

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN050420\
 Data File : VN061281.D
 Acq On : 4 May 2020 16:26
 Operator : JC/MD
 Sample : L2457-04
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1341

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042720W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.638	3	15	59	rBV	3684274	11533085	100.00%	54.630%
2	2.285	210	216	249	rVB	112811	255981	2.22%	1.213%
3	3.240	495	513	553	rBV	943139	2199782	19.07%	10.420%
4	6.776	1590	1613	1642	rBV2	83260	267117	2.32%	1.265%
5	7.548	1836	1853	1865	rBV	73310	183586	1.59%	0.870%
6	7.625	1865	1877	1899	rVB2	140649	330292	2.86%	1.565%
7	7.989	1973	1990	2009	rBV	101535	235725	2.04%	1.117%
8	8.551	2149	2165	2185	rBV	231212	475759	4.13%	2.254%
9	10.059	2619	2634	2652	rBV	364721	666437	5.78%	3.157%
10	11.381	3030	3045	3065	rBV	342991	600328	5.21%	2.844%
11	12.378	3343	3355	3373	rVB	272643	466681	4.05%	2.211%
12	13.236	3606	3622	3637	rVV	601714	973900	8.44%	4.613%
13	13.320	3637	3648	3658	rVV	339333	573047	4.97%	2.714%
14	13.381	3658	3667	3677	rVV	346115	577040	5.00%	2.733%
15	13.795	3775	3796	3808	rBV	178099	293882	2.55%	1.392%
16	14.040	3852	3872	3887	rBV	259573	422244	3.66%	2.000%
17	14.500	3999	4015	4025	rVB	555151	804371	6.97%	3.810%
18	16.197	4532	4543	4557	rBV	139233	251841	2.18%	1.193%

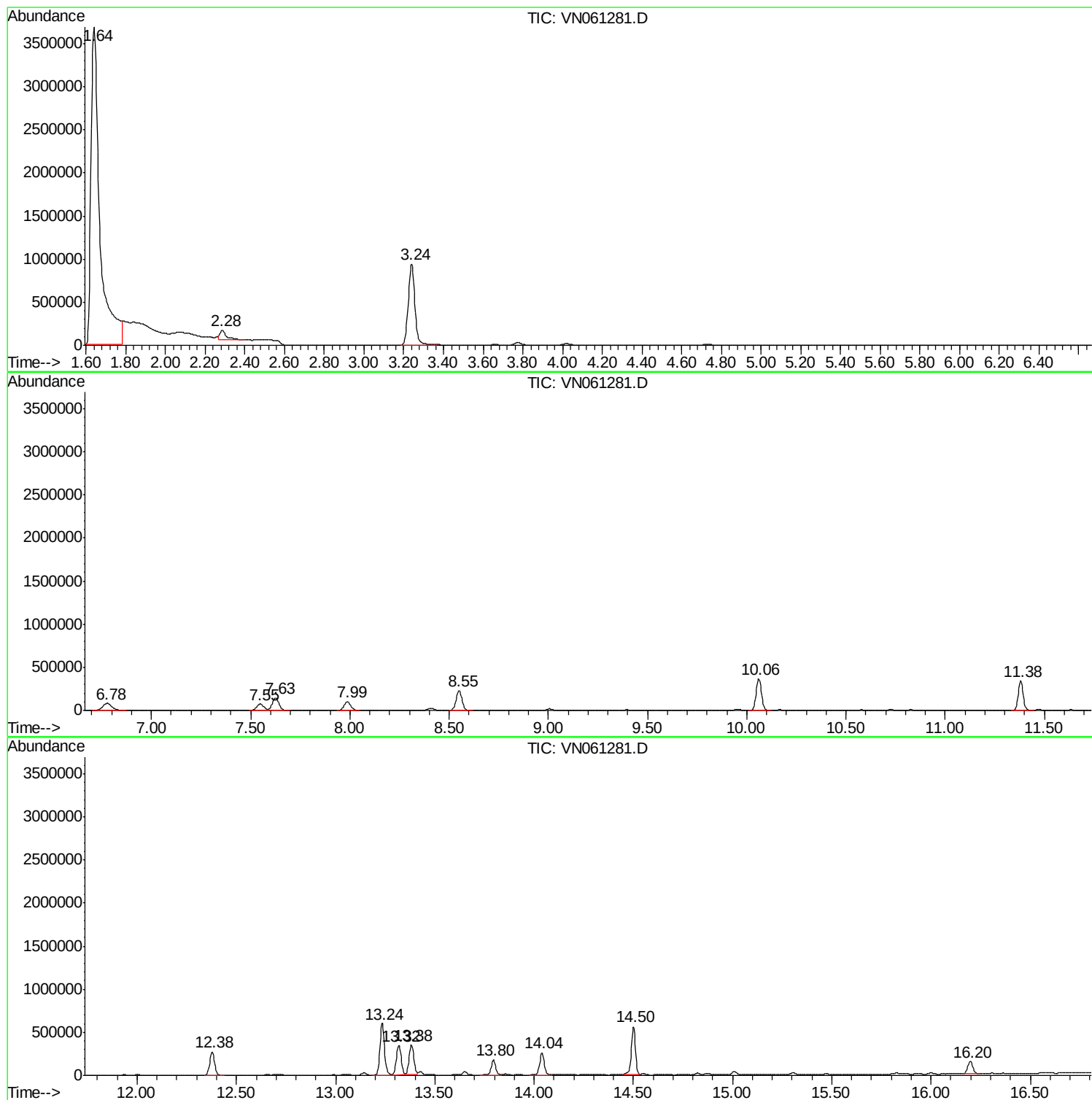
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N042720W.M
Quant Title : SW846 8260

