

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
 Data File : VN080836.D
 Acq On : 31 Jan 2024 13:33
 Operator : JC\MD
 Sample : P1284-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1248

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: VN080836.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	26	rBV	31097	46565	6.34%	0.849%
2	2.812	141	146	153	rVB6	7821	17062	2.32%	0.311%
3	4.424	409	420	432	rBV2	13485	40426	5.50%	0.737%
4	4.718	461	470	481	rVB3	5836	16385	2.23%	0.299%
5	7.224	886	896	905	rBV2	31105	80526	10.96%	1.468%
6	8.171	1045	1057	1061	rBV	74892	187954	25.57%	3.428%
7	8.224	1061	1066	1077	rVB2	128977	286184	38.94%	5.219%
8	8.524	1111	1117	1118	rBV2	8555	10999	1.50%	0.201%
9	8.577	1119	1126	1136	rVB2	91127	210077	28.58%	3.831%
10	9.100	1203	1215	1225	rBV	255955	522611	71.11%	9.530%
11	9.271	1235	1244	1250	rBV3	26078	56162	7.64%	1.024%
12	9.641	1300	1307	1313	rBV5	7061	16258	2.21%	0.296%
13	9.883	1342	1348	1360	rBV2	26651	51775	7.04%	0.944%
14	10.565	1456	1464	1473	rBV	343703	655149	89.14%	11.947%
15	11.865	1672	1685	1696	rBV	394945	734958	100.00%	13.403%
16	12.206	1738	1743	1749	rVB3	9449	15033	2.05%	0.274%
17	12.424	1774	1780	1787	rVB	58584	99123	13.49%	1.808%
18	12.847	1843	1852	1864	rBV	247693	464879	63.25%	8.478%
19	12.941	1864	1868	1874	rVV3	10758	18529	2.52%	0.338%
20	13.241	1911	1919	1922	rBV3	27883	50239	6.84%	0.916%
21	13.271	1922	1924	1929	rVV2	27951	36457	4.96%	0.665%
22	13.341	1929	1936	1944	rVB	377253	582231	79.22%	10.618%
23	13.482	1956	1960	1964	rBV4	4965	7563	1.03%	0.138%
24	13.629	1980	1985	1991	rBV5	4464	7561	1.03%	0.138%
25	13.794	2006	2013	2020	rBV	356750	607971	82.72%	11.087%
26	13.876	2020	2027	2036	rVV	235015	396228	53.91%	7.226%
27	13.953	2036	2040	2050	rVV7	11601	27581	3.75%	0.503%
28	14.259	2084	2092	2094	rBV7	6661	11853	1.61%	0.216%
29	15.394	2280	2285	2291	rVV2	61996	107943	14.69%	1.968%
30	15.823	2352	2358	2366	rVB5	19941	37262	5.07%	0.680%
31	15.941	2373	2378	2385	rVB5	23290	38852	5.29%	0.709%
32	16.117	2402	2408	2414	rBV5	15591	28029	3.81%	0.511%
33	16.259	2426	2432	2438	rBV5	6512	13210	1.80%	0.241%

