

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
 Data File : VN065940.D
 Acq On : 18 Feb 2021 15:00
 Operator : JC/MD
 Sample : M1425-12
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WATER-COMP

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\82N021721W.M
 Title : SW846 8260

Signal : TIC: VN065940.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.254	455	471	495	rBV	84383	204676	2.20%	0.832%
2	3.788	618	637	656	rBV	177794	458146	4.92%	1.863%
3	4.049	692	718	742	rVB2	51538	168951	1.82%	0.687%
4	7.550	1786	1807	1819	rBV	116029	291939	3.14%	1.187%
5	7.627	1819	1831	1851	rVB	224175	531609	5.71%	2.162%
6	7.991	1927	1944	1964	rBV2	141357	329141	3.54%	1.339%
7	8.550	2102	2118	2137	rBV	334036	699654	7.52%	2.846%
8	10.058	2572	2587	2601	rBV	529690	979830	10.53%	3.985%
9	10.576	2736	2748	2773	rVB	119355	216931	2.33%	0.882%
10	11.376	2982	2997	3022	rBV	472808	838724	9.01%	3.411%
11	11.585	3049	3062	3090	rVB	136396	235470	2.53%	0.958%
12	12.373	3294	3307	3327	rBV	347093	593192	6.37%	2.413%
13	12.788	3425	3436	3447	rVB2	72606	118452	1.27%	0.482%
14	13.312	3588	3599	3609	rBV	409433	702610	7.55%	2.858%
15	13.376	3609	3619	3628	rVV	1245156	2082574	22.37%	8.470%
16	13.421	3628	3633	3645	rVB	260708	390109	4.19%	1.587%
17	14.177	3857	3868	3889	rBV	224247	381121	4.09%	1.550%
18	14.283	3890	3901	3903	rBV	286907	378768	4.07%	1.540%
19	14.312	3904	3910	3932	rVB	781986	1323208	14.22%	5.382%
20	14.531	3969	3978	3991	rVB2	67844	123339	1.33%	0.502%
21	14.637	3991	4011	4036	rBV2	4063328	9307685	100.00%	37.855%
22	14.813	4057	4066	4088	rVB2	398509	886408	9.52%	3.605%
23	14.965	4089	4113	4120	rBV2	259426	686621	7.38%	2.793%
24	15.087	4145	4151	4155	rBV2	137533	195391	2.10%	0.795%
25	15.125	4156	4163	4192	rVB	598547	1136367	12.21%	4.622%
26	15.463	4256	4268	4296	rBV	605897	1120975	12.04%	4.559%
27	15.752	4348	4358	4367	rBV4	61766	111413	1.20%	0.453%
28	16.003	4429	4436	4451	rVB2	49673	94389	1.01%	0.384%

