

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091324\
 Data File : VN083876.D
 Acq On : 13 Sep 2024 17:43
 Operator : JC\MD
 Sample : P3956-01 5X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 EFF-WW

Integration Parameters: RTEINT3.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\624N090624W.M

Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

Signal : TIC: VN083876.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.424	409	420	443	rBV	395742	1193061	2.75%	1.061%
2	4.712	457	469	493	rBV	484649	1553592	3.58%	1.382%
3	7.241	885	899	924	rBV	1485951	4480276	10.33%	3.986%
4	7.788	980	992	1012	rBV2	193929	645380	1.49%	0.574%
5	9.435	1260	1272	1282	rBV	387568	809877	1.87%	0.721%
6	9.835	1329	1340	1348	rBV	10365680	19768810	45.58%	17.588%
7	9.912	1348	1353	1367	rVB	218534	464264	1.07%	0.413%
8	10.565	1458	1464	1470	rBV	293659	517198	1.19%	0.460%
9	10.877	1510	1517	1522	rBV	675634	1219019	2.81%	1.085%
10	10.924	1522	1525	1535	rVB	317863	549322	1.27%	0.489%
11	11.088	1543	1553	1562	rVB2	327590	951857	2.19%	0.847%
12	11.865	1674	1685	1692	rBV	264511	519389	1.20%	0.462%
13	12.376	1764	1772	1780	rBV	669774	1093269	2.52%	0.973%
14	12.506	1788	1794	1801	rVB	1667048	2634312	6.07%	2.344%
15	13.688	1988	1995	2001	rBV	262770	563713	1.30%	0.502%
16	13.876	2019	2027	2040	rBV	28334050	43368815	100.00%	38.584%
17	13.988	2041	2046	2053	rVB	585912	995752	2.30%	0.886%
18	14.141	2064	2072	2104	rVB	19086857	31074316	71.65%	27.646%

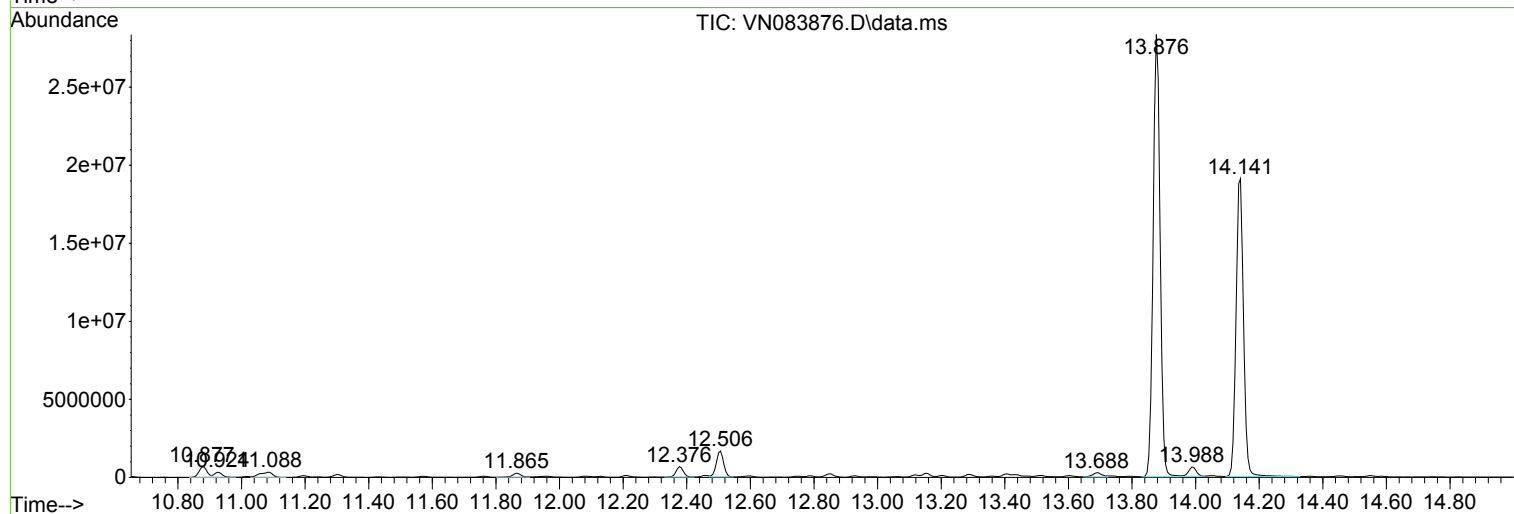
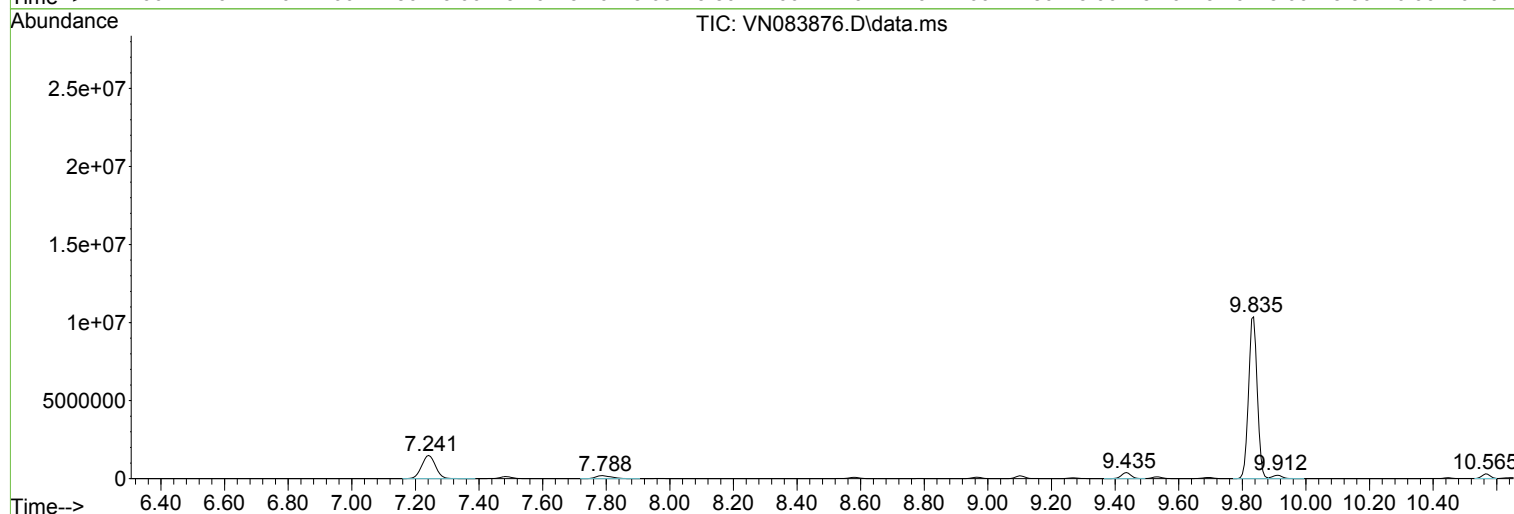
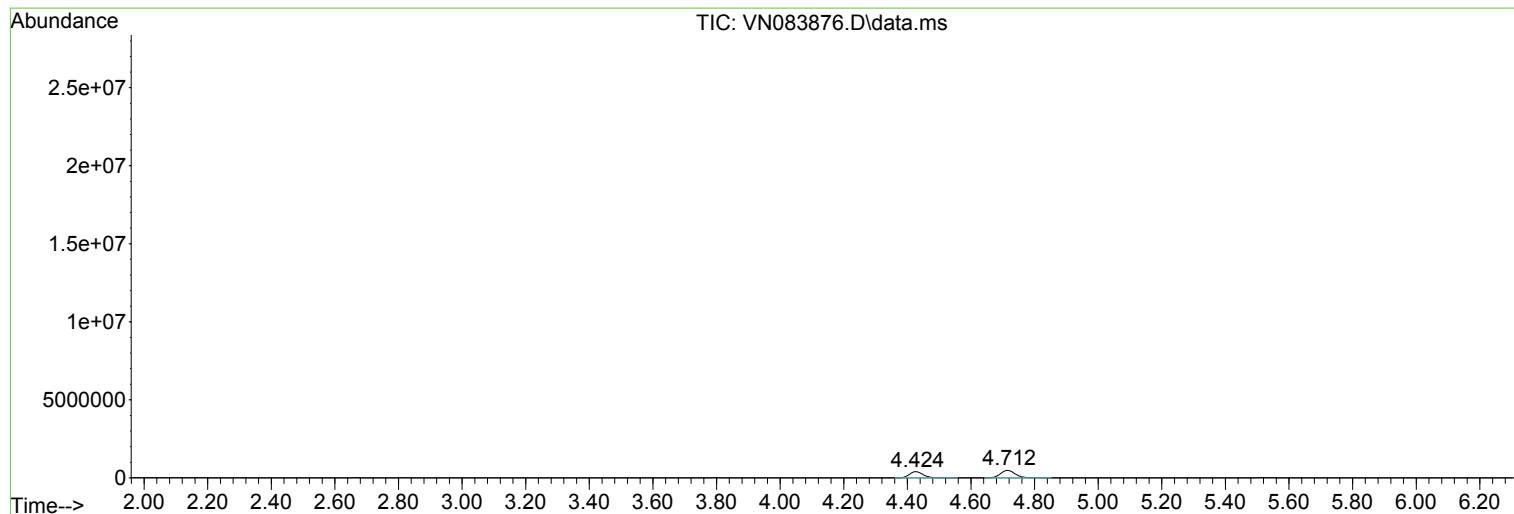
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\624N090624W.M
Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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



