

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102621\
 Data File : VN069168.D
 Acq On : 25 Oct 2021 22:21
 Operator : JC/MD
 Sample : M4284-08
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 17 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: VN069168.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.285	830	856	935	rBV	4387085	12969704	32.28%	5.534%
2	4.572	939	963	1031	rVB	891461	2842625	7.08%	1.213%
3	7.335	1963	1993	2037	rBV	510147	1400896	3.49%	0.598%
4	8.024	2228	2250	2261	rBV	263601	616390	1.53%	0.263%
5	8.088	2262	2274	2298	rVB	489869	1122339	2.79%	0.479%
6	8.440	2380	2405	2430	rBV	285004	668966	1.67%	0.285%
7	8.971	2581	2603	2629	rBV	726482	1506923	3.75%	0.643%
8	10.443	3126	3152	3171	rBV	1167268	2166676	5.39%	0.924%
9	11.087	3376	3392	3418	rBV	306667	531869	1.32%	0.227%
10	11.747	3614	3638	3657	rBV	1119918	2028452	5.05%	0.866%
11	12.353	3850	3864	3876	rBV	319582	520669	1.30%	0.222%
12	12.420	3876	3889	3909	rVV	544451	875685	2.18%	0.374%
13	12.554	3925	3939	3958	rBV	373184	594981	1.48%	0.254%
14	12.734	3982	4006	4026	rBV	924437	1623573	4.04%	0.693%
15	12.838	4029	4045	4055	rBV2	390430	730446	1.82%	0.312%
16	13.179	4156	4172	4194	rVB2	693982	1407267	3.50%	0.600%
17	13.412	4247	4259	4272	rBV	732713	1128884	2.81%	0.482%
18	13.495	4279	4290	4310	rVB2	433193	748687	1.86%	0.319%
19	13.619	4313	4336	4346	rBV	579467	1154422	2.87%	0.493%
20	13.675	4346	4357	4368	rVV	1088182	1786134	4.45%	0.762%
21	13.739	4368	4381	4408	rVB	8155705	14020580	34.90%	5.982%
22	14.142	4515	4531	4553	rBV2	8615115	13460119	33.50%	5.743%
23	14.257	4564	4574	4588	rBV4	287881	504681	1.26%	0.215%
24	14.348	4588	4608	4624	rBV2	3900336	9572480	23.83%	4.084%
25	14.423	4624	4636	4651	rVB	19185540	30310538	75.44%	12.933%
26	14.530	4666	4676	4683	rBV	4689003	7212888	17.95%	3.078%
27	14.635	4705	4715	4720	rBV3	6377123	9455887	23.54%	4.035%
28	14.675	4720	4730	4734	rBV	20710434	31026886	77.23%	13.239%
29	14.785	4761	4771	4800	rVB	9766747	16454685	40.96%	7.021%
30	14.997	4838	4850	4857	rBV2	2359689	4014635	9.99%	1.713%
31	15.204	4911	4927	4940	rBV2	7229759	13104311	32.62%	5.591%
32	15.257	4941	4947	4959	rVV2	582555	1001190	2.49%	0.427%
33	15.348	4960	4981	5015	rVV	23114953	40177050	100.00%	17.143%
34	15.480	5019	5030	5036	rVV	1483299	2589108	6.44%	1.105%
35	15.517	5037	5044	5078	rVB	2248905	4618374	11.50%	1.971%
36	15.885	5172	5181	5220	rVB3	196043	417817	1.04%	0.178%

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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

