

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122023\
 Data File : VU057086.D
 Acq On : 20 Dec 2023 12:51
 Operator : MD/SY
 Sample : 05771-06
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E0YA3

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: VU057086.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	32	rVB	103946	104233	15.38%	1.660%
2	1.489	55	62	68	rBV	60668	61469	9.07%	0.979%
3	1.599	87	96	111	rVB2	182945	203649	30.04%	3.243%
4	1.911	182	193	204	rBV	72129	97831	14.43%	1.558%
5	1.991	210	218	228	rVB	50144	66535	9.82%	1.059%
6	2.200	271	283	293	rVB	36911	54271	8.01%	0.864%
7	2.563	384	396	415	rBV	141920	232730	34.33%	3.706%
8	3.042	534	545	550	rBV7	3799	7353	1.08%	0.117%
9	3.078	550	556	565	rVV4	8247	15475	2.28%	0.246%
10	3.133	566	573	580	rVV7	4250	8400	1.24%	0.134%
11	3.174	581	586	601	rVB	4858	9774	1.44%	0.156%
12	3.358	633	643	656	rVB6	5044	11523	1.70%	0.183%
13	3.695	736	748	765	rBV5	6991	16755	2.47%	0.267%
14	4.528	993	1007	1020	rBV5	8651	20241	2.99%	0.322%
15	4.624	1023	1037	1075	rBV	72538	229201	33.81%	3.650%
16	5.055	1154	1171	1195	rBV	140298	325022	47.95%	5.176%
17	5.380	1259	1272	1287	rVB7	9712	21643	3.19%	0.345%
18	5.721	1355	1378	1409	rBV2	249587	677836	100.00%	10.794%
19	6.245	1526	1541	1564	rBV	236332	465907	68.73%	7.419%
20	6.538	1620	1632	1650	rBV2	43917	83669	12.34%	1.332%
21	6.682	1664	1677	1692	rBV	155083	307884	45.42%	4.903%
22	6.753	1693	1699	1710	rVB7	12327	24420	3.60%	0.389%
23	7.560	1938	1950	1969	rBV	74665	138248	20.40%	2.201%
24	7.894	2041	2054	2068	rBV	290792	520469	76.78%	8.288%
25	7.965	2068	2076	2093	rVB	36423	68851	10.16%	1.096%
