

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052924\
 Data File : VN082383.D
 Acq On : 29 May 2024 20:18
 Operator : JC\MD
 Sample : P2609-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 513

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\82N051524W.M
 Title : SW846 8260

Signal : TIC: VN082383.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	31	rVB2	16577	26097	1.43%	0.250%
2	4.436	413	422	431	rBV2	11609	33780	1.85%	0.324%
3	4.724	461	471	481	rBV3	8278	27511	1.50%	0.264%
4	6.142	702	712	725	rVB4	14086	46842	2.56%	0.449%
5	6.677	793	803	817	rBV4	17743	64760	3.54%	0.621%
6	7.224	884	896	910	rBV	682704	1828843	100.00%	17.534%
7	8.171	1047	1057	1061	rBV	164135	392008	21.43%	3.758%
8	8.224	1061	1066	1081	rVB	283169	635856	34.77%	6.096%
9	8.583	1109	1127	1134	rBV	198495	498518	27.26%	4.780%
10	8.665	1134	1141	1152	rBV5	23630	96141	5.26%	0.922%
11	9.100	1207	1215	1229	rBV	424782	881654	48.21%	8.453%
12	9.271	1236	1244	1257	rBV	141805	300666	16.44%	2.883%
13	9.653	1302	1309	1319	rBV2	44437	91733	5.02%	0.879%
14	10.571	1455	1465	1473	rBV	658215	1233275	67.43%	11.824%
15	11.865	1671	1685	1695	rBV	607304	1121441	61.32%	10.752%
16	12.418	1767	1779	1783	rBV6	9938	26749	1.46%	0.256%
17	12.853	1839	1853	1865	rBV	480004	834927	45.65%	8.005%
18	13.259	1916	1922	1931	rVV	63857	118909	6.50%	1.140%
19	13.341	1931	1936	1941	rVB2	12771	19507	1.07%	0.187%
20	13.500	1955	1963	1971	rBV3	26318	72100	3.94%	0.691%
21	13.688	1989	1995	2005	rVB2	47457	82166	4.49%	0.788%
22	13.794	2005	2013	2021	rBV	574179	1005374	54.97%	9.639%
23	13.876	2021	2027	2036	rVV	97394	175085	9.57%	1.679%
24	13.994	2043	2047	2061	rVB5	17773	47728	2.61%	0.458%
25	14.447	2119	2124	2128	rBV4	10964	19418	1.06%	0.186%
26	14.929	2201	2206	2210	rBV	26903	48272	2.64%	0.463%
27	15.053	2218	2227	2243	rBV4	51157	126309	6.91%	1.211%
28	15.212	2248	2254	2261	rVB3	55546	100361	5.49%	0.962%
29	15.347	2261	2277	2283	rBV10	39529	115838	6.33%	1.111%
30	15.441	2289	2293	2300	rVB4	14271	32840	1.80%	0.315%
31	15.582	2312	2317	2323	rBV7	9928	19259	1.05%	0.185%
32	15.647	2323	2328	2333	rVV2	17678	34019	1.86%	0.326%
33	15.829	2354	2359	2366	rVB8	13396	30993	1.69%	0.297%
34	15.941	2371	2378	2384	rBV3	17473	34196	1.87%	0.328%
35	16.170	2402	2417	2425	rBV4	39490	117005	6.40%	1.122%
36	16.506	2467	2474	2483	rBV5	25571	62089	3.39%	0.595%

