

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
 Data File : VN073749.D
 Acq On : 04 Aug 2022 20:26
 Operator : JC\MD
 Sample : N4056-01 100X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOTE

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\82N072822W.M
 Title : SW846 8260

Signal : TIC: VN073749.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.546	105	112	131	rBV	6263853	10777928	100.00%	34.433%
2	3.634	286	297	323	rBV	923933	2405853	22.32%	7.686%
3	4.081	363	373	385	rBV	104447	285862	2.65%	0.913%
4	4.222	388	397	413	rBV	317400	901677	8.37%	2.881%
5	4.510	435	446	462	rBV	158172	492596	4.57%	1.574%
6	6.986	857	867	890	rBV	186637	553379	5.13%	1.768%
7	7.951	1019	1031	1036	rBV	337567	804515	7.46%	2.570%
8	8.016	1036	1042	1062	rVB	608014	1412303	13.10%	4.512%
9	8.369	1092	1102	1116	rBV	321563	754423	7.00%	2.410%
10	8.904	1184	1193	1213	rVB	834773	1720405	15.96%	5.496%
11	9.092	1216	1225	1237	rBV2	49706	113561	1.05%	0.363%
12	9.469	1281	1289	1299	rBV	106178	215825	2.00%	0.690%
13	10.380	1432	1444	1451	rBV	1176161	2148358	19.93%	6.863%
14	11.686	1655	1666	1677	rBV	1161907	2032019	18.85%	6.492%
15	12.674	1823	1834	1842	rBV	999471	1679185	15.58%	5.365%
16	12.951	1872	1881	1887	rBV	99433	178453	1.66%	0.570%
17	13.421	1952	1961	1971	rBV3	205440	444564	4.12%	1.420%
18	13.557	1971	1984	1988	rVV	572781	1260352	11.69%	4.026%
19	13.615	1988	1994	2000	rVV	1298930	2139291	19.85%	6.834%
20	13.680	2000	2005	2016	rVB3	275576	589250	5.47%	1.882%
21	14.080	2065	2073	2082	rBV	153391	272030	2.52%	0.869%
22	15.433	2295	2303	2314	rVB	49827	119696	1.11%	0.382%

