

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042722\
 Data File : VN072224.D
 Acq On : 27 Apr 2022 18:29
 Operator : JC\MD
 Sample : N2575-02 10X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31799

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\82N042622W.M

Title : SW846 8260

Signal : TIC: VN072224.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.575	94	100	131	rBV	11885695	23052255	100.00%	65.432%
2	3.681	277	288	310	rBV	448107	1233045	5.35%	3.500%
3	8.016	1015	1025	1030	rBV	210251	501026	2.17%	1.422%
4	8.081	1030	1036	1051	rVV	385198	872789	3.79%	2.477%
5	8.245	1054	1064	1080	rBV	258091	592605	2.57%	1.682%
6	8.434	1086	1096	1107	rBV	244543	556429	2.41%	1.579%
7	8.963	1177	1186	1202	rBV	609392	1242152	5.39%	3.526%
8	10.439	1428	1437	1444	rBV	938465	1740718	7.55%	4.941%
9	11.739	1650	1658	1671	rBV	973167	1715839	7.44%	4.870%
10	12.727	1818	1826	1838	rBV	744951	1269971	5.51%	3.605%
11	13.669	1979	1986	1992	rBV	817235	1366564	5.93%	3.879%
12	13.733	1992	1997	2011	rVB2	325577	620338	2.69%	1.761%
13	14.351	2092	2102	2108	rBV7	62132	230609	1.00%	0.655%
14	15.198	2239	2246	2256	rBV	118445	236413	1.03%	0.671%

Sum of corrected areas: 35230753

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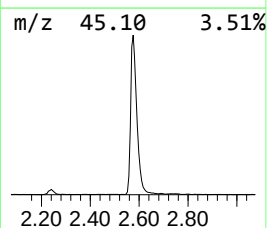
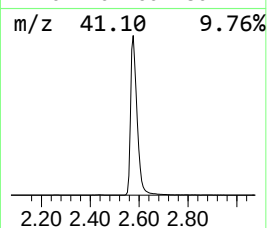
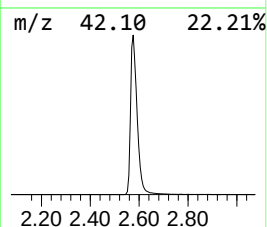
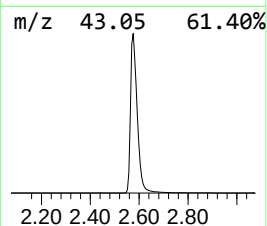
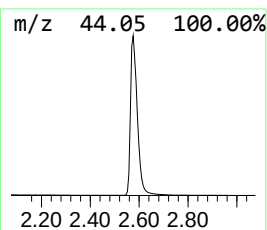
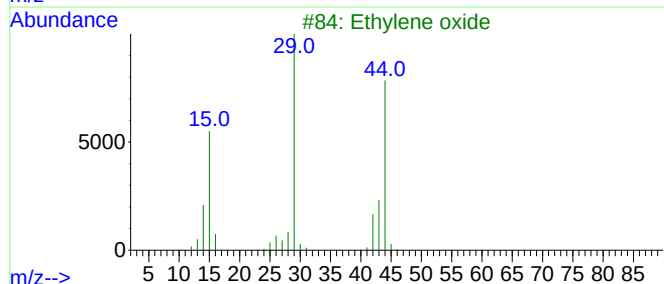
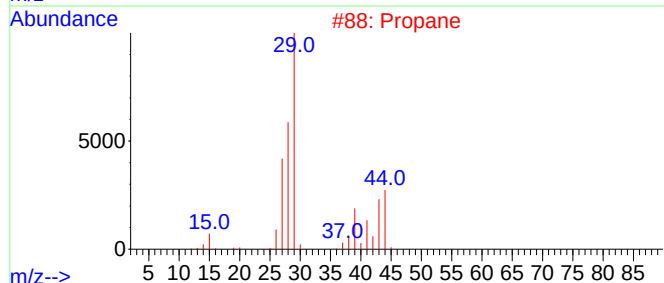
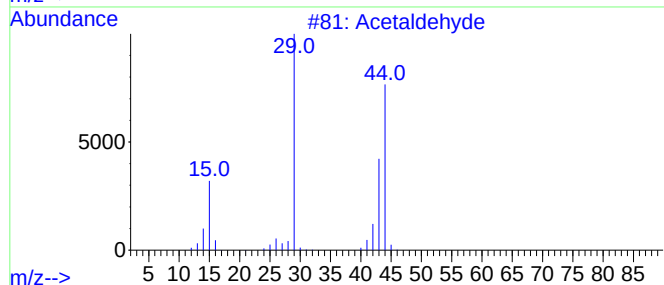
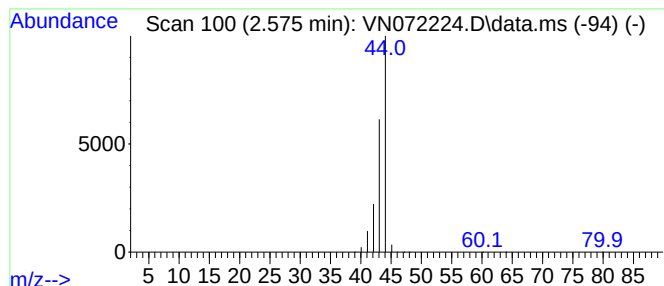
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Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.575	1320.61 ug/l	23052300	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Propane	44	C3H8	000074-98-6	5
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Alanine	89	C3H7NO2	000056-41-7	4
5			Hydrogen isocyanate	43	CHNO	000075-13-8	3



