

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121523\
 Data File : VU056912.D
 Acq On : 16 Dec 2023 04:55
 Operator : MD/SY
 Sample : 05771-05
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E0YA2

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: VU056912.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	rVB	341144	345687	37.83%	3.893%
2	1.486	54	61	68	rBV	209943	214045	23.42%	2.411%
3	1.599	86	96	108	rBV2	349427	384697	42.10%	4.332%
4	1.908	184	192	208	rVV	69226	97219	10.64%	1.095%
5	1.991	208	218	231	rVB	152391	215785	23.61%	2.430%
6	2.200	274	283	300	rVB	102856	146862	16.07%	1.654%
7	2.563	384	396	412	rBV	132824	217727	23.83%	2.452%
8	3.036	531	543	546	rBV5	8141	12785	1.40%	0.144%
9	3.078	549	556	564	rVV3	23679	43867	4.80%	0.494%
10	3.133	566	573	582	rVB3	13150	22632	2.48%	0.255%
11	3.358	626	643	654	rBV2	18819	39147	4.28%	0.441%
12	3.692	727	747	763	rBV4	21521	54423	5.96%	0.613%
13	4.525	988	1006	1025	rBV3	32651	78058	8.54%	0.879%
14	4.621	1025	1036	1070	rBV	126553	355214	38.87%	4.000%
15	5.055	1155	1171	1195	rBV	162878	386646	42.31%	4.354%
16	5.380	1258	1272	1286	rBV7	27451	64276	7.03%	0.724%
17	5.457	1288	1296	1309	rVB5	4642	9166	1.00%	0.103%
18	5.589	1326	1337	1349	rBV4	6512	14266	1.56%	0.161%
19	5.721	1357	1378	1409	rBV2	284349	832608	91.11%	9.377%
20	5.843	1410	1416	1427	rVV6	8151	16076	1.76%	0.181%
21	5.917	1431	1439	1449	rVV8	4633	9729	1.06%	0.110%
22	5.985	1449	1460	1475	rVB6	10476	21281	2.33%	0.240%
23	6.129	1496	1505	1523	rBV6	6811	14969	1.64%	0.169%
24	6.245	1528	1541	1569	rBV	261404	520361	56.94%	5.860%
25	6.541	1619	1633	1651	rBV	45422	90227	9.87%	1.016%
26	6.685	1664	1678	1691	rBV	187953	377198	41.28%	4.248%
27	6.756	1692	1700	1722	rVB4	39442	82476	9.03%	0.929%
28	6.978	1757	1769	1780	rBV6	4345	9358	1.02%	0.105%
29	7.563	1939	1951	1968	rBV2	81290	147872	16.18%	1.665%
30	7.894	2031	2054	2067	rBV	301956	552206	60.43%	6.219%
31	7.965	2067	2076	2096	rVB	127383	233072	25.51%	2.625%
32	8.177	2131	2142	2154	rBV	47809	84401	9.24%	0.951%
33	8.631	2272	2283	2316	rBV2	451522	913813	100.00%	10.291%
34	8.856	2347	2353	2363	rVB8	6613	10631	1.16%	0.120%
35	9.412	2514	2526	2548	rBV	378942	660471	72.28%	7.438%
36	9.570	2564	2575	2595	rVB2	37623	71582	7.83%	0.806%

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Smoothing : ON

Sampling : 1

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Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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Title : TRACE VOA SFAM1.0

37	9.689	2601	2612	2626	rBV	43849	78235	8.56%	0.881%
38	10.100	2728	2740	2754	rBV2	21414	38101	4.17%	0.429%
39	10.750	2929	2942	2962	rBV	152836	252372	27.62%	2.842%
40	10.898	2973	2988	3001	rBV8	8048	18652	2.04%	0.210%
41	10.994	3009	3018	3039	rBV5	7581	17414	1.91%	0.196%
42	11.807	3259	3271	3291	rBV	353371	579663	63.43%	6.528%
43	11.891	3291	3297	3308	rVB4	7420	12027	1.32%	0.135%
44	12.187	3377	3389	3407	rBV	312946	532204	58.24%	5.994%

