

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
 Data File : VN069121.D
 Acq On : 22 Oct 2021 5:52
 Operator : JC/MD
 Sample : M4284-08
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 20877

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\82N101221W.M
 Title : SW846 8260

Signal : TIC: VN069121.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.283	828	855	935	rBV	4217269	12329060	30.54%	5.219%
2	4.572	939	963	1007	rVB	881544	2764255	6.85%	1.170%
3	7.335	1964	1993	2038	rBV	485211	1320451	3.27%	0.559%
4	8.024	2229	2250	2261	rBV2	239911	568388	1.41%	0.241%
5	8.088	2262	2274	2303	rVB	458372	1035065	2.56%	0.438%
6	8.440	2378	2405	2429	rBV	265645	625158	1.55%	0.265%
7	8.968	2584	2602	2633	rBV2	670778	1386893	3.43%	0.587%
8	10.443	3125	3152	3170	rBV	1060038	1973888	4.89%	0.836%
9	11.087	3369	3392	3417	rBV	302131	534011	1.32%	0.226%
10	11.747	3617	3638	3658	rBV	986975	1800051	4.46%	0.762%
11	12.353	3849	3864	3877	rBV	379573	612039	1.52%	0.259%
12	12.420	3877	3889	3908	rVV	377537	630302	1.56%	0.267%
13	12.554	3925	3939	3955	rBV2	263234	418985	1.04%	0.177%
14	12.734	3981	4006	4026	rBV	834682	1469523	3.64%	0.622%
15	12.838	4029	4045	4055	rBV2	337965	629919	1.56%	0.267%
16	13.179	4157	4172	4194	rVB3	712598	1408065	3.49%	0.596%
17	13.412	4247	4259	4272	rBV	813135	1241182	3.07%	0.525%
18	13.495	4279	4290	4310	rVB3	412095	716996	1.78%	0.304%
19	13.619	4313	4336	4346	rBV	645010	1207722	2.99%	0.511%
20	13.678	4346	4358	4368	rVV	984857	1628639	4.03%	0.689%
21	13.742	4368	4382	4408	rVB	7943542	13781000	34.13%	5.834%
22	14.142	4515	4531	4553	rBV2	8955177	13926979	34.49%	5.895%
23	14.260	4564	4575	4588	rBV4	287143	511701	1.27%	0.217%
24	14.348	4589	4608	4624	rBV2	3994746	9692371	24.01%	4.103%
25	14.426	4624	4637	4651	rVB	19009671	30160899	74.70%	12.767%
26	14.530	4666	4676	4683	rBV	4611376	7063639	17.49%	2.990%
27	14.635	4705	4715	4720	rBV3	6323881	9214425	22.82%	3.900%
28	14.675	4721	4730	4735	rBV	21488062	33771233	83.64%	14.295%
29	14.788	4761	4772	4801	rVB	10171574	17021567	42.16%	7.205%
30	14.997	4838	4850	4858	rBV2	2549346	4444061	11.01%	1.881%
31	15.204	4912	4927	4940	rBV2	7233518	13174451	32.63%	5.577%
32	15.257	4942	4947	4959	rVV2	622591	1006762	2.49%	0.426%
33	15.351	4960	4982	5015	rVV	23393193	40375647	100.00%	17.091%
34	15.480	5019	5030	5036	rVV	1464931	2523498	6.25%	1.068%
35	15.517	5037	5044	5078	rVB2	2309996	4786445	11.85%	2.026%
36	15.888	5172	5182	5213	rVB2	238511	481927	1.19%	0.204%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Title : SW846 8260