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



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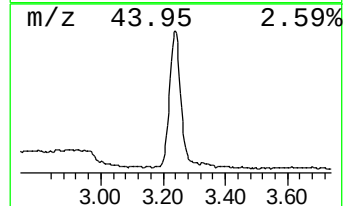
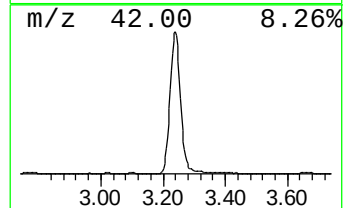
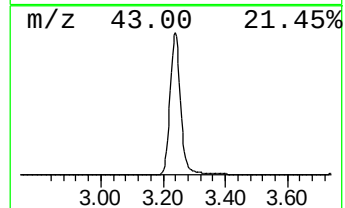
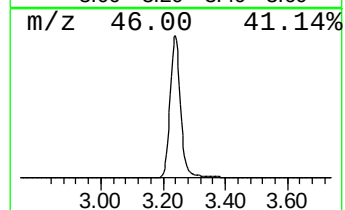
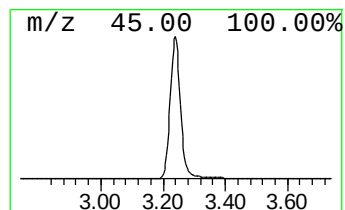
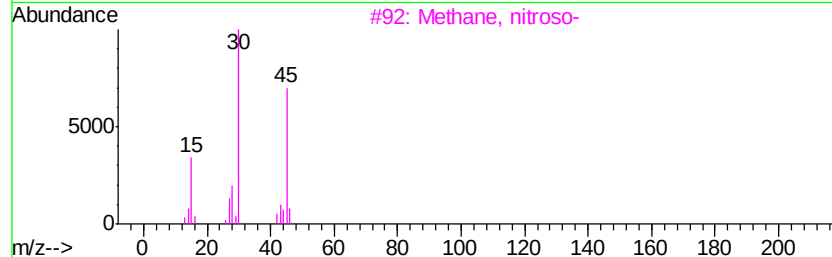
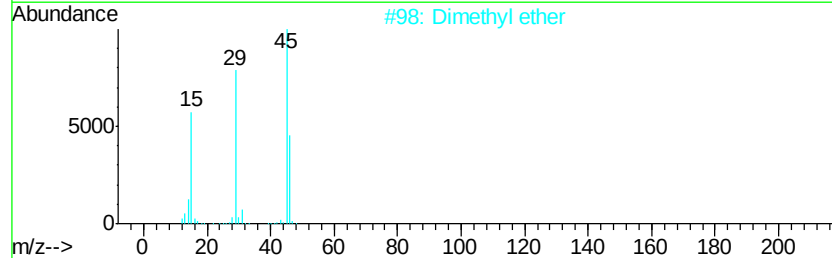
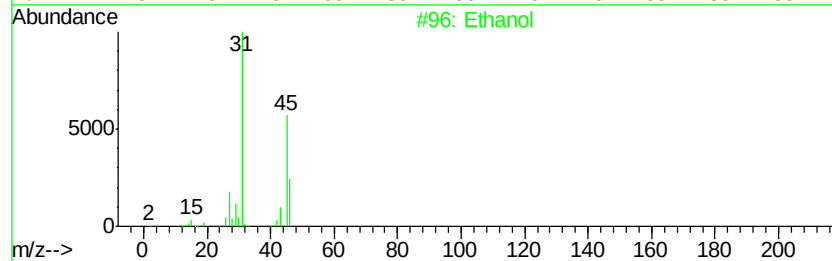
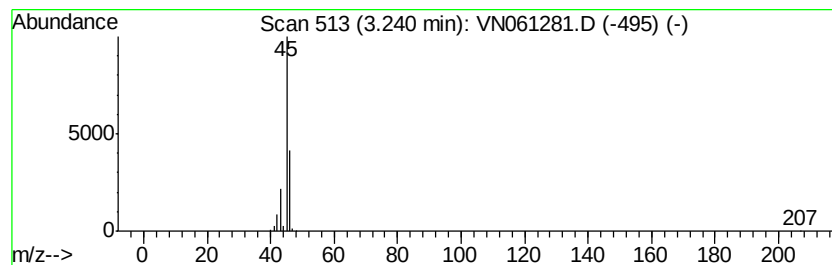
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.24	333.01 ug/l	2199780	Pentafluorobenzene	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol	46	C2H6O	000064-17-5	74
2		Dimethyl ether	46	C2H6O	000115-10-6	9
3		Methane, nitroso-	45	CH3NO	000865-40-7	4
4		Formic acid	46	CH2O2	000064-18-6	4
5		Oxalic acid	90	C2H2O4	000144-62-7	4