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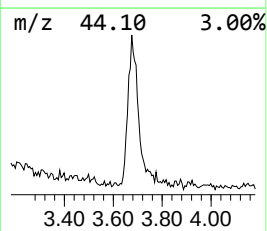
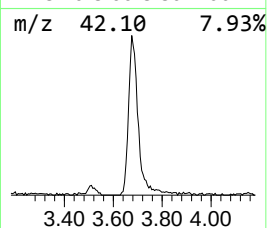
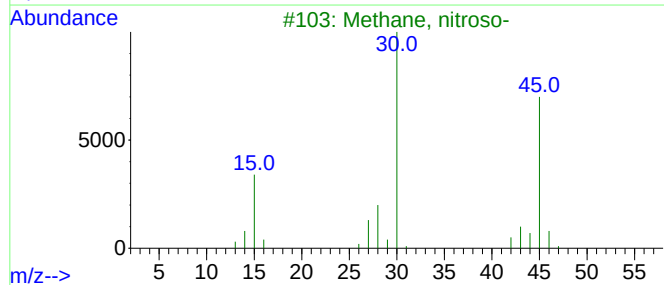
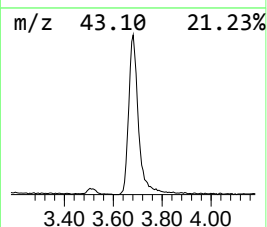
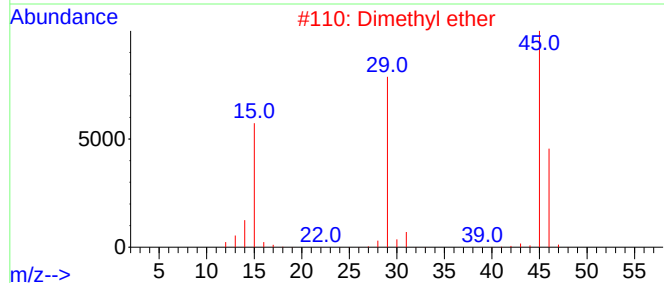
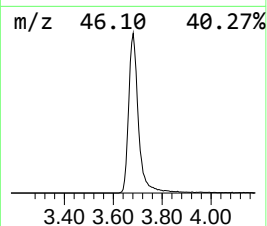
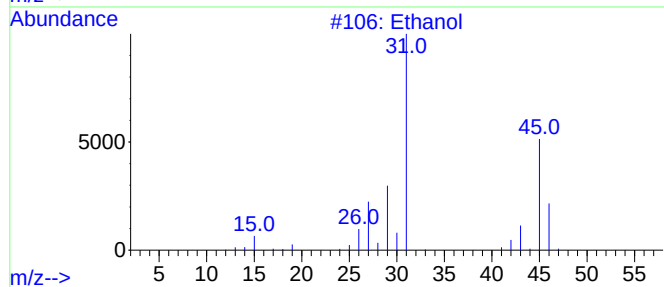
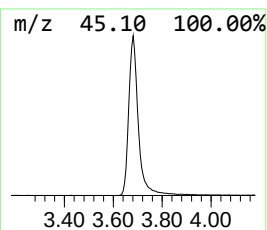
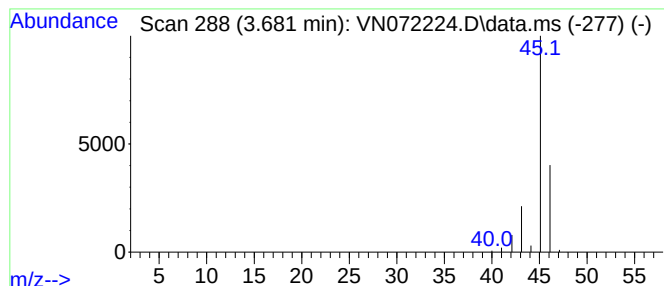
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Quant Title : SW846 8260