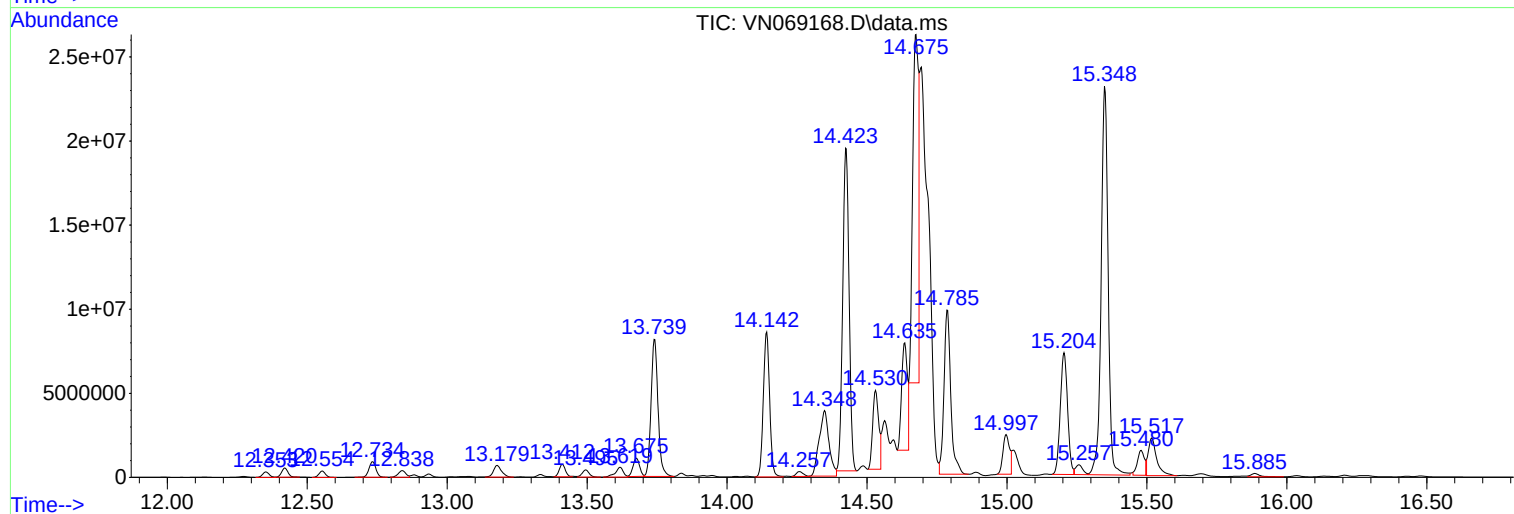
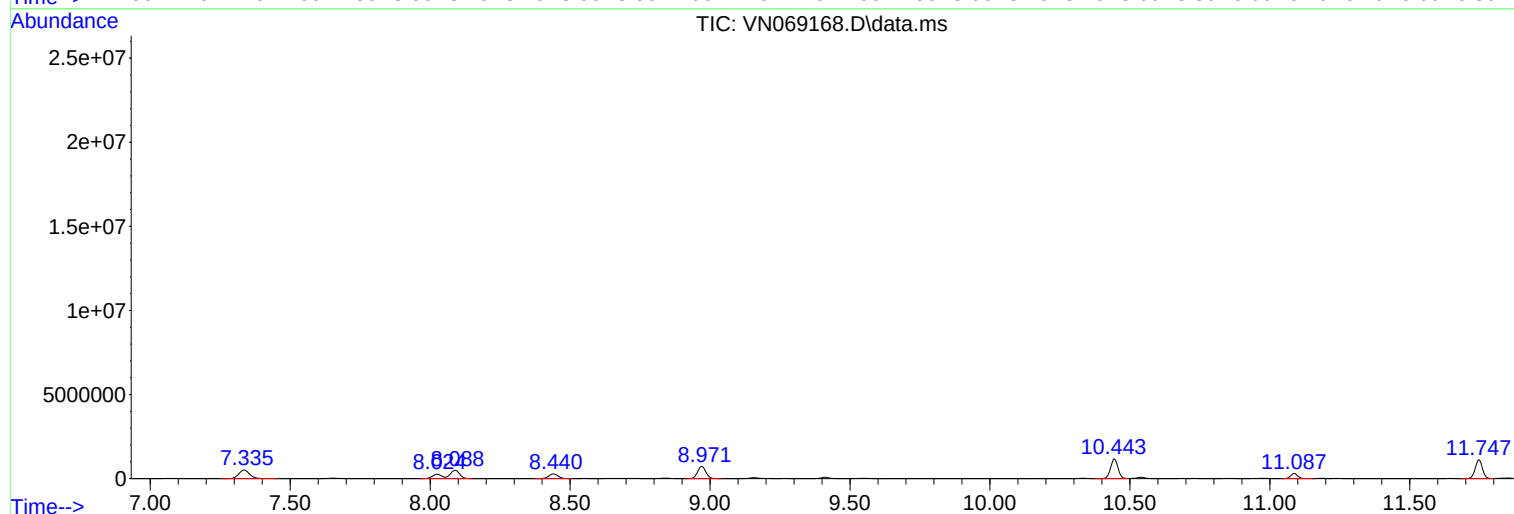
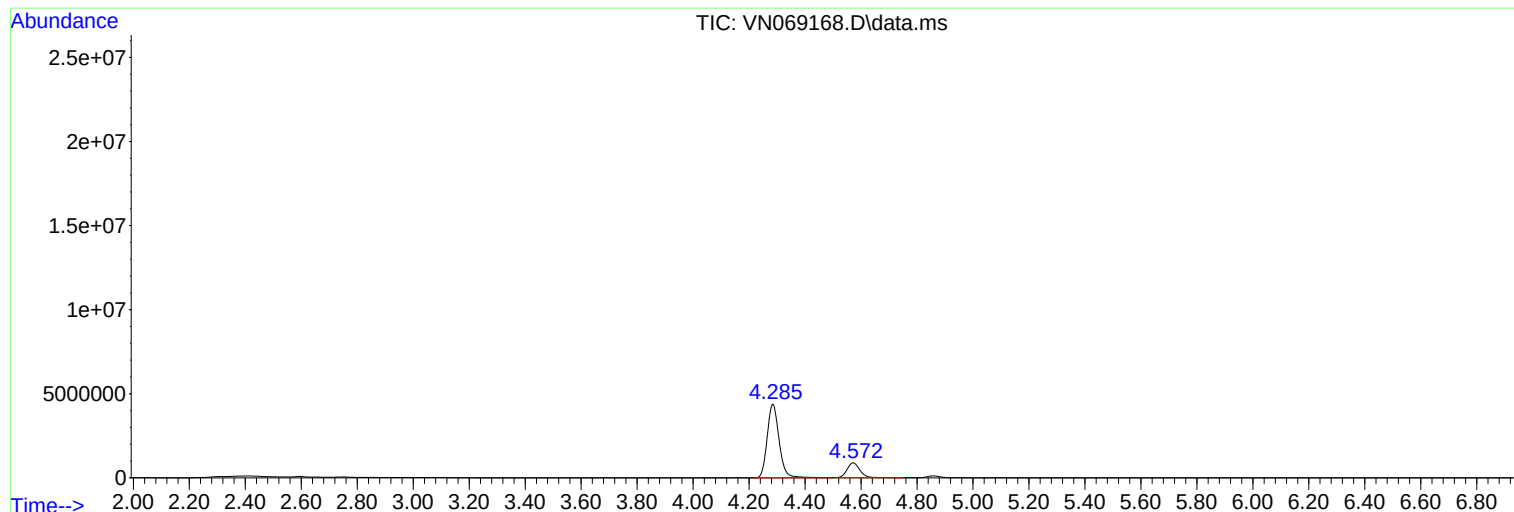
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
20877

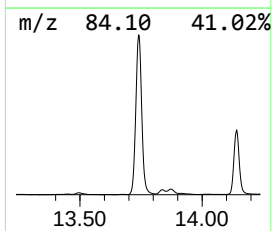
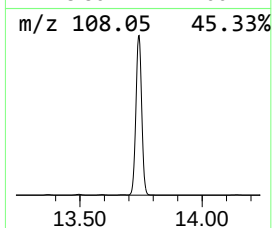
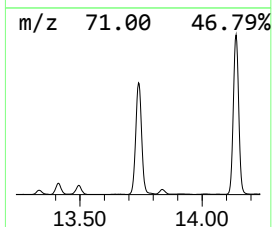
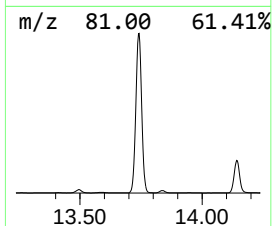
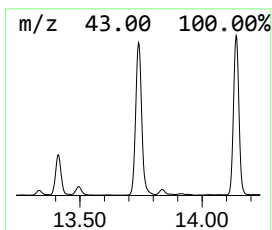
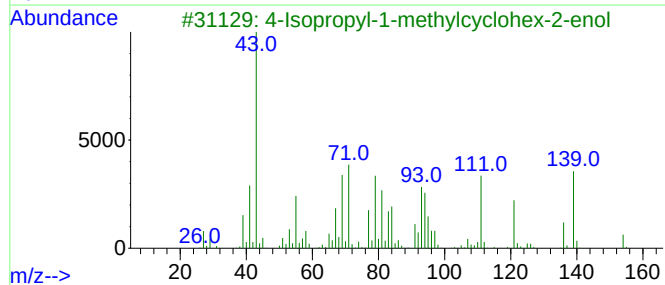
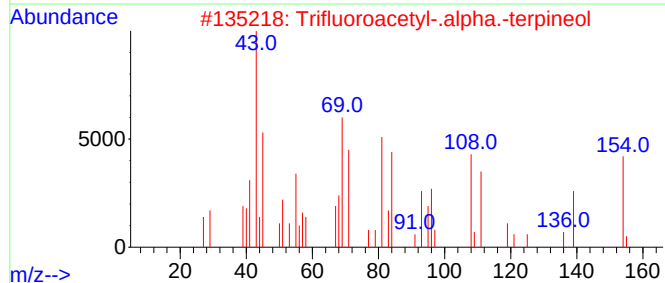
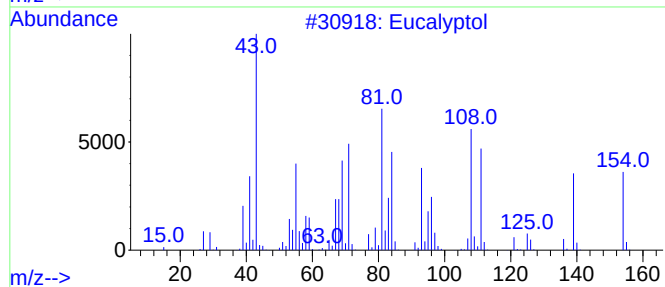
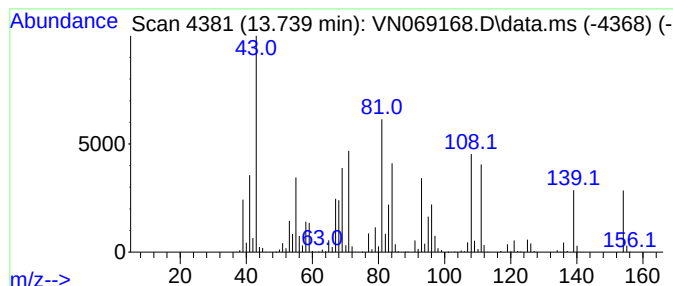
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 1 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	392.48 ug/l	14020600	1,4-Dichlorobenzene-d4	13.675

