

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110122\
 Data File : VU051663.D
 Acq On : 01 Nov 2022 18:55
 Operator : JC/MD
 Sample : N5353-19
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBXB2

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\SFAMUTR102822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051663.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	28	rVB	72518	75476	8.96%	0.948%
2	1.465	29	39	53	rBV	215943	415089	49.29%	5.214%
3	1.597	74	80	117	rVB3	195656	356124	42.29%	4.473%
4	1.909	170	177	194	rVB	89847	126155	14.98%	1.585%
5	1.993	197	203	217	rVB3	28102	41495	4.93%	0.521%
6	2.202	261	268	284	rVB2	34709	52092	6.19%	0.654%
7	2.565	369	381	394	rBV	163535	265990	31.58%	3.341%
8	2.629	394	401	414	rVB4	4222	9127	1.08%	0.115%
9	3.079	535	541	552	rVB3	5463	9581	1.14%	0.120%
10	3.353	615	626	644	rVB4	10458	23323	2.77%	0.293%
11	3.697	717	733	748	rBV6	7143	15485	1.84%	0.194%
12	3.874	759	788	812	rVB	12730	62569	7.43%	0.786%
13	4.620	1008	1020	1026	rBV	131518	267856	31.81%	3.364%
14	4.665	1028	1034	1056	rVB	176809	380273	45.15%	4.776%
15	5.060	1141	1157	1177	rBV2	164069	369521	43.88%	4.641%
16	5.722	1343	1363	1397	rBV2	312296	842158	100.00%	10.578%
17	6.247	1513	1526	1544	rBV	231347	442825	52.58%	5.562%
18	6.542	1605	1618	1640	rVB2	47411	88499	10.51%	1.112%
19	6.690	1647	1664	1693	rBV	198166	396768	47.11%	4.983%
20	7.565	1921	1936	1958	rBV2	88595	159779	18.97%	2.007%
21	7.896	2026	2039	2054	rBV	348638	608335	72.24%	7.641%
22	7.967	2056	2061	2075	rVB	12976	23287	2.77%	0.292%
23	8.179	2114	2127	2142	rBV2	53204	92444	10.98%	1.161%
24	8.472	2208	2218	2230	rVB3	7053	11819	1.40%	0.148%
25	8.552	2233	2243	2256	rBV2	50702	82341	9.78%	1.034%
26	8.632	2256	2268	2307	rBV	422983	795909	94.51%	9.997%
27	9.417	2498	2512	2535	rBV	349011	589419	69.99%	7.403%
28	10.754	2915	2928	2943	rBV	159631	259498	30.81%	3.259%
29	10.889	2961	2970	2984	rBV3	10668	17862	2.12%	0.224%
30	11.812	3245	3257	3281	rBV	297163	493336	58.58%	6.196%
31	12.063	3324	3335	3362	rBV3	26096	61745	7.33%	0.776%
32	12.192	3362	3375	3389	rBV	322929	525528	62.40%	6.601%