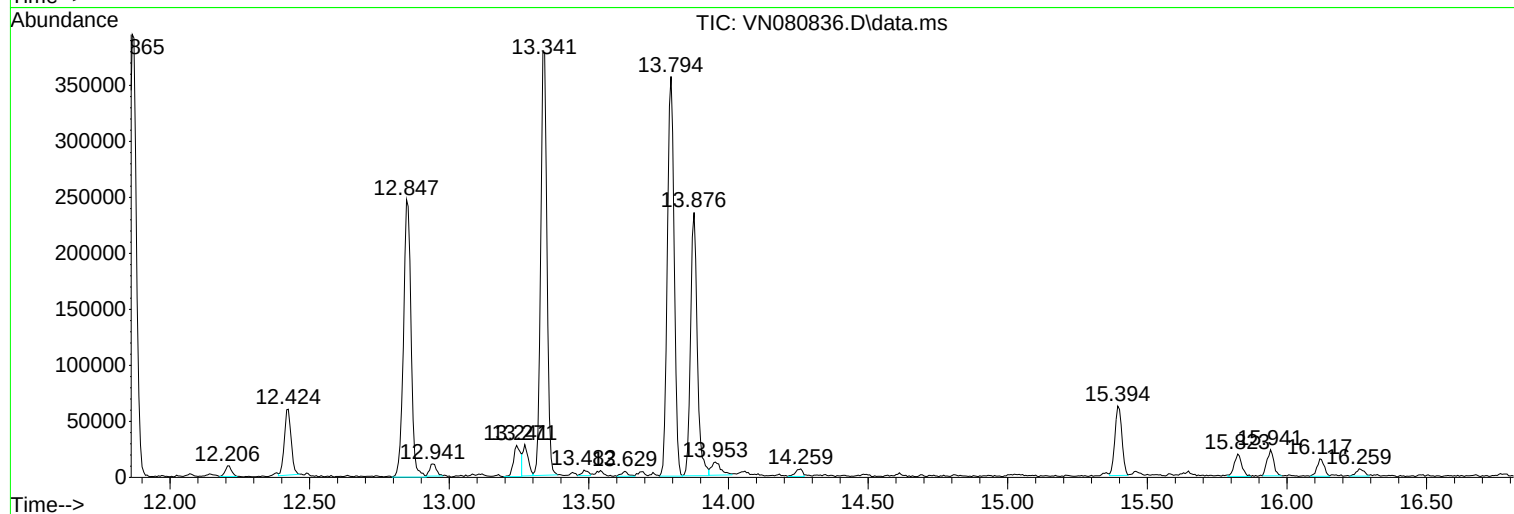
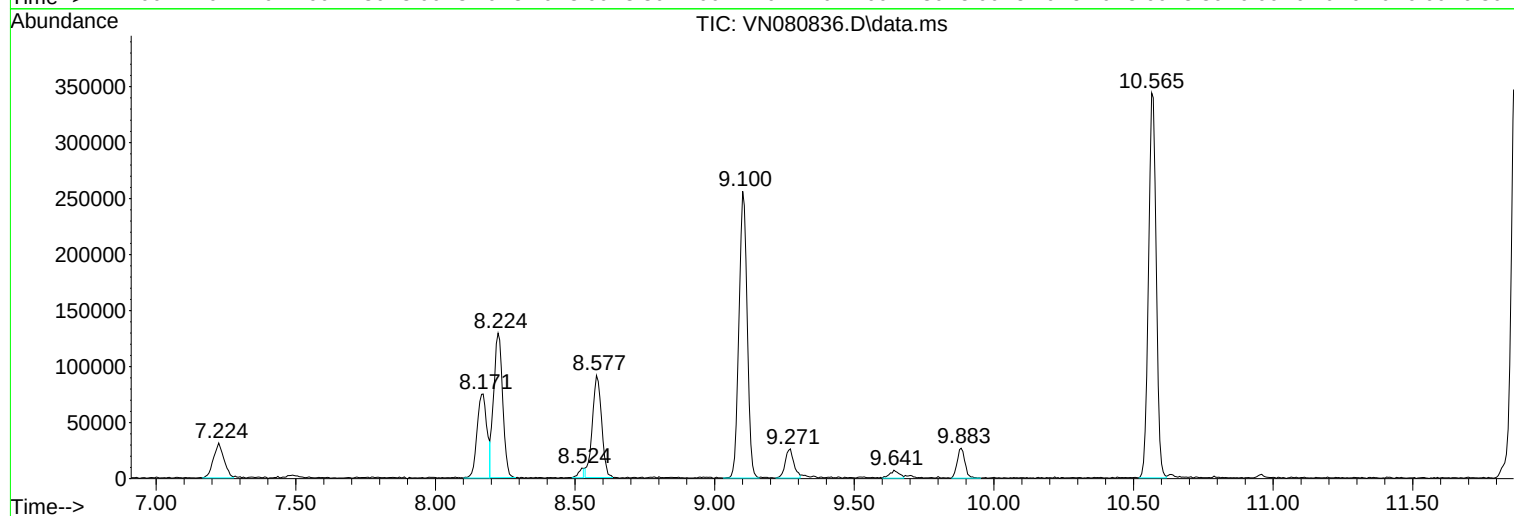
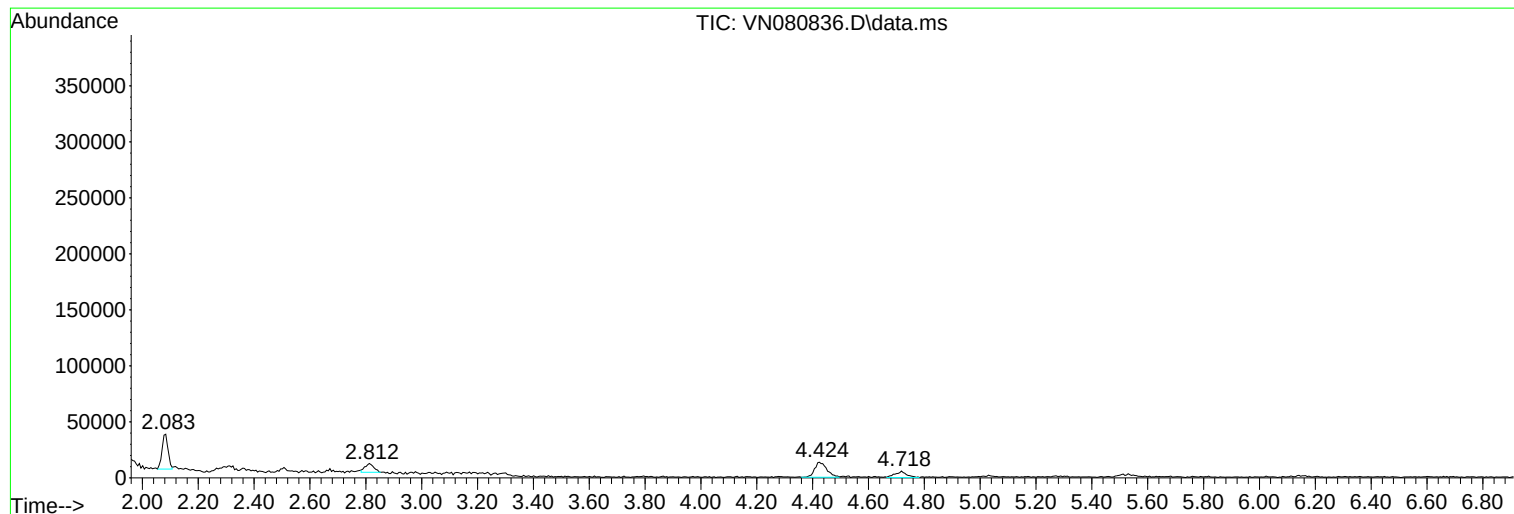
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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



