

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080321\
 Data File : VN067994.D
 Acq On : 3 Aug 2021 20:16
 Operator : JC/MD
 Sample : M3261-08
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41938

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\82N072921W.M
 Title : SW846 8260

Signal : TIC: VN067994.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.293	835	859	877	rBV2	137317	410579	1.46%	0.682%
2	8.024	2231	2250	2261	rBV3	246306	584416	2.08%	0.971%
3	8.086	2262	2273	2303	rVB2	426397	967903	3.44%	1.609%
4	8.440	2384	2405	2430	rBV	291264	665691	2.37%	1.106%
5	8.971	2584	2603	2630	rBV2	661448	1385780	4.93%	2.303%
6	10.443	3131	3152	3163	rBV	1089004	2019059	7.18%	3.356%
7	10.507	3163	3176	3225	rVB	6153485	11231929	39.95%	18.668%
8	11.746	3620	3638	3663	rBV	1034178	1864975	6.63%	3.100%
9	12.733	3990	4006	4024	rBV2	785635	1362150	4.84%	2.264%
10	13.010	4090	4109	4121	rBV2	703952	1241452	4.42%	2.063%
11	13.109	4134	4146	4171	rVB	901151	1788995	6.36%	2.973%
12	13.369	4228	4243	4274	rBV4	628653	1375554	4.89%	2.286%
13	13.592	4308	4326	4333	rBV	16271133	28114858	100.00%	46.728%
14	13.677	4348	4358	4375	rVB	1169363	1971976	7.01%	3.278%
15	13.836	4403	4417	4440	rBV	1567431	2494906	8.87%	4.147%
16	14.123	4510	4524	4537	rBV2	386028	651322	2.32%	1.083%
17	14.276	4568	4581	4594	rBV2	360294	583364	2.07%	0.970%
18	14.412	4612	4632	4645	rBV3	162943	350135	1.25%	0.582%
19	14.777	4755	4768	4777	rBV2	306983	495890	1.76%	0.824%
20	15.045	4857	4868	4879	rBV2	172226	287171	1.02%	0.477%
21	15.582	5054	5068	5083	rBV2	165424	318811	1.13%	0.530%

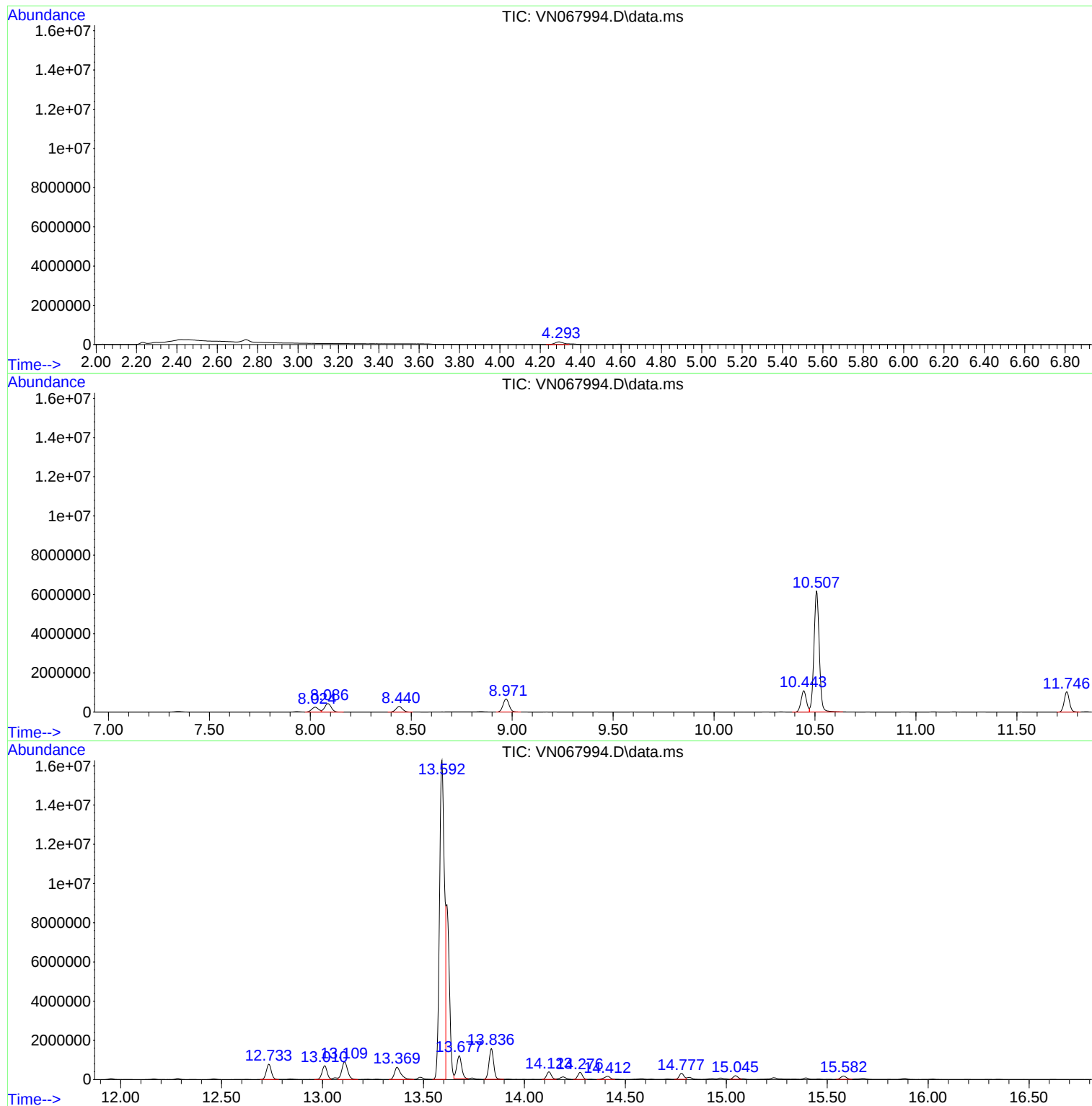
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072921W.M
Quant Title : SW846 8260

