

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121523\
 Data File : VU056914.D
 Acq On : 16 Dec 2023 05:43
 Operator : MD/SY
 Sample : 05771-07
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 50 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E0YA4

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: VU056914.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	13	21	38	rVB	391810	392031	42.49%	4.332%
2	1.490	54	62	82	rBV	245809	263694	28.58%	2.914%
3	1.599	87	96	106	rBV2	365522	403959	43.78%	4.464%
4	1.908	185	192	208	rVB	70230	96391	10.45%	1.065%
5	1.991	208	218	234	rVB	159319	224503	24.33%	2.481%
6	2.200	274	283	302	rVB	100029	146381	15.87%	1.617%
7	2.563	384	396	412	rBV	135594	226441	24.54%	2.502%
8	3.046	532	546	547	rBV7	9442	15314	1.66%	0.169%
9	3.078	549	556	566	rVV3	24923	47345	5.13%	0.523%
10	3.129	566	572	583	rVB2	11100	20426	2.21%	0.226%
11	3.354	629	642	659	rBV4	16639	38667	4.19%	0.427%
12	3.692	727	747	765	rBV2	21264	53239	5.77%	0.588%
13	4.528	991	1007	1023	rBV3	28760	69316	7.51%	0.766%
14	4.621	1023	1036	1066	rBV	128144	374090	40.54%	4.133%
15	5.055	1155	1171	1192	rBV	157354	359406	38.95%	3.971%
16	5.380	1258	1272	1288	rBV5	28357	65741	7.13%	0.726%
17	5.589	1325	1337	1346	rBV4	5663	12190	1.32%	0.135%
18	5.721	1358	1378	1391	rBV2	284294	769133	83.36%	8.498%
19	5.985	1450	1460	1470	rVB7	8068	15767	1.71%	0.174%
20	6.132	1497	1506	1516	rBV5	5934	11431	1.24%	0.126%
21	6.245	1528	1541	1572	rBV	257066	514293	55.74%	5.683%
22	6.538	1620	1632	1656	rBV2	84001	166679	18.07%	1.842%
23	6.685	1661	1678	1691	rBV	192581	376689	40.83%	4.162%
24	6.756	1692	1700	1720	rVB5	39074	84979	9.21%	0.939%
25	7.563	1939	1951	1973	rBV	77693	145877	15.81%	1.612%
26	7.894	2042	2054	2067	rVV	297406	535165	58.00%	5.913%
27	7.965	2067	2076	2104	rVB	157013	289874	31.42%	3.203%
28	8.177	2132	2142	2155	rBV	49783	87986	9.54%	0.972%