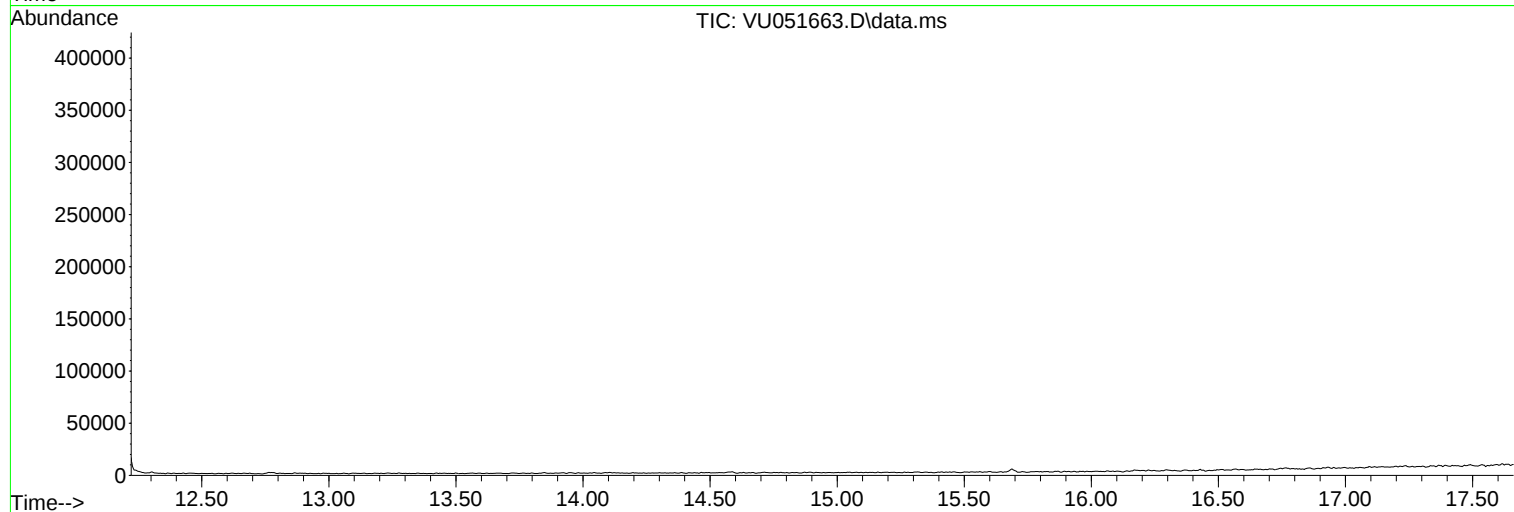
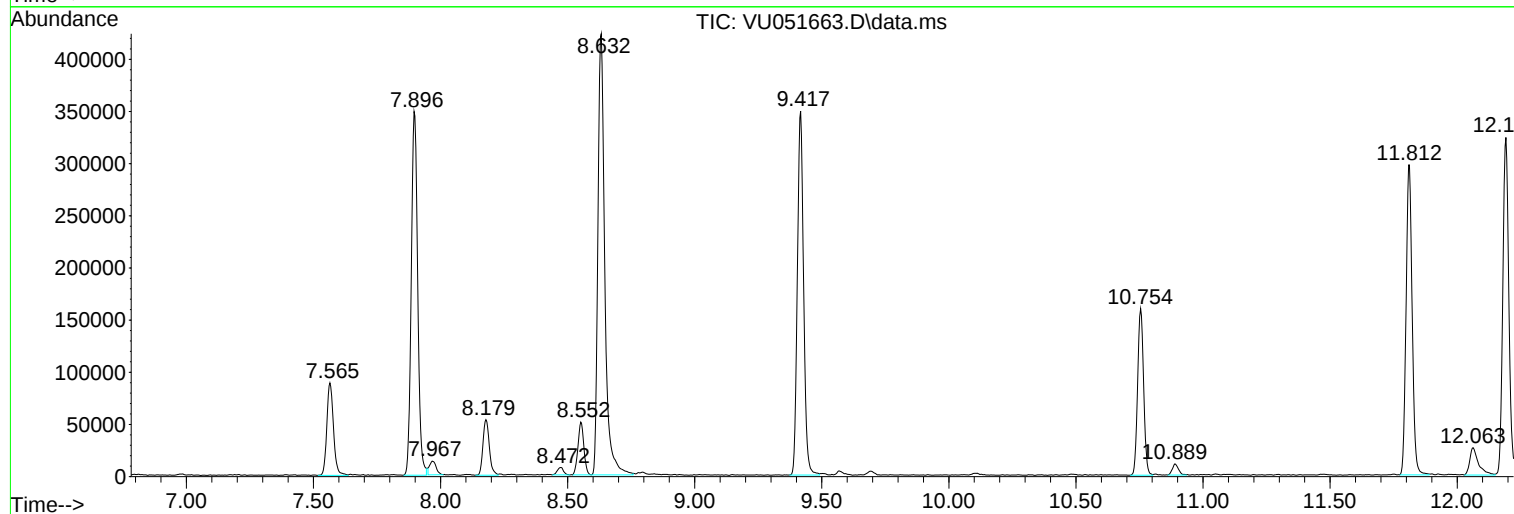
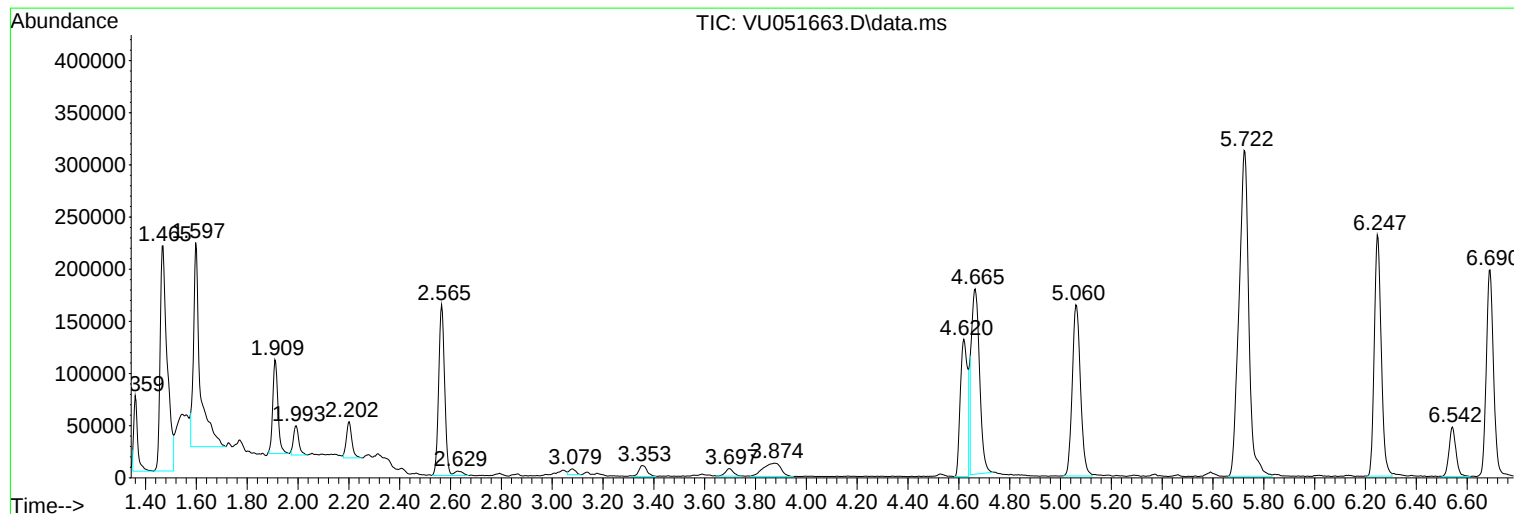
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Quant Title : TRACE VOA SFAM1.0

