

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
 Data File : VN080839.D
 Acq On : 31 Jan 2024 14:45
 Operator : JC\MD
 Sample : P1278-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 AUD-1316

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

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_N\methods\82N012924W.M
 Title : SW846 8260

Signal : TIC: VN080839.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	18	22	27	rVB	44053	64262	8.47%	1.297%
2	2.512	85	95	104	rBV4	9513	24745	3.26%	0.500%
3	2.665	115	121	127	rBV2	5330	9779	1.29%	0.197%
4	4.424	413	420	431	rBV2	7787	21758	2.87%	0.439%
5	7.224	883	896	906	rBV2	104166	287826	37.96%	5.810%
6	8.165	1047	1056	1061	rBV2	79567	190895	25.17%	3.854%
7	8.224	1061	1066	1076	rVB	142554	310129	40.90%	6.260%
8	8.577	1119	1126	1139	rVB3	103883	283888	37.44%	5.731%
9	9.100	1206	1215	1224	rBV	276059	556246	73.36%	11.229%
10	9.271	1238	1244	1250	rBV5	5107	9917	1.31%	0.200%
11	9.647	1300	1308	1316	rBV5	12353	32644	4.30%	0.659%
12	10.571	1456	1465	1471	rBV	338355	640018	84.40%	12.920%
13	10.635	1471	1476	1485	rVB3	26364	47873	6.31%	0.966%
14	11.300	1581	1589	1594	rBV5	25281	45566	6.01%	0.920%
15	11.865	1678	1685	1696	rBV	418825	758282	100.00%	15.307%
16	12.065	1712	1719	1727	rBV2	17820	33237	4.38%	0.671%
17	12.212	1737	1744	1747	rBV4	10063	17267	2.28%	0.349%
18	12.400	1769	1776	1777	rBV4	10164	14859	1.96%	0.300%
19	12.853	1845	1853	1863	rVB	247272	445530	58.76%	8.994%
20	13.341	1928	1936	1947	rBV	140039	228575	30.14%	4.614%
21	13.488	1956	1961	1965	rBV5	8352	13112	1.73%	0.265%
22	13.794	2006	2013	2022	rBV	372528	628863	82.93%	12.695%
23	13.870	2022	2026	2035	rVB3	20579	37742	4.98%	0.762%
24	14.959	2208	2211	2218	rVB5	6063	8189	1.08%	0.165%
25	15.035	2218	2224	2225	rBV2	7624	8525	1.12%	0.172%
26	15.059	2225	2228	2232	rVB4	7205	10716	1.41%	0.216%
