

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110222\
 Data File : VU051707.D
 Acq On : 02 Nov 2022 22:28
 Operator : JC/MD
 Sample : N5353-19
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 31 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: VU051707.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	21	rVB	65125	65786	9.16%	0.963%
2	1.469	31	40	55	rBV	217525	398914	55.53%	5.840%
3	1.597	73	80	90	rBV2	143185	177999	24.78%	2.606%
4	1.912	170	178	192	rVB	80267	106396	14.81%	1.558%
5	1.993	197	203	213	rVB	27595	37473	5.22%	0.549%
6	2.202	261	268	279	rVB	31481	44913	6.25%	0.658%
7	2.565	369	381	394	rBV	133839	216263	30.11%	3.166%
8	3.044	517	530	535	rBV9	3844	7735	1.08%	0.113%
9	3.079	536	541	550	rVB3	5561	8864	1.23%	0.130%
10	3.356	617	627	640	rVB3	8403	16956	2.36%	0.248%
11	3.694	720	732	746	rVB4	6697	15095	2.10%	0.221%
12	3.822	754	772	773	rBV	5319	9503	1.32%	0.139%
13	4.620	1009	1020	1026	rBV	114435	230661	32.11%	3.377%
14	4.665	1028	1034	1060	rVB	151283	331646	46.17%	4.856%
15	5.063	1141	1158	1177	rBV	141294	316673	44.08%	4.636%
16	5.594	1306	1323	1332	rBV7	4026	7849	1.09%	0.115%
17	5.722	1340	1363	1397	rBV3	264116	718336	100.00%	10.517%
18	6.247	1513	1526	1562	rBV	210671	414186	57.66%	6.064%
19	6.542	1607	1618	1631	rVB2	22009	41745	5.81%	0.611%
20	6.690	1649	1664	1684	rBV	173889	344324	47.93%	5.041%
21	7.565	1923	1936	1954	rBV	73238	131649	18.33%	1.927%
22	7.896	2026	2039	2056	rBV	284161	500549	69.68%	7.328%
23	7.970	2057	2062	2077	rVB2	8784	14107	1.96%	0.207%
24	8.179	2116	2127	2139	rBV2	44019	74959	10.44%	1.097%
25	8.552	2232	2243	2256	rBV2	44606	77551	10.80%	1.135%
