

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
 Data File : VX036318.D
 Acq On : 24 Jun 2023 17:48
 Operator : JC/MD
 Sample : 03379-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 230621028-02-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_X\Method\82X062323W.M
 Title : SW846 8260

Signal : TIC: VX036318.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.191	162	181	188	rBV3	23767	132710	3.00%	0.532%
2	2.398	207	215	231	rBV	501150	1231150	27.87%	4.932%
3	2.605	239	249	263	rBV3	17523	99465	2.25%	0.398%
4	3.001	297	314	348	rBV2	619158	2865385	64.87%	11.480%
5	4.574	557	572	590	rBV2	1271740	4417007	100.00%	17.696%
6	5.013	633	644	671	rBV3	268880	1073340	24.30%	4.300%
7	5.385	694	705	720	rVV2	139419	408806	9.26%	1.638%
8	5.550	720	732	751	rVB	211371	592870	13.42%	2.375%
9	5.952	788	798	807	rBV	167911	450357	10.20%	1.804%
10	6.257	840	848	858	rBV3	17484	56483	1.28%	0.226%
11	6.635	899	910	921	rBV2	34303	89897	2.04%	0.360%
12	6.763	921	931	947	rVB	325321	781648	17.70%	3.132%
13	7.251	1000	1011	1030	rBV2	70438	296129	6.70%	1.186%
14	7.458	1039	1045	1058	rVB	37864	86446	1.96%	0.346%
15	8.574	1221	1228	1234	rBV	65840	105180	2.38%	0.421%
16	8.647	1234	1240	1247	rVV	844916	1327812	30.06%	5.320%
17	8.720	1247	1252	1260	rVV	91485	176788	4.00%	0.708%
18	8.805	1261	1266	1270	rVV	43177	77039	1.74%	0.309%
19	9.378	1356	1360	1365	rVV	133092	197073	4.46%	0.790%
20	9.726	1411	1417	1425	rBV	33190	79673	1.80%	0.319%
21	10.055	1461	1471	1483	rBV	673526	1007532	22.81%	4.037%
22	10.195	1489	1494	1500	rBV2	62029	102454	2.32%	0.410%
23	10.299	1508	1511	1519	rVB	70528	104293	2.36%	0.418%
24	10.518	1538	1547	1550	rBV3	30944	68392	1.55%	0.274%
25	10.640	1563	1567	1571	rBV	58480	77054	1.74%	0.309%
26	10.768	1580	1588	1592	rBV	39144	65238	1.48%	0.261%
27	11.079	1634	1639	1645	rBV	631960	804377	18.21%	3.223%
28	11.506	1704	1709	1715	rBV	190225	252427	5.71%	1.011%
29	11.750	1740	1749	1753	rBV	30592	47365	1.07%	0.190%
30	11.884	1767	1771	1779	rVB	77193	104005	2.35%	0.417%
31	12.018	1788	1793	1801	rBV	659550	870265	19.70%	3.487%
32	12.103	1801	1807	1811	rBV2	297735	426351	9.65%	1.708%
33	12.244	1827	1830	1839	rVB	43735	69721	1.58%	0.279%
34	12.518	1871	1875	1878	rBV4	39054	64532	1.46%	0.259%
35	12.853	1926	1930	1933	rBV	30955	44238	1.00%	0.177%
36	12.902	1933	1938	1944	rVV	939562	1236934	28.00%	4.956%

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37	12.963	1944	1948	1952	rVB5	31944	47759	1.08%	0.191%
38	13.170	1977	1982	1986	rBV	273616	395417	8.95%	1.584%
39	13.213	1986	1989	1996	rVB4	55509	93090	2.11%	0.373%
40	13.335	2005	2009	2012	rBV	69502	88927	2.01%	0.356%
41	13.475	2027	2032	2033	rBV2	95427	123615	2.80%	0.495%
42	13.512	2033	2038	2044	rVV	1531669	2081741	47.13%	8.340%
43	13.591	2044	2051	2057	rVV3	203879	377225	8.54%	1.511%
44	13.658	2057	2062	2070	rVV	344266	566493	12.83%	2.270%
45	13.731	2070	2074	2077	rVV	225055	294445	6.67%	1.180%
46	13.774	2077	2081	2086	rVV	332165	423022	9.58%	1.695%
47	13.829	2086	2090	2094	rVV	53836	76302	1.73%	0.306%
48	13.878	2094	2098	2101	rVV	39576	58400	1.32%	0.234%
49	13.920	2101	2105	2115	rVB4	29267	76784	1.74%	0.308%
50	14.097	2127	2134	2147	rBV2	159551	245359	5.55%	0.983%
51	14.640	2218	2223	2226	rBV	36301	52248	1.18%	0.209%
52	15.597	2375	2380	2388	rBV	38704	68837	1.56%	0.276%