29	8.547	2246	2257	2269	rVB10	6806	12369	1.34%	0.137%
30	8.631	2269	2283	2311	rBV2	465195	922662	100.00%	10.195%
31	8.862	2344	2355	2364	rVB9	5504	9974	1.08%	0.110%
32	9.412	2511	2526	2545	rBV	366264	652551	70.72%	7.210%
33	9.570	2564	2575	2593	rBV2	36423	67553	7.32%	0.746%
34	9.689	2601	2612	2629	rBV2	52450	95180	10.32%	1.052%
35	10.097	2730	2739	2760	rVB2	22820	42274	4.58%	0.467%
36	10.750	2931	2942	2959	rBV	152876	250933	27.20%	2.773%

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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\SFAMUTR121123WMA.M
Title : TRACE VOA SFAM1.0

37	10.997	3012	3019	3037	rVB4	7661	15214	1.65%	0.168%
38	11.087	3037	3047	3064	rVB6	6383	12262	1.33%	0.135%
39	11.467	3156	3165	3177	rVB2	16873	26919	2.92%	0.297%
40	11.807	3259	3271	3290	rBV	340008	573826	62.19%	6.340%
41	11.891	3290	3297	3306	rVB4	7626	12583	1.36%	0.139%
42	12.068	3342	3352	3358	rBV4	9606	17403	1.89%	0.192%
