

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012924\
 Data File : VU057724.D
 Acq On : 29 Jan 2024 18:09
 Operator : MD/SY
 Sample : P1239-11
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0FB5

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\SFAMUTR012324WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU057724.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.358	14	21	31	rBV	50354	51667	25.24%	2.572%
2	1.490	56	62	75	rBV	15313	16348	7.99%	0.814%
3	1.599	84	96	108	rVV	82594	100471	49.08%	5.002%
4	1.657	108	114	125	rVB	5334	5538	2.71%	0.276%
5	1.728	130	136	144	rVB	4495	4840	2.36%	0.241%
6	1.911	184	193	207	rVB	24299	33396	16.31%	1.663%
7	1.991	207	218	228	rBV	25928	35247	17.22%	1.755%
8	2.149	260	267	274	rBV2	4178	6094	2.98%	0.303%
9	2.200	274	283	297	rVB	31692	47078	23.00%	2.344%
10	2.313	310	318	327	rBV2	3816	6093	2.98%	0.303%
11	2.409	340	348	357	rVV2	2868	4417	2.16%	0.220%
12	2.464	358	365	373	rVB2	1637	2263	1.11%	0.113%
13	2.560	385	395	409	rVB	47051	75872	37.07%	3.777%
14	2.679	422	432	452	rVB3	3866	6879	3.36%	0.342%
15	2.975	509	524	532	rBV6	1649	3986	1.95%	0.198%
16	3.078	545	556	566	rVV3	4957	9483	4.63%	0.472%
17	3.129	566	572	584	rVB7	1359	2935	1.43%	0.146%
18	3.355	630	642	656	rBV3	5439	11760	5.75%	0.585%
19	3.692	737	747	761	rBV	4563	9988	4.88%	0.497%
20	3.863	793	800	809	rBV3	1731	3262	1.59%	0.162%
21	4.567	1011	1019	1028	rVV4	1619	3172	1.55%	0.158%
22	4.628	1028	1038	1073	rVV2	21227	60722	29.66%	3.023%
23	5.055	1157	1171	1193	rVB	39579	87428	42.71%	4.352%
24	5.451	1285	1294	1307	rVB7	1132	2344	1.15%	0.117%
25	5.586	1328	1336	1345	rVB2	1933	3533	1.73%	0.176%
26	5.718	1359	1377	1406	rBV2	78958	204697	100.00%	10.190%
27	6.242	1529	1540	1567	rBV	78557	150703	73.62%	7.502%