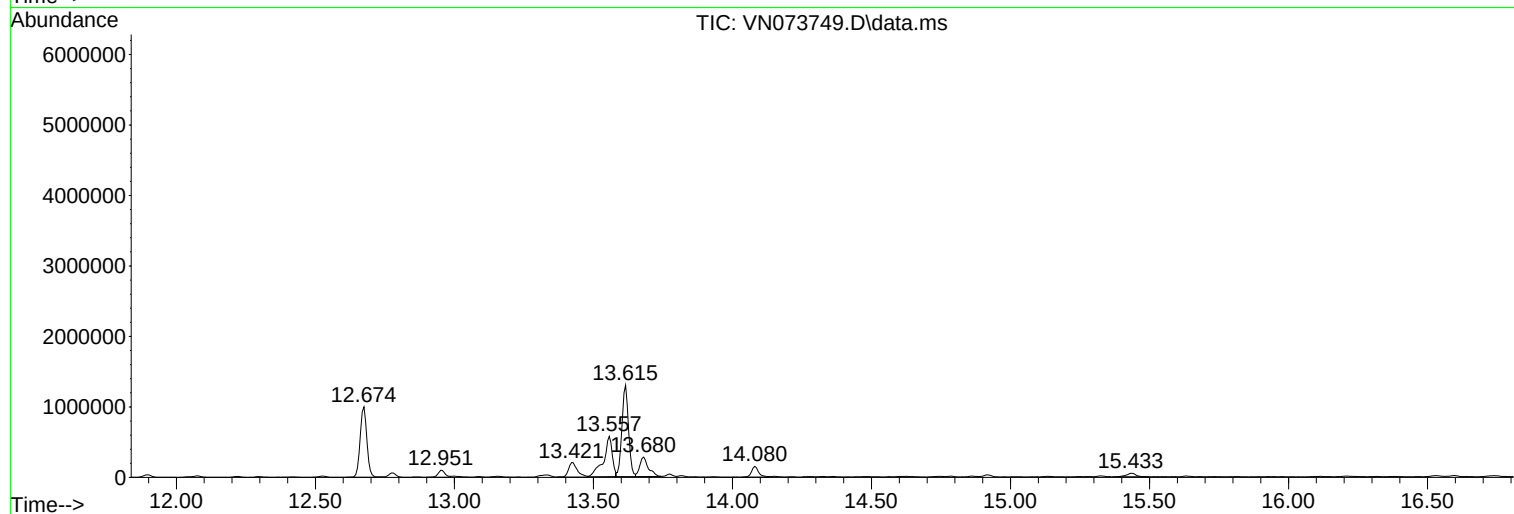
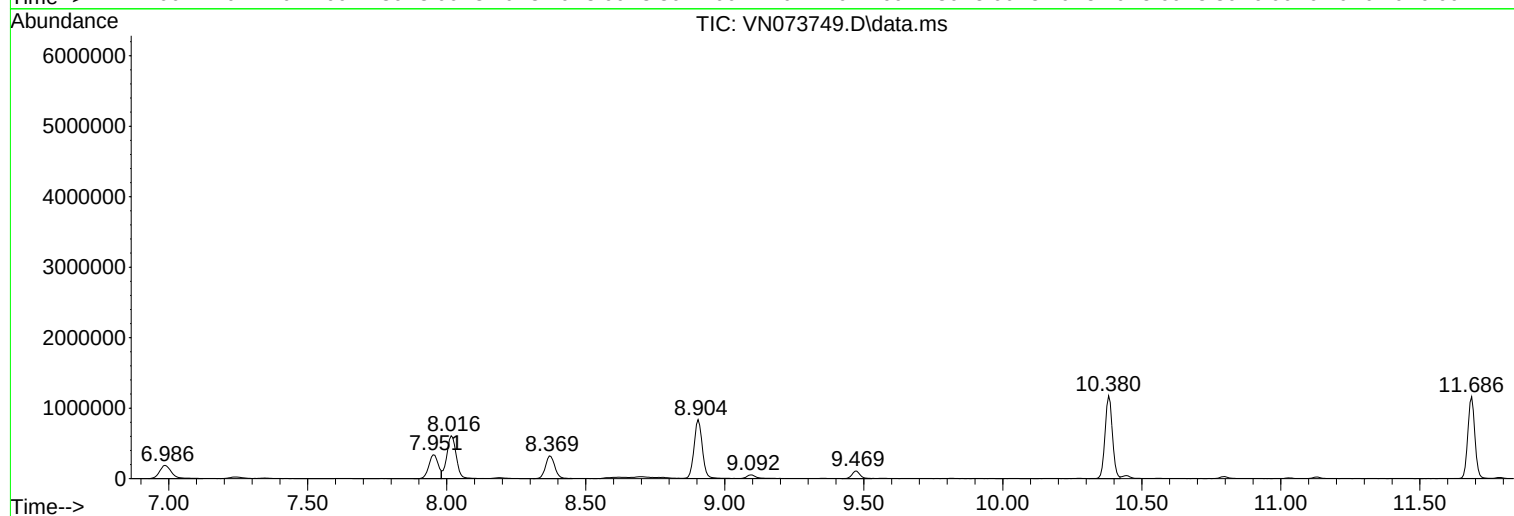
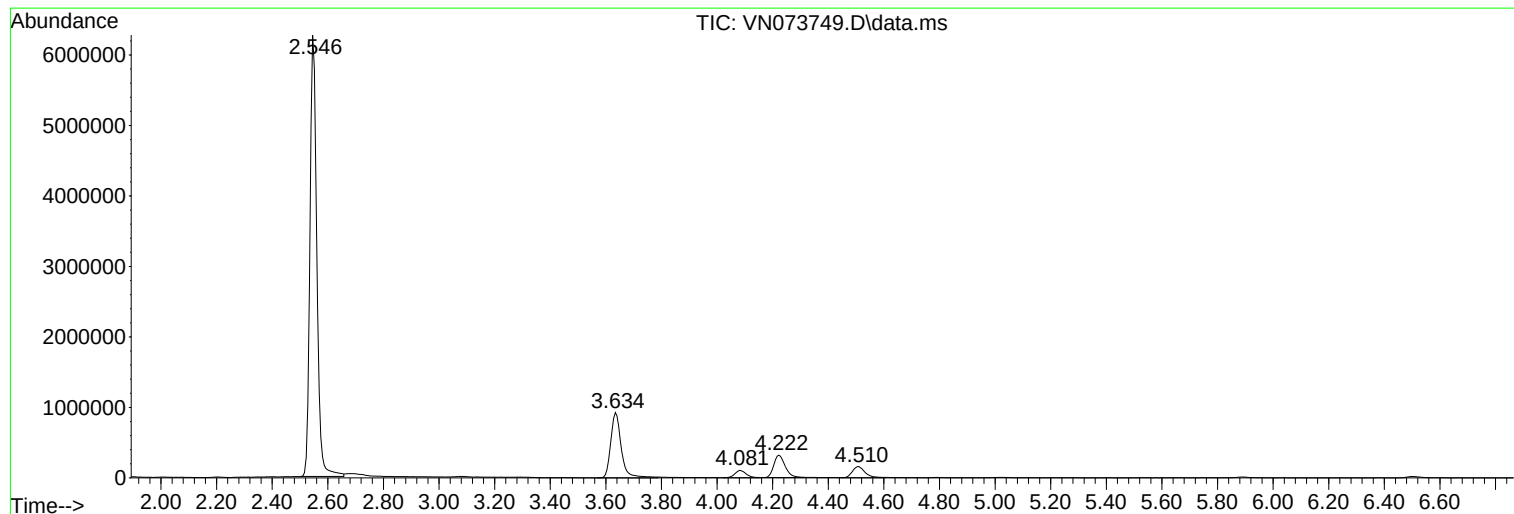
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



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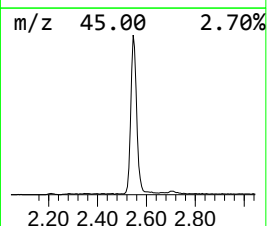
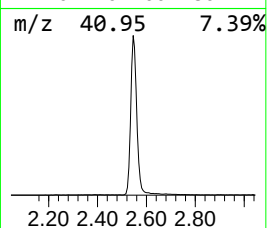
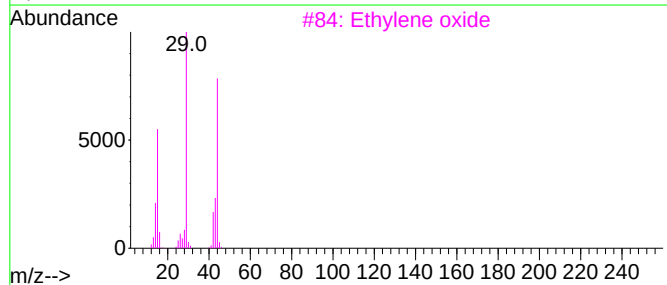
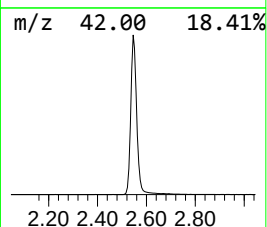
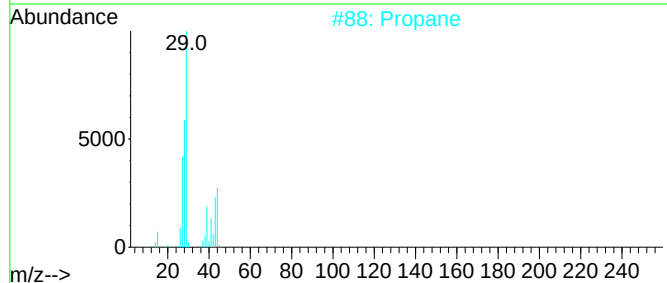
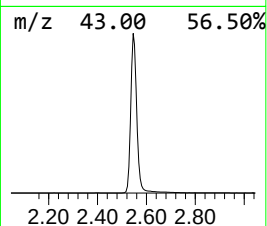
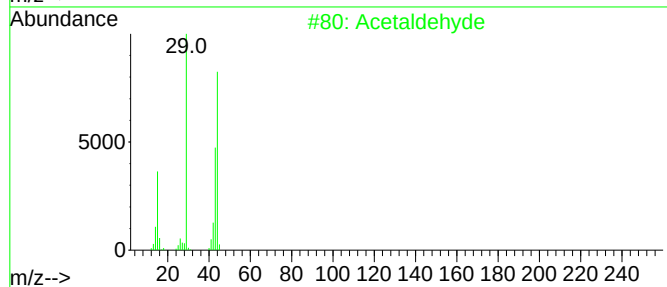
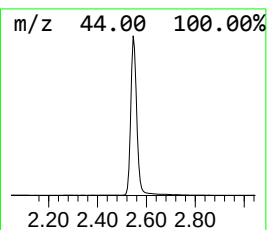
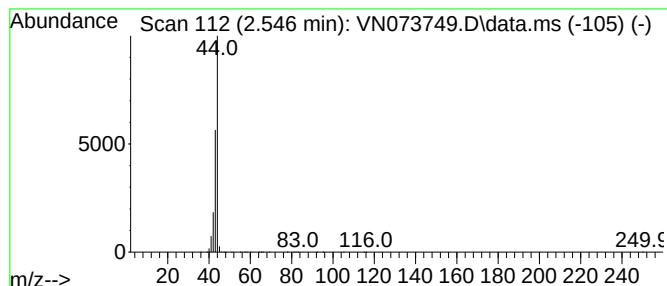
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.546	381.57 ug/l	10777900	Pentafluorobenzene	8.016

