

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
 Data File : VN080852.D
 Acq On : 31 Jan 2024 19:54
 Operator : JC\MD
 Sample : P1284-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1252

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: VN080852.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	16	22	29	rBV2	26569	42106	2.11%	0.526%
2	2.289	49	57	68	rBV	25205	65784	3.29%	0.822%
3	4.430	411	421	432	rBV3	17302	53552	2.68%	0.669%
4	7.224	887	896	909	rBV4	33612	92249	4.61%	1.153%
5	8.171	1046	1057	1061	rBV	80141	189913	9.50%	2.374%
6	8.229	1061	1067	1076	rVB2	127644	289472	14.48%	3.618%
7	8.529	1111	1118	1119	rBV	17453	25872	1.29%	0.323%
8	8.582	1121	1127	1134	rVB2	84634	193235	9.66%	2.415%
9	9.100	1205	1215	1225	rBV	248897	520774	26.04%	6.509%
10	9.271	1235	1244	1251	rBV2	38494	81228	4.06%	1.015%
11	9.882	1342	1348	1354	rVB3	12047	21357	1.07%	0.267%
12	10.571	1456	1465	1474	rBV	350000	648062	32.41%	8.100%
13	11.865	1673	1685	1694	rBV	404881	754289	37.72%	9.428%
14	12.212	1738	1744	1750	rVB4	11679	20947	1.05%	0.262%
15	12.423	1775	1780	1784	rBV	37944	58150	2.91%	0.727%
16	12.853	1844	1853	1863	rBV	260623	474889	23.75%	5.936%
17	13.082	1885	1892	1896	rBV5	12424	22298	1.12%	0.279%
18	13.264	1914	1923	1930	rBV	1222813	1999598	100.00%	24.993%
19	13.341	1930	1936	1944	rVB	355125	539777	26.99%	6.747%
20	13.506	1956	1964	1973	rBV2	265660	433638	21.69%	5.420%
21	13.611	1976	1982	1990	rVV4	48417	95175	4.76%	1.190%
22	13.688	1990	1995	2001	rVV4	25198	50006	2.50%	0.625%
23	13.794	2005	2013	2019	rBV	376950	642381	32.13%	8.029%
24	13.876	2019	2027	2035	rVV	213666	399197	19.96%	4.990%
25	14.241	2084	2089	2094	rBV7	11239	22287	1.11%	0.279%
26	14.935	2199	2207	2212	rBV6	15971	30227	1.51%	0.378%
27	15.094	2228	2234	2243	rVB10	6748	21698	1.09%	0.271%
28	15.394	2281	2285	2293	rVB3	50678	85203	4.26%	1.065%
29	15.511	2301	2305	2312	rVB9	15139	32224	1.61%	0.403%
30	15.600	2312	2320	2328	rBV10	11702	32798	1.64%	0.410%
31	15.823	2353	2358	2368	rVB7	15390	32950	1.65%	0.412%
32	15.947	2371	2379	2382	rBV5	15479	29268	1.46%	0.366%