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	43
3		4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	32
4		2-(3'-Oxo-butyl)-cyclopentanone	154	C9H14O2	1010143-37-2	25
5		2-Acetyl cyclohexanone	154	C9H14O2	006126-53-0	22



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ALS Vial : 17 Sample Multiplier: 1

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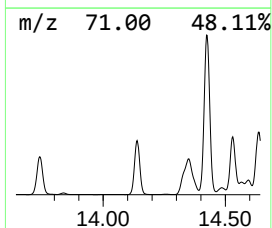
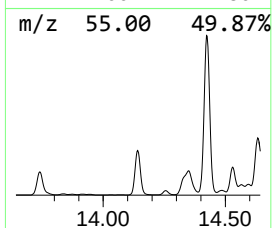
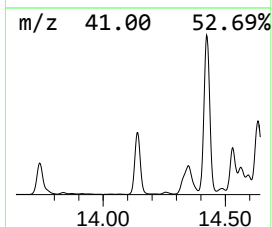
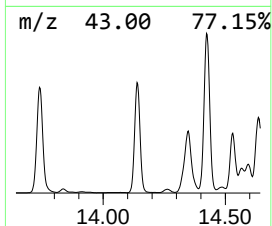
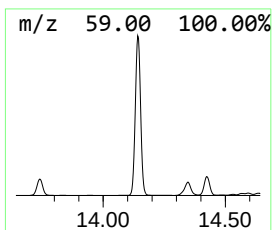
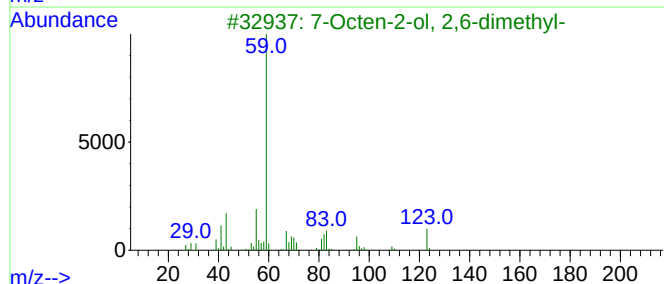
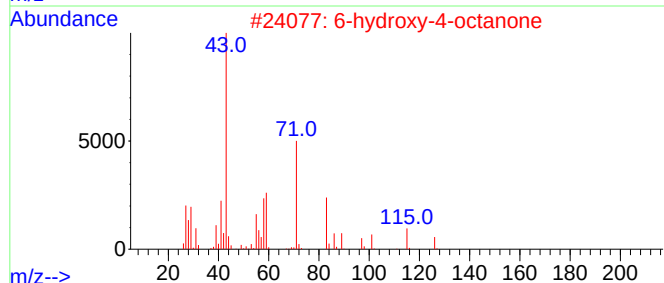
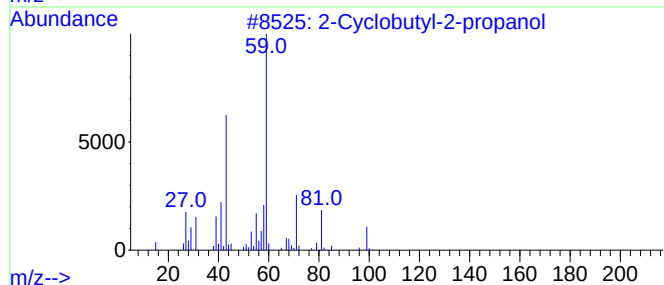
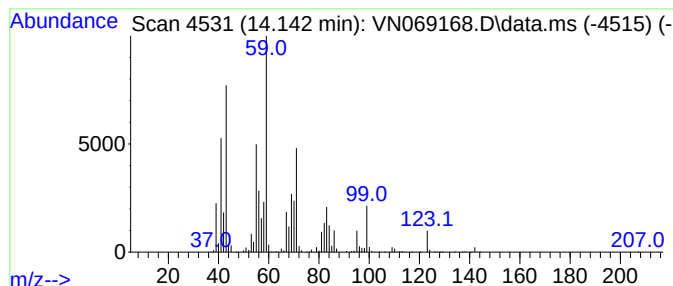
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown14.142 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.142	376.80 ug/l	13460100	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclobutyl-2-propanol	114	C7H14O	059383-67-4	37
2			6-hydroxy-4-octanone	144	C8H16O2	1000376-33-8	35
3			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	35
4			Formamide, N-formyl-N-methyl-	87	C3H5NO2	018197-25-6	27
5			N,N-Dimethylformamide-di-t-butyl...	203	C11H25NO2	036805-97-7	22