26	8.632	2256	2268	2297	rBV	371741	707577	98.50%	10.359%
27	9.417	2497	2512	2539	rBV	322122	558702	77.78%	8.180%
28	10.754	2915	2928	2949	rBV	151516	240559	33.49%	3.522%
29	10.893	2963	2971	2983	rVB3	5580	8813	1.23%	0.129%
30	11.809	3244	3256	3284	rBV	293000	485702	67.61%	7.111%
31	12.063	3325	3335	3354	rBV3	24489	52315	7.28%	0.766%
32	12.192	3361	3375	3398	rBV	278749	466463	64.94%	6.829%

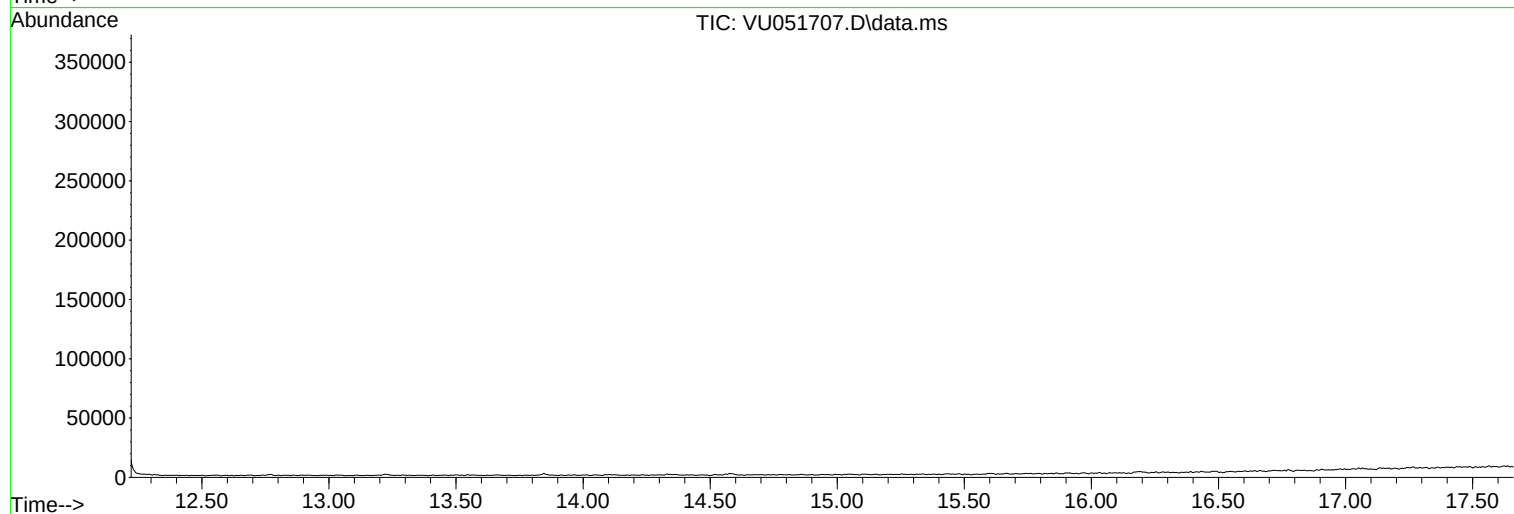
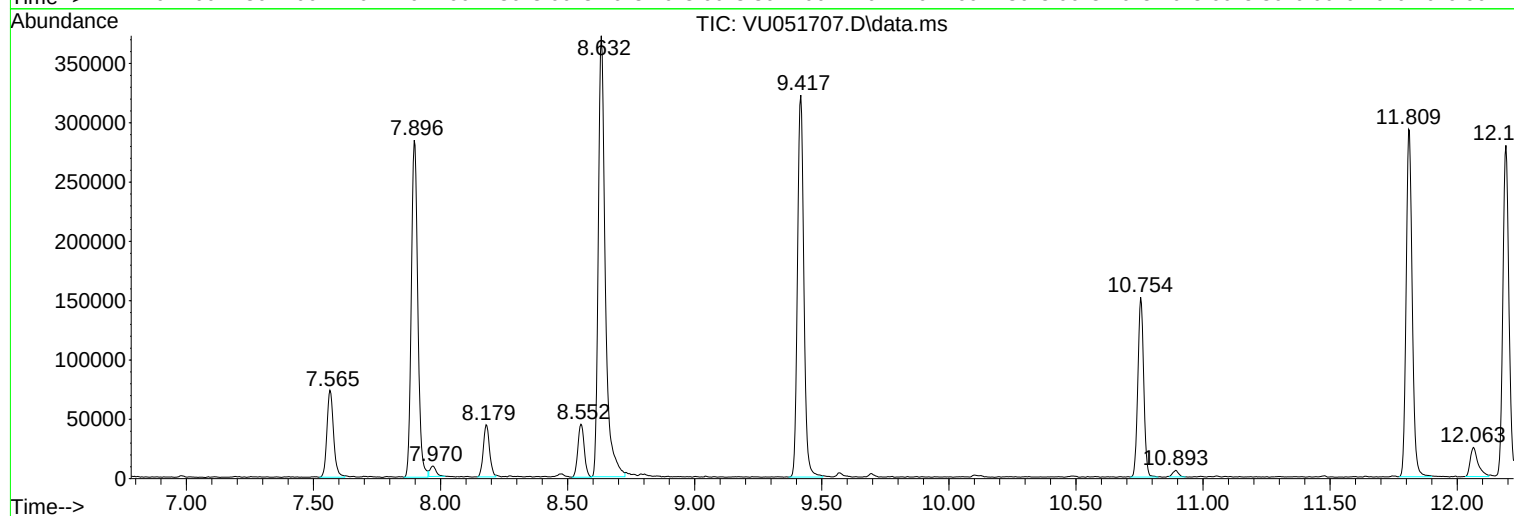
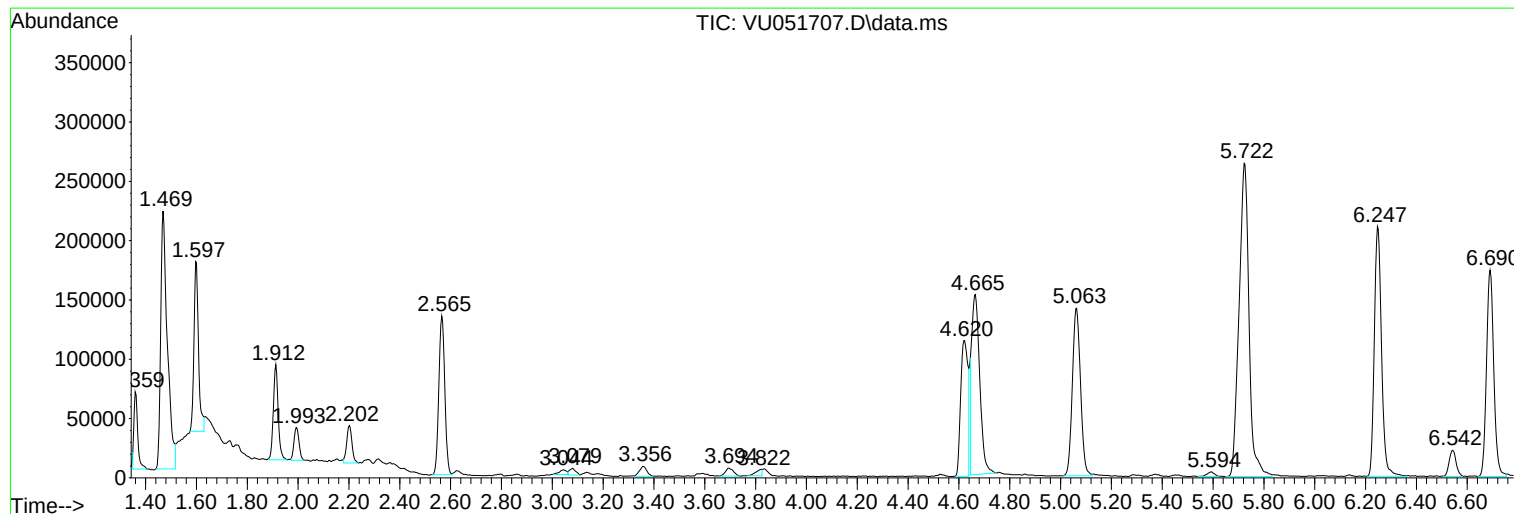
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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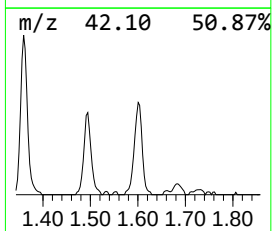
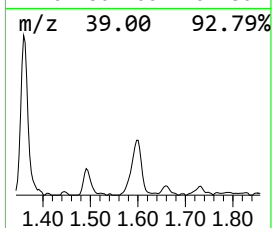
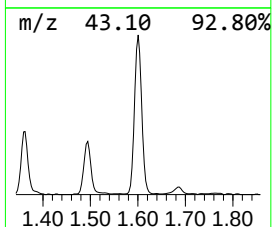
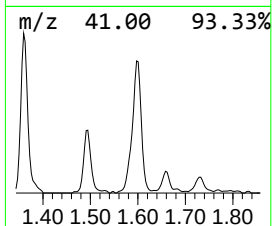
