

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062024\
 Data File : VN082664.D
 Acq On : 20 Jun 2024 13:34
 Operator : JC\MD
 Sample : P2981-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 240619096-02-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\82N061724W.M
 Title : SW846 8260

Signal : TIC: VN082664.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	53	58	66	rVB	138928	220487	4.20%	0.927%
2	2.824	139	148	160	rVB2	29840	82931	1.58%	0.349%
3	4.424	410	420	440	rBV	214036	658736	12.56%	2.770%
4	4.724	458	471	479	rBV2	25966	85376	1.63%	0.359%
5	5.524	590	607	641	rBV	1215418	4238429	80.79%	17.820%
6	7.441	920	933	951	rBV2	1722535	5245973	100.00%	22.056%
7	7.841	984	1001	1023	rBV	854372	2193251	41.81%	9.221%
8	8.171	1045	1057	1061	rBV2	129057	309935	5.91%	1.303%
9	8.230	1061	1067	1076	rVB	208394	473167	9.02%	1.989%
10	8.582	1117	1127	1136	rBV2	162343	479089	9.13%	2.014%
11	8.659	1136	1140	1146	rVB5	35847	80652	1.54%	0.339%
12	9.106	1207	1216	1225	rBV	325980	662104	12.62%	2.784%
13	9.535	1282	1289	1296	rVB	28910	56815	1.08%	0.239%
14	10.447	1433	1444	1454	rBV3	26987	65885	1.26%	0.277%
15	10.571	1457	1465	1471	rVV	531812	982705	18.73%	4.132%
16	10.635	1471	1476	1488	rVB3	62157	179738	3.43%	0.756%
17	11.171	1558	1567	1577	rVV	98160	198934	3.79%	0.836%
18	11.776	1662	1670	1675	rVV6	22670	60369	1.15%	0.254%
19	11.865	1675	1685	1694	rVV	478036	945548	18.02%	3.975%
20	11.965	1694	1702	1709	rVV2	83054	188378	3.59%	0.792%
21	12.071	1709	1720	1731	rVB4	76957	184286	3.51%	0.775%
22	12.400	1763	1776	1782	rBV	60892	113565	2.16%	0.477%
23	12.853	1846	1853	1861	rVB	383132	666620	12.71%	2.803%
24	13.482	1950	1960	1966	rBV2	36380	85644	1.63%	0.360%
25	13.612	1973	1982	1988	rBV3	55306	110214	2.10%	0.463%
26	13.729	1997	2002	2006	rBV2	32505	53760	1.02%	0.226%
27	13.794	2006	2013	2020	rVV	468048	879722	16.77%	3.699%
28	13.859	2020	2024	2036	rVB4	85010	190205	3.63%	0.800%
29	13.994	2042	2047	2062	rVB	37614	82488	1.57%	0.347%
30	14.247	2084	2090	2094	rBV3	71670	129408	2.47%	0.544%
31	14.300	2094	2099	2107	rVB2	73790	145526	2.77%	0.612%
32	14.453	2114	2125	2133	rVB7	38556	104372	1.99%	0.439%
33	14.676	2157	2163	2169	rVB	513189	821627	15.66%	3.454%
34	14.935	2202	2207	2214	rBV7	37054	68255	1.30%	0.287%
35	15.023	2216	2222	2229	rBV4	39373	81313	1.55%	0.342%
36	15.100	2229	2235	2241	rVB2	97950	169240	3.23%	0.712%

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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

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37	15.282	2258	2266	2268	rBV6	84884	201120	3.83%	0.846%
38	15.329	2268	2274	2278	rBV	709361	1327357	25.30%	5.581%
39	15.517	2301	2306	2312	rVB2	67171	110972	2.12%	0.467%
40	15.641	2317	2327	2335	rVB	250847	498290	9.50%	2.095%
41	15.794	2349	2353	2369	rVB5	54199	152851	2.91%	0.643%
42	16.011	2381	2390	2398	rBV2	92286	199948	3.81%	0.841%