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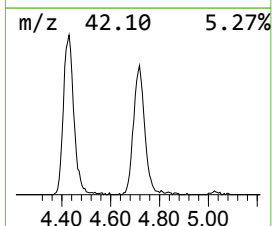
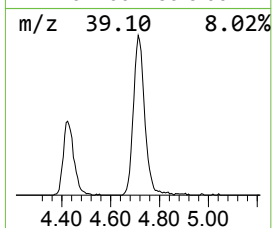
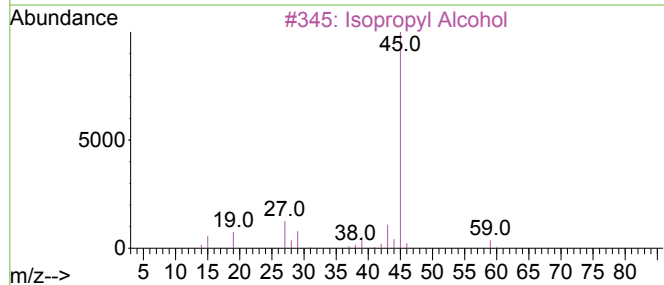
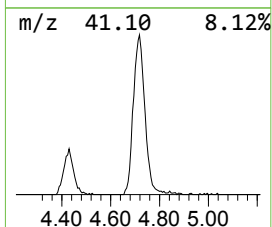
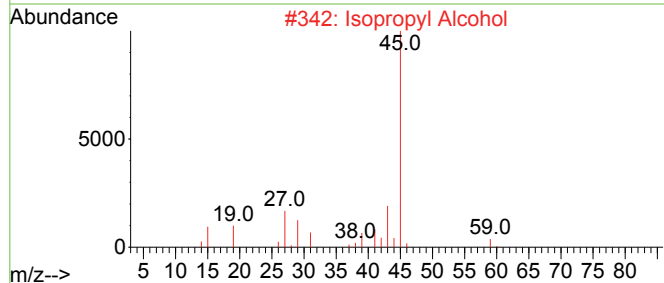
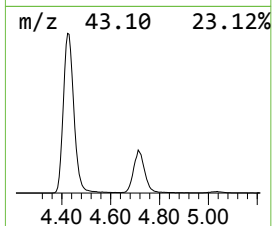
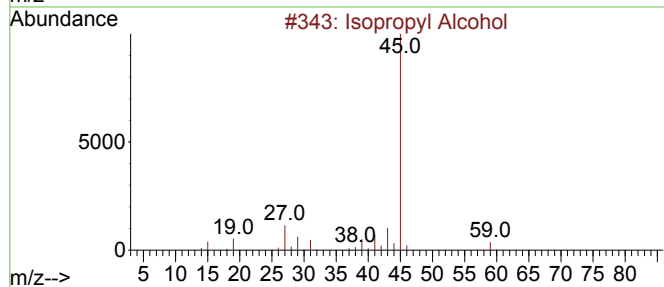
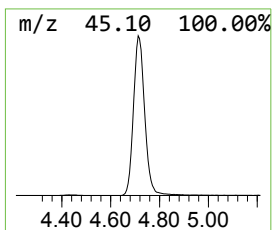
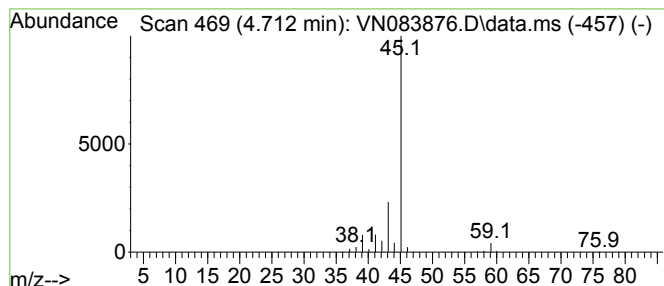
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.712	72.22 ug/l	1553590	Bromochloromethane	7.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43