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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\82N051524W.M
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37	16.782	2514	2521	2522	rBV2	19073	27870	1.52%	0.267%
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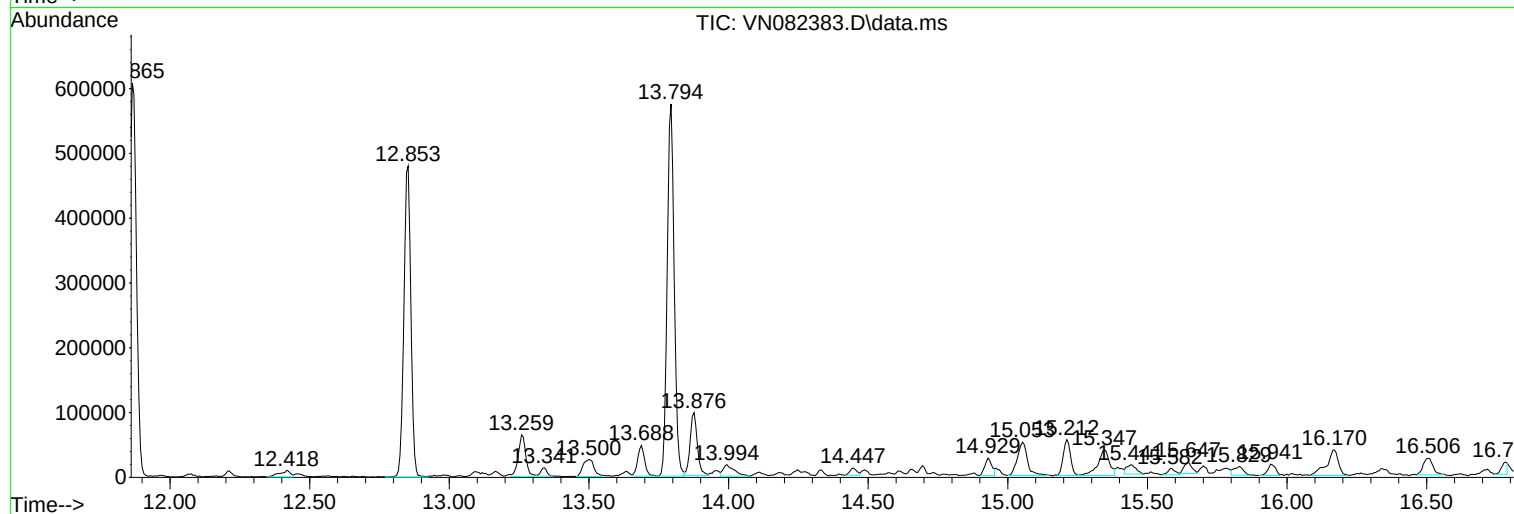
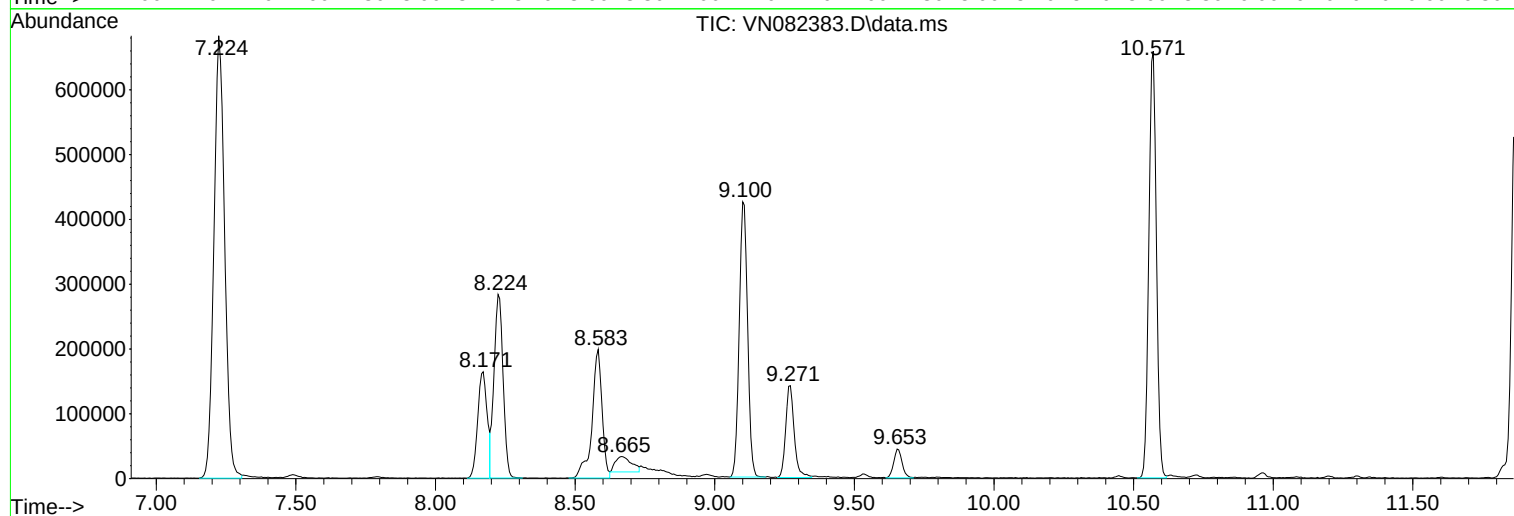
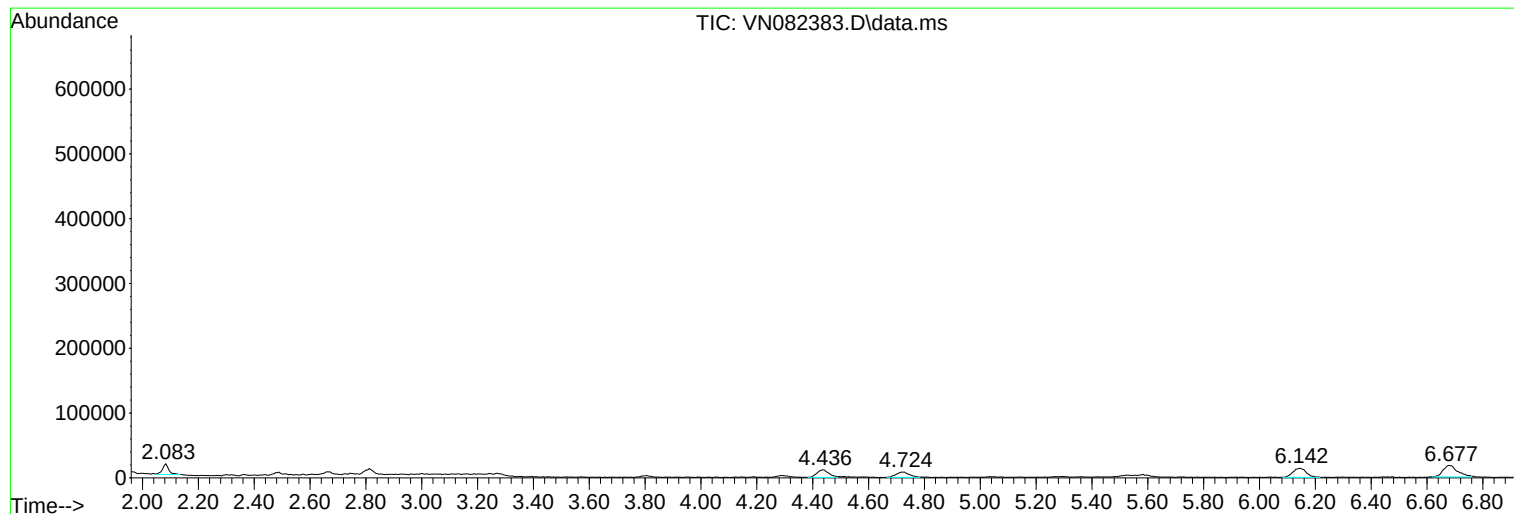
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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



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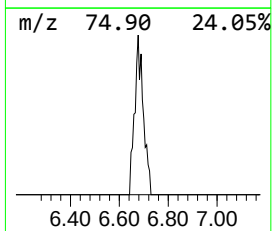
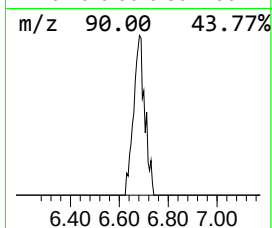
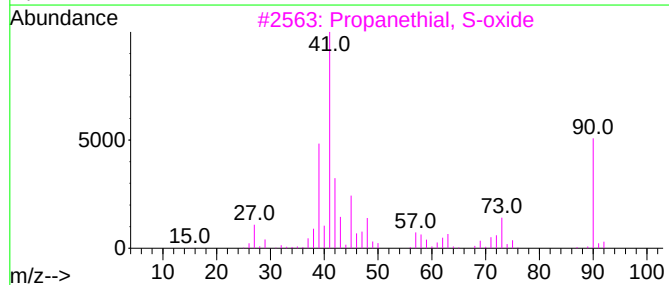
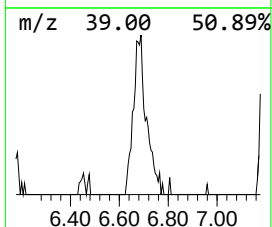
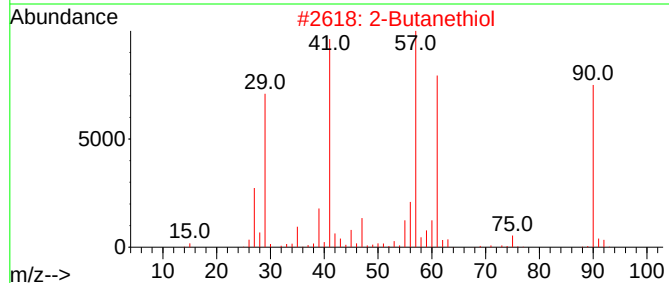
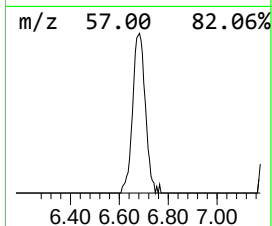
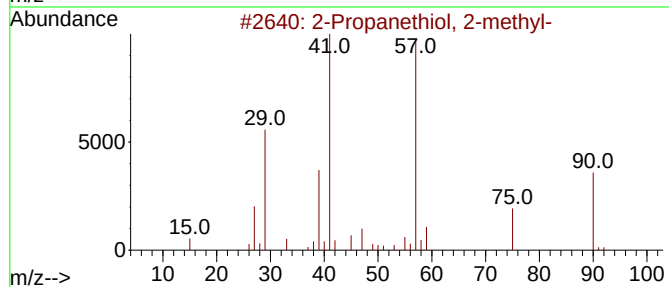
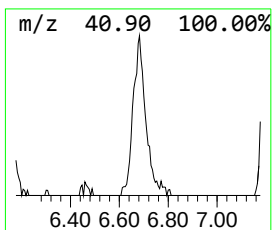
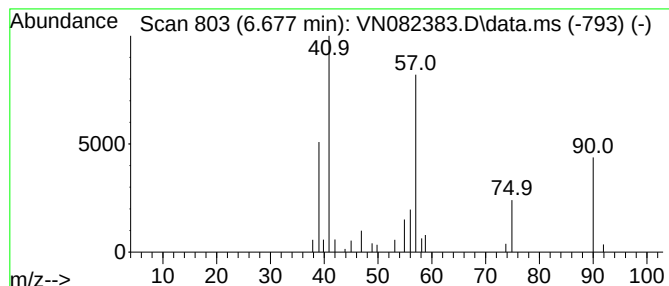
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Propanethiol, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.677	5.09 ug/l	64760	Pentafluorobenzene	8.230