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetaldehyde	44	C2H4O	000075-07-0	64
2		Propane	44	C3H8	000074-98-6	5
3		Ethylene oxide	44	C2H4O	000075-21-8	5
4		Alanine	89	C3H7NO2	000056-41-7	4
5		1,2-Propanediamine	74	C3H10N2	000078-90-0	4



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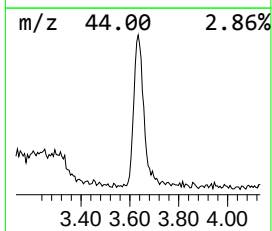
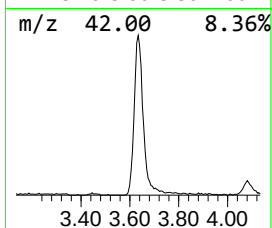
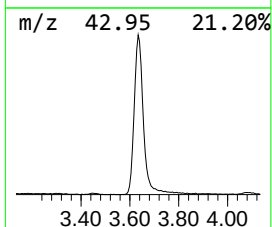
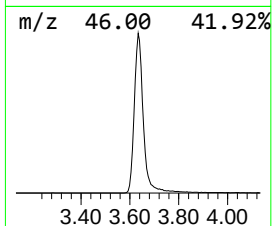
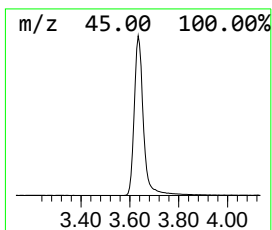
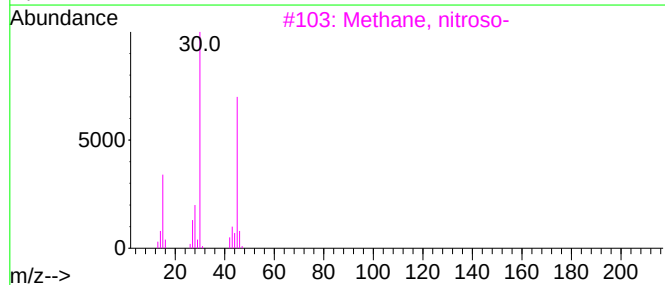
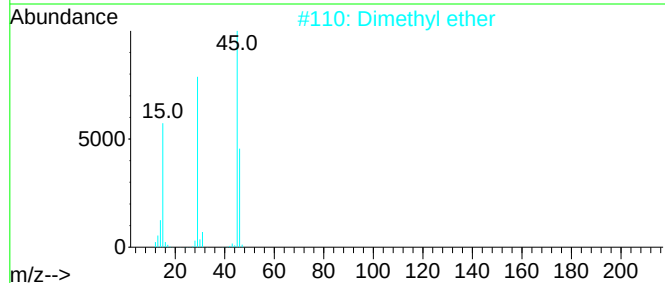
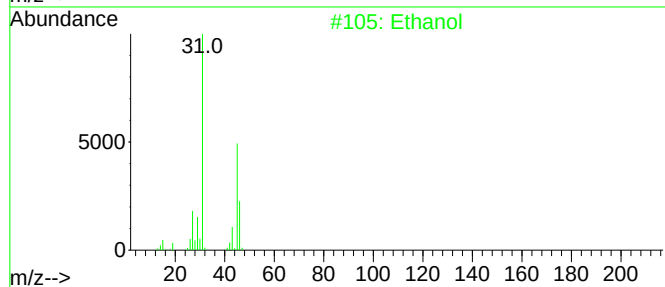
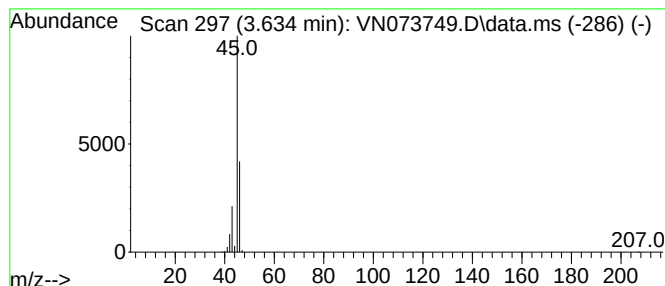
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.634	85.17 ug/l	2405850	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	83
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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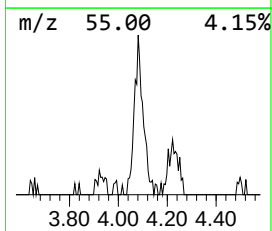
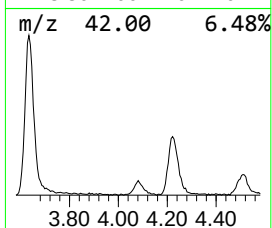
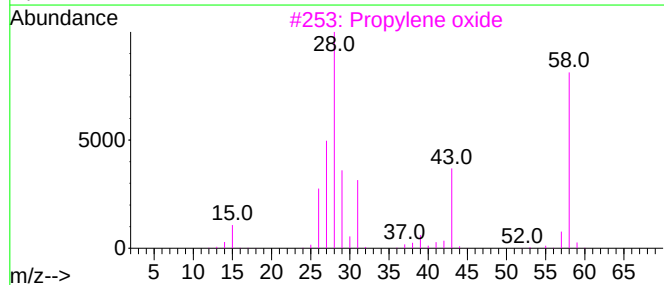
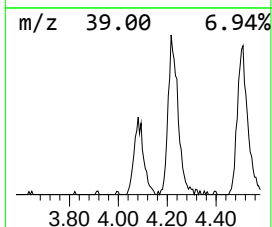
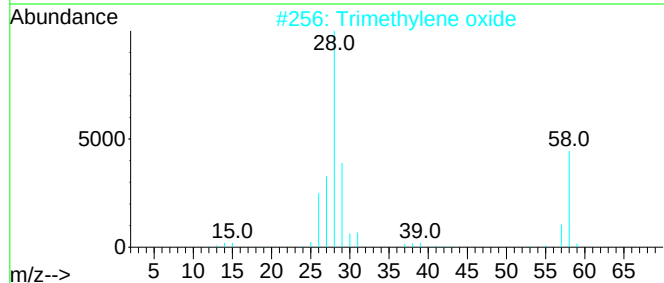
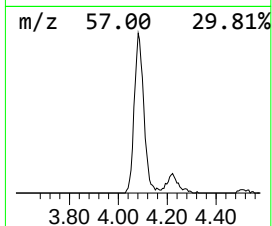
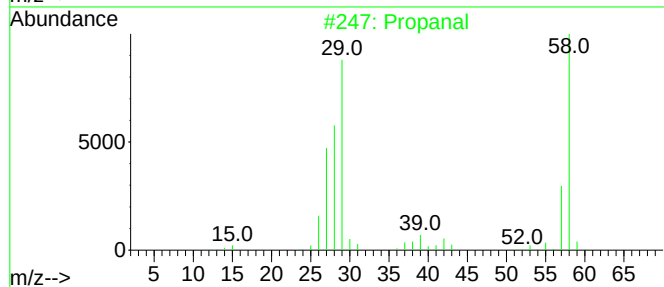
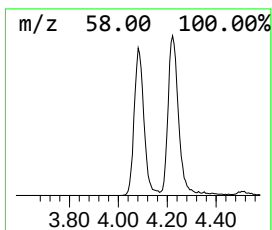