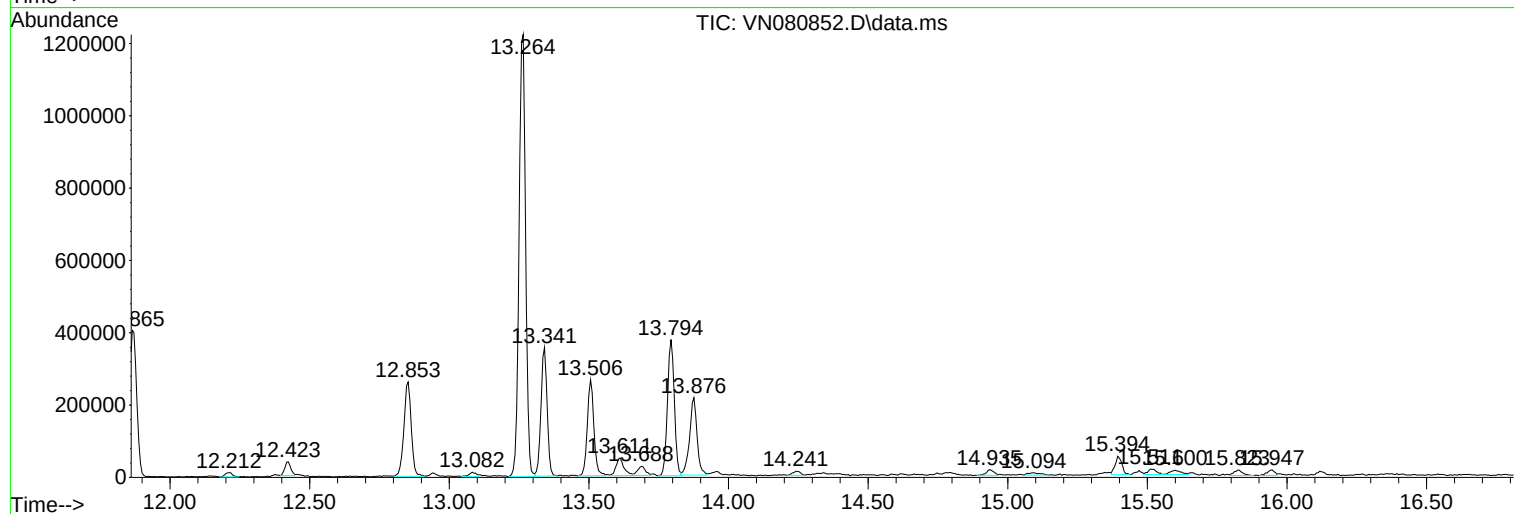
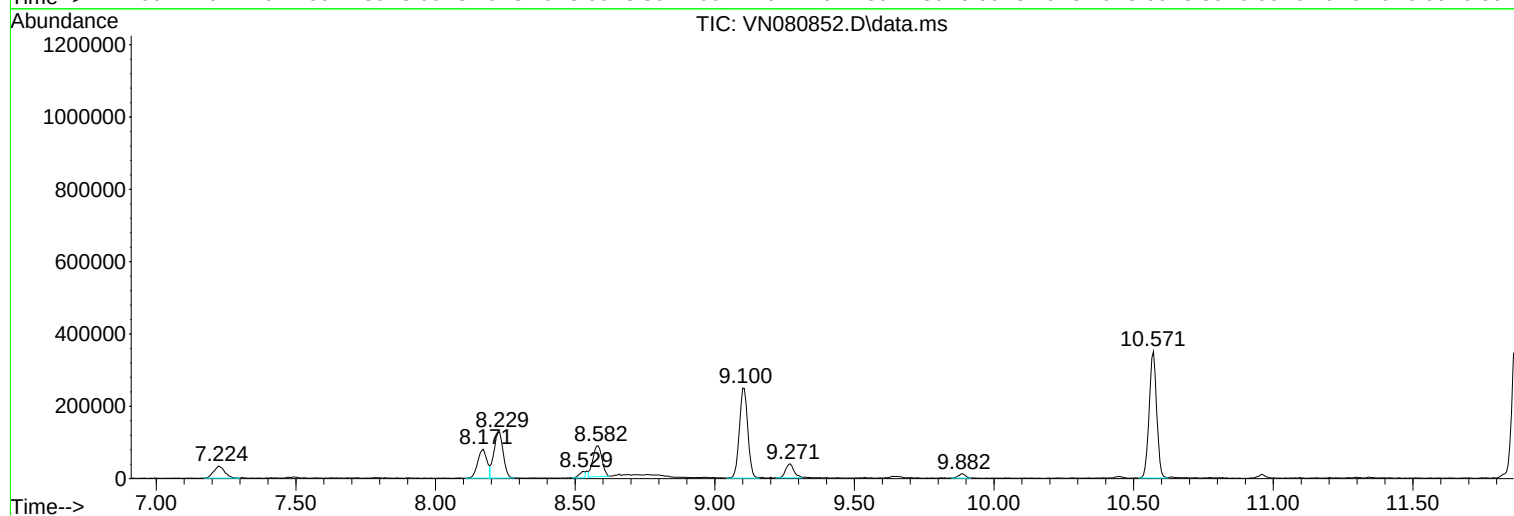
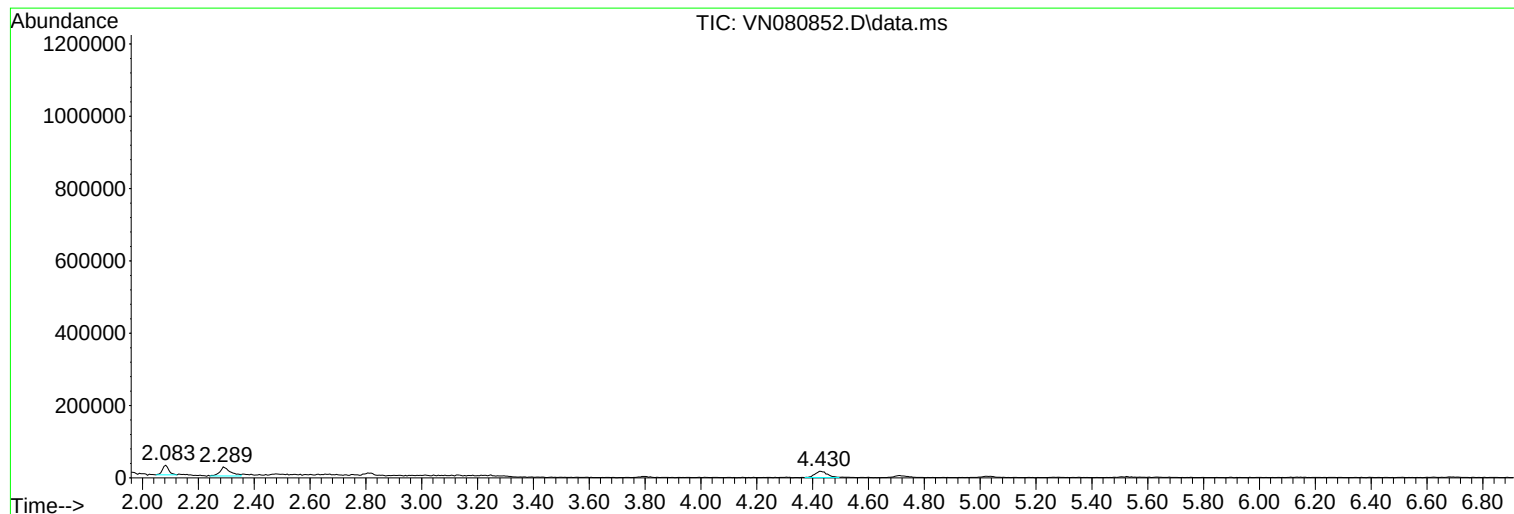
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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



