

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121223\
 Data File : VU056792.D
 Acq On : 12 Dec 2023 17:45
 Operator : MD/SY
 Sample : 05664-12
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E0Y70

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\SFAMUTR121123WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU056792.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	41	rVB2	141607	175512	17.14%	1.803%
2	1.441	42	47	54	rVB	10932	11322	1.11%	0.116%
3	1.486	54	61	67	rBV	74963	74552	7.28%	0.766%
4	1.515	67	70	80	rVB3	9916	11422	1.12%	0.117%
5	1.596	85	95	108	rBV	200943	243746	23.81%	2.504%
6	1.686	115	123	133	rBV	101807	129825	12.68%	1.334%
7	1.875	177	182	186	rBV	9241	10722	1.05%	0.110%
8	1.911	186	193	208	rVB	97739	130053	12.70%	1.336%
9	1.991	209	218	231	rVB2	52640	73519	7.18%	0.755%
10	2.200	274	283	303	rVB3	38410	61179	5.98%	0.628%
11	2.564	375	396	410	rBV2	211788	383318	37.44%	3.937%
12	2.637	410	419	438	rVB	24604	61008	5.96%	0.627%
13	2.789	454	466	481	rBV	51700	90540	8.84%	0.930%
14	3.081	549	557	566	rVB2	13446	23504	2.30%	0.241%
