

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101823\
 Data File : VV032463.D
 Acq On : 18 Oct 2023 11:53
 Operator : SY/MD
 Sample : 04903-15
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AF8

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_V\Method\SFAMVTR092923WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV032463.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.101	11	19	33	rVB2	12152	20104	4.26%	0.423%
2	1.281	67	75	92	rVV	74049	84354	17.87%	1.774%
3	1.355	92	98	105	rVV	15020	19473	4.13%	0.410%
4	1.391	105	109	117	rVB4	4650	6033	1.28%	0.127%
5	1.535	146	154	165	rVB	62055	73565	15.59%	1.547%
6	2.063	307	318	331	rBV	106476	158691	33.62%	3.338%
7	2.127	332	338	347	rVV	8687	15966	3.38%	0.336%
8	2.182	348	355	366	rVB2	7361	14149	3.00%	0.298%
9	2.712	505	520	535	rVB5	5169	12380	2.62%	0.260%
10	2.889	564	575	593	rBV2	17304	37213	7.88%	0.783%
11	3.802	848	859	892	rBV	53705	165807	35.13%	3.488%
12	4.275	982	1006	1026	rBV3	113575	408122	86.47%	8.585%
13	4.963	1202	1220	1238	rBV2	159846	413804	87.67%	8.704%
14	5.246	1297	1308	1326	rBV3	15184	39073	8.28%	0.822%
15	5.429	1352	1365	1382	rBV4	14492	36942	7.83%	0.777%
16	5.539	1386	1399	1416	rBV	118222	248104	52.57%	5.219%
17	5.995	1527	1541	1554	rBV	90649	192467	40.78%	4.049%
18	6.436	1664	1678	1692	rBV	89656	179932	38.12%	3.785%
19	6.921	1817	1829	1856	rVV2	40651	91369	19.36%	1.922%
20	7.188	1900	1912	1920	rBV	11907	23912	5.07%	0.503%
21	7.246	1920	1930	1950	rVV	186376	353050	74.80%	7.426%
22	7.371	1961	1969	1987	rVB2	16251	34373	7.28%	0.723%
23	7.561	2019	2028	2035	rBV	24712	43503	9.22%	0.915%
24	7.882	2115	2128	2146	rBV	26008	53783	11.39%	1.131%
25	8.030	2164	2174	2207	rBV	225804	471993	100.00%	9.928%
26	8.182	2210	2221	2245	rVB	82672	168160	35.63%	3.537%
27	8.789	2399	2410	2430	rBV	191110	341413	72.33%	7.182%
28	8.956	2455	2462	2472	rVB3	5380	9236	1.96%	0.194%
29	9.082	2488	2501	2517	rBV2	8918	16892	3.58%	0.355%
30	9.493	2619	2629	2638	rVB5	4505	8489	1.80%	0.179%