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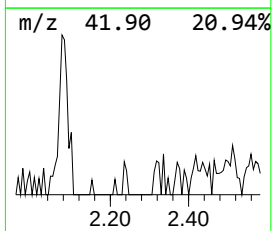
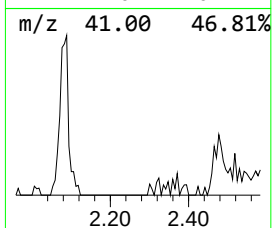
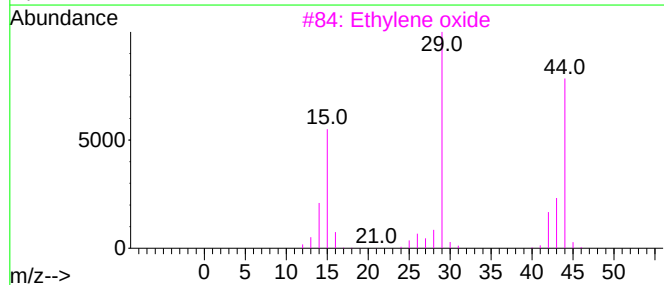
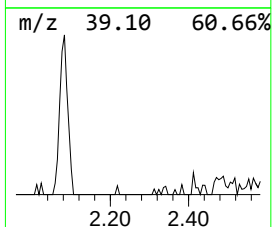
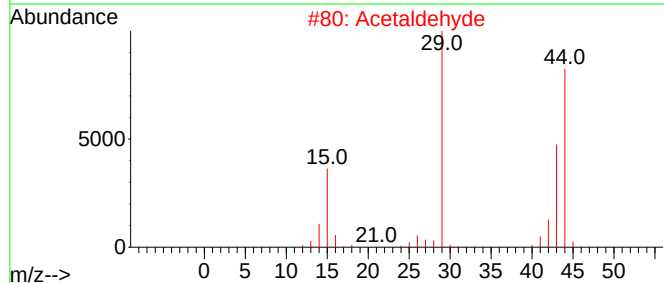
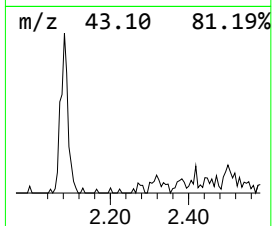
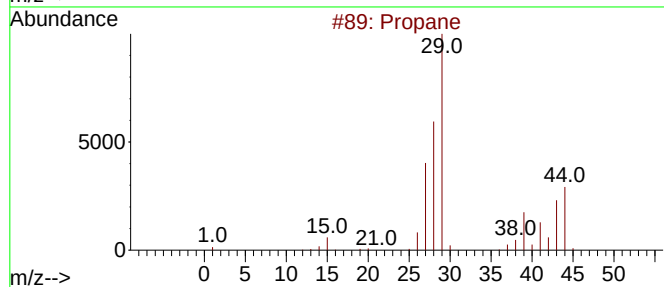
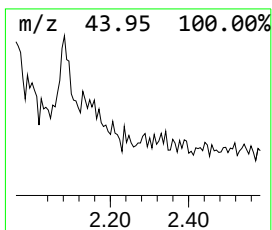
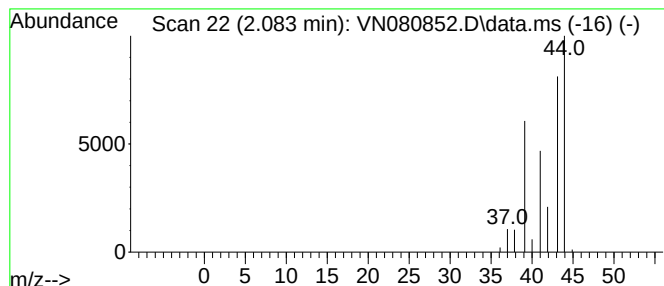
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	7.27 ug/l	42106	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	50
2			Acetaldehyde	44	C2H4O	000075-07-0	7
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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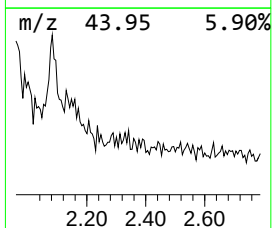
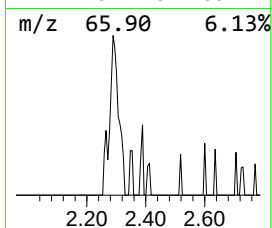
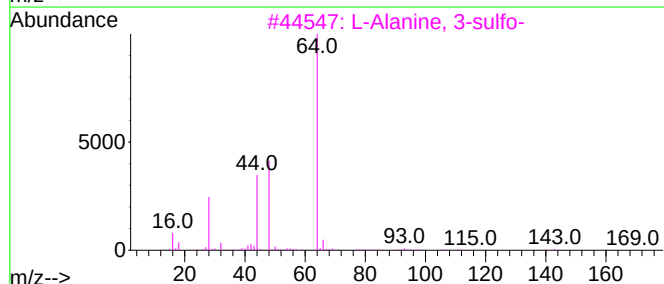
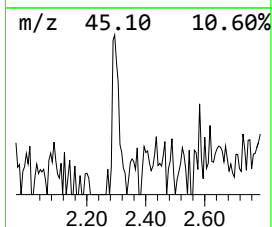
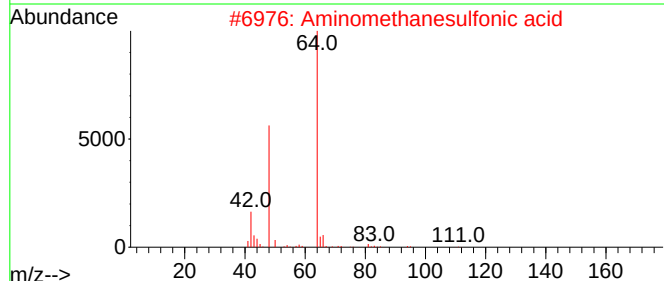
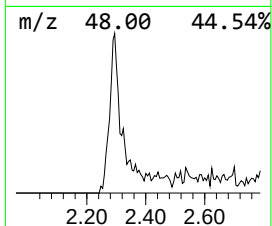
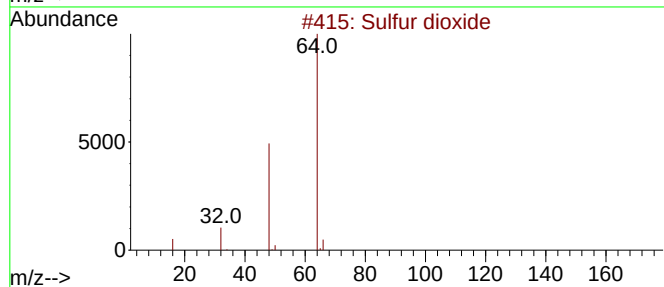
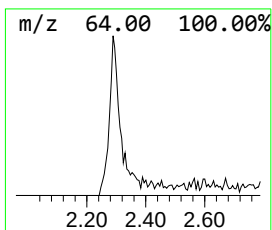
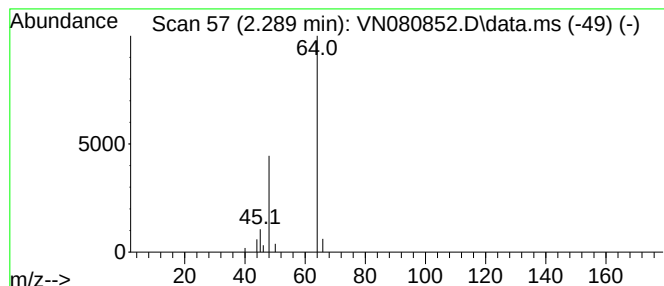
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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

Peak Number 2 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.289	11.36 ug/l	65784	Pentafluorobenzene	8.229