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



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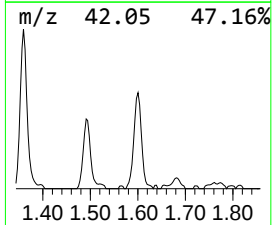
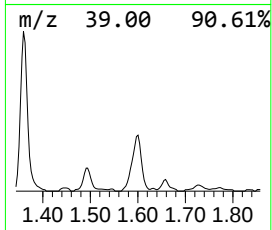
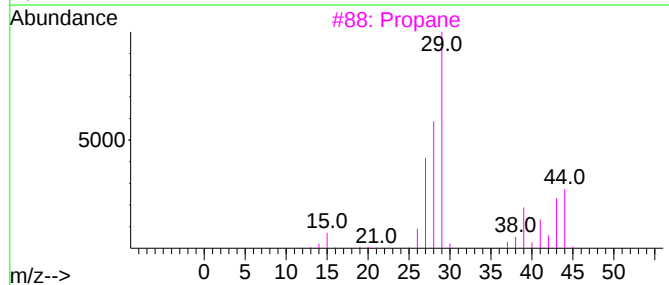
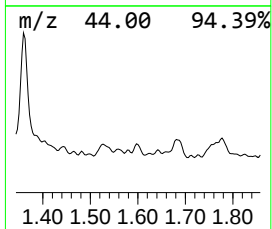
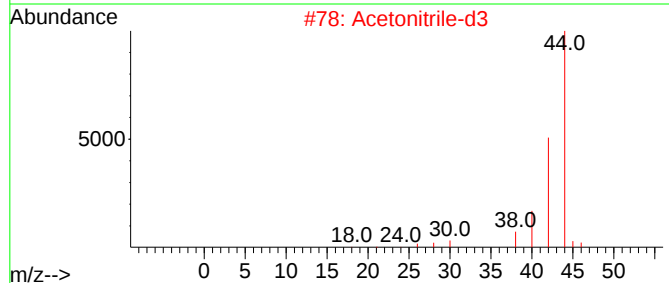
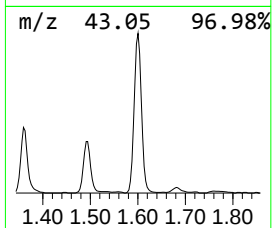
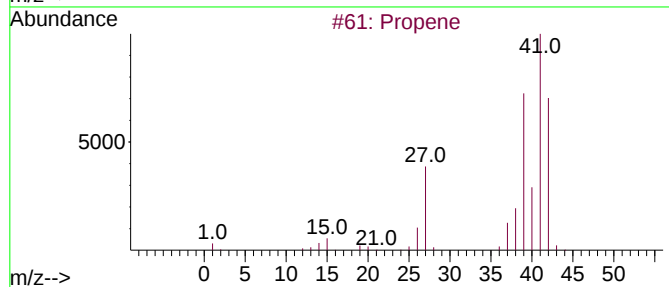
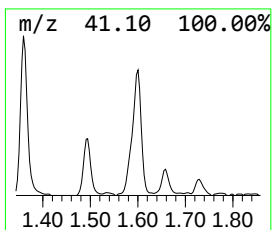
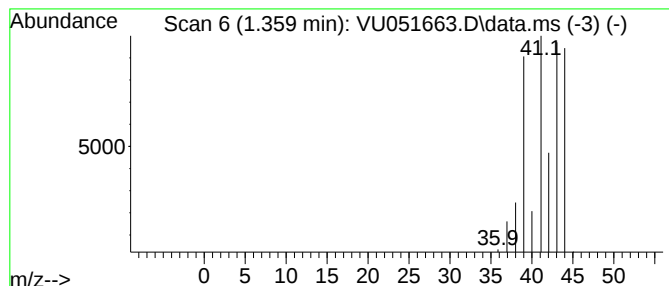
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	0.85 ug/L	75476	1,4-Difluorobenzene	6.247

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		Propane	44	C3H8	000074-98-6	7
4		Acetonitrile-d3	44	C2D3N	002206-26-0	4
5		Propane	44	C3H8	000074-98-6	4



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Instrument :
MSVOA_U
ClientSampleId :
DBXB2