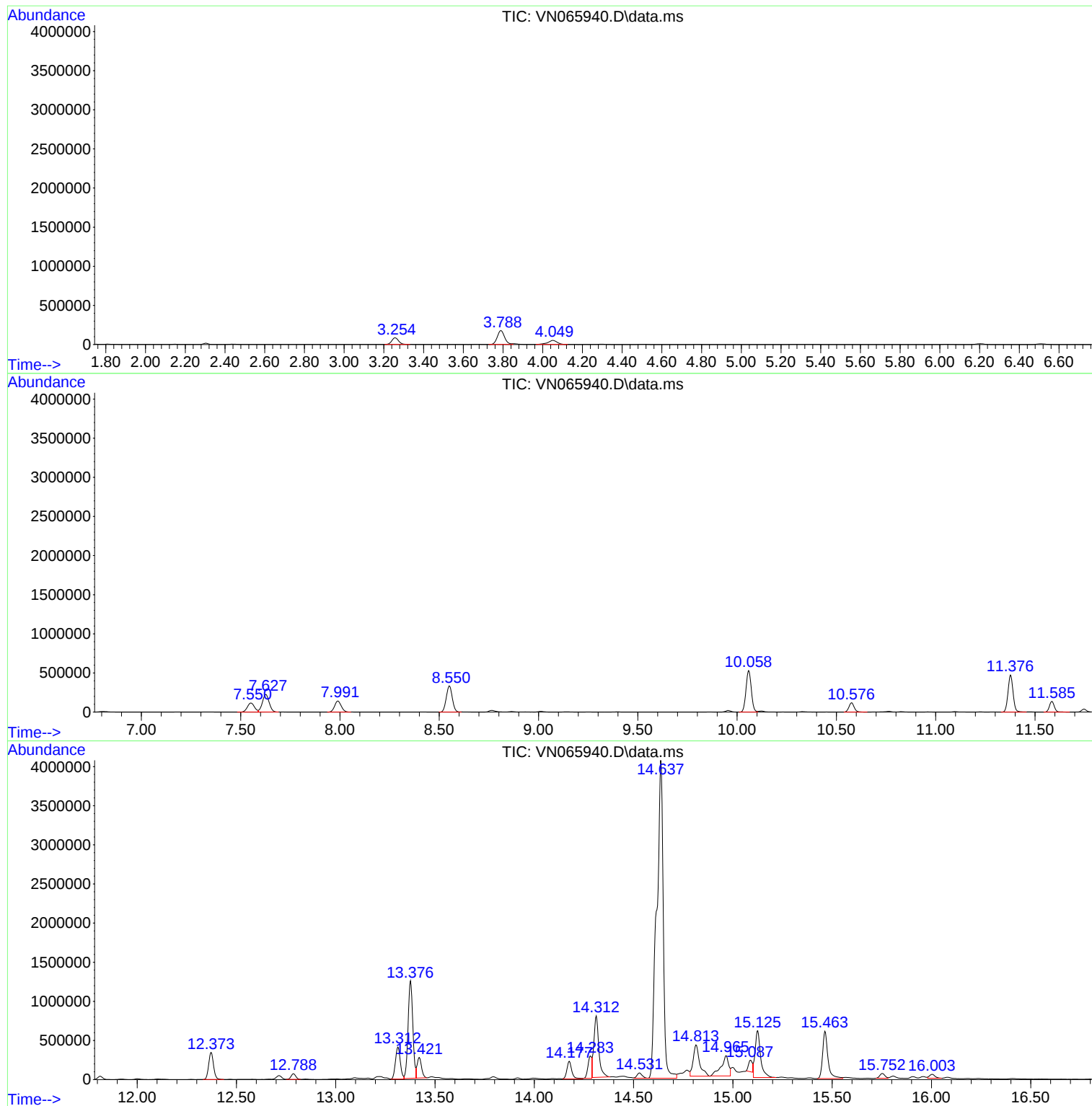
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WATER-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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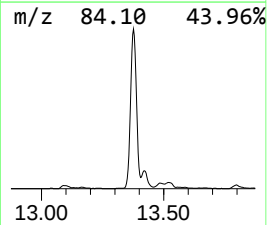
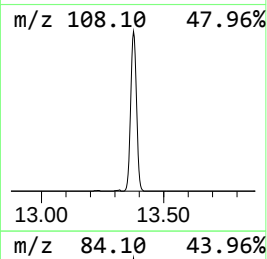
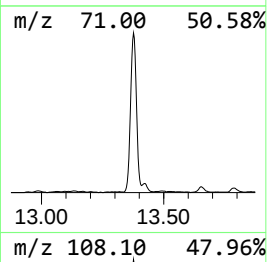
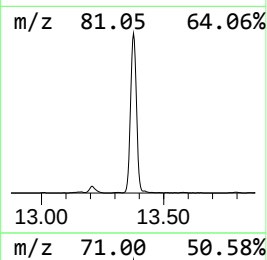
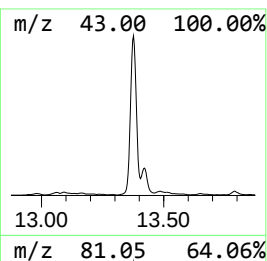
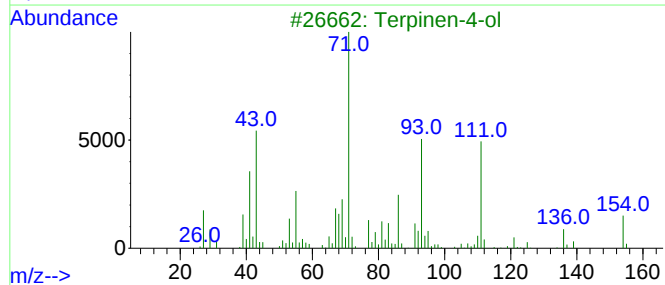
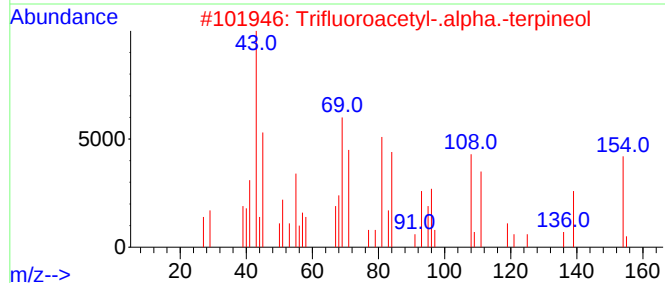
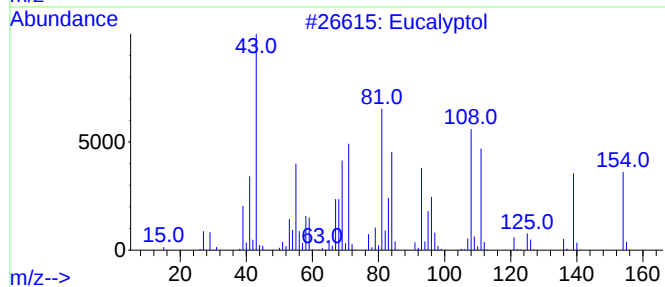
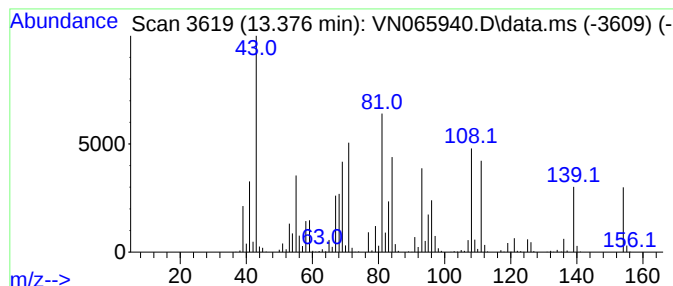
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Eucalyptol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.376	148.20 ug/l	2082570	1,4-Dichlorobenzene-d4	13.312

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	72
3			Terpinen-4-ol	154	C10H18O	000562-74-3	32
4			Sulfurous acid, 2-pentyl propyl ...	194	C8H18O3S	1000309-15-1	22
5			2-(3'-Oxo-butyl)-cyclopentanone	154	C9H14O2	1000143-37-2	16