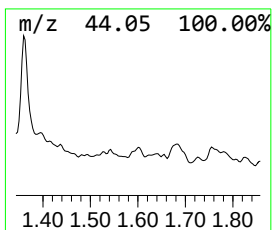
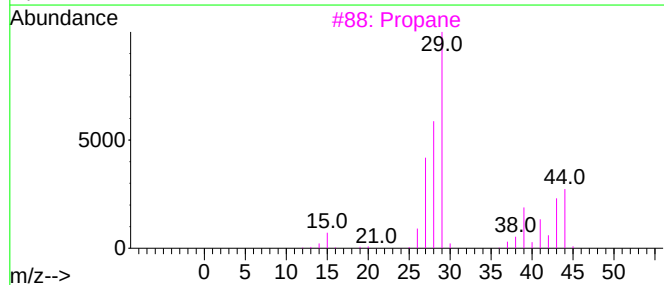
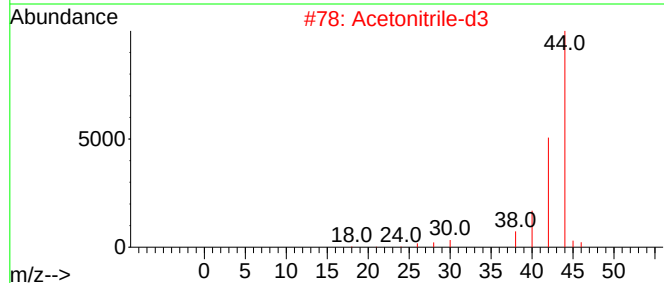
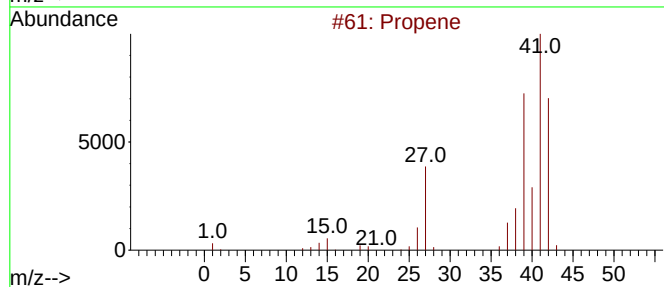
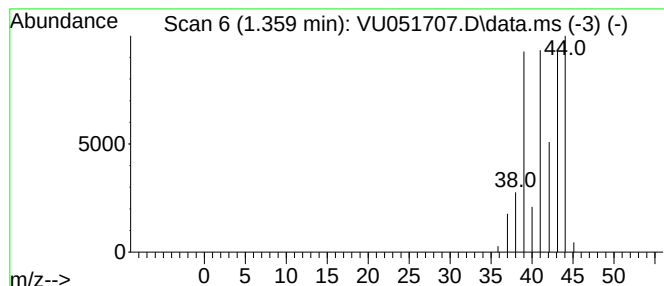
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	0.79 ug/L	65786	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	9
3			Propane	44	C3H8	000074-98-6	9
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

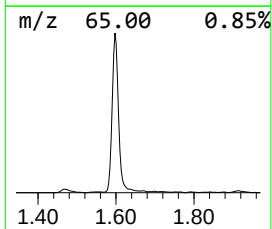
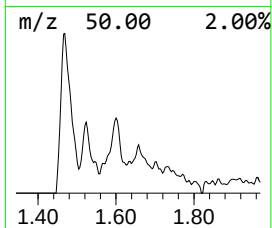
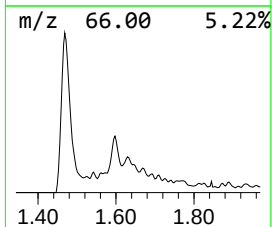
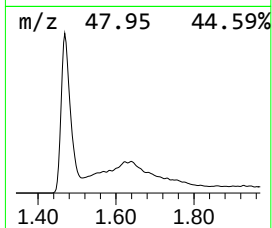
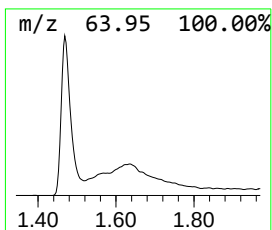
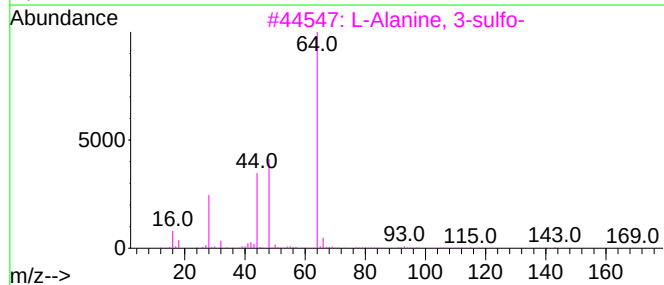
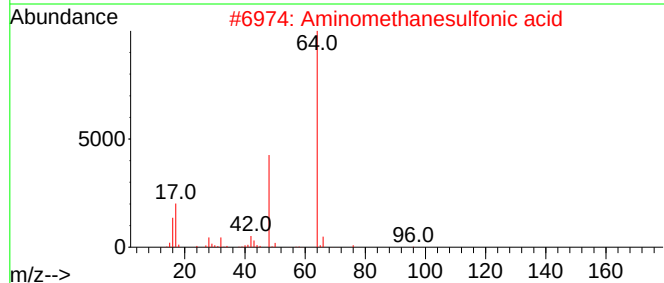
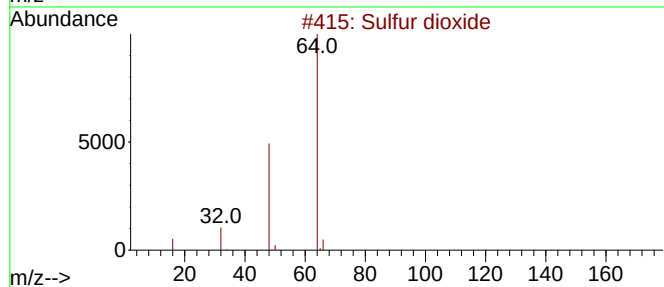
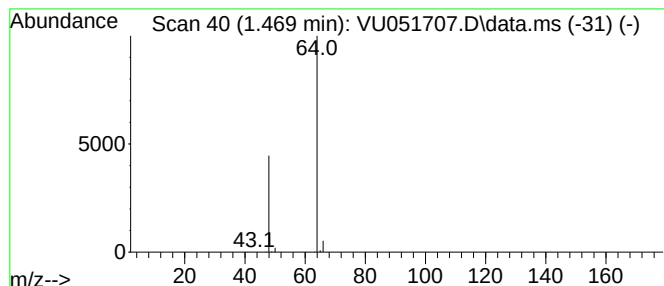