26	8.174	2131	2141	2157	rBV	44995	79634	11.75%	1.268%
27	8.631	2271	2283	2318	rBV2	283747	592948	87.48%	9.442%
28	9.412	2512	2526	2560	rBV	336638	592695	87.44%	9.438%
29	9.570	2566	2575	2597	rVB2	11961	23825	3.51%	0.379%
30	9.689	2600	2612	2626	rBV3	14594	24781	3.66%	0.395%
31	10.097	2730	2739	2748	rBV4	6691	11017	1.63%	0.175%
32	10.750	2931	2942	2960	rBV	115799	190194	28.06%	3.029%
33	11.470	3156	3166	3171	rBV4	4959	6897	1.02%	0.110%
34	11.807	3258	3271	3291	rBV	321053	521394	76.92%	8.302%
35	12.187	3377	3389	3405	rBV	281366	463216	68.34%	7.376%

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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

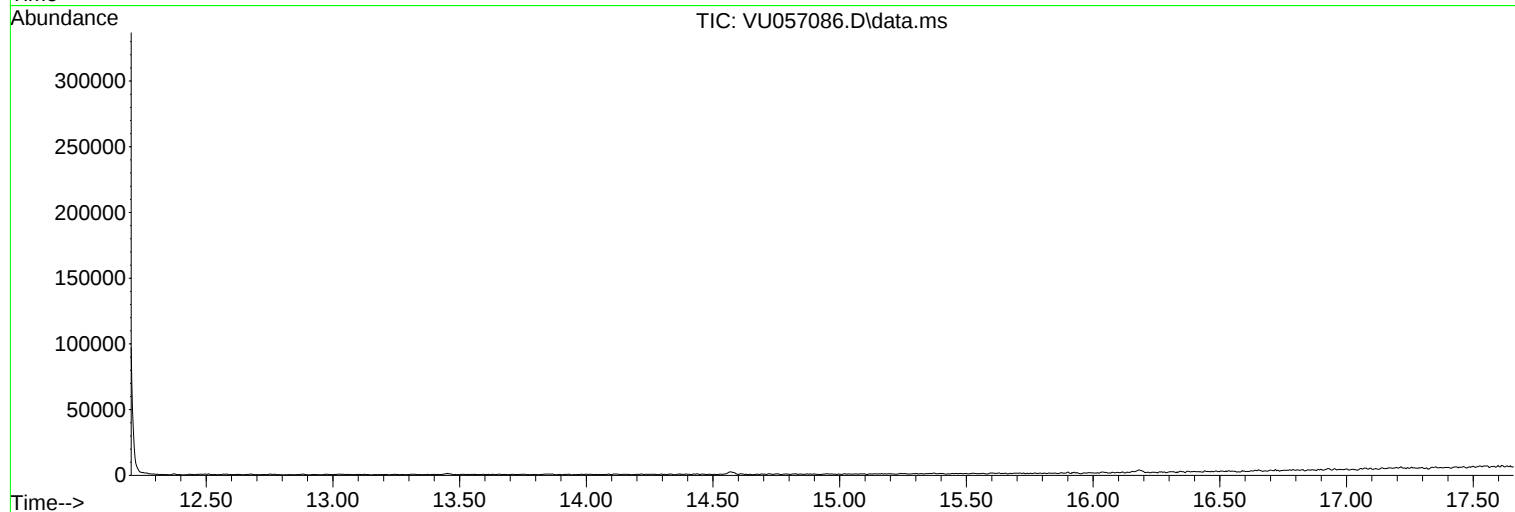
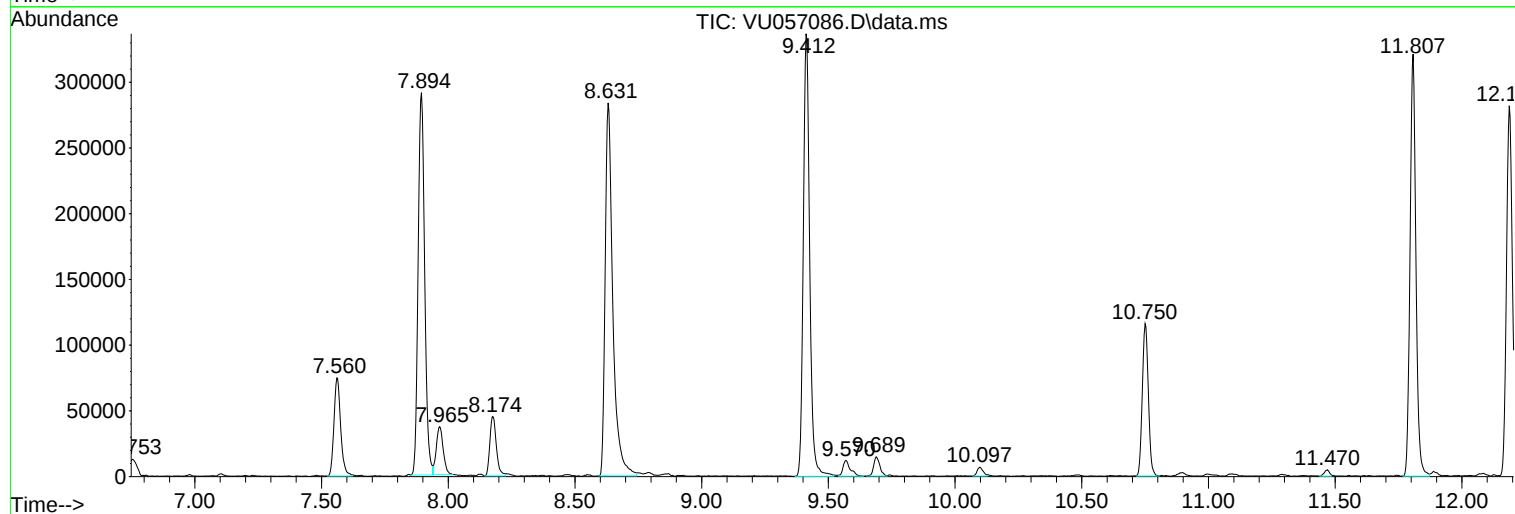
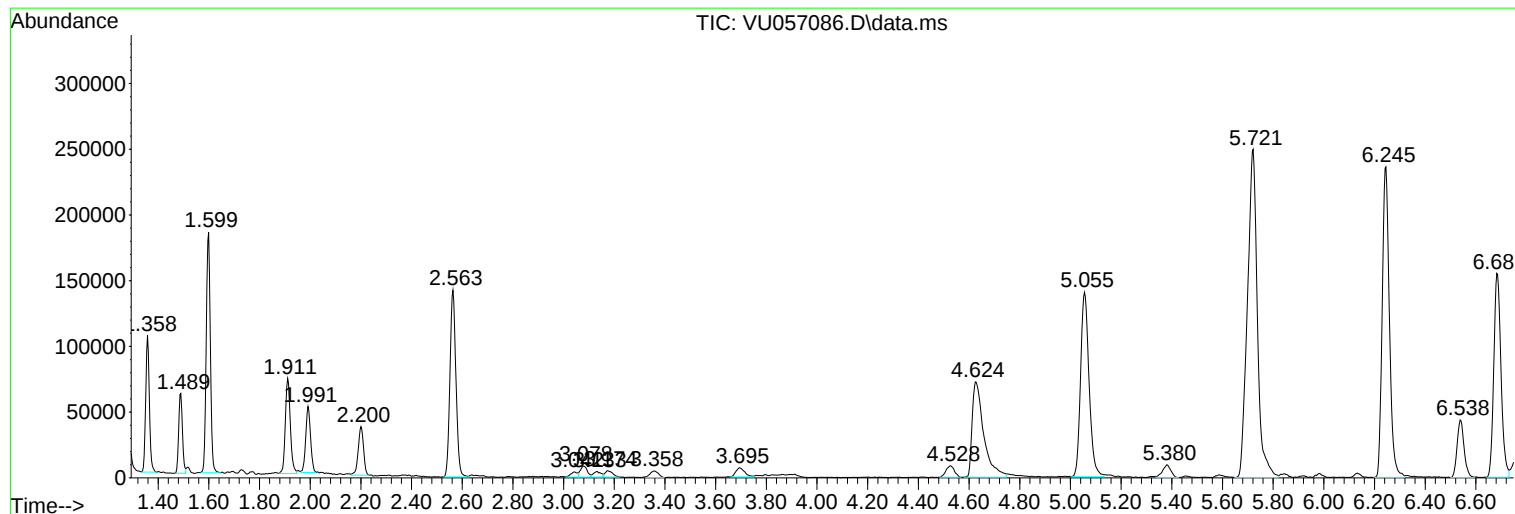