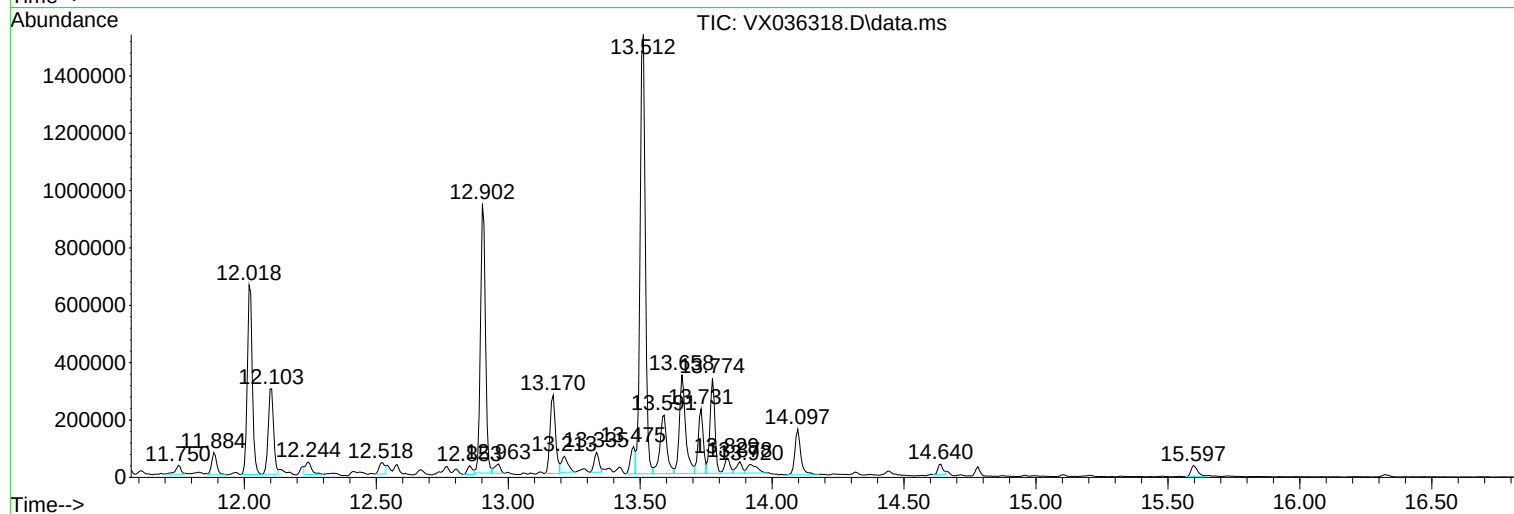
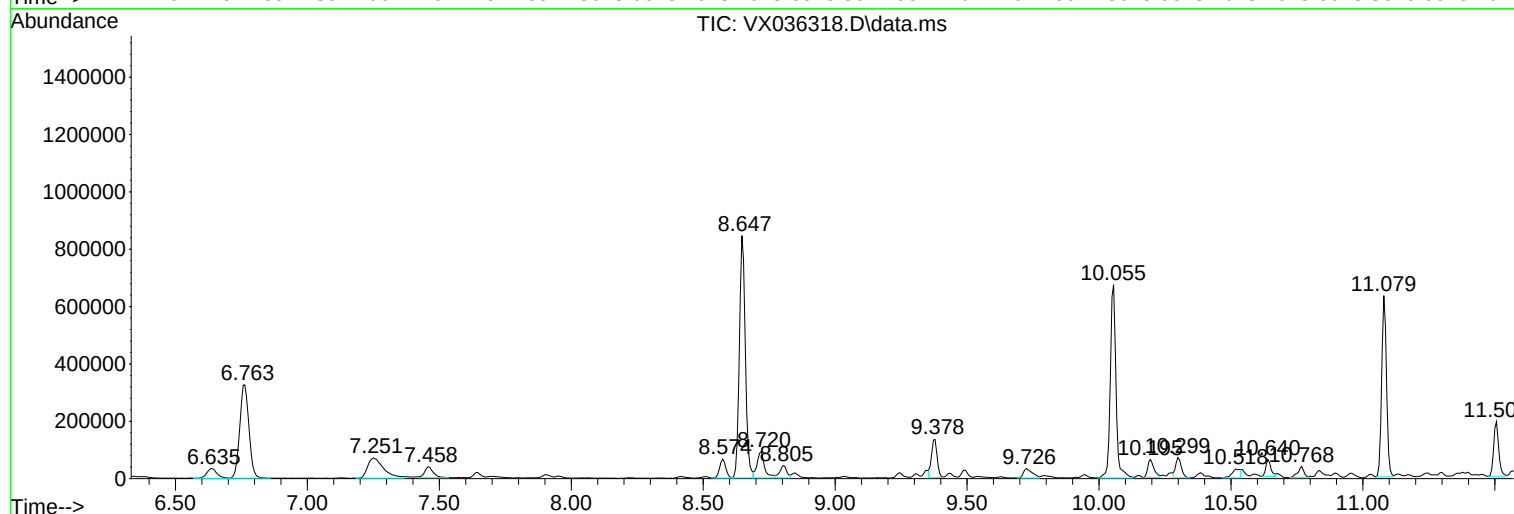
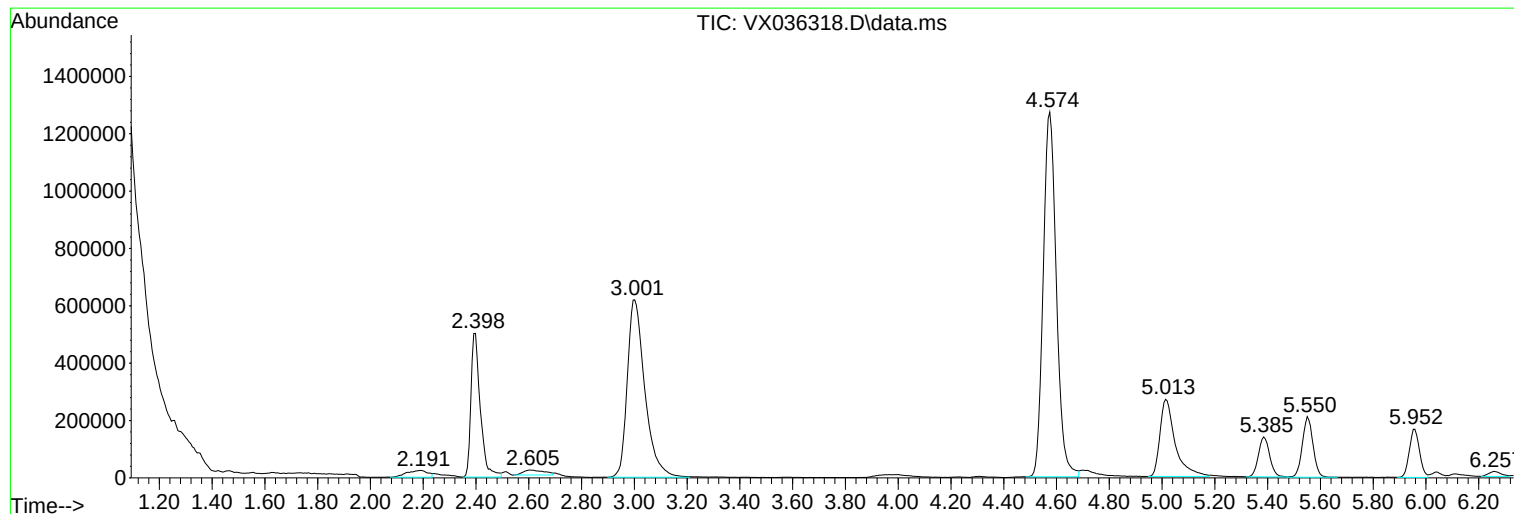
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Quant Title : SW846 8260

