

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020824\
 Data File : VN080967.D
 Acq On : 08 Feb 2024 16:34
 Operator : JC\MD
 Sample : P1415-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 240207098-02-VOA

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\82N020624W.M
 Title : SW846 8260

Signal : TIC: VN080967.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	52	58	66	rVB	106967	182649	2.02%	0.530%
2	2.818	139	147	153	rVB2	43007	104340	1.15%	0.303%
3	4.424	411	420	436	rBV2	128062	411534	4.55%	1.194%
4	5.518	590	606	625	rBV	2119326	7252395	80.18%	21.035%
5	7.435	917	932	946	rBV	3463571	9045020	100.00%	26.234%
6	7.553	946	952	962	rVB4	55666	164837	1.82%	0.478%
7	7.841	990	1001	1016	rBV	1150098	2955635	32.68%	8.573%
8	8.165	1046	1056	1061	rBV	296389	706115	7.81%	2.048%
9	8.224	1061	1066	1077	rVB	551056	1233209	13.63%	3.577%
10	8.582	1117	1127	1136	rBV3	315477	832562	9.20%	2.415%
11	9.106	1205	1216	1228	rBV	817682	1669738	18.46%	4.843%
12	10.570	1457	1465	1472	rBV	1029073	1910899	21.13%	5.542%
13	10.659	1472	1480	1490	rVB3	86581	213460	2.36%	0.619%
14	11.170	1557	1567	1578	rBV	149534	300946	3.33%	0.873%
15	11.870	1675	1686	1694	rBV	1038771	1956870	21.63%	5.676%
16	12.400	1770	1776	1781	rBV	73589	126101	1.39%	0.366%
17	12.853	1846	1853	1861	rVB	721383	1231913	13.62%	3.573%
18	13.188	1902	1910	1916	rBV4	43542	101961	1.13%	0.296%
19	13.611	1974	1982	1987	rBV	88333	154136	1.70%	0.447%
20	13.794	2005	2013	2021	rBV	944832	1678289	18.55%	4.868%
21	13.859	2021	2024	2036	rVB7	50161	133214	1.47%	0.386%
22	14.247	2085	2090	2096	rBV4	85541	177613	1.96%	0.515%
23	14.300	2096	2099	2110	rVB	69224	115843	1.28%	0.336%
24	14.447	2114	2124	2132	rBV7	46089	142043	1.57%	0.412%
25	14.676	2150	2163	2169	rBV	635111	1224078	13.53%	3.550%
26	15.288	2257	2267	2274	rBV6	78663	195760	2.16%	0.568%
27	15.376	2274	2282	2291	rBV7	103731	256537	2.84%	0.744%