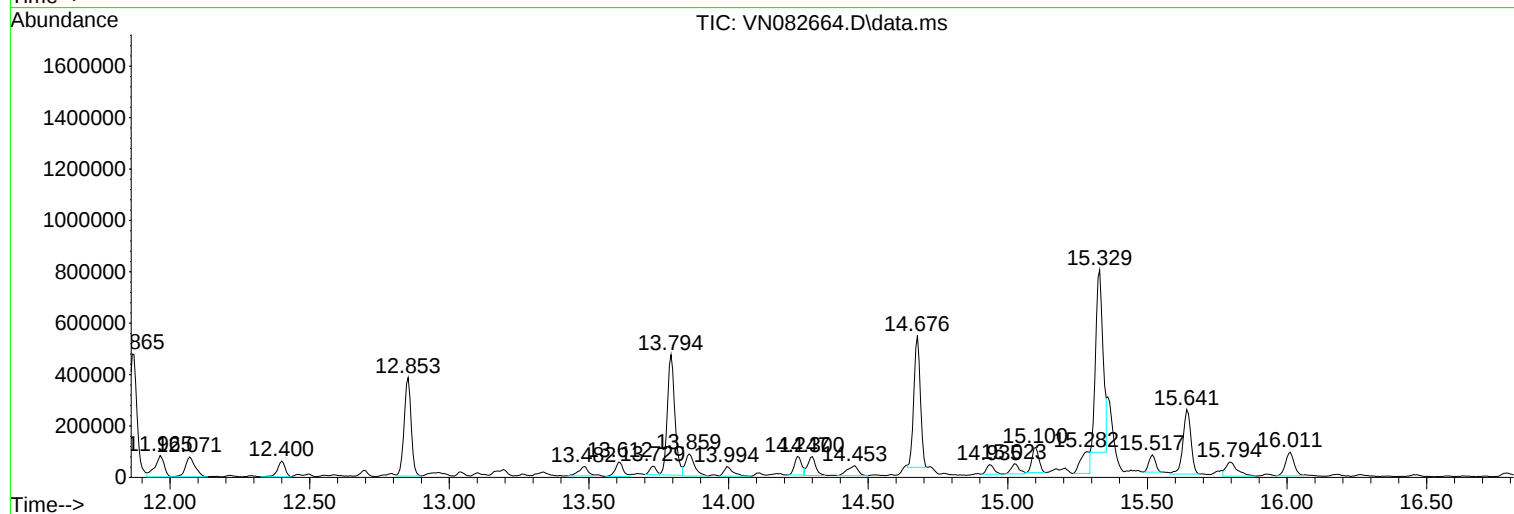
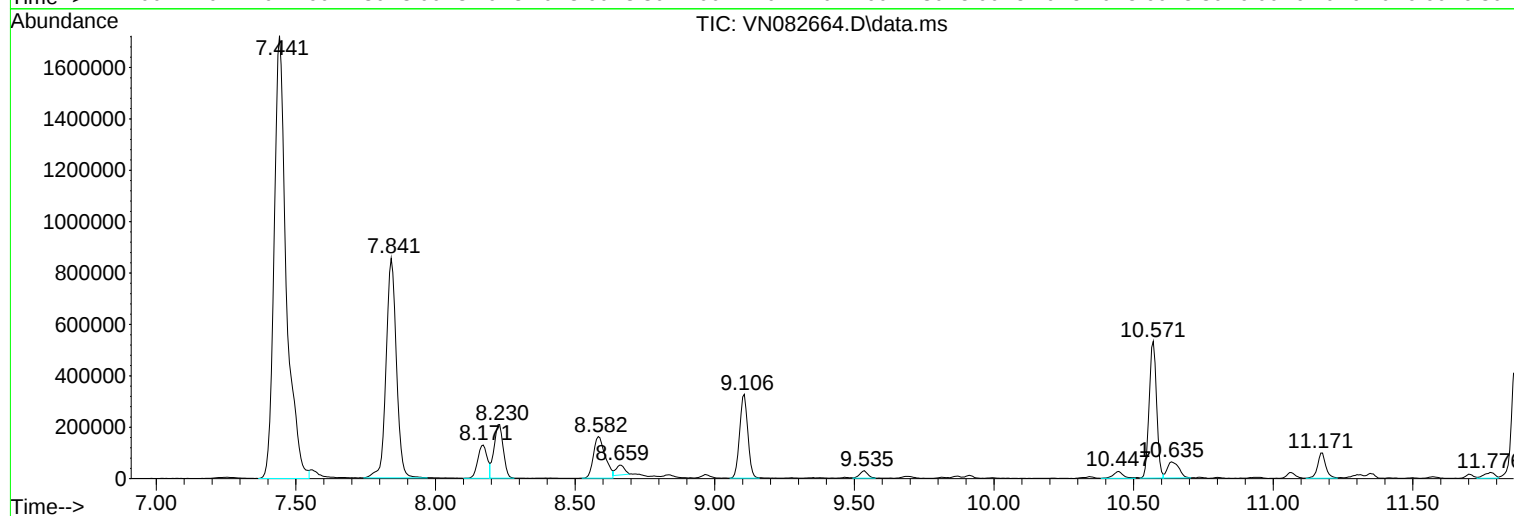
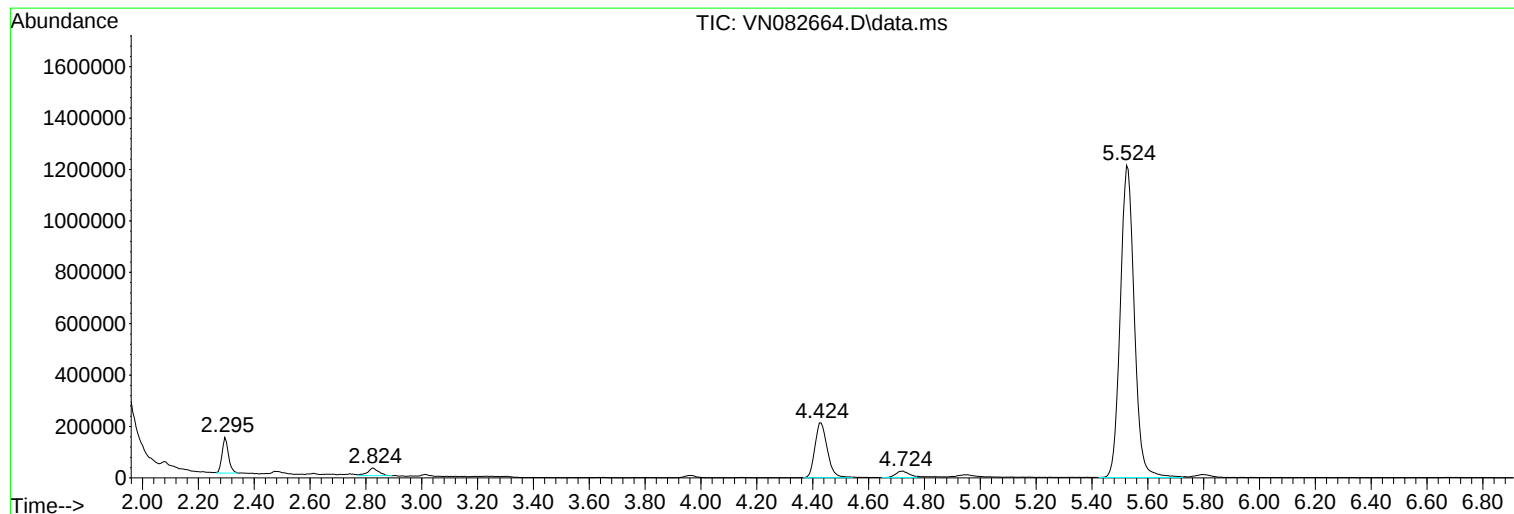
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Quant Title : SW846 8260

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



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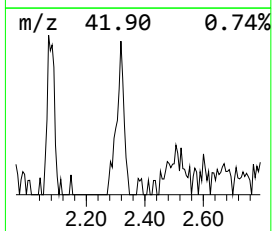
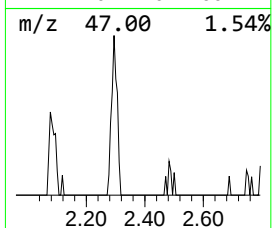
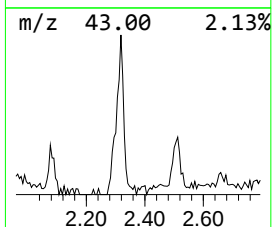
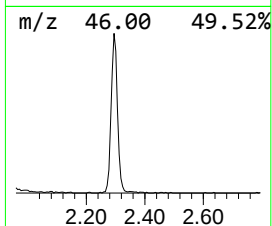
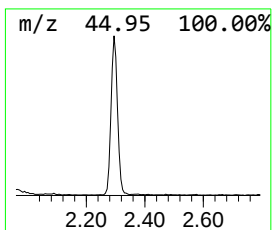
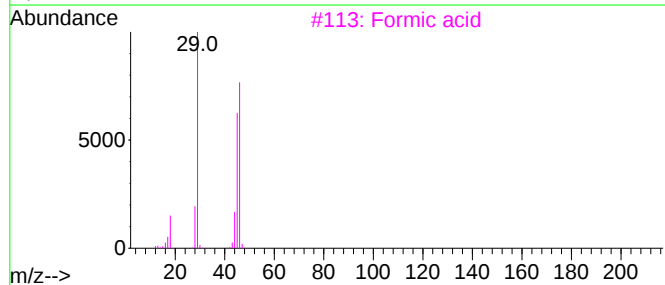
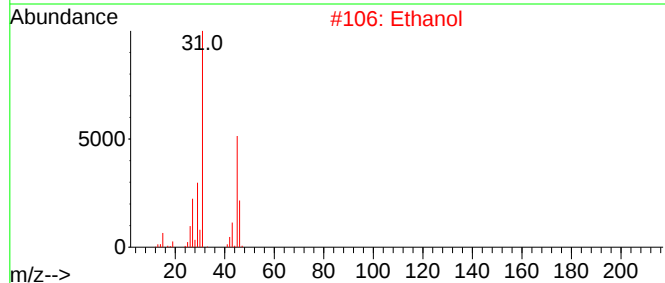
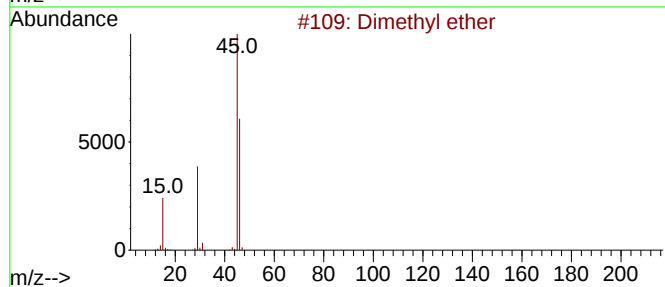
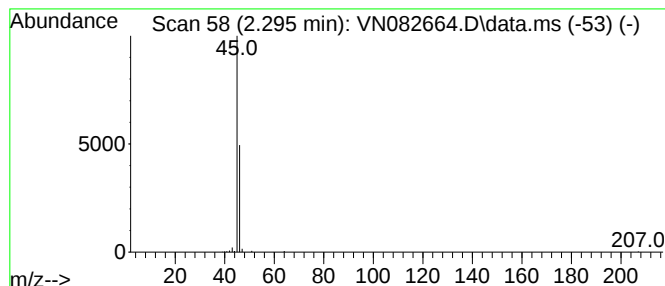
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061724W.M
Quant Title : SW846 8260

