

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN110724\
 Data File : VN084733.D
 Acq On : 07 Nov 2024 19:58
 Operator : JC\MD
 Sample : P4759-01 20X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MONTCLAIR-TOTE-1

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\82N103024W.M
 Title : SW846 8260

Signal : TIC: VN084733.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.654	111	119	141	rBV	1733356	3190069	10.83%	6.729%
2	8.165	1046	1056	1060	rBV	139832	332443	1.13%	0.701%
3	8.224	1060	1066	1078	rVB	246639	558997	1.90%	1.179%
4	8.577	1114	1126	1136	rBV	151586	337010	1.14%	0.711%
5	9.100	1206	1215	1235	rBV2	2876017	5890370	20.00%	12.426%
6	9.341	1249	1256	1271	rVB	444486	891164	3.03%	1.880%
7	10.565	1456	1464	1472	rBV	523762	962619	3.27%	2.031%
8	11.865	1677	1685	1692	rBV	498079	880235	2.99%	1.857%
9	12.676	1814	1823	1830	rBV	518118	969290	3.29%	2.045%
10	12.753	1830	1836	1845	rVV	712479	1196371	4.06%	2.524%
11	12.865	1845	1855	1866	rVV2	628071	1564795	5.31%	3.301%
12	13.788	2005	2012	2021	rBV	503392	853845	2.90%	1.801%
13	14.453	2116	2125	2137	rBV	19076073	29457387	100.00%	62.141%
14	14.582	2142	2147	2154	rVB2	183845	319843	1.09%	0.675%

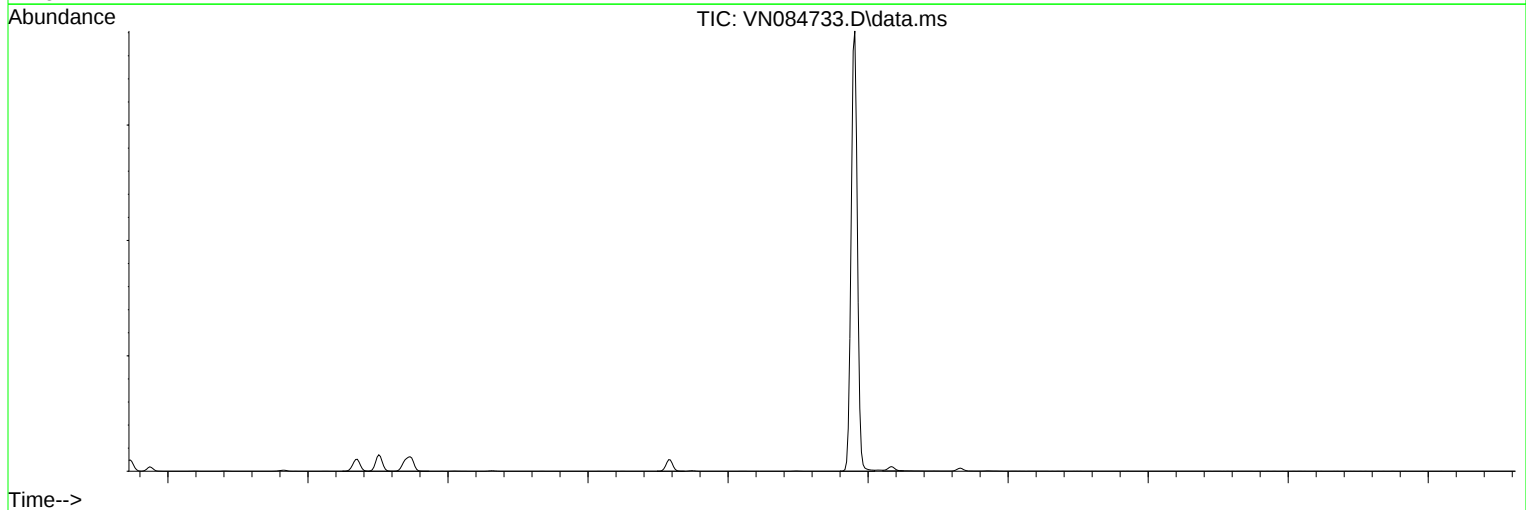
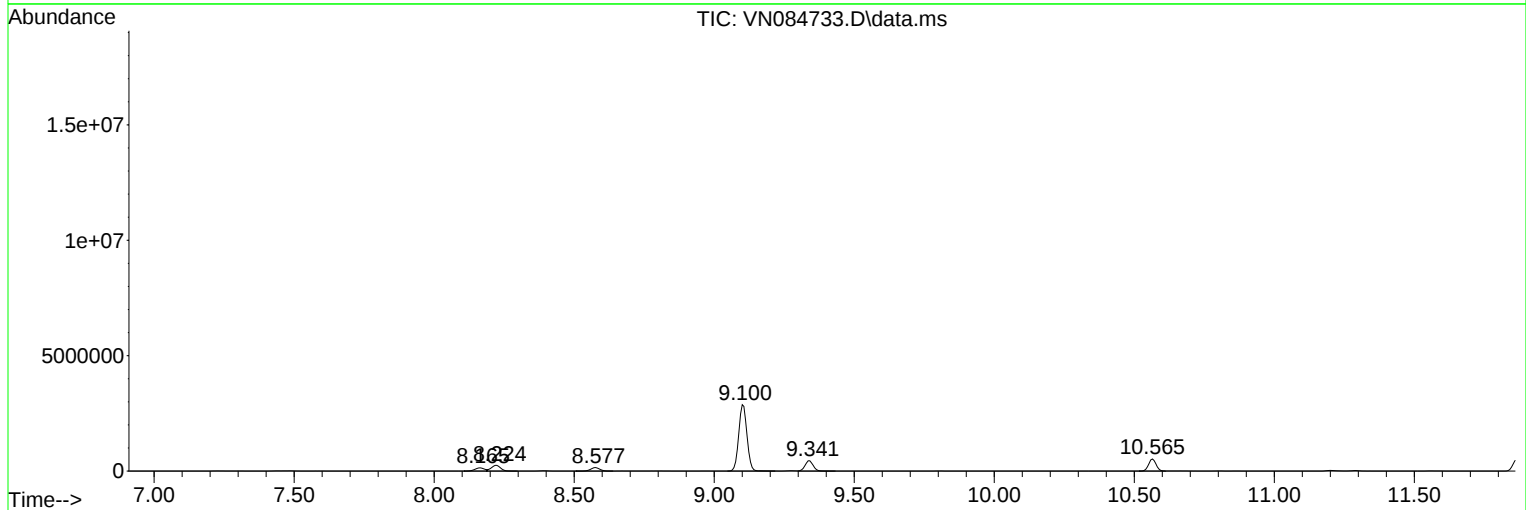
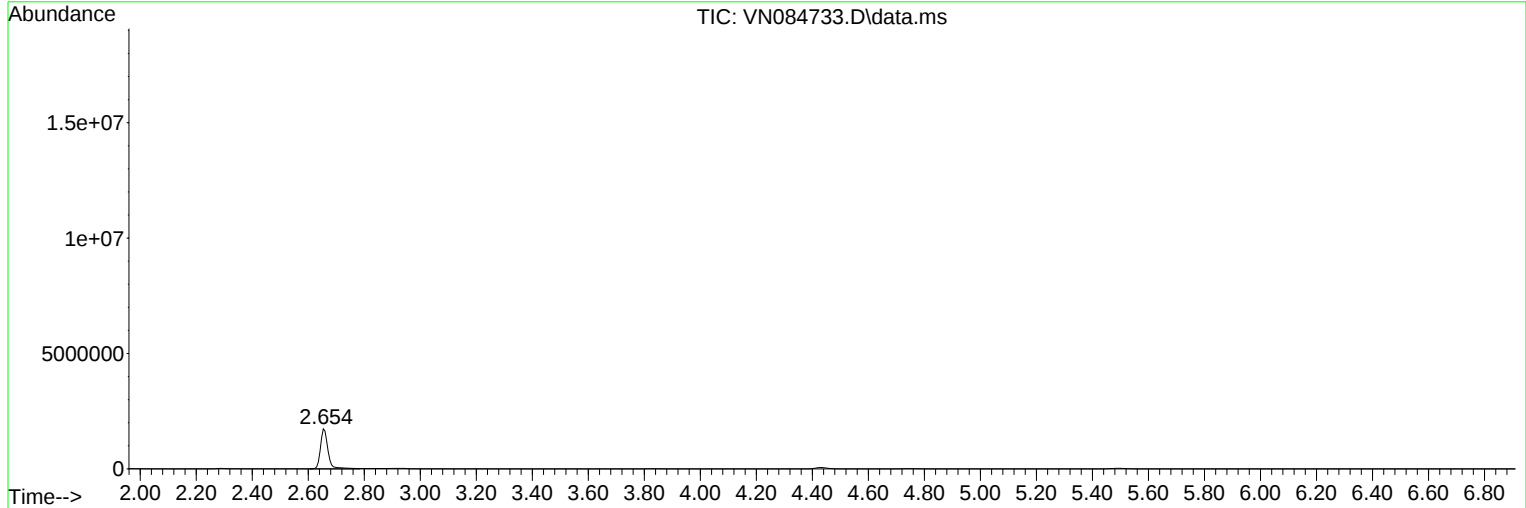
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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



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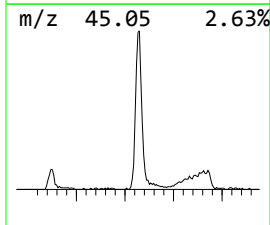
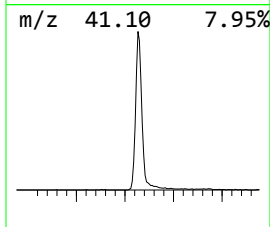
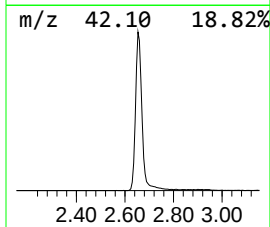
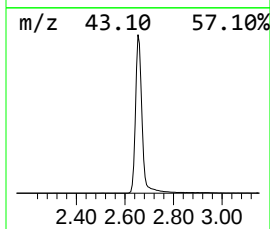
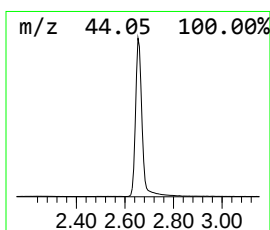
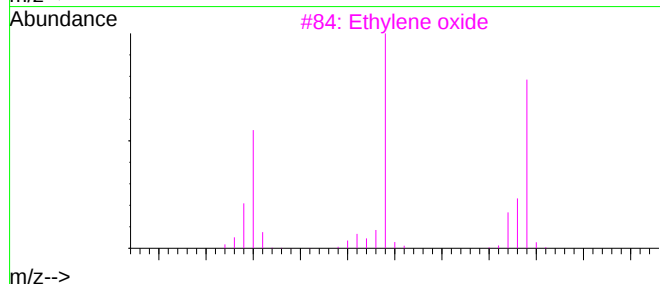
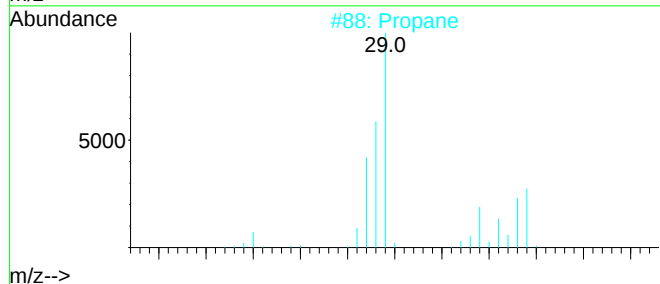
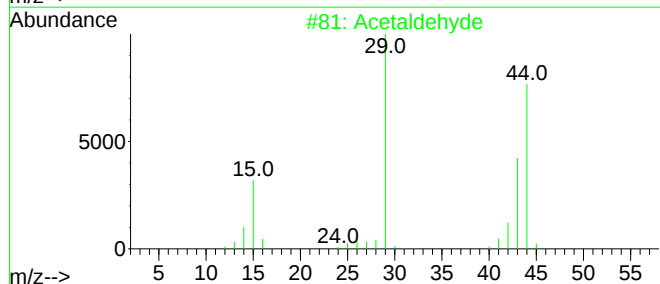
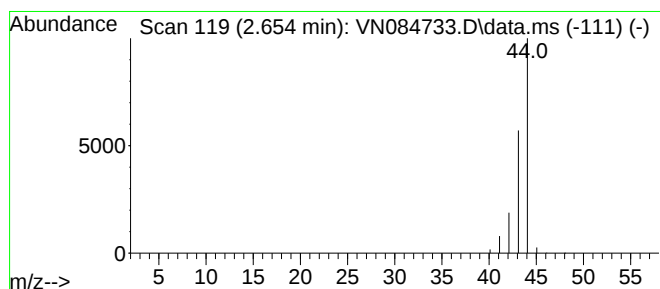
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.654	285.34 ug/l	3190070	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