31	9.670	2675	2684	2699	rBV	16605	27840	5.90%	0.586%
32	10.159	2823	2836	2852	rBV	72425	120428	25.51%	2.533%
33	10.329	2871	2889	2900	rBV2	53907	94899	20.11%	1.996%
34	10.394	2900	2909	2913	rBV8	3513	5305	1.12%	0.112%
35	10.455	2919	2928	2941	rVB2	16392	26488	5.61%	0.557%
36	10.680	2989	2998	3008	rVB2	2610	4733	1.00%	0.100%

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37	10.860	3044	3054	3062	rBV5	3744	5388	1.14%	0.113%
38	11.188	3145	3156	3177	rBV	203476	326519	69.18%	6.868%
39	11.500	3239	3253	3261	rBV6	9162	21649	4.59%	0.455%
40	11.564	3261	3273	3296	rVB	196525	319126	67.61%	6.713%
41	12.197	3460	3470	3483	rVB	24543	39333	8.33%	0.827%
42	12.297	3491	3501	3510	rBV	3510	6262	1.33%	0.132%
43	13.448	3852	3859	3868	rBV	5556	8681	1.84%	0.183%
44	13.988	4020	4027	4036	rBV3	3385	5027	1.07%	0.106%

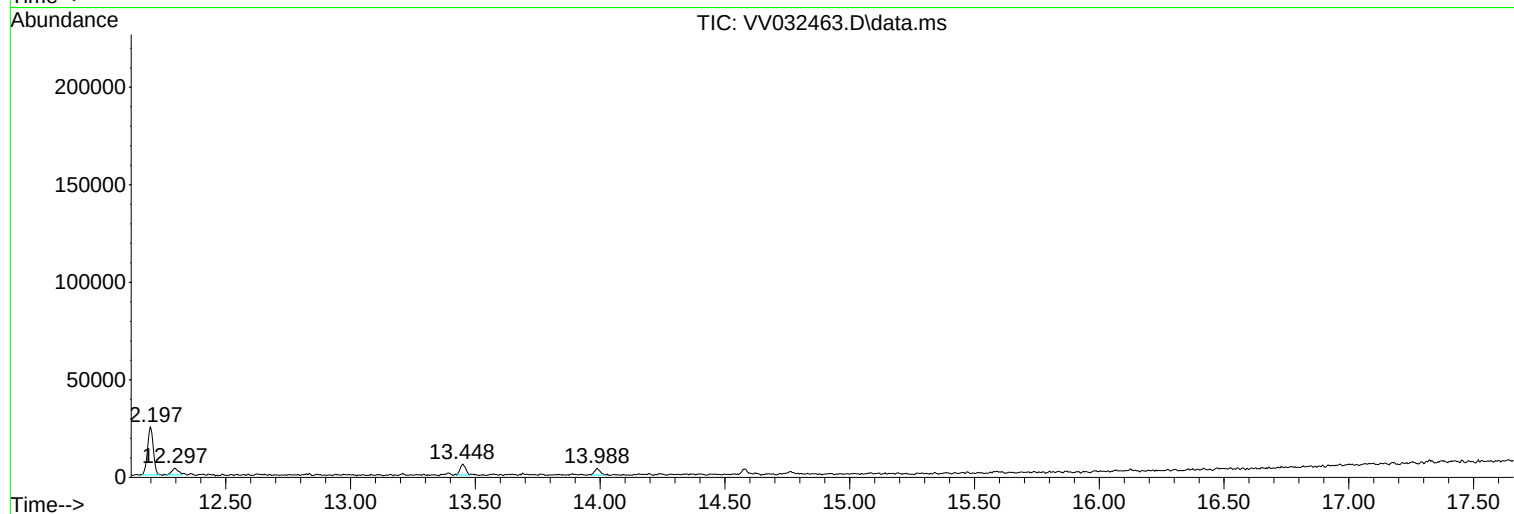
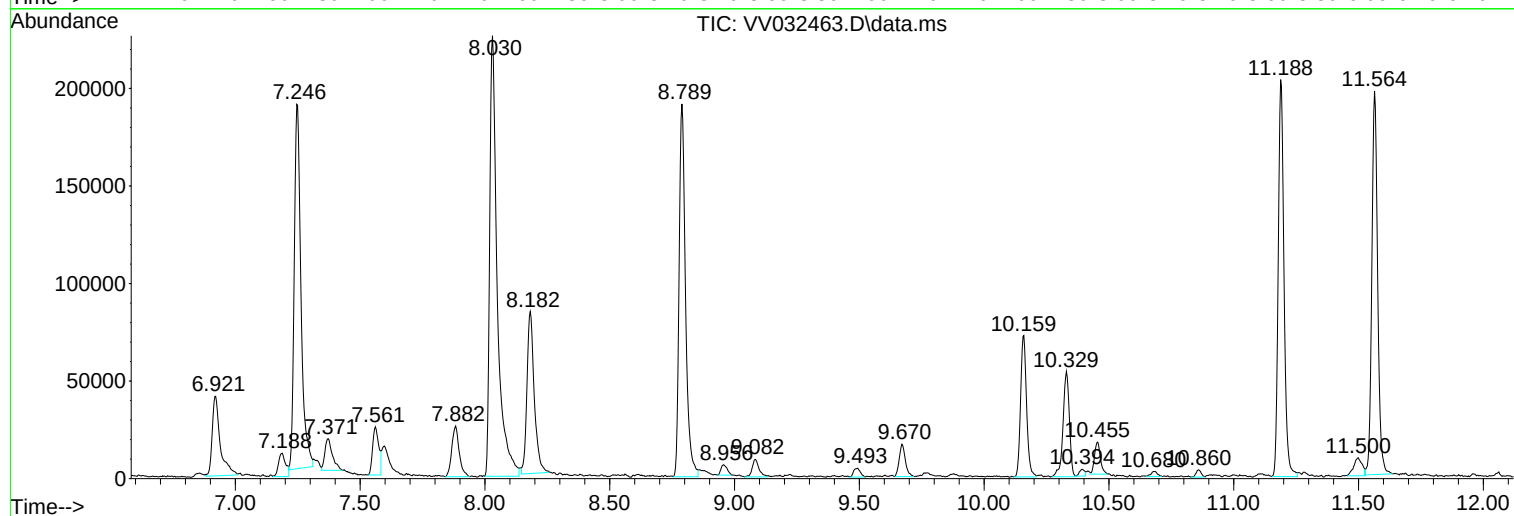
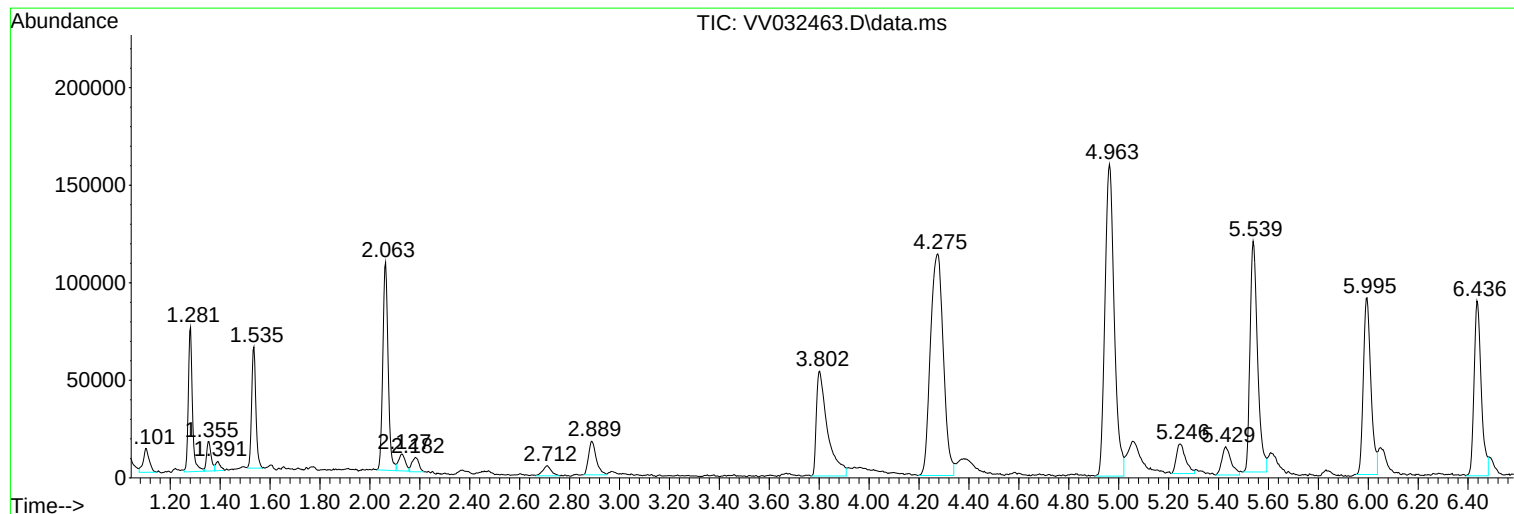