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	53
2		2-Butanethiol	90	C4H10S	000513-53-1	43
3		Propanethial, S-oxide	90	C3H6OS	032157-29-2	40
4		Butane, 2-nitro-	103	C4H9NO2	000600-24-8	10
5		1-Butanethiol	90	C4H10S	000109-79-5	9



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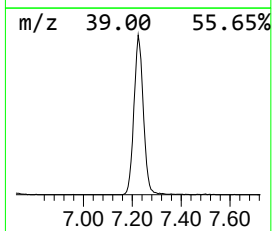
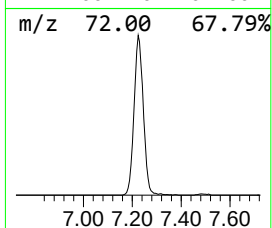
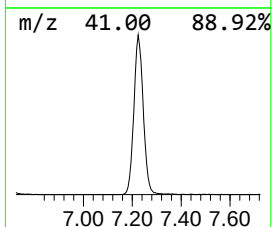
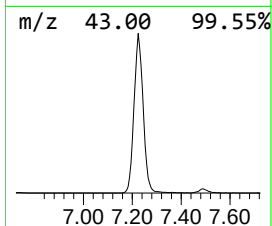
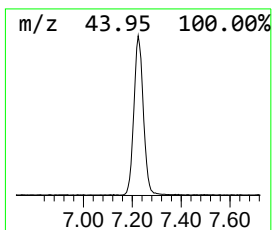
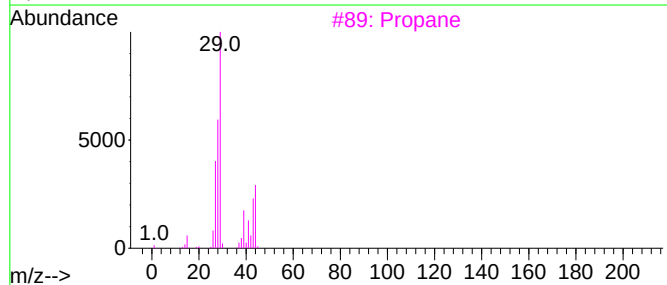
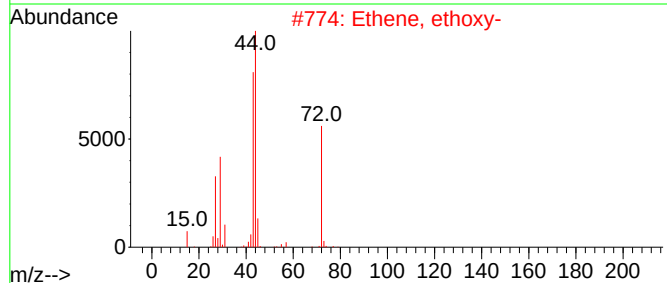
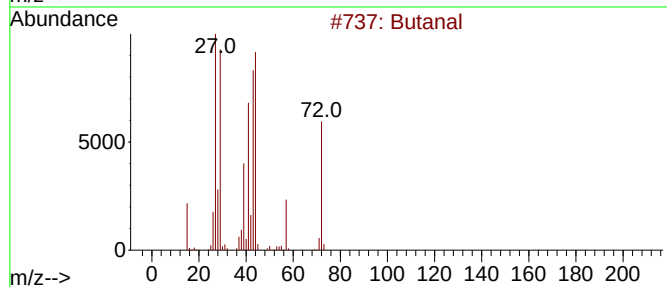
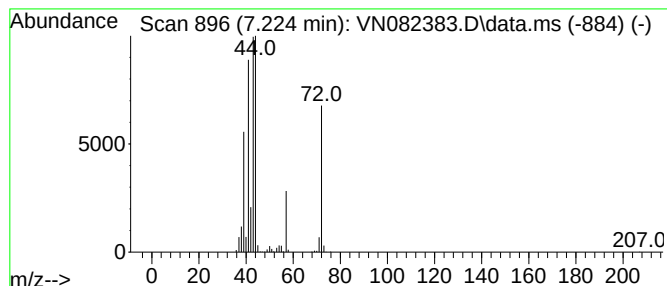
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Quant Title : SW846 8260

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

Peak Number 2 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	143.81 ug/l	1828840	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	49
3			Propane	44	C3H8	000074-98-6	47
4			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	25