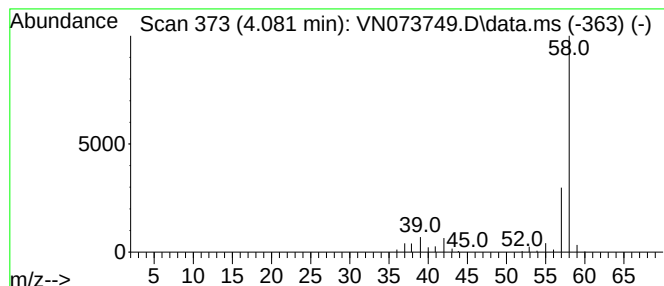
Instrument :
MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Propanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.081	10.12 ug/l	285862	Pentafluorobenzene	8.016	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	72
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	Propylene oxide	58	C3H6O	000075-56-9	7
4	Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	7
5	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	5



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ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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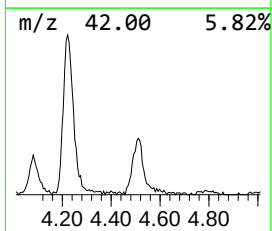
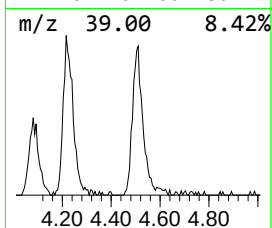
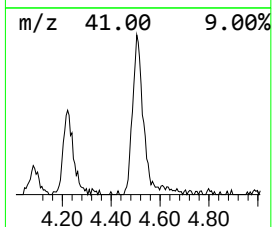
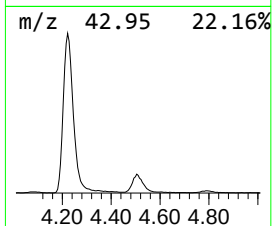
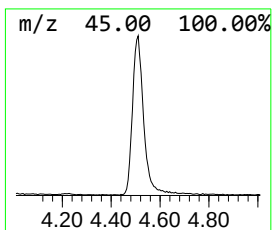
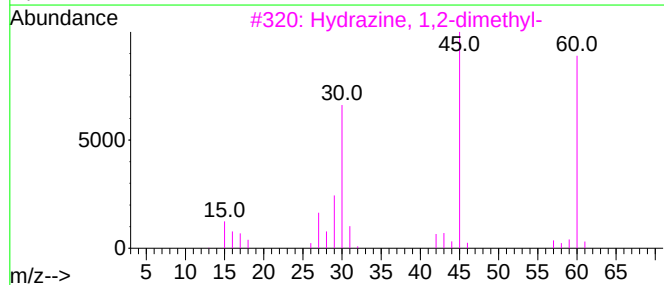
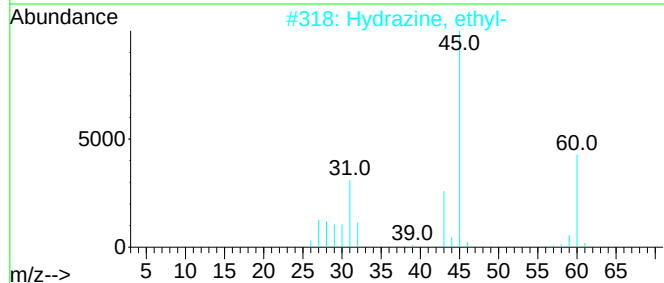
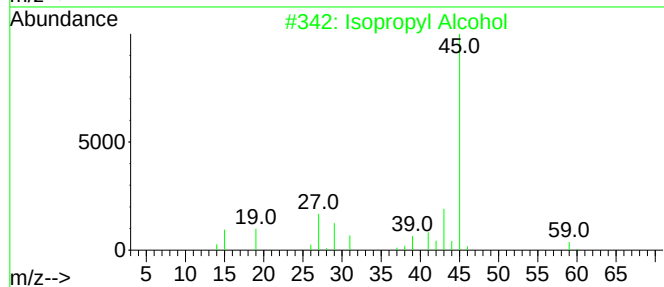
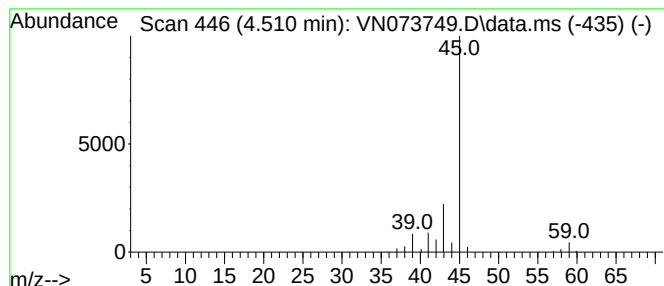
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	17.44 ug/l	492596	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4			Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4
5			4-Penten-2-ol	86	C5H10O	000625-31-0	4