15	3.178	581	587	606	rVB2	6674	13844	1.35%	0.142%
16	3.358	629	643	653	rBV3	9055	20569	2.01%	0.211%
17	3.576	699	711	727	rBV3	15079	37952	3.71%	0.390%
18	3.692	732	747	759	rBV5	13784	32762	3.20%	0.337%
19	4.448	968	982	994	rBV3	15373	37639	3.68%	0.387%
20	4.531	999	1008	1019	rVB4	8177	18927	1.85%	0.194%
21	4.625	1025	1037	1061	rBV2	127933	386288	37.73%	3.968%
22	5.055	1156	1171	1191	rBV	199802	441755	43.15%	4.538%
23	5.377	1253	1271	1284	rBV9	9486	22918	2.24%	0.235%
24	5.718	1357	1377	1410	rBV2	378708	1023842	100.00%	10.517%
25	5.975	1447	1457	1467	rBV8	6133	12492	1.22%	0.128%
26	6.133	1496	1506	1521	rBV6	9969	22927	2.24%	0.236%
27	6.245	1527	1541	1569	rBV	283014	558171	54.52%	5.733%
28	6.538	1621	1632	1643	rBV5	5260	10389	1.01%	0.107%
29	6.682	1664	1677	1692	rBV	234153	461458	45.07%	4.740%
30	6.759	1692	1701	1712	rVB5	16752	35054	3.42%	0.360%
31	6.878	1728	1738	1759	rBV4	15610	36437	3.56%	0.374%
32	6.968	1759	1766	1778	rVB8	7192	14242	1.39%	0.146%
33	7.560	1938	1950	1971	rBV	112464	205846	20.11%	2.114%
