

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070124\
 Data File : VU059679.D
 Acq On : 01 Jul 2024 12:58
 Operator : MD/SY
 Sample : P3059-12DL 4X
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E1GN3DL

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: VU059679.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	14	20	45	rBV	39544	56532	2.64%	0.697%
2	1.595	85	95	108	rBV	83875	101639	4.75%	1.253%
3	1.898	148	189	202	rBV	78951	230052	10.75%	2.836%
4	1.968	206	211	232	rVB3	55463	104041	4.86%	1.283%
5	2.184	270	278	289	rVB	25492	35595	1.66%	0.439%
6	2.438	343	357	380	rVB	691464	1130561	52.83%	13.939%
7	2.550	380	392	406	rVB2	80825	132786	6.21%	1.637%
8	2.631	406	417	447	rBV	29489	64870	3.03%	0.800%
9	2.798	450	469	480	rBV	625287	2139923	100.00%	26.385%
10	3.174	578	586	606	rVB	18175	44638	2.09%	0.550%
11	3.341	626	638	656	rVB2	40503	82846	3.87%	1.021%
12	4.653	1026	1046	1071	rBV3	135436	450897	21.07%	5.559%
13	5.052	1155	1170	1190	rBV	93425	206964	9.67%	2.552%
14	5.717	1355	1377	1409	rBV3	177188	463667	21.67%	5.717%
15	6.242	1523	1540	1565	rBV	167933	327105	15.29%	4.033%
16	6.537	1620	1632	1644	rBV3	32155	61958	2.90%	0.764%
17	6.682	1664	1677	1700	rBV2	112605	220906	10.32%	2.724%
18	7.560	1937	1950	1964	rBV	45816	82131	3.84%	1.013%
19	7.891	2041	2053	2073	rBV	200491	348438	16.28%	4.296%
20	8.177	2131	2142	2160	rBV2	27320	47080	2.20%	0.580%
21	8.634	2272	2284	2312	rBV	224428	477776	22.33%	5.891%
22	9.412	2514	2526	2550	rBV	245506	414085	19.35%	5.106%
23	9.688	2602	2612	2631	rVB	21513	37876	1.77%	0.467%