43	12.187	3377	3389	3408	rBV	308763	531521	57.61%	5.873%

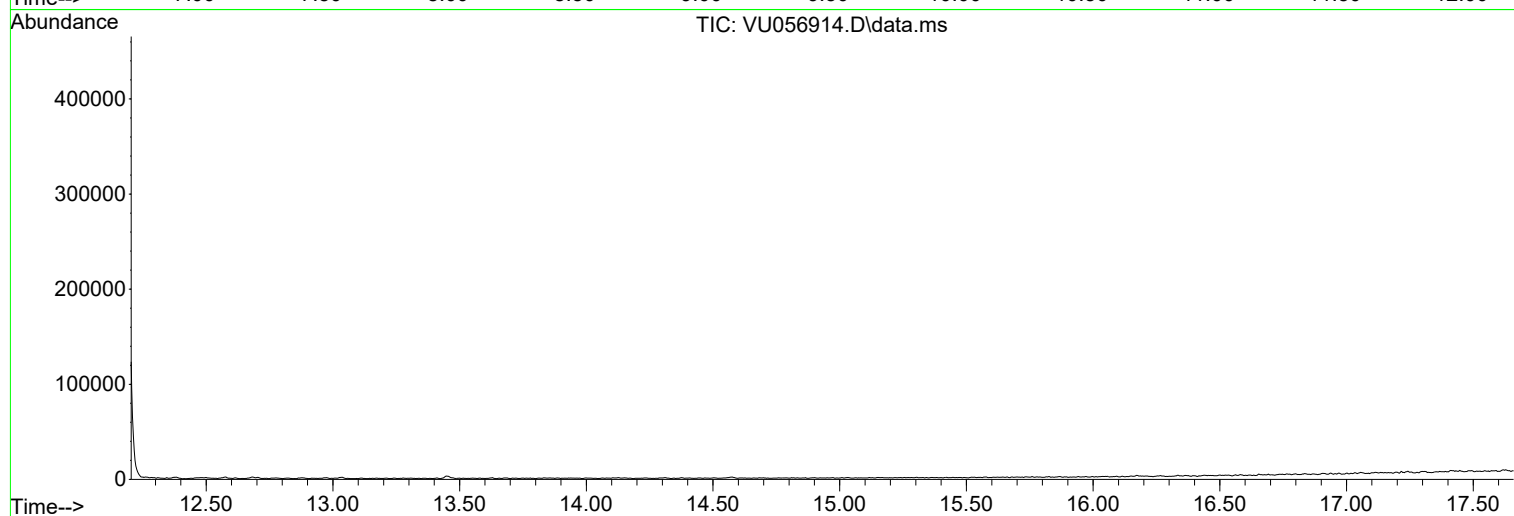
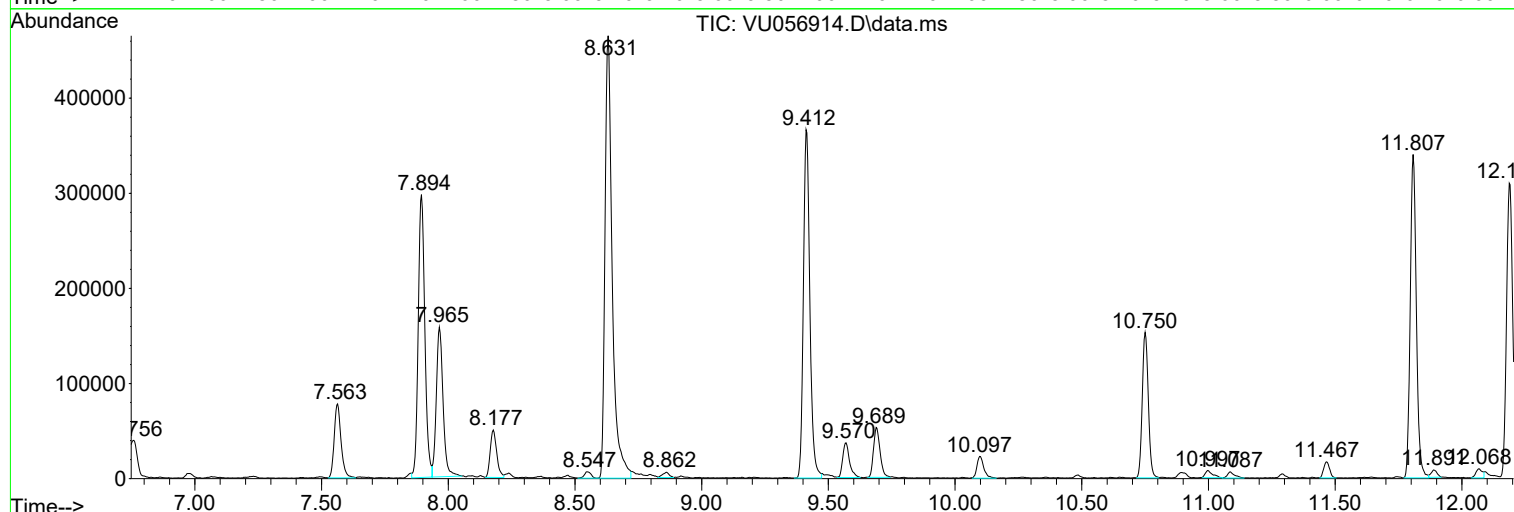
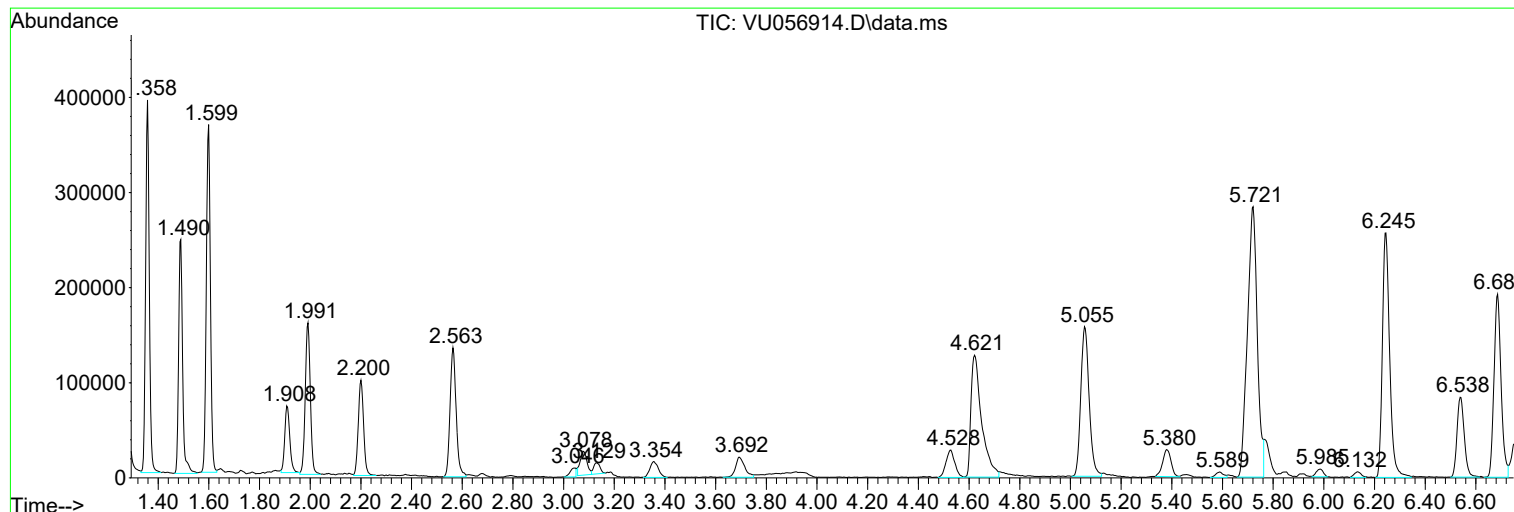
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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ClientSampleId :
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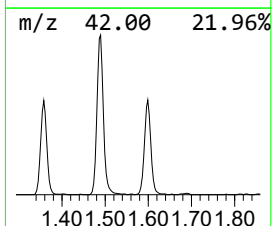
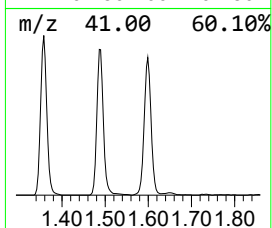
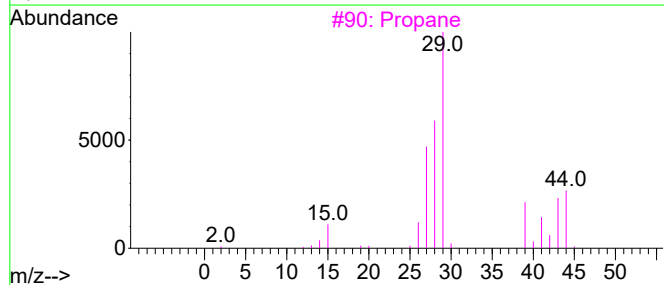
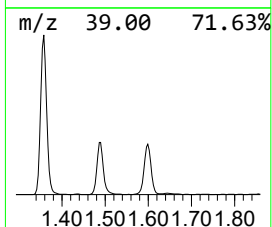
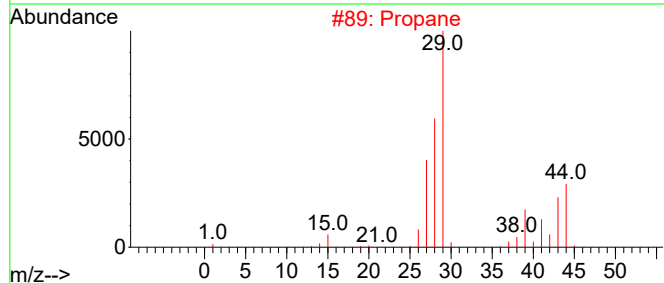
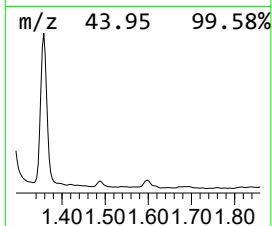
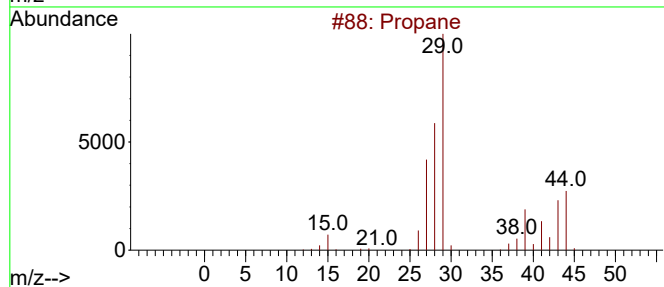
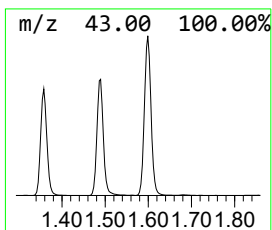
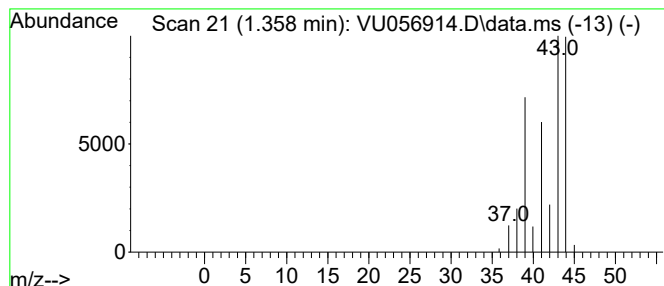
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.358	3.81 ug/L	392031	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane			44	C3H8	000074-98-6	90
2	Propane			44	C3H8	000074-98-6	83