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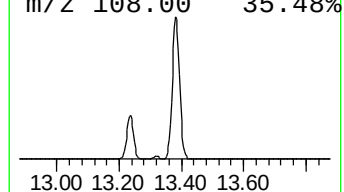
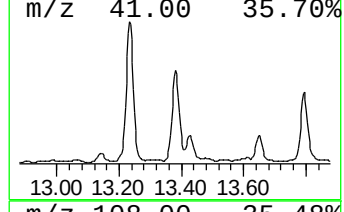
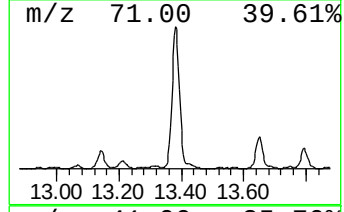
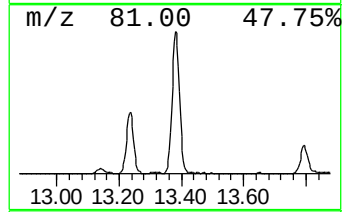
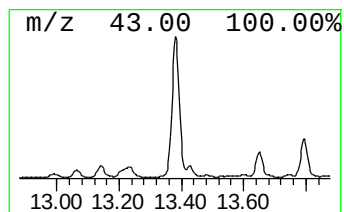
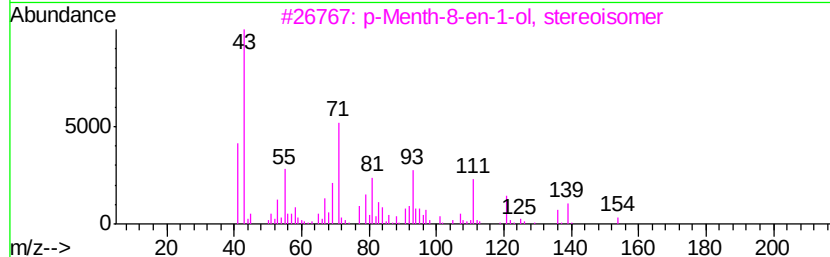
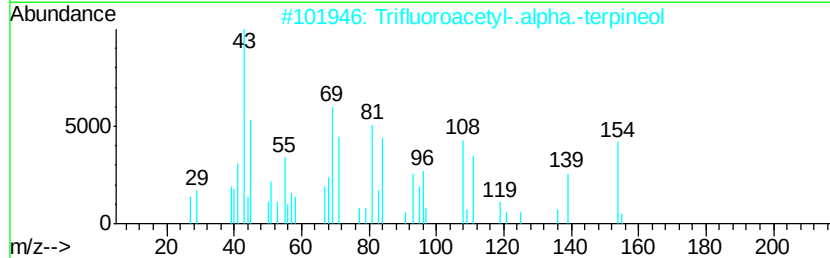
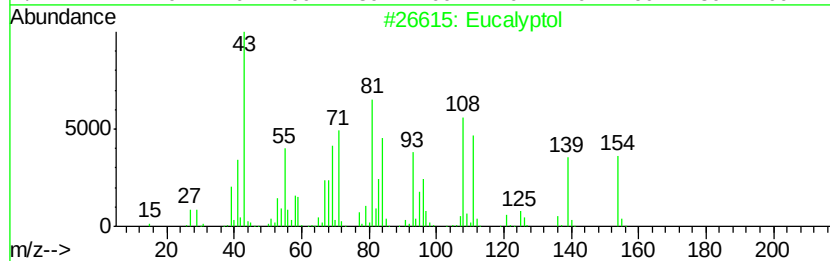
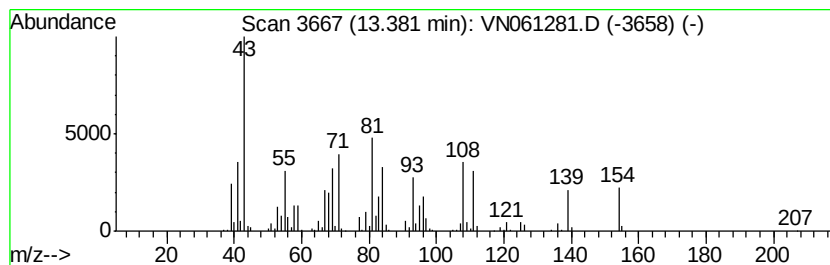
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Quant Title : SW846 8260