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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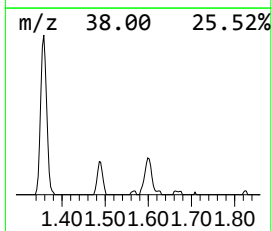
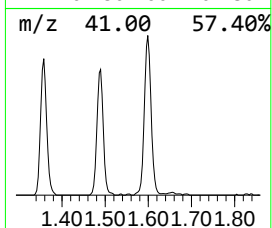
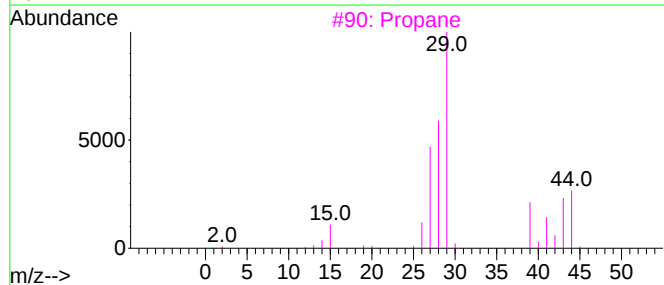
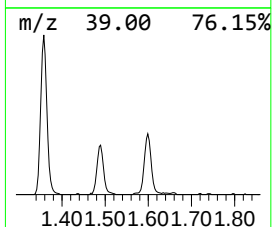
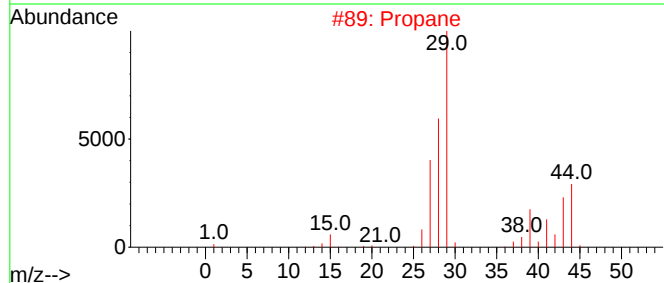
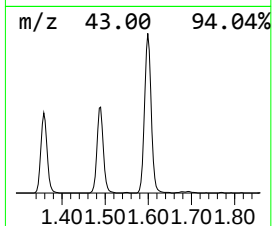
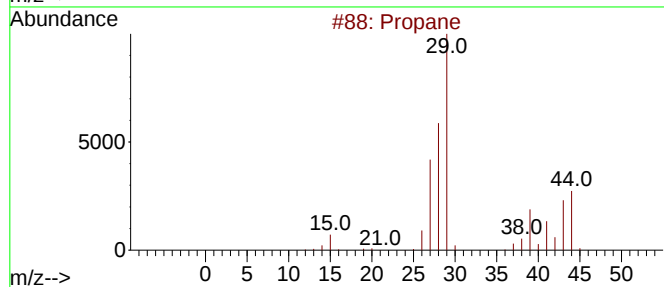
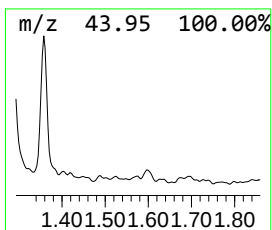
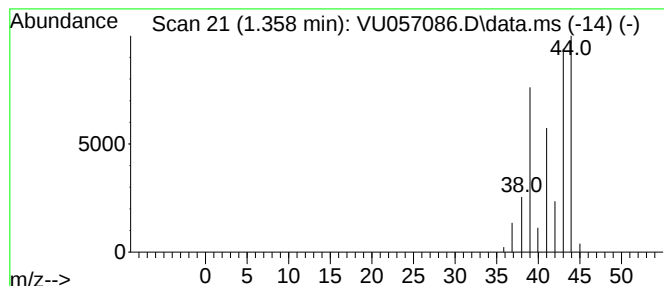
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.358	1.12 ug/L	104233	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	56
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
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Instrument :
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ClientSampleId :