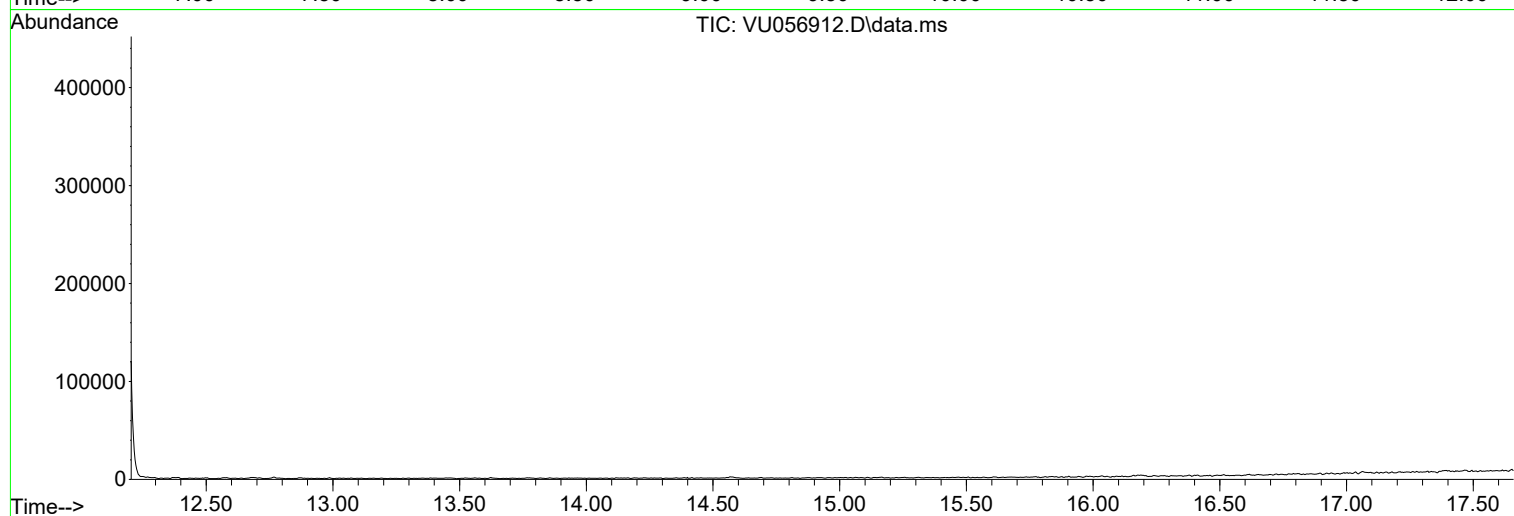
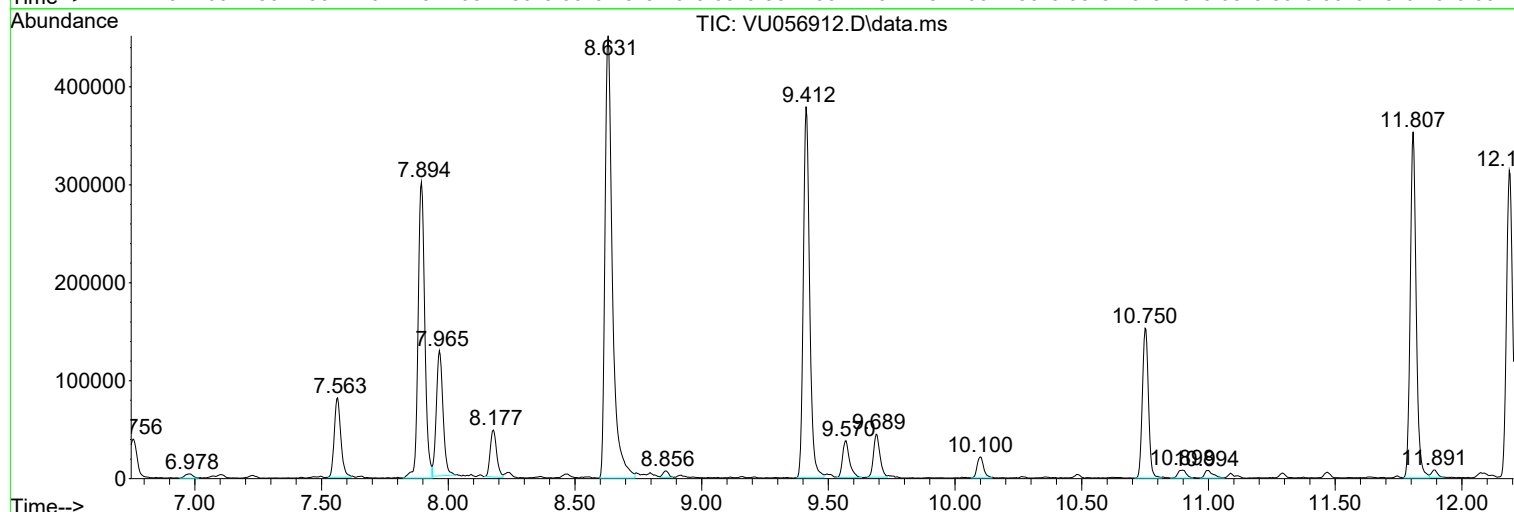
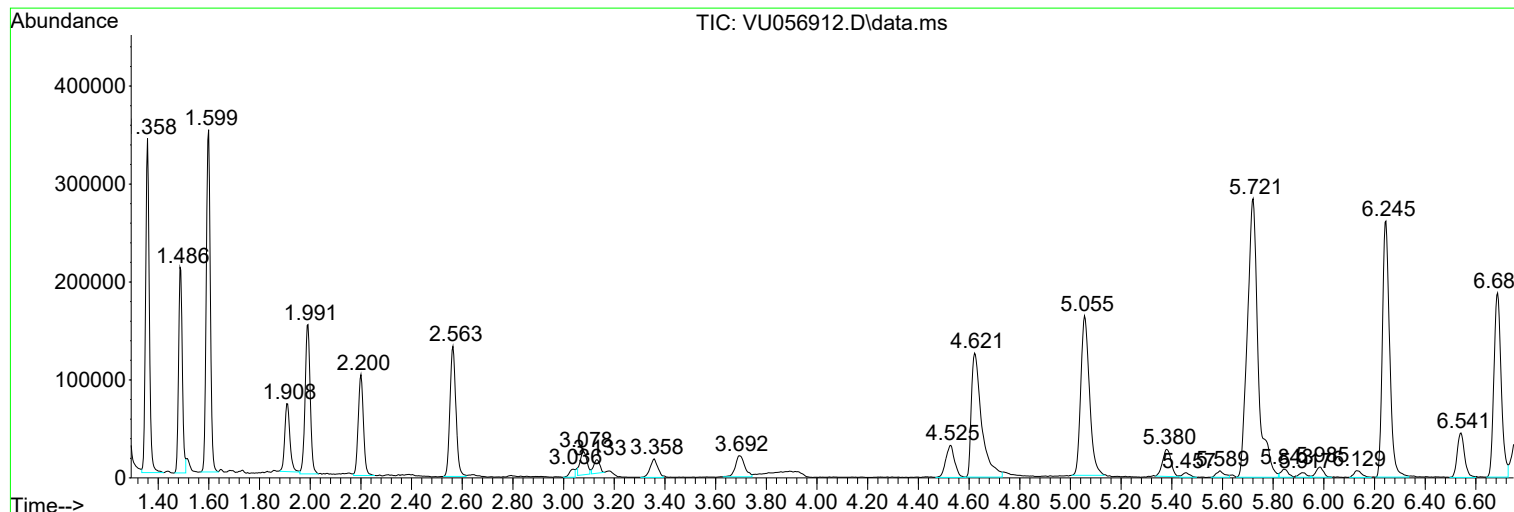
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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