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.469	4.82 ug/L	398914	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			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

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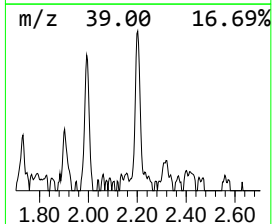
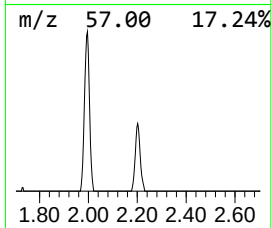
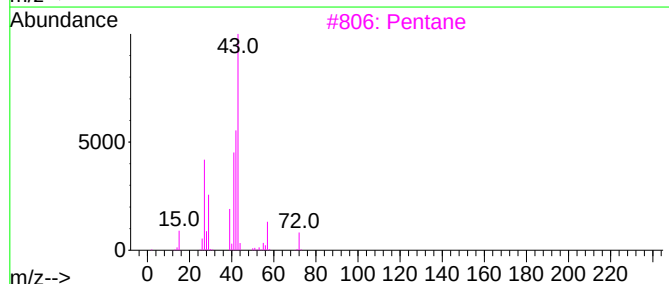
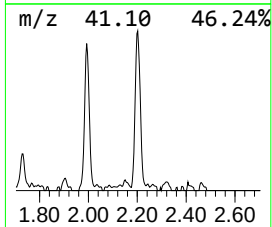
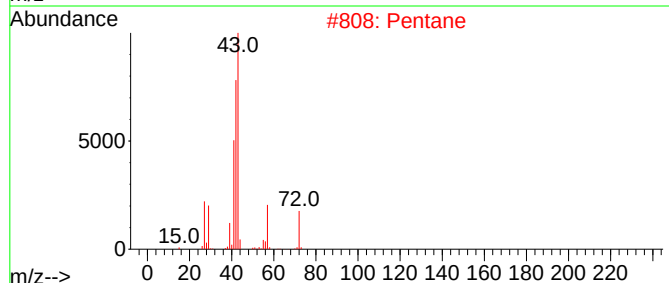
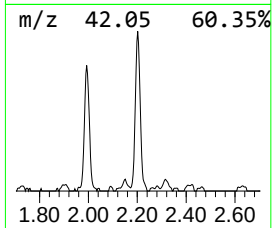
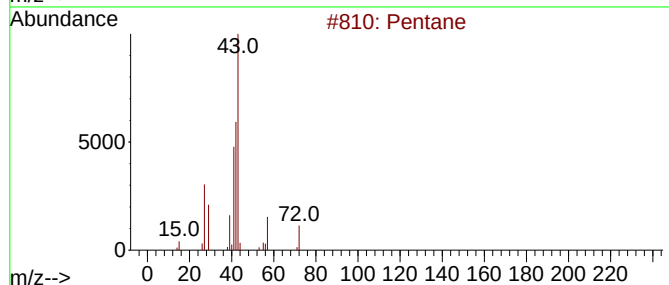
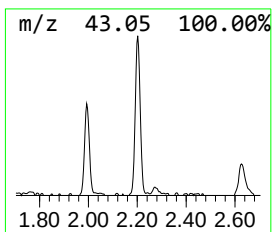
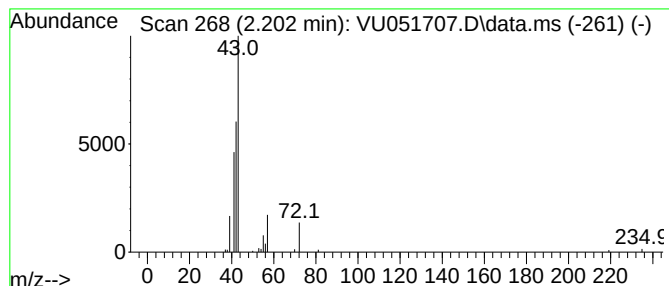
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.202	0.54 ug/L	44913	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	Pentane			72	C5H12	000109-66-0	78



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBXB2