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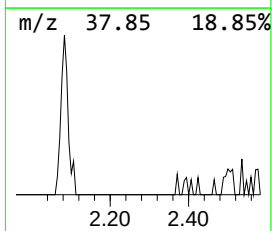
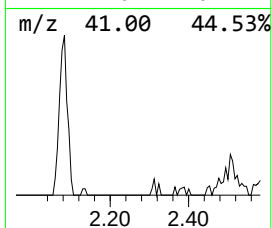
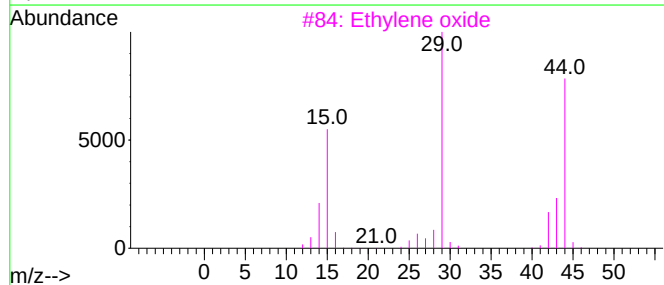
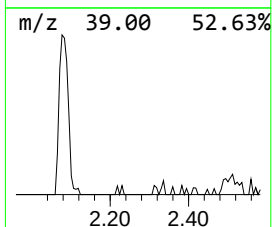
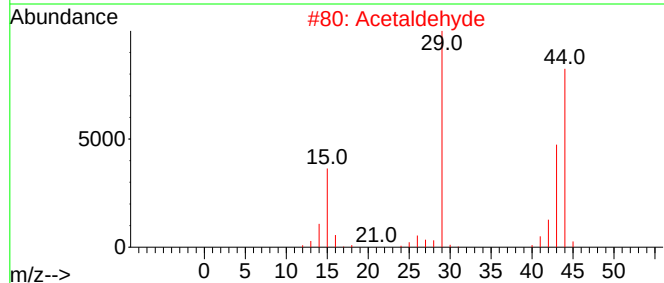
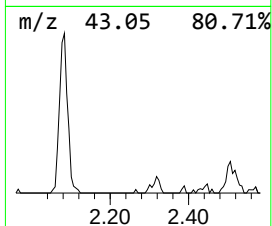
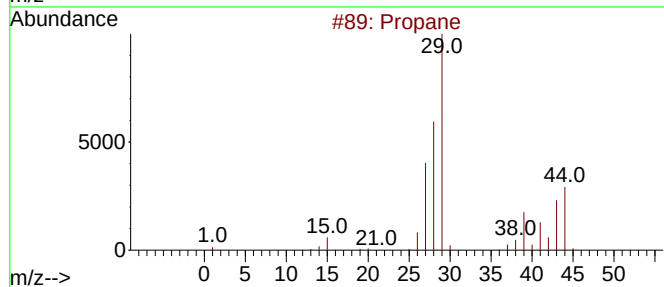
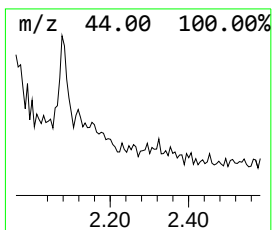
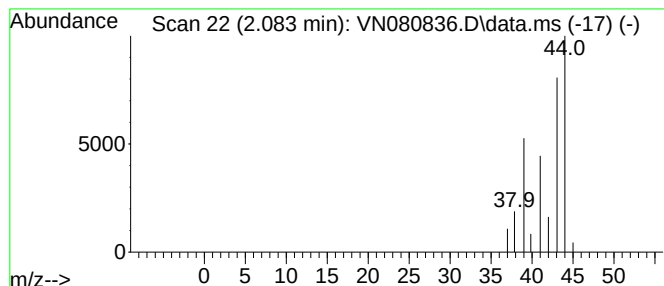
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	8.14 ug/l	46565	Pentafluorobenzene	8.224

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane			44	C3H8	000074-98-6	83
2	Acetaldehyde			44	C2H4O	000075-07-0	9
3	Ethylene oxide			44	C2H4O	000075-21-8	5
4	Cyclopropene			40	C3H4	002781-85-3	4
5	Ethyne, fluoro-			44	C2HF	002713-09-9	3