28	6.686	1666	1678	1697	rBV2	47428	91836	44.86%	4.572%
29	7.560	1940	1950	1968	rBV2	23785	42081	20.56%	2.095%
30	7.895	2041	2054	2070	rBV	102570	178847	87.37%	8.904%
31	8.178	2133	2142	2160	rVB	13202	22859	11.17%	1.138%
32	8.631	2273	2283	2316	rBV2	86366	175505	85.74%	8.737%
33	9.412	2515	2526	2551	rBV	103734	180129	88.00%	8.967%
34	10.750	2929	2942	2956	rBV	29964	47866	23.38%	2.383%
35	11.808	3260	3271	3289	rBV	106565	169342	82.73%	8.430%
36	12.058	3340	3349	3365	rBV4	3599	7441	3.64%	0.370%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Title : TRACE VOA SFAM1.0

37	12.187	3378	3389	3409	rVB	86831	140040	68.41%	6.972%
38	13.476	3783	3790	3797	rBV	1952	2562	1.25%	0.128%

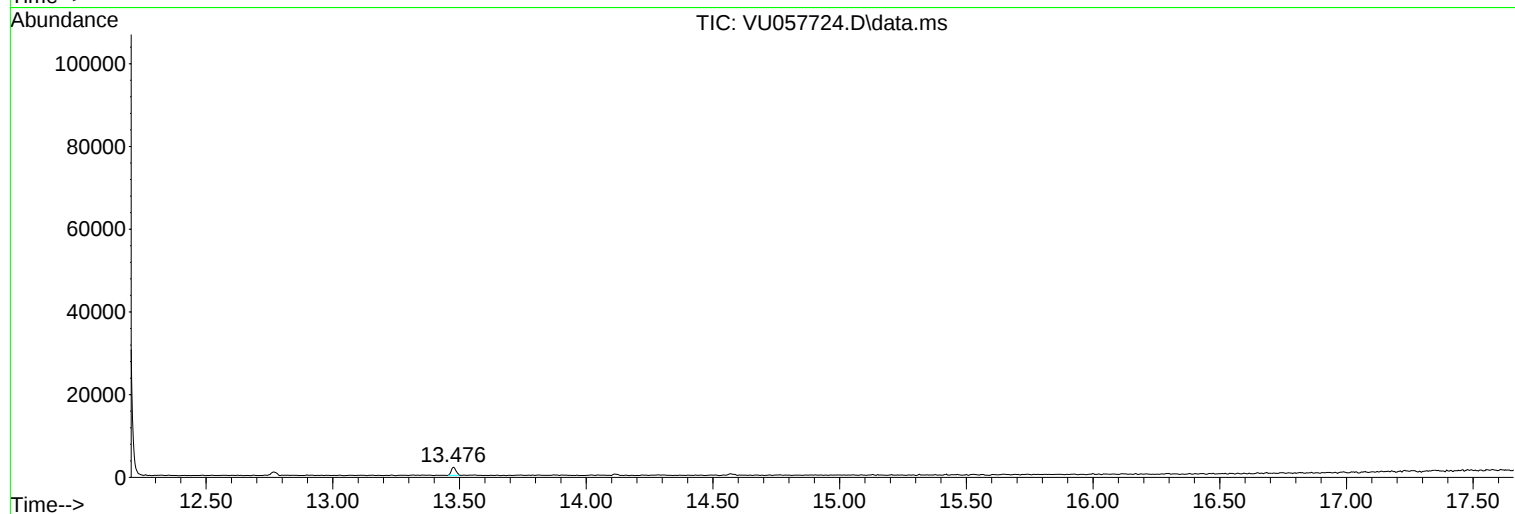
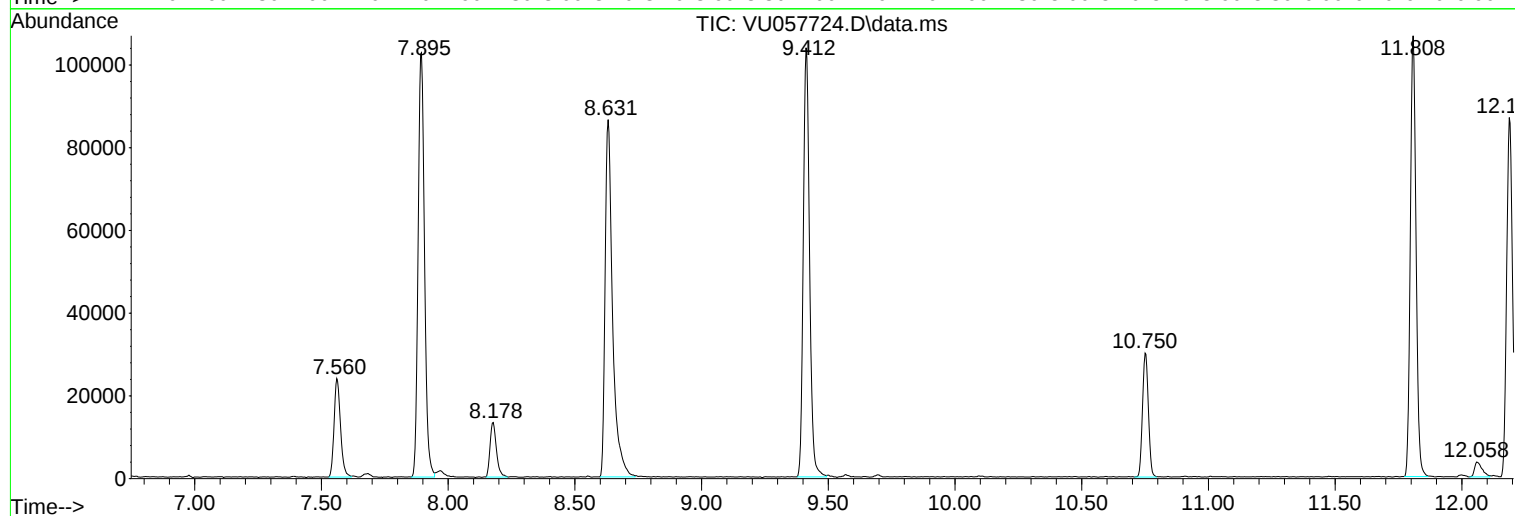
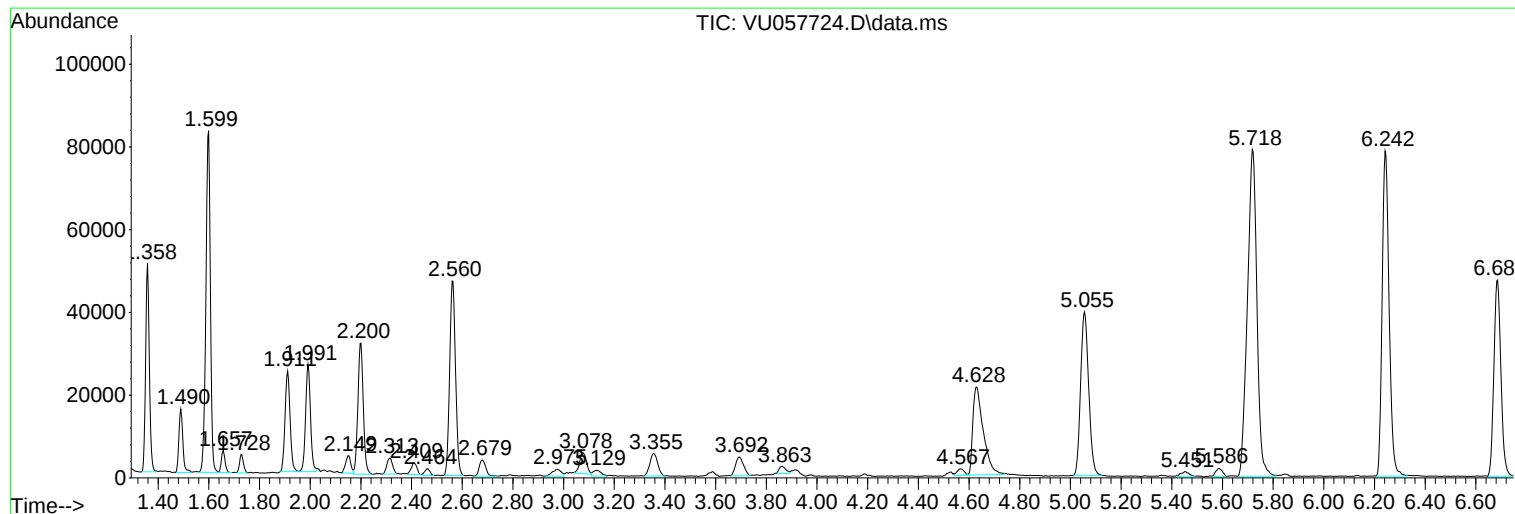