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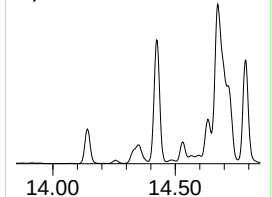
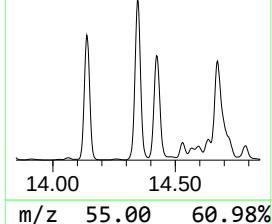
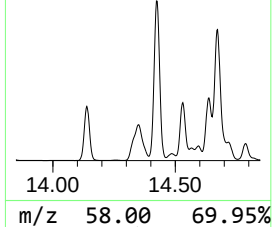
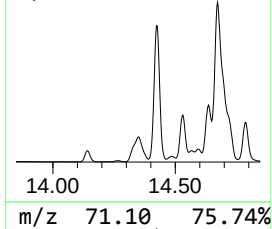
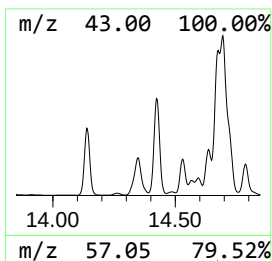
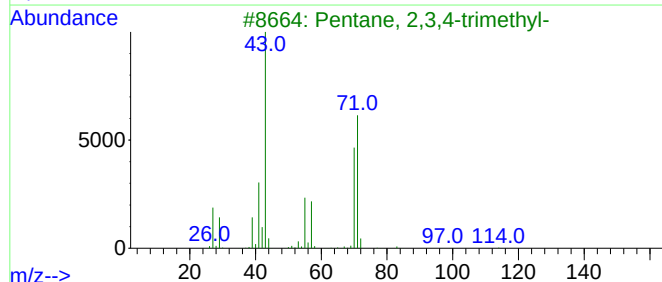
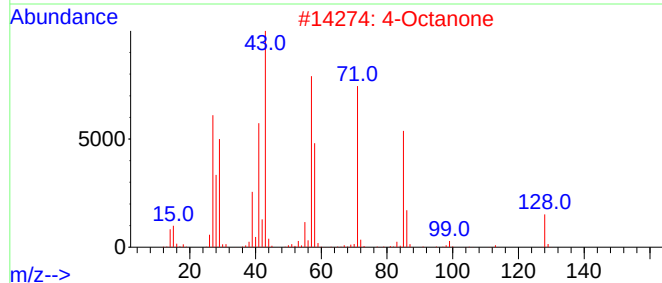
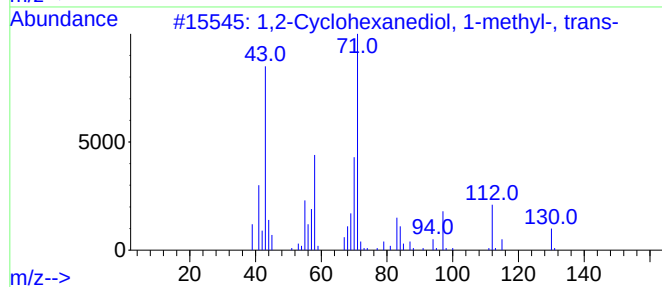
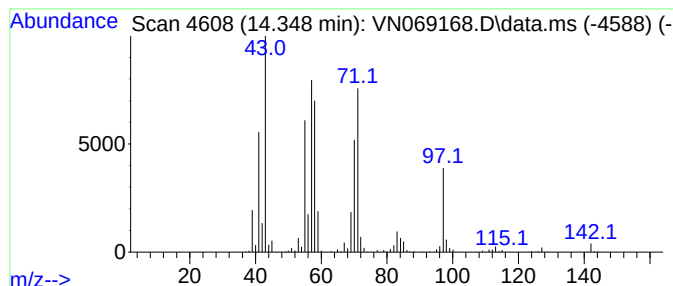
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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	267.97 ug/l	9572480	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Cyclohexanediol, 1-methyl-, ...	130	C7H14O2	019534-08-8	47
2			4-Octanone	128	C8H16O	000589-63-9	43
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	43
4			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	43
5			Heptane, 3,3-dimethyl-	128	C9H20	004032-86-4	43



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ALS Vial : 17 Sample Multiplier: 1

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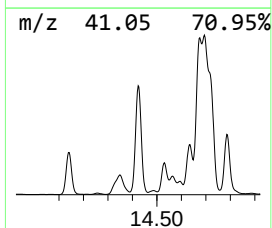
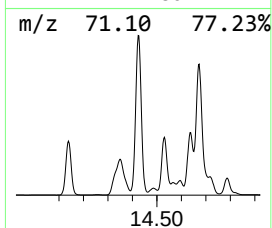
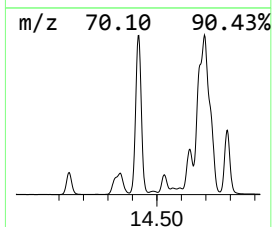
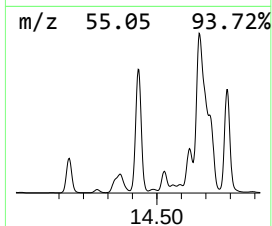
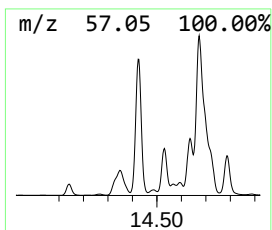
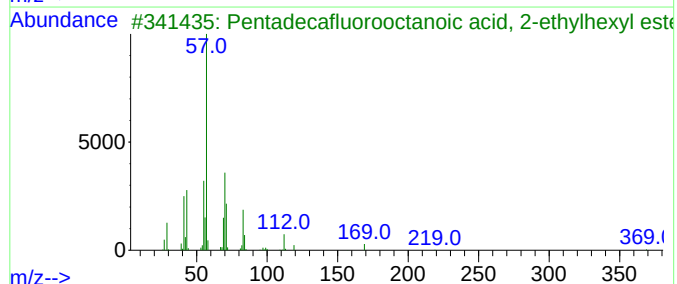
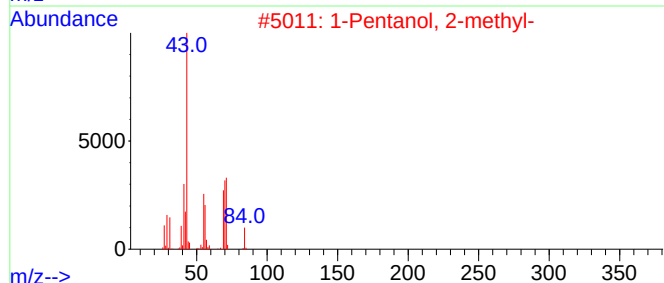
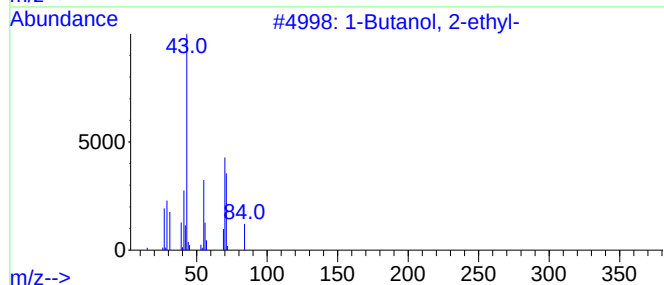
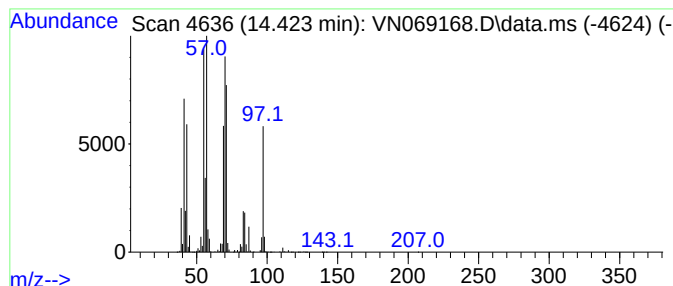
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Butanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.423	848.50 ug/l	30310500	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	50
2			1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	50
3			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	47
4			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	43
5			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	43