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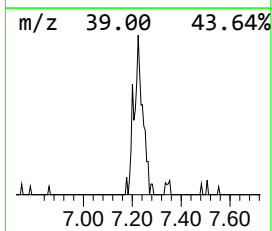
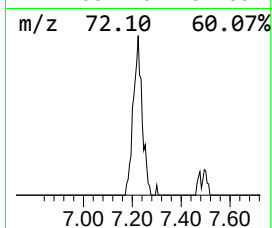
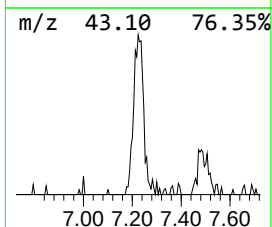
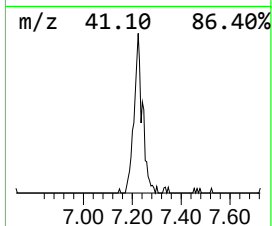
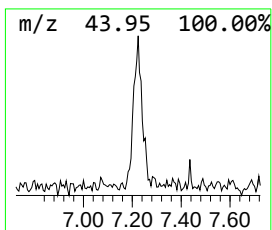
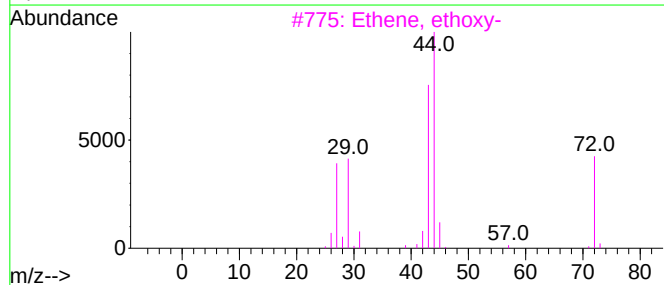
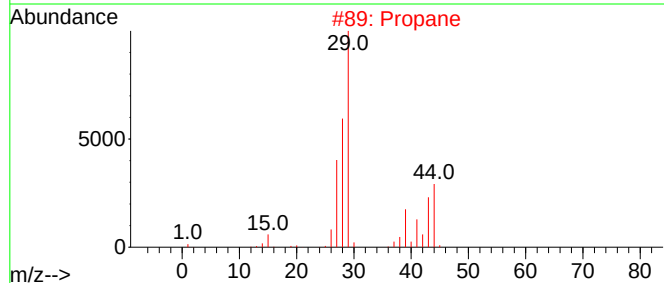
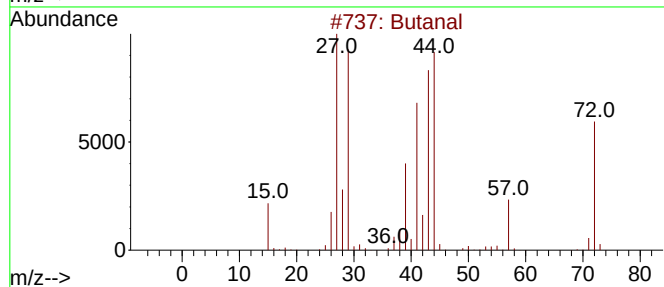
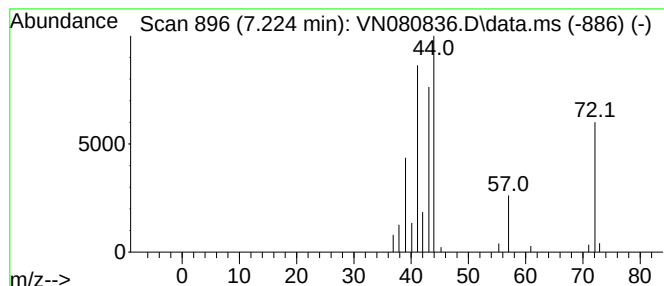
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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	14.07 ug/l	80526	Pentafluorobenzene	8.224

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	91
2		Propane	44	C3H8	000074-98-6	53
3		Ethene, ethoxy-	72	C4H8O	000109-92-2	50
4		Propanal, 2-methyl-	72	C4H8O	000078-84-2	35
5		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	35