24	10.753	2932	2943	2965	rVB	97386	161174	7.53%	1.987%
25	11.807	3258	3271	3295	rBV	221872	367056	17.15%	4.526%
26	12.190	3376	3390	3418	rBV	188789	319920	14.95%	3.945%

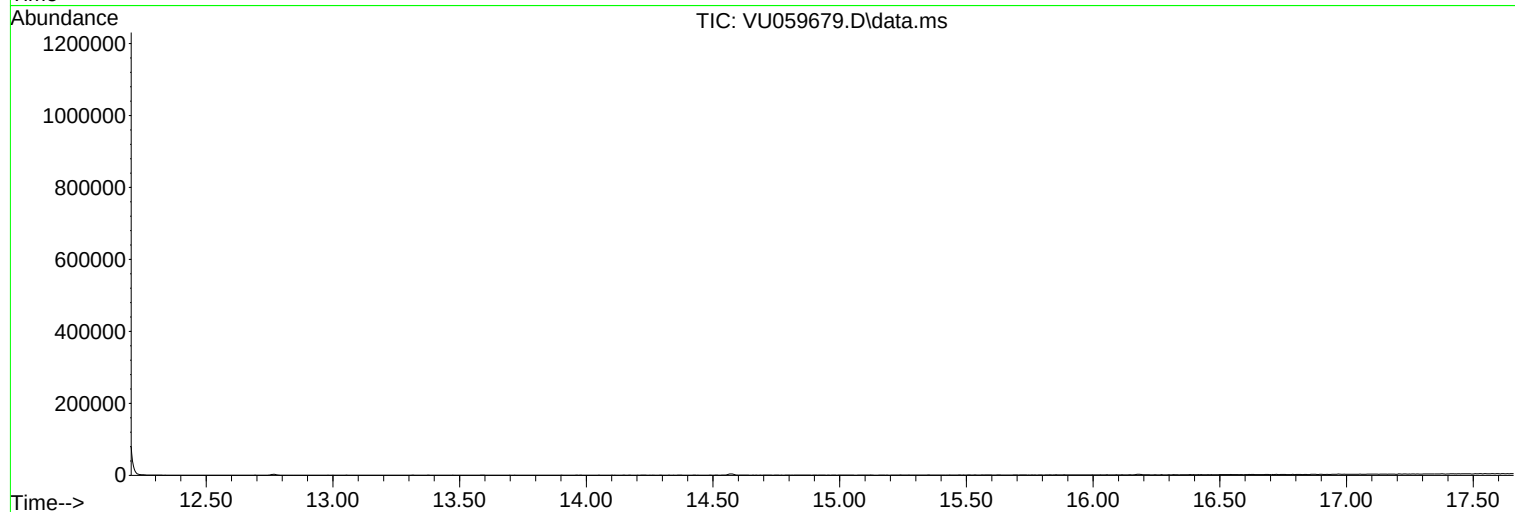
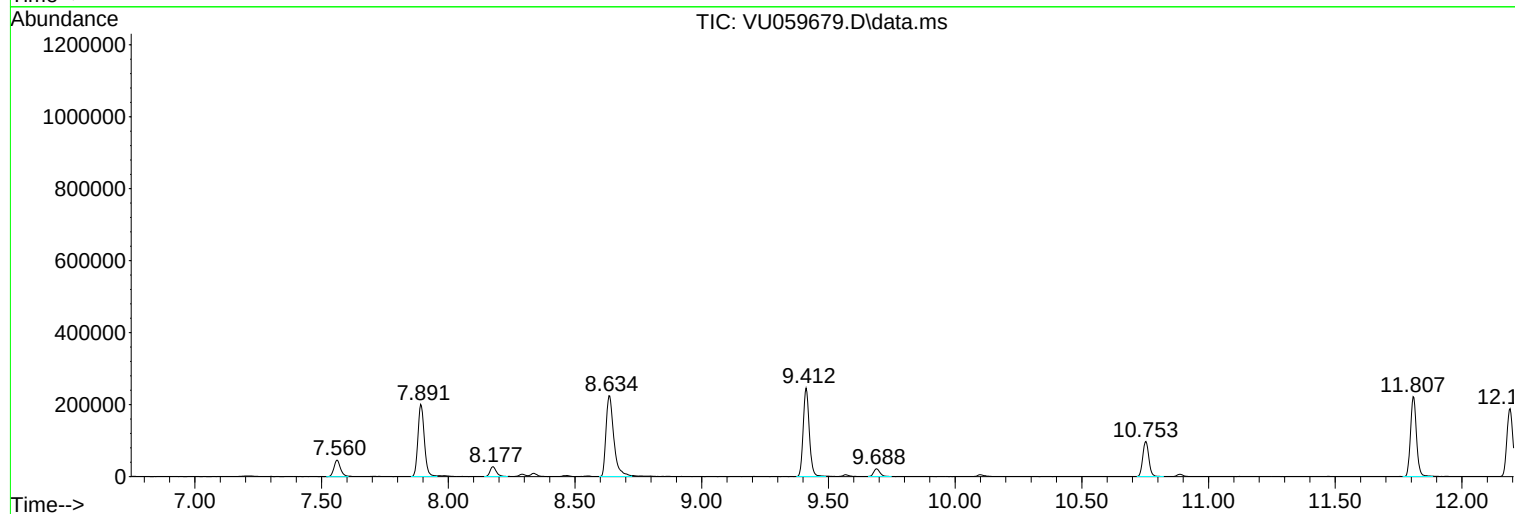
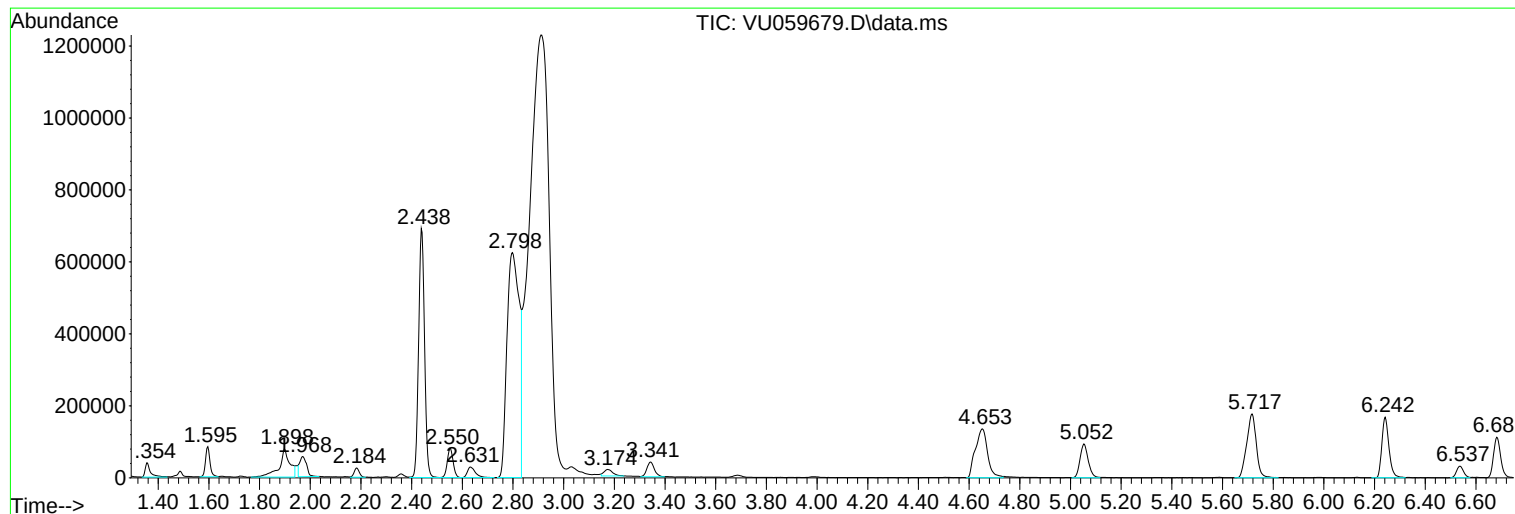
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E1GN3DL

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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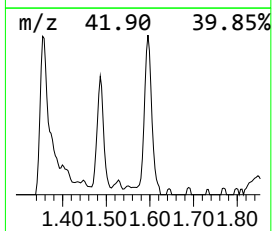
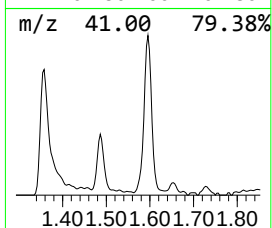
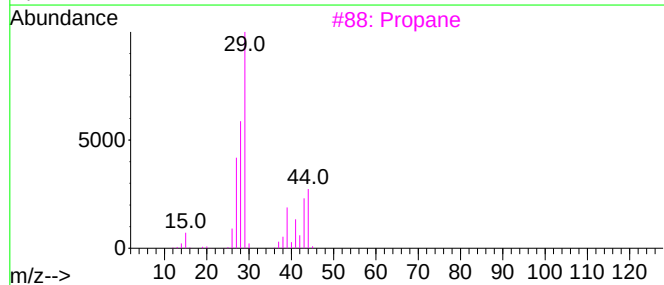
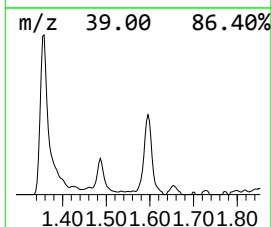
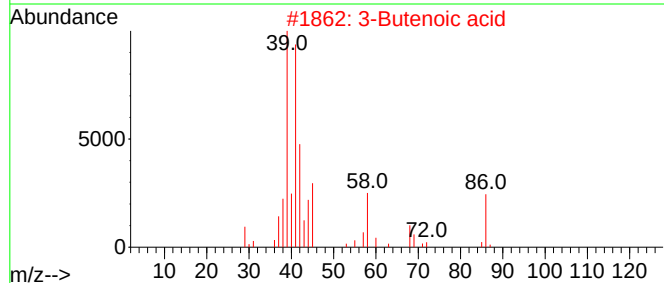
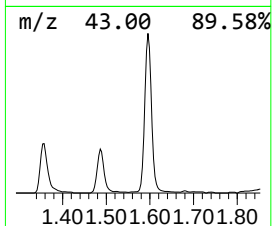
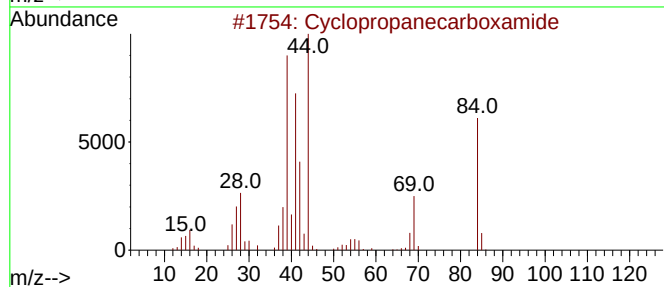
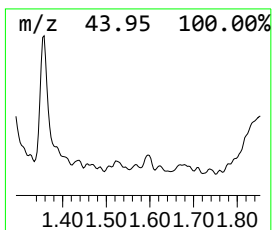