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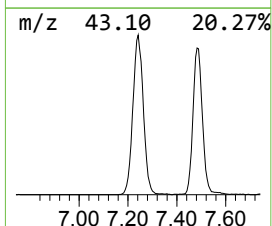
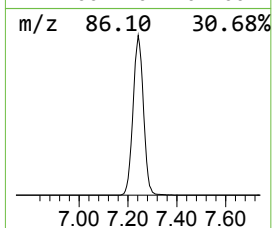
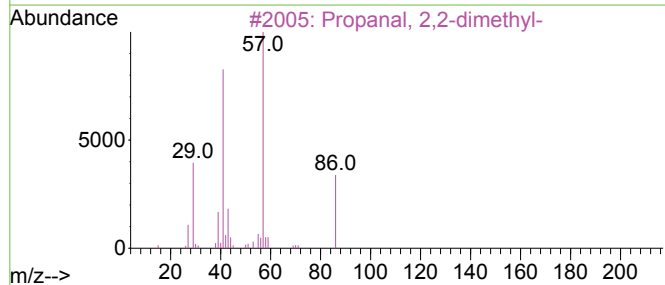
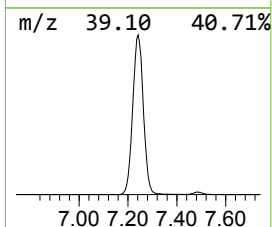
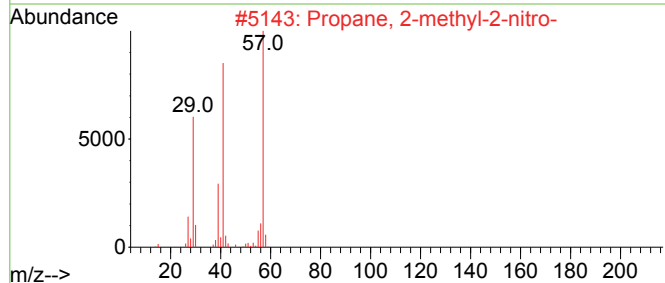
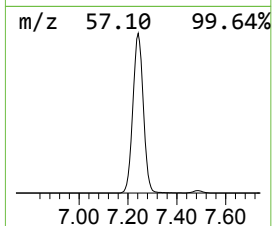
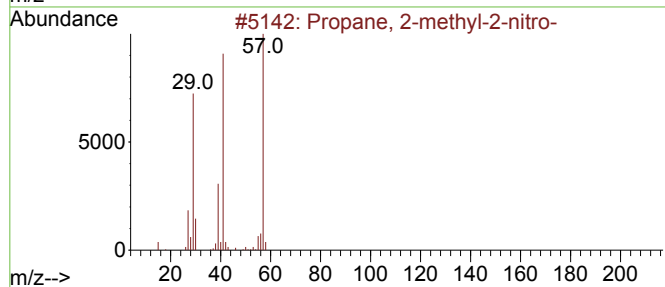
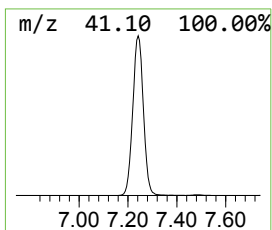
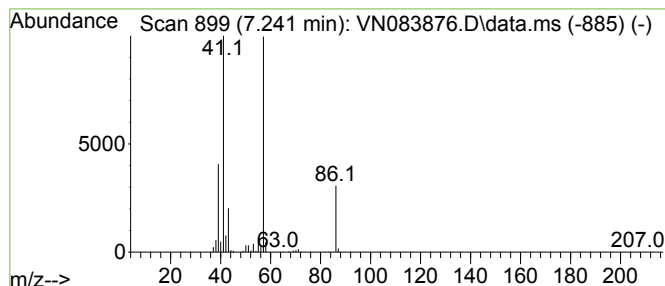
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 2 Propane, 2-methyl-2-nitro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.241	208.26 ug/l	4480280	Bromochloromethane	7.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
2			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38
3			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38
4			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	37
5			3-Pentanone	86	C5H10O	000096-22-0	32



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Instrument :
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ClientSampleId :
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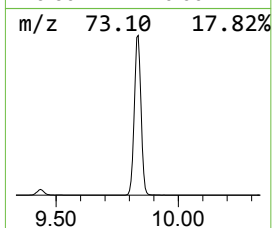
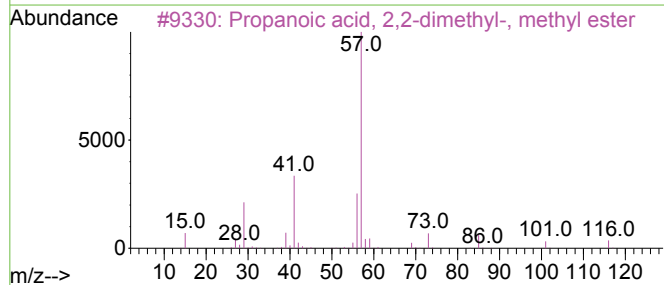
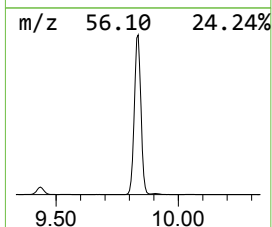
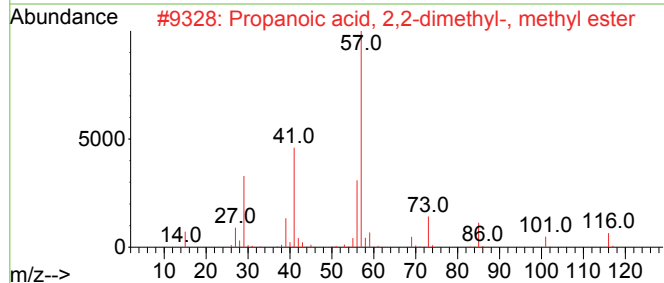
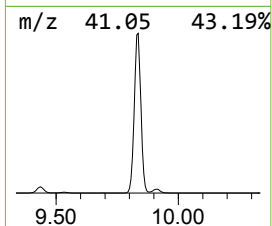
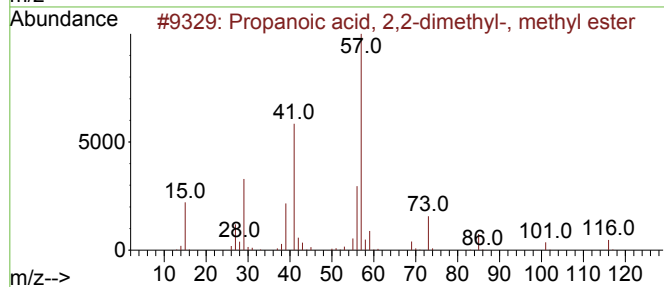
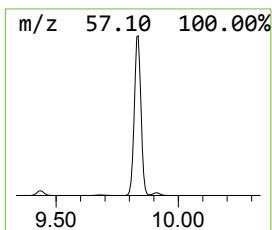
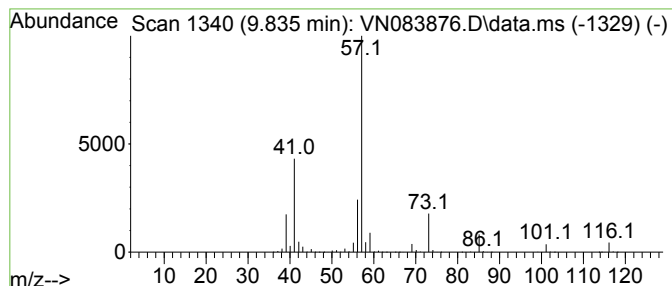
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 3 Propanoic acid, 2,2-dimethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.835	732.29 ug/l	19768800	1,4-Difluorobenzene	9.100