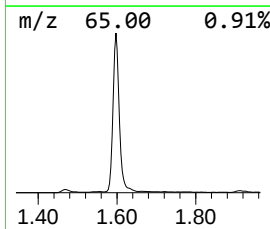
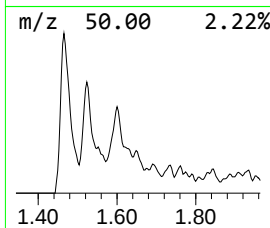
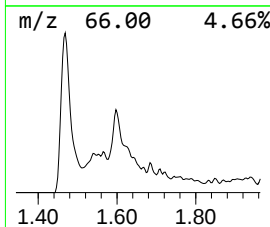
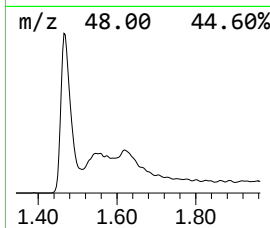
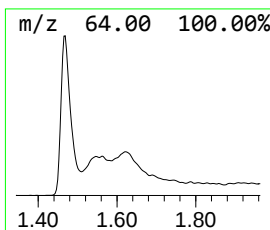
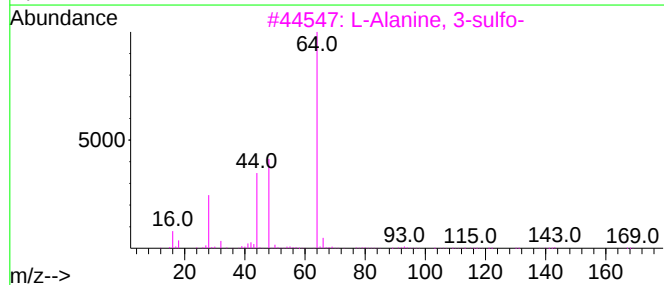
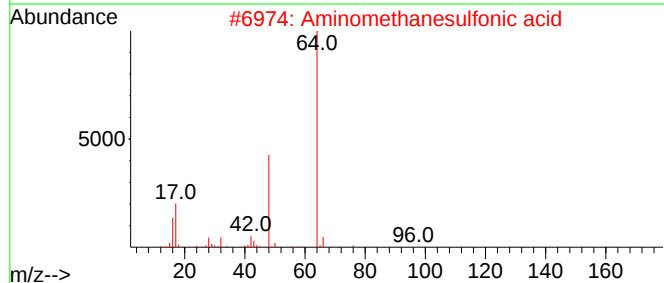
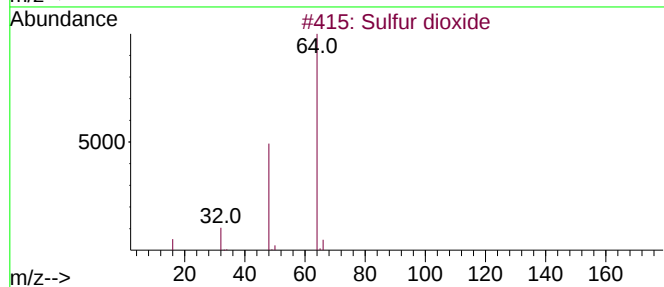
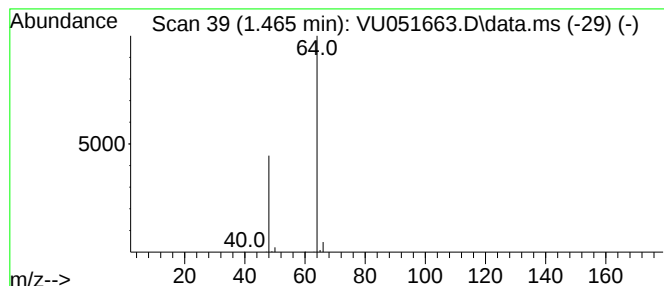
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.465	4.69 ug/L	415089	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBXB2