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

Peak Number 1 Dimethyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.295	23.30 ug/l	220487	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	64
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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Instrument :
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240619096-02-VOA

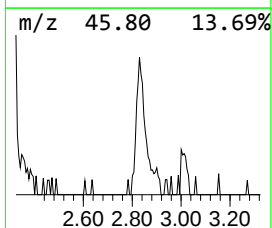
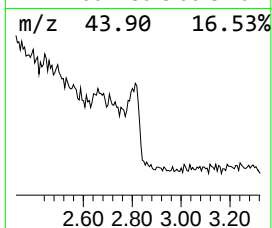
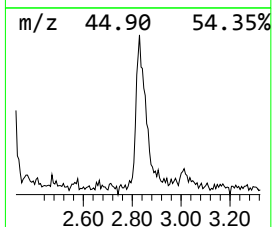
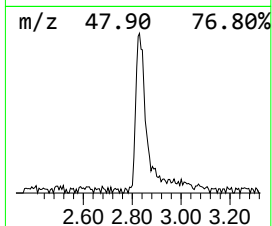
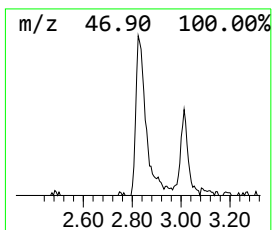
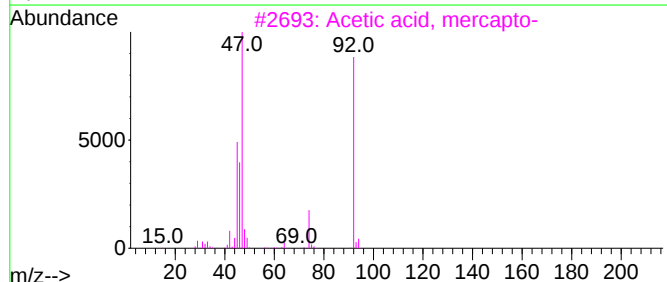
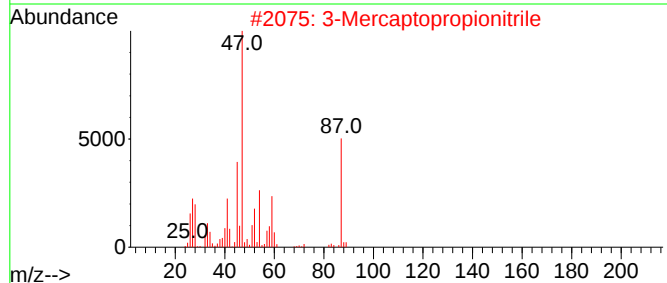
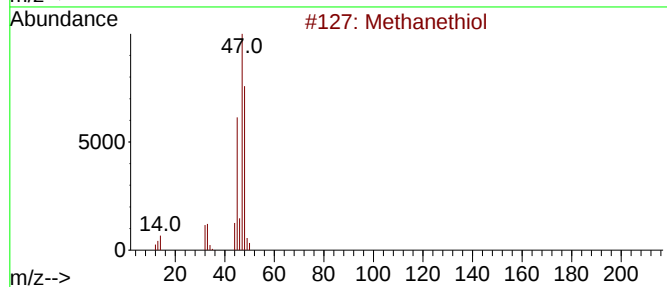
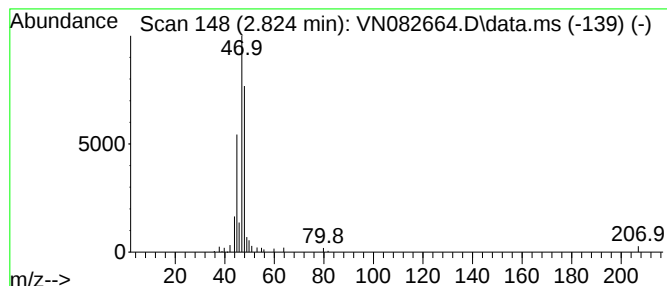
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061724W.M
Quant Title : SW846 8260

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

Peak Number 2 Methanethiol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.824	8.76 ug/l	82931	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	91
2			3-Mercaptopropionitrile	87	C3H5NS	001001-58-7	25
3			Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9
4			Methional	104	C4H8OS	003268-49-3	9
5			Ethanol	46	C2H6O	000064-17-5	5