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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MSVOA_U
ClientSampleId :
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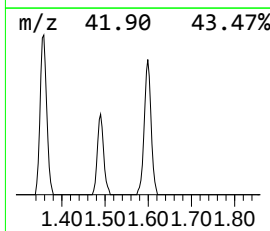
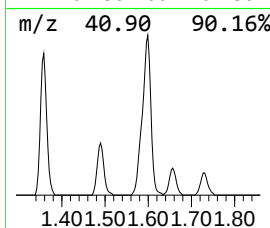
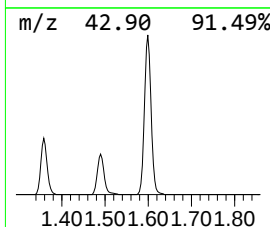
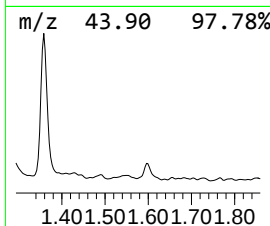
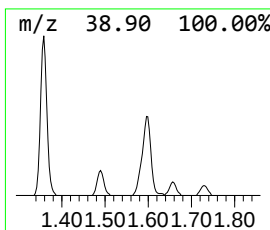
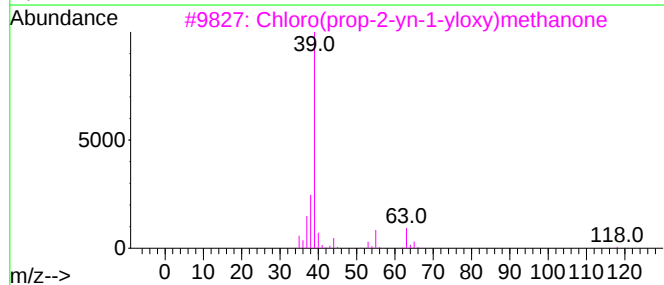
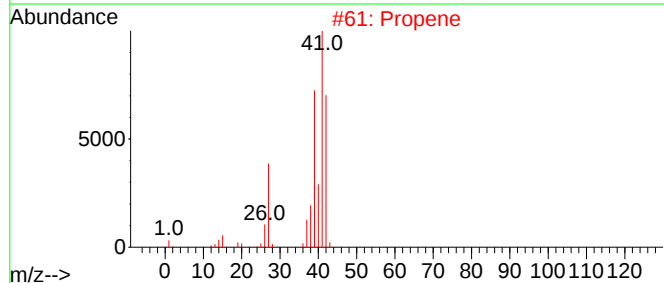
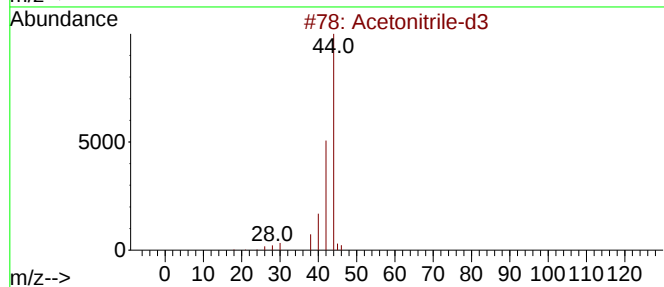
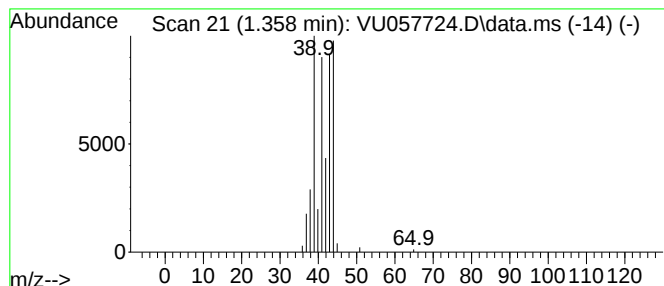
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.358	1.71 ug/L	51667	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetonitrile-d3	44	C2D3N	002206-26-0	9
2			Propene	42	C3H6	000115-07-1	9
3			Chloro(prop-2-yn-1-yloxy)methanone	118	C4H3ClO2	035718-08-2	9
4			Propane	44	C3H8	000074-98-6	5
5			Acetonitrile-d3	44	C2D3N	002206-26-0	4