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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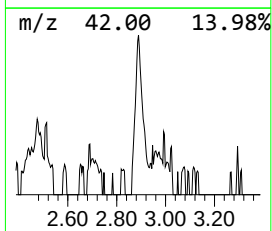
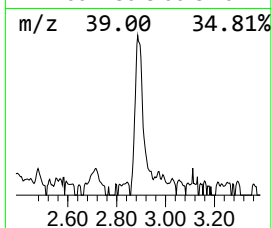
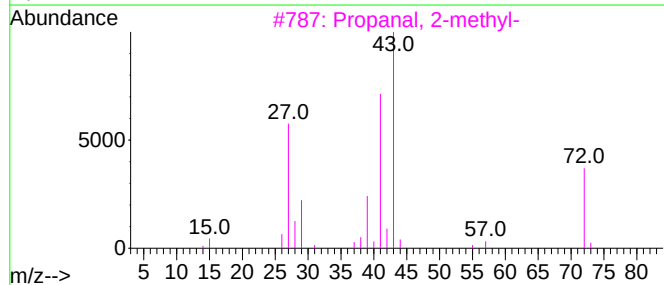
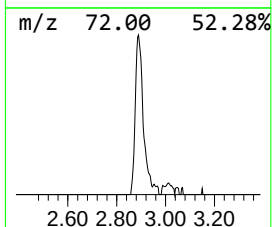
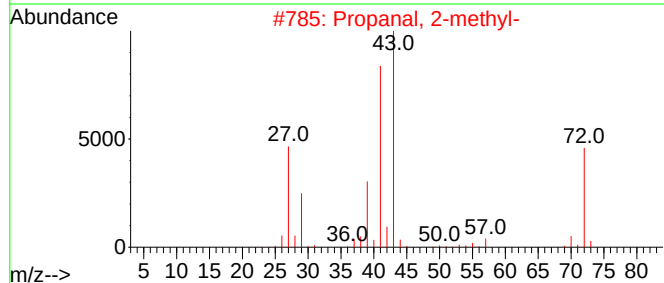
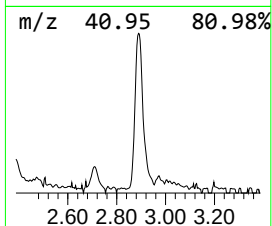
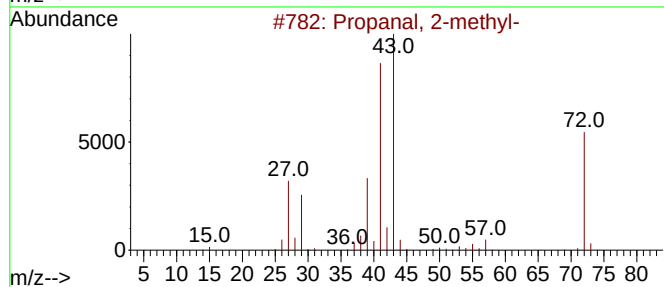
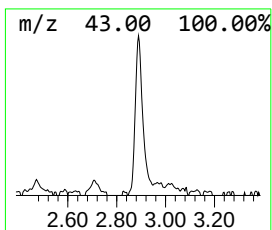
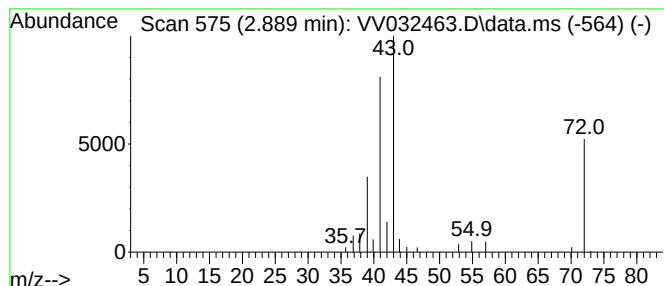
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Propanal, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.889	0.75 ug/L	37213	1,4-Difluorobenzene	5.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2-methyl-			72	C4H8O	000078-84-2	86
2	Propanal, 2-methyl-			72	C4H8O	000078-84-2	86
3	Propanal, 2-methyl-			72	C4H8O	000078-84-2	78
4	Propanal, 2-methyl-			72	C4H8O	000078-84-2	72
5	Butanal			72	C4H8O	000123-72-8	64



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Instrument :
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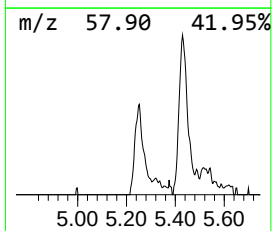