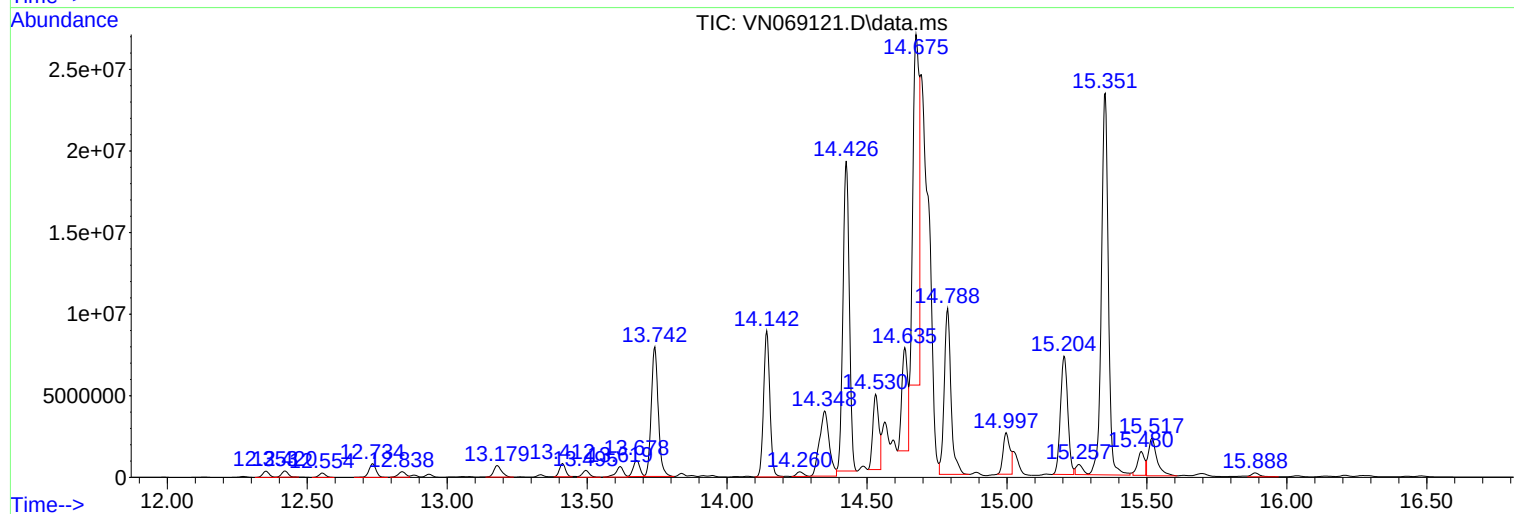
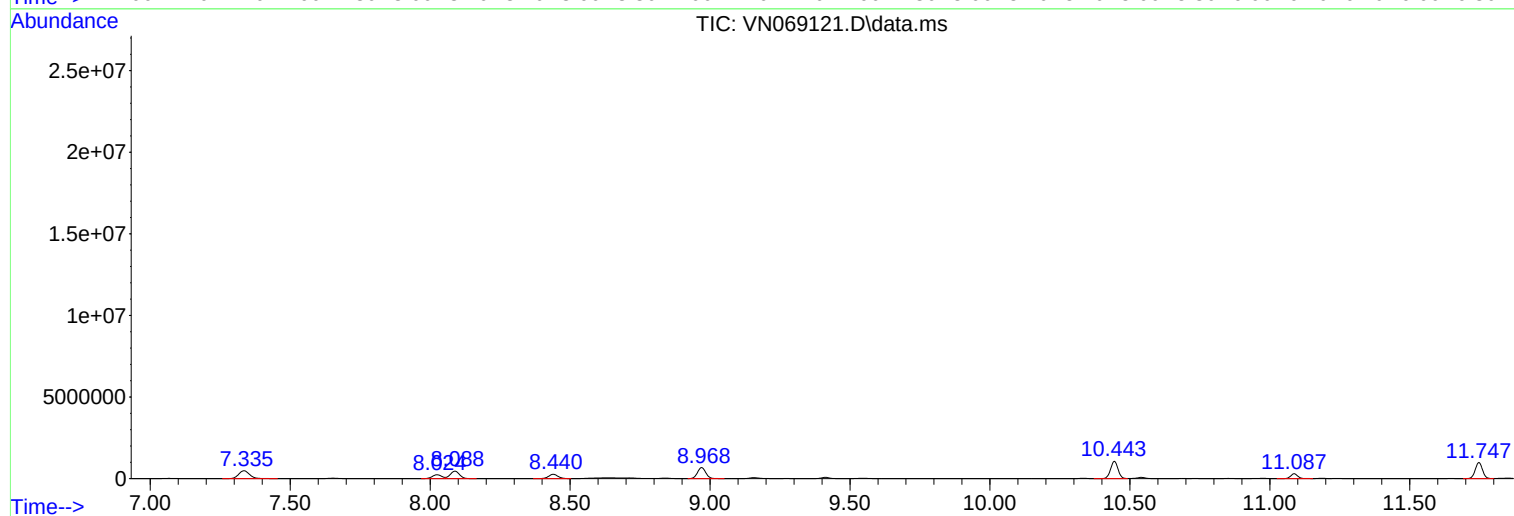
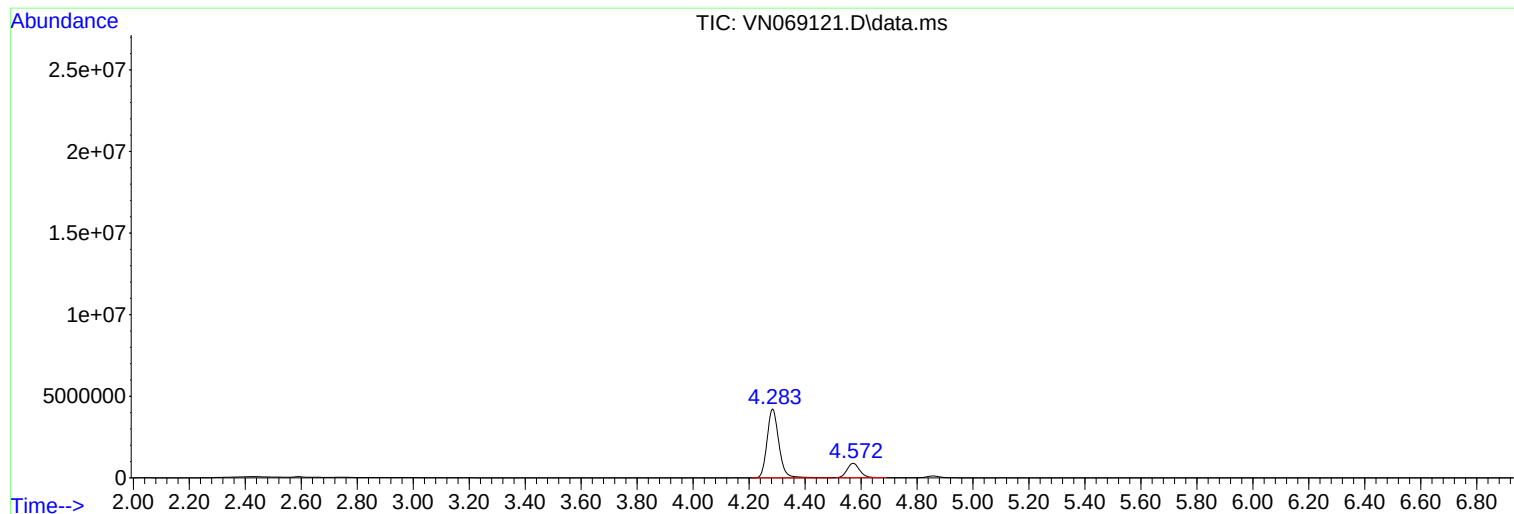
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_N
ClientSampled :
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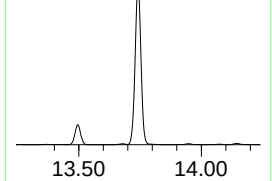
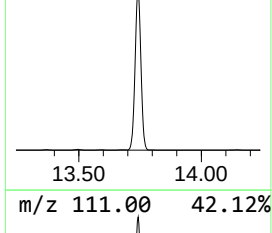
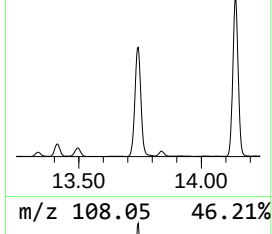
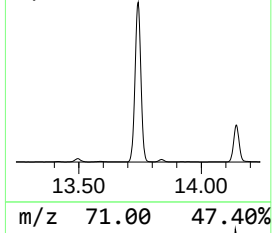
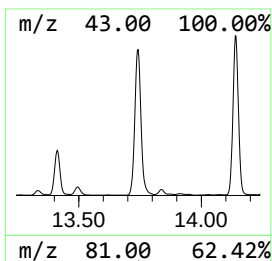
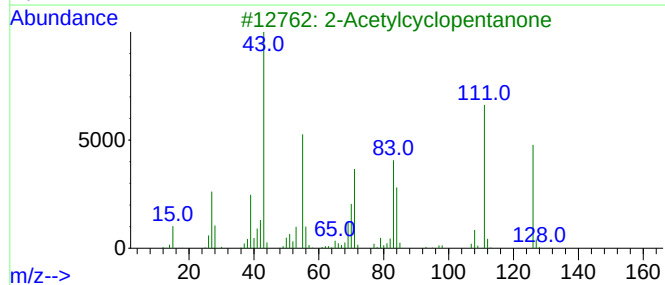
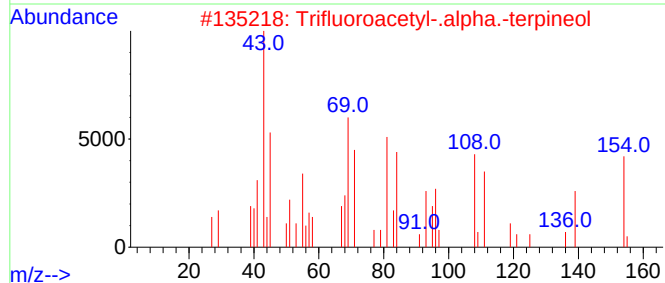
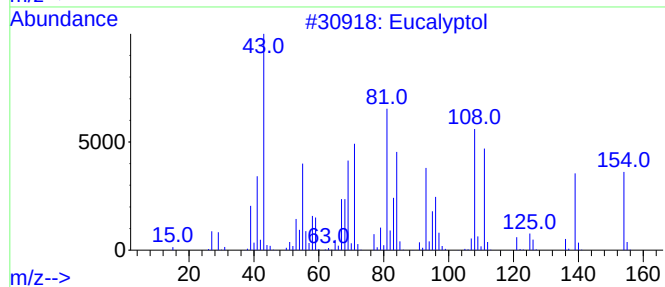
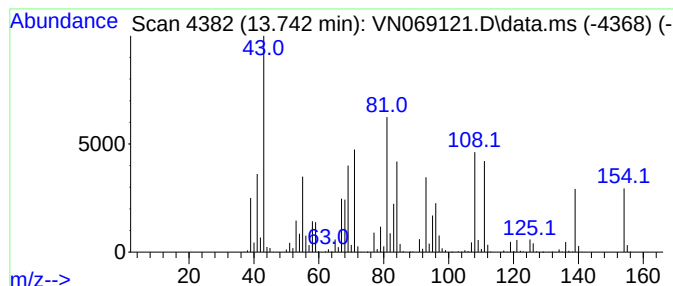
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 1 Eucalyptol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.742	423.08 ug/l	13781000	1,4-Dichlorobenzene-d4	13.678