34	7.792	2013	2022	2033	rBV4	12347	24086	2.35%	0.247%
35	7.894	2033	2054	2068	rVV	457972	817691	79.86%	8.399%
36	7.965	2068	2076	2089	rVB	74396	133315	13.02%	1.369%

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37	8.174	2131	2141	2155	rBV	66391	114778	11.21%	1.179%
38	8.631	2271	2283	2320	rBV2	472341	970584	94.80%	9.970%
39	8.785	2323	2331	2346	rVV3	27753	56177	5.49%	0.577%
40	9.412	2509	2526	2544	rBV	397827	700773	68.45%	7.198%
41	9.570	2564	2575	2590	rBV	34700	61151	5.97%	0.628%
42	9.692	2599	2613	2626	rBV	28598	56125	5.48%	0.577%
43	10.113	2730	2744	2765	rBV4	28141	73225	7.15%	0.752%
44	10.345	2802	2816	2838	rVB6	20064	41046	4.01%	0.422%
45	10.750	2930	2942	2960	rBV	172031	274765	26.84%	2.822%
46	10.898	2975	2988	3004	rVB4	6045	13906	1.36%	0.143%
47	10.997	3010	3019	3024	rBV2	8707	13713	1.34%	0.141%
48	11.463	3153	3164	3175	rBV2	23582	38019	3.71%	0.391%
49	11.685	3224	3233	3246	rBV5	18788	34386	3.36%	0.353%
50	11.808	3259	3271	3290	rBV	386126	641825	62.69%	6.593%
51	11.891	3290	3297	3307	rVB3	10059	15307	1.50%	0.157%
52	12.065	3340	3351	3369	rBV10	8544	25526	2.49%	0.262%
