

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
 Data File : VN081859.D
 Acq On : 25 Apr 2024 18:40
 Operator : JC\MD
 Sample : P2257-10
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 413C

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\82N042524W.M
 Title : SW846 8260

Signal : TIC: VN081859.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	17	22	29	rBV	70512	104225	5.43%	0.821%
2	4.430	413	421	430	rBV2	12613	38935	2.03%	0.307%
3	4.712	461	469	478	rVB4	10782	32361	1.69%	0.255%
4	7.224	884	896	906	rBV2	90236	254544	13.27%	2.005%
5	8.165	1046	1056	1061	rBV	174511	415403	21.65%	3.273%
6	8.224	1061	1066	1076	rVB2	320364	697148	36.33%	5.492%
7	8.577	1112	1126	1134	rBV	212608	491074	25.59%	3.869%
8	8.653	1134	1139	1140	rBV2	21838	27168	1.42%	0.214%
9	9.100	1207	1215	1228	rVB	498390	1019592	53.13%	8.033%
10	9.271	1238	1244	1257	rBV2	17012	41274	2.15%	0.325%
11	9.659	1304	1310	1316	rVB3	13073	24976	1.30%	0.197%
12	10.565	1456	1464	1472	rBV	725820	1402140	73.07%	11.046%
13	10.629	1472	1475	1482	rVB3	15760	27405	1.43%	0.216%
14	11.865	1671	1685	1696	rVB	660593	1280287	66.72%	10.086%
15	12.065	1714	1719	1726	rVB2	21892	44300	2.31%	0.349%
16	12.418	1768	1779	1789	rBV	161618	311665	16.24%	2.455%
17	12.853	1842	1853	1863	rBV	515677	942331	49.11%	7.424%
18	12.941	1863	1868	1873	rVV2	21691	34284	1.79%	0.270%
19	13.088	1886	1893	1897	rBV4	15123	28455	1.48%	0.224%
20	13.241	1912	1919	1922	rBV2	80425	135393	7.06%	1.067%
21	13.270	1922	1924	1929	rVV2	68237	89549	4.67%	0.705%
22	13.335	1929	1935	1943	rVB	1248050	1918910	100.00%	15.118%
23	13.482	1956	1960	1965	rBV3	19142	33816	1.76%	0.266%
24	13.535	1965	1969	1978	rVV4	21668	42041	2.19%	0.331%
25	13.629	1978	1985	1990	rVV8	8998	20602	1.07%	0.162%