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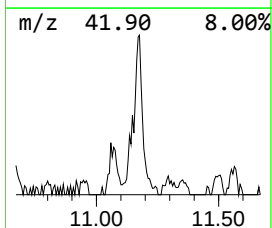
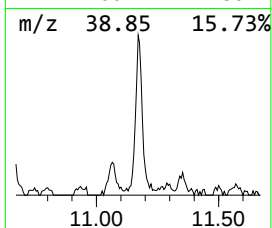
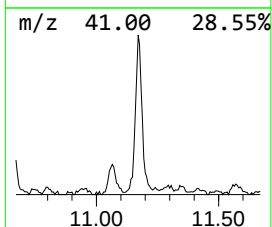
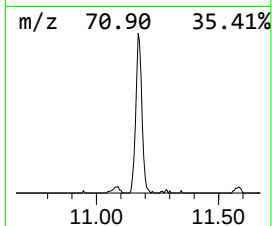
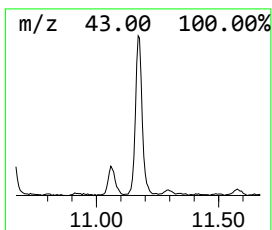
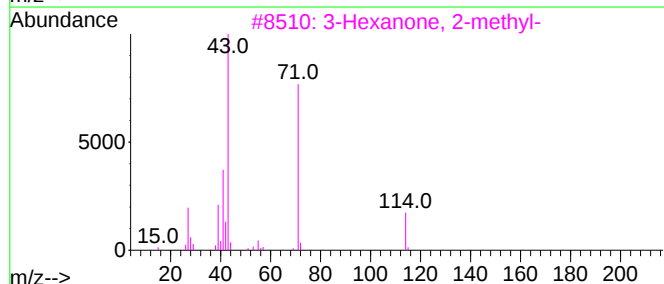
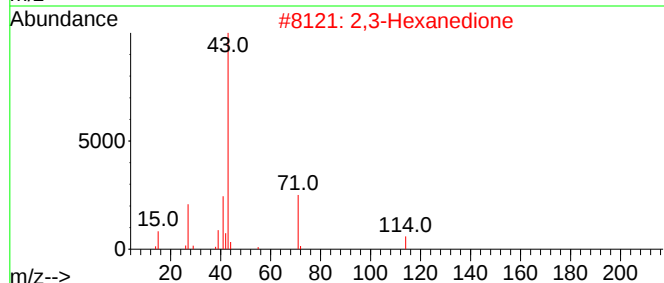
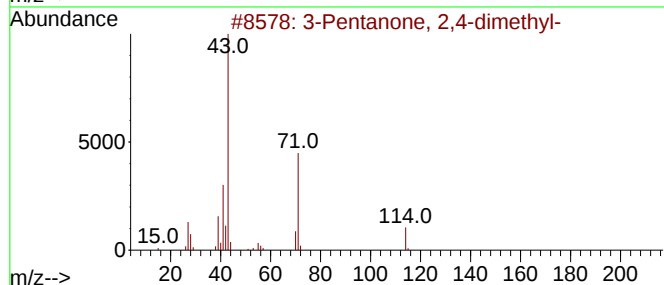
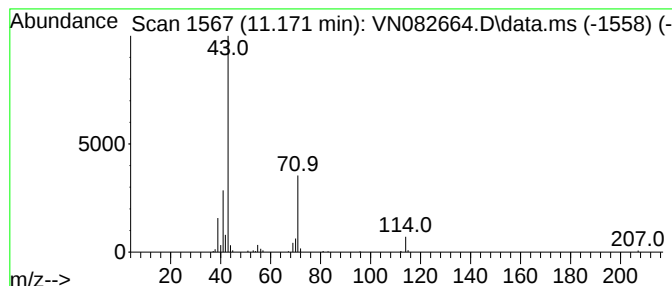
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061724W.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 3-Pentanone, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.171	10.52 ug/l	198934	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	81
2			2,3-Hexanedione	114	C6H10O2	003848-24-6	64
3			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	49
4			Sulfurous acid, pentyl 2-propyl ...	194	C8H18O3S	1000309-11-5	39
5			4-Heptanone	114	C7H14O	000123-19-3	38



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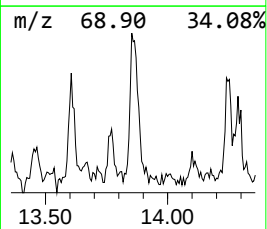
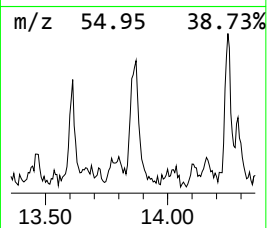
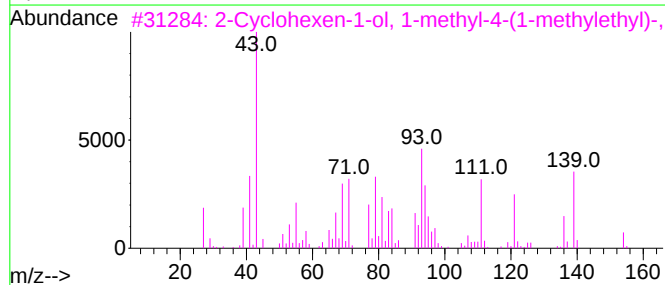
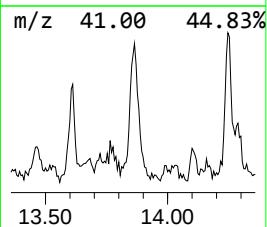
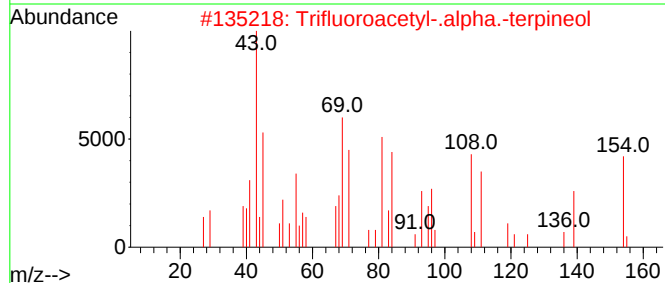
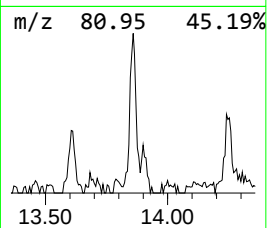
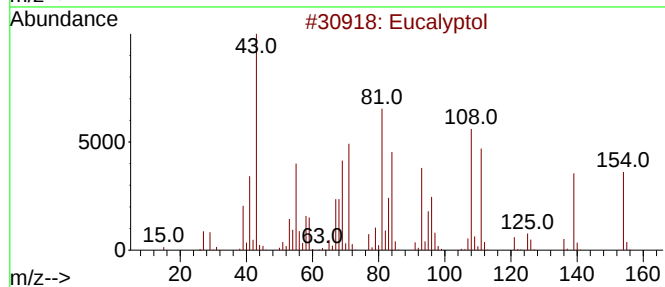
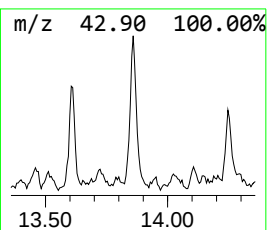
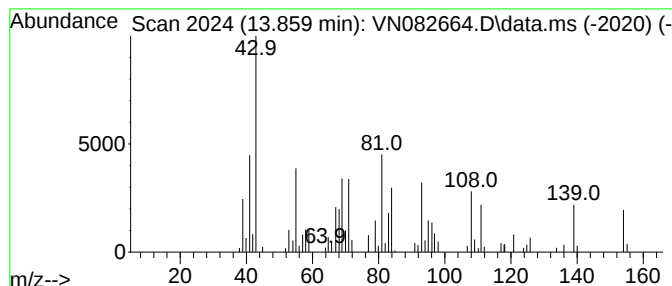
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Eucalyptol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.859	10.81 ug/l	190205	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	97
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	72
3			2-Cyclohexen-1-ol, 1-methyl-4-(1-methylethyl)-	154	C10H18O	029803-81-4	37
4			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	25
5			3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	18