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	91
2			Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	91
3			Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	91
4			Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	86
5			3,3-Dimethyl-2-oxobutanoic acid	130	C6H10O3	000815-17-8	38



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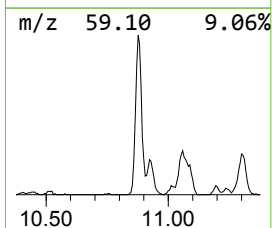
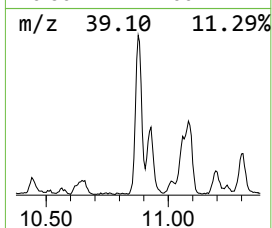
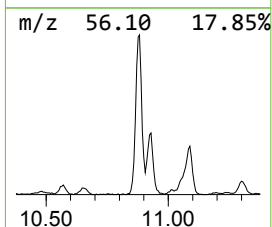
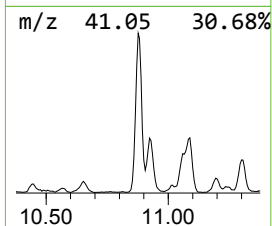
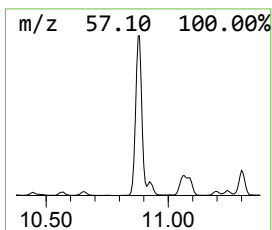
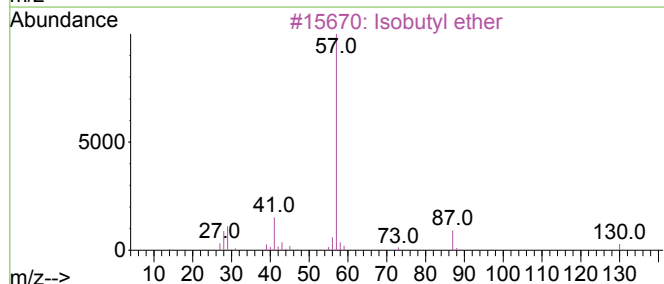
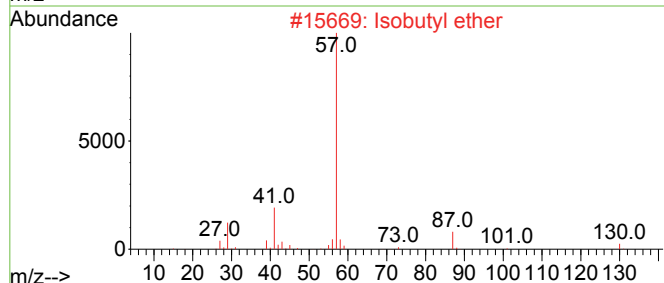
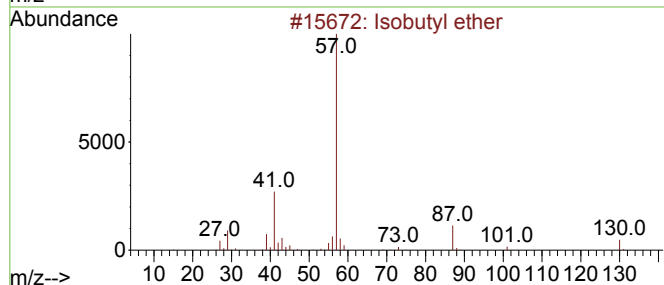
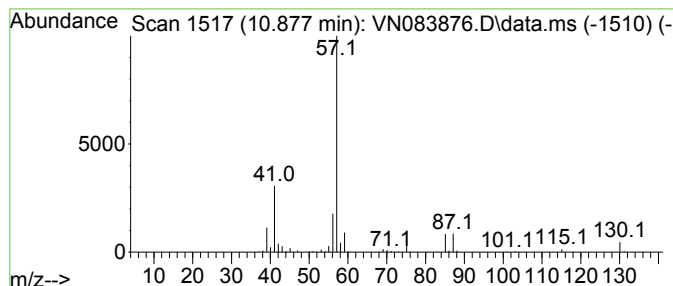
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 4 Isobutyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.877	70.41 ug/l	1219020	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl ether	130	C8H18O	000628-55-7	52
2			Isobutyl ether	130	C8H18O	000628-55-7	52
3			Isobutyl ether	130	C8H18O	000628-55-7	50
4			Isobutyl ether	130	C8H18O	000628-55-7	50
5			Propanoic acid, 2,2-dimethyl-, e...	130	C7H14O2	003938-95-2	50



