

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
 Data File : VU051742.D
 Acq On : 03 Nov 2022 18:40
 Operator : JC/MD
 Sample : N5407-03
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4Y3

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: VU051742.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.511	44	53	56	rBV	24840	35387	3.71%	0.517%
2	1.553	56	66	92	rVV	257916	955018	100.00%	13.954%
3	1.662	96	100	113	rVB	84105	122023	12.78%	1.783%
4	1.800	139	143	152	rVB	60412	70695	7.40%	1.033%
5	1.987	196	201	221	rVB2	80855	148895	15.59%	2.176%
6	2.655	399	409	422	rVB	125331	208767	21.86%	3.050%
7	2.887	473	481	494	rVB2	22300	38668	4.05%	0.565%
8	4.771	1051	1067	1101	rVB2	60801	251584	26.34%	3.676%
9	5.144	1171	1183	1206	rVB2	126569	286782	30.03%	4.190%
10	5.832	1375	1397	1412	rBV3	237979	613317	64.22%	8.962%
11	5.893	1412	1416	1431	rVB	21316	32480	3.40%	0.475%
12	6.347	1544	1557	1575	rBV	204040	378683	39.65%	5.533%
13	6.774	1675	1690	1708	rBV	155580	299391	31.35%	4.375%
14	7.620	1941	1953	1975	rBV	65068	115793	12.12%	1.692%
15	7.945	2041	2054	2068	rBV	244570	419977	43.98%	6.137%
16	8.015	2069	2076	2089	rVB	12583	21929	2.30%	0.320%
17	8.221	2128	2140	2154	rBV	40259	70188	7.35%	1.026%
18	8.671	2263	2280	2305	rBV	326191	662425	69.36%	9.679%
19	9.440	2506	2519	2534	rBV	290174	485942	50.88%	7.100%
20	9.990	2649	2690	2691	rBV4	41345	133600	13.99%	1.952%
21	10.764	2918	2931	2945	rVB	136457	217278	22.75%	3.175%
22	10.896	2963	2972	2986	rVB	11482	18743	1.96%	0.274%
23	11.758	3229	3240	3246	rBV9	6261	12837	1.34%	0.188%