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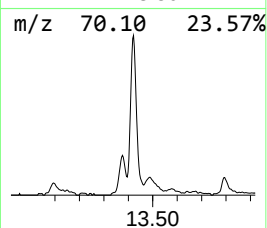
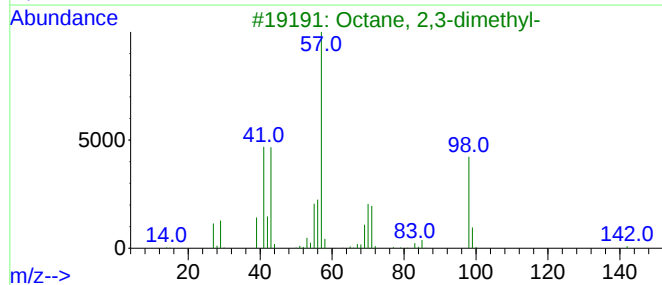
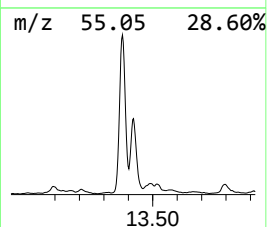
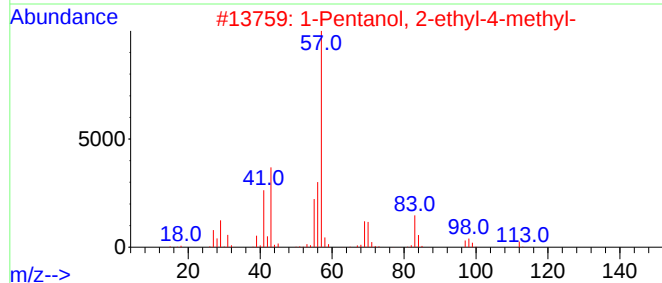
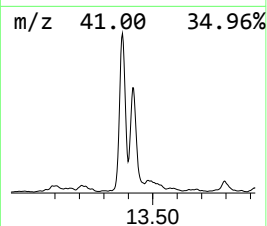
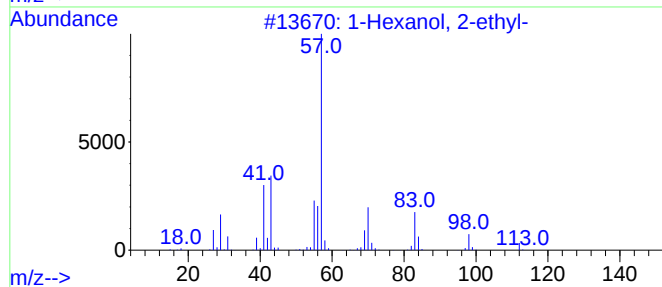
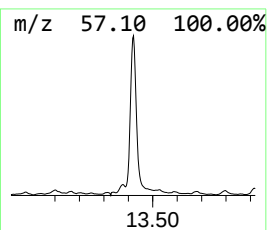
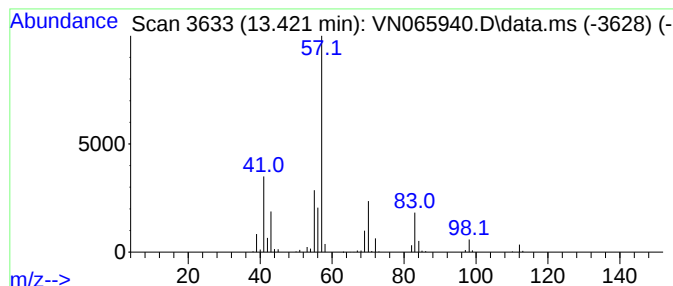
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.421	27.76 ug/l	390109	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	59
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	45



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WATER-COMP

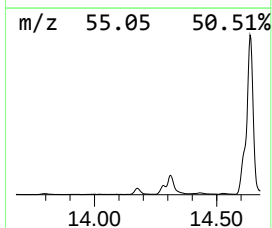
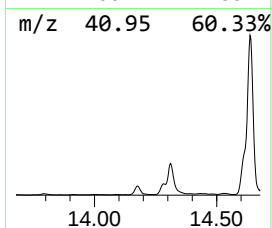
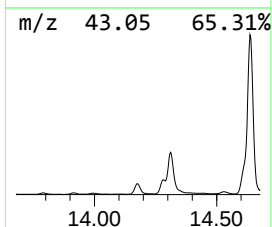
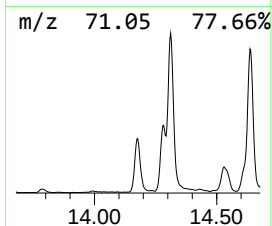
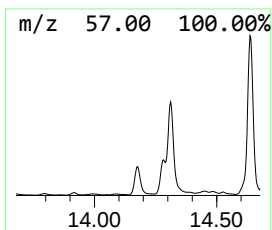
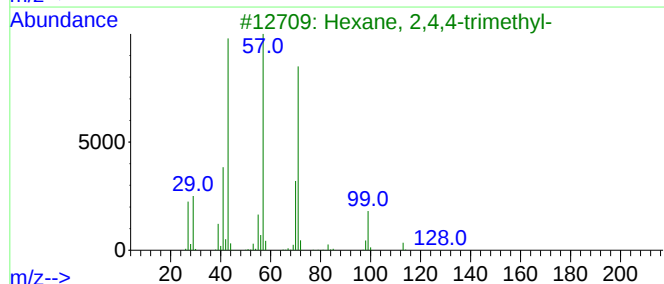
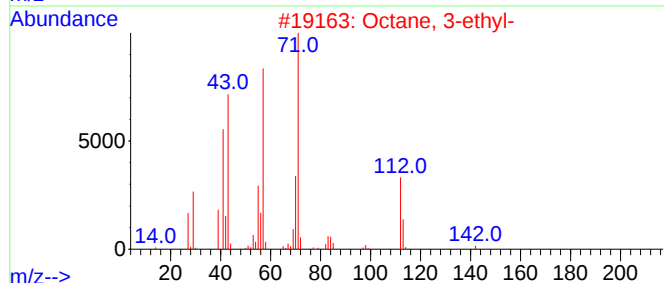
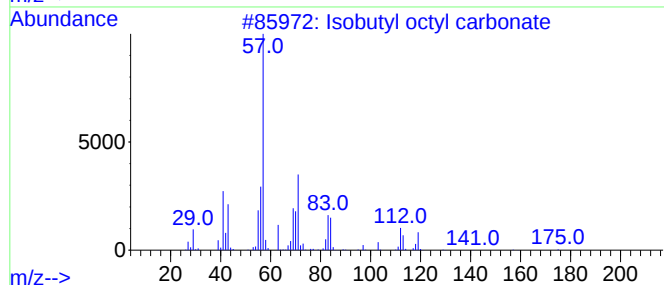
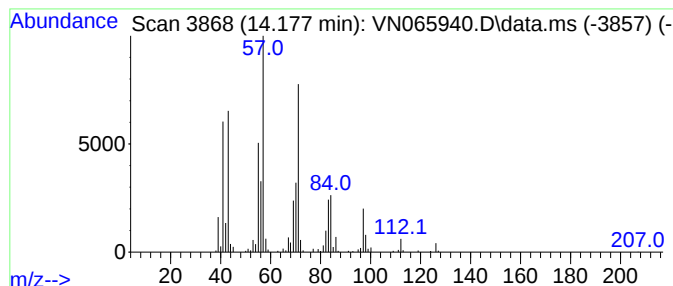
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Isobutyl octyl carbonate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.177	27.12 ug/l	381121	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl octyl carbonate	230	C13H26O3	1000372-74-6	52
2			Octane, 3-ethyl-	142	C10H22	005881-17-4	50
3			Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	43
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	43
5			1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
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Acq On : 18 Feb 2021 15:00
Operator : JC/MD
Sample : M1425-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WATER-COMP