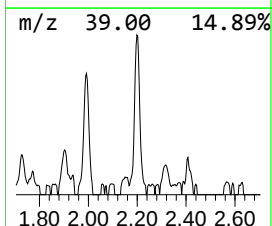
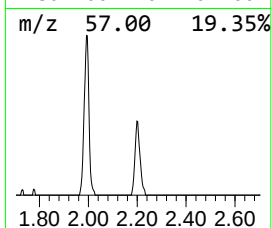
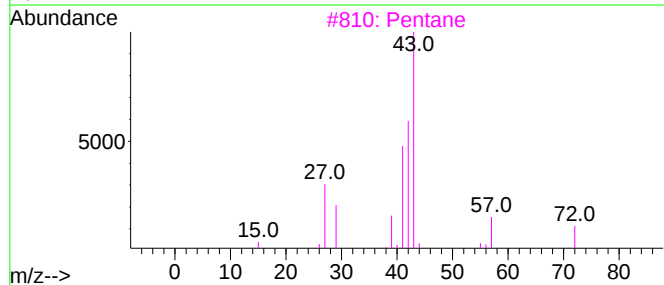
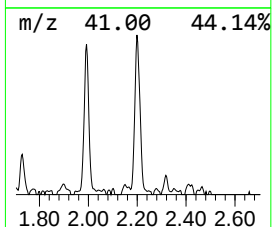
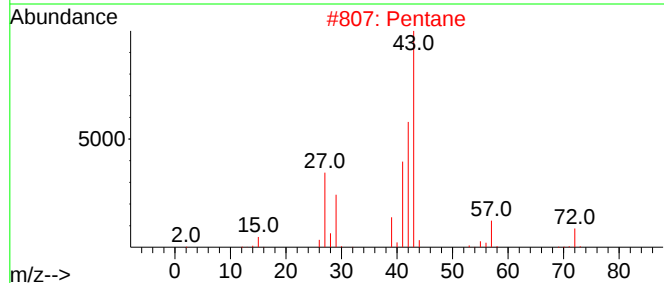
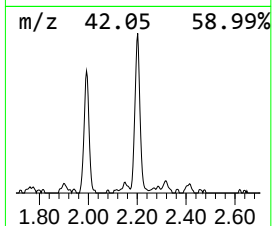
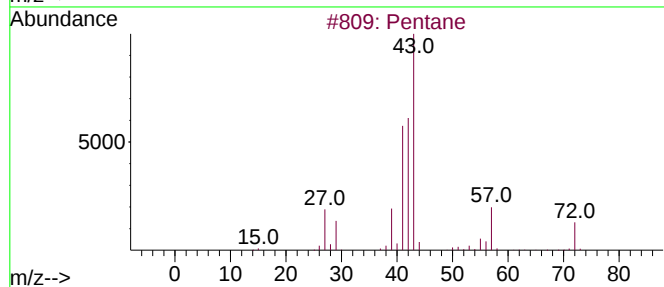
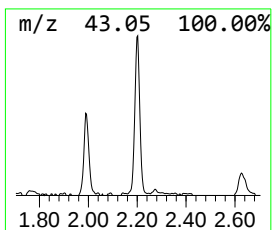
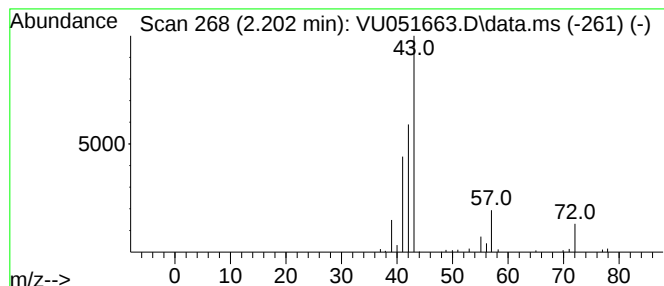
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.202	0.59 ug/L	52092	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane	72	C5H12	000109-66-0	86
2			Pentane	72	C5H12	000109-66-0	86
3			Pentane	72	C5H12	000109-66-0	86
4			Pentane	72	C5H12	000109-66-0	86
5			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	40



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Instrument :
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ClientSampleId :
DBXB2