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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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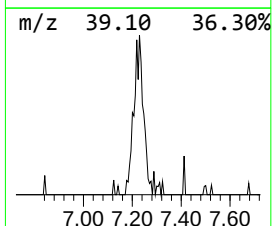
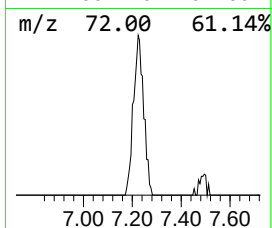
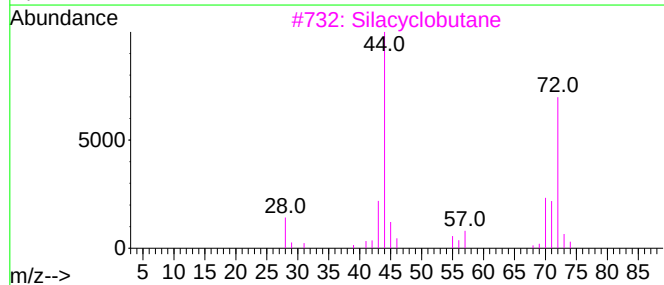
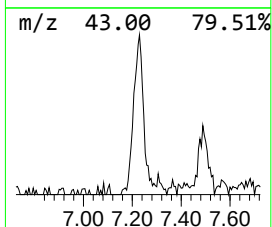
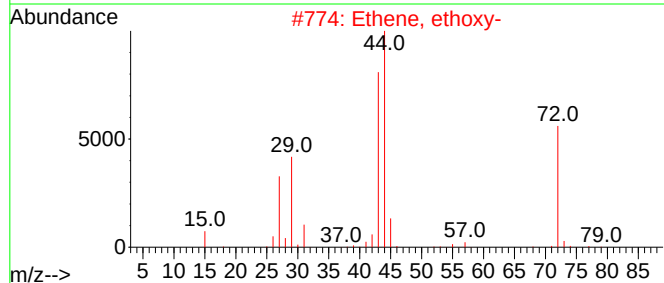
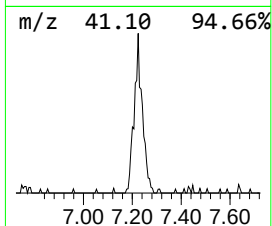
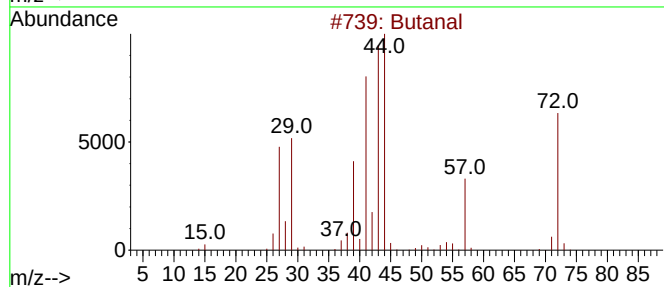
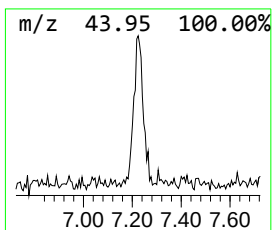
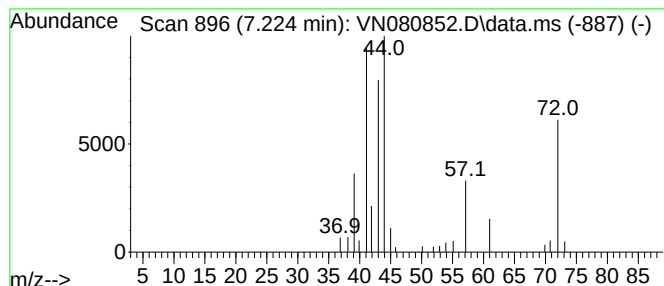
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Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	15.93 ug/l	92249	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	93
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	64
3			Silacyclobutane	72	C3H8Si	1000434-34-1	40
4			N-Formyl-dl-alanine	117	C4H7NO3	005893-10-7	28
5			Propanal, 2-methyl-	72	C4H8O	000078-84-2	27



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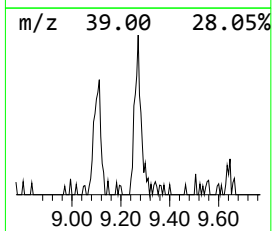
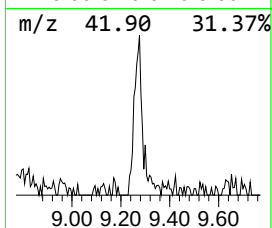
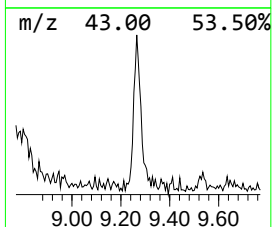
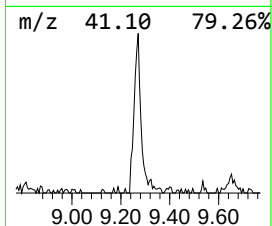
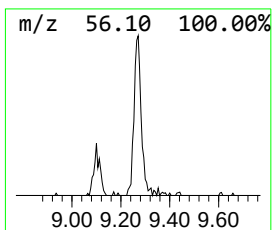
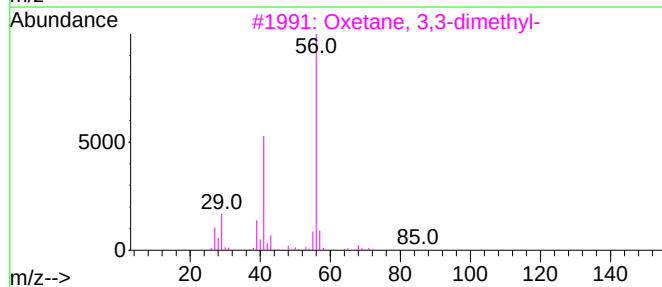
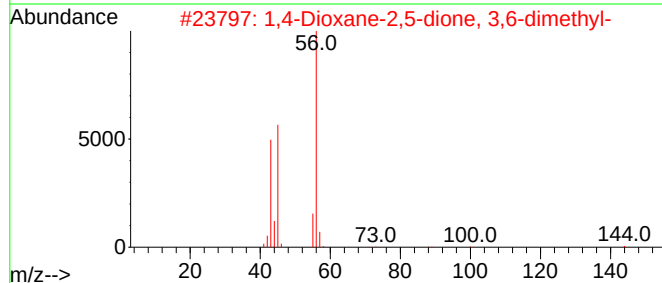
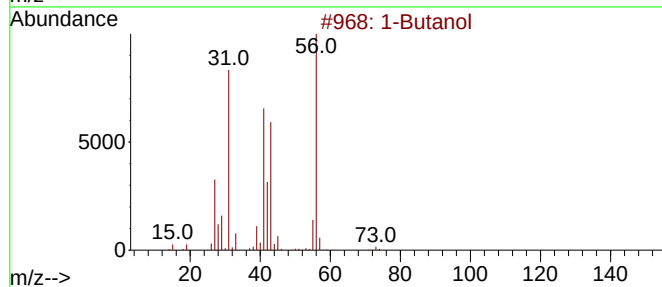
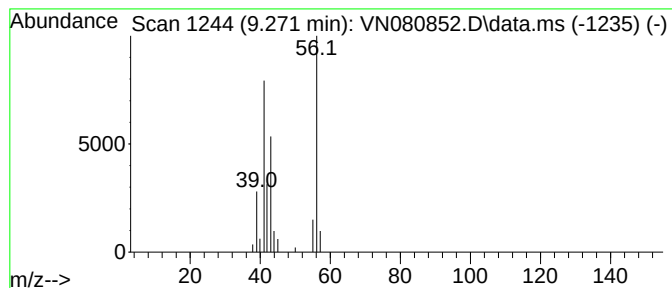
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.271	7.80 ug/l	81228	1,4-Difluorobenzene	9.106