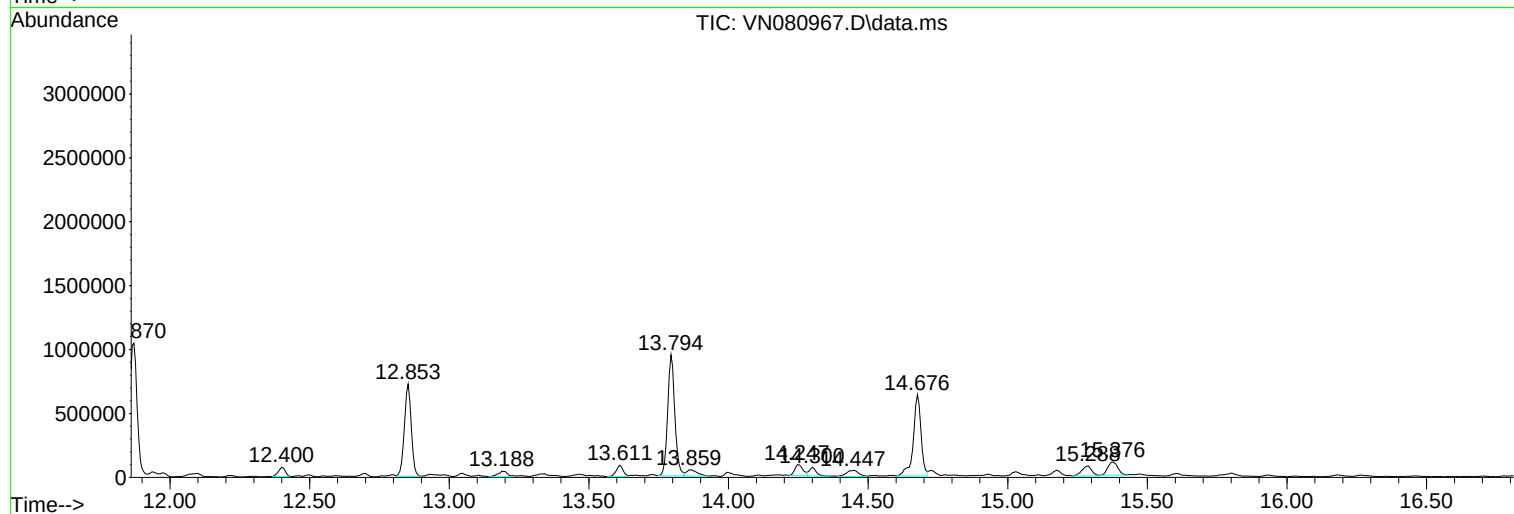
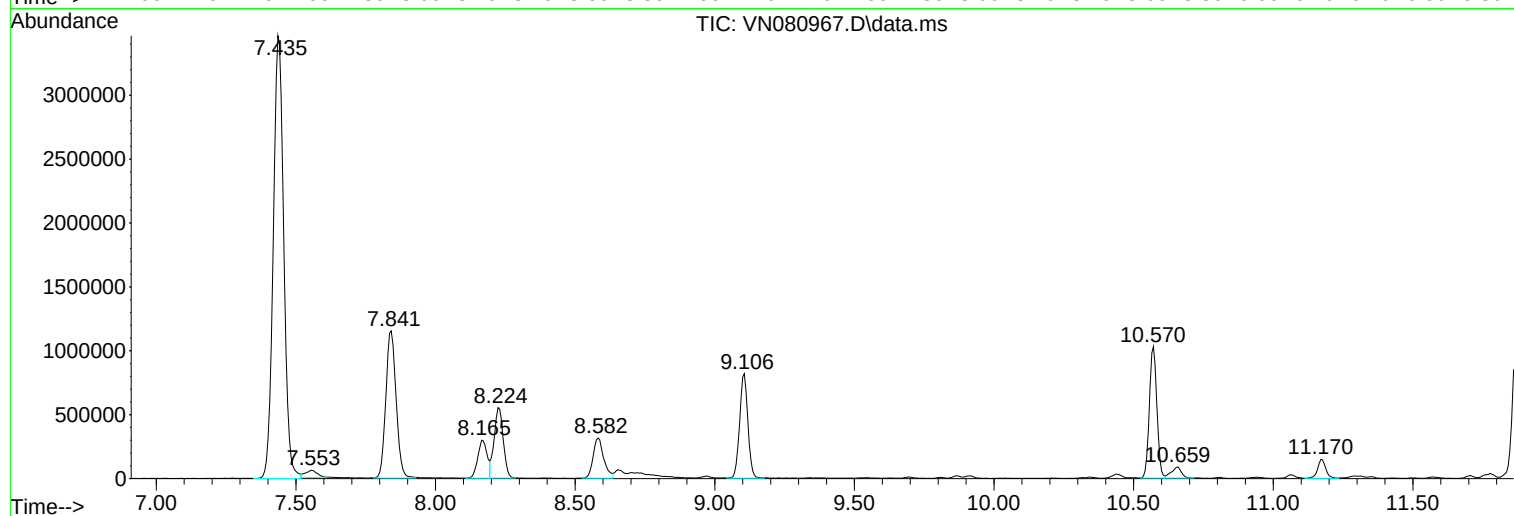
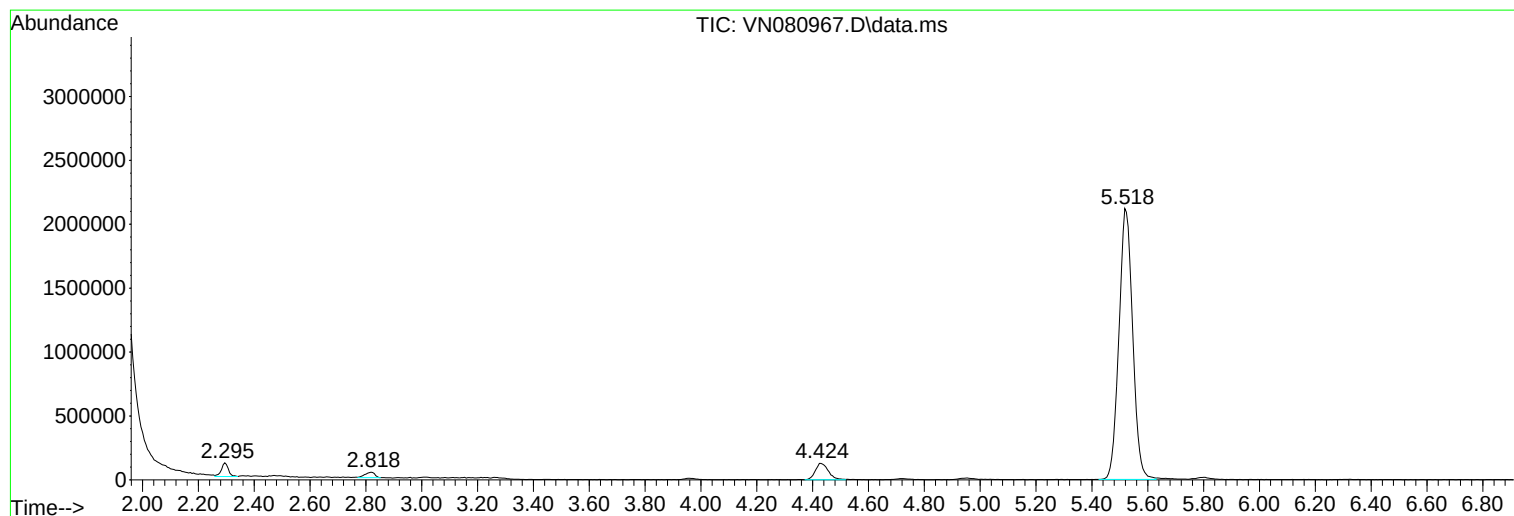
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M
Quant Title : SW846 8260

