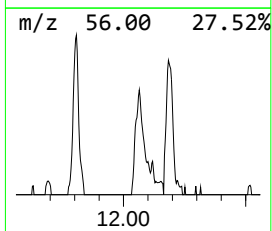
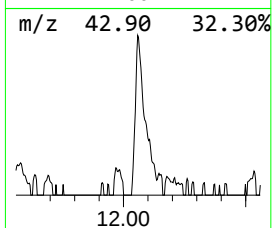
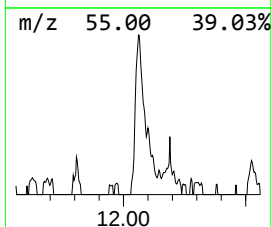
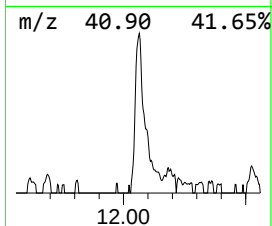
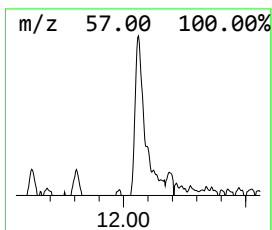
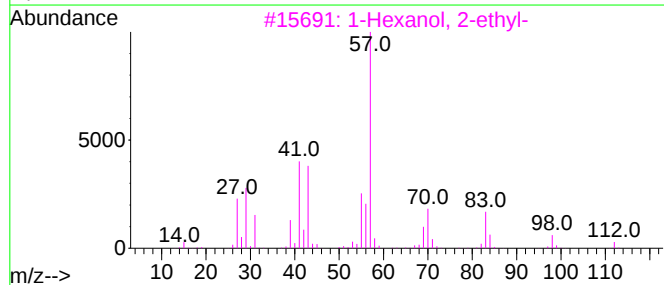
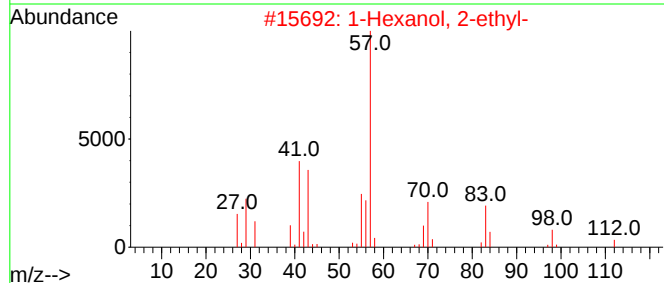
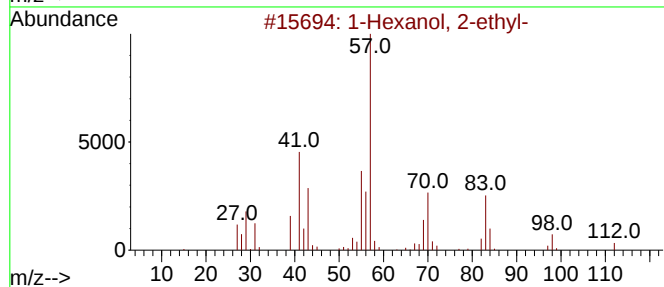
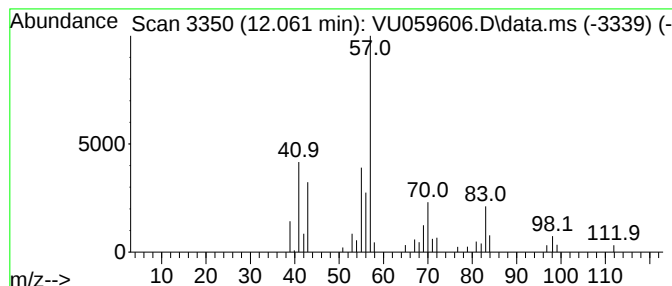
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.061	0.69 ug/L	53388	1,4-Dichlorobenzene-d4	11.807

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	78
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	59



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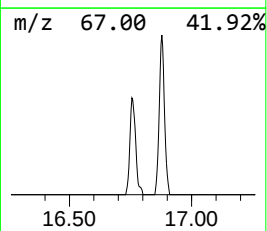
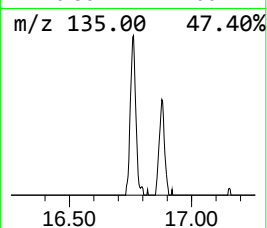
