

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062824\
 Data File : VU059578.D
 Acq On : 27 Jun 2024 21:28
 Operator : MD/SY
 Sample : P3006-18
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 JMRJ2

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: VU059578.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.393	25	32	46	rBV	29300	33557	6.91%	0.715%
2	1.624	93	104	120	rBV2	61627	92252	19.00%	1.966%
3	1.939	193	202	219	rBV	54517	79049	16.28%	1.684%
4	2.595	395	406	421	rVB	110571	178377	36.73%	3.800%
5	3.074	547	555	568	rVB3	8093	15813	3.26%	0.337%
6	3.380	642	650	660	rBV4	5833	10607	2.18%	0.226%
7	4.727	1048	1069	1106	rVB2	56746	247729	51.01%	5.278%
8	5.094	1162	1183	1208	rVB	90018	215812	44.44%	4.598%
9	5.775	1377	1395	1421	rBV2	193708	464919	95.73%	9.905%
10	6.290	1542	1555	1575	rBV	159468	297915	61.34%	6.347%
11	6.576	1632	1644	1657	rBV5	10166	18714	3.85%	0.399%
12	6.724	1677	1690	1712	rBV	115659	226652	46.67%	4.829%
13	7.135	1809	1818	1830	rBV2	4113	6809	1.40%	0.145%
14	7.589	1946	1959	1980	rBV	44489	78999	16.27%	1.683%
15	7.913	2048	2060	2073	rBV	211668	360169	74.16%	7.674%
16	7.984	2073	2082	2101	rVB	49463	87039	17.92%	1.854%
17	8.193	2135	2147	2163	rBV2	27612	47006	9.68%	1.002%
18	8.650	2274	2289	2326	rBV2	217772	485653	100.00%	10.347%
19	8.814	2330	2340	2356	rVB6	7465	16286	3.35%	0.347%
20	9.421	2517	2529	2551	rBV	233990	392960	80.91%	8.372%
21	10.756	2932	2944	2960	rVB	92530	153034	31.51%	3.261%
22	10.888	2975	2985	2995	rBV2	3662	5853	1.21%	0.125%