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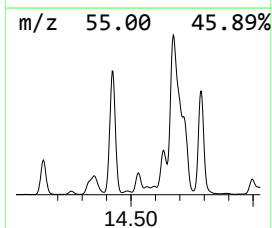
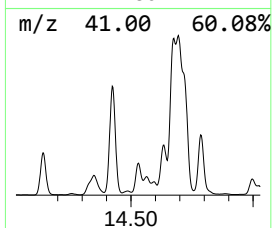
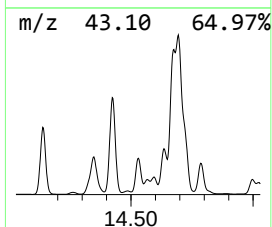
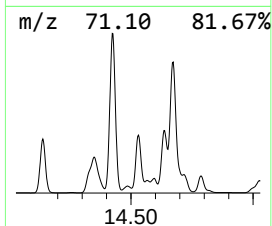
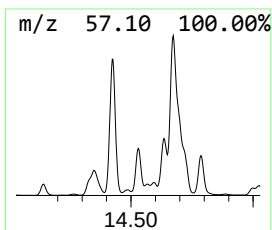
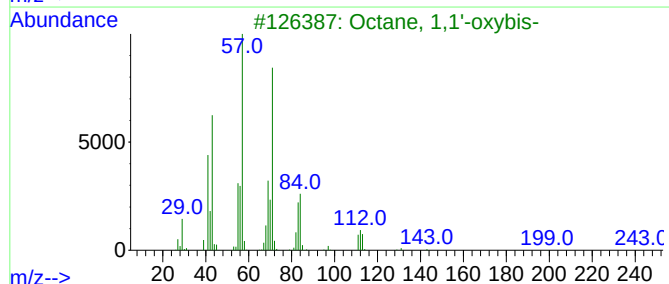
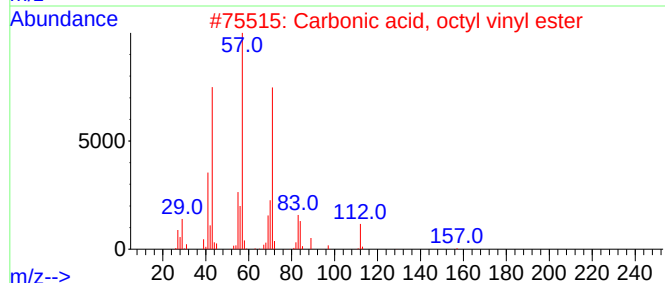
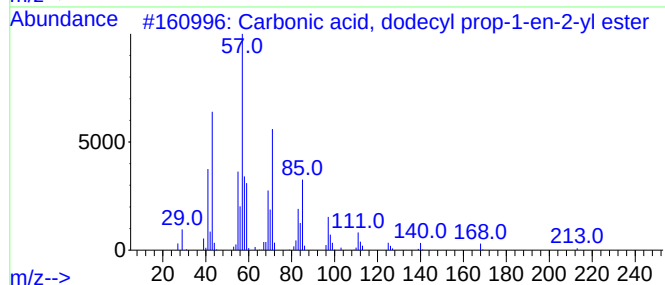
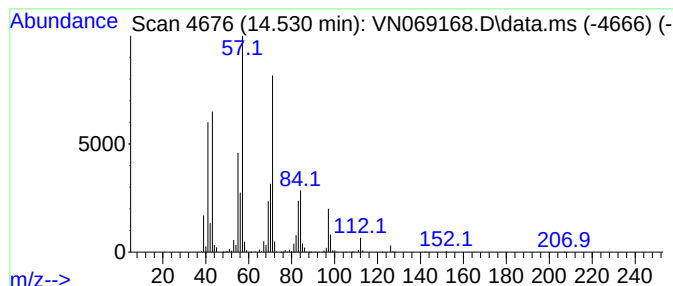
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 5 Carbonic acid, dodecyl prop... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.530	201.91 ug/l	7212890	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, dodecyl prop-1-en...	270	C16H30O3	1000382-90-7	72
2			Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	72
3			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	72
4			1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	53
5			Tetradecane	198	C14H30	000629-59-4	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102621\
Data File : VN069168.D
Acq On : 25 Oct 2021 22:21
Operator : JC/MD
Sample : M4284-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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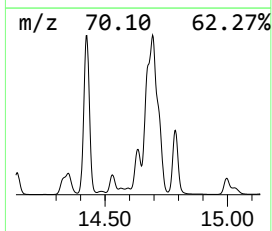
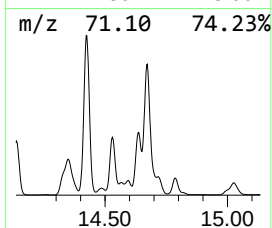
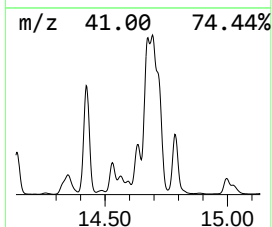
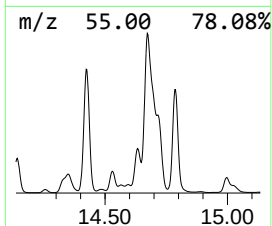
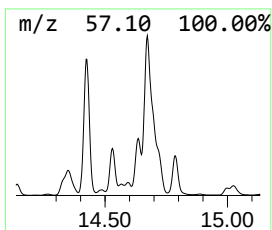
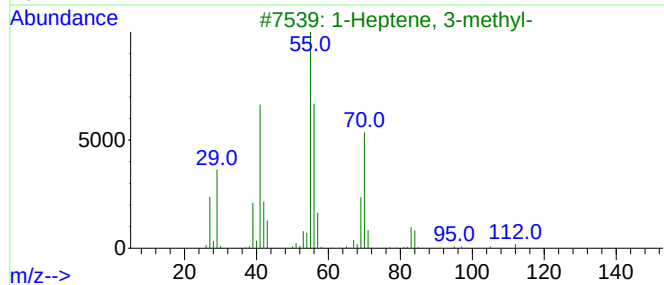
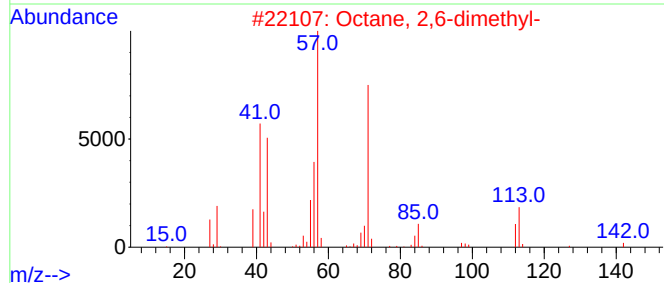
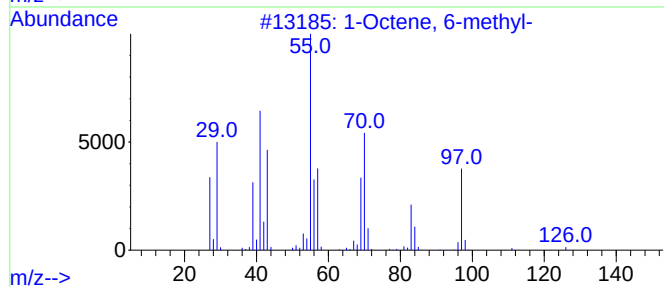
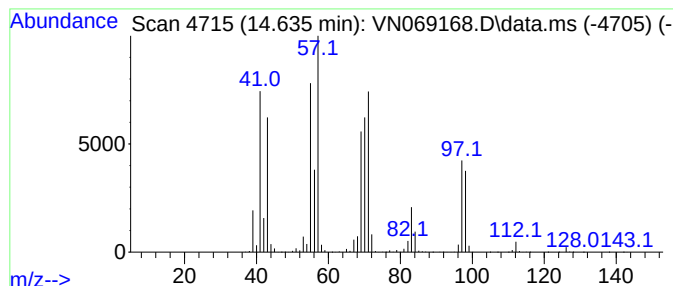
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Quant Title : SW846 8260