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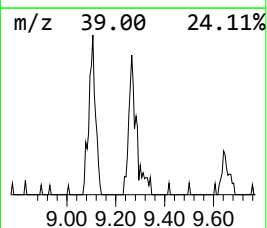
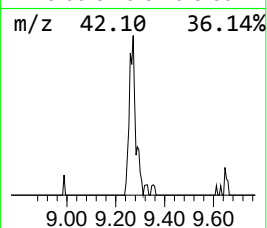
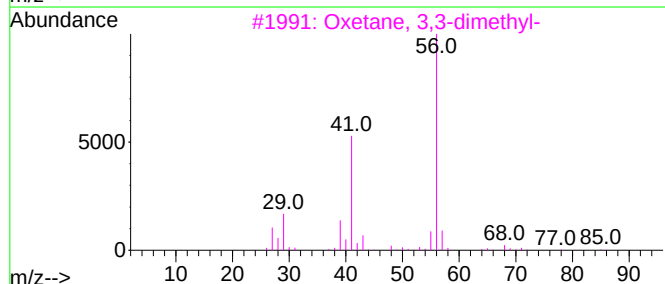
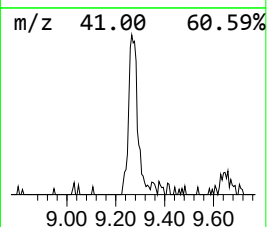
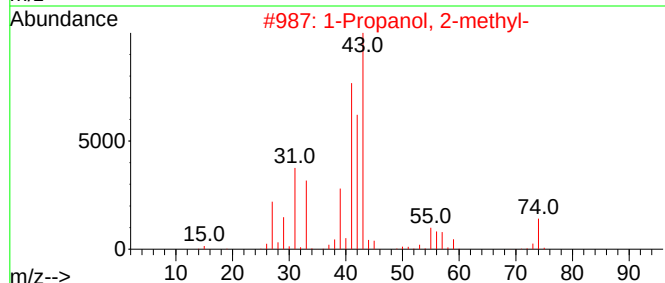
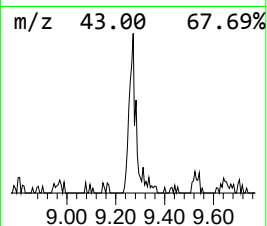
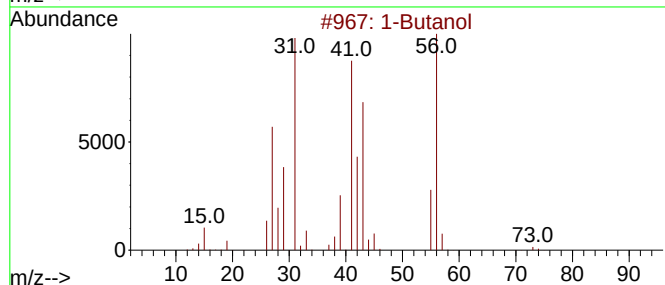
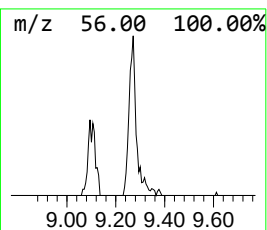
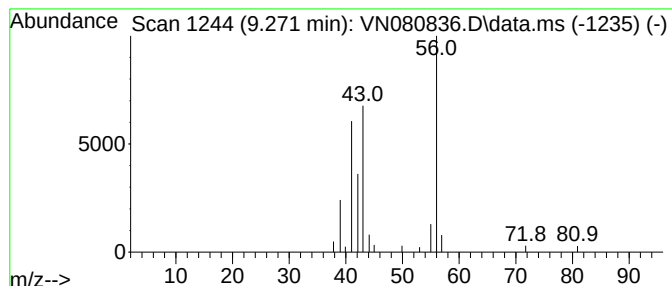
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Quant Title : SW846 8260

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

Peak Number 3 unknown9.271 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.271	5.37 ug/l	56162	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	43
2			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	12
3			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	9
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9