23	11.807	3260	3271	3287	rBV	214088	346347	71.32%	7.379%
24	12.068	3340	3352	3378	rBV4	18439	57646	11.87%	1.228%
25	12.190	3379	3390	3408	rVB	210631	344676	70.97%	7.344%
26	12.772	3563	3571	3581	rBV6	3429	5487	1.13%	0.117%
27	12.884	3599	3606	3617	rVB7	4311	6482	1.33%	0.138%
28	15.682	4469	4476	4485	rVB5	13037	18228	3.75%	0.388%
29	16.672	4778	4784	4791	rBV9	3627	4885	1.01%	0.104%
30	16.759	4803	4811	4822	rBV3	26834	38969	8.02%	0.830%
31	16.881	4835	4849	4866	rBV2	205087	355626	73.23%	7.577%

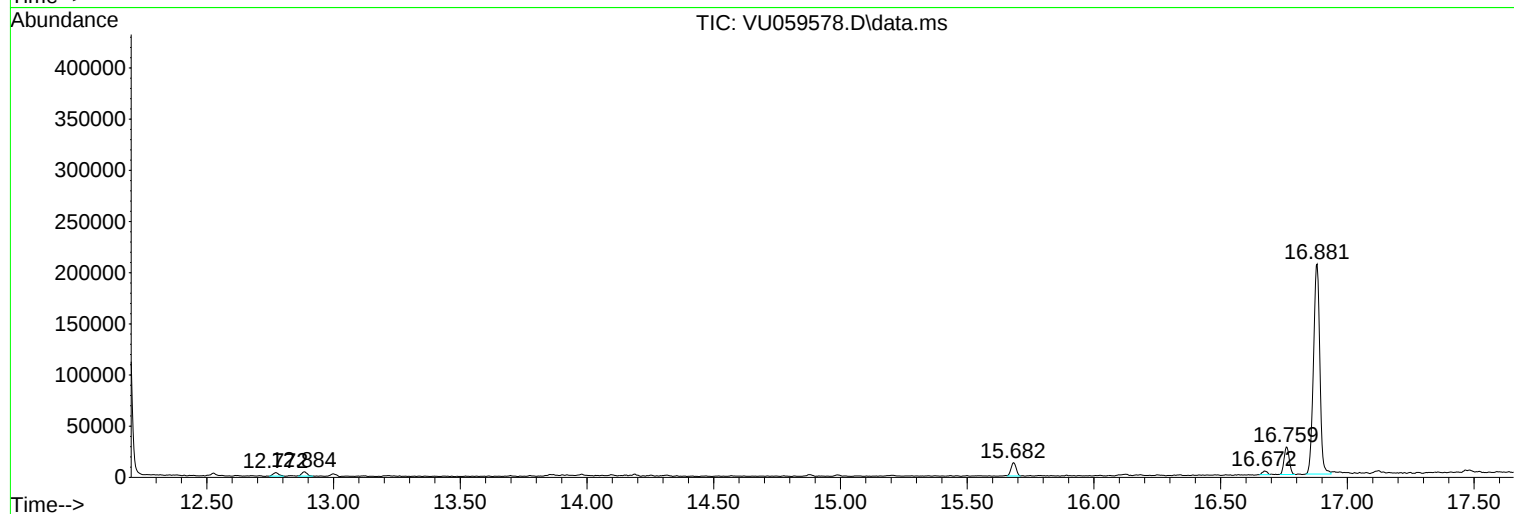
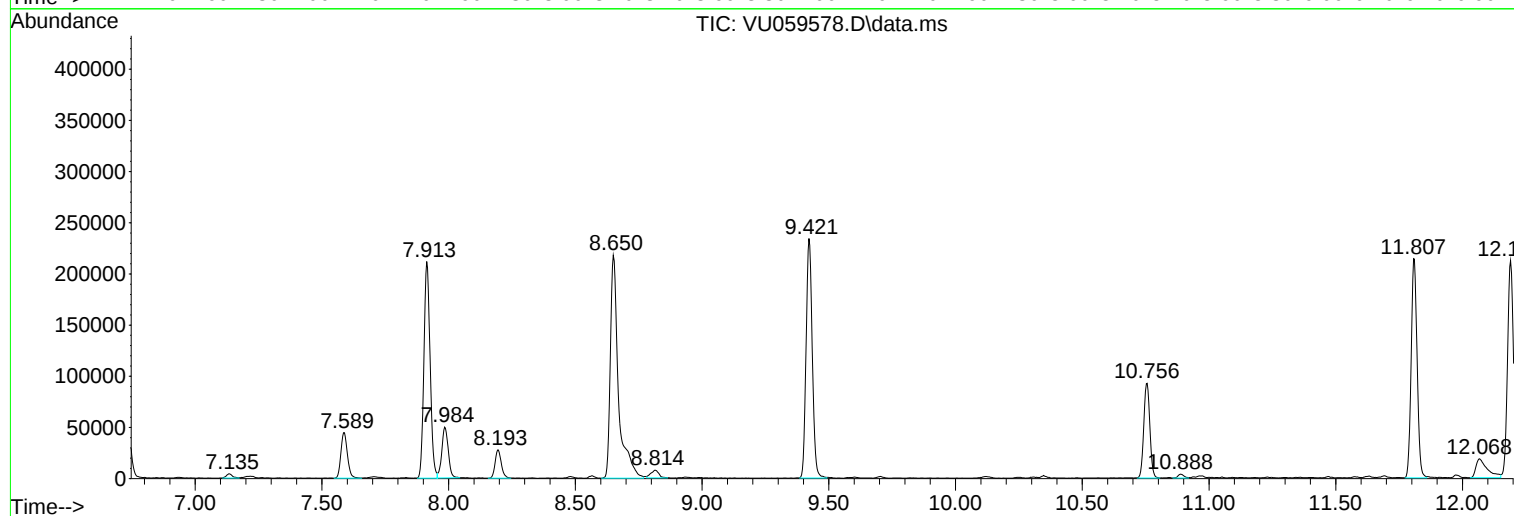
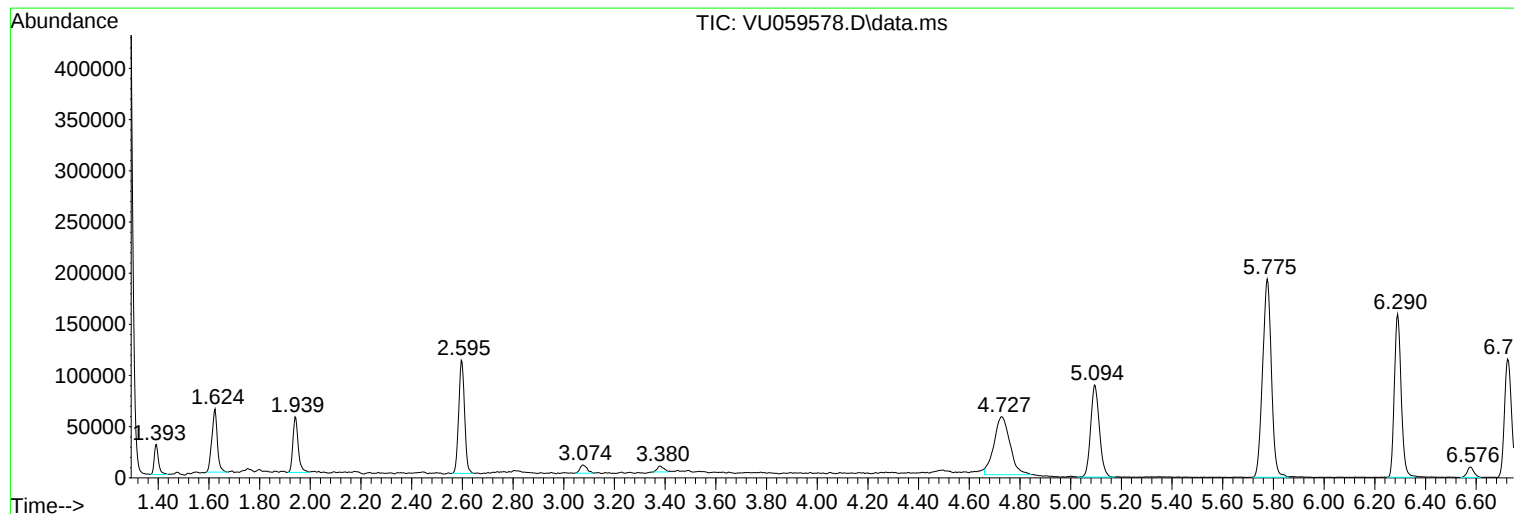
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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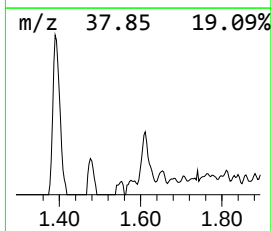