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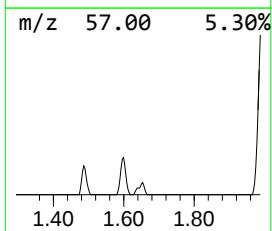
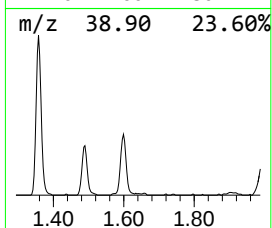
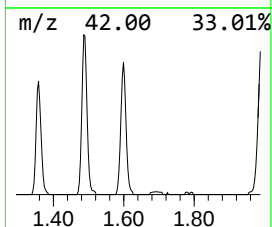
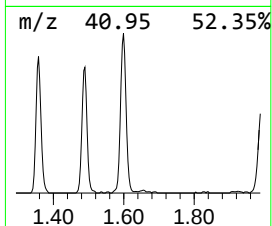
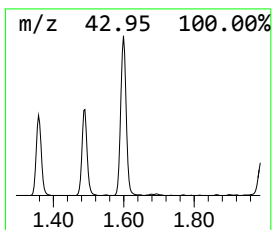
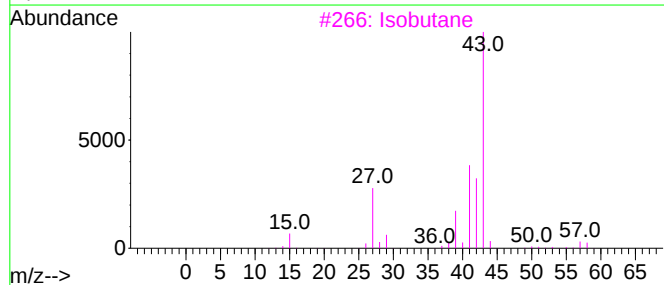
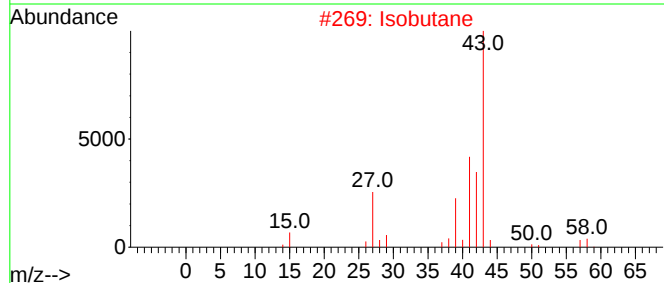
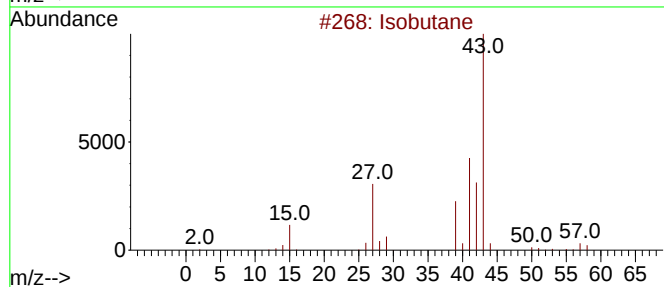
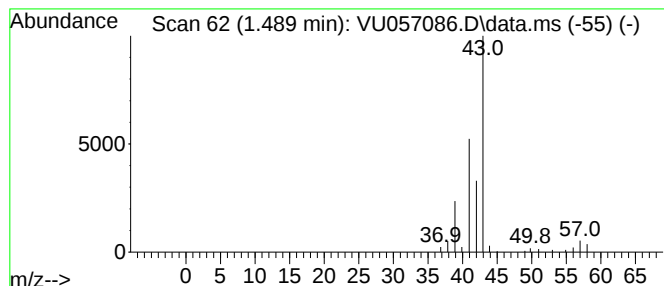
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.489	0.66 ug/L	61469	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	64
2		Isobutane	58	C4H10	000075-28-5	64
3		Isobutane	58	C4H10	000075-28-5	42
4		Isobutane	58	C4H10	000075-28-5	42
5		Isobutane	58	C4H10	000075-28-5	9



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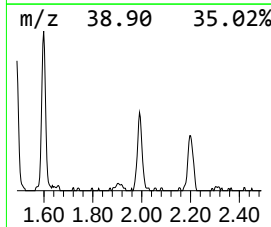
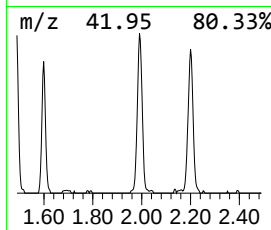