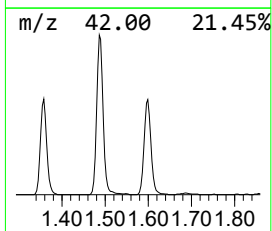
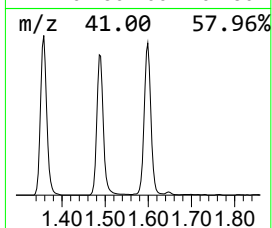
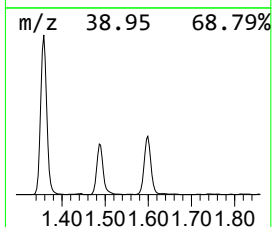
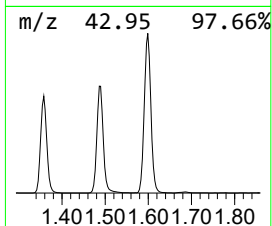
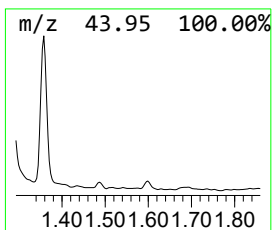
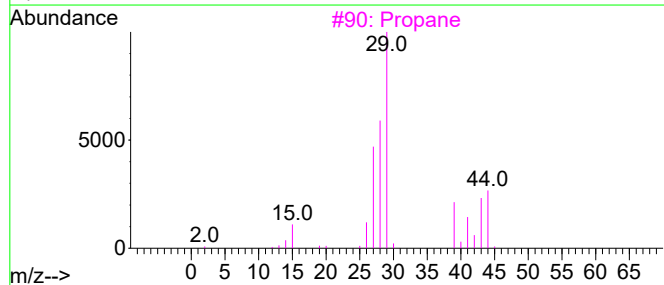