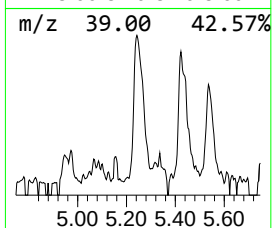
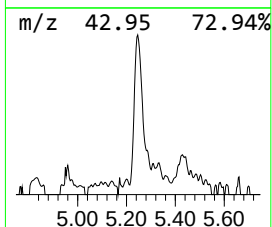
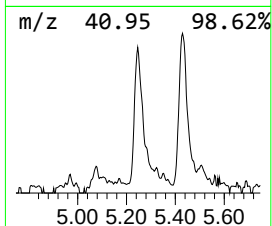
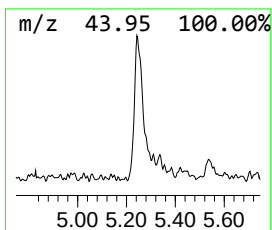
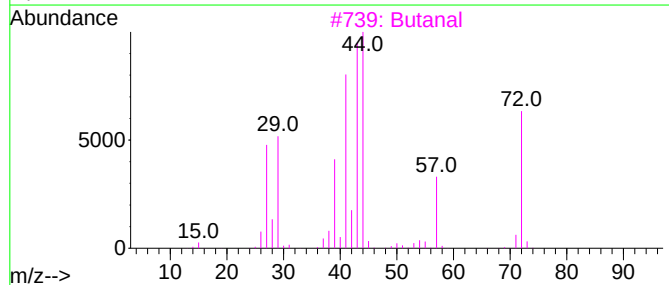
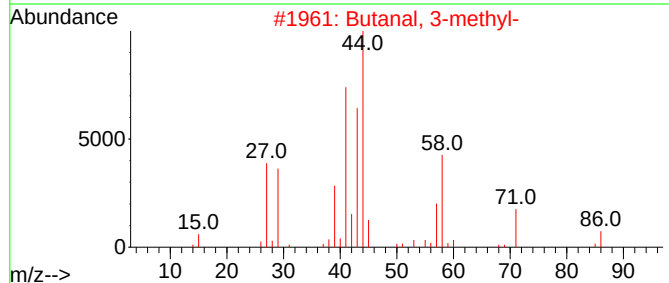
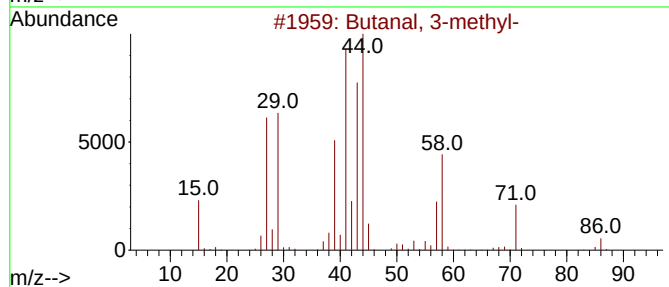
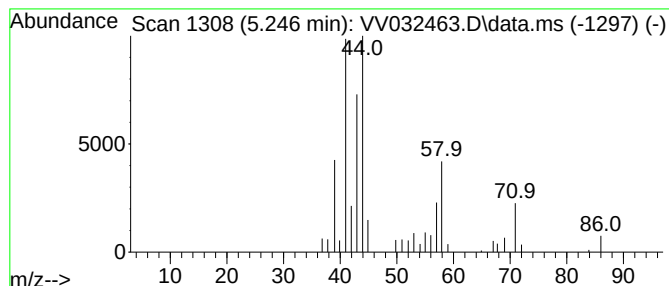
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Butanal, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.246	0.79 ug/L	39073	1,4-Difluorobenzene	5.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 3-methyl-	86	C5H10O	000590-86-3	94
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	81
3			Butanal	72	C4H8O	000123-72-8	47
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	46
5			Pentanal	86	C5H10O	000110-62-3	43



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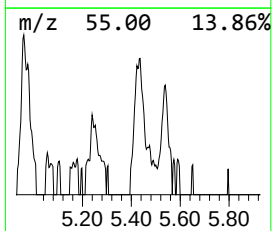
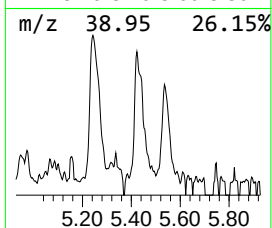
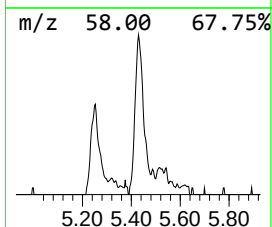