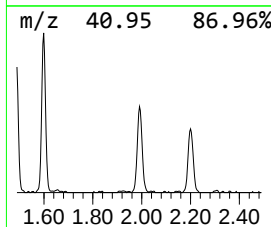
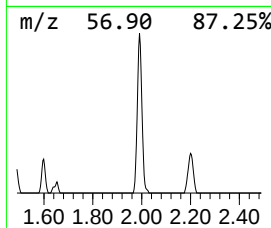
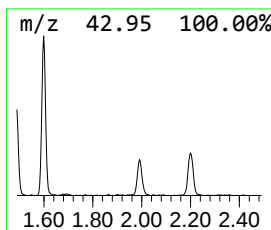
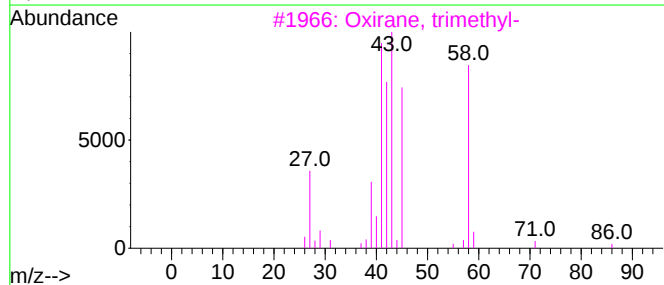
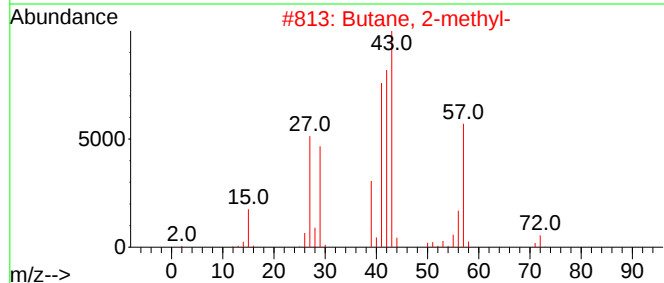
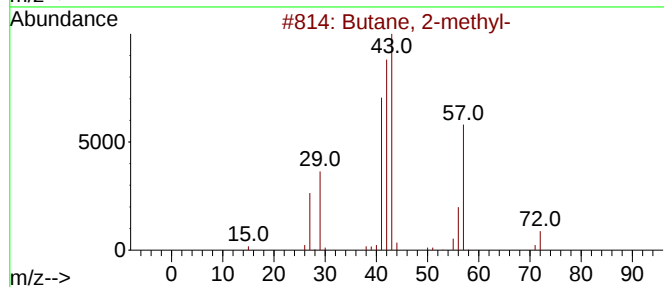
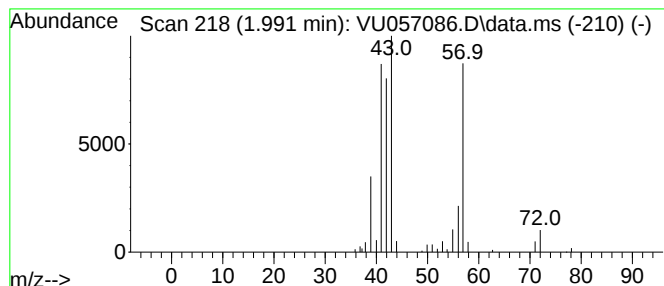
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.991	0.71 ug/L	66535	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	80
2		Butane, 2-methyl-	72	C5H12	000078-78-4	80
3		Oxirane, trimethyl-	86	C5H10O	005076-19-7	42
4		3-Buten-1-ol	72	C4H8O	000627-27-0	38
5		3-Buten-1-ol	72	C4H8O	000627-27-0	37



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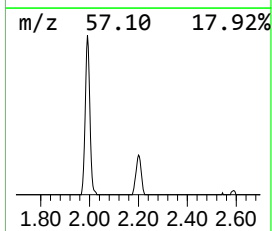
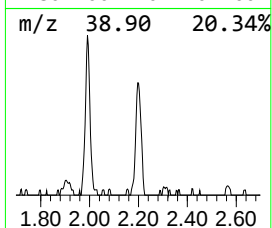
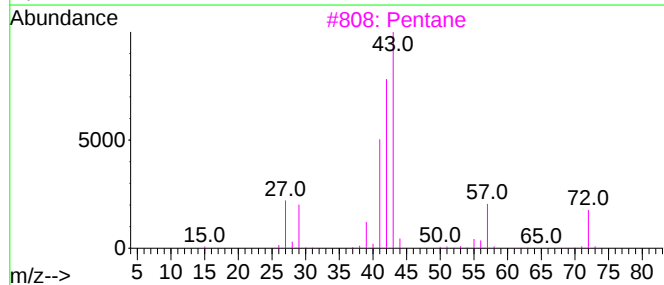
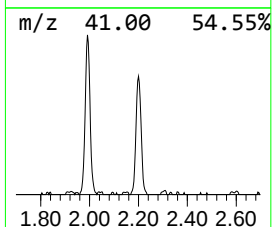