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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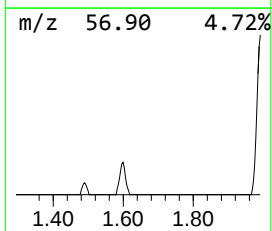
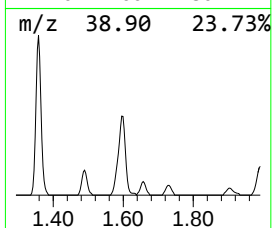
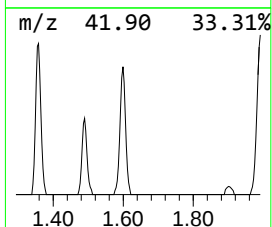
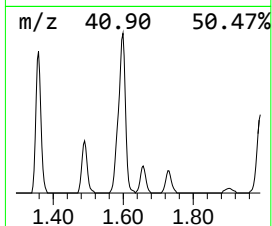
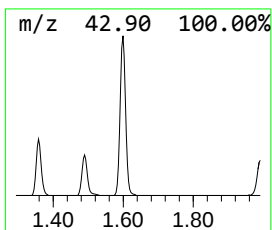
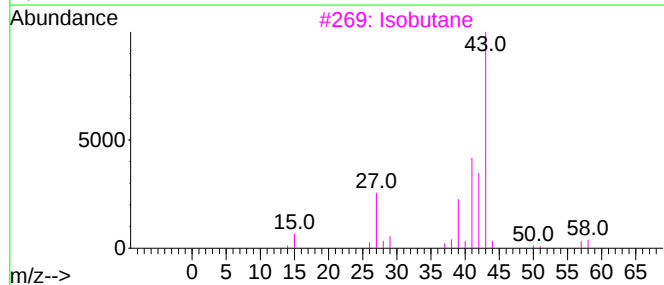
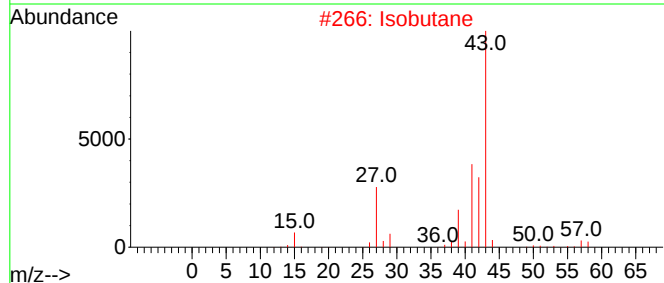
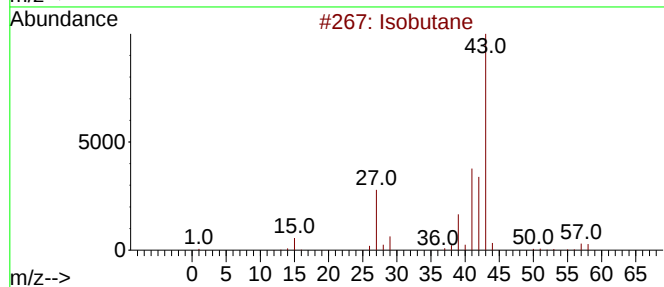
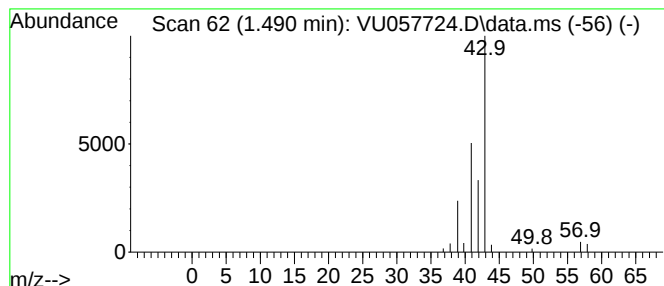
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.490	0.54 ug/L	16348	1,4-Difluorobenzene	6.242

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	78
2		Isobutane	58	C4H10	000075-28-5	72
3		Isobutane	58	C4H10	000075-28-5	72
4		Isobutane	58	C4H10	000075-28-5	72
5		Isobutane	58	C4H10	000075-28-5	9



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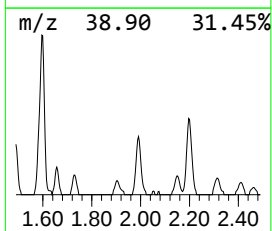