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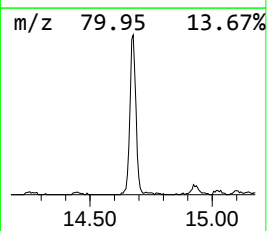
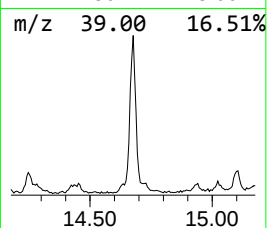
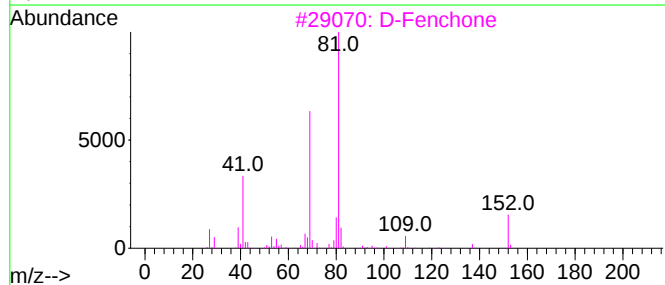
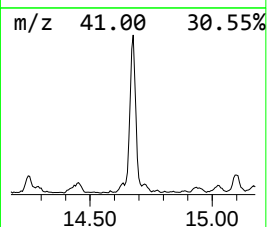
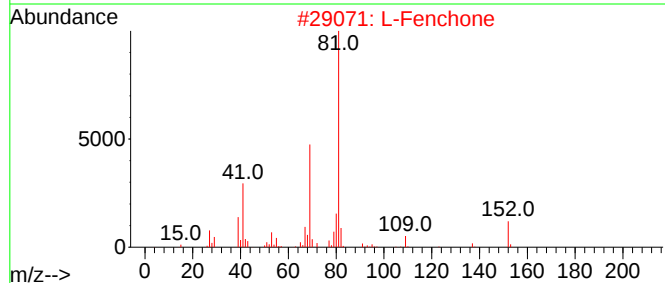
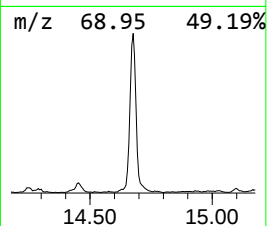
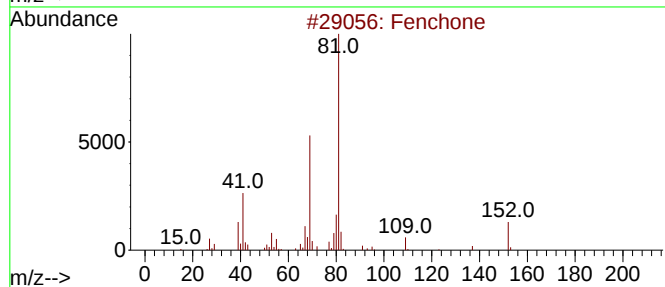
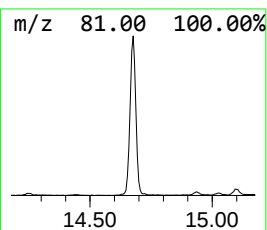
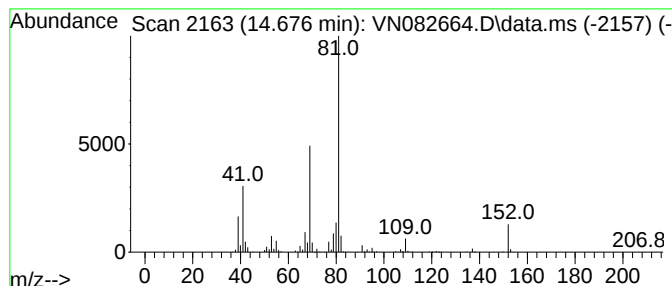
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Quant Title : SW846 8260

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

Peak Number 5 Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.676	46.70 ug/l	821627	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	95
3			D-Fenchone	152	C10H16O	004695-62-9	91
4			1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3NO2	1000301-43-3	50
5			Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062024\
Data File : VN082664.D
Acq On : 20 Jun 2024 13:34
Operator : JC\MD
Sample : P2981-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240619096-02-VOA

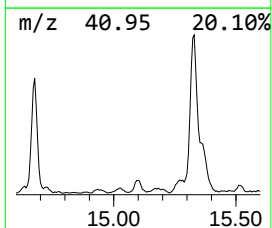
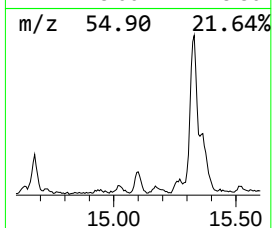
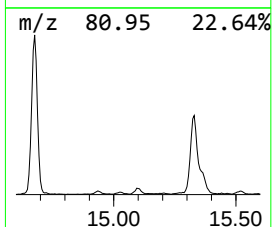
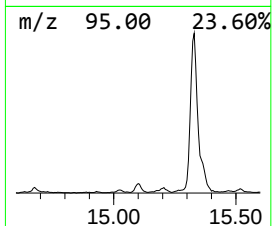
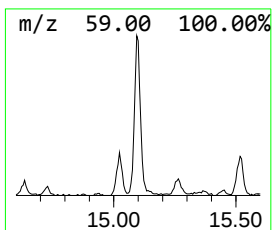
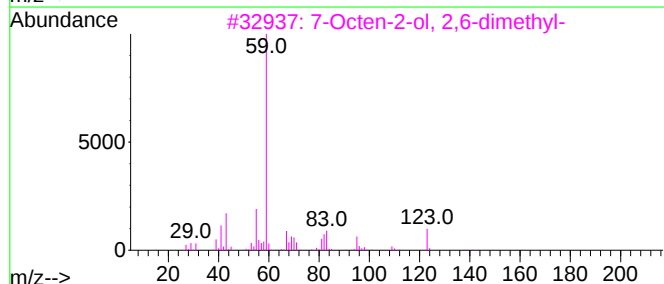
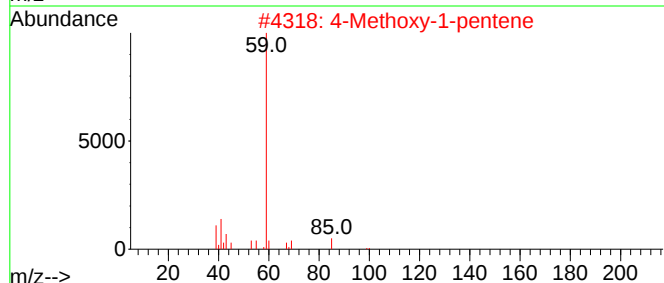
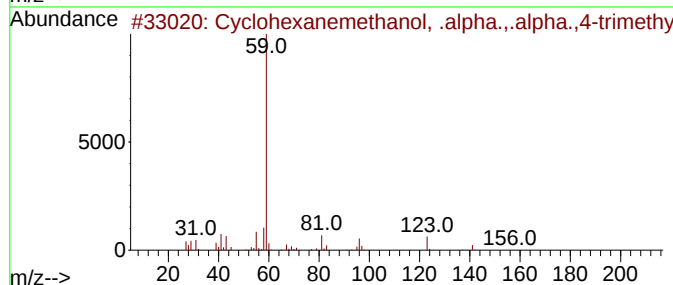
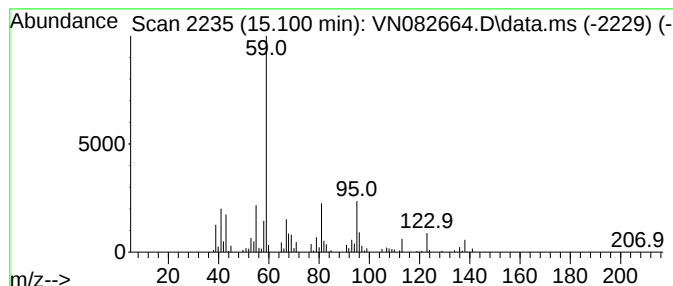
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Quant Title : SW846 8260