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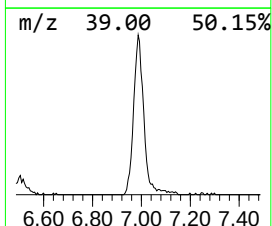
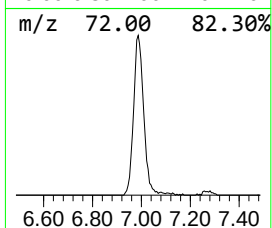
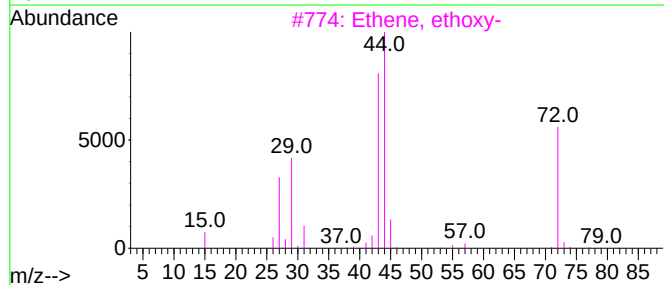
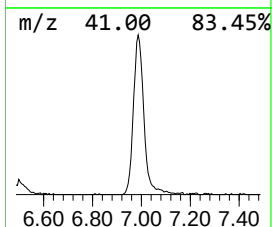
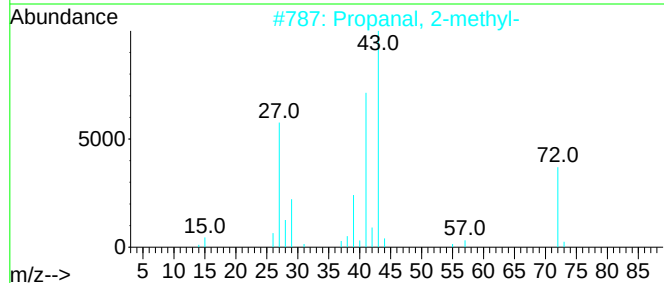
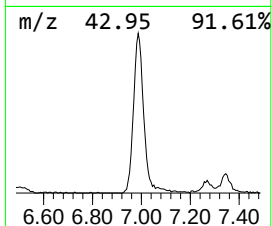
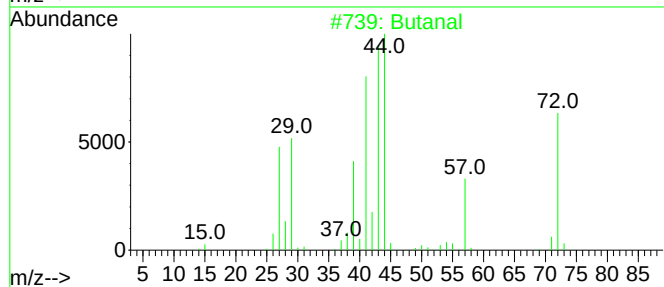
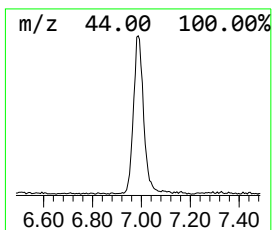
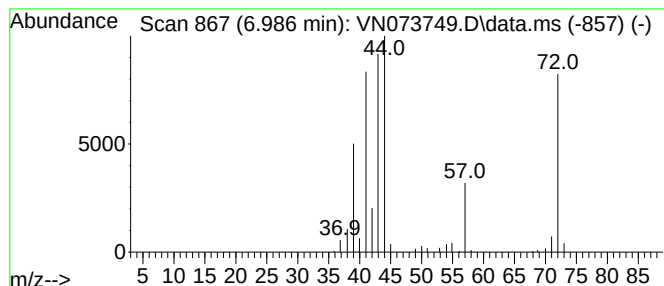
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Quant Title : SW846 8260

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

Peak Number 5 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.986	19.59 ug/l	553379	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	40
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37