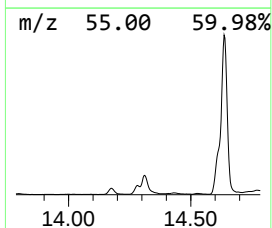
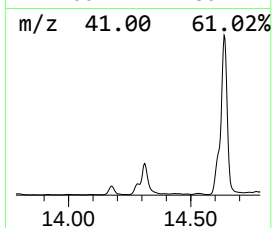
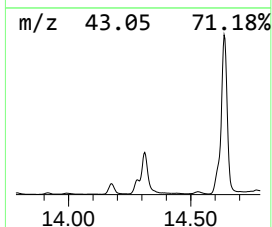
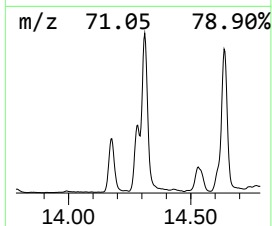
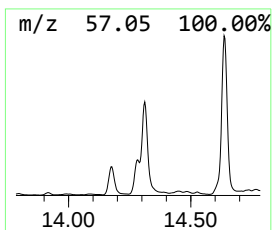
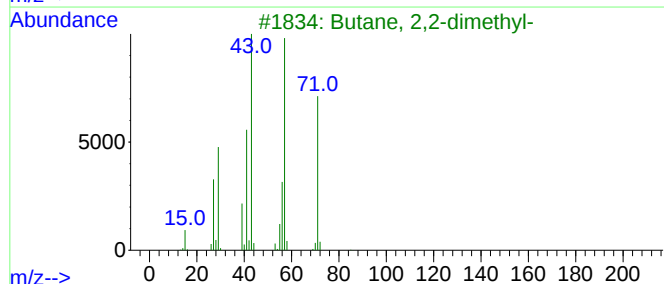
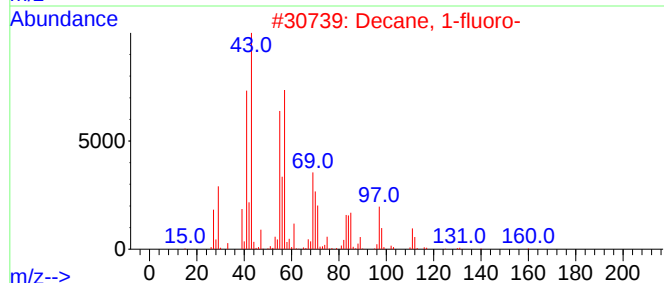
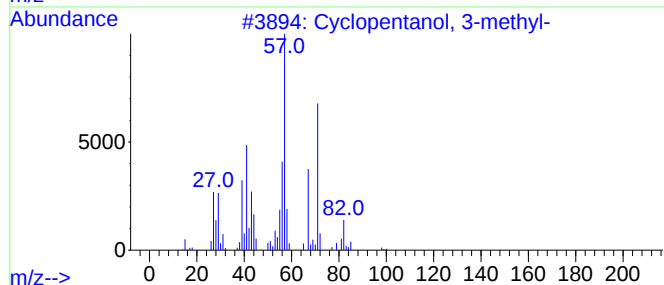
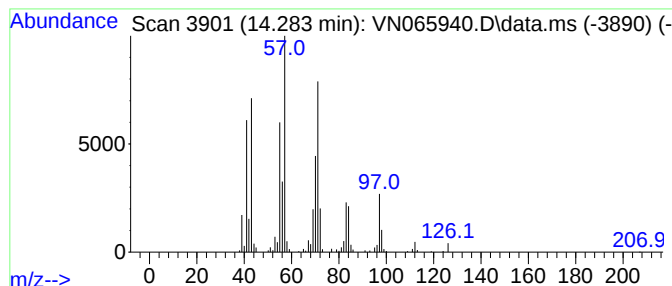
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.283 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.283	26.95 ug/l	378768	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanol, 3-methyl-	100	C6H12O	018729-48-1	43
2			Decane, 1-fluoro-	160	C10H21F	000334-56-5	43
3			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
4			1-Nonene	126	C9H18	000124-11-8	38
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	38