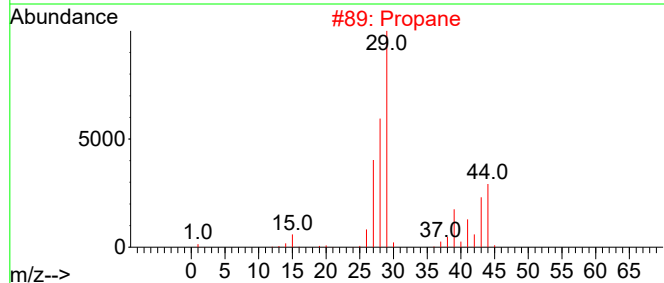
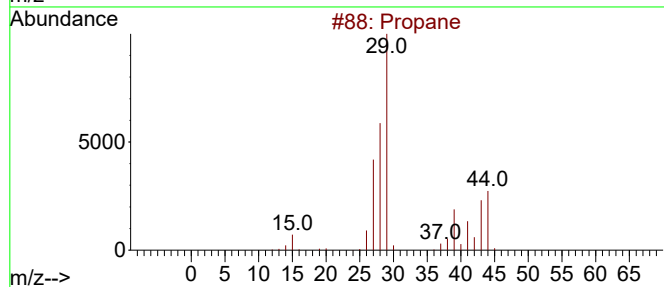
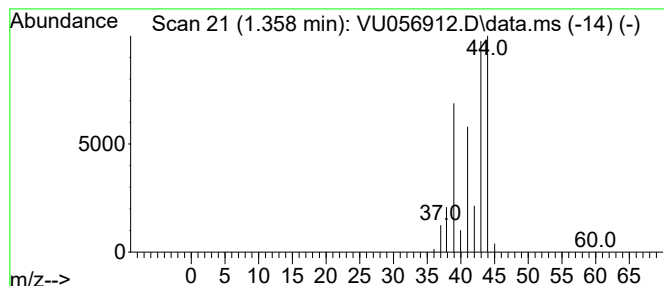
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Quant Title : TRACE VOA SFAM1.0