24	11.816	3247	3258	3276	rVB	296400	475093	49.75%	6.942%
25	12.063	3321	3335	3353	rBV2	38916	98253	10.29%	1.436%
26	12.195	3365	3376	3389	rBV	264289	420463	44.03%	6.144%
27	12.539	3474	3483	3504	rBV6	15152	34198	3.58%	0.500%
28	13.266	3700	3709	3724	rVB3	13116	25882	2.71%	0.378%
29	14.417	4059	4067	4075	rBV3	10080	15783	1.65%	0.231%
30	14.668	4132	4145	4151	rBV3	5997	13618	1.43%	0.199%
31	16.230	4624	4631	4642	rVV2	13358	19826	2.08%	0.290%
32	16.764	4787	4797	4808	rBV2	88204	140352	14.70%	2.051%

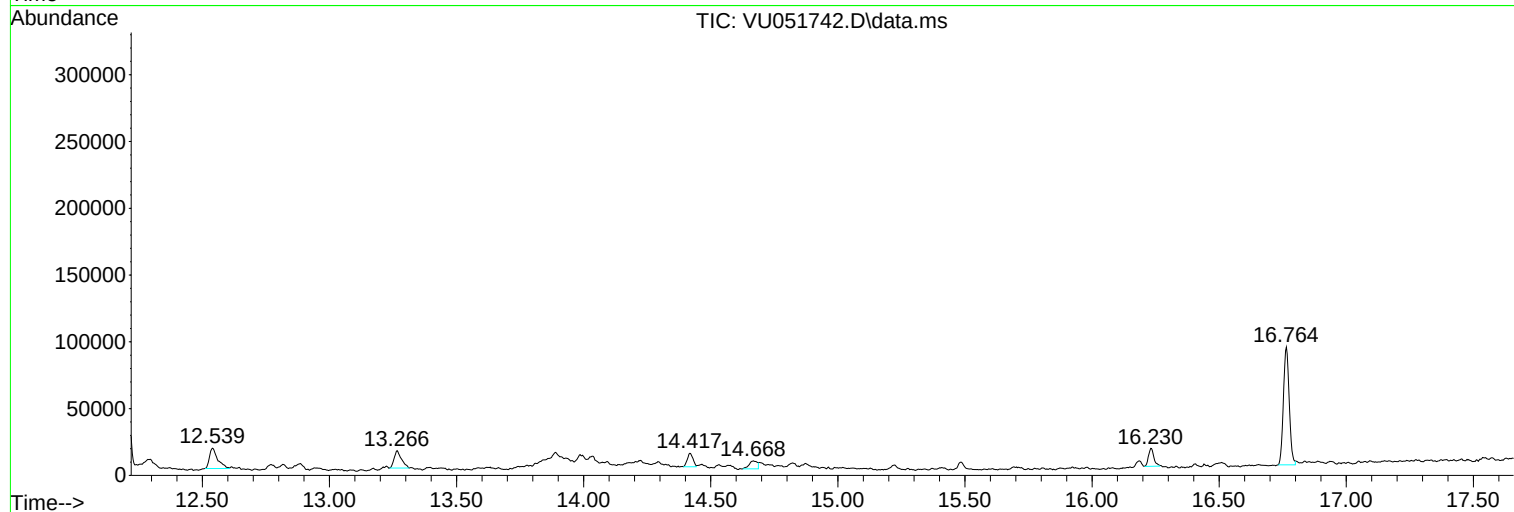
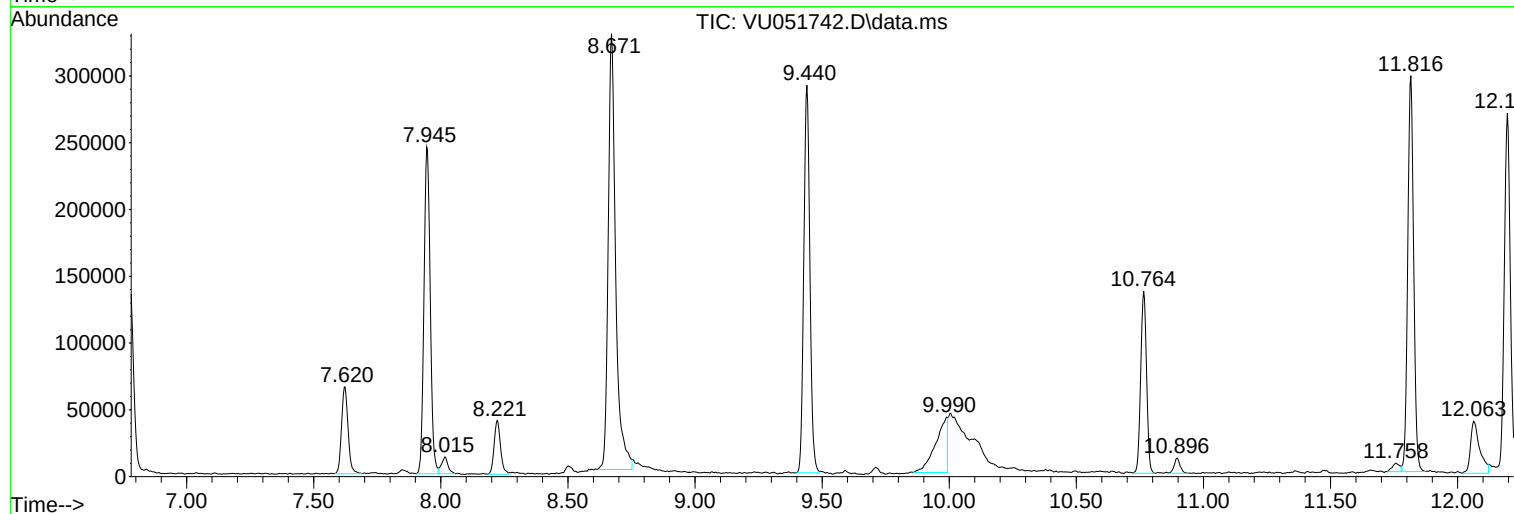
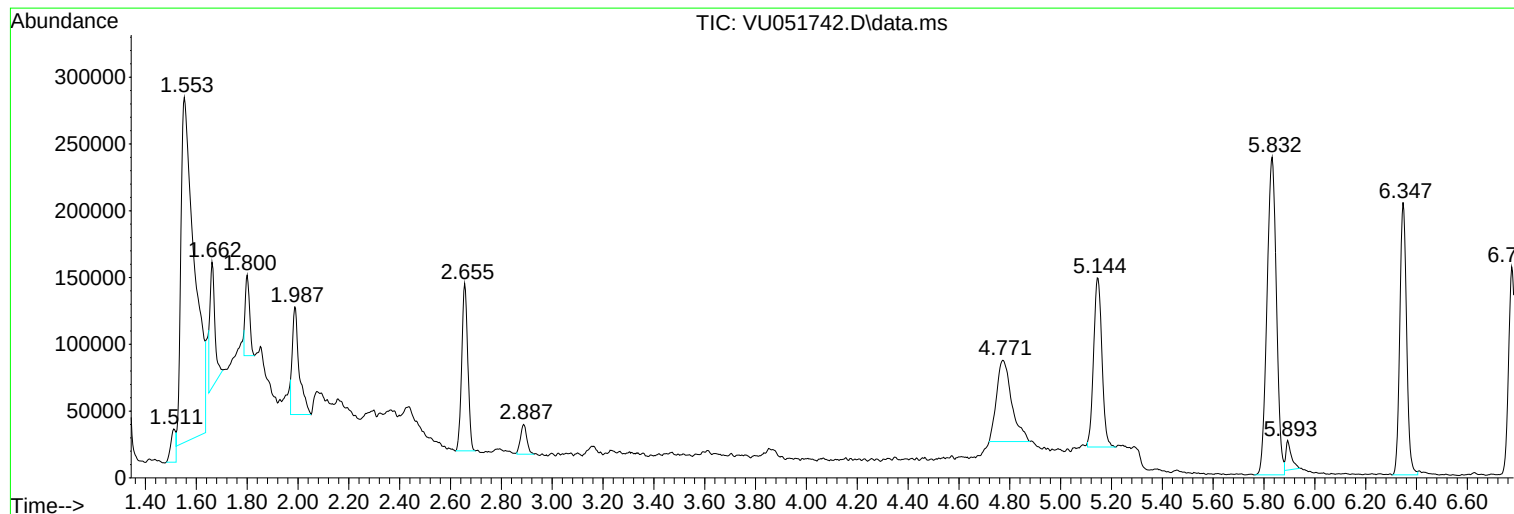
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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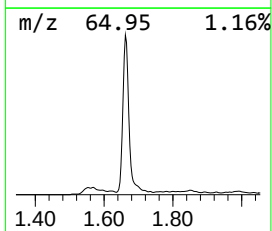