53	12.187	3377	3389	3410	rBV	409357	682974	66.71%	7.015%
54	12.885	3597	3606	3618	rBV7	12005	20536	2.01%	0.211%
55	12.971	3623	3633	3641	rBV3	7154	11029	1.08%	0.113%
56	13.444	3770	3780	3792	rVB6	9903	16366	1.60%	0.168%
57	14.087	3973	3980	3998	rVB	12736	24283	2.37%	0.249%

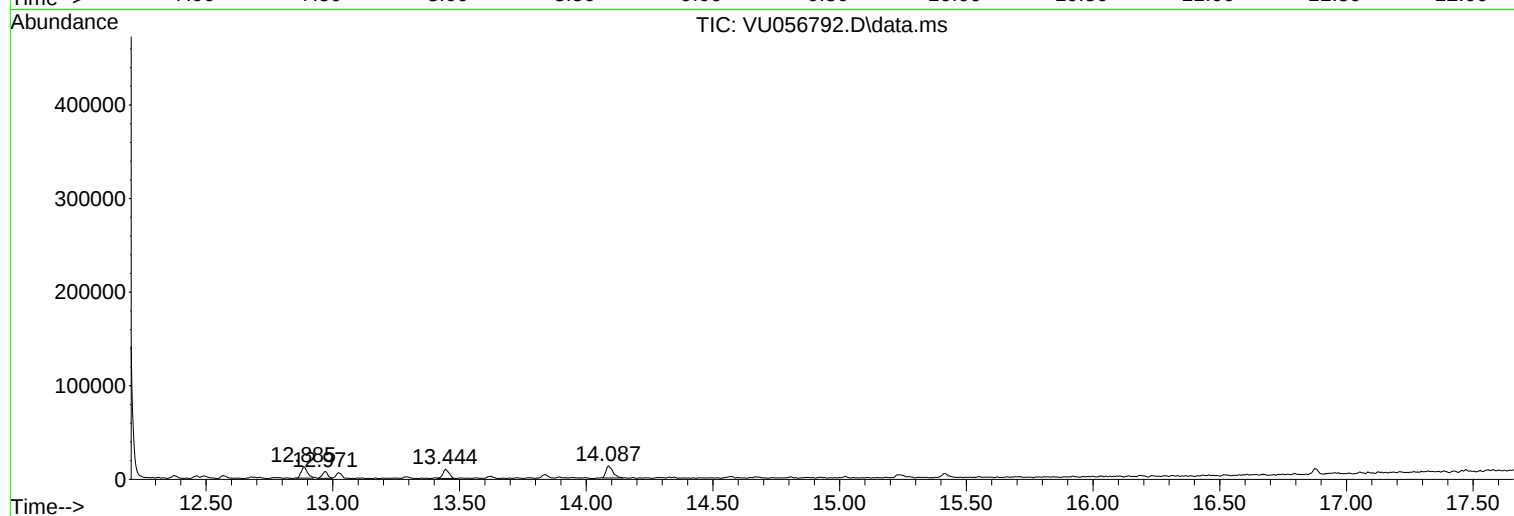
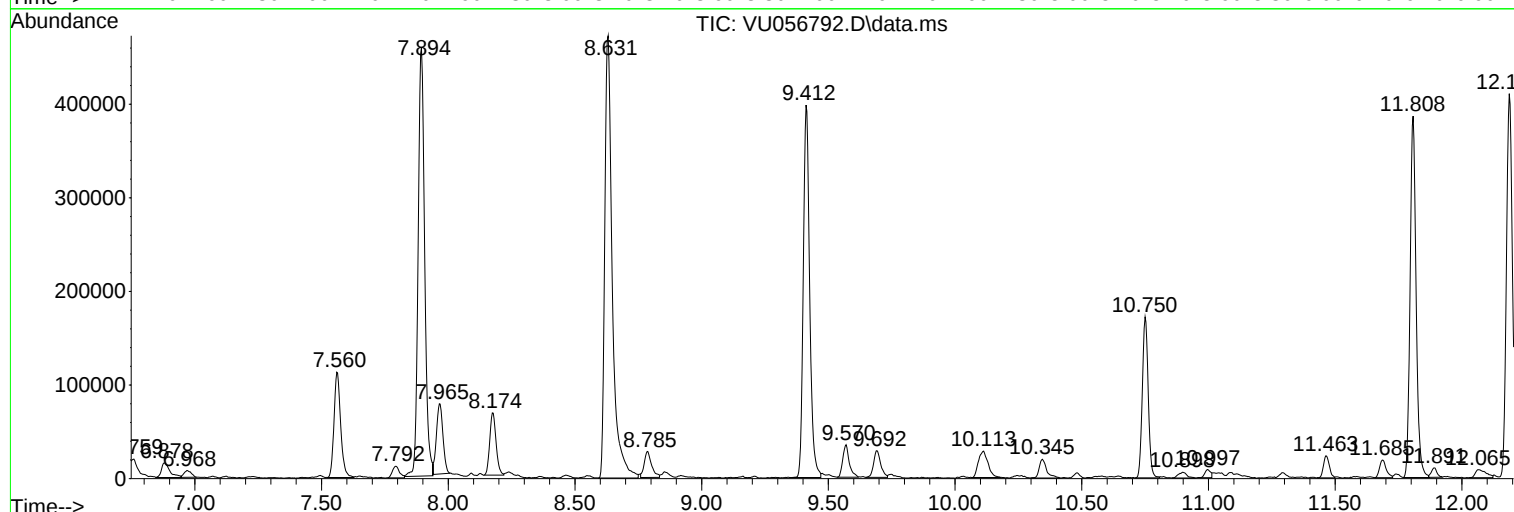
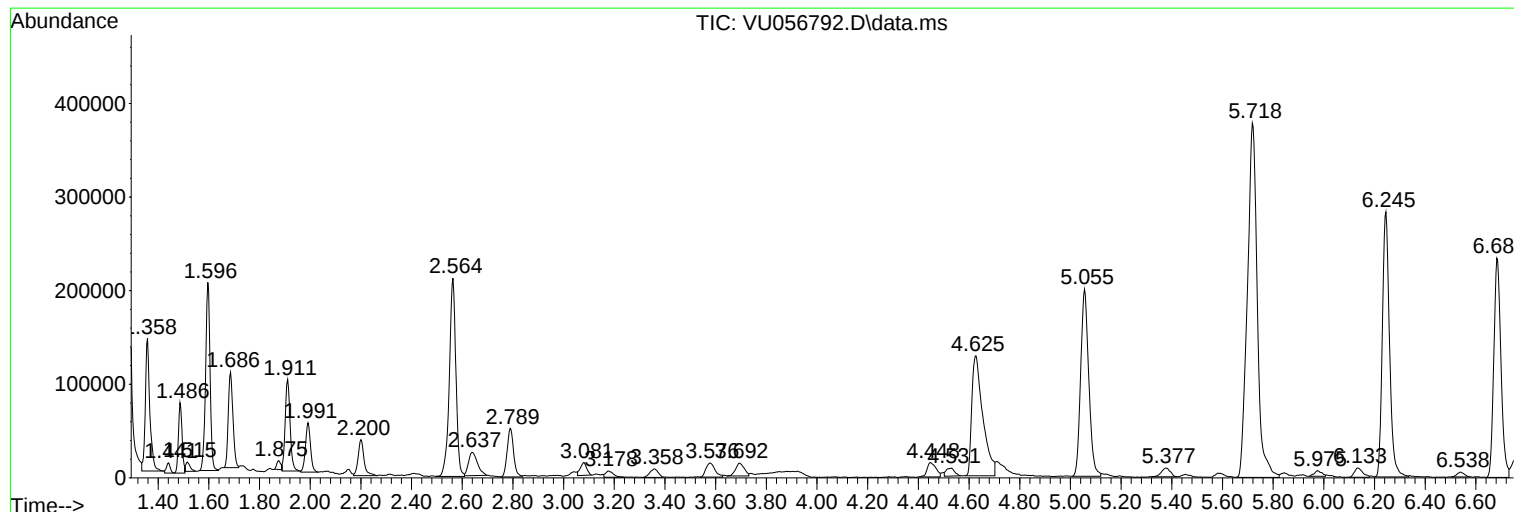
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Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
MSVOA_U
ClientSampleId :
E0Y70

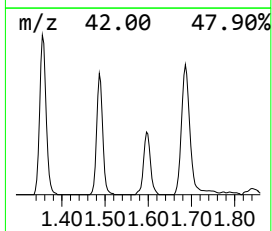
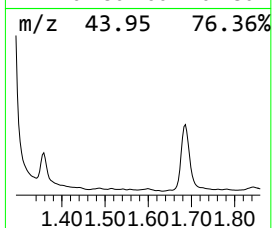
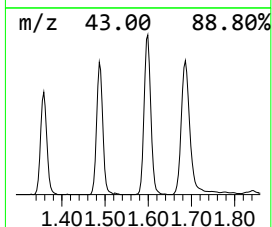
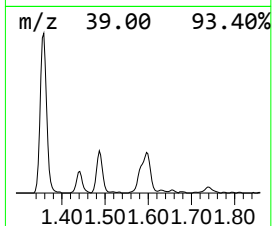
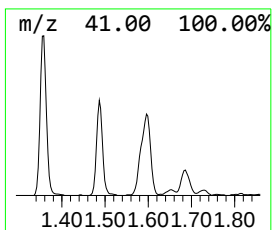
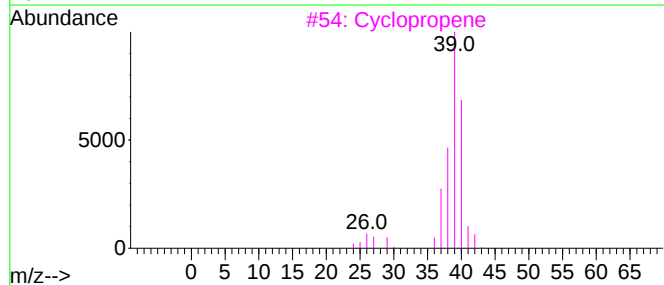
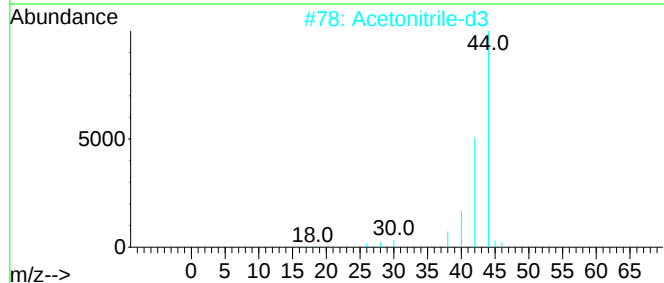
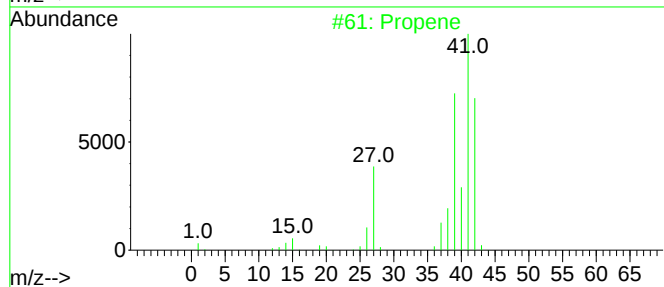
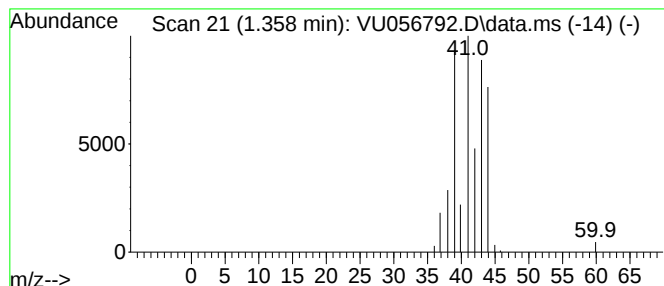
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Quant Title : TRACE VOA SFAM1.0

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.