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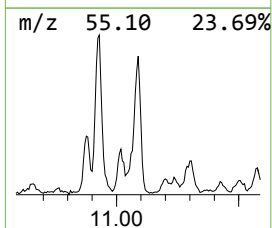
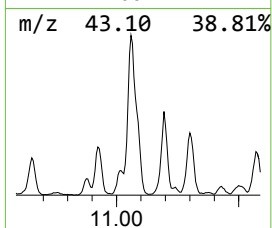
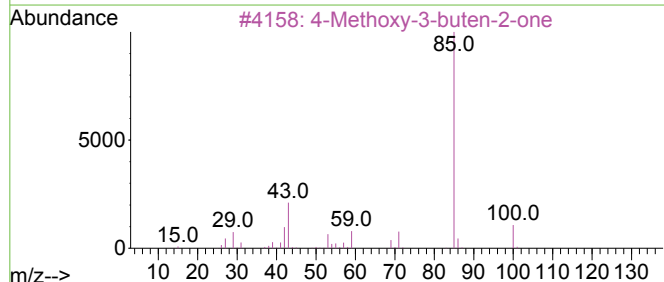
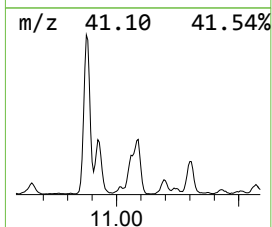
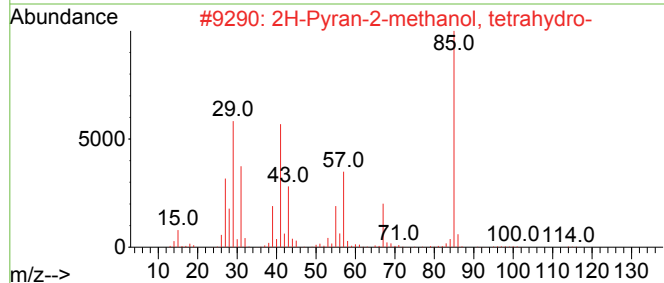
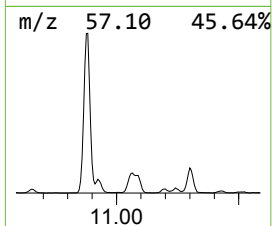
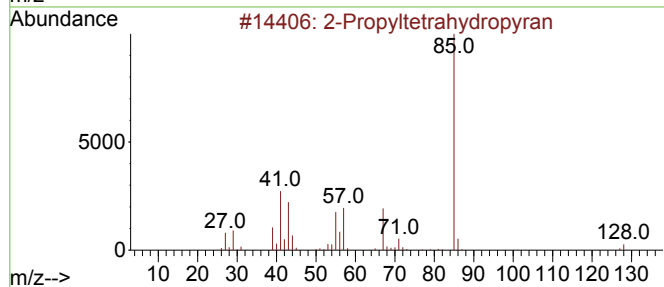
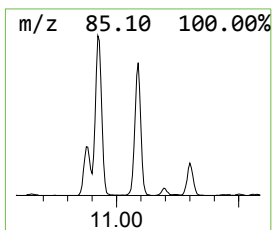
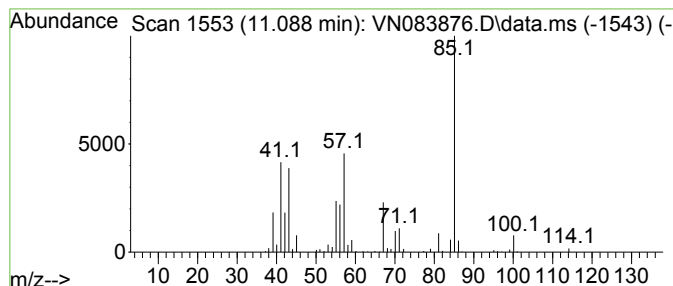
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Propyltetrahydropyran Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.088	54.98 ug/l	951857	Chlorobenzene-d5	11.865

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propyltetrahydropyran	128	C8H16O	003857-17-8	59
2		2H-Pyran-2-methanol, tetrahydro-	116	C6H12O2	000100-72-1	53
3		4-Methoxy-3-buten-2-one	100	C5H8O2	004652-27-1	50
4		trans-4-Methoxy-3-buten-2-one	100	C5H8O2	051731-17-0	47
5		2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	45



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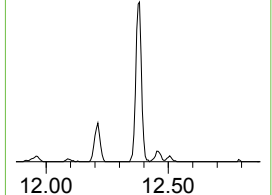
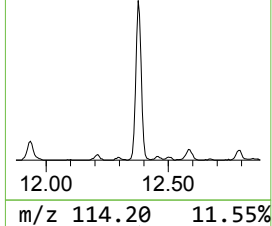
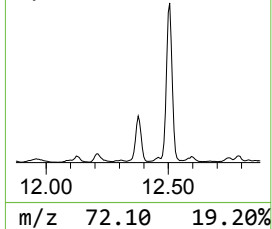
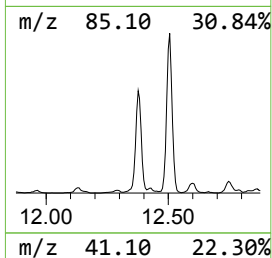
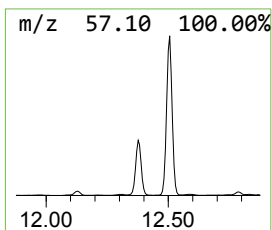
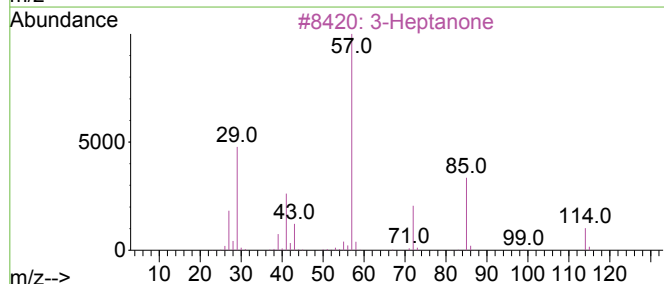
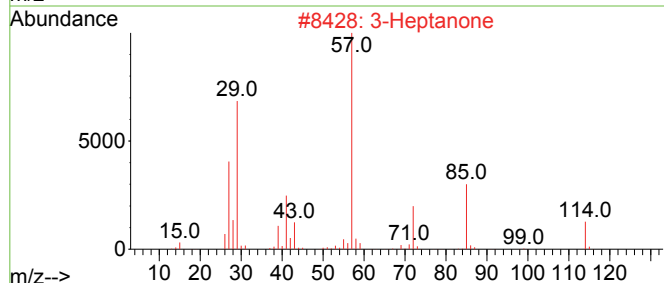
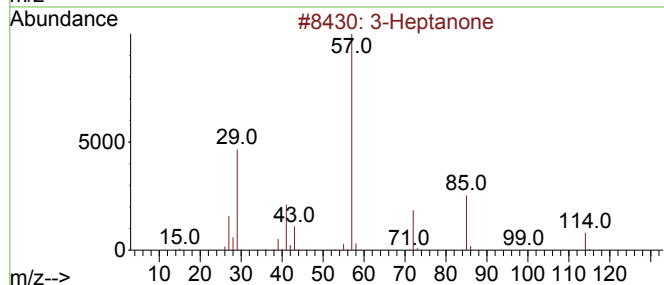
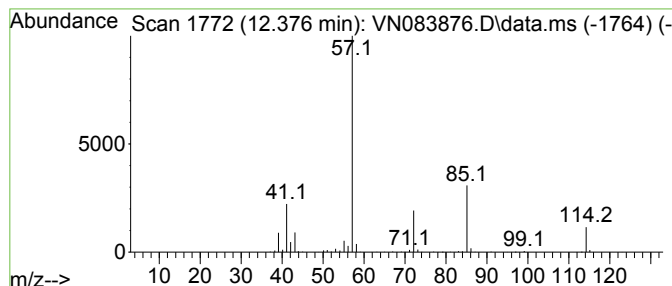
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 6 3-Heptanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.376	63.15 ug/l	1093270	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanone	114	C7H14O	000106-35-4	91
2			3-Heptanone	114	C7H14O	000106-35-4	91
3			3-Heptanone	114	C7H14O	000106-35-4	91
4			3-Heptanone	114	C7H14O	000106-35-4	80
5			4-Methyl-5-nonanone	156	C10H20O	035900-26-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091324\
Data File : VN083876.D
Acq On : 13 Sep 2024 17:43
Operator : JC\MD
Sample : P3956-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EFF-WW