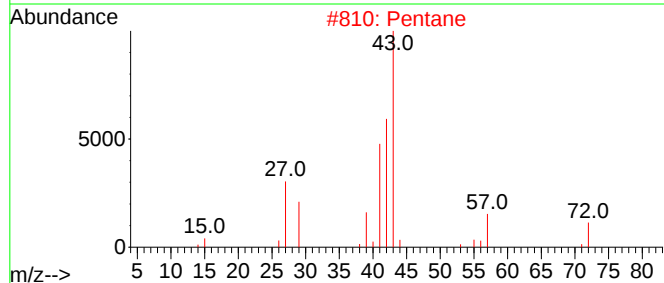
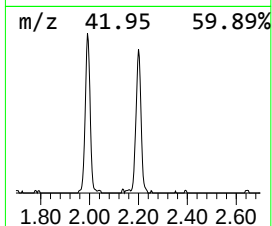
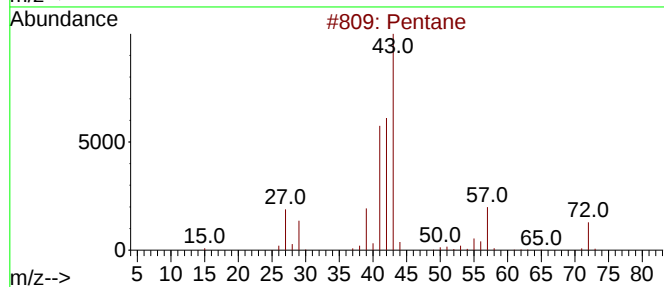
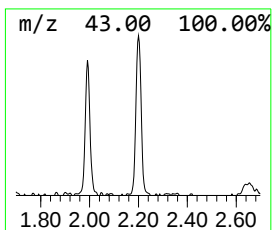
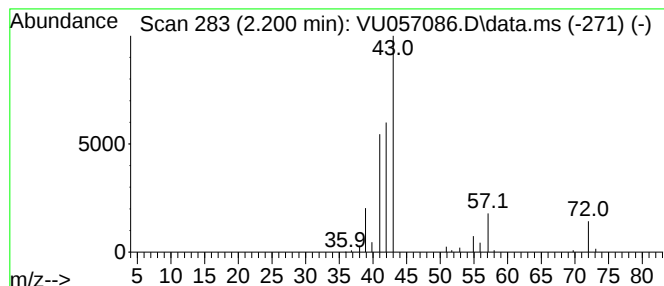
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Quant Title : TRACE VOA SFAM1.0

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.
2.200	0.58 ug/L	54271	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	86
4	Pentane			72	C5H12	000109-66-0	86
5	Pentane			72	C5H12	000109-66-0	78



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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	1.1	ug/L	104233	1	6.245	465907	5.0
(DEL) Alkane: S...	1.489	0.7	ug/L	61469	1	6.245	465907	5.0
(DEL) Alkane: S...	1.991	0.7	ug/L	66535	1	6.245	465907	5.0
(DEL) Alkane: S...	2.200	0.6	ug/L	54271	1	6.245	465907	5.0