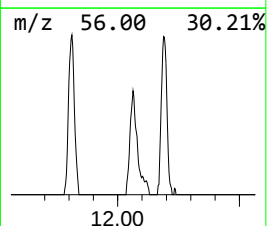
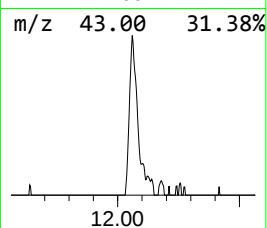
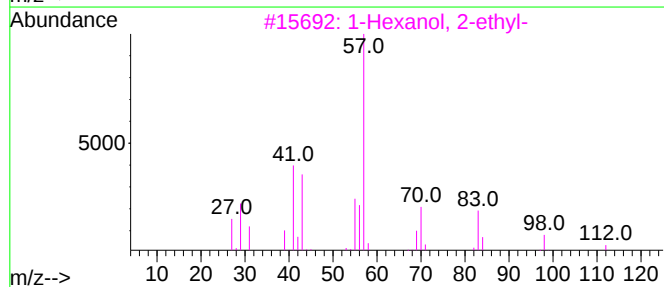
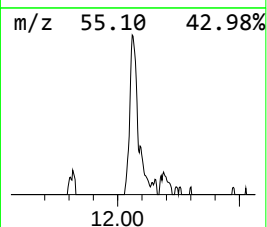
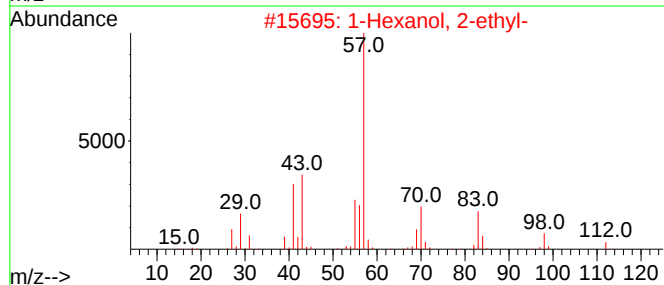
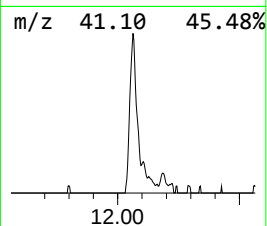
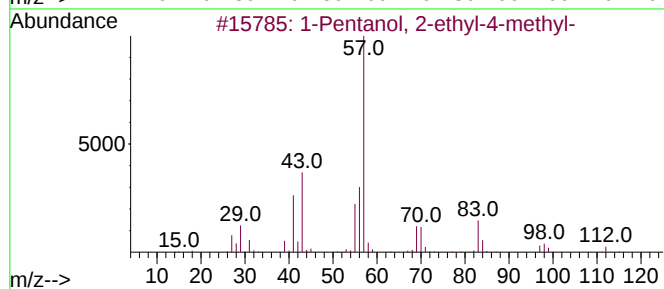
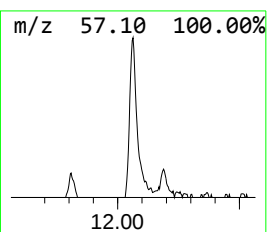
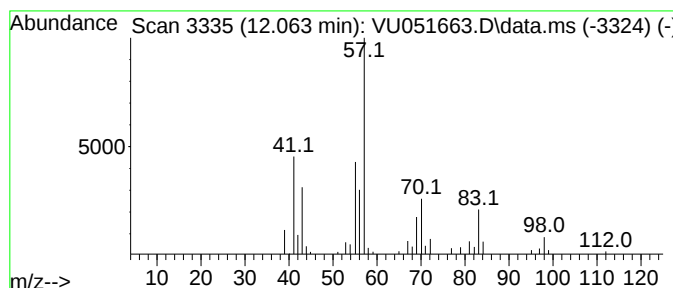
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 1-Pentanol, 2-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	0.63 ug/L	61745	1,4-Dichlorobenzene-d4	11.809

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50



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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...	1.359	0.8	ug/L	75476	1	6.247	442825	5.0
Sulfur dioxide	1.465	4.7	ug/L	415089	1	6.247	442825	5.0
(DEL) Alkane: S...	2.202	0.6	ug/L	52092	1	6.247	442825	5.0
1-Pentanol, 2-e...	12.063	0.6	ug/L	61745	3	11.809	493336	5.0