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	3.32 ug/L	345687	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			Acetaldehyde	44	C2H4O	000075-07-0	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0YA2

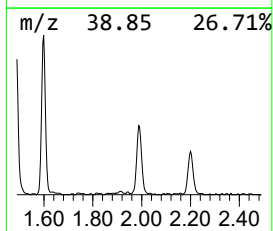
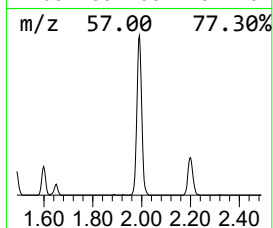
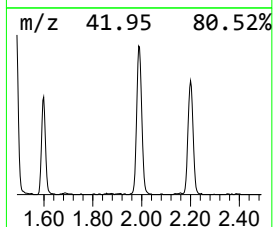
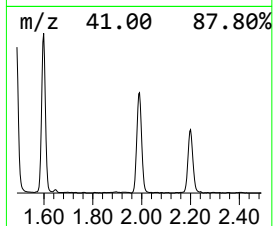
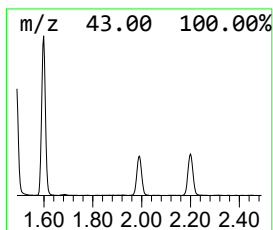
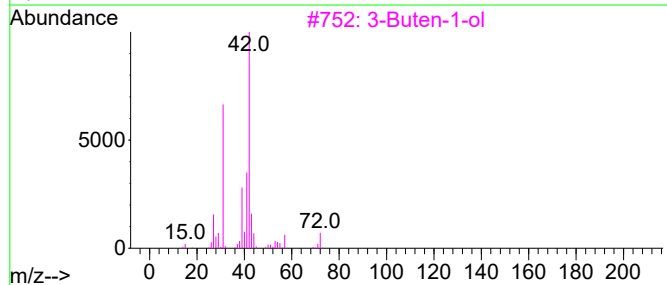
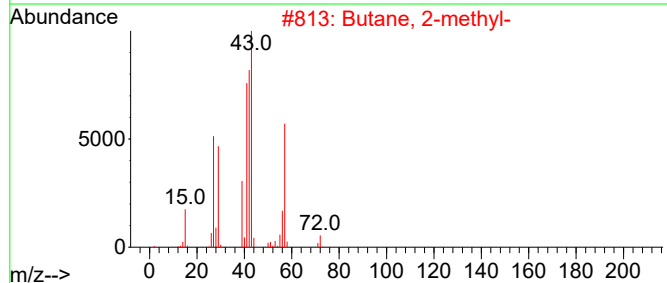
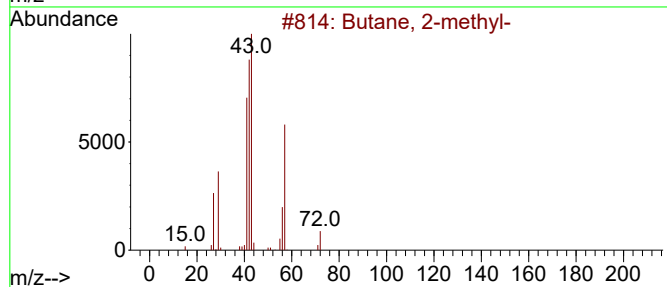
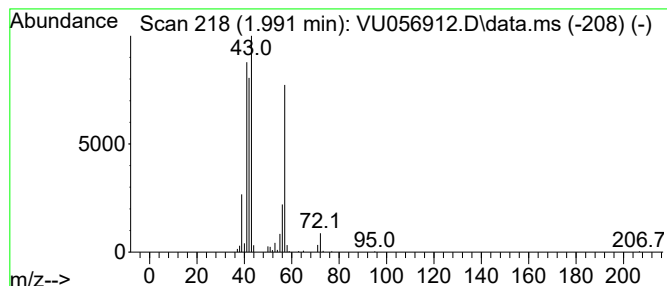
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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	2.07 ug/L	215785	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	91
2	Butane, 2-methyl-			72	C5H12	000078-78-4	90
3	3-Buten-1-ol			72	C4H8O	000627-27-0	43
4	Pentane			72	C5H12	000109-66-0	42
5	Pentane			72	C5H12	000109-66-0	42