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



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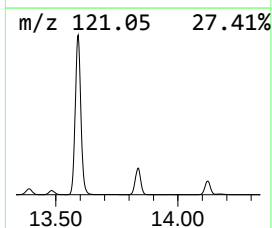
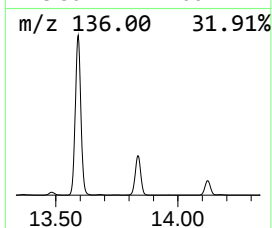
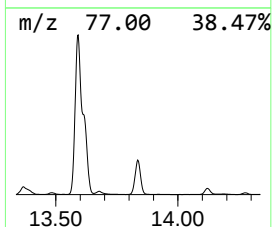
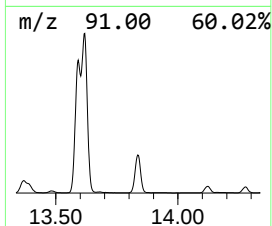
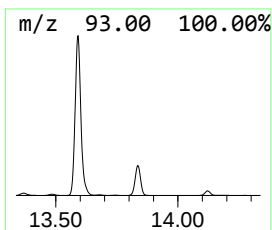
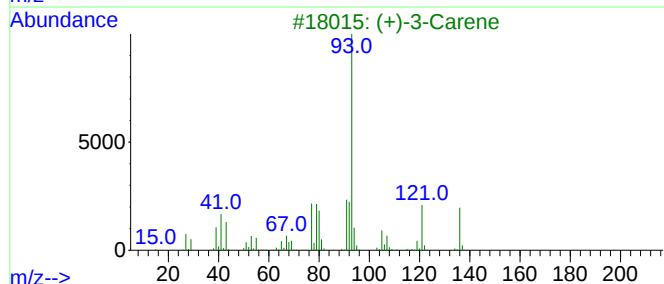
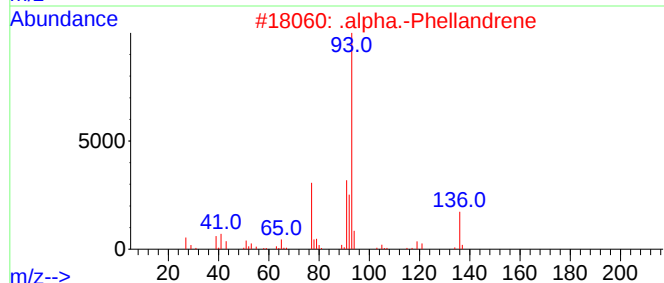
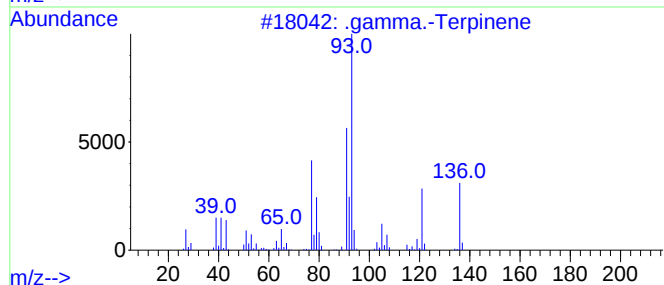
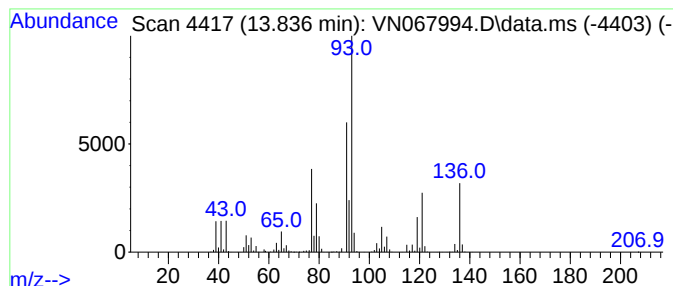
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072921W.M
Quant Title : SW846 8260