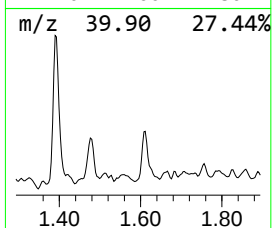
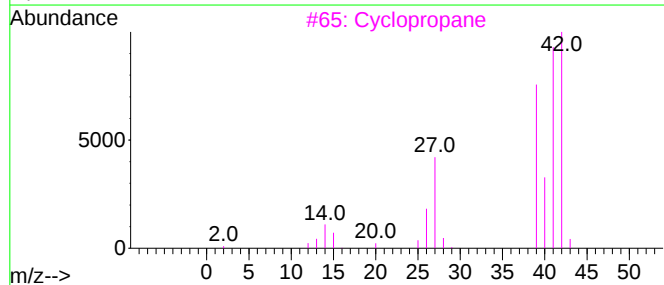
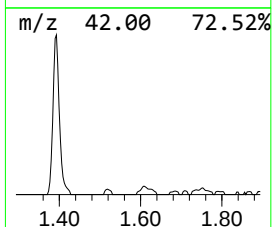
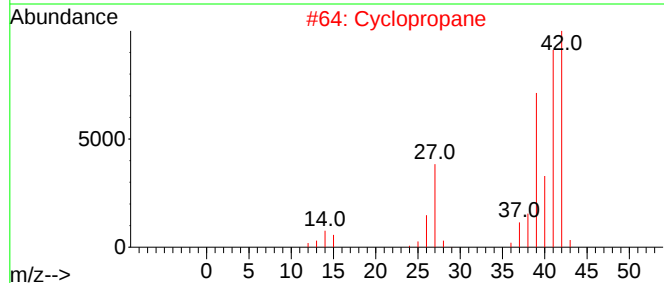
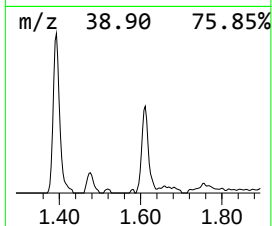
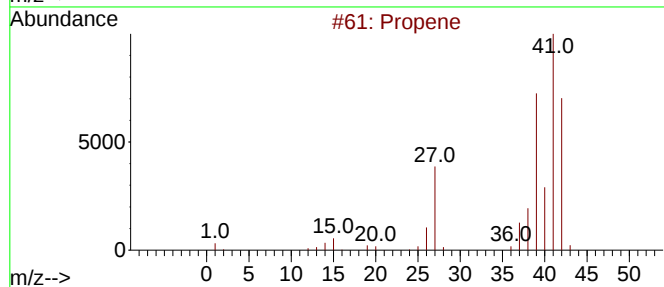
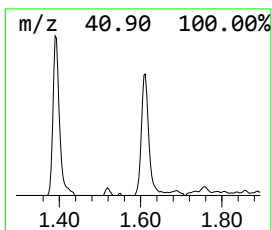
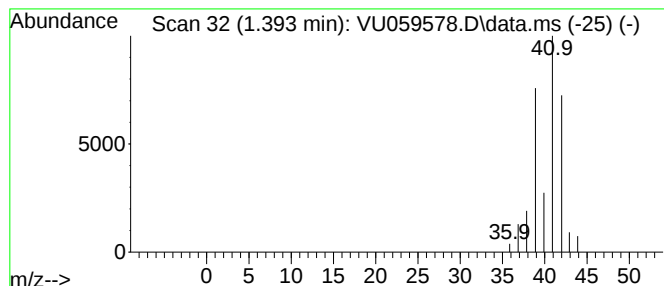
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.393	0.56 ug/L	33557	1,4-Difluorobenzene	6.290

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			Cyclopropane	42	C3H6	000075-19-4	59
4			Propene	42	C3H6	000115-07-1	45
5			Cyclopropene	40	C3H4	002781-85-3	10



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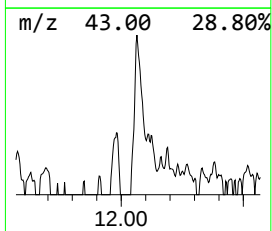
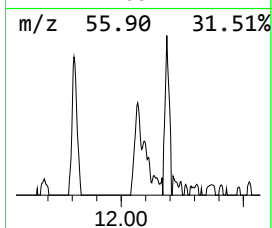
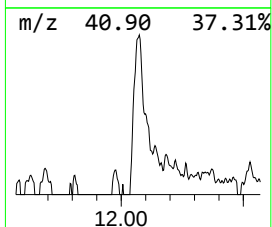