1.358	1.57 ug/L	175512	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	9
2			Acetonitrile-d3	44	C2D3N	002206-26-0	7
3			Cyclopropene	40	C3H4	002781-85-3	4
4			Propane	44	C3H8	000074-98-6	4
5			Propane	44	C3H8	000074-98-6	4



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Instrument :
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ClientSampleId :
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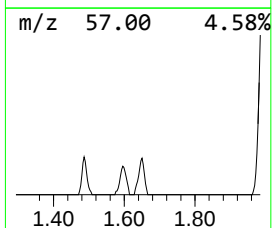
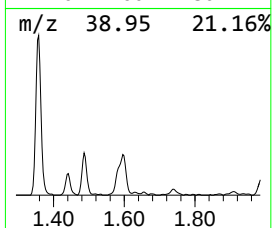
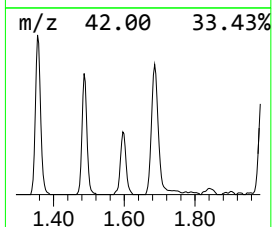
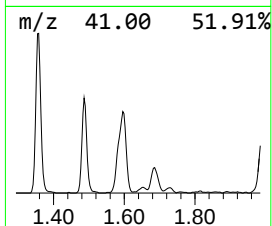
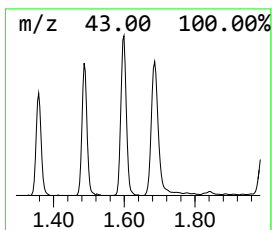
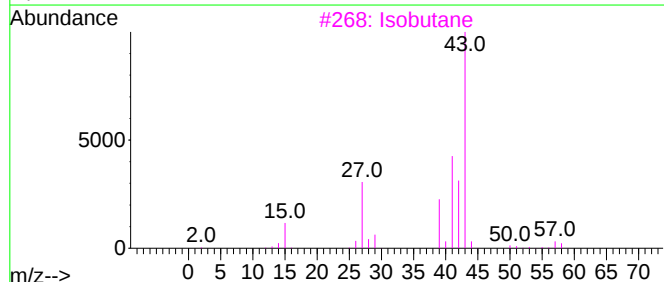
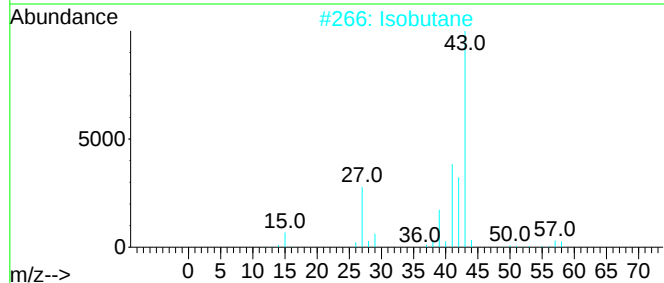
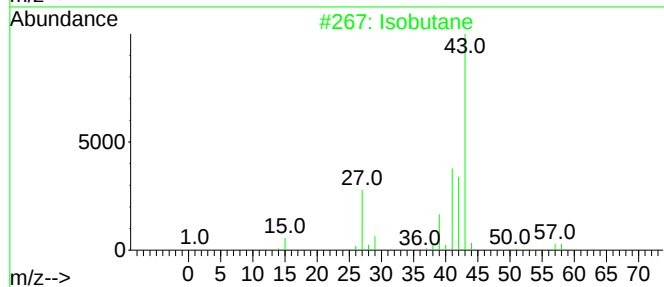
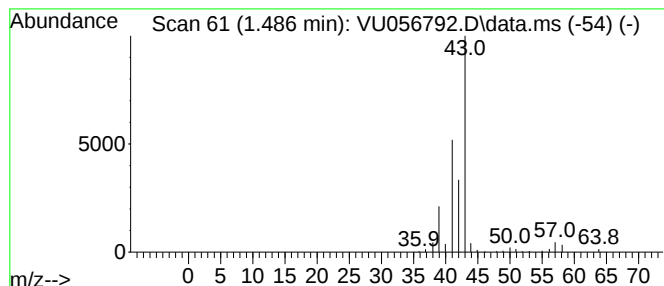
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.486	0.67 ug/L	74552	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	80
2		Isobutane	58	C4H10	000075-28-5	80