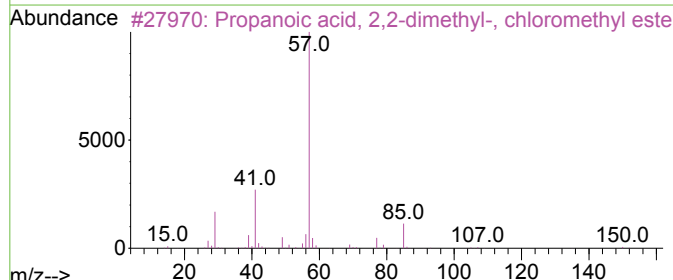
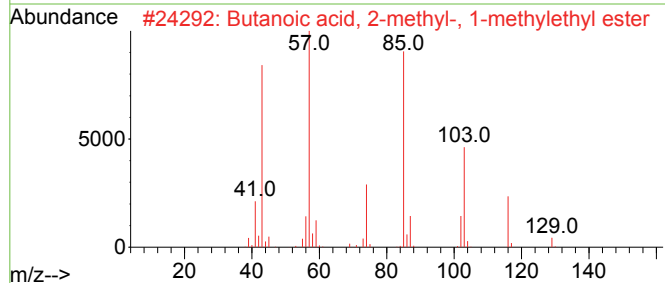
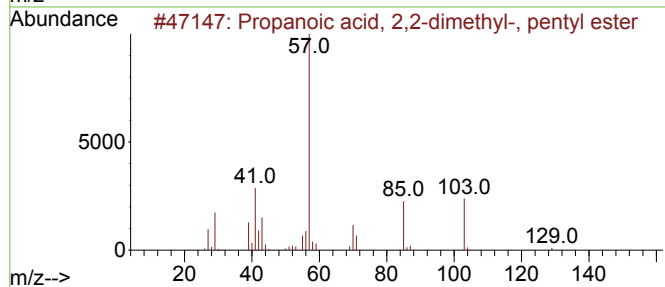
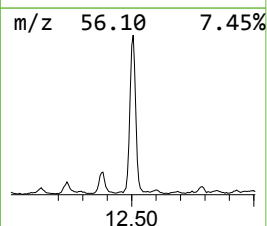
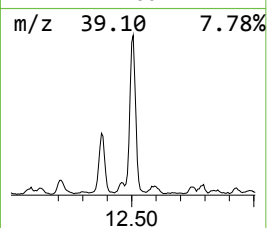
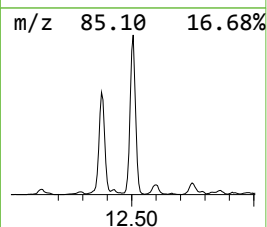
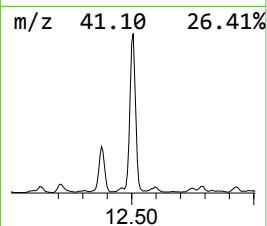
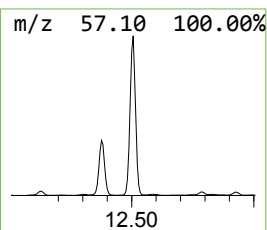
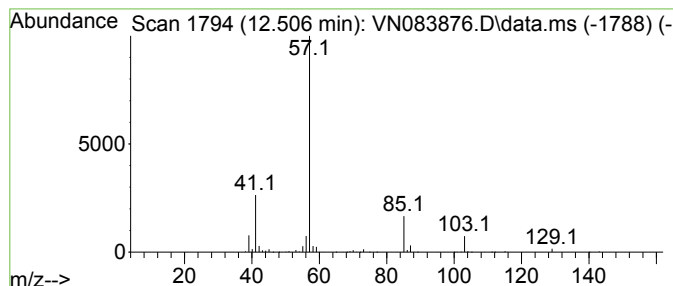
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 7 Propanoic acid, 2,2-dimethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.506	152.16 ug/l	2634310	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2-dimethyl-, p...	172	C10H20O2	002313-68-0	59
2			Butanoic acid, 2-methyl-, 1-meth...	144	C8H16O2	066576-71-4	42
3			Propanoic acid, 2,2-dimethyl-, c...	150	C6H11ClO2	018997-19-8	40
4			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	35
5			Cyclohexyl isovalerate	184	C11H20O2	007774-44-9	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091324\
Data File : VN083876.D
Acq On : 13 Sep 2024 17:43
Operator : JC\MD
Sample : P3956-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EFF-WW