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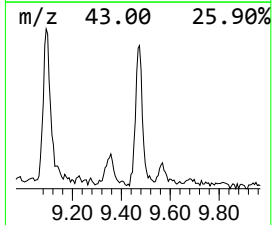
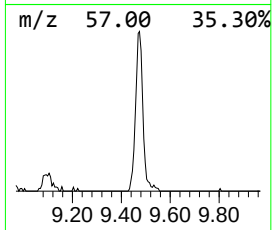
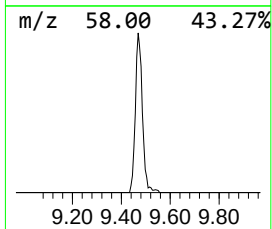
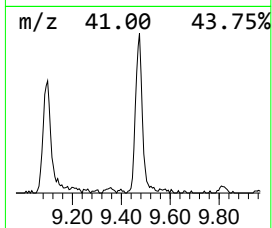
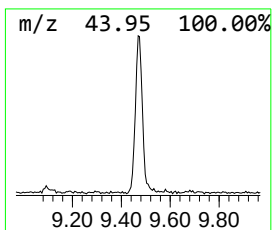
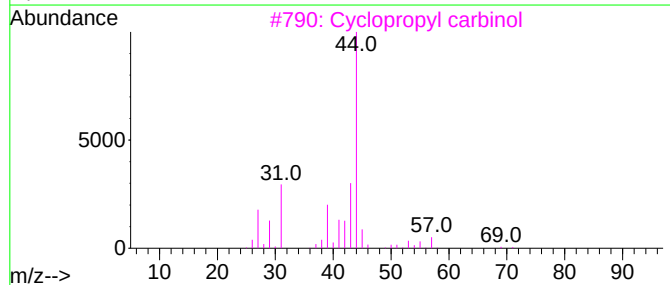
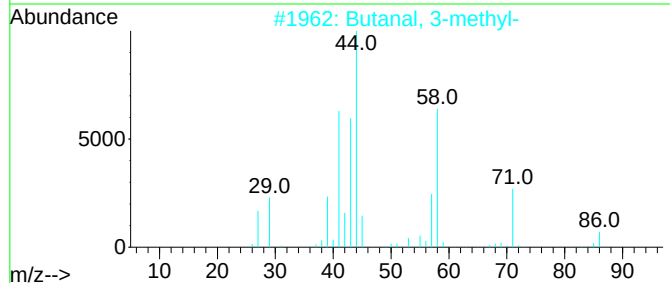
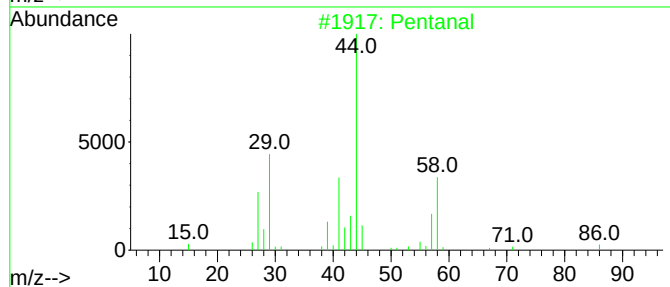
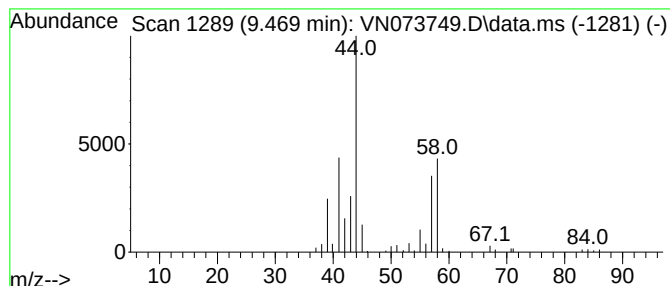
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Quant Title : SW846 8260

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

Peak Number 6 Pentanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.469	6.27 ug/l	215825	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	90
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	74
3			Cyclopropyl carbinol	72	C4H8O	002516-33-8	50
4			2-Formylhistamine	139	C6H9N3O	1000132-95-8	28
5			Ethylene oxide	44	C2H4O	000075-21-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073749.D
Acq On : 04 Aug 2022 20:26
Operator : JC\MD
Sample : N4056-01 100X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

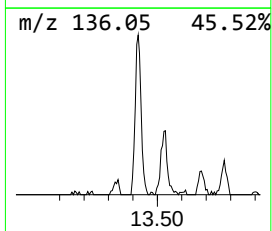
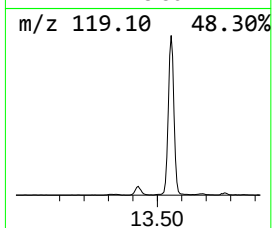
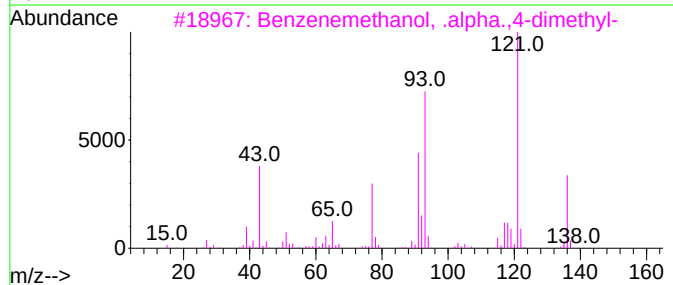
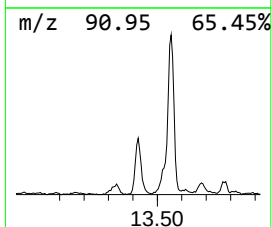
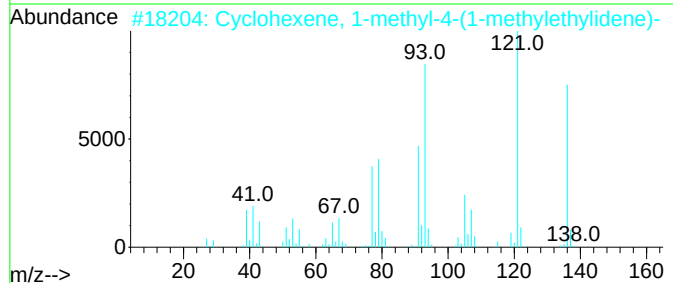
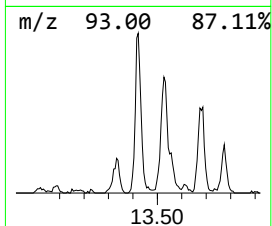
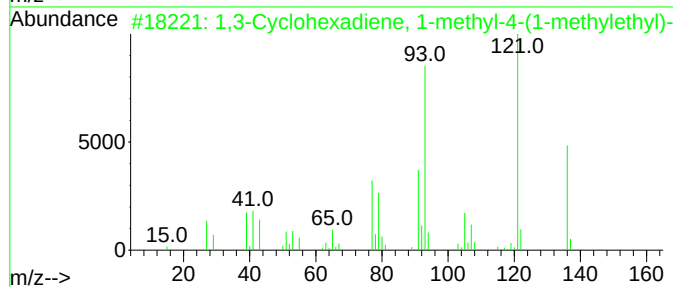
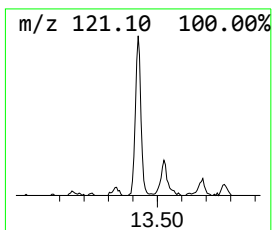
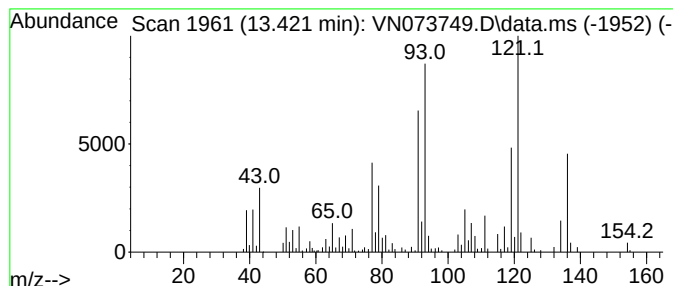
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ClientSampleId :
TOTE