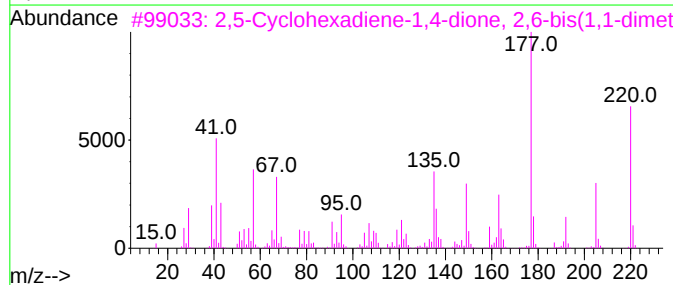
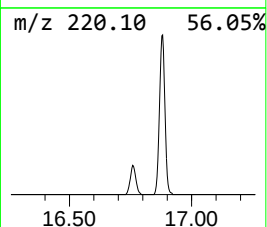
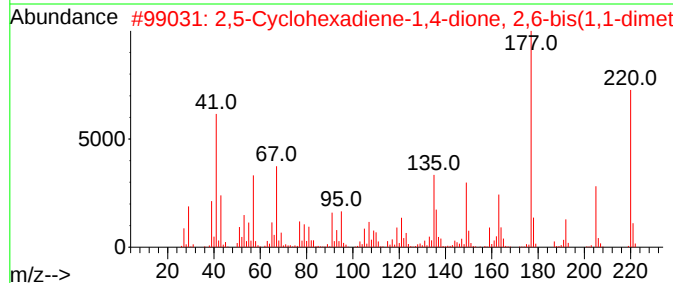
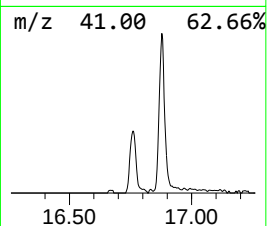
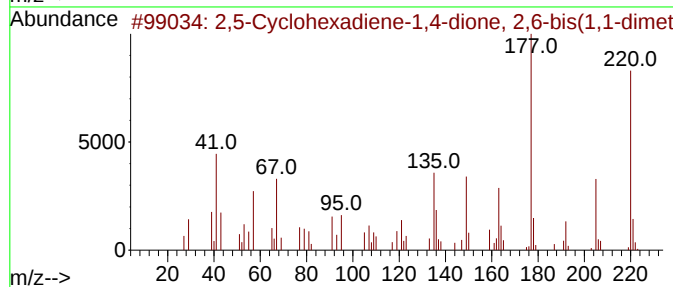
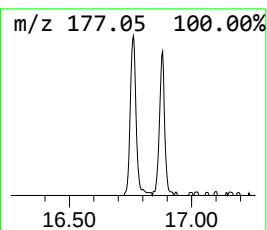
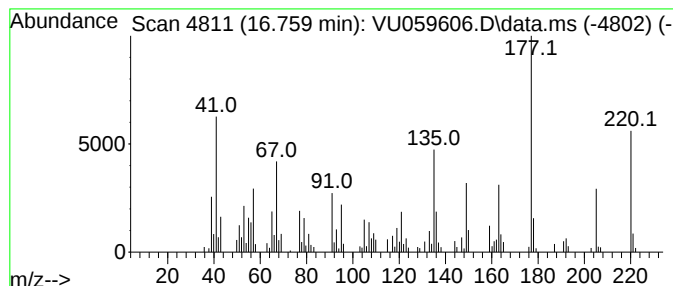
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
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Peak Number 4 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.759	1.31 ug/L	101818	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	90		



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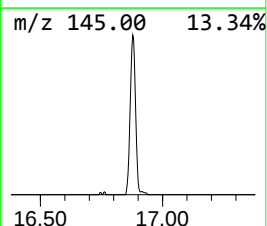
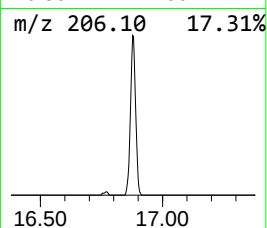
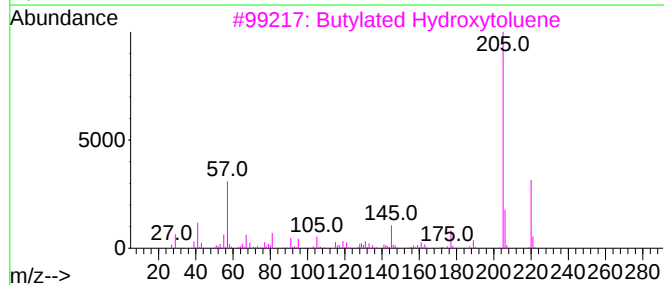
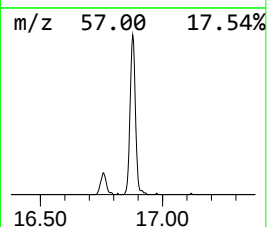