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



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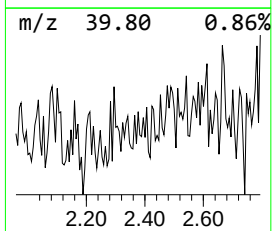
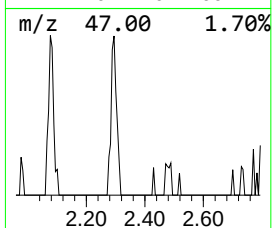
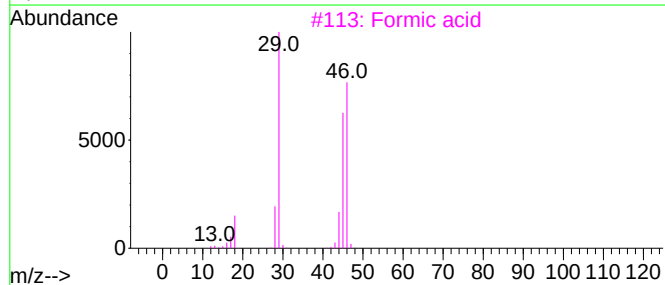
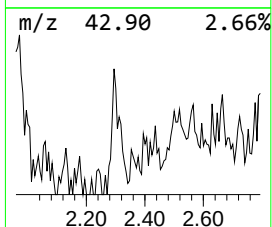
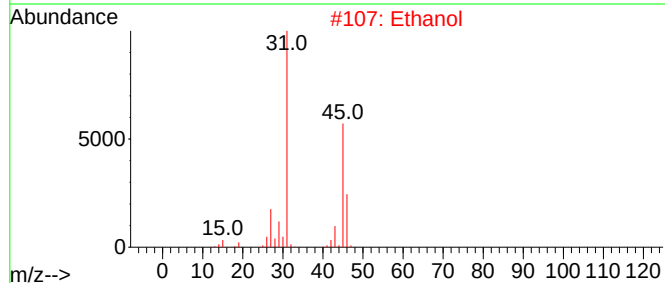
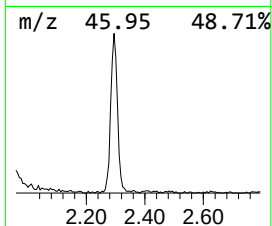
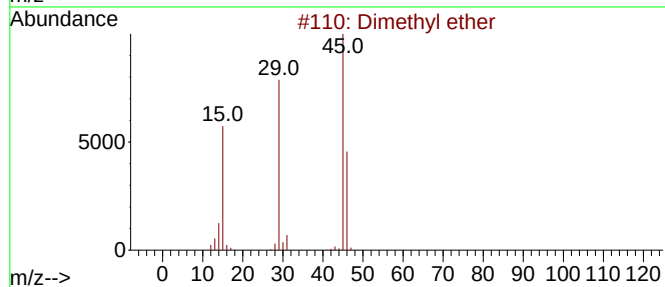
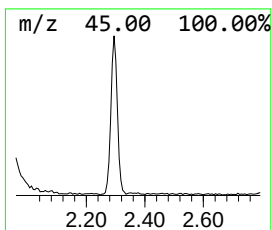
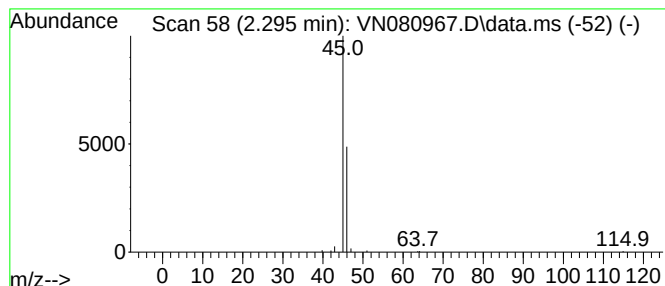
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Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.295	7.41 ug/l	182649	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	74
2			Ethanol	46	C2H6O	000064-17-5	7
3			Formic acid	46	CH2O2	000064-18-6	5
4			Oxalic acid	90	C2H2O4	000144-62-7	4
5			Propanedioic acid, dihydroxy-	136	C3H4O6	000560-27-0	4