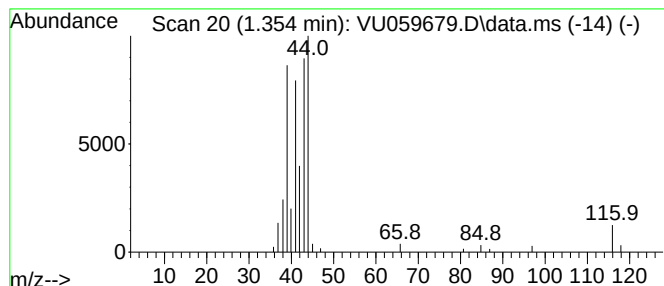
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Cyclopropanecarboxamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.354	0.86 ug/L	56532	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	64
2			3-Butenoic acid	86	C4H6O2	000625-38-7	64
3			Propane	44	C3H8	000074-98-6	64
4			2-Butenal, (E)-	70	C4H6O	000123-73-9	59
5			Thiocyanic acid, 2-propynyl ester	97	C4H3NS	024309-48-6	53



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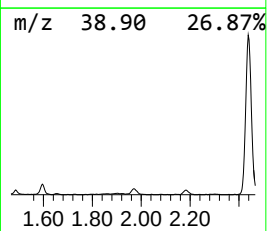
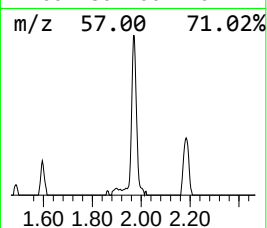
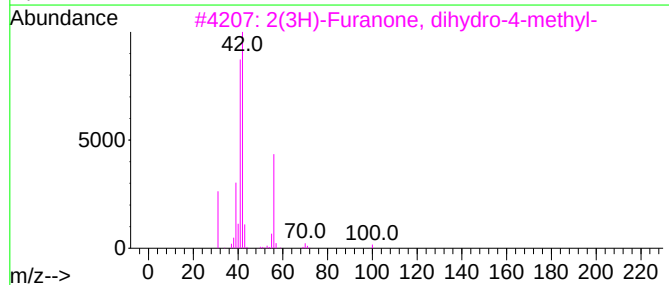
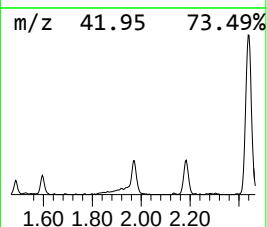
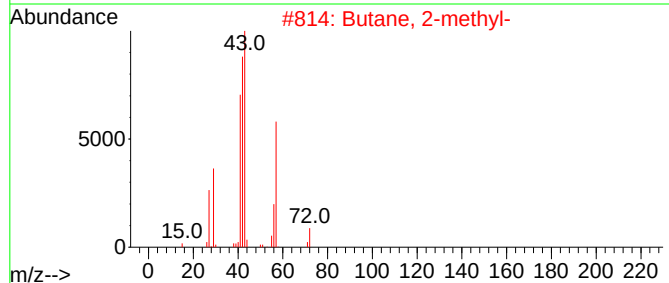
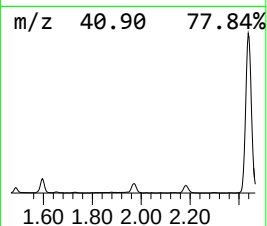
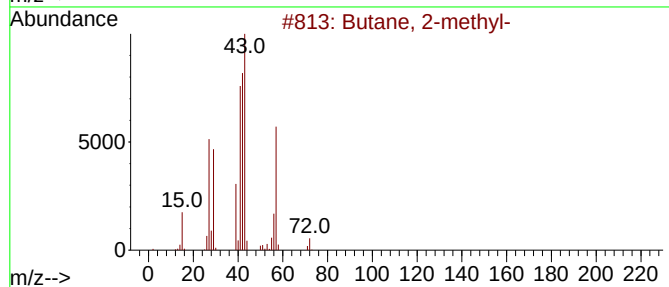