3		Isobutane	58	C4H10	000075-28-5	72
4		Isobutane	58	C4H10	000075-28-5	72
5		Isobutane	58	C4H10	000075-28-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121223\
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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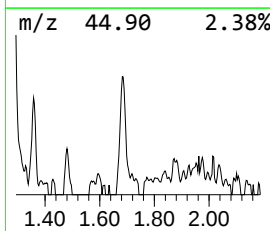
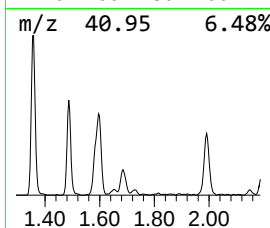
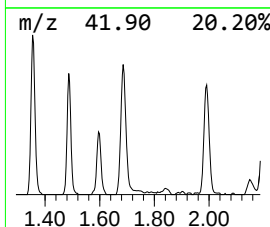
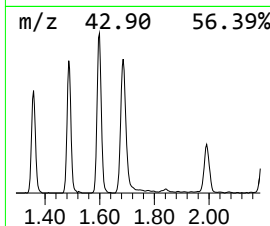
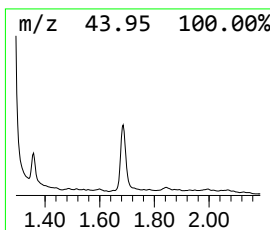
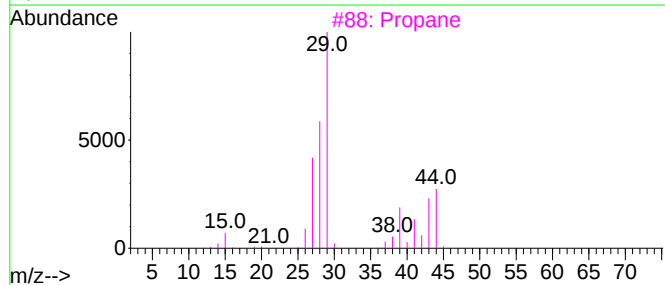
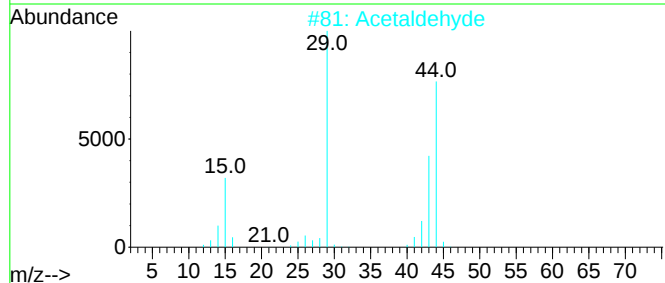
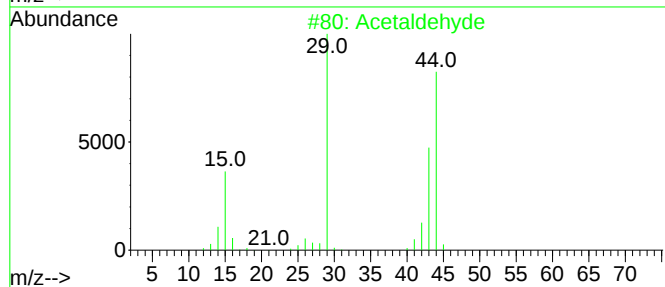
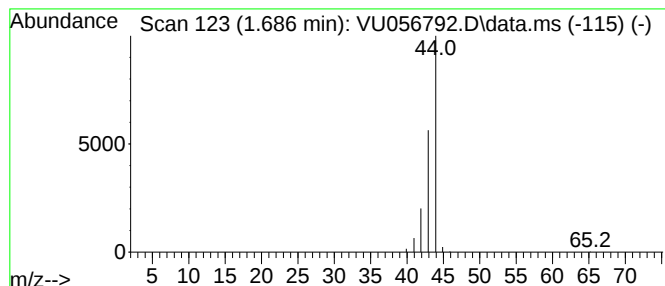
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.686	1.16 ug/L	129825	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	9
2			Acetaldehyde	44	C2H4O	000075-07-0	9
3			Propane	44	C3H8	000074-98-6	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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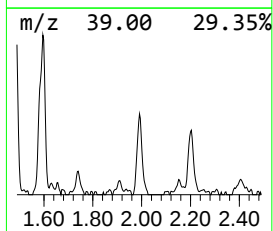