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WATER-COMP

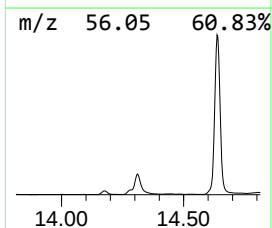
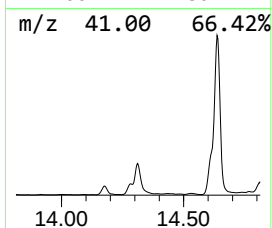
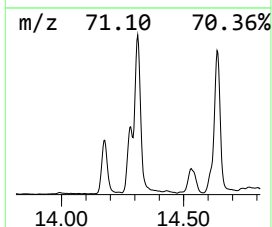
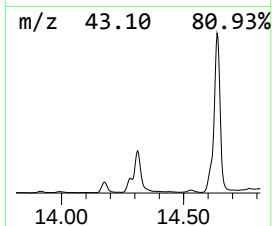
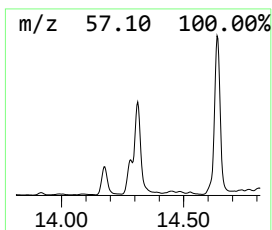
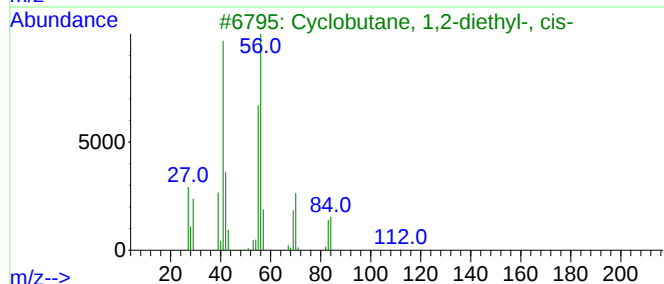
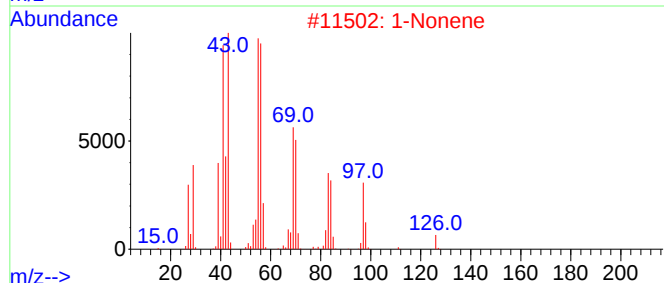
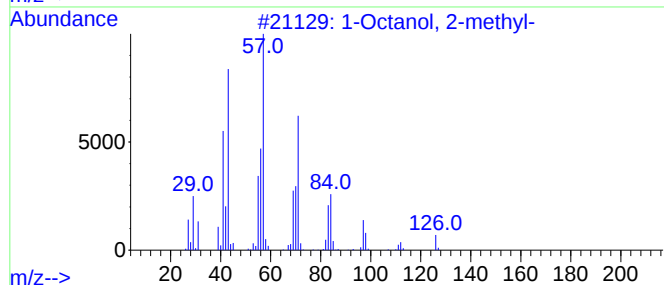
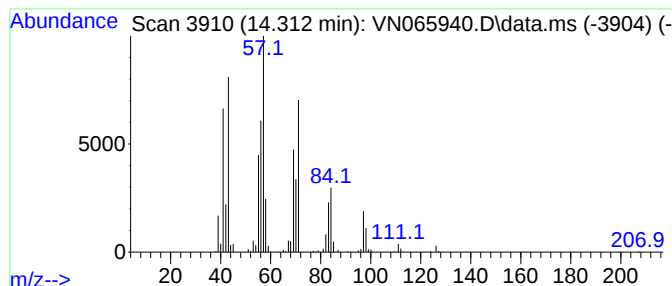
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Octanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.312	94.16 ug/l	1323210	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	86
2			1-Nonene	126	C9H18	000124-11-8	60
3			Cyclobutane, 1,2-diethyl-, cis-	112	C8H16	061141-50-2	49
4			Decane, 1-fluoro-	160	C10H21F	000334-56-5	47
5			Isooctyl mercaptoacetate	204	C10H20O2S	025103-09-7	38



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
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WATER-COMP

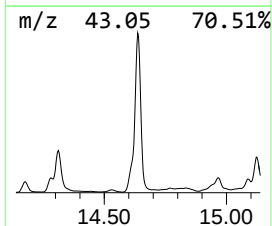
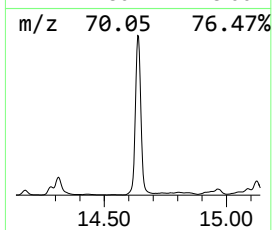
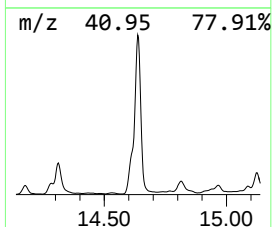
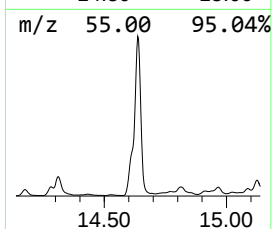
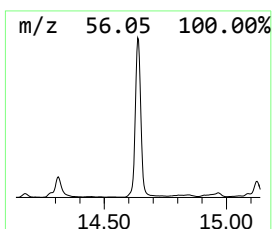
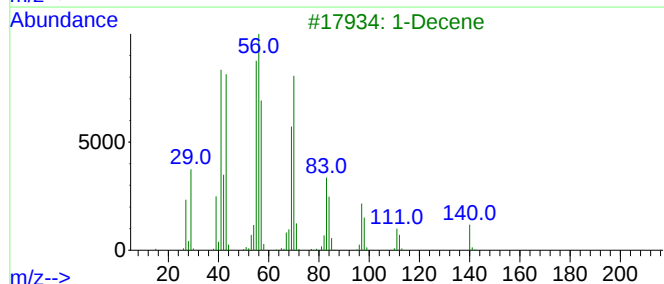
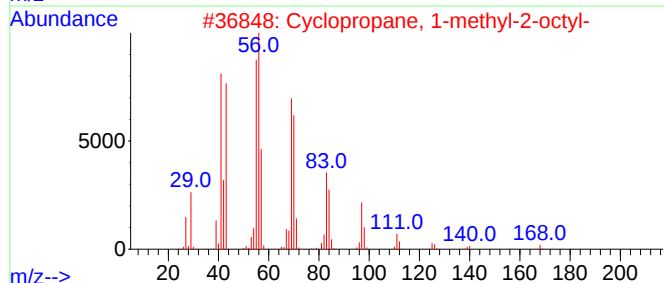
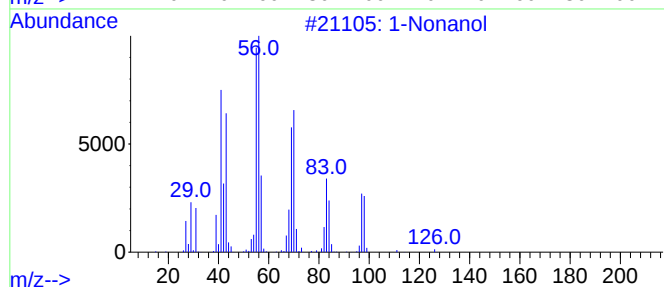
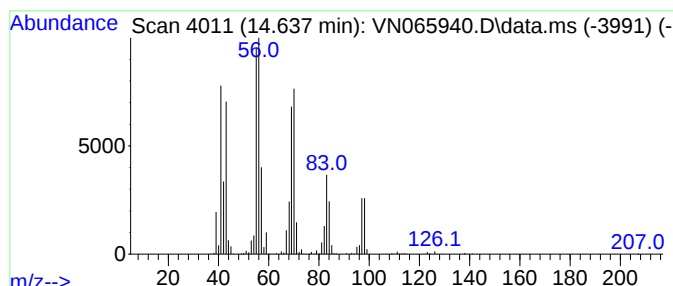
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.637	662.37 ug/l	9307690	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol			144	C9H20O	000143-08-8	91
2	Cyclopropane, 1-methyl-2-octyl-			168	C12H24	037617-26-8	80
3	1-Decene			140	C10H20	000872-05-9	72
4	Cycloheptane			98	C7H14	000291-64-5	68
5	Isopropylcyclobutane			98	C7H14	000872-56-0	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
Data File : VN065940.D
Acq On : 18 Feb 2021 15:00
Operator : JC/MD
Sample : M1425-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WATER-COMP