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	Hydrogen isocyanate	43	CHNO	000075-13-8	3



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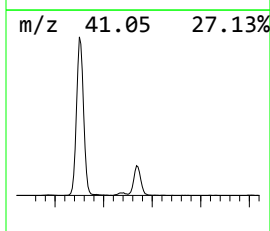
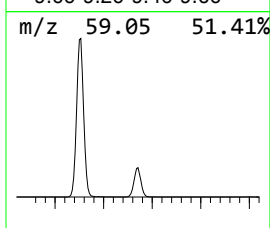
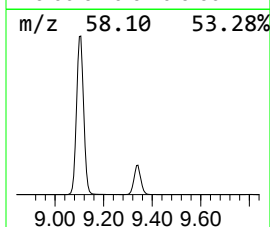
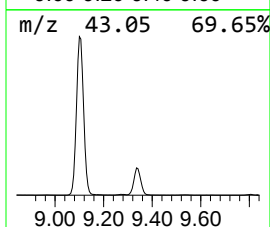
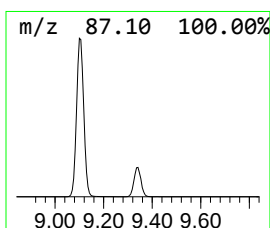
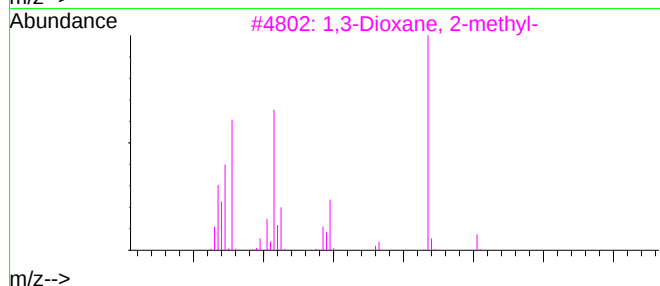
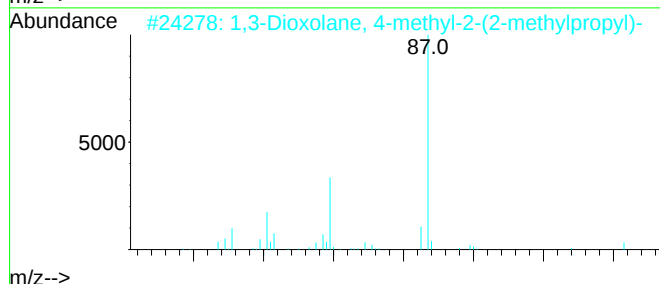
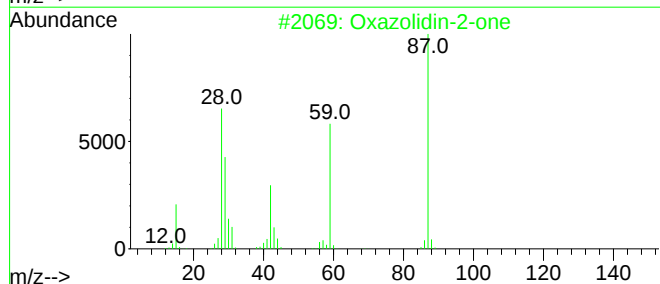
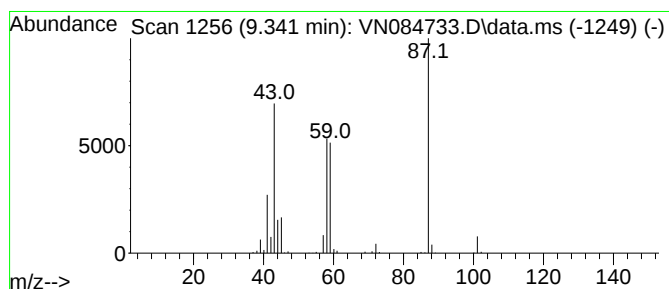
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Quant Title : SW846 8260

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

Peak Number 2 unknown9.341 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.341	7.56 ug/l	891164	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
2	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	40