3	Propane			44	C3H8	000074-98-6	9
4	Propene			42	C3H6	000115-07-1	9
5	Acetaldehyde			44	C2H4O	000075-07-0	5



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0YA4

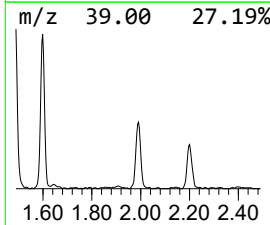
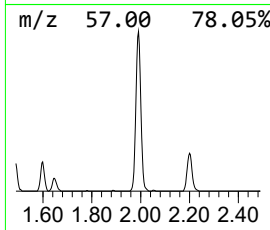
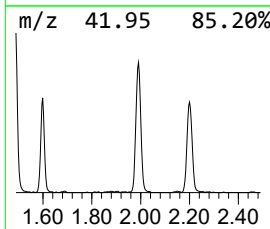
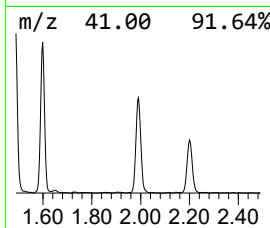
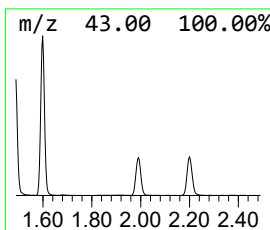
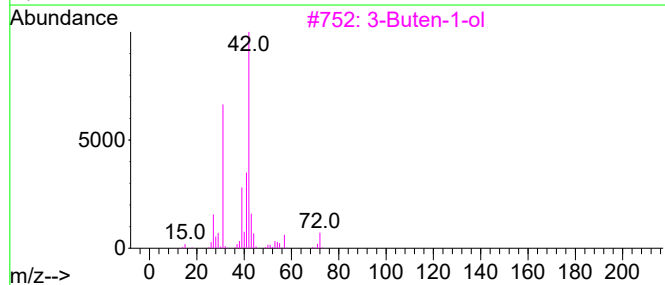
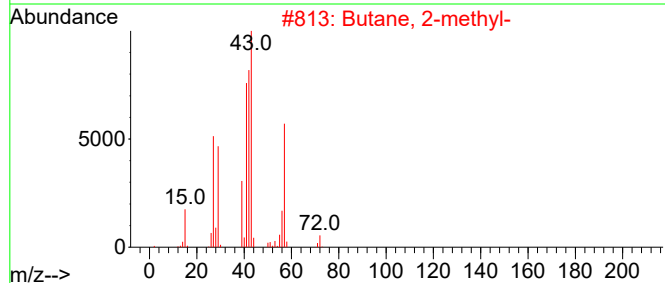
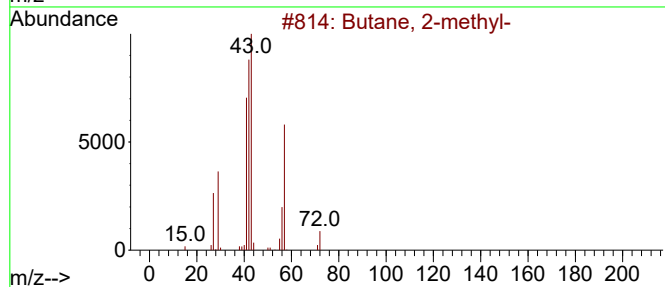
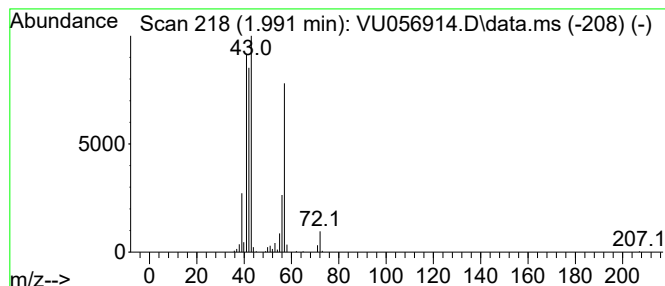
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.991	2.18 ug/L	224503	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	86
3			3-Buten-1-ol	72	C4H8O	000627-27-0	37
4			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33
5			Pentane	72	C5H12	000109-66-0	28



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0YA4

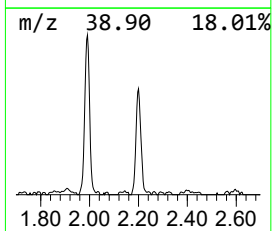
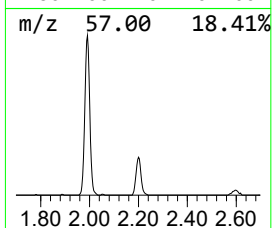