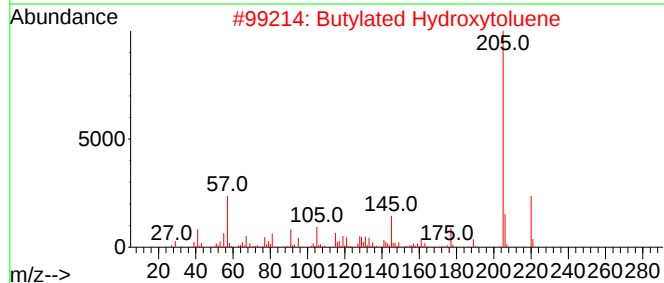
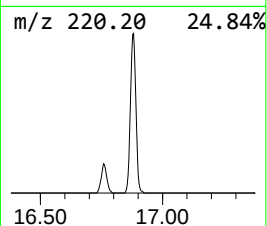
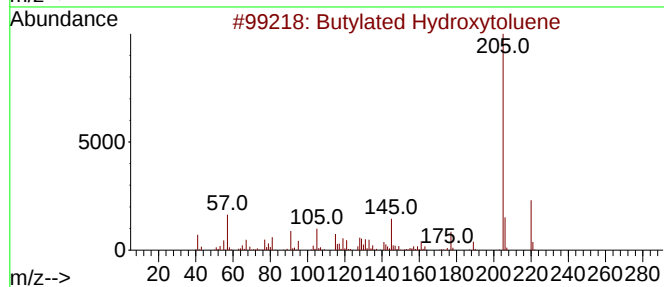
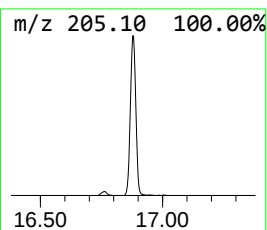
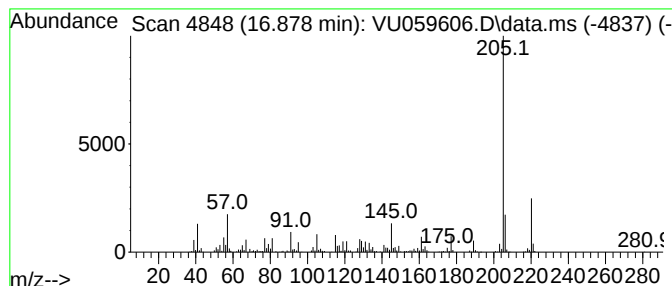
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.878	6.30 ug/L	489935	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
5			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	95



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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
(DEL) Alkane: S...	1.354	1.6	ug/L	106960	1	6.242	326891	5.0
1-Hexanol, 2-et...	12.061	0.7	ug/L	53388	3	11.807	388667	5.0
2,5-Cyclohexadi...	16.759	1.3	ug/L	101818	3	11.807	388667	5.0
Butylated Hydro...	16.878	6.3	ug/L	489935	3	11.807	388667	5.0