

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
 Data File : VN080853.D
 Acq On : 31 Jan 2024 20:18
 Operator : JC\MD
 Sample : P1284-07
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1253

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: VN080853.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	15	22	30	rVB	47806	74520	8.69%	1.167%
2	2.295	52	58	64	rBV2	19773	43467	5.07%	0.681%
3	2.806	139	145	146	rBV4	7911	11860	1.38%	0.186%
4	4.430	410	421	435	rBV2	33172	102272	11.93%	1.601%
5	5.018	513	521	533	rBV5	3183	10915	1.27%	0.171%
6	7.230	887	897	909	rBV5	44972	129089	15.05%	2.021%
7	7.489	934	941	950	rVB2	6076	15067	1.76%	0.236%
8	8.165	1047	1056	1061	rBV2	81701	200835	23.42%	3.145%
9	8.224	1061	1066	1075	rVB	137902	305793	35.66%	4.788%
10	8.577	1111	1126	1136	rBV2	108411	264893	30.89%	4.148%
11	8.671	1136	1142	1145	rBV5	4009	8670	1.01%	0.136%
12	9.100	1205	1215	1227	rBV	285715	596545	69.57%	9.341%
13	9.265	1234	1243	1251	rBV2	49368	99679	11.62%	1.561%
14	9.653	1302	1309	1314	rBV6	7451	18850	2.20%	0.295%
15	9.883	1342	1348	1355	rBV3	11642	23927	2.79%	0.375%
16	10.565	1456	1464	1473	rBV	378992	713563	83.21%	11.173%
17	10.959	1526	1531	1537	rBV3	8943	15779	1.84%	0.247%
18	11.865	1674	1685	1697	rVB	467045	857528	100.00%	13.428%
19	12.212	1738	1744	1754	rVB6	9486	20477	2.39%	0.321%
20	12.382	1769	1773	1775	rBV3	6535	10054	1.17%	0.157%
21	12.424	1775	1780	1784	rVB2	25141	40083	4.67%	0.628%
22	12.853	1843	1853	1863	rBV	311071	572042	66.71%	8.957%
23	12.941	1865	1868	1874	rVB3	11398	17978	2.10%	0.282%
24	13.253	1912	1921	1922	rBV4	17929	32270	3.76%	0.505%
25	13.271	1922	1924	1929	rVV4	17058	23267	2.71%	0.364%
26	13.341	1929	1936	1944	rVB	442330	661466	77.14%	10.358%
27	13.682	1993	1994	2003	rVB5	6002	8677	1.01%	0.136%
28	13.794	2005	2013	2020	rBV	474679	792013	92.36%	12.402%
29	13.876	2020	2027	2036	rVV	212278	356566	41.58%	5.583%
30	13.965	2036	2042	2052	rVB8	12966	29628	3.46%	0.464%
31	14.253	2087	2091	2093	rBV4	8826	9819	1.15%	0.154%
32	14.782	2171	2181	2192	rBV10	21670	72731	8.48%	1.139%
33	15.065	2220	2229	2232	rVV10	6117	14942	1.74%	0.234%
34	15.400	2279	2286	2292	rVV	74099	128016	14.93%	2.005%
35	15.464	2294	2297	2303	rVB6	7444	12106	1.41%	0.190%
36	15.823	2351	2358	2364	rBV5	15772	32286	3.77%	0.506%

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Instrument :
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ClientSampleId :
1253

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

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37	15.941	2371	2378	2387	rBV4	16029	30751	3.59%	0.482%
38	16.117	2403	2408	2415	rVB3	14417	27835	3.25%	0.436%