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

Peak Number 1 .gamma.-Terpinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.836	63.26 ug/l	2494910	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Terpinene	136	C10H16	000099-85-4	96
2			.alpha.-Phellandrene	136	C10H16	000099-83-2	83
3			(+)-3-Carene	136	C10H16	000498-15-7	81
4			3-Carene	136	C10H16	013466-78-9	76
5			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	76



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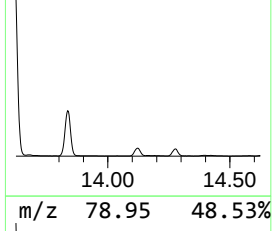
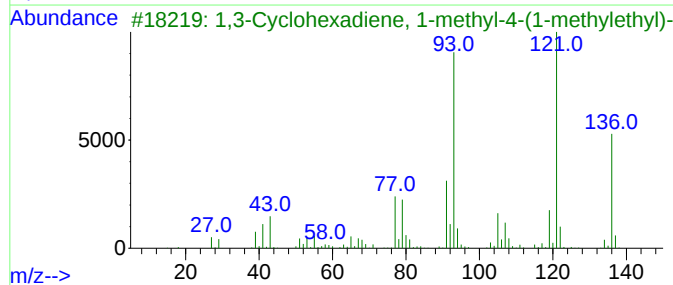
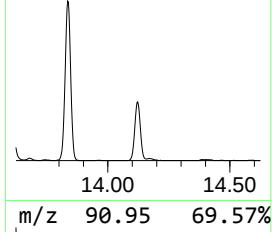
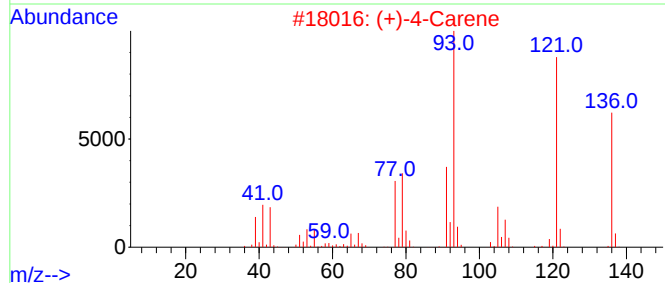
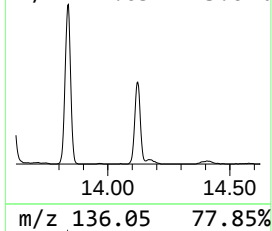
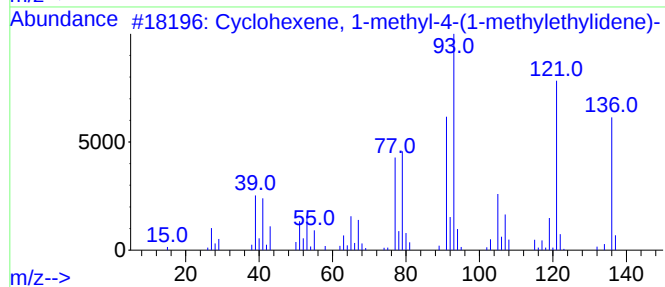
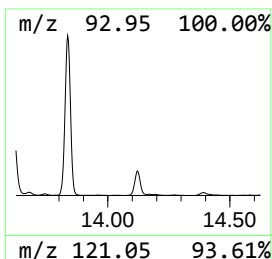
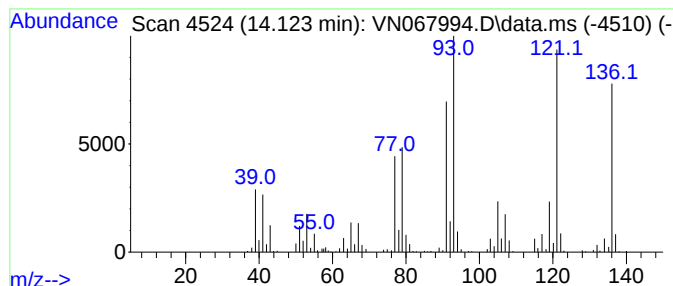
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072921W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.123	16.51 ug/l	651322	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	97
2			(+)-4-Carene	136	C10H16	029050-33-7	97
3			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	97
4			2-Carene	136	C10H16	000554-61-0	94
5			Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	000586-63-0	93