3	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	38
4	Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	36
5	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	33



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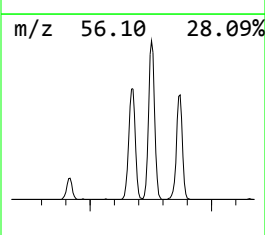
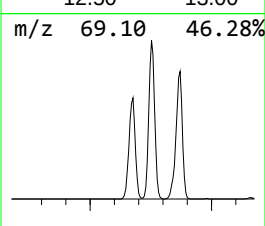
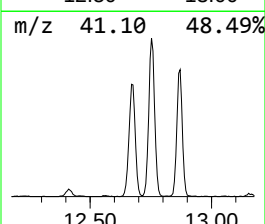
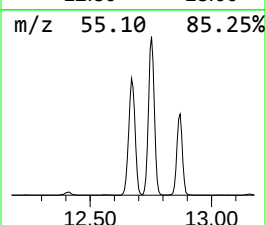
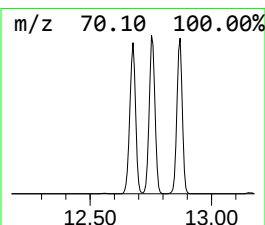
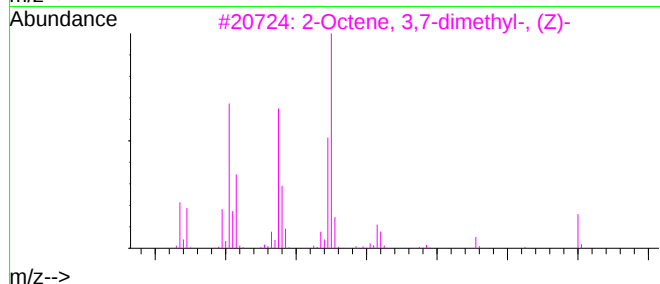
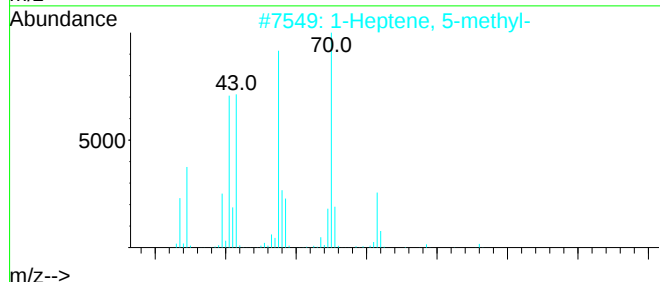
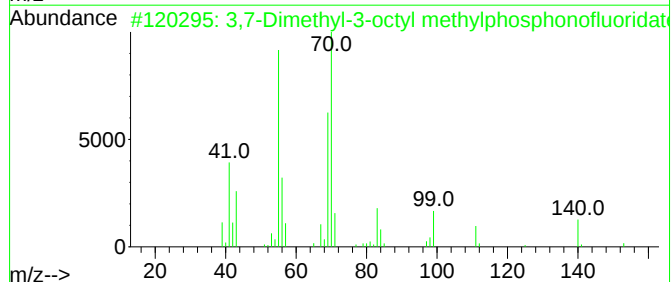
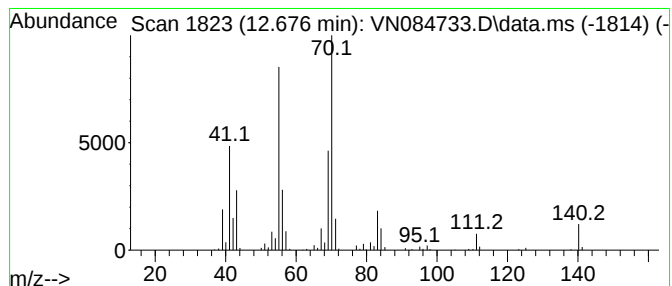
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TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 3,7-Dimethyl-3-octyl methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.676	55.06 ug/l	969290	Chlorobenzene-d5	11.865	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7-Dimethyl-3-octyl methylphosp...	238	C11H24F02P	159395-79-6	91
2	1-Heptene, 5-methyl-	112	C8H16	013151-04-7	90