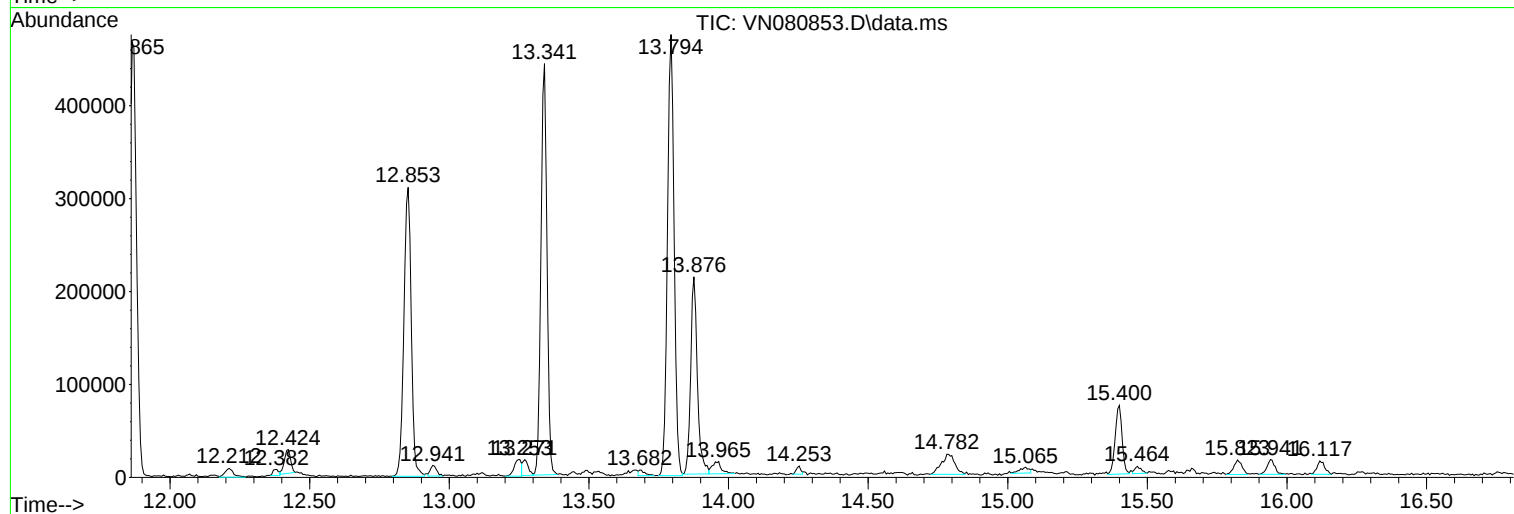
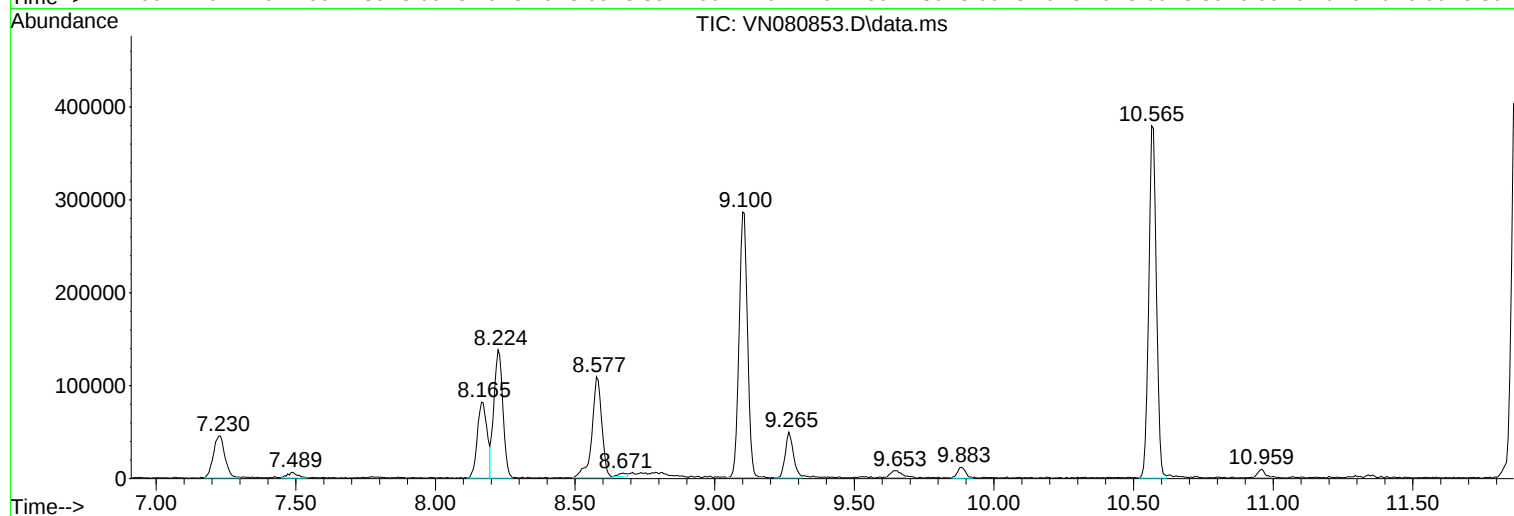
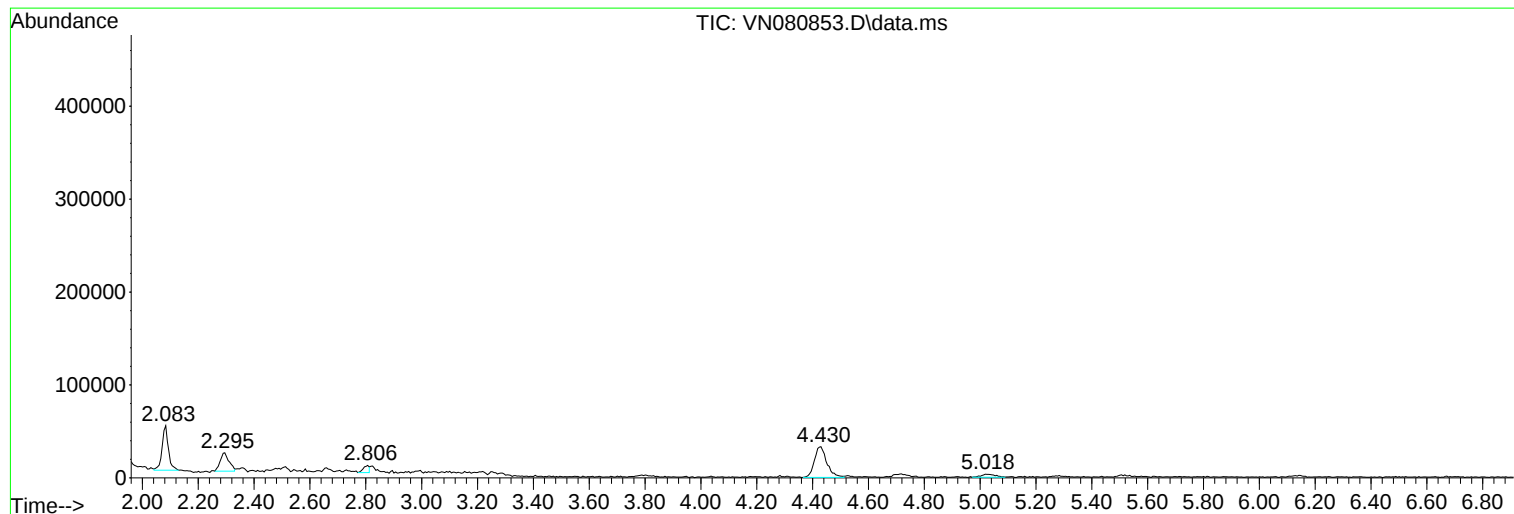
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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