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 48 Sample Multiplier: 1

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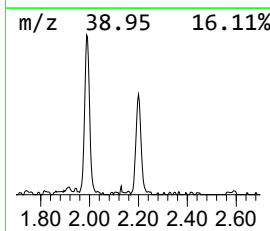
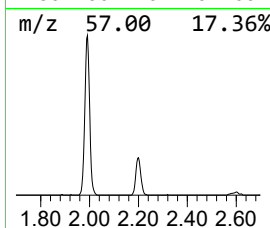
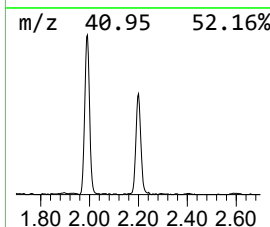
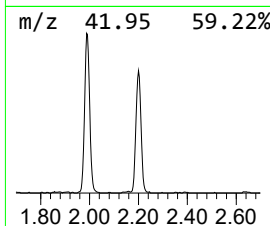
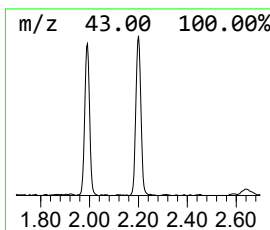
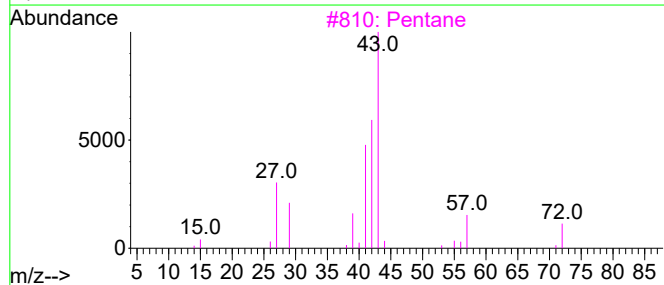
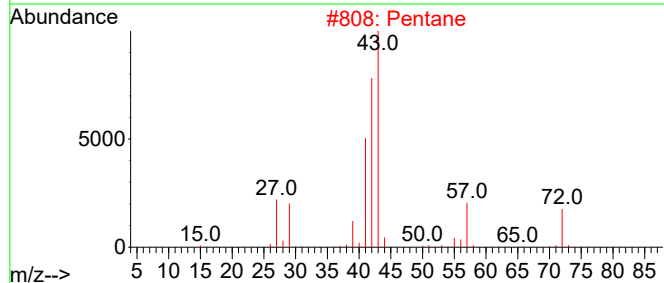
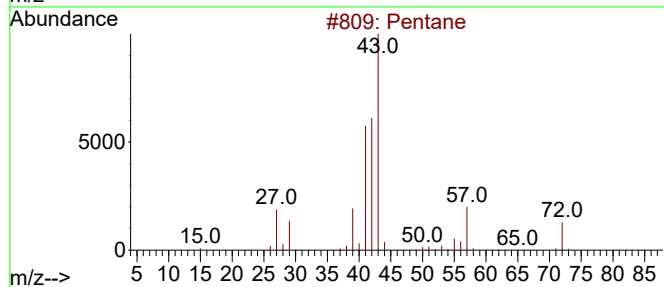
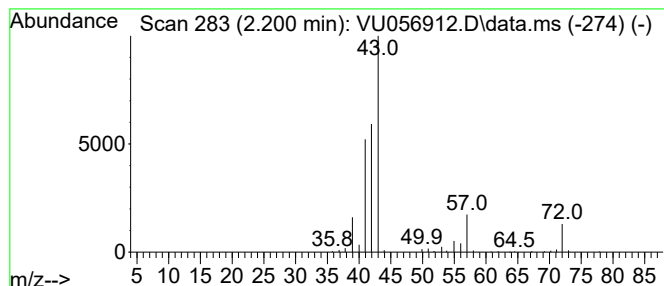
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.200	1.41 ug/L	146862	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	90
5	Pentane			72	C5H12	000109-66-0	86