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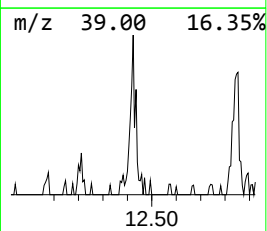
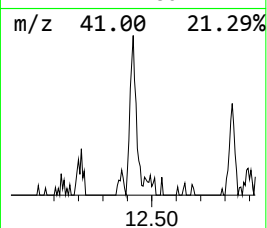
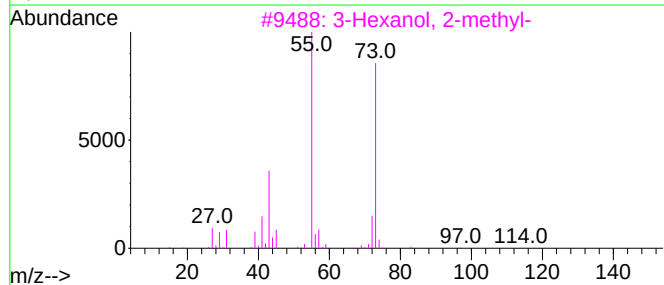
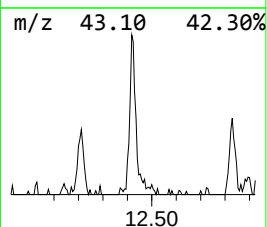
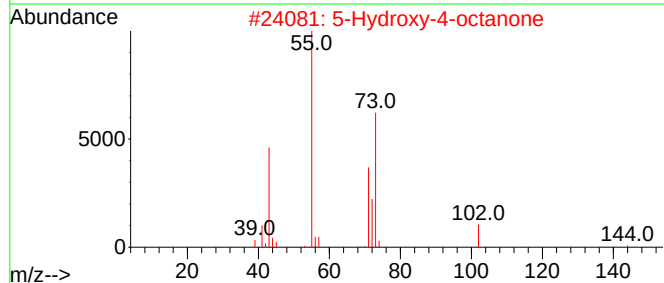
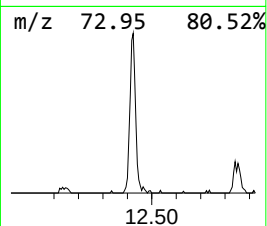
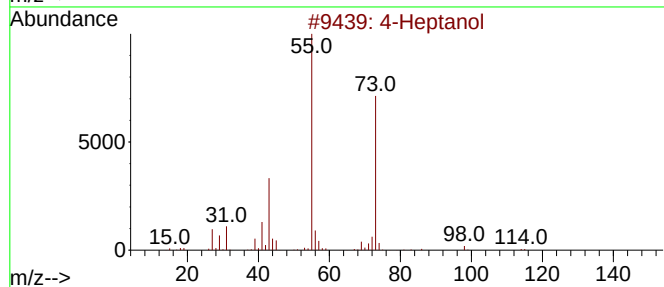
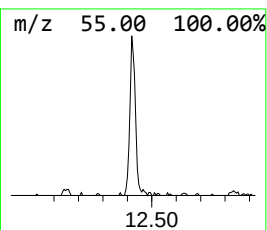
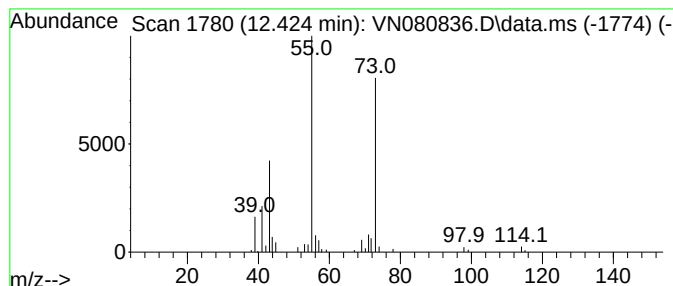
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Peak Number 4 4-Heptanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.424	6.74 ug/l	99123	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	72
2			5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	40
3			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	40
4			1-Hepten-4-ol	114	C7H14O	003521-91-3	36
5			4,5-Octanediol	146	C8H18O2	022607-10-9	23



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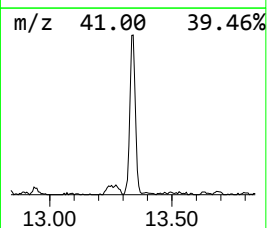
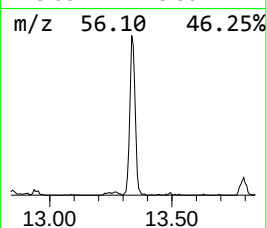
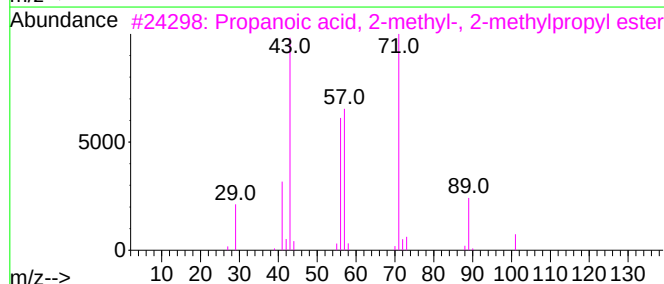
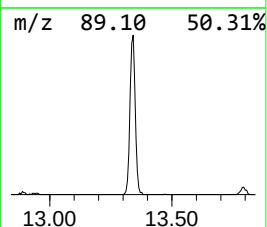
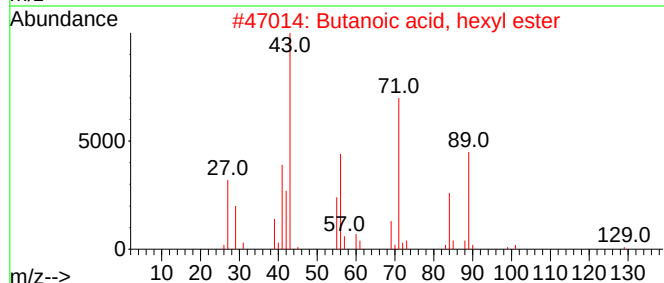
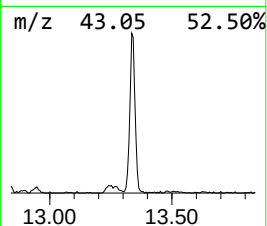
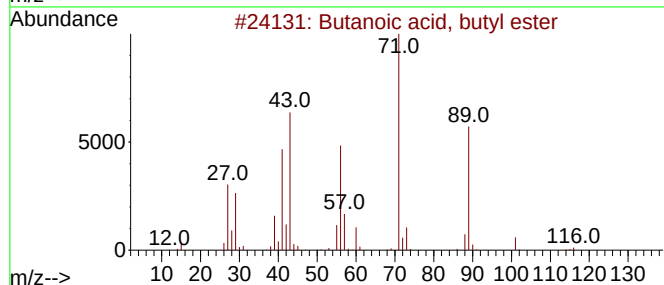
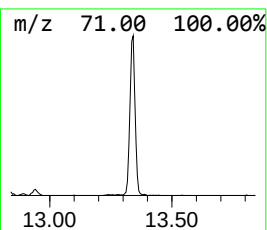
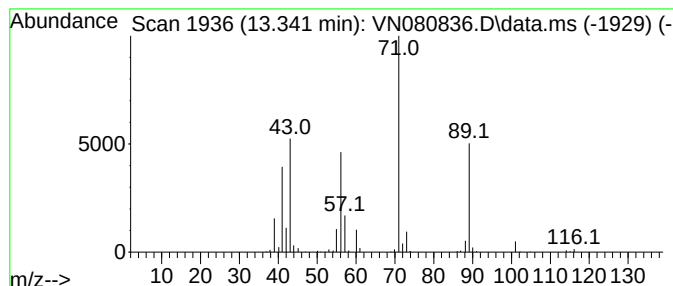
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Quant Title : SW846 8260