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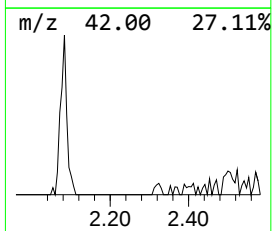
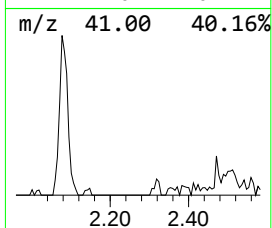
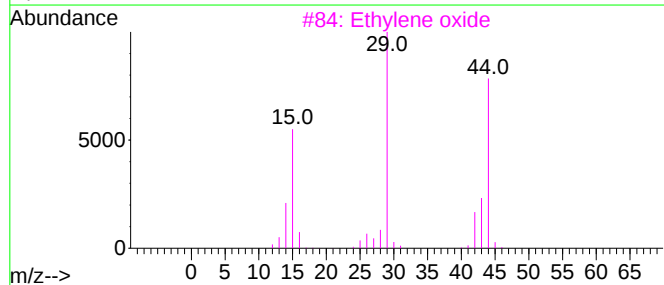
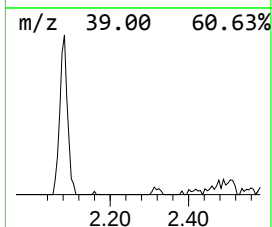
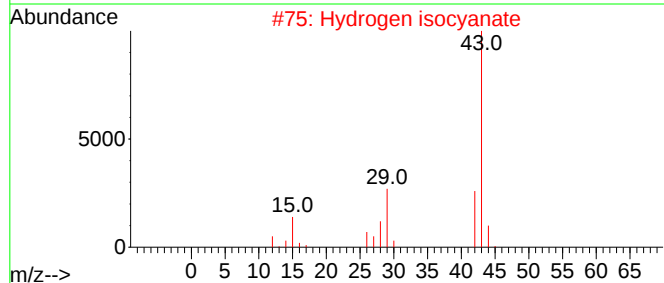
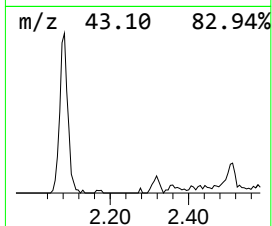
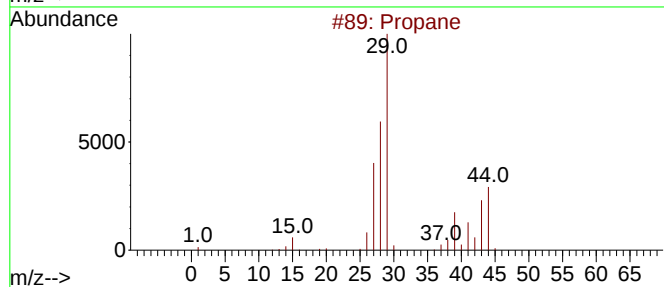
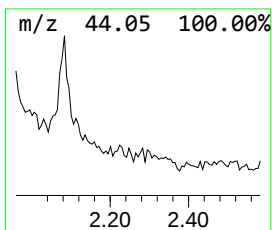
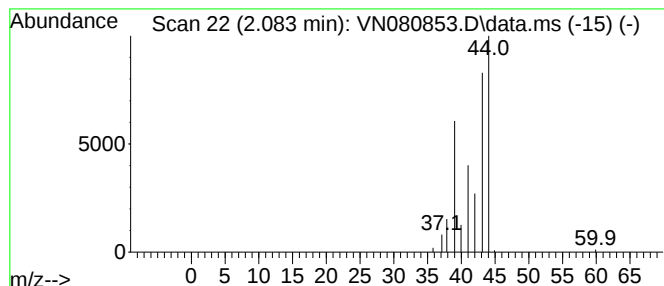
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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	12.18 ug/l	74520	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane			44	C3H8	000074-98-6	83
2	Hydrogen isocyanate			43	CHNO	000075-13-8	4
3	Ethylene oxide			44	C2H4O	000075-21-8	4
4	Propane, 2-nitro-			89	C3H7NO2	000079-46-9	4
5	Acetaldehyde			44	C2H4O	000075-07-0	4