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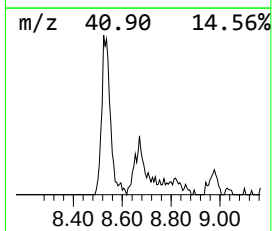
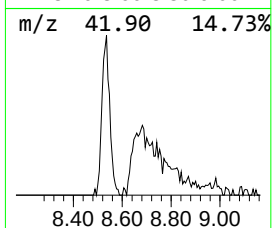
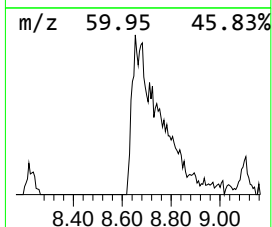
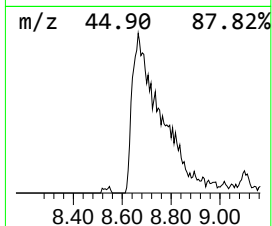
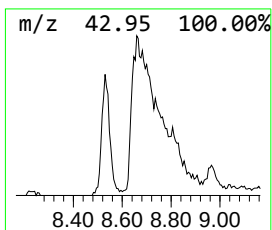
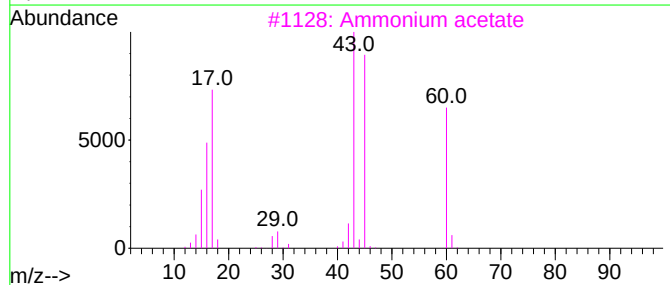
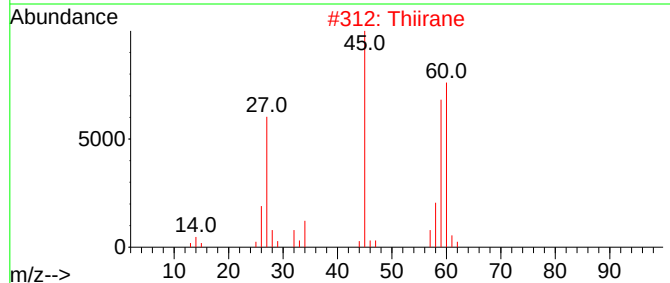
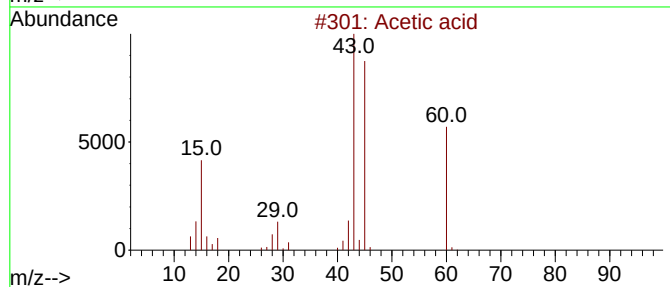
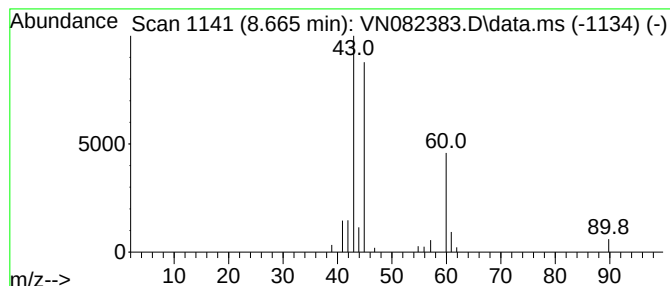
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Quant Title : SW846 8260

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

Peak Number 3 Acetic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.665	5.45 ug/l	96141	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	56
2			Thiirane	60	C2H4S	000420-12-2	53
3			Ammonium acetate	77	C2H7NO2	000631-61-8	43
4			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	9
5			Hydroperoxide, 1-methylpentyl	118	C6H14O2	024254-55-5	9



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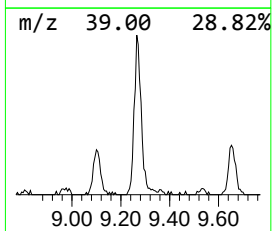
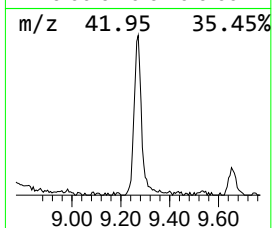
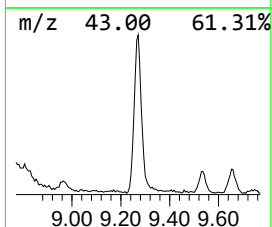
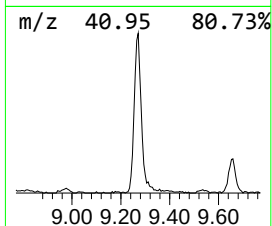
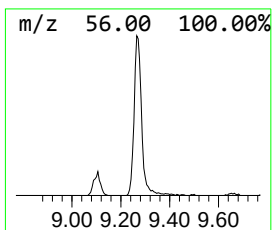
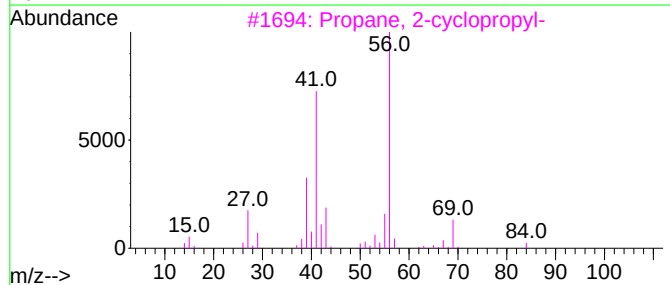
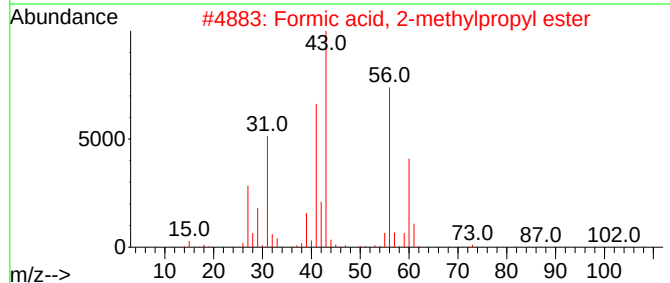
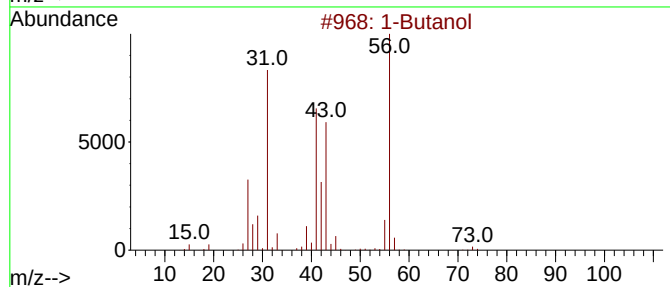
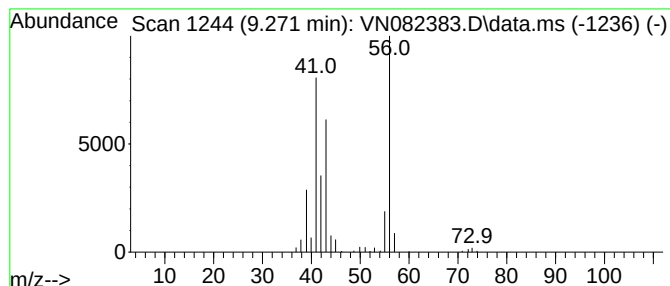
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Butanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.271	17.05 ug/l	300666	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			Formic acid, 2-methylpropyl ester	102	C5H10O2	000542-55-2	43
3			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
4			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	38
5			Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	9