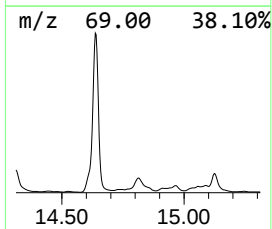
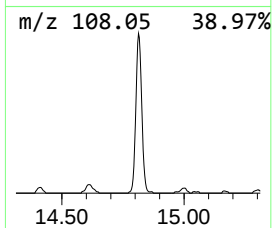
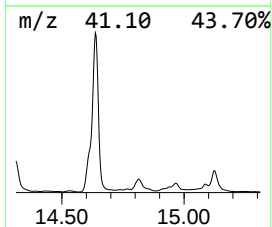
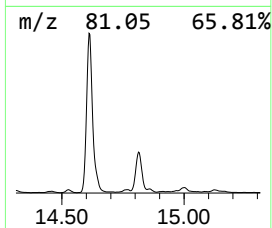
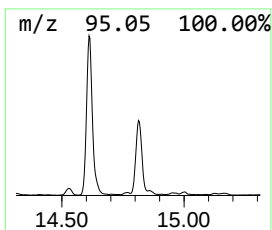
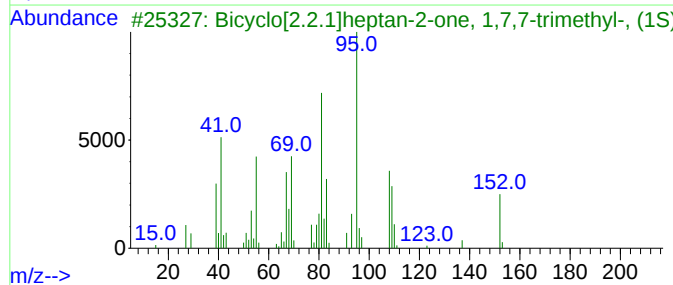
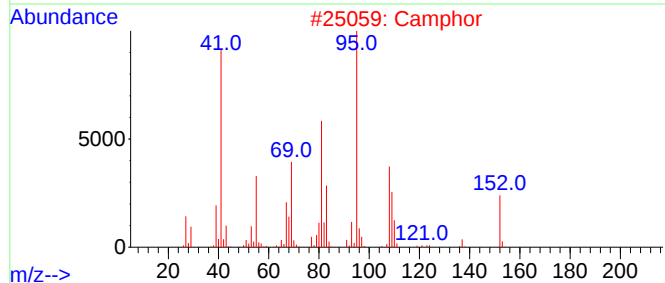
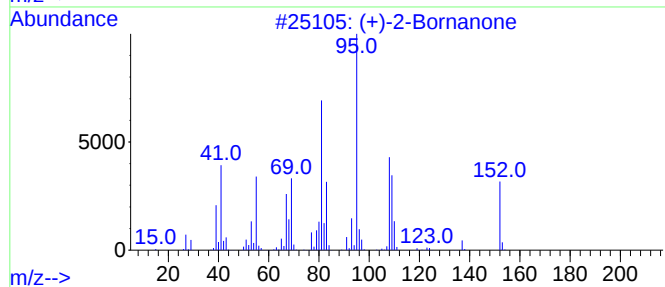
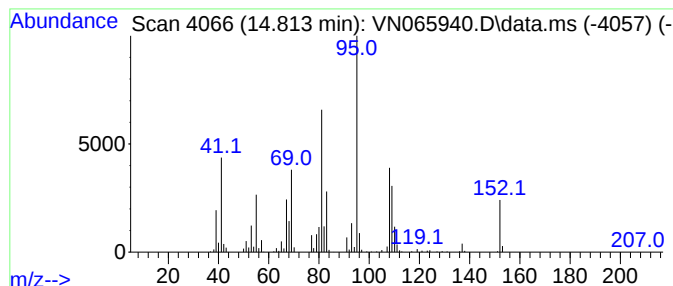
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 (+)-2-Bornanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.813	63.08 ug/l	886408	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-2-Bornanone	152	C10H16O	000464-49-3	95
2			Camphor	152	C10H16O	000076-22-2	95
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	94
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46
5			Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
Data File : VN065940.D
Acq On : 18 Feb 2021 15:00
Operator : JC/MD
Sample : M1425-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WATER-COMP