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



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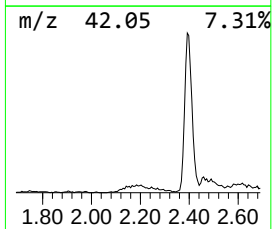
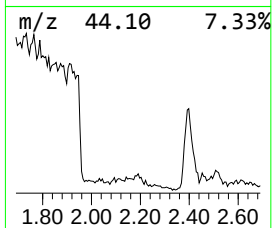
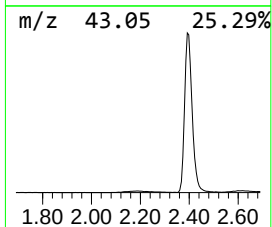
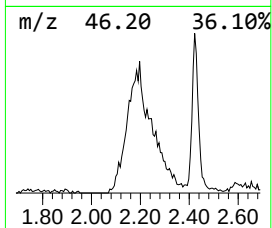
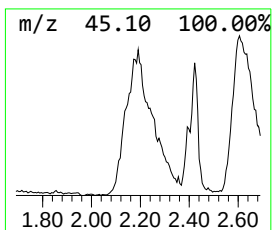
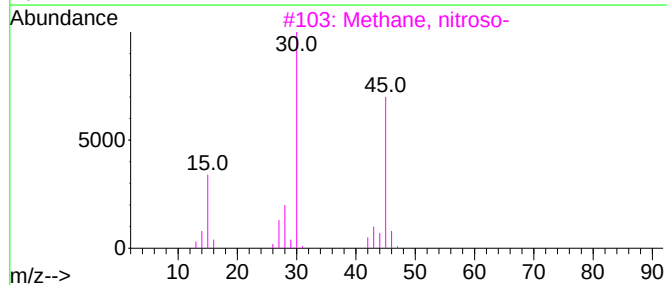
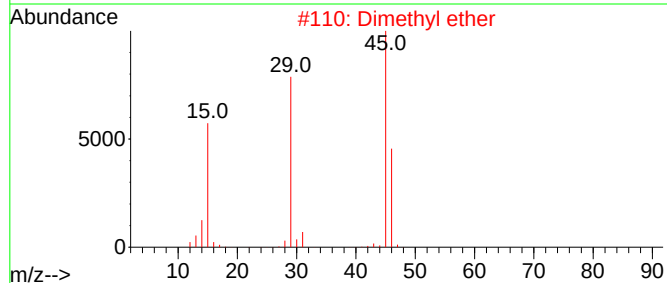
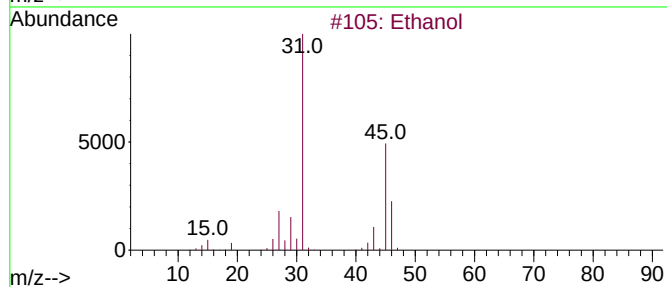
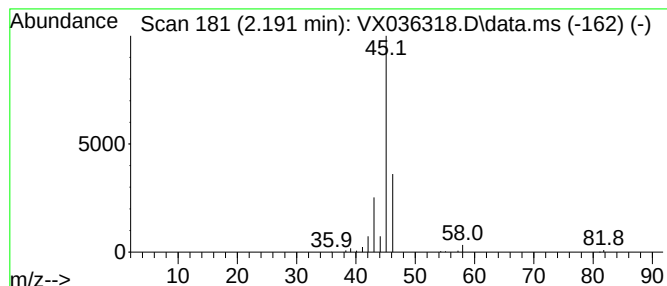
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Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.191	11.19 ug/l	132710	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	56
2			Dimethyl ether	46	C2H6O	000115-10-6	5
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Ethanol, 2-(2-hydroxyethoxy)-, 1...	151	C4H9NO5	020633-16-3	4



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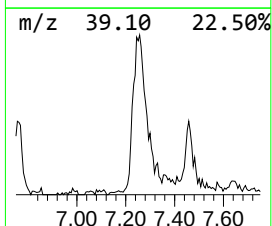
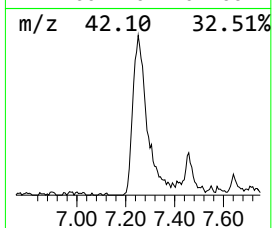
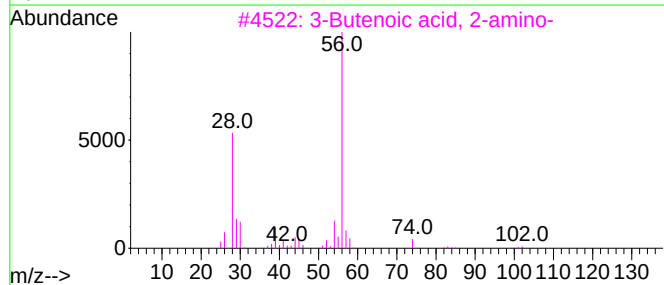
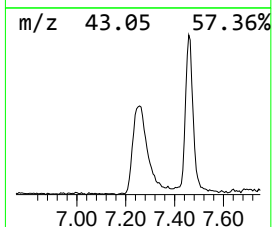
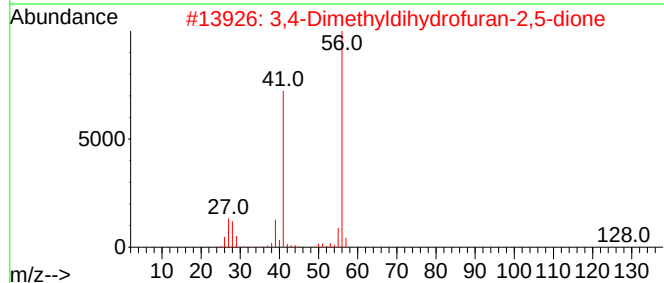
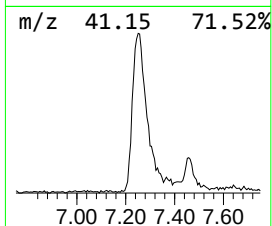
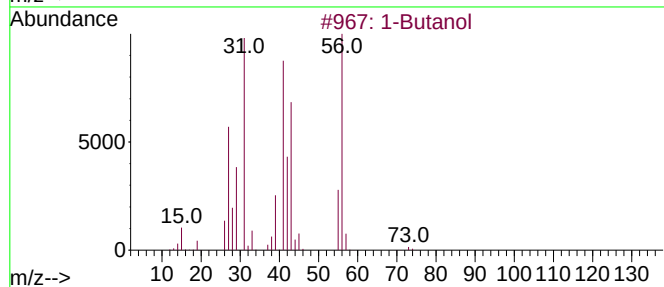
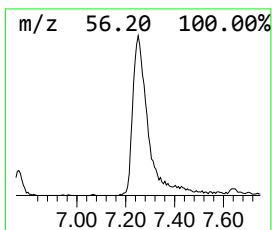
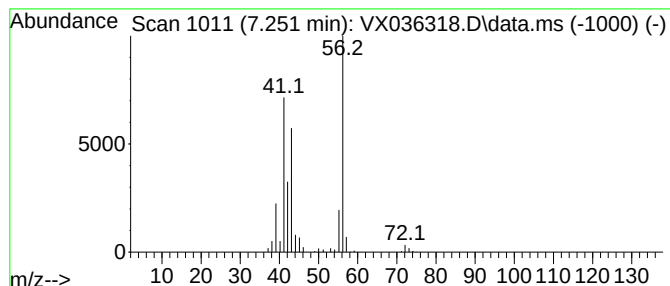
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.251	18.94 ug/l	296129	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	90
2	3,4-Dimethyldihydrofuran-2,5-dione			128	C6H8O3	007475-92-5	42
3	3-Butenoic acid, 2-amino-			101	C4H7NO2	056512-51-7	38
4	Propane, 2-cyclopropyl-			84	C6H12	003638-35-5	38
5	Cyclobutane, ethyl-			84	C6H12	004806-61-5	9