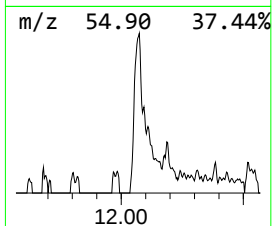
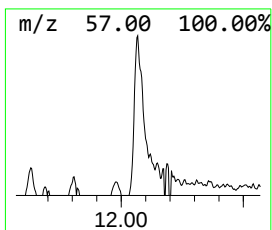
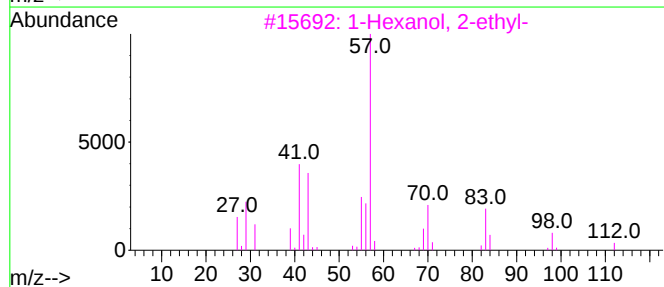
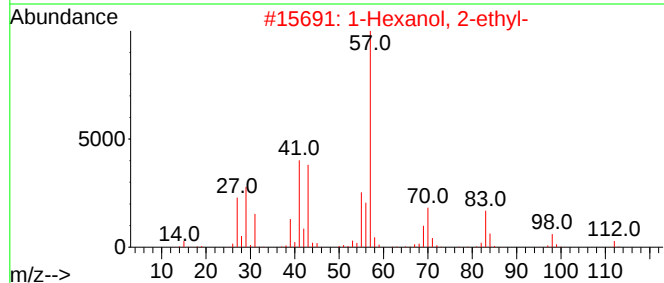
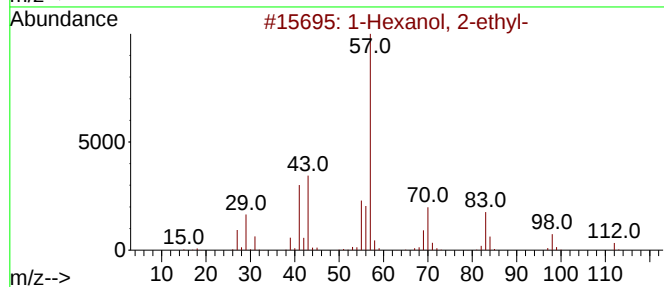
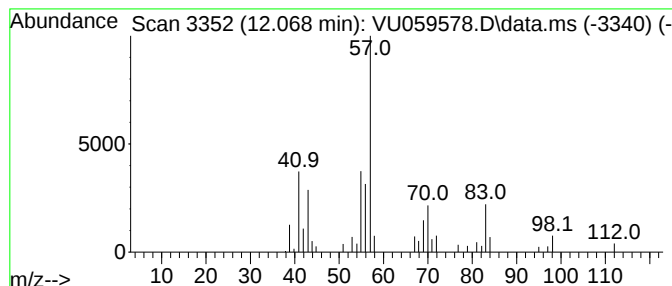
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.068	0.83 ug/L	57646	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
4	1-Pentanol, 2-ethyl-4-methyl-			130	C8H18O	000106-67-2	64
5	1-Pentanol, 2-ethyl-4-methyl-			130	C8H18O	000106-67-2	53



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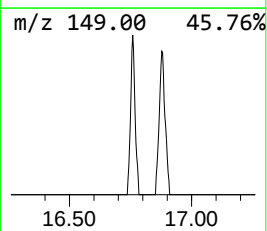
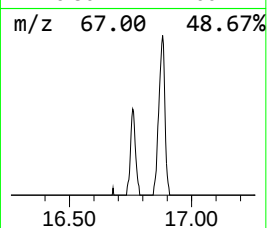
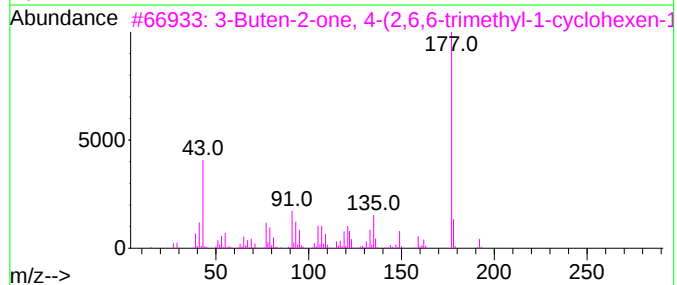
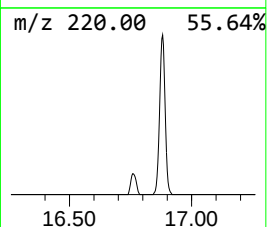
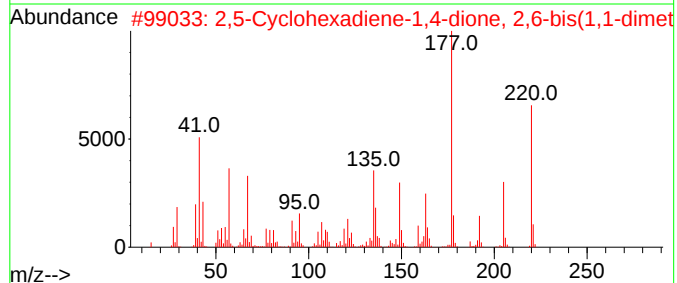