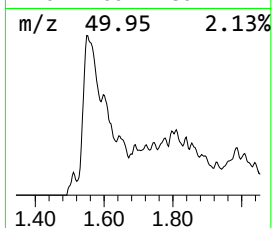
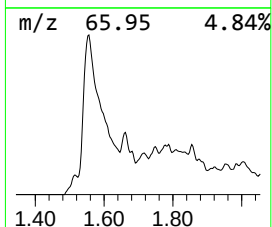
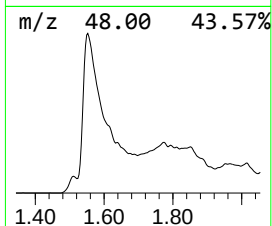
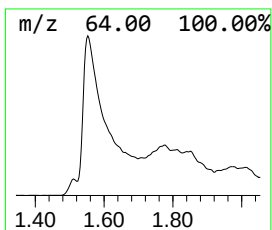
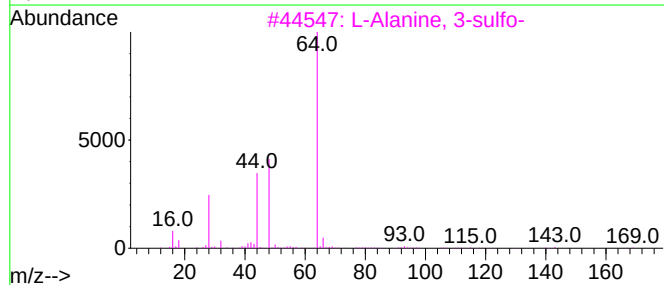
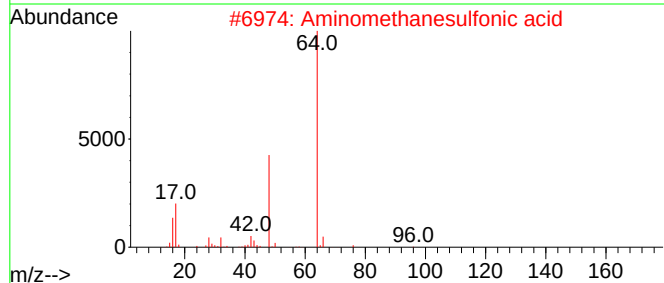
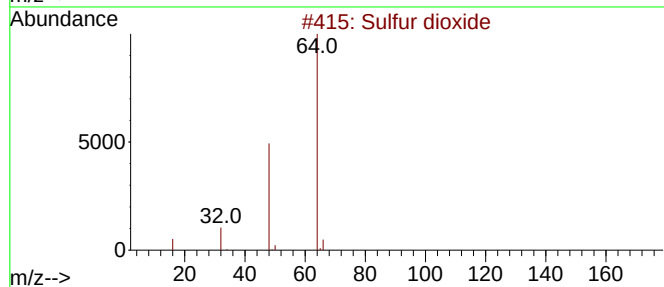
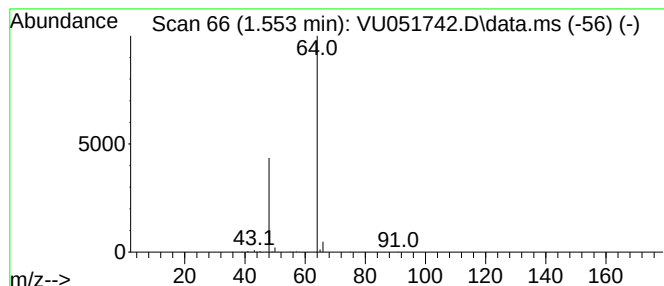
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.553	12.61 ug/L	955018	1,4-Difluorobenzene	6.347

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			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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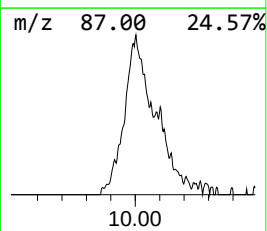
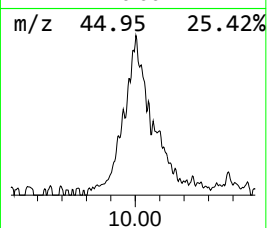
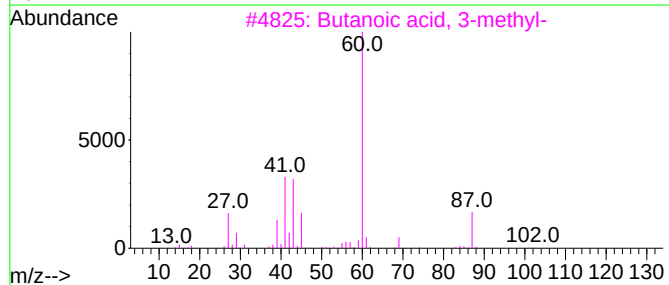