26	13.682	1990	1994	1999	rVB5	13200	26873	1.40%	0.212%
27	13.794	2006	2013	2020	rBV	593614	1040912	54.24%	8.201%
28	13.870	2020	2026	2034	rVV	1151732	1850162	96.42%	14.576%
29	13.953	2036	2040	2046	rVB5	36121	64889	3.38%	0.511%
30	14.176	2072	2078	2085	rBV7	9765	22446	1.17%	0.177%
31	14.253	2085	2091	2095	rBV4	22152	36823	1.92%	0.290%
32	14.753	2171	2176	2180	rBV4	24605	44240	2.31%	0.349%
33	15.394	2281	2285	2291	rVB3	30780	51392	2.68%	0.405%
34	15.464	2291	2297	2303	rBV5	25825	49539	2.58%	0.390%
35	15.653	2327	2329	2337	rVB7	12786	21082	1.10%	0.166%
36	16.117	2402	2408	2416	rVB6	14457	26957	1.40%	0.212%

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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\82N042524W.M
Title : SW846 8260

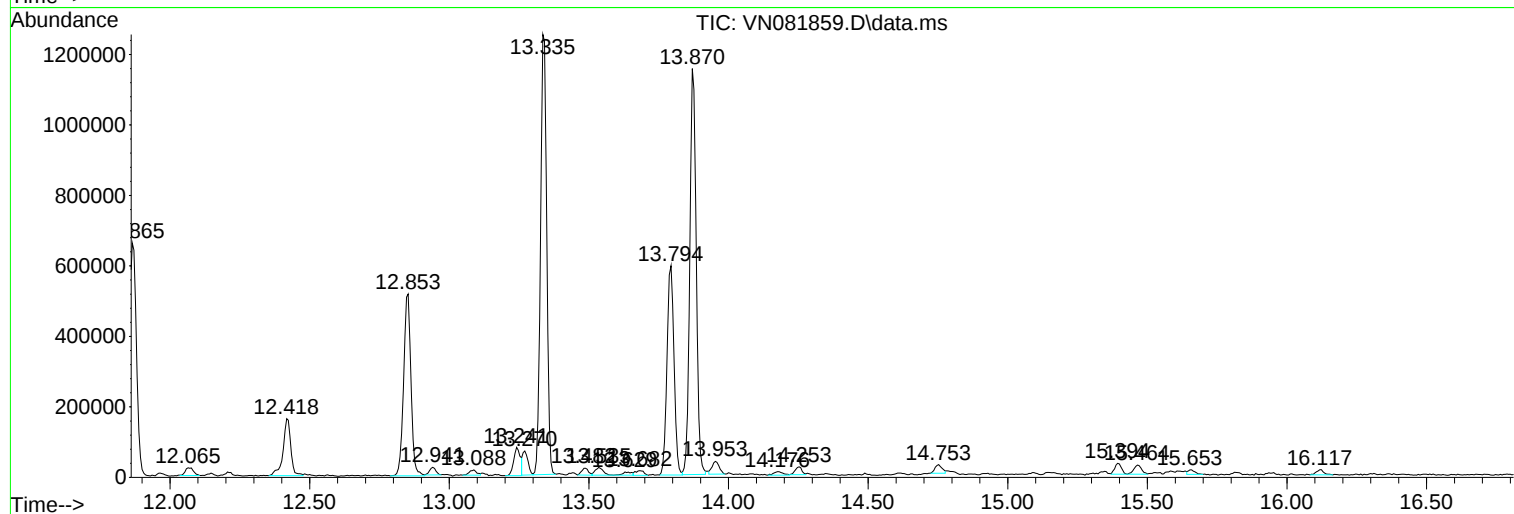
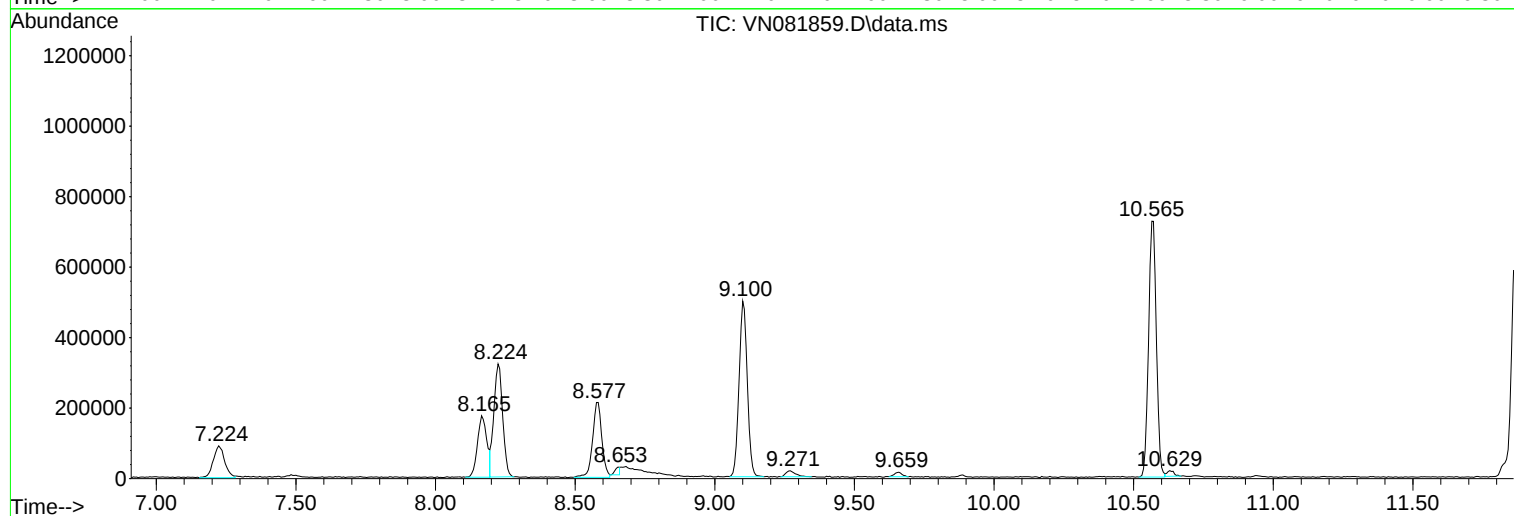
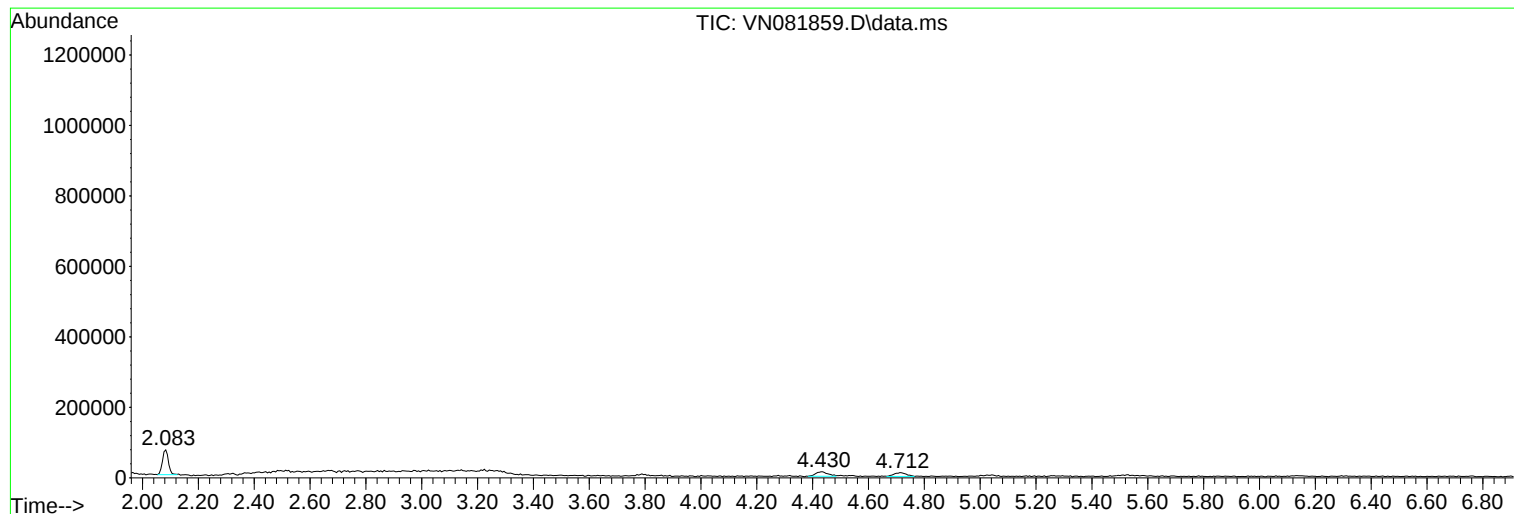