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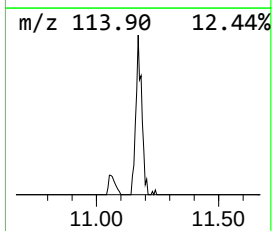
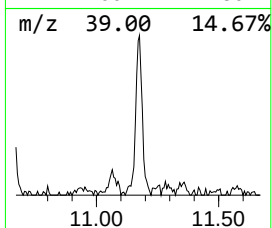
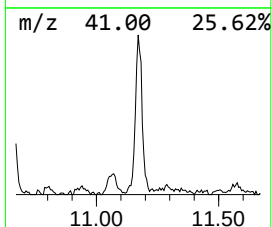
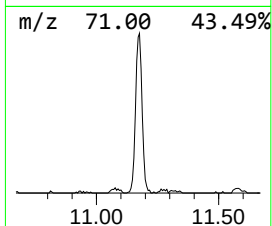
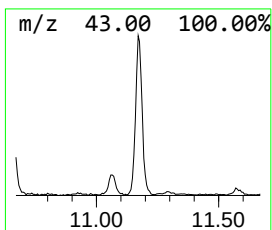
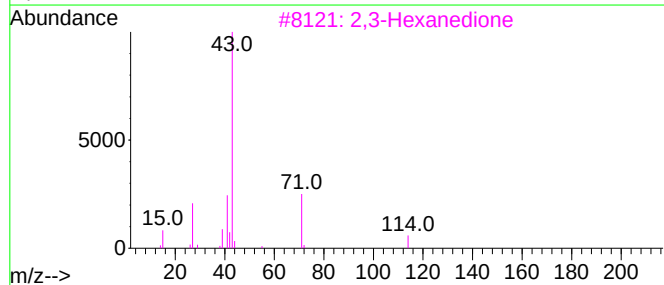
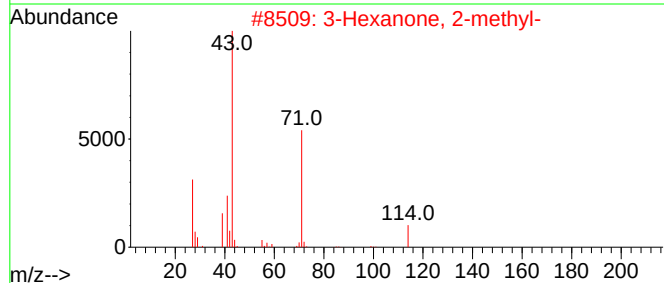
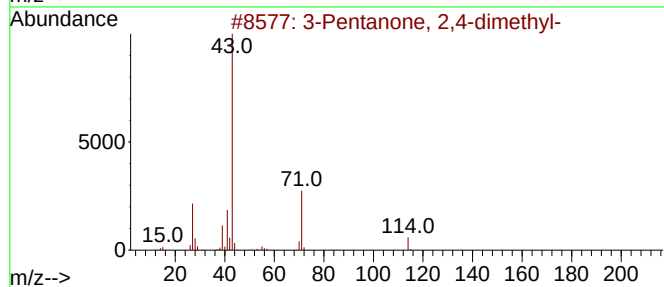
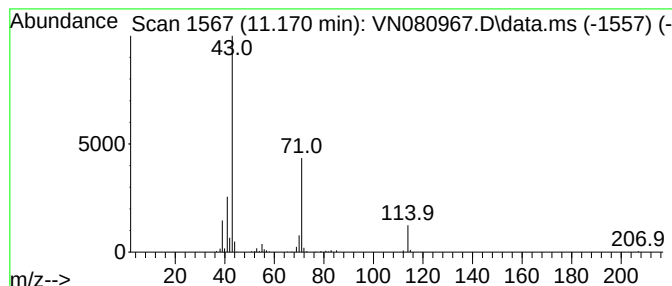
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Quant Title : SW846 8260