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 48 Sample Multiplier: 1

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E0YA2

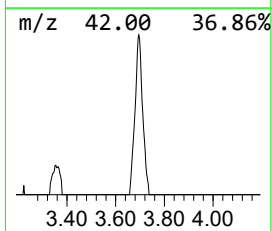
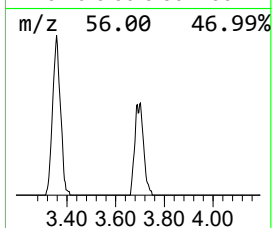
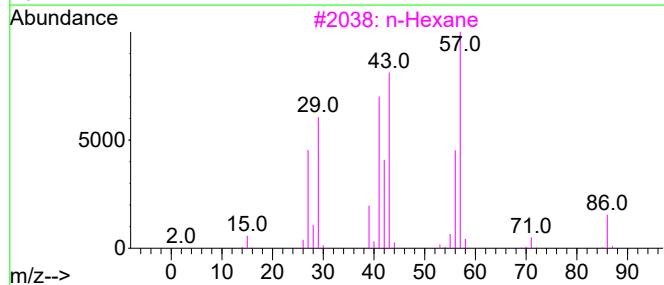
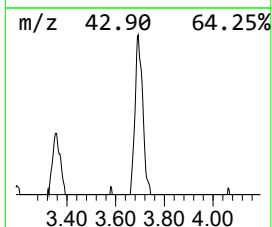
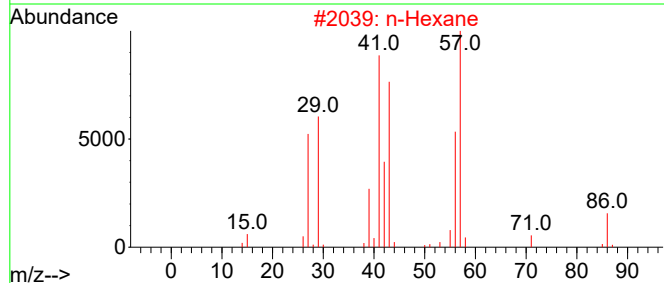
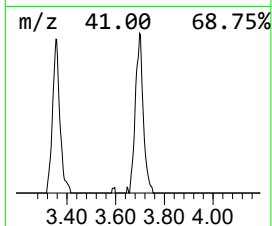
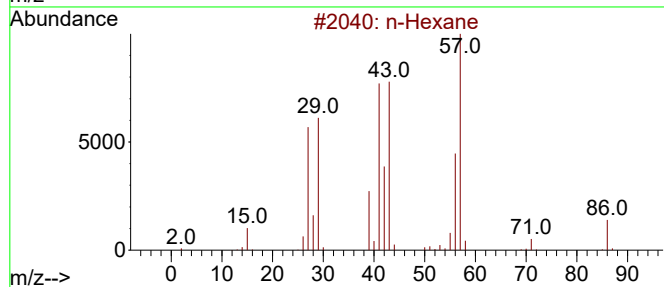
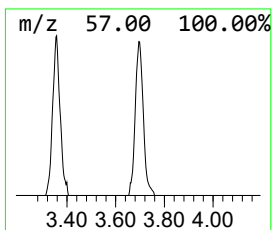
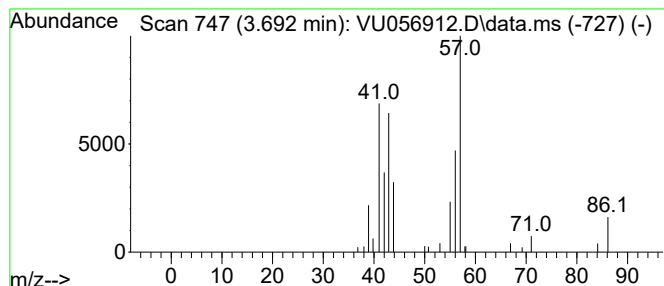
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Quant Title : TRACE VOA SFAM1.0

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	54423	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexane	86	C6H14	000110-54-3	68
2		n-Hexane	86	C6H14	000110-54-3	64
3		n-Hexane	86	C6H14	000110-54-3	64
4		n-Hexane	86	C6H14	000110-54-3	45
5		2-Ethyl-oxetane	86	C5H10O	1010386-40-2	45