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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



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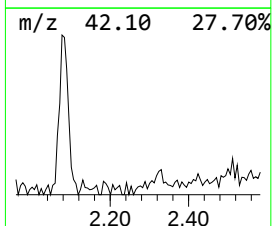
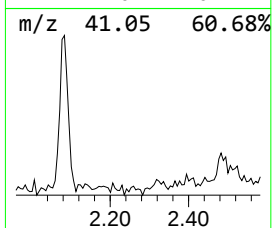
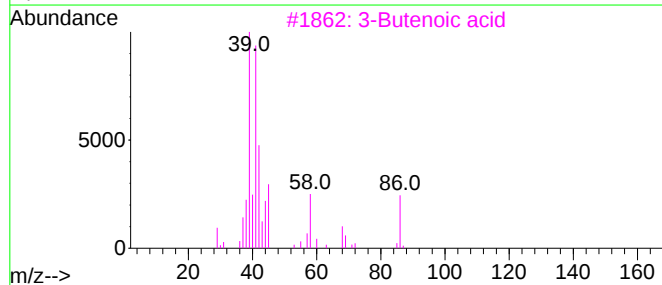
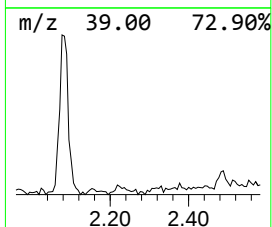
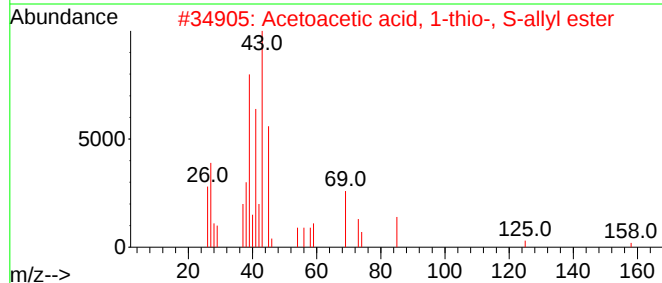
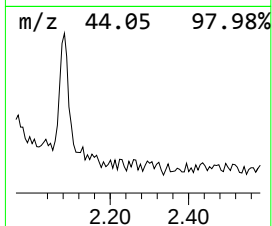
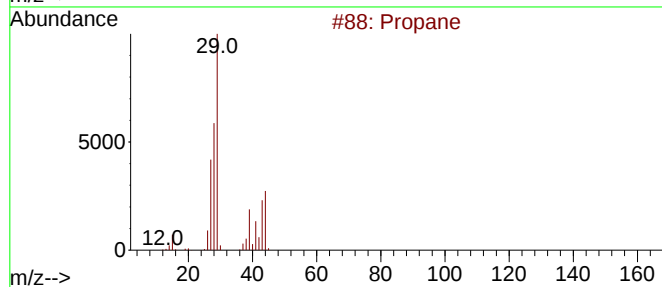
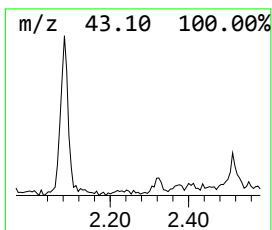
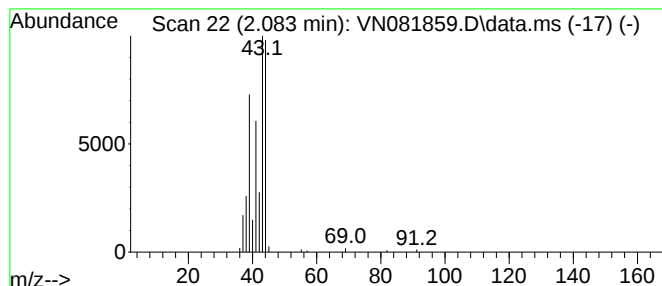
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	7.48 ug/l	104225	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	83
2			Acetoacetic acid, 1-thio-, S-all...	158	C7H10O2S	015780-65-1	40
3			3-Butenoic acid	86	C4H6O2	000625-38-7	16
4			2-Butynal	68	C4H4O	001119-19-3	9
5			2-Butenal	70	C4H6O	004170-30-3	9