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	64
3			2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	35
4			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	25
5			2-Acetylcyclohexanone	154	C9H14O2	006126-53-0	22



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Instrument :
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ClientSampleId :
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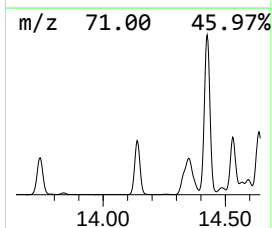
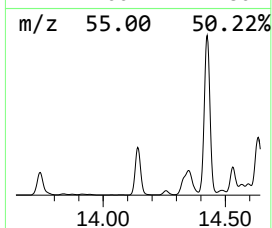
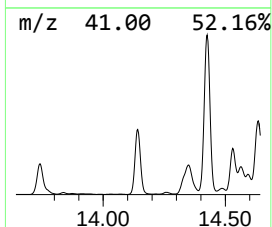
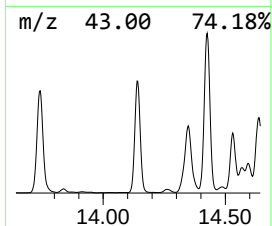
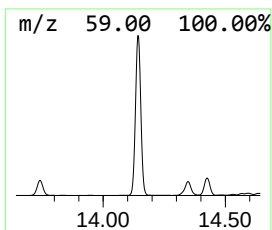
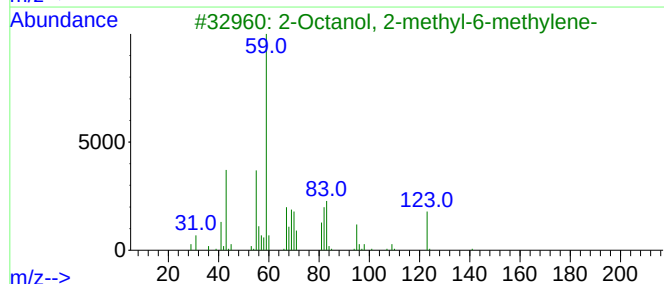
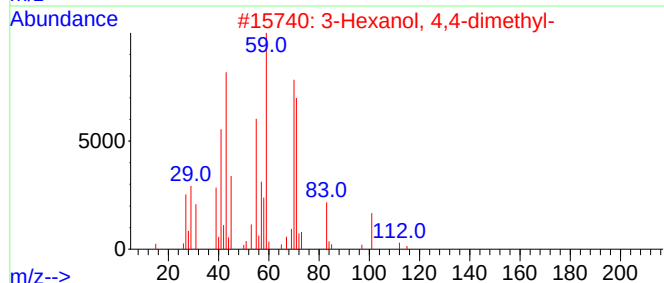
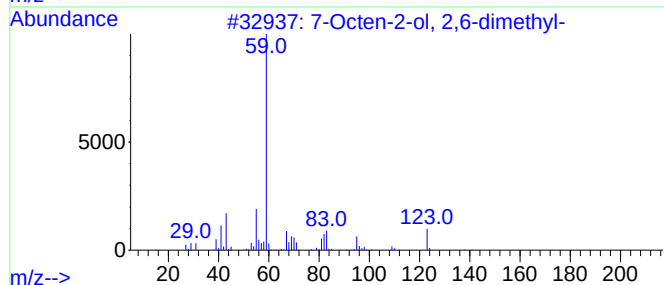
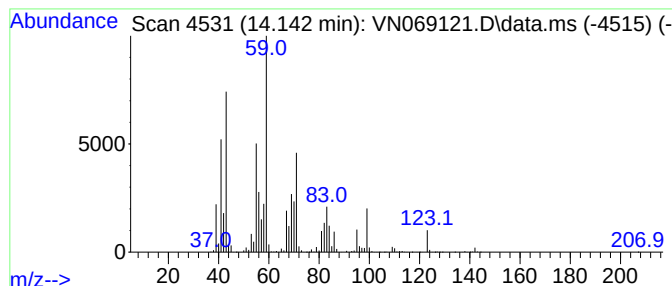
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown14.142 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.142	427.57 ug/l	13927000	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	43
2			3-Hexanol, 4,4-dimethyl-	130	C8H18O	019550-09-5	38
3			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	27
4			7-Oxabicyclo[4.1.0]heptane, 1,5-...	126	C8H14O	162239-52-3	27
5			Oxirane, tetramethyl-	100	C6H12O	005076-20-0	22