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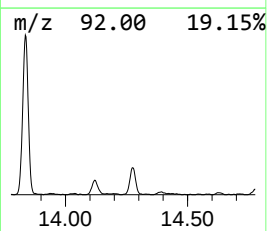
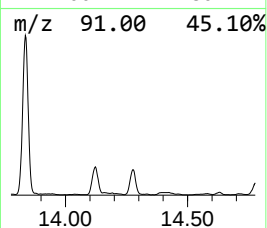
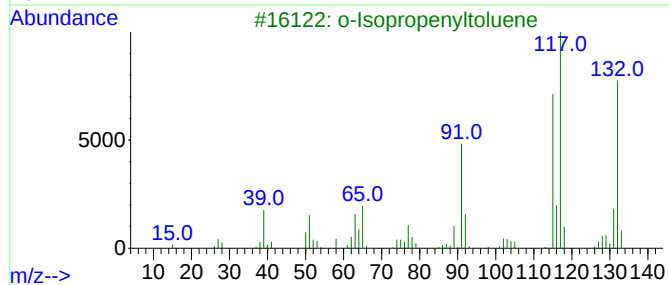
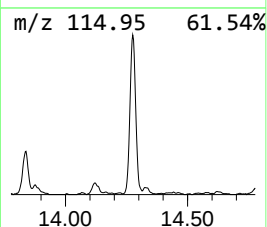
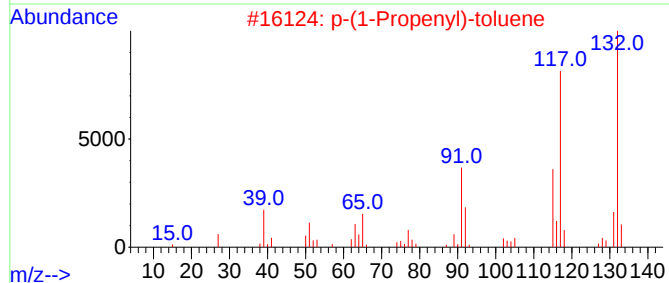
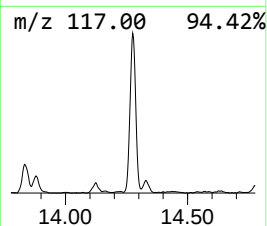
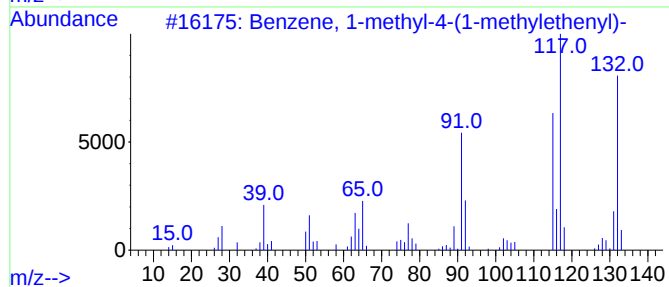
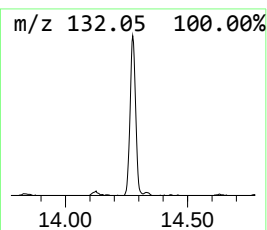
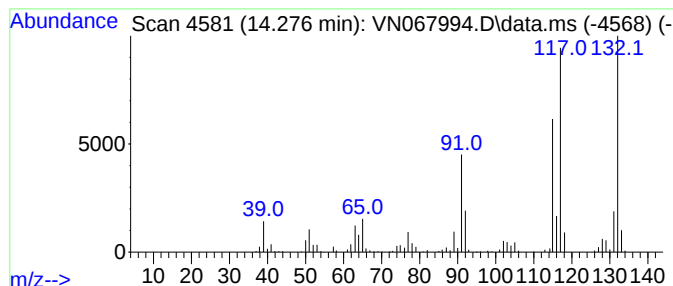
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-methyl-4-(1-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.276	14.79 ug/l	583364	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-(1-methyleth...	132	C10H12	001195-32-0	96
2			p-(1-Propenyl)-toluene	132	C10H12	1000429-54-9	96
3			o-Isopropenyltoluene	132	C10H12	007399-49-7	96
4			Benzene, 1-methyl-3-(1-methyleth...	132	C10H12	001124-20-5	93
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87