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

Peak Number 4 Eucalyptol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.38	50.35 ug/l	577040	1,4-Dichlorobenzene-d4	13.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol		154	C10H18O	000470-82-6	98
2	Trifluoroacetyl-.alpha.-terpineol		250	C12H17F3O2	1000058-17-6	78
3	p-Menth-8-en-1-ol, stereoisomer		154	C10H18O	007299-40-3	38
4	2-(3'-Oxo-butyl)-cyclopentanone		154	C9H14O2	1000143-37-2	18
5	3-Hepten-2-one, 3-propyl-		154	C10H18O	032064-69-0	15



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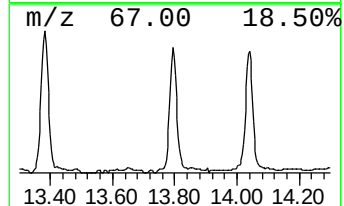
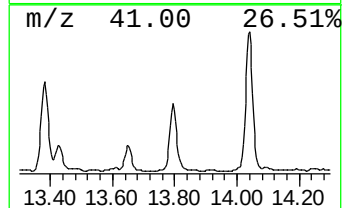
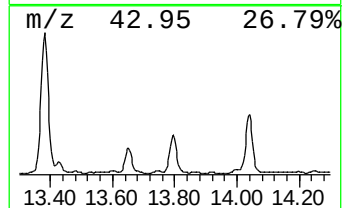
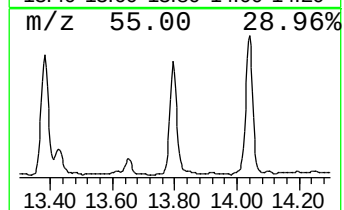
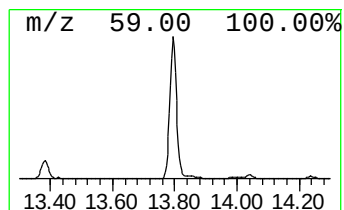
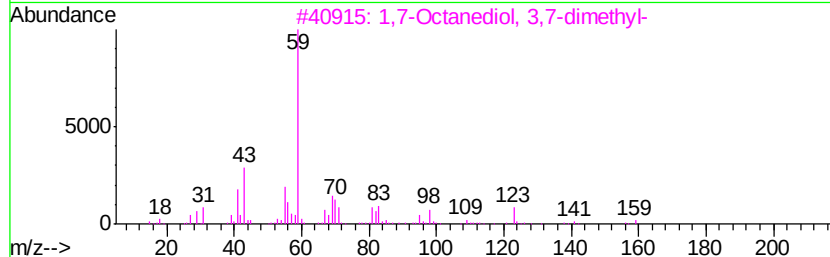
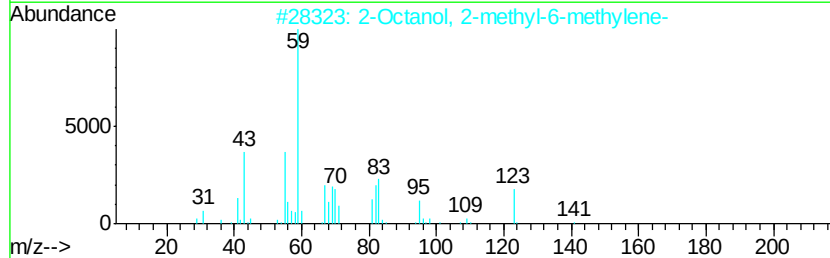
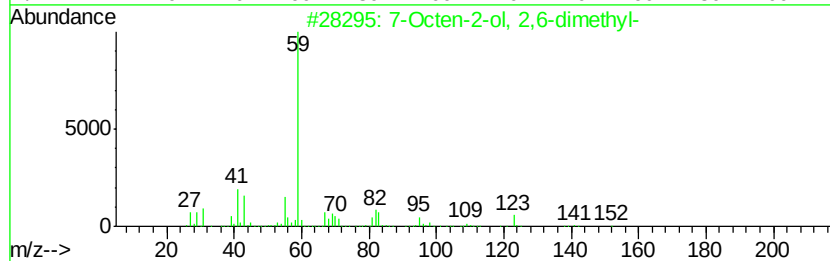
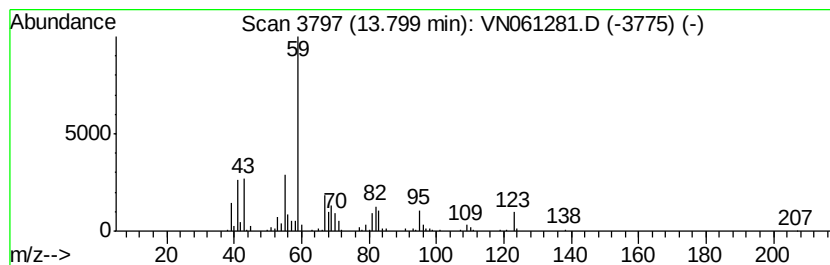
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Peak Number 5 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	25.64 ug/l	293882	1,4-Dichlorobenzene-d4	13.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
2		2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	53
3		1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	53
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	47
5		2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	38