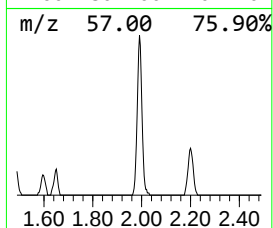
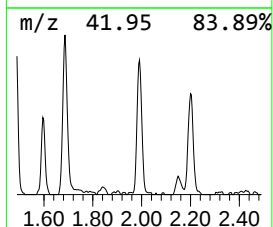
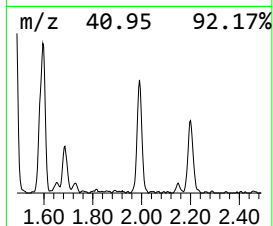
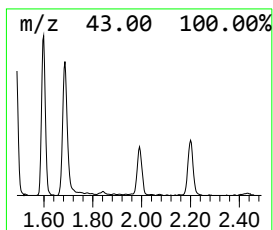
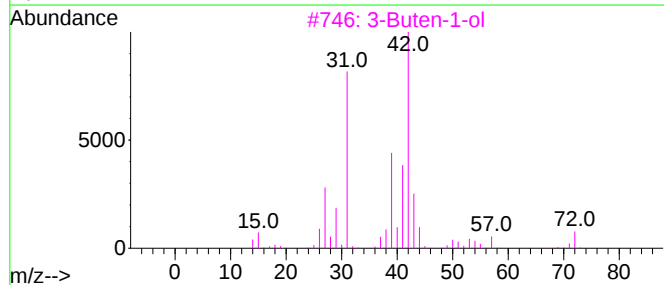
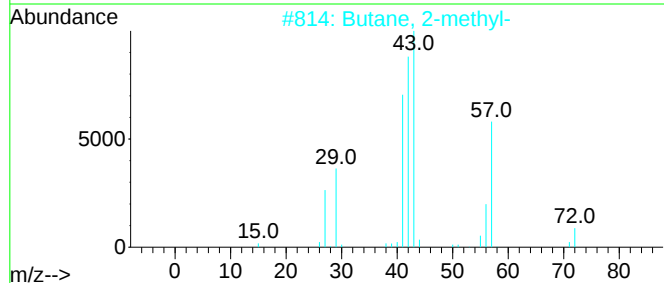
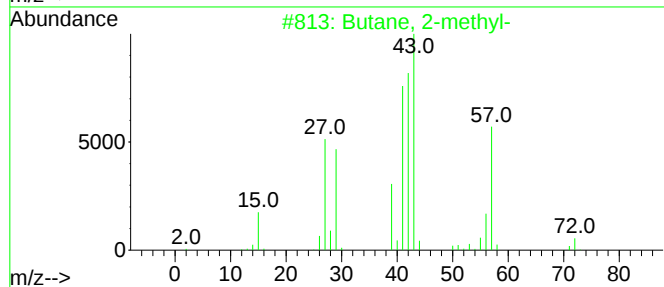
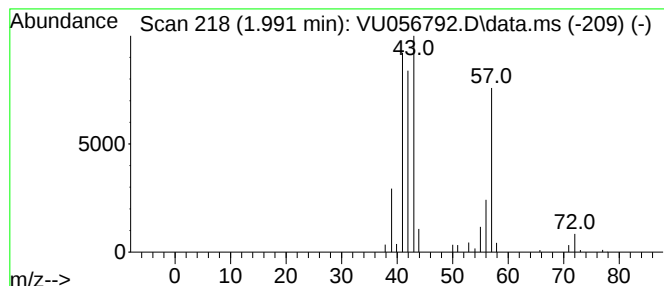
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.991	0.66 ug/L	73519	1,4-Difluorobenzene	6.245

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	37
4	Pentane			72	C5H12	000109-66-0	33
5	3-Buten-1-ol			72	C4H8O	000627-27-0	28



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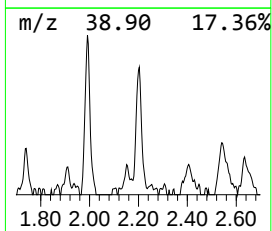
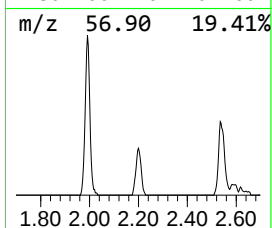
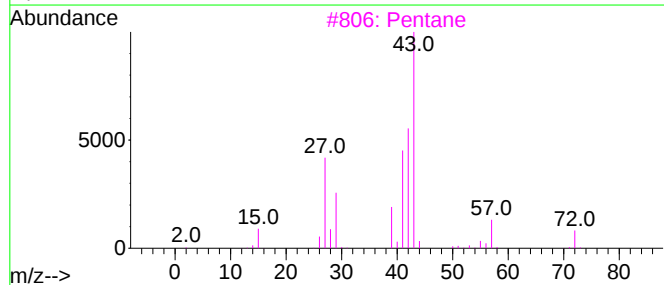
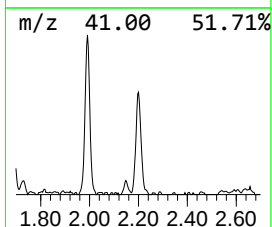
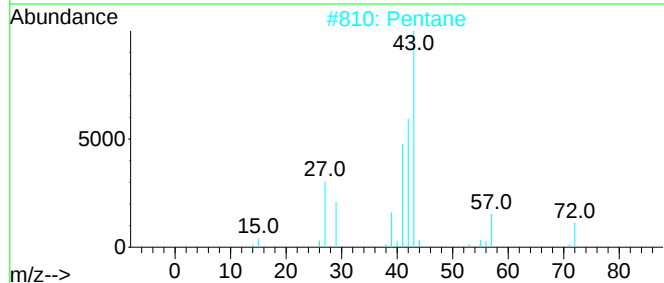
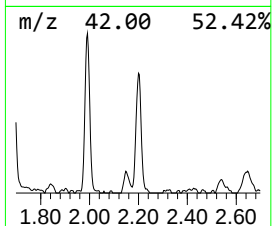
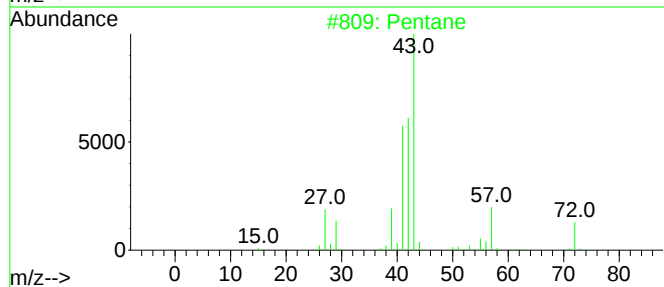