3	2-Octene, 3,7-dimethyl-, (Z)-	140	C10H20	006874-32-4	87
4	2-Nonene, 3-methyl-, (E)-	140	C10H20	017003-99-5	80
5	2-Heptene, 3-methyl-	112	C8H16	003404-75-9	64



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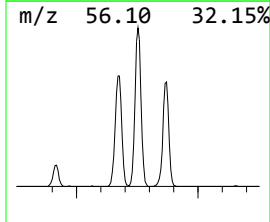
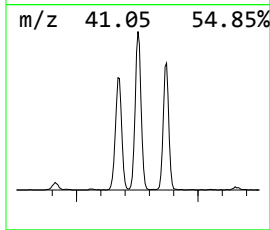
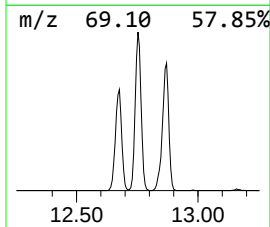
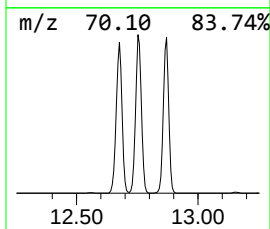
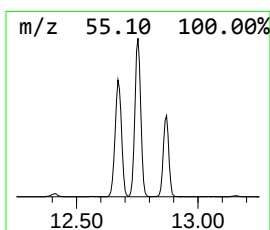
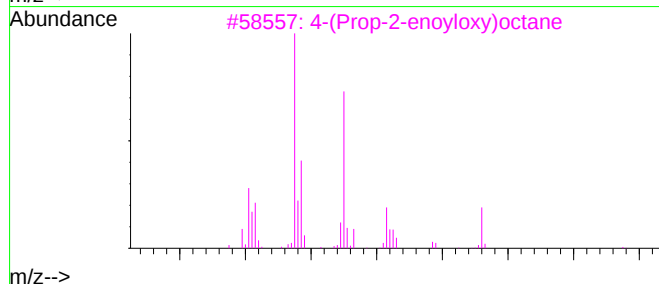
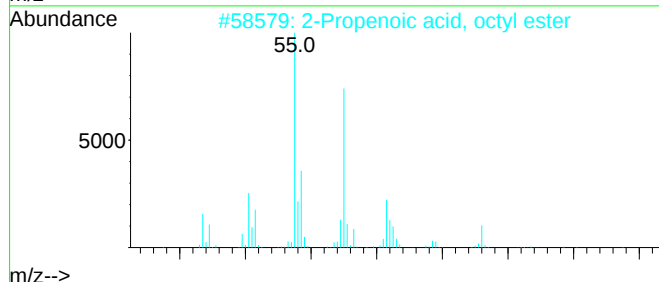
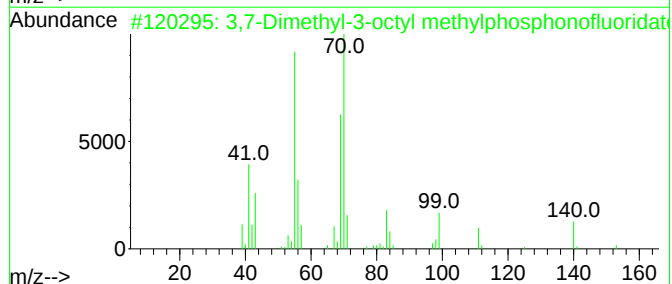
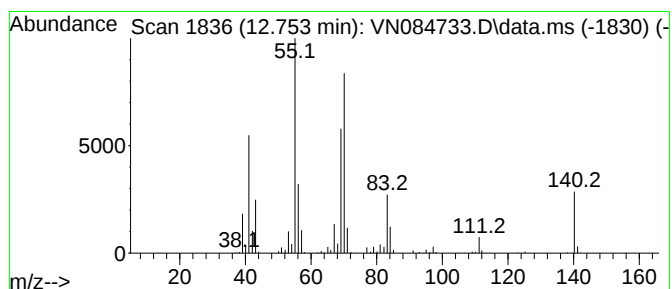
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TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Propenoic acid, octyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.753	67.96 ug/l	1196370	Chlorobenzene-d5	11.865	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7-Dimethyl-3-octyl methylphosp...	238	C11H24FO2P	159395-79-6	86