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Instrument :
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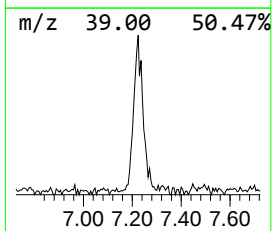
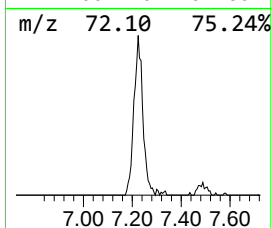
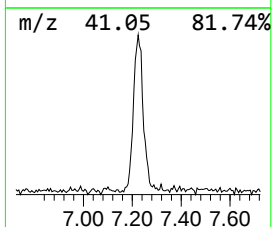
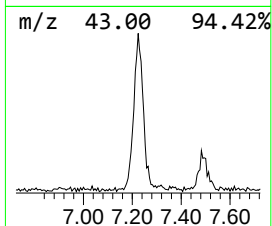
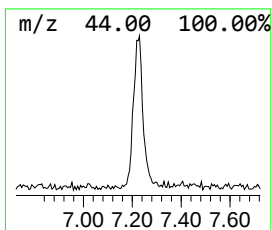
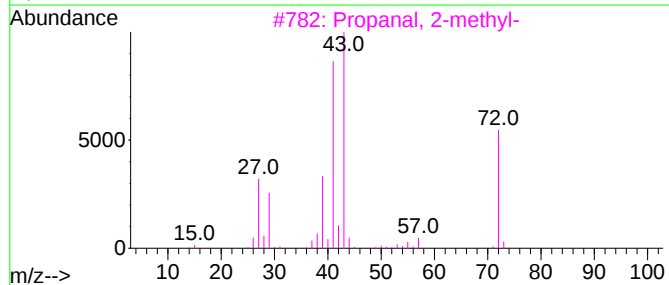
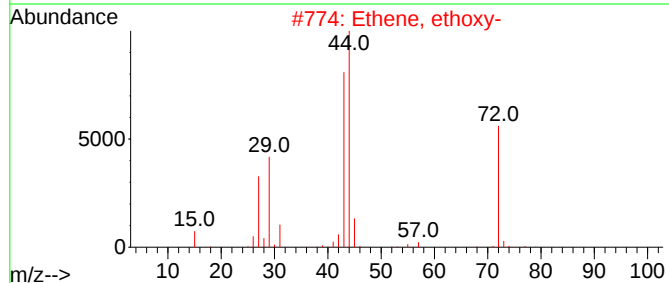
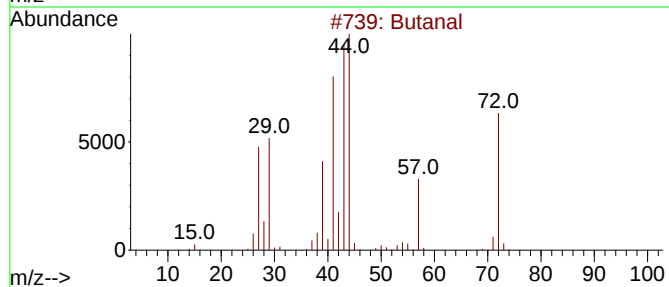
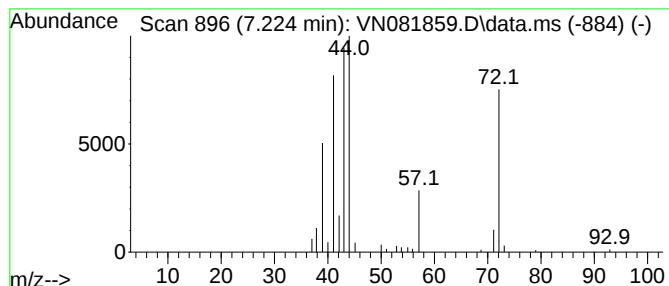
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	18.26 ug/l	254544	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			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	28



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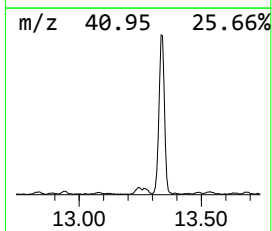
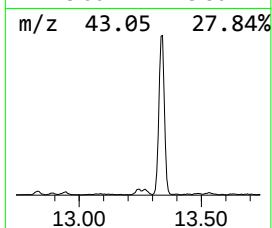
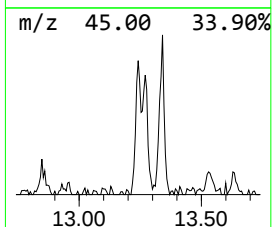