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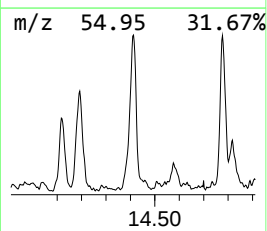
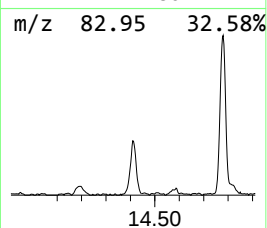
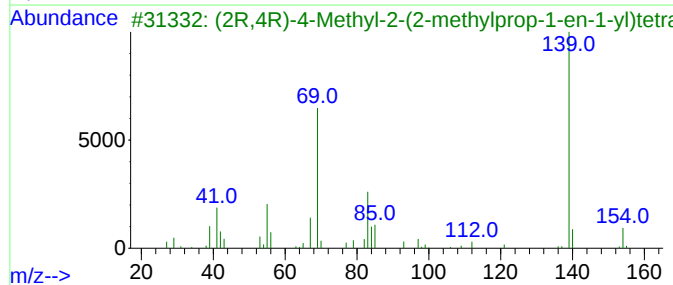
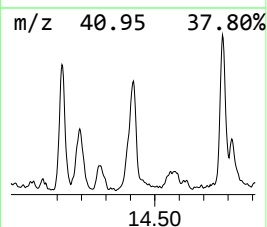
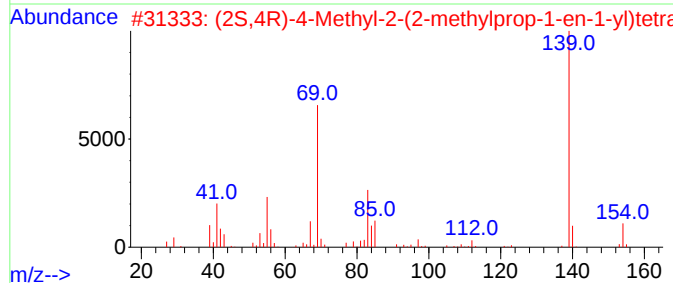
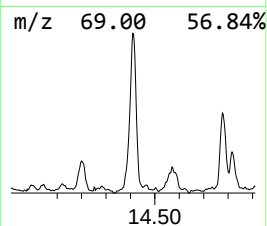
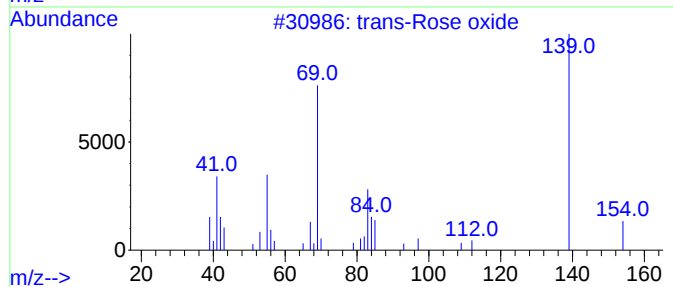
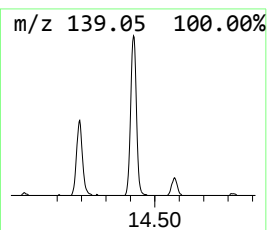
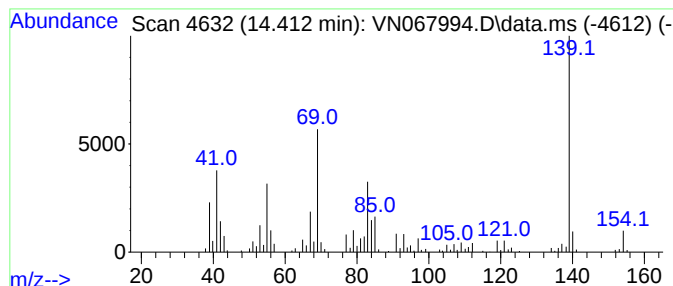
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TIC Integration Parameters: LSCINT.P

Peak Number 4 trans-Rose oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.412	8.88 ug/l	350135	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Rose oxide	154	C10H18O	000876-18-6	93
2			(2S,4R)-4-Methyl-2-(2-methylprop...	154	C10H18O	003033-23-6	90
3			(2R,4R)-4-Methyl-2-(2-methylprop...	154	C10H18O	005258-11-7	90
4			2H-Pyran, tetrahydro-4-methyl-2-...	154	C10H18O	016409-43-1	90
5			Methyl 5-[(4-fluorophenoxy)methy...	250	C13H11FO4	402739-03-1	47