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ALS Vial : 25 Sample Multiplier: 1

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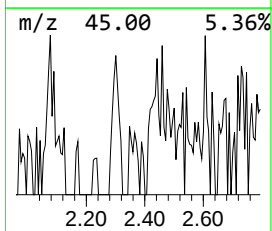
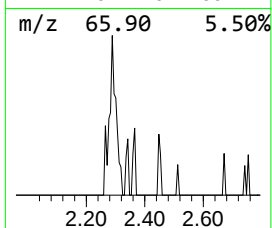
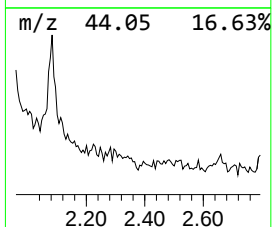
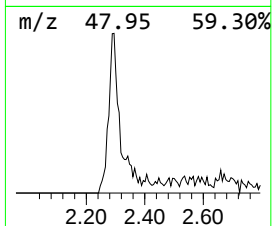
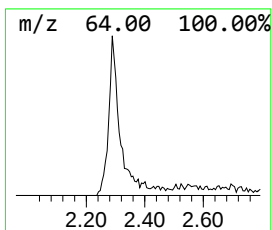
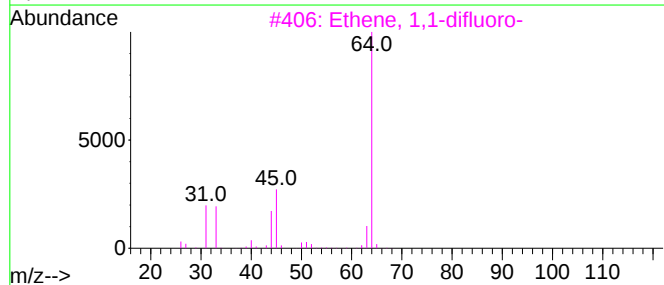
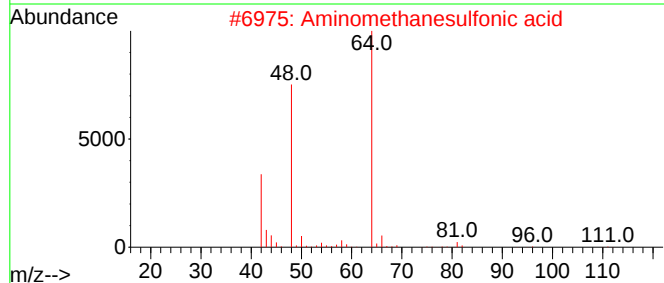
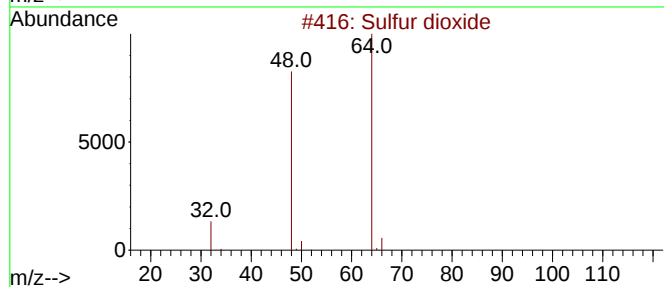
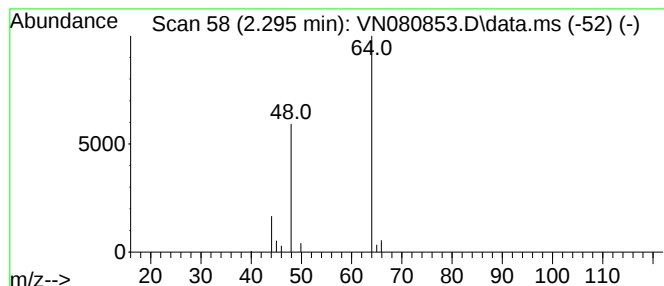
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.295	7.11 ug/l	43467	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	4