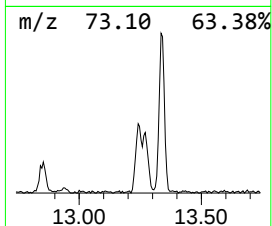
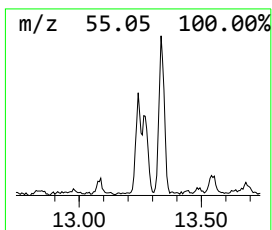
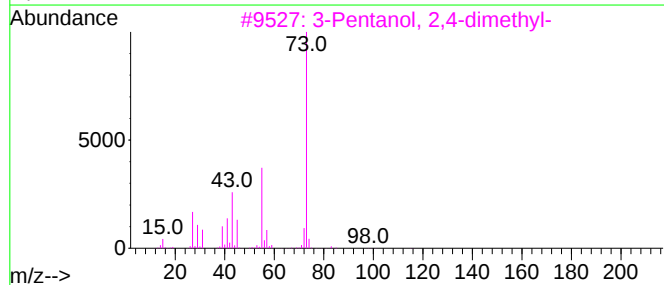
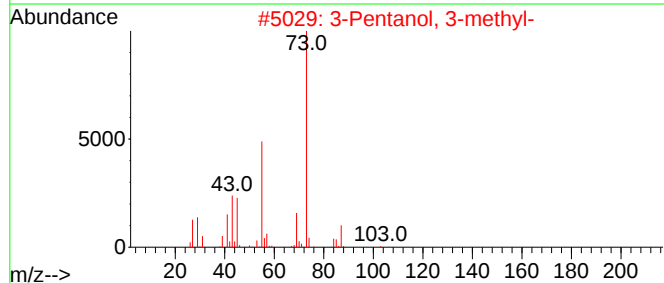
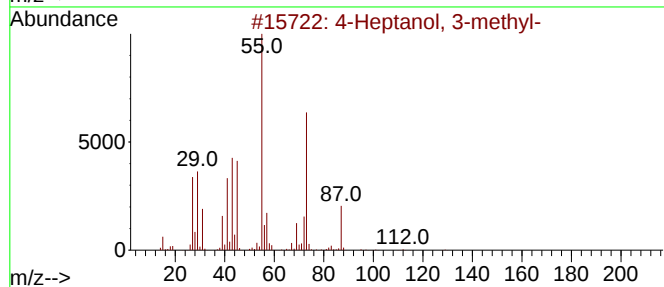
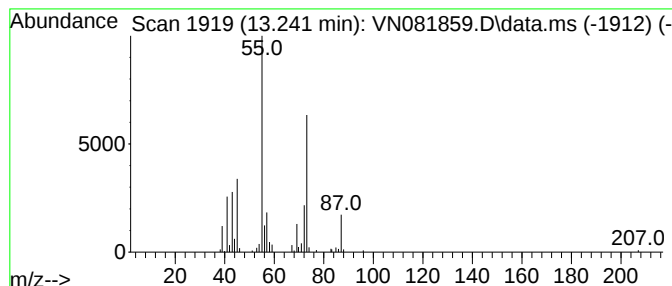
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4-Heptanol, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.241	6.50 ug/l	135393	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	83
2			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	50
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	42
4			4-Heptanol, 2-methyl-	130	C8H18O	021570-35-4	40
5			1-Butene, 3-propoxy-	114	C7H14O	037027-59-1	38



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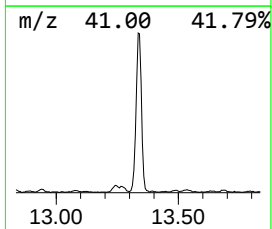
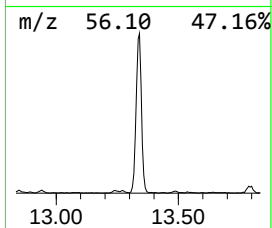
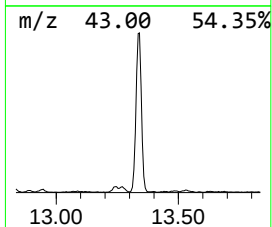
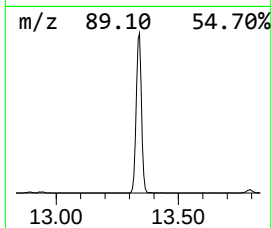