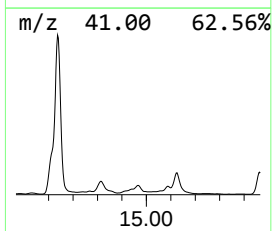
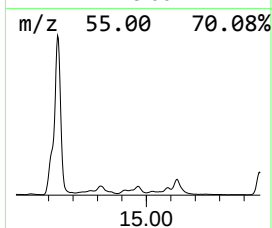
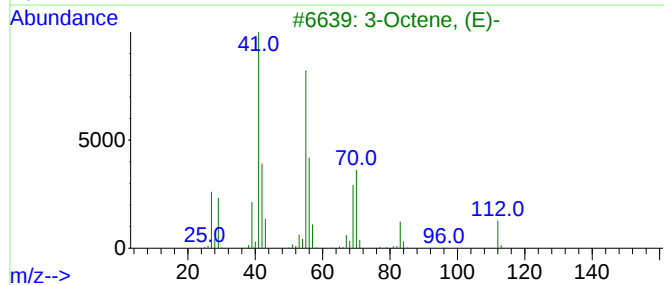
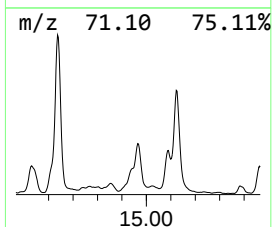
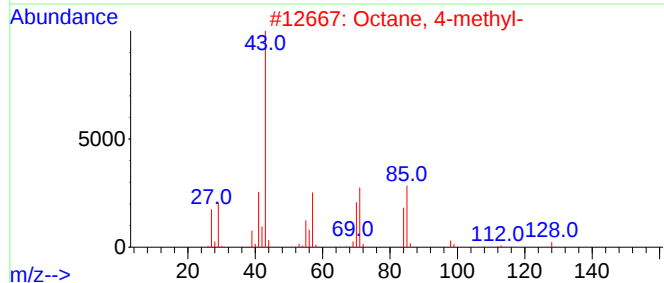
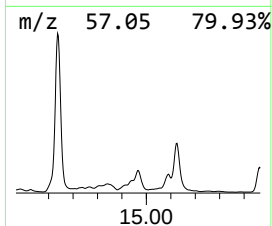
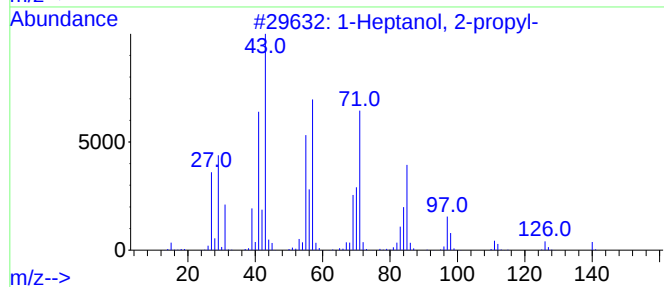
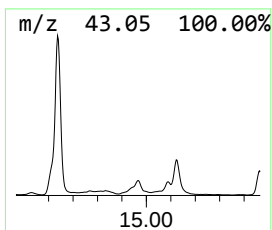
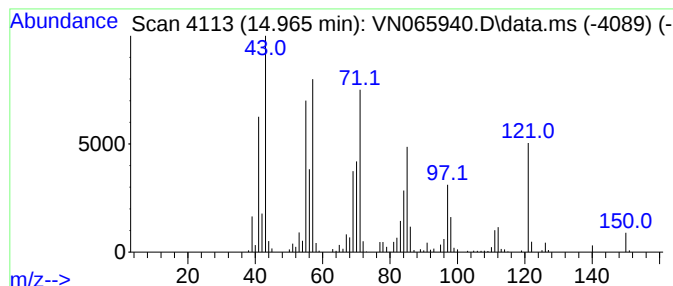
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Heptanol, 2-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.965	48.86 ug/l	686621	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	72
2			Octane, 4-methyl-	128	C9H20	002216-34-4	43
3			3-Octene, (E)-	112	C8H16	014919-01-8	38
4			3-Octene, (Z)-	112	C8H16	014850-22-7	38
5			Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
Data File : VN065940.D
Acq On : 18 Feb 2021 15:00
Operator : JC/MD
Sample : M1425-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WATER-COMP

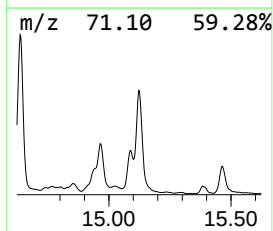
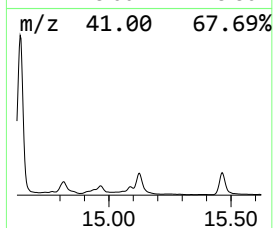
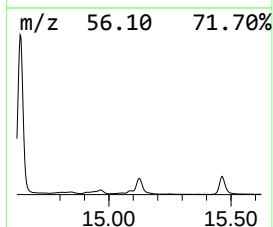
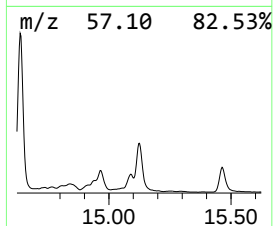
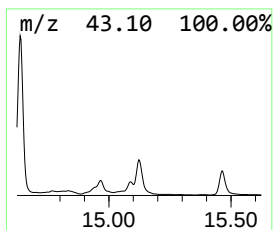
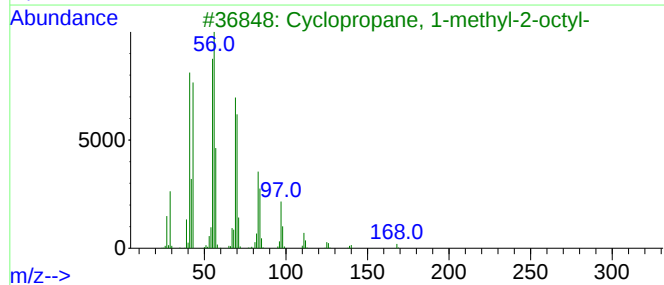
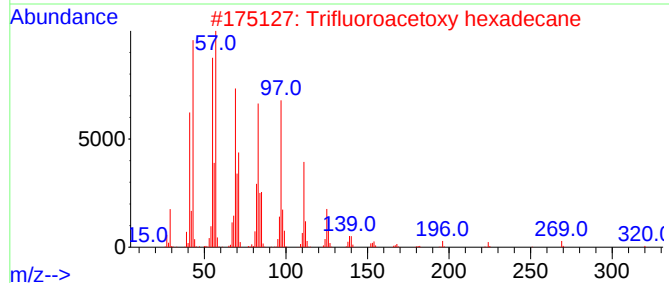
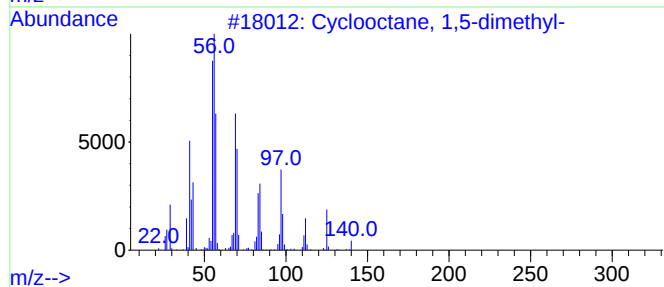
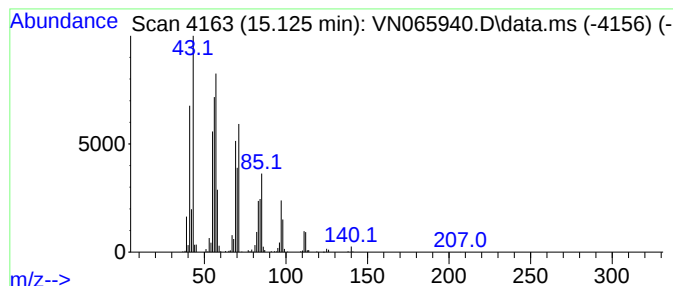
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Cyclooctane, 1,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.125	80.87 ug/l	1136370	1,4-Dichlorobenzene-d4	13.312