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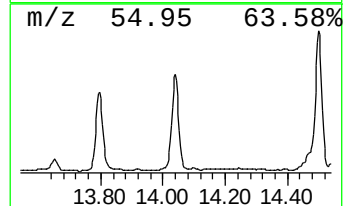
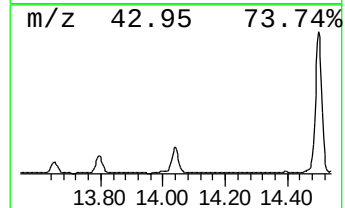
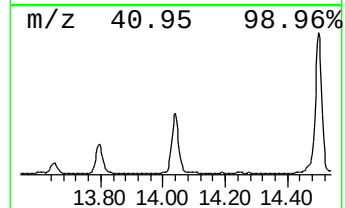
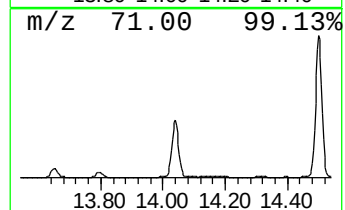
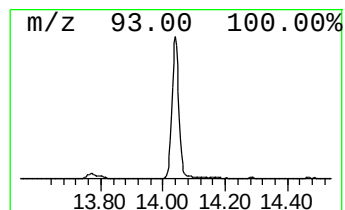
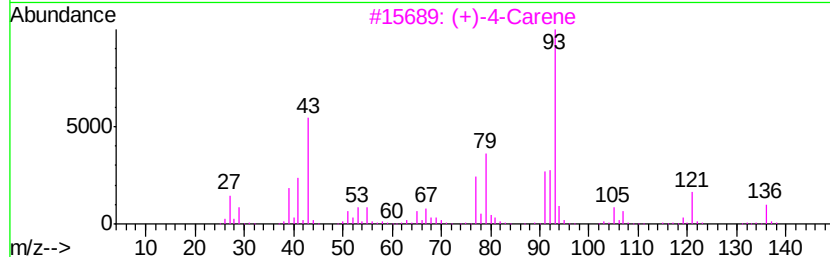
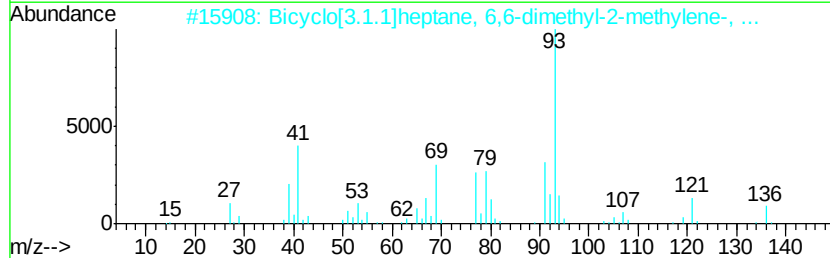
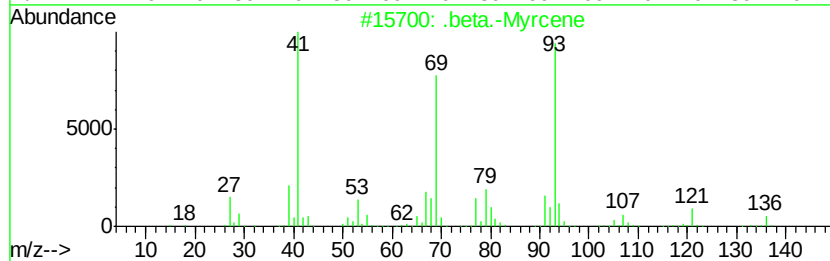
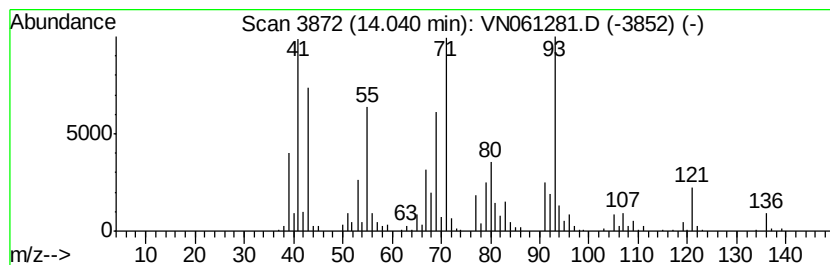
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown14.04 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	36.84 ug/l	422244	1,4-Dichlorobenzene-d4	13.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Myrcene	136	C10H16	000123-35-3	49
2		Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	49
3		(+)-4-Carene	136	C10H16	029050-33-7	46
4		.gamma.-Terpinene	136	C10H16	000099-85-4	46
5		(+)-3-Carene	136	C10H16	000498-15-7	46