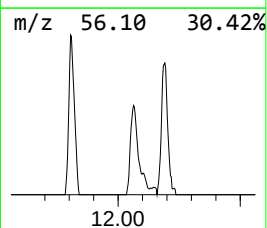
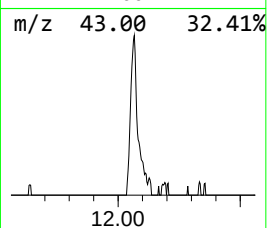
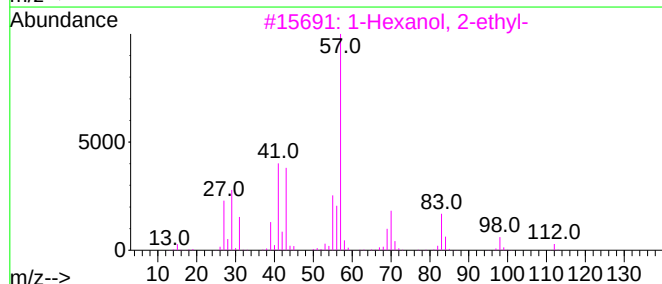
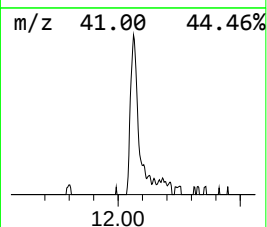
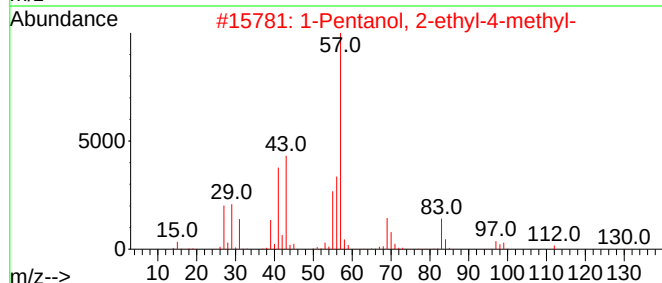
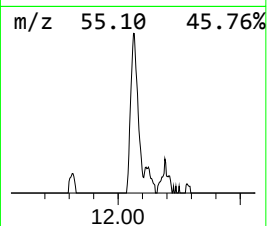
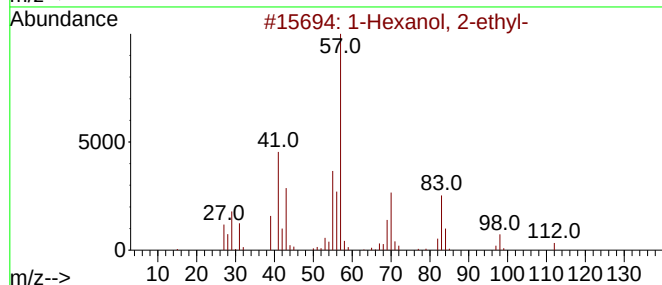
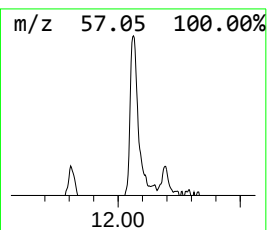
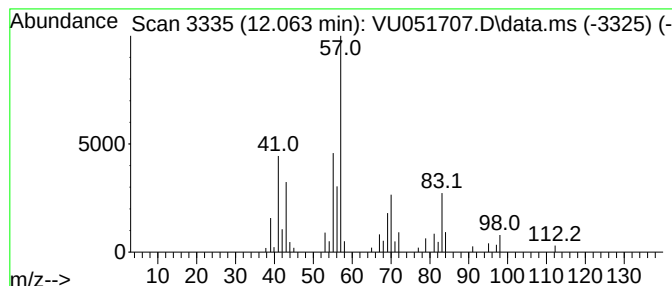
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	0.54 ug/L	52315	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	53



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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	65786	1	6.247	414186	5.0
Sulfur dioxide	1.469	4.8	ug/L	398914	1	6.247	414186	5.0
(DEL) Alkane: S...	2.202	0.5	ug/L	44913	1	6.247	414186	5.0
1-Hexanol, 2-et...	12.063	0.5	ug/L	52315	3	11.812	485702	5.0