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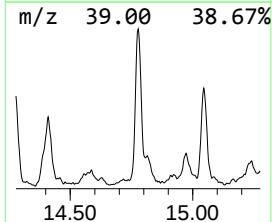
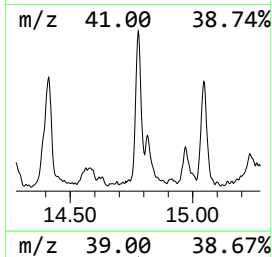
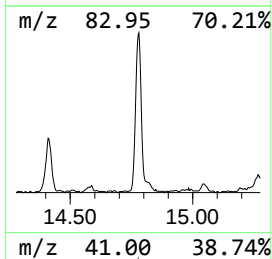
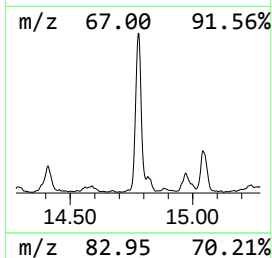
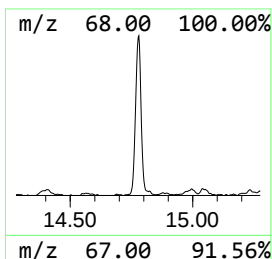
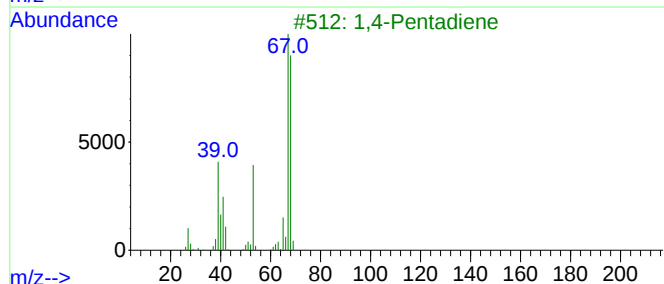
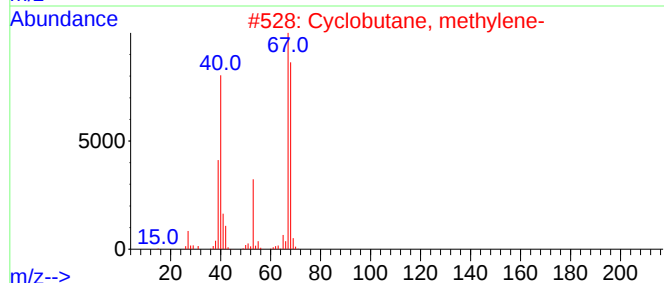
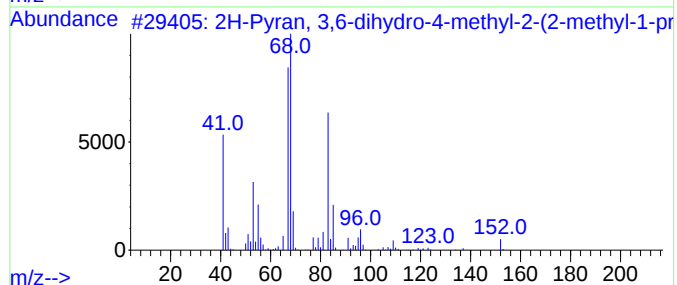
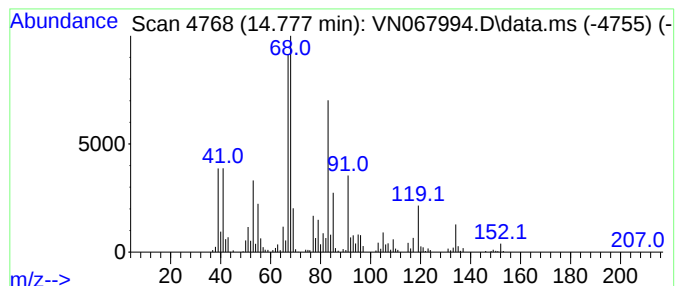
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Quant Title : SW846 8260

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

Peak Number 5 2H-Pyran, 3,6-dihydro-4-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.777	12.57 ug/l	495890	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Pyran, 3,6-dihydro-4-methyl-2...	152	C10H16O	001786-08-9	94
2			Cyclobutane, methylene-	68	C5H8	001120-56-5	52
3			1,4-Pentadiene	68	C5H8	000591-93-5	50
4			1,7-Octadiene, 3-methylene-	122	C9H14	068695-13-6	50
5			3-Octyne	110	C8H14	015232-76-5	43