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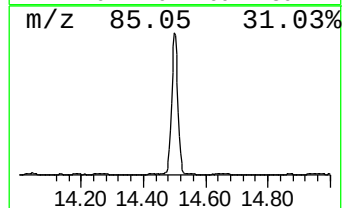
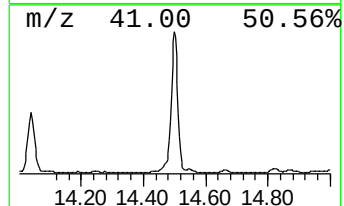
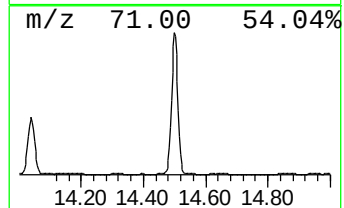
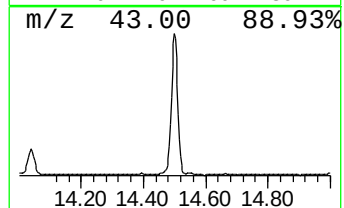
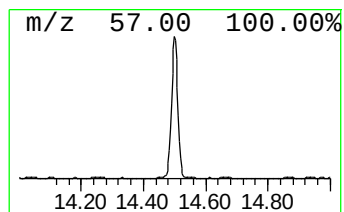
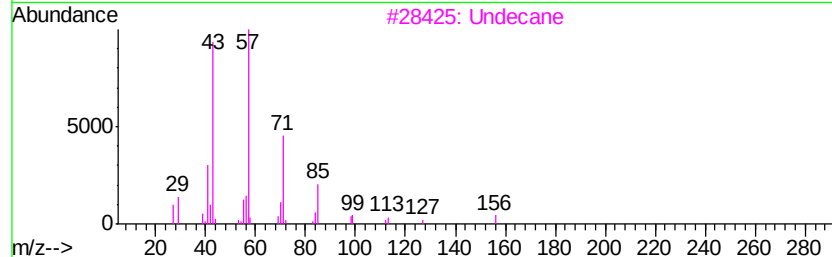
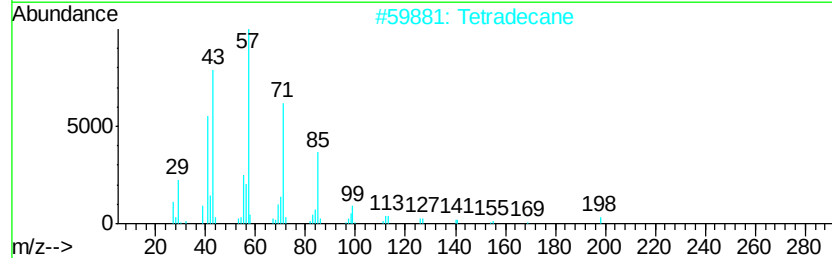
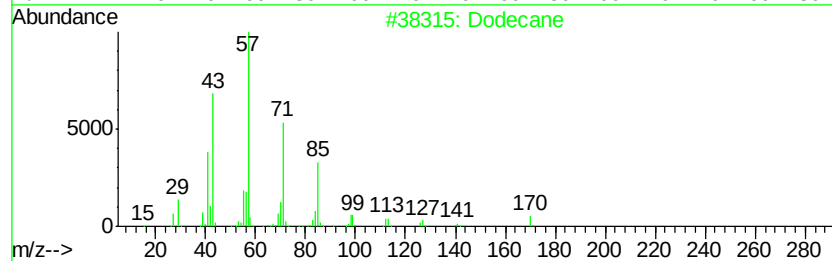
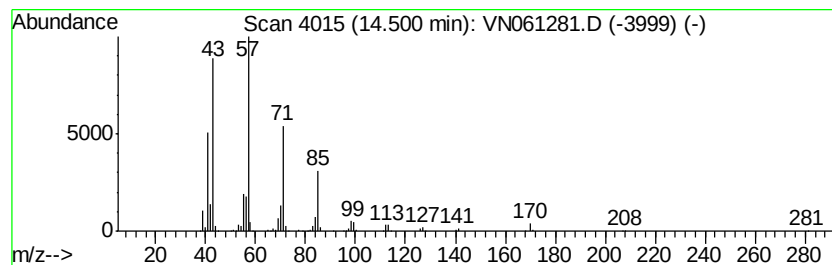
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Peak Number 7 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	70.18 ug/l	804371	1,4-Dichlorobenzene-d4	13.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane		170	C12H26	000112-40-3	95
2	Tetradecane		198	C14H30	000629-59-4	90
3	Undecane		156	C11H24	001120-21-4	86
4	Tridecane		184	C13H28	000629-50-5	86
5	Decane, 2,3,6-trimethyl-		184	C13H28	062238-12-4	83