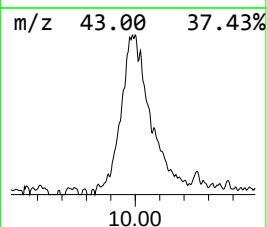
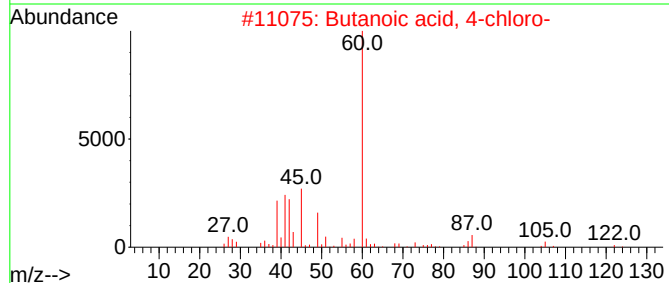
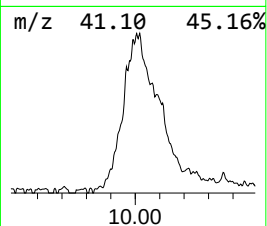
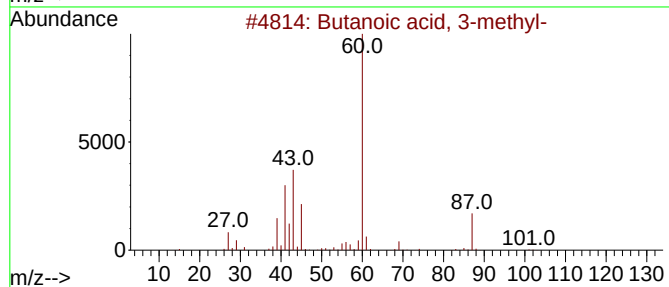
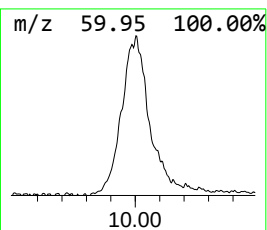
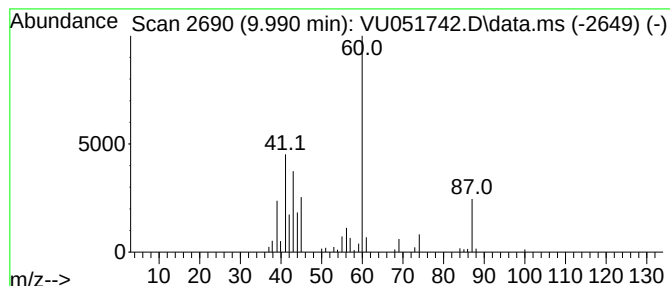
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Butanoic acid, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.990	1.37 ug/L	133600	Chlorobenzene-d5	9.440

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
2			Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	64
3			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59
4			Hexanoic acid	116	C6H12O2	000142-62-1	59
5			Pentanoic acid	102	C5H10O2	000109-52-4	59



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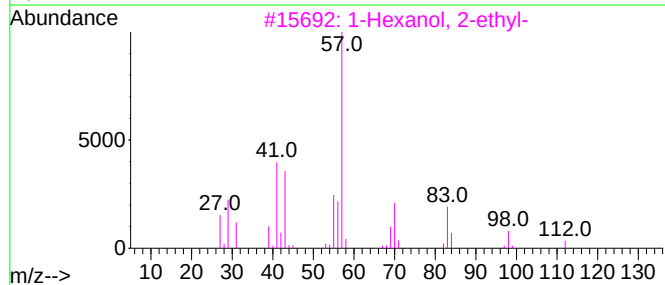