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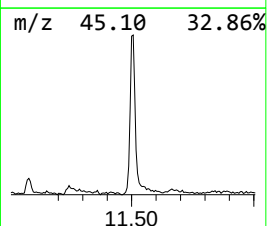
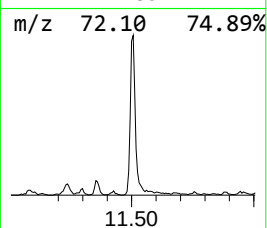
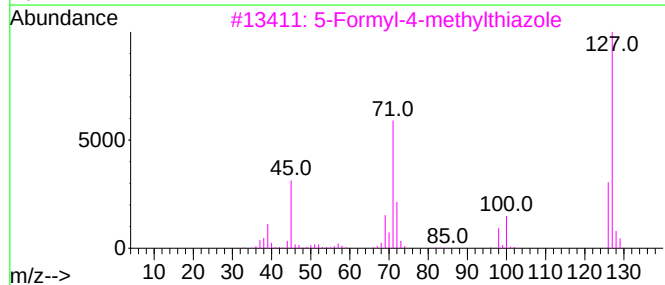
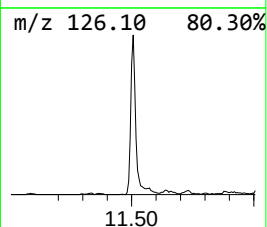
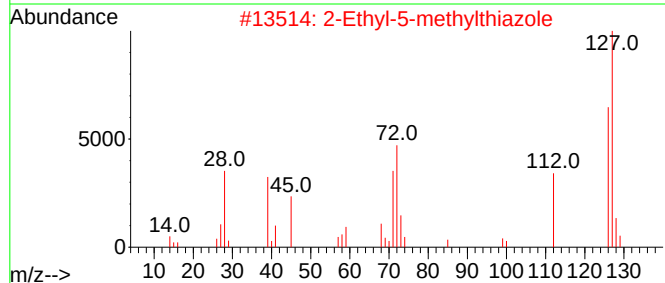
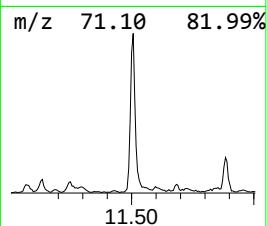
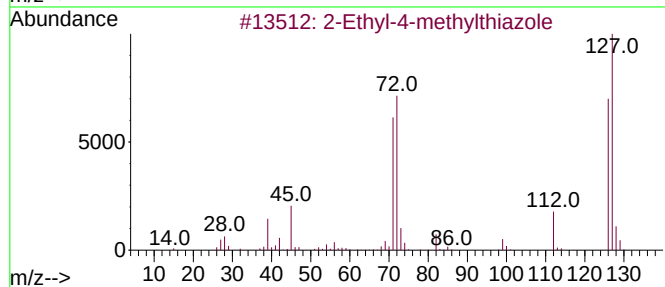
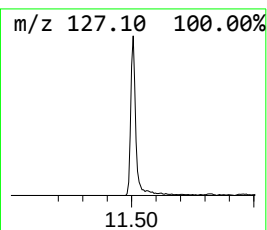
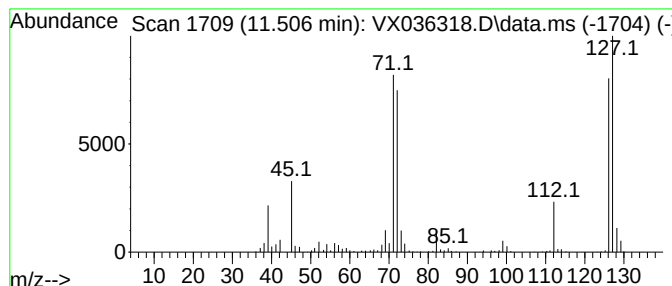
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Ethyl-4-methylthiazole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.506	14.50 ug/l	252427	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-4-methylthiazole	127	C6H9NS	015679-12-6	96
2			2-Ethyl-5-methylthiazole	127	C6H9NS	019961-53-6	50
3			5-Formyl-4-methylthiazole	127	C5H5NOS	082294-70-0	49
4			Thiazole, 2,4,5-trimethyl-	127	C6H9NS	013623-11-5	38
5			Thiazole, 4-ethyl-2-methyl-	127	C6H9NS	032272-48-3	38