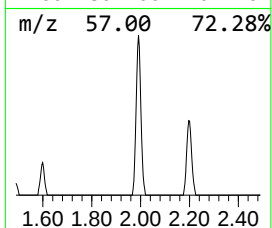
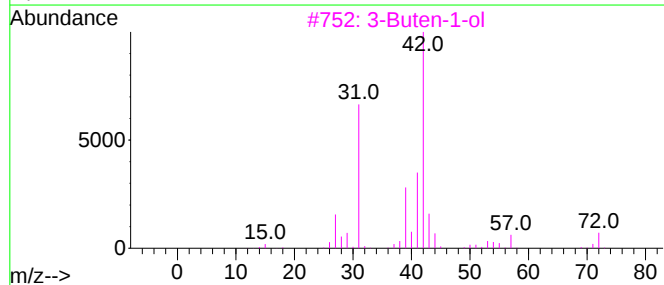
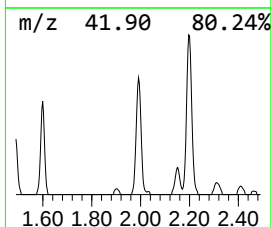
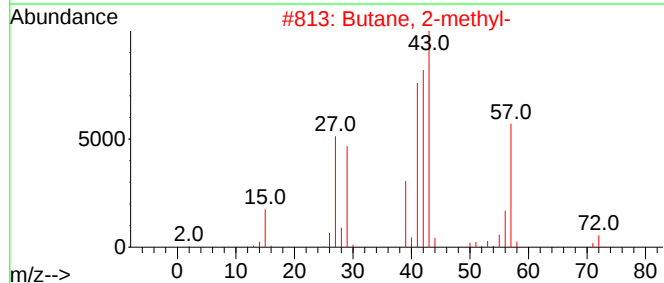
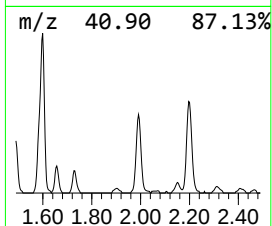
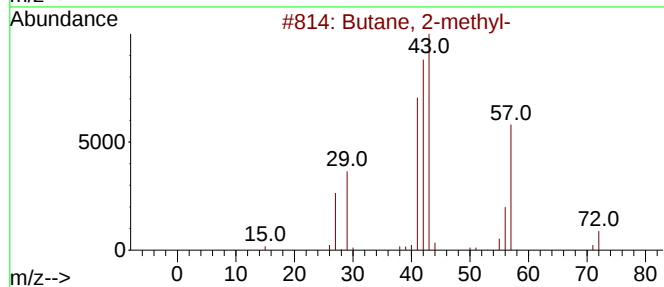
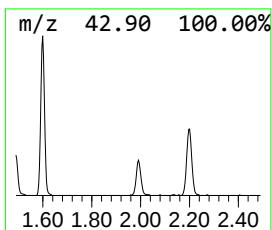
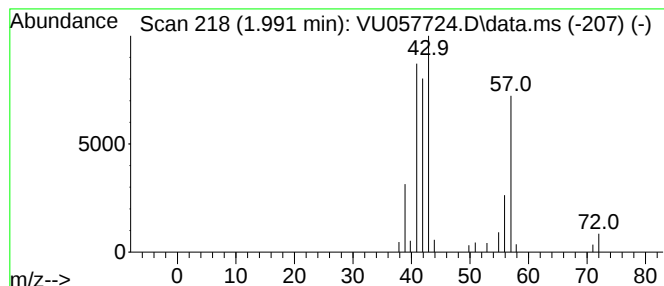
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.991	1.17 ug/L	35247	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	86
2	Butane, 2-methyl-			72	C5H12	000078-78-4	80
3	3-Buten-1-ol			72	C4H8O	000627-27-0	47
4	Oxirane, trimethyl-			86	C5H10O	005076-19-7	38
5	Pentane			72	C5H12	000109-66-0	33



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
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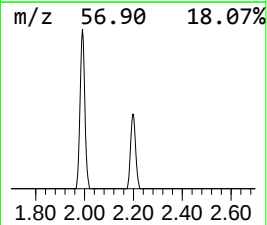
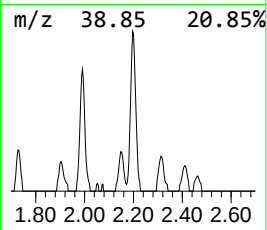
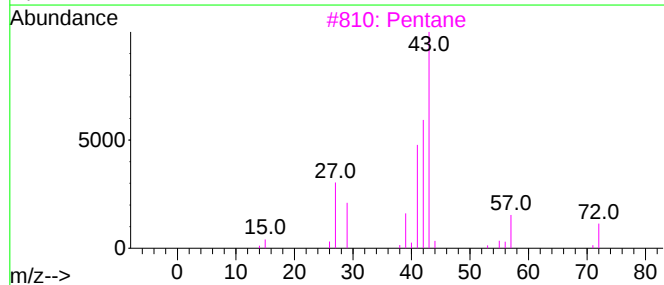