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	64
2			1,4-Dioxane-2,5-dione, 3,6-dimet...	144	C6H8O4	000095-96-5	9
3			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9
4			Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	5
5			Cyclobutane	56	C4H8	000287-23-0	4



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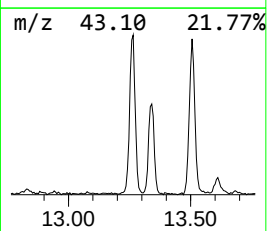
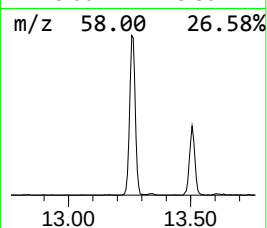
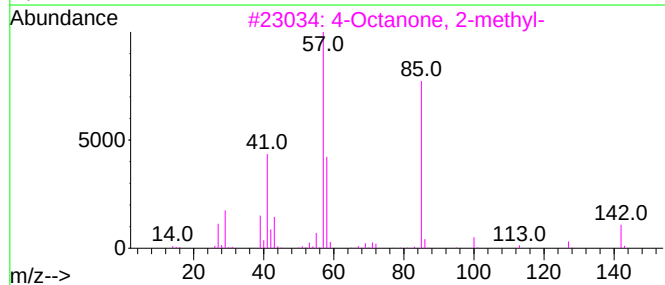
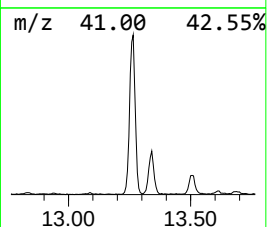
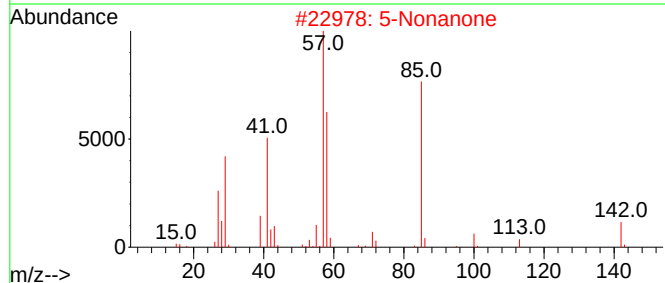
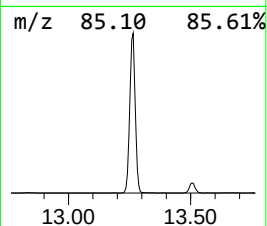
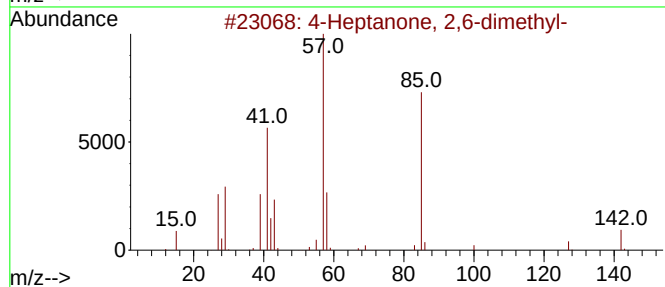
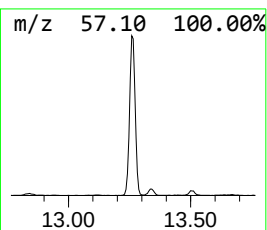
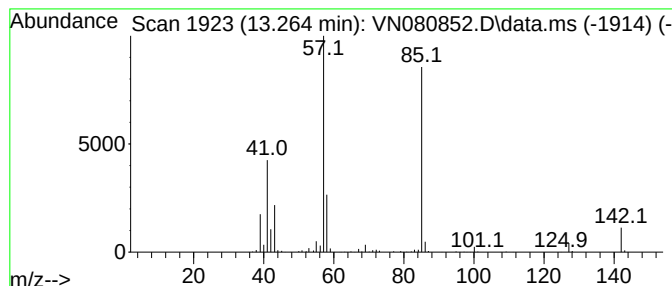
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Quant Title : SW846 8260

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

Peak Number 5 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.264	155.64 ug/l	1999600	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
2			5-Nonanone	142	C9H18O	000502-56-7	64
3			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	64
4			Allyl isovalerate	142	C8H14O2	002835-39-4	50
5			3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	50



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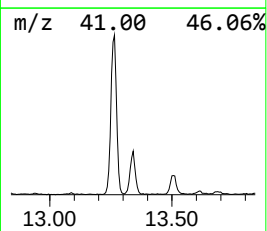
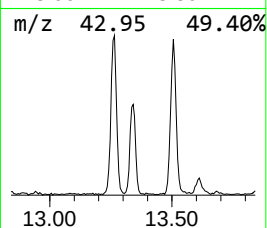
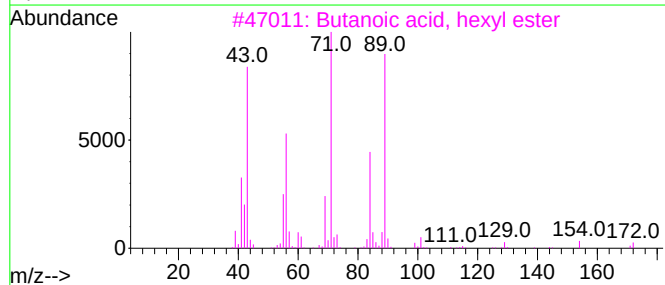
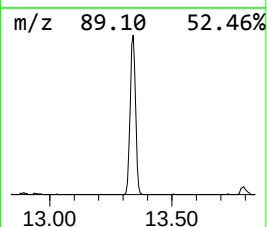
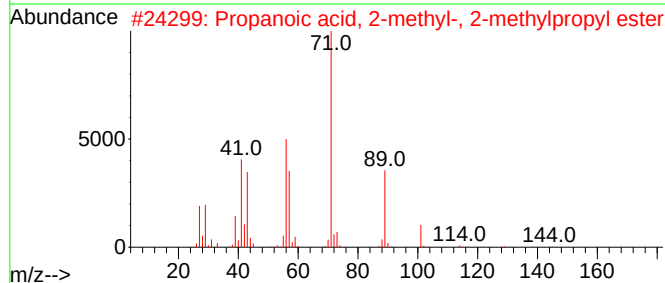
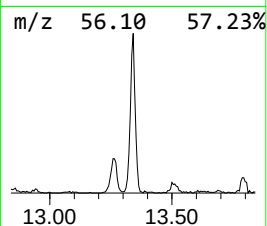
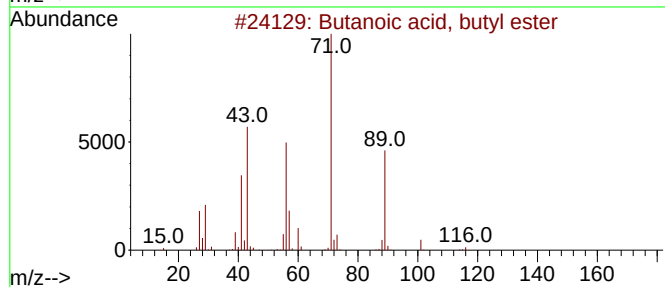
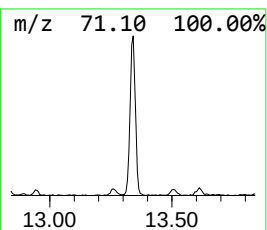
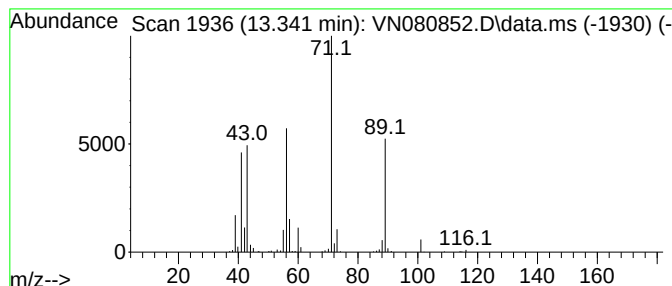
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Quant Title : SW846 8260