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Quant Title : SW846 8260

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

Peak Number 7 1,3-Cyclohexadiene, 1-methy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.421	10.39 ug/l	444564	1,4-Dichlorobenzene-d4	13.615	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	96
2	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	95
3	Benzenemethanol, .alpha.,4-dimet...	136	C9H12O	000536-50-5	81
4	Bicyclo[4.1.0]hept-2-ene, 3,7,7-...	136	C10H16	004497-92-1	76
5	(+)-4-Carene	136	C10H16	029050-33-7	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073749.D
Acq On : 04 Aug 2022 20:26
Operator : JC\MD
Sample : N4056-01 100X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOTE

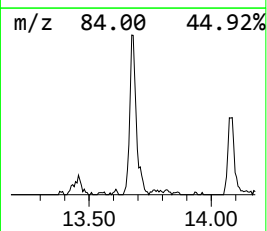
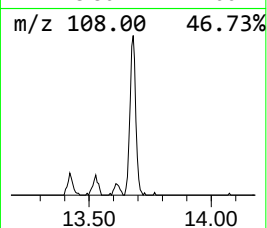
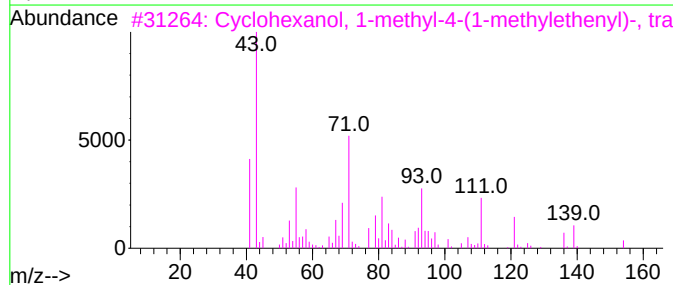
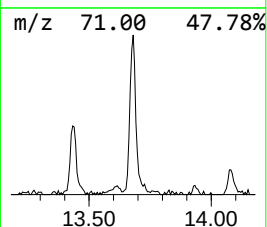
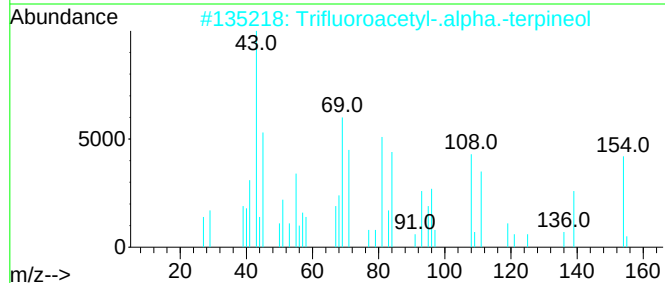
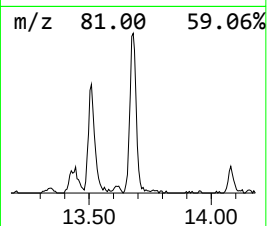
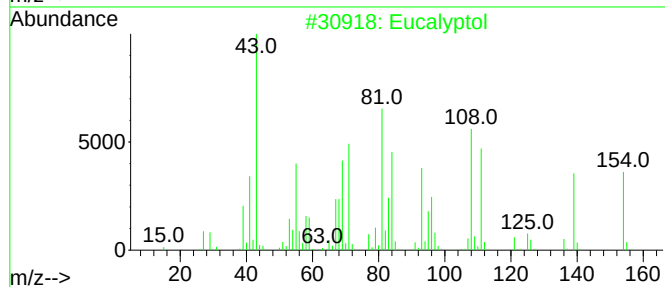
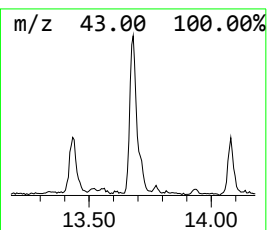
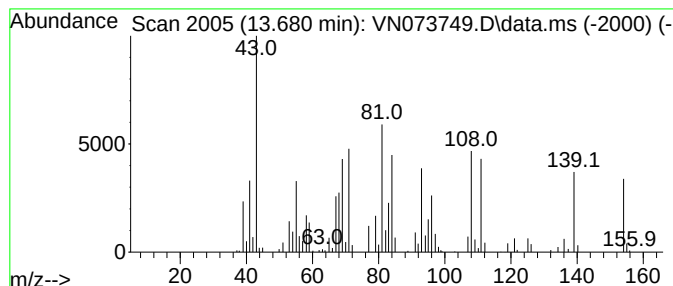
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Quant Title : SW846 8260