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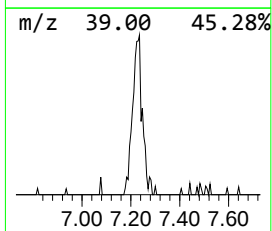
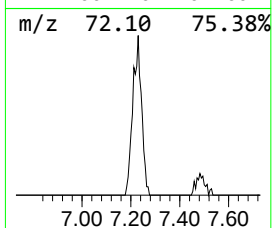
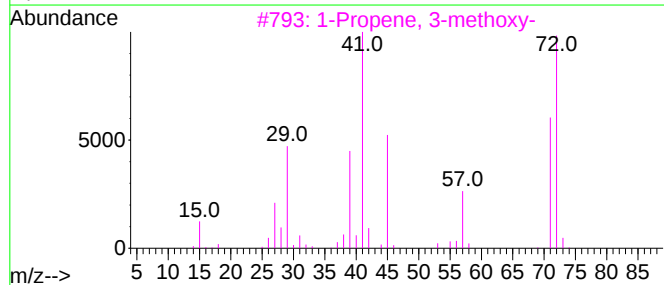
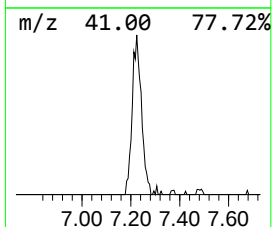
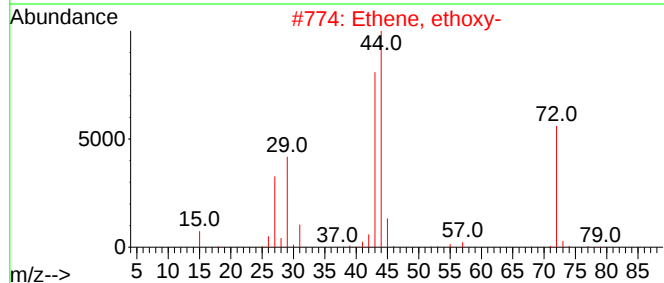
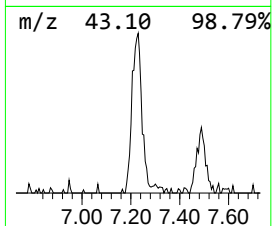
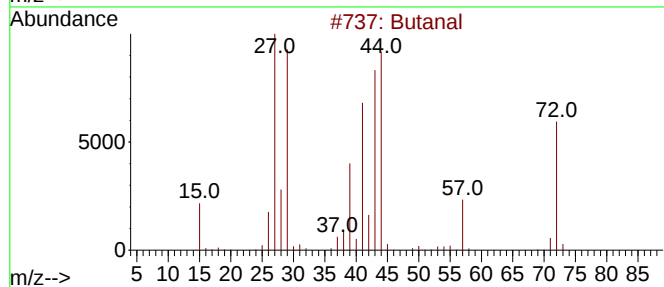
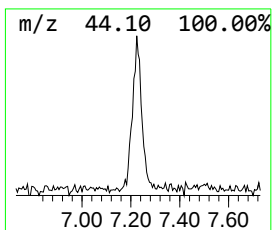
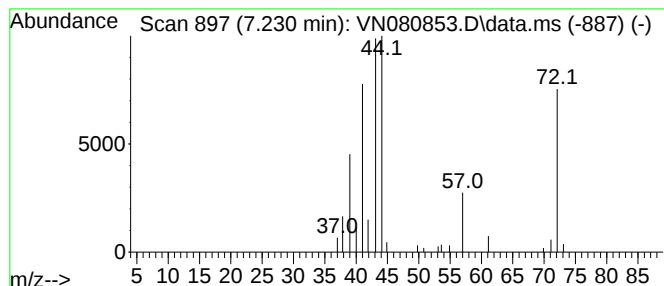
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.230	21.11 ug/l	129089	Pentafluorobenzene	8.230

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	53
3		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	47
4		Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
5		2-Propanone, hydrazone	72	C3H8N2	005281-20-9	37



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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1253