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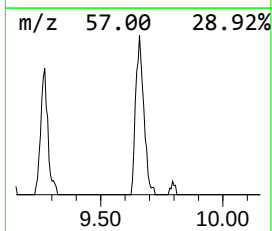
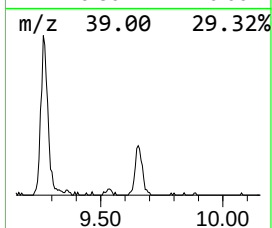
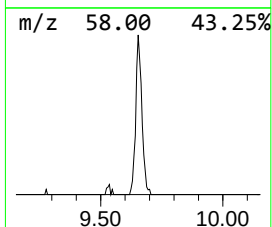
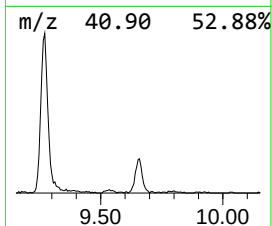
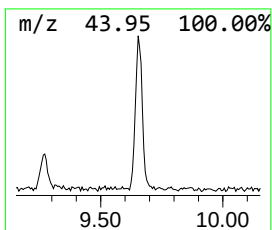
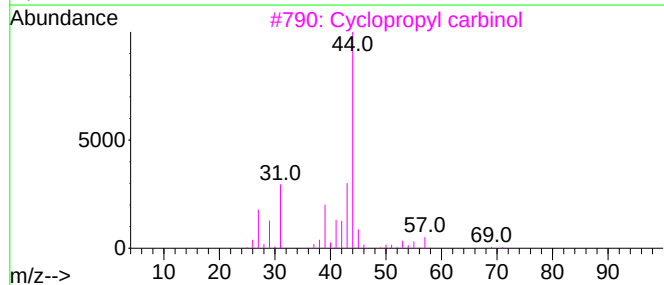
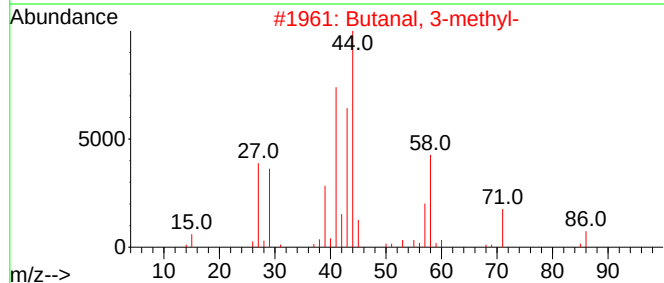
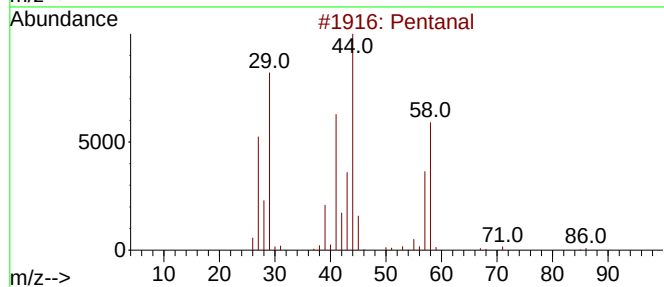
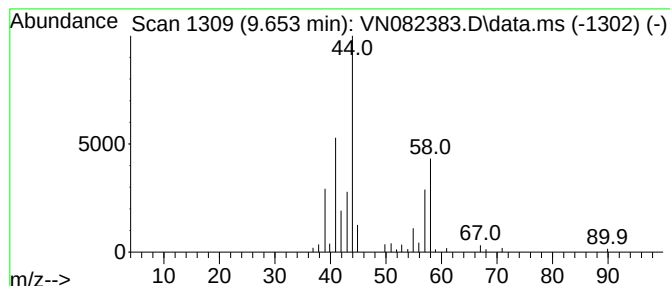
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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

Peak Number 5 Pentanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.653	5.20 ug/l	91733	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	72
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	64
3			Cyclopropyl carbinol	72	C4H8O	002516-33-8	28
4			1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	9
5			2-(4-Bromo-2-methylphenoxy)-N-me...	243	C10H14BrNO	915920-76-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052924\
Data File : VN082383.D
Acq On : 29 May 2024 20:18
Operator : JC\MD
Sample : P2609-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
513