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

Peak Number 6 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	42.01 ug/l	539777	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			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	42
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080852.D
Acq On : 31 Jan 2024 19:54
Operator : JC\MD
Sample : P1284-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1252

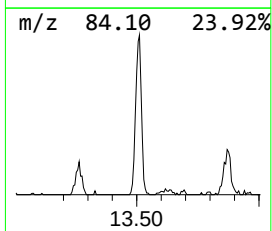
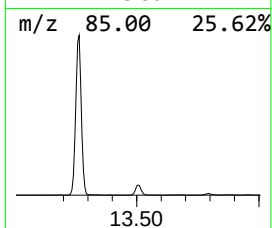
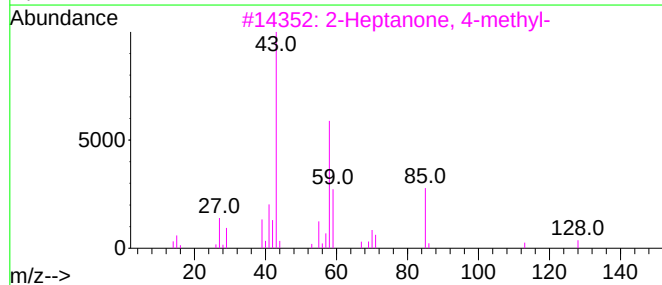
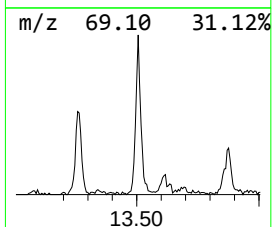
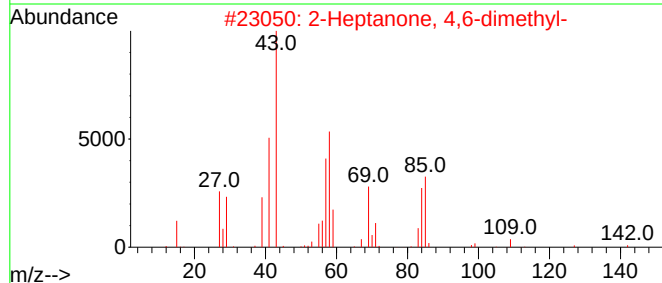
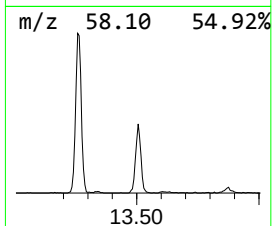
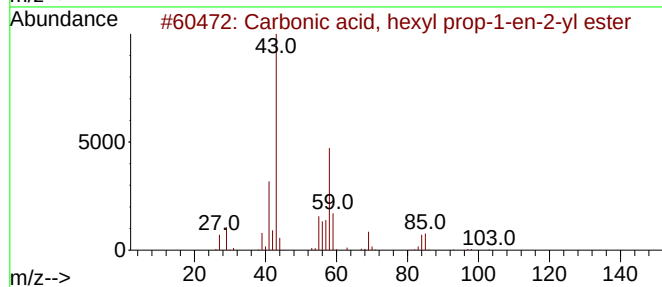
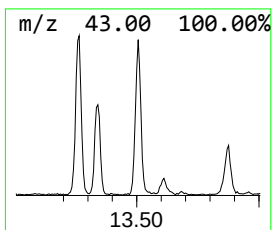
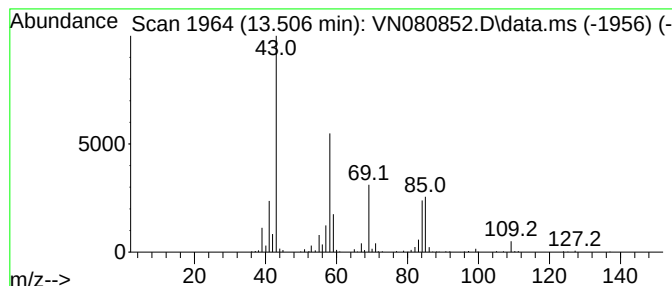
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Quant Title : SW846 8260