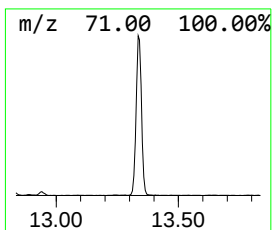
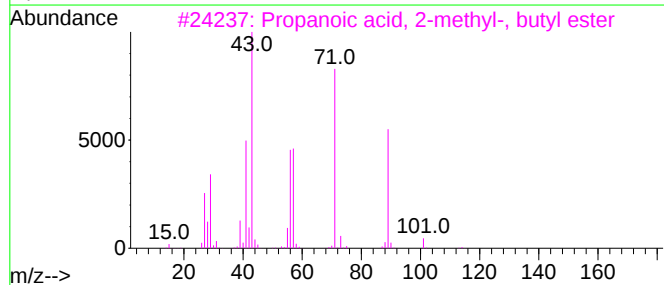
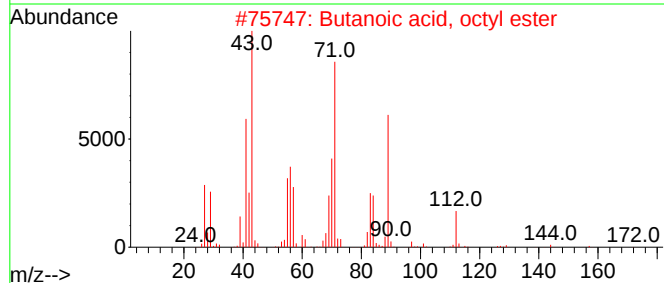
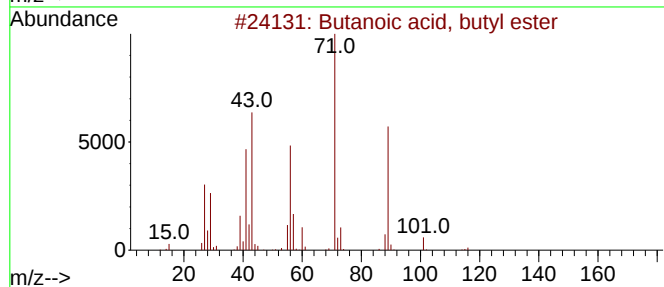
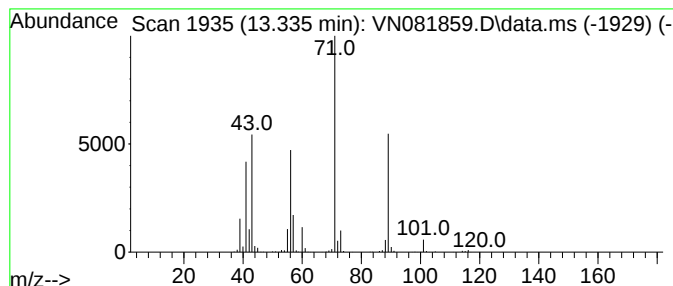
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	92.17 ug/l	1918910	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	91
2			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
3			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
5			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64



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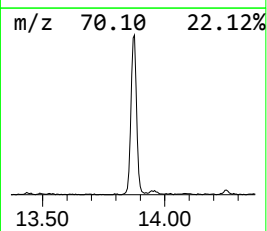
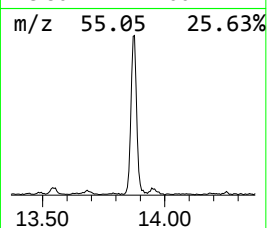
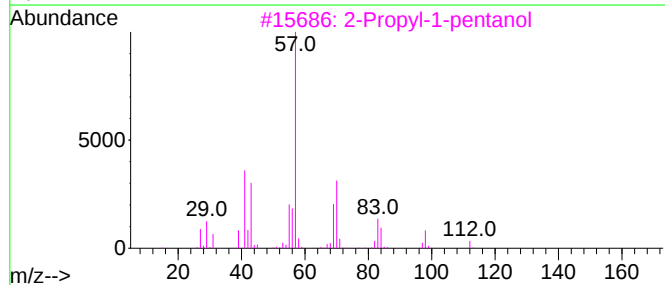
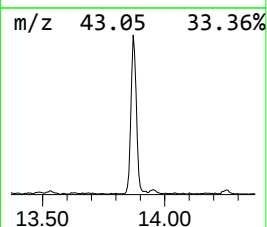
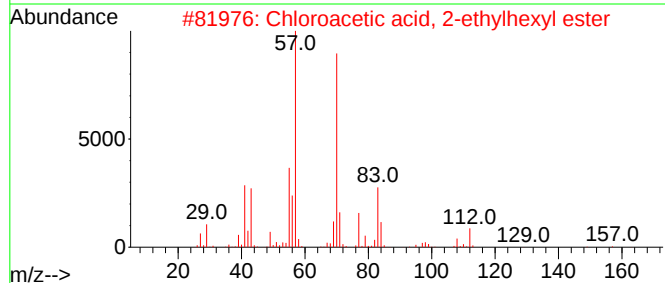
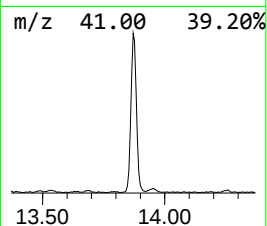
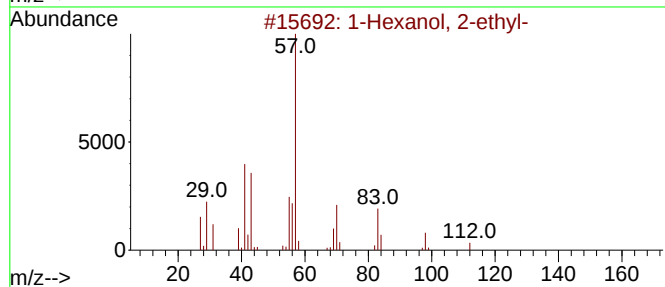