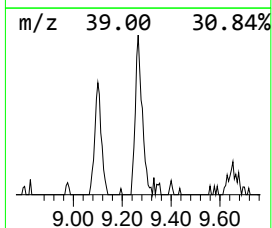
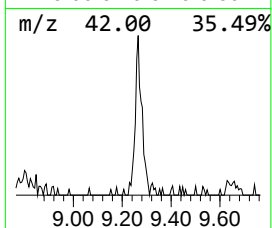
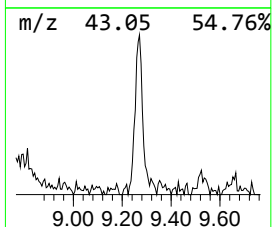
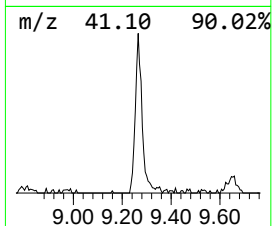
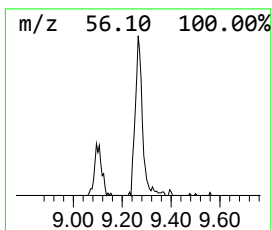
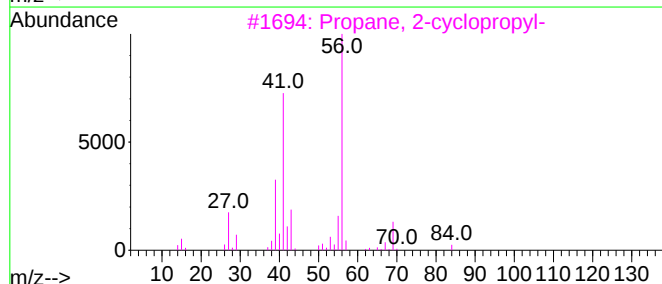
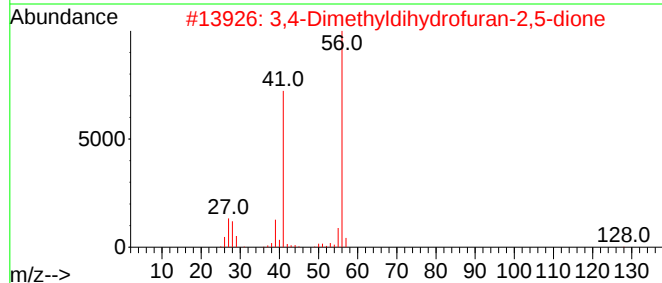
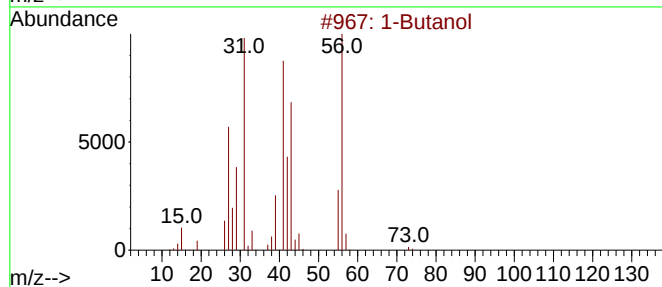
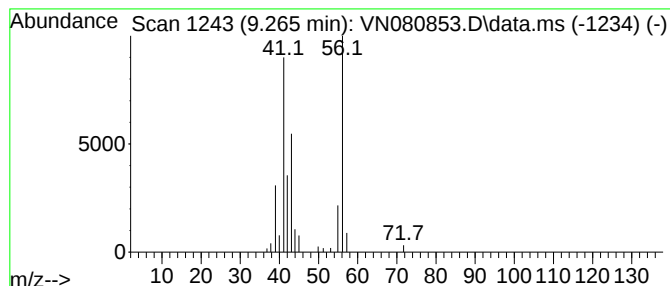
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.265	8.35 ug/l	99679	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	78
2			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	42
3			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
4			2-Butene, (Z)-	56	C4H8	000590-18-1	9
5			1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	9



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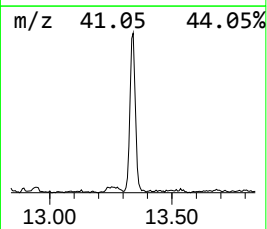
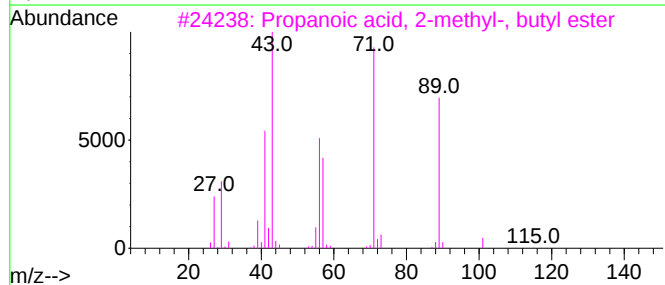
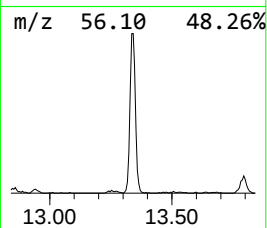
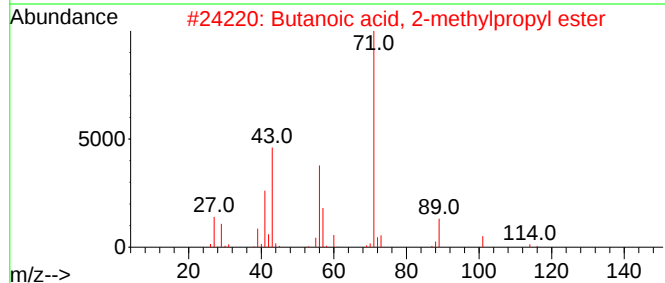
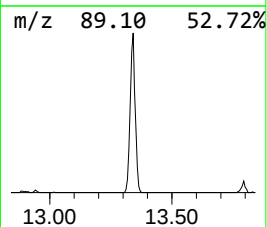
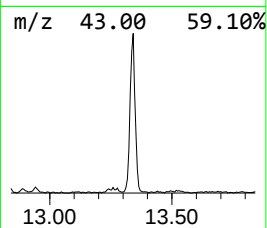
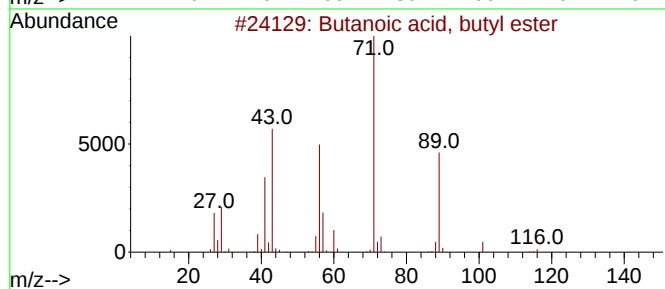
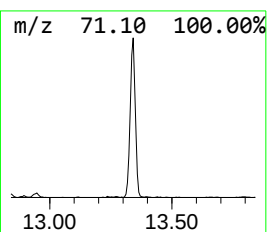
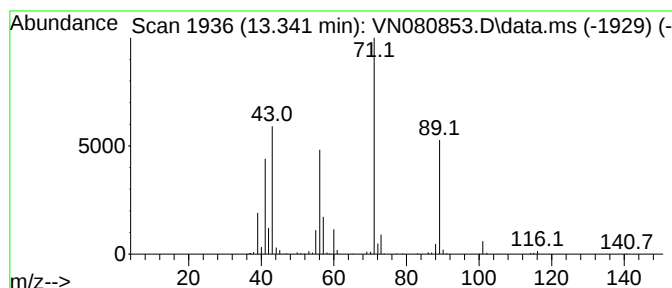
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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