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

Peak Number 6 Cyclohexanemethanol, .alpha... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.100	9.62 ug/l	169240	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	53
2			4-Methoxy-1-pentene	100	C6H12O	098386-09-5	43
3			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	42
4			Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	007322-63-6	40
5			trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1010281-69-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062024\
Data File : VN082664.D
Acq On : 20 Jun 2024 13:34
Operator : JC\MD
Sample : P2981-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240619096-02-VOA

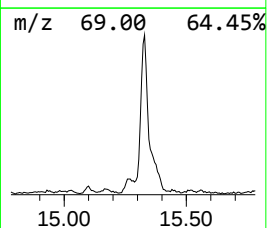
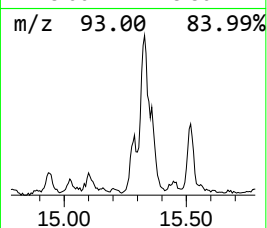
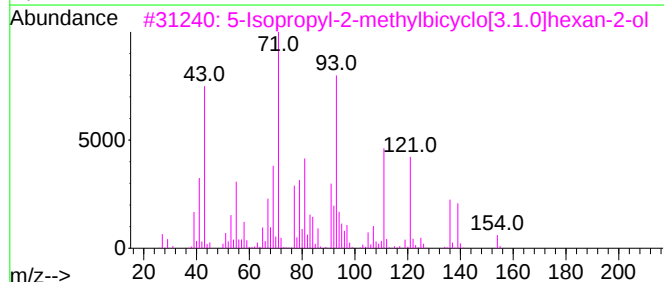
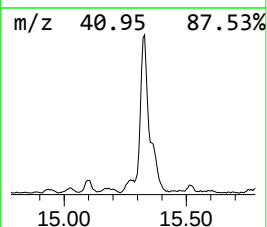
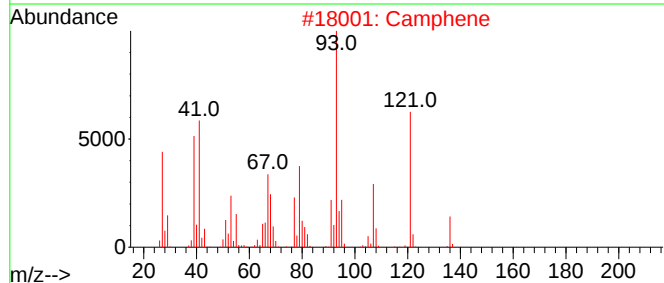
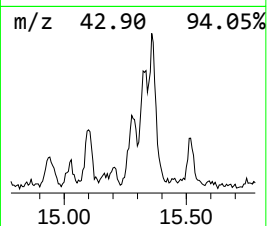
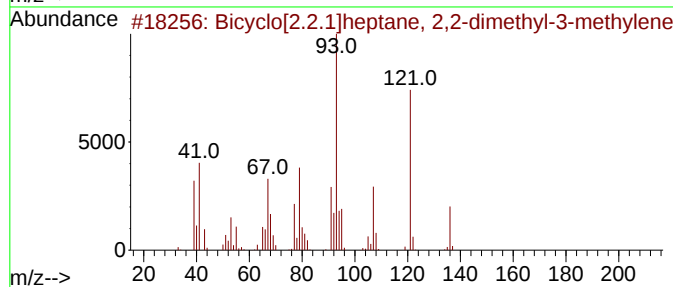
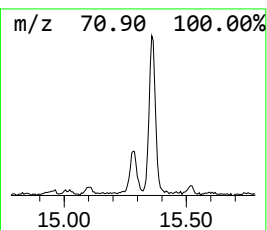
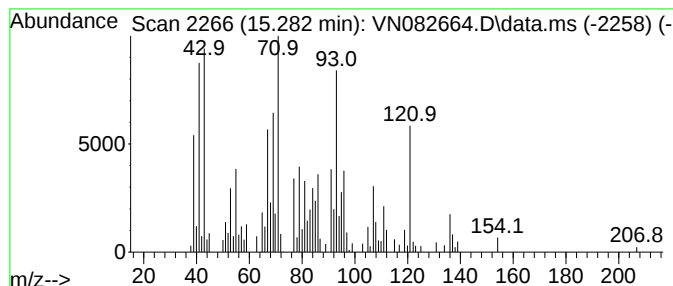
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Quant Title : SW846 8260

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

Peak Number 7 Bicyclo[2.2.1]heptane, 2,2-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.282	11.43 ug/l	201120	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	80
2			Camphene	136	C10H16	000079-92-5	70
3			5-Isopropyl-2-methylbicyclo[3.1....	154	C10H18O	000546-79-2	52
4			Bicyclo[4.1.0]heptan-3-ol, 4,7,7...	154	C10H18O	038748-96-8	46
5			Bicyclo[2.2.1]heptan-2-ol, 2,3,3...	154	C10H18O	000465-31-6	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062024\
Data File : VN082664.D
Acq On : 20 Jun 2024 13:34
Operator : JC\MD
Sample : P2981-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240619096-02-VOA