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Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.681	70.64 ug/l	1233050	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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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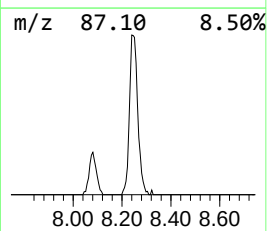
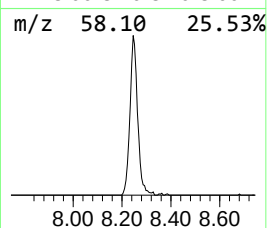
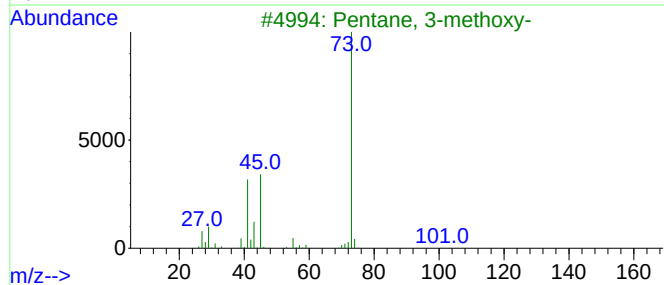
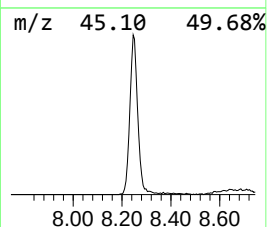
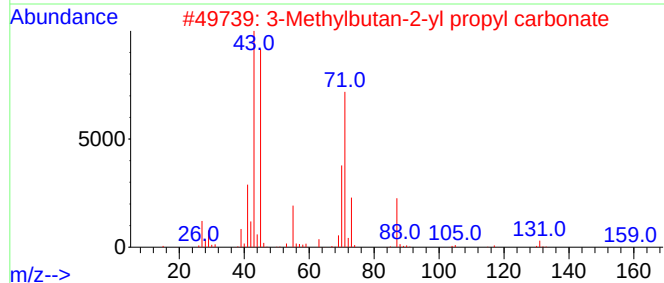
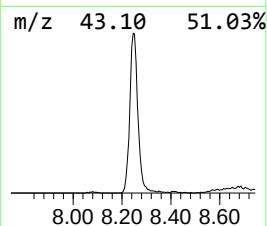
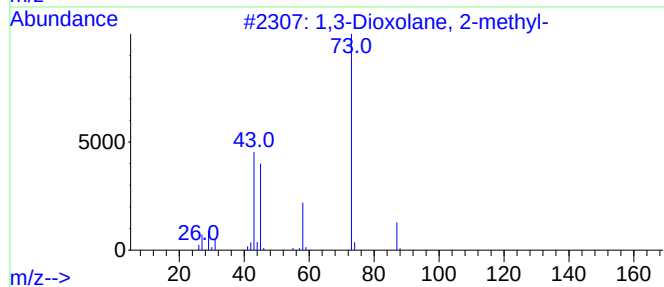
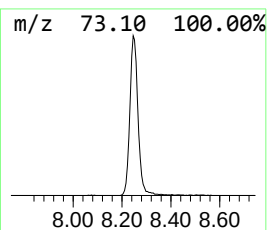
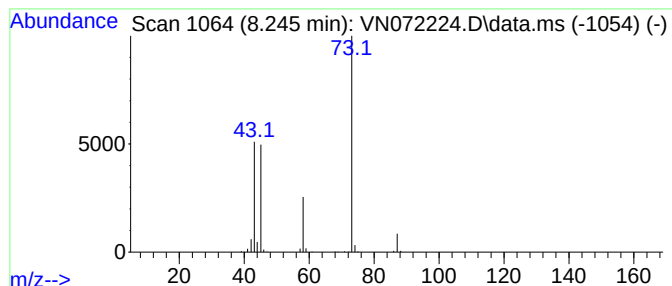
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 1,3-Dioxolane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.245	33.95 ug/l	592605	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	83
2			3-Methylbutan-2-yl propyl carbonate	174	C9H18O3	1000372-83-4	28
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	28
4			1,2-Propanediol, 1-acetate	118	C5H10O3	000627-69-0	28
5			2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	23