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

Peak Number 7 Carbonic acid, hexyl prop-1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.506	33.75 ug/l	433638	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, hexyl prop-1-en-2...	186	C10H18O3	1000382-54-2	64
2			2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	56
3			2-Heptanone, 4-methyl-	128	C8H16O	006137-06-0	50
4			Hexane, 3-ethyl-	114	C8H18	000619-99-8	38
5			1-Octene, 4-methyl-	126	C9H18	013151-12-7	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080852.D
Acq On : 31 Jan 2024 19:54
Operator : JC\MD
Sample : P1284-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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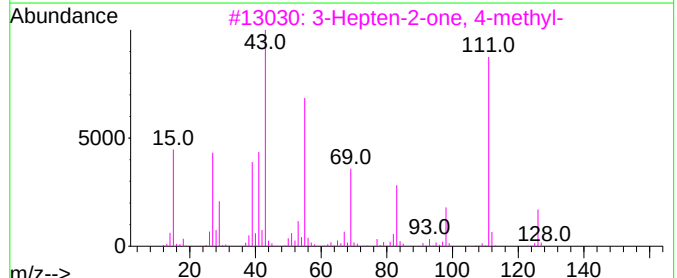
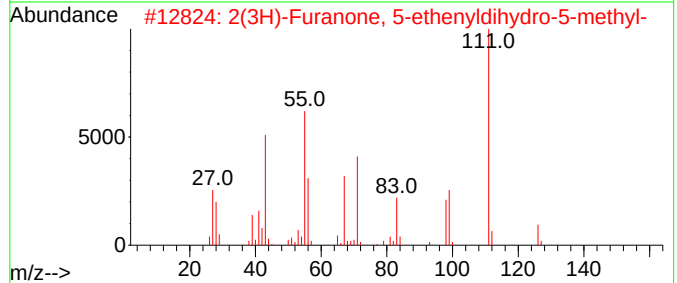
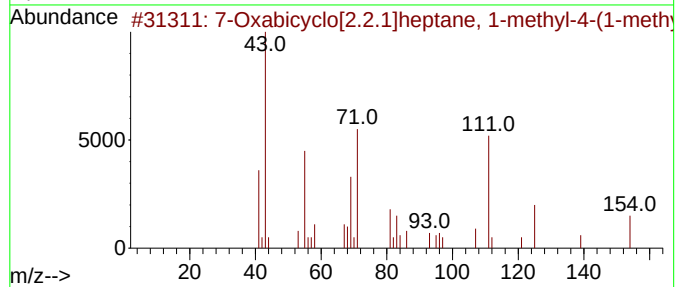
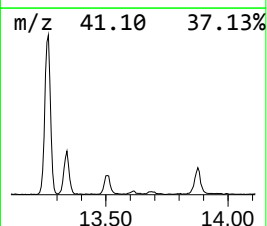
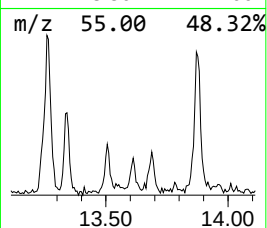
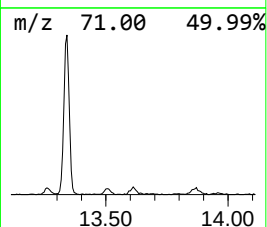
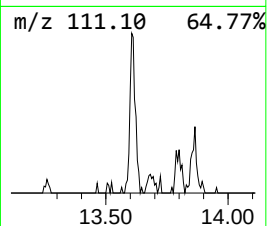
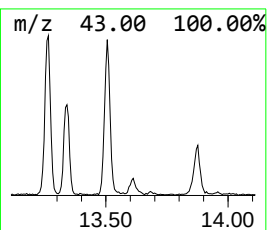
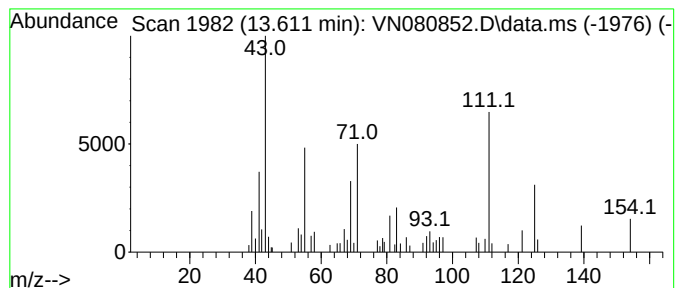
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Quant Title : SW846 8260

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

Peak Number 8 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.611	7.41 ug/l	95175	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	64
2		2(3H)-Furanone, 5-ethenyldihydro...	126	C7H10O2	001073-11-6	35
3		3-Hepten-2-one, 4-methyl-	126	C8H14O	022319-25-1	30
4		Isocytosine	111	C4H5N3O	000108-53-2	30
5		N-(2-Fluorophenyl)urea	154	C7H7FN2O	000656-31-5	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080852.D
Acq On : 31 Jan 2024 19:54
Operator : JC\MD
Sample : P1284-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1252

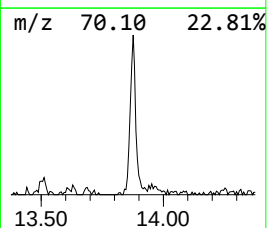
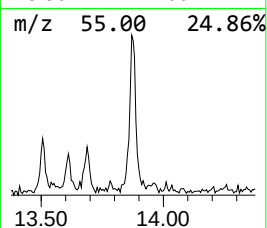
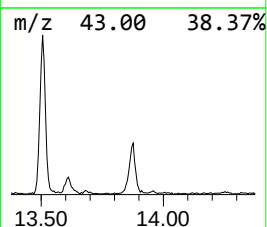
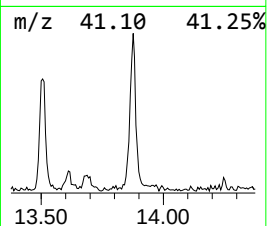
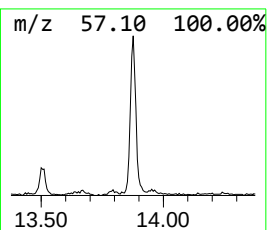
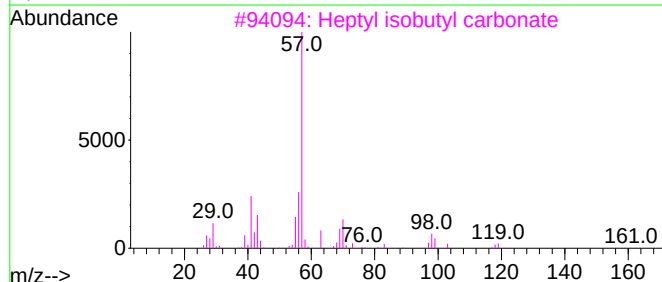
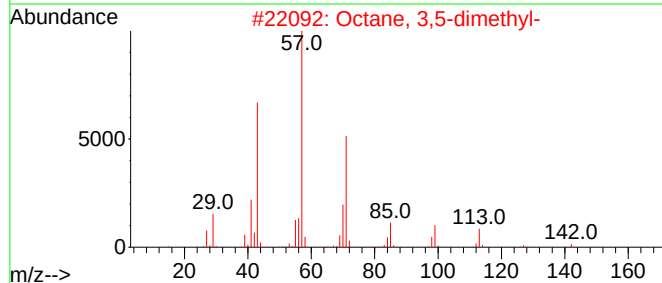
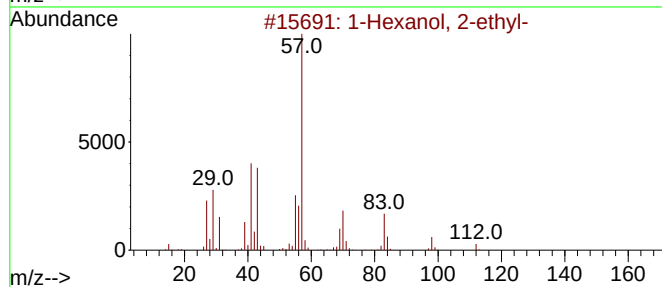
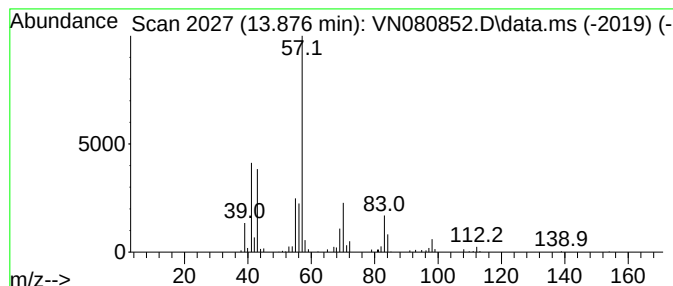
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Quant Title : SW846 8260