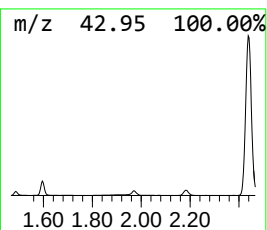
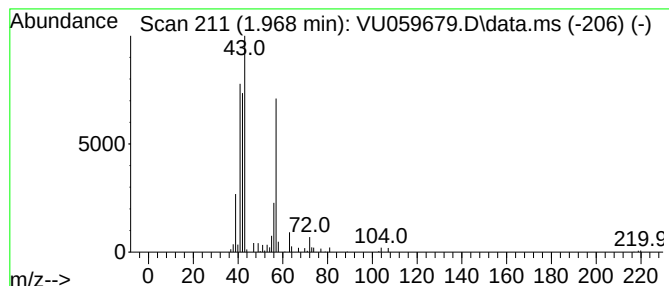
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.968	1.59 ug/L	104041	1,4-Difluorobenzene	6.242

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	64
2		Butane, 2-methyl-	72	C5H12	000078-78-4	56
3		2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	40
4		3-Buten-1-ol	72	C4H8O	000627-27-0	38
5		Pentane	72	C5H12	000109-66-0	36



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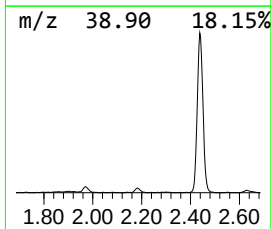
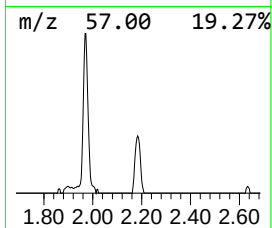
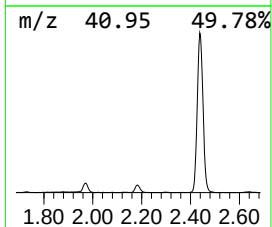
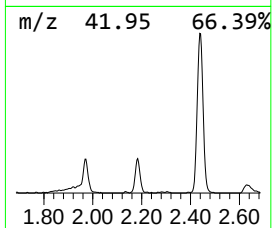
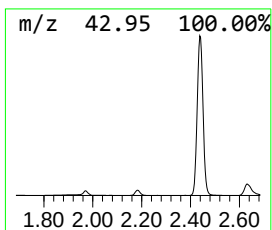
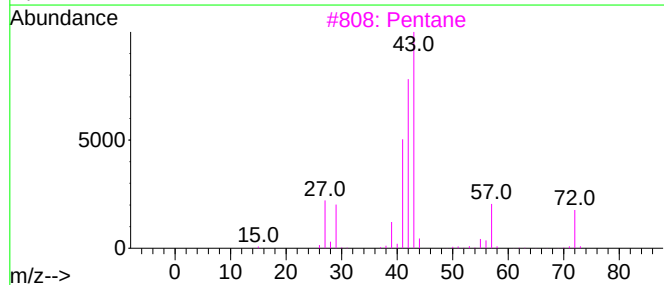
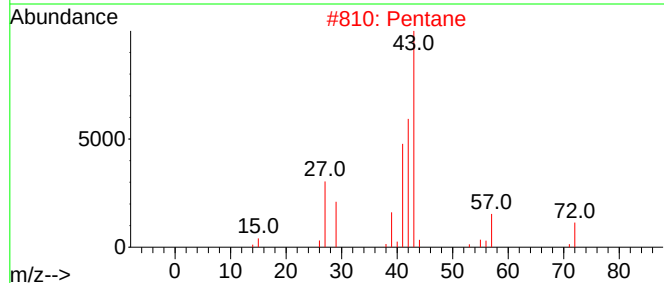