27	15.212	2249	2254	2261	rBV4	6643	11044	1.46%	0.223%
28	15.394	2280	2285	2290	rVV4	24310	37881	5.00%	0.765%
29	15.829	2356	2359	2364	rVB6	10560	15686	2.07%	0.317%
30	15.941	2373	2378	2384	rBV8	10564	21967	2.90%	0.443%
31	16.129	2401	2410	2412	rBV7	9566	21305	2.81%	0.430%
32	16.164	2412	2416	2423	rVB5	18418	36962	4.87%	0.746%
33	16.335	2439	2445	2450	rBV7	6795	14462	1.91%	0.292%
34	16.506	2466	2474	2483	rBV10	13345	32752	4.32%	0.661%
35	16.711	2502	2509	2515	rBV6	10013	20413	2.69%	0.412%
36	16.782	2515	2521	2522	rBV3	8642	10893	1.44%	0.220%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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_N\methods\82N012924W.M
Title : SW846 8260

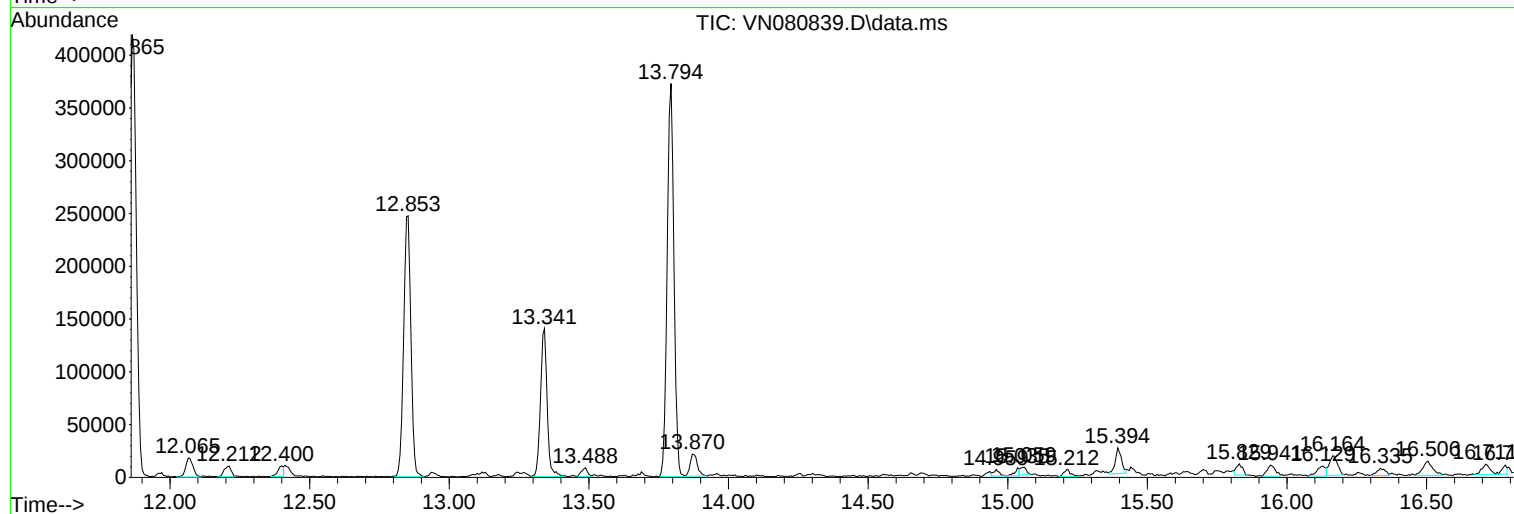
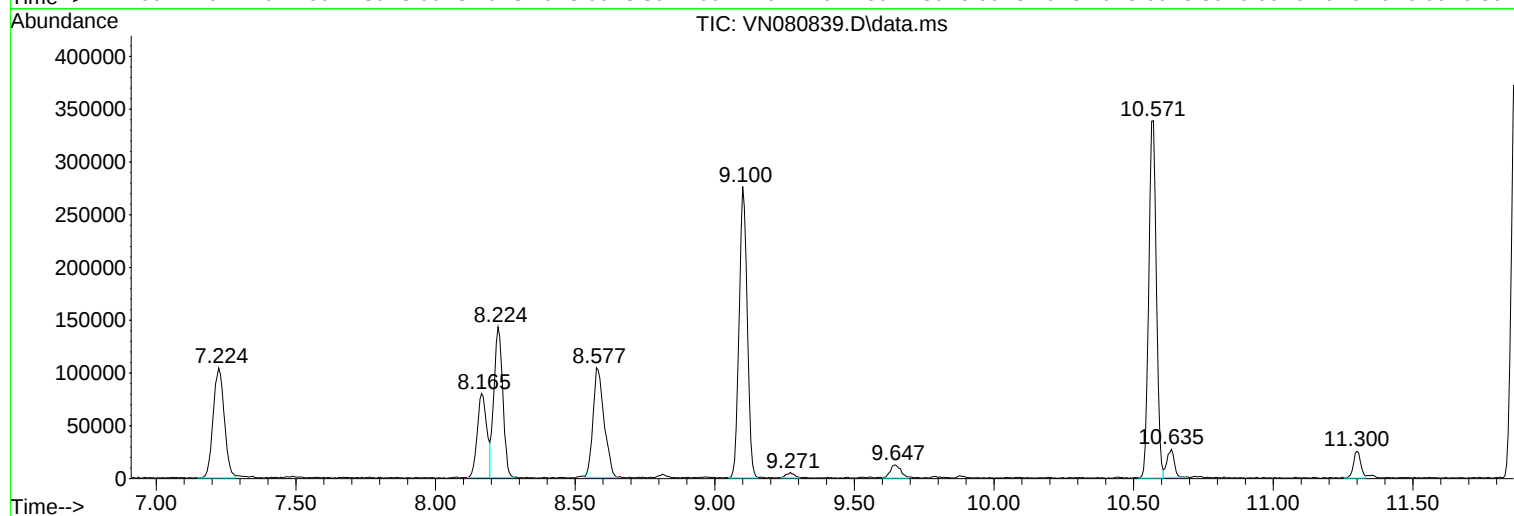
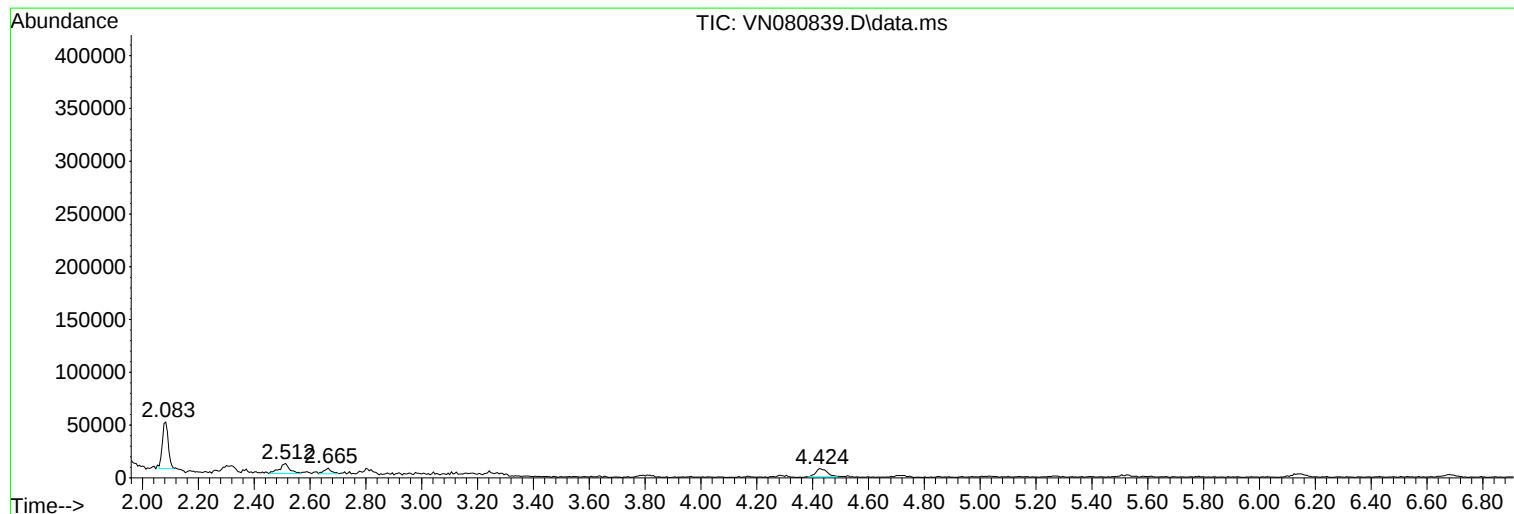
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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