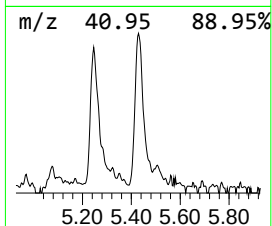
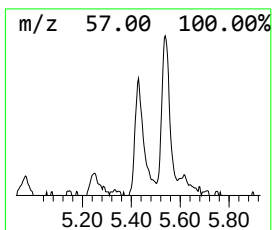
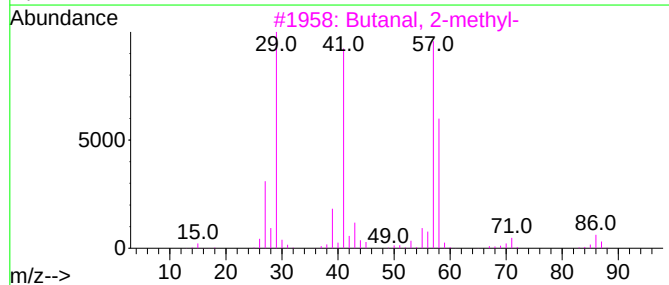
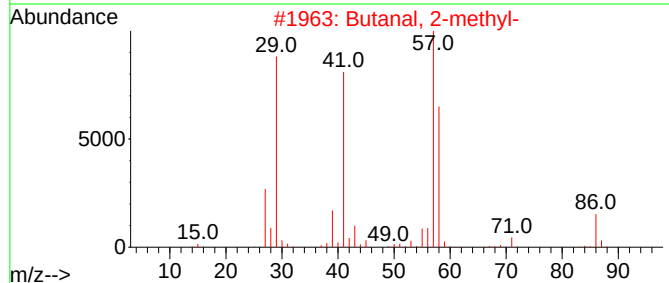
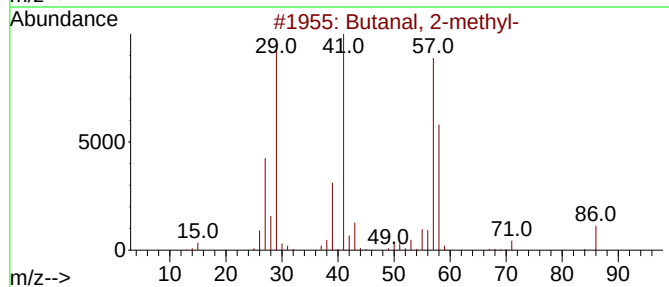
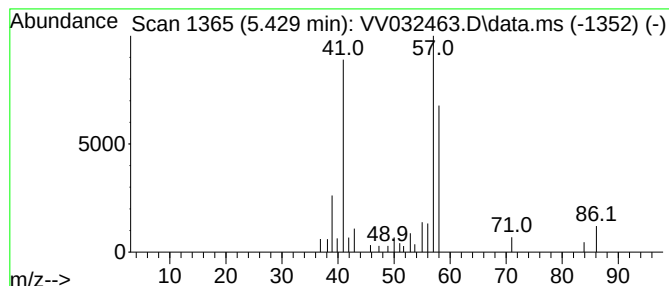
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanal, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.429	0.74 ug/L	36942	1,4-Difluorobenzene	5.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 2-methyl-	86	C5H10O	000096-17-3	80
2			Butanal, 2-methyl-	86	C5H10O	000096-17-3	80
3			Butanal, 2-methyl-	86	C5H10O	000096-17-3	72
4			Butane, 1-(2-propenyloxy)-	114	C7H14O	003739-64-8	38
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	35



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Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal, 2-met...	2.889	0.8	ug/L	37213	1	5.539	248104	5.0
Butanal, 3-methyl-	5.246	0.8	ug/L	39073	1	5.539	248104	5.0
Butanal, 2-methyl-	5.429	0.7	ug/L	36942	1	5.539	248104	5.0