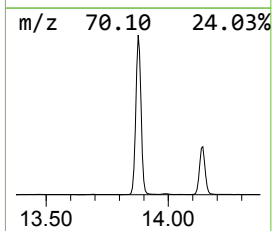
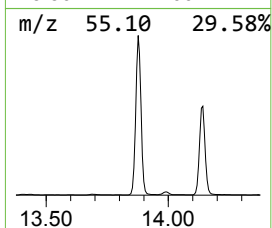
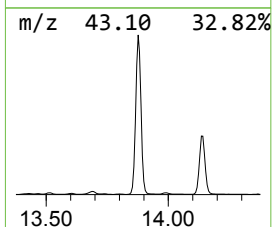
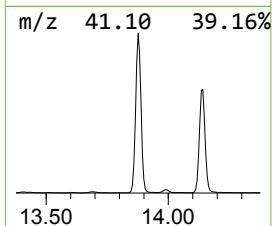
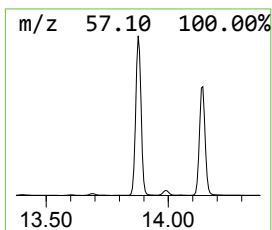
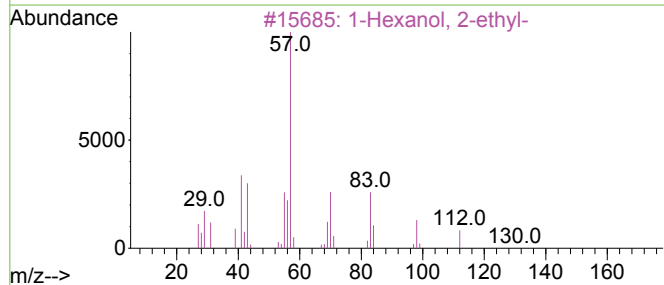
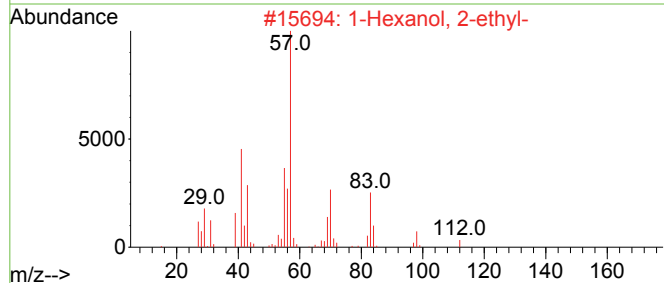
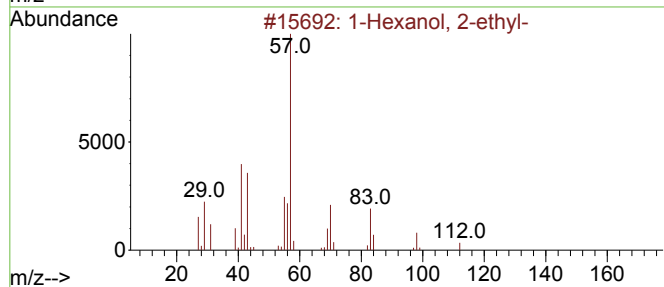
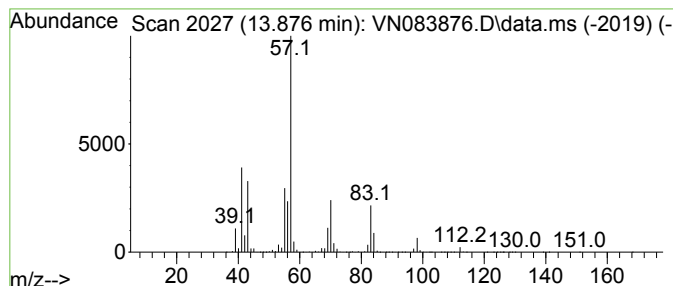
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	2504.99 ug/l	43368800	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	83	
2	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	78	
3	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	64	
4	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	64	
5	Pentadecafluorooctanoic acid, 2-...		526	C16H17F15O2	1000406-80-9	59	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091324\
Data File : VN083876.D
Acq On : 13 Sep 2024 17:43
Operator : JC\MD
Sample : P3956-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EFF-WW

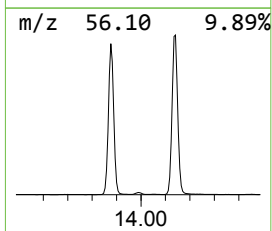
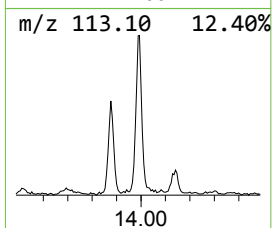
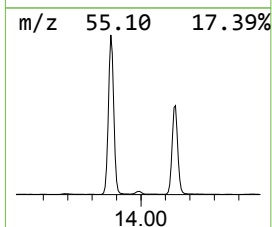
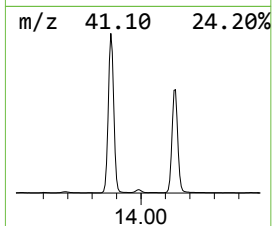
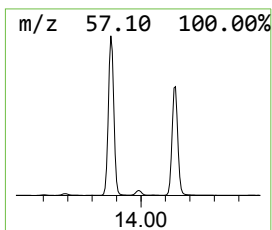
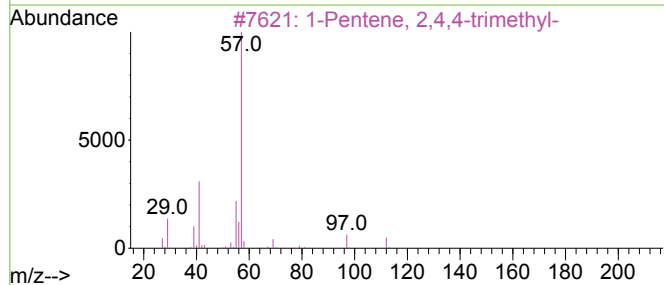
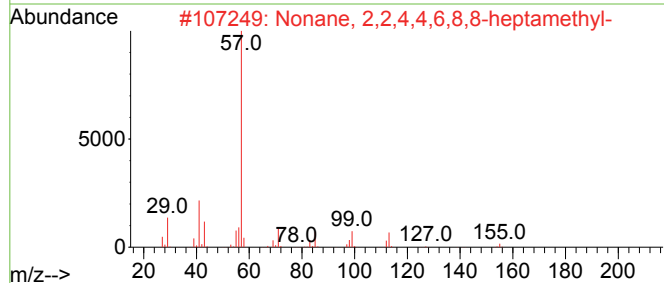
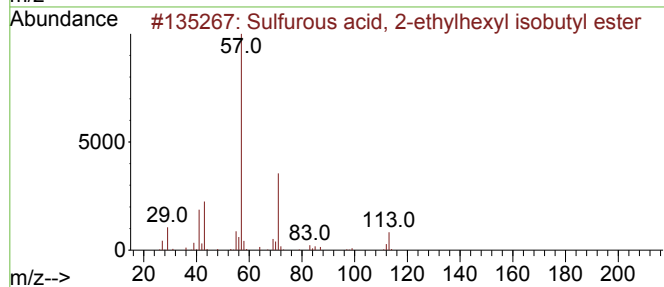
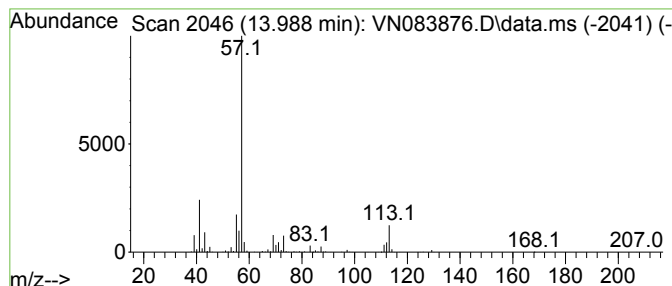
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Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 9 Sulfurous acid, 2-ethylhexy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.988	57.51 ug/l	995752	Chlorobenzene-d5	11.865