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

Peak Number 4 3-Pentanone, 2,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.170	7.69 ug/l	300946	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	90
2			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	86
3			2,3-Hexanedione	114	C6H10O2	003848-24-6	80
4			4-Heptanone	114	C7H14O	000123-19-3	64
5			Pyrrolidine	71	C4H9N	000123-75-1	53



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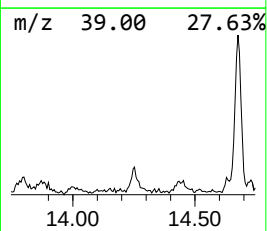
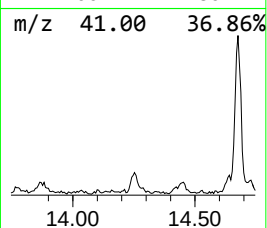
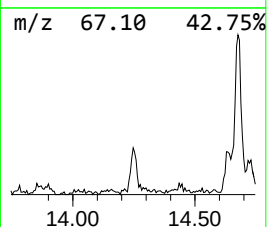
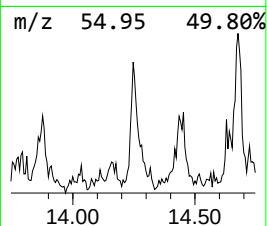
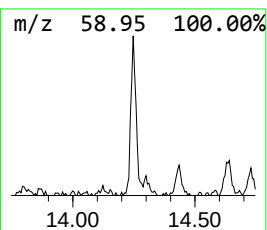
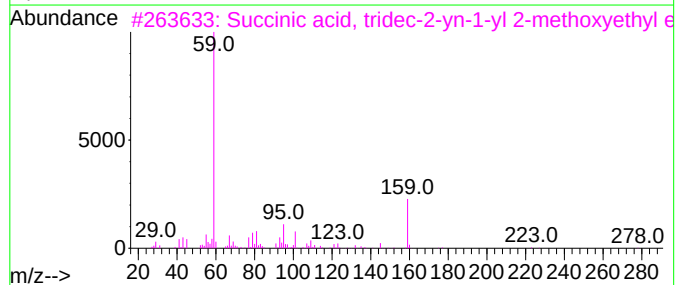
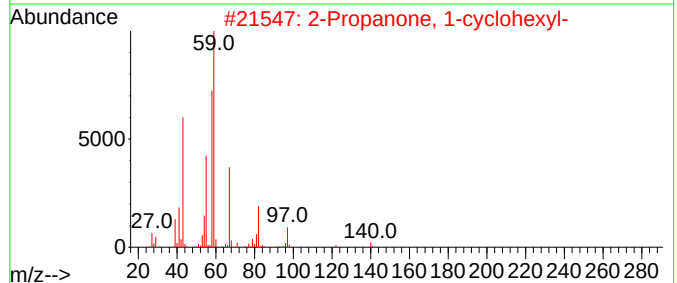
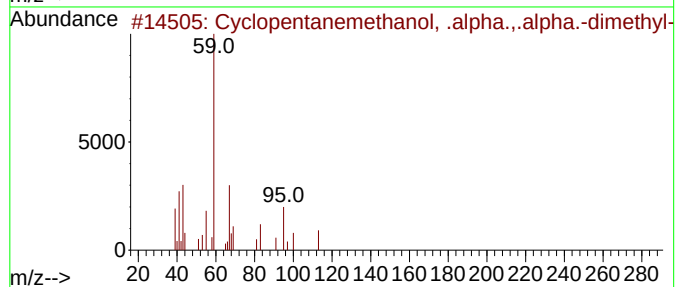
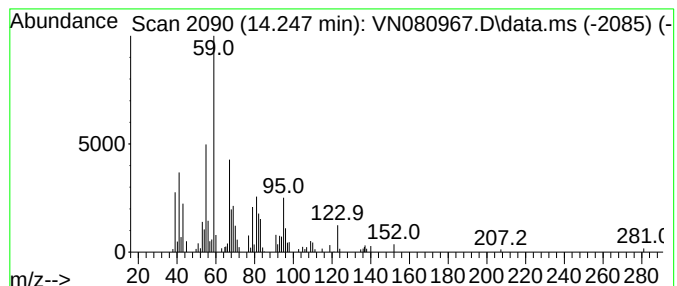
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Quant Title : SW846 8260