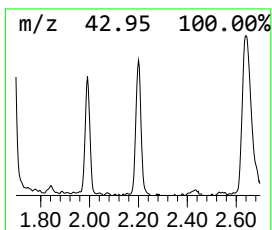
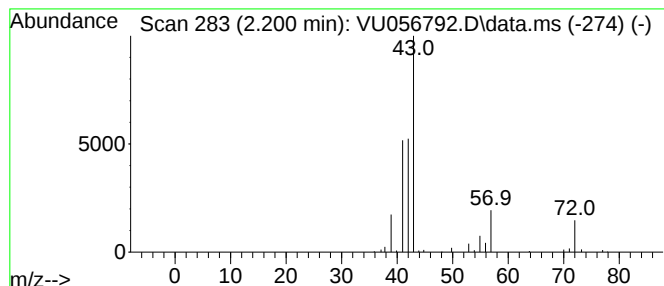
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.200	0.55 ug/L	61179	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	91
2	Pentane			72	C5H12	000109-66-0	86
3	Pentane			72	C5H12	000109-66-0	78
4	Pentane			72	C5H12	000109-66-0	72
5	Pentane			72	C5H12	000109-66-0	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121223\
Data File : VU056792.D
Acq On : 12 Dec 2023 17:45
Operator : MD/SY
Sample : 05664-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0Y70

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
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
(DEL) Alkane: S...	1.358	1.6	ug/L	175512	1	6.245	558171	5.0
(DEL) Alkane: S...	1.486	0.7	ug/L	74552	1	6.245	558171	5.0
unknown-01	1.686	1.2	ug/L	129825	1	6.245	558171	5.0
(DEL) Alkane: S...	1.991	0.7	ug/L	73519	1	6.245	558171	5.0
(DEL) Alkane: S...	2.200	0.6	ug/L	61179	1	6.245	558171	5.0