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Instrument :
MSVOA_N
ClientSampleId :
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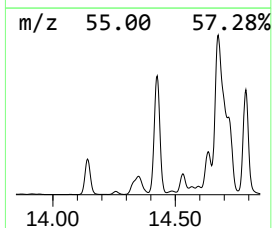
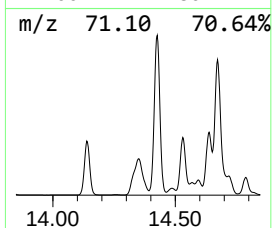
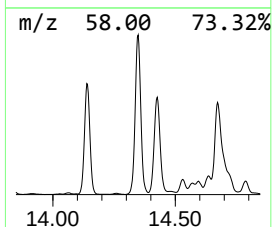
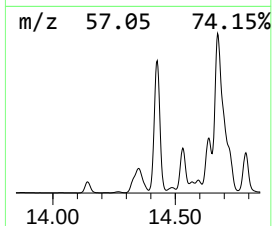
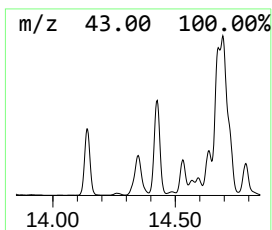
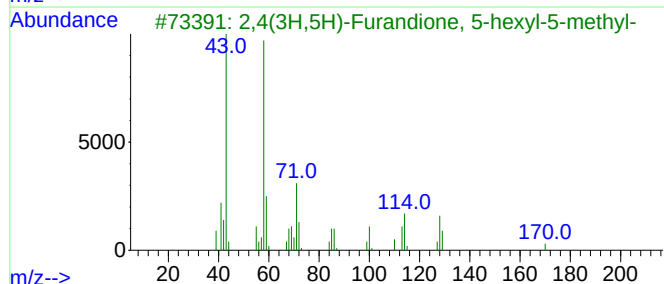
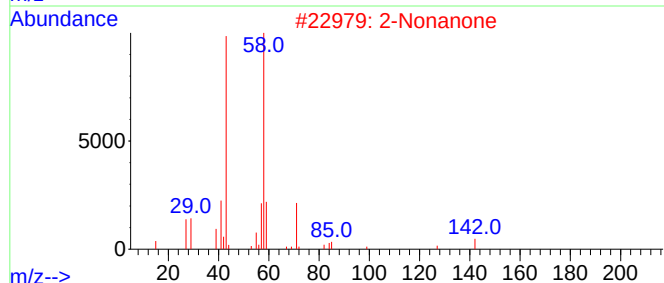
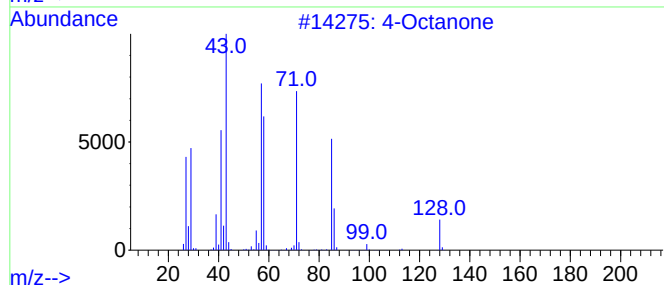
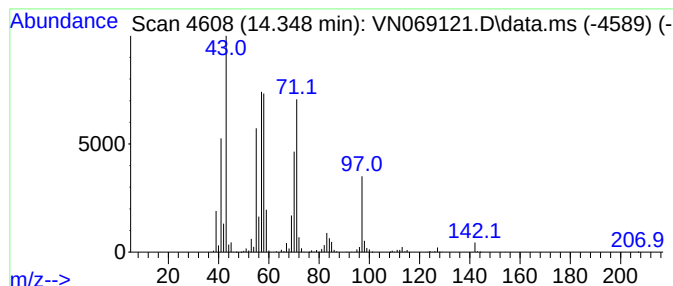
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown14.348 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.348	297.56 ug/l	9692370	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Octanone	128	C8H16O	000589-63-9	47
2			2-Nonanone	142	C9H18O	000821-55-6	46
3			2,4(3H,5H)-Furandione, 5-hexyl-5...	198	C11H18O3	054852-79-8	35
4			Heptane, 3,3-dimethyl-	128	C9H20	004032-86-4	27
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	25



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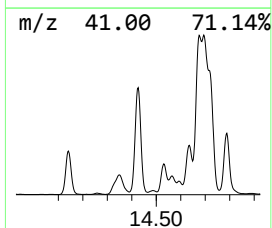
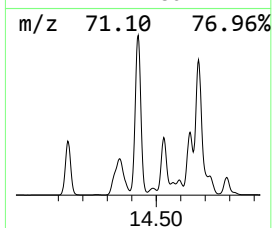
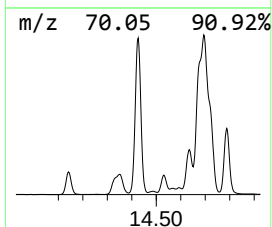
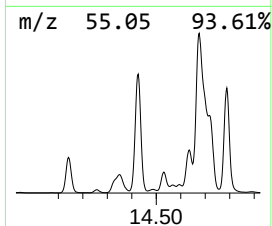
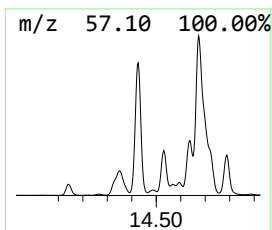
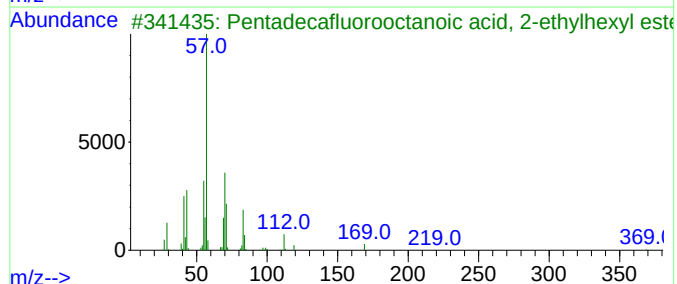
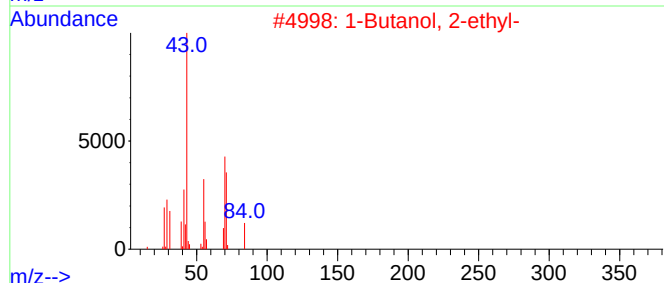
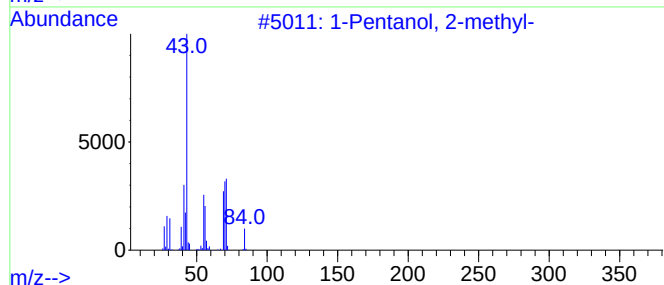
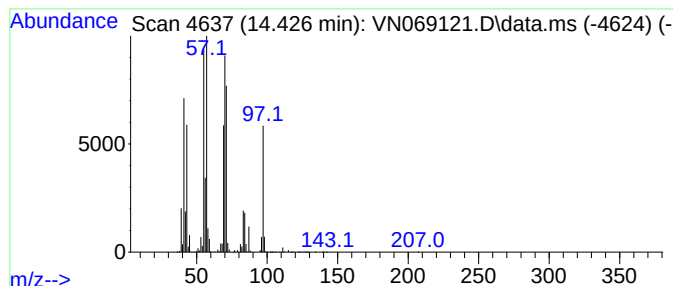
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Pentanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.426	925.95 ug/l	30160900	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 2-methyl-			102	C6H14O	000105-30-6	50
2	1-Butanol, 2-ethyl-			102	C6H14O	000097-95-0	47
3	Pentadecafluorooctanoic acid, 2-...			526	C16H17F15O2	1000406-80-9	43
4	Octane, 1,1'-oxybis-			242	C16H34O	000629-82-3	43
5	5-Ethyl-1-nonene			154	C11H22	019780-74-6	43