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	264.70 ug/l	9455890	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octene, 6-methyl-			126	C9H18	013151-10-5	53
2	Octane, 2,6-dimethyl-			142	C10H22	002051-30-1	43
3	1-Heptene, 3-methyl-			112	C8H16	004810-09-7	38
4	Butane, 2,2-dimethyl-			86	C6H14	000075-83-2	38
5	Carbonic acid, isobutyl 2-ethylh...			230	C13H26O3	1000383-13-3	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102621\
Data File : VN069168.D
Acq On : 25 Oct 2021 22:21
Operator : JC/MD
Sample : M4284-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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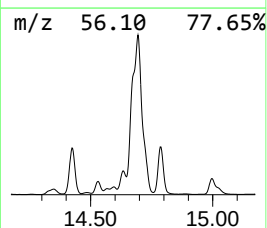
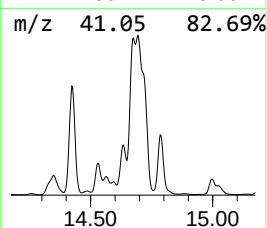
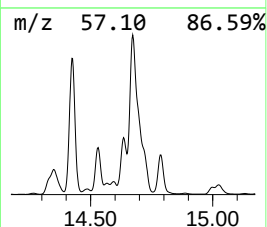
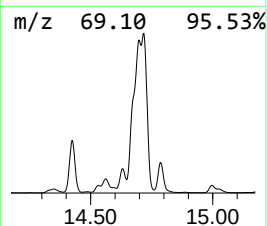
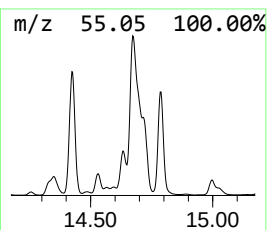
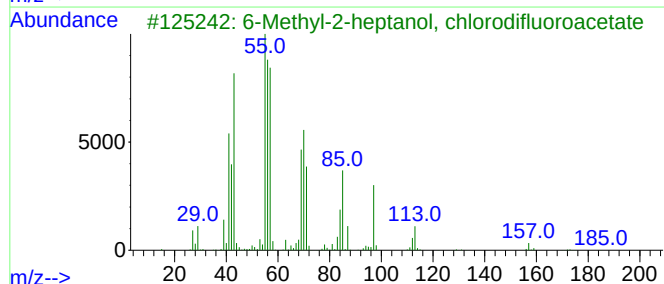
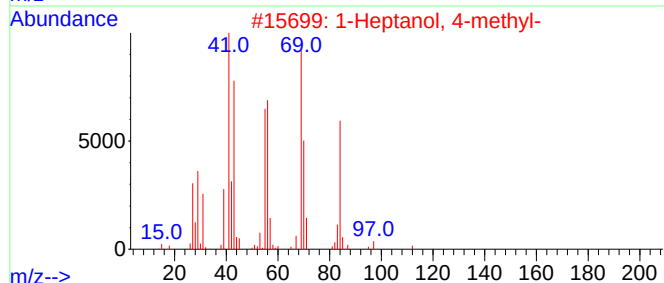
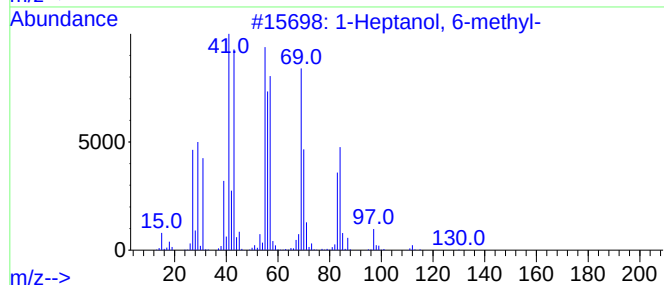
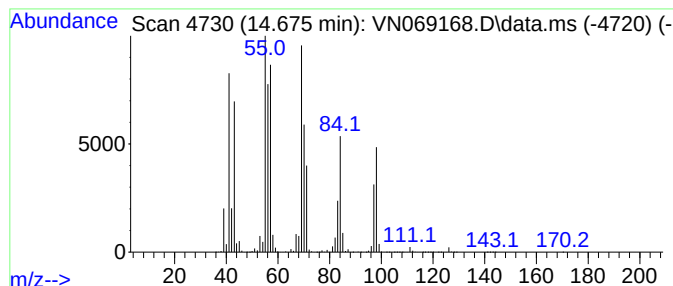
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Quant Title : SW846 8260