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

Peak Number 5 Cyclopentanemethanol, .alph... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.247	5.29 ug/l	177613	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	50
2			2-Propanone, 1-cyclohexyl-	140	C9H16O	000103-78-6	47
3			Succinic acid, tridec-2-yn-1-yl ...	354	C20H34O5	1000390-75-1	38
4			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	38
5			1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	35



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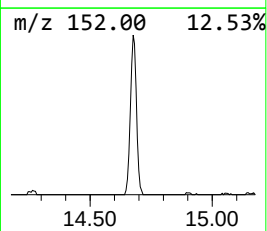
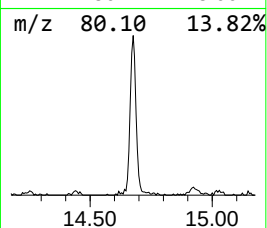
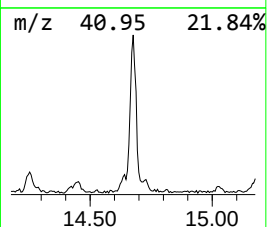
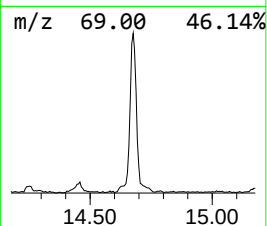
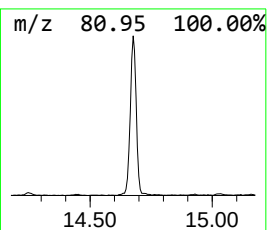
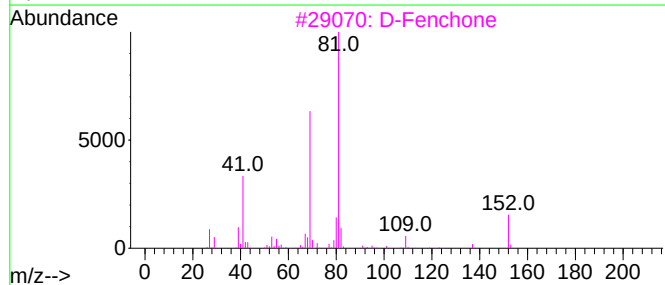
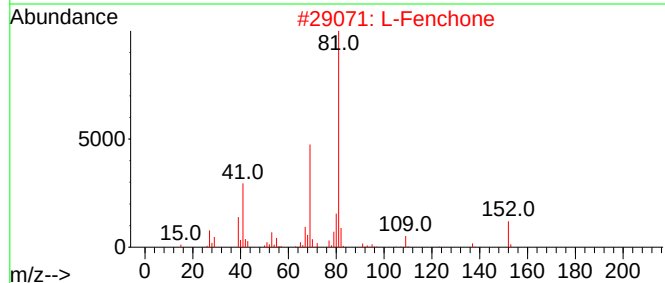
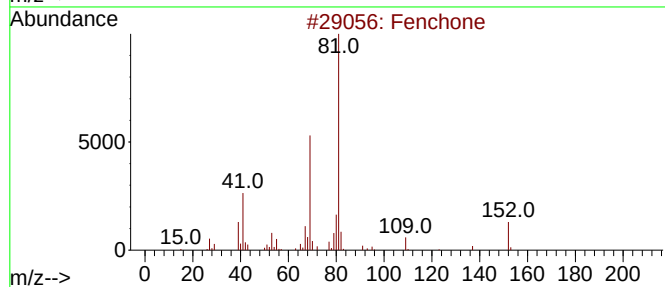
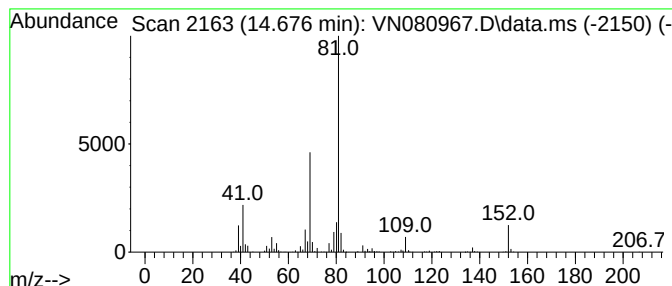
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Quant Title : SW846 8260

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

Peak Number 6 Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.676	36.47 ug/l	1224080	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	95
2			L-Fenchone	152	C10H16O	007787-20-4	94
3			D-Fenchone	152	C10H16O	004695-62-9	90
4			2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	47
5			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	42