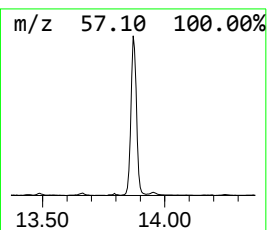
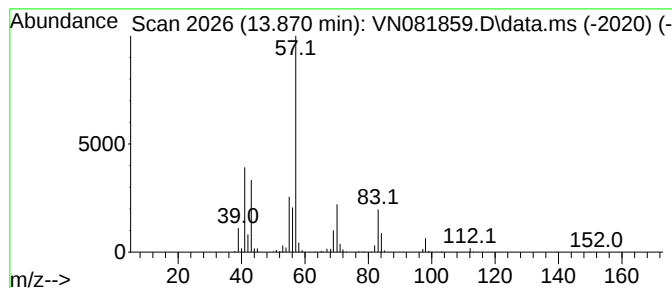
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.870	88.87 ug/l	1850160	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	59
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	50
5			Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042524\
Data File : VN081859.D
Acq On : 25 Apr 2024 18:40
Operator : JC\MD
Sample : P2257-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
413C

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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	7.5	ug/l	104225	1	8.224	697148	50.0
Butanal	7.224	18.3	ug/l	254544	1	8.224	697148	50.0
4-Heptanol, 3-m...	13.241	6.5	ug/l	135393	4	13.794	1040910	50.0
Butanoic acid, ...	13.335	92.2	ug/l	1918910	4	13.794	1040910	50.0
1-Hexanol, 2-et...	13.870	88.9	ug/l	1850160	4	13.794	1040910	50.0