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Instrument :
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ClientSampleId :
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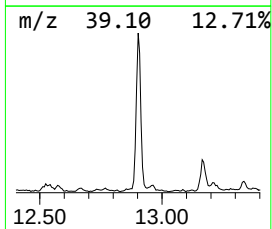
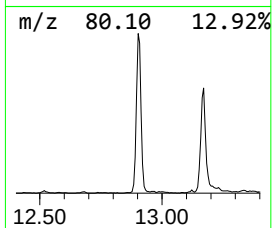
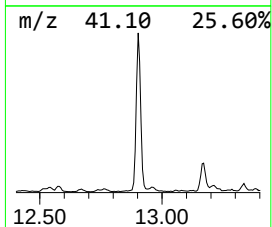
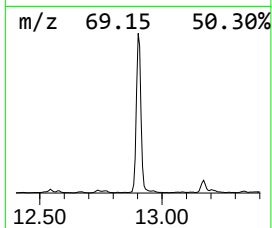
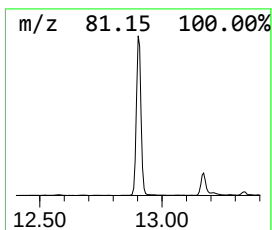
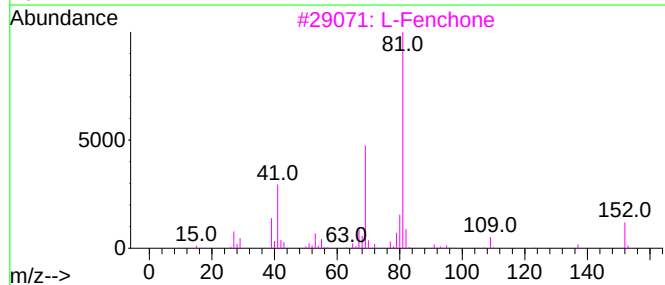
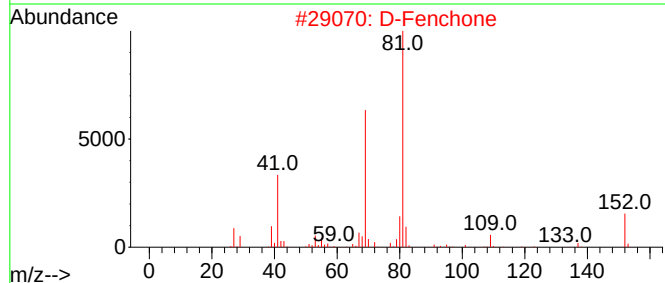
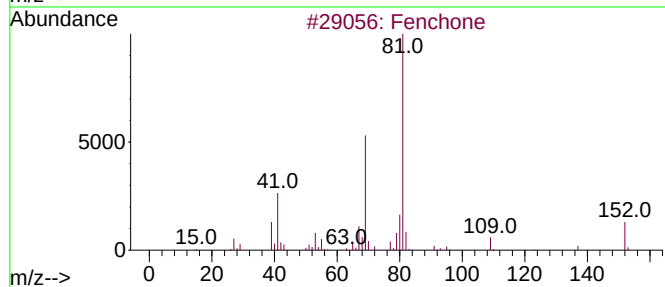
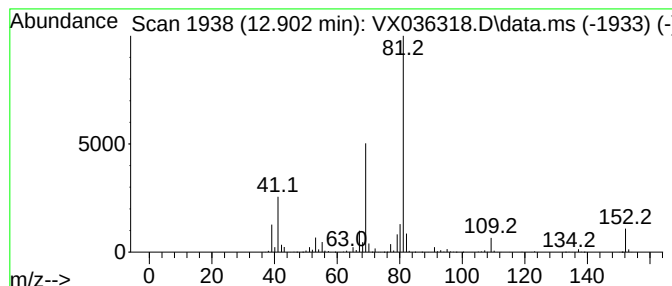
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Quant Title : SW846 8260

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.
12.902	71.07 ug/l	1236930	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	95
2			D-Fenchone	152	C10H16O	004695-62-9	94
3			L-Fenchone	152	C10H16O	007787-20-4	94
4			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	42
5			Cyclohexane, 1,3-dichloro-, trans-	152	C6H10Cl2	024955-62-2	36



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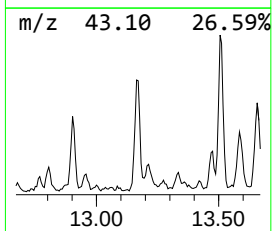
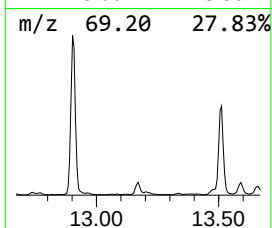
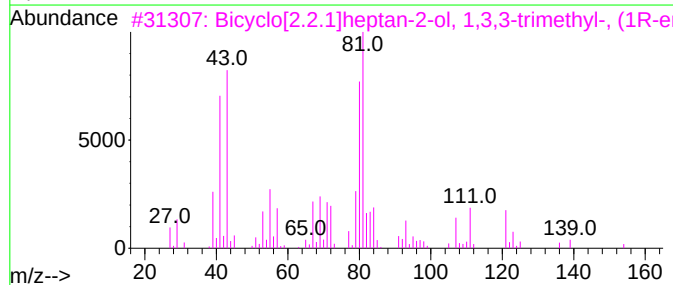
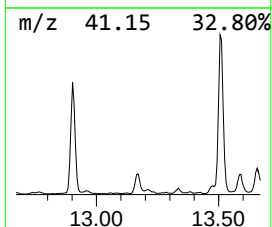
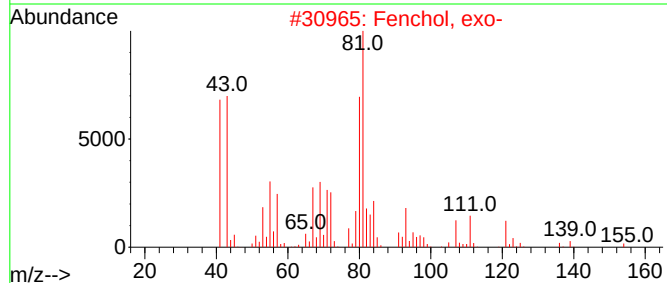
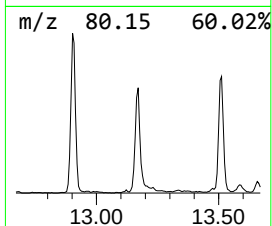
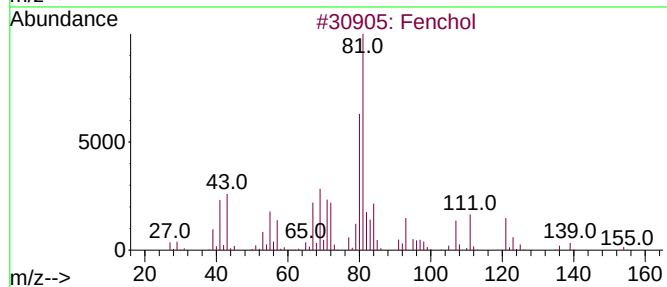
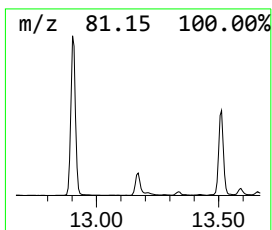
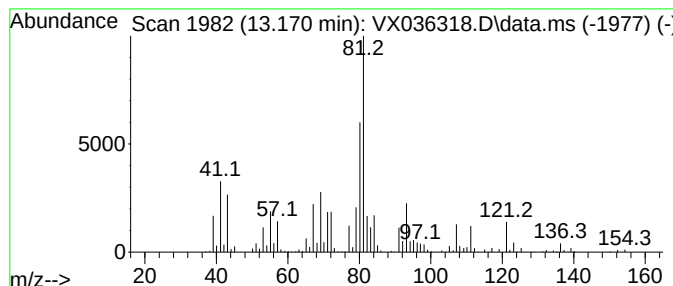
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Quant Title : SW846 8260