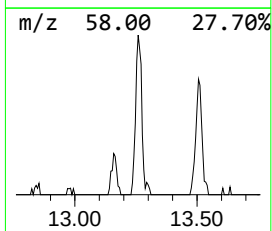
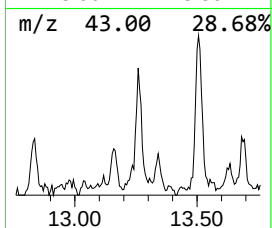
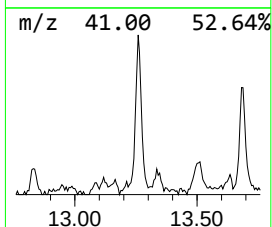
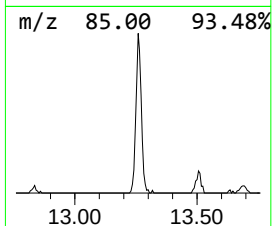
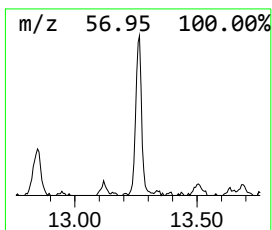
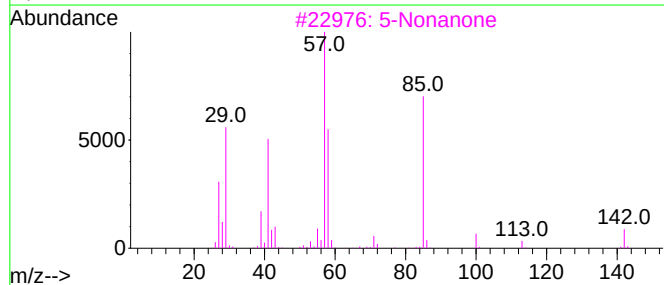
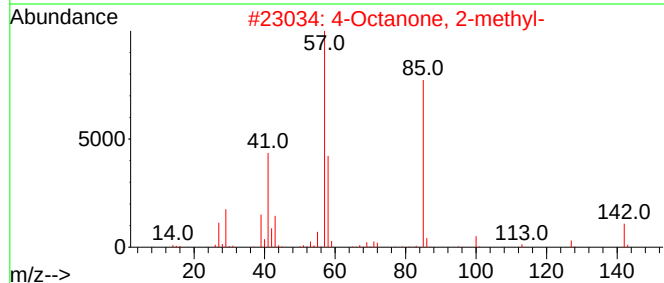
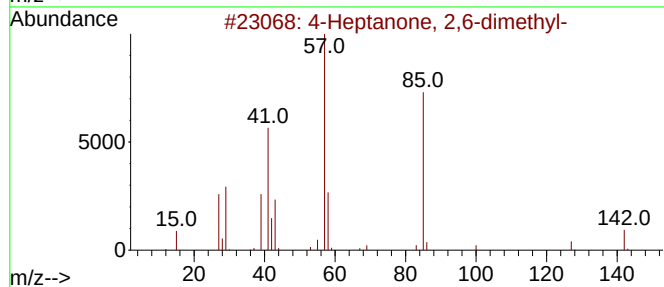
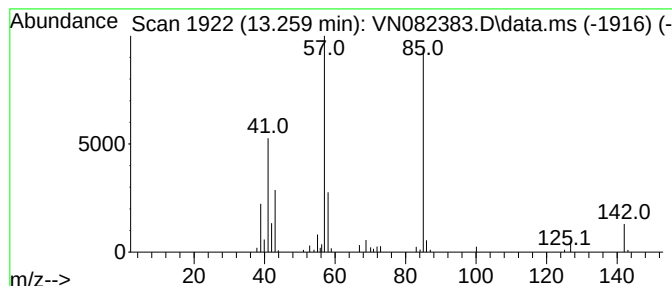
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	5.91 ug/l	118909	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			4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	80
3			5-Nonanone	142	C9H18O	000502-56-7	72
4			4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	64
5			Allyl isovalerate	142	C8H14O2	002835-39-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052924\
Data File : VN082383.D
Acq On : 29 May 2024 20:18
Operator : JC\MD
Sample : P2609-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
513

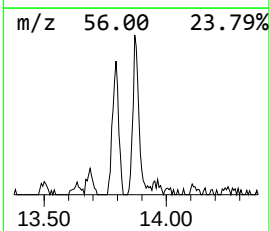
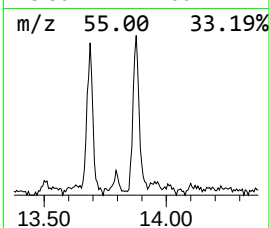
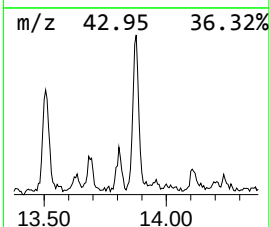
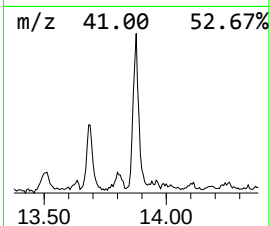
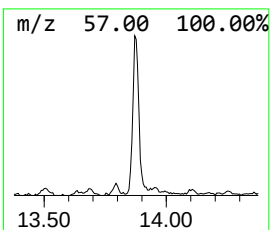
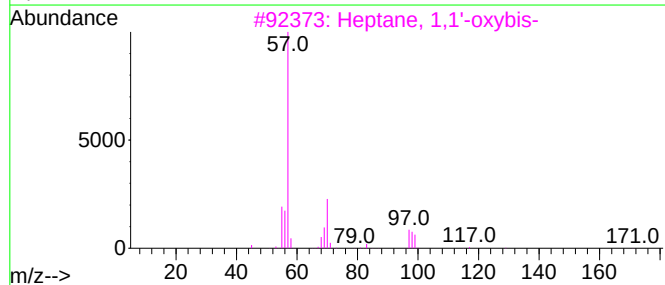
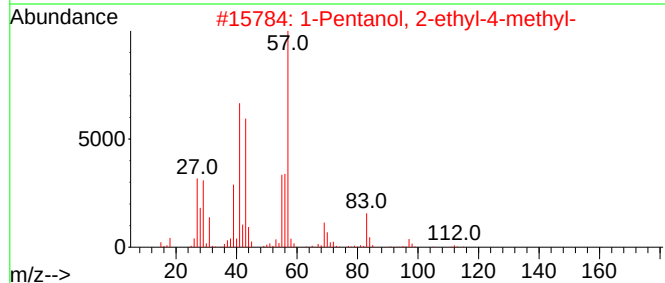
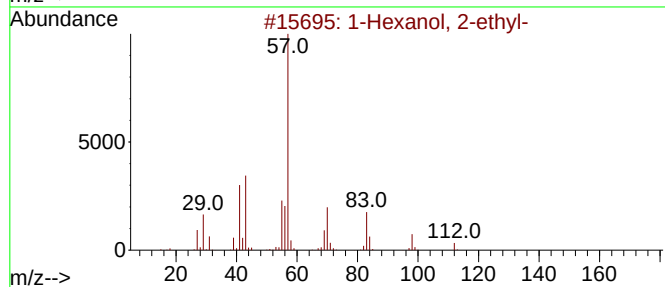
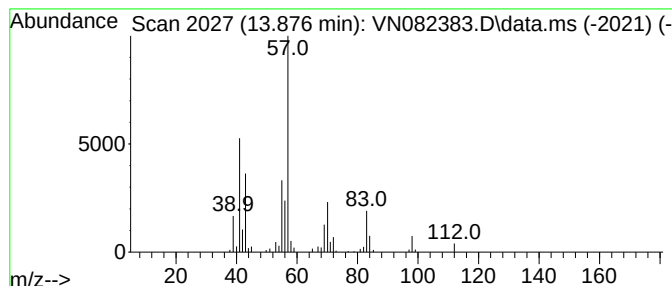
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Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	8.71 ug/l	175085	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	59
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			1-Hexene, 4-methyl-	98	C7H14	003769-23-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052924\
Data File : VN082383.D
Acq On : 29 May 2024 20:18
Operator : JC\MD
Sample : P2609-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
513