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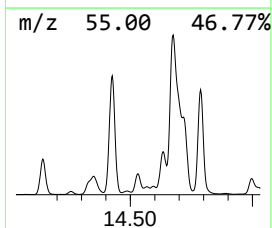
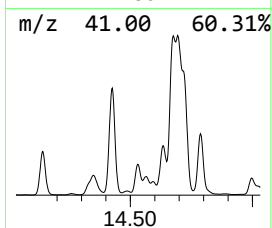
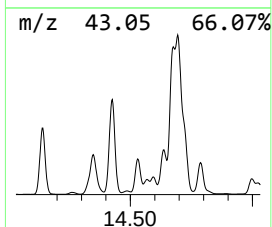
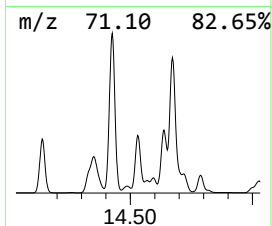
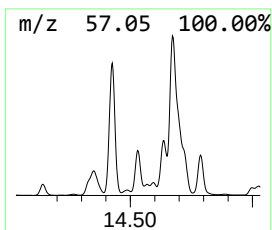
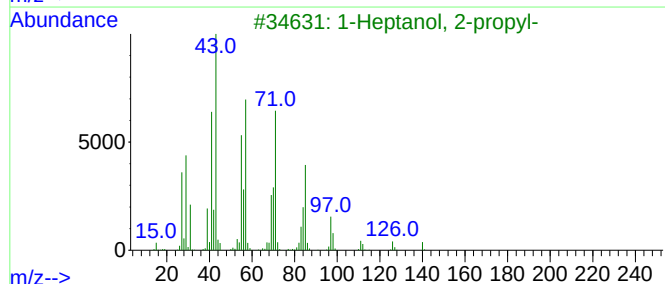
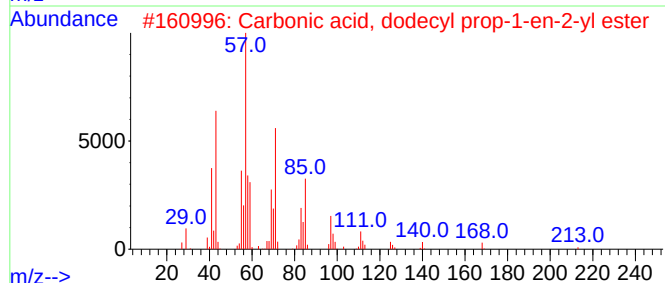
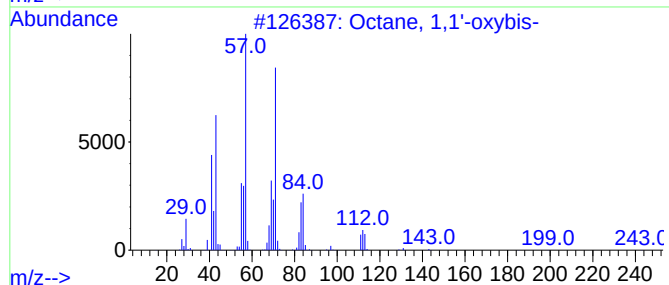
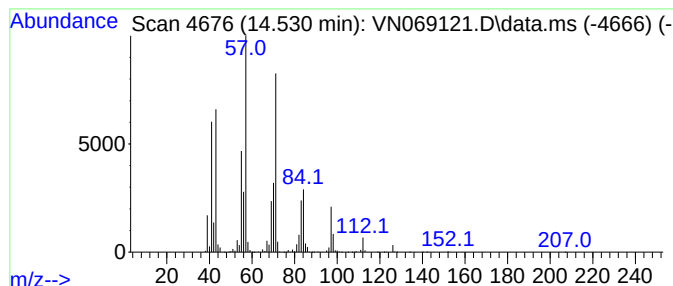
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 5 Octane, 1,1'-oxybis- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.531	216.86 ug/l	7063640	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	72
2			Carbonic acid, dodecyl prop-1-en-2-yl ester	270	C16H30O3	1000382-90-7	72
3			1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	53
4			Tetradecane	198	C14H30	000629-59-4	50
5			Octane, 3-ethyl-	142	C10H22	005881-17-4	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
Data File : VN069121.D
Acq On : 22 Oct 2021 5:52
Operator : JC/MD
Sample : M4284-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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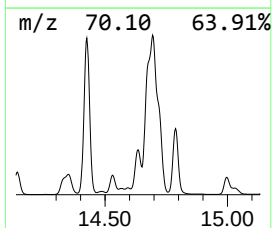
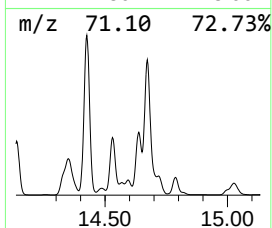
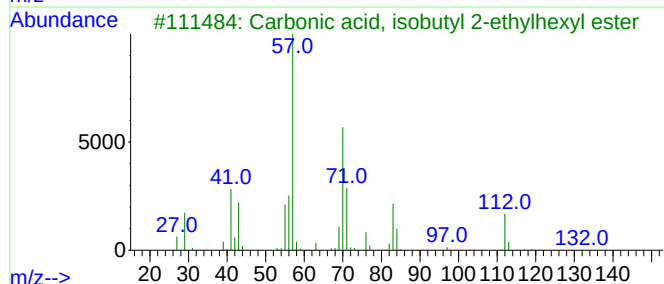
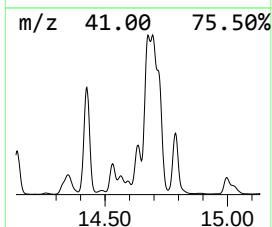
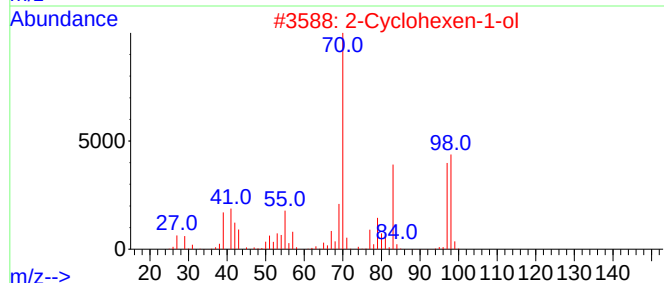
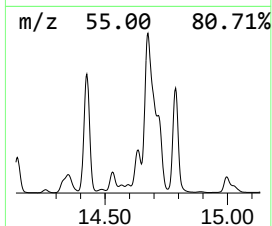
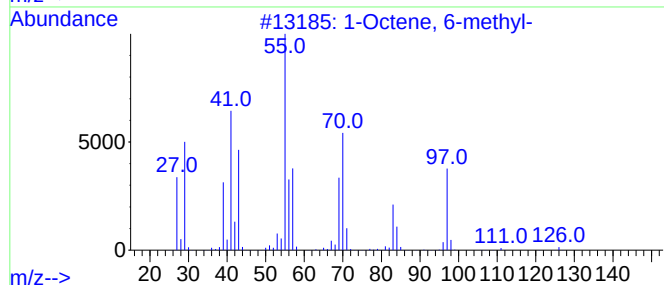
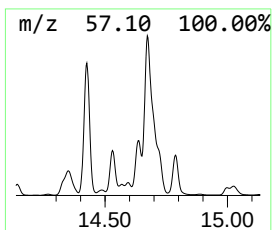
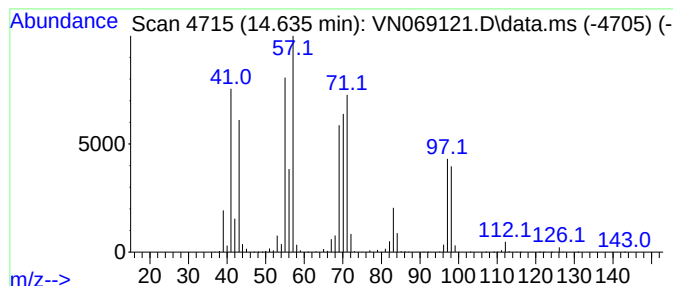
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Quant Title : SW846 8260