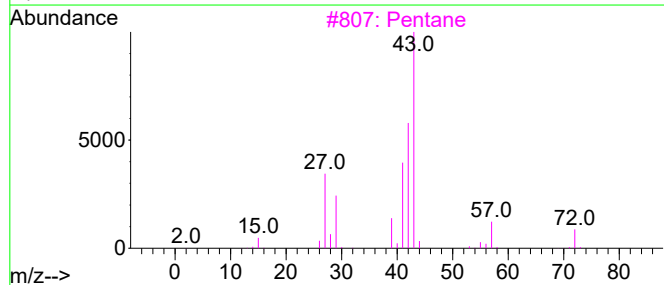
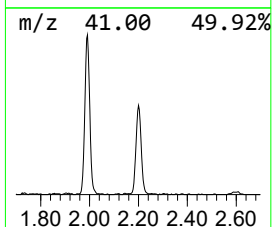
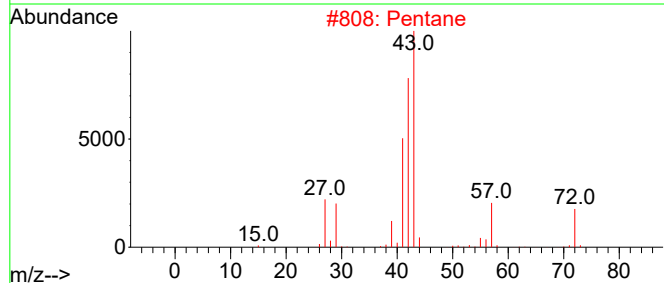
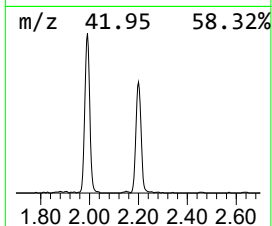
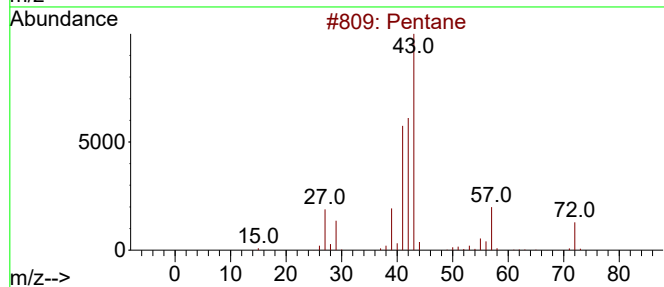
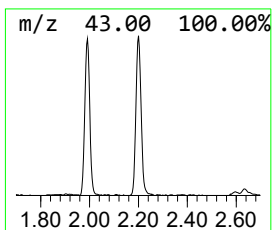
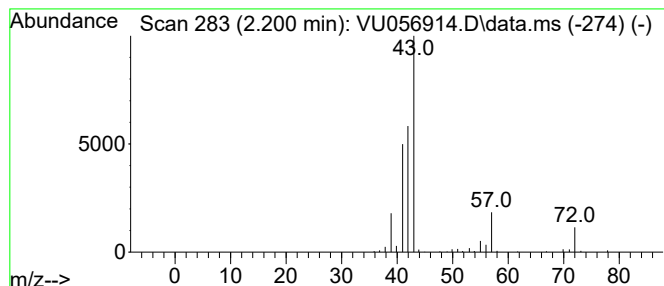
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.200	1.42 ug/L	146381	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	90
3	Pentane			72	C5H12	000109-66-0	90
4	Pentane			72	C5H12	000109-66-0	86
5	Pentane			72	C5H12	000109-66-0	86



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

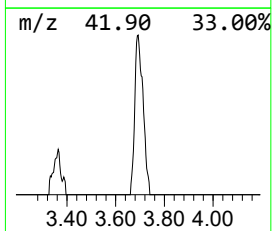
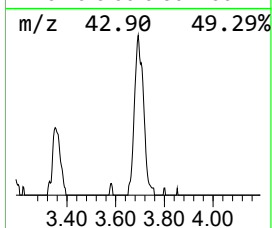
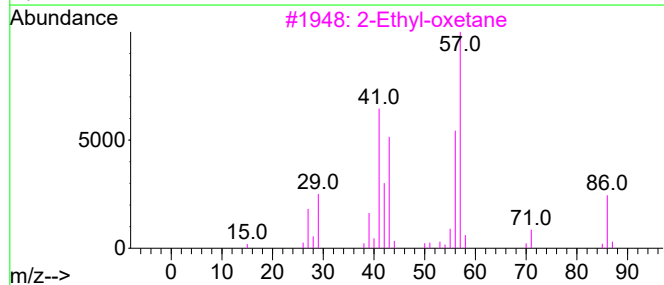
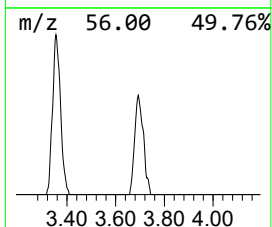
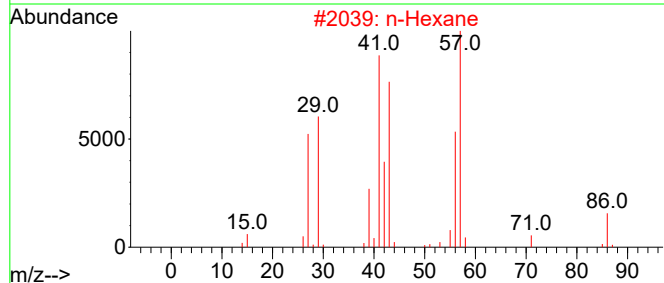
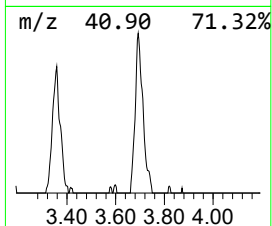
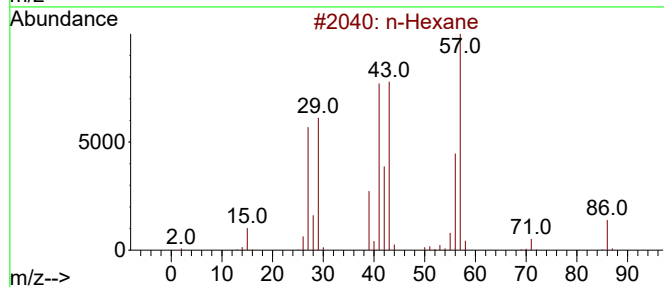
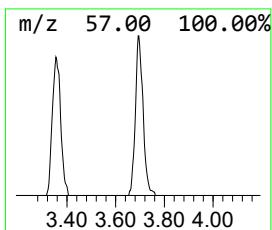