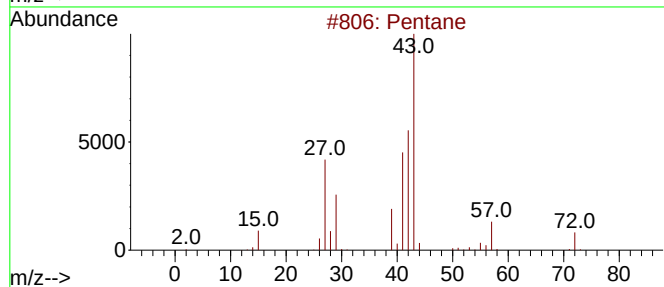
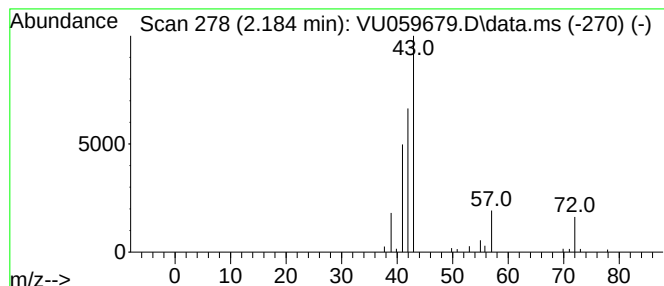
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.184	0.54 ug/L	35595	1,4-Difluorobenzene	6.242

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane		72	C5H12	000109-66-0	86
2	Pentane		72	C5H12	000109-66-0	86
3	Pentane		72	C5H12	000109-66-0	86
4	Pentane		72	C5H12	000109-66-0	86
5	Pentane		72	C5H12	000109-66-0	64



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MSVOA_U
ClientSampleId :
E1GN3DL

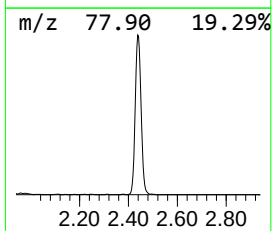
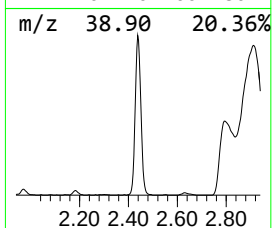
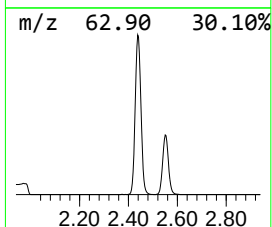
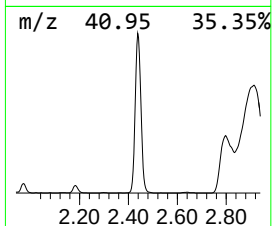
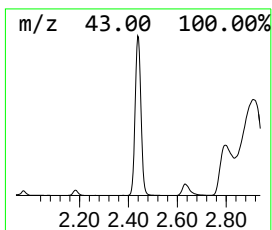
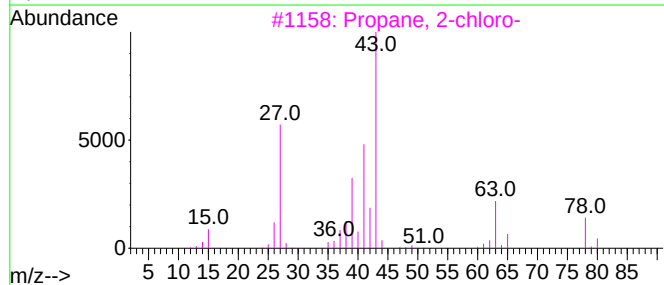
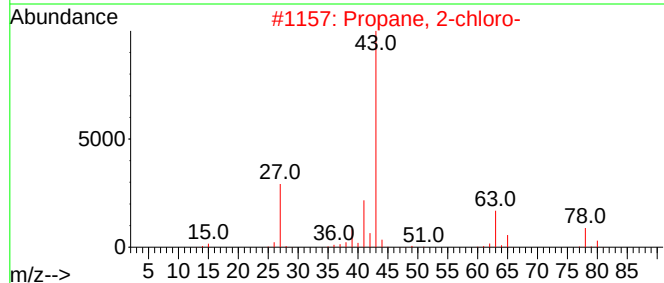