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Instrument :
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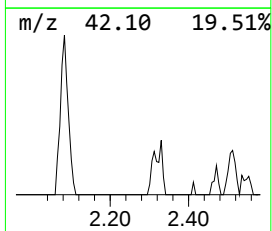
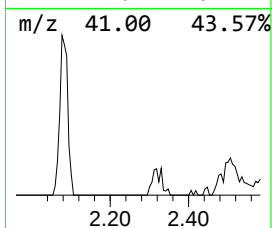
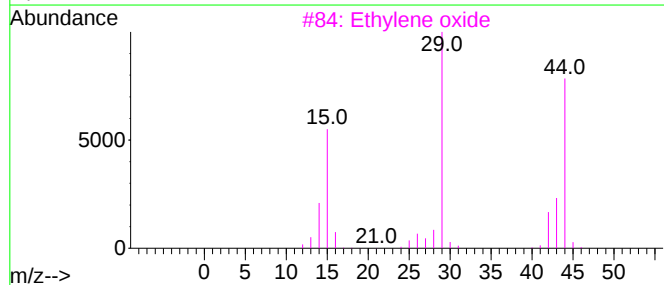
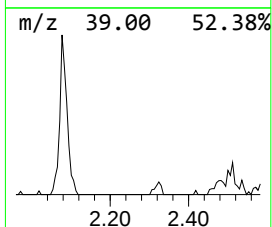
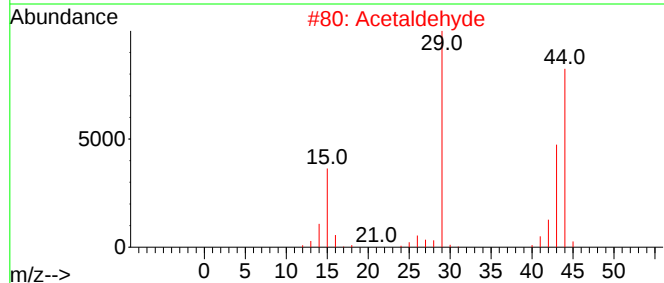
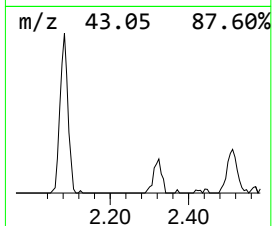
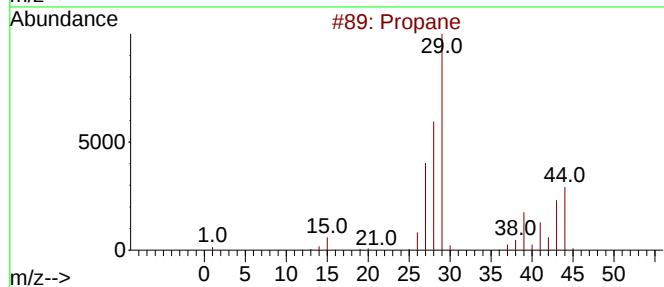
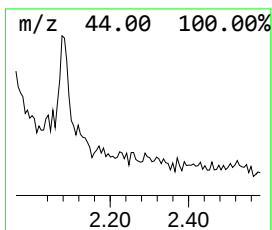
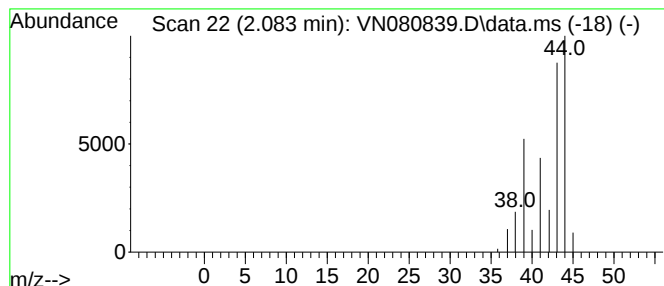
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	10.36 ug/l	64262	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	59
2			Acetaldehyde	44	C2H4O	000075-07-0	4
3			Ethylene oxide	44	C2H4O	000075-21-8	4
4			Hydrogen isocyanate	43	CHNO	000075-13-8	3
5			Acetonitrile-d3	44	C2D3N	002206-26-0	3



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Instrument :
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ClientSampleId :