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

Peak Number 6 1-Octene, 6-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.635	282.89 ug/l	9214430	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octene, 6-methyl-			126	C9H18	013151-10-5	64
2	2-Cyclohexen-1-ol			98	C6H10O	000822-67-3	38
3	Carbonic acid, isobutyl 2-ethylh...			230	C13H26O3	1000383-13-3	35
4	4-Methyl-2-hexene,c&t			98	C7H14	003404-55-5	35
5	2-Hexene, 4-methyl-, (E)-			98	C7H14	003683-22-5	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
Data File : VN069121.D
Acq On : 22 Oct 2021 5:52
Operator : JC/MD
Sample : M4284-08
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ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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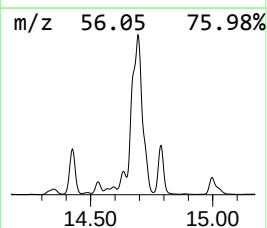
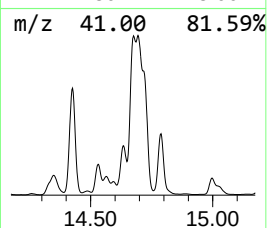
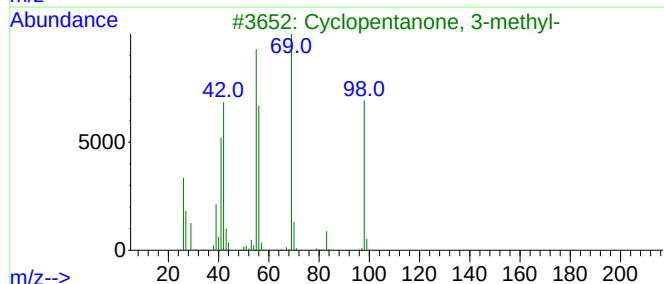
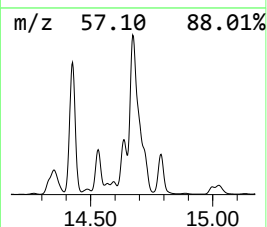
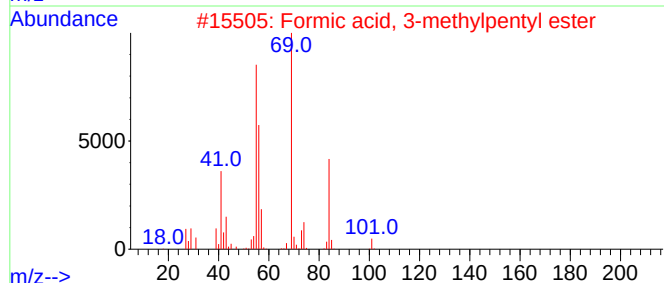
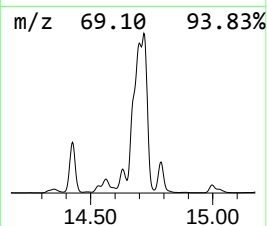
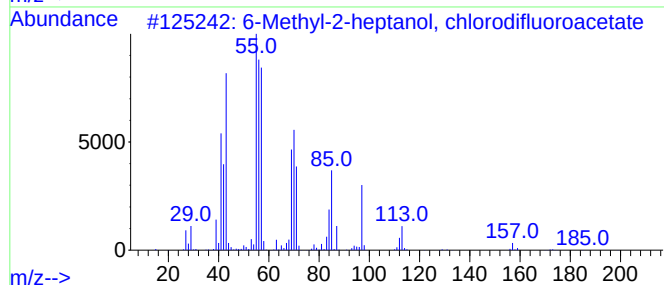
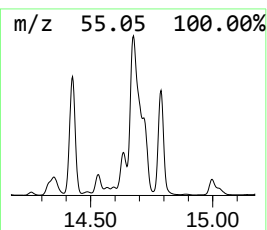
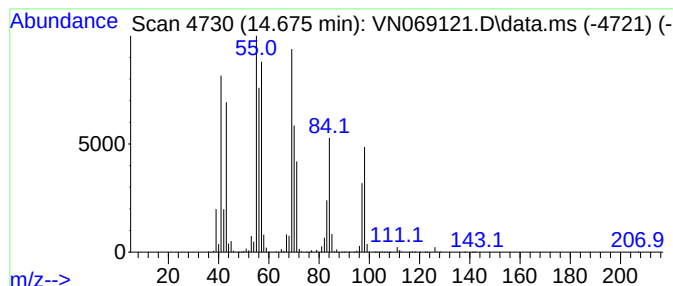
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.675 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.675	1036.79 ug/l	33771200	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Methyl-2-heptanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-5	47
2			Formic acid, 3-methylpentyl ester	130	C7H14O2	1000368-21-3	47
3			Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	47
4			Cycloheptane	98	C7H14	000291-64-5	43
5			2-Heptene	98	C7H14	000592-77-8	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
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Acq On : 22 Oct 2021 5:52
Operator : JC/MD
Sample : M4284-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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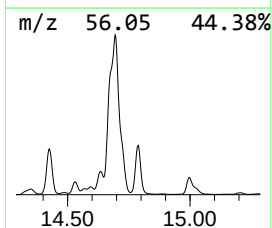
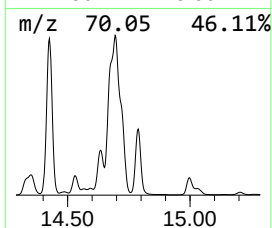
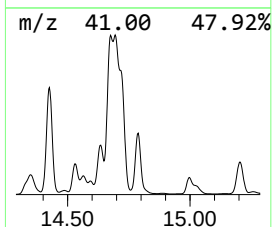
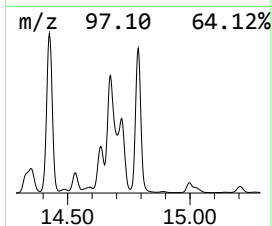
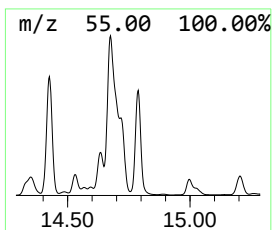
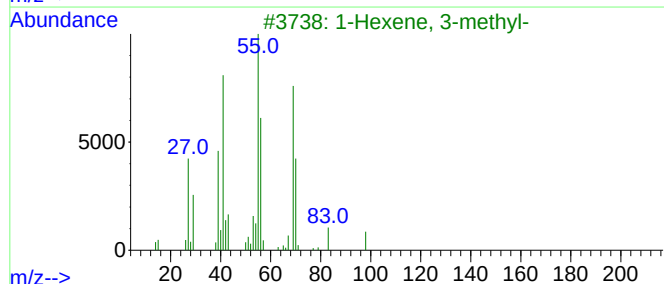
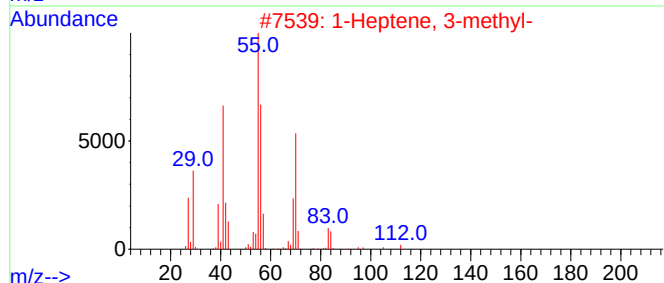
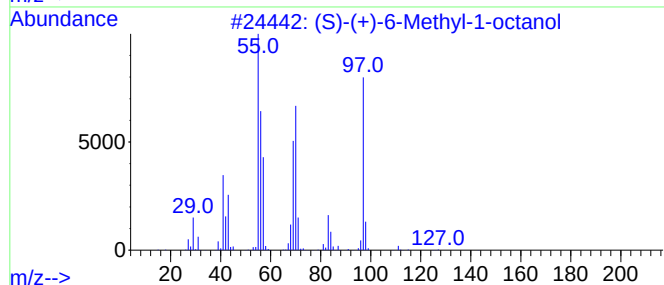
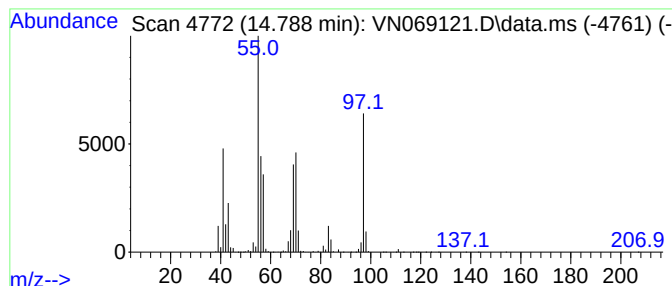
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Quant Title : SW846 8260