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

Peak Number 7 1-Heptanol, 6-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.675	868.55 ug/l	31026900	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	53
2			1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	50
3			6-Methyl-2-heptanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-5	47
4			Cycloheptane	98	C7H14	000291-64-5	43
5			3-Heptene, (E)-	98	C7H14	014686-14-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102621\
Data File : VN069168.D
Acq On : 25 Oct 2021 22:21
Operator : JC/MD
Sample : M4284-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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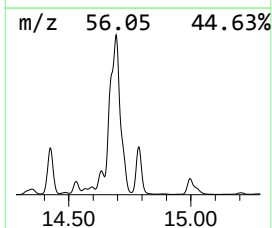
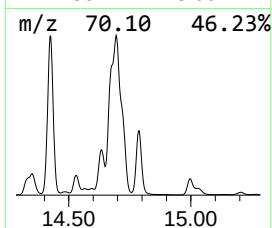
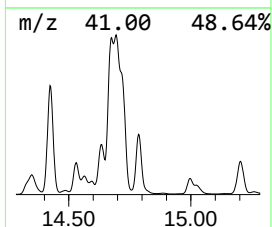
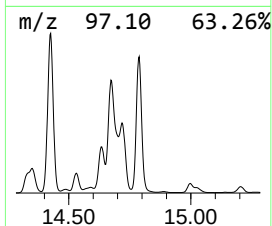
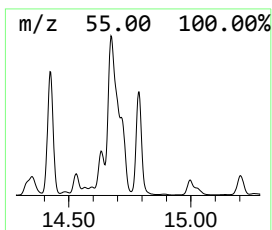
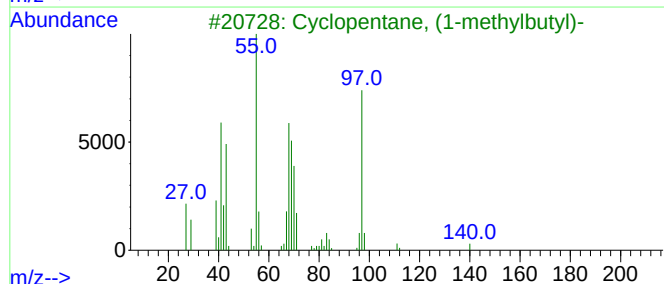
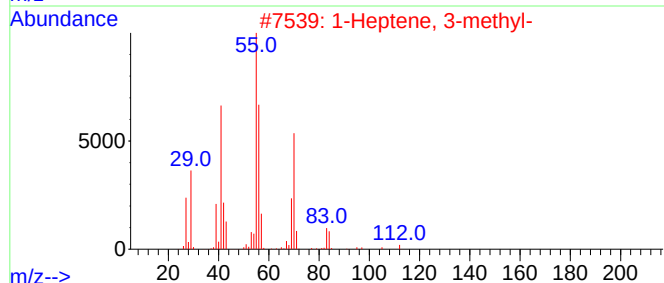
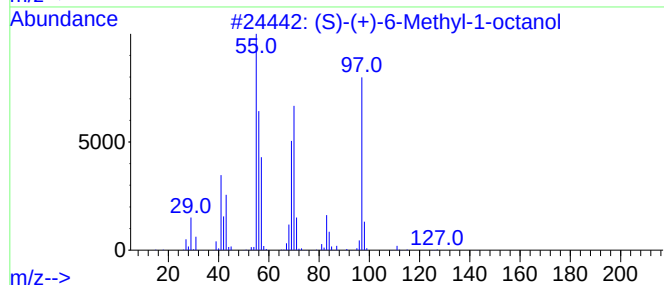
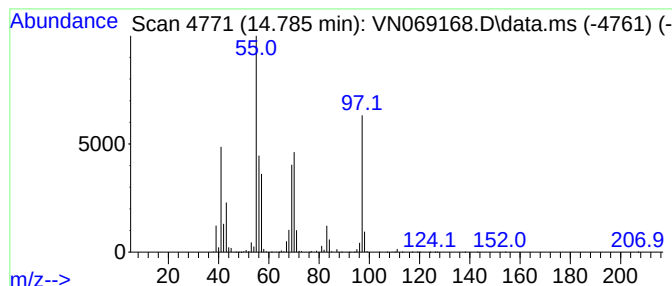
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Quant Title : SW846 8260

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.
14.785	460.62 ug/l	16454700	1,4-Dichlorobenzene-d4	13.675

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	Cyclopentane, (1-methylbutyl)-	140	C10H20	004737-43-3	42		
4	Cyclopentane, 1,2-dimethyl-3-(1-...	140	C10H20	000489-20-3	40		
5	6-Methyloctyl acetate	186	C11H22O2	1000439-66-5	40		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102621\
Data File : VN069168.D
Acq On : 25 Oct 2021 22:21
Operator : JC/MD
Sample : M4284-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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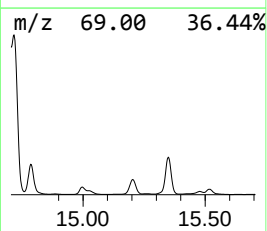
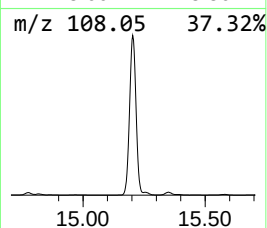
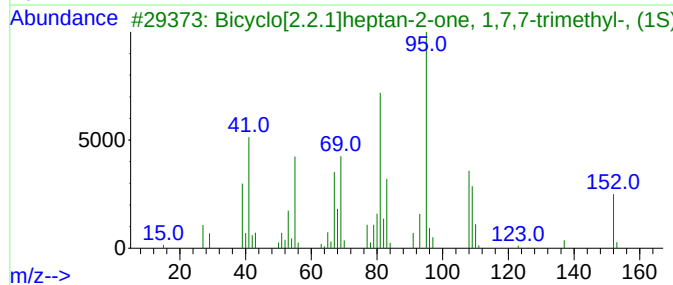
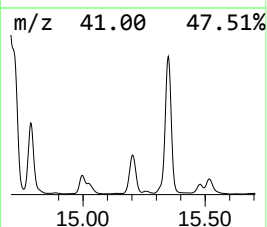
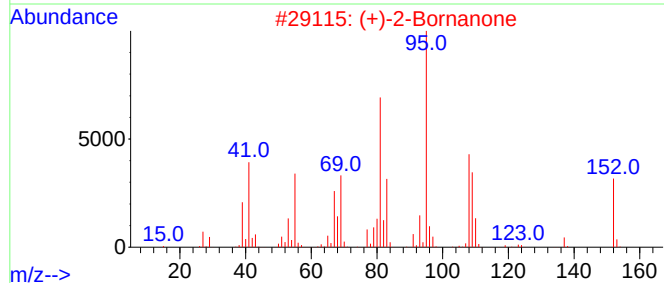
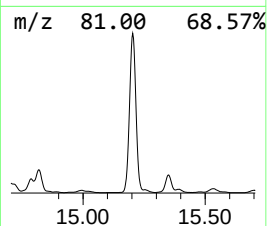
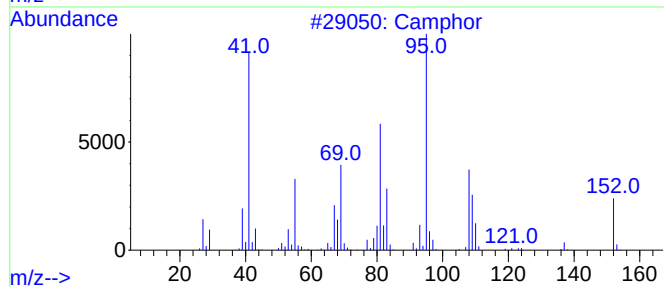
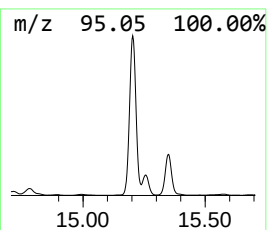
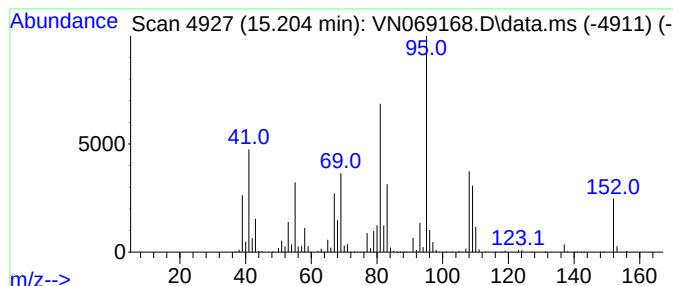
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Quant Title : SW846 8260