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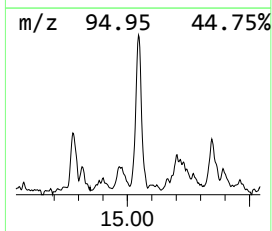
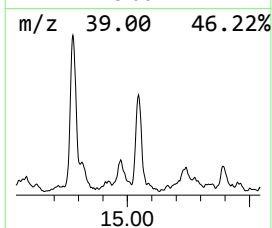
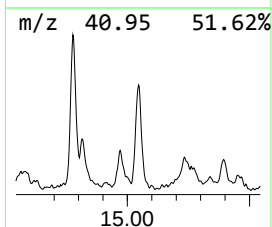
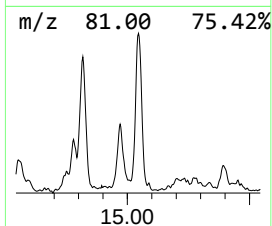
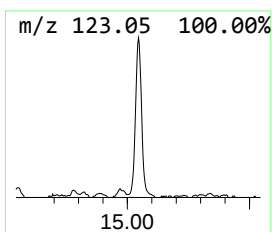
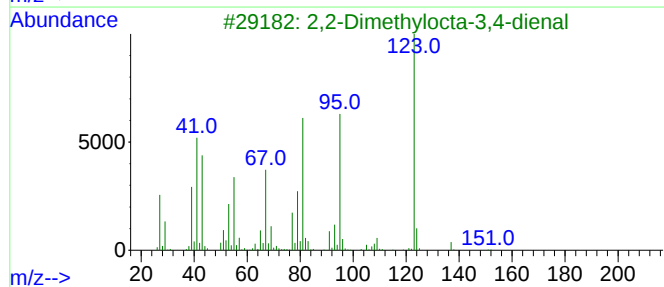
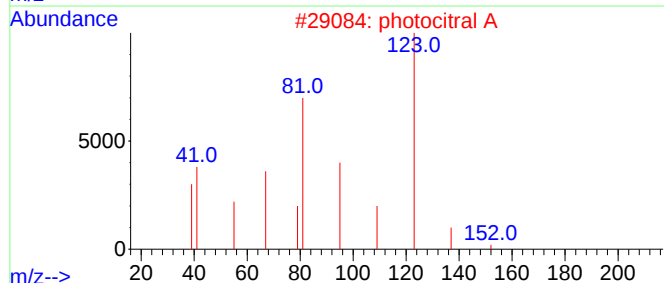
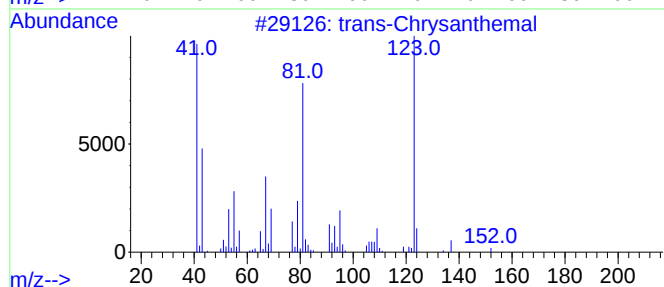
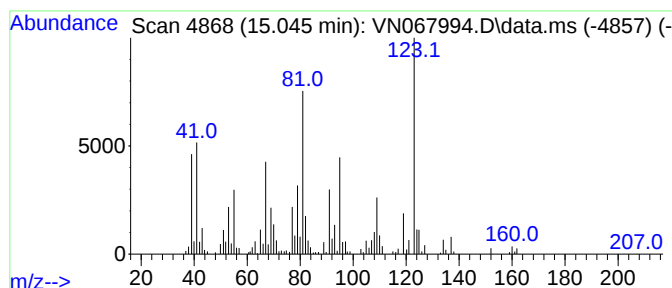
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Quant Title : SW846 8260

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

Peak Number 6 trans-Chrysanthemal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.045	7.28 ug/l	287171	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Chrysanthemal	152	C10H16O	020104-05-6	90
2			photocitral A	152	C10H16O	055253-28-6	74
3			2,2-Dimethylocta-3,4-dienal	152	C10H16O	000590-71-6	53
4			1-Cyclohexene-1-acetaldehyde, .a...	152	C10H16O	053155-80-9	53
5			Bicyclo[2.2.2]octane, 1-methyl-4...	202	C10H18O2S	069855-48-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080321\
Data File : VN067994.D
Acq On : 3 Aug 2021 20:16
Operator : JC/MD
Sample : M3261-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41938