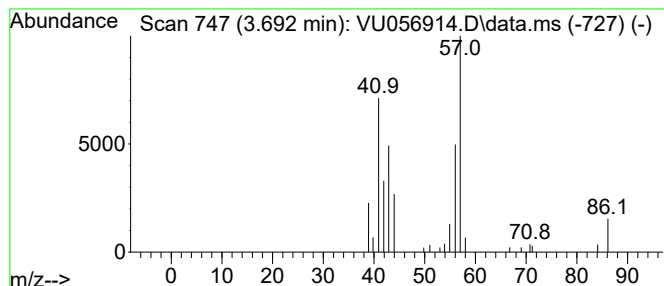
Instrument :
MSVOA_U
ClientSampleId :
E0YA4

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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 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.692	0.52 ug/L	53239	1,4-Difluorobenzene	6.245	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	64
2	n-Hexane	86	C6H14	000110-54-3	64
3	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	64
4	n-Hexane	86	C6H14	000110-54-3	59
5	n-Hexane	86	C6H14	000110-54-3	59



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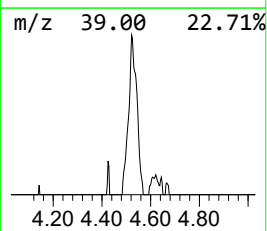
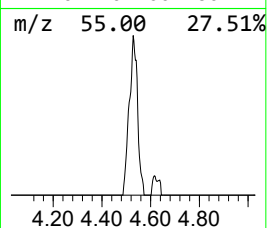
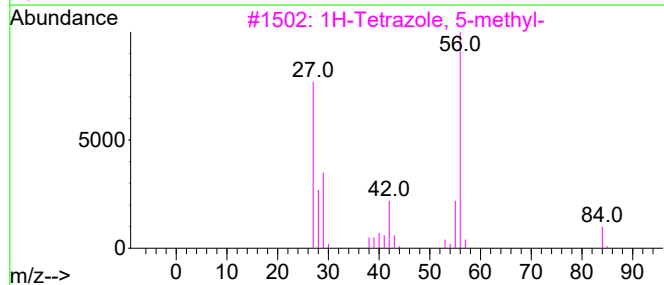
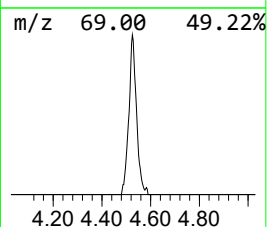
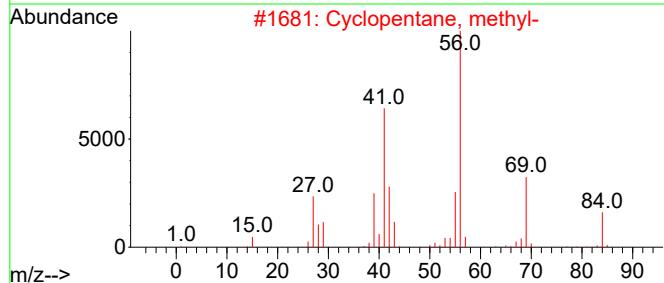
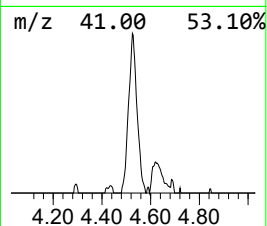
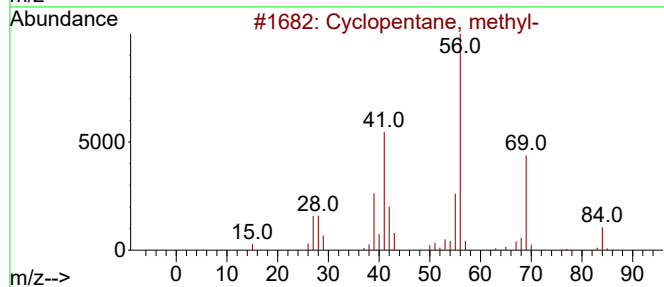
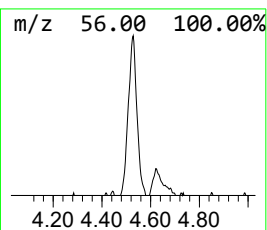
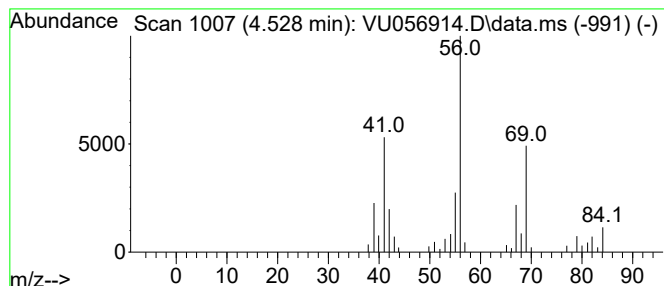
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 (DEL) Alkane: Cyclic4.528 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.528	0.67 ug/L	69316	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	74
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	58
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	52
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	52
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121523\
Data File : VU056914.D
Acq On : 16 Dec 2023 05:43
Operator : MD/SY
Sample : 05771-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0YA4

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	3.8	ug/L	392031	1	6.245	514293	5.0
(DEL) Alkane: S...	1.991	2.2	ug/L	224503	1	6.245	514293	5.0
(DEL) Alkane: S...	2.200	1.4	ug/L	146381	1	6.245	514293	5.0
(DEL) Alkane: S...	3.692	0.5	ug/L	53239	1	6.245	514293	5.0
(DEL) Alkane: C...	4.528	0.7	ug/L	69316	1	6.245	514293	5.0