Peak Number 5 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	41.76 ug/l	661466	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, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
5			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080853.D
Acq On : 31 Jan 2024 20:18
Operator : JC\MD
Sample : P1284-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1253

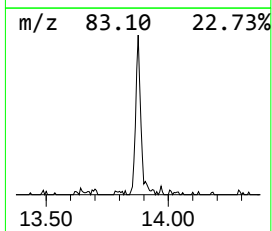
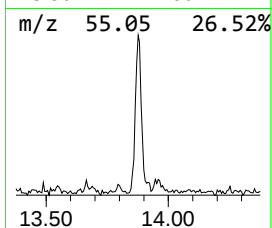
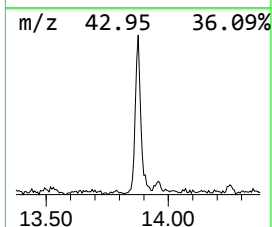
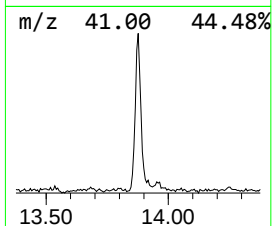
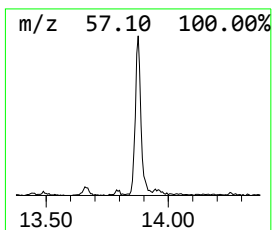
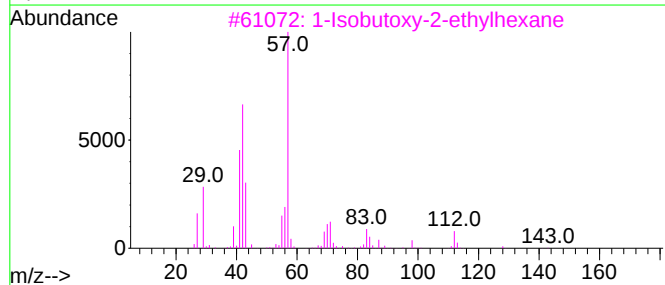
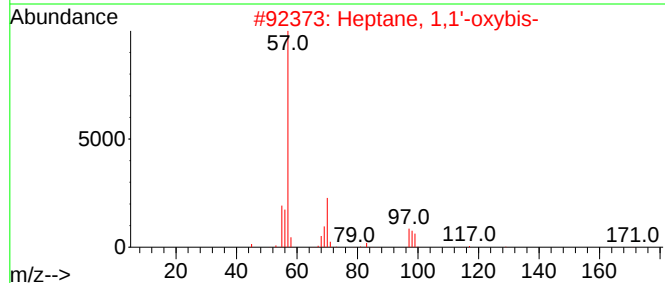
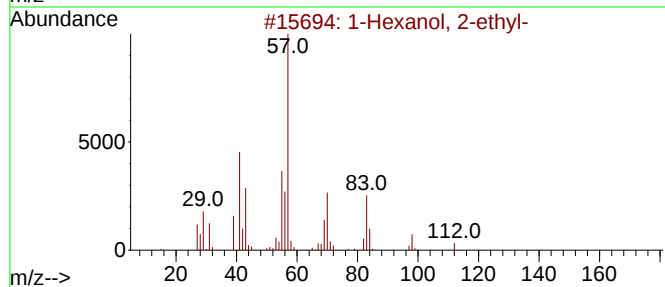
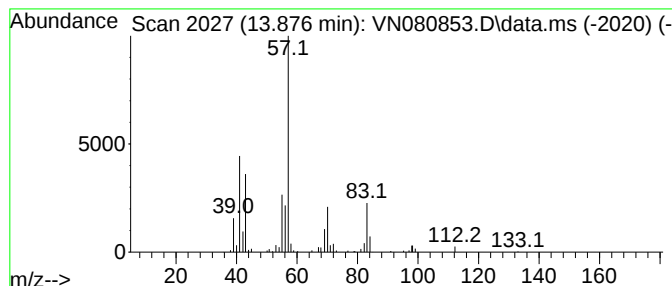
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Quant Title : SW846 8260