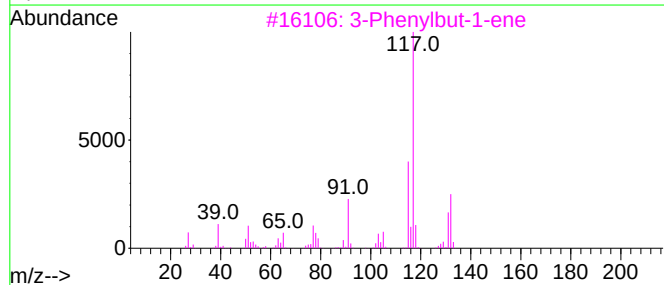
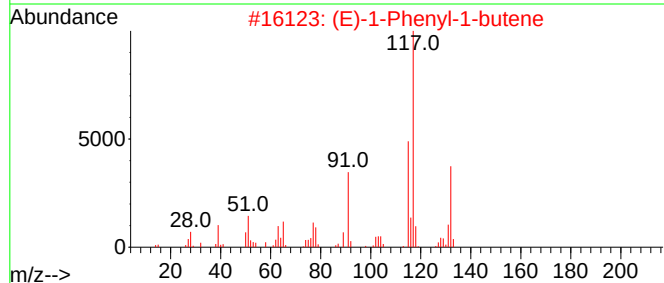
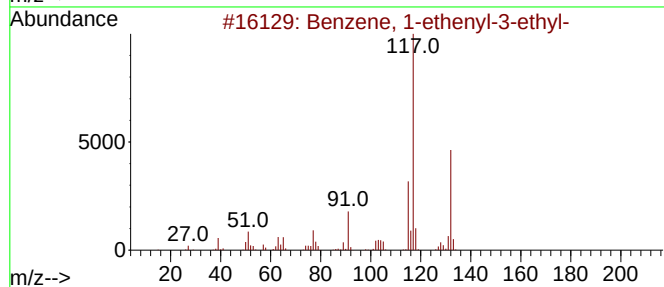
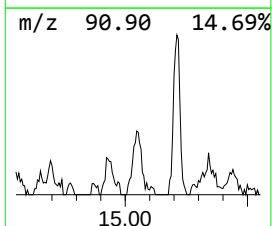
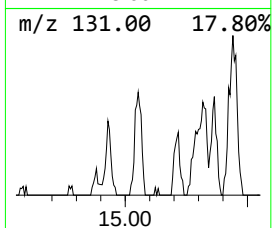
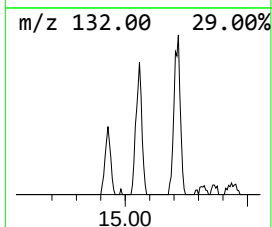
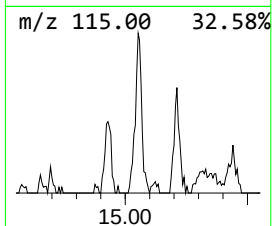
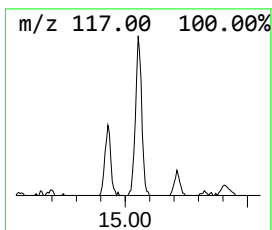
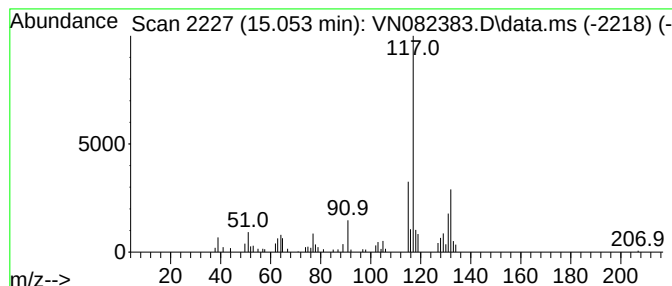
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Quant Title : SW846 8260

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

Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	6.28 ug/l	126309	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
2			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	90
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	90
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	87
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052924\
Data File : VN082383.D
Acq On : 29 May 2024 20:18
Operator : JC\MD
Sample : P2609-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
513

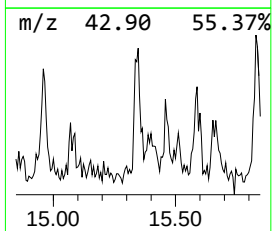
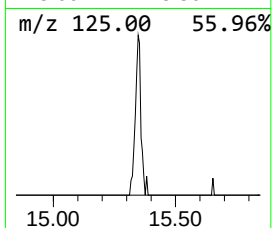
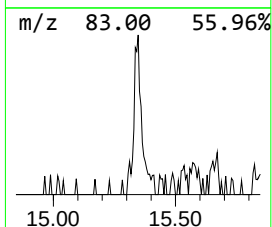
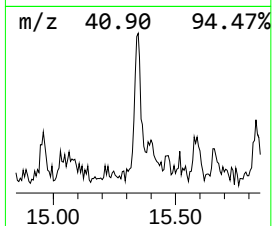
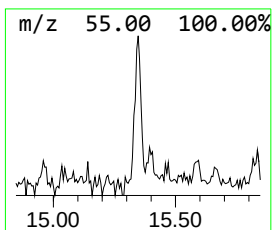
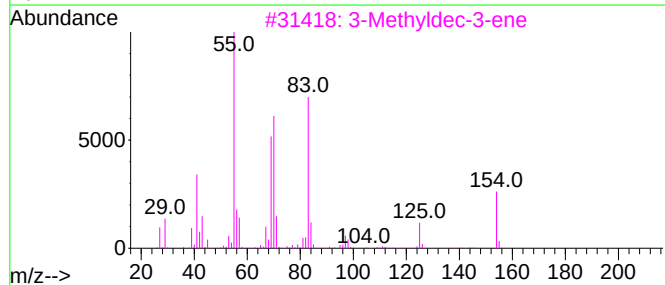
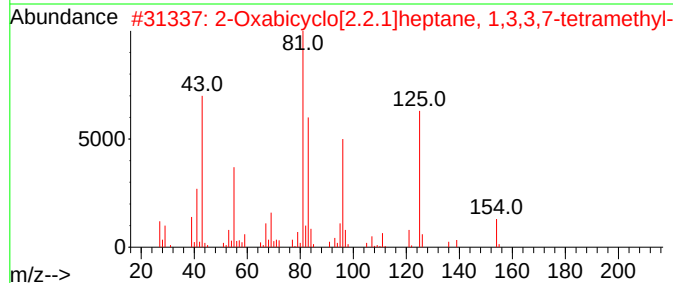
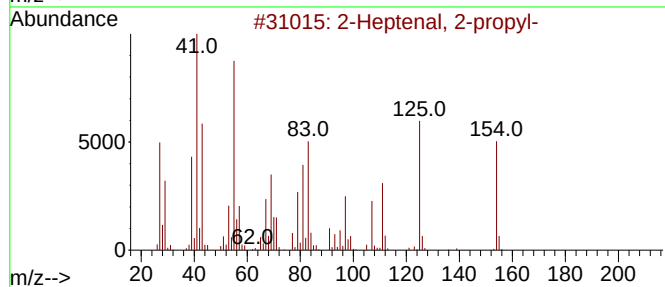
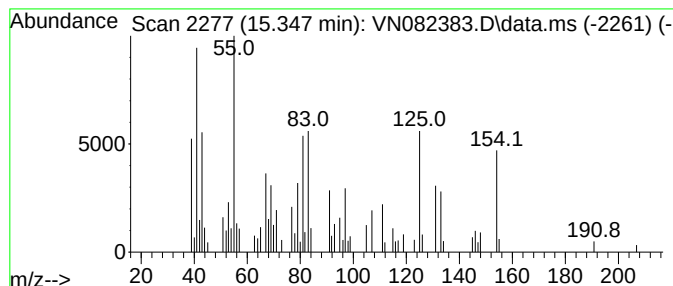
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Quant Title : SW846 8260