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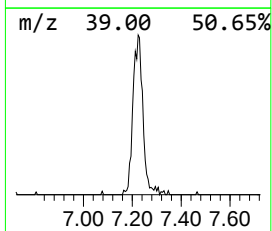
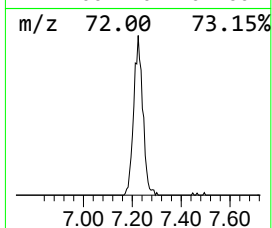
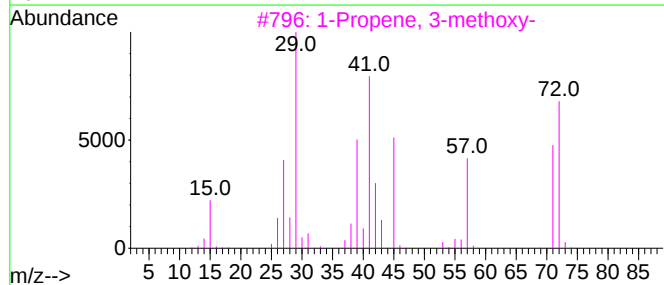
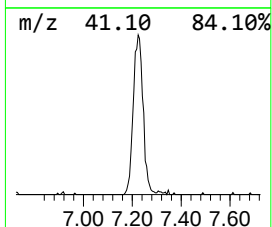
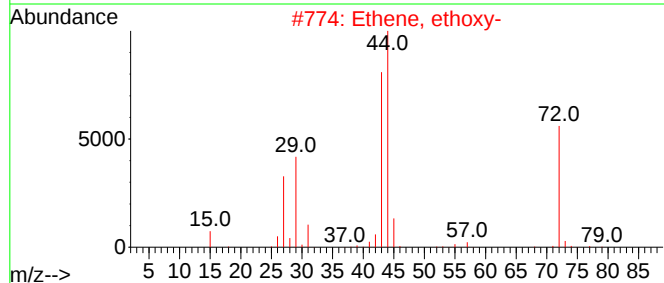
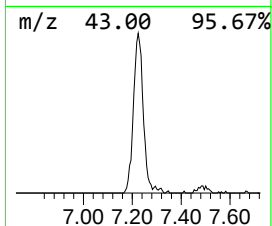
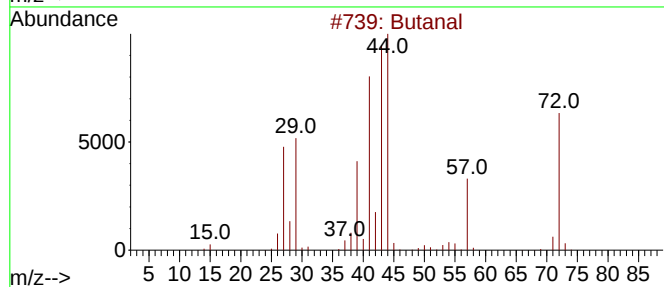
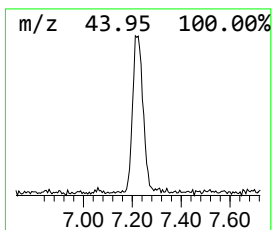
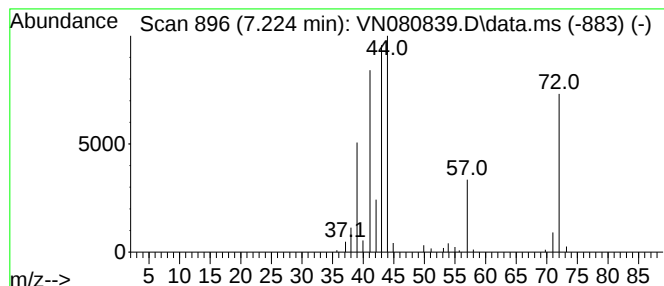
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Peak Number 2 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	46.40 ug/l	287826	Pentafluorobenzene	8.224

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	91
2		Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	49
4		Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5		Isobutylene epoxide	72	C4H8O	000558-30-5	16



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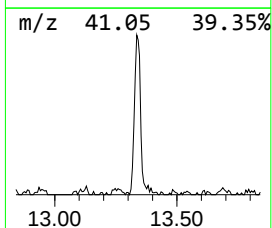