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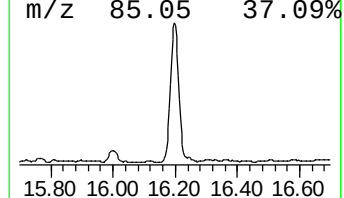
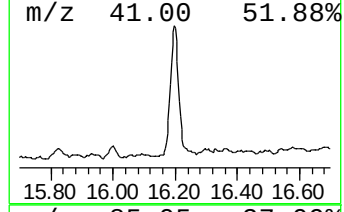
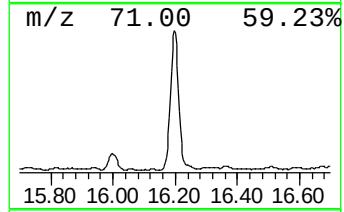
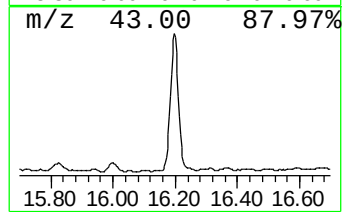
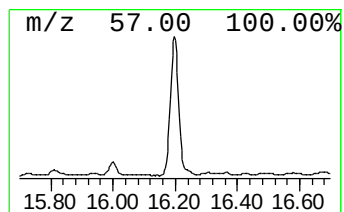
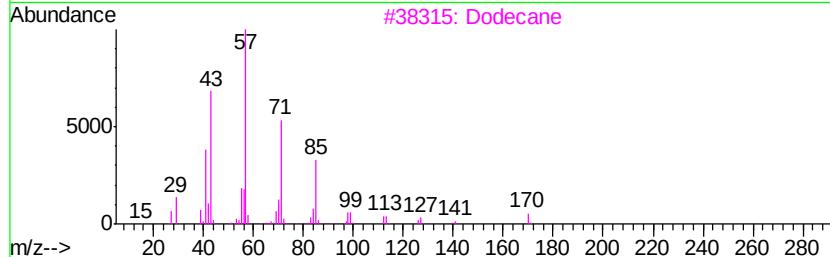
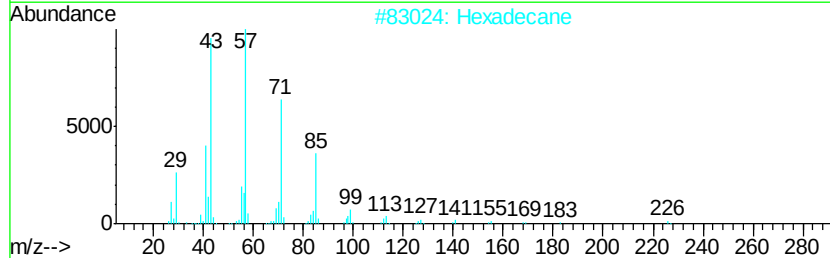
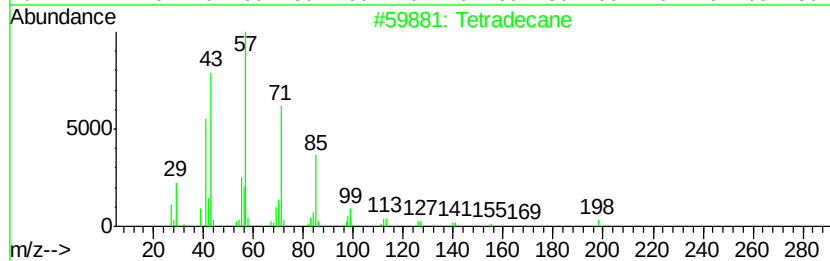
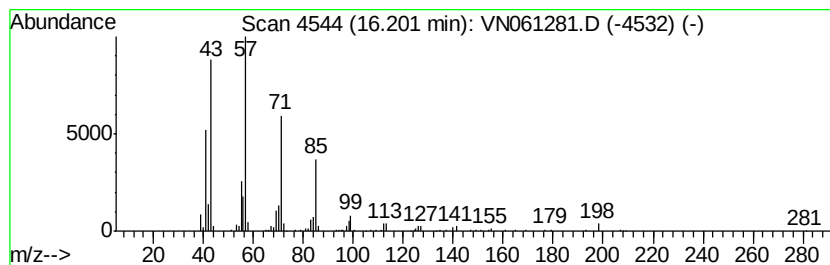
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 TIC Integration Parameters: LSCINT.P

 Peak Number 8 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.20	21.97 ug/l	251841	1,4-Dichlorobenzene-d4	13.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	98
2		Hexadecane	226	C16H34	000544-76-3	87
3		Dodecane	170	C12H26	000112-40-3	86
4		Tridecane	184	C13H28	000629-50-5	86
5		Undecane	156	C11H24	001120-21-4	86



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN050420\
Data File : VN061281.D
Acq On : 4 May 2020 16:26
Operator : JC/MD
Sample : L2457-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1341

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N042720W.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
Ethanol	3.24	333.0	ug/l	2199780	1	7.63	330292	50.0
Eucalyptol	13.38	50.4	ug/l	577040	4	13.32	573047	50.0
7-Octen-2-ol, 2,6...	13.80	25.6	ug/l	293882	4	13.32	573047	50.0
unknown14.04	14.04	36.8	ug/l	422244	4	13.32	573047	50.0
Dodecane	14.50	70.2	ug/l	804371	4	13.32	573047	50.0
Tetradecane	16.20	22.0	ug/l	251841	4	13.32	573047	50.0