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

Peak Number 5 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	47.88 ug/l	582231	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, hexyl ester	172	C10H20O2	002639-63-6	64
3			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	56



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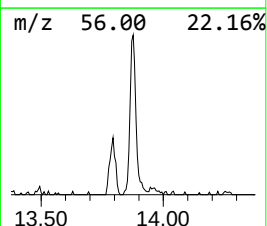
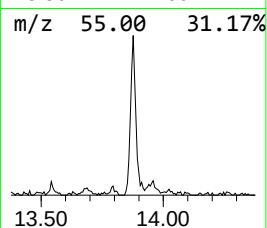
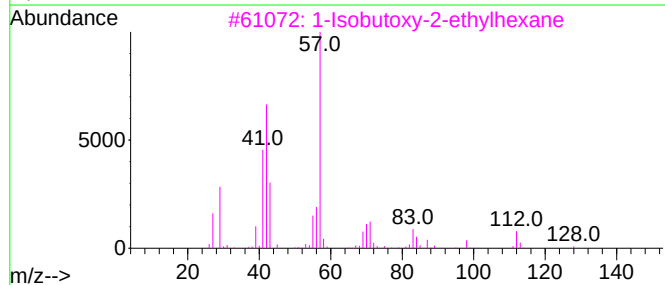
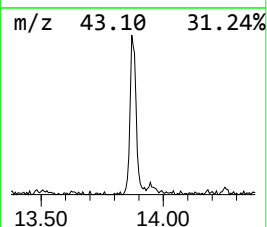
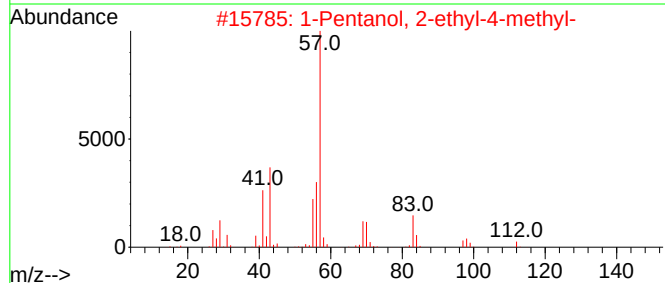
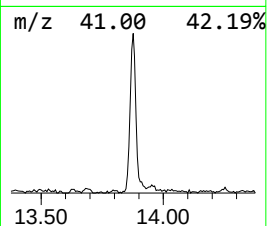
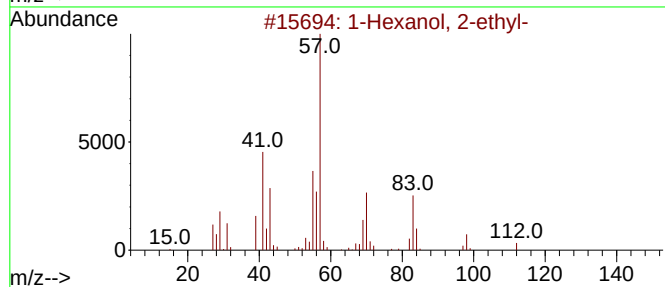
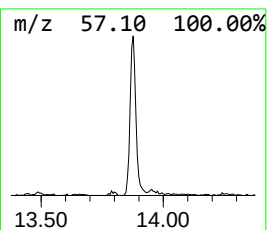
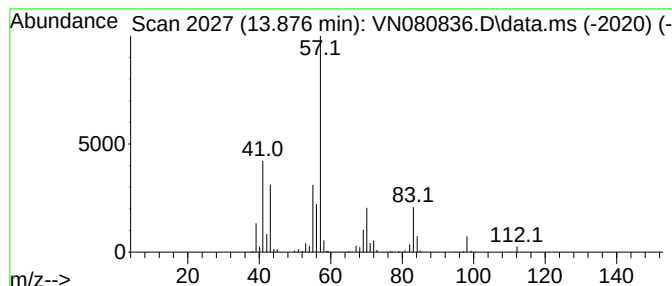
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Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	32.59 ug/l	396228	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			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080836.D
Acq On : 31 Jan 2024 13:33
Operator : JC\MD
Sample : P1284-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1248