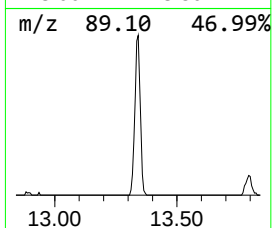
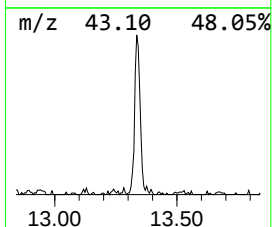
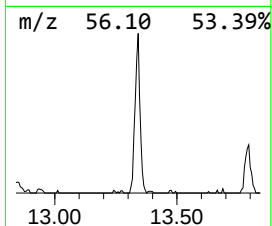
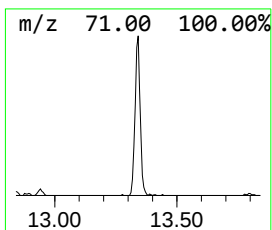
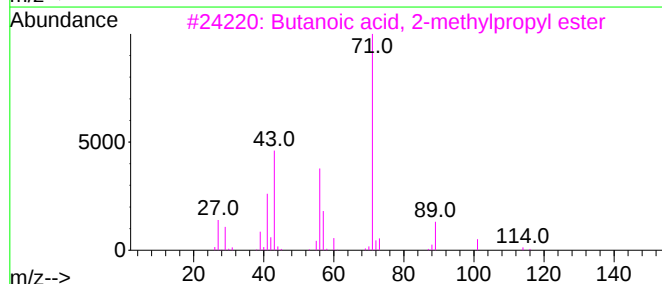
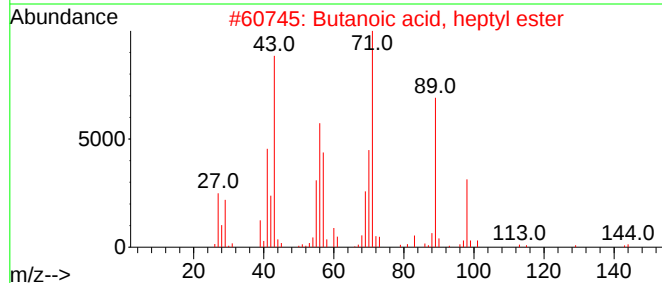
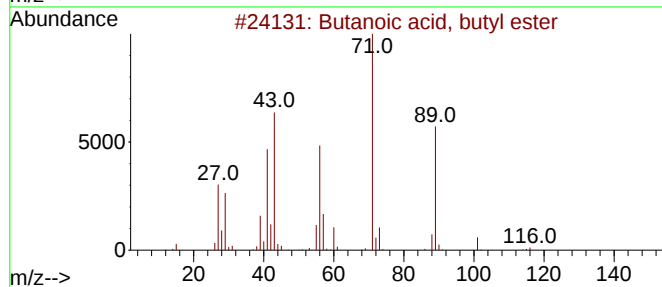
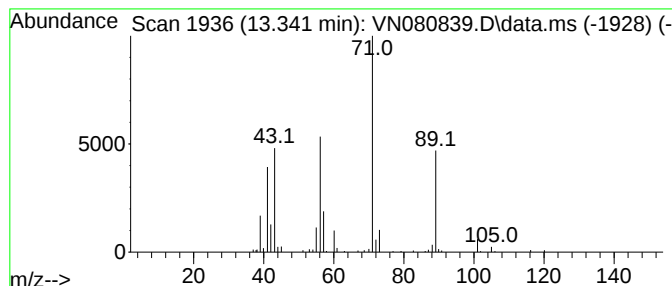
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	18.17 ug/l	228575	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
3			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
4			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
5			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	42



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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
Propane	2.083	10.4	ug/l	64262	1	8.224	310129	50.0
Butanal	7.224	46.4	ug/l	287826	1	8.224	310129	50.0
Butanoic acid, ...	13.341	18.2	ug/l	228575	4	13.794	628863	50.0