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

Peak Number 6 Fenchol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.170	22.72 ug/l	395417	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchol	154	C10H18O	001632-73-1	98
2			Fenchol, exo-	154	C10H18O	022627-95-8	98
3			Bicyclo[2.2.1]heptan-2-ol, 1,3,3...	154	C10H18O	002217-02-9	95
4			Cyclohexane, 1,2-dichloro-, cis-	152	C6H10Cl2	010498-35-8	50
5			Cyclohexane, 1,2-dichloro-	152	C6H10Cl2	001121-21-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036318.D
Acq On : 24 Jun 2023 17:48
Operator : JC/MD
Sample : 03379-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230621028-02-VOA

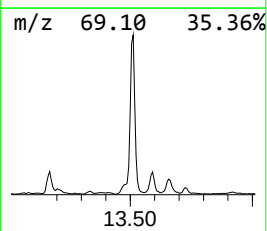
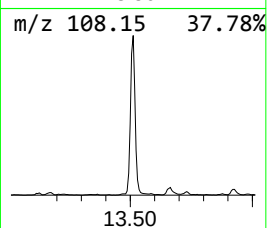
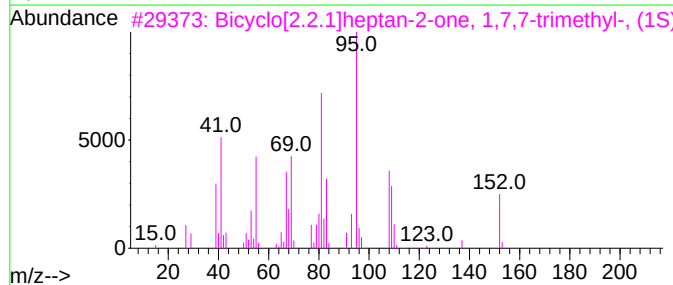
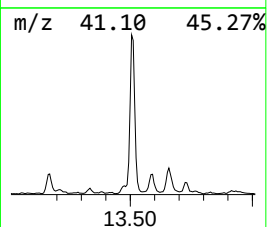
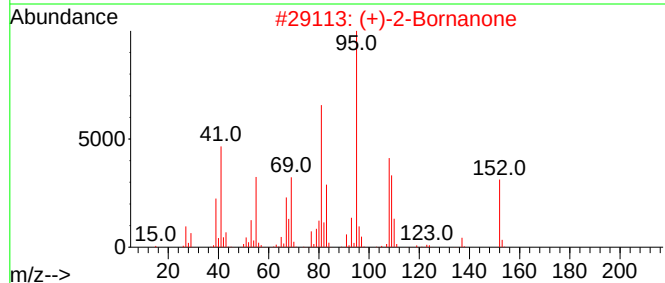
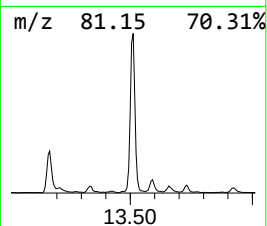
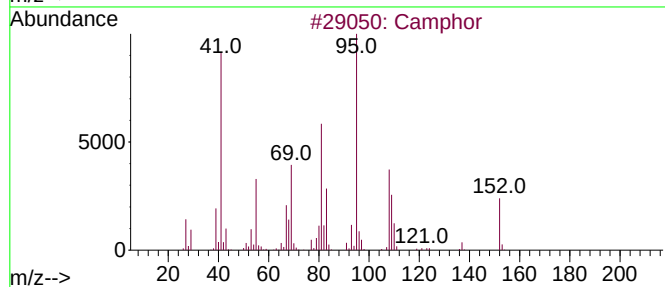
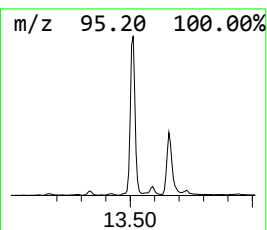
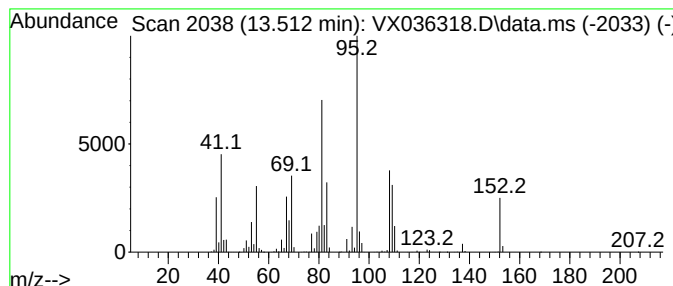
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Quant Title : SW846 8260

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

Peak Number 7 Camphor Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	119.60 ug/l	2081740	1,4-Dichlorobenzene-d4	12.024

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	98
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	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036318.D
Acq On : 24 Jun 2023 17:48
Operator : JC/MD
Sample : 03379-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230621028-02-VOA