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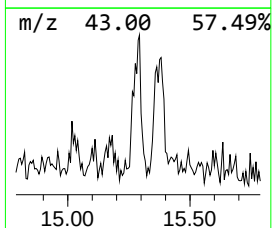
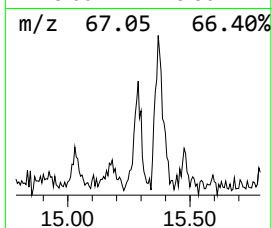
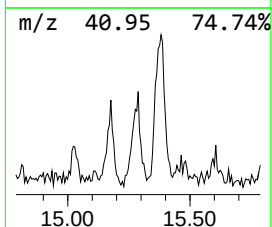
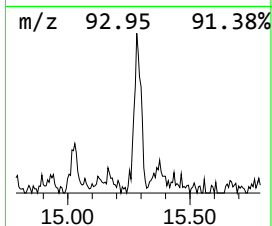
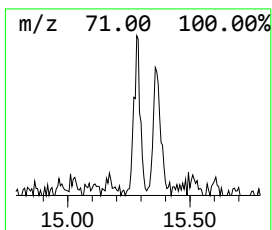
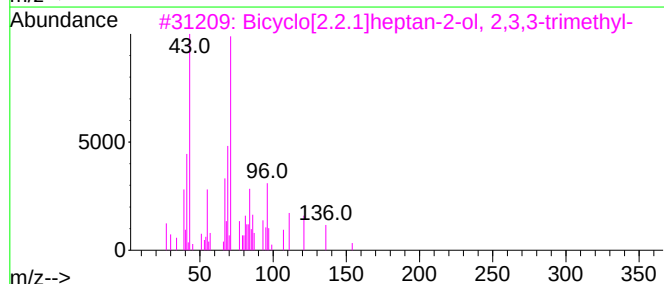
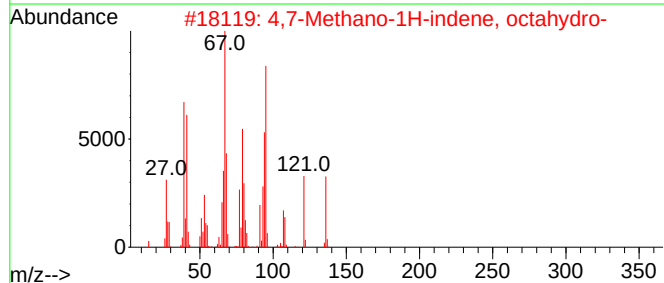
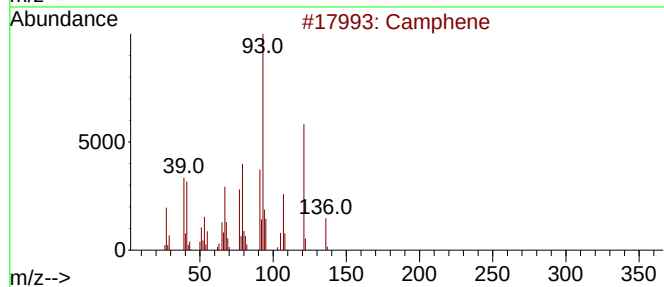
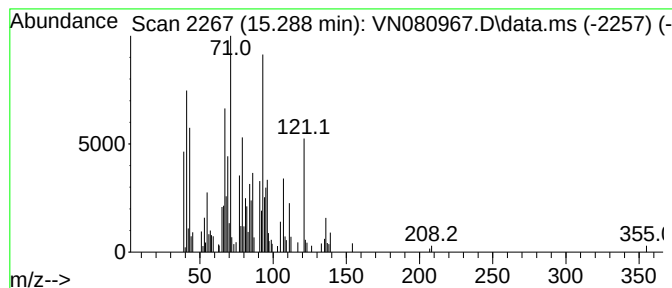
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M
Quant Title : SW846 8260

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

Peak Number 7 Camphene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.288	5.83 ug/l	195760	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphene	136	C10H16	000079-92-5	83
2			4,7-Methano-1H-indene, octahydro-	136	C10H16	006004-38-2	38
3			Bicyclo[2.2.1]heptan-2-ol, 2,3,3...	154	C10H18O	000465-31-6	30
4			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	30
5			1,6-Cyclodecadiene	136	C10H16	007049-13-0	25