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	31.07 ug/l	399197	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	64
2			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	59
3			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	50
4			Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	50
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080852.D
Acq On : 31 Jan 2024 19:54
Operator : JC\MD
Sample : P1284-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1252

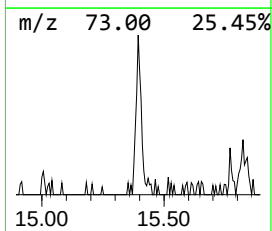
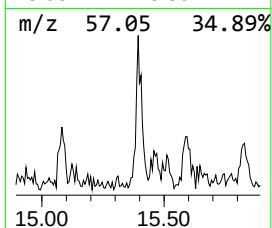
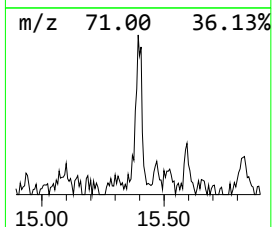
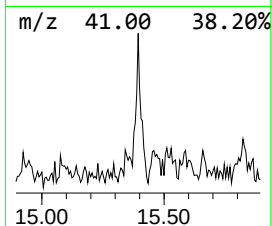
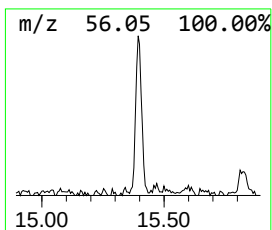
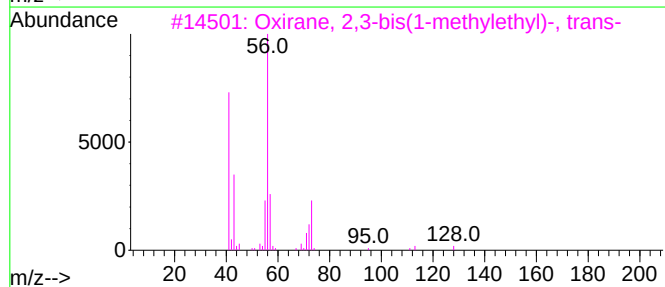
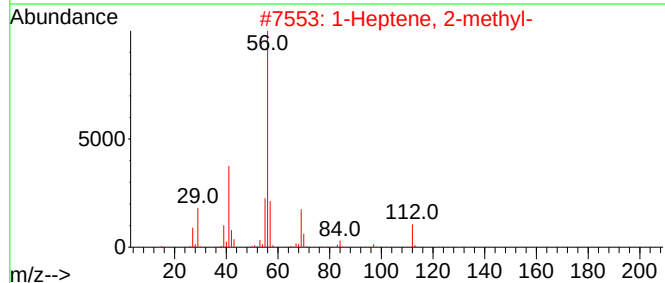
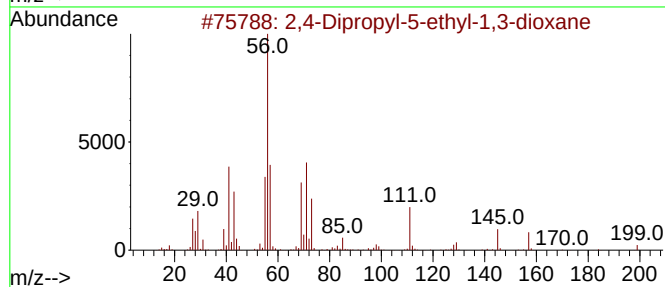
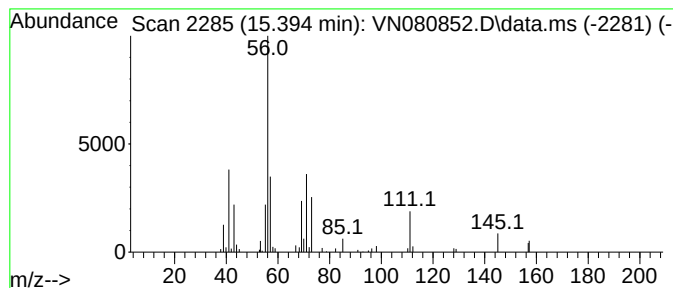
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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

Peak Number 10 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.394	6.63 ug/l	85203	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	83
2			1-Heptene, 2-methyl-	112	C8H16	015870-10-7	43
3			Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	40
4			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	33
5			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080852.D
Acq On : 31 Jan 2024 19:54
Operator : JC\MD
Sample : P1284-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1252

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	7.3	ug/l	42106	1	8.229	289472	50.0
Sulfur dioxide	2.289	11.4	ug/l	65784	1	8.229	289472	50.0
Butanal	7.224	15.9	ug/l	92249	1	8.229	289472	50.0
1-Butanol	9.271	7.8	ug/l	81228	2	9.106	520774	50.0
4-Heptanone, 2,...	13.264	155.6	ug/l	1999600	4	13.794	642381	50.0
Butanoic acid, ...	13.341	42.0	ug/l	539777	4	13.794	642381	50.0
Carbonic acid, ...	13.506	33.8	ug/l	433638	4	13.794	642381	50.0
7-Oxabicyclo[2....	13.611	7.4	ug/l	95175	4	13.794	642381	50.0
1-Hexanol, 2-et...	13.876	31.1	ug/l	399197	4	13.794	642381	50.0
2,4-Dipropyl-5-...	15.394	6.6	ug/l	85203	4	13.794	642381	50.0