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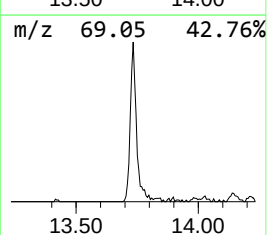
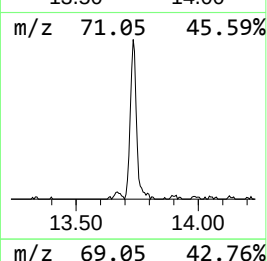
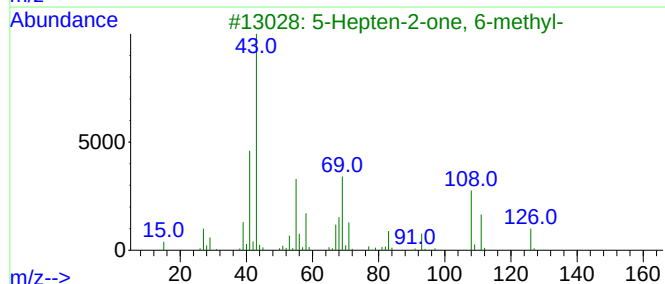
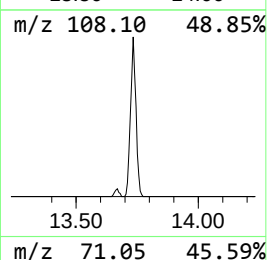
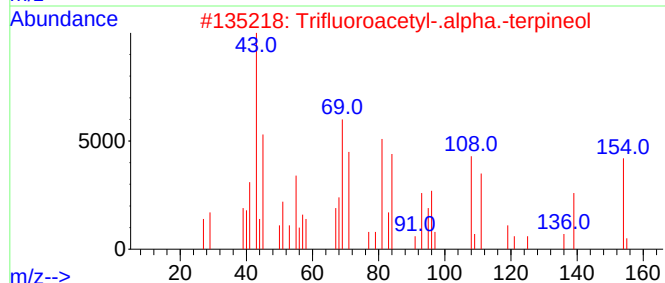
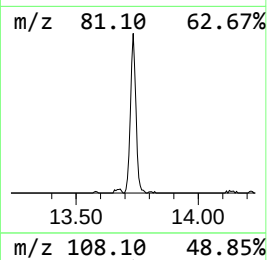
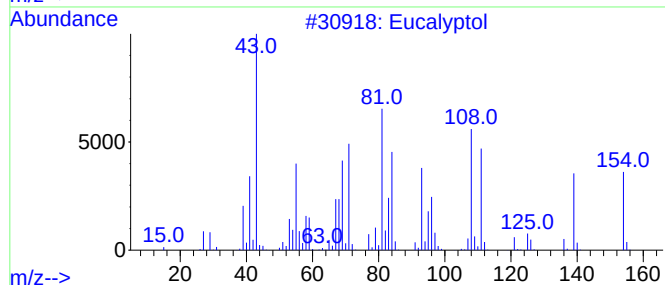
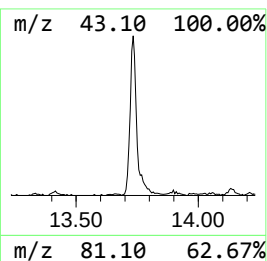
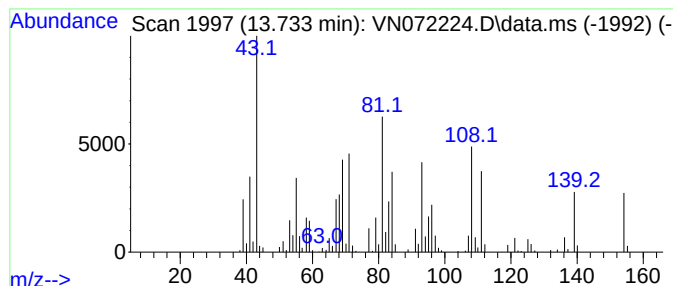
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eucalyptol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.733	22.70 ug/l	620338	1,4-Dichlorobenzene-d4	13.669

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	72
3			5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	25
4			trans-Cyclohexane-1,4-dimethanol...	228	C12H20O4	010412-78-9	22
5			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	22