2	2-Propenoic acid, octyl ester	184	C11H20O2	002499-59-4	72
3	4-(Prop-2-enoyloxy)octane	184	C11H20O2	042928-87-0	64
4	2-Ethylhexyl acrylate	184	C11H20O2	000103-11-7	64
5	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	60



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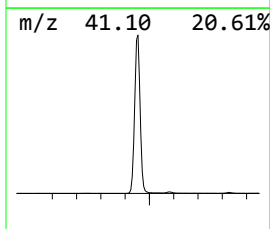
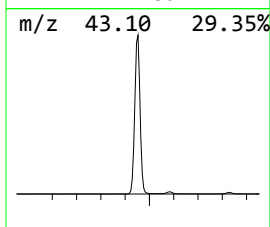
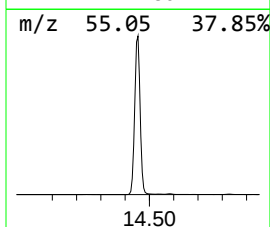
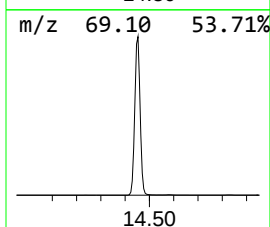
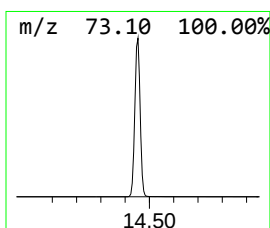
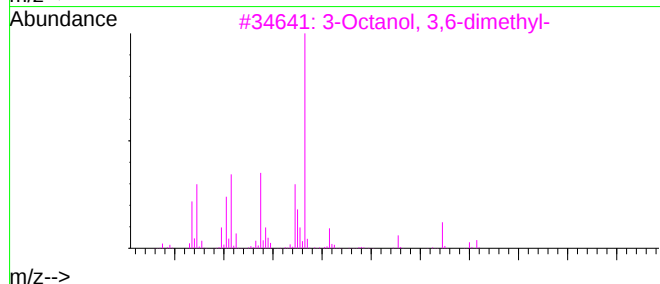
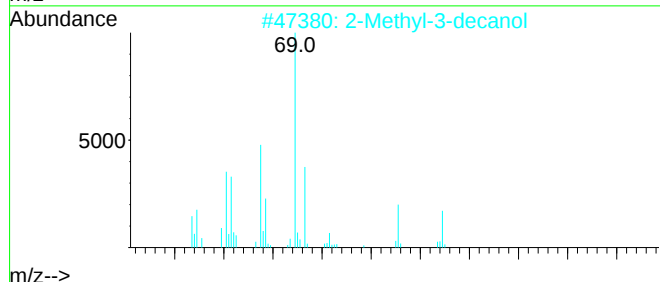
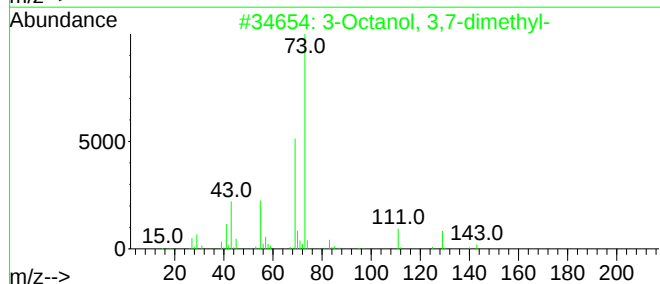
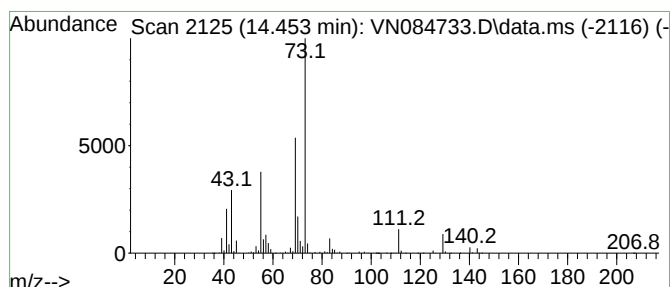
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TIC Integration Parameters: LSCINT.P

Peak Number 5 3-Octanol, 3,7-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.453	1724.98 ug/l	29457400	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanol, 3,7-dimethyl-	158	C10H22O	000078-69-3	80