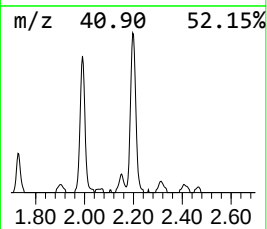
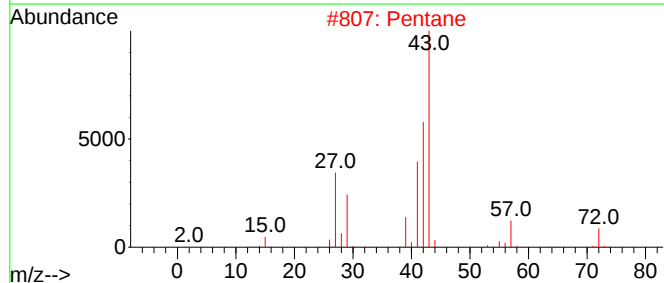
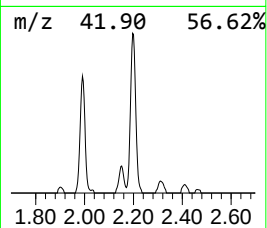
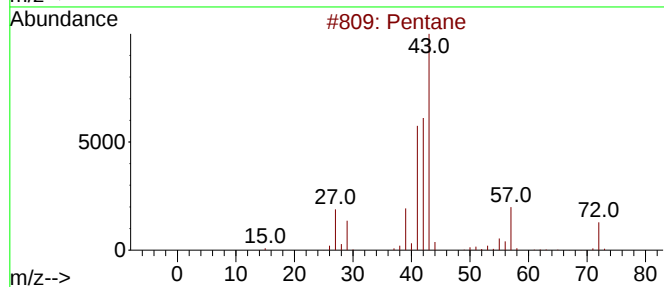
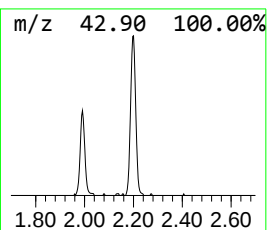
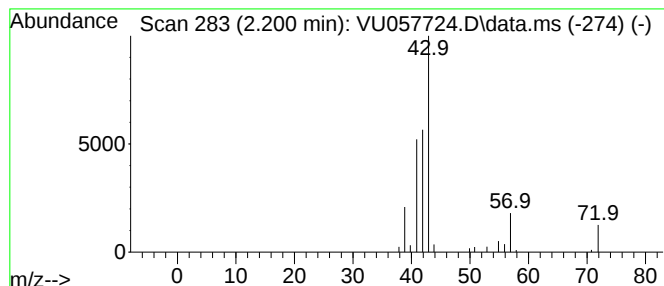
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.200	1.56 ug/L	47078	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	91
2	Pentane			72	C5H12	000109-66-0	90
3	Pentane			72	C5H12	000109-66-0	90
4	Pentane			72	C5H12	000109-66-0	90
5	Pentane			72	C5H12	000109-66-0	90



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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
unknown-01	1.358	1.7	ug/L	51667	1	6.242	150703	5.0
(DEL) Alkane: S...	1.490	0.5	ug/L	16348	1	6.242	150703	5.0
(DEL) Alkane: S...	1.991	1.2	ug/L	35247	1	6.242	150703	5.0
(DEL) Alkane: S...	2.200	1.6	ug/L	47078	1	6.242	150703	5.0