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctane, 1,5-dimethyl-	140	C10H20	021328-57-4	70
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	59
3			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	58
4			1-Decene	140	C10H20	000872-05-9	53
5			1-Dodecene	168	C12H24	000112-41-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
Data File : VN065940.D
Acq On : 18 Feb 2021 15:00
Operator : JC/MD
Sample : M1425-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WATER-COMP

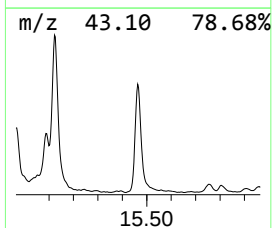
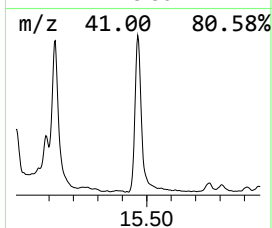
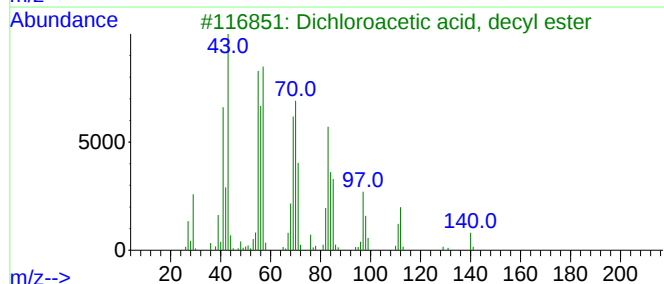
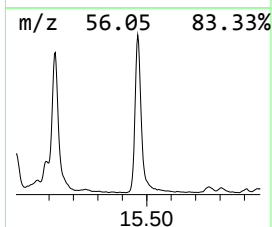
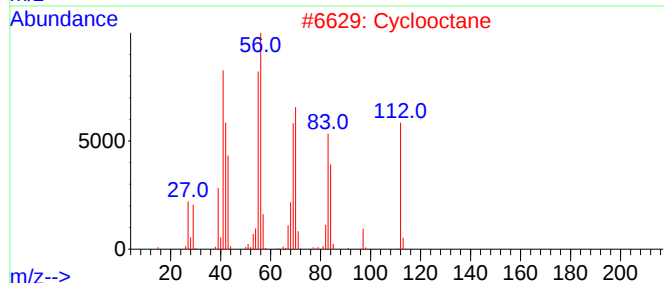
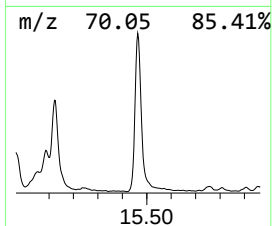
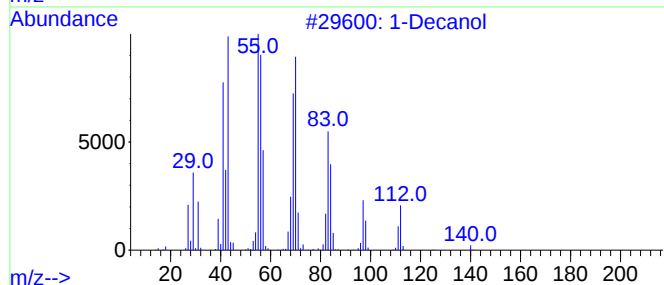
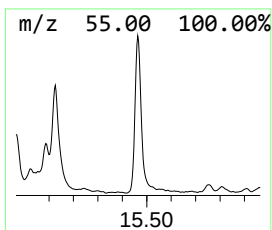
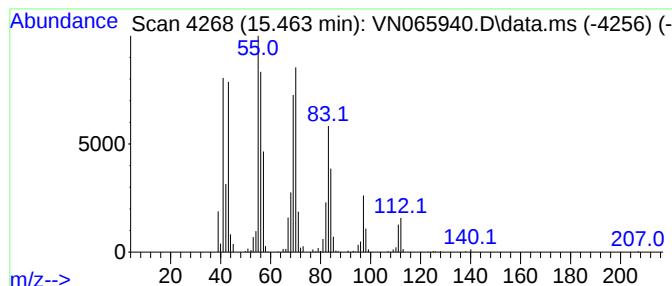
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1-Decanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.463	79.77 ug/l	1120980	1,4-Dichlorobenzene-d4	13.312

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Decanol	158	C10H22O	000112-30-1	91
2		Cyclooctane	112	C8H16	000292-64-8	87
3		Dichloroacetic acid, decyl ester	268	C12H22Cl2O2	083005-00-9	86
4		Formic acid, decyl ester	186	C11H22O2	005451-52-5	86
5		Cyclodecane	140	C10H20	000293-96-9	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021821\
Data File : VN065940.D
Acq On : 18 Feb 2021 15:00
Operator : JC/MD
Sample : M1425-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WATER-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021721W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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1-Hexanol, 2-et...	13.421	27.8	ug/l	390109	4	13.312	702610	50.0
Isobutyl octyl ...	14.177	27.1	ug/l	381121	4	13.312	702610	50.0
unknown14.283	14.283	26.9	ug/l	378768	4	13.312	702610	50.0
1-Octanol, 2-me...	14.312	94.2	ug/l	1323210	4	13.312	702610	50.0
1-Nonanol	14.637	662.4	ug/l	9307690	4	13.312	702610	50.0
(+)-2-Bornanone	14.813	63.1	ug/l	886408	4	13.312	702610	50.0
1-Heptanol, 2-p...	14.965	48.9	ug/l	686621	4	13.312	702610	50.0
Cyclooctane, 1,...	15.125	80.9	ug/l	1136370	4	13.312	702610	50.0
1-Decanol	15.463	79.8	ug/l	1120980	4	13.312	702610	50.0