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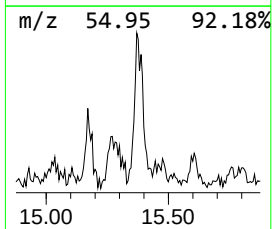
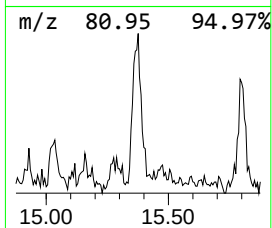
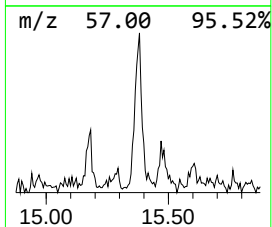
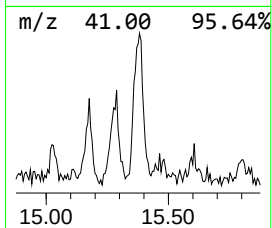
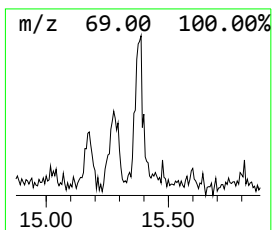
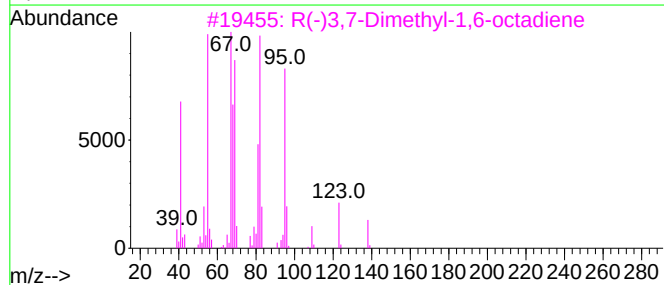
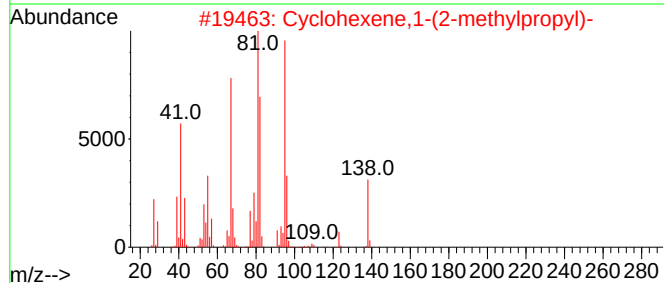
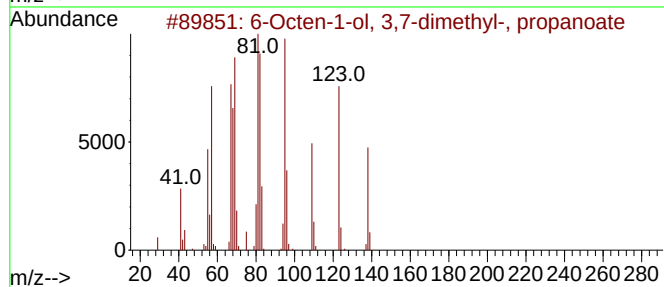
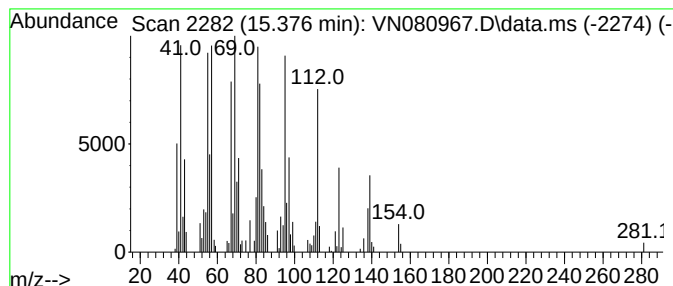
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Quant Title : SW846 8260

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

Peak Number 8 6-Octen-1-ol, 3,7-dimethyl-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.376	7.64 ug/l	256537	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Octen-1-ol, 3,7-dimethyl-, pro...	212	C13H24O2	000141-14-0	64
2			Cyclohexene,1-(2-methylpropyl)-	138	C10H18	003983-03-7	55
3			R(-)3,7-Dimethyl-1,6-octadiene	138	C10H18	010281-56-8	43
4			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-27-2	38
5			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN020824\
Data File : VN080967.D
Acq On : 08 Feb 2024 16:34
Operator : JC\MD
Sample : P1415-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240207098-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N020624W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl ether	2.295	7.4	ug/l	182649	1	8.229	1233210	50.0
3-Pentanone, 2,...	11.170	7.7	ug/l	300946	3	11.870	1956870	50.0
Cyclopentanemet...	14.247	5.3	ug/l	177613	4	13.794	1678290	50.0
Fenchone	14.676	36.5	ug/l	1224080	4	13.794	1678290	50.0
Camphene	15.288	5.8	ug/l	195760	4	13.794	1678290	50.0
6-Octen-1-ol, 3...	15.376	7.6	ug/l	256537	4	13.794	1678290	50.0