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	22.51 ug/l	356566	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			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50
4			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	50
5			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080853.D
Acq On : 31 Jan 2024 20:18
Operator : JC\MD
Sample : P1284-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1253

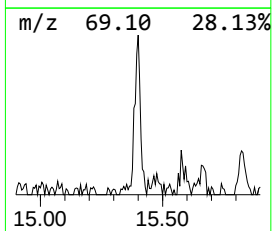
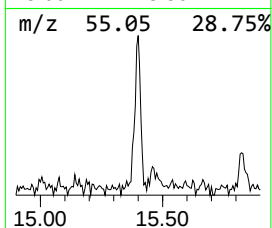
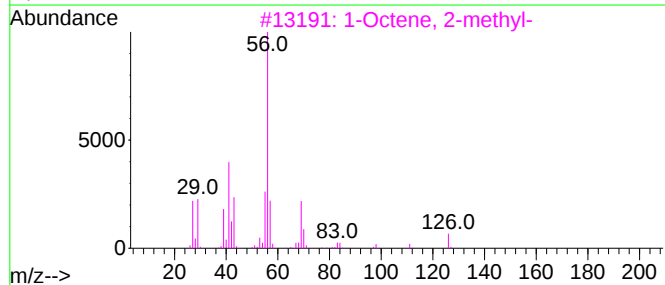
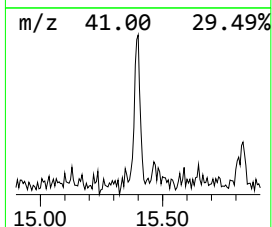
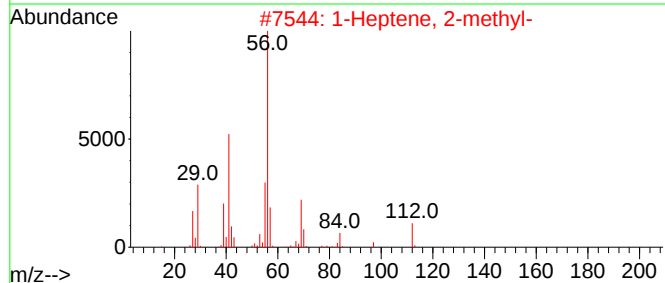
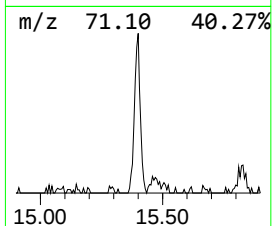
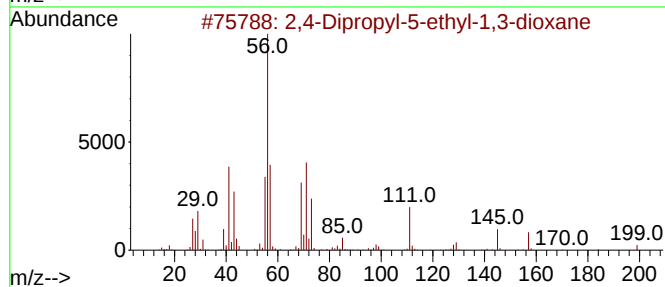
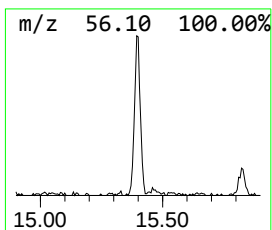
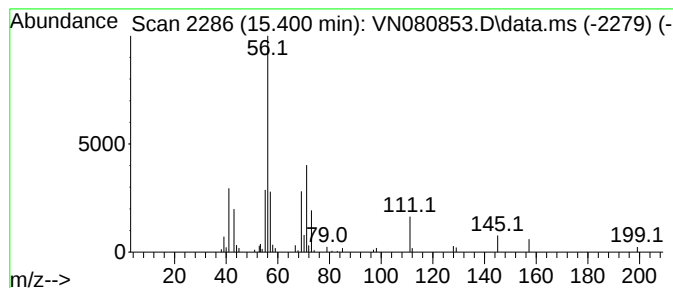
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.400 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.400	8.08 ug/l	128016	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	40
2		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	35
3		1-Octene, 2-methyl-	126	C9H18	004588-18-5	32
4		2-Methyl-1-nonene	140	C10H20	002980-71-4	25
5		1-Decene, 2-methyl-	154	C11H22	013151-27-4	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080853.D
Acq On : 31 Jan 2024 20:18
Operator : JC\MD
Sample : P1284-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1253

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	12.2	ug/l	74520	1	8.230	305793	50.0
Sulfur dioxide	2.295	7.1	ug/l	43467	1	8.230	305793	50.0
Butanal	7.230	21.1	ug/l	129089	1	8.230	305793	50.0
1-Butanol	9.265	8.3	ug/l	99679	2	9.100	596545	50.0
Butanoic acid, ...	13.341	41.8	ug/l	661466	4	13.794	792013	50.0
1-Hexanol, 2-et...	13.876	22.5	ug/l	356566	4	13.794	792013	50.0
unknown15.400	15.400	8.1	ug/l	128016	4	13.794	792013	50.0