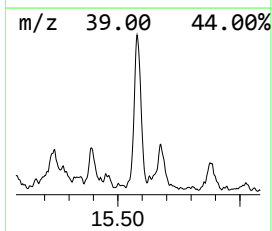
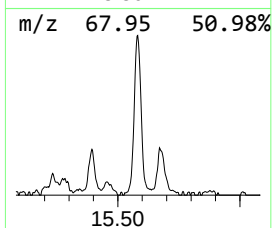
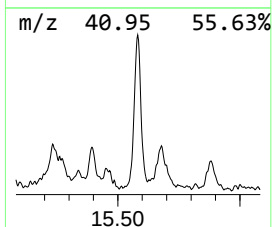
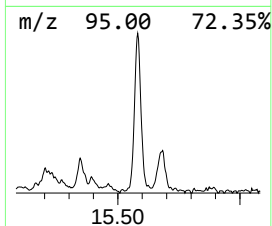
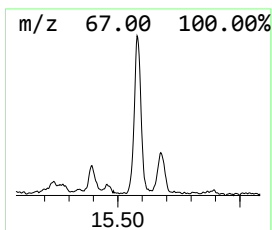
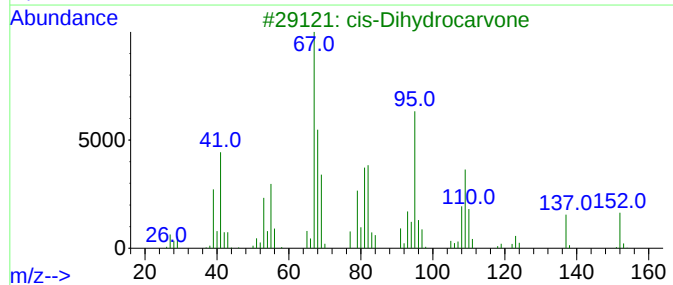
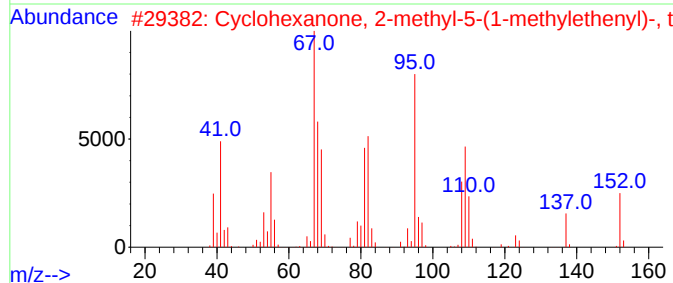
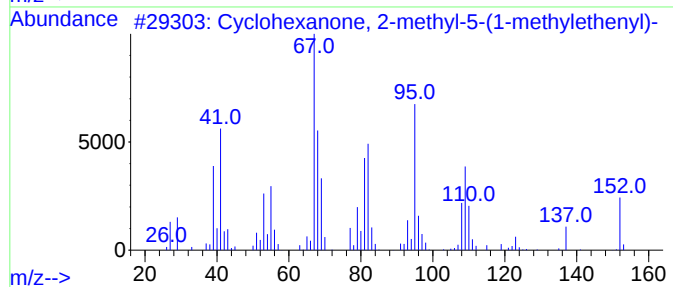
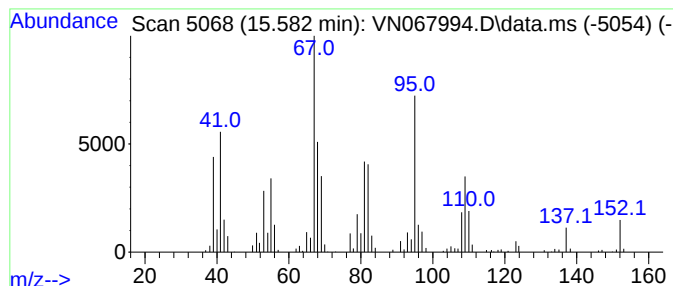
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexanone, 2-methyl-5-(... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.582	8.08 ug/l	318811	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	007764-50-3	97
2			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	005948-04-9	96
3			cis-Dihydrocarvone	152	C10H16O	003792-53-8	94
4			(+)-Dihydrocarvone	152	C10H16O	005524-05-0	90
5			3-Octyne	110	C8H14	015232-76-5	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080321\
Data File : VN067994.D
Acq On : 3 Aug 2021 20:16
Operator : JC/MD
Sample : M3261-08
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41938

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072921W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
.gamma.-Terpinene	13.836	63.3	ug/l	2494910	4	13.678	1971980	50.0
Cyclohexene, 1-...	14.123	16.5	ug/l	651322	4	13.678	1971980	50.0
Benzene, 1-meth...	14.276	14.8	ug/l	583364	4	13.678	1971980	50.0
trans-Rose oxide	14.412	8.9	ug/l	350135	4	13.678	1971980	50.0
2H-Pyran, 3,6-d...	14.777	12.6	ug/l	495890	4	13.678	1971980	50.0
trans-Chrysanth...	15.045	7.3	ug/l	287171	4	13.678	1971980	50.0
Cyclohexanone, ...	15.582	8.1	ug/l	318811	4	13.678	1971980	50.0