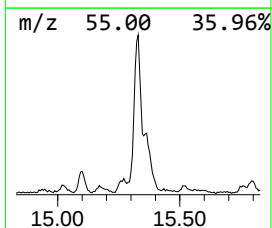
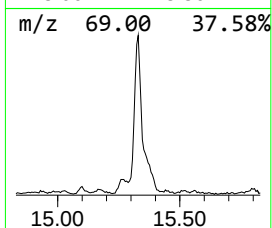
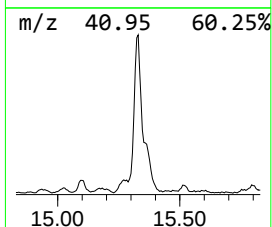
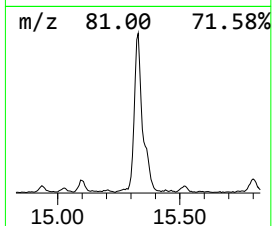
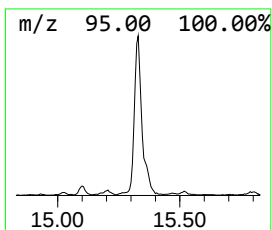
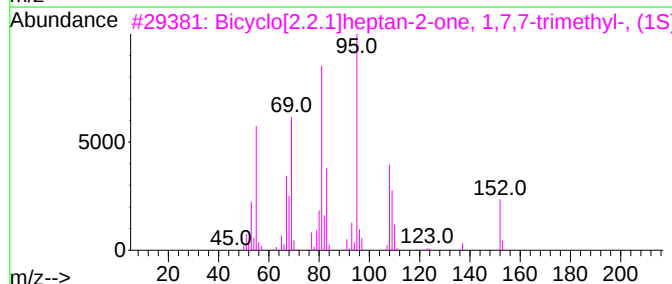
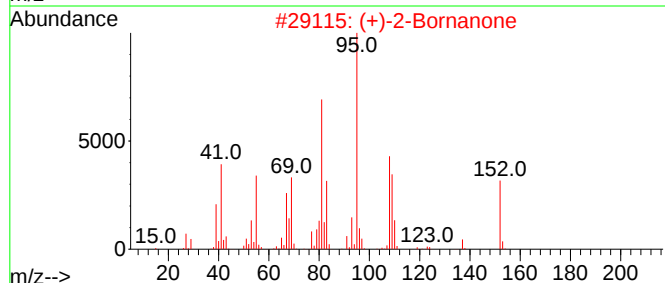
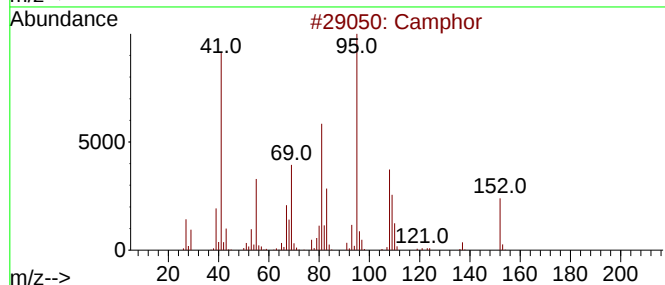
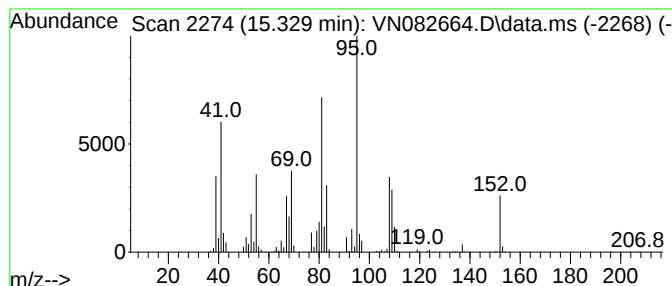
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Quant Title : SW846 8260

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

Peak Number 8 Camphor Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.329	75.44 ug/l	1327360	1,4-Dichlorobenzene-d4	13.794

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	94
4			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062024\
Data File : VN082664.D
Acq On : 20 Jun 2024 13:34
Operator : JC\MD
Sample : P2981-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240619096-02-VOA

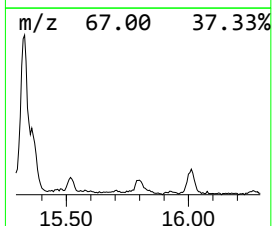
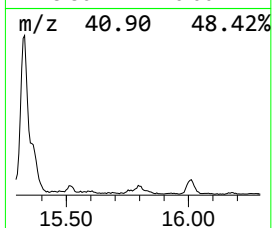
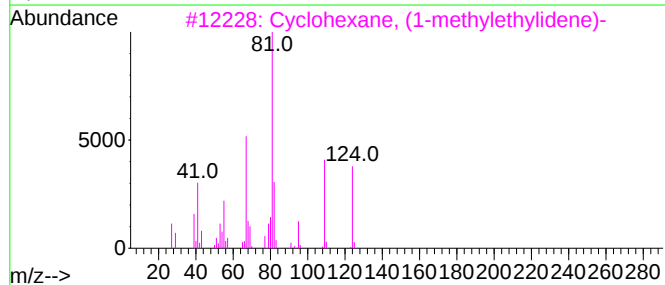
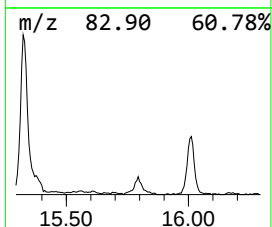
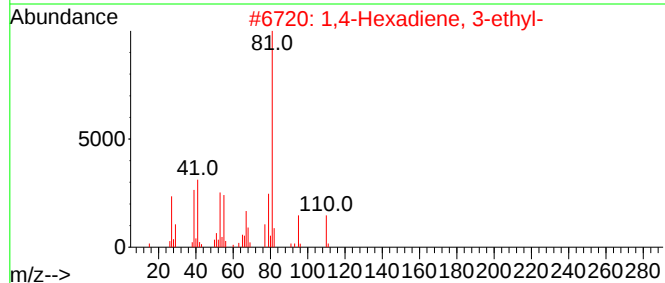
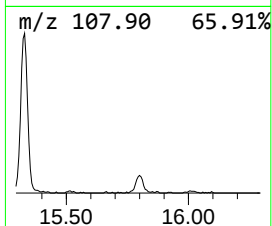
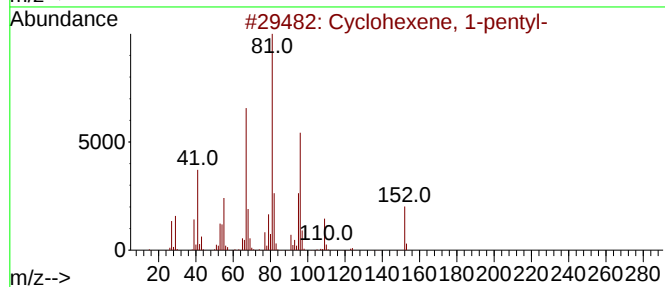
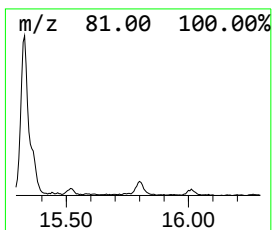
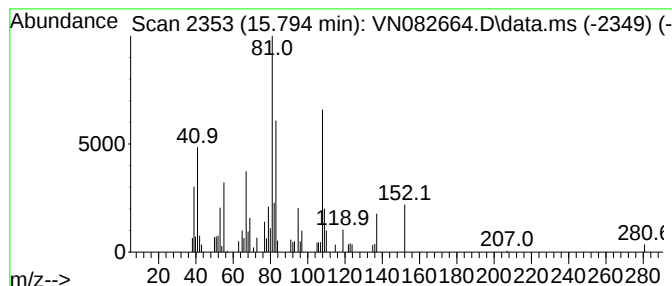
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Quant Title : SW846 8260