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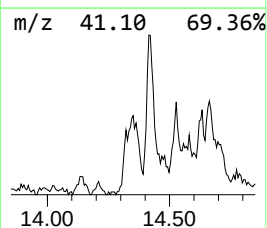
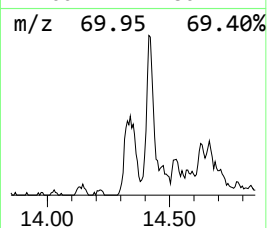
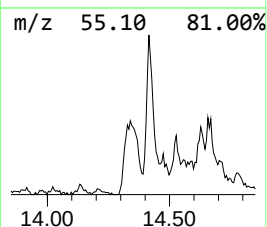
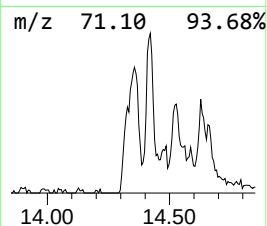
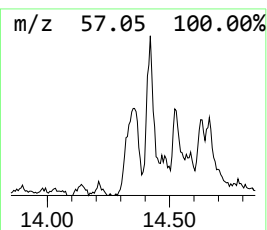
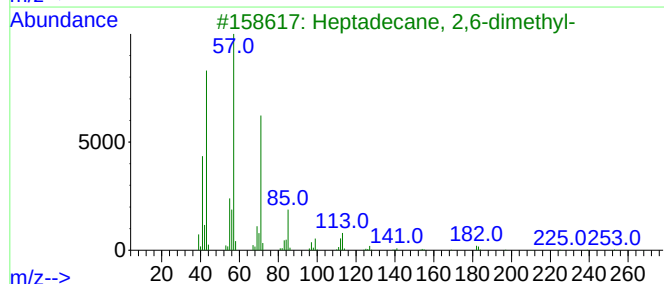
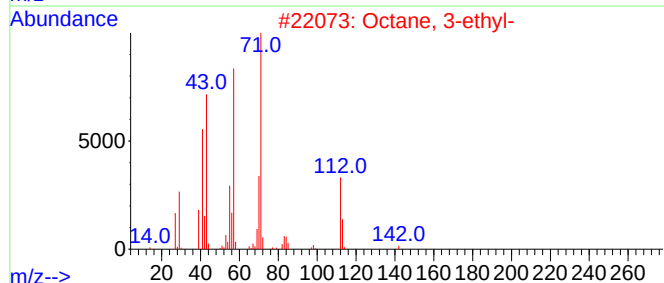
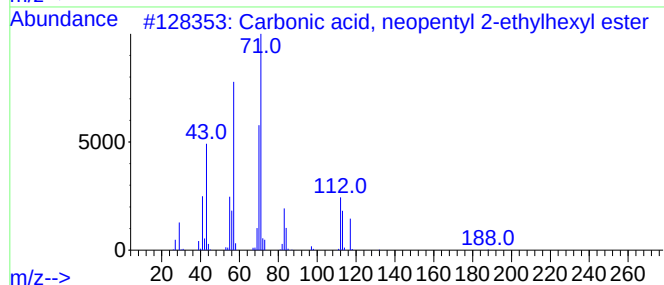
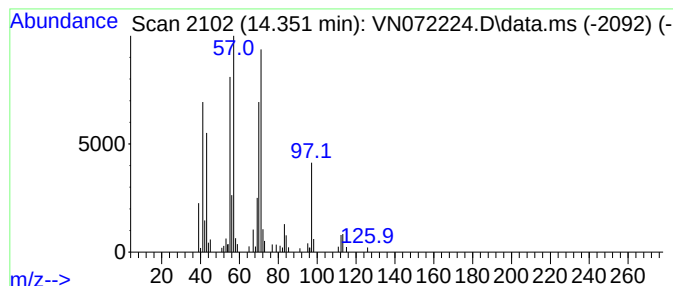
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Carbonic acid, neopentyl 2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.351	8.44 ug/l	230609	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, neopentyl 2-ethyl...	244	C14H28O3	1000357-85-7	53
2			Octane, 3-ethyl-	142	C10H22	005881-17-4	47
3			Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	43
4			Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	38
5			Hexane, 3-ethyl-4-methyl-	128	C9H20	003074-77-9	35