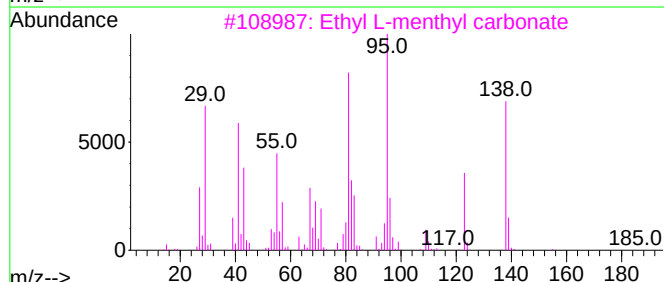
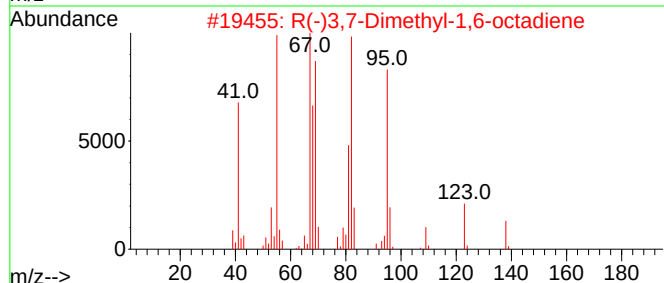
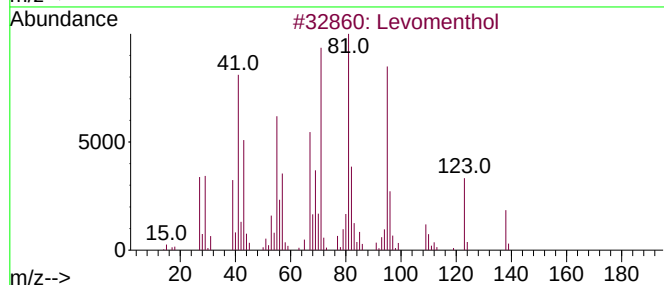
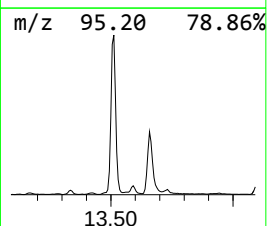
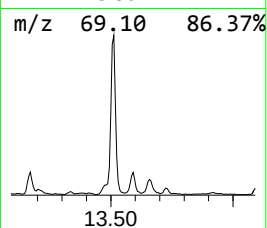
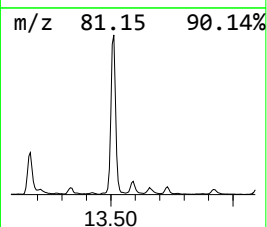
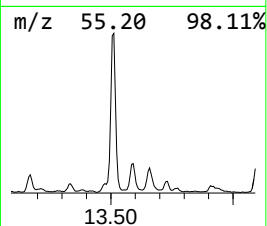
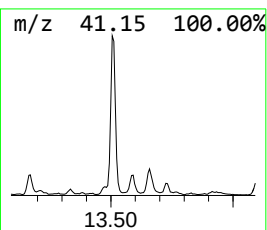
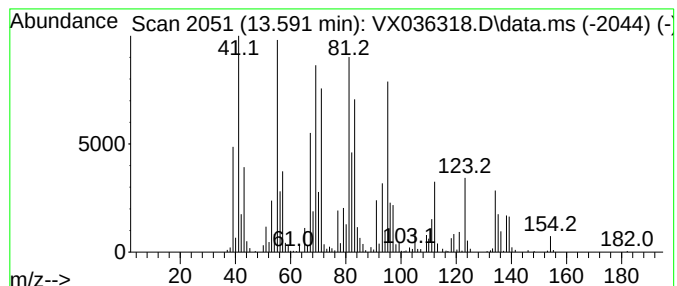
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.591 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	21.67 ug/l	377225	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Levomenthol	156	C10H20O	002216-51-5	49
2			R(-)3,7-Dimethyl-1,6-octadiene	138	C10H18	010281-56-8	46
3			Ethyl L-menthyl carbonate	228	C13H24O3	035106-15-1	43
4			Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-27-2	42
5			Cyclohexene,1-(2-methylpropyl)-	138	C10H18	003983-03-7	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036318.D
Acq On : 24 Jun 2023 17:48
Operator : JC/MD
Sample : 03379-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230621028-02-VOA

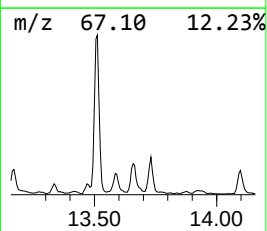
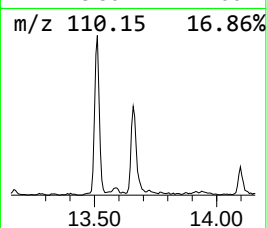
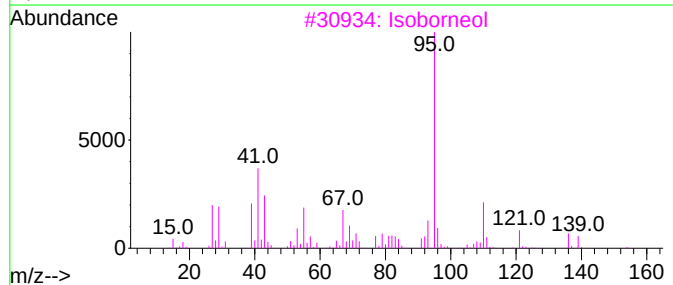
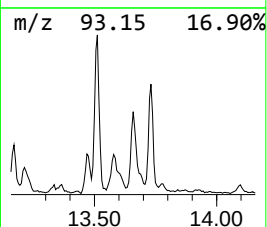
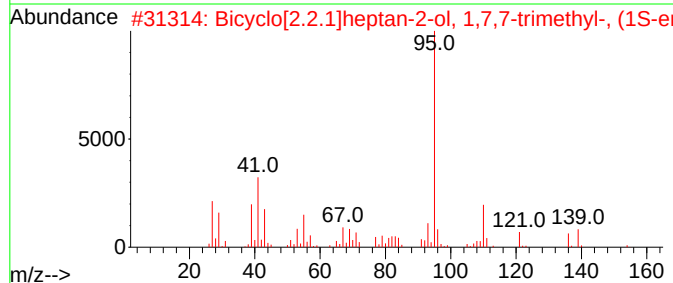
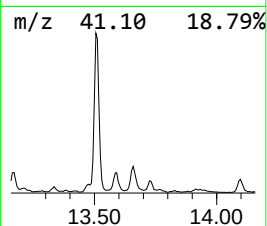
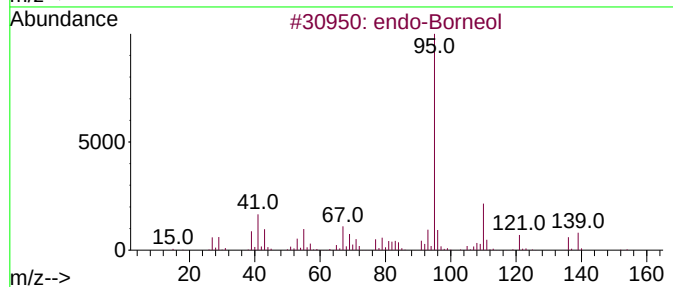
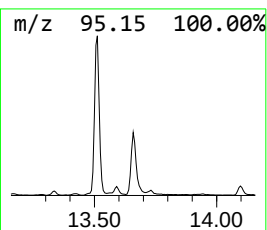
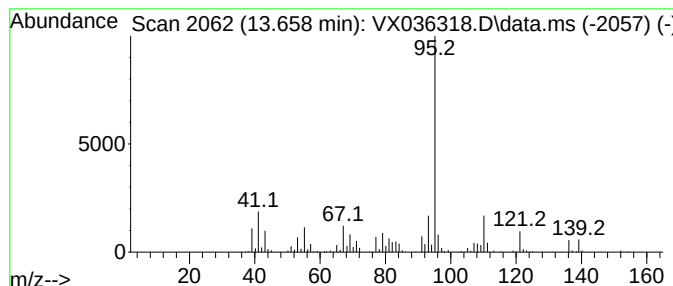
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Quant Title : SW846 8260