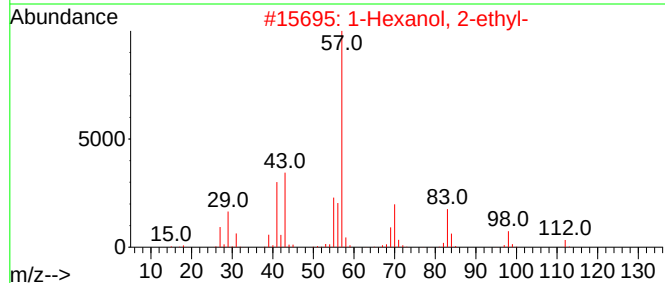
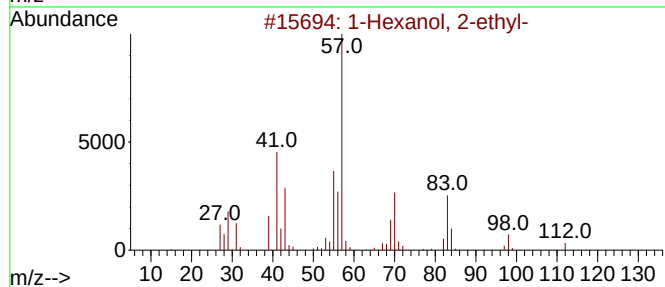
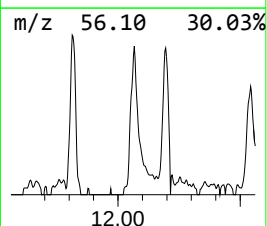
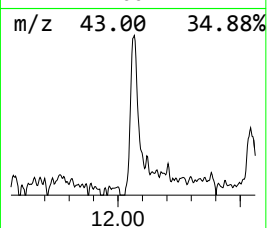
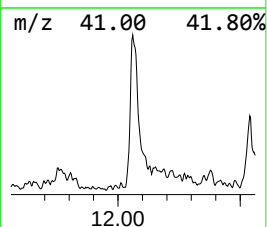
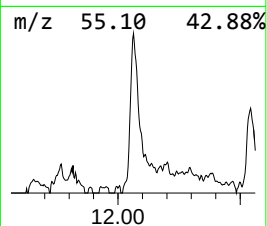
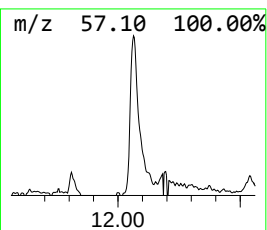
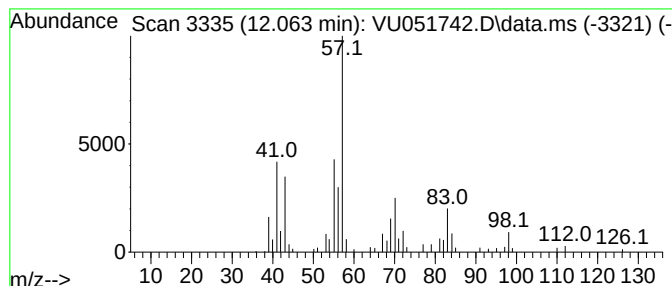
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	1.03 ug/L	98253	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	80
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	53
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53



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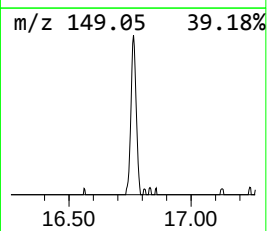
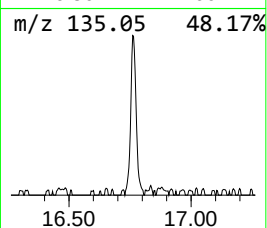
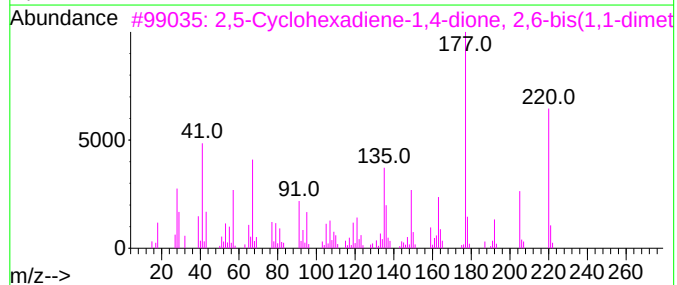