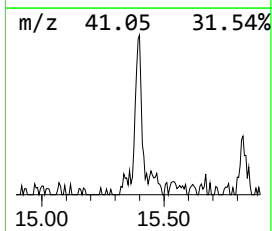
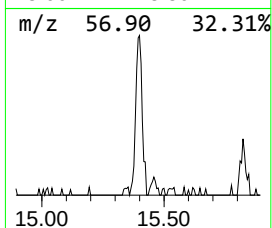
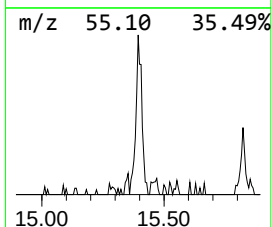
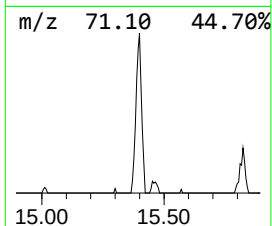
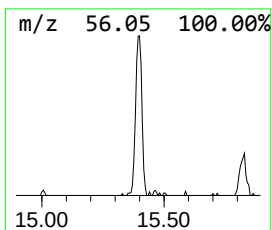
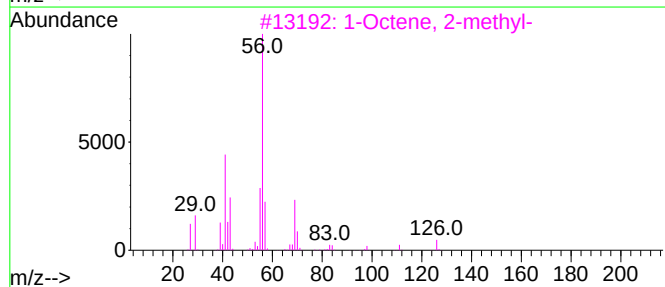
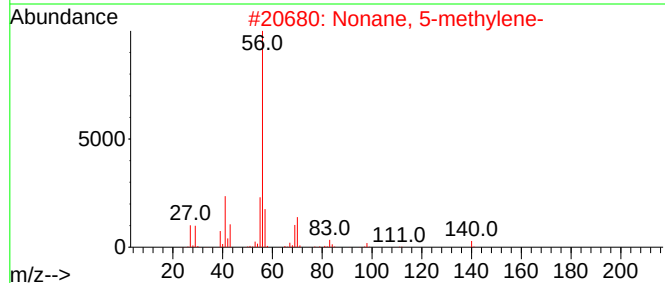
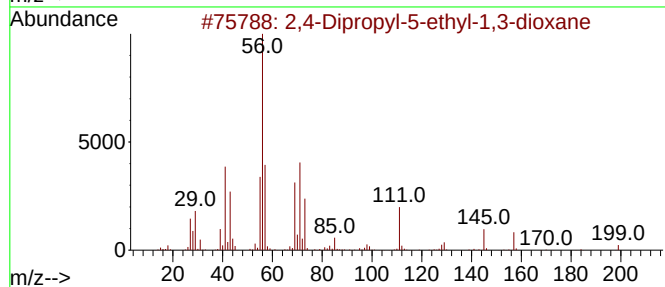
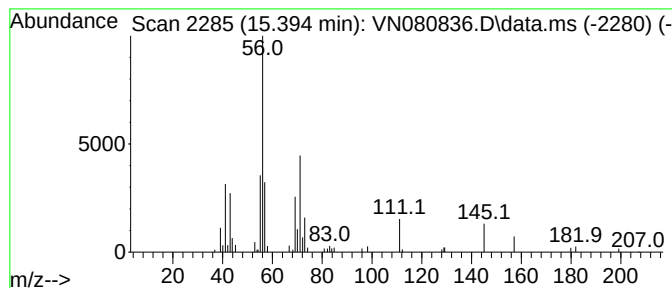
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.394 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.394	8.88 ug/l	107943	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	37
2		Nonane, 5-methylene-	140	C10H20	006795-79-5	32
3		1-Octene, 2-methyl-	126	C9H18	004588-18-5	32
4		1-Decene, 2-methyl-	154	C11H22	013151-27-4	32
5		2-Methyl-1-nonene	140	C10H20	002980-71-4	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080836.D
Acq On : 31 Jan 2024 13:33
Operator : JC\MD
Sample : P1284-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1248

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane	2.083	8.1	ug/l	46565	1	8.224	286184	50.0
Butanal	7.224	14.1	ug/l	80526	1	8.224	286184	50.0
unknown9.271	9.271	5.4	ug/l	56162	2	9.100	522611	50.0
4-Heptanol	12.424	6.7	ug/l	99123	3	11.871	734958	50.0
Butanoic acid, ...	13.341	47.9	ug/l	582231	4	13.794	607971	50.0
1-Hexanol, 2-et...	13.876	32.6	ug/l	396228	4	13.794	607971	50.0
unknown15.394	15.394	8.9	ug/l	107943	4	13.794	607971	50.0