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

Peak Number 8 (S)-(+)-6-Methyl-1-octanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.788	522.57 ug/l	17021600	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	91		
2	1-Heptene, 3-methyl-	112	C8H16	004810-09-7	50		
3	1-Hexene, 3-methyl-	98	C7H14	003404-61-3	43		
4	Cyclopentane, (1-methylbutyl)-	140	C10H20	004737-43-3	42		
5	6-Methyloctyl acetate	186	C11H22O2	1000439-66-5	40		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
Data File : VN069121.D
Acq On : 22 Oct 2021 5:52
Operator : JC/MD
Sample : M4284-08
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ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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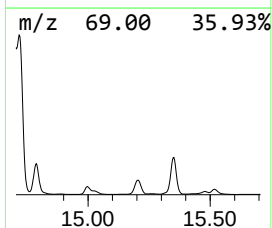
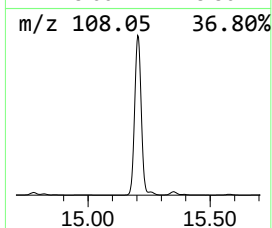
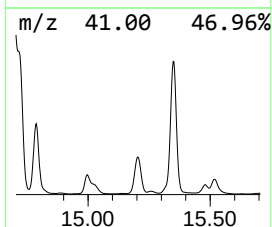
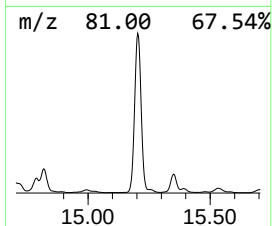
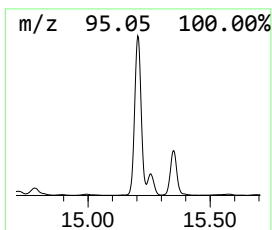
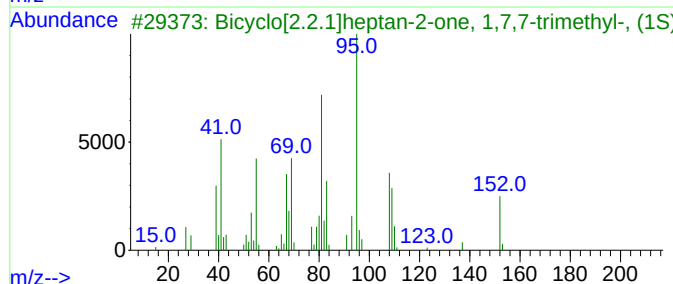
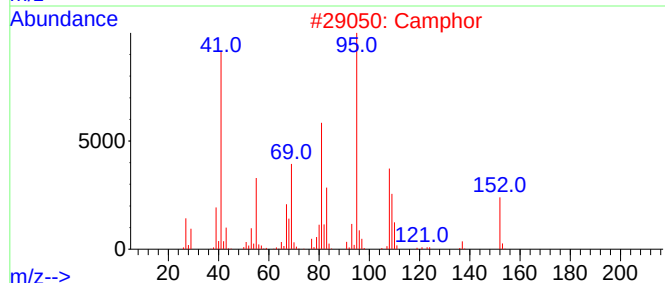
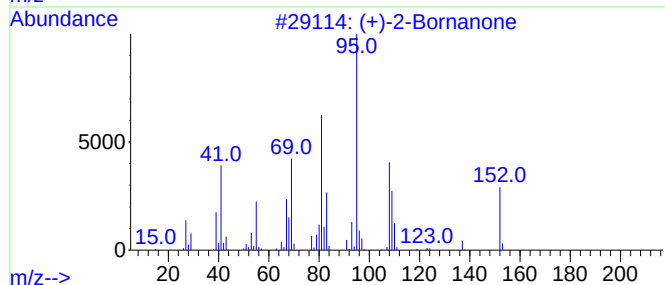
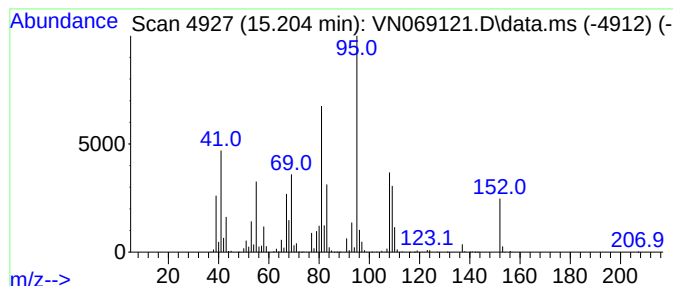
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Quant Title : SW846 8260