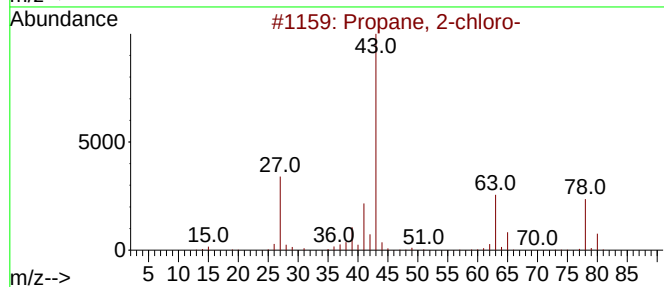
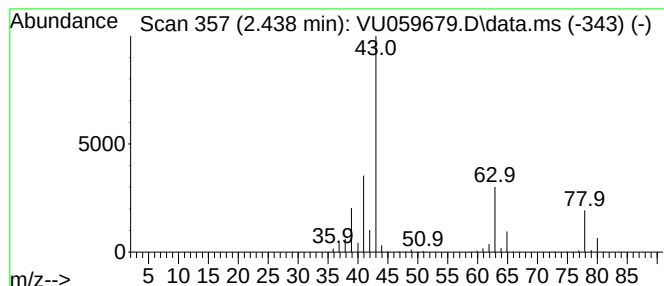
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Propane, 2-chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.438	17.28 ug/L	1130560	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-chloro-	78	C3H7Cl	000075-29-6	91
2			Propane, 2-chloro-	78	C3H7Cl	000075-29-6	64
3			Propane, 2-chloro-	78	C3H7Cl	000075-29-6	42
4			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
5			Acetyl chloride	78	C2H3ClO	000075-36-5	9



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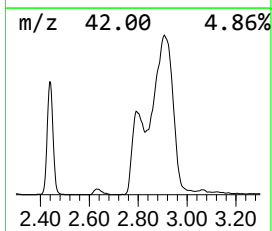
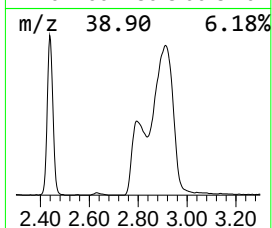
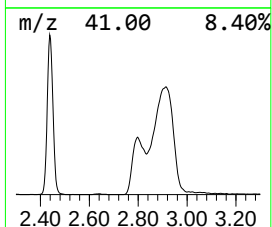
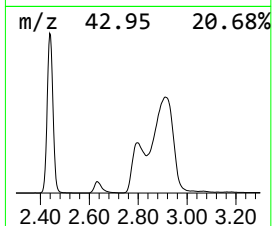
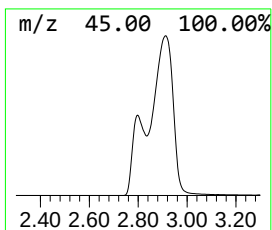