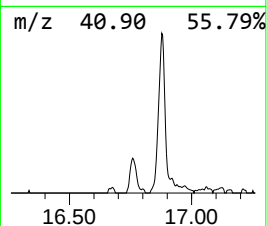
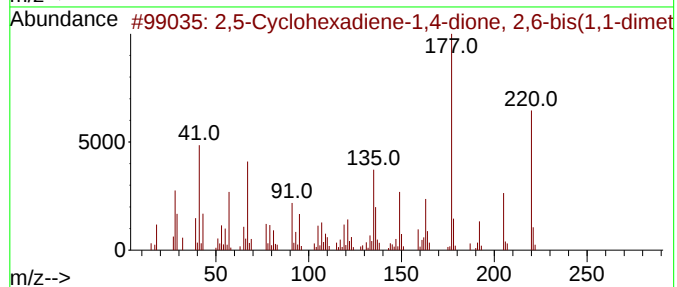
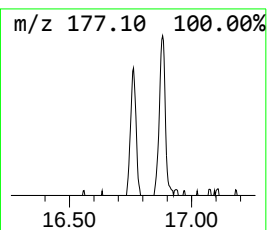
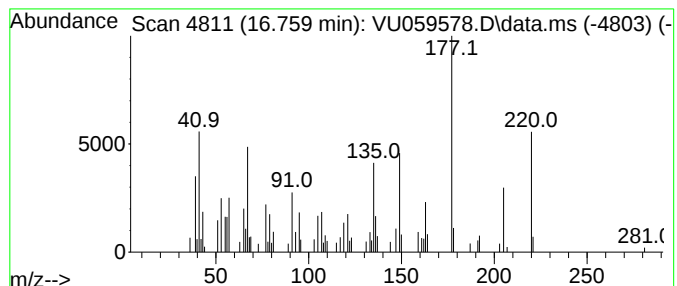
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Quant Title : TRACE VOA SFAM1.0

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.759	0.56 ug/L	38969	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	87		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	83		
3	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H200	014901-07-6	55		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	49		
5	2-Acetyl-3,4,5,6-tetrafluorobenz...	220	C9H4F402	1000461-12-2	46		



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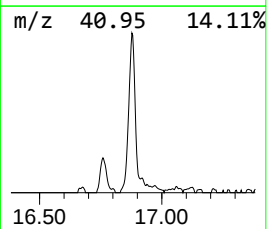