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

Peak Number 9 unknown15.794 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.794	8.69 ug/l	152851	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1-pentyl-	152	C11H20	015232-85-6	43
2			1,4-Hexadiene, 3-ethyl-	110	C8H14	002080-89-9	30
3			Cyclohexane, (1-methylethylidene)-	124	C9H16	005749-72-4	27
4			Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	27
5			Cyclopentene, 3-methyl-1-(1-meth...	124	C9H16	051115-02-7	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062024\
Data File : VN082664.D
Acq On : 20 Jun 2024 13:34
Operator : JC\MD
Sample : P2981-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240619096-02-VOA

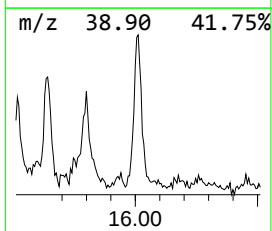
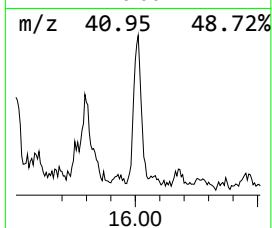
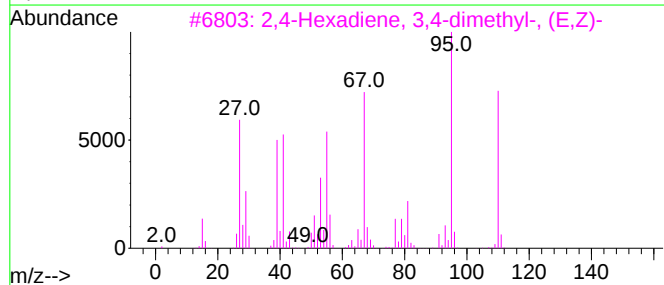
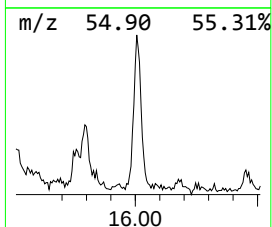
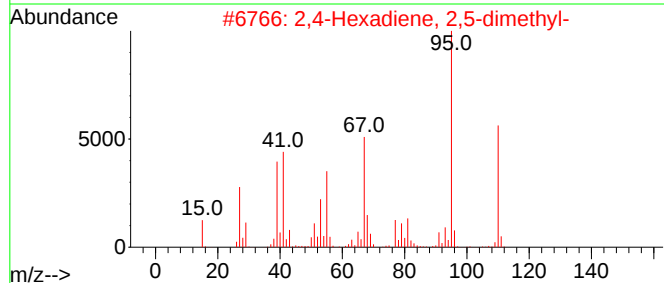
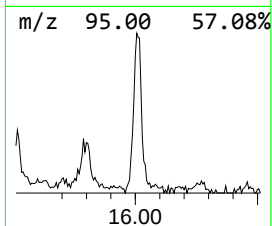
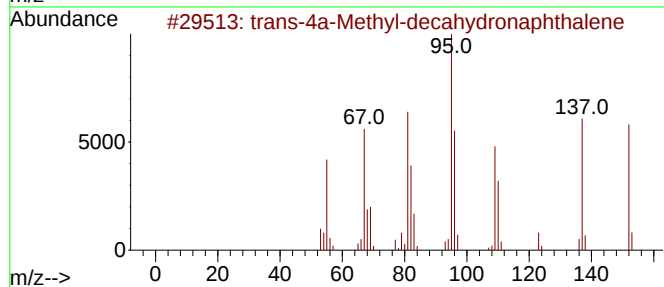
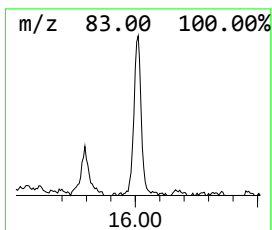
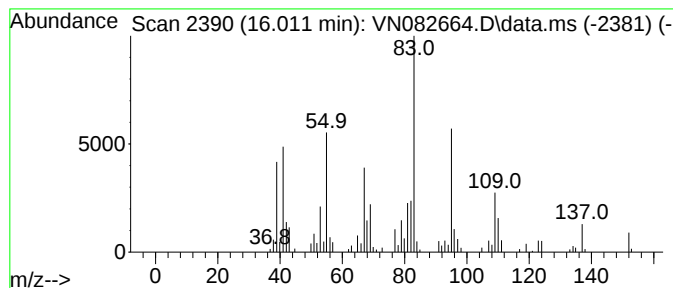
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Quant Title : SW846 8260

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

Peak Number 10 unknown16.011 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.011	11.36 ug/l	199948	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	45
2			2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	42
3			2,4-Hexadiene, 3,4-dimethyl-, (E...	110	C8H14	002417-88-1	30
4			4-Methyl-1,3-heptadiene	110	C8H14	017603-57-5	25
5			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062024\
Data File : VN082664.D
Acq On : 20 Jun 2024 13:34
Operator : JC\MD
Sample : P2981-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240619096-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061724W.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
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Methanethiol	2.824	8.8	ug/l	82931	1	8.230	473167	50.0
3-Pentanone, 2,...	11.171	10.5	ug/l	198934	3	11.871	945548	50.0
Eucalyptol	13.859	10.8	ug/l	190205	4	13.794	879722	50.0
Fenchone	14.676	46.7	ug/l	821627	4	13.794	879722	50.0
Cyclohexanemeth...	15.100	9.6	ug/l	169240	4	13.794	879722	50.0
Bicyclo[2.2.1]h...	15.282	11.4	ug/l	201120	4	13.794	879722	50.0
Camphor	15.329	75.4	ug/l	1327360	4	13.794	879722	50.0
unknown15.794	15.794	8.7	ug/l	152851	4	13.794	879722	50.0
unknown16.011	16.011	11.4	ug/l	199948	4	13.794	879722	50.0