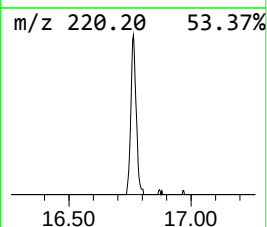
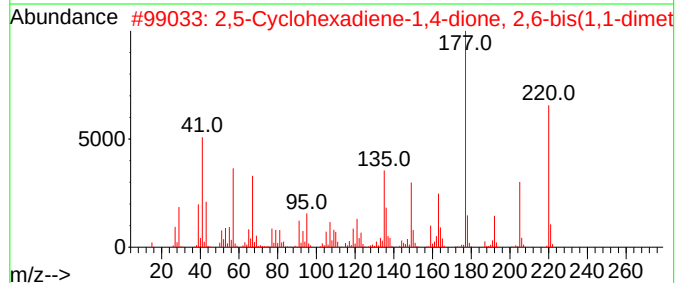
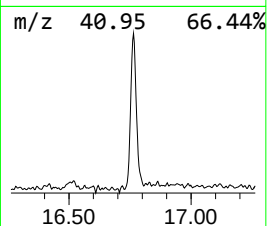
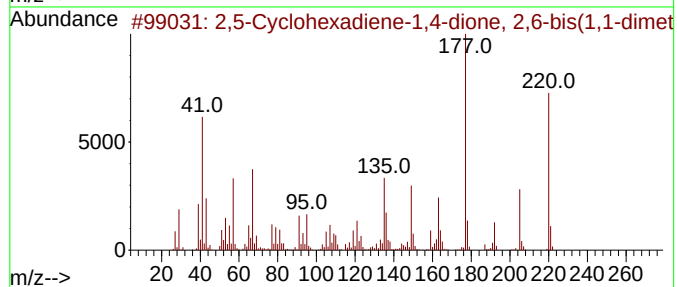
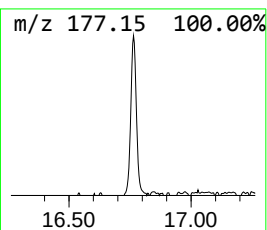
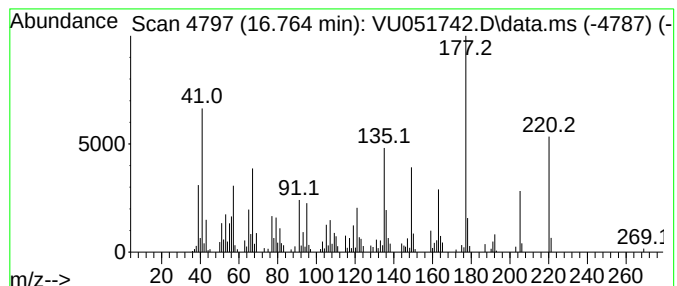
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.764	1.48 ug/L	140352	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	93		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	90		
5	2-Acetyl-3,4,5,6-tetrafluorobenz...	220	C9H4F402	1000461-12-2	45		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.553	12.6	ug/L	955018	1	6.347	378683	5.0
Butanoic acid, ...	9.990	1.4	ug/L	133600	2	9.440	485942	5.0
1-Hexanol, 2-et...	12.063	1.0	ug/L	98253	3	11.816	475093	5.0
2,5-Cyclohexadi...	16.764	1.5	ug/L	140352	3	11.816	475093	5.0