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl iso...	250	C12H26O3S	1000309-18-7	53
2			Nonane, 2,2,4,4,6,8,8-heptamethyl-	226	C16H34	004390-04-9	50
3			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	38
4			2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17FO2	1000365-51-0	38
5			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091324\
Data File : VN083876.D
Acq On : 13 Sep 2024 17:43
Operator : JC\MD
Sample : P3956-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EFF-WW

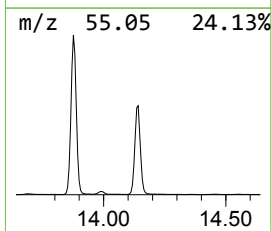
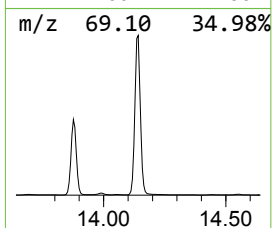
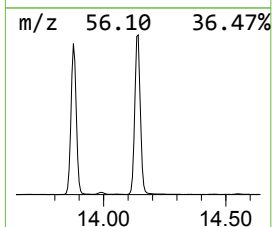
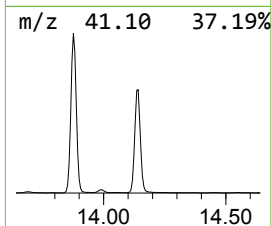
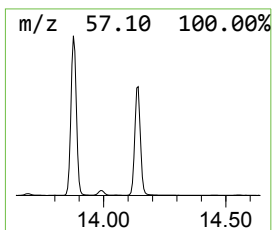
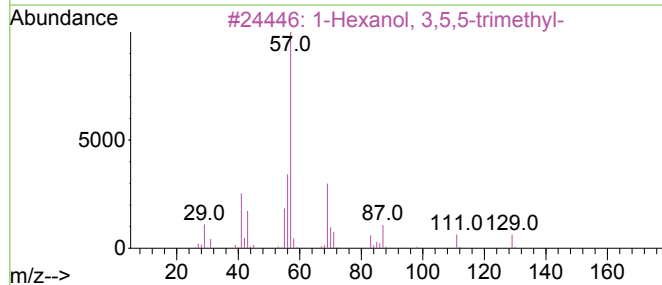
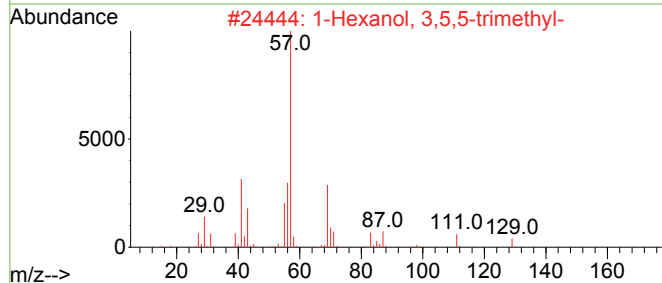
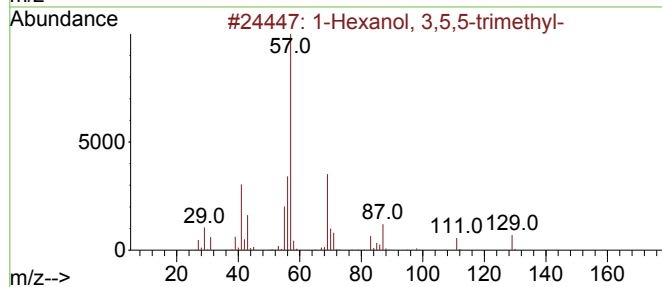
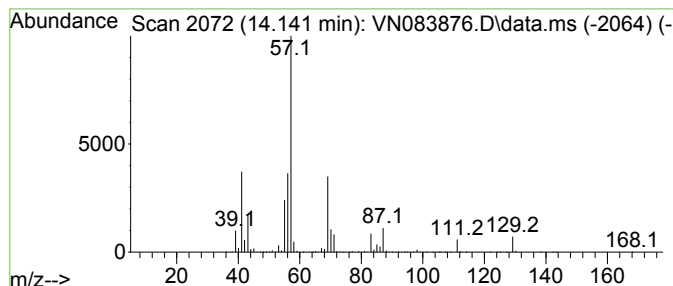
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\624N090624W.M
Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

Peak Number 10 1-Hexanol, 3,5,5-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.141	1794.86 ug/l	31074300	Chlorobenzene-d5	11.865

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 3,5,5-trimethyl-	144	C9H20O	003452-97-9	90
2		1-Hexanol, 3,5,5-trimethyl-	144	C9H20O	003452-97-9	90
3		1-Hexanol, 3,5,5-trimethyl-	144	C9H20O	003452-97-9	90
4		1-Hexanol, 3,5,5-trimethyl-	144	C9H20O	003452-97-9	86
5		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091324\
Data File : VN083876.D
Acq On : 13 Sep 2024 17:43
Operator : JC\MD
Sample : P3956-01 5X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
EFF-WW

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\624N090624W.M
Quant Title : METHOD 624 VOLATILE ORGANIC ANALYSIS

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	4.712	72.2	ug/l	1553590	1	7.812	645380	30.0
Propane, 2-meth...	7.241	208.3	ug/l	4480280	1	7.812	645380	30.0
Propanoic acid,...	9.835	732.3	ug/l	19768800	2	9.100	809877	30.0
Isobutyl ether	10.877	70.4	ug/l	1219020	3	11.865	519389	30.0
2-Propyltetrahy...	11.088	55.0	ug/l	951857	3	11.865	519389	30.0
3-Heptanone	12.376	63.1	ug/l	1093270	3	11.865	519389	30.0
Propanoic acid,...	12.506	152.2	ug/l	2634310	3	11.865	519389	30.0
1-Hexanol, 2-et...	13.876	2505.0	ug/l	43368800	3	11.865	519389	30.0
Sulfurous acid,...	13.988	57.5	ug/l	995752	3	11.865	519389	30.0
1-Hexanol, 3,5,...	14.141	1794.9	ug/l	31074300	3	11.865	519389	30.0