2	2-Methyl-3-decanol	172	C11H24O	083909-79-9	59
3	3-Octanol, 3,6-dimethyl-	158	C10H22O	000151-19-9	43
4	Dichloroacetic acid, 6-ethyl-3-o...	268	C12H22Cl2O2	1000282-56-6	38
5	1-Undecyn-4-ol	168	C11H20O	022127-86-2	35



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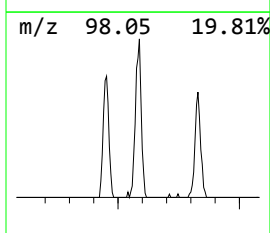
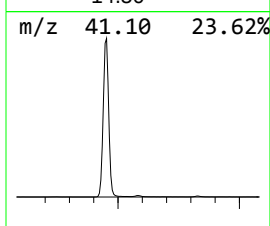
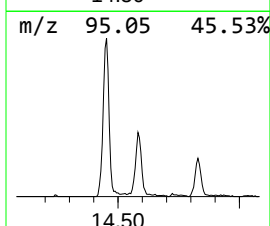
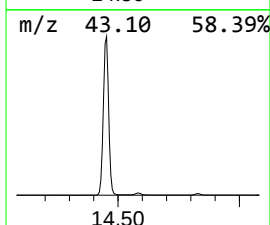
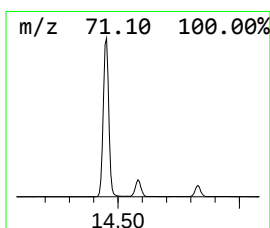
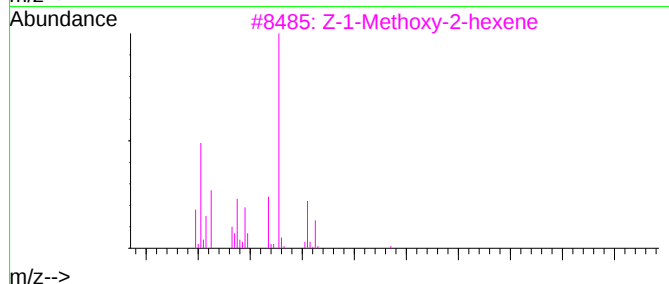
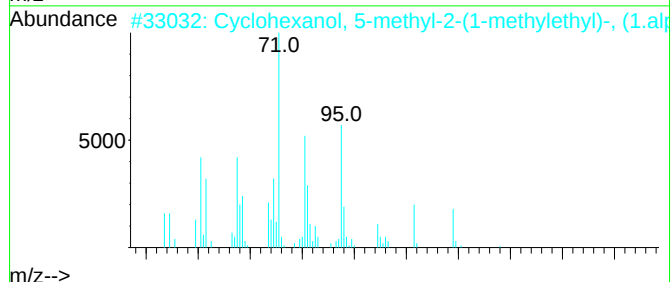
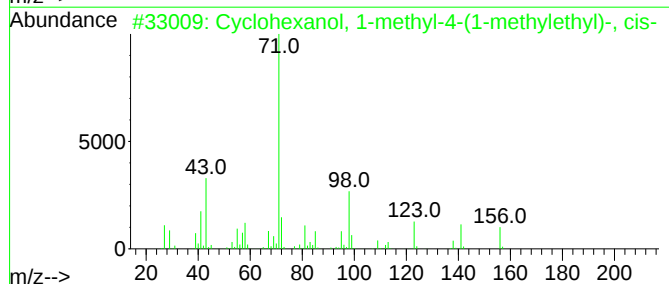
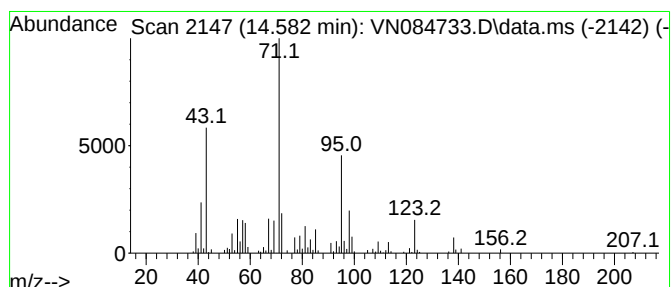
Instrument :
MSVOA_N
ClientSampleId :
MONTCLAIR-TOTE-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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

Peak Number 6 Cyclohexanol, 1-methyl-4-(1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.582	18.73 ug/l	319843	1,4-Dichlorobenzene-d4	13.788	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 1-methyl-4-(1-meth...	156	C10H20O	003901-95-9	58
2	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	000491-02-1	45
3	Z-1-Methoxy-2-hexene	114	C7H14O	1000279-60-9	43
4	Cyclohexanol, 1-methyl-4-(1-meth...	156	C10H20O	003901-93-7	40
5	Z-1-Methoxy-2-pentene	100	C6H12O	1000279-59-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN110724\
Data File : VN084733.D
Acq On : 07 Nov 2024 19:58
Operator : JC\MD
Sample : P4759-01 20X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MONTCLAIR-TOTE-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.654	285.3	ug/l	3190070	1	8.224	558997	50.0
unknown9.341	9.341	7.6	ug/l	891164	2	9.100	5890370	50.0
3,7-Dimethyl-3-...	12.676	55.1	ug/l	969290	3	11.865	880235	50.0
2-Propenoic aci...	12.753	68.0	ug/l	1196370	3	11.865	880235	50.0
3-Octanol, 3,7-...	14.453	1725.0	ug/l	29457400	4	13.788	853845	50.0
Cyclohexanol, 1...	14.582	18.7	ug/l	319843	4	13.788	853845	50.0