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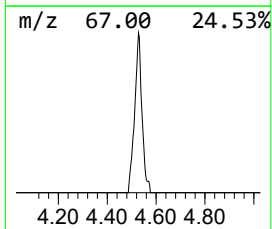
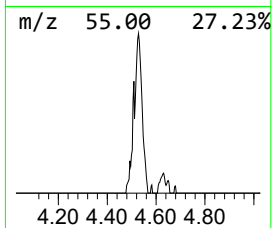
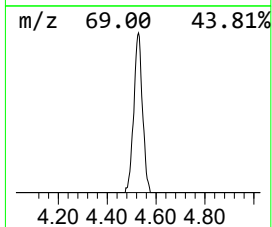
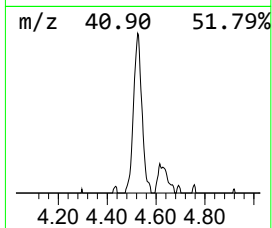
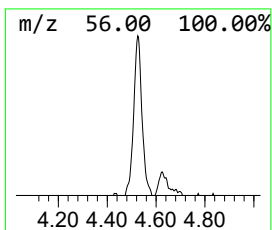
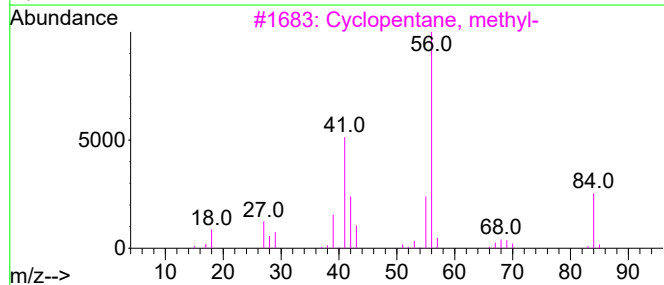
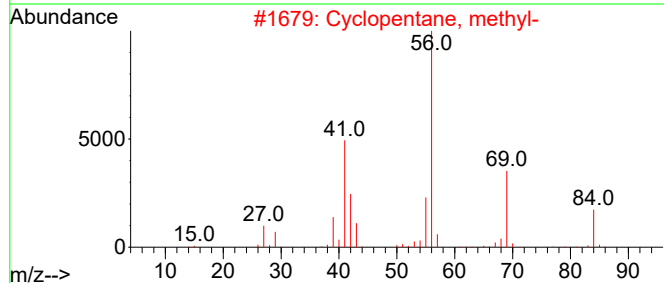
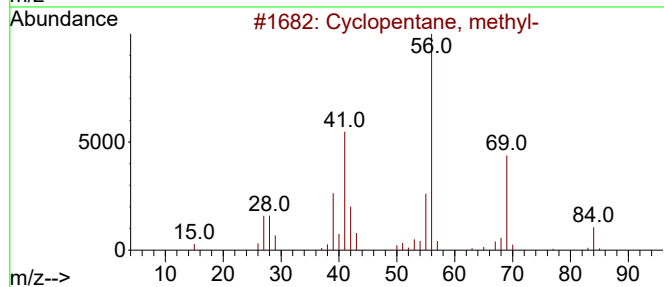
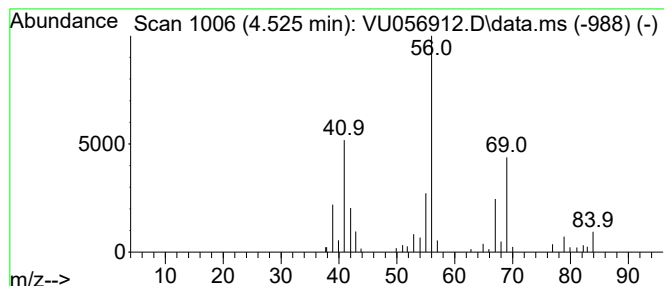
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 (DEL) Alkane: Cyclic4.525 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.525	0.75 ug/L	78058	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	81
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	64
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	59
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	52
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121523\
Data File : VU056912.D
Acq On : 16 Dec 2023 04:55
Operator : MD/SY
Sample : 05771-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E0YA2

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

					--Internal Standard--			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	1.358	3.3	ug/L	345687	1	6.245	520361	5.0
(DEL) Alkane: S...	1.991	2.1	ug/L	215785	1	6.245	520361	5.0
(DEL) Alkane: S...	2.200	1.4	ug/L	146862	1	6.245	520361	5.0
(DEL) Alkane: S...	3.692	0.5	ug/L	54423	1	6.245	520361	5.0
(DEL) Alkane: C...	4.525	0.8	ug/L	78058	1	6.245	520361	5.0