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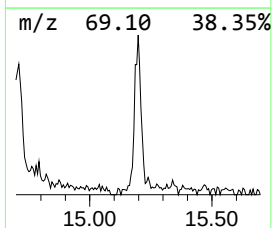
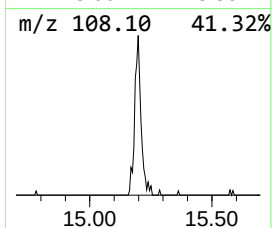
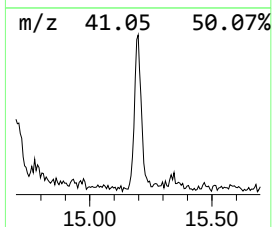
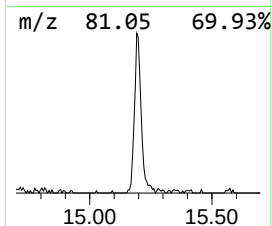
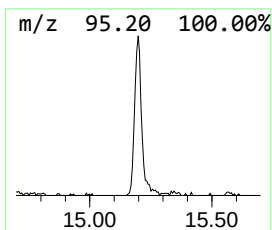
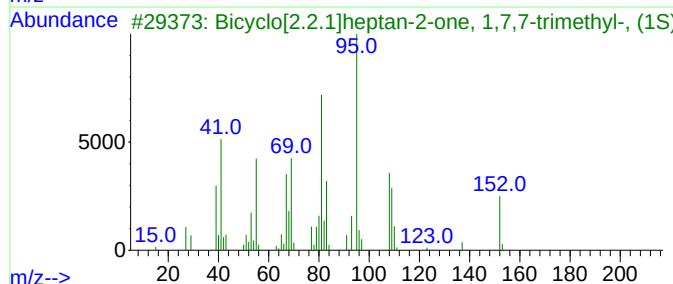
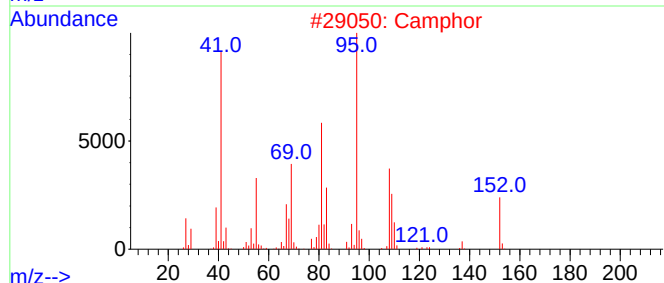
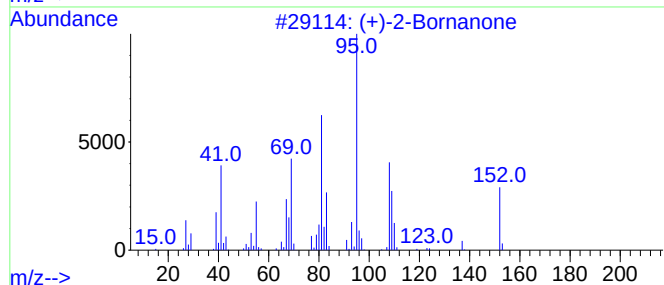
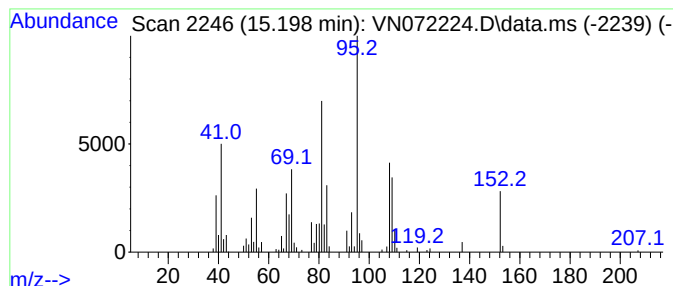
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Peak Number 6 (+)-2-Bornanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	8.65 ug/l	236413	1,4-Dichlorobenzene-d4	13.669

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	97
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	96
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46
5			5-Hepten-2-ol, 6-methyl-	128	C8H16O	001569-60-4	35



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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
Acetaldehyde	2.575	1320.6	ug/l	23052300	1	8.081	872789	50.0
Ethanol	3.681	70.6	ug/l	1233050	1	8.081	872789	50.0
1,3-Dioxolane, ...	8.245	34.0	ug/l	592605	1	8.081	872789	50.0
Eucalyptol	13.733	22.7	ug/l	620338	4	13.669	1366560	50.0
Carbonic acid, ...	14.351	8.4	ug/l	230609	4	13.669	1366560	50.0
(+)-2-Bornanone	15.198	8.7	ug/l	236413	4	13.669	1366560	50.0