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

Peak Number 9 Camphor Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	366.83 ug/l	13104300	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphor	152	C10H16O	000076-22-2	98
2			(+)-2-Bornanone	152	C10H16O	000464-49-3	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			Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102621\
Data File : VN069168.D
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Operator : JC/MD
Sample : M4284-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

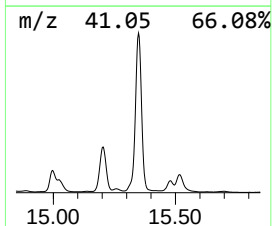
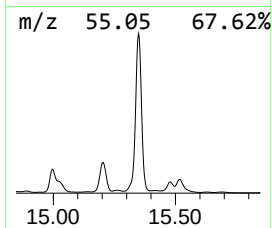
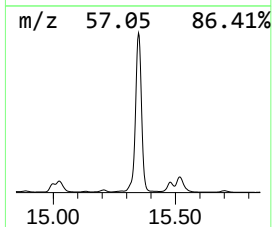
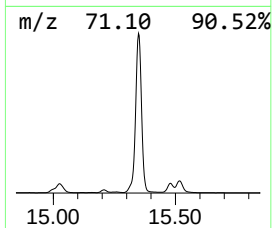
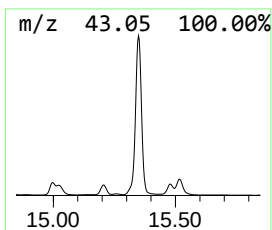
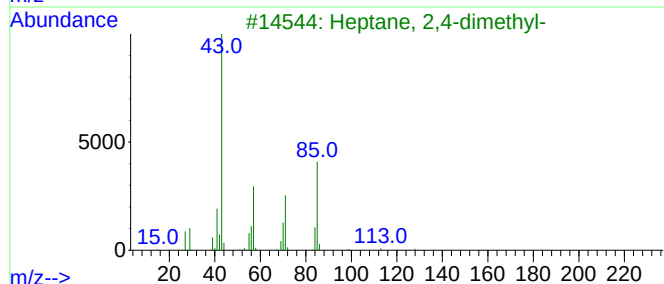
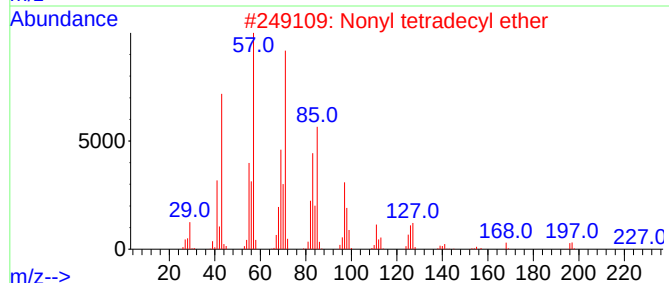
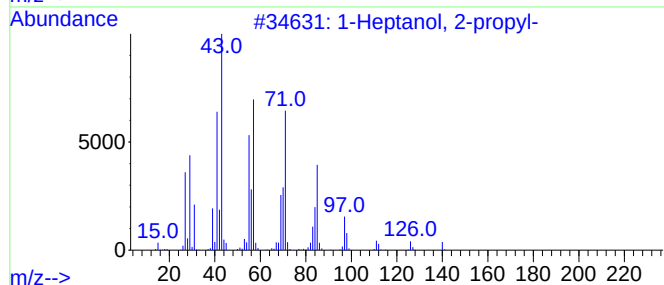
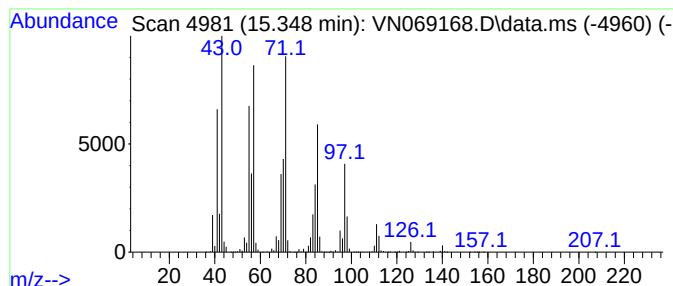
Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

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

Peak Number 10 1-Heptanol, 2-propyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.348	1124.69 ug/l	40177100	1,4-Dichlorobenzene-d4		13.675	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Heptanol, 2-propyl-		158	C10H22O	010042-59-8	72
2	Nonyl tetradecyl ether		340	C23H48O	1000406-37-6	64
3	Heptane, 2,4-dimethyl-		128	C9H20	002213-23-2	58
4	Octane, 1,1'-oxybis-		242	C16H34O	000629-82-3	38
5	2,4,4-Trimethyl-1-hexene		126	C9H18	051174-12-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102621\
Data File : VN069168.D
Acq On : 25 Oct 2021 22:21
Operator : JC/MD
Sample : M4284-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 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	376.8	ug/l	13460100	4	13.675	1786130	50.0
unknown14.348	14.348	268.0	ug/l	9572480	4	13.675	1786130	50.0
1-Butanol, 2-et...	14.423	848.5	ug/l	30310500	4	13.675	1786130	50.0
Carbonic acid, ...	14.530	201.9	ug/l	7212890	4	13.675	1786130	50.0
1-Octene, 6-met...	14.635	264.7	ug/l	9455890	4	13.675	1786130	50.0
1-Heptanol, 6-m...	14.675	868.5	ug/l	31026900	4	13.675	1786130	50.0
(S)-(+)-6-Methy...	14.785	460.6	ug/l	16454700	4	13.675	1786130	50.0
Camphor	15.204	366.8	ug/l	13104300	4	13.675	1786130	50.0
1-Heptanol, 2-p...	15.348	1124.7	ug/l	40177100	4	13.675	1786130	50.0