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

Peak Number 9 endo-Borneol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.658	32.55 ug/l	566493	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			endo-Borneol	154	C10H18O	000507-70-0	94
2			Bicyclo[2.2.1]heptan-2-ol, 1,7,7...	154	C10H18O	000464-45-9	91
3			Isoborneol	154	C10H18O	000124-76-5	87
4			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	62
5			Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036318.D
Acq On : 24 Jun 2023 17:48
Operator : JC/MD
Sample : 03379-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230621028-02-VOA

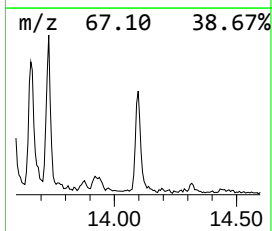
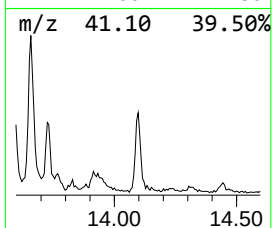
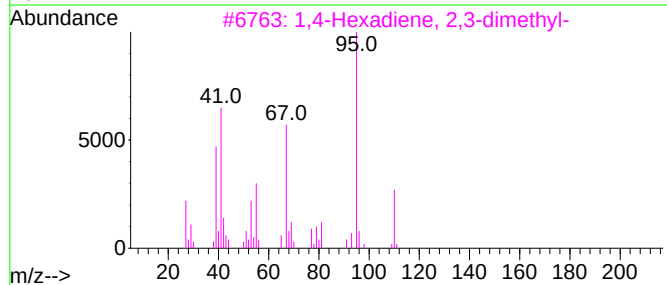
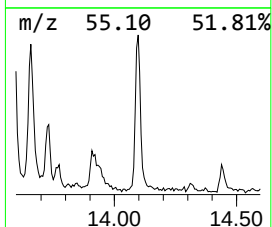
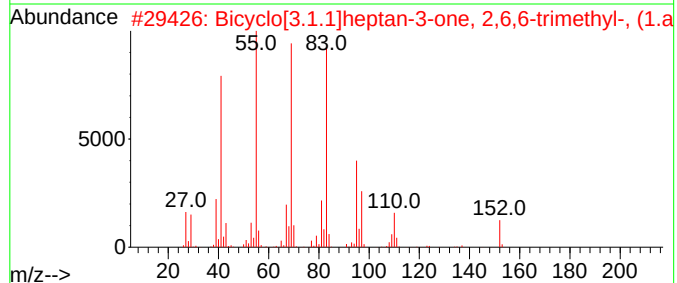
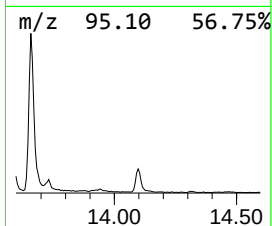
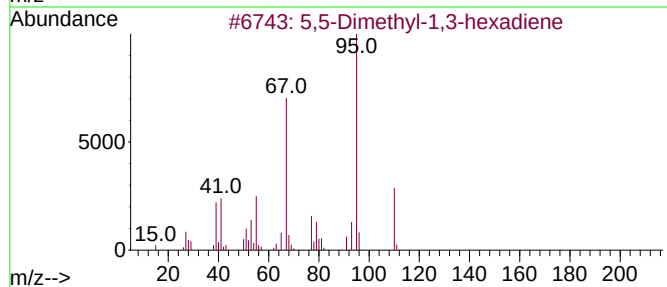
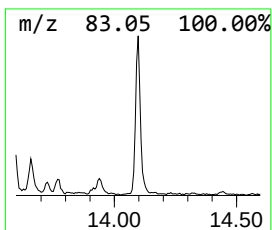
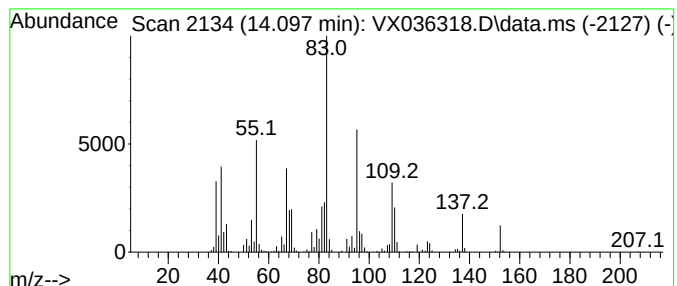
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

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

Peak Number 10 5,5-Dimethyl-1,3-hexadiene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.097	14.10 ug/l	245359	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	80
2			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	62
3			1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	42
4			2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	38
5			2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036318.D
Acq On : 24 Jun 2023 17:48
Operator : JC/MD
Sample : 03379-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230621028-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.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
Ethanol	2.191	11.2	ug/l	132710	1	5.550	592870	50.0
1-Butanol	7.251	18.9	ug/l	296129	2	6.763	781648	50.0
2-Ethyl-4-methy...	11.506	14.5	ug/l	252427	4	12.024	870265	50.0
Eucalyptol	12.104	24.5	ug/l	426351	4	12.024	870265	50.0
Fenchone	12.902	71.1	ug/l	1236930	4	12.024	870265	50.0
Fenchol	13.170	22.7	ug/l	395417	4	12.024	870265	50.0
Camphor	13.512	119.6	ug/l	2081740	4	12.024	870265	50.0
unknown13.591	13.591	21.7	ug/l	377225	4	12.024	870265	50.0
endo-Borneol	13.658	32.5	ug/l	566493	4	12.024	870265	50.0
5,5-Dimethyl-1,...	14.097	14.1	ug/l	245359	4	12.024	870265	50.0