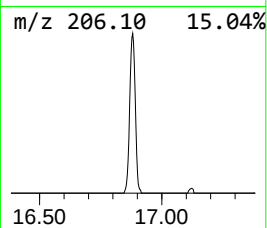
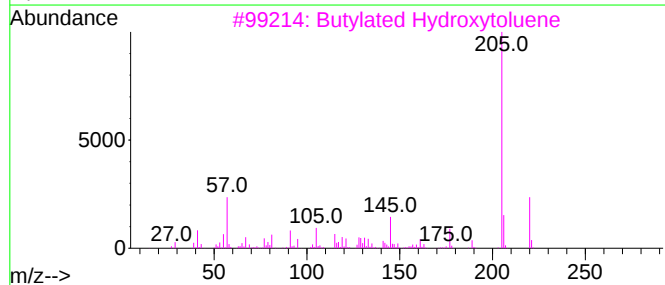
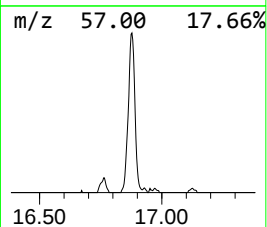
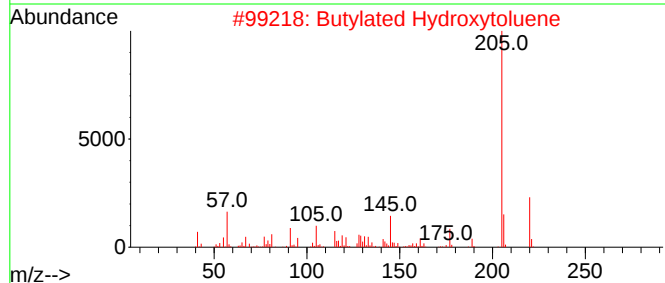
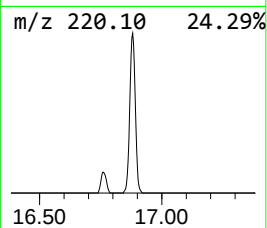
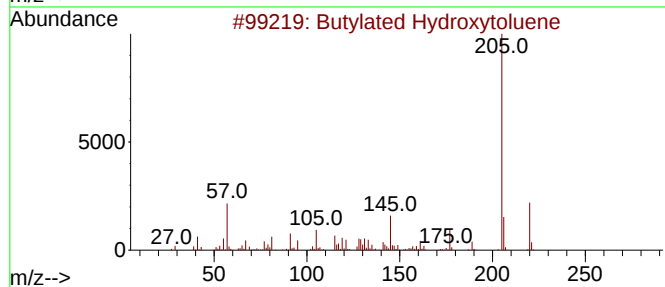
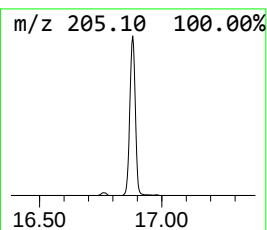
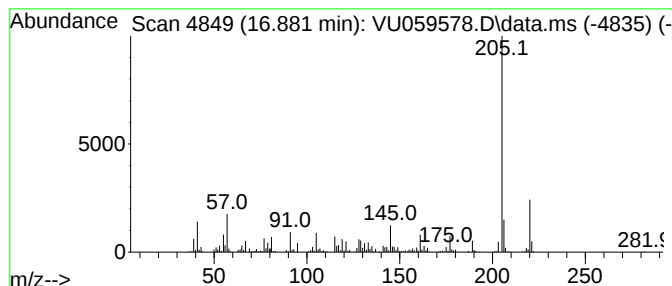
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.881	5.13 ug/L	355626	1,4-Dichlorobenzene-d4	11.810

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



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.393	0.6	ug/L	33557	1	6.290	297915	5.0
1-Hexanol, 2-et...	12.068	0.8	ug/L	57646	3	11.810	346347	5.0
2,5-Cyclohexadi...	16.759	0.6	ug/L	38969	3	11.810	346347	5.0
Butylated Hydro...	16.881	5.1	ug/L	355626	3	11.810	346347	5.0