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

Peak Number 9 2-Heptenal, 2-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.347	5.76 ug/l	115838	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptenal, 2-propyl-	154	C10H18O	034880-43-8	70
2			2-Oxabicyclo[2.2.1]heptane, 1,3,...	154	C10H18O	015404-57-6	35
3			3-Methyldec-3-ene	154	C11H22	036969-75-2	30
4			3-Cyclopentylpropionic acid, 3-t...	324	C21H40O2	1000293-56-8	22
5			1,2,4-Triazine-3,5(2H,4H)-dione,...	169	C7H11N3O2	052236-30-3	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052924\
Data File : VN082383.D
Acq On : 29 May 2024 20:18
Operator : JC\MD
Sample : P2609-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
513

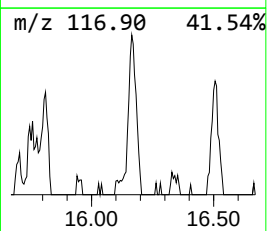
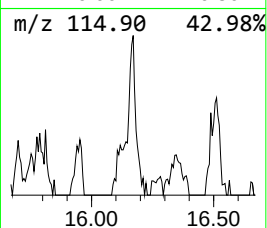
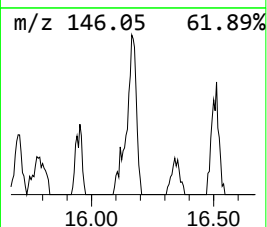
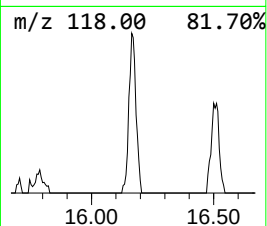
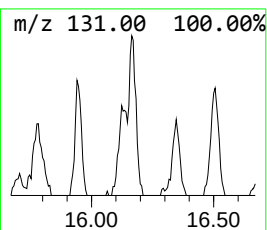
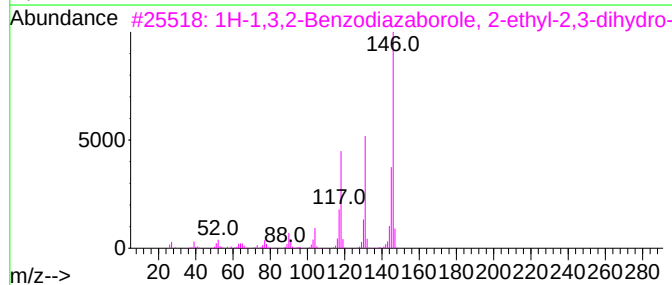
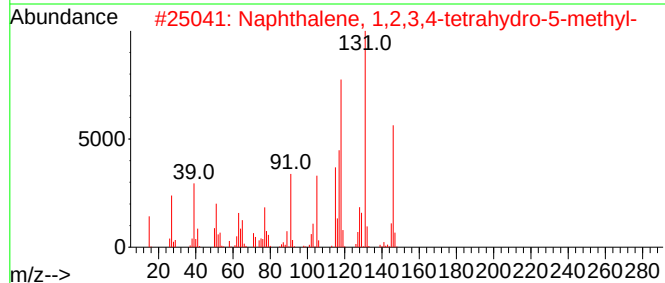
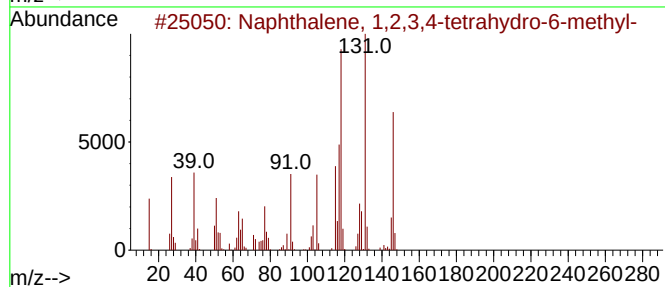
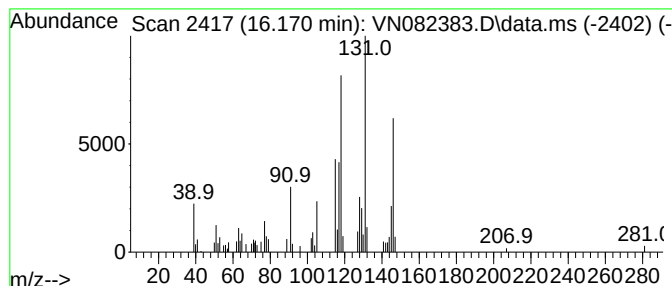
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	5.82 ug/l	117005	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	94
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	91
3			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	62
4			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	58
5			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052924\
Data File : VN082383.D
Acq On : 29 May 2024 20:18
Operator : JC\MD
Sample : P2609-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.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
2-Propanethiol,...	6.677	5.1	ug/l	64760	1	8.230	635856	50.0
Butanal	7.224	143.8	ug/l	1828840	1	8.230	635856	50.0
Acetic acid	8.665	5.5	ug/l	96141	2	9.100	881654	50.0
1-Butanol	9.271	17.1	ug/l	300666	2	9.100	881654	50.0
Pentanal	9.653	5.2	ug/l	91733	2	9.100	881654	50.0
4-Heptanone, 2,...	13.259	5.9	ug/l	118909	4	13.794	1005370	50.0
1-Hexanol, 2-et...	13.876	8.7	ug/l	175085	4	13.794	1005370	50.0
Benzene, 1-ethe...	15.053	6.3	ug/l	126309	4	13.794	1005370	50.0
2-Heptenal, 2-p...	15.347	5.8	ug/l	115838	4	13.794	1005370	50.0
Naphthalene, 1,...	16.170	5.8	ug/l	117005	4	13.794	1005370	50.0