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

Peak Number 9 (+)-2-Bornanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	404.46 ug/l	13174500	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2			Camphor	152	C10H16O	000076-22-2	98
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
4			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5			1-Adamantanol	152	C10H16O	000768-95-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
Data File : VN069121.D
Acq On : 22 Oct 2021 5:52
Operator : JC/MD
Sample : M4284-08
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ALS Vial : 47 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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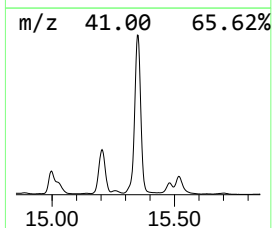
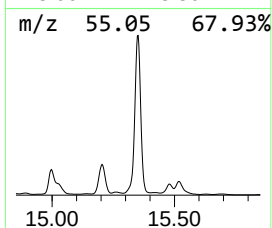
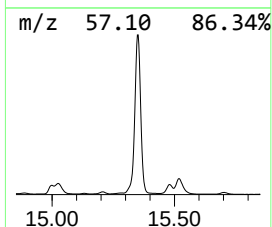
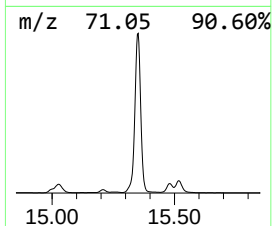
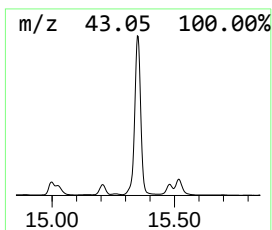
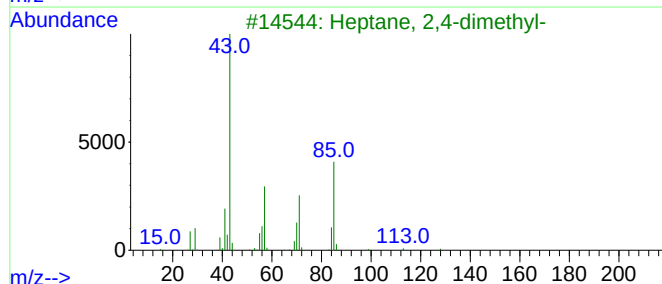
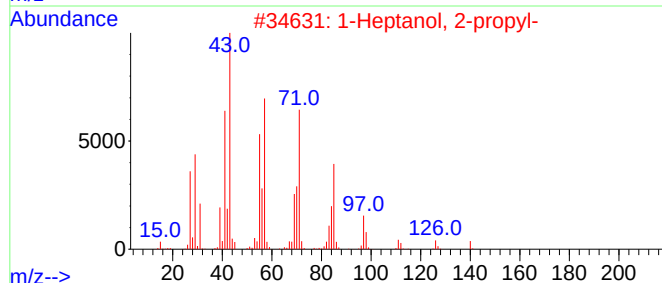
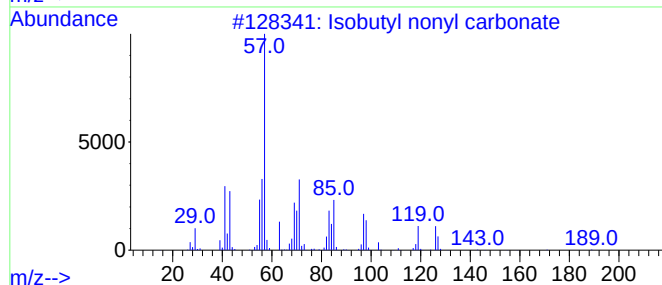
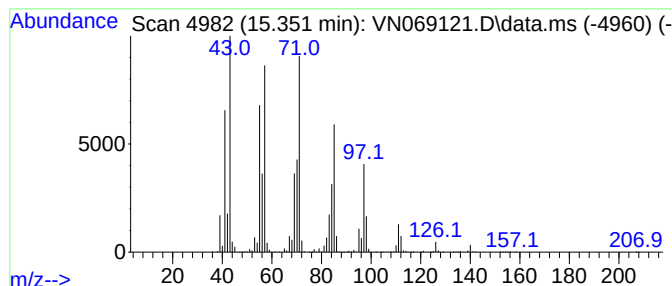
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Quant Title : SW846 8260

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

Peak Number 10 Isobutyl nonyl carbonate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	1239.55 ug/l	40375600	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl nonyl carbonate	244	C14H28O3	959311-27-4	86
2			1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	72
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	58
4			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	38
5			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102121\
Data File : VN069121.D
Acq On : 22 Oct 2021 5:52
Operator : JC/MD
Sample : M4284-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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					#	RT	Resp	Conc
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unknown14.142	14.142	427.6	ug/l	13927000	4	13.678	1628640	50.0
unknown14.348	14.348	297.6	ug/l	9692370	4	13.678	1628640	50.0
1-Pentanol, 2-m...	14.426	926.0	ug/l	30160900	4	13.678	1628640	50.0
Octane, 1,1'-ox...	14.531	216.9	ug/l	7063640	4	13.678	1628640	50.0
1-Octene, 6-met...	14.635	282.9	ug/l	9214430	4	13.678	1628640	50.0
unknown14.675	14.675	1036.8	ug/l	33771200	4	13.678	1628640	50.0
(S)-(+)-6-Methy...	14.788	522.6	ug/l	17021600	4	13.678	1628640	50.0
(+)-2-Bornanone	15.204	404.5	ug/l	13174500	4	13.678	1628640	50.0
Isobutyl nonyl ...	15.351	1239.6	ug/l	40375600	4	13.678	1628640	50.0