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

Peak Number 8 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.680	13.77 ug/l	589250	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	74
3			Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-40-3	37
4			Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-41-4	37
5			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073749.D
Acq On : 04 Aug 2022 20:26
Operator : JC\MD
Sample : N4056-01 100X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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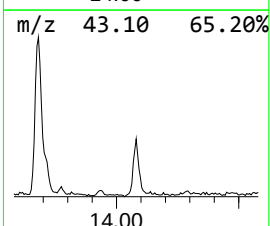
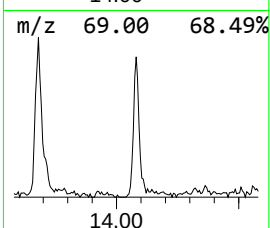
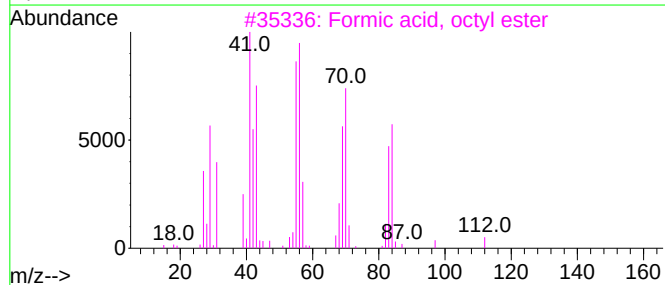
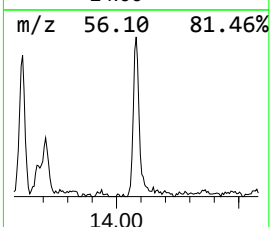
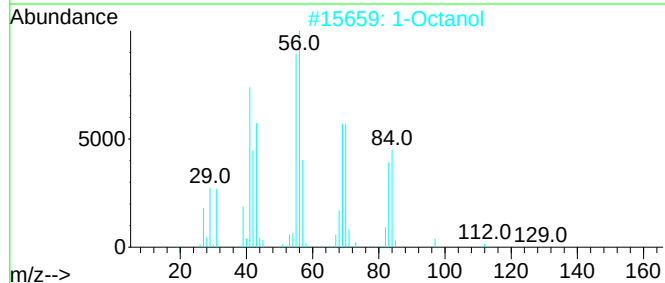
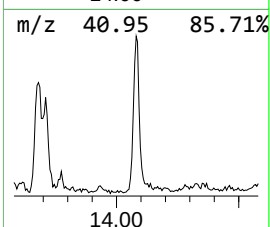
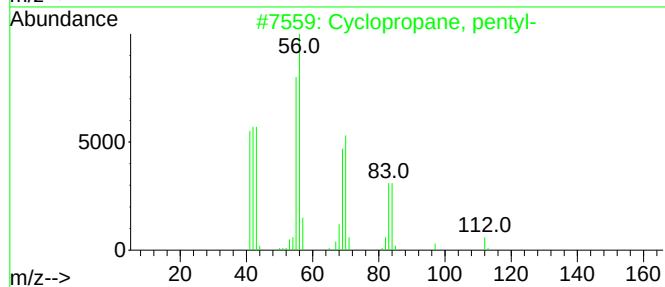
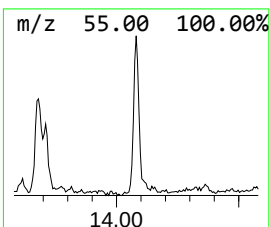
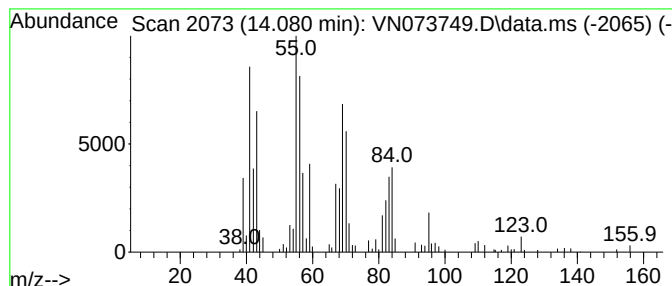
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Quant Title : SW846 8260

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

Peak Number 9 Cyclopropane, pentyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.080	6.36 ug/l	272030	1,4-Dichlorobenzene-d4	13.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, pentyl-	112	C8H16	002511-91-3	58
2			1-Octanol	130	C8H18O	000111-87-5	58
3			Formic acid, octyl ester	158	C9H18O2	000112-32-3	53
4			1-Hexene	84	C6H12	000592-41-6	38
5			1-Octene	112	C8H16	000111-66-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080422\
Data File : VN073749.D
Acq On : 04 Aug 2022 20:26
Operator : JC\MD
Sample : N4056-01 100X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOTE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.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
Acetaldehyde	2.546	381.6	ug/l	10777900	1	8.016	1412300	50.0
Ethanol	3.634	85.2	ug/l	2405850	1	8.016	1412300	50.0
Propanal	4.081	10.1	ug/l	285862	1	8.016	1412300	50.0
Isopropyl Alcohol	4.510	17.4	ug/l	492596	1	8.016	1412300	50.0
Butanal	6.986	19.6	ug/l	553379	1	8.016	1412300	50.0
Pentanal	9.469	6.3	ug/l	215825	2	8.904	1720410	50.0
1,3-Cyclohexadi...	13.421	10.4	ug/l	444564	4	13.615	2139290	50.0
Eucalyptol	13.680	13.8	ug/l	589250	4	13.615	2139290	50.0
Cyclopropane, p...	14.080	6.4	ug/l	272030	4	13.615	2139290	50.0