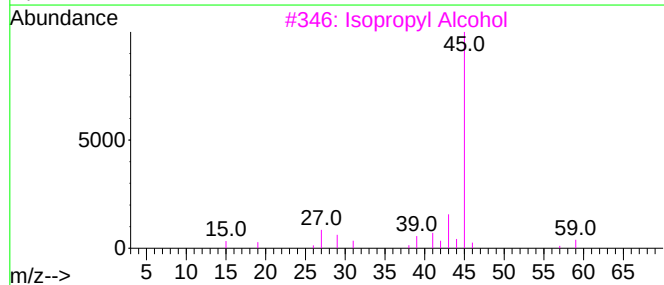
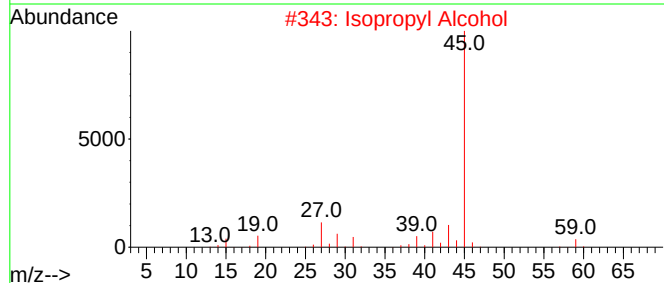
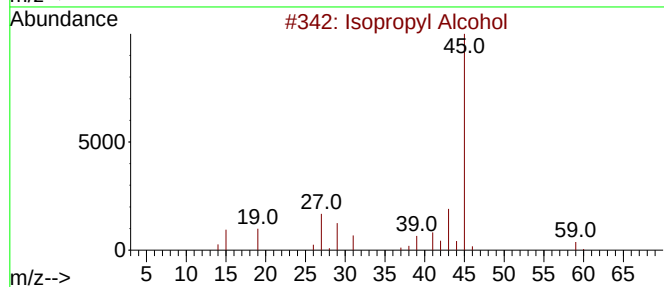
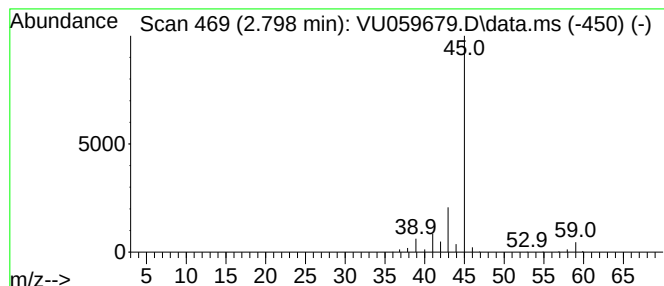
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.798	32.71 ug/L	2139920	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
5			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40



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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
Cyclopropanecar...	1.354	0.9	ug/L	56532	1	6.242	327105	5.0
(DEL) Alkane: S...	1.968	1.6	ug/L	104041	1	6.242	327105	5.0
(DEL) Alkane: S...	2.184	0.5	ug/L	35595	1	6.242	327105	5.0
Propane, 2-chloro-	2.438	17.3	ug/L	1130560	1	6.242	327105	5.0
Isopropyl Alcohol	2.798	32.7	ug/L	2139920	1	6.242	327105	5.0